

## Supporting Information Material

# Pharmacophore-based discovery of FXR-agonists. Part I: Model development and experimental validation

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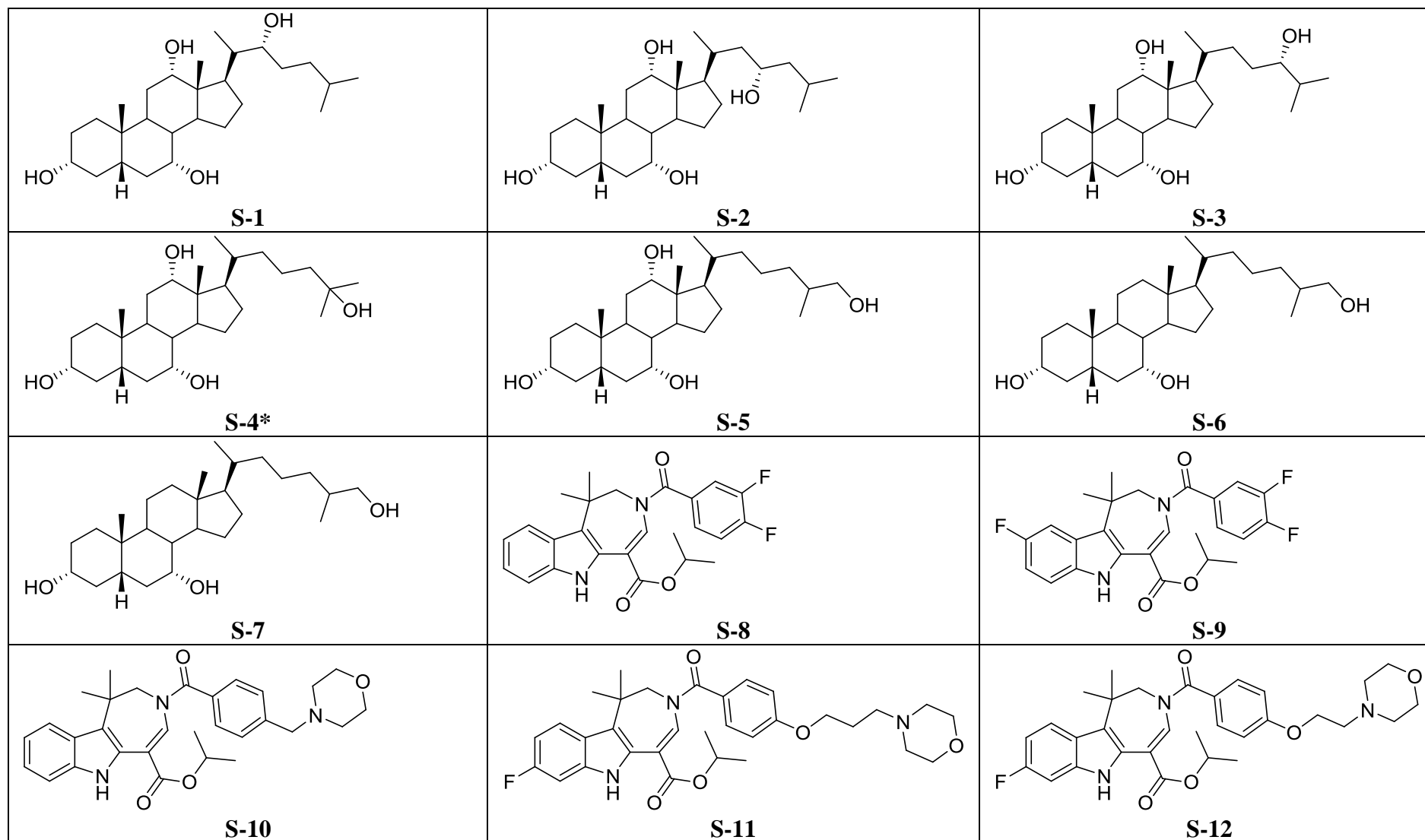
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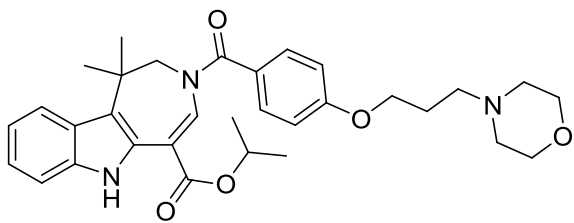
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## Supporting references (FXR ligand sources in the ChEMBL database): <sup>1-16</sup>

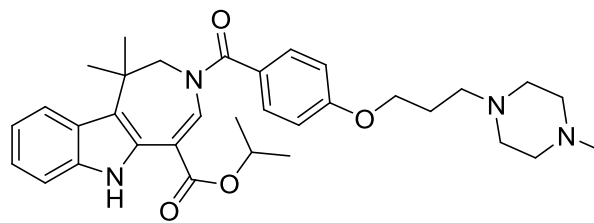
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**Chart S-1.** FXR ligands from recent literature used for theoretical model validation.

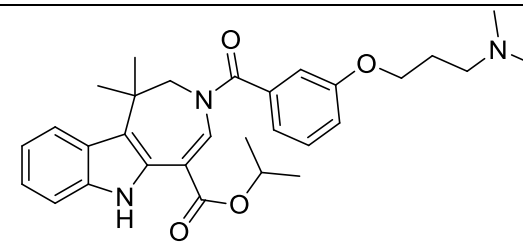




**S-13**



**S-14**



**S-15**

\* **S-4** was not recognized by the FXR pharmacophore model collection.