German Centre for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig
Puschstraße 4, 04103 Leipzig, Germany

sDiv working group meeting summary

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

General working atmosphere. The meeting was a mixed in-person and remote format, with the majority of participants attending in person. The atmosphere in Leipzig was extremely productive and dynamic (in part because it was the first time in two years that people had been let loose on the world!), but this did hinder participation for remote attendees - particularly during briefing sessions where there were many participants in the room (which inevitably introduced some chatter and background noise).

sDiv support. Excellent support all-round, from preparation (help with flights, hotels, etc.), to food, to IT, to expenses. We had a few teething problems with technology and building access (we suspect because the building was new). It was also a shame that another sDiv group had their meeting at the same time, which we didn't know when selecting dates - in fact, two attendees were participants in both meetings and struggled to balance time between them.

General format. We started with a general introduction (PIs Tom Walker and Franzi Schrodt, plus sDiv host Nicole van Dam) and short briefings on each of the topics covered (data product: Kristian Peters; handbook: Sue Marr; systematic review: Franzi Schrodt; new studies: Tom Walker; data platform: Dale Forrister). Following this, we continued with a parallel session format (this year with only two parallel sessions at once) with daily briefings and recaps. Sessions were planned dynamically to allow ideas to flourish and effort to migrate to where it was needed most. However, we focused particularly on the following main objectives and made substantial progress on all of them.

Topic 1 | data upload. **Progress since last sDiv meeting:** *Nature Scientific Data* paper idea accepted; some data uploaded to MetaboLights. **Meeting aims:** Collect all outstanding data; develop structure of paper; plan timetable to submission. **Progress made:** After updating participants on this topic, it was felt that this activity could continue without much group input. While some parallel sessions occurred, the majority of work took place between sessions - led mostly by Kristian Peters and Emmanuel Defossez. In addition to identifying more datasets to upload, the concept and structure of the *Nature Scientific Data* paper was finalized. **Balance between activities:** 30% brainstorming/exchange; 70% work on outputs. **Actions prior to next sDiv meeting:** Finish uploading data to Metabolights; write draft paper.

Topic 2 | eco-metabolomics handbook. **Progress since last sDiv meeting:** Structure planned; some writing teams identified; instructions for authors written. **Meeting aims:** Kick-start writing on all sections; finalize timetable to submission. **Progress made:** This topic was a main focus for parallel sessions. After identifying writing teams for all sections and sharing instructions, participants worked on drafting sections during the meeting. Some were completed at the meeting, but most were started with plans made to finish afterwards. **Balance between activities:** 40% brainstorming/exchange; 60% work on outputs. **Actions prior to next sDiv meeting:** Finish all sections; write paper; submit paper.

Topic 3 | systematic review. **Progress since last sDiv meeting:** Structure planned; search protocol identified; review criteria established; initial literature search undertaken. **Meeting**

aims: Introduce search protocol to participants and get participants to test it on a subset of selected papers. **Progress made:** After an update on progress and a discussion on the review protocol (taking one parallel session), participants were given 20 papers to review as a test of the protocol. This exercise was balanced between free time and one or two further parallel sessions. **Balance between activities:** 20% brainstorming/exchange; 80% work on outputs. **Actions prior to next sDiv meeting:** Finalize protocol in light of test; do literature search; finish systematic review; draft paper skeleton.

Topic 4 | eco-metabolomics data platform. **Progress since last sDiv meeting:** New activity since last meeting; introduction planned; leads identified. **Meeting aims:** Plan scope; identify participants; partition workload. **Progress made:** This was a new topic for this year (to fit within the data framework of the sDiv proposal), so it was a main focus of parallel sessions. Most effort was spent discussing what a data platform would look like, how it would function and making a plan to develop it. **Balance between activities:** 100% brainstorming/exchange. **Actions prior to next sDiv meeting:** Create dummy dataset for road-testing data platform; software development on metabolomics/traits backend; tentative prototype platform in place.

Topic 5 | kick-starting new ideas. **Progress since last sDiv meeting:** None (new topic). **Meeting aims:** Pick low-hanging fruit using data already assembled for the metabolites-traits paper (see below). **Progress made:** This topic built from the success of last year's "new hypothesis" session, which yielded two review papers (one published, one in development). It was therefore a main focus of parallel sessions, during which participants discussed ideas and formalized three into paper plans: (i) chemical vs. trait niches; (ii) the biogeography of the metabolome; and (iii) the metabolomes of invasive vs. endangered species. **Balance between activities:** 100% brainstorming/exchange. **Actions prior to next sDiv meeting:** Bottom-out ideas and discard if not tenable; develop plan into skeleton; perform preliminary data analyses.

Completed projects from sDiv 2020

- Walker *et al.* (in revision) The metabolism of plant form and function. *Nat. Ecol. Ecol. sDiv 2020 topic 2*.
- Walker *et al.* (2022) Functional traits 2.0: the power of the metabolome for ecology. *Journal of Ecology* **110**, 4-20. *sDiv 2020 topic 4(i).*

Successes between sDiv meetings. Apart from direct sDiv activities, collaborations among working group members have led to several publications. These early successes are a huge testament to the energy and positivity of this working group and we thank all of our members for their participation. Some examples include:

Endara, M., Soule, A. J., Forrister, D. L., Dexter, K. G., Pennington, R. T., Nicholls, J. A., Loiseau, O., Kursar, T. A., & Coley, P. D. (2021). The role of plant secondary metabolites in shaping regional and local plant community assembly. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13646

Fernandez-Conradi, P., Defossez, E., Delavallade, A., Descombes, P., Pitteloud, C., Glauser, G., Pellissier, L., & Rasmann, S. (2021). The effect of community-wide phytochemical diversity on herbivory reverses from low to high elevation. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13649

Philbin, C. S., Dyer, L. A., Jeffrey, C. S., Glassmire, A. E., & Richards, L. A. (2021). Structural and compositional dimensions of phytochemical diversity in the genus Piper reflect distinct ecological modes of action. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13691

Rawlings, A., O'Connor, E., Moody, S. C., Dudley, E., Boddy, L., Fowler, M. S., Fitzpatrick, D. A., Doyle, S., & Eastwood, D. C. (2021). Metabolic responses of two pioneer wood decay fungi to diurnally cycling temperature. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13716

Sytiuk, A., Céréghino, R., Hamard, S., Delarue, F., Guittet, A., Barel, J. M., Dorrepaal, E., Küttim, M., Lamentowicz, M., Pourrut, B., Robroek, B. J. M., Tuittila, E., & Jassey, V. E. J. (2021). Predicting the structure and functions of peatland microbial communities from Sphagnum phylogeny, anatomical and morphological traits and metabolites. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13728

Weinhold, A., Döll, S., Liu, M., Schedl, A., Pöschl, Y., Xu, X., Neumann, S., & Dam, N. M. van. (2021). Tree species richness differentially affects the chemical composition of leaves, roots and root exudates in four subtropical tree species. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13777

Williams, A., Langridge, H., Straathof, A. L., Muhamadali, H., Hollywood, K. A., Goodacre, R., & Vries, F. T. (2021). Root functional traits explain root exudation rate and composition across a range of grassland species. *Journal of Ecology*. https://doi.org/10.1111/1365-2745.13630