

PK-DB 2.0: An Open Pharmacokinetics and Pharmacodynamics Database for Pharmacometric Modeling, AI, and Digital Twins



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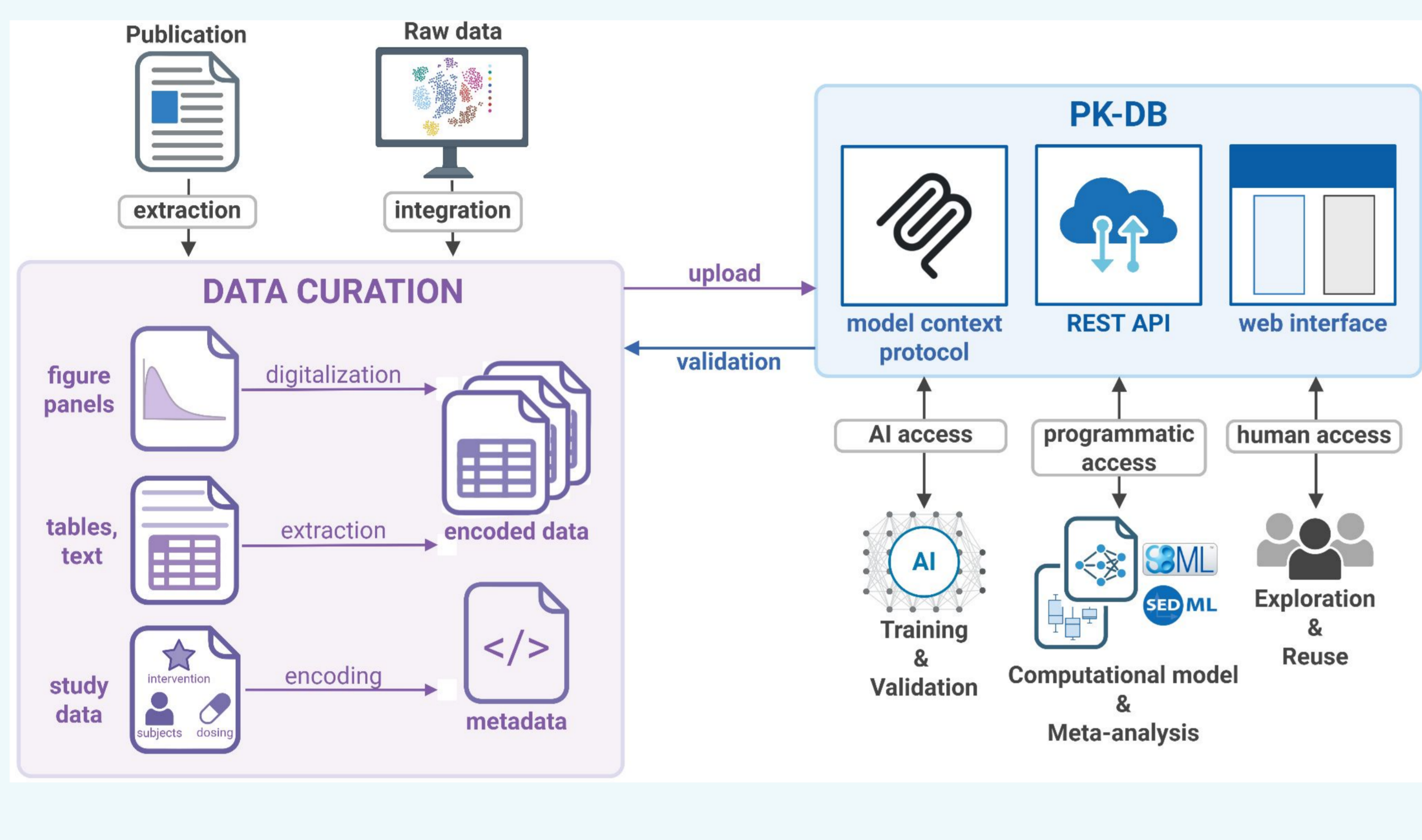
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1. BACKGROUND

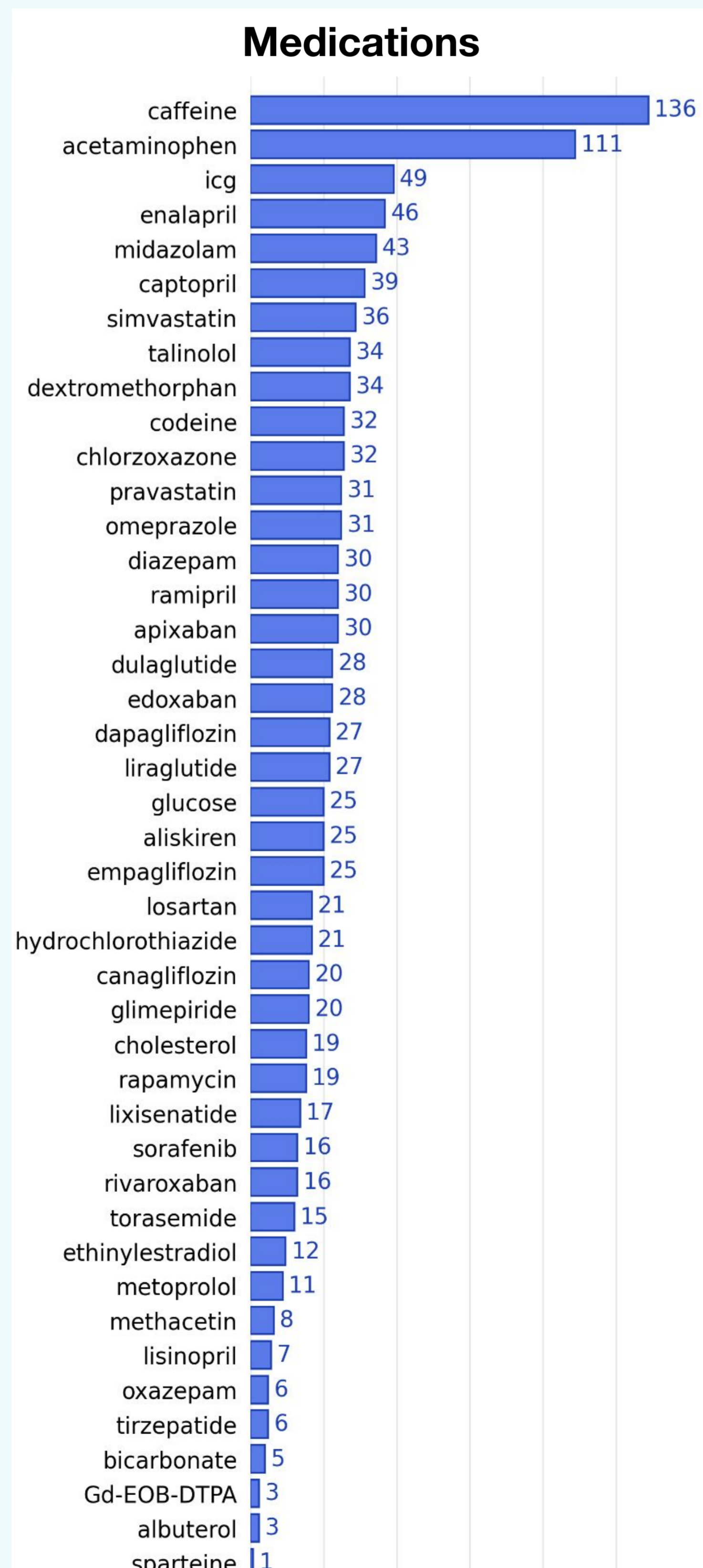
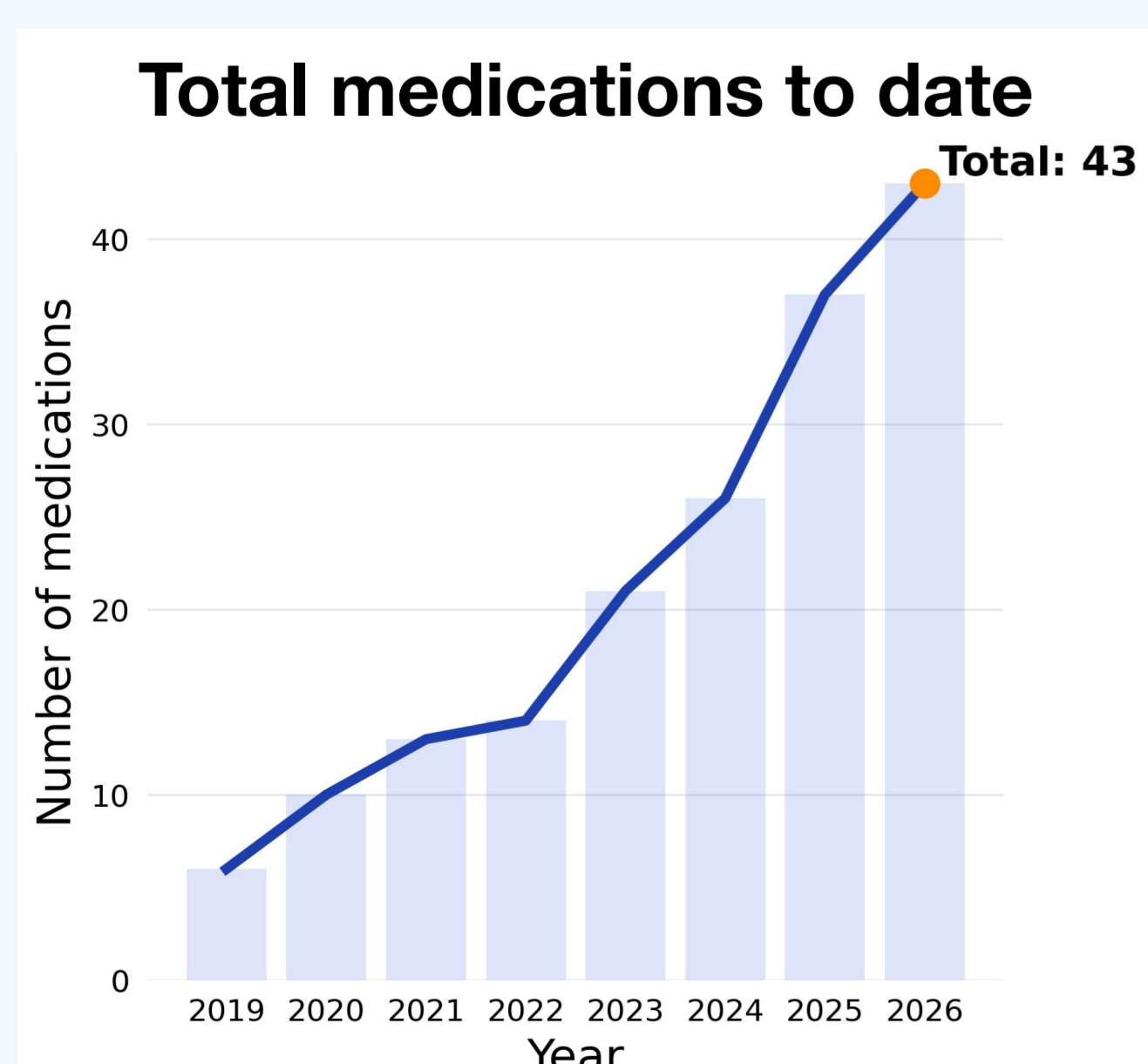
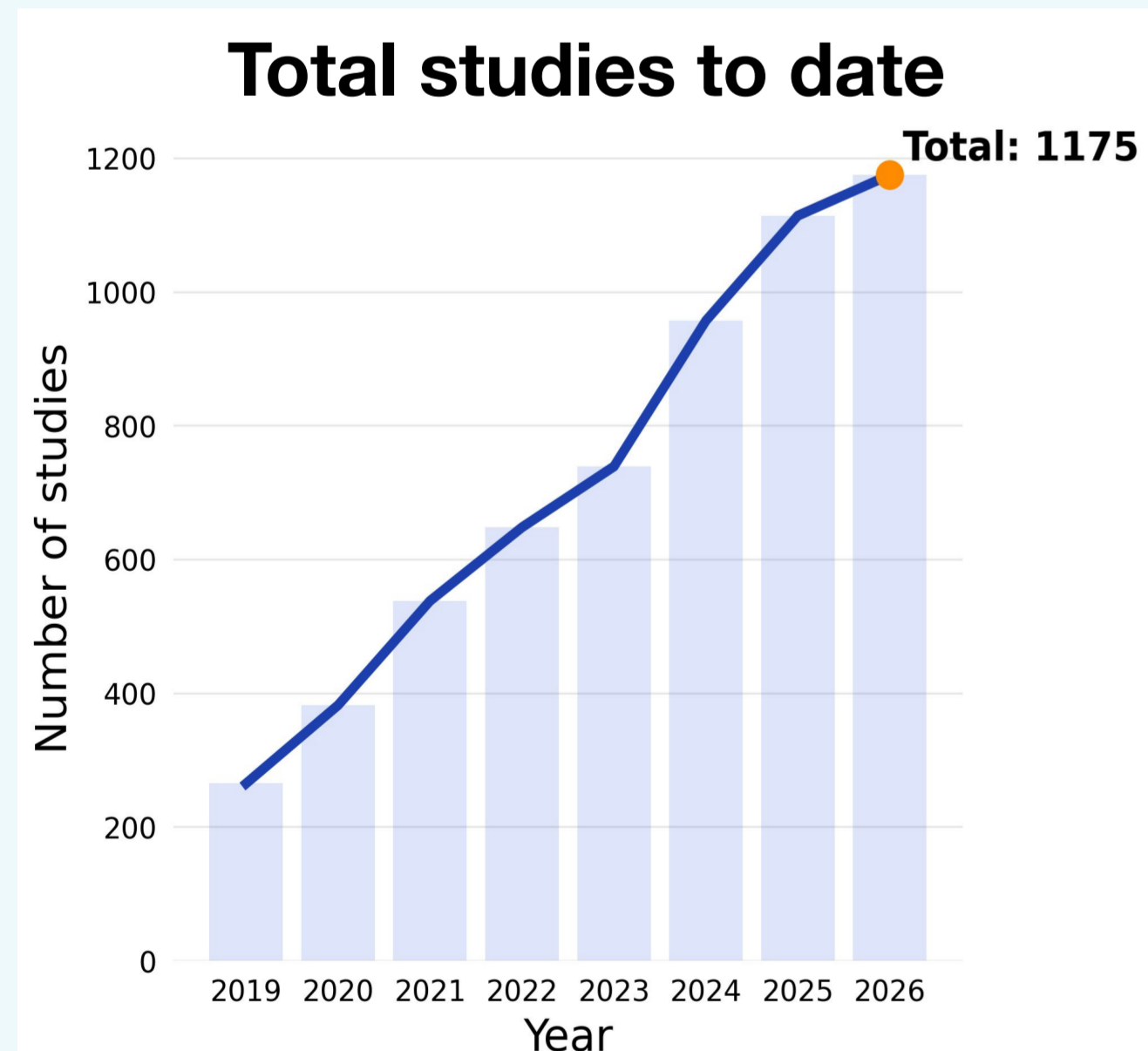
PK-DB 2.0 aims to provide an **open, standardized, and computationally accessible PK/PD platform** tailored to pharmacometric modeling, automated workflows, artificial intelligence, and digital twin development, with a focus on data quality, interoperability, and machine-readability [1,2].

2. METHODS



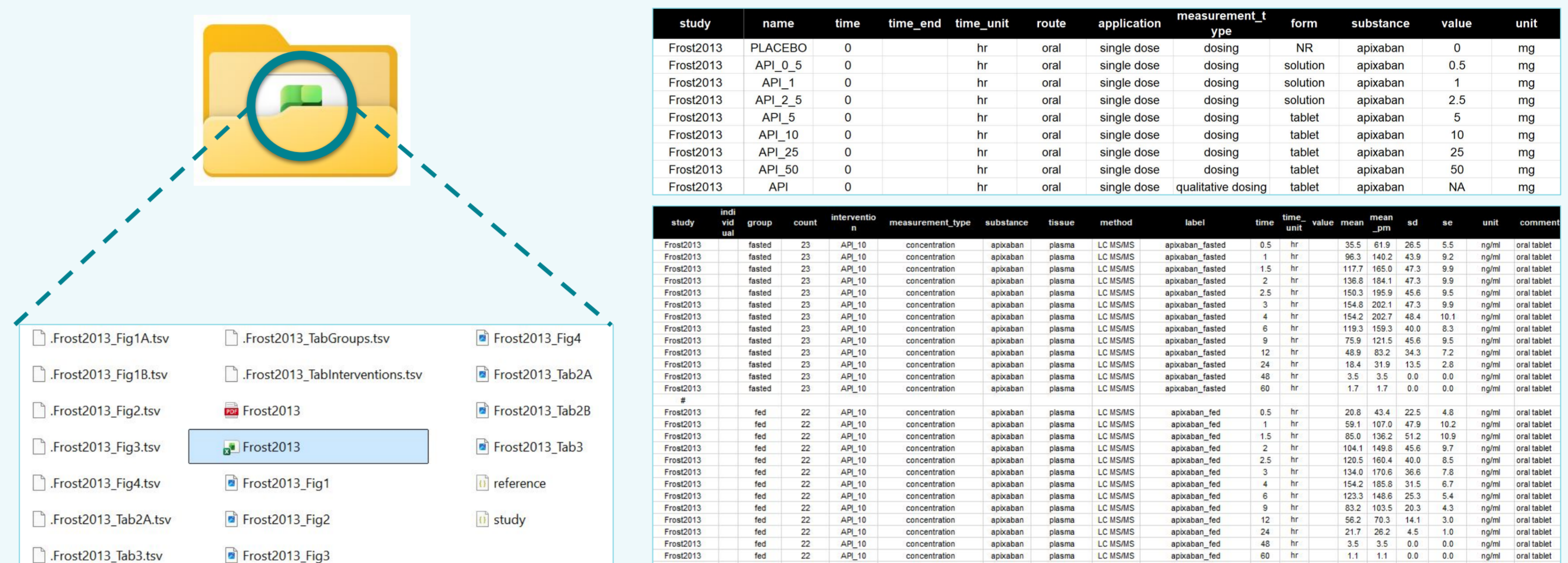
3. RESULTS

Overview of the database structure and its evolution over time. PK-DB 2.0 contains 1175 studies focused on 43 medications. Curated data describes their pharmacokinetics, pharmacodynamics, and drug-drug interactions.



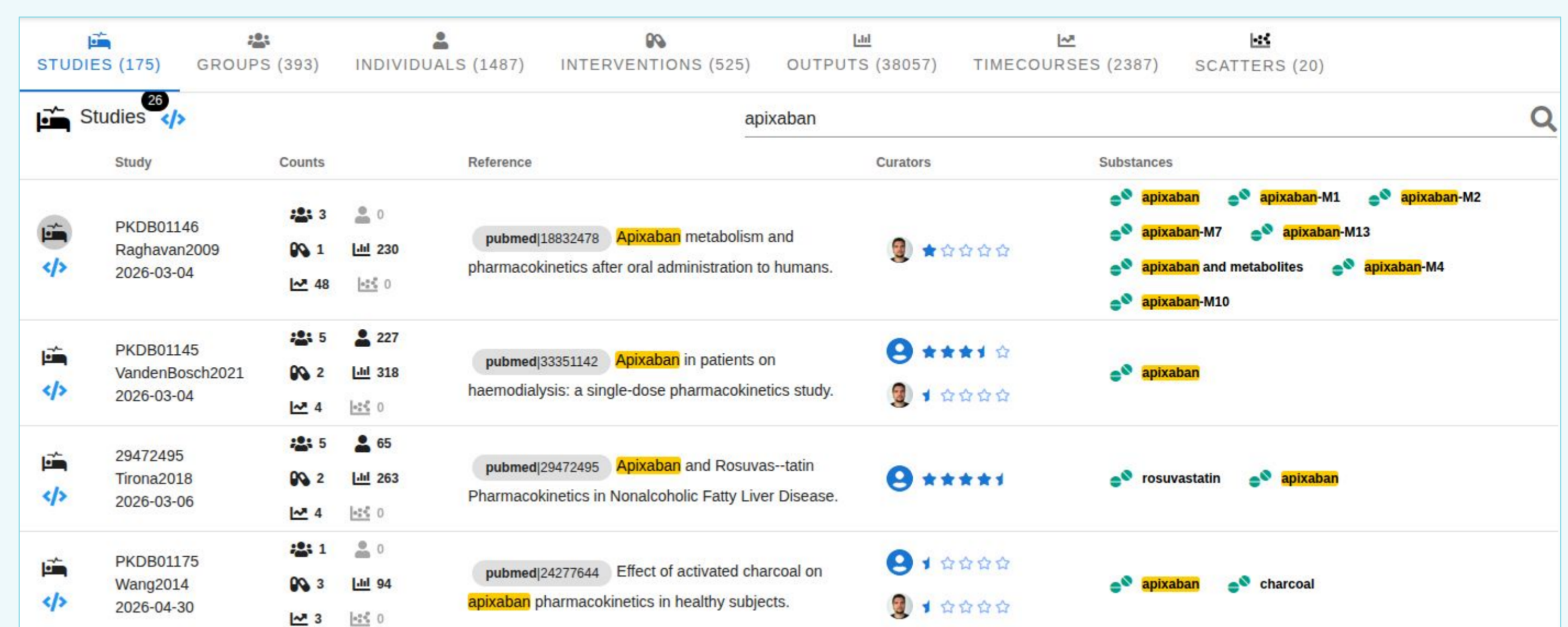
4. EXAMPLE

Data curation



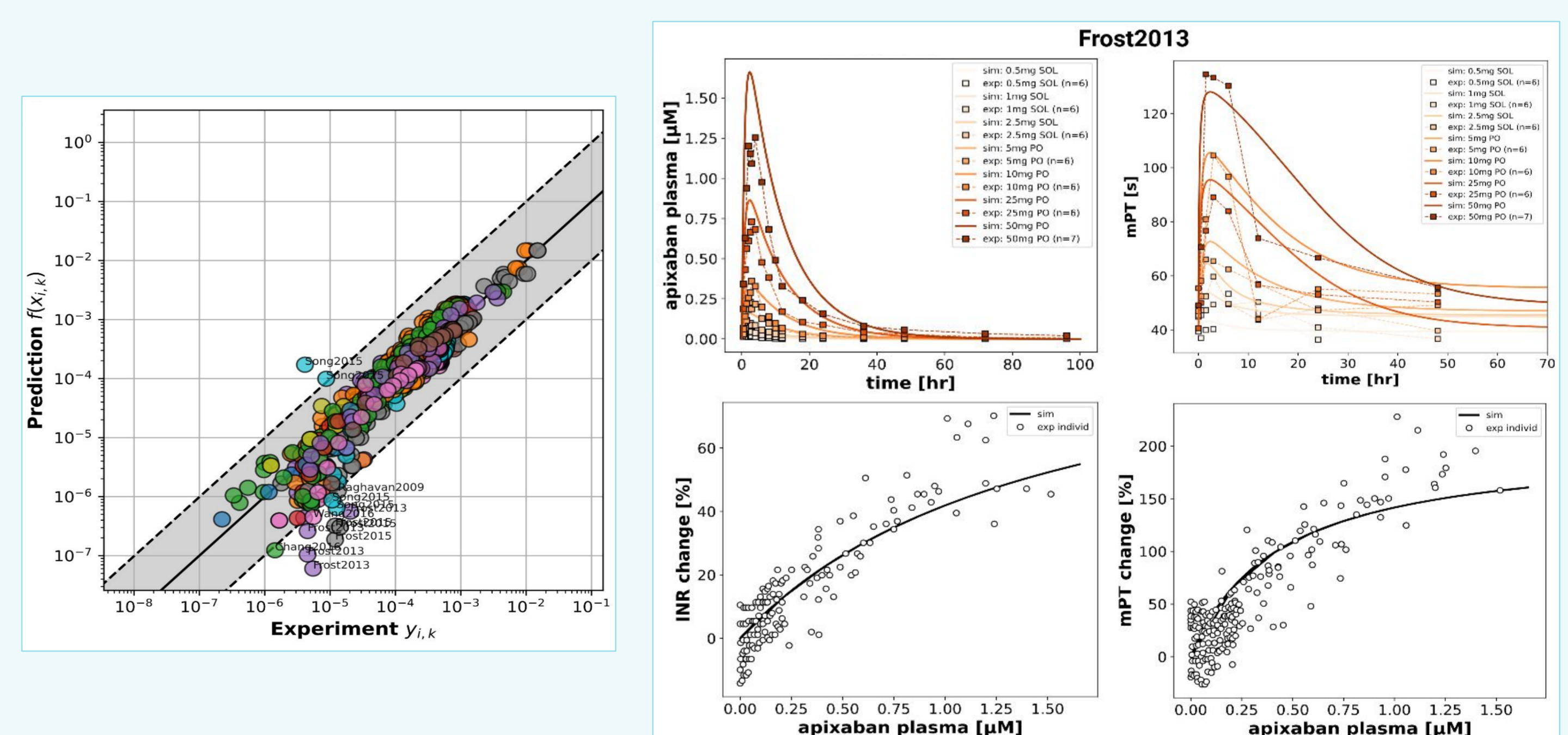
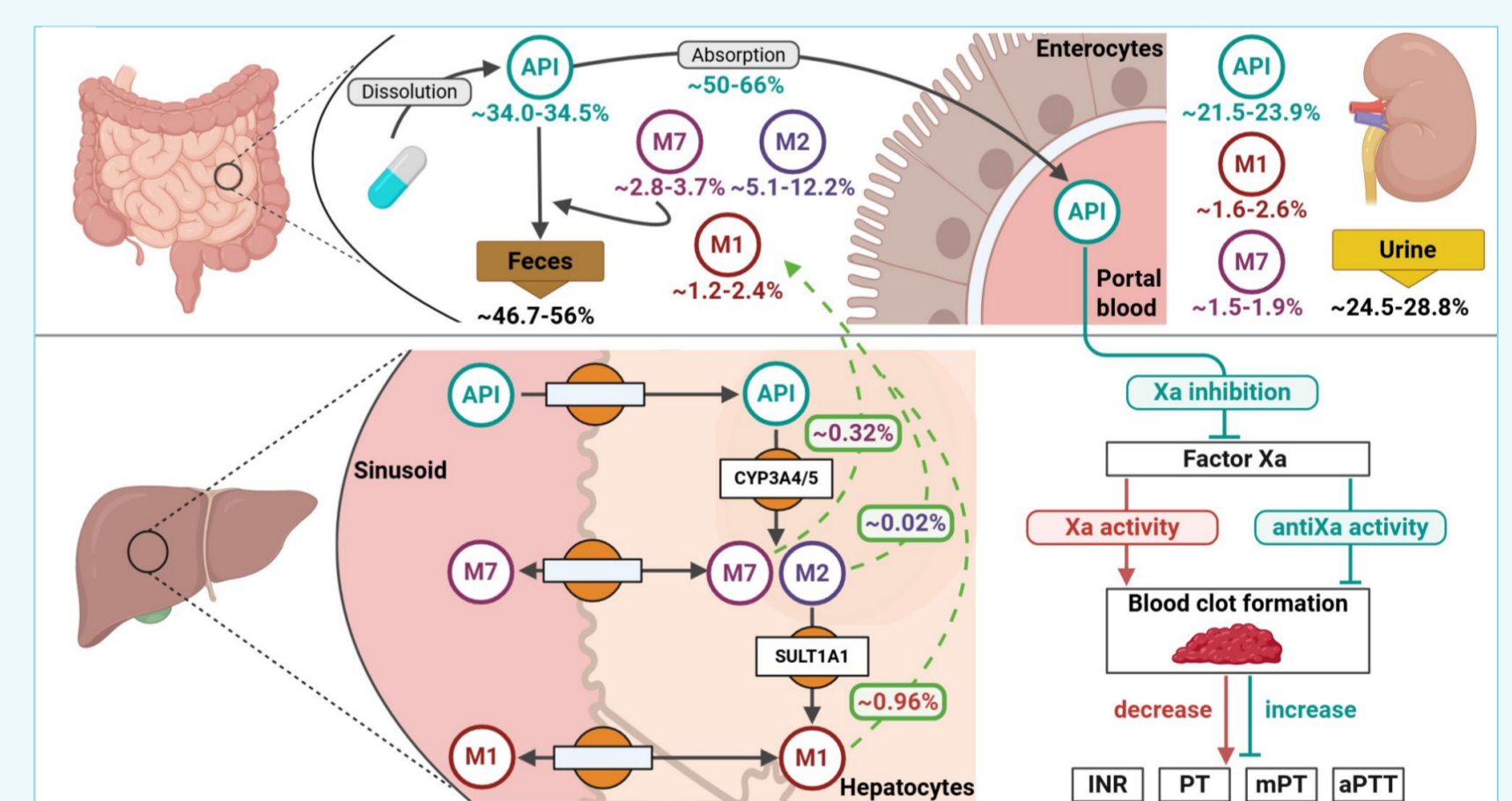
Example of curated study. Folder structure and encoded intervention and pharmacokinetic/pharmacodynamic data [3].

PK-DB web interface



PK-DB usage in model development

PBPK/PD model of apixaban. Model structure (on the right) and usage of the apixaban data from PK-PD database for model optimization and evaluation (below) [4].



5. CONCLUSIONS

PK-DB 2.0 provides a unified, machine-readable PK/PD data infrastructure for modern pharmacometrics. By combining rigorous curation, standardized representation, and explicit AI integration through a dedicated MCP server, the platform supports reproducible model development, cross-study analyses, and next-generation AI- and Digital Twin-enabled decision support.

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