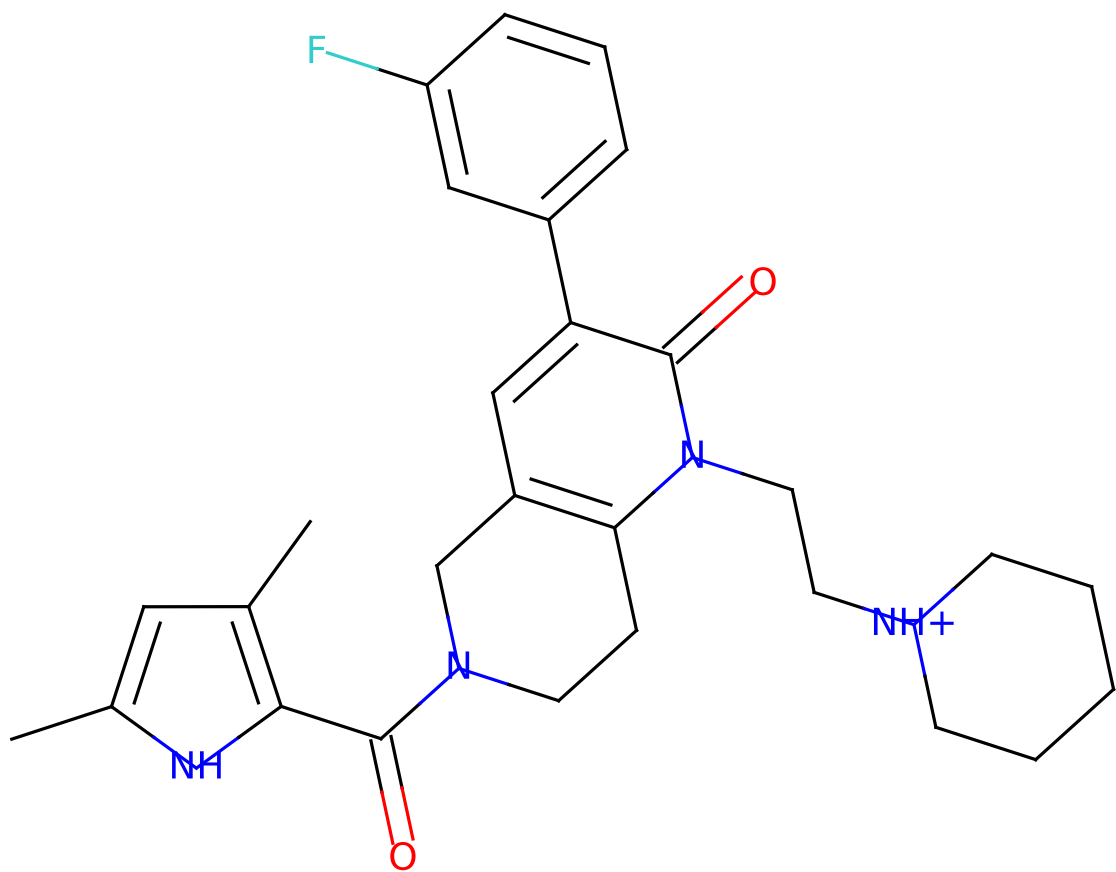1

MolLogP: 5.8548000000000044 | QED: 0.21272800874019035

c1ccc(cc1)Cn2c(nnc2SCC(=O)c3c[nH]c4c3cccc4)Cc5c[nH]c6c5cccc6
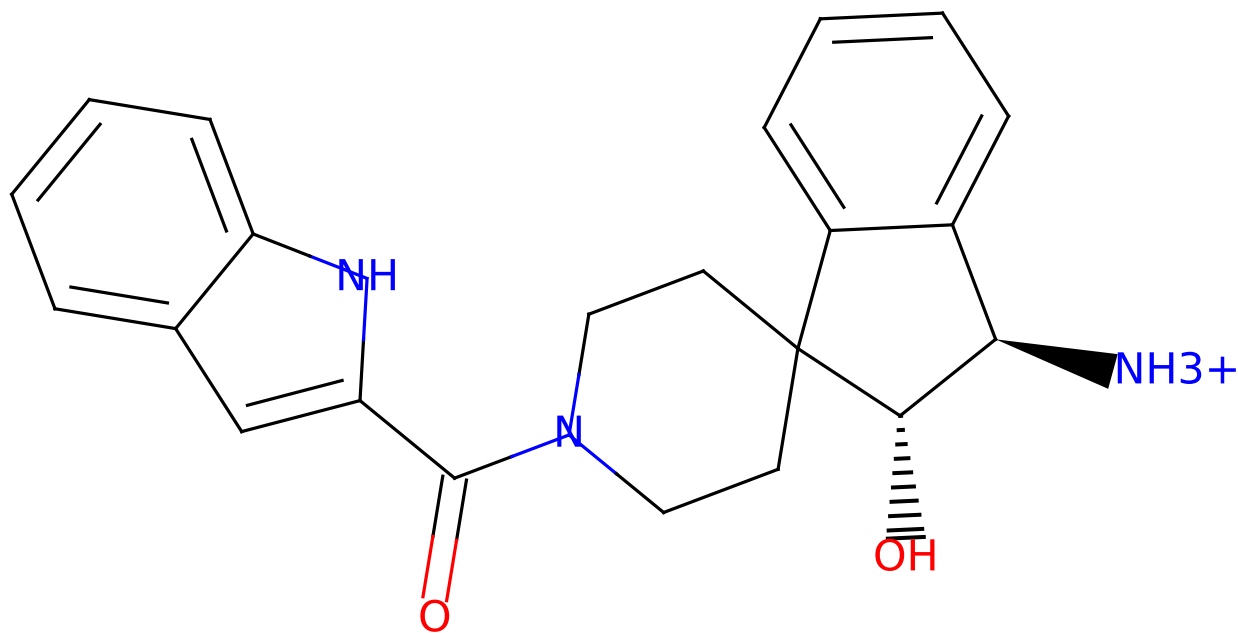
ORD-MCULE-2017284421_1

MolLogP: 2.866640000000001 | QED: 0.5937830397355752

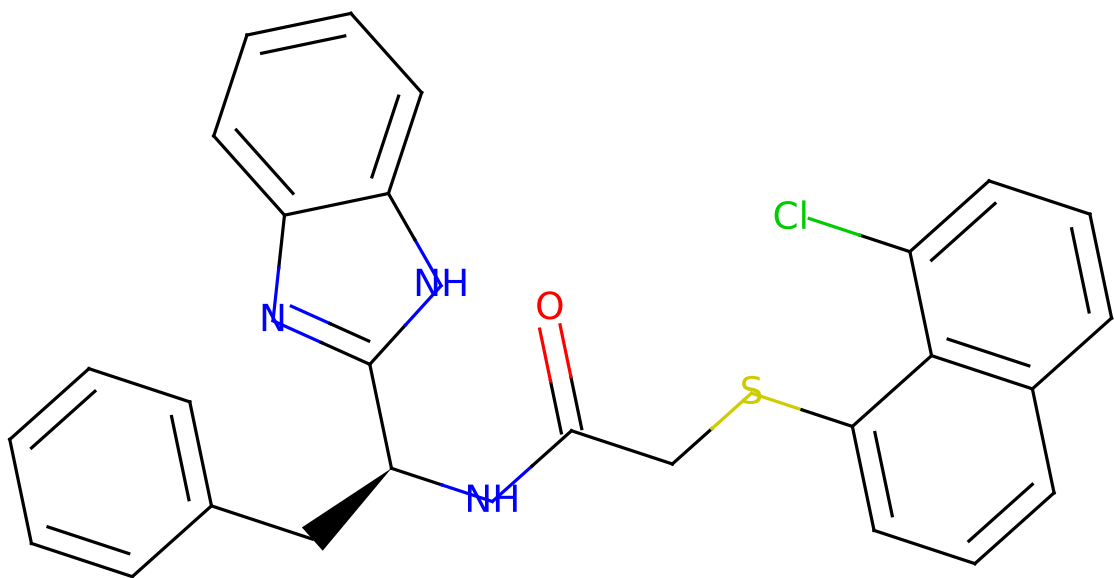Cc1cc([nH]c1C(=O)N2CCc3c(cc(c(=O)n3CC[NH+]4CCCCC4)c5cccc(c5)F)C2)C

ORD-MCULE-8927634984_1

3

MolLogP: 1.9993999999999992 | QED: 0.6185886642817092

c1ccc2c(c1)cc([nH]2)C(=O)N3CCC4(CC3)c5ccccc5[C@H]([C@@H]4O)[NH3+]
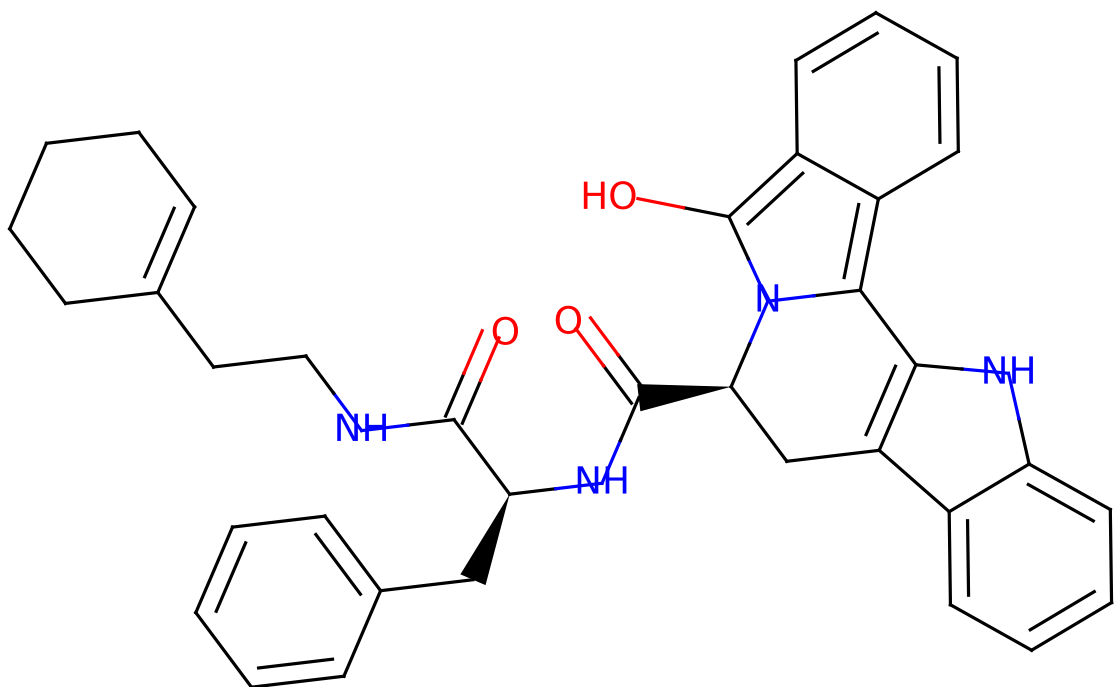
ORD-MCULE-2501948372_1

MolLogP: 6.561800000000004 | QED: 0.26406471710612306

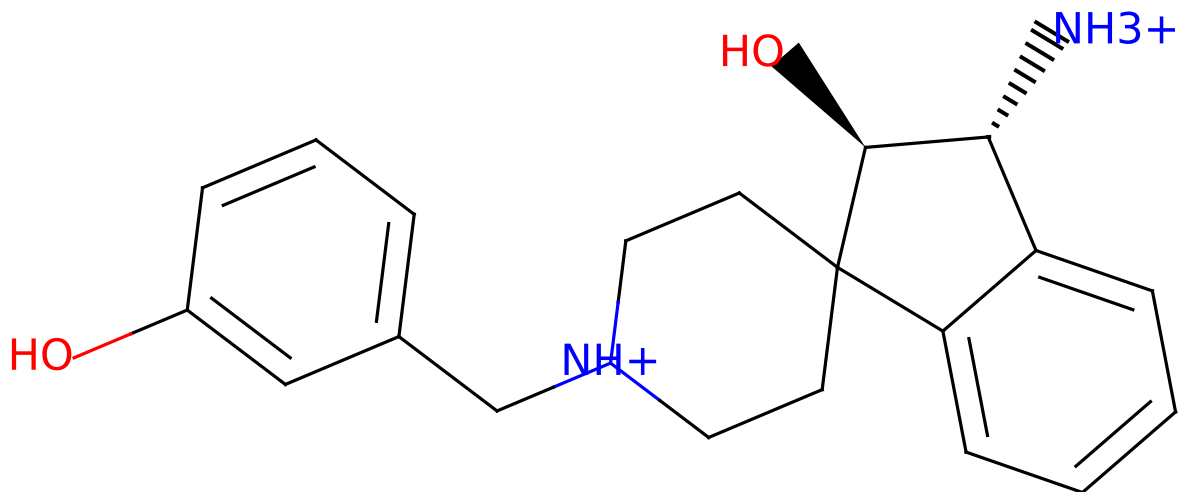c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)CSc4cccc5c4c(ccc5)Cl

ORD-MCULE-6426577239_1

MolLogP: 6.326600000000007 | QED: 0.163672300852651

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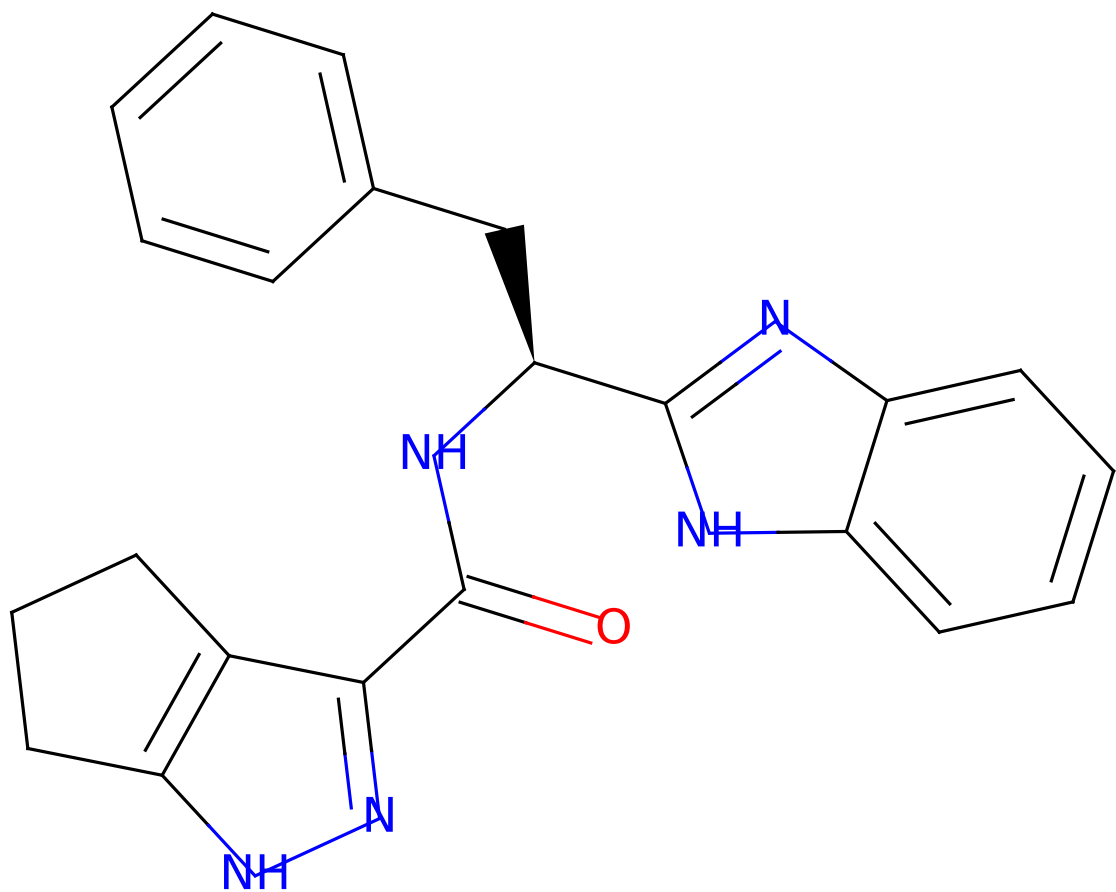
ORD-MCULE-2409941333_1

MolLogP: 0.1664000000000006 | QED: 0.6350962382114449

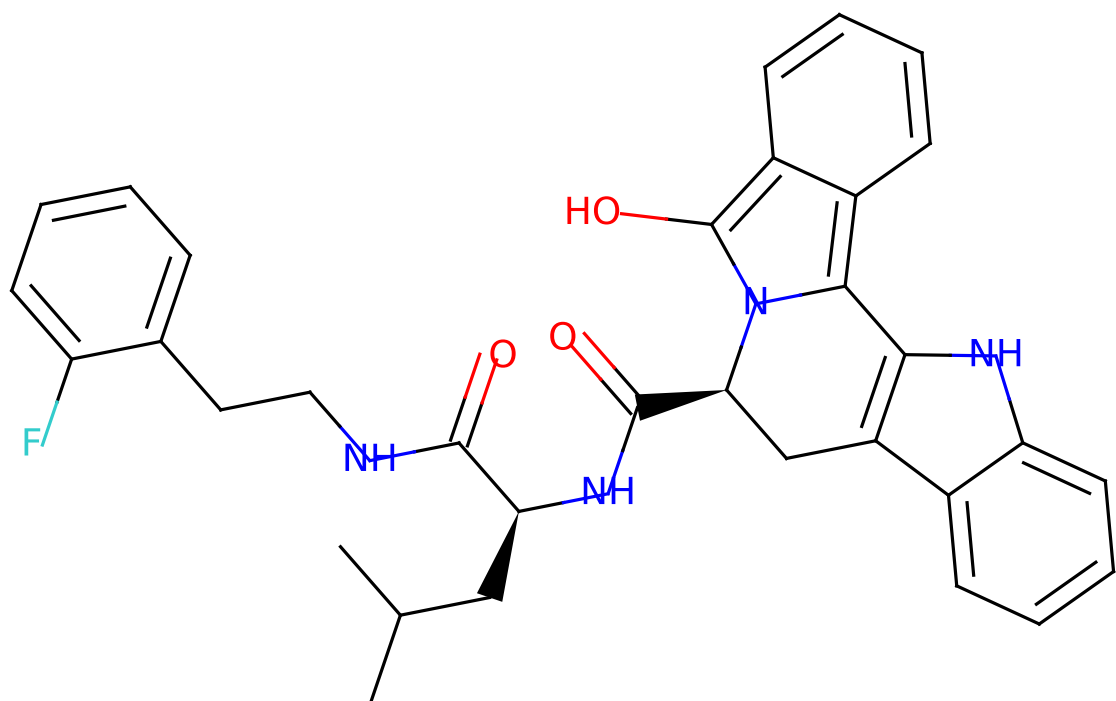c1ccc2c(c1)[C@H]([C@@H](C23CC[NH+](CC3)Cc4cccc(c4)O)O)[NH3+]

ORD-MCULE-1732713950_1

MolLogP: 3.488500000000001 | QED: 0.5018558408043431

c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4c5c([nH]n4)CCC5
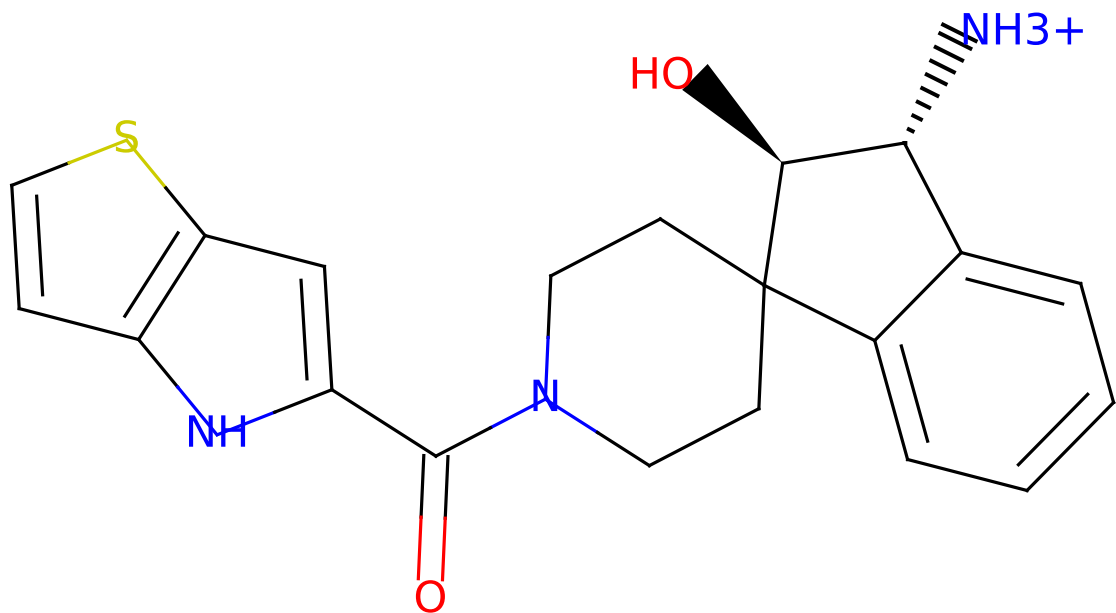
ORD-MCULE-3980688822_1

MolLogP: 5.621300000000006 | QED: 0.20107182839149487

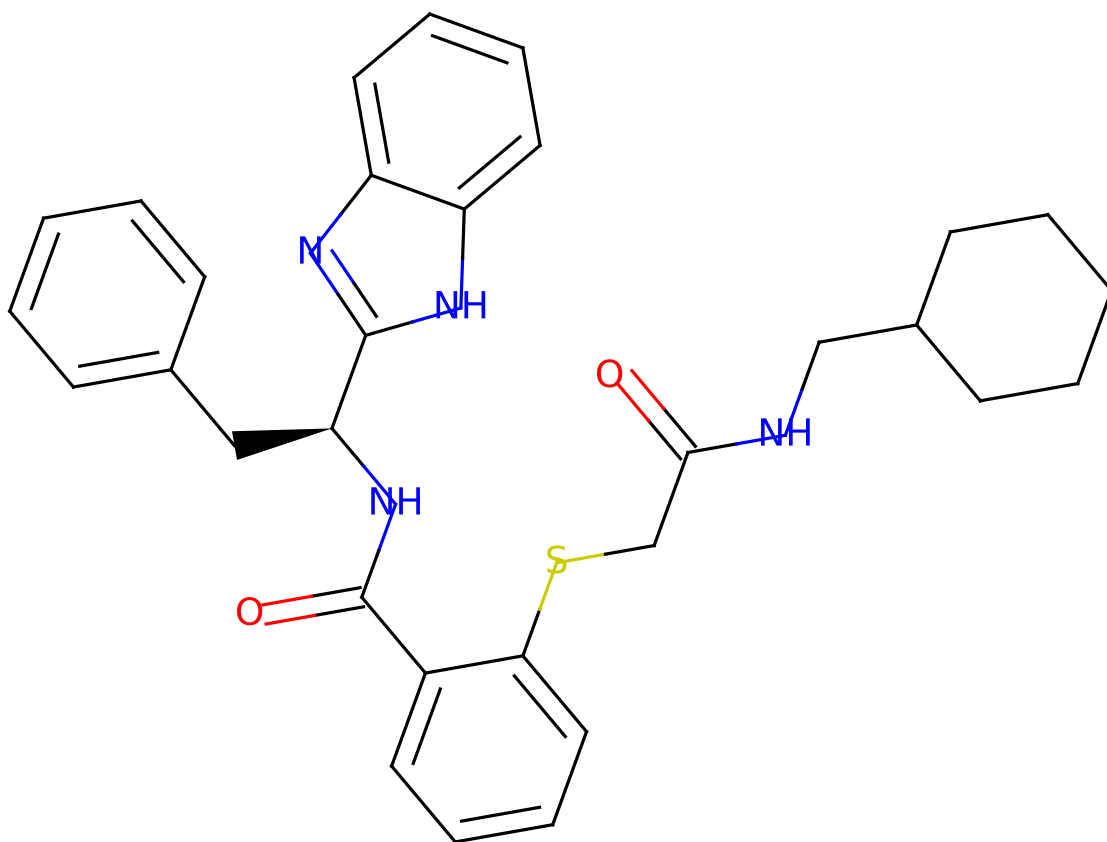CC(C)C[C@@H](C(=O)NCCc1ccccc1F)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O

ORD-MCULE-9438397769_1

MolLogP: 2.0608999999999997 | QED: 0.6142566250775262

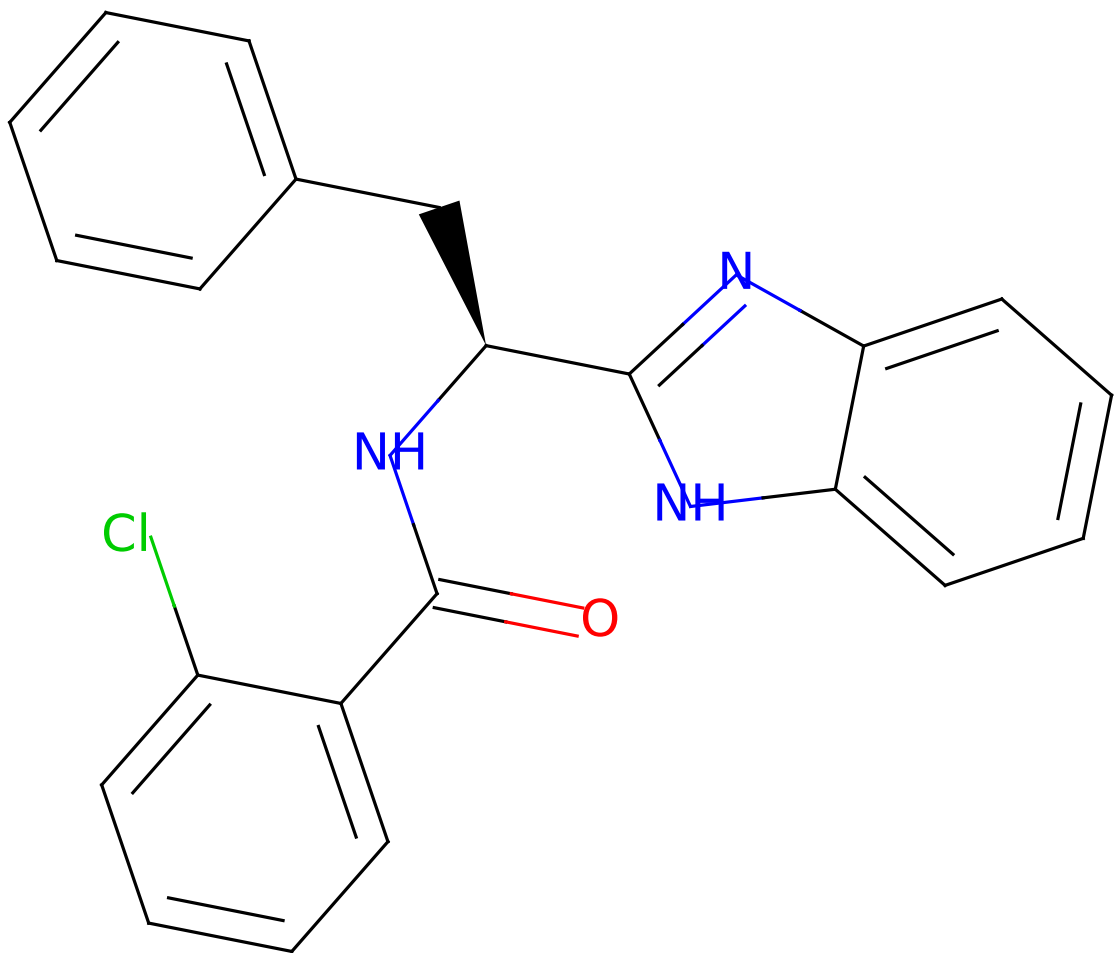c1ccc2c(c1)[C@H]([C@@H](C23CCN(CC3)C(=O)c4cc5c([nH]4)ccs5)O)[NH3+]

ORD-MCULE-1278004987_1

MolLogP: 6.065300000000004 | QED: 0.21912555782077076

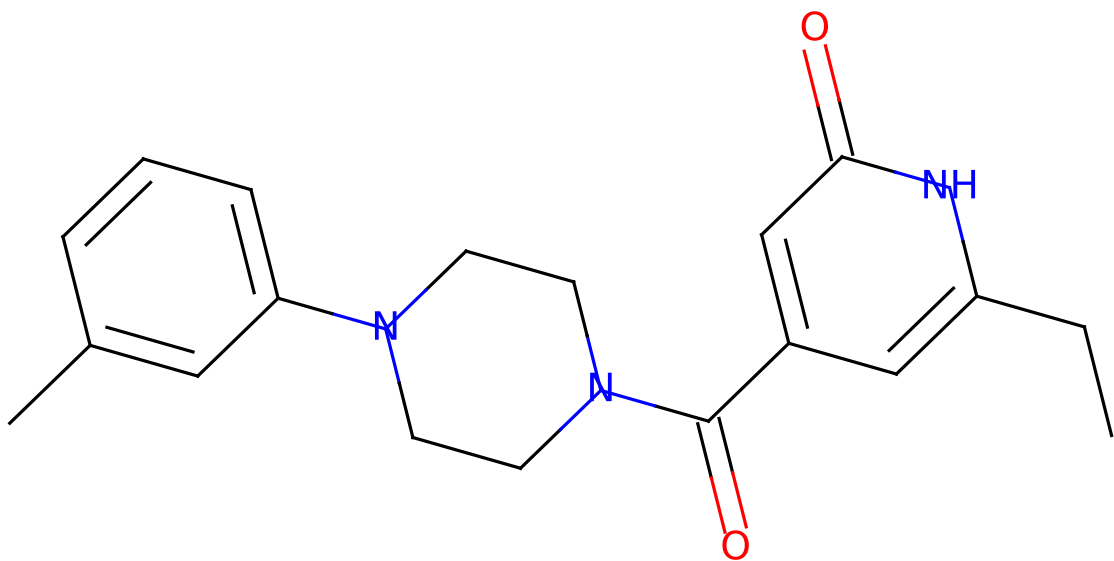c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4ccccc4SCC(=O)NCC5CCCCC5

ORD-MCULE-5858157644_1

MolLogP: 4.930100000000003 | QED: 0.5192510599861315
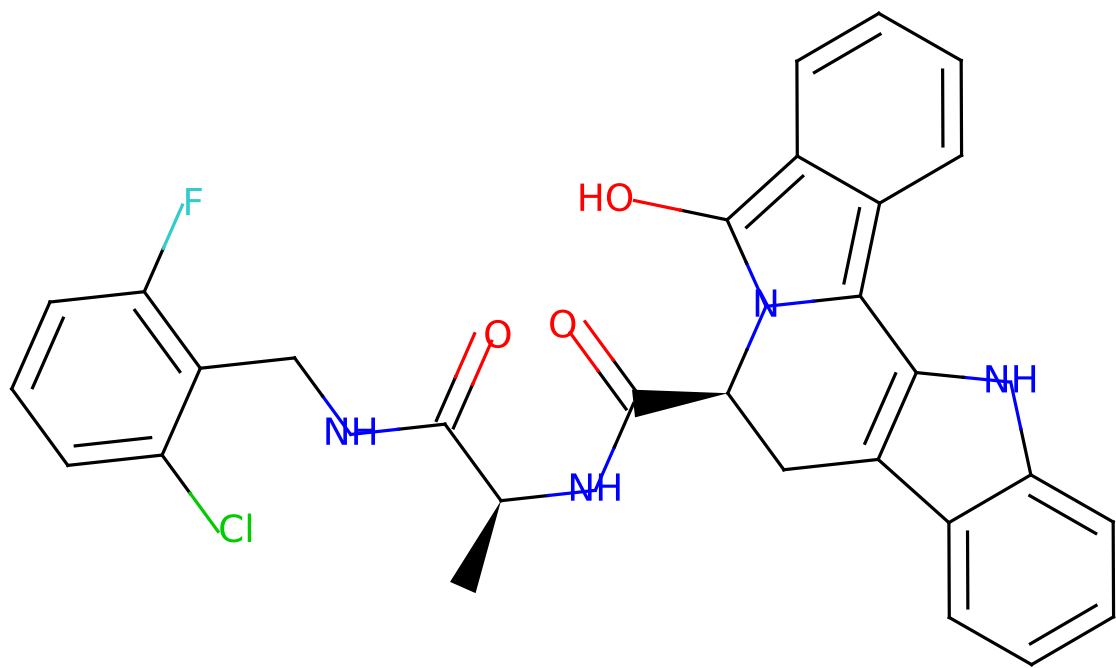
c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4ccccc4Cl

ORD-MCULE-3102049132_1

MolLogP: 2.20812 | QED: 0.9411763351761466

CCc1cc(cc(=O)[nH]1)C(=O)N2CCN(CC2)c3cccc(c3)C
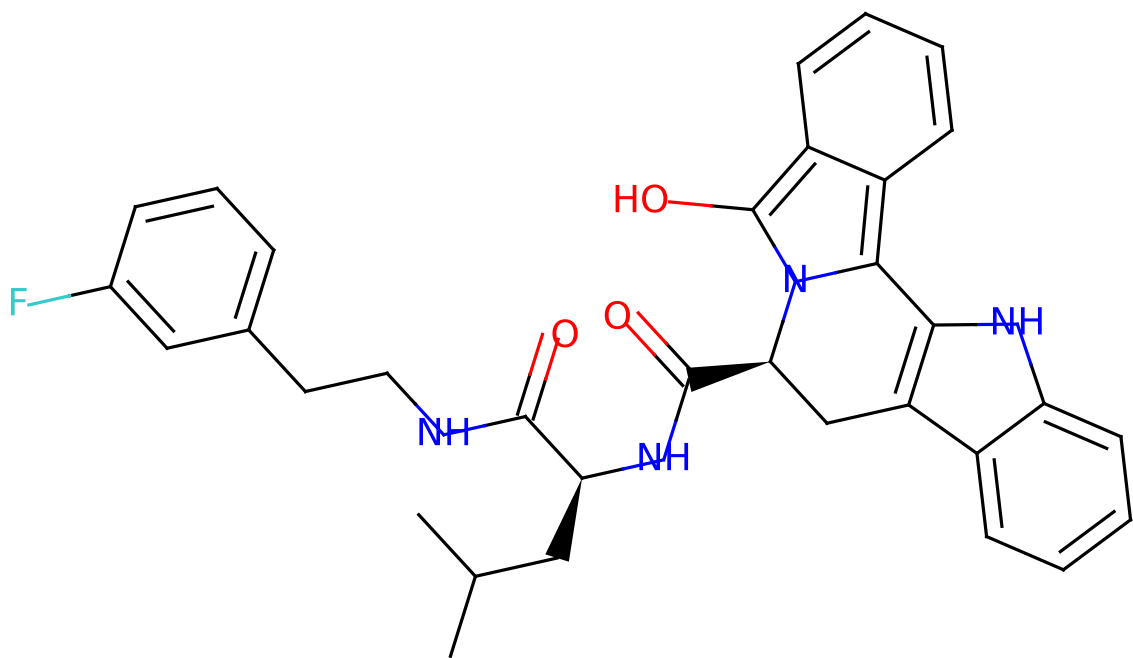
ORD-MCULE-8841098920_1

13

MolLogP: 5.206000000000005 | QED: 0.2510218746481418

C[C@@H](C(=O)NCc1c(cccc1Cl)F)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O
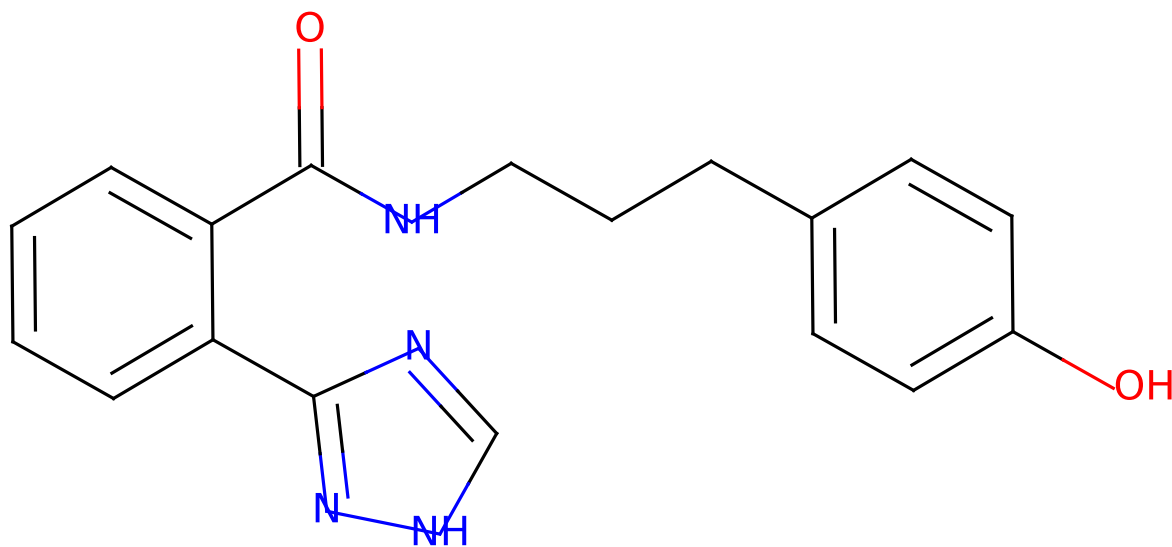
ORD-MCULE-3098689138_1

MolLogP: 5.077000000000003 | QED: 0.3514266685198548

c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)CCc4c[nH]c5c4cccc5

ORD-MCULE-3593629191_1

15

MolLogP: 5.621300000000006 | QED: 0.20107182839149487

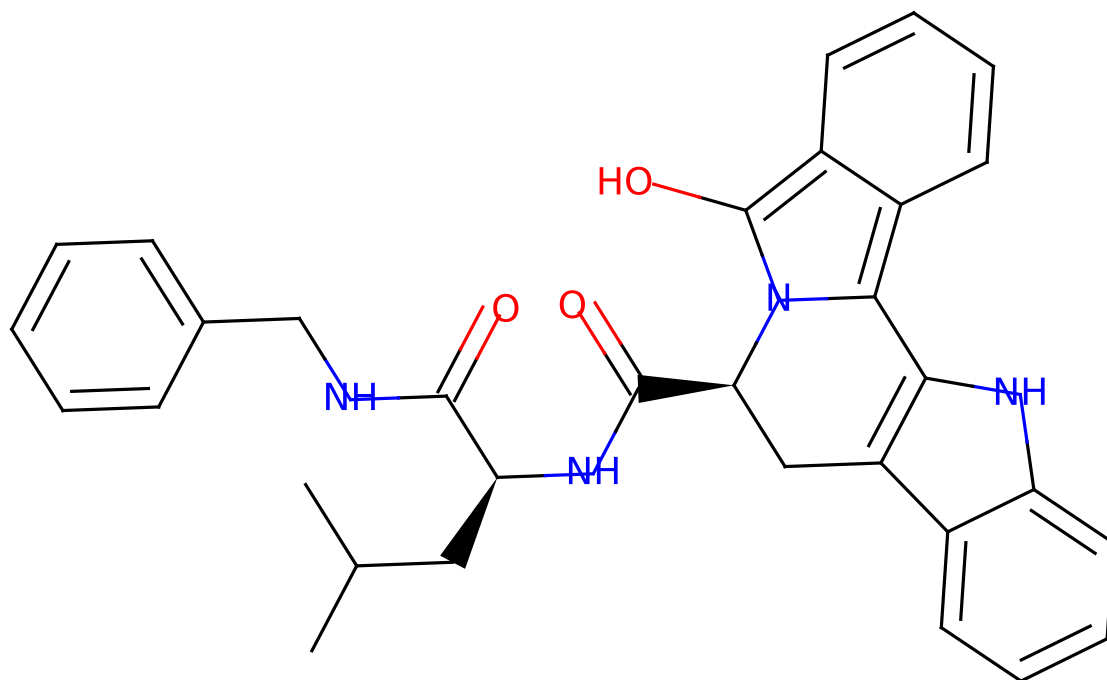CC(C)C[C@@H](C(=O)NCCc1cccc(c1)F)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O

ORD-MCULE-9212942515_1

MolLogP: 2.5399000000000007 | QED: 0.6082699718104049
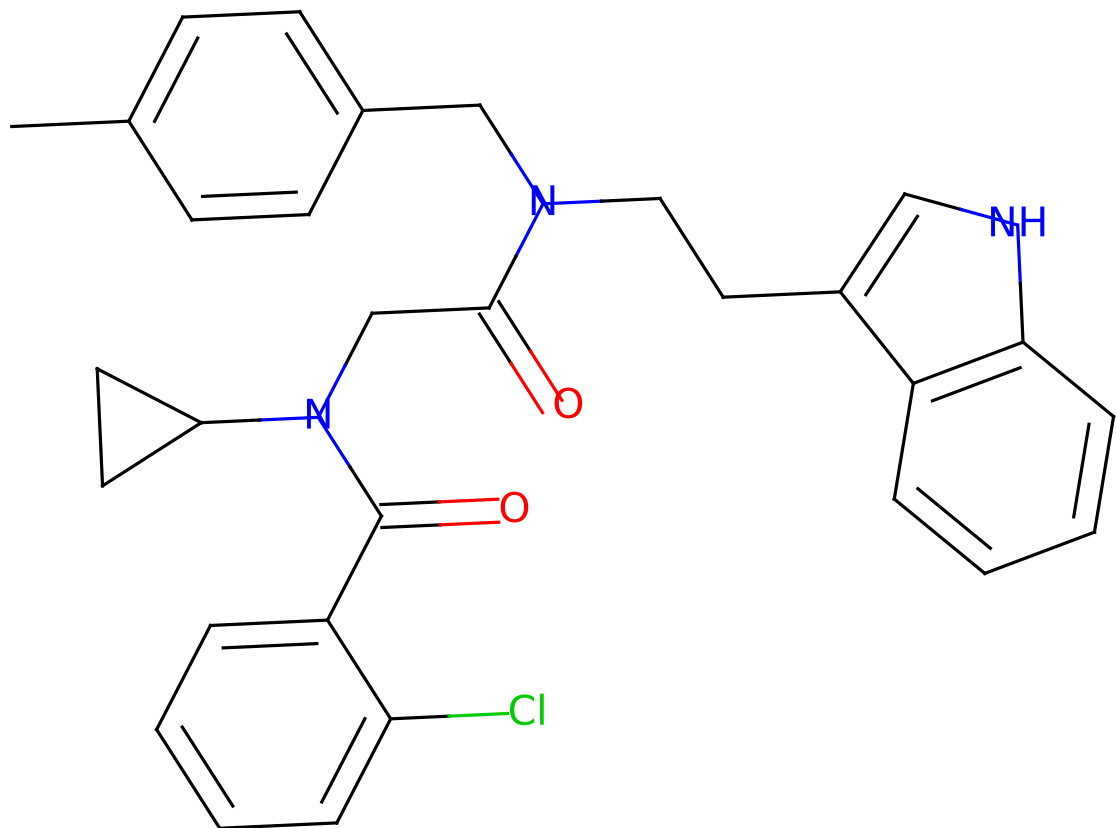
c1ccc(c(c1)c2nc[nH]n2)C(=O)NCCCc3ccc(cc3)O

ORD-MCULE-8568450548_2

17

MolLogP: 5.439700000000005 | QED: 0.22997913326523065

CC(C)C[C@@H](C(=O)NCc1ccccc1)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O
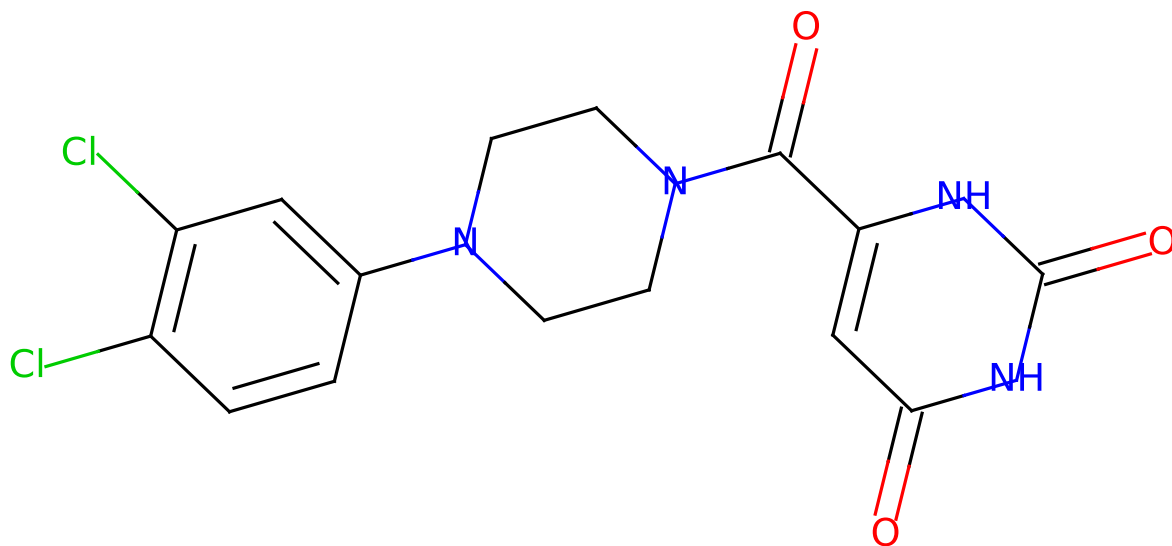
ORD-MCULE-1429565079_1

18

MolLogP: 6.005820000000006 | QED: 0.3065717951069043

Cc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)CN(C4CC4)C(=O)c5ccccc5Cl
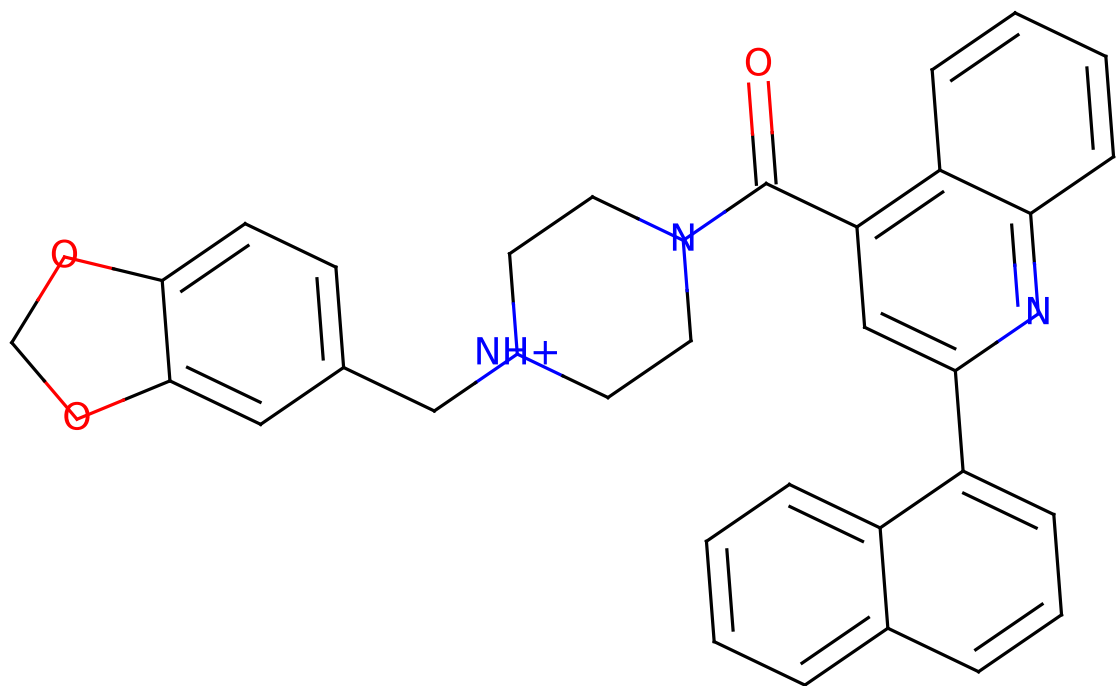
ORD-MCULE-9466928660_1

19

MolLogP: 1.3323999999999998 | QED: 0.8361136071388907

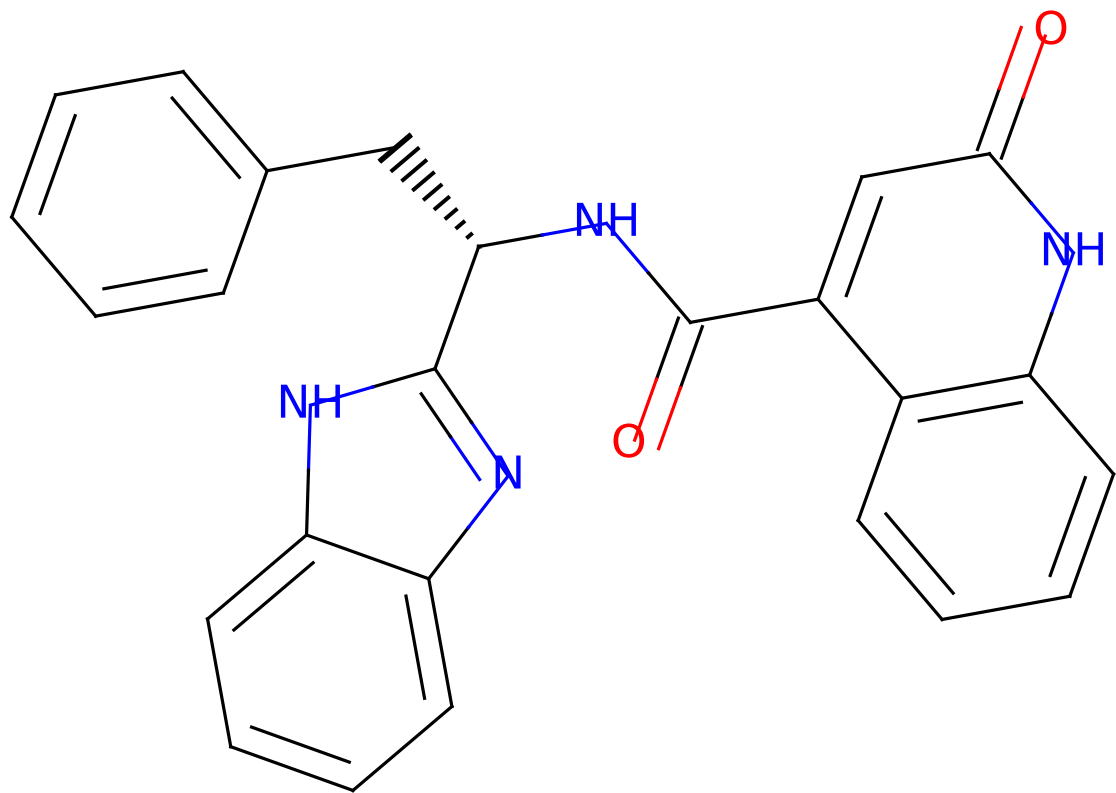c1cc(c(cc1N2CCN(CC2)C(=O)c3cc(=O)[nH]c(=O)[nH]3)Cl)Cl

ORD-MCULE-5948770040_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

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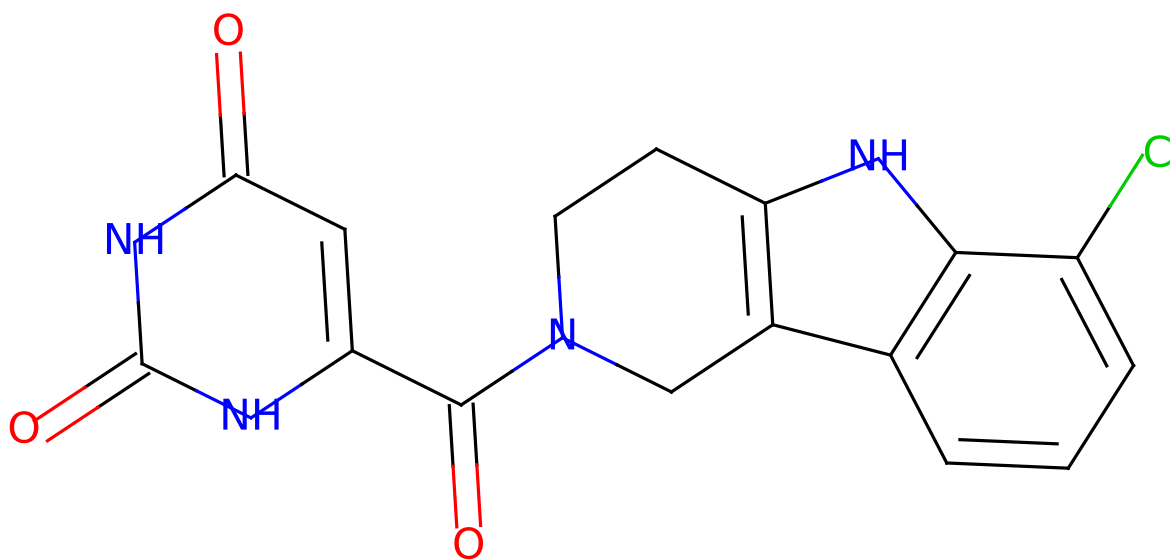
ORD-MCULE-3696478799_1

21

MolLogP: 4.118200000000002 | QED: 0.4085896962540062

c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4cc(=O)[nH]c5c4cccc5
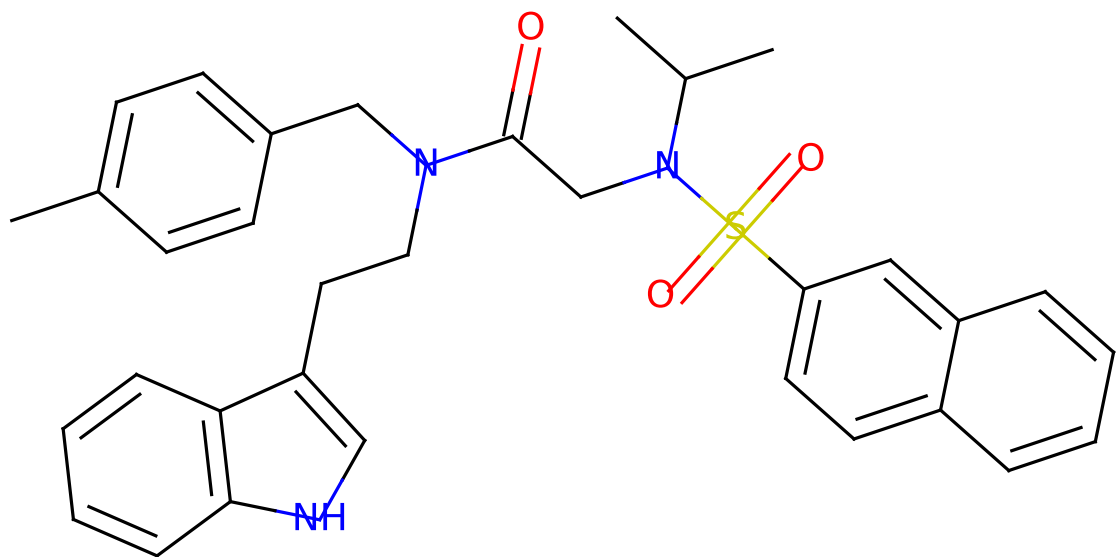
ORD-MCULE-2354836978_1

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

23

MolLogP: 1.3963999999999992 | QED: 0.6214150570244427

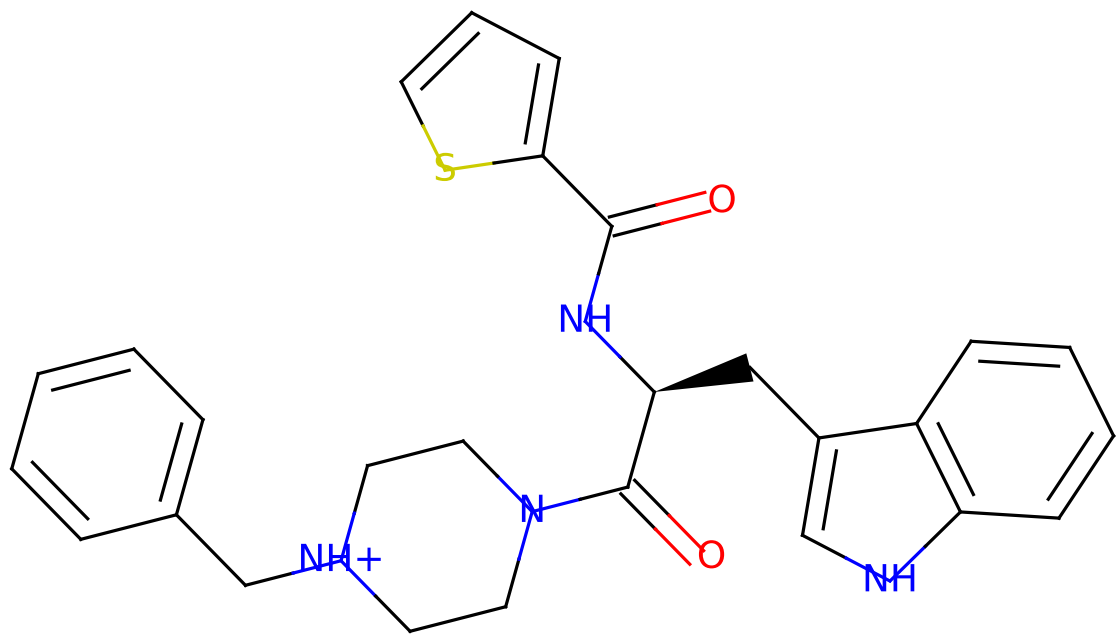c1cc2c3c([nH]c2c(c1)Cl)CCN(C3)C(=O)c4cc(=O)[nH]c(=O)[nH]4

ORD-MCULE-8437712869_1

MolLogP: 6.300120000000007 | QED: 0.2205978344284386

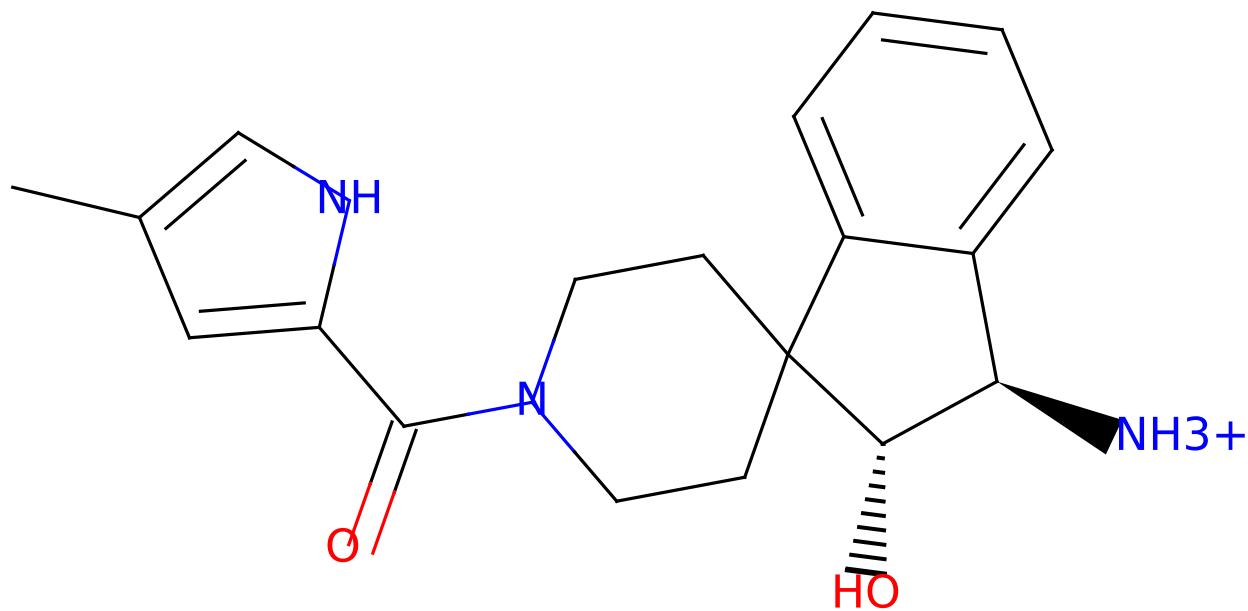Cc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)C[N@@](C(C)C)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-8798249417_1

MolLogP: 2.4978000000000016 | QED: 0.386099483933206

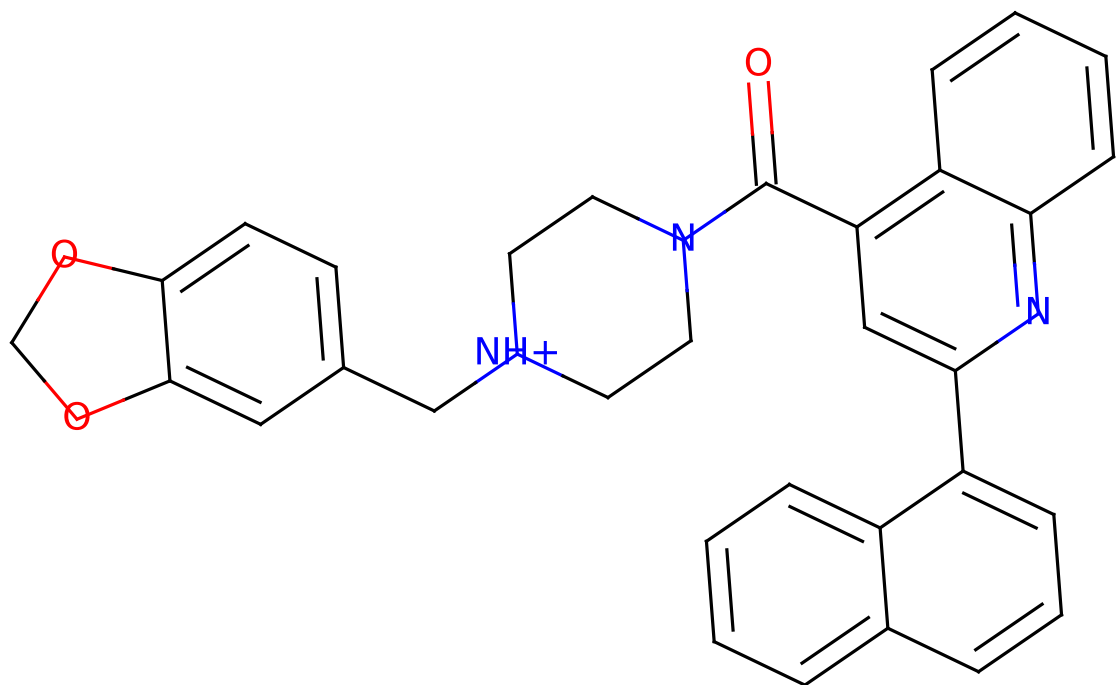c1ccc(cc1)C[NH+]2CCN(CC2)C(=O)[C@H](Cc3c[nH]c4c3cccc4)NC(=O)c5cccs5

ORD-MCULE-1316421825_1

MolLogP: 1.1546199999999995 | QED: 0.7344909610737468

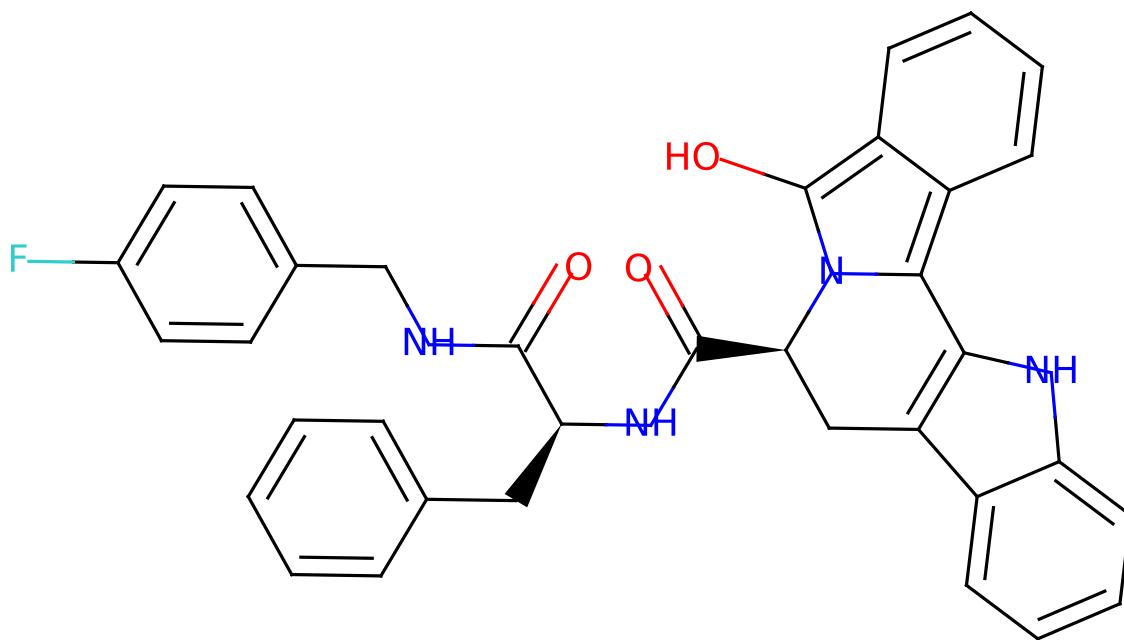Cc1cc([nH]c1)C(=O)N2CCC3(CC2)c4ccccc4[C@H]([C@@H]3O)[NH3+]

ORD-MCULE-8962808574_1

MolLogP: 4.324600000000004 | QED: 0.3977358166273845

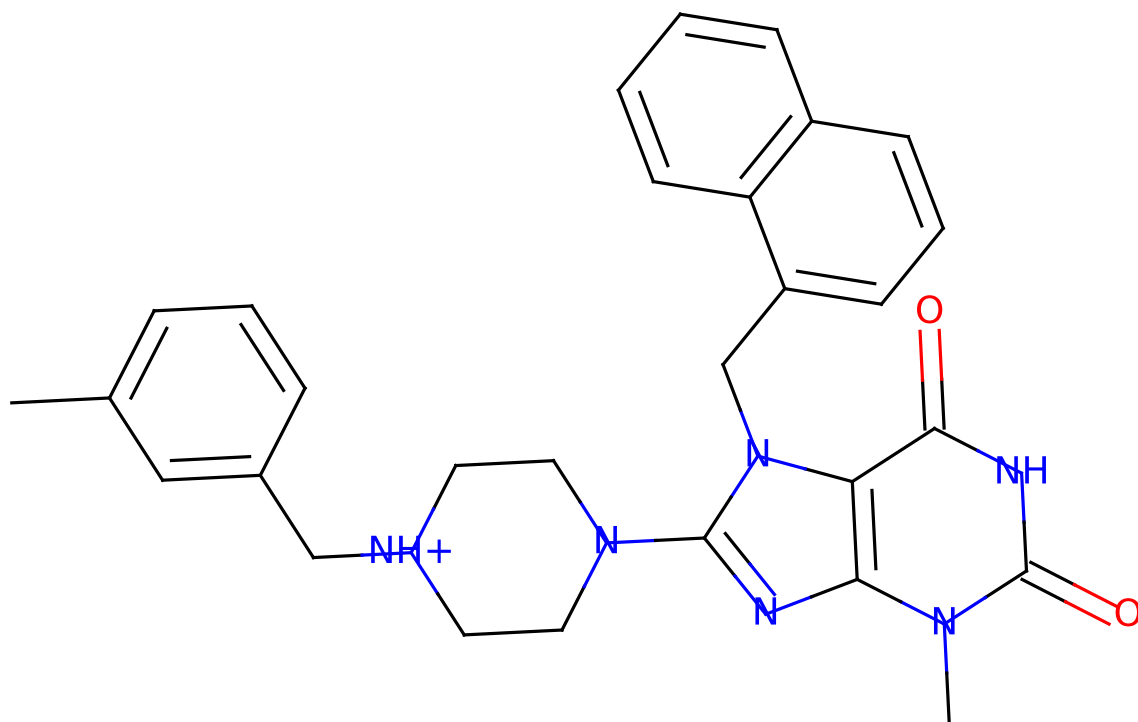c1ccc2c(c1)cccc2c3cc(c4ccccc4n3)C(=O)N5CC[NH+](CC5)Cc6ccc7c(c6)OCO7

ORD-MCULE-4959815000_1

28

MolLogP: 5.775400000000006 | QED: 0.19535260854802458

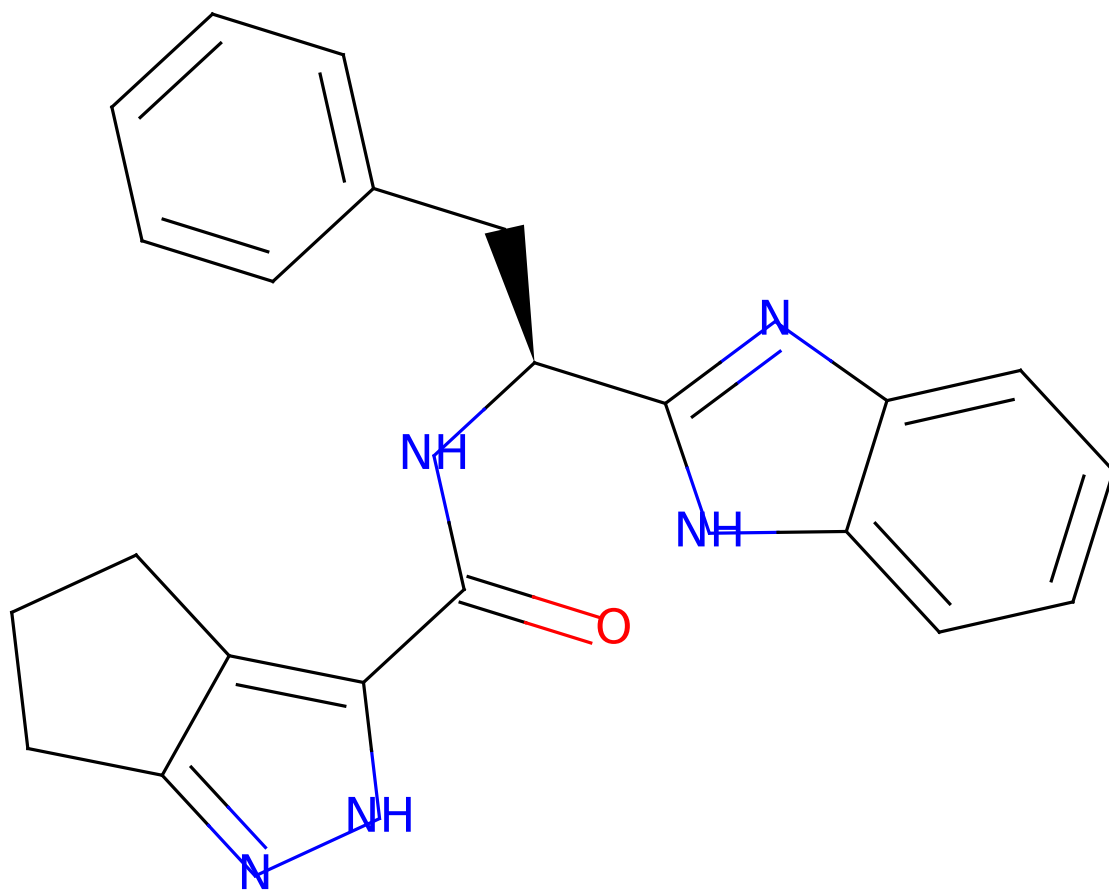c1ccc(cc1)C[C@@H](C(=O)NCc2ccc(cc2)F)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-6477680903_1

MolLogP: 1.8383199999999995 | QED: 0.3900645932426038

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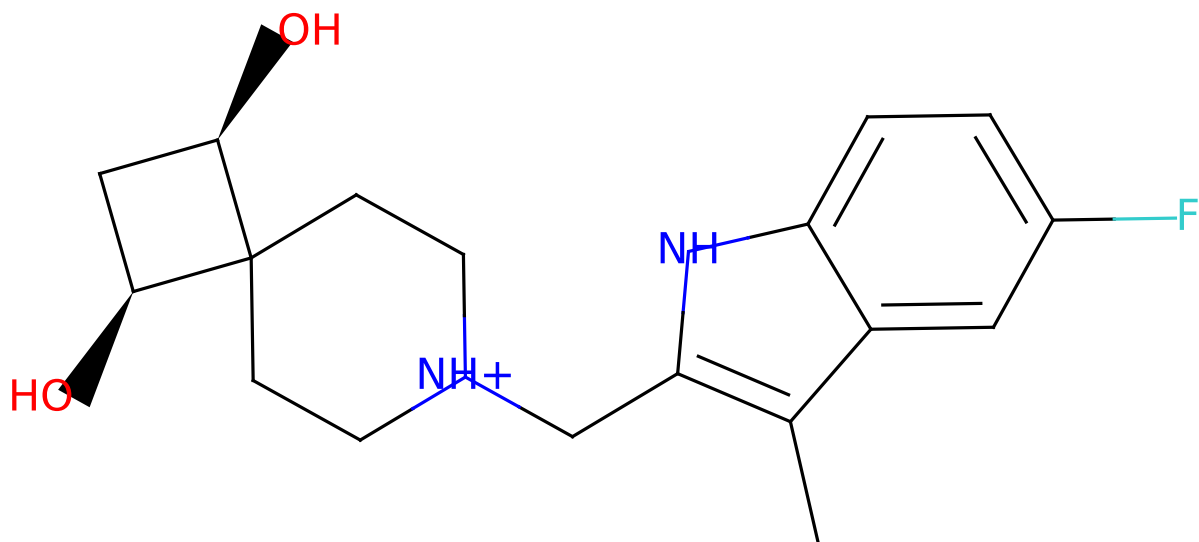
ORD-MCULE-9311937068_1

MolLogP: 3.488500000000001 | QED: 0.5018558408043431

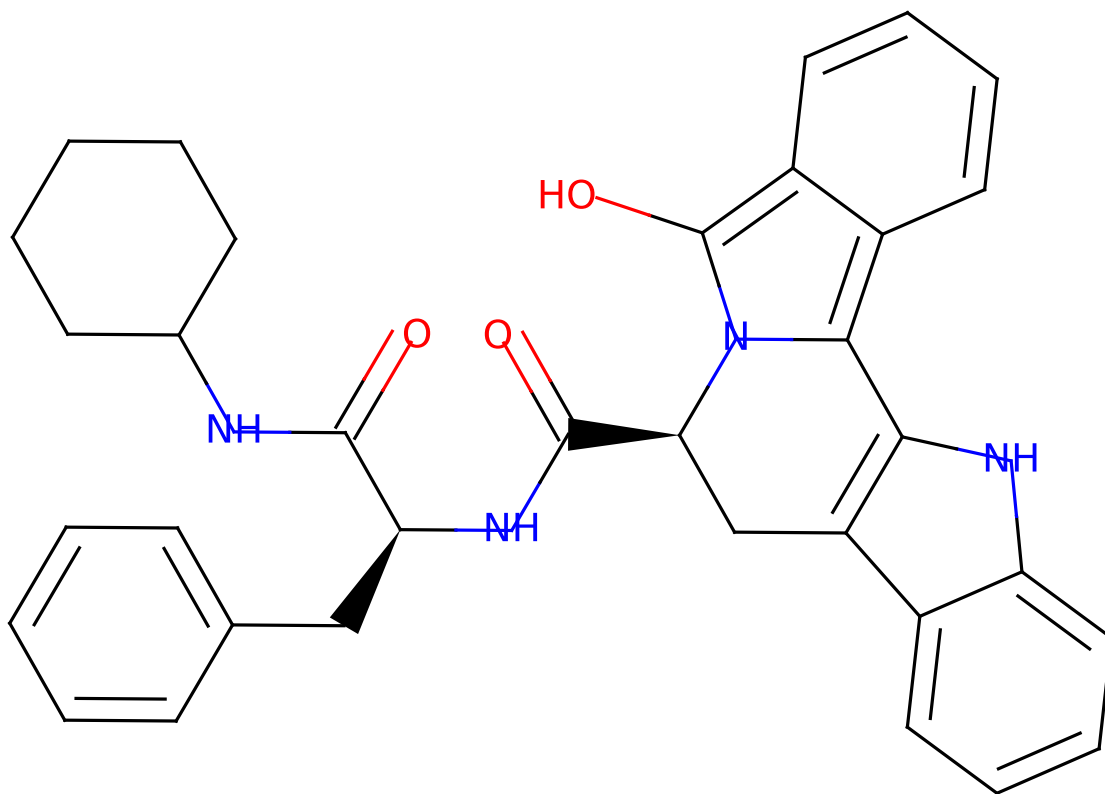c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4c5c(n[nH]4)CCC5

ORD-MCULE-3980688822_2

MolLogP: 0.9060199999999996 | QED: 0.6648399620688924

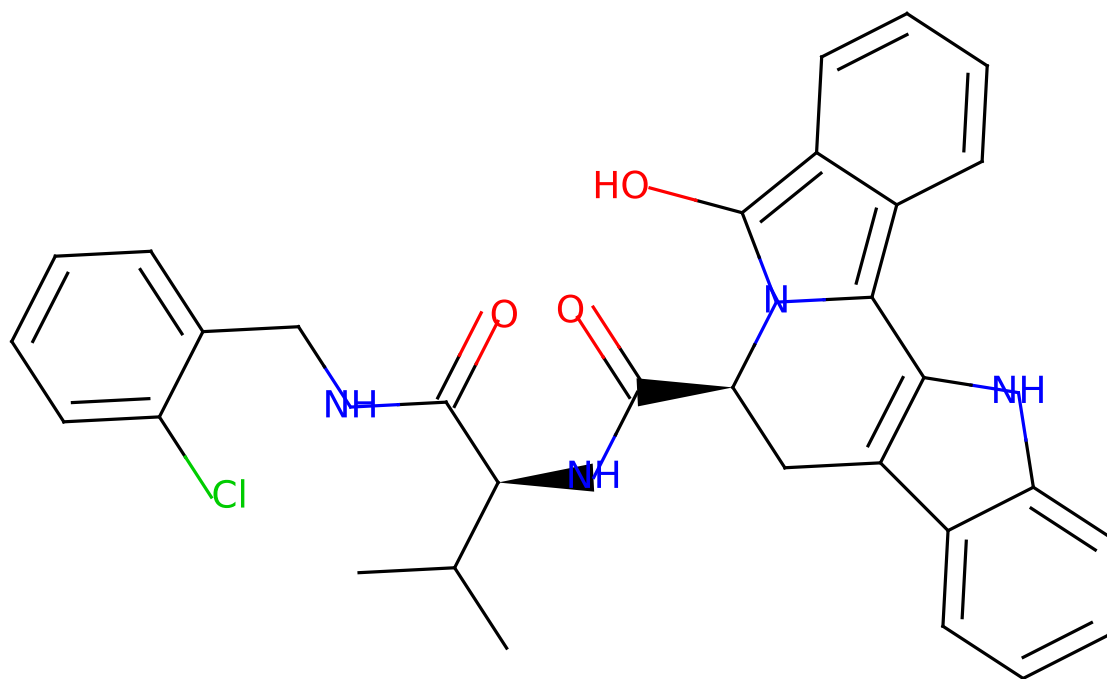Cc1c2cc(ccc2[nH]c1C[NH+]3CCC4(CC3)[C@@H](C[C@@H]4O)O)F

ORD-MCULE-6381989453_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
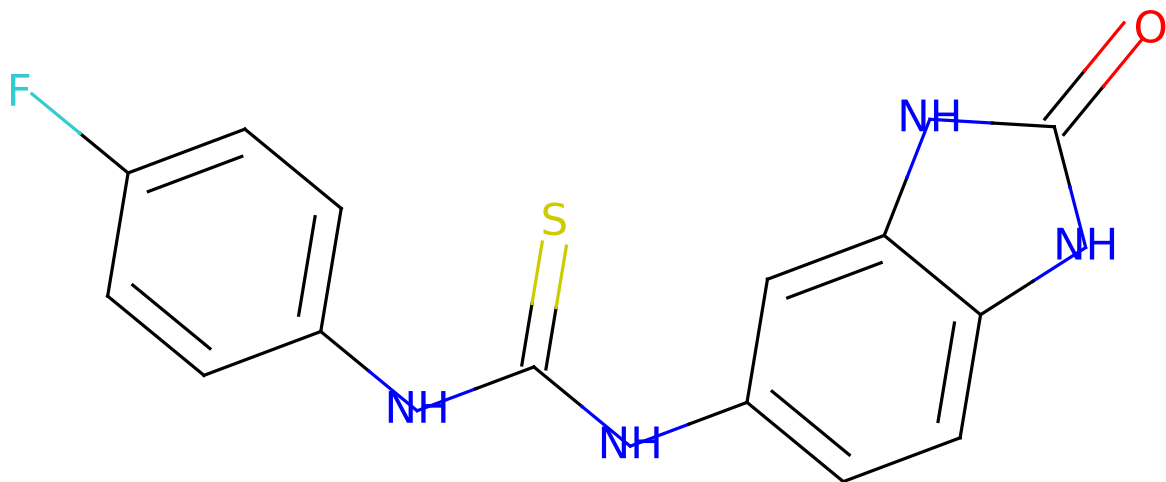
ORD-MCULE-9395623979_1

MolLogP: 5.7030000000000065 | QED: 0.22209215464218618

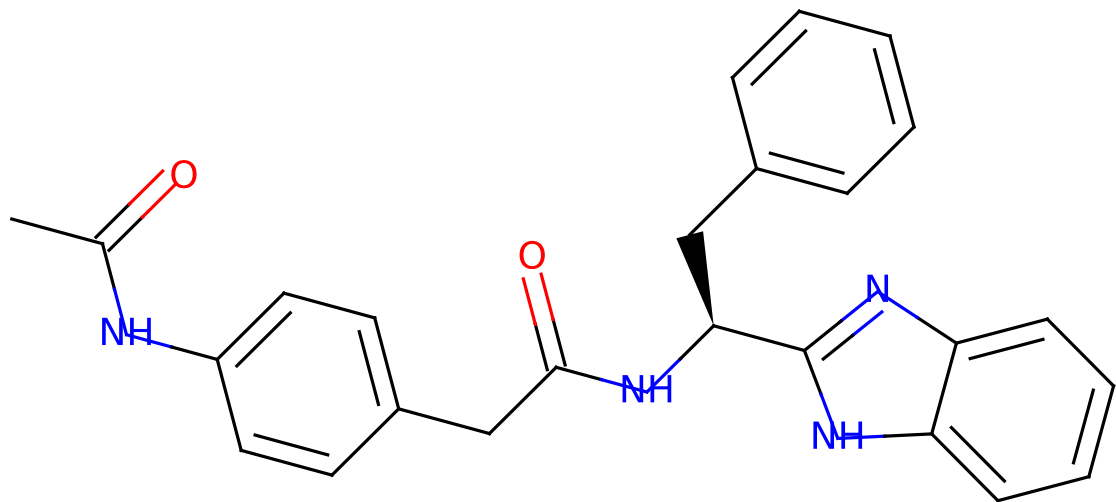CC(C)[C@@H](C(=O)NCc1ccccc1Cl)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O

ORD-MCULE-3474145980_1

MolLogP: 2.8042 | QED: 0.5493193398397668

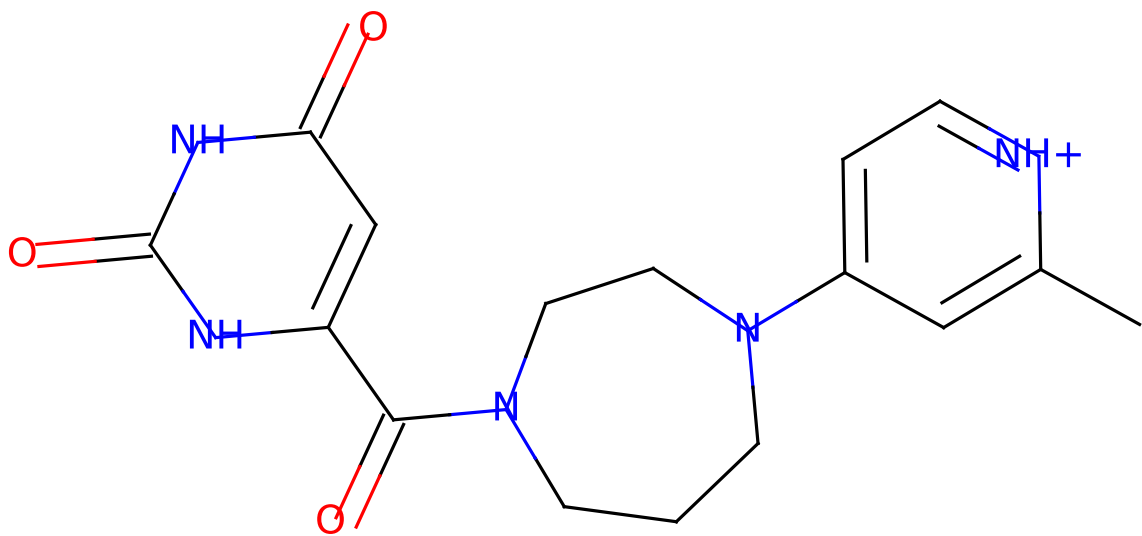c1cc(ccc1NC(=S)Nc2ccc3c(c2)[nH]c(=O)[nH]3)F

ORD-MCULE-1797511267_1

MolLogP: 4.164000000000002 | QED: 0.42587160458676115

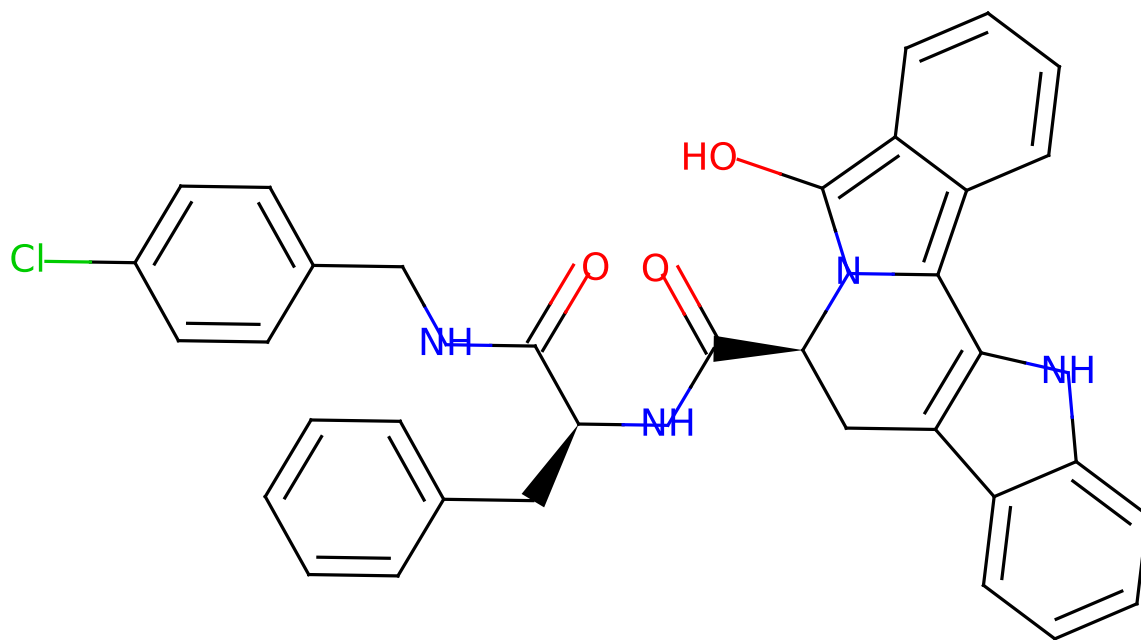CC(=O)Nc1ccc(cc1)CC(=O)N[C@@H](Cc2ccccc2)c3[nH]c4ccccc4n3

ORD-MCULE-9073095150_1

MolLogP: -0.4617799999999987 | QED: 0.7772996204300281

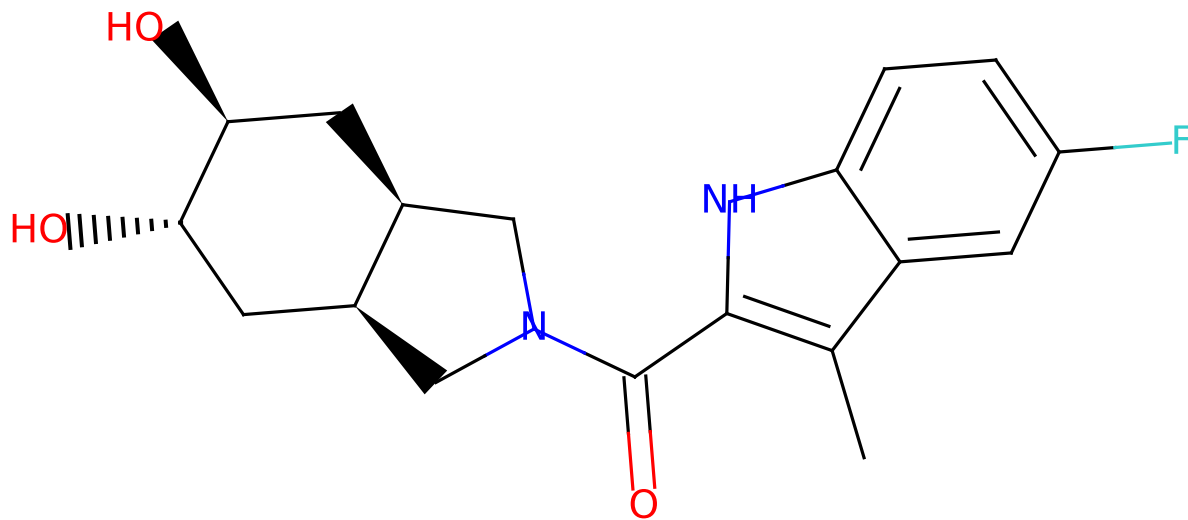Cc1cc(cc[nH+]1)N2CCCN(CC2)C(=O)c3cc(=O)[nH]c(=O)[nH]3

ORD-MCULE-5271818360_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
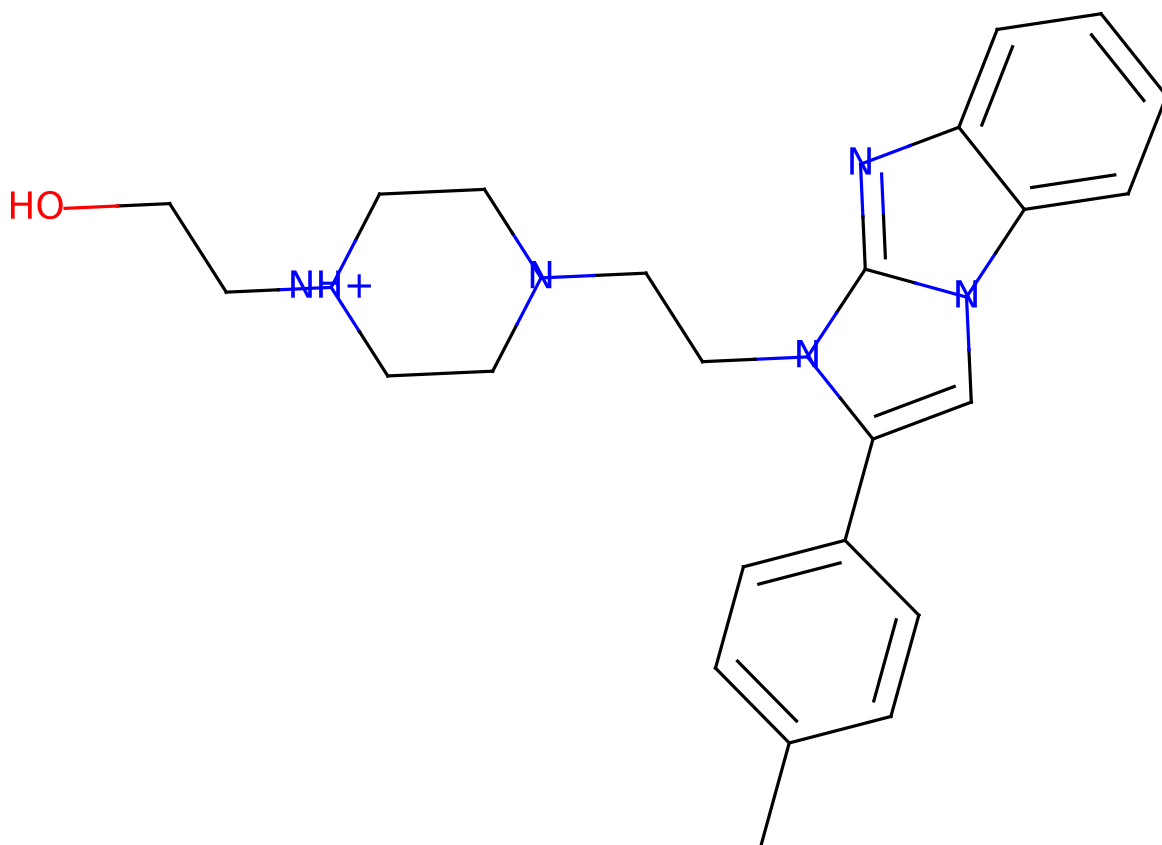
ORD-MCULE-6977725985_1

MolLogP: 1.8192199999999996 | QED: 0.7454546925399498

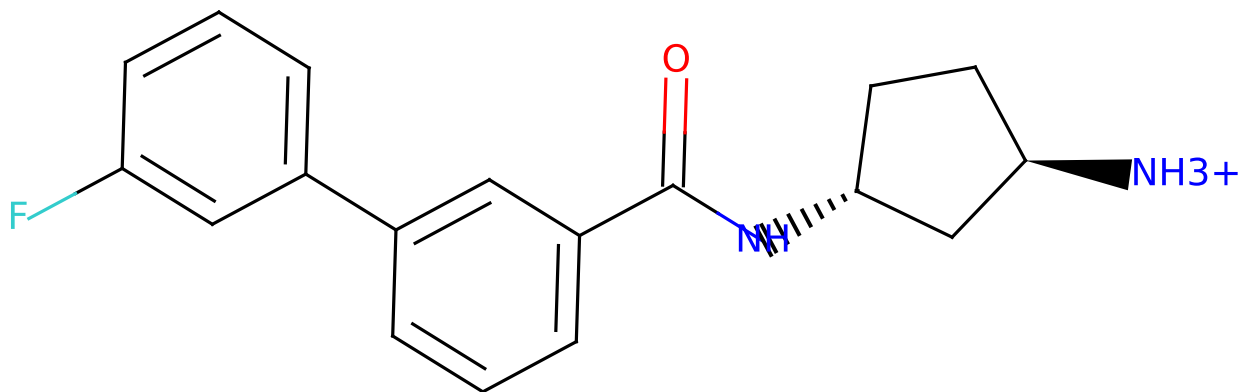Cc1c2cc(ccc2[nH]c1C(=O)N3C[C@H]4C[C@@H]([C@H](C[C@H]4C3)O)O)F

ORD-MCULE-2853315083_1

MolLogP: 1.457219999999999 | QED: 0.5116138122864926
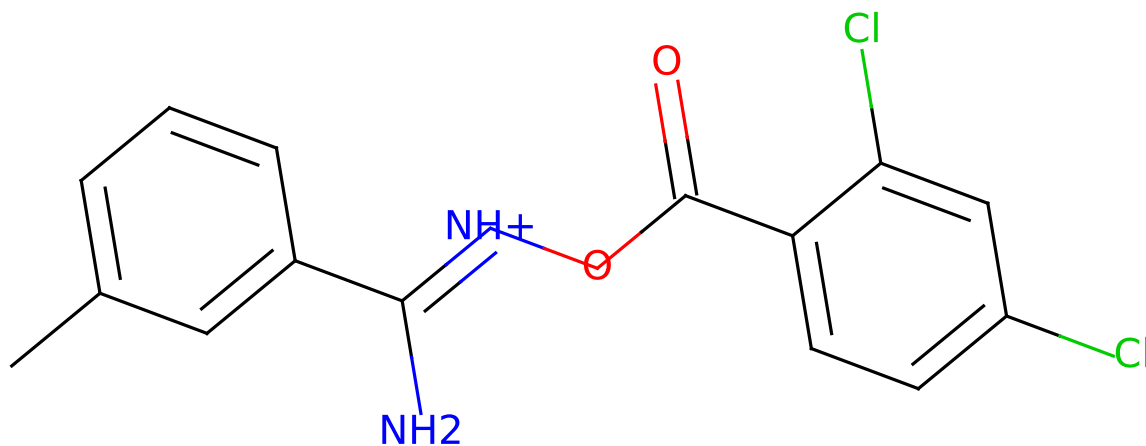
Cc1ccc(cc1)c2cn3c4ccccc4nc3n2CCN5CC[NH+](CC5)CCO

ORD-MCULE-8833230269_1

MolLogP: 2.3854999999999995 | QED: 0.8980472991550998

c1cc(cc(c1)C(=O)N[C@@H]2CC[C@H](C2)[NH3+])c3cccc(c3)F

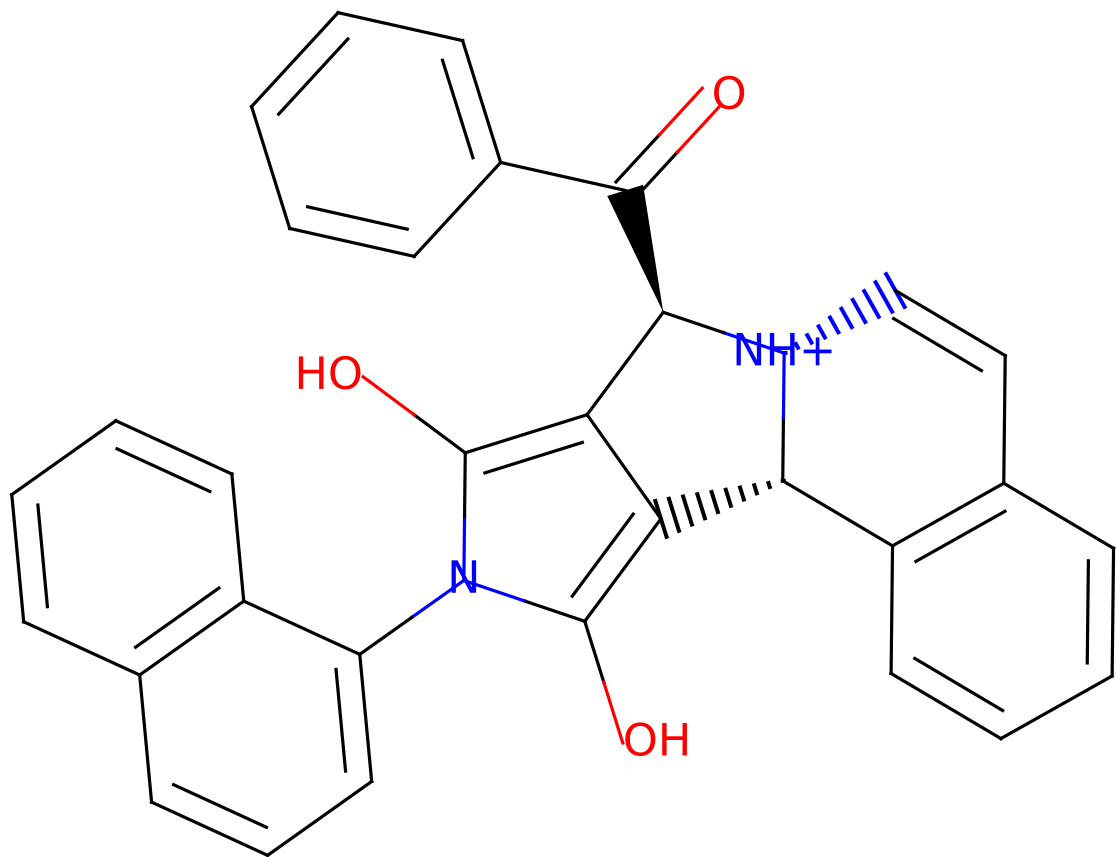ORD-MCULE-6036933641_1

MolLogP: 1.8597199999999996 | QED: 0.3919487272743939

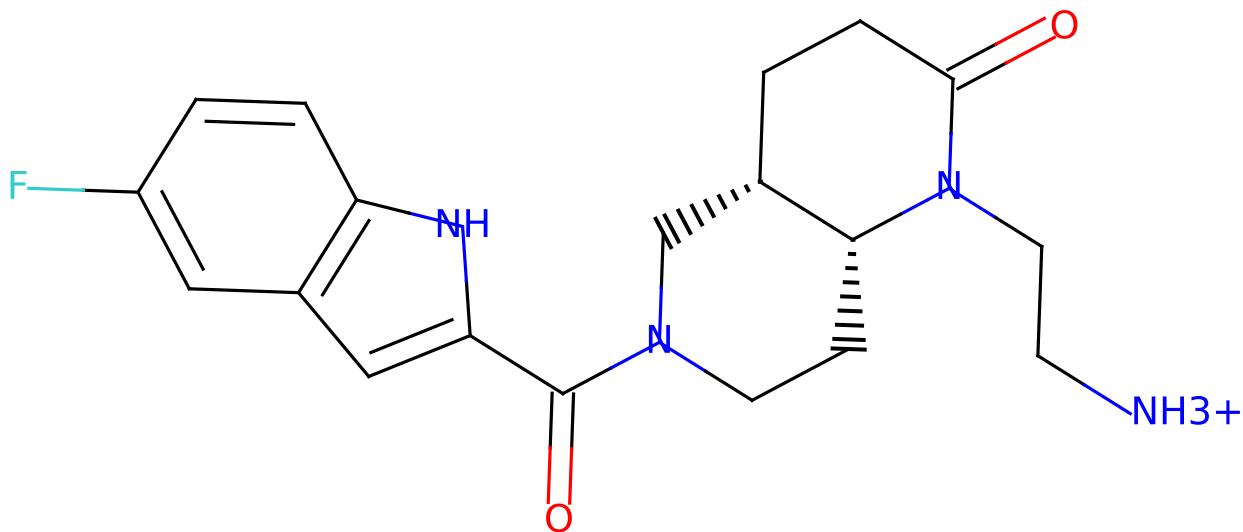Cc1cccc(c1)/C(=[NH+]/OC(=O)c2ccc(cc2Cl)Cl)/N

ORD-MCULE-5145994619_1

MolLogP: 4.937900000000005 | QED: 0.32678562838553826

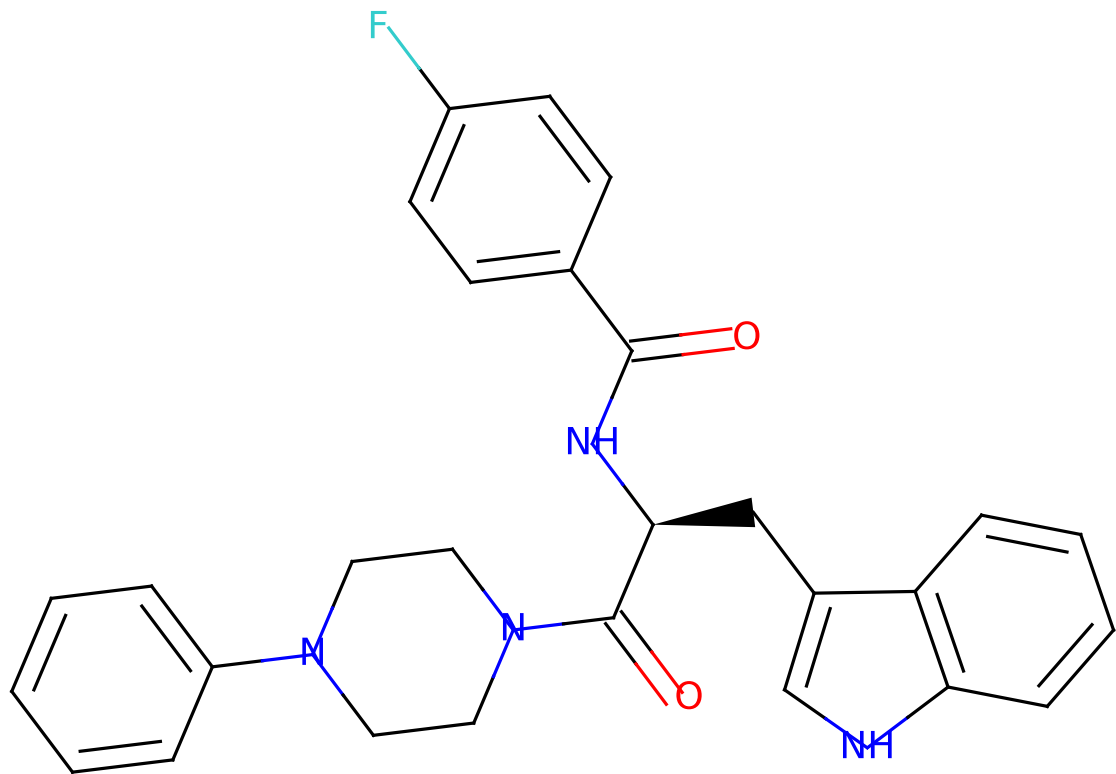c1ccc(cc1)C(=O)[C@@H]2c3c(c(n(c3O)c4cccc5c4cccc5)O)[C@@H]6[N@H+]2C=Cc7c6cccc7

ORD-MCULE-7416131701_1

MolLogP: 1.0020000000000002 | QED: 0.85696777313891

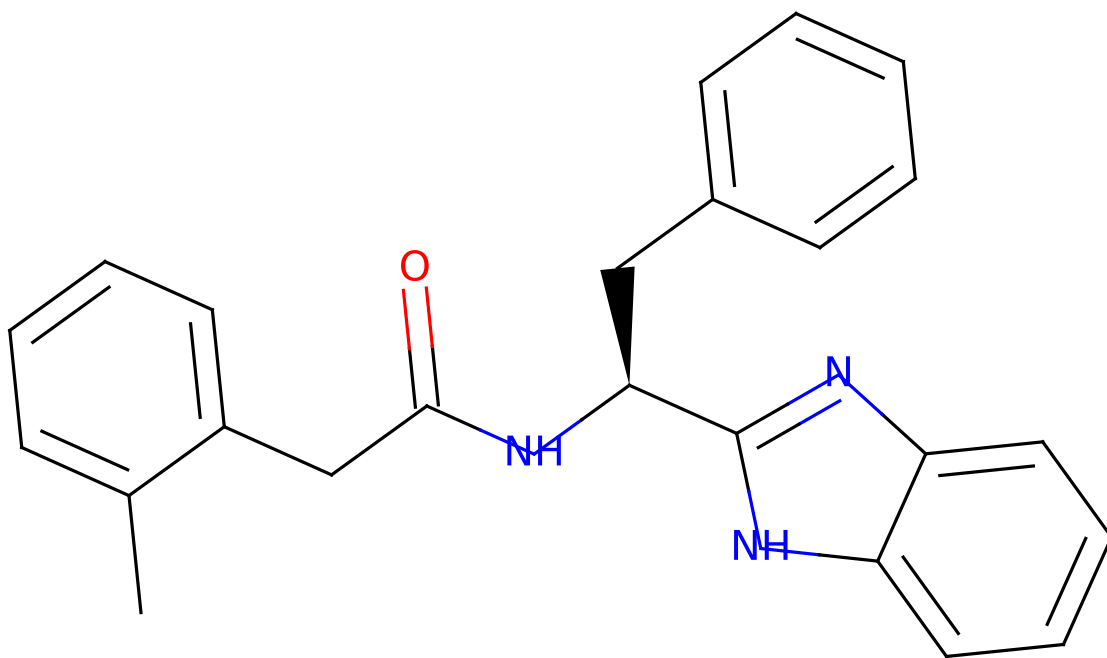c1cc2c(cc1F)cc([nH]2)C(=O)N3CC[C@@H]4[C@H](C3)CCC(=O)N4CC[NH3+]

ORD-MCULE-5223569619_1

MolLogP: 3.996900000000002 | QED: 0.44774588382557573

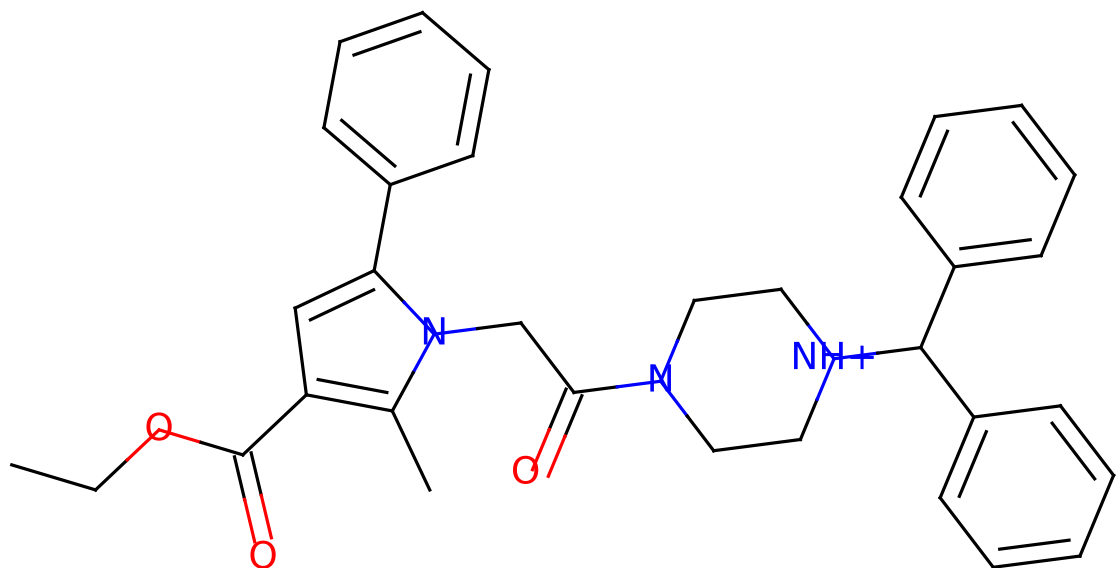c1ccc(cc1)N2CCN(CC2)C(=O)[C@H](Cc3c[nH]c4c3cccc4)NC(=O)c5ccc(cc5)F

ORD-MCULE-1314415937_1

MolLogP: 4.514020000000003 | QED: 0.5251456893780476

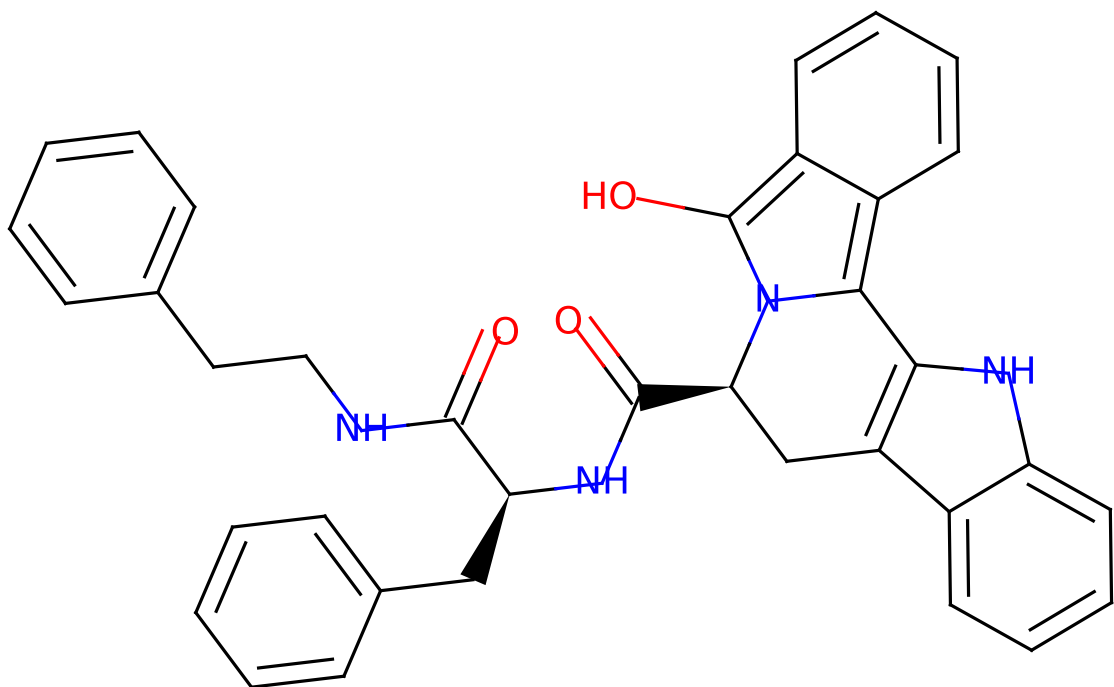Cc1ccccc1CC(=O)N[C@@H](Cc2ccccc2)c3[nH]c4ccccc4n3

ORD-MCULE-2322094178_1

MolLogP: 4.156920000000005 | QED: 0.3538541391422037

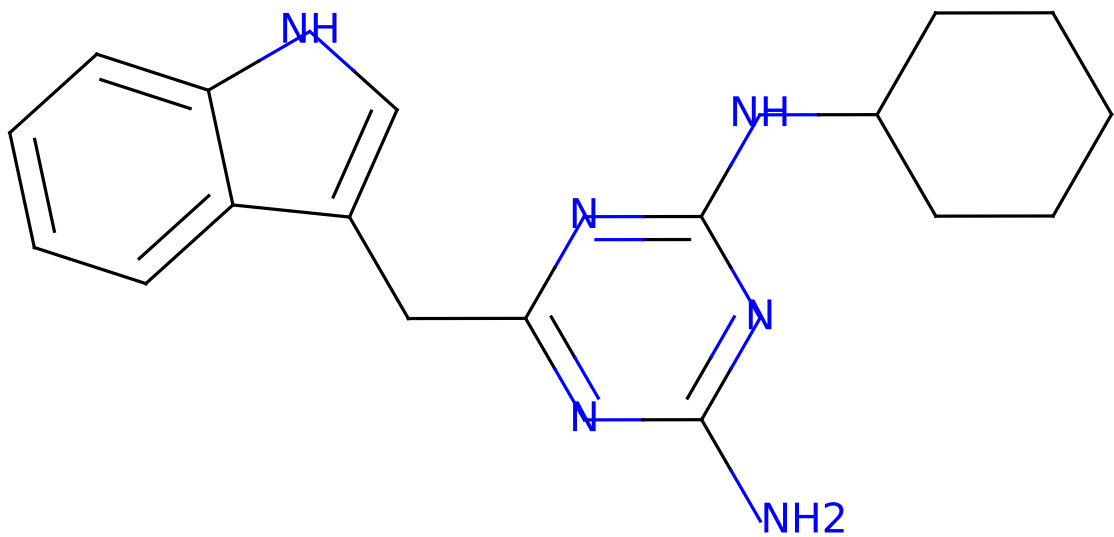CCOC(=O)c1cc(n(c1C)CC(=O)N2CC[NH+](CC2)C(c3ccccc3)c4ccccc4)c5ccccc5

ORD-MCULE-1955508051_1

MolLogP: 5.678800000000005 | QED: 0.1901898602150378

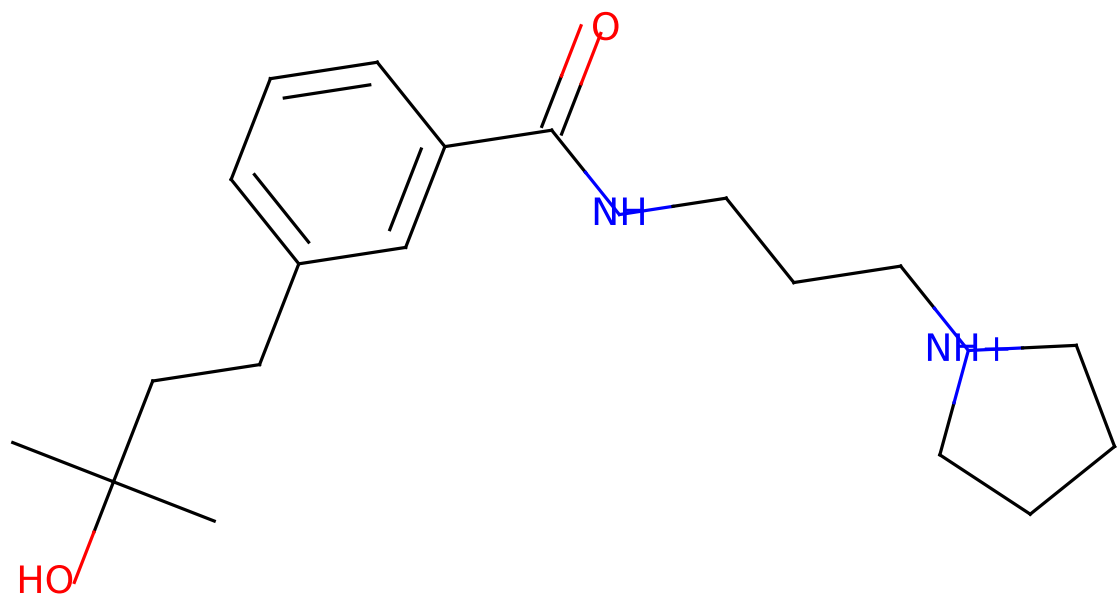c1ccc(cc1)CCNC(=O)[C@H](Cc2ccccc2)NC(=O)[C@@H]3Cc4c5ccccc5[nH]c4-c6n3c(c7c6cccc7)O

ORD-MCULE-1662960575_1

MolLogP: 3.2705 | QED: 0.6853336260666155
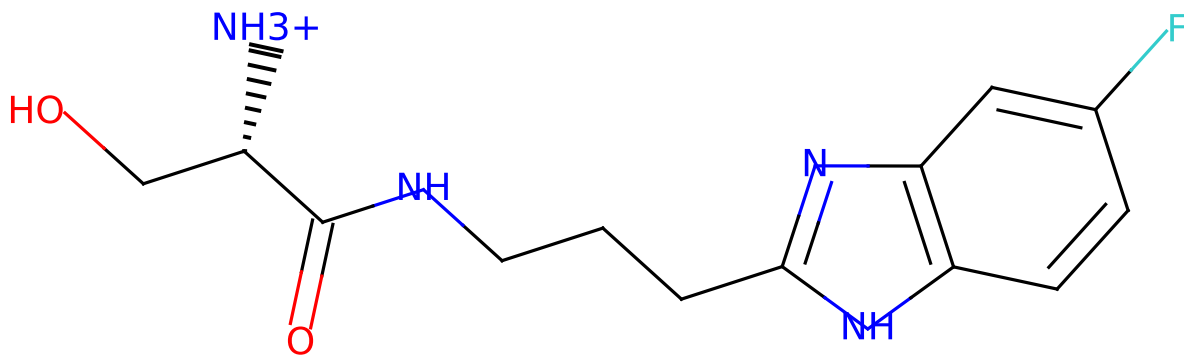
c1ccc2c(c1)c(c[nH]2)Cc3nc(nc(n3)NC4CCCCC4)N

ORD-MCULE-6998567671_1

MolLogP: 1.1887 | QED: 0.6305650027117164

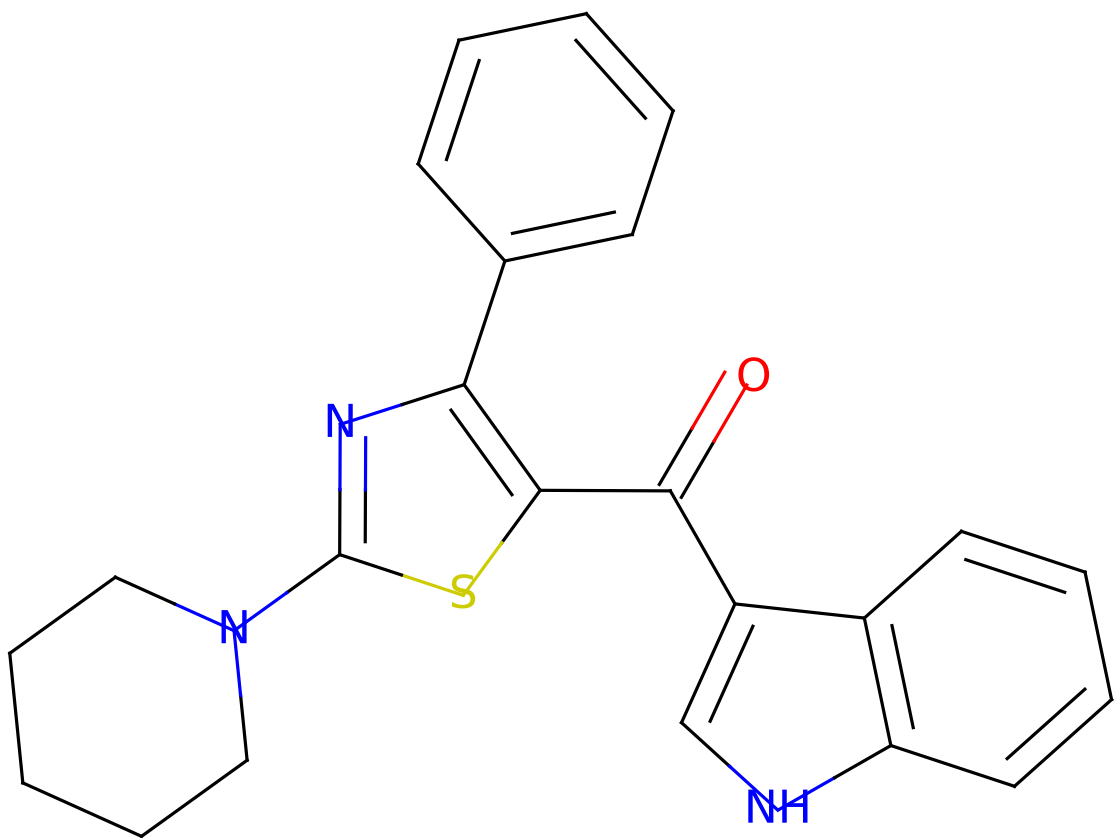CC(C)(CCc1cccc(c1)C(=O)NCCC[NH+]2CCCC2)O

ORD-MCULE-3927034065_1

MolLogP: -0.6463999999999992 | QED: 0.5288104160101527

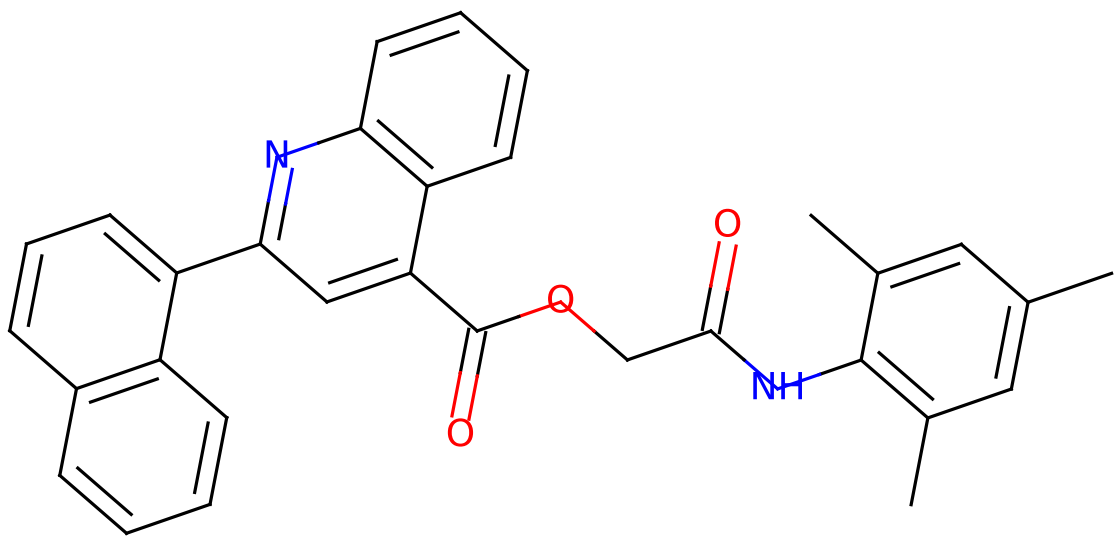c1cc2c(cc1F)nc([nH]2)CCCNC(=O)[C@H](CO)[NH3+]

ORD-MCULE-2168809409_2

MolLogP: 5.512700000000004 | QED: 0.46961092394706994

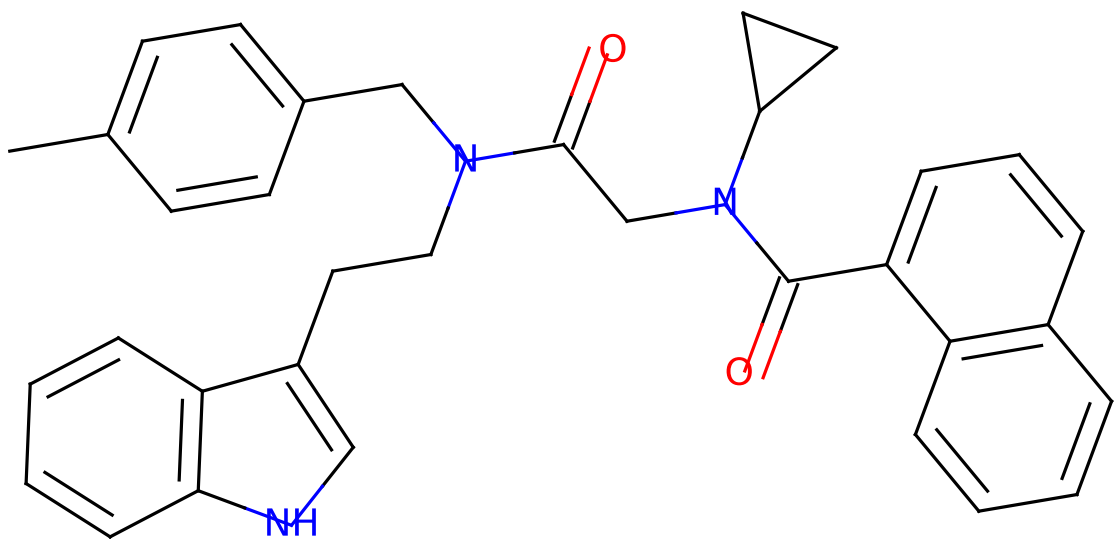c1ccc(cc1)c2c(sc(n2)N3CCCCC3)C(=O)c4c[nH]c5c4cccc5

ORD-MCULE-2310276978_1

MolLogP: 6.775760000000005 | QED: 0.28530611753059815

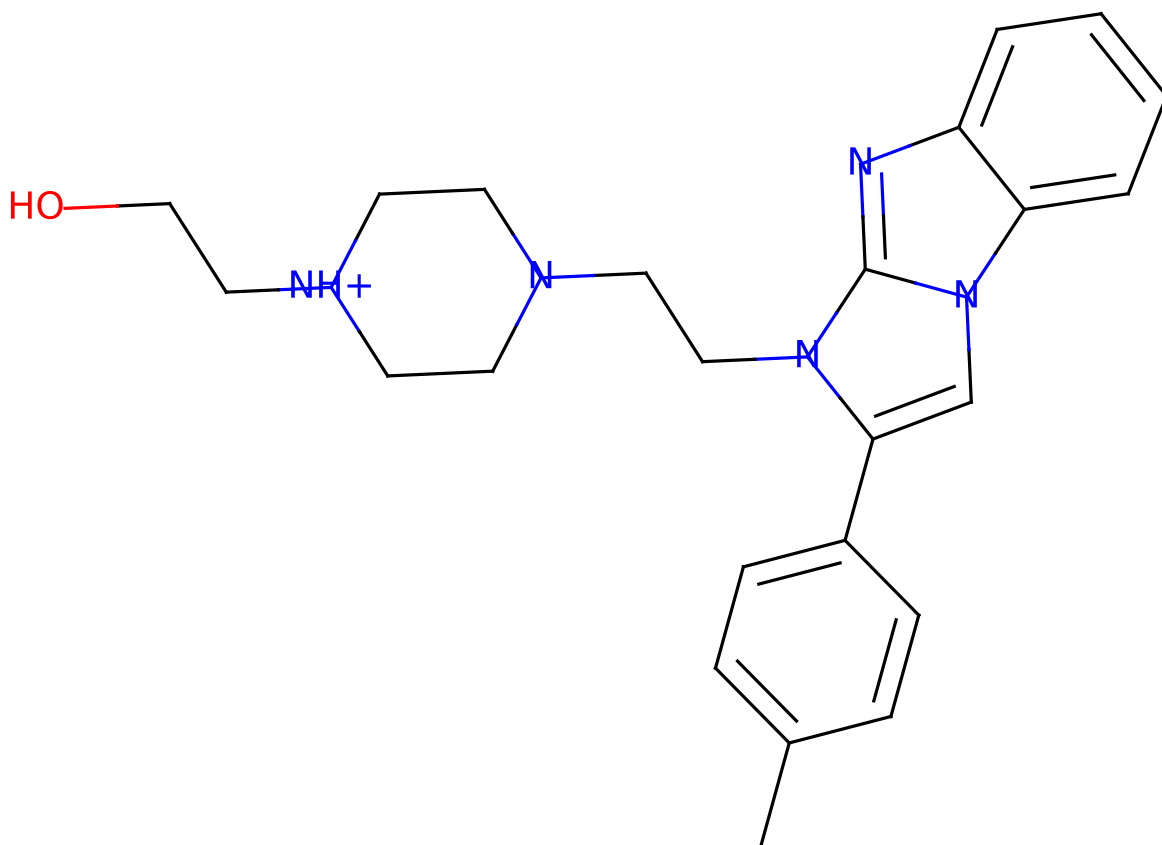Cc1cc(c(c(c1)C)NC(=O)COC(=O)c2cc(nc3c2cccc3)c4cccc5c4cccc5)C

ORD-MCULE-2281744958_1

53

MolLogP: 6.505620000000007 | QED: 0.2434419591344794

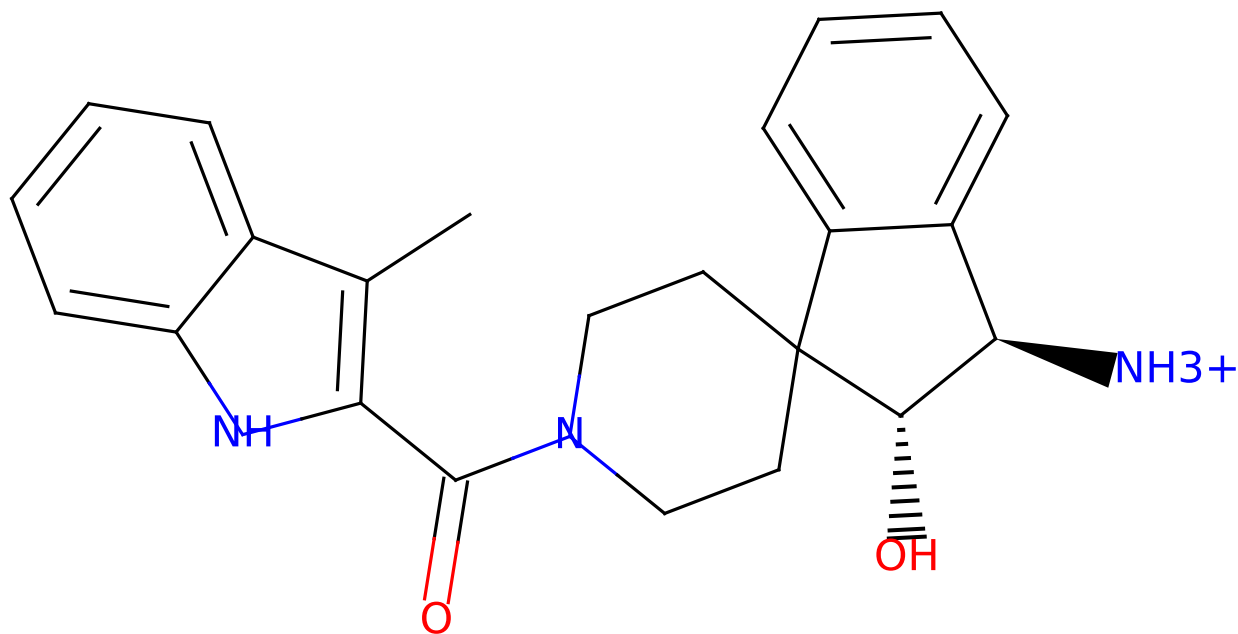Cc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)CN(C4CC4)C(=O)c5cccc6c5cccc6

ORD-MCULE-2519953694_1

MolLogP: 1.457219999999999 | QED: 0.5116138122864926
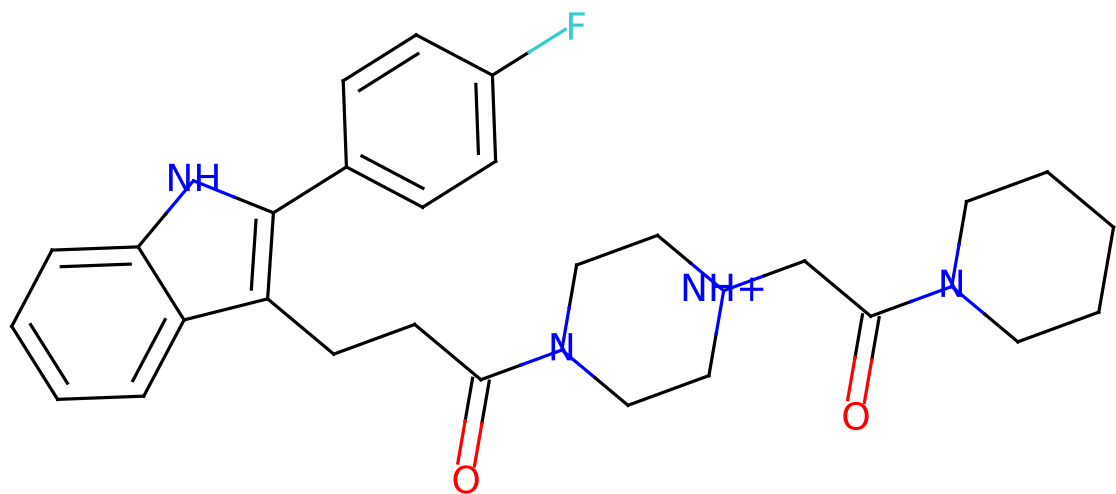
Cc1ccc(cc1)c2cn3c4ccccc4nc3n2CCN5CC[NH+](CC5)CCO

ORD-MCULE-1979616796_1

MolLogP: 2.307819999999999 | QED: 0.6088973921864737

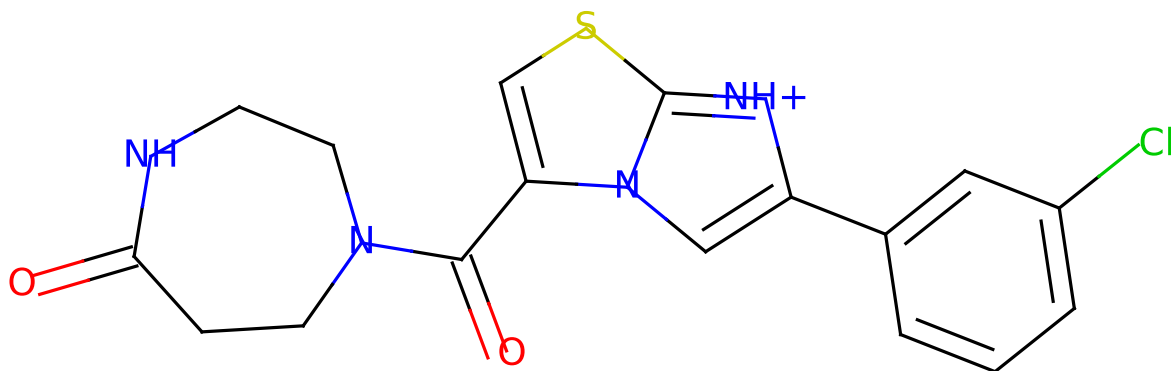Cc1c2ccccc2[nH]c1C(=O)N3CCC4(CC3)c5ccccc5[C@H]([C@@H]4O)[NH3+]

ORD-MCULE-6516517118_1

MolLogP: 2.6462000000000003 | QED: 0.5736027253089309

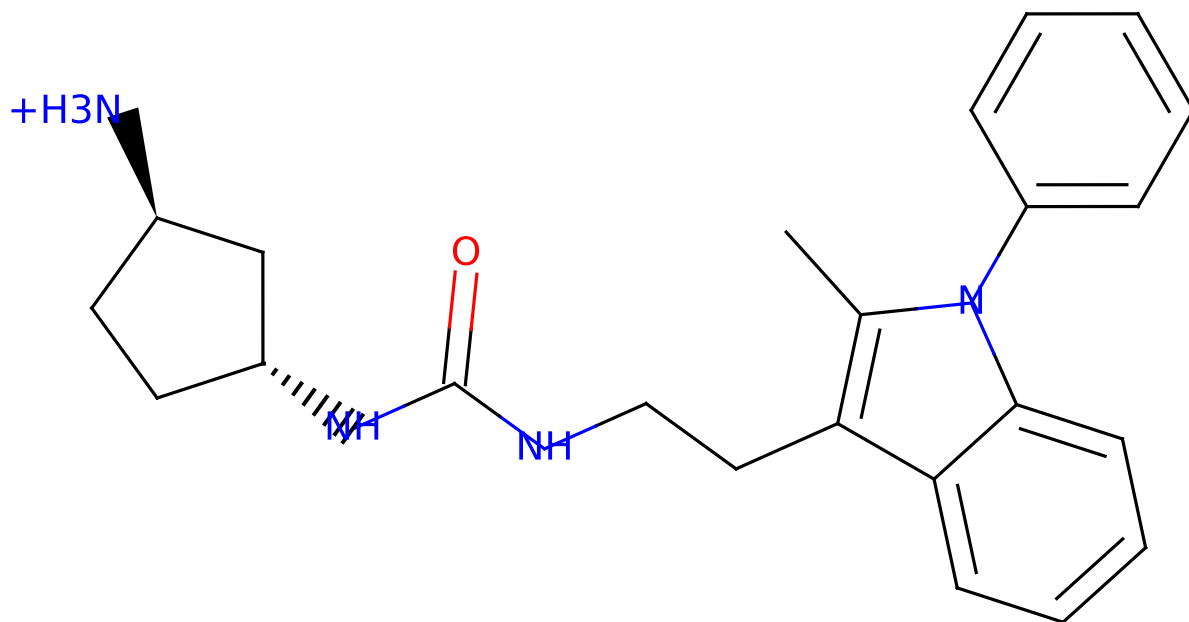c1ccc2c(c1)c(c([nH]2)c3ccc(cc3)F)CCC(=O)N4CC[NH+](CC4)CC(=O)N5CCCCC5

ORD-MCULE-6805927393_1

MolLogP: 2.0974000000000004 | QED: 0.7448757747391636
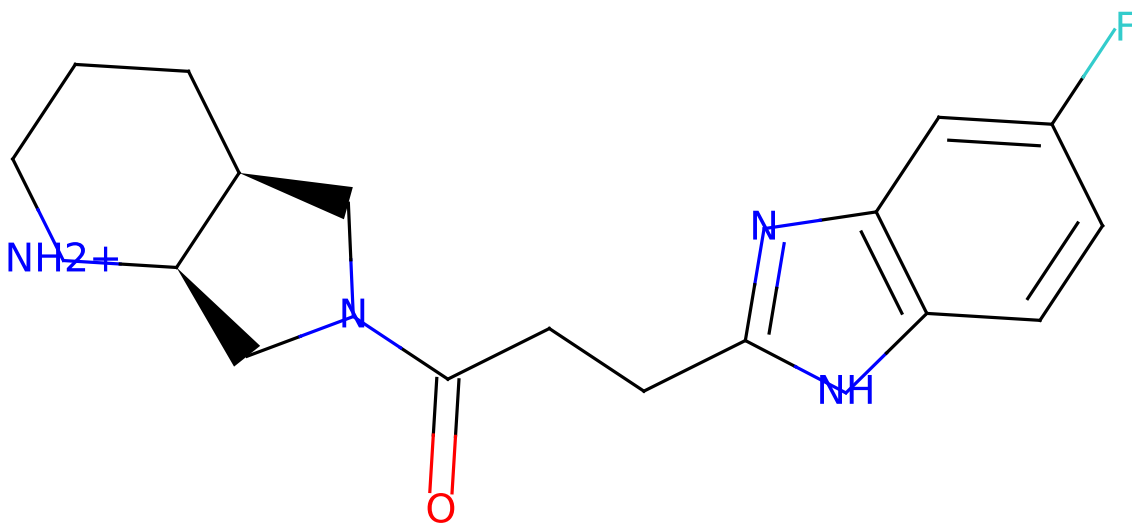
c1cc(cc(c1)Cl)c2cn3c(csc3[nH+]2)C(=O)N4CCC(=O)NCC4

ORD-MCULE-5189722048_1

MolLogP: 2.94362 | QED: 0.6283459342713494

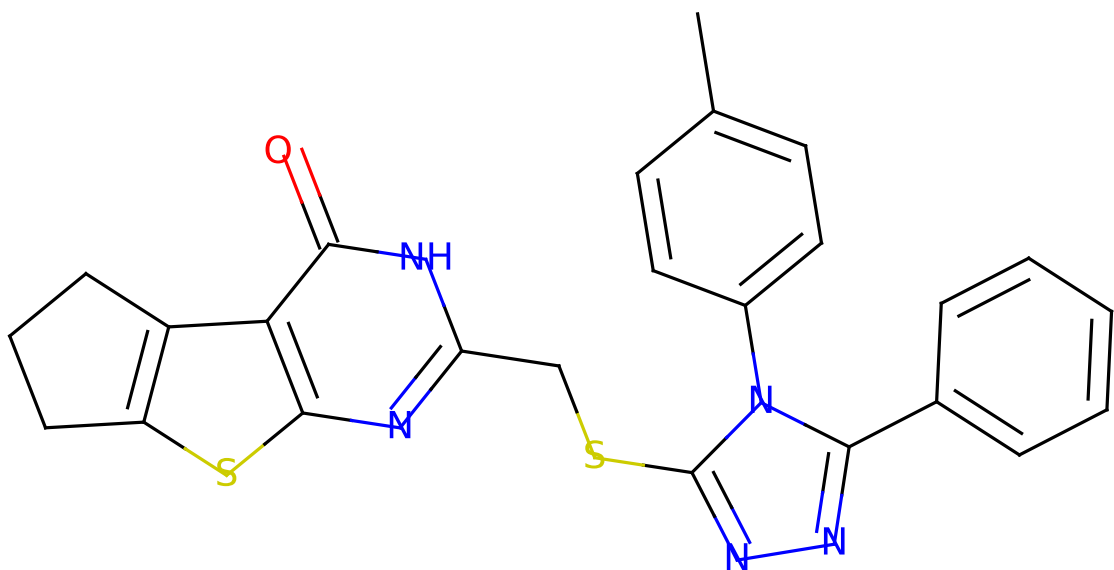Cc1c(c2ccccc2n1c3ccccc3)CCNC(=O)N[C@@H]4CC[C@H](C4)[NH3+]

ORD-MCULE-8224909414_1

MolLogP: 0.8188000000000001 | QED: 0.8800768463511687

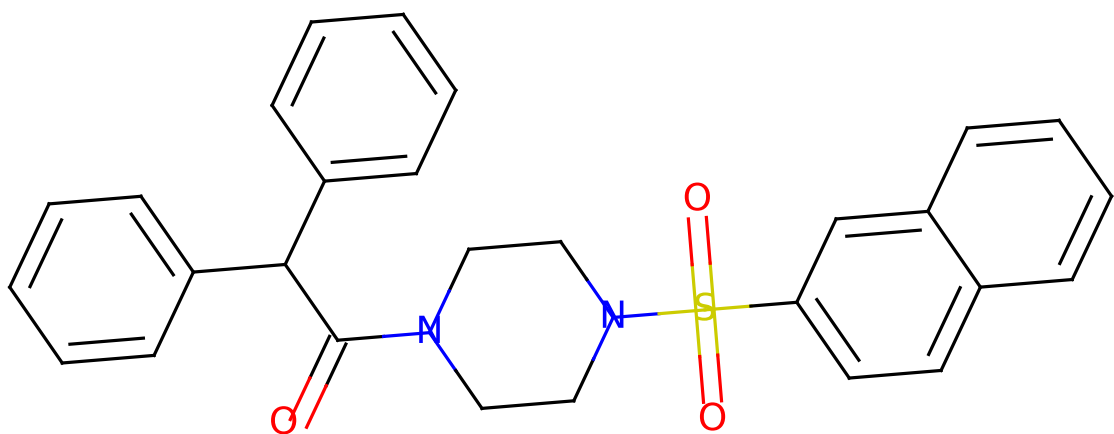c1cc2c(cc1F)nc([nH]2)CCC(=O)N3C[C@@H]4CCC[NH2+][C@@H]4C3

ORD-MCULE-7193355722_2

MolLogP: 5.3217200000000044 | QED: 0.35110179262542385
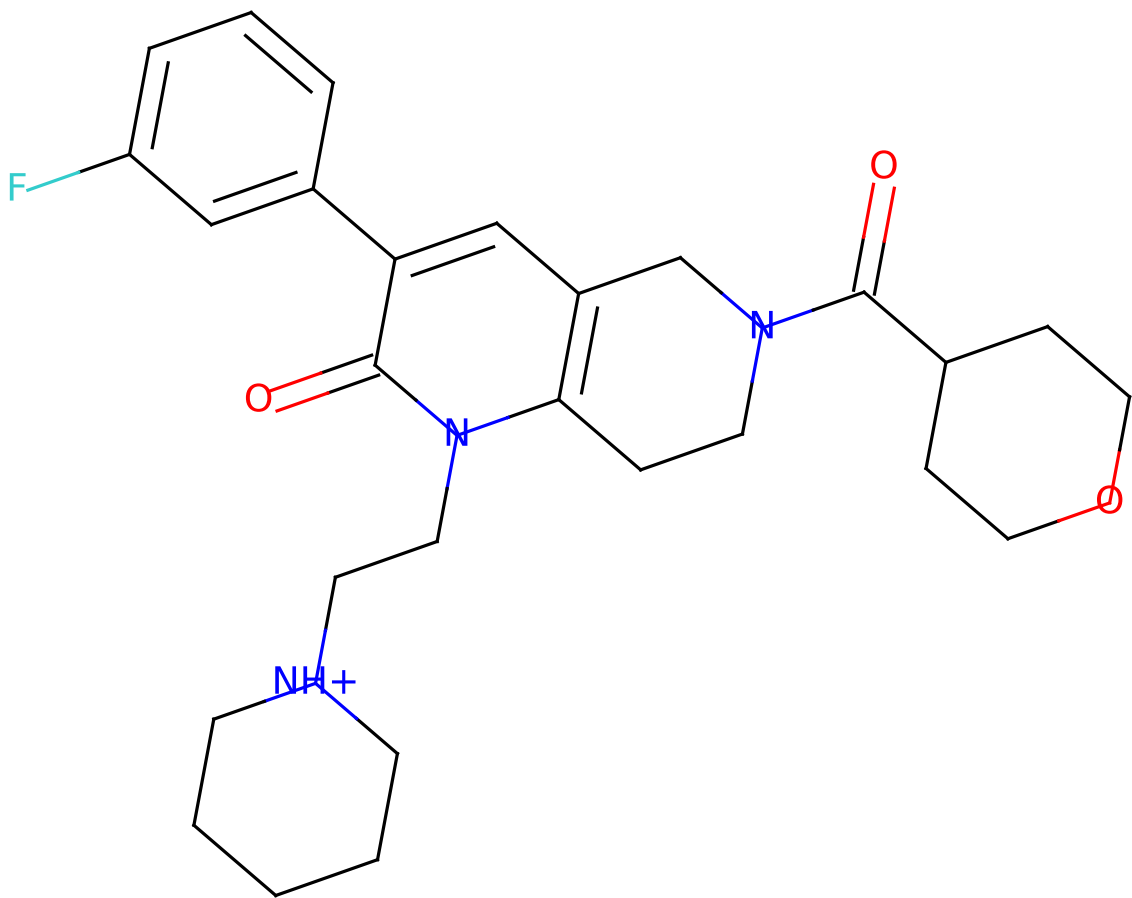
Cc1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4c5c(sc4n3)CCC5)c6ccccc6

ORD-MCULE-1034841344_1

61

MolLogP: 4.504800000000004 | QED: 0.43144005118053486

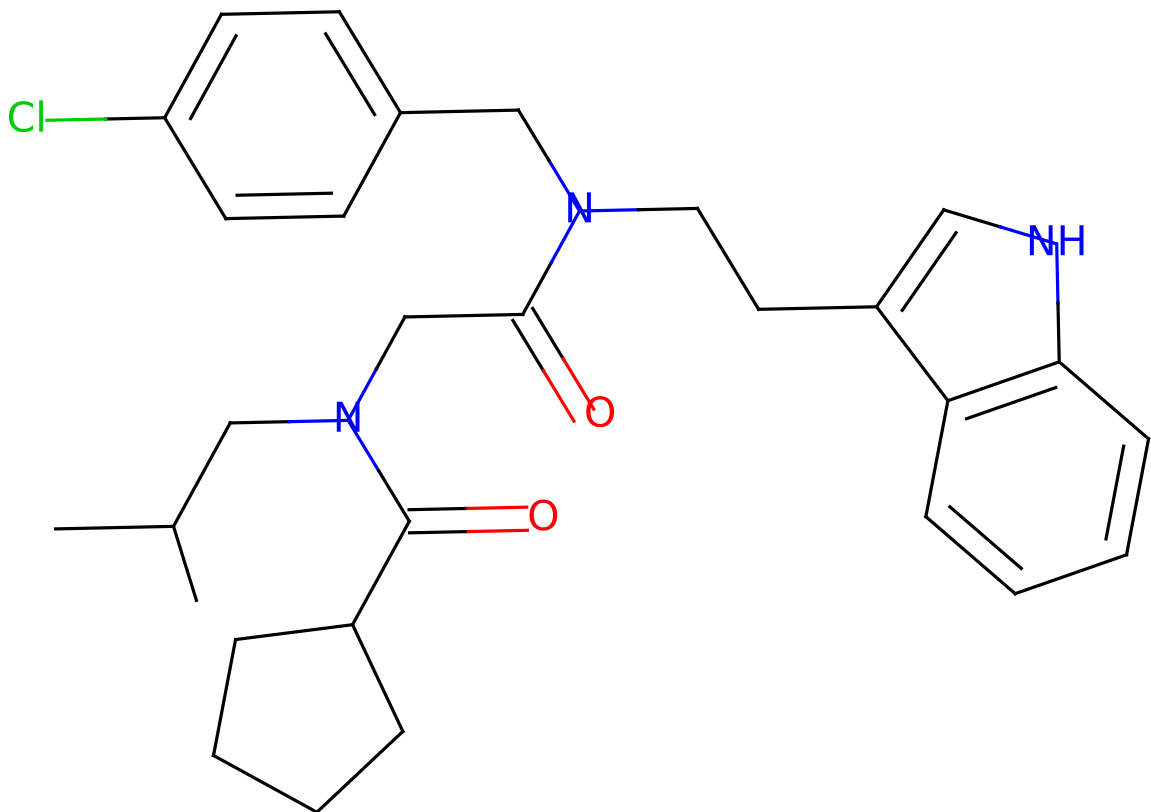c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)S(=O)(=O)c4ccc5ccccc5c4

ORD-MCULE-9717306826_1

MolLogP: 2.0344999999999995 | QED: 0.7308722123771373

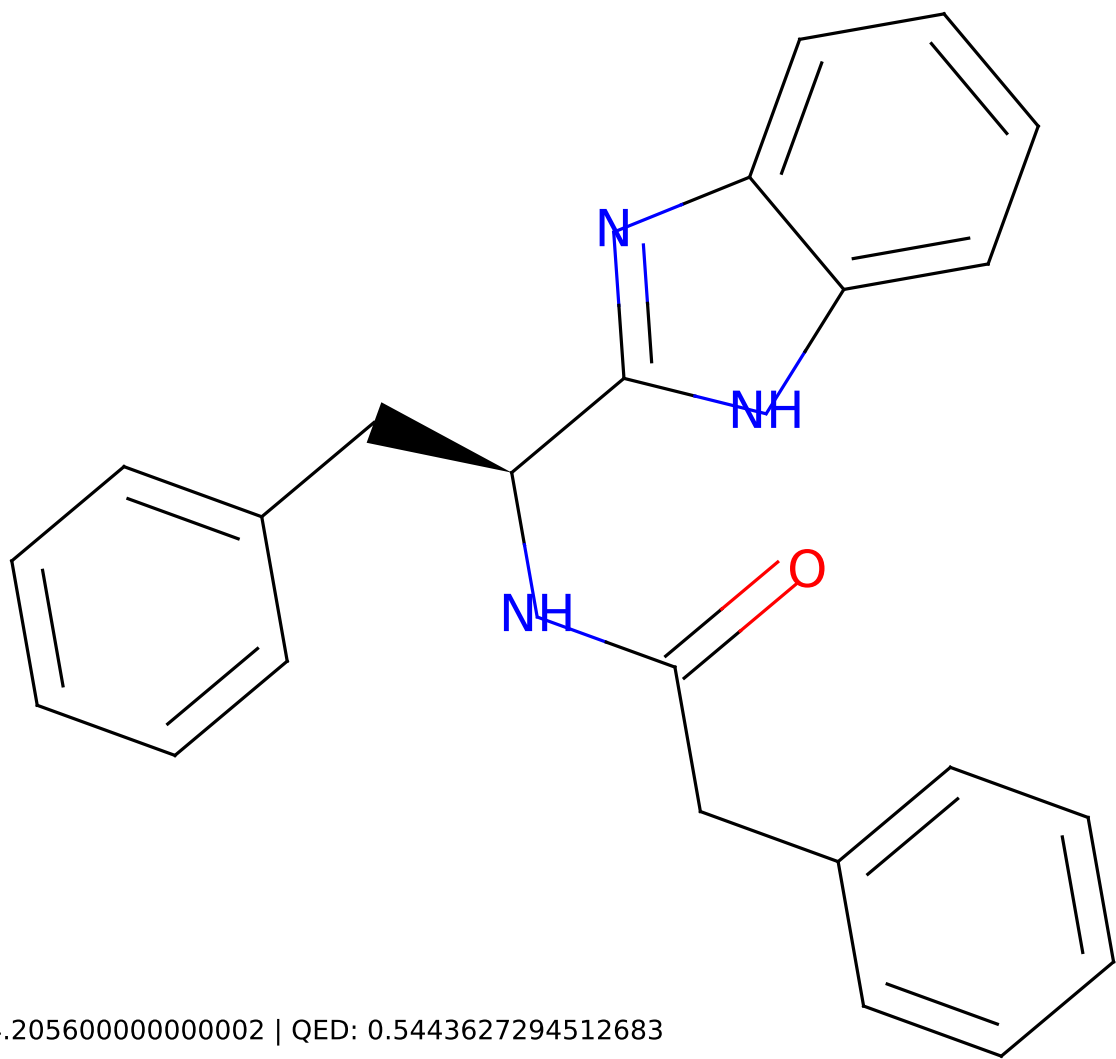c1cc(cc(c1)F)c2cc3c(n(c2=O)CC[NH+]4CCCCC4)CCN(C3)C(=O)C5CCOCC5

ORD-MCULE-5517230918_1

MolLogP: 6.067400000000006 | QED: 0.3724918485885742

CC(C)CN(CC(=O)N(CCc1c[nH]c2c1cccc2)Cc3ccc(cc3)Cl)C(=O)C4CCCC4
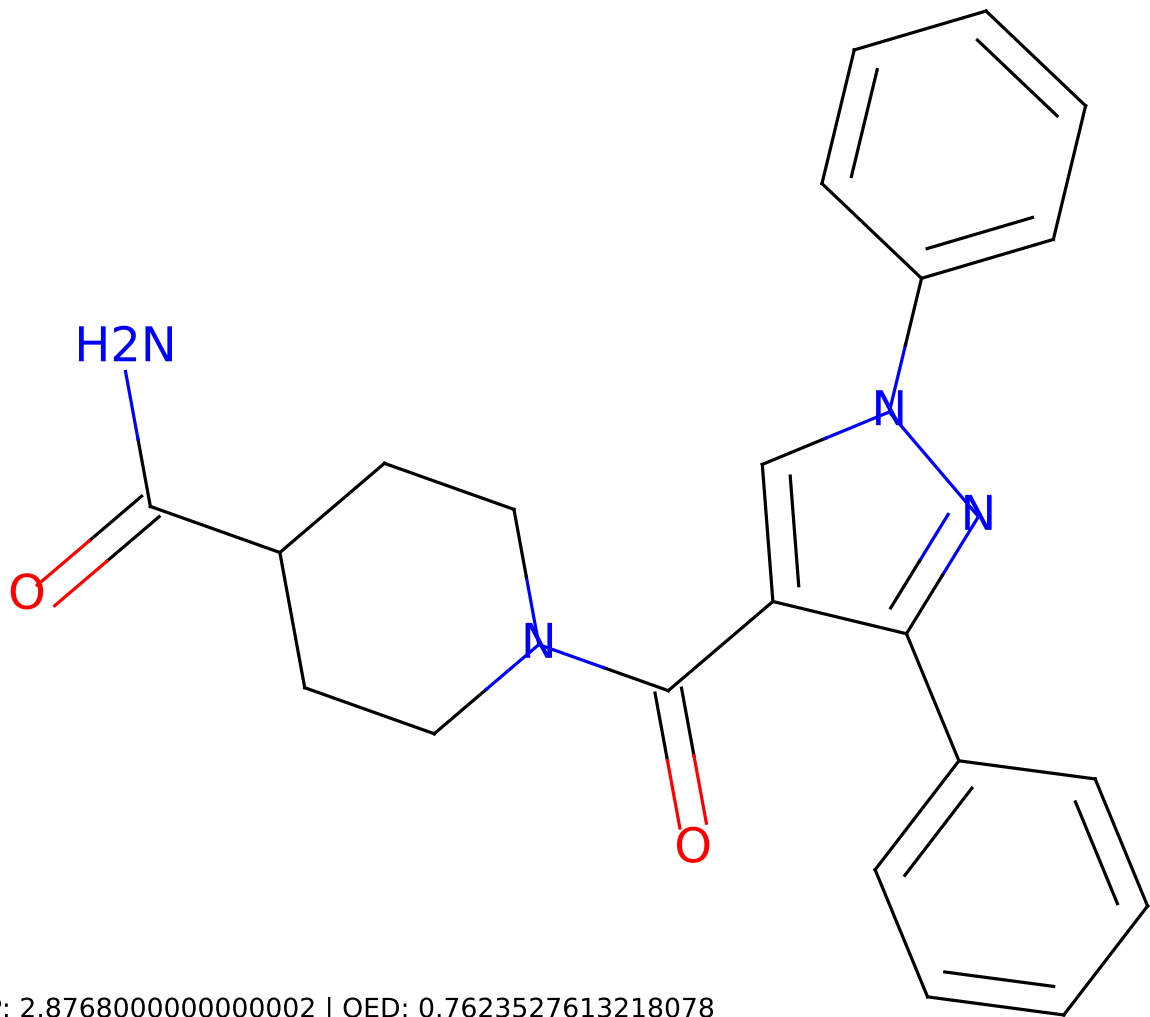
ORD-MCULE-6156881199_1

MolLogP: 4.205600000000002 | QED: 0.5443627294512683

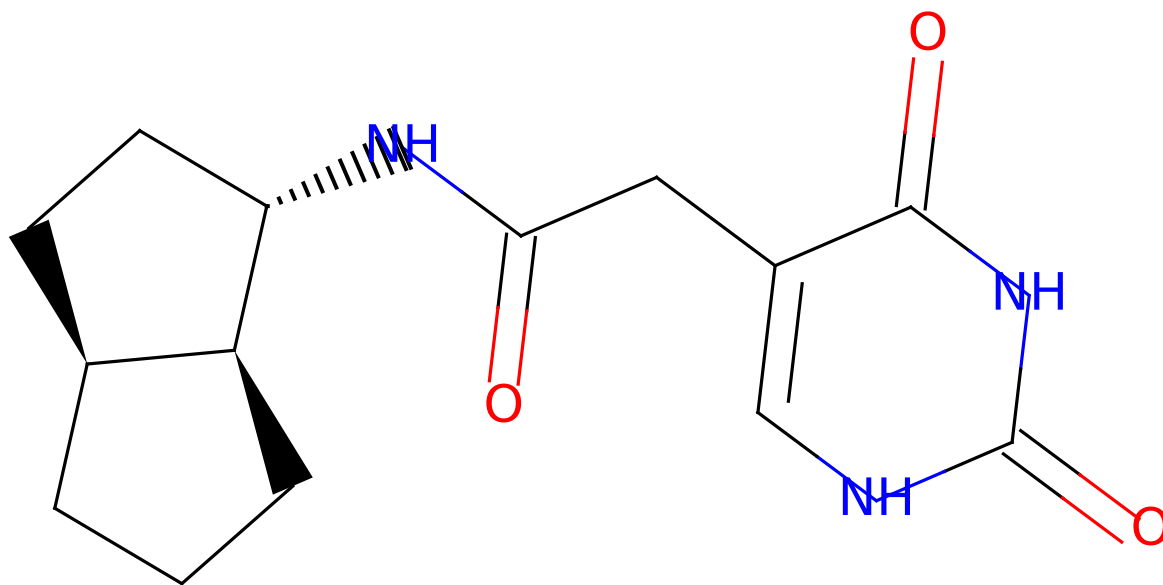c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)Cc4ccccc4

ORD-MCULE-7344200039_1

MolLogP: 2.8768000000000002 | QED: 0.7623527613218078
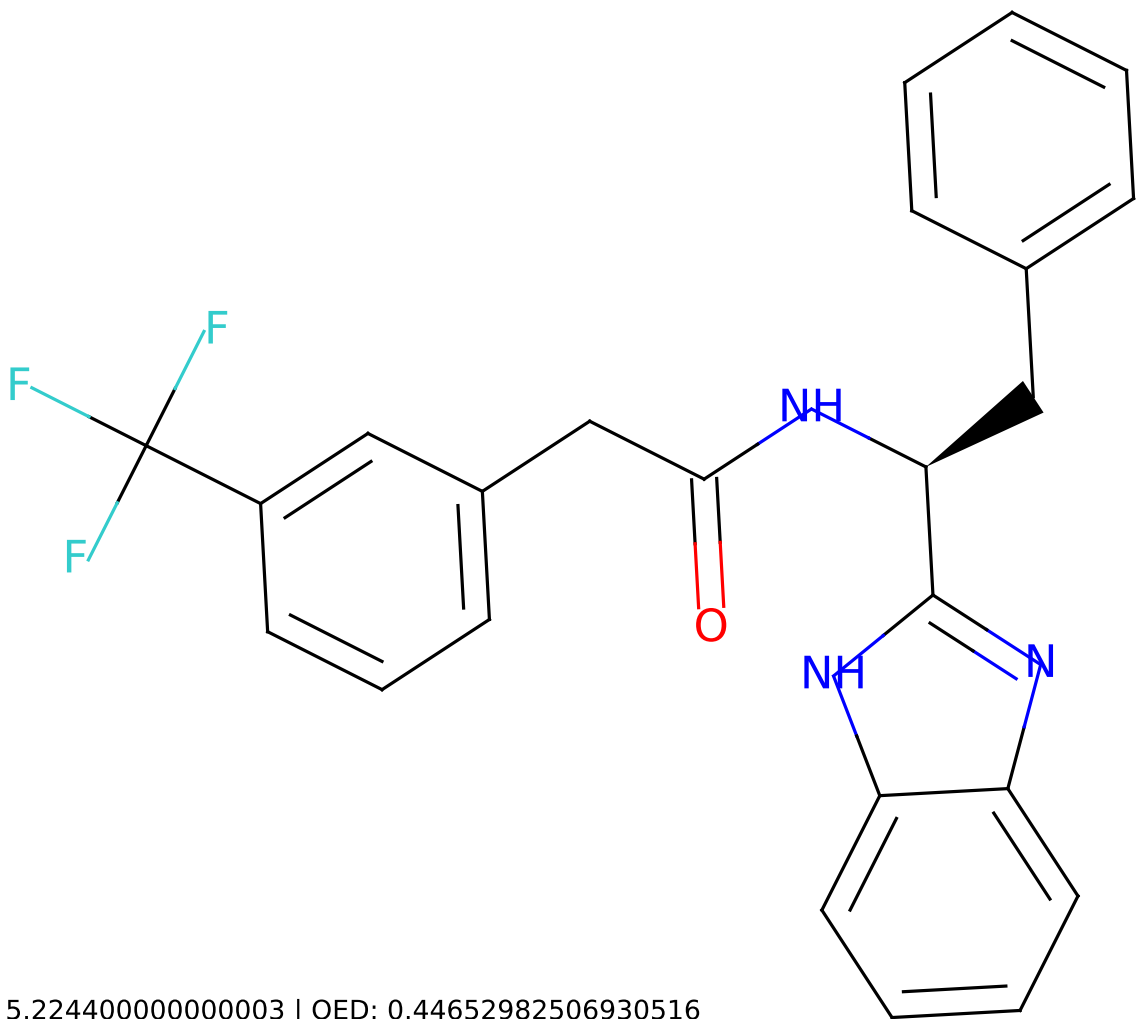
c1ccc(cc1)c2c(cn(n2)c3ccccc3)C(=O)N4CCC(CC4)C(=O)N

ORD-MCULE-8349729891_1

MolLogP: 0.30059999999999953 | QED: 0.7413021226835171

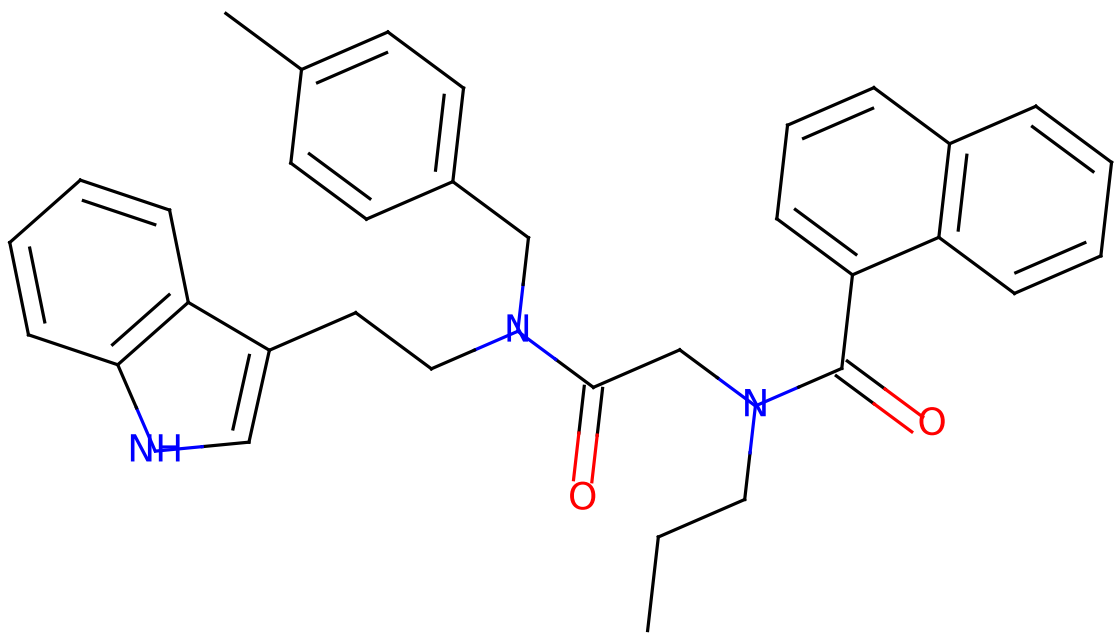c1c(c(=O)[nH]c(=O)[nH]1)CC(=O)N[C@H]2CC[C@H]3[C@@H]2CCC3

ORD-MCULE-3980028168_1

MolLogP: 5.224400000000003 | QED: 0.44652982506930516

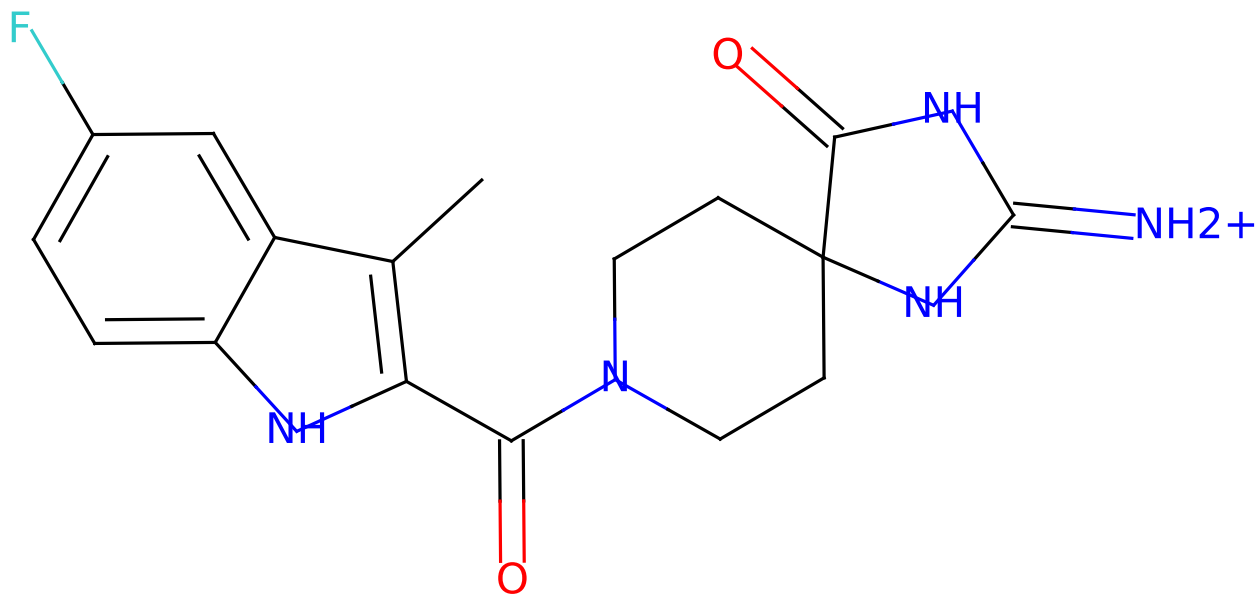c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)Cc4cccc(c4)C(F)(F)F

ORD-MCULE-4125658730_1

68

MolLogP: 6.753220000000007 | QED: 0.22269048177123804

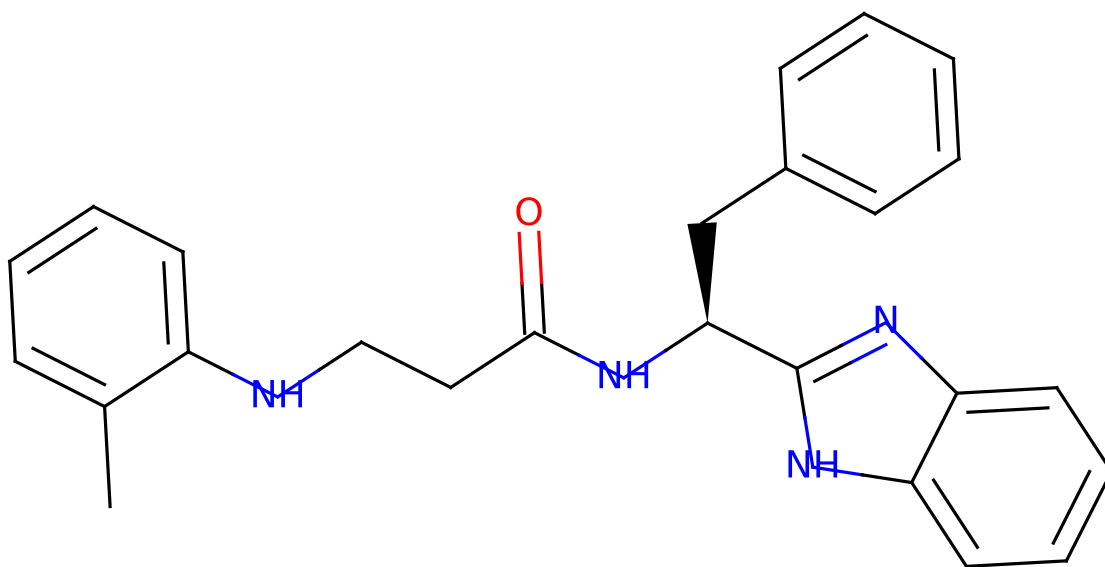CCCN(CC(=O)N(CCc1c[nH]c2c1cccc2)Cc3ccc(cc3)C)C(=O)c4cccc5c4cccc5

ORD-MCULE-6912999917_1

69

MolLogP: -0.5752799999999987 | QED: 0.5567411639689259

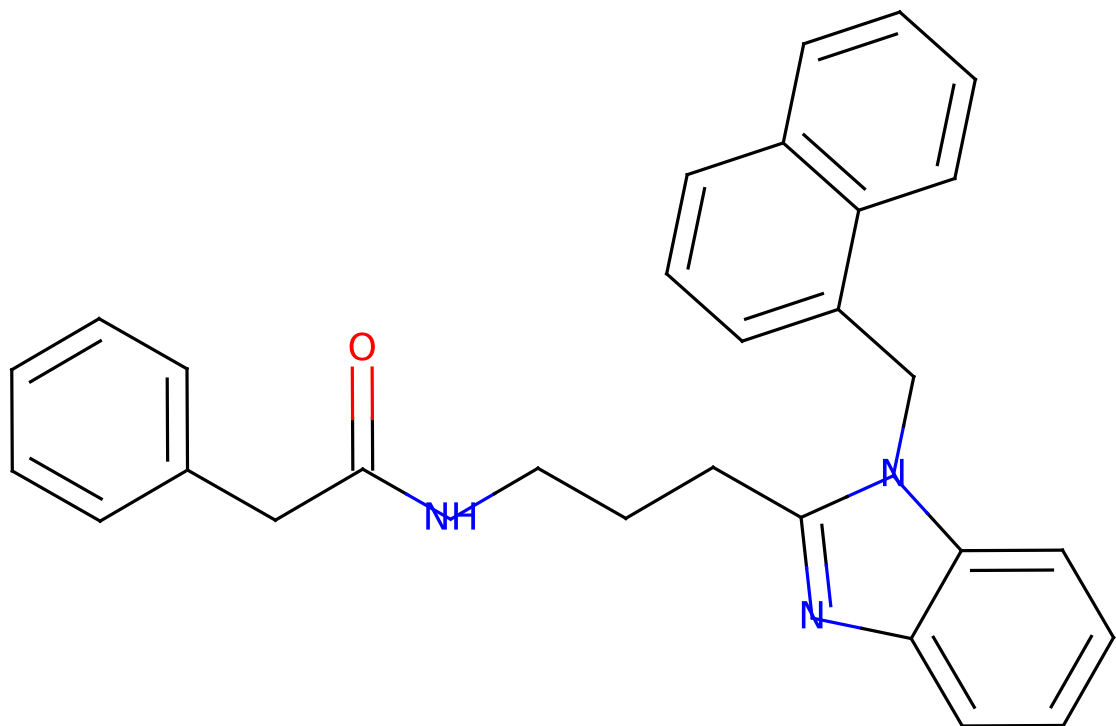Cc1c2cc(ccc2[nH]c1C(=O)N3CCC4(CC3)C(=O)NC(=[NH2+])N4)F

ORD-MCULE-5493358376_2

MolLogP: 4.773520000000003 | QED: 0.4002438598311808

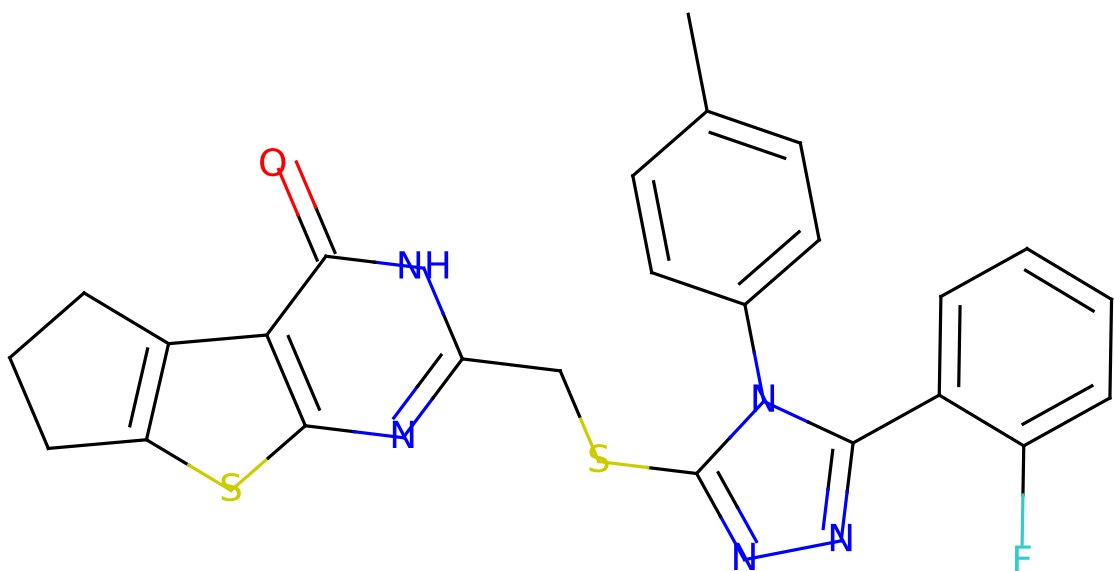Cc1ccccc1NCCC(=O)N[C@@H](Cc2ccccc2)c3[nH]c4ccccc4n3

ORD-MCULE-9437816791_1

MolLogP: 5.529300000000005 | QED: 0.32718667928035094

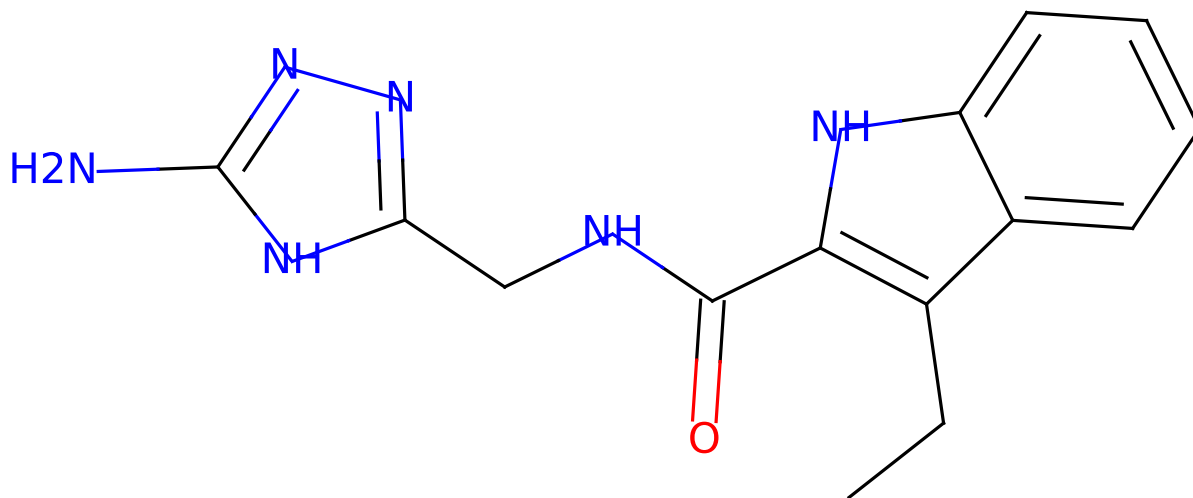c1ccc(cc1)CC(=O)NCCCc2nc3ccccc3n2Cc4cccc5c4cccc5

ORD-MCULE-9349708949_1

MolLogP: 5.460820000000004 | QED: 0.33185428545886714

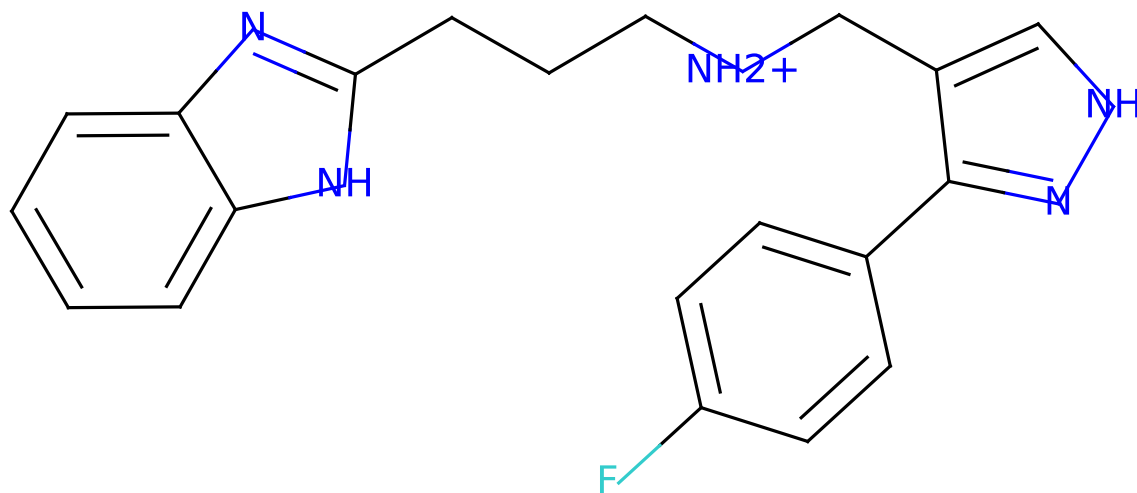Cc1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4c5c(sc4n3)CCC5)c6ccccc6F

ORD-MCULE-4573025143_1

MolLogP: 1.3606000000000003 | QED: 0.5790569204754366

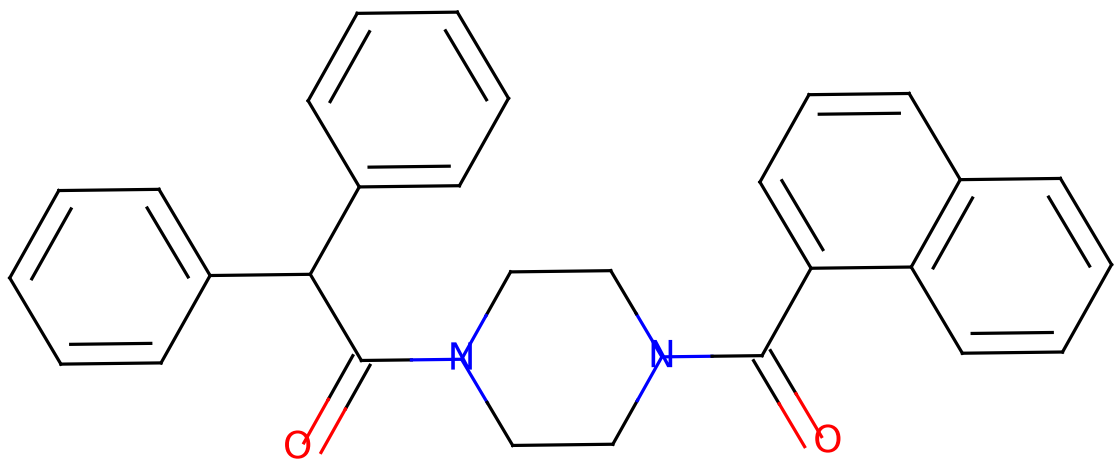CCc1c2ccccc2[nH]c1C(=O)NCc3[nH]c(nn3)N

ORD-MCULE-1055493247_3

MolLogP: 2.7883000000000004 | QED: 0.44848198893249597
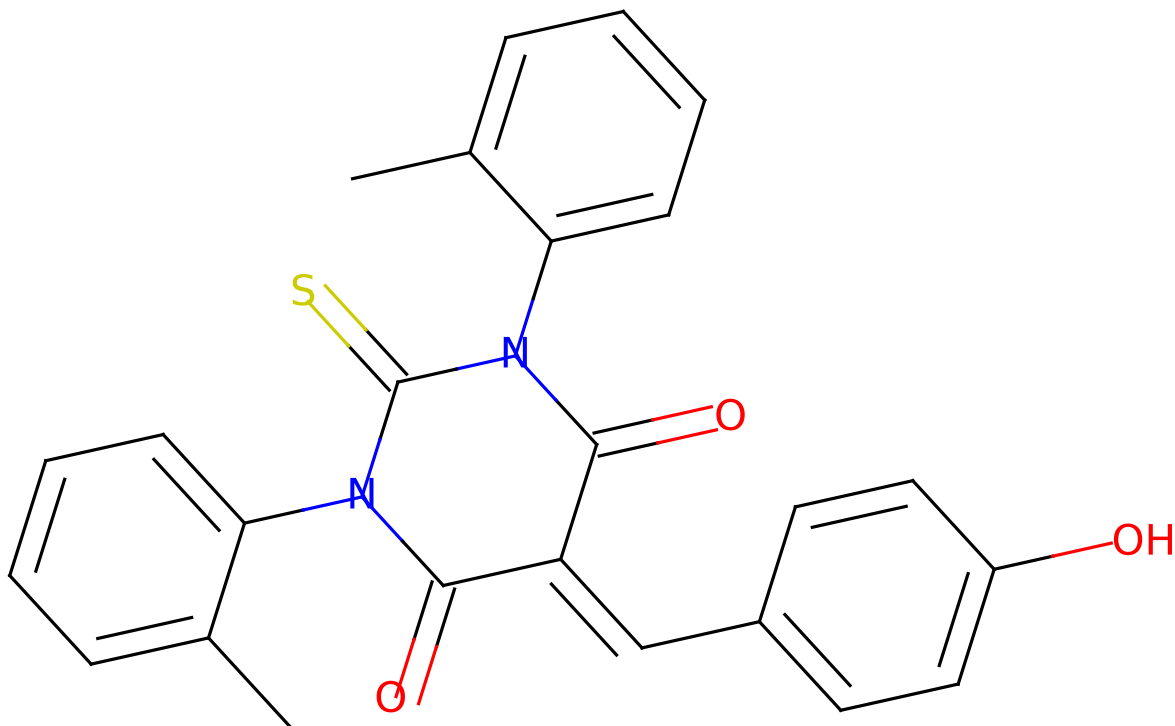
c1ccc2c(c1)[nH]c(n2)CCC[NH2+]Cc3c[nH]nc3c4ccc(cc4)F

ORD-MCULE-3429761171_2

MolLogP: 4.956300000000004 | QED: 0.45571063266576933

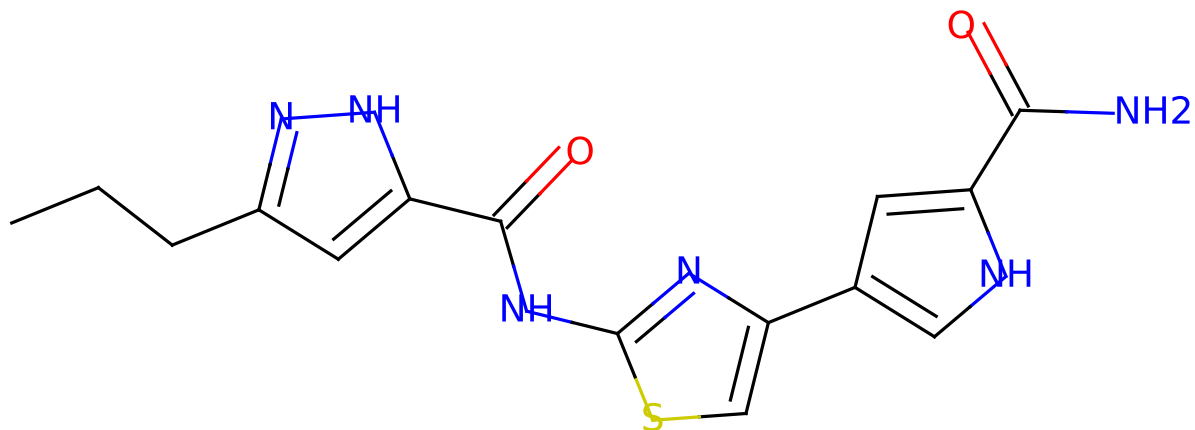c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4cccc5c4cccc5

ORD-MCULE-4705080812_1

MolLogP: 4.757340000000004 | QED: 0.37131368628186073

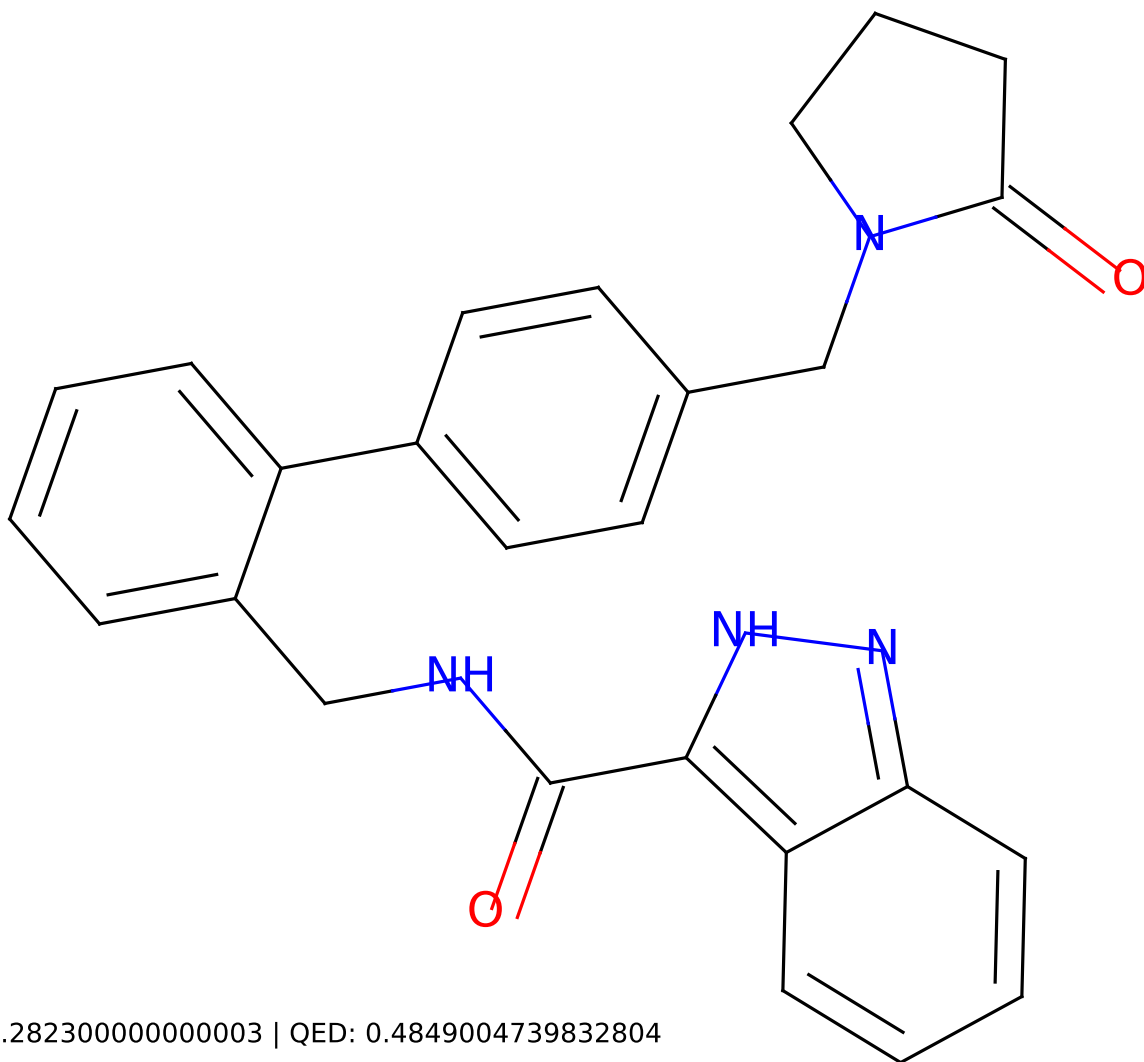Cc1ccccc1N2C(=O)C(=Cc3ccc(cc3)O)C(=O)N(C2=S)c4ccccc4C

ORD-MCULE-6554581903_1

MolLogP: 2.165 | QED: 0.5457063523155568
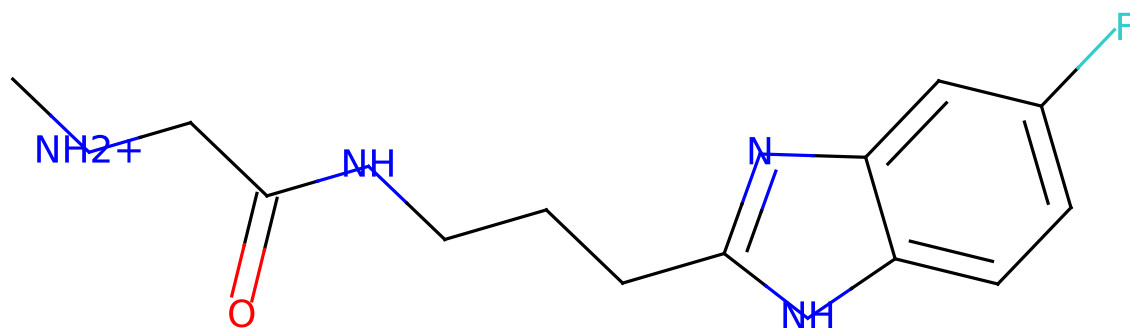
CCCc1cc([nH]n1)C(=O)Nc2nc(cs2)c3cc([nH]c3)C(=O)N

ORD-MCULE-9221479095_2

MolLogP: 4.282300000000003 | QED: 0.4849004739832804
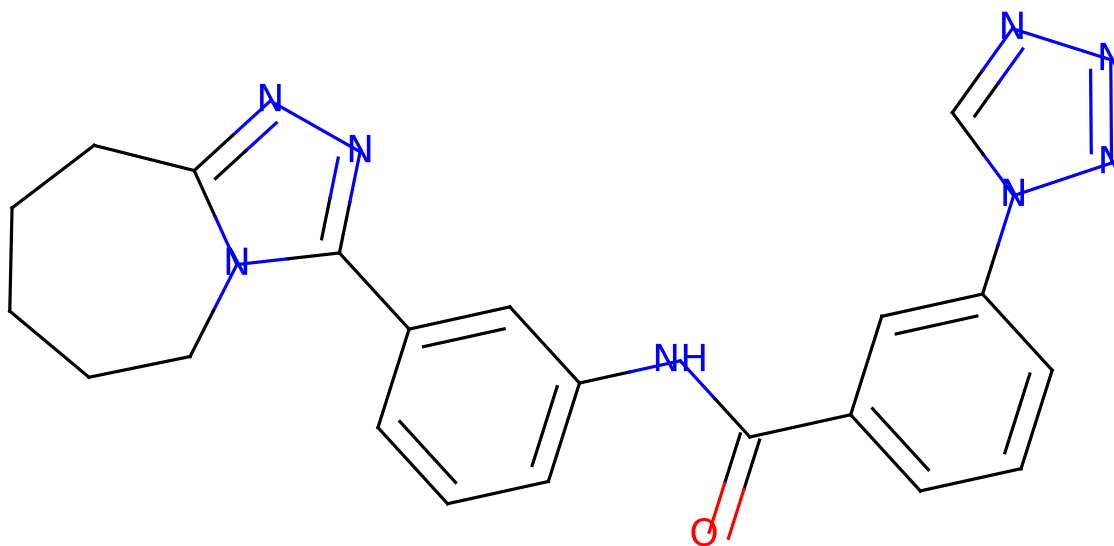
c1ccc(c(c1)CNC(=O)c2c3ccccc3n[nH]2)c4ccc(cc4)CN5CCCC5=O

ORD-MCULE-6144665861_2

MolLogP: -0.0559999999999977 | QED: 0.6403435644960167
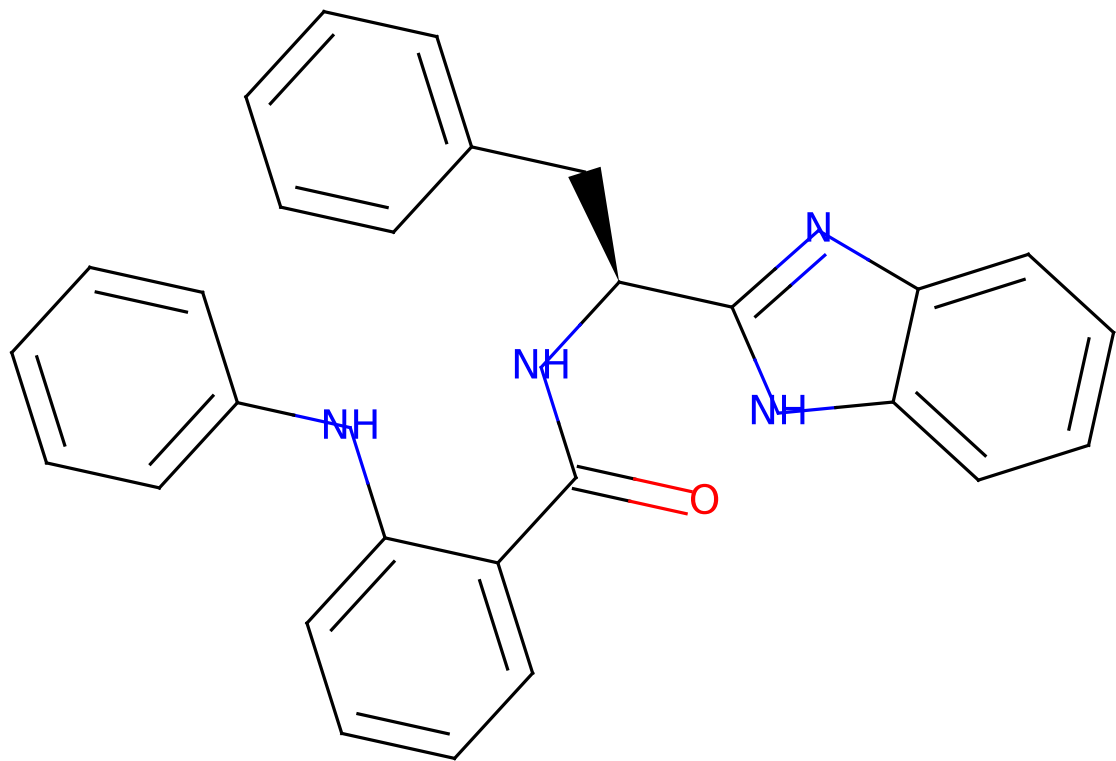
C[NH2+]CC(=O)NCCCc1[nH]c2ccc(cc2n1)F

ORD-MCULE-5985443175_2

MolLogP: 2.8995000000000006 | QED: 0.564916346720981
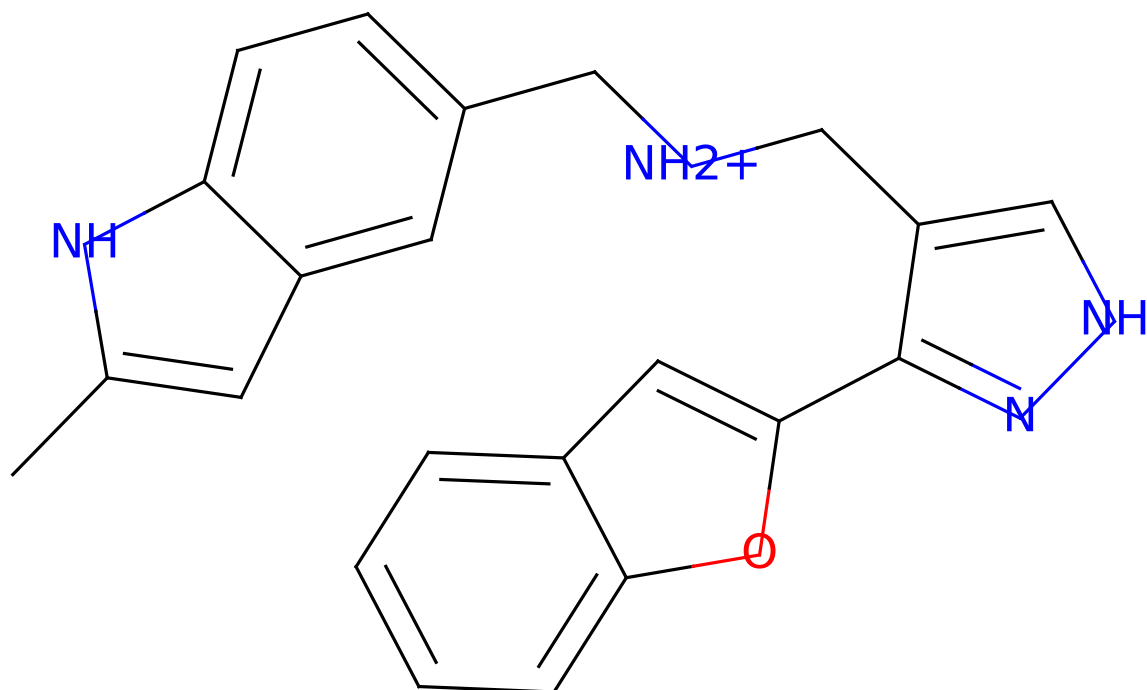
c1cc(cc(c1)NC(=O)c2cccc(c2)n3cnnn3)c4nnc5n4CCCCC5

ORD-MCULE-2036827873_1

MolLogP: 6.020300000000004 | QED: 0.2944823282671522

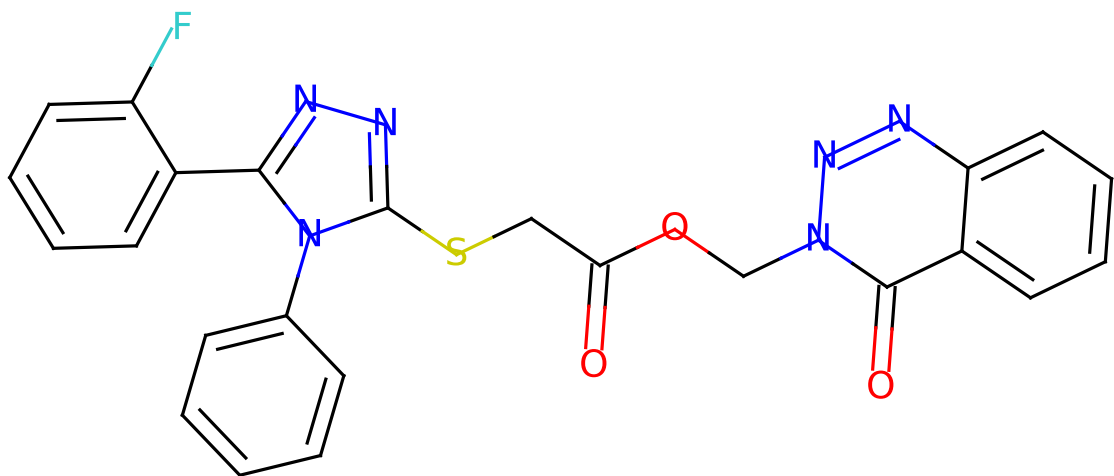c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4ccccc4Nc5ccccc5

ORD-MCULE-8785708058_1

MolLogP: 3.8762200000000018 | QED: 0.4465288488541507
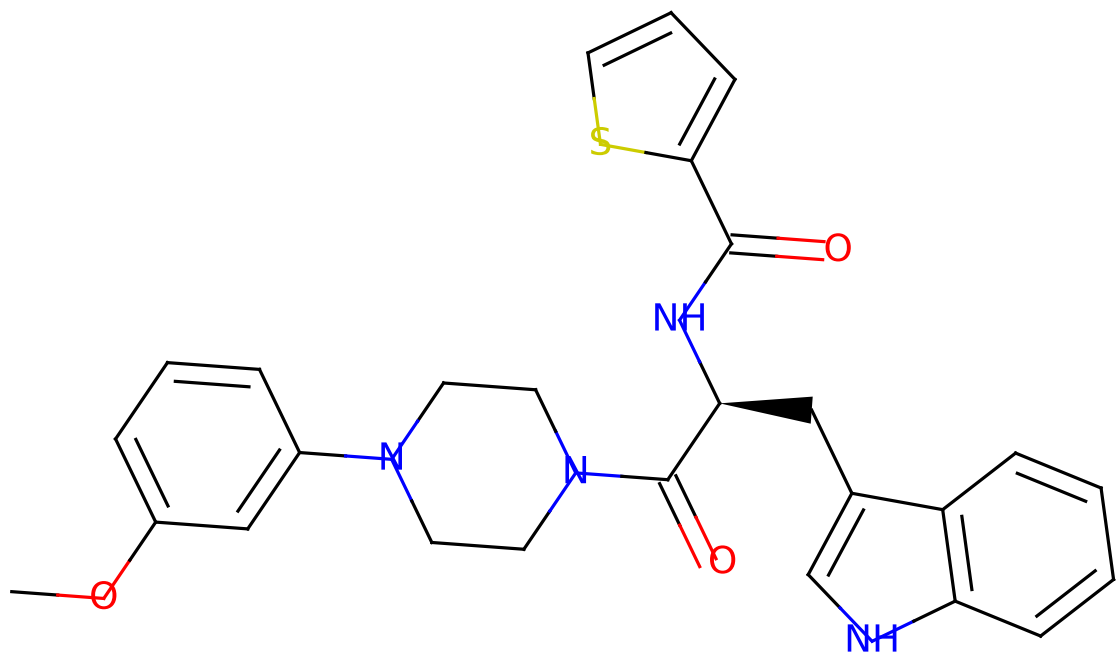
Cc1cc2cc(ccc2[nH]1)C[NH2+]Cc3c[nH]nc3c4cc5ccccc5o4

ORD-MCULE-8751974401_2

83

MolLogP: 3.471300000000002 | QED: 0.25337500540496866

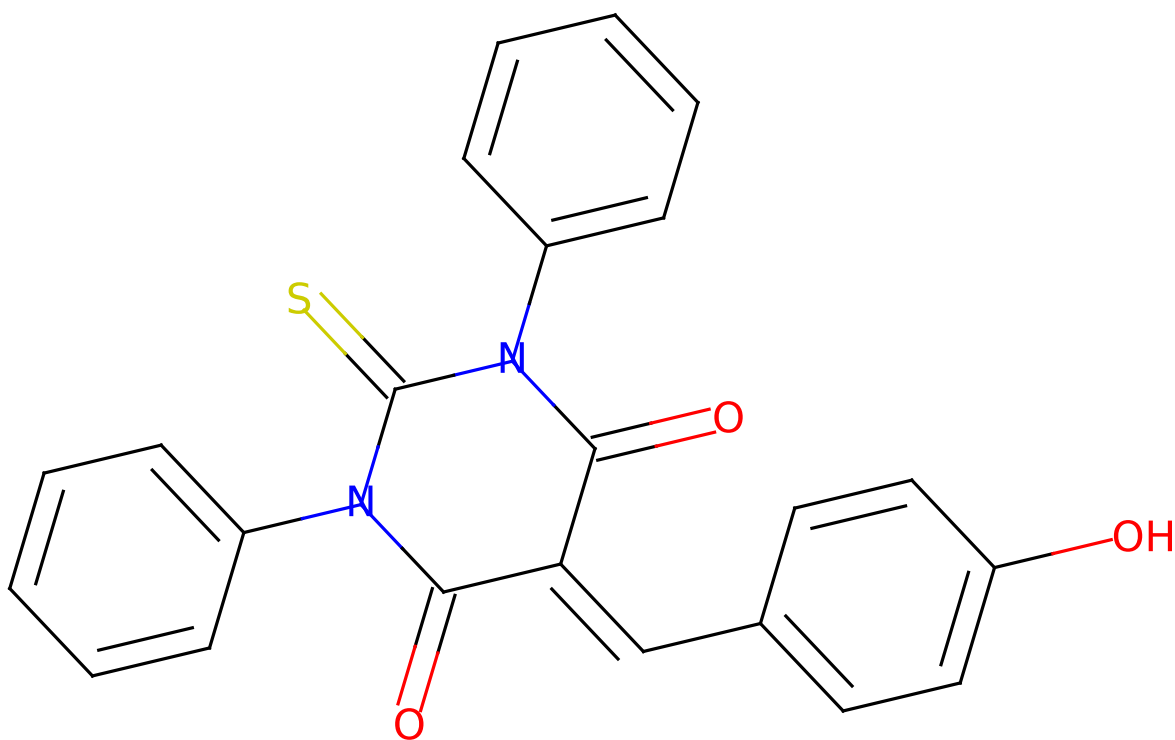c1ccc(cc1)n2c(nnc2SCC(=O)OCn3c(=O)c4ccccc4nn3)c5ccccc5F

ORD-MCULE-3885560687_1

MolLogP: 3.927900000000003 | QED: 0.41334145973930614

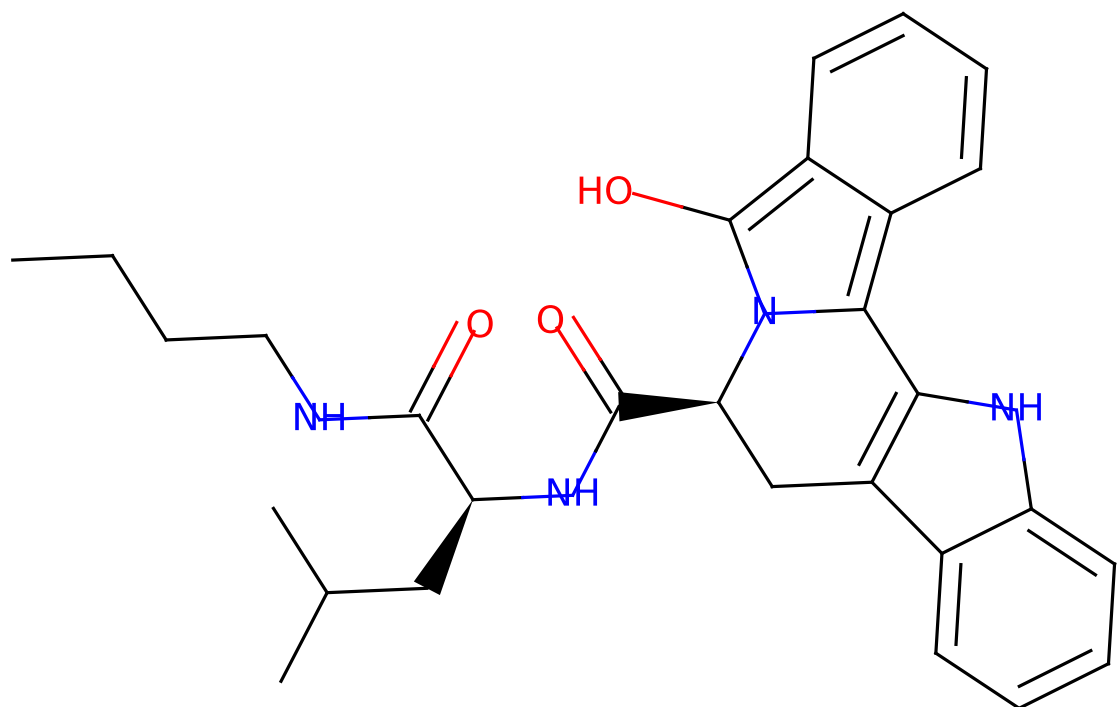COc1cccc(c1)N2CCN(CC2)C(=O)[C@H](Cc3c[nH]c4c3cccc4)NC(=O)c5cccs5

ORD-MCULE-5744155890_1

MolLogP: 4.140500000000002 | QED: 0.40781038035980627

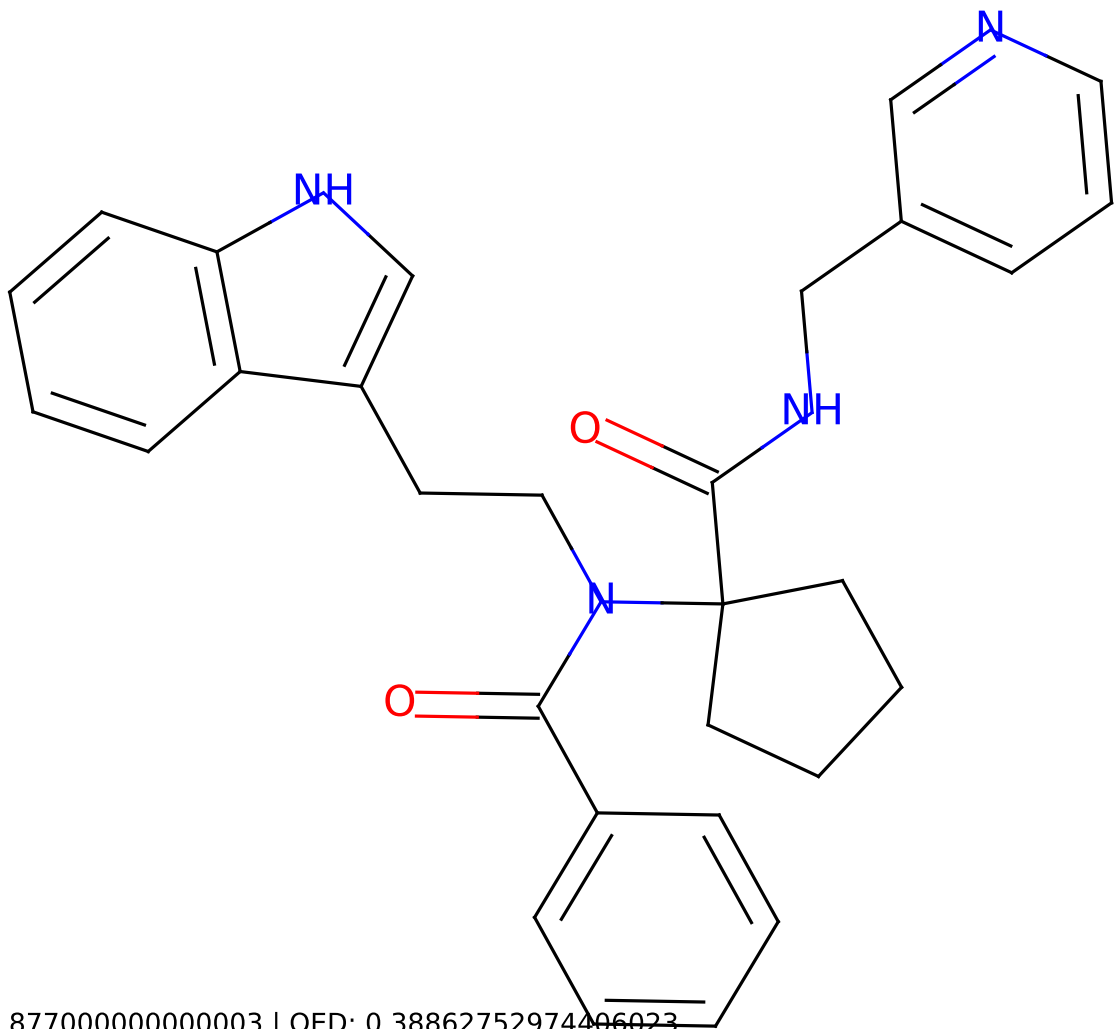c1ccc(cc1)N2C(=O)C(=Cc3ccc(cc3)O)C(=O)N(C2=S)c4ccccc4

ORD-MCULE-2963351147_1

MolLogP: 5.0396000000000045 | QED: 0.2626498348566446

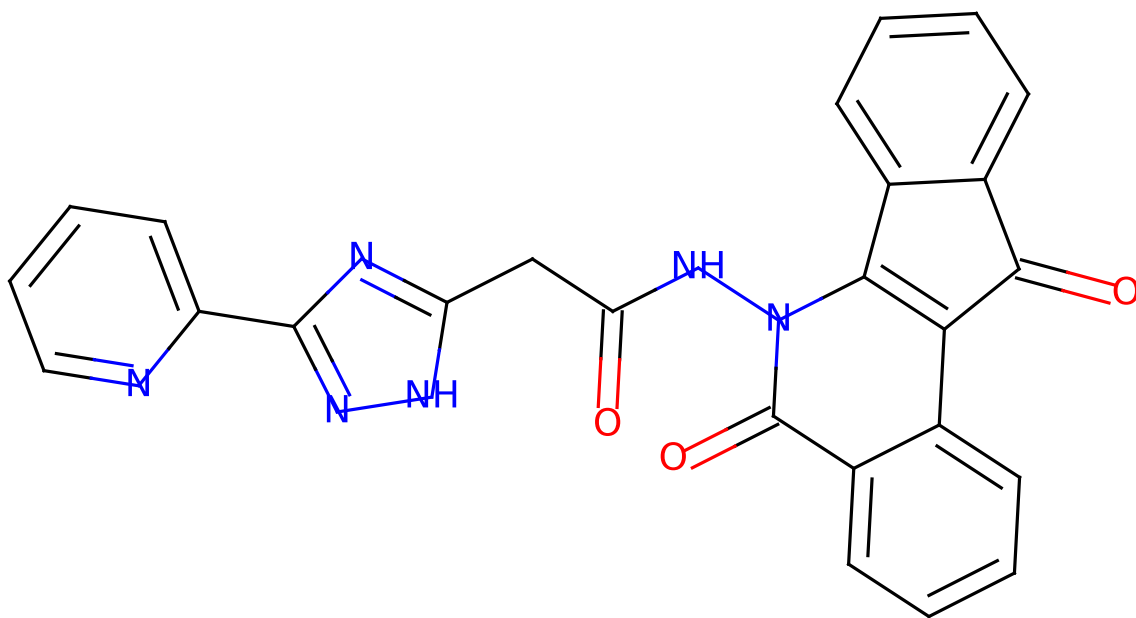CCCCNC(=O)[C@H](CC(C)C)NC(=O)[C@@H]1Cc2c3ccccc3[nH]c2-c4n1c(c5c4cccc5)O

ORD-MCULE-3907045269_1

MolLogP: 4.877000000000003 | QED: 0.38862752974406023

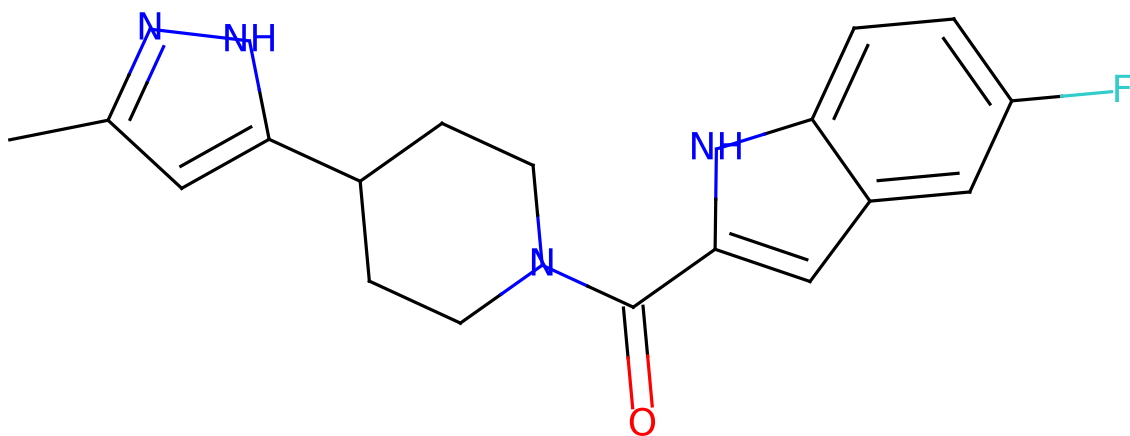c1ccc(cc1)C(=O)N(CCc2c[nH]c3c2cccc3)C4(CCCC4)C(=O)NCc5cccnc5

ORD-MCULE-6383481281_1

MolLogP: 2.705800000000001 | QED: 0.4275564127608206

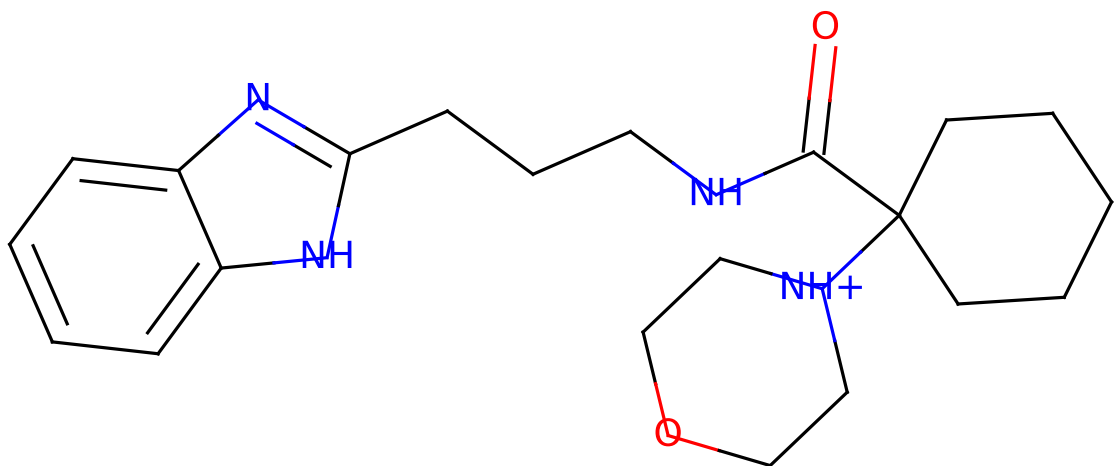c1ccc2c(c1)c3c(n(c2=O)NC(=O)Cc4[nH]nc(n4)c5ccccn5)-c6ccccc6C3=O

ORD-MCULE-1087797516_1

MolLogP: 3.3583200000000017 | QED: 0.7582549149593061

Cc1cc([nH]n1)C2CCN(CC2)C(=O)c3cc4cc(ccc4[nH]3)F
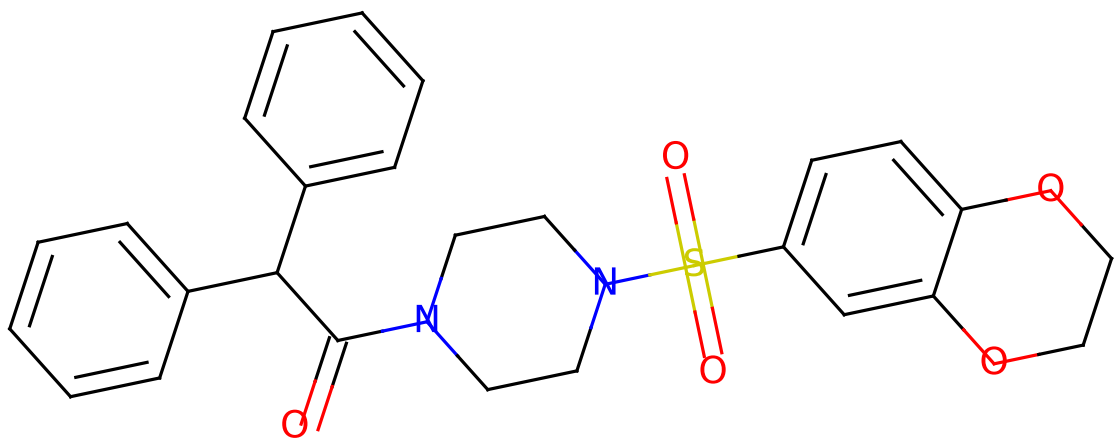
ORD-MCULE-1224951145_2

MolLogP: 1.2297000000000005 | QED: 0.6690861441540914

c1ccc2c(c1)[nH]c(n2)CCCNC(=O)C3(CCCCC3)[NH+]4CCOCC4

ORD-MCULE-2015327629_1

MolLogP: 1.4353999999999996 | QED: 0.7509950151336577

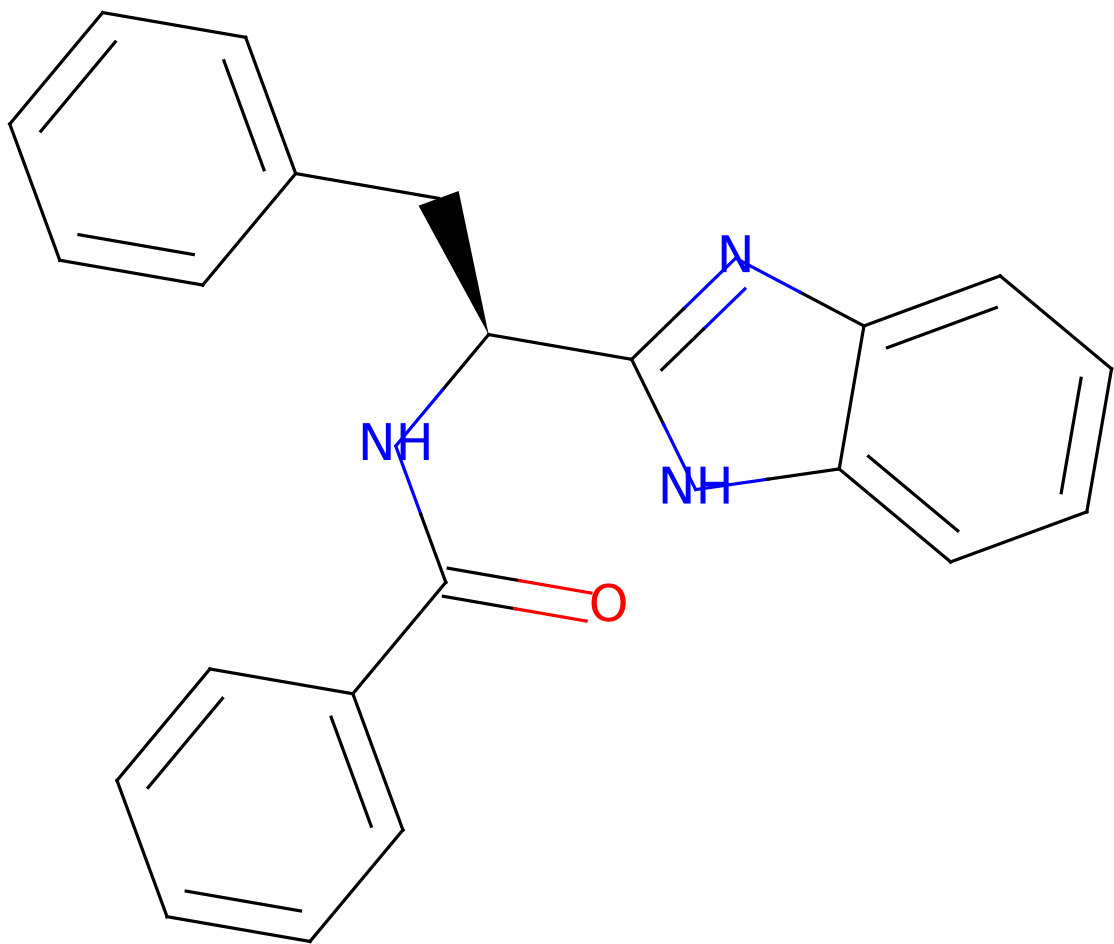c1cc2c(cc1Cl)cc([nH]2)C(=O)N3CCC4(CC3)[C@@H](C[C@@H]4OCC[NH3+])O

ORD-MCULE-3838004698_1

MolLogP: 3.1228000000000016 | QED: 0.5633261375042687

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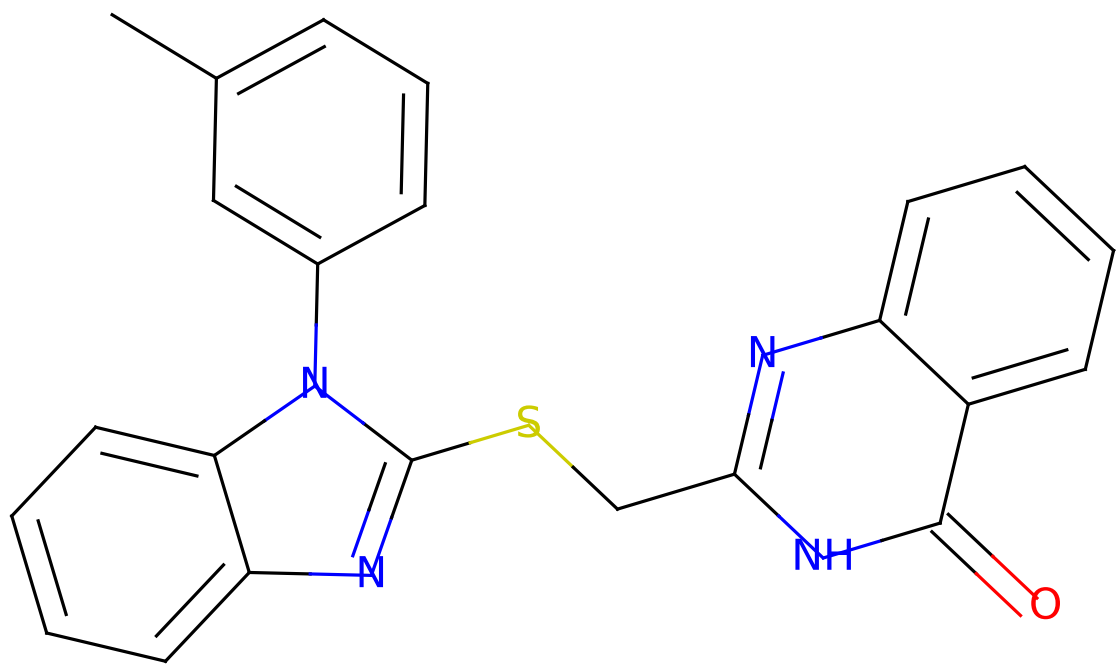
ORD-MCULE-1904175079_1

MolLogP: 4.276700000000003 | QED: 0.5692049669555924

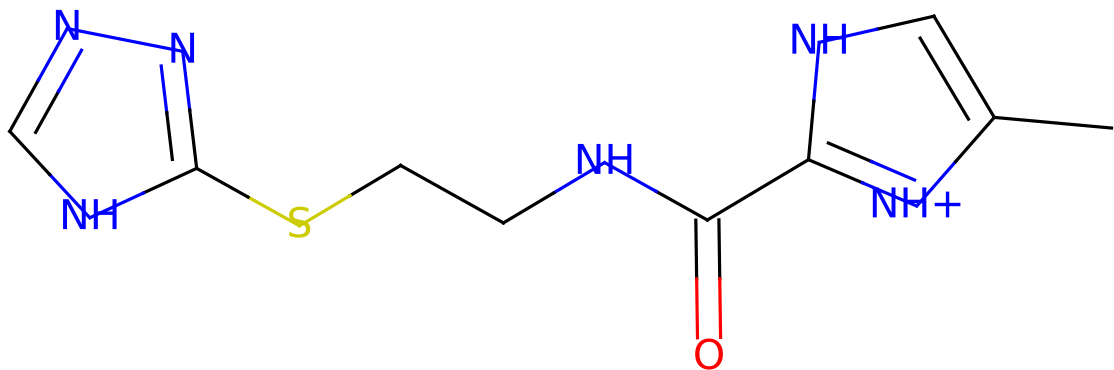c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4ccccc4

ORD-MCULE-4489145056_1

MolLogP: 4.862720000000003 | QED: 0.439123236596394

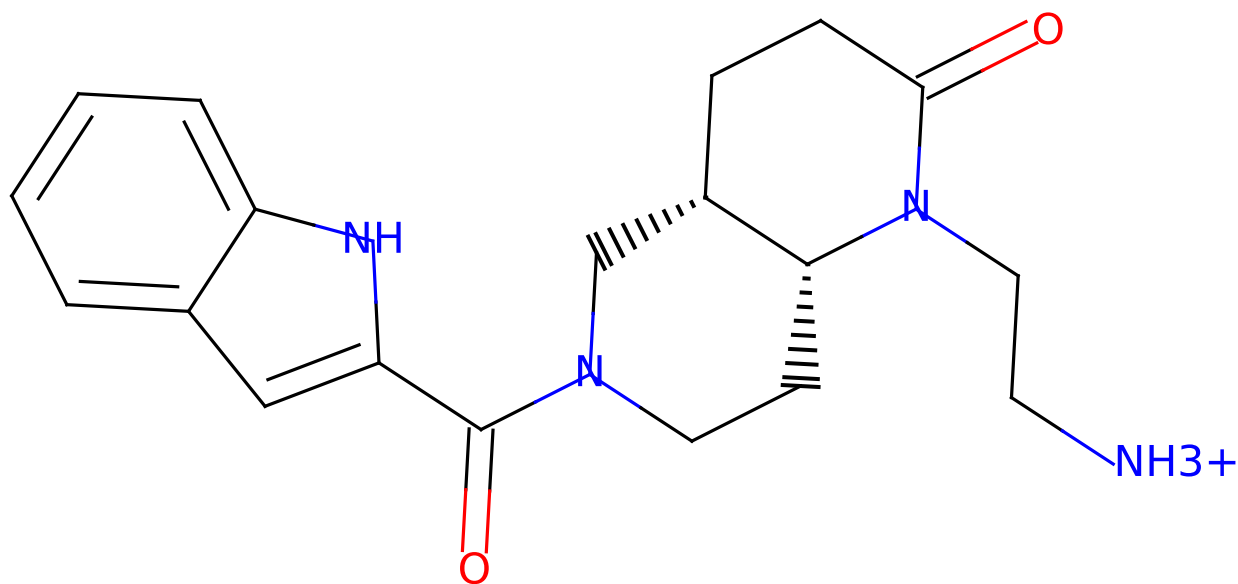Cc1cccc(c1)n2c3ccccc3nc2SCc4[nH]c(=O)c5ccccc5n4

ORD-MCULE-1819742436_1

MolLogP: -0.2225800000000006 | QED: 0.5061753470565761
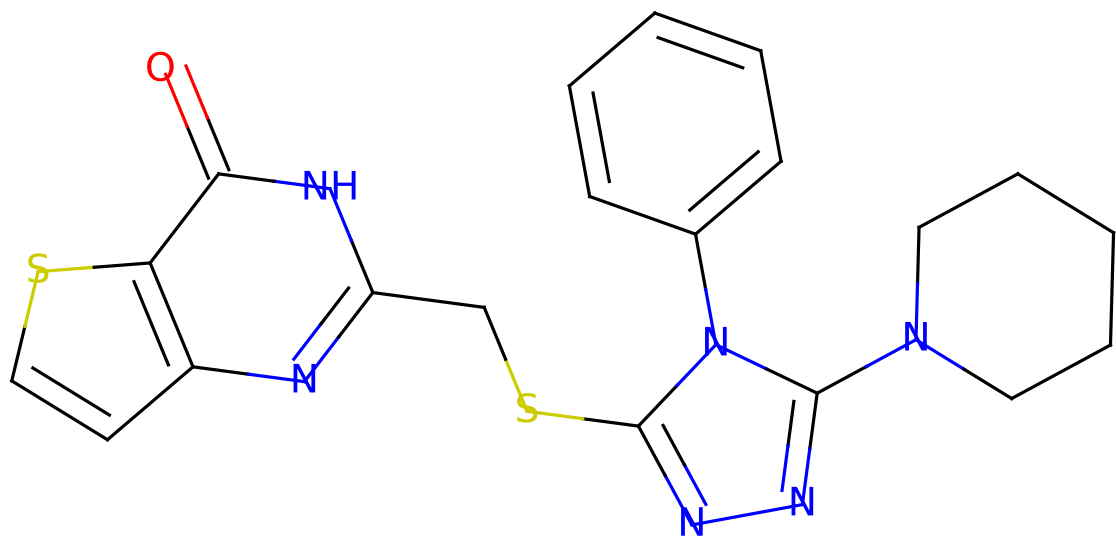
Cc1c[nH]c([nH+]1)C(=O)NCCSc2[nH]cnn2

ORD-MCULE-3031881642_6

MolLogP: 0.8629000000000007 | QED: 0.8678648239017707

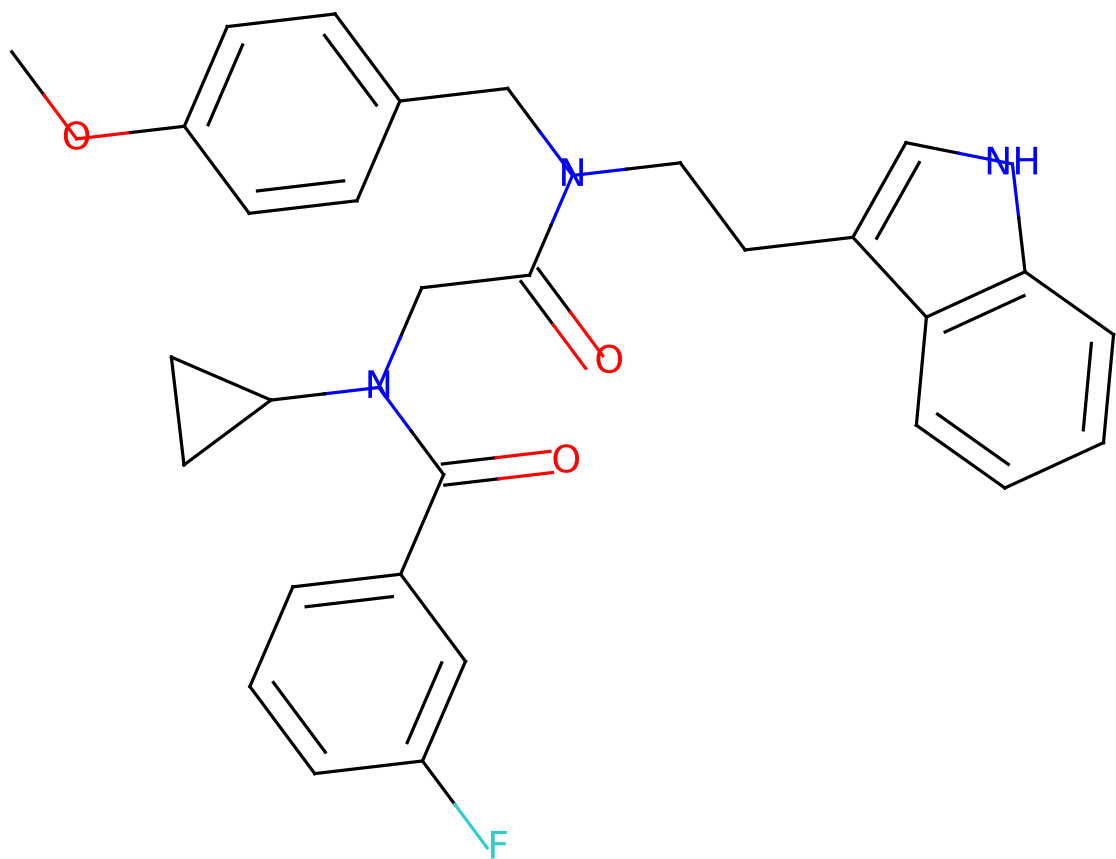c1ccc2c(c1)cc([nH]2)C(=O)N3CC[C@@H]4[C@H](C3)CCC(=O)N4CC[NH3+]

ORD-MCULE-6453287452_1

MolLogP: 3.847900000000002 | QED: 0.4903952442933713

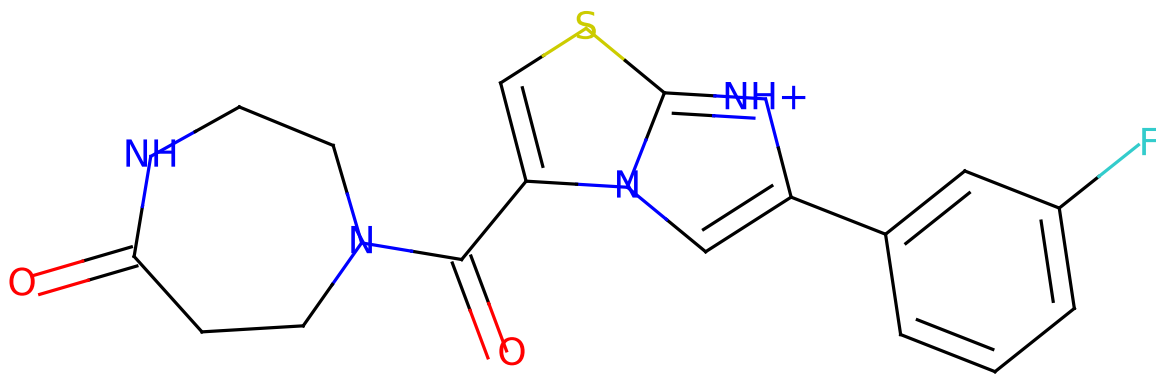c1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4c(n3)ccs4)N5CCCCC5

ORD-MCULE-1821738086_1

98

MolLogP: 5.191700000000005 | QED: 0.326572692572572

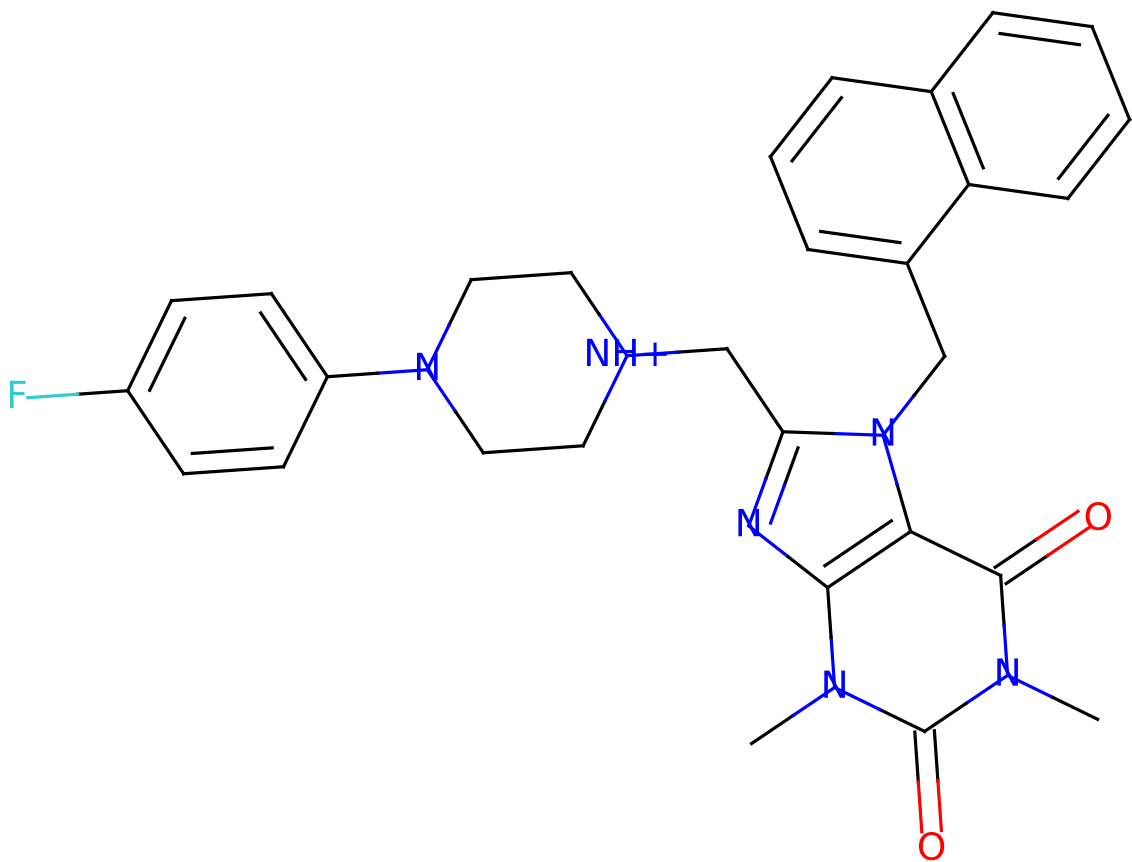COc1ccc(cc1)CN(CCc2c[nH]c3c2cccc3)C(=O)CN(C4CC4)C(=O)c5cccc(c5)F

ORD-MCULE-3860138249_1

MolLogP: 1.5831 | QED: 0.7549046916536171

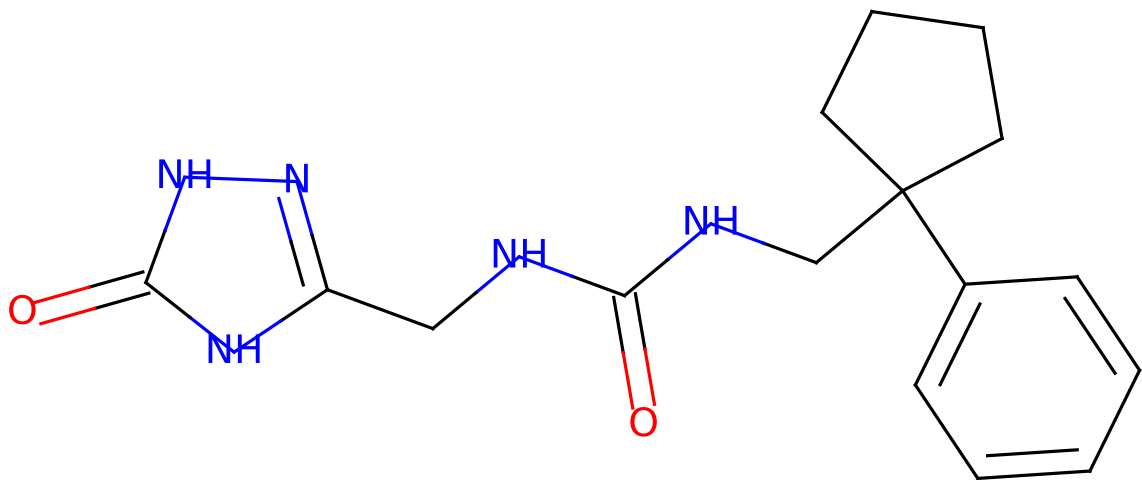c1cc(cc(c1)F)c2cn3c(csc3[nH+]2)C(=O)N4CCC(=O)NCC4

ORD-MCULE-6537132306_1

MolLogP: 1.679400000000001 | QED: 0.3884656547732727

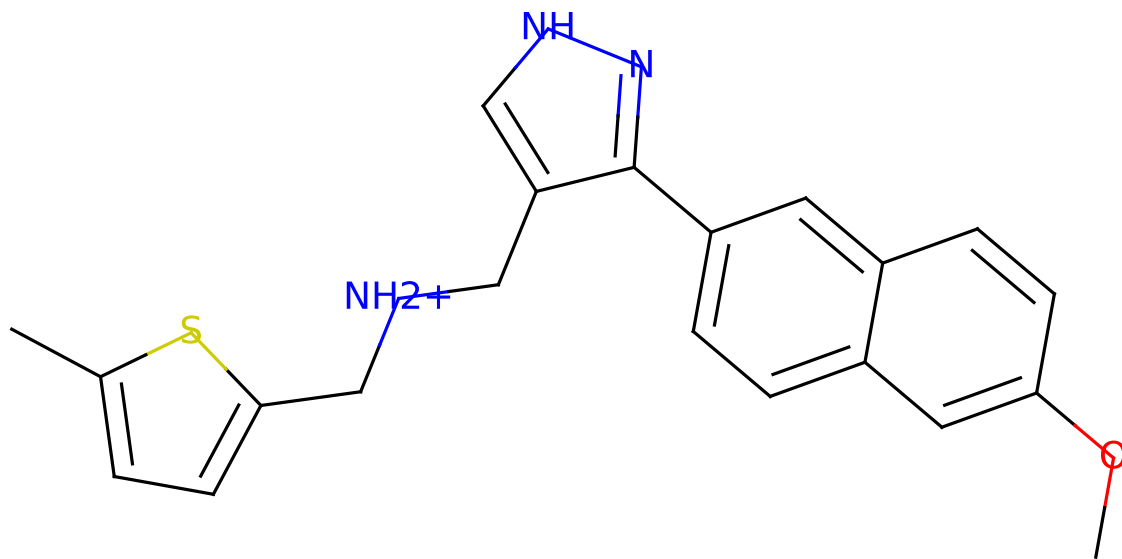Cn1c2c(c(=O)n(c1=O)C)n(c(n2)C[NH+]3CCN(CC3)c4ccc(cc4)F)Cc5cccc6c5cccc6

ORD-MCULE-9488978359_1

MolLogP: 1.4091999999999993 | QED: 0.6705060922590245
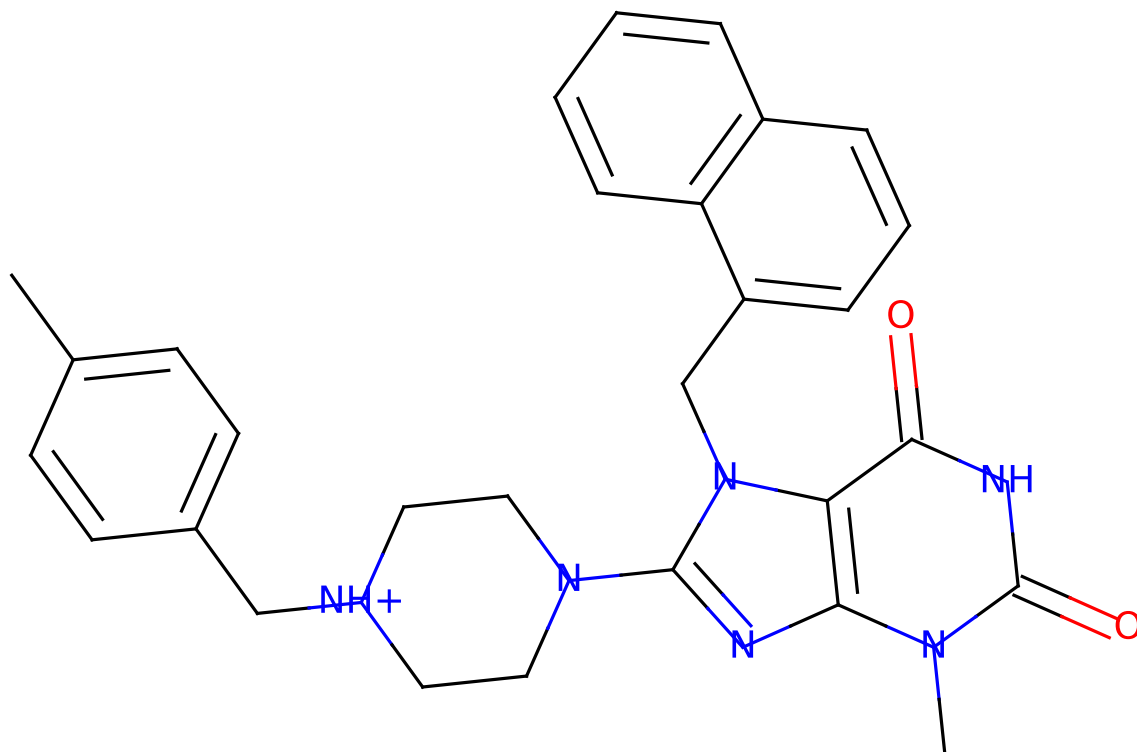
c1ccc(cc1)C2(CCCC2)CNC(=O)NCc3[nH]c(=O)[nH]n3

ORD-MCULE-8823736514_1

MolLogP: 3.872020000000002 | QED: 0.5455855495375038

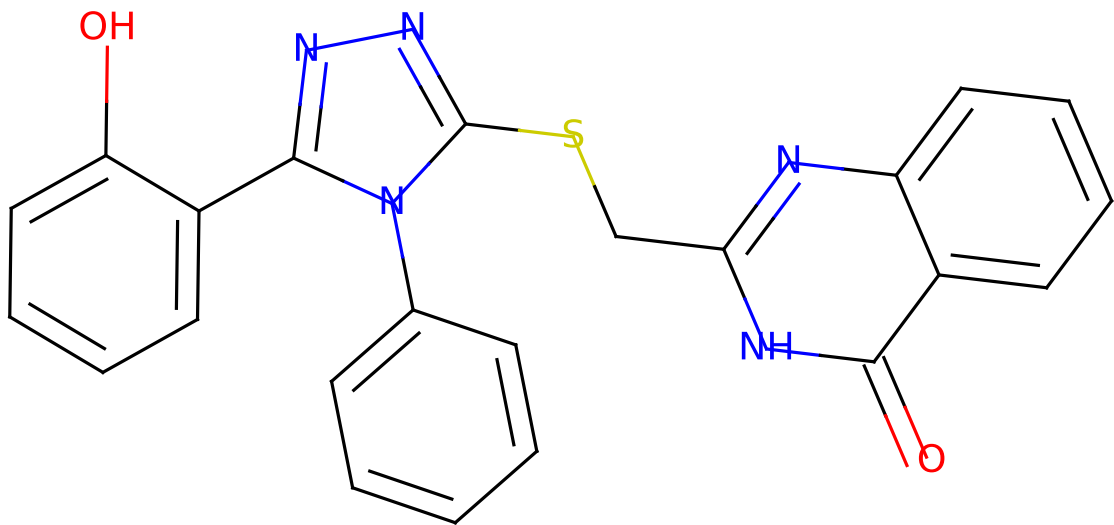Cc1ccc(s1)C[NH2+]Cc2c[nH]nc2c3ccc4cc(ccc4c3)OC

ORD-MCULE-5957284691_2

103

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: 1.4775000000000003 | QED: 0.33193936612782626

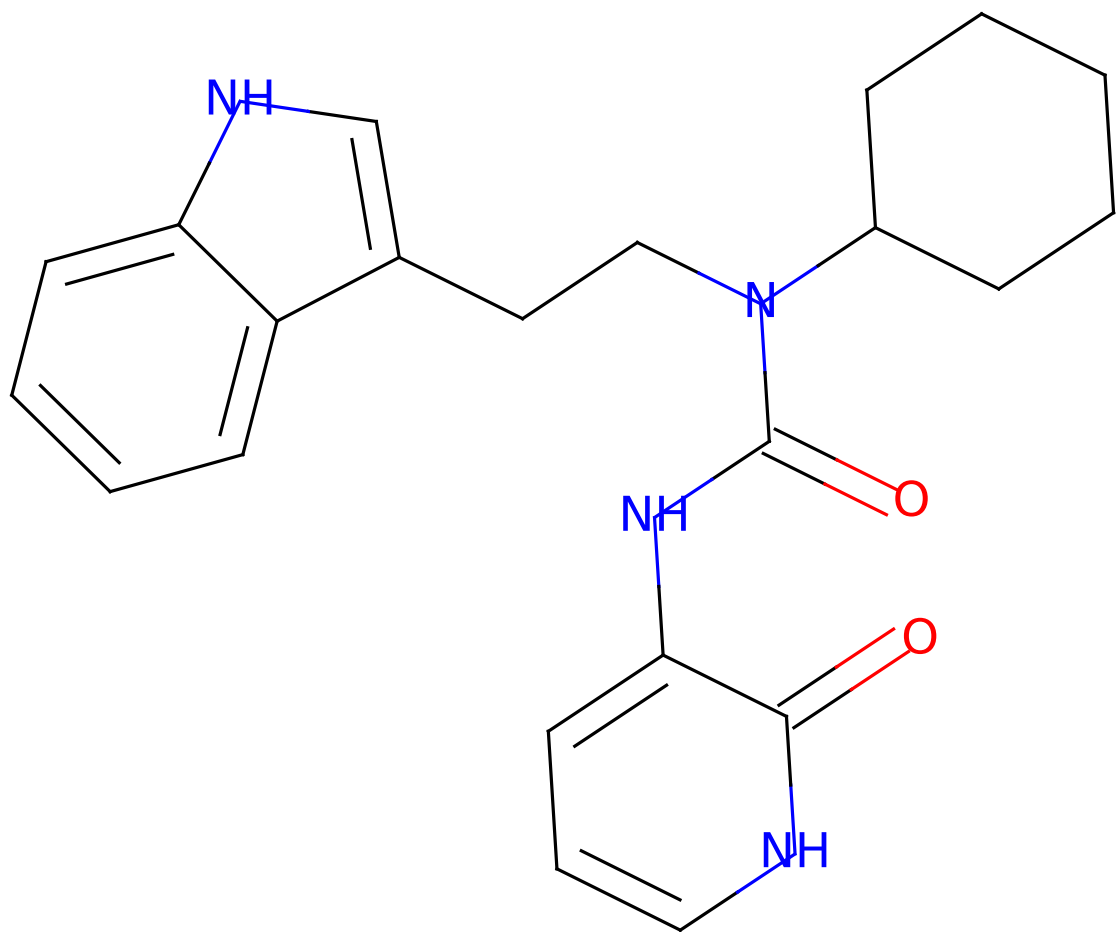COc1ccc(cc1)CCNC(=O)c2cc3c(nc4ccccn4c3=O)n(c2=[NH2+])Cc5ccc(cc5)F

ORD-MCULE-6887706487_1

MolLogP: 4.168700000000002 | QED: 0.40881200045573285

c1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4ccccc4n3)c5ccccc5O
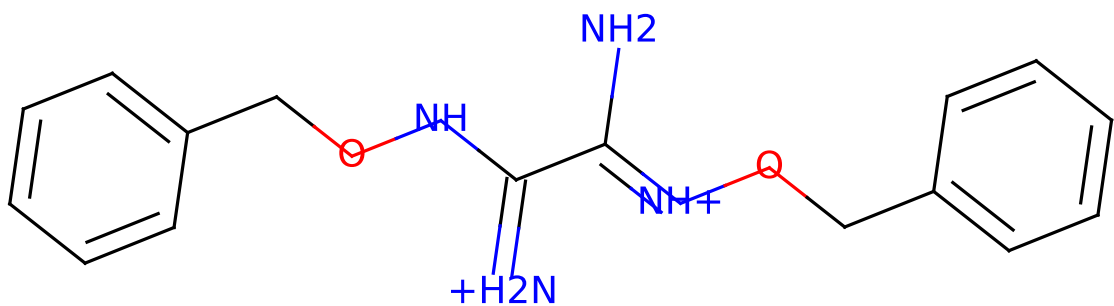
ORD-MCULE-9878325632_1

106

MolLogP: 4.265500000000002 | QED: 0.6197897825841696

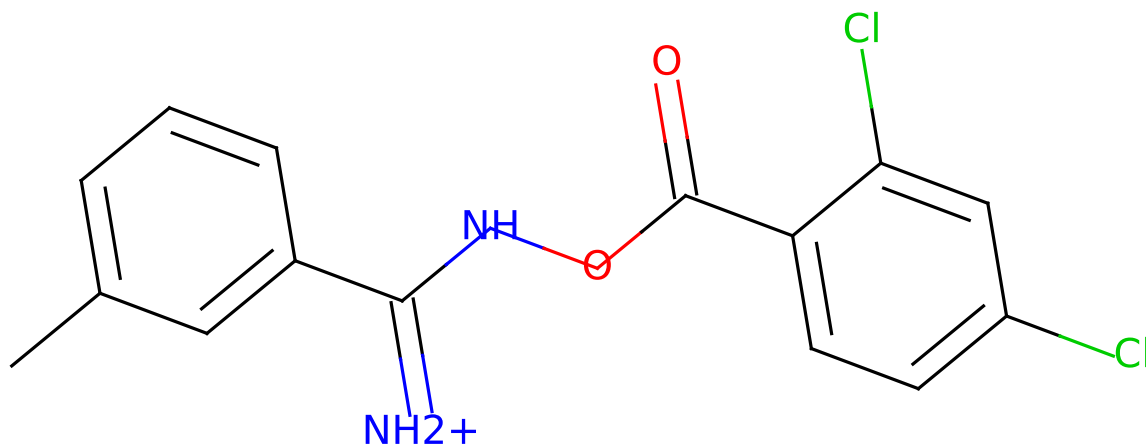c1ccc2c(c1)c(c[nH]2)CCN(C3CCCCC3)C(=O)Nc4ccc[nH]c4=O

ORD-MCULE-2083056029_1

MolLogP: -1.5649999999999962 | QED: 0.2945290701347922

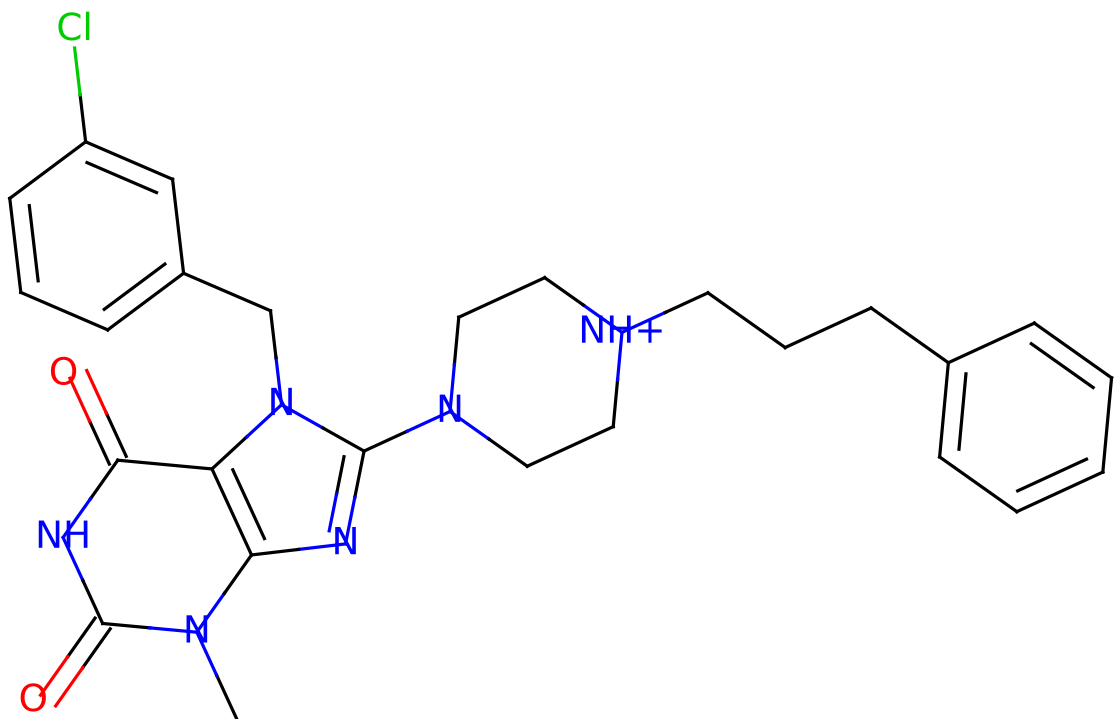c1ccc(cc1)CONC(=[NH2+])/C(=[NH+]/OCc2ccccc2)/N

ORD-MCULE-6929749068_2

MolLogP: 2.1691199999999995 | QED: 0.5055005573998982
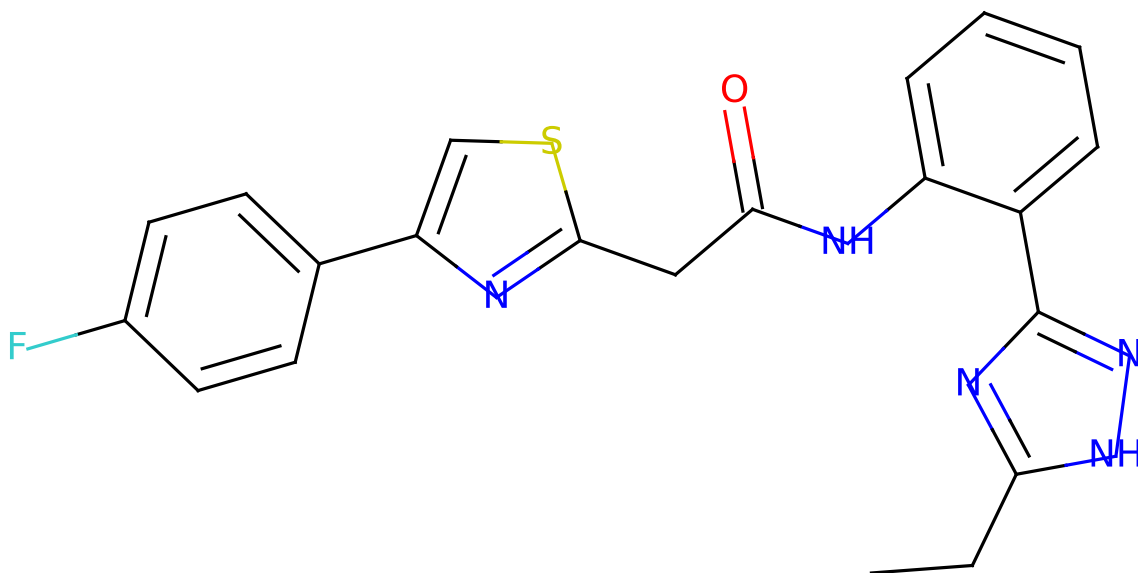
Cc1cccc(c1)C(=[NH2+])NOC(=O)c2ccc(cc2Cl)Cl

ORD-MCULE-5145994619_2

MolLogP: 1.4627000000000023 | QED: 0.40834176238750675

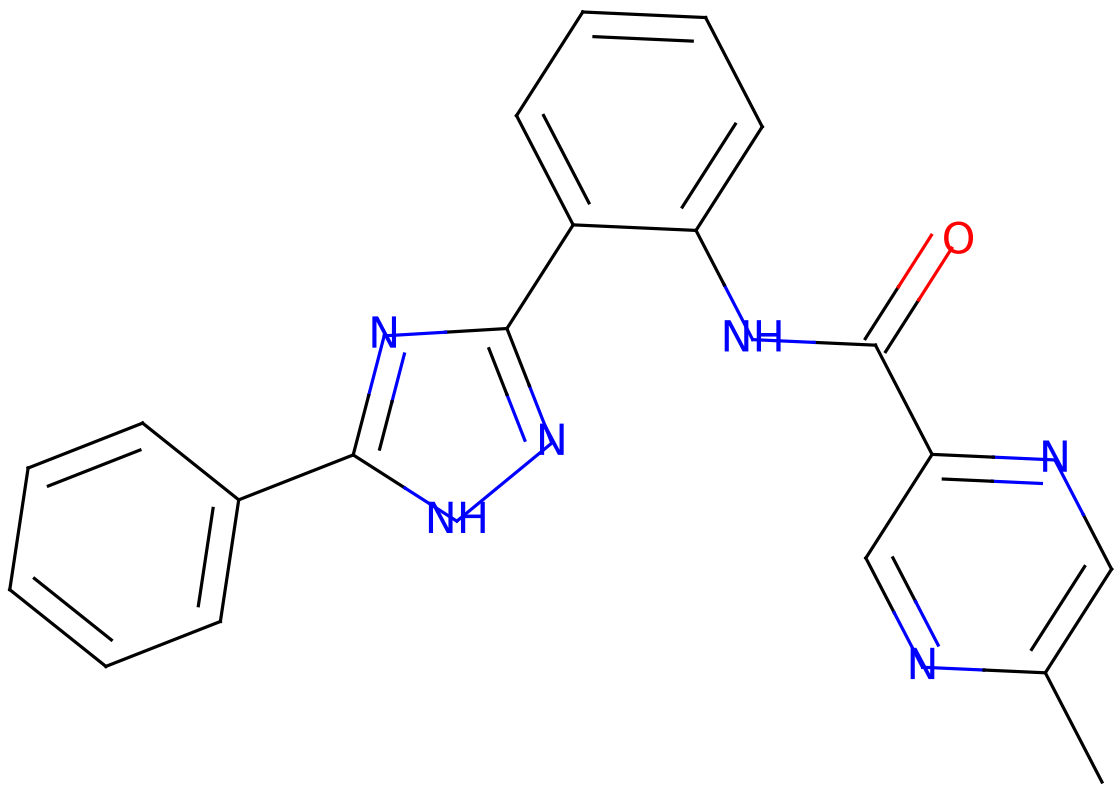Cn1c2c(c(=O)[nH]c1=O)n(c(n2)N3CC[NH+](CC3)CCCc4ccccc4)Cc5cccc(c5)Cl

ORD-MCULE-9446460441_1

MolLogP: 4.477900000000003 | QED: 0.4936757474816063
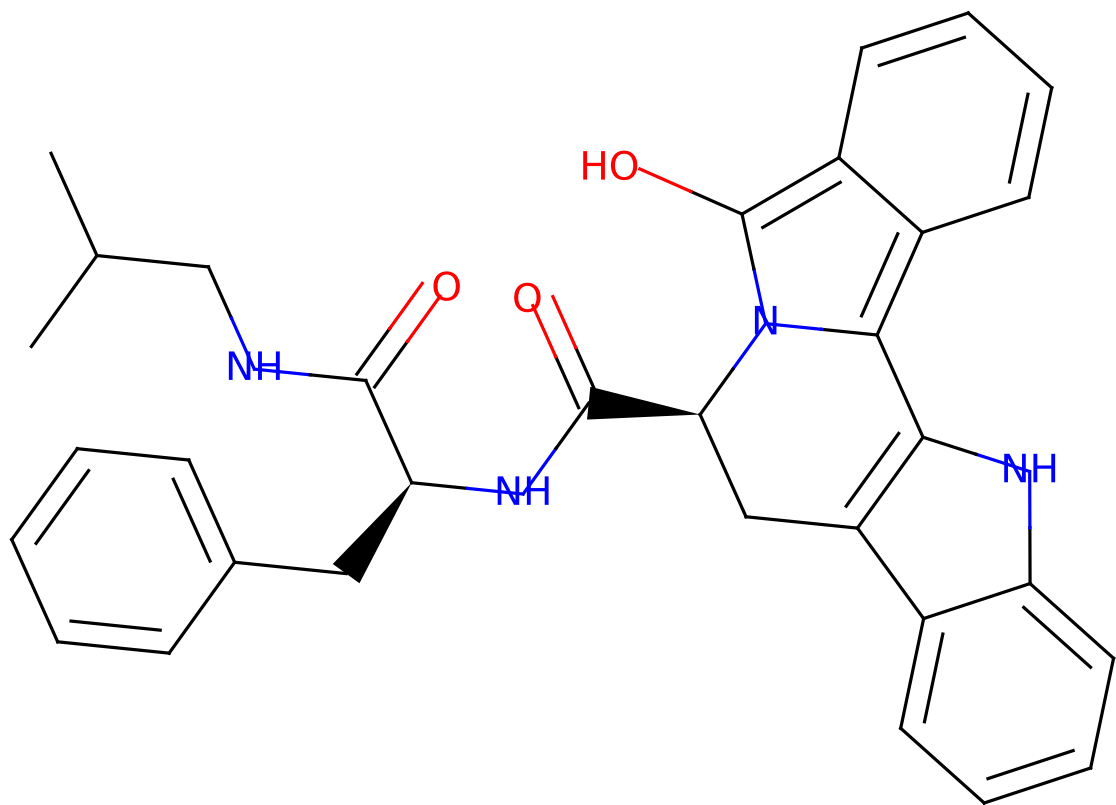
CCc1[nH]nc(n1)c2ccccc2NC(=O)Cc3nc(cs3)c4ccc(cc4)F

ORD-MCULE-5637537904_1

MolLogP: 3.4894200000000017 | QED: 0.5833527144726719
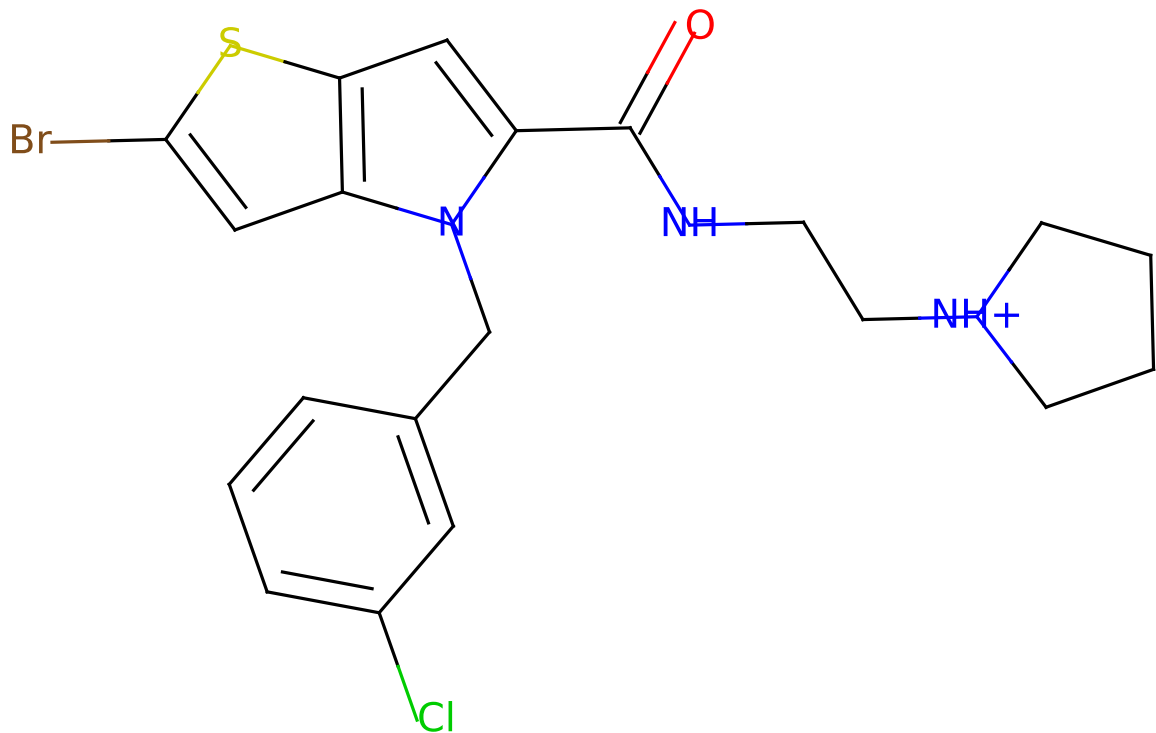
Cc1cnc(cn1)C(=O)Nc2ccccc2c3nc([nH]n3)c4ccccc4

ORD-MCULE-5087943183_2

112

MolLogP: 5.092100000000004 | QED: 0.24051335775492633

CC(C)CNC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O
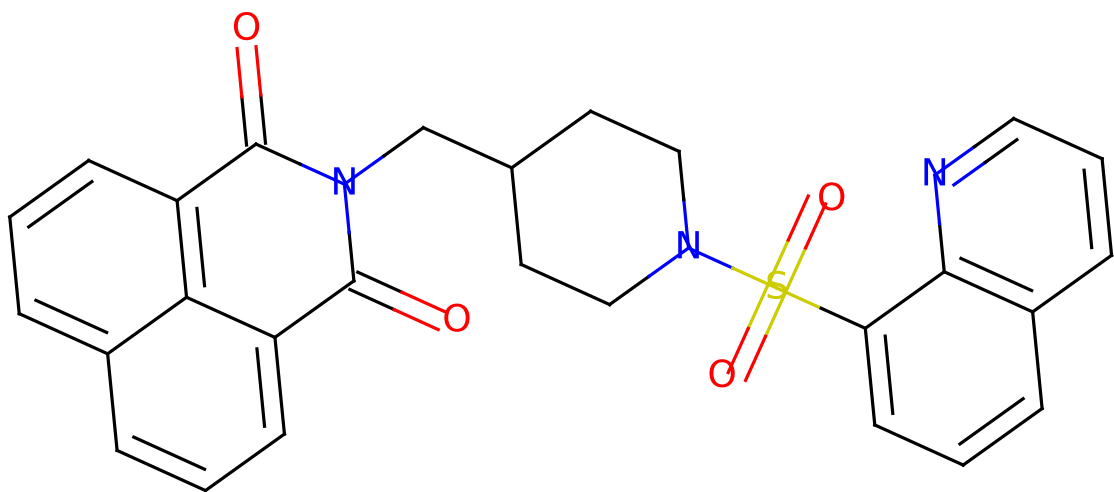
ORD-MCULE-5744226570_1

113

MolLogP: 3.5755000000000017 | QED: 0.5713670532654103
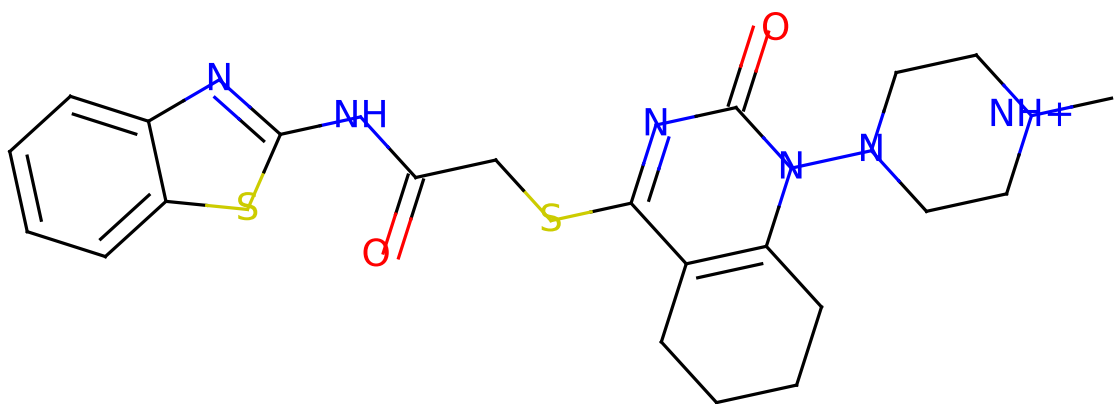
c1cc(cc(c1)Cl)Cn2c3cc(sc3cc2C(=O)NCC[NH+]4CCCC4)Br

ORD-MCULE-8462272476_1

MolLogP: 4.084900000000004 | QED: 0.4065854846130124

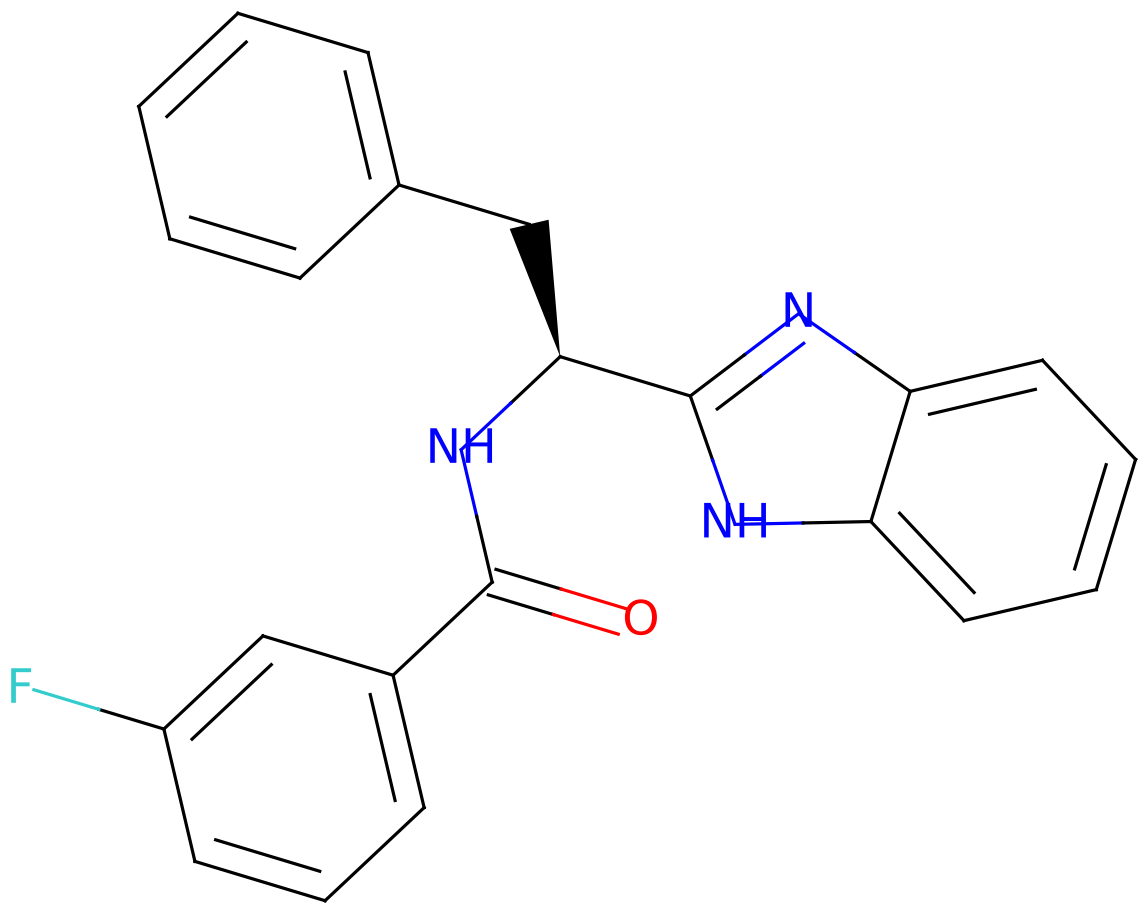c1cc2cccc3c2c(c1)C(=O)N(C3=O)CC4CCN(CC4)S(=O)(=O)c5cccc6c5nccc6

ORD-MCULE-4940228361_1

MolLogP: 0.928900000000001 | QED: 0.4255211702032764

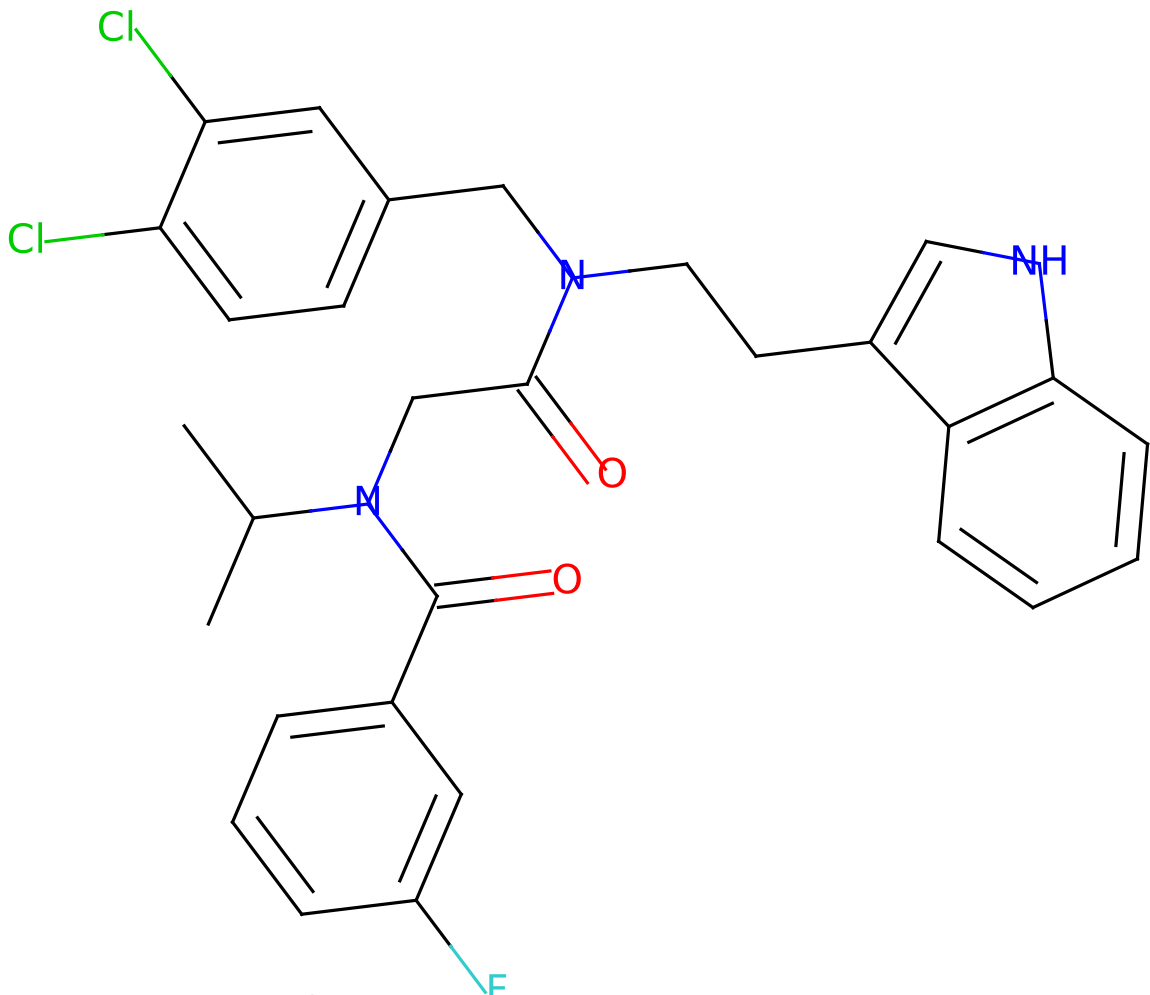C[NH+]1CCN(CC1)n2c3c(c(nc2=O)SCC(=O)Nc4nc5ccccc5s4)CCCC3

ORD-MCULE-5552350264_1

MolLogP: 4.415800000000003 | QED: 0.5542691106258936

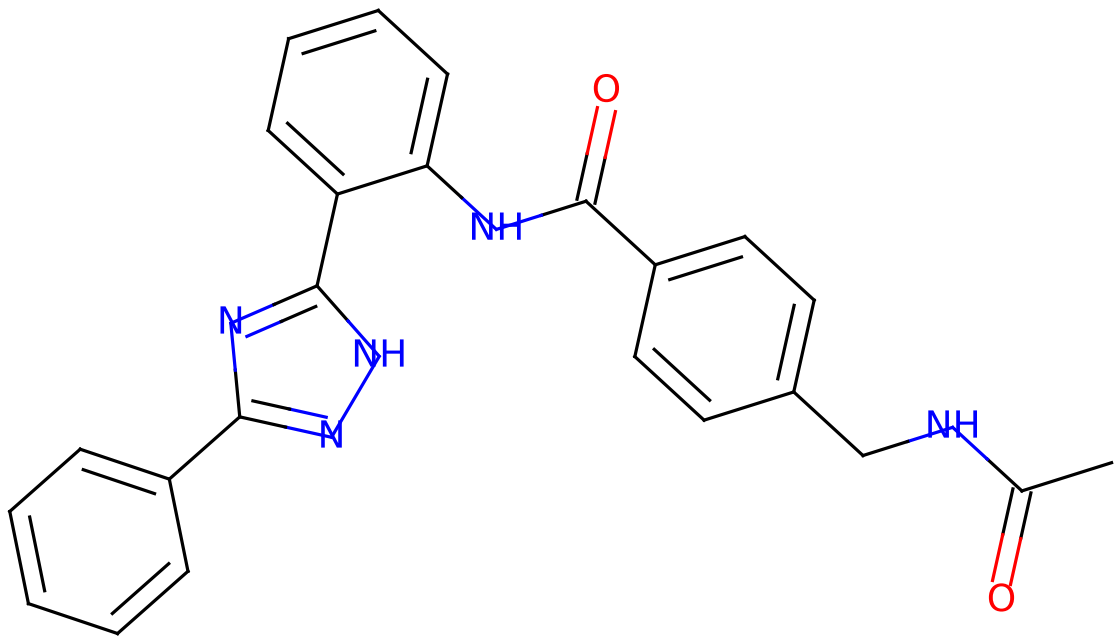c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)c4cccc(c4)F

ORD-MCULE-6499664919_1

117

MolLogP: 6.735900000000006 | QED: 0.25587382028192834

CC(C)N(CC(=O)N(CCc1c[nH]c2c1cccc2)Cc3ccc(c(c3)Cl)Cl)C(=O)c4cccc(c4)F
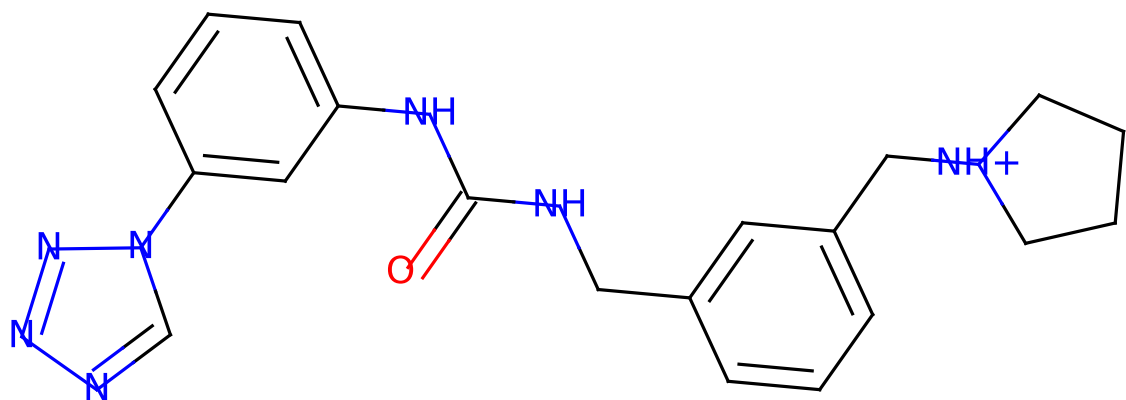
ORD-MCULE-1618528086_1

MolLogP: 4.027100000000002 | QED: 0.44600141958321116

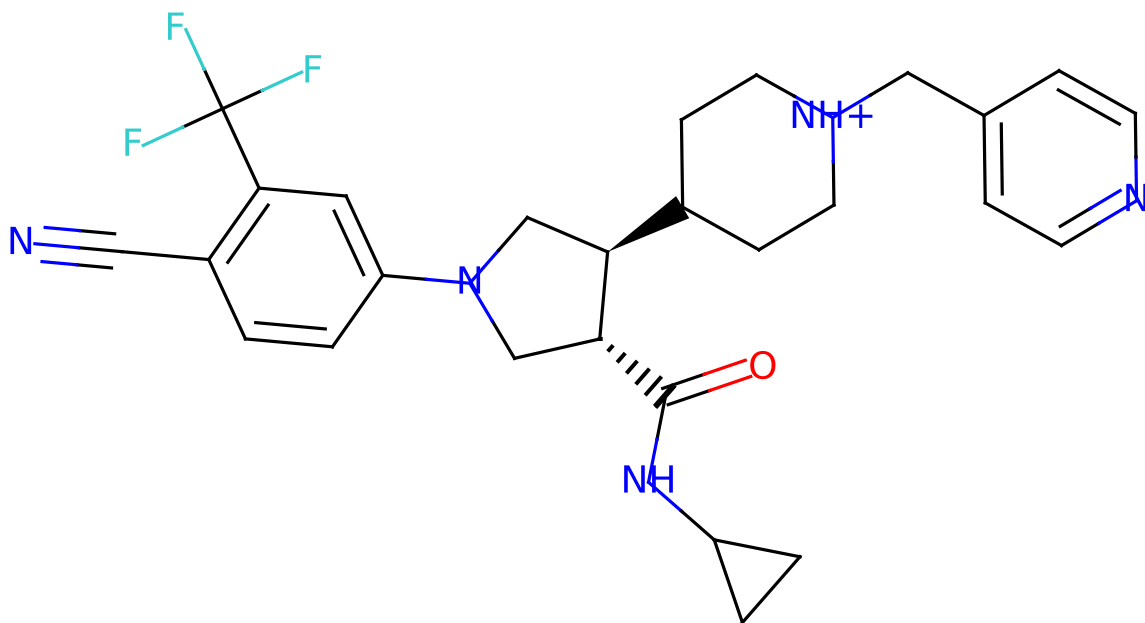CC(=O)NCc1ccc(cc1)C(=O)Nc2ccccc2c3[nH]nc(n3)c4ccccc4

ORD-MCULE-7152686229_1

MolLogP: 1.162699999999999 | QED: 0.6006008381376307
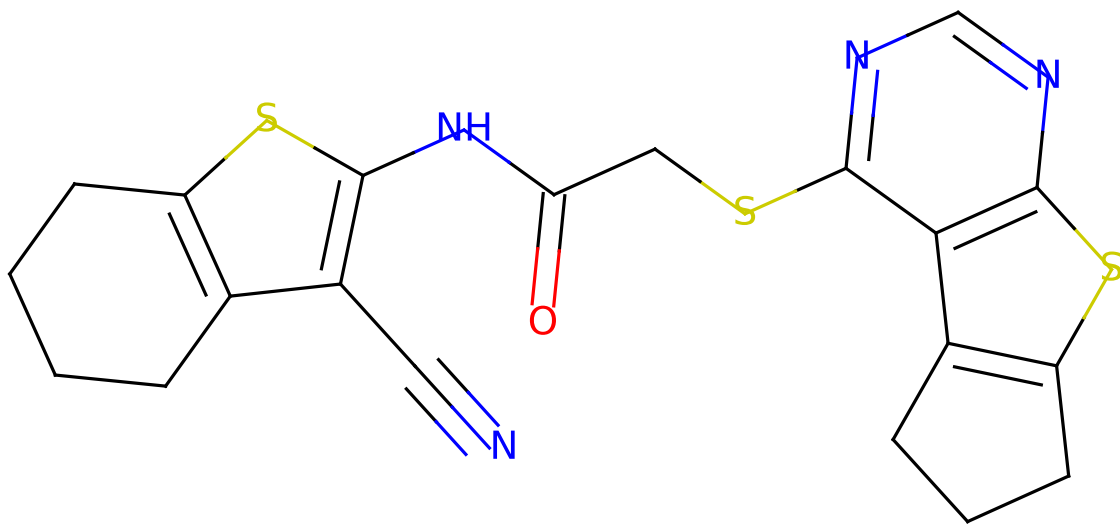
c1cc(cc(c1)C[NH+]2CCCC2)CNC(=O)Nc3cccc(c3)n4cnnn4

ORD-MCULE-1562586832_1

120

MolLogP: 2.798180000000001 | QED: 0.6427003035078636

c1cc(c(cc1N2C[C@H]([C@@H](C2)C(=O)NC3CC3)C4CC[NH+](CC4)Cc5ccncc5)C(F)(F)F)C#N
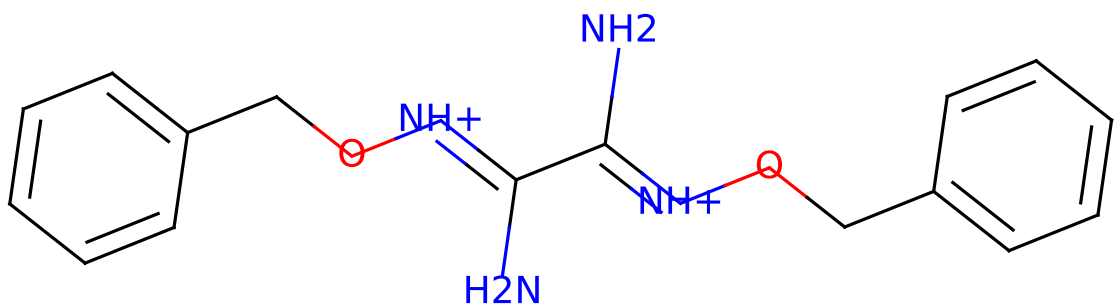
ORD-MCULE-2750885730_1

MolLogP: 4.722780000000003 | QED: 0.4822073179363986

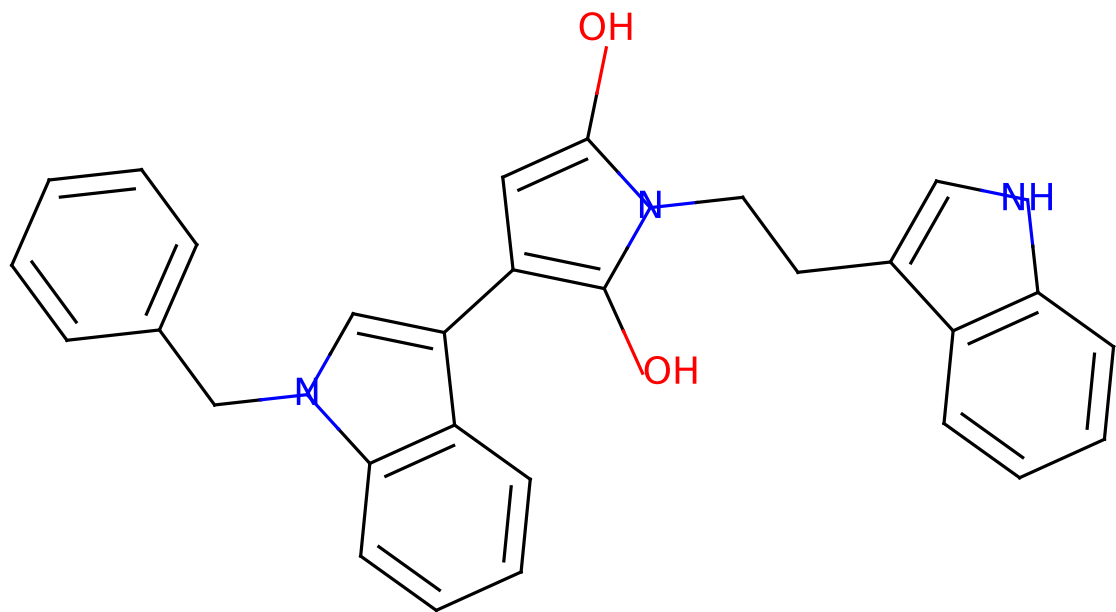c1nc2c(c3c(s2)CCC3)c(n1)SCC(=O)Nc4c(c5c(s4)CCCC5)C#N

ORD-MCULE-4016357234_1

122

MolLogP: -1.874399999999996 | QED: 0.28519401198506406

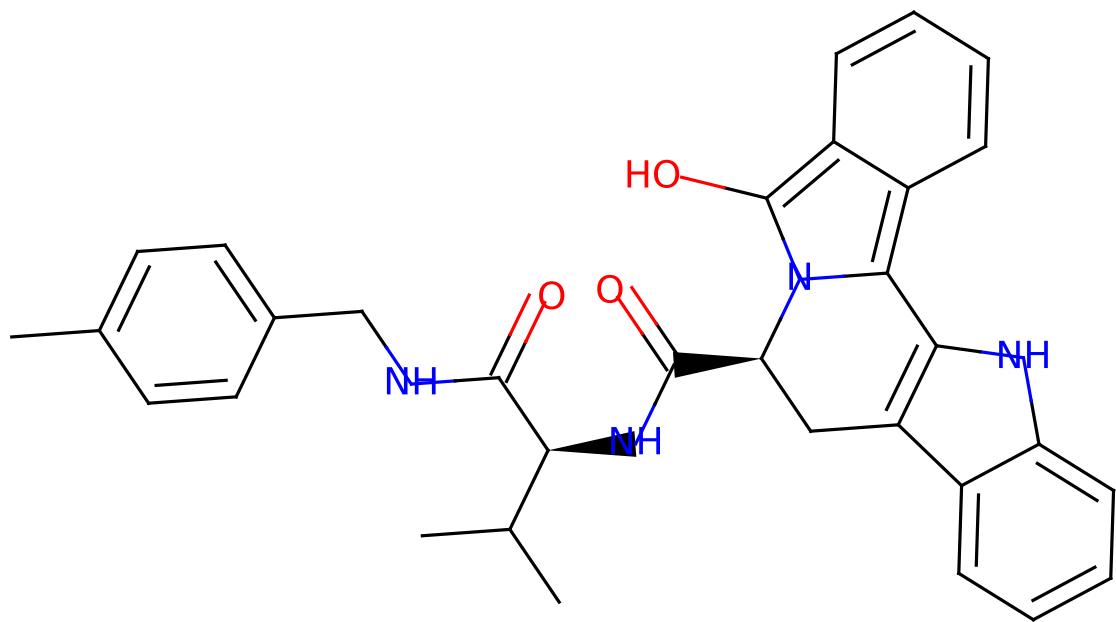c1ccc(cc1)CO/[NH+]=C(\N)/C(=[NH+]/OCc2ccccc2)/N

ORD-MCULE-6929749068_1

MolLogP: 6.2933000000000066 | QED: 0.28074538236838986

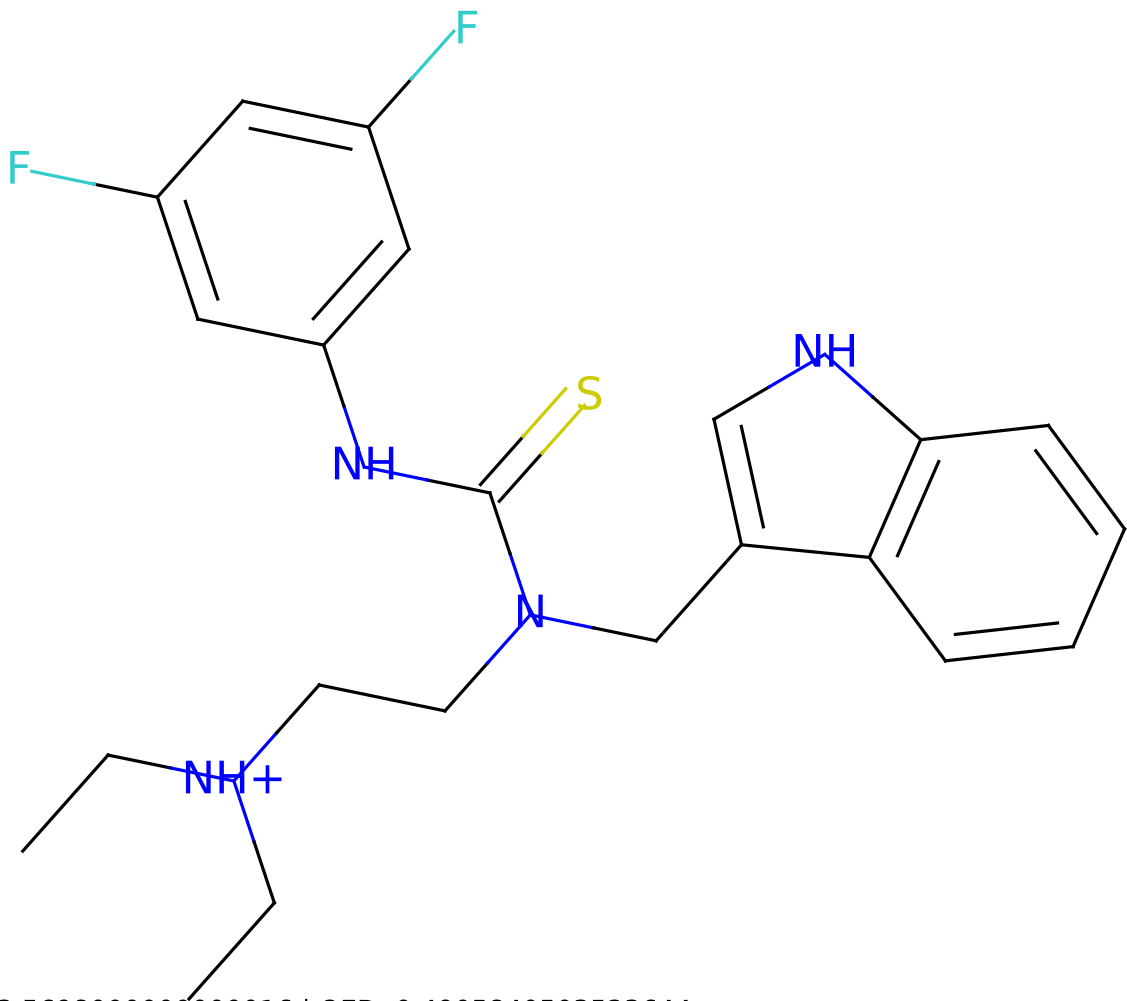c1ccc(cc1)Cn2cc(c3c2cccc3)c4cc(n(c4O)CCc5c[nH]c6c5cccc6)O

ORD-MCULE-8667499303_1

124

MolLogP: 5.358020000000005 | QED: 0.24263328233406037

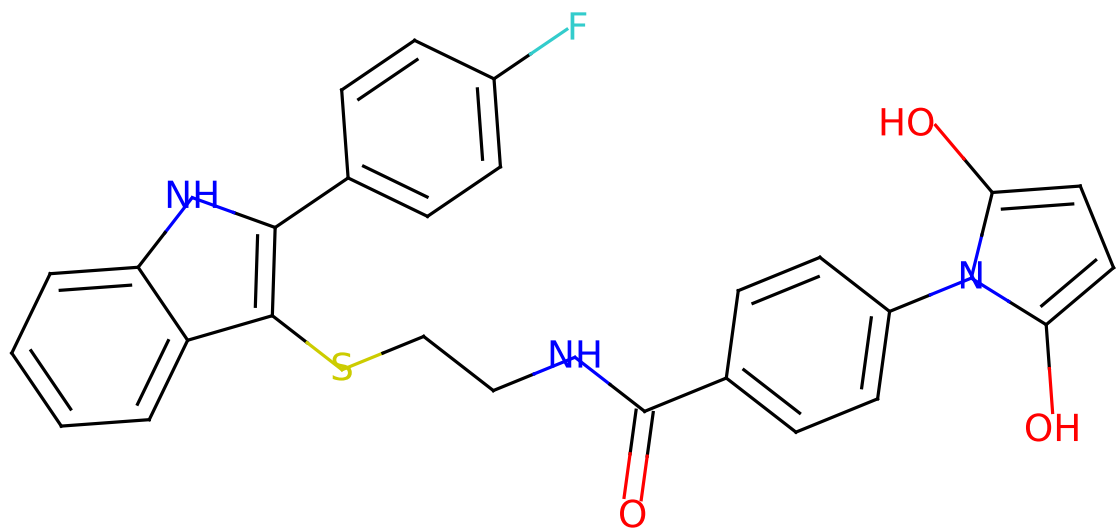Cc1ccc(cc1)CNC(=O)[C@H](C(C)C)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O

ORD-MCULE-8649642231_1

MolLogP: 3.5698000000000016 | QED: 0.4905840503523644

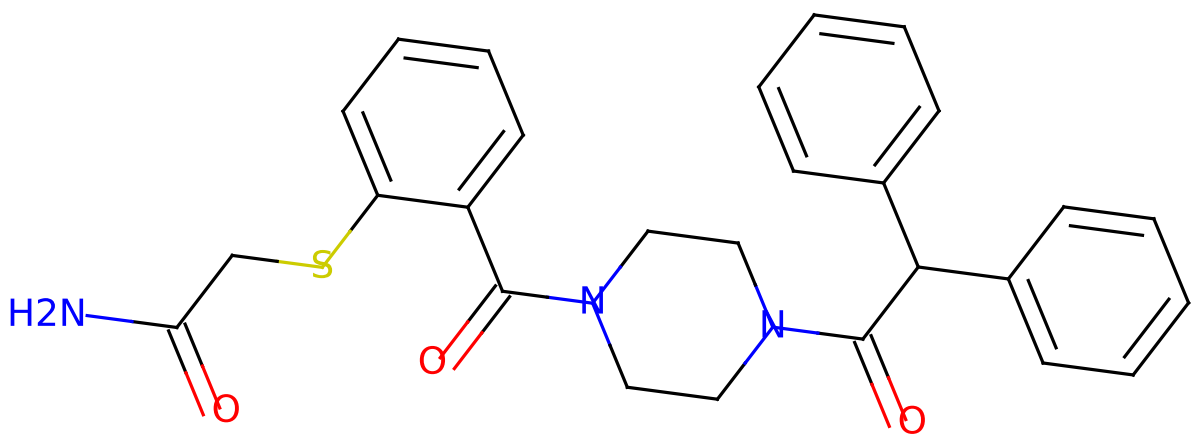CC[NH+](CC)CCN(Cc1c[nH]c2c1cccc2)C(=S)Nc3cc(cc(c3)F)F

ORD-MCULE-6419793505_1

MolLogP: 5.698000000000006 | QED: 0.1751712265847373

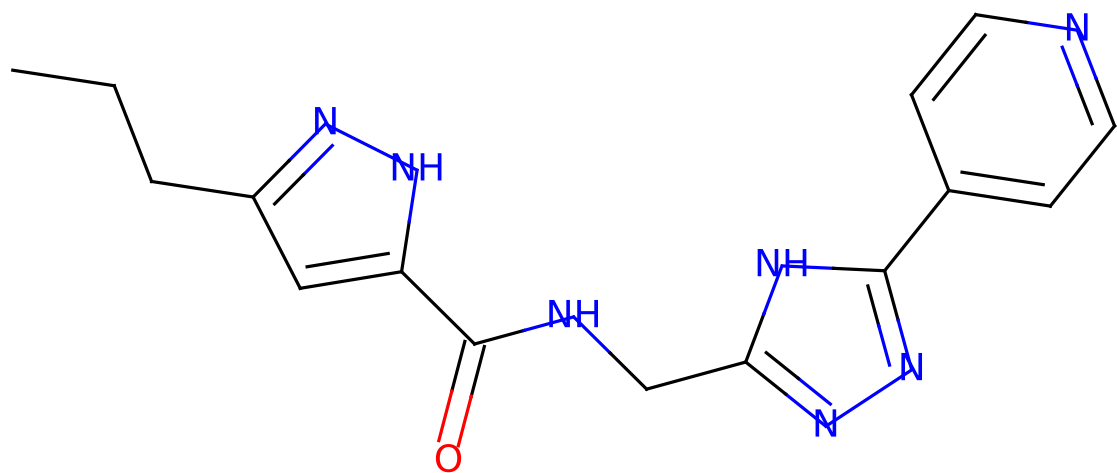c1ccc2c(c1)c(c([nH]2)c3ccc(cc3)F)SCCNC(=O)c4ccc(cc4)n5c(ccc5O)O

ORD-MCULE-8115904674_1

127

MolLogP: 3.3805000000000005 | QED: 0.5334780547848035

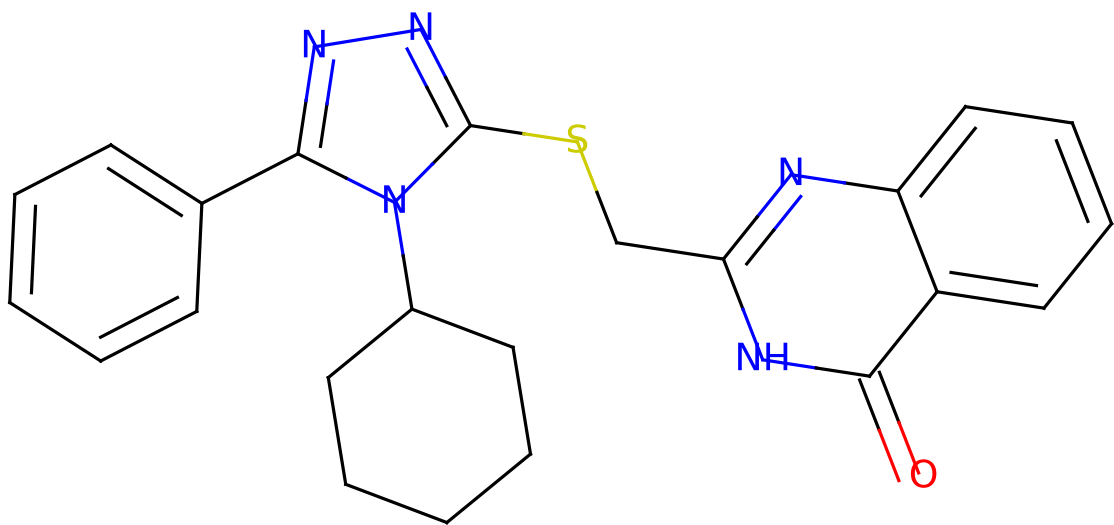c1ccc(cc1)C(c2ccccc2)C(=O)N3CCN(CC3)C(=O)c4ccccc4SCC(=O)N

ORD-MCULE-2742509230_1

MolLogP: 1.4722999999999997 | QED: 0.637925488109036

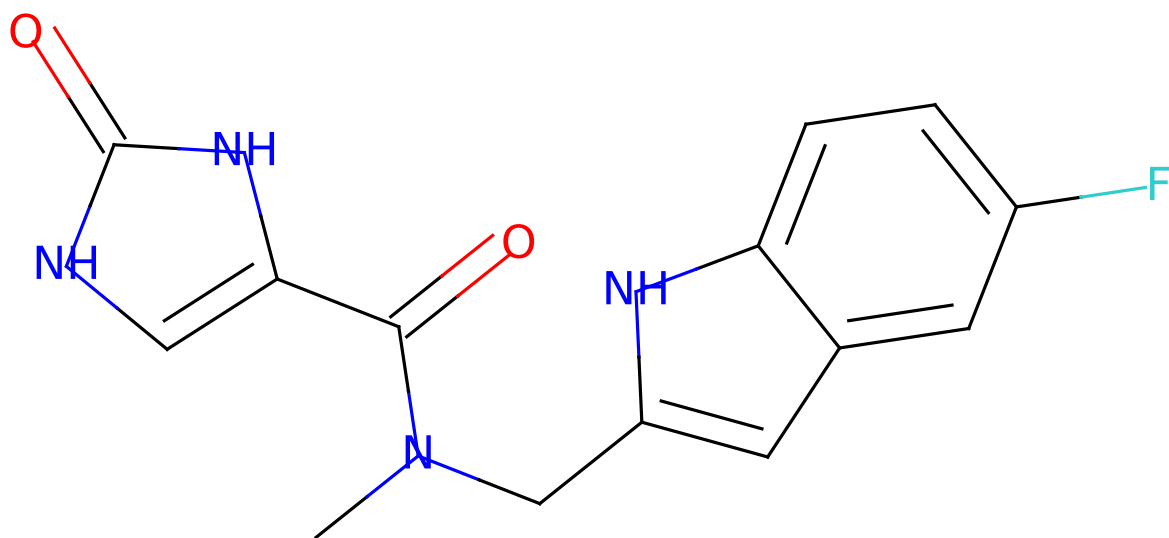CCCc1cc([nH]n1)C(=O)NCc2[nH]c(nn2)c3ccncc3

ORD-MCULE-9274314730_6

MolLogP: 4.979100000000003 | QED: 0.4635852670383765

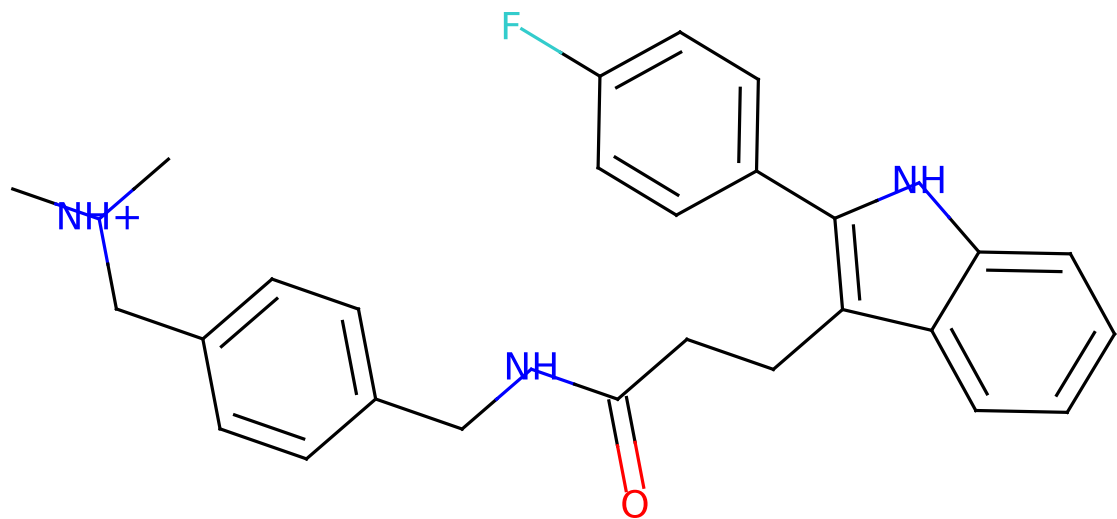c1ccc(cc1)c2nnc(n2C3CCCCC3)SCc4[nH]c(=O)c5ccccc5n4

ORD-MCULE-4525414745_1

MolLogP: 1.5955999999999997 | QED: 0.6835212266203077

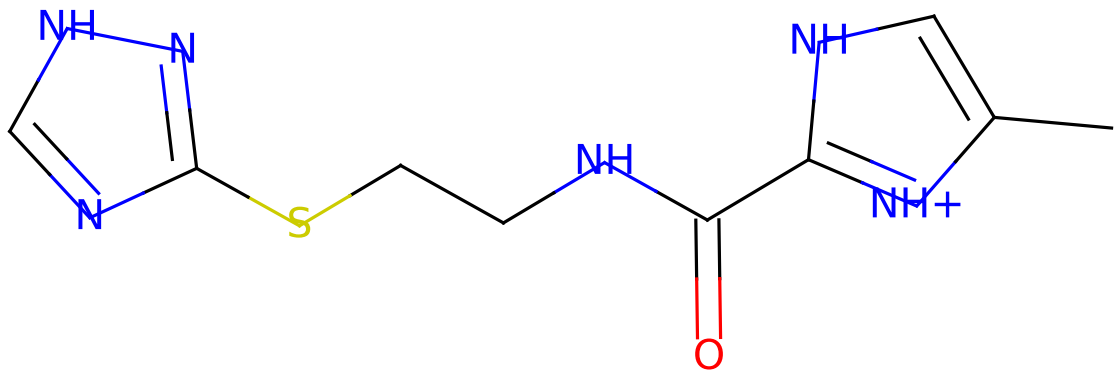CN(Cc1cc2cc(ccc2[nH]1)F)C(=O)c3c[nH]c(=O)[nH]3

ORD-MCULE-4793474277_1

MolLogP: 3.8675000000000024 | QED: 0.3905849596735302

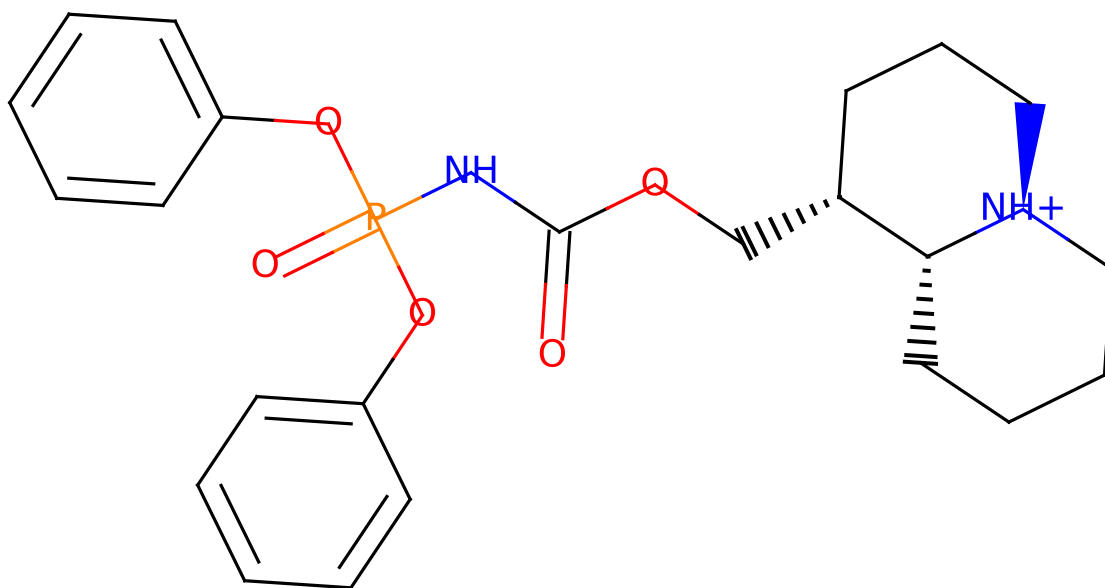C[NH+](C)Cc1ccc(cc1)CNC(=O)CCc2c3ccccc3[nH]c2c4ccc(cc4)F

ORD-MCULE-8278306247_1

MolLogP: -0.2225800000000006 | QED: 0.5061753470565761
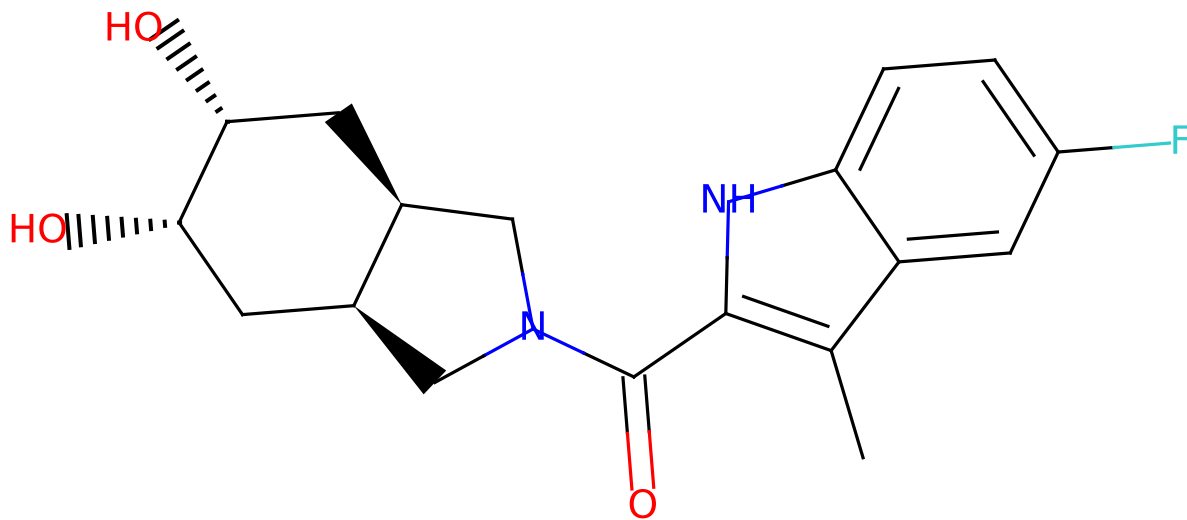
Cc1c[nH]c([nH+]1)C(=O)NCCSc2nc[nH]n2

ORD-MCULE-3031881642_5

133

MolLogP: 3.826100000000002 | QED: 0.633786993463605

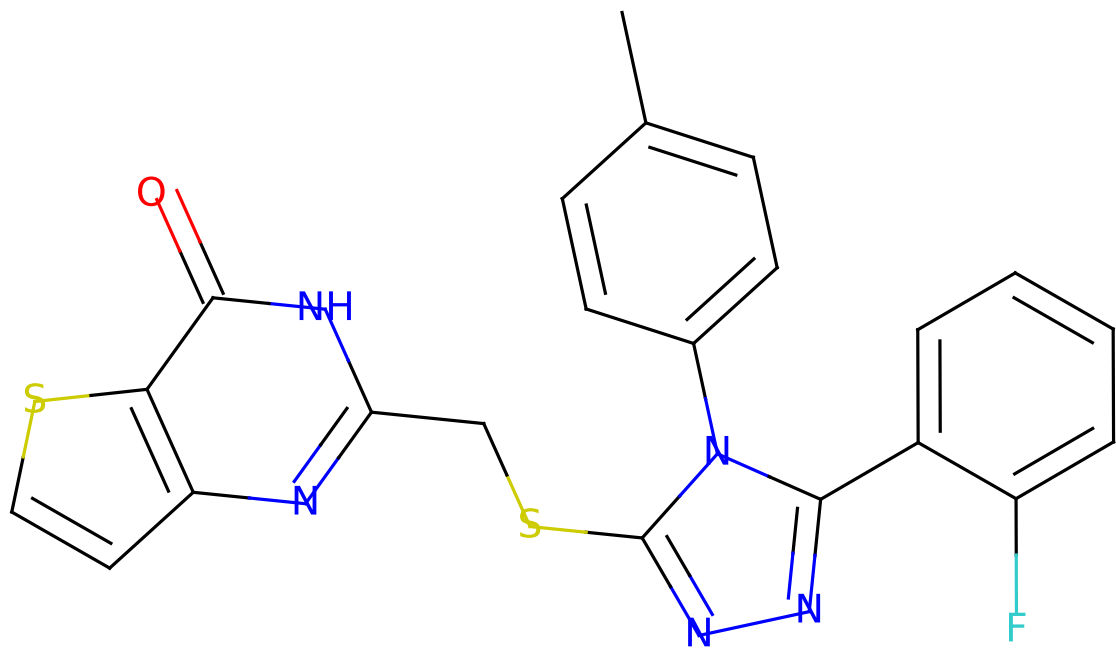c1ccc(cc1)OP(=O)(NC(=O)OC[C@@H]2CCC[N@@H+]3[C@@H]2CCCC3)Oc4ccccc4

ORD-MCULE-4122169139_1

MolLogP: 1.8192199999999996 | QED: 0.7454546925399498

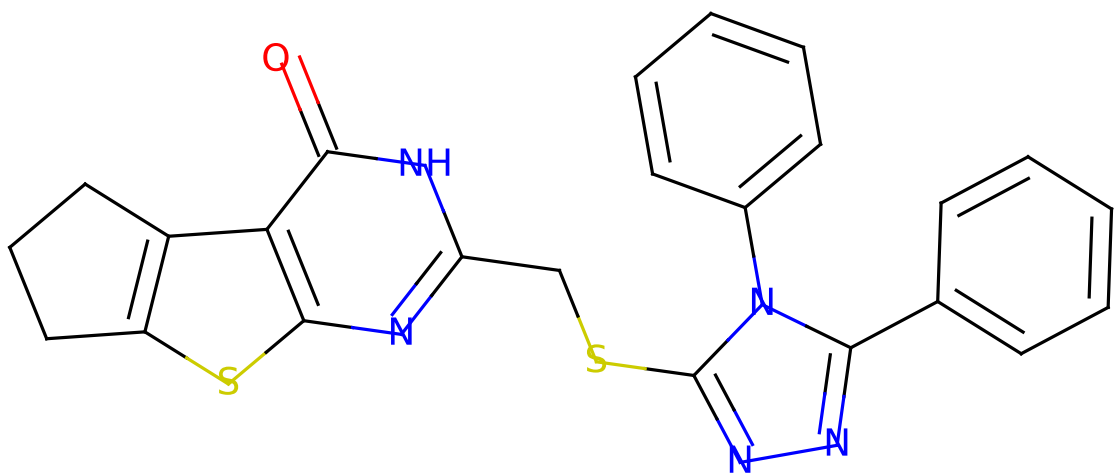Cc1c2cc(ccc2[nH]c1C(=O)N3C[C@H]4C[C@@H]([C@@H](C[C@H]4C3)O)O)F

ORD-MCULE-7272550771_1

MolLogP: 4.972120000000003 | QED: 0.38342429300269104

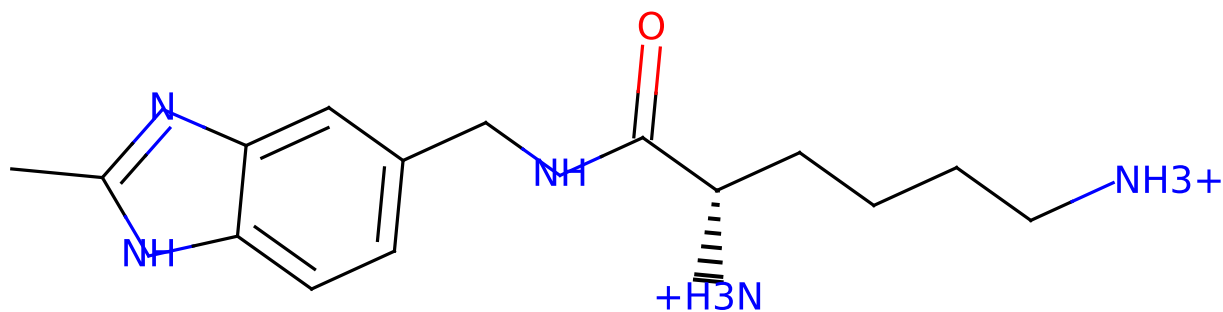Cc1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4c(n3)ccs4)c5ccccc5F

ORD-MCULE-7430389497_1

136

MolLogP: 5.013300000000003 | QED: 0.37541396911851704

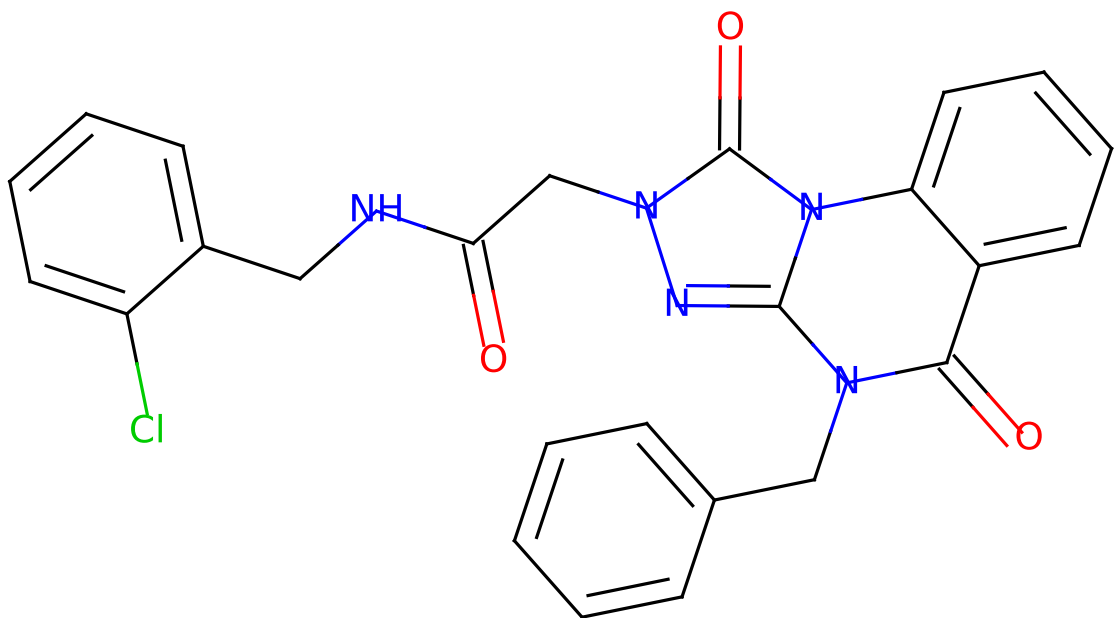c1ccc(cc1)c2nnc(n2c3ccccc3)SCc4[nH]c(=O)c5c6c(sc5n4)CCC6

ORD-MCULE-5456008772_1

MolLogP: -0.4897799999999974 | QED: 0.5158008337340667

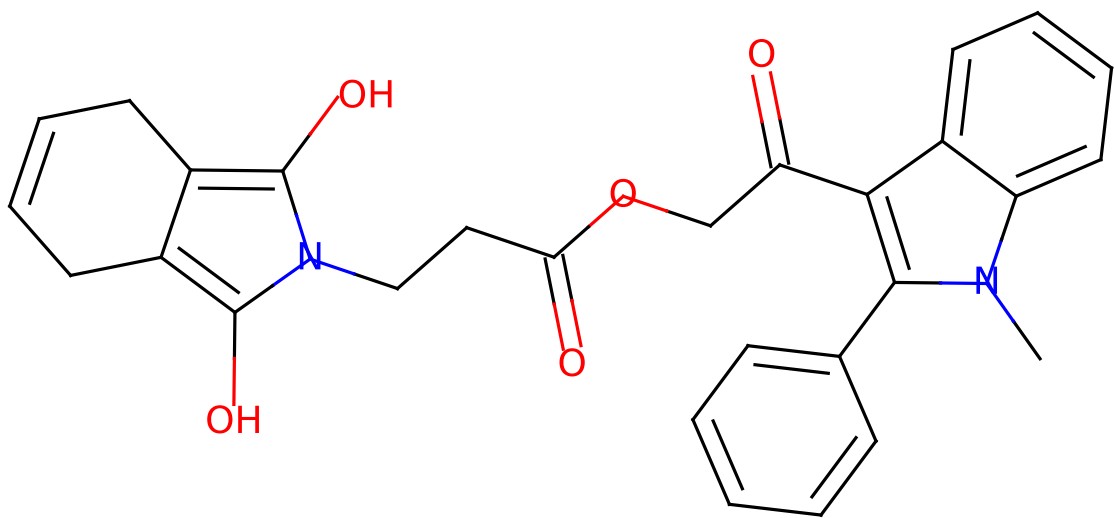Cc1[nH]c2ccc(cc2n1)CNC(=O)[C@H](CCCC[NH3+])[NH3+]

ORD-MCULE-7841773146_2

MolLogP: 2.8290000000000006 | QED: 0.41036881357903016

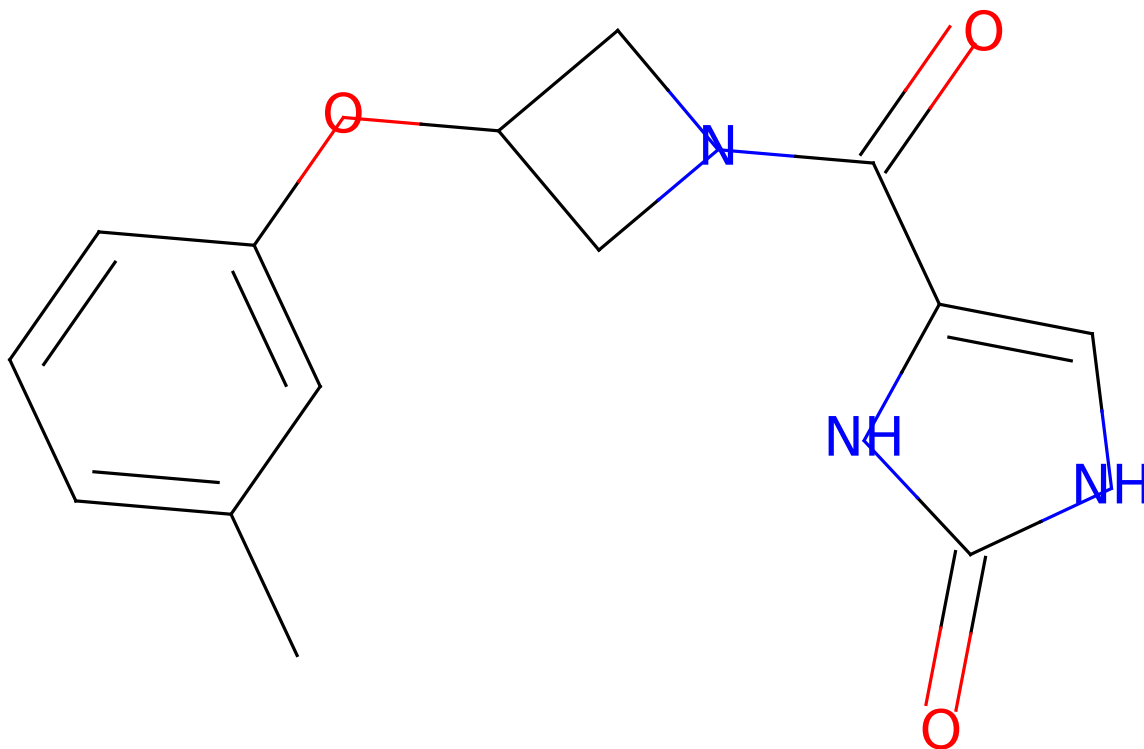c1ccc(cc1)Cn2c(=O)c3ccccc3n4c2nn(c4=O)CC(=O)NCc5ccccc5Cl

ORD-MCULE-9240489399_1

MolLogP: 4.529000000000005 | QED: 0.23518885305592843

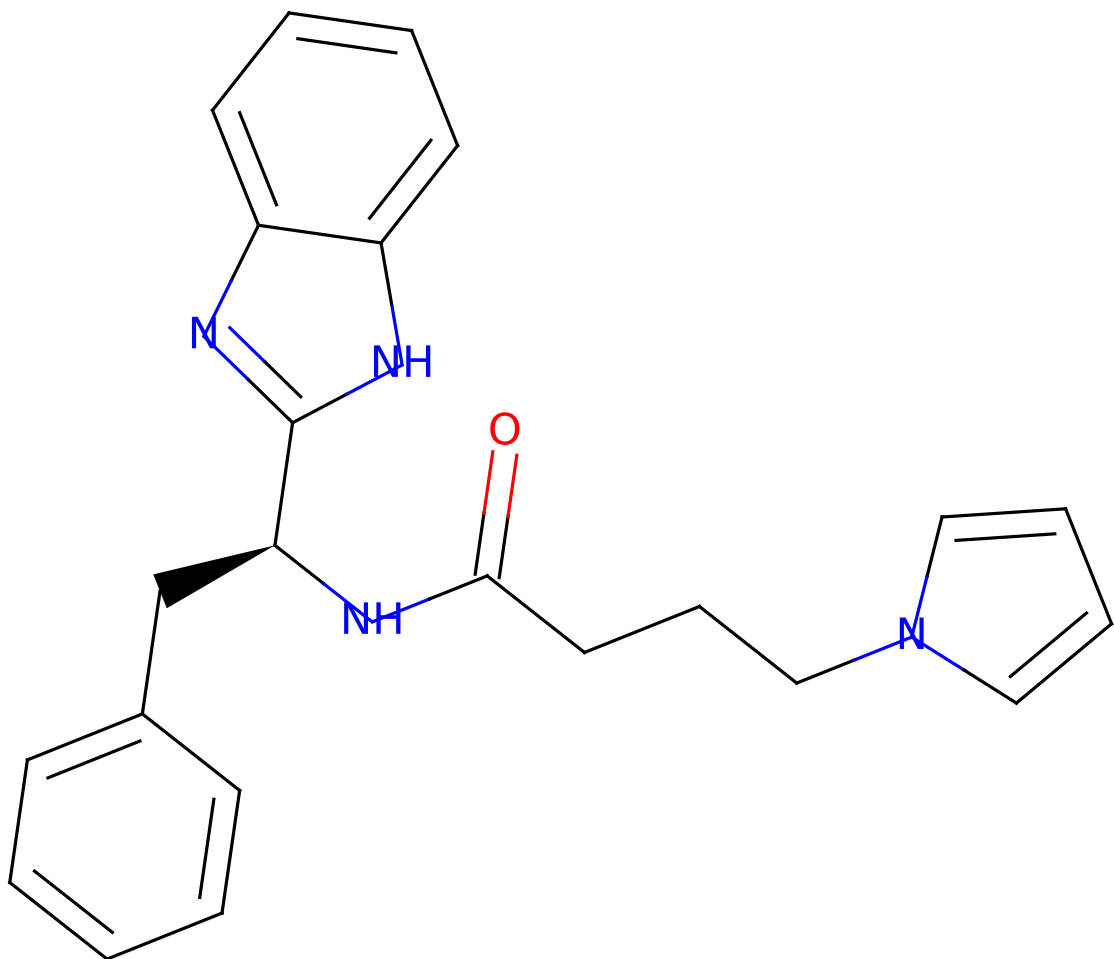Cn1c2ccccc2c(c1c3ccccc3)C(=O)COC(=O)CCn4c(c5c(c4O)CC=CC5)O

ORD-MCULE-2859578203_1

MolLogP: 0.9148199999999995 | QED: 0.8723455942903283

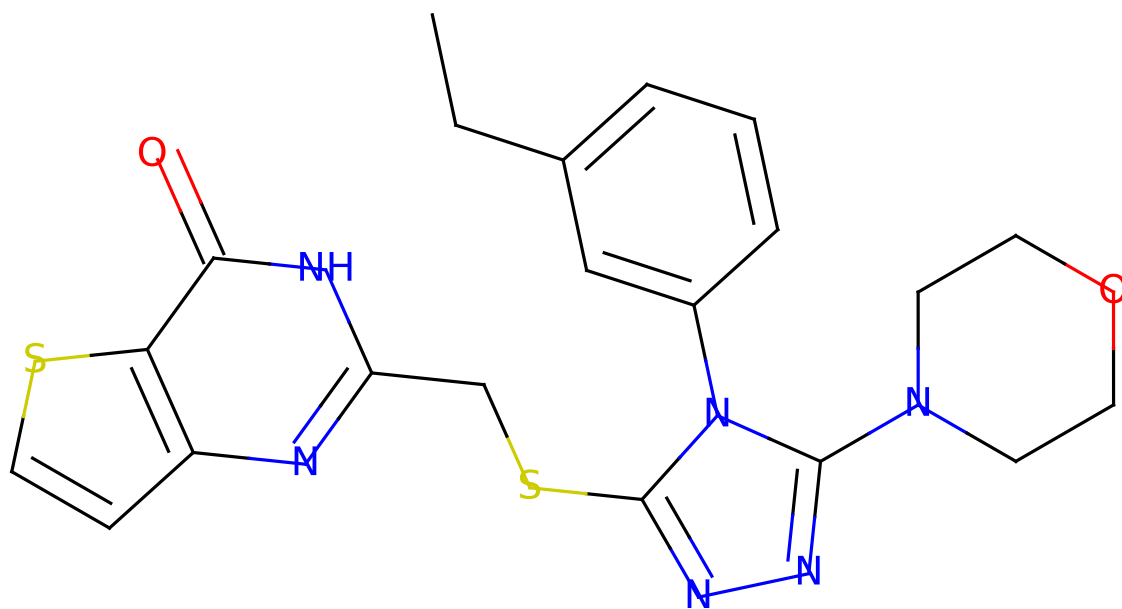Cc1cccc(c1)OC2CN(C2)C(=O)c3c[nH]c(=O)[nH]3

ORD-MCULE-3526061706_1

MolLogP: 4.244800000000002 | QED: 0.48575188876455516

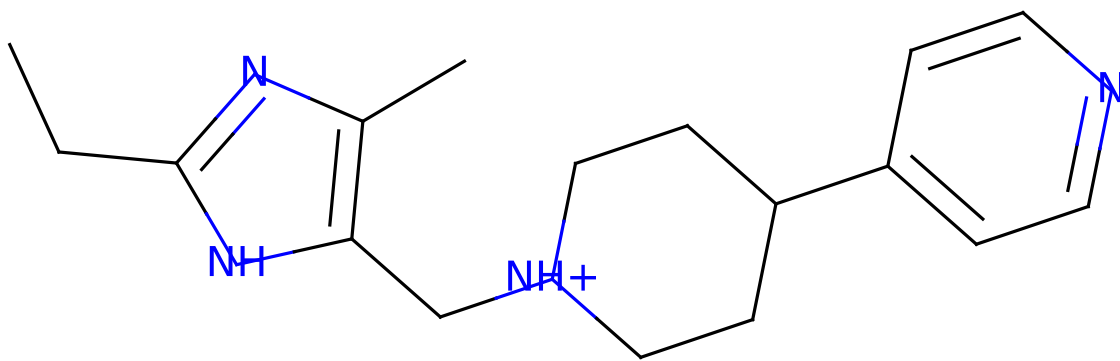c1ccc(cc1)C[C@@H](c2[nH]c3ccccc3n2)NC(=O)CCCn4cccc4

ORD-MCULE-4811796101_1

MolLogP: 3.2566000000000015 | QED: 0.44743771673666255

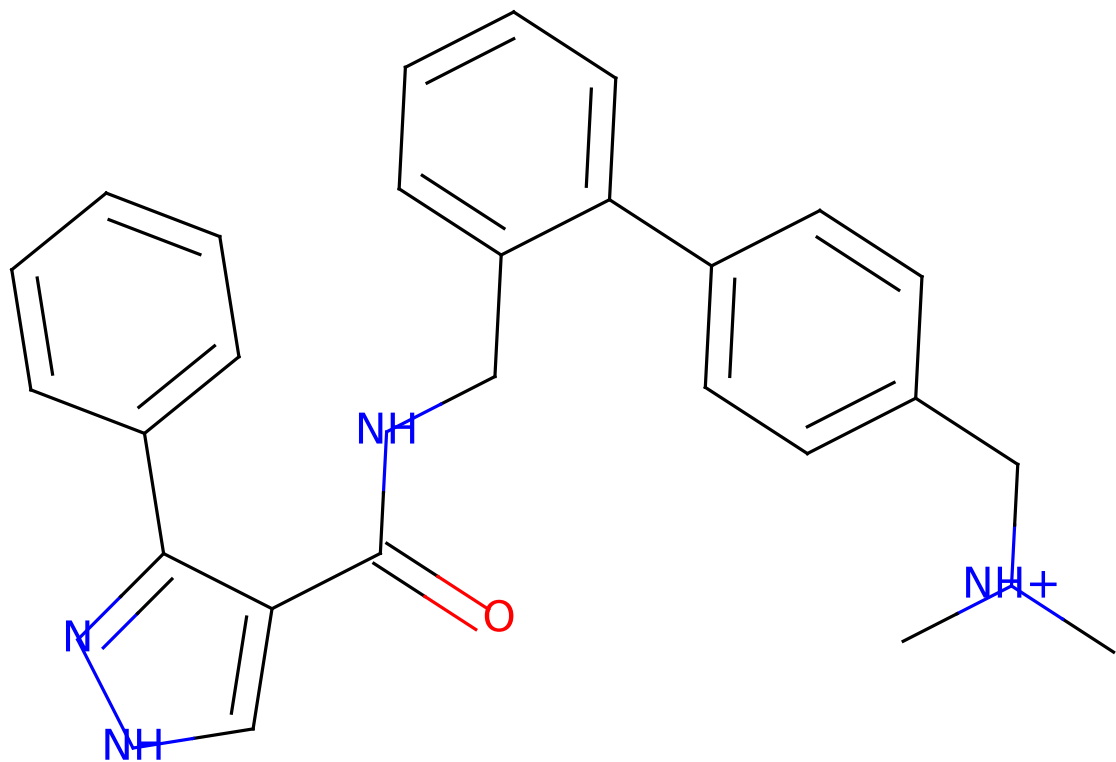CCc1cccc(c1)n2c(nnc2SCc3[nH]c(=O)c4c(n3)ccs4)N5CCOCC5

ORD-MCULE-1301409427_1

MolLogP: 1.6380199999999994 | QED: 0.8968518845054934

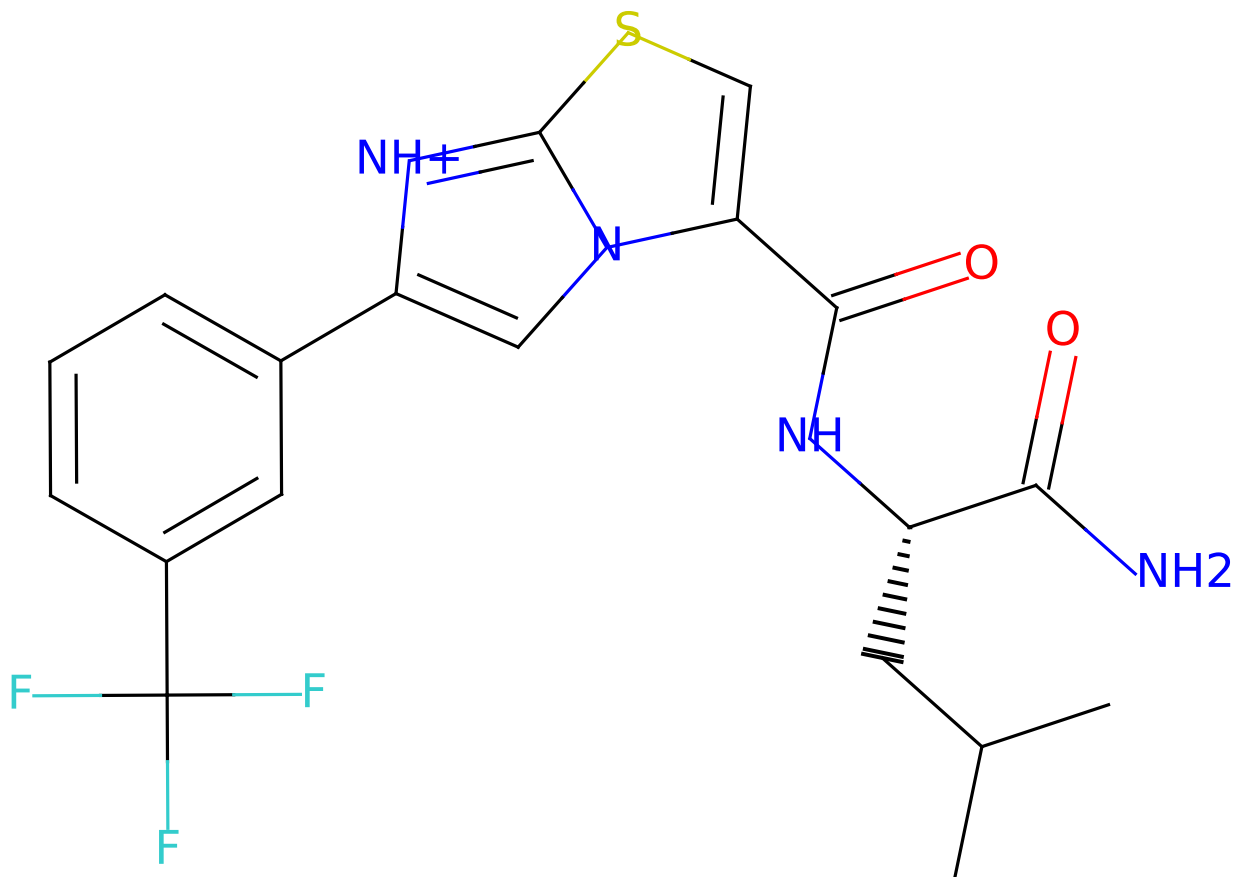CCc1[nH]c(c(n1)C)C[NH+]2CCC(CC2)c3ccncc3

ORD-MCULE-1222418359_2

MolLogP: 3.318200000000002 | QED: 0.4369107040448897
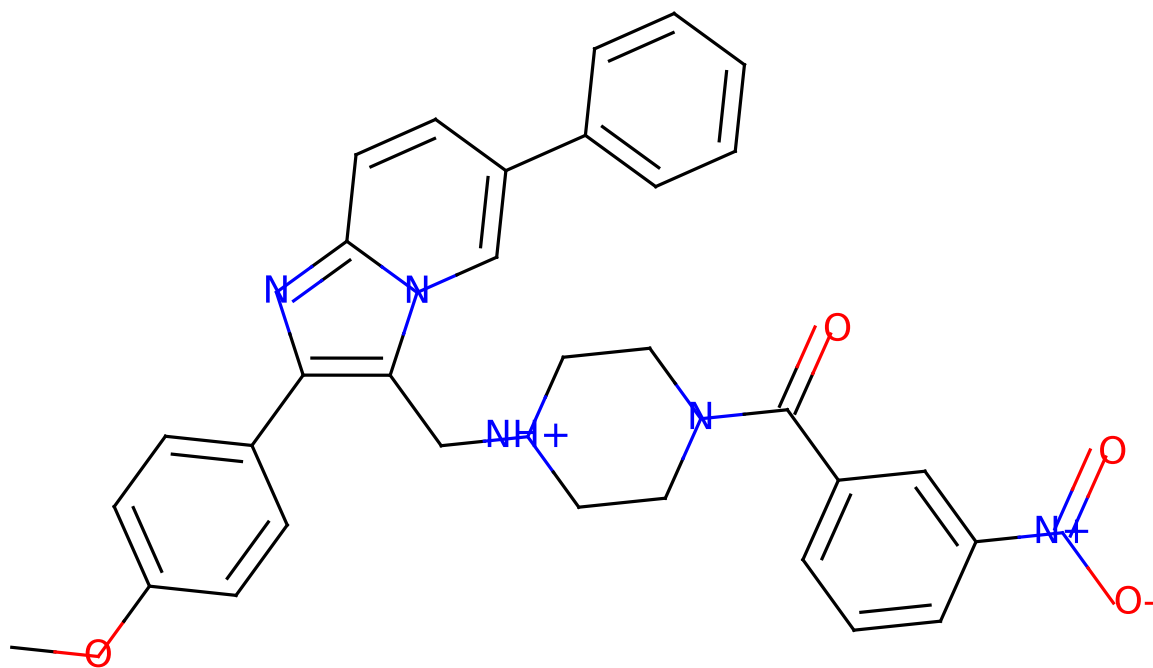
C[NH+](C)Cc1ccc(cc1)c2ccccc2CNC(=O)c3c[nH]nc3c4ccccc4

ORD-MCULE-5308855700_2

MolLogP: 3.1305000000000014 | QED: 0.6353316346922763

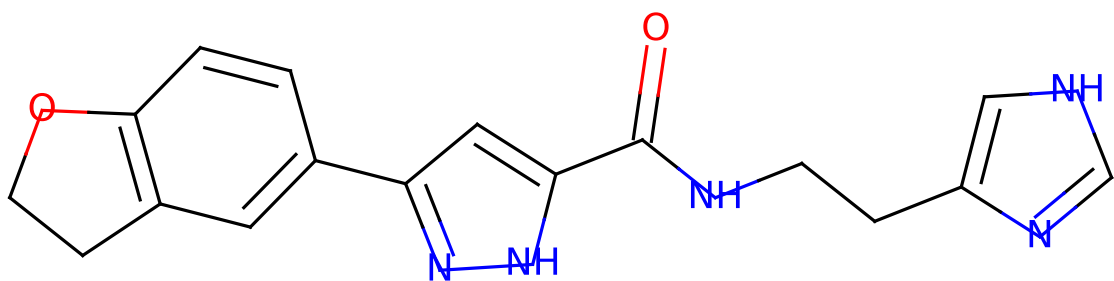CC(C)C[C@@H](C(=O)N)NC(=O)c1csc2n1cc([nH+]2)c3cccc(c3)C(F)(F)F

ORD-MCULE-9635688656_1

MolLogP: 4.126000000000003 | QED: 0.2439331506700583

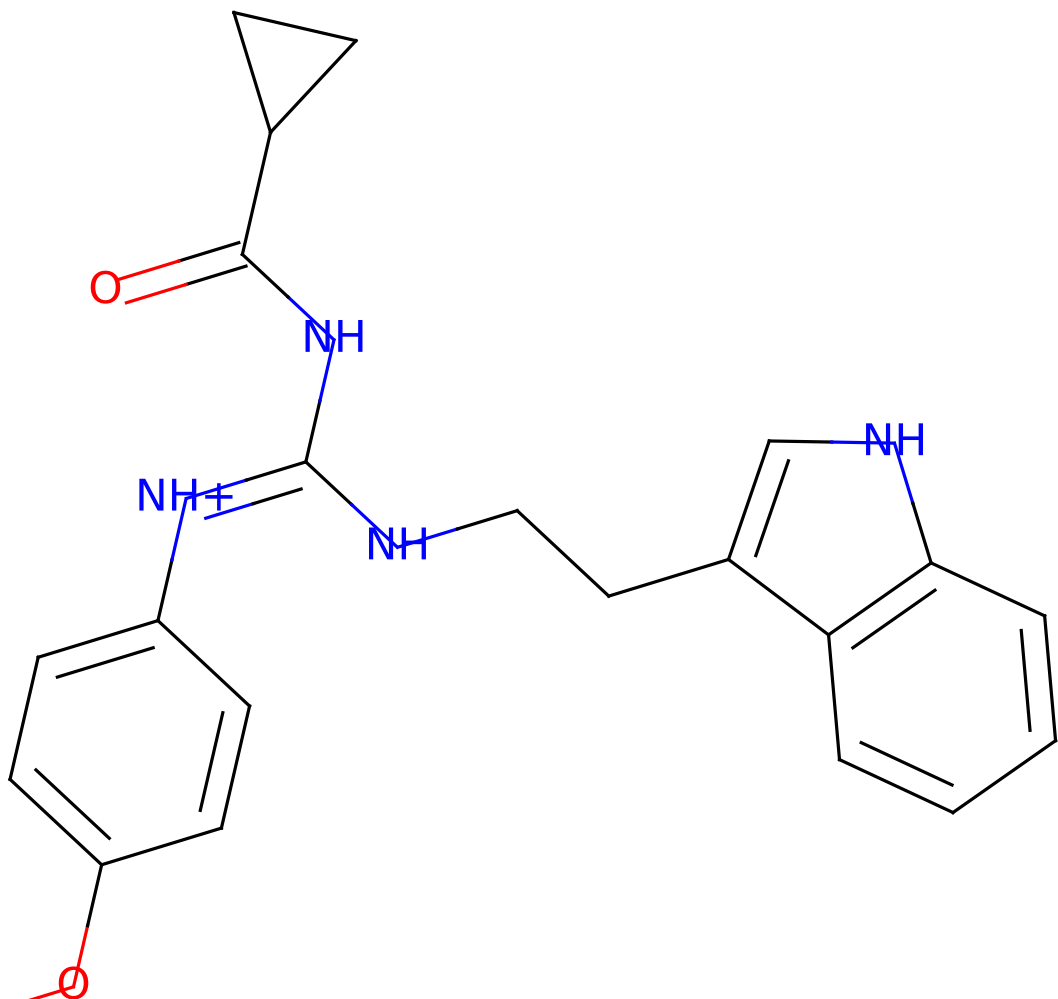COc1ccc(cc1)c2c(n3cc(ccc3n2)c4ccccc4)C[NH+]5CCN(CC5)C(=O)c6cccc(c6)N(=O)=O

ORD-MCULE-5878589304_1

MolLogP: 1.7071999999999998 | QED: 0.665828249386189
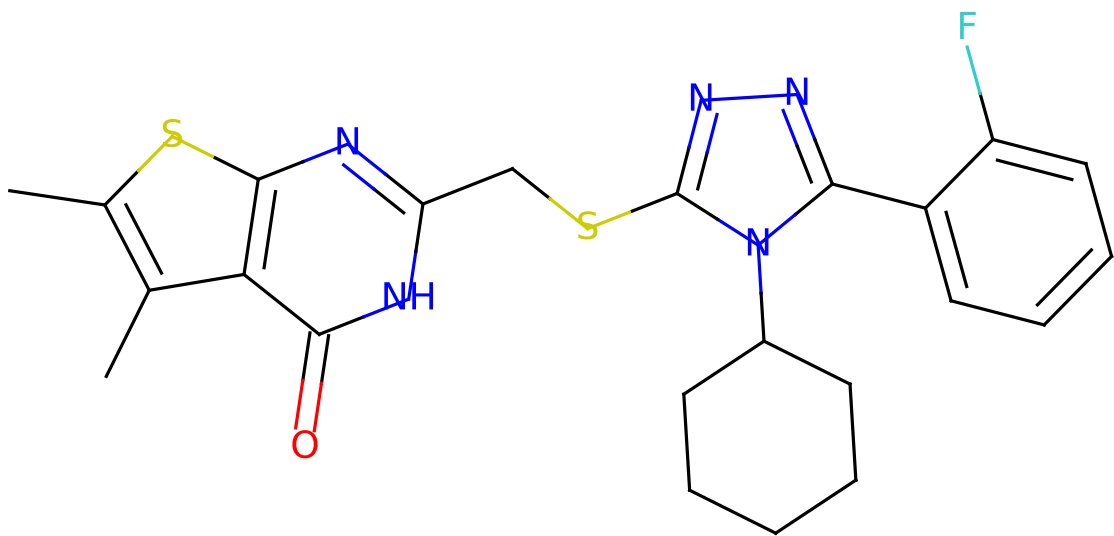
c1cc2c(cc1c3cc([nH]n3)C(=O)NCCc4c[nH]cn4)CCO2

ORD-MCULE-1691783948_2

MolLogP: 1.6030999999999997 | QED: 0.3891835901506976

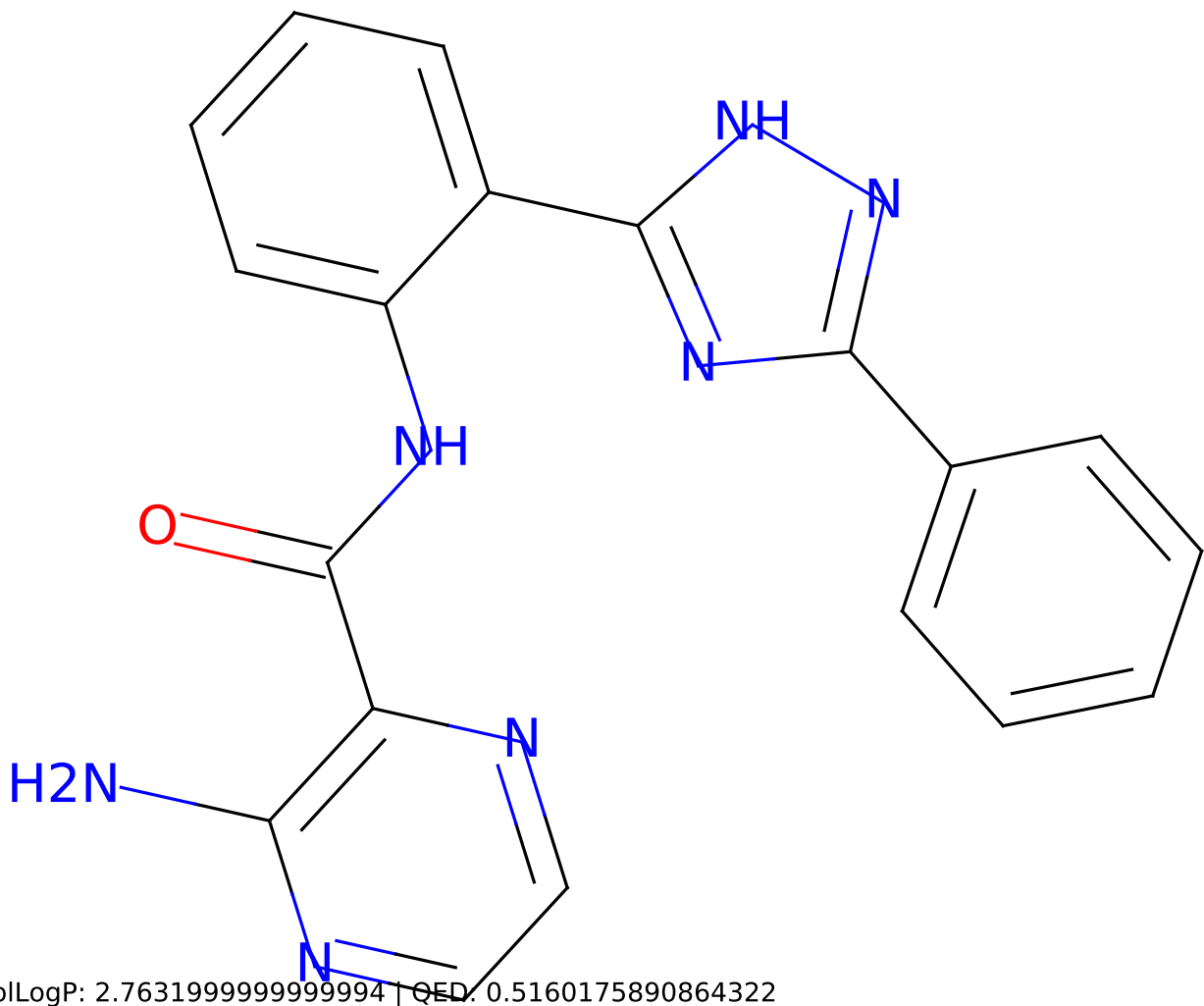COc1ccc(cc1)/[NH+]=C(\NCCc2c[nH]c3c2cccc3)/NC(=O)C4CC4

ORD-MCULE-1633632758_2

MolLogP: 5.796540000000005 | QED: 0.3741050130956263
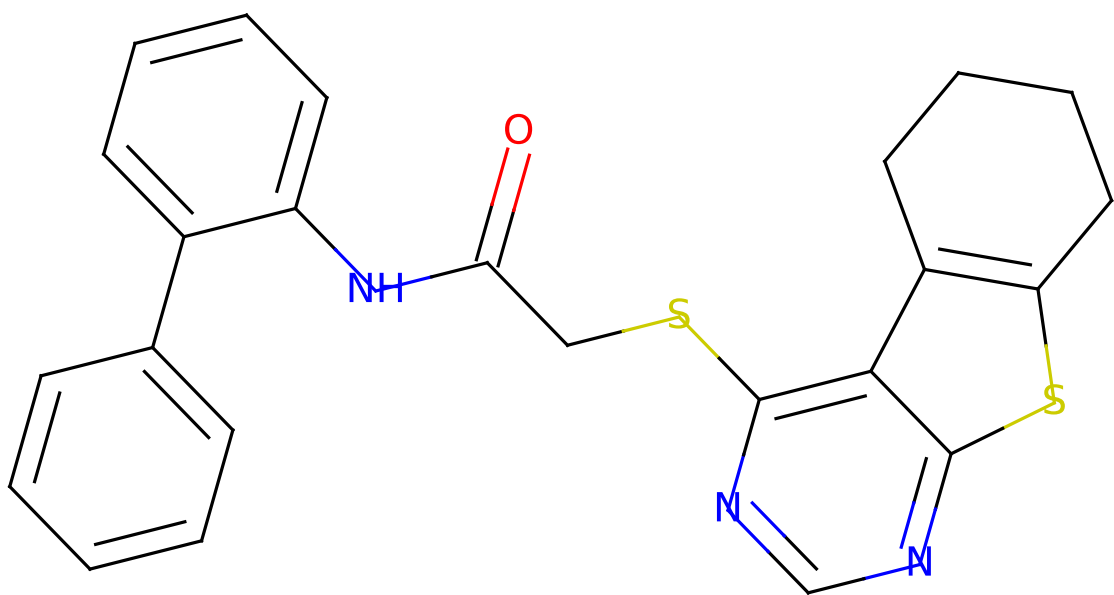
Cc1c(sc2c1c(=O)[nH]c(n2)CSc3nnc(n3C4CCCCC4)c5ccccc5F)C

ORD-MCULE-4930584650_1

150

MolLogP: 2.763199999999994 | QED: 0.5160175890864322

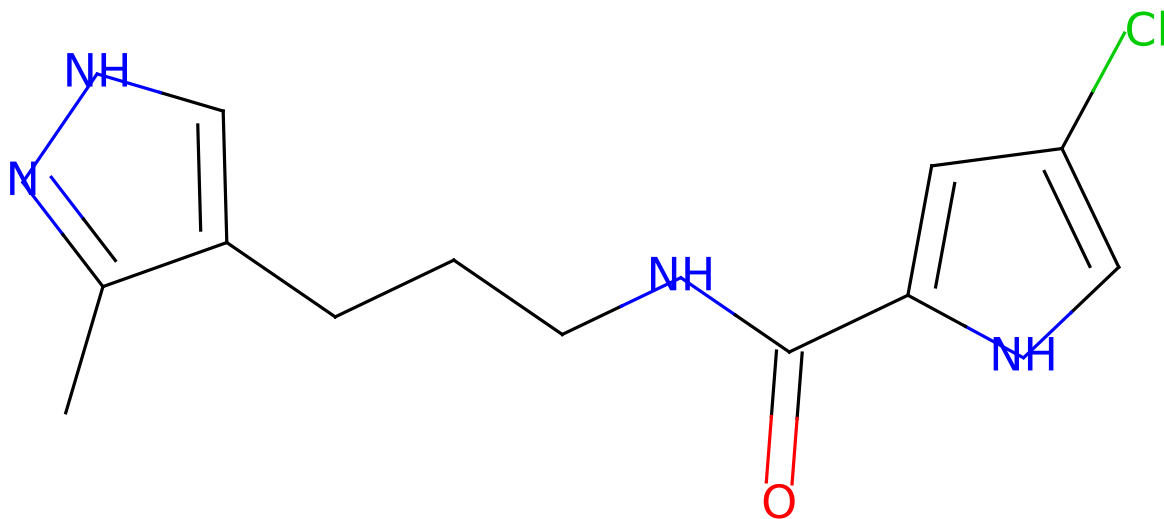c1ccc(cc1)c2nc([nH]n2)c3ccccc3NC(=O)c4c(nccn4)N

ORD-MCULE-1569445415_1

MolLogP: 5.967900000000003 | QED: 0.3124787410843783
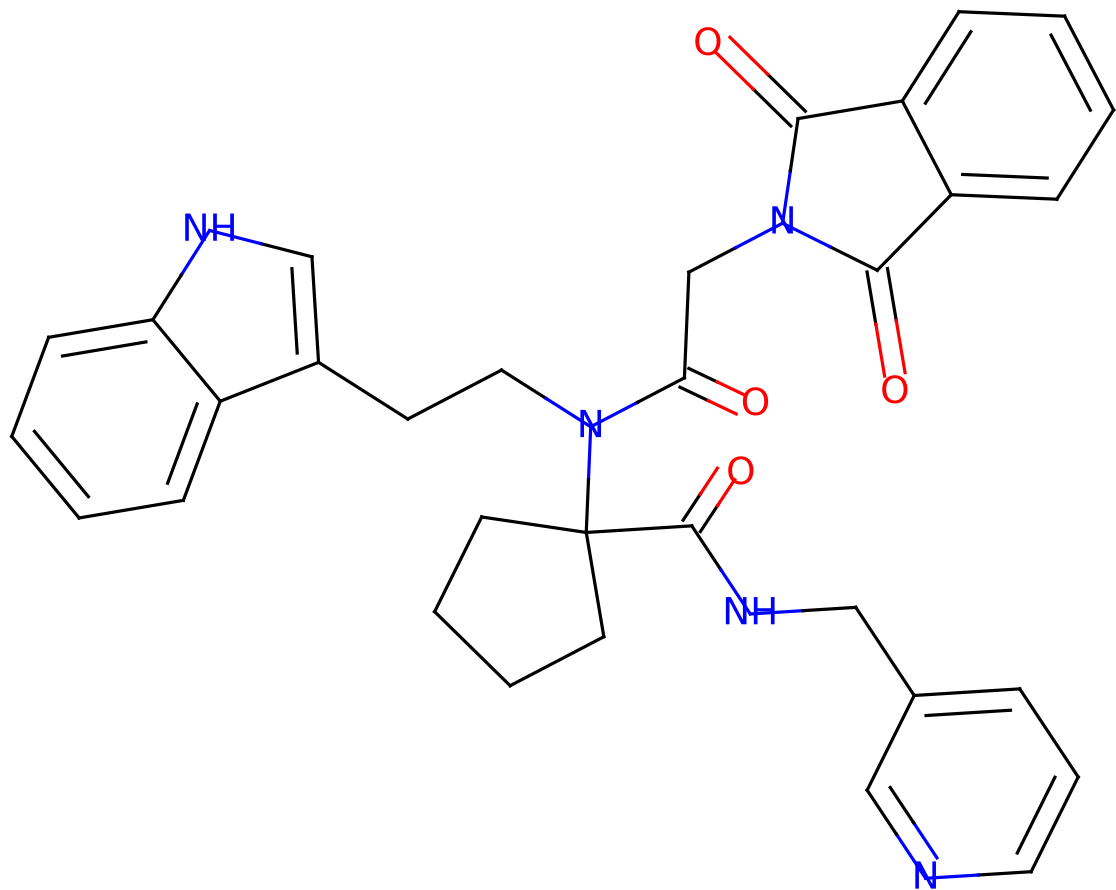
c1ccc(cc1)c2ccccc2NC(=O)CSc3c4c5c(sc4ncn3)CCCC5

ORD-MCULE-3168694897_1

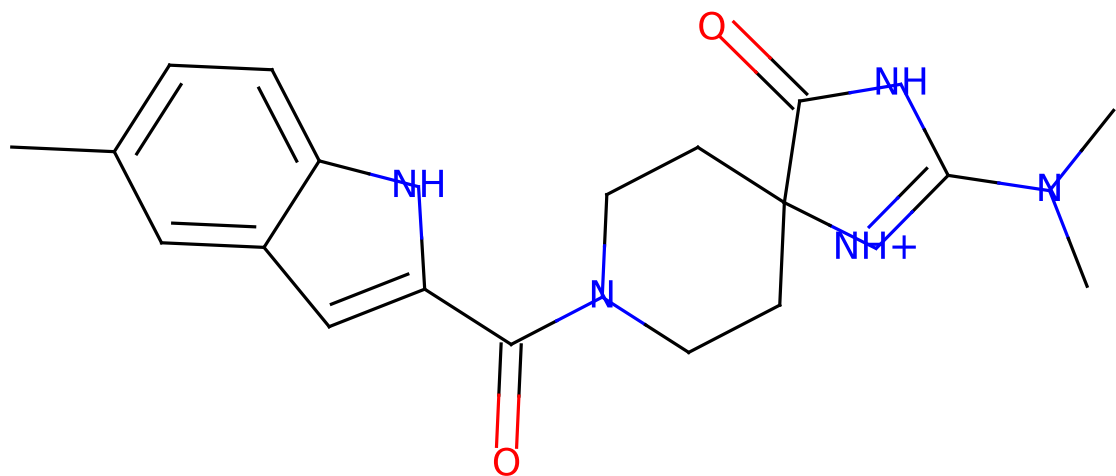MolLogP: 2.06222 | QED: 0.7249799798021191

Cc1c(c[nH]n1)CCCNC(=O)c2cc(c[nH]2)Cl

ORD-MCULE-7291272788_2

153

MolLogP: 3.8594000000000026 | QED: 0.30783163269976804

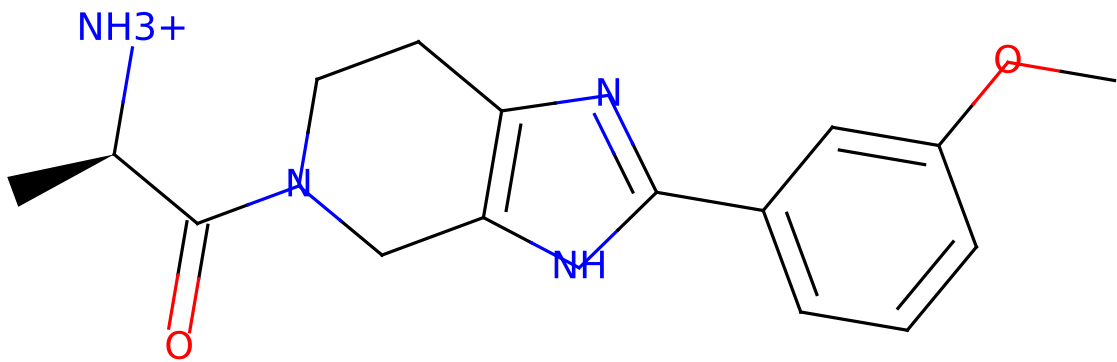c1ccc2c(c1)c(c[nH]2)CCN(C(=O)CN3C(=O)c4ccccc4C3=O)C5(CCCC5)C(=O)NCc6cccnc6

ORD-MCULE-9783175038_1

MolLogP: -0.42087999999999726 | QED: 0.650528335907669

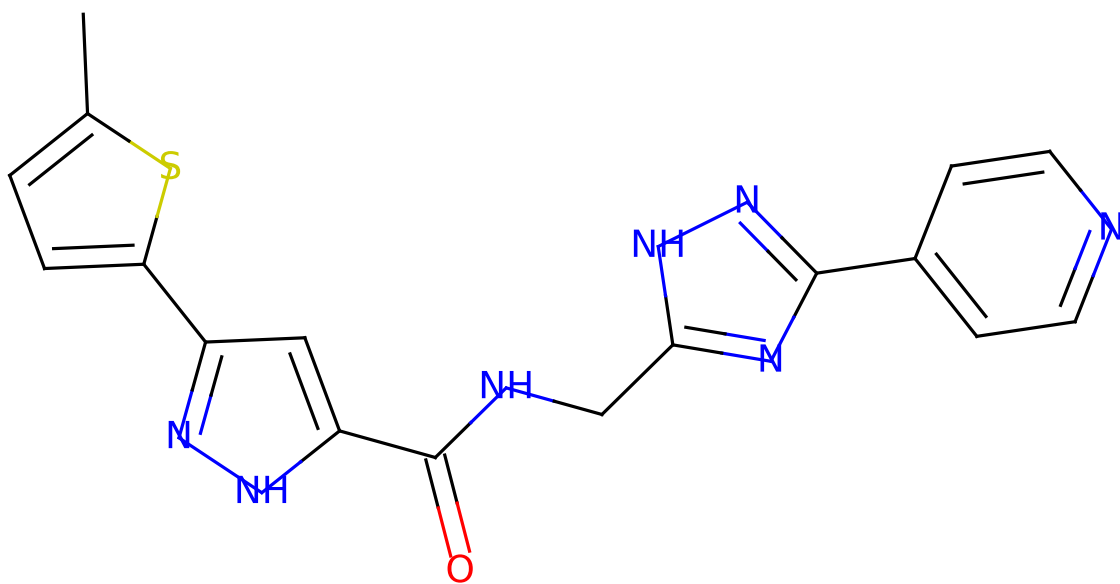Cc1ccc2c(c1)cc([nH]2)C(=O)N3CCC4(CC3)C(=O)NC(=[NH+]4)N(C)C

ORD-MCULE-4563504276_1

MolLogP: 0.6004 | QED: 0.8702502574304508
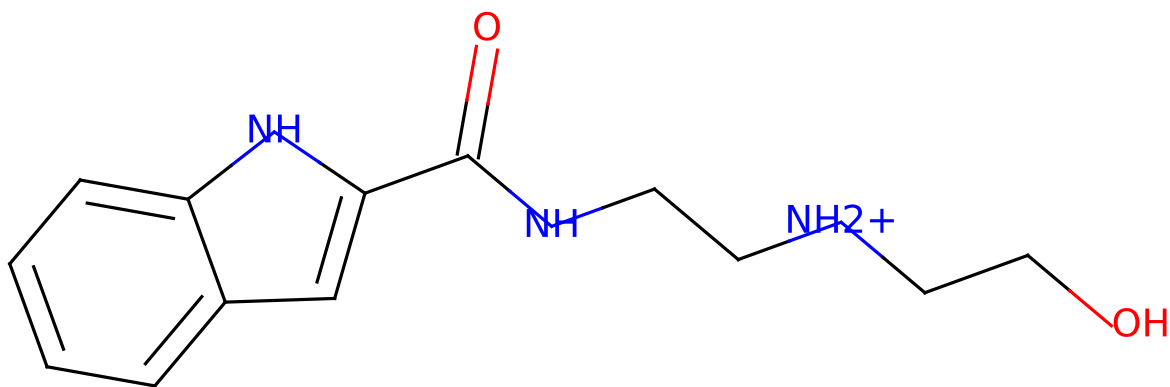
C[C@H](C(=O)N1CCc2c([nH]c(n2)c3cccc(c3)OC)C1)[NH3+]

ORD-MCULE-6534865045_1

156

MolLogP: 2.5567200000000003 | QED: 0.5030636309757494

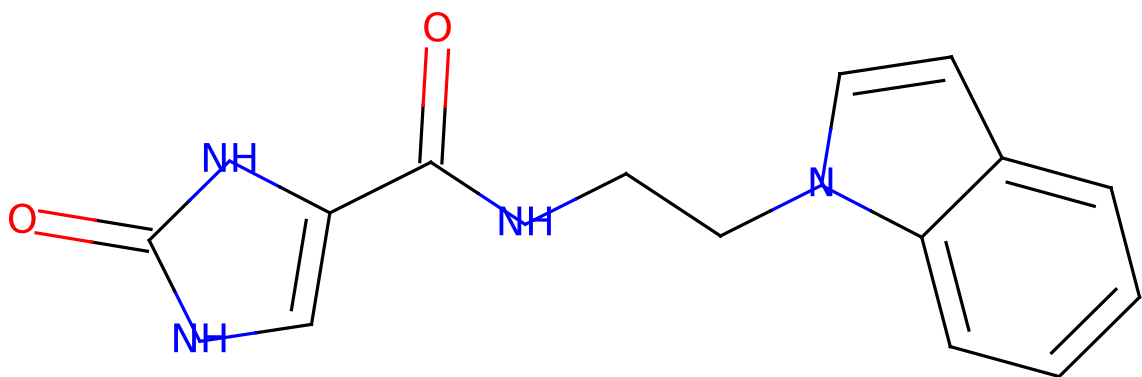Cc1ccc(s1)c2cc([nH]n2)C(=O)NCc3[nH]nc(n3)c4ccncc4

ORD-MCULE-4883931485_4

MolLogP: -0.5465999999999993 | QED: 0.5175460145680517
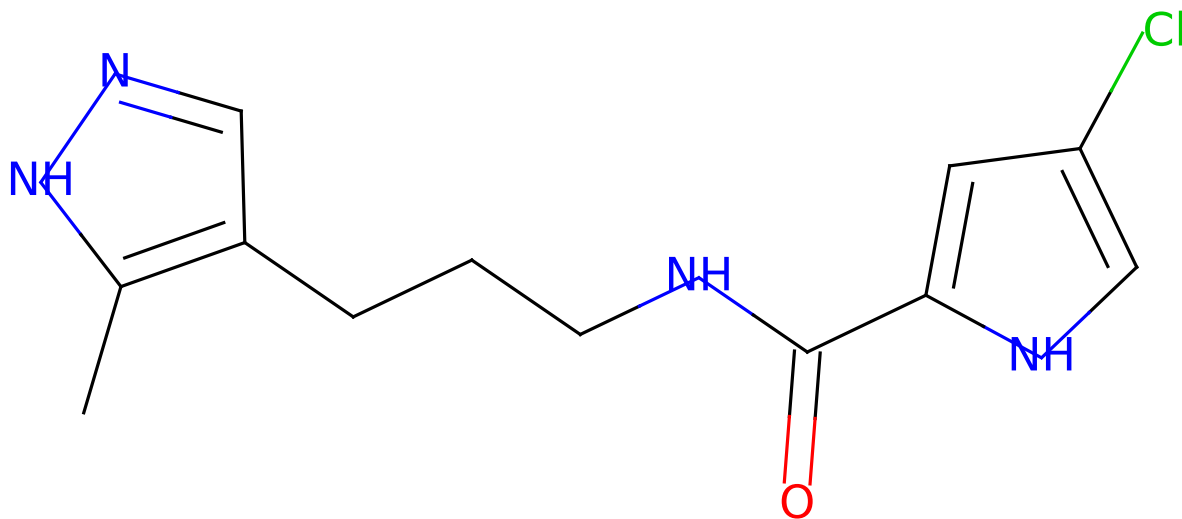
c1ccc2c(c1)cc([nH]2)C(=O)NCC[NH2+]CCO

ORD-MCULE-1189442017_1

MolLogP: 1.0876999999999992 | QED: 0.6628257497555063
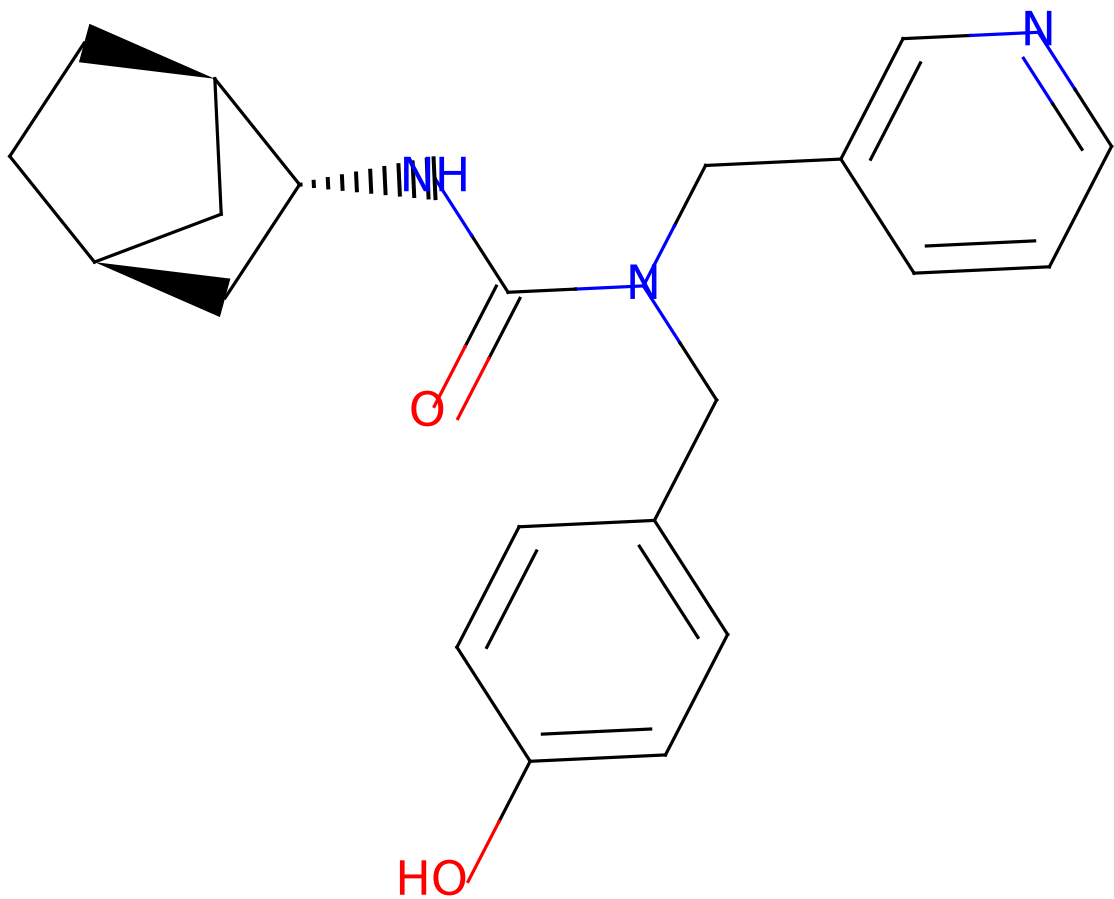
c1ccc2c(c1)ccn2CCNC(=O)c3c[nH]c(=O)[nH]3

ORD-MCULE-4890372754_1

MolLogP: 2.06222 | QED: 0.7249799798021191

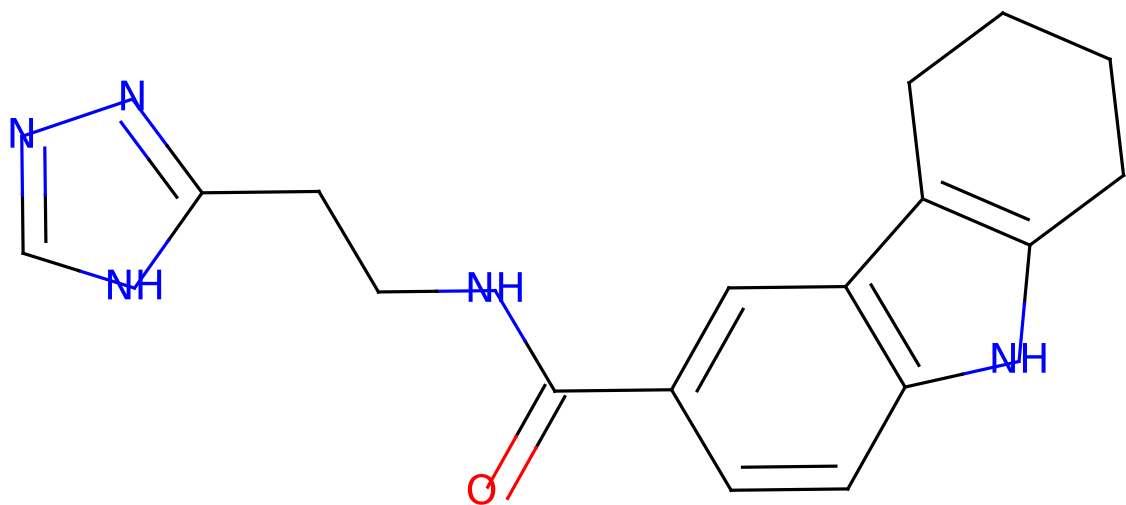Cc1c(cn[nH]1)CCCNC(=O)c2cc(c[nH]2)Cl

ORD-MCULE-7291272788_1

MolLogP: 3.6876000000000024 | QED: 0.8633635995240779

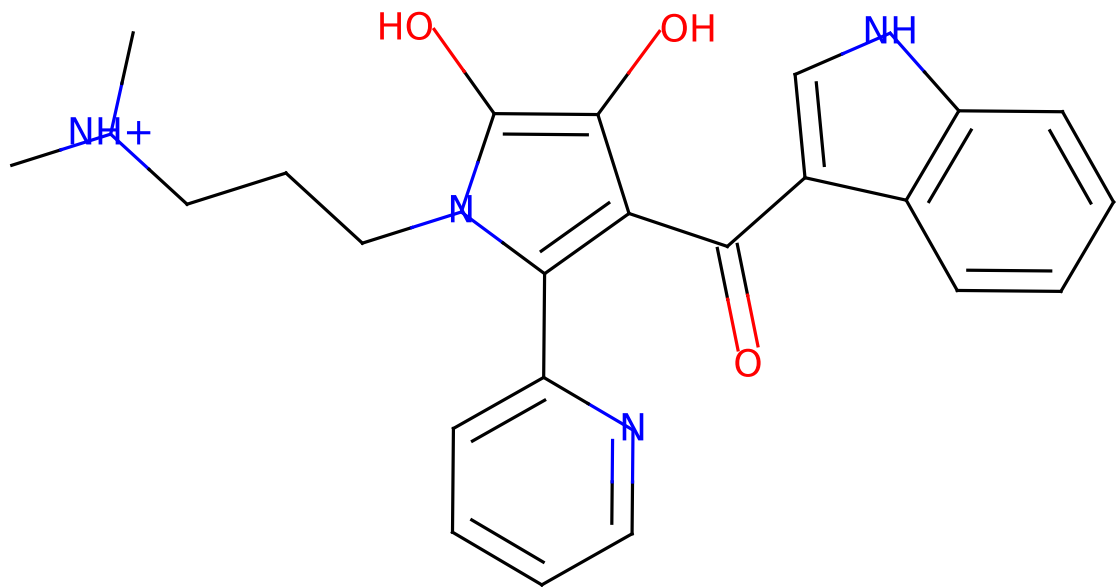c1cc(cnc1)CN(Cc2ccc(cc2)O)C(=O)N[C@@H]3C[C@H]4CC[C@@H]3C4

ORD-MCULE-6576711707_1

MolLogP: 2.1372999999999998 | QED: 0.6898435106729162
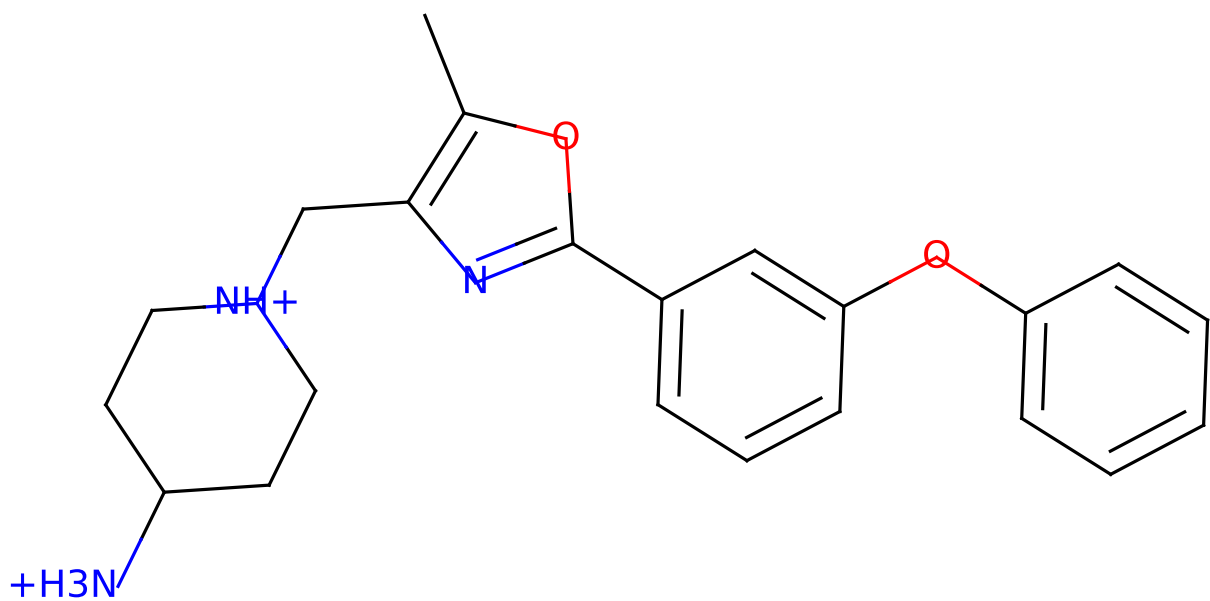
c1cc2c(cc1C(=O)NCCc3[nH]cnn3)c4c([nH]2)CCCC4

ORD-MCULE-5529773957_3

162

MolLogP: 2.2081999999999997 | QED: 0.35465254250339956

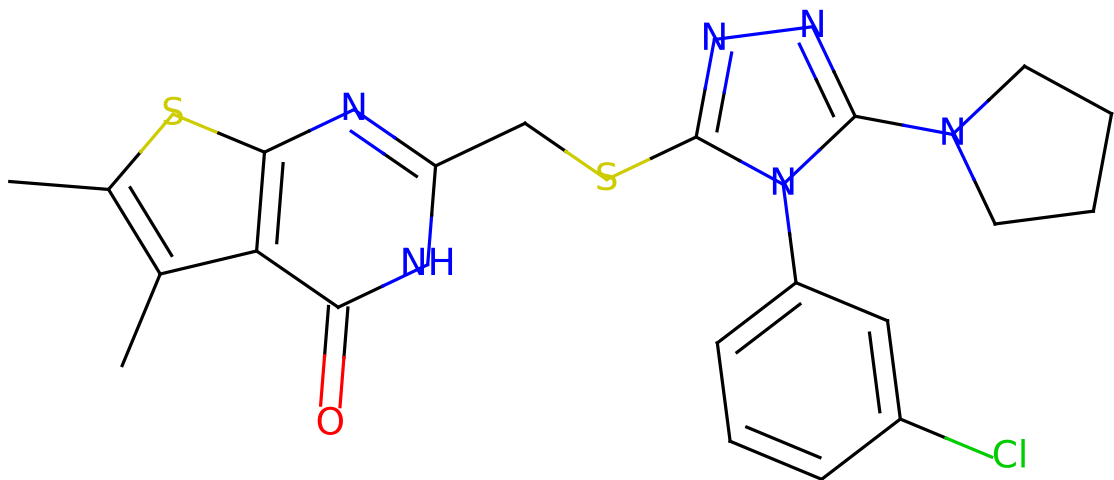C[NH+](C)CCCn1c(c(c(c1O)O)C(=O)c2c[nH]c3c2cccc3)c4ccccn4

ORD-MCULE-2111961046_1

MolLogP: 2.23152 | QED: 0.728608613493782
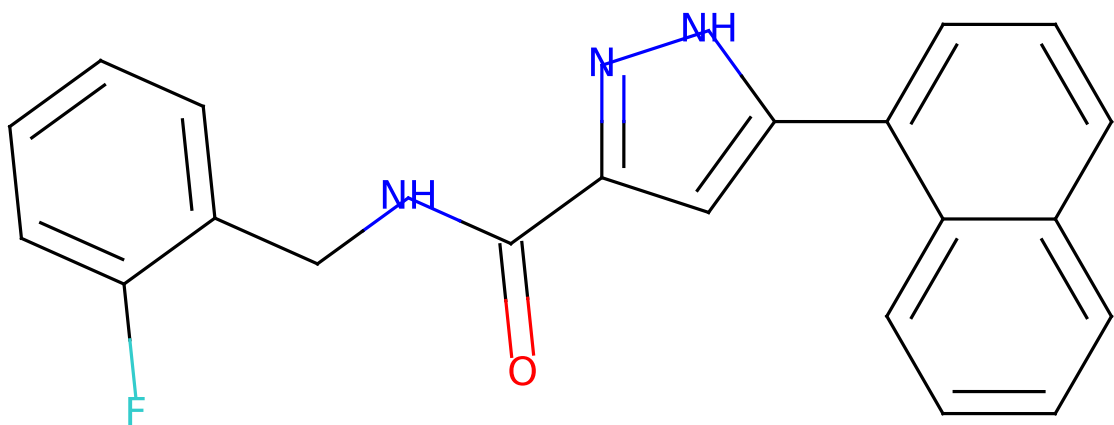
Cc1c(nc(o1)c2cccc(c2)Oc3ccccc3)C[NH+]4CCC(CC4)[NH3+]

ORD-MCULE-2649592665_1

164

MolLogP: 4.728040000000004 | QED: 0.4228846148248437

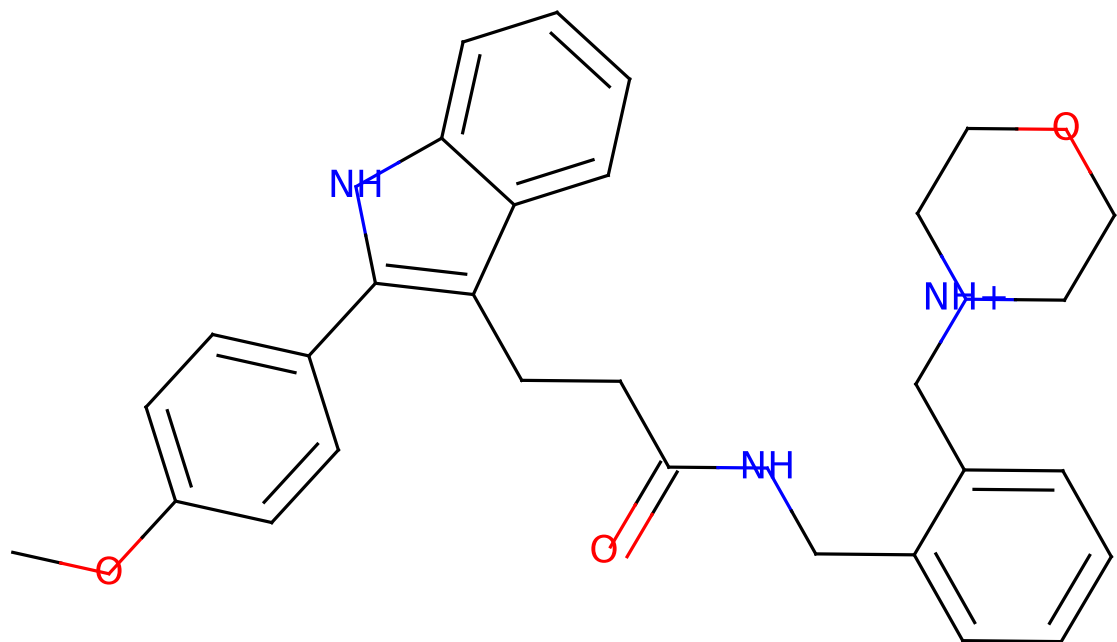Cc1c(sc2c1c(=O)[nH]c(n2)CSc3nnc(n3c4cccc(c4)Cl)N5CCCC5)C

ORD-MCULE-3115407234_1

MolLogP: 4.299000000000002 | QED: 0.5793088677435203

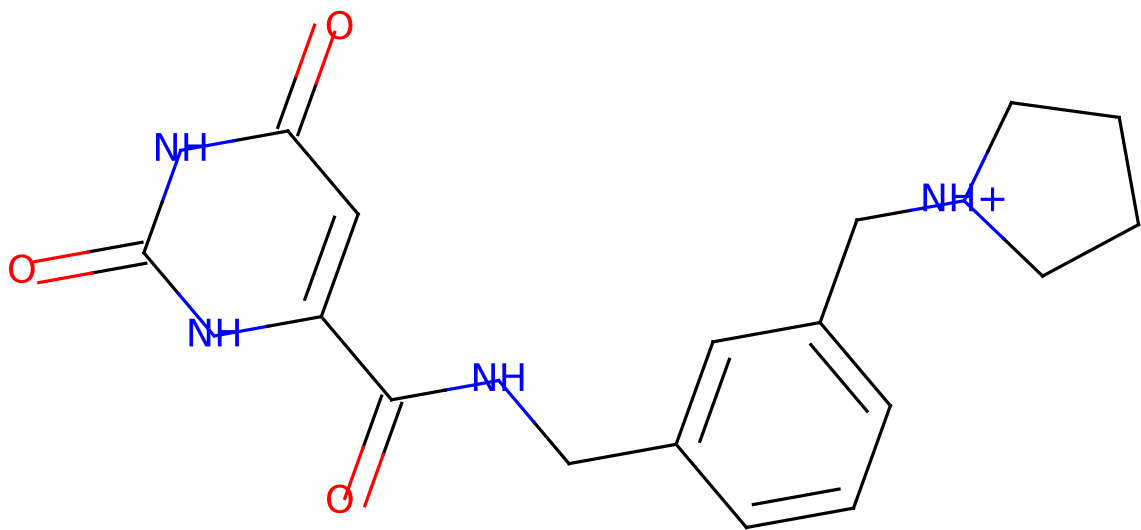c1ccc2c(c1)cccc2c3cc(n[nH]3)C(=O)NCc4ccccc4F

ORD-MCULE-7679599807_2

MolLogP: 3.507600000000001 | QED: 0.34067725093396733

COc1ccc(cc1)c2c(c3ccccc3[nH]2)CCC(=O)NCc4ccccc4C[NH+]5CCOCC5
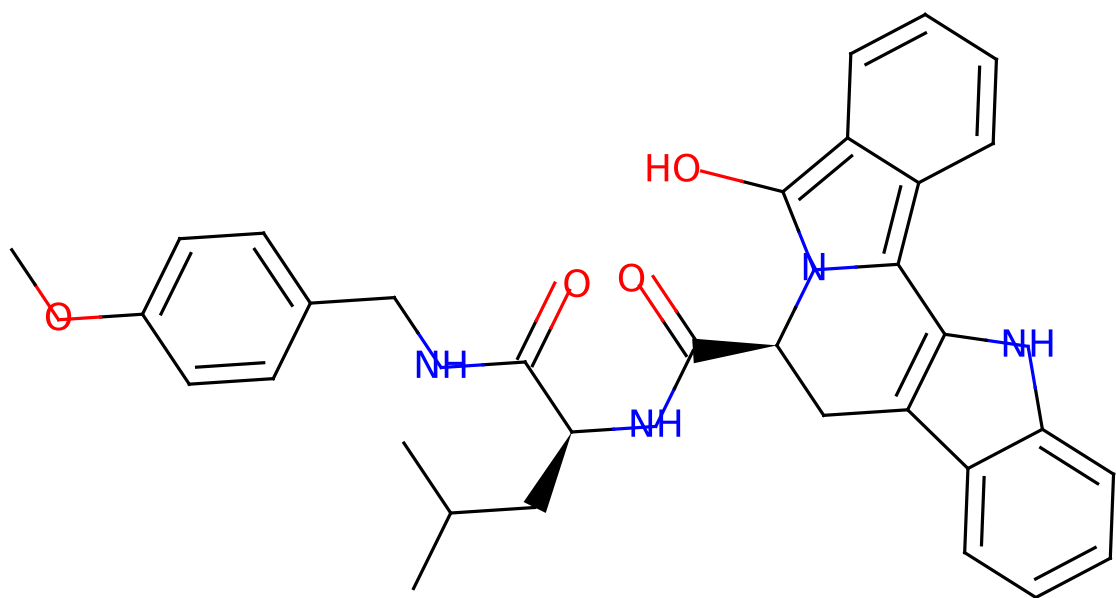
ORD-MCULE-9997038445_1

MolLogP: -0.8280999999999985 | QED: 0.5761956647652665

c1cc(cc(c1)C[NH+]2CCCC2)CNC(=O)c3cc(=O)[nH]c(=O)[nH]3
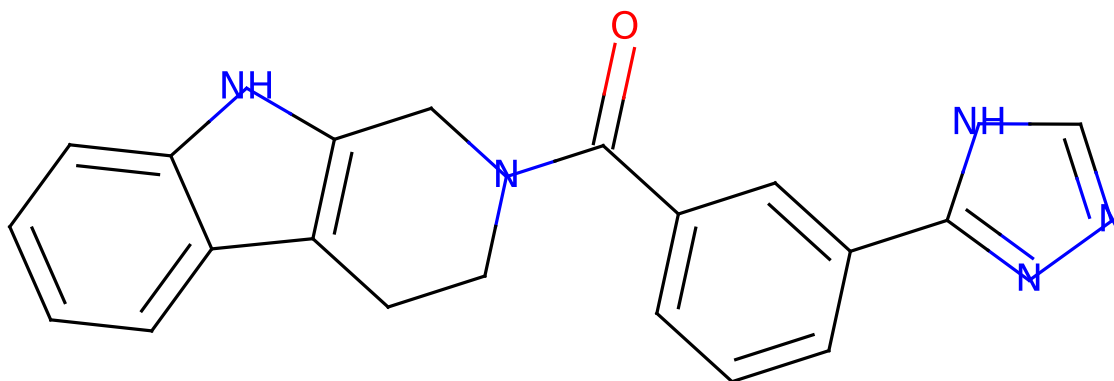
ORD-MCULE-1515849673_1

MolLogP: 4.227720000000003 | QED: 0.4413876056422959

Cc1ccccc1N2CCN(CC2)C(=O)[C@H](Cc3c[nH]c4c3cccc4)NC(=O)c5cccs5

ORD-MCULE-4776089530_1

169

MolLogP: 5.448300000000005 | QED: 0.2060938306399034

CC(C)C[C@@H](C(=O)NCc1ccc(cc1)OC)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O
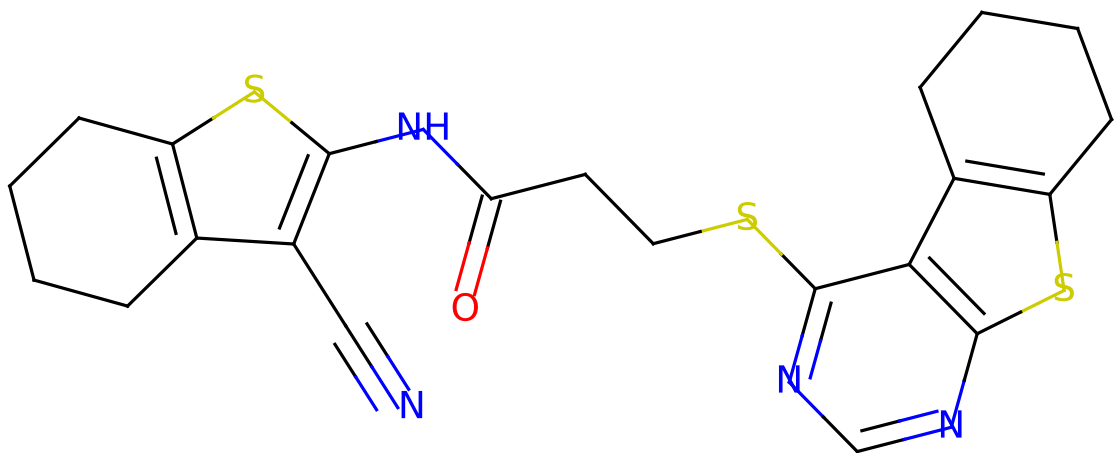
ORD-MCULE-2416817574_1

MolLogP: 3.1515000000000013 | QED: 0.5868071970006061
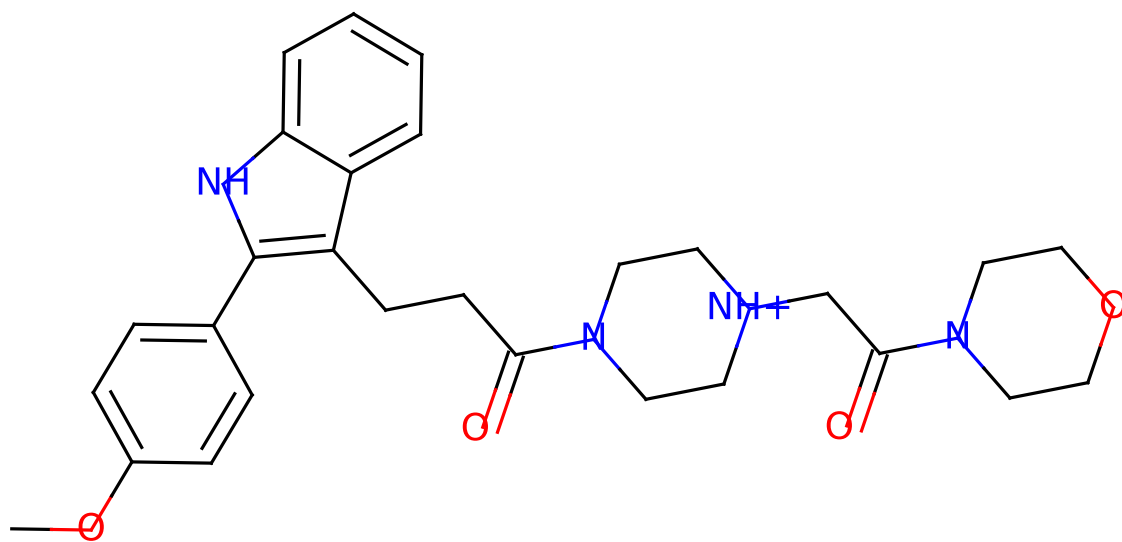
c1ccc2c(c1)c3c([nH]2)CN(CC3)C(=O)c4cccc(c4)c5[nH]cnn5

ORD-MCULE-9392421513_3

171

MolLogP: 5.5029800000000035 | QED: 0.4065448408945222
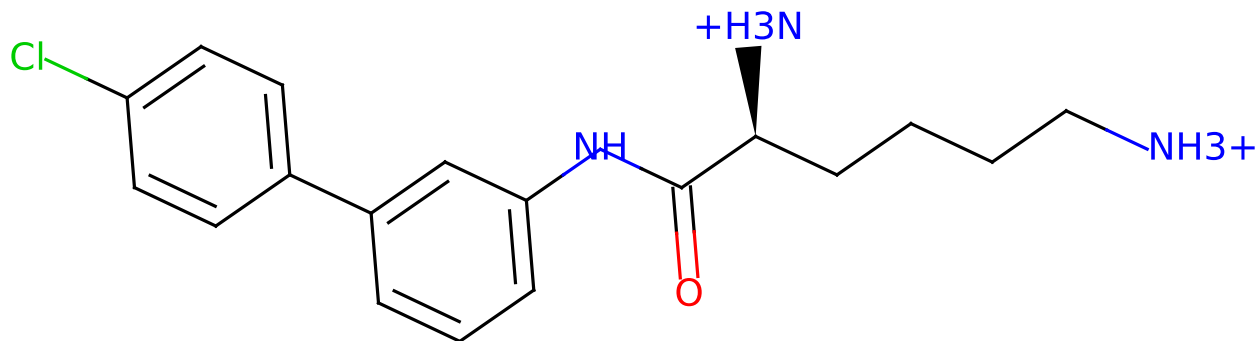
c1nc2c(c3c(s2)CCCC3)c(n1)SCCC(=O)Nc4c(c5c(s4)CCCC5)C#N

ORD-MCULE-3751444125_1

MolLogP: 1.362000000000001 | QED: 0.5233311781906421

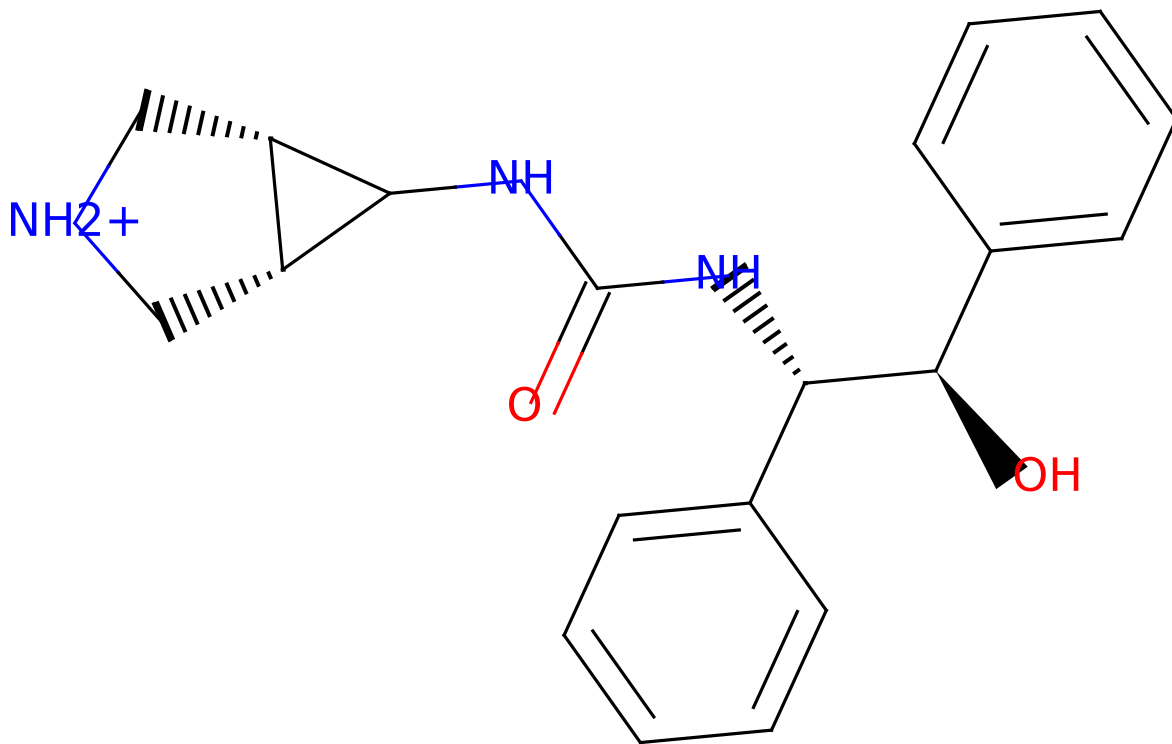COc1ccc(cc1)c2c(c3ccccc3[nH]2)CCC(=O)N4CC[NH+](CC4)CC(=O)N5CCOCC5

ORD-MCULE-3773841872_1

MolLogP: 1.9682000000000006 | QED: 0.6648487288742537

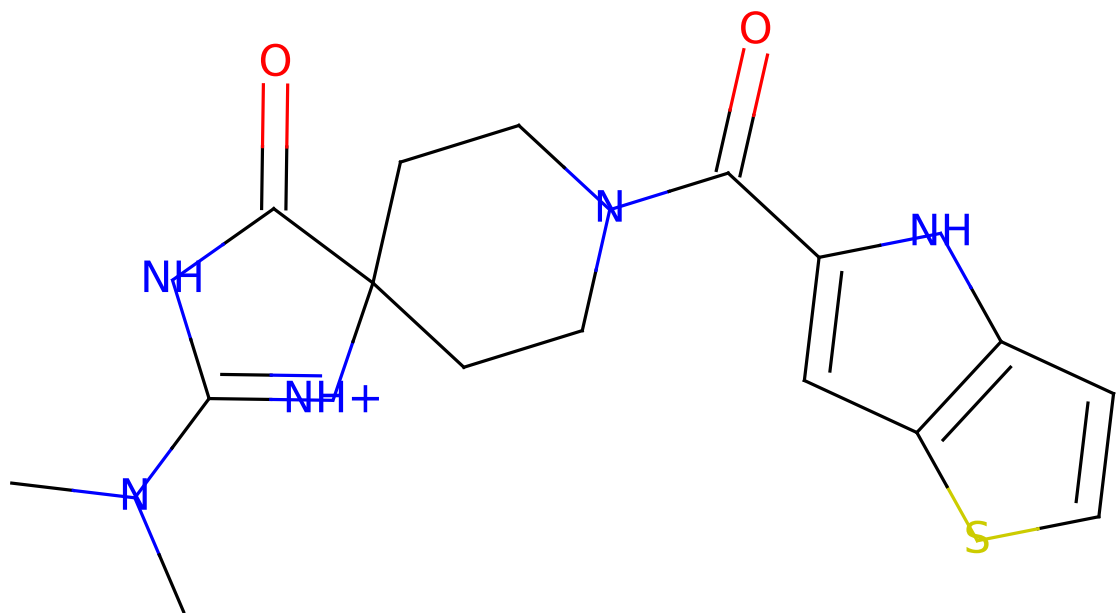c1cc(cc(c1)NC(=O)[C@H](CCCC[NH3+])[NH3+])c2ccc(cc2)Cl

ORD-MCULE-8425442450_1

MolLogP: 0.9520999999999997 | QED: 0.6550749011853475

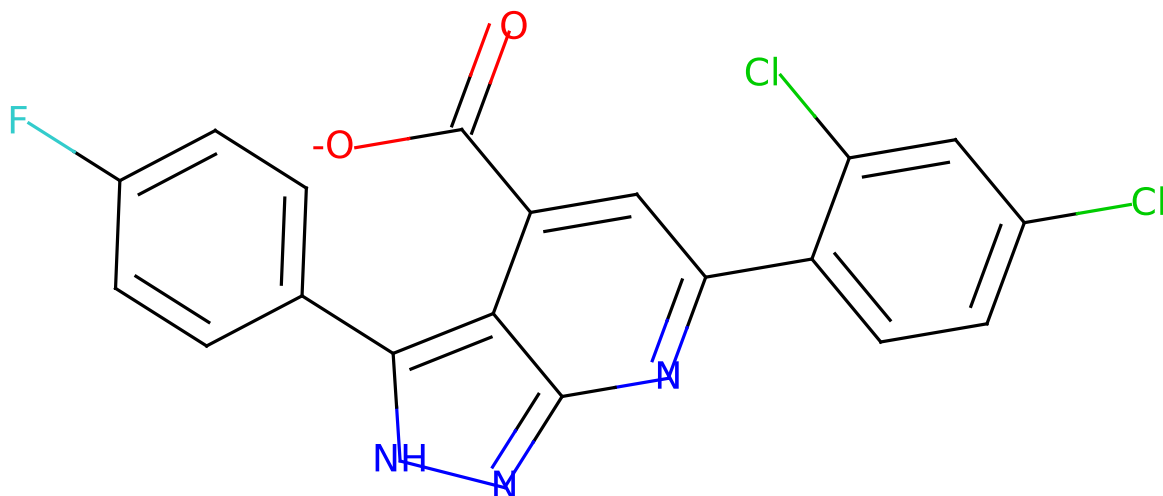c1ccc(cc1)[C@@H]([C@@H](c2ccccc2)O)NC(=O)NC3[C@H]4[C@@H]3C[NH2+]C4

ORD-MCULE-3076850808_1

175

MolLogP: -0.667799999999998 | QED: 0.6406640817072597

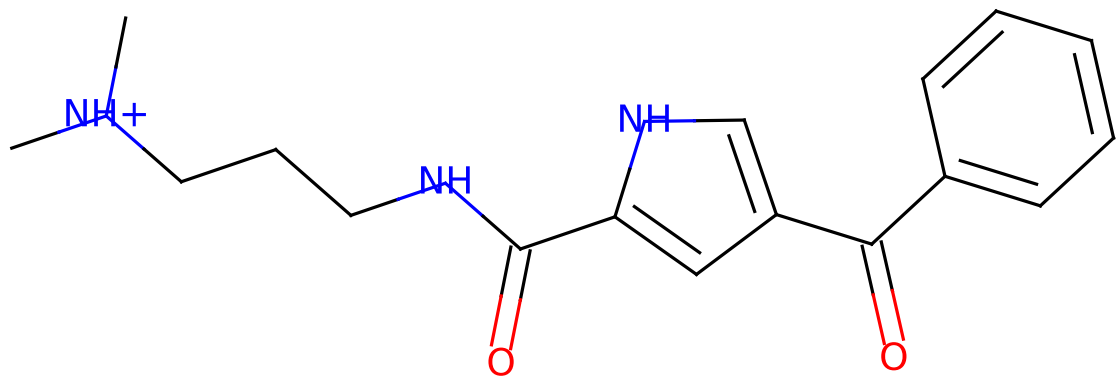CN(C)C1=[NH+]C2(CCN(CC2)C(=O)c3cc4c([nH]3)ccs4)C(=O)N1

ORD-MCULE-5592055088_1

MolLogP: 4.101300000000001 | QED: 0.5605562382060875
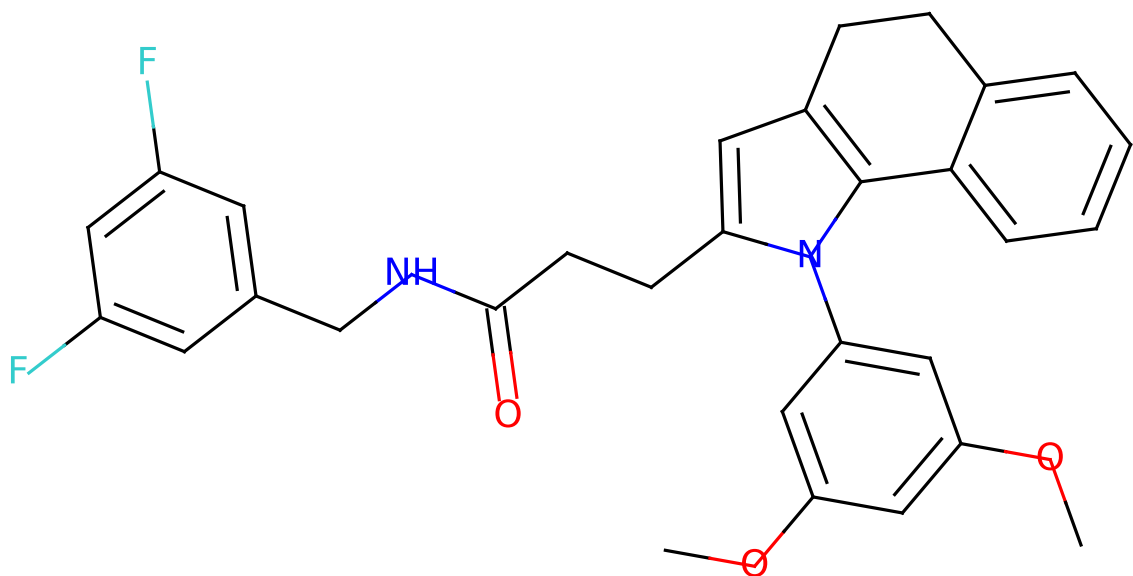
c1cc(ccc1c2c3c(cc(nc3n[nH]2)c4ccc(cc4Cl)Cl)C(=O)[O-])F

ORD-MCULE-9333872893_1

177

MolLogP: 0.5101000000000013 | QED: 0.515135413748422
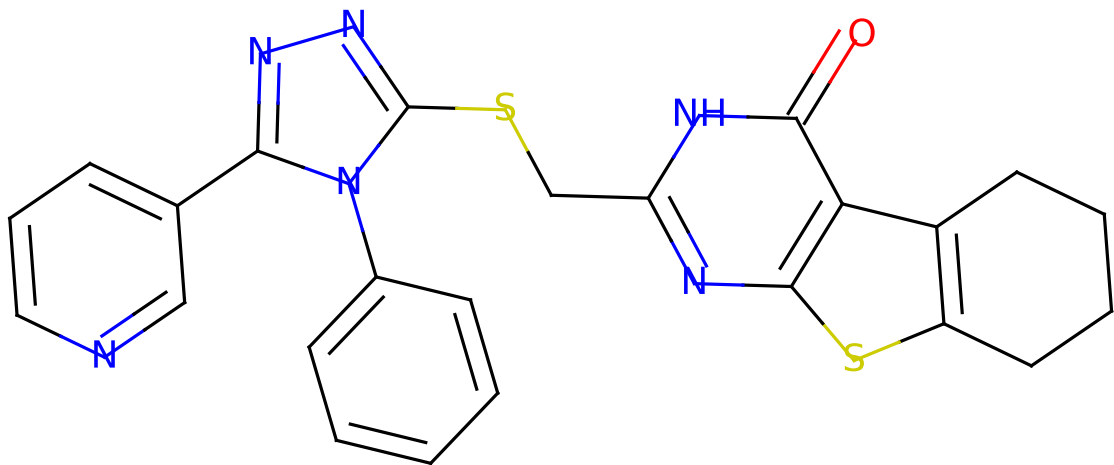
C[NH+](C)CCCNC(=O)c1cc(c[nH]1)C(=O)c2ccccc2

ORD-MCULE-9796670140_1

MolLogP: 5.7873000000000046 | QED: 0.33203587335464885

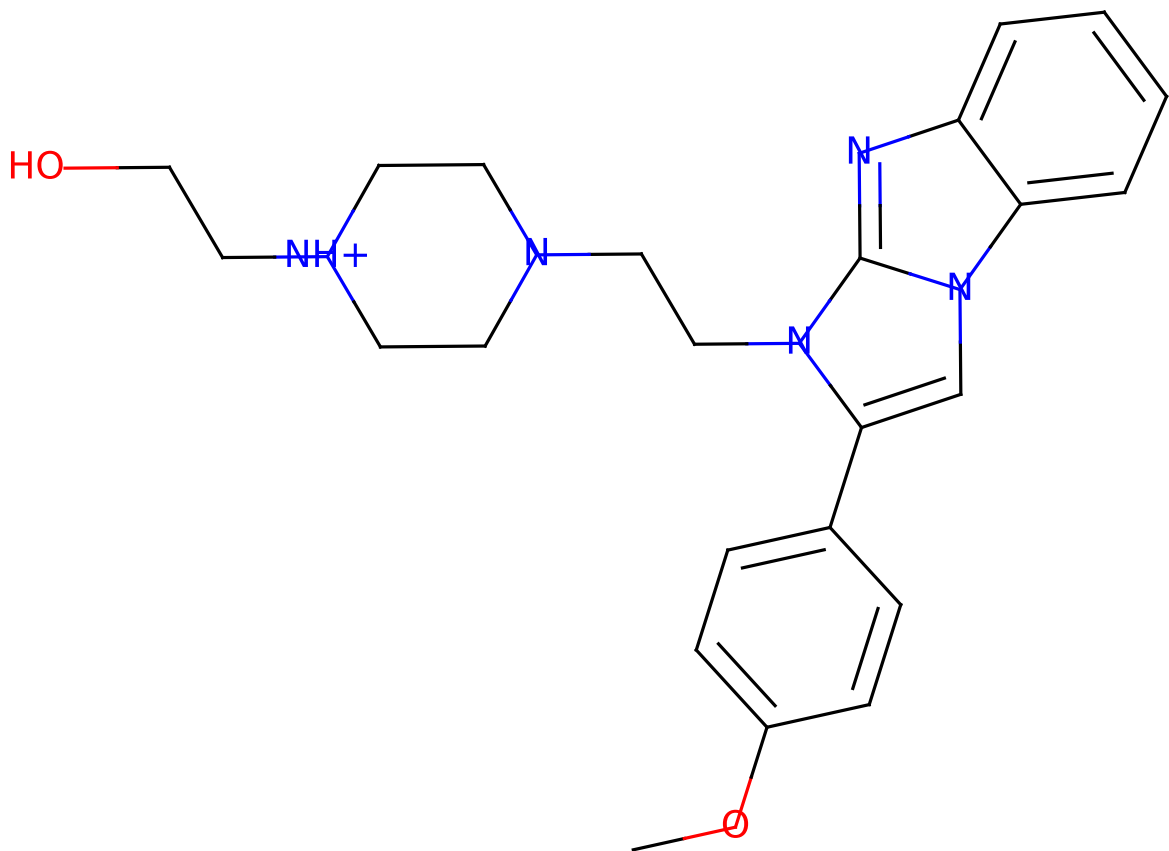COc1cc(cc(c1)OC)n2c(cc3c2-c4ccccc4CC3)CCC(=O)NCc5cc(cc(c5)F)F

ORD-MCULE-6553444445_1

MolLogP: 4.7984000000000036 | QED: 0.3697739660005106

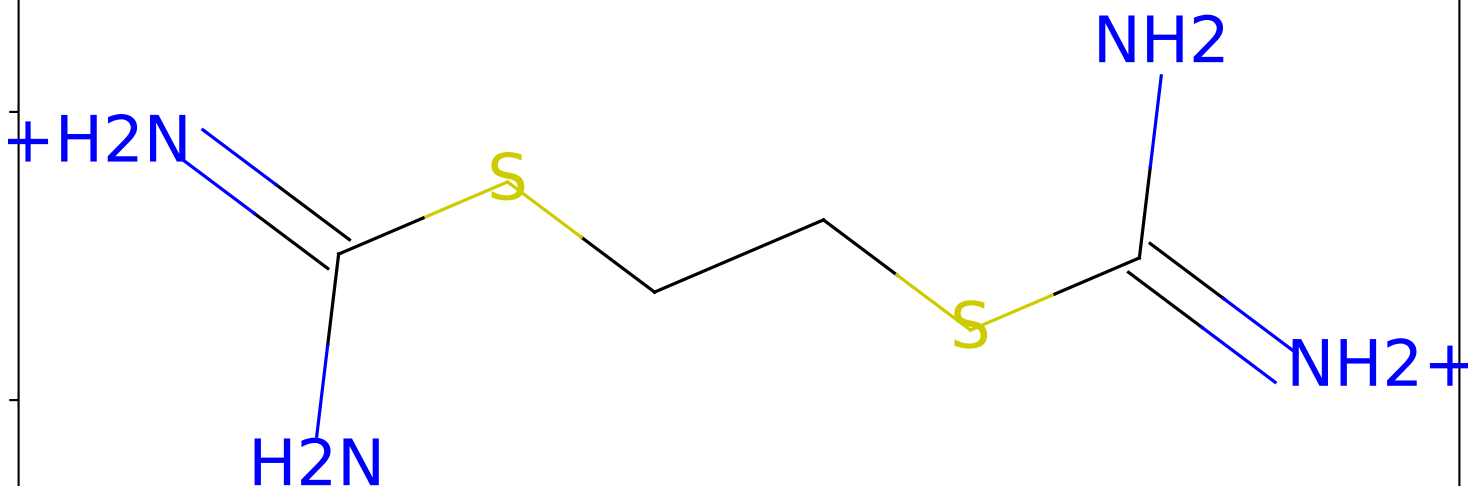c1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4c5c(sc4n3)CCCC5)c6cccnc6

ORD-MCULE-7538303993_1

MolLogP: 1.1573999999999989 | QED: 0.4711511261739625
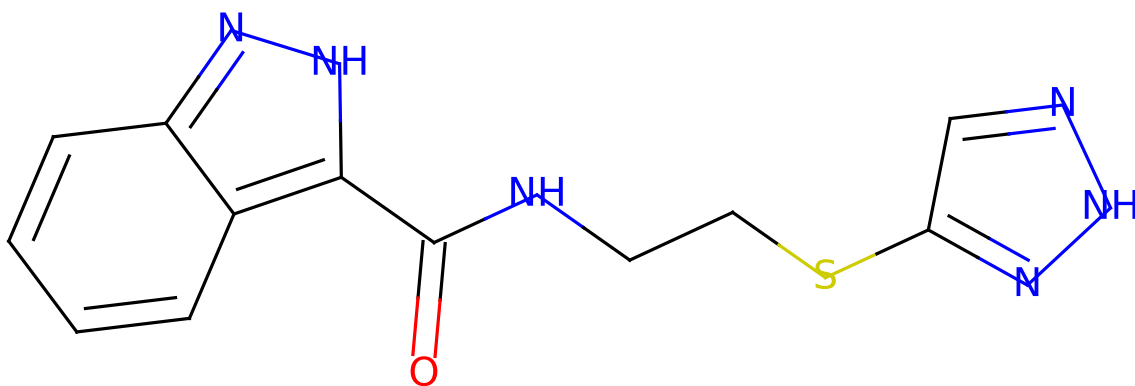
COc1ccc(cc1)c2cn3c4ccccc4nc3n2CCN5CC[NH+](CC5)CCO

ORD-MCULE-3060397501_1

181

MolLogP: -3.3959999999999995 | QED: 0.20640969285637883
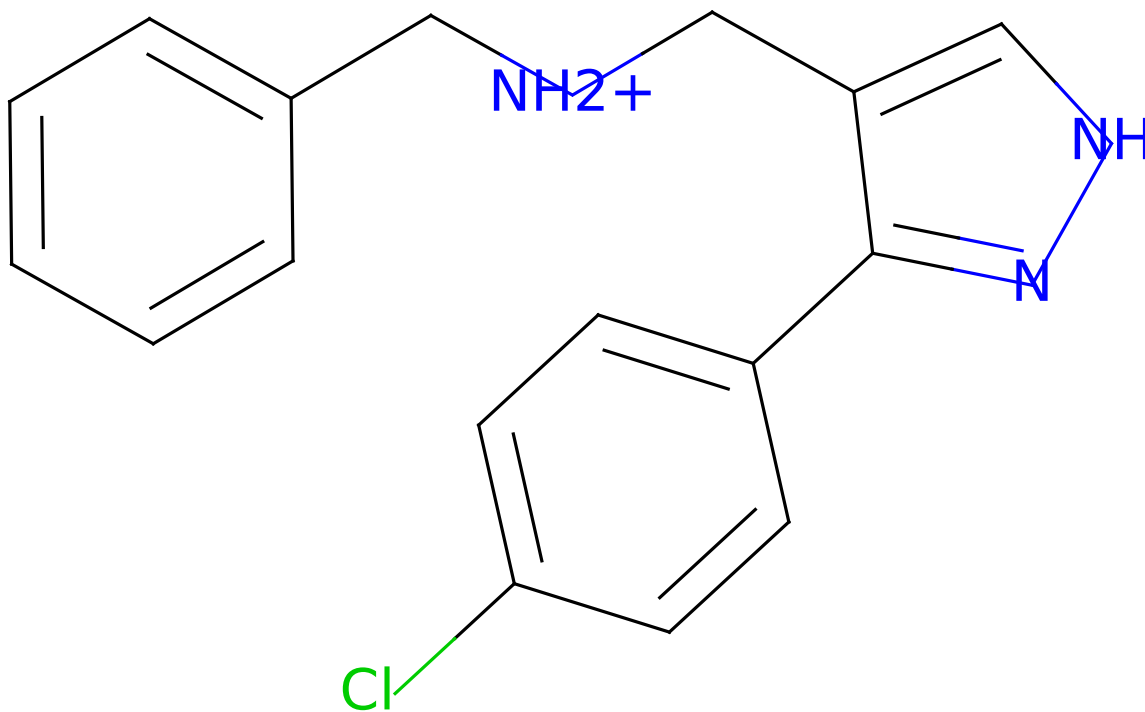
C(CSC(=[NH2+])N)SC(=[NH2+])N

ORD-MCULE-6143797504_1

MolLogP: 1.2030999999999998 | QED: 0.48377262508697316
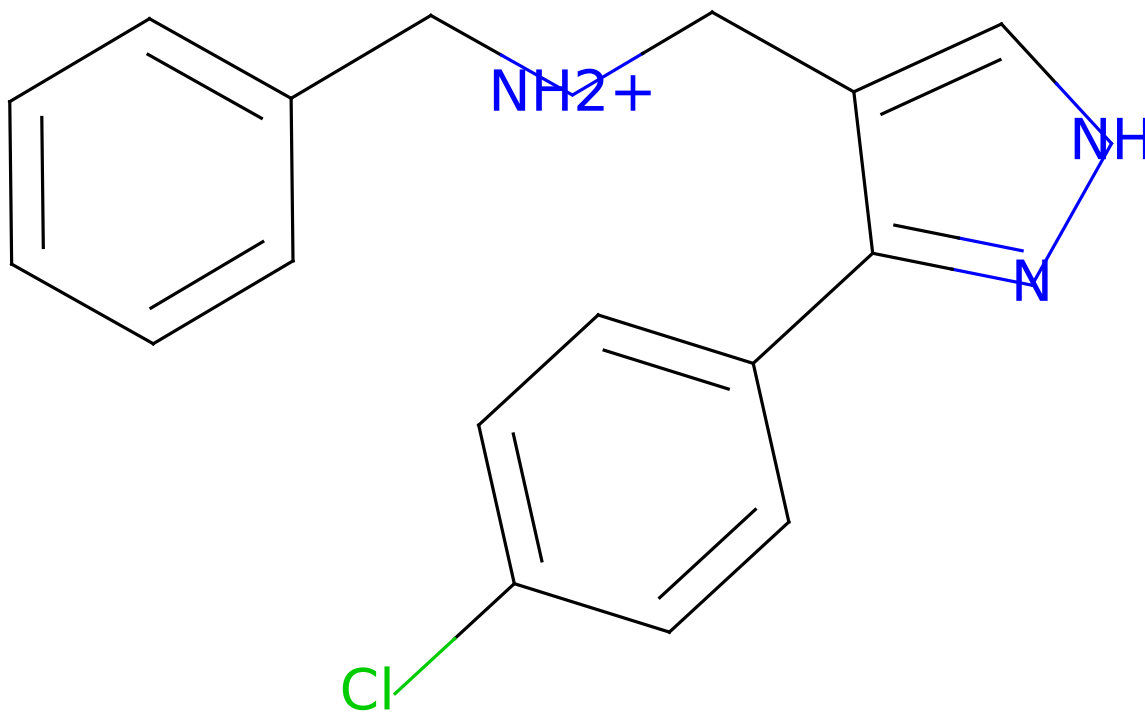
c1ccc2c(c1)c([nH]n2)C(=O)NCCSc3cn[nH]n3

ORD-MCULE-4087160291_2

MolLogP: 2.9937000000000005 | QED: 0.7471396874116025
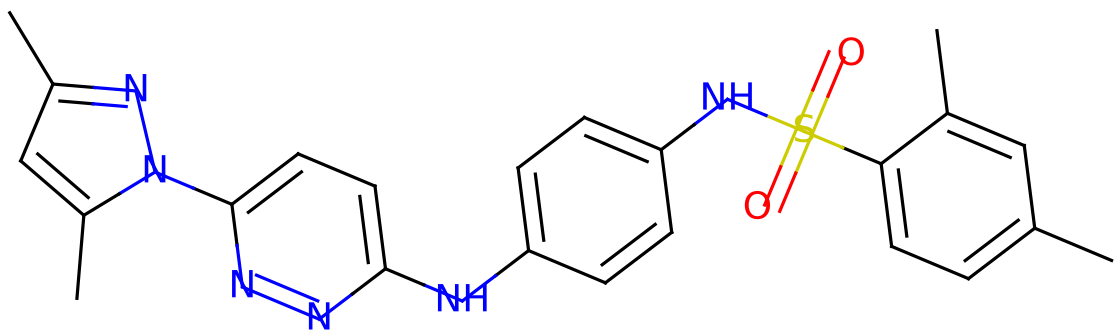
c1ccc(cc1)C[NH2+]Cc2c[nH]nc2c3ccc(cc3)Cl

ORD-MCULE-7943829824_2

MolLogP: 2.9937000000000005 | QED: 0.7471396874116025
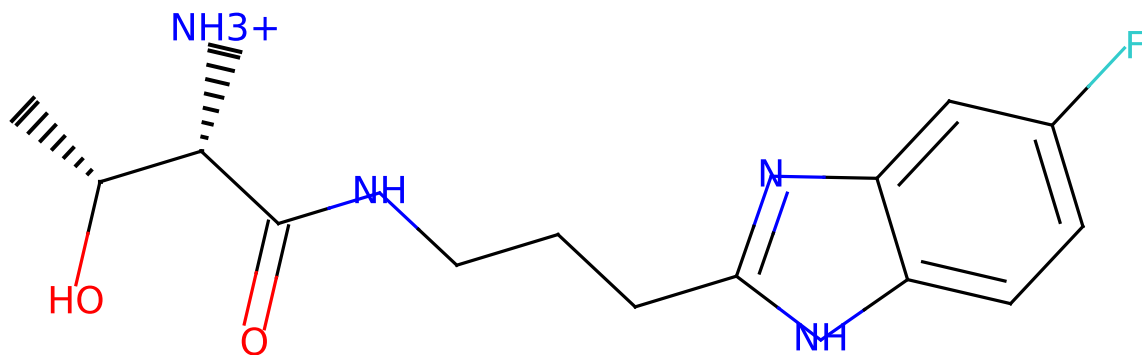
c1ccc(cc1)C[NH2+]Cc2c[nH]nc2c3ccc(cc3)Cl

ORD-MCULE-1543150755_2

MolLogP: 4.440380000000002 | QED: 0.45212526711587675

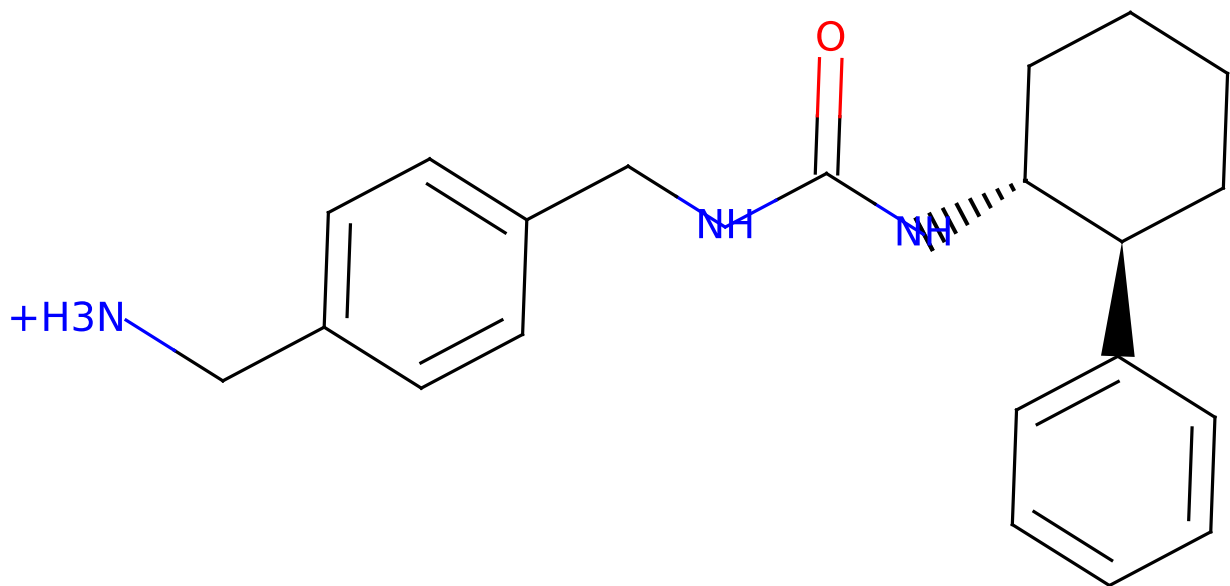Cc1ccc(c(c1)C)S(=O)(=O)Nc2ccc(cc2)Nc3ccc(nn3)n4c(cc(n4)C)C

ORD-MCULE-1431143843_1

MolLogP: -0.2578999999999998 | QED: 0.5517583186893628

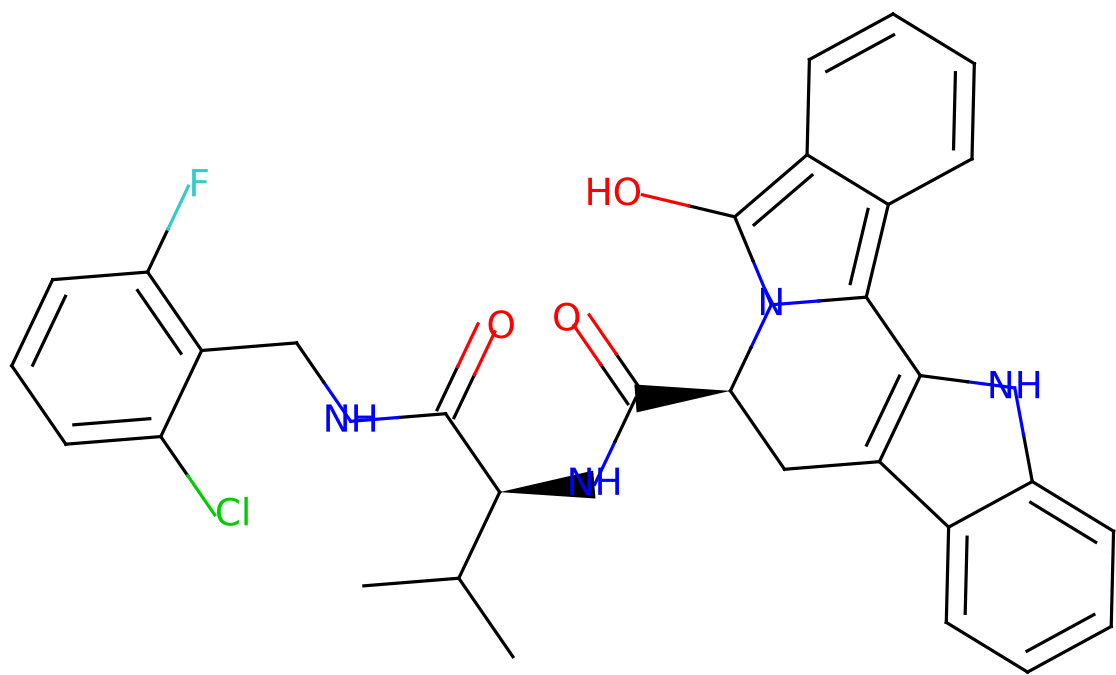C[C@H]([C@@H](C(=O)NCCCc1[nH]c2ccc(cc2n1)F)[NH3+])O

ORD-MCULE-2801087464_2

MolLogP: 2.9540999999999995 | QED: 0.7706756725762592

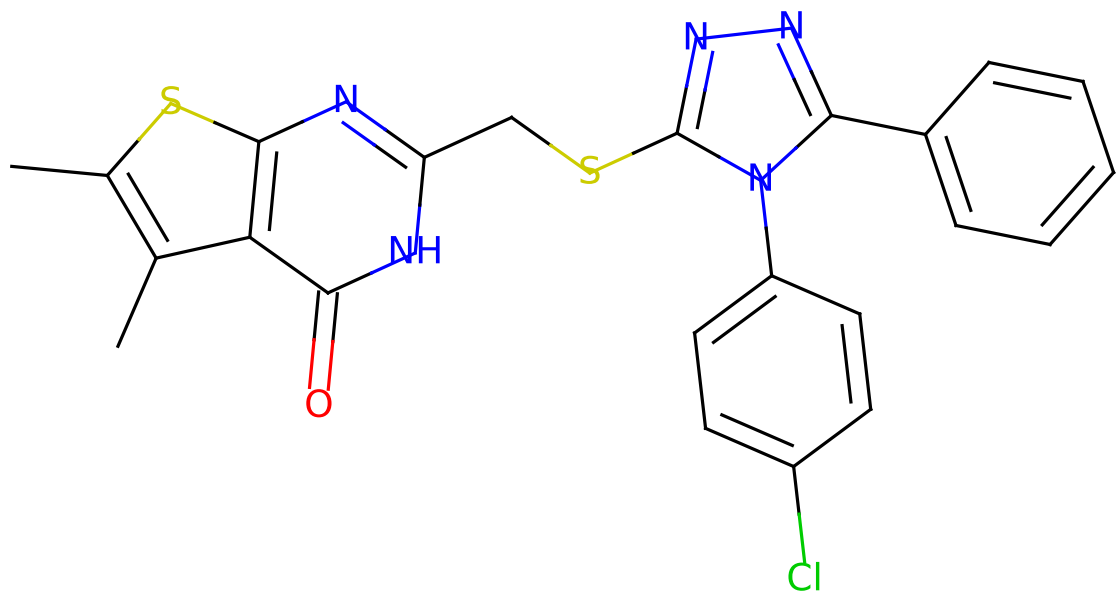c1ccc(cc1)[C@@H]2CCCC[C@H]2NC(=O)NCc3ccc(cc3)C[NH3+]

ORD-MCULE-5985705514_1

MolLogP: 5.842100000000006 | QED: 0.2105388748100887

CC(C)[C@@H](C(=O)NCc1c(cccc1Cl)F)NC(=O)[C@@H]2Cc3c4ccccc4[nH]c3-c5n2c(c6c5cccc6)O
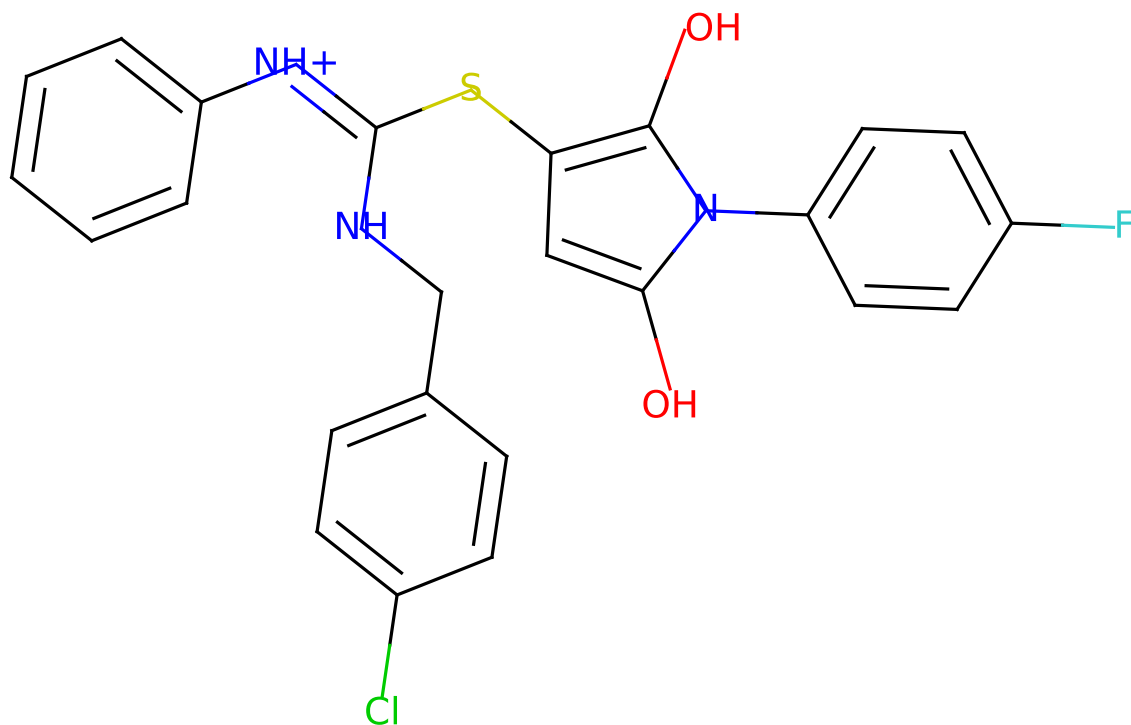
ORD-MCULE-8258045284_1

MolLogP: 5.794840000000004 | QED: 0.32246728257767643

Cc1c(sc2c1c(=O)[nH]c(n2)CSc3nnc(n3c4ccc(cc4)Cl)c5ccccc5)C

ORD-MCULE-4200535063_1

MolLogP: 1.1573999999999989 | QED: 0.4711511261739625

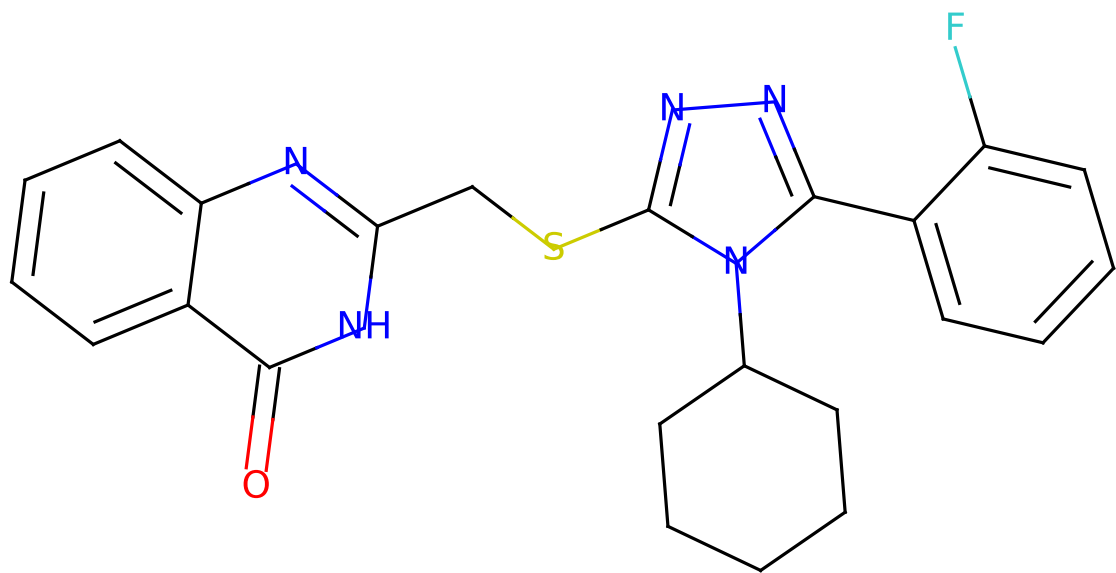COc1ccc(cc1)c2cn3c4ccccc4nc3n2CCN5CC[NH+](CC5)CCO

ORD-MCULE-4391248609_1

MolLogP: 4.3312000000000035 | QED: 0.19976136878195225

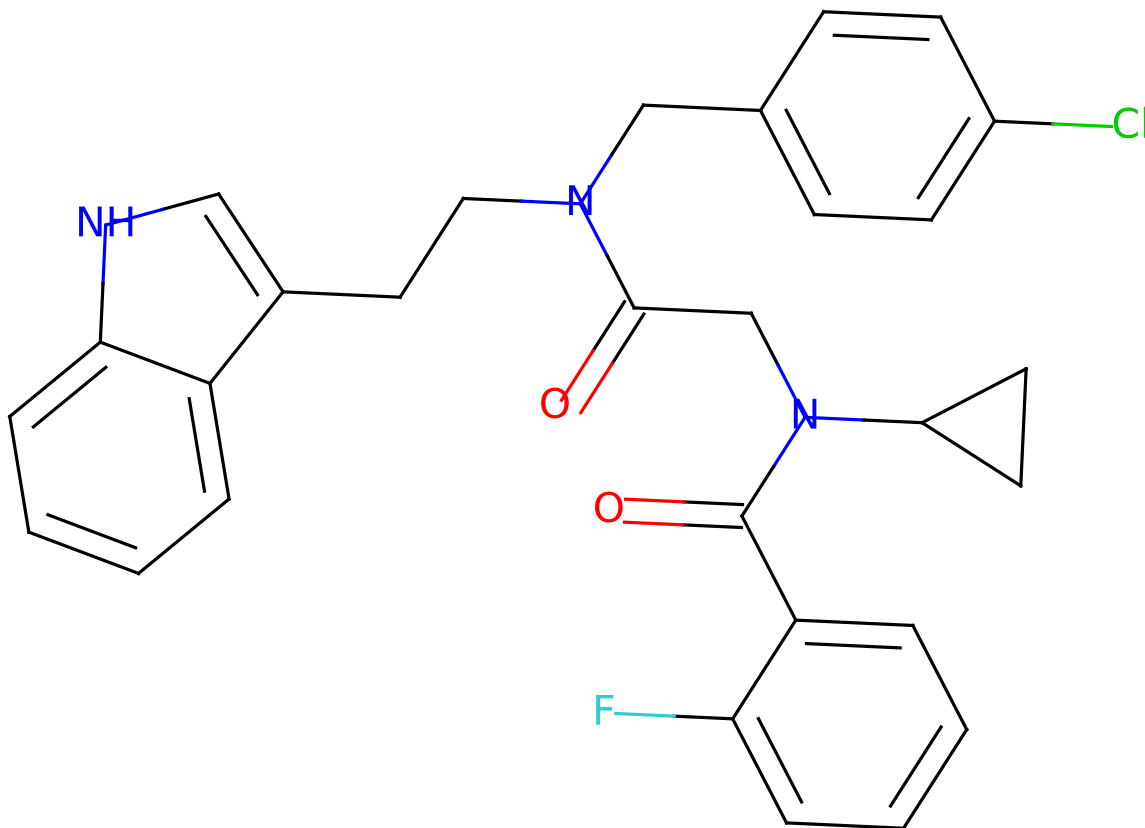c1ccc(cc1)/[NH+]=C(\NCc2ccc(cc2)Cl)/Sc3cc(n(c3O)c4ccc(cc4)F)O

ORD-MCULE-3082269743_2

MolLogP: 5.118200000000003 | QED: 0.44053341797173784

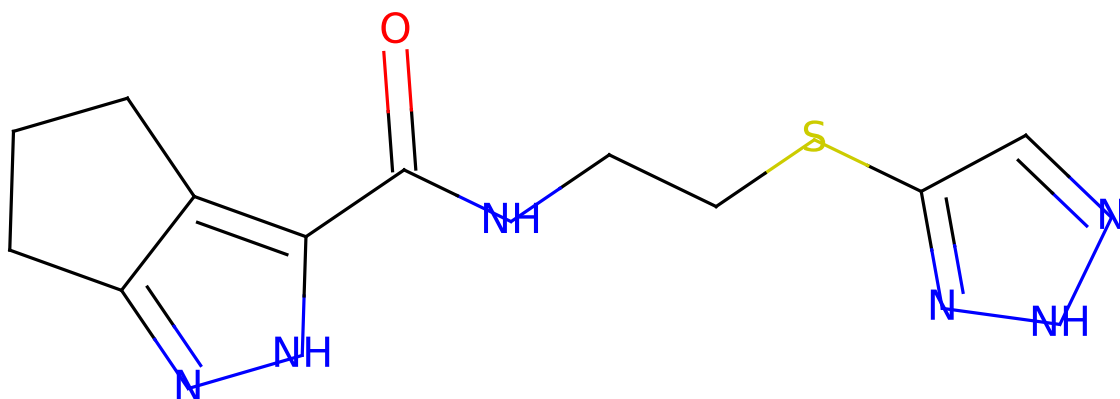c1ccc2c(c1)c(=O)[nH]c(n2)CSc3nnc(n3C4CCCCC4)c5ccccc5F

ORD-MCULE-3688813370_1

MolLogP: 5.8365000000000045 | QED: 0.31193101256435674

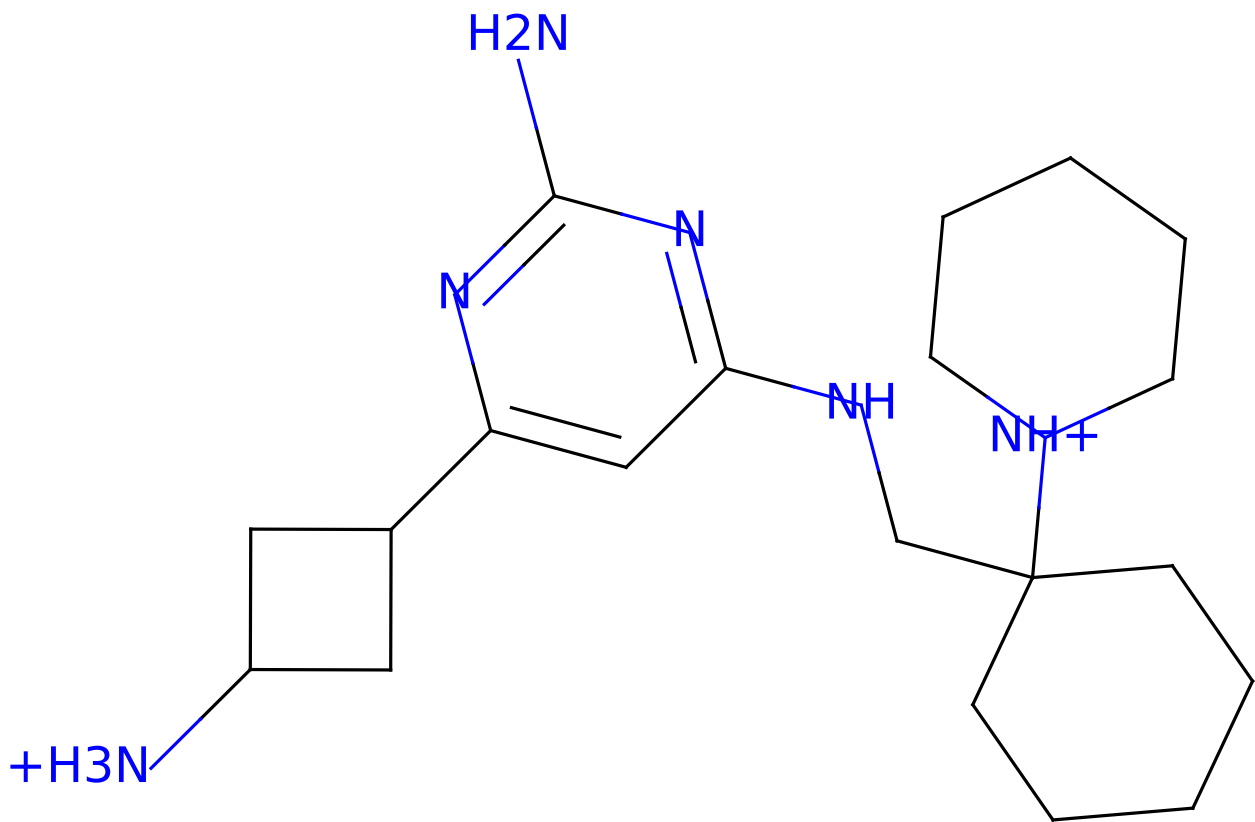c1ccc2c(c1)c(c[nH]2)CCN(Cc3ccc(cc3)Cl)C(=O)CN(C4CC4)C(=O)c5ccccc5F

ORD-MCULE-2191192499_1

194

MolLogP: 0.5385999999999996 | QED: 0.5473356614179136
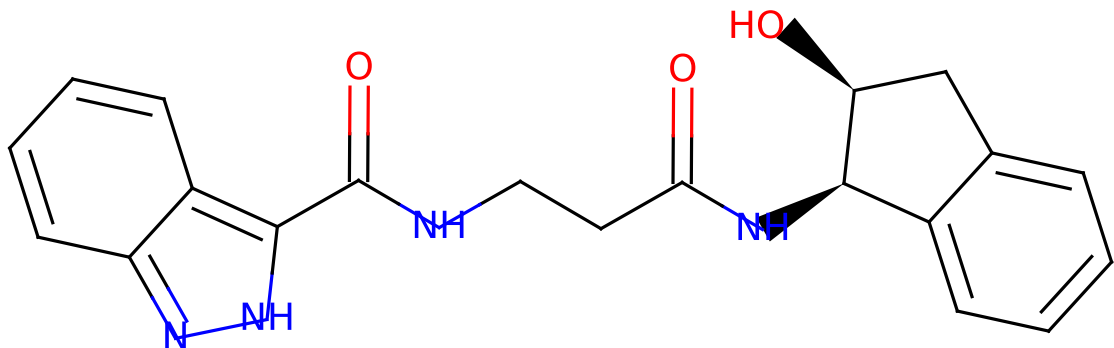
c1c(n[nH]n1)SCCNC(=O)c2c3c(n[nH]2)CCC3

ORD-MCULE-7076725470_2

MolLogP: 0.7303000000000031 | QED: 0.6224096899439784

c1c(nc(nc1NCC2(CCCCC2)[NH+]3CCCCC3)N)C4CC(C4)[NH3+]
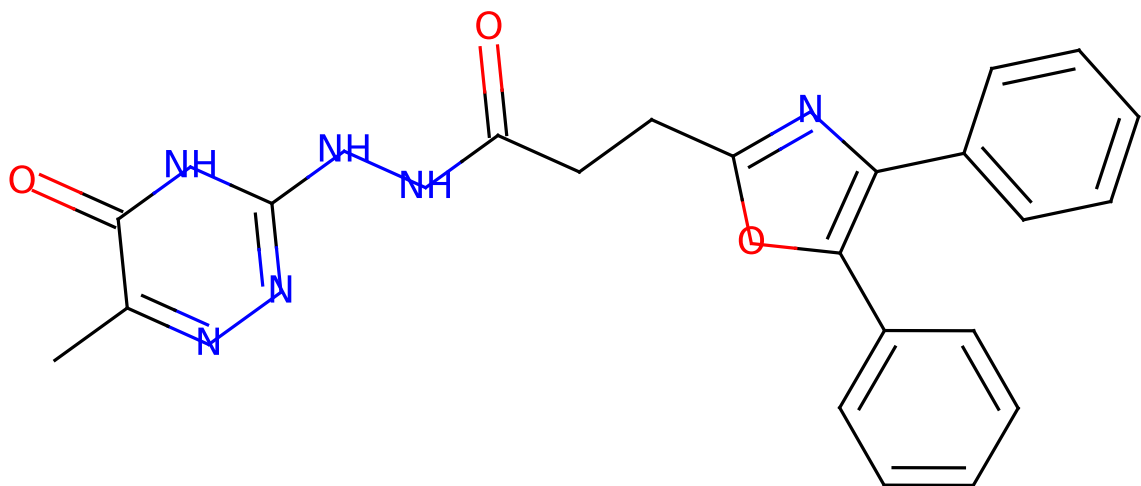
ORD-MCULE-4013099548_1

MolLogP: 1.4572999999999998 | QED: 0.5496662419492623

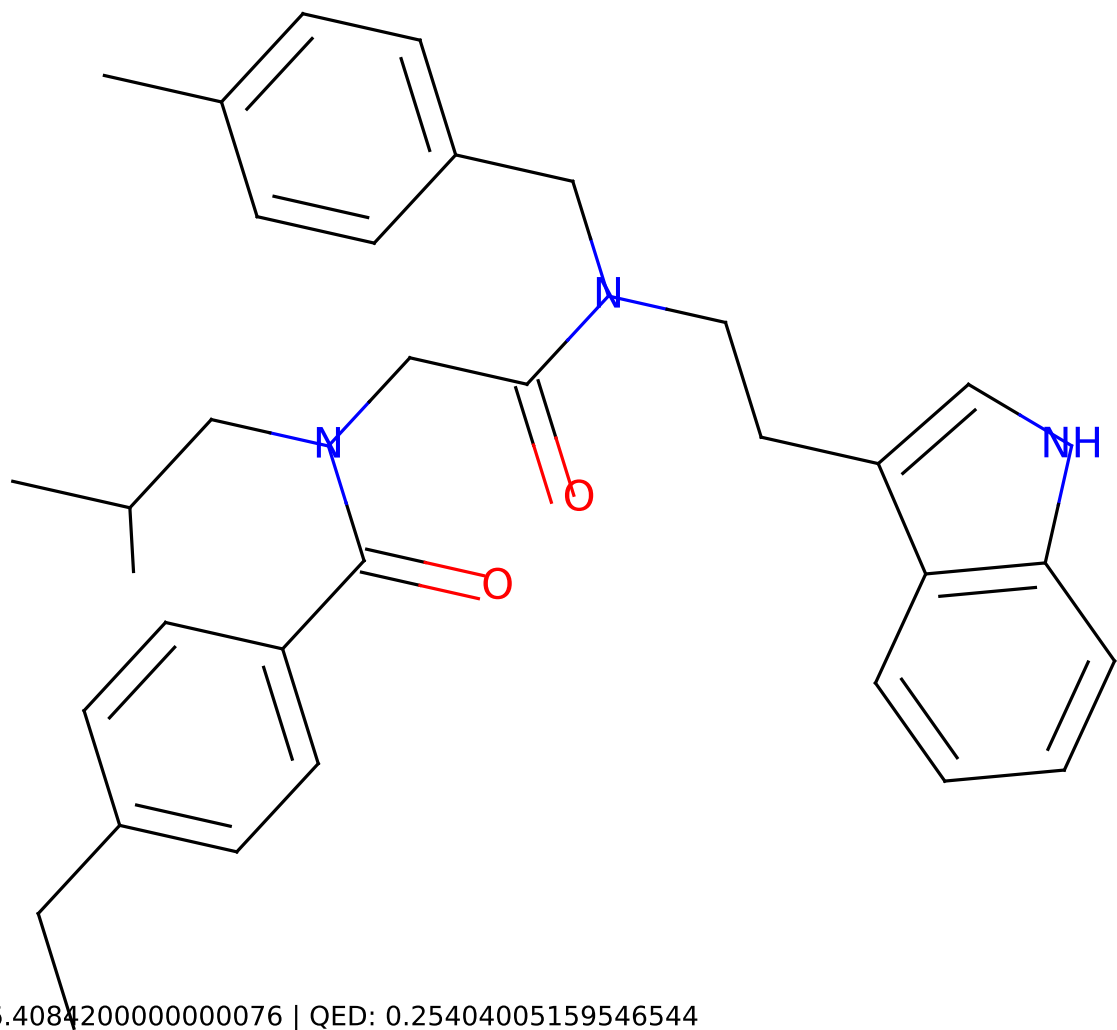c1ccc2c(c1)C[C@@H]([C@@H]2NC(=O)CCNC(=O)c3c4ccccc4n[nH]3)O

ORD-MCULE-3840831569_2

MolLogP: 2.87122 | QED: 0.39553410644706627

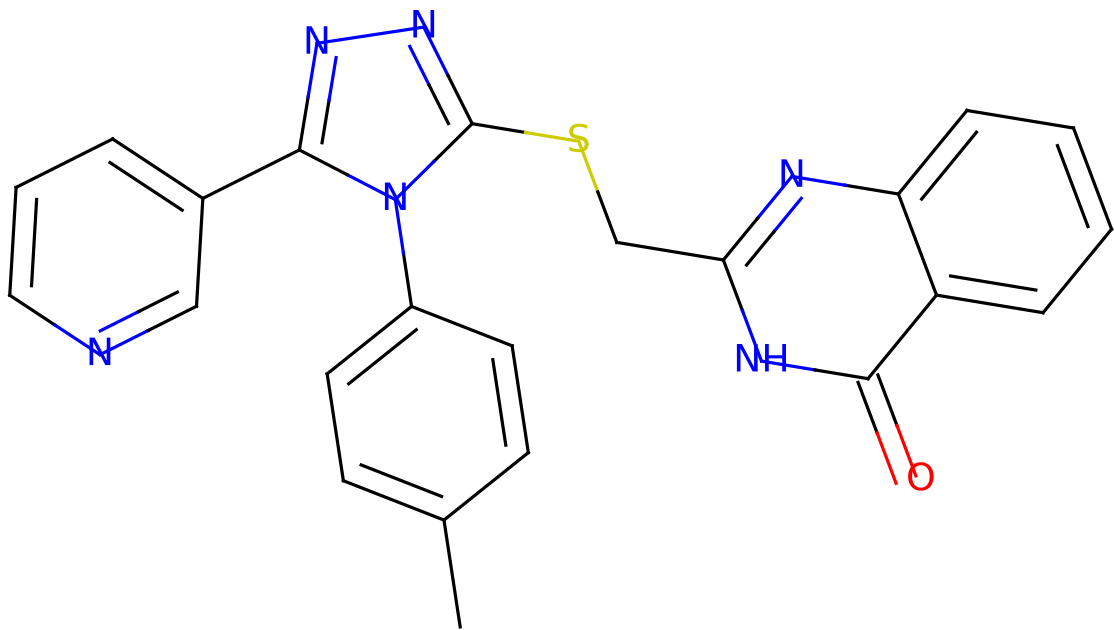Cc1c(=O)[nH]c(nn1)NNC(=O)CCc2nc(c(o2)c3ccccc3)c4ccccc4

ORD-MCULE-2018561625_1

MolLogP: 6.4084200000000076 | QED: 0.25404005159546544

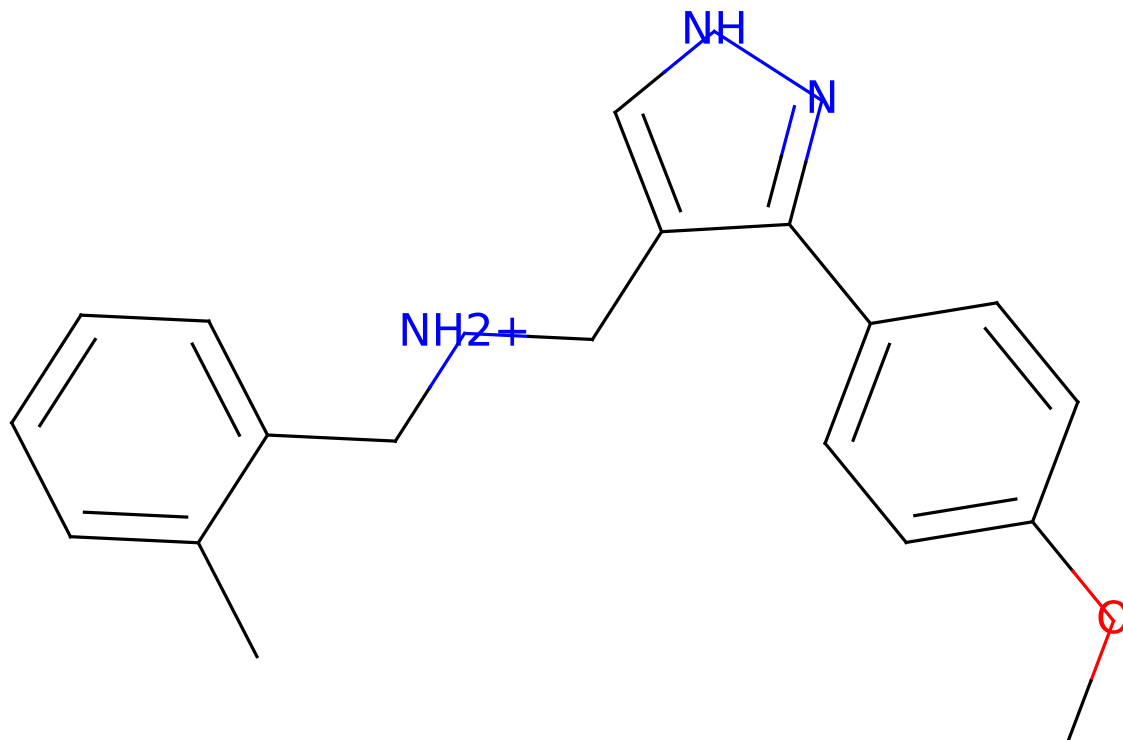CCc1ccc(cc1)C(=O)N(CC(C)C)CC(=O)N(CCc2c[nH]c3c2cccc3)Cc4ccc(cc4)C

ORD-MCULE-3489359328_1

MolLogP: 4.166520000000002 | QED: 0.42448353309437625
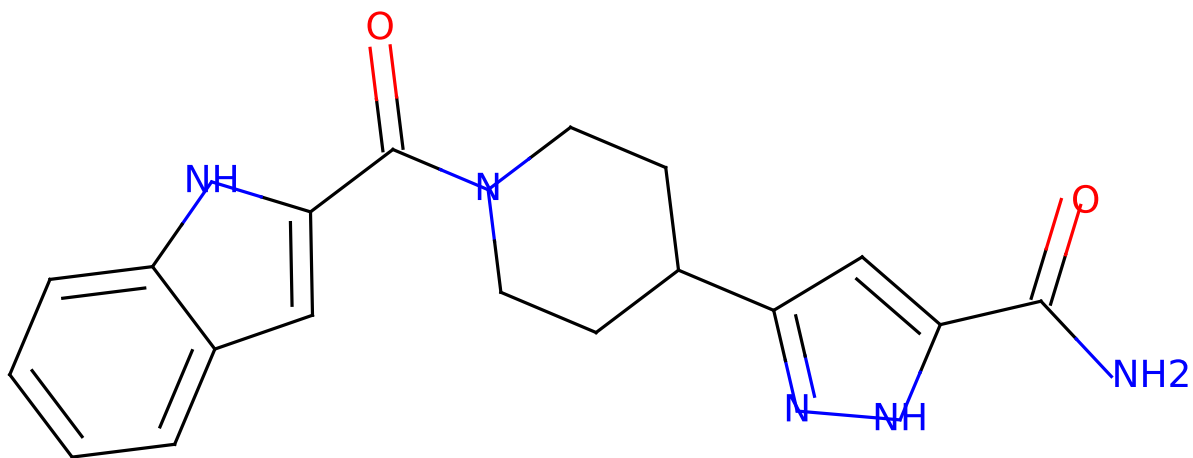
Cc1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4ccccc4n3)c5cccnc5

ORD-MCULE-9348026124_1

MolLogP: 2.6573200000000003 | QED: 0.7353755142198527
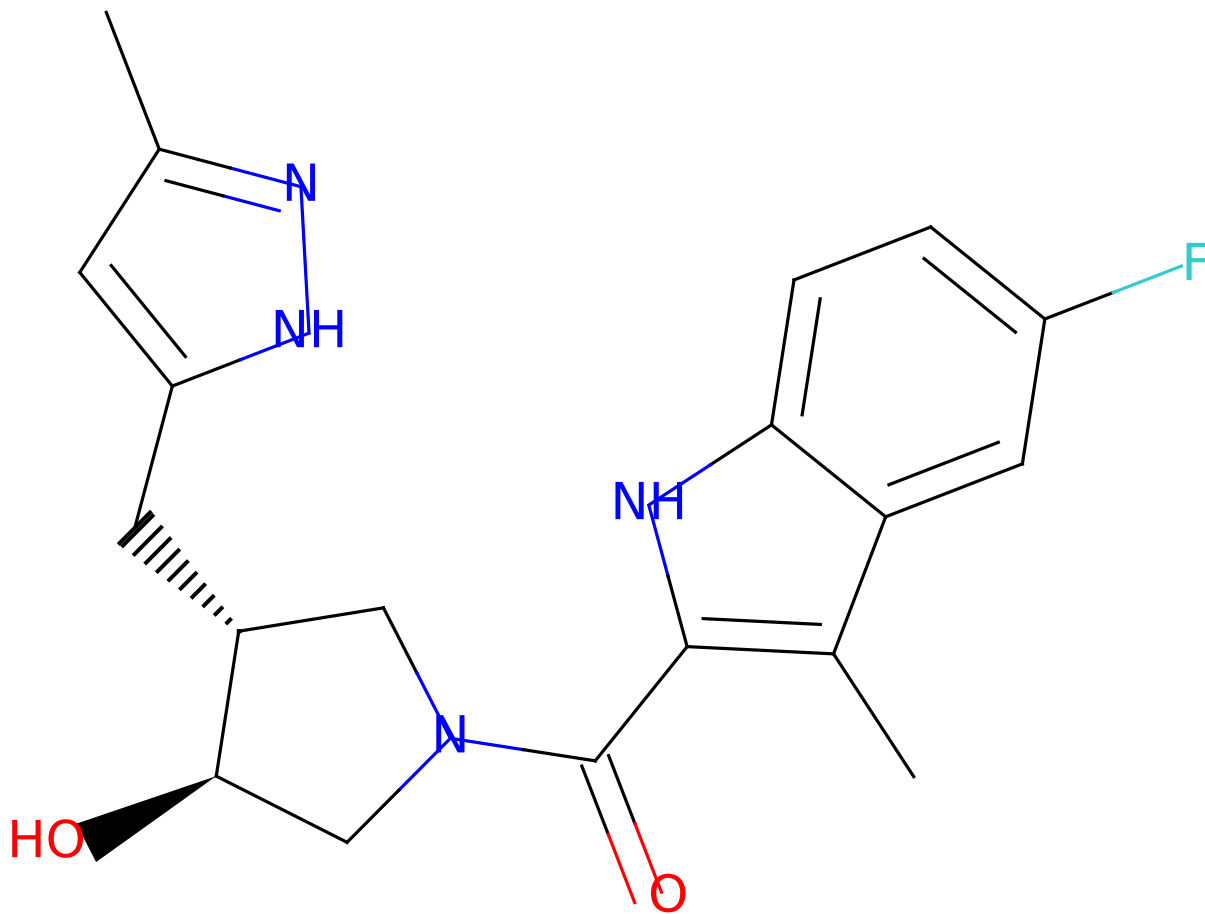
Cc1ccccc1C[NH2+]Cc2c[nH]nc2c3ccc(cc3)OC

ORD-MCULE-5715268546_2

201

MolLogP: 2.009699999999999 | QED: 0.6800421176747338
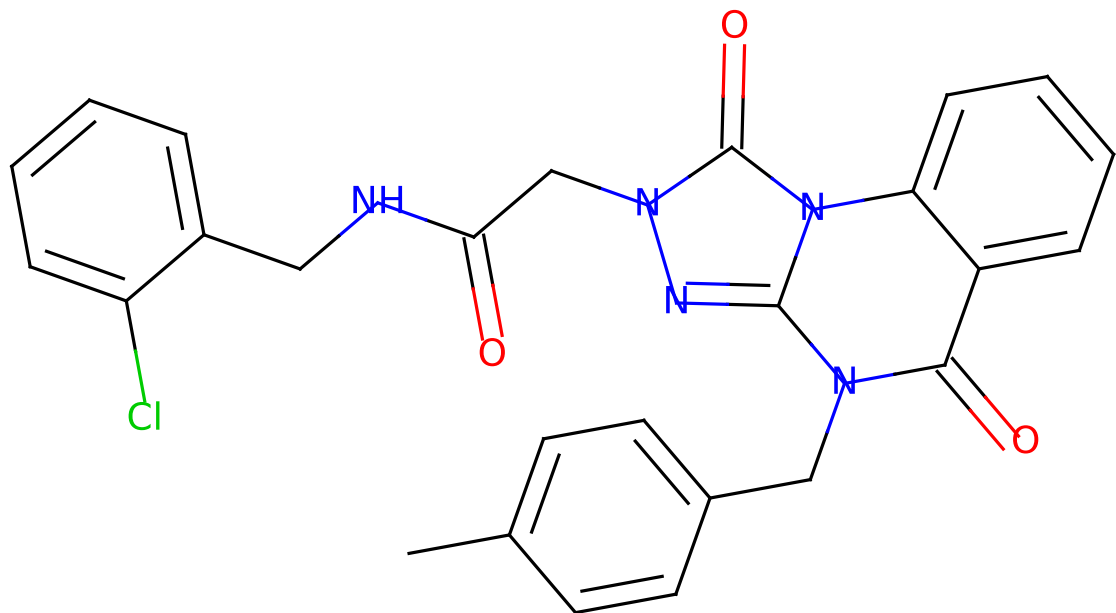
c1ccc2c(c1)cc([nH]2)C(=O)N3CCC(CC3)c4cc([nH]n4)C(=O)N

ORD-MCULE-1541843003_1

MolLogP: 2.322540000000001 | QED: 0.6732574964382159

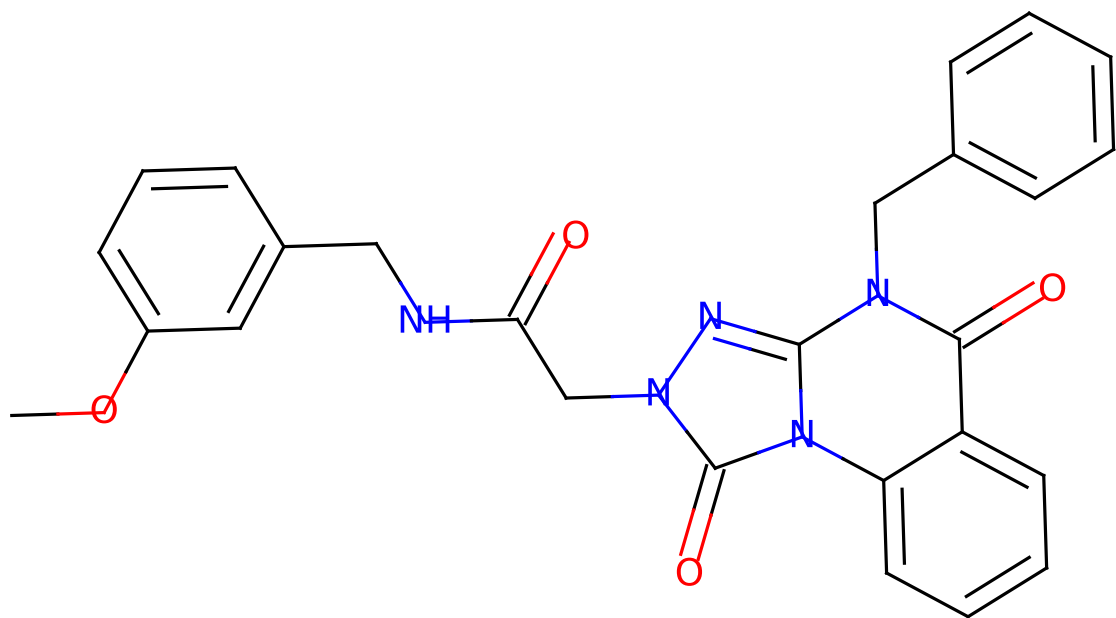Cc1cc([nH]n1)C[C@@H]2CN(C[C@H]2O)C(=O)c3c(c4cc(ccc4[nH]3)F)C

ORD-MCULE-1415496642_2

MolLogP: 3.1374200000000014 | QED: 0.3981895620447937

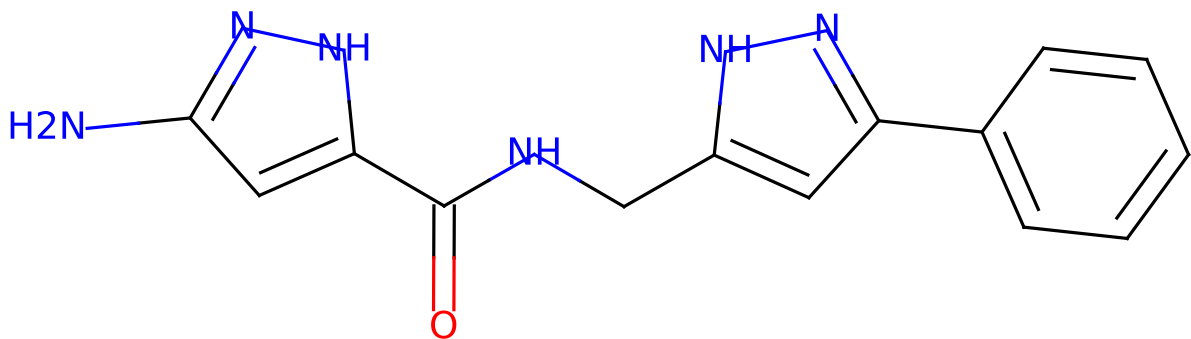Cc1ccc(cc1)Cn2c(=O)c3ccccc3n4c2nn(c4=O)CC(=O)NCc5ccccc5Cl

ORD-MCULE-1519514142_1

204

MolLogP: 2.1841999999999997 | QED: 0.3939687915568442

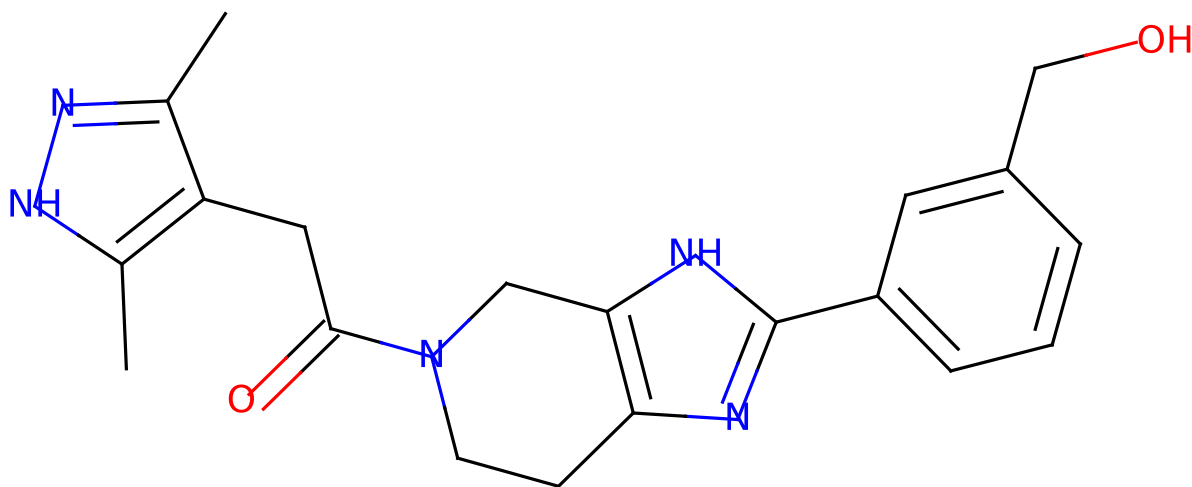COc1cccc(c1)CNC(=O)Cn2c(=O)n3c4ccccc4c(=O)n(c3n2)Cc5ccccc5

ORD-MCULE-4293042328_1

205

MolLogP: 1.3119999999999996 | QED: 0.5775560590322325
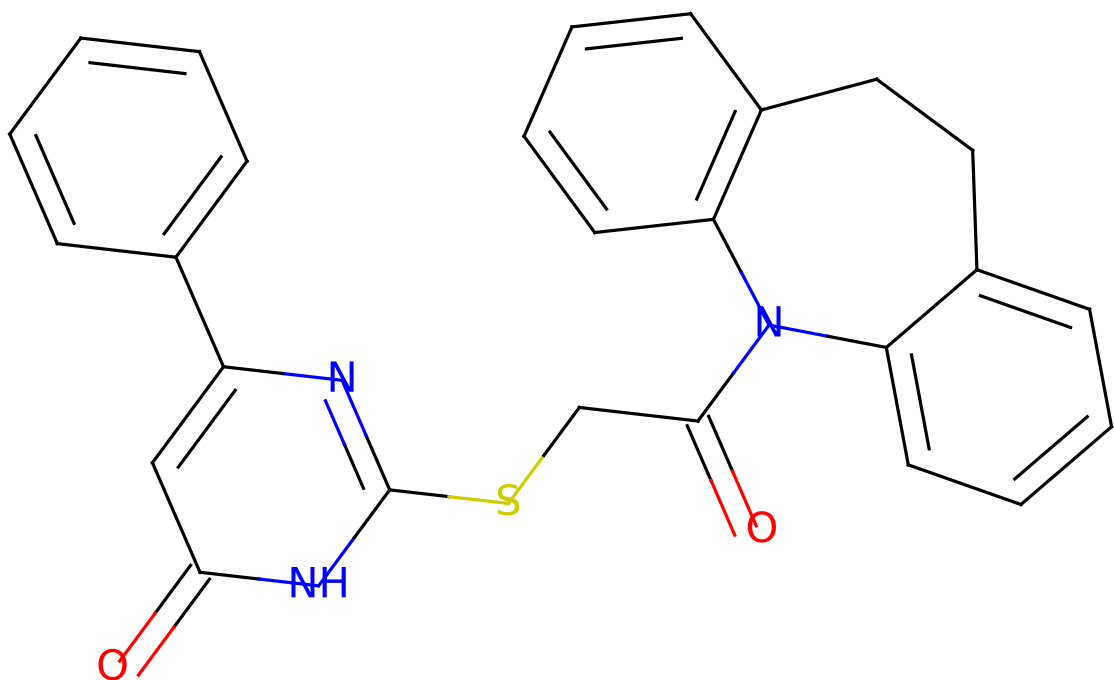
c1ccc(cc1)c2cc([nH]n2)CNC(=O)c3cc(n[nH]3)N

ORD-MCULE-7367467944_1

MolLogP: 2.03634 | QED: 0.6588826857001278

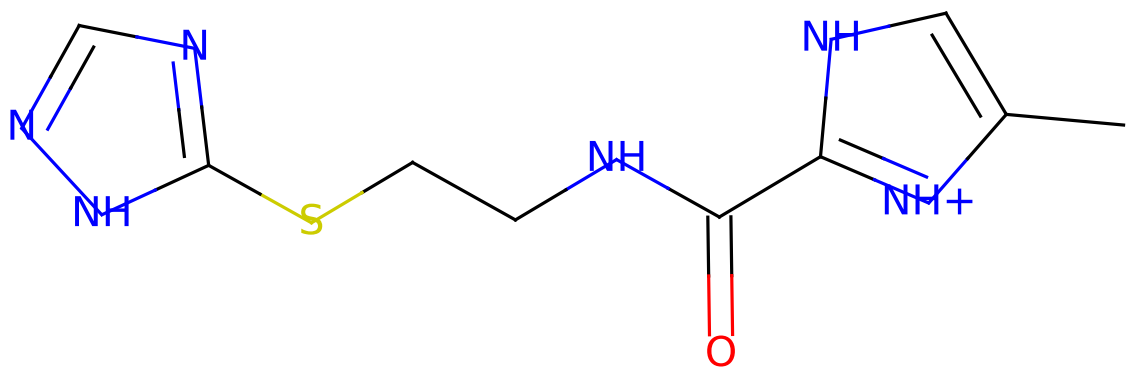Cc1c(c(n[nH]1)C)CC(=O)N2CCc3c([nH]c(n3)c4cccc(c4)CO)C2

ORD-MCULE-6069061169_1

MolLogP: 4.992500000000004 | QED: 0.3592735625430039
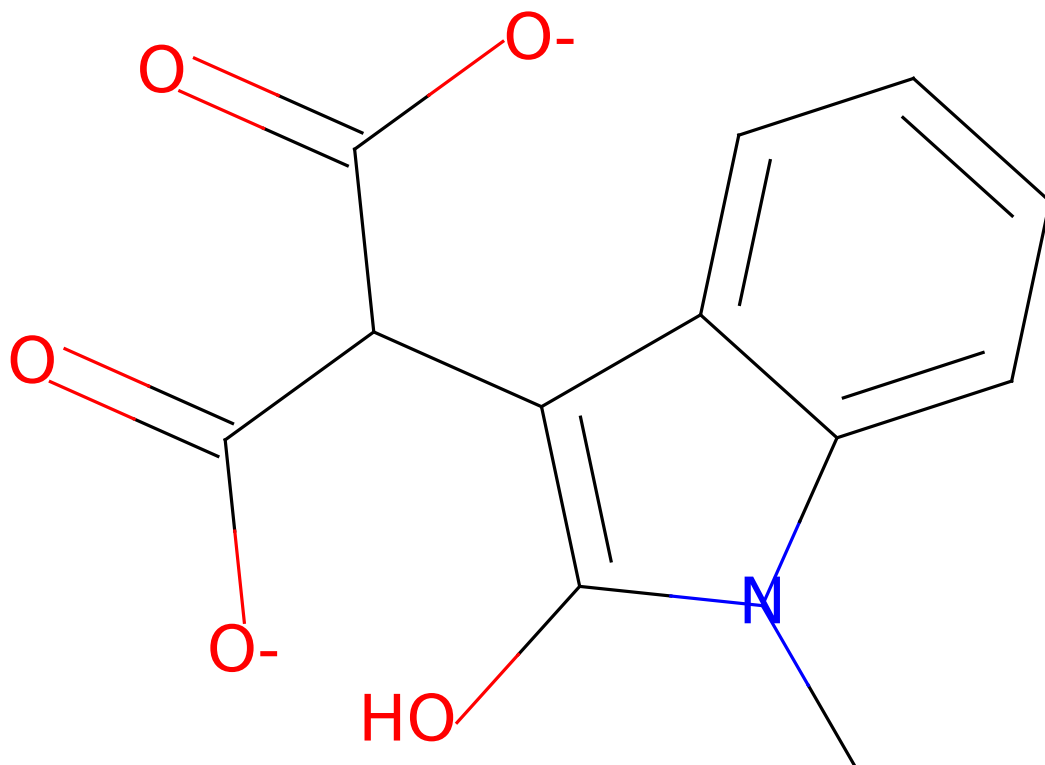
c1ccc(cc1)c2cc(=O)[nH]c(n2)SCC(=O)N3c4ccccc4CCc5c3cccc5

ORD-MCULE-5745284403_1

MolLogP: -0.22257999999999972 | QED: 0.5061753470565761
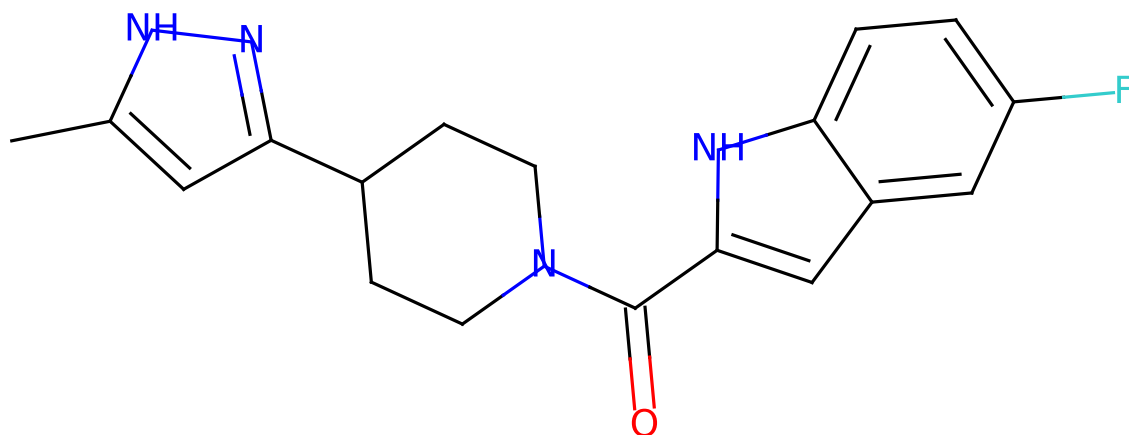
Cc1c[nH]c([nH+]1)C(=O)NCCSc2[nH]ncn2

ORD-MCULE-3031881642_4

MolLogP: -1.5327000000000002 | QED: 0.6620379444743765
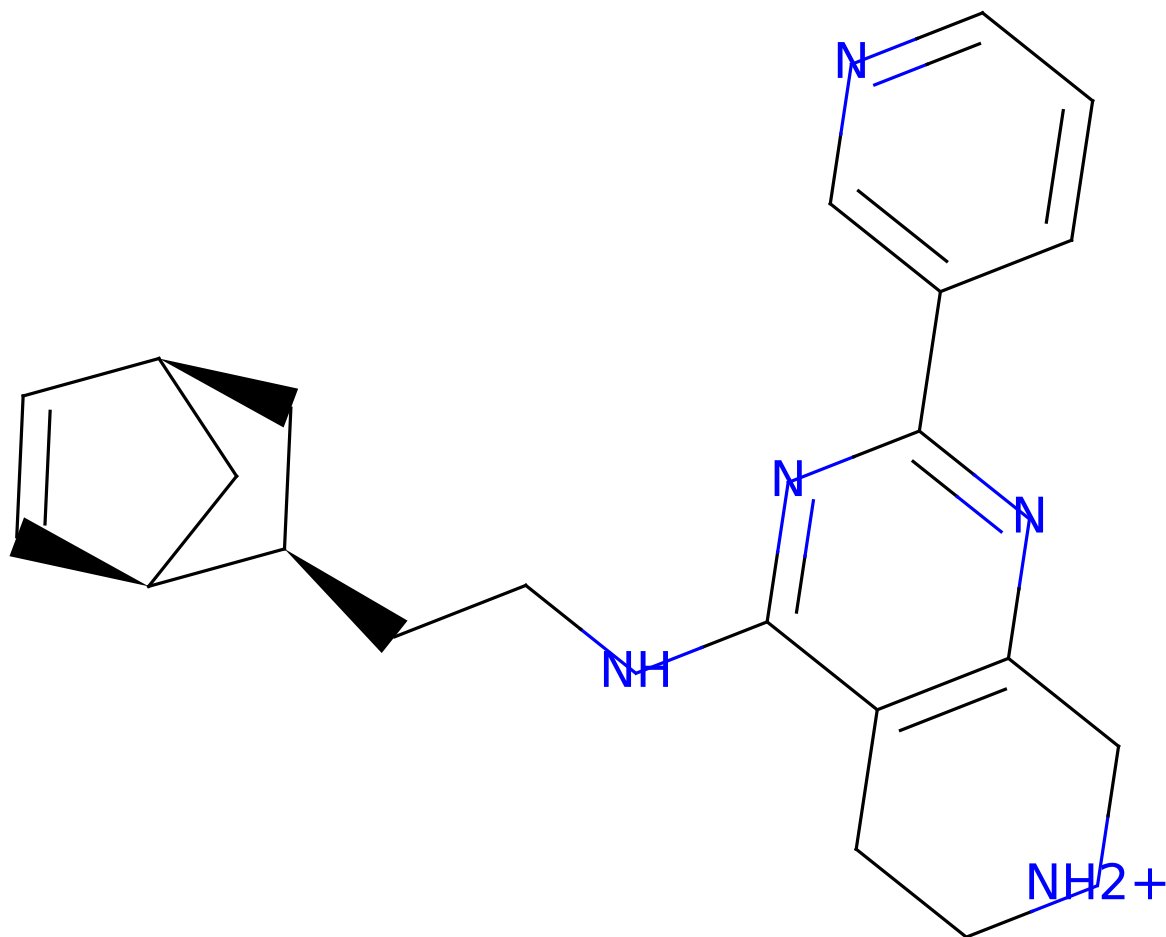
Cn1c2ccccc2c(c1O)C(C(=O)[O-])C(=O)[O-]

ORD-MCULE-6430306176_1

MolLogP: 3.3583200000000017 | QED: 0.7582549149593061
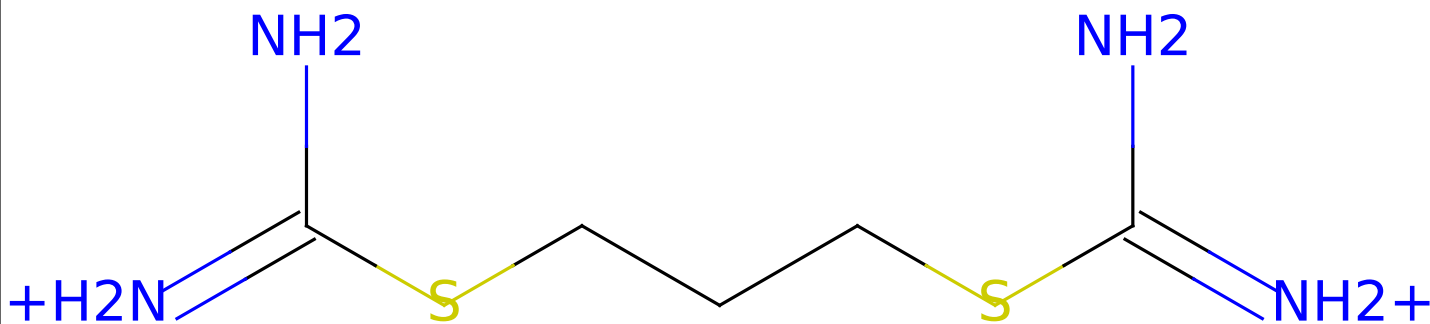
Cc1cc(n[nH]1)C2CCN(CC2)C(=O)c3cc4cc(ccc4[nH]3)F

ORD-MCULE-1224951145_1

MolLogP: 2.1723 | QED: 0.812915759881308

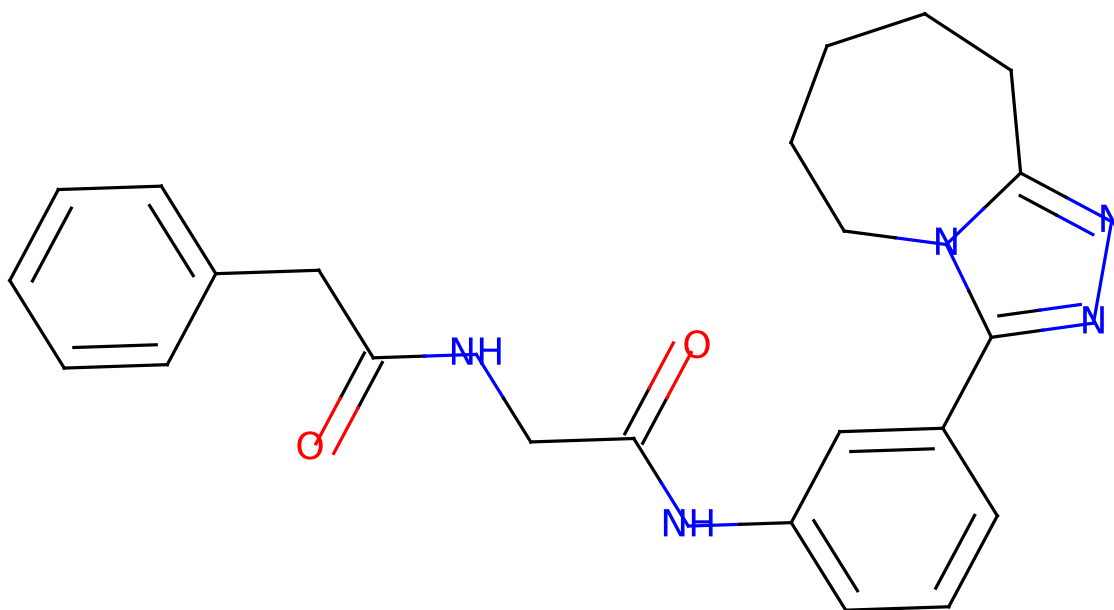c1cc(cnc1)c2nc3c(c(n2)NCC[C@@H]4C[C@H]5C[C@@H]4C=C5)CC[NH2+]C3

ORD-MCULE-5739750381_1

MolLogP: -3.009499999999999 | QED: 0.21733625653293873
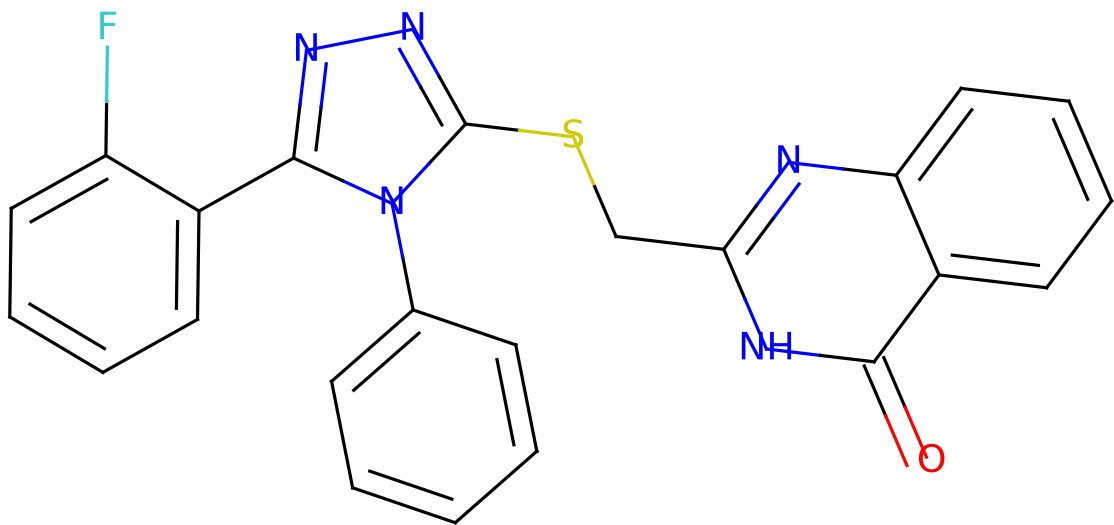
C(CSC(=[NH2+])N)CSC(=[NH2+])N

ORD-MCULE-2100796872_1

MolLogP: 2.9689000000000014 | QED: 0.6622517052186552

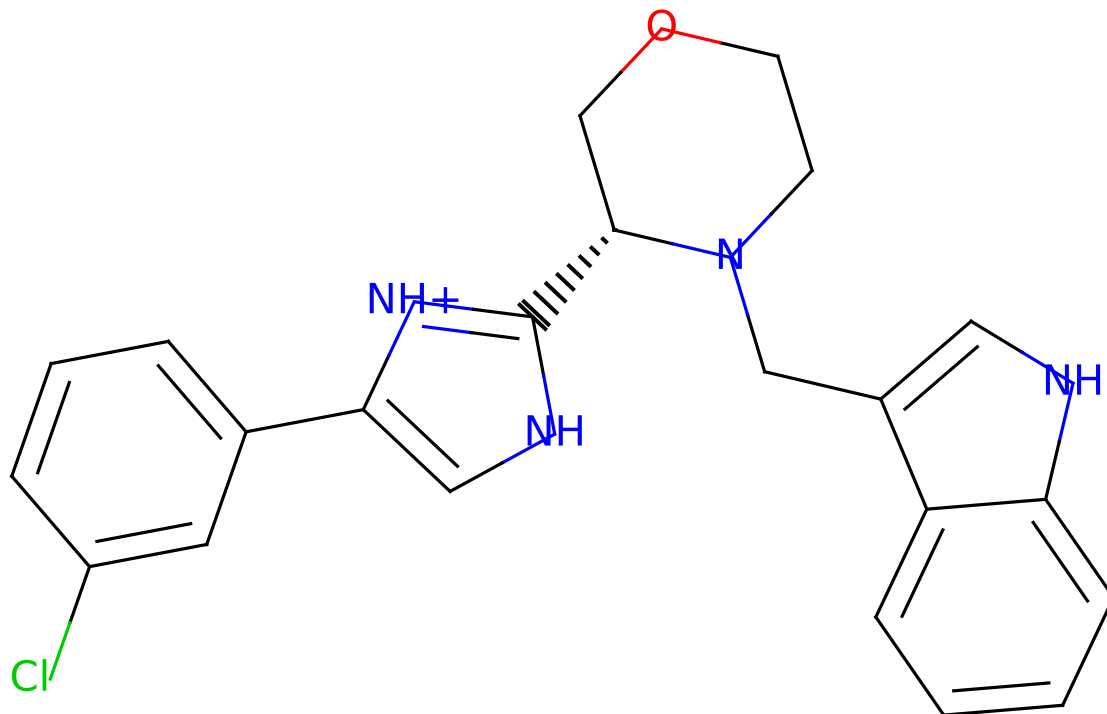c1ccc(cc1)CC(=O)NCC(=O)Nc2cccc(c2)c3nnc4n3CCCCC4

ORD-MCULE-1216711339_1

214

MolLogP: 4.602200000000002 | QED: 0.413298001078919

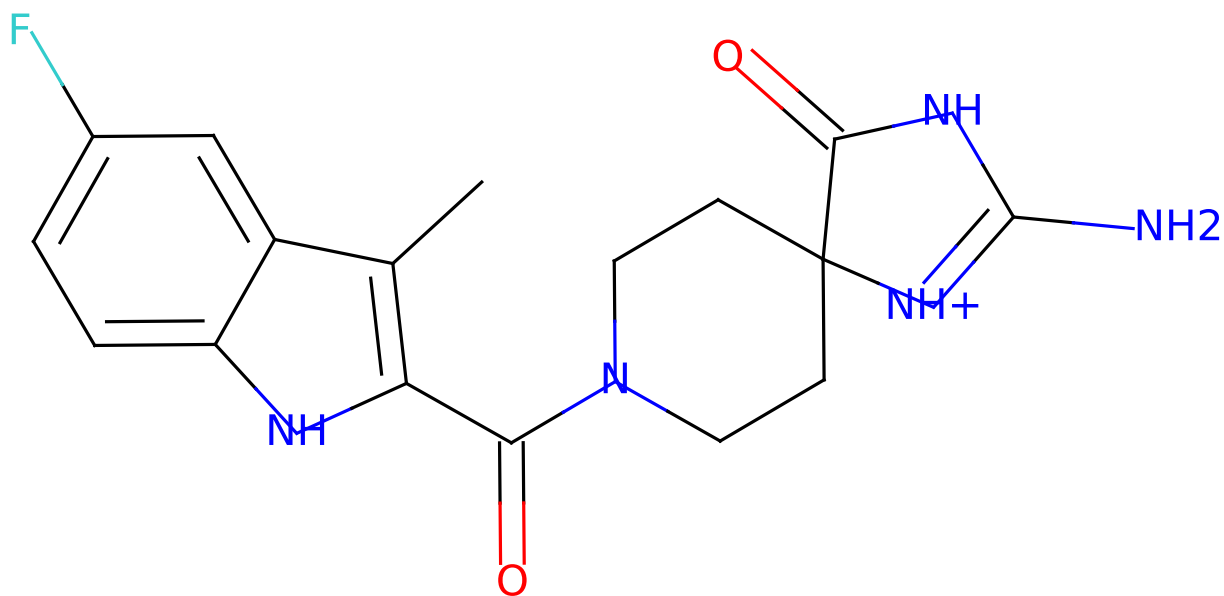c1ccc(cc1)n2c(nnc2SCc3[nH]c(=O)c4ccccc4n3)c5ccccc5F

ORD-MCULE-6571557424_1

MolLogP: 4.204000000000002 | QED: 0.545453988440908

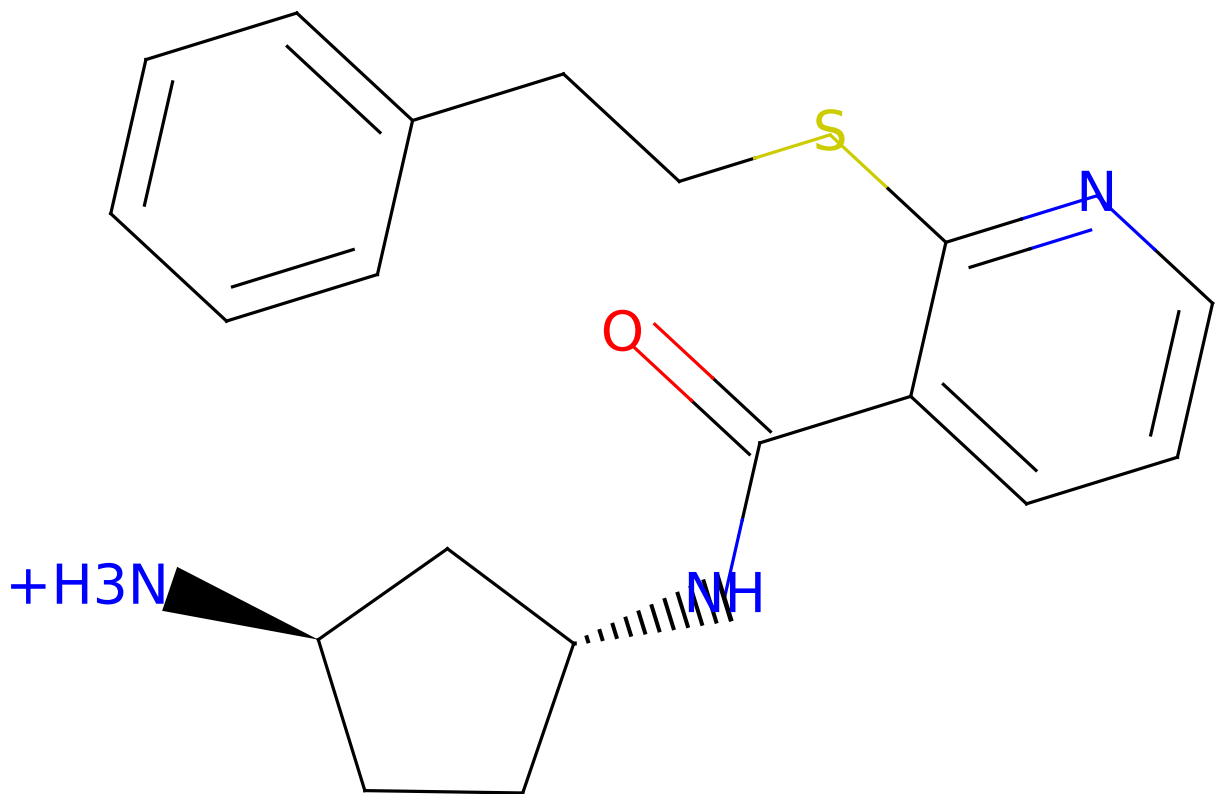c1ccc2c(c1)c(c[nH]2)C[N@@]3CCOC[C@H]3c4[nH]cc([nH+]4)c5cccc(c5)Cl

ORD-MCULE-2988500623_2

216

MolLogP: -0.8846799999999984 | QED: 0.5395798621431691

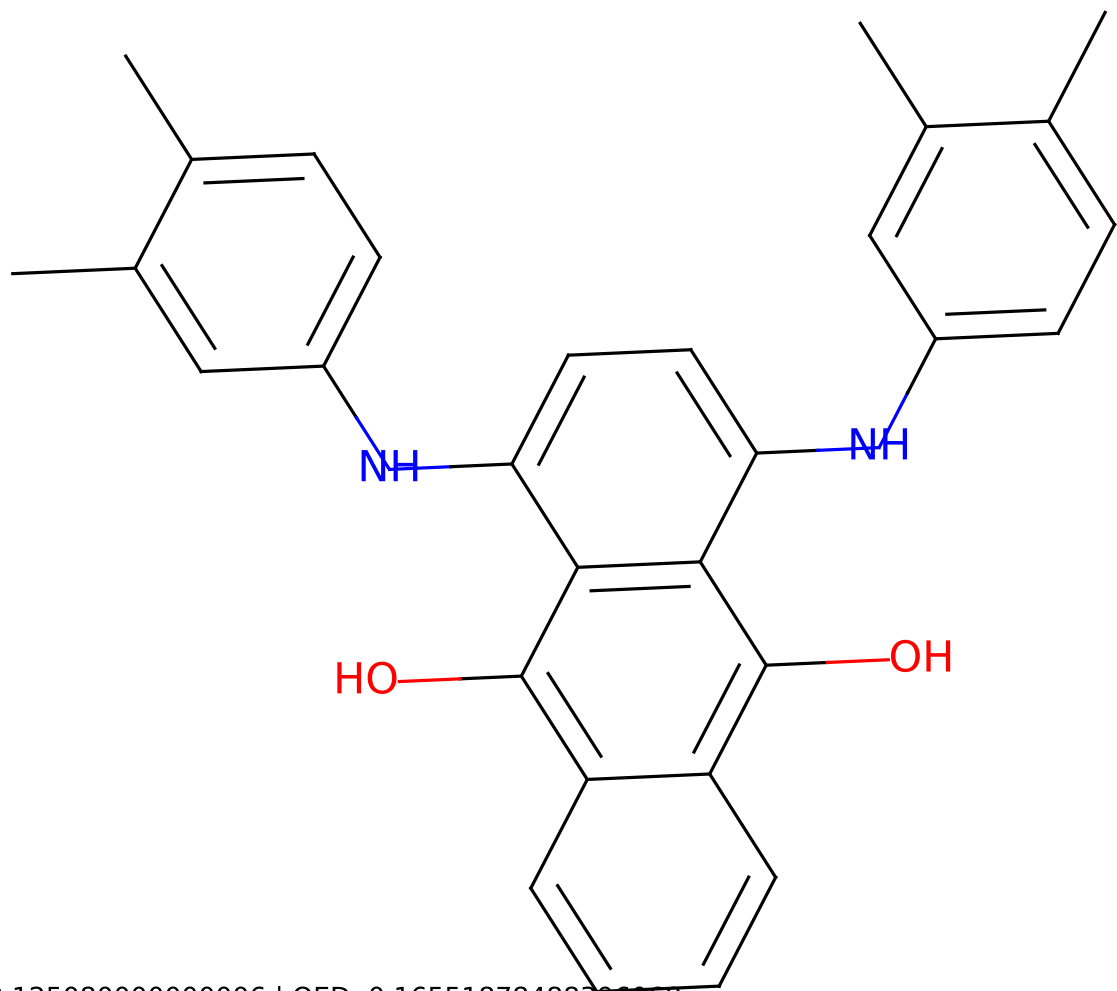Cc1c2cc(ccc2[nH]c1C(=O)N3CCC4(CC3)C(=O)NC(=[NH+]4)N)F

ORD-MCULE-5493358376_1

MolLogP: 2.3091999999999993 | QED: 0.7916274143548181

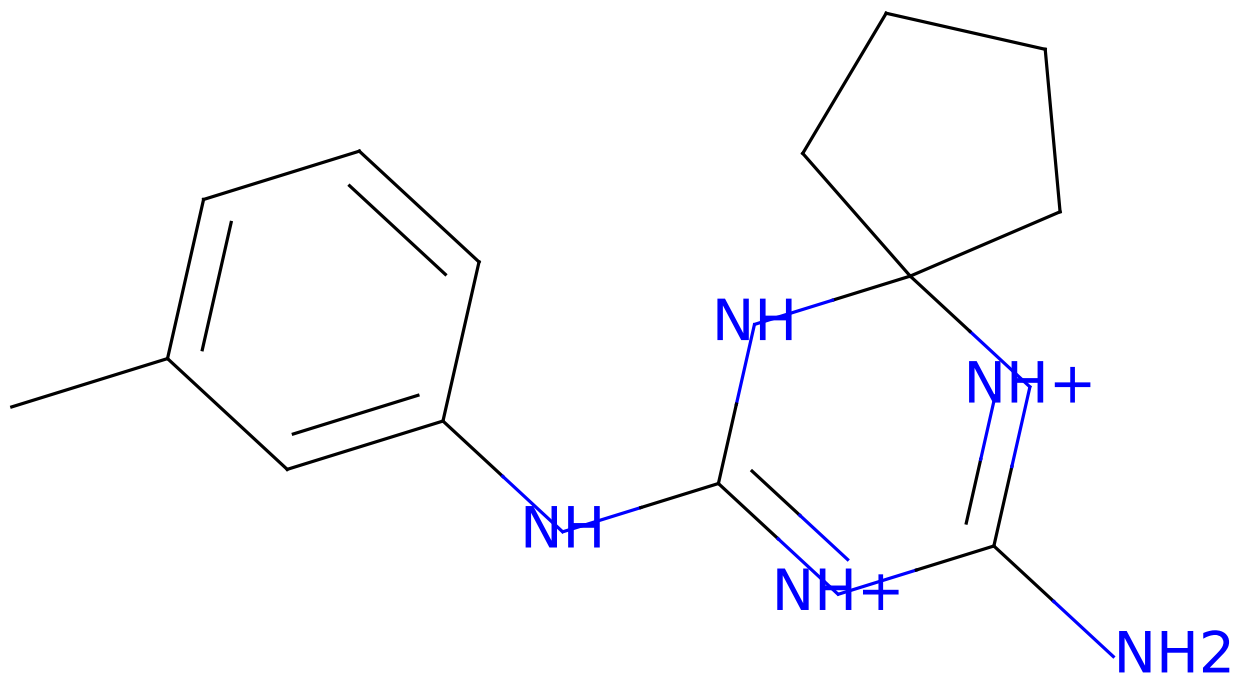c1ccc(cc1)CCSc2c(cccn2)C(=O)N[C@@H]3CC[C@H](C3)[NH3+]

ORD-MCULE-8438239678_1

MolLogP: 8.125080000000006 | QED: 0.1655187848396068

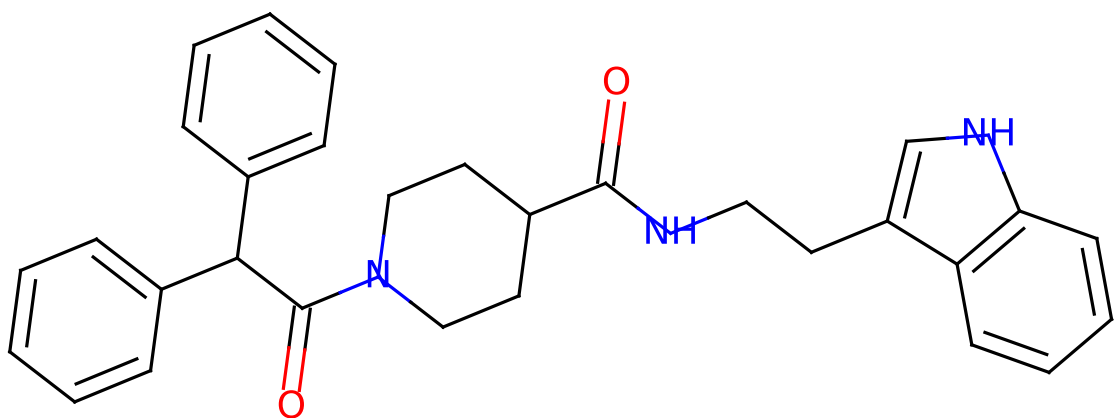Cc1ccc(cc1C)Nc2ccc(c3c2c(c4ccccc4c3O)O)Nc5ccc(c(c5)C)C

ORD-MCULE-7183554266_1

MolLogP: -1.887679999999997 | QED: 0.4092714343340848
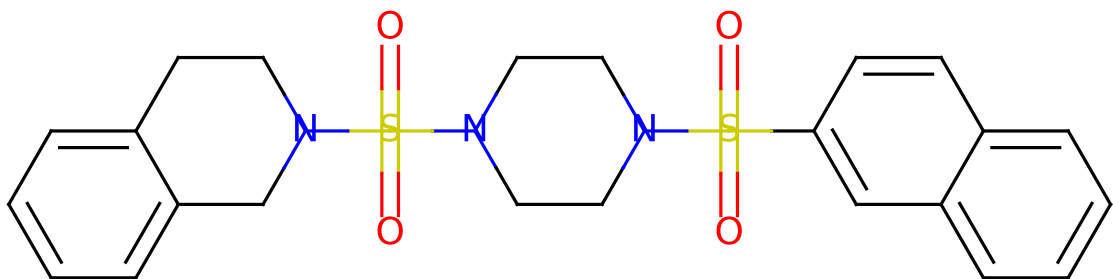
Cc1cccc(c1)NC2=[NH+]C(=[NH+]C3(N2)CCCC3)N

ORD-MCULE-9408357356_3

MolLogP: 4.897300000000003 | QED: 0.40786292071408126

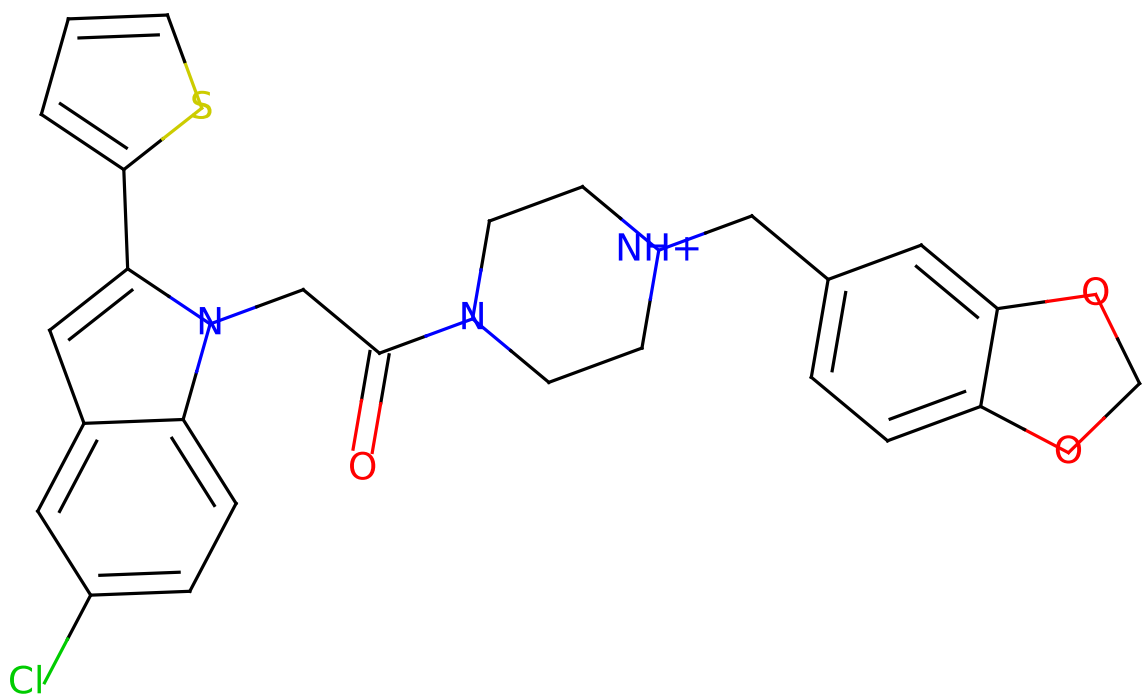c1ccc(cc1)C(c2ccccc2)C(=O)N3CCC(CC3)C(=O)NCCc4c[nH]c5c4cccc5

ORD-MCULE-9130199918_1

221

MolLogP: 2.4492000000000003 | QED: 0.5856933574669014

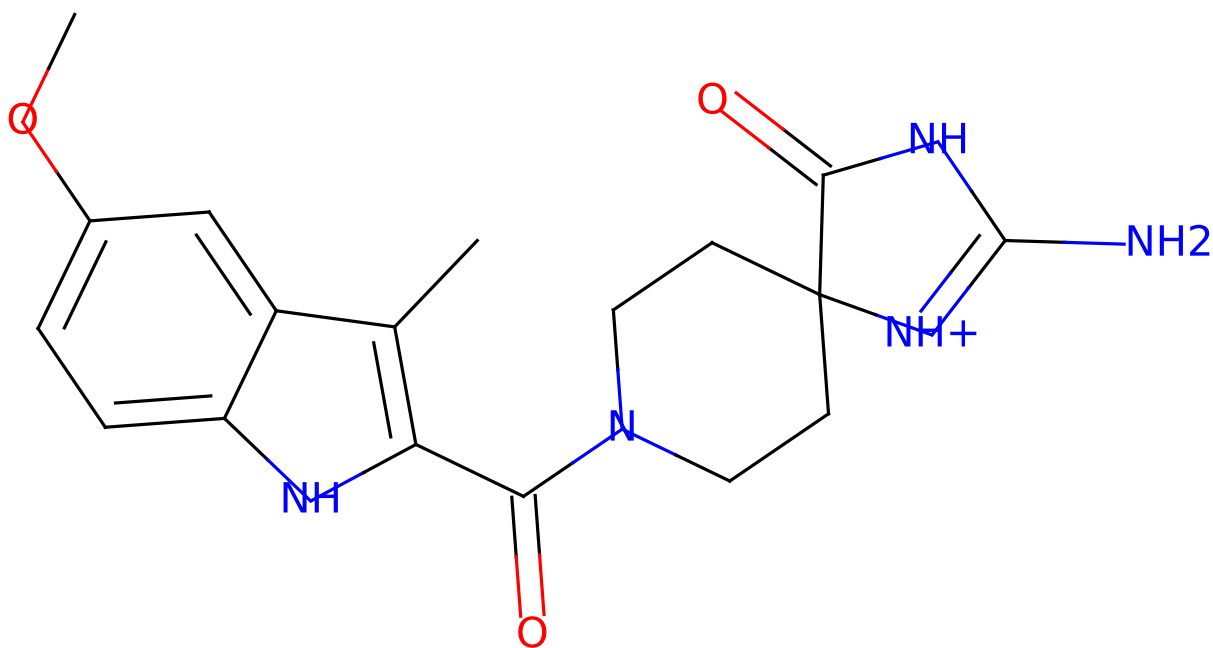c1ccc2cc(ccc2c1)S(=O)(=O)N3CCN(CC3)S(=O)(=O)[N@@]4CCc5ccccc5C4

ORD-MCULE-4597039646_1

MolLogP: 3.6792000000000016 | QED: 0.46023888484418957

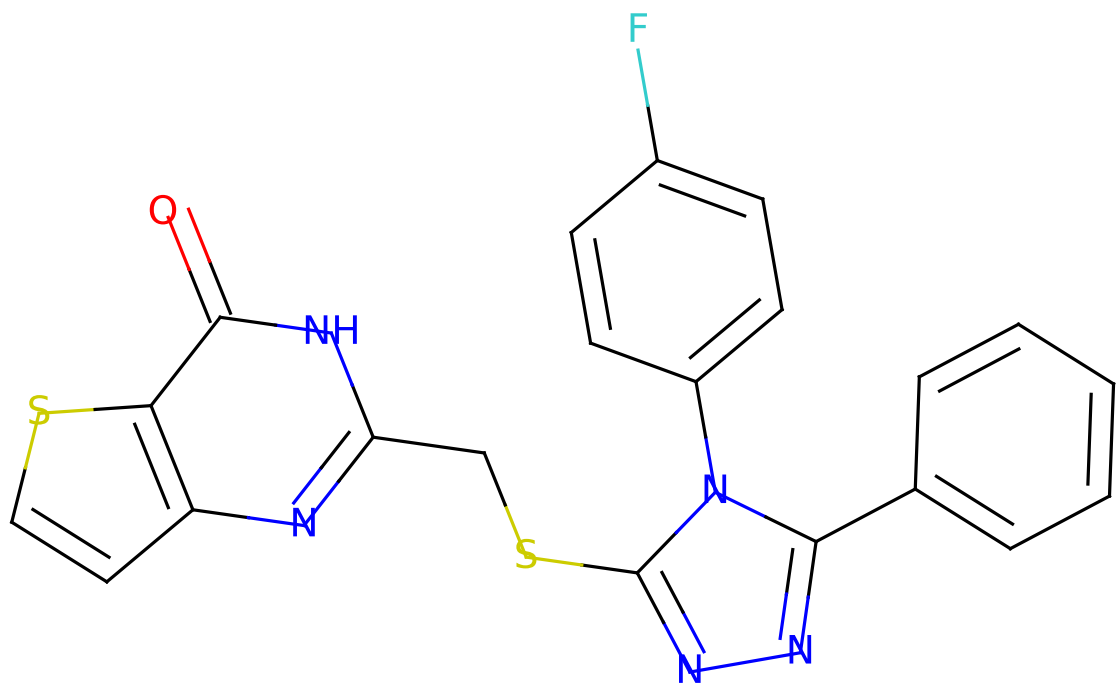c1cc(sc1)c2cc3cc(ccc3n2CC(=O)N4CC[NH+](CC4)Cc5ccc6c(c5)OCO6)Cl

ORD-MCULE-8022118059_1

223

MolLogP: -1.015179999999998 | QED: 0.5516408221661389

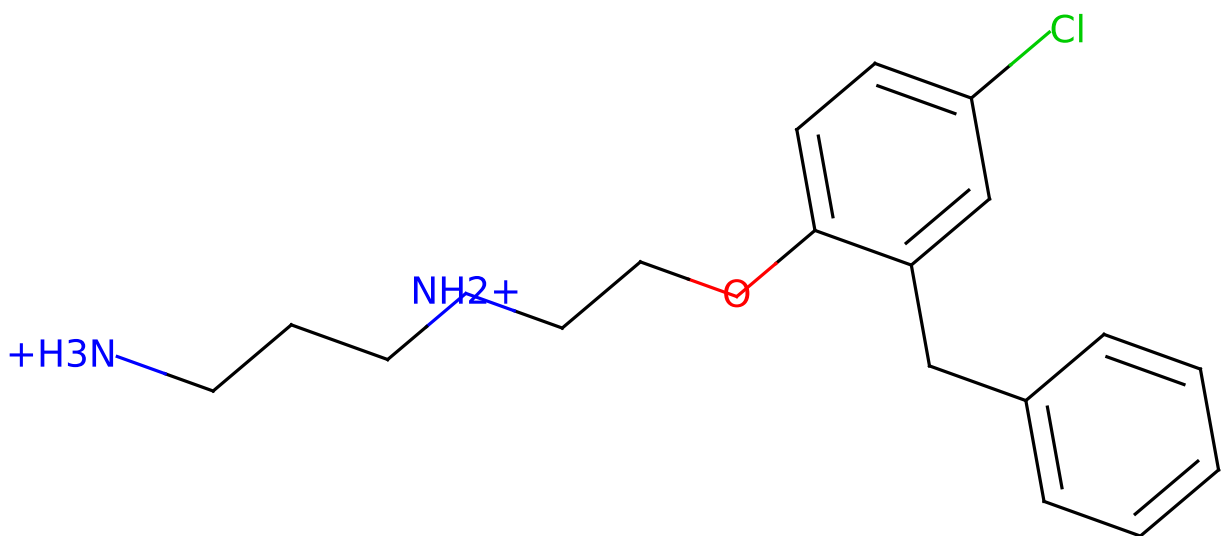Cc1c2cc(ccc2[nH]c1C(=O)N3CCC4(CC3)C(=O)NC(=[NH+]4)N)OC

ORD-MCULE-4669669279_1

224

MolLogP: 4.663700000000002 | QED: 0.4063509953205324

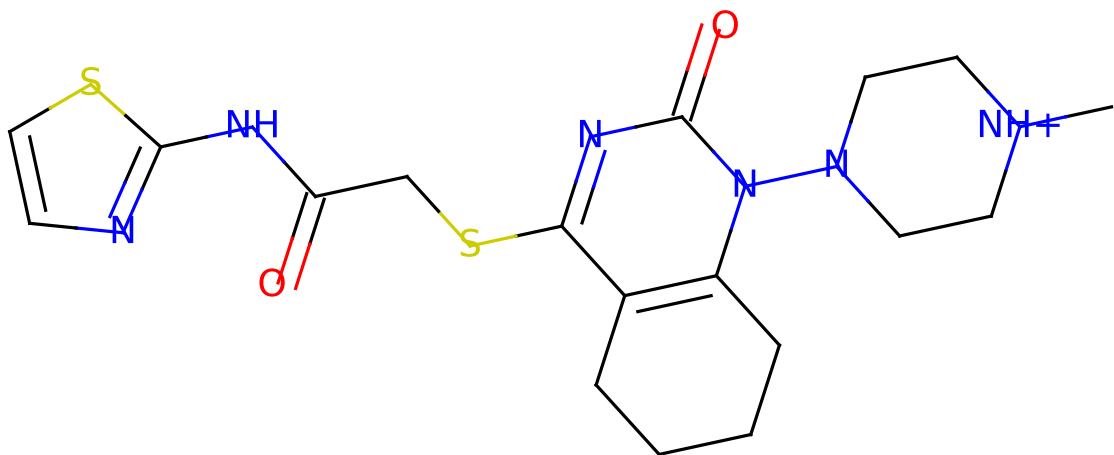c1ccc(cc1)c2nnc(n2c3ccc(cc3)F)SCc4[nH]c(=O)c5c(n4)ccs5

ORD-MCULE-9631221861_1

MolLogP: 1.5049999999999992 | QED: 0.6760516897747543
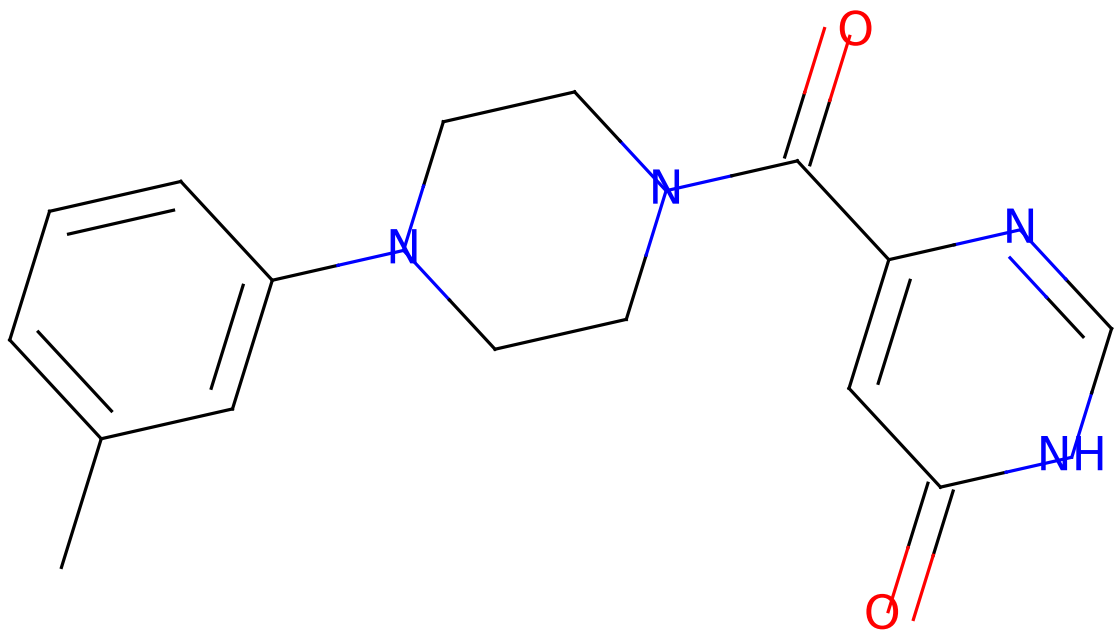
c1ccc(cc1)Cc2cc(ccc2OCC[NH2+]CCC[NH3+])Cl

ORD-MCULE-2027483325_1

MolLogP: -0.22429999999999795 | QED: 0.512858888603975
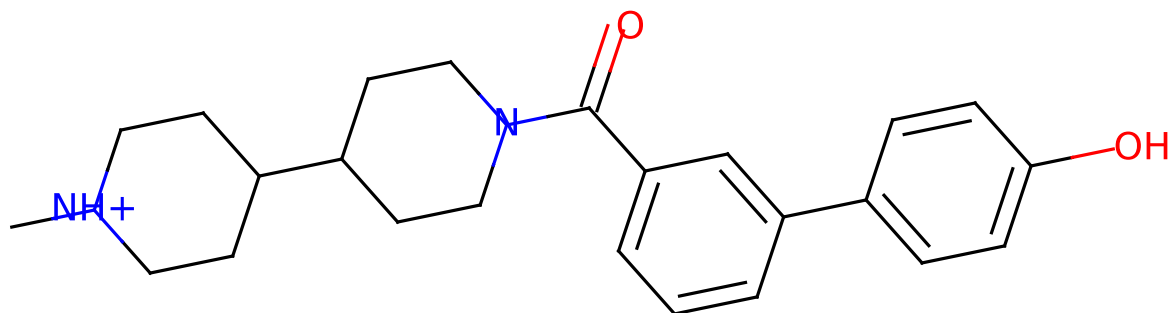
C[NH+]1CCN(CC1)n2c3c(c(nc2=O)SCC(=O)Nc4nccs4)CCCC3

ORD-MCULE-7119626278_1

227

MolLogP: 1.0407199999999999 | QED: 0.8992243633579676
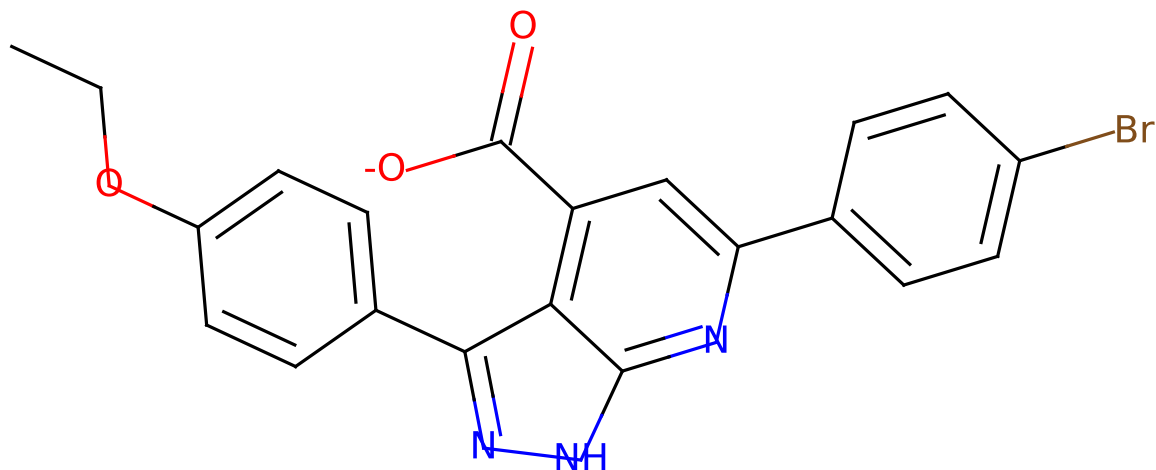
Cc1cccc(c1)N2CCN(CC2)C(=O)c3cc(=O)[nH]cn3

ORD-MCULE-7522626224_1

228

MolLogP: 2.8361000000000014 | QED: 0.8614065159940071

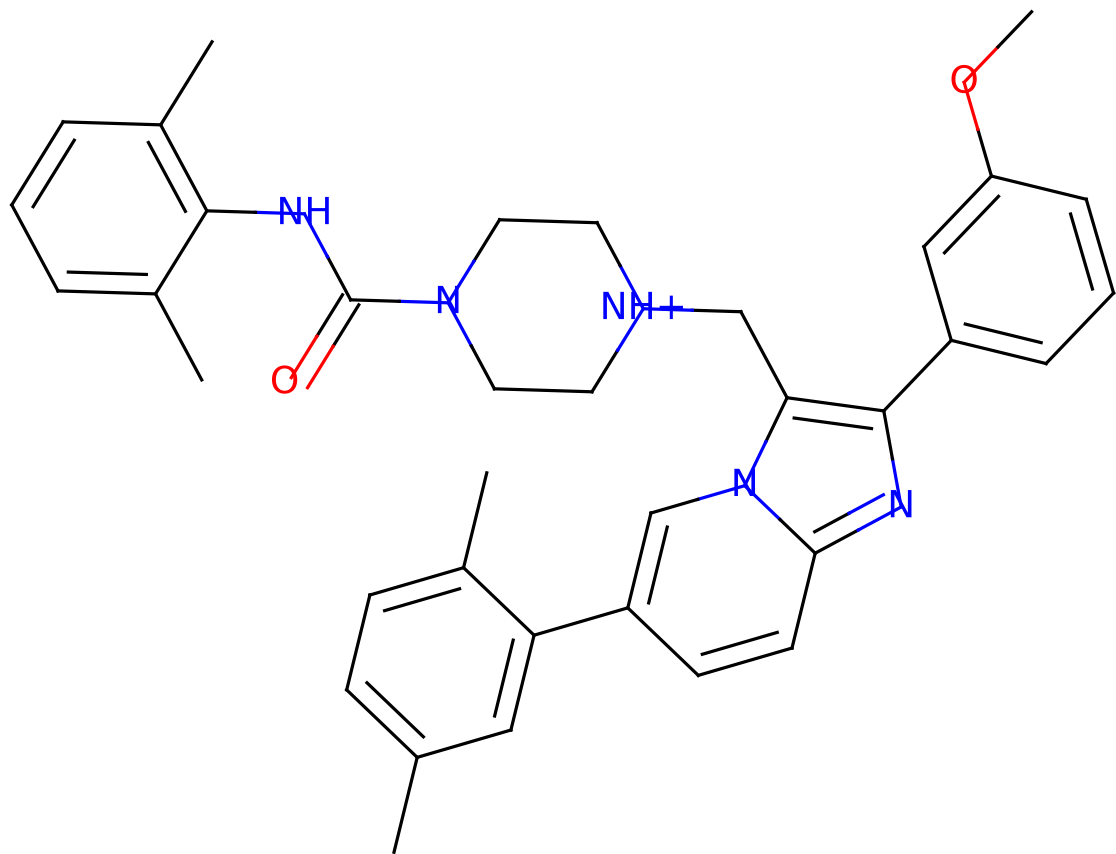C[NH+]1CCC(CC1)C2CCN(CC2)C(=O)c3cccc(c3)c4ccc(cc4)O

ORD-MCULE-4074523091_1

MolLogP: 3.816600000000002 | QED: 0.5128556740600366

CCOc1ccc(cc1)c2c3c(cc(nc3[nH]n2)c4ccc(cc4)Br)C(=O)[O-]
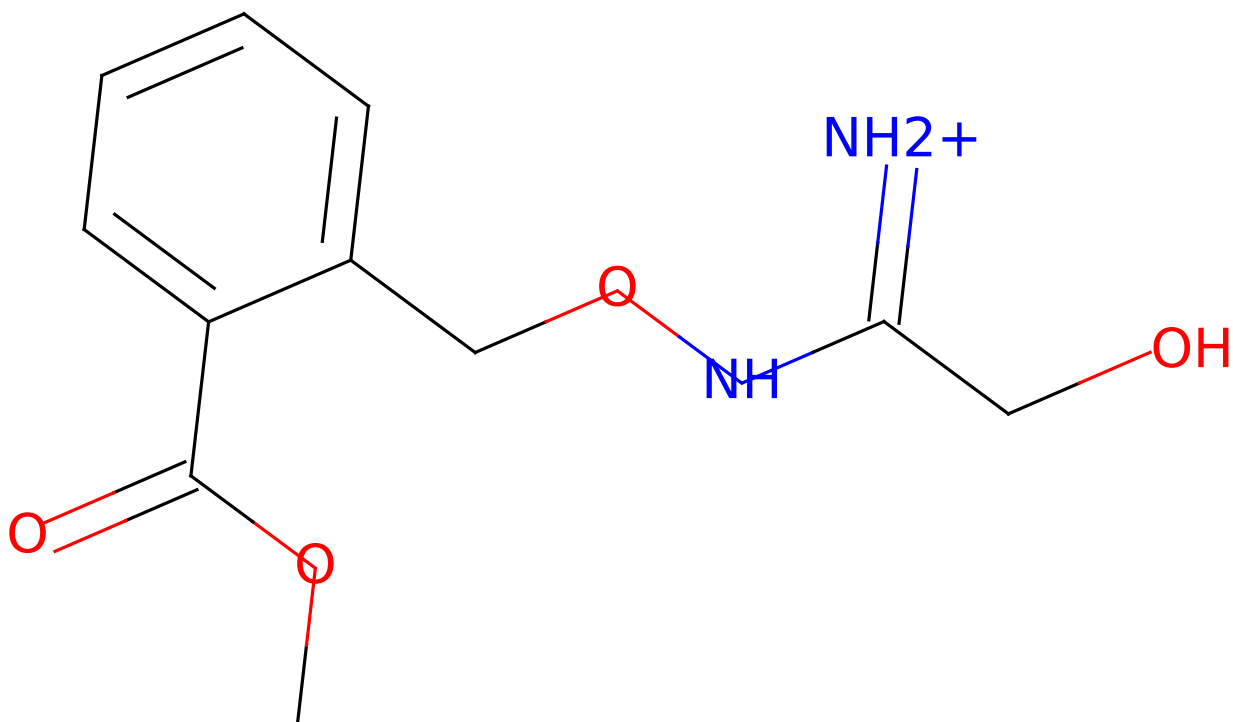
ORD-MCULE-6920424942_2

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
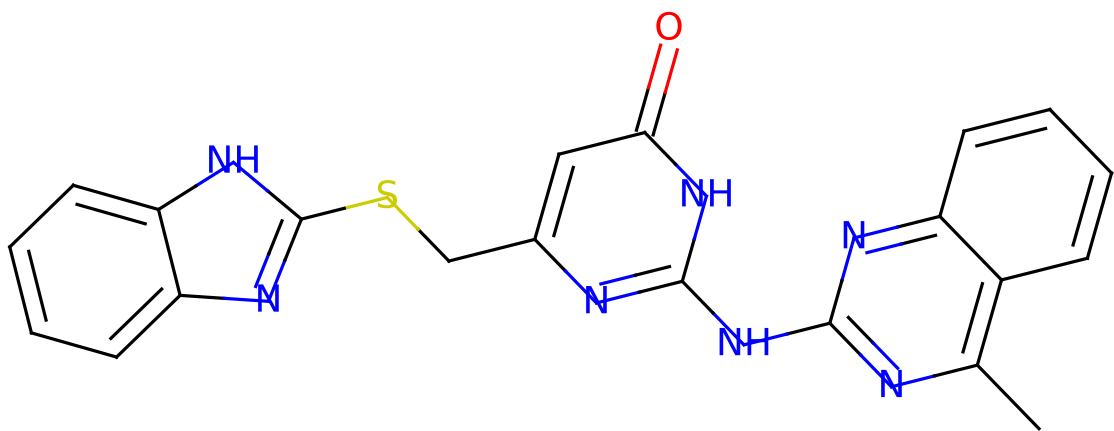
ORD-MCULE-1845027027_1

MolLogP: 2.0513999999999992 | QED: 0.49799599747758305

c1cc(ccc1c2c(c3cc(ccc3[nH]2)F)CCC(=O)N4CC[NH+](CC4)CC(=O)NC5CC5)F

ORD-MCULE-3182061958_1

MolLogP: -1.3556999999999981 | QED: 0.2553941368529607
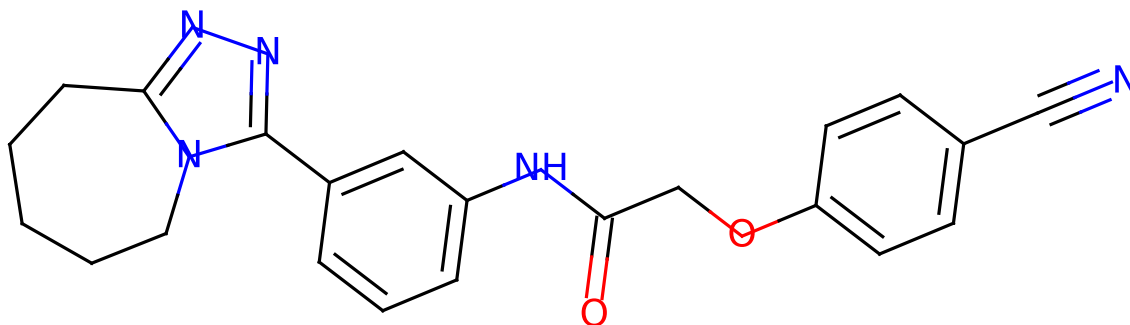
COC(=O)c1ccccc1CONC(=[NH2+])CO

ORD-MCULE-6958584111_2

MolLogP: 3.933720000000001 | QED: 0.3728174639709249

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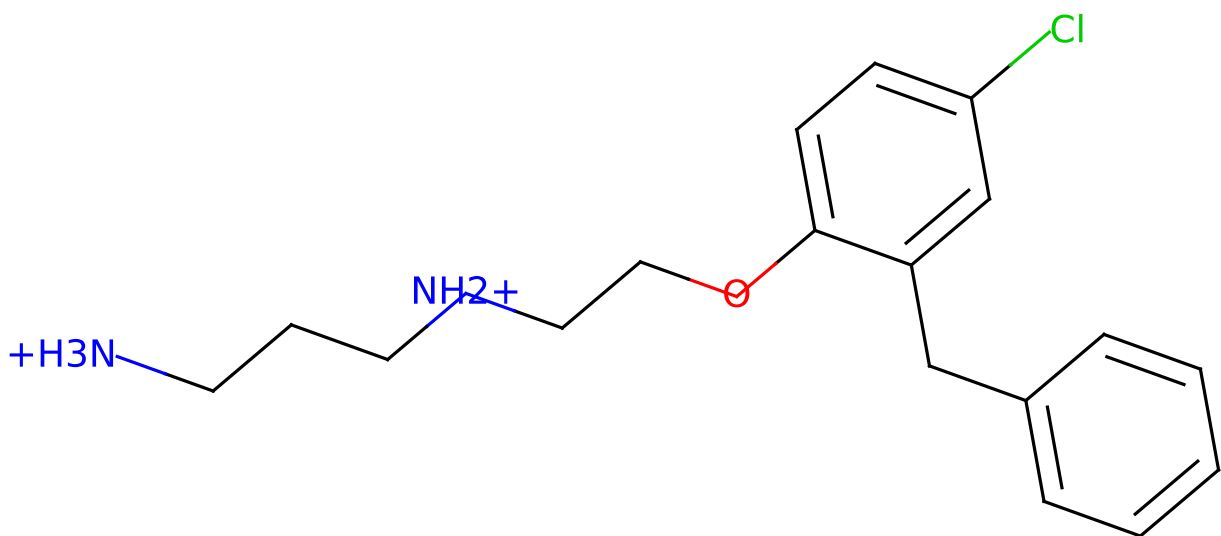
ORD-MCULE-6515729583_1

MolLogP: 3.5606800000000023 | QED: 0.7224907060425046
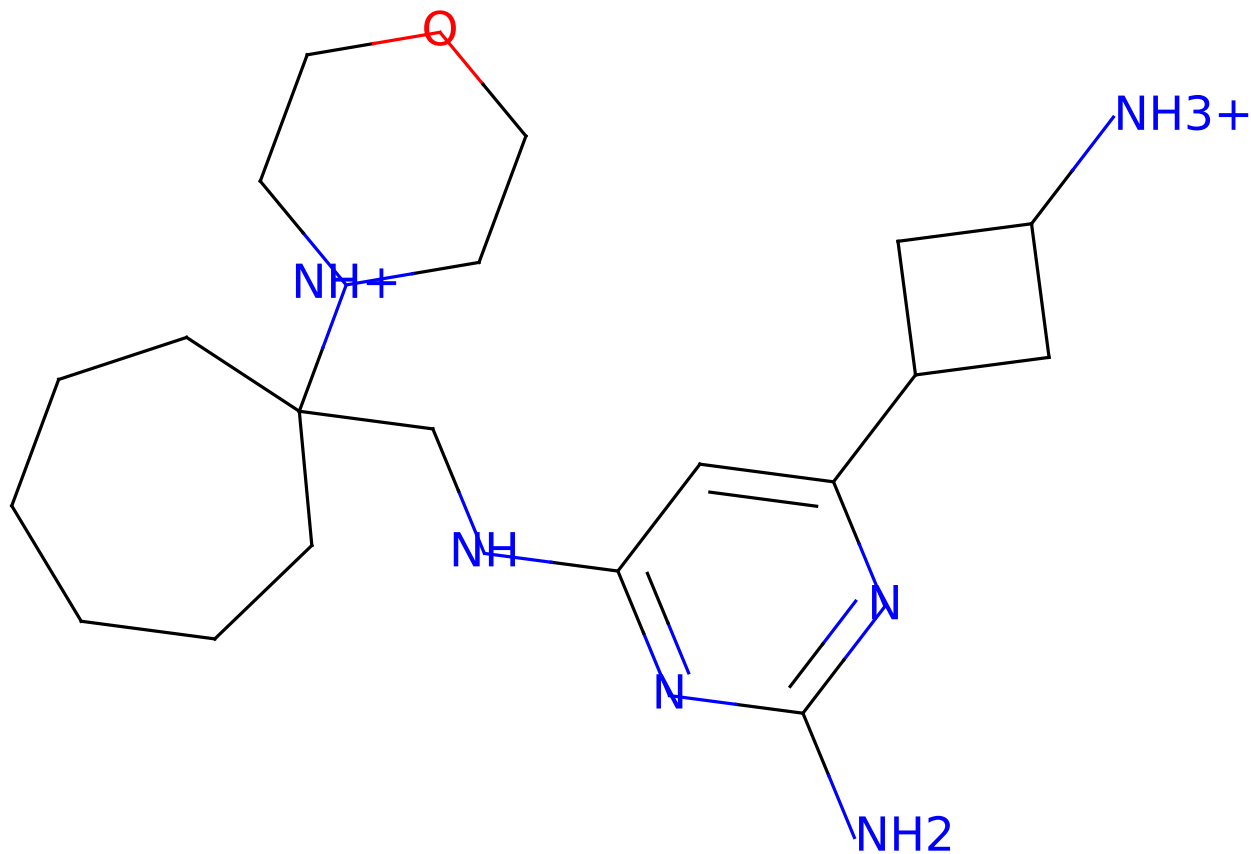
c1cc(cc(c1)NC(=O)COc2ccc(cc2)C#N)c3nnc4n3CCCCC4

ORD-MCULE-9347356531_1

MolLogP: 1.5049999999999992 | QED: 0.6760516897747543
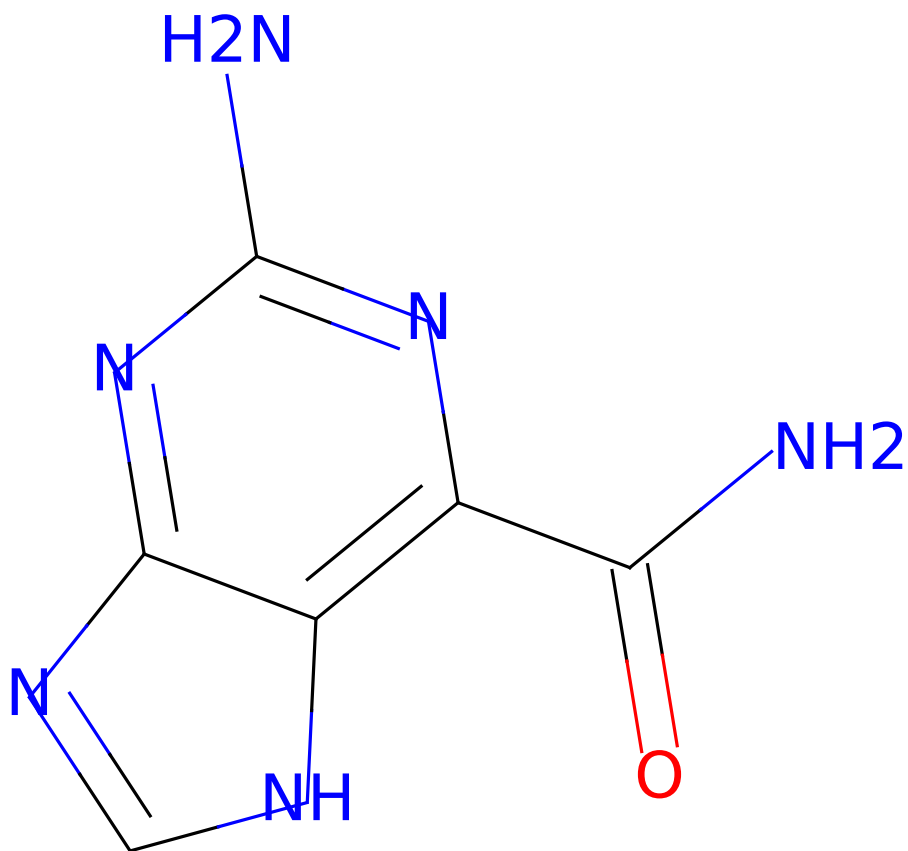
c1ccc(cc1)Cc2cc(ccc2OCC[NH2+]CCC[NH3+])Cl

ORD-MCULE-6607100517_1

MolLogP: -0.033299999999995944 | QED: 0.5401807256548551
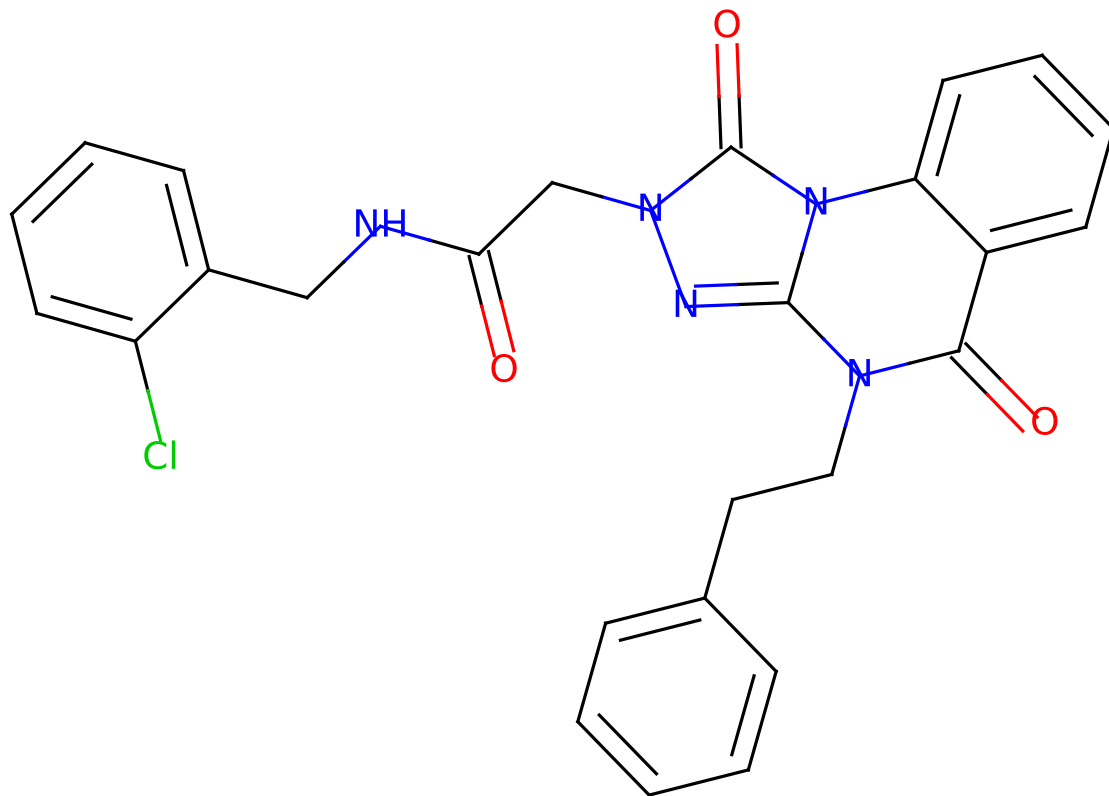
c1c(nc(nc1NCC2(CCCCC2)[NH+]3CCOCC3)N)C4CC(C4)[NH3+]

ORD-MCULE-6145847171_1

H2N

N

N

NH2

N

NH

O

MolLogP: -0.966000000000002 | QED: 0.5180752253839909

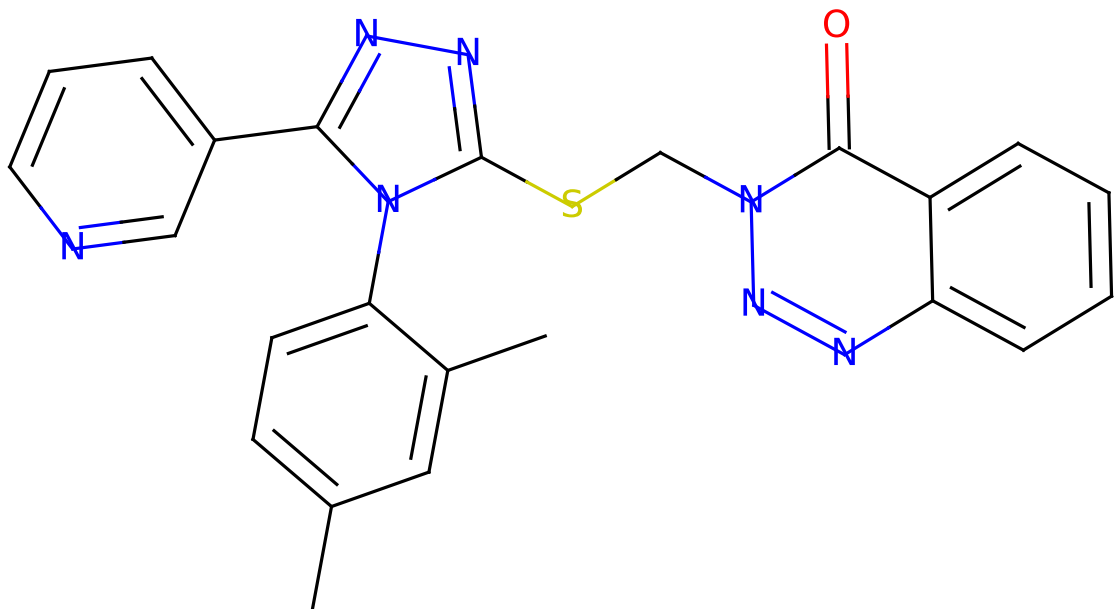c1[nH]c2c(nc(nc2n1)N)C(=O)N

ORD-MCULE-1089692040_1

MolLogP: 3.0234000000000005 | QED: 0.38187236877306086

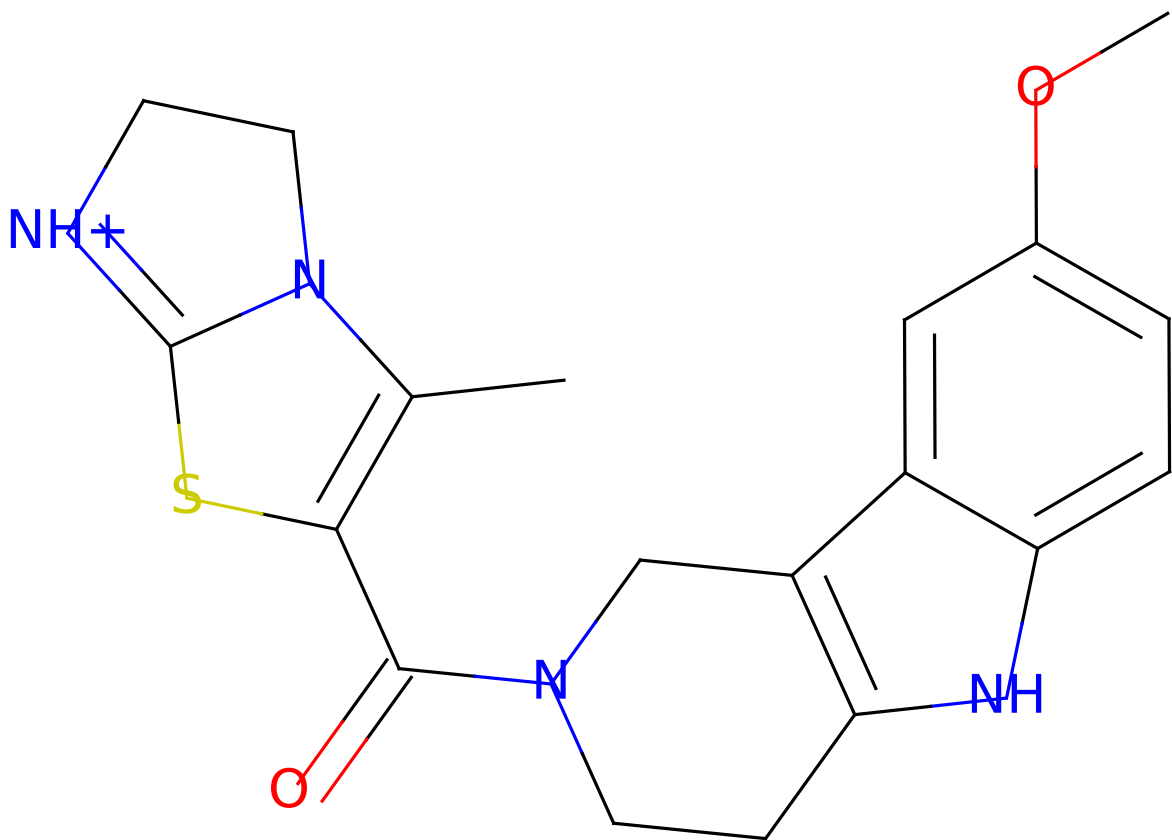c1ccc(cc1)CCn2c(=O)c3ccccc3n4c2nn(c4=O)CC(=O)NCc5ccccc5Cl

ORD-MCULE-5959851446_1

MolLogP: 3.8008400000000018 | QED: 0.3831563866893923

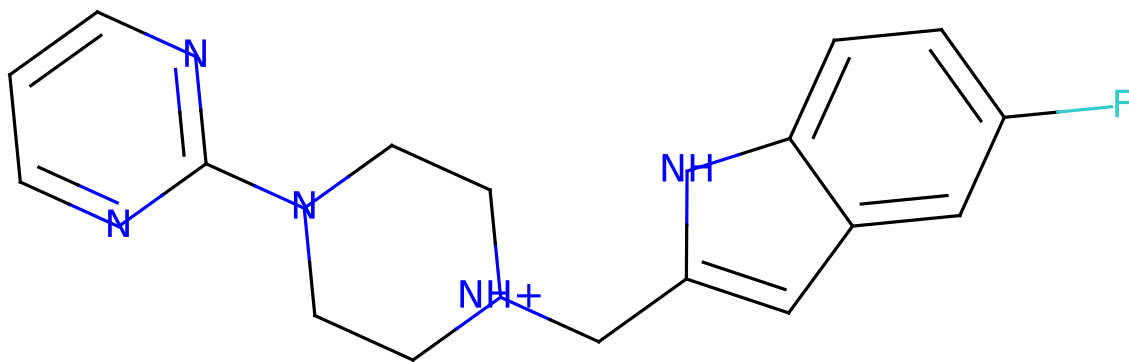Cc1ccc(c(c1)C)n2c(nnc2SCn3c(=O)c4ccccc4nn3)c5cccnc5

ORD-MCULE-9552168897_1

240

MolLogP: 0.7917000000000001 | QED: 0.8218110020883408

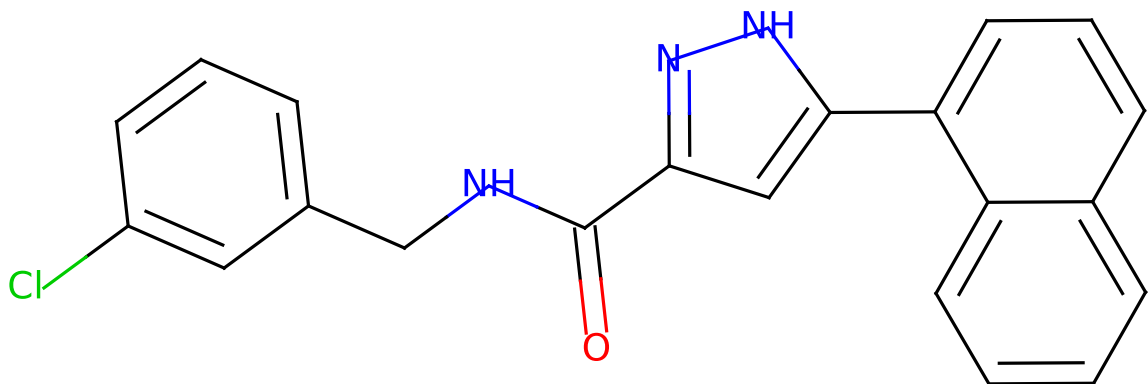CC1=C(SC2=[NH+]CCN12)C(=O)N3CCc4c(c5cc(ccc5[nH]4)OC)C3

ORD-MCULE-3259407472_1

MolLogP: 1.0020999999999998 | QED: 0.7585712959964838

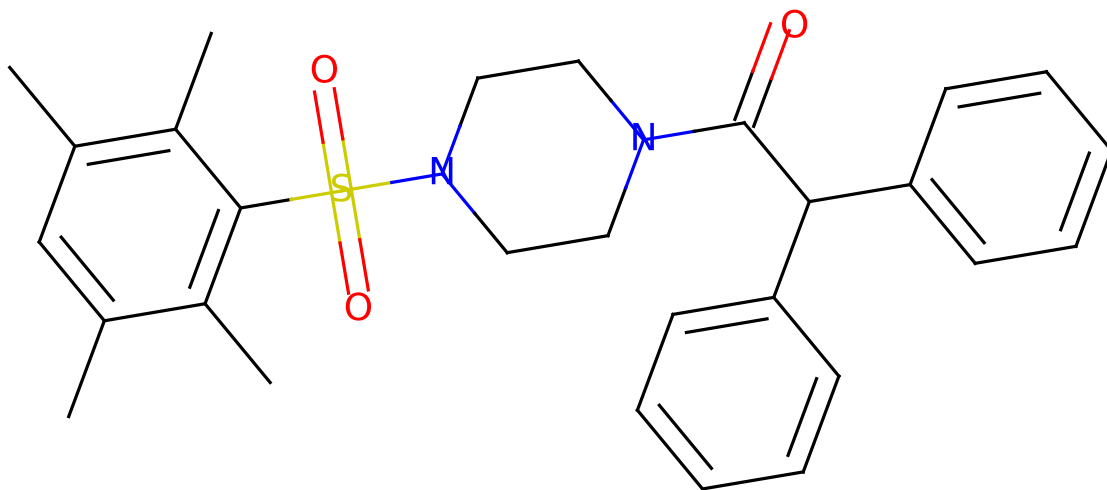c1cnc(nc1)N2CC[NH+](CC2)Cc3cc4cc(ccc4[nH]3)F

ORD-MCULE-7360443270_1

MolLogP: 4.813300000000002 | QED: 0.5474981448162837

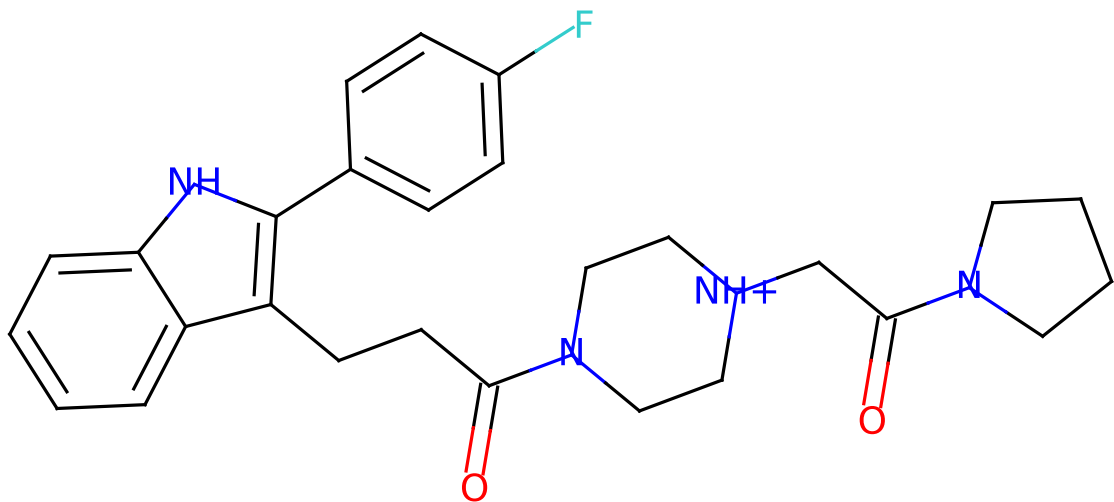c1ccc2c(c1)cccc2c3cc(n[nH]3)C(=O)NCc4cccc(c4)Cl

ORD-MCULE-3021913260_2

243

MolLogP: 4.5852800000000045 | QED: 0.541437412840622

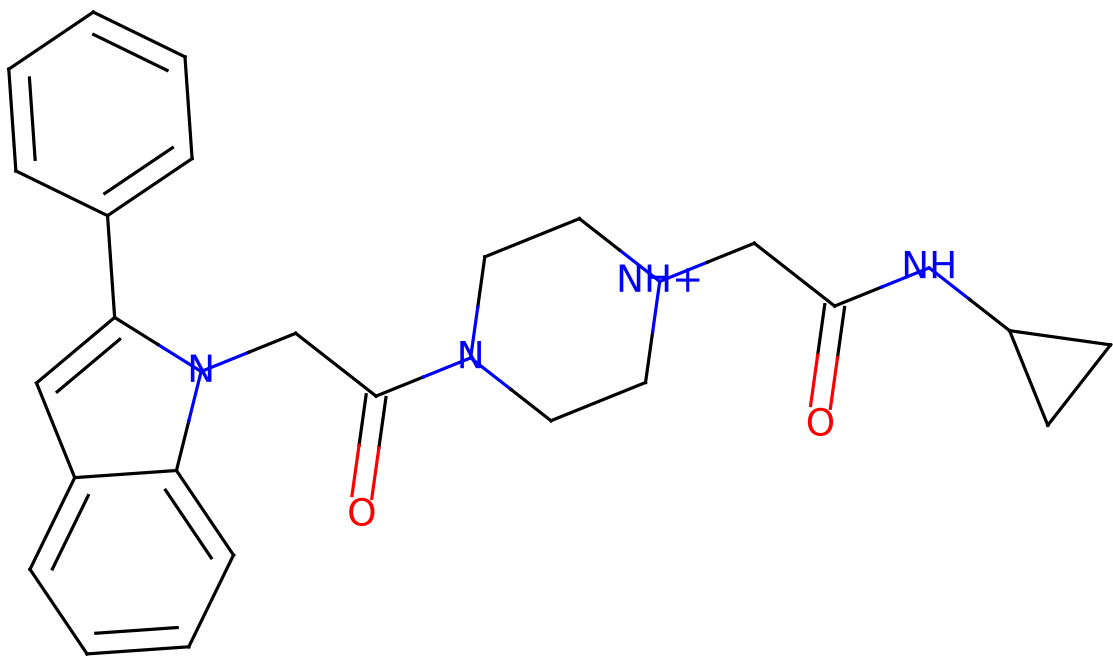Cc1cc(c(c(c1C)S(=O)(=O)N2CCN(CC2)C(=O)C(c3ccccc3)c4ccccc4)C)C

ORD-MCULE-2055004350_1

MolLogP: 2.256099999999999 | QED: 0.5892811568593804

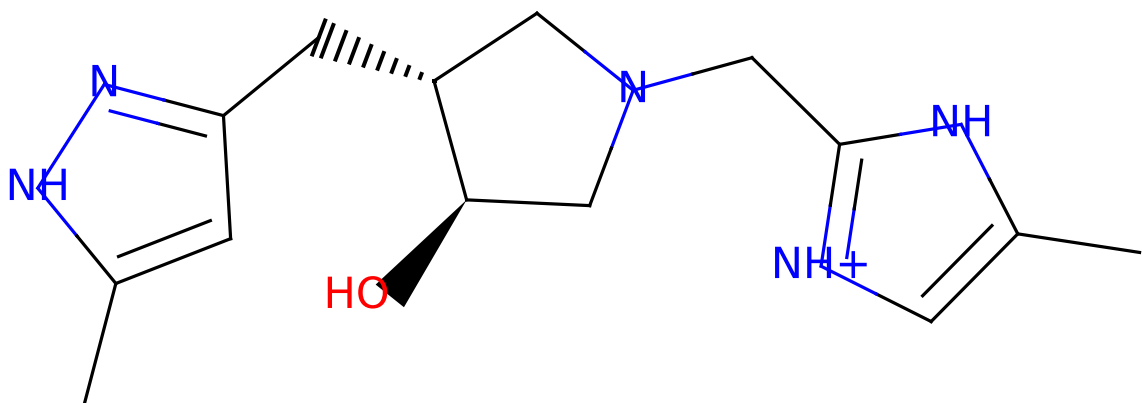c1ccc2c(c1)c(c([nH]2)c3ccc(cc3)F)CCC(=O)N4CC[NH+](CC4)CC(=O)N5CCCC5

ORD-MCULE-3657624205_1

MolLogP: 1.314 | QED: 0.6355823751893853

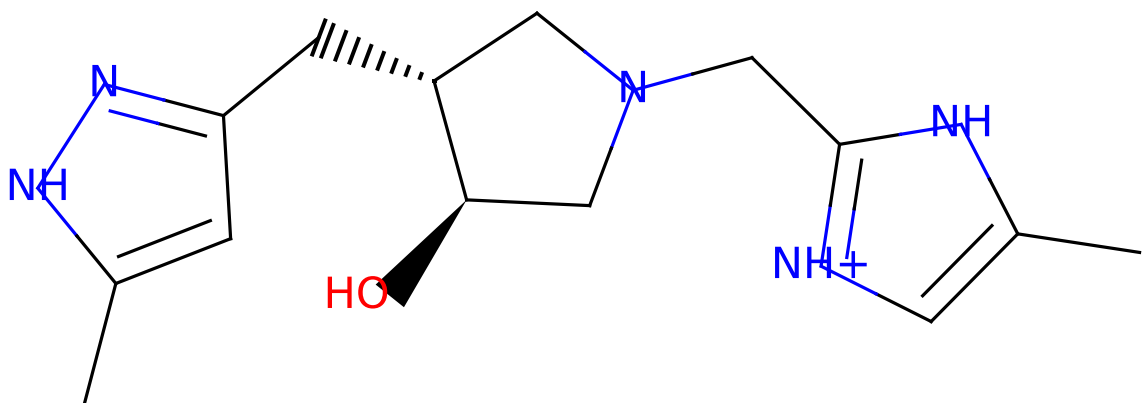c1ccc(cc1)c2cc3ccccc3n2CC(=O)N4CC[NH+](CC4)CC(=O)NC5CC5

ORD-MCULE-1009794542_1

246

MolLogP: 0.2041400000000005 | QED: 0.7460837063757351

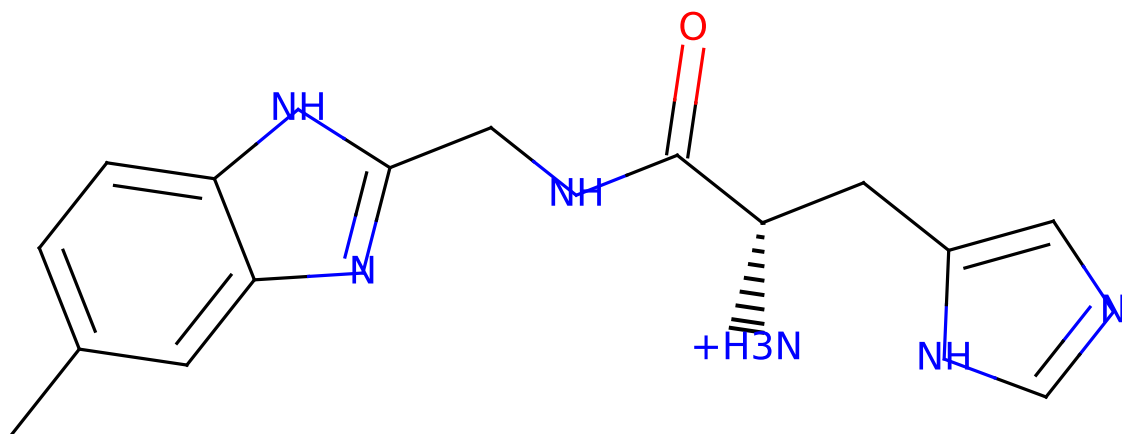Cc1cc(n[nH]1)C[C@@H]2C[N@](C[C@H]2O)Cc3[nH]c(c[nH+]3)C

ORD-MCULE-3967726014_1

MolLogP: 0.2041400000000005 | QED: 0.7460837063757351

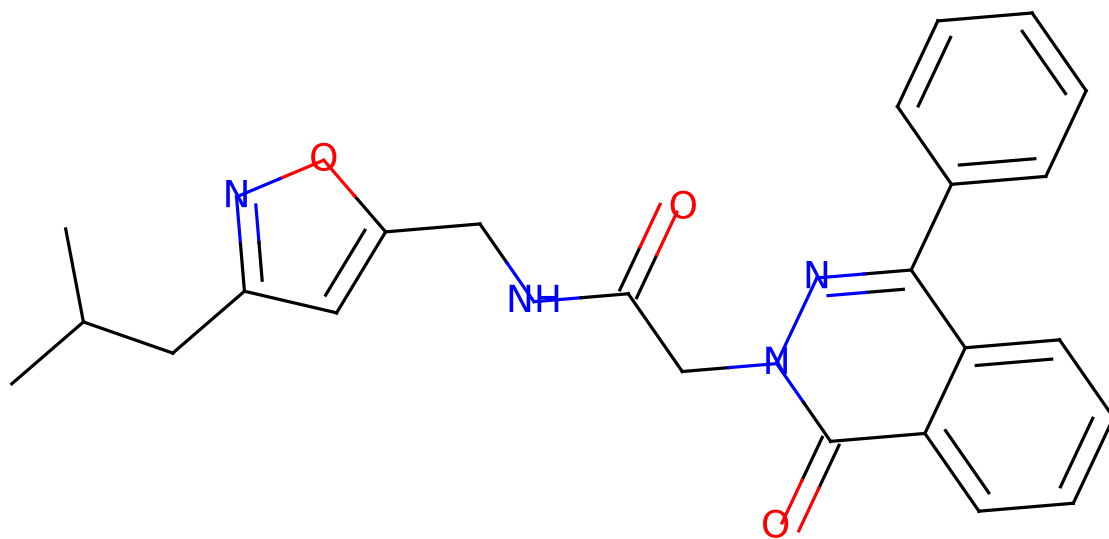Cc1cc(n[nH]1)C[C@@H]2C[N@@](C[C@H]2O)Cc3[nH]c(c[nH+]3)C

ORD-MCULE-3967726014_1

MolLogP: 0.06382000000000104 | QED: 0.5339791274710981

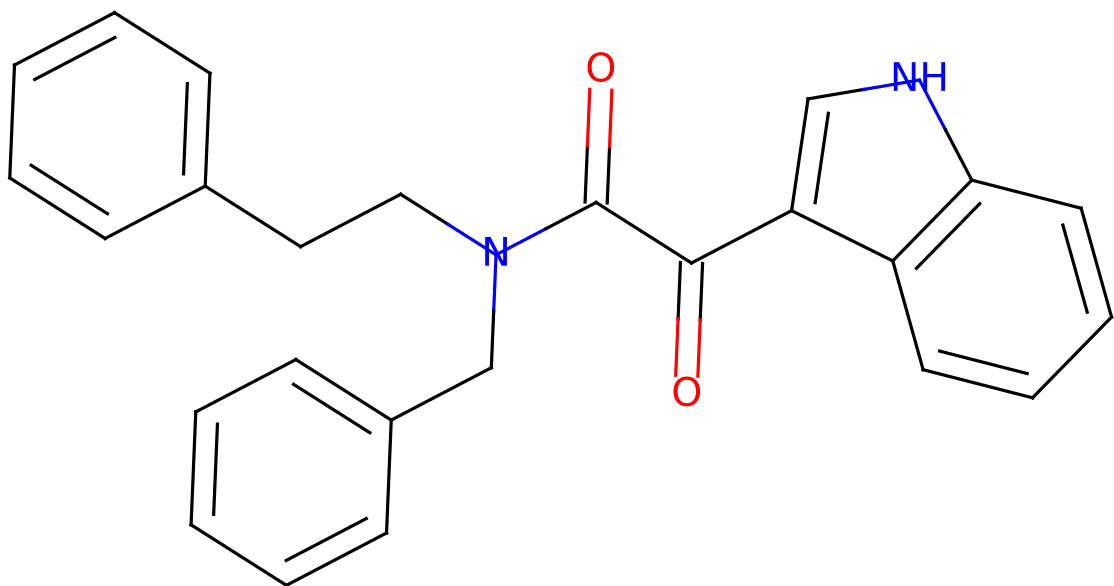Cc1ccc2c(c1)nc([nH]2)CNC(=O)[C@H](Cc3cnc[nH]3)[NH3+]

ORD-MCULE-7818026901_2

MolLogP: 3.5664000000000016 | QED: 0.4974502112146776
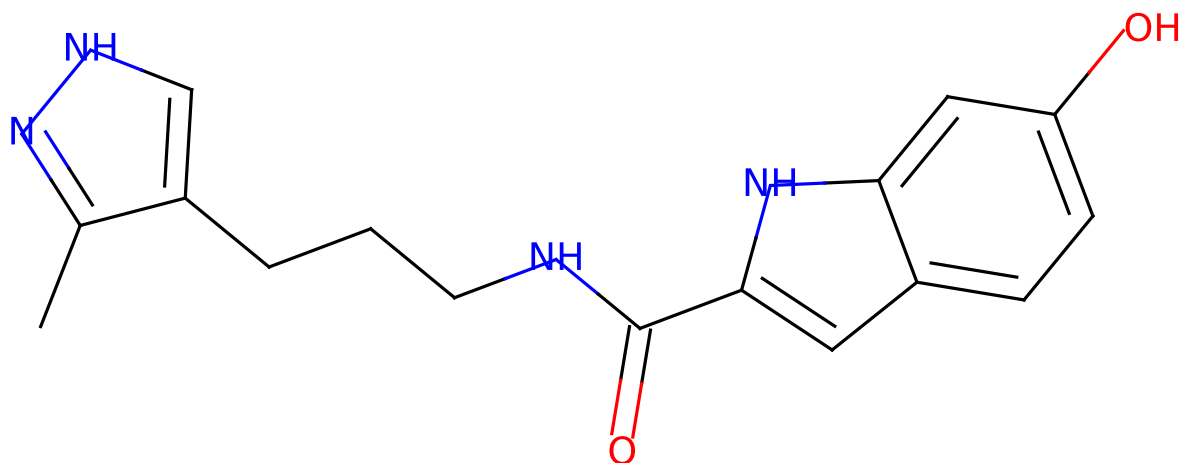
CC(C)Cc1cc(on1)CNC(=O)Cn2c(=O)c3ccccc3c(n2)c4ccccc4

ORD-MCULE-3335564164_1

MolLogP: 4.622100000000003 | QED: 0.3744573878138413

c1ccc(cc1)CCN(Cc2ccccc2)C(=O)C(=O)c3c[nH]c4c3cccc4

ORD-MCULE-8417802339_1

251

MolLogP: 2.2676200000000004 | QED: 0.5442475309965601

Cc1c(c[nH]n1)CCCNC(=O)c2cc3ccc(cc3[nH]2)O

ORD-MCULE-4353393377_2