Oxford, 10 April 2016

Minutes of the WG4 (Computational Methods) Meeting

of COST Action BM1403
"Native Mass Spectrometry and Related Methods for Structural Biology”

Meeting place and date: Oxford, UK, 10 April 2016, 10:30-20:30

1. Welcome to participants

The participants were welcomed by Prof Justin Benesch (Local Organizer) and Prof Frank Sobott (Chair).

2. Aim of the WG4 Meeting

The goal of this Meeting was to discuss the use of computational methods in native mass spectrometry. There was a particular focus on the challenges the field faces, and discussion of potential solutions, as well as on developing an EU-based framework for on-going collaborative work.

3. Format of the WG4 Meeting

The meeting took place in round-table format, with five key topics considered in depth. Each topic was kick-started by a 15 minute presentation by a speaker, who then led, together with a designated chair, the ensuing discussion.

4. Programme of the WG4 Meeting

10:30 - 10:45: Tea and coffee

10:45 - 11:00: Overview and agenda Chair: Justin Benesch

11:00 - 12:15: ***Quantifying native IM-MS data*** Chair: Perdita Barran, Speaker: Brandon Ruotolo (Invited Speaker)

12:15 - 13:15: Working lunch and general discussion

13:15 - 14:30: ***Calculating CCSs*** Chair: Bela Paizs, Speaker: Carlos Larriba-Andaluz (Invited Speaker)

14:30 - 15:45: ***Charging in native MS*** Chair: Frank Sobott, Speaker: Matt Bush (Invited Speaker)

15:45 - 16:00: Tea and coffee

16:00 - 17:15: ***Native MS for protein structure*** Chair: Kostas Thalassinos, Speaker: Argyris Politis

17:15 - 18:30: ***MD using native MS data*** Chair: Valerie Gabelica, Speaker: Erik Marklund

19:30 - 20:30: Networking Dinner

**5. Participants**

Frank Sobott (Antwerp); Bela Paizs (Bangor); Kevin Pagel (Berlin); Valerie Gabelica, Massimiliano Porrini, Frederic Rosu (Bordeaux); Giulia Rosetti (Juelich); Antoni Borysik, Argyris Politis (King’s, London); Alison Ashcroft (Leeds); Emeline Hanozin (Liege); Alexander Kulesza (Lyon); Perdita Barran, Lukasz Migas (Manchester); Jasper Boschmans (Owlstone); Tim Allison, Justin Benesch, Matteo Degiacomi; Michael Landreh, Erik Marklund (Oxford); Carlos Larriba-Andaluz (Purdue); Kostas Thalassinos (UCL, London); Brandon Ruotolo (Michigan); Matt Bush (Washington).

**6. Outcomes**

The discussion raised a number of important points relating to the Action goals, e.g. the need for a unified data standard as input for processing of ion mobility data (-> compare with Skyline at PNNL). Data standards are also sometimes required for journals (e.g. Elsevier) to deposit or visualize data, and funding agencies increasingly request this.
But e.g. metabolomics vs. protein structure data have very different requirements.

Different software strategies for structural modeling based on native MS and ion mobility data were discussed and compared. The need for a unified strategy, involving all key players in software development (many of which were present) was identified, to avoid duplication and develop urgently needed tools.

**7. Action points**

- Take stock of currently existing computational strategies and their capabilities and limitations, by preparing publications which summarize the status quo (Justin)

- Propose a data notation format to the community (Perdi)

- Try to obtain funding as a community for software development, by applying together for a grant in upcoming “computational tools in the life sciences” call in the UK (Kostas)