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Supplementary Information for

Molecular signature of organic nitrogen in septic-impacted groundwater

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Environmental Science: Processes & Impacts

Dendrogram from Cluster Analysis (Figure S1)

Van Krevelen diagrams (Figures S2-S7)

p. S2
p. S3

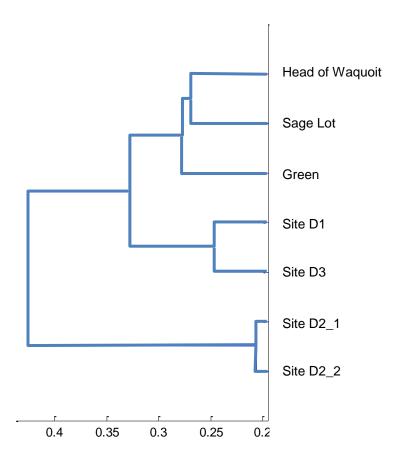
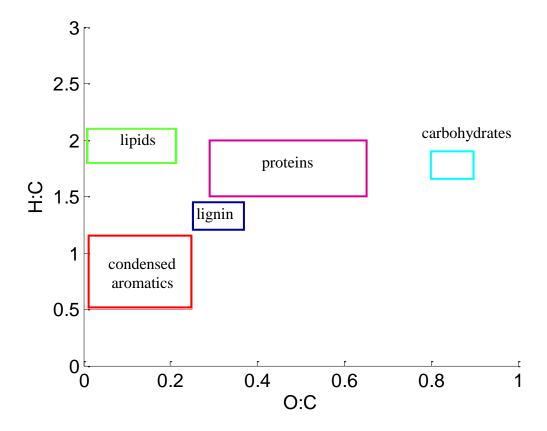


Figure S1. Dendrogram derived from cluster analysis determined from the FTICR-MS data from the six samples. The sample for Site D2 was analyzed twice, and the close association of the replicates indicates limited instrument variability.

Van Krevelen diagrams

In the following van Krevelen diagrams, the left hand plot contains all of the identified features for which formulas were assigned. The plot on the right hand side contains only N-containing features. The rectangles indicate regions associated with condensed hydrocarbons (red), lignin (dark blue), lipids (green), proteins (pink), and carbohydrates (light blue), as shown below.



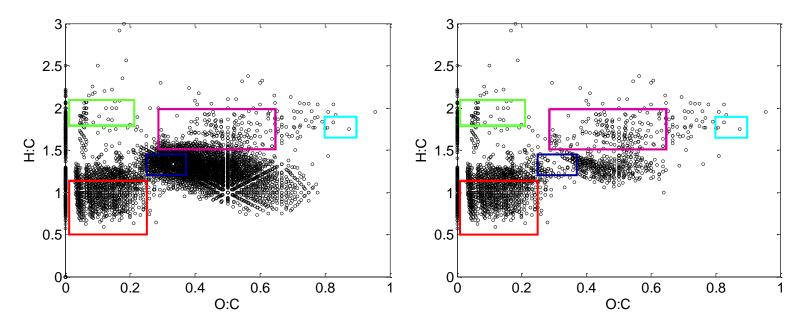


Figure S2. Van Krevelen diagrams for the Waquoit ground water samples.

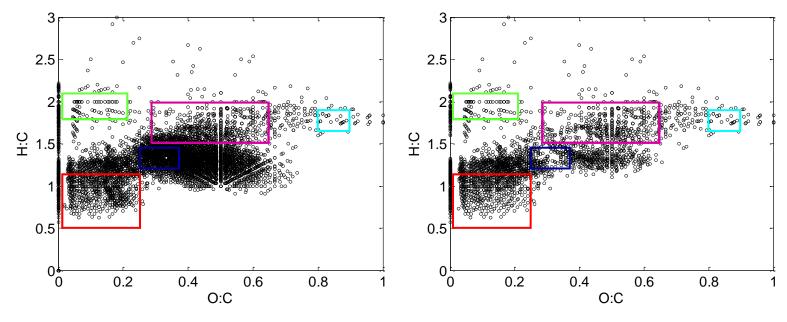


Figure S3. Van Krevelen diagrams for the Sage Lot ground water samples.

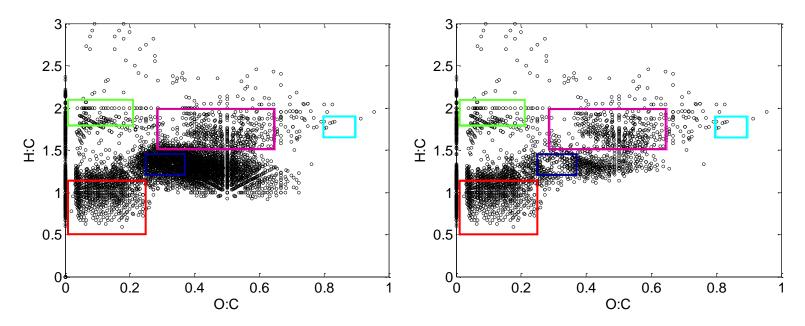


Figure S4. Van Krevelen diagrams for the Green Pond ground water samples.

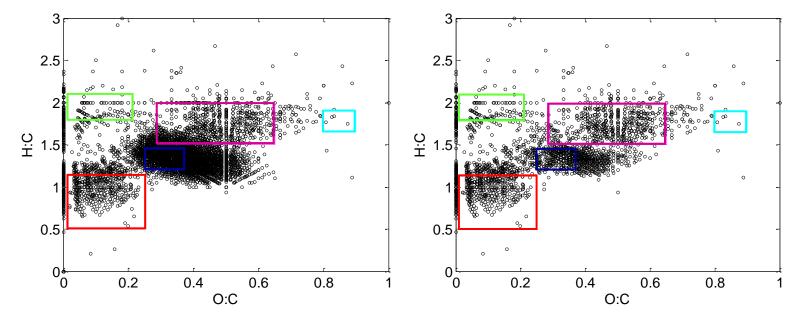


Figure S5. Van Krevelen diagrams for the Site D1 ground water samples.

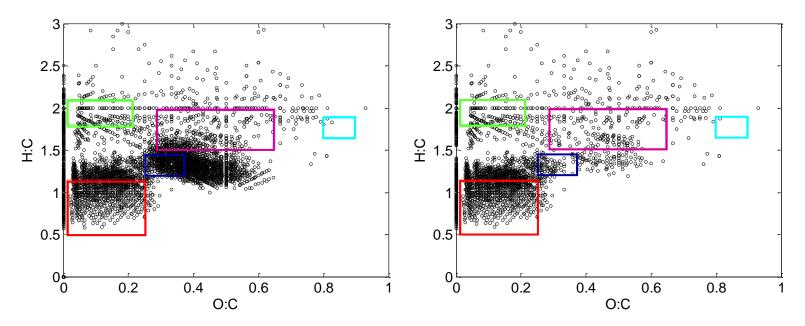


Figure S6. Van Krevelen diagrams for the Site D2 ground water samples.

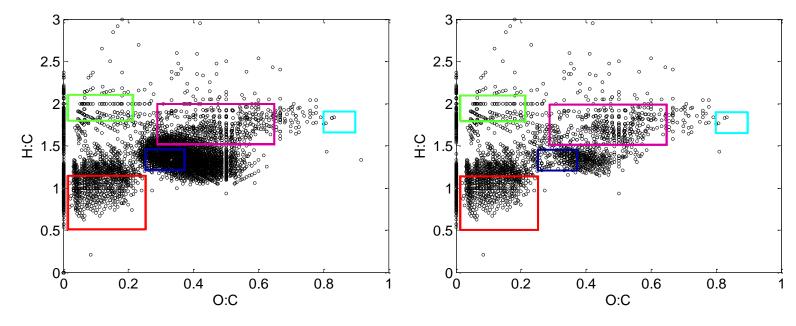


Figure S7. Van Krevelen diagrams for the Site D3 ground water samples.