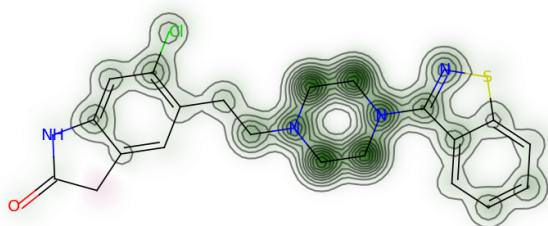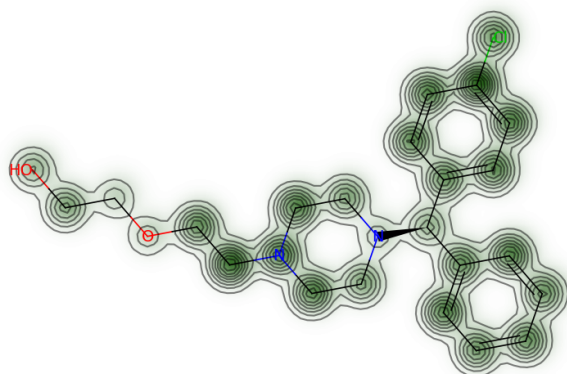zinc_id: ZINC000003986735
smiles: Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCO)CC2)n1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
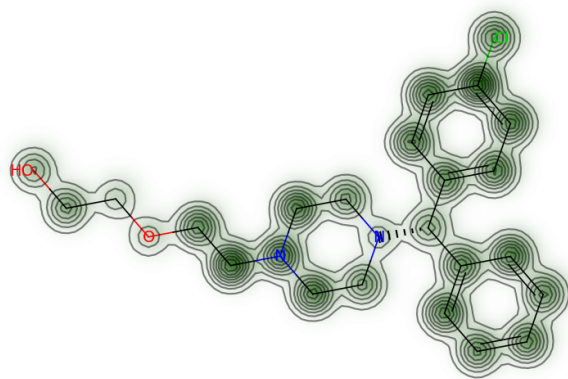Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 1.0

zinc_id: ZINC000000538550
smiles: O=C1Cc2cc(CCN3CCN(c4nsc5ccccc45)CC3)c(Cl)cc2N1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.33784

zinc_id: ZINC000019364224
smiles: OCCOCCN1CCN([C@H](c2ccccc2)c2ccc(Cl)cc2)CC1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
Fingerprint: FCFP4-like Morgan 2048 bits
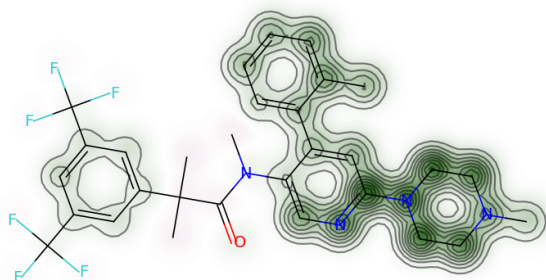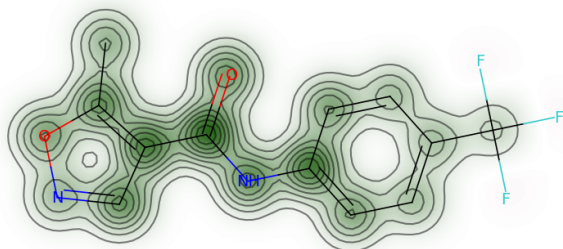TanimotoSimilarity: 0.30769

zinc_id: ZINC000019364222
smiles: OCCOCCN1CCN([C@@H](c2ccccc2)c2ccc(Cl)cc2)CC1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
Fingerprint: FCFP4-like Morgan 2048 bits
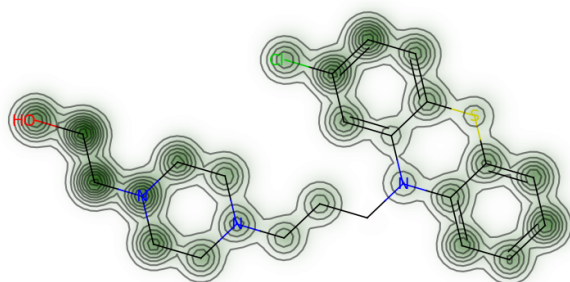TanimotoSimilarity: 0.30769

4

zinc_id: ZINC000011681563
smiles: Cc1ccccc1-c1cc(N2CCN(C)CC2)ncc1N(C)C(=O)C(C)(C)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
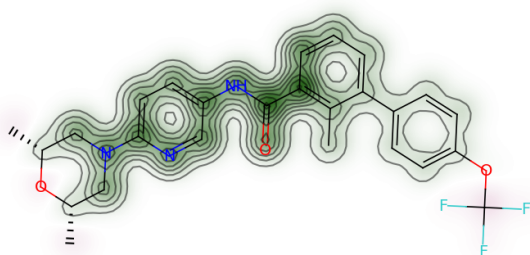Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.30263

5

zinc_id: ZINC000000004840
smiles: Cc1oncc1C(=O)Nc1ccc(C(F)(F)F)cc1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
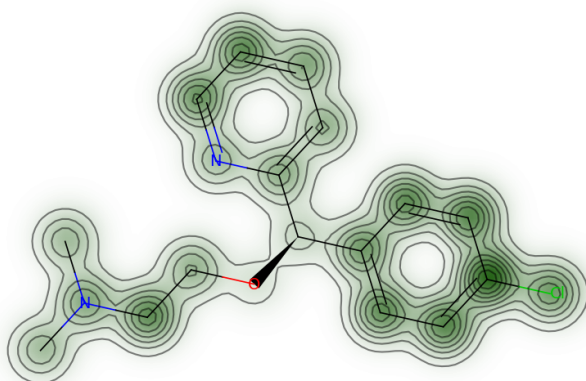Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.30159

6

zinc_id: ZINC000019228902
smiles: OCCN1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc32)CC1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
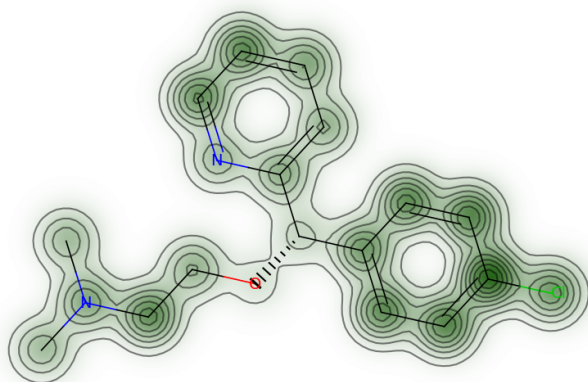Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.29851

7

zinc_id: ZINC000068202099
smiles: Cc1c(C(=O)Nc2ccc(N3C[C@H](C)O[C@H](C)C3)nc2)cccc1-c1ccc(OC(F)(F)F)cc1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.2963

8

zinc_id: ZINC000000002043
smiles: CN(C)CCO[C@H](c1ccc(Cl)cc1)c1ccccn1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.29412

9

zinc_id: ZINC000000000122
smiles: CN(C)CCO[C@@H](c1ccc(Cl)cc1)c1ccccn1
QuerySmiles: Cc1cccc(c1NC(=O)c2cnc(s2)Nc3cc(nc(n3)C)N4CCN(CC4)CCO)Cl
Fingerprint: FCFP4-like Morgan 2048 bits
TanimotoSimilarity: 0.29412

10