Opening up the Lab Notebook: Publishing Experimental & Supplementary Information

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Supplementary Information supporting publications is not uniform across journals, is generally not 100% representative of the work undertaken, is not structured or comprehensive and therefore is often not fully considered in review. In chemistry articles where characterisation techniques are applied widely, crystallography is the exception in that there are universally agreed processes and protocols for presenting the scientific findings and the supporting data. Crystallography can therefore lead the way! Our approach to solving the broader problem of availability of supporting information is to expose the observations of the researchers who conducted the work when it was performed. By combining these observations with related data (e.g. in information management systems) and linking these with the article there is the potential for a much richer system for data supporting a publication. The Electronic Laboratory Notebook (ELN) plays a key role by establishing authenticity, adding structure to the record and having the capacity to be made open. We present a formal publication in Chemistry Central Journal (http://journal.chemistrycentral.com/content/7/1/182) which is a collaborative piece of work between the UK National Crystallography Service (University of Southampton) and the University of Greenwich, where the data supporting the article is not contained within it, but is openly exposed at source by an ELN and a crystal structure repository. We draw on the experience of crystallographic publishing and aligning that with the other characterisation techniques alongside which crystal structures are routinely published and related. The article presents all the supplementary information (some 35 or so data sources) in a single graphical approach, which permits examination of synthesis, spectra & structures in-line and provides a link to the original ELN record. All records are assigned a Digital Object Identifier (DOI) by a system established within the University.

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