Use of Artificial Intelligence in Drug Development

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Purpose:

The purpose of this study was to investigate the potential of artificial intelligence (AI) in streamlining pharmacokinetic (PK) non-compartmental analysis (NCA) and data cleaning tasks. The goal was to assess whether AI could enhance efficiency and accuracy in these complex tasks, which traditionally require significant manual effort and expertise.

Objectives:

1. Create an analysis ready dataset for a single dose study
2. Calculate Pharmacokinetic Parameters for each Study
3. Generate Tables, Figures and Listings of Study data

For non-compartmental analysis, samples that are BLQ prior to T_{max} should be set to zero, concentrations that are BLQ after T_{max} should be set to missing.

Methods:

The study employed an AI to tested on a variety of tasks, including data cleaning, pharmacokinetic non-compartmental analysis and data tabulation. The system's adaptability was also assessed by introducing unexpected scenarios and changes in the data structure. The aim was to evaluate how well the AI system could adapt to these changes and continue to perform its tasks effectively.

AI tools evaluated included Chat GPT, Co-pilot, Perplexity, Claude 3.5 Sonnet and Poe

Workflow:

Upload datasets and PK SOP

Set concentrations prior to Tmax to zero and after T_{max} to missing per SOP

Request calculation of PK parameters C_{max}, T_{max}, AUC_{last}, AUC_{inf} and $T_{1/2}$ per SOP

Request TFLs

Example Prompts:

Pharmacokinetic data are contained within the PK merge file. TIME and TIMEU columns represent actual time of the PK sample and the units of time respectively.

For non-compartmental analysis, samples that are BLQ prior to Tmax should be set to zero, concentrations that are BLQ after Tmax should be set to missing

This is my standard operating procedure for calculating pharmacokinetic parameters, can you calculate Cmax,Tmax, AUClast, AUCinf, t1/2 and report lambda z, lambda z lower, labmda z upper, span, Rsq adjusted.

Generate and individual subject pharmacokinetic parameter table

Results:

Example PK Parameter Table

ID	Cmax (ng/mL)	Tmax (hr)	AUClast (ng*hr/mL)	AUCinf (ng*hr/mL)	t1/2 (hr)	Lambda_z (hr^-1)	Lambda_z_lower (hr)	Lambda_z_upper (hr)	Span (hr)	Rsq_adjusted
111-004-2001	6390	1	14856.2	14902.7	2.426	0.2857	4	12	8	0.9959
111-004-2002	3280	1.7	6421.555	6446.165	2.588	0.2679	4	12.3	8.3	0.9947
111-004-2003	7330	1	16569.95	16611.0	2.405	0.2883	4	12	8	0.9985
111-004-2004	4130	1	7041.545	7058.453	2.207	0.3141	4	10	6	0.9993
111-004-2005	6450	1.5	12844.8	12861.613	2.124	0.3264	4	10	6	0.9999
111-004-2006	6010	2	12300.79	12326.377	2.392	0.2898	4	12	8	0.9958

Key Take Aways:

The AI methodology evaluated herein are currently not ready for use for facile and standard NCA analysis. Additional software modification and beta testing is necessary

Prompts need to be written with sufficient detail to avoid misinterpretation

Several AIs were able to create a PK analysis and reporting ready dataset for basic requests e.g. BLQ handling

C_{max} and T_{max} was generally calculated in a reliable manner. Incorrect calculations of AUC and $t_{1/2}$ were frequent

Generation of tables was accurate based on what calculated values that were generated

In general AI performed poorly at mathematical calculations. Further human verification is required to ensure correct calculations