CODE	3DV5 (PDB)	Resolution	3
Name		Ring size	16
Formula	C29H49N3O3	# Ligand atoms	32
Type	macrocycle	Scorpion Score	10

Mol. Weight (Da)	487,37	Saturated/ Unsaturated	U
cLogP	6.9188		
tPSA	81.67	Chiral centres.ring	3
#HBD's	3	Chiral centres.sub	1
#HBA's	2		
$N_{RB\ (RING)}$	14	$N_{RB\ (SUBSTITUENT)}$	6

Number of substituents	1	P/NP balance, substituents	2/12
Large (≥5HA)	1	P/NP balance, peripheral groups	2/5
Small (2-4HA)	-		
Proportion HA in substituents	44%	Degrees of unsaturation ring	7
Number of peripheral groups	5	N:O ratio	2:3
		Chiral centres	4

Polarity distribution ligand atoms

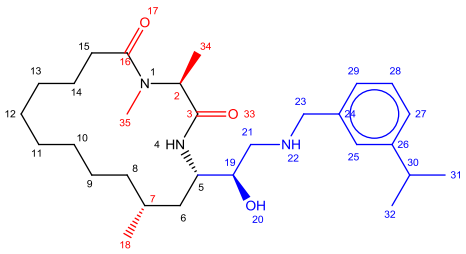
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	14	-	5
Substituent	2	12	2	4
Peripheral groups	2	3	2	2
Total	6	29	4	11

Protein name	BACE-1
Organism	Homo sapiens
Classification	Hydrolase
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	18

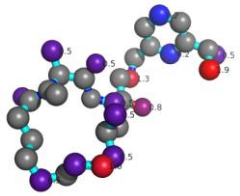
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	5	Hydrogen donor-π	2
Ionic interaction	1	π-π	2
Cation-dipole	-	VdW interaction	12
Cation-π	-	Unfavourable	5
Dipolar interaction	-	Poor-angle	3
Halogen bond	-	Unclassified	1
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



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

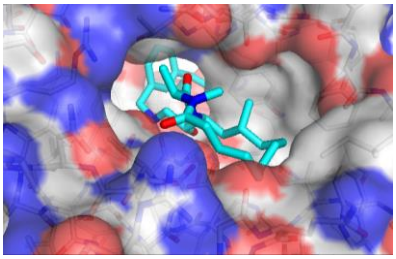


Physicochemical properties

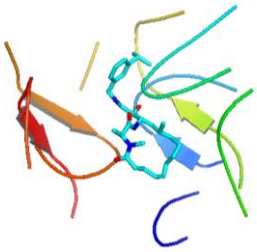
'click for publication'

IC50 (µM):	
BACE-1	0,022
Abeta40CHO	0,045
CathD	1,4

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis