

Lies, Damned Lies and Statistics in Molecular Modeling

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What is the most useful skill that you should develop to become effective at molecular modeling? It could be knowledge of the many software programs used in the field, their strengths and weaknesses and when to apply them. It could be a deep understanding of the physical principles underlying drug action or of the biological pathways of life. Or it could be the facility to assess data, to turn it into information and knowledge. In my presentation I will make the case that the latter is the most important skill that should be brought into the field of computational chemistry, and that a firm knowledge of statistics is the foundation of such a skill set. Examples will be given of practical utility and also of the issues of empirical fields that lack statistical support.

"Confidence Limits, Error Bars and Method Comparison in Molecular Modeling.
Part 1: The calculation of confidence intervals."

<http://link.springer.com/article/10.1007%2Fs10822-014-9753-z>