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# Molecular Design of Novel Micellar Timed-Release Drug Delivery

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Conventional drug delivery methods such as tablets, capsules, or injections are well understood and have been the major drug delivery vehicle for most of modern science. Consequently, new drug delivery methods are being studied that may improve upon the conventional methods. This study focused on a newer form of drug delivery that utilizes the unique free assembly characteristic of micelles. These micelles are aimed towards drugs that poorly soluble in water, and are able to dramatically increase drug solubility inside the micellar core thus increasing the bioavailability of the drug to the body. The drug/surfactant combination of interest used in this study was ibuprofen (0.021 g/L solubility) and $C_{12}E_8$. To this end, the thermodynamics of micellization, and the kinetics of drug release are points of interest. A thermodynamic model was created to calculate the gibb's free energy of micellization as a function of micellar shape, core minor radius, composition, and counter ion binding. This model consisted of six smaller free energies associated with the assembly of the dual micelle, and was expressed as :

$$g_{mic} = g_{trans} + g_{pack} + g_{int} + g_{st} + g_{elec} + g_{ent}$$

The model calculates the gibb's free energy of micellization, and thus minimizing the function based on the four parameters yields the micelle that is most optimal. From the gibb's free energy of micellization, it is possible to calculate the micellar solubility of ibuprofen.

It was found that for composition 0.5 – 0.54 (mole fraction $C_{12}E_8$), the predicted solubility of ibuprofen ranged from 176.12 g/L to 191.43 g/L (0.854 M to 0.928 M). The next step for this project would be the experimental verification of the thermodynamic model as well as development and refinement of a drug release kinetics model. The $g_{mic}$ model in theory does well to predict ibuprofen solubility, but a working kinetic model would be instrumental in the promoting of micellar drug delivery systems.

I will be presenting my findings at the upcoming AIChE annual conference on October 29th and also expect to publish a paper with Dr. Gow sometime in the future.

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