

MolLogP: 3.996900000000002 | QED: 0.44774588382557573

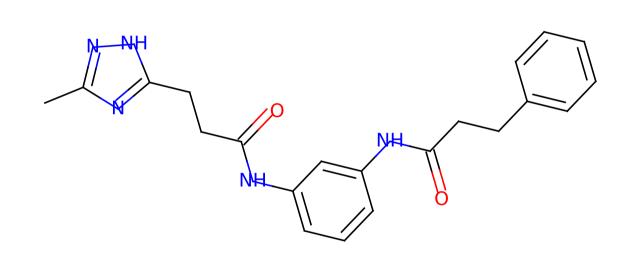
c1ccc(cc1)N2CCN(CC2)C(=0)[C@H](Cc3c[nH]c4c3cccc4)NC(=0)c5ccc(cc5)F

ORD-MCULE-1314415937_1

MolLogP: 6.278400000000006 | QED: 0.1536402815353809

 $\verb|c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)c4ccc(c(c4)n5c(=O)c6cccc6c(n5)c7ccc(cc7)CI)N(=O)=O|$

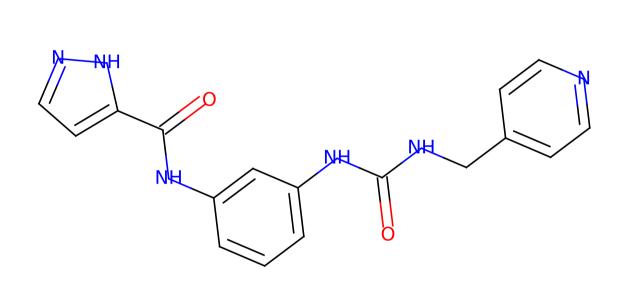
ORD-MCULE-1708960826_1



MolLogP: 3.255720000000002 | QED: 0.5609005544471908

Cclnc([nH]n1)CCC(=O)Nc2cccc(c2)NC(=O)CCc3ccccc3

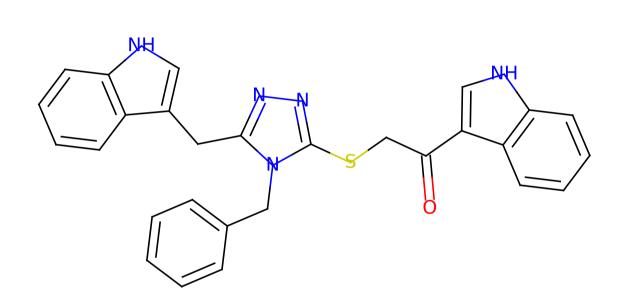
ORD-MCULE-7553698642_2



MolLogP: 2.3787000000000003 | QED: 0.5728605502990787

 $\verb|clcc|| clcc|| clcc|$

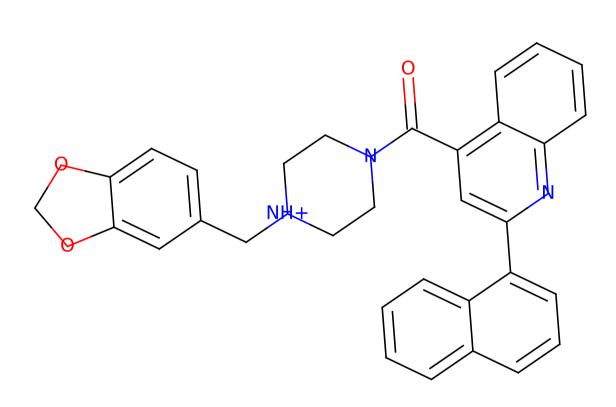
ORD-MCULE-7513600470_1



MolLogP: 5.8548000000000044 | QED: 0.21272800874019035

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

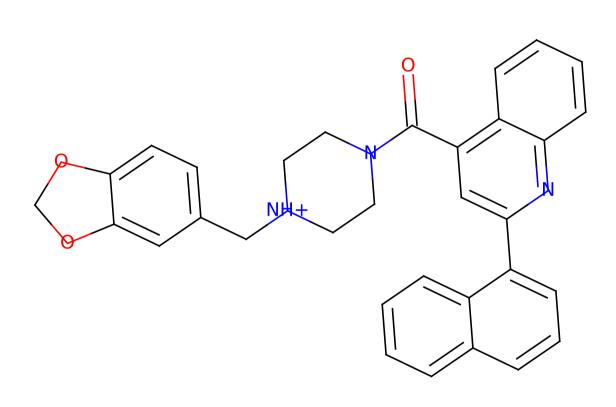
ORD-MCULE-2017284421_1



MolLogP: 4.324600000000004 | QED: 0.3977358166273845

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

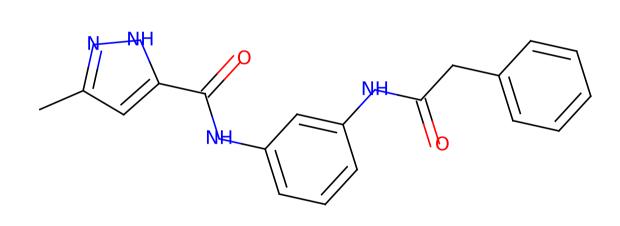
ORD-MCULE-3696478799_1



MolLogP: 4.324600000000004 | QED: 0.3977358166273845

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

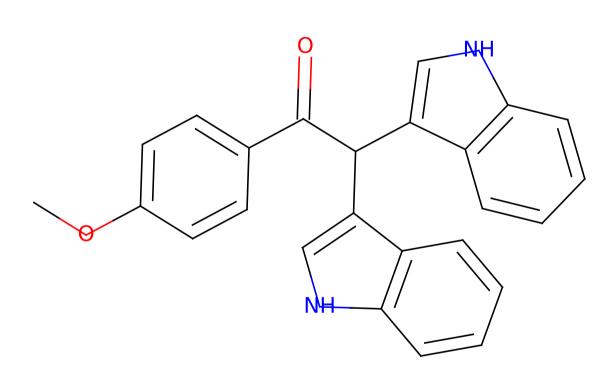
ORD-MCULE-4959815000_1



MolLogP: 3.151620000000001 | QED: 0.6696813920700114

Cc1cc([nH]n1)C(=O)Nc2cccc(c2)NC(=O)Cc3ccccc3

ORD-MCULE-3510580523_2



MolLogP: 5.672600000000004 | QED: 0.3858691235836935

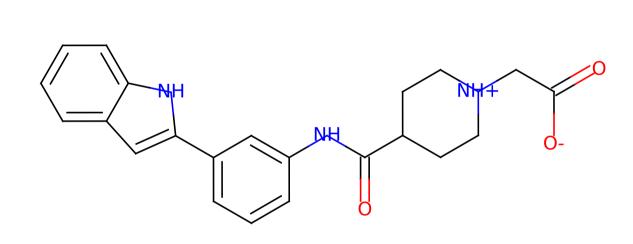
COc1ccc(cc1)C(=0)C(c2c[nH]c3c2cccc3)c4c[nH]c5c4cccc5

ORD-MCULE-5951889621_1

MolLogP: 5.523620000000003 | QED: 0.4255453099531194

Cc1cc(cc(c1O)c2nc3ccccc3o2)NC(=O)c4cccc(c4)Br

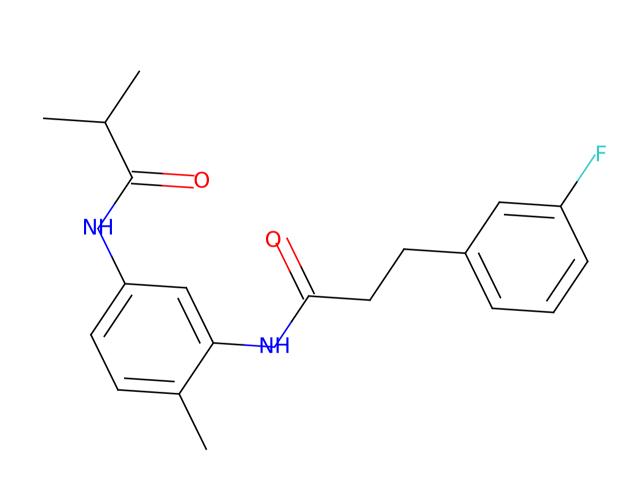
ORD-MCULE-3754289526_1



MolLogP: 0.8181999999999999 | QED: 0.6149652607656041

c1ccc2c(c1)cc([nH]2)c3cccc(c3)NC(=O)C4CC[NH+](CC4)CC(=O)[O-]

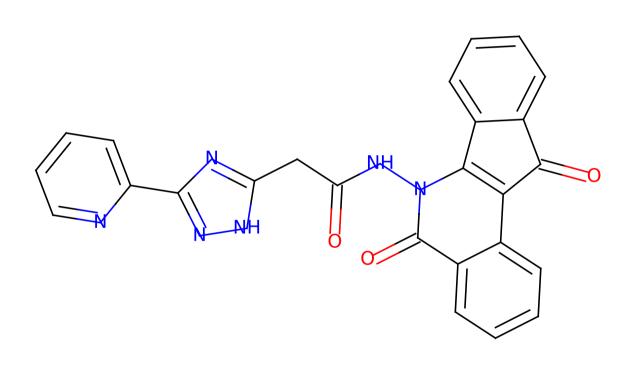
ORD-MCULE-7204065904_1



MolLogP: 4.299920000000002 | QED: 0.8221477477273719

Cc1ccc(cc1NC(=O)CCc2cccc(c2)F)NC(=O)C(C)C

ORD-MCULE-7213991237_1



MolLogP: 2.705800000000001 | QED: 0.4275564127608206

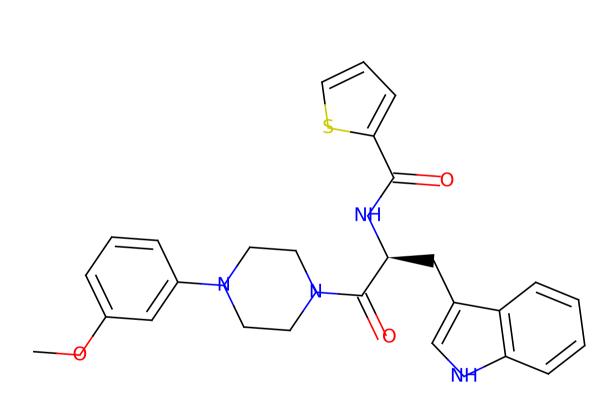
c1ccc2c(c1)c3c(n(c2=O)NC(=O)Cc4[nH]nc(n4)c5ccccn5)-c6ccccc6C3=O

ORD-MCULE-1087797516_1

MolLogP: 3.03902 | QED: 0.619385059261453

Cc1ccc(cc1)C(=O)Nc2cccc(c2)NC(=O)[C@H](Cc3ccccc3)[NH3+]

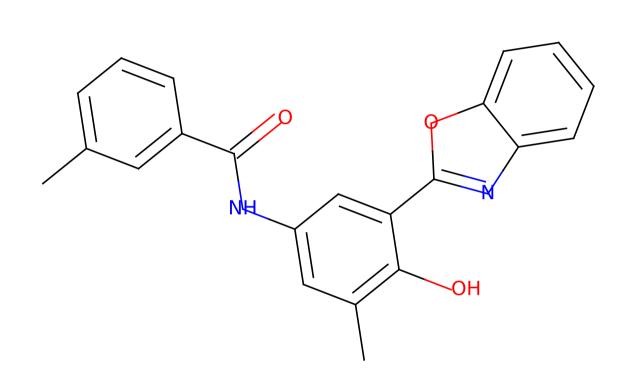
ORD-MCULE-3922106238_1



MolLogP: 3.927900000000003 | QED: 0.41334145973930614

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

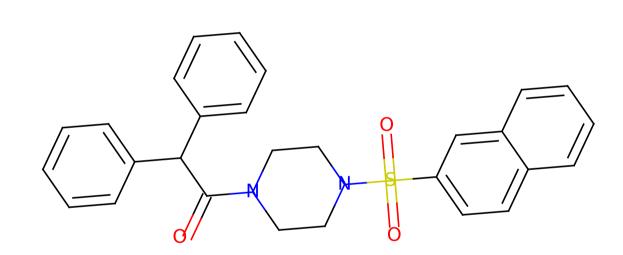
ORD-MCULE-5744155890_1



MolLogP: 5.069540000000004 | QED: 0.501451148111379

Cc1cccc(c1)C(=O)Nc2cc(c(c(c2)c3nc4ccccc4o3)O)C

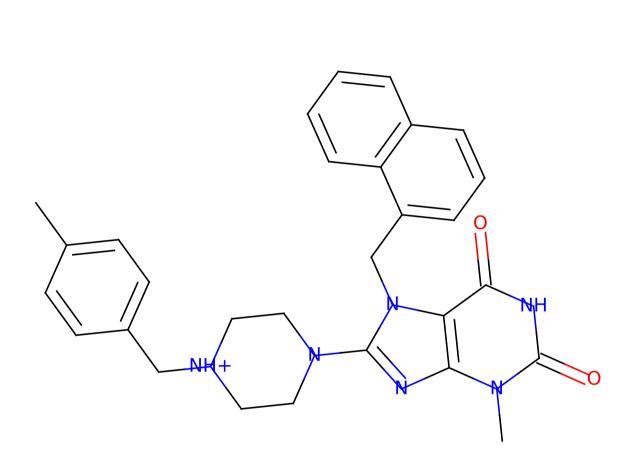
ORD-MCULE-3619815540_1



MolLogP: 4.504800000000004 | QED: 0.43144005118053486

c1ccc(cc1)C(c2cccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5cccc5c4

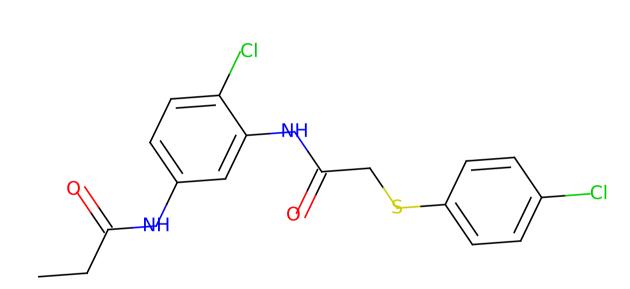
ORD-MCULE-9717306826_1



MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

 $\label{eq:condition} Cc1ccc(cc1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C$

ORD-MCULE-8959718627_1



MolLogP: 5.072700000000003 | QED: 0.6848468242287495

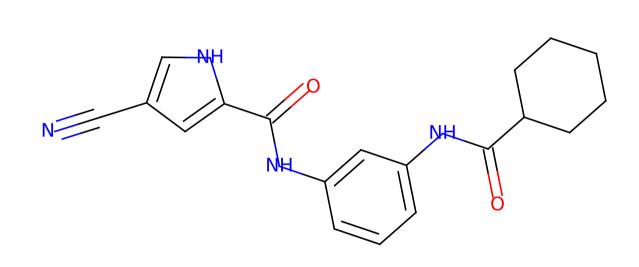
 $\mathsf{CCC}(=\mathsf{O})\mathsf{Nc1}\mathsf{ccc}(\mathsf{c(c1)NC}(=\mathsf{O})\mathsf{CSc2}\mathsf{ccc}(\mathsf{cc2})\mathsf{CI})\mathsf{CI}$

ORD-MCULE-9993059218_1

MolLogP: 2.960820000000001 | QED: 0.6386998682150667

Cc1[nH]c(c[nH+]1)C(=O)Nc2cccc(c2)NC(=O)CCc3ccccc3

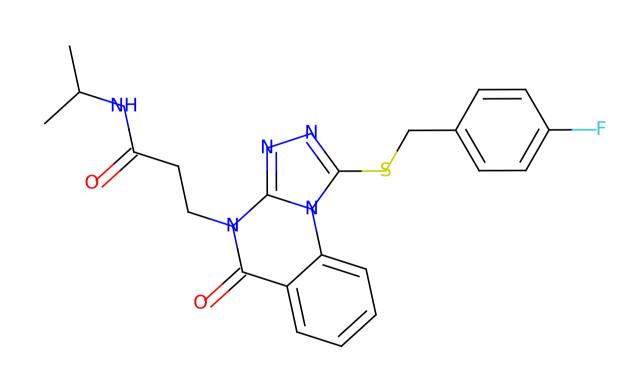
ORD-MCULE-1363662852_1



MolLogP: 3.6574800000000014 | QED: 0.7944424049877485

c1cc(cc(c1)NC(=0)C2CCCC2)NC(=0)c3cc(c[nH]3)C#N

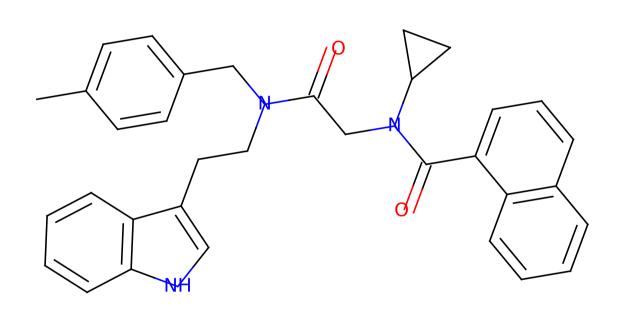
ORD-MCULE-1584805944_1



MolLogP: 3.3903000000000016 | QED: 0.4466230004287319

CC(C)NC(=O)CCn1c(=O)c2cccc2n3c1nnc3SCc4ccc(cc4)F

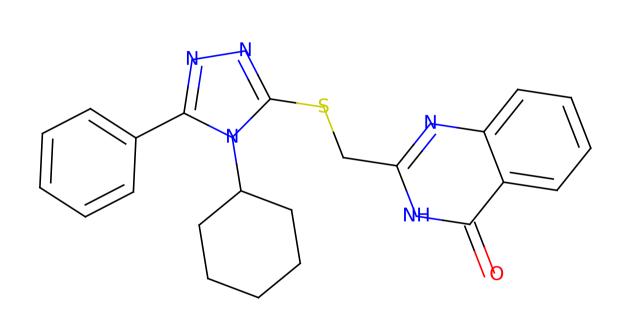
ORD-MCULE-7198549483_1



MolLogP: 6.505620000000007 | QED: 0.2434419591344794

 $\label{eq:c1ccc} Cc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)CN(C4CC4)C(=O)c5cccc6c5cccc6$

ORD-MCULE-2519953694_1



MolLogP: 4.979100000000003 | QED: 0.4635852670383765

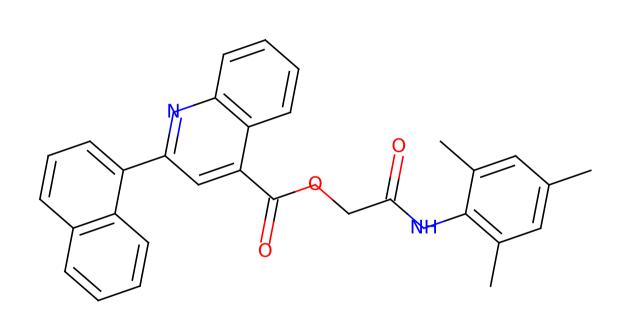
c1ccc(cc1)c2nnc(n2C3CCCC3)SCc4[nH]c(=O)c5cccc5n4

ORD-MCULE-4525414745_1

MolLogP: 4.3312000000000035 | QED: 0.19976136878195225

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

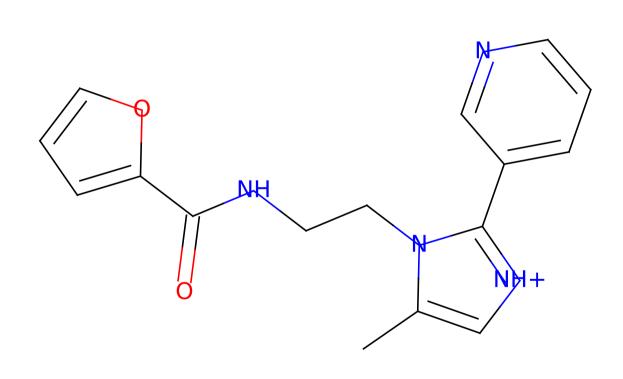
ORD-MCULE-3082269743_2



MolLogP: 6.775760000000005 | QED: 0.28530611753059815

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

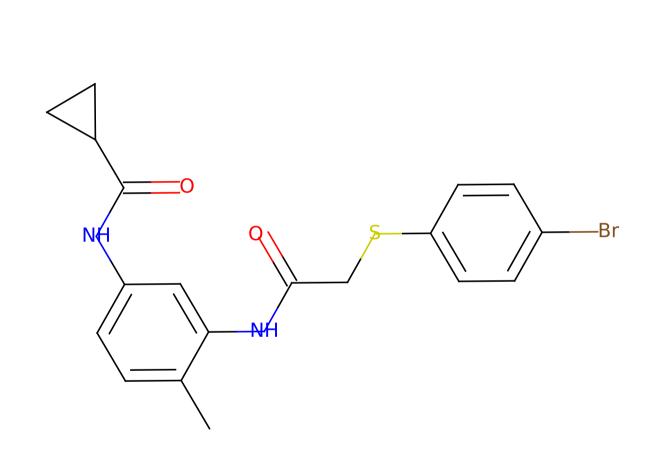
ORD-MCULE-2281744958_1



MolLogP: 1.6956199999999997 | QED: 0.7785628587123187

Cc1c[nH+]c(n1CCNC(=O)c2ccco2)c3cccnc3

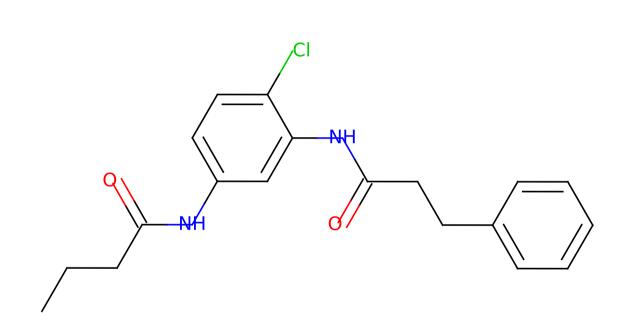
ORD-MCULE-7907421198_1



MolLogP: 4.836820000000002 | QED: 0.6593998471722905

Cc1ccc(cc1NC(=O)CSc2ccc(cc2)Br)NC(=O)C3CC3

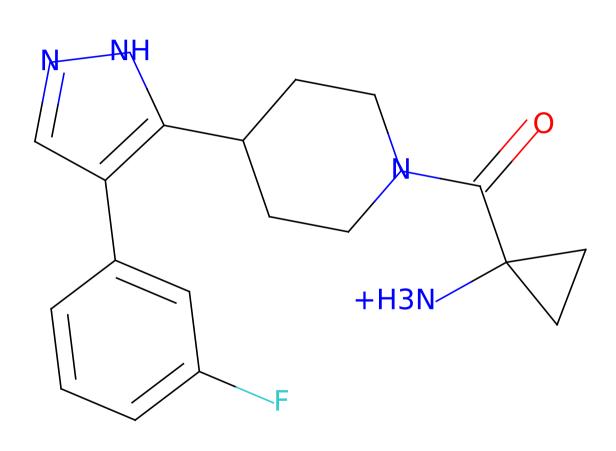
ORD-MCULE-6851258613_1



MolLogP: 4.649900000000003 | QED: 0.7676539659220933

 $\mathsf{CCCC}(=\mathsf{O})\mathsf{Nc1ccc}(\mathsf{c}(\mathsf{c1})\mathsf{NC}(=\mathsf{O})\mathsf{CCc2cccc2})\mathsf{CI}$

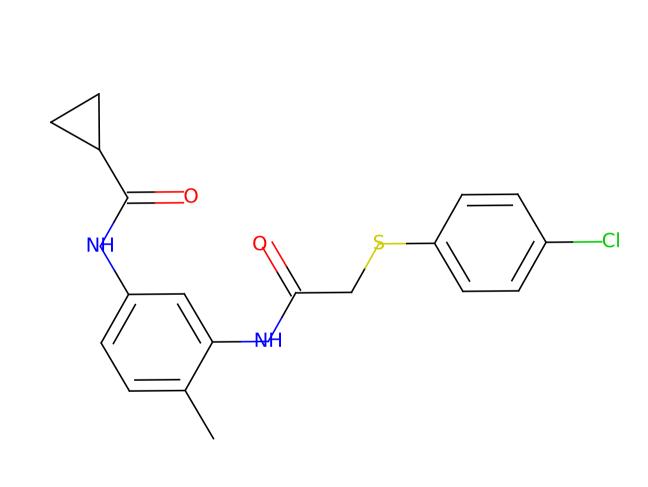
ORD-MCULE-6733900362_1



MolLogP: 1.6962999999999999 | QED: 0.8989870465496963

c1cc(cc(c1)F)c2cn[nH]c2C3CCN(CC3)C(=O)C4(CC4)[NH3+]

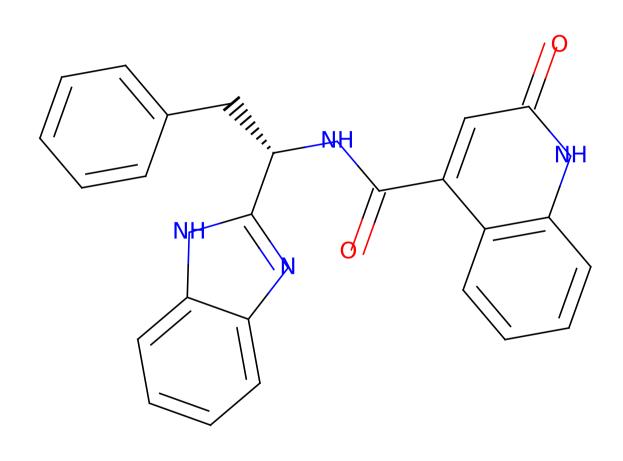
ORD-MCULE-1209624973_1



MolLogP: 4.727720000000002 | QED: 0.7185501495685765

Cc1ccc(cc1NC(=O)CSc2ccc(cc2)Cl)NC(=O)C3CC3

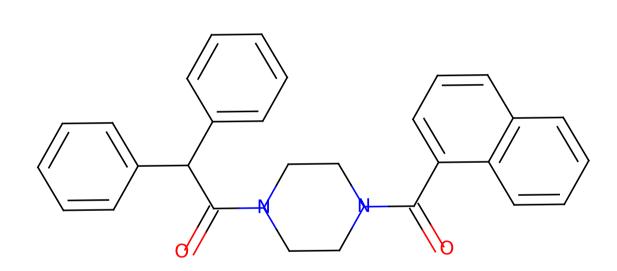
ORD-MCULE-7789954188_1



MolLogP: 4.118200000000002 | QED: 0.4085896962540062

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

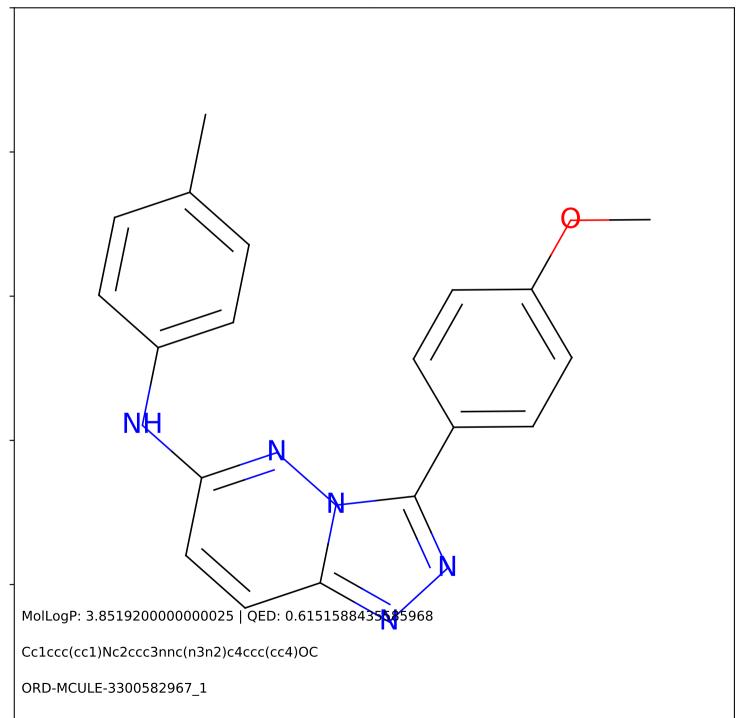
ORD-MCULE-2354836978_1

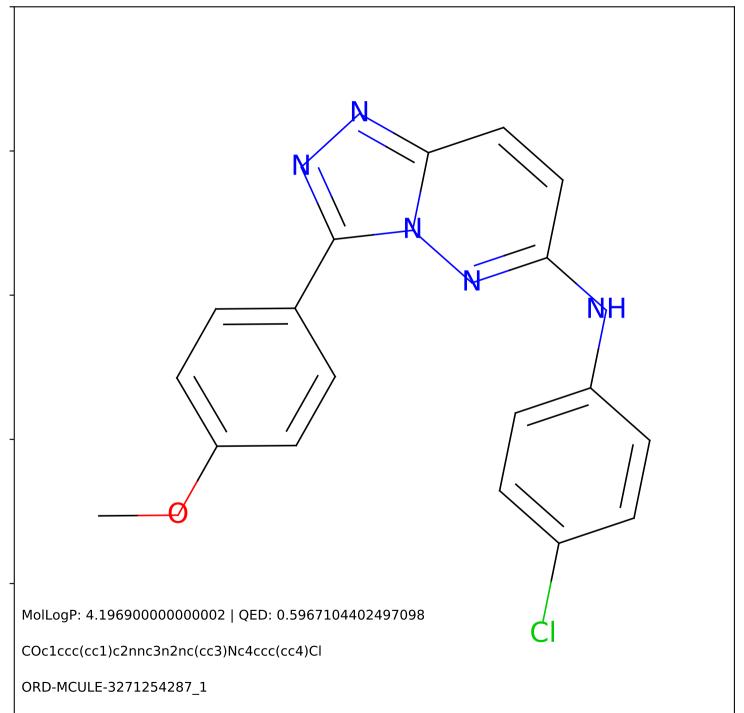


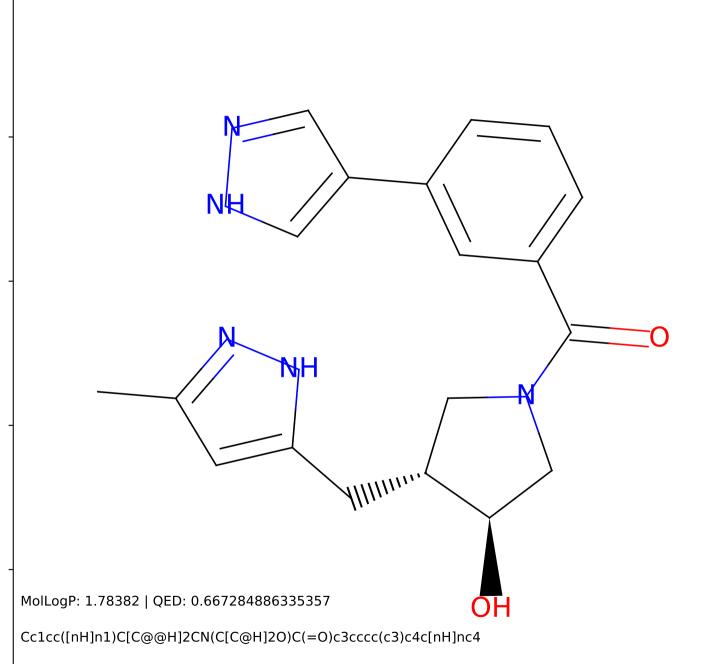
MolLogP: 4.956300000000004 | QED: 0.45571063266576933

c1ccc(cc1)C(c2cccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

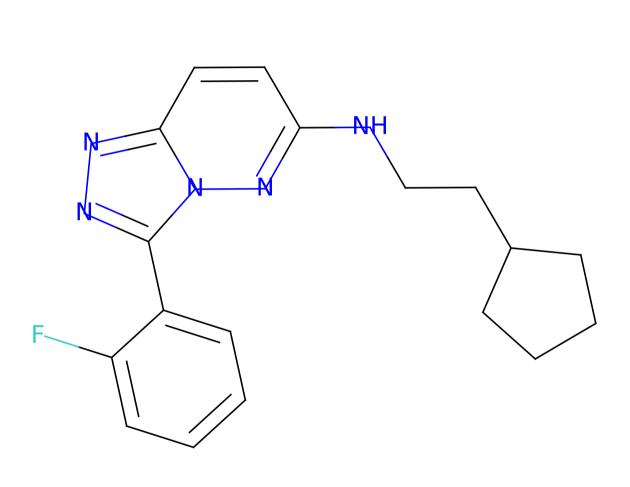
ORD-MCULE-4705080812_1







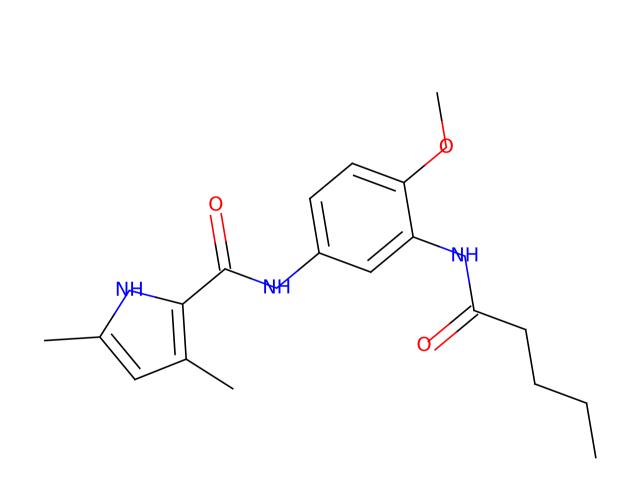
ORD-MCULE-6602067988_2



MolLogP: 3.922600000000002 | QED: 0.7722355966003347

c1ccc(c(c1)c2nnc3n2nc(cc3)NCCC4CCC4)F

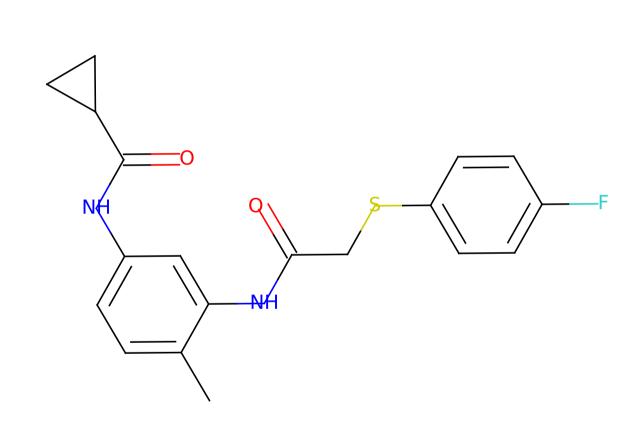
ORD-MCULE-5630254852_1



MolLogP: 4.021140000000003 | QED: 0.7097899893457638

 $\mathsf{CCCCC}(=\mathsf{O})\mathsf{Nc1cc}(\mathsf{ccc1OC})\mathsf{NC}(=\mathsf{O})\mathsf{c2c}(\mathsf{cc}([\mathsf{nH}]2)\mathsf{C})\mathsf{C}$

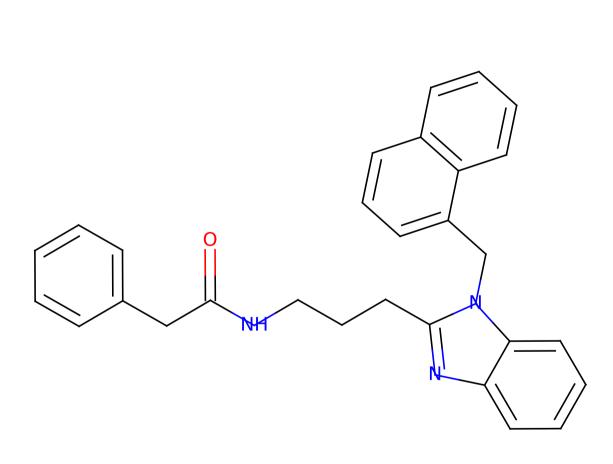
ORD-MCULE-5916323629_1



MolLogP: 4.213420000000002 | QED: 0.7605680072129353

Cc1ccc(cc1NC(=O)CSc2ccc(cc2)F)NC(=O)C3CC3

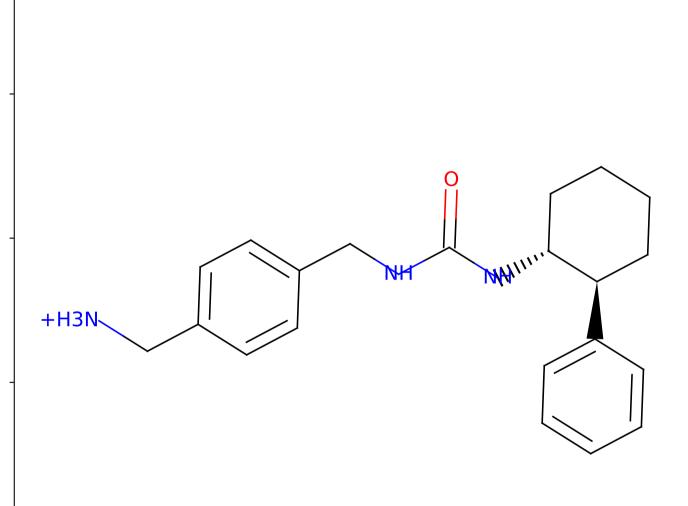
ORD-MCULE-5225269073_1



MolLogP: 5.529300000000005 | QED: 0.32718667928035094

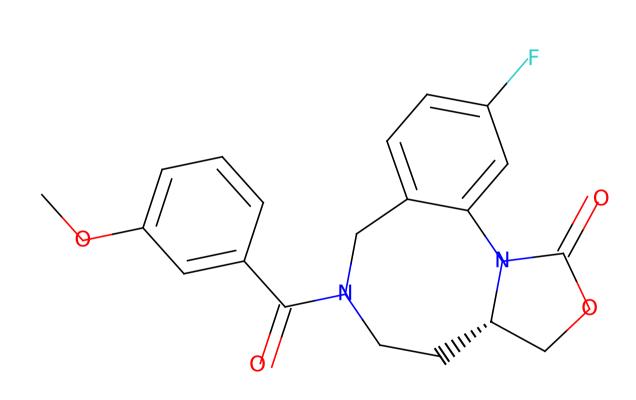
c1ccc(cc1)CC(=O)NCCCc2nc3ccccc3n2Cc4cccc5c4cccc5

ORD-MCULE-9349708949_1



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

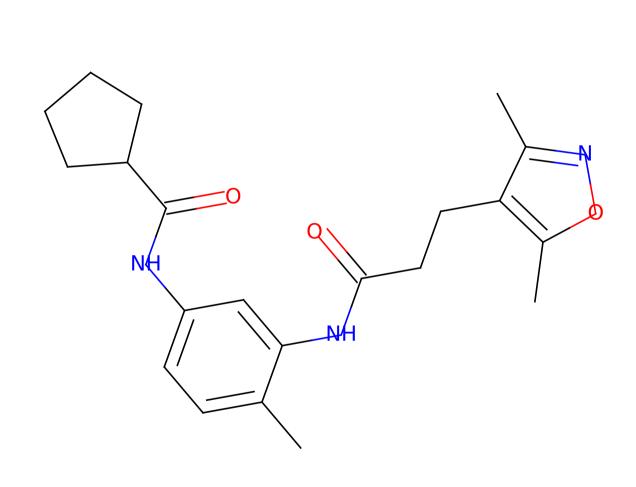
ORD-MCULE-5985705514_1



MolLogP: 3.2056000000000013 | QED: 0.8145962020967583

COc1cccc(c1)C(=O)N2CC[C@H]3COC(=O)N3c4cc(ccc4C2)F

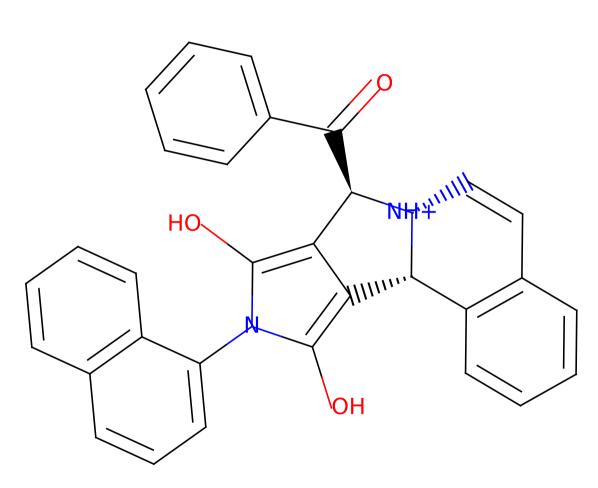
ORD-MCULE-6145200920_1



MolLogP: 4.299860000000003 | QED: 0.7949686710997425

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

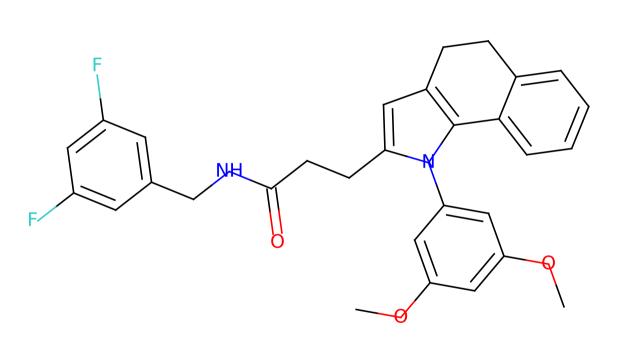
ORD-MCULE-7968599617_1



MolLogP: 4.937900000000005 | QED: 0.32678562838553826

 $\verb|c1ccc(cc1)C(=0)[C@@H]2c3c(c(n(c30)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7||\\$

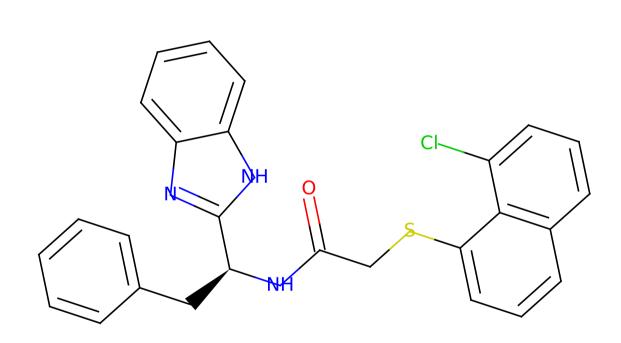
ORD-MCULE-7416131701_1



MolLogP: 5.7873000000000046 | QED: 0.33203587335464885

COc1cc(cc(c1)OC)n2c(cc3c2-c4cccc4CC3)CCC(=O)NCc5cc(cc(c5)F)F

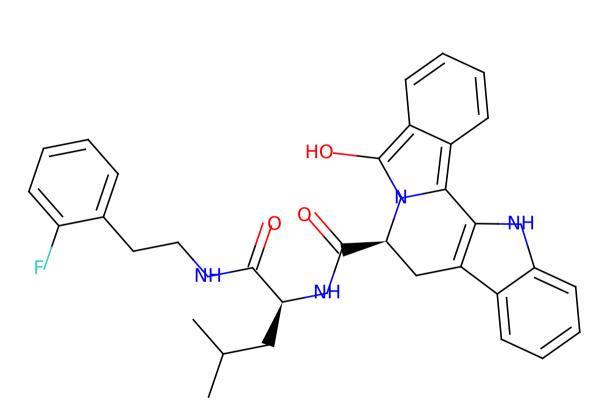
ORD-MCULE-6553444445_1



MolLogP: 6.561800000000004 | QED: 0.26406471710612306

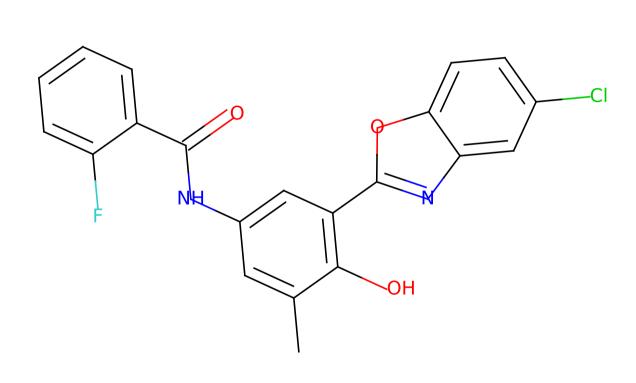
c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)CSc4cccc5c4c(ccc5)Cl

ORD-MCULE-6426577239_1



MolLogP: 5.621300000000006 | QED: 0.20107182839149487

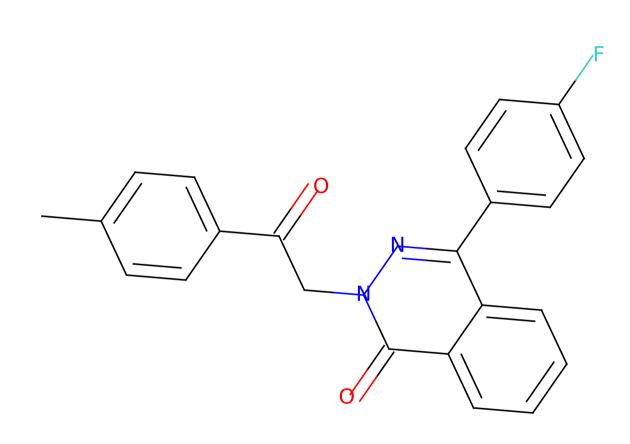
ORD-MCULE-9438397769_1



MolLogP: 5.553620000000003 | QED: 0.44479111691834555

Cc1cc(cc(c10)c2nc3cc(ccc3o2)CI)NC(=0)c4cccc4F

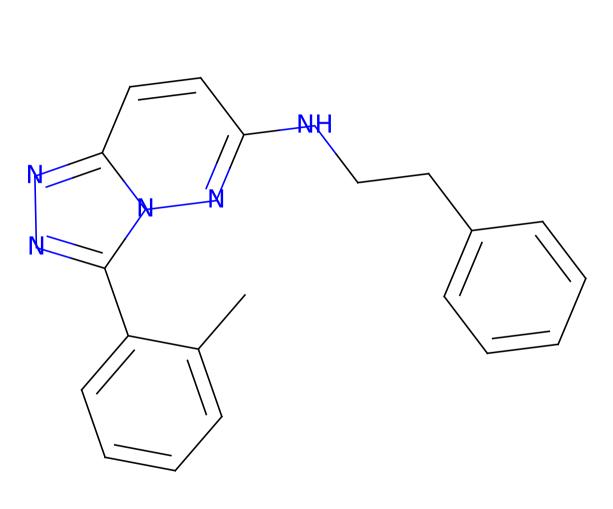
ORD-MCULE-1411882390_1



MolLogP: 4.393920000000003 | QED: 0.49926272810105116

Cc1ccc(cc1)C(=O)Cn2c(=O)c3ccccc3c(n2)c4ccc(cc4)F

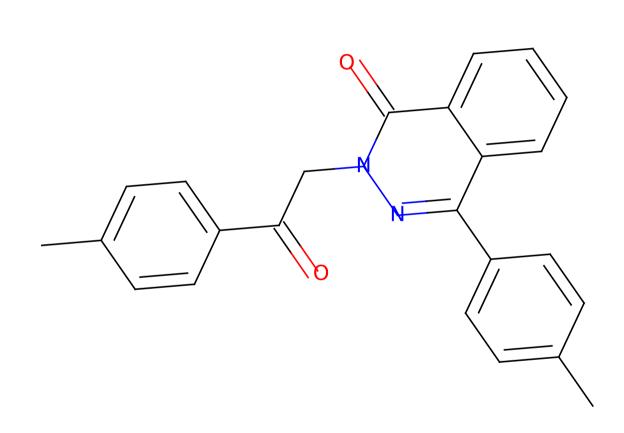
ORD-MCULE-4318132863_1



MolLogP: 3.7543200000000017 | QED: 0.605659512601071

Cc1cccc1c2nnc3n2nc(cc3)NCCc4cccc4

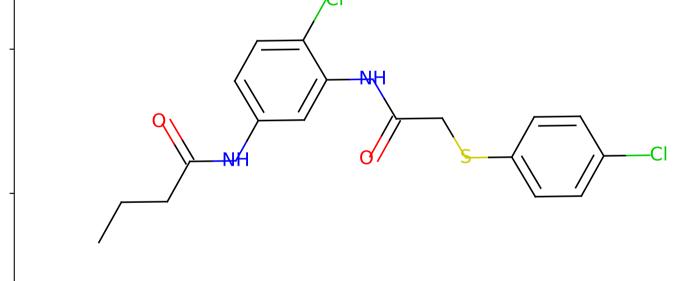
ORD-MCULE-2174983984_1



MolLogP: 4.563240000000004 | QED: 0.49617569404605777

Cc1ccc(cc1)c2c3ccccc3c(=O)n(n2)CC(=O)c4ccc(cc4)C

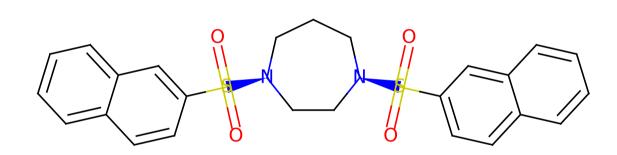
ORD-MCULE-9614379555_1



MolLogP: 5.462800000000002 | QED: 0.6100241423306323

CCCC(=O)Nc1ccc(c(c1)NC(=O)CSc2ccc(cc2)CI)CI

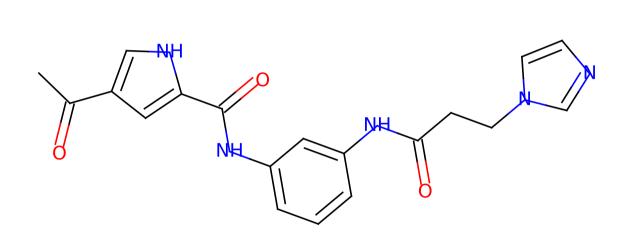
ORD-MCULE-4706668103_1



MolLogP: 4.078300000000003 | QED: 0.441202265024148

c1ccc2cc(ccc2c1)S(=O)(=O)[N@@]3CCC[N@](CC3)S(=O)(=O)c4ccc5cccc5c4

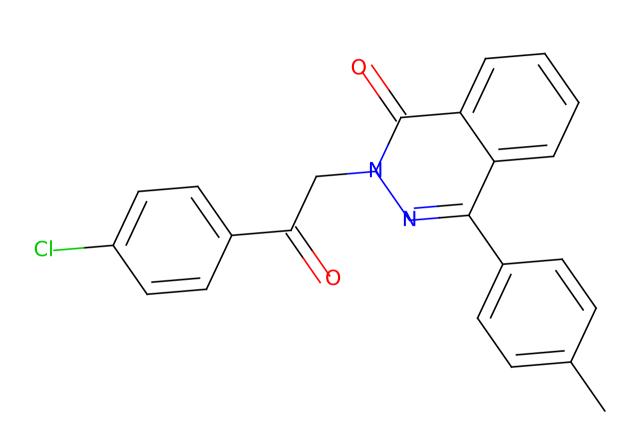
ORD-MCULE-4262091783_1



MolLogP: 2.6949000000000005 | QED: 0.5593182677576637

CC(=O)c1cc([nH]c1)C(=O)Nc2cccc(c2)NC(=O)CCn3ccnc3

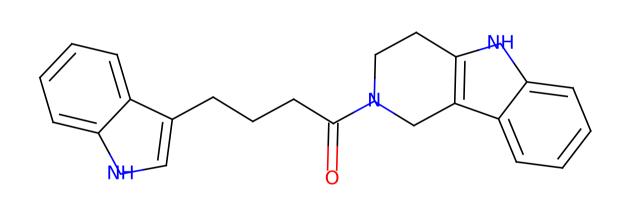
ORD-MCULE-2010508719_1



MolLogP: 4.908220000000004 | QED: 0.46667037300893904

Cc1ccc(cc1)c2c3cccc3c(=O)n(n2)CC(=O)c4ccc(cc4)Cl

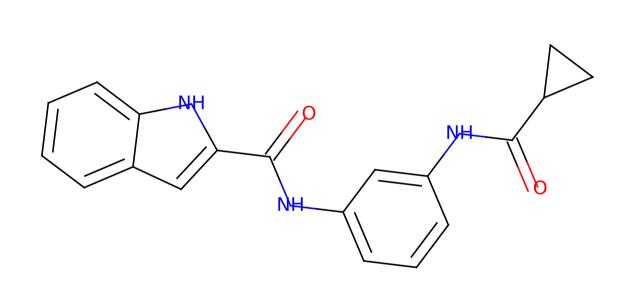
ORD-MCULE-2709561402_1



MolLogP: 4.556800000000003 | QED: 0.5527480330596802

c1ccc2c(c1)c(c[nH]2)CCCC(=O)N3CCc4c(c5ccccc5[nH]4)C3

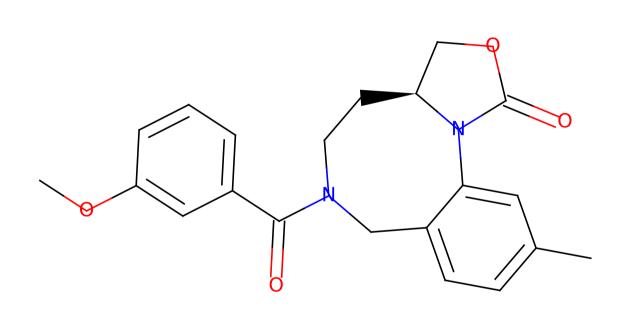
ORD-MCULE-6844818866_1



MolLogP: 3.768700000000001 | QED: 0.6846113766118399

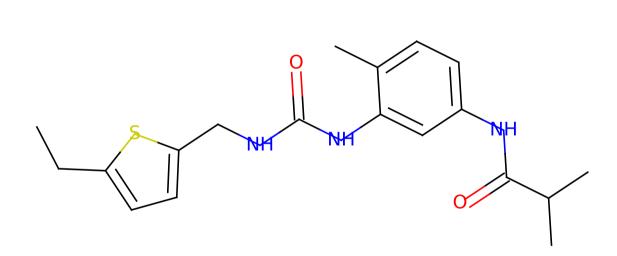
 $\verb|c1ccc2c(c1)cc([nH]2)C(=O)Nc3cccc(c3)NC(=O)C4CC4|\\$

ORD-MCULE-3820145843_1



MolLogP: 3.374920000000002 | QED: 0.8176099573772637

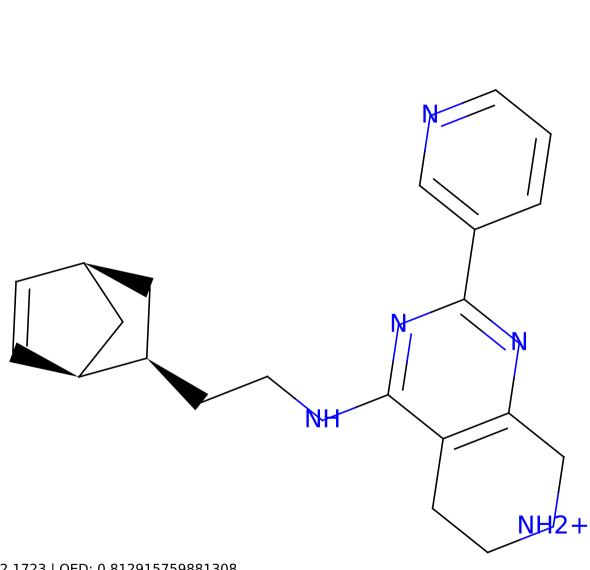
ORD-MCULE-4911470400_1



MolLogP: 4.535120000000003 | QED: 0.7087373697322665

 $\mathsf{CCc1ccc}(\mathsf{s1})\mathsf{CNC}(=\mathsf{O})\mathsf{Nc2cc}(\mathsf{ccc2C})\mathsf{NC}(=\mathsf{O})\mathsf{C}(\mathsf{C})\mathsf{C}$

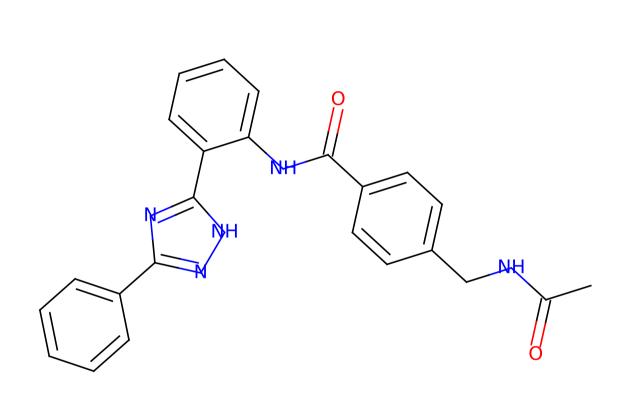
ORD-MCULE-2174198710_1



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

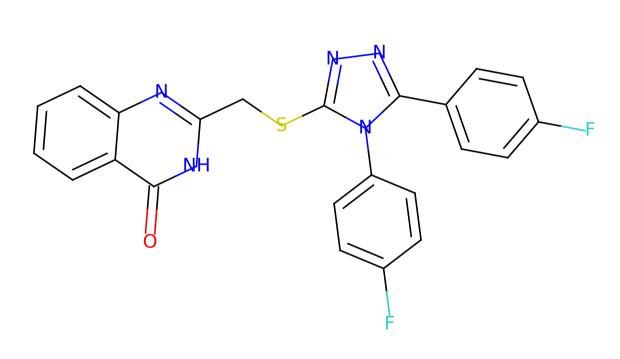
ORD-MCULE-5739750381_1



MolLogP: 4.027100000000002 | QED: 0.44600141958321116

CC(=O)NCc1ccc(cc1)C(=O)Nc2cccc2c3[nH]nc(n3)c4cccc4

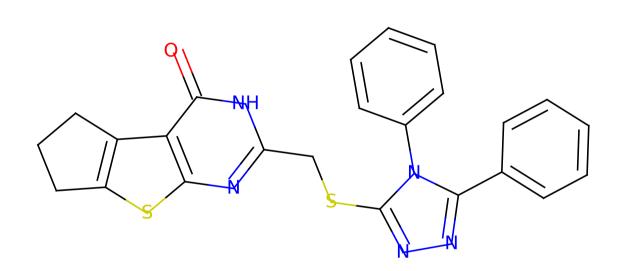
ORD-MCULE-7152686229_1



MolLogP: 4.7413000000000025 | QED: 0.3939745845285081

c1ccc2c(c1)c(=0)[nH]c(n2)CSc3nnc(n3c4ccc(cc4)F)c5ccc(cc5)F

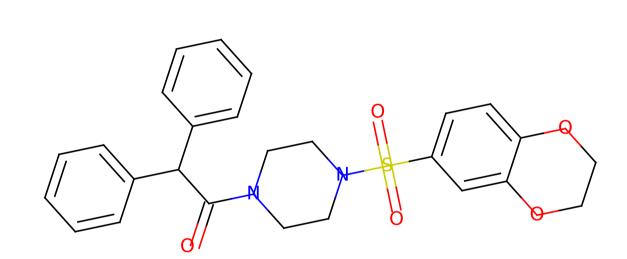
ORD-MCULE-5900515006_1



MolLogP: 5.013300000000003 | QED: 0.37541396911851704

c1ccc(cc1)c2nnc(n2c3ccccc3)SCc4[nH]c(=0)c5c6c(sc5n4)CCC6

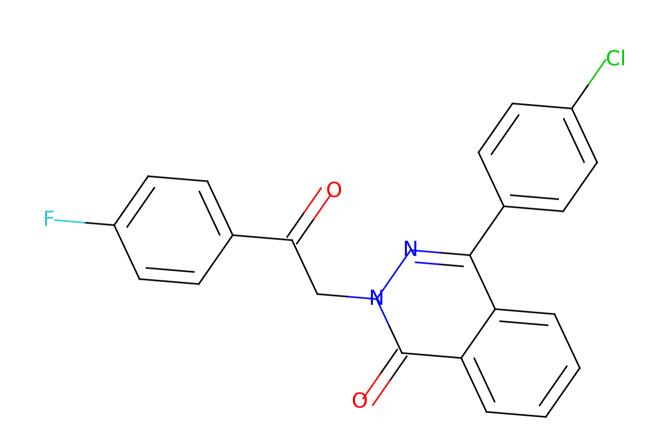
ORD-MCULE-5456008772_1



MolLogP: 3.122800000000016 | QED: 0.5633261375042687

c1ccc(cc1)C(c2cccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5c(c4)OCCO5

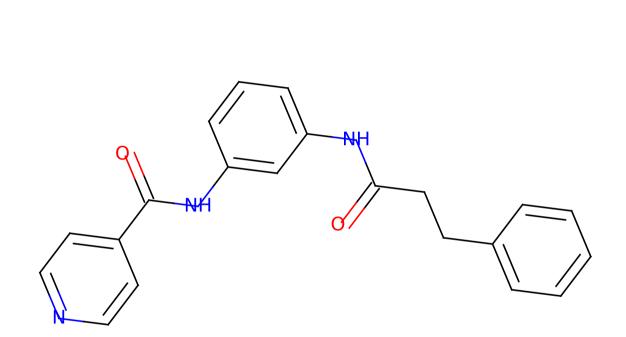
ORD-MCULE-1904175079_1



MolLogP: 4.738900000000003 | QED: 0.47127673315402185

c1ccc2c(c1)c(nn(c2=0)CC(=0)c3ccc(cc3)F)c4ccc(cc4)Cl

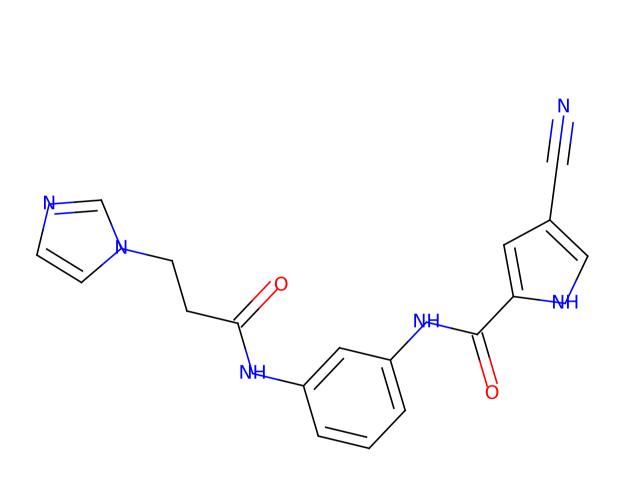
ORD-MCULE-4965151625_1



MolLogP: 3.9052000000000024 | QED: 0.7115155585770637

c1ccc(cc1)CCC(=0)Nc2cccc(c2)NC(=0)c3ccncc3

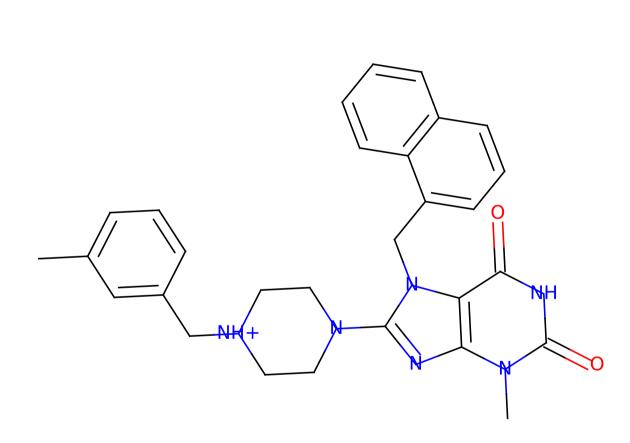
ORD-MCULE-3836592429_1



MolLogP: 2.3639799999999997 | QED: 0.6339198492190868

c1cc(cc(c1)NC(=O)c2cc(c[nH]2)C#N)NC(=O)CCn3ccnc3

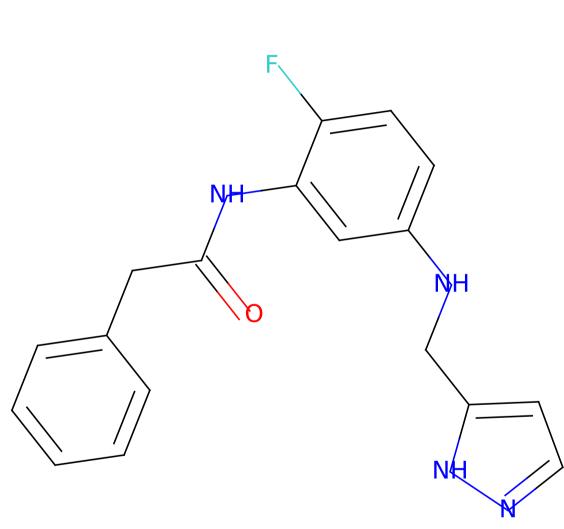
ORD-MCULE-1695331164_1



MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

Cc1cccc(c1)C[NH+]2CCN(CC2)c3nc4c(n3Cc5cccc6c5cccc6)c(=O)[nH]c(=O)n4C

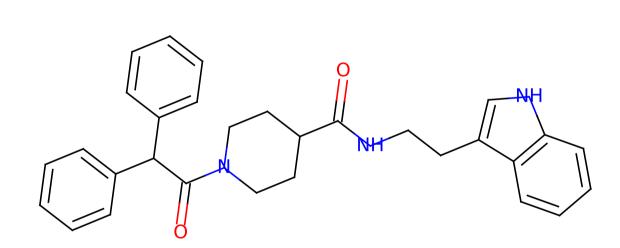
ORD-MCULE-9311937068_1



MolLogP: 3.3421000000000003 | QED: 0.6511474358760188

c1ccc(cc1)CC(=O)Nc2cc(ccc2F)NCc3ccn[nH]3

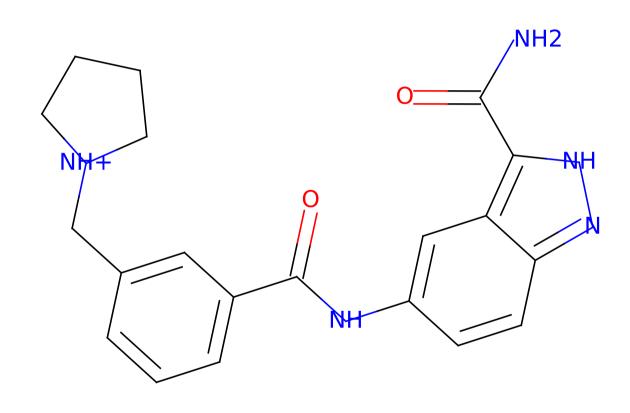
ORD-MCULE-6966320943_1



MolLogP: 4.897300000000003 | QED: 0.40786292071408126

c1ccc(cc1)C(c2cccc2)C(=O)N3CCC(CC3)C(=O)NCCc4c[nH]c5c4ccc5

ORD-MCULE-9130199918_1



MolLogP: 1.0927999999999999 | QED: 0.5445620954382201

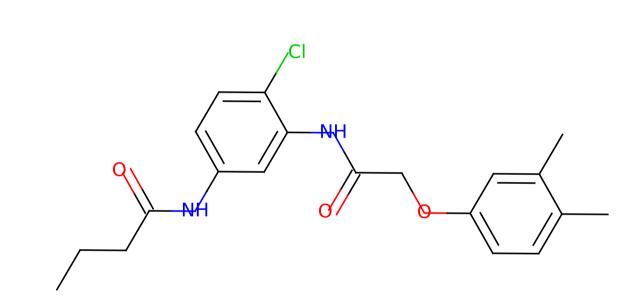
c1cc(cc(c1)C(=0)Nc2ccc3c(c2)c([nH]n3)C(=0)N)C[NH+]4CCCC4

ORD-MCULE-1647109669_2

MolLogP: 3.773000000000015 | QED: 0.6492918937523862

c1cc(cnc1)CCC(=0)Nc2cc(ccc2F)NC(=0)c3ccc4c(c3)OCO4

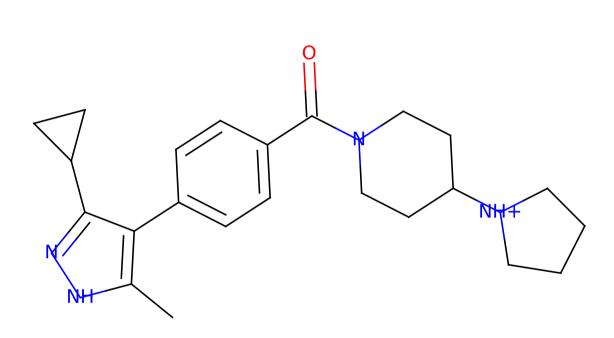
ORD-MCULE-9133488145_1



MolLogP: 4.712940000000003 | QED: 0.7368131788510064

 $\mathsf{CCCC}(=\mathsf{O})\mathsf{Nc1}\mathsf{ccc}(\mathsf{c(c1)NC}(=\mathsf{O})\mathsf{COc2}\mathsf{ccc}(\mathsf{c(c2)C})\mathsf{C})\mathsf{C}\mathsf{I}$

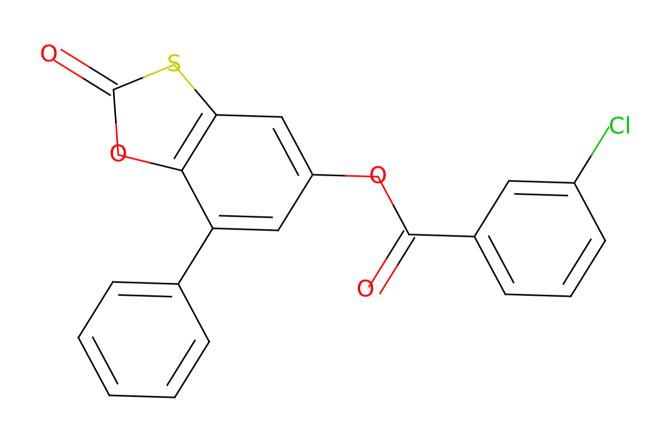
ORD-MCULE-8562081414_1



MolLogP: 2.54582 | QED: 0.8578099200835345

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

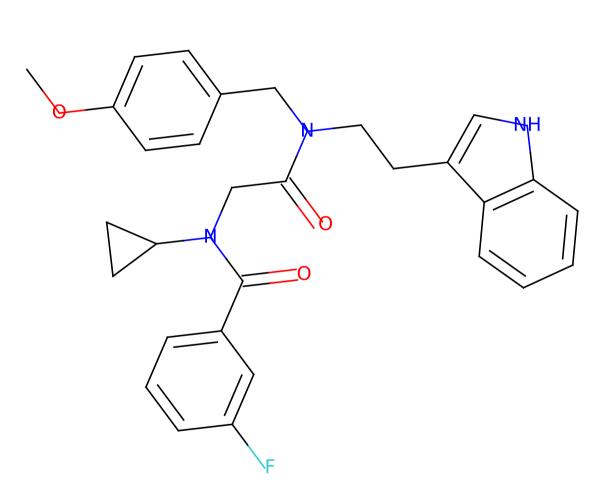
ORD-MCULE-3417237209_1



MolLogP: 5.394100000000034 | QED: 0.35166099869276446

 $\verb|c1ccc(cc1)c2cc(cc3c2oc(=O)s3)OC(=O)c4cccc(c4)Cl|\\$

ORD-MCULE-7866332805_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