Supplemental Material to

Retention Database for Prediction, Simulation and Optimization of GC Separations

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Introduction:

The supporting informations includes the following files:

CSV Files:

- Database_measurements.csv: Database including only the data of our own measurements.
- Database_all.csv: Database including all data from the literature and measurements
- Dabase_verficated.csv: Database including only data that pass the verification process.

HTML-Files:

You can watch the HTML files easily in your Browser.

- Notebook_PCA.html: Static Pluto Notebook, including the Database, some 3D plots of the data and processing steps of the PCA analysis. Use the Table of Content menu on the right hand side to navigate through the document.
- Figure S3.html: 3D plot of the ABC parameters compound category
- Figure S4.html: 3D plot of the K-centric parameters sorted by compound category
- Figure S5.html: Chromatogram of the measurement and simulation of FAMEs with focus on the simulation of unsaturated FAMES such as C18:1, C18:2, C18:3 and C20 derivates.

$\ln k$ Values of Measurements

The ln k values of all measured compounds can be found at
https://github.com/JanLeppert/RetentionData/tree/main/Databases/Measurements

Lambert W function

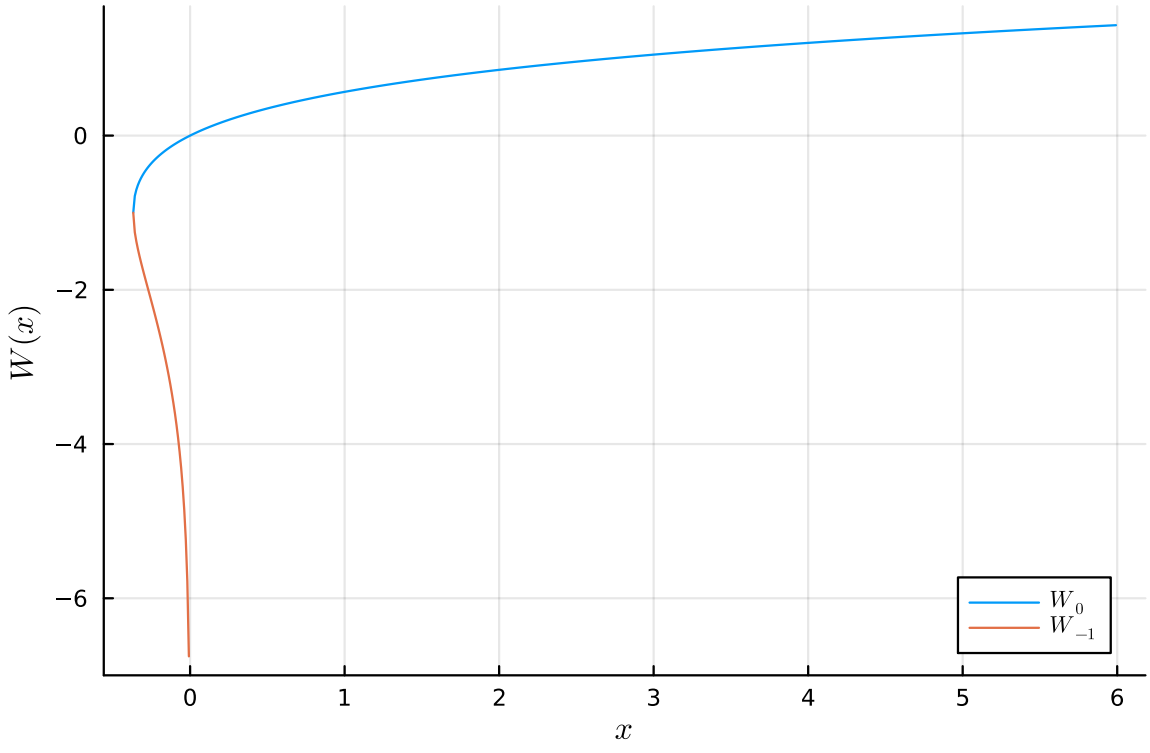

Figure S1 Plot of the Lambert W function with its to branches W_0 and W_{-1}.

Results of PCA for ABC parameters

PCA(indim = 3, outdim = 1, principalratio = 0.9999871043651598)

Pattern matrix (unstandardized loadings):

	PC1
1	-35.9871
2	4495.83
3	4.62894

Importance of components:

	PC1
SS Loadings (Eigenvalues)	2.02138 e7
Variance explained	0.999987
Cumulative variance	0.999987
Proportion explained	1.0
Cumulative proportion	1.0

Results of PCA for K-centric parameters

PCA(indim = 3, outdim = 2, principalratio = 0.9989824070935823)

Pattern matrix (unstandardized loadings):

	PC1	PC2
1	78.3826	-11.8578
2	4.10909	0.109094
3	27.8943	33.3364

Importance of components:

	PC1	PC2
SS Loadings (Eigenvalues)	6938.81	1251.94
Variance explained	0.846314	0.152696
Cumulative variance	0.846314	0.99901
Proportion explained	0.847152	0.152848
Cumulative proportion	0.847152	1.0

Fast GC Measurement via FF TG GC

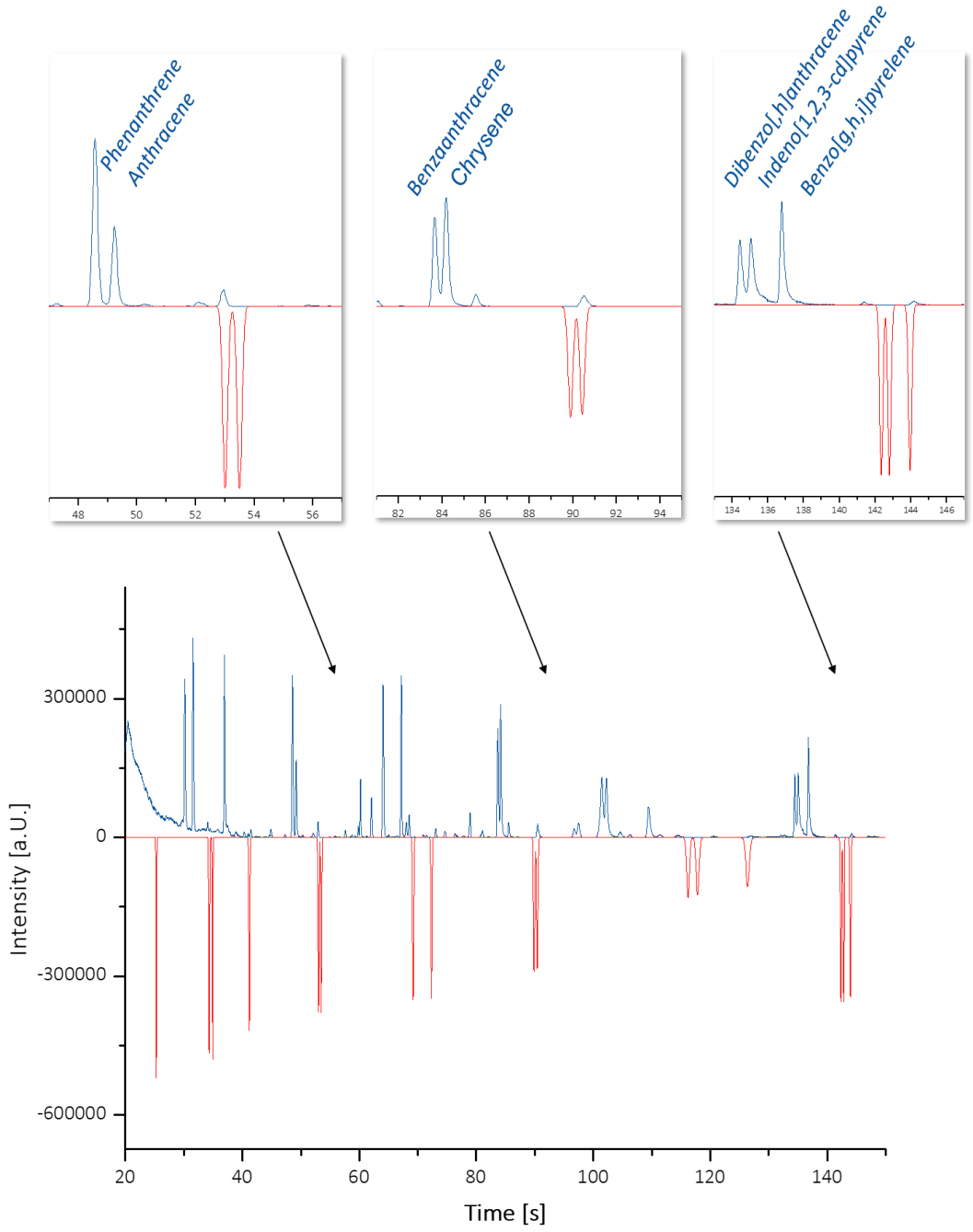

Figure S2: Comparison between simulated (red) and measured (blue) chromatogram of Flow Field Thermal Gradient separation of 16 EPA PAH on ZB-PAH-CT column (4 m, ϐ=0.001).