

Target Name	HCV NS5B Polymerase
Target TTD ID	TTDC00001

Target Species	Hepatitis C virus
Chemical Type	Thiazolones derivatives
Mode of Action	Inhibitor
QSAR Model 1	$-\log IC_{50} = 2.303 + 1.0117(\pm 0.2009)XRO + 0.6914(\pm 0.2198)PRZ + 0.7499(\pm 0.2282)OXA - 1.6371(\pm 0.6206) xen$ $N = 26, Se = 0.1743, r^2 = 0.75, r^2_{cv} = 0.5691, F = 16.5022$
QSAR Model 2	$-\log IC_{50} = 0.7947 + 1.2648(\pm 0.2139)GGI4 + 0.072(\pm 0.0182)RDF115e - 1.583(\pm 0.2891)H4u - 0.656(\pm 0.2793)Mor16v - 52.2558(\pm 9.9329)R6u +$ $N = 26, Se = 0.1782, r^2 = 0.7387, r^2_{cv} = 0.596, F = 11.8759$
QSAR Model 3	$-\log IC_{50} = 0.558 + 1.0977(\pm 0.1154)XRO + 0.6823(\pm 0.1590)TEN - 0.3872(\pm 0.0929)psychotic-80 + 0.0459(\pm 0.0105)RDF115e + 0.761(\pm 0.1675)Mor30m$ $N = 26, Se = 0.1141, r^2 = 0.8929, r^2_{cv} = 0.8215, F = 35.0183$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>GGI4- is the topological charge index of order 4; RDF115e- is the Radial distribution on function - 1/5 weighted by atomic Sanderson electronegativities; H4u- is the H autocorrelation of lag 4/unweighted; Mor16v- is the 3D-MoRSE - signal 16 / weighted by atomic van der Waals volume; R6u+- is the Maximal-autocorrelation of log 6/unweighted; xen - is the 100 . max. atomic electrophilic reaction index for N atoms; XRO- is the parabolic function 100 .Maximum atomic one electron reaction index for Oxygen Atom; PRZ - is the parabolic function 0.001 . sup (area of</p>

	molecular surface) . neu (area of neutral surface)product; OXA- is the parabolic function of percent of oxygen. Average charge for Oxygen atoms; Psychotic-80 - is the Ghose Vishwandhan wedoloskin antipsychotic like index 80%; Mor30m- is the 3D Morse signal 30/weighted by atomic masses; TEN- is the parabolic function of total energy /1000; XRO- is the parabolic function 100 .Maximum atomic one electron reaction index for Oxygen Atom.
Reference	Comparative QSAR Studies on the Novel Series of Thiazolones and Tetrazole Derivatives as HCV NS5B Polymerase Allosteric Inhibitors. <i>Letters in Drug Design & Discovery</i> , 2009, 6, 286-297

Target Species	Hepatitis C virus
Chemical Type	Tetrazole derivatives
Mode of Action	Inhibitor
QSAR Model 1	$-\log IC_{50} = 2.303 + 1.0117(\pm 0.2009)XRO + 0.6914(\pm 0.2198) PRZ + 0.7499(\pm 0.2282) OXA - 1.6371(\pm 0.6206) xen$ <p>$N = 26, Se = 0.1743, r^2 = 0.75, r^2_{cv} = 0.5691, F = 16.5022$</p>
QSAR Model 2	$-\log IC_{50} = 0.7947 + 1.2648(\pm 0.2139)GGI4 + 0.072(\pm 0.0182) RDF115e - 1.583(\pm 0.2891)H4u - 0.656(\pm 0.2793)Mor16v - 52.2558(\pm 9.9329) R6u +$ <p>$N = 26, Se = 0.1782, r^2 = 0.7387, r^2_{cv} = 0.596, F = 11.8759$</p>
QSAR Model 3	$-\log IC_{50} = 0.558 + 1.0977(\pm 0.1154)XRO + 0.6823(\pm 0.1590) TEN - 0.3872(\pm 0.0929) psychotic-80 + 0.0459(\pm 0.0105) RDF115e + 0.761(\pm 0.1675) Mor30m$ <p>$N = 26, Se = 0.1141, r^2 = 0.8929, r^2_{cv} = 0.8215, F = 35.0183$</p>
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>GGI4- is the topological charge index of order 4; RDF115e- is the Radial distribution on function - 11/5 weighted by atomic Sanderson electronegativities; H4u- is the H autocorrelation of lag 4/unweighted; Mor16v- is the 3D-MoRSE - signal 16 / weighted by atomic van der Waals volume;</p>

	<p>R_{6u+-} is the Maximal-autocorrelation of log ϕ/unweighted; χ_{en} - is the 100 . max. atomic electrophilic reaction index for N atoms; XRO- is the parabolic function 100 .Maximum atomic one electron reaction index for Oxygen Atom; PRZ - is the parabolic function 0.001 . sup (area of molecular surface) . neu (area of neutral surface)product; OXA- is the parabolic function of percent of oxygen. Average charge for Oxygen atoms; Psychotic-80 - is the Ghose Vishwandhan wedoloskin antipsychotic like index 80%; Mor30m- is the 3D Morse signal 30/weighted by atomic masses; TEN- is the parabolic function of total energy /1000; XRO- is the parabolic function 100 .Maximum atomic one electron reaction index for Oxygen Atom.</p>
Reference	<p>Comparative QSAR Studies on the Novel Series of Thiazolones and Tetrazole Derivatives as HCV NS5B Polymerase Allosteric Inhibitors. <i>Letters in Drug Design & Discovery</i>, 2009, 6, 286-297</p>