

## Supporting information for

# Molecular level insights into gas oil hydrodenitrogenation by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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**Supporting information 1 : HT-GCxGC coupled by Simulated Distillation analyses of the gas oil feed and the 80% HDN conversion effluent**

In order to evaluate the conversion by cracking reactions and hydrocarbon composition after hydrotreatment, the gas oil feed and the hydrotreated effluent at 79.5% HDN conversion were analyzed by high-temperature comprehensive two dimensional chromatography (HT-GCxGC) coupled with simulated distillation. The configuration of GCxGC was described as following:

Parameters	Microfluidic modulator
<b>Instrument</b>	Agilent 7890A
<b>Injector</b>	MMA split mode 400°C split ration 25 2µL
<b>First column</b>	DB1 HT 15m 0.1mm 0.1µm
<b>Second column</b>	ZB35 HT 5m 0.25mm 0.18µm
<b>Carrier gas</b>	Hydrogène 0.14mL/min et 24mL/min
<b>Oven temperature</b>	100°C 2min 400°C at 2.2°C/min
<b>Modulation time</b>	8.965s
<b>Detector</b>	FID 100Hz

The chromatograms of the 80% HDN conversion effluent is given below:

**Figure S1: HT-GCxGC-FID chromatogram of the 79.5% HDN conversion liquid effluent**

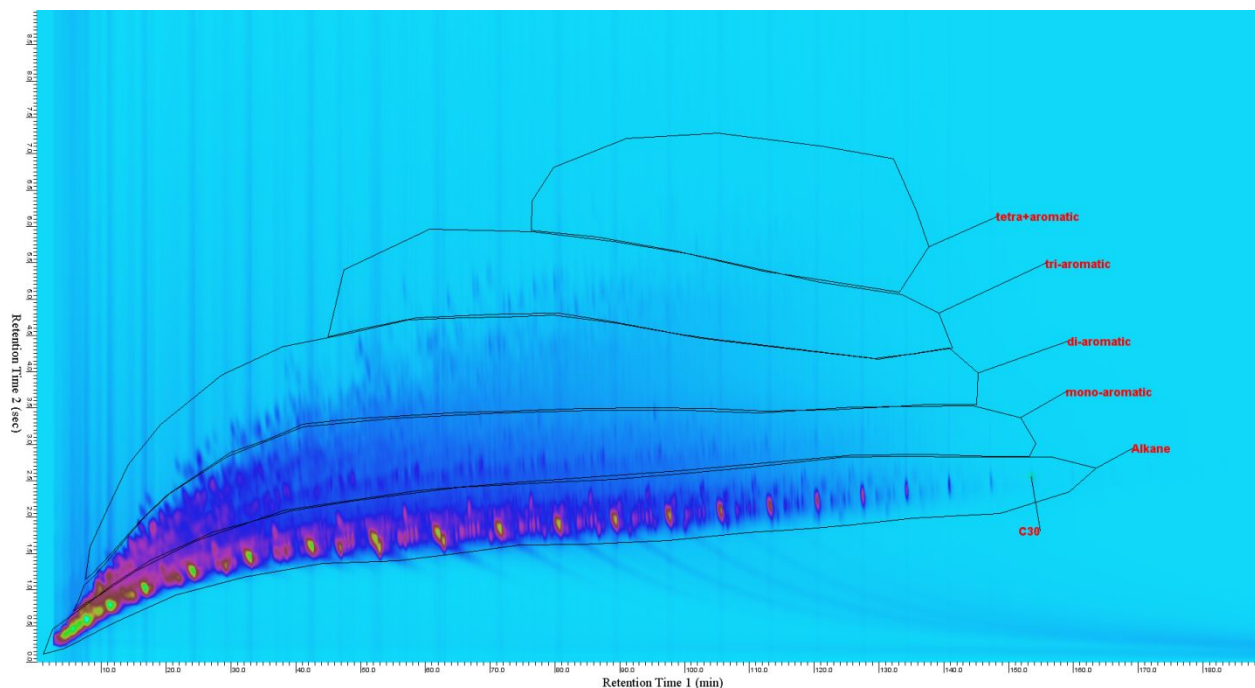
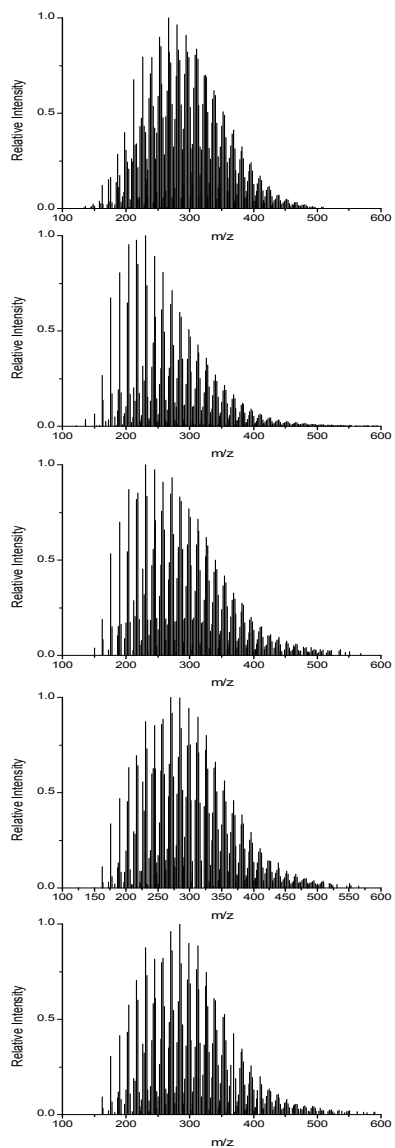
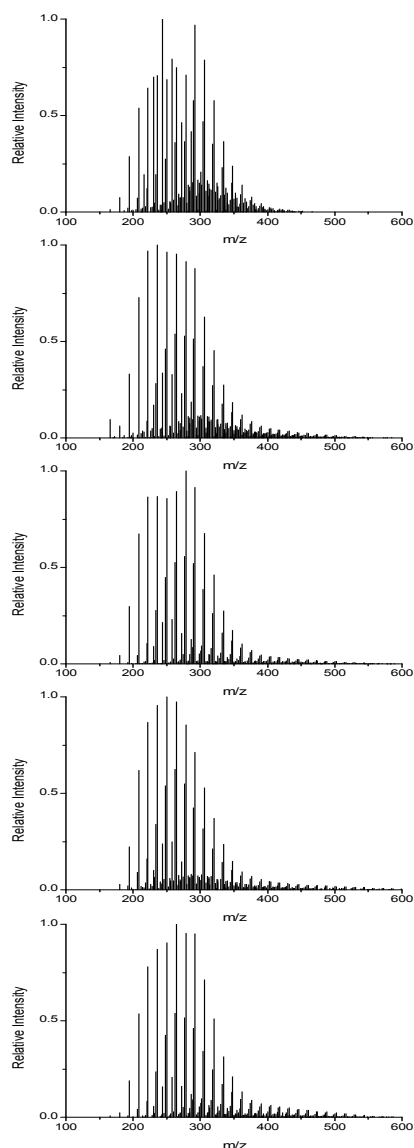


Figure S2 : FT-ICR/MS raw spectra of the gas oil feed and of the hydrotreated effluents: (a): ESI(+)-FT-ICR/MS spectra, (b): ESI(-)-FT-ICR/MS spectra. From top to bottom: spectra of the gas oil feed, 71%, 74%, 80% and 89% HDN conversion effluents.

(a)



(b)



**Figure S3 : Distribution of N1 and polyheteroatom families of nitrogen compounds in the feed and in the hydrotreated liquid effluents: (a) ESI(+) FT-ICR/MS; (b) ESI(-) FT-ICR/MS**

