

## Supplementary Material

### Design and evaluation of the performance of an NMR screening fragment library

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SMILES of 24 common hitters (hit in > 90% of screens)

NC1=NC2=CC3=C(OCCO3)C=C2S1  
NC1=CC=C(C=C1)C1=NC2=CC=CC=C2N1  
OC1=CC=CC=C1NS(=O)(=O)C1=CC=CC=C1  
COC1=CC=C(C=C1)C1=C(C)SC(N)=N1  
CC1=C(N=C(N)S1)C1=CC=CC=C1  
OC1=CC=C(C=C1)C1CCC=C1  
OC1=CC=CC(=C1)C1=NC2=CC=CC=C2N1  
CC1=CC(=NN1)C1=CC=CC=C1  
NC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(N)C=C1  
FC1=CC=CC(NC(=O)C2=CC=CO2)=C1  
COC1=CC=C(C=C1)C1=NN=C(N)S1  
NC1=NN=C(S1)C1=CC=CC=C1  
CC1=CC=C(NC(=O)C2=CC=CC(N)=C2)C=C1  
CNS(=O)(=O)C1=CC=C(SC)C=C1  
NS(=O)(=O)C1=C2C=CC=CC2=CC=C1  
CC(NC(C)=O)C1=CC=C(Br)C=C1  
CC1=NN=C2SC(CC3=CC=CC=C3)=NN12  
NC1=CC=CC(=C1)C1=NC2=CC=CC=C2N1  
CC1=CC(=CO1)C(=O)NC1=CC=CC(O)=C1  
CC1=NNC2=C1C(=O)CC(C2)C1=CC=CC=C1  
CNC(=O)C1=C(OC)C=C2C=CC=CC2=C1  
CCC1=NNC(N)=C1C1=CC=C(OC)C=C1  
CC1=C(N)NN=C1C1=CC=C(Cl)C=C1  
COC1=CC=C(C2=NN=C(N)S2)C(OC)=C1

Structures of 24 common hitters (hit in > 90% of screens)

