NTGS00/1 Analysis Summary

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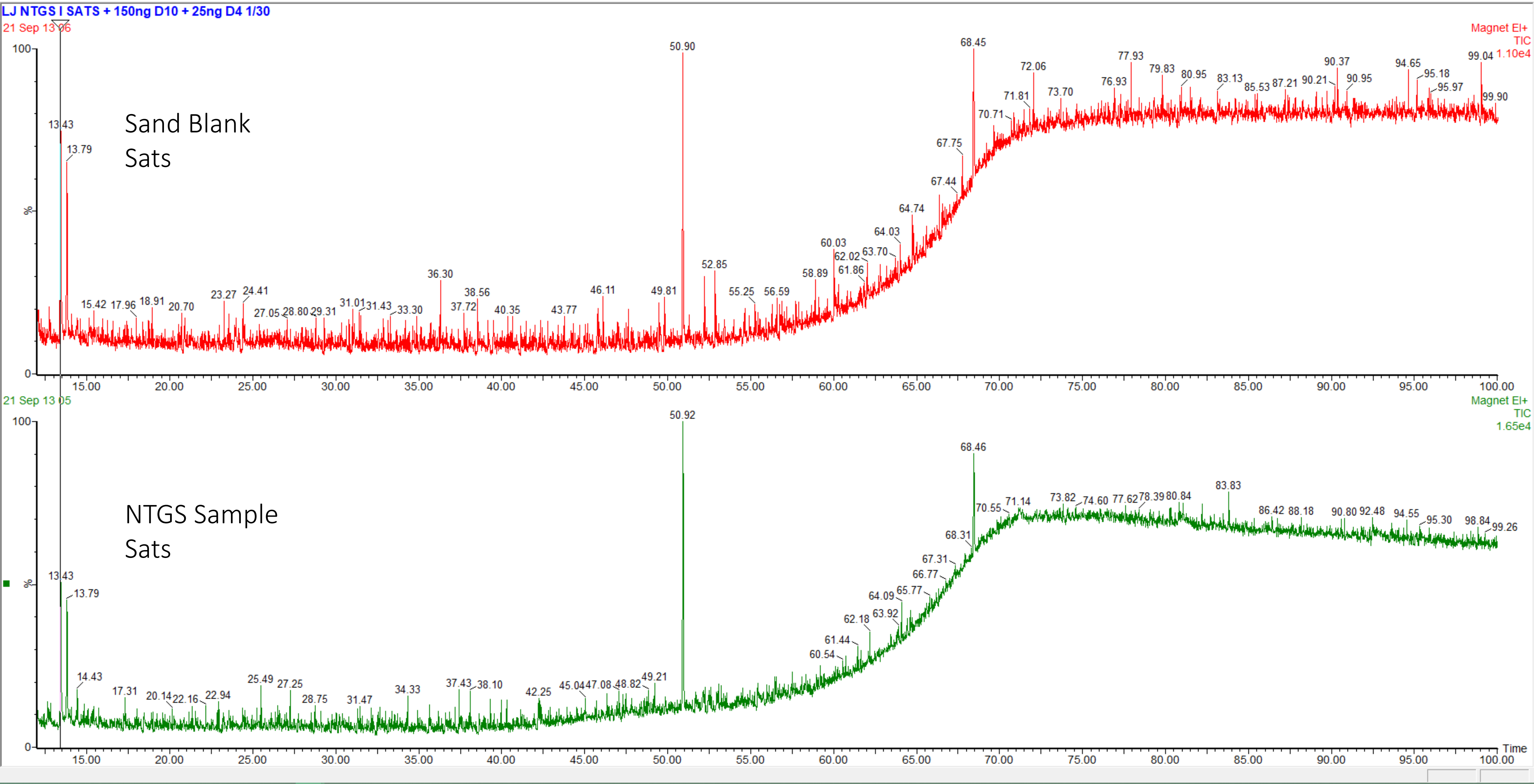
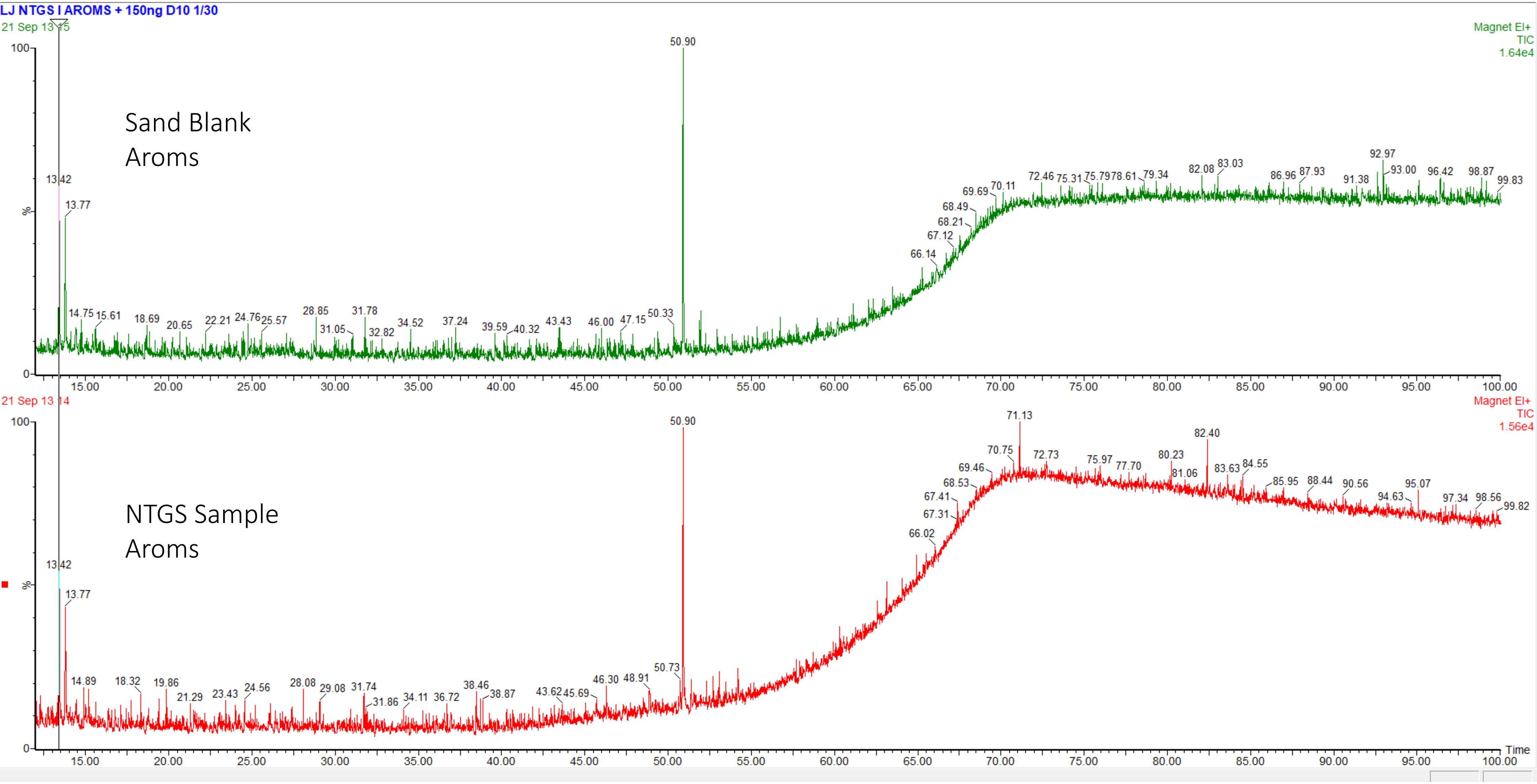
Figure 1

Summary

- This PowerPoint provides a summary of the biomarkers analysed in the ≈ 1.3-1.4 billion year old South Nicholson Basin sample, NTGS00/1 provided by NTGS.
- The majority of the peaks visible in the sample are likely contamination either from the laboratory or the sample itself.
- This is supported by the existence of steranes which only appear in the molecular fossil record later than the age of the sample (Brocks et al. 2017), especially the C29 steranes. Furthermore, analysis of the geological equivalent Velkerri formation in the adjacent McArthur basin contains no detectable steranes (Jarrett et al. 2019).
- Almost all biologically significant peaks have a blank to extract ratio > than 5% indicating that at least some of the contamination is derived from the laboratory.
- Finally, the thermal maturity indicated by phenanthrenes (P) and methylphenanthrenes (MP) indicates that the sample is of mid-maturity. However, the sample looks deformed and metamorphic (Figure 1) and yielded very little bitumen (Figure 2) indicating it is of very high maturity. The thermal maturity indicated by the P and MP molecules are likely a proxy for the thermal exposure of the contaminant.

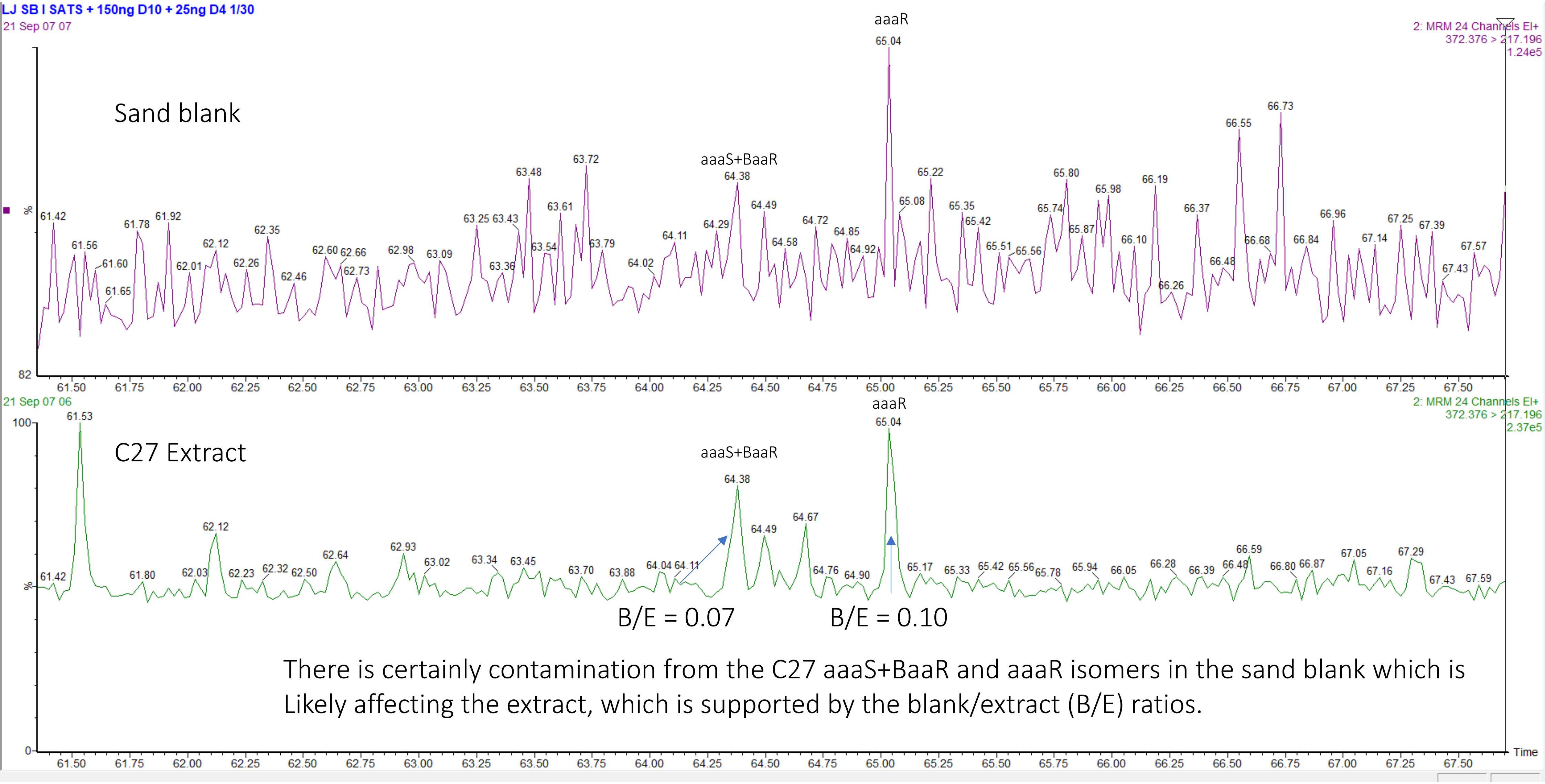
Full Scans

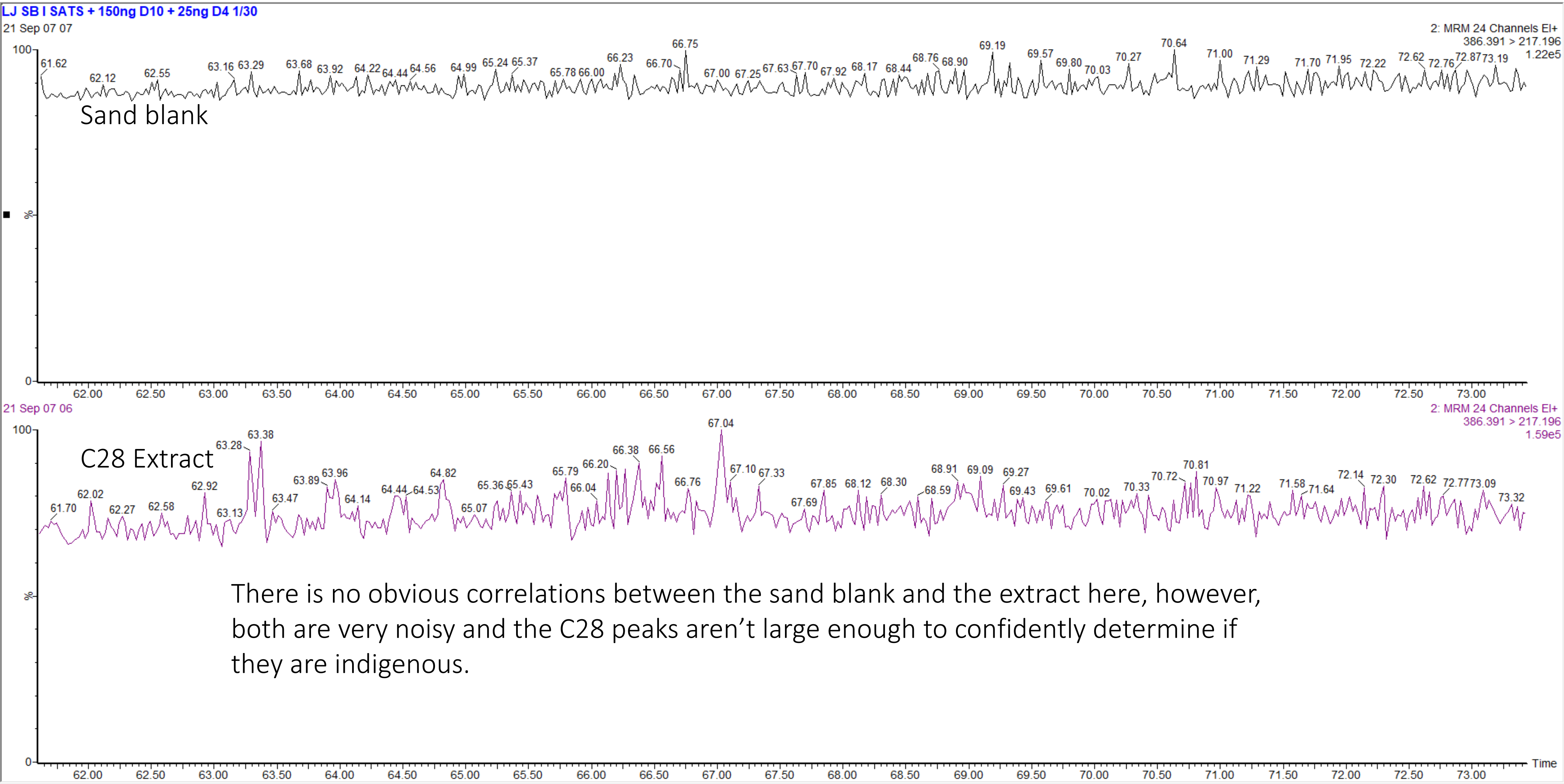

LJ NTGS I SATS + 150ng D10 + 25ng D4 1/30
21 Sep 13 06
Magnet EI+
TIC
1.10e4
Sand Blank
Sats
13.43
13.79
15.42
17.96
18.91
20.70
23.27
24.41
27.05
28.80
29.31
31.01
31.43
33.30
36.30
37.72
38.56
40.35
43.77
46.11
49.81
50.90
52.85
55.25
56.59
58.89
60.03
61.86
62.02
63.70
64.03
64.74
67.44
67.75
68.45
70.71
71.81
72.06
73.70
76.93
77.93
79.83
80.95
83.13
85.53
87.21
90.21
90.37
90.95
94.65
95.18
95.97
99.04
99.90
100
%
0
15.00
20.00
25.00
30.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
70.00
75.00
80.00
85.00
90.00
95.00
100.00
21 Sep 13 05
Magnet EI+
TIC
1.65e4
NTGS Sample
Sats
13.43
13.79
14.43
17.31
20.14
22.16
22.94
25.49
27.25
28.75
31.47
34.33
37.43
38.10
42.25
45.04
47.08
48.82
49.21
50.92
60.54
61.44
62.18
63.92
64.09
65.77
66.77
67.31
68.31
68.46
70.55
71.14
73.82
74.60
77.62
78.39
80.84
83.83
86.42
88.18
90.80
92.48
94.55
95.30
98.84
99.26
100
%
0
15.00
20.00
25.00
30.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
70.00
75.00
80.00
85.00
90.00
95.00
100.00
Time



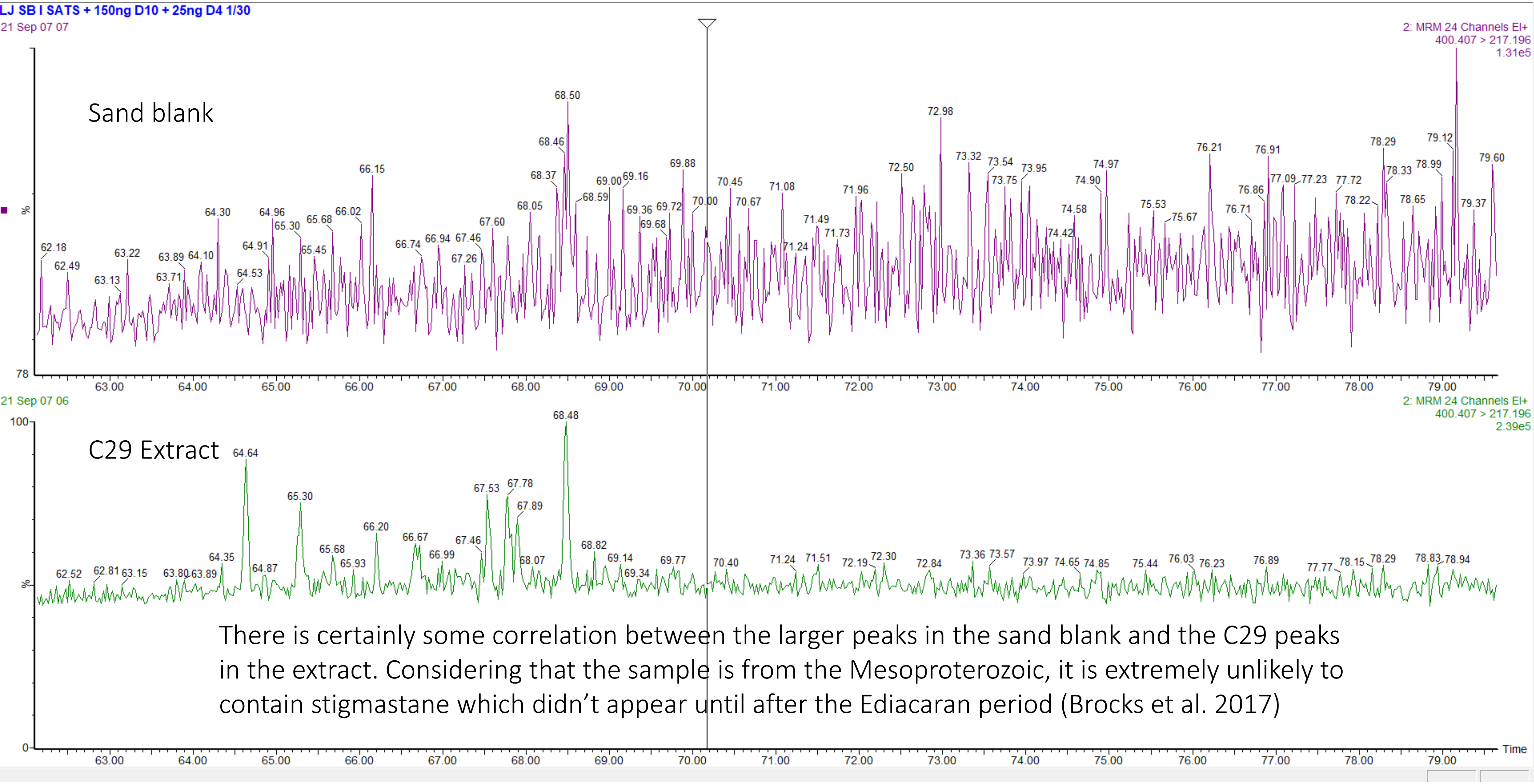
LJ NTGS I AROMS + 150ng D10 1/30
21 Sep 13 15
Magnet EI+
TIC
1.64e4
Sand Blank
Aroms
50.90
13.42
13.77
14.75 15.61
18.69
20.65
22.21 24.76 25.57
28.85
31.05
31.78
32.82
34.52
37.24
39.59 40.32
43.43
46.00 47.15 50.33
66.14
67.12
68.21
68.49
69.69 70.11
72.46 75.31 75.79 78.61 79.34
82.08 83.03
86.96 87.93
91.38
92.97
93.00
96.42
98.87
99.83
100
%
0
21 Sep 13 14
Magnet EI+
TIC
1.56e4
NTGS Sample
Aroms
50.90
13.42
13.77
14.89
18.32
19.86
21.29
23.43
24.56
28.08
29.08
31.74
31.86
34.11 36.72
38.46
38.87
43.62 45.69
46.30 48.91
50.73
66.02
67.31
67.41
68.53
69.46
70.75
71.13
72.73
75.97 77.70
80.23
81.06
82.40
83.63 84.55
85.95 88.44
90.56
94.63
95.07
97.34 98.56
99.82
15.00
20.00
25.00
30.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
70.00
75.00
80.00
85.00
90.00
95.00
100.00
Time

Steranes


LJ SB I SATS + 150ng D10 + 25ng D4 1/30
21 Sep 07 07
2: MRM 24 Channels EI+
372.376 > 217.196
1.24e5
Sand blank
aaaR
65.04
aaaS+BaaR
64.38
21 Sep 07 06
2: MRM 24 Channels EI+
372.376 > 217.196
2.37e5
C27 Extract
aaaR
65.04
aaaS+BaaR
64.38
B/E = 0.07
B/E = 0.10
There is certainly contamination from the C27 aaaS+BaaR and aaaR isomers in the sand blank which is
Likely affecting the extract, which is supported by the blank/extract (B/E) ratios.
Time

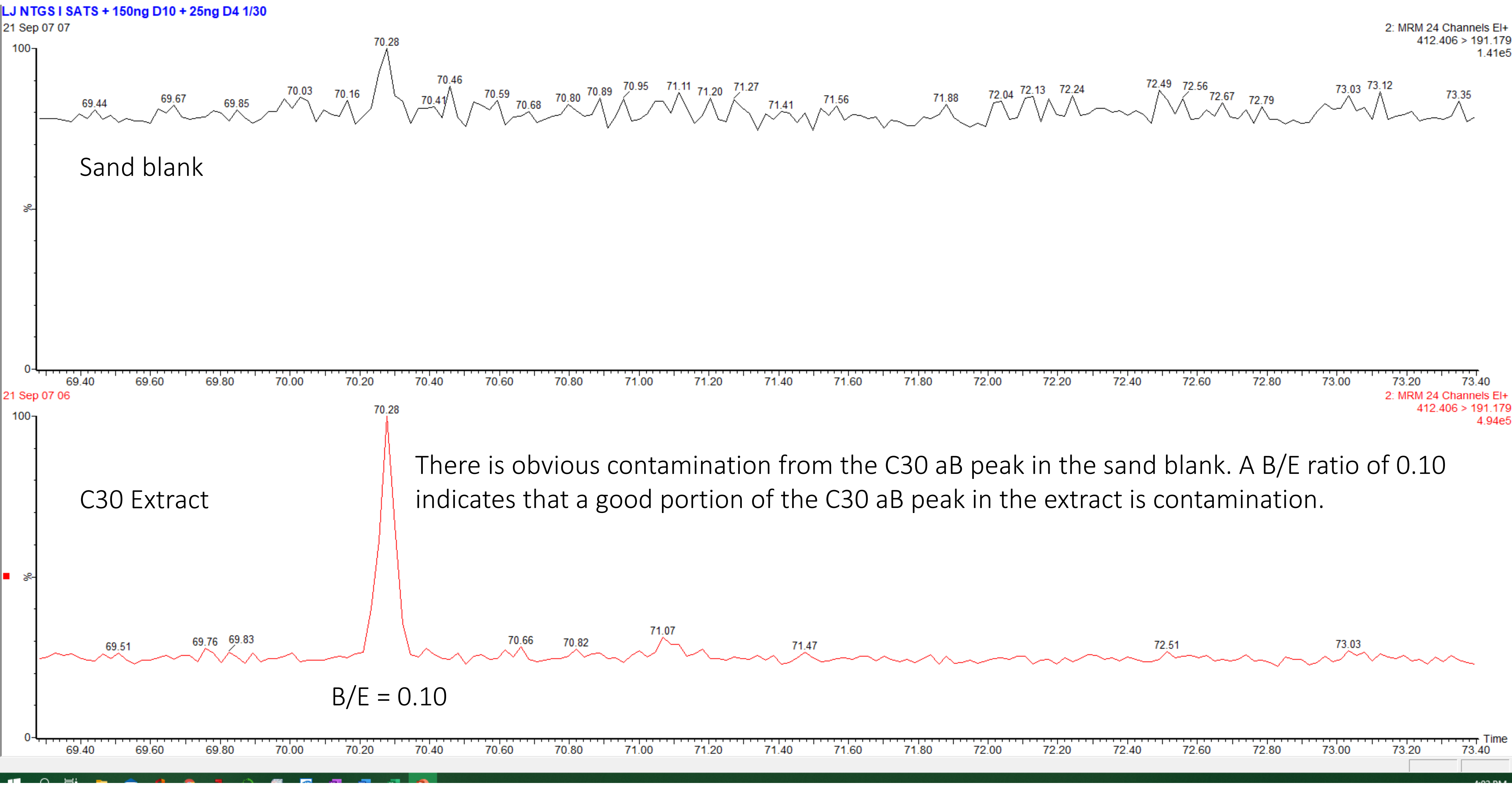


There is no obvious correlations between the sand blank and the extract here, however, both are very noisy and the C28 peaks aren't large enough to confidently determine if they are indigenous.

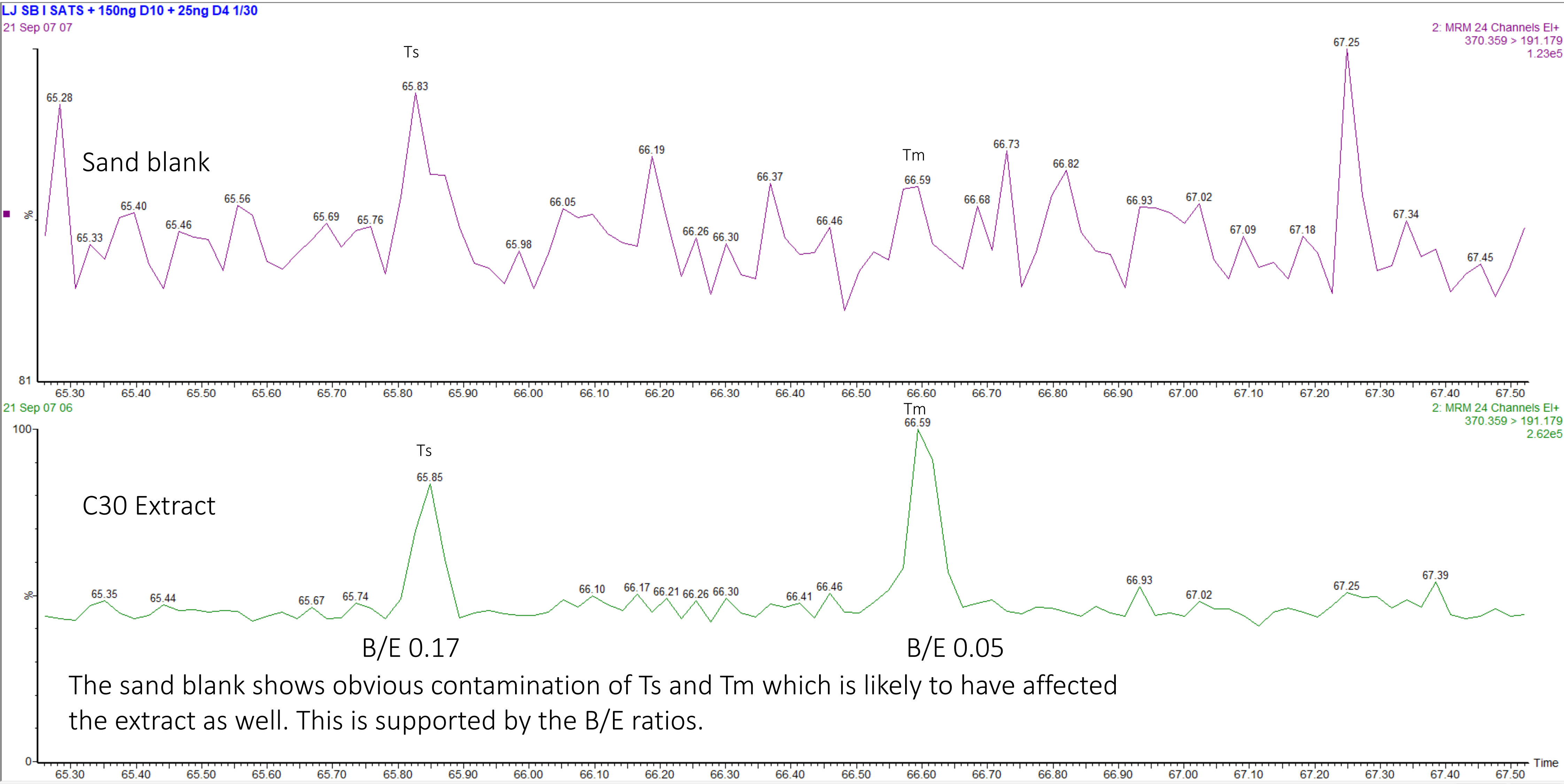


There is certainly some correlation between the larger peaks in the sand blank and the C29 peaks in the extract. Considering that the sample is from the Mesoproterozoic, it is extremely unlikely to contain stigmastane which didn't appear until after the Ediacaran period (Brocks et al. 2017)

Hopanes

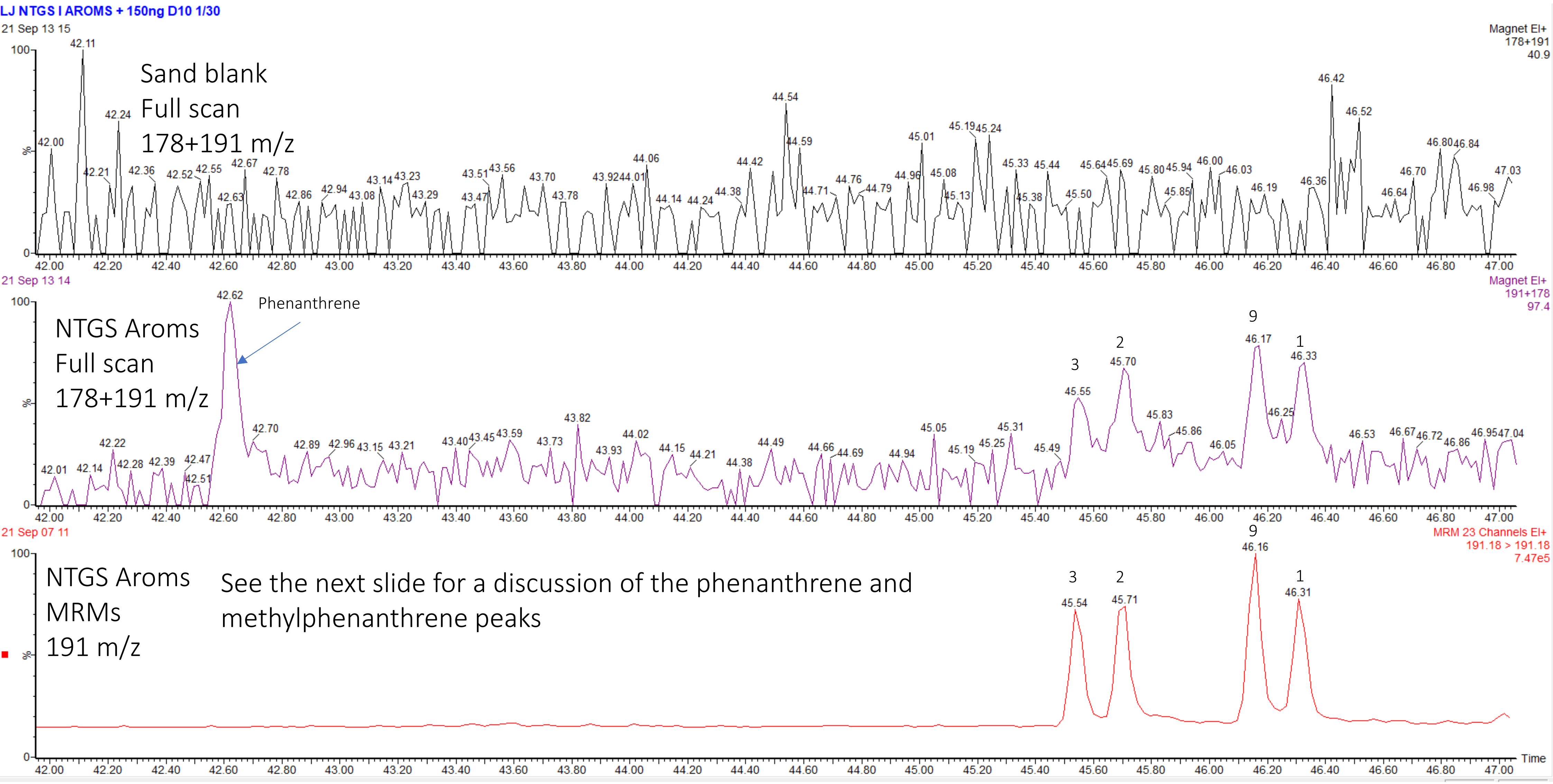


There is obvious contamination from the C30 aB peak in the sand blank. A B/E ratio of 0.10 indicates that a good portion of the C30 aB peak in the extract is contamination.



The sand blank shows obvious contamination of Ts and Tm which is likely to have affected the extract as well. This is supported by the B/E ratios.

Thermal maturity


LJ NTGS I AROMS + 150ng D10 1/30
21 Sep 13 15
Magnet EI+
178+191
40.9
Sand blank
Full scan
178+191 m/z
21 Sep 13 14
Magnet EI+
191+178
97.4
42.62
Phenanthrene
NTGS Aroms
Full scan
178+191 m/z
3
45.55
2
45.70
9
46.17
1
46.33
21 Sep 07 11
MRM 23 Channels EI+
191.18 > 191.18
7.47e5
NTGS Aroms
MRMs
191 m/z
See the next slide for a discussion of the phenanthrene and methylphenanthrene peaks
3
45.54
2
45.71
9
46.16
1
46.31
Time

9, 1-methylphenanthrenes are less thermally stable compared to 3, 2-methylphenanthrenes which means that they will decrease as a function of thermal exposure. The pattern of methylphenanthrenes here indicates mid-maturity since all four isomers are a similar height. This is further supported by the phenanthrene parent peak. As the methylphenanthrenes are exposed to heat, the methyl bond eventually breaks and the molecule converts to the phenanthrene parent peak. Since the parent peak is not exceptionally higher than the methylphenanthrene peaks, it indicates mid-maturity. This is likely the maturity measurement of some contaminant since the sample looked fairly deformed and metamorphic (See figure 1) and the extracted material was colourless indicating that it yielded very little bitumen (See figure 2). Based on these observations, we expected much higher thermal maturity the what is measured.

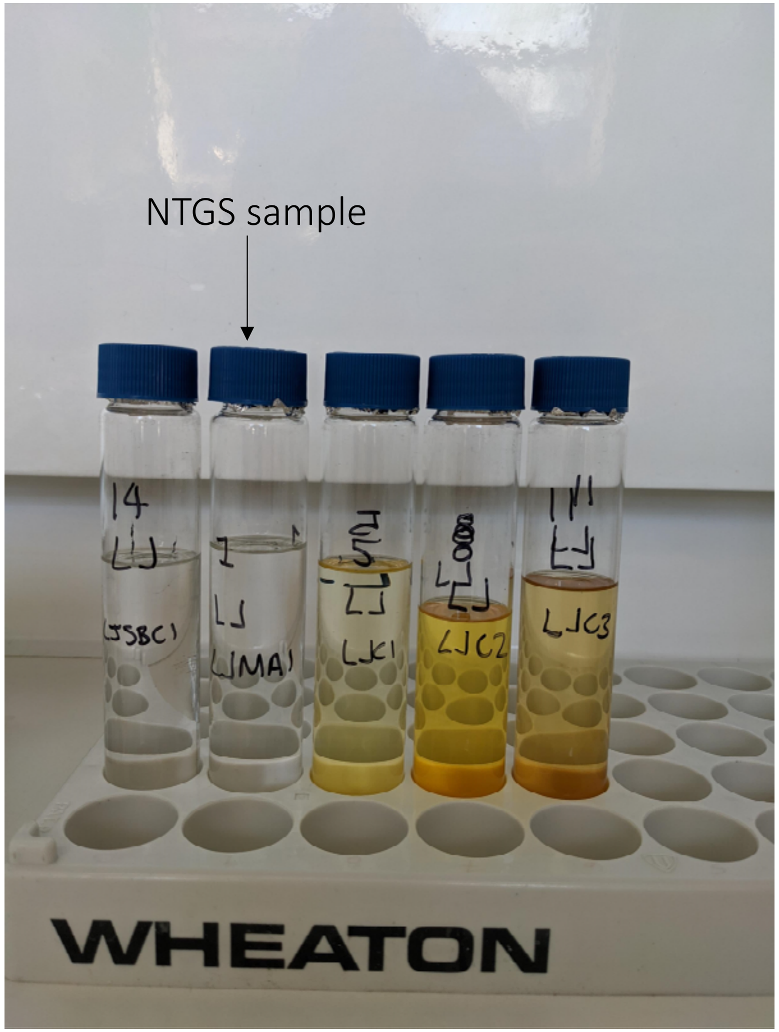


Figure 2

References

Brocks, J.J., Jarrett, A.J.M., Sirantoine, E., Hallmann, C., Hoshino, Y., Liyanage, T., 2017. The rise of algae in Cryogenian oceans and the emergence of animals. Nature 548, 578–581. https://doi.org/10.1038/nature23457

Jarrett, A.J.M., Cox, G.M., Brocks, J.J., Grosjean, E., Boreham, C.J., Edwards, D.S., 2019. Microbial assemblage and palaeoenvironmental reconstruction of the 1.38 Ga Velkerri Formation, McArthur Basin, northern Australia. Geobiology 17, 360–380. https://doi.org/10.1111/gbi.12331