chem-bla-ics

Fast molecular similarity with a new 3D shape descriptor

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Abstract

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.

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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 ;)