Supporting Information for:

Sub ppt determination of butyltins, methylmercury and inorganic mercury in natural waters by dynamic headspace in-tube extraction and GC-ICPMS detection

Jing Hu[a, b], Enea Pagliano[b], Xiandeng Hou[a], Chengbin Zheng[a], Lu Yang[b]* and Zoltan Mester[b]

[a] Analytical & Testing Center, Sichuan University, 29 Wangjiang Rd, Chengdu, Sichuan 610064, China.

[b] National Research Council Canada, 1200 Montreal Rd, Ottawa, Ontario, K1A 0R6, Canada.

Supporting Information (SI) Contents:

Table S1. GC-ICPMS and EIMS operating parameters

GC	Column	Zebron ZB-5MS (30 m ×0.25 mm × 0.25 µm)
	Injection mode	Splitless
	Inlet temperature	260 °C
	Carrier gas	Helium, 1 mL min^{-1}
	Oven program	60 °C (hold for 1 min), 25 °C /min to 260 °C (hold for 6 min)
	Transfer line temperature	260 °C
ICP-MS	RF power	820 W
	RF matching	1.77 V
	Sample depth	7.5 mm
	Torch-H	0.3 mm
	Torch-V	-1.4 mm
	Carrier gas	1.23 L/min
EIMS	Source temperature	230 °C
	EM volts	1628 V
	Electron energy	70 eV
	Ion polarity	Positive
	Detector temperature	250 °C

Table S2. Properties of sorbent materials used (manufacturer's data)

Sorbent	Sorbent type	Surface area (m^2 g^{-1})	Temperature limit (^oC)	Water affinity	application
Carbopack C	non-porous graphitized carbon black	10	500	relatively low	low to medium boilers (C12~C20)
Carboxen 1000	carbon molecular sieve	1200	225	moderate	very volatile compounds (C2-C5)
Molecular sieve 5A	crystalline metal aluminosilicates	NA	NA	NA	NA
Carbosieve S III	carbon molecular sieve	975	400	moderate	volatile organics (C2-C5)
Tenax TA/Carbosieve S III	porous organic polymer/carbon molecular	NA	NA	NA	NA
Carbopack C/Carbosieve S III	sieve non-porous graphitized carbon black/carbon molecular sieve	NA	NA	NA	NA
Molecular sieve 5A	crystalline metal aluminosilicates	NA	NA	NA	NA
Tenax GR/Carbosieve S III	70% porous organic polymer-30% graphitized carbon/carbon molecular sieve	24	350	low	volatiles, flavors
Tenax TA	porous organic polymer	35	350	low	volatiles and semivolatiles (C7-C26)

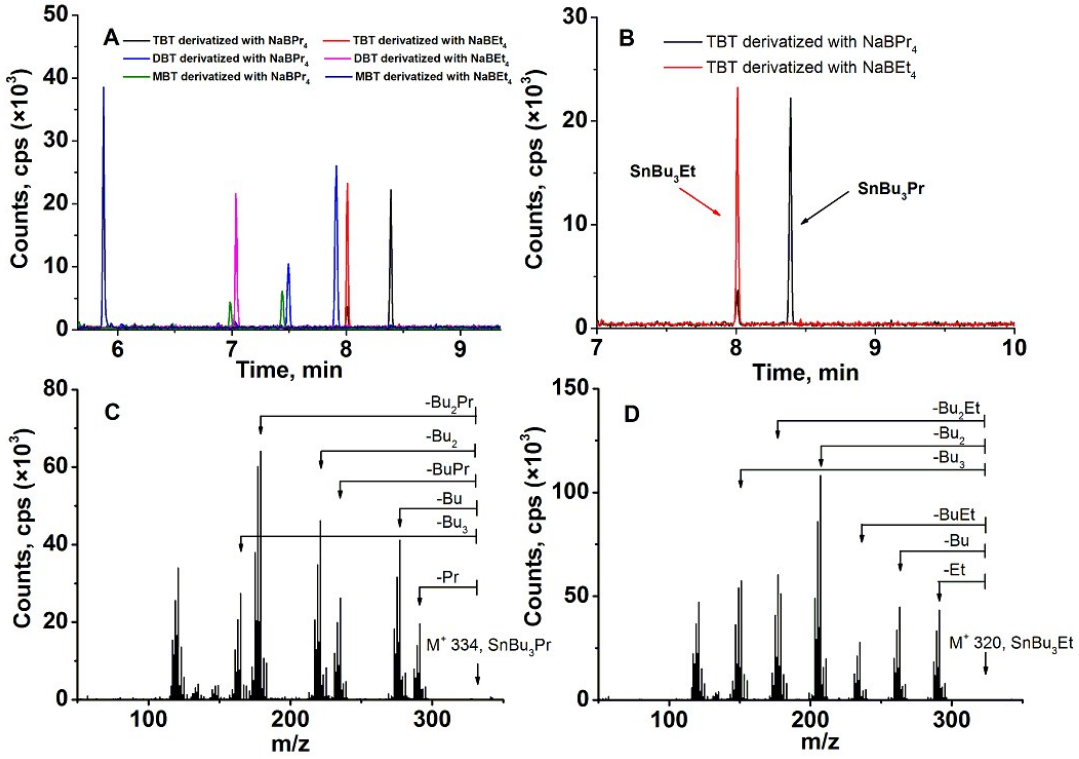

Figure S1. GC-MS chromatograms of (A) propylated and ethylated TBT, DBT and MBT, and (B) propylated and ethylated TBT in full scan mode; Extracted peak spectra of (C) propylated TBT and (D) ethylated TBT.

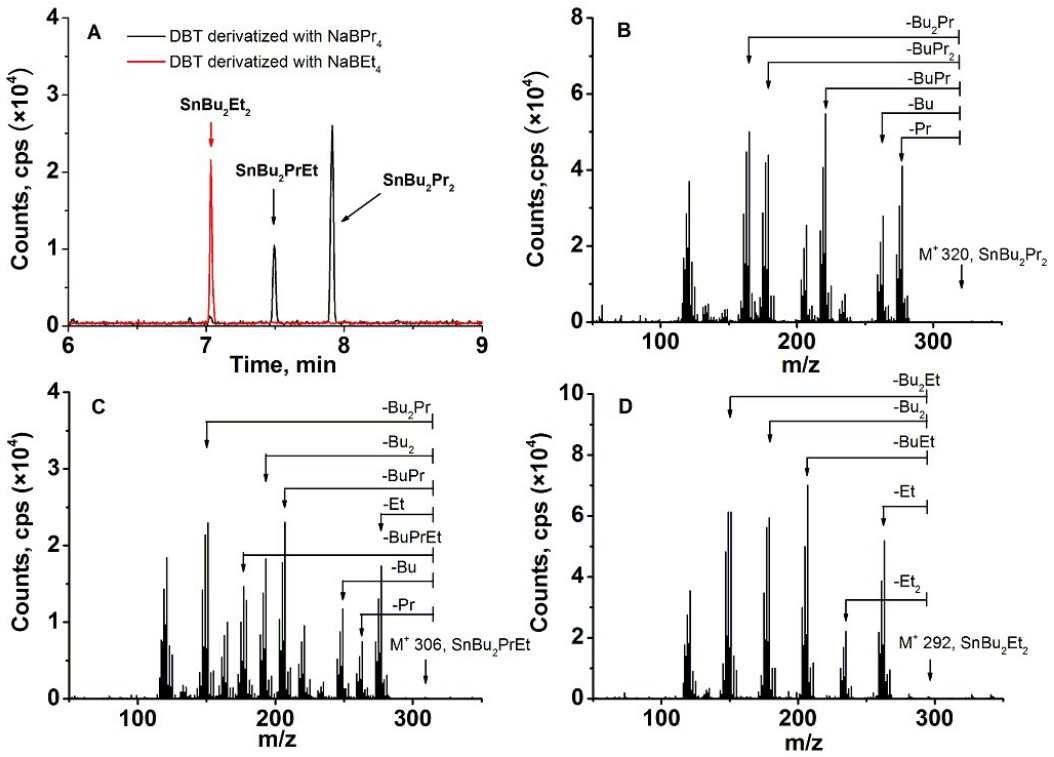

Figure S2. GC-MS chromatogram of propylated and ethylated DBT in full scan mode (A) and extracted peak spectra of propylated DBT (B, C, D).

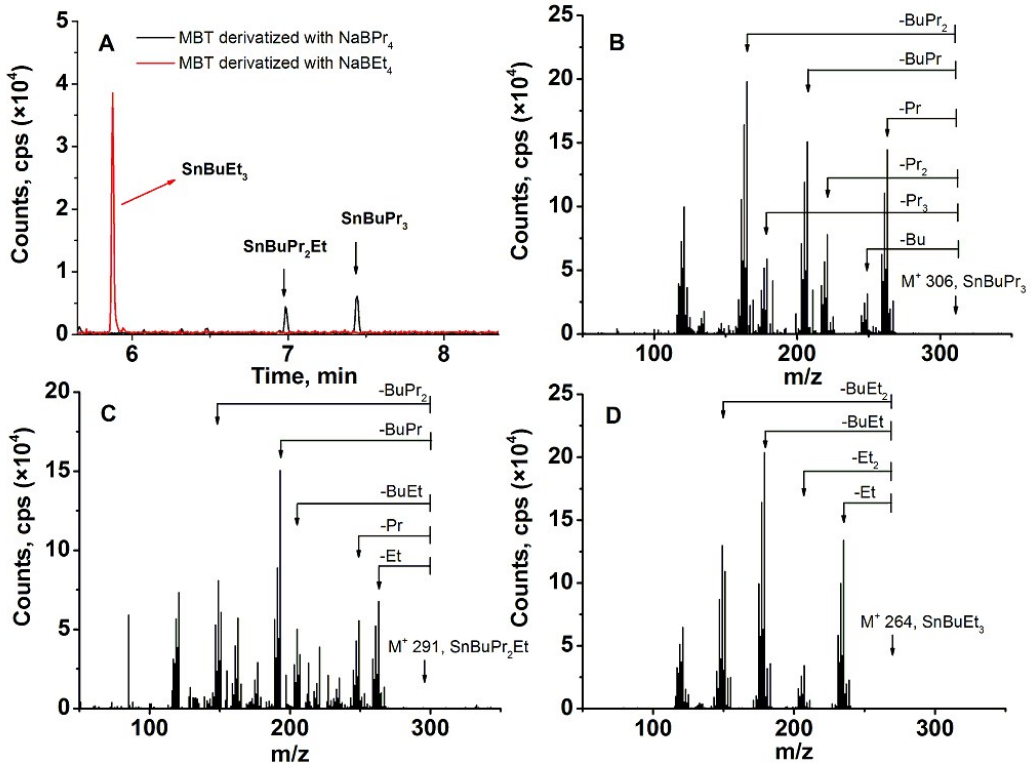

Figure S3. GC-MS chromatogram of propylated and ethylated MBT in full scan mode (A) and extracted peak spectra of propylated MBT (B, C, D). The difference in intensities was due to the different concentration of MBT used in ethylation (2 µg ml^{-1}) and proylation (0.5 µg ml^{-1}).