Table S1. The parameters and their acceptable values employed through QikProp module.

Parameter	Description	Acceptable values
#amine	Number of non-conjugated amine groups	0-1
#amidine	Number of amidine and guanidine groups.	0
#acid	Number of carboxylic acid groups	0 – 1
#amide	Number of non-conjugated amide groups.	0 – 1
#rotor	Number of non-trivial (not CX3), non-hindered (not alkene, amide, small ring) rotatable bonds	0 – 15
#rtvFG	Number of reactive functional groups	0 – 2
CNS	Predicted central nervous system activity on a –2 (inactive) to +2 (active) scale.	–2 (inactive), +2 (active)
mol_MW	Molecular weight of the molecule	130.0 – 725.0
dipole	Computed dipole moment of the molecule	1.0 – 12.5
SASA	Total solvent accessible surface area (SASA) in square angstroms using a probe with a 1.4 Å radius.	300.0 – 1000.0
FOSA	Hydrophobic component of the SASA (saturated carbon and attached hydrogen).	0.0 – 750.0
FISA	Hydrophilic component of the SASA (SASA on N, O, H on heteroatoms, carbonyl C).	7.0 – 330.0
PISA	π (carbon and attached hydrogen) component of the SASA.	0.0 – 450.0
WPSA	Weakly polar component of the SASA (halogens, P, and S).	0.0 – 175.0
Volume	Total solvent-accessible volume in cubic angstroms using a probe with a 1.4 Å radius.	500.0 – 2000.0
donorHB	Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution.	0.0 – 6.0
accptHB	Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution.	2.0 – 20.0
Dip^2/V	Square of the dipole moment divided by the molecular volume.	0.0 – 0.13
ACxDN^.5/SA	Index of cohesive interaction in solids.	0.0 – 0.05
glob	Globularity descriptor	0.75 – 0.95
QPpolrz	Predicted polarizability in cubic angstroms.	13.0 – 70.0
QPlogPC16	Predicted hexadecane/gas partition coefficient.	4.0 – 18.0
QPlogoct	Predicted octanol/gas partition coefficient.	8.0 – 35.0
QPlogPw	Predicted water/gas partition coefficient.	4.0 – 45.0
QPlogPo/w	Predicted octanol/water partition coefficient.	–2.0 – 6.5
QPlogS	Predicted aqueous solubility, log S.	–6.5 – 0.5
CIQPlogS	Conformation-independent predicted aqueous solubility	–6.5 – 0.5
QPlogHERG	Predicted IC50 value for blockage of HERG K^+ channels.	concern below –5
QPPCaco	Predicted apparent Caco-2 cell permeability in nm/sec.	<25 poor, >500 great
QPlogBB	Predicted brain/blood partition coefficient.	–3.0 – 1.2
QPPMDCK	Predicted apparent MDCK cell permeability in nm/sec.	<25 poor, >500 great
QPlogKp	Predicted skin permeability, log Kp.	–8.0 – –1.0
IP(eV)	PM3 calculated ionization potential (negative of HOMO energy).	7.9 – 10.5
EA(eV)	PM3 calculated electron affinity (negative of LUMO energy).	–0.9 – 1.7

#metab	Number of likely metabolic reactions.	1 – 8
QPlogKhsa	Prediction of binding to human serum albumin.	–1.5 – 1.5
HumanOralAbsoprtion	Predicted qualitative human oral absorption	1, 2, or 3 for low, medium, or high
PercentHumanOralAbsoprtion	Predicted human oral absorption on 0 to 100% scale.	>80% is high <25% is poor
SAfluorine	Solvent-accessible surface area of fluorine atoms.	0.0 – 100.0
SAamideO	Solvent-accessible surface area of amide oxygen atoms.	0.0 – 35.0
PSA	Van der Waals surface area of polar nitrogen and oxygen atoms and carbonyl carbon atoms.	7.0 – 200.0
#NandO	Number of nitrogen and oxygen atoms.	2 – 15
RuleOfFive	Number of violations of Lipinski's rule of five	maximum is 4
RuleOfThree	Number of violations of Jorgensen's rule of three.	maximum is 3
#ringatoms	Number of atoms in a ring	
#in34	Number of atoms in 3- or 4-membered rings	
#in56	Number of atoms in 5- or 6-membered rings	
#nonHatm	Number of heavy atoms (nonhydrogen atoms)	
Jm	Predicted maximum transdermal transport rate	

Table S2. The predicted ADME properties for top 20 best compounds including reference compound from the SwissADME server.

Compound	GI absorption	BBB permeant	CYP1A2	CYP2C19	CYP2C9	CYP2D6	CYP3A4	Lipinksi rule	PAINS	Brenk
Crystal Structure (PDB ID:6W6Y)	Low	No	No	No	No	No	No	Yes; 1 violation: NorO>10	0 alert	1 alert: phosphor
ZINC000000082673	High	No	Yes	No	Yes	Yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000036569382	High	No	No	No	No	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000003830180	Low	No	No	No	No	No	No	Yes; 1 violation: NorO>10	0 alert	1 alert: phosphor
ZINC000006112607	High	No	Yes	No	No	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000014116837	High	No	No	Yes	Yes	No	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000121003678	High	Yes	Yes	Yes	Yes	Yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000217844024	High	No	Yes	No	No	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000096223736	High	No	Yes	Yes	Yes	Yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000097036564	High	No	Yes	No	No	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000237938532	High	No	No	No	No	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000096232566	High	No	Yes	No	No	Yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000003869813	Low	No	No	No	No	No	No	Yes; 1 violation: NorO>10	0 alert	1 alert: phosphor
ZINC000097036607	High	No	No	No	No	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000097036605	High	No	No	Yes	Yes	No	No	Yes; 0 violation	0 alert	0 alert
ZINC000079784201	High	No	Yes	Yes	No	Yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000426746041	High	No	Yes	Yes	No	yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000113844870	Low	No	No	No	No	No	No	Yes; 1 violation: NorO>10	0 alert	2 alerts: het-C-het_not_in_ring, phosphor
ZINC000000001793	Low	No	No	No	No	No	No	Yes; 0 violation	0 alert	1 alert: isolated_alkene
ZINC000009504042	High	No	Yes	Yes	Yes	Yes	Yes	Yes; 0 violation	0 alert	0 alert
ZINC000005615258	Low	No	No	No	No	No	No	Yes; 1 violation: NorO>10	0 alert	1 alert: phosphor

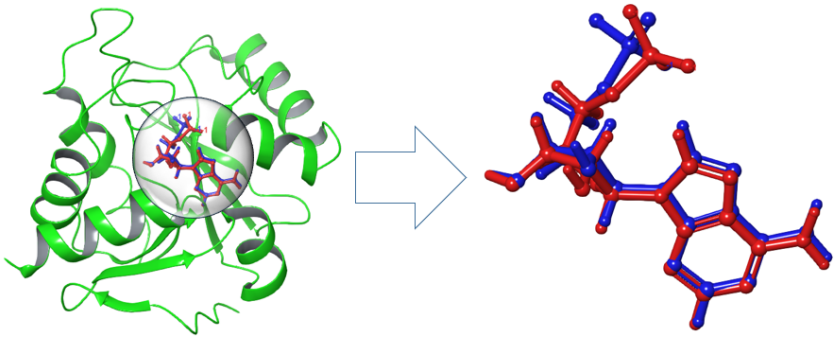


Figure S1. Comparison between the docked pose (red) and the crystal (blue) binding pose of ADP to NSP3 (ADP ribose phosphatase, PDB ID: 6W6Y).

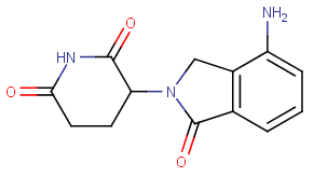
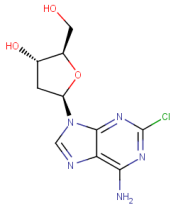
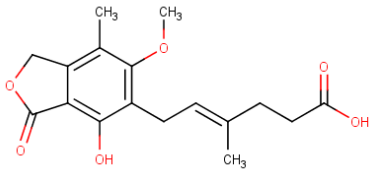
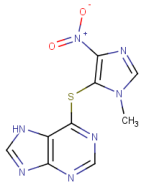
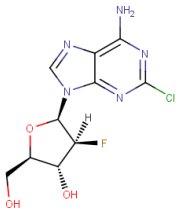
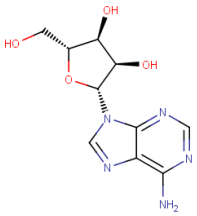
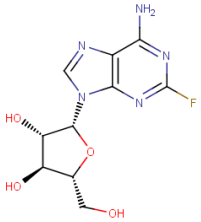
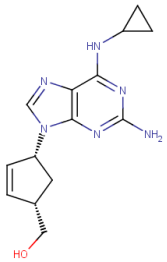
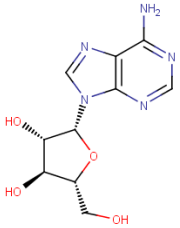
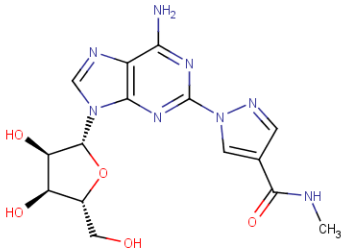
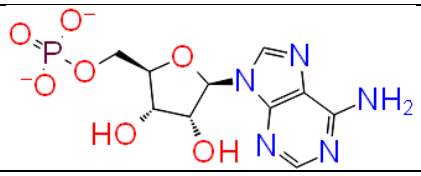
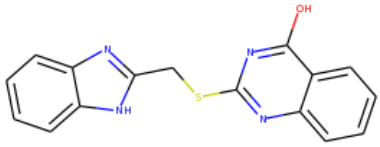
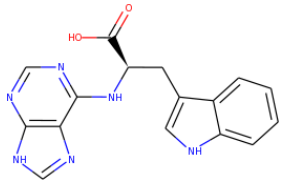
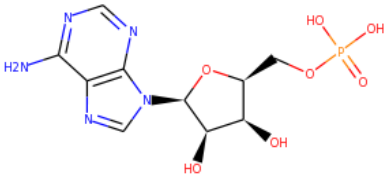
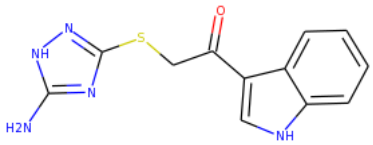
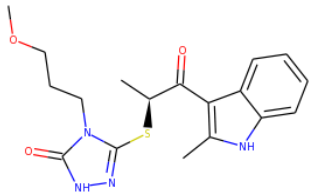
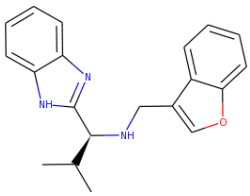
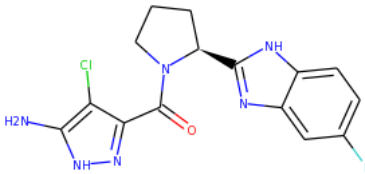
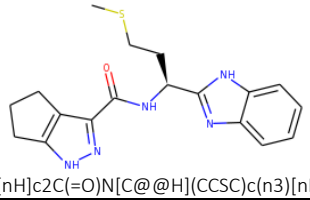
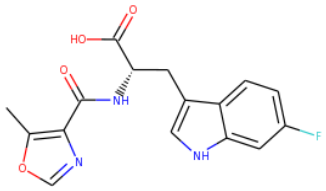
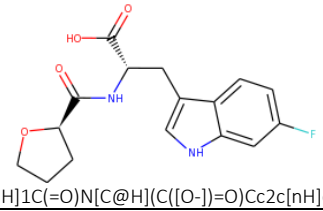
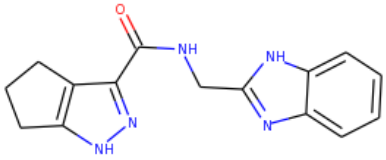
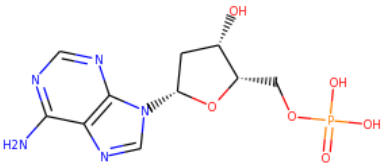
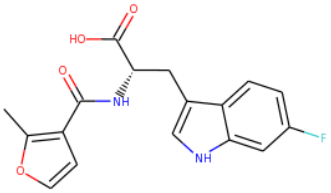
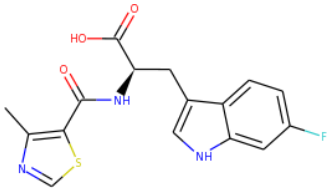
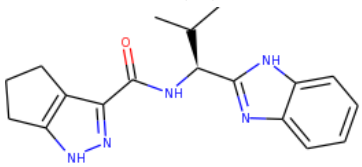
No	FDA approved drugs/ Structure/ Docking score	No	FDA approved drugs/ Structure/ Docking score
1	Ladevina; Lenangio  Docking Score: -7.788 kcal/mol	6	Cladribine  Docking Score: -7.626 kcal/mol
2	Mycophenolic acid  Docking Score: -7.758 kcal/mol	7	Azathioprine  Docking Score: -7.610 kcal/mol
3	Clofarabine  Docking Score: -7.757 kcal/mol	8	Adenosine  Docking Score: -7.573 kcal/mol
4	Fludarabine  Docking Score: -7.709 kcal/mol	9	Abacavir  Docking Score: -7.251 kcal/mol
5	Vidarabine  Docking Score: -7.700 kcal/mol	10	Regadenoson  Docking Score: -7.201 kcal/mol

Figure S2. Top ten hits from the FDA approved drug compounds.

No	Zinc ID/ Structure/ SMILE_code	Docking score	# STAR	# Cluster ID	Centroid
Ref. Comp		-9.752 kcal/mol	0	11	No Centroid
1	ZINC000000082673  c1cccc(c12)[nH]c(n2)CSc([nH]c3=O)nc(c34)cccc4	−11.691 kcal/mol	0	11	No Centroid
2	ZINC000036569382  n1c[nH]c(c12)ncnc2N[C@@H](C([O-])=O)Cc3c[nH]c(c34)cccc4	−11.642 kcal/mol	0	11	No Centroid
3	ZINC000003830180  [O-]P([O-])(=O)OC[C@H]1[C@@H](O)[C@@H](O)[C@H](O1)n(cn2)c(c23)ncnc3N	−11.050 kcal/mol	0	11	No Centroid
4	ZINC000006112607  Nc1nc([nH]n1)SCC(=O)c2c[nH]c(c23)cccc3	−10.952 kcal/mol	0	11	No Centroid
5	ZINC000014116837  c1cccc(c12)[nH]c(C)c2C(=O)[C@H](C)Sc(n[nH]3)n(c3=O)CCCOC	−10.909 kcal/mol	0	11	No Centroid
6	ZINC000121003678  c1cccc(c12)[nH]c(n2)[C@H](C(C)C)NCc3coc(c34)cccc4	−10.772 kcal/mol	0	11	No Centroid
7	ZINC000217844024  [nH]1nc(N)c(Cl)c1C(=O)N2CCC[C@H]2c(n3)[nH]c(c34)ccc(F)c4	−10.765 kcal/mol	0	11	No Centroid

8	ZINC000096223736  C1CCc(c12)n[nH]c2C(=O)N[C@@H](CCSC)c(n3)[nH]c(c34)cccc4	−10.486 kcal/mol	0	11	No Centroid
9	ZINC000097036564  n1coc(C)c1C(=O)N[C@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3	−10.427 kcal/mol	0	11	No Centroid
10	ZINC000237938532  O1CCC[C@@H]1C(=O)N[C@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3	−10.414 kcal/mol	0	11	No Centroid
11	ZINC000096232566  C1CCc(c12)n[nH]c2C(=O)NCc(n3)[nH]c(c34)cccc4	−10.411 kcal/mol	0	11	No Centroid
12	ZINC000003869813  [O-]P([O-])(=O)OC[C@H]1[C@@H](O)C[C@H](O1)n(cn2)c(c23)ncnc3N	−10.409 kcal/mol	0	11	No Centroid
13	ZINC000097036607  c1coc(C)c1C(=O)N[C@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3	−10.373 kcal/mol	0	11	No Centroid
14	ZINC000097036605  s1cnc(C)c1C(=O)N[C@@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3	−10.344 kcal/mol	0	11	No Centroid
15	ZINC000079784201  C1CCc(c12)n[nH]c2C(=O)N[C@@H](C(C)C)c(n3)[nH]c(c34)cccc4	−10.336 kcal/mol	0	11	No Centroid

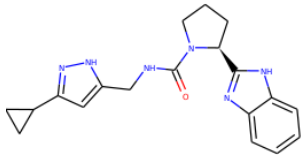
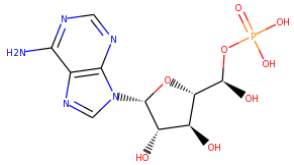
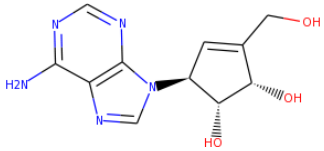
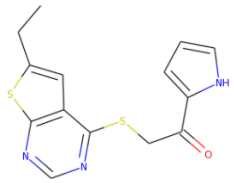
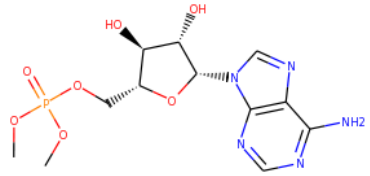
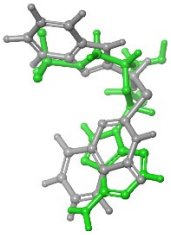
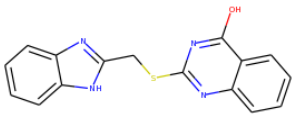
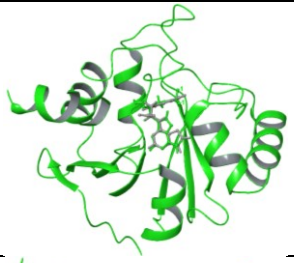
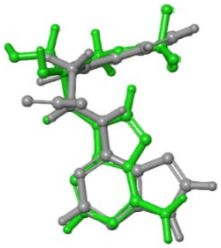
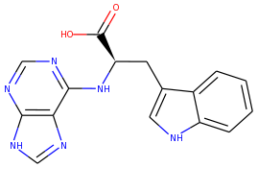
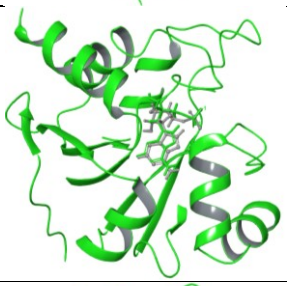
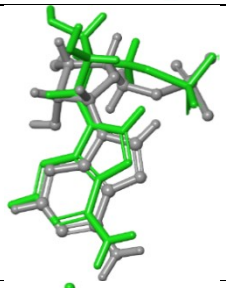
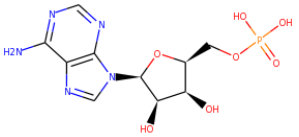
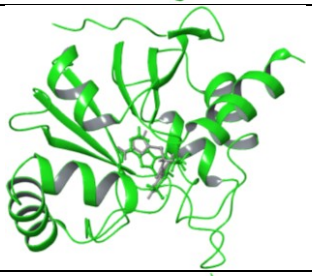
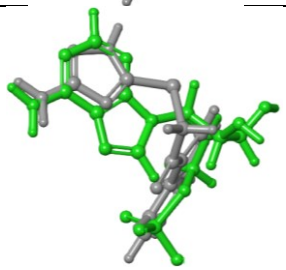
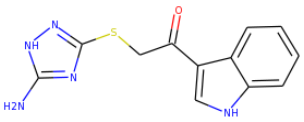
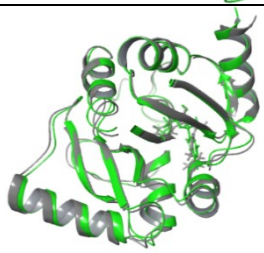
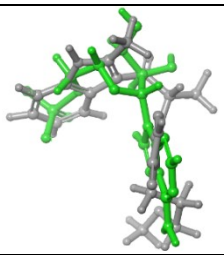
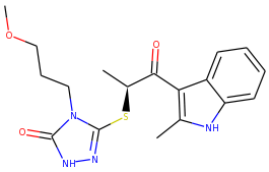
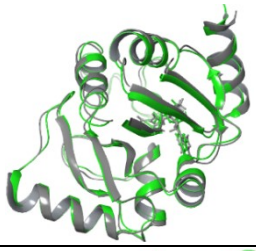
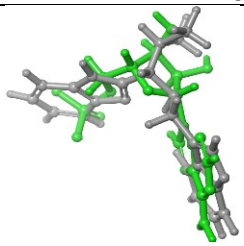
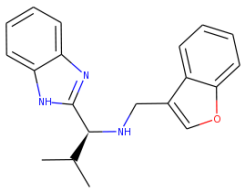
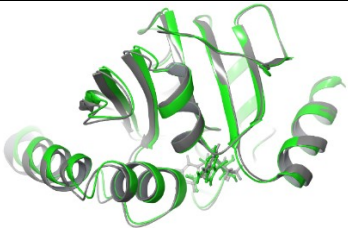
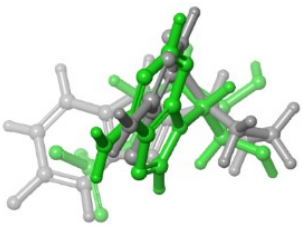
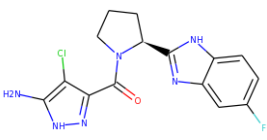
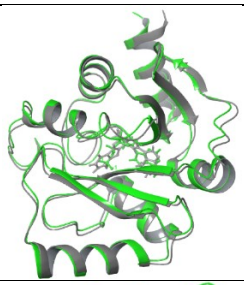
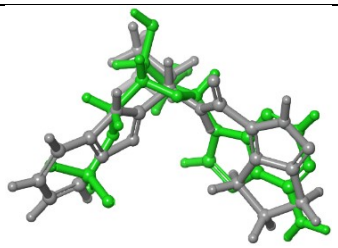
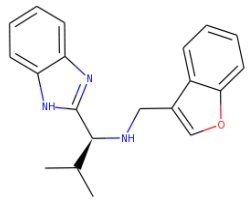
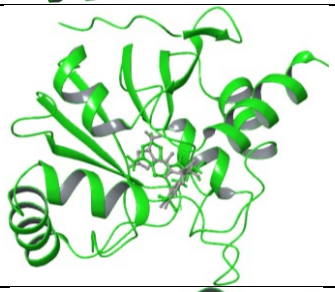
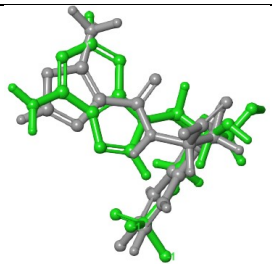
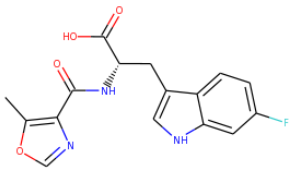
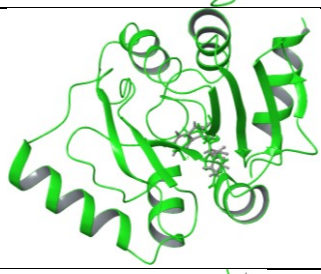
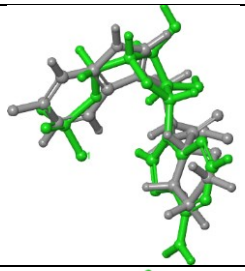
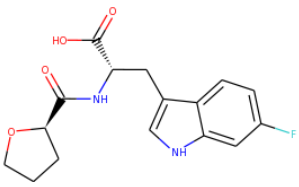
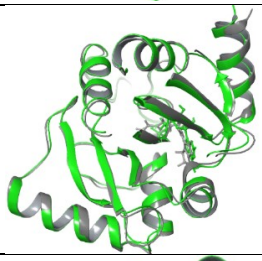
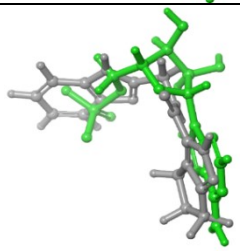
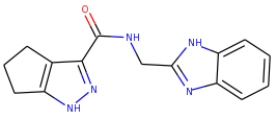
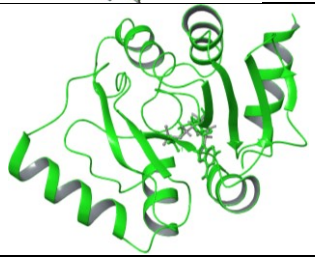
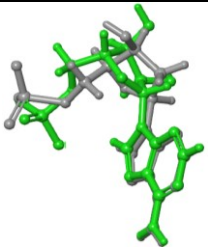
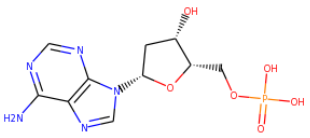
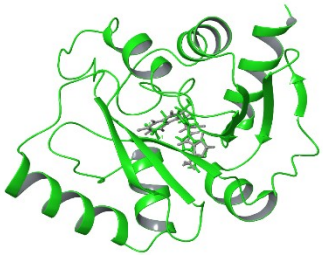
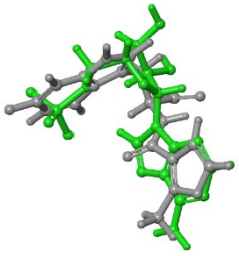
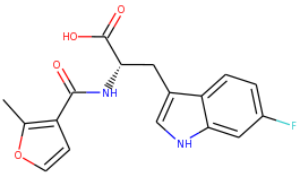
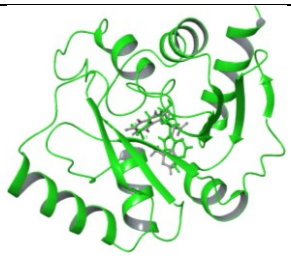
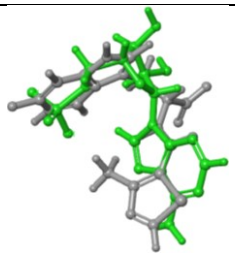
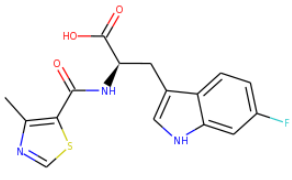
16	ZINC000426746041  C1CC1c([nH]n2)cc2CNC(=O)N3CCC[C@H]3c(n4)[nH]c(c45)cccc5	−10.300 kcal/mol	0	11	No Centroid
17	ZINC000113844870  [O-]P([O-])(=O)O[C@@H](O)[C@@H]1[C@@H](O)[C@H](O)[C@@H](O1)n(cn2)c(c23)ncnc3N	−10.229 kcal/mol	3	11	No Centroid
18	ZINC000000001793  OCC1=C[C@@H]([C@@H](O)[C@H]1O)n(cn2)c(c23)ncnc3N	−10.202 kcal/mol	0	11	No Centroid
19	ZINC000009504042  [nH]1cccc1C(=O)CSc2ncnc(c23)sc(c3)CC	−10.195 kcal/mol	0	11	No Centroid
20	ZINC000005615258  COP(=O)(OC)OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O1)n(cn2)c(c23)ncnc3N	−9.897 kcal/mol	0	11	No Centroid

Figure S3. The table represents Zinc ID, structure, SMILE code, docking score, numbers of STARs (represent if the molecule is drug like), cluster IDs (ligand similarity clustering is based on Canvas), and centroid (measures distances to the arithmetic means of clusters) of the top twenty zinc compounds including the reference compound.

	Protein-Ligand Complexes	Crystal Ligand Structure	Ligand Interaction
ZINC000082673			
ZINC036569382			
ZINC003830180			
ZINC006112607			
ZINC014116837			
ZINC121003678			
ZINC217844024			

ZINC096223736			
ZINC097036564			
ZINC237938532			
ZINC096232566			
ZINC003869813			
ZINC097036607			
ZINC097036605			

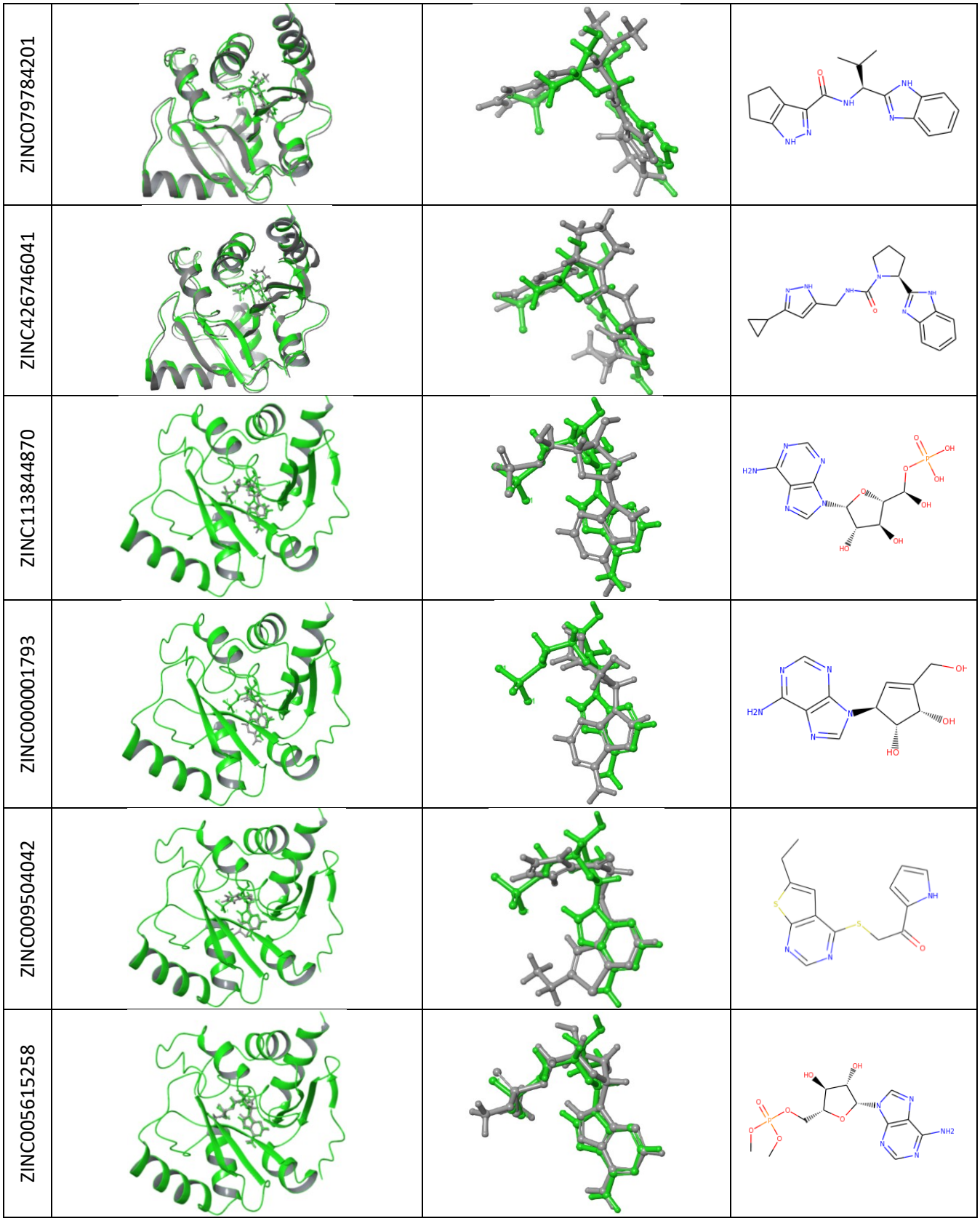
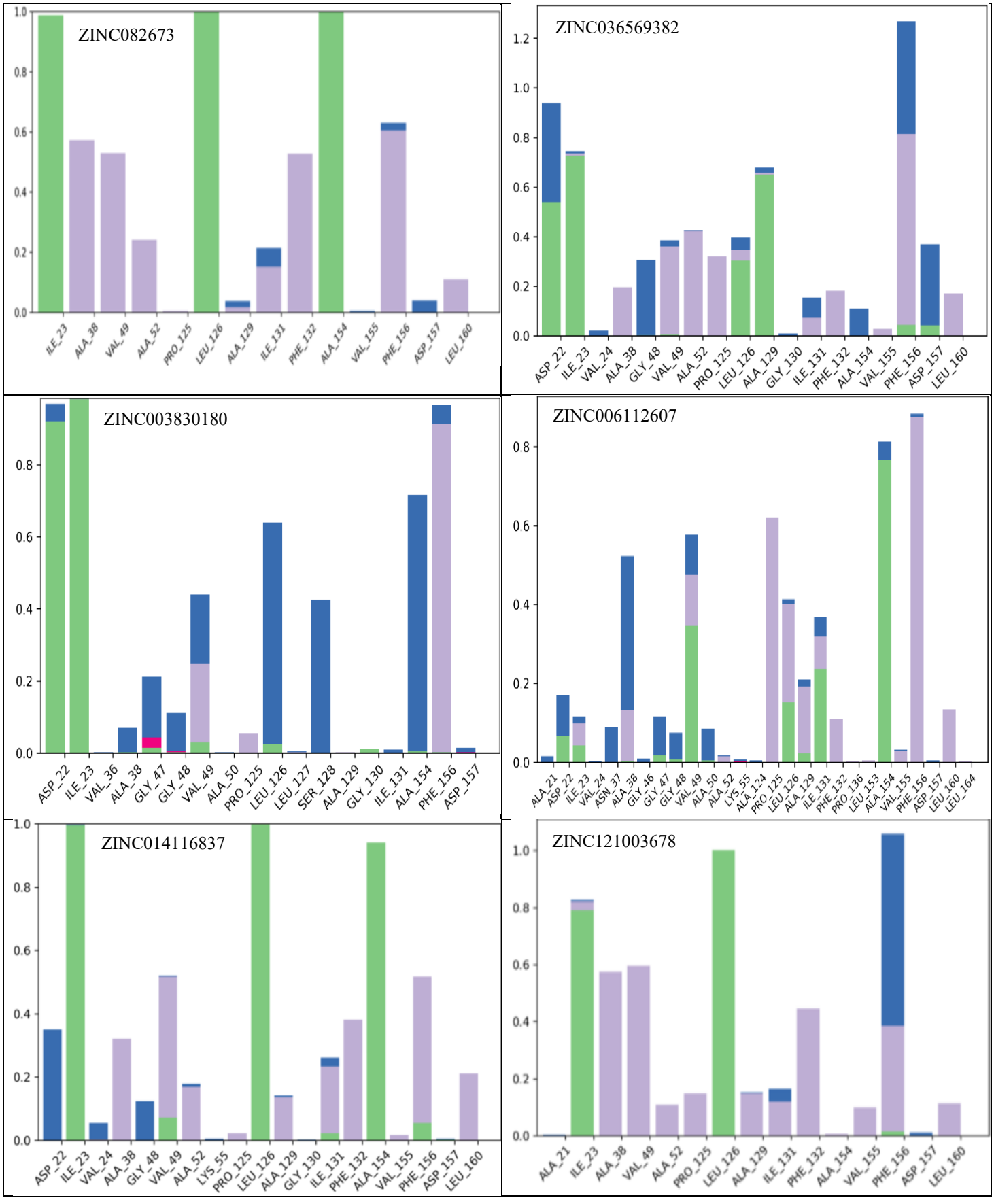


Figure S4. Comparison between the docked complex (gray) of the top twenty ligands and the crystal complex structure (green). The last column represents the ligand chemical structure.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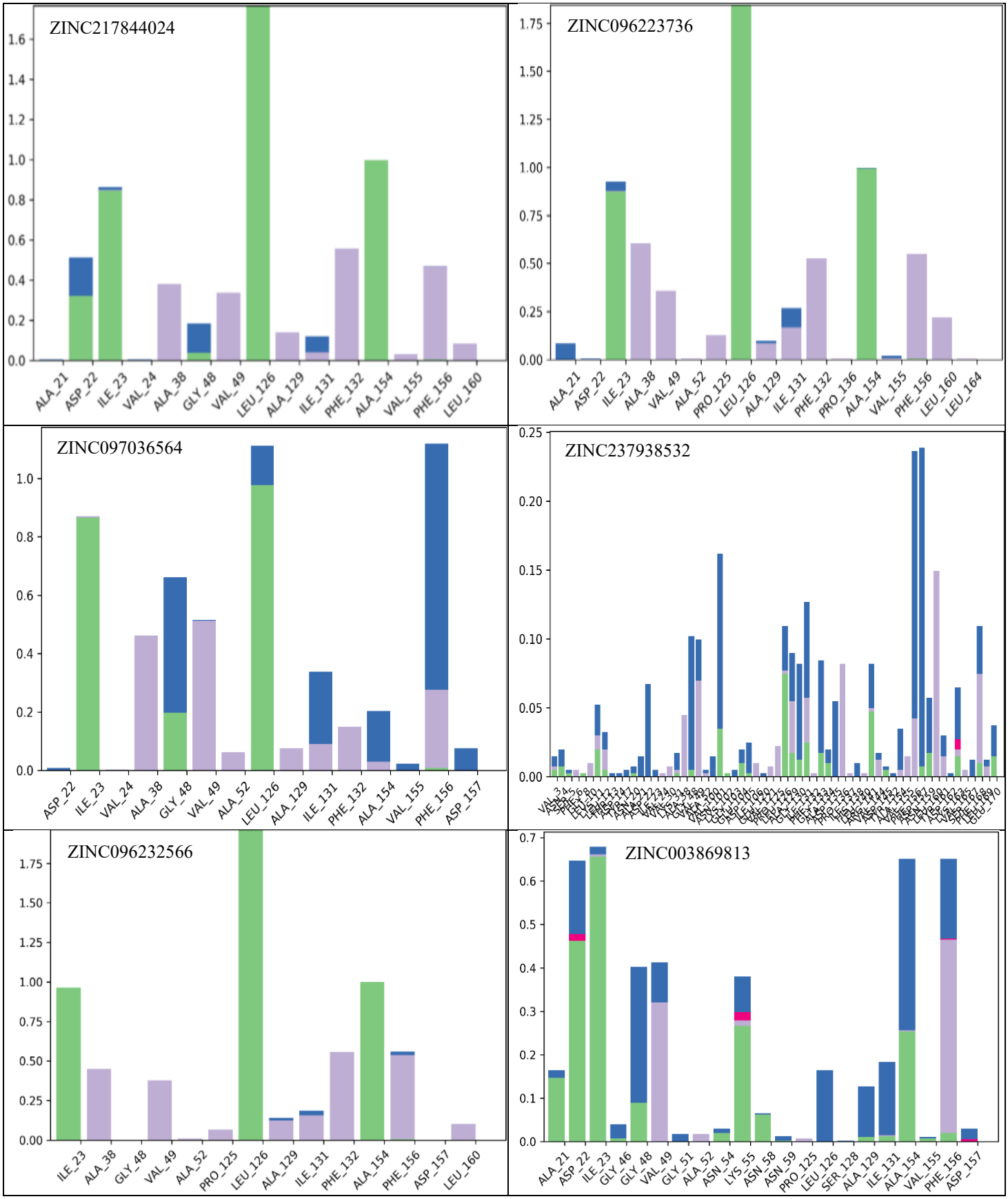
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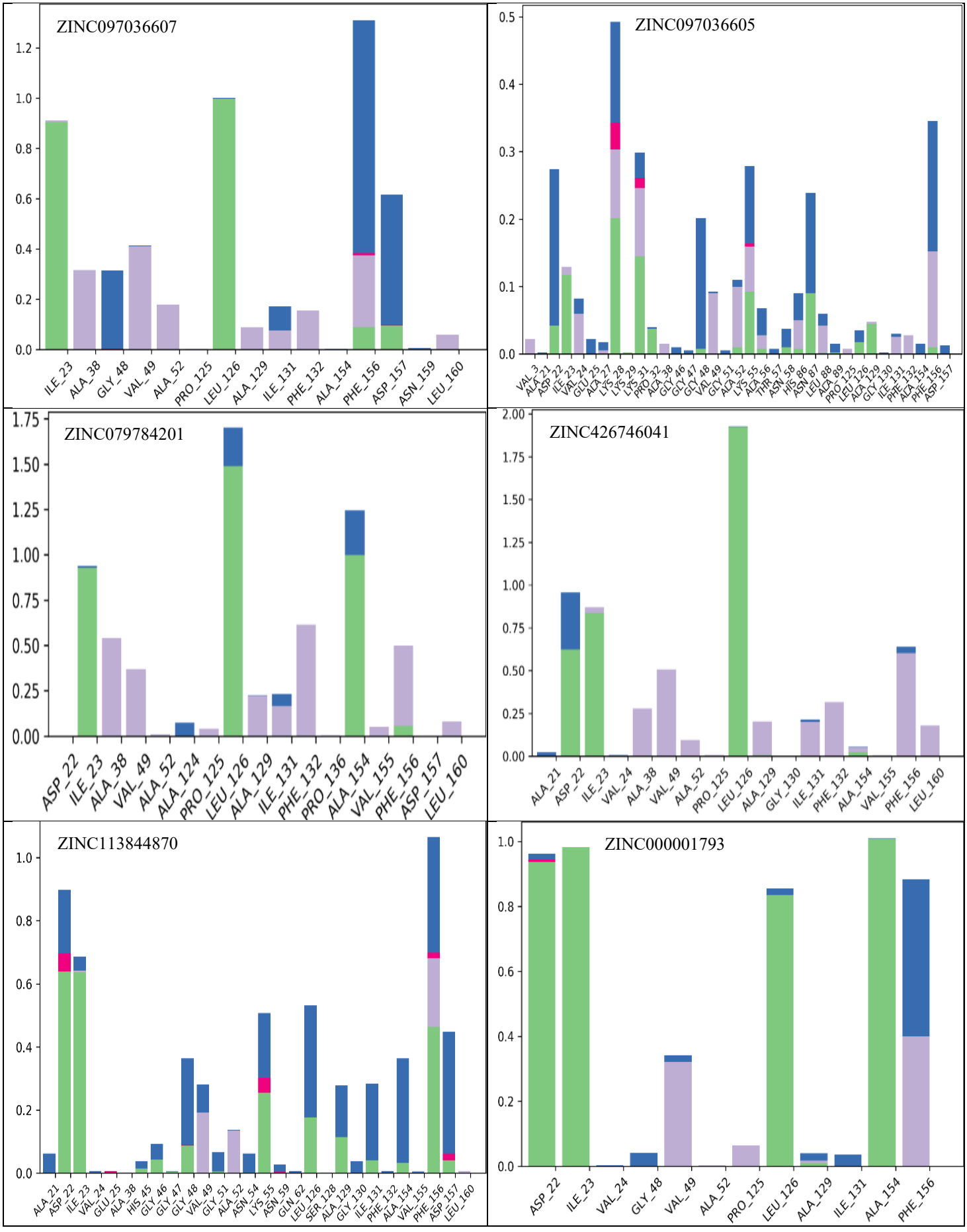
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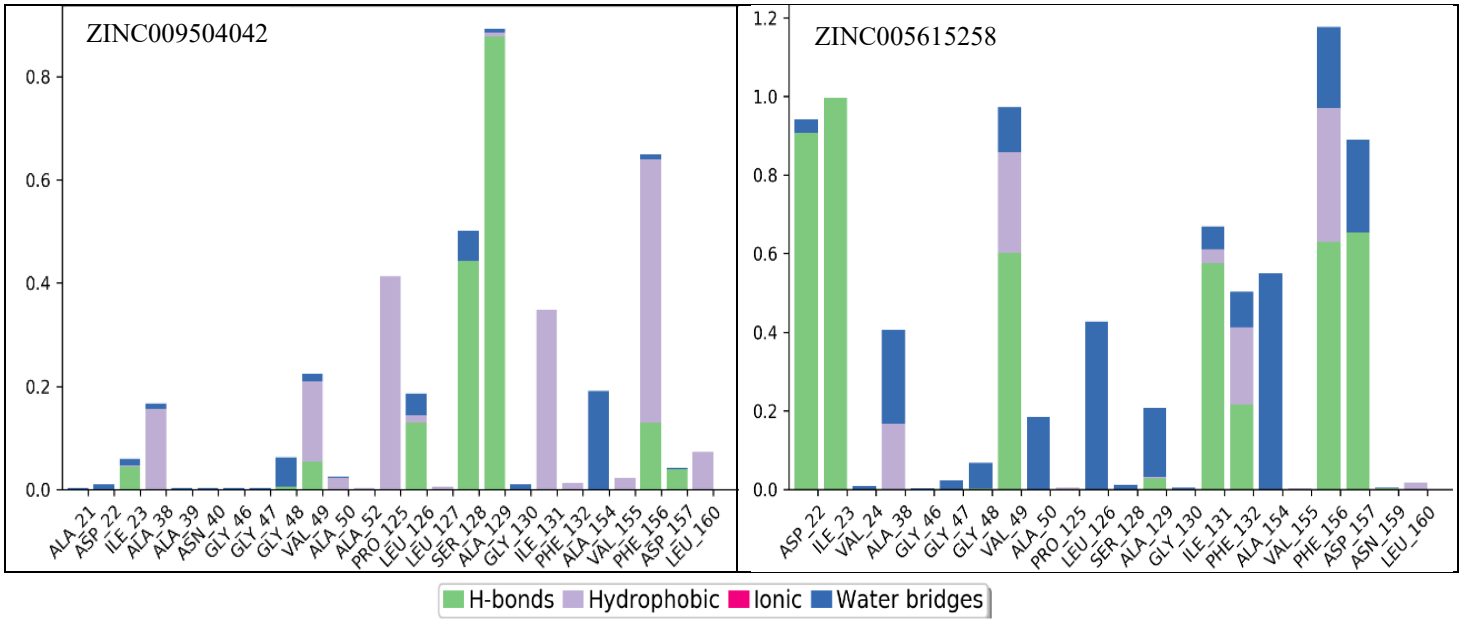
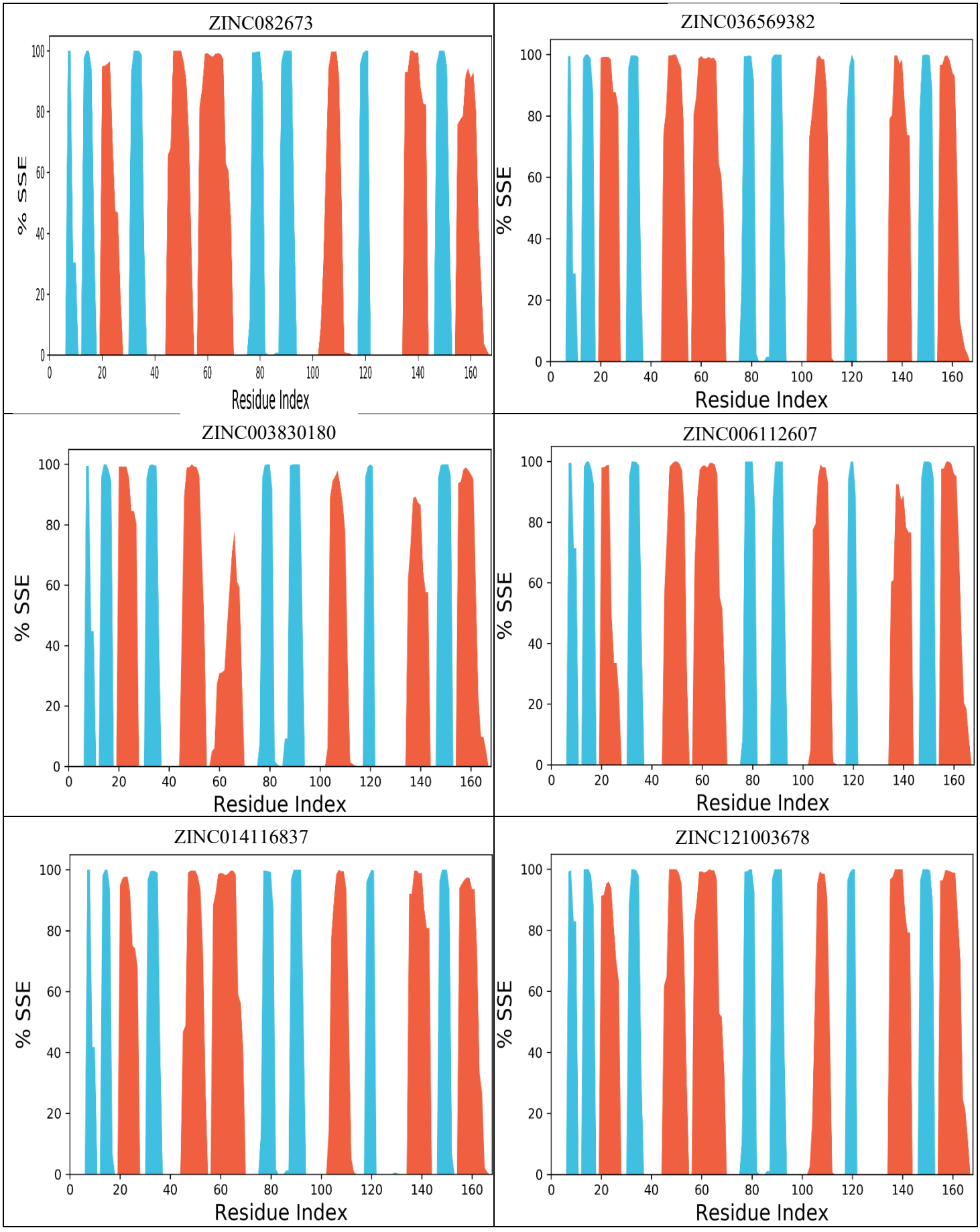


Figure S5. Protein-Ligand contacts during MD simulations for top eight compounds. Interaction fraction greater than 1 is possible because of multiple contacts on one residue.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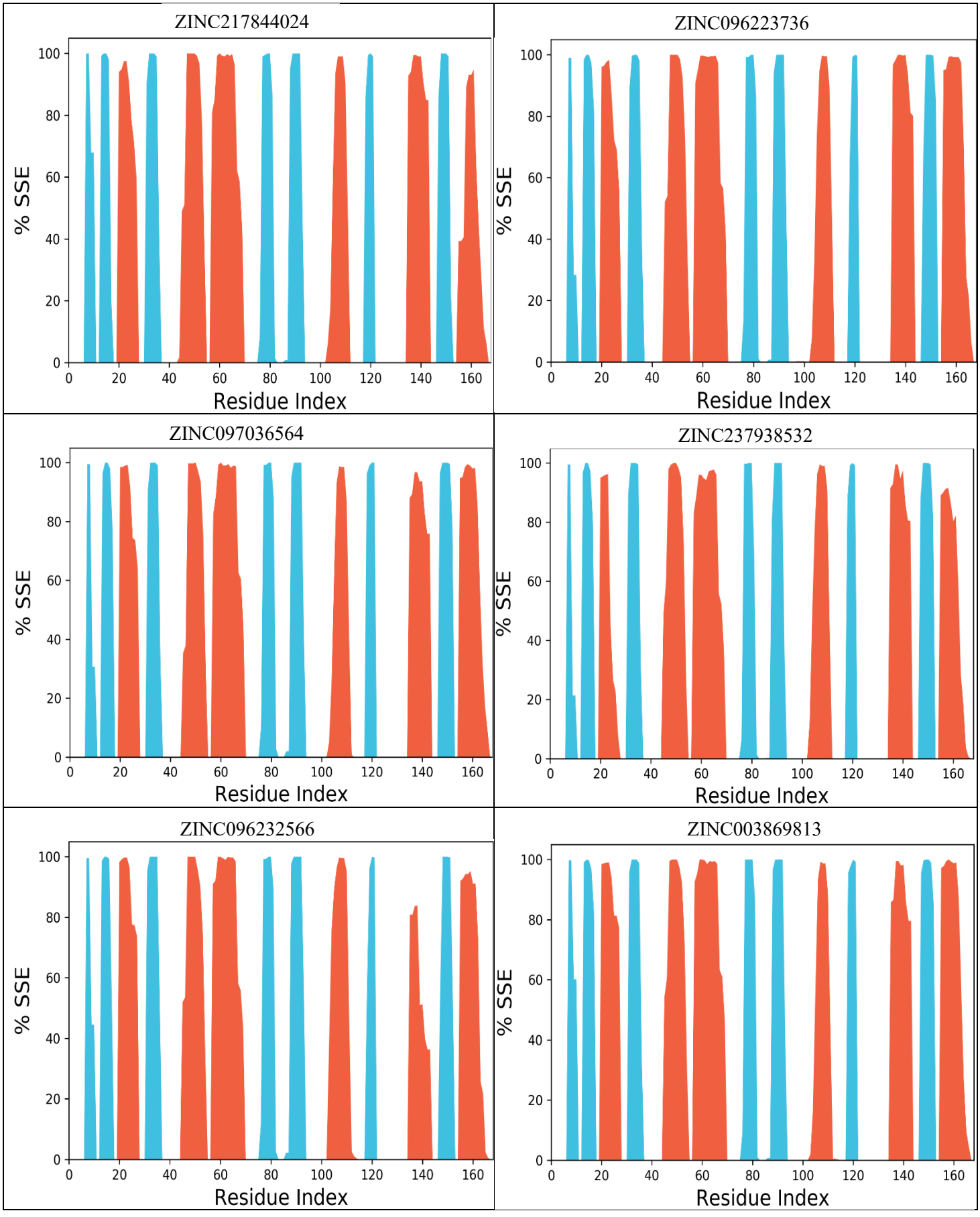
% SSE
Residue Index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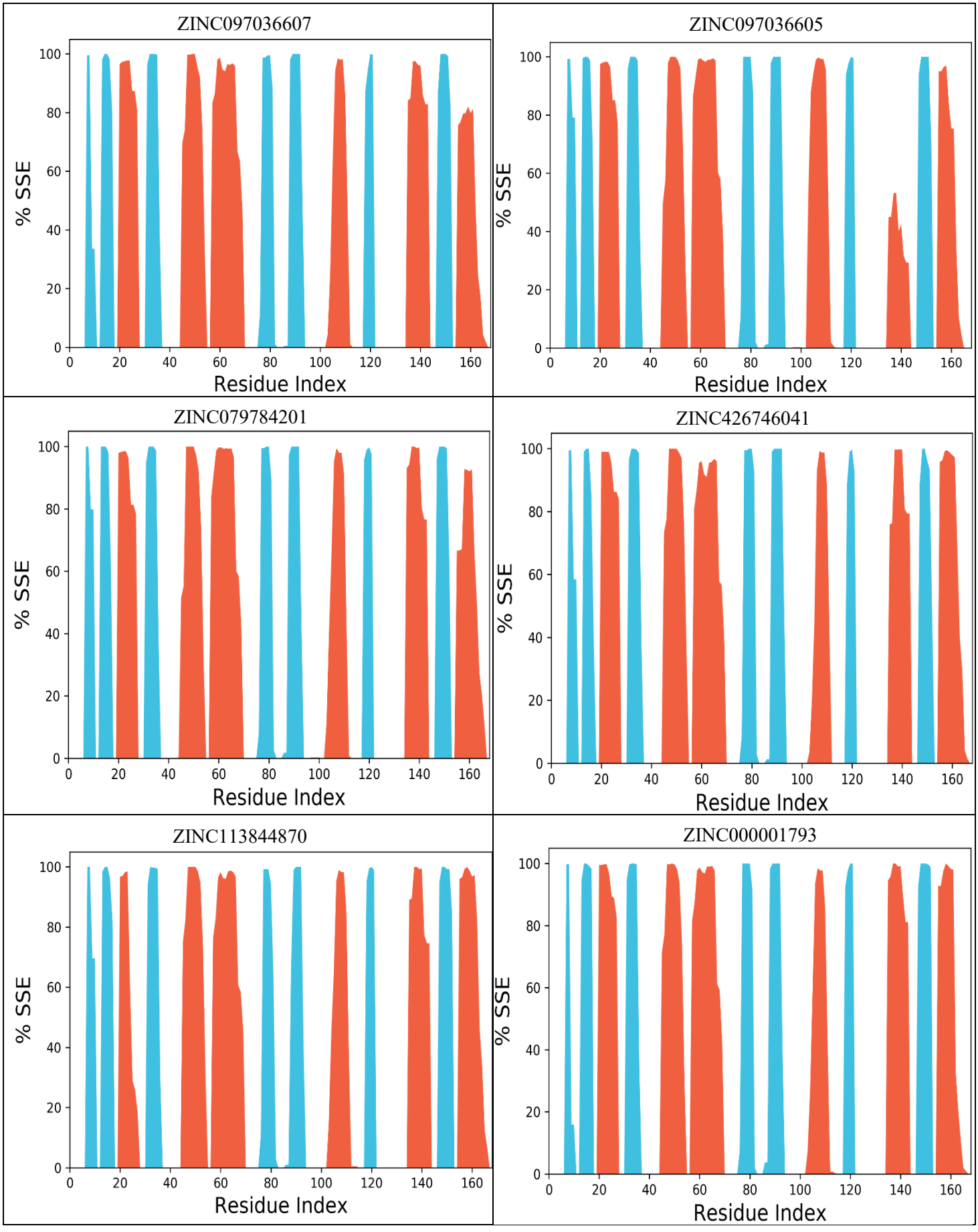
% SSE
Residue Index
0
20
40
60
80
100
120
140
160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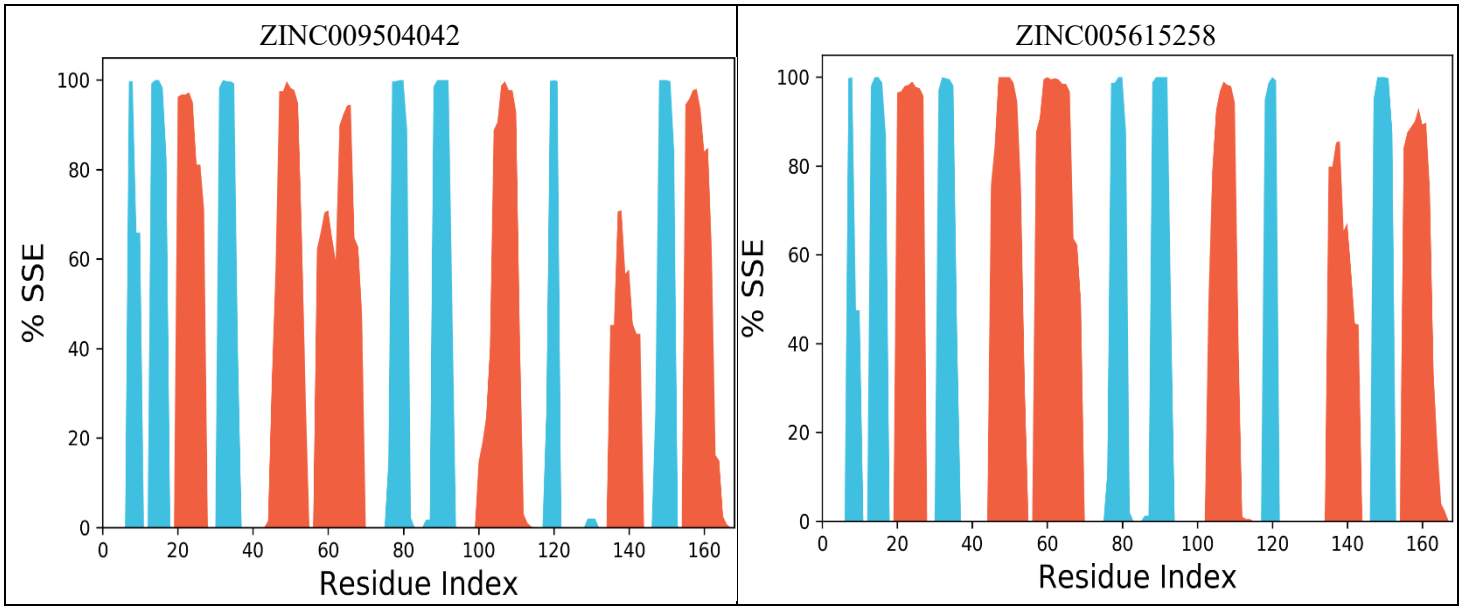


Figure S6. Protein Secondary Structure elements for the top twenty compounds. Red represents alpha helices and blue represents beta sheets and the white places represent random coil.

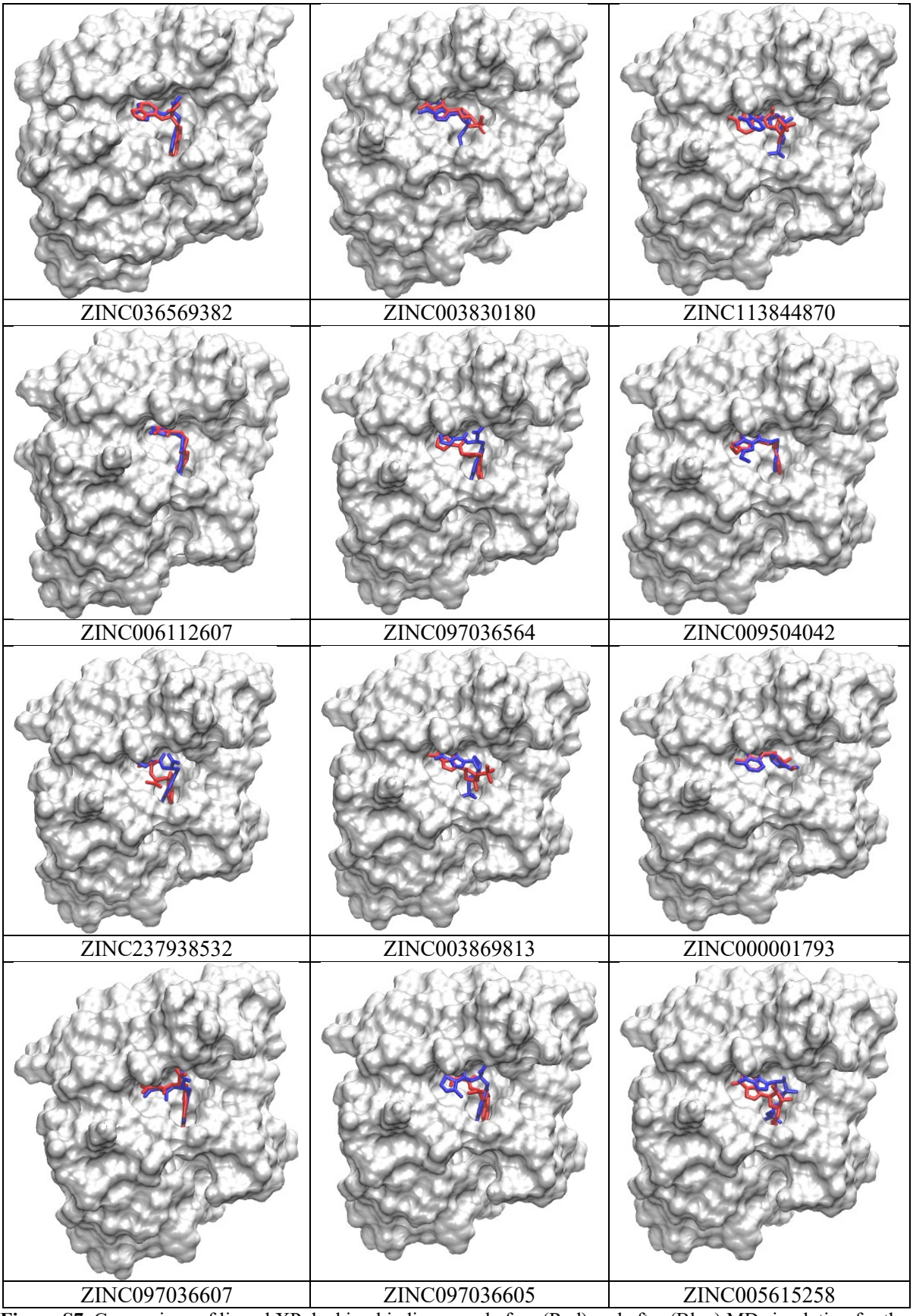
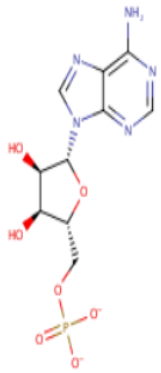
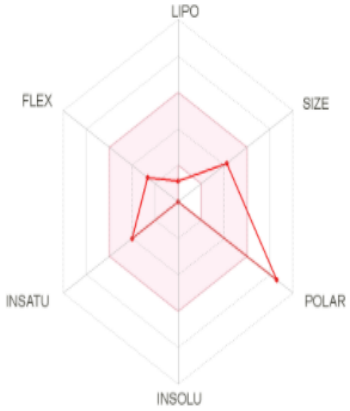


Figure S7. Comparison of ligand XP docking binding pose before (Red) and after (Blue) MD simulation for the twelve ligands.

Ref. Compound	6W6Y	[O-]P([O-])(=O)OC[C@@H]1[C@@H](O)[C@@H](O)[C@@H](O1)n(cn2)c(c23)ncnc3N

Reference Molecule (6W6Y)





SMILES O[C@@H]1[C@H](O)[C@H](O[C@H]1n1cnc2c1ncnc2N)COP(=O)([O-])[O-]

Physicochemical Properties	
Formula	C10H12N5O7P
Molecular weight	345.21 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	9
Fraction Csp3	0.50
Num. rotatable bonds	4
Num. H-bond acceptors	10
Num. H-bond donors	3
Molar Refractivity	70.52
TPSA	201.54 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	-0.59
Log $P_{o/w}$ (XLOGP3)	-3.52
Log $P_{o/w}$ (WLOGP)	-1.30
Log $P_{o/w}$ (MLOGP)	-3.06
Log $P_{o/w}$ (SILICOS-IT)	-3.53
Consensus Log $P_{o/w}$	-2.40

Water Solubility	
Log S (ESOL)	0.21
Solubility	5.62e+02 mg/ml ; 1.63e+00 mol/l
Class	Highly soluble
Log S (Ali)	-0.13
Solubility	2.55e+02 mg/ml ; 7.40e-01 mol/l
Class	Very soluble
Log S (SILICOS-IT)	1.26
Solubility	6.34e+03 mg/ml ; 1.84e+01 mol/l
Class	Soluble

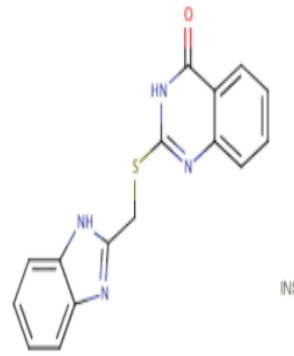
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-10.90 cm/s

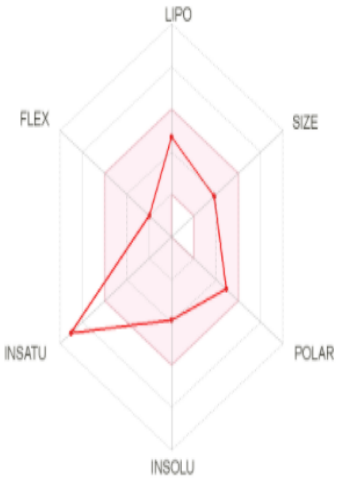
Druglikeness	
Lipinski	Yes; 1 violation: NorO>10
Ghose	No; 1 violation: WLOGP<-0.4
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 2 violations: XLOGP3<-2, TPSA>150
Bioavailability Score	0.11

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: phosphor
Leadlikeness	Yes
Synthetic accessibility	4.28

1	ZINC000000082673	c1cccc(c12)[nH]c(n2)CSc([nH]c3=O)nc(c34)cccc4

2-[(4-Azidosulfanylphenoxy)methyl]quinoline





SMILES O=c1[nH]c(SCc2nc3c([nH]2)cccc3)nc2c1cccc2

Physicochemical Properties	
Formula	C16H12N4OS
Molecular weight	308.36 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	19
Fraction Csp3	0.06
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	2
Molar Refractivity	88.22
TPSA	99.73 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.81
Log $P_{o/w}$ (XLOGP3)	2.73
Log $P_{o/w}$ (WLOGP)	2.94
Log $P_{o/w}$ (MLOGP)	1.84
Log $P_{o/w}$ (SILICOS-IT)	4.00
Consensus Log $P_{o/w}$	2.66

Water Solubility	
Log *S* (ESOL)	-3.91
Solubility	3.77e-02 mg/ml ; 1.22e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.48
Solubility	1.02e-02 mg/ml ; 3.32e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.77
Solubility	5.27e-05 mg/ml ; 1.71e-07 mol/l
Class	Poorly soluble

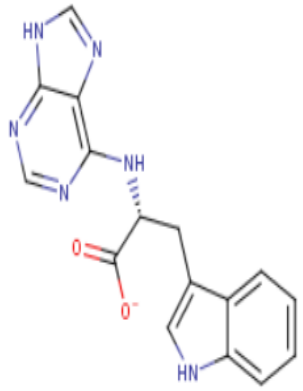
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.24 cm/s

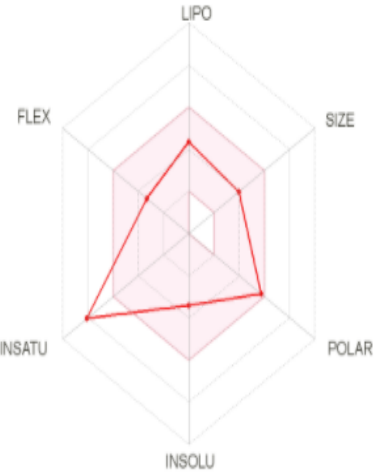
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	2.63

2	ZINC000036569382	n1c[nH]c(c12)ncnc2N[C@@H](C([O-])=O)Cc3c[nH]c(c34)cccc4

Molecule 1





SMILES [O-]C(=O)[C@H](Nc1ncnc2c1nc[nH]2)Cc1c[nH]c2c1cccc2

Physicochemical Properties	
Formula	C16H13N6O2
Molecular weight	321.31 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	18
Fraction Csp3	0.12
Num. rotatable bonds	5
Num. H-bond acceptors	5
Num. H-bond donors	3
Molar Refractivity	86.78
TPSA	122.41 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.65
Log $P_{o/w}$ (XLOGP3)	2.13
Log $P_{o/w}$ (WLOGP)	0.42
Log $P_{o/w}$ (MLOGP)	-1.52
Log $P_{o/w}$ (SILICOS-IT)	2.00
Consensus Log $P_{o/w}$	0.74

Water Solubility	
Log *S* (ESOL)	-3.40
Solubility	1.28e-01 mg/ml ; 3.99e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.33
Solubility	1.50e-02 mg/ml ; 4.65e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.43
Solubility	1.20e-03 mg/ml ; 3.75e-06 mol/l
Class	Moderately soluble

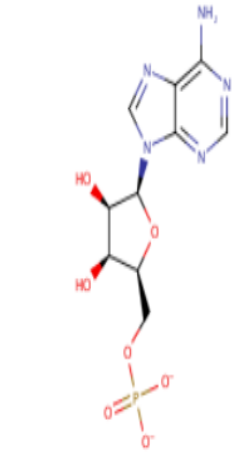
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.75 cm/s

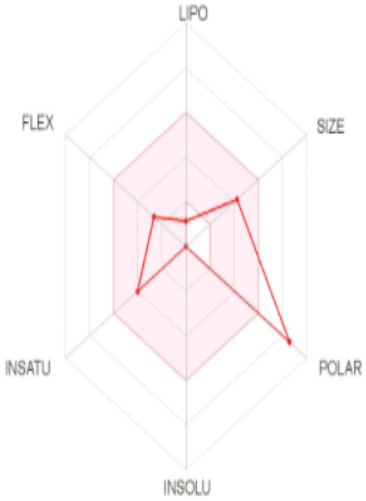
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	2.94

3	ZINC000003830180	[O-]P([O-])(=O)OC[C@H]1[C@@H](O)[C@@H](O)[C@H](O1)n(cn2)c(c23)ncnc3N

Cyclic guanosine monophosphate





SMILES O[C@@H]1[C@H](O)[C@@H](O[C@@H]1n1cnc2c1ncnc2N)COP(=O)([O-])[O-]

Physicochemical Properties	
Formula	C10H12N5O7P
Molecular weight	345.21 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	9
Fraction Csp3	0.50
Num. rotatable bonds	4
Num. H-bond acceptors	10
Num. H-bond donors	3
Molar Refractivity	70.52
TPSA	201.54 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	-1.52
Log $P_{o/w}$ (XLOGP3)	-3.52
Log $P_{o/w}$ (WLOGP)	-1.30
Log $P_{o/w}$ (MLOGP)	-3.06
Log $P_{o/w}$ (SILICOS-IT)	-3.53
Consensus Log $P_{o/w}$	-2.59

Water Solubility	
Log *S* (ESOL)	0.21
Solubility	5.62e+02 mg/ml ; 1.63e+00 mol/l
Class	Highly soluble
Log *S* (Ali)	-0.13
Solubility	2.55e+02 mg/ml ; 7.40e-01 mol/l
Class	Very soluble
Log *S* (SILICOS-IT)	1.26
Solubility	6.34e+03 mg/ml ; 1.84e+01 mol/l
Class	Soluble

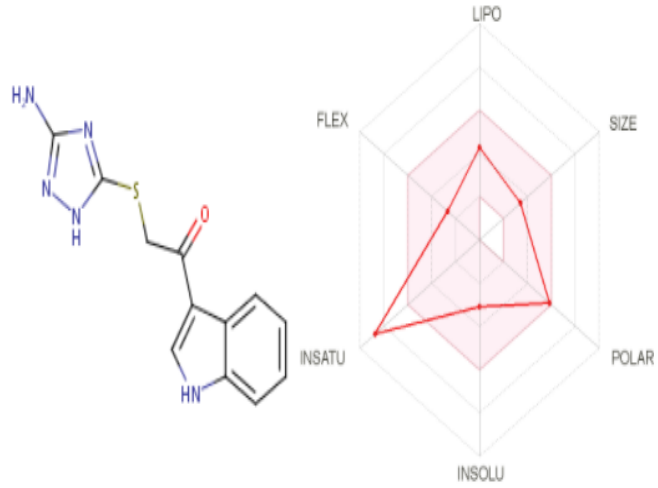
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-10.90 cm/s

Druglikeness	
Lipinski	Yes; 1 violation: NorO>10
Ghose	No; 1 violation: WLOGP<-0.4
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 2 violations: XLOGP3<-2, TPSA>150
Bioavailability Score	0.11

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: phosphor
Leadlikeness	Yes
Synthetic accessibility	4.28

4	ZINC000006112607	Nc1nc([nH]n1)SCC(=O)c2c[nH]c(c23)cccc3

Molecule 1



SMILES Nc1n[nH]c(n1)SCC(=O)c1c[nH]c2c1cccc2

Physicochemical Properties	
Formula	C12H11N5OS
Molecular weight	273.31 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	14
Fraction Csp3	0.08
Num. rotatable bonds	4
Num. H-bond acceptors	3
Num. H-bond donors	3
Molar Refractivity	74.08
TPSA	125.75 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.76
Log $P_{o/w}$ (XLOGP3)	2.02
Log $P_{o/w}$ (WLOGP)	1.85
Log $P_{o/w}$ (MLOGP)	0.34
Log $P_{o/w}$ (SILICOS-IT)	2.13
Consensus Log $P_{o/w}$	1.42

Water Solubility	
Log *S* (ESOL)	-3.09
Solubility	2.23e-01 mg/ml ; 8.16e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.29
Solubility	1.41e-02 mg/ml ; 5.15e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-4.37
Solubility	1.16e-02 mg/ml ; 4.26e-05 mol/l
Class	Moderately soluble

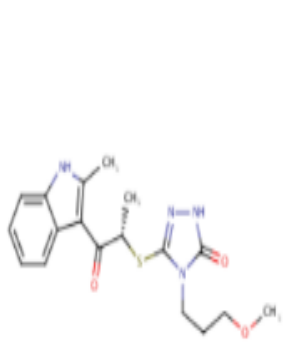
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.53 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	2.48

5	ZINC000014116837	c1cccc(c12)[nH]c(C)c2C(=O)[C@H](C)Sc(n[nH]3)n(c3=O)CCCOC

Molecule 1



SMILES COCCCn1c(n[nH]c1=O)S[C@H](C(=O)c1c(C)[nH]c2c1cccc2)C

Physicochemical Properties	
Formula	C18H22N4O3S
Molecular weight	374.46 g/mol
Num. heavy atoms	26
Num. arom. heavy atoms	14
Fraction Csp3	0.39
Num. rotatable bonds	8
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	102.68
TPSA	118.07 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.37
Log $P_{o/w}$ (XLOGP3)	2.87
Log $P_{o/w}$ (WLOGP)	2.76
Log $P_{o/w}$ (MLOGP)	1.54
Log $P_{o/w}$ (SILICOS-IT)	3.84
Consensus Log $P_{o/w}$	2.67

Water Solubility	
Log *S* (ESOL)	-3.84
Solubility	5.41e-02 mg/ml ; 1.44e-04 mol/l
Class	Soluble
Log *S* (Ali)	-5.01
Solubility	3.67e-03 mg/ml ; 9.80e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.51
Solubility	1.14e-03 mg/ml ; 3.05e-06 mol/l
Class	Moderately soluble

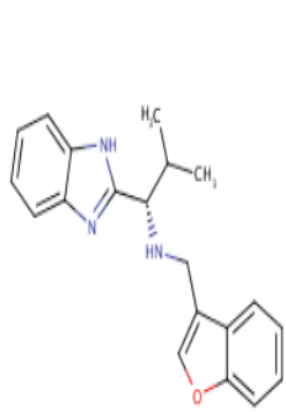
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.55 cm/s

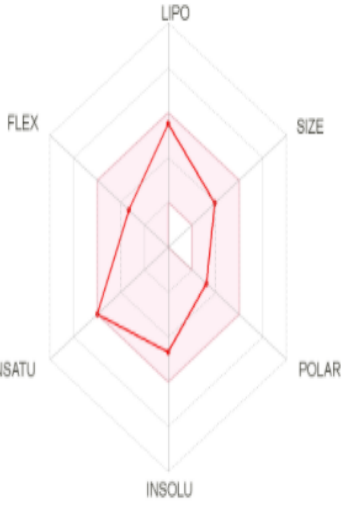
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 2 violations: MW>350, Rotors>7
Synthetic accessibility	3.69

6	ZINC000121003678	c1cccc(c12)[nH]c(n2)[C@H](C(C)C)NCc3coc(c34)cccc4

Molecule 1





SMILES CC([C@@H](c1nc2c([nH]1)cccc2)NCc1coc2c1cccc2)C

Physicochemical Properties	
Formula	C20H21N3O
Molecular weight	319.40 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	18
Fraction Csp3	0.25
Num. rotatable bonds	5
Num. H-bond acceptors	3
Num. H-bond donors	2
Molar Refractivity	97.35
TPSA	53.85 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.99
Log $P_{o/w}$ (XLOGP3)	4.15
Log $P_{o/w}$ (WLOGP)	4.32
Log $P_{o/w}$ (MLOGP)	2.64
Log $P_{o/w}$ (SILICOS-IT)	4.65
Consensus Log $P_{o/w}$	3.75

Water Solubility	
Log *S* (ESOL)	-4.66
Solubility	6.99e-03 mg/ml ; 2.19e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-4.99
Solubility	3.28e-03 mg/ml ; 1.03e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-7.62
Solubility	7.59e-06 mg/ml ; 2.38e-08 mol/l
Class	Poorly soluble

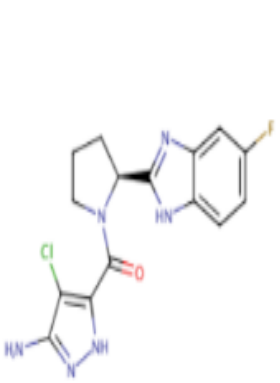
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-5.30 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.40

7	ZINC000217844024	[nH]1nc(N)c(Cl)c1C(=O)N2CCC[C@H]2c(n3)[nH]c(c34)ccc(F)c4

Molecule 1



SMILES Fc1ccc2c(c1)nc([nH]2)[C@@H]1CCCN1C(=O)c1[nH]nc(c1Cl)N

Physicochemical Properties	
Formula	C15H14ClFN6O
Molecular weight	348.76 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	14
Fraction Csp3	0.27
Num. rotatable bonds	3
Num. H-bond acceptors	4
Num. H-bond donors	3
Molar Refractivity	91.41
TPSA	103.69 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.50
Log $P_{o/w}$ (XLOGP3)	2.01
Log $P_{o/w}$ (WLOGP)	2.36
Log $P_{o/w}$ (MLOGP)	1.92
Log $P_{o/w}$ (SILICOS-IT)	2.60
Consensus Log $P_{o/w}$	2.08

Water Solubility	
Log *S* (ESOL)	-3.50
Solubility	1.10e-01 mg/ml ; 3.15e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.81
Solubility	5.35e-02 mg/ml ; 1.53e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-4.93
Solubility	4.12e-03 mg/ml ; 1.18e-05 mol/l
Class	Moderately soluble

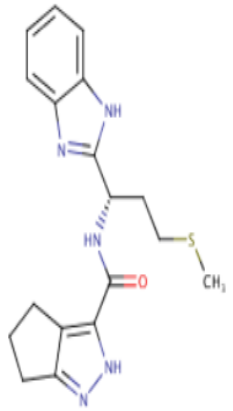
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-7.00 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	3.12

8	ZINC000096223736	C1CCc(c12)n[nH]c2C(=O)N[C@@H](CCSC)c(n3)[nH]c(c34)cccc4

Molecule 1



SMILES CSCC[C@@H](c1nc2c([nH]1)cccc2)NC(=O)c1[nH]nc2c1CCC2

Physicochemical Properties	
Formula	C18H21N5OS
Molecular weight	355.46 g/mol
Num. heavy atoms	25
Num. arom. heavy atoms	14
Fraction Csp3	0.39
Num. rotatable bonds	7
Num. H-bond acceptors	3
Num. H-bond donors	3
Molar Refractivity	100.36
TPSA	111.76 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.80
Log $P_{o/w}$ (XLOGP3)	2.65
Log $P_{o/w}$ (WLOGP)	2.67
Log $P_{o/w}$ (MLOGP)	1.87
Log $P_{o/w}$ (SILICOS-IT)	4.13
Consensus Log $P_{o/w}$	2.62

Water Solubility	
Log *S* (ESOL)	-3.67
Solubility	7.67e-02 mg/ml ; 2.16e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.65
Solubility	7.99e-03 mg/ml ; 2.25e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.41
Solubility	1.39e-04 mg/ml ; 3.90e-07 mol/l
Class	Poorly soluble

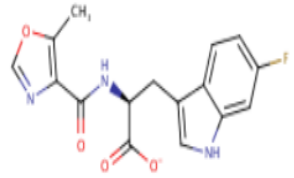
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.59 cm/s

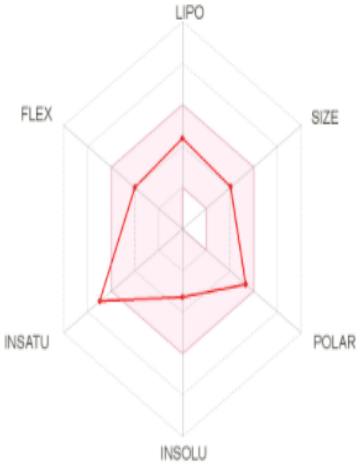
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	3.52

9	ZINC000097036564	n1coc(C)c1C(=O)N[C@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3

Molecule 1





SMILES [O-]C(=O)[C@H](Cc1c[nH]c2c1ccc(c2)F)NC(=O)c1ncoc1C

Physicochemical Properties	
Formula	C16H13FN3O4
Molecular weight	330.29 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	14
Fraction Csp3	0.19
Num. rotatable bonds	6
Num. H-bond acceptors	6
Num. H-bond donors	2
Molar Refractivity	80.21
TPSA	111.05 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.83
Log $P_{o/w}$ (XLOGP3)	2.16
Log $P_{o/w}$ (WLOGP)	1.11
Log $P_{o/w}$ (MLOGP)	0.63
Log $P_{o/w}$ (SILICOS-IT)	2.81
Consensus Log $P_{o/w}$	1.71

Water Solubility	
Log *S* (ESOL)	-3.28
Solubility	1.72e-01 mg/ml ; 5.20e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.12
Solubility	2.48e-02 mg/ml ; 7.50e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.11
Solubility	2.57e-03 mg/ml ; 7.78e-06 mol/l
Class	Moderately soluble

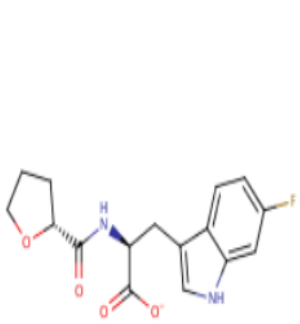
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.78 cm/s

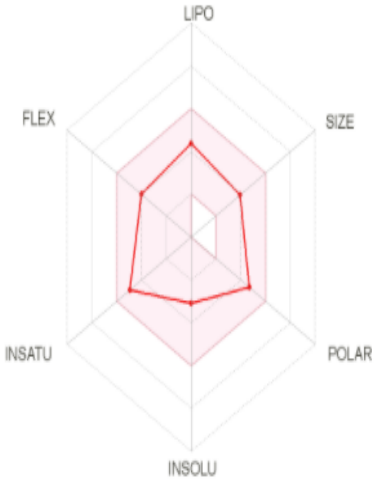
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.56

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	3.09

10	ZINC000237938532	O1CCC[C@@H]1C(=O)N[C@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3

Molecule 1





SMILES [O-]C(=O)[C@H](Cc1c[nH]c2c1ccc(c2)F)NC(=O)[C@H]1CCCO1

Physicochemical Properties	
Formula	C16H16FN2O4
Molecular weight	319.31 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	9
Fraction Csp3	0.38
Num. rotatable bonds	6
Num. H-bond acceptors	5
Num. H-bond donors	2
Molar Refractivity	78.67
TPSA	94.25 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.91
Log $P_{o/w}$ (XLOGP3)	2.16
Log $P_{o/w}$ (WLOGP)	0.68
Log $P_{o/w}$ (MLOGP)	0.95
Log $P_{o/w}$ (SILICOS-IT)	2.69
Consensus Log $P_{o/w}$	1.48

Water Solubility	
Log S (ESOL)	-3.07
Solubility	2.69e-01 mg/ml ; 8.43e-04 mol/l
Class	Soluble
Log S (Ali)	-3.77
Solubility	5.40e-02 mg/ml ; 1.69e-04 mol/l
Class	Soluble
Log S (SILICOS-IT)	-3.99
Solubility	3.28e-02 mg/ml ; 1.03e-04 mol/l
Class	Soluble

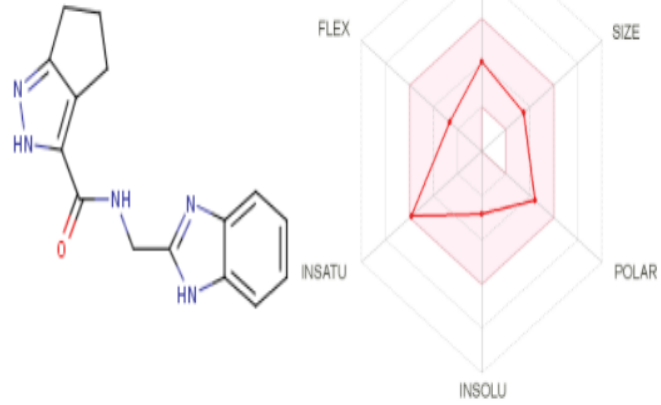
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.71 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.56

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	3.14

11	ZINC000096232566	C1CCc(c12)n[nH]c2C(=O)NCc(n3)[nH]c(c34)cccc4

Molecule 1



SMILES O=C(c1[nH]nc2c1CCC2)NCc1nc2c([nH]1)cccc2

Physicochemical Properties	
Formula	C15H15N5O
Molecular weight	281.31 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	14
Fraction Csp3	0.27
Num. rotatable bonds	4
Num. H-bond acceptors	3
Num. H-bond donors	3
Molar Refractivity	78.35
TPSA	86.46 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.24
Log $P_{o/w}$ (XLOGP3)	1.61
Log $P_{o/w}$ (WLOGP)	1.55
Log $P_{o/w}$ (MLOGP)	1.14
Log $P_{o/w}$ (SILICOS-IT)	3.09
Consensus Log $P_{o/w}$	1.73

Water Solubility	
Log *S* (ESOL)	-2.83
Solubility	4.18e-01 mg/ml ; 1.49e-03 mol/l
Class	Soluble
Log *S* (Ali)	-3.04
Solubility	2.58e-01 mg/ml ; 9.17e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-5.50
Solubility	8.94e-04 mg/ml ; 3.18e-06 mol/l
Class	Moderately soluble

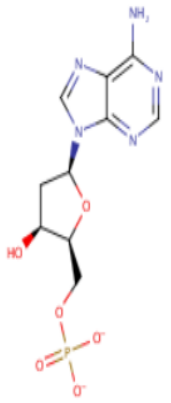
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.87 cm/s

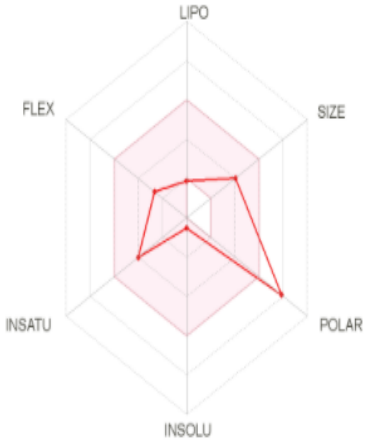
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	2.61

12	ZINC000003869813	[O-]P([O-])(=O)OC[C@H]1[C@@H](O)C[C@H](O1)n(cn2)c(c23)ncnc3N

Cyclic adenosine monophosphate





SMILES O[C@H]1C[C@H](O[C@H]1COP(=O)([O-])[O-])n1cnc2c1ncnc2N

Physicochemical Properties	
Formula	C10H12N5O6P
Molecular weight	329.21 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	9
Fraction Csp3	0.50
Num. rotatable bonds	4
Num. H-bond acceptors	9
Num. H-bond donors	2
Molar Refractivity	69.36
TPSA	181.31 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	-0.16
Log $P_{o/w}$ (XLOGP3)	-2.20
Log $P_{o/w}$ (WLOGP)	-0.27
Log $P_{o/w}$ (MLOGP)	-2.31
Log $P_{o/w}$ (SILICOS-IT)	-2.66
Consensus Log $P_{o/w}$	-1.52

Water Solubility	
Log *S* (ESOL)	-0.53
Solubility	9.63e+01 mg/ml ; 2.93e-01 mol/l
Class	Very soluble
Log *S* (Ali)	-1.08
Solubility	2.77e+01 mg/ml ; 8.40e-02 mol/l
Class	Very soluble
Log *S* (SILICOS-IT)	0.45
Solubility	9.26e+02 mg/ml ; 2.81e+00 mol/l
Class	Soluble

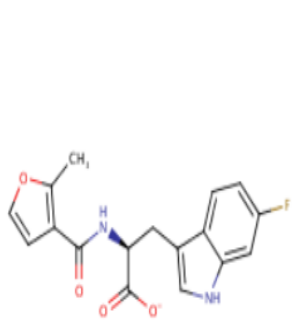
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-9.87 cm/s

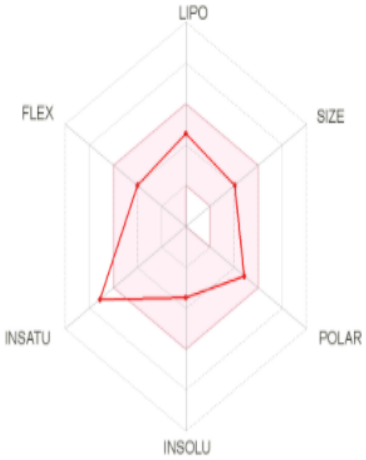
Druglikeness	
Lipinski	Yes; 1 violation: NorO>10
Ghose	Yes
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 2 violations: XLOGP3<-2, TPSA>150
Bioavailability Score	0.11

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: phosphor
Leadlikeness	Yes
Synthetic accessibility	4.04

13	ZINC000097036607	c1coc(C)c1C(=O)N[C@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3

Molecule 1





SMILES [O-]C(=O)[C@H](Cc1c[nH]c2c1ccc(c2)F)NC(=O)c1ccoc1C

Physicochemical Properties	
Formula	C17H14FN2O4
Molecular weight	329.30 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	14
Fraction Csp3	0.18
Num. rotatable bonds	6
Num. H-bond acceptors	5
Num. H-bond donors	2
Molar Refractivity	82.42
TPSA	98.16 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.92
Log $P_{o/w}$ (XLOGP3)	2.48
Log $P_{o/w}$ (WLOGP)	1.72
Log $P_{o/w}$ (MLOGP)	1.27
Log $P_{o/w}$ (SILICOS-IT)	3.36
Consensus Log $P_{o/w}$	2.15

Water Solubility	
Log *S* (ESOL)	-3.48
Solubility	1.09e-01 mg/ml ; 3.31e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.19
Solubility	2.15e-02 mg/ml ; 6.52e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.48
Solubility	1.09e-03 mg/ml ; 3.30e-06 mol/l
Class	Moderately soluble

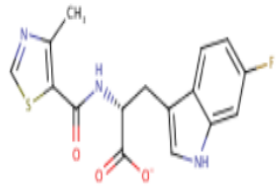
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.55 cm/s

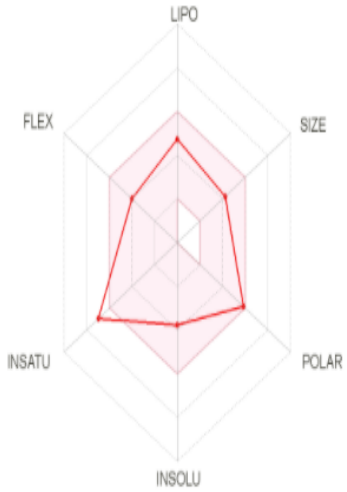
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.56

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	3.14

14	ZINC000097036605	s1cnc(C)c1C(=O)N[C@@H](C([O-])=O)Cc2c[nH]c(c23)cc(F)cc3

Molecule 1





SMILES [O-]C(=O)[C@@H](Cc1c[nH]c2c1ccc(c2)F)NC(=O)c1scnc1C

Physicochemical Properties	
Formula	C16H13FN3O3S
Molecular weight	346.36 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	14
Fraction Csp3	0.19
Num. rotatable bonds	6
Num. H-bond acceptors	5
Num. H-bond donors	2
Molar Refractivity	85.82
TPSA	126.15 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.57
Log $P_{o/w}$ (XLOGP3)	2.78
Log $P_{o/w}$ (WLOGP)	1.58
Log $P_{o/w}$ (MLOGP)	1.03
Log $P_{o/w}$ (SILICOS-IT)	4.06
Consensus Log $P_{o/w}$	2.20

Water Solubility	
Log *S* (ESOL)	-3.77
Solubility	5.82e-02 mg/ml ; 1.68e-04 mol/l
Class	Soluble
Log *S* (Ali)	-5.09
Solubility	2.85e-03 mg/ml ; 8.22e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.15
Solubility	2.43e-03 mg/ml ; 7.01e-06 mol/l
Class	Moderately soluble

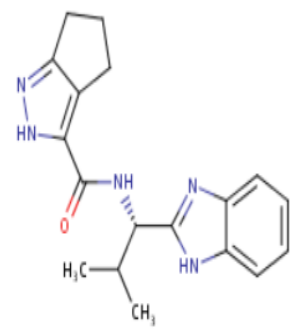
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.44 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.56

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	3.12

15	ZINC000079784201	C1CCc(c12)n[nH]c2C(=O)N[C@@H](C(C)C)c(n3)[nH]c(c34)cccc4

Molecule 1



SMILES O=C(c1[nH]nc2c1CCC2)N[C@H](c1nc2c([nH]1)cccc2)C(C)C

Physicochemical Properties	
Formula	C18H21N5O
Molecular weight	323.39 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	14
Fraction Csp3	0.39
Num. rotatable bonds	5
Num. H-bond acceptors	3
Num. H-bond donors	3
Molar Refractivity	92.77
TPSA	86.46 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.73
Log $P_{o/w}$ (XLOGP3)	2.97
Log $P_{o/w}$ (WLOGP)	2.58
Log $P_{o/w}$ (MLOGP)	1.87
Log $P_{o/w}$ (SILICOS-IT)	3.86
Consensus Log $P_{o/w}$	2.60

Water Solubility	
Log *S* (ESOL)	-3.82
Solubility	4.92e-02 mg/ml ; 1.52e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.45
Solubility	1.15e-02 mg/ml ; 3.56e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.95
Solubility	3.67e-04 mg/ml ; 1.14e-06 mol/l
Class	Moderately soluble

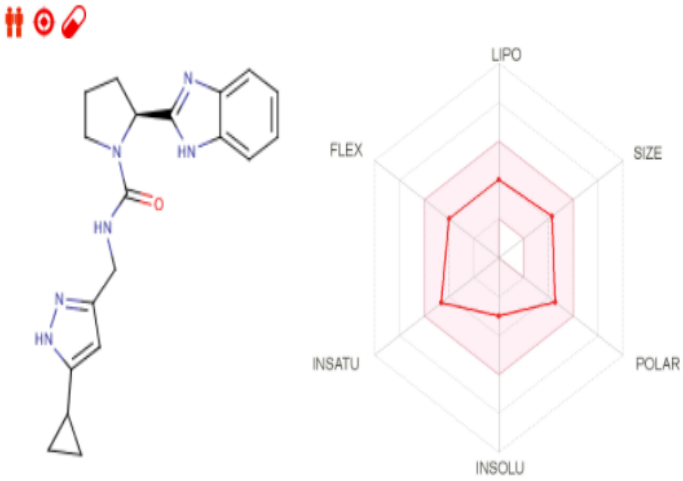
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.16 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	Yes
Synthetic accessibility	3.39

16	ZINC000426746041	C1CC1c([nH]n2)cc2CNC(=O)N3CCC[C@H]3c(n4)[nH]c(c45)cccc5

Molecule 1



SMILES O=C(N1CCC[C@H]1c1nc2c([nH]1)cccc2)NCc1n[nH]c(c1)C1CC1

Physicochemical Properties	
Formula	C19H22N6O
Molecular weight	350.42 g/mol
Num. heavy atoms	26
Num. arom. heavy atoms	14
Fraction Csp3	0.42
Num. rotatable bonds	6
Num. H-bond acceptors	3
Num. H-bond donors	3
Molar Refractivity	102.28
TPSA	89.70 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.62
Log $P_{o/w}$ (XLOGP3)	1.57
Log $P_{o/w}$ (WLOGP)	2.29
Log $P_{o/w}$ (MLOGP)	1.84
Log $P_{o/w}$ (SILICOS-IT)	2.79
Consensus Log $P_{o/w}$	2.22

Water Solubility	
Log *S* (ESOL)	-3.00
Solubility	3.47e-01 mg/ml ; 9.90e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.06
Solubility	3.02e-01 mg/ml ; 8.63e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-5.45
Solubility	1.25e-03 mg/ml ; 3.58e-06 mol/l
Class	Moderately soluble

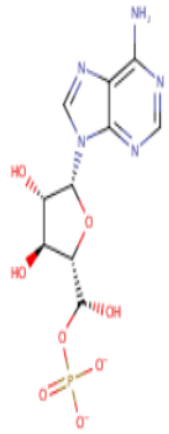
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-7.32 cm/s

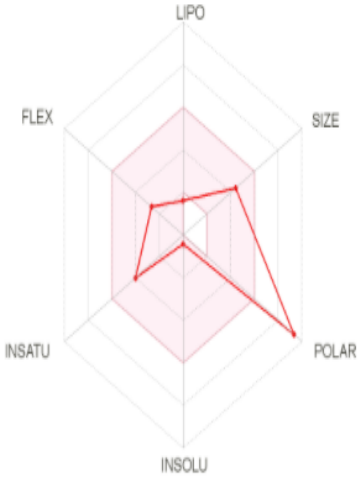
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	3.39

17 (3 stars)*	ZINC000113844870	[O-]P([O-])(=O)O[C@@H](O)[C@@H]1[C@@H](O)[C@H](O)[C@@H](O1)n(cn2)c(c2 3)ncnc3N

Molecule 1





SMILES O[C@@H]([C@H]1O[C@H]([C@H]([C@@H]1O)O)n1cnc2c1ncnc2N)OP(=O)([O-])[O-]

Physicochemical Properties	
Formula	C10H12N5O8P
Molecular weight	361.20 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	9
Fraction Csp3	0.50
Num. rotatable bonds	4
Num. H-bond acceptors	11
Num. H-bond donors	4
Molar Refractivity	71.68
TPSA	221.77 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	-0.15
Log $P_{o/w}$ (XLOGP3)	-2.67
Log $P_{o/w}$ (WLOGP)	-1.98
Log $P_{o/w}$ (MLOGP)	-3.40
Log $P_{o/w}$ (SILICOS-IT)	-4.29
Consensus Log $P_{o/w}$	-2.50

Water Solubility	
Log *S* (ESOL)	-0.41
Solubility	1.40e+02 mg/ml ; 3.88e-01 mol/l
Class	Very soluble
Log *S* (Ali)	-1.44
Solubility	1.32e+01 mg/ml ; 3.65e-02 mol/l
Class	Very soluble
Log *S* (SILICOS-IT)	2.21
Solubility	5.82e+04 mg/ml ; 1.61e+02 mol/l
Class	Soluble

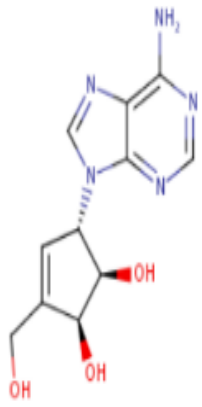
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-10.40 cm/s

Druglikeness	
Lipinski	Yes; 1 violation: NorO>10
Ghose	No; 1 violation: WLOGP<-0.4
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 3 violations: XLOGP3<-2, TPSA>150, H-acc>10
Bioavailability Score	0.11

Medicinal Chemistry	
PAINS	0 alert
Brenk	2 alerts: het-C-het_not_in_ring, phosphor
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	4.47

18	ZINC000000001793	OCC1=C[C@@H]([C@@H](O)[C@H]1O)n(cn2)c(c23)ncnc3N

Molecule 1



SMILES OCC1=C[C@@H]([C@H]([C@H]1O)O)n1cnc2c1ncnc2N

Physicochemical Properties	
Formula	C11H13N5O3
Molecular weight	263.25 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	9
Fraction Csp3	0.36
Num. rotatable bonds	2
Num. H-bond acceptors	6
Num. H-bond donors	4
Molar Refractivity	65.92
TPSA	130.31 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.98
Log $P_{o/w}$ (XLOGP3)	-1.98
Log $P_{o/w}$ (WLOGP)	-1.39
Log $P_{o/w}$ (MLOGP)	-1.73
Log $P_{o/w}$ (SILICOS-IT)	-1.81
Consensus Log $P_{o/w}$	-1.19

Water Solubility	
Log *S* (ESOL)	-0.44
Solubility	9.49e+01 mg/ml ; 3.60e-01 mol/l
Class	Very soluble
Log *S* (Ali)	-0.23
Solubility	1.54e+02 mg/ml ; 5.85e-01 mol/l
Class	Very soluble
Log *S* (SILICOS-IT)	-0.11
Solubility	2.03e+02 mg/ml ; 7.73e-01 mol/l
Class	Soluble

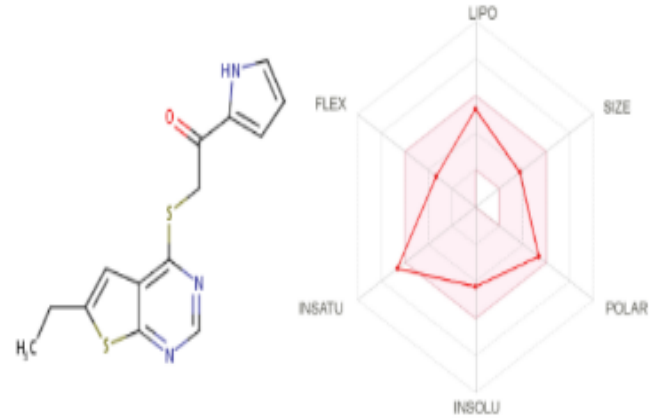
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-9.31 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: WLOGP<-0.4
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	Yes
Synthetic accessibility	3.87

19	ZINC000009504042	[nH]1cccc1C(=O)CSc2ncnc(c23)sc(c3)CC

Molecule 1



SMILES CCc1sc2c(c1)c(ncn2)SCC(=O)c1ccc[nH]1

Physicochemical Properties	
Formula	C14H13N3OS2
Molecular weight	303.40 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	14
Fraction Csp3	0.21
Num. rotatable bonds	5
Num. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	82.98
TPSA	112.18 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.41
Log $P_{o/w}$ (XLOGP3)	3.77
Log $P_{o/w}$ (WLOGP)	3.56
Log $P_{o/w}$ (MLOGP)	1.30
Log $P_{o/w}$ (SILICOS-IT)	4.82
Consensus Log $P_{o/w}$	3.17

Water Solubility	
Log S (ESOL)	-4.28
Solubility	1.58e-02 mg/ml ; 5.20e-05 mol/l
Class	Moderately soluble
Log S (Ali)	-5.82
Solubility	4.60e-04 mg/ml ; 1.52e-06 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-5.57
Solubility	8.19e-04 mg/ml ; 2.70e-06 mol/l
Class	Moderately soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-5.47 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.08

20	ZINC000005615258	COP(=O)(OC)OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O1)n(cn2)c(c23)ncnc3N

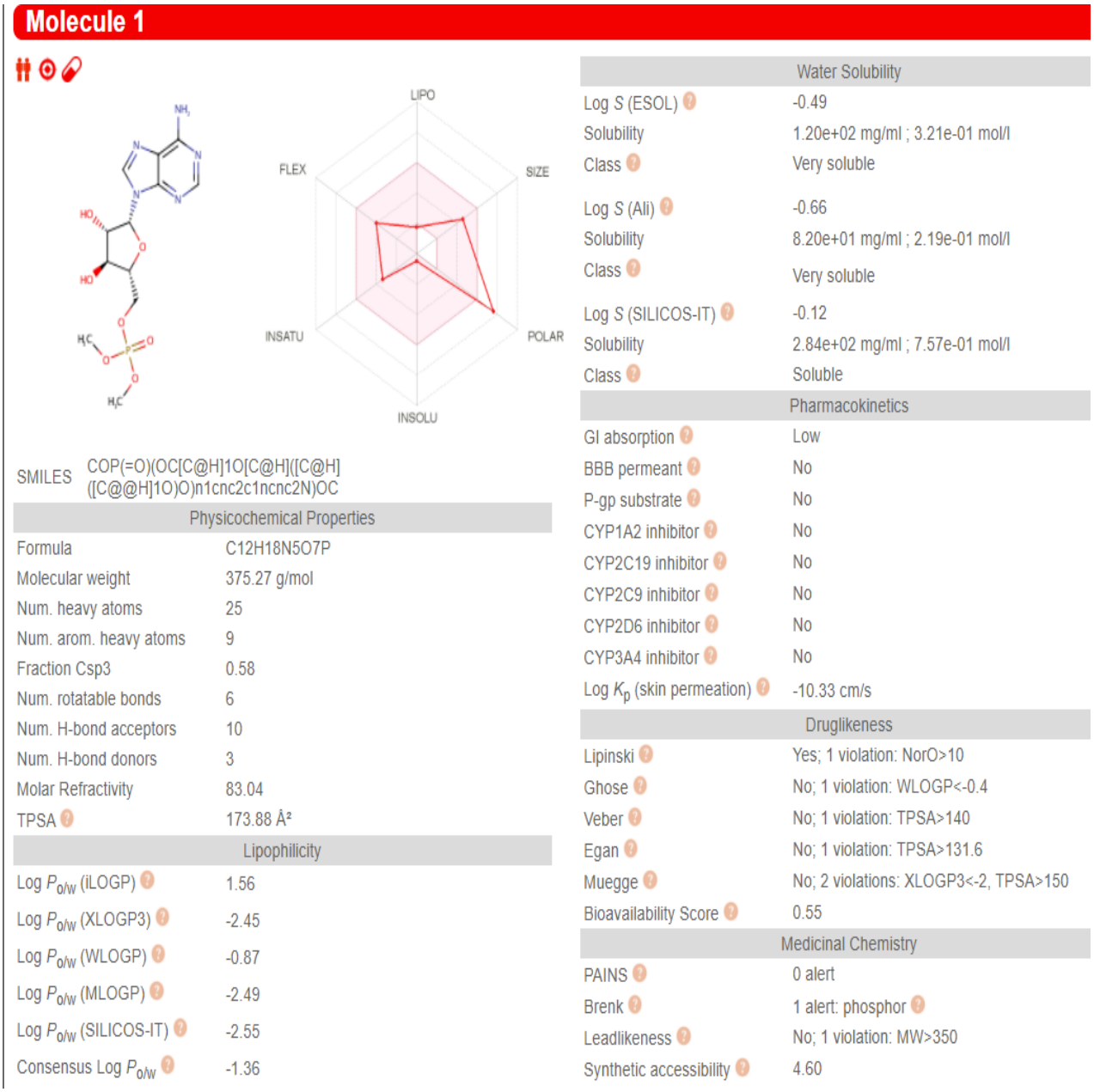


Figure S9. The predicted ADME properties for the top 20 best compounds including the reference compound from the SwissADME server.