chem-bla-ics

UU Cheminformatics Journal Club

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Keywords

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Following the steps of the IU Cheminformatics Journal Club, I have started a UU Cheminformatics Journal Club:

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Hi all,

after repeated questions from various people around asking about some
educational thingy on cheminformatics, and now that I have two
students I want to educate, I am starting a cheminformatics journal
club, as it is nicely called... we'll discuss cheminformatics
literature biweekly.

No worries if you skip or meeting or so, but when you join, you *must*
have read the paper. Additionally, it is expected that you attempted
to understand the paper, by looking up cited references and methods.
That said, you are not expected to spend a week of literature mining
on the paper (depending on the topic and your backgroun, a day or two
at most will do); instead, you are required to form an opinion on the
paper. Preferably, those opinions are written down before the meeting,
to force you to actually formulate them.

During a meeting, we'll discuss the paper then, identifying strong and
week points of the paper, and one of us (rotating) will make notes,
and write up a (public, OA) review on the paper based on our
discussion.

Everyone is invited to join in. Please do let me know which dates you
will attend. Meetings are from 10-11 am.

* Thu, 11/2: Towards pharmacogenomics knowledge discovery with the
  semantic web, doi:10.1093/bib/bbn056
* Thu, 25/2: Small Molecule Subgraph Detector (SMSD) toolkit,
  doi:10.1186/1758-2946-1-12
* Thu, 11/3: Virtual screening of bioassay data, doi:10.1186/1758-2946-1-21

As you see, the list is a mix of various subfields of molecular
chemometrics: the first is around knowledge management (RDF), the
second around chemical graph theory, and the last about statistics
(Bayes, SVM, RF). This covers about the three pillars of current
cheminformatics research.
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