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Project acronym: NaToxAq

Marie Skłodowska-Curie Action

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Deliverable reference number and title

D6.15 Upload of data to databases and archives 4

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Organisation name of lead beneficiary for this deliverable:

Helmholtz Centre for Environmental Research (UFZ) supported by Federal Department of Economic Affairs, Education and Research (WBF)

Project co-funded by the European Commission within the Horizon 2020 Programme		
Dissemination Level		
PU	Public	X
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

1. Introduction and Objective(s)

In agreement with the DOW, NaToxAq successfully uploaded several mass spectra of natural toxins to the European MassBank (<https://massbank.eu/MassBank>) allowing the share, exchange and free access of the scientific community to these data and supporting and stimulating the collaboration and exchange within the project. To facilitate a broader sharing and re-use of the raw mass spectral used for deriving the mass spectral library records, UFZ considers to upload the raw mass spectral data and related peak-lists to the Global Natural Products Social Molecular Networking (GNPS) database (<https://gnps.ucsd.edu/ProteoSAFe/static/gnps-splash.jsp>).

2. Strategy for solving the task

The lead beneficiary UFZ is collecting standard substances of other NaToxAq partners for LC-HRMS analysis and processing of MassBank spectra in order to facilitate the task. UFZ started first discussions with GNPS maintainers how to integrate the raw mass spectral data of NaToxAq in GNPS.

3. Delays and difficulties

There are no delays and difficulties in deriving and uploading mass spectral records in MassBank. The NaToxAq partners Agroscope, Recetox, UCPH and UFZ provided analytical standards to UFZ which are measured, processed and uploded to MassBank in batches.

4. Result

In this deliverable we report the availability of almost 2000 mass spectra (see attached spreadsheet) to the specific NaToxAq database in MassBank (<https://massbank.eu/MassBank>). The compounds representing pyrrolizidine and quinolizidine alkaloids as well as glycoalkaloids were selected due to their natural origin and because of their environmental concern.

The records can be reached by the Record Index (<https://massbank.eu/MassBank/RecordIndex>) list or via the Search (<https://massbank.eu/MassBank/Search>). The attached spreadsheet contains a deep link to each NaToxAq entry in MassBank. The landing page of the NaToxAq representation on MassBank is directly reachable via <https://goo.gl/joofrG>. The landing page of each record contains meta data regarding the chemical identity, instruments, analytical conditions and the mass spectral data itself. The records were automatically derived from the raw data files using RMassBank 2.12.0 [1; <https://github.com/MassBank/RMassBank>].

See <https://natoxaq.ku.dk/toxins/> for an excel sheet of MassBank accessions.

References

1. Stravs, M.A., et al., *Automatic recalibration and processing of tandem mass spectra using formula annotation*. *Journal of Mass Spectrometry*, 2013. **48**(1): p. 89-99.