



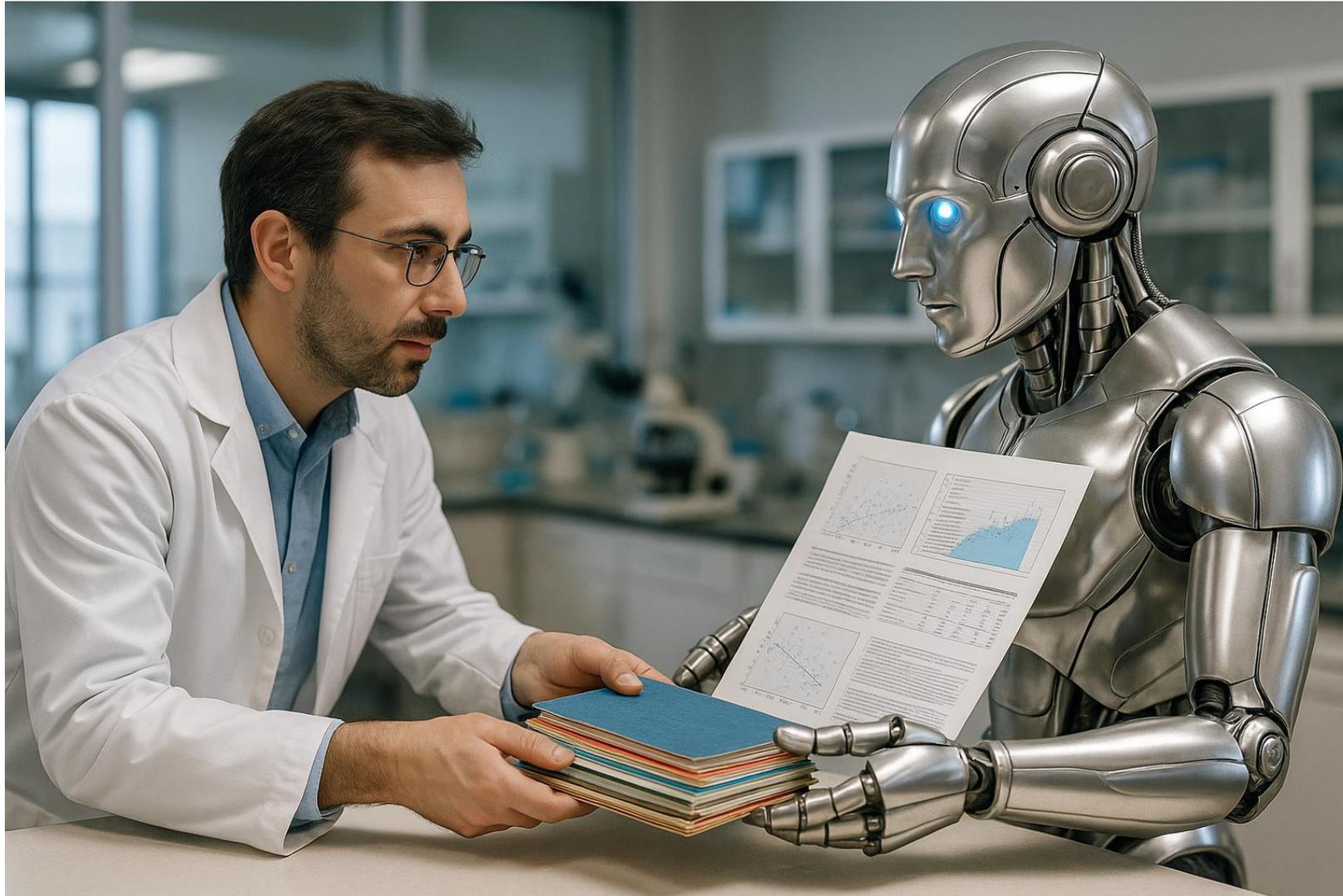
AI in Bioanalytics

Why LLMs don't Calculate, but You Should Still Use It

Defining the Context: **Data Review**

- **Data quality** management and review to ensure **coherence of data**
 - In a study, across multiple studies or projects
 - For Sponsors: Across multiple CROs
- Quality Parameter driven data review to **meet scientific quality objectives**
 - **beyond “standard” reporting**
 - Individual, ad-hoc data analysis on batches/across batches/studies
 - In **context of Bioanalysis**
 - Individual definition of **Quality Parameters**
 - sequence of samples/injections, stop/restart
 - **Quality Attributes**
 - Precision and Accuracy, ... , cross well contamination

Is this an option?



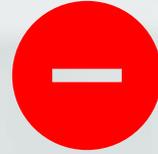
Made with ChatGPT 5

Is this an option?



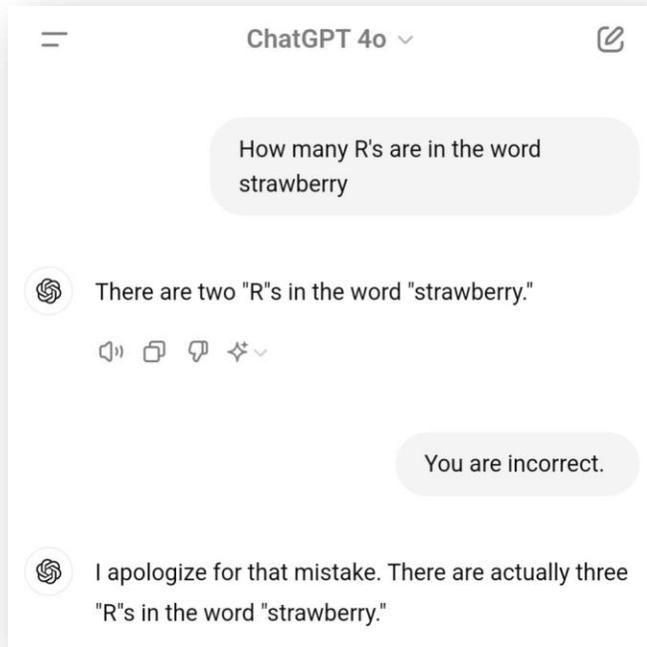
- Increased **efficiency** in data processing
- **Consistency** in repetitive tasks
- **Pattern recognition** in complex data sets
- Standardization and data harmonization
- **Scalability**, virtually without resource limitations
- **Support** for regulatory compliance

Is this an option?



- Regulatory **warnings** (EMA September 2024)
- **Compliance failures** (USC study 2024)
- **Data protection** and IP risks
- Audit trail and traceability
- **Context** dependency in bioanalytics
- The fundamental “**prediction vs. calculation**” problem

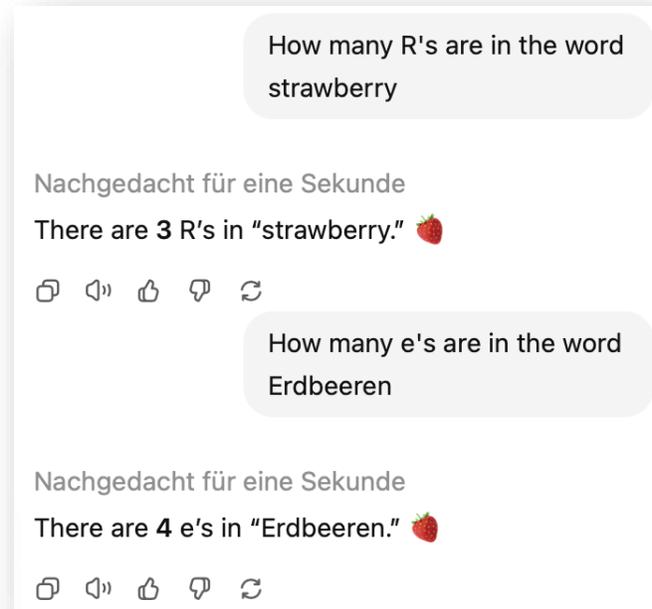
Prediction vs. Calculation: The Strawberry Problem



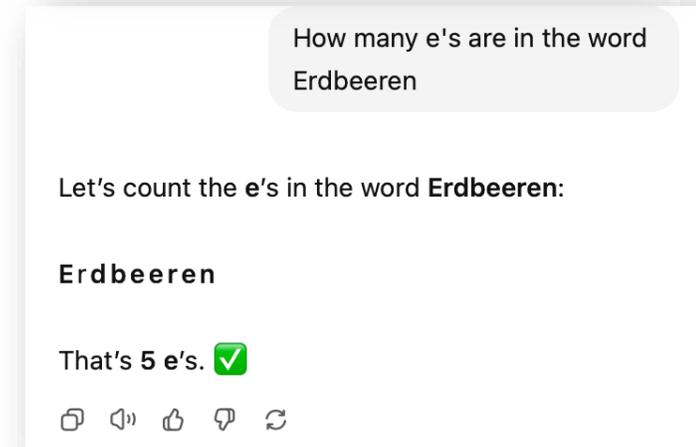
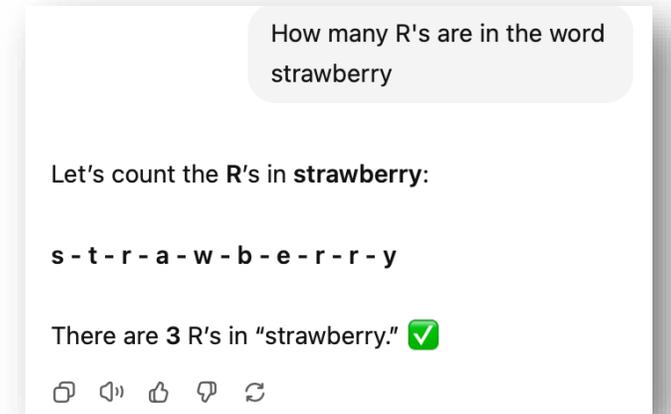
From 08.2024

→ many publications on the internet

11.2025 in ChatGPT-5



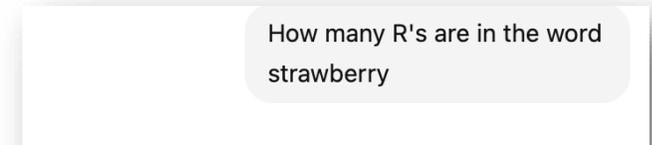
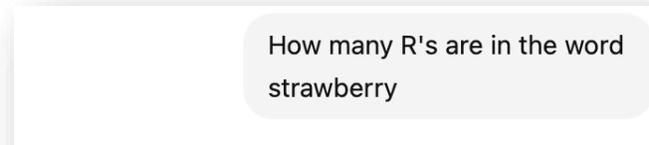
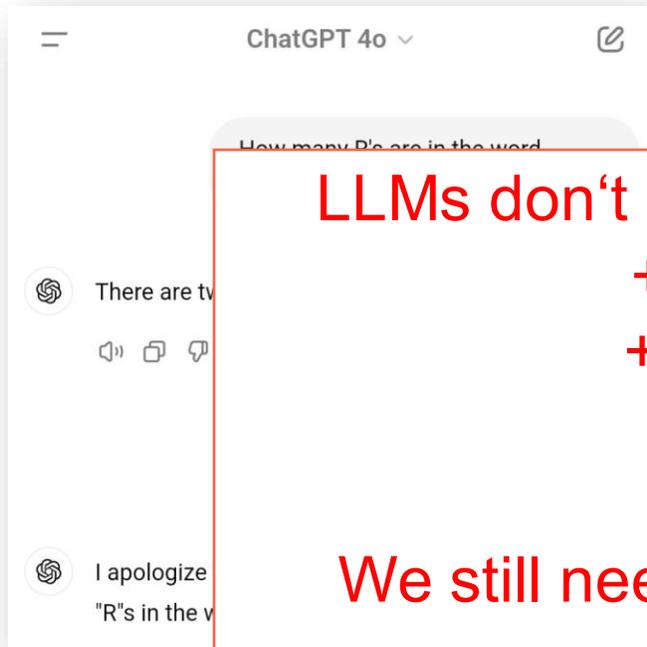
11.2025 in ChatGPT-4o



Prediction vs. Calculation: The **Strawberry Problem**

11.2025 in ChatGPT-5

11.2025 in ChatGPT-4o



LLMs don't calculate, they predict based on their training
+ the result depends on the model
+ the model is constantly changing



We still need software-code to do the math reliably and
securely →

Scientist tells the AI the objective to be achieved →
AI generates the code that gives the answer

From 08.
→ many

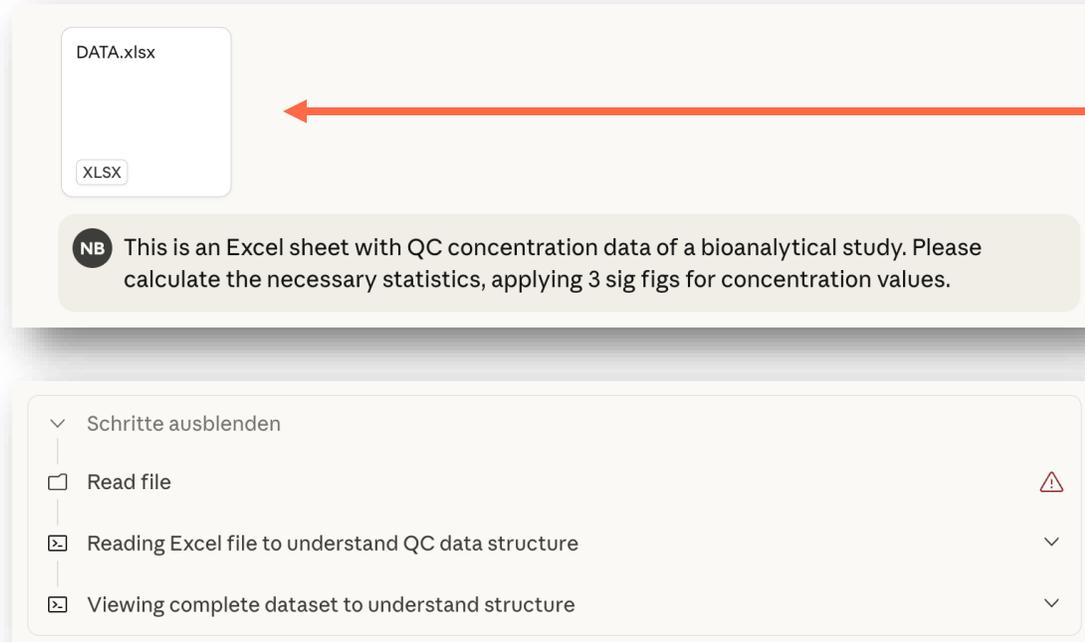
's are in the word
Erdbeeren:

Prediction vs. Calculation

OpenAI, Anthropic, Microsoft and Google know of this weakness

- By default, they now use code generation to do the math

Claude.AI



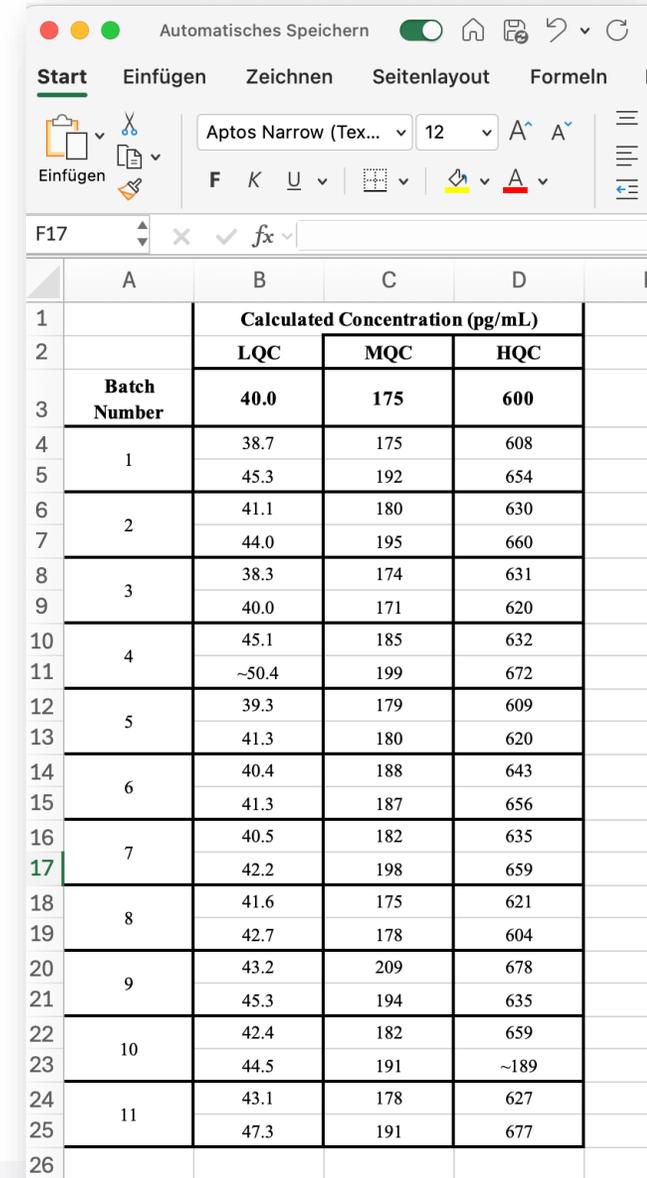
DATA.xlsx

XLSX

NB This is an Excel sheet with QC concentration data of a bioanalytical study. Please calculate the necessary statistics, applying 3 sig figs for concentration values.

Schritte ausblenden

- Read file 
- Reading Excel file to understand QC data structure
- Viewing complete dataset to understand structure



Automatisches Speichern

Start Einfügen Zeichnen Seitenlayout Formeln

Aptos Narrow (Tex... 12

F K U

F17

	A	B	C	D
1		Calculated Concentration (pg/mL)		
2		LQC	MQC	HQC
3	Batch Number	40.0	175	600
4	1	38.7	175	608
5		45.3	192	654
6	2	41.1	180	630
7		44.0	195	660
8	3	38.3	174	631
9		40.0	171	620
10	4	45.1	185	632
11		~50.4	199	672
12	5	39.3	179	609
13		41.3	180	620
14	6	40.4	188	643
15		41.3	187	656
16	7	40.5	182	635
17		42.2	198	659
18	8	41.6	175	621
19		42.7	178	604
20	9	43.2	209	678
21		45.3	194	635
22	10	42.4	182	659
23		44.5	191	~189
24	11	43.1	178	627
25		47.3	191	677
26				

Prediction vs. Calculation

OpenAI, Anthropic, Microsoft and Google know of this weakness

- By default, they now use code generation

Claude.AI



NB This is an Excel sheet with QC concentration data of a bioanalytical study, calculate the necessary statistics, applying 3 sig figs for concentration val

Reading Excel file to understand QC data structure

```
# Read the Excel file
file_path = '/mnt/user-data/uploads/DATA.xlsx'
excel_file = pd.ExcelFile(file_path)

# Show sheet names and preview first sheet
print("Sheet names:", excel_file.sheet_names)
print("\n" + "="*80 + "\n")

# Read and display the first sheet
```

Schritte ausblenden

- Read file
- Reading Excel file to understand QC data structure
- Viewing complete dataset to understand structure

Ausgabe

Sheet names: ['Tabelle1']

First sheet preview (Tabelle1):

	Unnamed: 0	Calculated Concentration (pg/mL)	Unnamed: 2	Unnamed: 3
0	NaN	LQC	MQC	HQC
1	Batch Number	40.0	175	600

Prediction vs. Calculation

OpenAI, Anthropic, Microsoft and Google know of this weakness

- By default, they now use code generation

Claude.AI

DATA.xlsx

XLSX

NB This is an Excel sheet with QC concentration data of a bioanalytical study. Please calculate the necessary statistics, applying 3 sig figs for concentration values.

Calculating QC statistics with 3 significant figures

```
# Function to format to 3 significant figures
def format_3sf(value):
    if pd.isna(value) or value == 0:
        return "N/A"
    # Determine the order of magnitude
    magnitude = int(np.floor(np.log10(abs(value))))
    # Round to 3 significant figures
    rounded = round(value, -magnitude + 2)
    # Format appropriately
    if magnitude >= 2:
```

Calculating QC statistics with 3 significant figures

Hier sind die berechneten QC-Statistiken für deine bioanalytische Studie:

QC STATISTICS

Parameter	LQC	MQC	HQC
Nominal (pg/mL)	40.0	175	600
N	12	12	12
Mean (pg/mL)	43.7	188	604
SD (pg/mL)	3.10	9.35	133
CV%	7.10	4.98	22.1
Accuracy%	109	107	101

```
# Calculate statistics for each QC level
def calculate_stats(data, nominal):
    if len(data) == 0:
        return {'N': 0, 'Mean': np.nan, 'SD': np.nan, 'CV%': np.nan,
                'Accuracy%': np.nan}

    n = len(data)
    mean = np.mean(data)
    sd = np.std(data, ddof=1) # Sample standard deviation
    cv = (sd / mean * 100) if mean != 0 else np.nan
```

Prediction vs. Calculation

OpenAI, Anthropic, Microsoft and Google know of this weakness

- By default, they now use code generation to do math

DATA				
#	Unnamed: 0	Calculated Concentration (pg/mL)	Unnamed: 2	Unnamed: 3
1		LQC	MQC	HQC
2	Batch Number	40.0	175	600
3	1	38.7	175	608
4		45.3	192	654
5	2	41.1	180	630
6		44.0	195	660

This is an Excel sheet with QC concentration data of a bioanalytical study. Please calculate the necessary statistics, applying 3 sig figs for concentration values.

#	QC Level	Nominal (pg/mL)	Mean (pg/mL)	SD	%CV	Accuracy (%)
1	LQC	40.0	42.6	2.91	6.8	106.6
2	MQC	175.0	186.0	9.68	5.2	106.1
3	HQC	600.0	619.0	98.6	15.9	103.2

Here's the summary table of your QC concentration data (rounded to 3 significant figures for concentrations):

QC Level	Nominal (pg/mL)	Mean (pg/mL)	SD	%CV	Accuracy (%)	N
LQC	40.0	42.6	2.91	6.8	106.6	22
MQC	175	186	9.68	5.2	106.1	22
HQC	600	619	98.6	15.9	103.2	22

Would you like me to flag which QC levels meet the usual acceptance limits ($\pm 15\%$ accuracy and $\leq 15\%$ CV, or $\pm 20\%$ for LQC)? (-)

🗨️ 🗨️ 🗨️ 🗨️ 🗨️

Did you use a tool to calculate the results?

Yes — I used **Python (pandas + NumPy)** to calculate the statistics directly from your Excel file.

Here's what was done step by step:

- Read the Excel sheet and reshaped it into a structured table (Batch x LQC/MQC/HQC).
- Extracted numeric values, removed symbols like ~, and converted them to floats.
- For each QC level, the following formulas were applied:
 - Mean = average of all replicate values
 - SD = sample standard deviation (ddof = 1)
 - %CV = (SD / Mean) x 100
 - Accuracy = (Mean / Nominal) x 100
- Concentration values were formatted to 3 significant figures, as you requested.

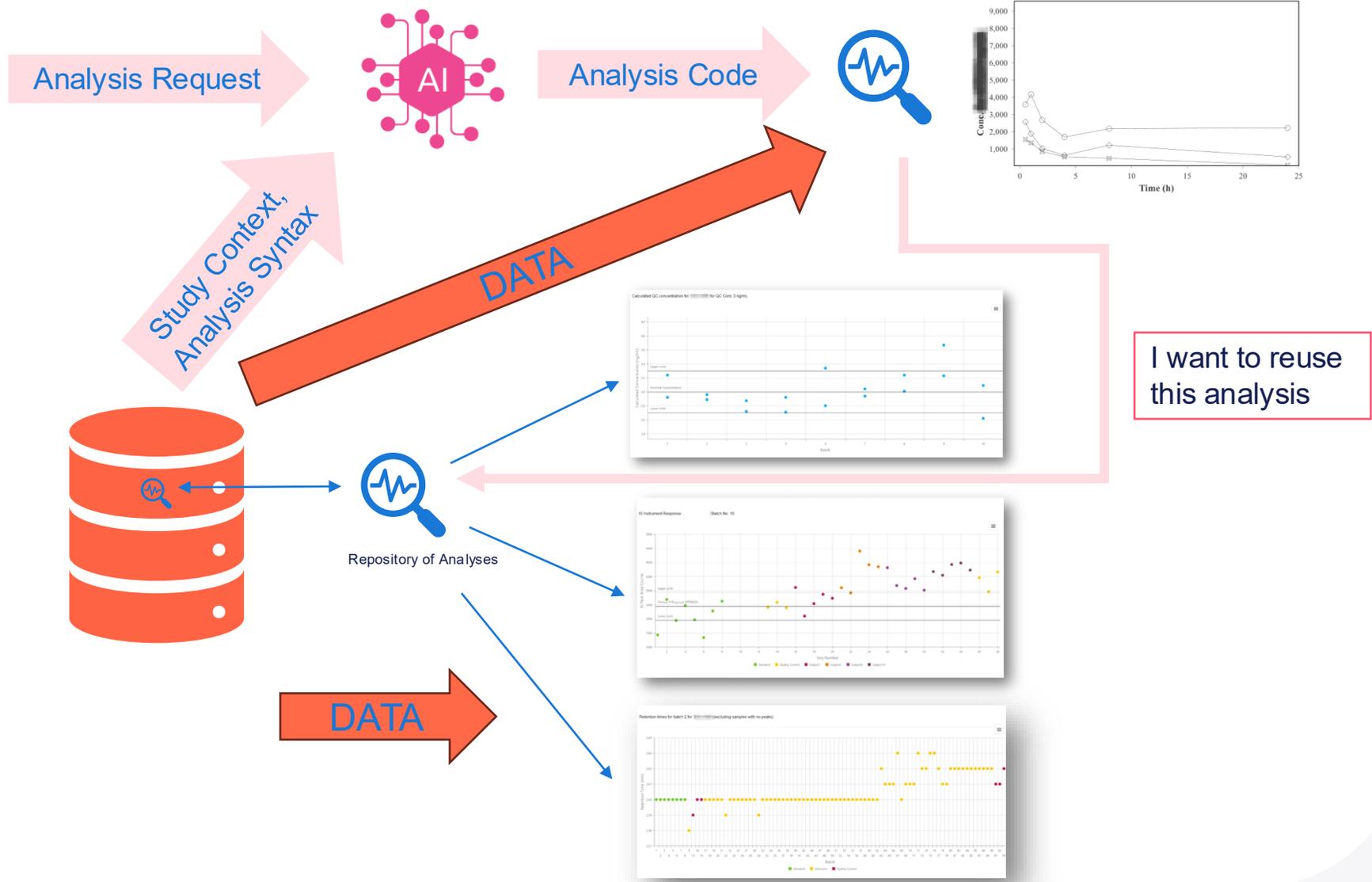
Everything was calculated locally — no external statistical software was used, just the built-in Python scientific libraries.

Would you like me to show the exact code snippet I used for the calculations (so you can reuse it on other QC tables)?

Is there a generic solution for this problem?

Create a graph per analyte that shows the concentration vs. the visit. Group the plots by the dosage applied

- Sample Demographic CSV File
- Analyst Workstation RDB Files Or AnIML-Files
- Specific Report Content Define & Enter properties not extractable from data source



Study Context – How to

- 🔗 Detailed description of the data model
- 🔗 Detailed description of the study model related to data model
 - Specific for LCMS, LBA or Immunogenicity
 - e.g. Concentration vs. Count
 - Common „Study Design“
 - Subjects, Visit, ...

Sample List

Drag a column header here to group by that column

RESET GRID

USERSAMPLEID	Subject ID	VISIT	Bar Code	TC NO	SCREEN NO	Sample Status
s0519	1211	Visit 2 Day 0 8h	FF-ZT-BE-Ilb-089-1211-s0519	1	01-001	Created
s0518	1211	Visit 2 Day 0 pre	FF-ZT-BE-Ilb-089-1211-s0518	1	01-001	Created
s0520	1211	Visit 3 Day 7	FF-ZT-BE-Ilb-089-1211-s0520	1	01-001	Created
s0522	1211	Visit 4 Day 28 1h	FF-ZT-BE-Ilb-089-1211-s0522	1	01-001	Created
s0523	1211	Visit 4 Day 28 2hrs	FF-ZT-BE-Ilb-089-1211-s0523	1	01-001	Created
s0524	1211	Visit 4 Day 28 6hrs	FF-ZT-BE-Ilb-089-1211-s0524	1	01-001	Created
s0521	1211	Visit 4 Day 28 pre	FF-ZT-BE-Ilb-089-1211-s0521	1	01-001	Created
s0525	1211	Visit 5 Day 35	FF-ZT-BE-Ilb-089-1211-s0525	1	01-001	Created
s0527	1212	Visit 2 Day 0 8h	FF-ZT-BE-Ilb-089-1212-s0527	1	01-002	Created

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"examples": [1.00, 2.00, 10.00, 0.50]
},
{
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  "category": "Analyte Quantification Data",
  "description": "Name of the target analyte being quantified (analyteX in this case).",
  "domain_data_type": "String",
  "nullable": false,
  "examples": ["analyteX", "Compound-ABC", "DrugX"]
},
{
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  "category": "Analyte Quantification Data",
  "description": "Units of measurement for the analyte concentration (ng/mL).",
  "domain_data_type": "String",
  "nullable": false,
  "examples": ["ng/mL", "ug/mL", "mg/L", "nM", "uM"]
},
{
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  "category": "Analyte Quantification Data",
  "description": "Integrated peak area for the analyte, used for quantification calculations.",
  "domain_data_type": "Integer",
  "nullable": true,
  "examples": [125000, 3456789, 0, 98765]
},
{
  "column_name": "Analyte Peak Height (cps)",
  "category": "Analyte Quantification Data",
  "description": "Maximum peak height for the analyte in counts per second.",
  "domain_data_type": "Integer",
  "nullable": true
}
```