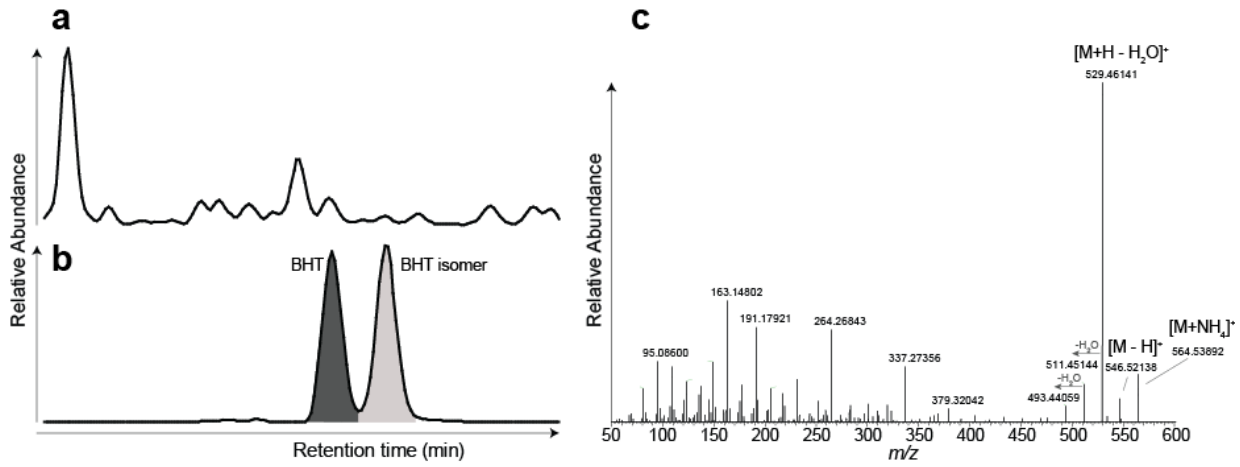
Sup Fig 1.


a
b
Relative Abundance
BHT
BHT isomer
Retention time (min)
c
Relative Abundance
[M+H - H2O]+
529.46141
163.14802
191.17921
264.26843
95.08600
337.27356
379.32042
493.44059
511.45144
546.52138
564.53892
[M - H]+
[M+NH4]+
-H2O
-H2O
50 100 150 200 250 300 350 400 450 500 550 600
m/z

Supplemental Figure 1. Base peak chromatogram (a) and combined extracted ion currents (within 3 ppm) of protonated, ammoniated, and sodiated adducts (*m/z* 547.47209 + 564.49864 + 569.45403, respectively) (b) of non-derivatised BHT and BHT isomer in sediment from 64PE406-E1 core depth 46 – 47 cm. (c) Combined orbitrap $HRMS^2$ of 6 scan events over the ammoniated adduct ($[M+NH_4]^+$; *m/z* 564.49864) of BHT isomer.