

Interactive comment on “UManSysProp: an online facility for molecular property prediction and atmospheric aerosol calculations” by D. Topping et al.

D. Topping et al.

david.topping@manchester.ac.uk

Received and published: 25 January 2016

We would like to thank the Editor for very helpful comments, which we have addressed in the new version as detailed below.

Editor comment: *The main paper must give the model name and version number (or other unique identifier) in the title.* **Response:** This has now been corrected and the title now reads ‘UManSysProp v1.0, an online and open-source facility for molecular property prediction and atmospheric aerosol calculations.’

Editor comment: *All papers must include a section, at the end of the paper, entitled*

C3787

‘Code availability’. Here, either instructions for obtaining the code, or the reasons why the code is not available should be clearly stated. It is preferred for the code to be uploaded as a supplement or to be made available at a data repository with an associated DOI (digital object identifier) for the exact model version described in the paper. Alternatively, for established models, there may be an existing means of accessing the code through a particular system. In this case, there must exist a means of permanently accessing the precise model version described in the paper. In some cases, authors may prefer to put models on their own website, or to act as a point of contact for obtaining the code. Given the impermanence of websites and email addresses, this is not encouraged, and authors should consider improving the availability with a more permanent arrangement. After the paper is accepted the model archive should be updated to include a link to the GMD paper.”

Response: In addition to providing the online portal for users who do not want to use source code, and the JSON API for linking with our web portal without using a web browser, we also now provide the source code for all predictive techniques provided on the site. We have released this via a github repository that has an associated DOI 10.5281/zenodo.45143 as requested by GMD. This information has now been added to the introduction and abstract via the text below, on the web site and in a new section entitled ‘Code Availability’ at the end:

‘In addition to providing the online portal for users who do not want to use source code, and the JSON API for linking with our web portal without using a web browser, we also provide the source code for all predictive techniques provided on the site, covered by the GNU GPL license to encourage development of a user community. We have released this via a Github repository https://github.com/loftytopping/UManSysProp_public.git, that has an associated DOI for the exact model version given in this paper as provided by the Zenodo service (DOI 10.5281/zenodo.45143)”

Interactive comment on Geosci. Model Dev. Discuss., 8, 9669, 2015.

C3788