Computational Pharmaceutics
Application of Molecular Modelling in Drug Delivery

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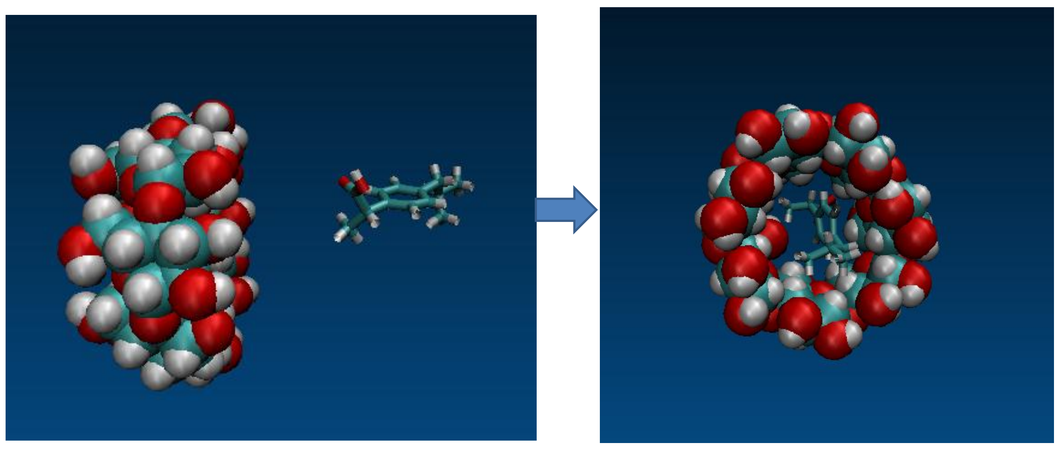
Dr Defang Ouyang's research interests focus on computational pharmaceutics, which combines computer modelling and experimental techniques to explore the mechanisms of drug delivery on a molecular level and then develop novel drug delivery systems, including cyclodextron formulations, solid dispersions and non-viral siRNA delivery systems.

Cyclodextrin-Drug Complexes

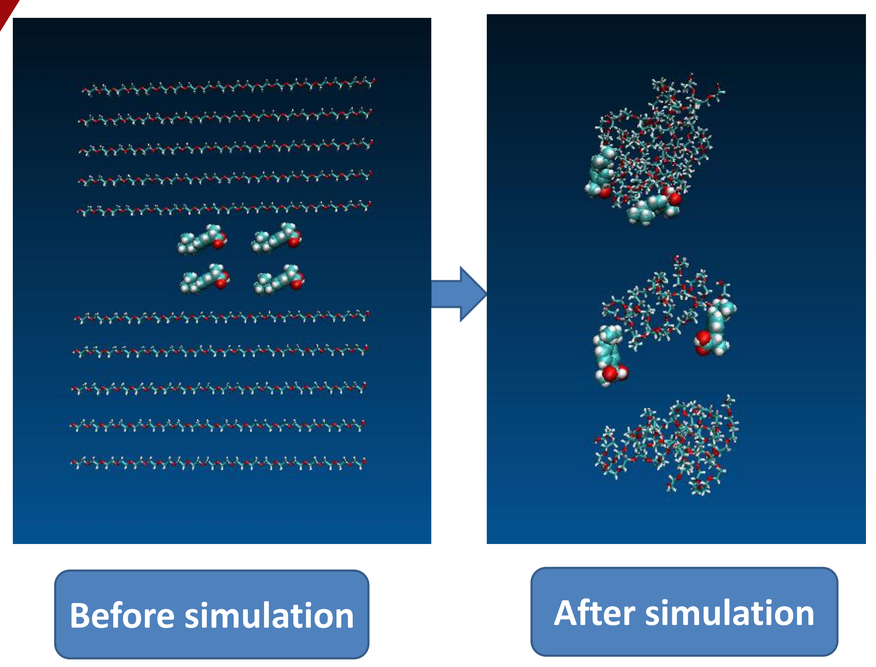


(left) Snapshots of β-cyclodextrin-ibuprofen complex at 0 ns; (right) Snapshots of β-cyclodextrin-ibuprofen complex at 10 ns.

(water molecules are omitted for clarity)

Cyclodextrins can be used for the solubilization of poor-soluble drugs and improvement of their bioavailability. MD simulation can investigate the structure, dynamics and energetics of cyclodextrin-drug complexes.

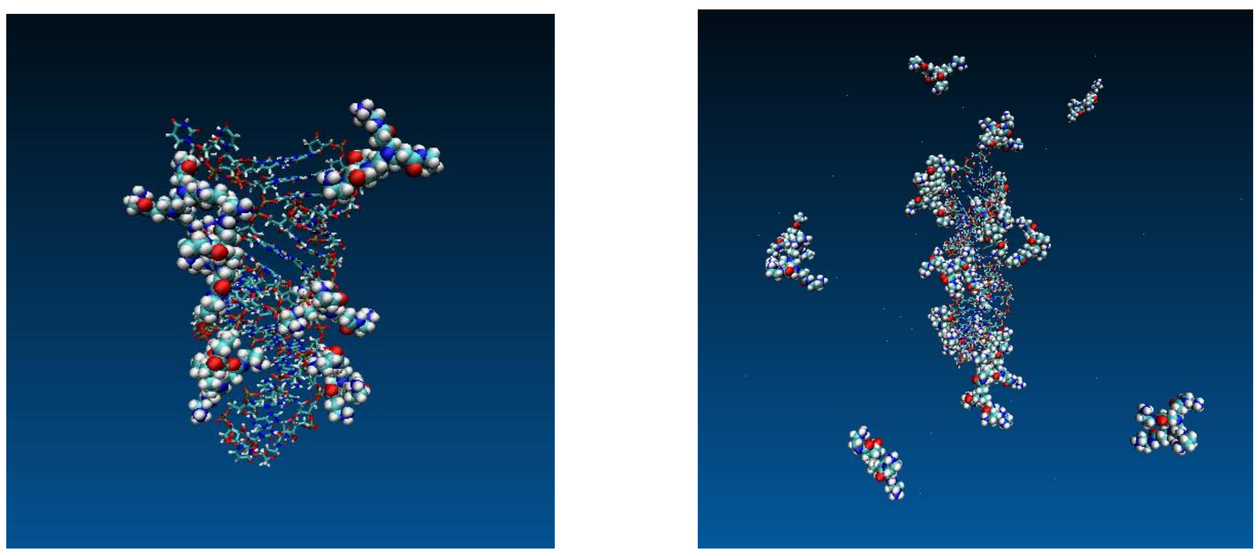
Solid Dispersions



(left) Snapshots of polyethylene glycol (PEG) -ibuprofen solid dispersion at 0 ns; (right) Snapshots of polyethylene glycol (PEG) -ibuprofen solid dispersion after the simulated annealing simulation.

Solid dispersion is a dispersion of one or more active ingredients in an inert carrier at the solid state. Molecular simulation can help us to explore the molecular state of solid dispersion by simulated annealing methods.

Non-viral siRNA Delivery Systems



(left) Snapshots of 4+polymer-siRNA complex at 10 ns at charge ratio of 0.6/1 (molecular ratio 6/1);
(right) Snapshots of 4+polymer-siRNA complex at 10 ns at charge ratio of 2/1 (molecular ratio 20/1).
(water molecules and counterions are omitted for clarity)

Both experimental approaches and computer modeling are combined to investigate the mechanism of polymer-siRNA complexation for the development of novel siRNA delivery systems.

Conclusions

Molecular modelling technique is a powerful technique to investigate the mechanism of drug delivery at the molecular level.

References: *Aust. J. Chem*. 2009;62(9):1054-1061; *J. Phys. Chem. B.* 2010;114(28):9220-9230.
J. Phys. Chem. B. 2010;114(28):9231-9237; *Biophys. Chem.* 2011;158(2-3):126-133.