Article title: In silico hit optimization towards AKT inhibition: Fragment-based approach, molecular docking and molecular dynamics study

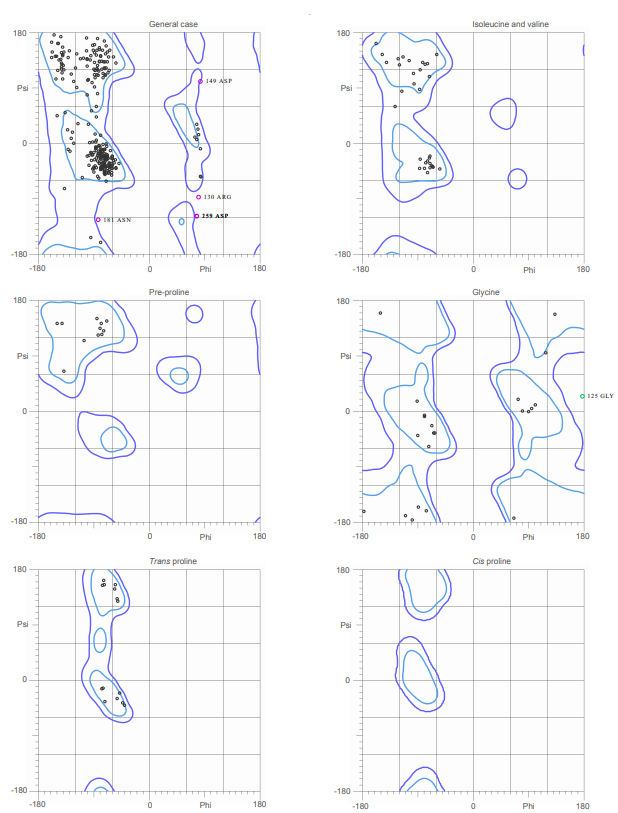
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Supporting Information

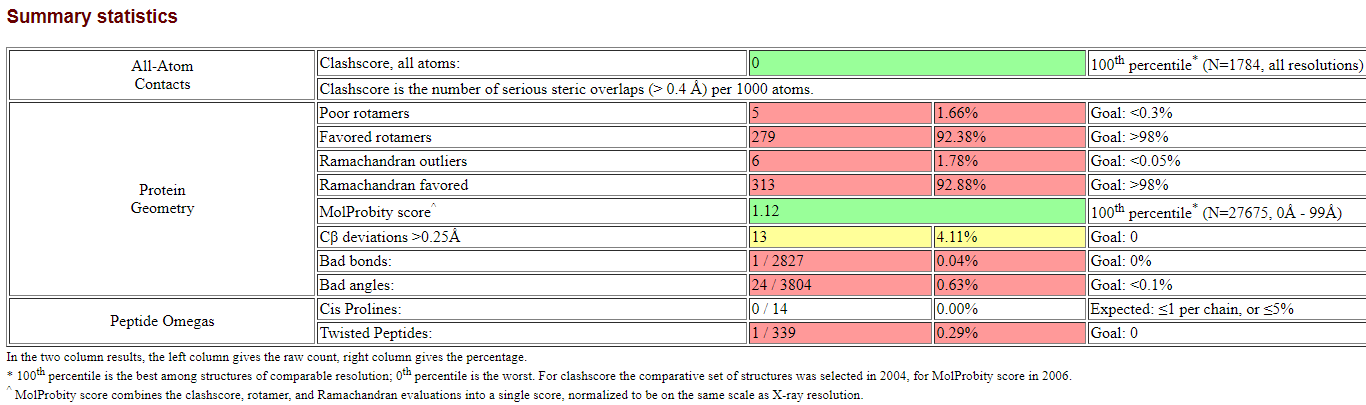


Figure S1. Validation of AKT3homology model.

2E in AKT1





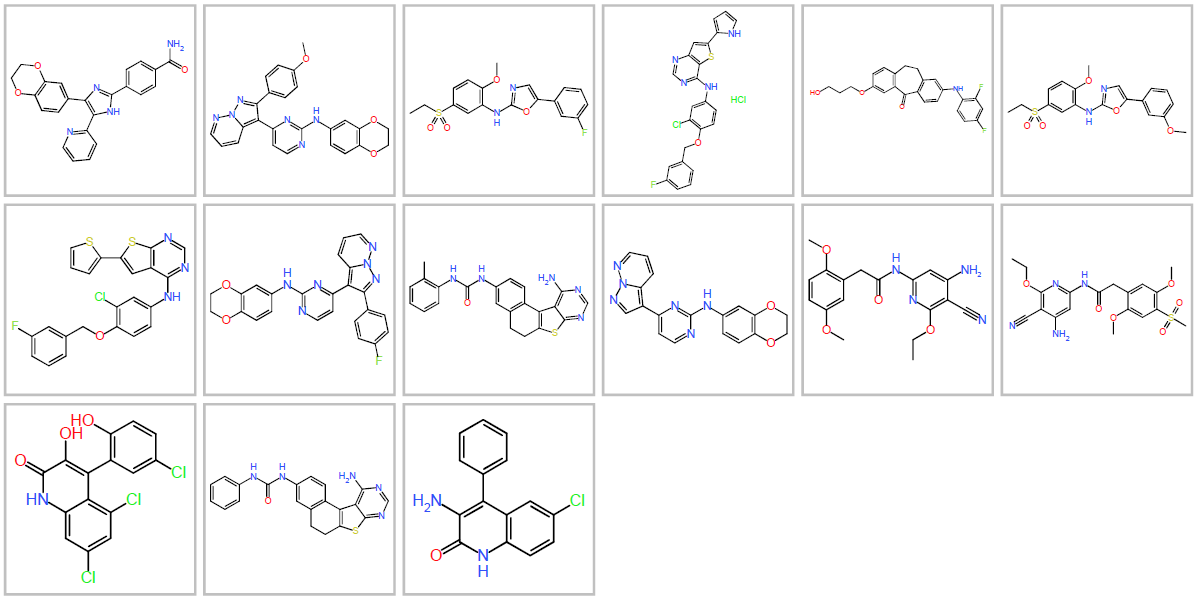
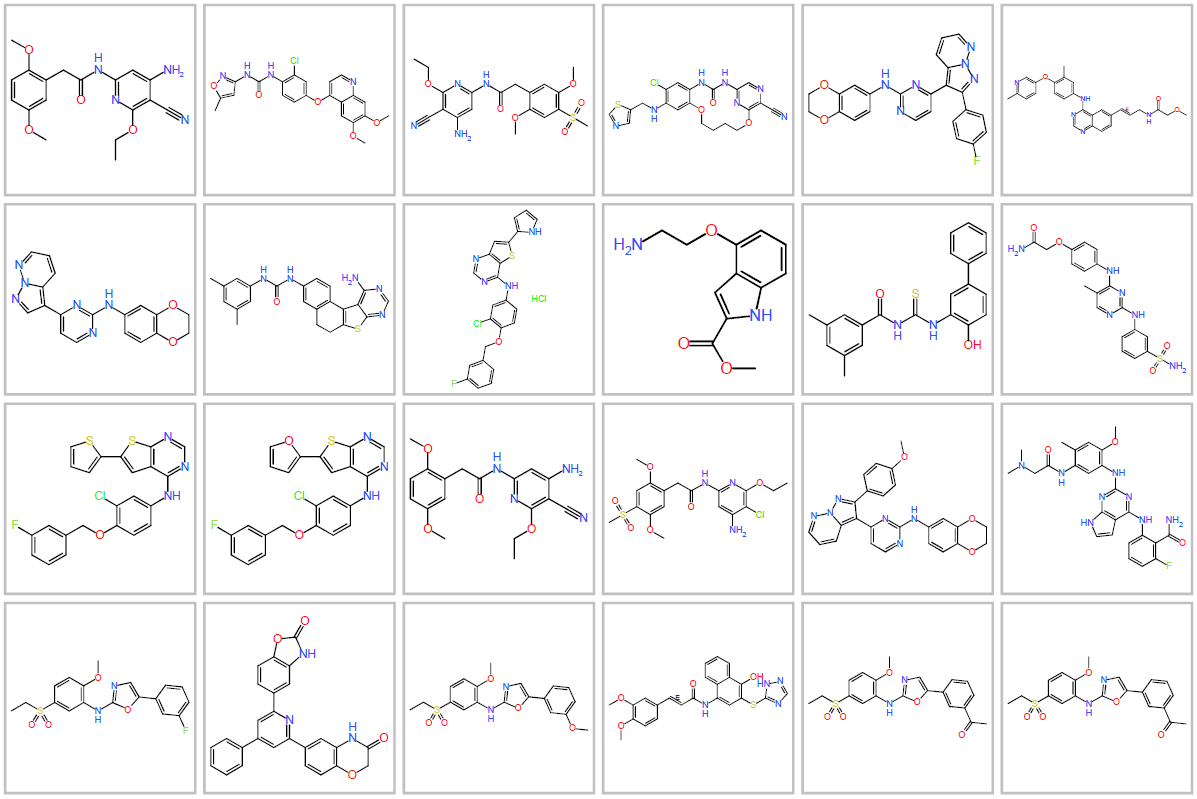
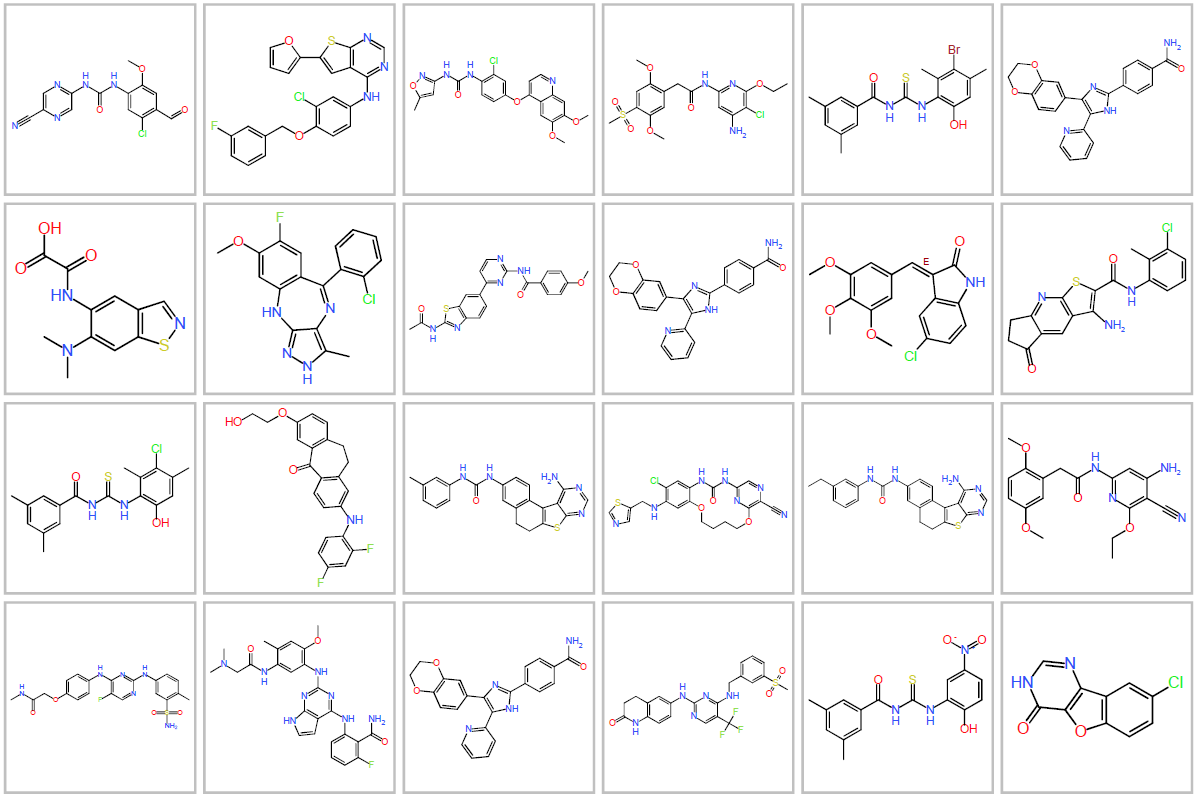
1E in AKT1



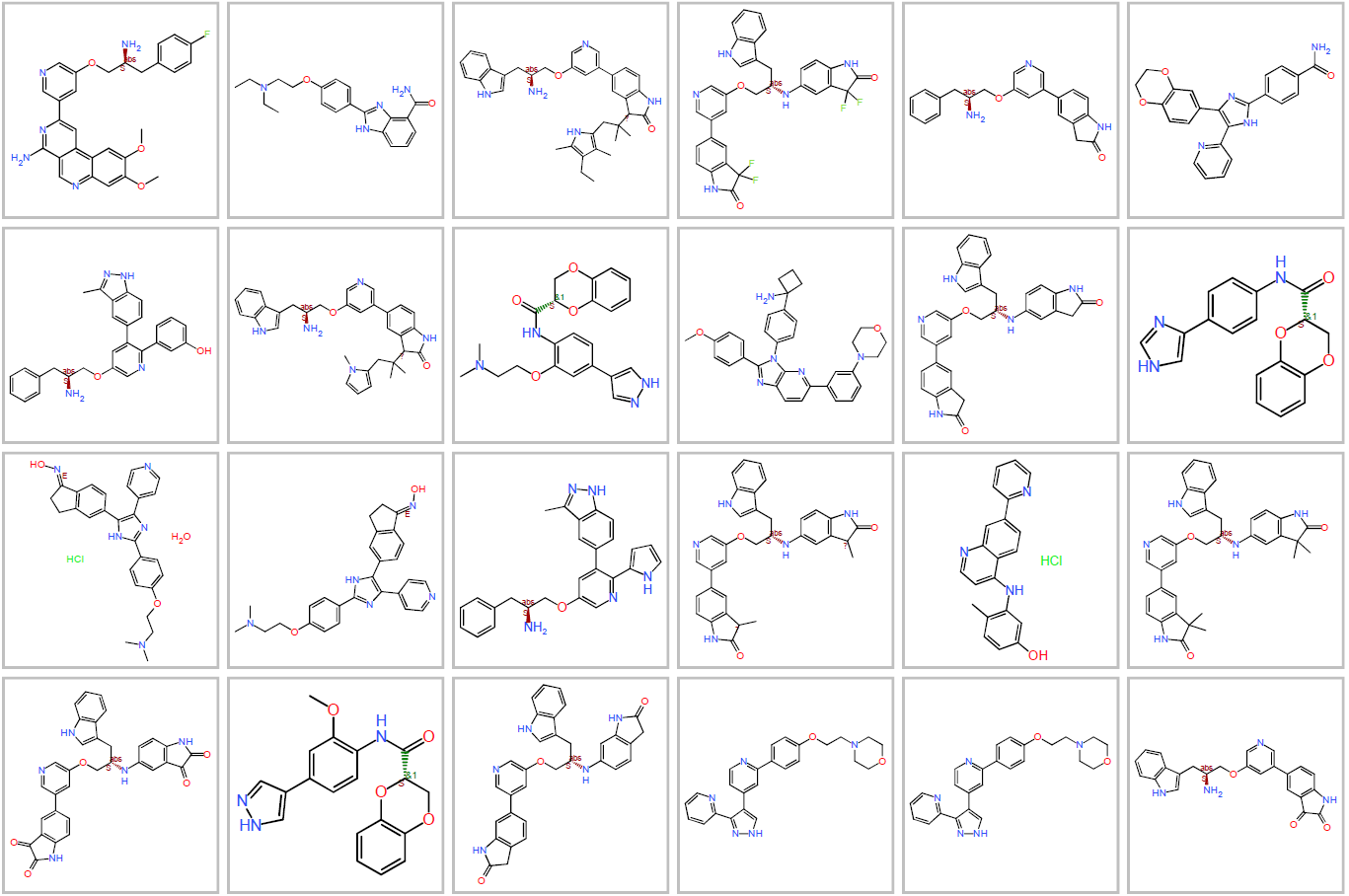
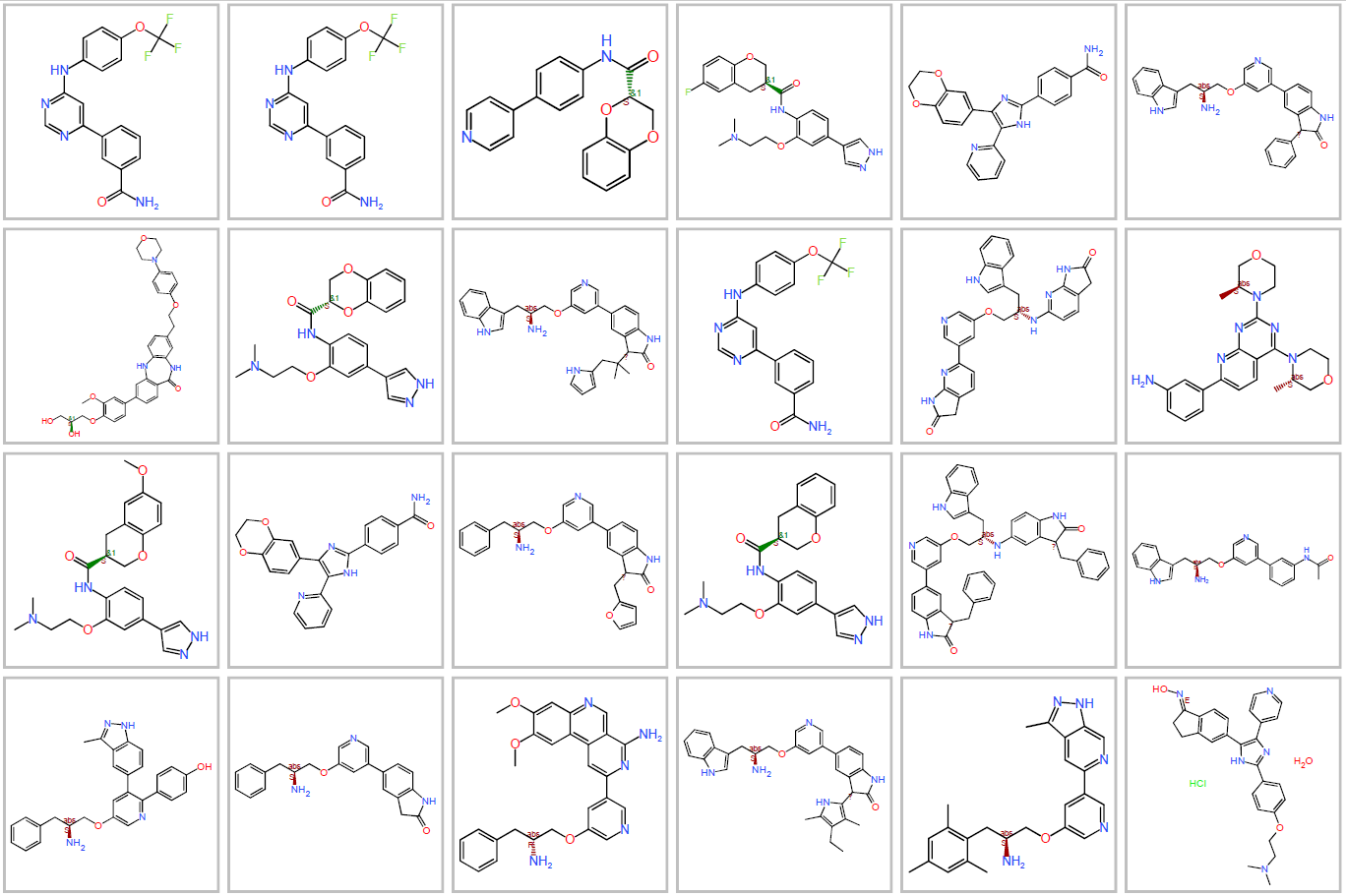
3E in AKT1



FragFp

PathFp



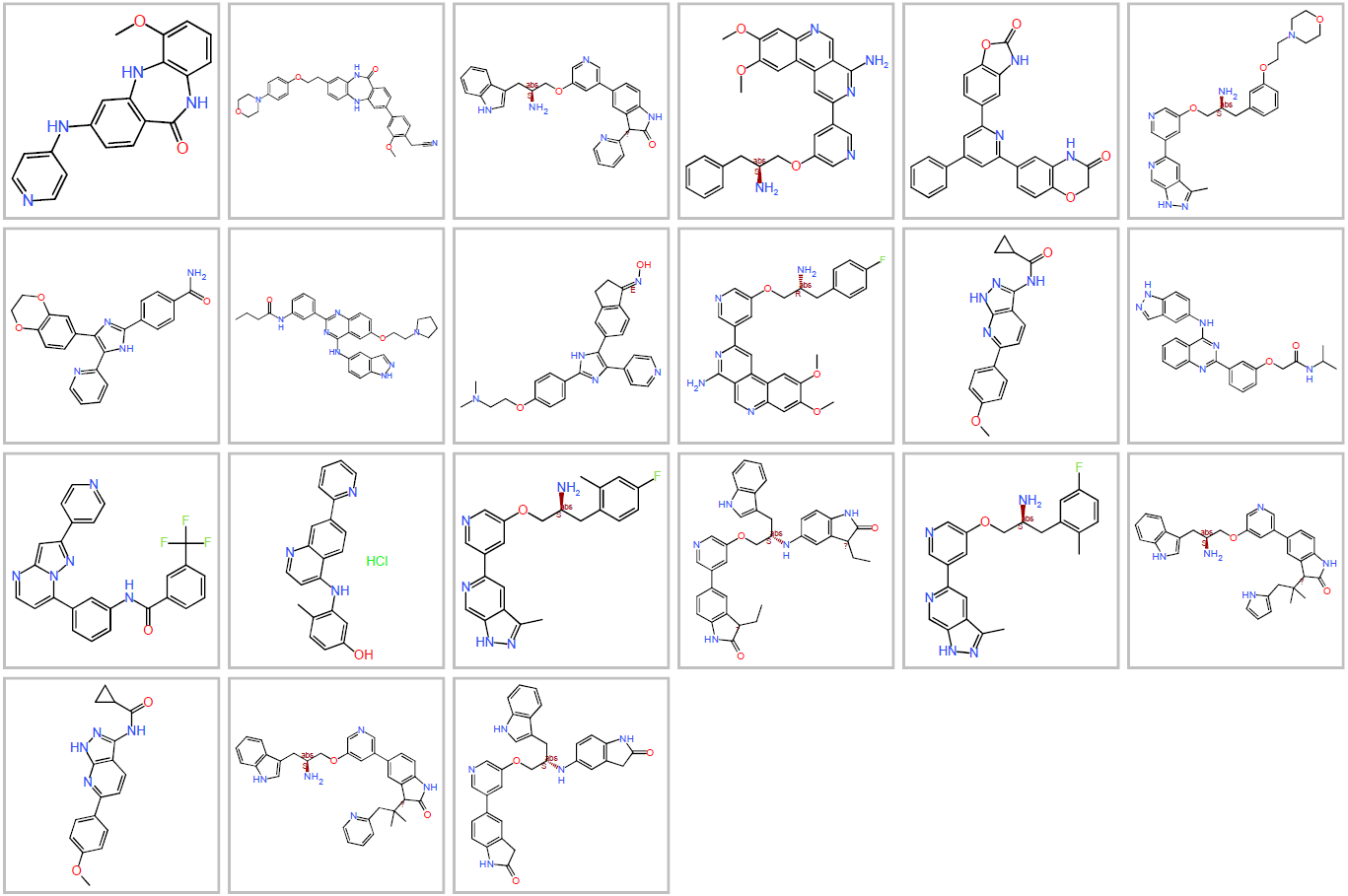
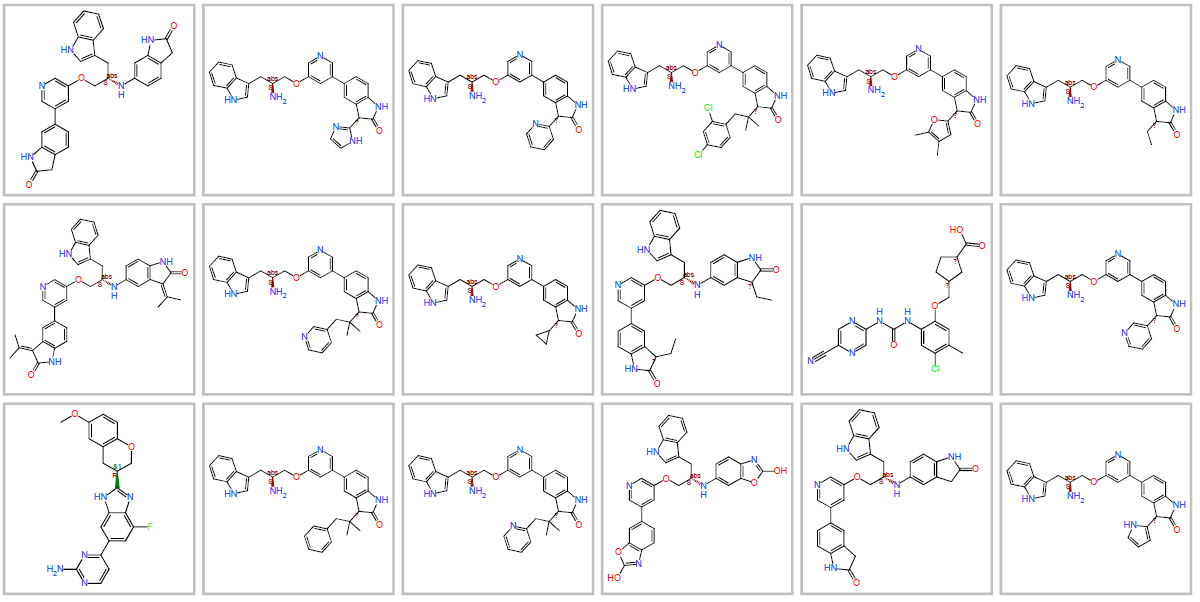
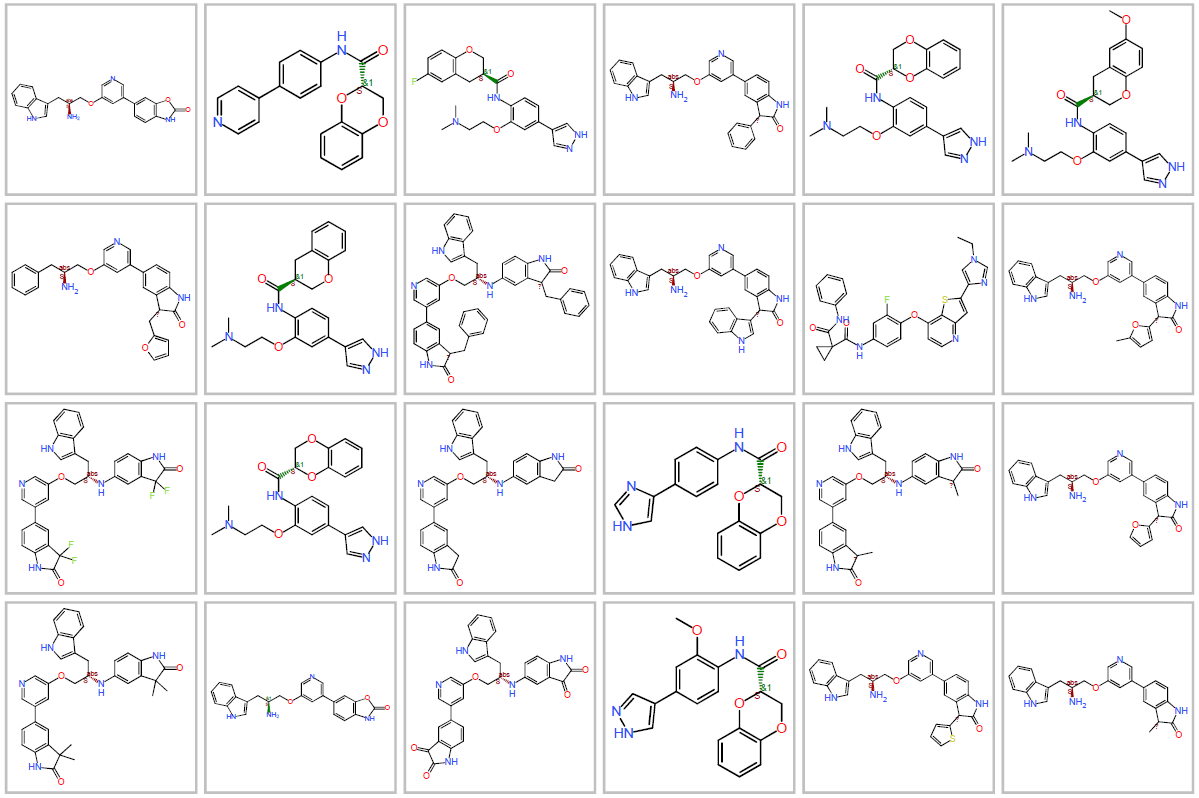
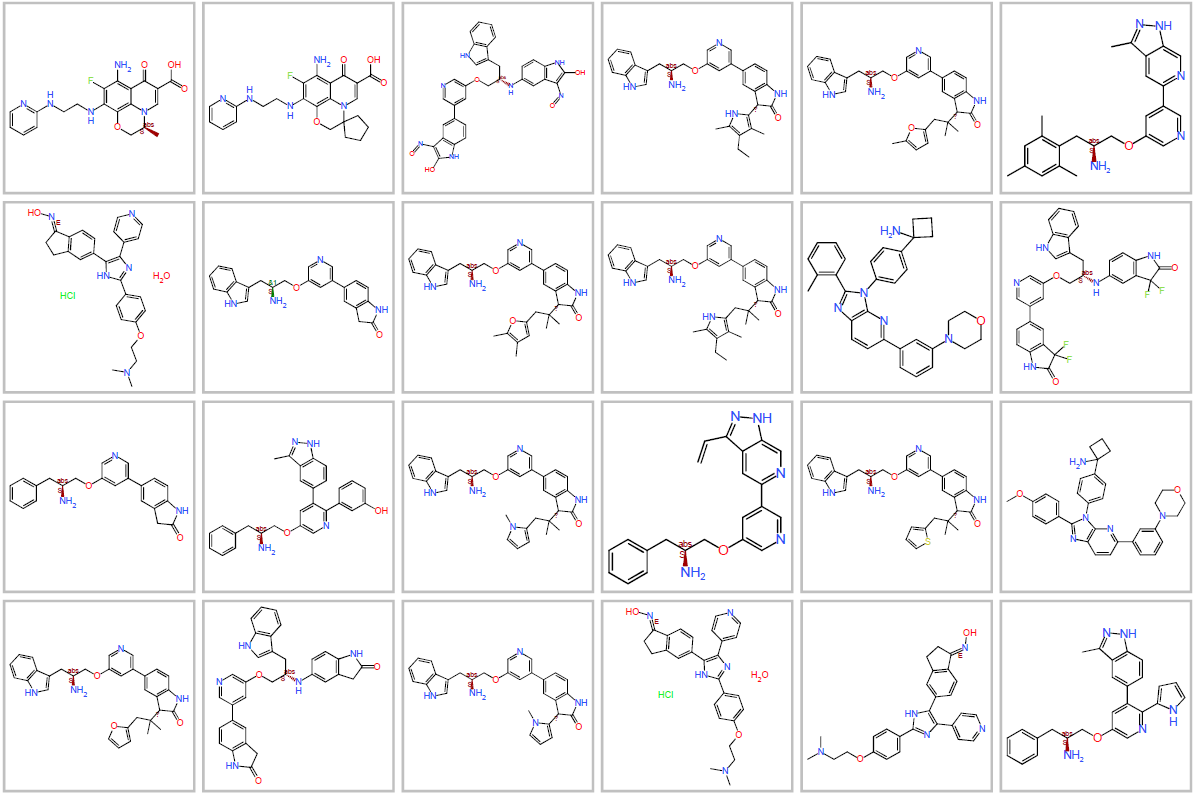
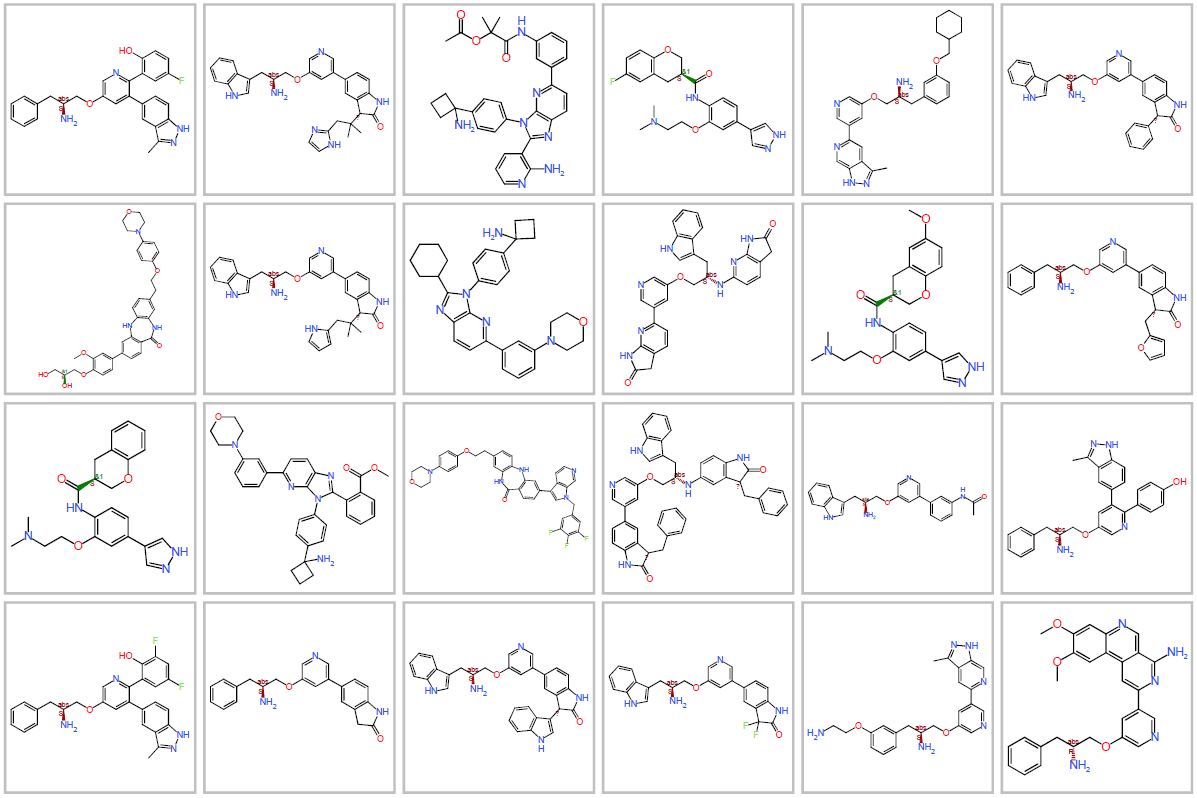


Figura S3.1. Structures with a Tanimoto coefficient of 0.6 for series A using FragFp and PathFp.

FragFp



PathFp



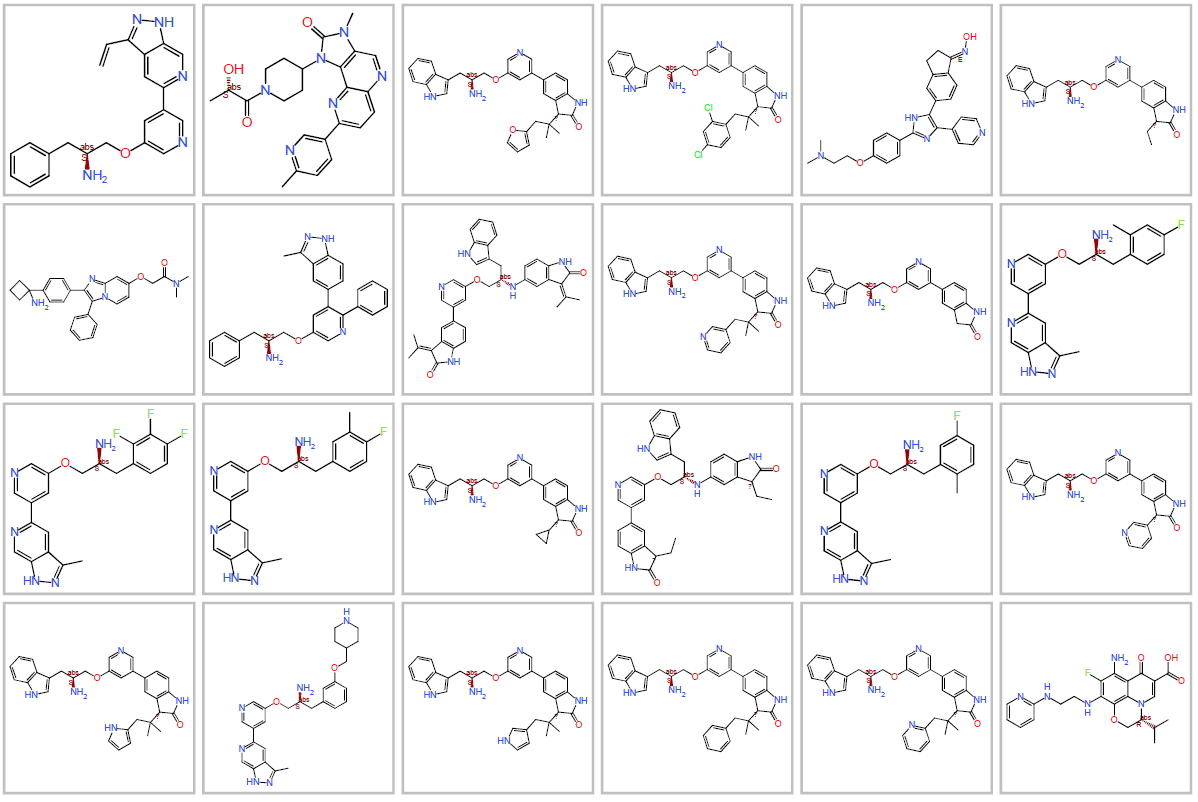
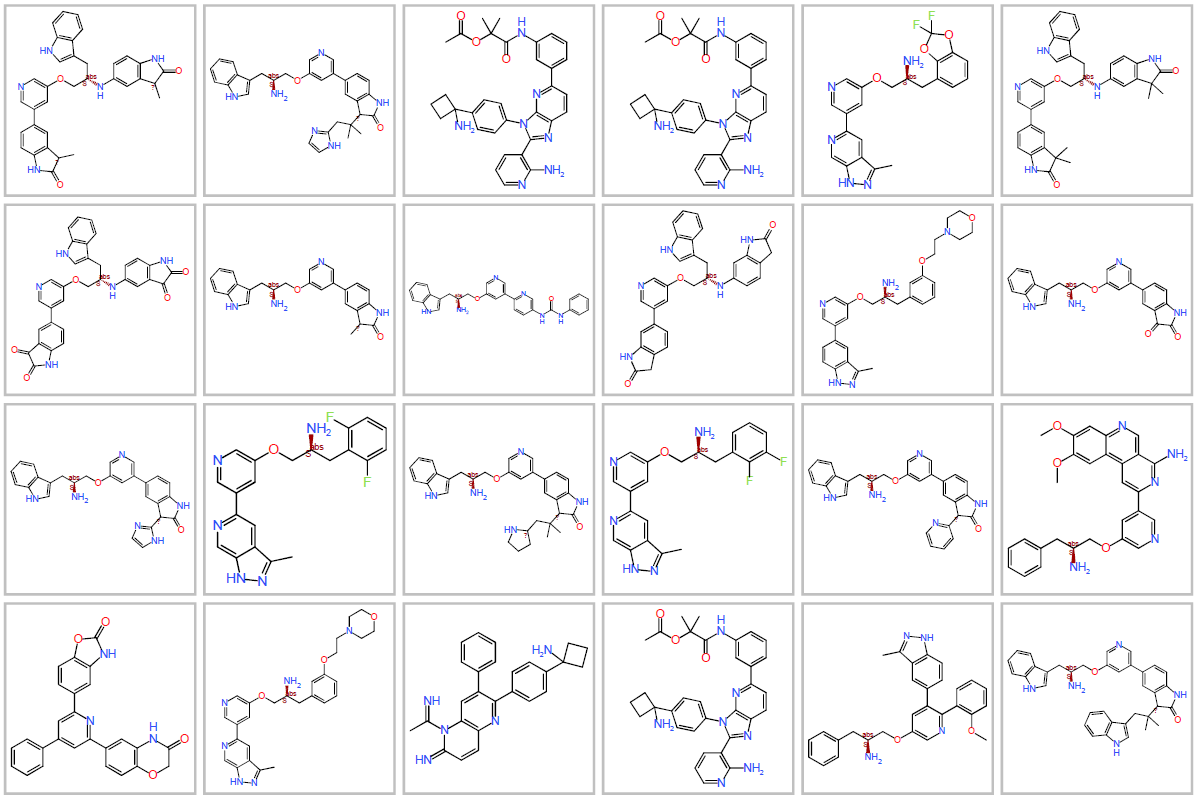
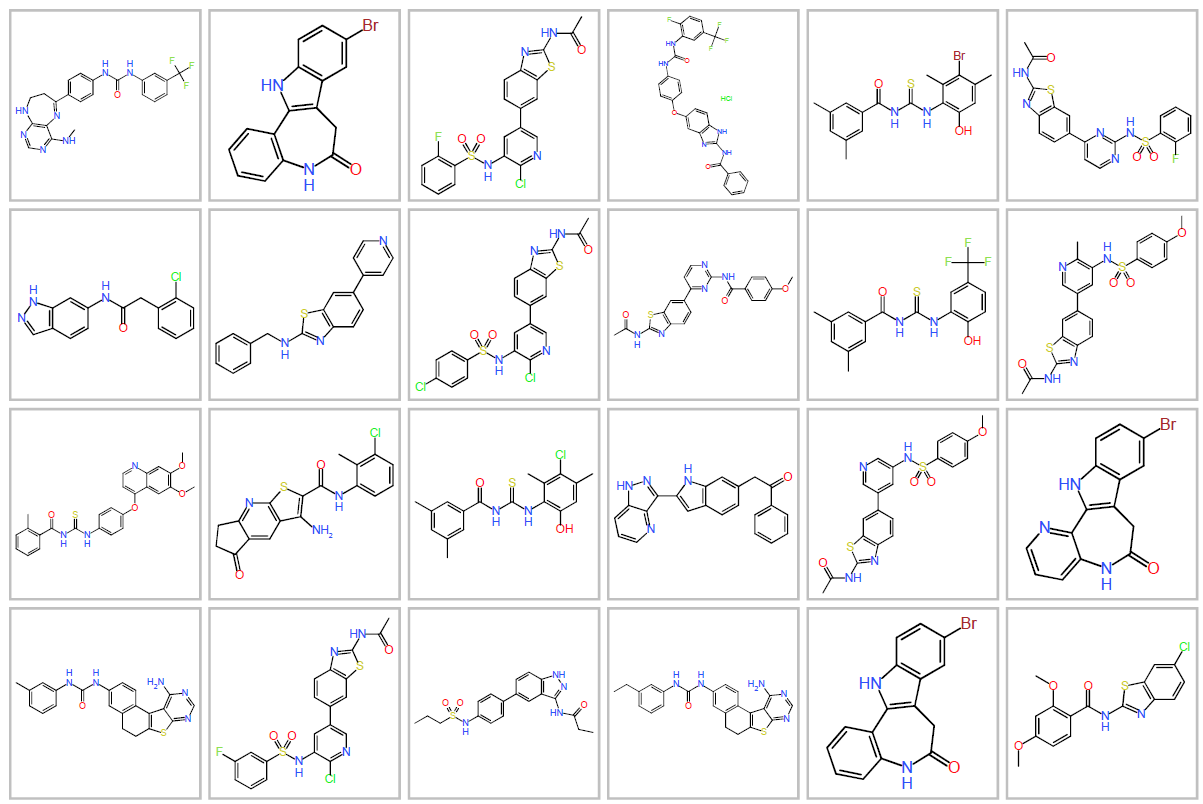
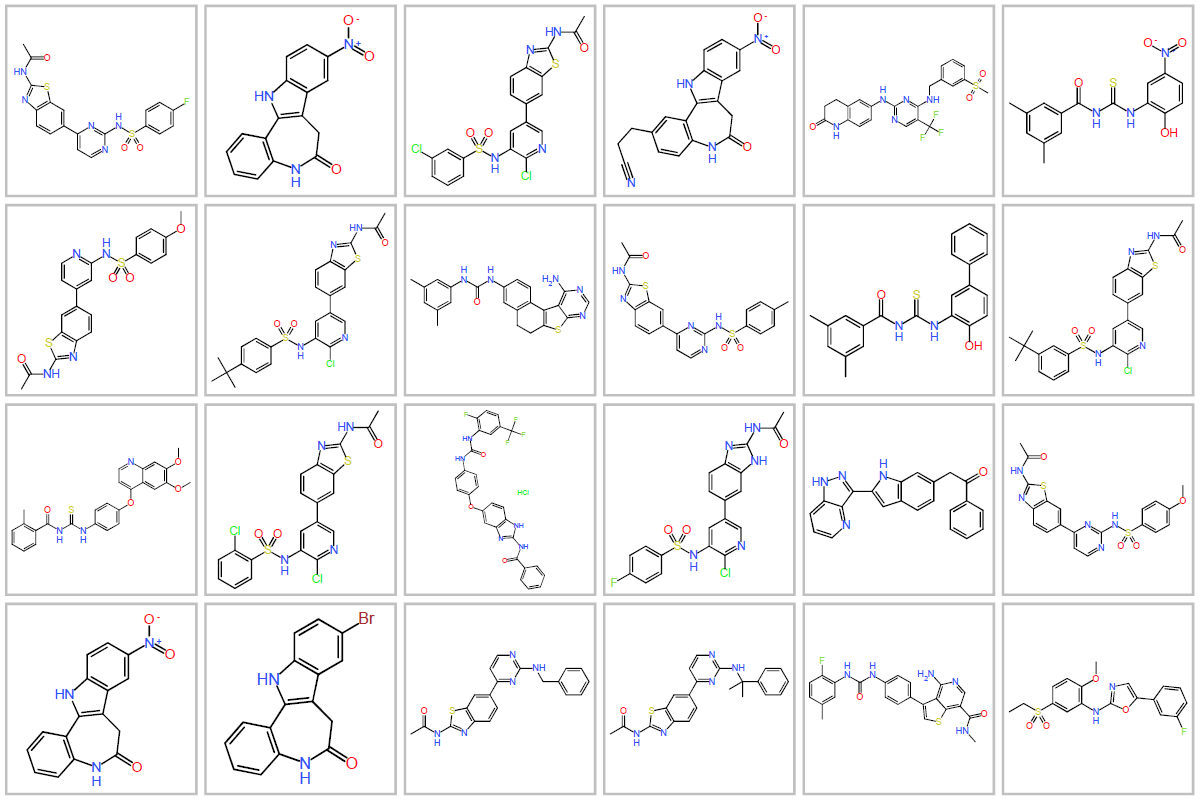
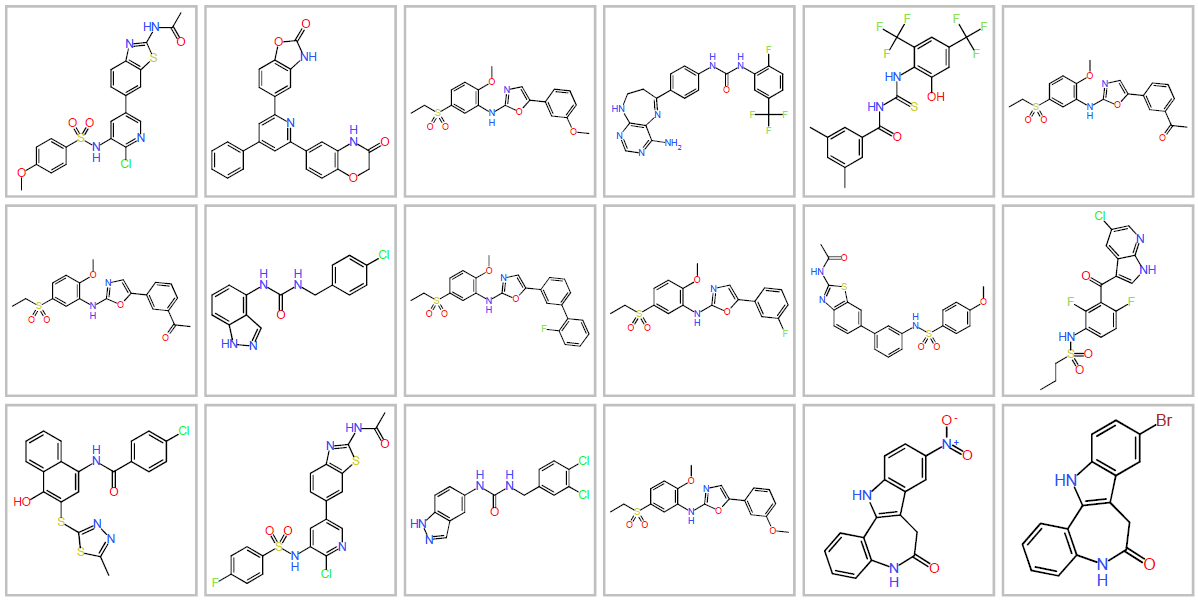
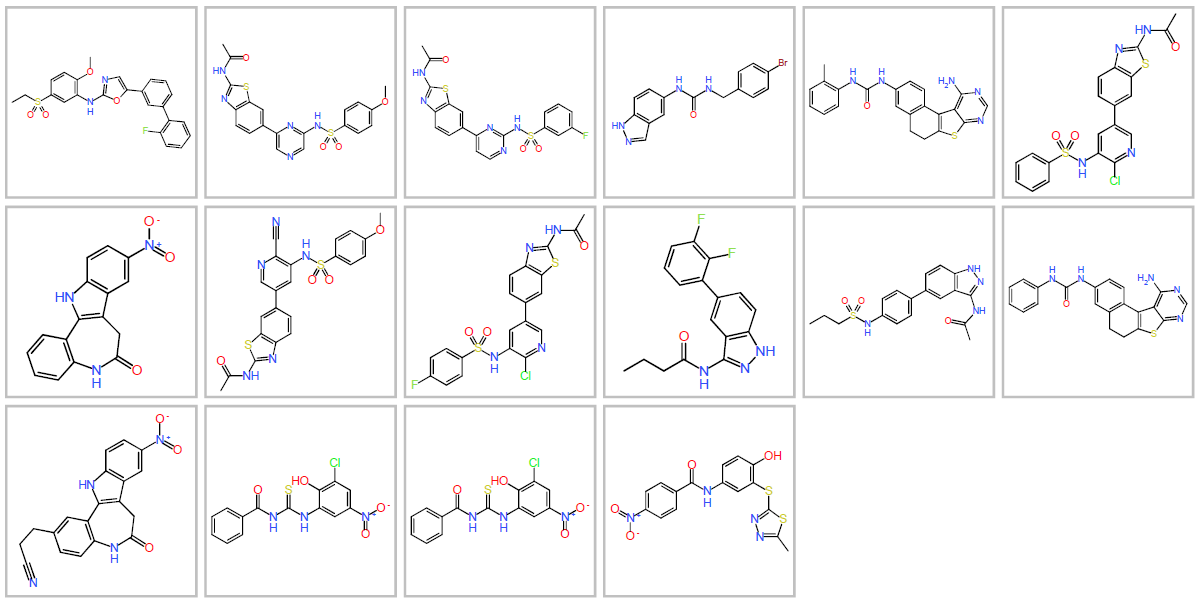


Figura S3.2. Structures with a Tanimoto coefficient of 0.6 for series C using FragFp and PathFp.

FragFp



PathFp

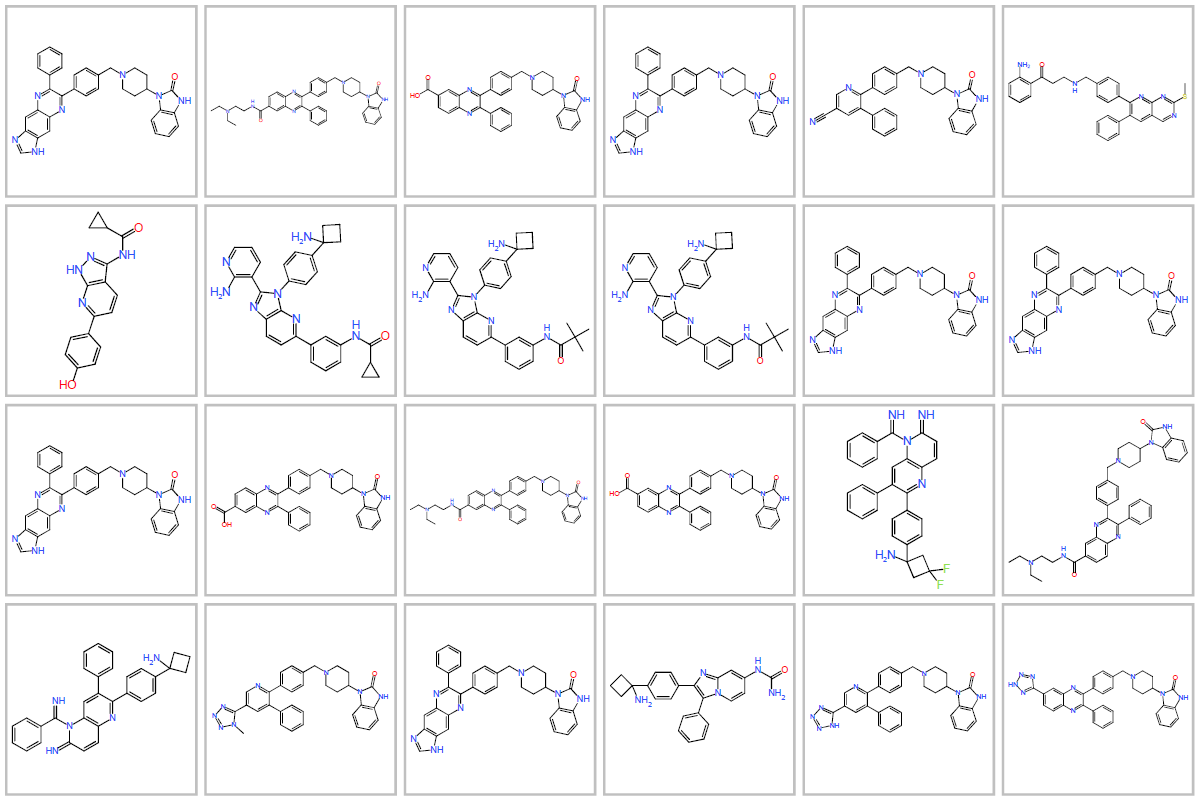
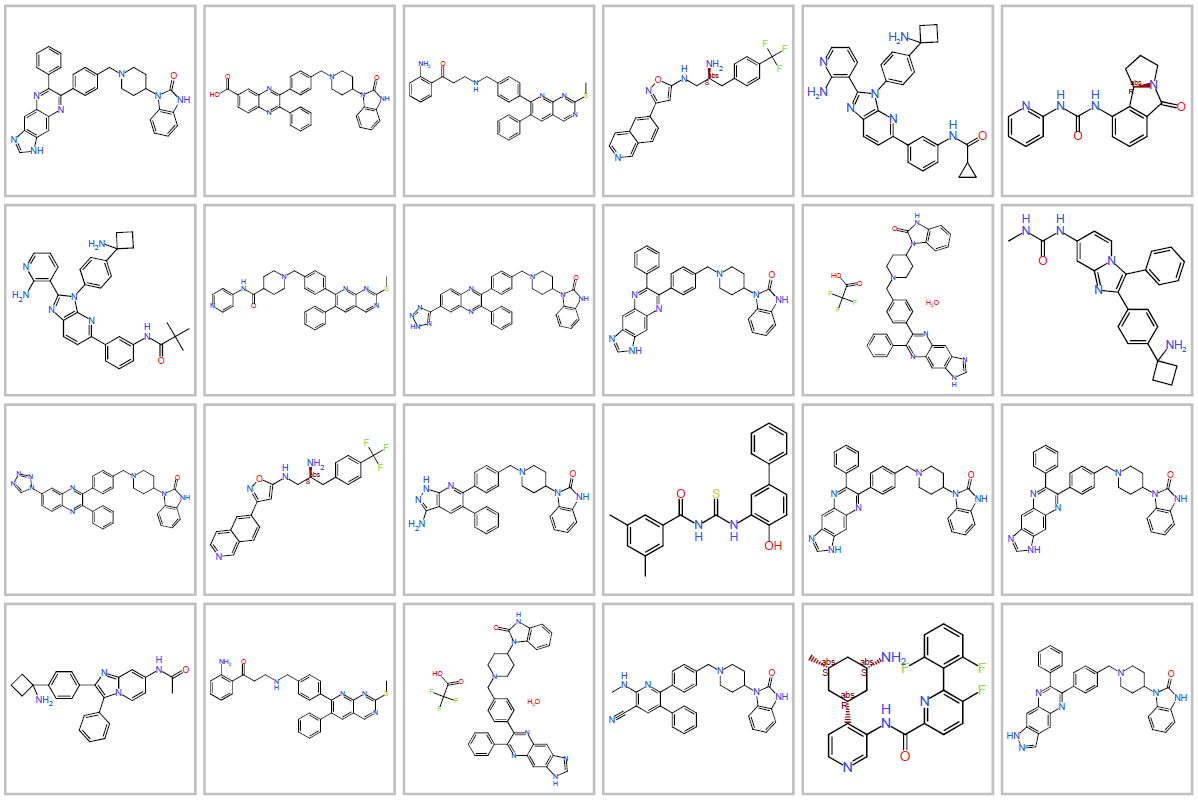
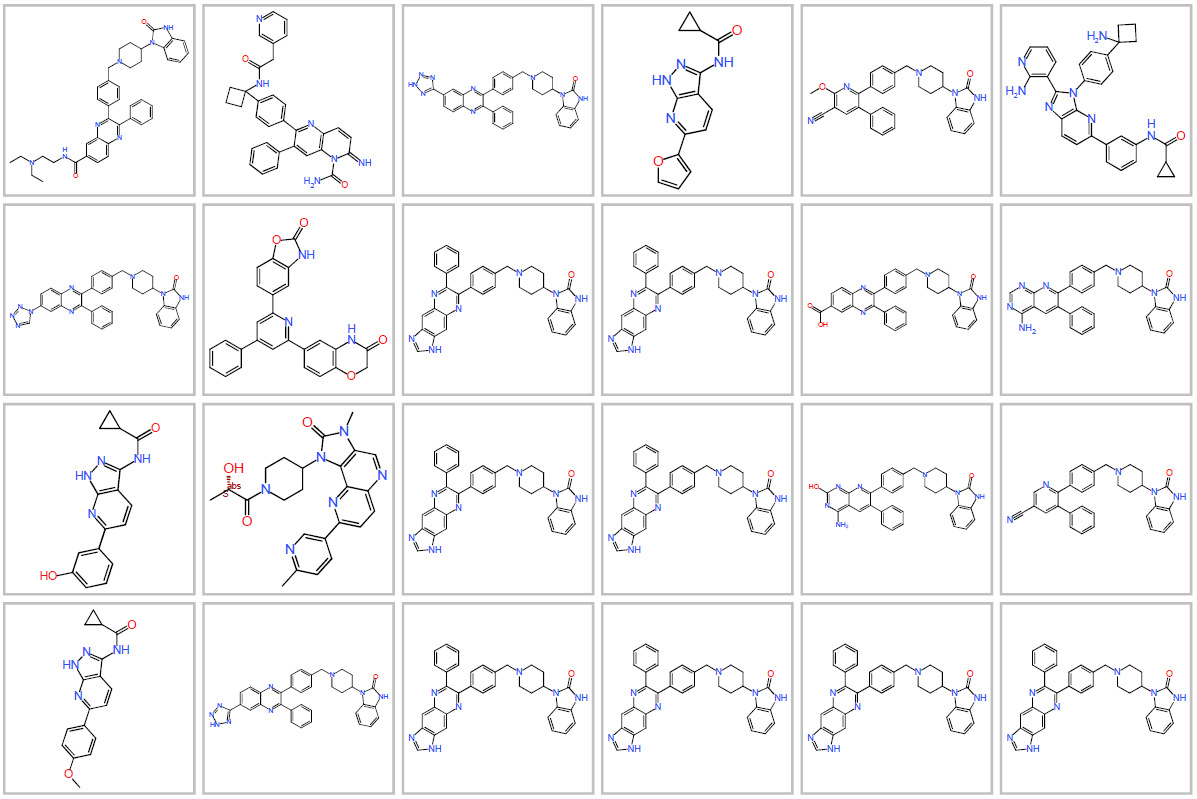
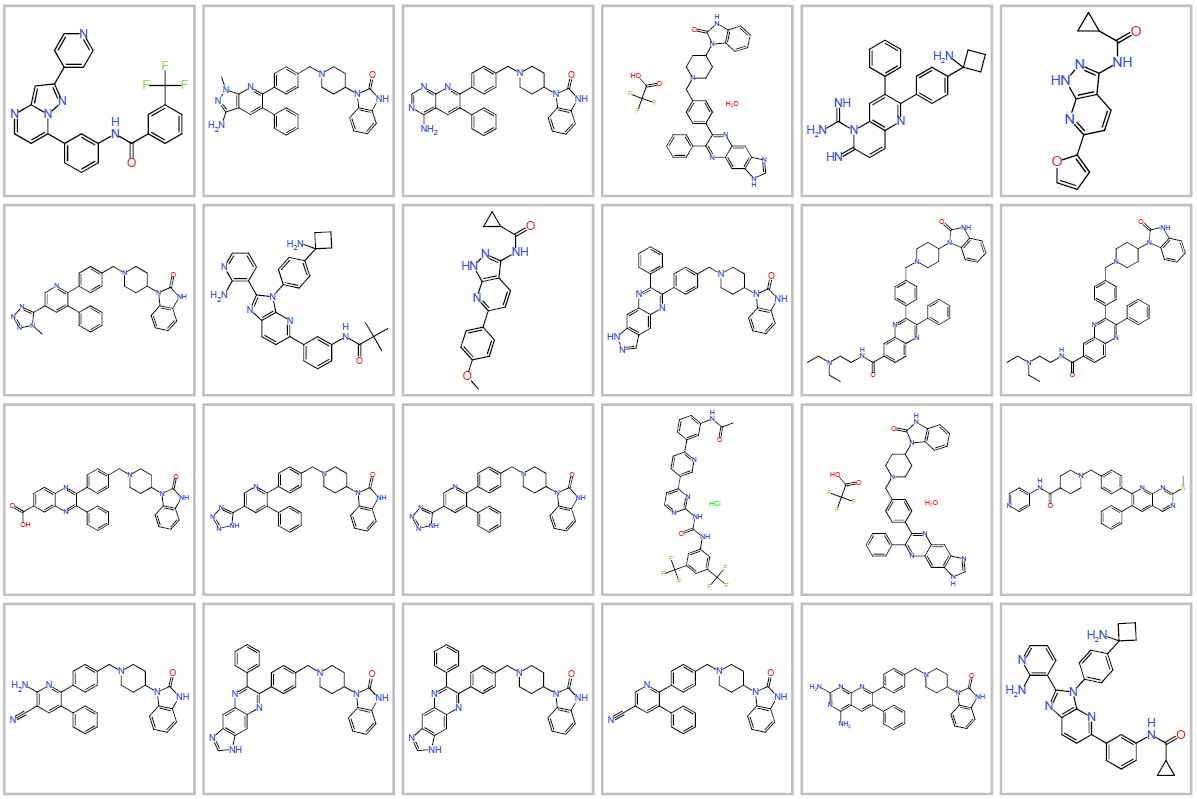
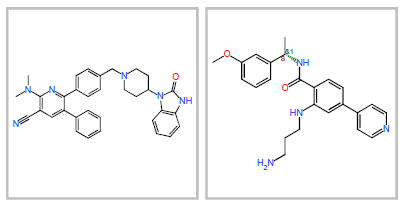
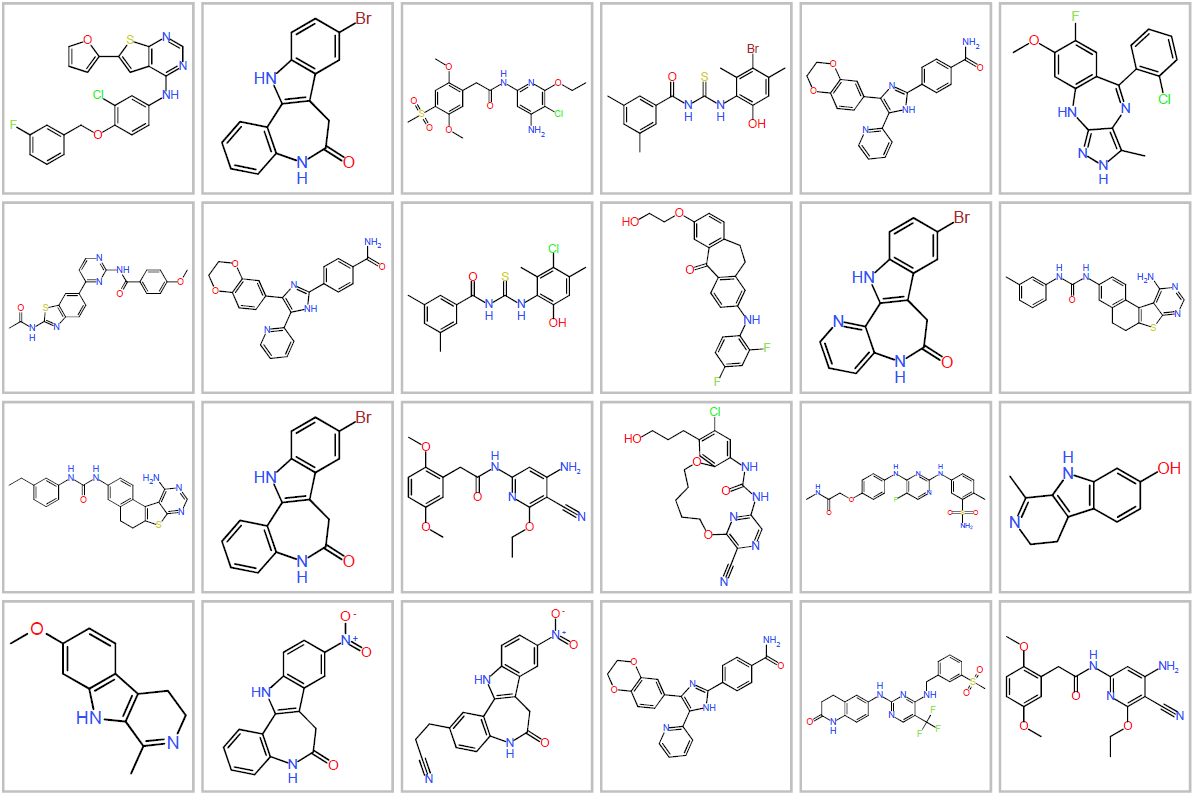
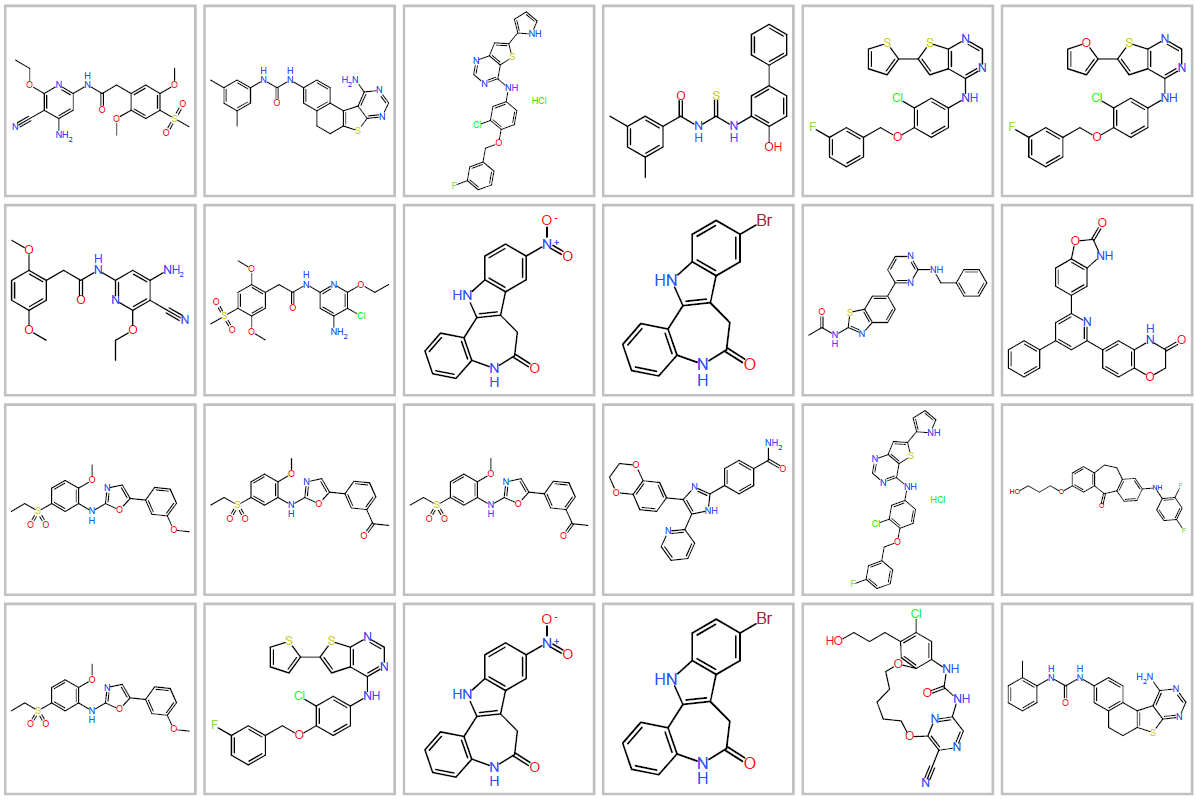
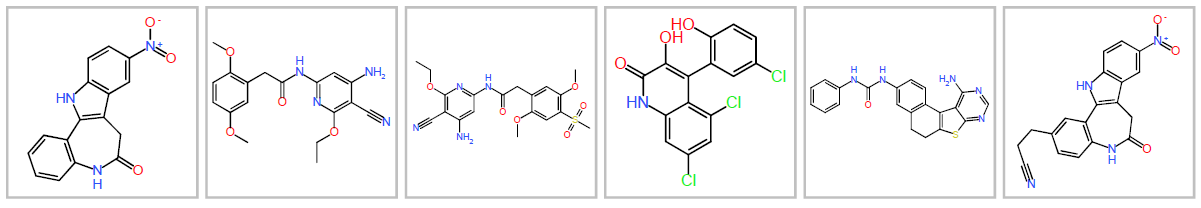
    

Figura S3.3. Structures with a Tanimoto coefficient of 0.6 for series D using FragFp and PathFp.

FragFp

PathFp

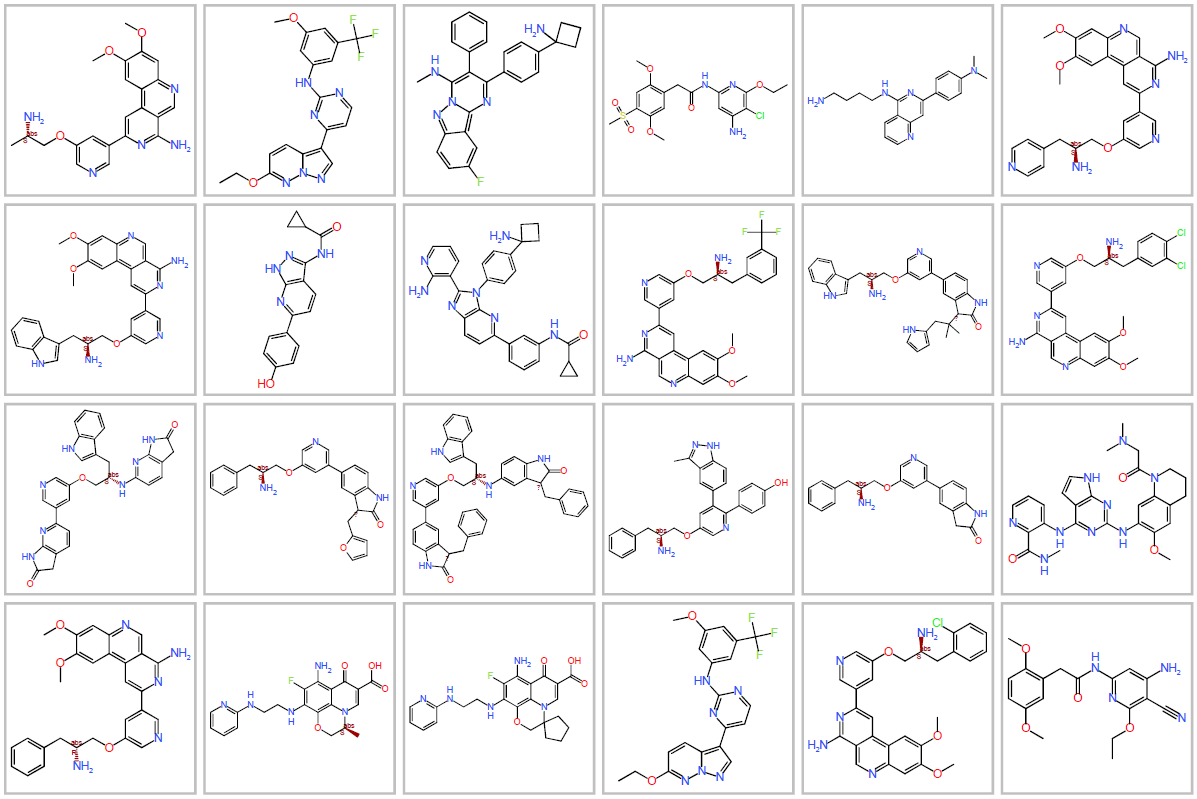
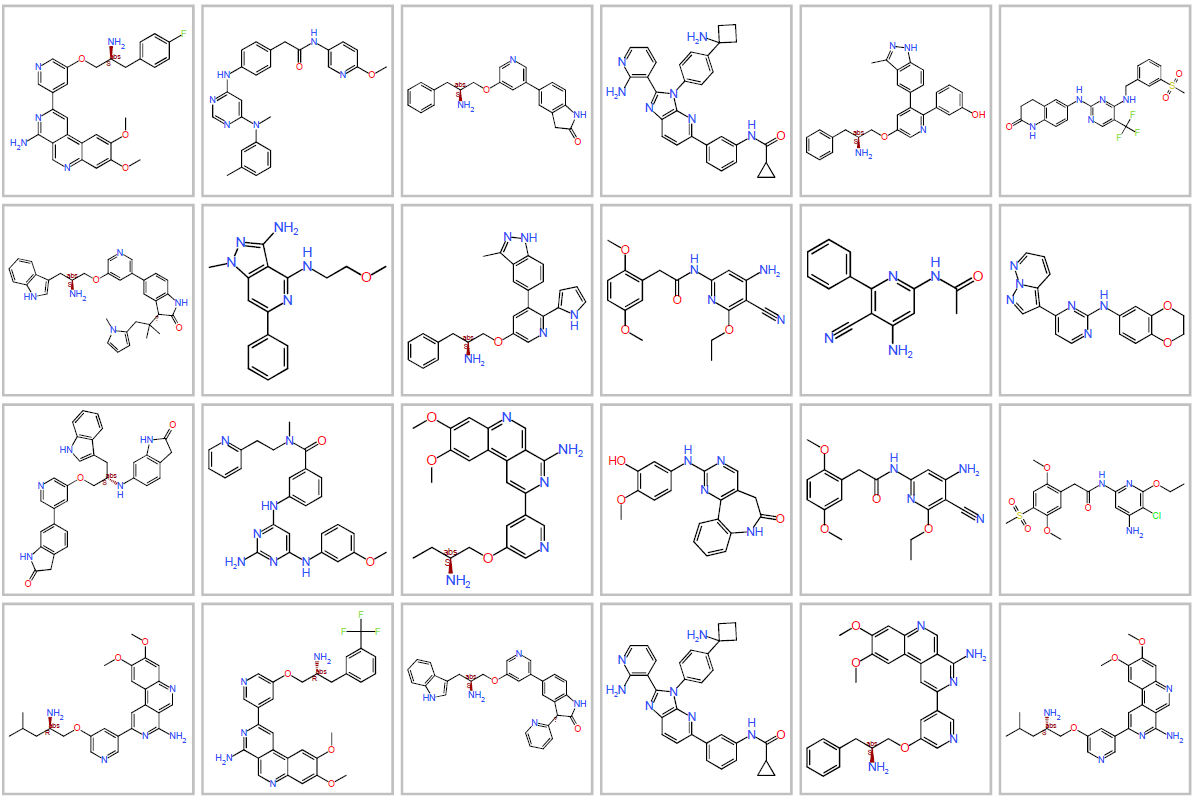
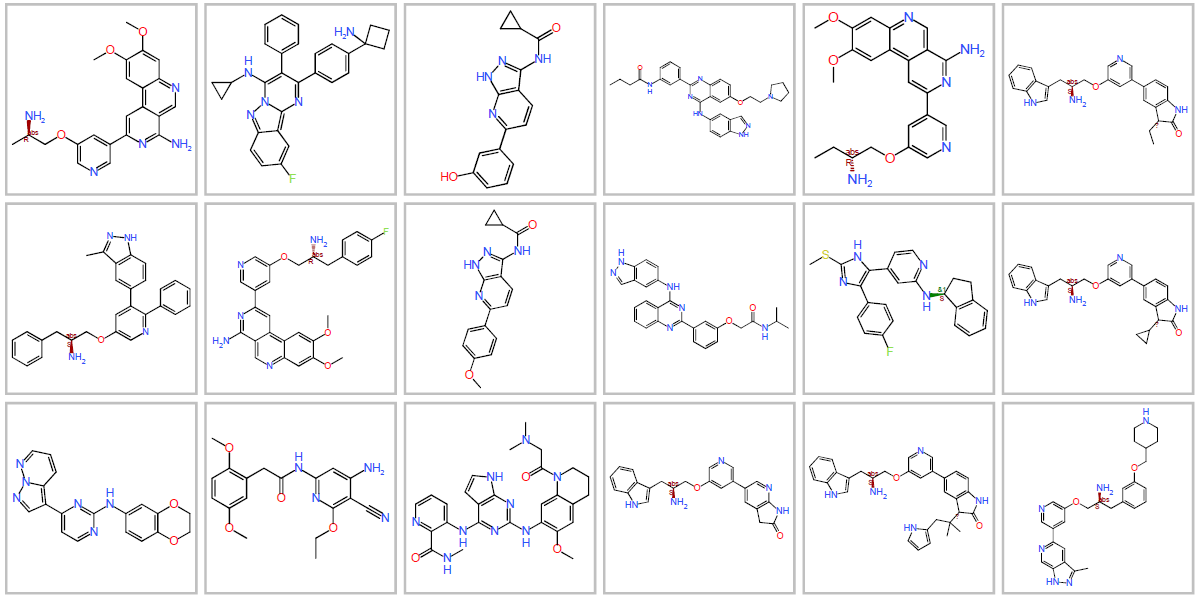
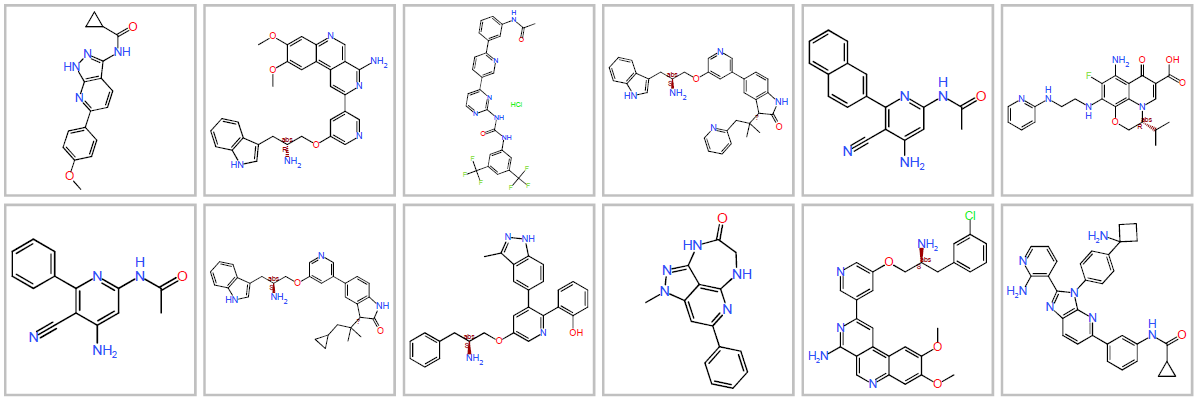
   

Figura S3.4. Structures with a Tanimoto coefficient of 0.6 for series E using FragFp and PathFp.