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| **Data set** | **SMILES** |
| **1** | NCC=1NC(=O)NC(=O)C=1Cl |
| **2** | O=C1NC(=O)C(Cl)=C(CNC)N1 |
| **3** | O=C1NC(CNCC)=C(Cl)C(=O)N1 |
| **4** | O=C1NC(CNC(C)C)=C(Cl)C(=O)N1 |
| **5** | O=C1NC(CNCCCO)=C(Cl)C(=O)N1 |
| **6** | O=C1NC(CNCCN)=C(Cl)C(=O)N1 |
| **7** | O=C1NC(CN(C)C)=C(Cl)C(=O)N1 |
| **8** | ClC1=C(NC(=O)NC1=O)CN2CCC2 |
| **9** | ClC1=C(NC(=O)NC1=O)CN2CCCC2 |
| **10** | ClC1=C(NC(=O)NC1=O)CN2CCCCC2 |
| **11** | O=C1NC(CCN(C)C)=C(Cl)C(=O)N1 |
| **12** | ClC1=C(NC(=O)NC1=O)CN2CCCC2C |
| **13** | ClC1=C(NC(=O)NC1=O)Cn2ccnc2 |
| **14** | ClC1=C(NC(=O)NC1=O)Cn2ccnc2C |
| **15** | O=C2NC(=O)NC(CN1CCCC1)=C2 |
| **16** | BrC1=C(NC(=O)NC1=O)CN2CCCC2 |
| **17** | IC1=C(NC(=O)NC1=O)CN2CCCC2 |
| **18** | CC1=C(NC(=O)NC1=O)CN2CCCC2 |
| **19** | O=C1NC(CN\C=N\N)=C(Cl)C(=O)N1 |
| **20** | O=C1NC(CN\C=N\NC)=C(Cl)C(=O)N1 |
| **21** | O=C2NC(CNC1=NCCN1)=C(Cl)C(=O)N2 |
| **22** | O=C1NC(CN\C=N\C)=C(Cl)C(=O)N1 |
| **23** | O=C1NC(CN(C)\C=N\N)=C(Cl)C(=O)N1 |
| **24** | O=C1NC(CS\C=N\N)=C(Cl)C(=O)N1 |
| **25** | O=C1NC(CS\C=N\NC)=C(Cl)C(=O)N1 |
| **26** | O=C2NC(CSC1=NCCN1)=C(Cl)C(=O)N2 |
| **27** | ClC1=C(NC(=O)NC1=O)CN2CCNC2=N |
| **28** | BrC1=C(NC(=O)NC1=O)CN2CCNC2=N |
| **29** | ClC1=C(NC(=O)NC1=O)CN2CCN(C)C2=N |
| **30** | ClC1=C(NC(=O)NC1=O)CN2CCN(CC)C2=N |
| **31** | CC(C)N2CCN(CC=1NC(=O)NC(=O)C=1Cl)C2=N |
| **32** | ClC1=C(NC(=O)NC1=O)CN2C=CN(C)C2=N |
| **33** | ClC1=C(NC(=O)NC1=O)CN2CCN(CC)C2=N |
| **34** | ClC1=C(NC(=O)NC1=O)CN2CCCC2=N |
| **35** | CC1=C(NC(=O)NC1=O)CN2CCCC2=N |
| **36** | BrC1=C(NC(=O)NC1=O)CN2CCCC2=N |
| **37** | O=C1NC(CNC)=C(Cl)C(=O)N1 |
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| **Virtual screening data set** | **SMILES** |
| **38** | ClC1=C(N=CNC1=O)CN2CCCC2=N |
| **39** | ClC1=C(NC(=O)NC1=O)CN2CCCC2N |
| **40** | ClC1=C(NC(=O)NC1=O)CN2C=NCC2 |
| **41** | ClC1=C(NC(=O)NC1=O)CN2CC(CO)C(O)C2 |
| **42** | ClC1=C(NC(=O)NC1=O)CN2CCN=C2N |
| **43** | O=C1C=C(NC(=O)N1)CN2CCCCC2 |
| **44** | O=C1C=C(NC(=O)N1)CN2CCC(C)CC2 |
| **45** | O=C1C=C(NC(=O)N1)CN2CCCCC2C |
| **46** | O=C2C=C(CN1CCCCCC1)NC(=O)N2 |
| **47** | ClC1=C(NC(=O)NC1=O)CN2CC=NC2N |
| **48** | O=C1NC(CN(CCC)CCC)=CC(=O)N1 |
| **49** | O=C1C=C(NC(=O)N1)CN2CCCC(C)C2 |