CODE	4KE0(PDB)	Resolution	2.3
Name		Ring size	13
Formula	C31H42N2O3	# Ligand atoms	36
Type	Macrocycle	Scorpion Score	10.3

Mol. Weight (Da)	491	Saturated/ Unsaturated	U
cLogP	6.17		
tPSA	71	Chiral centres.ring	1
#HBD's	3	Chiral centres.sub	2
#HBA's	5		
$N_{RB\ (RING)}$	10	$N_{RB\ (SUBSTITUENT)}$	5
Number of substituents	2	P/NP balance, substituents	3/19
Large (≥5HA)	1	P/NP balance, peripheral groups	1/0
Small (2-4HA)	1		
Proportion HA in substituents	61.1%	Degrees of unsaturation ring	12
Number of peripheral groups	1	N:O ratio	2:3
		Chiral centres	3

Polarity distribution ligand atoms

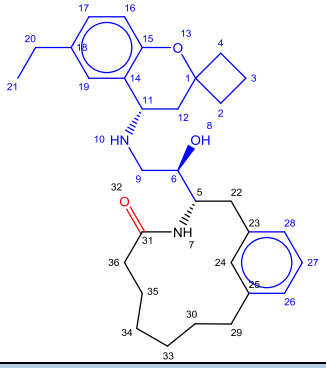
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	1	12	-	6
Substituent	3	19	3	6
Peripheral groups	1	-	1	-
Total	5	31	4	12

Protein name	BACE1
Organism	Homo sapiens
Classification	Hydrolase/ hydrolase inhibitor
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	15

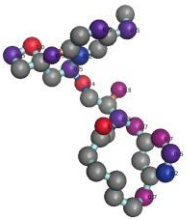
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	5	Hydrogen donor-π	1
Ionic interaction	1	π-π	3
Cation-dipole		VdW interaction	11
Cation-π		Unfavourable	4
Dipolar interaction		Poor-angle	2
Halogen bond		Unclassified	1
Water-mediated interaction	0		

2D-STRUCTURE LIGAND



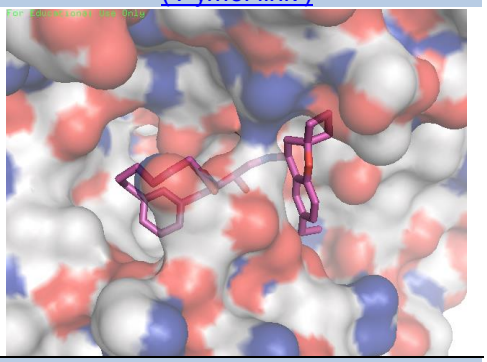
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



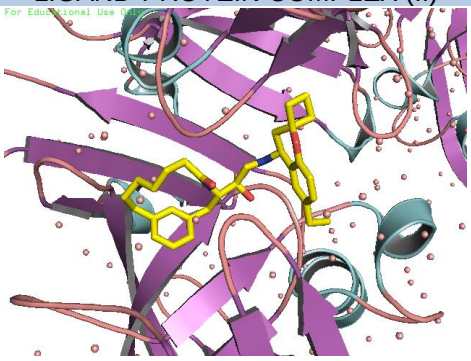
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis