Target Name	3-hydroxy-3-methyl-glutaryl coenzyme A reductase
Target TTD ID	TTDS00195

Target Species	Human
Chemical Type	Statins derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\text{HMGRI-score} = 0.169 \cdot \text{Cc} - 0.029 \cdot \text{Svd} + 0.561 \cdot D - 0.002 \cdot W - 3.992 \cdot \text{Nrc} + 12.415 \cdot \text{Bn} + 12.167$ $N = 183 \quad \text{Rc} = 0.7 \quad \lambda = 0.54 \quad F = 25.15 \quad p\text{-level} < 0.001$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** N is the number of compounds used for training, Rc is the canonical regression coefficient, λ is the Wilks's statistic parameter, F is the Fisher ratio and p is the level of error. Cluster count (Cc), sum of valence degree (Svd), Wiener index (W), number of R centers (Nrc) and normal chiral/non-chiral balance (Bn). W: Wiener index; J: Balaban index; Cc: Cluster count; Svd: Sum of valence degree; D: Diameter; R: Radius; Sha: Shape attribute; Shc: Shape coefficient; Sod: Sum of degree; Mti: Molecular topological index; Nrb: Number of Rotable Bonds; Tc: Total connectivity; Tvc: Total valence connectivity; Ntc: Number of total centers; Ncc: Number of chiral centers; Nncc: Number of non-chiral centers; Nsc: Number of S centers; Nrc: Number of R centers; Bg = Nncc – Ncc: General chiral/non-chiral balance; Bn = (Ncc - Nncc)/Ntc: Normal chiral/non-chiral balance; Brs = (Nrc - Nsc)/(Ncc + 1): Relative RS balance; Inv: In vivo test indicator; Psa: Polar surface area
Reference	QSAR and complex network study of the chiral HMGR inhibitor structural diversity. *Bioorganic & Medicinal Chemistry* 17 (2009) 165–175