

		Conc.
Peaks	t _R (min)	(ng/mL)
1. 3-MCPD-d5 PBA derivative	4.143	100
2. 3-MCPD PBA derivative	4.169	200
3. 2-MCPD-d5 PBA derivative	4.388	100
4. 2-MCPD PBA derivative	4.418	100

Rxi-17Sil MS, 20 m, 0.18 mm ID, 0.18 µm (cat.# 14102)

Sample Diluent: See notes Isooctane

Injection

Inj. Vol.: 1 µL PTV split (split ratio 10:1)
Liner: Topaz 2.0 mm ID straight inlet liner w/wool (cat.# 23314)
Inlet Temp. Program: 120 °C to 165 °C at 300 °C/min (hold 10 min) to 320 °C at 300 °C/min (hold 8 min) Oven

 $120~^{\circ}\text{C}$ (hold 0.5 min) to 200 $^{\circ}\text{C}$ at 18.5 $^{\circ}\text{C/min}$ to 330 $^{\circ}\text{C}$ at 35 $^{\circ}\text{C/min}$ He, constant flow 1 mL/min Oven Temp.:

Carrier Gas Flow Rate: Detector MS SIM

Mode: SIM Program: 147, 150, 196, 201 m/z, 50 ms dwell

Transfer Line Temp.: 320 °C Analyzer Type: Quadrupole Source Type: Source Temp.: Inert 230 °C Quad Temp.: Ionization Mode: 150 °C ΕI

Instrument Agilent 7890A GC & 5975C MSD

Notes 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.