Supporting Information

Towards a new pseudo-quantitative approach to evaluate the ionization response of nitrogen compounds in complex matrices

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Figure S1: Initial GC×GC-NCD identification blobs

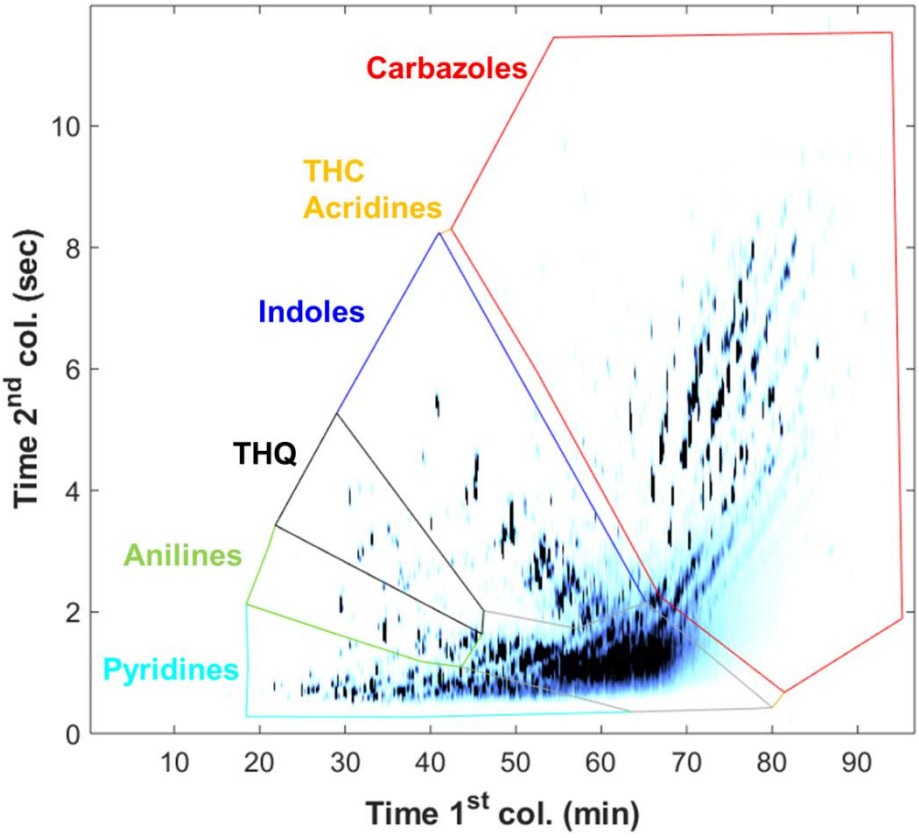

Figure S2: Comparison of the F3F4F5 solutions and whole gas oils analysis in ESI(+) mode

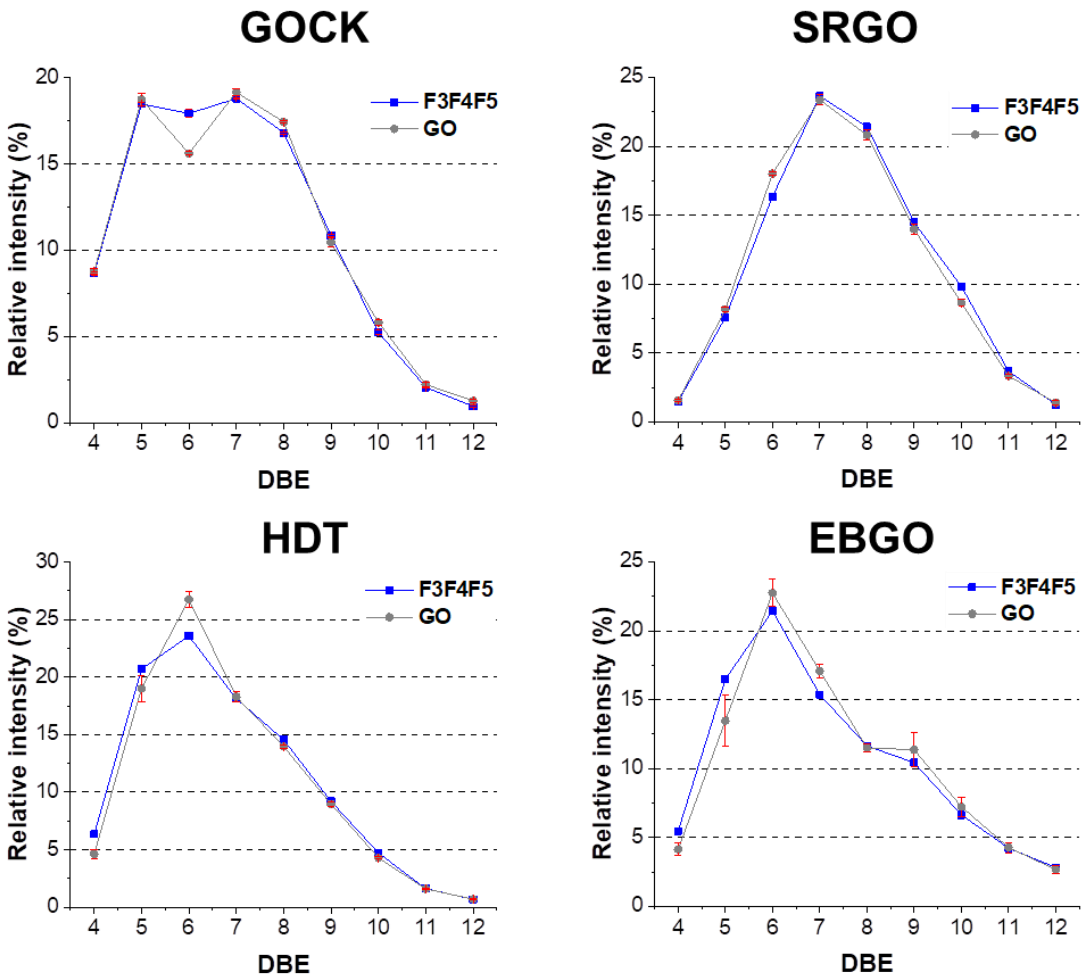

Figure S3: Comparison of the F3F4F5 solutions and whole gas oils analysis in ESI(-) mode

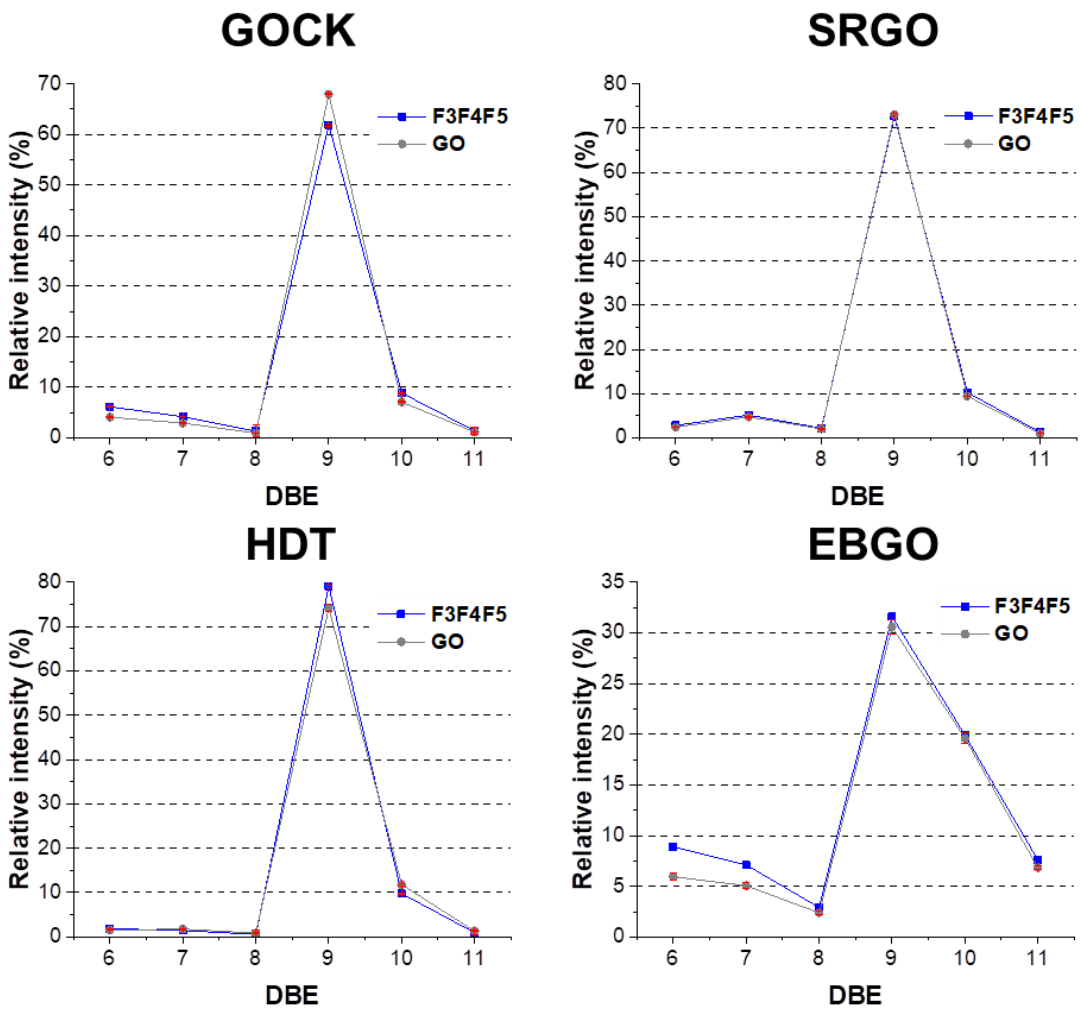

Figure S4: (A) Mass spectra obtained and (B) their corresponding DBE=f(#C) plots for the N1[H] class in ESI(+) mode for 4 types of different gas oils. (C) Number of N1[H] compounds identified depending on the gas oil considered.

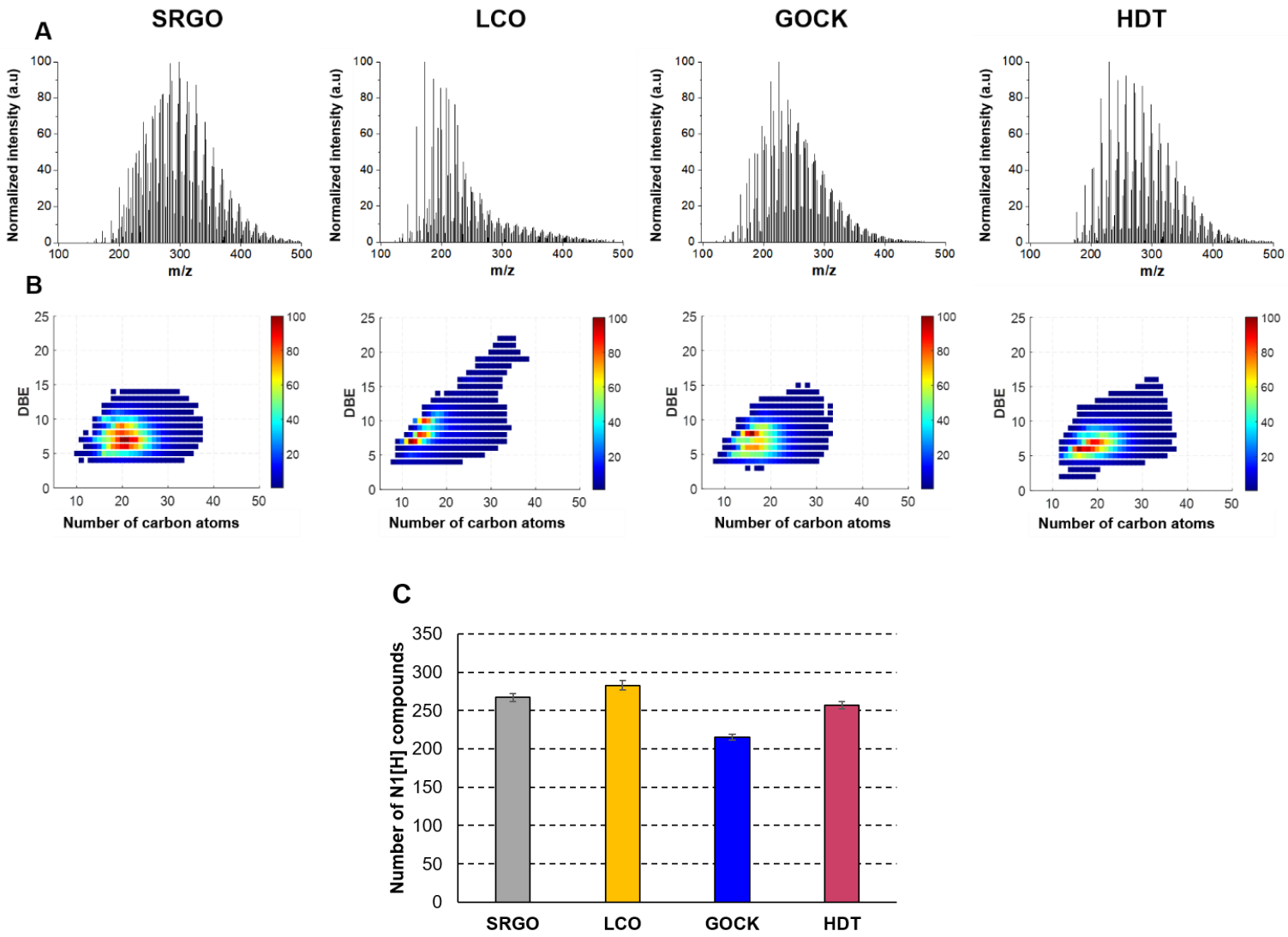

Figure S5: (A) Mass spectra obtained and (B) their corresponding DBE=f(#C) plots for the N1[H] class in ESI(-) mode for 4 types of different gas oils. (C) Number of N1[H] compounds identified depending on the gas oil considered.

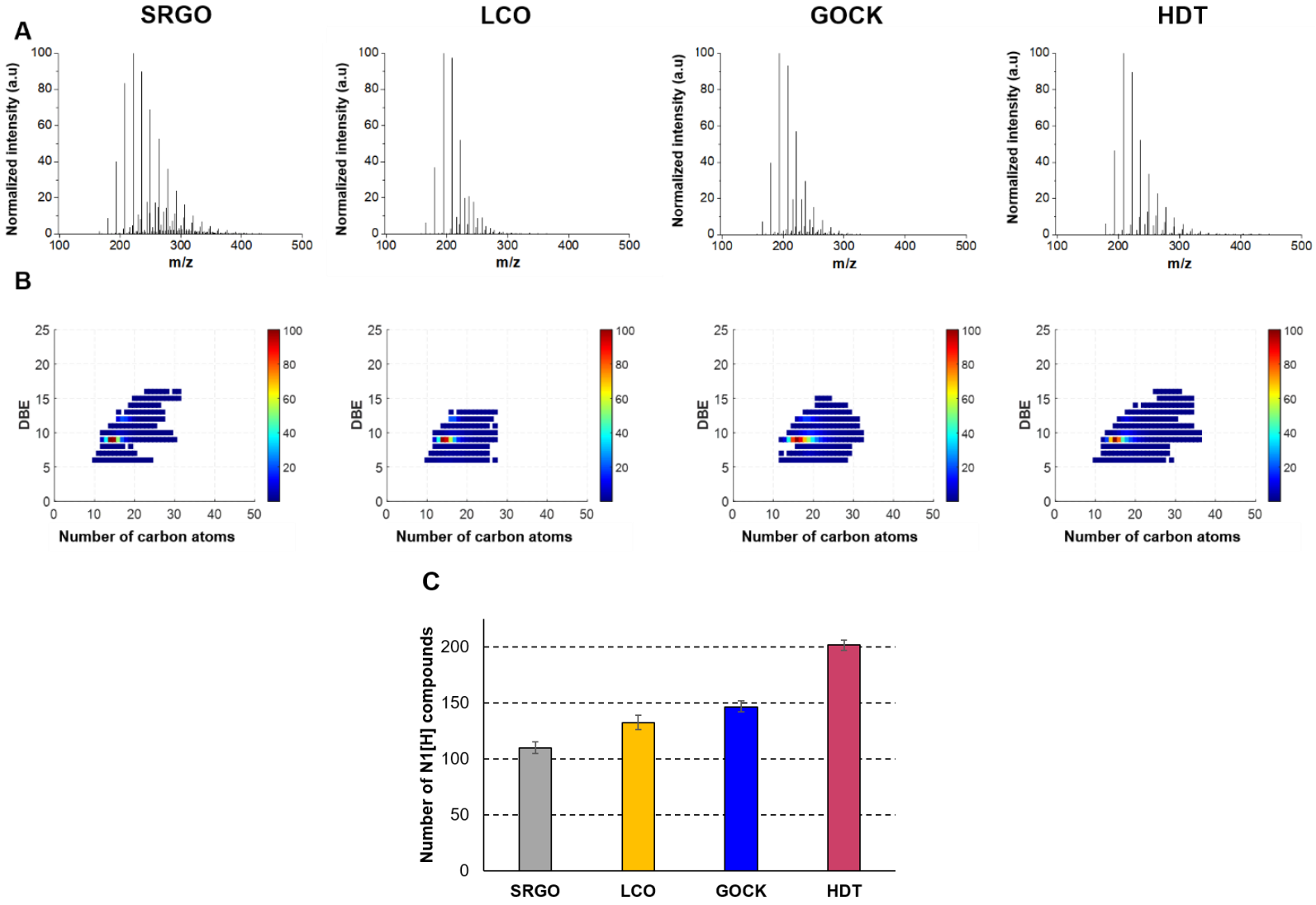

Table S1. Characteristics of MLR models. *: the reference error of the GC×GC-NCD method was assumed to be equal to 10%.

Criteria	Indoles	Carbazoles	THQ Ani Pyr	Quinolines	Acridines
Outliers	GO 1, GO 7, GO 21	GO 4, GO 6, GO 18	GO 6, GO 11, GO 18	GO 4, GO 6	GO 1, GO 4
RMSEC (ppm)	19	57	18	15	10
RMSECV (ppm)	20	70	23	20	14
Concentration range (ppm)	0-270	0-1000	0-400	0-650	0-170
Robustness criteria (RMSECV/RMSEC)	1.05	1.22	1.32	1.26	1.35
Cross validation bias (%)	0.047	0.511	0.159	-0.263	-0.640
Bias	0	1.14E-13	1.42E-14	2.84E-14	2.13E-14
$R^2_{calibration}$	0.939	0.932	0.965	0.991	0.947
$R^2_{cross\ validation}$	0.932	0.898	0.938	0.986	0.902
CV: Number of splits	8	10	5	8	6
CV: Samples per blind	2	1	3	2	2
GC×GC-NCD Error (%)	10*	10*	10*	10*	10*

Figure S6: Comparison of the evolution of the nitrogen pseudo-concentration as a function of number of carbon atoms for the quinolines and acridines families for the samples GO 3 (SRGO) and GO 5 (LCO)