Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting Information

Physical Separation of Highly PAXH Contaminated Soil as Well as Analysis of Its Fractions and Corresponding Water Phase Using Fourier Transform Mass Spectrometry

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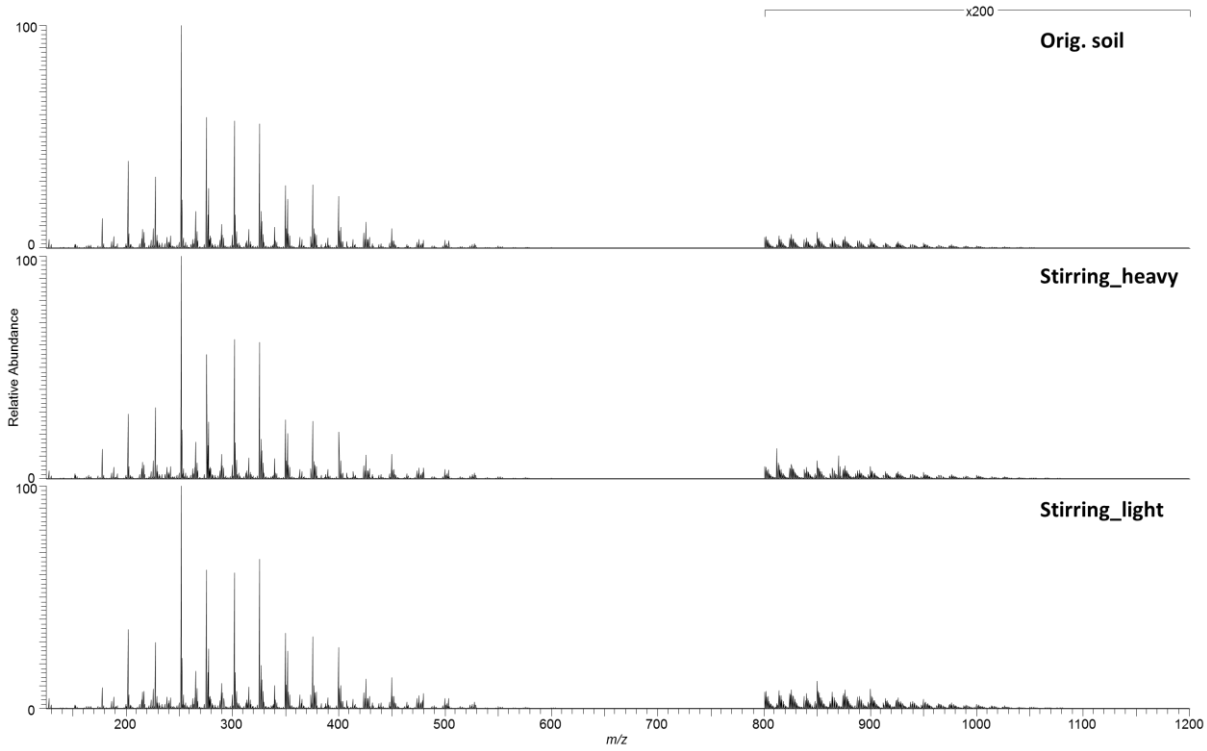

Figure S1. Recombined positive mode APPI mass spectra for original soil (top), its heavy (middle) and light (bottom) fractions after stirring.

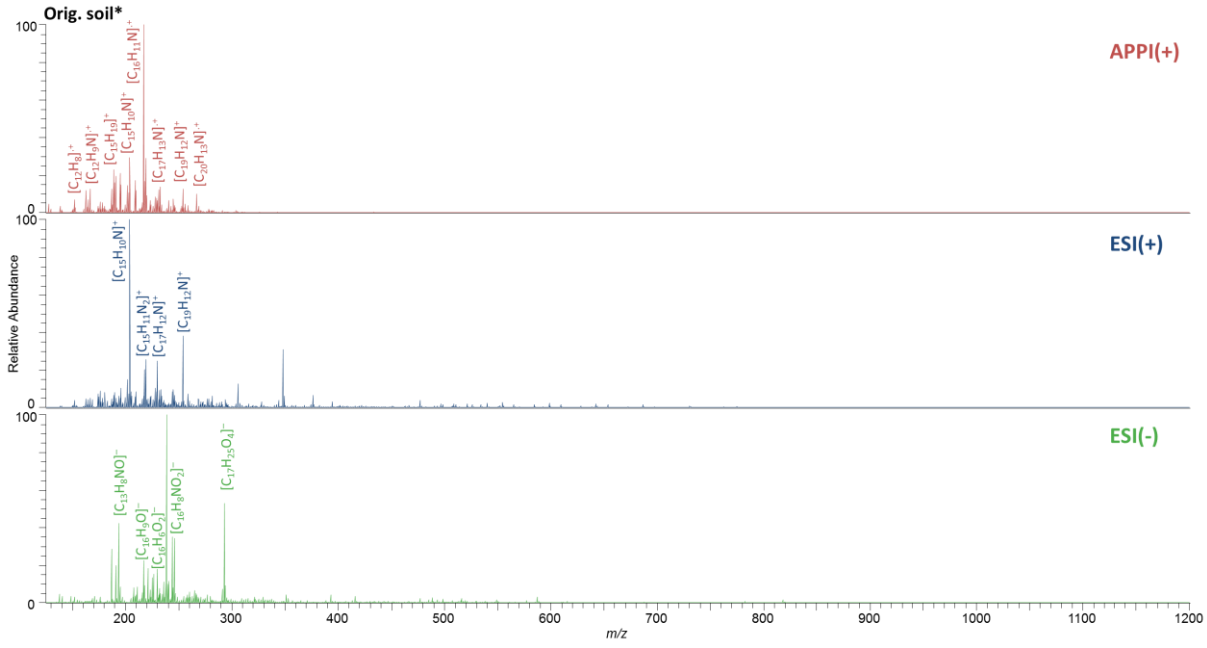

Figure S2. Recombined mass spectra for the original soil Soxhlet extracted using water, analyzed by FT Orbitrap MS using positive mode APPI (top), ESI (middle) and negative mode ESI (bottom).

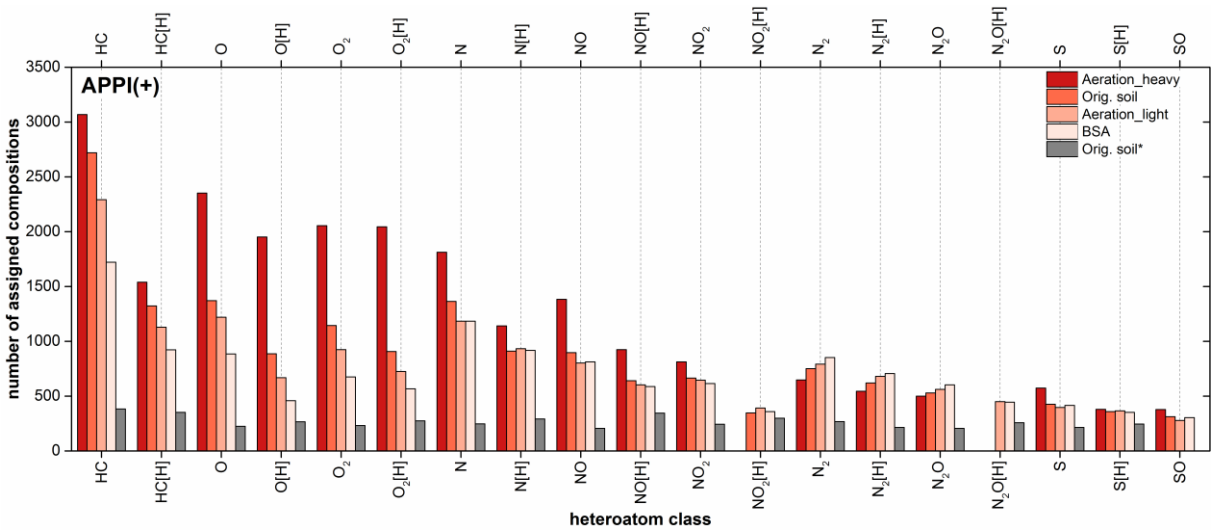

Figure S3. Class distributions for the heavy fraction after aeration, original soil, light fraction after aeration and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using positive mode APPI FT Orbitrap MS.

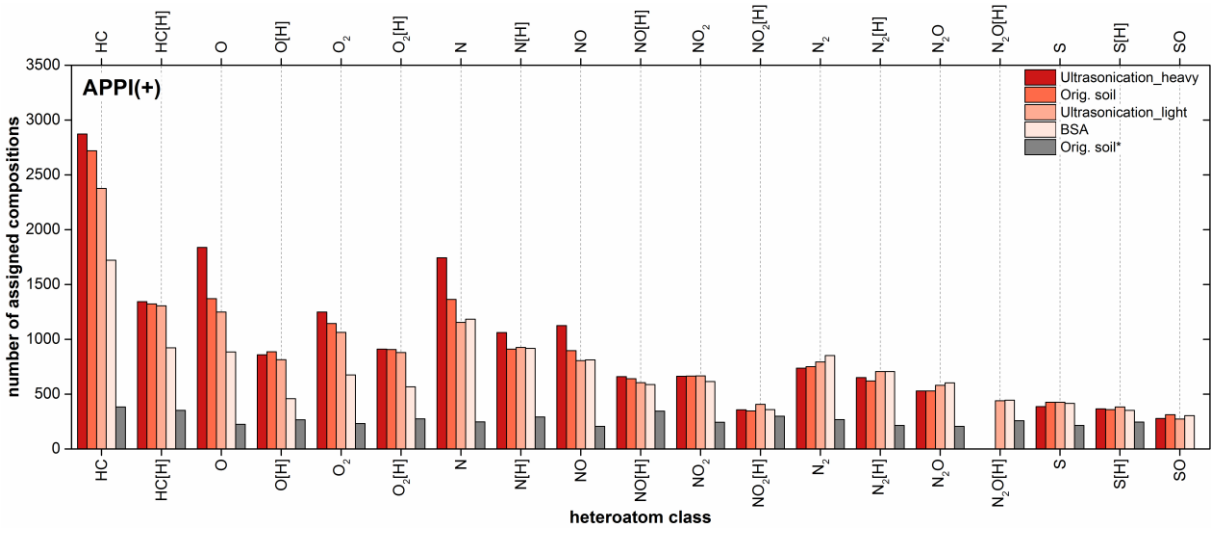

Figure S4. Class distributions for the heavy fraction after ultrasonication, original soil, light fraction after ultrasonication and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using positive mode APPI FT Orbitrap MS.

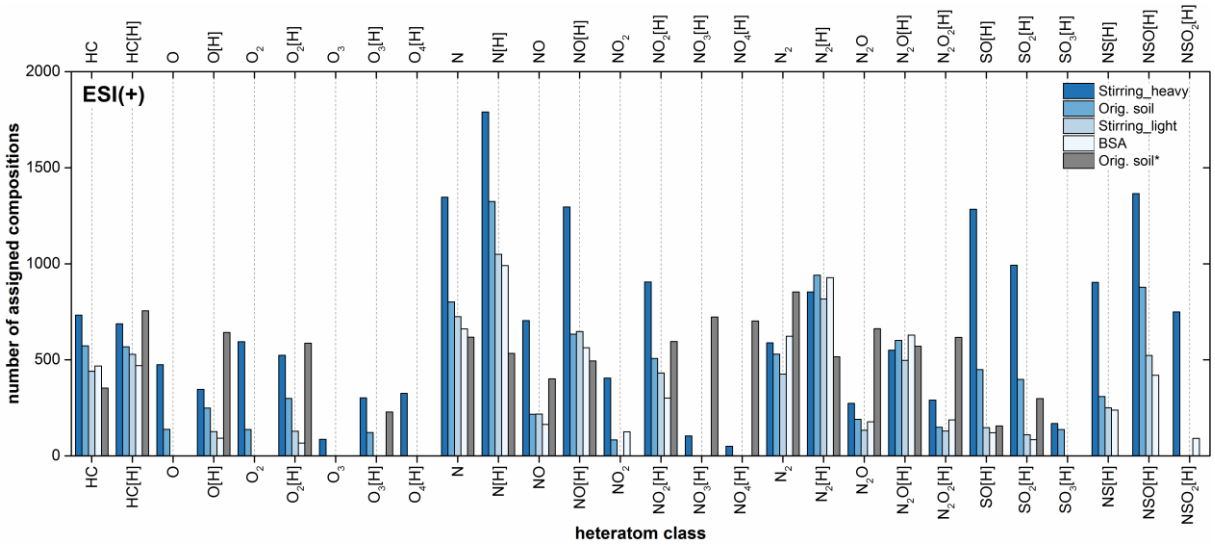

Figure S5. Class distributions for the heavy fraction after stirring, original soil, light fraction after stirring and the black solid aggregate (from dark to light blue) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using positive mode ESI FT Orbitrap MS.

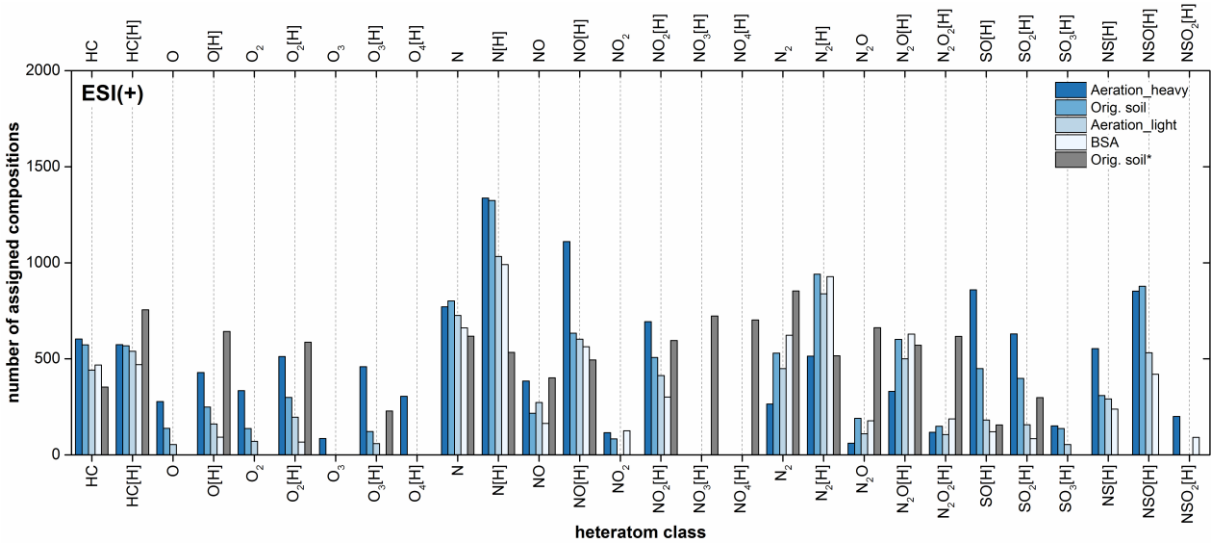

Figure S6. Class distributions for the heavy fraction after aeration, original soil, light fraction after aeration and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using positive mode ESI FT Orbitrap MS.

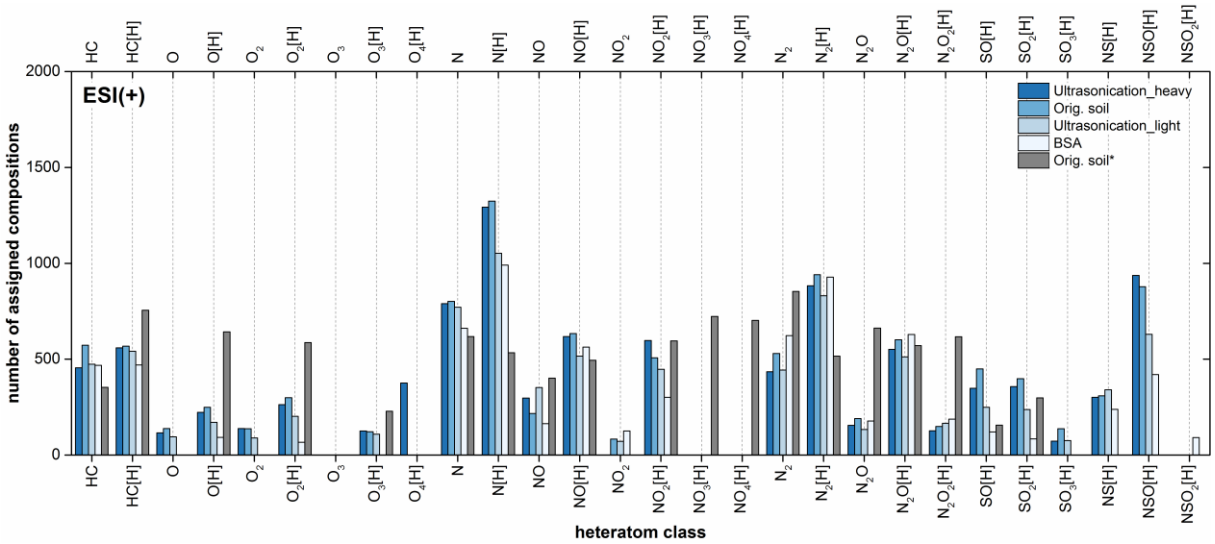

Figure S7. Class distributions for the heavy fraction after ultrasonication, original soil, light fraction after ultrasonication and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using positive mode ESII FT Orbitrap MS.

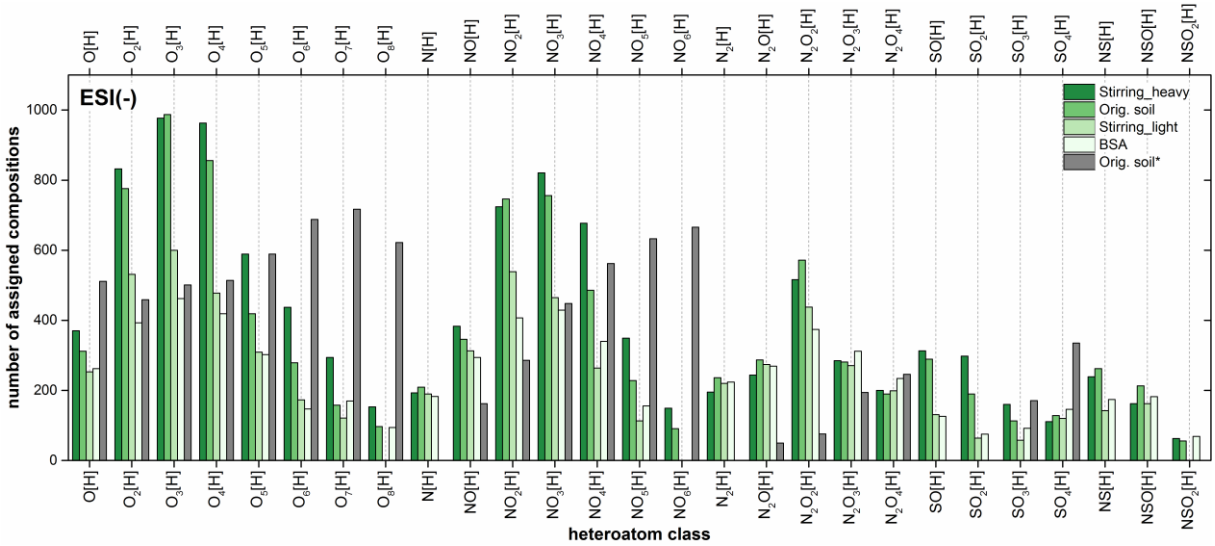

Figure S8. Class distributions for the heavy fraction after stirring, original soil, light fraction after stirring and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using negative mode ESI FT Orbitrap MS.

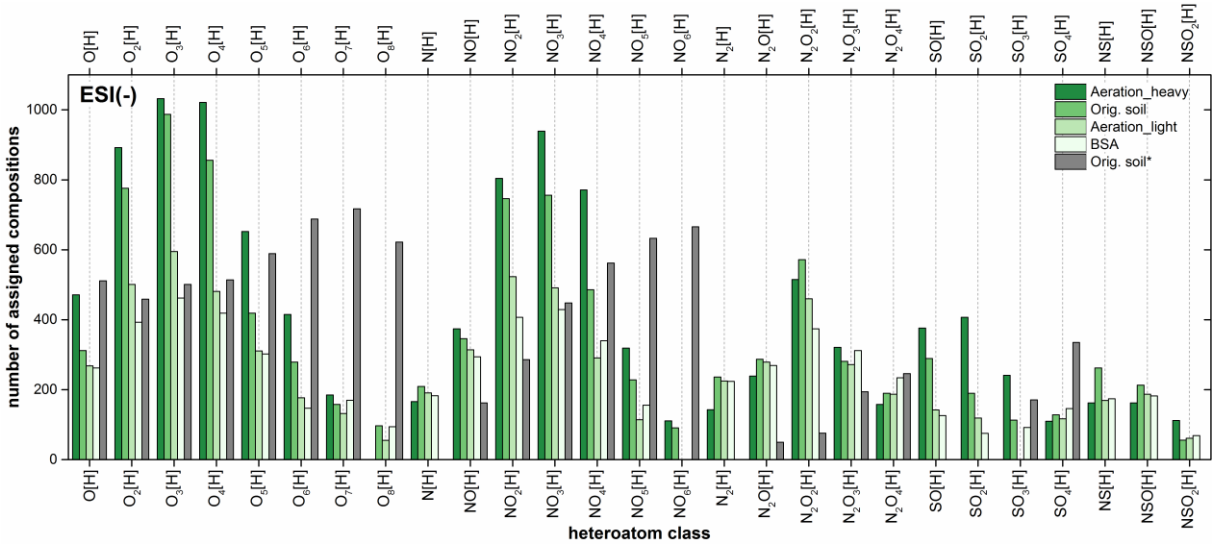

Figure S9. Class distributions for the heavy fraction after aeration, original soil, light fraction after aeration and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using negative mode ESI FT Orbitrap MS.

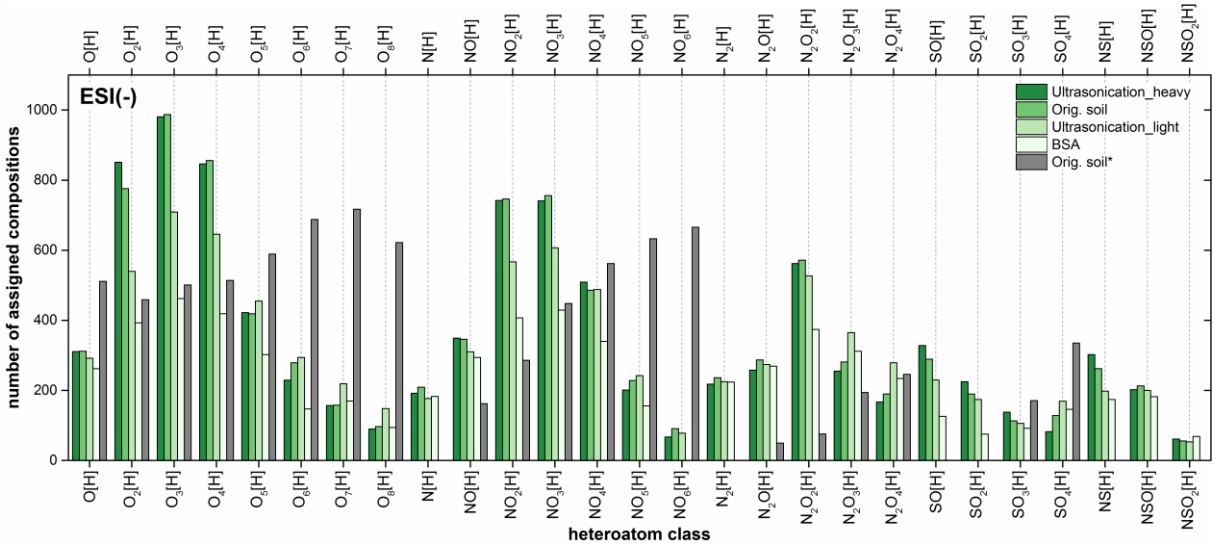

Figure S10. Class distributions for the heavy fraction after ultrasonication, original soil, light fraction after ultrasonication and the black solid aggregate (from dark to light red) as well as the water extract (selected classes only) denoted as orig. soil*, analyzed using negative mode ESI FT Orbitrap MS.

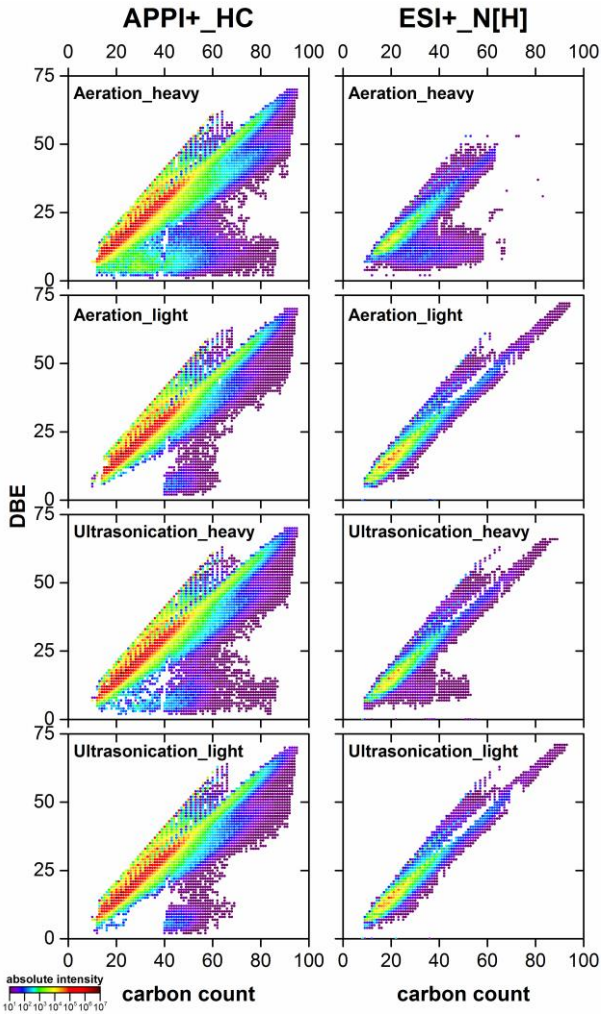

Figure S 11. DBE vs. carbon number plots for radical hydrocarbon (left column) and protonated nitrogen (right column) classes from the heavy and light fractions after aeration and ultrasonication (from top to bottom), analyzed using positive mode APP and ESI Orbitrap MS.

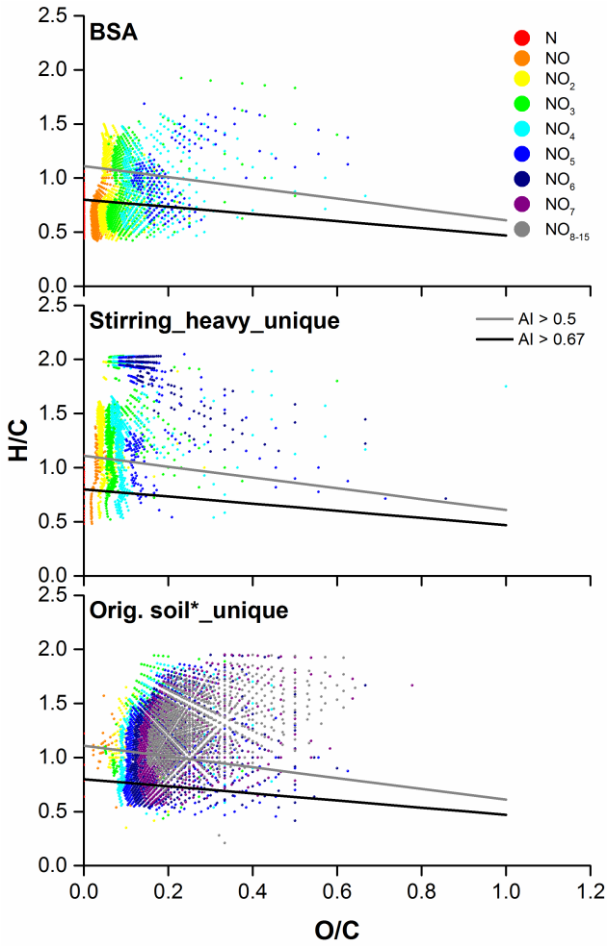

Figure S12. Van Krevelen plots for the black solid aggregate (top), the unique compositions from the heavy fraction after stirring (middle), and the original soil Soxhlet extracted using water (bottom, denoted as orig. soil*), compared with the black solid aggregate, analyzed by negative mode ESI FT Orbitrap MS. Compositions below the gray or black line have a AI higher than 0.5 or 0.67, respectively.

Table S 1. The number of NO_x class compositions detected in total, AI > 0.5 or > 0.67 (proportion to total number in bracket) for different samples.

NO_x classes	Number of compositions in			
	total	AI < 0.5	0.5 ≤ AI < 0.67	AI ≥ 0.67
BSA	1809	486 (27%)	559 (31%)	764 (42%)
Stirring_heavy	3296	1659 (50%)	850 (26%)	787 (24%)
Orig. soil*	4531	2826 (62%)	1138 (25%)	567 (13%)