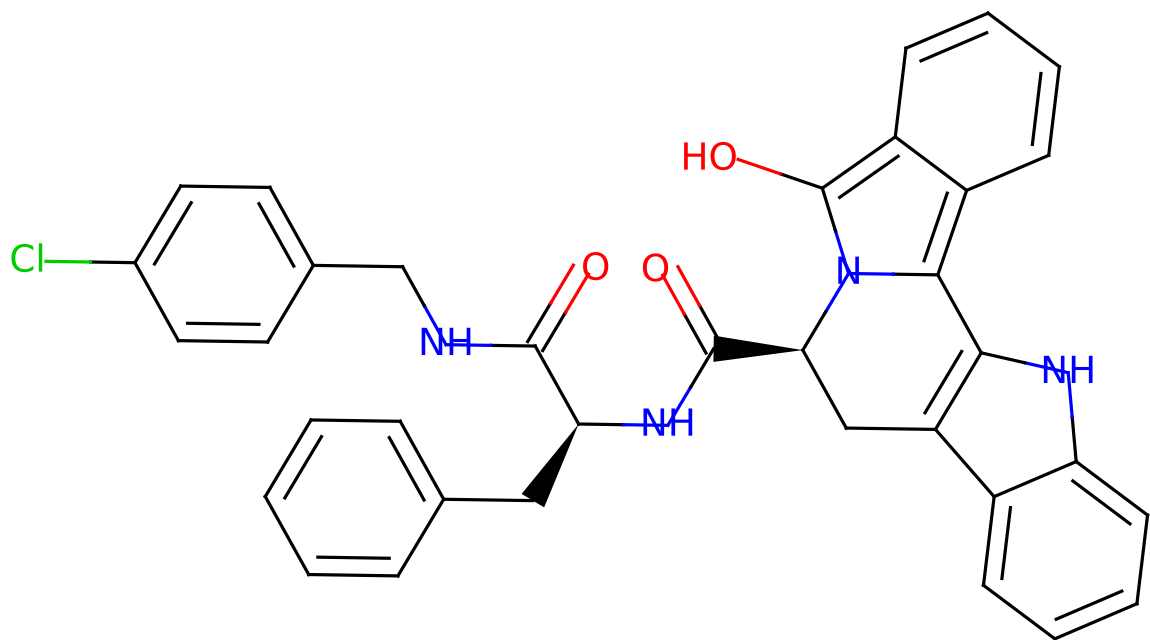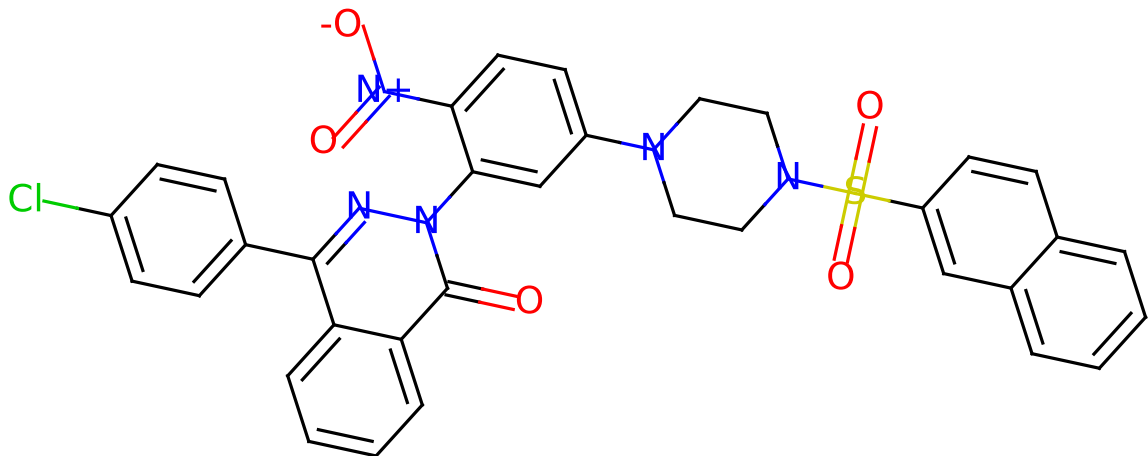('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 6.289700000000006 | QED: 0.1763358576321032

c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)Cl)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-6977725985_1

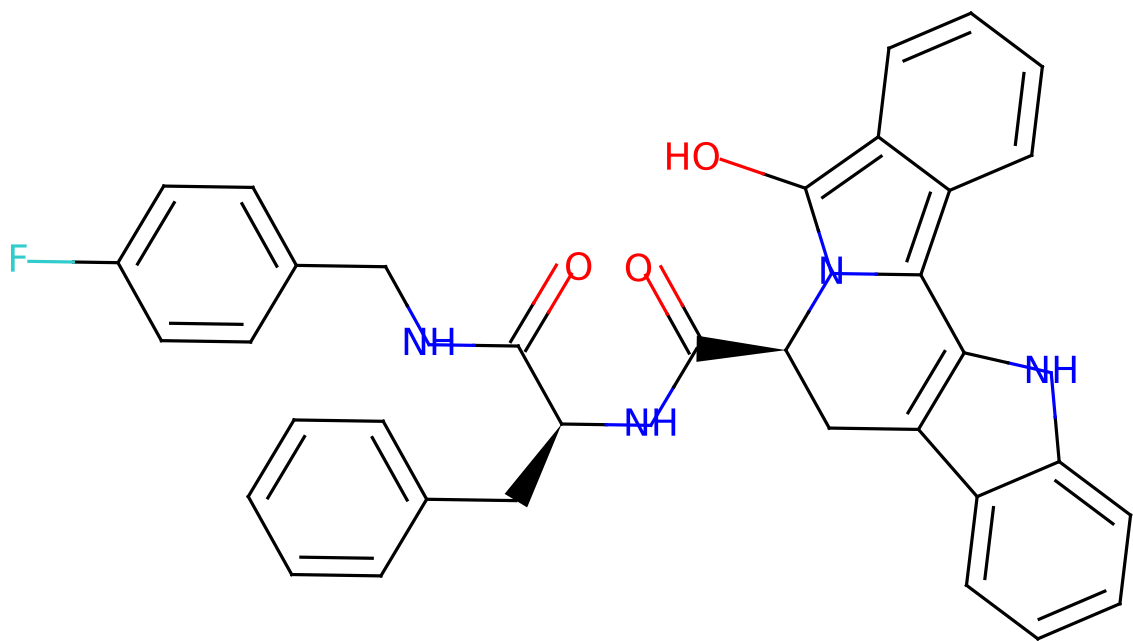('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6ccccc6c(n5)c7ccc(cc7)Cl)N(=O)=O

ORD-MCULE-1708960826_1
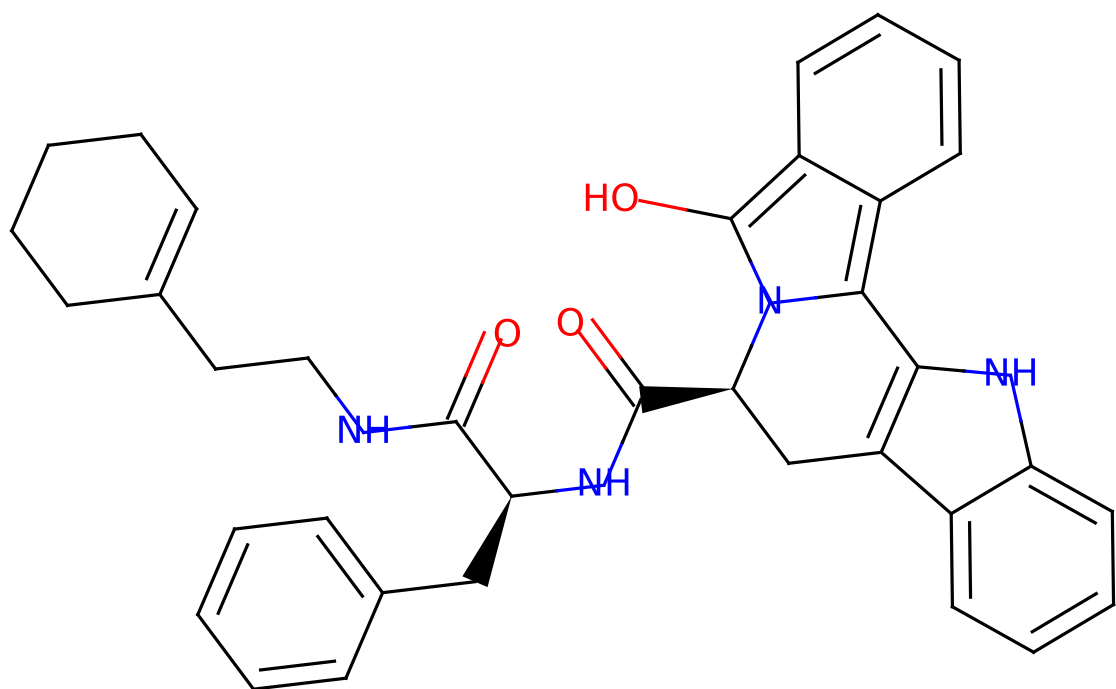
('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 5.775400000000006 | QED: 0.19535260854802458

c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)F)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O
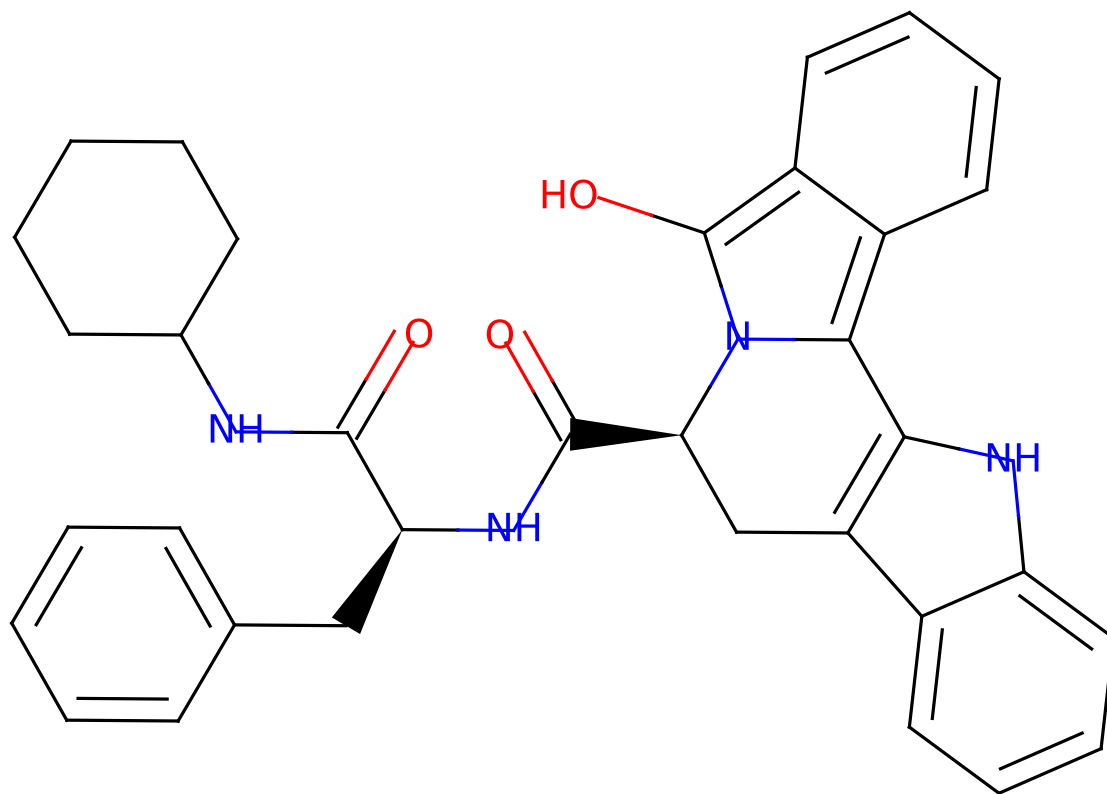
ORD-MCULE-6477680903_1

MolLogP: 6.326600000000007 | QED: 0.163672300852651

c1ccc(cc1)C[C@@H](C(=O)NCCC2=CCCCC2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-2409941333_1

MolLogP: 5.768800000000006 | QED: 0.2176477509654081

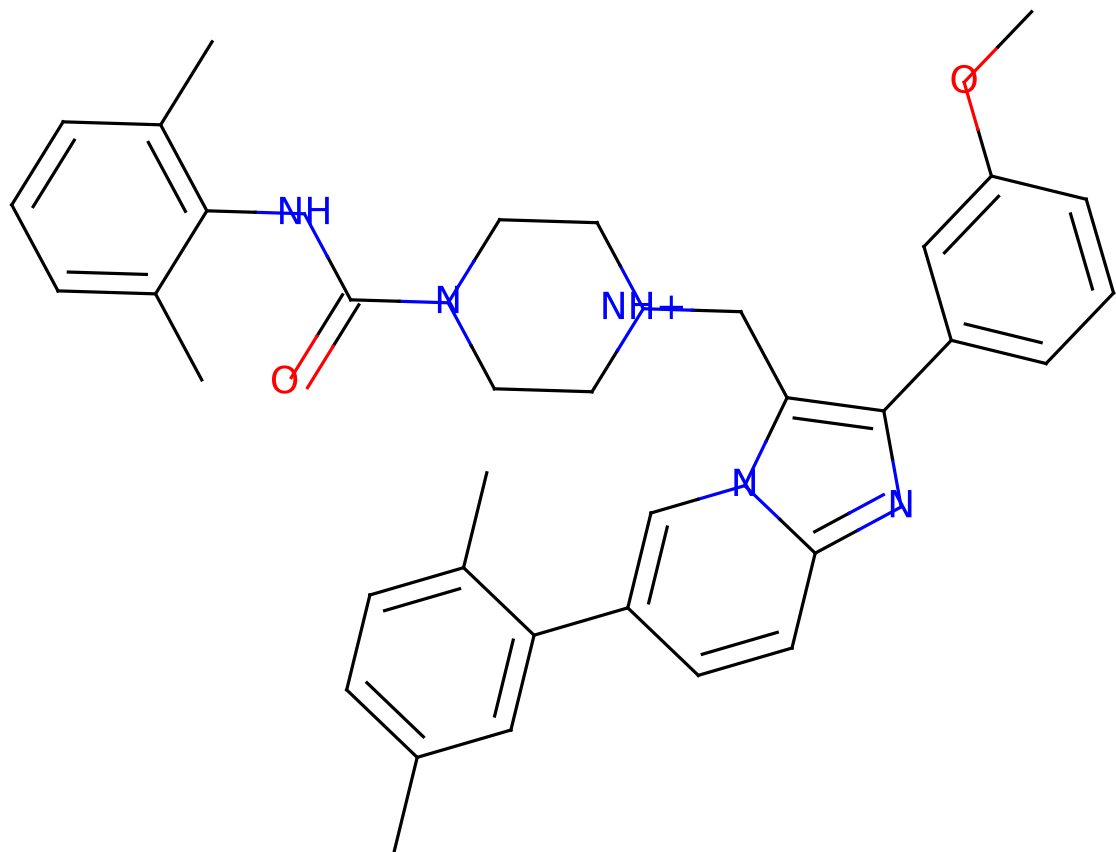c1ccc(cc1)C[C@@H](C(=O)NC2CCCCC2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-9395623979_1

('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7

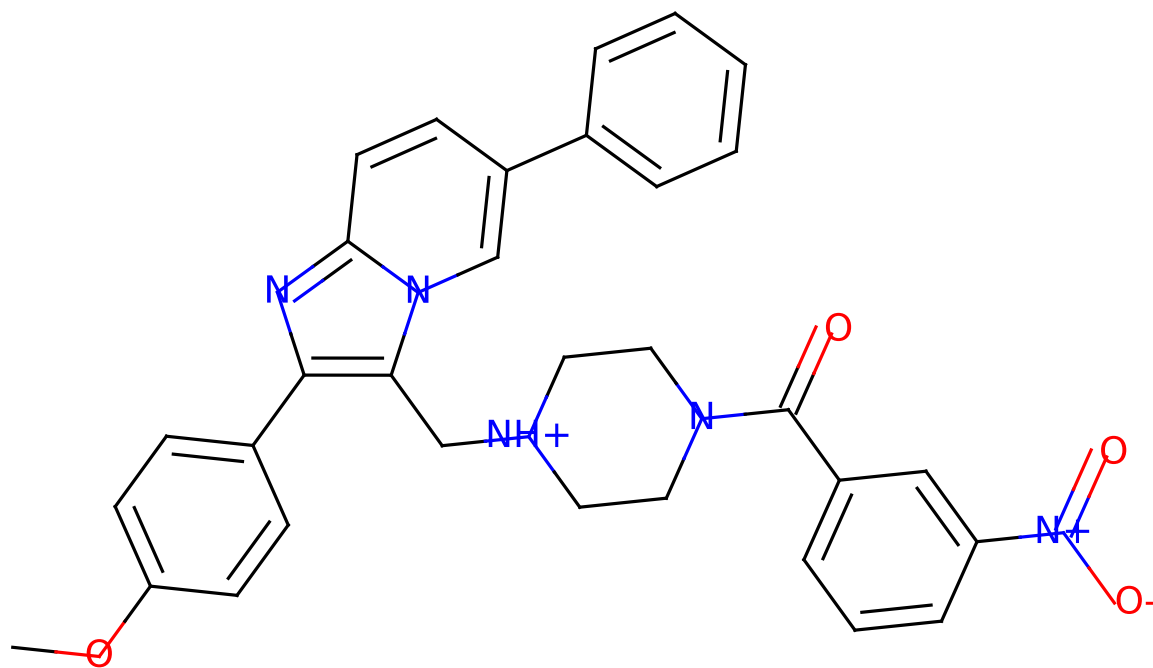ORD-MCULE-7416131701_1

('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 5.843180000000006 | QED: 0.2678094183325389

Cc1ccc(c(c1)c2ccc3nc(c(n3c2)C[NH+]4CCN(CC4)C(=O)Nc5c(cccc5C)C)c6cccc(c6)OC)C
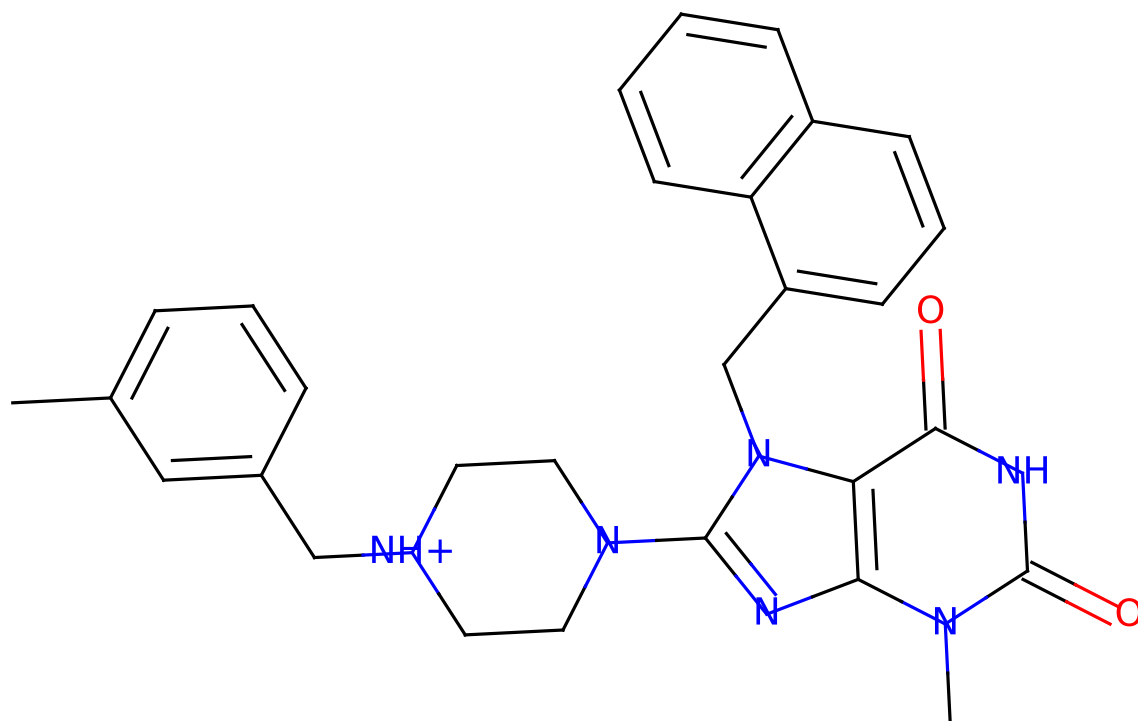
ORD-MCULE-1845027027_1

MolLogP: 4.126000000000003 | QED: 0.2439331506700583

COc1ccc(cc1)c2c(n3cc(ccc3n2)c4ccccc4)C[NH+]5CCN(CC5)C(=O)c6cccc(c6)N(=O)=O
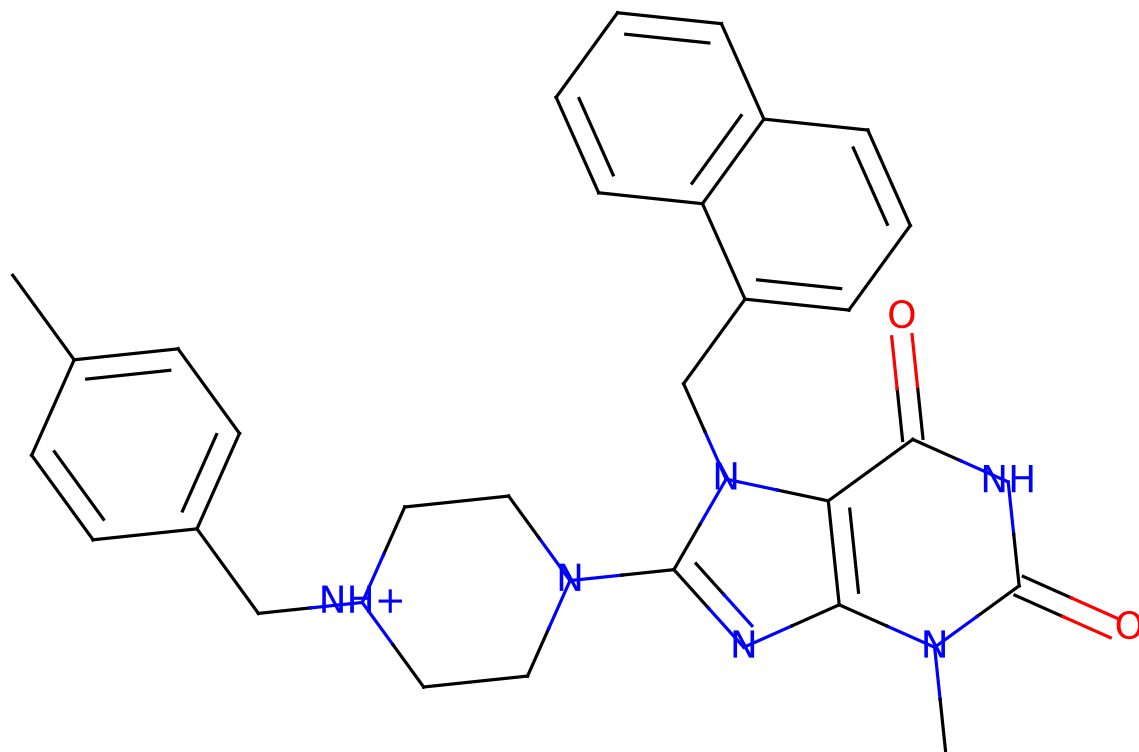
ORD-MCULE-5878589304_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
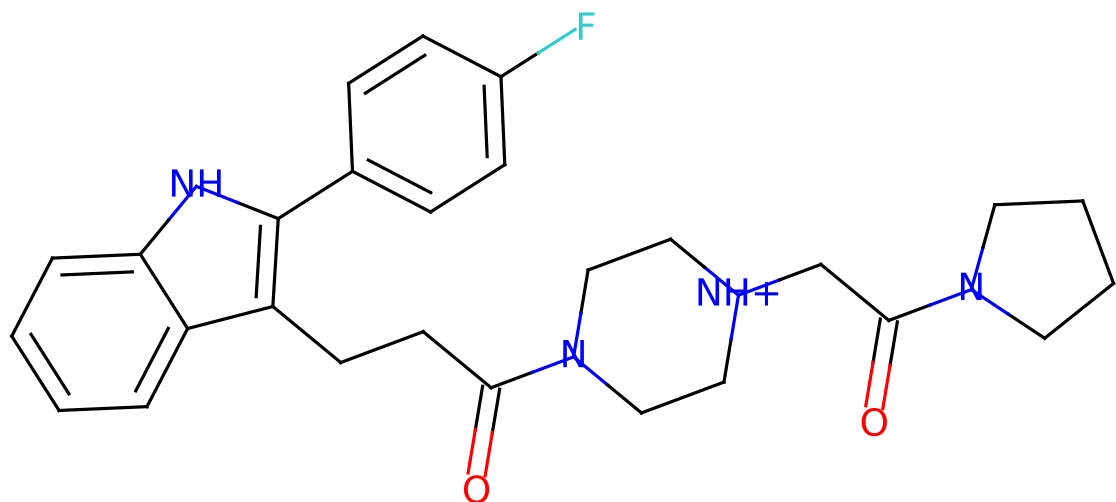
ORD-MCULE-9311937068_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C

ORD-MCULE-8959718627_1

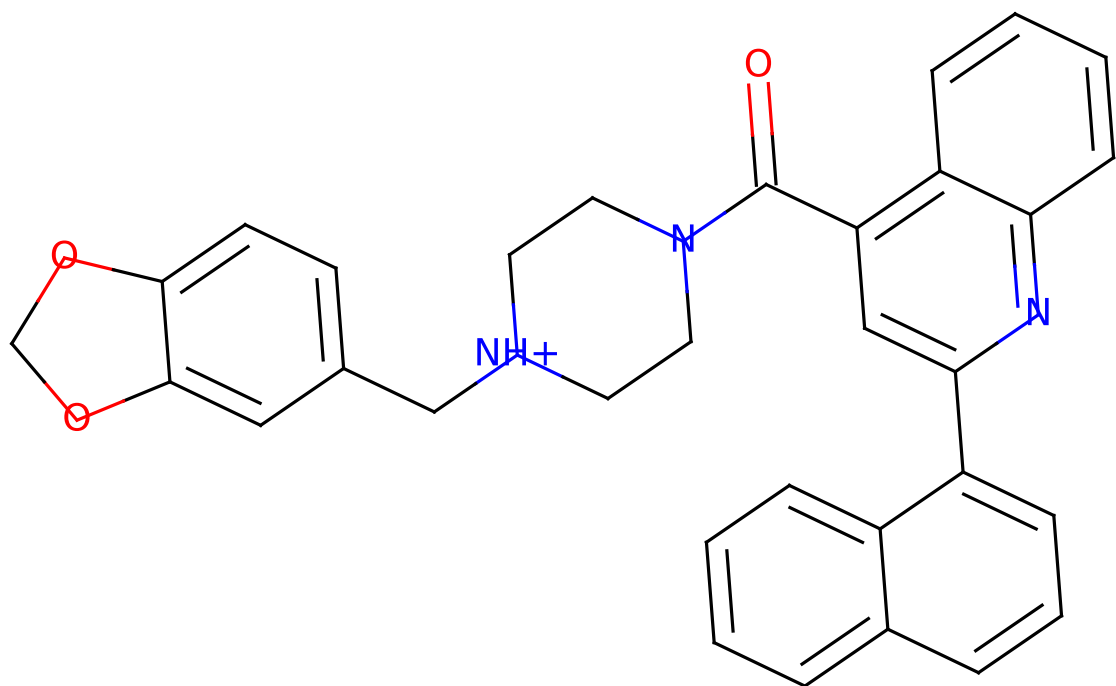('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 2.256099999999999 | QED: 0.5892811568593804

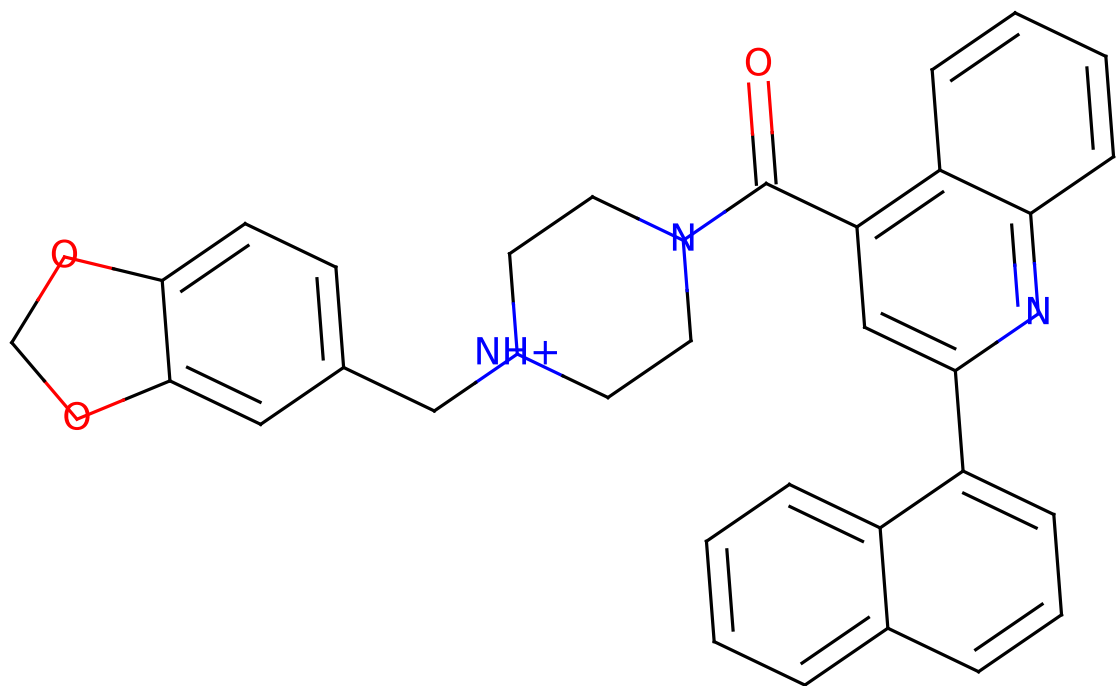c1ccc2c(c1)c(c([nH]2)c3ccc(cc3)F)CCC(=O)N4CC[NH+](CC4)CC(=O)N5CCCC5

ORD-MCULE-3657624205_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-4959815000_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-3696478799_1

MolLogP: 1.362000000000001 | QED: 0.5233311781906421

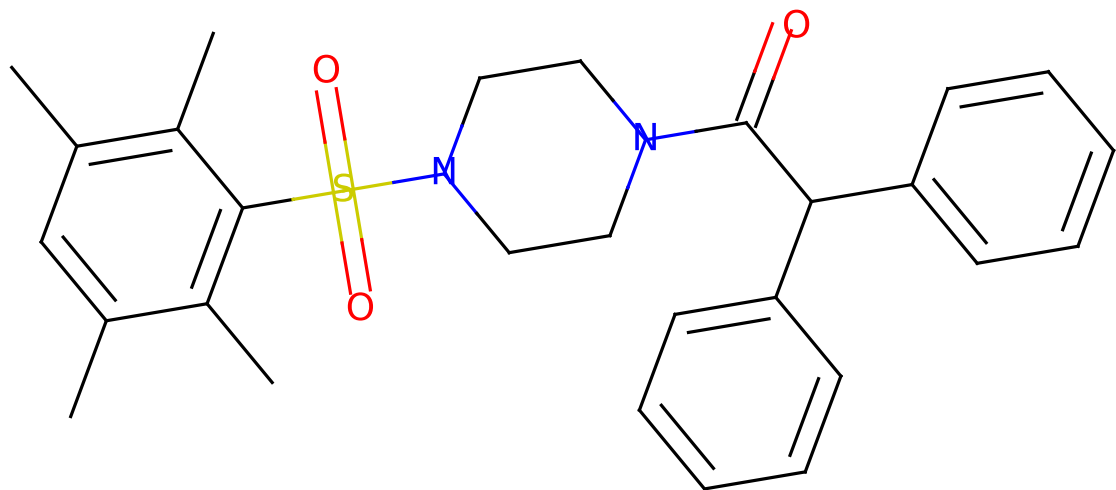COc1ccc(cc1)c2c(c3ccccc3[nH]2)CCC(=O)N4CC[NH+](CC4)CC(=O)N5CCOCC5

ORD-MCULE-3773841872_1
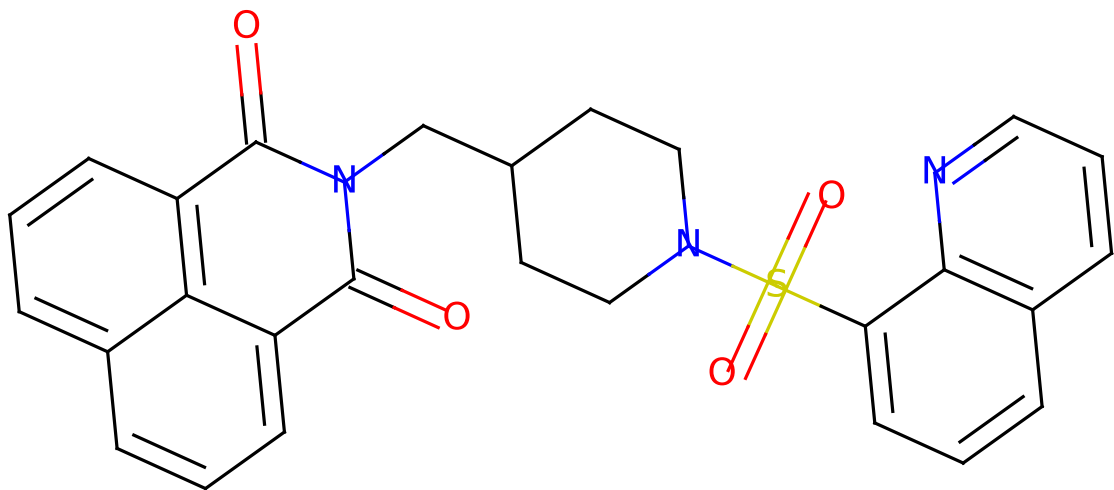
MolLogP: 4.084900000000004 | QED: 0.4065854846130124

c1cc2cccc3c2c(c1)C(=O)N(C3=O)CC4CCN(CC4)S(=O)(=O)c5cccc6c5nccc6

ORD-MCULE-4940228361_1
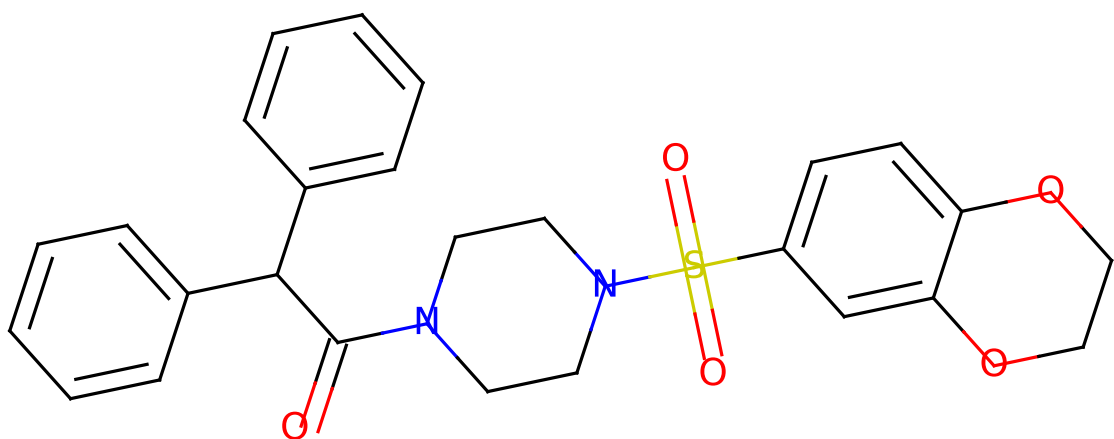
MolLogP: 4.5852800000000045 | QED: 0.541437412840622

Cc1cc(c(c(c1C)S(=O)(=O)N2CCN(CC2)C(=O)C(c3ccccc3)c4ccccc4)C)C

ORD-MCULE-2055004350_1
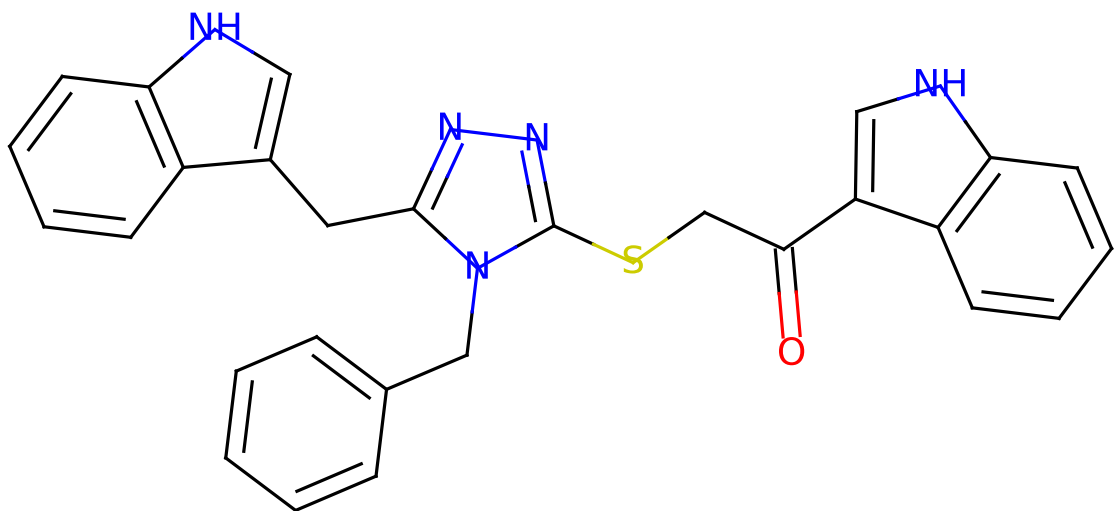
MolLogP: 3.1228000000000016 | QED: 0.5633261375042687

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5c(c4)OCCO5
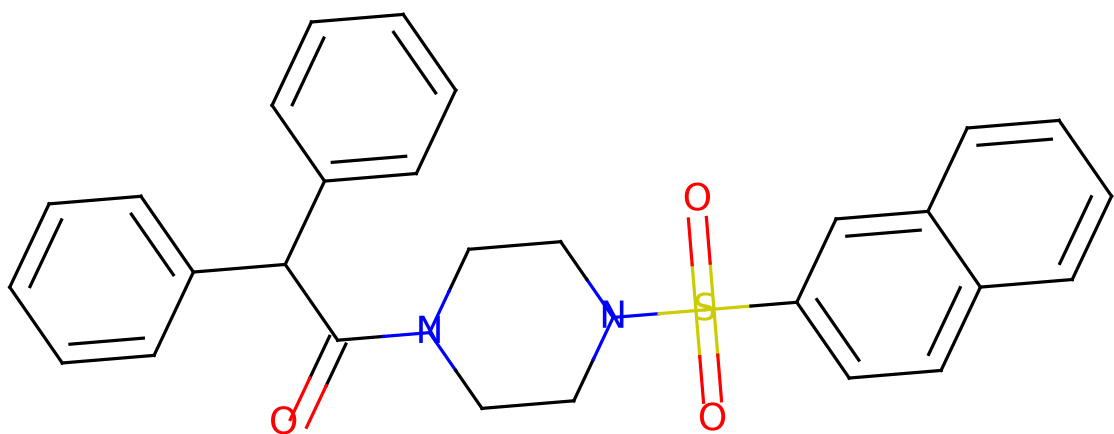
ORD-MCULE-1904175079_1

MolLogP: 5.8548000000000044 | QED: 0.21272800874019035

c1ccc(cc1)Cn2c(nnc2SCC(=O)c3c[nH]c4c3cccc4)Cc5c[nH]c6c5cccc6

ORD-MCULE-2017284421_1

('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')
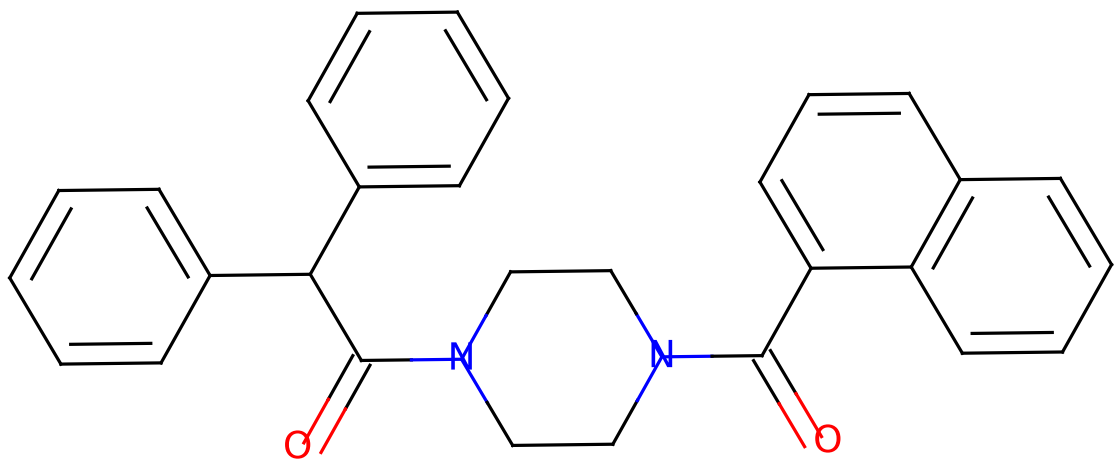
MolLogP: 4.504800000000004 | QED: 0.43144005118053486

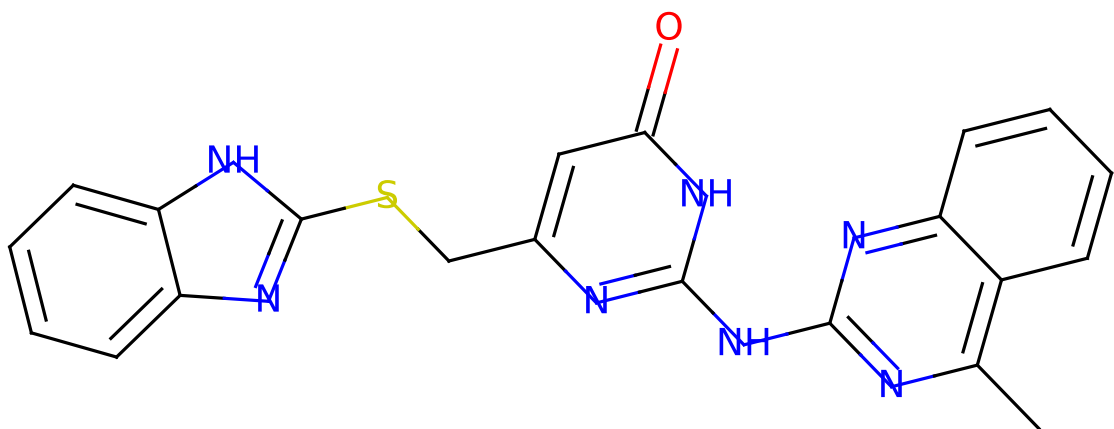c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-9717306826_1

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

ORD-MCULE-4705080812_1

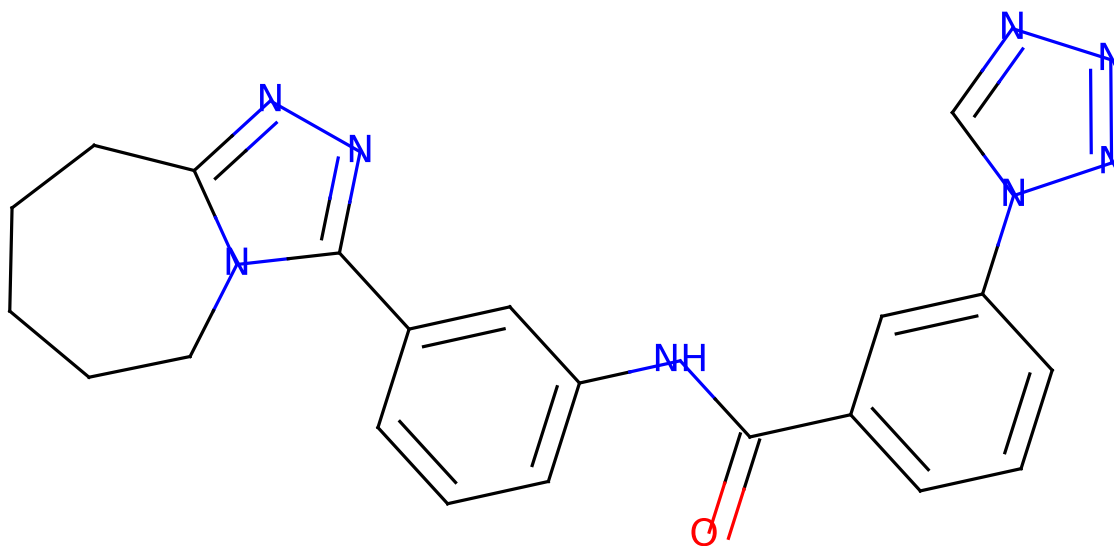('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 3.933720000000001 | QED: 0.3728174639709249

Cc1c2ccccc2nc(n1)Nc3[nH]c(=O)cc(n3)CSc4[nH]c5ccccc5n4
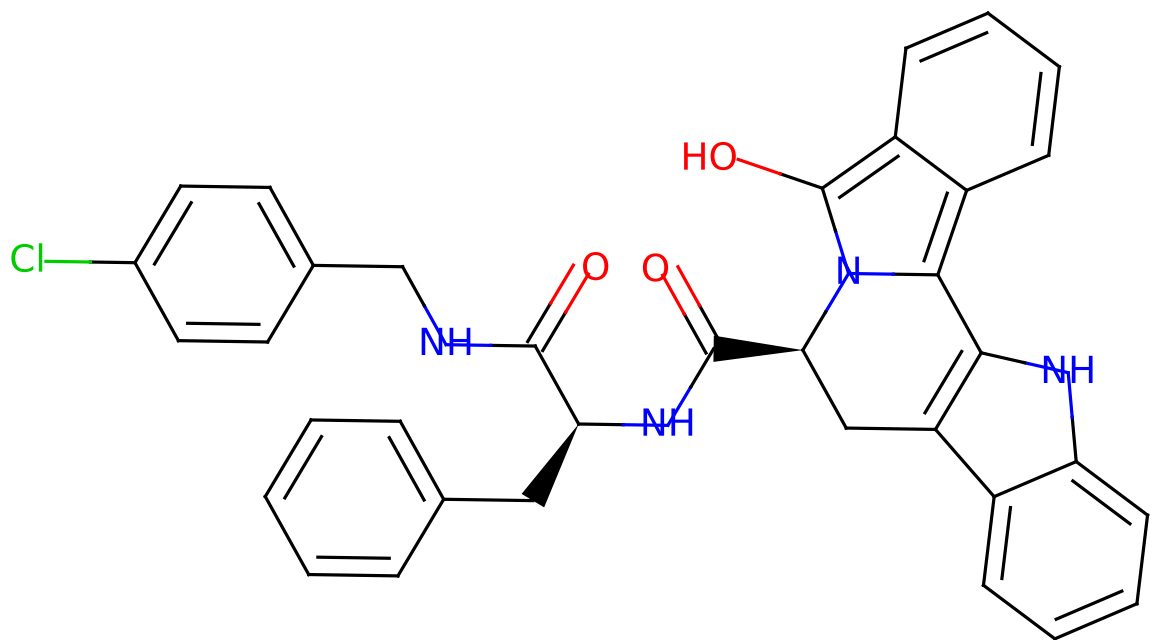
ORD-MCULE-6515729583_1

('NSP15_6W01_AB_1_F', '3CLPro_7BQY_A_1_F')

MolLogP: 2.8995000000000006 | QED: 0.564916346720981

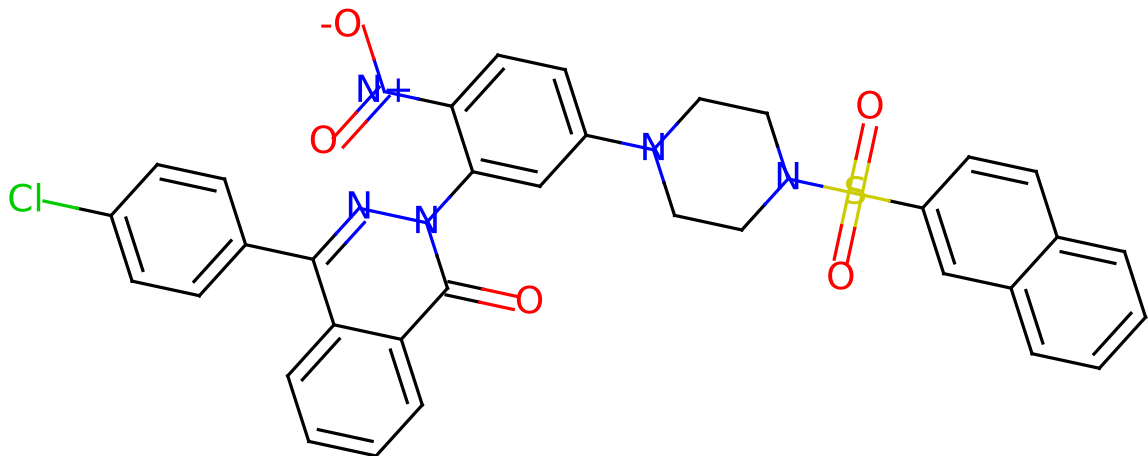c1cc(cc(c1)NC(=O)c2cccc(c2)n3cnnn3)c4nnc5n4CCCCC5

ORD-MCULE-2036827873_1

MolLogP: 6.289700000000006 | QED: 0.1763358576321032

c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)Cl)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-6977725985_1
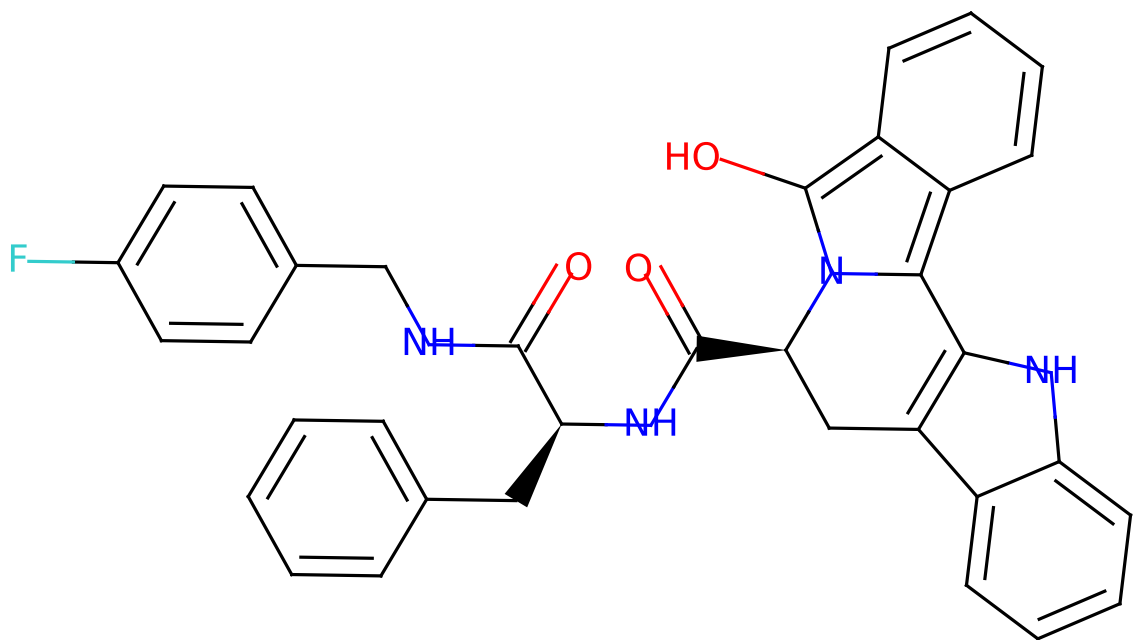
('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6ccccc6c(n5)c7ccc(cc7)Cl)N(=O)=O
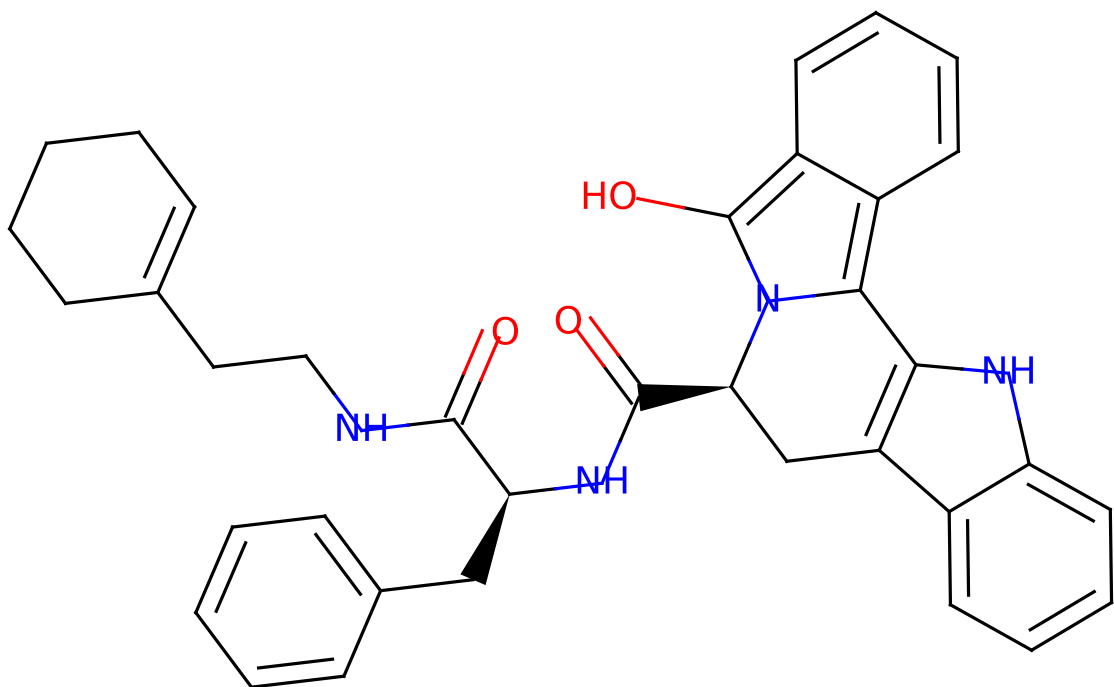
ORD-MCULE-1708960826_1

MolLogP: 5.775400000000006 | QED: 0.19535260854802458

c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)F)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

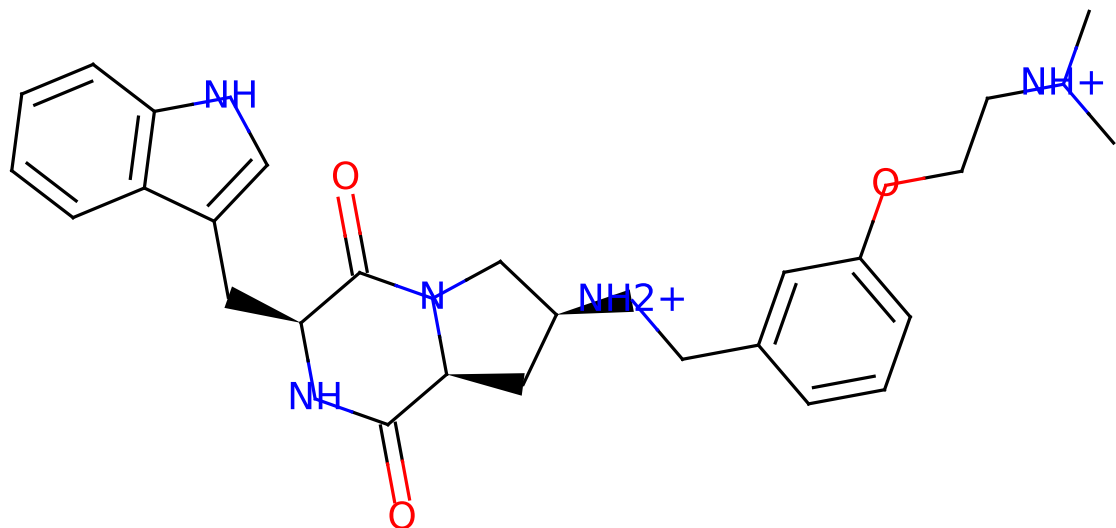ORD-MCULE-6477680903_1

('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 6.326600000000007 | QED: 0.163672300852651

c1ccc(cc1)C[C@@H](C(=O)NCCC2=CCCCC2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O
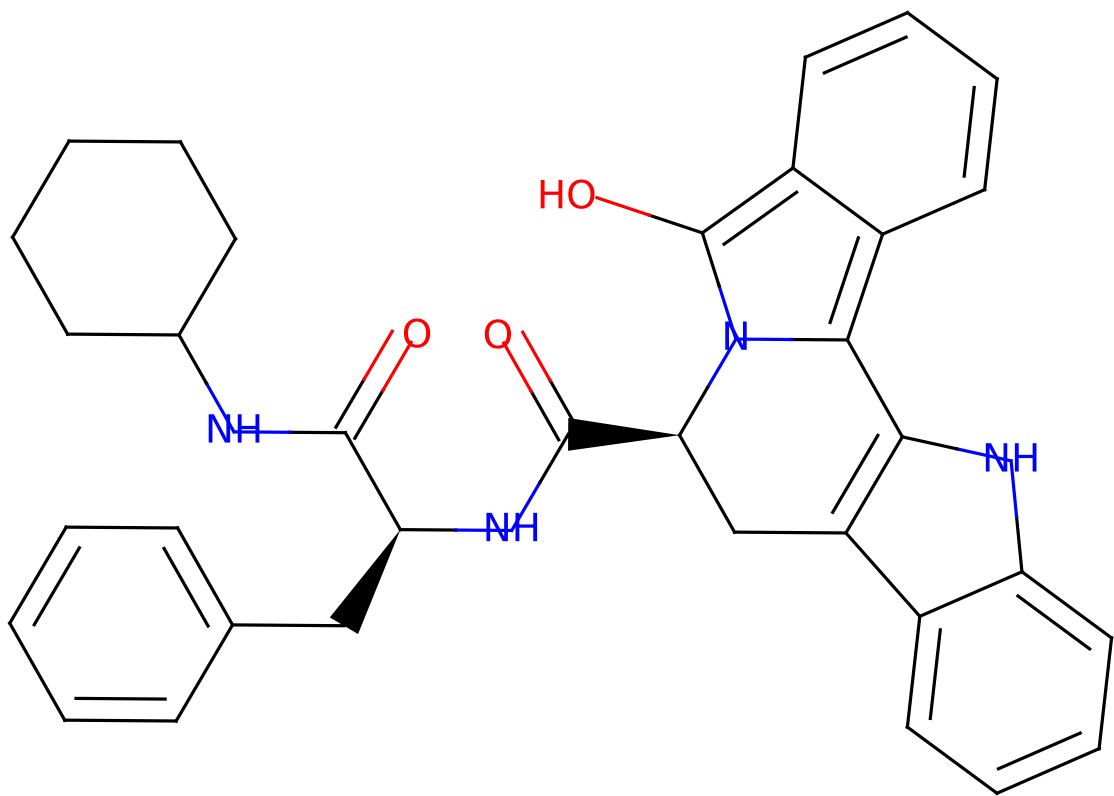
ORD-MCULE-2409941333_1

MolLogP: -0.5347999999999931 | QED: 0.33363924899756003

C[NH+](C)CCOc1cccc(c1)C[NH2+][C@H]2C[C@H]3C(=O)N[C@H](C(=O)N3C2)Cc4c[nH]c5c4cccc5

ORD-MCULE-1689748277_1

MolLogP: 5.768800000000006 | QED: 0.2176477509654081

c1ccc(cc1)C[C@@H](C(=O)NC2CCCCC2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-9395623979_1

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7

ORD-MCULE-7416131701_1

('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')
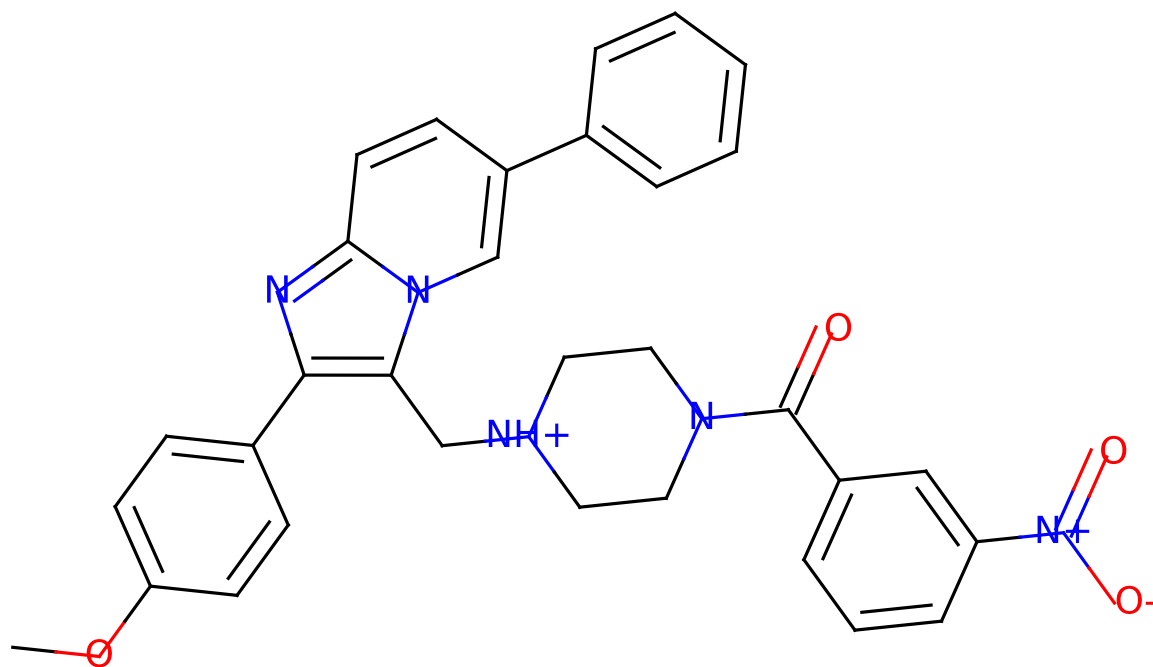
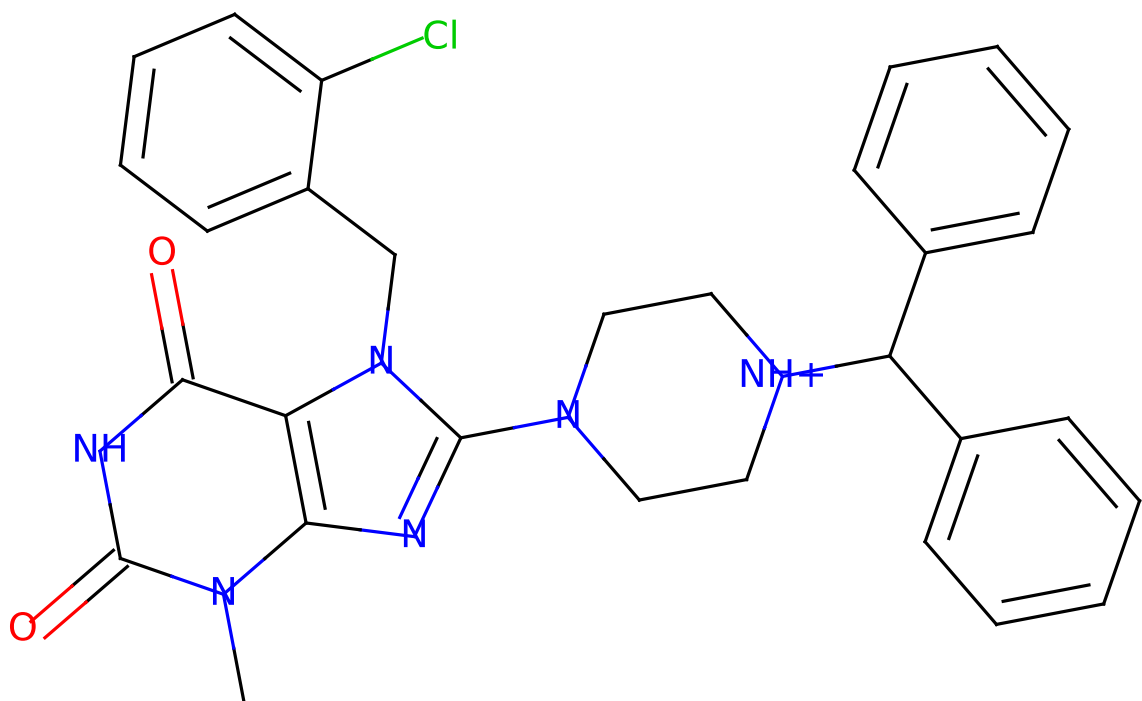MolLogP: 4.126000000000003 | QED: 0.2439331506700583

COc1ccc(cc1)c2c(n3cc(ccc3n2)c4ccccc4)C[NH+]5CCN(CC5)C(=O)c6cccc(c6)N(=O)=O

ORD-MCULE-5878589304_1
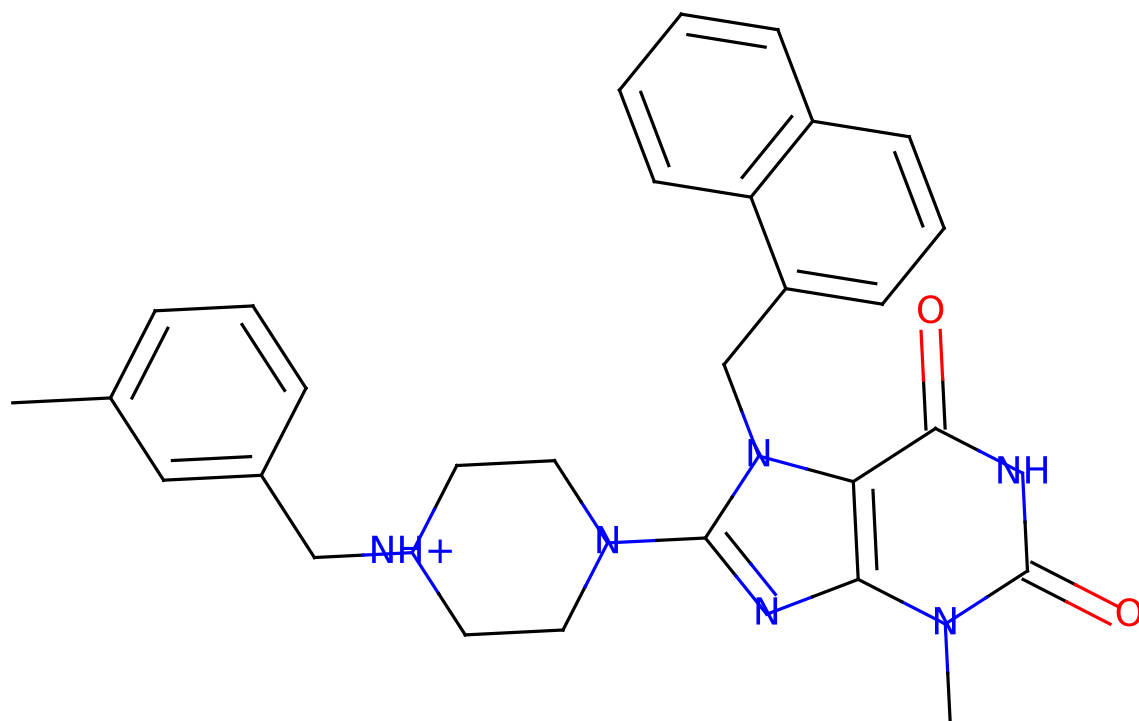
('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 2.619500000000003 | QED: 0.34626772452730337

Cn1c2c(c(=O)[nH]c1=O)n(c(n2)N3CC[NH+](CC3)C(c4ccccc4)c5ccccc5)Cc6ccccc6Cl
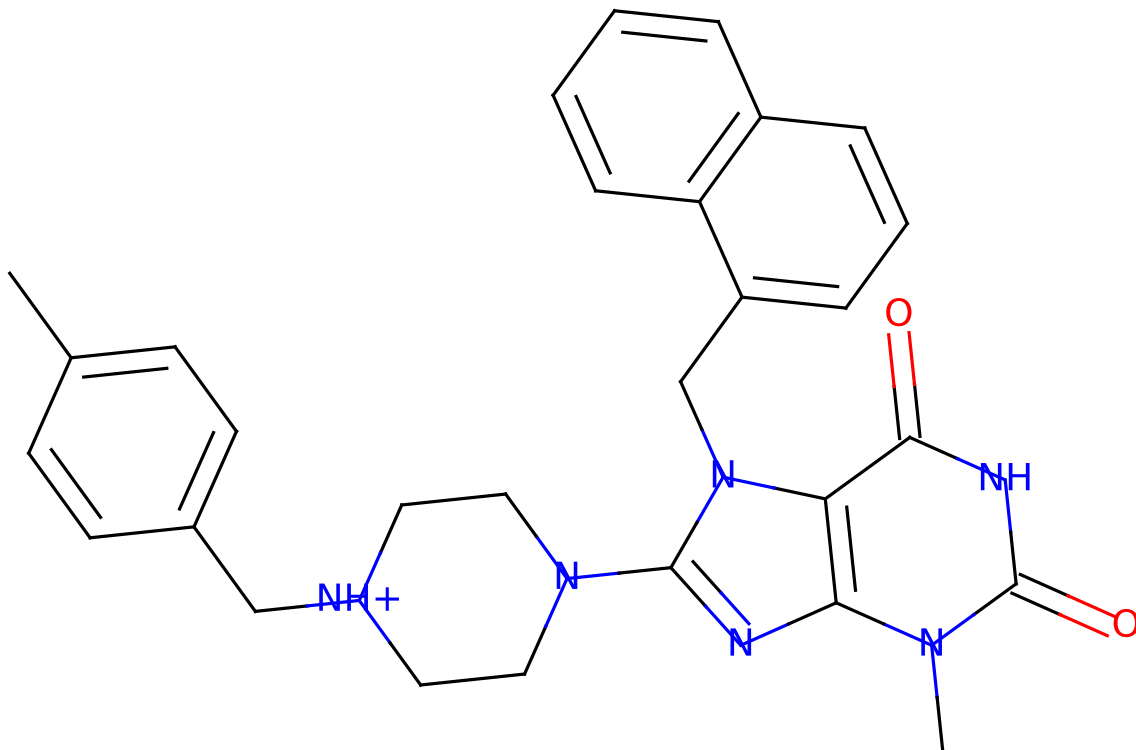
ORD-MCULE-5585700293_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
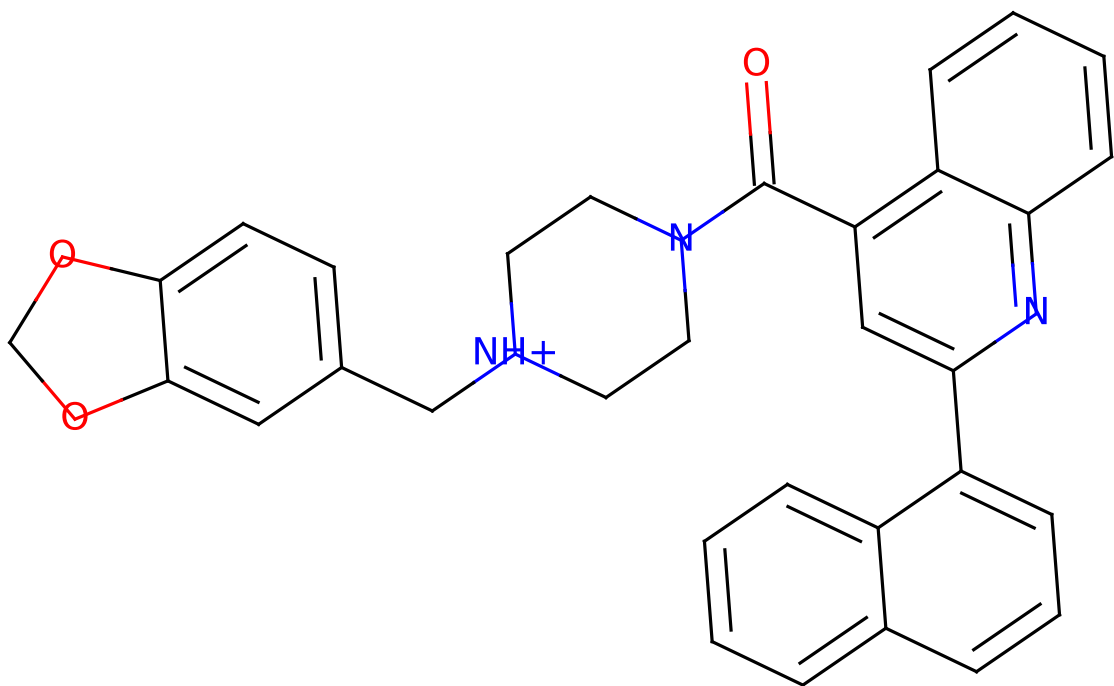
ORD-MCULE-9311937068_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

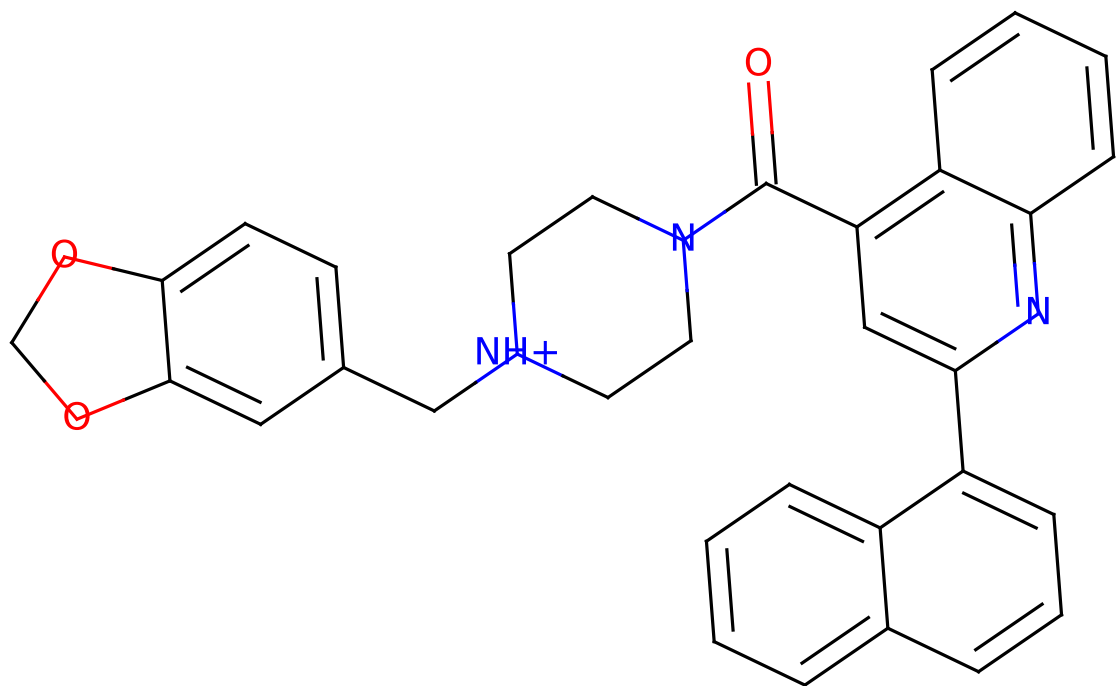Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C

ORD-MCULE-8959718627_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

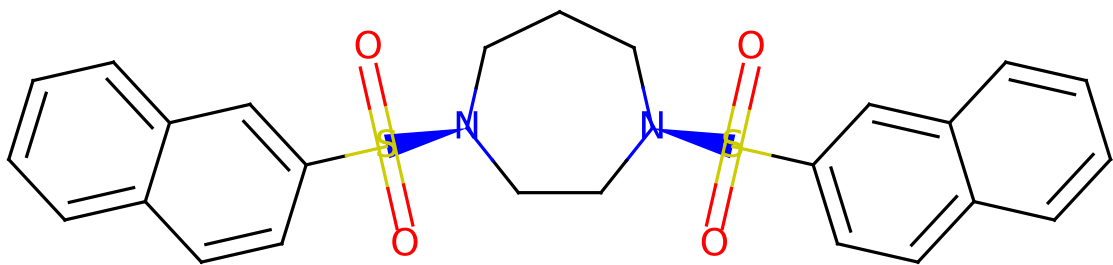c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-4959815000_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7
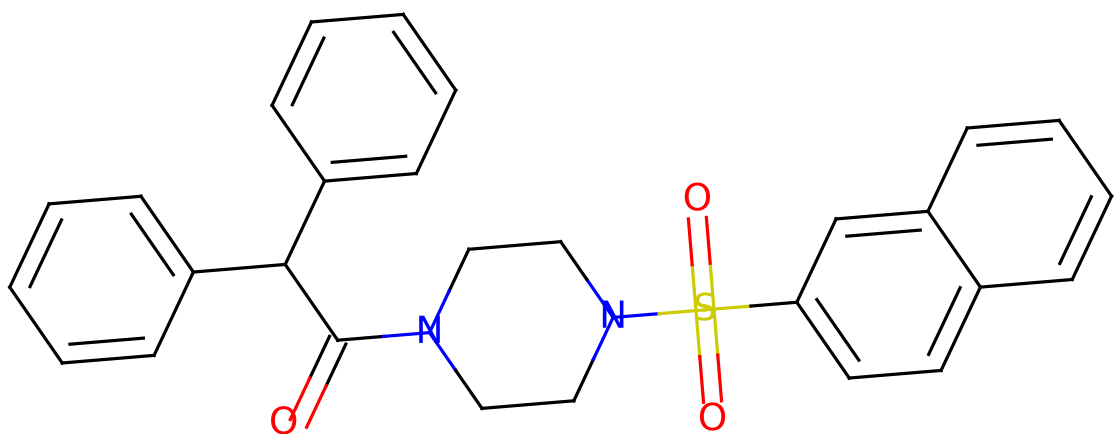
ORD-MCULE-3696478799_1

MolLogP: 4.078300000000003 | QED: 0.441202265024148

c1ccc2cc(ccc2c1)S(=O)(=O)[N@@]3CCC[N@](CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-4262091783_1
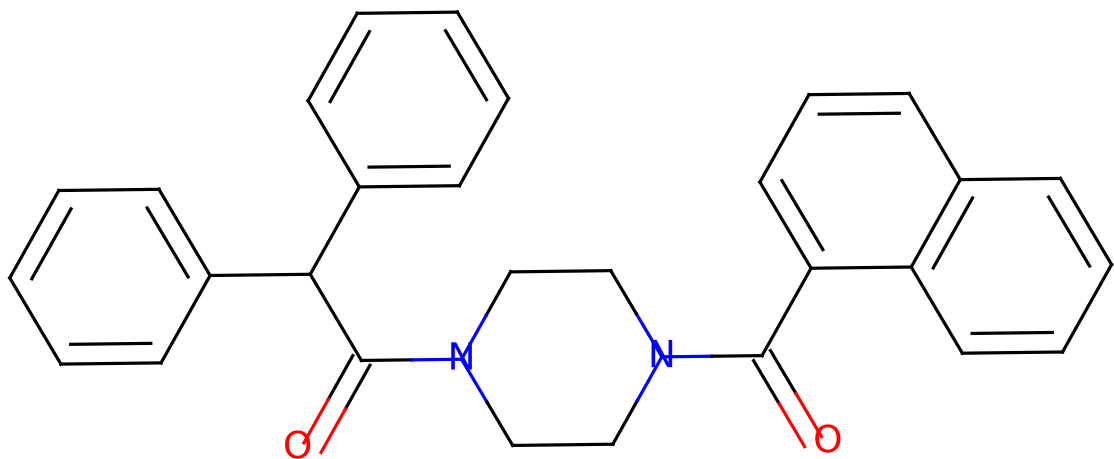
('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 4.504800000000004 | QED: 0.43144005118053486

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-9717306826_1
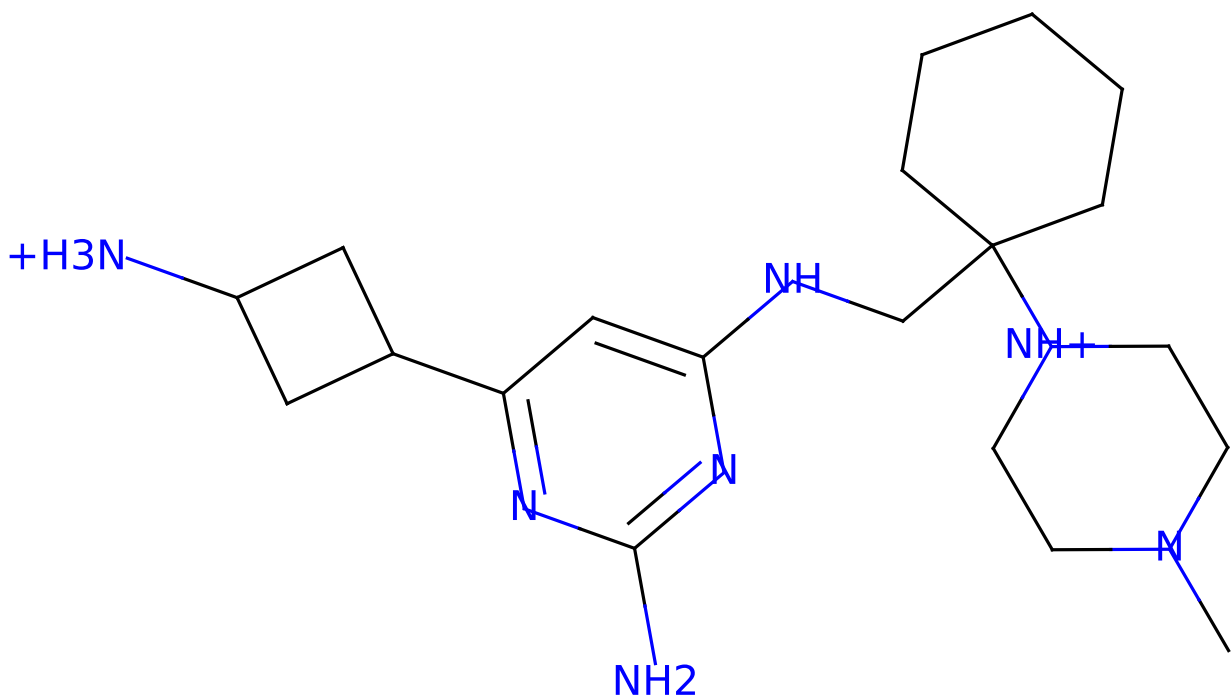
('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5
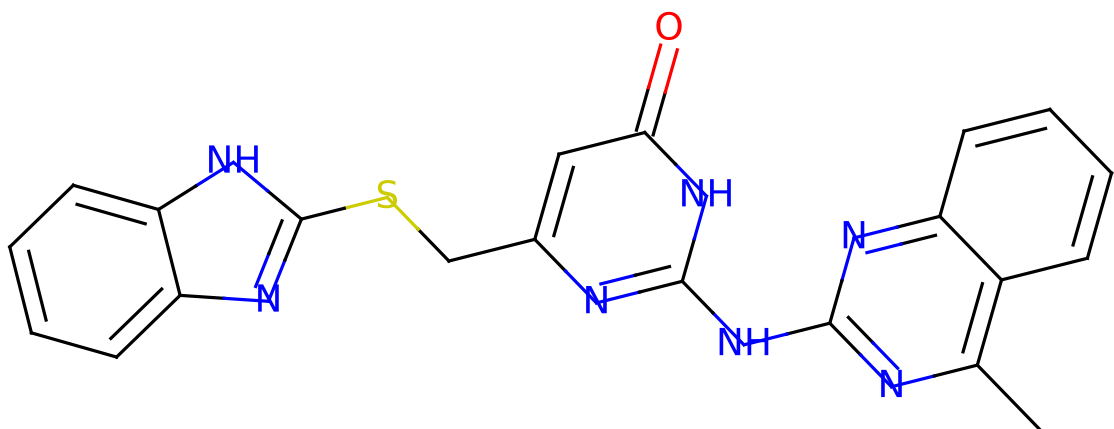
ORD-MCULE-4705080812_1

MolLogP: -0.5081999999999955 | QED: 0.5556824916141568

CN1CC[NH+](CC1)C2(CCCCC2)CNc3cc(nc(n3)N)C4CC(C4)[NH3+]

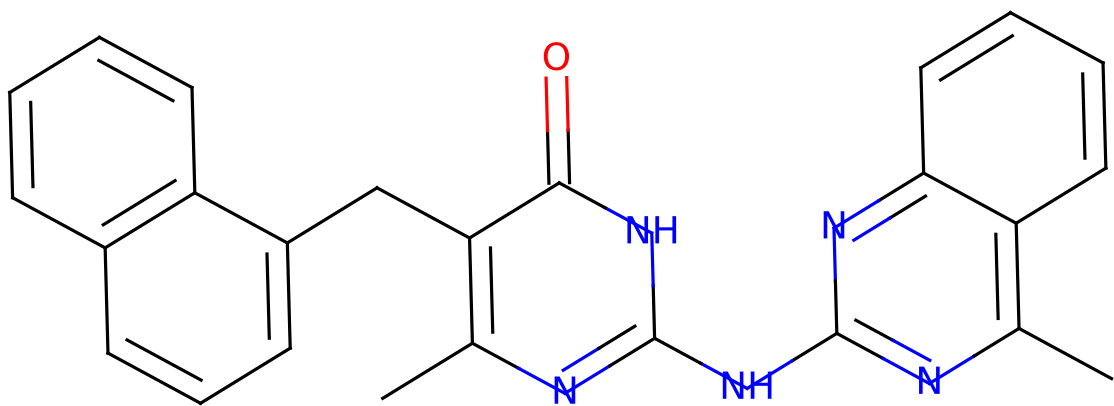ORD-MCULE-6677911371_1

('NSP15_6W01_AB_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 3.933720000000001 | QED: 0.3728174639709249

Cc1c2ccccc2nc(n1)Nc3[nH]c(=O)cc(n3)CSc4[nH]c5ccccc5n4

ORD-MCULE-6515729583_1
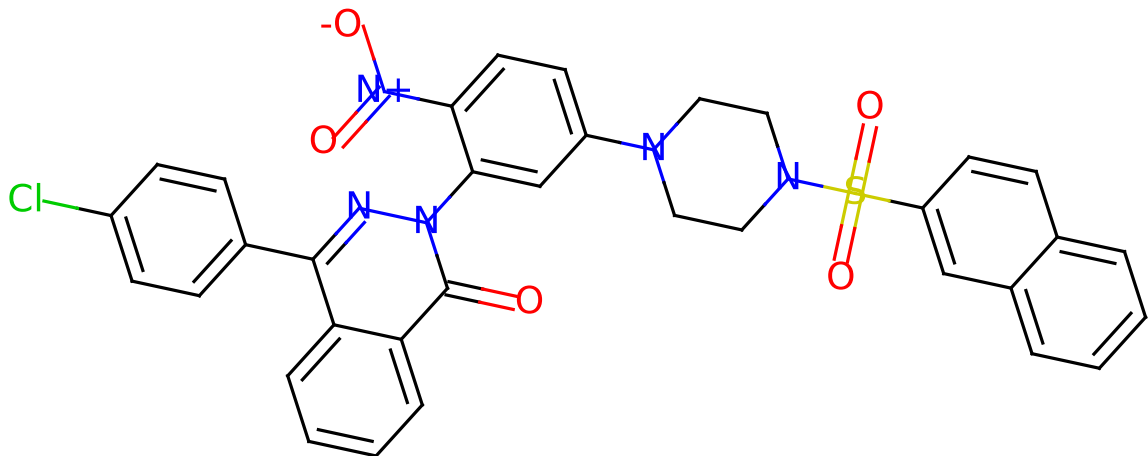
MolLogP: 4.817540000000003 | QED: 0.44632759624472335

Cc1c2ccccc2nc(n1)Nc3[nH]c(=O)c(c(n3)C)Cc4cccc5c4cccc5

ORD-MCULE-8965057287_1

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6ccccc6c(n5)c7ccc(cc7)Cl)N(=O)=O

ORD-MCULE-1708960826_1

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7
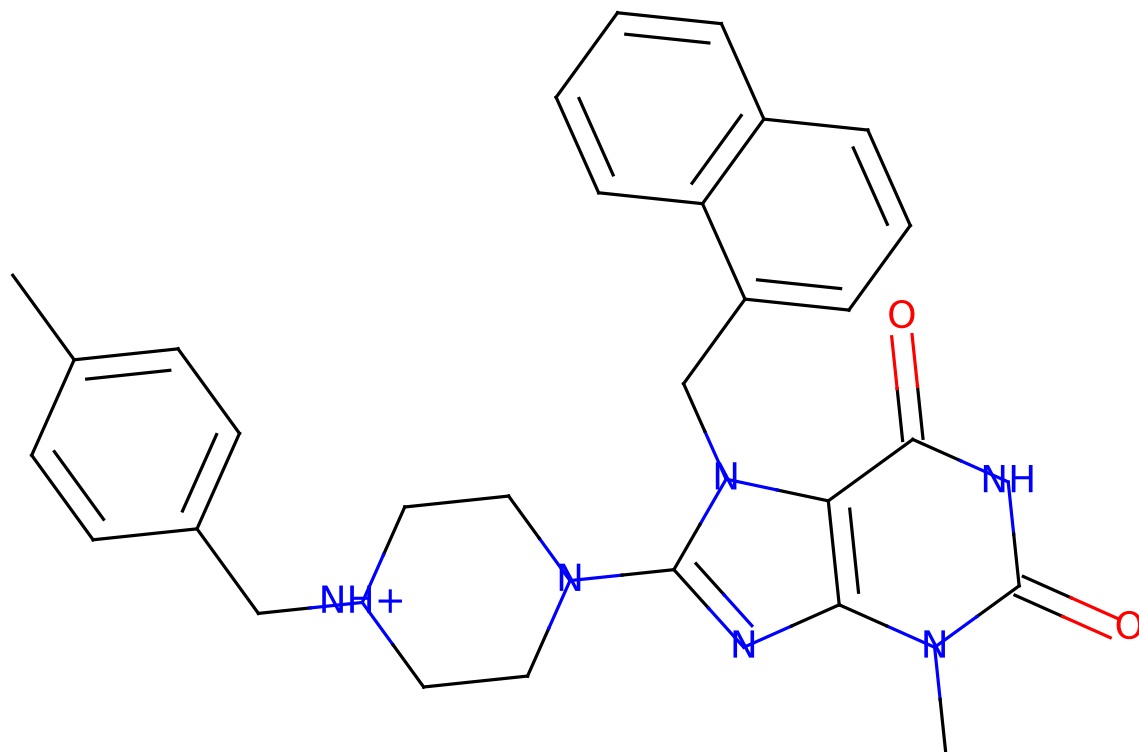
ORD-MCULE-7416131701_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
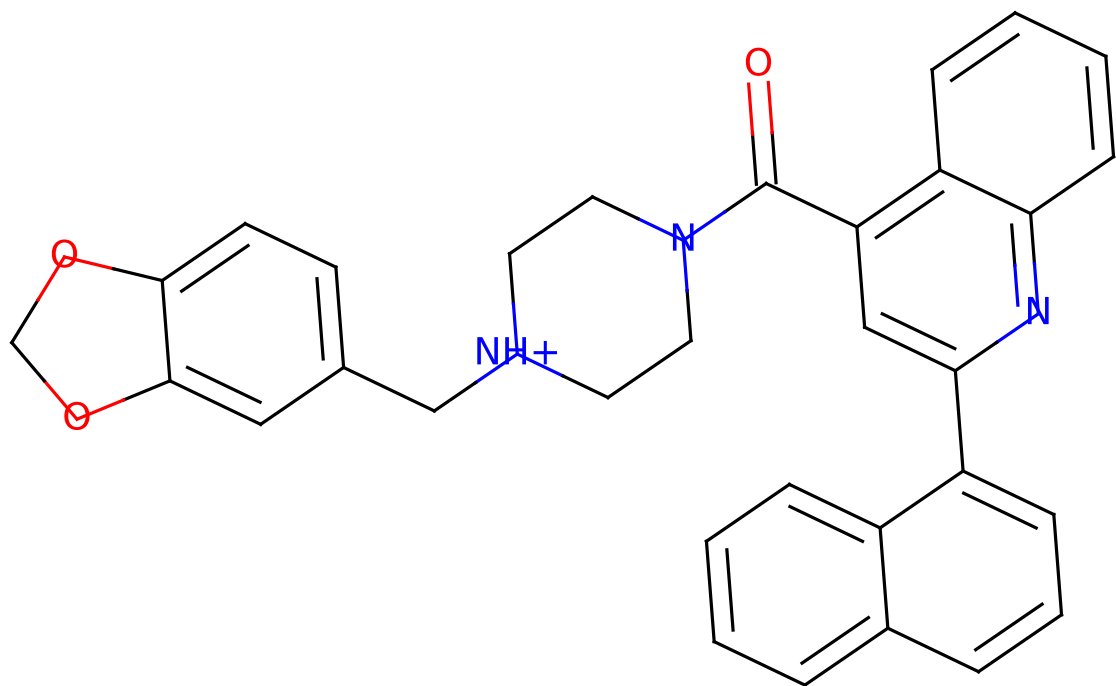
ORD-MCULE-9311937068_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

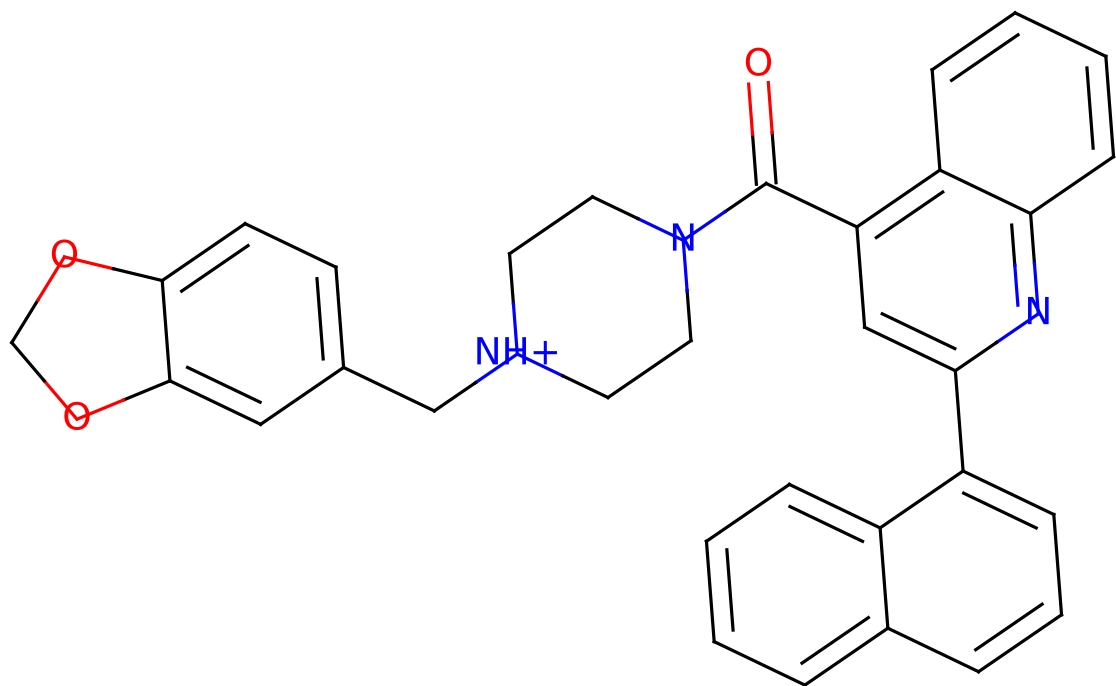Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C

ORD-MCULE-8959718627_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

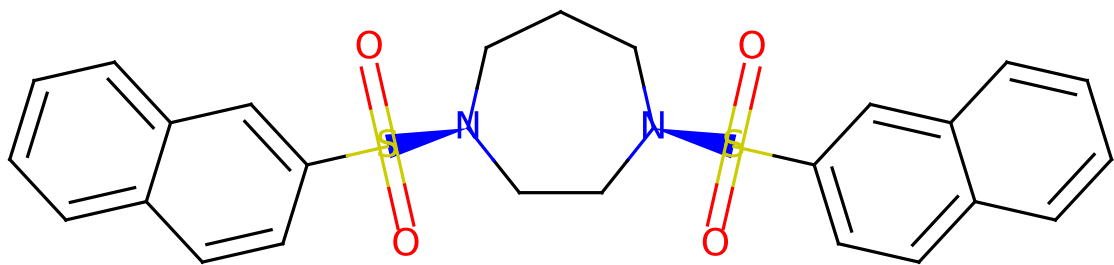c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-4959815000_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

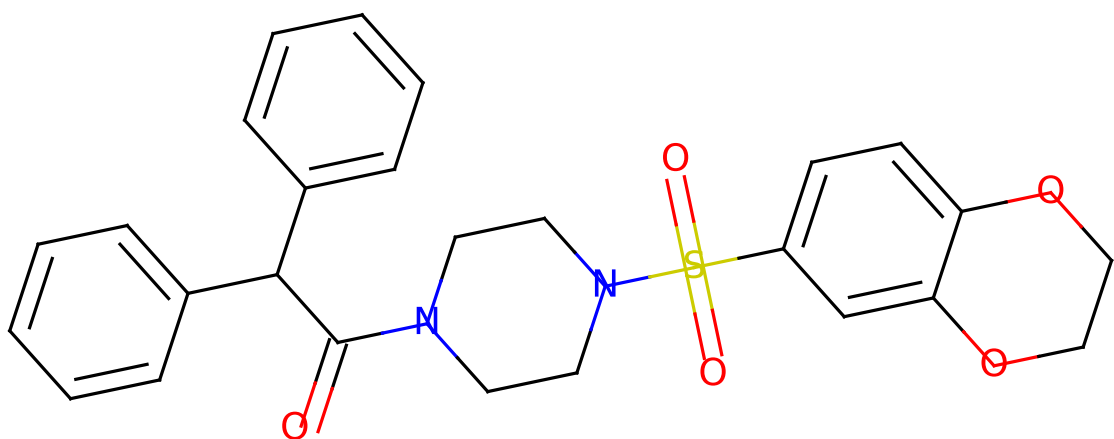c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-3696478799_1

MolLogP: 4.078300000000003 | QED: 0.441202265024148

c1ccc2cc(ccc2c1)S(=O)(=O)[N@@]3CCC[N@](CC3)S(=O)(=O)c4ccc5ccccc5c4
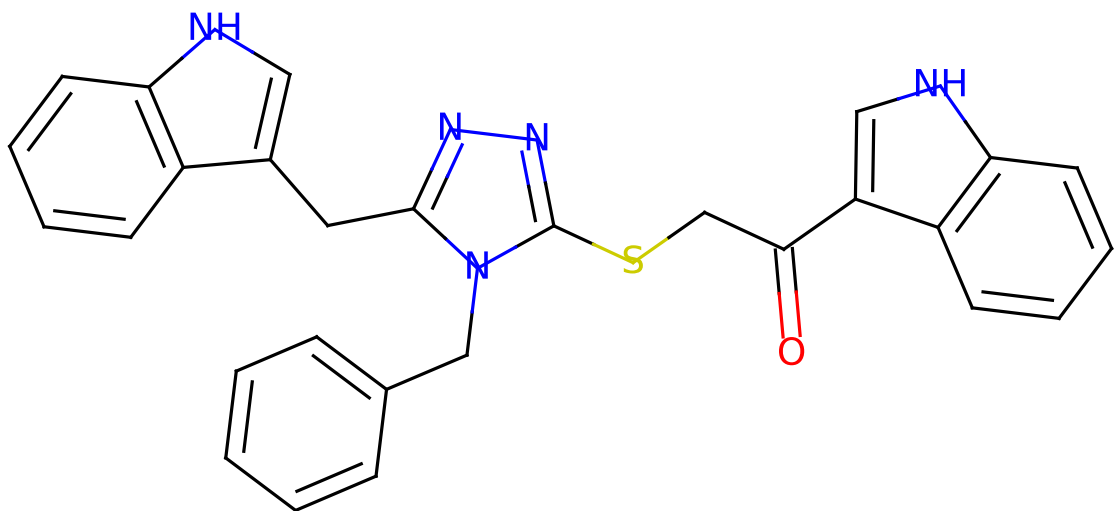
ORD-MCULE-4262091783_1

MolLogP: 3.1228000000000016 | QED: 0.5633261375042687

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5c(c4)OCCO5

ORD-MCULE-1904175079_1
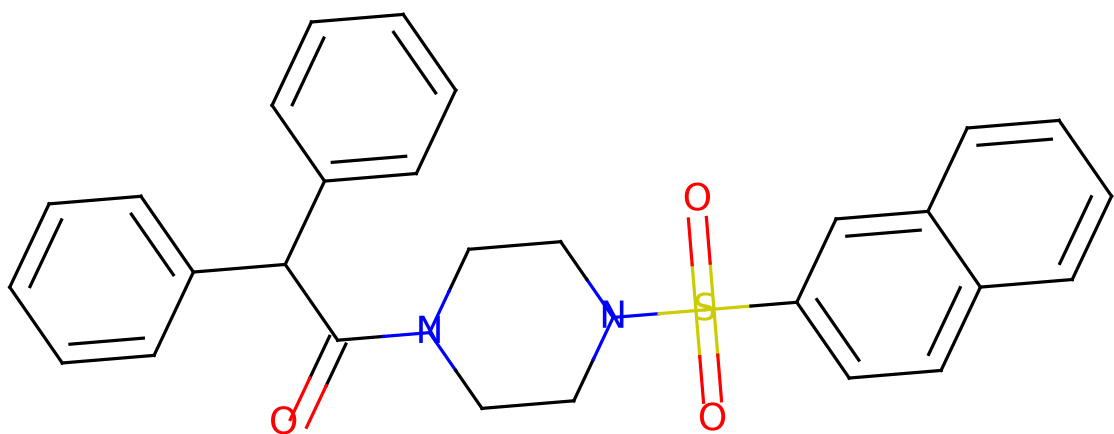
('NSP15_6W01_AB_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 5.8548000000000044 | QED: 0.21272800874019035

c1ccc(cc1)Cn2c(nnc2SCC(=O)c3c[nH]c4c3cccc4)Cc5c[nH]c6c5cccc6

ORD-MCULE-2017284421_1
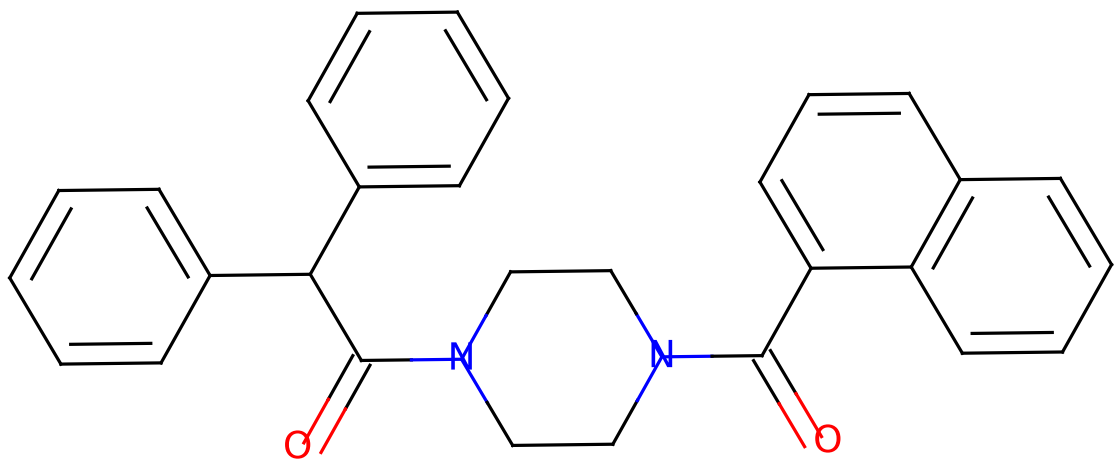
('NSP15_6W01_AB_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 4.504800000000004 | QED: 0.43144005118053486

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4
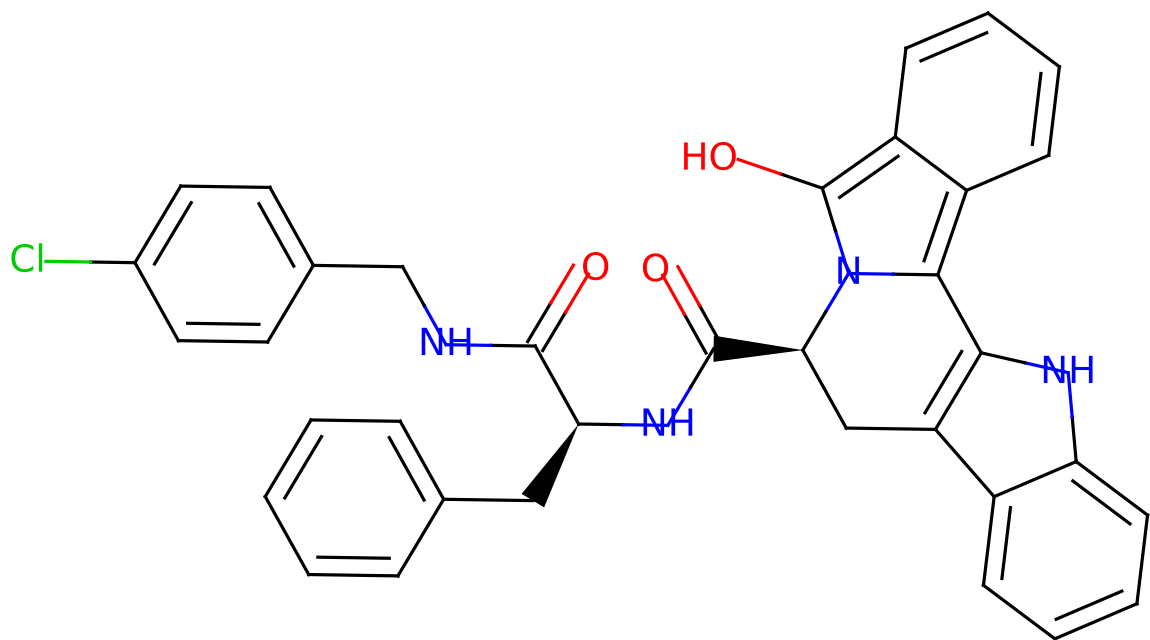
ORD-MCULE-9717306826_1

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

ORD-MCULE-4705080812_1
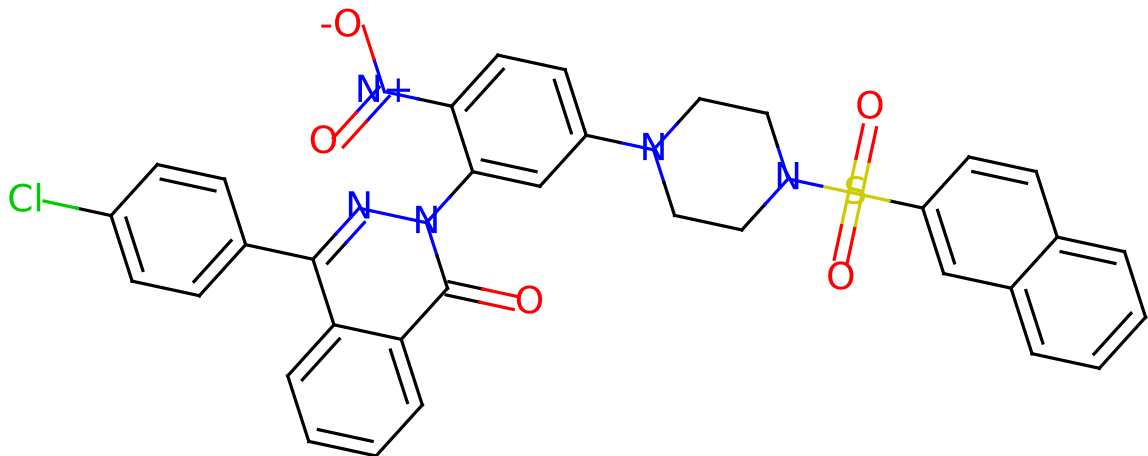
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 6.289700000000006 | QED: 0.1763358576321032

c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)Cl)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O
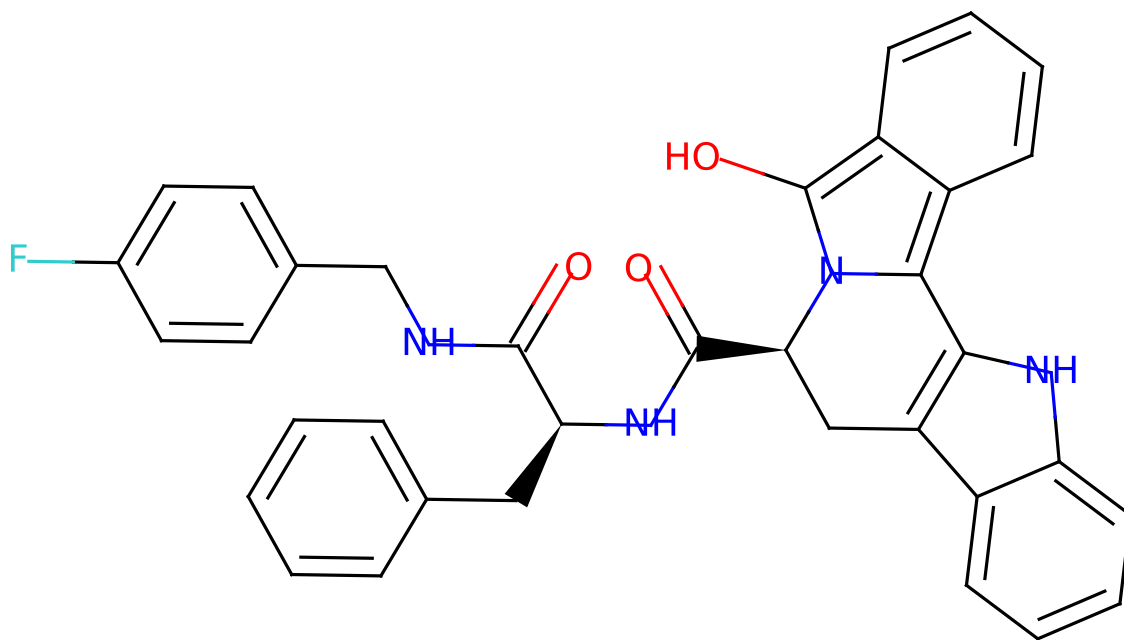
ORD-MCULE-6977725985_1

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6ccccc6c(n5)c7ccc(cc7)Cl)N(=O)=O

ORD-MCULE-1708960826_1
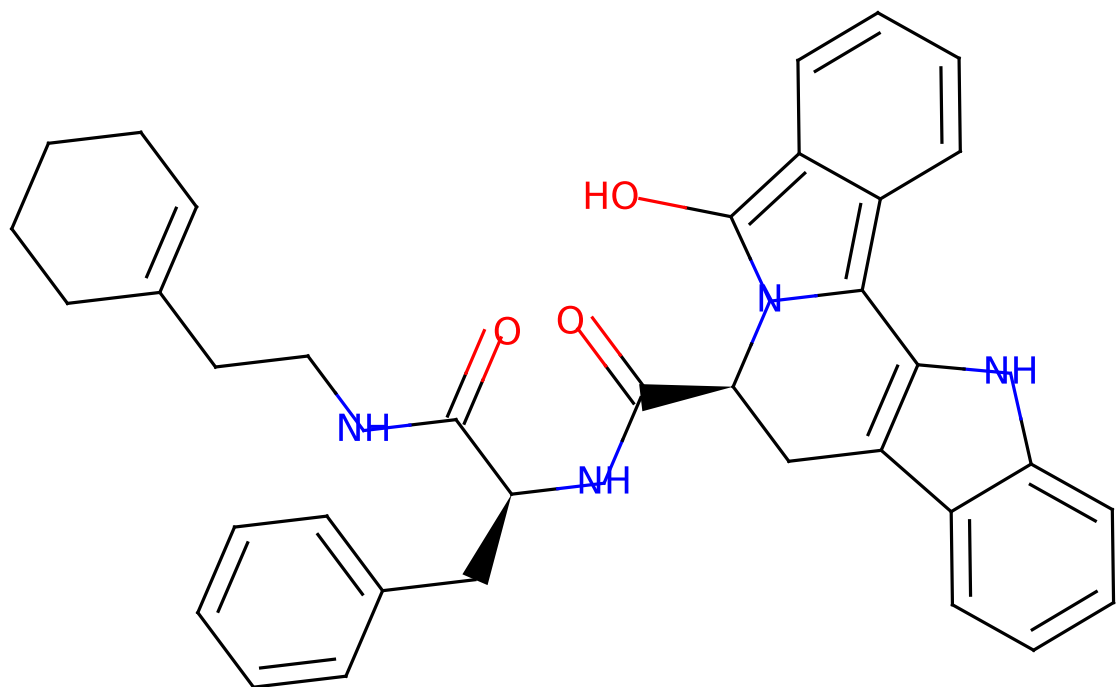
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 5.775400000000006 | QED: 0.19535260854802458

c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)F)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O
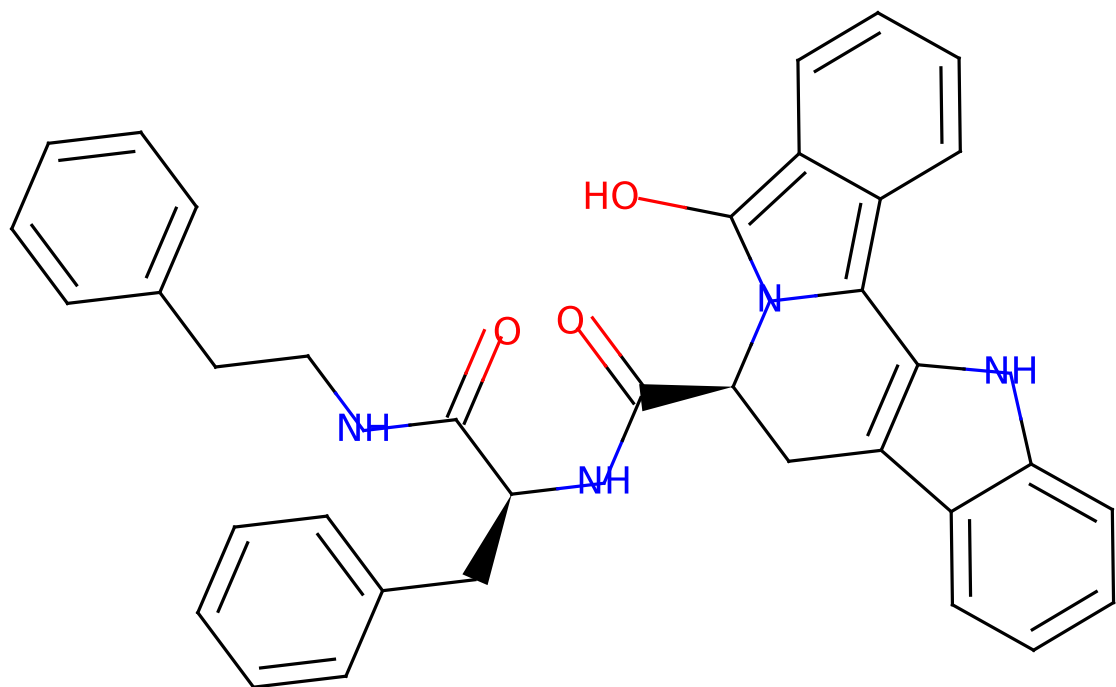
ORD-MCULE-6477680903_1

MolLogP: 6.326600000000007 | QED: 0.163672300852651

c1ccc(cc1)C[C@@H](C(=O)NCCC2=CCCCC2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

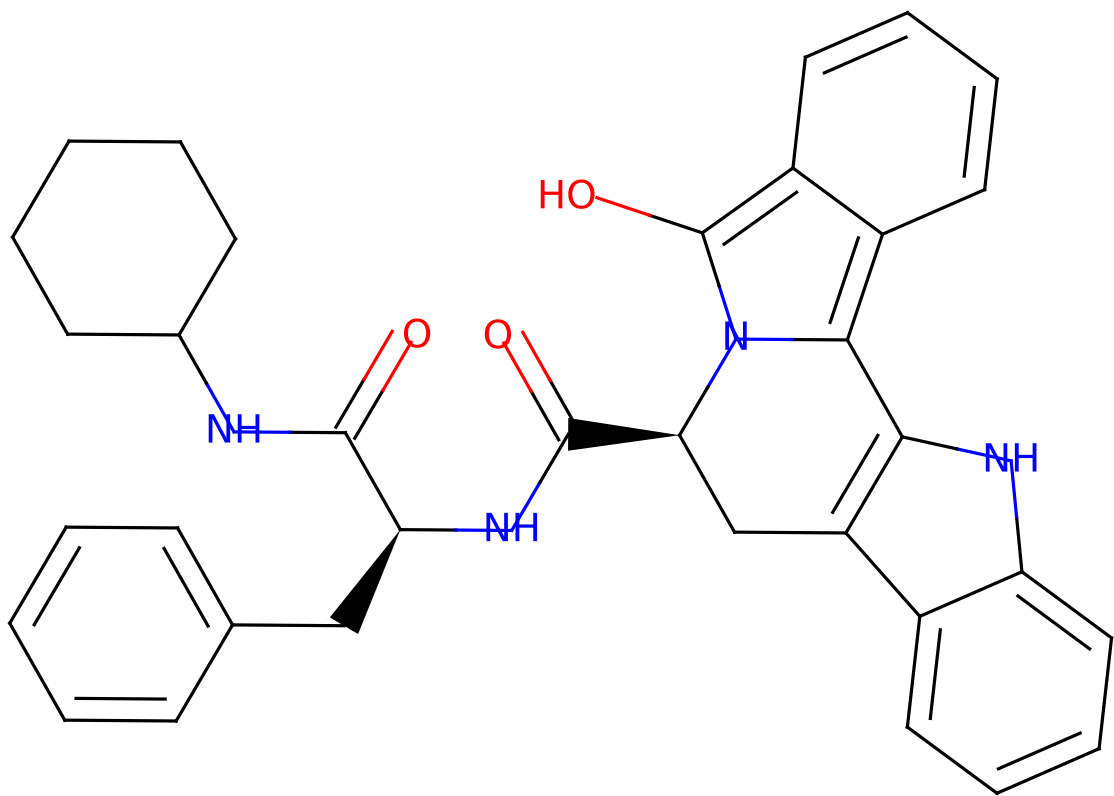ORD-MCULE-2409941333_1

('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 5.678800000000005 | QED: 0.1901898602150378

c1ccc(cc1)CCNC(=O)[C@H](Cc2ccccc2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-1662960575_1
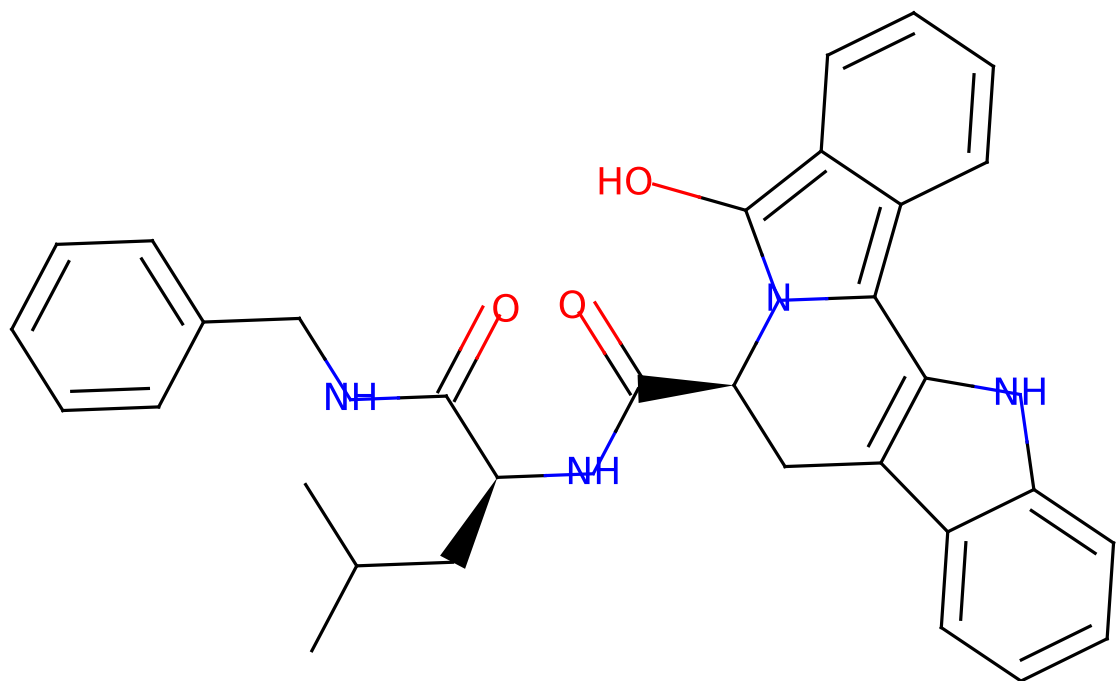
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 5.768800000000006 | QED: 0.2176477509654081

c1ccc(cc1)C[C@@H](C(=O)NC2CCCCC2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-9395623979_1

MolLogP: 5.439700000000005 | QED: 0.22997913326523065

CC(C)C[C@@H](C(=O)NCc1ccccc1)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O

ORD-MCULE-1429565079_1

('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7

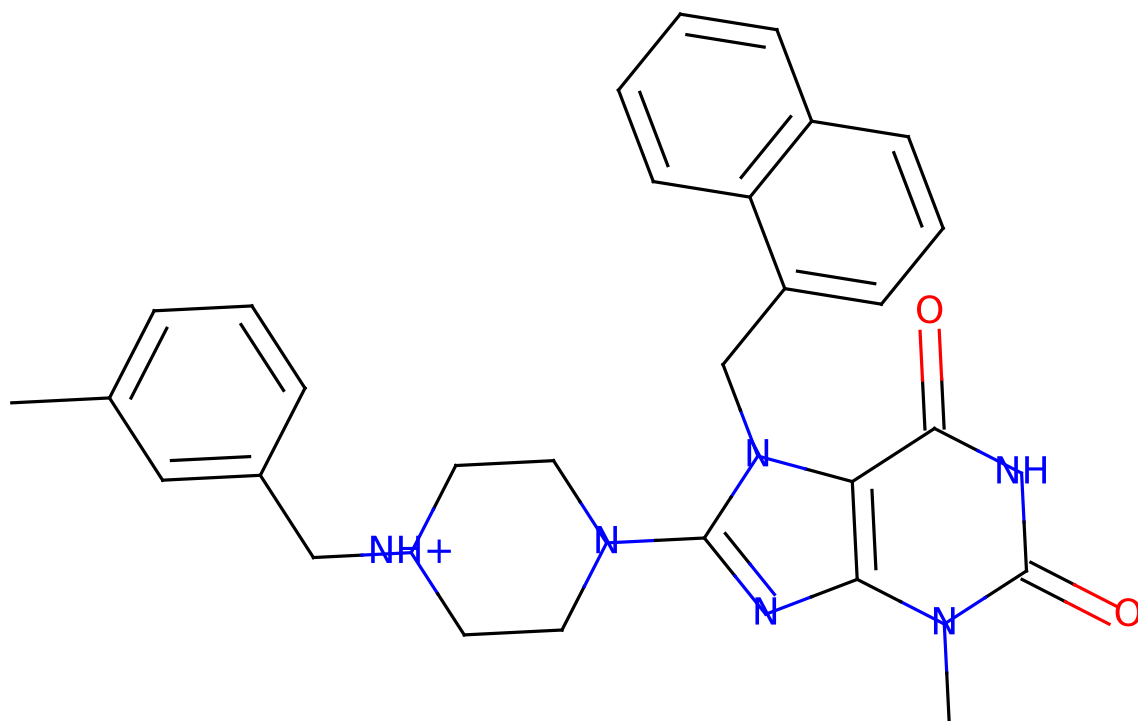ORD-MCULE-7416131701_1

('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')
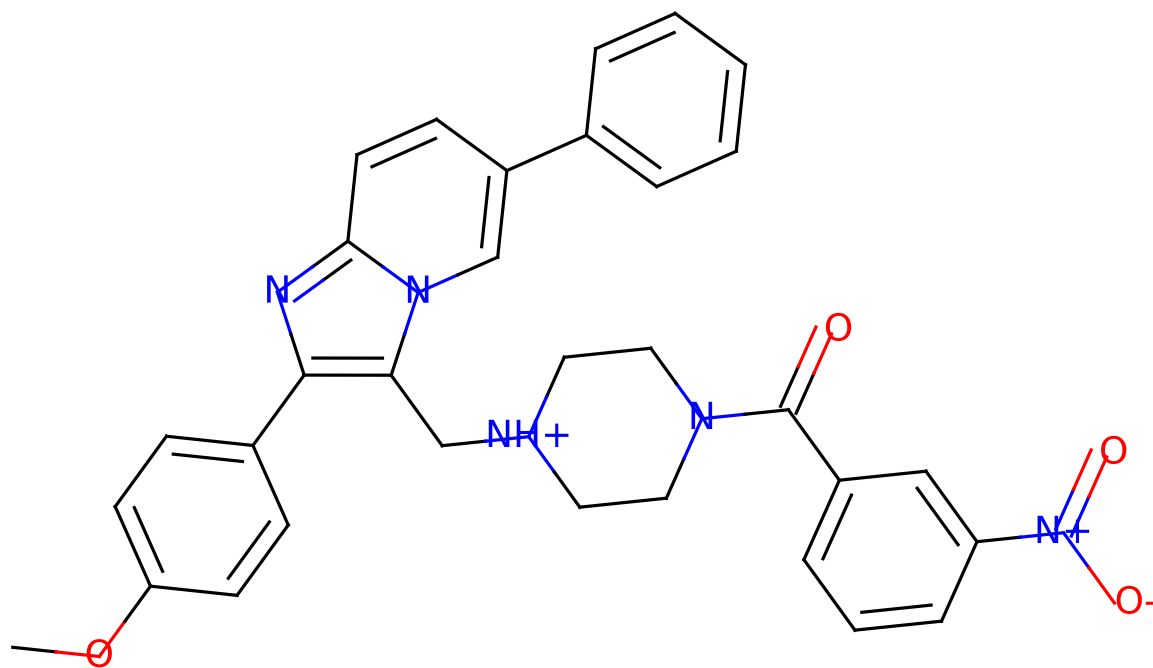
MolLogP: 4.126000000000003 | QED: 0.2439331506700583

COc1ccc(cc1)c2c(n3cc(ccc3n2)c4ccccc4)C[NH+]5CCN(CC5)C(=O)c6cccc(c6)N(=O)=O

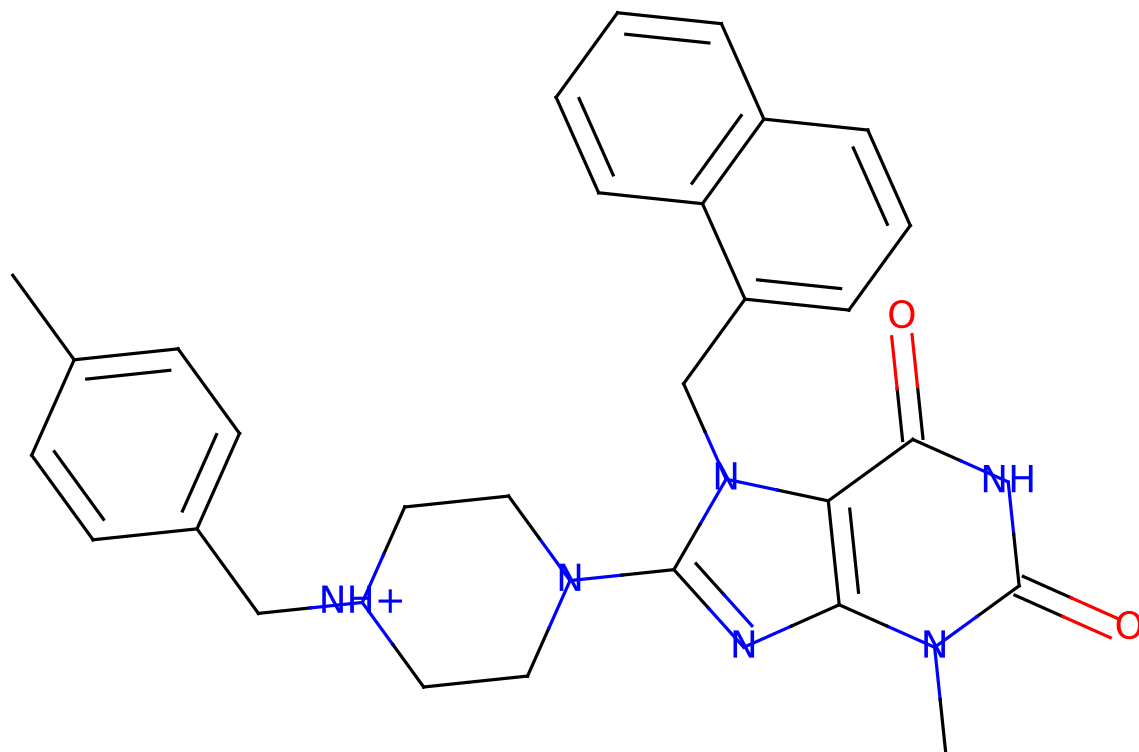ORD-MCULE-5878589304_1

('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
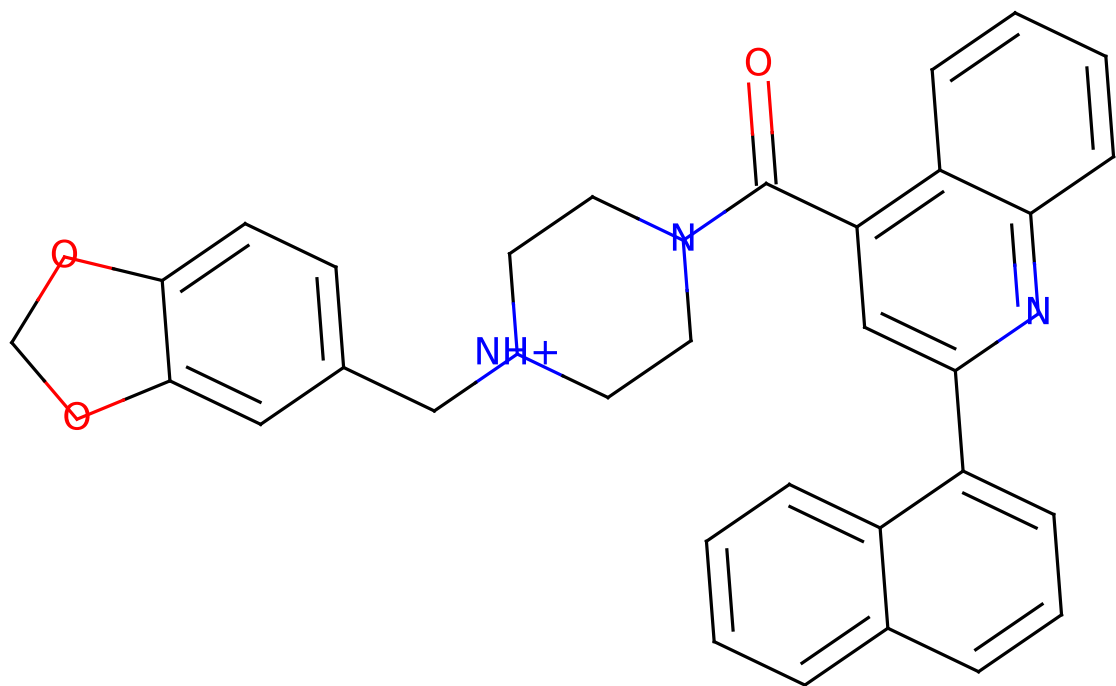
ORD-MCULE-9311937068_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
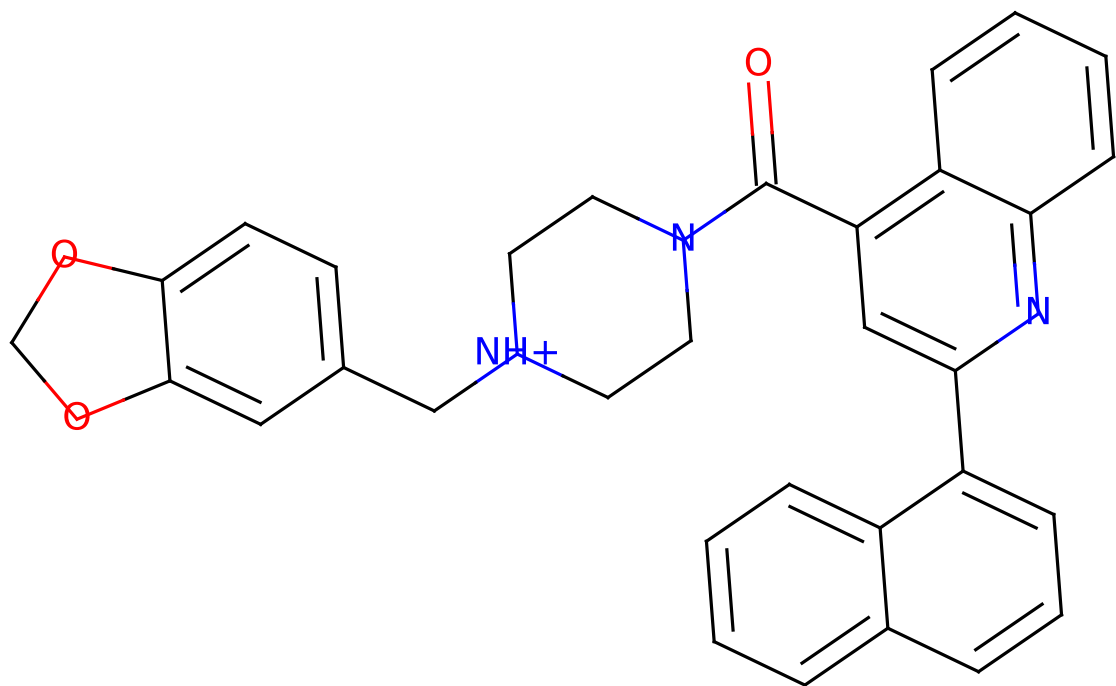
ORD-MCULE-8959718627_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7
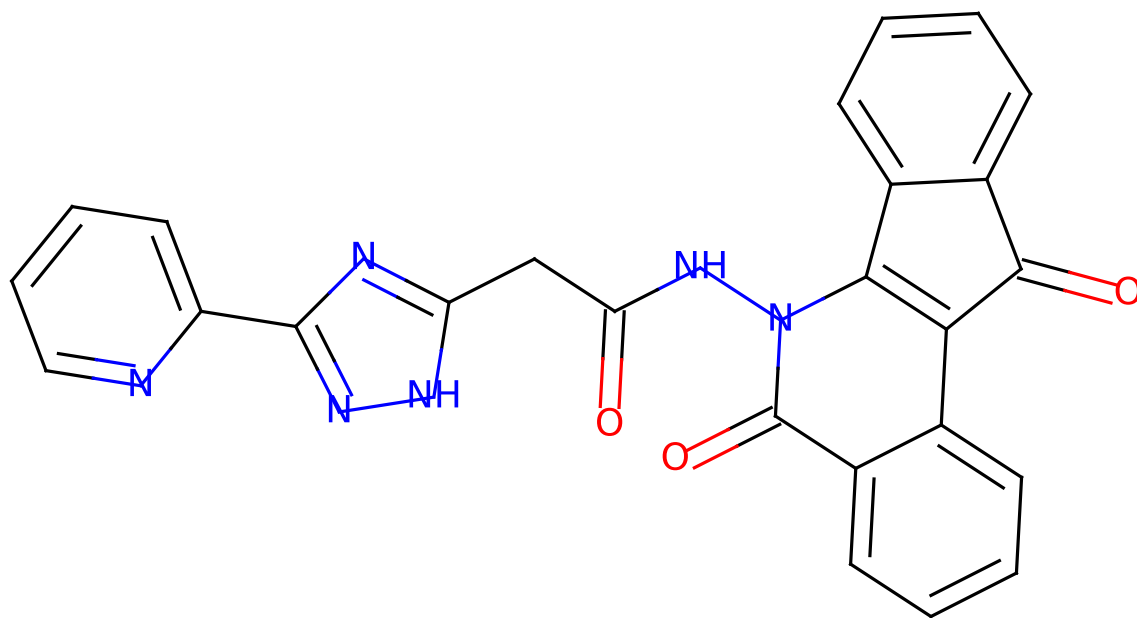
ORD-MCULE-4959815000_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7
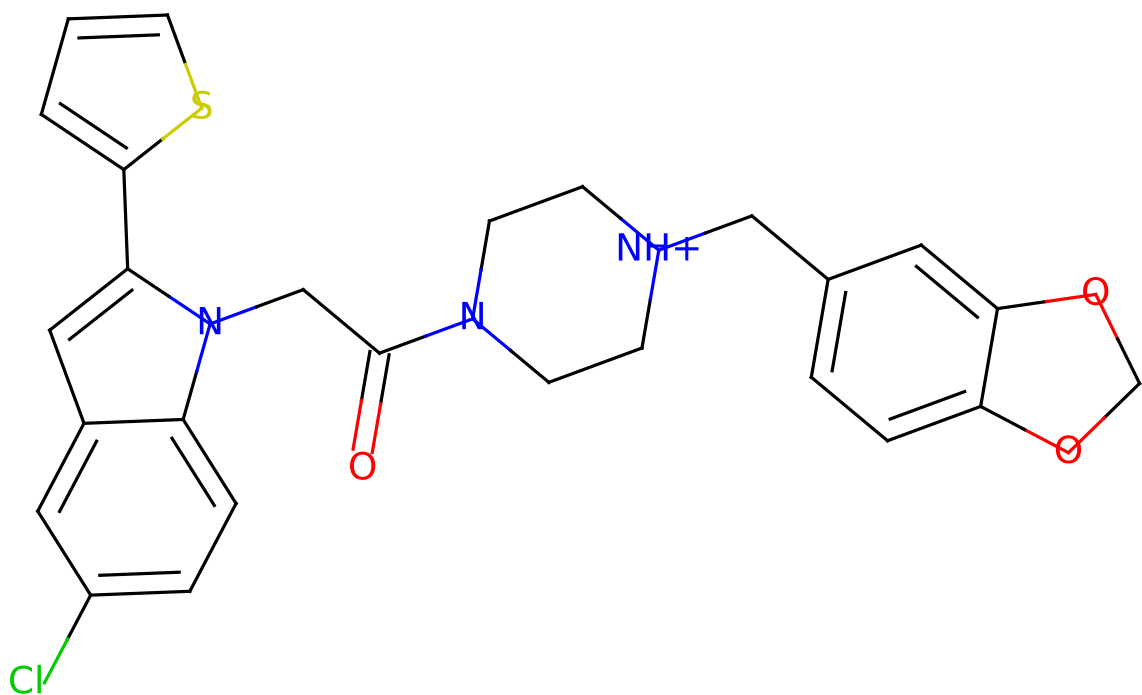
ORD-MCULE-3696478799_1

MolLogP: 2.705800000000001 | QED: 0.4275564127608206

c1ccc2c(c1)c3c(n(c2=O)NC(=O)Cc4[nH]nc(n4)c5ccccn5)-c6ccccc6C3=O

ORD-MCULE-1087797516_1
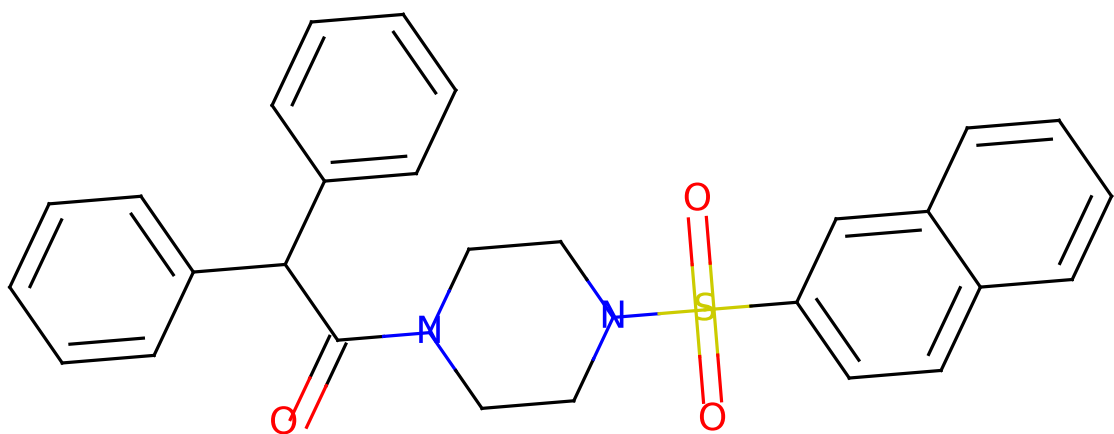
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 3.6792000000000016 | QED: 0.46023888484418957

c1cc(sc1)c2cc3cc(ccc3n2CC(=O)N4CC[NH+](CC4)Cc5ccc6c(c5)OCO6)Cl
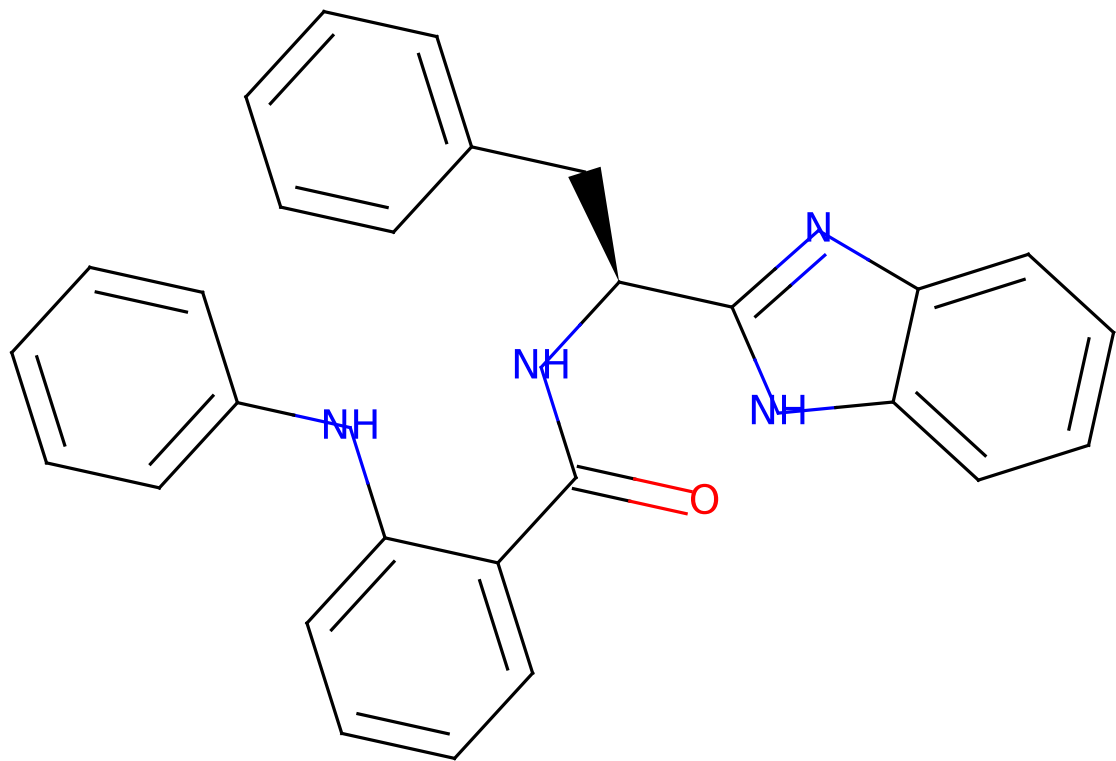
ORD-MCULE-8022118059_1

MolLogP: 4.504800000000004 | QED: 0.43144005118053486

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-9717306826_1
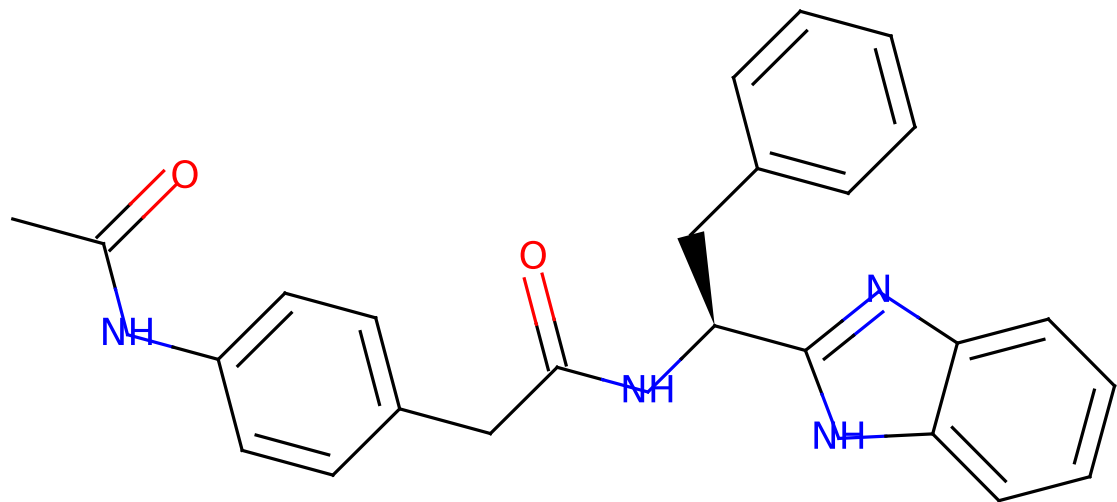
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 6.020300000000004 | QED: 0.2944823282671522

c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4ccccc4Nc5ccccc5

ORD-MCULE-8785708058_1
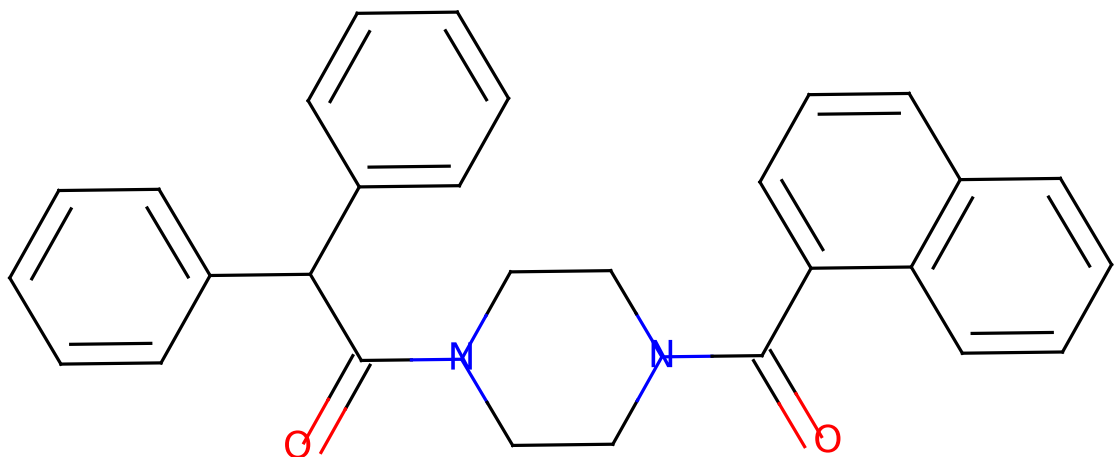
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 4.164000000000002 | QED: 0.42587160458676115

CC(=O)Nc1ccc(cc1)CC(=O)N[C@@H](Cc2ccccc2)c3[nH]c4ccccc4n3
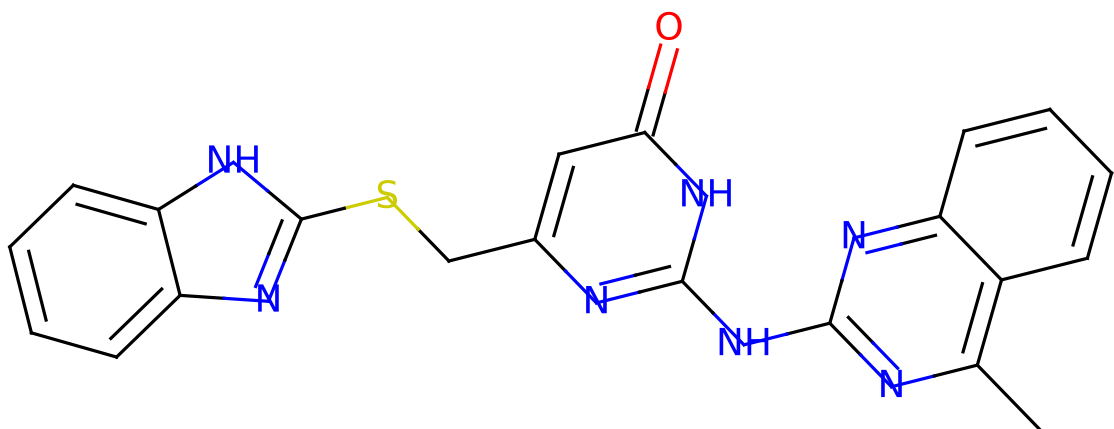
ORD-MCULE-9073095150_1

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

ORD-MCULE-4705080812_1
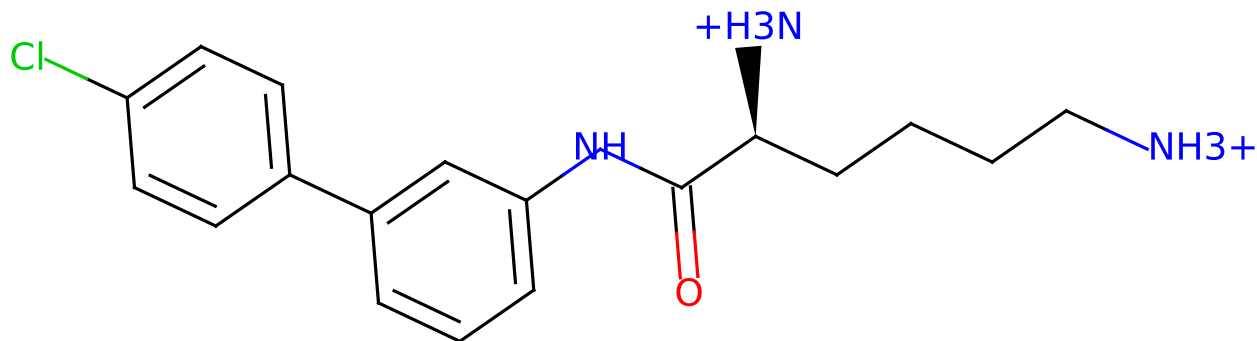
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 3.933720000000001 | QED: 0.3728174639709249

Cc1c2ccccc2nc(n1)Nc3[nH]c(=O)cc(n3)CSc4[nH]c5ccccc5n4
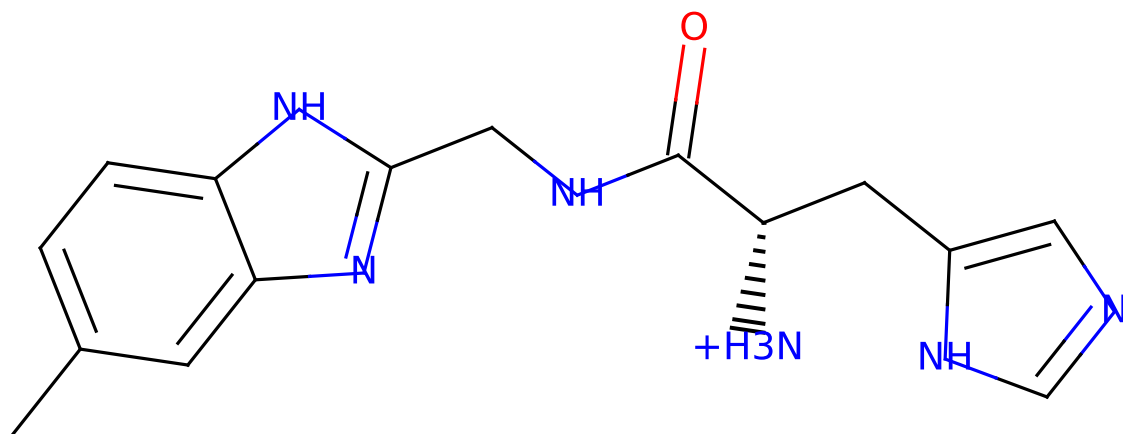
ORD-MCULE-6515729583_1

MolLogP: 1.9682000000000006 | QED: 0.6648487288742537

c1cc(cc(c1)NC(=O)[C@H](CCCC[NH3+])[NH3+])c2ccc(cc2)Cl

ORD-MCULE-8425442450_1
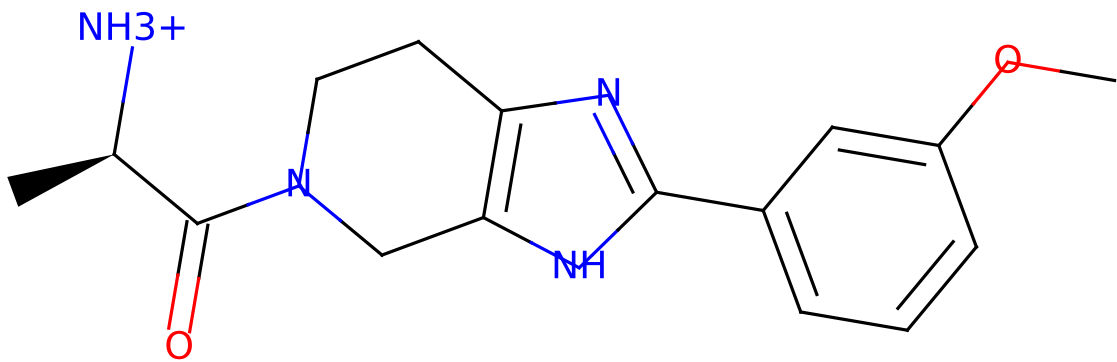
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 0.06382000000000104 | QED: 0.5339791274710981

Cc1ccc2c(c1)nc([nH]2)CNC(=O)[C@H](Cc3cnc[nH]3)[NH3+]

ORD-MCULE-7818026901_2
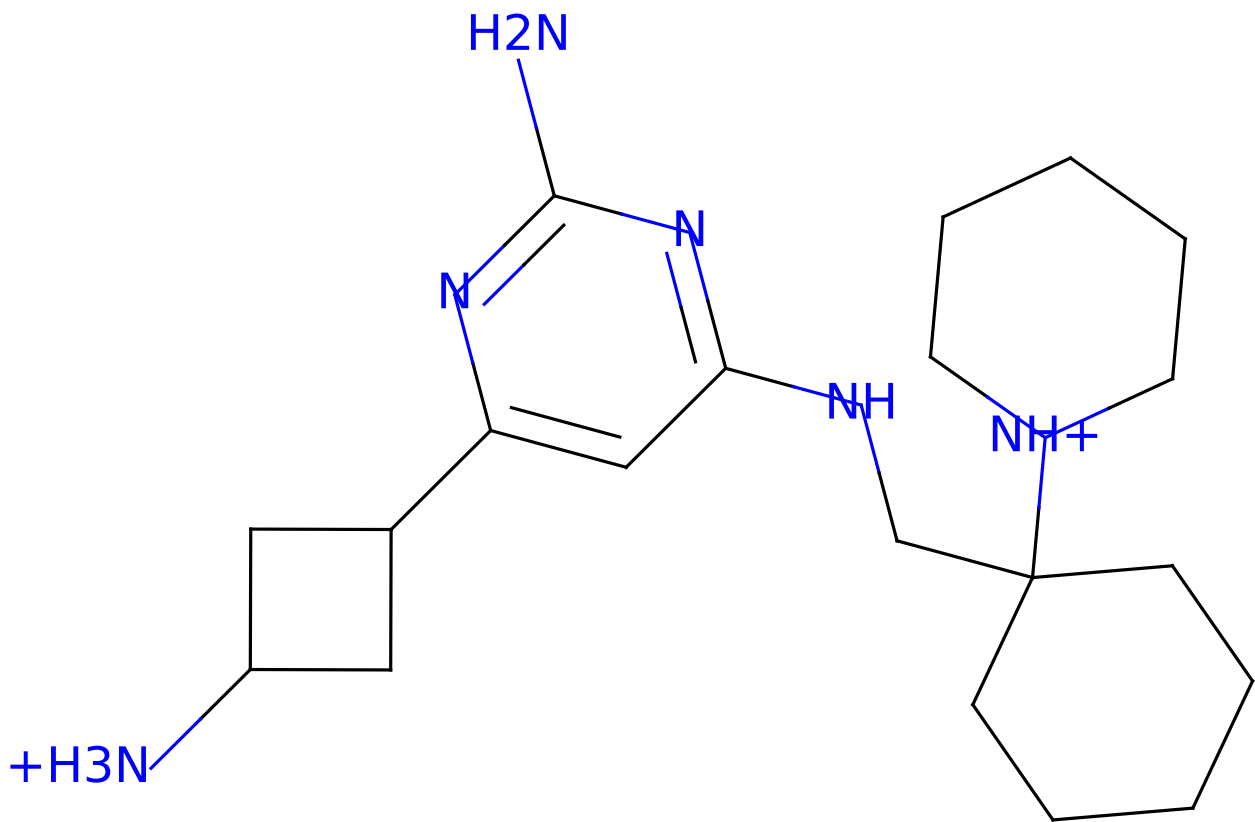
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 0.6004 | QED: 0.8702502574304508

C[C@H](C(=O)N1CCc2c([nH]c(n2)c3cccc(c3)OC)C1)[NH3+]

ORD-MCULE-6534865045_1
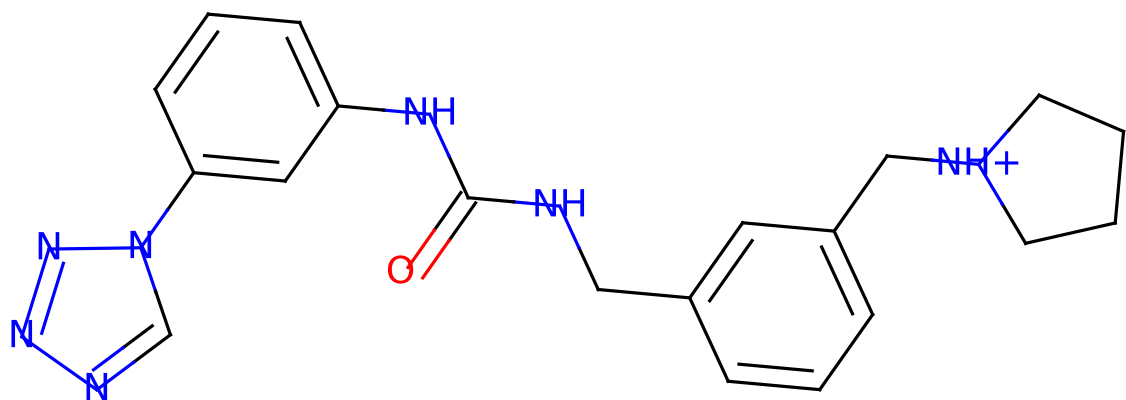
H2N

N

N

NH

NH+

+H3N

MolLogP: 0.7303000000000031 | QED: 0.6224096899439784

c1c(nc(nc1NCC2(CCCCC2)[NH+]3CCCCC3)N)C4CC(C4)[NH3+]

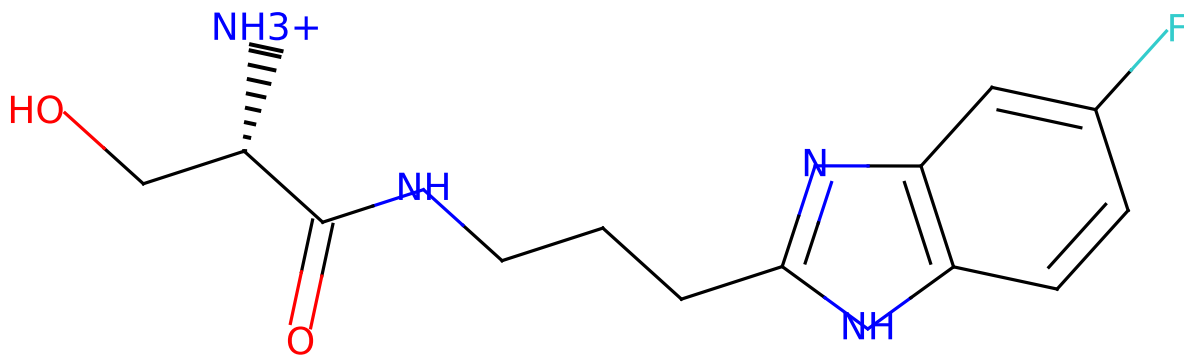ORD-MCULE-4013099548_1

('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 1.162699999999999 | QED: 0.6006008381376307

c1cc(cc(c1)C[NH+]2CCCC2)CNC(=O)Nc3cccc(c3)n4cnnn4

ORD-MCULE-1562586832_1
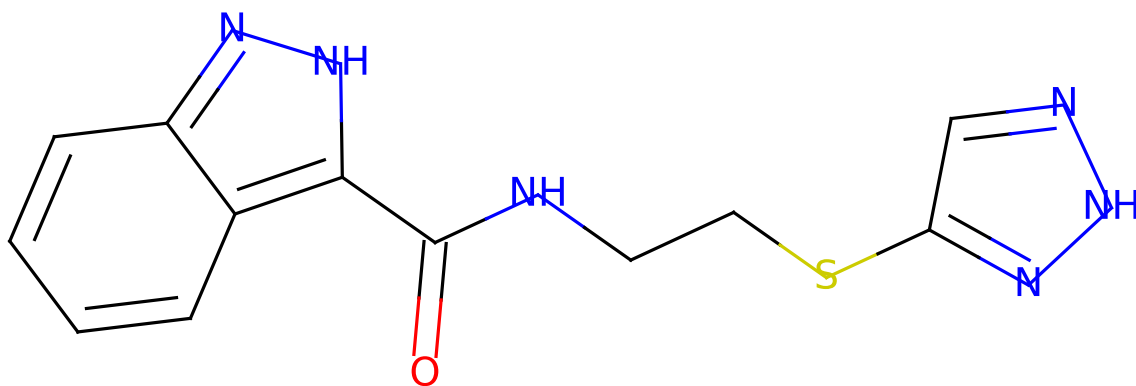
('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: -0.6463999999999992 | QED: 0.5288104160101527

c1cc2c(cc1F)nc([nH]2)CCCNC(=O)[C@H](CO)[NH3+]

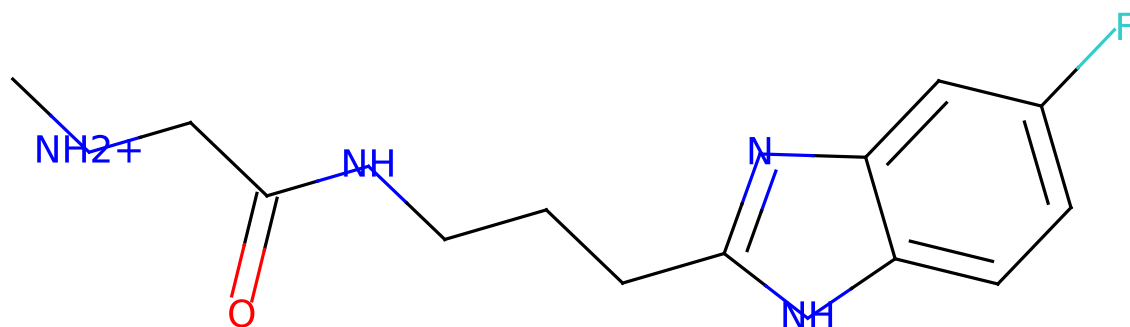ORD-MCULE-2168809409_2

('3CLPro_7BQY_A_1_F', 'NSP16_6W61_A_1_H')

MolLogP: 1.2030999999999998 | QED: 0.48377262508697316

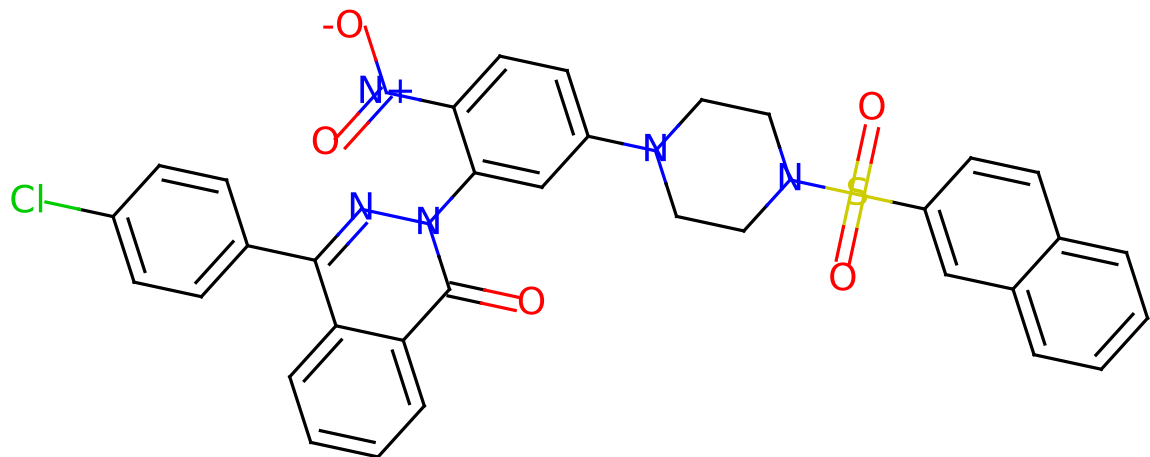c1ccc2c(c1)c([nH]n2)C(=O)NCCSc3cn[nH]n3

ORD-MCULE-4087160291_2

MolLogP: -0.05599999999999977 | QED: 0.6403435644960167

C[NH2+]CC(=O)NCCCc1[nH]c2ccc(cc2n1)F

ORD-MCULE-5985443175_2
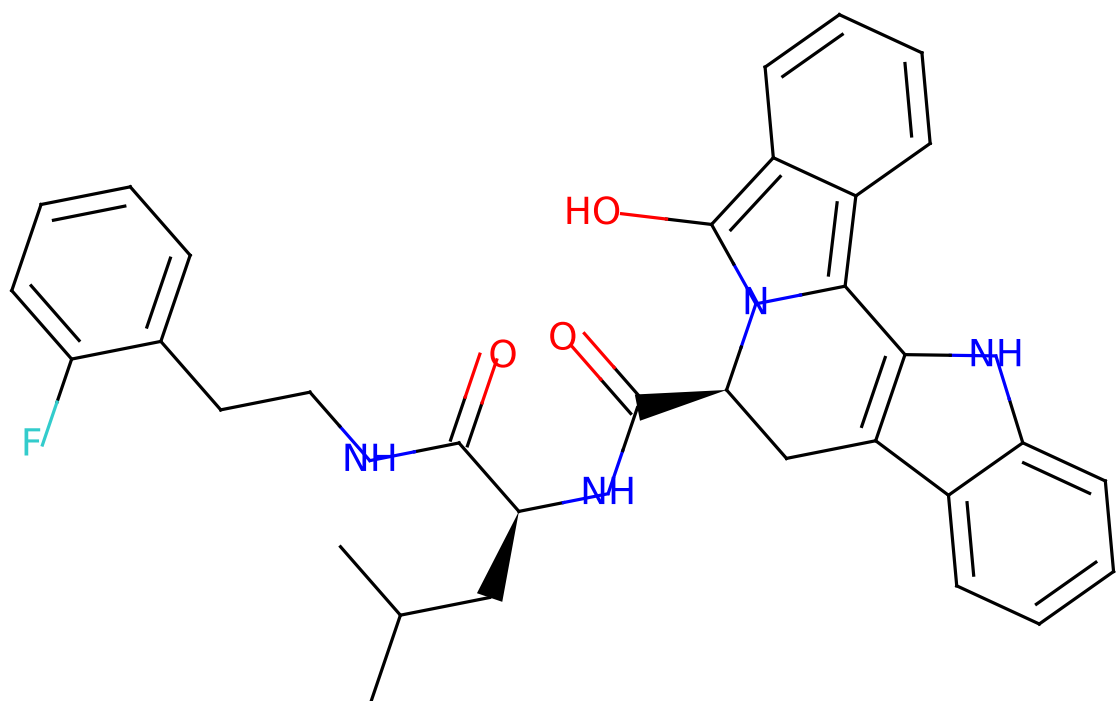
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6ccccc6c(n5)c7ccc(cc7)Cl)N(=O)=O
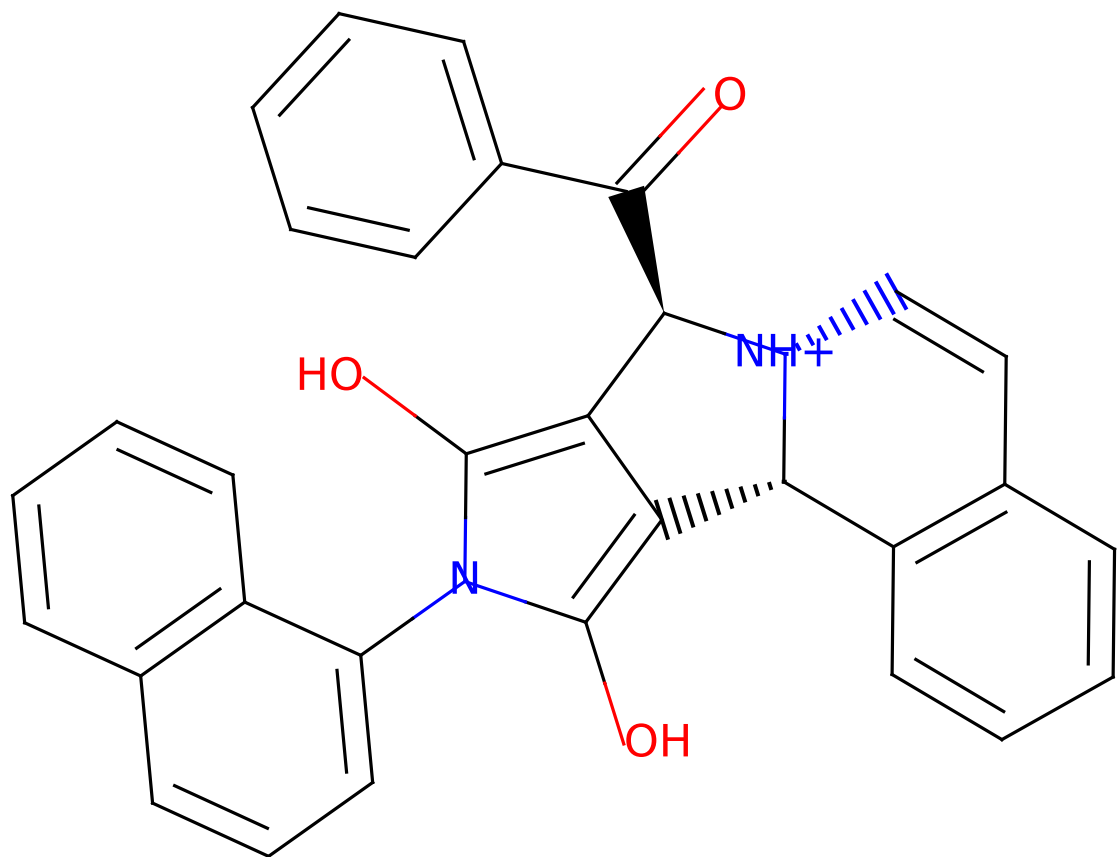
ORD-MCULE-1708960826_1

MolLogP: 5.621300000000006 | QED: 0.20107182839149487

CC(C)C[C@@H](C(=O)NCCc1ccccc1F)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O

ORD-MCULE-9438397769_1

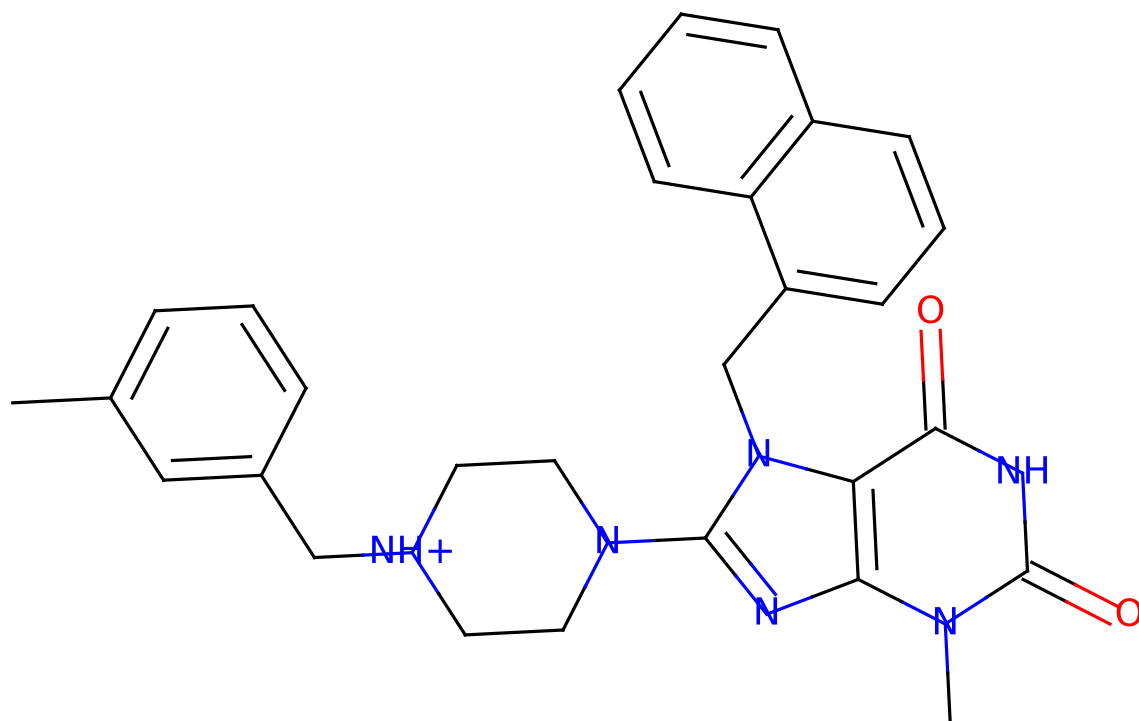('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7

ORD-MCULE-7416131701_1

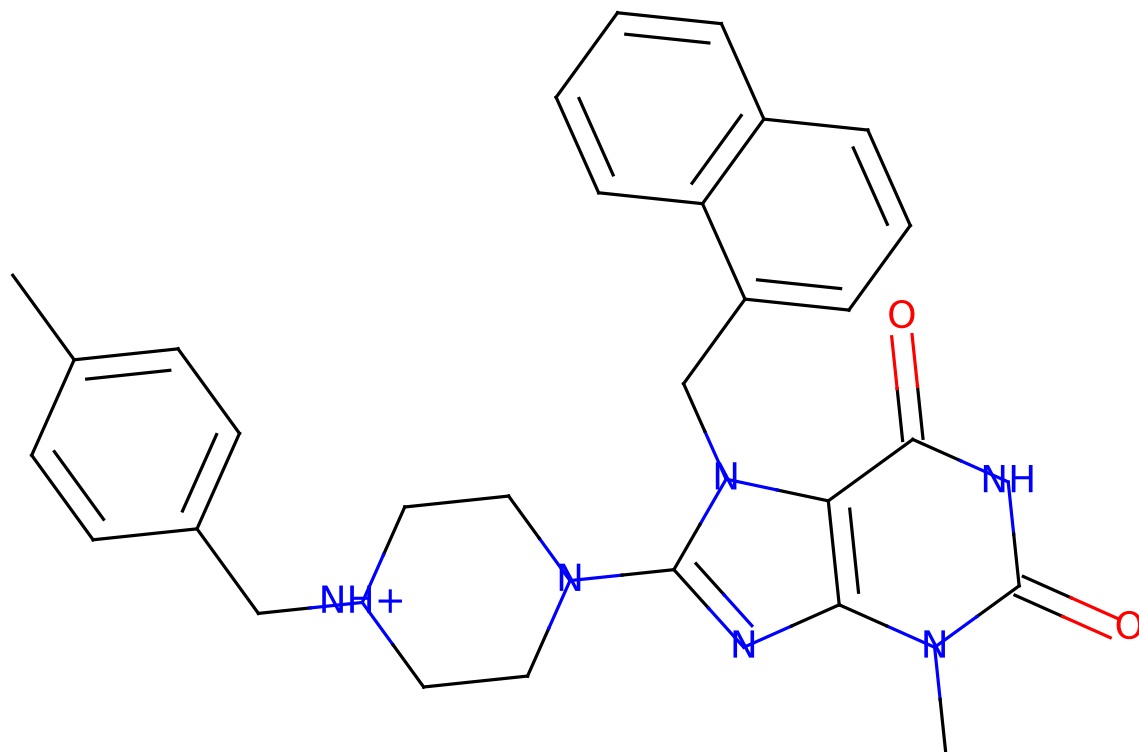MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
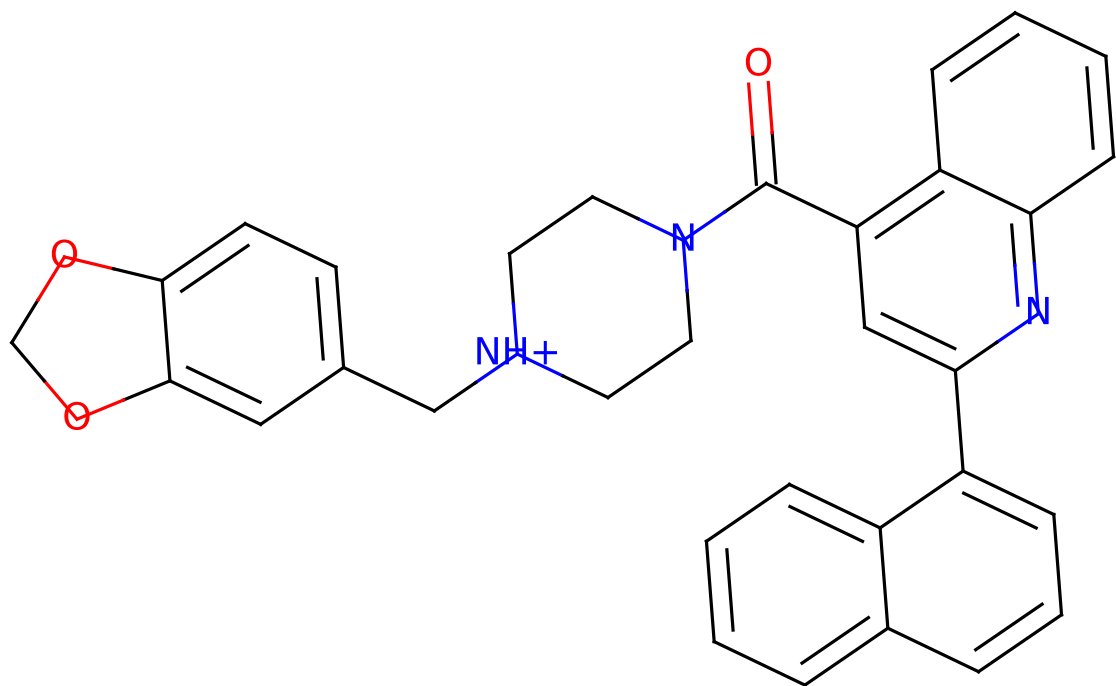
ORD-MCULE-9311937068_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
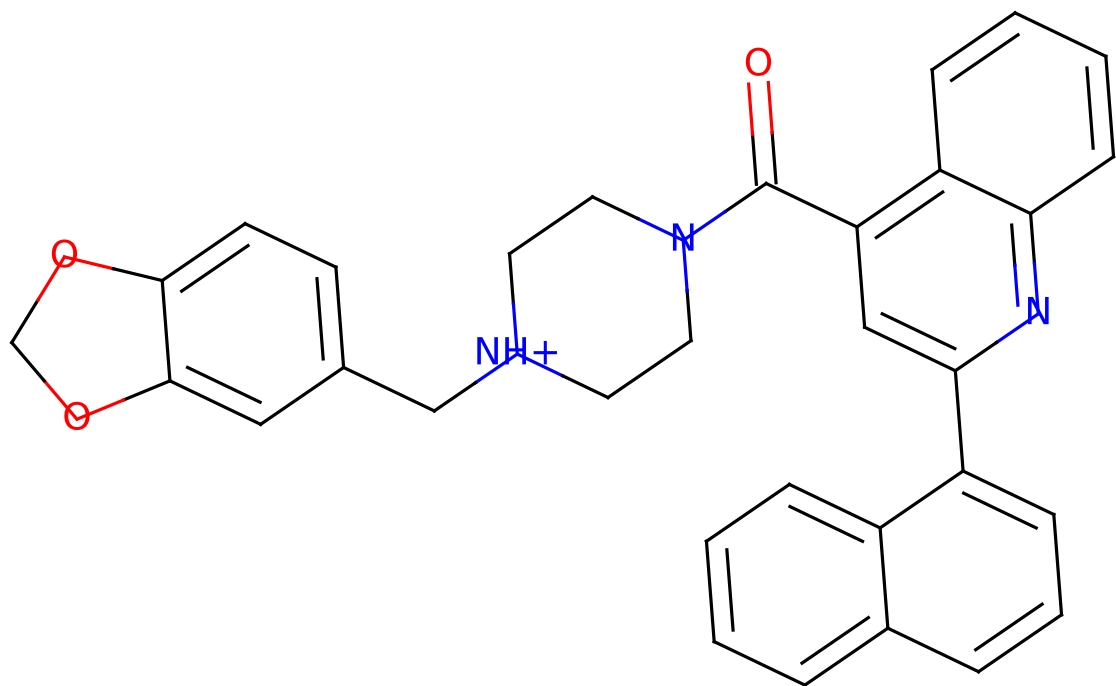
ORD-MCULE-8959718627_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7
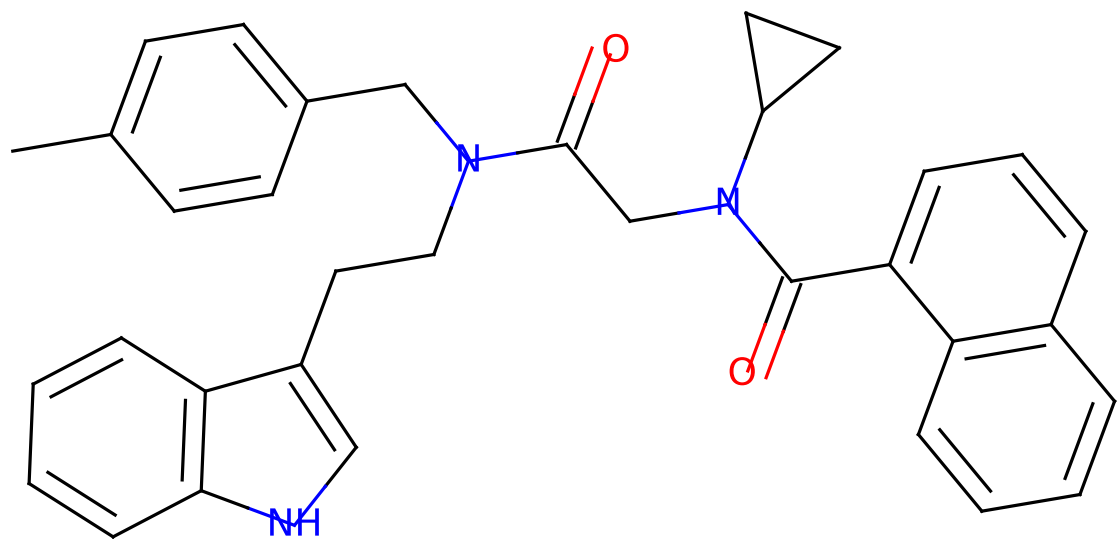
ORD-MCULE-4959815000_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-3696478799_1
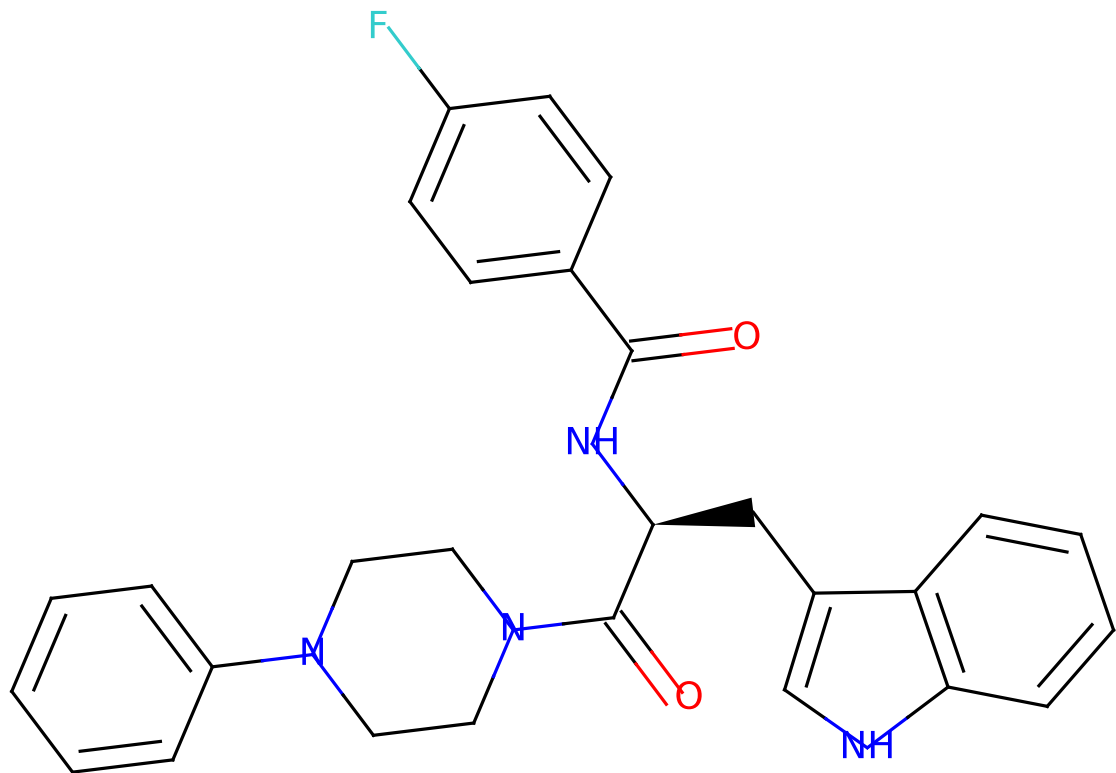
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 6.505620000000007 | QED: 0.2434419591344794

Cc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)CN(C4CC4)C(=O)c5cccc6c5cccc6

ORD-MCULE-2519953694_1
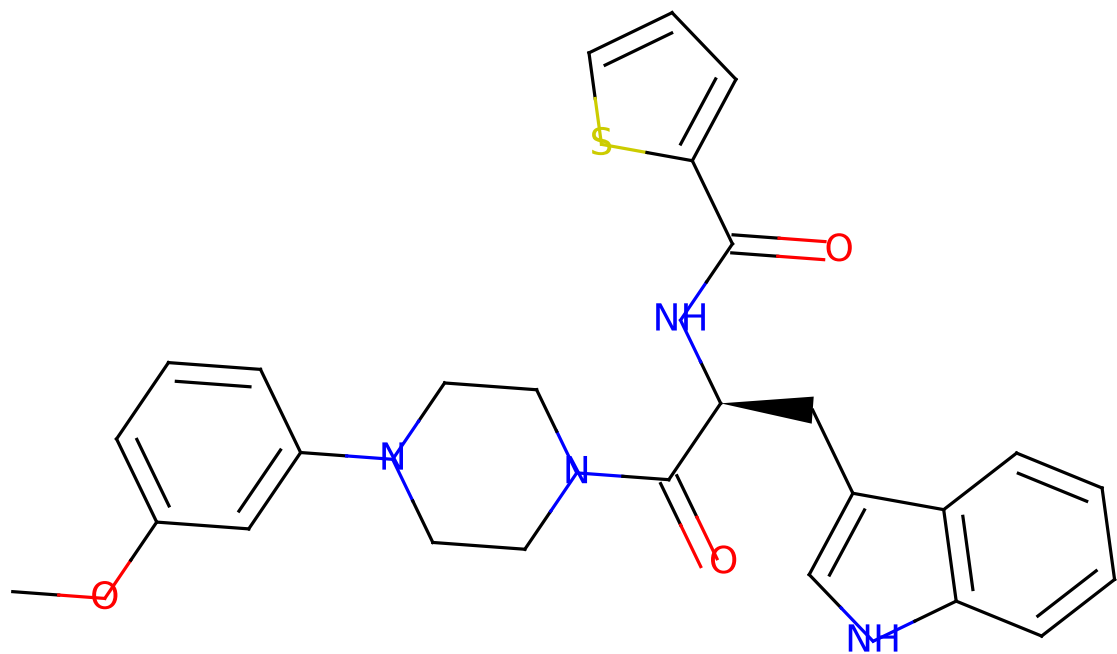
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 3.996900000000002 | QED: 0.44774588382557573

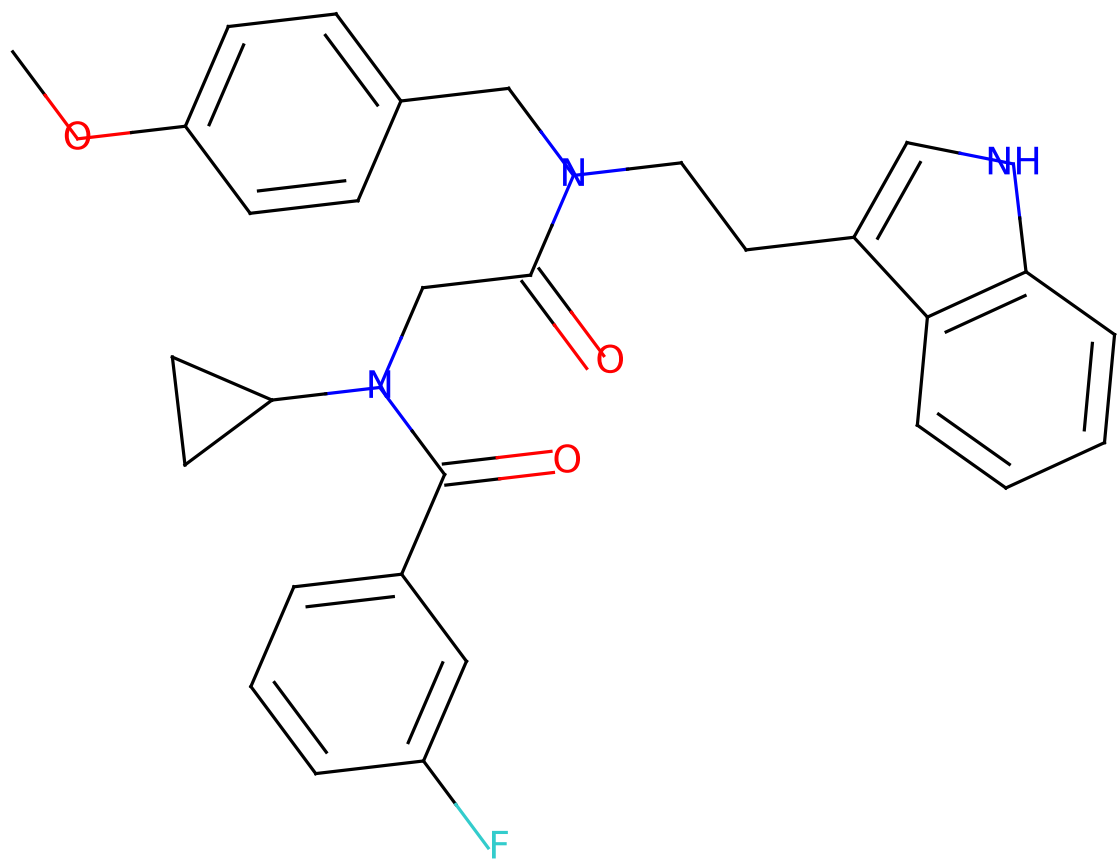c1ccc(cc1)N2CCN(CC2)C(=O)[C@H](Cc3c[nH]c4c3cccc4)NC(=O)c5ccc(cc5)F

ORD-MCULE-1314415937_1

MolLogP: 3.927900000000003 | QED: 0.41334145973930614

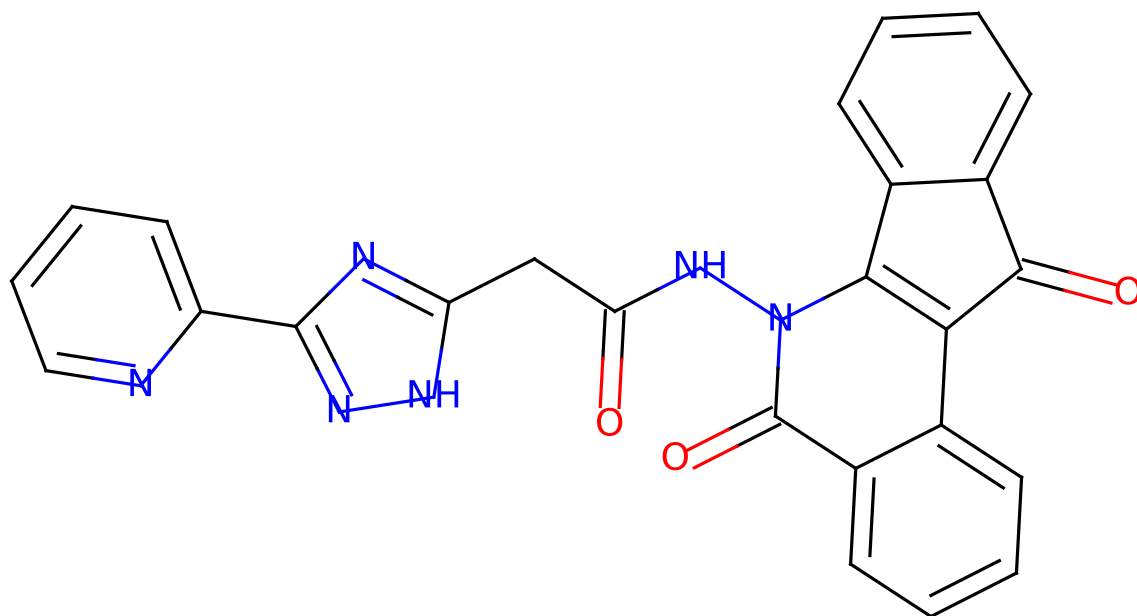COc1cccc(c1)N2CCN(CC2)C(=O)[C@H](Cc3c[nH]c4c3cccc4)NC(=O)c5cccs5

ORD-MCULE-5744155890_1

MolLogP: 5.191700000000005 | QED: 0.326572692572572

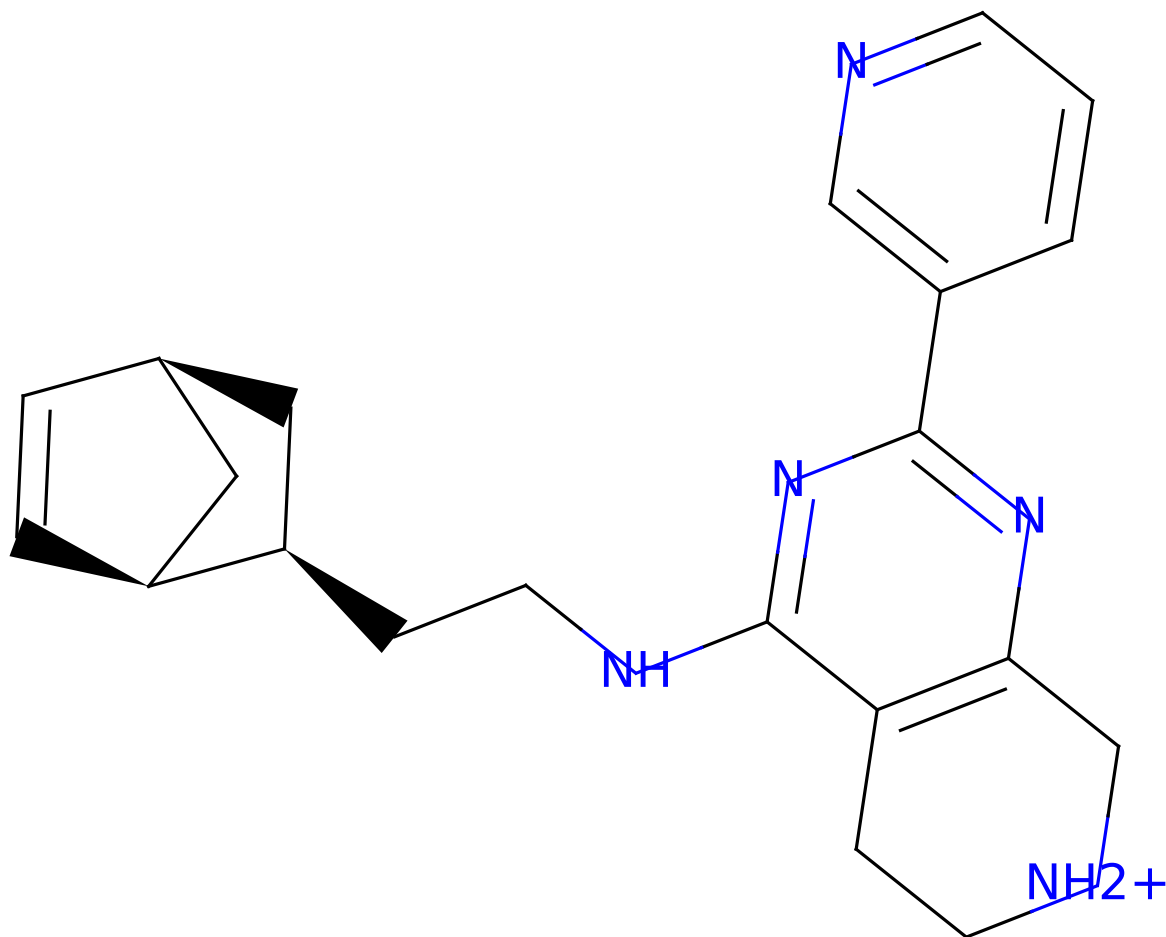COc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)CN(C4CC4)C(=O)c5cccc(c5)F

ORD-MCULE-3860138249_1

MolLogP: 2.705800000000001 | QED: 0.4275564127608206

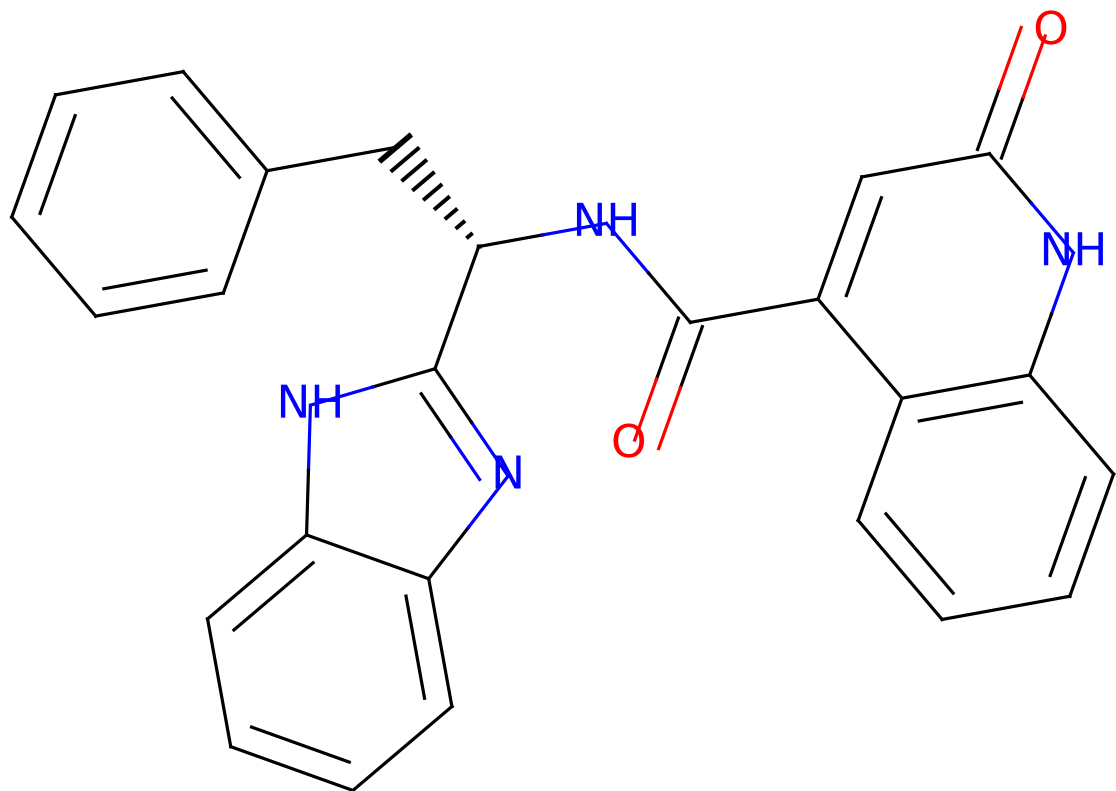c1ccc2c(c1)c3c(n(c2=O)NC(=O)Cc4[nH]nc(n4)c5ccccn5)-c6ccccc6C3=O

ORD-MCULE-1087797516_1

MolLogP: 2.1723 | QED: 0.812915759881308

c1cc(cnc1)c2nc3c(c(n2)NCC[C@@H]4C[C@H]5C[C@@H]4C=C5)CC[NH2+]C3
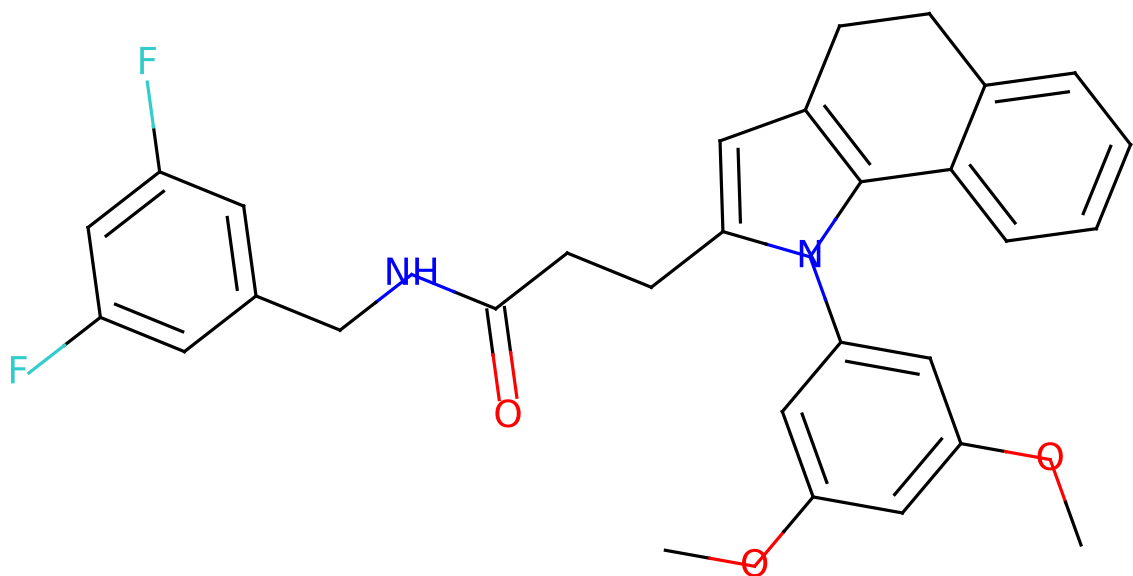
ORD-MCULE-5739750381_1

MolLogP: 4.118200000000002 | QED: 0.4085896962540062

c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4cc(=O)[nH]c5c4cccc5

ORD-MCULE-2354836978_1
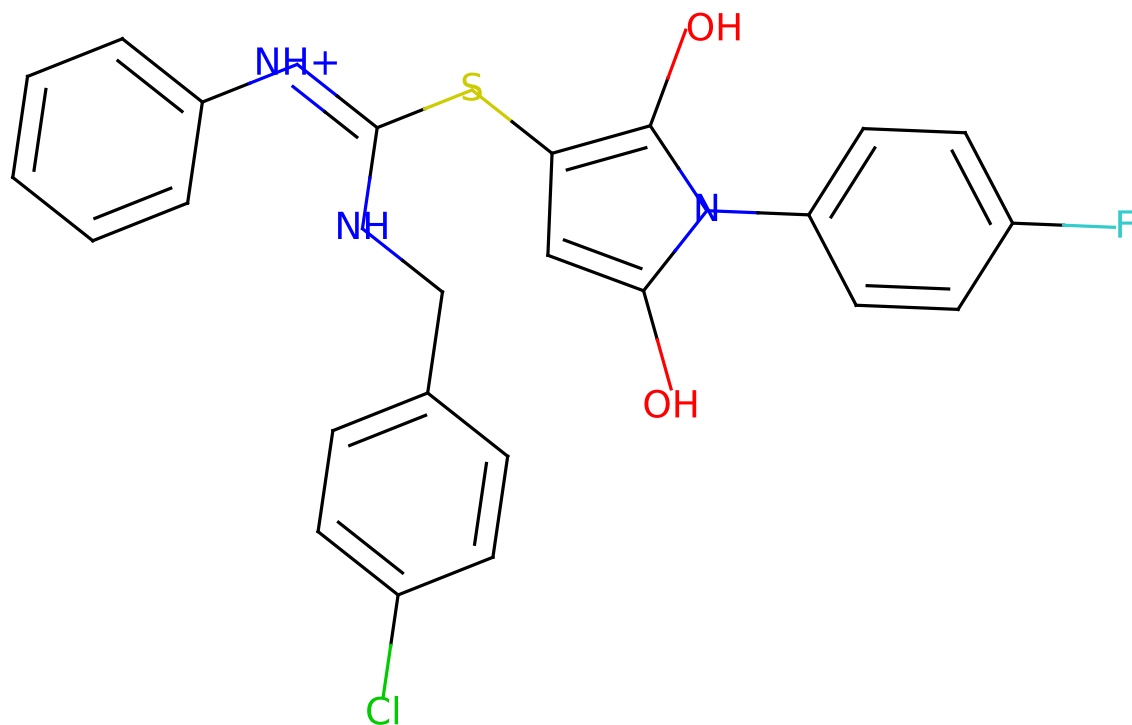
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 5.7873000000000046 | QED: 0.33203587335464885

COc1cc(cc(c1)OC)n2c(cc3c2-c4ccccc4CC3)CCC(=O)NCc5cc(cc(c5)F)F

ORD-MCULE-6553444445_1
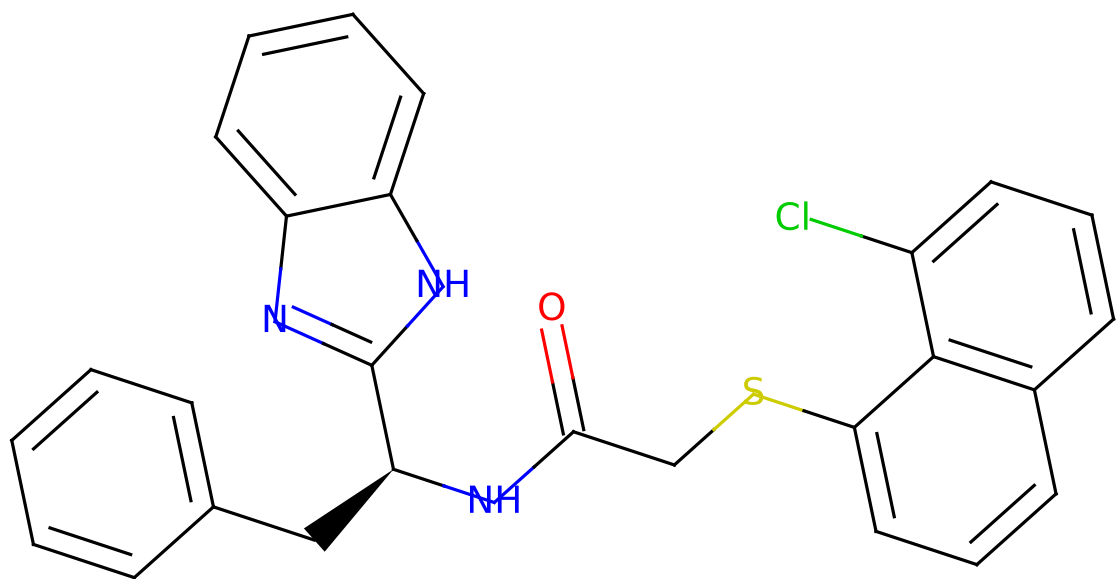
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 4.3312000000000035 | QED: 0.19976136878195225

c1ccc(cc1)/[NH+]=C(\NCc2ccc(cc2)Cl)/Sc3cc(n(c3O)c4ccc(cc4)F)O

ORD-MCULE-3082269743_2
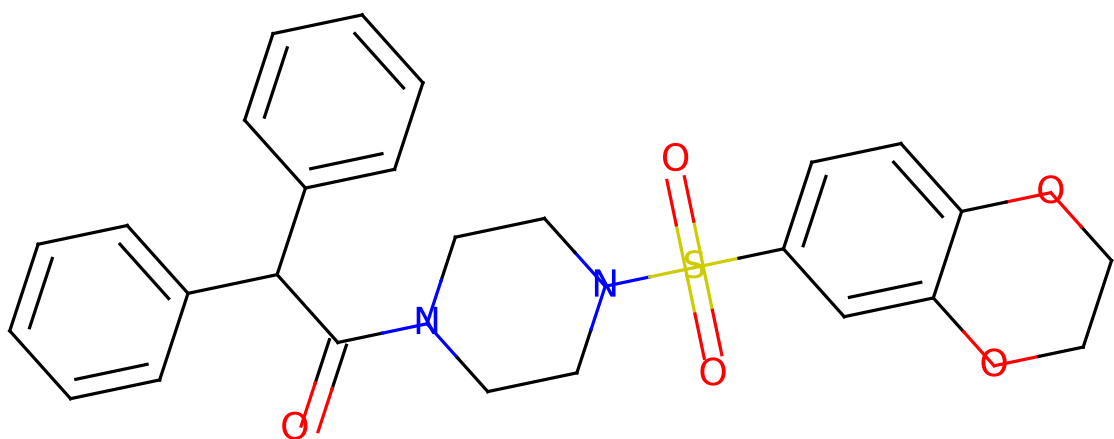
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 6.561800000000004 | QED: 0.26406471710612306

c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)CSc4cccc5c4c(ccc5)Cl

ORD-MCULE-6426577239_1
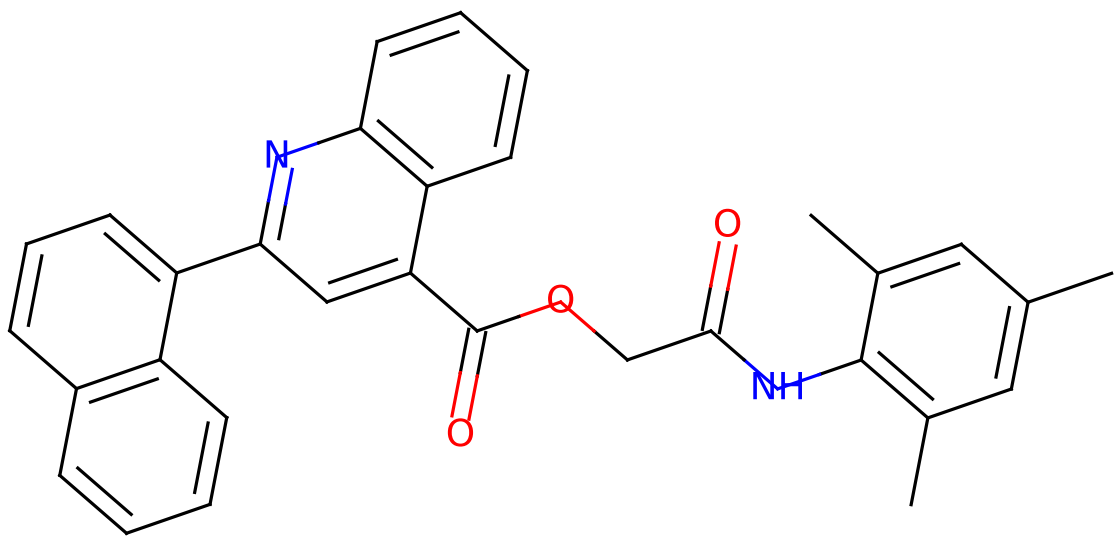
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 3.1228000000000016 | QED: 0.5633261375042687

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5c(c4)OCCO5

ORD-MCULE-1904175079_1
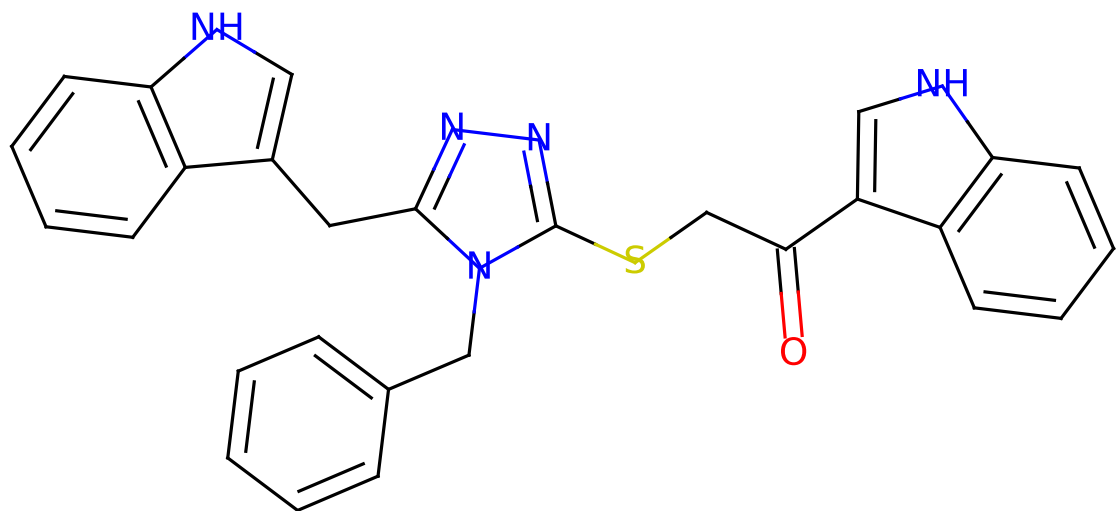
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 6.775760000000005 | QED: 0.28530611753059815

Cc1cc(c(c(c1)C)NC(=O)COC(=O)c2cc(nc3c2cccc3)c4cccc5c4cccc5)C

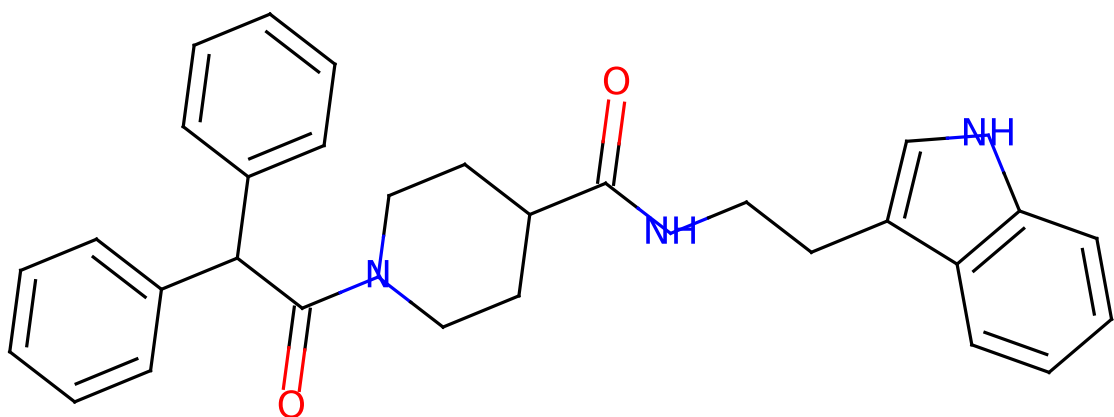ORD-MCULE-2281744958_1

('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 5.8548000000000044 | QED: 0.21272800874019035

c1ccc(cc1)Cn2c(nnc2SCC(=O)c3c[nH]c4c3cccc4)Cc5c[nH]c6c5cccc6

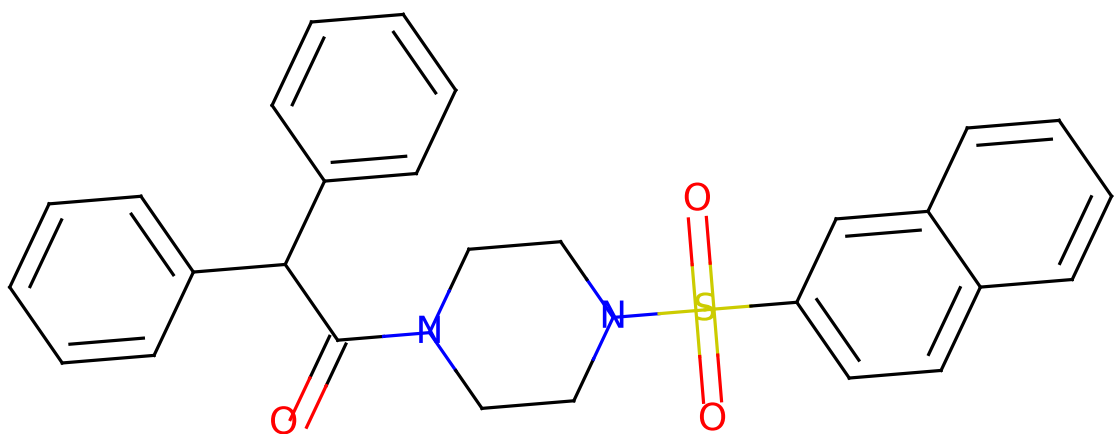ORD-MCULE-2017284421_1

('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 4.897300000000003 | QED: 0.40786292071408126

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCC(CC3)C(=O)NCCc4c[nH]c5c4cccc5
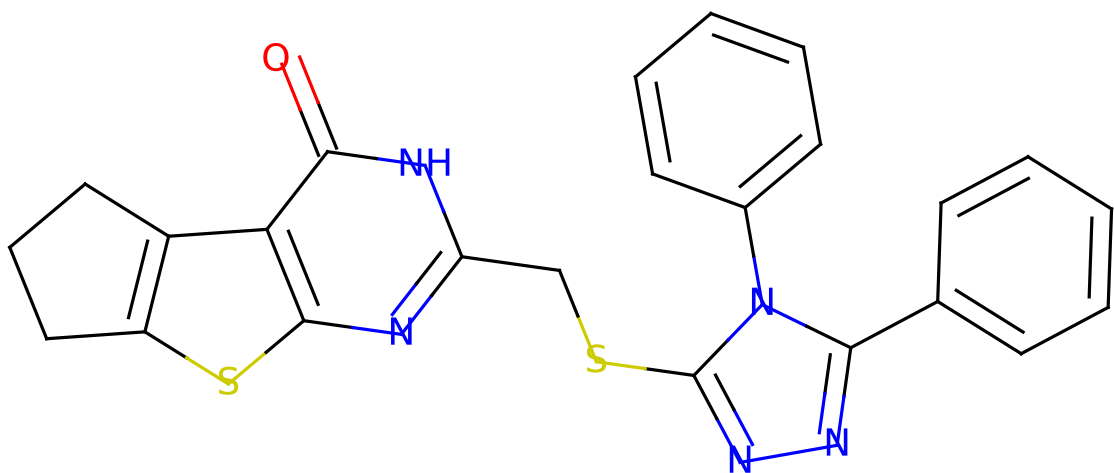
ORD-MCULE-9130199918_1

MolLogP: 4.504800000000004 | QED: 0.43144005118053486

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-9717306826_1

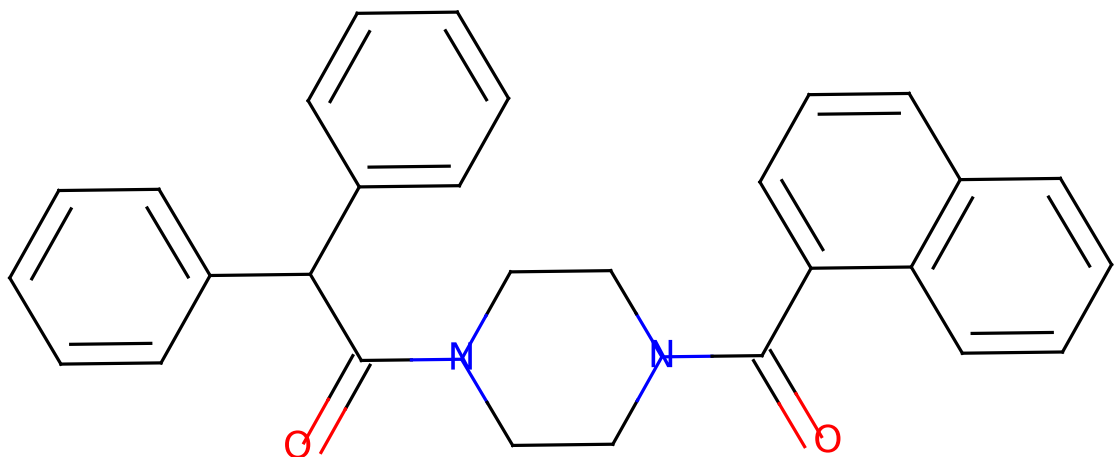('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 5.013300000000003 | QED: 0.37541396911851704

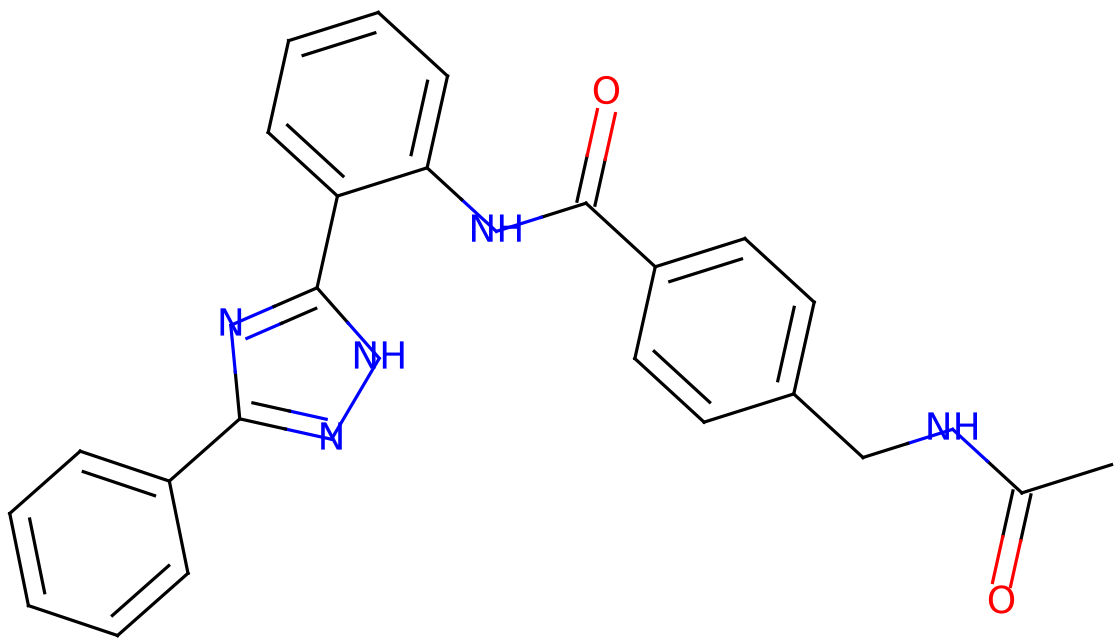c1ccc(cc1)c2nnc(n2c3ccccc3)SCc4[nH]c(=O)c5c6c(sc5n4)CCC6

ORD-MCULE-5456008772_1

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

ORD-MCULE-4705080812_1
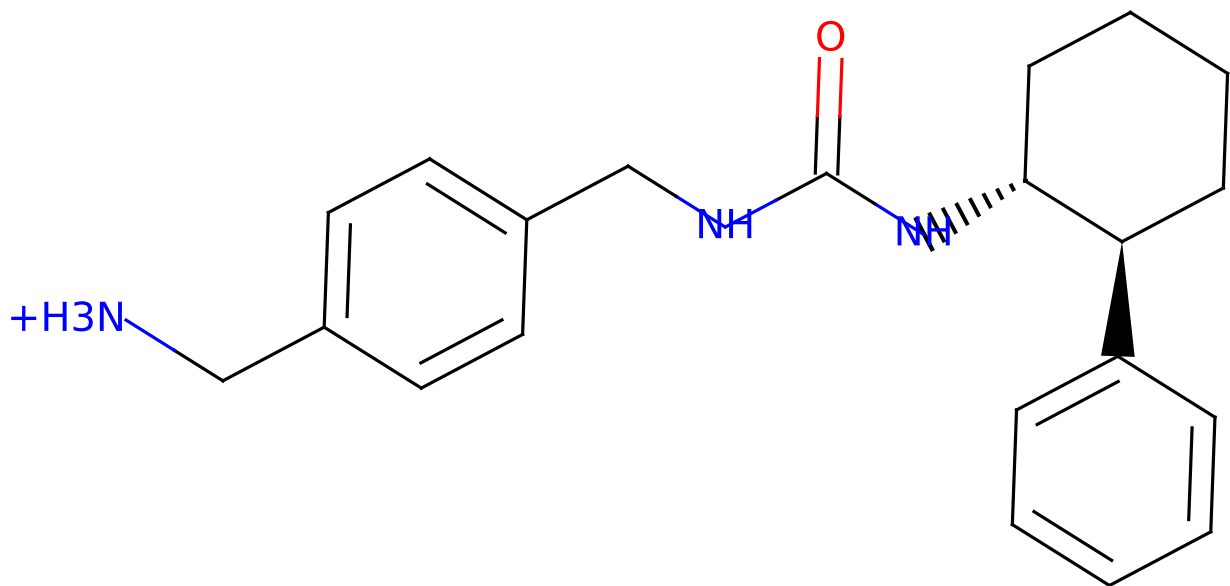
MolLogP: 4.027100000000002 | QED: 0.44600141958321116

CC(=O)NCc1ccc(cc1)C(=O)Nc2ccccc2c3[nH]nc(n3)c4ccccc4
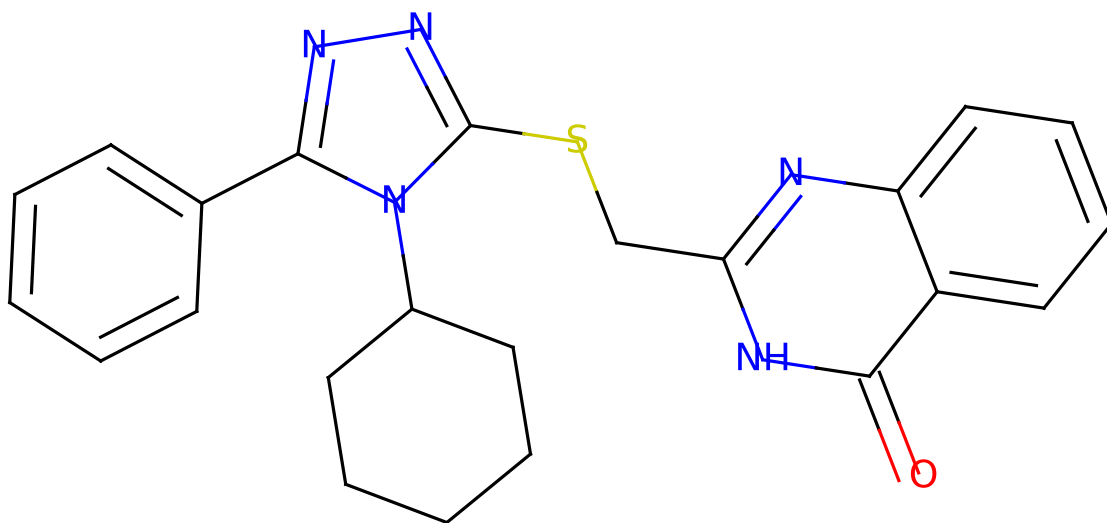
ORD-MCULE-7152686229_1

MolLogP: 2.9540999999999995 | QED: 0.7706756725762592

c1ccc(cc1)[C@@H]2CCCC[C@H]2NC(=O)NCc3ccc(cc3)C[NH3+]

ORD-MCULE-5985705514_1
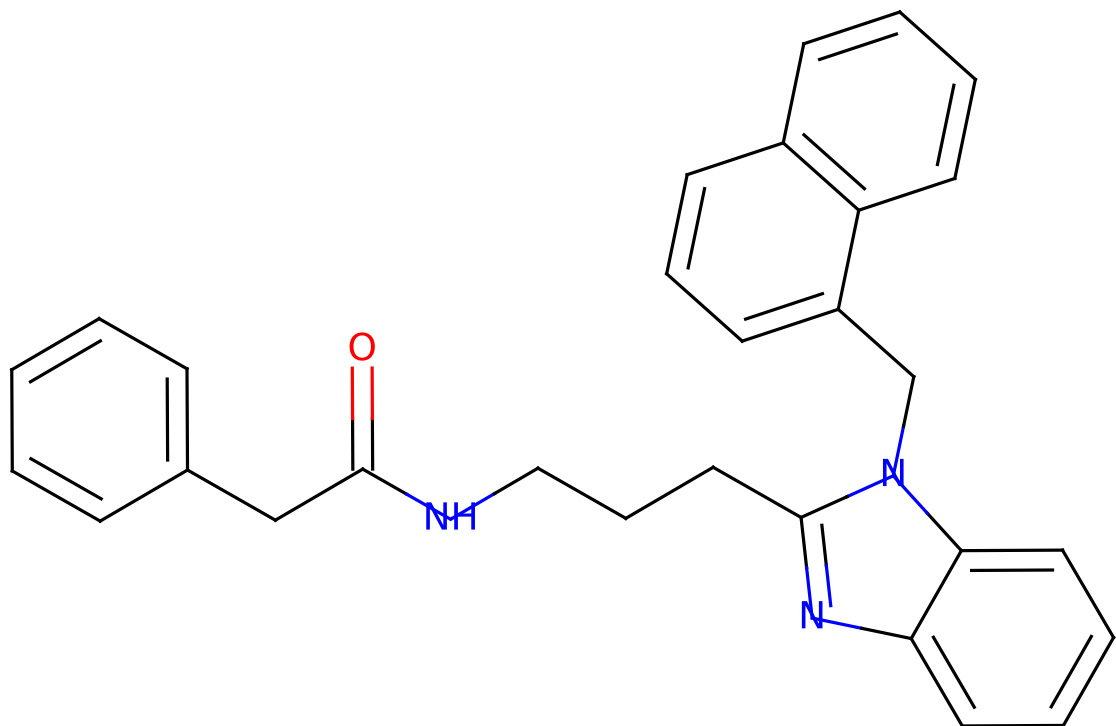
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 4.979100000000003 | QED: 0.4635852670383765

c1ccc(cc1)c2nnc(n2C3CCCCC3)SCc4[nH]c(=O)c5ccccc5n4

ORD-MCULE-4525414745_1
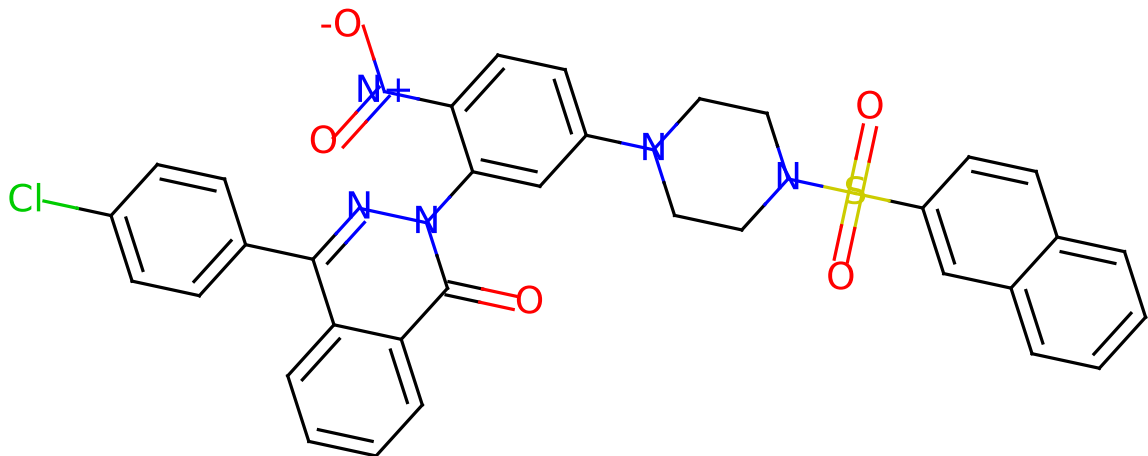
('3CLPro_7BQY_A_1_F', 'PLPro_6W9C_A_2_F')

MolLogP: 5.529300000000005 | QED: 0.32718667928035094

c1ccc(cc1)CC(=O)NCCCc2nc3ccccc3n2Cc4cccc5c4cccc5

ORD-MCULE-9349708949_1
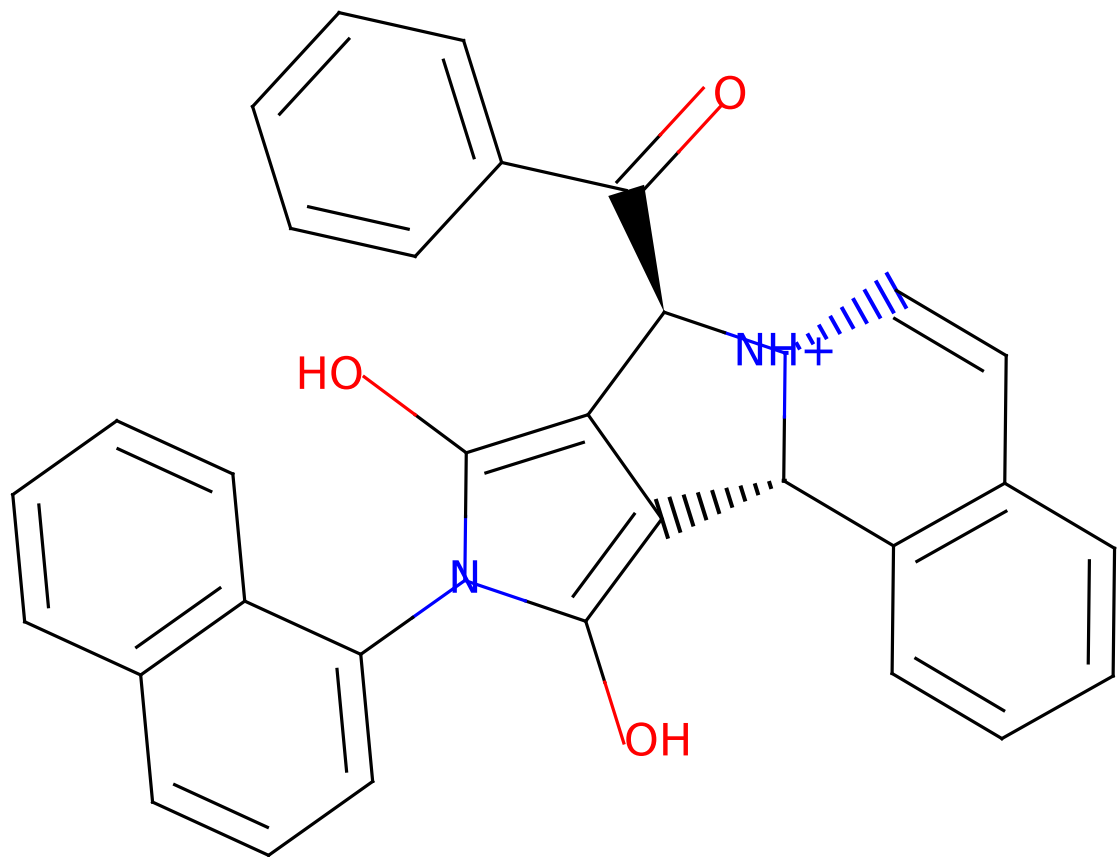
('NSP16_6W61_A_1_H', 'PLPro_6W9C_A_2_F')

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6ccccc6c(n5)c7ccc(cc7)Cl)N(=O)=O

ORD-MCULE-1708960826_1
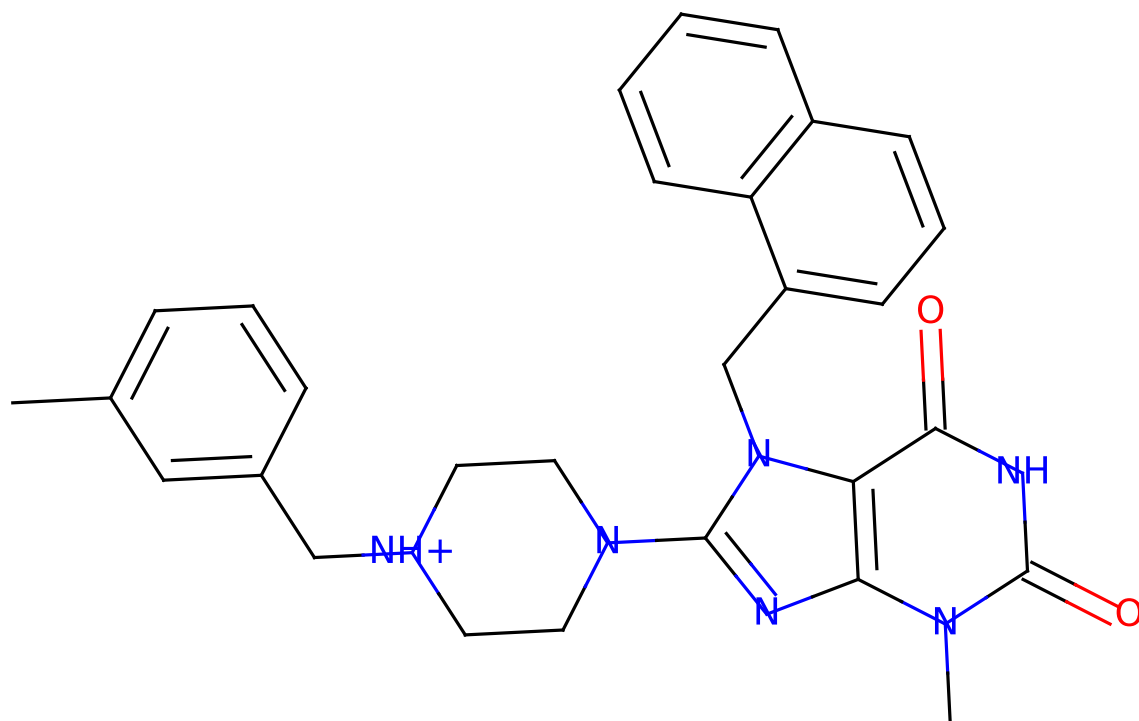
('NSP16_6W61_A_1_H', 'PLPro_6W9C_A_2_F')

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7

ORD-MCULE-7416131701_1

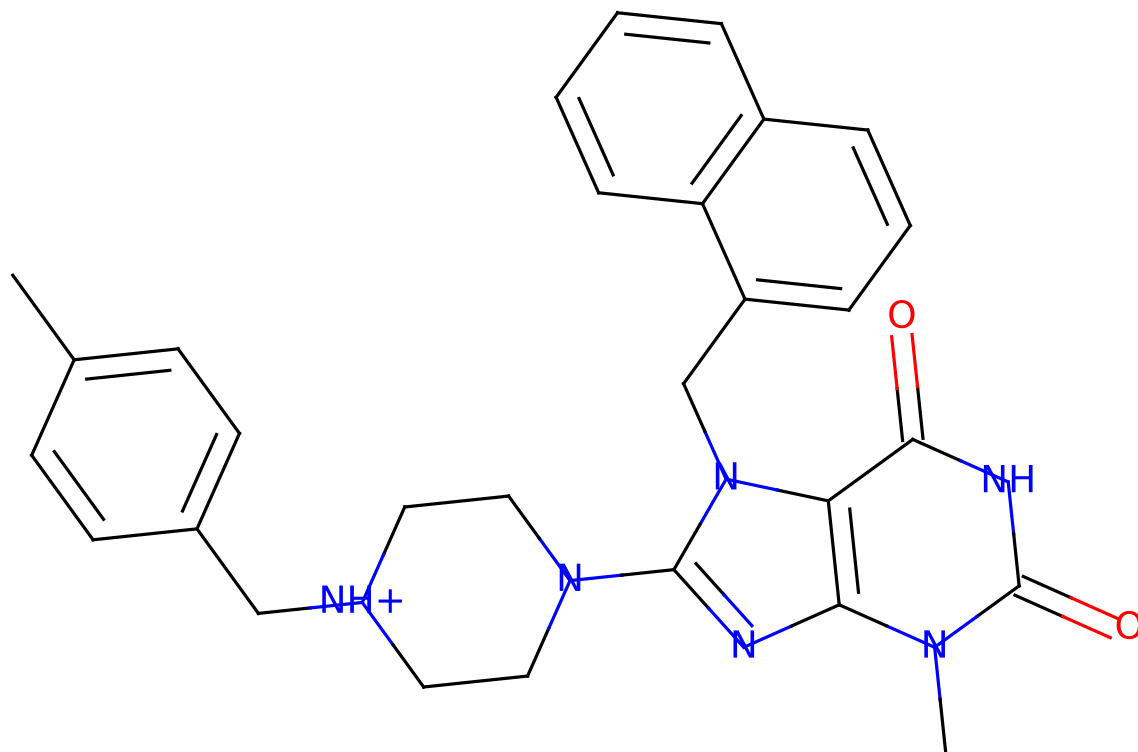MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
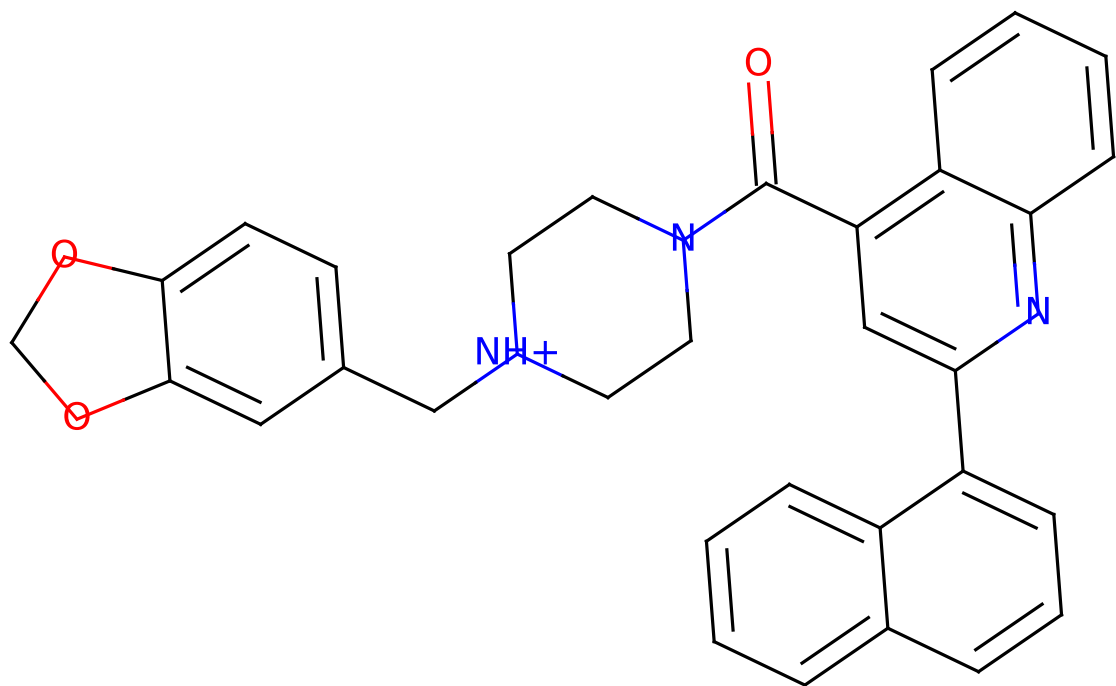
ORD-MCULE-9311937068_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C
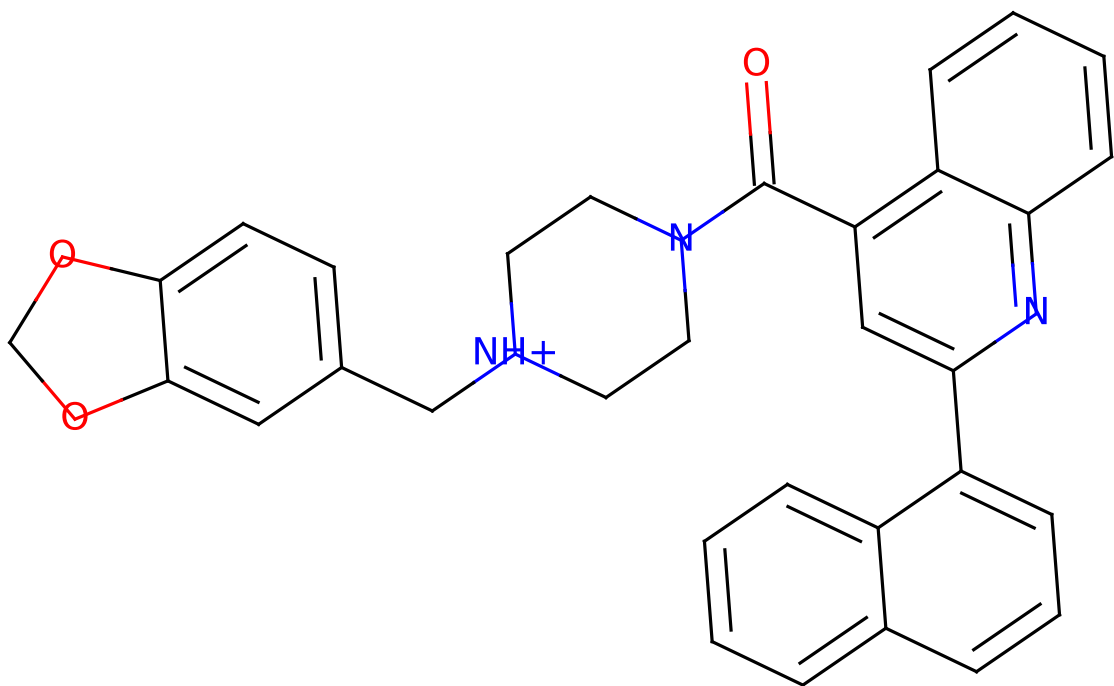
ORD-MCULE-8959718627_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-4959815000_1
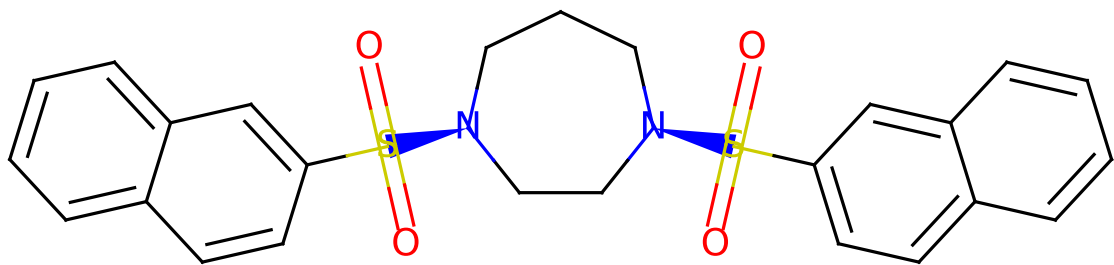
('NSP16_6W61_A_1_H', 'PLPro_6W9C_A_2_F')

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

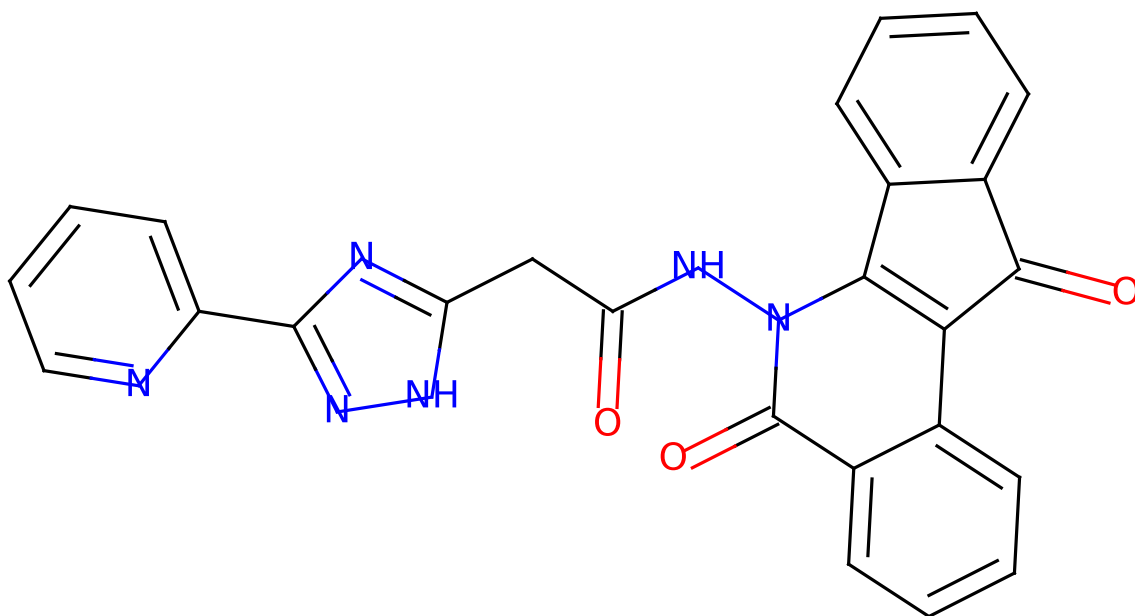c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-3696478799_1

MolLogP: 4.078300000000003 | QED: 0.441202265024148

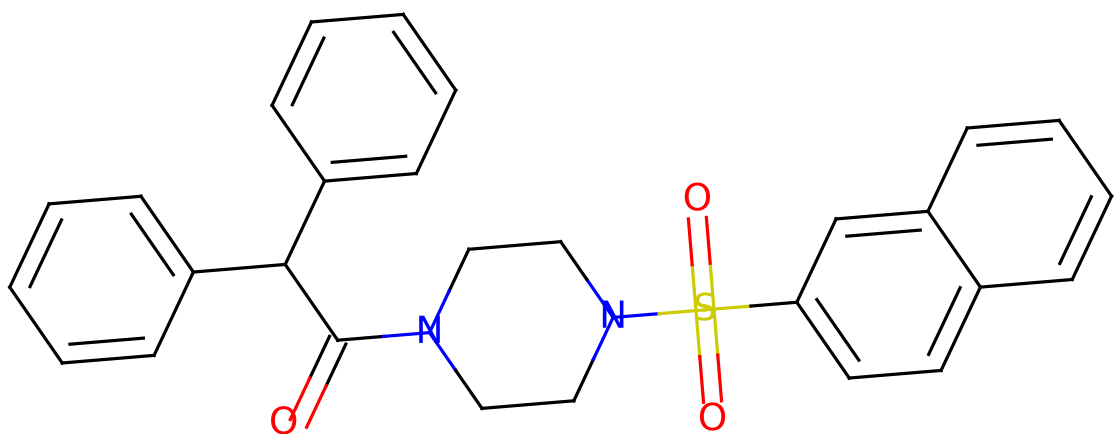c1ccc2cc(ccc2c1)S(=O)(=O)[N@@]3CCC[N@](CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-4262091783_1

MolLogP: 2.705800000000001 | QED: 0.4275564127608206

c1ccc2c(c1)c3c(n(c2=O)NC(=O)Cc4[nH]nc(n4)c5ccccn5)-c6ccccc6C3=O
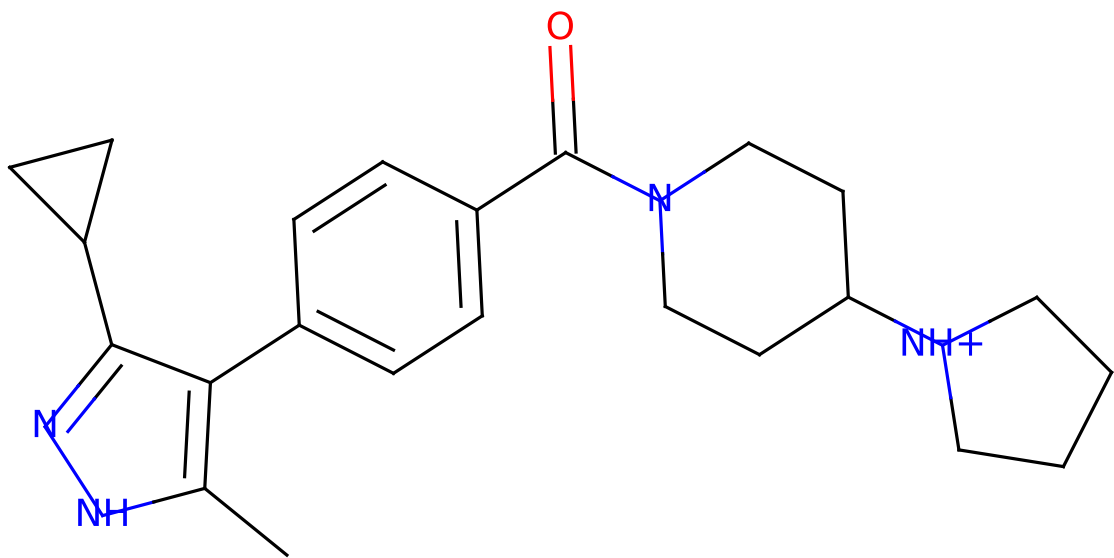
ORD-MCULE-1087797516_1

MolLogP: 4.504800000000004 | QED: 0.43144005118053486

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-9717306826_1
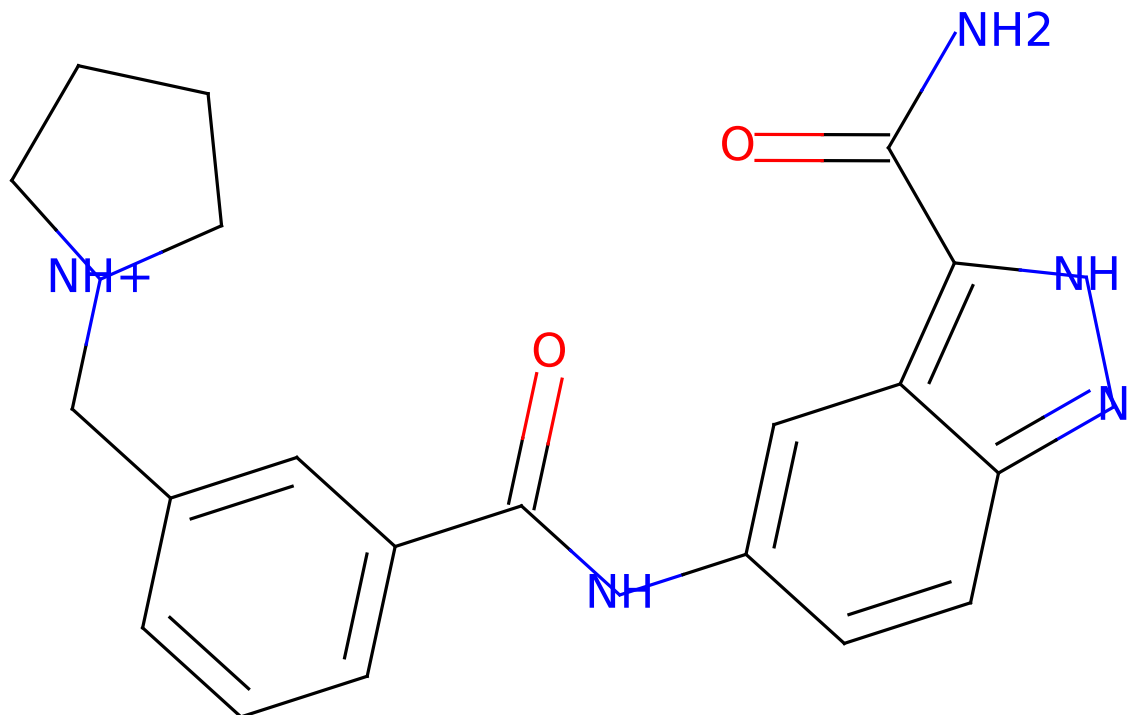
('NSP16_6W61_A_1_H', 'PLPro_6W9C_A_2_F')

MolLogP: 2.54582 | QED: 0.8578099200835345

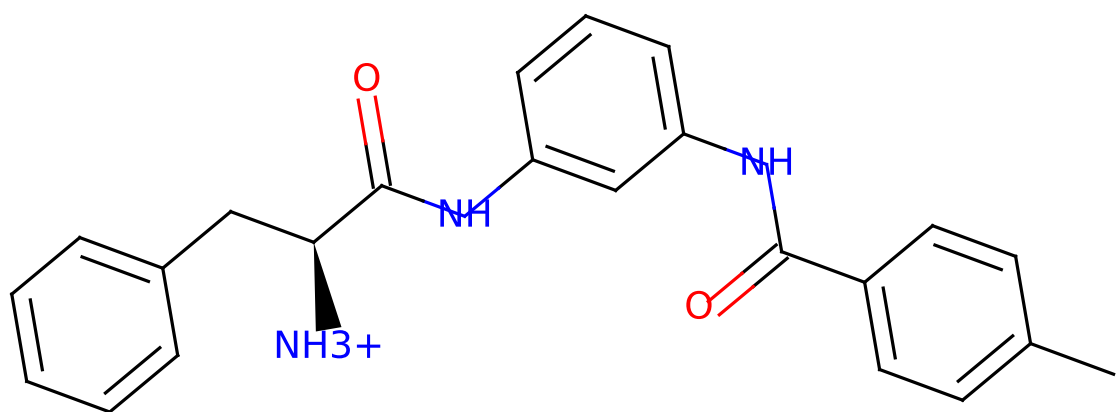Cc1c(c(n[nH]1)C2CC2)c3ccc(cc3)C(=O)N4CCC(CC4)[NH+]5CCCC5

ORD-MCULE-3417237209_1

MolLogP: 1.0927999999999995 | QED: 0.5445620954382201

c1cc(cc(c1)C(=O)Nc2ccc3c(c2)c([nH]n3)C(=O)N)C[NH+]4CCCC4

ORD-MCULE-1647109669_2
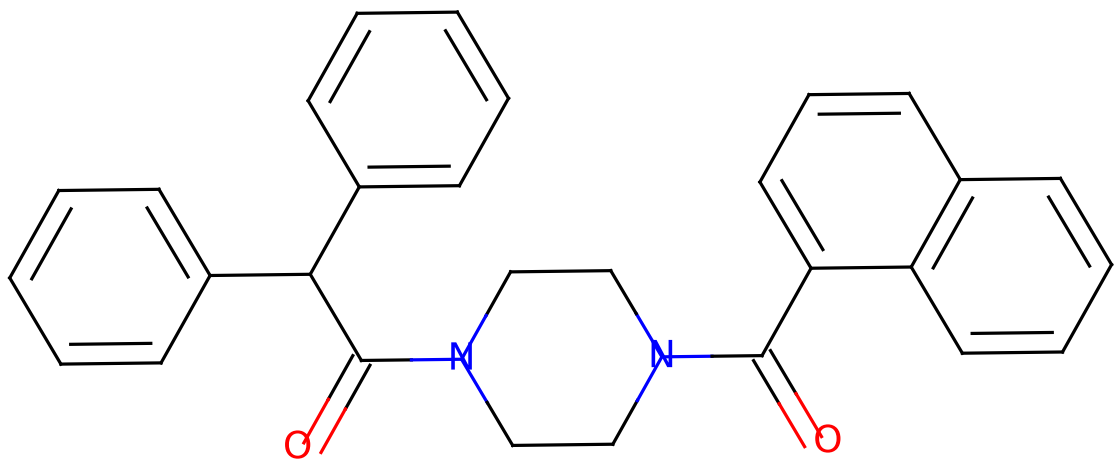
MolLogP: 3.03902 | QED: 0.619385059261453

Cc1ccc(cc1)C(=O)Nc2cccc(c2)NC(=O)[C@H](Cc3ccccc3)[NH3+]
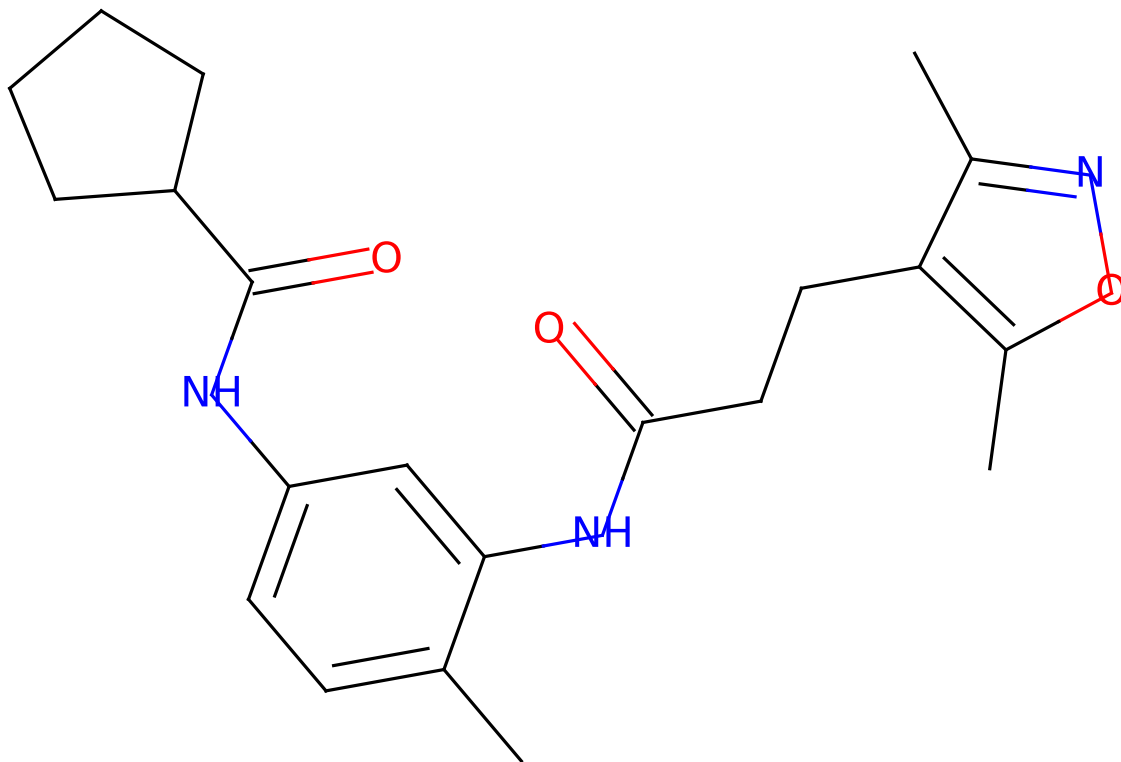
ORD-MCULE-3922106238_1

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

ORD-MCULE-4705080812_1

('NSP16_6W61_A_1_H', 'PLPro_6W9C_A_2_F')

MolLogP: 4.299860000000003 | QED: 0.7949686710997425

Cc1ccc(cc1NC(=O)CCc2c(noc2C)C)NC(=O)C3CCCC3

ORD-MCULE-7968599617_1