**Supplementary Material for Grouping of Complex Substances Using Analytical Chemistry Data: A Framework for Quantitative Evaluation and Visualization**

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The R Markdown documentation of unsupervised and supervised analysis workflow can be accessed through <http://parametric.tamu.edu/research/Onel_etAl_2019_Rmarkdown.html>

The GC-MS, GCxGC-FID, and IM-MS data of Petroleum UVCB, and GC-MS data of SRM samples can be downloaded from http://paroc.tamu.edu/Software/Onel\_etAl\_2019\_data.zip