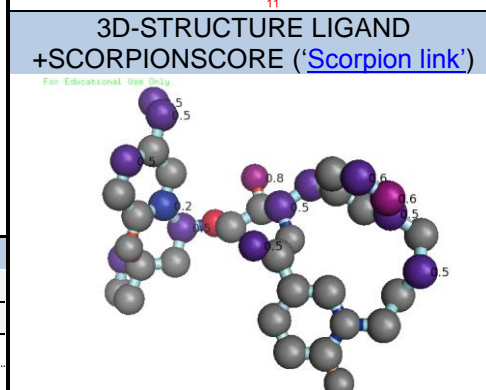
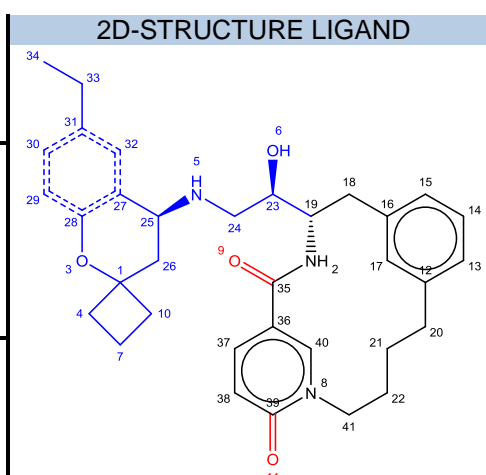


CODE	4KE1(PDB)	Resolution	1.9	
Name		Ring size	14	
Formula	C34H41N3O4	# Ligand atoms	41	
Type	Macrocycle	Scorpion Score	8.6	
Mol. Weight (Da)	556	Saturated/ Unsaturated	U	
cLogP	5.0	Chiral centres.ring	1	
tPSA	93	Chiral centres.sub	2	
#HBD's	4			
#HBA's	7			
N _{RB} (RING)	9	N _{RB} (SUBSTITUENT)	5	
Number of substituents	1	P/NP balance, substituents	3/16	
Large (≥5HA)	1	P/NP balance, peripheral groups	2/0	
Small (2-4HA)	-	Degrees of unsaturation ring	16	
Proportion HA in substituents	46.3%	N:O ratio	3:4	
Number of peripheral groups	2	Chiral centres	3	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	2	18	-	6
Substituent	3	16	2	6
Peripheral groups	2	-	1	-
Total	7	34	3	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	4	Hydrogen donor-π	1	
Ionic interaction	1	π-π	3	
Cation-dipole		VdW interaction	9	
Cation-π		Unfavourable	5	
Dipolar interaction	1	Poor-angle	2	
Halogen bond		Unclassified	2	
Water-mediated interaction	0			



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