CODE	4CTC (PDB)	Resolution	2.14
Name		Ring size	12
Formula	C23H24FN5O2	# Ligand atoms	31
Type	Macrocycle	Scorpion Score	11.1

Mol. Weight (Da)	421.19	Saturated/ Unsaturated	U
cLogP	2.9997		
tPSA	83.52	Chiral centres.ring	1
#HBD's	2	Chiral centres.sub	0
#HBA's	6		
$N_{RB\ (RING)}$	7	$N_{RB\ (SUBSTITUENT)}$	9

Number of substituents	3	P/NP balance, substituents	5/11
Large (≥5HA)	2	P/NP balance, peripheral groups	2/1
Small (2-4HA)	1		
Proportion HA in substituents	52%	Degrees of unsaturation ring	14
Number of peripheral groups	3	N:O ratio	5/2
		Chiral centres	1

Polarity distribution ligand atoms

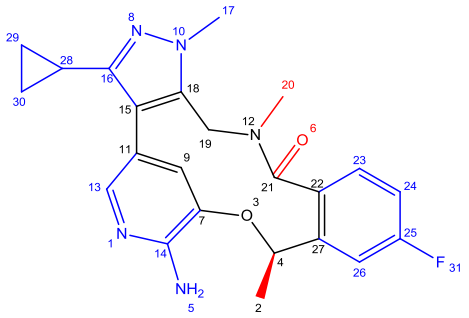
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	10	-	3
Substituent	5	11	3	9
Peripheral groups	1	2	-	1
Total	8	23	3	13

Protein name	Human Anaplastic Lymphoma Kinase
Organism	Homo sapiens
Classification	Tranferase
Binding mode	Edge- on
Receptor secondary structure topology	
Number of residue 'hotspots'	10

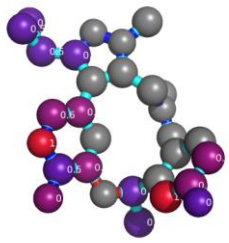
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	3	Hydrogen donor-π	
Ionic interaction		π-π	
Cation-dipole		VdW interaction	15
Cation-π		Unfavourable	1
Dipolar interaction	1	Poor-angle	1
Halogen bond		Unclassified	1
Water-mediated interaction	2		

2D-STRUCTURE LIGAND



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

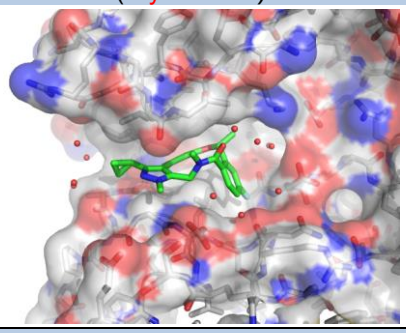


Physicochemical properties

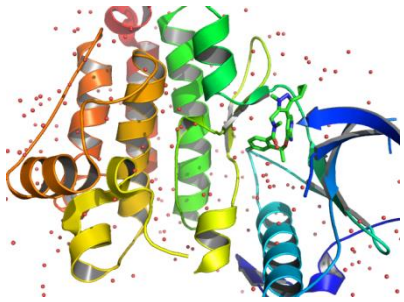
'click for publication'

K_i ALK-L1196M (nM)	<0,1
IC50 pALK-L1196M (nM)	5,8
log D	2,9

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis