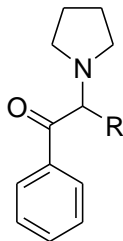


**Table S1.** pIC<sub>50</sub> values, volume, and  $\pi$  values used in the QSAR investigation.



R	pIC <sub>50</sub> DAT	Volume (Å <sup>3</sup> )	Lipophilicity ( $\pi$ ) <sup>a</sup>
-H	5.49	175.39	0
-CH <sub>3</sub>	6.70	189.05	0.46
-CH <sub>2</sub> CH <sub>3</sub>	7.20	211.61	1.02
-CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	7.74	229.00	1.55
-CH(CH <sub>3</sub> ) <sub>2</sub>	7.04	231.20	1.53
-CH <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	7.92	246.19	2.13
-C <sub>5</sub> H <sub>9</sub>	7.77	253.22	2.14
-C <sub>6</sub> H <sub>11</sub>	8.10	270.47	2.82

<sup>a</sup> Hansch, C.; Leo, A.; Unger, S. H.; Kim, K. H.; Nikaitani, D.; Lien, E. J. (1973) "Aromatic" substituent constants for structure-activity correlations. *J. Med. Chem.* 16, 1207–1216.