

Supporting Information

Exploration of the reactivity of heteroatomic compounds contained in vacuum gas oils during hydrotreatment using FT-ICR MS

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Table S1: Additional informations about the considered samples. NA: Not available

Sample	Type	Total aromatics (% w/w) by UV <i>Ref. method:</i> <i>ASTM D2269</i>	Oxygen content (% w/w) by IR <i>Ref. method:</i> <i>MLE-MO-LAB-048</i>
VGO 1	SRVGO – Safaniya	47	0.18
VGO 2	SRVGO – Arabian Light & Irak	51	NA
VGO 3	80% SRVGO 1 + 20% GO Safaniya	47	0.19
HDT 1a	HDT from VGO 1 <i>Middle temperature</i>	48	0.18
HDT 1b	HDT from VGO 1 <i>High temperature</i>	46	< 0.1
HDT 2	HDT from VGO 2 <i>Middle temperature</i>	44	< 0.1
HDT 3	HDT from VGO 3 <i>Middle temperature</i>	45	0.25

Figure S1: DBE=f(#C) plots of N1[H] compounds in ESI(-) mode

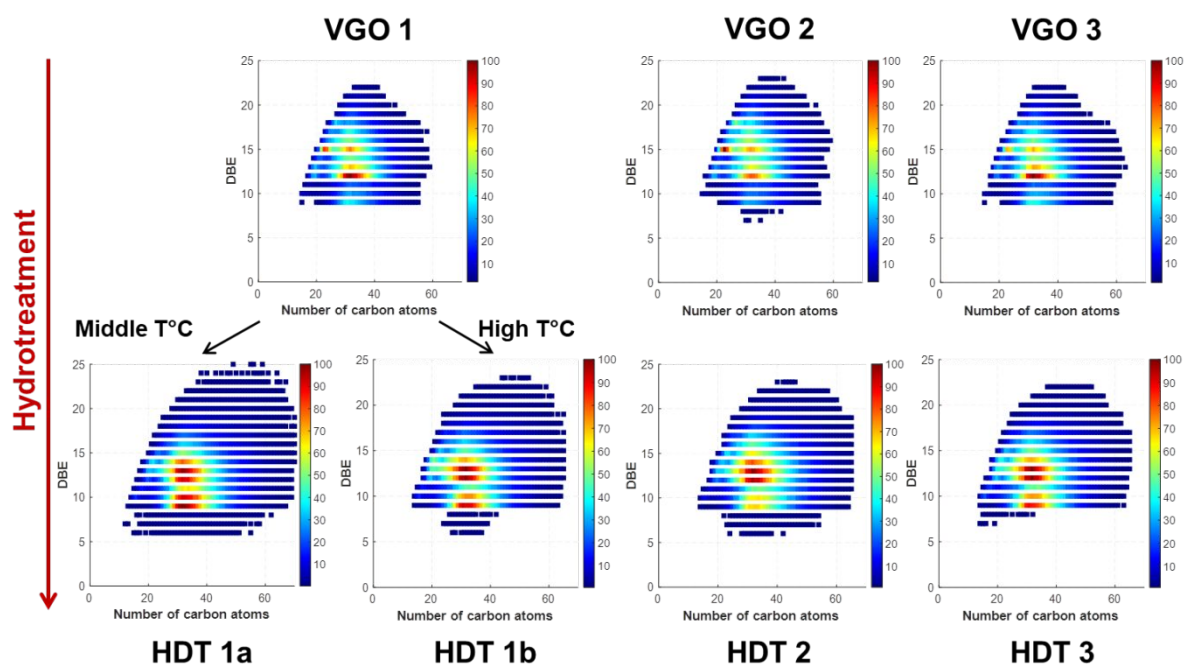


Figure S2: DBE=f(#C) plots of N1[H] compounds in ESI(+) mode

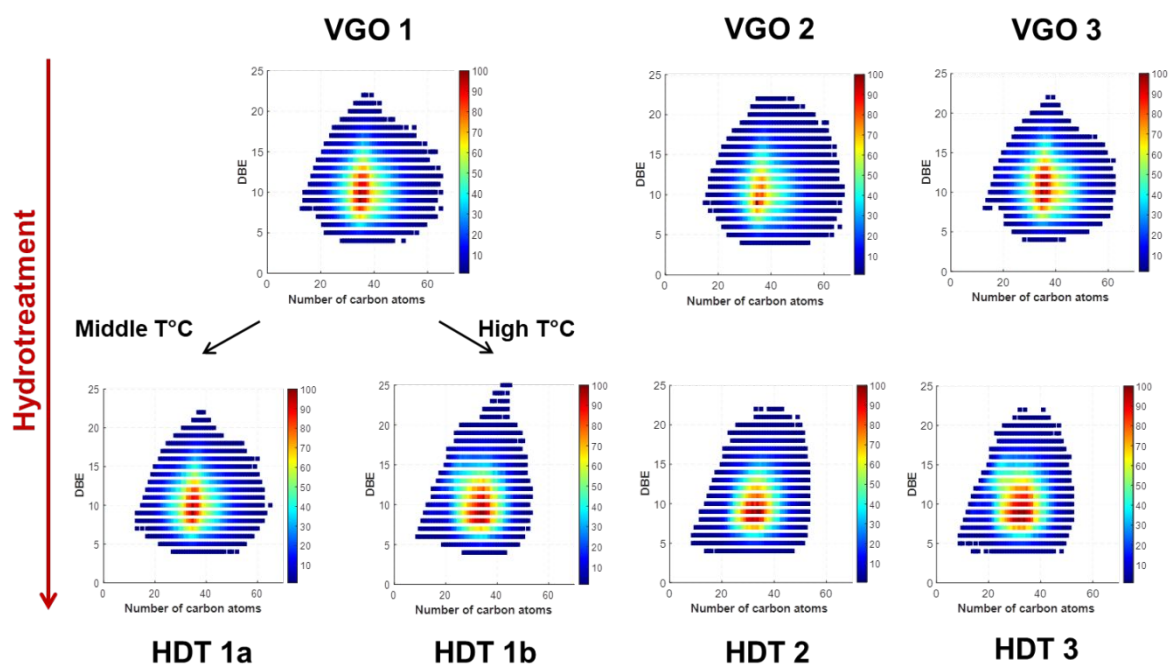


Figure S3: Evolution of the relative intensities of the DBE (A) and the number of carbon atoms (B) of the N1O1[H] compounds for the different feeds in ESI(-) mode.

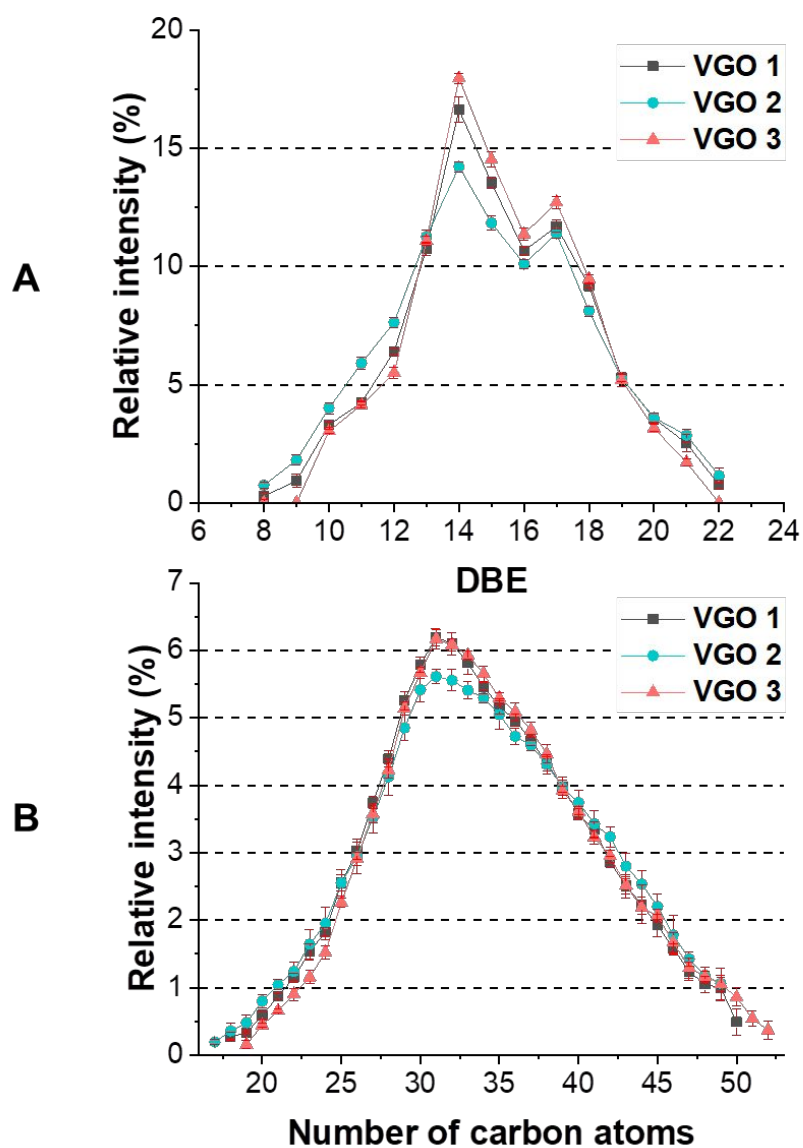


Figure S4: DBE=f(#C) plots of O1N2[H] and N1O2[H] compounds in the feeds

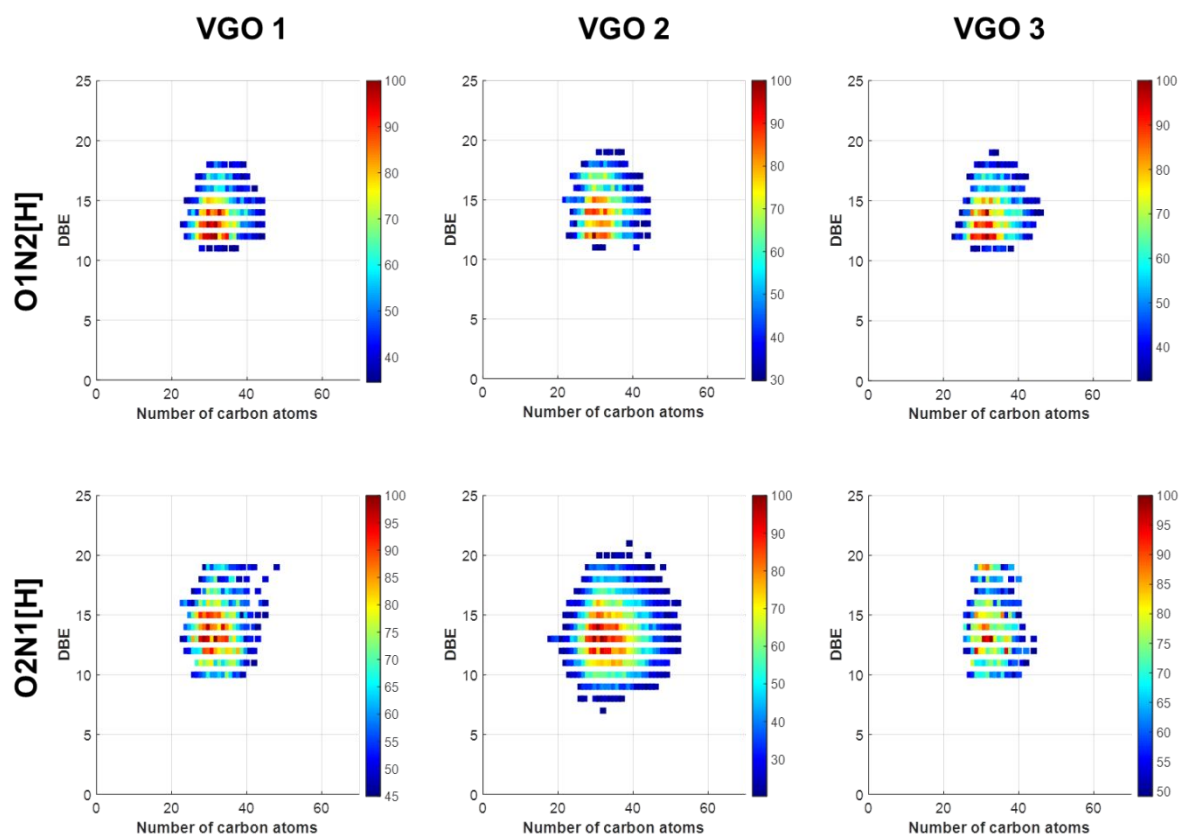


Figure S5: DBE=f(#C) plots of O1N1[H] compounds in ESI(+) mode

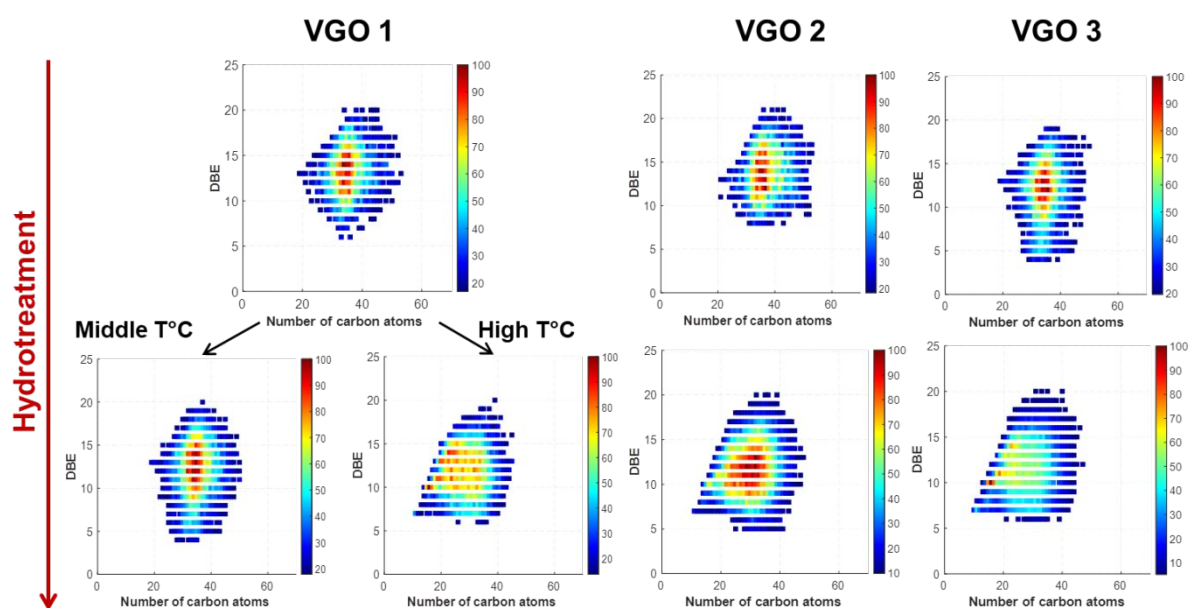


Figure S6: Evolution of the relative intensities of the DBE (A) and the number of carbon atoms (B) of the O1S1[Na] compounds for the different feedstocks and O1S1[H] for the hydrotreated samples in ESI(+) mode.

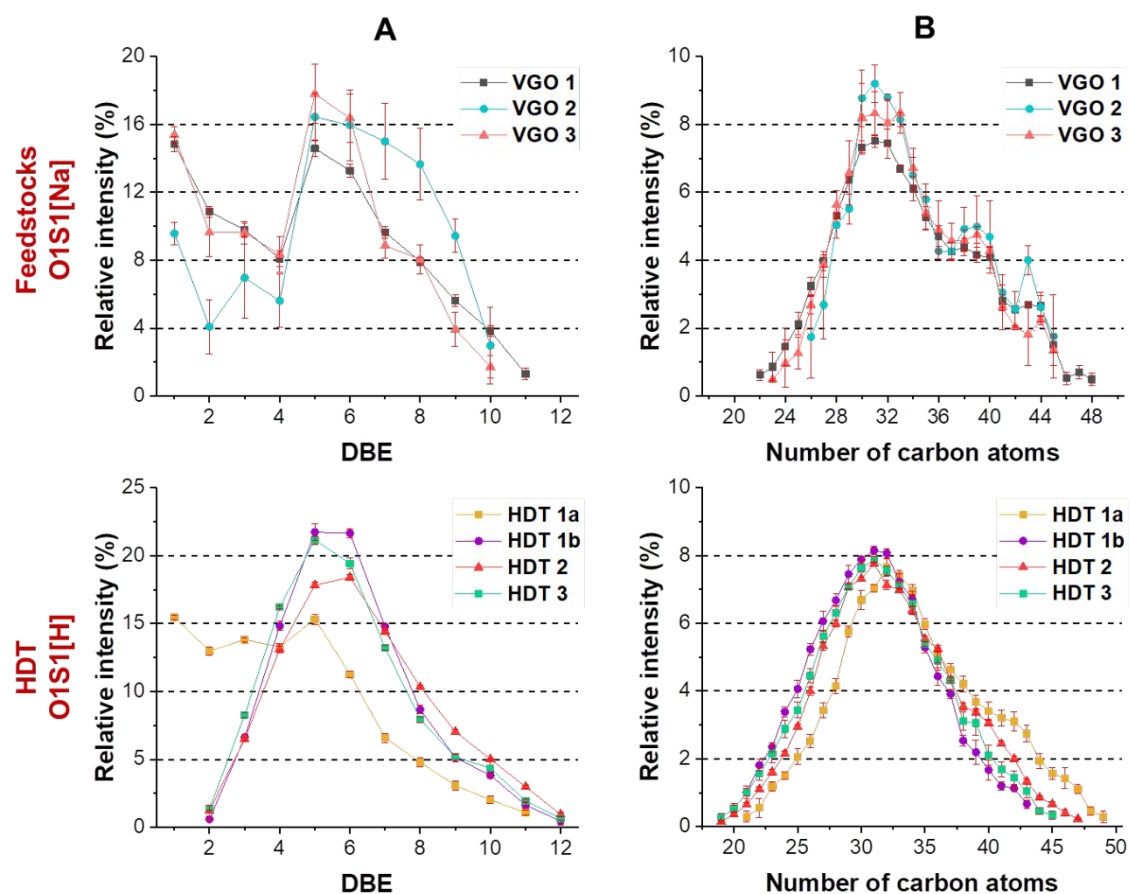


Figure S7: Evolution of the relative intensities of the DBE (A) and the number of carbon atoms (B) of the N1S1[H] compounds for the different feeds in ESI(+) mode.

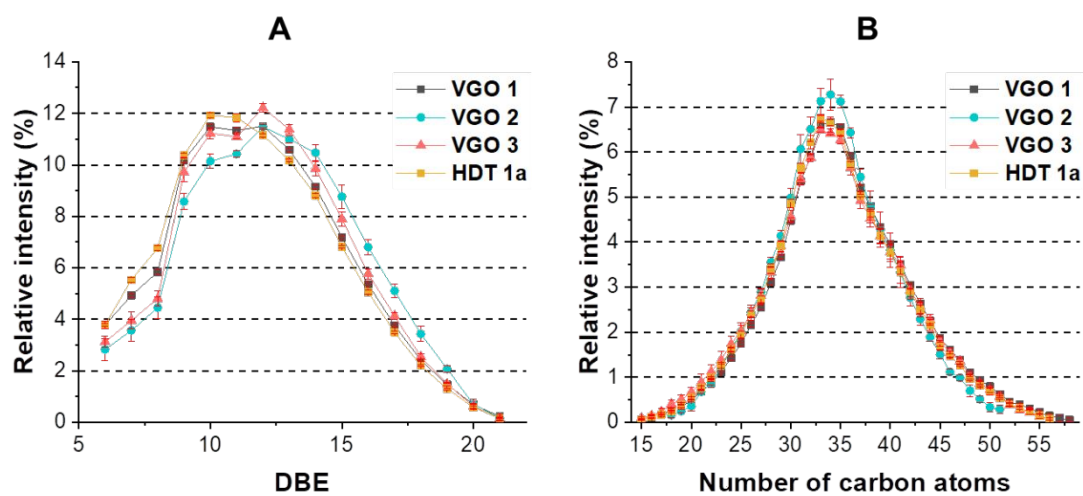


Figure S8: Evolution of the relative intensities of the DBE (A) and the number of carbon atoms (B) of the O1[H] compounds for the different feeds and hydrotreated samples in ESI(-) mode.

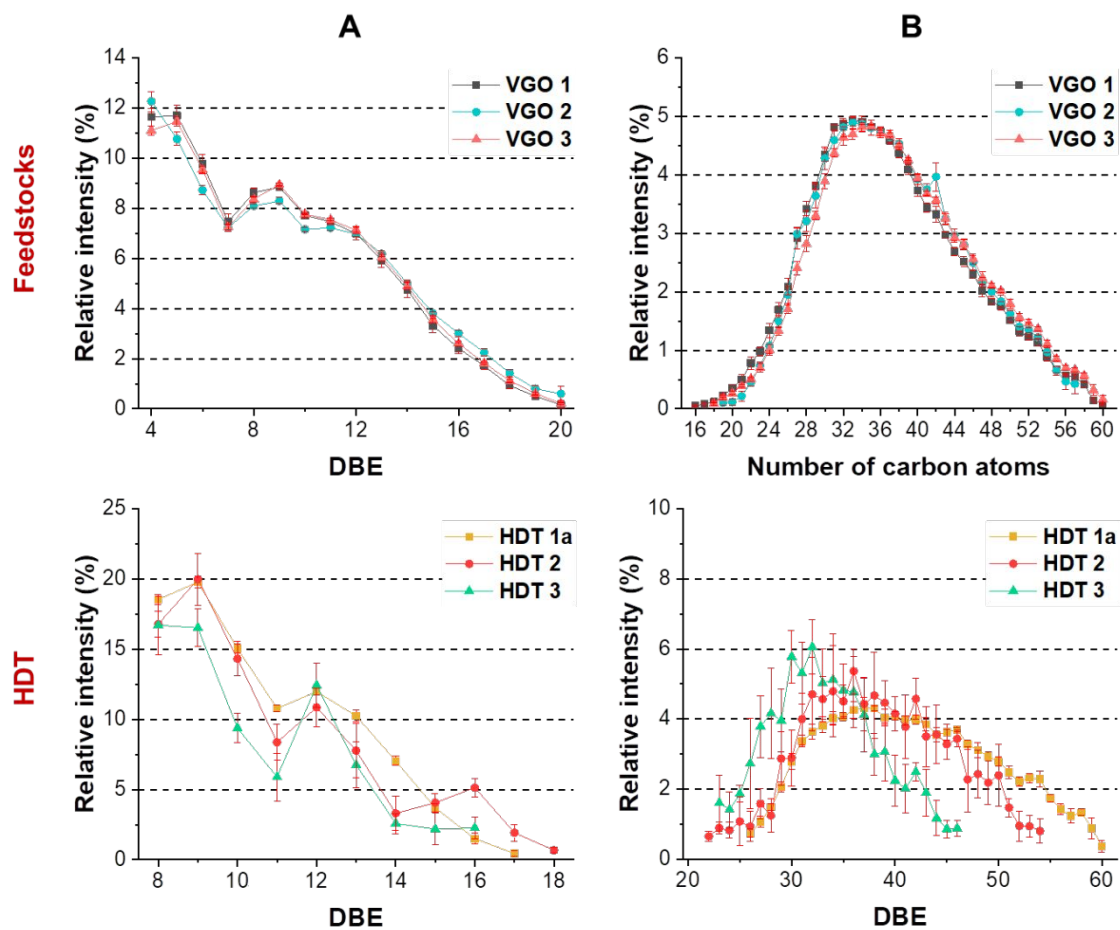


Figure S9: Evolution of the relative intensities of the DBE (A) and the number of carbon atoms (B) of the O2[H] compounds for the different feeds in ESI(-) mode.

