Asclepius – A Custom GPT for Open Systems Pharmacology

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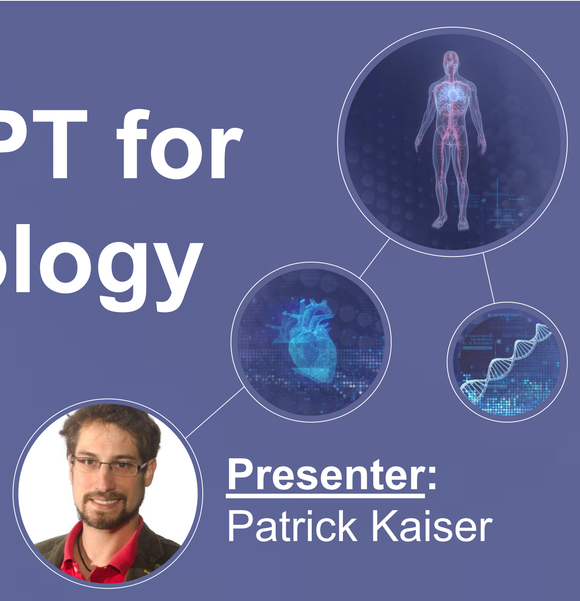

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Introduction

Asclepius is a custom GPT "chatbot" to support Physiologically Based (PB) Pharmacokinetic (PK) and Pharmacodynamic (PD) modeling with the Open Systems Pharmacology (OSP) suite. It provides expert guidance on PK-Sim®, MoBi®, and the R packages ecosystem, generating answers from the official OSP documentation and the GitHub forum knowledge base.

Methods – Context engineering

What is context engineering? It's the practice of shaping what the model "sees" at answer time — by curating trusted sources, retrieving only the most relevant passages, and prompting the model to cite them — to maximize accuracy, reproducibility, and user trust. In **Asclepius**, context engineering aligns the model with OSP usage: scope the task, retrieve authoritative snippets, and answer with sources. This reduces hallucinations, keeps answers tool-specific (PK-Sim/MoBi/R packages), and makes outputs reproducible.

How it works (high level). We maintain a curated corpus (official docs, tutorials, release notes, forum Q&A, key GitHub repos). At question time, **Asclepius** performs retrieval-augmented generation (RAG): it selects the most relevant passages and injects them into the model's working context, then produces a concise, cited answer. Lightweight metadata (tool, version, doc type) helps disambiguate similar topics and keeps responses scoped to the user's task.

Why we need it for OSP. OSP's breadth and depth make free-form search inefficient; critical instructions often live in specific sections of the docs or in forum threads. Context engineering converts that dispersed knowledge into a reliable, auditable answer stream—so modelers can focus on modeling rather than documentation hunting.

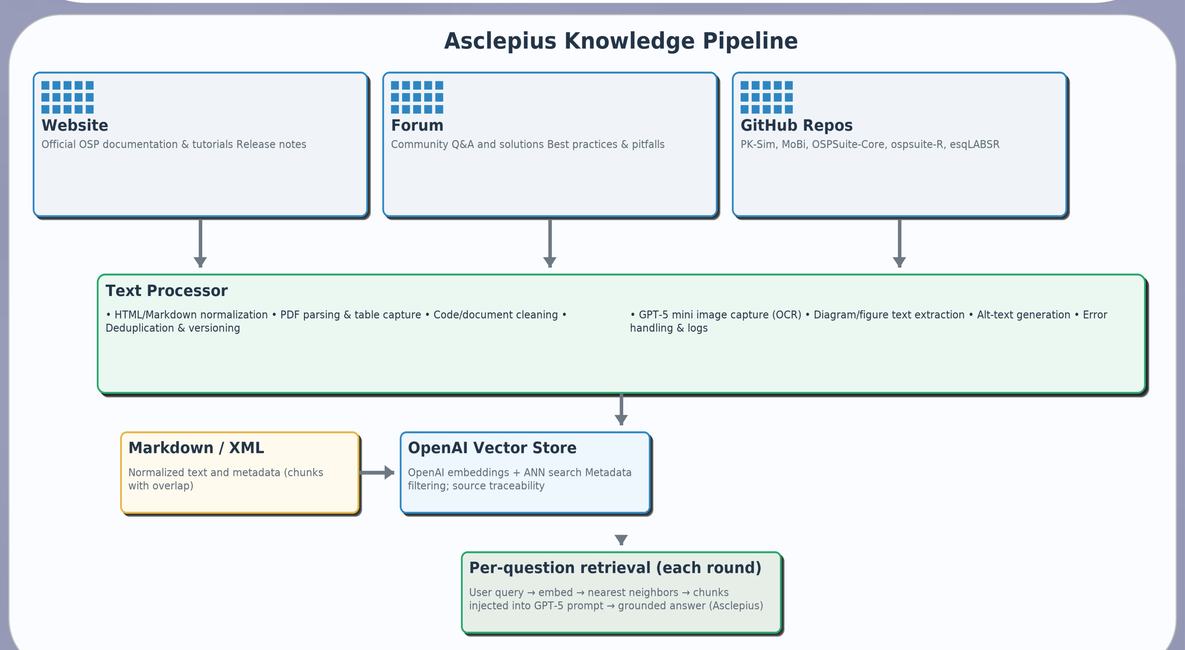

Figure 1: Context pipeline – sources → parsing/OCR → chunking/metadata → embeddings → vector store → RAG with GPT-5.

Usage

Scan the QR-Code to connect with Asclepius >>

Follow these guidelines to get the best results when using Asclepius:

- Formulate clear, specific prompts. Focus on one task at a time (e.g., model setup, parameterization, simulation).
- Provide all necessary context. For PK/PD workflows, mention the OSP tool (PK-Sim, MoBi, ospsuite-R, Reporting Engine).
- Request structured outputs. Ask for step-by-step instructions, tables, or lists if needed.
- Use the assistant for documentation-supported tasks only. If the information is missing, Asclepius will indicate it.
- Keep prompts concise and professional. Avoid unnecessary details or unrelated topics.

Asclepius: Domain-Tuned GPT for PBPK/QSP Workflows

Figure 3: Access Asclepius via QR

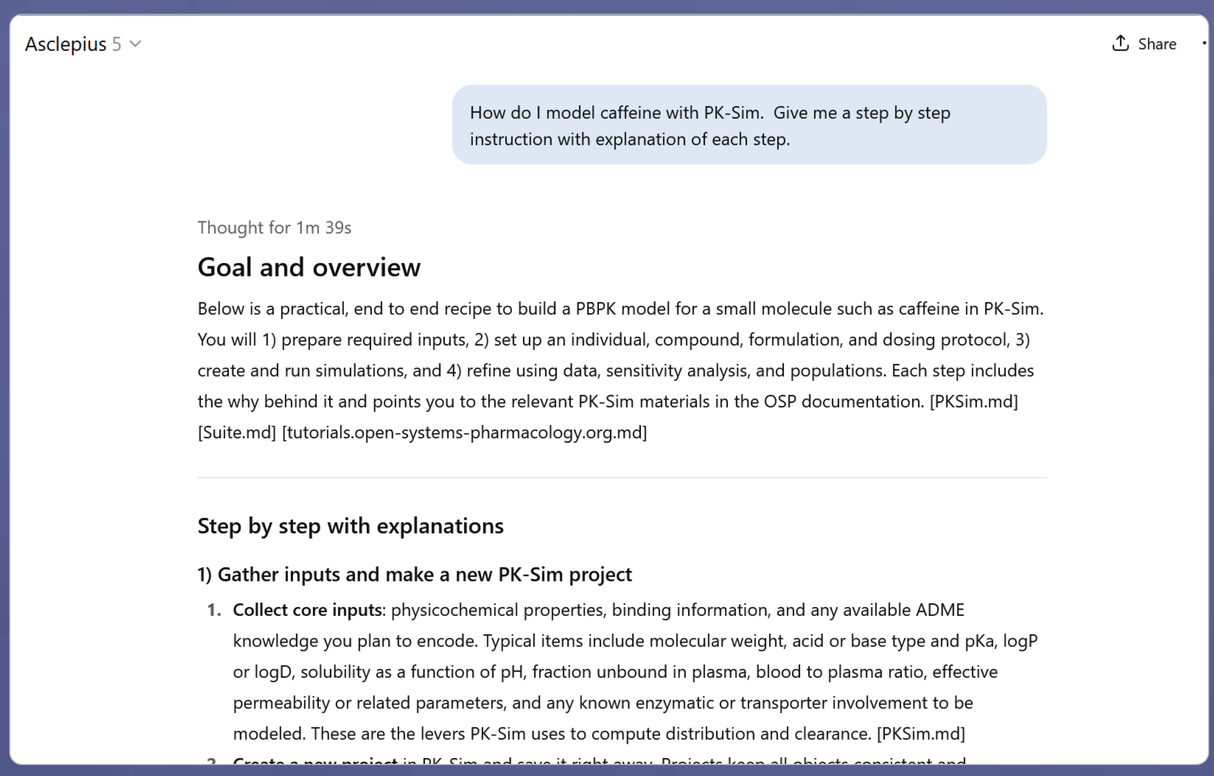

Figure 2: Asclepius in ChatGPT – structured answer grounded in OSP documentation.

Conclusion & Outlook

Today. Asclepius combines GPT-5 with an audited OSP knowledge base to deliver accurate, cited guidance and reproducible R code for typical PK/PD and PBPK/QSP workflows.

Next. Extensions of this approach include **autonomous researcher agents** that can query public biomedical resources (e.g., PubMed, Europe PMC, ChEMBL, DrugBank, ClinicalTrials.gov) to surface literature-derived model parameters and related evidence for OSP tasks — always with provenance and citations. Likewise, **internal AI assistants** can be built to provide governed access to organizational knowledge bases and documentation (e.g., policies, SOPs, templates, code examples).

Together, these applications illustrate how domain-tuned assistants can expand evidence-seeking beyond OSP documentation, keep analyses auditable via source-linked outputs, and accelerate onboarding while standardizing best practices across projects.

Modeling Scaling Coding

Supporting the open-source development of:
PK-Sim® MoBi® OSP Open Systems Pharmacology Software Suite
www.open-systems-pharmacology.org

Presented at OSPCC 2025, Paris, France;

www.ESQlabs.com