QSAR STUDIES ON ANTIMICROBIAL ACTIVITY OF BENZOXAZINDIONE ANALOGUES



Milena JADRIJEVIĆ-MLADAR TAKAČ, Ivan KOS, Vedran TAKAČ Faculty of Pharmacy and Biochemistry, University of Zagreb, 10000 Zagreb, Croatia mladar@pharma.hr; cpf.centar@gmail.com

188 **000 1**1 888 **000** 81

INTRODUCTION

Recently, different benzoxazindione analogues were investigated for their antiviral, antiallergic and tocolytic oxytocin receptor activities. The benzoxazinone analogue efavirenz, *i.e.* 6-chloro-4-(cycloprophylethynyl)-1,4-dihydro-4-(trifluoromethyl)-2H-3,1-benzoxazin-2-one, was approved as antiretroviral drug, a non-nucleoside type of reverse transcriptase inhibitor.

In extension of our previous QSAR studies using topological indices, TIs (W, χ 1, J), the QSAR of 1,4 benzoxazin-2,3-dione (1 - 35) and 3,1-benzoxazin-2,4-dione (36 - 62) analogues (Table 1) were explored using 67 different computed molecular descriptors (MDs) and experimentally obtained parameters (MIC) for antimicrobial activity against 7 microorganisms (Table 2).



			MIC x 10 ⁻³ mol dm ⁻³								
Compd.	SARCINA LUTEA ATCC 9341	STAPHILOCOCCUS AUREUS ATCC 56511	BACILLUS SUBTILIS ATCC 8236	KLEBSIELLA PNEUMONIAE ATCC 10031	ESCHERICHIA COLI ATCC 99-1	ESCHERICHIA COLI ATCC 0536	CANDIDA MONOSA				
21	-	3,38	3,38	3,38	1,62		3,38				
22	-	3,09	3,09	3,09	1,55		3,09				
23	4,8	3,39	3,39	3,39	1,7		3,39				
24	-	3,09	3,09	3,09	1,55		1,55				
25	-	2,96	2,96	2,96	1,48		2,96				
26	-	2,85	2,85	2,85	1,43		2,85				
27	-	2,49	2,49	2,49	+		1,25				
28	-	2,49	2,49	2,49	1,25		2,49				
30	-	2,44	2,44	2,44	1,22		1,22				
32	-	3,11	3,11	3,11	2,12		2,12				
33	-	3,43	3,43	3,43	1,58		3,43				
44	3,28	3,28	-	1,64	-		1,64				
49		3,99	-	3,99	-	3,99					
50	3,78	3,78	-	3,78	-	3,78					
51	3,59	3,59	-	3,59	-	3,59					
53	3,08	3,08	-	3,08	-	3,08					
56	1,21	1,21	-	0,6	-	1,21	0,3				
60	4,23	4,23	-	2,12	-	4,23	2,12				
61	1,6	1,6	-	0,79	-	1,59	0,79				
62	24	48	-	24	-	24	12				

RESULTS

2D and 3D Correlations with biological activities against Staphylococcus aureus, ATCC 56511





Figure 1. Synthesis of N-Mannich bases from 1,4-benzoxazin-2,3-dione and 3,1-benzoxazin-2,4-dione

METUODO

	Chemical st	tructures of 1,4-benzoxazin-	-2,3-dione (1-35) and 3,1-benzoxazin-2,4-dione (36-62)	10 22,61	38,02 0,61	344 946 1,978	78 42,121 21,2	,275 10,13 65,405 0,917	-0,62 0,385	~ 4 J		e e e e e e e e e e e e e e e e e e e
			$R \rightarrow Q \rightarrow R^1$	11 26,32	45,11 0,6	386 1334 2,065	5 47,973 24,2	,252 11,562 74,816 0,698 -	-0,624 0,389	ol dm		
			N O	12 26,7	43,11 0,64 33	37,21 1334 2,065	5 47,973 24,2	,252 11,562 81,18 2,678	1,783 3,18	. ŭ 		
			R2	13 24,7	40,57 0,62	36b 1031 1,668 340 1174 1.00	6 44,895 22,3	,283 10,648 67,916 1,793 (0,916 0,839	2 - 2 WIC		
N ₀	R	R ¹	R ²	14 26,29 15 22.02	43,40 0,61 3 35.7 0.67	454 1196 1.603	47,011 23, 3 46,61 23,	.261 10.859 69.829 3.871	3.684 13.569			50 60 70 2,5 ^{°°}
1	H	0	CH ₂ NHCH ₂ CH ₂ OH	16 31,34	51,99 0,63	548 2473 1,684	34 60,52 30.5	,213 14,329 92,59 2,869	2,726 7,43			$2M_{OD}$ 80 $_{90}$ $_{100}$ 0,0 1,0 $_{NO}$
2	Н	0	CH ₂ N(CH ₂ CH ₂ Cl) ₂	17 31,23	48,78 0,64	534 2240 1,42	2 59,557 29,5	,224 13,915 89,961 3,236	3,492 12,196	0 40	50 60 70 80 90 100	
3	Н	0	CH ₂ —NO	18 31,32	50,3 0,64	502 2240 1,42	2 59,557 29,2	,224 13,915 89,961 4,225	4,722 22,295		χMOD	
				19 24,53	38,36 0,66	432 1345 1,617	7 48,715 24,2	,253 11,507 74,482 2,539	2,619 6,861	Figure 6. 2D	Correlation of modified Randic connectivity index	Figure 7. 3D Correlation of modified Randic connectivity index
4	Н	NO ₂	CH ₂ —N	20 14,74	23,61 0,67	388 412 2,037	37 31,904 16,3	,372 7,503 49,509 1,342 (0,799 0,638	(χMOD) and M aureus, ATCC	MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus</i>	(χMOD), lipophylicity (AlogP) and MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus aureus</i> , ATCC 56511
				21 19,36	32,25 0,65	438 944 1,979	'9 41,79 21,2 0 45,704 004	,275 9,897 65,443 0,855 (0,053 0,003			
5	Н	0	$CH_2 - N - C_6H_5$	22 22,55	38,01 0,63 4	454 1268 1,913	3 45,781 23,2	,243 10,935 72,002 1,407 (0,653 0,426	1~	Staphylococcus aureus ATCC 5651	
6	Н	NNHCH ₃	Н	23 19,64 24 20.96	35.13 0.64	442 1112 1.922	2 43.791 22.2	.255 10.397 68.443 1.136 (0.088 0.008		r = -0.86517 n = 20	
7	Н	NNHCH ₃	CH ₂ N(CH ₂ CH ₂ OH) ₂	25 24,15	40,9 0,62	454 1341 2,038	88 47,463 24,2	,248 11,218 73,325 1,671	1,274 1,622	4 -		Ϋ́ε
8	н	NNHCH	CH ₂ -N	26 25,75	43,78 0,61	458 1526 2,016	6 49,468 25,2	,236 11,701 76,224 1,927	1,662 2,764	ې بې		
0				27 27,06	43,34 0,66	436 2000 1,695	5 56,262 28,2	,229 13,236 85,904 2,137	1,276 1,627	3 mol c	•	
9	Н	NNHCOCH ₃	Н	28 27,06	43,34 0,6	536 2000 1,695	5 56,262 28,2	,229 13,236 85,904 2,137	1,276 1,627	- 2 - [C/10 ⁻		
10	Н	NNHCOCH ₃	CH ₂ NHCH ₂ CH ₂ OH	29 19,3	30,66 0,67 36	68,445 813 1,986	36 39,78 20,	0,29 9,397 64,379 1,294 (0,917 0,842	≥		0,60 0.62 226283032
11	Н	NNHCOCH ₃	CH ₂ N(CH ₂ CH ₂ OH) ₂	30 28,81	47,95 0,62 48	84,445 2042 2,116	6 55,345 28,2	,222 13,112 88,194 1,625	1,393 1,939			0.64 0.66 0.68 $1.16^{18} 20^{22^4}$ 5^{1}
12	Н	NNHCOCH ₃	CH ₂ N(CH ₂ CH ₂ CI) ₂	31 28,46	47,19 0,61 31	14,445 1292 2,128	28 47,628 24,2	,259 11,307 74,397 2,435 2	2,597 6,742	0 +	2 14 16 18 20 22 24 26 28 30 32	0,70 12 14
13	н	NNHCOCH ₂	CH ₂ -N	32 25,32	43,1 0,6	388 1138 2,131	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	200 10.050 65.371 1.756	2,372 5,627		Sv	
				33 21,33	42.41 0.64 41	12 445 1463 1.702	2 50.611 25.5	256 11.952 80.24 1.685	1,381 1,300			
14	Н	NNHCOCH ₃	CH ₂ -N	35 25,51	42,19 0,64 47	74,445 1680 2,079	'9 51,496 26,2	,234 12,201 82,73 1,105 (0,549 0,302	Figure 8. 2D volumes (Sv)	Correlation of sum of atomic van der Waals and MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus</i>	Figure 9. 3D Correlation of sum of atomic van der Waals
		CF3		36 27,1	45,91 0,59	300 956 2,207	43,287 22,2	,294 10,015 63,091 3,48	3,402 11,57	aureus ATCC	56511	(10 ⁻³ mol dm ⁻³) against <i>Staphylococcus aureus</i> , ATCC 56511
15	Н	N	Н	37 20,62	33,81 0,62	314 674 1,663	3 39,127 19,5	,324 9,254 59,645 1,303	1,227 1,505			
		CF3		38 21,73	37,03 0,6 3	328 794 2,024	4 40,09 20,2	,295 9,668 62,545 0,936	0,46 0,212			
16	Н	N	CH ₂ N(CH ₂ CH ₂ OH) ₂	39 23,1	37,12 0,64 29	93,21 908 2,048	8 42,121 21,2	,285 10,206 72,824 3,027	2,954 8,728	2D and 3	D Correlations with biological acti	vities against Klebsiella pneumoniae,
		CF3		40 25,18	40,87 0,63 34	44,445 1194 1,638	88 47,016 23,2	,266 11,148 74,515 1,195	1,345 1,81	AICC 10	031	
17	Н	N	CH ₂ -N_O	41 19,44	32,8 0,63	390 813 2,002	2 39,954 20,2	,292 9,541 62,86 1,262 (0,358 0,128			
10		CF3		42 23,15	39,9 0,61	432 1180 2,062	2 45,805 23,2	,262 10,973 72,271 1,084 (0,345 0,126	l l		4
18	П			43 21,53	38.24 0.62	362 893 1,686 386 1028 1,686	42,727 21,2 19 44,842 22,4	233 10,059 65,371 2,162 283 10,559 68,371 2,425	2 35 5 525		_	
19	Н		Н	44 23,13 45 22.04	36.69 0.63	418 1028 1,669	44,043 22,2 9 44,843 22,2	,283 10,559 69,371 1,423	2,33 5,525 1,121 1,257	4 -		°
		O ₂ N		46 28.52	48,78 0,59	404 1394 2.215	5 49,002 25	5,26 11,319 72,817 3.566	3,296 10,863	ې ب		
20	NO ₂	0	Н	47 23,53	37,89 0,65 38	83,21 1180 2,062	2 45,805 23,2	,262 10,973 78,635 3,074	2,762 7,627	nol dr		WIC/IC
21	NO ₂	0	CH ₂ NHCH ₂ COOH	48 29,72	47,23 0,65	468 2177 1,322	2 57,634 28,2	,215 13,525 86,744 2,933	3,063 9,38	°-01/;	•	0,70
22	NO ₂	0	CH ₂ NHCH ₂ COOC ₂ H ₅	49 17,94	29,37 0,64	334 613 1,931	31 36,073 18,3	,312 8,592 55,717 1,113 (0,673 0,452	WC		0 10 0,68 0,66 0,66 0,66 0,66 0,66 0,66 0,6
23	NO ₂	0	CH ₂ NHCH ₂ CONH ₂	50 19,54	32,26 0,63	340 702 1,964	37,898 19,3	,301 9,003 58,135 1,394	1,05 1,103		• •	C_{10}^{40} $_{50}^{50}$ $_{60}^{0,62}$ N^{1}
24	NO ₂	0	CH ₂ NHCH ₂ CH ₂ CH ₂ COOH	51 21,13	35,14 0,62 3	350 866 1,845	5 40,064 20,2	,269 9,63 62,276 1,666	1,272 1,619	o 🕂		-
25	NO ₂	0	CH ₂ NHCH(COOH)CH(CH ₃) ₂	52 21,13	35,14 0,62	342 894 1,788	8 40,075 2,2	,26 9,592 61,717 1,666	1,029 1,058	, i i i i i i i i i i i i i i i i i i i	CID	
26	NO ₂	0	CH ₂ NHCH(COOH)CH ₂ CH(CH ₃) ₂	53 23,82	39,1 0,63 34	48,455 1087 1,934 508 1530 2.011	4 43,92 22,2 1 49,466 25 4	,256 10,541 73,398 1,929 1 235 11 701 77 00 0.600	1,377 1,897	Figure 10, 2D	Correlation of Randic ID number (CID) and MIC	Figure 11, 3D Correlation of Randic ID number (CID), mean
27	NO ₂	0	CH ₂ NHCH(COOH)CH(OH)C ₆ H ₅	55 22.98	38,79 0.64	524 1530 2.011	1 49,466 25,	.235 11.701 77.379 1.105	0.3 0.09	(10 ⁻³ mol dm ⁻³	3) against Klebsiella pneumoniae ATCC 10031	atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³)
28	NO ₂	0	CH ₂ NHCH(COOH)CH(OH)C ₆ H ₅	56 30,74	49,88 0,64	538 2556 1,638	88 60,439 30,2	,207 14,312 92,833 2,607	2,765 7,646			against Mebsiella prieumoniae ATCC 10031
29	NO ₂	NNHCSNH ₂	Н	57 11,72	17,85 0,69	224 179 2,015	5 24,352 12,4	,491 5,771 37,005 1,384	1,212 1,469			
30	H	NNHCSNH ₂	CH ₂ NHCH(COOH)CH(CH ₃) ₂	58 17,94	29,37 0,64	334 613 1,931	31 36,073 18,3	312 8.592 55.671 1.519 (0,702 0,493	4		4
31	Н		CH_N/CH(CH_)_/									
		2		59 14,8	23,01 0,04	230 286 1,991	1 28,394 14,4	,414 6,809 43,713 1,726	1,052 1,107			
32	NO ₂	0	$CH_2N/CH(CH_3)_2/_2$	59 14,8 60 16,28	23,61 0,64 2 24,91 0,68 25	230 286 1,991 54,44 436 1,92	1 28,394 14,4 2 32,235 16,5	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277	1,052 1,107 1,331 1,771	٣-		
32 33	NO ₂ NO ₂	0	CH ₂ -N	59 14,8 60 16,28 61 22,93 62 12,14	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4	230 286 1,991 254,44 436 1,92 422 1188 1,623 230 249 4,006	1 28,394 14,4 2 32,235 16,5 23 46,888 23,5	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696	1,052 1,107 1,331 1,771 2,927 8,568 1,400 1,224	3 mol dm -3		
32	NO ₂ NO ₂	0	CH ₂ N/CH(CH ₃) ₂ / ₂ CH ₂ -N	59 14,8 60 16,28 61 22,93 62 13,14	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 6 30,065 15,3	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 2	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224	MIC/10 ⁻³ mol dm ⁻³		WICC10 ² m ¹
32 33 34	NO ₂ NO ₂ NO ₂	O O NNHCSNH ₂	CH ₂ -N CH ₂ -N CH ₂ -N	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular 5	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 36 30,065 15,3 gend 14,4	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224	MIC/10 ⁻³ mol dm ⁻³		With the second
32 33 34 35	NO ₂ NO ₂ NO ₂ NO ₂	O O NNHCSNH ₂ NNHCSNH ₂	CH2N/CH(CH3)2/2 CH2N/CH(CH3)2/2 CH2N/CH(CH3)2/2 CH2N/CH(CH3)2/2 NHCH(CH3)COOH	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular Des	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg escriptor name	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 36 30,065 15,3 gend 1 1	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224	E-mp lon grand day 2 1214		mu 2 mo 2 mo 0,0 1,0 1,0 1,0 1,0 1,0 1,0 1,0 1,0 1,0
32 33 34 35	NO ₂ NO ₂ NO ₂ NO ₂	O O NNHCSNH ₂ NNHCSNH ₂	CH ₂ N/CH(CH ₃) ₂ / ₂ CH ₂ -N CH ₂ -N CH ₂ -N	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular Des Wi	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg escriptor name /iener W index	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 96 30,065 15,3 gend 100 100	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4 Descriptor type topological description topological description	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e otor	E-up ou qu 2 10 12 14	$16_{18_{20}_{22}_{24}_{26}_{28}_{28}_{30}_{32}}$	$\left(\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$
32 33 34 35	NO ₂ NO ₂ NO ₂ NO ₂	O O NNHCSNH ₂ NNHCSNH ₂	$\frac{CH_{2}NCH(CH_{3})_{2}}{CH_{2}-N}$ $CH_{2}-N$ $CH_{2}-N$ $NHCH(CH_{3})COOH$ $R_{+} \int_{V_{1}}^{R_{1}}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Wi Sum of atomic	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg escriptor name Viener W index c van der Waals	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 36 30,065 15,3 gend	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4 Descriptor type topological descriptor Constitutional descriptor (Carbon atom)	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e otor (scaled on	E-mp lom 2 12 14	$10^{-10^{-10^{-10^{-10^{-10^{-10^{-10^{-$	$\left(\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$
32 33 34 35	NO ₂ NO ₂ NO ₂ NO ₂	O O NNHCSNH ₂ NNHCSNH ₂	$\frac{CH_{2}NCH(CH_{3})_{2}}{CH_{2}N/CH(CH_{3})_{2}/2}$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $NHCH(CH_{3})COOH$ $R + \int_{R^{+}} \int_{R^$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Wi Sum of atomic	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg escriptor name 'iener W index c van der Waals	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 96 30,065 15,3 gend	x414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4 Descriptor type topological descriptor (Constitutional descriptor (Constitutional descriptor atom) Constitutional descriptor (Carbon atom)	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	E-up and dm 2 MIC/10-3 mol dm -12 12 ₁₄	16 + 10 + 10 + 10 + 10 + 10 + 10 + 10 +	r_{u} r_{u
32 33 34 35 35 36	NO ₂ NO ₂ NO ₂ NO ₂ H	O O NNHCSNH ₂ NNHCSNH ₂	$\frac{1}{CH_2N/CH(CH_3)_2/2}$ CH_2-N CH_2-N CH_2-N $NHCH(CH_3)COOH$ $R + \int_{R^2} \int$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Wi Sum of atomic sum of atomic Sa Sa	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg escriptor name Viener W index c van der Waals anderson electro	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 36 30,065 15,3 gend	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4 Descriptor type topological descriptor topological descriptor topological descriptor constitutional descriptor Carbon atom) constitutional descriptor constitutional descriptor	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	E ^{-up low} ² ¹² 14, ¹² 14,	Correlation of sum of atomic van der Waals	Figure 13. 3D Correlation of sum of atomic van der Waals
32 33 34 35 35 36 37	NO ₂ NO ₂ NO ₂ NO ₂ H H	0 0 NNHCSNH ₂ NNHCSNH ₂ 0 0	$\frac{1}{CH_2 N/CH(CH_3)_2/2}$ $CH_2 N/CH(CH_3)_2/2$ $CH_2 N/CH(CH_3)COOH$ $R + \int_{R^2} \int_{R^2}^{R^2} CH_2 N/CH(CH_3)_2/2$ $CH_2 N/CH(CH_3)_2/2$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Sum of atomic Wi sum of atomic Sa mean atomic Mi	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptor name 'iener W index c van der Waals anderson electro c van der Waals	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 96 30,065 15,3 gend	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4 Descriptor type topological descriptor topological descriptor topological descriptor constitutional descriptor Carbon atom) constitutional descriptor constitutional descriptor constitutional descriptor (scaled on Carbon atom) atom atom atom	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv),	O Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10-3 mol dm-3) against Klebsiella preumoniae ATCC 10031
32 33 34 35 35 36 37 38	NO ₂ NO ₂ NO ₂ NO ₂ H H	0 0 NNHCSNH ₂ NNHCSNH ₂ 0 0	$= \frac{CH_2NCH(CH_3)_{2'2}}{CH_2N/CH(CH_3)_{2'2}}$ $= \frac{CH_2-N}{CH_2-N}$ $= \frac{CH_2-N}{CH_2-N}$ $= \frac{CH_2N/CH(CH_3)COOH}{CH_2N/CH(CH_3)_{2'2}}$ $= \frac{CH_2N/CH(CH_3)_{2'2}}{CH_2-N}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular Des Sum of atomic Sa sum of atomic Sa mean atomic Sa	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1000000000000000000000000000000000000	1 28,394 14,4 2 32,235 16,3 23 46,888 23,3 36 30,065 15,3 gend	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 7 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 7 Descriptor type topological descriptor topological descriptor topological descriptor constitutional descriptor Carbon atom) constitutional descriptor constitutional descriptor constitutional descriptor (scaled on Carbon atom) a	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, A	O Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10-3 mol dm-3) against Klebsiella ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against Klebssiella pneumoniae ATCC 10031
32 33 34 35 35 36 37 38 38 30	NO ₂ NO ₂ NO ₂ NO ₂ H H	0 0 NNHCSNH ₂ NNHCSNH ₂ 0 0 0	$\frac{CH_{2}NCH(CH_{3})_{2}}{CH_{2}N/CH(CH_{3})_{2}/2}$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}N/CH(CH_{3})_{2}/2$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$ $CH_{2}-N$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Des Wi sum of atomic Sa first Zagreb index Index	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1000 1000 escriptor name 1000 1000 iener W index 1000 1000 c van der Waals 1000 1000 anderson electro 1000 1000 c van der Waals 1000 1000 x by valence verf 1000 1000	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend	,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 7 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 7 Constitutional descriptor type topological descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom)	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, A	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (C (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031
32 33 34 35 36 37 38 39	NO ₂ NO ₂ NO ₂ NO ₂ H H H H	0 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	$\frac{1}{CH_2N/CH(CH_3)_2/2}$ CH_2-N CH_2-N CH_2-N $R + \int_{R^2} \int_{R^2} \int_{R^2} \int_{R^2} CH_2N/CH(CH_3)_2/2$ $CH_2N/CH(CH_3)_2/2$ $CH_2-N = O$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Sum of atomic Sa sum of atomic Sa first Zagreb index Rar	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1000000000000000000000000000000000000	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend	,414 6,809 43,713 1,726 4 ,349 7,665 51,874 1,277 4 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 4 Descriptor type topological descrip constitutional descrip constitutional descrip constitutional descrip Carbon atom) constitutional descrip constitutional descrip constitutional descrip (scaled on Carbon atom) constitutional descrip constitutional descrip walk and path cour walk and path cour constitutional descrip constitutional descrip	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, A	CIUSIONS	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031
32 33 34 35 36 37 38 39 40	NO ₂ NO ₂ NO ₂ NO ₂ H H H H	0 0 NNHCSNH ₂ NNHCSNH ₂ 0 0 0 0 0 0 N-OH NNHCSNH ₂	$\frac{CH_{2}NCH(CH_{3})_{2}/_{2}}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}-N}{R^{2}}$ $\frac{CH_{2}N/CH(CH_{3})_{2}/_{2}}{CH_{2}-N}$ $\frac{CH_{2}-N}{O}$ $\frac{CH_{2}N(CH_{2}CH_{2}OH)_{2}}{CH_{2}-N}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID γ1	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des Des Wi sum of atomic Sa first Zagreb index Ran connectivity index Ran	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1000 1000 escriptor name 1000 1000 iener W index 1000 1000 c van der Waals 1000 1000 anderson electro 1000 1000 c van der Waals 1000 1000 ex by valence verfandic ID number 1000 1000	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend	,414 6,809 43,713 1,726 1 ,349 7,665 51,874 1,277 1 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 1 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (constit	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, A	CCUSIONS	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against Klebsiella pneumoniae ATCC 10031
32 33 34 35 35 36 37 38 38 39 40 41	NO ₂ NO ₂ NO ₂ NO ₂ H H H H H	0 0 NNHCSNH ₂ NNHCSNH ₂ 0 0 0 0 0 N-OH NNHCSNH ₂	$\frac{1}{CH_2N/CH(CH_3)_2/2}$ $\frac{1}{CH_2-N_1}$ $\frac{1}{CH_2-N_1}$ $\frac{1}{CH_2-N_1}$ $\frac{1}{CH_2-N_1}$ $\frac{1}{CH_2-N_1}$ $\frac{1}{CH_2N/CH(CH_3)_2/2}$ $\frac{1}{CH_2N/CH(CH_3)_2/2}$ $\frac{1}{CH_2-N_1O}$ $\frac{1}{CH_2N(CH_2CH_2OH)_2}$ $\frac{1}{CH_2N(CH_2CH_2CH)_2}$ $\frac{1}{CH_2-N_1O}$ $\frac{1}{CH_2-N_1O}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v χ1	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular 0 Des Wi sum of atomic Sa first Zagreb index Ran connectivity index Ran	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1 scriptor name 1 'iener W index 1 c van der Waals 1 anderson electro 1 c van der Waals 1 ex by valence verf 1 ndic ID number 1 ex chi-1 (Randic or index) 1	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend	3414 6,809 43,713 1,726 1 349 7,665 51,874 1,277 1 364 11,08 71,703 2,696 2 388 7,075 46,73 1,431 1 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a constitutional descriptor a 1 1 constitutional descriptor (scaled on Carbon a constitutional descriptor a) 1 1 constitutional descriptor (scaled on Carbon a constitutional descriptor a) 1 1 constitutional descriptor (scaled on Carbon a) 1 1 1	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, A Previo	Correlation of sum of atomic van der Waals (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
32 33 34 35 35 36 37 38 38 39 40 41 41 42	NO ₂ NO ₂ NO ₂ NO ₂ H H H H H	O O NNHCSNH2 NNHCSNH2 NNHCSNH2 O O O O NNHCSNH2 NNHCSNH2 O	$\frac{CH_{2}NCH(CH_{3})_{2}}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}-N}{CH_{2}-N}$ $\frac{CH_{2}N(CH(CH_{3})_{2}/_{2})}{CH_{2}-N}$ $\frac{CH_{2}N(CH_{2}CH_{2}OH)_{2}}{CH_{2}-N}$ $\frac{CH_{2}-N}{O}$ $\frac{CH_{2}N(CH_{2}CH_{2}OH)_{2}}{CH_{2}-N}$ $\frac{CH_{2}-N}{O}$ $\frac{CH_{2}N(CH_{2}CH_{2}OH)_{2}}{CH_{2}-N}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v χ1 XMOD	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular 0 Des 0 sum of atomic 0 sum of atomic 0 first Zagreb index Ran connectivity index 0 modified Ra 0	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1000 1000 escriptor name 1000 1000 iener W index 1000 1000 c van der Waals v 1000 1000 anderson electro 1000 1000 c van der Waals v 1000 1000 ex by valence verf 1000 1000 ex chi-1 (Randic of index) 1000 1000 andic connectivity 1000 1000	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 96 30,065 15,3 gend	3414 6,809 43,713 1,726 3 ,349 7,665 51,874 1,277 3 ,264 11,08 71,703 2,696 3 ,388 7,075 46,73 1,431 3 Descriptor type topological descrip constitutional descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) walk and path courd walk and path courd connectivity indescriptor connectivity indescriptor	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee	Correlation of sum of atomic van der Waals (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031
32 33 34 35 35 36 37 38 38 39 40 40 41 42	NO ₂ NO ₂ NO ₂ NO ₂ H H H H H H	O O O O NNHCSNH ₂ NNHCSNH ₂ O O O O O O NNHCSNH ₂ O O O O O O O O O O O O O O O O O O O O O O O O O O O	$\frac{CH_2N/CH(CH_3)_2/2}{CH_2N/CH(CH_3)_2/2}$ $\frac{CH_2-N_1^{-1}}{CH_2-N_1^{-1}}$ $\frac{CH_2-N_1^{-1}}{CH_2-N_1^{-1}}$ $\frac{CH_2-N_1^{-1}}{CH_2}$ $\frac{CH_2N/CH(CH_3)_2/2}{CH_2-N_1^{-1}}$ $\frac{CH_2-N_1^{-1}}{CH_2-N_1^{-1}}$ $\frac{CH_2N(CH_2CH_2OH)_2}{CH_2-N_1^{-1}}$ $\frac{CH_2-N_1^{-1}}{CH_2-N_1^{-1}}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1	23,61 0,64 24 24,91 0,68 28 35,48 0,67 4 20,72 0,69 4 puted molecular 0 Des 0 sum of atomic 0 sum of atomic 0 first Zagreb index Ran connectivity inde 0 modified Ra Randic-type eige	2302861,99154,444361,9242211881,6233283481,996descriptors' legscriptor name'iener W indexc van der Waals vanderson electroc van der Waals vanderson electroandic ID numberex by valence verfandic ID numberandic connectivityandic connectivity	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend	3414 6,809 43,713 1,726 1 ,349 7,665 51,874 1,277 1 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 1 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Procee	Correlation of sum of atomic van der Waals (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031 CLUSIONS us 2D QSAR results have antimicrobial activity (Noted to the construction of the construction o	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> <i>pneumoniae</i> ATCC 10031
32 33 34 35 36 37 38 39 40 41 42 43	NO ₂ NO ₂ NO ₂ NO ₂ H H H H H H H	O O O O NNHCSNH2 NNHCSNH2 O O O O O O NNHCSNH2 O O O O O O O O O NNHCSNH2 O O O O O O O O O O O O O O O O O O O O O	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1	23,61 0,64 24 24,91 0,68 28 35,48 0,67 4 20,72 0,69 3 puted molecular 0 Sum of atomic 0 sum of atomic 0 first Zagreb index Ran connectivity index Ran Randic-type eig adj adj	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1,996 scriptor name 1,996 'iener W index 1,096 c van der Waals v 1,096 anderson electro 1,096 c van der Waals v 1,096 anderson electro 1,096 ex by valence verf 1,096 ndic ID number 1,096 ex chi-1 (Randic of index) 1,096 andic connectivity 1,096 andic connectivity 1,096	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend	3414 6,809 43,713 1,726 3 ,349 7,665 51,874 1,277 3 ,264 11,08 71,703 2,696 3 ,388 7,075 46,73 1,431 3 Descriptor type topological descrip constitutional descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon a Constitutional descriptor (Scaled on Carbon a use topological descriptor (Scaled on Carbon a Connectivity indescriptor (Scaled on Carbon a	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, J Previou betwee •Prese	Correlation of sum of atomic van der Waals (10 ³ mol dm ³) against <i>Klebsiella</i> (10 ³ mol dm ³) against <i>klebsiella</i> (1	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 E shown significant correlation MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> greement with previously
32 33 34 35 36 37 38 39 40 41 42 43	NO ₂ NO ₂ NO ₂ NO ₂ H H H H H H H H H	0 0 NNHCSNH ₂ NNHCSNH ₂ 0 0 0 0 0 N-OH NNHCSNH ₂ 0 0 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 puted molecular 0 0 sum of atomic 0 0 sum of atomic 0 0 first Zagreb index Ran connectivity inde Ran modified Ra Randic-type eig adj Balaban dist	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1,996 escriptor name 1,996 escriptor nam	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 volumes 14,4 volumes 14,4 volumes 15,3 volumes 15,3 volumes 14,4 volumes 15,3 volume 15,3 volume 14,4 volumes 15,3 volume 14,4	,414 6,809 43,713 1,726 3 ,349 7,665 51,874 1,277 3 ,264 11,08 71,703 2,696 3 ,388 7,075 46,73 1,431 3 Descriptor type topological descrip constitutional descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a constitutional descriptor (scaled on Carbon a topological descriptor (scaled on Carbon a constitutional descriptor (scaled on Carbon a walk and path courd connectivity inde eigenvalue-based in connectivity inde	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine	Correlation of sum of atomic van der Waals (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebssiella pneumoniae</i> ATCC 10031 E shown significant correlation (TIS) and topological indices (TIS) agreement with previously
32 33 34 35 36 37 38 39 40 41 42 43 44	NO2 NO2 NO2 NO2 NO2 H H H H H H H H	0 0 NNHCSNH2 NNHCSNH2 0	$\frac{CH_{2}NCH(CH_{3})_{2}}{CH_{2}-N_{2}}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID	23,61 0,64 24 24,91 0,68 28 35,48 0,67 4 20,72 0,69 4 puted molecular Des sum of atomic Wi sum of atomic Sa first Zagreb index Ran connectivity inde Ran And Connectivity inde And Balaban dist And Balaban dist Bala	2302861,991254,444361,9242211881,6233283481,996descriptors' legescriptor namefiener W indexc van der Waals vanderson electroc van der Waals vanderson electroc van der Waals vex by valence verfndic ID numberex chi-1 (Randic ofindex)andic connectivitygenvector-basedjacency matrixtance connectivityaban ID number	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 volumes 14,4 volumes 14,4 volumes 15,3 volumes 15,3 volumes 14,4 volumes 15,3 volumes 15,3 volumes 14,4 volumes 15,3 volume 15,3 volume 14,4 volume 14,4 <t< th=""><th>3414 6,809 43,713 1,726 3 349 7,665 51,874 1,277 3 264 11,08 71,703 2,696 2 388 7,075 46,73 1,431 3 Descriptor type topological descrip constitutional descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Connectivity inde walk and path cou Connectivity inde connectivity inde Connectivity inde eigenvalue-based in Connectivity inde</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Previo betwee •Prese obtaine •3D QS</th><th>Correlation of sum of atomic van der Waals (10³ mol dm⁻³) against <i>Klebsiella</i> ATCC 10031</th><th>Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation ATCC 10031 the preference of biological indices (TIs) agreement with previously</th></t<>	3414 6,809 43,713 1,726 3 349 7,665 51,874 1,277 3 264 11,08 71,703 2,696 2 388 7,075 46,73 1,431 3 Descriptor type topological descrip constitutional descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon a Connectivity inde walk and path cou Connectivity inde connectivity inde Connectivity inde eigenvalue-based in Connectivity inde	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Previo betwee •Prese obtaine •3D QS	Correlation of sum of atomic van der Waals (10 ³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation ATCC 10031 the preference of biological indices (TIs) agreement with previously
32 33 34 35 36 37 38 39 40 41 42 43 44 45	NO2 NO2 NO2 NO2 NO2 H H H H H H H H H	0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP	23,61 0,64 24 24,91 0,68 28 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 Jourge for the second se	2302861,991254,444361,9242211881,6233283481,996descriptors' legscriptor name'iener W indexc van der Waals vanderson electroc van der Waals vanderson electroc van der Waals vex by valence verfndic ID numberex chi-1 (Randic orindex)andic connectivitygenvector-basedjacency matrixtance connectivityaban ID numberol-water partition	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 volumes 14,4 volumes 14,4 volumes 15,3 volumes 15,3 volumes 14,4 volumes 15,3 volumes 15,3 volumes 14,4 volumes 14,4 volume 14,4 <t< th=""><th>3414 6,809 43,713 1,726 3,349 349 7,665 51,874 1,277 3,388 7,075 46,73 1,431 3,388 7,075 46,73 1,431 3,388 7,075 46,73 1,431 3,388 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde co</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, J CON •Previo betwee •Prese obtaine •3D QS activity</th><th>Correlation of sum of atomic van der Waals (C 10⁻³ mol dm⁻³) against <i>Klebsiella</i> ACC 10031 CLUSIONS US 2D QSAR results have antimicrobial activity (No nt 2D results are in good ed. AR correlations indicate prediction on the basis of</th><th>Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AIC() and topological indices (TIs) agreement with previously the preference of biological for the preference of biological for the more than one MD and their</th></t<>	3414 6,809 43,713 1,726 3,349 349 7,665 51,874 1,277 3,388 7,075 46,73 1,431 3,388 7,075 46,73 1,431 3,388 7,075 46,73 1,431 3,388 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde co	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, J CON •Previo betwee •Prese obtaine •3D QS activity	Correlation of sum of atomic van der Waals (C 10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ACC 10031 CLUSIONS US 2D QSAR results have antimicrobial activity (No nt 2D results are in good ed. AR correlations indicate prediction on the basis of	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AIC() and topological indices (TIs) agreement with previously the preference of biological for the preference of biological for the more than one MD and their
32 33 34 35 36 37 38 39 40 41 42 43 44 45	NO2 NO2 NO2 NO2 NO2 H H H H H H H H H	0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0	$\frac{1}{CH_2N/CH(CH_3)_{2/2}}$ $\frac{1}{CH_2N/CH(CH_3)_{2/2}}$ $\frac{1}{CH_2N/CH(CH_3)COOH}$ $\frac{1}{r_1+r_1}$ $\frac{1}{r_1+r_2}$ $\frac{1}{r_1+r_2}$ $\frac{1}{r_1+r_2}$ $\frac{1}{r_1+r_2}$ $\frac{1}{r_2}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP ALOGP	23,61 0,64 24 24,91 0,68 28 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 puted molecular 0 0 sum of atomic 0 0 sum of atomic 0 0 first Zagreb index Ran connectivity inde Ran Randic-type eig adj Balaban dist Bala Moriguchi octano 0 Ghose-Crippen of 0	2302861,991254,444361,9242211881,6233283481,996descriptors' legescriptor namefiener W indexc van der Waals vanderson electroc van der Waals vex by valence verfndic ID numberex chi-1 (Randic ofindex)andic connectivitygenvector-basedjacency matrixtance connectivityoctanol-water partition	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 volumes 14,4 volumes 15,3 volumes 15,3 volumes 15,3 volumes 14,4 volumes 15,3 volumes 15,3 volumes 14,4 volumes 14,4 volume 14,4 <t< th=""><th>3414 6,809 43,713 1,726 3,349 ,349 7,665 51,874 1,277 3,388 ,388 7,075 46,73 1,431 3,388 7,075 46,73 1,431 3,388 3,388 7,075 46,73 1,431 3,388 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom)</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D QS activity influen</th><th>Correlation of sum of atomic van der Waals (first Zagreb index by valence vertex degrees) (C (10³ mol dm³) against <i>Klebsiella</i> ATCC 10031</th><th>Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological former than one MD and their as it is combination of</th></t<>	3414 6,809 43,713 1,726 3,349 ,349 7,665 51,874 1,277 3,388 ,388 7,075 46,73 1,431 3,388 7,075 46,73 1,431 3,388 3,388 7,075 46,73 1,431 3,388 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom)	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D QS activity influen	Correlation of sum of atomic van der Waals (first Zagreb index by valence vertex degrees) (C (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological former than one MD and their as it is combination of
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46	NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c} CH_{2}N/CH(CH_{3})_{2/2} \\ \hline \\ CH_{2}-N/CH(CH_{3})_{2/2} \\ \hline \\ CH_{2}-N/CH(CH_{3})COOH \\ \hline \\ \\ R \\ + \\ + \\ + \\ + \\ + \\ + \\ + \\ + \\$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP ALOGP	23,61 0,64 24 24,91 0,68 28 35,48 0,67 4 20,72 0,69 3 puted molecular Des wi sum of atomic S sum of atomic Sa first Zagreb index Ran connectivity inde Ran modified Ra Adj Balaban dist Bala Moriguchi octano Ghose-Crippen of	2302861,991254,444361,9242211881,6233283481,996descriptors' legescriptor namefener W indexc van der Waals vanderson electroc van der Waals vex by valence verfndic ID numberex chi-1 (Randic ofindex)andic connectivitygenvector-basedjacency matrixtance connectivityoctanol-water partitionoctanol-water partition	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 volumes 14,4 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 16,3 volume 16,3 <tr< th=""><th>3,302 30,001 1,010 1,010 ,414 6,809 43,713 1,726 1,349 ,349 7,665 51,874 1,277 1,388 ,388 7,075 46,73 1,431 1,431 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descrip (scaled on Carbon atom) constitutional descrip walk and path cour connectivity inde connectivity ind</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influent</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees NC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> ATCC 10031</th><th> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation MIC) and topological indices (TIs) agreement with previously the preference of biological form of the preference of the preferen</th></tr<>	3,302 30,001 1,010 1,010 ,414 6,809 43,713 1,726 1,349 ,349 7,665 51,874 1,277 1,388 ,388 7,075 46,73 1,431 1,431 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descrip (scaled on Carbon atom) constitutional descrip walk and path cour connectivity inde connectivity ind	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influent	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees NC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation MIC) and topological indices (TIs) agreement with previously the preference of biological form of the preference of the preferen
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46 47	NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des j 0,61 1 j 0,69 3 j j Des j j Norig j sum of atomic Sa mean atomic j first Zagreb index Ran j connectivity inde Ran i connectivity inde adj j Balaban dist Bala Moriguchi octano Ghose-Crippen of Ga i Squared Ghose Squared Ghose	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 escriptor name 9 iener W index 9 c van der Waals v 9 anderson electro 9 c van der Waals v 9 ex by valence verf 9 ndic ID number 9 ex chi-1 (Randic of index) 9 andic connectivity 9 genvector-based 9 jacency matrix 1 tance connectivity 1 aban ID number 9 octanol-water partition 1 octanol-water partition 1 octanol-water partition 1	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 2 32,235 16,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 15,3 volumes 16,3 volume 16,3 <th>10,002 0,001 1,000 1,000 ,414 6,809 43,713 1,726 1,349 ,264 11,08 71,703 2,696 2,269 ,388 7,075 46,73 1,431 2,269 ,388 7,075 46,73 1,431 2,269 ,388 7,075 46,73 1,431 2,269 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 ,388 7,075 46,73 1,431 ,389</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •Prese obtaine •Prese obtaine •aactivity influene</th> <th>Correlation of sum of atomic van der Waals (C 10⁻³ mol dm⁻³) against <i>Klebsiella</i> ATCC 10031 CLUSIONS US 2D QSAR results have antimicrobial activity (No ant 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topolog</th> <th> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological formore than one MD and their as it is combination of gical (W, ZMV1,), and wher</th>	10,002 0,001 1,000 1,000 ,414 6,809 43,713 1,726 1,349 ,264 11,08 71,703 2,696 2,269 ,388 7,075 46,73 1,431 2,269 ,388 7,075 46,73 1,431 2,269 ,388 7,075 46,73 1,431 2,269 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 46,73 1,431 2,2696 ,388 7,075 ,388 7,075 46,73 1,431 ,389	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •Prese obtaine •Prese obtaine •aactivity influene	Correlation of sum of atomic van der Waals (C 10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031 CLUSIONS US 2D QSAR results have antimicrobial activity (No ant 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topolog	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological formore than one MD and their as it is combination of gical (W, ZMV1,), and wher
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46 47 48	NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular 0 5 puted molecular 0 0 sum of atomic Sa 0 5 first Zagreb index Ran connectivity inde Ran modified Ra Randic-type eig adj Balaban dist Moriguchi octano Ghose-Crippen of Squared Ghose partitio	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 scriptor name 1 'iener W index 1 c van der Waals 's 1 anderson electro 1 c van der Waals 's 1 anderson electro 1 ex by valence verf 1 ndic ID number 1 ex chi-1 (Randic of index) 1 andic connectivity 1 genvector-based 1 jacency matrix 1 tance connectivity 1 octanol-water partition 1 octanol-water partition 1 octanol-water partition 1 octanol-water partition 1 on coeff. (logP') 1	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 23 46,888 23,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 15,3 volumes 16,3 volume 16,3 </th <th>10,002 0,001 1,000 1,000 ,414 6,809 43,713 1,726 1,349 ,264 11,08 71,703 2,696 2,269 ,388 7,075 46,73 1,431 1,727 ,388 7,075 46,73 1,431 1,726 constitutional descriptor type topological descriptor (Carbon atom) 1,431 1,737 constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) 1,600 1,600 constitutional descriptor (scaled on Carbon atom) 1,000 1,000 1,000 constitutional descriptor (scaled on Carbon atom) 1,000 1,000 1,000 constitutional descriptor (scaled on Carbon atom) 1,000 1,000 1,000 connectivity inde connectivity inde 1,000 1,000 1,000 connectivity inde 1,000 1,000 1,000 1,000 1,000 connectivity inde 1,000 1,000 1,000 1,000 1,000 1,000 connectivity inde</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •3D QS activity influent constitu</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ATCC 10031 CCLUSIONS Dus 2D QSAR results have an antimicrobial activity (Nont 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologian are properties (AlogP, ML</th> <th> Figure 13. 3D Correlation of sum of atomic van der Waats volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological for the ir as it is combination of gical (W, ZMIV1,), and topological (W, ZMIV1,), and topology) descriptors. </th>	10,002 0,001 1,000 1,000 ,414 6,809 43,713 1,726 1,349 ,264 11,08 71,703 2,696 2,269 ,388 7,075 46,73 1,431 1,727 ,388 7,075 46,73 1,431 1,726 constitutional descriptor type topological descriptor (Carbon atom) 1,431 1,737 constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) 1,600 1,600 constitutional descriptor (scaled on Carbon atom) 1,000 1,000 1,000 constitutional descriptor (scaled on Carbon atom) 1,000 1,000 1,000 constitutional descriptor (scaled on Carbon atom) 1,000 1,000 1,000 connectivity inde connectivity inde 1,000 1,000 1,000 connectivity inde 1,000 1,000 1,000 1,000 1,000 connectivity inde 1,000 1,000 1,000 1,000 1,000 1,000 connectivity inde	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •3D QS activity influent constitu	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ATCC 10031 CCLUSIONS Dus 2D QSAR results have an antimicrobial activity (Nont 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologian are properties (AlogP, ML	 Figure 13. 3D Correlation of sum of atomic van der Waats volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological for the ir as it is combination of gical (W, ZMIV1,), and topological (W, ZMIV1,), and topology) descriptors.
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49	NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H H	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c} \begin{array}{c} CH_{2}NCH(CH_{3})_{2}2 \\ \hline \\ CH_{2}NCH(CH_{3})_{2}2 \\ \hline \\ \\ CH_{2}-N \\ \hline \\ \end{array} \\ \hline \\ \hline \\ CH_{2}-N \\ \hline \\ \end{array} \\ \hline \\ \hline \\ \hline \\ \\ CH_{2}-N \\ \hline \\ \hline \\ \hline \\ \hline \\ \\ \hline \\ \\ \hline \\ \hline \\ \hline \\ \\ \hline \\ \hline \\ \\ \hline \hline \\ \hline \\ \hline \\ \hline \\ \hline \hline \\ \hline \\ \hline \\ \hline \hline \\ \hline \hline \\ \hline \\ \hline \hline \hline \\ \hline \hline \hline \\ \hline \hline \hline \\ \hline \hline \hline \hline \\ \hline \hline \hline \hline \hline \\ \hline \hline$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 4 puted molecular Des puted molecular 0 Sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Randic first Zagreb index Randic Sandic-type eig adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghos partitic	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 scriptor name 9 'iener W index 1 c van der Waals 's 9 anderson electro 1 c van der Waals 's 9 anderson electro 9 ex by valence verf 9 ndic ID number 9 ex chi-1 (Randic of index) 9 andic connectivity 9 genvector-based 9 jacency matrix 1 tance connectivity 9 genvector-based 9 jacency matrix 1 tance connectivity 9 octanol-water partition 9 octanol-water partition 9 octanol-water partition 9 octanol-water partition 9	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 3 46,888 23,3 3 46,888 23,3 3 30,065 15,3 gend 30,065 15,3 gend 30,065 15,3 yolumes 14,4 14,4 yolumes 15,3 yolumes 15,3 yolume 14,3 yolume <t< th=""><th>3412 0,001 1,000 1,000 414 6,809 43,713 1,726 1 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 1 Constitutional descriptor type topological descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon at constitutional descriptor (scaled on Carbon at constitutional descriptor (scaled on Carbon at connectivity indescriptor (scaled on Carbon at cource) topological descriptor (scaled on Carbon at connectivity indescriptor (scaled on Carbon at cource) at copological descriptor (scaled on Carbon at cource) walk and path cource connectivity indescriptor (scaled on Carbon at cource) at copological descriptor (scaled on Carbon at cource) walk and path cource molecular proper molecular proper</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D QS activity influent constitu molecu •3D CO</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 10031 CCURSIONS US 2D QSAR results have en antimicrobial activity (No int 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topolog alar properties (AlogP, ML relations allow better spa</th><th> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological for the irrest is combination of gical (W, ZMV1,), and topological (W, ZMV1,), and topological indices (TIS) and the irrest is combination of gical (W, ZMV1,), and topological (W, ZMV1,), and topological indices (TIS) and the irrest is combination of gical (W, ZMV1,), and the irrest is combination of gical (W, ZMV1,</th></t<>	3412 0,001 1,000 1,000 414 6,809 43,713 1,726 1 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 1 Constitutional descriptor type topological descriptor (Carbon atom) Constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon at constitutional descriptor (scaled on Carbon at constitutional descriptor (scaled on Carbon at connectivity indescriptor (scaled on Carbon at cource) topological descriptor (scaled on Carbon at connectivity indescriptor (scaled on Carbon at cource) at copological descriptor (scaled on Carbon at cource) walk and path cource connectivity indescriptor (scaled on Carbon at cource) at copological descriptor (scaled on Carbon at cource) walk and path cource molecular proper molecular proper	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D QS activity influent constitu molecu •3D CO	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 10031 CCURSIONS US 2D QSAR results have en antimicrobial activity (No int 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topolog alar properties (AlogP, ML relations allow better spa	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AICC) and topological indices (TIs) agreement with previously the preference of biological for the irrest is combination of gical (W, ZMV1,), and topological (W, ZMV1,), and topological indices (TIS) and the irrest is combination of gical (W, ZMV1,), and topological (W, ZMV1,), and topological indices (TIS) and the irrest is combination of gical (W, ZMV1,), and the irrest is combination of gical (W, ZMV1,
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50	NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ 1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 5 puted molecular 0 6 Sum of atomic 0 0 sum of atomic 0 0 first Zagreb index Ran connectivity inde 8 modified Ra Randic-type eig adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghose partition	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 scriptor name 9 iener W index 9 c van der Waals v anderson electro c van der Waals v anderson electro x by valence verf ndic ID number ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity genvector-based jacency matrix tance connectivity genvector-based jacency matrix tance connectivity octanol-water partition octanol-water partition octanol-water partition octanol-water partition	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 3 46,888 23,3 3 46,888 23,3 3 30,065 15,3 gend 14,4 volumes 15,3 volumes 16,3 volume	3412 0,002 0,011 1,010 1,414 4,809 43,713 1,726 1,349 349 7,665 51,874 1,277 1,264 388 7,075 46,73 1,431 1,338 Descriptor type topological descrip constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descrip walk and path cou connectivity inde connectivity inde <td< th=""><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •Prese obtaine •Prese obtaine •3D QS activity influen constitu molecu</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> ATCC 10031</th><th> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AlC) and topological indices (TIs) agreement with previously the preference of biological for more than one MD and their as it is combination of gical (W, ZMV1,), and cogP,) descriptors. atial dispersion and thus provide QSAR study. </th></td<>	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •Prese obtaine •Prese obtaine •3D QS activity influen constitu molecu	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AlC) and topological indices (TIs) agreement with previously the preference of biological for more than one MD and their as it is combination of gical (W, ZMV1,), and cogP,) descriptors. atial dispersion and thus provide QSAR study.
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51	NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv ZM1v CID χ 1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 25 35,48 0,67 35 20,72 0,69 35 puted molecular 0 35 puted molecular 0 35 sum of atomic 0 35 sum of atomic 35 35 sum of atomic 35 35 first Zagreb 1 gagreb 1 2 first Zagreb 1 gagreb 1 2 first Zagreb 1 gagreb 1 3 first Zagreb 1 gagreb 1 3 first Zagreb 1 gagreb 1 3 gagreb 3 3 <t< th=""><th>230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 scriptor name 9 iener W index 9 c van der Waals * 9 anderson electro 9 c van der Waals * 9 ex by valence verf 9 ndic ID number 9 ex chi-1 (Randic of index) 9 andic connectivity 9 genvector-based 9 jacency matrix 1 tance connectivity 9 octanol-water partition 9 octanol-water partition 9 octanol-water partition 9 se-Crippen octar 9 on coeff. (logP^2 9</th><th>1 28,394 14,9 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,9 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolume 16,3 yolume 16,3</th><th>3412 34,002 35,011 1,010 1,414 6,809 43,713 1,726 1,277 1,264 ,264 11,08 71,703 2,696 2,388 ,388 7,075 46,73 1,431 1,431 Descriptor type 1,431 1,431 Constitutional descriptor (Carbon atom)) Constitutional descriptor (Scaled on Carbon atom)) constitutional descriptor (Scaled on Carbon atom)) Constitutional descriptor (Scaled on Carbon atom)) 1,000 constitutional descriptor (Scaled on Carbon atom)) 1,000 1,000 constitutional descriptor (Scaled on Carbon atom)) 1,000 1,000 constitutional descriptor (Scaled on Carbon atom) 1,000 1,000 connectivity indescriptor 1,000</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previo betwee •Prese obtaine •3D QS activity influen constitu molecu •3D con an opti •Good</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees MC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> ATCC 10031</th><th> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> e shown significant correlation AllC) and topological indices (TIs) agreement with previously the preference of biological for their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide QSAR study. atudy were observed using </th></t<>	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 scriptor name 9 iener W index 9 c van der Waals * 9 anderson electro 9 c van der Waals * 9 ex by valence verf 9 ndic ID number 9 ex chi-1 (Randic of index) 9 andic connectivity 9 genvector-based 9 jacency matrix 1 tance connectivity 9 octanol-water partition 9 octanol-water partition 9 octanol-water partition 9 se-Crippen octar 9 on coeff. (logP^2 9	1 28,394 14,9 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,9 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolume 16,3	3412 34,002 35,011 1,010 1,414 6,809 43,713 1,726 1,277 1,264 ,264 11,08 71,703 2,696 2,388 ,388 7,075 46,73 1,431 1,431 Descriptor type 1,431 1,431 Constitutional descriptor (Carbon atom)) Constitutional descriptor (Scaled on Carbon atom)) constitutional descriptor (Scaled on Carbon atom)) Constitutional descriptor (Scaled on Carbon atom)) 1,000 constitutional descriptor (Scaled on Carbon atom)) 1,000 1,000 constitutional descriptor (Scaled on Carbon atom)) 1,000 1,000 constitutional descriptor (Scaled on Carbon atom) 1,000 1,000 connectivity indescriptor 1,000	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previo betwee •Prese obtaine •3D QS activity influen constitu molecu •3D con an opti •Good	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees MC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> ATCC 10031	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> e shown significant correlation AllC) and topological indices (TIs) agreement with previously the preference of biological for their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide QSAR study. atudy were observed using
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 44 45 46 47 48 49 50 51 52	NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2 NO2	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ 1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular Des sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Ran connectivity inde Ran Randic-type eig adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghos partition	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 9 escriptor name 9 iener W index 9 c van der Waals 9 anderson electro 9 c van der Waals 9 ex by valence verf 9 ndic ID number 9 ex chi-1 (Randic of index) 9 andic connectivity 9 genvector-based 9 jacency matrix 1 tance connectivity 9 octanol-water partition 9 octanol-water partition 9 octanol-water partition 9 se-Crippen octar 9 on coeff. (logP^2 9	1 28,394 14,9 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,9 yolumes 14,9 yolumes 14,9 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolumes 15,3 yolume 16,3	3412 34,001 34,001 1,010 ,414 6,809 43,713 1,726 1 ,264 11,08 71,703 2,696 2 ,388 7,075 46,73 1,431 1 Constitutional descriptor (pological descriptor (pological descriptor (pological descriptor (scaled on Carbon atom)) Constitutional descriptor (scaled on Carbon atom)) Constitutional descriptor (scaled on Carbon atom) Constitutional descriptor (scaled on Carbon atom) Constitutional descriptor (scaled on Carbon atom) Connectivity index Connectivity index Connectivity index Connectivity index Connectivity index eigenvalue-based in topological descrip walk and path cour molecular proper molecular proper molecular proper	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •Prese obtaine •3D Q activity influen constitu molecu •3D con an opti •Good constitu	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees IC (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031 CLUSIONS US 2D QSAR results have an antimicrobial activity (Mathematical ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topological and selection of MDs in G correlations in this QSAR utional (Sv, Mv). topological	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation MIC) and topological indices (TIs) agreement with previously the preference of biological for more than one MD and their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide QSAR study. study were observed using cal (W), connectivity (γ1. γMOD).
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53	NO2 NO2 NO2 NO2 NO2 NO2 H <t< th=""><th>0 0 0 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c c c c c c c c c c c c c c c c c c c$</th><th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv CID χ1 XMOD VRA1 BID MLOGP ALOGP2</th><th>23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular Des puted molecular 1 Sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Ran connectivity inde Ran Randic-type eig adj Balaban dist Bala Moriguchi octano Ghose-Crippen d Squared Ghose partitic Squared Ghose partitic</th><th>230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1,996 scriptor name 1 'iener W index 1 c van der Waals 's 1 anderson electro 1 c van der Waals 's 1 andic ID number 1 ex by valence verf 1 ndic ID number 1 ex chi-1 (Randic of index) 1 andic connectivity 1 genvector-based 1 jacency matrix 1 tance connectivity 1 genvector-based 1 jacency matrix 1 tance connectivity 1 octanol-water partition 1 octanol-water partition 1 octanol-water partition 1 se-Crippen octar 1 on coeff. (logP^2 1</th><th>1 28,394 14,9 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,9 volumes 14,9 volumes 14,9 volumes 15,3 volumes 15,3 volumes 16,3 volume 16,3</th><th>0,010 0,011 1,010 ,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 2,388 ,388 7,075 46,73 1,431 1,331 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde connectivity inde eigenvalue-based in molecular proper molecular</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D Volumes (Sv), ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •Prese obtaine •3D QS activity influen constitu molecu •3D con an opti •Good</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ATCC 10031 CCUCUSIONS ATCC 10031 CUCUSIONS ATCC 10031 CUCUSIONS ATCC 10031 ATCC 10031 ATCC</th><th> Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AlC() and topological indices (TIs) agreement with previously the preference of biological for their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide DSAR study. study were observed using cal (W), connectivity (χ1, χMOD), tors with antimicrobial activity. </th></t<>	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv CID χ1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 5 puted molecular Des puted molecular 1 Sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Ran connectivity inde Ran Randic-type eig adj Balaban dist Bala Moriguchi octano Ghose-Crippen d Squared Ghose partitic Squared Ghose partitic	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 1,996 scriptor name 1 'iener W index 1 c van der Waals 's 1 anderson electro 1 c van der Waals 's 1 andic ID number 1 ex by valence verf 1 ndic ID number 1 ex chi-1 (Randic of index) 1 andic connectivity 1 genvector-based 1 jacency matrix 1 tance connectivity 1 genvector-based 1 jacency matrix 1 tance connectivity 1 octanol-water partition 1 octanol-water partition 1 octanol-water partition 1 se-Crippen octar 1 on coeff. (logP^2 1	1 28,394 14,9 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,9 volumes 14,9 volumes 14,9 volumes 15,3 volumes 15,3 volumes 16,3 volume 16,3	0,010 0,011 1,010 ,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 2,388 ,388 7,075 46,73 1,431 1,331 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde connectivity inde eigenvalue-based in molecular proper molecular	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D Volumes (Sv), ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •Prese obtaine •3D QS activity influen constitu molecu •3D con an opti •Good	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ATCC 10031 CCUCUSIONS ATCC 10031 CUCUSIONS ATCC 10031 CUCUSIONS ATCC 10031 ATCC	 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation AlC() and topological indices (TIs) agreement with previously the preference of biological for their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide DSAR study. study were observed using cal (W), connectivity (χ1, χMOD), tors with antimicrobial activity.
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 44 45 46 47 48 49 50 51 52 53 54	NO2 NO3 NO4 H <th>0 0 0 NNHCSNH2 NNHCSNH2 0</th> <th>$\begin{array}{c} CH_2 N(CH(CH_3)_2/2 \\ CH_2 N(CH(CH_3)_2/2 \\ CH_2 N(CH(CH_3)_2/2 \\ CH_2 - N \\ \end{array} \\ \hline \\ CH_2 - N \\ \hline \\ \\ \hline \\ \\ CH_2 N(CH_2 CH_3) COOH \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1 XMOD VRA1 BID MLOGP ALOGP2</th> <th>23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 4 puted molecular 0 puted molecular 0 sum of atomic Sa 0 sum of atomic Sa 0 first Zagreb index Ran connectivity inde Ran Moriguchi octano adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghos partitio Abri, et al., Eur Cabri, et al., Eur abri, et al., Sohou Cabri, et al., Eur</th> <th>230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptor name 'iener W index c van der Waals 's anderson electro c van der Waals 's anderson electro c van der Waals 's ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity genvector-based jacency matrix tance connectivity octanol-water partition octanol-water partition</th> <th>1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 32,235 16,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 14,4 volumes 15,3 volume 16,3 volume 16,3</th> <th>0,000 0,000 1,000 ,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 2,388 ,388 7,075 46,73 1,431 1,331 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde connectivity inde connectivity inde connectivity inde connectivity inde</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •Prese obtaine •3D Q activity influen constitu molecu •3D con an opti •Good constitu</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10³ mol dm³) against <i>Klebsiella</i> ATCC 10031</th> <th></th>	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c} CH_2 N(CH(CH_3)_2/2 \\ CH_2 N(CH(CH_3)_2/2 \\ CH_2 N(CH(CH_3)_2/2 \\ CH_2 - N \\ \end{array} \\ \hline \\ CH_2 - N \\ \hline \\ \\ \hline \\ \\ CH_2 N(CH_2 CH_3) COOH \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ 1 XMOD VRA1 BID MLOGP ALOGP2	23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 4 puted molecular 0 puted molecular 0 sum of atomic Sa 0 sum of atomic Sa 0 first Zagreb index Ran connectivity inde Ran Moriguchi octano adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghos partitio Abri, et al., Eur Cabri, et al., Eur abri, et al., Sohou Cabri, et al., Eur	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptor name 'iener W index c van der Waals 's anderson electro c van der Waals 's anderson electro c van der Waals 's ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity genvector-based jacency matrix tance connectivity octanol-water partition	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 32,235 16,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 14,4 volumes 15,3 volume 16,3	0,000 0,000 1,000 ,414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 2,388 ,388 7,075 46,73 1,431 1,331 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde connectivity inde connectivity inde connectivity inde connectivity inde	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •Prese obtaine •3D Q activity influen constitu molecu •3D con an opti •Good constitu	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031	
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 44 45 46 47 48 49 50 51 52 53 54	NO2 NO2 NO2 NO2 NO2 NO2 H <t< th=""><th>0 0 0 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}-N \\ \end{array}$</th><th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv CID χ1 XMOD VRA1 J BID MLOGP ALOGP2 ALOGP2 SV. K. Agg 2919-29</th><th>23,61 0,64 2 24,91 0,68 26 35,48 0,67 2 20,72 0,69 3 puted molecular Des puted molecular Wi sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Randic forst Zagreb index Randic Andrigue chi octano Ghose - Crippen of Squared Ghose partition Squared Ghose partition Abri, et al., Eur Squared Ghose 26. Solution</th><th>230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 328 348 1,996 descriptors' leg scriptors' leg scriptor name fener W index c van der Waals v anderson electro c van der Waals v andic ID number ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity andic connectivity genvector-based jacency matrix tance connectivity aban ID number octanol-water partition octanol-water partition octanol-vater partition</th><th>1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 23 46,888 23,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 16,3 volume 16,3 index from 16,3 index from 16,3 index from 16,3 of coeff (logP) 16,3 artition coeff. 10,3 on adikar, Bio 10,3</th><th>0,001 1,010 414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 2,388 7,075 46,73 1,431 1,431 1,431 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde eigenvalue-based in molecular proper molecu</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu and lip (MIC) a</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10³ mol dm³) against <i>Klebsiella</i> ATCC 10031</th><th></th></t<>	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c} CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}-N \\ \end{array}$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv CID χ 1 XMOD VRA1 J BID MLOGP ALOGP2 ALOGP2 SV. K. Agg 2919-29	23,61 0,64 2 24,91 0,68 26 35,48 0,67 2 20,72 0,69 3 puted molecular Des puted molecular Wi sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Randic forst Zagreb index Randic Andrigue chi octano Ghose - Crippen of Squared Ghose partition Squared Ghose partition Abri, et al., Eur Squared Ghose 26. Solution	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 328 348 1,996 descriptors' leg scriptors' leg scriptor name fener W index c van der Waals v anderson electro c van der Waals v andic ID number ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity andic connectivity genvector-based jacency matrix tance connectivity aban ID number octanol-water partition octanol-water partition octanol-vater partition	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 36 30,065 15,3 gend 14,4 23 46,888 23,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 16,3 volume 16,3 index from 16,3 index from 16,3 index from 16,3 of coeff (logP) 16,3 artition coeff. 10,3 on adikar, Bio 10,3	0,001 1,010 414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 2,388 7,075 46,73 1,431 1,431 1,431 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde eigenvalue-based in molecular proper molecu	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu and lip (MIC) a	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (IC (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031	
32 33 34 35 35 36 37 38 39 40 41 42 43 44 45 44 45 46 47 48 49 50 51 52 53 54 55	NO2 H <td< th=""><th>О О О О О О О О О О О О О О О О О О О</th><th>$\begin{array}{c c c c c c c c c c c c c c c c c c c$</th><th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7.0</th><th>23,61 0,64 2 24,91 0,68 26 35,48 0,67 4 20,72 0,69 5 puted molecular Des Sum of atomic Sa wi sum of atomic Sa mean atomic first Zagreb index Ran connectivity inde Ran Moriguchi octano Ghose-Crippen of Squared Ghose partition Squared Ghose partition Squared Ghose partition Consectivity inde Consectivity inde Ghose-Crippen of Consectivity inde Squared Ghose Calaba Squared Ghose Calaba Squared Ghose Calaba Contract of Calaba Calaba Squared Ghose Calaba Contract of Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Cal</th><th>230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 348 1,996 descriptors' leg 356 1,996 scriptor name 1,996 'iener W index 1,996 c van der Waals 's 1,996 anderson electro 1,996 c van der Waals 's 1,996 anderson electro 1,996 c van der Waals 's 1,996 anderson electro 1,996 c van der Waals 's 1,996 ex by valence verf 1,996 ndic ID number 1,996 ex chi-1 (Randic of index) 1,996 andic connectivity 1,996 genvector-based 1,996 jacency matrix 1,996 tance connectivity 1,996 octanol-water partition 1,997 octanol-water partition 1,996 octanol-water partition 1,997 see-Crippen octar 1,997 andic connectivity 1,996</th></td<> <th>28,394 14,4 232,235 16,3 332,235 15,3 36 30,065 15,3 gend 1 volumes 1 volumes 1 volume 1 connectivity 1 artition coeff 1 nol-water 1 artition coeff 1 006) 0</th> <th>1010 1010 414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 1,338 7,075 46,73 1,431 1 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde connectivity inde eigenvalue-based in connectivity inde walk and path cou molecular proper molecular proper molecular proper molecular proper molecular proper</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •3D QS activity influent constitu molecu •3D con an opti •Good constitu and lip (MIC) a</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 100³ mol dm³) against <i>Klebsiella</i> ATCC 1003 CLUSIONS US 2D QSAR results have an antimicrobial activity (Material 20 results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologic alar properties (AlogP, ML rrelations allow better spa mal selection of MDs in G correlations in this QSAR utional (Sv, Mv), topologic ophylicity (AlogP) descrip against <i>Staphylococcus</i> a ested method can be usef</th> <th></th>	О О О О О О О О О О О О О О О О О О О	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7.0	23,61 0,64 2 24,91 0,68 26 35,48 0,67 4 20,72 0,69 5 puted molecular Des Sum of atomic Sa wi sum of atomic Sa mean atomic first Zagreb index Ran connectivity inde Ran Moriguchi octano Ghose-Crippen of Squared Ghose partition Squared Ghose partition Squared Ghose partition Consectivity inde Consectivity inde Ghose-Crippen of Consectivity inde Squared Ghose Calaba Squared Ghose Calaba Squared Ghose Calaba Contract of Calaba Calaba Squared Ghose Calaba Contract of Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Calaba Cal	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 348 1,996 descriptors' leg 356 1,996 scriptor name 1,996 'iener W index 1,996 c van der Waals 's 1,996 anderson electro 1,996 c van der Waals 's 1,996 anderson electro 1,996 c van der Waals 's 1,996 anderson electro 1,996 c van der Waals 's 1,996 ex by valence verf 1,996 ndic ID number 1,996 ex chi-1 (Randic of index) 1,996 andic connectivity 1,996 genvector-based 1,996 jacency matrix 1,996 tance connectivity 1,996 octanol-water partition 1,997 octanol-water partition 1,996 octanol-water partition 1,997 see-Crippen octar 1,997 andic connectivity 1,996	28,394 14,4 232,235 16,3 332,235 15,3 36 30,065 15,3 gend 1 volumes 1 volumes 1 volume 1 connectivity 1 artition coeff 1 nol-water 1 artition coeff 1 006) 0	1010 1010 414 6,809 43,713 1,726 ,349 7,665 51,874 1,277 1,264 ,264 11,08 71,703 2,696 1,338 7,075 46,73 1,431 1 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) constitutional descriptor (Scaled on Carbon atom) connectivity inde connectivity inde connectivity inde eigenvalue-based in connectivity inde walk and path cou molecular proper molecular proper molecular proper molecular proper molecular proper	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •3D QS activity influent constitu molecu •3D con an opti •Good constitu and lip (MIC) a	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 100 ³ mol dm ³) against <i>Klebsiella</i> ATCC 1003 CLUSIONS US 2D QSAR results have an antimicrobial activity (Material 20 results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologic alar properties (AlogP, ML rrelations allow better spa mal selection of MDs in G correlations in this QSAR utional (Sv, Mv), topologic ophylicity (AlogP) descrip against <i>Staphylococcus</i> a ested method can be usef	
32 33 34 35 35 35 36 37 38 39 40 41 42 43 44 45 44 45 44 50 51 52 53 54 55 56	NO2 NO3 NO4 H	0 0 0 NNHCSNH₂ NNHCSNH₂ 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ 1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222	23,61 0,64 2 24,91 0,68 26 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 sum of atomic Sa 0 0 sum of atomic Sa mean atomic 0 first Zagreb index Ran 0 connectivity inde 8 0 Moriguchi octano Ghose-Crippen of 0 Squared Ghose partition 0 Squared Ghose 0 0 Consectivity inde 0 0 Ghose-Crippen of 0 0 Squared Ghose 0 0 Squared Ghose 0 0 26. 56,914 (J. Torre 0 245, http://www 0 0	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg scriptor name 1 scriptor name 1 1 1 iener W index c van der Waals for anderson electron 1 c van der Waals for anderson electron anderson electron 1 c van der Waals for anderson electron 1 1 ex by valence verfandic ID number 1 1 ex chi-1 (Randic of index) 1 1 andic connectivity 1 1 genvector-based 1 1 andic connectivity 1 1 genvector-based 1 1 andic logP) 1 1 octanol-water partition 1 1 octanol-water partition 1 1 octanol-water partition 1 1 octanol-water partition 1 1 octanol-water partentso 1	28,394 14,4 232,235 16,3 346,888 23,3 36 30,065 15,3 gend 1 volumes 1 volumes 1 volume 1 index from 1 artition coeff. 1 nol-water 1 006) 006) 006) 006) 006) 006)	1002 0001 1000 414 6,809 43,713 1,726 349 7,665 51,874 1,277 1 264 11,08 71,703 2,696 2 388 7,075 46,73 1,431 1 Descriptor type topological descriptor (Carbon atom) constitutional descriptor (Carbon atom) constitutional descriptor (scaled on Carbon atom) connectivity indescriptor (scaled on Carbon atom) connectivity inde	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previou betwee •Prese obtaine •3D QS activity influent constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees MIC (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031	
32 333 34 35 35 36 37 38 39 40 41 42 43 44 42 43 50 51 52 53 54 55 56 57	NO2 H <th>0 0 0 NNHCSNH₂ NNHCSNH₂ 0</th> <th>$\begin{array}{c c c c c c c c c c c c c c c c c c c$</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mlog J BID MLOGP2 ALOGP2 S. USP 7,0 4. EP11222 5. M. Movr</th> <th>23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 3 puted molecular Des sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Randic-type eig connectivity inde Balaban dist Moriguchi octano Ghose-Crippen of Squared Ghose partition sum of al., Eur Squared Ghose fabri, et al., Eur Squared Ghose abri, et al., Eur Squared Ghose fabri, et al., Eur Soly fabri,</th> <th>230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptor name iener W index c c van der Waals v anderson electro c van der Waals v anderson electro c van der Waals v andic ID number ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity genvector-based jacency matrix tance connectivity genvector-based jacency matrix tance connectivity octanol-water partition octanol-water partition</th> <th>28,394 14,4 232,235 16,3 332,235 15,3 36 30,065 15,3 gend 1 volumes 1 volumes 1 volume 1 index from 1 artition coeff. 1 nol-water 1 006) 006) online.com/ 1 Maysinger; 1</th> <th>Image Image Image 414 6,809 43,713 1,726 1,349 349 7,665 51,874 1,277 1,338 264 11,08 71,703 2,696 2,338 7,075 46,73 1,431 1,331 1,331 Descriptor type topological descrip constitutional descriptor (scaled on Carbon atom) constitutional descrip (scaled on Carbon atom) constitutional descrip walk and path cou connectivity inde eigenvalue-based in topological descrip walk and path cou connectivity inde eigenvalue-based in molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previou betwee •Prese obtaine •3D Q activity influent constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 1003 COMPARTING ACC 1003 CONTRICTIONS CLUSSIONS ACC 1003 CONTRICTIONS ACC 1003 CONTR</th> <th></th>	0 0 0 NNHCSNH₂ NNHCSNH₂ 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mlog J BID MLOGP2 ALOGP2 S. USP 7,0 4. EP11222 5. M. Movr	23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 3 puted molecular Des sum of atomic Sa Wi sum of atomic Sa mean atomic first Zagreb index Randic-type eig connectivity inde Balaban dist Moriguchi octano Ghose-Crippen of Squared Ghose partition sum of al., Eur Squared Ghose fabri, et al., Eur Squared Ghose abri, et al., Eur Squared Ghose fabri, et al., Eur Soly fabri,	230 286 1,991 54,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptor name iener W index c c van der Waals v anderson electro c van der Waals v anderson electro c van der Waals v andic ID number ex by valence verf ndic ID number ex chi-1 (Randic of index) andic connectivity genvector-based jacency matrix tance connectivity genvector-based jacency matrix tance connectivity octanol-water partition	28,394 14,4 232,235 16,3 332,235 15,3 36 30,065 15,3 gend 1 volumes 1 volumes 1 volume 1 index from 1 artition coeff. 1 nol-water 1 006) 006) online.com/ 1 Maysinger; 1	Image Image Image 414 6,809 43,713 1,726 1,349 349 7,665 51,874 1,277 1,338 264 11,08 71,703 2,696 2,338 7,075 46,73 1,431 1,331 1,331 Descriptor type topological descrip constitutional descriptor (scaled on Carbon atom) constitutional descrip (scaled on Carbon atom) constitutional descrip walk and path cou connectivity inde eigenvalue-based in topological descrip walk and path cou connectivity inde eigenvalue-based in molecular proper molecular proper	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previou betwee •Prese obtaine •3D Q activity influent constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 1003 COMPARTING ACC 1003 CONTRICTIONS CLUSSIONS ACC 1003 CONTRICTIONS ACC 1003 CONTR	
32 333 34 35 35 36 37 38 39 40 41 42 43 44 45 44 45 44 50 51 52 53 54 55 56 57 58	NO2 NO3 NO4 H </th <th>0 0 0 NNHCSNH2 NNHCSNH2 0</th> <th>$\begin{array}{c c c c c c c c c c c c c c c c c c c$</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv CID $\chi1$ XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202</th> <th>23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 puted molecular 0 0 sum of atomic Sa 0 0 sum of atomic Sa 0 0 first Zagreb index Ran 0 connectivity inde 0 0 modified Ra Randic-type eig 0 Moriguchi octano 0 0 Ghose-Crippen of 0 0 Squared Ghose 0 0 abri, et al., Eur 0 0 abri, M. Jadrijevid 0 0 <</th> <th>230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors / leg scriptor name fiener W index c van der Waals ? anderson electro c van der Waals ? anderson electro c van der Waals ? ander connectivity andic connectivity andic connectivity genvector-based jacency matrix tance connectivity jacency matrix <</th> <th>28,394 14,4 232,235 16,3 30,065 15,3 gend 30,065 yolumes 14,4 yolumes 14,4 yolumes 15,3 yolumes 14,4 yolumes 15,3 yolumes 14,4 yolumes 15,3 yolumes 14,4 yolume 14,4</th> <th>Initial Initial Initial 414 6,809 43,713 1,726 1 349 7,665 51,874 1,277 1 264 11,08 71,703 2,696 1 388 7,075 46,73 1,431 1 Descriptor type topological descriptor (Carbon atom) Constitutional descriptor (scaled on Carbon atom) constitutional description (scaled on Carbon atom) atopological description (scaled on Carbon atom) constitutional description (scaled on Carbon atom) atopological description (scaled on Carbon atom) connectivity indeference connectivity indeference atopological description (scaled on Carbon atom) connectivity indeference connectivity indeference connectivity indeference atopological description molecular propere molecular propere molecular propere molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previou betwee •Prese obtaine •3D QS activity influen constitu molecu •3D con an opti •3D con an opti •Good constitu molecu •3D con an opti •Good constitu molecu •3D con</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (C (10³ mol dm³) against <i>Klebsiella</i> ATCC 10031</th> <th></th>	0 0 0 NNHCSNH2 NNHCSNH2 0	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv CID $\chi1$ XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202	23,61 0,64 24 24,91 0,68 25 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 puted molecular 0 0 sum of atomic Sa 0 0 sum of atomic Sa 0 0 first Zagreb index Ran 0 connectivity inde 0 0 modified Ra Randic-type eig 0 Moriguchi octano 0 0 Ghose-Crippen of 0 0 Squared Ghose 0 0 abri, et al., Eur 0 0 abri, M. Jadrijevid 0 0 <	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors / leg scriptor name fiener W index c van der Waals ? anderson electro c van der Waals ? anderson electro c van der Waals ? ander connectivity andic connectivity andic connectivity genvector-based jacency matrix tance connectivity jacency matrix <	28,394 14,4 232,235 16,3 30,065 15,3 gend 30,065 yolumes 14,4 yolumes 14,4 yolumes 15,3 yolumes 14,4 yolumes 15,3 yolumes 14,4 yolumes 15,3 yolumes 14,4 yolume 14,4	Initial Initial Initial 414 6,809 43,713 1,726 1 349 7,665 51,874 1,277 1 264 11,08 71,703 2,696 1 388 7,075 46,73 1,431 1 Descriptor type topological descriptor (Carbon atom) Constitutional descriptor (scaled on Carbon atom) constitutional description (scaled on Carbon atom) atopological description (scaled on Carbon atom) constitutional description (scaled on Carbon atom) atopological description (scaled on Carbon atom) connectivity indeference connectivity indeference atopological description (scaled on Carbon atom) connectivity indeference connectivity indeference connectivity indeference atopological description molecular propere molecular propere molecular propere molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper molecular proper	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, Previou betwee •Prese obtaine •3D QS activity influen constitu molecu •3D con an opti •3D con an opti •Good constitu molecu •3D con an opti •Good constitu molecu •3D con	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees (C (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031	
32 333 34 35 35 36 37 38 39 40 41 42 43 44 42 43 44 50 51 52 53 54 55 56 57 58 59	NO2 NO3 H <th>0 0 0 NNHCSNH₂ NNHCSNH₂ 0</th> <th>$\begin{array}{c} CH_{2}NCH(CH_{3})_{2}^{2} \\ \hline CH_{3}NCH(CH_{3})_{2}^{2} \\ \hline CH_{4}^{2} \\ \hline CH_{2} \\ \hline CH_{4} \\ \hline CH_$</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Se Mv <math>Sr Sr </math></th> <th>23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 4 puted molecular 0 puted molecular 0 sum of atomic 0 sum of atomic 0 first Zagreb index Ran connectivity inde Ran connectivity inde adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghose partition abri, et al., Eur adj abri, M. Jadrijević adj </th> <th>230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg scriptor name 1 iener W index c van der Waals for anderson electron anderson electron c van der Waals for anderson electron andic ID number ex by valence verfandic ID number andic connectivity andic connectivity genvector-based jacency matrix tance connectivity aban ID number octanol-water partition octanol-water partition octanol-water partition oc-Mladar, D. N</th> <th>1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,7 gend 15,3 gend 16,3 gend</th> <th>10000 10000 10000 414 6,809 43,713 1,726 349 7,665 51,874 1,277 1 264 11,08 71,703 2,696 1 388 7,075 46,73 1,431 1 Descriptor type topological descriptor (Constitutional descriptor (connectivity inde connectivity inde connectivity inde cong. Med. Chem. 10 (20 Cherges/</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •3D QS activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 1003 mol dm³) against <i>Klebsiella</i> ATCC 1003 CLUSIONS US 2D QSAR results have an antimicrobial activity (Not and 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologic alar properties (AlogP, ML rrelations allow better spat mal selection of MDs in G correlations in this QSAR utional (Sv, Mv), topologic ophylicity (AlogP) descrip against <i>Staphylococcus a</i> ested method can be usef cal properties and/or biolo ing for new lead compour unds.</th> <th></th>	0 0 0 NNHCSNH₂ NNHCSNH₂ 0	$\begin{array}{c} CH_{2}NCH(CH_{3})_{2}^{2} \\ \hline CH_{3}NCH(CH_{3})_{2}^{2} \\ \hline CH_{4}^{2} \\ \hline CH_{2} \\ \hline CH_{4} \\ \hline CH_$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Se Mv $Sr Sr $	23,61 0,64 2 24,91 0,68 25 35,48 0,67 4 20,72 0,69 4 puted molecular 0 puted molecular 0 sum of atomic 0 sum of atomic 0 first Zagreb index Ran connectivity inde Ran connectivity inde adj Balaban dist Bala Moriguchi octano Ghose-Crippen of Squared Ghose partition abri, et al., Eur adj abri, M. Jadrijević adj	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg scriptor name 1 iener W index c van der Waals for anderson electron anderson electron c van der Waals for anderson electron andic ID number ex by valence verfandic ID number andic connectivity andic connectivity genvector-based jacency matrix tance connectivity aban ID number octanol-water partition octanol-water partition octanol-water partition oc-Mladar, D. N	1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,7 gend 15,3 gend 16,3 gend	10000 10000 10000 414 6,809 43,713 1,726 349 7,665 51,874 1,277 1 264 11,08 71,703 2,696 1 388 7,075 46,73 1,431 1 Descriptor type topological descriptor (Constitutional descriptor (connectivity inde connectivity inde connectivity inde cong. Med. Chem. 10 (20 Cherges/	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and M pneumoniae, Previou betwee •Prese obtaine •3D QS activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees ACC 1003 mol dm ³) against <i>Klebsiella</i> ATCC 1003 CLUSIONS US 2D QSAR results have an antimicrobial activity (Not and 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologic alar properties (AlogP, ML rrelations allow better spat mal selection of MDs in G correlations in this QSAR utional (Sv, Mv), topologic ophylicity (AlogP) descrip against <i>Staphylococcus a</i> ested method can be usef cal properties and/or biolo ing for new lead compour unds.	
32 333 34 35 35 36 37 38 39 40 41 42 43 44 45 44 45 44 50 51 52 53 54 55 56 57 58 59 60	NO2 H </th <th>0 0 0 NNHCSNH₂ NNHCSNH₂ 0</th> <th>$\begin{array}{c} CH_{2}NCH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{3}N(CH_{2}CH_{2}OOH) \\ CH_{3}NHCH_{3}COOOH \\ CH_{3}NHCH_{2}COOH \\ CH_{3}NHCH_{2}CH_{3}NHCH_{2}COOH \\ CH_{3}NHCH_{2}OH)_{2}NHCH_{2}OOH \\ CH_{3}NHCH_{2}OOH \\ CH_{3}NHCH_{2}OOH \\ CH_{$</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv $ZM1v$ CID $\chi1$ XMOD $\chi1$ XMOD VRA1 J BID MLOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st</th> <th>23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 puted molecular 0 0 sum of atomic Sa 0 0 sum of atomic Sa 0 0 first Zagreb index Ran 0 first Zagreb index Ran 0 forst Zagreb index Ran 0 first Zagreb index Ran 0 first Zagreb index Ran 0 Gonnectivity inde 0 0 Moriguchi octano 0 0 Ghose-Crippen of 0 0 Squared Ghose 0 0 partition 0 0 fin, M. Jadrijević 0 0 in, M. Jadrijević 0 0</th> <th>230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptors' leg scriptor name scriptor name iener W index c c van der Waals scriptor anderson electro s c van der Waals s andic ID number s ex by valence verf s ndic ID number s ex chi-1 (Randic of index) s andic connectivity seed jacency matrix tance connectivity seed jacency matrix tance connectivity see Crippen octar on coeff. (logP^2 s f. Med. Che s y.freepatentso s c'-Mladar, D. N s c-Mladar; Pha softward softward, Softward softward</th> <th>1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,4 32,235 16,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 14,4 volume 15,3 volume 14,4 volume</th> <th>Initial Otolia Otolia</th> <th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th> <th>Figure 12. 3D Volumes (SV), ZM1V) and M pneumoniae, CON Previo betwee Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu</th> <th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees IC (10³ mol dm³) against <i>Klebsiella</i> ATCC 1003 CLUSIONS Dus 2D QSAR results have en antimicrobial activity (M int 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologic lar properties (AlogP, ML rrelations allow better spa mal selection of MDs in G correlations in this QSAR utional (Sv, Mv), topologic ophylicity (AlogP) descrip against <i>Staphylococcus</i> a ested method can be usef cal properties and/or biolo ing for new lead compour unds.</th> <th></th>	0 0 0 NNHCSNH₂ NNHCSNH₂ 0	$\begin{array}{c} CH_{2}NCH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH(CH_{3})_{2}^{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{3}N(CH_{2}CH_{2}OOH) \\ CH_{3}NHCH_{3}COOOH \\ CH_{3}NHCH_{2}COOH \\ CH_{3}NHCH_{2}CH_{3}NHCH_{2}COOH \\ CH_{3}NHCH_{2}OH)_{2}NHCH_{2}OOH \\ CH_{3}NHCH_{2}OOH \\ CH_{3}NHCH_{2}OOH \\ CH_{$	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv $ZM1v$ CID $\chi1$ XMOD $\chi1$ XMOD VRA1 J BID MLOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st	23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 3 puted molecular 0 0 puted molecular 0 0 sum of atomic Sa 0 0 sum of atomic Sa 0 0 first Zagreb index Ran 0 first Zagreb index Ran 0 forst Zagreb index Ran 0 first Zagreb index Ran 0 first Zagreb index Ran 0 Gonnectivity inde 0 0 Moriguchi octano 0 0 Ghose-Crippen of 0 0 Squared Ghose 0 0 partition 0 0 fin, M. Jadrijević 0 0 in, M. Jadrijević 0 0	230 286 1,991 254,44 436 1,92 422 1188 1,623 328 348 1,996 descriptors' leg scriptors' leg scriptor name scriptor name iener W index c c van der Waals scriptor anderson electro s c van der Waals s andic ID number s ex by valence verf s ndic ID number s ex chi-1 (Randic of index) s andic connectivity seed jacency matrix tance connectivity seed jacency matrix tance connectivity see Crippen octar on coeff. (logP^2 s f. Med. Che s y.freepatentso s c'-Mladar, D. N s c-Mladar; Pha softward softward, Softward softward	1 28,394 14,4 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,4 32,235 16,3 30,065 15,3 gend 14,4 volumes 15,3 volumes 14,4 volume 15,3 volume 14,4 volume	Initial Otolia	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D Volumes (SV), ZM1V) and M pneumoniae, CON Previo betwee Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees IC (10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 1003 CLUSIONS Dus 2D QSAR results have en antimicrobial activity (M int 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topologic lar properties (AlogP, ML rrelations allow better spa mal selection of MDs in G correlations in this QSAR utional (Sv, Mv), topologic ophylicity (AlogP) descrip against <i>Staphylococcus</i> a ested method can be usef cal properties and/or biolo ing for new lead compour unds.	
32 333 34 35 35 36 37 38 39 40 41 42 43 44 42 43 44 45 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61	NO2 NO3 H </th <th>$\begin{array}{c c}$</th> <th>CH_NCH(CH_3)/2 CH_NCH(CH_3)/2 OH_H OH_H</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 3. USP 7,0 4. EP11222 5. M. Movr 2919-29 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete str Version str</th> <th>23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 5 puted molecular 0 sum of atomic 5 sum of atomic 5 first Zagreb index Ran connectivity inde Ran modified Ra Randic-type eig Moriguchi octano Ghose-Crippen of Squared Ghose partitio Squared Ghose partitio fin, M. Jadrijević 5 abri, et al., Eur 5 abri, et al., Fur 5 fabri, et al., Eur 5 abri, bragon for Wa</th> <th>230 286 1,991 2422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptor name 1 1 1 scriptor name 1 1 1 scriptor name 1 1 1 scriptor name 1 1 1 1 anderson electro 1 1 1 1 1 anderson electro 1 <td< th=""><th>1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,7 gend 15,3 volumes 15,3 volume 16,3 volume 16,3 volume 16,3 volume 16,3 volume 16,3 ty index from 16,3 index from 16,3 artition coeff. 10,3 pol-bysinger; 10,3 armazie 38 38 vare for molectivit/ 38</th><th>Initial Otolia Otolia</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, CON Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees MCC 1003 CONTRELEDGEMENTS</th><th>Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> <i>preumoniae</i> ATCC 10031</th></td<></th>	$ \begin{array}{c c} $	CH_NCH(CH_3)/2 CH_NCH(CH_3)/2 OH_H	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ 1 XMOD VRA1 J BID MLOGP2 3. USP 7,0 4. EP11222 5. M. Movr 2919-29 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete str Version str	23,61 0,64 24 24,91 0,68 26 35,48 0,67 4 20,72 0,69 5 puted molecular 0 sum of atomic 5 sum of atomic 5 first Zagreb index Ran connectivity inde Ran modified Ra Randic-type eig Moriguchi octano Ghose-Crippen of Squared Ghose partitio Squared Ghose partitio fin, M. Jadrijević 5 abri, et al., Eur 5 abri, et al., Fur 5 fabri, et al., Eur 5 abri, bragon for Wa	230 286 1,991 2422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptor name 1 1 1 scriptor name 1 1 1 scriptor name 1 1 1 scriptor name 1 1 1 1 anderson electro 1 1 1 1 1 anderson electro 1 <td< th=""><th>1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,7 gend 15,3 volumes 15,3 volume 16,3 volume 16,3 volume 16,3 volume 16,3 volume 16,3 ty index from 16,3 index from 16,3 artition coeff. 10,3 pol-bysinger; 10,3 armazie 38 38 vare for molectivit/ 38</th><th>Initial Otolia Otolia</th><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, CON Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees MCC 1003 CONTRELEDGEMENTS</th><th>Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella</i> <i>preumoniae</i> ATCC 10031</th></td<>	1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,7 gend 15,3 volumes 15,3 volume 16,3 volume 16,3 volume 16,3 volume 16,3 volume 16,3 ty index from 16,3 index from 16,3 artition coeff. 10,3 pol-bysinger; 10,3 armazie 38 38 vare for molectivit/ 38	Initial Otolia	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3D volumes (Sv), (ZM1V) and W pneumoniae, CON Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees MCC 1003 CONTRELEDGEMENTS	Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Sv), AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella</i> <i>preumoniae</i> ATCC 10031
32 333 34 35 35 36 37 38 39 40 41 42 43 44 42 43 44 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61	NO2 NO3 NO4 H <th>$\begin{array}{c c}$</th> <th>CH₂NCH(CH₃)½ CH₂NCH(CH₃)½ CH₂NCH(CH₃CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH₂CH)₂ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH₂CH₃CH₂COH CH₂NHCH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂CO</th> <th>59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete str Version str</th> <th>23,61 0,64 24 24,91 0,68 26 35,48 0,67 26 20,72 0,69 35 puted molecular 0 puted molecular 0 sum of atomic Sa 0 sum of atomic Sa 0 first Zagreb index Ran connectivity inde Ran connectivity inde 0 Moriguchi octano Ghose-Crippen of Squared Ghose partition abri, et al., Eur Eur abri, et al., Eur 245, http://www in, M. Jadrijević 0 . 56,914 (J. Torre 245, http://www 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0</th> <th>230 286 1,991 2422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptor name 1 1 1 iener W index c van der Waals for ander son electron 1 anderson electron c van der Waals for ander son electron 1 1 andic ID number 1 1 1 1 ex by valence verf ndic ID number 1 1 1 ex chi-1 (Randic of index) 1 1 1 1 1 genvector-based jacency matrix 1</th> <th>1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,4 yolumes 14,7 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volume 16,3 volume<</th> <th>Initial Otoline <t< th=""><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3 volumes (Sv), ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu and lipe (MIC) a</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees at C(10³ mol dm³) against <i>Klebsiella</i> ATCC 10031 CCUUSIONS Sus 2D QSAR results have an antimicrobial activity (Nat 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topological activity (AlogP, ML, rrelations allow better spatial selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description and selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description and selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description against <i>Staphylococcus</i> are better and/or biological activity (AlogP) description and the description of the basis of correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description against <i>Staphylococcus</i> are better and/or biological activity (AlogP) description and the description and</th><th>the preference of biological former than one MD and their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide SAR study. Study were observed using cal (W), connectivity (χ1, χMOD), tors with antimicrobial activity <i>ureus</i> ATCC5611 full in prediction of physico-gical activity parameters in ad among investigated</th></t<></th>	$ \begin{array}{c c} $	CH₂NCH(CH₃)½ CH₂NCH(CH₃CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH)₂ CH₂N(CH₂CH₂CH₂CH)₂ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH(CH₃)½ CH₂NHCH₂CH₃CH₂COH CH₂NHCH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂COH CH₂NHCH(COOH)CH₂CO	59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ 1 XMOD VRA1 J BID MLOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete str Version str	23,61 0,64 24 24,91 0,68 26 35,48 0,67 26 20,72 0,69 35 puted molecular 0 puted molecular 0 sum of atomic Sa 0 sum of atomic Sa 0 first Zagreb index Ran connectivity inde Ran connectivity inde 0 Moriguchi octano Ghose-Crippen of Squared Ghose partition abri, et al., Eur Eur abri, et al., Eur 245, http://www in, M. Jadrijević 0 . 56,914 (J. Torre 245, http://www 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0	230 286 1,991 2422 1188 1,623 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptors' leg 328 348 1,996 descriptor name 1 1 1 iener W index c van der Waals for ander son electron 1 anderson electron c van der Waals for ander son electron 1 1 andic ID number 1 1 1 1 ex by valence verf ndic ID number 1 1 1 ex chi-1 (Randic of index) 1 1 1 1 1 genvector-based jacency matrix 1	1 28,394 14,7 2 32,235 16,3 3 46,888 23,3 30,065 15,3 gend 14,4 yolumes 14,7 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volumes 15,3 volume 16,3 volume<	Initial Otoline Otoline <t< th=""><th>1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e </th><th>Figure 12. 3 volumes (Sv), ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu and lipe (MIC) a</th><th>Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees at C(10³ mol dm³) against <i>Klebsiella</i> ATCC 10031 CCUUSIONS Sus 2D QSAR results have an antimicrobial activity (Nat 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topological activity (AlogP, ML, rrelations allow better spatial selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description and selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description and selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description against <i>Staphylococcus</i> are better and/or biological activity (AlogP) description and the description of the basis of correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description against <i>Staphylococcus</i> are better and/or biological activity (AlogP) description and the description and</th><th>the preference of biological former than one MD and their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide SAR study. Study were observed using cal (W), connectivity (χ1, χMOD), tors with antimicrobial activity <i>ureus</i> ATCC5611 full in prediction of physico-gical activity parameters in ad among investigated</th></t<>	1,052 1,107 1,331 1,771 2,927 8,568 1,106 1,224 e	Figure 12. 3 volumes (Sv), ZM1V) and M pneumoniae, Previo betwee •Prese obtaine •3D Q activity influen constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu molecu •3D co an opti •Good constitu and lipe (MIC) a	Correlation of sum of atomic van der Waals first Zagreb index by valence vertex degrees at C(10 ³ mol dm ³) against <i>Klebsiella</i> ATCC 10031 CCUUSIONS Sus 2D QSAR results have an antimicrobial activity (Nat 2D results are in good ed. SAR correlations indicate prediction on the basis of ce on particular system, a utional (Sv, Se,), topological activity (AlogP, ML, rrelations allow better spatial selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description and selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description and selection of MDs in G correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description against <i>Staphylococcus</i> are better and/or biological activity (AlogP) description and the description of the basis of correlations in this QSAR utional (Sv, Mv), topological activity (AlogP) description against <i>Staphylococcus</i> are better and/or biological activity (AlogP) description and the description and	the preference of biological former than one MD and their as it is combination of gical (W, ZMV1,), and ogP,) descriptors. atial dispersion and thus provide SAR study. Study were observed using cal (W), connectivity (χ 1, χ MOD), tors with antimicrobial activity <i>ureus</i> ATCC5611 full in prediction of physico-gical activity parameters in ad among investigated

Table 3. Computed molecular descriptors

| |
 |

 | | Compd. Sv
 | Se Mv ZM1v | W J CID
 | BID χ^1 XMOD MLOG ALOG ALOG D | | ⁸ 9 10 11 2,0 1,5 ^{2,0} |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |

--
--
--
--
--
--
--

--|---
---	---	---
--
--
--
--
--
--
--
---|---|--
--|--|--|---|---|--
---|---|---|--|--|--|--|---
--|--|---|--|---|---|--|--|---|---
---|--|---|--|---|---|---|--|---
---|---|--|--
--|---
---|---|--|--|---|---|--|--
--|---|--
---	--	---	---	---	---	---	---	---	---	---	---
--											
The biol											
 |

 | r C(1) and C() test besterie (Table 2) and Cardida | 1 18,02
 | 29,93 0,62 268 | 512 1,965 34,241 17
 | P P P2 7,337 8,236 53,134 0,736 -0,05 0,003 | | z' 11 12 13 14 15 0,0 0,5 1,0 NOS |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| I he biol | ogical act
 | ctivity were evaluated using

 | g G(+) and G(-) test bacteria (Table 2) and Candida | 2 22,11
 | 35,02 65 279,21 | 789 2,035 40,092 20
 | 0,297 9,9668 68,909 2,581 2,354 5,539 | 6 8 10 12 14 | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| RID Sv | $Se and \Delta$
 | ALOGP) using multiple

 | linear regression analysis | 3 20,62
 | 33,81 0,62 314 | 670 1,672 39,129 19
 | 9,326 9,254 59,645 0,897 0,713 0,508 | χ | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 010, 30, |
 | ALOOT,) using multiple

 | intear regression analysis. | 4 21,71
 | 35,37 0,62 282 | 670 1,672 39,129 19
 | 9,326 9,254 58,645 1,933 1,942 3,773 | Figure 4. 2D Correlation of valence connectivity index (χ 1) and MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus aureus</i> ATCC | Figure 5. 3D Correlation of valence connectivity index (χ 1),
AlogP and MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus aureus</i> |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| Molecul | ar descrip
 | otors were calculated with

 | DRAGON [®] software, and multiple regression analyses | 5 28,3
 | 44,36 0,64 364 | 1576 1,316 51,92 25
 | 5,238 12,22 77,018 2,408 2,655 7,047 5,394 7,236 46,492 1,623 0,744 0,554 | 56511 | ATCC 56511 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| using O | riginPro 7
 | 7.5 [®] .

 | | 7 24,8
 | 42,79 0,59 334 | 1028 2,075 44,132 22
 | 2,275 10,706 69,253 0,857 -0,214 0,046 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| Ŭ | Ŭ
 |

 | | 8 27,78
 | 41,13 0,6 288 | 890 1,685 43,169 51
 | 1,299 10,292 65,354 2,229 1,783 3,177 | ⁶ Staphylococcus aureus ATCC 5651
Y = 7.35268 - 0.06072 X | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 |

 | | 9 17,91
 | 28,82 0,64 292 | 514 1,946 34,065 17
 | 7,333 8,092 52,055 1,466 0,334 0,111 | r = -0.88495
n = 20 | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| Table 1. C | Chemical st
 | tructures of 1,4-benzoxazin-2,

 | 3-dione (1-35) and 3,1-benzoxazin-2,4-dione (36-62) | 10 22,61
 | 38,02 0,61 344 | 946 1,978 42,121 21
 | 1,275 10,13 65,405 0,917 -0,62 0,385 4,252 11,562 74,816 0,698 -0,624 0,389 | m 4- | e e e e e e e e e e e e e e e e e e e |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 | R、

 | \mathcal{A} | 12 26,32
 | 43,11 0,64 337,21 | 1334 2,065 47,973 24
 | 4,252 11,562 74,816 0,698 -0,624 0,389 4,252 11,562 81,18 2,678 1,783 3,18 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 |

 | | 13 24,7
 | 40,57 0,62 366 | 1031 1,668 44,895 22
 | 2,283 10,648 67,916 1,793 0,916 0,839 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| No | R
 | R ¹

 | R ² | 14 26,29
 | 43,46 0,61 340 | 1174 1,66 47,011 2
 | 23,27 11,148 70,916 2,043 1,372 1,883 | | 40 50 50 2,0 ^{3,0} |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 1 | Н
 | 0

 | CH ₂ NHCH ₂ CH ₂ OH | 15 22,93
 | 35,7 0,67 454 | 1196 1,603 46,61 23
 | 3,261 10,859 69,829 3,871 3,684 13,569 | | $2M_{00}$ 80_{90} $0.5^{1,0}$ 1.5_{00} |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 2 | Н
 | 0

 | CH ₂ N(CH ₂ CH ₂ CI) ₂ | 16 31,34
17 31,23
 | 51,99 0,63 548 48,78 0.64 534 | 2473 1,684 60,52 30
 | 0,213 14,329 92,59 2,869 2,726 7,43
9 224 13 915 89 961 3 236 3 492 12 196 | 0 | 100 0,0 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 3 | Н
 | 0

 | CH ₂ —NO | 18 31,32
 | 50,3 0,64 502 | 2240 1,42 59,557 29
 | 9,224 13,915 89,961 4,225 4,722 22,295 | χMOD | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 |

 | | 19 24,53
 | 38,36 0,66 432 | 1345 1,617 48,715 24
 | 4,253 11,507 74,482 2,539 2,619 6,861 | Figure 6. 2D Correlation of modified Randic connectivity index | Figure 7. 3D Correlation of modified Randic connectivity index |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 4 | Н
 | NO ₂

 | CH ₂ —N | 20 14,74
 | 23,61 0,67 388 | 412 2,037 31,904 16
 | 6,372 7,503 49,509 1,342 0,799 0,638 | (χ MOD) and MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus</i> aureus ATCC 56511 | (χMOD), lipophylicity (AlogP) and MIC (10 ⁻³ mol dm ⁻³) against |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 |

 | | 21 19,36
 | 32,25 0,65 438 | 944 1,979 41,79 21
 | 1,275 9,897 65,443 0,855 0,053 0,003 2,242 40,025 70,020 4,407 0,053 0,003 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 5 | Н
 | 0

 | | 22 22,55
23 19.84
 | 33.02 0.64 422 | 944 1.979 4.79 21
 | 3,243 10,933 72,002 1,407 0,833 0,426 1,275 9,897 65,154 0.449 -0.549 0.301 | Staphylococcus aureus ATCC 5651
Y = 6.87674 - 0.16685 X | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 6 | Н
 | NNHCH ₃

 | Н | 24 20,96
 | 35,13 0,64 442 | 1112 1,922 43,791 22
 | 2,255 10,397 68,443 1,136 0,088 0,008 | r = -0.86517
n = 20 | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 7 | Н
 | NNHCH ₃

 | CH ₂ N(CH ₂ CH ₂ OH) ₂ | 25 24,15
 | 40,9 0,62 454 | 1341 2,038 47,463 24
 | 4,248 11,218 73,325 1,671 1,274 1,622 | | Ϋ́Ę |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 8 | Н
 | NNHCH ₃

 | CH ₂ -N | 26 25,75
 | 43,78 0,61 458 | 1526 2,016 49,468 25
 | 5,236 11,701 76,224 1,927 1,662 2,764 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 9 | н
 | NNHCOCH.

 | Н | 27 27,06
 | 43,34 0,66 436 | 2000 1,695 56,262 28
 | 8,229 13,236 85,904 2,137 1,276 1,627
8,229 13,236 85,904 2,137 1,276 1,627 | | MIC |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 10 | Н
 | NNHCOCH ₂

 | CH ₂ NHCH ₂ CH ₂ OH | 29 19,3
 | 30,66 0,67 368,445 | 813 1,986 39,78 2
 | 20,29 9,397 64,379 1,294 0,917 0,842 | | 0,60 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 11 | Н
 | NNHCOCH ₃

 | CH ₂ N(CH ₂ CH ₂ OH) ₂ | 30 28,81
 | 47,95 0,62 484,445 | 2042 2,116 55,345 28
 | 8,222 13,112 88,194 1,625 1,393 1,939 | | 0,62
0,64
0,66
18 ^{20²²⁴} |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 12 | Н
 | NNHCOCH ₃

 | CH ₂ N(CH ₂ CH ₂ CI) ₂ | 31 28,46
 | 47,19 0,61 314,445 | 1292 2,128 47,628 24
 | 4,259 11,307 74,397 2,435 2,597 6,742 | | ¹ // ₁₂ 0,68 0,70 12 14 16 5 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 13 | Н
 | NNHCOCH

 | | 32 25,32
 | 43,1 0,6 388 | 1138 2,131 45,462 23 893 1,684 42,720 64
 | 3,271 10,718 69,254 2,668 2,372 5,627 1,299 10,059 65,371 1,756 1,384 4,000 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 |

 | | 34 26,09
 | 42,41 0,64 412,445 | 1463 1,702 50.611 25
 | 5,256 11,952 80,24 1,685 1,499 2.248 | Figure 9, 2D Correlation of automatic termination in 144 mil | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 14 | Н
 | NNHCOCH ₃

 | CH ₂ -N | 35 25,51
 | 42,19 0,64 474,445 | 1680 2,079 51,496 26
 | 6,234 12,201 82,73 1,105 0,549 0,302 | volumes (Sv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus</i> | Figure 9. 3D Correlation of sum of atomic van der Waals volumes (Sv), mean atomic van der Waals volume (Mv) and MIC |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 15 |
 | CF ₃

 | | 36 27,1
 | 45,91 0,59 300 | 956 2,207 43,287 22
 | 2,294 10,015 63,091 3,48 3,402 11,57 | aureus ATCC 56511 | (10 ⁻³ mol dm ⁻³) against <i>Staphylococcus aureus</i> , ATCC 56511 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 15 | Н
 | N

 | Н | 37 20,62
 | 33,81 0,62 314 37,03 0.6 200 | 674 1,663 39,127 19 794 2,024 40,000 60
 | 9,324 9,254 59,645 1,303 1,227 1,505 0,295 9,668 62,545 0,026 0,40 0,040 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 16 | Н
 |

 | CH ₂ N(CH ₂ CH ₂ OH) ₂ | 30 21,73
39 23.1
 | 37,03 0,6 328 37,12 0,64 293,21 | 908 2,024 40,09 20
 | 0,230 0,000 02,545 0,936 0,46 0,212 1,285 10,206 72,824 3,027 2,954 8,728 | 2D and 3D Correlations with biological acti | vities against Klebsiella pneumoniae. |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| |
 |

 | | 40 25,18
 | 40,87 0,63 344,445 | 1194 1,638 47,016 23
 | 3,266 11,148 74,515 1,195 1,345 1,81 | ATCC 10031 | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 17 | Н
 | N-

 | CH ₂ —N_O | 41 19,44
 | 32,8 0,63 390 | 813 2,002 39,954 20
 | 0,292 9,541 62,86 1,262 0,358 0,128 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 10 |
 | CF3

 | CH | 42 23,15
 | 39,9 0,61 432 | 1180 2,062 45,805 23
 | 3,262 10,973 72,271 1,084 0,345 0,126 1,000 10,050 65,271 2,462 1,804 2,588 | | 4 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 10 | п
 |

 | | 43 21,55
44 23,13
 | 35,36 0,63 382 38,24 0,63 386 | 1028 1.669 44.843 22
 | 1,299 10,059 65,371 2,162 1,694 5,566 2,283 10,559 68,371 2,425 2,35 5,525 | 4■ | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 19 | н
 |

 | Н | 45 22,04
 | 36,69 0,63 418 | 1028 1,669 44,843 22
 | 2,283 10,559 69,371 1,423 1,121 1,257 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 20 | NO.
 | 0 ₂ N

 | Н | 46 28,52
 | 48,78 0,59 404 | 1394 2,215 49,002 2
 | 25,26 11,319 72,817 3,566 3,296 10,863 | లా - | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 21 | NO ₂
 | 0

 | CH ₂ NHCH ₂ COOH | 47 23,53
 | 37,89 0,65 383,21 | 1180 2,062 45,805 23
 | 3,262 10,973 78,635 3,074 2,762 7,627 8,245 12,525 86,744 2,022 2,062 0,28 | ာ
မ
ကို 2 - | Ŭ
■ |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 22 | NO ₂
 | 0

 | CH ₂ NHCH ₂ COOC ₂ H ₅ | 40 29,72
49 17.94
 | 29,37 0,64 334 | 2117 1,322 57,634 28 613 1,931 36.073 18
 | 8,312 8,592 55,717 1,113 0,673 0.452 | MC/1 | 0 10 0,70 0,68 0,70 0,68 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 23 | NO ₂
 | 0

 | CH ₂ NHCH ₂ CONH ₂ | 50 19,54
 | 32,26 0,63 340 | 702 1,964 37,898 19
 | 9,301 9,003 58,135 1,394 1,05 1,103 | · · | C_{10}^{30} $_{50}^{40}$ $_{50}^{0,62}$ $_{10}^{0,64}$ |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 24 | NO ₂
 | 0

 | CH ₂ NHCH ₂ CH ₂ CH ₂ COOH | 51 21,13
 | 35,14 0,62 350 | 866 1,845 40,064 20
 | 0,269 9,63 62,276 1,666 1,272 1,619 | | 60 0,60 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 25 | NO ₂
 | 0

 | CH ₂ NHCH(COOH)CH(CH ₃) ₂ | 52 21,13
 | 35,14 0,62 342 39,1 0,62 249,455 | 894 1,788 40,075 2 1087 1,934 42,02 00
 | 2,26 9,592 61,717 1,666 1,029 1,058 2,256 10,541 73,398 1,020 1,277 1,057 | CID | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 26 | NO ₂
 | 0

 | CH ₂ NHCH(COOH)CH ₂ CH(CH ₃) ₂ | 33 23,82
 | 0,03 348,455 | 43,92 22
 | 2,200 10,041 10,030 1,929 1,377 1,897 | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 07 |
 | 0

 | | 54 23,46
 | 39,50 0,63 508 | 1530 2,011 49,466 25
 | 5,235 11,701 77,09 0,699 -0,302 0,091 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC | Figure 11. 3D Correlation of Randic ID number (CID), mean |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 | NO ₂
 | 0

 | CH_NHCH(COOH)CH(OH)C_H | 54 23,46 55 22,98
 | 39,56 0,63 508 38,79 0,64 524 | 1530 2,011 49,466 25 1530 2,011 49,466 25
 | 5,23511,70177,090,699-0,3020,0915,23511,70177,3791,1050,30,09 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³)
against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27
28
29 | NO ₂
NO ₂
NO ₂
 | O
O
NNHCSNH ₂

 | CH ₂ NHCH(COOH)CH(OH)C ₆ H ₅
CH ₂ NHCH(COOH)CH(OH)C ₆ H ₅
H | 54 23,46 55 22,98 56 30,74
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³)
against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27
28
29
30 | NO ₂
NO ₂
NO ₂
H
 | O
O
NNHCSNH ₂
NNHCSNH ₂

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_6H_5\\ \\ CH_2NHCH(COOH)CH(OH)C_6H_5\\ \\ \\ H\\ \\ \\ CH_2NHCH(COOH)CH(CH_3)_2 \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18
 | 5,23511,70177,090,699-0,3020,0915,23511,70177,3791,1050,30,090,20714,31292,8332,6072,7657,6462,4915,77137,0051,3841,2121,4698,3128,59255,6711,5190,7020,493 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³)
against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27
28
29
30
31 | NO ₂
NO ₂
NO ₂
H
H
 | O
O
NNHCSNH ₂
NNHCSNH ₂
NNHCSNH ₂

 | $\frac{CH_2NHCH(COOH)CH(OH)C_6H_5}{CH_2NHCH(COOH)CH(OH)C_6H_5}$ $\frac{H}{CH_2NHCH(COOH)CH(CH_3)_2}$ $CH_2N/CH(CH_3)_2/_2$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14
 | 5,23511,70177,090,699-0,3020,0915,23511,70177,3791,1050,30,090,20714,31292,8332,6072,7657,6462,4915,77137,0051,3841,2121,4698,3128,59255,6711,5190,7020,4934,4146,80943,7131,7261,0521,107 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 4 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 | NO ₂
NO ₂
NO ₂
H
H
NO ₂
 | O
O
NNHCSNH ₂
NNHCSNH ₂
NNHCSNH ₂
O

 | $\begin{array}{c} \begin{array}{c} CH_2 NHCH(COOH)CH(OH)C_6 H_5 \\ \hline \\ CH_2 NHCH(COOH)CH(OH)C_6 H_5 \\ \hline \\ H \\ \hline \\ CH_2 NHCH(COOH)CH(CH_3)_2 \\ \hline \\ CH_2 N/CH(CH_3)_2 /_2 \\ \hline \\ CH_2 N/CH(CH_3)_2 /_2 \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16
 | 5,23511,70177,090,699-0,3020,0915,23511,70177,3791,1050,30,090,20714,31292,8332,6072,7657,6462,4915,77137,0051,3841,2121,4698,3128,59255,6711,5190,7020,4934,4146,80943,7131,7261,0521,1076,3497,66551,8741,2771,3311,771 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | A A A A A A A A A A A A A A A A A A A |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27
28
29
30
31
32
33 | NO2 NO2 NO2 H H NO2 NO2
 | O
O
NNHCSNH ₂
NNHCSNH ₂
NNHCSNH ₂
O
O

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ H \\ \hline \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ \hline \\ CH_{2}N/CH(CH_{3})_{2}/_{2} \\ \hline \\ CH_{2}N/CH(CH_{3})_{2}/_{2} \\ \hline \\ \hline \\ CH_{2}-N \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10^{-3} mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 | NO ₂
NO ₂
NO ₂
H
H
NO ₂
NO ₂
 | O
O
NNHCSNH ₂
NNHCSNH ₂
NNHCSNH ₂
O
O

 | $\begin{array}{c} CH_2 NHCH(COOH)CH(OH)C_6 H_5 \\ \hline CH_2 NHCH(COOH)CH(OH)C_6 H_5 \\ \hline H \\ \hline CH_2 NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2 NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2 N/CH(CH_3)_2 /_2 \\ \hline CH_2 N/CH(CH_3)_2 /_2 \\ \hline CH_2 - N \\ \hline \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 348 1,996 30,065 15
 | 5,23511,70177,090,699-0,3020,0915,23511,70177,3791,1050,30,090,20714,31292,8332,6072,7657,6462,4915,77137,0051,3841,2121,4698,3128,59255,6711,5190,7020,4934,4146,80943,7131,7261,0521,1076,3497,66551,8741,2771,3311,7713,26411,0871,7032,6962,9278,5685,3887,07546,731,4311,1061,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10^{-3} mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 NO2
 | O
O
NNHCSNH ₂
NNHCSNH ₂
O
O
NNHCSNH ₂

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2-N \\ \hline CH_2-N \\ \hline \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 | NO2 NO2 NO2 H H NO2
 | O
O
NNHCSNH ₂
NNHCSNH ₂
NNHCSNH ₂
O
NNHCSNH ₂

 | $CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5}$ $CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5}$ H $CH_{2}NHCH(COOH)CH(CH_{3})_{2}$ $CH_{2}N/CH(CH_{3})_{2}/_{2}$ $CH_{2}N/CH(CH_{3})_{2}/_{2}$ $CH_{2}-N$ $CH_{2}-N$ $NHCH(CH_{3})COOH$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Descrip | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 M index 1 5 5
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 | NO2 NO2 NO2 H H NO2
 | O
O
NNHCSNH ₂
NNHCSNH ₂
O
O
O
NNHCSNH ₂

 | $CH_2NHCH(COOH)CH(OH)C_6H_5$ $CH_2NHCH(COOH)CH(OH)C_6H_5$ H $CH_2NHCH(COOH)CH(CH_3)_2$ $CH_2N/CH(CH_3)_2/2$ $CH_2N/CH(CH_3)_2/2$ CH_2-N CH_2-N CH_2-N | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Wiener Sum of atomic yan | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 Vindex 4 4 4
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against Klebsiella pneumoniae ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 | $\frac{NO_2}{NO_2}$ $\frac{NO_2}{H}$ $\frac{H}{NO_2}$ $\frac{NO_2}{NO_2}$ $\frac{NO_2}{NO_2}$
 | O
O
NNHCSNH ₂
NNHCSNH ₂
O
O
O
NNHCSNH ₂
NNHCSNH ₂

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2-N \\ \hline CH_2-N \\ \hline \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Wiener Sum of atomic van | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 V index 4 4 4
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10^{-3} mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 36 | NO2 NO2 NO2 H H NO2
 | O
O
NNHCSNH ₂
NNHCSNH ₂
O
O
O
NNHCSNH ₂
R

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2/_2 \\ \hline CH_2N/CH(CH_3)_2/_2 \\ \hline CH_2-N \\ \hline CH_2-N \\ \hline \\ \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Wiener Sum of atomic van sum of atomic van | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 30 30,065 15 otor Name 30 30,065 15 stor name 30,065 15 30,065 15 otor name 30,065 15 30 30 otor name 30 30 30 30 ot
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against Klebsiella pneumoniae ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | |
 |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | | |
 | |
| 27 28 29 30 31 32 33 34 35 36 | NO2 NO2 NO2 H H NO2
 | O O NNHCSNH2 NNHCSNH2 NNHCSNH2 O O O NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2

 | $CH_2NHCH(COOH)CH(OH)C_6H_5$ $CH_2NHCH(COOH)CH(OH)C_6H_5$ H $CH_2NHCH(COOH)CH(CH_3)_2$ $CH_2N/CH(CH_3)_2/2$ $CH_2N/CH(CH_3)_2/2$ CH_2-N CH_2-N CH_2-N CH_2-N CH_2-N CH_2-N | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Wiener sum of atomic van Sande | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 V index 4 4 5 a der Waals volumes 5 5
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (MV) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 36 37 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H
 | O
O
NNHCSNH ₂
NNHCSNH ₂
O
O
O
NNHCSNH ₂
NNHCSNH ₂
R.

 | $\frac{CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5}}{CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5}}$ $\frac{CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5}}{H}$ $\frac{CH_{2}NHCH(COOH)CH(CH_{3})_{2}}{CH_{2}N/CH(CH_{3})_{2}/2}$ $\frac{CH_{2}N/CH(CH_{3})_{2}/2}{CH_{2}-N}$ $\frac{CH_{2}-N}{C}$ $\frac{CH_{2}-N}{C}$ $\frac{CH_{2}-N}{C}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Duted molecular desc Descrip Sum of atomic van Wiener sum of atomic van mean atomic van | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 Criptors' legend 7 7 7 Vindex 4 4 1,996 30,065 15 Criptors' legend 7 7 7 7 7 Vindex 7 4 7 7 7 10 7 7 7 7 7 1188 1,623 46,888 23 7 1188 1,996 30,065 15 7 149 7 7 7 7 7 15 7 7 7 7 7 15 7<
 | 5,235 11,701 77,09 0,699 -0,302 0,091 $5,235$ 11,701 77,379 1,105 0,3 0,09 $0,207$ 14,312 92,833 2,607 2,765 7,646 $2,491$ $5,771$ $37,005$ 1,384 1,212 1,469 $8,312$ $8,592$ $55,671$ 1,519 0,702 0,493 $4,414$ $6,809$ $43,713$ 1,726 1,052 1,107 $6,349$ $7,665$ $51,874$ 1,277 1,331 1,771 $3,264$ 11,08 $71,703$ $2,696$ $2,927$ $8,568$ $5,388$ $7,075$ $46,73$ 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) | Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degreess (ZM1V) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10^{-3} mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 36 37 38 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H H H H
 | О О NNHCSNH2 NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 O NNHCSNH2 O O O O O NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 O O O O O O

 | $\frac{CH_2NHCH(COOH)CH(OH)C_6H_5}{CH_2NHCH(COOH)CH(OH)C_6H_5}$ H $CH_2NHCH(COOH)CH(CH_3)_2$ $CH_2N/CH(CH_3)_2/2$ $CH_2N/CH(CH_3)_2/2$ CH_2-N | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Cont Descriptor W Sv Se Mv ZM1v
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Duted molecular desc Descrip Sum of atomic van Wiener sum of atomic van mean atomic van first Zagreb index by preserve 10 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 30,065 15 v index ader Waals volumes ader Waals volumes
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) topological descriptor (scaled on Carbon atom) topological descriptor topological descriptor (scaled on Carbon atom) topological descriptor | Figure 12. 3D Correlation of Sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10^{-3} mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 H H H H H H H H H H H H H H H
 | О О NNHCSNH2 NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 O NNHCSNH2 O O NNHCSNH2

 | $\begin{array}{c} \begin{array}{c} CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline \\ CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline \\ CH_2N/CH(CH_3)_{2/2} \\ \hline \\ CH_2N/CH(CH_3)_{2/2} \\ \hline \\ CH_2-N \\ \hline \\ CH_2-N(CH_2CH_2OH)_2 \\ \hline \\ CH_2N(CH_2CH_2OH)_2 \\ \hline \\ CH_2N(CH_2CH_2C)_2 \\ \hline \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Str Str Sc Mv ZM1v
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Duted molecular desc Descrip Wiener Sum of atomic van sum of atomic van mean atomic van first Zagreb index by v Randic I | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 30 30,065 15 otor Name 30 30 16 otor Name 30 30 16 otor Name 30 30 16 otor Name 30 30 30 otor Name 30 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607
2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Topological descriptor Constitutional descriptor (scaled on Carbon atom)) Constitutional descriptor (scaled on Carbon atom) Constitutional descriptor (scaled on Carbon atom) Constitutional descriptor < | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 13. 3D Correlation of sum of atomic van der Waals volumes (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | | |

 | | | | | | | | | | | | |
 | | | | | | |
 | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | | |
 | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | | |
 | |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 H
 | О О NNHCSNH2 NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 O NNHCSNH2 NNHCSNH2 O NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2

 | $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v CID χ1
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Sum of atomic van Sum of atomic van Wiener sum of atomic van mean atomic van first Zagreb index by v Randic I Connectivity index chi Connectivity index chi | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 348 1,996 30,065 otor name 30,065 15 otor name 30 30 otor name 30 30 otor name 30 30 otor name 30 30 otor name
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type Constitutional descriptor (scaled on Carbon atom) Mathematical descriptor walk and path counts Connectivity index | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 13. 3D Correlation of Randic ID humber (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | |
 |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | | |
 | |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 H
 | 0
0
NNHCSNH ₂
NNHCSNH ₂
0
0
0
NNHCSNH ₂
R.
0
0
0
0
0
0
0
0
0
0
0
0
0
0

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2-N/CH(CH_3)_{2/2} \\ \hline CH_2-N/CH(CH_2)_{2/2} \\ \hline CH_2-N/CH(CH_2)_{2/2} \\ \hline CH_2-N/CH(CH_2CH_2OH)_2 \\ \hline CH_2-N$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Cont Descriptor W Sv Sv State Mv ZM1v $\chi 1$
 | 39,50 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip 328 Descrip Wiener Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by v Randic I connectivity index chi ind | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 348 1,996 30,065 valence vertex legrees 30,065 15 ot der Waals volumes 30 30 ot der Waals volumes 30 30 ot der Waals volume 30 30 ot der Waals volume 30 30 30 ot der Waals vo | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) topological descriptor walk and path counts connectivity index
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 13. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: style="text-align: center;"> | | |

 |
 | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | |
 | | | | | | | | | | | |
 | | | | | | |
 | | |
 | | | | | | | | |
 | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | |
 |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 | NO2 NO2 NO2 H H NO2 NO3 H
 | O O NNHCSNH2 NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 O

 | $\begin{array}{c} \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2 \\ \hline CH_2 \\ \hline CH_$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v $\chi 1$
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Wiener sum of atomic van sum of atomic van first Zagreb index by v Randic I connectivity index chi index modified Randic Index | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30 15 otor name 7 7 16 valencex valencex 15 15 oder Waals volumes 15 15 15 oder Waals volumes 15 15 15 oder Waals volume 16 16 16 oder Waals volume 17 17 16 17 oder Waals volume 16 16 16 16 oder Waals volume 16 16 16 16 oder Waals volume 16 16 16 16 oder Waals volume </th <th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index</th> <th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th> <th>Figure 13. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: state of the state</th> | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031
 | Figure 13. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: state of the state | | |

 | |
 | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | |
 | | | | | |
 | | | |
 | | | | | | | | | |
 | | | | | | | | | | |
 | | | | | | |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 | NO2 NO2 NO2 H H NO2 NO2 NO2 NO2 NO2 NO2 NO2 H <th>0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th> <th>$\begin{array}{c} \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2 \\ \hline CH_2N/CH(CH_2OH)_2 \\ \hline CH_2N(CH_2CH_2OH)_2 \\ \hline CH_2N(CH_2CH_2OH)_2$</th> <th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Con Descriptor W Sv Sv Se Mv ZM1v $\chi 1$ XMOD VRA1</th> <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Viener Sum of atomic van sum of atomic van sum of atomic van first Zagreb index by v Randic I connectivity index chi ind modified Randic Randic I</th> <th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 5 5 5 otor Name 5 5 5</th> <th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type Constitutional descriptor (scaled on Carbon atom) Constitutional descriptor Walk and path counts Connectivity index Connectivity index Example a connectivity index Example a connectivity index Example a connectivity index<th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>Figure 11. 3D Correlation of Randic ID number (CID), mean
atomic van der Waals volume (Mv) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: style sty</th></th> | 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_6H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2 \\ \hline CH_2N/CH(CH_2OH)_2 \\ \hline CH_2N(CH_2CH_2OH)_2 \\ \hline CH_2N(CH_2CH_2OH)_2$
 | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Con Descriptor W Sv Sv Se Mv ZM1v $\chi 1$ XMOD VRA1 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Viener Sum of atomic van sum of atomic van sum of atomic van first Zagreb index by v Randic I connectivity index chi ind modified Randic Randic I | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 5 5 5
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type Constitutional descriptor (scaled on Carbon atom) Constitutional descriptor Walk and path counts Connectivity index Connectivity index Example a connectivity index Example a connectivity index Example a connectivity index <th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031</th> <th>Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: style sty</th> | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: style sty | | |

 |
 | |
 | | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | | | | |
 | | | | | | | |
 | | | |
 | | | | | | |
 | | |
 | | | | | | | | | | | | |
 | | | | | | | | | | | | |
 |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 | NO2 NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0

 | $\frac{CH_2NHCH(COOH)CH(OH)C_6H_5}{CH_2NHCH(COOH)CH(OH)C_6H_5}$ $\frac{CH_2NHCH(COOH)CH(OH)C_6H_5}{H}$ $\frac{H}{H}$ $\frac{CH_2NHCH(COOH)CH(CH_3)_2}{CH_2N/CH(CH_3)_2/2}$ $\frac{CH_2N/CH(CH_3)_2/2}{CH_2N/CH(CH_3)_2/2}$ $\frac{CH_2-N_2}{CH_2-N_2}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv ZM1v χ1 XMOD VRA1
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name 7 7 7 oter Waals volumes 7 7 oter Waals volumes 7 7 oter Waals volume 7 7 valence vertex degrees 7 D number 7 7 i-1 (Randic connectivity index 7 ector-based index from 7 ory matrix 7
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) connec | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 13. 3D Correlation of standic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: standard content of the standard conte | | |

 |
 | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | |
 | | | | | | | | | | |
 | | | | | | |
 | | | |
 | | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | |
 |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 | NO2 NO2 H H NO2 H
 | О NNHCSNH2 NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 O NNHCSNH2 NNHCSNH2 O NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 O OOO<

 | $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Sc X1 XMOD VRA1
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Wiener sum of atomic van sum of atomic van first Zagreb index by v Randic I connectivity index chi ind modified Randic Randic I Balaban distance adjacen | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 Criptors' legend 30,065 15 Otor name * * * * W index * * * * der Waals volumes * * * ader Waals volume * * * der Waals volume * * * ader Waals volume * <
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type < | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against Klebsiella pneumoniae ATCC 10031 | Figure 13. 3D Correlation of Kandic ID number (CID), mean against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: Constraint of the standic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: Constraint of the standic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: Constraint of the standic ID number (CID) and topological indices (TIs) agreement with previously | |
 |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | | |
 | |
| 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 | NO2 NO2 NO2 H H NO2 H
 | O O NNHCSNH2 NNHCSNH2 NNHCSNH2 O O NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 O

 | $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Sc XMOD XMOD VRA1
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 Descrip Wiener sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by v Randic I connectivity index chi ind modified Randic Balaban distance Balaban distance Balaban | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 Criptors' legend 30,065 15 otor name 7 7 7 * W index 4 1,996 30,065 15 otor name 7 7 7 7 otor name 7 7 7 7 otor vallence vertex degrees 7 7 7 otor vallence vertex degrees 7 7 7 i-1 (Randic connectivity index 7 7 7 i-1 (Randic connectivity index 7 7 7 i-1 (Randic connectivity index 7 7 7 i-1 (Randic c
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index eigenvalue-base | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against Klebsiella pneumoniae ATCC 10031 | Figure 13. 3D Correlation of Kandic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 1 28 1 29 1 30 1 31 1 32 1 33 1 34 1 35 1 36 1 37 1 38 1 39 1 40 1 40 1 42 1 42 1 43 1 44 1 45 1 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_9H_5 \\ CH_2NHCH(COOH)CH(OH)C_8H_5 \\ H \\ CH_2NHCH(COOH)CH(CH_3)_2 \\ CH_2N/CH(CH_3)_{2/2} \\ CH_2N/CH(CH_3)_{2/2} \\ CH_2N/CH(CH_3)_{2/2} \\ CH_2N/CH(CH_3)_{2/2} \\ CH_2N/CH(CH_3)COOH \\ \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Cont Descriptor W Sv Se Mv Slave XMOD χ1 XMOD VRA1 BID MLOGP
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip Wiener Sum of atomic van sum of atomic van Sum of atomic van first Zagreb index by v Randic I connectivity index chi ind modified Randic Randic I Modified Randic Balaban distance Balaban distance Agiacen | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * W index * * * * der Waals volumes * * * der Waals volume * * * der Waals volume * * * valence vertex degrees * D number * * i-1 (Randic connectivity idex) * * connectivity index *
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index Connectivity index eigenvalue-based index eigenvalue-based index molecular property < | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Kandic ID number (CID), mean atomic van der Waals volume (Mv) and MIC (10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: style sty | | |

 |
 | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | |
 | | | | | | | | | | |
 | | | | | | |
 | | | |
 | | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | |
 |
| 27 28 29 30 31 32 33 33 34 35 36 37 36 37 38 39 40 41 42 43 44 42 43 44 45 46 | NO2 NO2 NO2 H H NO2 H </th <th>0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 NNHCSNH2 0 NNHCSNH2 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0</th> <th>$\begin{array}{c} \hline CH_2NHCH(COOH)CH(OH)C_9H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_9H_5 \\ \hline H \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_{2N/CH(CH_{3})COOH \\ \hline \\$</th> <th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Contr Descriptor Descriptor W Sv State Mv Sv State Mv State Mu State Mu State Mu State Mu State Mu State State State State State State State State State State State State State State</th> <th>39,56 0,63 508 38,79 0,64 524 49,88 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic van Randic van first Zagreb index by van Randic randic Gonnectivity index chi ind adjacen Balaban distance Moriguchi octanol-wat Ghose-Crippen octanol-wat</th> <th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * W index * * * • der Waals volumes * * * valence vertex degrees * * * oder Waals volume * * valence vertex degrees * * * oder Waals volume *<th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type
topological descriptor constitutional descriptor (scaled on Carbon atom) Constitutional descriptor constitutional descriptor (scaled on Carbon atom) Connectivity index connectivity index eigenvalue-based index eigenvalue-based index molecular property molecular property</th><th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th> Figure 11. 3D Correlation of Randic ID humber (CID), mean atomic van der Waals volume (Mv) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: the state of the state</th></th> | 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 NNHCSNH2 0 NNHCSNH2 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} \hline CH_2NHCH(COOH)CH(OH)C_9H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_9H_5 \\ \hline H \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_2N/CH(CH_3)_{2/2} \\ \hline CH_{2N/CH(CH_{3})COOH \\ \hline \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Contr Descriptor Descriptor W Sv State Mv Sv State Mv State Mu State Mu State Mu State Mu State Mu State State
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic van Randic van first Zagreb index by van Randic randic Gonnectivity index chi ind adjacen Balaban distance Moriguchi octanol-wat Ghose-Crippen octanol-wat | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * W index * * * • der Waals volumes * * * valence vertex degrees * * * oder Waals volume * * valence vertex degrees * * * oder Waals volume * <th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) Constitutional descriptor constitutional descriptor (scaled on Carbon atom) Connectivity index connectivity index eigenvalue-based index eigenvalue-based index molecular property molecular property</th> <th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th> <th> Figure 11. 3D Correlation of Randic ID humber (CID), mean atomic van der Waals volume (Mv) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: the state of the state</th> | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) Constitutional descriptor constitutional descriptor (scaled on Carbon atom) Connectivity index connectivity index eigenvalue-based index eigenvalue-based index molecular property molecular property | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031
 | Figure 11. 3D Correlation of Randic ID humber (CID), mean atomic van der Waals volume (Mv) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: the state of the state | | |

 | |
 | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | |
 | | | | | |
 | | | | | |
 | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | |
| 27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 44 41 42 43 44 47 | NO2 NO2 NO2 H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} \hline CH_2NHCH(COOH)CH(OH)C_9H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_9H_5 \\ \hline H \\ \hline \\ CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline \\ CH_2N/CH(CH_3)_2/2 \\ \hline \\ CH_2N(CH_2CH_2OH)_2 \\ \hline \\ CH_2N(CH(CH_3)_2/2 \\ \hline \\ CH_2N(CH(CH_3)_2/2 \\ \hline \\ CH_2N(CH(CH_3)_2/2 \\ \hline \\ CH_2N(CH(CH_2CH_2CH_2OH)_2 \\ \hline \\ \hline \\ CH_2N(CH(CH_2CH_2CH_2OH)_2 \\ \hline \\ \hline \\ CH_2N(CH(CH_3)_2/2 \\ \hline \\ CH_2N(CH(CH_3)_2/2 \\ \hline \\ CH_2N(CH(CH_2CH_2CH_2OH)_2 \\ \hline \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor Descriptor W Sv S SV S S
 | 39,56 0,63 508 38,79 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic van Sande first Zagreb index by van Randic I connectivity index chi index mean atomic van index first Zagreb index by van Randic I Ghose-Crippen octan adjacen Moriguchi octanol-wat Salaban Moriguchi octanol-wat Ghose-Crippen octan | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * oder Waals volumes * * oder Waals volume * * valence vertex degrees * * D number * * i-1 (Randic connectivity * oconnectivity index * * econnectivity index * * econnectivity index * * iD number * * iD number * * iD number * * iD number | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional
descriptor (scaled on Carbon atom) (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ⁻³ mol dm ⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Figure 11. 3D Correlation of Randic ID humber (CID), mean atomic van der Waals volume (MV) and MIDC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: the second secon | | |

 |
 | | | | | | | | | | | |
 | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | |
 | | |
 | | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | |
 |
| 272829303132323334353637383940414243444243444445464748 | NO2 NO2 NO2 H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_8H_5 \\ \hline CH_2NHCH(COOH)CH(OH)C_8H_5 \\ \hline H \\ \hline CH_2NHCH(COOH)CH(CH_3)_2 \\ \hline CH_2N/CH(CH_3)_2/2 \\ \hline CH_2N/CH_2CH_2OH)_2 \\ \hline CH_2N/CH_2CH_2OH)_2 \\ \hline CH_2N(CH_2CH_2OH)_2 \\ \hline CH_2N(CH_2OH)_2 \\ \hline $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Com Descriptor W Sv Sv
 | 39,56 0,63 508 38,79 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip Viener Sum of atomic van sum of atomic van Sande first Zagreb index by van Randic I modified Randic ind Randic-type eigenver adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 16 otor name * * * oder Waals volumes * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * <th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor</th> <th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10³ mol dm³) against Klebsiella pneumoniae ATCC 10031</th> <th> Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (W) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: the second second</th> | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ³ mol dm ³) against Klebsiella pneumoniae ATCC 10031
 | Figure 11. 3D Correlation of Randic ID number (CID), mean atomic van der Waals volume (W) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: the second second | | |

 | |
 | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | |
 | | | | | |
 | | | | | |
 | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | |
| 27 1 28 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 42 1 44 1 42 1 44 1 44 1 44 1 44 1 44 1 445 1 446 1 448 1 449 1 | NO2 NO2 H H NO2 H </th <th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <tr td=""></tr></th> <th>$\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_{B}H_{5} \\ \hline \\ CH_2NHCH(COOH)CH(OH)C_{B}H_{5} \\ \hline \\ H \\ \hline \\ CH_2NHCH(COOH)CH(CH_{3})_{2} \\ \hline \\ CH_2N/CH(CH_{3})_{2}/2 \\ \hline \\ CH_2N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{3}))_{2}/2 \\ \hline \\ CH_{2}N(CH(CH_{3}))_{2}/2 \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ \hline \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\$</th> <th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Cont Descriptor W Sv Sv J XMOD J BID MLOGP ALOGP2 ALOGP2 Sv</th> <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Secrip sum of atomic van Sum of atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Moriguchi octanol-wat Balaban Moriguchi octanol-wat Squared Ghose-Criper octanol</th> <th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * Windex * * * * der Waals volumes * * * der Waals volume * * valence vertex degrees * * * der Waals volume * * valence vertex degrees * * * der Waals volume * * valence vertex degrees * * * onnectivity index * * * onnectivity index * * * onnectivity index *</th> <th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312
 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom)) constitutional descriptor (scaled on Carbon atom) (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) (scaled on Carbon atom) topological descriptor walk and path counts connectivity index eigenvalue-based index eigenvalue-based index walk and path counts molecular property molecular property molecular property mo</th> <th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10-3 mol dm-3) against Klebsiella pneumoniae ATCC 10031</th> <th> Figure 11. 3D Correlation of Rando D number (CDD), mean atomic van der Waals volume (WV) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation <i>MIC</i> (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 the preference of biological indices (TIs) agreement with previously the preference of biological findices (W, ZMV1,), and togP,) descriptors. atial dispersion and thus provide </th> | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <tr td=""></tr>

 | $\begin{array}{c} CH_2NHCH(COOH)CH(OH)C_{B}H_{5} \\ \hline \\ CH_2NHCH(COOH)CH(OH)C_{B}H_{5} \\ \hline \\ H \\ \hline \\ CH_2NHCH(COOH)CH(CH_{3})_{2} \\ \hline \\ CH_2N/CH(CH_{3})_{2}/2 \\ \hline \\ CH_2N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{3}))_{2}/2 \\ \hline \\ CH_{2}N(CH(CH_{3}))_{2}/2 \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ \hline \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ \hline \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Cont Descriptor W Sv Sv J XMOD J BID MLOGP ALOGP2 ALOGP2 Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Secrip sum of atomic van Sum of atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Moriguchi octanol-wat Balaban Moriguchi octanol-wat Squared Ghose-Criper octanol | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * Windex * * * * der Waals volumes * * * der Waals volume * * valence vertex degrees * * * der Waals volume * * valence vertex degrees * * * der Waals volume * * valence vertex degrees * * * onnectivity index * * * onnectivity index * * * onnectivity index * | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom)) constitutional descriptor (scaled on Carbon atom) (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) (scaled on Carbon atom) topological descriptor walk and path counts connectivity index eigenvalue-based index eigenvalue-based index walk and path counts molecular property molecular property molecular property mo
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10-3 mol dm-3) against Klebsiella pneumoniae ATCC 10031 | Figure 11. 3D Correlation of Rando D number (CDD), mean atomic van der Waals volume (WV) and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation <i>MIC</i> (10⁻³ mol dm⁻³) against <i>Klebsiella pneumoniae</i> ATCC 10031 the preference of biological indices (TIs) agreement with previously the preference of biological findices (W, ZMV1,), and togP,) descriptors. atial dispersion and thus provide | | |

 |
 | | | | | | | | | | | | |
 | | | | | |
 | | | | | | | | |
 | | | | | | | | | | |
 | | | | | | |
 | | | |
 | | | | | | | |
 | | |
 | | | | | | | | | | | | |
 | | | | | | | | | | |
 |
| |
 |

 | |
 | |
 | | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 272829303131323334353637383940414243404142434444454647484950 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <tr td=""></tr>

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}COH \\ \hline \\ CH_{2}NHCH(CH_{3})COOH \\ \hline \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Cont Descriptor W Sv Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Van Randic I connectivity index by van Randic I modified Randic Randic I Randic-type eigenver
adjacen adjacen Balaban distance Balaban Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * W index - - - • der Waals volumes * * * * der Waals volume * * * valence vertex degrees * * * ID number * * * i-1 (Randic connectivity index * * econnectivity index * * econnectivity index * * econnectivity index * * iD number * * * | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom)) constitutional descriptor (scaled on Carbon atom) (scaled on Carbon atom) constitutional
descriptor (scaled on Carbon atom) (scaled on Carbon atom) und path counts connectivity index eigenvalue-based index eigenvalue-based index eigenvalue-based index eigenvalue-based index molecular property molecular property molecular property molec | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10-3 mol dm-3) against Klebsiella pneumoniae ATCC 10031 | Figure 11. 3D Correlation of Rando D number (CD), mean atomic van der Waals volume (WW) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 13. 3D Correlation of sum of atomic van der Waals volumes (SV), AlogP and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 e shown significant correlation <i>MIC</i> (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 the preference of biological indices (TIs) agreement with previously the preference of biological findices (V, ZMV1,), and their as it is combination of gical (W, ZMV1,), and thus provide QSAR study. | | |

 |
 | |
 | | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | | | | |
 | | | | | | | |
 | | | |
 | | | | | | |
 | | |
 | | | | | | | | | | | | |
 | | | | | | | | | | | | |
 |
| |
 |

 | |
 | |
 | | | |
 | |

 | |
 | | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | | |
 | | |
| 27 1 29 1 30 1 31 1 32 1 33 1 33 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 44 1 45 1 49 1 50 <td< th=""><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ \\ CH_{2}N(CH(CH_{2}OH)_{2} \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ \\ \\ \\ \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Struttor XNV CID χ1 XMOD VRA1 BID ALOGP2 ALOGP2</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) topological descriptor walk and path counts connectivity index eige</th><th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>representation of kande D number (cD), mean atomic van der Waals volume (WW) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031</th></td<> | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ \\ CH_{2}N/CH(CH_{3})_{2} \\ \\ \\ CH_{2}N(CH(CH_{2}OH)_{2} \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \\ \\ CH_{2}N(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ \\ \\ \\ \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Struttor XNV CID χ1 XMOD VRA1 BID ALOGP2 ALOGP2
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701
 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) topological descriptor walk and path counts connectivity index eige | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10-3 mol dm-3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | representation of kande D number (cD), mean atomic van der Waals volume (WW) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | |
 |

 | | | | | | | | | | | | |
 | | | | | | |
 | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | | |
 | |
| 27128129130131132133134135136137138139140141243144142143145146147148150515152 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 0 NNHCSNH2 0 0 NNHCSNH2 0 NNHCSNH2 0

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{5} \\ H \\ \hline \\ CH_{2}NICH(COOH)CH(CH_{3})_{2} \\ CH_{2}NICH(CH_{3})_{2} \\ \hline \\ CH_{2}NICH(CH_{3})_{2} \\ \hline \\ CH_{2}NICH(CH_{3})_{2} \\ \hline \\ CH_{2}NICH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH_{2}COH)_{2} \\ \hline \\ CH_{2}NHCH_{2}COOH \\ \hline \\ \hline \\ \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv State Mv State X1 XMOD X1 State J ALOGP ALOGP2
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van first Zagreb index by Randic I connectivity index chi ind mean atomic van modified Randic Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Squared Ghose-Cripperi octan (IC Squared Ghose-Cripperi octan IC | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) Constitutional descriptor atom constitutional descriptor (scaled on Carbon atom)
 constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index eigenvalue-based index eigenvalue-based index molecular property molecular pro | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | Pigure 11. 3D Correlation of Rando D number (CID), mean atomic van der Waals volume (WW) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 | | |

 |
 | |
 | | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | | | | |
 | | | | | | | |
 | | | |
 | | | | | | |
 | | |
 | | | | | | | | | | | | |
 | | | | | | | | | | | | |
 |
| 27 1 29 1 30 1 31 1 32 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 2 53 1 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 <tr td=""> <th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\$</th><th>54 23,46 555 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv S S S</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic van Randic I connectivity index chi ind first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octanol-wat Balaban Moriguchi octanol-wat Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat Moriguchi octanol-wat Squared Ghose-Crippen octanol-wat abri, et al., <i>Eur. J.</i> Can atom con </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * Windex * * * * der Waals volumes * * * der Waals volume * * valence vertex degrees * * D number * * i-1 (Randic connectivity * * connectivity index * * open * * open <</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th><th>regime 11. 3D Correlation of Kando D Jumber (Clo³ mol dm³)
against Klebsiella pneumoniae ATCC 10031</th></tr> <tr><th>27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 9 40 41 42 43 50 51 52 53 54</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 <tr td=""> <th>$\begin{array}{c}
CH_{2}NHCH(COOH)CH(OH)C_{2}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2})$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th><th>right of the second se</th></th></tr><tr><th>27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 50 51 52 53 54 55</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline H \\ \hline CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2}/2 \\ \hline CH_{2}N/CH(CH_{2}OH)_{2} \\ \hline CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{3})COH \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippe eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Squared Ghose-Cripartition co squared Ghose-Crippen octan gatora abri, et al., Eur. J. fawal, R. Sohguara 26. 54.914 (J. Torrens </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 vindex 46 46 6 oder Waals volumes 5 5 5 valence vertex degrees 5 5 5 10 number 5 5 5 i-1 (Randic connectivity index 5 5 oconnectivity index 5 5 oconnectivity index 5 5 ider Waals volume 5 5 valence vertex degrees 5 5 id number 5 6</th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index eigenvalue-based index topological descriptor walk and path counts molecular property molecular property <pmolecular p="" property<=""> molecular property <th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study.</th></pmolecular></th></tr><tr><th>27 1 28 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1
37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 5 56 1</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ H $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}N(CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CCOH$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Su ZM1v CID χ1 XMOD VRA1 Su J BID MLOGP2 ALOGP2 3. USP 7,0 3. USP 7,0 4. EP11222 Su</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Sq914</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 16 windex ader Waals volumes 5 16 otder Waals volume 5 5 16 valence vertex degrees 5 5 10 number 5 5 5 5 i-1 (Randic connectivity index 5 5 5 iD number 5 5 5 5 iopp) 5 5 5 5 5 iopp) 5 6 6 6 6 iopp)</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously
the preference of biological of the previously of the preference of biological of the previously of the previo</th></tr><tr><th>2728293031323333343536373839404142434445464748495051525354555657</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ H \\ CH_{3}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}COH) \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr S. Movr</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi incomolified Randic Type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Ghose-Crippen octan (Ic Squared Ghose-Cripartition cc Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc fabri, et al., <i>Eur. J.</i> Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 5 vindex 46,888 23 ader Waals volumes 5 5 valence vertex degrees 5 D number 5 i-1 (Randic connectivity index 5 connectivity index 5 oconnectivity index 5 iD number 5 ici (logP^2) 5 opp) 5 rippen octanol-water opp) 5 opp) 5 opp) 5</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702
0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>right first and correlation of kande ID number (CID), mean atomic van der Waals volume (My and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$</th></tr><tr><th>272829303132333334353637383940414243444546474849505152535455565758</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>CH2NHCH(COOH)CH(OH)C8H5 CH2NHCH(COOH)CH(OH)C8H5 H CH2NHCH(COOH)CH(OH)22 CH2NCH(CH3)22 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2C</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Sv Se Mv State Mv Sc Mv State Mv Sc Se Mv State XMOD X1 Sc Sate MLOGP ALOGP2 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. M. Movr 193-202</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octan adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Abri, et al., <i>Eur. J.</i> fawal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free fin, M. Jadrijević-MI </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property molecular property</th><th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>regime 11. 3D Correlation of Rando ID number (CID), mean atomic value (W) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int \frac{1}{\sqrt{9}} \int$</th></tr><tr><th>27 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 1 55 5 56 1 59 1 </th><th>NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H H H H H H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <td< th=""><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, <</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996
 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of value (W) and MIC (10³ mol dm³)
against <i>Klebsiella pneumoniae</i> ATCC 10031</th></td<></th></tr><tr><th>27 1 28 1 30 1 31 1 32 1 32 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 45 1 44 1 45 1 50 1 51 1 52 1 54 1 55 1 56 1 57 58 59 1 60 1</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ H \\ CH_{3}NHCH(COOH)CH(OH)_{2}H_{3} \\ CH_{3}N/CH(CH_{3})_{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}(COH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH(COH)(CH_{4}COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ \end{array}$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv ZM1v CID $\chi1$ MCOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi index modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan maxal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free in, M. Jadrijević-MI </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5.235 11.701 77,09 0,699 -0,302 0,091 5.235 11.701 77,379 1,105 0,3 0,09 0.207 14,312 92,833 2,607 2,765 7,646 2,441 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,776 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) (sconnectivity index (scaled on Carbon a</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML 3D correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of Rando ID number (CH), mean atomic value (W) and MIC (10³ mol dm³) against <i>Klebsiella</i> pneumoniae ATCC 10031</th></tr><tr><th>271281293303313323333343353363373383940142340142353144142350151253354555556157558159606161</th><th>NO2 NO2 H H NO2 H</th><th></th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Corr Descriptor W Sv Sv Sv</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip sum of atomic van sum of atomic van sum of atomic Van sum of atomic van first Zagreb index by van Randic I connectivity index chi index
 first Zagreb index by van Randic I connectivity index chi index geore adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan in, M. Jadrijević-MI jadrijević-MI in, M. Jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 12 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5.235 11,701 77,09 0,699 -0,302 0,091
5.235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,441 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,776 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML - 3D correlations allow better spata an optimal selection of MDs in C. Good correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i> - Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>Piper Pit. 3D Correlation of Xande ID number (CH2), mean atomic van der Waals volume (My) and MIC (10³) mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$</th></tr></th></tr> | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ $ | 54 23,46 555 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv S S S
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic van Randic I connectivity index chi ind first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octanol-wat Balaban Moriguchi octanol-wat Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat Moriguchi octanol-wat Squared Ghose-Crippen octanol-wat abri, et al., <i>Eur. J.</i> Can atom con | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * Windex * * * * der Waals volumes * * * der Waals volume * * valence vertex degrees * * D number * * i-1 (Randic connectivity * * connectivity index * * open * * open < | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031 | regime 11. 3D Correlation of Kando D Jumber (Clo ³ mol dm ³)
against Klebsiella pneumoniae ATCC 10031 | 27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 9 40 41 42 43 50 51 52 53 54 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 <tr td=""> <th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{2}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2})$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th><th>right of the second se</th></th></tr> <tr><th>27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 50 51 52 53 54 55</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline H \\ \hline CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2}/2 \\ \hline CH_{2}N/CH(CH_{2}OH)_{2} \\ \hline
CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{3})COH \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippe eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Squared Ghose-Cripartition co squared Ghose-Crippen octan gatora abri, et al., Eur. J. fawal, R. Sohguara 26. 54.914 (J. Torrens </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 vindex 46 46 6 oder Waals volumes 5 5 5 valence vertex degrees 5 5 5 10 number 5 5 5 i-1 (Randic connectivity index 5 5 oconnectivity index 5 5 oconnectivity index 5 5 ider Waals volume 5 5 valence vertex degrees 5 5 id number 5 6</th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index eigenvalue-based index topological descriptor walk and path counts molecular property molecular property <pmolecular p="" property<=""> molecular property <th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study.</th></pmolecular></th></tr> <tr><th>27 1 28 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 5 56 1</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ H $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}N(CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CCOH$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Su ZM1v CID χ1 XMOD VRA1 Su J BID MLOGP2 ALOGP2 3. USP 7,0 3. USP 7,0 4. EP11222 Su</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Sq914</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638
60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 16 windex ader Waals volumes 5 16 otder Waals volume 5 5 16 valence vertex degrees 5 5 10 number 5 5 5 5 i-1 (Randic connectivity index 5 5 5 iD number 5 5 5 5 iopp) 5 5 5 5 5 iopp) 5 6 6 6 6 iopp)</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously
the preference of biological of the previously of the preference of biological of the previously of the previo</th></tr> <tr><th>2728293031323333343536373839404142434445464748495051525354555657</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ H \\ CH_{3}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}COH) \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr S. Movr</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi incomolified Randic Type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Ghose-Crippen octan (Ic Squared Ghose-Cripartition cc Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc fabri, et al., <i>Eur. J.</i> Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 5 vindex 46,888 23 ader Waals volumes 5 5 valence vertex degrees 5 D number 5 i-1 (Randic connectivity index 5 connectivity index 5 oconnectivity index 5 iD number 5 ici (logP^2) 5 opp) 5 rippen octanol-water opp) 5 opp) 5 opp) 5</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>right first and correlation of kande ID number (CID), mean atomic van der Waals volume (My and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$</th></tr> <tr><th>272829303132333334353637383940414243444546474849505152535455565758</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>CH2NHCH(COOH)CH(OH)C8H5 CH2NHCH(COOH)CH(OH)C8H5 H CH2NHCH(COOH)CH(OH)22 CH2NCH(CH3)22 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2C</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Sv Se Mv State Mv Sc Mv State Mv Sc Se Mv State XMOD X1 Sc Sate MLOGP ALOGP2 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. M. Movr 193-202</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octan adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Abri, et al., <i>Eur. J.</i> fawal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free fin, M. Jadrijević-MI </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701
77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property molecular property</th><th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>regime 11. 3D Correlation of Rando ID number (CID), mean atomic value (W) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int \frac{1}{\sqrt{9}} \int$</th></tr> <tr><th>27 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 1 55 5 56 1 59 1 </th><th>NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H H H H H H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <td< th=""><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, <</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of value (W) and MIC (10³ mol dm³)
against <i>Klebsiella pneumoniae</i> ATCC 10031</th></td<></th></tr> <tr><th>27 1 28 1 30 1 31 1 32 1 32 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 45 1 44 1 45 1 50 1 51 1 52 1 54 1 55 1 56 1 57 58 59 1 60 1</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ H \\ CH_{3}NHCH(COOH)CH(OH)_{2}H_{3} \\ CH_{3}N/CH(CH_{3})_{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}(COH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\
CH_{4}N(CH(COH)(CH_{4}COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ \end{array}$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv ZM1v CID $\chi1$ MCOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi index modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan maxal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free in, M. Jadrijević-MI </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5.235 11.701 77,09 0,699 -0,302 0,091 5.235 11.701 77,379 1,105 0,3 0,09 0.207 14,312 92,833 2,607 2,765 7,646 2,441 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,776 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) (sconnectivity index (scaled on Carbon a</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML 3D correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of Rando ID number (CH), mean atomic value (W) and MIC (10³ mol dm³) against <i>Klebsiella</i> pneumoniae ATCC 10031</th></tr> <tr><th>271281293303313323333343353363373383940142340142353144142350151253354555556157558159606161</th><th>NO2 NO2 H H NO2 H</th><th></th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Corr Descriptor W Sv Sv Sv</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip sum of atomic van sum of atomic van sum of atomic Van sum of atomic van first Zagreb index by van Randic I connectivity index chi index first Zagreb index by van Randic I connectivity index chi index geore adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan in, M. Jadrijević-MI jadrijević-MI in, M. Jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 12 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5.235 11,701 77,09 0,699 -0,302 0,091
5.235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,441 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,776 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML - 3D correlations allow better spata an optimal selection of MDs in C. Good correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i> - Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>Piper Pit. 3D Correlation of Xande ID number (CH2), mean atomic van der Waals volume (My) and MIC (10³) mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$</th></tr> | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{2}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van
 Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara </th> <th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th> <th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th> <th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th> <th>right of the second se</th> | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031 | right of the second se | 27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 50 51 52 53 54 55 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline H \\ \hline CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2}/2 \\ \hline CH_{2}N/CH(CH_{2}OH)_{2} \\ \hline CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{3})COH \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippe eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Squared Ghose-Cripartition co squared Ghose-Crippen octan gatora abri, et al., Eur. J. fawal, R. Sohguara 26. 54.914 (J. Torrens | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638
 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 vindex 46 46 6 oder Waals volumes 5 5 5 valence vertex degrees 5 5 5 10 number 5 5 5 i-1 (Randic connectivity index 5 5 oconnectivity index 5 5 oconnectivity index 5 5 ider Waals volume 5 5 valence vertex degrees 5 5 id number 5 6 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index eigenvalue-based index topological descriptor walk and path counts molecular property molecular property <pmolecular p="" property<=""> molecular property <th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study.</th></pmolecular> | Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study. | 27 1 28 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 5 56 1 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ H $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}N(CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CCOH$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Su ZM1v CID χ1 XMOD VRA1 Su J BID MLOGP2 ALOGP2 3. USP 7,0 3. USP 7,0 4. EP11222 Su | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37
 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Sq914 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 16 windex ader Waals volumes 5 16 otder Waals volume 5 5 16 valence vertex degrees 5 5 10 number 5 5 5 5 i-1 (Randic connectivity index 5 5 5 iD number 5 5 5 5 iopp) 5 5 5 5 5 iopp) 5 6 6 6 6 iopp) | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | response to the preference of biological indices (TIs) agreement with previously
the preference of biological of the previously of the preference of biological of the previously of the previo | 2728293031323333343536373839404142434445464748495051525354555657 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ H \\ CH_{3}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}COH) \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr S. Movr | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi incomolified Randic Type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Ghose-Crippen octan (Ic Squared Ghose-Cripartition cc Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc fabri, et al., <i>Eur. J.</i> Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 5 vindex 46,888 23 ader Waals volumes 5 5 valence vertex degrees 5 D number 5 i-1 (Randic connectivity index 5 connectivity index 5 oconnectivity index 5 iD number 5 ici (logP^2) 5 opp) 5 rippen octanol-water opp) 5 opp) 5 opp) 5 | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | right first and correlation of kande ID number (CID), mean atomic van der Waals volume (My and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$ | 272829303132333334353637383940414243444546474849505152535455565758
 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | CH2NHCH(COOH)CH(OH)C8H5 CH2NHCH(COOH)CH(OH)C8H5 H CH2NHCH(COOH)CH(OH)22 CH2NCH(CH3)22 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2C | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Sv Se Mv State Mv Sc Mv State Mv Sc Se Mv State
XMOD X1 Sc Sate MLOGP ALOGP2 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. M. Movr 193-202 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octan adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Abri, et al., <i>Eur. J.</i> fawal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free fin, M. Jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property molecular property | Figure 10. 2D Correlation of Randie ID number (CID) and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | regime 11. 3D Correlation of Rando ID number (CID), mean atomic value (W) and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int \frac{1}{\sqrt{9}} \int $ | 27 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 1 55 5 56 1 59 1 | NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H H H H H H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <td< th=""><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, <</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular
properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of value (W) and MIC (10³ mol dm³)
against <i>Klebsiella pneumoniae</i> ATCC 10031</th></td<> | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, < | 1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002) | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | regime 11. 3D Correlation of value (W) and MIC (10 ³ mol dm ³)
against <i>Klebsiella pneumoniae</i> ATCC 10031 | 27 1 28 1 30 1 31 1 32 1 32 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 45 1 44 1 45 1 50 1 51 1 52 1 54 1 55 1 56 1 57 58 59 1 60 1 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ H \\ CH_{3}NHCH(COOH)CH(OH)_{2}H_{3} \\ CH_{3}N/CH(CH_{3})_{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}(COH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH(COH)(CH_{4}COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv ZM1v CID $\chi1$ MCOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi index modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan maxal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free in, M. Jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5.235 11.701 77,09 0,699 -0,302 0,091 5.235
11.701 77,379 1,105 0,3 0,09 0.207 14,312 92,833 2,607 2,765 7,646 2,441 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,776 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) (sconnectivity index (scaled on Carbon a | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML 3D correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | regime 11. 3D Correlation of Rando ID number (CH), mean atomic value (W) and MIC (10 ³ mol dm ³) against <i>Klebsiella</i> pneumoniae ATCC 10031 | 271281293303313323333343353363373383940142340142353144142350151253354555556157558159606161 | NO2 NO2 H H NO2 H | | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Corr Descriptor W Sv Sv Sv | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip sum of atomic van sum of atomic van sum of atomic Van sum of atomic van first Zagreb index by van Randic I connectivity index chi index first Zagreb index by van Randic I connectivity index chi index geore adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan in, M. Jadrijević-MI jadrijević-MI in, M. Jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 12 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5.235 11,701 77,09 0,699 -0,302 0,091
5.235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,441 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,776 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML - 3D correlations allow better spata an optimal selection of MDs in C. Good correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i> - Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | Piper Pit. 3D Correlation of Xande ID number (CH2), mean atomic van der Waals volume (My) and MIC (10 ³) mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$ |
| $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ CH_{2}NCH(CH_{3})_{2} \\ \hline \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}OH)_{2} \\ \hline \\ CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ \hline \\ CH_{2}NHCH(COOH) \\ \hline \\ $ | 54 23,46 555 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv S S S
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 mouted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic van Randic I connectivity index chi ind first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octanol-wat Balaban Moriguchi octanol-wat Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat Ghose-Crippen octanol-wat Moriguchi octanol-wat Squared Ghose-Crippen octanol-wat abri, et al., <i>Eur. J.</i> Can atom con

 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 30,065 15 otor name * * * * Windex * * * * der Waals volumes * * * der Waals volume * * valence vertex degrees * * D number * * i-1 (Randic connectivity * * connectivity index * * open * * open < | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031 | regime 11. 3D Correlation of Kando D Jumber (Clo ³ mol dm ³)
against Klebsiella pneumoniae ATCC 10031 |
 | | | | |

 |
 | | | | | | | | | | | |
 | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | |
 |
| 27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 9 40 41 42 43 50 51 52 53 54 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 <tr td=""> <th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{2}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2})$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th><th>right of the second se</th></th></tr> <tr><th>27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 50 51 52 53 54 55</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline H \\ \hline CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2}/2 \\ \hline CH_{2}N/CH(CH_{2}OH)_{2} \\ \hline CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{3})COH \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline
CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippe eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Squared Ghose-Cripartition co squared Ghose-Crippen octan gatora abri, et al., Eur. J. fawal, R. Sohguara 26. 54.914 (J. Torrens </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 vindex 46 46 6 oder Waals volumes 5 5 5 valence vertex degrees 5 5 5 10 number 5 5 5 i-1 (Randic connectivity index 5 5 oconnectivity index 5 5 oconnectivity index 5 5 ider Waals volume 5 5 valence vertex degrees 5 5 id number 5 6</th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index eigenvalue-based index topological descriptor walk and path counts molecular property molecular property <pmolecular p="" property<=""> molecular property <th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study.</th></pmolecular></th></tr> <tr><th>27 1 28 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 5 56 1</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ H $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}N(CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CCOH$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Su ZM1v CID χ1 XMOD VRA1 Su J BID MLOGP2 ALOGP2 3. USP 7,0 3. USP 7,0 4. EP11222 Su</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Sq914</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15
 criptors' legend 5 5 16 otor name 5 5 16 windex ader Waals volumes 5 16 otder Waals volume 5 5 16 valence vertex degrees 5 5 10 number 5 5 5 5 i-1 (Randic connectivity index 5 5 5 iD number 5 5 5 5 iopp) 5 5 5 5 5 iopp) 5 6 6 6 6 iopp)</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously
the preference of biological of the previously of the preference of biological of the previously of the previo</th></tr> <tr><th>2728293031323333343536373839404142434445464748495051525354555657</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ H \\ CH_{3}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}COH) \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr S. Movr</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi incomolified Randic Type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Ghose-Crippen octan (Ic Squared Ghose-Cripartition cc Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc fabri, et al., <i>Eur. J.</i> Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 5 vindex 46,888 23 ader Waals volumes 5 5 valence vertex degrees 5 D number 5 i-1 (Randic connectivity index 5 connectivity index 5 oconnectivity index 5 iD number 5 ici (logP^2) 5 opp) 5 rippen octanol-water opp) 5 opp) 5 opp) 5</th><th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th>Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>right first and correlation of kande ID number (CID), mean atomic van der Waals volume (My and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$</th></tr> <tr><th>272829303132333334353637383940414243444546474849505152535455565758</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>CH2NHCH(COOH)CH(OH)C8H5 CH2NHCH(COOH)CH(OH)C8H5 H CH2NHCH(COOH)CH(OH)22 CH2NCH(CH3)22 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2C</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Sv Se Mv State Mv Sc Mv State Mv Sc Se Mv State XMOD X1 Sc Sate MLOGP ALOGP2 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. M. Movr 193-202</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octan adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Abri, et al., <i>Eur. J.</i> fawal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free fin, M. Jadrijević-MI </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809
43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property molecular property</th><th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>regime 11. 3D Correlation of Rando ID number (CID), mean atomic value (W) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int \frac{1}{\sqrt{9}} \int$</th></tr> <tr><th>27 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 1 55 5 56 1 59 1 </th><th>NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H H H H H H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <td< th=""><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, <</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of value (W) and MIC (10³ mol dm³)
against <i>Klebsiella pneumoniae</i> ATCC 10031</th></td<></th></tr> <tr><th>27 1 28 1 30 1 31 1 32 1 32 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 45 1 44 1 45 1 50 1 51 1 52 1 54 1 55 1 56 1 57 58 59 1 60 1</th><th>NO2 NO2 H H NO2 H</th><th>0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0</th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ H \\ CH_{3}NHCH(COOH)CH(OH)_{2}H_{3} \\ CH_{3}N/CH(CH_{3})_{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}(COH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH(COH)(CH_{4}COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ \end{array}$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60
 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv ZM1v CID $\chi1$ MCOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi index modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan maxal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free in, M. Jadrijević-MI </th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5.235 11.701 77,09 0,699 -0,302 0,091 5.235 11.701 77,379 1,105 0,3 0,09 0.207 14,312 92,833 2,607 2,765 7,646 2,441 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,776 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) (sconnectivity index (scaled on Carbon a</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML 3D correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of Rando ID number (CH), mean atomic value (W) and MIC (10³ mol dm³) against <i>Klebsiella</i> pneumoniae ATCC 10031</th></tr> <tr><th>271281293303313323333343353363373383940142340142353144142350151253354555556157558159606161</th><th>NO2 NO2 H H NO2 H</th><th></th><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Corr Descriptor W Sv Sv Sv</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip sum of atomic van sum of atomic van sum of atomic Van sum of atomic van first Zagreb index by van Randic I connectivity index chi index first Zagreb index by van Randic I connectivity index chi index geore adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan in, M. Jadrijević-MI jadrijević-MI in, M. Jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 12 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5.235 11,701 77,09 0,699 -0,302 0,091
5.235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,441 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,776 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML - 3D correlations allow better spata an optimal selection of MDs in C. Good correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i> - Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>Piper Pit. 3D Correlation of Xande ID number (CH2), mean atomic van der Waals volume (My) and MIC (10³) mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$</th></tr>
 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{2}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara </th> <th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931
 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th> <th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th> <th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th> <th>right of the second se</th> | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031 | right of the second se | 27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 50 51 52 53 54 55 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline H \\ \hline CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2}/2 \\ \hline CH_{2}N/CH(CH_{2}OH)_{2} \\ \hline CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{3})COH \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippe eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Squared Ghose-Cripartition co squared Ghose-Crippen octan gatora abri, et al., Eur. J. fawal, R. Sohguara 26. 54.914 (J. Torrens | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 vindex 46 46 6 oder Waals volumes 5 5 5 valence vertex degrees 5 5 5 10 number 5 5 5 i-1 (Randic connectivity index 5 5 oconnectivity index 5 5 oconnectivity index 5 5 ider Waals volume 5 5 valence vertex degrees 5 5 id number 5 6 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index eigenvalue-based index topological descriptor walk and path counts molecular property molecular property <pmolecular p="" property<=""> molecular property <th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study.</th></pmolecular> | Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study. | 27 1 28 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 5 56 1 | NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H
 H H H H H H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ H $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}N(CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CCOH$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Su ZM1v CID χ1 XMOD VRA1 Su J BID MLOGP2 ALOGP2 3. USP 7,0 3. USP 7,0 4. EP11222 Su | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Sq914 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 16 windex ader Waals volumes 5 16 otder Waals volume 5 5 16 valence vertex degrees 5 5 10 number 5 5 5 5 i-1 (Randic connectivity index 5 5 5 iD number 5 5 5 5 iopp) 5 5 5 5 5 iopp) 5 6 6 6 6 iopp) | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | response to the preference of biological indices (TIs) agreement with previously
the preference of biological of the previously of the preference of biological of the previously of the previo | 2728293031323333343536373839404142434445464748495051525354555657 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 0 0 0 0 0 0 0 0 0 0 0
 0 0 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ H \\ CH_{3}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}COH) \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr S. Movr | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi incomolified Randic Type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Ghose-Crippen octan (Ic Squared Ghose-Cripartition cc Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc fabri, et al., <i>Eur. J.</i> Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 5 vindex 46,888 23 ader Waals volumes 5 5 valence vertex degrees 5 D number 5 i-1 (Randic connectivity index 5 connectivity index 5 oconnectivity index 5 iD number 5 ici (logP^2) 5 opp) 5 rippen octanol-water opp) 5 opp) 5 opp) 5 | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | right first and correlation of kande ID number (CID), mean atomic van der Waals volume (My and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$ | 272829303132333334353637383940414243444546474849505152535455565758 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0 | CH2NHCH(COOH)CH(OH)C8H5 CH2NHCH(COOH)CH(OH)C8H5 H CH2NHCH(COOH)CH(OH)22 CH2NCH(CH3)22 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2C | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Sv Se Mv State Mv Sc Mv State Mv Sc Se Mv State XMOD X1 Sc Sate MLOGP ALOGP2 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. M. Movr 193-202 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octan adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Abri, et al., <i>Eur. J.</i> fawal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free fin, M. Jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property molecular property | Figure 10. 2D Correlation of Randie ID number (CID) and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | regime 11. 3D Correlation of Rando ID number (CID), mean atomic value (W) and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int \frac{1}{\sqrt{9}} \int $ | 27 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 1 55 5 56 1 59 1 | NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H H H H H H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <td< th=""><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, <</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of value (W) and MIC (10³ mol dm³)
against <i>Klebsiella pneumoniae</i> ATCC 10031</th></td<> | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, < | 1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613
1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002) | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | regime 11. 3D Correlation of value (W) and MIC (10 ³ mol dm ³)
against <i>Klebsiella pneumoniae</i> ATCC 10031 | 27 1 28 1 30 1 31 1 32 1 32 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 45 1 44 1 45 1 50 1 51 1 52 1 54 1 55 1 56 1 57 58 59 1 60 1 | NO2 NO2 H H NO2 H | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0
 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ H \\ CH_{3}NHCH(COOH)CH(OH)_{2}H_{3} \\ CH_{3}N/CH(CH_{3})_{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}(COH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH(COH)(CH_{4}COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv ZM1v CID $\chi1$ MCOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi index modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan maxal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free in, M. Jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5.235 11.701 77,09 0,699 -0,302 0,091 5.235 11.701 77,379 1,105 0,3 0,09 0.207 14,312 92,833 2,607 2,765 7,646 2,441 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,776 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) (sconnectivity index (scaled on Carbon a | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML 3D correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | regime 11. 3D Correlation of Rando ID number (CH), mean atomic value (W) and MIC (10 ³ mol dm ³) against <i>Klebsiella</i> pneumoniae ATCC 10031 | 271281293303313323333343353363373383940142340142353144142350151253354555556157558159606161
 | NO2 NO2 H H NO2 H | | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Corr Descriptor W Sv Sv Sv | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip sum of atomic van sum of atomic van sum of atomic Van sum of atomic van first Zagreb index by van Randic I connectivity index chi index first Zagreb index by van Randic I connectivity index chi index geore adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan in, M. Jadrijević-MI jadrijević-MI in, M. Jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 12 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5.235 11,701 77,09 0,699 -0,302 0,091
5.235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,441 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,776 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML - 3D correlations allow better spata an optimal selection of MDs in C. Good correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i> - Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | Piper Pit. 3D Correlation of Xande ID number (CH2), mean atomic van der Waals volume (My) and MIC (10 ³) mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$ | | | | | | | |
 | | |
| $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{2}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH_{2}CH_{2}OH \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2})_{2} \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) \\ CH_{2}N/CH(CH_{2}) $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv Sv <th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara </th> <th>1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th> <th>5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224</th> <th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031</th> <th>right of the second se</th> | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Jose crip Sum of atomic van Sum of atomic van sum of atomic Sande Mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Id Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Squared Ghose-Crippen octan (Id Abri, et al., Eur. J. Saval, R. Sohguara

 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend
 | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Image: ATCC 10031 | right of the second se
 | | |
 | | |

 | |
 | | | | | | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | |
 | | | | | | | | | | | |
 | | | |
| 27 28 29 30 31 32 33 33 34 35 36 37 38 39 40 41 42 38 39 40 41 42 43 50 51 52 53 54 55 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{4}H_{5} \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline H \\ \hline CH_{2}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2}/2 \\ \hline CH_{2}N/CH(CH_{2}OH)_{2} \\ \hline CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{2}CH_{2}OH) \\ \hline CH_{2}N(CH(CH_{3})_{2}/2 \\ \hline CH_{2}N(CH(CH_{3})COH \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}COH) \\ \hline CH_{2}N(CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_{2}COH \\ \hline CH_{2}N(CH_{2}CH_$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippe eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Squared Ghose-Cripartition co squared Ghose-Crippen octan gatora abri, et al., Eur. J. fawal, R. Sohguara 26. 54.914 (J. Torrens | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name 5 5 5 vindex 46 46 6 oder Waals volumes 5 5 5 valence vertex degrees 5 5 5 10 number 5 5 5 i-1 (Randic connectivity index 5 5 oconnectivity index 5 5 oconnectivity index 5 5 ider Waals volume 5 5 valence vertex degrees 5 5 id number 5 6 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index eigenvalue-based index topological descriptor walk and path counts molecular property molecular property <pmolecular p="" property<=""> molecular property <th>Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031</th><th>response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference
of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study.</th></pmolecular> | Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | response to the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological indices (TIs) agreement with previously the preference of biological (W, ZMIV1,), and to provide QSAR study. | | |

 |
 | | | | | | | | | | | |
 | | | | | |
 | | | | | | | |
 | | | | | | | | | | | |
 | | | | | | |
 | | |
 | | | | | | | | |
 | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | |
 |
| 27 1 28 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 37 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 5 56 1 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ H $CH_{n}NHCH(COOH)CH(OH)C_{n}H_{n}$ $CH_{n}NHCH(COOH)CH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}NCH(CH_{n})/2$ $CH_{n}N(CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CH_{n}CCH_{n}CCH_{n}CCH_{n}CCH_{n}CH_{n}CCOH$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Su ZM1v CID χ1 XMOD VRA1 Su J BID MLOGP2 ALOGP2 3. USP 7,0 3. USP 7,0 4. EP11222 Su
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Sq914 | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 16 windex ader Waals volumes 5 16 otder Waals volume 5 5 16 valence vertex degrees 5 5 10 number 5 5 5 5 i-1 (Randic connectivity index 5 5 5 iD number 5 5 5 5 iopp) 5 5 5 5 5 iopp) 5 6 6 6 6 iopp)
 | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randie ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | response to the preference of biological indices (TIs) agreement with previously
the preference of biological of the previously of the preference of biological of the previously of the previo | | |

 |
 | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | |
 | | | | | | | | | | |
 | | | | | | |
 | | | |
 | | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | |
 |
| 2728293031323333343536373839404142434445464748495051525354555657 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{0}H_{2} \\ H \\ CH_{3}NHCH(COOH)CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{3})_{2} \\ CH_{2}N/CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}CH_{2}COH) \\ CH_{2}N(CH_{2}COH) \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv ZM1v CID χ1 XMOD VRA1 J BID MLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr S. Movr
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by van Randic I connectivity index chi incomolified Randic Type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Ghose-Crippen octan (Ic Squared Ghose-Cripartition cc Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc fabri, et al., <i>Eur. J.</i> Squared Ghose-Cripartition cc adjacen Squared Ghose-Cripartition cc | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 16 otor name 5 5 5 vindex 46,888 23 ader Waals volumes 5 5 valence vertex degrees 5 D number 5 i-1 (Randic connectivity index 5 connectivity index 5 oconnectivity index 5 iD number 5 ici (logP^2) 5 opp) 5 rippen octanol-water opp) 5 opp) 5 opp) 5 | 5,235 11,701 77,09 0,699 -0,302 0,091
5,235 11,701 77,379 1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,491 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,726 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC
(10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | right first and correlation of kande ID number (CID), mean atomic van der Waals volume (My and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$ | | |

 | |
 | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | |
 | | |
 | | | | | | |
 | | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | |
| 272829303132333334353637383940414243444546474849505152535455565758 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | CH2NHCH(COOH)CH(OH)C8H5 CH2NHCH(COOH)CH(OH)C8H5 H CH2NHCH(COOH)CH(OH)22 CH2NCH(CH3)22 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2C)2 CH2NCH(CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2CH2C | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv Sv Se Mv Sv Se Mv State Mv Sc Mv State Mv Sc Se Mv State XMOD X1 Sc Sate MLOGP ALOGP2 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. USP 7,0 S. M. Movr 193-202
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van Sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi ind modified Randic Randic I Ghose-Crippen octan adjacen Balaban distance Balaban Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Squared Ghose-Crippen octan (Ic Abri, et al., <i>Eur. J.</i> fawal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free fin, M. Jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend 5 5 5 otor name
 | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor constitutional descriptor (scaled on Carbon atom) constitutional descriptor (scaled on Carbon atom) constitutional descriptor constitutional descriptor (scaled on Carbon atom) connectivity index connectivity index connectivity index connectivity index eigenvalue-based index molecular property molecular property molecular property molecular property | Figure 10. 2D Correlation of Randie ID number (CID) and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031 | regime 11. 3D Correlation of Rando ID number (CID), mean atomic value (W) and MIC (10 ³ mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int \frac{1}{\sqrt{9}} \int $ | | |

 | |
 | | | | | | | | | | | |
 | | | | | | |
 | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | |
 | | |
 | | | | | | |
 | | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | |
| 27 1 29 1 30 1 31 1 32 1 33 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 42 1 43 1 44 1 45 1 46 1 47 1 48 1 49 1 50 1 51 1 52 1 53 1 54 1 55 5 56 1 59 1 | NO2 NO2 H H NO2 H H H H H H H H H H H H H H H H H H H H H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 0 <td< th=""><th>$\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$</th><th>54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT</th><th>39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, <</th><th>1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend </th><th>5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)</th><th> Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. </th><th>regime 11. 3D Correlation of value (W) and MIC (10³ mol dm³)
against <i>Klebsiella
pneumoniae</i> ATCC 10031</th></td<>

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{2} \\ H \\ CH_{2}NCH(CH(OOH)CH(OH)_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}NCH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{3})/_{2} \\ CH_{2}N(CH(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}CH_{2}OH)_{2} \\ CH_{2}N(CH_{2}COH \\ CH_{2}N(CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}COOH \\ CH_{2}NHCH(COOH)CH_{2}OOH \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ H \\ CH_{2}NHCH(CH_{2})_{3}OOH \\ CH_{2}NHCH(CH_{2})_{3}OO$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Se Mv SE Mv State $\chi 1$ XMOD $\chi 1$ SMLOGP2 ALOGP2 3. USP 7,0 4. EP11222 5. M. MOVT 193-202 6. M. MOVT
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 muted molecular desc Descrip wiener sum of atomic van sum of atomic sande mean atomic van first Zagreb index by van Randic I connectivity index chi ind modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC Squared Ghose-Crippen octan (IC fin, M. Jadrijević-MI (IC staf, R. Sohguara 26. 56,914 (J. Torrens, < | 1530 2,011 49,466 25 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5,235 11,701 77,09 0,699 -0,302 0,091 5,235 11,701 77,379 1,105 0,3 0,09 0,207 14,312 92,833 2,607 2,765 7,646 2,491 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,726 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) constitutional descriptor walk and path counts connectivity index connectivity index eigenvalue-based index itopological descriptor walk and path counts molecular property molecular property molecular property molecular property molecular property McCoorg. Med. Chem. 10 (2002)
 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 figure 12. 3D Correlation of sum of atomic van der Waals volumes (Sv), first Zagreb index by valence vertex degrees (ZM1V) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML, 3D correlations in this QSAR constitutional (Sv, Mv), topologia and pipophylicity (AlogP) descrip (MIC) against <i>Staphylococccus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | regime 11. 3D Correlation of value (W) and MIC (10 ³ mol dm ³)
against <i>Klebsiella pneumoniae</i> ATCC 10031 | | |

 |
 | | | | | | | | | | | |
 | | | | | |
 | | | | | | | | | |
 | | | | | | | | | |
 | | | | | | | | |
 | | |
 | | | | | | |
 | | | |
 | | | | | | | | | | | |
 | | | | | | | | | | |
 |
| 27 1 28 1 30 1 31 1 32 1 32 1 33 1 34 1 35 1 36 1 36 1 37 1 36 1 37 1 38 1 39 1 40 1 41 1 42 1 43 1 44 1 45 1 44 1 45 1 50 1 51 1 52 1 54 1 55 1 56 1 57 58 59 1 60 1 | NO2 NO2 H H NO2 H
 | 0 0 NNHCSNH2 NNHCSNH2 0 0 0 0 0 NNHCSNH2 0 NNHCSNH2 NNHCSNH2 NNHCSNH2 0

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ CH_{2}NHCH(COOH)CH(OH)C_{8}H_{3} \\ H \\ CH_{3}NHCH(COOH)CH(OH)_{2}H_{3} \\ CH_{3}N/CH(CH_{3})_{2} \\ CH_{3}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH) \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH_{2}CH_{2}OH)_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{3})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}/_{2} \\ CH_{4}N(CH(CH_{4})_{2}(COH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH_{4}COOH) \\ CH_{4}N(CH(COH)(CH_{4}COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ CH_{4}N(CH(CH_{4})(COOH) \\ \\ \end{array}$ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Com Descriptor W Sv Sv Se Mv Se Mv ZM1v CID $\chi1$ MCOGP ALOGP2 3. USP 7,0 4. EP11222 5. M. Movr 193-202 6. M. Movr 7. Talete st
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip Sum of atomic van sum of atomic van sum of atomic Sande mean atomic van first Zagreb index by var Randic I connectivity index chi index modified Randic Randic I Randic-type eigenve adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan maxal, R. Sohguara 26. 56,914 (J. Torrens, 245, http://www.free in, M. Jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 14 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5.235 11.701 77,09 0,699 -0,302 0,091 5.235 11.701 77,379 1,105 0,3 0,09
0.207 14,312 92,833 2,607 2,765 7,646 2,441 5,771 37,005 1,384 1,212 1,469 8,312 8,592 55,671 1,519 0,702 0,493 4,414 6,809 43,713 1,776 1,052 1,107 6,349 7,665 51,874 1,277 1,331 1,771 3,264 11,08 71,703 2,696 2,927 8,568 5,388 7,075 46,73 1,431 1,106 1,224 Descriptor type topological descriptor (scaled on Carbon atom) (sconnectivity index (scaled on Carbon a | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10³ mol dm³) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML 3D correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i>. Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | regime 11. 3D Correlation of Rando ID number (CH), mean atomic value (W) and MIC (10 ³ mol dm ³) against <i>Klebsiella</i> pneumoniae ATCC 10031 | | |

 |
 | |
 | | | | | | | | | | | | | |
 | | | | | |
 | | | | | | | | | | | |
 | | | | | | | |
 | | | |
 | | | | | | |
 | | |
 | | | | | | | | | | | |
 | | | | | | | | | | | | | |
 |
| 271281293303313323333343353363373383940142340142353144142350151253354555556157558159606161 | NO2 NO2 H H NO2 H
 |

 | $\begin{array}{c} CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ \hline \\ CH_{2}NHCH(COOH)CH(OH)C_{6}H_{5} \\ H \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ CH_{2}NCH(CH_{3})/_{2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $ | 54 23,46 55 22,98 56 30,74 57 11,72 58 17,94 59 14,8 60 16,28 61 22,93 62 13,14 Table 4. Corr Descriptor W Sv Sv Sv
 | 39,56 0,63 508 38,79 0,64 524 49,88 0,64 538 17,85 0,69 224 29,37 0,64 334 23,61 0,64 230 24,91 0,68 254,44 35,48 0,67 422 20,72 0,69 328 puted molecular desc Descrip sum of atomic van sum of atomic van sum of atomic Van sum of atomic van first Zagreb index by van Randic I connectivity index chi index first Zagreb index by van Randic I connectivity index chi index geore adjacen Balaban distance Balaban Moriguchi octanol-wat Ghose-Crippen octan Moriguchi octanol-wat Ghose-Crippen octan in, M. Jadrijević-MI jadrijević-MI in, M. Jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI jadrijević-MI | 1530 2,011 49,466 25 1530 2,011 49,466 25 2556 1,638 60,439 30 179 2,015 24,352 12 613 1,931 36,073 18 286 1,991 28,394 12 436 1,92 32,235 16 1188 1,623 46,888 23 348 1,996 30,065 15 criptors' legend | 5.235 11,701 77,09 0,699 -0,302 0,091
5.235 11,701 77,379
1,105 0,3 0,09
0,207 14,312 92,833 2,607 2,765 7,646
2,441 5,771 37,005 1,384 1,212 1,469
8,312 8,592 55,671 1,519 0,702 0,493
4,414 6,809 43,713 1,776 1,052 1,107
6,349 7,665 51,874 1,277 1,331 1,771
3,264 11,08 71,703 2,696 2,927 8,568
5,388 7,075 46,73 1,431 1,106 1,224 | Figure 10. 2D Correlation of Randic ID number (CID) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i> ATCC 10031 Figure 12. 3D Correlation of sum of atomic van der Waals volumes (SV), first Zagreb index by valence vertex degrees (ZMV) and MIC (10.3 mol dm.3) against <i>Klebsiella pneumoniae</i>, ATCC 10031 CONCLUSIONS Previous 2D QSAR results hav between antimicrobial activity (M. Present 2D results are in good obtained. 3D QSAR correlations indicate activity prediction on the basis of influence on particular system, a constitutional (Sv, Se,), topolo molecular properties (AlogP, ML - 3D correlations allow better spata an optimal selection of MDs in C. Good correlations in this QSAR constitutional (Sv, Mv), topologic and lipophylicity (AlogP) descript (MIC) against <i>Staphylococcus a</i> - Suggested method can be used chemical properties and/or bioloc searching for new lead compounds. | Piper Pit. 3D Correlation of Xande ID number (CH2), mean atomic van der Waals volume (My) and MIC (10 ³) mol dm ³) against <i>Klebsiella pneumoniae</i> ATCC 10031
$\int_{0}^{0} \int_{0}^{0} \int_{$ | | |

 |
 | | | | | | | | | | | | |
 | | | | | |
 | | | | | | | | |
 | | | | | | | | | | |
 | | | | | | | |
 | | |
 | | | | | | | |
 | | |
 | | | | | | | | | | | | |
 | | | | | | | | | | |
 |