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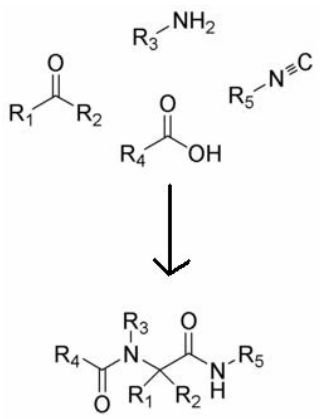
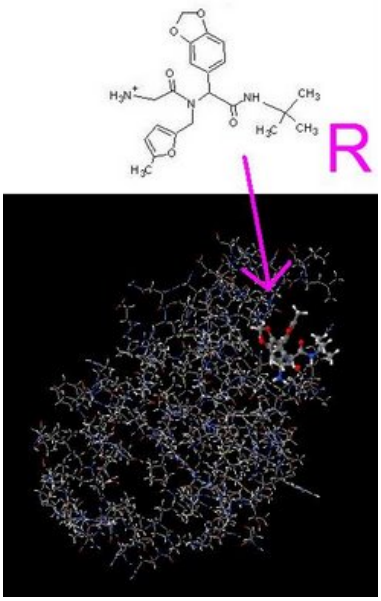
Current Research

The main focus of my research group is currently the synthesis of novel anti-malarial agents from virtual combinatorial libraries of Ugi products. We use the Ugi reaction because it is experimentally simple to execute and affords a great diversity from four pools of readily available starting materials: aldehydes or ketones, amines, carboxylic acids and isonitriles.



Based on feedback from our docking collaborators, targets from the virtual library are selected for synthesis then sent for testing. For example, the image below shows the docking of one of our Ugi products within enoyl reductase, an enzyme used by the malarial parasite to build its cell wall. (from Too-Tsu Tan).



Open Notebook Science

There is currently a growing movement in science to make research results more accessible, fueled in part by pressure from funding agencies such as the National Institutes of Health.

I have extended this concept of transparency in research to include the public sharing of all laboratory experiments in real time and have coined the term "Open Notebook Science" to distinguish this from other more limited forms of "Open Science".

We have found that social software tools such as blogs, wikis and mailing lists can be used very effectively to disseminate active research prior to publication in traditional journals. A wiki can serve as a convenient online laboratory notebook, with each experiment recorded on a new page. Additions and changes to the wiki are easily tracked with its built-in version tracking system. The use of a hosted wiki further affords third-party time stamps to prove who knew what when. The blog component serves as a convenient vehicle to report milestones and discuss project ideas, linking back to specific experimental details in the wiki.

The use of such a system allows other researchers to benefit from information gleaned from "failed" or incomplete experiments. Perhaps of even greater importance, working openly can catalyze the forging of new collaborations that would not otherwise have formed. All of the docking and testing collaborations that we currently have came about as a result of disseminating our results using social software.

The current interest in Open Notebook Science, and our application of it to malaria research under the project term UsefulChem, is reflected by citations of our work in Wired Magazine, Nature blogs, Cell, Chemical & Engineering News, Per Contra, Assignment Zero, National Public Radio's Marketplace, Chemistry Central and 3Quarks Daily.

References

Bradley, Jean-Claude. Open Notebook Science Using Blogs and Wikis. Available from Nature Precedings <http://dx.doi.org/10.1038/npre.2007.39.1> (2007)

http://usefulchem.wikispaces.com