GC2 DOI Abstract

Title: Drug Design Data Resource Grand Challenge 2 Dataset: Farnesoid X Receptor
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The Farnesoid X receptor (FXR) dataset, contributed by Roche, comprises 36 co-crystal structures of FXR with chemically varied ligands, one apo structure, and 102 IC50s measured with a Scintillation Proximity Assay. Among these compounds, 96 belong to four chemical series (benzimidazoles, isoxazoles, spiros and sulfonamides) and six are classified as miscellaneous. For 92 of the compounds, IC50 values range from 0.000335 to 62.37 μM, while the remaining ten IC50s are greater than 100 μM. Some of the compounds were synthesized as racemates, diastereomers and epimers, as noted within the dataset. The 37 co-crystal and apo structures have resolutions ranging from 1.8 to 2.6 Å and contain representatives from each of the four chemical series.