Target Name	Adenosine A_3 receptor
Target TTD ID	TTDS00189

Target Species	Human
Chemical Type	Thiazole derivatives
Mode of Action	Antagonist
Activity Type	Adenosine A_3 binding affinity
QSAR Model 1	$\mathrm{p}K_\mathrm{i} = -3.951(\pm2.415)q_2 - 2.623(\pm2.136)q_5 + 2.441(\pm1.489)q_7 - 0.275(\pm0.261)\log P$ $- 1.498(\pm0.763)I_{\mathrm{OBu\_t}} + 0.895(\pm0.614)I_{\mathrm{Me\_Et}} + 4.030$ $n = 30,\quad R_a^2 = 0.744,\ R^2 = 0.797,\ R = 0.893,\ F = 15.0(\mathrm{df}6, 23),\ s = 0.483,$ $Q^2 = 0.689,\ \mathrm{SDEP} = 0.523,\ S_{\mathrm{PRESS}} = 0.597,\ \mathrm{PRESS} = 8.2,\ \mathrm{bs}r^2(\pm\mathrm{sd}) = 0.798(\pm0.007)$
QSAR Model 2	$\mathrm{p}K_\mathrm{i} = 0.280(\pm0.118)f2 + 0.415(\pm0.118)f3 - 0.368(\pm0.118)f4 - 0.239(\pm0.118)f6$ $- 0.424(\pm0.118)f7 + 0.459(\pm0.118)f8 + 4.401$ $n = 30,\quad R_a^2 = 0.895,\ R^2 = 0.916,\ R = 0.957,\ F = 42.0(\mathrm{df}6, 23),\ s = 0.310,$ $Q^2 = 0.870,\ \mathrm{SDEP} = 0.338,\ S_{\mathrm{PRESS}} = 0.386,\ \mathrm{PRESS} = 3.4,\ \mathrm{bs}r^2(\pm\mathrm{sd}) = 0.917(\pm0.001)$
QSAR Model 3	$\mathrm{p}K_\mathrm{i} = -1.940(\pm2.072)q_2 - 11.413(\pm3.878)q_8 - 13.611(\pm5.005)q_9 - 0.038(\pm0.029)[\log P]^2$ $- 1.556(\pm0.722)I_{\mathrm{OBu\_t}} + 3.083$ $n = 30,\quad R_a^2 = 0.775,\ R^2 = 0.814,\ R = 0.902,\ F = 21.0(\mathrm{df}5, 24),\ s = 0.452,$ $Q^2 = 0.753,\ \mathrm{SDEP} = 0.466,\ S_{\mathrm{PRESS}} = 0.521,\ \mathrm{PRESS} = 6.5,\ \mathrm{bs}r^2(\pm\mathrm{sd}) = 0.814(\pm0.007)$

QSAR Model 4	$pK_i = -1.932(\pm 2.150)q_2 - 11.413(\pm 4.012)q_8 - 13.741(\pm 5.189)q_9 - 0.311(\pm 0.260)\log P$ $- 1.518(\pm 0.747)I_{OBu\_t} + 3.686$ $n = 30,\quad R_a^2 = 0.762,\ R^2 = 0.803,\ R = 0.896, F = 19.6(df5, 24),\ s = 0.465,$ $Q^2 = 0.739,\ SDEP = 0.479,\ S_{PRESS} = 0.536,\ PRESS = 6.9,\ bsr^2(\pm sd) = 0.804(\pm 0.007)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** q_x: Wang-Ford charge of atom x (x may take values 1 to 14). I_{OBu_t}: Indicator variable having value 1 if tert-butyloxy group is present at R position, 0 otherwise. I_X: Indicator variable having value 1 if X =N, value 0 otherwise. I_{Me_Et}: Indicator variable having value 1 if R = methyl or ethyl, value 0 otherwise.
Reference	Exploring QSAR of thiazole and thiadiazole derivatives as potent and selective human adenosine A3 receptor antagonists using FA and GFA techniques. Bioorganic & Medicinal Chemistry 13 (2005) 1159–1165

Target Species	Human
Chemical Type	Thiadiazole derivatives
Mode of Action	Antagonist
Activity Type	Adenosine A_3 binding affinity
QSAR Model 1	$pK_i = -3.951(\pm 2.415)q_2 - 2.623(\pm 2.136)q_5 + 2.441(\pm 1.489)q_7 - 0.275(\pm 0.261)\log P$ $- 1.498(\pm 0.763)I_{OBu\_t} + 0.895(\pm 0.614)I_{Me\_Et} + 4.030$ $n = 30,\quad R_a^2 = 0.744,\ R^2 = 0.797,\ R = 0.893, F = 15.0(df6, 23),\ s = 0.483,$ $Q^2 = 0.689,\ SDEP = 0.523,\ S_{PRESS} = 0.597,\ PRESS = 8.2,\ bsr^2(\pm sd) = 0.798(\pm 0.007)$

QSAR Model 2	$pK_i = 0.280(\pm0.118)f2 + 0.415(\pm0.118)f3 - 0.368(\pm0.118)f4 - 0.239(\pm0.118)f6 - 0.424(\pm0.118)f7 + 0.459(\pm0.118)f8 + 4.401$ $n = 30,\ \ R_a^2 = 0.895,\ R^2 = 0.916,\ R = 0.957,\ F = 42.0(\mathrm{df}6, 23),\ s = 0.310,$ $Q^2 = 0.870,\ \mathrm{SDEP} = 0.338,\ S_{\mathrm{PRESS}} = 0.386,\ \mathrm{PRESS} = 3.4,\ \mathrm{bs}r^2(\pm\mathrm{sd}) = 0.917(\pm0.001)$
QSAR Model 3	$pK_i = -1.940(\pm2.072)q_2 - 11.413(\pm3.878)q_8 - 13.611(\pm5.005)q_9 - 0.038(\pm0.029)[\log P]^2 - 1.556(\pm0.722)I_{\mathrm{OBu\_t}} + 3.083$ $n = 30,\ \ R_a^2 = 0.775,\ R^2 = 0.814,\ R = 0.902,\ F = 21.0(\mathrm{df}5, 24),\ s = 0.452,$ $Q^2 = 0.753,\ \mathrm{SDEP} = 0.466,\ S_{\mathrm{PRESS}} = 0.521,\ \mathrm{PRESS} = 6.5,\ \mathrm{bs}r^2(\pm\mathrm{sd}) = 0.814(\pm0.007)$
QSAR Model 4	$pK_i = -1.932(\pm2.150)q_2 - 11.413(\pm4.012)q_8 - 13.741(\pm5.189)q_9 - 0.311(\pm0.260)\log P - 1.518(\pm0.747)I_{\mathrm{OBu\_t}} + 3.686$ $n = 30,\ \ R_a^2 = 0.762,\ R^2 = 0.803,\ R = 0.896, F = 19.6(\mathrm{df}5, 24),\ s = 0.465,$ $Q^2 = 0.739,\ \mathrm{SDEP} = 0.479,\ S_{\mathrm{PRESS}} = 0.536,\ \mathrm{PRESS} = 6.9,\ \mathrm{bs}r^2(\pm\mathrm{sd}) = 0.804(\pm0.007)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** q_x: Wang-Ford charge of atom x (x may take values 1 to 14). I_{OBu_t}: Indicator variable having value 1 if tert-butyloxy group is present at R position, 0 otherwise. I_X: Indicator variable having value 1 if X =N, value 0 otherwise. I_{Me_Et}: Indicator variable having value 1 if R = methyl or ethyl, value 0 otherwise.
Reference	Exploring QSAR of thiazole and thiadiazole derivatives as potent and selective human adenosine A3 receptor antagonists using FA and GFA techniques. Bioorganic & Medicinal Chemistry 13 (2005) 1159–1165

Target Species	Human
Chemical Type	1,2,4-triazolo[4,3-a]quinoxalin-1-one derivatives

Mode of Action	Antagonist
QSAR Model 1	$pK_i = 1.913\sigma_p + 0.684I_{NO_2} + 4.654$ $n = 17,\quad R_a^2 = 0.726,\quad R^2 = 0.760,\quad R = 0.872,\ F = 22.2(\text{df } 2, 14),\quad s = 0.465,$ $Q^2 = 0.653,\quad \text{SDEP} = 0.507,\quad S_{\text{PRESS}} = 0.559,\ \text{PRESS} = 4.4$
QSAR Model 2	$pK_i = 0.320f3 + 0.518f4 + 0.332f5 + 0.396f6 - 0.187f7 + 4.294$ $n = 17,\quad R_a^2 = 0.786,\quad R^2 = 0.853,\quad R = 0.923,\ F = 12.7(\text{df } 5, 11),\quad s = 0.411,$ $Q^2 = 0.631,\quad \text{SDEP} = 0.524,\quad S_{\text{PRESS}} = 0.651,\ \text{PRESS} = 4.6$
QSAR Model 3	$pK_i = 1.847\sigma_p + 0.792I_{NO_2} - 2.375q_{15} + 2.507q_{19} + 4.452$ $n = 17,\quad R_a^2 = 0.744,\quad R^2 = 0.808,\quad R = 0.899,$ $Q^2 = 0.648,\quad \text{LSE} = 0.143,\quad \text{SDEP} = 0.511,\ S_{\text{PRESS}} = 0.608,\quad \text{PRESS} = 4.4$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** q_x: Wang–Ford charge of atom x (x may take values 1–20) I_{NO2}: Indicator variable having value 1 if nitro group is present at the R1 position, value 0 otherwise I_{NH2}: Indicator variable having value 1 if amino group is present at the R1 position, value 0 otherwise I'_{NH2}: Indicator variable having value 1 if amino group present at position 8, value 0 otherwise
Reference	QSAR of adenosine A3 receptor antagonist 1,2,4-triazolo[4,3-a]quinoxalin-1-one derivatives using chemometric tools. Bioorganic & Medicinal Chemistry Letters 15 (2005) 3737–3743

Target Species	Rat
Chemical Type	Adenosine analogues
Mode of Action	Agonist
Activity	Displacement of specified [^{125}I] AB-MECA binding at rat A_3 receptors expressed in CHO cells

Type	
QSAR Model 1	$\log(K_i) = 11.619 + 4.204 \cdot BELm7 + 11.721 \cdot BELv2 -$ $7.415 \cdot BEHe7 + 5.610 \cdot BEHp3 + 13.131 \cdot BELp5 - 7.010 \cdot BELp6$ $N = 32\ R = 0.899\ S = 0.322\ F_{exp} = 17.535\ p < 10^{-5}\ q^2_{LOO} = 0.724\ S_{cv\text{-}LOO} = 0.385$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Constitutional: nCIC, RBF, nDB, nS, nR05, nR06 Topological: X4A, X5A, Lop, IC3, IC5, T(N..S) Molecular walk count: MWC05, MWC08, MWC10, SRW05, SRW07, SRW10 BCUT: BEHm8, BELm1, BELm2, BEHe7, BEHp5, BEHp7 Galvez topological charge indices: GGI4, GGI6, GGI7, JGI1, JGI8, JGI9 2D autocorrelations: MATS3m, MATS1e, MATS2e, MATS1p, GATS8v, GATS8v Randic ´molecular profiles: DP04, DP06, SP01, SP02, SP03, SHP2 Geometrical: J3D, MAXDN, MAXDP, MEcc, G(N..N), G(O..I) RDF: RDF130u, RDF140v, RDF050v, RDF050p, RDF140p, RDF155p 3D-MORSE: Mor16m, Mor18m, Mor20m, Mor08e, Mor12e, Mor10p WHIM: E1v, L2e, G3m, L2p, E1s, Gm GETAWAY: R3u+, R1m+, R3v+, R3e+, R5e+, R7e+
Reference	Quantitative Structure Activity Relationships as Useful Tools for the Design of New Adenosine Receptor Ligands. 1. Agonist. *Current Medicinal Chemistry*, 2006, 13, 2253-2266