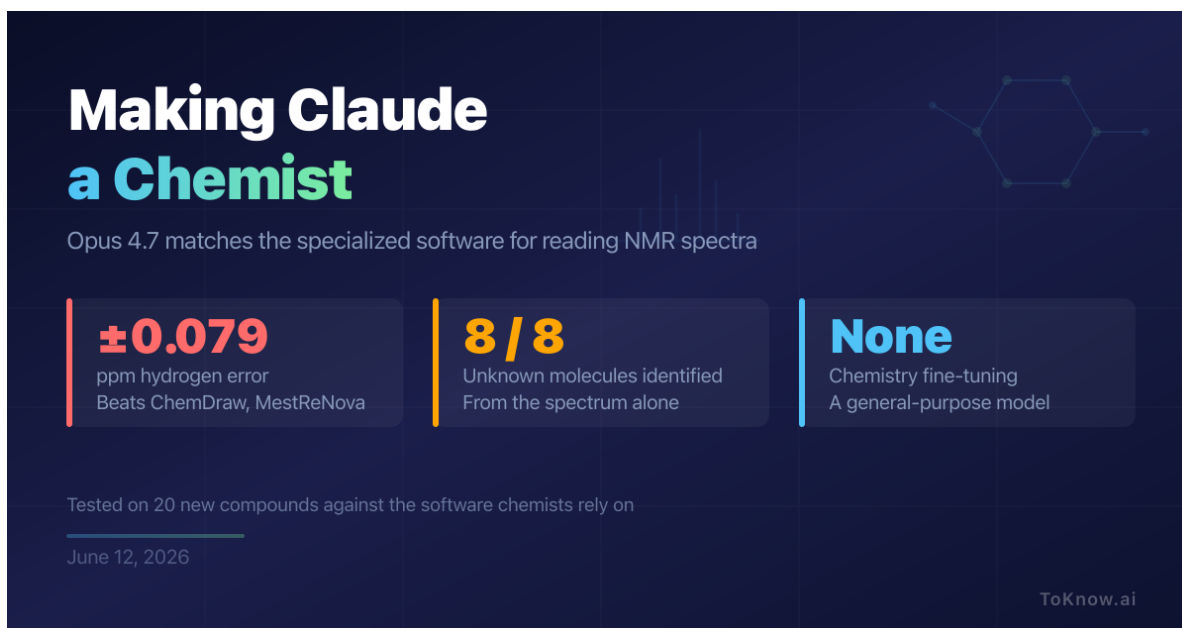


Claude Now Matches the Specialized Software Chemists Use to Identify Molecules

Kabui, Charles

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Anthropic published its first chemistry white paper, testing whether Claude can read an NMR spectrum, the magnetic-resonance readout chemists use to work out a molecule's structure. Reading one by hand means matching every peak to an atom in the proposed structure, one of chemistry's slowest steps. Anthropic chemist David Kamber pitted three Claude models

against ChemDraw and MestReNova, the desktop software built for the job, on 20 new compounds from preprints published after the models' training cutoff. Given a molecule as a line of text, Claude Opus 4.7 placed each hydrogen peak with an average error of ± 0.079 ppm, edging out both programs, and tied MestReNova on carbon. Handed only a spectrum and a chemical formula, it recovered all eight simpler unknown structures on every attempt.

What stands out is that Opus 4.7 had no chemistry-specific training, yet it competes with software written for this one job. For a working chemist, pasting a peak list and a formula into a chat can confirm a known compound or propose an unknown one, with no special setup. Dedicated structure-elucidation tools have existed for decades but need richer two-dimensional data; Claude works from the same basic readout already on screen.

The result reframes how AI is reaching the lab. Rather than a model fine-tuned for chemistry, a general assistant matches software built for one narrow task. The limit now is trust, not raw skill: on the hardest unknowns Claude sometimes reasoned in circles without committing, so a chemist still checks the answer.

Read More: [GPT-Rosalind: OpenAI's Specialized Model for Life Sciences and Drug Discovery](#)

Sources:

- [Making Claude a chemist \(Anthropic\)](#)
- [Claude vs. ChemDraw on NMR prediction and structure elucidation, full white paper \(Anthropic, PDF\)](#)
- [Anthropic AI for Science program](#)
- [Anthropic's announcement \(X\)](#)

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