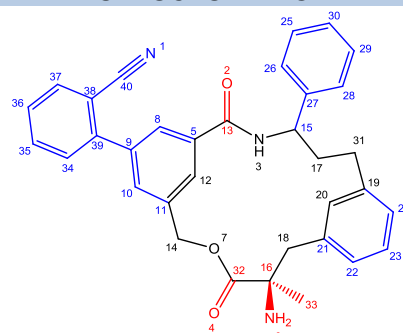
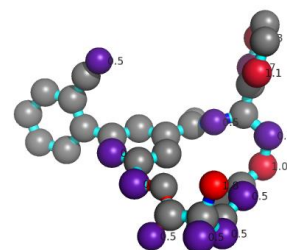
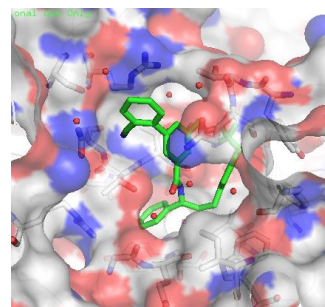
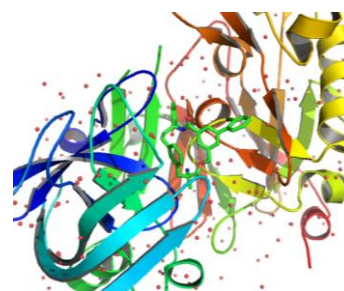


CODE	2QZK(PDB)	Resolution		
Name	COMP 1b	Ring size	16	
Formula	C34H31N3O3	# Ligand atoms	57	
Type	macrocycle	Scorpion Score	15.6	
Mol. Weight (Da)	529,63	Saturated/ Unsaturated	U	
cLogP	5.3922	Chiral centres.ring	2	
tPSA	105.21	Chiral centres.sub	0	
#HBD's	3			
#HBA's	4			
N _{RB} (RING)	10	N _{RB} (SUBSTITUENT)	2	
Number of substituents	3	P/NP balance, substituents	1/19	
<i>Large (≥5HA)</i>	2	P/NP balance, peripheral groups	3/1	
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	21	
Proportion HA in substituents	35	N:O ratio	3:3	
Number of peripheral groups	4	Chiral centres	2	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	2	14	1	7
Substituent	1	19	1	3
Peripheral groups	3	1	2	1
Total	6	34	4	11
Protein name	human Beta Secretase complexed			
Organism	Homo sapiens			
Classification	Hydrolase			
Binding mode	Compact			
Receptor secondary structure topology				
Number of residue 'hotspots'	17			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	5	Hydrogen donor-π	1	
Ionic interaction	2	π-π	3	
Cation-dipole	-	VdW interaction	12	
Cation-π	1	Unfavourable	2	
Dipolar interaction	2	Poor-angle	7	
Halogen bond	-	Unclassified	1	
Water-mediated interaction	3			

2D-STRUCTURE LIGAND

3D-STRUCTURE LIGAND
+SCORPIONSORE ('Scorpion link')Physicochemical properties
'click for publication'IC₅₀= 27nMLIGAND-PROTEIN COMPLEX (I)
('Pymol link')

LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis