CODE	4DRU (PDB)	Resolution	2.1
Name	Indol inhibitor	Ring size	16
Formula	C32H38N4O5S	# Ligand atoms	42
Type	MACROCYCLE	Scorpion Score	11.6

Mol. Weight (Da)	590.73	Saturated/ Unsaturated	U
cLogP	7.1333		
tPSA	99.26	Chiral centres.ring	0
#HBD's	1	Chiral centres.sub	0
#HBA's	9		
$N_{RB\ (RING)}$	9	$N_{RB\ (SUBSTITUENT)}$	2
Number of substituents	1	P/NP balance, substituents	1/19
Large (≥5HA)	1	P/NP balance, peripheral groups	4/2
Small (2-4HA)	-		
Proportion HA in substituents	48%	Degrees of unsaturation ring	16
Number of peripheral groups	6	N:O ratio	4:5
		Chiral centres	0

Polarity distribution ligand atoms

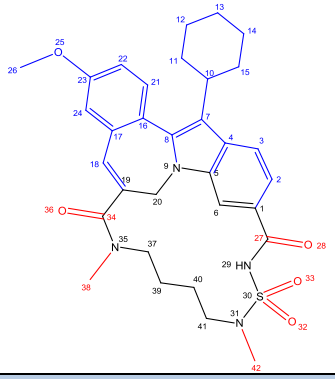
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	5	11	-	2
Substituent	1	19	1	12
Peripheral groups	4	2	2	-
Total	10	32	3	14

Protein name	HCV NS5B
Organism	Hepatitis C virus
Classification	Transferase / inhibitor
Binding mode	Face on
Receptor secondary structure topology	
Number of residue 'hotspots'	12

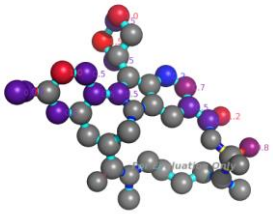
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	3	Hydrogen donor-π	-
Ionic interaction	-	π-π	2
Cation-dipole	-	VdW interaction	17
Cation-π	-	Unfavourable	2
Dipolar interaction	-	Poor-angle	-
Halogen bond	-	Unclassified	-
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



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

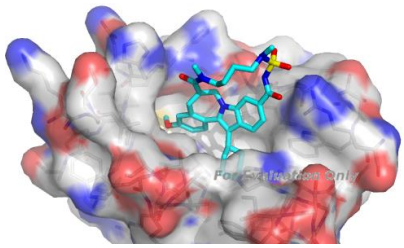


Physicochemical properties

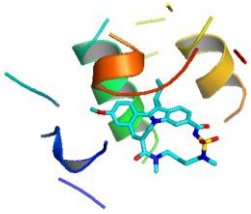
'click for publication'

K_d	2.4nm
IC_{50}	26nm
EC_{50}	75nm

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis