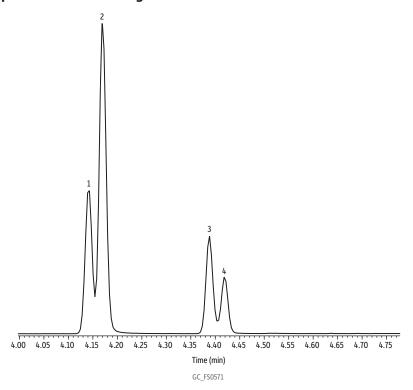


## **Experimental Chromatogram**



Rxi-17Sil MS, 20 m, 0.18 mm ID, 0.18 µm (cat.# 14102) Column Standard/Sample See notes Diluent:

Inj. Vol.:

 $1\,\mu L$  PTV split (split ratio 10:1) Topaz 2.0 mm lD straight inlet liner w/wool (cat.# 23314) 120 °C to 165 °C at 300 °C/min (hold 10 min) to 320 °C at 300 °C/min Inlet Temp. Program:

(hold 8 min)

Oven Oven Temp.: 120 °C (hold 0.5 min) to 200 °C at 18.5 °C/min to 330 °C at 35 °C/min

**Carrier Gas** He, constant flow 1 mL/min Flow Rate: Detector MS

Mode: SIM Program: 147, 150, 196, 201 m/z, 50 ms dwell Transfer Line Temp.: 320 °C Analyzer Type: Quadrupole Inert 230 °C Source Type: Source Temp.: Quad Temp.: 150 °C Ionization Mode:

Notes

Instrument **Sample Preparation** 

Agilent 7890A GC & 5975C MSD
Standards were derivatized with 20 µL phenylboronic acid (saturated solution in diethyl ether), dried, and then reconstituted in 1 mL isooctane. Final concentrations are given in the peak table. Compounds and retention times in the peak list are from the actual chromatographic analysis. PBA derivatives of 3-MBPD-d5 and 3-MBPD were included in the Pro EZGC model, but not in the experimental

analysis.



Injection