CODE	**3OWN** (PDB)	Resolution	2.0
Name		Ring size	15
Formula	C37H48N4O7S	# Ligand atoms	49
Type	Macrocycle	Scorpion Score	12.7

Mol. Weight (Da)	693	Saturated/ Unsaturated	U
cLogP	3.49		
tPSA	154	Chiral centres.ring	2
#HBD's	4	Chiral centres.sub	2
#HBA's	10		
$N_{RB\ (RING)}$	9	$N_{RB\ (SUBSTITUENT)}$	10
Number of substituents	4	P/NP balance, substituents	6/26
Large (≥5HA)	3	P/NP balance, peripheral groups	2/0
Small (2-4HA)	1		
Proportion HA in substituents	65.3%	Degrees of unsaturation ring	16
Number of peripheral groups	2	N:O ratio	4:7
		Chiral centres	4

Polarity distribution ligand atoms

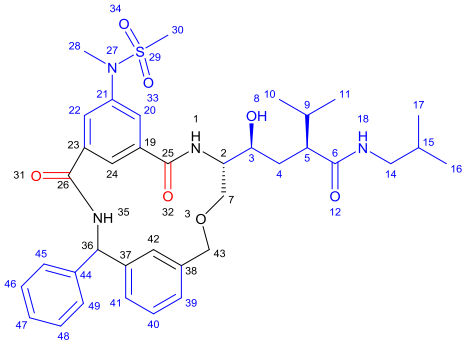
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	12	-	3
Substituent	6	26	3	10
Peripheral groups	2	-	1	-
Total	11	38	4	13

Protein name	Renin
Organism	Homo sapiens
Classification	Hydrolase/ Hydrolase inhibitor
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	17

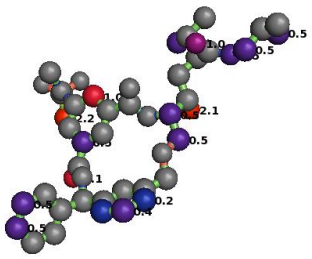
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	9	Hydrogen donor-π	4
Ionic interaction		π-π	4
Cation-dipole		VdW interaction	13
Cation-π		Unfavourable	6
Dipolar interaction		Poor-angle	3
Halogen bond		Unclassified	2
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



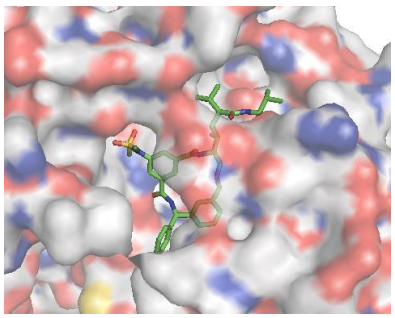
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



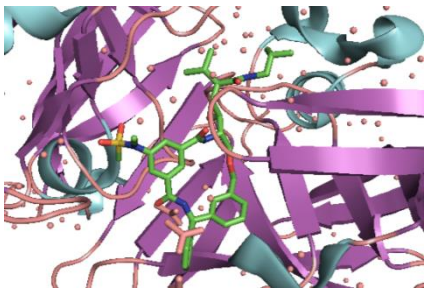
Physicochemical properties
'click for publication'

Renin Ki (nM)	34
Cathepsin D Ki (nM)	200
BACE-1 IC50 (nM)	3700

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis