Supporting Information

Evaluating the benefits of data fusion and PARAFAC for the chemometric analysis of FT-ICR MS datasets from gas oils samples

Julie Guillemant[†], Marion Lacoue-Nègre^{*†}, Alexandra Berlioz-Barbier[†], Luis Pereira de

Oliveira[†], Florian Albrieux[†], Jean-François Joly[†], and Ludovic Duponchel[‡]

† IFPEN, Etablissement de Lyon, Rond-Point de l'Echangeur de Solaize, BP 3 69360 Solaize, France

‡ Univ. Lille, CNRS, UMR 8516 - LASIR - Laboratoire de Spectrochimie Infrarouge et Raman, F-59000 Lille, France

* Correspondence should be addressed to Dr. Marion Lacoue-Nègre:

Marion.lacoue-negre@ifpen.fr

Figure/Table	Reference	Page
Evolution of basic nitrogen		
families for the different	Figure S1	S-2
hydrotreated samples		
Comparison of the compositions of		
the nitrogen and sulfur families for	Figure S2	S-3
the different types of gas oils		
PC3-PC4 score plot from ESI(+)-	Figure S3	S-4
FT-ICR MS analysis		
PC3-PC4 score plot from ESI(-)-	Figure S4	S-5
FT-ICR MS analysis		
PC1-PC2 and PC3-PC4 scores		
plots from APPI(+)-FT-ICR MS	Figure S5	S-6
analysis	-	

Table of contents





Figure S2: Comparison of the compositions of the nitrogen and sulfur families for the different types of gas oils



Figure S3: PC3-PC4 score plot from ESI(+)-FT-ICR MS analysis and its corresponding loadings plots



Figure S4: PC3-PC4 score plot from ESI(-)-FT-ICR MS analysis and its corresponding loadings plots





Figure S5: PC1-PC2 and PC3-PC4 scores plots from APPI(+)-FT-ICR MS analysis and its corresponding loadings plots.

