Quorum Sensing Molecules for Unicellular Organisms: Spectroscopic and Computational Study of Conformational Behavior

Dan Tollefson (Dr. John Thoemke) Daniel.Tollefson@mnsu.edu
Department of Chemistry and Geology - Minnesota State University, Mankato

Background
Quorum sensing plays a vital role in unicellular communications. It has been recently found that unicellular bacteria produce as small molecules that are created and released into the extracellular environment. Detailed knowledge regarding the interactions of these small molecules with the molecular and cellular-scale environments can potentially lead to the manipulation of quorum sensing within a population. Studies have focused on the application of QS manipulation in phenol-degrading activated sludge in waste water treatment facilities. Bio-char sequestering of QS molecules for agricultural purposes, and pharmaceutical applications. The function of these molecules requires that they can readily diffuse through the polar environment of aqueous solution and the nonpolar environment of cell membranes.

Methodology
- For FT-IR analysis, solutions of QS molecules were prepared in deuterated water and octanol.
- Nicolet S10 spectrometer with a single bounce ATR (Smart iTR module).
- Search for low energy conformers and solvation
- Theoretical Vibrational Analysis

Results

Future Work
The shortcomings of this research can largely be overcome by using larger and more complex mathematical models along with newer and more advanced software. All of this requires a higher computational cost. More accurate results can be obtained using DFT methods at the B3LYP/6-31+G* level. These calculations would not only use larger basis sets, it would also take into the account of electron correlation and excited states. This would also lead to much more accurate calculated vibrational frequencies.

References
(7) HyperChem™ Professional v. 5.1, HyperCube Inc., 115 NW 4th St., Gainesville, FL 32601, USA.

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