SESSION 4

SECONDARY CYANOMETABOLITES – STRUCTURE, BIOSYNTHESIS, PHYSIOLOGICAL FUNCTION, ENVIRONMENTAL SIGNIFICANCE AND BIOTECHNICAL APPLICATION

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Increasing confidence in identifying cyanobacterial metabolites to study their occurrence and behavior

Cyanobacteria and their unique secondary metabolites offer many opportunities for research across disciplines. Over the past decades, a legion of new cyanobacterial metabolites has been identified but we often do not know yet what their concentrations and behaviour in the environment are. We often point to the key challenge of the lack of reference standards and thus the high analytical requirements for identification and quantification before further studies of these compounds become feasible. Until recently, even a comprehensive list of all known cyanobacterial metabolites was not openly available. As a result of the 11th ICTC in Krakow (2019) we started a collaborative effort to merge, expand, and validate existing private and public datasets into one open access structural database: CyanoMetDB. The 2021 version of CyanoMetDB contains complete structural and literature information for more than 2000 secondary metabolites from cyanobacteria. We actively facilitated the integration of CyanoMetDB into other platforms (e.g., PubChem, The Natural Products Atlas, MetFrag, Norman List Exchange, CompTox). We continue updating CyanoMetDB to include information and compounds currently missing.

A structural suspect list such as CyanoMetDB is essential for dereplication work on cyano-metabolites using mass spectrometry. However, to improve our confidence of compound identification, we need to be able to compare empirical fragmentation data to available reference spectra, when no authentic standard is directly available. Currently, reference spectra are publicly available for a small fraction of the metabolites listed in CyanoMetDB. One main shortcoming is the lack of commercially available reference standards or high costs associated with these materials. Metabolites identified in extracts that have not been purified often do not meet the quality standards of spectral databases. This dilemma prevents making cyanobacterial metabolite identification more widely available. The CyanoMetDB team now takes on the next challenge to systematically record mass spectral reference data of available standards, purified bioreagents and compounds identified with high certainty in cyanobacterial extracts.

We will share the reference data through open access spectral databases open to such data to enhance dereplication of known cyanobacterial metabolites. The availability of reference spectra offers many new opportunities including studies of compound- and class-specific gas phase fragmentation patterns. Without the collaborative and often selfless work of the researchers involved, these efforts would not be possible. CyanoMetDB is open to all community members to contribute to and support our efforts.