Expansion of Chenomx NMR Compound Library with publicly available compound databases.

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SUMMARY:

One dimensional proton (1H) NMR spectra of biological mixtures (i.e. serum, plasma, CSF, urine) can easily be analyzed using Chenomx's NMR Suite. The Profiler module, coupled with a sophisticated and flexible *multi*-frequency compound library database, allows for spectral deconvolution, identification and quantification of single metabolites.

Chenomx has developed an integrated software suite and over 330 detailed signatures of common compounds used for metabolomics research. Spectral models of reference compounds can be searched and overlaid on the experimental spectra to interactively validate or invalidate potential metabolites. However, burdensome external web searches based on observed peak positions are required to search for metabolites not currently in the library.

In an ongoing effort to simplify the identification of metabolites directly in Profiler in a convivial and effortless way, Chenomx has begun a compound library expansion program using public NMR compound databases. An automated approach combining Chenomx's existing algorithms and technologies has been developed and tested on the Human Metabolome Database (www.hmdb.ca). Focusing strictly on spectra acquired in water, about 335 new compound signatures were added, effectively doubling the size of available compounds in Chenomx's library.

Public Human Metabolome Database (HMDB) library

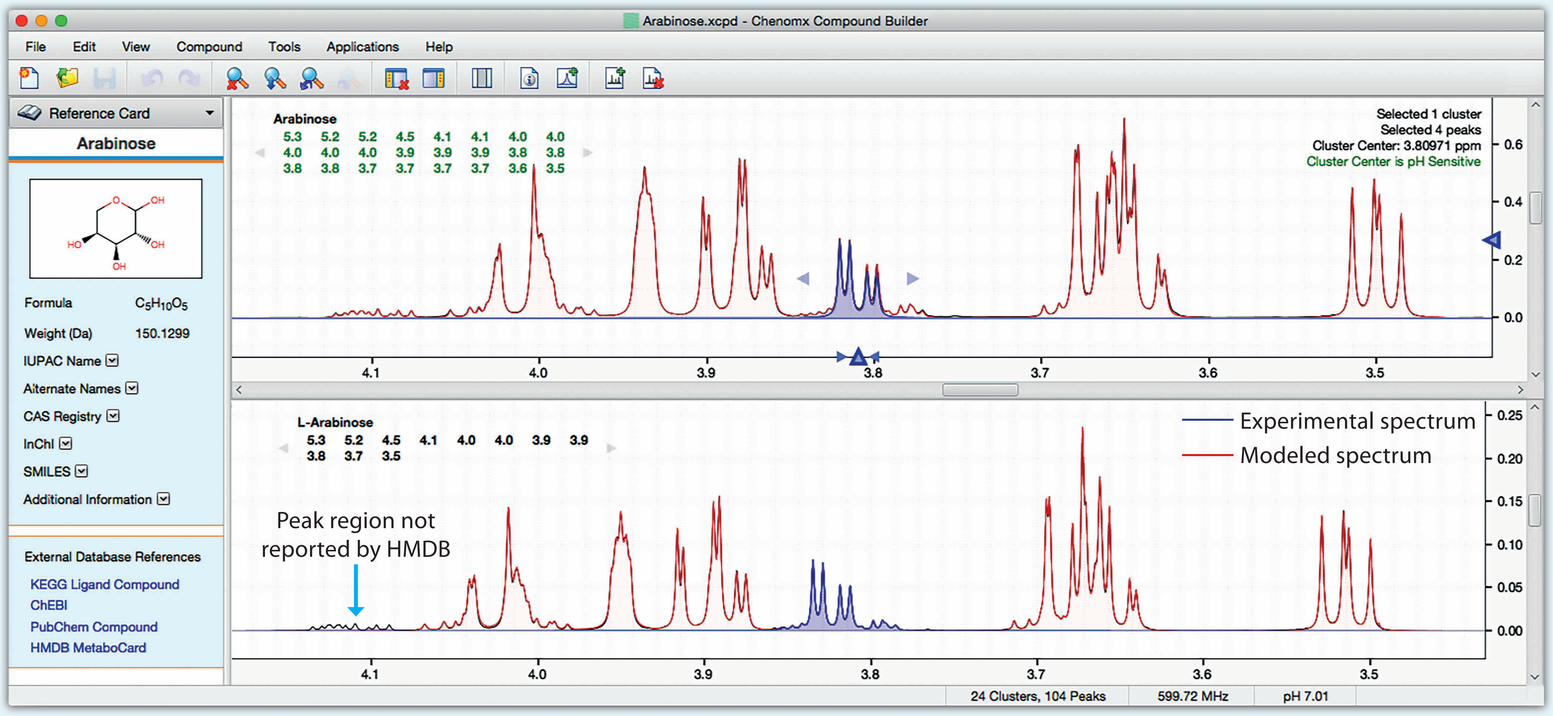
	HMDB raw Bruker/ Varian spectra	Spectra information (xml)	Metabolite card
Extracted Information	• Vendor type • Pulse sequence name and parameters • Raw free induction decay	• Conditions *(pH, solvent, temperature)* • Compound concentration • Peak centers	• Compound name and synonyms • Compound chemical formula, mass • Smiles, Inchi, CAS, etc.
Automated Processing	• Phasing • Baseline Correction • Reference Deconvolution	• Peak picking around suggested centers • Peak fitting • Peak clustering	• Creation of Chenomx compound card with Reference Card Editor
Output	• Chenomx CNX processed spectrum	• Chenomx peak-based compound entry • Native at original HMDB spectrum frequency, and simulated at all others	• Chenomx compound card

673 HMDB reference compounds† imported into a separate Chenomx library and available for identification and quantification in Profiler (~ 325 were already present in the Chenomx proprietary library)

†Available to Chenomx users upon request

EXAMPLE OF AUTOMATIC COMPOUND SIGNATURE CREATION FOR ARABINOSE

TOP: Chenomx native signature
BOTTOM: HMDB auto-generated signature



HMDB entries:

- High fidelity spectral reconstruction using pure lorentzian peak shapes.
- Line widths automatically adjusted to magnet shimming conditions.
- Peak clustering based on peak proximity and agnostic of chemical structure *(may be different than Chenomx)*.
- Single pH *(vast majority at neutral pH)*.
- Highly dependent on raw data quality (fid) and reported peaks.
- Absolute quantification not tested by Chenomx.

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