• **Artificial Intelligence in MS Instrumentation and Applications**

Vibe Coding Mass Spectrometry Tools (I'm Sorry) *and how I put them online!*

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Reprints: https://reprints.katzlab.org/

https://reprints.katzlab.org/asms-2026-vibecoding/

Introduction

There are admittedly a myriad of tools to do things like calculate PPM, MW, etc., and, honestly, it is pretty easy to create these in a spreadsheet. Nevertheless I found myself wanting to do simple calculations from my phone, or, otherwise wanting to perform calculations with more reactive interfaces.

You all know how to use Claude/ChatGPT, etc. I used ChatGPT.

What I share that I felt would be useful was how to take the output from your session and easily and cheaply host it for mass consumption! Here I show my workflow for this using CloudFlare.

TL;DR: The examples to create MS tools are useful, but, the workflows for their creation/hosting are perhaps something you haven't seen.

Methods

1) Start with an idea for a tool you want.
2) Prompt ChatGPT to code your idea.
   a) Ask for standalone HTML/JavaScript (if you dont, it really wants to use Vite/Next.js/some other tool that needs you to "build" your web page – Im not that clever).
   b) To save time, I also have it code my logo in.
   c) If you include a screen shot of an existing page, you can request it match your color scheme.
3) Test your Code!
   a) Save your code as **index.html** in some directory
   b) Run **python3 -m http.server** in that directory
   c) Point your browser to **localhost:8000**
   d) If it doesn't work, prompt for fixes
4) Get a CloudFlare account if you dont have one
   a) Get a domain name if you want one (not required, but, cooler….. CloudFlare offers this at cost)
   b)
5) Using 'wrangler' on the commandline, upload your project to CloudFlare.
   a) If you want, you can also just use the web interface and upload a zip file of your resources
6) Use the project URL, or, link it to your custom URL
7) Share with your friends.

Results

The fruits of this activity have yielded several tools.

You can use the tools described at:

https://katzlab.org/

Access to the tools is provided through **CloudFlare**, which, because of the usage, only costs the price of the domain name itself ($10.12/yr). **I would like to stress, I consider none of these tools novel or terribly improved over what exists (except for HMDBSEARCH, I friggin' love that). The main point of this conversation is to show how to easily put your own tools on the Internet.**

Here are the current tools:

Hmdbsearch: Search the HMDB for a given mass with a PPM error. Seriously, have you every made a measurement and wanted to search HMDB for the compound? Been frustrated as you manually calculate an upper and lower range? **NO MORE!** My favorite tool :)

PPM: Given a true and measured mass, calculate the PPM. Yawn.

Molecular Weight Calculator: Formula to Mass. Given a chemical formula, calculate the monoisotopic exact mass. Want adducts (H^+, H^+ and Na^+, Pull a Proton?), no problem. D2O? Sure thing for [13]C. Options to report Neutral and m/z.

Molecular Formula Calculator: Mass to Formula. Have a mass, want to figure out a formula? Have a mass delta, want to try to figure out what it is? This tool could be your friend. It takes a collection of elements and ranges (you can also select default ranges) and generates a list of formulae ordered by error. It also calculates some sanity checks (DBE, various element ratios). The mass can also be "Math" such as "195.0879 - H+", "200-10.3234".

Two fun things:
1) This can also calculate element losses to get to your mass delta.
2) You can click on the reported formula to do a PubChem Search.

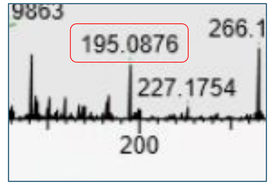
Conflict of Interest

I own some CloudFlare stock. I bought it a few years ago because I liked their product and I had fun drinking their Kool-Aid; my cousin the big time stock investor thought I was stupid.

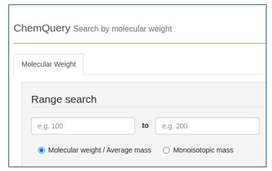
Acknowledgement

I would like to thank my friends and colleagues that have dogfooded these tools and help to make them better, notably, Mario Alba, Ethan Canfield, Kruttika Dabke, Jennifer Kyle, Jiajun Lei, Tao Liu, Layla Phillips and Cara Sake.

1- Sample Tool Development Workflow



Hmm… What compound is this?



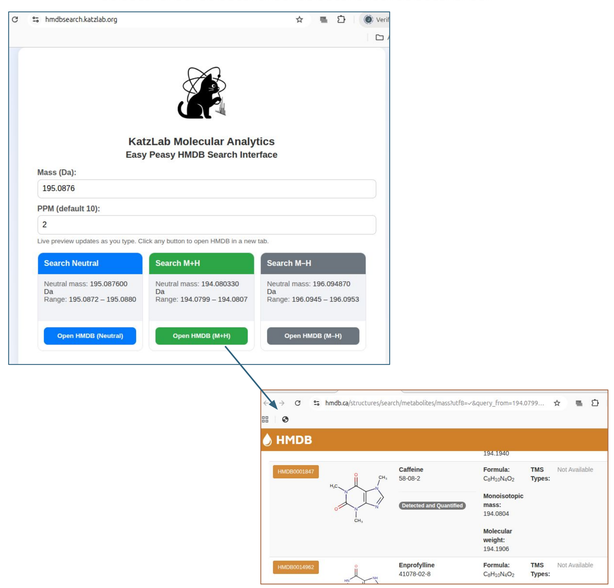
HMDB.CA

I just want to put in the m/z I measured! Why do I have to math a range? Why is "Average" the default?

Hi Chat! lets create a javascript webpage…. it has a form that asks for a mass and a ppm then it generates a URL and sends you to a page as follows: https://hmdb.ca/structures/search/metabolites/mass?utf8=%E2%9C%93&query_from=488.2032&query_to=488.2048&search_type=monoisotopic&commit=Search#results where 488.2032 and 488.2048 are replaced by the mass +/- the ppm as inputted in the URL

Chat GPT WORKING PROTOTYPE

you are SO good at this that I want to add a feature… under the mass, you can say "correct for an H+ adduct" and "correct for an H- adduct". if they click one of these buttons, add or subtract 1.00727 from the mass respectively before doing the calculation, please. Also, let's default the PPM error to 10….



Shown in **Figure 1** is a sample workflow from problem realization through tool creation. The problem shown is the measurement of a mass and the desire to search HMDB. HMDB's interface requires a range rather than a mass with an error tolerance. The mass also needs to be neutral. Shown is the ChatGPT prompt to create a web page to accomplish this goal. The major iterations are included but some refinements are removed for simplicity (like adding ioncat.png).

The final web interface is shown as well as the output produced when using the program.

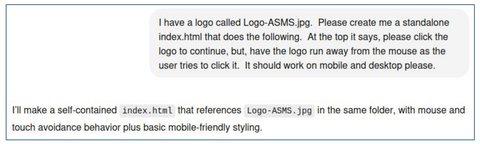
You ALREADY know **Claude** and **ChatGPT**….

Pause here to learn **my easy way** to put tools in the web from Idea to DONE in **15 minutes**!

https://katzlab.org/

2- 15 min to Create and Publish Your Tool Online!

A) Create your App…



B) Download. Test (if desired)

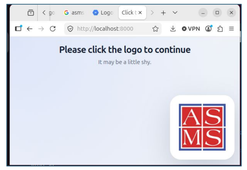
```
$ mkdir ASMS_DEMO
$ mv ~/Downloads/index.html ASMS_DEMO
$ mv ~/Downloads/Logo-ASMS.jpg ASMS_DEMO
$ cd ASMS_DEMO
$ python3 -m http.server
Serving HTTP on 0.0.0.0 port 8000 (http://0.0.0.0:8000/) ...
```

The example shown was from a Linux environment with python3 installed (to create a local http server).

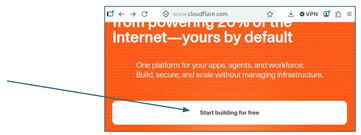
Neither is required for the subsequent steps.

Just place all files in their own directory for use in step 2F.

Testing can always be done "live".



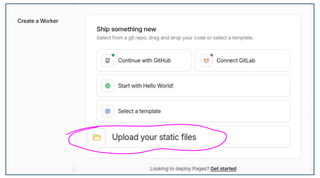
C) Get your account at **cloudflare.com**



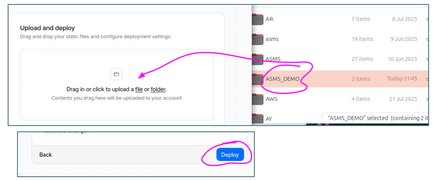
D) Get your custom domain if desired.

E) Create a "page" application

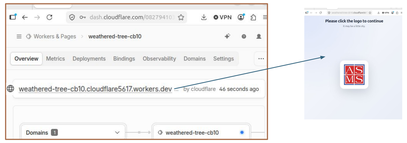
F) Upload Content



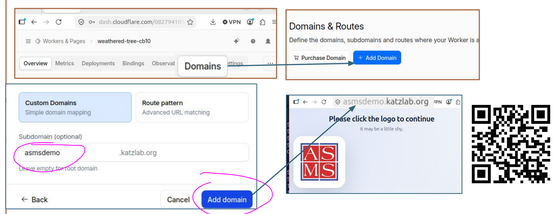
In this case I will be using static content, just dragging in the folder. But, notice that you can link to github, or download their command line tools to build and manage projects. Easy to start, maintainable when you want it to scale.



G) Test (or use if you don't have a domain)



H) Map to your domain!



Shown in **Figure 2** are seven steps demonstrating the process of creating an application, staging it on your local computer and testing it (2A,2B). Steps 2C and 2D outline the creation of a CloudFlare account (free) and acquiring a domain (~$10/yr). Finally, steps 2E-2H demonstrate how to upload your web page and map it to your custom domain (if desired).

3- Prompting and Debuging of KatzLab.org

For the curious, more details on the prompting performed for building the katzlab.org tools are available on the reprint link for this poster.

It probably goes without saying, but, constant and through testing are imperative for any AI generated code base. There were definitely some amusing fights in the creation of some of these tools.

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