

Supplementary material

Table 1: Comparative characteristics of IDV and novel hit

Molecular properties	IDV	Novel hit
Atoms	92	63
MW (≤ 500)	613.8 [†]	494.6
TPSA (\AA^2)	118	181
cLogP (≤ 5)	2.9	2.4
HBD (≤ 5)	4	4
HBA (≤ 10)	7	6
NI ¹	0	0
PI ²	2	3
Docking results		
MolDock Score	-	-185.7
Rerank Score	-	-148.5
Docking Score	-	-191.6
H-bond energy	-	-12.8
Flexible torsions	-	8
Energy Minimum	-15.1	-13.8
ADME/Tox		
Cramer rules	Class 3	Class 3
Biodegradability	Class 2	Class 2
Carcinogenicity	no	no

[†]negative ionizable groups; ²positive ionizable groups