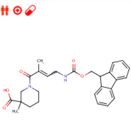
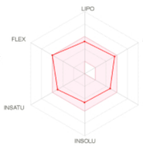
## Molecule 1



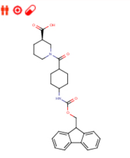



SMILES O=C(OCC1c2ccccc2c2c1ccc2)NC/C=C/(C(=O)N1CCCC(C1)C)C(=O)O)C

| Physicochemical Properties | |
|---|---|
| Formula | C27H30N2O5 |
| Molecular weight | 462.54 g/mol |
| Num. heavy atoms | 34 |
| Num. arom. heavy atoms | 12 |
| Fraction Csp3 | 0.37 |
| Num. rotatable bonds | 9 |
| Num. H-bond acceptors | 5 |
| Num. H-bond donors | 2 |
| Molar Refractivity | 132.60 |
| TPSA | 95.94 Å² |
| **Lipophilicity** | |
| Log $P_{o/w}$ (ILOGP) | 3.02 |
| Log $P_{o/w}$ (XLOGP3) | 3.57 |
| Log $P_{o/w}$ (WLOGP) | 3.80 |
| Log $P_{o/w}$ (MLOGP) | 2.90 |
| Log $P_{o/w}$ (SILICOS-IT) | 3.85 |
| Consensus Log $P_{o/w}$ | 3.43 |

| Water Solubility | |
|---|---|
| Log *S* (ESOL) | -4.62 |
| Solubility | 1.10e-02 mg/ml ; 2.38e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -5.27 |
| Solubility | 2.48e-03 mg/ml ; 5.36e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -6.27 |
| Solubility | 2.50e-04 mg/ml ; 5.40e-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 | Yes |
| CYP2D6 inhibitor | Yes |
| CYP3A4 inhibitor | Yes |
| Log $K_p$ (skin permeation) | -6.59 cm/s |
| **Druglikeness** | |
| Lipinski | Yes; 0 violation |
| Ghose | No; 1 violation: MR>130 |
| Veber | Yes |
| Egan | Yes |
| Muegge | Yes |
| Bioavailability Score | 0.56 |
| **Medicinal Chemistry** | |
| PAINS | 0 alert |
| Brenk | 1 alert: michael_acceptor_1 |
| Leadlikeness | No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.60 |

## Molecule 2

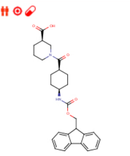



SMILES O=C(NC1CCC(CC1)C(=O)N1CCC[C@H](C1)C(=O)O)OCC1c2ccccc2c2c1cccc2

| Physicochemical Properties | |
|---|---|
| Formula | C28H32N2O5 |
| Molecular weight | 476.56 g/mol |
| Num. heavy atoms | 35 |
| Num. arom. heavy atoms | 12 |
| Fraction Csp3 | 0.46 |
| Num. rotatable bonds | 8 |
| Num. H-bond acceptors | 5 |
| Num. H-bond donors | 2 |
| Molar Refractivity | 136.02 |
| TPSA | 95.94 Å² |
| **Lipophilicity** | |
| Log $P_{o/w}$ (ILOGP) | 2.73 |
| Log $P_{o/w}$ (XLOGP3) | 3.81 |
| Log $P_{o/w}$ (WLOGP) | 4.03 |
| Log $P_{o/w}$ (MLOGP) | 3.18 |
| Log $P_{o/w}$ (SILICOS-IT) | 3.33 |
| Consensus Log $P_{o/w}$ | 3.41 |

| Water Solubility | |
|---|---|
| Log *S* (ESOL) | -4.92 |
| Solubility | 5.72e-03 mg/ml ; 1.20e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -5.52 |
| Solubility | 1.44e-03 mg/ml ; 3.02e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -5.97 |
| Solubility | 5.09e-04 mg/ml ; 1.07e-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) | -6.50 cm/s |
| **Druglikeness** | |
| Lipinski | Yes; 0 violation |
| Ghose | No; 1 violation: MR>130 |
| Veber | Yes |
| Egan | Yes |
| Muegge | Yes |
| Bioavailability Score | 0.56 |
| **Medicinal Chemistry** | |
| PAINS | 0 alert |
| Brenk | 0 alert |
| Leadlikeness | No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.87 |

## Molecule 3

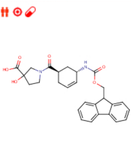


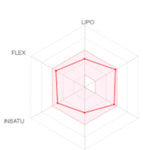

SMILES O=C(N[C@@H]1CC[C@@H](CC1)C(=O)N1CCC[C@H](C1)C(=O)O)OCC1c2ccccc2c2c1cccc2

| Physicochemical Properties | |
|---|---|
| Formula | C28H32N2O5 |
| Molecular weight | 476.56 g/mol |
| Num. heavy atoms | 35 |
| Num. arom. heavy atoms | 12 |
| Fraction Csp3 | 0.46 |
| Num. rotatable bonds | 8 |
| Num. H-bond acceptors | 5 |
| Num. H-bond donors | 2 |
| Molar Refractivity | 136.02 |
| TPSA | 95.94 Å² |
| **Lipophilicity** | |
| Log $P_{o/w}$ (ILOGP) | 3.13 |
| Log $P_{o/w}$ (XLOGP3) | 3.81 |
| Log $P_{o/w}$ (WLOGP) | 4.03 |
| Log $P_{o/w}$ (MLOGP) | 3.18 |
| Log $P_{o/w}$ (SILICOS-IT) | 3.33 |
| Consensus Log $P_{o/w}$ | 3.49 |

| Water Solubility | |
|---|---|
| Log *S* (ESOL) | -4.92 |
| Solubility | 5.72e-03 mg/ml ; 1.20e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -5.52 |
| Solubility | 1.44e-03 mg/ml ; 3.02e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -5.97 |
| Solubility | 5.09e-04 mg/ml ; 1.07e-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) | -6.50 cm/s |
| **Druglikeness** | |
| Lipinski | Yes; 0 violation |
| Ghose | No; 1 violation: MR>130 |
| Veber | Yes |
| Egan | Yes |
| Muegge | Yes |
| Bioavailability Score | 0.56 |
| **Medicinal Chemistry** | |
| PAINS | 0 alert |
| Brenk | 0 alert |
| Leadlikeness | No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.87 |

## Molecule 4



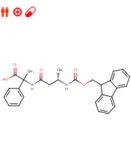


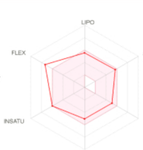

SMILES O=C[N[C@@H]1C=CC[C@H](C1)C(=O)N1CCC(C1)O)C(=O)O)OCC1c2ccccc2c2c1cccc2

| Physicochemical Properties | |
|---|---|
| Formula | C27H28N2O6 |
| Molecular weight | 476.52 g/mol |
| Num. heavy atoms | 35 |
| Num. arom. heavy atoms | 12 |
| Fraction Csp3 | 0.37 |
| Num. rotatable bonds | 8 |
| Num. H-bond acceptors | 6 |
| Num. H-bond donors | 3 |
| Molar Refractivity | 131.94 |
| TPSA | 116.17 Å² |
| **Lipophilicity** | |
| Log $P_{o/w}$ (ILOGP) | 2.36 |
| Log $P_{o/w}$ (XLOGP3) | 2.51 |
| Log $P_{o/w}$ (WLOGP) | 2.53 |
| Log $P_{o/w}$ (MLOGP) | 2.12 |
| Log $P_{o/w}$ (SILICOS-IT) | 2.19 |
| Consensus Log $P_{o/w}$ | 2.34 |

| Water Solubility | |
|---|---|
| Log *S* (ESOL) | -4.10 |
| Solubility | 3.77e-02 mg/ml ; 7.92e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -4.60 |
| Solubility | 1.21e-02 mg/ml ; 2.54e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -4.87 |
| Solubility | 6.46e-03 mg/ml ; 1.36e-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 | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log $K_p$ (skin permeation) | -7.42 cm/s |
| **Druglikeness** | |
| Lipinski | Yes; 0 violation |
| Ghose | No; 1 violation: MR>130 |
| Veber | Yes |
| Egan | Yes |
| Muegge | Yes |
| Bioavailability Score | 0.56 |
| **Medicinal Chemistry** | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated_alkene |
| Leadlikeness | No; 2 violations: MW>350, Rotors>7 |
| Synthetic accessibility | 5.11 |

## Molecule 5






SMILES C[C@@H](CC(=O)NC(c1ccccc1)(C(=O)O)C)NC(=O)OCC1c2ccccc2c2c1cccc2

| Physicochemical Properties | |
|---|---|
| Formula | C28H28N2O5 |
| Molecular weight | 472.53 g/mol |
| Num. heavy atoms | 35 |
| Num. arom. heavy atoms | 18 |
| Fraction Csp3 | 0.25 |
| Num. rotatable bonds | 11 |
| Num. H-bond acceptors | 5 |
| Num. H-bond donors | 3 |
| Molar Refractivity | 131.77 |
| TPSA | 104.73 Å² |
| **Lipophilicity** | |
| Log $P_{o/w}$ (ILOGP) | 2.74 |
| Log $P_{o/w}$ (XLOGP3) | 4.22 |
| Log $P_{o/w}$ (WLOGP) | 4.31 |
| Log $P_{o/w}$ (MLOGP) | 2.96 |
| Log $P_{o/w}$ (SILICOS-IT) | 4.11 |
| Consensus Log $P_{o/w}$ | 3.67 |

| Water Solubility | |
|---|---|
| Log *S* (ESOL) | -5.08 |
| Solubility | 3.90e-03 mg/ml ; 8.26e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -6.13 |
| Solubility | 3.51e-04 mg/ml ; 7.42e-07 mol/l |
| Class | Poorly soluble |
| Log *S* (SILICOS-IT) | -8.12 |
| Solubility | 3.58e-06 mg/ml ; 7.57e-09 mol/l |
| Class | Poorly 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) | -6.19 cm/s |
| **Druglikeness** | |
| Lipinski | Yes; 0 violation |
| Ghose | No; 1 violation: MR>130 |
| Veber | No; 1 violation: Rotors>10 |
| Egan | Yes |
| Muegge | Yes |
| Bioavailability Score | 0.56 |
| **Medicinal Chemistry** | |
| PAINS | 0 alert |
| Brenk | 0 alert |
| Leadlikeness | No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.51 |