

Supporting Information

A chemometric exploration of APPI(+)-FT-ICR MS data sets for a comprehensive study of aromatic sulfur compounds in gas oils

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Table of contents

Figure/Table	Reference	Page
Data processing workflow used	Figure S1	2
PC1-PC2 score plot from PCA considering only LCO samples. PC2 loadings plot highlighting C14 and C15-DBT importance	Figure S2	3
C3-DBT relative intensity in samples	Figure S3	4
PC3-PC4 and PC5-PC6 score plots	Figure S4	5
PC3, PC4, PC5 and PC6 loadings plot	Figure S5	6
Q-residual contributions of different gas oils samples	Figure S6	7

Figure S1: Data processing workflow used

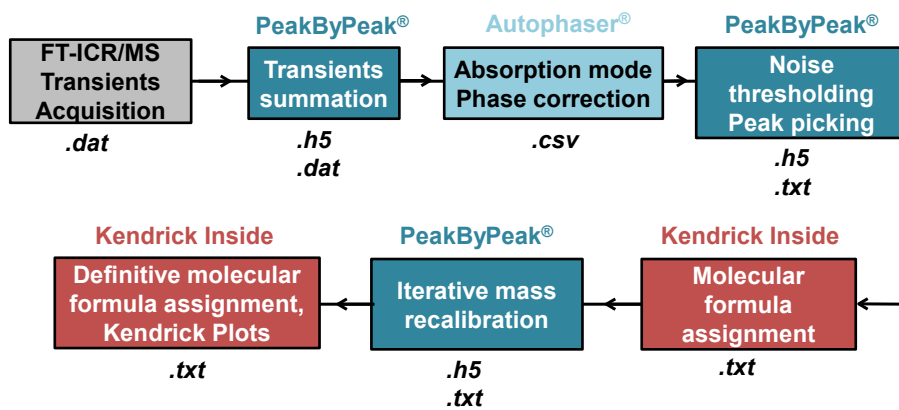


Figure S2: (A) PC1-PC2 score plot from PCA considering only LCO samples that shows the deviation over time of the several replicates of GO 8 (corresponding to samples 43, 44, 45, 46, 47 and 48). (B) PC2 loadings plot highlighting C14 and C15-DBT importance. (C) Evolution of sulfur pseudo-concentrations for the several replicates according to the number of carbon atoms of DBE 9-DBT family. 1-6 corresponds to the different replicates analysis numbers.

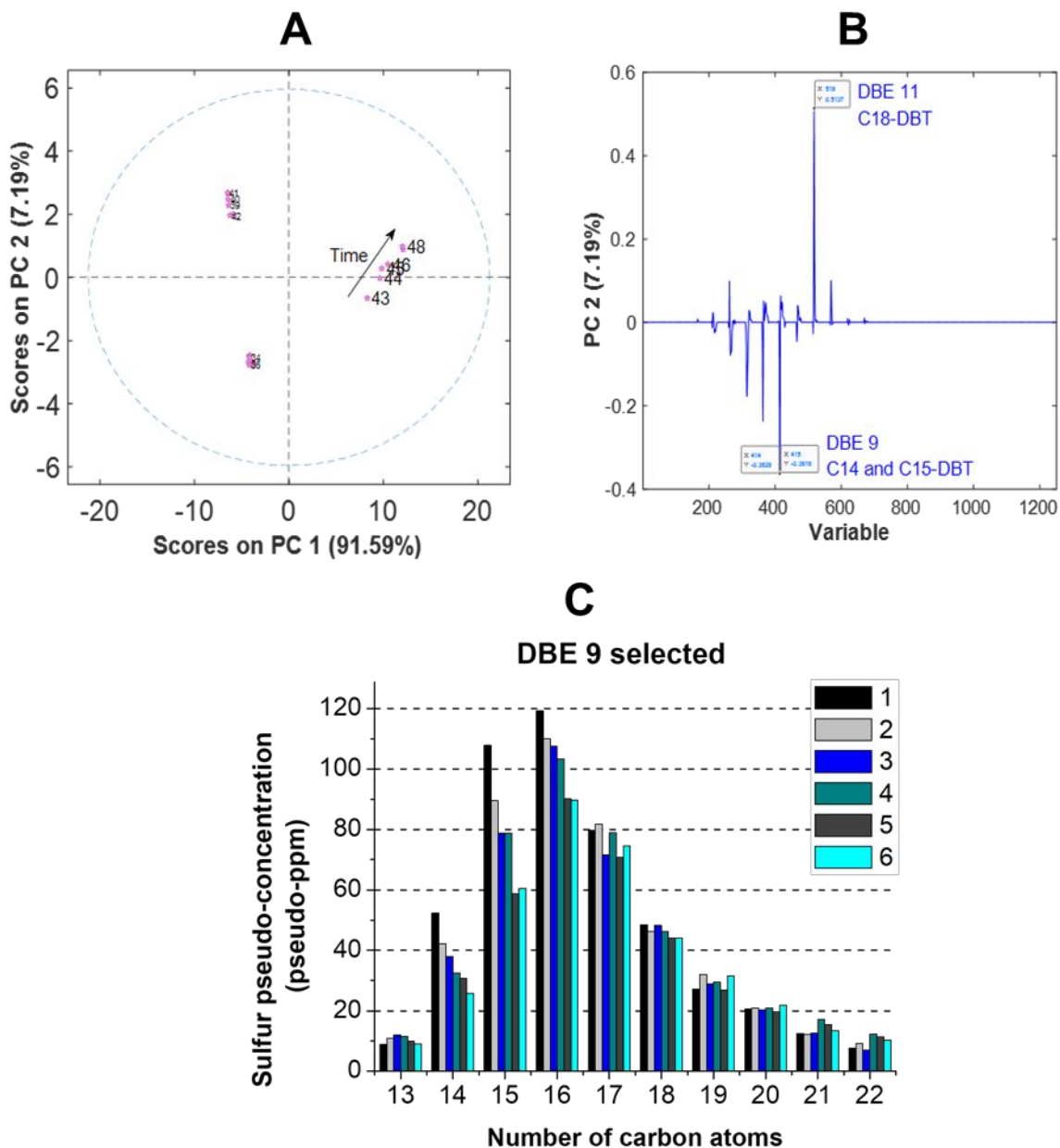


Figure S3: C3-DBT relative intensity in samples

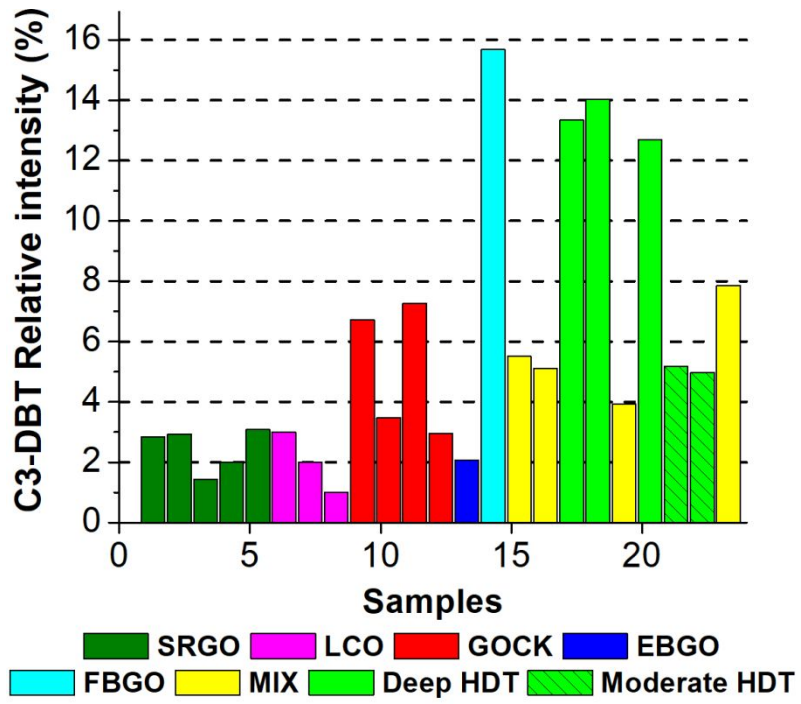


Figure S4: (A) PC3-PC4 and (B) PC5-PC6 Score plots

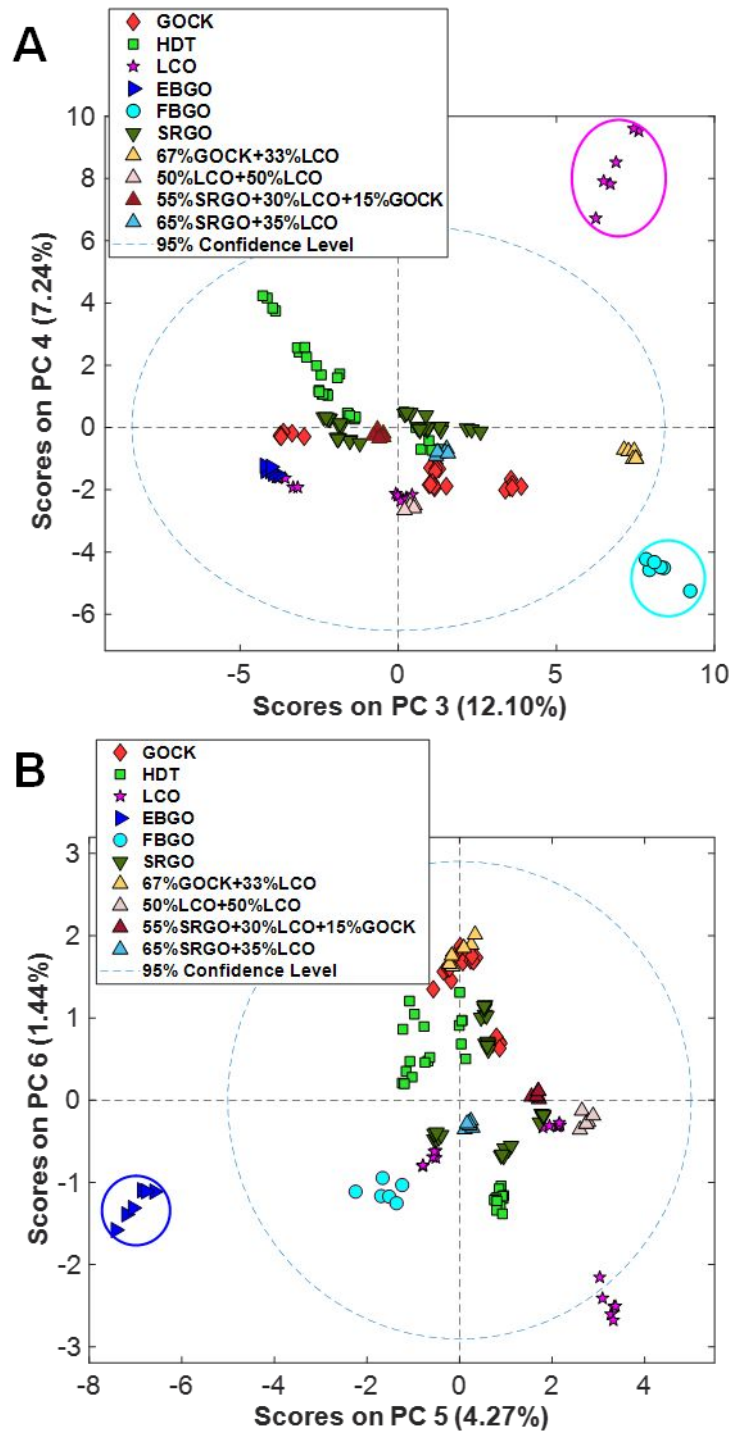


Figure S5: (A) PC3 Loadings plot. (B) PC4 Loadings plot. (C) PC5 Loadings plot. (D) PC6 Loadings plot

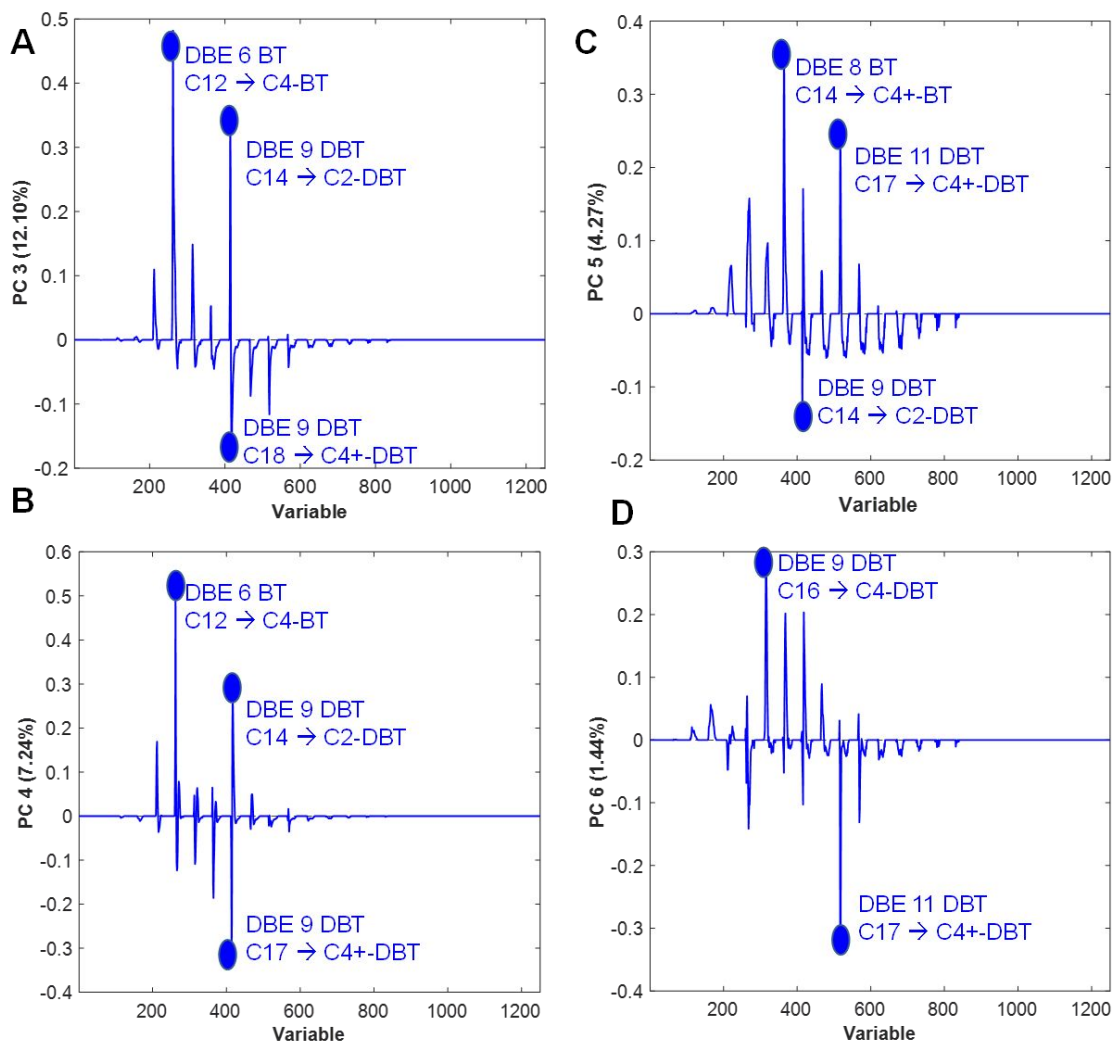


Figure S6: Q-residual contributions of different gas oils samples.

