

Fast molecular similarity with a new 3D shape descriptor

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chem-bla-ics

Jim reported about [SPECTRa being in the news](#) and ./ about [Toward a 3D Search Engine](#). These two items have in coming that they deal with the article *Ultrafast shape recognition for similarity search in molecular databases* by Ballester and Richards (DOI:[10.1098/rspa.2007.1823](#)). The NewScientist wrote up [their angle on it](#), with a quote from [Henry Rzepa](#).

The article proposes a new shape descriptor which is requires little computational resources to be calculated. It consists of 12 numbers describing the shape, and a simple similarity measure converts it into similarities. The results shown in the article, and replicated in the NewScientist article linked above, are interesting enough for me to wonder if I could [Federico](#), one of our [CUBIC](#) students, to work on this in the last two weeks of his practical.

BTW, [Andreas](#), don't those review articles (viz. DOI:[10.1039/b409813g](#)) work out good for your citation count ;)