Structural analysis of heavy oil fractions after hydrodenitrogenation by high-resolution tandem mass spectrometry and ion mobility spectrometry.

Johann Le Maître[1,2,3], Marie Hubert-Roux[1,3], Benoit Paupy[2,3], Sabrina Marceau[2,3], Christopher Rüger[1], Carlos Afonso[1,3], Pierre Giusti[2,3]

[1], Normandie Université, COBRA, UMR 6014 et FR 3038; Université de Rouen;

INSA de Rouen; CNRS, IRCOF, Mont Saint Aignan Cedex, France

[2]TOTAL Refining & Chemicals, Total Research & Technology Gonfreville, BP 27, 76700 Harfleur, France.

[3]CNRS Joint Laboratory C2MC, Complex Matrices Molecular Characterization - CNRS (France) BP 27, 76700 Harfleur, France

Supporting Information

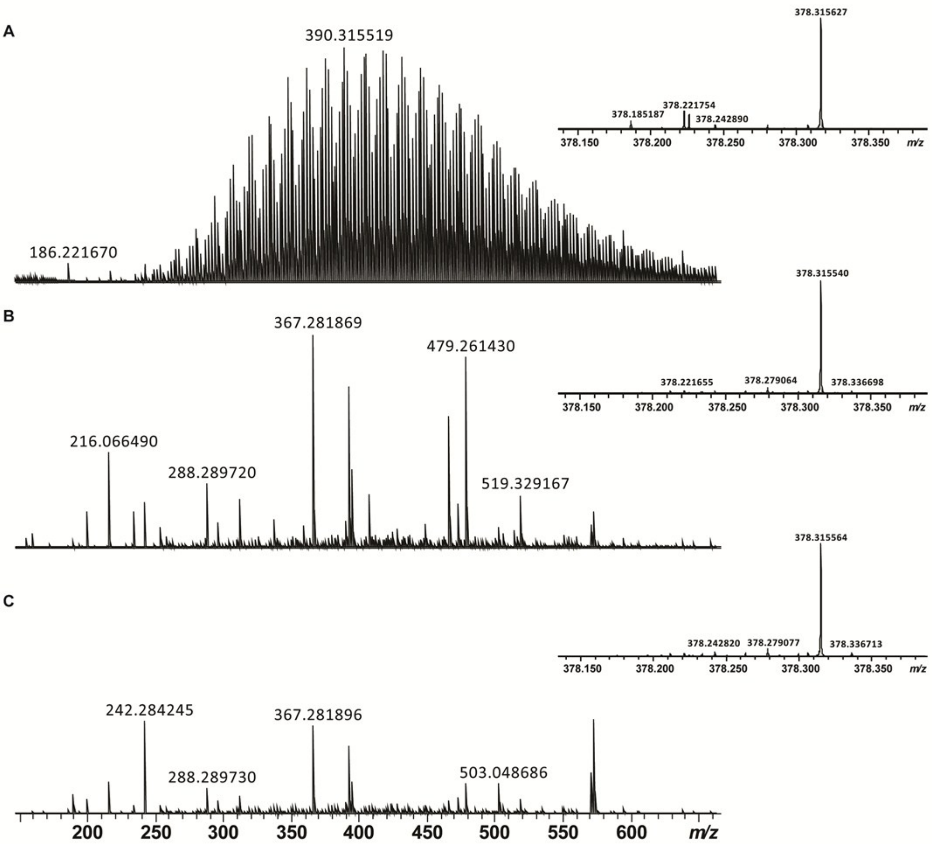


Figure S1. ESI(+) mass spectra of the feed VGO (A), Effluent 70 ppm (B) and Effluent 10 ppm (C) recorded by FTICRMS.

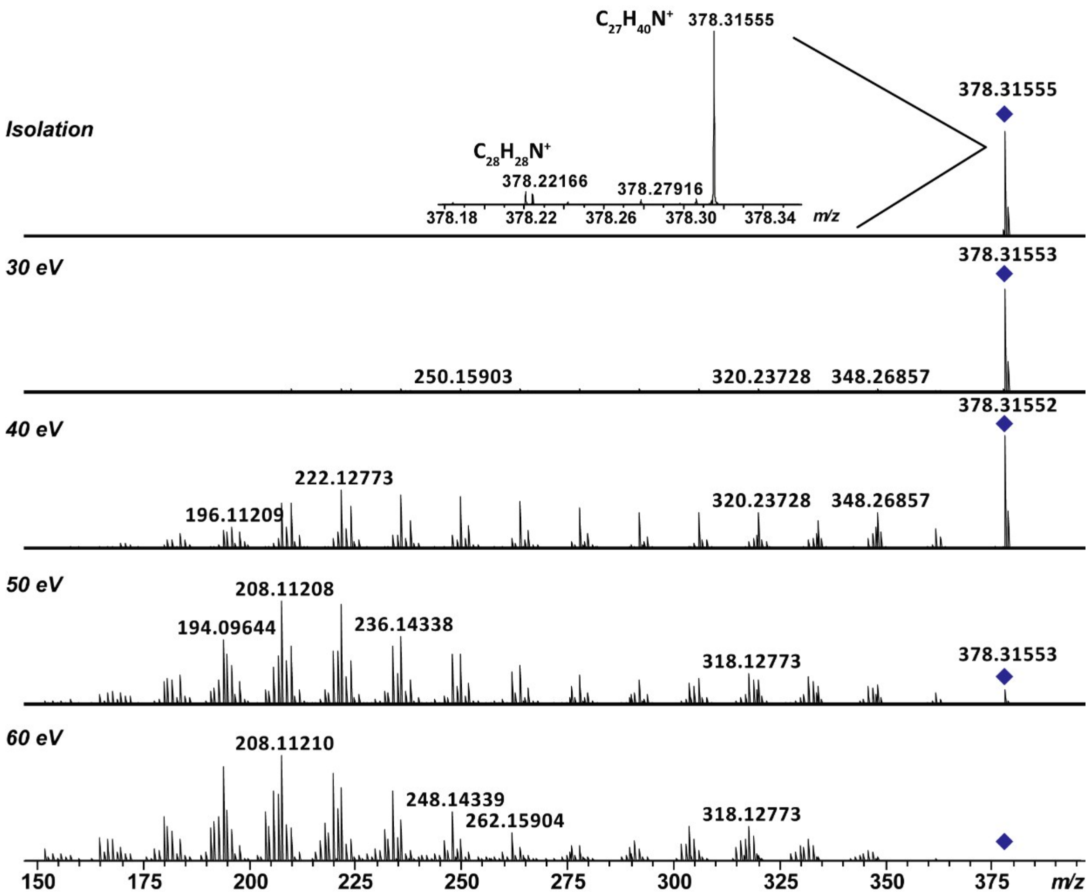
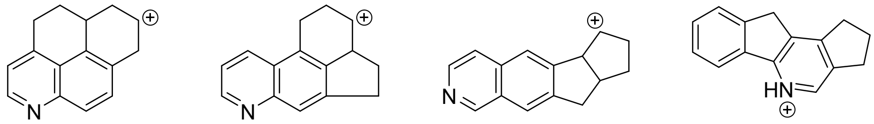
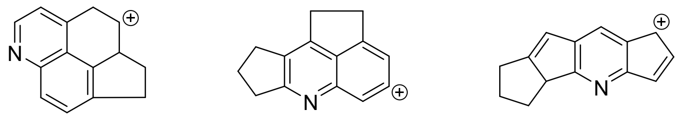


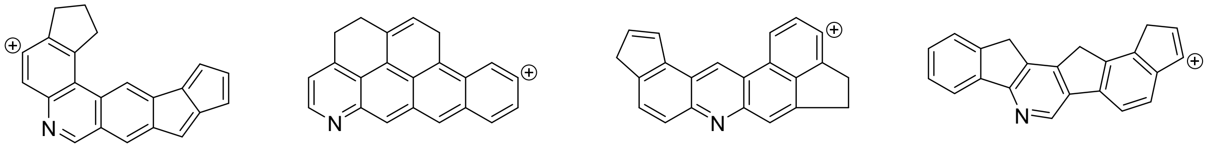
Figure S2. ESI/MS/MS spectra of the precursor ion at *m/z* 378.31553 ($C_{27}H_{40}N^+$, DBE 9) and *m/z* 378.22166 ($C_{28}H_{28}N^+$, DBE 16) at collision energies 30 eV, 40 eV, 50 eV and 60 eV.



Chemical Formula: $C_{15}H_{14}N^+$
Exact Mass: 208.11208
DBE 10



Chemical Formula: $C_{14}H_{12}N^+$
Exact Mass: 194.09643
DBE 10



Chemical Formula: $C_{22}H_{14}N^+$
Exact Mass: 292.11208
DBE 17

Figure S3. Hypothetical structures of the molecular nuclei of the most abundant fragment ions.

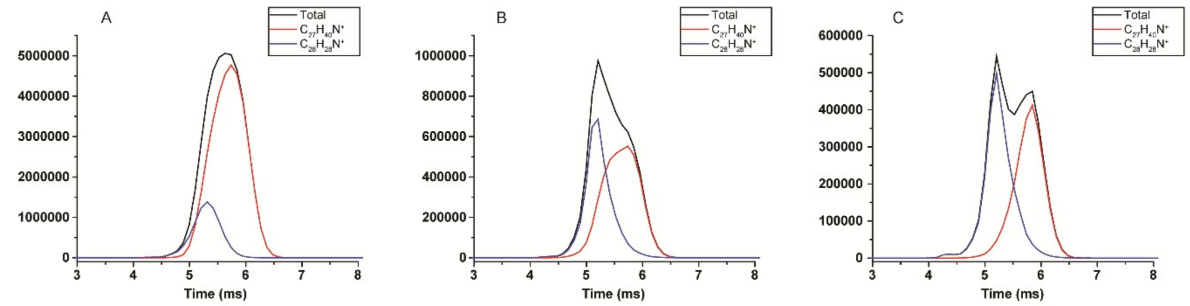


Figure S4. Superposition of the ion mobility spectra of the isobars of *m/z* 378 for (A) VGO, (B) effluent mild HDN (70 ppm) and (C) effluent deep HDN (10 ppm) process (*m/z* 378.31553 ($C_{27}H_{40}N^+$, DBE 9) in blue and *m/z* 378.22166 ($C_{28}H_{28}N^+$, DBE 16) in red)

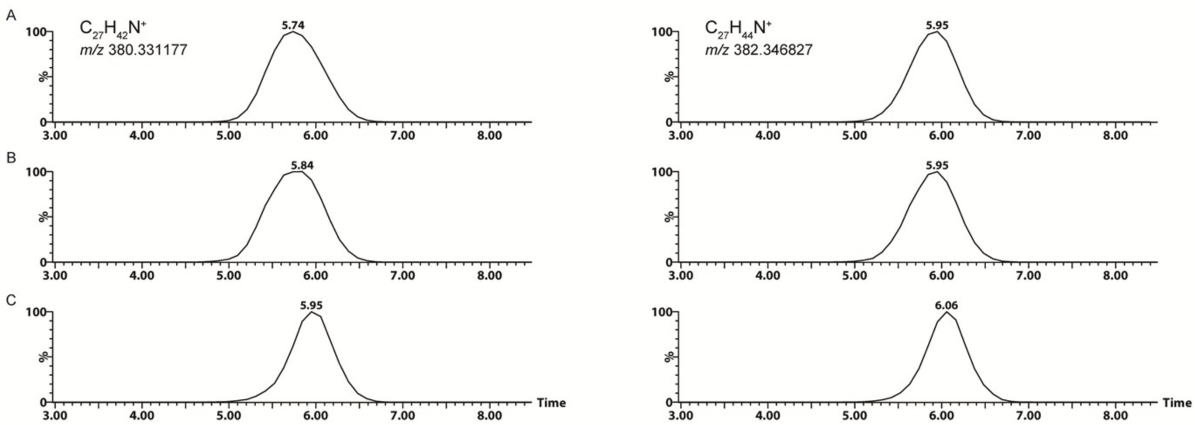


Figure S5. Ion mobility spectra of the *m/z* 380.331177 ($C_{27}H_{42}N^+$, DBE 8) and *m/z* 382.346827 ($C_{27}H_{44}N^+$, DBE 7) selected in the quadrupole for VGO (A), Effluent 70 ppm (B) and Effluent 10 ppm (C) process.

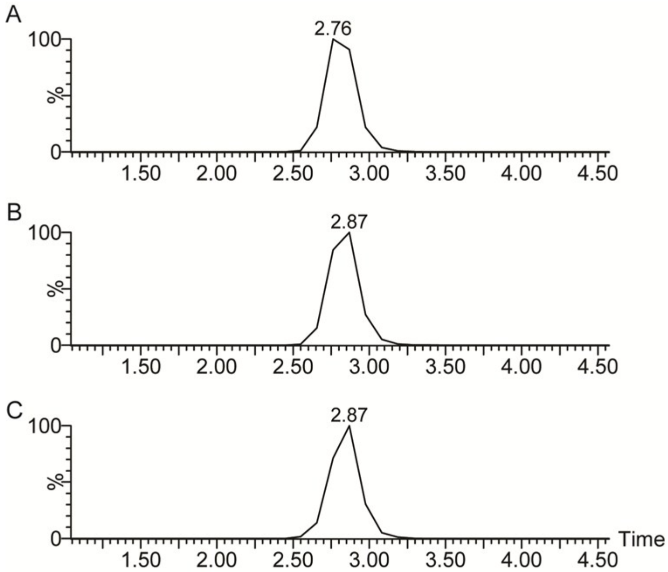


Figure S6. Ion mobility spectra of $C_{15}H_{14}N^{+}$ *m/z* 208.11208 (DBE 10) fragment ion from refractory precursor ions fragmented in the 70eV *Trap* for (A) VGO, (B) effluent mild HDN (70 ppm) and (C) effluent deep HDN (10 ppm) process.