

Investigating the trace polar species present in diesel using high resolution mass spectrometry and selective ionization techniques

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Supporting Information

Table S1. Mass spectral peaks that were used for the internal calibration of FT-ICRMS data.

ESI-positive		ESI-negative	
m/z	sum formula	m/z	sum formula
134.097	C ₉ H ₁₂ N	183.0116	C ₈ H ₇ O ₃ S
160.1126	C ₁₁ H ₁₄ N	205.1229	C ₁₃ H ₁₇ O ₂
176.1439	C ₁₂ H ₁₈ N	221.1542	C ₁₄ H ₂₁ O ₂
202.1596	C ₁₄ H ₂₀ N	261.2218	C ₁₈ H ₂₉ O
256.2065	C ₁₈ H ₂₆ N	281.2481	C ₁₈ H ₃₃ O ₂
312.2691	C ₂₂ H ₃₄ N	301.2168	C ₂₀ H ₂₉ O ₂
438.41	C ₃₁ H ₅₂ N	317.2844	C ₂₂ H ₃₇ O
471.4178	C ₃₀ H ₅₆ O ₂ Na	329.2844	C ₂₃ H ₃₇ O
		345.3157	C ₂₄ H ₄₁ O
		367.3576	C ₂₄ H ₄₇ O ₂

Table S2. Ion transmission settings for FT-ICRMS data acquisition (n.a. – not available, n.p. not present in the instrument).

Assembly	Part	ESI (solarix)		APCI (apeX)
		(+)	(-)	(+)
Source Optics	Funnel RF Amplitude	40 Vpp	40 Vpp	150 Vpp
Octopole/Hexapole	Frequency	5 MHz	5 MHz	5 MHz
	RF Amplitude	300 Vpp	300 Vpp	400 Vpp
Collision cell	Frequency	2 MHz	2 MHz	n.a.
	RF Amplitude	1000 Vpp	1000 Vpp	800 Vpp
Transfer optics	Time of flight	0.6 ms	0.6 ms	0.7 ms
	Frequency	6 MHz	6 MHz	n.p.
	RF Amplitude	400 Vpp	400 Vpp	n.p.

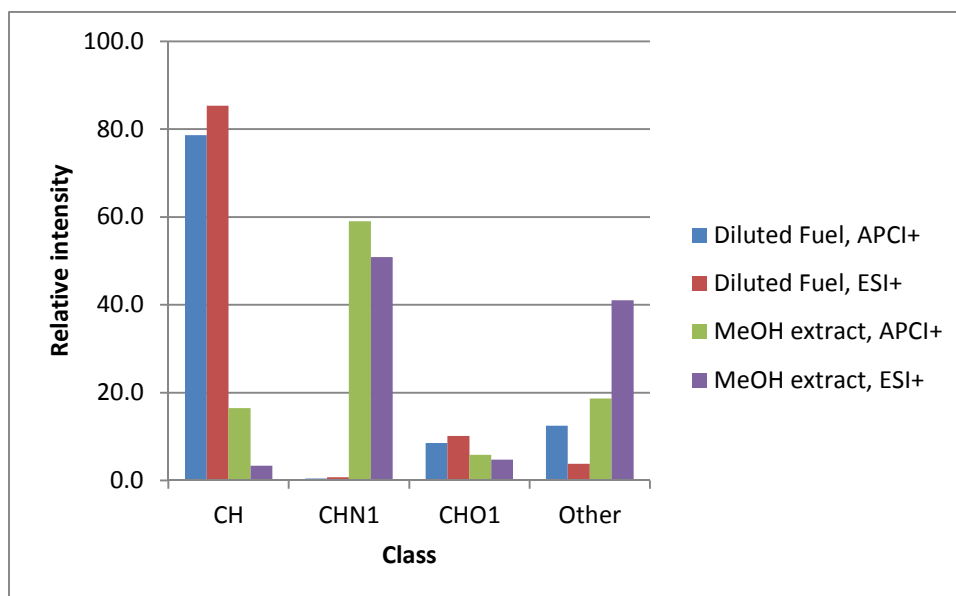


Figure S1. Relative intensities of ion classes observed for diluted fuels and methanol extracts when analyzed with ESCI-TOFMS. Similar parameters as discussed in the Experimental section (ESI-TOFMS) were used. The results show that many species forming part of the CH-class were not extracted efficiently with methanol. For the methanol extract, the CH-class was more prominent in the APCI spectrum, therefore showing the selectivity of the different ionization techniques.