

Supplementary Information for “Online SFE-LC-FTMS for sensitive and comprehensive characterization of soil organic matter”

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Table S1. Comparison of the compounds assigned for high-C peat soil using SFE (CO₂) and LSE with different solvents (MeOH, ACN, H₂O and hexane)¹. A) Compound classes of formulas assigned using FTICR MS, and B) compositional distribution.

A)

Extraction method	Lipid %	Unsaturated Hydrocarbon %	Protein %	Lignin %	Carbo-hydrate %	Amino sugar %	Tannin %	Condensed hydrocarbon %	Other %
SFE-CO ₂	54	4	15	22	1	1	0	1	2
LSE-MeOH	44	5	7	10	1	2	1	7	23
LSE-CAN	24	10	3	16	1	0	3	14	29
LSE-H ₂ O	2	4	11	33	9	5	6	10	20
LSE-hexane	54	3	21	4	0	2	0	1	14

B)

Extraction method	# of assigned formulas	CHO %	CHON %	CHOS %	CHOP %	CHONP %	CHOSP %	CHONS %	CHONSP %	Other %
SFE-CO ₂	6414	66	7	2	6	10	1	8	2	0
LSE-MeOH	3135	37	41	9	1	6	0	2	3	0
LSE-ACN	3638	37	24	9	3	9	2	8	8	0
LSE-H ₂ O	2642	40	39	2	0	5	5	7	0	0
LSE-hexane	625	54	14	12	3	7	2	5	3	0
LSE Combined	5800	46	30	6	1	6	3	6	3	0

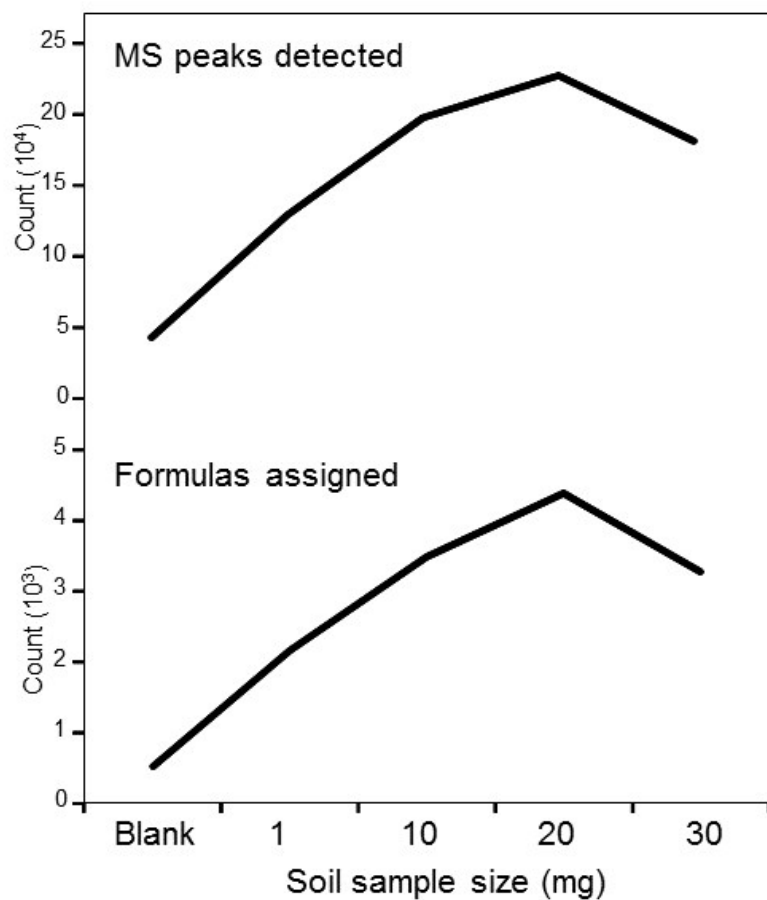


Figure S1. The number of MS peaks detected and molecular formulas assigned varied with the amount of soil available for extraction. The highest number of MS peaks detected and formulas assigned was attained with 20 mg of soil undergoing extraction. Experimental conditions are detailed in the text.

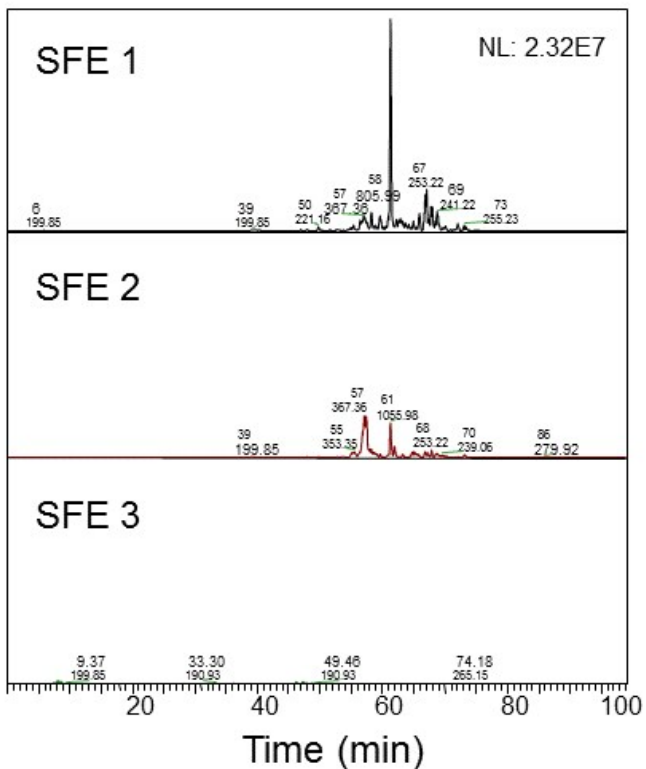


Figure S2. Recovery for SFE of low C soil. A SRS soil (20 mg) was extracted three times (SFE 1-3) and residues left after each extraction examined using LC-FTMS residues. The three LCMS base peak chromatograms are depicted at the same intensity scale (i.e., 2.32×10^7). Very little organic matter can be detected after the third extraction.

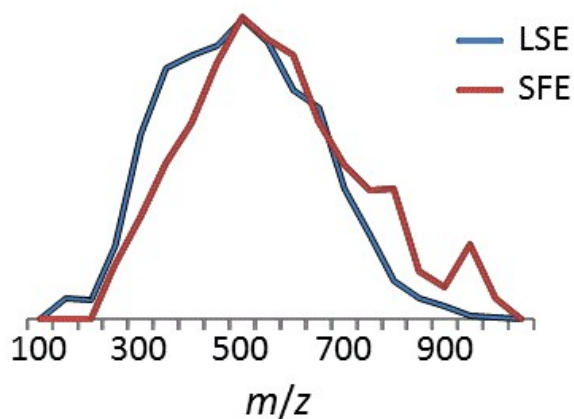


Figure S3. Comparison of the normalized m/z distribution of the molecular species identified by LSE and SFE techniques for high C peat. LSE preferentially extracts molecules with mass between $300 < m/z < 400$ whereas SFE preferentially extracts molecules with $m/z > 650$.

- (1) Tfaily, M. M.; Chu, R. K.; Tolic, N.; Roscioli, K. M.; Anderton, C. R.; Pasa-Tolic, L.; Robinson, E. W.; Hess, N. J. Advanced solvent based methods for molecular characterization of soil organic matter by high-resolution mass spectrometry. *Analytical chemistry* **2015**, *87* (10), 5206.