

Supporting information for resubmission of manuscript ac-2013-01061q:

New Spectral Deconvolution Algorithms for the Analysis of Polycyclic Aromatic Hydrocarbons and Sulfur Heterocycles by Comprehensive Two-Dimensional Gas Chromatography/Mass Spectrometry

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Table S-1 lists the instrumental parameters for the GC/MS and GC×GC/MS methods used in this study.

Table S1. GC/MS and GC×GC/MS instrument parameters

GC Parameters	GC×GC/MS Method	GC/MS Method
Injection Mode	Splitless	Splitless
Injection Volume	1 µL	1 µL
Inlet Program	-20°C, 12°C/min, 320°C (5 min)	300°C
Carrier Gas	Constant Flow, 1 mL/min He	Constant Flow, 1.5 mL/min He
Column 1	30 m x 0.25 mm ID x 1.0 µm DB-5MS Ultra Inert	30 m x 0.25 mm ID x 0.25 µm DB-5
Column 2	1 m x 0.18 mm ID x 0.36 µm RXI-17SilMS	N/A
Transfer Line Temperature	300°C	290°C
Modulation Time	8 sec	N/A
Hot Jet Temperature	310°C	N/A
Cryogen Flow	15 L/min	N/A
Temperature Program	60°C (1 min), 6.5°C/min, 325°C (20 min)	60°C (1 min), 5°C/min, 340°C (0 min), -20°C/min, 300°C (5 min)
Run Time	61.77 min	64 min
MS Parameters	GC×GC/MS Method	GC/MS Method
Solvent Delay	17 min	8 min
Mass Range	50-350 m/z	50-450 m/z
Scan Rate	19.79 scans/sec	8.3 scans/sec
Quadrupole Temperature	150°C	150°C
Ion Source Temperature	230°C	230°C