Direct sulfur-containing compounds speciation in crude oils and high-boiling fractions by APCI (+) FT-ICR Mass Spectrometry

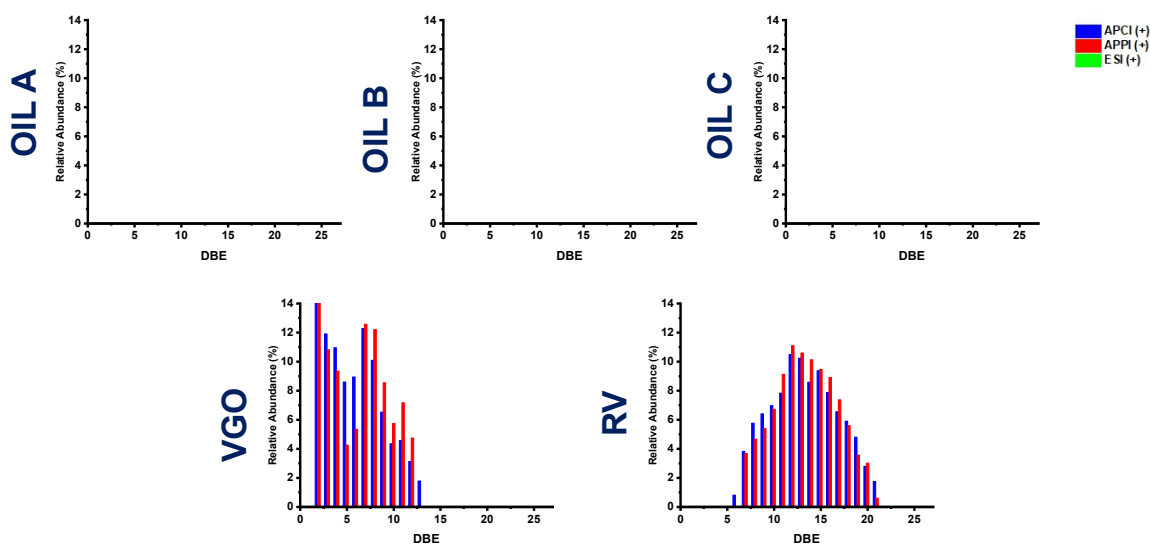Danielle Mitze Muller Franco[a], Taynara Rodrigues Covas[a], Rosana Cardoso Lopes Pereira[a], Lidya Cardozo da Silva[a], Mario Duncan Rangel[a], Rosineide Costa Simas[b], Gabriel Henry Morais Dufrayer[a], Boniek Gontijo Vaz[a]*

Table S1: Individual results obtained on one day five times for Oil D in APCI (+) for REPE data.

	S[H] (%)	S• (%)
OIL D (R1)	3.35	1.06
OIL D (R2)	3.96	1.00
OIL D (R3)	3.73	0.91
OIL D (R4)	3.54	0.94
OIL D (R5)	3.37	0.99
Mean	3.59	0.98
DP	0.23	0.05
CV(%)	6.41	5.28

Table S2: Individual Results obtained on twelve different days for Oil D in APCI (+) for REPRO data.

	S[H] (%)	S• (%)
OIL D (Day 1)	3.73	0.79
OIL D (Day 2)	3.72	0.74
OIL D (Day 3)	3.49	0.76
OIL D (Day 4)	3.79	0.83
OIL D (Day 5)	3.58	0.78
OIL D (Day 6)	3.39	0.69
OIL D (Day 7)	3.10	0.72
OIL D (Day 8)	3.43	0.74
OIL D (Day 9)	3.62	0.50
OIL D (Day 10)	3.49	0.73
OIL D (Day 11)	3.14	0.79
OIL D (Day 12)	3.37	0.99
Mean	3.49	0.76
DP	0.21	0.11
CV(%)	6.01	14.07

Figure S1: Distribution of DBE (double bonds equivalents = ring plus double bonds to carbon) distribution for members of S2 class all in positive mode ESI, APP.I and, APC.I 7-T Fourier transform ion cyclotron resonance of samples.