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| **Target Name** | CXCR3 receptor |
| **Target TTD ID** | TTDC00125 |

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| **Target Species** | Human |
| **Chemical Type** | 4-*N*-aryl-[1,4] diazepane ureas |
| **Mode of Action** | Inhibitor |
| **QSAR Model 1** | $\log(1/IC_{50}) = 3.99 - 2.58\,\text{ChiInf0} - 2.35\,\text{ChiInf8} - 8.85\times10^{-3}\,\text{AtomCompTot} + 7.78\times10^{-1}\,{}^{3}k + 1.94\times10^{-1}\,\text{ClogP}$<br>$R^2 = 0.82 \quad \text{RMS} = 0.21 \quad F = 16.94 \quad R^2_{\text{LOO}} = 0.71 \quad \text{SDEP} = 0.23$<br>$S_{\text{PRESS}} = 0.27 \quad n = 25$ |
| **QSAR Model 2** | $\log(1/IC_{50}) = -0.25\,\text{ChiInf0} - 0.50\,\text{ChiInf8} - 0.31\,\text{AtomCompTot} + 0.93\,{}^{3}k + 0.34\,\text{ClogP}$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br><br>Physicochemical constants, topological and structural descriptors: Description [Notation]<br><br>Molar refractivity [MR]; Diameter [Diam]; Partition coefficient (octanolewater) [ClogP]; Molecular topological index [TIndx]; Principal moment of inertia Z [PMIZ]; Number of rotatable bonds [NRBo]; Principal moment of inertia Y [PMIY]; Polar surface area [PSAr]; Principal moment of inertia [PMIX]; Radius [Rad]; Connolly accessible area [SAS]; Shape attribute [ShpA]; Connolly molecular area [MS]; Shape coefficient [ShpC]; Total energy [TotE]; Sum of valence degrees [SVDe]; LUMO energy [LUMO]; Total connectivity [TCon]; HOMO energy [HOMO]; Total valence connectivity [TVCon]; Balaban index [BIndx]; Wiener index [WIndx]; Cluster count [ClsC]; Randic 0 [Chi0]; Randic 1 [Chi1]; Randic 2 [Chi2]; Randic 3 [Chi3]; Randic 4 [Chi4]; Randic information 0 [ChiInf0]; Randic information 1 [ChiInf1]; Randic information 2 [ChiInf2]; Randic information 3 |

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| | [ChiInf3]; Randic information 4 [ChiInf4]; KiereHall 0 [Ki0]; Randic Mod [ChiMod]; Xu1 [Xu1]; Xu2 [Xu2]; Xu3 [Xu3]; Balaban topological [TopoJ]; Topological radius [TopoRad]; Topological diameter [TopoDia]; Number of clusters [NClusters]; Number of rings [NRings]; Wiener Dim [Wiener Dim]; Bertz [Bertz]; AtomCompMean [AtomCompMean]; AtomCompTot [AtomCompTot]; Zagreb1 [Zagreb1]; Zagreb2 [Zagreb2]; Quadratic [Quadr]; ScHultz [ScHultz]; Kappa1 [1k]; Kappa3 [3k]; Kappa2 [2k]; Wiener distance [WienerDistCode]; Wiener information [InfWiener]; DistEqMean [DistEqMean]; DistEqTotal [DistEqTotal]; InfMagnitDistTot [InfMagnitDistTot]; Polarity [Polarity]; Gordon [Gordon]; Randic information 8 [ChiInf8] |
| **Reference** | A novel QSAR model for predicting the inhibition of CXCR3 receptor by 4-N-aryl-[1,4] diazepane ureas. *European Journal of Medicinal Chemistry* 44 (2009) 877-884 |