

## Supporting Information

### Insights from nitrogen compounds in gas oils highlighted by high-resolution Fourier transform mass spectrometry

Julie Guillemant<sup>†</sup>, Florian Albrieux<sup>†</sup>, Luis P. de Oliveira<sup>\*†</sup>, Marion Lacoue-Nègre<sup>†</sup>, Ludovic Duponchel<sup>‡</sup> and Jean-François Joly<sup>†</sup>

<sup>†</sup> IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France

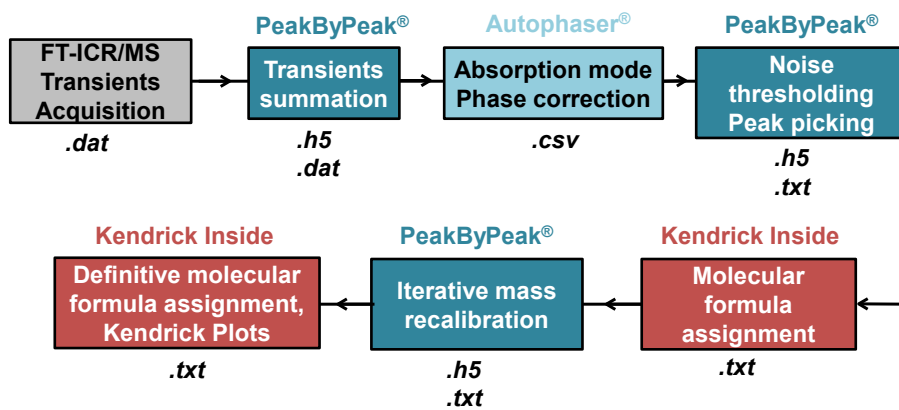
<sup>‡</sup> Univ. Lille, CNRS, UMR 8516 - LASIR – Laboratoire de Spectrochimie Infrarouge et Raman, , F-59000 Lille, France

\* Correspondence should be addressed to Dr. Luis Pereira de Oliveira:  
luis.pereira-oliveira@ifpen.fr

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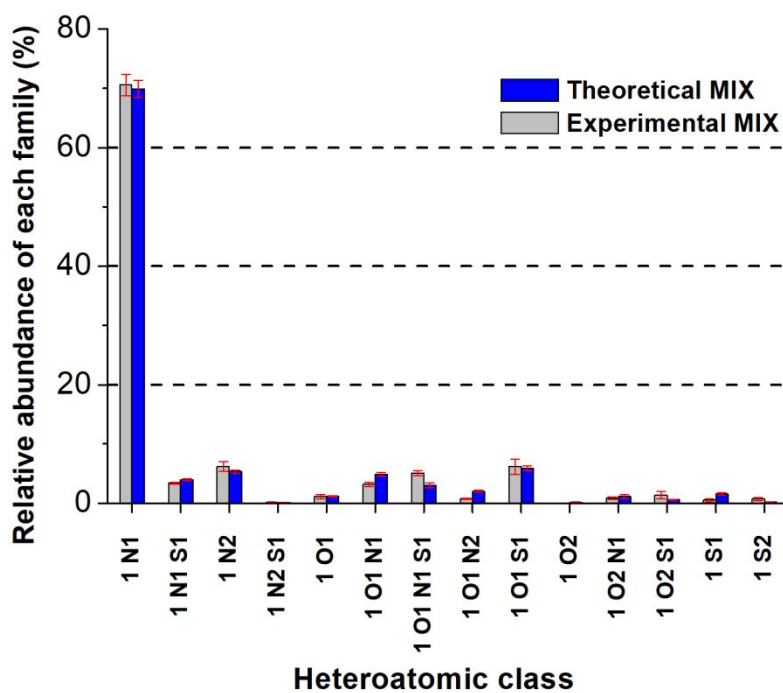
Figure S1: Data processing workflow used



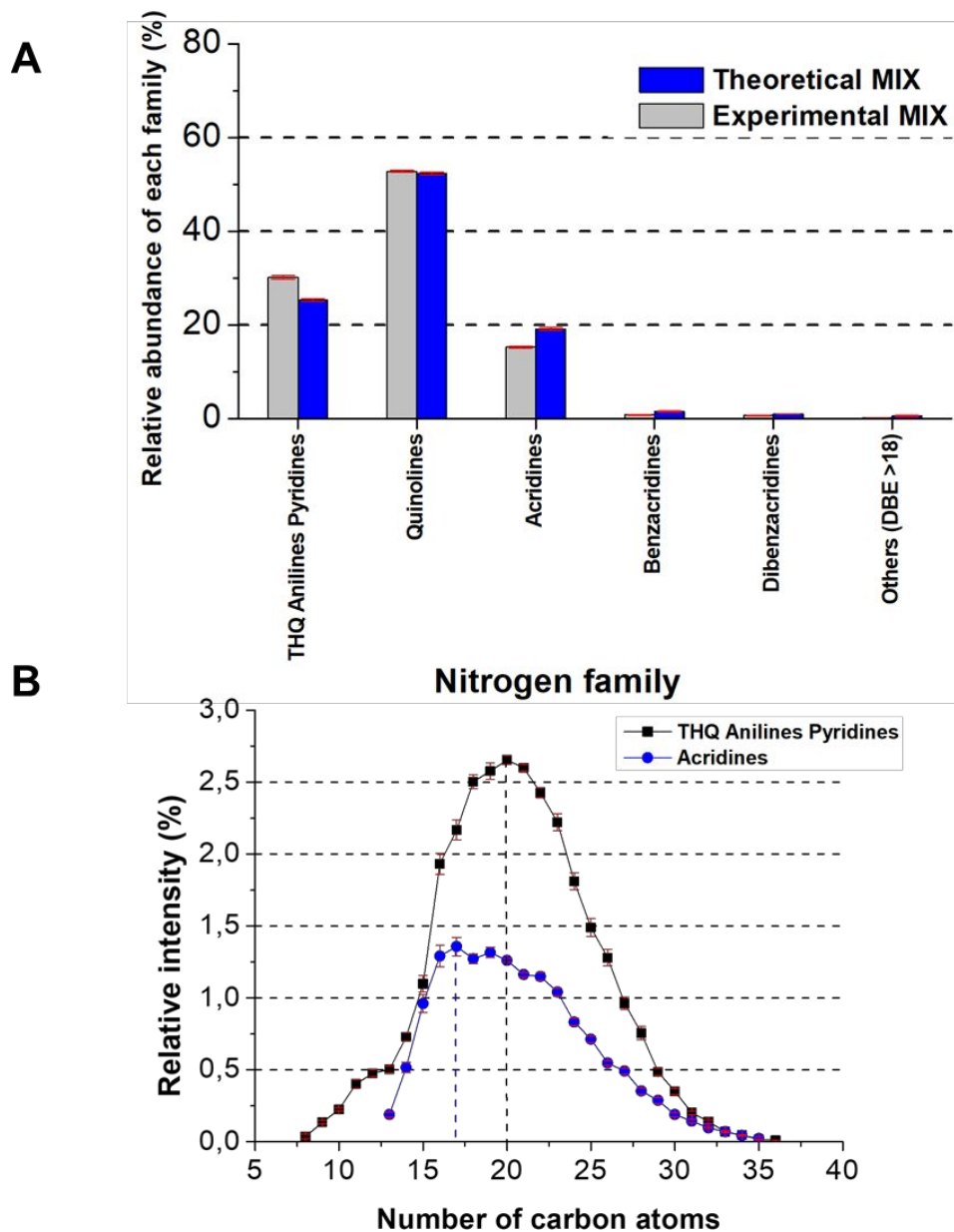
**Table S1: RSD values obtained for every sample in both ESI modes. Minimal and maximal RSD values for each mode are indicated with (\*) and (\*\*) respectively.**

<b>Sample</b>	<b>Gas oil Type</b>	<b>RSD (%) for ESI(+) Data</b>	<b>RSD (%) for ESI(-) Data</b>
GO 1	SR	2.16	1.37
GO 2	SR	0.98	2.50
GO 3	SR	0.66	1.03
GO 4	SR	0.38 (*)	1.60
GO 5	SR	1.14	1.83
GO 6	LCO	3.48	4.26
GO 7	LCO	2.79	4.29
GO 8	LCO	5.09	1.59
GO 9	GOCK	2.89	0.71
GO 10	GOCK	5.37	2.49
GO 11	GOCK	1.76	0.69 (*)
GO 12	GOCK	2.72	0.84
GO 13	H-OIL	4.96	6.51 (**)
GO 14	HYVAHL	2.69	1.05
GO 15	MIX	0.86	2.38
GO 16	MIX	0.63	0.61
GO 17	HDT	0.92	1.29
GO 18	HDT	0.97	3.47
GO 19	MIX	1.42	1.99
GO 20	HDT	2.95	5.16
GO 21	HDT	5.98 (**)	4.48
GO 22	HDT	1.13	3.69
GO 23	MIX	1.46	4.15
	<b>Mean</b>	<b>2.32</b>	<b>2.52</b>

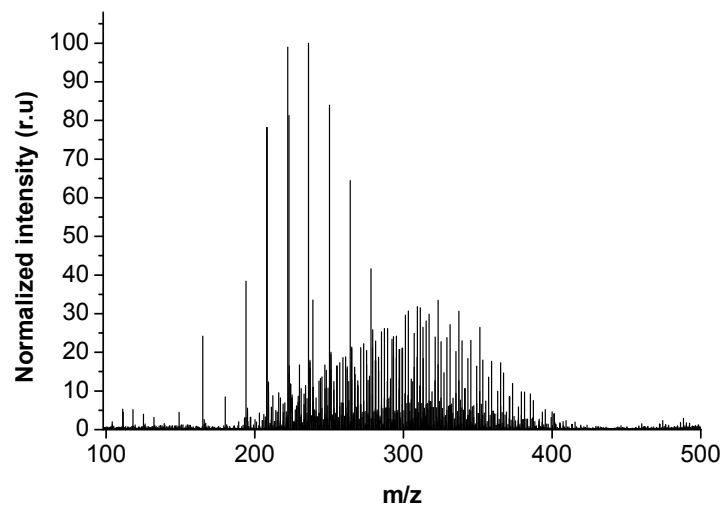
**Figure S2: Comparison of experimental and theoretical MIX heteroatomic classes relative abundances for ESI(+). The standard deviation error bars colored in red have been added on the figure.**



**Figure S3: (A) Comparison of theoretical and experimental MIX compositions for basic nitrogen families. (B) Comparison of the distribution of relative intensity according to the number of carbon atoms of the molecules for the THQ Anilines Pyridines and Acridines for MIX sample. The standard deviation error bars colored in red have been added on both figures.**



**Figure S4: ESI(-)-FT-ICR MS spectra from SRGO Sample 3**



**Figure S5: DBE vs carbon numbers plot of 1N1 family in SR Sample 3 obtained with ESI(-)-FT-ICR MS and corresponding core structures**

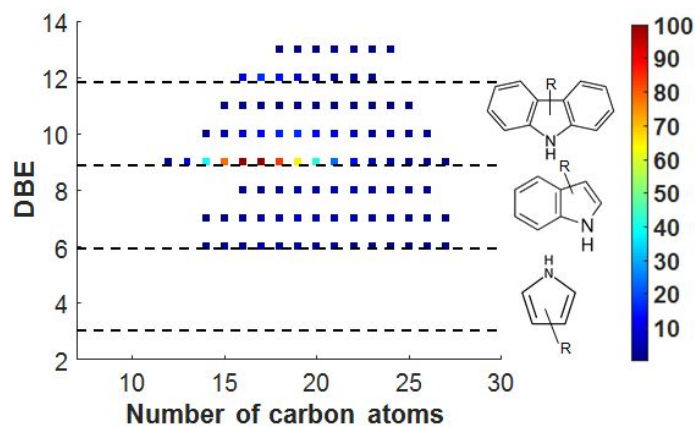
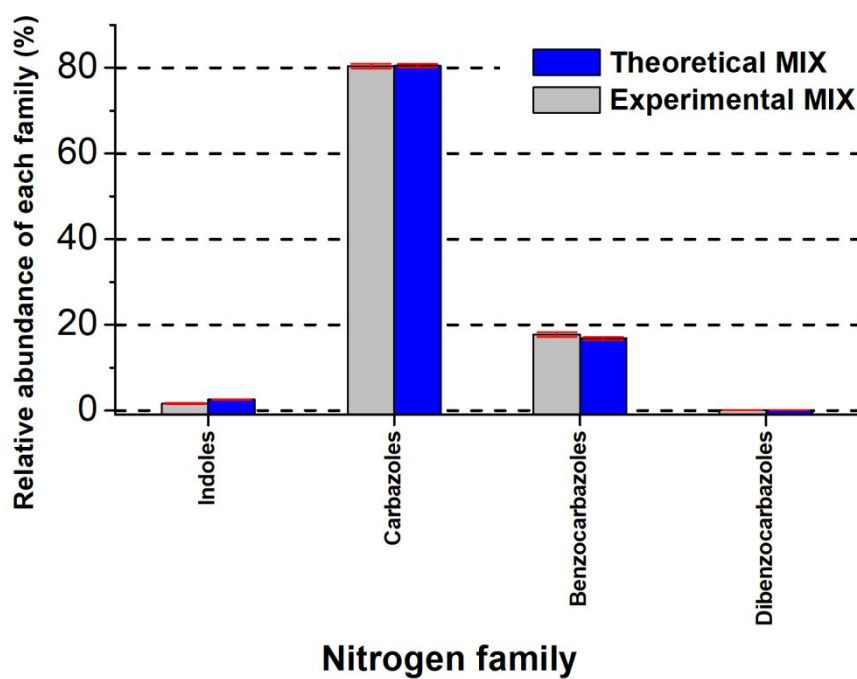


Figure S6: Comparison of theoretical and experimental MIX compositions for neutral nitrogen families





**Figure S7: Hydrodenitrogenation mechanisms of Carbazoles (Top) and Acridines (Bottom) compounds according to DBE evolution.** Adapted with permission from **Molecular-Level Insights into Coker/Straight-Run Gas Oil Hydrodenitrogenation by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**, Nguyen, M.T.; Pirngruber, G.; Chainet, F.; Albrieux, F.; Tayakout-Fayolle, M.; Geantet, C., *Energy Fuels* 2019. Copyright 2019 American Chemical Society.

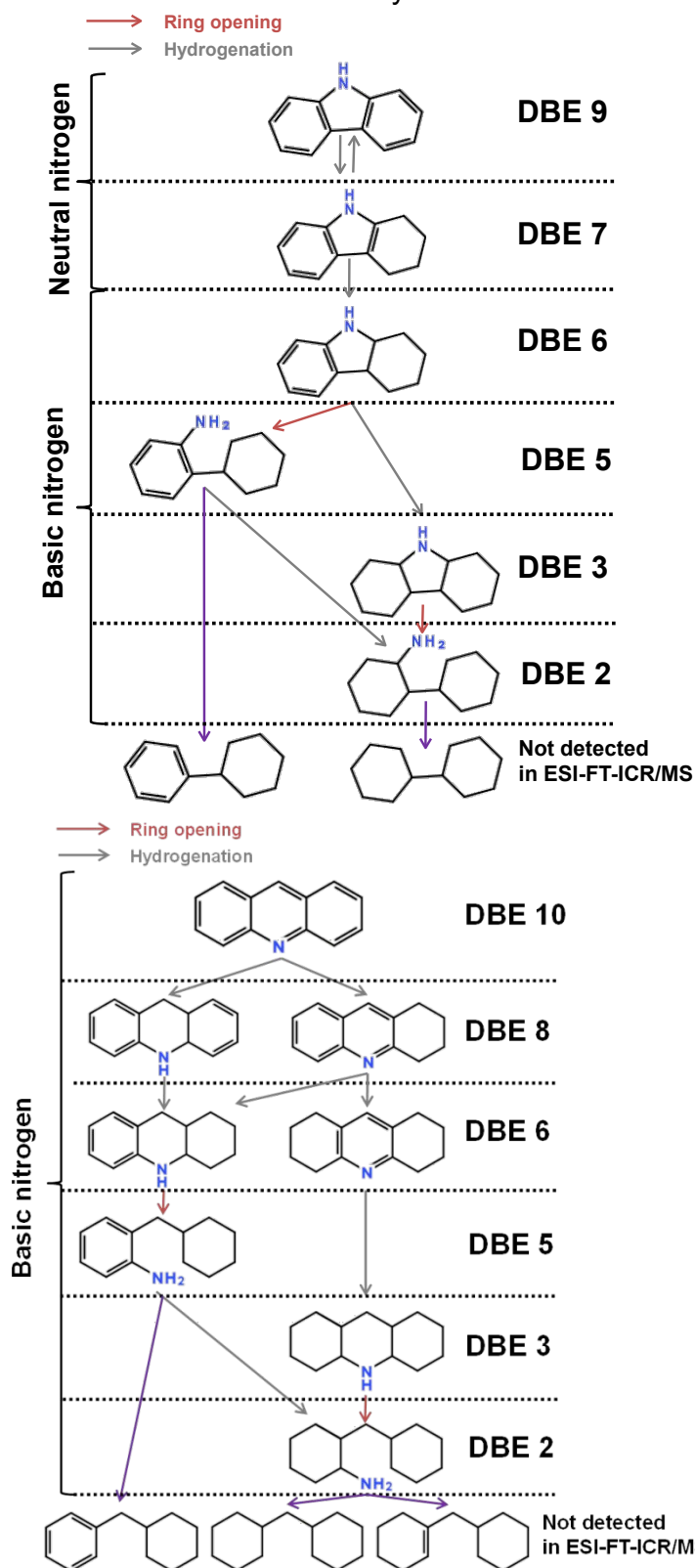


Figure S8: (A) Evolution of RINNC (*Relative Intensity Normalized to Nitrogen Content*) for the different basic families. (B) Evolution of RINNC (*Relative Intensity Normalized to Nitrogen Content*) as a function of the number of carbon atoms of the molecules for basic compounds

