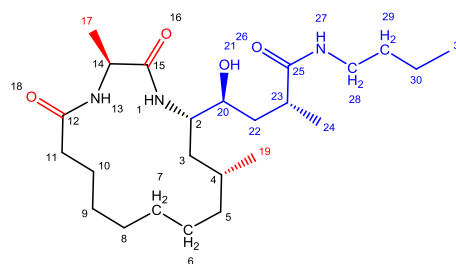


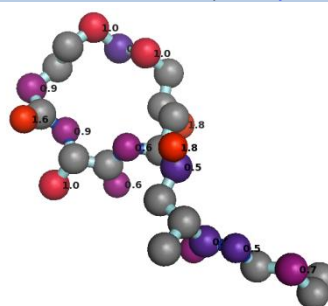
CODE	3DV1(PDB)	Resolution	2.1	
Name	NVP-ARV999	Ring size	15	
Formula	C24H45N3O4	# Ligand atoms	31	
Type	Macrocycle	Scorpion Score	15	
Mol. Weight (Da)	440	Saturated/Unsaturated	S	
cLogP	4.3	Chiral centres.ring	3	
tPSA	108	Chiral centres.sub	2	
#HBD's	4			
#HBA's	7			
N _{RB} (RING)	13	N _{RB} (SUBSTITUENT)	7	
Number of substituents	1	P/NP balance, substituents	3/9	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	2/2	
<i>Small (2-4HA)</i>	-	Degrees of unsaturation ring	4	
Proportion HA in substituents	38.7%	N:O ratio	3:4	
Number of peripheral groups	4	Chiral centres	5	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	2	13	2	4
Substituent	3	9	-	6
Peripheral groups	2	2	2	2
Total	7	24	4	12

Protein name	Human beta-secretase		
Organism	Homo sapiens		
Classification	Hydrolase		
Binding mode	Face-on/ compact		
Receptor secondary structure topology			
Number of residue 'hotspots'	15		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	9	Hydrogen donor-π	1
Ionic interaction		π-π	
Cation-dipole		VdW interaction	12
Cation-π		Unfavourable	1
Dipolar interaction	1	Poor-angle	1
Halogen bond		Unclassified	1
Water-mediated interaction	6		

2D-STRUCTURE LIGAND



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

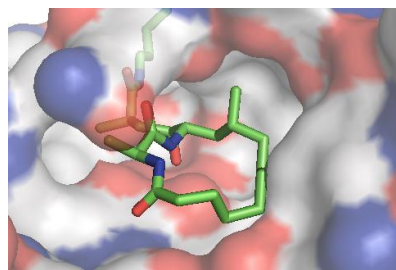


Physicochemical properties

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IC50 (h BACE-1) (μM)	0,59
IC50 (Abeta40CHO) (μM)	>10
IC50 (hCathD FQ) (μM)	>10

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



LIGAND-PROTEIN COMPLEX (II)

