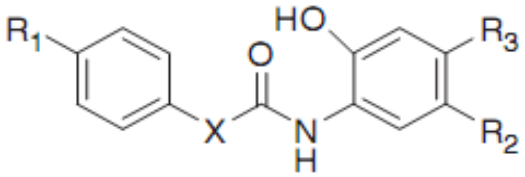
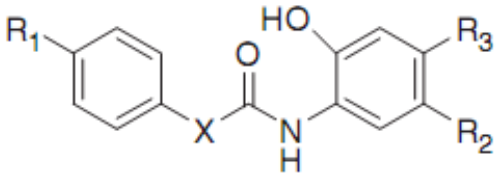

QSAR APPLICATION

Table 2. Training set of compounds, biological activity and parameters used in Equation (1).

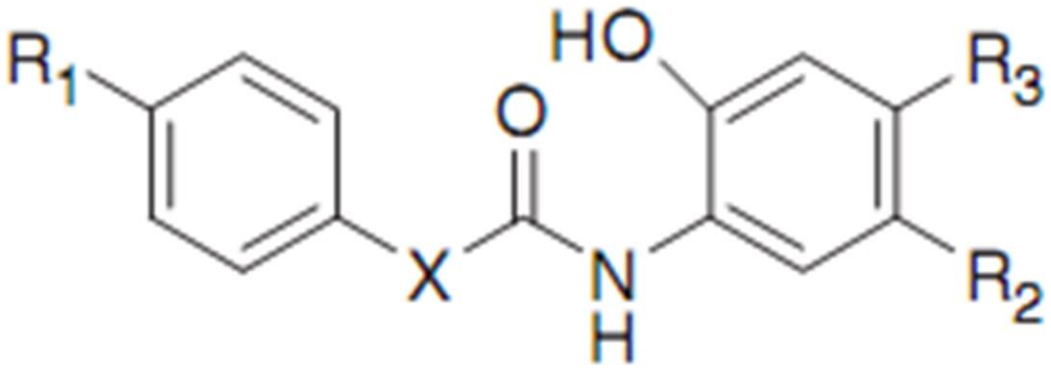


Comp. Nos	R_1	R_2	R_3	X	*MIC* $\mu g\,ml^{-1}$	*Ix*	σR_3	$B1_{R1}$
1	$C(CH_3)_3$	H	NO_2	–	1.95	0	0.78	2.59
2	H	H	NO_2	–	125	0	0.78	1
5	H	NO_2	H	–	15.6	0	0	1
6	C_2H_5	NO_2	H	–	7.8	0	0	1.52
7	F	NO_2	H	–	15.6	0	0	1.35
8	Br	H	NO_2	CH_2	125	1	0.78	1.95
9	Cl	H	NO_2	CH_2	125	1	0.78	1.80
12	CH_3	NO_2	H	CH_2	125	1	0	1.52
15	H	H	NH_2	–	15.6	0	−0.66	1
16	F	H	NH_2	–	15.6	0	−0.66	1.35
18	C_2H_5	H	NH_2	–	7.8	0	−0.66	1.52
19	H	NH_2	H	–	31.25	0	0	1
20	C_2H_5	NH_2	H	–	15.6	0	0	1.52
21	F	NH_2	H	–	15.6	0	0	1.35
22	Br	H	NH_2	CH_2	31.25	1	−0.66	1.95
23	Cl	H	NH_2	CH_2	31.25	1	−0.66	1.80
24	CH_3	H	NH_2	CH_2	62.5	1	−0.66	1.52
25	F	H	NH_2	CH_2	62.5	1	−0.66	1.35
26	CH_3	NH_2	H	CH_2	62.5	1	0	1.52

Table 2. Training set of compounds, biological activity and parameters used in Equation (1).



Comp. Nos	R_1	R_2	R_3	X	*MIC* $\mu g\,ml^{-1}$	*Ix*	σR_3	$B1_{R1}$	*Observed log 1/C*
1	$C(CH_3)_3$	H	NO_2	–	1.95	0	0.78	2.59	5.207
2	H	H	NO_2	–	125	0	0.78	1	3.315
5	H	NO_2	H	–	15.6	0	0	1	4.219
6	C_2H_5	NO_2	H	–	7.8	0	0	1.52	4.563
7	F	NO_2	H	–	15.6	0	0	1.35	4.248
8	Br	H	NO_2	CH_2	125	1	0.78	1.95	3.448
9	Cl	H	NO_2	CH_2	125	1	0.78	1.80	3.389
12	CH_3	NO_2	H	CH_2	125	1	0	1.52	3.360
15	H	H	NH_2	–	15.6	0	−0.66	1	4.165
16	F	H	NH_2	–	15.6	0	−0.66	1.35	4.198
18	C_2H_5	H	NH_2	–	7.8	0	−0.66	1.52	4.516
19	H	NH_2	H	–	31.25	0	0	1	3.863
20	C_2H_5	NH_2	H	–	15.6	0	0	1.52	4.215
21	F	NH_2	H	–	15.6	0	0	1.35	4.198
22	Br	H	NH_2	CH_2	31.25	1	−0.66	1.95	4.012
23	Cl	H	NH_2	CH_2	31.25	1	−0.66	1.80	3.946
24	CH_3	H	NH_2	CH_2	62.5	1	−0.66	1.52	3.612
25	F	H	NH_2	CH_2	62.5	1	−0.66	1.35	3.619
26	CH_3	NH_2	H	CH_2	62.5	1	0	1.52	3.612

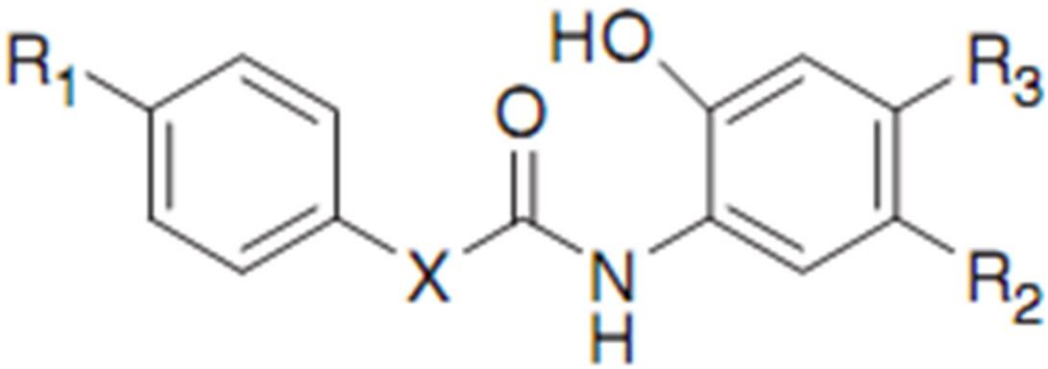


$$\log\ 1/C = 2{,}92 + 0{,}951\ B1R_1 - 0{,}937\ Ix - 0{,}372\ \sigma R_3$$

$R^2 = 0{,}90$ $S = 0{,}165$

Table 4. Observed and calculated log $1/C$ values with residuals obtained from Equation (1).

Comp. Nos	*Observed log 1/C*	*Predicted log 1/C*	*Residuals*
1	5.207	5.091	0.116
2	3.315	3.578	−0.263
5	4.219	3.869	0.350
6	4.563	4.363	0.200
7	4.248	4.202	0.046
8	3.448	3.544	−0.096
9	3.389	3.402	−0.013
12	3.360	3.426	−0.066
15	4.165	4.114	0.051
16	4.198	4.447	−0.249
18	4.516	4.609	−0.093
19	3.863	3.869	−0.006
20	4.215	4.363	−0.148
21	4.198	4.202	−0.004
22	4.012	4.081	−0.069
23	3.946	3.938	0.008
24	3.612	3.672	−0.060
25	3.619	3.510	0.109
26	3.612	3.426	0.186



$$\log\ 1/C = 2{,}92 + 0{,}951\ B1R_1 - 0{,}937\ Ix - 0{,}372\ \sigma R_3$$

Design a new molecule that you think has a high biological activity.