

sDiv working group meeting summary

“sMile: Synthesising plant Metabolomics into biodiversity, Life history & Ecology”

General working atmosphere. This was the first sDiv working group meeting and the first time most group members met. Despite the entire meeting being remote, it was a huge success and participation was generally high throughout the five days. People were engaged and interested, with attendance chiefly varying due to time zone differences between the US and Europe. However, the remote format also gave participants the opportunity to occasionally sneak away to other commitments - good for participants but not ideal for the workshop.

sDiv support. Support from sDiv was excellent to prepare for the meeting and for adapting strategies and expectations to an online format. Apart from the housekeeping introduction from Marten and an occasional sDiv appearance/email, we had no further contact during the week - none was needed!

General format. After a general introduction (PIs Tom Walker and Franzi Schrodt) and short briefings on each of the topics being covered (data upload: Kristian Peters; group paper: Tom Walker; handbook: Henriette Uthe; new hypotheses: Nicole van Dam), the meeting took the format of a mini-conference with parallel sessions and a debrief at the end of the day (CET). This gave participants the opportunity of contributing to multiple topics and to dip in and out of sessions as required. **Pros:** participants could pick which sessions to attend and move between topics as desired. **Cons:** too many parallel sessions (max. three) meant that some participants felt they couldn't contribute to everything they wanted to.

Topic 1 | data upload. **Meeting aims:** Decide on how, in what format and where to upload the metabolomics dataset being used for the sDiv working group. If possible, begin this process. **Progress made:** After initial discussion about the current status of data (format, location, type, etc.), an early decision was made to upload all data to Metabolights. The group spent the rest of the week defining an upload protocol, road-testing it and beginning the upload process. The idea of a paper describing the datasets was floated, possibly to submit to *Nature Scientific Data*. **Balance between activities:** 10% brainstorming/exchange; 90% work on outputs. **Actions prior to next sDiv meeting:** Continue data upload; bottom-out possible paper for active development next year.

Topic 2 | metabolome traits paper. **Meeting aims:** Build skeleton and identify outstanding tasks for paper linking the metabolome to plant functional traits. **Progress made:** Skeleton was built, including sketches for all figures, and writing started on the Introduction section. Exploratory analyses were undertaken and actions/leads were assigned. **Balance between activities:** 30% brainstorming/exchange; 70% work on outputs. **Actions prior to next sDiv meeting:** Finish analyses; write paper; submit paper.

Topic 3 | eco-metabolomics handbook. **Meeting aims:** Explore the potential value of and content for a handbook on eco-metabolomics, and build a plan of action to realise it. **Progress made:** There was rapid consensus that such a handbook would be valuable, albeit challenging to deliver. Remaining sessions on this topic centered on brainstorming potential content and identifying how to move forwards, including assigning actions/leads. **Balance between**

activities: 70% brainstorming/exchange; 30% work on outputs. **Actions prior to next sDiv meeting:** Formalise structure; identify writing teams; write detailed instructions for authors.

Topic 4 | new hypotheses. **WMeeting aimshat:** Building on the diverse interdisciplinary expertise in the sDiv working group, identify low-hanging fruit for new studies to be performed as a working group. **Progress made:** Most sessions on this topic were discussion-based and focused on identifying and bottoming-out potential (and realistic) ideas. Two ideas crystallised: (i) the outline for a review paper on the power of the metabolome for ecology (already part of the sDiv proposal); and (ii) a systematic review of how the metabolome has been used to study biodiversity and ecosystem functioning. Actions/leads were assigned for both. **Balance between activities:** 90% brainstorming/exchange; 10% work on outputs. **Actions prior to next sDiv meeting:** Write standard review; submit standard review; develop protocol for systematic review; do literature search for systematic review.