Research identifies easier way to predict how chemical compounds will interact

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New research has revealed that simple, commercially available computer programmes could be used to design next generation drug-delivery systems by predicting more easily how different chemical compounds interact.

Led by Dr Jennifer Hiscock of the University of Kent, a team of researchers has identified a new more cost-effective way of predicting how compounds known as amphiphiles will interact with each other to impart specific physical properties to a solution.

The study, entitled Towards the prediction of global solution state properties for hydrogen bonded, self-associating amphiphiles, has revealed for the first time the potential for simple, easily accessible new methods of predicting on a computer how the compounds will behave.

The research involved the team using computer modelling to exhibit desired, pre-programmed properties before the chemical compounds even exist in real life.

The research is likely speed up the development - and decrease costs - associated with developing new methods of delivering drugs and medical-grade soaps and gels.

More information: Lisa White et al, Towards the prediction of global solution state properties for hydrogen bonded, self-associating amphiphiles, *Chemistry - A European Journal* (2018). DOI:

10.1002/chem.201801280