**Multi-Modal Chemical Imaging of Molecular Messengers in Emerging *Pseudomonas aeruginosa* Microbial Communities**

Nameera F. Baig¹*, Sage J. B. Dunham²*, Nydia Morales-Soto³, Joshua D. Shrout³, Jonathan V. Sweedler²y, and Paul W. Bohn¹y

¹Department of Chemistry and Biochemistry and Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556

²Department of Chemistry and Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL 61801

³Department of Civil and Environmental Engineering and Earth Sciences and Department of Biological Sciences, University of Notre Dame, Notre Dame, IN 46556

**Supplemental Information**

**Figure S1.** Tandem mass spectrometry of analytes from Table 1
Multimodal Chemical Imaging of Molecular Messengers

Product of 244, 7-hour film, 25 eV

2-heptyl-4-quinoline
[M+H]^+ m/z calculated: 244.17
[M+H]^+ m/z observed: 244.17

[HHQ-C6H12]^+

Product of 260, 7-hour film, 25 eV

4-hydroxy-2-heptylquinoline-N-oxide
[M+H]^+ m/z calculated: 260.17
[M+H]^+ m/z observed: 260.18

[HQNO-C6H12O]^+

2-heptyl-3-hydroxyquinolone
[M+H]^+ m/z calculated: 260.17
[M+H]^+ m/z observed: 260.18

[PQS-C6H12]^+
Multimodal Chemical Imaging of Molecular Messengers

Product of 270, 7-hour film, 25 eV

2-nonenyl-4-quinoline
[M+H]^+ m/z calculated: 270.19
[M+H]^+ m/z observed: 272.19

Product of 272, 7-hour film, 25 eV

2-nonyl-4-quinoline
[M+H]^+ m/z calculated: 272.20
[M+H]^+ m/z observed: 272.21
Multimodal Chemical Imaging of Molecular Messengers

Product of 286, 7-hour film, 25 eV

4-hydroxy-2-nonenylquinoline-N-oxide
[M+H]^+ m/z calculated: 286.18
[M+H]^+ m/z observed: 286.19

Product of 288, 7-hour film, 25 eV

4-hydroxy-2-heptylquinoline-N-oxide
[M+H]^+ m/z calculated: 288.20
[M+H]^+ m/z observed: 260.20

[C₉₋₁-NQNO-C₇H₁₄O]^+

[C₉₋₁-NQNO-C₆H₁₄O]^+

[C₉₋₁-NQNO-C₆H₁₂O]^+

[C₉₋₁-NQNO-C₆H₁₂O]^+

[C₉₋₁-NQNO-C₆H₁₀O]^+

[C₉₋₁-NQNO-C₆H₁₀O]^+

[C₉₋₁-NQNO-C₆H₁₀O]^+

[C₉₋₁-NQNO-C₆H₁₀O]^+
2-undecenyl-4-quinoline

\[ [M+H]^+ \text{ m/z calculated: 270.19} \]

\[ [M+H]^+ \text{ m/z observed: 272.19} \]
Figure S2. Line-scans of $m/z$ 288.21 on the 7-hour biofilm of Figure 2.
Figure S3. Raman spectra of quiolone standards (i) HQNO and (ii) PQS.