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

Supporting Information

Barium ion adduct mass spectrometry to identify carboxylic acid photoproducts from crude oil-water systems under solar irradiation

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Iteration Number	Element	Minimum	Maximum
1)	C	1	100
	H	4	200
	N	0	1
	O	0	6
	S	0	1
	138 Ba	1	2
	137 Ba	0	0
2)	C	1	100
	H	4	200
	N	0	2
	O	0	6
	S	0	2
	138 Ba	0	0
	137 Ba	0	0
3)	C	1	100
	H	4	200
	N	0	2
	O	0	15
	S	0	2
	138 Ba	0	0
	137 Ba	0	0
4)	C	1	100
	H	4	200
	N	0	2
	O	0	15
	S	0	2
	138 Ba	1	2
	137 Ba	0	0
5)	C	1	100
	H	4	200
	N	0	2
	O	0	15
	S	0	2
	138 Ba	1	2
	137 Ba	1	2

Table S1: Elemental constraints for each molecular assignment iteration.

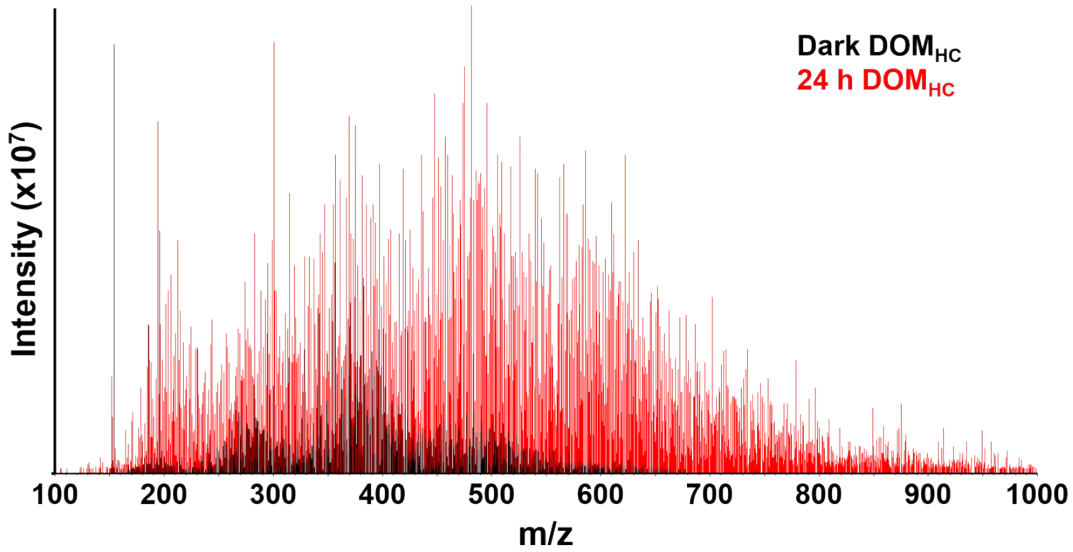

Figure S1: Overlay of spectra comparing derivatized samples at 25 ppm C of precursor ion scan of m/z 155 showing possible $[M-H+Ba]^+$ peaks for dark (black) and irradiated DOM_{HC} (red) produced after 24 h of sunlight exposure on an AbSciex 3200 Qtrap using (+) ESI MS/MS.

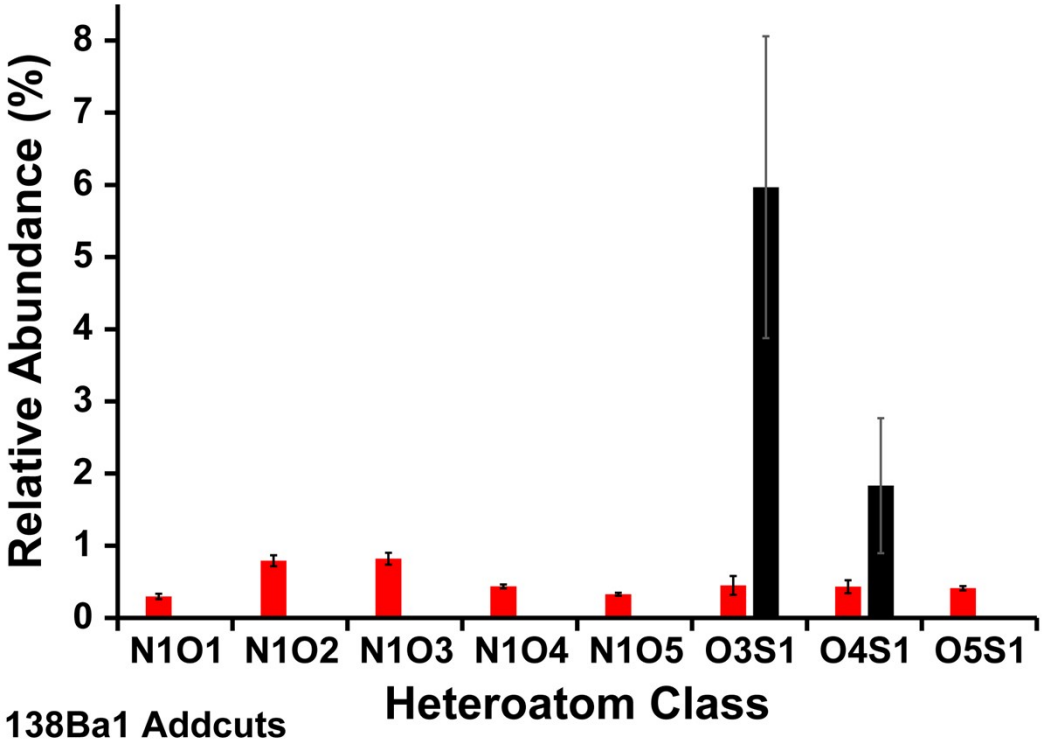

Figure S2. Heteroatom class distribution for barium 138 containing adducts detected in the dark (black) and irradiated (red) DOM_{HC}. Error bars represent standard deviation (n=3).

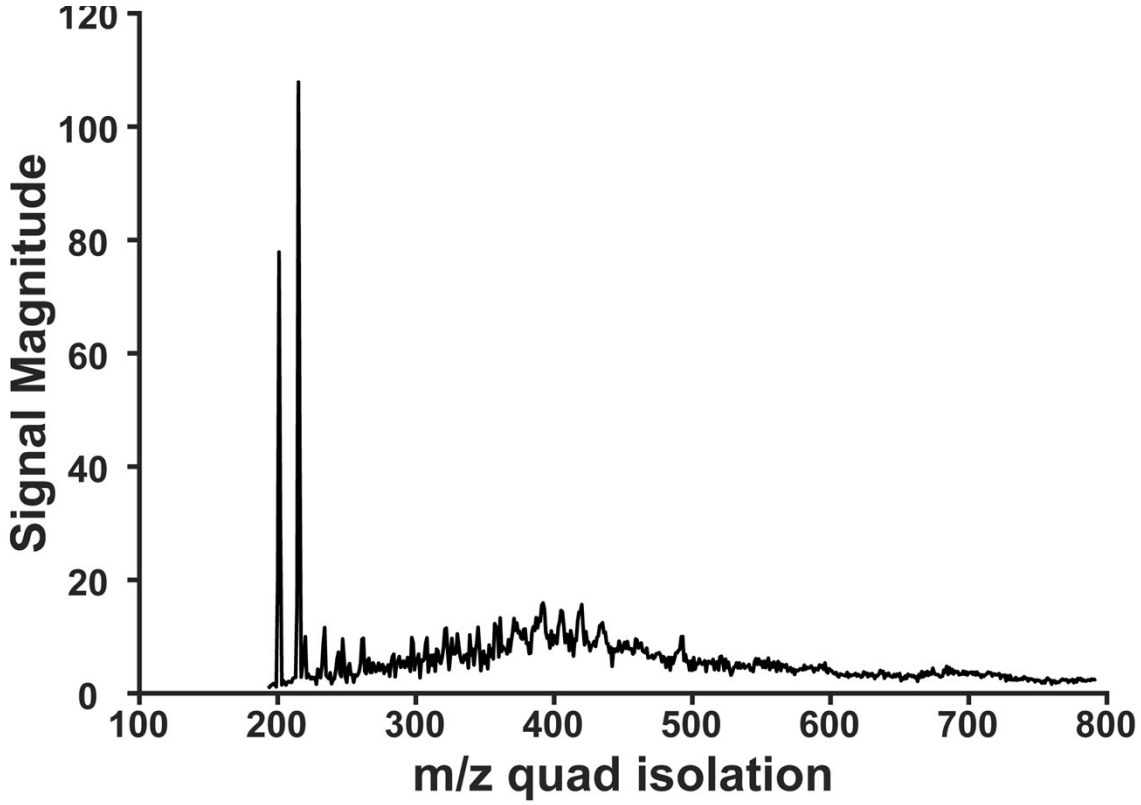

Figure S3. Plot of m/z quad isolation vs. signal magnitude for m/z 196.918 ($C_2H_3O_2{}^{138}Ba^+$) detected in the DOM_{HC} after light exposure using FT-ICR MS/IRMPD.