## **Supporting Information**

Combined Data-driven and Mechanism-based

Approaches for Human-Intestinal-Absorption

Prediction in Early Drug-Discovery Stage

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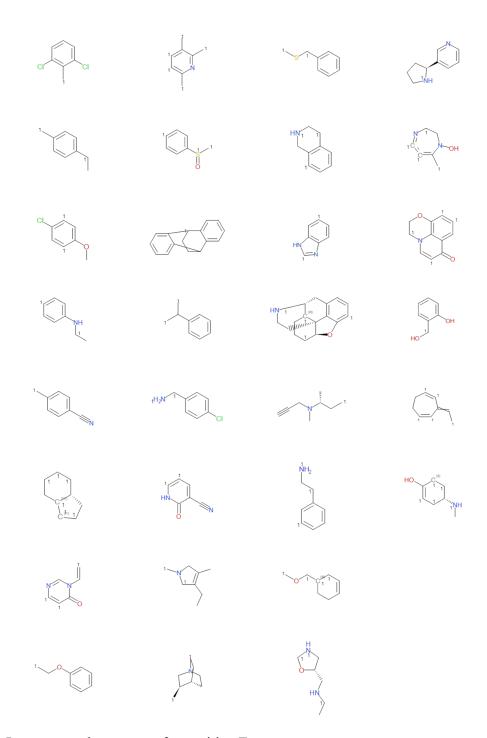


Figure S1 Important substructures for positive Fa

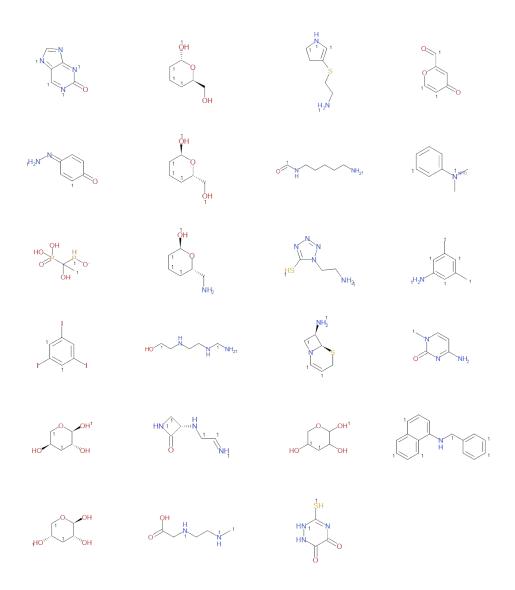


Figure S2 Important substructures for negative Fa