Supplementary Material

Synthesis of reference organosulfates and optimization of UPLC-ESI-MS/MS method for their quantification in environmental samples: Its application for determination of organosulfates in $PM_{2.5}$

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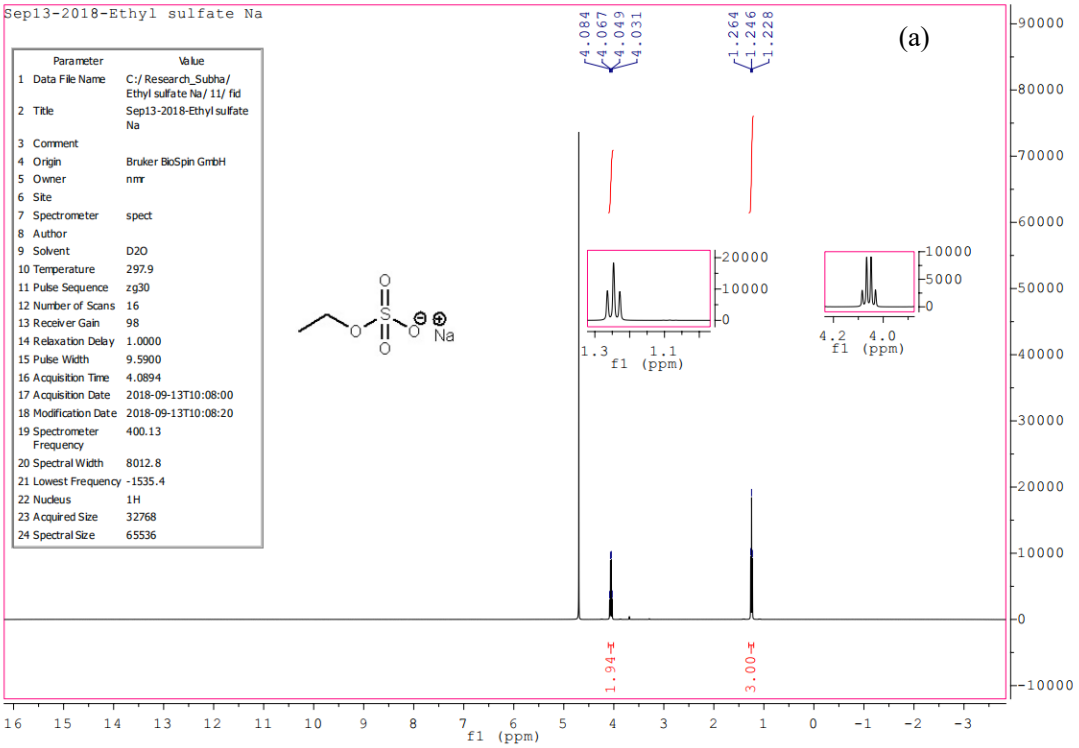

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5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	D2O
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	98
14 Relaxation Delay	1.0000
15 Pulse Width	9.5900
16 Acquisition Time	4.0894
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18 Modification Date	2018-09-13T10:08:20
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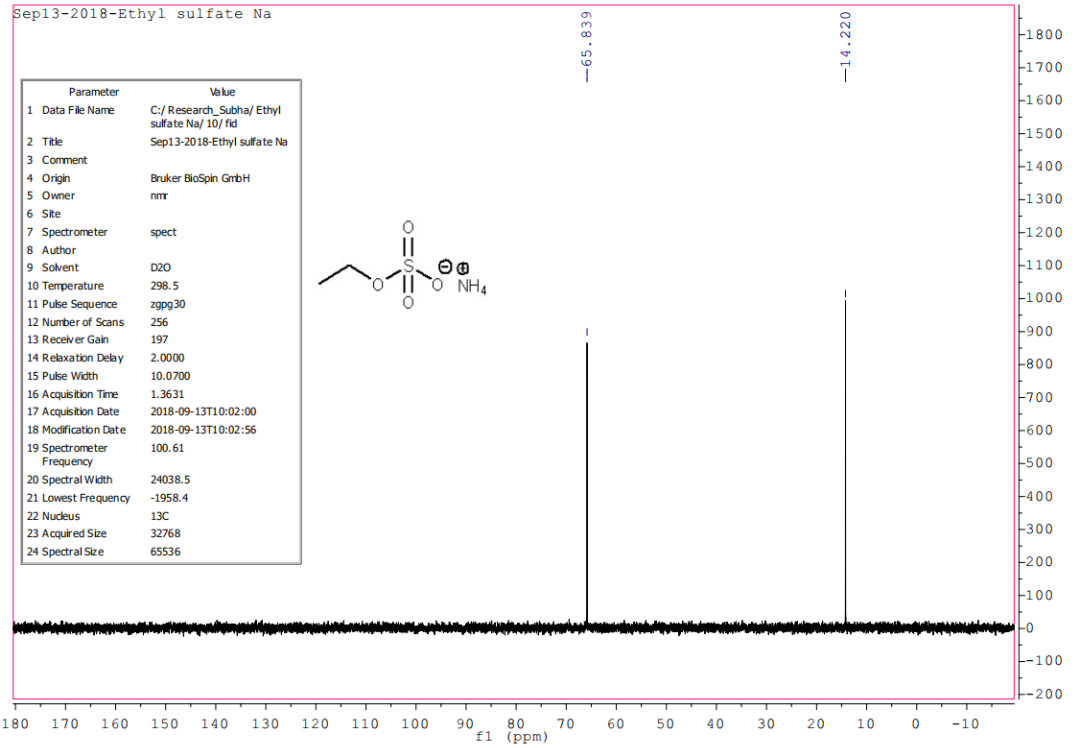
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



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6 Site	
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13 Receiver Gain	197
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15 Pulse Width	10.0700
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18 Modification Date	2018-09-13T10:02:56
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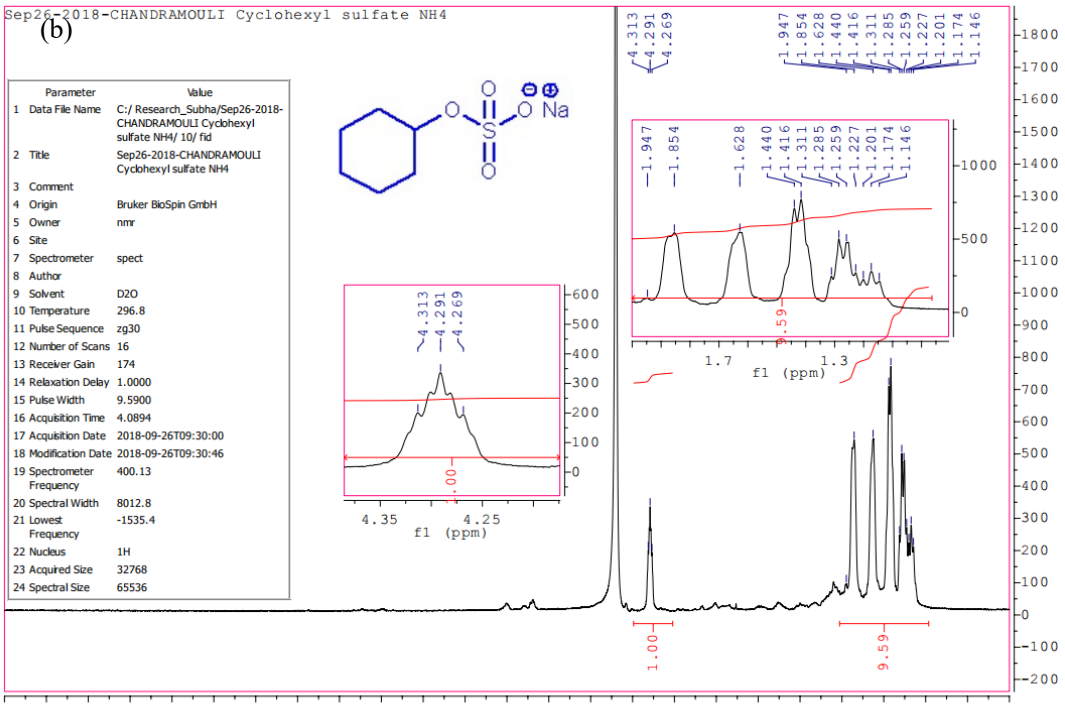
21 Lowest Frequency	-1958.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

(b)



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5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	D2O
10	Temperature	296.8
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	174
14	Relaxation Delay	1.0000
15	Pulse Width	9.5900
16	Acquisition Time	4.0894
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22	Nucleus	1H
23	Acquired Size	32768
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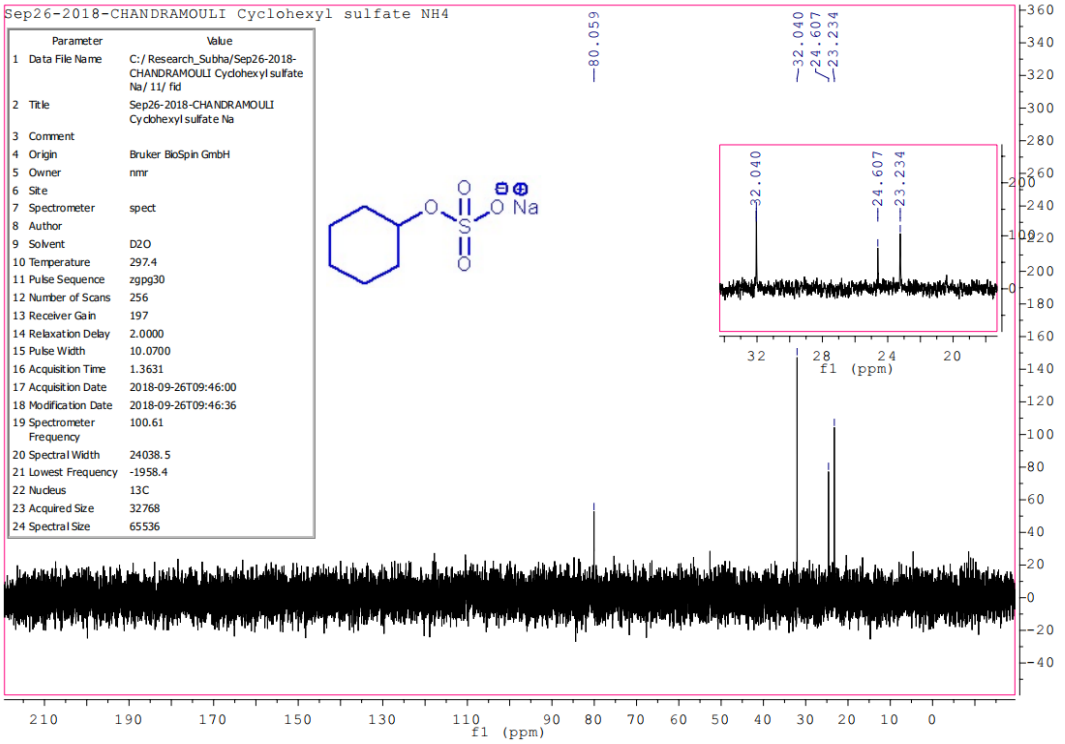

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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	D2O
10	Temperature	297.4
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	197
14	Relaxation Delay	2.0000
15	Pulse Width	10.0700
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19	Spectrometer Frequency	100.61
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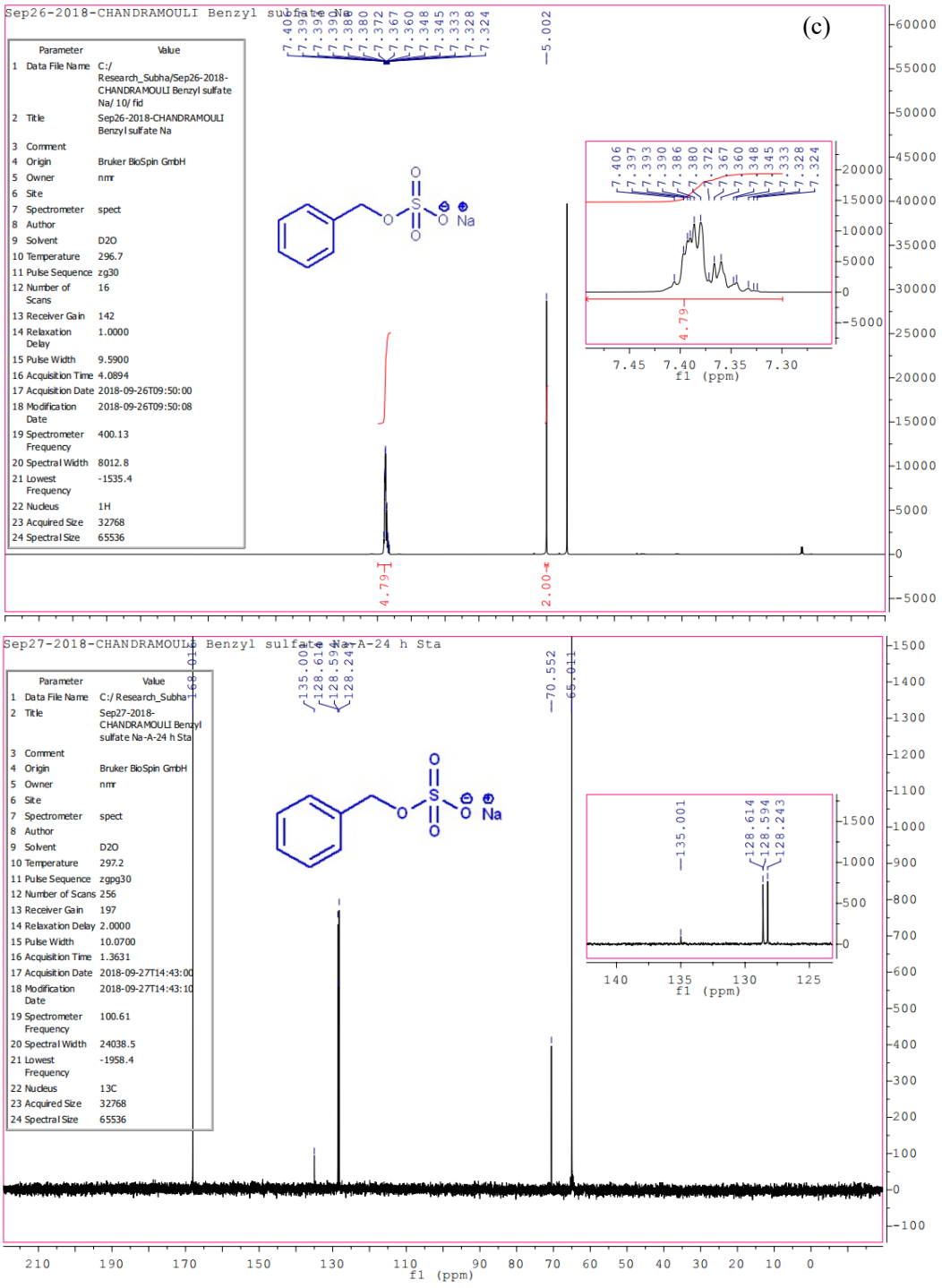
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536


(c)
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3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent D2O
10 Temperature 296.7
11 Pulse Sequence zg30
12 Number of Scans 16
13 Receiver Gain 142
14 Relaxation Delay 1.0000
15 Pulse Width 9.5900
16 Acquisition Time 4.0894
17 Acquisition Date 2018-09-26T09:50:00
18 Modification Date 2018-09-26T09:50:08
19 Spectrometer Frequency 400.13
20 Spectral Width 8012.8
21 Lowest Frequency -1535.4
22 Nucleus 1H
23 Acquired Size 32768
24 Spectral Size 65536
7.406 7.397 7.393 7.390 7.386 7.380 7.372 7.367 7.360 7.348 7.345 7.333 7.328 7.324
5.002
4.79
2.00
O S O Na
f1 (ppm)
Sep27-2018-CHANDRAMOULI Benzyl sulfate Na-A-24 h Sta
Parameter Value
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3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent D2O
10 Temperature 297.2
11 Pulse Sequence zgpg30
12 Number of Scans 256
13 Receiver Gain 197
14 Relaxation Delay 2.0000
15 Pulse Width 10.0700
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21 Lowest Frequency -1958.4
22 Nucleus 13C
23 Acquired Size 32768
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128.243
70.552
68.011
O S O Na
f1 (ppm)

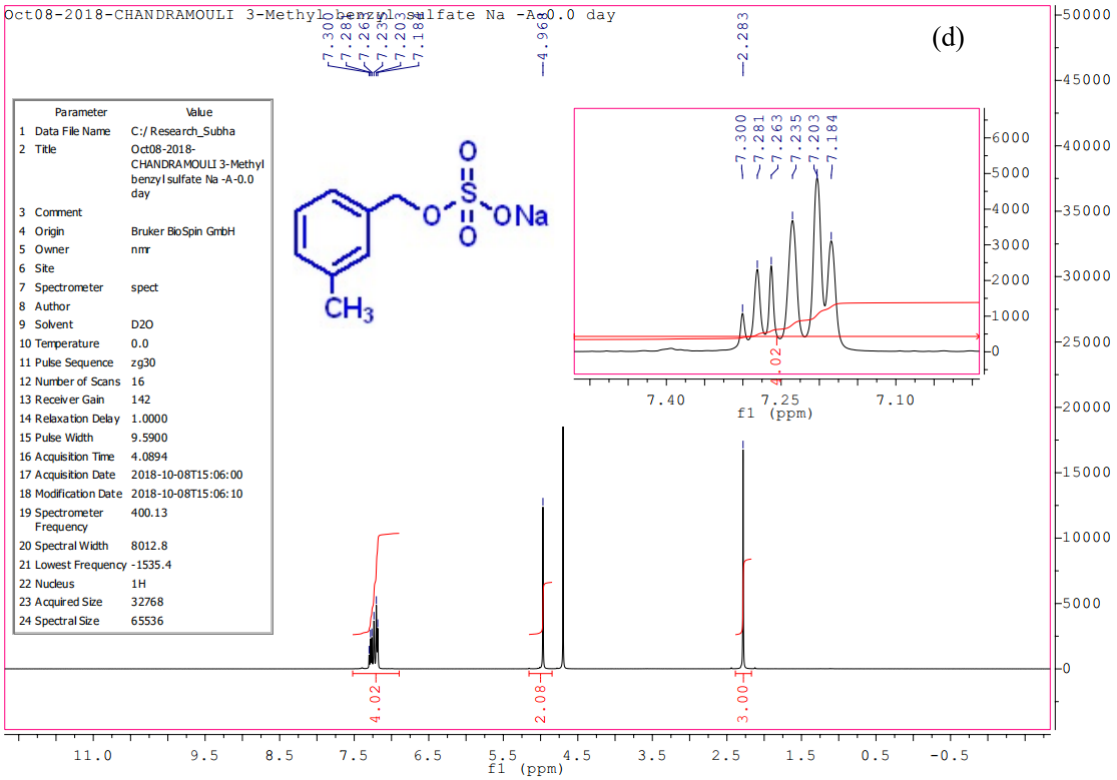

Figure. S1 HNMR (400 MHz, D_2O) and CNMR (100 MHz, D_2O) spectra for sodium or ammonium salts of ethyl (a), benzyl (b), cyclohexyl (c), and 3-methylbenzyl (d).