

Figure 10 Additional file 2.1 Randomly selected structures generated by the canonical Prior.

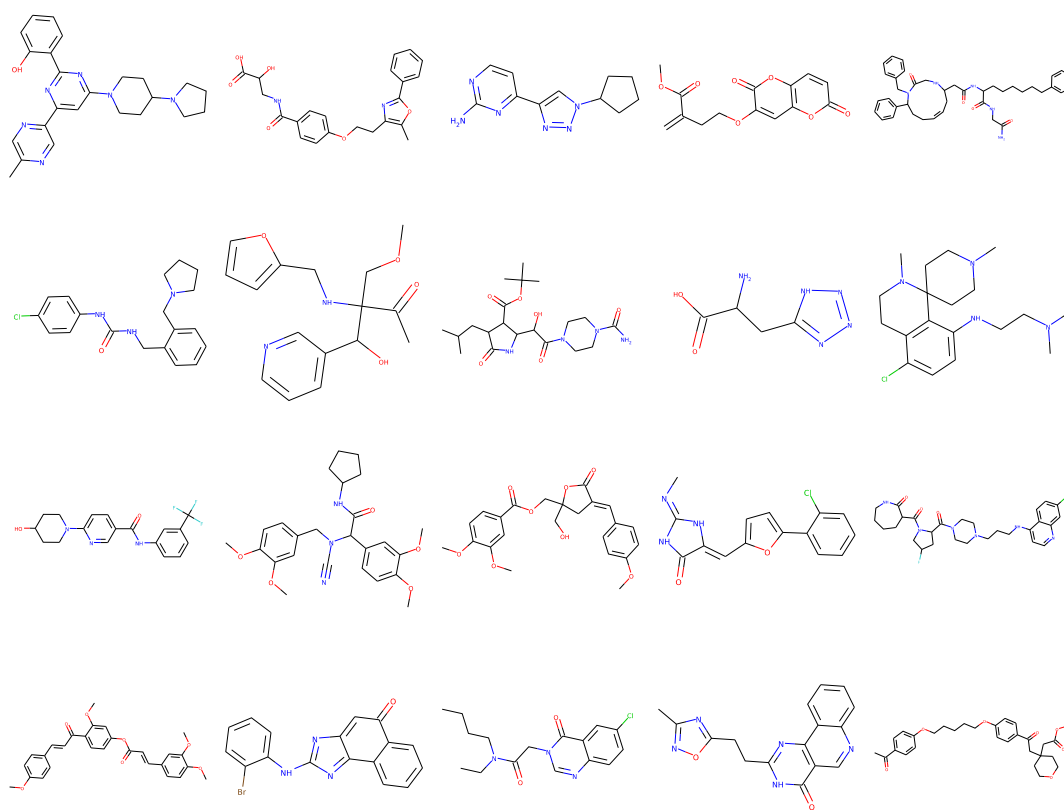


Figure 11 Additional file 2.2 Randomly selected structures generated by the Agent trained to avoid sulphur.

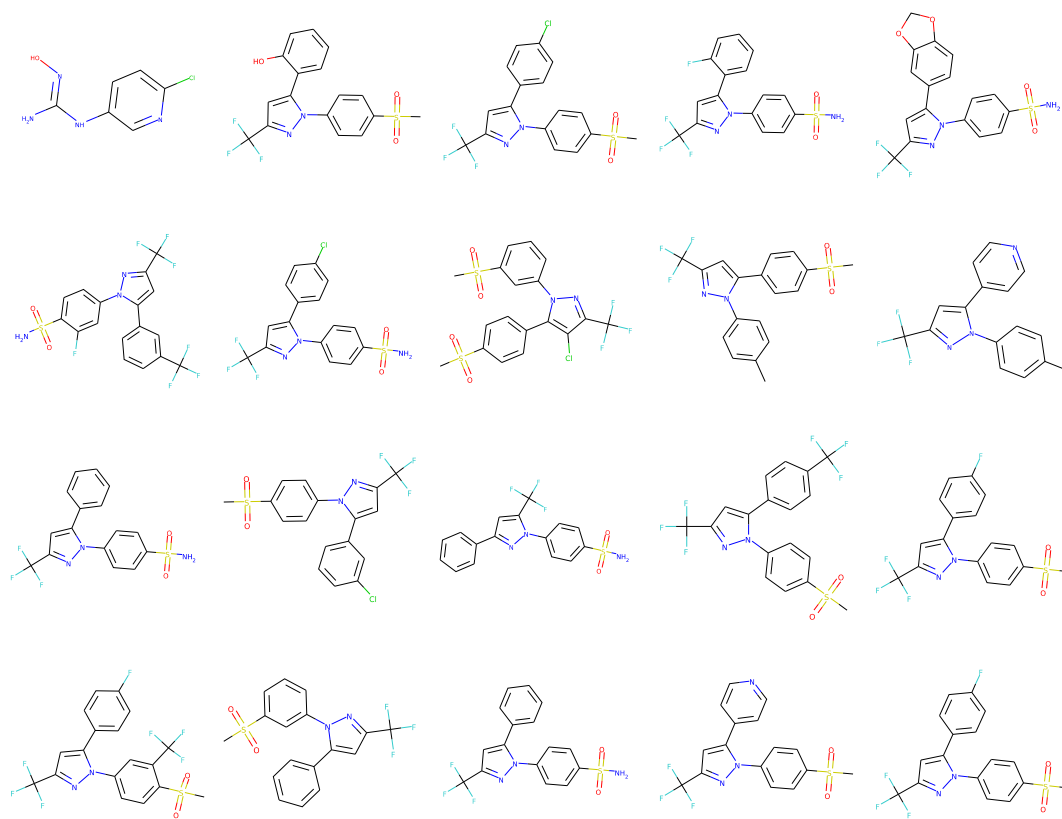


Figure 12 Additional file 2.3 Randomly selected structures generated by the Agent based on the reduced Prior trained to design analogues of Celecoxib.

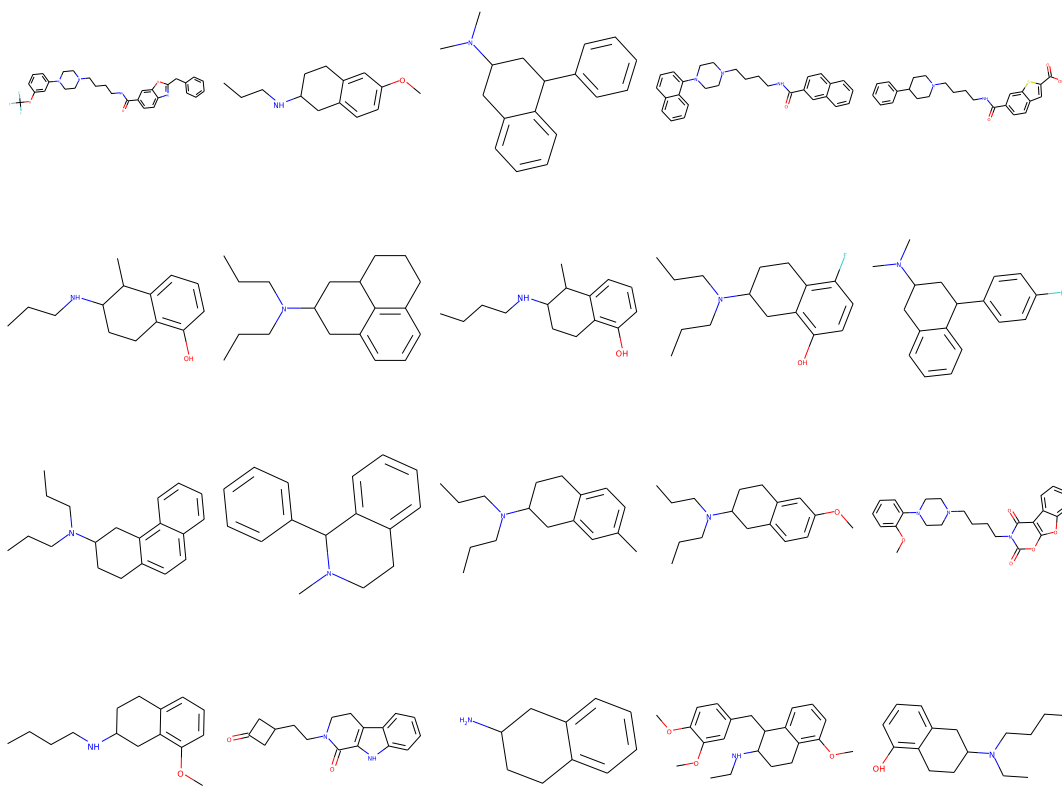


Figure 13 Additional file 2.4 Randomly selected structures generated by the Agent based on the reduced Prior trained to design actives against DRD2.