Supplementary Figures

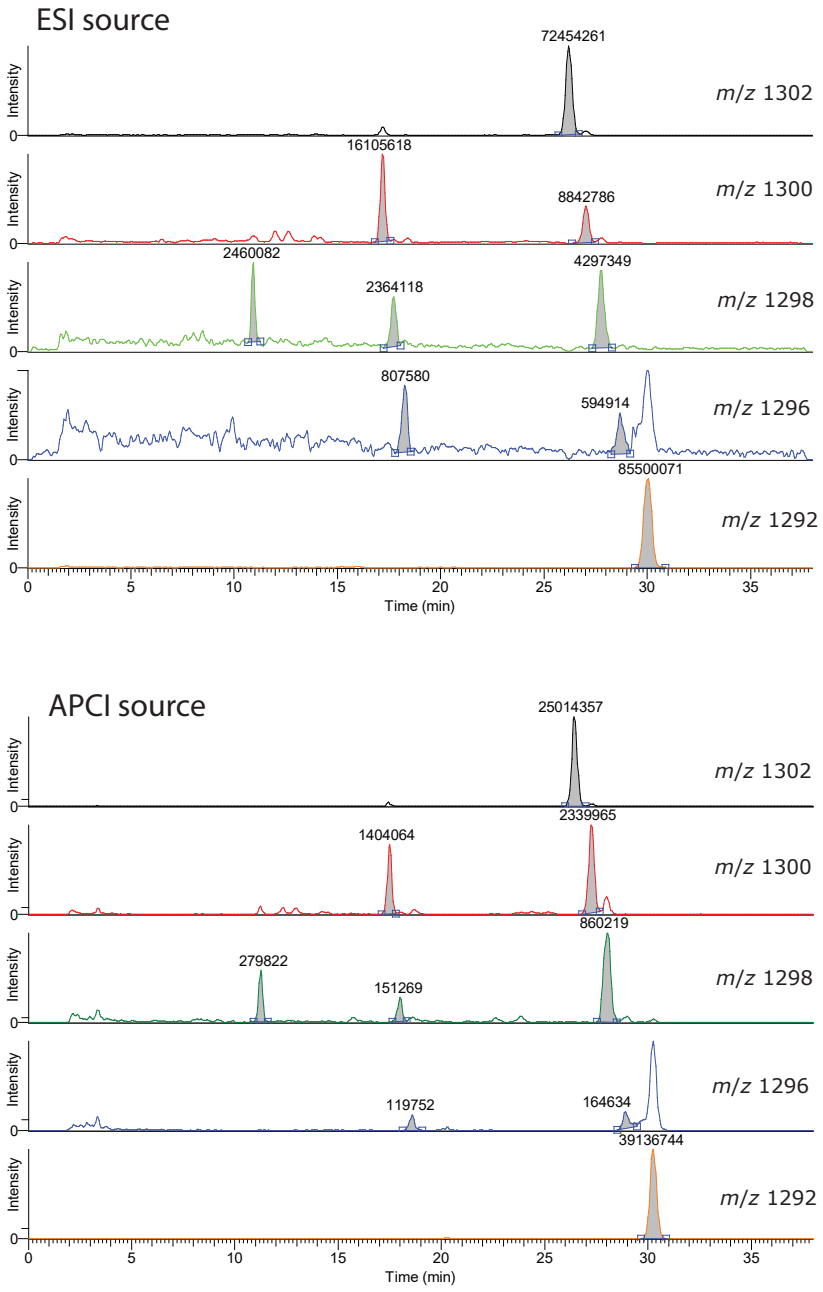
Separation of branched and isoprenoid glycerol dialkyl glycerol tetraether (GDGT) isomers in peat soils and marine sediments using reverse phase chromatography.

Jayne E. Rattray[1,2] and Rienk H. Smittenberg[1]

[1]Department of Geological Sciences, Stockholm University, Svante Arrhenius väg 8C, SE 106 91, Stockholm, Sweden.

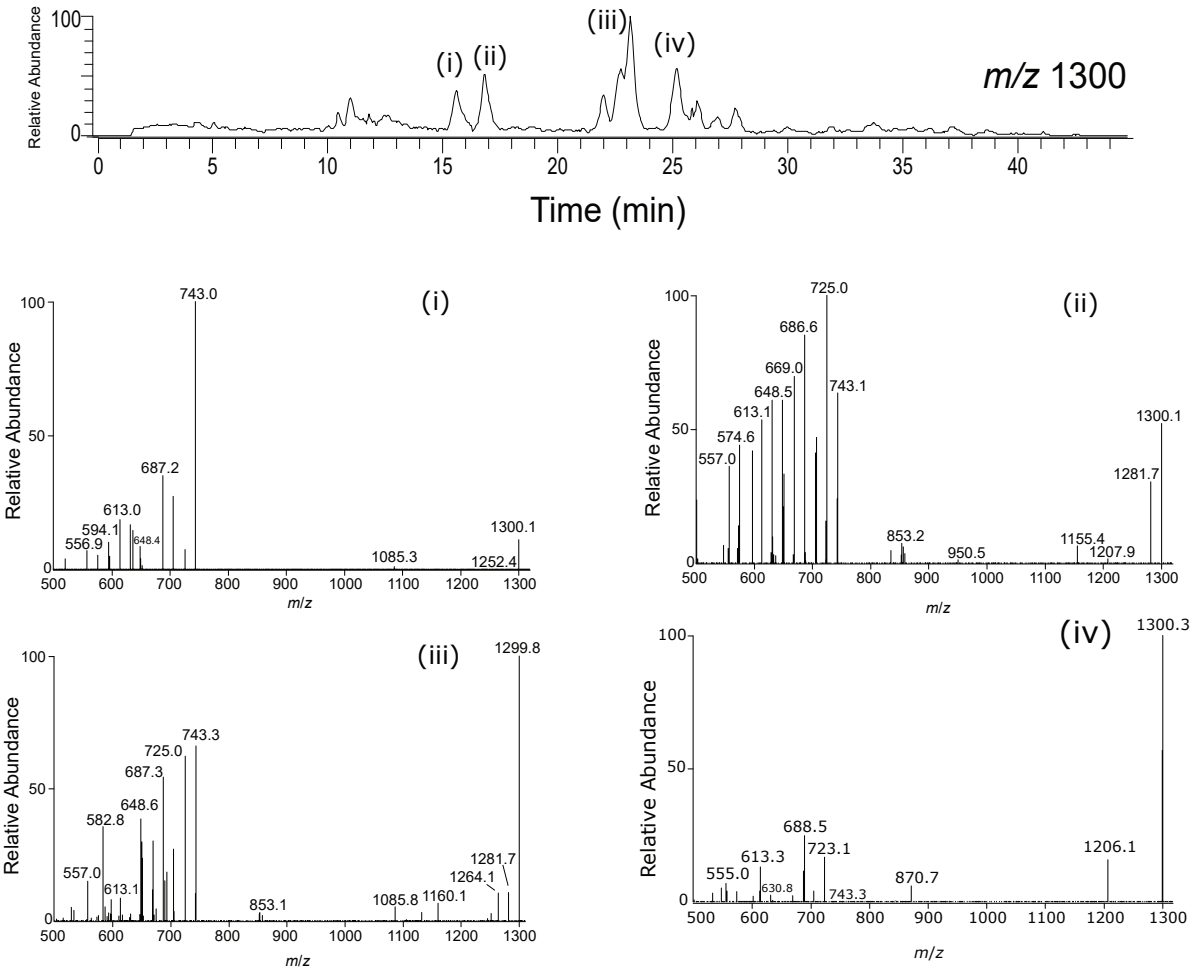
[2] Currently at: Department of Biological Sciences, University of Calgary, Canada.

SI Fig 1. Chromatograms of isoprenoid GDGTs in a Black Sea extract tested usingAPCI vs ESI sources



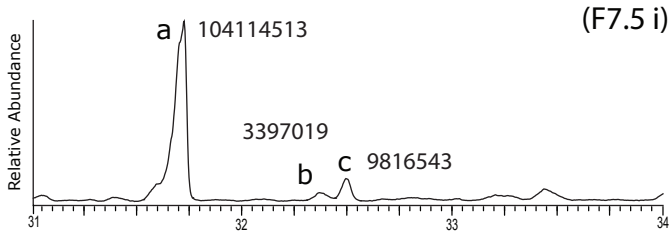
SI. Fig. 2

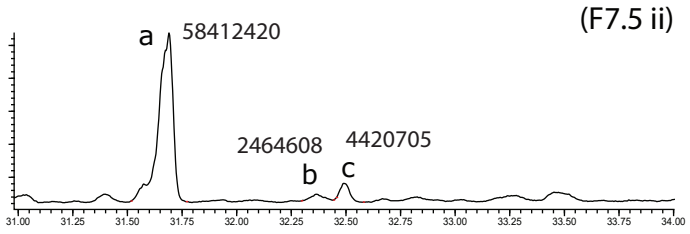
Mass spectra from GDGT isomers eluting at *m/z* 1300 in a Swedish peat bog lipid extract



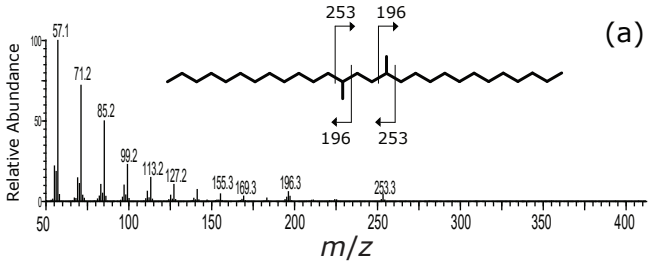
SI Fig 3.

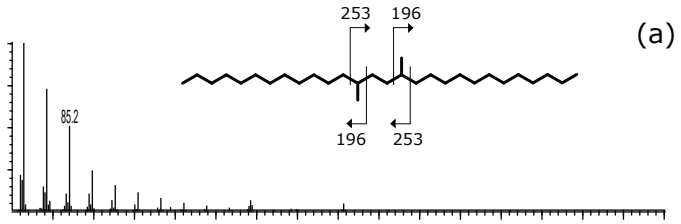
GC/MS chromatograms HPLC fraction F7.5 minutes

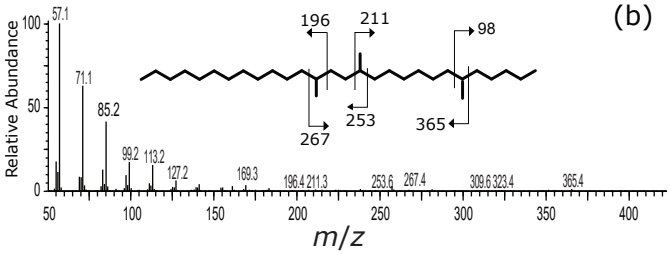


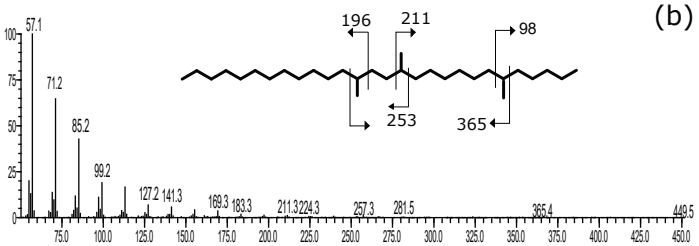


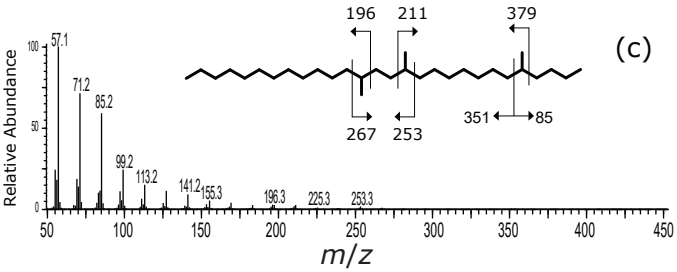
GC/MS spectra F7.5





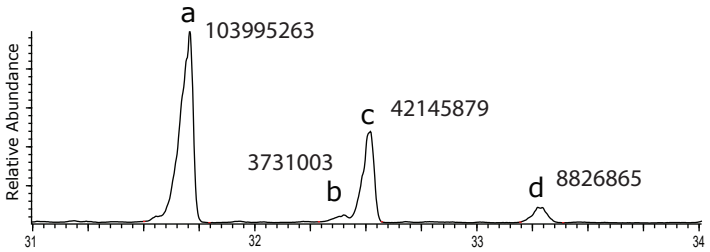




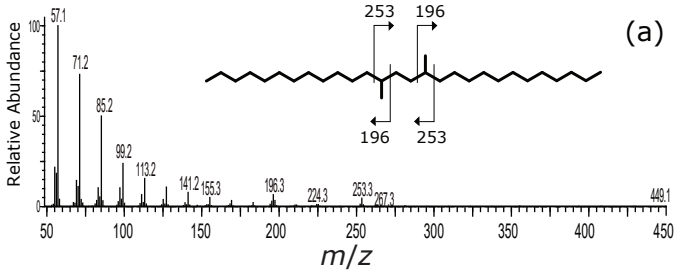


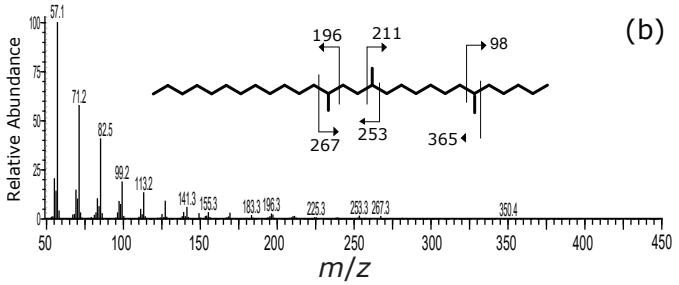
SI Fig 4.

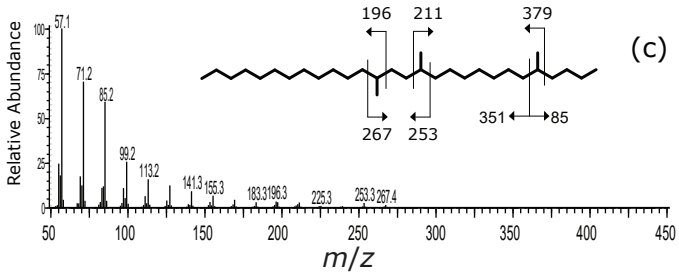
GC/MS chromatograms HPLC fraction F12 minutes (ii)

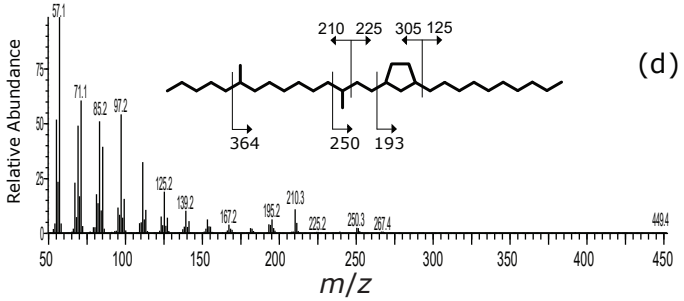


GC/MS spectra F12(ii)



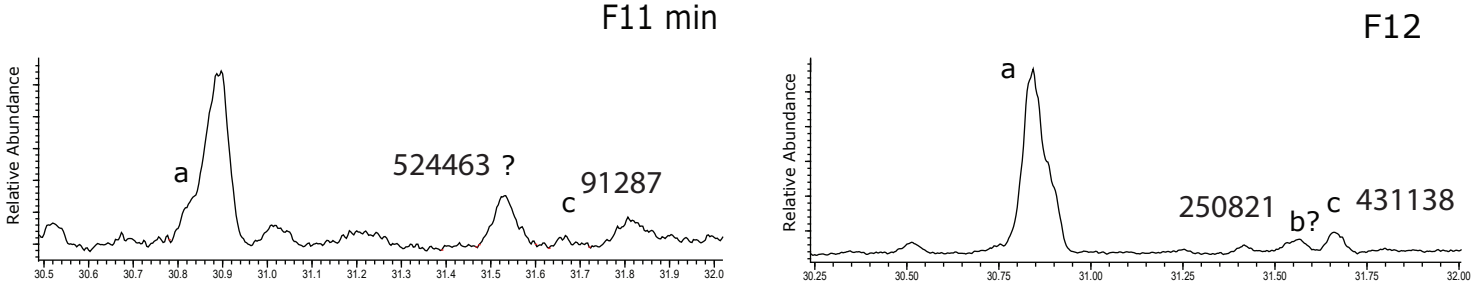




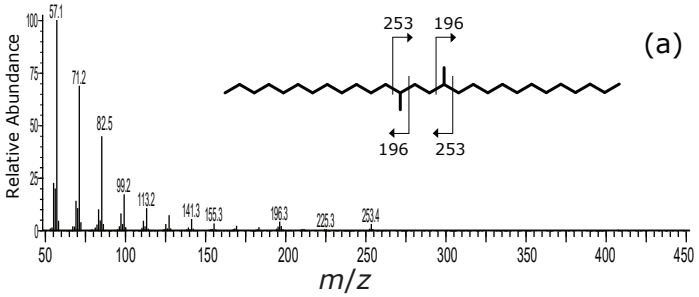


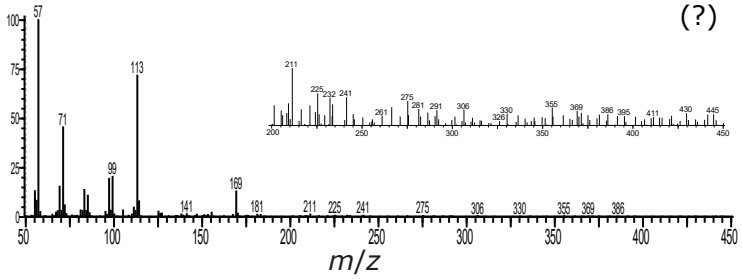
SI Fig. 5

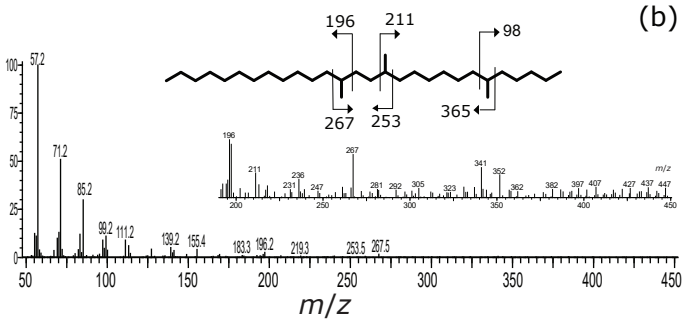
GC/MS chromatogram NTP lacustrine extract HPLC fractions

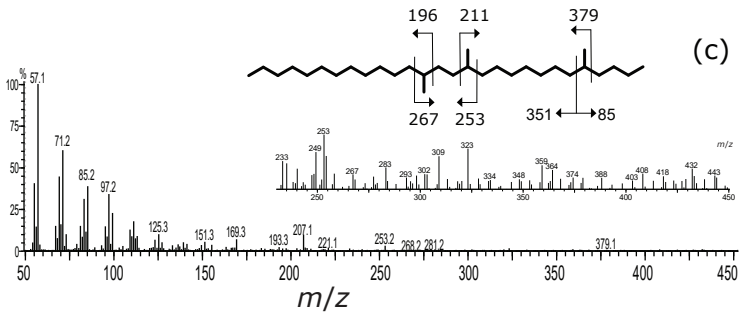


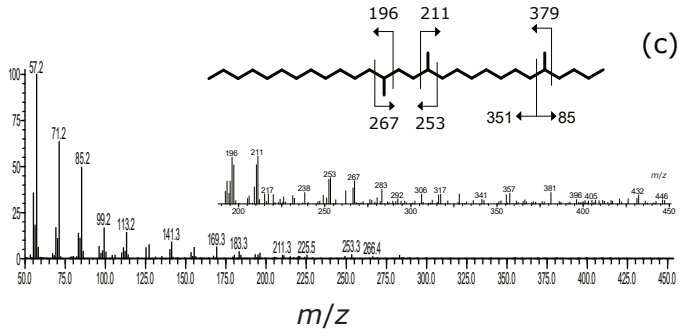
GC/MS spectra NTP lacustrine extract HPLC fractions

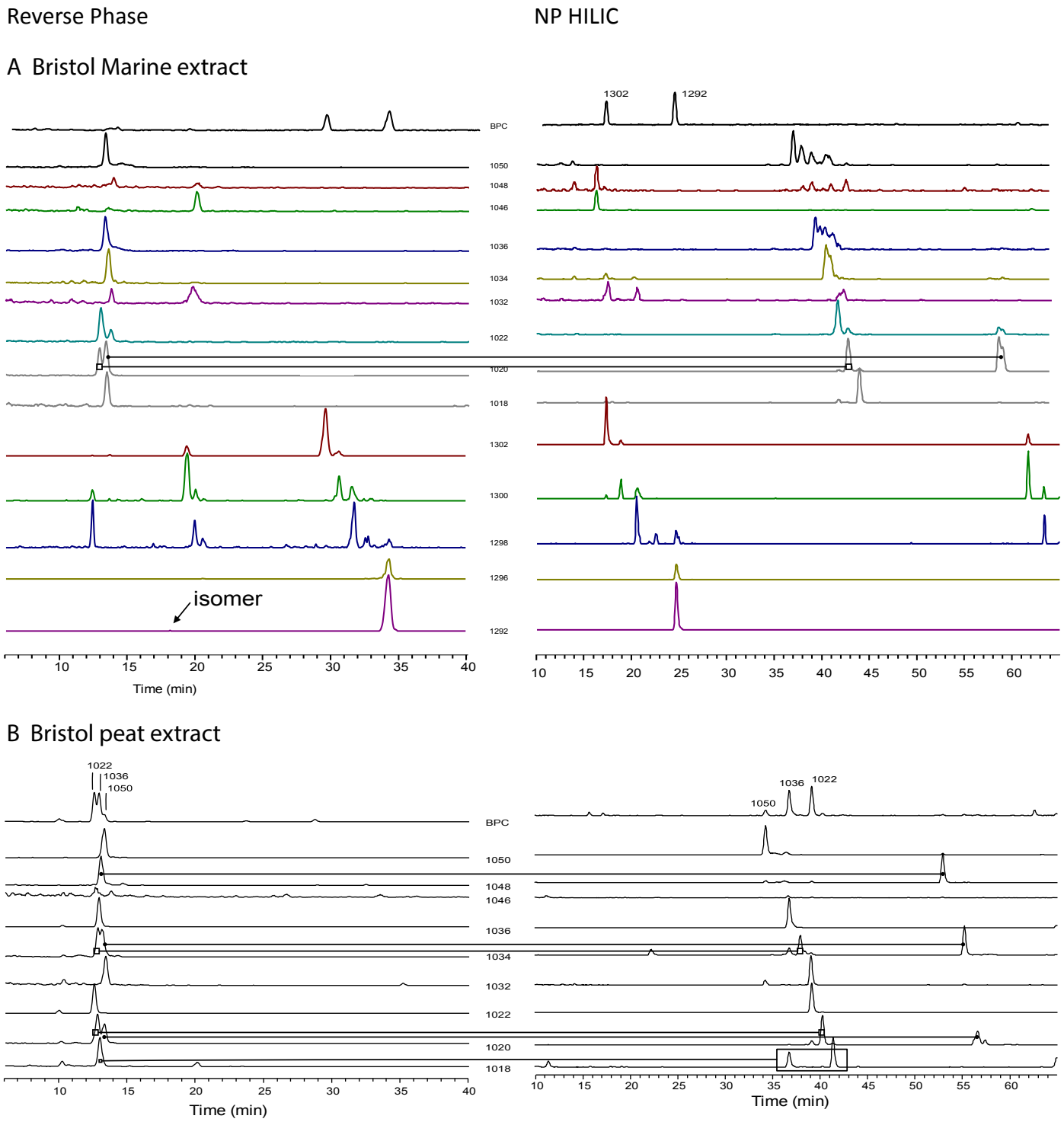






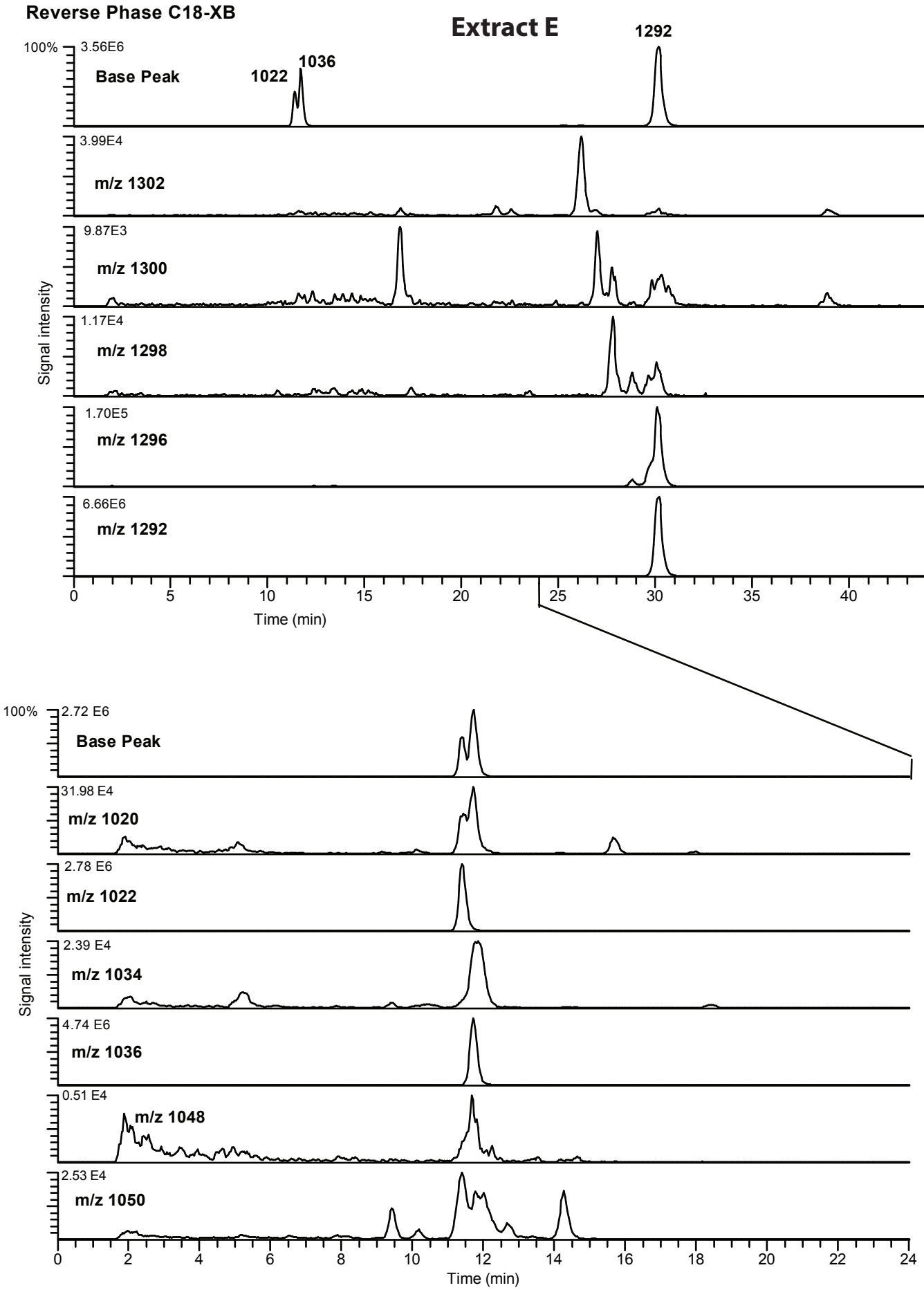






SI Fig. 6. HPLC-MS ion chromatograms for A) the Bristol Marine standard sample and B) the Bristol peat sample run both using NP HILIC (right) and C18-XB RP (left). For the peat sample, the RP method shows near-eluting double peaks for 1020 and 1034. In HILIC, 1034, 1020 but also 1048 show a 'normal' eluting peak but also a late eluting. From these samples it looks like the 5,6- etc isomers separating in the HILIC methods elute in one peak in the RP method, but that some other, later eluting GDGTs in HILIC also come out in RP. For the marine sample, the HILIC method results in separation of many brGDGT isomers between 37-45 min. Surprisingly, these did not show up in the RP method. m/z 1020 has two peaks eluting close to each other in RP, in HILIC there is one late eluting 1020. Isoprenoid GDGTs clearly elute in more than one group with RP. In HILIC, m/z 1300 and 1298 show two very late eluting peaks. In HILIC, the crenarchaeol isomer elutes as usual. In RP, a small peak elutes around 18min which likely is the same isomer.

SI Fig. 7


Reverse Phase C18-XB
Extract E
100%
3.56E6
Base Peak
1022
1036
1292
3.99E4
m/z 1302
9.87E3
m/z 1300
1.17E4
m/z 1298
1.70E5
m/z 1296
6.66E6
m/z 1292
Signal intensity
0
5
10
15
20
25
30
35
40
Time (min)
100%
2.72 E6
Base Peak
31.98 E4
m/z 1020
2.78 E6
m/z 1022
2.39 E4
m/z 1034
4.74 E6
m/z 1036
0.51 E4
m/z 1048
2.53 E4
m/z 1050
Signal intensity
0
2
4
6
8
10
12
14
16
18
20
22
24
Time (min)