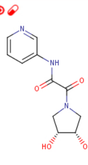
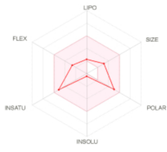
Molecule 1





SMILES O[C@@H]1CN(C[C@@H]1O)C(=O)C(=O)Nc1ccccc1

Physicochemical Properties	
Formula	C11H13N3O4
Molecular weight	251.24 g/mol
Num. heavy atoms	18
Num. arom. heavy atoms	6
Fraction Csp3	0.36
Num. rotatable bonds	4
Num. H-bond acceptors	5
Num. H-bond donors	3
Molar Refractivity	65.00
TPSA	102.76 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.67
Log $P_{o/w}$ (XLOGP3)	-1.54
Log $P_{o/w}$ (WLOGP)	-1.99
Log $P_{o/w}$ (MLOGP)	-1.81
Log $P_{o/w}$ (SILICOS-IT)	-1.07
Consensus Log $P_{o/w}$	-1.15

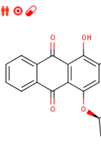
Water Solubility	
Log *S* (ESOL)	-0.41
Solubility	9.77e+01 mg/ml ; 3.89e-01 mol/l
Class	Very soluble
Log *S* (Ali)	-0.11
Solubility	1.95e+02 mg/ml ; 7.74e-01 mol/l
Class	Very soluble
Log *S* (SILICOS-IT)	-0.81
Solubility	3.86e+01 mg/ml ; 1.53e-01 mol/l
Class	Soluble

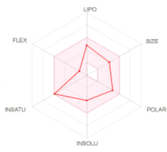
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-8.93 cm/s

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: diketo_group
Leadlikeness	Yes
Synthetic accessibility	2.87

Molecule 2





SMILES C[C@@H]1CNC[C@H]1Oc1cc(O)c(c2c1C(=O)c1cccc1C2=O)O

Physicochemical Properties	
Formula	C19H17NO5
Molecular weight	339.34 g/mol
Num. heavy atoms	25
Num. arom. heavy atoms	12
Fraction Csp3	0.26
Num. rotatable bonds	2
Num. H-bond acceptors	6
Num. H-bond donors	3
Molar Refractivity	94.12
TPSA	95.86 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.81
Log $P_{o/w}$ (XLOGP3)	2.88
Log $P_{o/w}$ (WLOGP)	1.48
Log $P_{o/w}$ (MLOGP)	0.51
Log $P_{o/w}$ (SILICOS-IT)	2.65
Consensus Log $P_{o/w}$	1.87

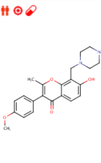
Water Solubility	
Log *S* (ESOL)	-3.98
Solubility	3.54e-02 mg/ml ; 1.04e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.55
Solubility	9.50e-03 mg/ml ; 2.80e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-4.89
Solubility	4.39e-03 mg/ml ; 1.29e-05 mol/l
Class	Moderately soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.33 cm/s

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

Medicinal Chemistry	
PAINS	2 alerts: catechol_A, quinone_A
Brenk	1 alert: catechol
Leadlikeness	Yes
Synthetic accessibility	3.72

Molecule 3



SMILES OCCN1CCN(CC1)Cc1c(O)ccc2c1oc(C)c(c2=O)c1ccc(cc1)OC

Physicochemical Properties	
Formula	C24H28N2O5
Molecular weight	424.49 g/mol
Num. heavy atoms	31
Num. arom. heavy atoms	16
Fraction Csp3	0.38
Num. rotatable bonds	6
Num. H-bond acceptors	7
Num. H-bond donors	2
Molar Refractivity	127.88
TPSA	86.38 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.66
Log $P_{o/w}$ (XLOGP3)	2.13
Log $P_{o/w}$ (WLOGP)	1.68
Log $P_{o/w}$ (MLOGP)	0.70
Log $P_{o/w}$ (SILICOS-IT)	3.74
Consensus Log $P_{o/w}$	2.38

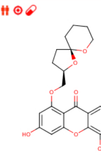
Water Solubility	
Log *S* (ESOL)	-3.80
Solubility	6.73e-02 mg/ml ; 1.59e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.58
Solubility	1.13e-01 mg/ml ; 2.66e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-6.39
Solubility	1.73e-04 mg/ml ; 4.08e-07 mol/l
Class	Poorly soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-7.38 cm/s

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

Medicinal Chemistry	
PAINS	1 alert: mannich_A
Brenk	0 alert
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	3.89

Molecule 4



SMILES Oc1cc(OC[C@H]2CC[C@]3(O2)CCCCO3)c2c(c1)oc1c(c2=O)cccc1O

Physicochemical Properties	
Formula	C22H22O7
Molecular weight	398.41 g/mol
Num. heavy atoms	29
Num. arom. heavy atoms	14
Fraction Csp3	0.41
Num. rotatable bonds	3
Num. H-bond acceptors	7
Num. H-bond donors	2
Molar Refractivity	106.96
TPSA	98.36 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.75
Log $P_{o/w}$ (XLOGP3)	3.31
Log $P_{o/w}$ (WLOGP)	3.81
Log $P_{o/w}$ (MLOGP)	1.25
Log $P_{o/w}$ (SILICOS-IT)	3.67
Consensus Log $P_{o/w}$	2.96

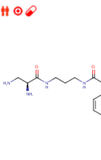
Water Solubility	
Log *S* (ESOL)	-4.55
Solubility	1.11e-02 mg/ml ; 2.79e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-5.05
Solubility	3.54e-03 mg/ml ; 8.88e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.66
Solubility	8.66e-04 mg/ml ; 2.17e-06 mol/l
Class	Moderately soluble

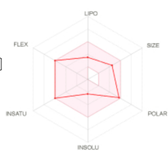
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.38 cm/s

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

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: polycyclic_aromatic_hydrocarbon_2
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	5.20

Molecule 5





SMILES NC[C@@H](C(=O)NCCCNC(=O)c1c2ccccc2nc2c1cccc2)N

Physicochemical Properties	
Formula	C20H23N5O2
Molecular weight	365.43 g/mol
Num. heavy atoms	27
Num. arom. heavy atoms	14
Fraction Csp3	0.25
Num. rotatable bonds	9
Num. H-bond acceptors	5
Num. H-bond donors	4
Molar Refractivity	104.70
TPSA	123.13 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.93
Log $P_{o/w}$ (XLOGP3)	0.66
Log $P_{o/w}$ (WLOGP)	0.91
Log $P_{o/w}$ (MLOGP)	0.60
Log $P_{o/w}$ (SILICOS-IT)	1.86
Consensus Log $P_{o/w}$	1.19

Water Solubility	
Log *S* (ESOL)	-2.31
Solubility	1.79e+00 mg/ml ; 4.88e-03 mol/l
Class	Soluble
Log *S* (Ali)	-2.82
Solubility	5.51e-01 mg/ml ; 1.51e-03 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-6.28
Solubility	1.93e-04 mg/ml ; 5.28e-07 mol/l
Class	Poorly soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-8.06 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	1 alert: polycyclic_aromatic_hydrocarbon_2
Leadlikeness	No; 2 violations: MW>350, Rotors>7
Synthetic accessibility	2.70