CODE	**3G60**(PDB)	Resolution	4.4
Name		Ring size	18
Formula	C24H30N6O3Se3	# Ligand atoms	36
Type	Cyclic peptide	Scorpion Score	13.5

Mol. Weight (Da)	687	Saturated/ Unsaturated	U
cLogP	3.59		
tPSA	126	Chiral centres.ring	3
#HBD's	3	Chiral centres.sub	0
#HBA's	12 (incl. Se)		
N_{RB}			

Number of substituents	6	P/NP balance, substituents	3/12
Large (≥5HA)	0	P/NP balance, peripheral groups	3/0
Small (2-4HA)	6		
Proportion HA in substituents	41.6%	Degrees of unsaturation ring	13
Number of peripheral groups	3	N:O ratio	6:3
		Chiral centres	3

Polarity distribution ligand atoms

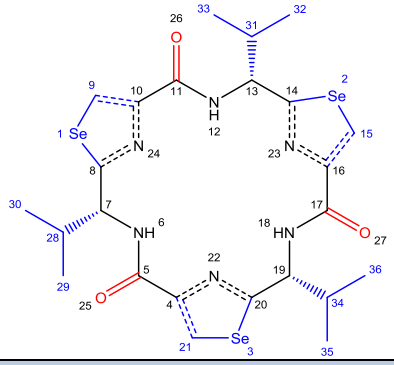
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	6	12	2	2
Substituent	3	12	-	6
Peripheral groups	3	0	-	-
Total	9	24	2	8

Protein name	P-glycoprotein
Organism	Mus musculus
Classification	Membrane protein
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	13

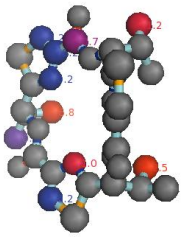
Number of protein-ligand interactions* ('Database link')

Hydrogen bond		Hydrogen donor-π	
Ionic interaction		π-π	5
Cation-dipole		VdW interaction	15
Cation-π		Unfavourable	4
Dipolar interaction		Poor-angle	
Halogen bond		Unclassified	2
Water-mediated interaction			

2D-STRUCTURE LIGAND

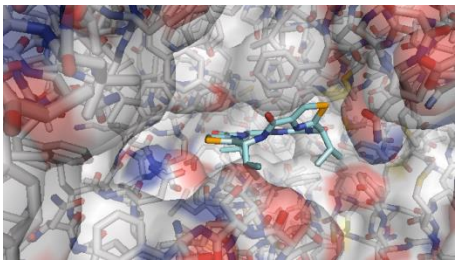


3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

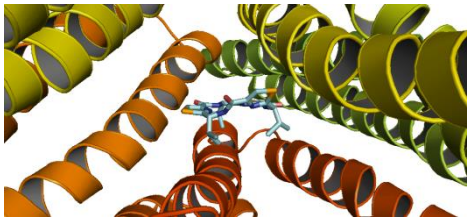


Physicochemical properties 'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis