

From Prompt to Platform: Vibe Coding Mass Spectrometry Tools

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Introduction

There are admittedly a myriad of mass spectrometry tools (calculate PPM, MW, etc.). Sometimes the tools are not quite a match for desired workflows or for solving niche problems, so, you vibe code a new tool using AI (Claude/ChatGPT etc). If you made a great new tool and want to share it, that path is less well known. Here we demonstrate facile and inexpensive ways to make your tools available for common use, including a complete walkthrough from "idea" to "product" that can be performed in **15 minutes** by **anyone that can use a browser**.

Methods

Like you, we use a generative AI. Possibly like you, we do AI assisted programming workflows to develop tools. Because we are targeting final access/availability on a standalone website, we are specifically prompting for lightweight, browser-based computational tools that can run in a browser environment. We often test applications locally before deployment using a Python HTTP server, iterating for feature correctness and desired functionality scope.

Post development, tools are deployed as static web pages either on the Cloudflare Pages infrastructure or via Github Pages. Access is either through a free public URL or custom domain. The advantage of the Git repository is that it is inherently version-controlled and often a familiar environment to many developers. Each committed change to the Github repository triggers automatic redeployment, similar to cloudflare, tools can be served as paths under a single domain or separated across multiple domain names. Neither route requires a conventional software build framework, enabling rapid iteration from specification to deployed tool.

Results

The overall workflow: You start with an awesome idea, which you develop into a standalone HTML/JavaScript using your favorite AI model, create free Cloudflare or Github accounts, optionally buy a custom domain or use a free Cloudflare/Git URL and deploy directly using just Cloudflare or a Github repository which also enables maintaining and developing code iteratively, documenting code history, automating deployment and collaborating with others.

Two tools are presented here as representative examples of this approach and to share our learned lessons in development.

Tool 1 – Easy Peasy HMDB Search (ChatGPT, Cloudflare Pages): HMDB searches require neutral monoisotopic mass and absolute tolerance, while compounds are typically reported as observed m/z and ppm tolerance (UG! SO MUCH MATH). The tool converts a single observed m/z into search windows for neutral, [M+H], and [M-H] interpretations and generates direct HMDB queries, simplifying calculations.

Tool 2 – Concentration calculator (ClaudeCode, Git Repo + Cloudflare Pages): Tools exist (e.g. TraceFinder) for calculating concentrations of unknown compounds from standard curves for those who do this on a daily basis. But for a lab that has to do these calculations sparingly, spending >\$5,000 to use those tools is ouchy costly. Our tool takes input directly from Skyline and after plugging in some metadata, calculates concentrations, flags outliers and visualizes results. Users can choose different models for calculations, interact with the standard curves to drop points from a fit and decide on data visualization from a set of options. Results can be shared as downloadable PDFs, CSVs or a snapshot of results in JSON format viewable by anyone on the website.

Happy hour drinking and prompting end up as real tools...

Tool 1: I wish HMDB was easy to search...

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?

Tool 2: I need an easy way to calc std curves and []'s

How do I calculate conc. of hundreds of compounds, visualize results and share reports *easily* with others at \$0 cost and minimal time/effort?

Use your excellent prompt writing skills to ask Claude/Chat to generate a javascript webpage

Claude/Chat GPT WORKING PROTOTYPE

Iterate / Add more cool features / Add cool logos (bonus-points if based on a real cat)

