CODE	4DPF(PDB)	Resolution	1.8
Name		Ring size	15
Formula	C35H46N4O6S	# Ligand atoms	46
Type	macrocycle	Scorpion Score	11.7

Mol. Weight (Da)	651	Saturated/ Unsaturated	U
cLogP	4.17		
tPSA	137	Chiral centres.ring	2
#HBD's	4	Chiral centres.sub	1
#HBA's	10		
$N_{RB\ (RING)}$	11	$N_{RB\ (SUBSTITUENTS)}$	9

Number of substituents	3	P/NP balance, substituents	5/24
Large (≥5HA)	3	P/NP balance, peripheral groups	2/0
Small (2-4HA)	-		
Proportion HA in substituents	63.0%	Degrees of unsaturation ring	15
Number of peripheral groups	2	N:O ratio	4:6
		Chiral centres	3

Polarity distribution ligand atoms

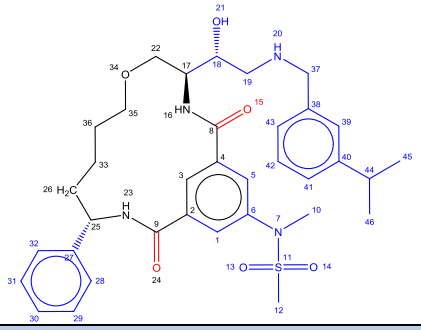
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	12	-	6
Substituent	5	23	4	9
Peripheral groups	2	-	2	-
Total	10	35	6	15

Protein name	BACE-1
Organism	Homo Sapiens
Classification	Hydrolase/ hydrolase inhibitor
Binding mode	compact
Receptor secondary structure topology	
Number of residue 'hotspots'	20

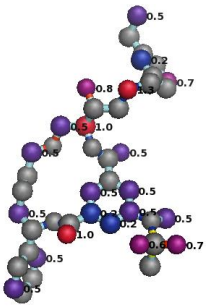
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	7	Hydrogen donor-π	3
Ionic interaction	1	π-π	4
Cation-dipole		VdW interaction	14
Cation-π		Unfavourable	5
Dipolar interaction	1	Poor-angle	4
Halogen bond		Unclassified	1
Water-mediated interaction	5		

2D-STRUCTURE LIGAND



3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

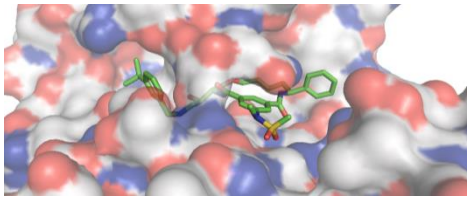


Physicochemical properties

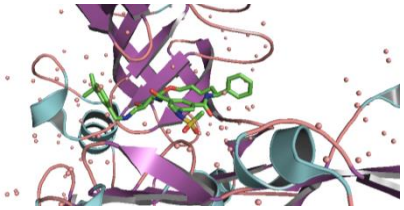
'click for publication'

IC50 enzyme (nM)	400
IC50 cell (nM)	260

LIGAND-PROTEIN COMPLEX (I) ('Pymol link')



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis