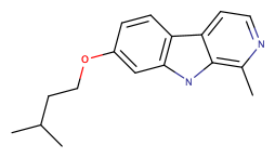
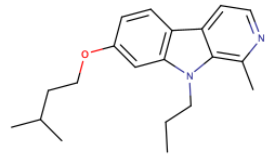
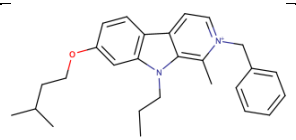
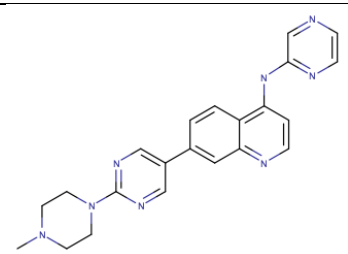
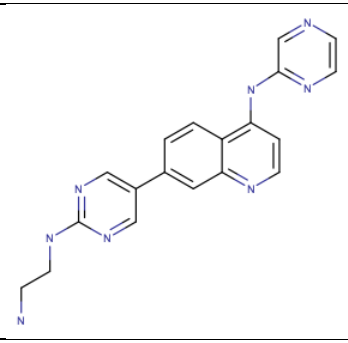
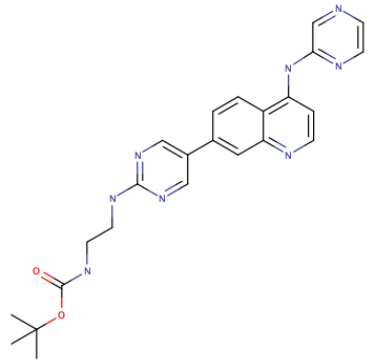
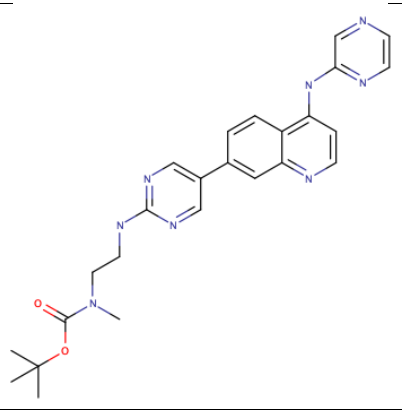
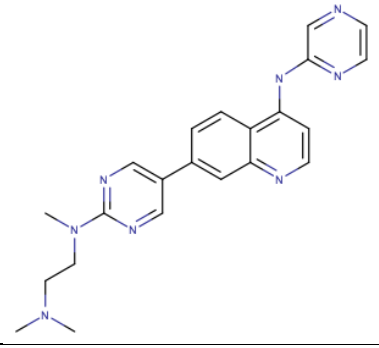
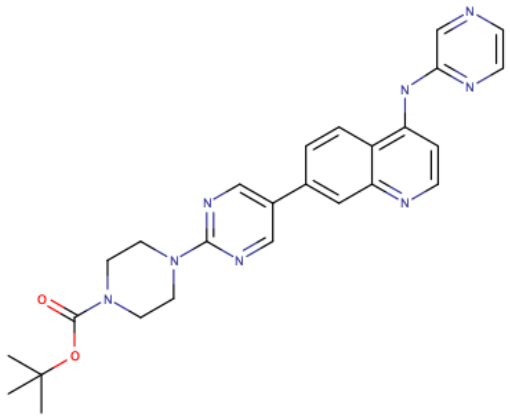
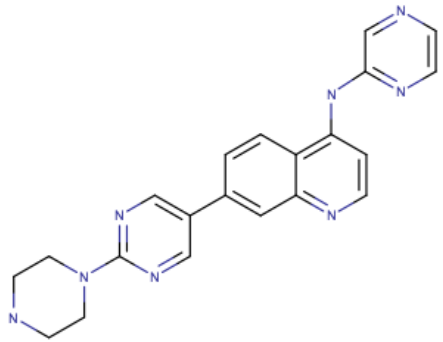
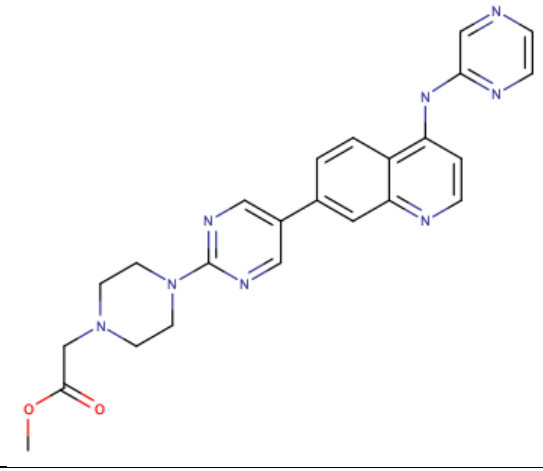
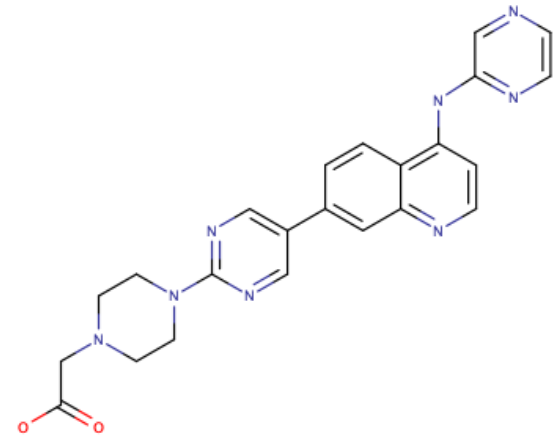
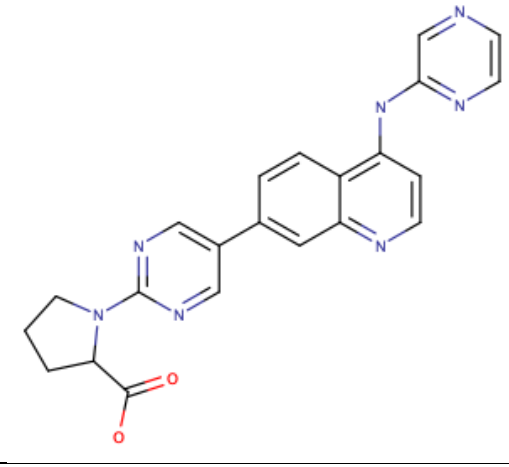
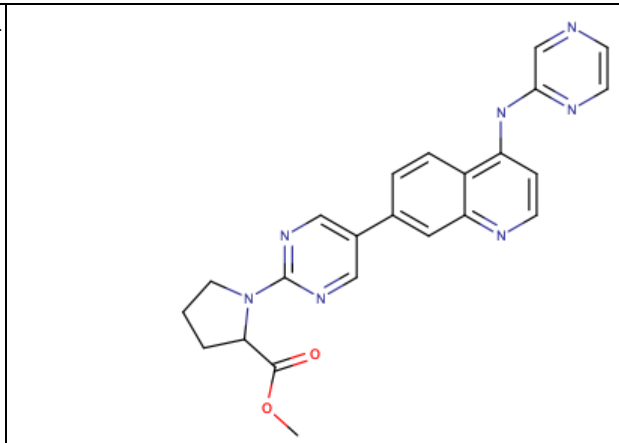
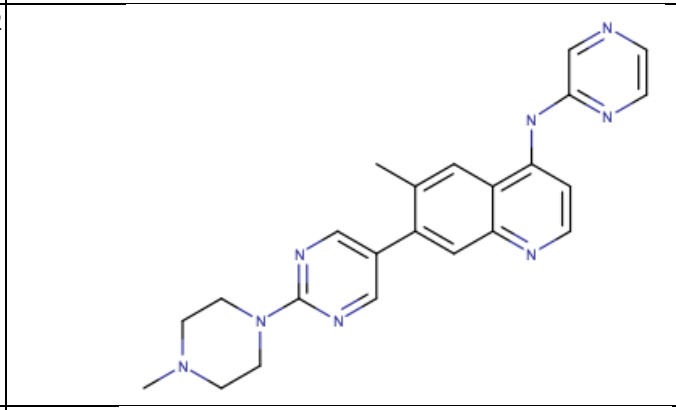
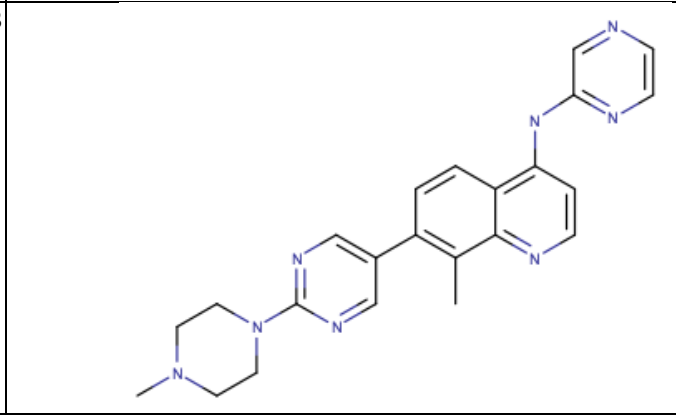
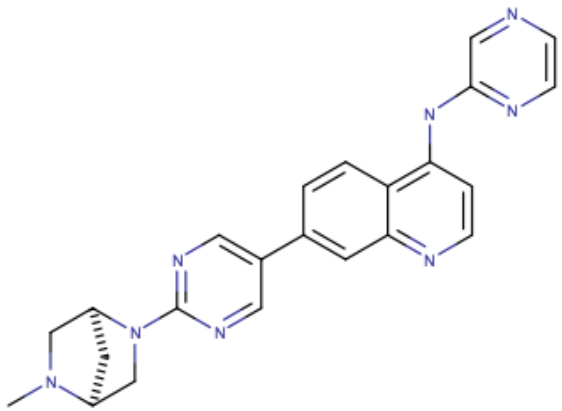
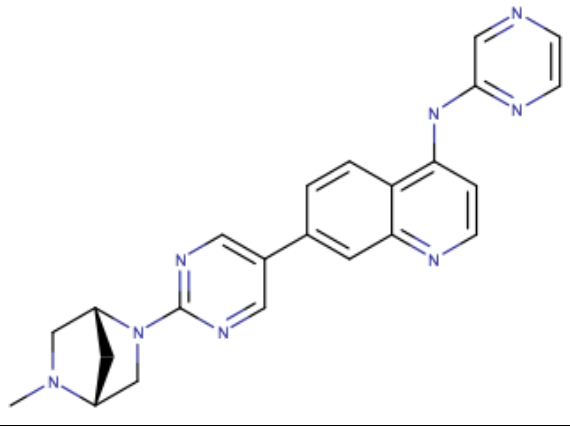
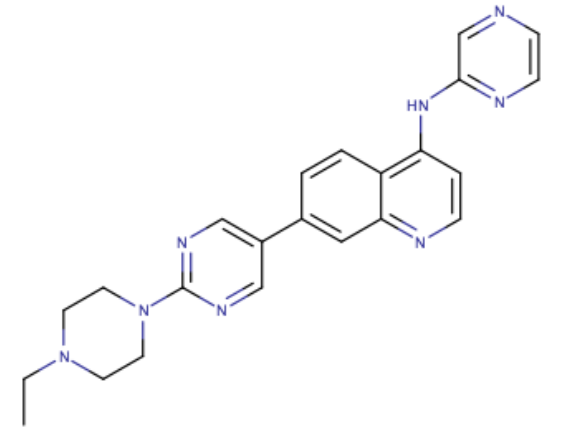
ID	Chemical Structure	SMILES	Experimental solubility, S (mol/l)
CN_S001_C001		CC(C)CCOC1=CC2=C(C=C1)C1=CC=NC(C)=C1N2	7.45E-05
CN_S001_C002		CCCN1C2=C(C=CC(OCCC(C)C)=C2)C2=CC=NC(C)=C12	6.44E-06
CN_S001_C003		CCCN1C2=C(C=CC(OCCC(C)C)=C2)C2=CC=[N+](CC3=CC=CC=C3)C(C)=C12	2.64E-03
CN_S002_C001		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	4.40E-05
CN_S002_C002		NCCNC1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.80E-05

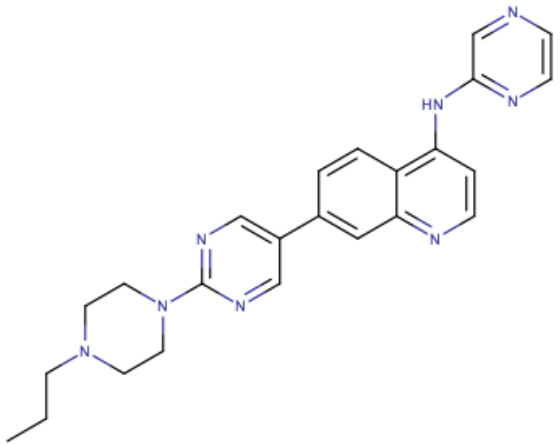
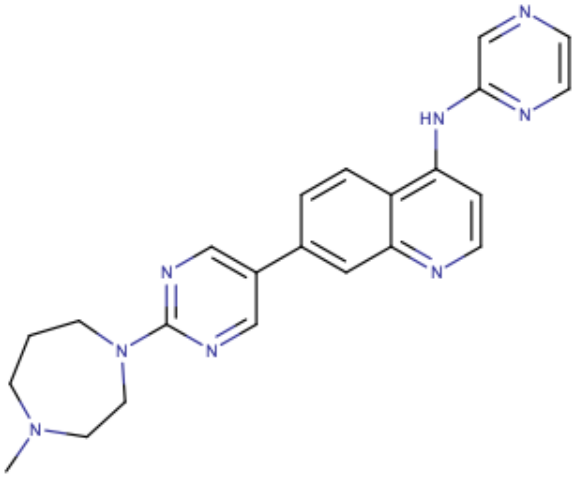
CN_S002_C003		CC(C)(C)OC(=O)NCCNC1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	2.00E-07
CN_S002_C004		CN(CCNC1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1)C(=O)OC(C)(C)C	3.00E-06
CN_S002_C005		CN(C)CCN(C)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	6.30E-04

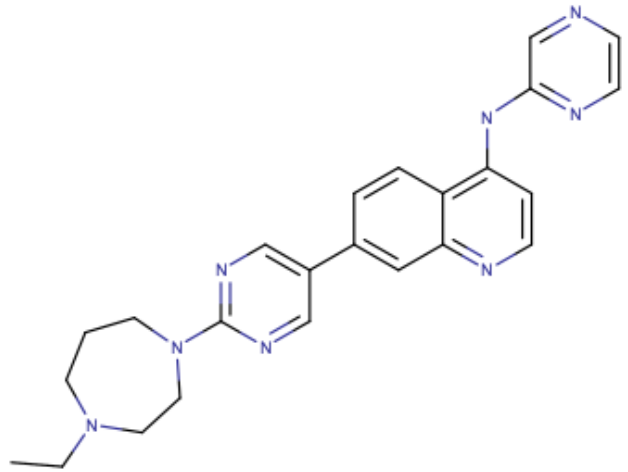
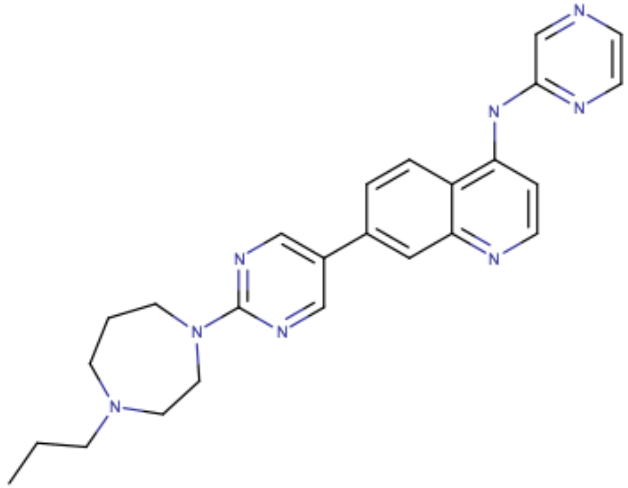
CN_S002_C006		CC(C)(C)OC(=O)N1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.00E-07
CN_S002_C007		C1CN(CCN1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	3.90E-05
CN_S002_C008		COC(=O)CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.60E-05

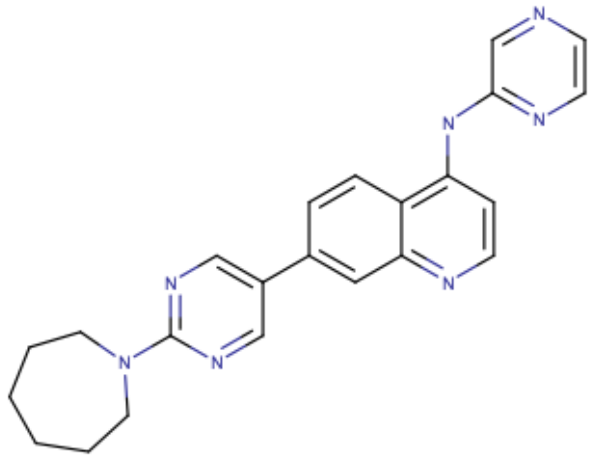
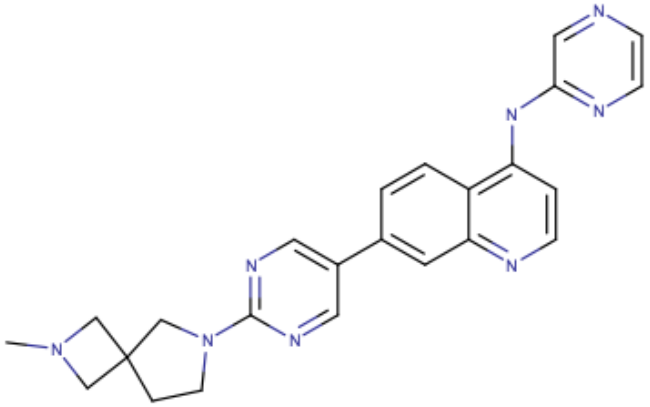
CN_S002_C009		OC(=O)CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.70E-05
CN_S002_C010		OC(=O)C1CCCN1C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	4.20E-05

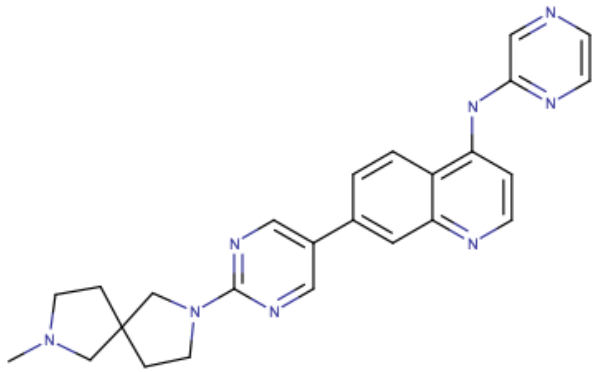
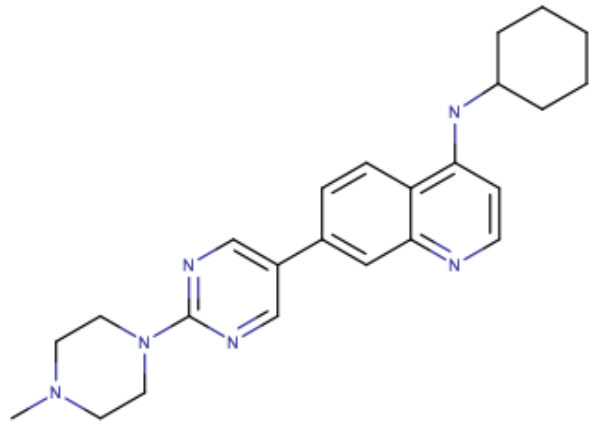
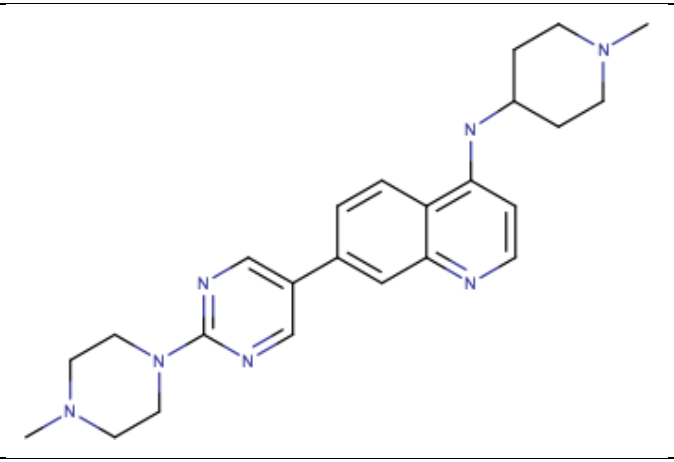
CN_S002_C011		COC(=O)C1CCCN1C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	3.00E-07
CN_S002_C012		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1C	2.00E-08
CN_S002_C013		CN1CCN(CC1)C1=NC=C(C=N1)C1=C(C)C2=NC=CC(NC3=NC=CN=C3)=C2C=C1	5.00E-06

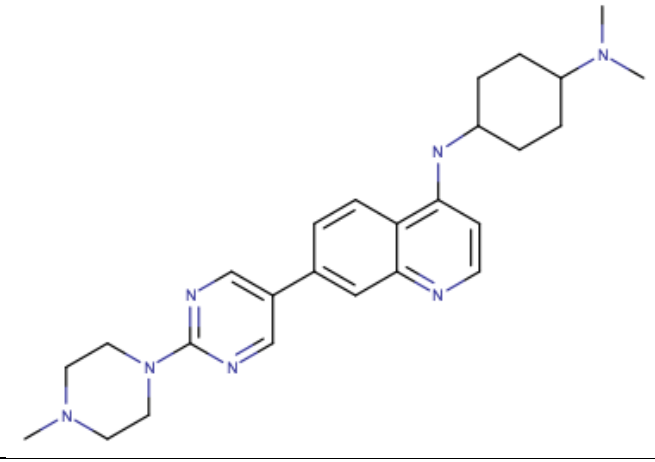
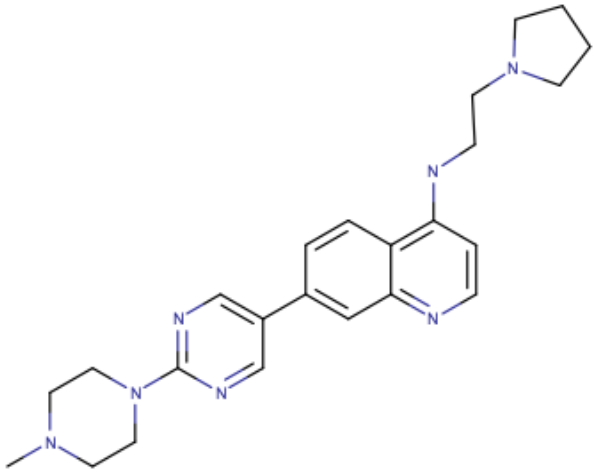
CN_S002_C014		CN1CC2CC1CN2C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	9.10E-04
CN_S002_C015		CN1C[C@H]2C[C@@H]1CN2C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	9.60E-04
CN_S002_C016		CCN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.40E-05

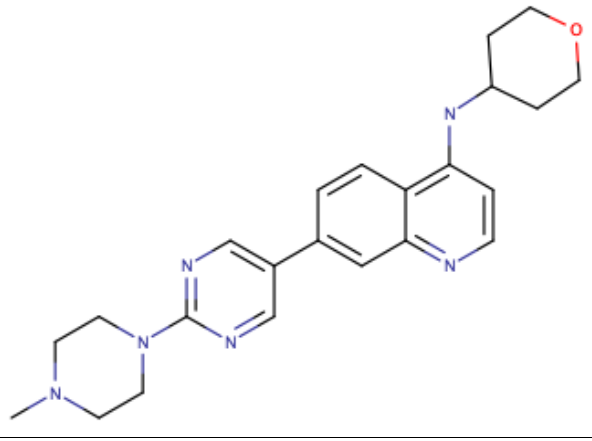
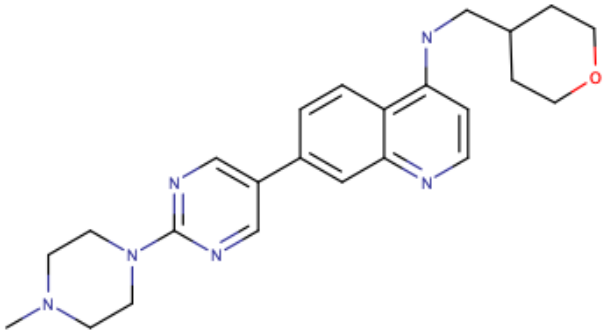
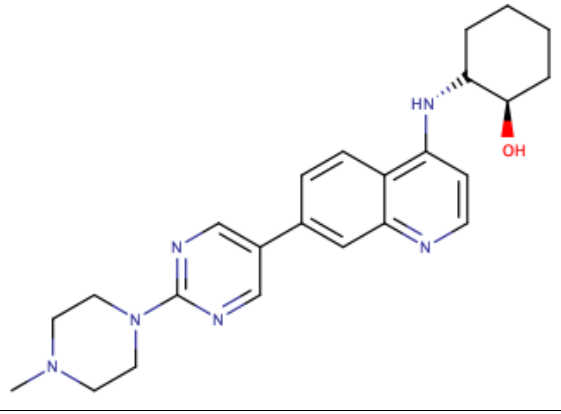
CN_S002_C017		CCCN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	4.40E-05
CN_S002_C018		CN1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	9.90E-04

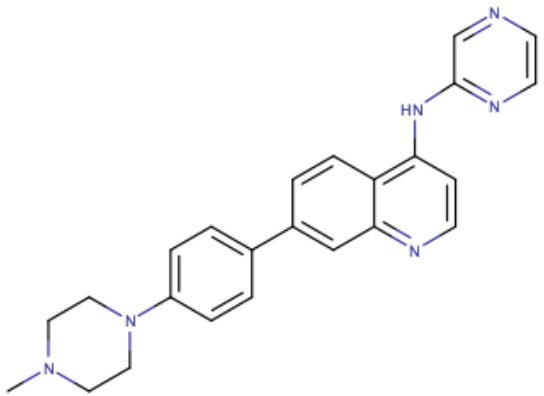
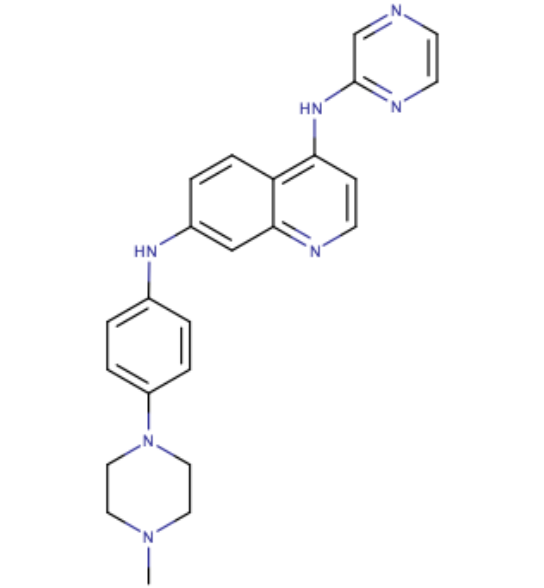
CN_S002_C019		CCN1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	8.00E-04
CN_S002_C020		CCCN1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	7.80E-05

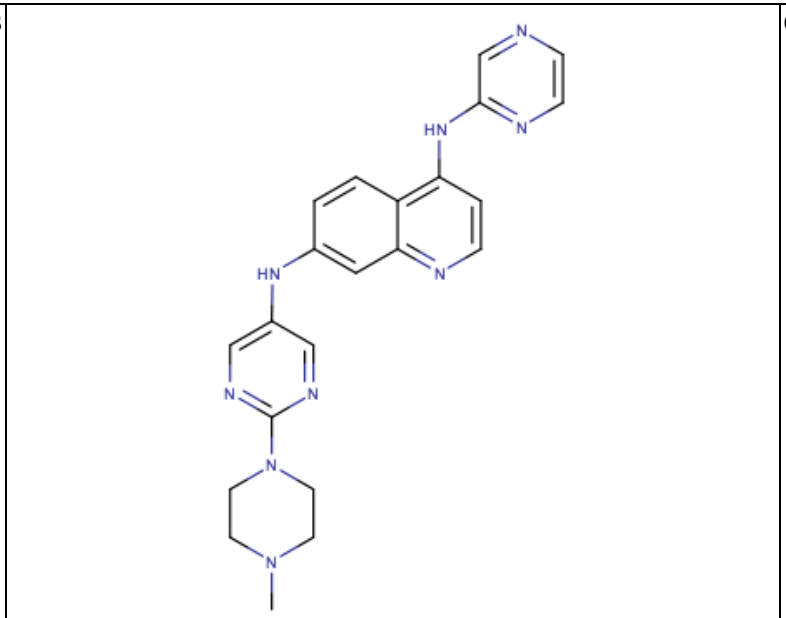
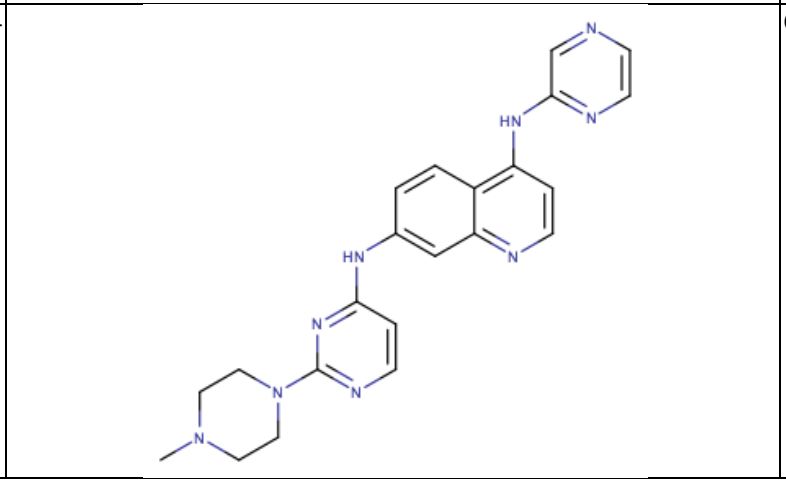
CN_S002_C021		C1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	2.00E-06
CN_S002_C022		CN1CC2(C1)CCN(C2)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	6.90E-04

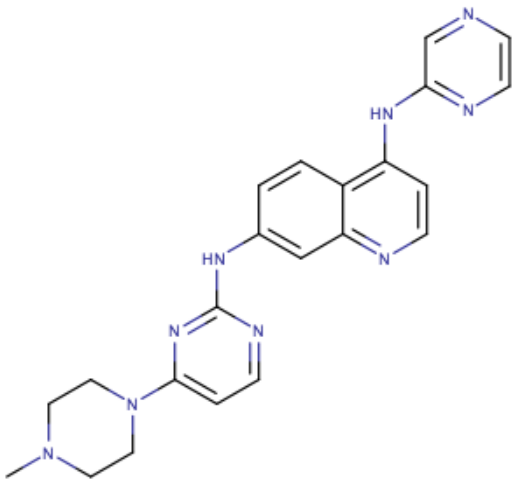
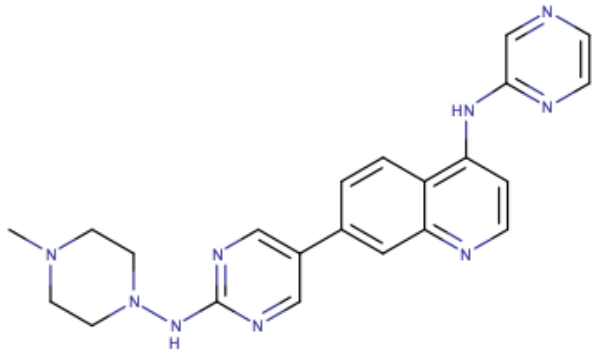
CN_S002_C023		CN1CCC2(CCN(C2)C2=NC=C(C=N2)C2=CC3=NC=CC(NC4=NC=CN=C4)=C3C=C2)C1	7.00E-04
CN_S002_C024		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3CCCCC3)=C2C=C1	9.80E-05
CN_S002_C025		CN1CCC(CC1)NC1=C2C=CC(=CC2=NC=C1)C1=CN=C(N=C1)N1CCN(C)CC1	1.00E-03

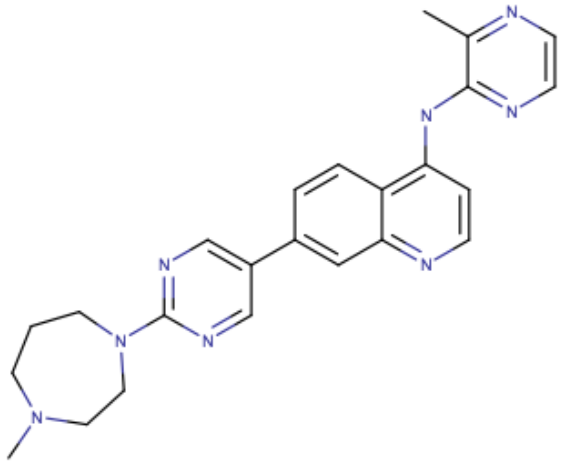
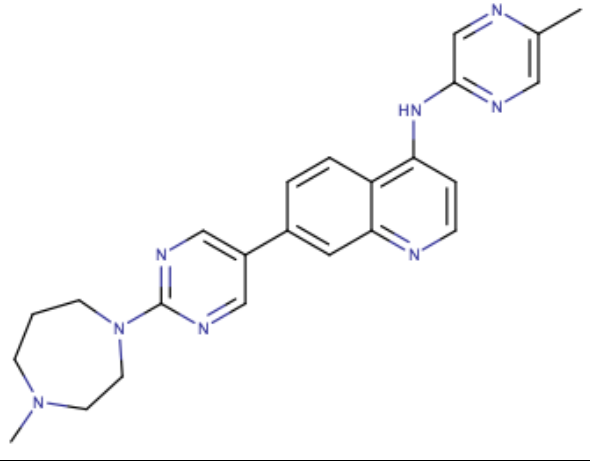
CN_S002_C026		CN(C)C1CCC(CC1)NC1=C2C=CC(=CC2=NC=C1)C1=CN=C(N=C1)N1CCN(C)CC1	6.60E-04
CN_S002_C027		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NCCN3CCCC3)=C2C=C1	5.90E-04

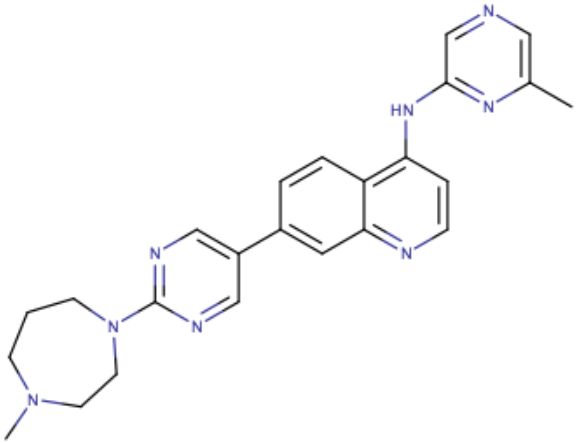
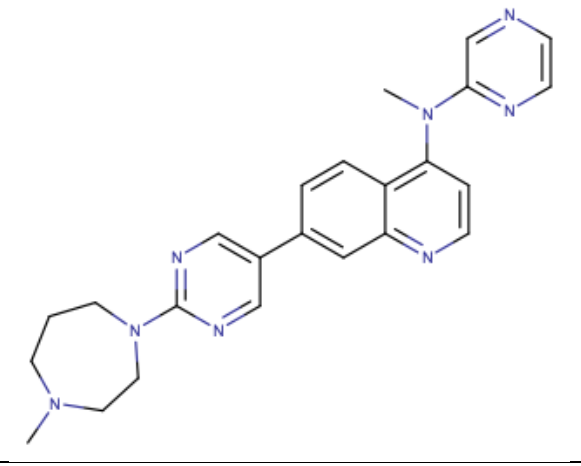
CN_S002_C028		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3CCOCC3)=C2C=C1	7.60E-04
CN_S002_C029		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NCC3CCOCC3)=C2C=C1	7.60E-04
CN_S002_C030		CN1CCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3CCCC[C@H]3O)=C2C=C1	9.80E-04

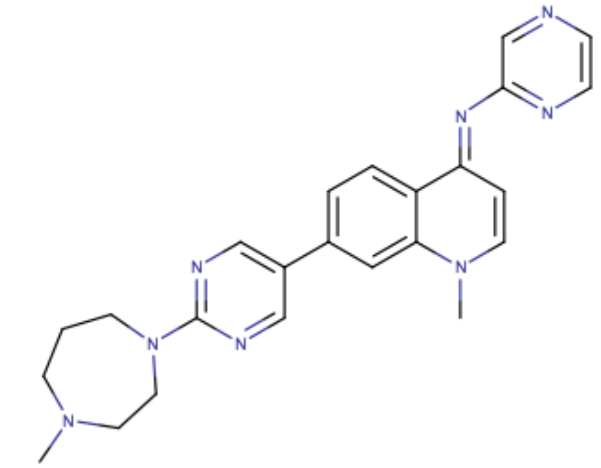
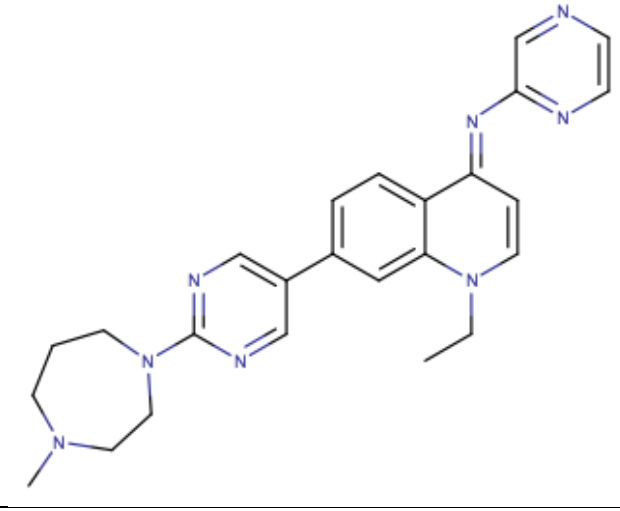
CN_S002_C031		CN1CCN(CC1)C1=CC=C(C=C1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.70E-06
CN_S002_C032		CN1CCN(CC1)C1=CC=C(NC2=CC3=NC=CC(NC4=NC=CN=C4)=C3C=C2)C=C1	8.10E-04

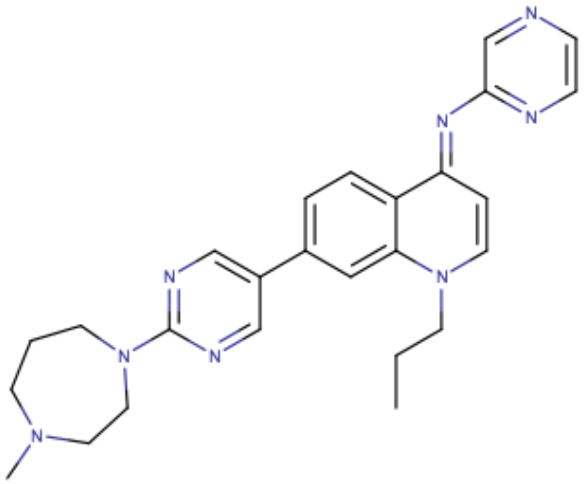
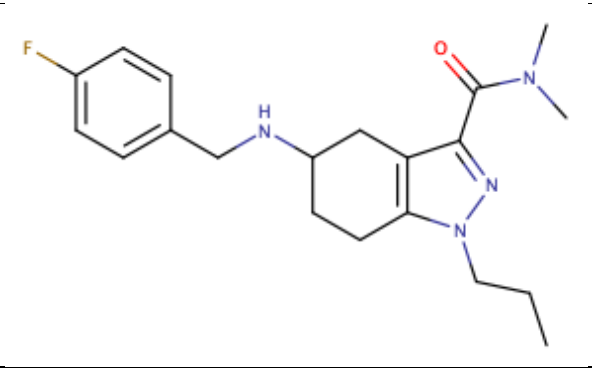
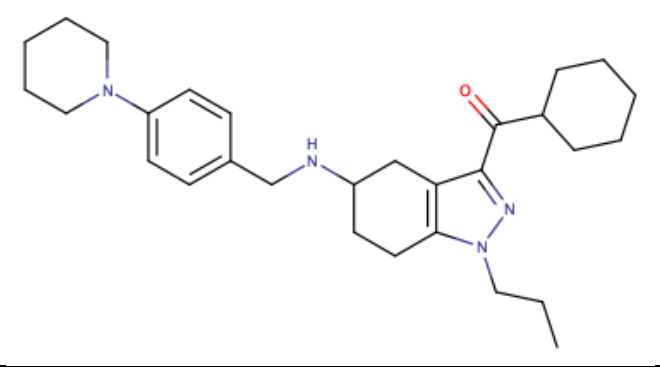
CN_S002_C033		CN1CCN(CC1)C1=NC=C(NC2=CC3=NC=CC(NC4=NC=CN=C4)=C3C=C2)C=N1	1.30E-04
CN_S002_C034		CN1CCN(CC1)C1=NC=CC(NC2=CC3=NC=CC(NC4=NC=CN=C4)=C3C=C2)=N1	2.00E-06

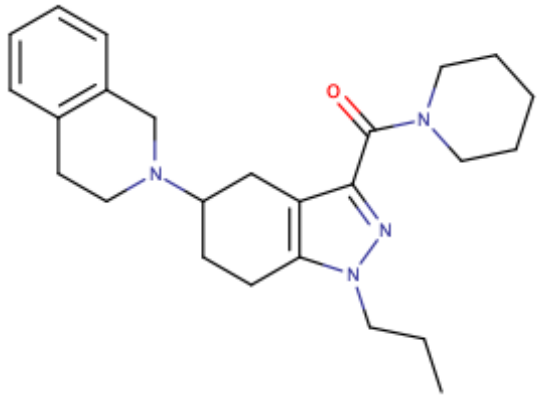
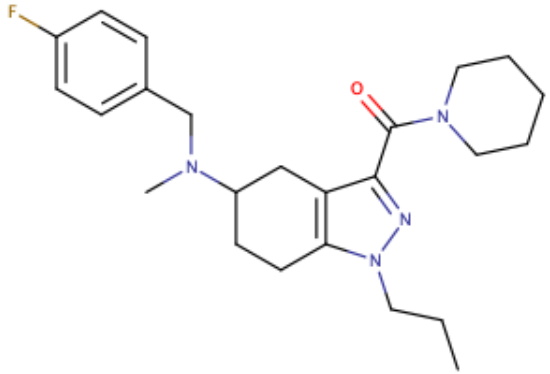
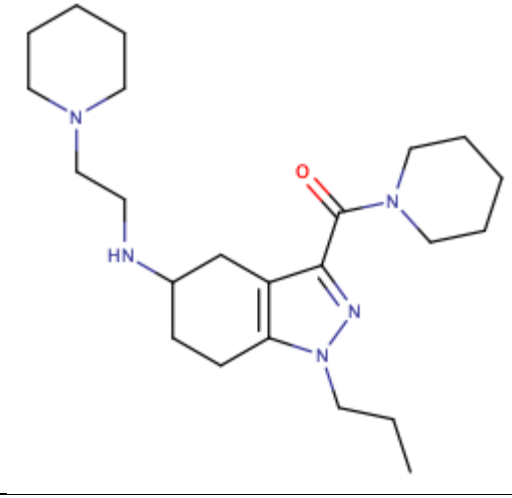
CN_S002_C035		CN1CCN(CC1)C1=CC=NC(NC2=CC3=NC=CC(NC4=NC=CN=C4)=C3C=C2)=N1	2.60E-05
CN_S002_C036		CN1CCN(CC1)NC1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3)=C2C=C1	1.00E-03

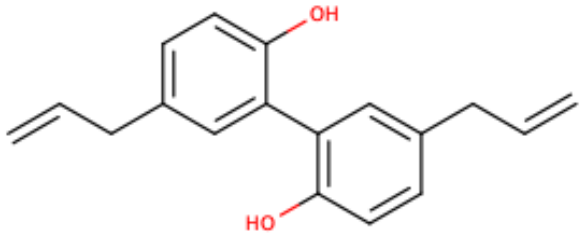
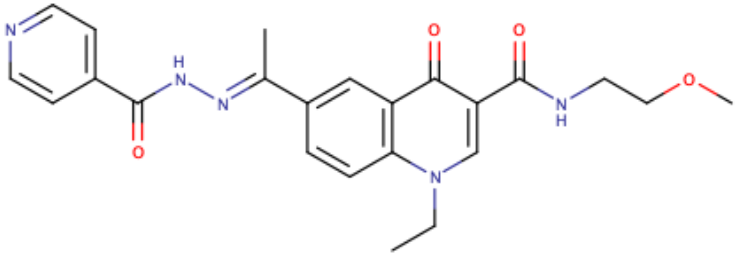
CN_S002_C037		CN1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=CN=C3C)=C2C=C1	8.30E-04
CN_S002_C038		CN1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC=C(C)N=C3)=C2C=C1	6.50E-04

CN_S002_C039		CN1CCCN(CC1)C1=NC=C(C=N1)C1=CC2=NC=CC(NC3=NC(C)=CN=C3)=C2C=C1	1.00E-03
CN_S002_C040		CN(C1=NC=CN=C1)C1=C2C=CC(=CC2=NC=C1)C1=CN=C(N=C1)N1CCCN(C)CC1	8.10E-04

CN_S002_C041		CN1C=C\C(=N/C2=NC=CN=C2)C2=CC=C(C=C12)C1=CN=C(N=C1)N1CCCN(C)CC1	8.80E-04
CN_S002_C042		CCN1C=C\C(=N/C2=NC=CN=C2)C2=CC=C(C=C12)C1=CN=C(N=C1)N1CCCN(C)CC1	1.00E-03

CN_S002_C043		CCCN1C=C\C(=N/C2=NC=CN=C2)C2=CC=C(C=C12)C1=CN=C(N=C1)N1CCCN(C)CC1	8.90E-04
CN_S003_C001		CCCN1N=C(C(=O)N(C)C)C2=C1CCC(C2)NCC1=CC=C(F)C=C1	1.78E-03
CN_S003_C002		CCCN1N=C(C(=O)C2CCCCC2)C2=C1CCC(C2)NCC1=CC=C(C=C1)N1CCCCC1	4.63E-04

CN_S003_C003		CCCN1N=C(C(=O)N2CCCCC2)C2=C1CCC(C2)N1CCC2=C(C1)C=CC=C2	7.13E-04
CN_S003_C004		CCCN1N=C(C(=O)N2CCCCC2)C2=C1CCC(C2)N(C)CC1=CC=C(F)C=C1	2.42E-03
CN_S003_C005		CCCN1N=C(C(=O)N2CCCCC2)C2=C1CCC(C2)NCCN1CCCCC1	1.74E-03

CN_S004_C001		OC1=CC=C(CC=C)C=C1C1=C(O)C=CC(CC=C)=C1	2.25E-04
CN_S005_C001		CCN1C=C(C(=O)NCCOC)C(=O)C2=C1C=CC(=C2)C(\C)=N\NC(=O)C1=CC=NC=C1	9.50E-05