Supporting Information

Characterization of oil sands naphthenic acids by negative-ion electrospray ionization mass spectrometry: influence of acidic versus basic transfer solvent

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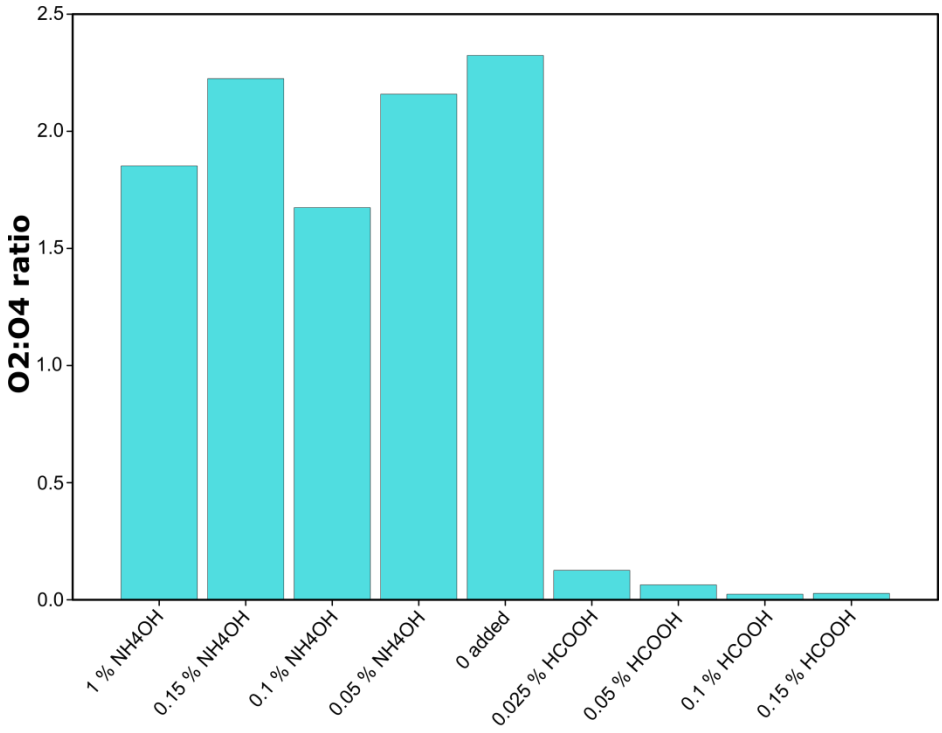


Figure S1: Bar chart showing O_2/O_4 ratio for FT-ICR MS data, as a function of base or acid added to OSPW

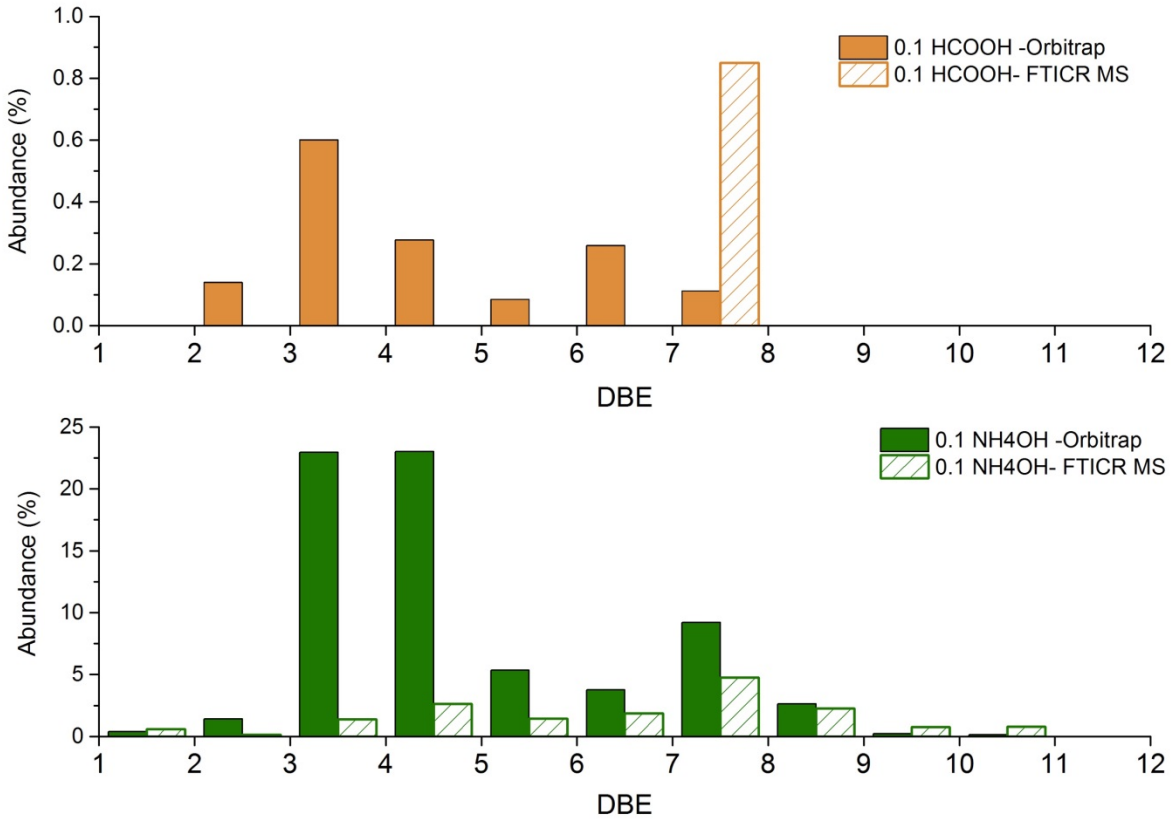
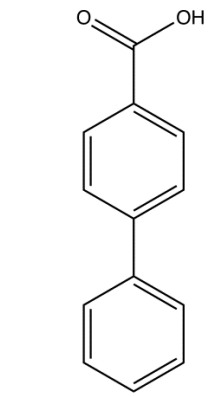


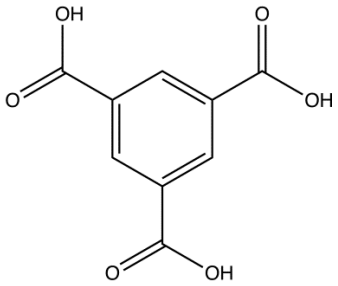
Figure S2: O_2 DBE distributions obtained from negative-ion ESI Orbitrap and FT-ICR MS data using acid pH mobile phase (top) and basic pH mobile phase (bottom) with OSPW extract

Table S1: O_2, O_4, and O_6 compounds run using FT-ICR MS to monitor signal response as a function of additives used

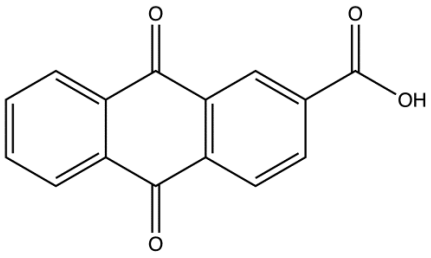
Compound	Additive	Intensity / a.u.	Apparent pH
Biphenyl-4-carboxylic acid ($C_{13}H_{10}O_2$)	0.1 % NH_4OH	5.34E+10	8.91
	0.1 % HCOOH	4.79E+08	3.52
Anthraquinone-2-carboxylic acid ($C_{15}H_8O_4$)	0.1 % NH_4OH	5.46E+10	9.19
	0.1 % HCOOH	3.31E+09	3.68
Trimesic acid ($C_9H_6O_6$)	0.1 % NH_4OH	2.81E+10	8.75
	0.1 % HCOOH	1.86E+10	3.59



Biphenyl-4-carboxylic acid



Trimesic acid



Anthraquinone-2-carboxylic acid

Figure S3: Structures of the three compounds used to study signal intensity as a function of the additives used

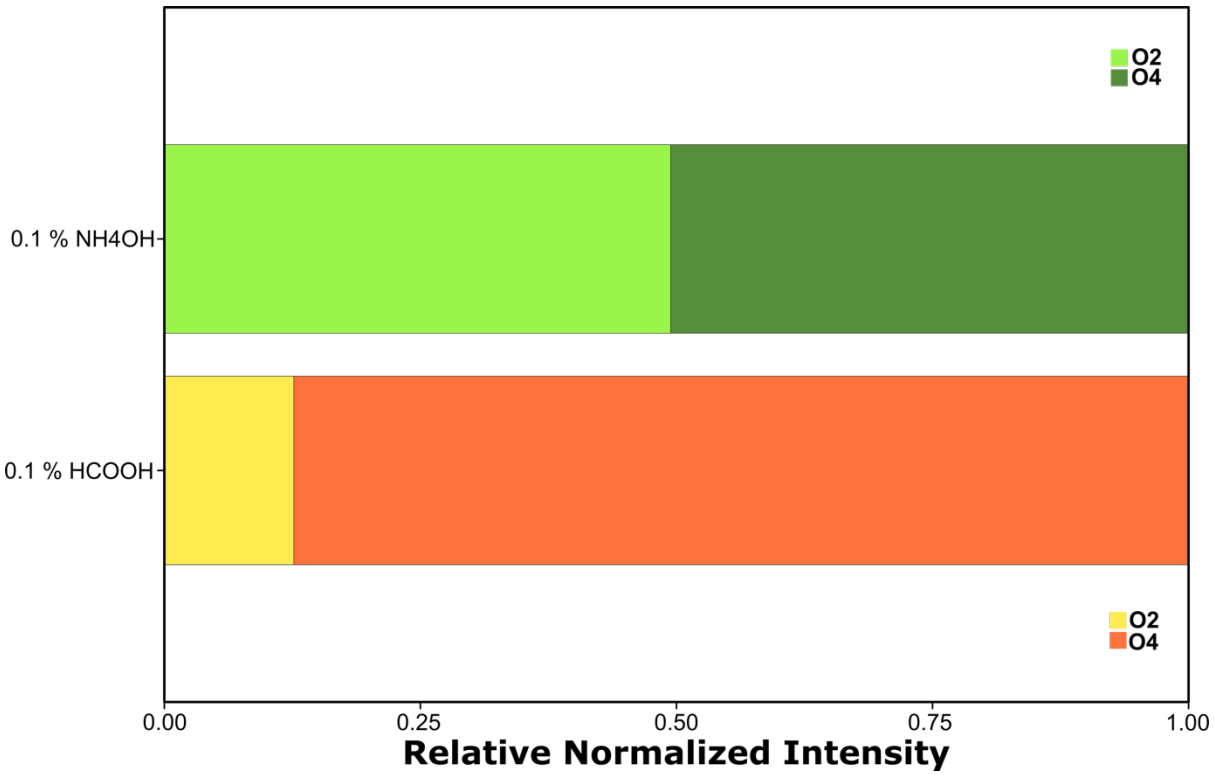


Figure S4: Normalized bar chart showing signal ratios acquired by FT-ICR MS of only the individual O_2 and O_4 compounds, for comparison with the results using the OSPW sample

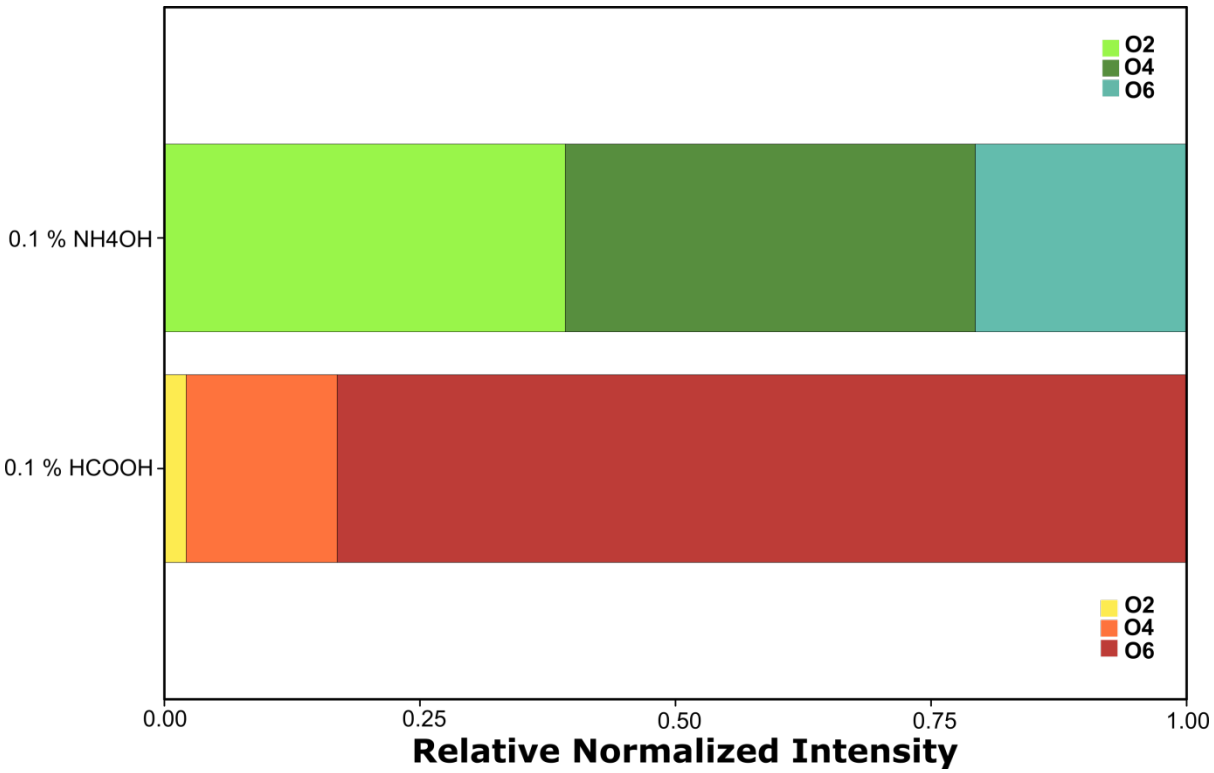


Figure S5: Normalized bar chart showing signal ratios acquired by FT-ICR MS of individual O_2, O_4, and O_6 compounds

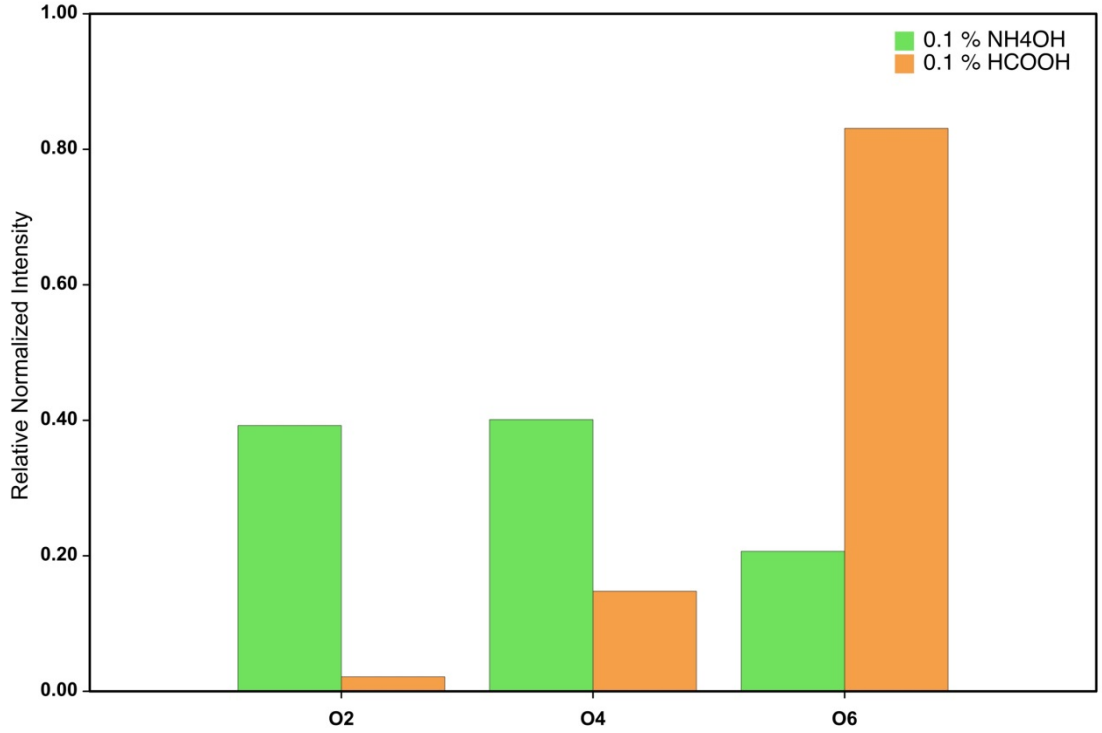


Figure S6: Relative normalized signals acquired by FT-ICR MS of the individual O_2, O_4, and O_6 compounds; alternative representation of data shown in Figure S5

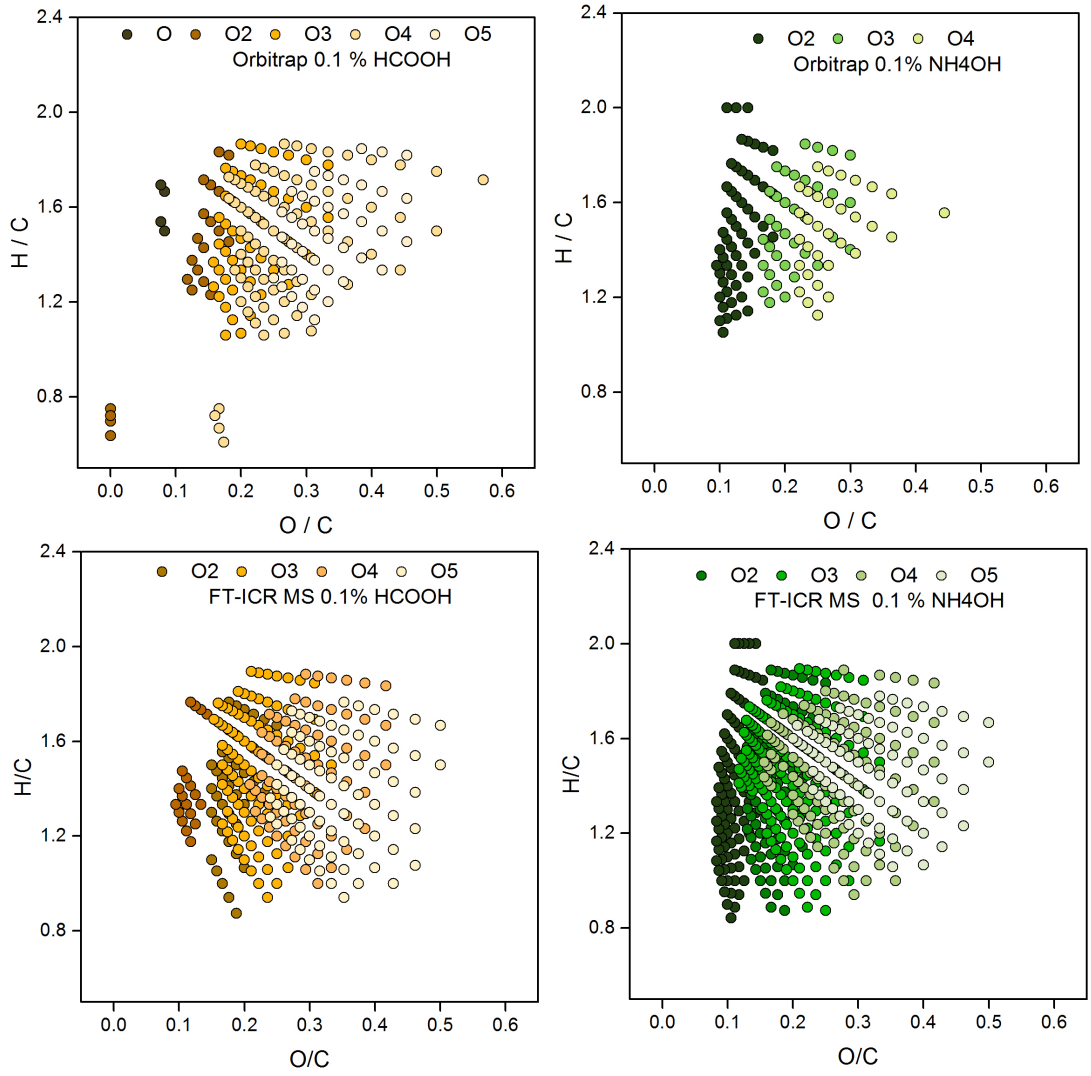


Figure S7: H/C against O/C van Krevelen plots for the 0.1% HCOOH and 0.1% NH_4OH solutions. Note that the number of relevant molecular compositions used will be higher than the number of data points within the plots; multiple molecular compositions may have the same H/C and O/C ratios, thus resulting in overlapping data points