chem-bla-ics

Open Access / Open Data leads to added value

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Two companies recently showed two things:

- · open access and open data allow adding value
- · adding value is easier by forking

Rich' MetaMolecular set up Chempedia which combines a substructure-searchable chemical Wikipedia. There is also a page to make links to new Wikipedia monographs. Not sure why Rich chose CAS instead of the InChI, given the recent controversy on validity of CAS numbers in Wikipedia... realize that this page is for new monograph, of which the CAS number is likely not verified yet, or? On the other hand, the InChI or InChIKey is not so abundant in Wikipedia yet (I really must make an updated list).

ChemSpider has been using a similar approach to add value to existing resources. The interesting thing in this case, is that these substructure searchable versions, have an interesting spin off: it allows ChemSpider to build a valuable DOI-InChI table. So far, I spotted:

- iucr.chemspider.com (Antony's story)
- molbank.chemspider.com (Antony's story)
- motd.chemspider.com (Antony's story)

If you wonder how to integrate all data again when things are so distributed, just consider userscripts.