HMDB Compounds – Release 2

A second version of the HMDB compound packs is now available to Chenomx users.

Our automated conversion procedure has been corrected and enhanced to produce more accurate compound signatures.

The produced compound entries depend heavily on the provided data by HMDB, mainly the quality of the raw spectra and the accuracy of the reported peak positions.

Since our initial release of the HMDB compound packs, several issues were identified with the HMDB database, which made some compounds difficult or impossible to import. We have made modifications to address these issues. A total of 16 compounds were removed from our initial release

The HMDB compound packs are complementary to the proprietary Chenomx libraries. A comprehensive list of all the included compounds in both sets is available for viewing or downloading on our web site. Additionally, a table comparing fundamental differences between both libraries is provided below. When performing spectral fitting, we strongly recommend using the Chenomx compound entries when available.

Installation instructions:
Using the Library Manager module, remove any previously installed HMDB compounds (Choose Library in the application menu bar, Remove compounds)
Install the new compound packs by using Add Compounds from the Library menu

HMDB Reference Cards
Once it is downloaded, extract the contents of the zip file to your Chenomx Reference Card location. This is typically located in your user profile as a folder called "Chenomx Reference Cards". If you are unsure of where this is on your system, open Library Manager's Preferences and you will see the location. You may need to create this folder if you have never used it before.

Differences between the HMDB and Chenomx compound signatures

Functionality	**HMDB signatures**	**Chenomx proprietary signatures**
Pulse sequence	Mixture, not-standardized	Standardized
Pulse Sequence parameters	Mixture, not-standardized	Standardized
Multi-frequency	Raw data at 500 **or** 600 MHz All other frequencies simulated	Native raw data at 400, 500, 600, 700 **and** 800 MHz All other frequencies simulated
pH sensitive	No, single pH All cluster transform windows set to ± 0.025 ppm	Yes, multi-pH pH-adapted cluster transform windows
Peak cluster definition	Automated peak clustering Not-related to compound chemical structures	Related to the expected peak multiplets from the compound chemical structure