

Supplementary Data Tables

The supplementary tables below summarize the results of our manuscript’s systematic analysis of 28 AI use cases in drug discovery. The original anonymized data table where the summarized results come from is also provided in the supplementary material of this manuscript in a csv file format.

Table S1: AI Use Cases Requiring Multiple Model Deployments.

The table shows the distribution of 28 identified AI use cases based on whether they require the deployment of more than one model.

No	9	32.1%
Yes	17	60.7%
I do not know	1	3.6%
N/A	1	3.6%
TOTAL	28	100.0%

Table S2: Distribution of AI Use Cases by Drug Discovery Phase

The table breaks down the 28 identified AI use cases by whether they primarily focus on the preclinical phase of drug discovery.

Yes	18	64.3%
No	10	35.7%
TOTAL	28	100.0%

Table S3: Expected End-User Impact of AI Use Cases

The table categorizes the 28 AI use cases based on whether they are expected to impact less than 50 end users.

Yes	19	67.9%
No	9	32.1%
TOTAL	28	100.0%

Table S4: Computational Requirements for AI Use Cases (GPU/CUDA)

The table categorizes the 28 AI use cases based on whether they need CUDA drivers, which indicates a requirement for GPU access.

Yes	11	39.3%
No	15	53.6%
I do not know, N/A	2	7.1%
TOTAL	28	100.0%

Table S5: Model Re-training Requirements for AI Use Cases

The table shows the distribution of the 28 AI use cases based on the anticipated need for frequent or automated model re-training.

Yes	18	64.3%
No	8	28.6%
I do not know, N/A	2	7.1%
TOTAL	28	

Table S6: Input Data Modalities Required by AI Use Cases

The table illustrates the variety of input data modalities (tabular, image, text, molecules) required by the 28 AI use cases.

Image	5	17.9%
Tabular	14	50.0%
Text	5	17.9%
Molecules	1	3.6%
tbd, N/A	3	10.7%
TOTAL	28	100.0%

Table S7: Programming Languages Used for Model Development

The table shows the distribution of programming languages (Python, R, MATLAB) used to develop the models for the 28 AI use cases.

Python	15	53.6%
R	9	32.1%
MATLAB	1	3.6%
tbd	3	10.7%
TOTAL	28	100.0%