Session 6 - GC-/LC-MS profiling (Co-chairs: Robbat/Fiehn)

06-01: MassBank of North America: using untargeted metabolomics and multistage fragmentation mass spectral libraries to annotate natural products in plants

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Plants produce thousands of natural products for specific biological functions in their ecosphere. To structurally annotate these metabolites, large mass spectral libraries are required to develop fragmentation rules to detail relationships of substructures. At UC Davis, we developed a range of informatics resources to catalog mass spectra of both known and unknown plant metabolites. First, the new BinVestigate web interface enables users to screen our BinBase resource that we have built over the past 15 years, with currently 2,500 studies and over 150,000 samples. Second, we developed the open access MS-DIAL data processing along with MS-FINDER compound identification software, in collaboration with the RIKEN plant science center in Japan. Third, we collated all publicly available mass spectra resources into a unified database, MassBank of North America (MoNA). MoNA now contains more than 260,000 mass spectra, including over 35,000 QTOF, ion trap MS^n and Q-Exactive HF mass spectra of natural products. We present a range of examples how plant natural products are identified through multiple extraction solvents, high resolution mass spectral platforms, and MS library searching, including the NIST standard reference material 3291 of bilberry extracts, complex foods and the identification of plant products in human upper intestinal tract samples or plasma extracts.