

Supplemental Figures

Effects on membrane lateral pressure suggest permeation mechanisms for bacterial quorum signaling molecules

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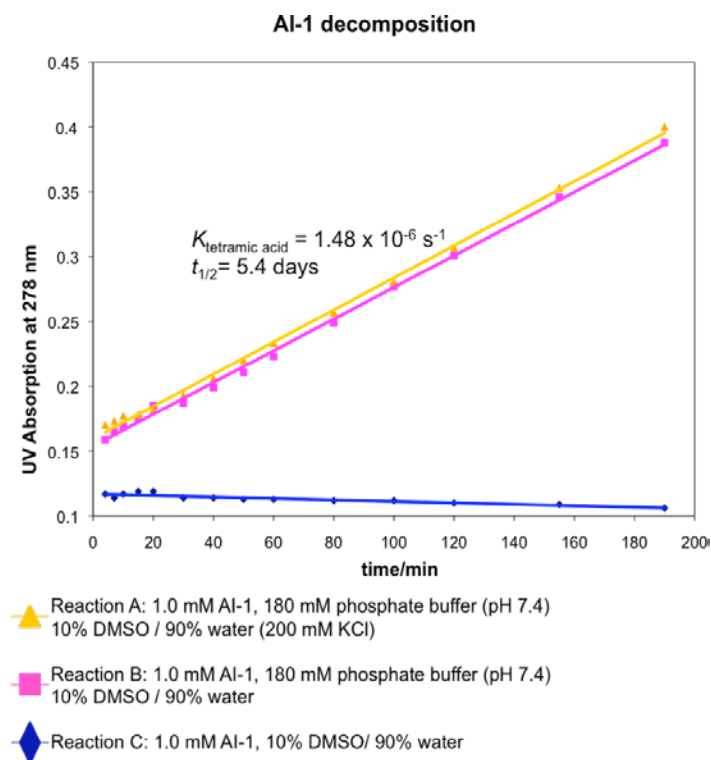


Figure S1. 3-oxo- C_{12} -AHL (AI-1) does not decompose into tetramic acid at neutral pH (7.0). Solid 3-oxo- C_{12} -AHL (AI-1) was stored at -20°C and a 20 mM stock solution in DMSO was always freshly prepared and used immediately. Reactions A-C (100 μL , in UV cuvettes (10 mm pathlength), temperature = 25°C) were monitored by following the UV absorbance of tetramic acid at 278 nm ($\epsilon = 13,900 \text{ M}^{-1}\text{cm}^{-1}$, see Kaufmann et al. *Proc. Natl. Acad. Sci. USA*. 2005, 102(2), 309-14). The rate constants for reactions A (phosphate buffer + KCl) and B (phosphate buffer) were both determined to be $1.48 \times 10^{-6} \text{ s}^{-1}$ (similar to the value, $1.49 \times 10^{-6} \text{ s}^{-1}$, reported in ref. 1). Interestingly, no decomposition of 3-oxo- C_{12} -AHL into tetramic acid was observed when the reaction was conducted in 10% DMSO/ 90% deionized water (reaction C).

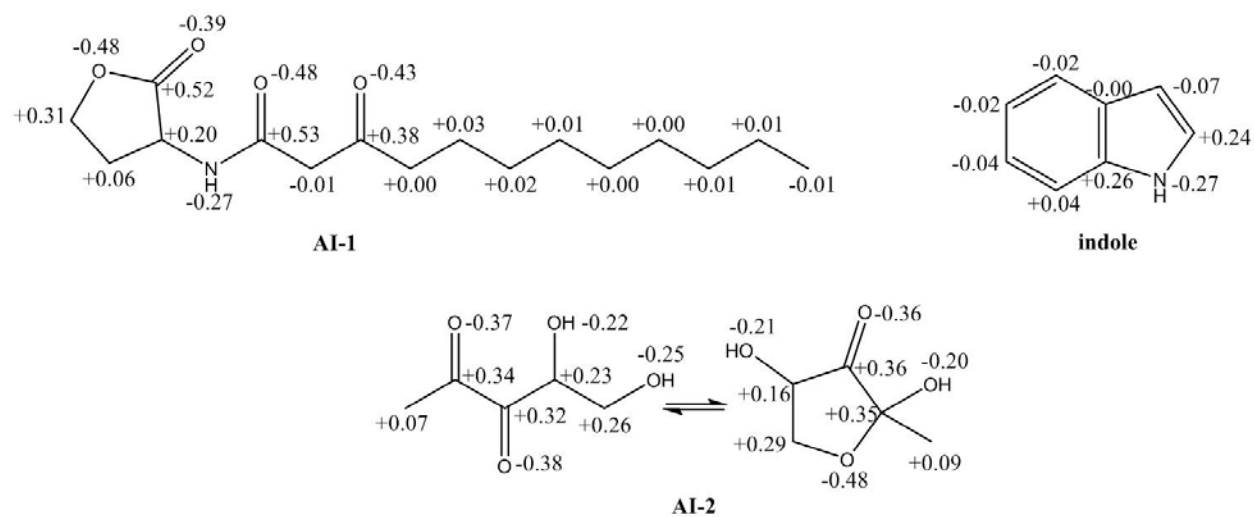


Figure S2. Chemical structures and partial charges for the natural AIs. The atomic charges were calculated with Gaussian 09 software (11) at B3LYP/6-31G(d) level. All the hydrogen charges were summed into the adjacent heavy atoms such as C, N and O.

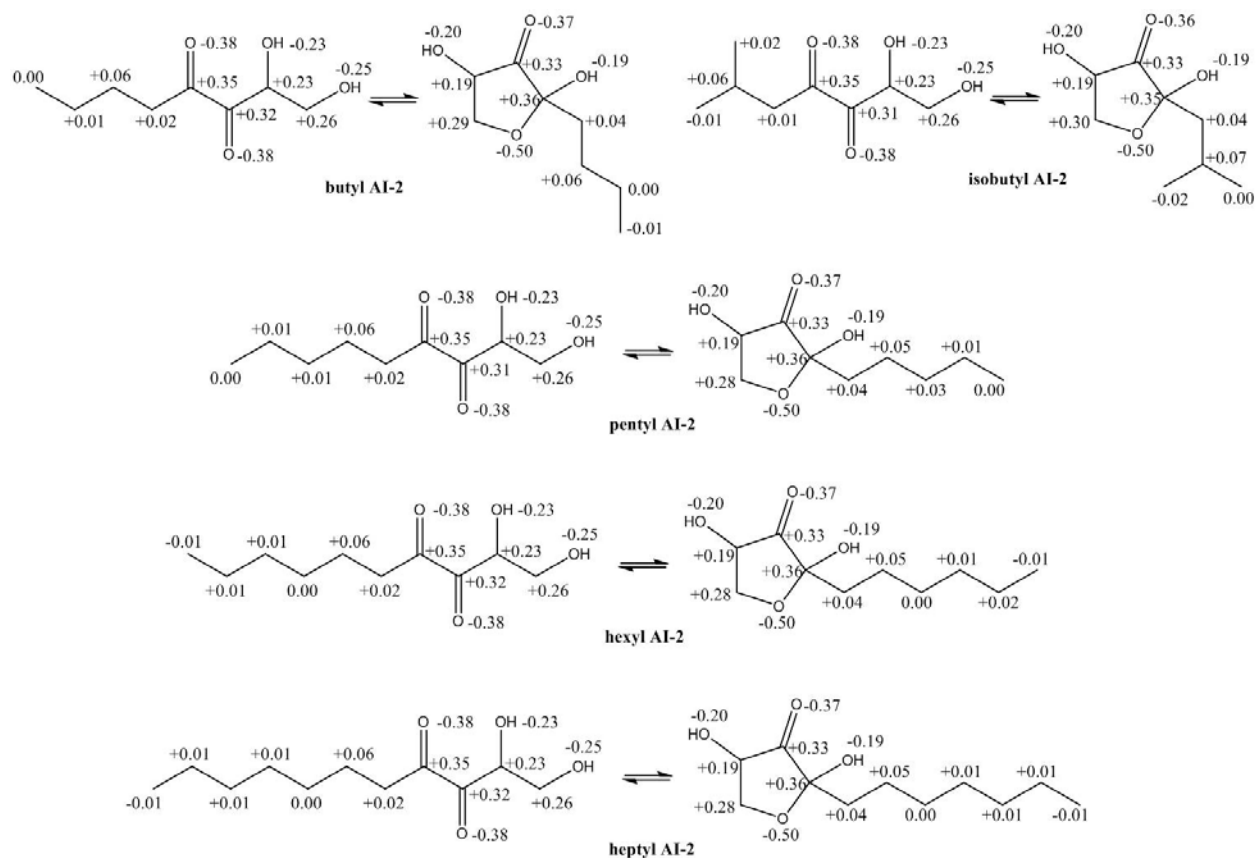


Figure S3. Chemical structures and partial charges for alkylated analogs of AI-2. The atomic charges were calculated with Gaussian 09 software (11) at B3LYP/6-31G(d) level. All the hydrogen charges were summed into the adjacent heavy atoms such as C, N and O.