Electronic Supplementary Information

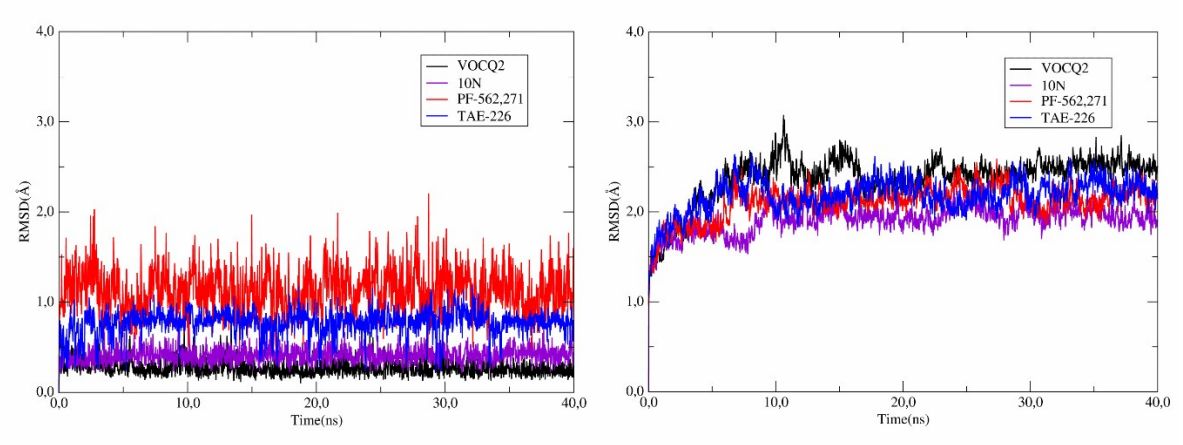

Figure SM1. RMSD profiles of ligands (left) and FAK Kinase Domain (right) as a time function during equilibration/production period.

Lig. / Res.	TAE-226	PF-562,271	10N	$VO(CQ)_2$
Ile428	side chain:2-methoxy-aniline (HC) side chain:morpholine (HC)	side chain:amino-oxindole (HC)	side chain:7-azaindole side chain:phenyl (HC)	side chain:quinoline (HC) O: pyrimidine ring (CHB)
Leu501	side chain:pyrimidine (HC)	side chain:amino-oxindole (HC)	side chain:7-azaindole (HC)	side chain:quinoline (HC)
Cys502	NH:N3 (HB) O:HN2 (HB)	NH:N5(HB) O:HN6 (HB)	NH:N2 (HB) O:HN5 (HB)	O:Cl (HalB)
Gly505	side main:2-methoxy-aniline (HC)	side main:amino-oxindole (HC)	side main:phenyl (HC)	side main:quinoline (HC)
Glu506	side chain:morpholine (HC)	side chain:amino-oxindole (HC)	side chain:phenyl (HC)	side chain:quinoline (HC)
Asn551	OD1-O:N-methylformamide group (CHB)	HA:O=S (CHB)	OD1:methylsulfonamide group (CHB)	OD1:pyridine ring (CHB)
Leu553	side chain:pyrimidine (HC)	side chain:diaminopyridine side chain:trifluoro-methyl group (HC)	side chain:7-azaindole (HC)	side chain:quinoline (HC)
Gly563	HA1:O=C (CHB) HA2:O=C (CHB)	side main: methyl-pyridinyl-sulfonamide (HC)	side main:phenyl (HC)	low interaction
Asp564	NH:O=C (HB)	NH:F (HB) NH:O=S (HB)	NH:N1 (HB)	low interaction
Leu567	side chain: 4-aniline (HC)	side chain:pyridinyl (HC)	side chain:phenyl (HC)	side chain:quinoline (HC)
Tyr570	-----	-----	-----	side chain:pyrimidine ring (HC)

Lys581	-----	-----	-----	side chain:clioquinolate (HC)

Table SM1. Interactions for each inhibitor and FAK, atom and moiety implicated. Hydrogen bond (HB), Halogen bond (HalB), Hydrophobic contact (HC), Carbon Hydrogen bond (CHB).

	DFT $VO(CQ)_2$ structure	Bis- (2-methyl-8-quinolinolato)oxovanadium(IV) X-ray structure
Bond length/Å		
N – V	2.094	2.137
O – V	1.943	1.921
(O-V)	1.597	1.600
Angle/º		
N – V – O	80.1	80.6
N – V – O’	89.1	91.0
O – (V-O)	112.0	116.4
N – (V-O)	104.5	99.5

Table SM2. Comparison of bis (2-methyl-8-quinolinolato)oxovanadium(IV) X-ray structure and $VO(CQ)_2$ structure, calculated with DFT. Vanadyl oxygen is inside parenthesis, the prime emphasizes that this atom belongs to another ligand.