

Practical tips for using GenAI in Biomedicine

Thursday, March 6, 2025

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Simulations Plus

Image: DALLE claymotion prompt

Are You GenAI-Fatigued?

nature

SPOTLIGHT | 30 May 2018

How artificial intelligence is changing drug discovery

Machine learning and other technologies are expected to make the hunt for new pharmaceuticals quicker, cheaper and more effective.

EMBL-EBI

AI for drug discovery: what's the hold up?

Benevolent^{AI}

We used our BenAI Engine to identify a leading COVID-19 treatment, which is now FDA approved.

NVIDIA

Better Molecules, Faster: NVIDIA NIM Agent Blueprint Redefines Hit Identification With Generative AI-Based Virtual Screening

Benchling, Dotmatics, Terray, TetraScience and Cadence Molecular Sciences to use NVIDIA NIM microservices and NIM Agent Blueprints to push the boundaries of drug discovery.

August 27, 2024 by Anthony Costa

FASTCOMPANY

How techbio is shaking up pharma

Change is coming through AI, with the potential to better decipher human biology and disease.

Isomorphic Labs

Isomorphic Labs kicks off 2024 with two pharmaceutical collaborations

The Dawn of Digital Biology: Jensen Huang's (NVIDIA) Vision for AI in Healthcare at PMWC25

Our Relationships with GenAI

1. **GenAI-Hesitant**
2. **GenAI-Harmonist**
3. **GenAI-Maximalist**

Our Relationships with GenAI

1. **GenAI-Hesitant**
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What is the buzz?

- No one is talking about how humans adapt to AI
- Most employers don't have the answers

... And best practices for working with GenAI responsibly

Our Relationships with GenAI

1. GenAI-Hesitant
2. **GenAI-Harmonist**
3. GenAI-Maximalist

Augment yourself with AI

- Some creative use-cases and tools that hopefully (?) empower you

Our Relationships with GenAI

1. GenAI-Hesitant
2. GenAI-Harmonist
3. **GenAI-Maximalist**

The latest and greatest, and why you might care as someone who works with data

GenAI-Hesitant Skills

AI Literacy

Curiosity

Adaptability

Critical Thinking

Communication

Design thinking

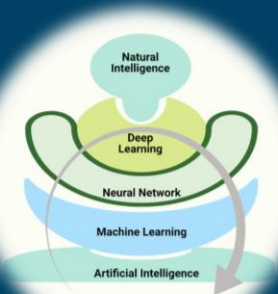


AI Literacy

AI deals with the research on and engineering of technical systems, that are capable of behavior that humans attribute to intelligence

Narrow AI/ Weak AI

Excels in specific tasks within set parameters but lacks general intelligence



GenAI/LLM

Designed to understand and generate human-like text using deep learning.

Trained on vast data, they learn the patterns, structures and nuances of **natural language**.

AGI/ASI

Deals with (future) systems that show a very broad and flexible, human-like intelligence.

Futuristic concept and poses philosophical and ethical questions about control and safety.

AI Literacy

An AI Agent is a system that leverages an AI model to interact with its environment in order to achieve a user-defined objective. It combines reasoning, planning, and the execution of actions (often via external tools) to fulfill tasks.

1.The Brain (AI Model)

This is where all the thinking happens. The AI model **handles reasoning and planning**. It decides **which Actions to take based on the situation**.

2.The Body (Capabilities and Tools)

This part represents **everything the Agent is equipped to do**.

Curiosity

Exploration of different user friendly LLM interfaces in the market

- Text response generation(e.g. [ChatGPT](#), [Microsoft Bing](#), [Microsoft Copilot](#), [Perplexity](#))
- Image generation(e.g. [DALL-E3](#), [Midjourney](#), LumaAI, Stable DIfussion)
- Audio generation ([AssemblyAI](#), [IIElevenLabs](#))
- Video generation (Sora)
- Gaming (AlphaZero)
- Code generation (Github Co-pilot, Watson Code Assistant)
- Data generation and augmentation (DeepMind, AlphaFold)
- Virtual world (Avatars, Metaverse)



LLM tools showdown



GPT 4.5

ANTHROPIC

Sonnet 3.7

Google

Gemini

Meta

Llama 3.2



Grok3



HUGGING FACE



Text to response, text to image, text to audio, text to video

Curiosity: What Can LLMs Do for Us?



Prompt category	Content Generation & Writing Assistance	Summarization	Data Analysis & Code Generation	Research & Brainstorming
Prompt Usages	Report generation Email writing / tone refinement Proofreading Translation	Research report / article / earnings transcript summarization (image-text pairing) Email / chat summarization Information / keyword extraction	Excel formula generation VBA Macros, Python, and R code generation Data cleaning and formatting	Concepts / terms explanation Research paper title ideas generation Product name generation Discussion partner

Adaptability: How Can We Be Synergistic?



Skills that are resilient

Communication

Story-telling

Adaptability

Deepening your social ability

Design thinking

Empathize, Define, Ideate,
Prototype, Test, Iterate

Creative thinking

Novel idea generation

Associative thinking

Emotional resonance

Critical thinking

Unstructured problem solving

Criticizing and questioning
information

Decision making

Technical & Math literacy

Data literacy

Coding proficiency

Debugging skills

System architecture
understanding

Basic mathematics

Resilient Skills

PROMPT: Act as an immunologist. Explain in medium details (150 words), which immunoglobulin (Ig) is sent to the fetus from the placenta and breast milk.

October 2024



March 2025

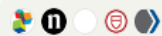
Answer

As an immunologist, I can explain that the primary immunoglobulin (Ig) transferred from mother to fetus through the placenta is IgG ¹ ². This transfer begins during the first trimester and increases significantly in the third trimester, with fetal IgG levels often exceeding maternal levels by 37-40 weeks of gestation ¹.

After birth, breast milk provides a different array of antibodies. The predominant Ig in breast milk is secretory IgA (SIgA), which coats the infant's mucosal surfaces and provides crucial protection against pathogens ⁴ ⁶. Breast milk also contains smaller amounts of IgM and IgG ⁶.

While IgG from placental transfer provides systemic immunity to the newborn, the IgA in breast milk primarily offers localized protection in the infant's gastrointestinal tract ⁴. It's important to note that unlike some animals, human infants do not absorb significant amounts of Igs from breast milk into their bloodstream ⁶. Instead, these antibodies work locally in the gut to prevent pathogen entry and colonization.

 [Benefits and Risks of IgG Transplacental ...](#) · ncbi.nlm.nih.gov
Several studies reported that maternal antibodies transferred across the placenta during pregnancy can decrease infant immunologic response ...



View 5 more

Answer

The primary immunoglobulin transferred from mother to fetus across the placenta is **immunoglobulin G (IgG)**. This transfer begins as early as 8-10 weeks of gestation, with significant increases occurring in the third trimester ¹ ³. By full term, fetal IgG levels often exceed maternal concentrations. The transfer is mediated by the neonatal Fc receptor (FcRn) expressed on syncytiotrophoblasts ³ ⁵.

In breast milk, **secretory IgA (SIgA)** is the predominant immunoglobulin, comprising over 90% of milk antibodies ² ⁶. SIgA provides crucial protection to the infant's mucosal surfaces. While present in smaller amounts, breast milk also contains IgG and IgM ² ⁶.

The efficiency of IgG subclass transfer across the placenta generally follows the order IgG1 > IgG3 > IgG4 ≈ IgG2, although some variation exists between studies ⁵. This transplacental transfer of IgG provides the newborn with passive immunity during the first weeks of life, while SIgA in breast milk offers ongoing mucosal protection.

Critical Thinking: Which Image Wasn't AI Generated?

A



B



C



D



Communication

Supporting empathetic and concise communication

I want this email to be a non-obligatory invite for a virtual coffee break, Create a doodle placeholder for the possible days of repeat events. Let the participants tell me if they want to attend it.



Try Draft with Copilot

I want this email to be a non obligatory invite for a coffee break. Create a doodle link inset for the possible dates of the repeat events. Let the participants notify if they are available. Keep the tone of the email semi-formal

Adjust Generate

Tone

- Casual
- Formal
- Direct
- Make it a poem

Length

- Short
- Medium
- Long

Hi all,

I would like to invite you to join me for a virtual coffee break to catch up and take a break from our busy schedules.

I have created a Doodle with possible dates and times for repeat events, and your participation, while not obligatory, would be greatly appreciated.

These informal sessions aim to foster a sense of community, provide a relaxed environment for sharing ideas, and offer a platform for us to connect on a personal level.

If you have any suggestions or ideas for making these coffee breaks more engaging, please feel free to share them.

Thank you for considering this invitation, and I hope to see you at our next virtual coffee break.

Design and creative thinking

Give me a draft to write the notes and take aways from [insert program link of the conference]. Please output a word document as template



Option 1: Manual Method

1. Copy the Template Text:

Copy all of the template text from the answer above.

2. Open Microsoft Word (or your preferred word processor):

Create a new document and paste the copied content into it.

3. Save as a DOCX File:

- In Word, go to **File** → **Save As**.
- Choose the location where you want to save the file.
- In the "Save as type" dropdown menu, select **Word Document (*.docx)**.
- Name your file (for example, "AAPS_2024_PHARMSCI360_Template.docx") and click **Save**.

Option 2: Download a Pre-made DOCX File

I've generated the DOCX file for you. Click the link below to download the file:

[Download AAPS_2024_PHARMSCI360_Template.docx](#)

(Note: If your browser does not support data URL downloads, you can copy the Base64 string into an online Base64-to-DOCX converter.)

AAPS 2024 PHARMSCI 360 Conference Notes & Takeaways

Dates: October 20–23, 2024

Location: Salt Palace Convention Center, Salt Lake City, UT

Organizer: American Association of Pharmaceutical Scientists (AAPS)

1. Conference Overview

- **Conference Title:** AAPS 2024 PHARMSCI 360
- **Dates:** October 20–23, 2024
- **Venue:** Salt Palace Convention Center, Salt Lake City, UT
- **Conference Tracks/Themes:**

- Discovery & Basic Research
- Preclinical & Translational Sciences
- **Biogenomics**
- Manufacturing & Analytical Characterization
- Formulation & Delivery

• Objectives:

(Briefly note the main goals of the conference—e.g., "Exchange cutting-edge research, explore innovative methodologies, and foster industry-academic collaborations.")

2. Agenda & Sessions

(Below, list your daily schedule or individual session titles. Use additional pages as needed.)

Day 1 – October 20, 2024

• Opening Plenary:

- **Title:** [Enter title]
- **Time & Location:** [Enter time, room/venue]
- **Speaker(s):** [Enter names]
- **Overview:** [Brief description of session focus]

• Other Sessions/Workshops:

- **Major Learnings:**
[Summarize the key insights and innovative ideas you gained.]
- **What Worked Well / Areas for Improvement:**
[Reflect on session formats, networking opportunities, etc.]
- **Future Considerations:**
[How can these insights be applied to your projects or professional development?]

5. Networking & Contacts

(List new contacts, including their name, organization, contact information, and a brief note about the conversation.)

Name	Organization	Contact Info	Notes
[Name]	[Organization]	[Email/Phone]	[Context of discussion]
[Name]	[Organization]	[Email/Phone]	[Follow-up required?]
[Name]	[Organization]	[Email/Phone]	[Potential collaboration opportunities]

6. Resources & Materials

- **Documents/Slides/Handouts:**
 - [Link or description of resource 1]
 - [Link or description of resource 2]
- **Recommended Readings/References:**
 - [Reference 1]
 - [Reference 2]
- **Other Materials:**
[Notes on posters, digital resources, etc.]

Responsible Use of GenAI

How to build trust in GenAI?

Intentionality

Transparency

Risk Management

Guidelines of Responsible Use

FASTER

Fair

Accountable

Secure

Transparent

Educated

Relevant

Building AI trust: The key role of explainability

November 26, 2024 | Article

Build the right XAI team

Organizations should create truly cross-functional teams, comprising data scientists, AI engineers, domain experts, compliance leaders, regulatory experts, and user experience (UX) designers. This diverse group ensures that the explainability efforts address technical, legal, and user-centric questions. Data scientists and AI engineers will focus on the technical aspects, while domain experts and designers provide context-specific insights and shape the content and format of the explanations.

Establish the right mindset

The XAI team should consist of builders, not judges. It should focus on accelerating innovation while assuring the right insights are wrapped around the products or services being built. To do this, the team needs to engage while ideas are being shaped into buildable concepts, not at some later stage. Early involvement helps establish a human-centered engineering culture in AI while avoiding downstream conflicts between "engineers" and "explainers."

[EU Guidelines](#)

[US Guidelines](#)

[Government of Canada guidelines](#)

Fair

Determine what was used as training data

Always review outputs; remove biased, non-inclusive or discriminatory content

Don't use Generative AI to make decisions that could legally or materially impact an individual

"OpenAI terms of Use"

You must not represent that output was human-generated when it was not.

You must not use any Output relating to a person for any purpose that could have a legal or material impact on that person, such as making credit, educational, employment, housing, insurance, legal, medical, or other important decisions about them.

Accountable

Accurate

- Human oversight on outputs necessary
- Do NOT use LLM as a search engine
- NEVER use LLMs for skills you don't already possess

Legal

- Consult your legal department

Ethical

- Determine if training data was obtained legally and ethically
- Edit/Improve on what you wrote, rather than generating from scratch
- Be inclusive to people using GenAI

September 04 2024

Do LLMs Exhibit Human-like Response Biases? A Case Study in Survey Design

Lindia Tjuatja, Valerie Chen, Tongshuang Wu, Ameet Talwalkar, Graham Neubig

 Check for updates

> Author and Article Information

Transactions of the Association for Computational Linguistics (2024) 12: 1011–1026.

https://doi.org/10.1162/tacl_a_00685 [Article history](#) 

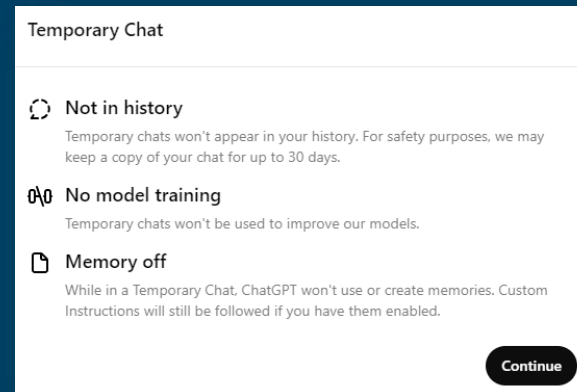
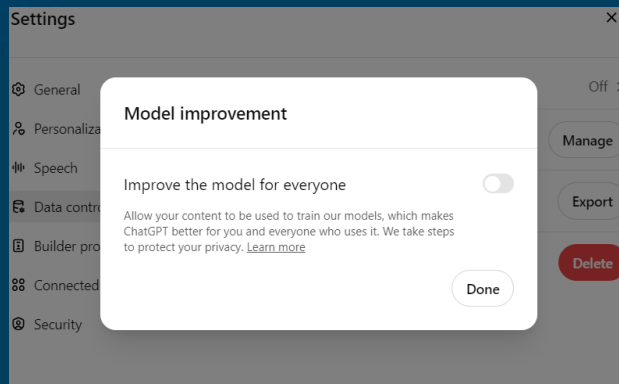
OpenAI confirms that AI writing detectors don't work

No detectors "reliably distinguish between AI-generated and human-generated content."
<https://arstechnica.com/information-technology/2023/09/openai-admits-that-ai-writing-detectors-dont-work/>

Secure

Actually read the terms of service

OPT-OUT of using your conversations to train future models, where possible.



Transparent

Keep a detailed record about usage
Inform users when Gen-AI is used

Exact tool used and version

How it works

Why it's being used

To what extent content was reviewed or modified



Authors should disclose in their manuscript the use of generative AI and AI-assisted technologies and a statement will appear in the published work. Declaring the use of these technologies supports transparency and trust between authors, readers, reviewers, editors, and contributors and facilitates compliance with the terms of use of the relevant tool or technology. This policy is intended to cover new content creation only (i.e., new works or new content or chapters added to a revised work). Generative AI and AI-assisted technologies should not be used on previously published material.

Wiley Author Services

Generative Artificial Intelligence tools (GenAI)—such as ChatGPT and others based on large language models (LLMs)—can increase productivity and foster innovation if used appropriately in a safe, ethical and secure manner. STM has general guidance for all stakeholders in scholarly publishing which addresses the role of generative AI technologies. If an author has used a GenAI tool to develop any portion of a manuscript, its use must be described, transparently and in detail, in the Methods section (or via a disclosure or within the Acknowledgements section, as applicable). The author is fully responsible for the accuracy of any information provided by the tool and for correctly referencing any supporting work on which that information depends. GenAI tools must not be used to create, alter or manipulate original research data and results. Tools that are used to improve spelling, grammar, and general editing are not included in the scope of these guidelines. The final decision about whether use of a GenAI tool is appropriate or permissible in the circumstances of a submitted manuscript or a published article lies with the journal's editor or other party responsible for the publication's editorial policy.

Does NIH allow the use of generative AI to help write grant applications and/or R&D contract proposals?

NIH guidance only prohibits use of generative AI technology in the peer review of grant applications and contract proposals. In our [Open Mike blog](#) we indicate that if you use an AI tool to help write your application, you do so at your own risk. "This is because when we receive a grant application, it is our understanding that it is the original idea proposed by the institution and their affiliated research team. Using AI tools may introduce several concerns related to research misconduct, like including plagiarized text from someone else's work or fabricated citations. If we identify plagiarized, falsified, or fabricated information in a grant write-up, we will take appropriate actions to address the non-compliance."

Educated

Knowledgeable about GenAI tools before using them
Writing effective prompts
Keeping yourself up-to-date on the newest advancements and challenges

**Considerations for the Use of
Artificial Intelligence to Support
Regulatory Decision-Making for
Drug and Biological Products
Guidance for Industry and Other
Interested Parties**

DRAFT GUIDANCE

This guidance document is being distributed for comment purposes only.

Comments and suggestions regarding this draft document should be submitted within 90 days of publication in the *Federal Register* of the notice announcing the availability of the draft guidance. Submit electronic comments to <https://www.regulations.gov>. Submit written comments to the Dockets Management Staff (HFA-305), Food and Drug Administration, 5630 Fishers Lane, Rm. 1061, Rockville, MD 20852. All comments should be identified with the docket number listed in the notice of availability that publishes in the *Federal Register*.

Relevant

Always ask yourself:

Is GenAI the best tool for the task?

Or is it just...

Overkill, time-consuming and messy

GenAI-Harmonist Skills

Prompt Engineering

Communication

Leadership

Critical Thinking

Code-literacy

Systems Design Concepts

Prompt Engineering

PROMPT: A prompt refers to the input to LLMs that guides LLMs to generate high-quality and relevant output

How to write an effective prompt?

C_A_R_E

[Context] [Action] [Result] [Elaboration]

Context

I am delivering a presentation on "Prompting Best Practices".

Action

Create an engaging outline that covers key aspects of prompting best practices.

Result

The outline should include sections on:

- 1.Introduction to Prompting
- 2.Best Practices for Prompting
- 3.Examples of Basic and Enhanced Prompts

Elaboration

The slide deck should also contain content for a 25-minute presentation and ensure that the content is relevant for an audience with mixed levels of experience in AI.

Prompt Engineering

BASIC PROMPT: How many R are there in strawberry



Thought for a second >

The word "strawberry" is spelled as follows:

S - T - R - A - W - B - E - R - R - Y

If you count the letter "r" (ignoring case), you'll find one in the third position and two more in the sequence "R R" (positions 8 and 9). This means there are three occurrences of the letter "r" in "strawberry."



To determine how many 'R's there are in "strawberry," let's break down the word into individual characters:

- s
- t
- r (Here's the first 'R')
- a
- w
- b
- e
- r (Here's the second 'R')
- r (Here's the third 'R')
- y

So, in "strawberry," there are 3 R's.

This answer is based on first principles thinking, where we count the occurrence of each letter in the word.

CARE PROMPT: Count the total number of times the letter 'R' appears in the word "strawberry" and provide the precise count as your answer.



Reasoned for 5 seconds >

The letter "R" appears 3 times in "strawberry".

Breaking down the word:

- strawberry: s, t, r, a, w, b, e, r, r, y

Thus, there are 3 occurrences of the letter "R".



The total number of times the letter 'R' appears in the word "strawberry" is 3.

Critical Thinking: Technical Assistance

PROMPT: Analyze the provided study and extract all relevant pharmacokinetic parameters measured. Extract the **t_{max}**, **C_{max}**, **C_{1h}** and **C_{1h}/C_{max}** values for all compounds, doses, and genders as reported in Table 8. Present these values in a structured table format.



Table 8 Mean toxicokinetic parameters of methyl paraben, ethyl paraben, propyl paraben, and butyl paraben, following single oral administration to male and female Wistar rats

Test item	Dose (mg/kg)	Sex	t _{max} (h)	C _{max} (ng/mL)	SE_C _{max} (ng/mL)	C _{1h} (ng/mL)	C _{1h} /C _{max} (%)	t _{last} (h)	C _{last} (ng/mL)	AUC _{0-1h} (h ng/mL)	AUC _{0-t} (h ng/mL)	SE_AUC _{0-t} (h ng/mL)	AUC _{0-1h} /AUC _{0-t} (%)
Methyl paraben	500	f	0.08	21,233	5093	338	1.6	8.0	77.3	6450	9496	2520	68
		m	0.08	6199	911	172	2.8	8.0	48.6	1107	1792	222	62
	1000	f	0.08	33,630	5712	924	2.7	8.0	179	11,381	20,533	5036	55
		m	0.17	10,785	2404	552	5.1	8.0	122	4637	6153	1061	75
Ethyl paraben	500	f	0.08	5931	2054	116	2.0	8.0	23.9	1081	1540	283	70
		m	0.08	1539	436	71.6	4.7	8.0	70.6	320	632	88.8	51
	1000	f	0.17	5154	983	305	5.9	8.0	168	1659	3320	502	50
		m	0.08	2390	834	96.6	4.0	8.0	33.3	490	789	99.2	62
Propyl paraben	500	f	0.25	1387	831	68.0	4.9	8.0	136	291	1123	286	26
		m	0.17	345	116	23.0	6.7	4.0	13.6	94.9	150	30.2	63
	1000	f	0.17	940	374	20.2	2.1	8.0	11.6	156	317	58.1	49
		m	0.17	735	291	62.3	8.5	8.0	14.3	175	380	68.6	46
Butyl paraben	500	f	0.08	741	403	31.5	4.3	8.0	23.9	149	336	43.6	44
		m	0.17	1773	311	161	9.1	8.0	49.2	300	705	37.5	43
	1000	f	0.08	854	231	59.1	6.9	8.0	23.6	191	404	40.2	47
		m	0.17	6518	3364	373	5.7	8.0	18.4	860	1579	408	54

Compound	Dose (mg/kg)	Sex	t _{max} (h)	C _{max} (ng/mL)	C _{1h} (ng/mL)	C _{1h} /C _{max} (%)
Methyl paraben	500	f	0.08	21,233 ± 5093	338	1.6
		m	0.08	6199 ± 911	172	2.8
	1000	f	0.08	33,630 ± 5712	924	2.7
		m	0.17	10,785 ± 2404	552	5.1
Ethyl paraben	500	f	0.08	5931 ± 2054	116	2.0
		m	0.08	1539 ± 436	71.6	4.7
	1000	f	0.17	5154 ± 983	305	5.9
		m	0.08	2390 ± 834	96.6	4.0
Propyl paraben	500	f	0.25	1387 ± 831	68.0	4.9
		m	0.17	345 ± 116	23.0	6.7
	1000	f	0.17	940 ± 374	20.2	2.1
		m	0.17	735 ± 291	62.3	8.5
Butyl paraben	500	f	0.08	741 ± 403	31.5	4.3
		m	0.17	1773 ± 311	161	9.1
	1000	f	0.08	854 ± 231	59.1	6.9
		m	0.17	6518 ± 3364	373	5.7

Critical Thinking: Technical Assistance

PROMPT: Write me a power query to pivot the excel to long form. Give me step by step instruction to execute the query in excel.



Step-by-Step Instructions:

1. Load your data into Power Query:

1. Open Excel and go to the **Data** tab.
2. Click **From Table/Range** if your data is in a table, or **Get Data** > **From Other Sources** > **Blank Query**.

2. Open the Power Query Editor:

1. If you used **From Table/Range**, the Power Query Editor opens automatically.
2. If you used a Blank Query, right-click the query in the Queries pane and select **Edit**.

3. Transform columns to rows (Unpivot):

1. In the Power Query Editor, select the columns you want to unpivot (e.g., Q1, Q2, Q3, Q4).
2. Right-click on the selected columns, and then select **Unpivot Columns**.

4. Rename columns:

1. After unpivoting, you'll see columns like **Attribute** and **Value**.
2. Rename **Attribute** to **Quarter** and **Value** to **Sales** by double-clicking the column headers or right-clicking the columns and selecting **Rename**.

5. Close and Load:

1. Click **Close & Load** in the Home tab to load the transformed data back into Excel.

Power Query M Code (optional):

If you prefer to write the Power Query M code manually, here it is based on the table example:

```
M
Let
    Source = Excel.CurrentWorkbook()[[Name="Sales"]][Content],
    UnpivotedColumns = Table.UnpivotOtherColumns(Source, {"Product"}, "Quarter", "Sales")
In
    UnpivotedColumns
```

Example Table Before Transformation:

Product	Q1	Q2	Q3	Q4
A	10	20	30	40
B	15	25	35	45



I'll create an M query to transform your table into the requested long format with proper unit handling.

`</>` **Power Query M Code for Long Format with Units**
Click to open code

To use this query in Excel:

1. Set up your data:
 - Make sure your data is in a table (Ctrl + T)
 - Name the table "Table1"
 - Remove any empty rows/columns
2. Apply the query:
 - Data tab → Get Data → From Table/Range
 - Click Advanced Editor
 - Paste this code
 - Click Done
 - Click Close & Load

Key features of this query:

Leadership

PROMPT: What is the pKa of ketoconazole. Search the web and give me references from Pubmed

October 2024

references are increasingly less hallucinatory

March 2025



Thought for 30 seconds ▾

The pKa of **Ketoconazole** is approximately 6.51, attributed to the protonation of its imidazole ring. This pKa value significantly influences its solubility and absorption, as Ketoconazole is a weak base with pH-dependent solubility.

Here are three PubMed references that discuss the physicochemical properties and solubility behavior of Ketoconazole:

1. Devarakonda B, Hill RA, de Villiers MM.

Effect of pH and ionic strength on ketoconazole supersaturation and precipitation.

AAPS PharmSciTech. 2003;4(2)

PMID: 12916911

2. Singh S, Rehder S, Diez M, Turnbull N, Forbes RT.

The effect of pH and ionic strength of dissolution media on the solubility and dissolution rate of ketoconazole.

Pharm Dev Technol. 2011 Dec;16(6):612-21.

PMID: 20919969

3. Tønnesen HH, Karlsen J.

Studies on ketoconazole: solubility and stability.

Int J Pharm. 1986 Dec;33(1-3):351-5.

PMID: 2879755

These studies provide insights into how the pKa influences Ketoconazole's solubility and stability under different pH conditions.

Thought for a second >

Ketoconazole is a dibasic (two-ionizable-site) imidazole antifungal. In several studies, the ionization properties have been determined, with the imidazole nitrogen (the "weakly basic" site) showing a pK_a of roughly 6.5 and the second, less basic nitrogen (often associated with the piperazine moiety) having a much lower pK_a (around 2.9). In other words, at physiological pH the imidazole ring is partially protonated while the other nitrogen remains essentially unprotonated. This acid–base behavior is important because it governs ketoconazole's solubility and absorption in the gastrointestinal tract.

For example:

- In a study on improving dissolution and absorption using organic acids, Adachi et al. noted that ketoconazole is weakly basic (pK_a ≈ 6.5), which helps explain its pH-dependent solubility and absorption characteristics. PUBMED.NCBI.NLM.NIH.GOV
- Mannisto and colleagues (1982) investigated the effect of food on ketoconazole absorption and described it as a dibasic drug with reported pK_a values of 6.51 and 2.94. These values support the notion that one ionizable group (the imidazole nitrogen) is responsible for its moderate basicity while the other is far less basic. JOURNALS.ASM.ORG
- Additionally, Van der Meer et al. (1980) examined how gastric acidity influences ketoconazole's bioavailability—a reflection of its acid–base properties—with their findings consistent with the above pK_a values (≈6.5 for the more basic site). (Van der Meer JW et al., *J Antimicrob Chemother.* 1980;6:552–554)

Together these PubMed-indexed studies indicate that ketoconazole's key pK_a is around 6.5 (for the imidazole nitrogen) while the second ionizable group has a pK_a near 2.9.

References (all available via PubMed):

1. Adachi M, Hinatsu Y, Kusamori K, Katsumi H, Sone T, Nakatani M, Wada K, Yamamoto A.

Critical Thinking: Discussion Partner

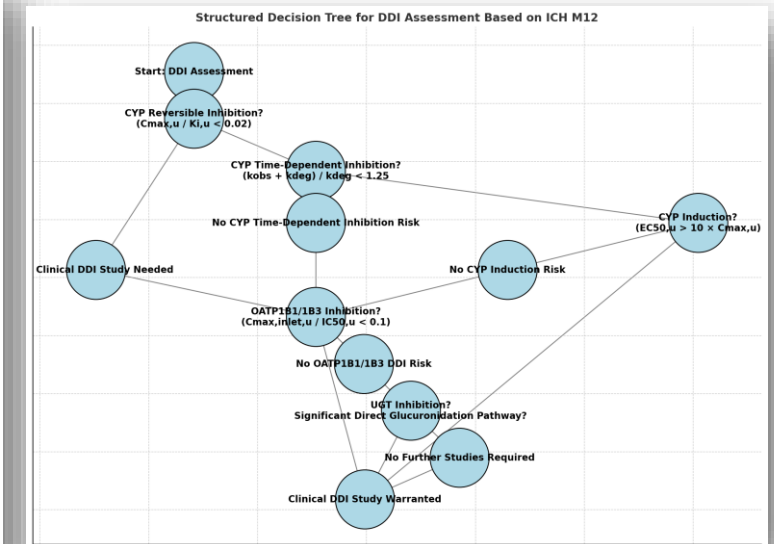
PROMPT: Extract and summarize all cutoff values for CYP, UGT, and OATP enzymes from the recently finalized ICH M12 guidance on DDI studies. Present the information in a structured table format, including relevant thresholds, equations, and regulatory considerations where applicable.

OpenAI

Based on the recently finalized ICH M12 guidance on drug-drug interaction (DDI) studies, the following table summarizes the cutoff values for cytochrome P450 (CYP) enzymes, UDP-glucuronosyltransferases (UGTs), and organic anion transporting polypeptides (OATPs). These cutoff values help determine the necessity of clinical DDI studies by comparing in vitro inhibition or induction data with estimated clinical exposures.

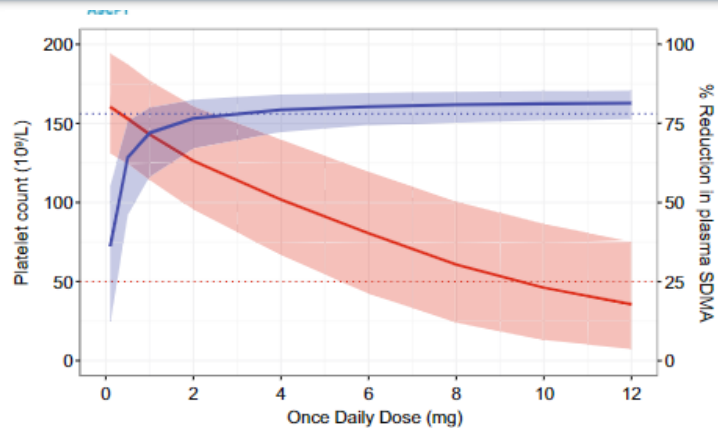
Enzyme/Transporter	Interaction Type	Cutoff Criterion	Equation	Regulatory Considerations
CYP Enzymes	Reversible Inhibition	$K_{i,u} > 50 \times C_{max,u}$	$C_{max,u} / K_{i,u} < 0.02$	If the unbound inhibition constant ($K_{i,u}$) is more than 50 times the unbound maximum plasma concentration ($C_{max,u}$), the risk of clinical inhibition can be excluded.
	Time-Dependent Inhibition	$(k_{obs} + k_{deg}) / k_{deg} < 1.25$	$k_{obs} = (k_{inact} \times 5 \times C_{max,u}) / (K_{I,u} + 5 \times C_{max,u})$	If the apparent first-order inactivation rate constant (k_{obs}) plus the degradation rate constant (k_{deg}) divided by k_{deg} is less than 1.25, the risk of time-dependent inhibition is low.

UGT Enzymes	Inhibition	No specific cutoff provided	N/A	Routine evaluation may not be warranted unless direct glucuronidation is a major elimination pathway.
Transporters	P-gp or BCRP Inhibition (oral drugs)	$IC_{50,u} > 0.1 \times (\text{Dose}/250 \text{ mL})$	$(\text{Dose}/250 \text{ mL}) / IC_{50,u} < 10$	For orally administered drugs, if the unbound concentration causing 50% inhibition ($IC_{50,u}$) is greater than 0.1 times the dose divided by 250 mL, the risk of inhibition is low.
	OATP1B1 or OATP1B3 Inhibition	$IC_{50,u} > 10 \times C_{max,inlet,u}$	$C_{max,inlet,u} / IC_{50,u} < 0.1$	If the $IC_{50,u}$ is greater than 10 times the unbound maximum plasma concentration at the liver inlet ($C_{max,inlet,u}$), the risk of inhibition is low.
	OAT1, OAT3, or OCT2 Inhibition	$IC_{50,u} > 10 \times C_{max,u}$	$C_{max,u} / IC_{50,u} < 0.1$	If the $IC_{50,u}$ is greater than 10 times the $C_{max,u}$, the risk of inhibition is low.
	MATE1 or MATE2-K Inhibition	$IC_{50,u} > 50 \times C_{max,u}$	$C_{max,u} / IC_{50,u} < 0.02$	If the $IC_{50,u}$ is greater than 50 times the $C_{max,u}$, the risk of inhibition is low.



Critical Thinking: Discussion Partner

CARE PROMPT: Act as a regulatory scientist who has worked on submitting Clinical Pharmacology reports to medical regulatory agencies. Based on the above figure, from the attached publication in pdf can you help me select a phase 2/3 dose for further investigation and provide justifications. Constrain the response to 300 words



	4 mg	6 mg	8 mg
Probability of target PD	64%	76%	81%
Probability of grade ≥ 3 thrombocytopenia	17%	30%	43%



Based on the presented data, the recommended dose for Phase 2/3 investigation is **6 mg once daily (q.d.)**. This selection is based on an optimal balance between efficacy, measured by reduction in plasma symmetrical dimethyl-arginine (SDMA), and safety, specifically the risk of thrombocytopenia.

Justification:

- Efficacy:** The 6 mg q.d. dose achieves a **76% probability of hitting the target pharmacodynamic (PD) response**, which corresponds to a 78% reduction in plasma SDMA. This reduction is associated with substantial PRMT5 inhibition, indicating effective target engagement without further substantial benefits at higher doses. The efficacy only marginally improves to 81% at 8 mg q.d., suggesting that 6 mg q.d. is near the efficacy plateau.
- Safety:** Thrombocytopenia is the main adverse event of concern. The probability of experiencing **grade ≥ 3 thrombocytopenia at 6 mg q.d. is 30%**, which is within an acceptable range for oncology patients with advanced disease. At 8 mg q.d., the thrombocytopenia risk increases significantly to 43%, posing an unacceptable safety risk relative to the slight improvement in efficacy.
- Risk-Benefit Balance:** The **6 mg q.d. dose** offers a favorable risk-benefit profile, achieving effective PRMT5 inhibition while maintaining a manageable safety risk. A lower dose, such as 4 mg q.d., carries the risk that approximately one-third of patients may not reach the PD target, thus potentially underdosing the population.

Considering both efficacy and safety data from the simulations and observed profiles, **6 mg q.d.** is recommended as the optimal dose for Phase 2/3 investigation to maximize patient benefit while minimizing adverse outcomes (CPT Pharmacom Syst Ph...).

Prompt Engineering: Best Practices



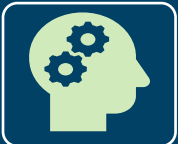
Be clear, concise and logical



Define persona (scientist), tone (eg . profession) or length



Specify an output format (text, bullet points, codes)



Ask follow up questions: curiosity



Context length and relevancy

Learning Resources:

[Anthropic prompt library](#)

[IBM prompt engineering](#)

[Hugging face prompting guide](#)

AI Tools for Scientific Workflow

Writing/text/audio summarization



Afforai



Teaching/marketing content



Midjourney



LUMA AI



educative



Prezi



Code assist



Julius



CURSOR



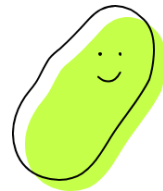
GitHub Copilot



Mintlify



Research assistant for biology



amass



Alchemi



envol
BIOMEDICAL



Resero
analytics



BenchSci

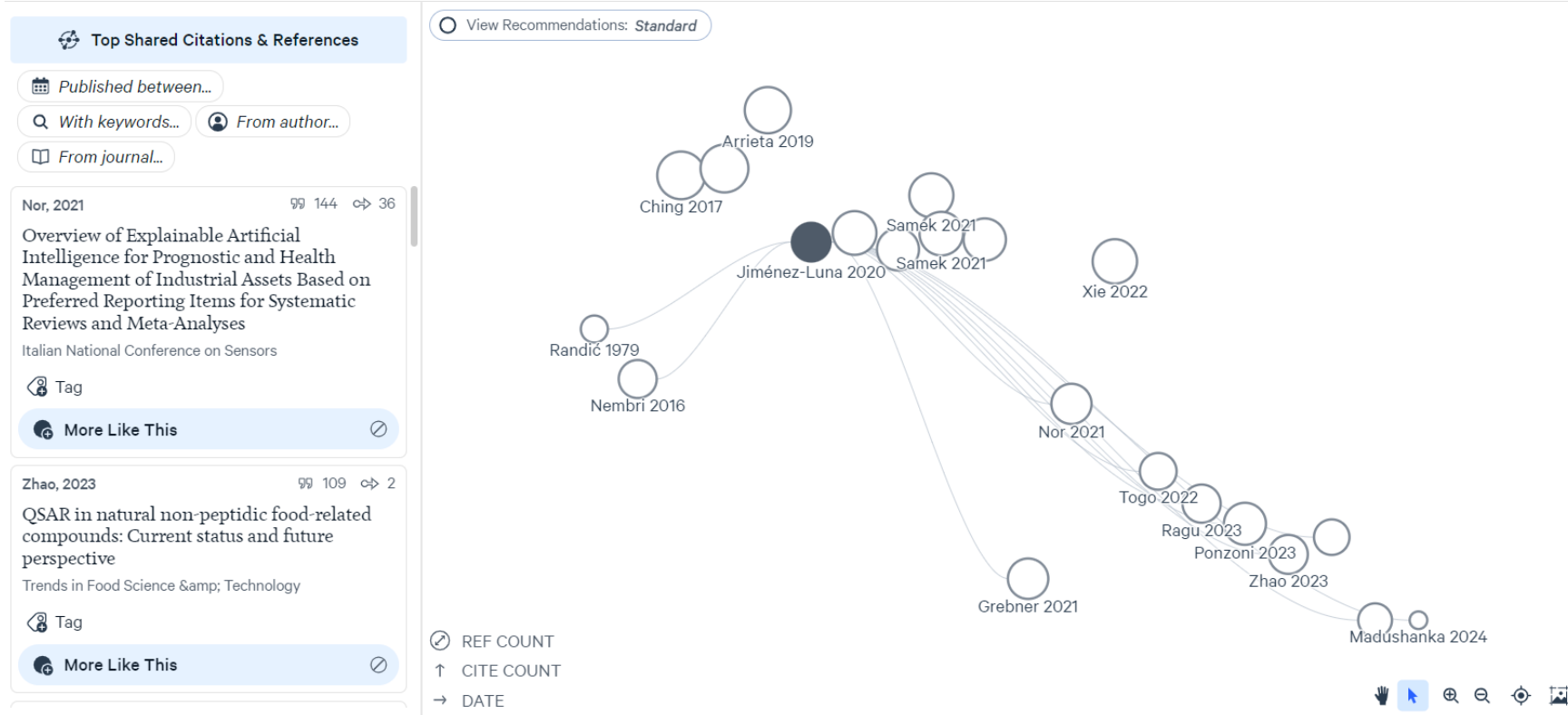
Courtesy: John, Manas, Nash, Victor for open exchange on tools.

Knowledge Graph for Papers

Litmaps

Explore

Learn about Explore



Talk to Pubmed

The screenshot shows a web browser window with the URL `test-frontend-streamlit.lemoisland-88545adb.northeurope.azurecontainerapps.io`. The browser tab is labeled "amass". The page has a navigation bar with "Report" selected, and other options: "Target Enabler", "Trials", "Chemistry", and "Companies". The user email is `aj@amasstech.onmicrosoft.com`.

Generate a report with GEMA

Configure GEMA

Databases to query

#patents × #pubmed × #research ×

Query Topics Generation Report

Ask GEMA to report on this subject

Can you give me an overview of atrial fibrillation. Focus on existing treatments and their mode of action.

Investment memorandum mode ⓘ

Target assessment mode ⓘ

Report generation options

Generate topics

Past generated reports by GEMA

Today's conversations

- Current Treatments and Emerging Perspectives in Heart Failure with Preserved Ejection Fraction (HFpEF) ×

Previous 7 days' conversations

- Investigating PI3K Alpha-Specific Inhibitors: A Targeted Approach ×
- Therapeutic Specific Agent ×

A circular profile picture of a man is visible in the bottom left of the sidebar.

Automated reporting: Turbo Platform



From raw data to complete reports in minutes

LLM models in TurboToxicology

Claude 3.5 Sonnet

OpenAI GPT-4

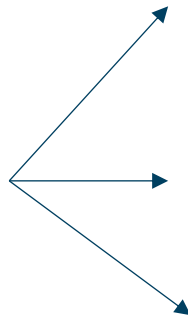
Meta LLaMA 3

... many other foundation models

... optional: client proprietary models

LLM models enhance report text

- Organizes content into categories
- Formats content into paragraphs
- Much more readable text
- Editable; regenerate from edited



- 50 mg/kg/dose:
 - Thin in 2 males began Day 22 no longer observed Day 43, and in 7 females began Day 22 no longer observed Day 93.
 - Hunched posture in 15 males began Day 25 through Day 148, and in 15 females began Day 25 through Day 148.
 - Discolored in 7 females began Day 29 no longer observed Day 85.
 - Salivation in 16 males began Day 15 no longer observed Day 83, and in 16 females began Day 16 no longer observed Day 83.
 - Staining in 16 males began Day 15 through Day 148, and in 14 females began Day 22 through Day 148.
 - Ungroomed in 16 males began Day 28 through Day 148, and in 16 females began Day 29 through Day 148.
 - Swollen in 9 males began Day 37 no longer observed Day 91, and in 5 females began Day 36 no longer observed Day 50.



User selections:
Model, Organize By, Format

Clinical Observations

Model: Organize By: Format:

Physical Condition and Appearance

At the 50 mg/kg/dose level, changes in physical condition were observed in both sexes. Thin appearance developed in 2 males and 7 females, first noted on Day 22. This condition resolved by Day 43 in males and by Day 93 in females. Additionally, ungroomed coat was noted in 16 males beginning Day 28 and persisting through Day 148, and in 16 females from Day 29 through Day 148. Body staining was also present in 16 males from Day 15 through Day 148, and in 14 females from Day 22 through Day 148.

Posture and General Demeanor

Changes in posture were apparent, with hunched posture observed in 15 males and 15 females, beginning on Day 25 and continuing through Day 148. Secretions and Discoloration Excessive salivation was recorded in 16 males from Day 15 to Day 83 and in 16 females from Day 16 to Day 83. In addition, discoloration of the coat was observed in 7 females, first noted on Day 29 and resolving by Day 85.

Swelling

Localized swelling was documented in 9 males, appearing on Day 37 and resolving by Day 91, and in 5 females, starting Day 36 and resolving by Day 50.

GenAI-Maximalist Skills

Craft LLM prompts

Experience

Software DevOps

Complex AI Tasks

Collaboration

Systems Level Design

Experience: training/teaching

AI tool for synthesizing new audio/image/avatars for training Teaching and training content generation will be changing

ElevenLabs

English



German

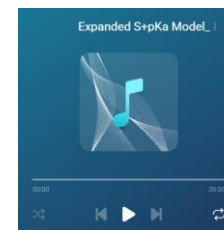


Play buttons to hear my synthetic voice used to create multilingual educational content on Ozempic



Create realistic image content: for business cases

NotebookLM



AI in Toxicology and Risk Assessment

Create podcasts: for business cases or just to hear the publication you couldn't read on your walks



Craft LLM Prompts: Shiny Assistant

Andrej Karpathy @karpathy

There's a new kind of coding I call "vibe coding", where you fully give in to the vibes, embrace exponentials, and forget that the code even exists. It's possible because the LLMs (e.g. Cursor Composer w Sonnet) are getting too good. Also I just talk to Composer with SuperWhisper so I barely even touch the keyboard. I ask for the dumbest things like "decrease the padding on the sidebar by half" because I'm too lazy to find it. I "Accept All" always, I don't read the diffs anymore. When I get error messages I just copy paste them in with no comment, usually that fixes it. The code grows beyond my usual comprehension, I'd have to really read through it for a while. Sometimes the LLMs can't fix a bug so I just work around it or ask for random changes until it goes away. It's not too bad for throwaway weekend projects, but still quite amusing. I'm building a project or webapp, but it's not really coding - I just see stuff, say stuff, run stuff, and copy paste stuff, and it mostly works.

12:17 AM · Feb 3, 2025 · 3.8M Views

The screenshot displays the Shiny Assistant interface. On the left, a code editor shows R code for a Shiny app. In the center, a list of six key changes is provided, detailing the removal of date-related functionality and updates to the CSV upload and visualization components. On the right, the 'Data Visualization App' is shown, featuring a 'Sankey Diagram' and a 'Bar Graph'. The bar graph displays 'Total Value' on the y-axis (ranging from 0e+00 to 1e+05) and 'Category' on the x-axis, with categories '(mg)', '(ng/mL)', and '(ug/mL)'. The interface includes a 'Run app' button, a 'Generate Sankey Diagram' button, and a 'Generate Bar Graph' button. A message input field at the bottom left contains the text 'Enter a message...'. The bottom of the image features a blue banner with the text 'CAREER DEVELOPMENT' and the 'aaps' logo.

Python Concise

```
theme_minimal() +
labs(title = "Bar Graph", x
})
})
}
shinyApp(ui, server)
```

Run app →

Here are the key changes I've made to remove date-related functionality:

1. Removed the `library(Lubridate)` import as it's no longer needed.
2. Removed the "Generate Time Series Graph" button from the UI.
3. Removed the Time Series Graph card from the layout.
4. Removed the date column selection from the column mapping UI.
5. Updated the CSV template download to not include a date column.
6. Removed the time series plot generation code from the server function.

This modified version of the app now focuses solely on the Sankey diagram and bar graph visualizations, without any date-related components. Users can still upload CSV files, map columns for source, target, value, and category, and generate Sankey diagrams and bar graphs based on their data.

Enter a message...

Shiny for R

```
app.R
18 card(
19   card_header("Sankey Diagram"),
20   sankeyNetworkOutput("sankey_plot")
21 ),
22 ),
23 card_header("Bar Graph"),
24 plotOutput("bar_plot")
25 )
26 )
27 )
28
29 server <- function(input, output, session) {
30   data <- reactiveVal(NULL)
31
32   observeEvent(input$csv_file, {
33     req(input$csv_file)
34     data(read_csv(input$csv_file$datapath))
35
36     # Update column mapping UI
37     output$column_mapping <- renderUI({
38       req(data())
39       column_names <- colnames(data())
40       tagList(
41         selectInput("source_col", "Source Column",
42                   column_names),
43         selectInput("target_col", "Target Column",
44                   column_names),
45         selectInput("value_col", "Value Column",
46                   column_names),
47         selectInput("category_col", "Category Column",
48                   column_names)
49       )
50     })
51
52     output$download_template <- downloadHandler(
53       filename = function() {
54         # ...
55       }
56     )
57   })
58 }
```

Data Visualization App

Upload CSV File

Browse... | Zolpide

Upload complete

Download CSV Template

Source Column: RECORDC

Target Column: VAR

Value Column: TIME

Category Column: UNIT

Generate Sankey Diagram

Generate Bar Graph

Sankey Diagram

Bar Graph

Total Value

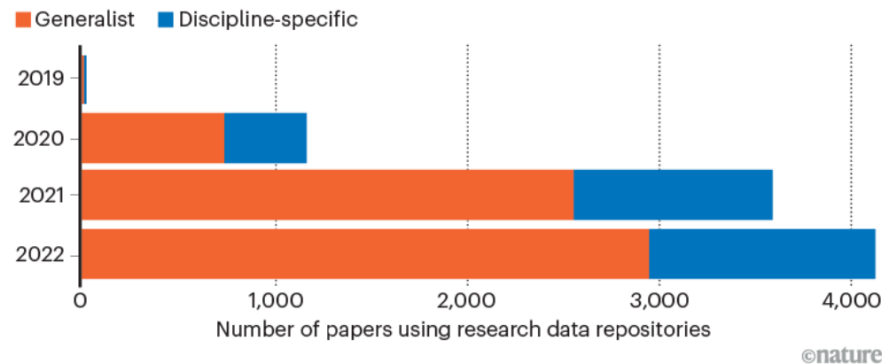
Category

(mg) (ng/mL) (ug/mL)

Data is the New Oil: LLMs are the Combustion Engines

RISE IN DATA ARCHIVING

Researchers are increasingly depositing data in repositories to widen access, but mostly in generalist rather than discipline-specific ones that offer curation. This can be seen in the top 15 repositories used in primary-research papers published in American Geophysical Union journals between 2019 and 2022.



FAIR and OPEN Data for AI and ML:

- Publicly available datasets for benchmark training data are lacking in our field
- Available data sources, types, formats are not interoperable
- Available data are not analysis ready (Labels lacking, structure unsuitable)
- Pretrained models that can be adapted for biological observations are lacking

<https://doi.org/10.1038/s42256-024-00911-w>

A call for an industry-led initiative to critically assess machine learning for real-world drug discovery

NIH Data Sharing Index (S-index) Challenge

Promoting data sharing and developing a robust metric to reward exemplary data sharers.

This Challenge aims to incentivize and reward data sharing excellence, promoting a new metric for assessing how effectively researchers share valuable data, driving a culture of openness in science.

Kindly provided by Shelly Stall

Hanson et al. Nature 623, 28-31 (2023)

doi: <https://doi.org/10.1038/d41586-023-03316-8>

Maskey, M., Alemohammad, H., Murphy, K. J., and Ramachandran, R. (2020), Advancing AI for Earth science: A data systems perspective, Eos, 101, <https://doi.org/10.1029/2020EO151245>. Published on 06 November 2020

Explainable AI (XAI): Small Steps

As the LLMs have gotten progressively larger, they have begun to surpass some repeatable human performance, however they show plagiarism, bias, are black box like and hallucinate thus area of active research

BioGPT and human annotator have comparable performance in biomedical research test

Selected performances on PubMedQA, which tests biomedical language processing

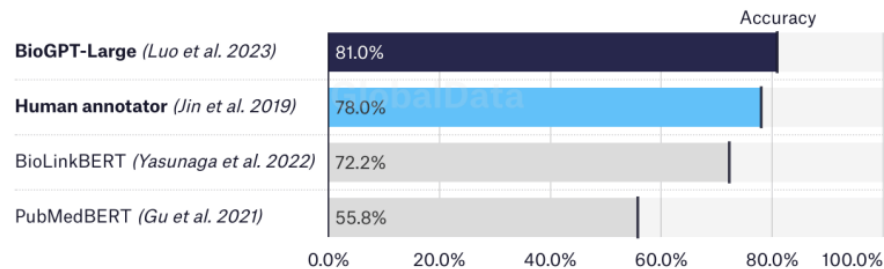


Chart: GlobalData • Source: PubMedQA

Table 2. Application of specialized LLMs in different fields of medical science

Sl. no.	LLM	Year of release	Remarks	Reference
1.	PMC-LLaMA	2023	PMC-LLaMA, an open-source language model that is developed by refinement of an open-source language model on a total of 4.8 million biomedical academic papers for added injecting medical knowledge, improving its capability in the medical domain.	Wu et al. ⁹⁶
2.	ClinicalCamel	2023	It is an open LLM obviously tailored for clinical research. Fine-tuned from LLaMA-2 using QLoRA, Clinical Camel achieves state-of-the-art performance across medical benchmarks among openly available medical LLMs. Leveraging efficient single-GPU training.	Toma et al. ⁹⁷
3.	MedAlpaca	2023	MedAlpaca was developed by instruction fine-tuning of the LLaMA 13B and 7B models on Medical Meadow data. It is also the assembly of reformatted instruction-response pairs with datasets for medical NLP tasks and data derived from various internet sources.	Han et al. ⁹⁸
4.	BioGPT	2023	BioGPT is a domain-specific GPT language model for biomedical text generation and mining. BioGPT follows the transformer language model backbone, and is pre-trained on 15M PubMed abstracts from scratch.	Luo et al. ⁹⁹
5.	BioMedLM	2022	BioMedLM is based on a HuggingFace GPT model (decoder-only transformer) with 2.7B parameters and a maximum context length of 1,024 tokens. It also uses a custom biomedical tokenizer trained on PubMed abstracts with a vocabulary size of 28,896.	Karkera et al. ¹⁰⁰
6.	Med-PaLM2	2022	Med-PaLM is a large language model (LLM) designed to provide high quality answers to medical questions. It is also available to Google Cloud customers, who are able to explore a range of applications, from basic tasks to complex workflows. It has been aligned to the medical domain and evaluated using medical exams, medical research, and consumer queries.	Luo et al. ¹⁰¹
7.	ChatDoctor	2023	This is a specified language model with improved accuracy in medical advice refining the large language model meta-AI (LLaMA) by a large dataset of patient-doctor dialogs obtained from a widely used online medical consultation platform.	Li et al. ¹⁰²

Human-in-the-Loop: Where We Stand

HITL integrates human input and expertise into the lifecycle of ML and AI systems. This includes approaches like:

Active learning (AL): humans label data at the systems request

Interactive machine learning (IML): Users interact frequently with the learning system, providing information incrementally to guide the learning process.

Machine teaching (MT): Human experts define and transfer specific knowledge to the machine learning model, giving them more direct control over what is learned.

Human-in-the-loop assisted de novo molecular design

[Iiris Sundin](#) ✉, [Alexey Voronov](#) ✉, [Haoping Xiao](#), [Kostas Papadopoulos](#), [Esben Jannik Bjerrum](#), [Markus Heinonen](#), [Atanas Patronov](#), [Samuel Kaski](#) & [Ola Engkvist](#)

Journal of Cheminformatics **14**, Article number: 86 (2022) | [Cite this article](#)

5529 Accesses | 13 Citations | 25 Altmetric | [Metrics](#)

An algorithmic framework for synthetic cost-aware decision making in molecular design

[Jenna C. Fromer](#) & [Connor W. Coley](#) ✉

Nature Computational Science **4**, 440–450 (2024) | [Cite this article](#)

The AI-driven Drug Design (AIDD) platform: an interactive multi-parameter optimization system integrating molecular evolution with physiologically based pharmacokinetic simulations

Published: 19 March 2024

Volume 38, article number 14, (2024) | [Cite this article](#)

[Jeremy Jones](#) ✉, [Robert D. Clark](#), [Michael S. Lawless](#), [David W. Miller](#) & [Marvin Waldman](#)

Clinical Pharmacology & Therapeutics

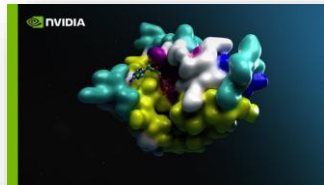
State of the Art Review

Current Status and Future Directions: The Application of Artificial Intelligence/Machine Learning for Precision Medicine

[Kunal Naik](#), [Rahul K. Goyal](#), [Luca Foschini](#), [Choi Wai Chak](#), [Christian Thielscher](#), [Hao Zhu](#), [James Lu](#), [Joseph Lehár](#), [Michael A. Pacanoswki](#), [Nadia Terranova](#), [Neha Mehta](#), [Niklas Korsbo](#), [Tala Fakhouri](#), [Qi Liu](#), [Jogarao Gobburu](#) ✉ ... [See fewer authors](#) ^

Explainable LLMs: Multi-Modal Information

AI in medicine and drug discovery is a single mode story- But over time that narrowness and constraint may well be alleviated.

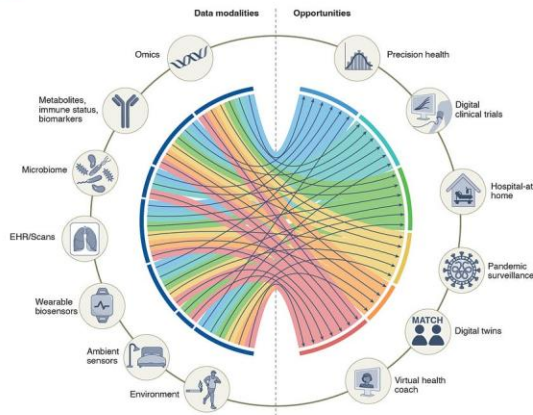


Get Started With NVIDIA BioNeMo

NVIDIA BioNeMo™ is an AI platform for drug discovery that simplifies and accelerates the building and training of models using your own data and scaling the deployment of models for drug discovery applications.

nature
medicine

Multimodal biomedical AI



Acosta J et al,
September 2022

MedQwen3B-Reasoner

A 3B parameter LLM that learns to reason across domains and express uncertainty
Trained using continual cross domain reinforcement fine-tuning (GAPQ)

Medical Domain 70% + Math Domain 30% + Cross-Domain Reasoning

Mathematical Reasoning	Medical Research	Clinical Decision
<p>How much money did Agatha have at first for her bike purchase? Agatha spends \$15 on frame, \$25 on front wheel, with \$20 left for seat and handlebar tape.</p> <p><reasoning> To determine how much money Agatha initially had, we need to add up the amount she spent on the frame, the front wheel, and the remaining money she has left to spend on a seat and handlebar tape. The total amount spent on the frame and the front wheel is: $\\$15 + \\$25 = \\$40$ The remaining money she has left is \$20. Therefore, the initial amount of money Agatha had is the sum of the money she has spent and the money she has left. $\\$40 + \\$20 = \\$60$ </reasoning> <answer> Agatha initially had \$60. </answer></p>	<p>Does BMP2/7 expression predict tumor recurrence time? Study examined BMP expression in bladder cancer patients after TURBT surgery.</p> <p><reasoning> The study indicates that high expression of BMP2 and BMP7 correlated with prolonged time to recurrence (log-rank: $p = 0.01$ and $p = 0.03$ respectively). This means that the gene expression levels of BMP2 and BMP7 were significantly associated with the time to recurrence, with higher expression leading to a longer time to recurrence. Therefore, based on the statistical significance (p-values < 0.05) it is reasonable to conclude that the expression of bone morphogenetic protein-2 and -7 in urinary bladder cancer patients predicts time to tumor recurrence. </reasoning> <answer> yes </answer></p>	<p>Best vaccination strategy for hesitant parents? Choose between: strict schedule, flexible timing, alternative schedules, or patient dismissal.</p> <p><reasoning> The strategy recommended by pediatricians to encourage vaccination among hesitant parents should not lead to the abandonment or dismissal of families as it can undermine the critical role of pediatricians in protecting children's health. Option D can harm the trust between the pediatrician and the parent, potentially alienating them. Options B and C might create confusion or threaten parents' trust in the recommended vaccination schedule. Option A, on the other hand, provides an evidence-based compromise that allows some flexibility while ensuring coverage for essential vaccines, which can be respected by hesitant parents as it balances their concerns with public health needs. This approach respects the autonomy of parents while providing relevant information and reassurance, which can help in addressing their hesitations, making Option A the most suitable strategy. </reasoning> <answer> A </answer></p>

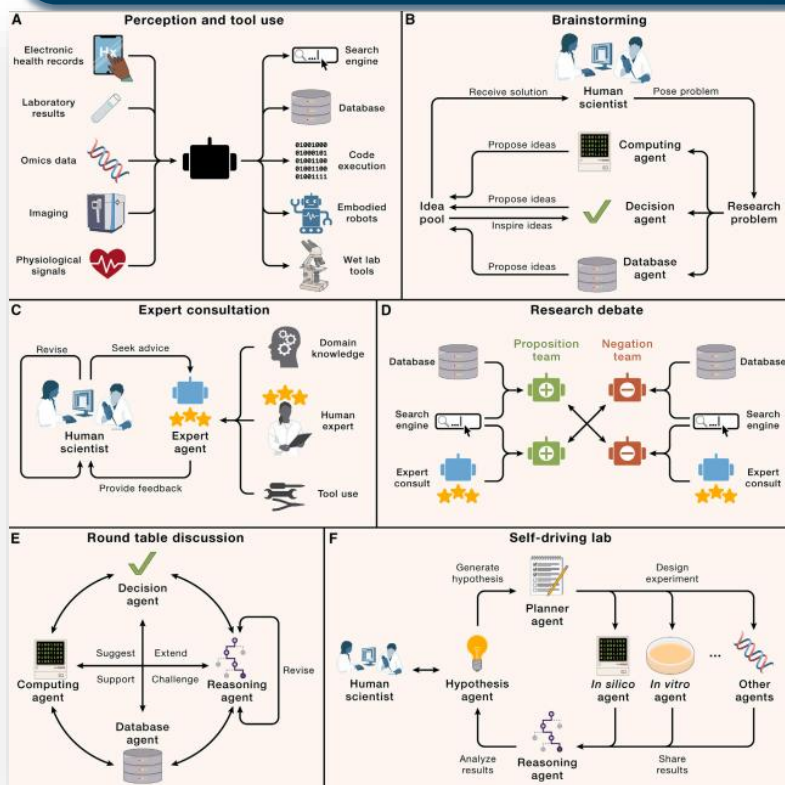
<https://nvidianews.nvidia.com/news/nvidia-unveils-large-language-models-and-generative-ai-services-to-advance-life-sciences-r-d>

Acosta, J.N., Falcone, G.J., Rajpurkar, P. et al. Multimodal biomedical AI. Nat Med 28, 1773–1784 (2022). <https://doi.org/10.1038/s41591-022-01981-2>

<https://huggingface.co/hooman650/MedQwen3B-Reasoner>

The current future: AI Scientist

systems capable of skeptical learning and reasoning that empower biomedical research through collaborative agents that integrate AI models and biomedical tools with experimental platforms. Rather than taking humans out of the discovery process, biomedical AI agents combine human creativity and expertise with AI's ability to analyze large datasets, navigate hypothesis spaces, and execute repetitive tasks.



Autonomous chemical research with large language models

<https://doi.org/10.1038/s41586-023-06792-0> Daniil A. Boiko¹, Robert MacKnight¹, Ben Kline² & Gabe Gomes^{1,3,4,5,6}
Received: 20 April 2023

A REVIEW OF LARGE LANGUAGE MODELS AND AUTONOMOUS AGENTS IN CHEMISTRY

A PREPRINT

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November 18, 2024

Digital medicine

The rise of agentic AI teammates in medicine

Medicine is in the dawn of a fundamental shift from using artificial intelligence (AI) as tools to deploying AI as agents. When used as a tool, AI is passive and reactive. Even powerful medical AI foundation models today remain tools that depend on human users to provide input and context, interpret its output, and take follow-up steps. To fully unlock AI's potential in medicine, clinicians need to make the key conceptual shift: from using AI as sophisticated calculators to embracing AI as health-care teammates. Unlike tools, agentic AI has the potential to take initiatives; rather than waiting for queries and data, agents can proactively monitor and pull data from the health-care system to identify issues and propose solutions. An AI agent can maintain long-term memory and context, tracking complex patient histories and interactions over time. Furthermore, it can autonomously navigate databases such as electronic health records and orchestrate various tools, including specialised AI algorithms for specific subtasks. Much more work is needed to develop AI agents, but ongoing research shows key agentic capabilities. First, most AI agents are large language models (LLMs) and LLMs have rapidly improved their reasoning and problem-solving abilities. For instance, by leveraging longer reasoning chains, LLMs have achieved high performances on mathematical examinations and in making differential diagnoses in pathology. Second, LLMs have become more adept at interacting with the external environment and using tools, for example, the ability to directly use computers to fill out web forms. Medical LLMs have also improved their reliability by using search engine tools to retrieve relevant medical knowledge. Third, collaborations between multiple AI agents with complementary expertise have expanded their capability to address open-ended challenges. This is illustrated by preliminary research from a virtual laboratory, in which an AI professor agent led a team of AI scientists to design new nanobody binders for SARS-CoV-2 variants. Yet such research still requires further verification and validation. By harnessing these advances, AI agents have the potential to become valuable teammates to human clinicians. While separate AI tools exist for tasks such as transcribing patient meetings, analysing medical images, and searching clinical guidelines, in the future an AI clinical manager agent might be able to orchestrate these tools while maintaining an understanding of patient histories and clinical visits. Instead of juggling multiple tools, the clinician could interact with a single manager agent. In this scenario, human clinicians would supervise AI agents. Such agents could address the fragmentation of medical data by aggregating central information and facilitating communication between specialists, health-care providers, and databases.

Agentic AI in medicine poses exciting opportunities but also new challenges that require careful investigation. We will need new frameworks for evaluating and regulating AI agents to ensure responsible use. Notably, in the USA, the Food and Drug Administration's review of medical AI devices treats each AI as a tool for tackling a specific task. Thus, existing assessments typically focus on AI performance for a narrow medical output. New evaluation frameworks for AI agents could draw inspiration from more holistic assessments and extended real-world residences that are integral to medical students' training. Additionally, conflation by AI agents is a risk and continuous performance monitoring will be essential. Multi-agent systems could play a part here with specialised safety or reliability agents assisting human supervisors in continuously evaluating AI agent's behaviour (figure). Defining appropriate use cases and establishing boundaries for AI agent autonomy will also be crucial. Initial deployments might focus on low-risk administrative tasks in controlled virtual environments. Health-care professionals would also need training to effectively collaborate with these semi-autonomous AI teammates. Undoubtedly, some reasonable concerns about AI by the medical community will be exacerbated by an extension of AI that is more autonomous. This is why compelling evidence of enhanced accuracy, productivity, and safety will be required to accept a new era of agentic medicine. The time to prepare for this future is now.

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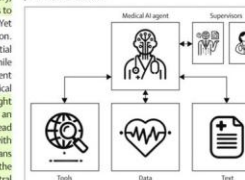


Figure: Medical AI agent orchestrating tools and data while monitored by human clinician and AI reviewer

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Gao S, Fang A, Huang Y, Giunchiglia V, Noori A, Schwarz JR, Ektefaie Y, Kondic J, Zitnik M. Empowering biomedical discovery with AI agents. Cell. 2024 Oct 31;187(22):6125-6151. doi: 10.1016/j.cell.2024.09.022. PMID: 39486399.

The rise of agentic AI teammates in medicine. Zou, James et al. The Lancet, Volume 405, Issue 10477, 457

Key Skills: Context is the Endgame

Understand Market Needs

Attend conferences, webinars, and network with AI experts to identify skill gaps and align expertise.

Continuous Learning

Take courses on LLM methodologies aligned with your interests.

Use AI Strategically

Focus on solving clinical and medical challenges without adding complexity.

Understand Data Quality

Evaluate data quality, regulatory, and ethical aspects.

Select Tools and Techniques

Identify suitable algorithms, frameworks, and relevant tools (e.g., Python/R/Javascript) for healthcare applications.

Collaborate and Iterate

Work with interdisciplinary teams, test prototypes, and refine solutions for better usability. Balance critical thinking, adaptability, communication, curiosity, and technical proficiency

Learn APIs

Understand wrappers and APIs to enhance system integration.

Questions & Contact



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Dream Weather Artisan

Asian-inspired dreamy weather visuals with literary facts and spiritual depth.

By Priyata Kalra 20+



PBPK First-in-Human Guide

By Priyata Kalra X

A PBPK assistant for first-in-human drug prediction brainstorming.

The Allies of this talk

John DiBella
Haiying Zhou
Christina Hendrickson
Vladimir Chupakhin
Rafal Bachorz
Manas Shah
Andrea Ceja
Nash DelCamp
Victor Aguilar
Melissa Van Bussel (Health Canada)
Thomas Hartung (JHU)
Jurgen Pahle (University of Heidelberg)
Shelly Stall (NASA)
Thomas Leuchtefeld (inSilica)
Allen Lat (Corcept Therapeutics)
David Watson (Resero Analytics)
Jubin Shah (molecular Health)
AAPS Community: Tina Morris, Joy Davis, Rebecca Stauffer, Stacey Royson

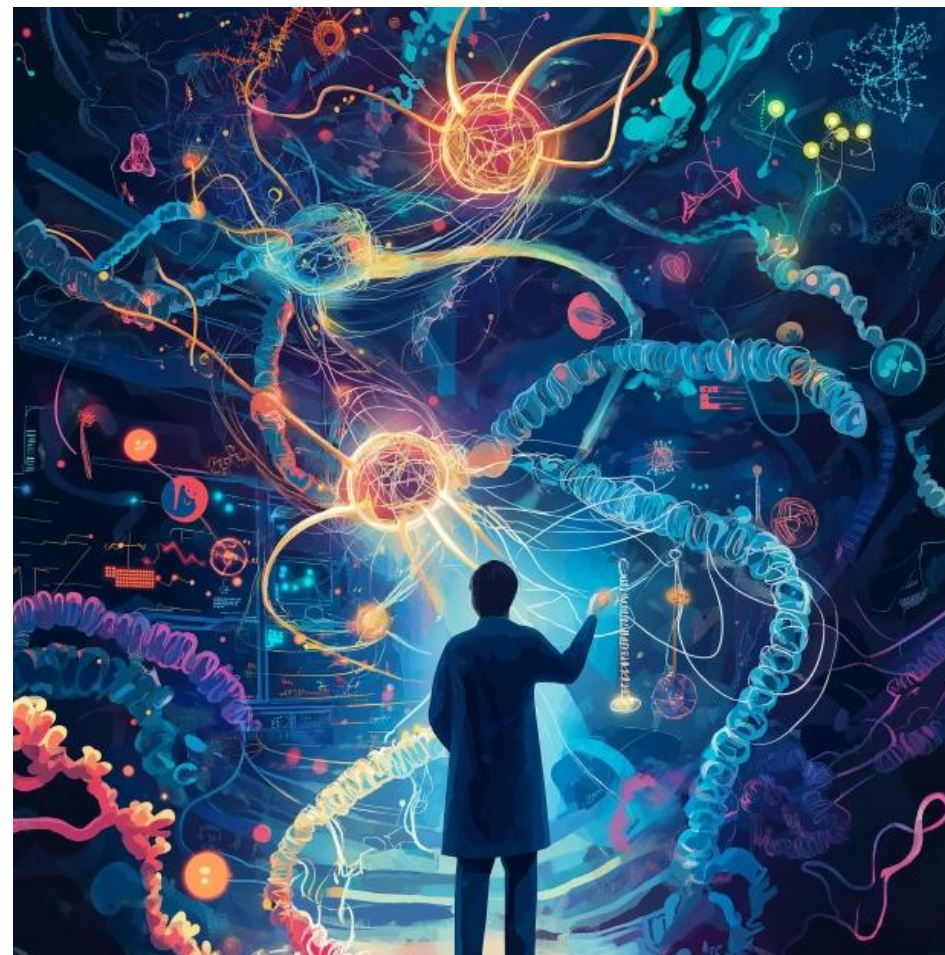


Image: Midjourney

Agenda: Skills for Future of Work?

Humanics

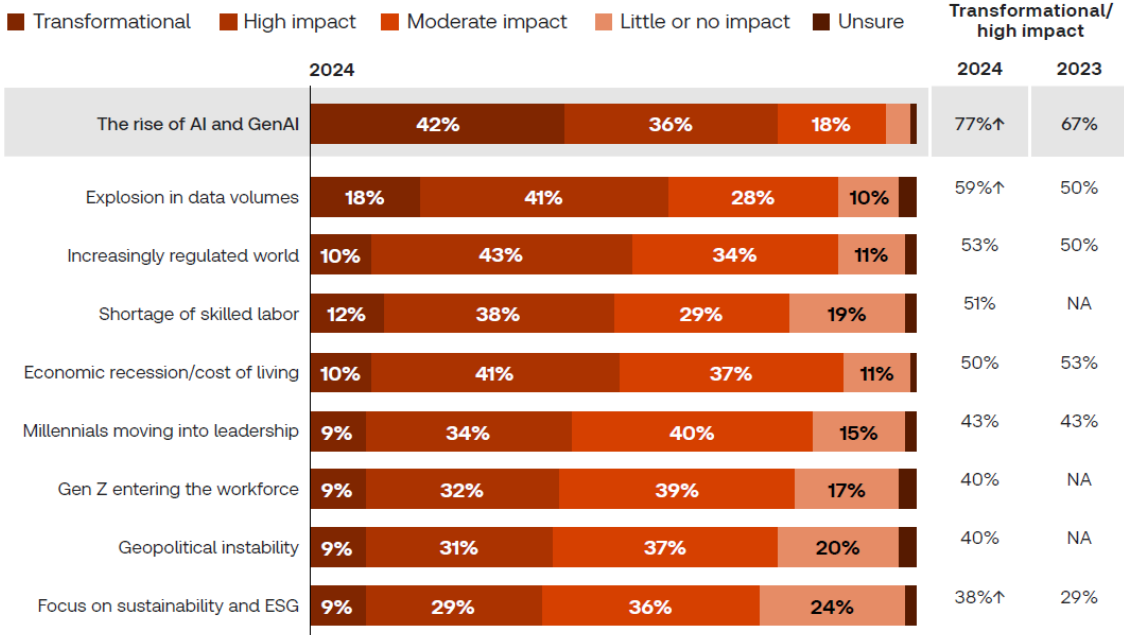
Nurture human nature and affair.

Knowledge

Increase knowledge on the edge of rare problems.

The Rise of GenAI

To what extent do you think the following trends will impact your profession over the next five years?



Source: Thomson Reuters 2024

Generative AI could:

- Produce **\$60 billion to \$110 billion** in annual revenue across the pharmaceutical industry value chain
- **Impact 10% of the tasks** carried out daily by 80% of the workers

Human side: 70 percent of digital transformations fail not because of technical issues but because leaders ignored the importance of managing change.

Humanics

Critical Thinking

Analyze problems from multiple angles.

Communication

Articulate ideas clearly to diverse audiences.

Adaptability

Learn to leverage AI for greater productivity.

Curiosity

Embrace continuous learning and exploration.

Experience

Reimagining our education and empathy.

Knowledge

AI Basics

Understand foundational AI concepts and capabilities.

Prompt Engineering

Craft effective prompts to maximize AI output.

AI Tool Familiarity

Gain acquaintance with emerging AI applications

Tech Literacy

Stay current with evolving digital technologies.

Math

Numeracy with statistics and basic math.

Desire to Learn- how I do it?

Permissionless Apprenticeship

Dive in and learn by doing, then build theory.

Learning Resources

Leverage online courses, podcasts, and social networks.

Learn in Public

Have a habit of creating.

Learn for necessity

Top-down approach for busy work

OpenAI confirms that AI writing detectors don't work

No detectors "reliably distinguish between AI-generated and human-generated content."

<https://arstechnica.com/information-technology/2023/09/openai-admits-that-ai-writing-detectors-dont-work/>

Craft LLM Prompts: 4o canvas

design elements. Here is an updated CSS file that you can add:

Website Styles

I've added a CSS file to style your HTML similar to the Simulations Plus website. It includes a gradient banner, modern typography, hexagonal images, and a cookie banner. Let me know if you need any further modifications or adjustments!

give me the updated files as .html and .css

I've saved the updated HTML and CSS files for you. You can download them using the links below:

- index.html
- styles.css

Let me know if you need further adjustments or additional features! [🗨️]

```
1 /* styles.css */
2
3 body {
4   font-family: 'Roboto', sans-serif;
5   margin: 0;
6   padding: 0;
7   box-sizing: border-box;
8   background-color: #f4f4f4;
9   color: #333;
10  }
11
12 header {
13   background: #002a4e;
14   color: #fff;
15   padding: 20px 0;
16  }
17
18 .navbar .container {
19   display: flex;
20   align-items: center;
21   justify-content: space-between;
22  }
23
24 .logo {
25   font-size: 1.8em;
26   font-weight: bold;
27  }
28
29 nav ul {
30   list-style: none;
31   display: flex;
32   gap: 20px;
33  }
34
35 nav ul li a {
36   color: #fff;
37   text-decoration: none;
38   font-weight: 500;
39   transition: color 0.3s;
40  }
41
42 nav ul li a:hover {
43   color: #ffd700;
44  }
45
```

- PHP
- C++
- Python
- JavaScript
- TypeScript
- Java

