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Supplement of

Molecular characterization of organic matter mobilized from Bangladeshi aquifer sediment: tracking carbon compositional change during microbial utilization

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Section S1: Calculation of organic carbon in sediment

Sediment Porewater Organic Carbon (DOC) = 0.33 ± 0.06 mg OC g⁻¹ sediment

Sediment Organic Matter (LOI) = 6.5 ± 1.5 mg/g

Using van Bemmelen factor (Burt, 2011) (58% OM = OC) to estimate sediment OC:

$$6.5 \text{ mg/g} * 0.58 = 3.77 \text{ mg OC/g sed}$$

DOC in sediment porewater as percent of sediment OC:

$$0.33/3.77 * 100 = 8.75 \%$$

Error for the above calculation:

$$\text{Err}_{\text{DOC}} = 0.06/3.77 = 0.0159$$

$$\text{Err}_{\text{OC}} = 0.33/(3.77^2) * (0.58 * 1.5) = 0.0202$$

$$\text{Err} = \sqrt{[(0.06/3.77)^2 + (0.33/(3.77^2) * (0.58 * 1.5))^2]}$$

$$= 0.0257 \text{ mg OC/g sed}$$

$$0.0257/3.77 * 100 = 0.68 \%$$

DOC in sediment porewater represented $8.8 \pm 0.7 \%$ of OC in sediment.

Table S1. Dissolved organic carbon concentrations in initial waters (mg-C L⁻¹)*

Initial Waters	Pond Recharge	Rice Field Recharge	Sediment Porewater
Rep 1	27.0	12.3	856
Rep 2	29.0	25.3	1103
Rep 3	33.1		1219

* Samples combined together during processing of FT-ICR-MS data are grouped together with thick lines.

Table S2. Dissolved organic carbon concentrations in incubation waters (mg-C L⁻¹)*

		1.5 days	17 days	18 days	19 days	20 days	80 days	81 days	91 days	184 days
Pond Recharge, Sterilized Sediment	Rep 1	212.9	219.30		254.6			253.4	184.7	222.9
	Rep 2	202.7	230.68		238.4			240.5		
	Avg. (stdev)	207.8 (7.2)	235.8 (14.8)			226.2 (36.5)				
Rice Recharge, Sterilized Sediment	Rep 1	226.0	213.48			264.9		230.7	201.8	247.4
	Rep 2	369.3	220.73			216.0		245.5		
	Avg. (stdev)	297.7 (101.4)	228.8 (24.3)			226.0 (22.2)				
Pond Recharge, Native Sediment	Rep 1	145.0		162.9	153.8		50.9		40.0	
	Rep 2	147.0		161.6	155.6					
	Avg. (stdev)	146.0 (1.4)	158.5 (4.5)			45.5 (7.7)				
Rice Recharge, Native Sediment	Rep 1	135.5		145.0		148.6	37.3		26.67	20.75
	Rep 2	142.6		174.2		140.8	31.5			
	Avg. (stdev)	139.1 (5.0)	152.1 (15.1)			31.77 (5.3)				

* Samples combined together during processing of FT-ICR-MS data are grouped together with thick lines.

Table S3. Methane concentrations in incubation bottles (mg-C L⁻¹)

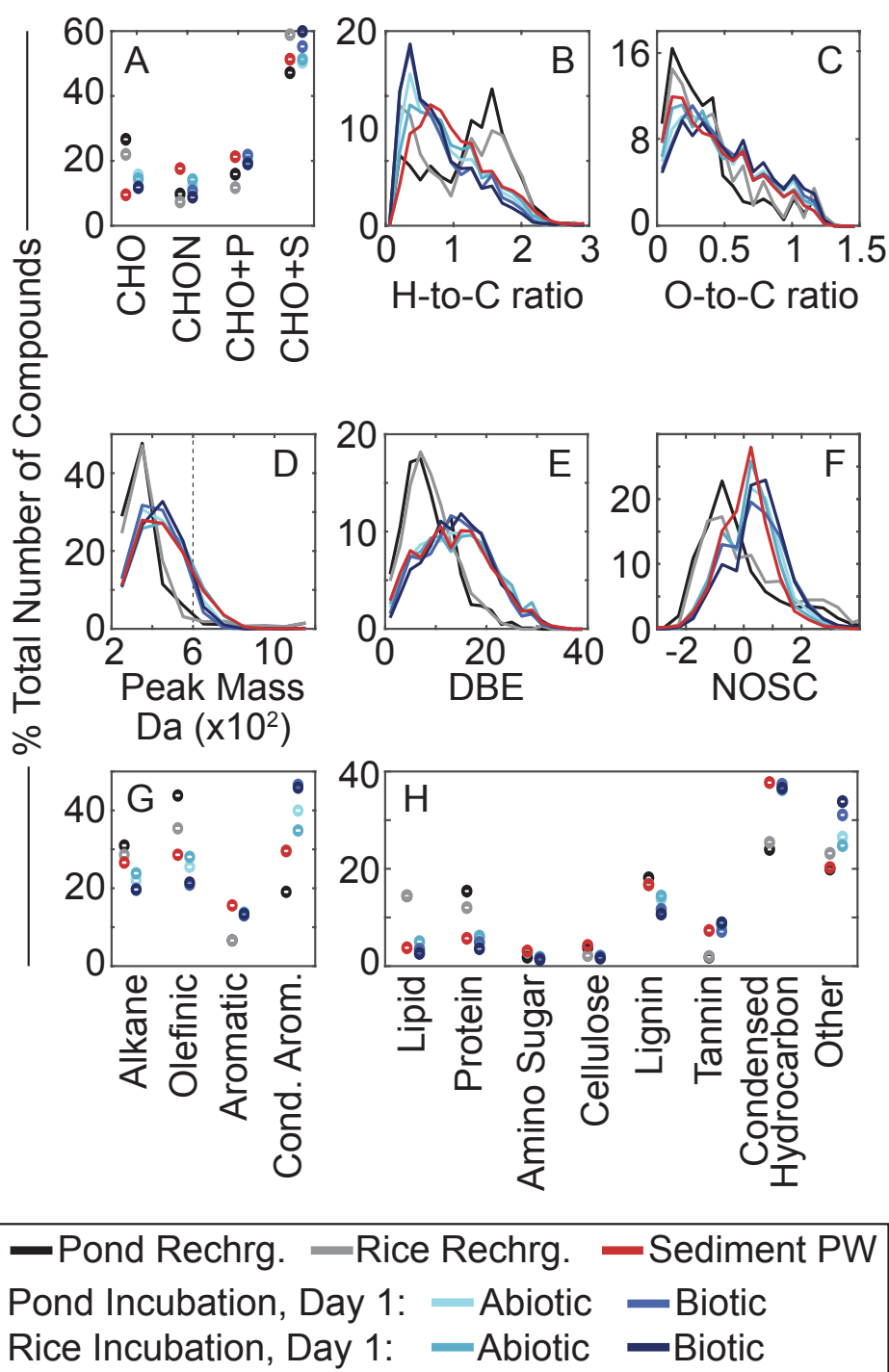
	18 days	273 days
Pond Recharge, Sterilized Sediment	Below detection	Below detection
Rice Recharge, Sterilized Sediment	Below detection	Below detection
Pond Recharge, Native Sediment	Below detection	198 ±46
Rice Recharge, Native Sediment	Below detection	368 ±45

Table S4. Compound Class Assignment

Compound Class	H-to-C ratio range	O-to-C ratio range
Lipid-like	1.5 – 2.3	0 – 0.2
Protein-like	1.5 – 2.2	0.2 – 0.5
Amino sugar-like	1.5 – 2.2	0.5 – 0.7
Carbohydrate-like	1.5 – 2.3	0.7 – 1.1
Lignin-like	0.8 – 1.5	0.25 – 0.67
Tannin-like	0.6 – 1.2	0.67 – 0.95
Condensed hydrocarbon-like	0.8 – 1.2 0 – 0.8	0 – 0.25 0 – 0.5

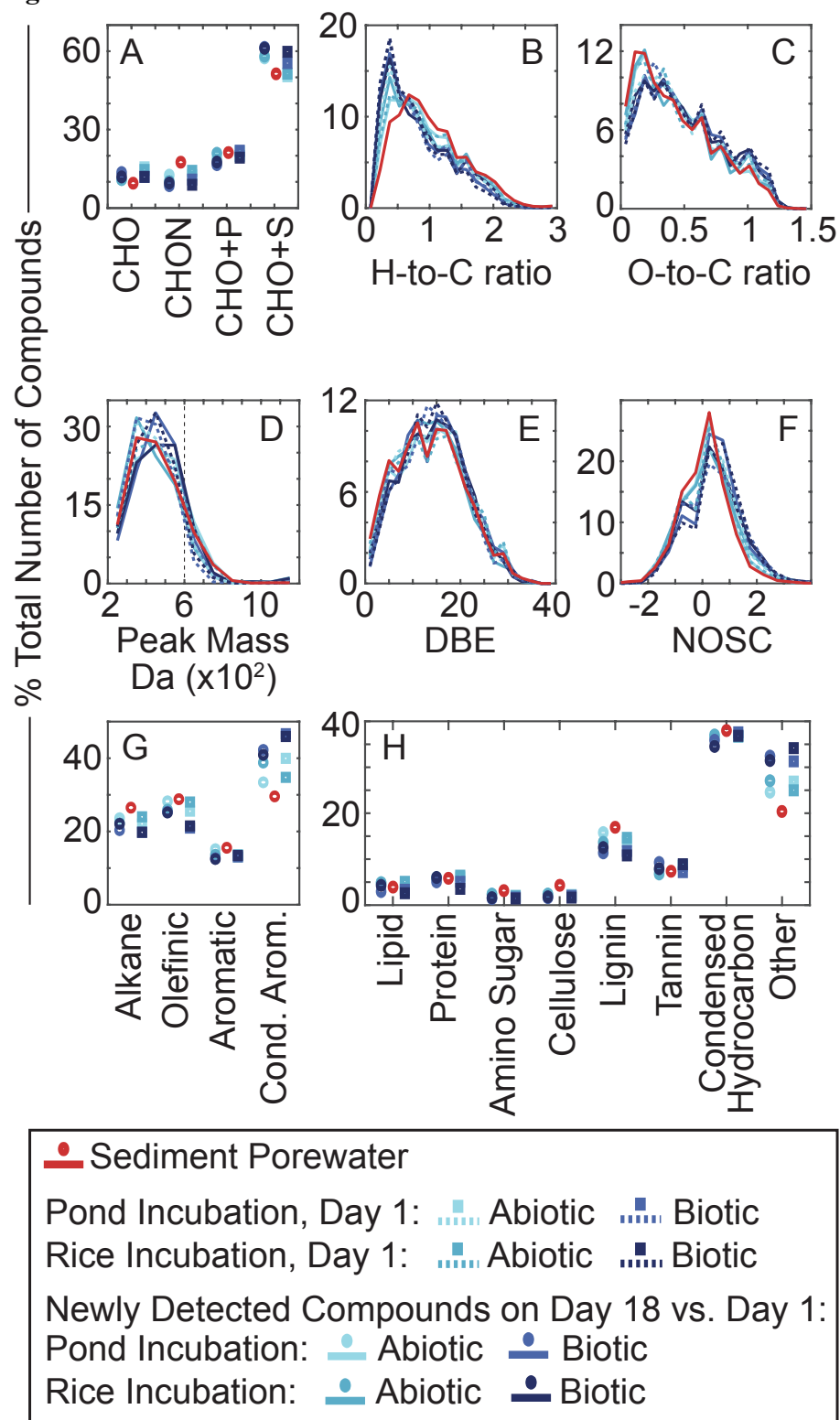
- Based on D'Andrilli et al. (2015).
- Compounds falling outside of designated ratios ranges were classified as 'other'

Figure S1



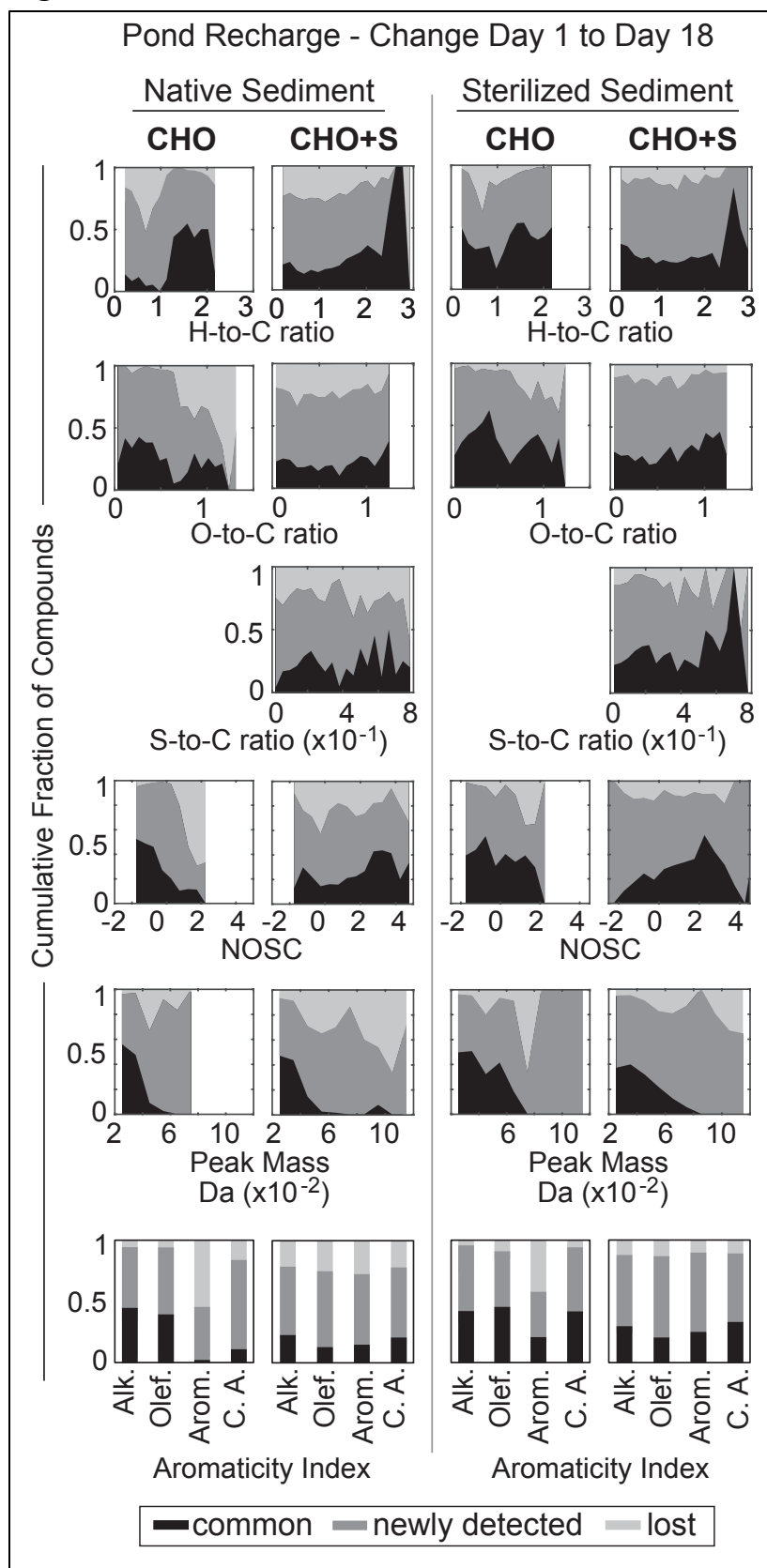
Chemical characteristics of mobilized SOC (red), DOC in pond recharge water (black), DOC in rice field recharge water (grey), and DOC in day-1 incubation waters (blues). **(a)** Percent of identified compounds in heteroatom groups. Proportional distributions of **(b)** H-to-C ratios, **(c)** O-to-C ratios, **(d)** peak mass, **(e)** double bond equivalents, and **(f)** nominal oxidation states of carbon. Percent of identified compounds in groupings based on **(g)** AI (alkanes, AI=0; olefinics, $0 < AI \leq 0.5$; aromatics, $AI > 0.5$; condensed aromatics, $AI \geq 0.67$) and **(h)** compound classifications (Table S4).

Figure S2



Chemical characteristics of mobilized SOC (red), DOC in incubation waters from day 1 (dashed blues, squares), and newly detected compounds on incubation day 18 that were not detected on incubation day 1 (solid blues, circles). Panels as identified in Figure S1.

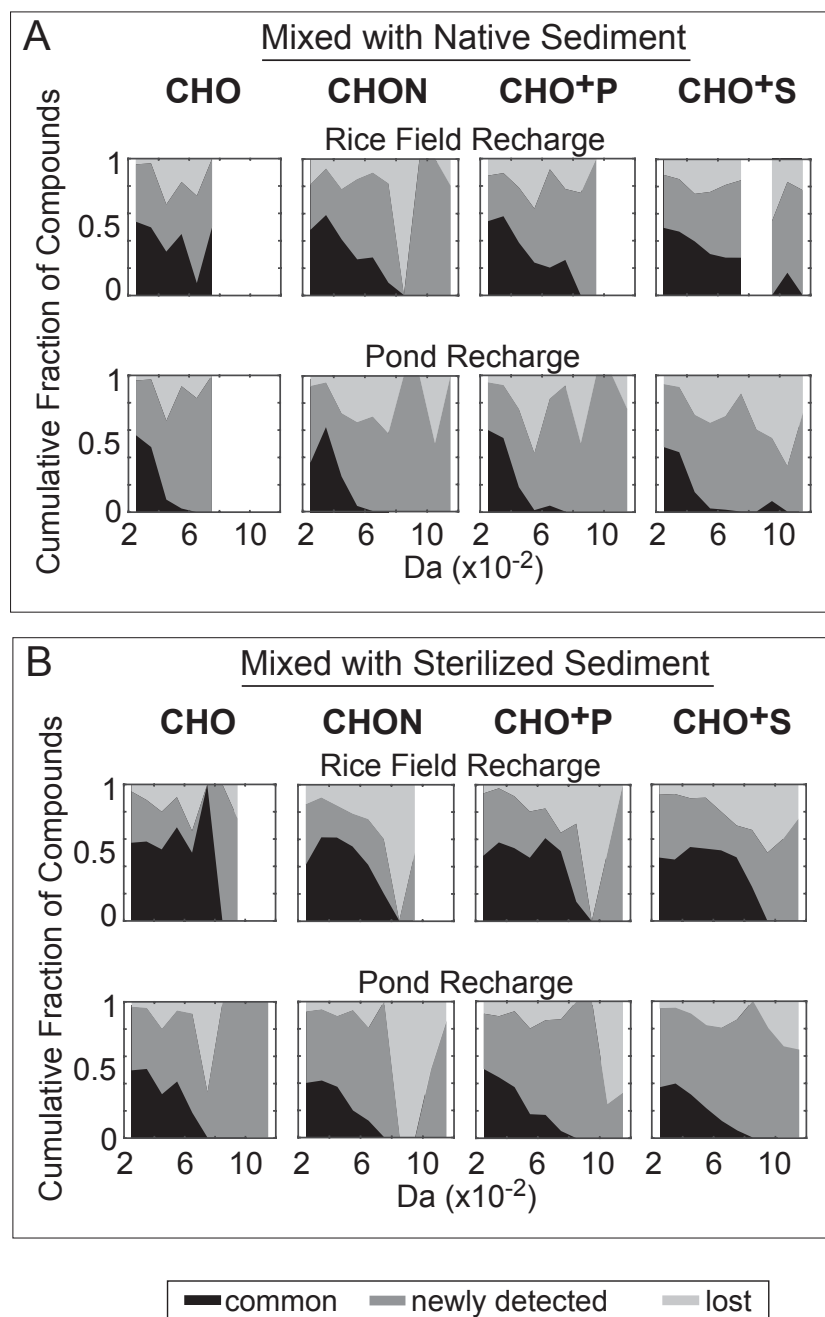
Figure S3



Relative change in chemical indices between day 1 and day 18 for pond recharge water incubated with native sediment and sterilized sediment. Plotted are the cumulative fractions of compounds that were identified at both time points, i.e., common (black), identified at the second time point but not at the first, i.e., newly detected (dark grey), and identified at the first time point but not at the second, i.e., lost (light grey). Compounds were separated by heteroatom group (CHO and CHO+S groups are shown) and characterized based on H-to-C ratio, O-to-C ratio, S-to-C ratio, nominal oxidation state of carbon (NOSC), peak mass, and aromaticity index.

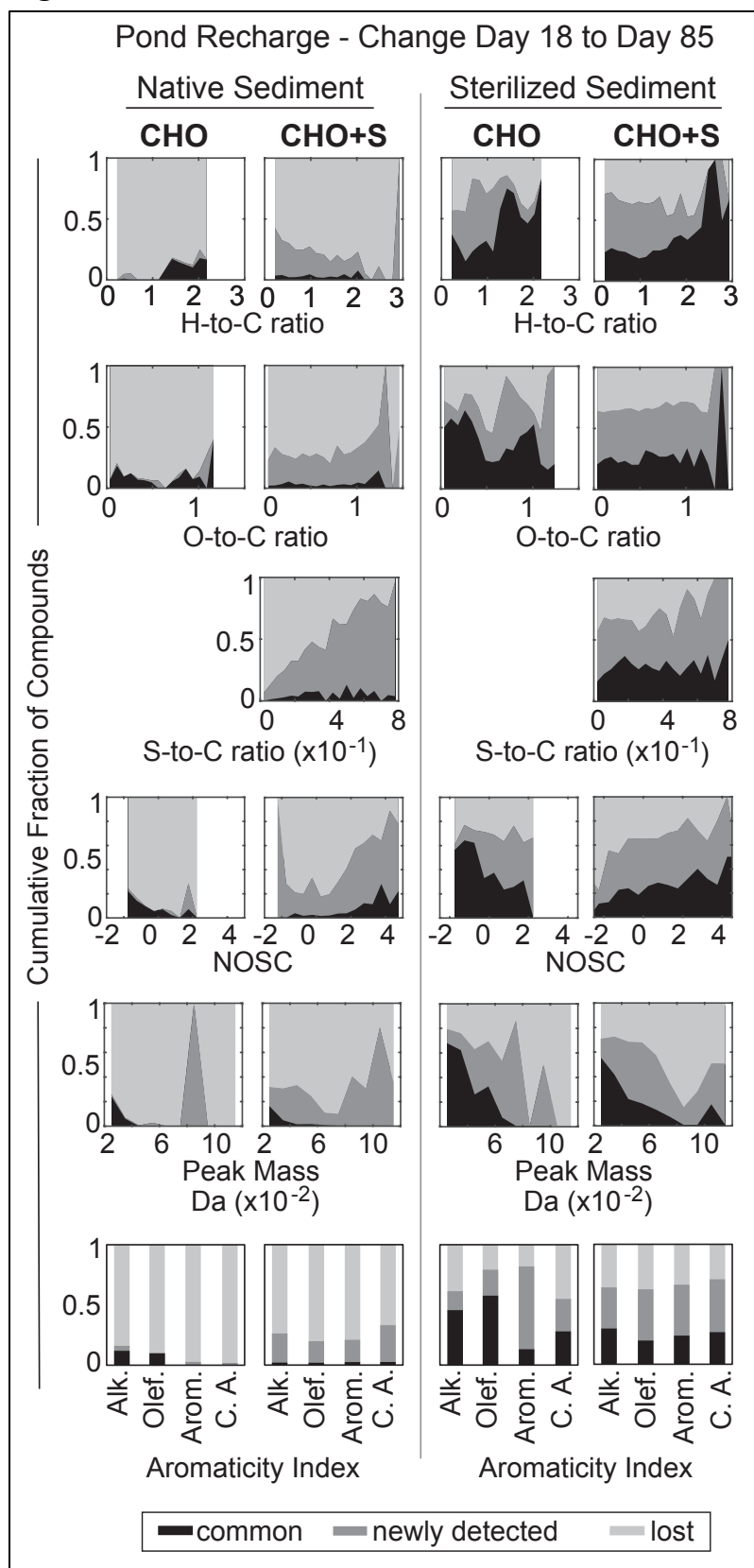
Figure S4

Peak Mass — Change from Day 1 to Day 18



Relative change in peak mass between day 1 and day 18 for both rice field recharge water (top row) and pond recharge water (bottom row) incubated with (a) native sediment and (b) sterilized sediment. Plotted are the cumulative fractions of compounds that were identified at both time points, i.e., common (black), identified at the second time point but not at the first, i.e., newly detected (dark grey), and identified at the first time point but not at the second, i.e., lost (light grey). Compounds were separated by heteroatom group (CHO, CHON, CHO+P, CHO+S).

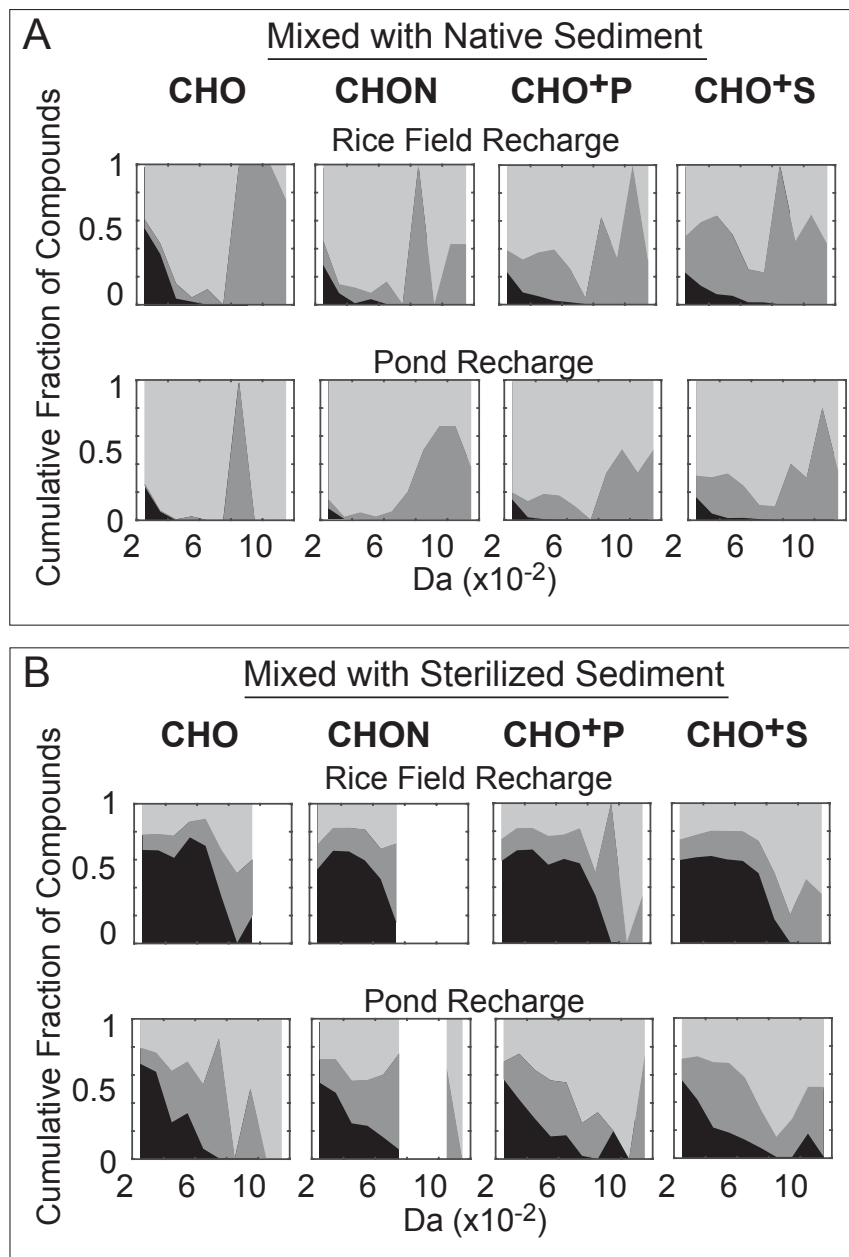
Figure S5



Relative change in chemical indices between day 18 and day 85 for pond recharge water incubated with native sediment and sterilized sediment. Plotted are the cumulative fractions of compounds that were identified at both time points, i.e., common (black), identified at the second time point but not at the first, i.e., newly detected (dark grey), and identified at the first time point but not at the second, i.e., lost (light grey). Compounds were separated by heteroatom group (CHO and CHO+S groups are shown) and characterized based on H-to-C ratio, O-to-C ratio, S-to-C ratio, nominal oxidation state of carbon (NOSC), peak mass, and aromaticity index.

Figure S6

Peak Mass — Change from Day 18 to Day 85



Relative change in peak mass between day 18 and day 85 for both rice field recharge water (top row) and pond recharge water (bottom row) incubated with **(a)** native sediment and **(b)** sterilized sediment. Plotted are the cumulative fractions of compounds that were identified at both time points, i.e., common (black), identified at the second time point but not at the first, i.e., newly detected (dark grey), and identified at the first time point but not at the second, i.e., lost (light grey). Compounds were separated by heteroatom group (CHO, CHON, CHO+P, CHO+S).

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