

**Table 3. Experimental and predicted MIC ( $\mu\text{g/mL}$ ) values of training set and test set molecules based on atom based 3D-QSAR model (Antibacterial activity).**

<b>Compound code</b>	<b><i>B.subtilis</i> MIC (<math>\mu\text{g/mL}</math>)</b>	<b>Experimental <math>-\log(\text{MIC})</math></b>	<b>Predicted <math>-\log(\text{MIC})</math> (Training set)</b>	<b>Predicted <math>-\log(\text{MIC})</math> (Test set)</b>
A1	32	-1.505	-1.74	
A2	256	-2.408	-2.11	
A3	16	-1.204	-1.19	
A4	64	-1.806		-1.31
A5	32	-1.505	-1.50	
A6	16	-1.204	-1.29	
A7	256	-2.408	-2.44	
A8	128	-2.107		-2.17
A9	64	-1.806	-1.71	
A10	256	-2.408	-2.34	
A11	128	-2.107	-2.07	
A12	128	-2.107	-2.10	
A13	256	-2.408	-2.47	
A14	128	-2.107		-2.35
A15	64	-1.806		-1.83
A16	64	-1.806		-1.93
A17	64	-1.806	-1.71	
A18	128	-2.107	-2.05	
A19	128	-2.107	-2.06	
A20	64	-1.806		-2.04
A21	256	-2.408	-2.50	
A22	128	-2.107		-2.03
A23	256	-2.408	-2.43	
A24	264	-2.422	-2.48	
A25	64	-1.806	-1.95	

**Table 4. Experimental and predicted MIC ( $\mu\text{g/mL}$ ) values of training set and test set molecules based on atom based 3D-QSAR model (Antibacterial activity).**

<b>Compound code</b>	<b><i>S. aureus</i> MIC (<math>\mu\text{g/mL}</math>)</b>	<b>Experimental <math>-\log(\text{MIC})</math></b>	<b>Predicted <math>-\log(\text{MIC})</math> (Training set)</b>	<b>Predicted <math>-\log(\text{MIC})</math> (Test set)</b>
A1	32	-1.50515	-1.55	
A2	128	-2.10721	-1.94	
A3	16	-1.20412	-1.26	
A4	64	-1.80618	-1.78	
A5	32	-1.50515	-1.71	
A6	16	-1.20412	-1.26	
A7	128	-2.10721		-2.2
A8	128	-2.10721	-1.91	
A9	64	-1.80618		-1.95
A10	256	-2.40824	-2.27	
A11	64	-1.80618	-1.71	
A12	128	-2.10721		-2.02
A13	128	-2.10721		-2.28
A14	128	-2.10721	-2.08	
A15	128	-2.10721	-2.18	
A16	128	-2.10721		-1.95
A17	128	-2.10721	-2.04	
A18	256	-2.40824	-2.5	
A19	256	-2.40824	-2.48	
A20	128	-2.10721		-2.05
A21	256	-2.40824	-2.43	
A22	256	-2.40824	-2.33	
A23	128	-2.10721		-2.25
A24	128	-2.10721	-2.3	
A25	64	-1.80618		-1.55

**Table 5. Experimental and predicted MIC ( $\mu\text{g/mL}$ ) values of training set and test set molecules based on atom based 3D-QSAR model (Antibacterial activity).**

<b>Compound code</b>	<b><i>E. coli</i> MIC (<math>\mu\text{g/mL}</math>)</b>	<b>Experimental <math>-\log(\text{MIC})</math></b>	<b>Predicted <math>-\log(\text{MIC})</math> (Training set)</b>	<b>Predicted <math>-\log(\text{MIC})</math> (Test set)</b>
A1	64	-1.806	-1.82	
A2	128	-2.107	-2.37	
A3	16	-1.204		-1.42
A4	128	-2.107	-1.99	
A5	64	-1.806	-1.76	
A6	16	-1.204	-1.50	
A7	256	-2.408		-2.64
A8	128	-2.107		-2.32
A9	64	-1.806	-1.75	
A10	128	-2.107	-2.34	
A11	64	-1.806		-1.78
A12	256	-2.408	-2.26	
A13	256	-2.408	-2.35	
A14	128	-2.107	-2.31	
A15	64	-1.806		-1.71
A16	128	-2.107	-2.12	
A17	128	-2.107	-1.86	
A18	128	-2.107		-2.46
A19	256	-2.408	-2.28	
A20	64	-1.806	-1.75	
A21	64	-1.806	-1.79	
A22	128	-2.107		-2.32
A23	128	-2.107		-2.29
A24	64	-1.806	-1.92	
A25	32	-1.505	-1.43	

**Table 6. Experimental and predicted MIC ( $\mu\text{g/mL}$ ) values of training set and test set molecules based on atom based 3D-QSAR model (Antibacterial activity).**

<b>Compound code</b>	<b><i>P. vulgaris</i> MIC (<math>\mu\text{g/mL}</math>)</b>	<b>Experimental <math>-\log(\text{MIC})</math></b>	<b>Predicted <math>-\log(\text{MIC})</math> (Training set)</b>	<b>Predicted <math>-\log(\text{MIC})</math> (Test set)</b>
A1	64	-1.806		-1.826
A2	128	-2.107		-2.35
A3	16	-1.204	-1.48	
A4	128	-2.107	-1.95	
A5	64	-1.806	-1.78	
A6	16	-1.204	-1.52	
A7	256	-2.408	-2.22	
A8	128	-2.107		-2.21
A9	64	-1.806	-1.75	
A10	256	-2.408	-2.48	
A11	128	-2.107	-2.31	
A12	128	-2.107		-2.31
A13	128	-2.107		-2.39
A14	256	-2.408	-2.38	
A15	128	-2.107	-2.21	
A16	64	-1.806	-1.75	
A17	64	-1.806	-1.89	
A18	256	-2.408	-2.46	
A19	256	-2.408	-2.26	
A20	128	-2.107	-2.15	
A21	64	-1.806		-1.86
A22	128	-2.107	-2.18	
A23	256	-2.408		-2.28
A24	64	-1.806		-1.69
A25	32	-1.505	-1.68	

**Table 7. Experimental and predicted MIC ( $\mu\text{g/mL}$ ) values of training set and test set molecules based on atom based 3D-QSAR model (Antifungal activity).**

<b>Compound code</b>	<b><i>A. niger</i> MIC (<math>\mu\text{g/mL}</math>)</b>	<b>Experimental <math>-\log(\text{MIC})</math></b>	<b>Predicted <math>-\log(\text{MIC})</math> (Training set)</b>	<b>Predicted <math>-\log(\text{MIC})</math> (Test set)</b>
A1	32	-1.505	-1.51	
A2	256	-2.408	-2.42	
A3	16	-1.204	-1.21	
A4	64	-1.806		-1.44
A5	16	-1.204	-1.21	
A6	16	-1.204	-1.19	
A7	128	-2.107	-2.08	
A8	64	-1.806		-1.64
A9	128	-2.107	-2.02	
A10	128	-2.107	-2.16	
A11	64	-1.806	-1.81	
A12	32	-1.505	-1.50	
A13	64	-1.806		-1.35
A14	32	-1.505	-1.55	
A15	32	-1.505	-1.47	
A16	64	-1.806		-1.51
A17	32	-1.505	-1.56	
A18	64	-1.806		-1.44
A19	32	-1.505	-1.49	
A20	64	-1.806		-1.54
A21	64	-1.806		-2.18
A22	32	-1.505	-1.51	
A23	128	-2.107	-2.14	
A24	64	-1.806	-1.78	
A25	64	-1.806		-1.56

**Table 8. Experimental and predicted MIC ( $\mu\text{g/mL}$ ) values of training set and test set molecules based on atom based 3D-QSAR model (Antifungal activity).**

<b>Compound code</b>	<b><i>C. tropicalis</i> MIC (<math>\mu\text{g/mL}</math>)</b>	<b>Experimental <math>-\log(\text{MIC})</math></b>	<b>Predicted <math>-\log(\text{MIC})</math> (Training set)</b>	<b>Predicted <math>-\log(\text{MIC})</math> (Test set)</b>
A1	64	-1.806	-1.959	
A2	256	-2.408	-2.52	
A3	16	-1.204		-1.31
A4	64	-1.806		-1.99
A5	32	-1.505	-1.47	
A6	16	-1.204	-1.31	
A7	64	-1.806	-1.99	
A8	128	-2.107		-2.32
A9	128	-2.107	-2.35	
A10	64	-1.806		-1.68
A11	64	-1.806	-2.01	
A12	16	-1.204	-1.46	
A13	128	-2.107	-2.36	
A14	32	-1.505	-1.45	
A15	64	-1.806	-2.04	
A16	128	-2.107	-2.25	
A17	16	-1.204	-1.42	
A18	32	-1.505		-1.59
A19	64	-1.806	-1.93	
A20	32	-1.505	-1.64	
A21	128	-2.107		-2.34
A22	32	-1.505	-1.45	
A23	64	-1.806		-1.98
A24	32	-1.505	-1.45	
A25	32	-1.505		-1.72