

Target Name	Histamine H1 receptor
Target TTD ID	TTDS00086

Target Species	Rat
Target Location	Brain
Chemical Type	Phenylaminotetralines
Mode of Action	Binder
QSAR Model 1	$pK_{0.5} = -20.5562 (\pm 2.6662)MRI + 1.8364 (\pm 0.1917)Ip_1 + 12.2214$ $n = 26, Se = 0.4621, R_A^2 = 0.8192, R = 0.9130, F = 56.621$
QSAR Model 2	$pK_{0.5} = -20.7518 (\pm 2.7753)MRI + 1.9821 (\pm 0.2185)Ip_1 - 0.3822 (\pm 0.2890)Ip_2 + 12.5220$ $n = 26, Se = 0.4547, R_A^2 = 0.8249, R = 0.9197, F = 40.247,$
QSAR Model 3	$pK_{0.5} = -19.2614 (\pm 2.9358)MRI + 1.7606 (\pm 0.2045)Ip_1 + 0.2958 (\pm 0.2831)Ip_3 + 11.8731$ $n = 26, Se = 0.4612, R_A^2 = 0.8199, R = 0.9173, F = 38.928$
QSAR model 4	$pK_{0.5} = -22.2297 (\pm 2.7997)MRI + 1.7591 (\pm 0.1925)Ip_1 - 0.3789 (\pm 0.2426)Ip_4 + 12.9920$ $n = 26, Se = 0.4482, R_A^2 = 0.8298, R = 0.9221, F = 41.632$
Molecular description	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p>Negentropy(N), molecular redundancy index (MRI), first-order valence connectivity index (<math>{}^1\chi^v</math>),</p>

	Wiener (W), and Szeged (Sz) indices.
Reference	QSAR Study on Competition Binding of Rodenticides (PATs) to H1 Receptor in Rat and Guinea Pig Brain. <i>Bioorganic &amp; Medicinal Chemistry</i> 10 (2002) 2913–2918

Target Species	Guinea pig
Target Location	Brain
Chemical Type	Phenylaminotetralines
Mode of Action	Binder
QSAR Model 1	$pK_{0.5} = -20.5562 (\pm 2.6662)MRI + 1.8364 (\pm 0.1917)Ip_1 + 12.2214$ $n = 26, Se = 0.4621, R_A^2 = 0.8192, R = 0.9130, F = 56.621$
QSAR Model 2	$pK_{0.5} = -20.7518 (\pm 2.7753)MRI + 1.9821 (\pm 0.2185)Ip_1 - 0.3822 (\pm 0.2890)Ip_2 + 12.5220$ $n = 26, Se = 0.4547, R_A^2 = 0.8249, R = 0.9197, F = 40.247,$
QSAR Model 3	$pK_{0.5} = -19.2614 (\pm 2.9358)MRI + 1.7606 (\pm 0.2045)Ip_1 + 0.2958 (\pm 0.2831)Ip_3 + 11.8731$ $n = 26, Se = 0.4612, R_A^2 = 0.8199, R = 0.9173, F = 38.928$
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Molecular description	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p>Negentropy(N), molecular redundancy index (MRI), first-order valence connectivity index (<math>{}^1\chi^v</math>), Wiener (W), and Szeged (Sz) indices.</p>

<b>Reference</b>	QSAR Study on Competition Binding of Rodenticides (PATs) to H1 Receptor in Rat and Guinea Pig Brain. <i>Bioorganic &amp; Medicinal Chemistry</i> 10 (2002) 2913–2918
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