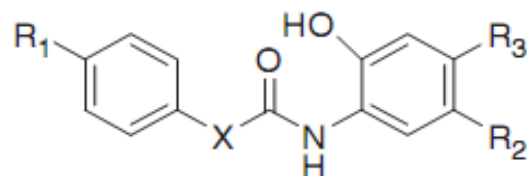


A laboratory setting featuring various pieces of glassware. In the foreground, there are several beakers and flasks containing liquids of different colors: blue, orange, yellow, and green. A large graduated cylinder on the right contains a dark orange liquid. In the background, a large flask contains a red liquid. The scene is lit with dramatic, low-key lighting, creating strong highlights and deep shadows. A red banner with white text is overlaid across the middle of the image.

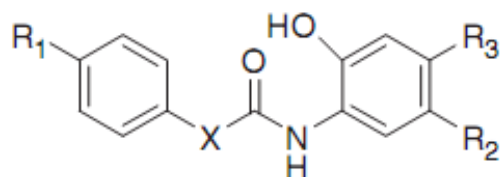
# QSAR APPLICATION

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

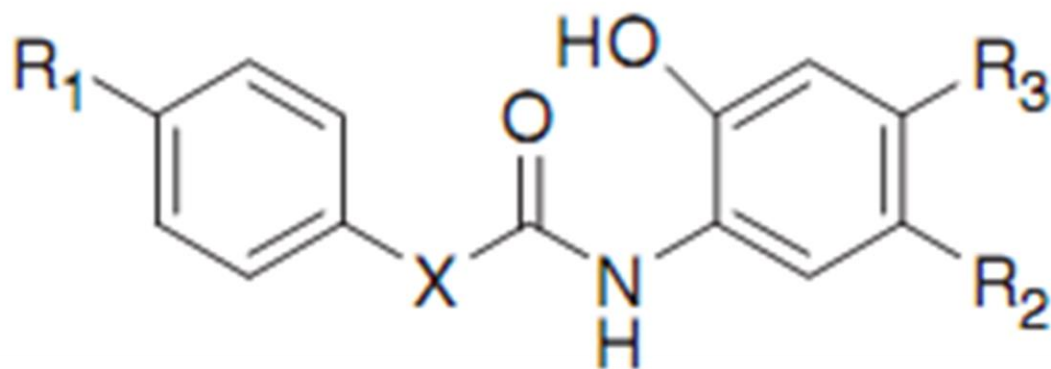


Comp. Nos	$R_1$	$R_2$	$R_3$	X	MIC $\mu\text{g ml}^{-1}$	$I_x$	$\sigma R_3$	$BI_{R1}$
1	C(CH <sub>3</sub> ) <sub>3</sub>	H	NO <sub>2</sub>	–	1.95	0	0.78	2.59
2	H	H	NO <sub>2</sub>	–	125	0	0.78	1
5	H	NO <sub>2</sub>	H	–	15.6	0	0	1
6	C <sub>2</sub> H <sub>5</sub>	NO <sub>2</sub>	H	–	7.8	0	0	1.52
7	F	NO <sub>2</sub>	H	–	15.6	0	0	1.35
8	Br	H	NO <sub>2</sub>	CH <sub>2</sub>	125	1	0.78	1.95
9	Cl	H	NO <sub>2</sub>	CH <sub>2</sub>	125	1	0.78	1.80
12	CH <sub>3</sub>	NO <sub>2</sub>	H	CH <sub>2</sub>	125	1	0	1.52
15	H	H	NH <sub>2</sub>	–	15.6	0	–0.66	1
16	F	H	NH <sub>2</sub>	–	15.6	0	–0.66	1.35
18	C <sub>2</sub> H <sub>5</sub>	H	NH <sub>2</sub>	–	7.8	0	–0.66	1.52
19	H	NH <sub>2</sub>	H	–	31.25	0	0	1
20	C <sub>2</sub> H <sub>5</sub>	NH <sub>2</sub>	H	–	15.6	0	0	1.52
21	F	NH <sub>2</sub>	H	–	15.6	0	0	1.35
22	Br	H	NH <sub>2</sub>	CH <sub>2</sub>	31.25	1	–0.66	1.95
23	Cl	H	NH <sub>2</sub>	CH <sub>2</sub>	31.25	1	–0.66	1.80
24	CH <sub>3</sub>	H	NH <sub>2</sub>	CH <sub>2</sub>	62.5	1	–0.66	1.52
25	F	H	NH <sub>2</sub>	CH <sub>2</sub>	62.5	1	–0.66	1.35
26	CH <sub>3</sub>	NH <sub>2</sub>	H	CH <sub>2</sub>	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	$MIC$ $\mu g ml^{-1}$	$I_x$	$\sigma R_3$	$BI_{R1}$	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



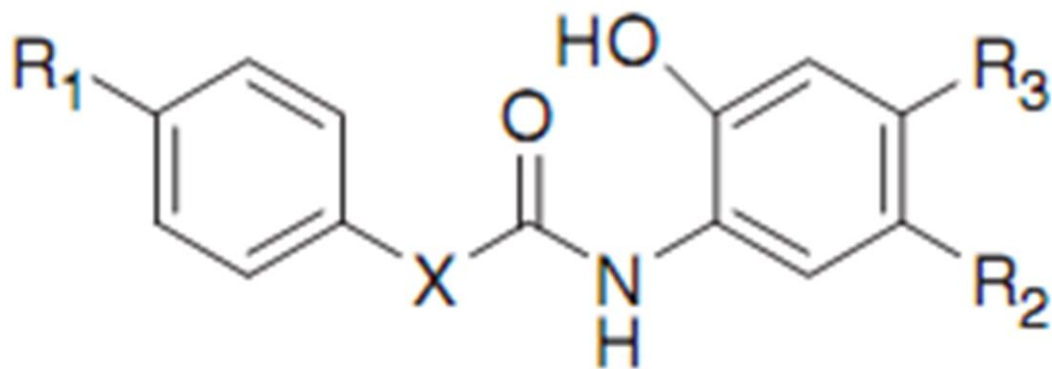
$$\log 1/C = 2,92 + 0,951 B1R_1 - 0,937 I_x - 0,372 \sigma R_3$$

$$R^2 = 0,90 \quad S = 0,165$$



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

<i>Comp. Nos</i>	<i>Observed <math>\log 1/C</math></i>	<i>Predicted <math>\log 1/C</math></i>	<i>Residuals</i>
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



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

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