Target Name	Acetylcholinesterase (AChE)
Target TTD ID	TTDS00140

Target Species	Human
Chemical Type	Tacrine derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log RA = -5.094(\pm0.456) + 0.207(\pm0.047)\log P - 0.017(\pm0.008)SE + 0.679(\pm0.096)VCI1 - 0.258(\pm0.040)SIK1 - 0.112(\pm0.013)SFE$ $n = 68,\ R = 0.978,\ R^2 = 0.957,\ Q^2 = 0.946,\ SE = 0.404,\ F = 278.5$ (df 5, 62), PRESS = 10.101, SDEP = 0.224.
QSAR Model 2	$\log RA = -1.993(\pm0.561) + 0.764(\pm0.218)SIKA3 + 0.104(\pm0.262)NORB - 0.081(\pm0.013)SFE - 0.027(\pm0.003)VDWSURFA + 0.027(\pm0.004)WNSA1$ $n = 68,\ R = 0.979,\ R^2 = 0.959,\ Q^2 = 0.952,\ SE = 0.395,\ F = 290.8$ (df 5, 62), PRESS = 9.691, SDEP = 0.233.
QSAR Model 3	$\log RA = -3.588(\pm0.359) + 0.129(\pm0.054)\log P + 0.111(\pm0.028)NORB - 0.096(\pm0.012)SFE - 0.017(\pm0.003)VDWSURFA + 0.020(\pm0.005)WNSA1$ $n = 68,\ R = 0.977,\ R^2 = 0.955,\ Q^2 = 0.945,\ SE = 0.415$, RMSEP = 0.440, SDEP = 0.223, $F = 263.3$ (df 5, 62), PRESS = 10.655.
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** LogP: Octanol–water partition coefficient, calculated by Ghose's atom additive method SE: Steric energy (kcal/mol), the optimization to find a low-energy structure SIK1: Shape index of order 1 (j1), quantifying the number of cycles in the chemical sample SIKA3: Shape index of order 3 (j3), quantifying the degree of branching toward the center of the chemical sample VCI1: First-order (bond) valence molecular connectivity index (1vV) for the chemical sample VDWSURFA: Two-dimensional van der Waals surface area

	NORB: Number of rigid bonds WNSA1: Surface-weighted charged partial negative surface area, first type SFE: Water solvation free energy, calculated by Ghose's atom additive method
Reference	Quantitative structure–activity relationship (QSAR) of tacrine derivatives against acetylcholinesterase (AChE) activity using variable selections. *Bioorganic & Medicinal Chemistry Letters* 17 (2007) 1082–1090