CODE	3ZPT (PDB)	Resolution	1.6
Name	Compound 19(a)	Ring size	15
Formula	C36H54BrN5O6	# Ligand atoms	48
Type	macrocycle	Scorpion Score	13.2

Mol. Weight (Da)	733	Saturated/ Unsaturated	U
cLogP	6.03		
tPSA	149	Chiral centres.ring	2
#HBD's	5	Chiral centres.sub	1
#HBA's	12		
$N_{RB\ (RING)}$	9	$N_{RB\ (SUBSTITUENT)}$	12
Number of substituents	3	P/NP balance, substituents	7/23
Large (≥5HA)	1	P/NP balance, peripheral groups	3/0
Small (2-4HA)	2		
Proportion HA in substituents	62.5%	Degrees of unsaturation ring	12
Number of peripheral groups	3	N:O ratio	5/6
		Chiral centres	3

Polarity distribution ligand atoms

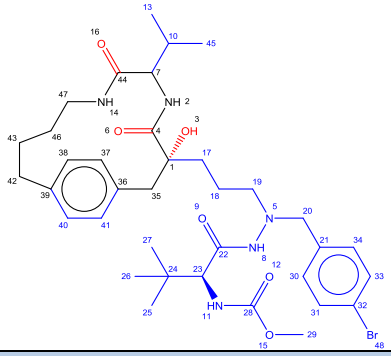
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	13	1	4
Substituent	7	23	4	8
Peripheral groups	3	-	3	-
Total	12	36	8	12

Protein name	HIV-1 Protease
Organism	Human immunodeficiency virus 1
Classification	Hydrolase
Binding mode	compact
Receptor secondary structure topology	
Number of residue 'hotspots'	21

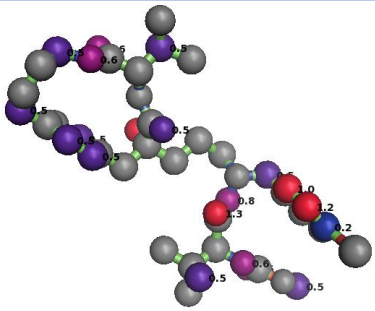
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	8	Hydrogen donor-π	
Ionic interaction		π-π	2
Cation-dipole		VdW interaction	13
Cation-π		Unfavourable	1
Dipolar interaction	1	Poor-angle	2
Halogen bond		Unclassified	2
Water-mediated interaction	3		

2D-STRUCTURE LIGAND



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

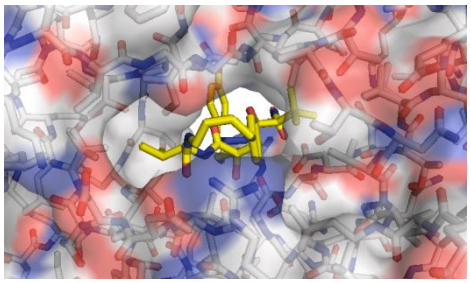


Physicochemical properties

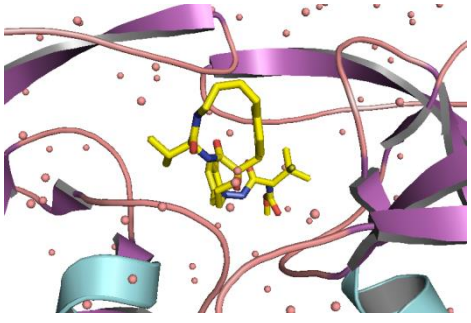
'click for publication'

Ki (nM)	3.1
EC50 (µM)	0.37
CC50 (µM)	>50

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis