
The Metabolomics Standards Initiative

To the editor:

The standards papers that *Nature Biotechnology* hosted online as part of a community consultation (<http://www.nature.com/nbt/consult/index.html>), in particular those by the Human Proteome Organization Proteomics Standardization Initiative (HUPO-PSI)^{1,2} and the Functional Genomics Experiment (FuGE)³ working groups, represent an important first step toward permitting the sharing of high-quality, structured data. We particularly applaud the open consultation solicited by *Nature Biotechnology* and

advocate the early-community-involvement approach taken by HUPO-PSI, FuGE and the other working groups in the development of such guidelines and standards. These are the most effective ways to ensure that the output generated is pragmatic and the standards are both useful and widely accepted by the community.

As representatives of the nascent Metabolomics Standards Initiative (MSI)⁴, we are following closely the work of the FuGE and the PSI working groups, leveraging on their work where commonality exists, such as the mass

Nature Biotechnology's online community consultation initiative (<http://www.nature.com/nbt/consult/index.html>) is intended to encourage researchers to participate in the development of guidelines/standards.

spectrometry and the sample preparation domains. MSI combines and thereby strengthens several preexisting groups and initiatives (including Standard Metabolic Reporting Structure (SMRS), ArMet and MIAMET)⁵⁻⁷ in a concerted effort under the aegis of the Metabolomics Society⁸. As with other functional genomic approaches, we envisage a great deal of commonality in terms of experimental description.

The MSI working groups have drafted a series of manuscripts, outlining the work to date, and we intend to work closely with PSI working groups towards the development of common or interoperable standards. It is our view that reporting standards (checklists), syntax (format) and semantics (controlled vocabulary or ontology) should be reused across the functional genomics and systems biology standards communities, where applicable. This would benefit the entire scientific community by facilitating publication and dissemination of the results and simplifying the job of data integration⁹. From a technical perspective, it will be necessary to both remove redundancies and fill gaps between the domains that are covered by checklists, exchange formats and terminologies developed. These are certainly difficult but not insurmountable tasks and FuGE, developed and endorsed by many communities to 'unify' the exchange formats, is the first good exemplar project.

We would also like to highlight that the sociological barriers involved in these large-scale open standards efforts, such as PSI, can be extremely challenging, and thus will require extensive liaison between communities. With our experience in MSI,

we are aware that managing this process of consensus building from start to finish takes time, resources and expertise. The time invested in these efforts to build commonalities and synergies among initiatives (e.g., between PSI and MSI) is often little, or at least not as continuous as it should be, due to lack of resources.

For these reasons, we express our appreciation for the efforts that each individual has put into the work behind FuGE and PSI guidelines. We take this opportunity also to encourage individuals or groups to join these initiatives, bringing with them their requirements, suggestions or critiques, and contributing to the development process in a constructive manner.

COMPETING INTERESTS STATEMENT [AU: Please complete and return form]

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1. http://www.nature.com/nbt/consult/pdf/Taylor_et_al.pdf
2. http://www.nature.com/nbt/consult/pdf/Taylor_et_al_2.pdf
3. Jones, A.R. *et al.* *OMICS* **10**, 179–184 (2006).
4. <http://msi-workgroups.sourceforge.net>
5. Lindon, J.C. *et al.* *Nat. Biotechnol.* **23**, 833–828 (2005).
6. Jenkins, H. *et al.* *Nat. Biotechnol.* **22**, 1601–1606 (2004).
7. Bino, R.J. *et al.* *Trends Plant Sci.* **9**, 418–425 (2004).
8. <http://metabolomicsociety.org/>
9. Quackenbush, J. *Nat. Biotechnol.* **22**, 613–614 (2004).