**Supporting Information**

# Structure Property Relationships of *N*-Acylsulfonamides and Related Bioisosteres

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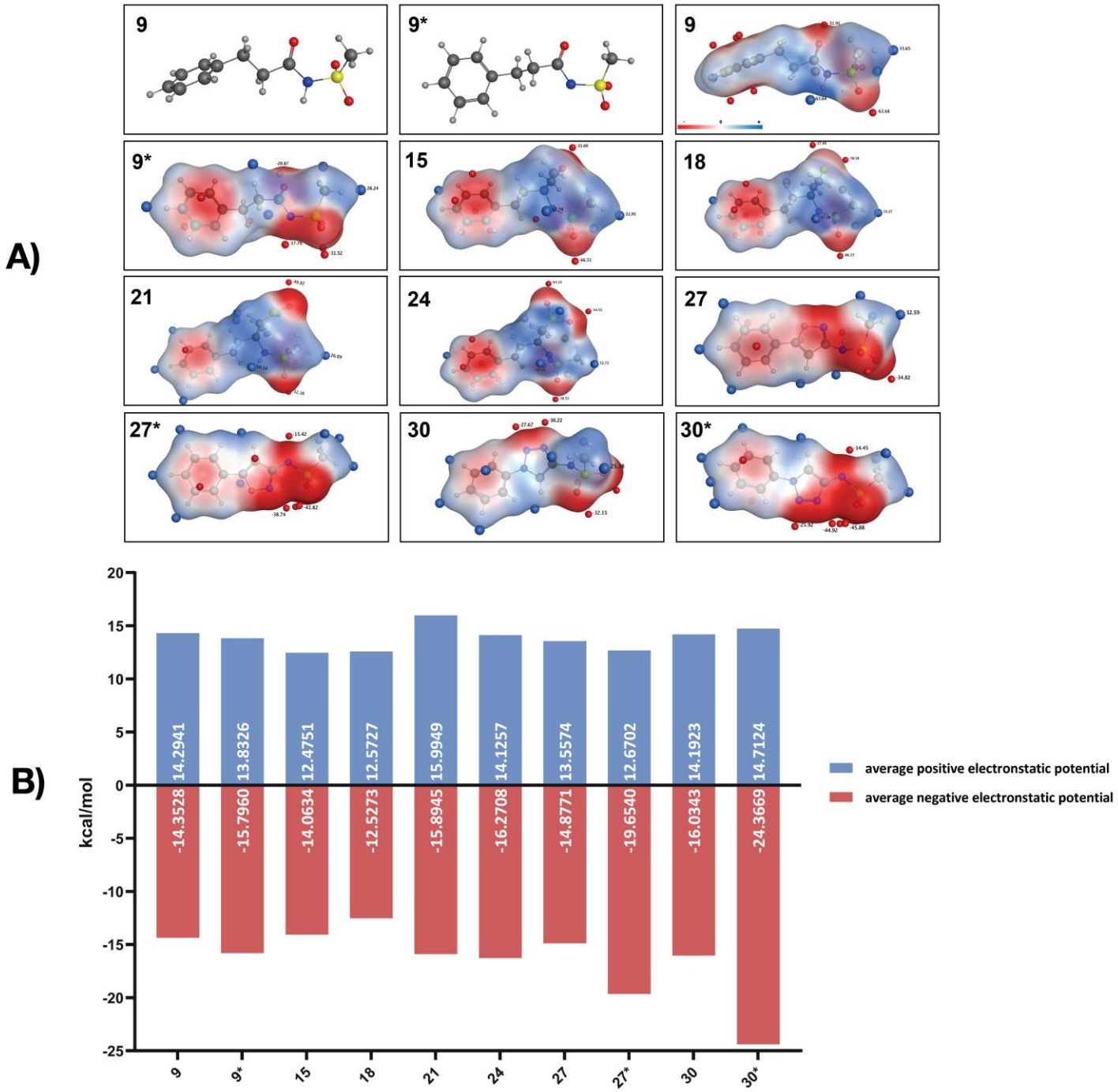



**Figure S1.** (*A*) comparison of Gaussian-optimized geometry and electrostatic potential maps of *N*-acylsulfonamide **9** and its derivatives **15**, **18**, **21**, **24**, **27** and **30**. Compounds that based on p$K_a$ determinations are expected to be mostly charged at physiological pH are shown both in their neutral (*i.e.*, **9**, **27** and **30**) and deprotonated (*i.e.*, **9***, **27*** and **30***) forms. (*B*) Average electrostatic potential values of the gaussian-optimized structure showing positive and negative average ESP values of each compound.

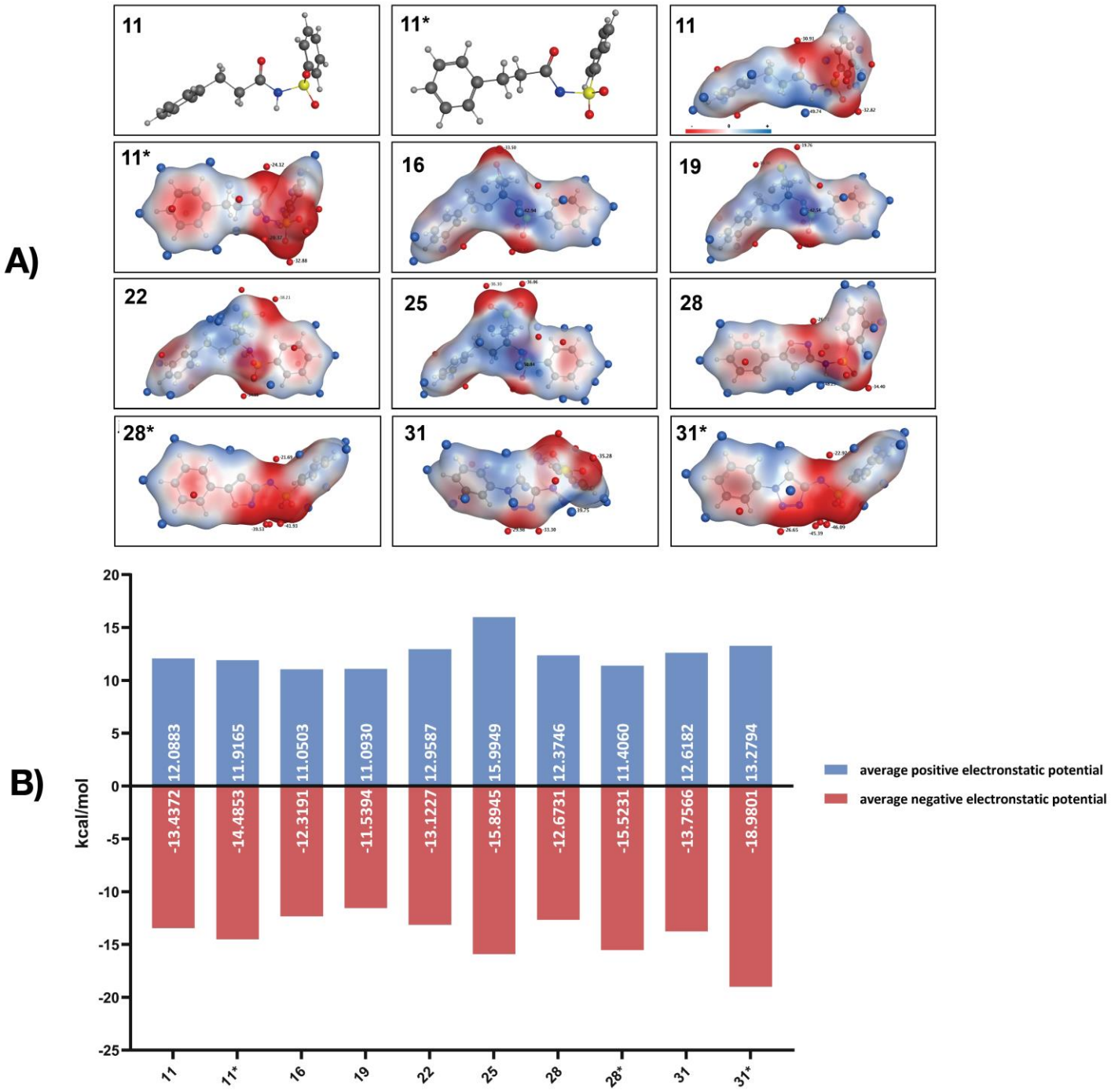



**Figure S2**. (*A*) comparison of Gaussian-optimized geometry and electrostatic potential maps of *N*-acylsulfonamide **11** and its derivatives **16**, **19**, **22**, **25**, **28** and **31**. Compounds that based on p$K_a$ determinations are expected to be mostly charged at physiological pH are shown both in their neutral (*i.e.*, **11**, **28** and **31**) and deprotonated (*i.e.*, **11***, **28*** and **31***) forms. (*B*) Average electrostatic potential values of the gaussian-optimized structure showing positive and negative average ESP values of each compound.

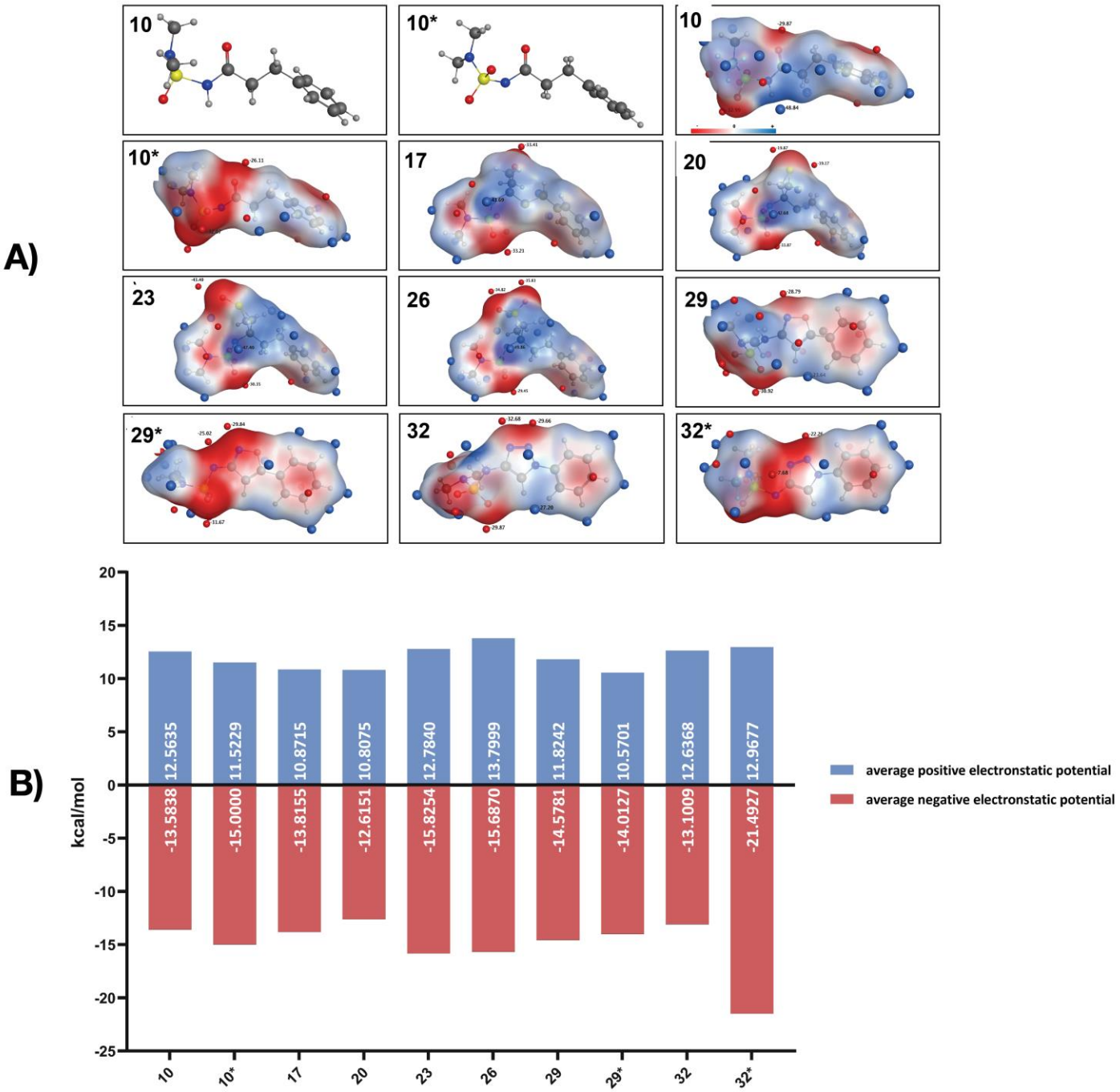
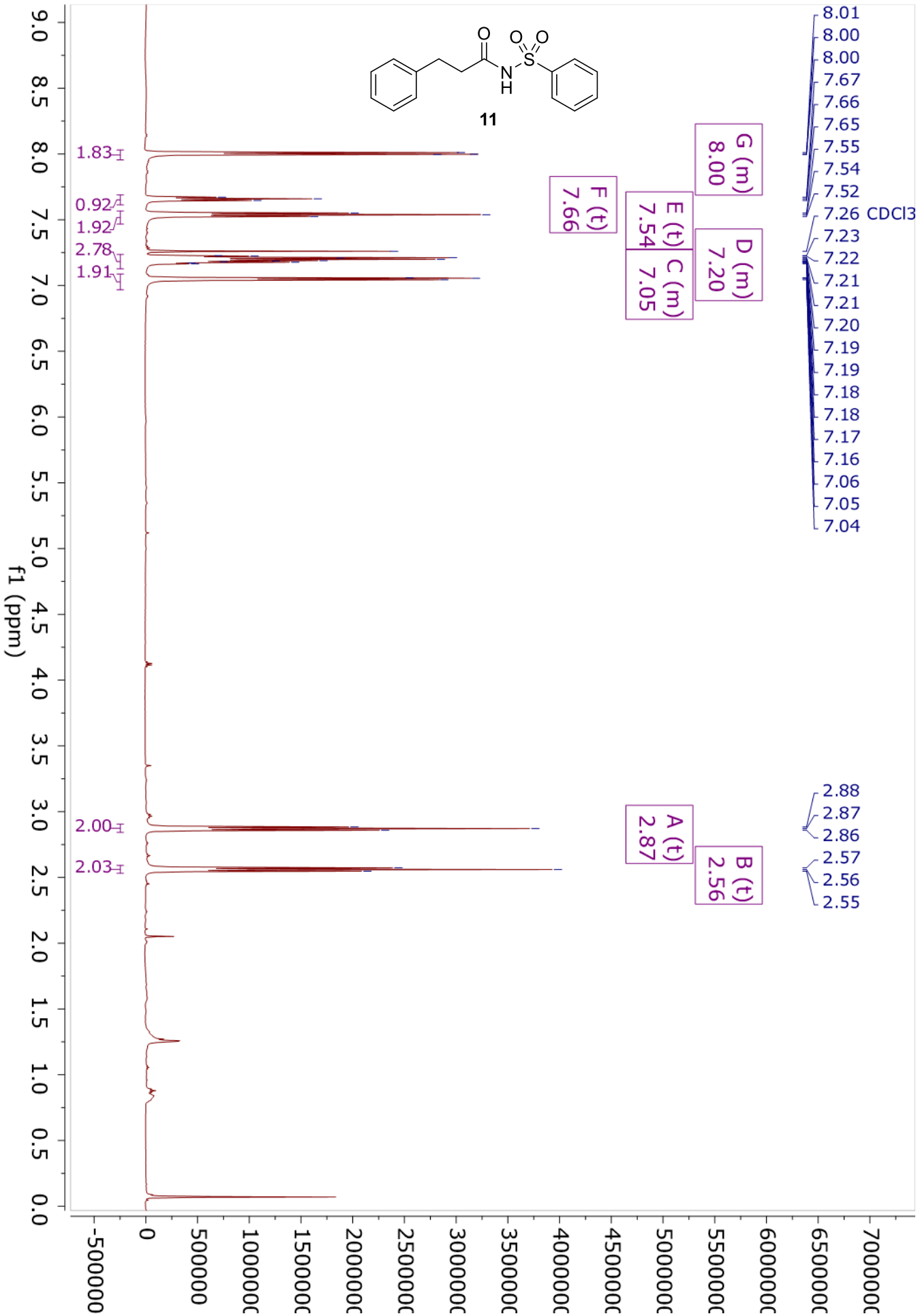
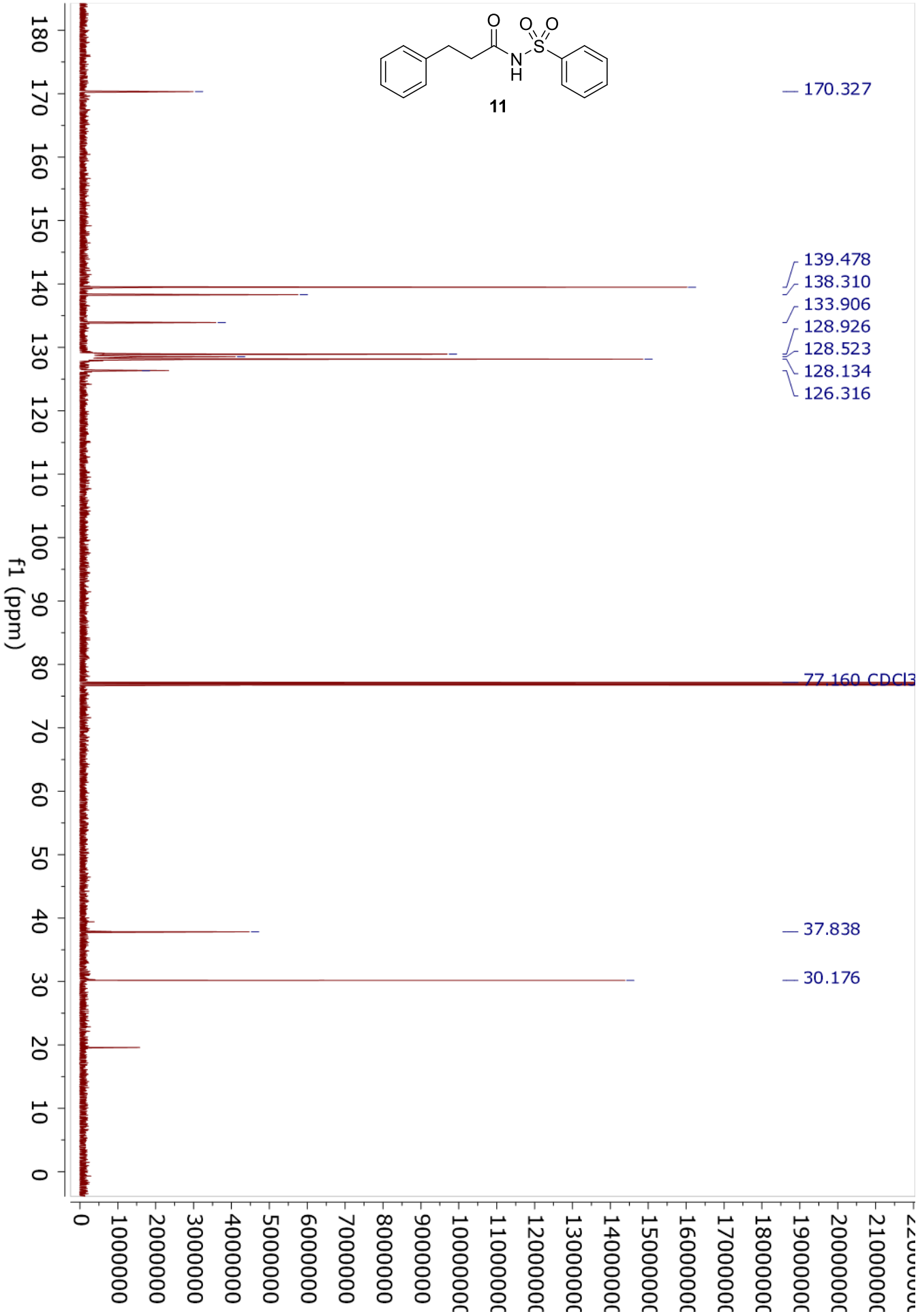
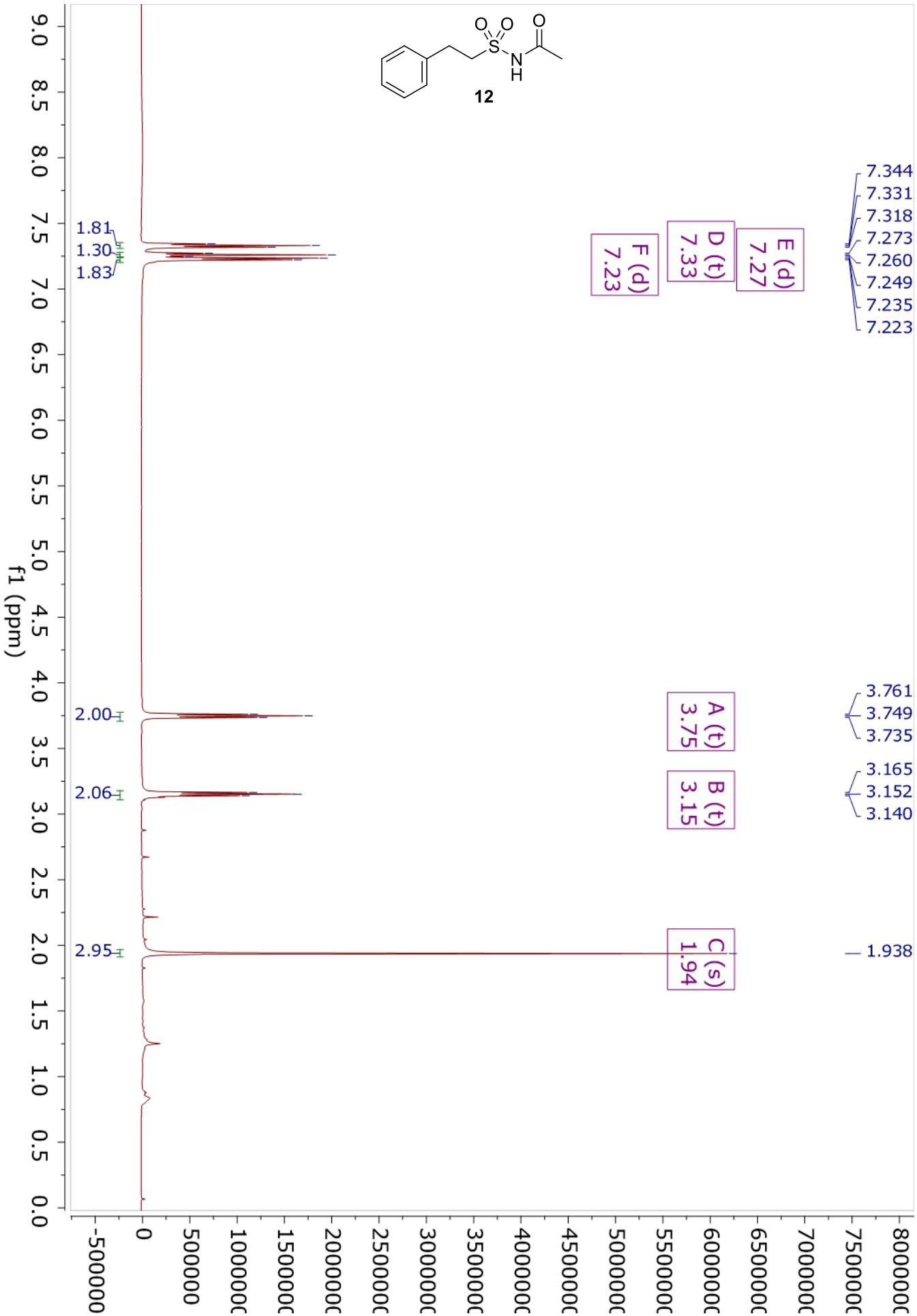
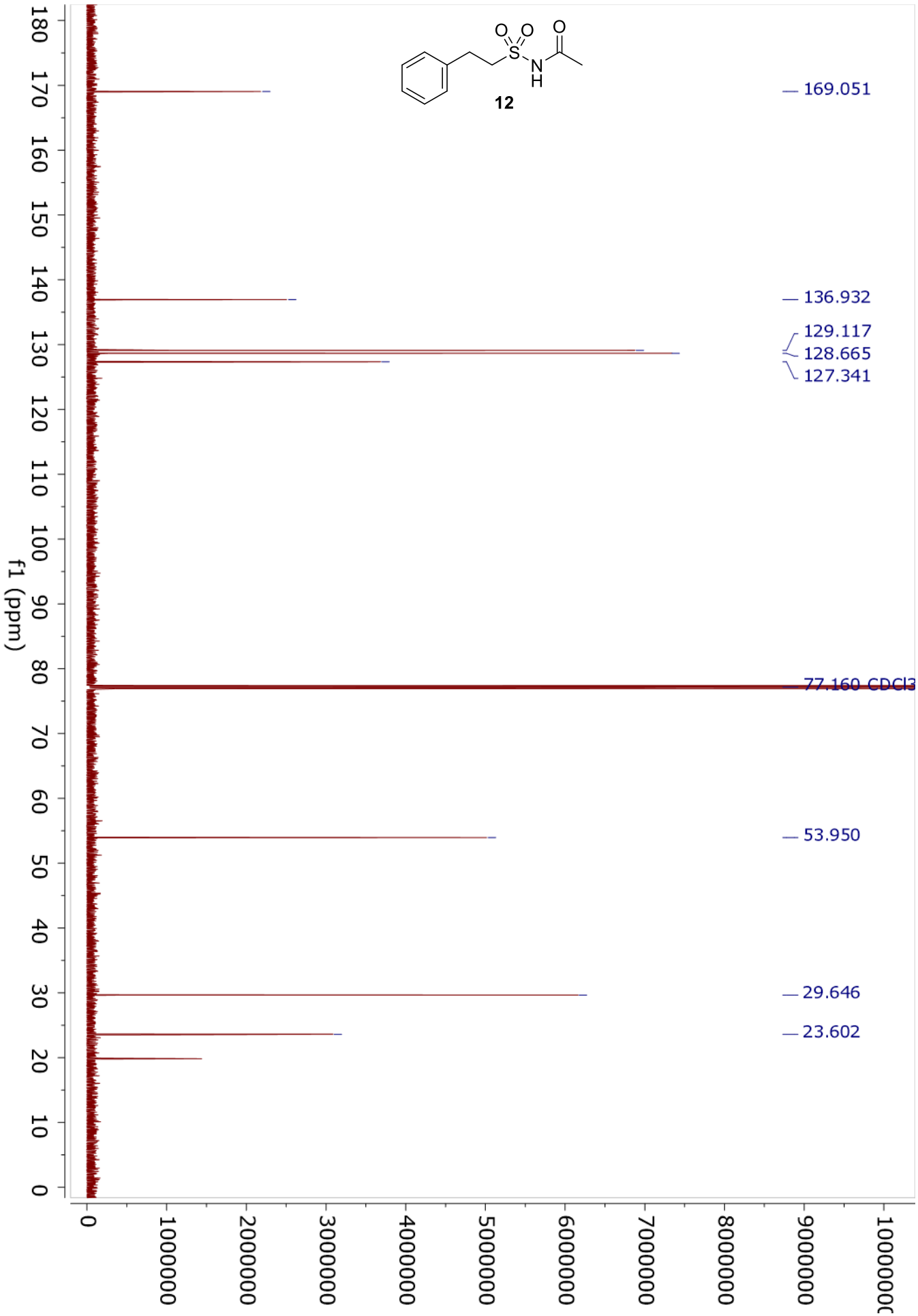



**Figure S3**. (*A*) comparison of Gaussian-optimized geometry and electrostatic potential maps of *N*-acylsulfonamide **10** and its derivatives **17**, **20**, **23**, **26**, **29** and **32**. Compounds that based on p$K_a$ determinations are expected to be mostly charged at physiological pH are shown both in their neutral (*i.e.*, **10**, **29** and **32**) and deprotonated (*i.e.*, **10***, **29*** and **32***) forms. (*B*) Average electrostatic potential values of the gaussian-optimized structure showing positive and negative average ESP values of each compound.


11
1.83
0.92
1.92
2.78
1.91
2.00
2.03
G (m) 8.00
F (t) 7.66
E (t) 7.54
C (m) 7.05
D (m) 7.20
A (t) 2.87
B (t) 2.56
8.01
8.00
8.00
7.67
7.66
7.65
7.55
7.54
7.52
7.26 CDCl3
7.23
7.22
7.21
7.21
7.20
7.19
7.19
7.18
7.18
7.17
7.16
7.06
7.05
7.04
2.88
2.87
2.86
2.57
2.56
2.55
f1 (ppm)


11
170.327
139.478
138.310
133.906
128.926
128.523
128.134
126.316
77.160 CDCl3
37.838
30.176
f1 (ppm)


12
f1 (ppm)
1.81
1.30
1.83
2.00
2.06
2.95
F (d) 7.23
D (t) 7.33
E (d) 7.27
A (t) 3.75
B (t) 3.15
C (s) 1.94
7.344
7.331
7.318
7.273
7.260
7.249
7.235
7.223
3.761
3.749
3.735
3.165
3.152
3.140
1.938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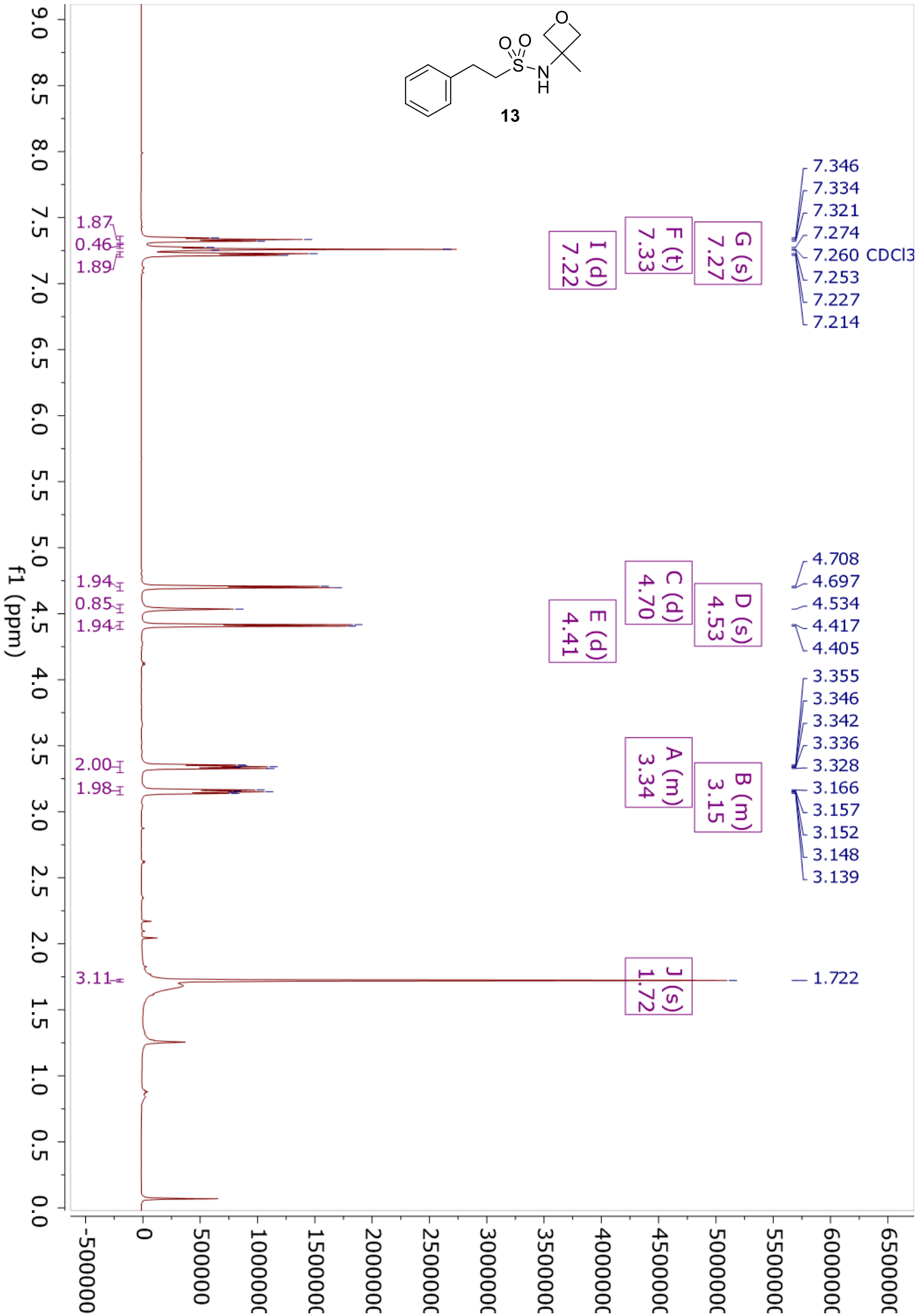
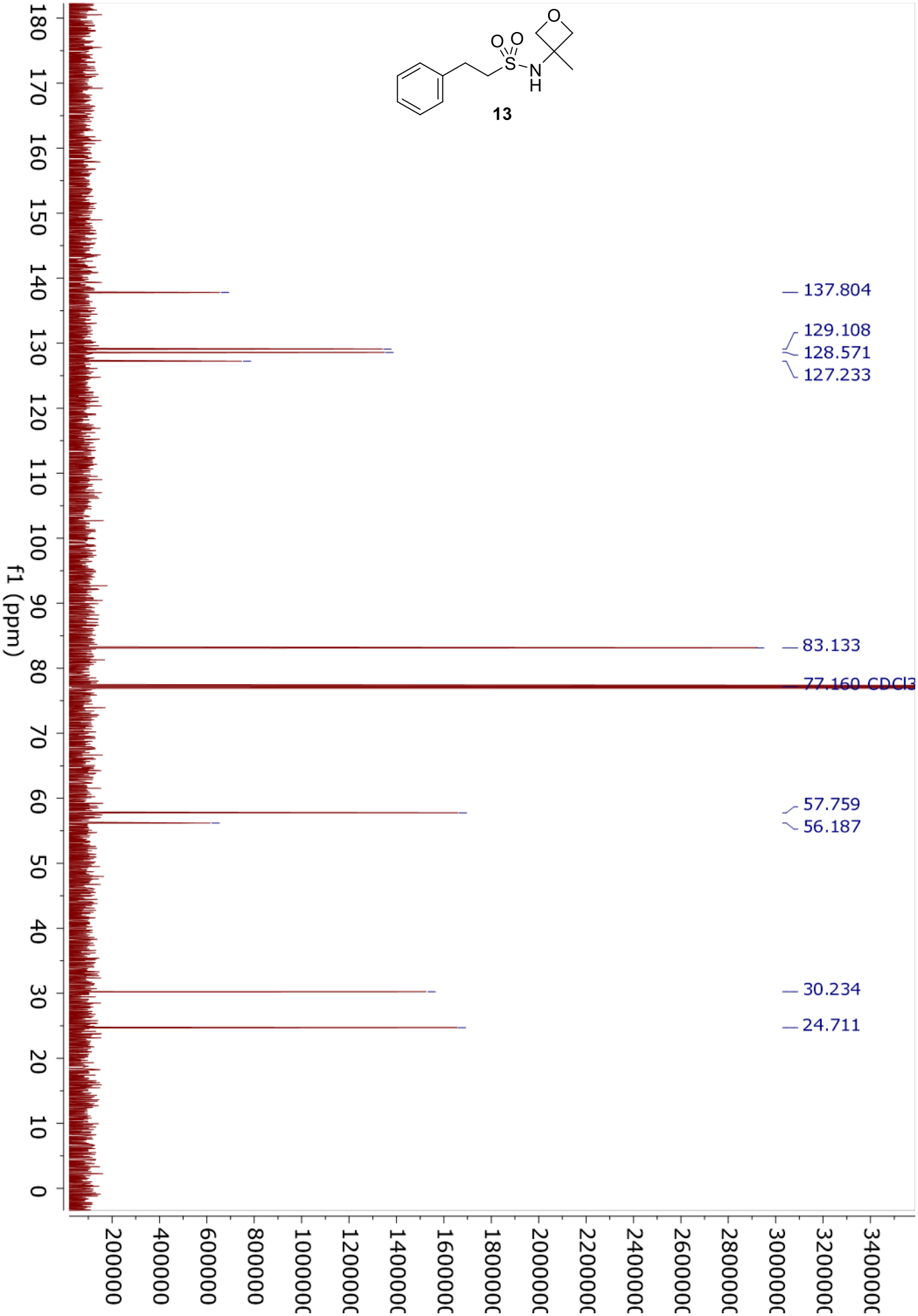
169.051
136.932
129.117
128.665
127.341
77.160 CDCl3
53.950
29.646
23.602
f1 (ppm)


13
f1 (ppm)
1.87
0.46
1.89
1.94
0.85
1.94
2.00
1.98
3.11
I (d) 7.22
F (t) 7.33
G (s) 7.27
C (d) 4.70
E (d) 4.41
D (s) 4.53
A (m) 3.34
B (m) 3.15
J (s) 1.72
7.346
7.334
7.321
7.274
7.260 CDCl3
7.253
7.227
7.214
4.708
4.697
4.534
4.417
4.405
3.355
3.346
3.342
3.336
3.328
3.166
3.157
3.152
3.148
3.139
1.722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137.804
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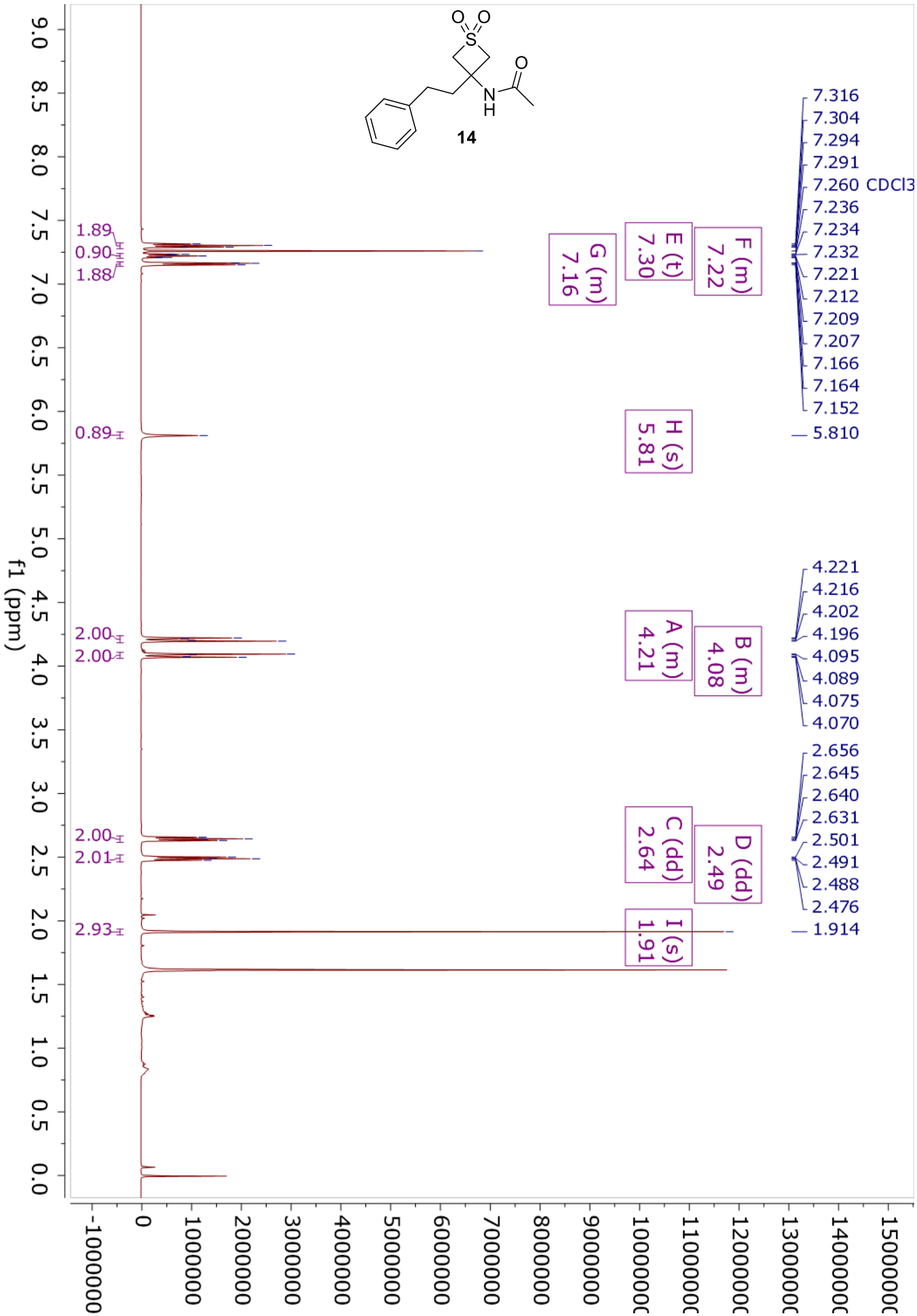
128.571
127.233
83.133
77.160 CDCl3
57.759
56.187
30.234
24.711
f1 (ppm)


14
7.316
7.304
7.294
7.291
7.260 CDCl3
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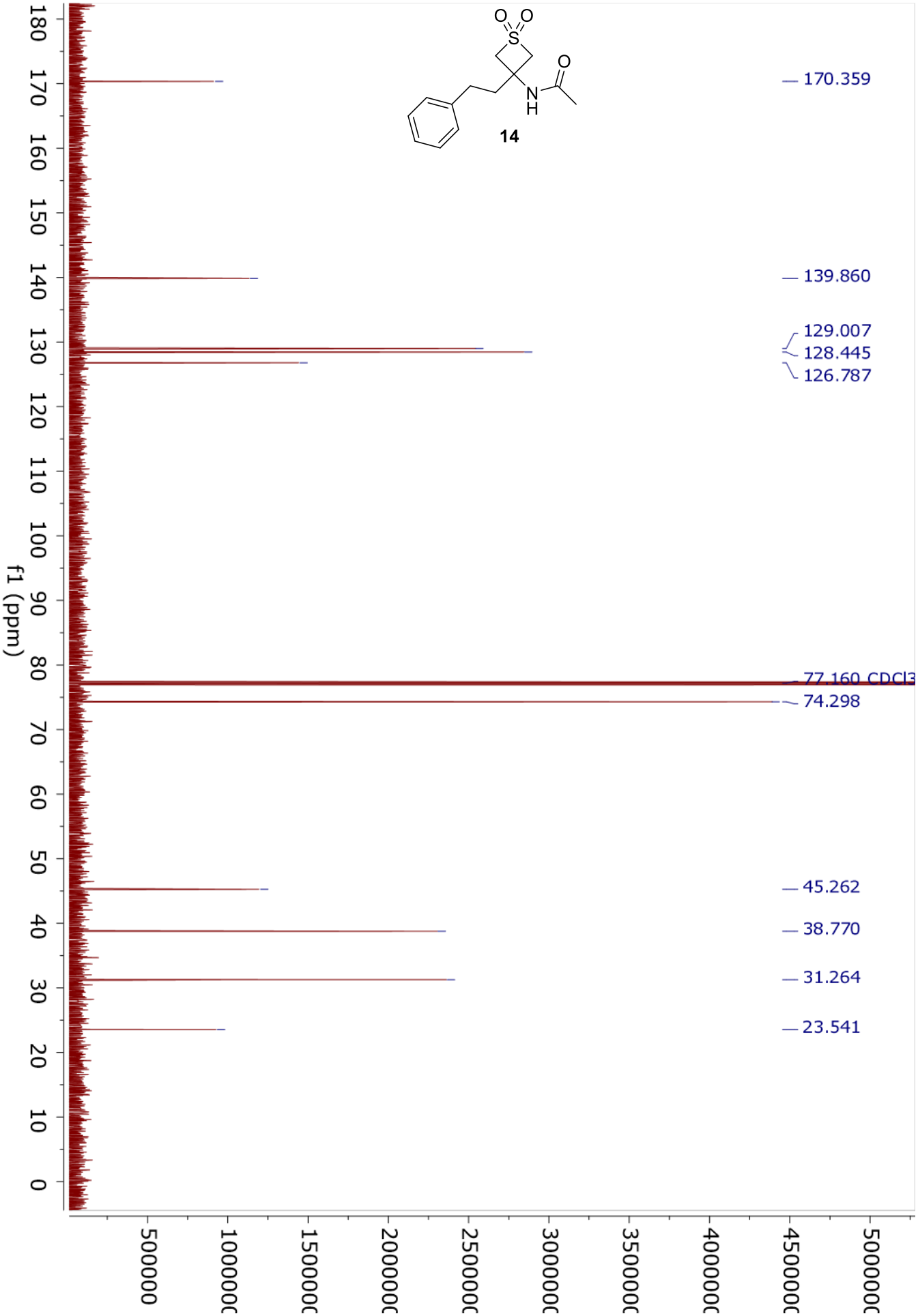
7.234
7.232
7.221
7.212
7.209
7.207
7.166
7.164
7.152
5.810
4.221
4.216
4.202
4.196
4.095
4.089
4.075
4.070
2.656
2.645
2.640
2.631
2.501
2.491
2.488
2.476
1.914
F (m) 7.22
E (t) 7.30
G (m) 7.16
H (s) 5.81
B (m) 4.08
A (m) 4.21
D (dd) 2.49
C (dd) 2.64
I (s) 1.91
1.89
0.90
1.88
0.89
2.00
2.00
2.00
2.01
2.93
f1 (ppm)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170.359
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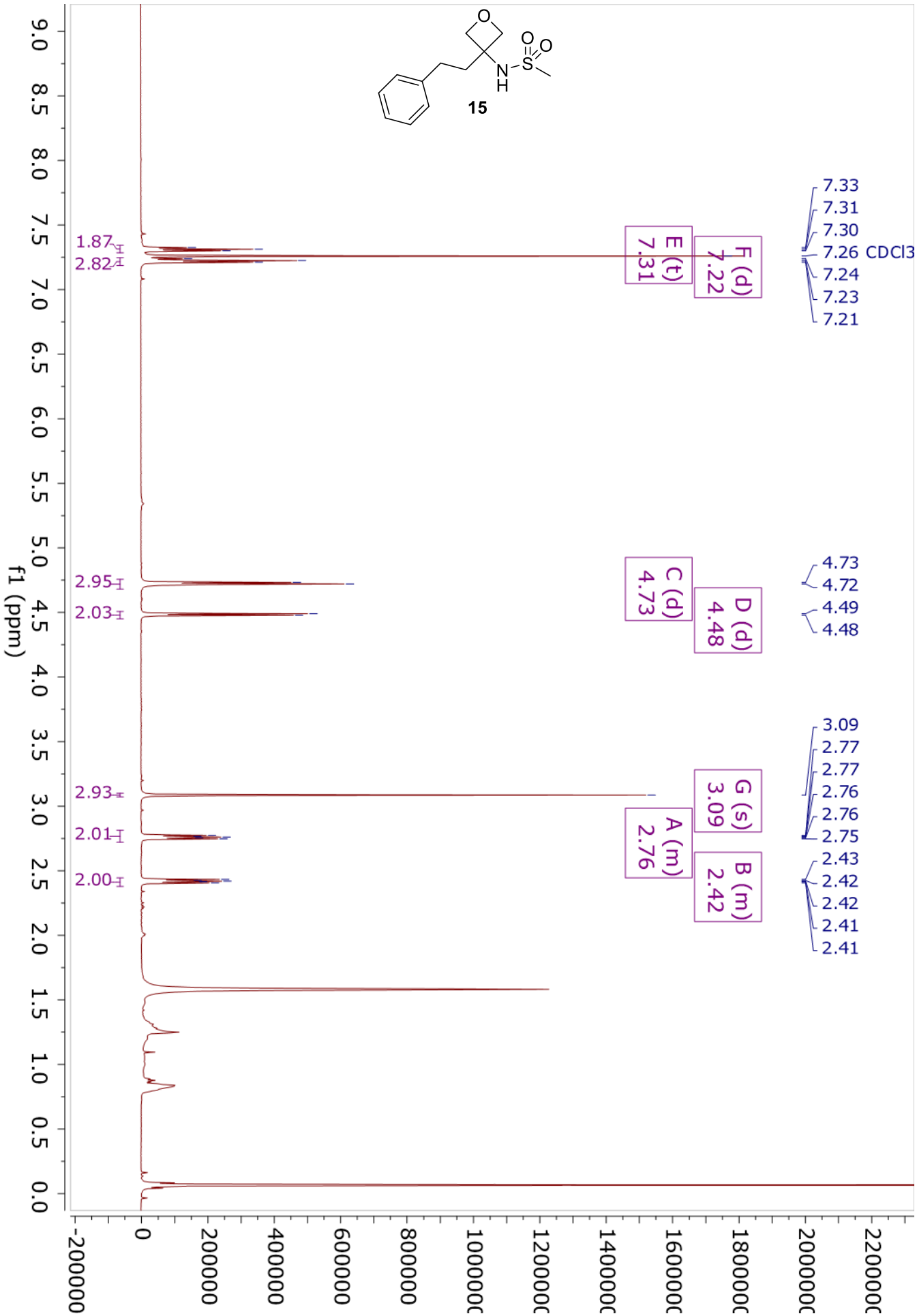
129.007
128.445
126.787
77.160 CDCl3
74.298
45.262
38.770
31.264
23.541
f1 (ppm)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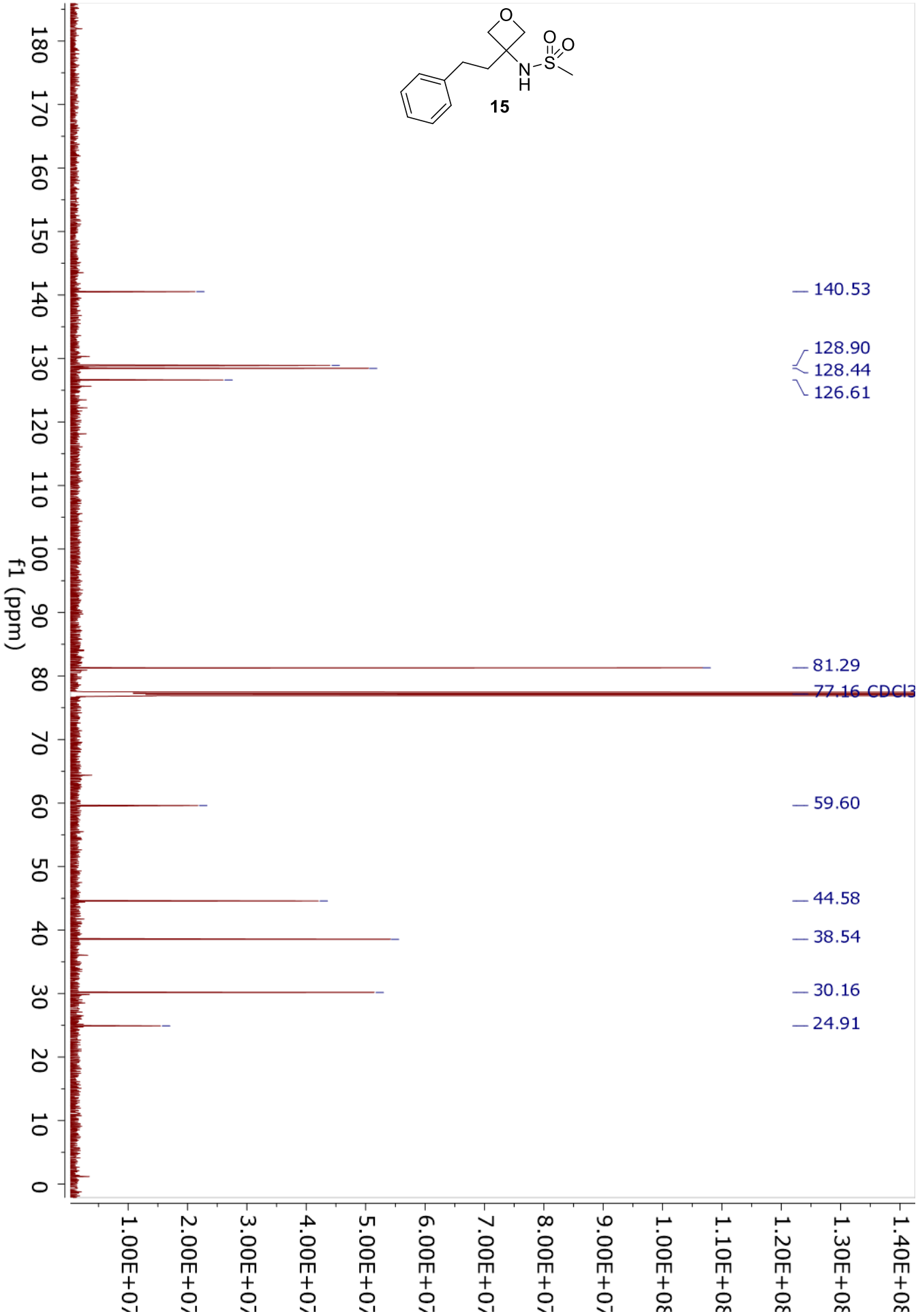
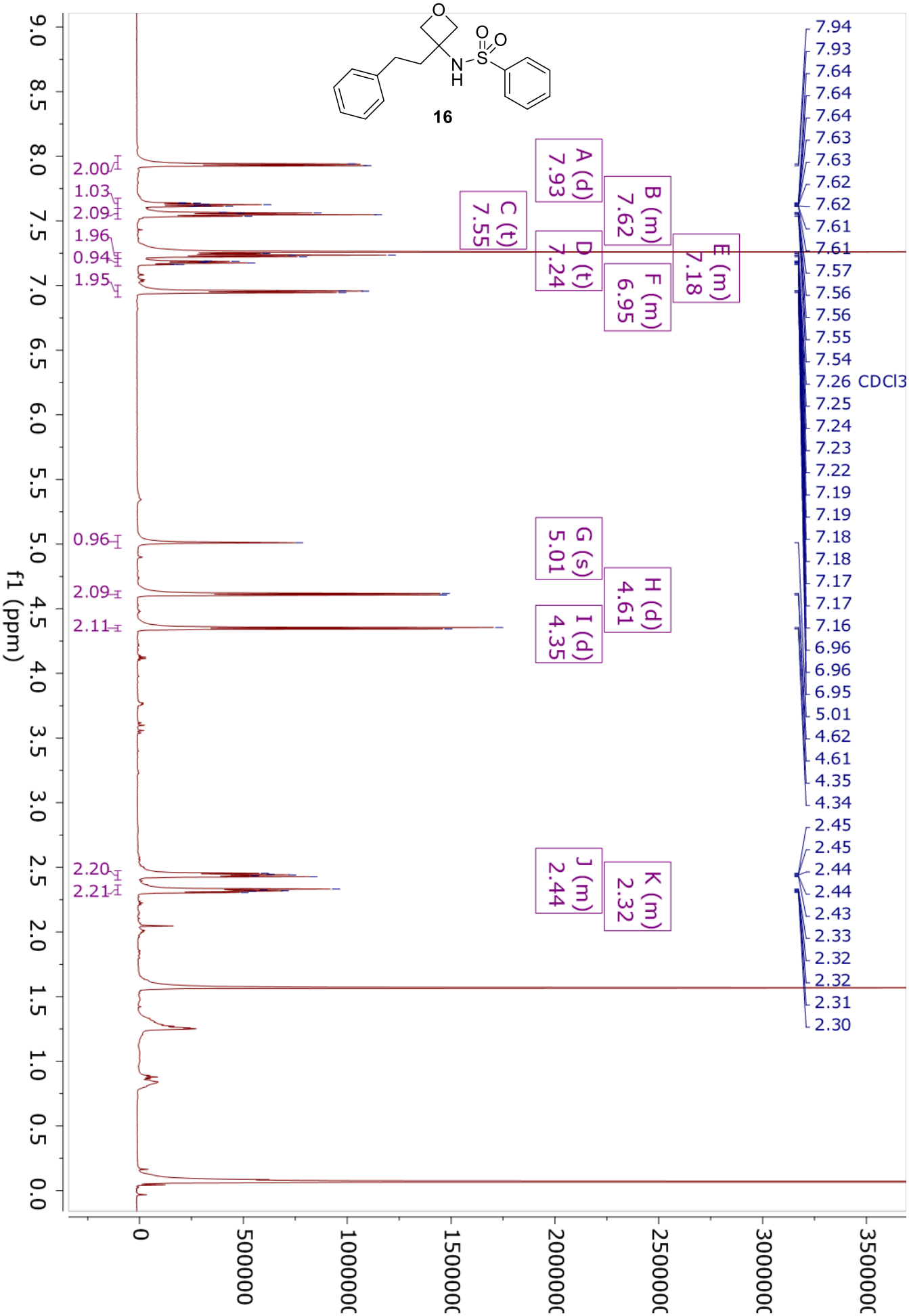
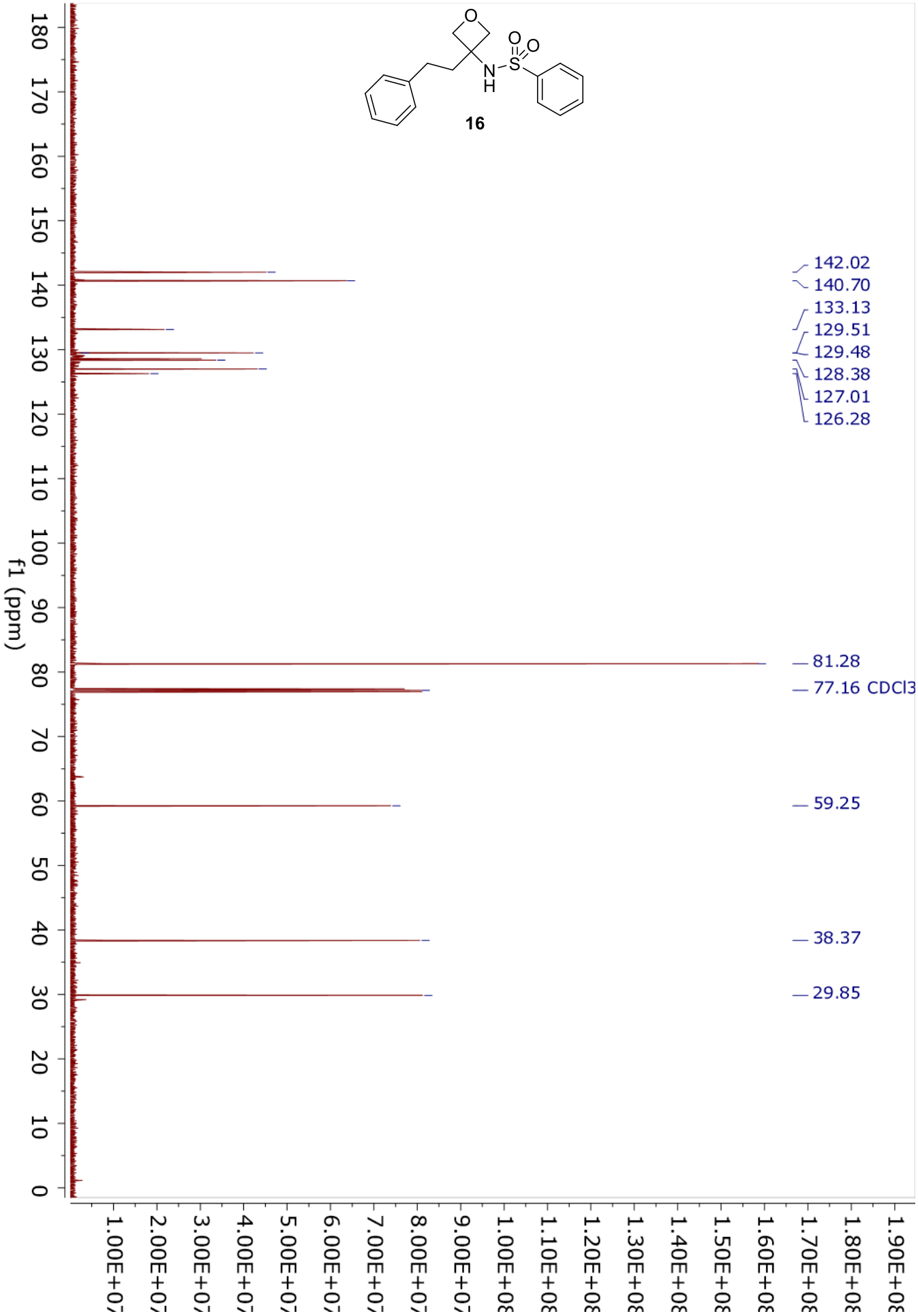
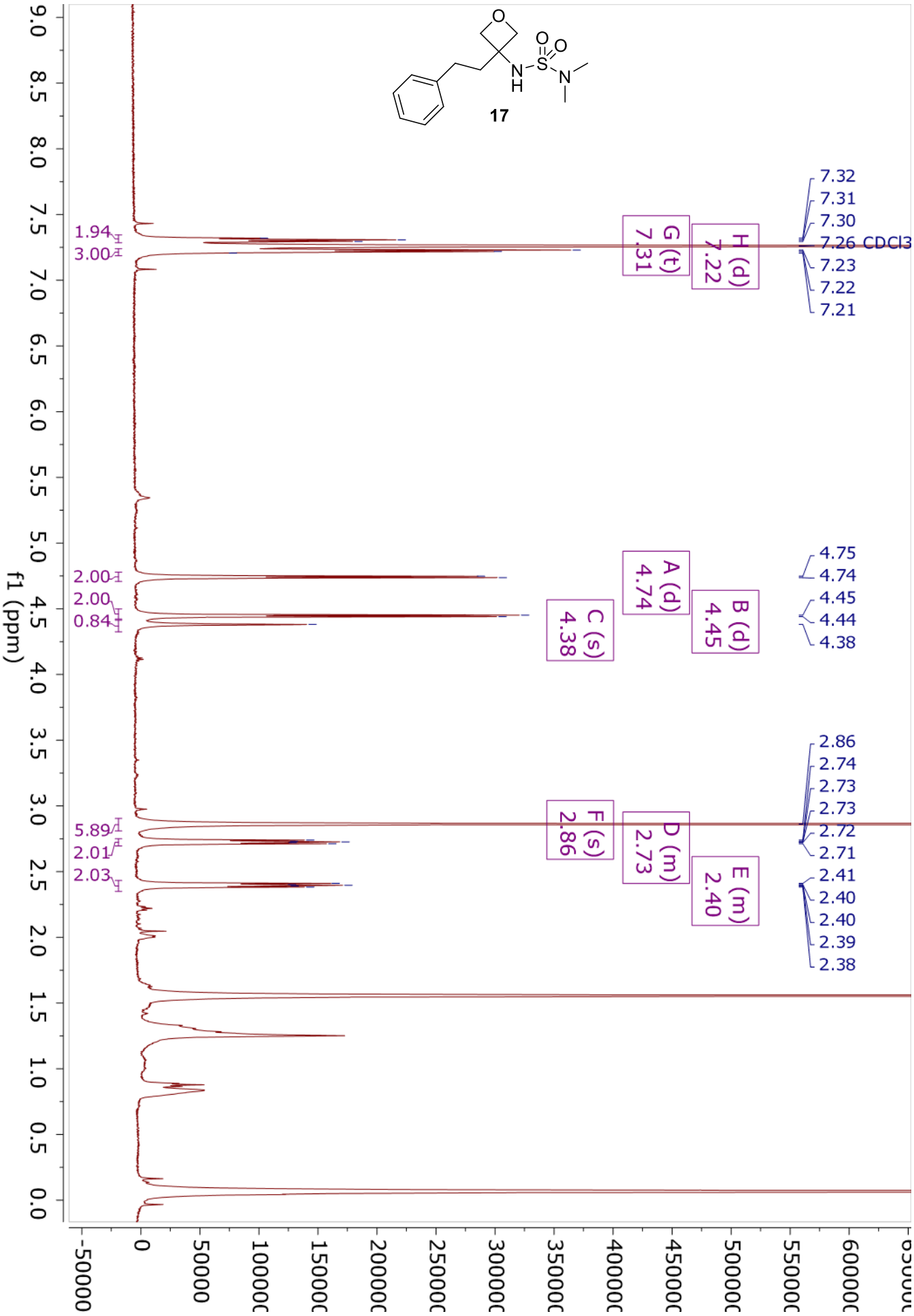
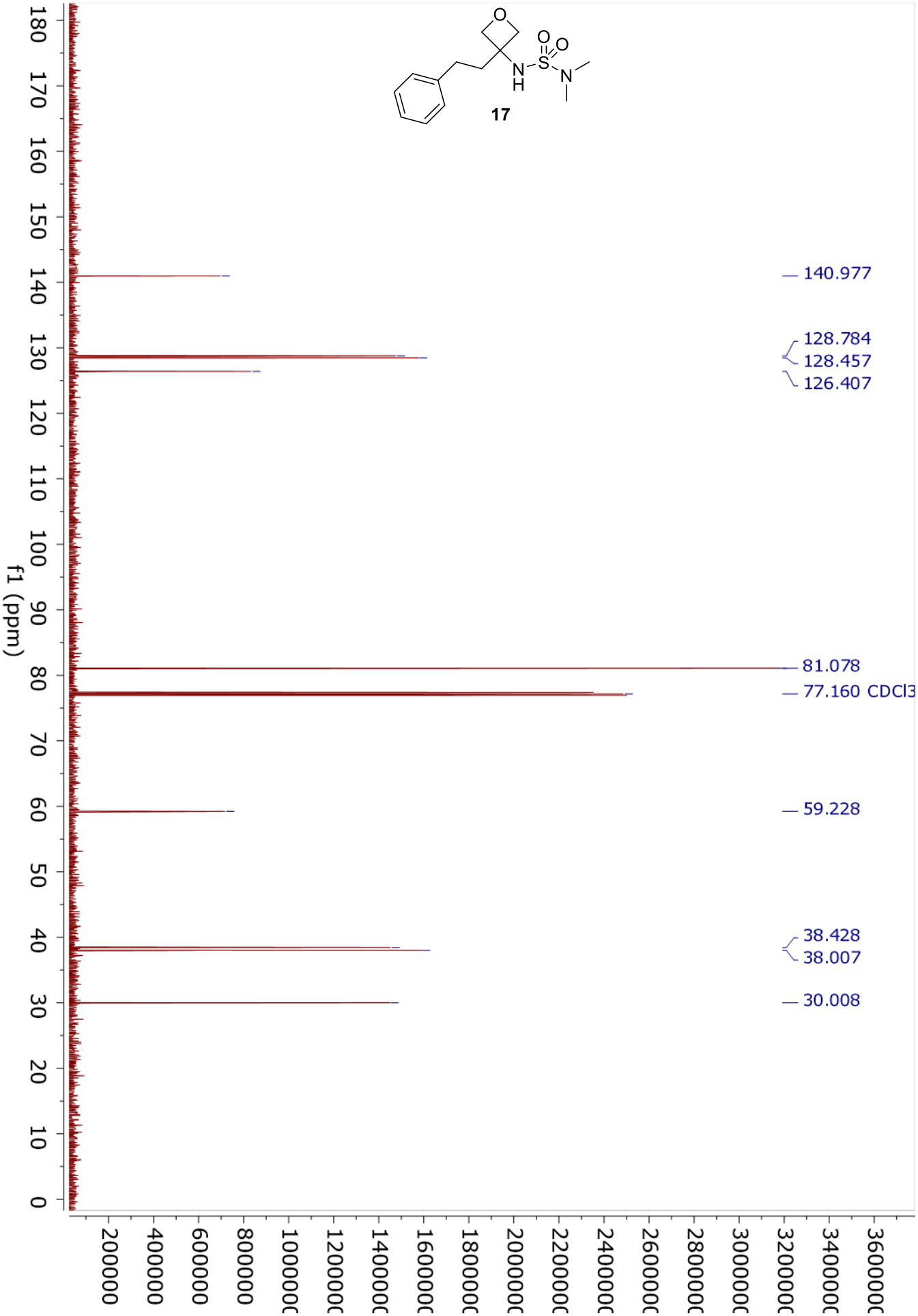
f1 (ppm)
1.87
2.82
2.95
2.03
2.93
2.01
2.00
E (t) 7.31
F (d) 7.22
C (d) 4.73
D (d) 4.48
G (s) 3.09
A (m) 2.76
B (m) 2.42
7.33
7.31
7.30
7.26 CDCl3
7.24
7.23
7.21
4.73
4.72
4.49
4.48
3.09
2.77
2.77
2.76
2.76
2.75
2.43
2.42
2.42
2.41
2.41

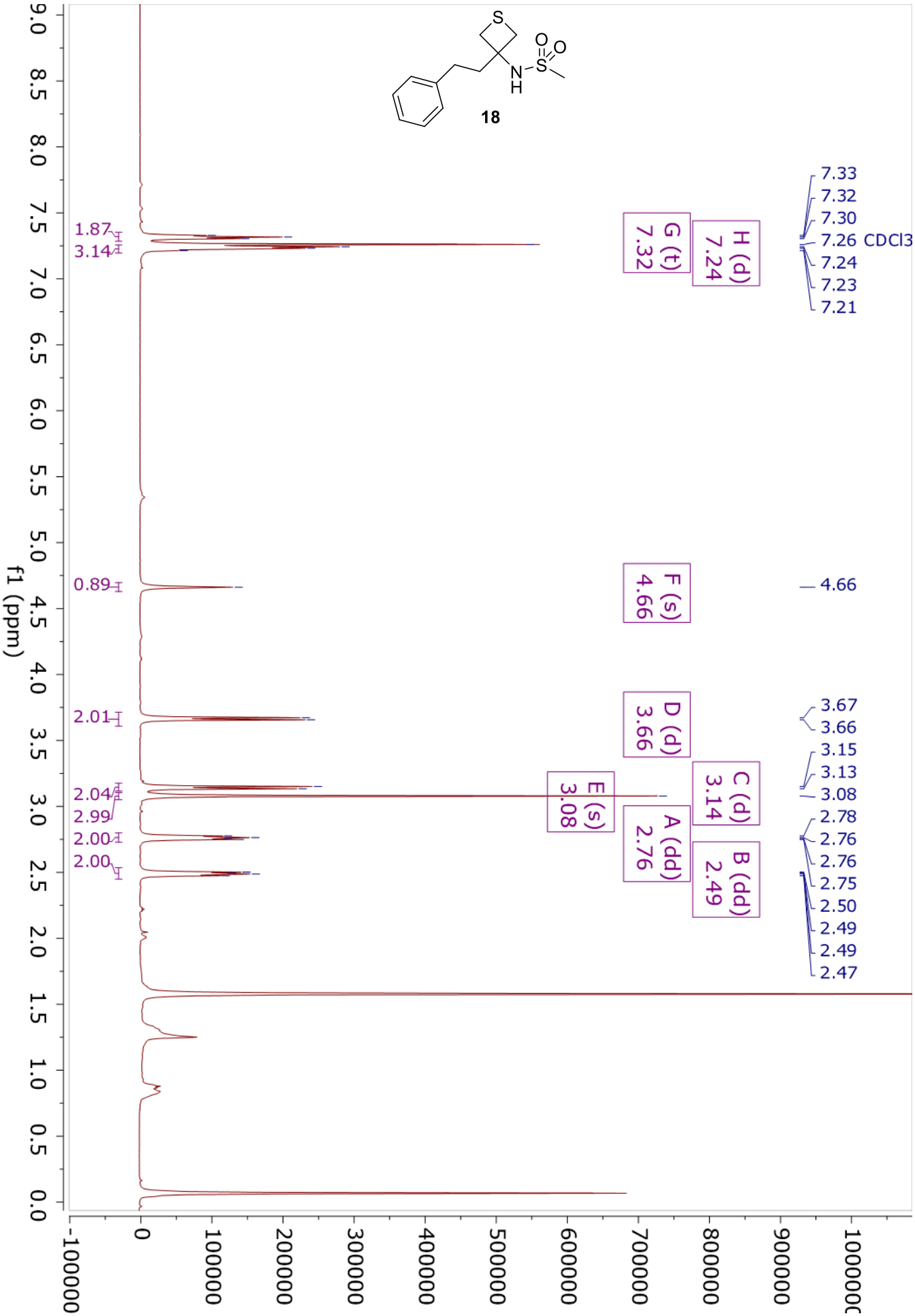

15
140.53
128.90
128.44
126.61
81.29
77.16 CDCl3
59.60
44.58
38.54
30.16
24.91
f1 (ppm)

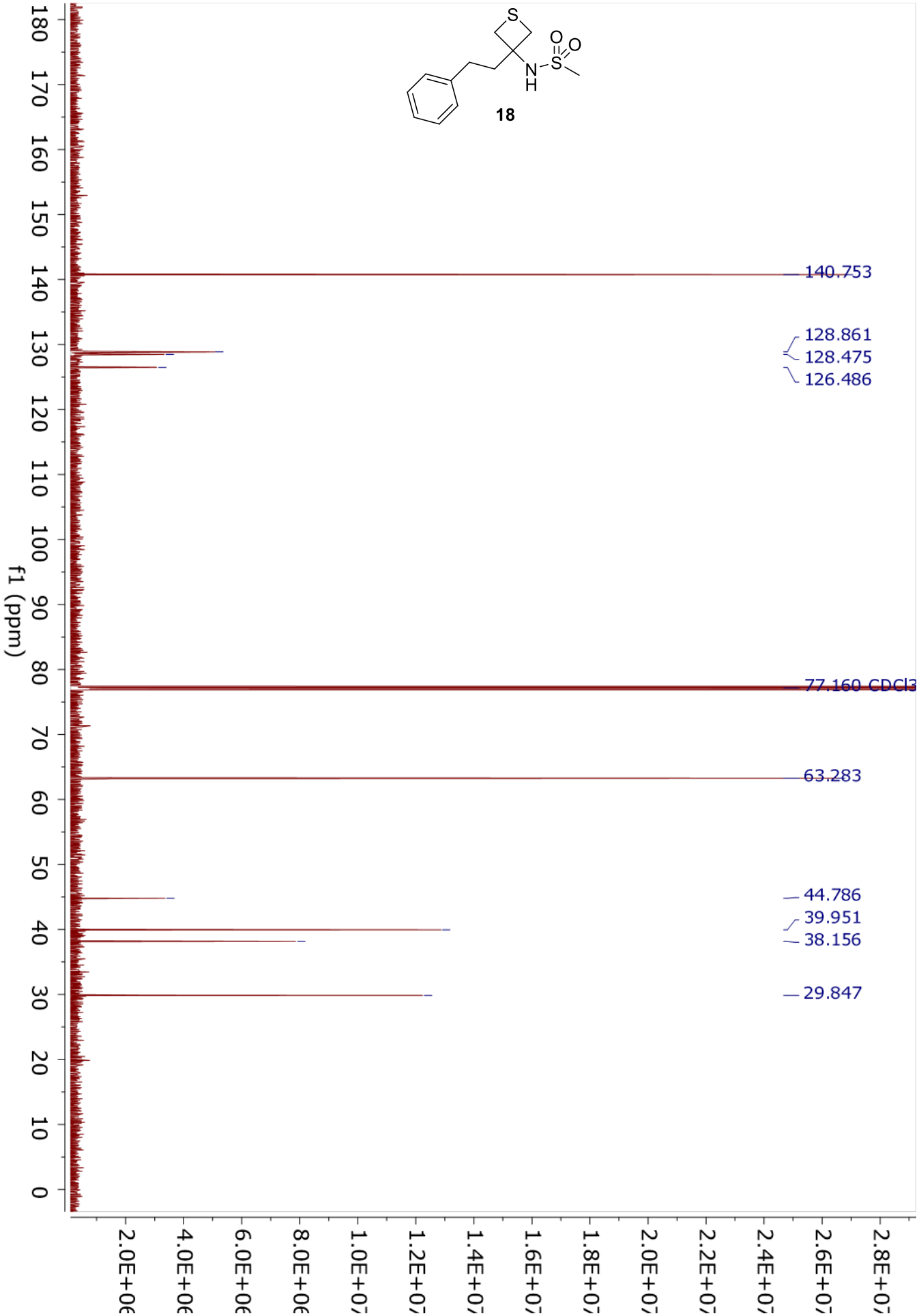

16
A (d) 7.93
B (m) 7.62
C (t) 7.55
D (t) 7.24
E (m) 7.18
F (m) 6.95
G (s) 5.01
H (d) 4.61
I (d) 4.35
J (m) 2.44
K (m) 2.32
CDCl3
f1 (ppm)

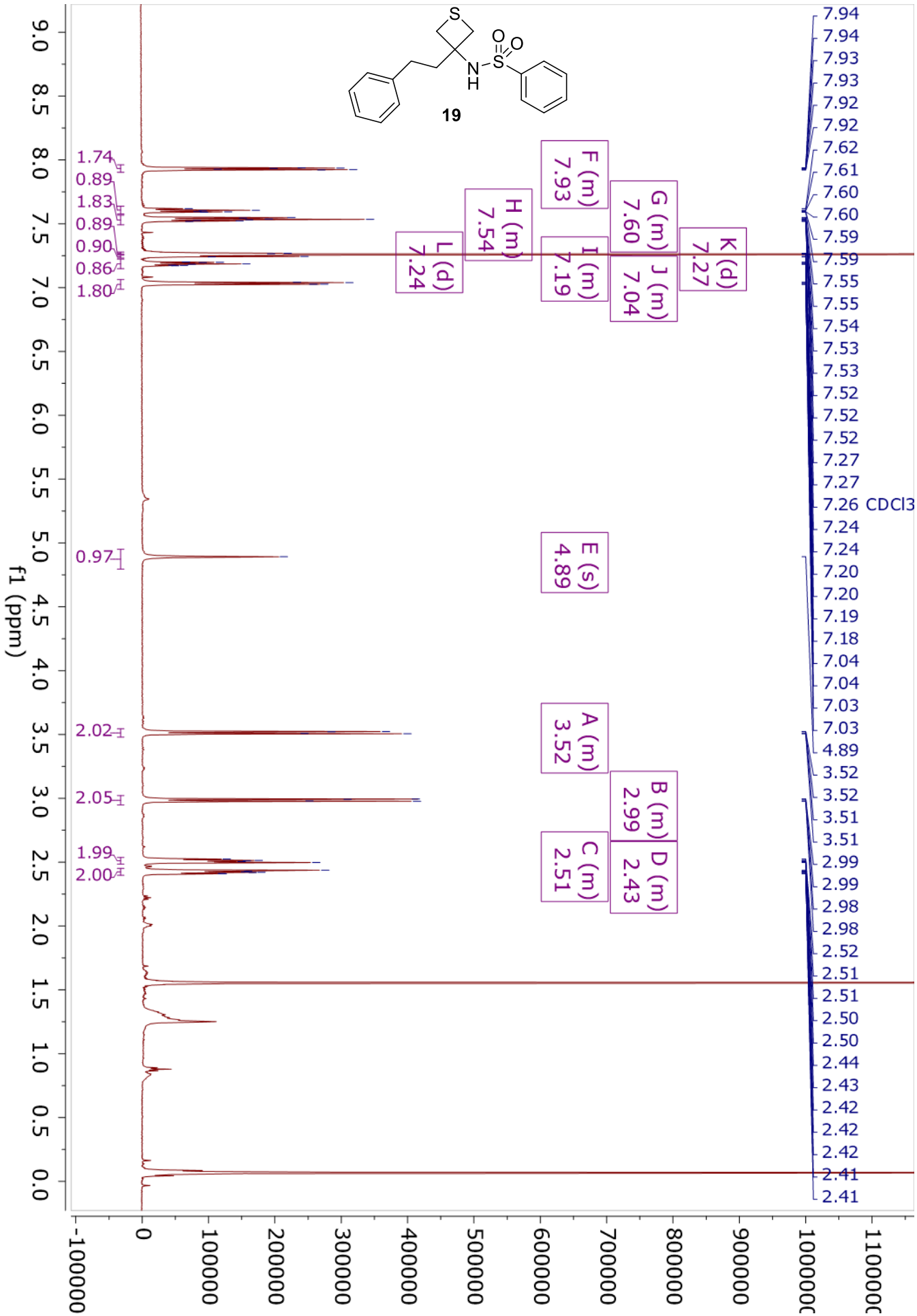

16
142.02
140.70
133.13
129.51
129.48
128.38
127.01
126.28
81.28
77.16 CDCl3
59.25
38.37
29.85
f1 (ppm)

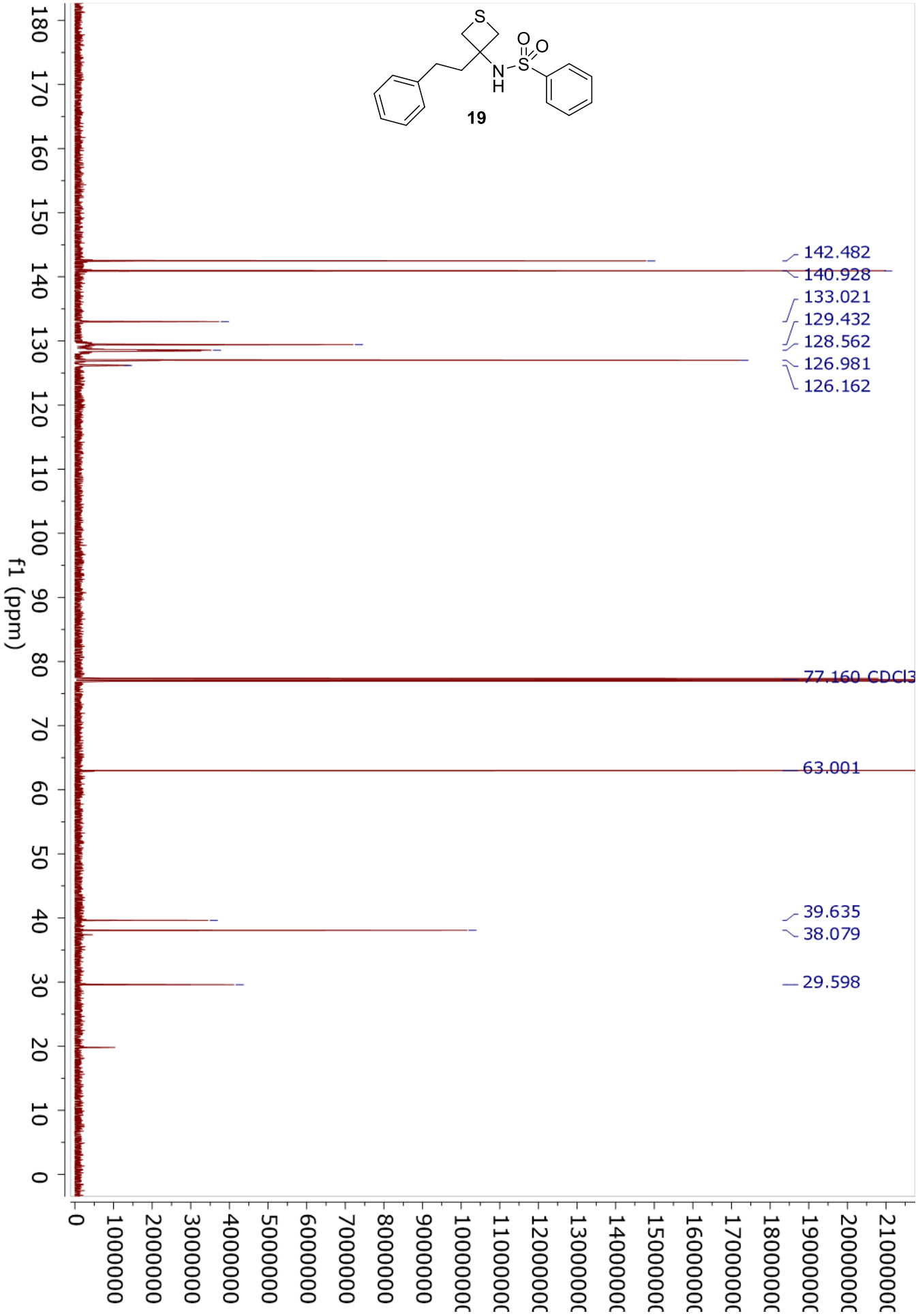

17
7.32
7.31
7.30
7.26 CDCl3
7.23
7.22
7.21
4.75
4.74
4.45
4.44
4.38
2.86
2.74
2.73
2.73
2.72
2.71
2.41
2.40
2.40
2.39
2.38
G (t) 7.31
H (d) 7.22
A (d) 4.74
B (d) 4.45
C (s) 4.38
F (s) 2.86
D (m) 2.73
E (m) 2.40
1.94
3.00
2.00
2.00
0.84
5.89
2.01
2.03
f1 (ppm)


17
140.977
128.784
128.457
126.407
81.078
77.160 CDCl3
59.228
38.428
38.007
30.008
f1 (ppm)


18
f1 (ppm)
1.87
3.14
0.89
2.01
2.04
2.99
2.00
2.00
G (t) 7.32
H (d) 7.24
F (s) 4.66
D (d) 3.66
E (s) 3.08
C (d) 3.14
A (dd) 2.76
B (dd) 2.49
7.33
7.32
7.30
7.26 CDCl3
7.24
7.23
7.21
4.66
3.67
3.66
3.15
3.13
3.08
2.78
2.76
2.76
2.75
2.50
2.49
2.49
2.47


S
O
O
S
N
H
18
140.753
128.861
128.475
126.486
77.160 CDCl3
63.283
44.786
39.951
38.156
29.847
f1 (ppm)


19
F (m) 7.93
G (m) 7.60
H (m) 7.54
I (m) 7.19
J (m) 7.04
K (d) 7.27
L (d) 7.24
E (s) 4.89
A (m) 3.52
B (m) 2.99
C (m) 2.51
D (m) 2.43
CDCl3
f1 (ppm)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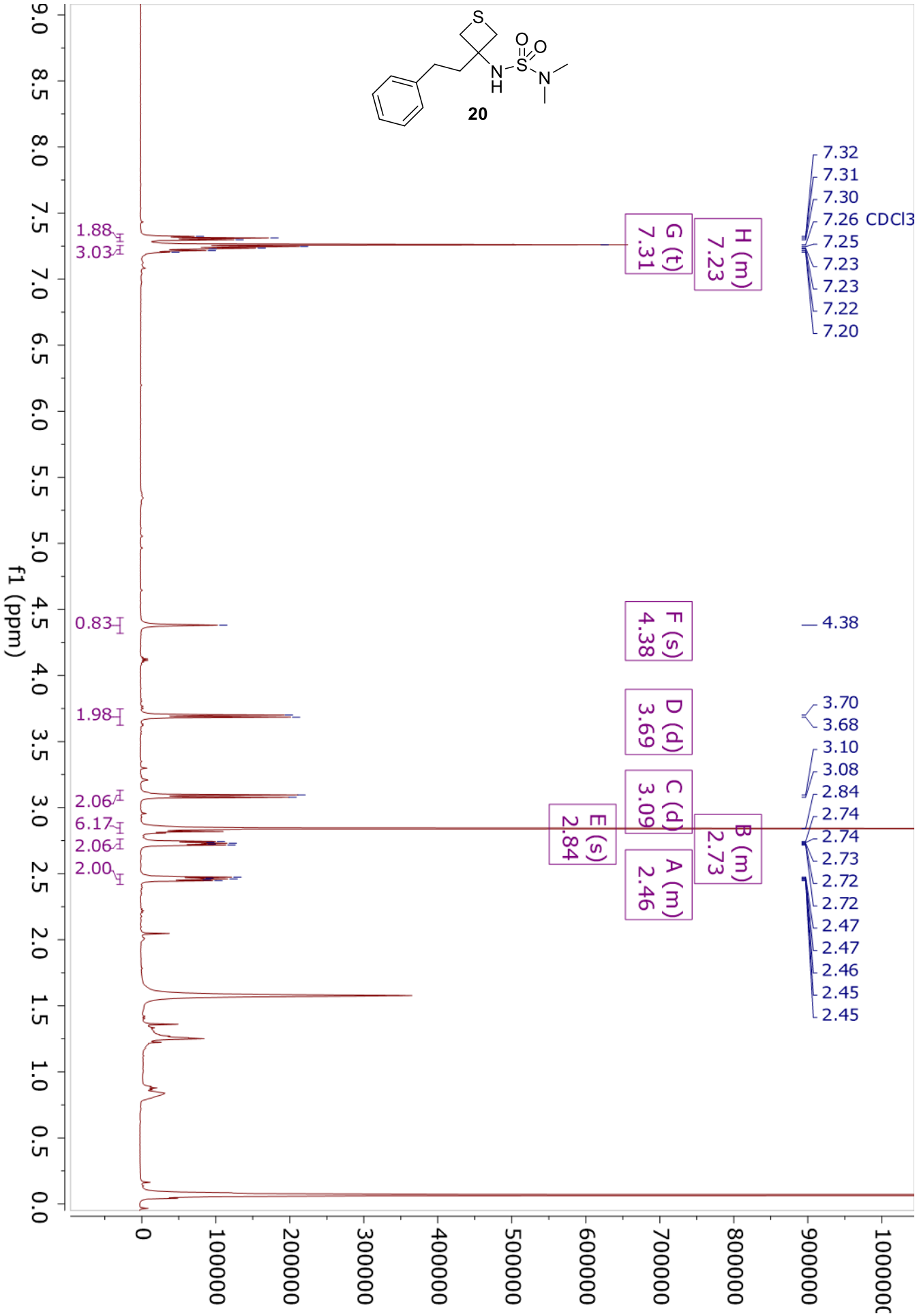
142.482
140.928
133.021
129.432
128.562
126.981
126.162
77.160 CDCl3
63.001
39.635
38.079
29.598
f1 (ppm)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f1 (ppm)
1.88
3.03
0.83
1.98
2.06
6.17
2.06
2.00
G (t) 7.31
H (m) 7.23
F (s) 4.38
D (d) 3.69
C (d) 3.09
E (s) 2.84
B (m) 2.73
A (m) 2.46
7.32
7.31
7.30
7.26 CDCl3
7.25
7.23
7.23
7.22
7.20
4.38
3.70
3.68
3.10
3.08
2.84
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2.74
2.73
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2.72
2.47
2.47
2.46
2.45
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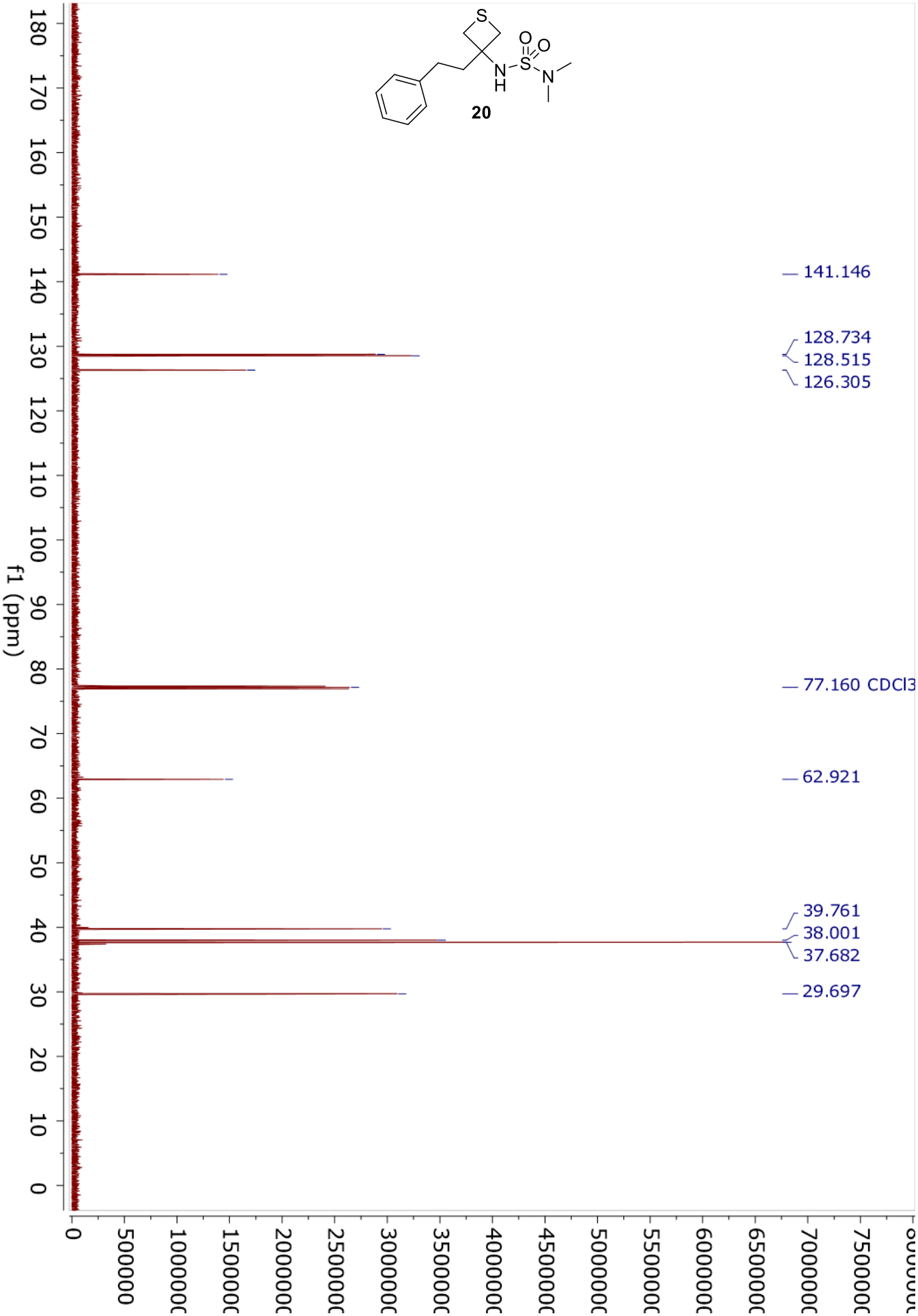
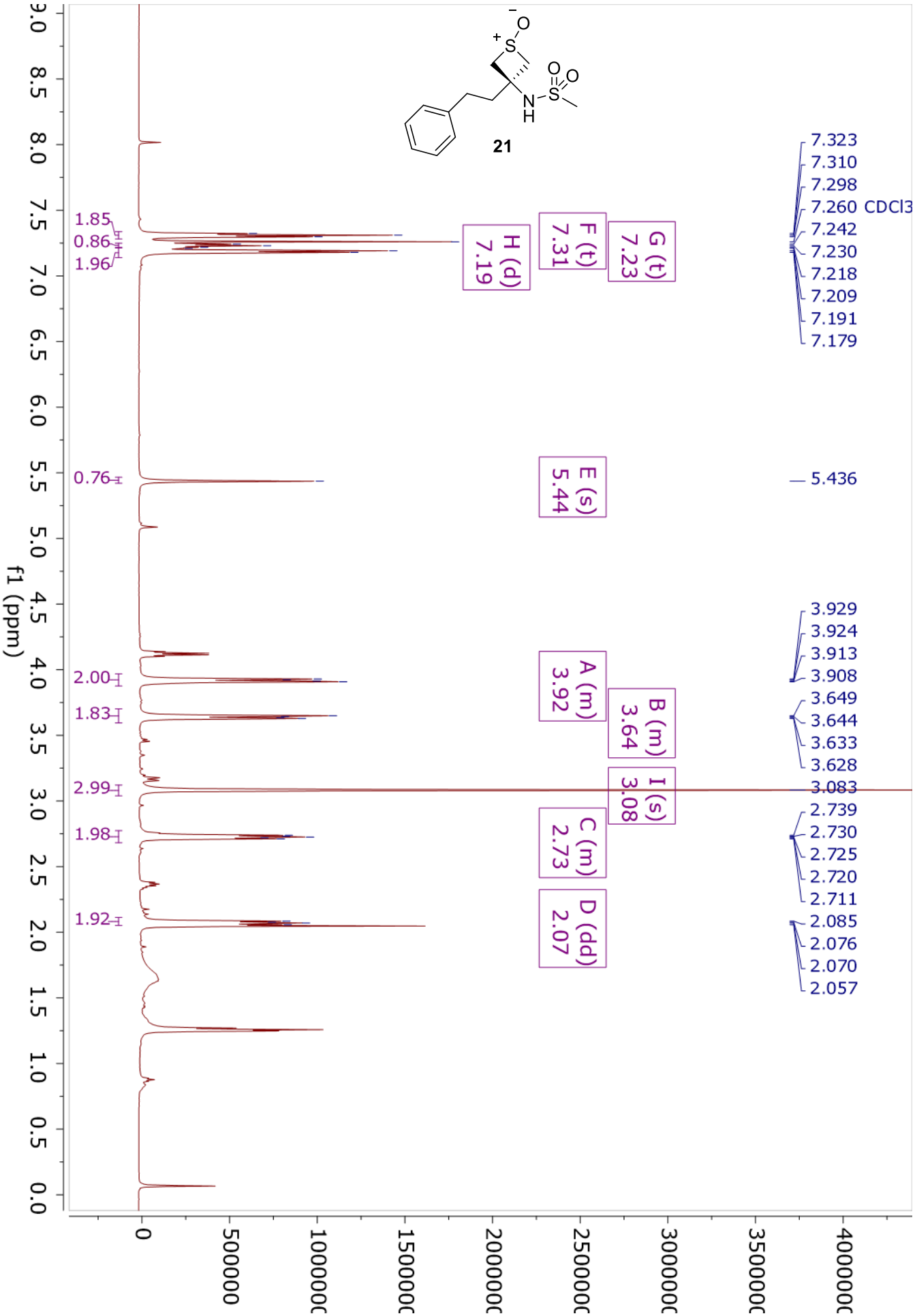

S
O
O
S
N
H
N
20
141.146
128.734
128.515
126.305
77.160 CDCl3
62.921
39.761
38.001
37.682
29.697
f1 (ppm)


21
f1 (ppm)
A (m) 3.92
B (m) 3.64
C (m) 2.73
D (dd) 2.07
E (s) 5.44
F (t) 7.31
G (t) 7.23
H (d) 7.19
I (s) 3.08
1.85
0.86
1.96
0.76
2.00
1.83
2.99
1.98
1.92
7.323
7.310
7.298
7.260 CDCl3
7.242
7.230
7.218
7.209
7.191
7.179
5.436
3.929
3.924
3.913
3.908
3.649
3.644
3.633
3.628
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2.739
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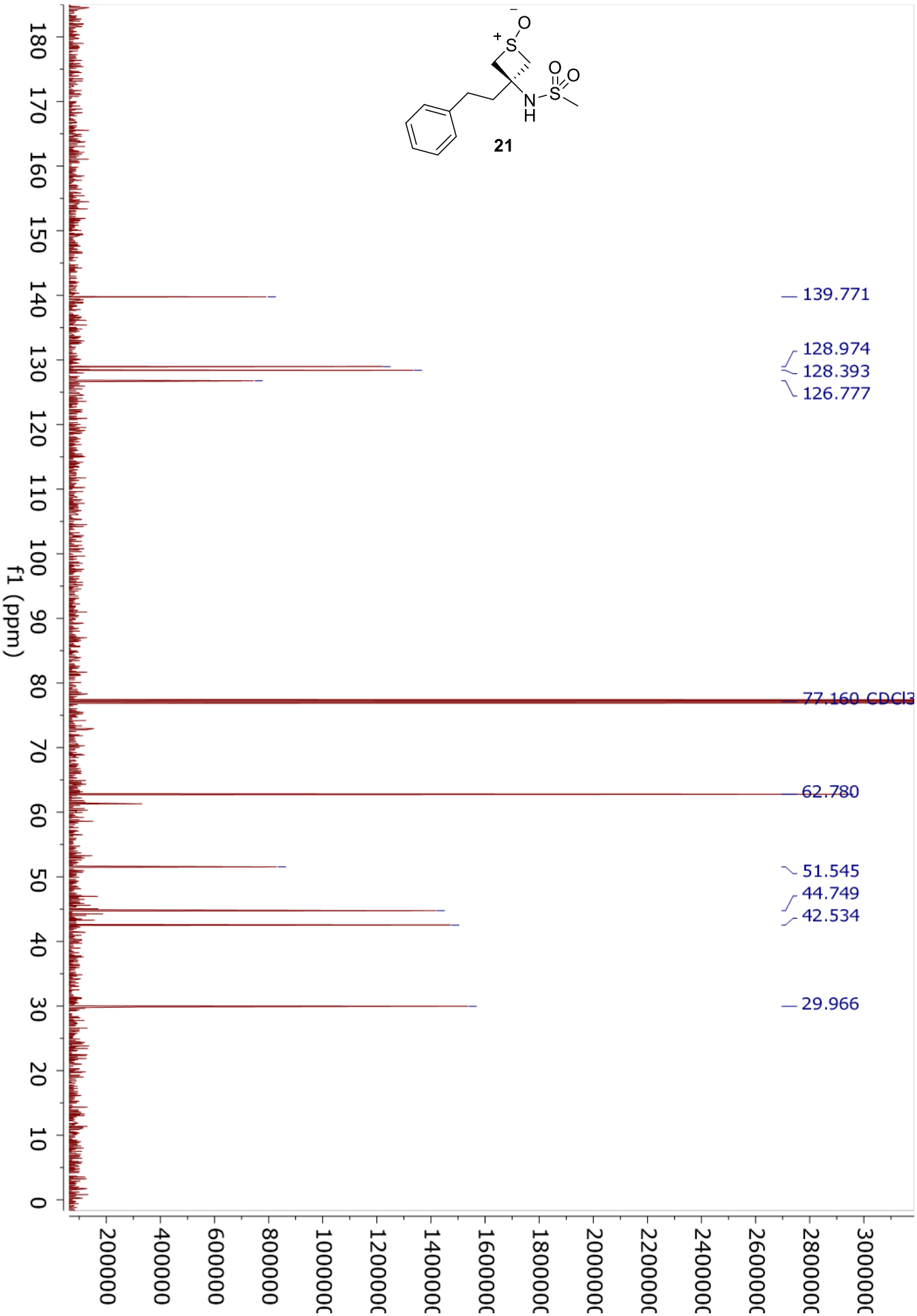
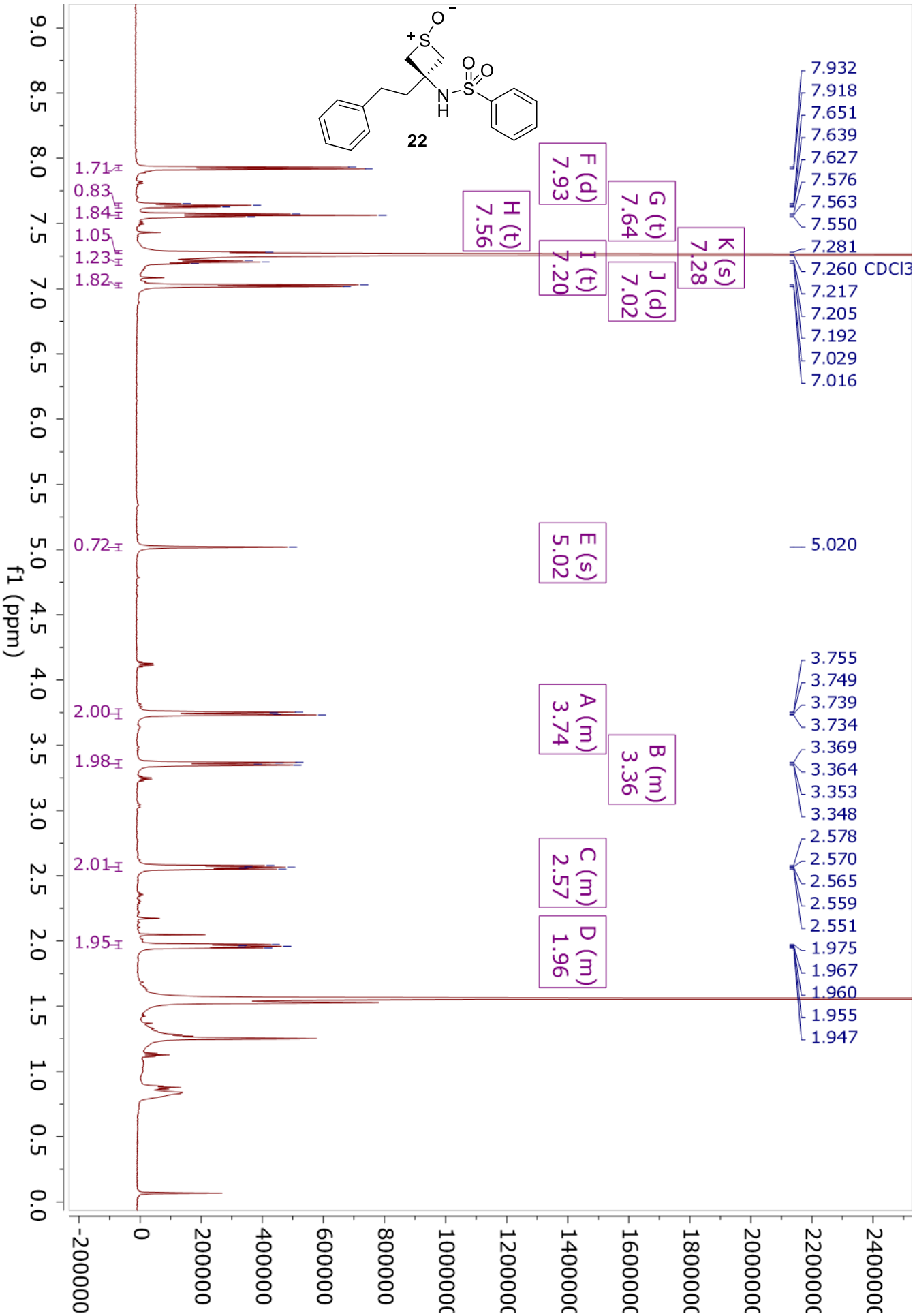
2.720
2.711
2.085
2.076
2.070
2.057


21
139.771
128.974
128.393
126.777
77.160 CDCl3
62.780
51.545
44.749
42.534
29.966
f1 (ppm)


22
F (d) 7.93
G (t) 7.64
H (t) 7.56
I (t) 7.20
J (d) 7.02
K (s) 7.28
E (s) 5.02
A (m) 3.74
B (m) 3.36
C (m) 2.57
D (m) 1.96
1.71
0.83
1.84
1.05
1.23
1.82
0.72
2.00
1.98
2.01
1.95
7.932
7.918
7.651
7.639
7.627
7.576
7.563
7.550
7.281
7.260 CDCl3
7.217
7.205
7.192
7.029
7.016
5.020
3.755
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3.739
3.734
3.369
3.364
3.353
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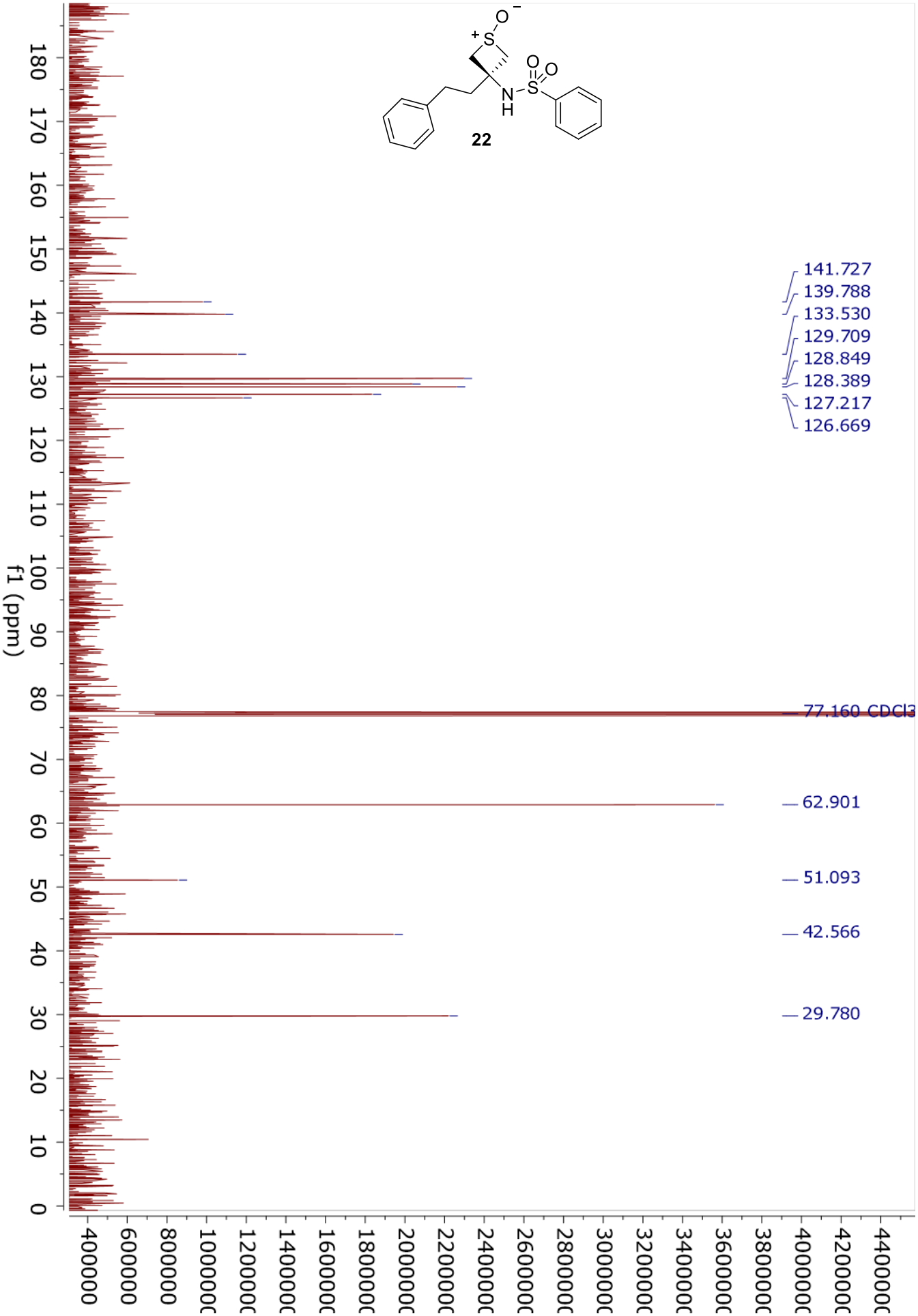
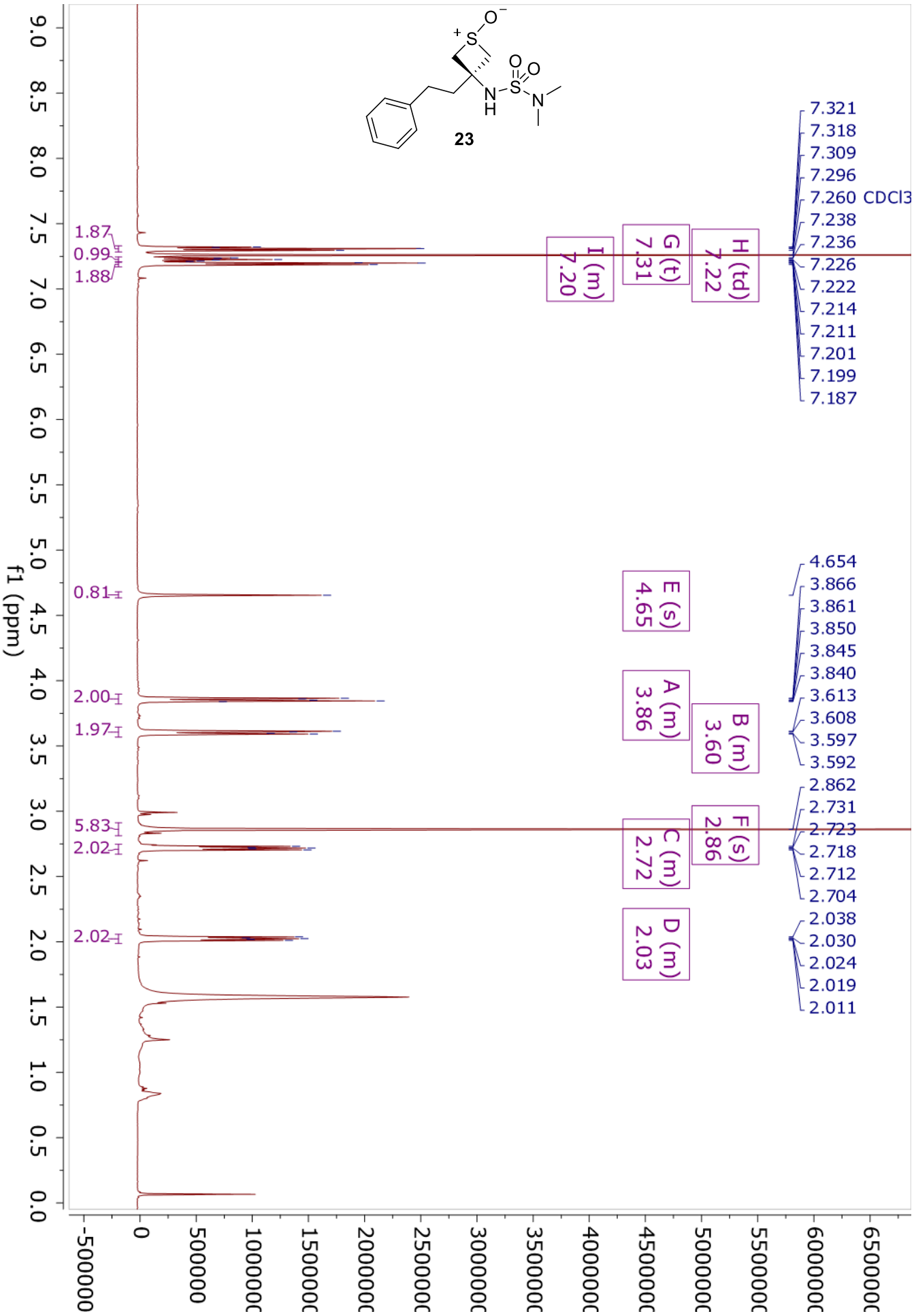
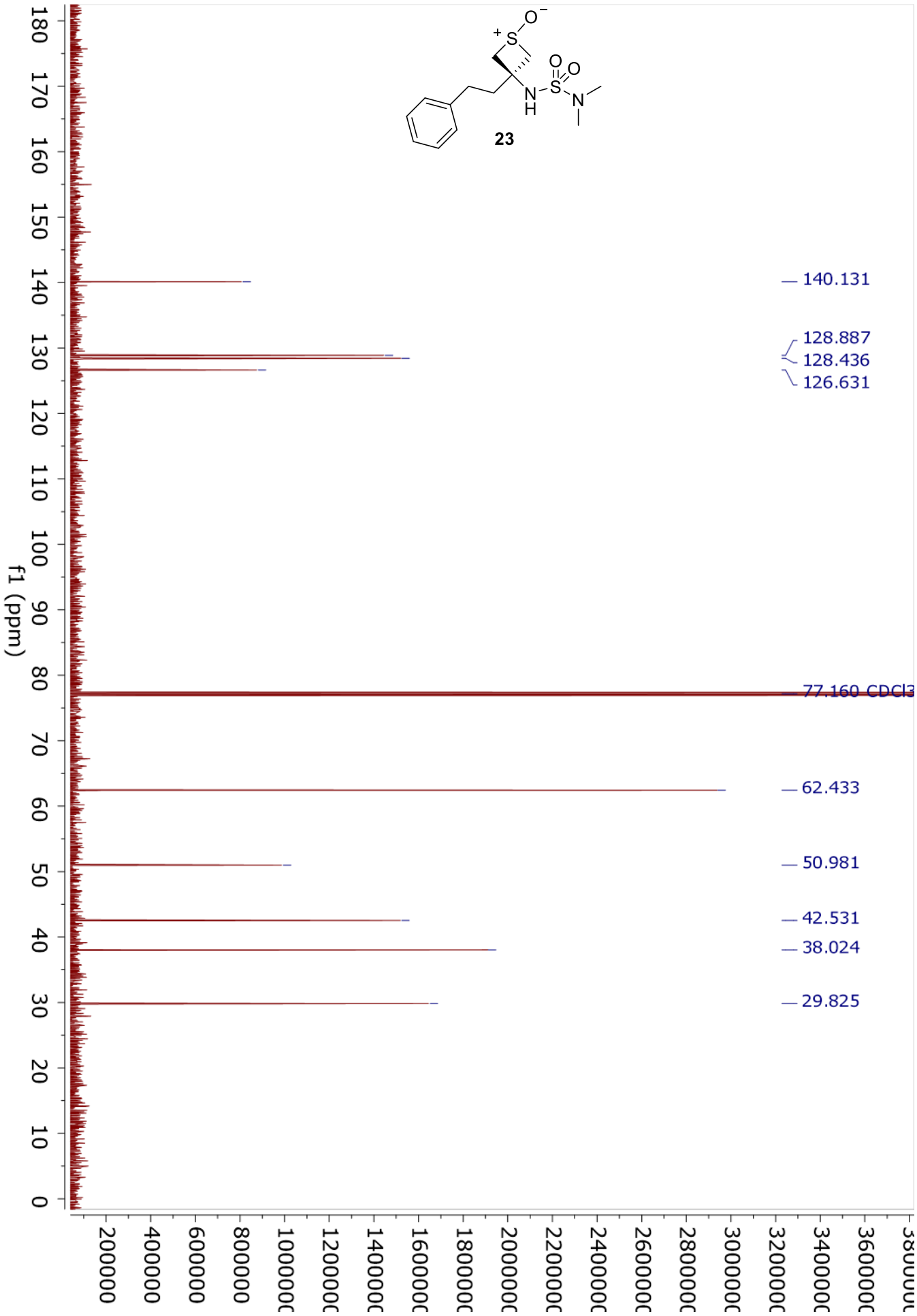
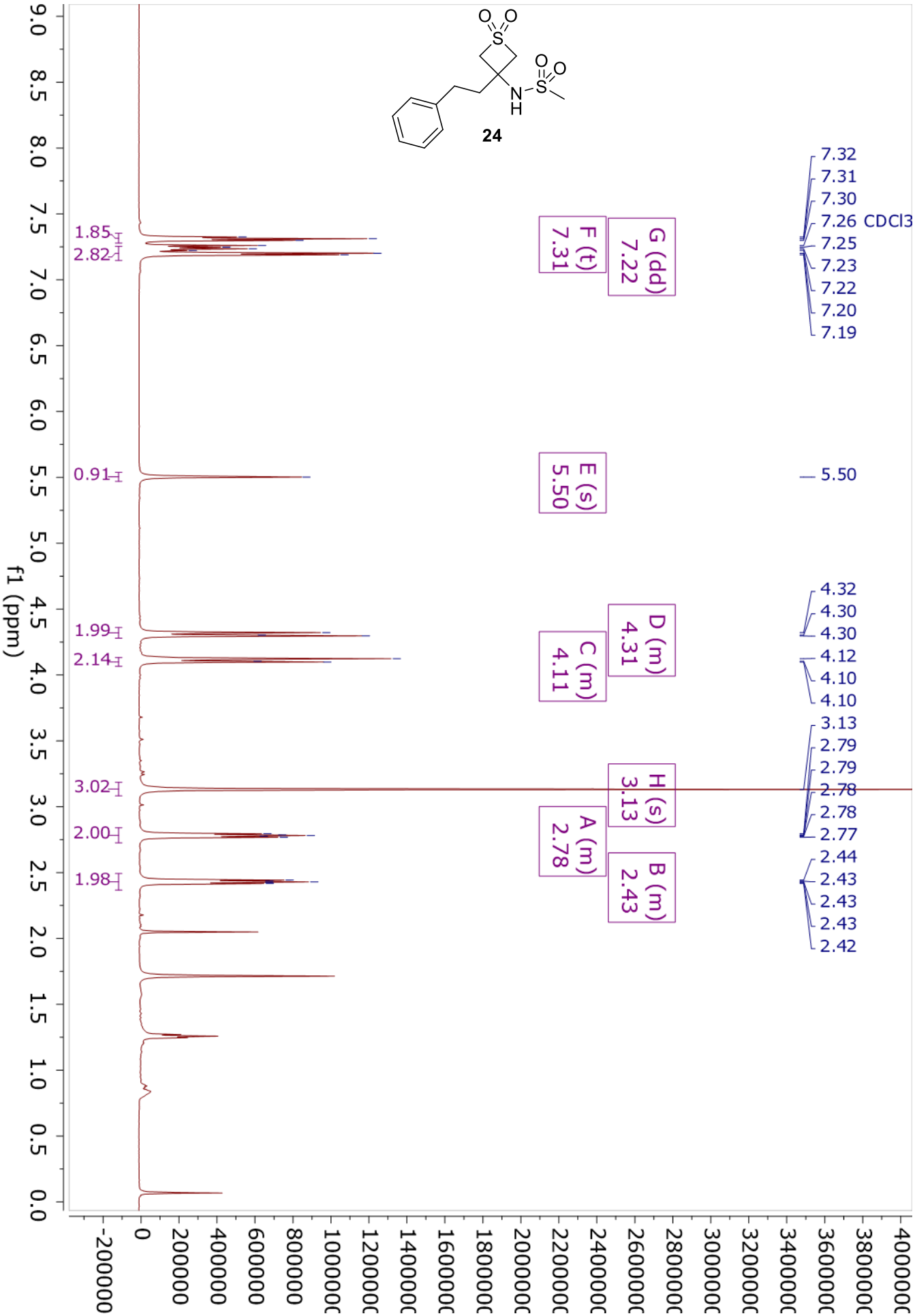
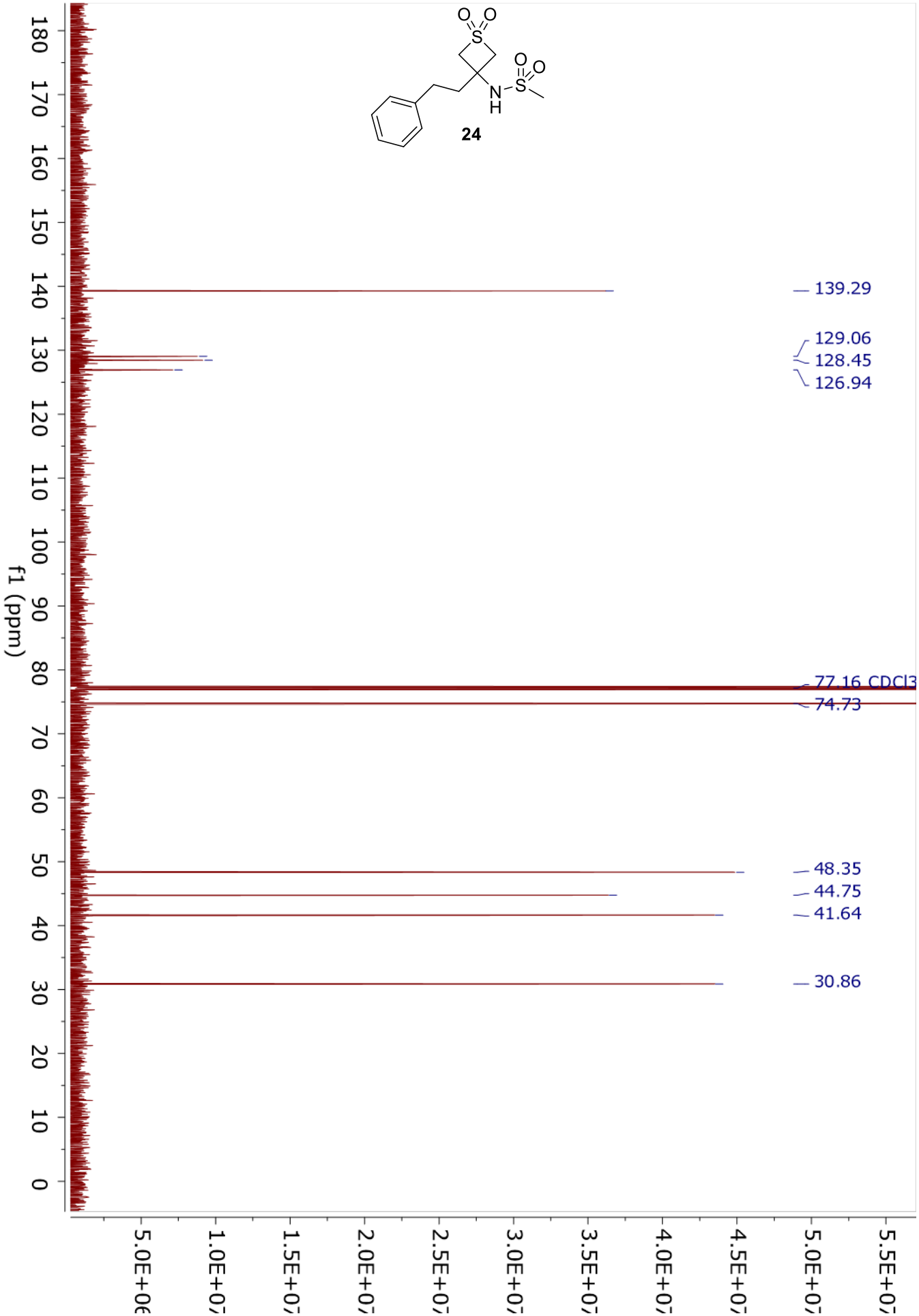
f1 (ppm)

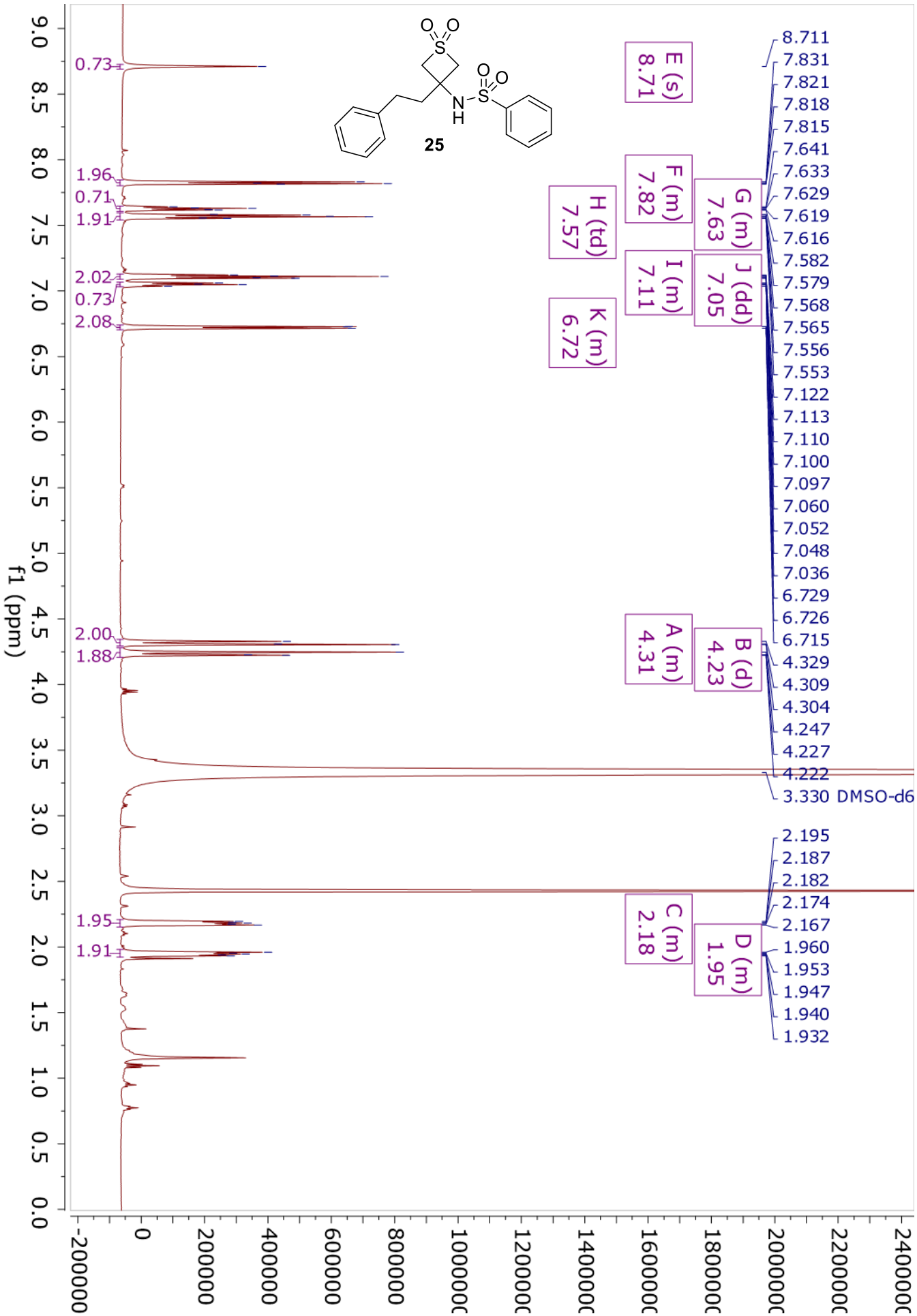

22
141.727
139.788
133.530
129.709
128.849
128.389
127.217
126.669
77.160 CDCl3
62.901
51.093
42.566
29.780
f1 (ppm)

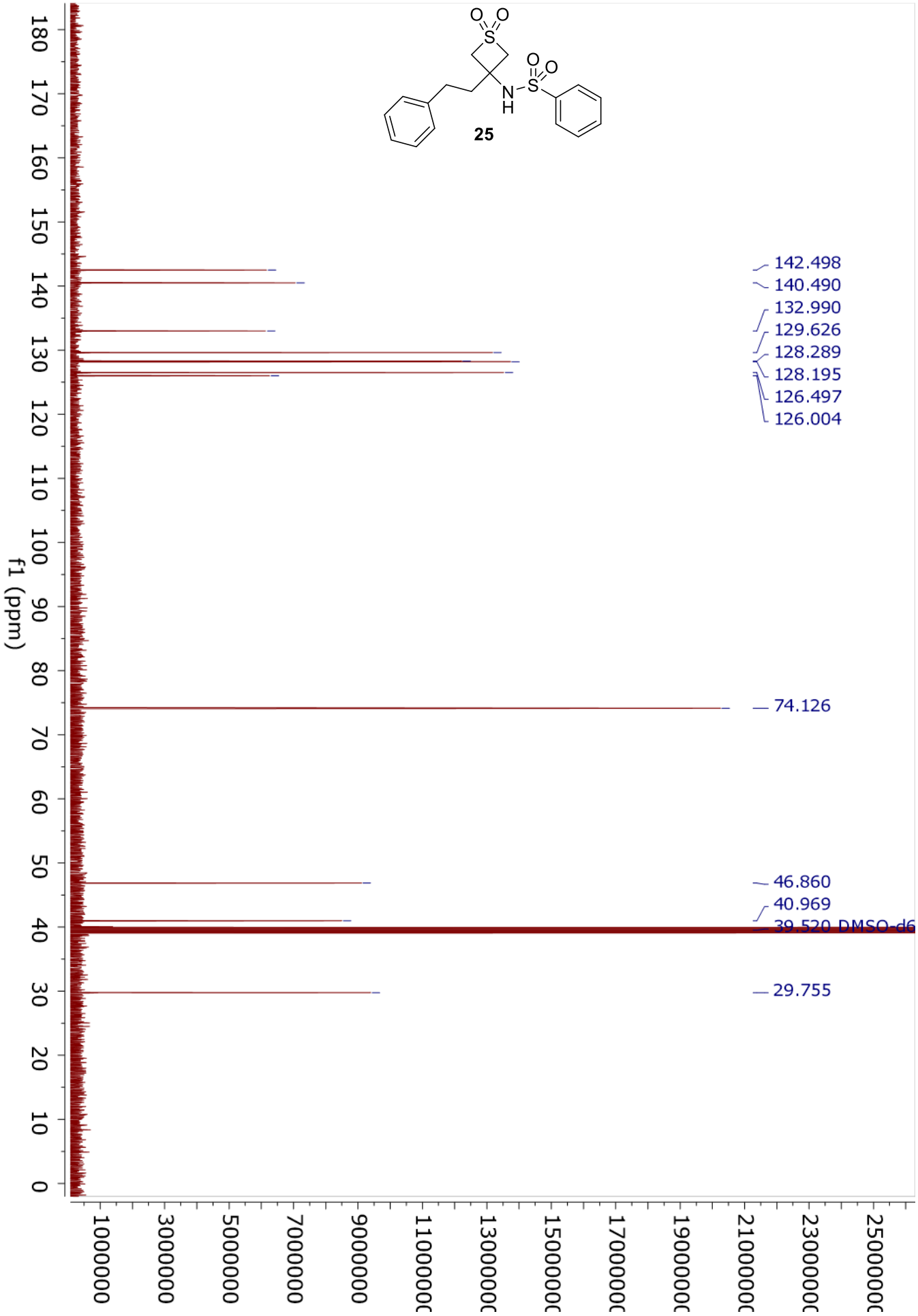

23
f1 (ppm)
7.321
7.318
7.309
7.296
7.260 CDCl3
7.238
7.236
7.226
7.222
7.214
7.211
7.201
7.199
7.187
4.654
3.866
3.861
3.850
3.845
3.840
3.613
3.608
3.597
3.592
2.862
2.731
2.723
2.718
2.712
2.704
2.038
2.030
2.024
2.019
2.011
1.87
0.99
1.88
0.81
2.00
1.97
5.83
2.02
2.02
G (t) 7.31
H (td) 7.22
I (m) 7.20
E (s) 4.65
A (m) 3.86
B (m) 3.60
F (s) 2.86
C (m) 2.72
D (m) 2.03

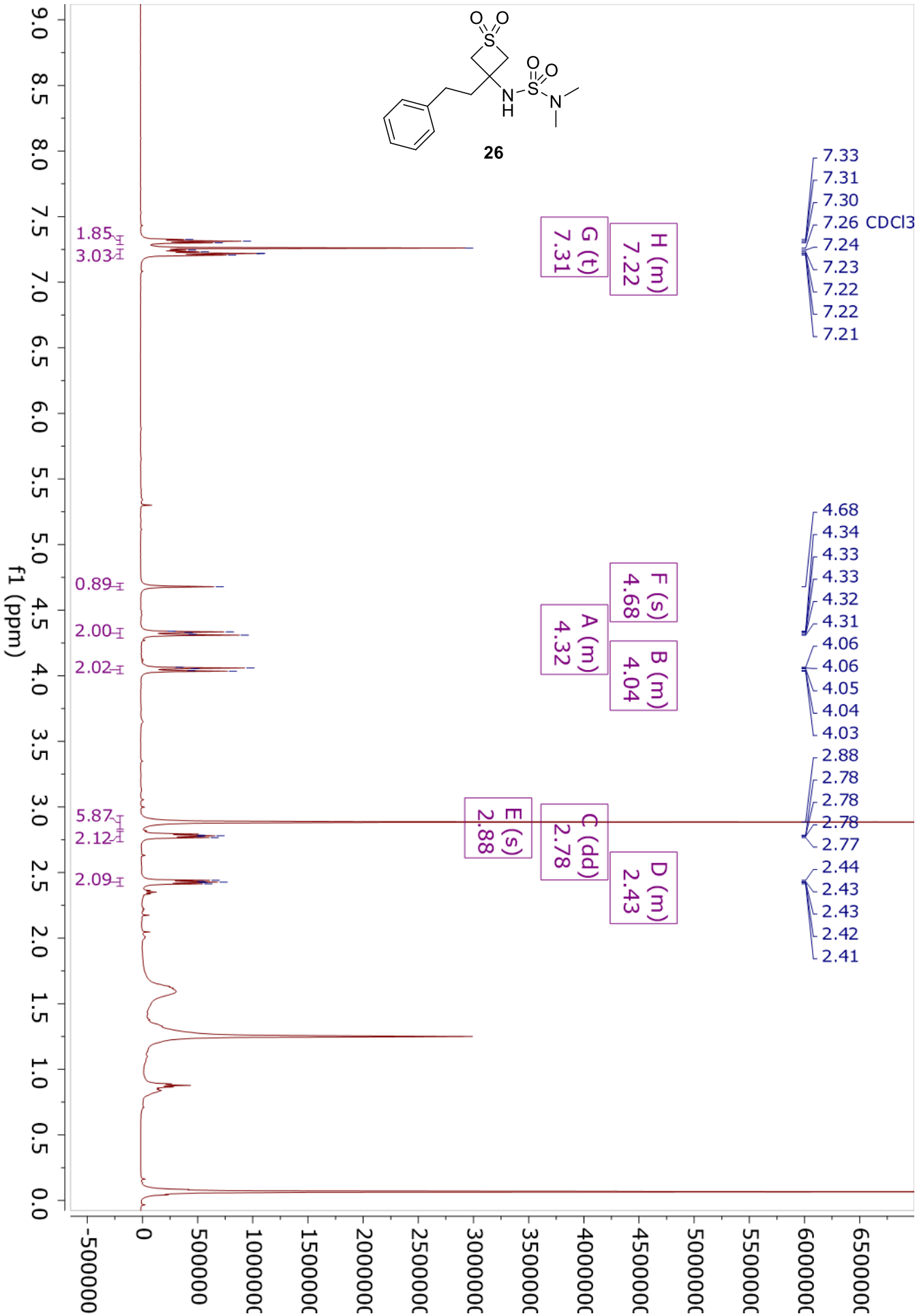

23
140.131
128.887
128.436
126.631
77.160 CDCl3
62.433
50.981
42.531
38.024
29.825
f1 (ppm)

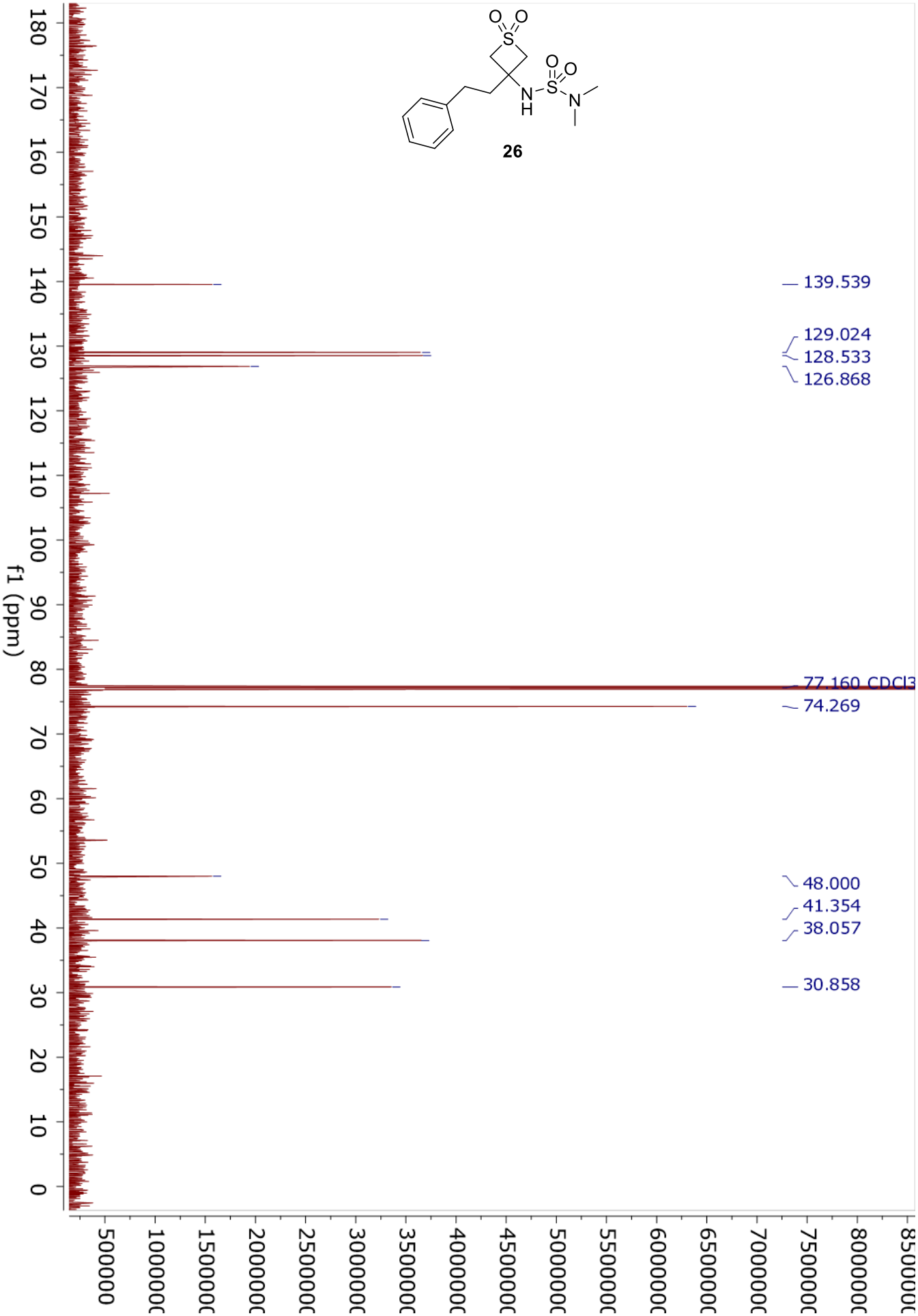

24
f1 (ppm)
1.85
2.82
0.91
1.99
2.14
3.02
2.00
1.98
F (t) 7.31
G (dd) 7.22
E (s) 5.50
D (m) 4.31
C (m) 4.11
H (s) 3.13
A (m) 2.78
B (m) 2.43
7.32
7.31
7.30
7.26 CDCl3
7.25
7.23
7.22
7.20
7.19
5.50
4.32
4.30
4.30
4.12
4.10
4.10
3.13
2.79
2.79
2.78
2.78
2.77
2.44
2.43
2.43
2.43
2.42

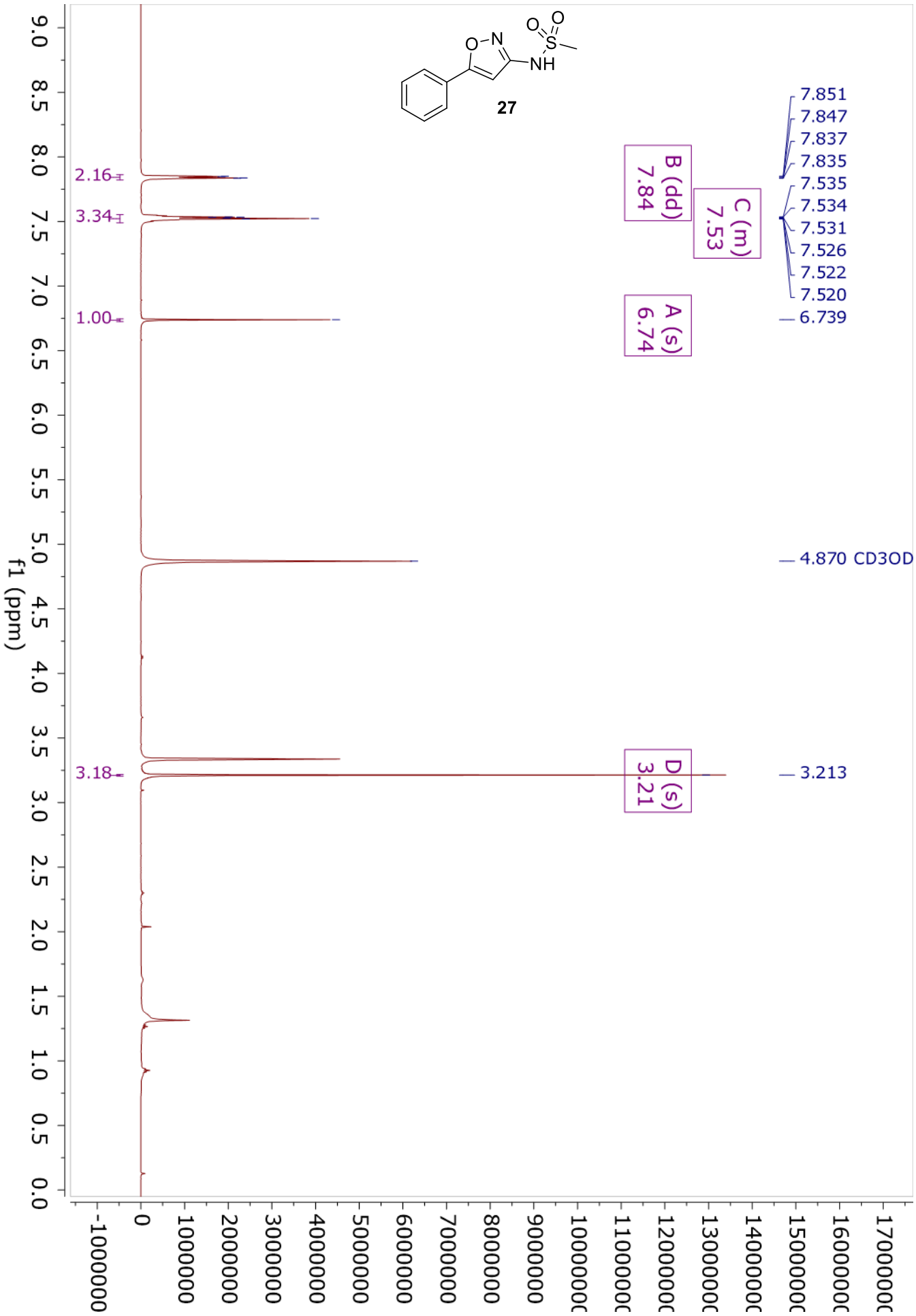

24
139.29
129.06
128.45
126.94
77.16 CDCl3
74.73
48.35
44.75
41.64
30.86
f1 (ppm)

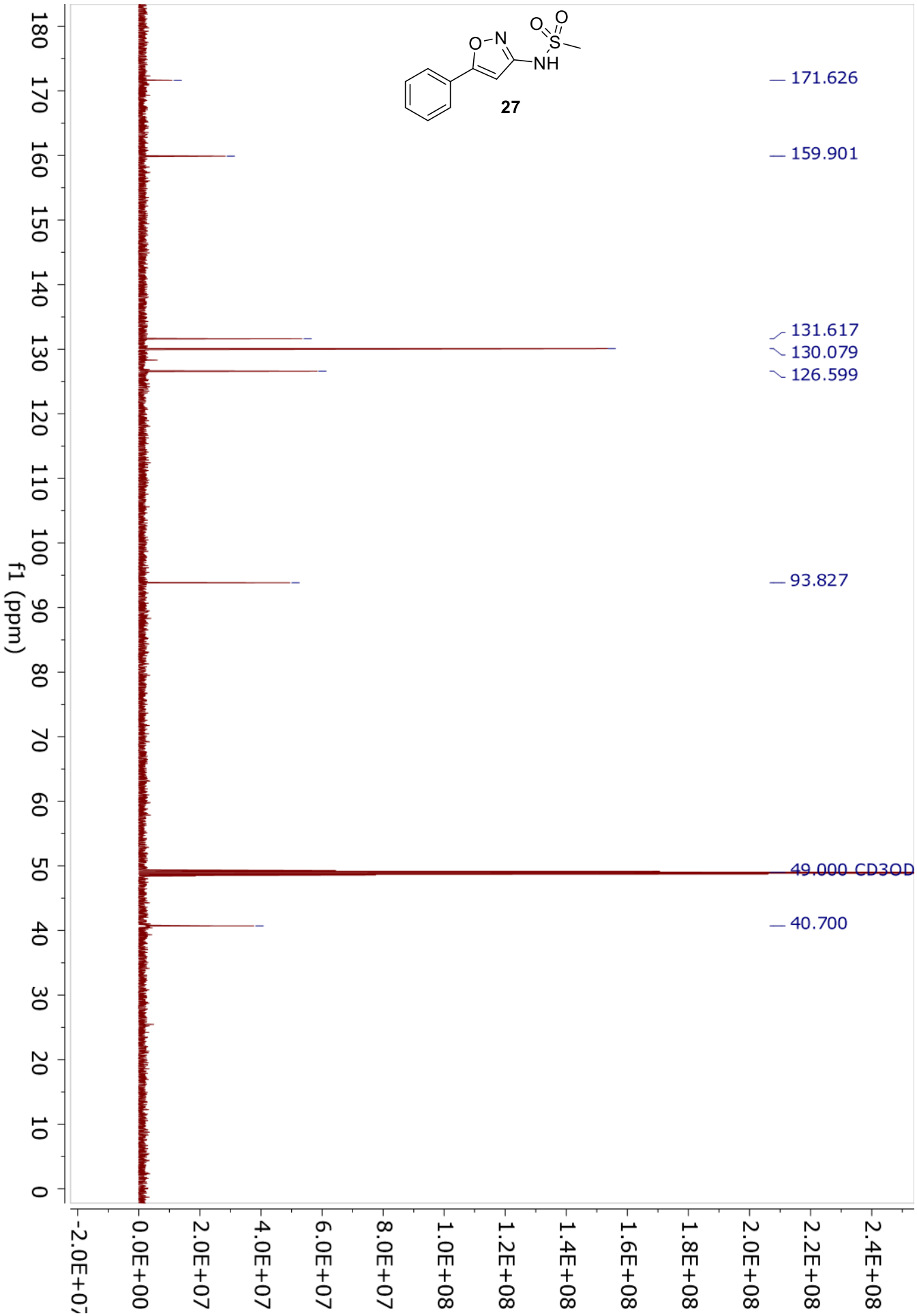

25
E (s) 8.71
F (m) 7.82
G (m) 7.63
H (td) 7.57
I (m) 7.11
J (dd) 7.05
K (m) 6.72
A (m) 4.31
B (d) 4.23
C (m) 2.18
D (m) 1.95
DMSO-d6
f1 (ppm)

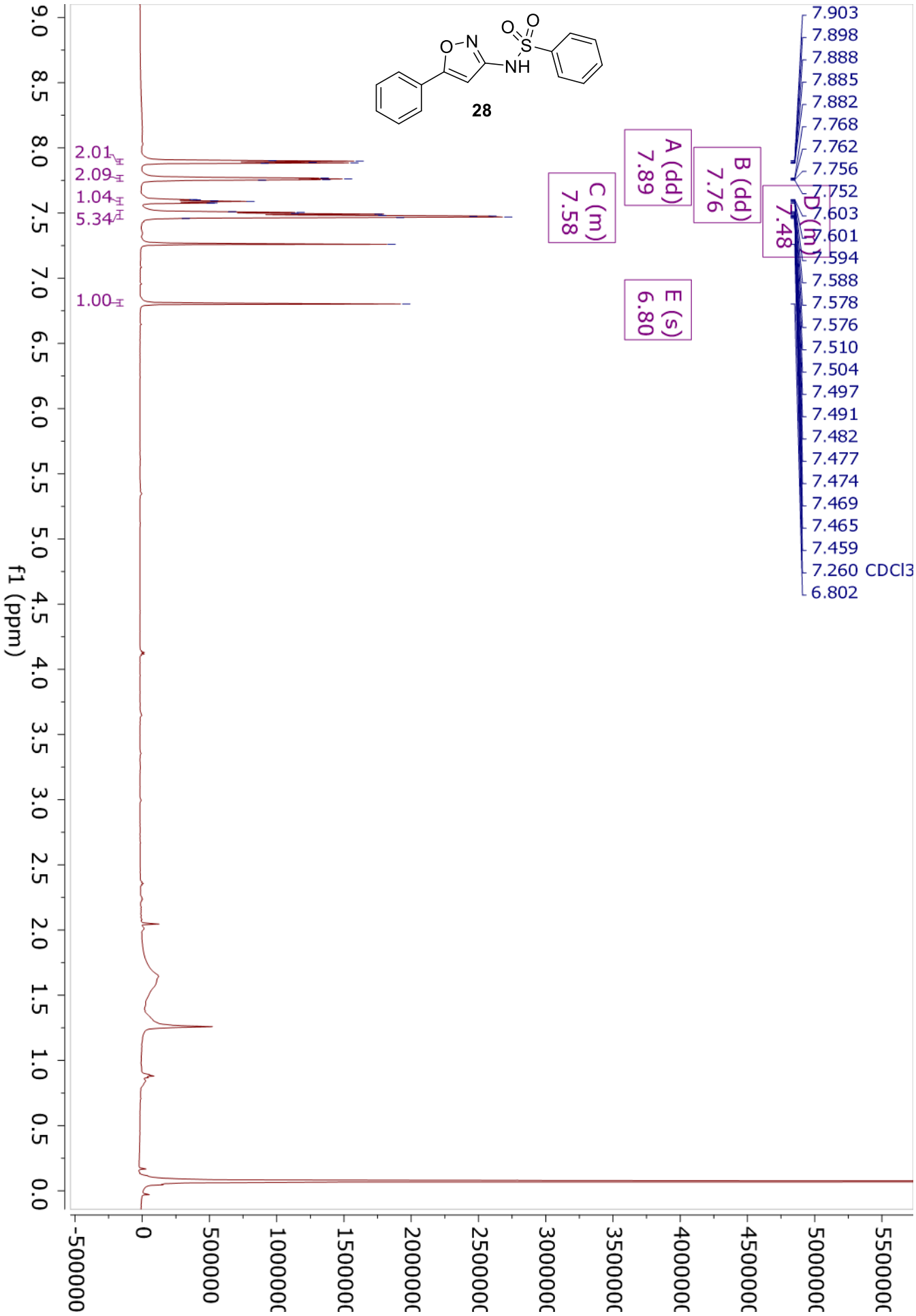

25
142.498
140.490
132.990
129.626
128.289
128.195
126.497
126.004
74.126
46.860
40.969
39.520 DMSO-d6
29.755
f1 (ppm)

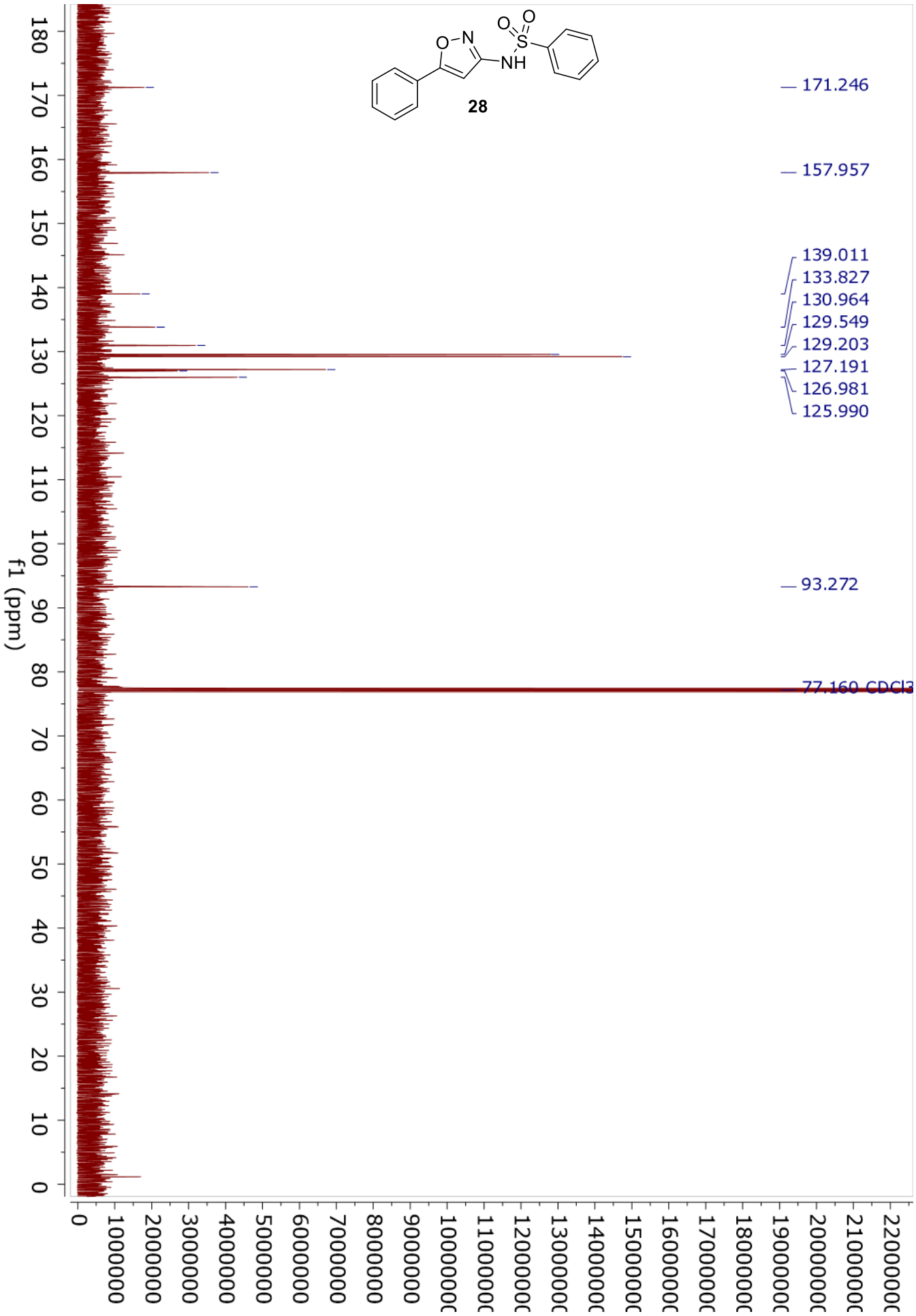

26
7.33
7.31
7.30
7.26 CDCl3
7.24
7.23
7.22
7.22
7.21
4.68
4.34
4.33
4.33
4.32
4.31
4.06
4.06
4.05
4.04
4.03
2.88
2.78
2.78
2.78
2.77
2.44
2.43
2.43
2.42
2.41
H (m) 7.22
G (t) 7.31
F (s) 4.68
A (m) 4.32
B (m) 4.04
E (s) 2.88
C (dd) 2.78
D (m) 2.43
1.85
3.03
0.89
2.00
2.02
5.87
2.12
2.09
f1 (ppm)

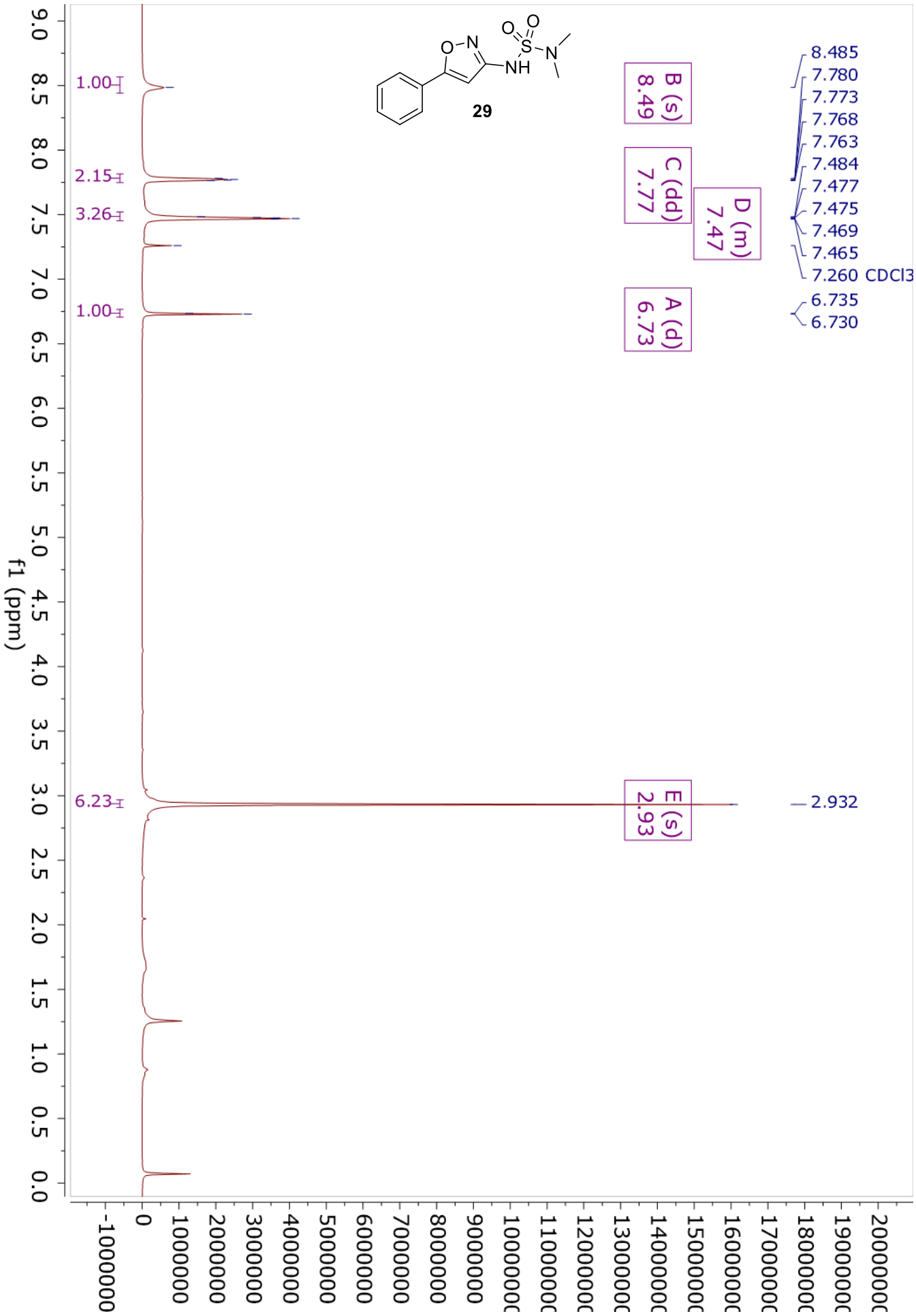

26
139.539
129.024
128.533
126.868
77.160 CDCl3
74.269
48.000
41.354
38.057
30.858
f1 (ppm)

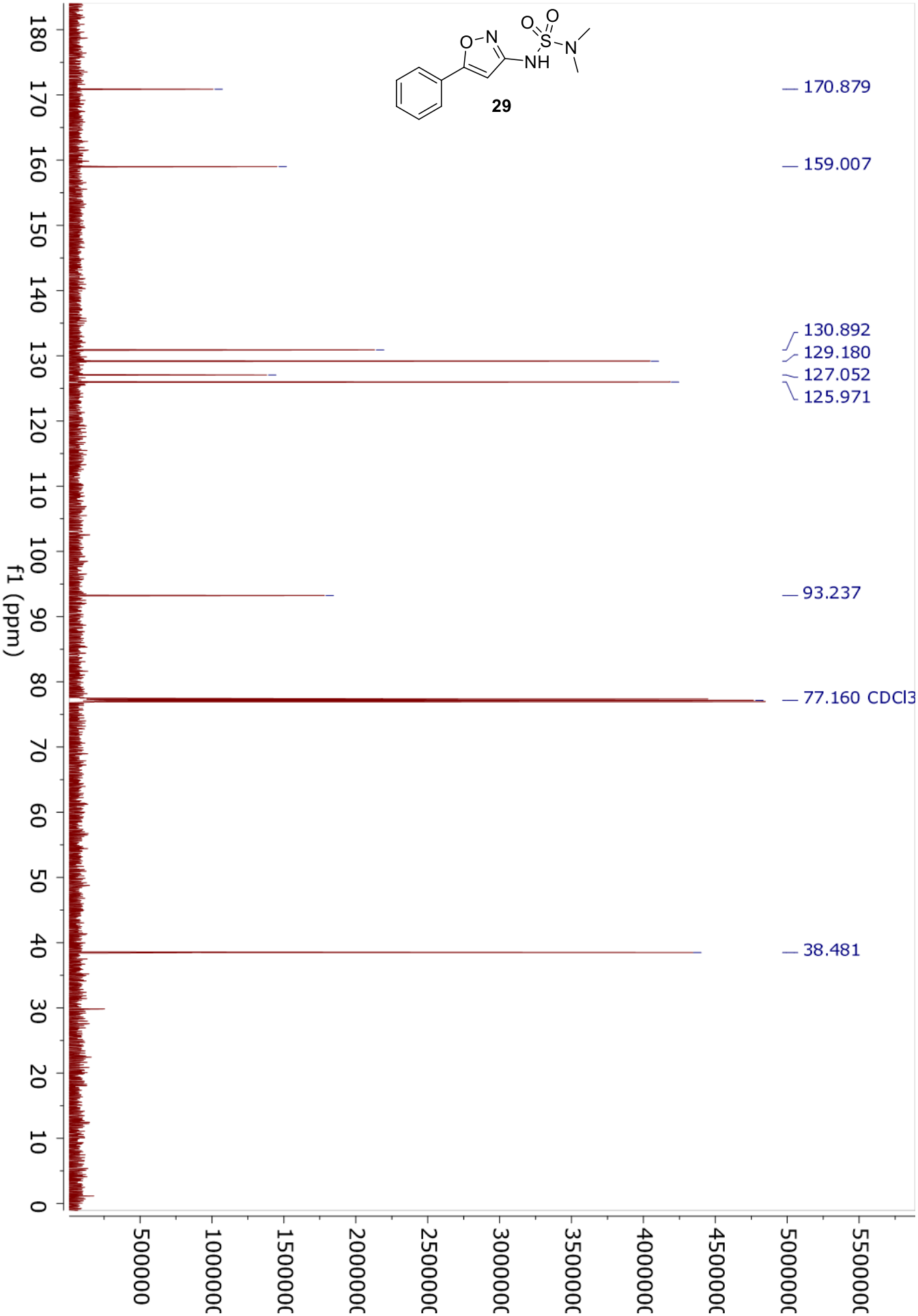

27
7.851
7.847
7.837
7.835
7.535
7.534
7.531
7.526
7.522
7.520
6.739
4.870 CD3OD
3.213
B (dd)
7.84
C (m)
7.53
A (s)
6.74
D (s)
3.21
2.16
3.34
1.00
3.18
f1 (ppm)

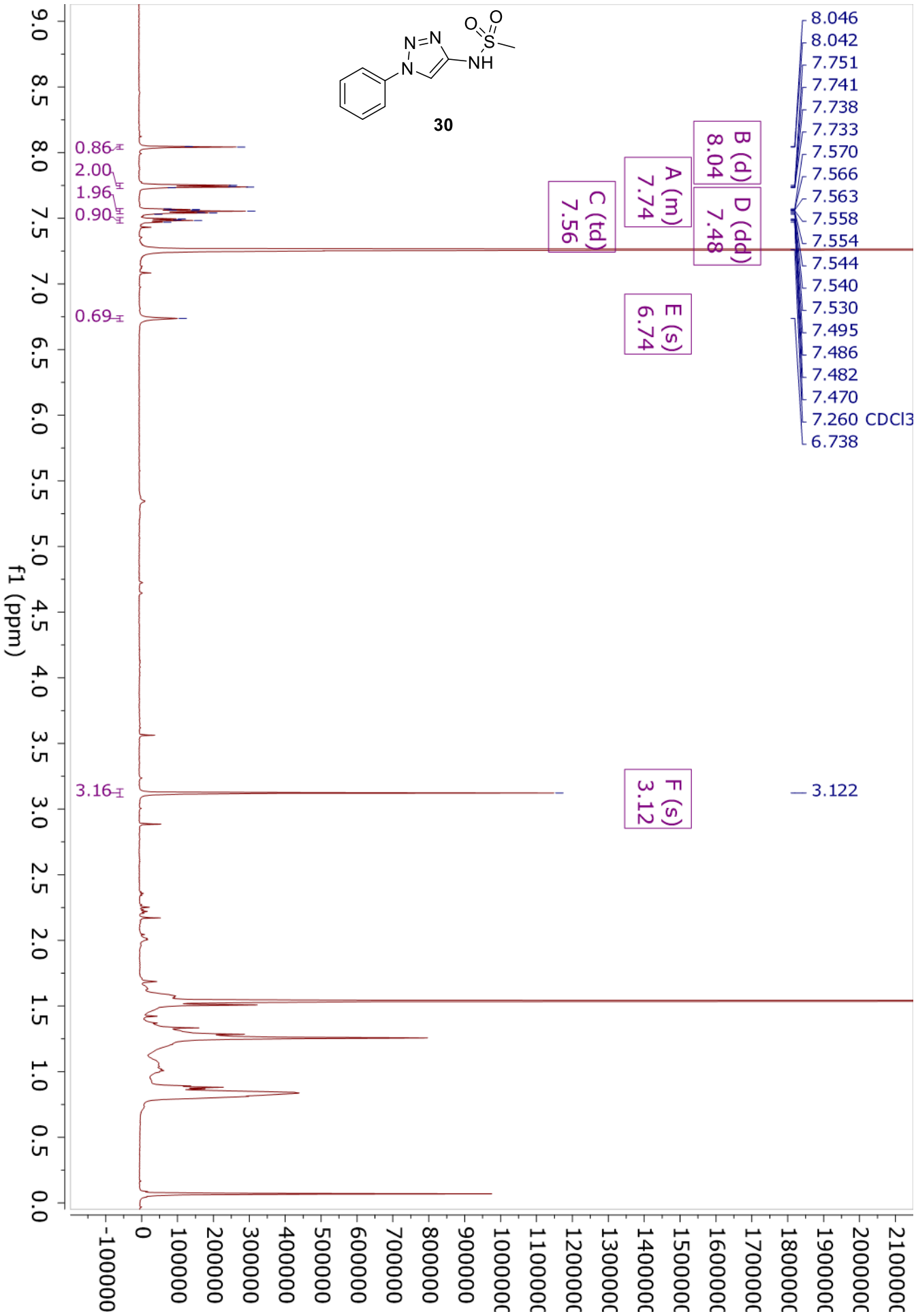

27
171.626
159.901
131.617
130.079
126.599
93.827
49.000 CD3OD
40.700
f1 (ppm)

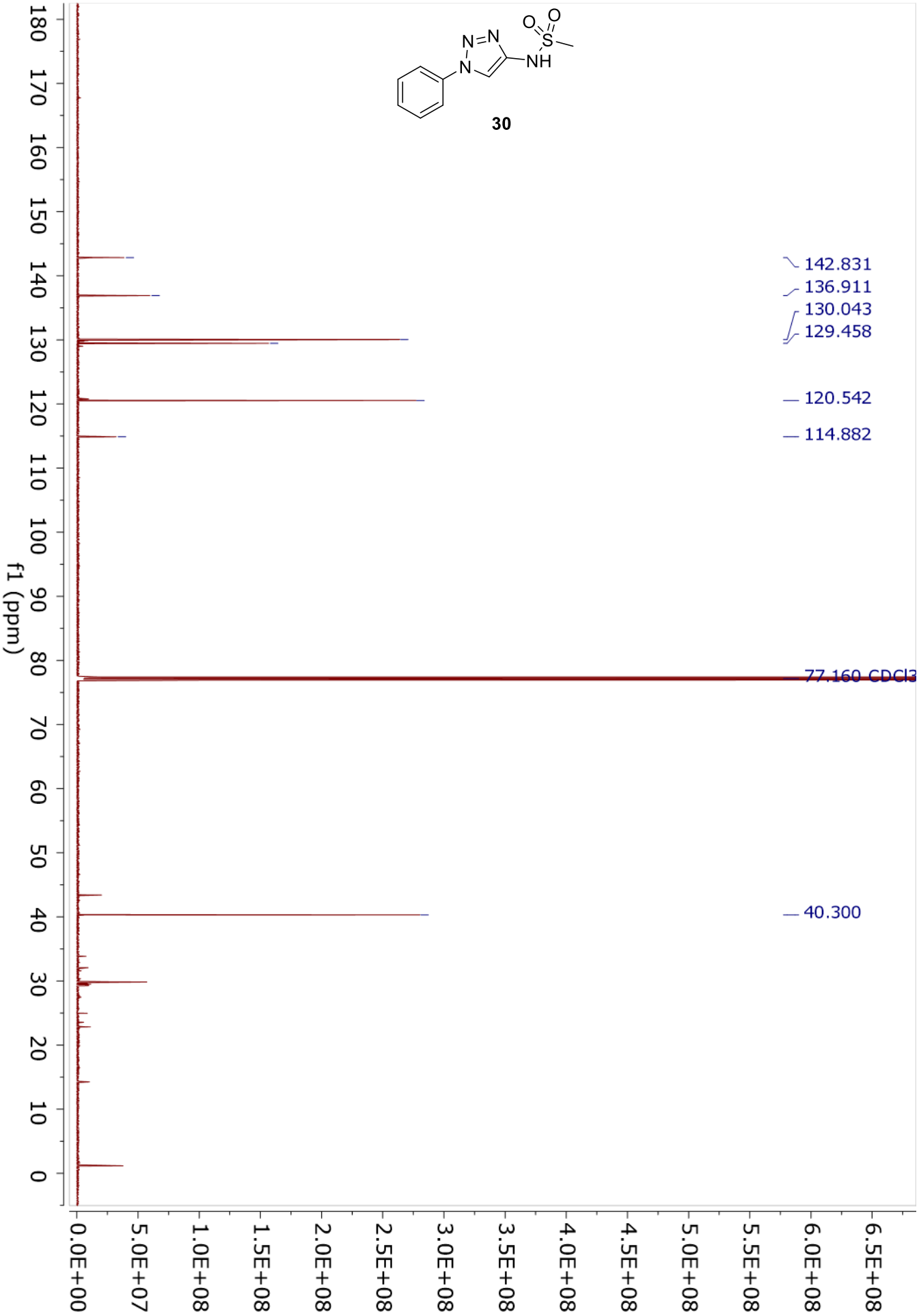

28
A (dd) 7.89
B (dd) 7.76
C (m) 7.58
D (m) 7.48
E (s) 6.80
2.01
2.09
1.04
5.34
1.00
7.903
7.898
7.888
7.885
7.882
7.768
7.762
7.756
7.752
7.603
7.601
7.594
7.588
7.578
7.576
7.510
7.504
7.497
7.491
7.482
7.477
7.474
7.469
7.465
7.459
7.260 CDCl3
6.802
f1 (ppm)

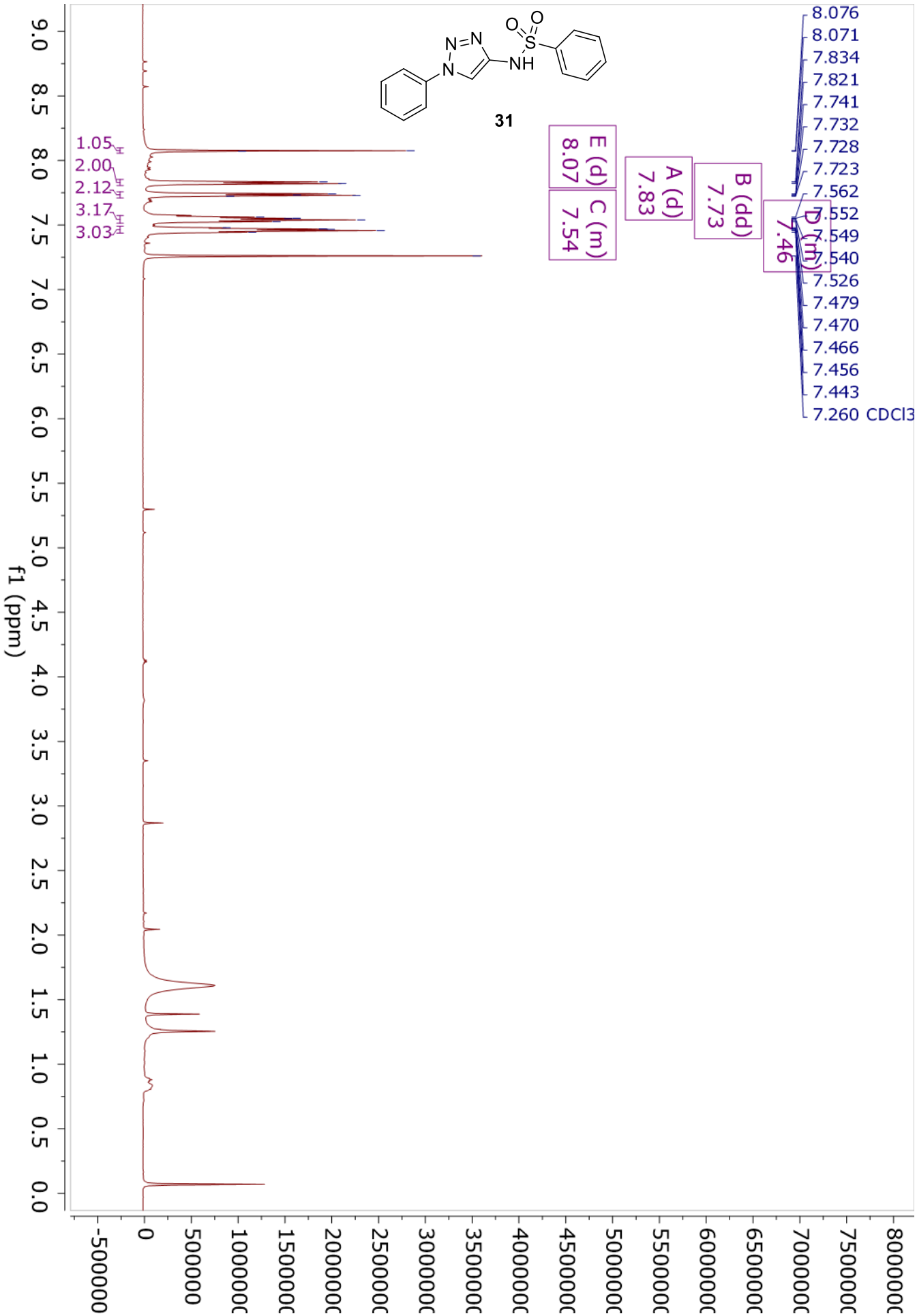

28
171.246
157.957
139.011
133.827
130.964
129.549
129.203
127.191
126.981
125.990
93.272
77.160 CDCl3
f1 (ppm)

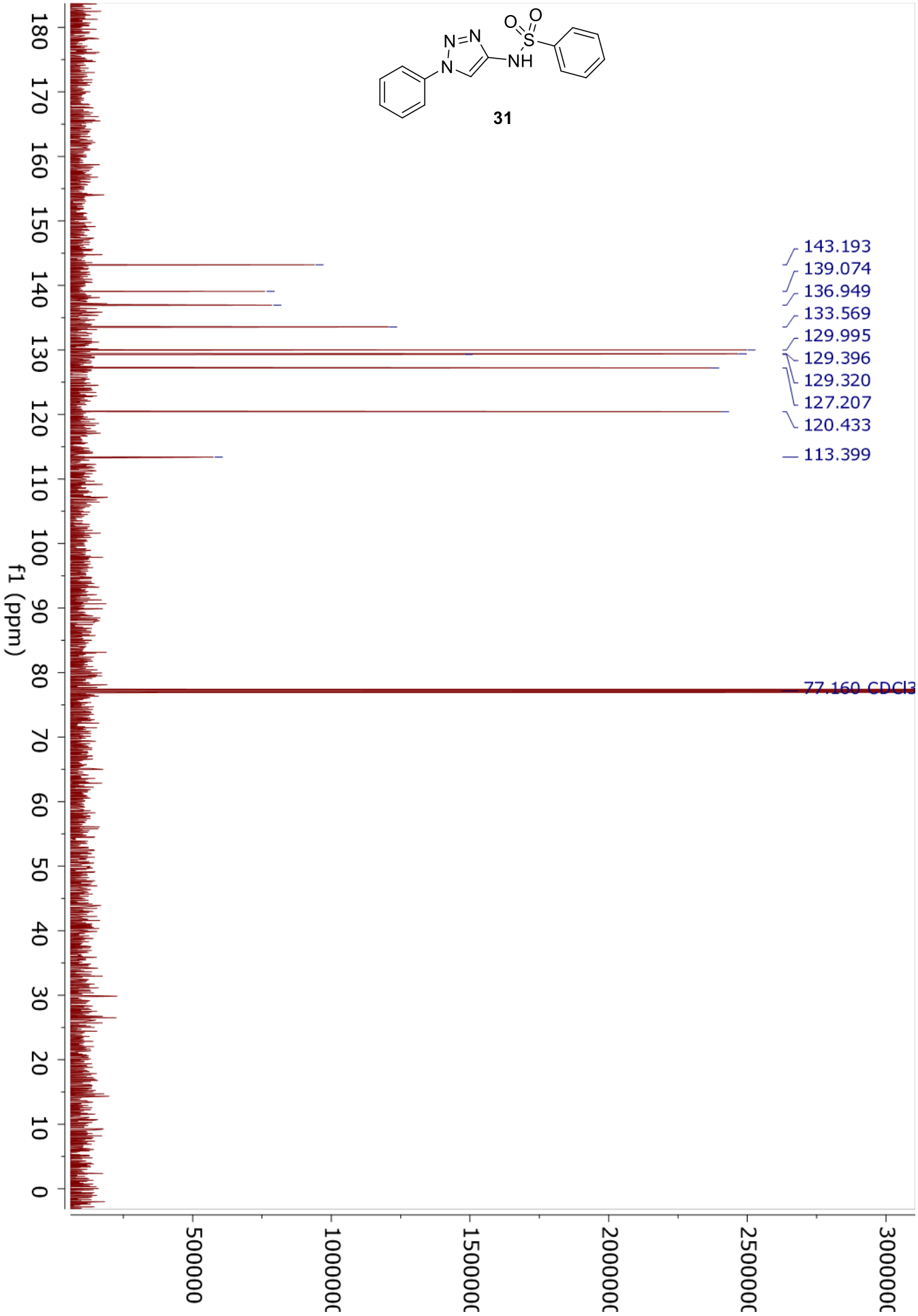

29
B (s) 8.49
C (dd) 7.77
D (m) 7.47
A (d) 6.73
E (s) 2.93
8.485
7.780
7.773
7.768
7.763
7.484
7.477
7.475
7.469
7.465
7.260 CDCl3
6.735
6.730
2.932
1.00
2.15
3.26
1.00
6.23
f1 (ppm)

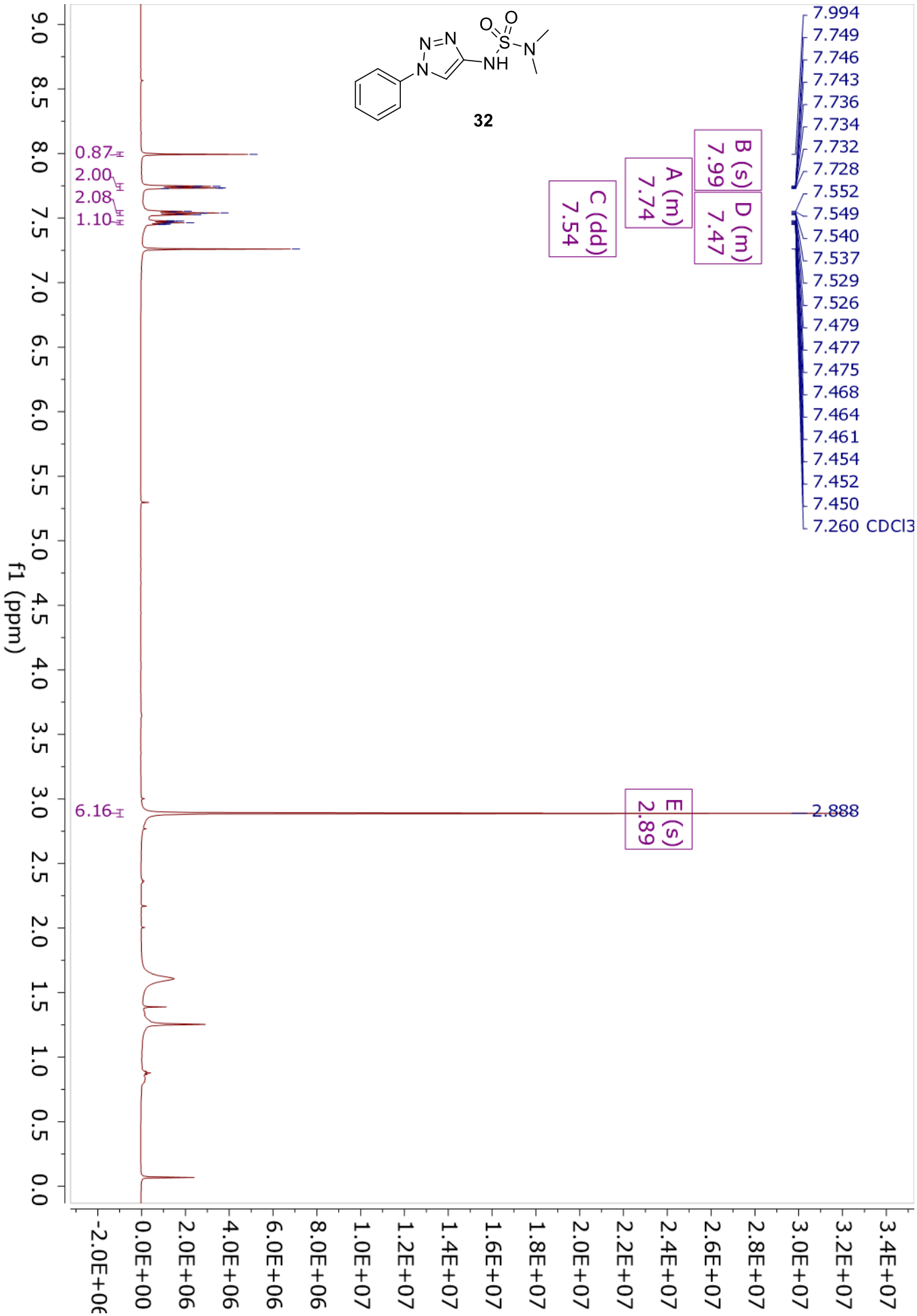

29
170.879
159.007
130.892
129.180
127.052
125.971
93.237
77.160 CDCl3
38.481
f1 (ppm)

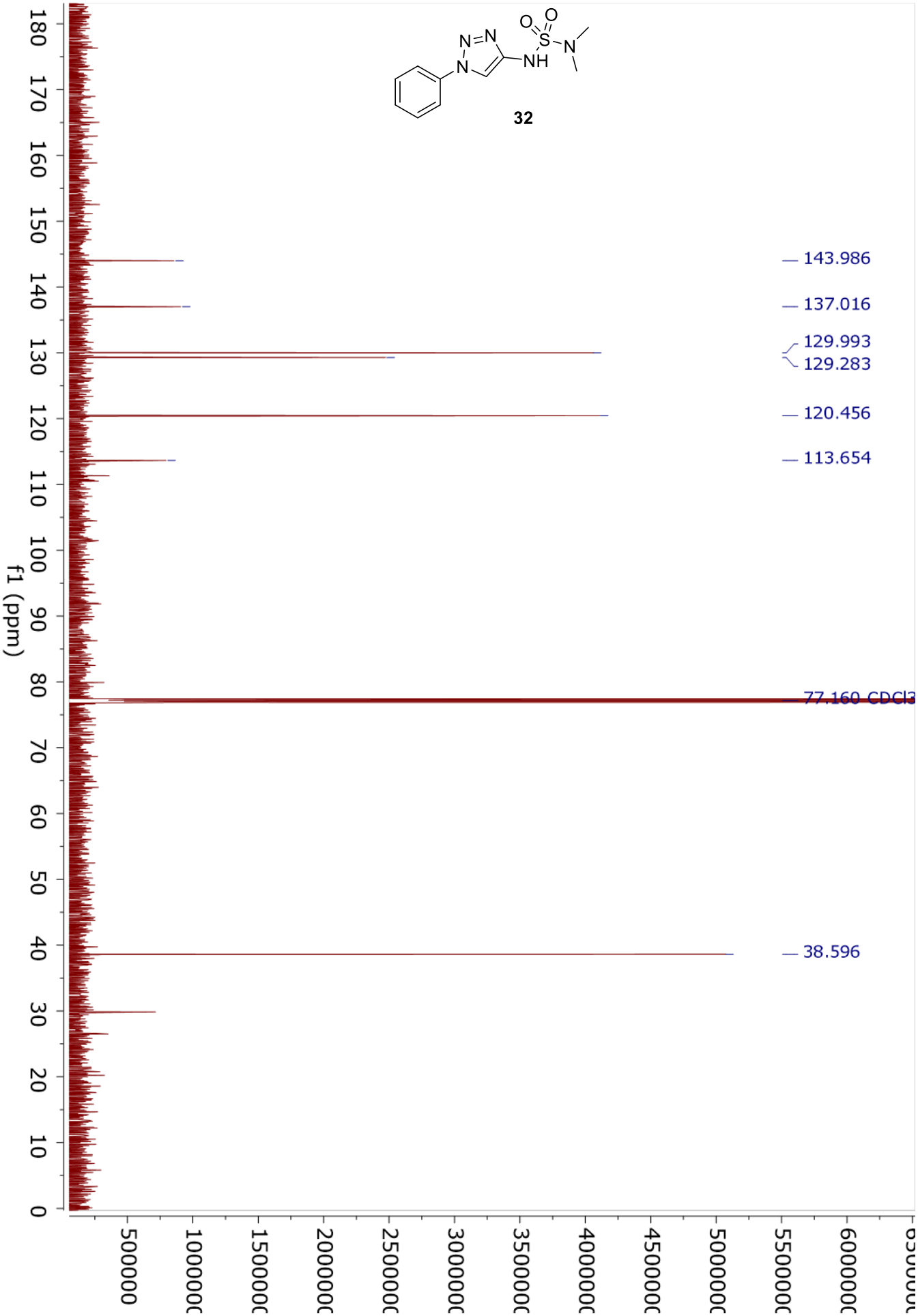

30
0.86
2.00
1.96
0.90
0.69
3.16
A (m) 7.74
B (d) 8.04
C (td) 7.56
D (dd) 7.48
E (s) 6.74
F (s) 3.12
8.046
8.042
7.751
7.741
7.738
7.733
7.570
7.566
7.563
7.558
7.554
7.544
7.540
7.530
7.495
7.486
7.482
7.470
7.260 CDCl3
6.738
3.122
f1 (ppm)


30
142.831
136.911
130.043
129.458
120.542
114.882
77.160 CDCl3
40.300
f1 (ppm)


31
1.05
2.00
2.12
3.17
3.03
E (d) 8.07
C (m) 7.54
A (d) 7.83
B (dd) 7.73
D (m) 7.46
8.076
8.071
7.834
7.821
7.741
7.732
7.728
7.723
7.562
7.552
7.549
7.540
7.526
7.479
7.470
7.466
7.456
7.443
7.260 CDCl3
f1 (ppm)


31
143.193
139.074
136.949
133.569
129.995
129.396
129.320
127.207
120.433
113.399
77.160 CDCl3
f1 (ppm)


32
7.994
7.749
7.746
7.743
7.736
7.734
7.732
7.728
7.552
7.549
7.540
7.537
7.529
7.526
7.479
7.477
7.475
7.468
7.464
7.461
7.454
7.452
7.450
7.260 CDCl3
2.888
B (s) 7.99
D (m) 7.47
A (m) 7.74
C (dd) 7.54
E (s) 2.89
0.87
2.00
2.08
1.10
6.16
f1 (ppm)


32
143.986
137.016
129.993
129.283
120.456
113.654
77.160 CDCl3
38.596
f1 (ppm)

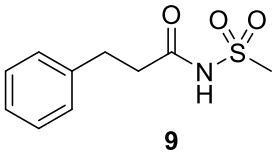
pH-metric Result

Sample name: **BL-0393 (Cpd 9)**
Assay name: **pH-metric pKa**
Assay ID: **20D-20005**
Filename:

Experiment start time: **4/20/2020 2:05:41 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 4.75 ±0.01 (n=50)
RMSD 0.102

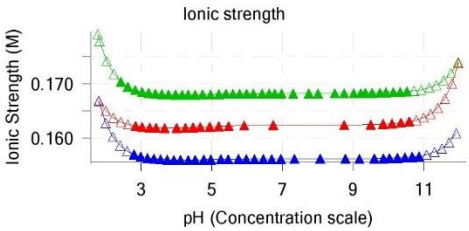


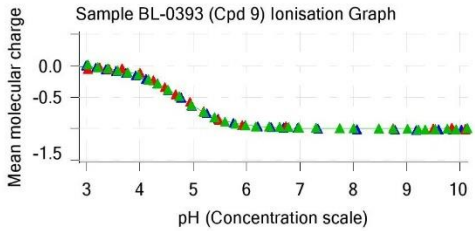
**9**

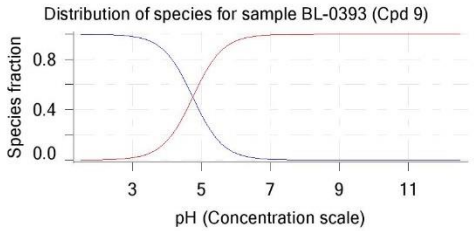
## Warnings and errors

Errors None
Warnings None

## Graphs



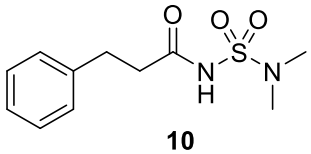



Sample name: **BL-0344 (Cpd 10)**
Assay name: **pH-metric pKa**
Assay ID: **20D-20006**
Filename:

Experiment start time: **4/20/2020 3:02:57 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 5.79 ±0.01 (n=49)
RMSD 0.168

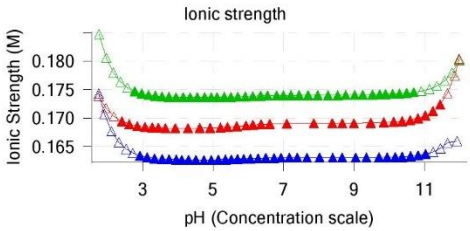


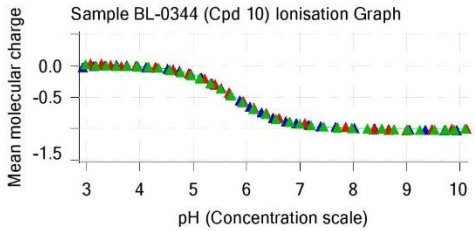
**10**

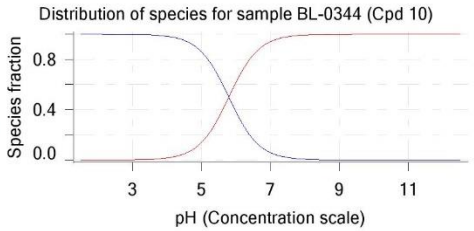
## Warnings and errors

Errors None
Warnings None

## Graphs



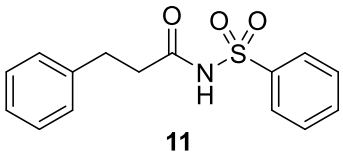
pH-metric Result

Sample name: **BL-0664 (Cpd 11)**
Assay name: **pH-metric pKa**
Assay ID: **19B-19008**
Filename:

Experiment start time: **2/19/2019 1:57:00 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 4.49 ±0.04 (n=49)
RMSD 0.605

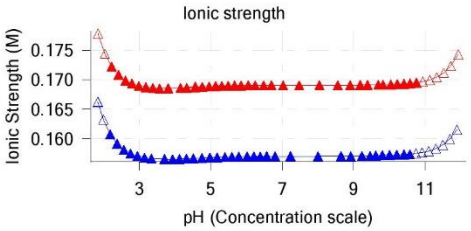


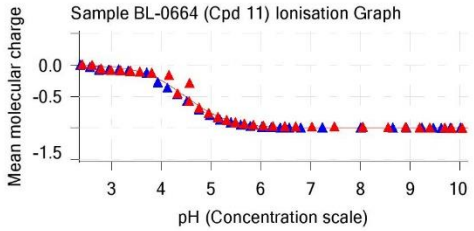
**11**

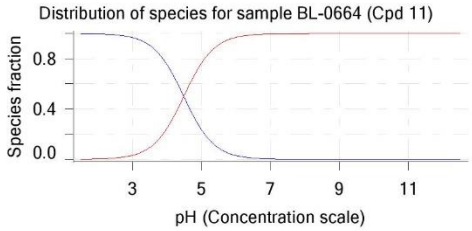
## Warnings and errors

Errors None
Warnings None

## Graphs



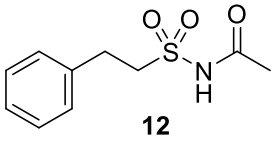



Sample name: **BL-0822 (Cpd 12)**
Assay name: **pH-metric pKa**
Assay ID: **20C-23007**
Filename:

Experiment start time: **3/23/2020 1:19:23 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 4.91 ±0.01 (n=50)
RMSD 0.174

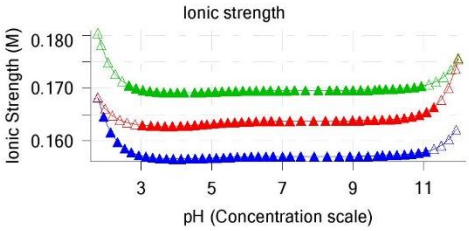


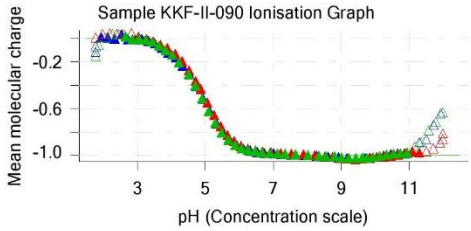

**12**

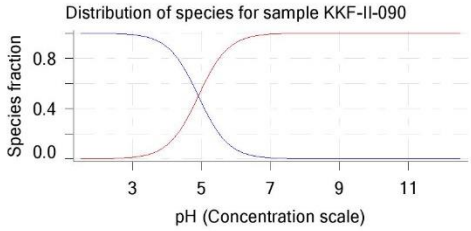
## Warnings and errors

Errors None
Warnings None

## Graphs



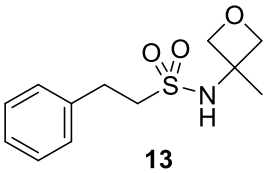



Sample name: **BL-0789 (Cpd 13)**
Assay name: **pH-metric pKa**
Assay ID: **20A-31002**
Filename:

Experiment start time: **1/31/2020 8:34:52 AM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 10.45 ±0.01 (n=50)
RMSD 0.252

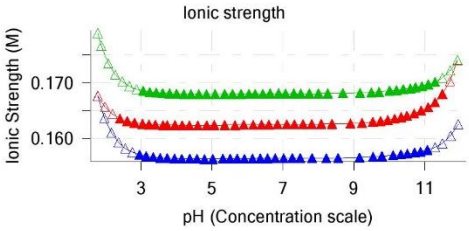


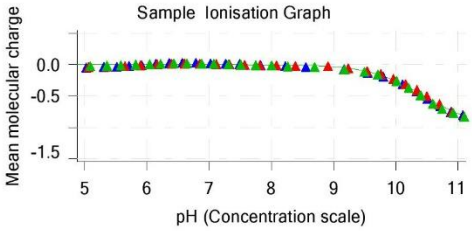
**13**

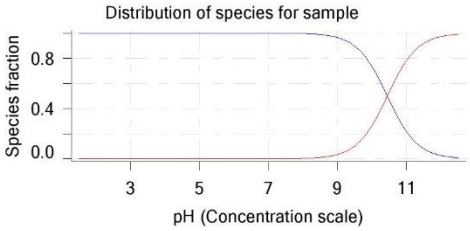
## Warnings and errors

Errors None
Warnings None

## Graphs



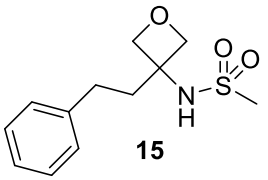
pH-metric Result

Sample name: **BL-0650 (Cpd 15)**
Assay name: **pH-metric pKa**
Assay ID: **18I-12002**
Filename:

Experiment start time: **9/12/2018 2:55:21 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 10.05 ±0.01 (n=49)
RMSD 0.100

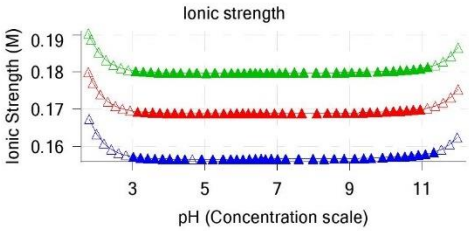


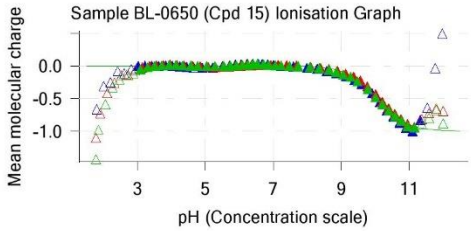

**15**

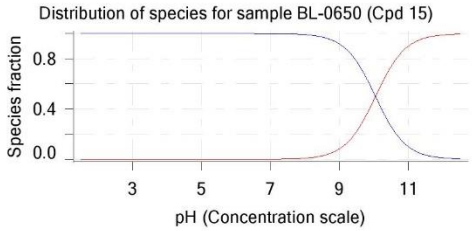
## Warnings and errors

Errors None
Warnings None

## Graphs



# Yasuda-Shedlovsky Result

Sample name: **BL-0658 (Cpd 16)**
Assay name: **pH-metric psKa**
Assay ID: **19B-19012**
Filename:

Experiment start time: **2/19/2019 6:35:49 PM**
Analyst:
Instrument ID: **T317135**

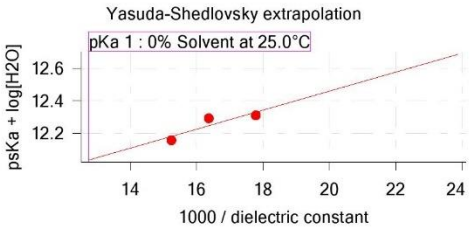
## Yasuda-Shedlovsky result

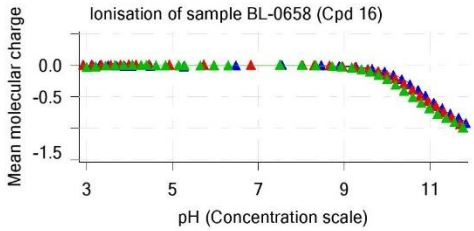
| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 10.29 | ±0.12 | 11.29 | 58.6190 | 0.7880 | 0.170 M | 25.0°C |

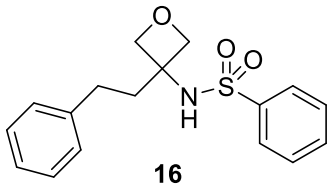
## Warnings and errors

Errors None
Warnings None

## Graphs




**16**

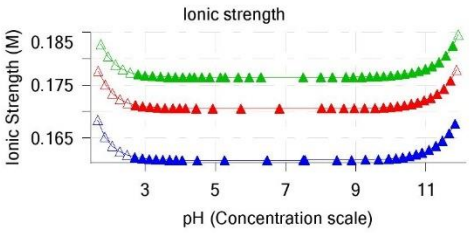
## pH-metric Result

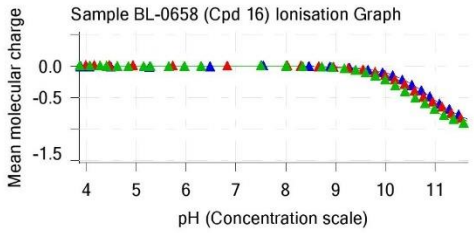
RMSD 0.440

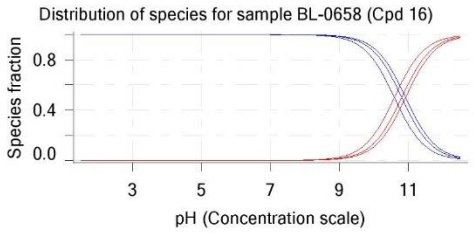
## Warnings and errors

Errors None
Warnings None

## Graphs



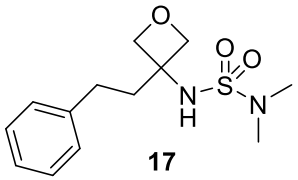



Sample name: **BL-0663 (Cpd 17)**
Assay name: **pH-metric pKa**
Assay ID: **19C-06002**
Filename:

Experiment start time: **3/6/2019 12:17:05 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 11.02 ±0.01 (n=50)
RMSD 0.567

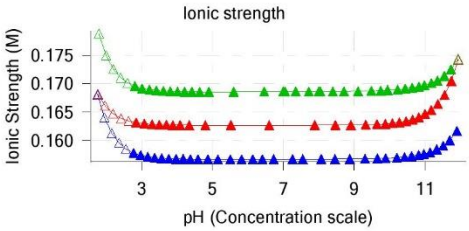


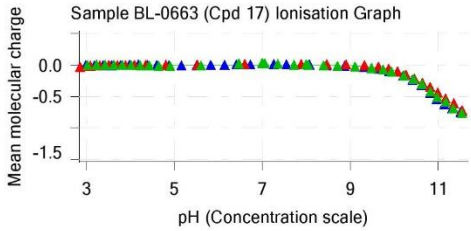
**17**

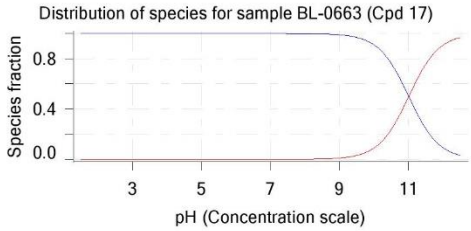
## Warnings and errors

Errors None
Warnings None

## Graphs



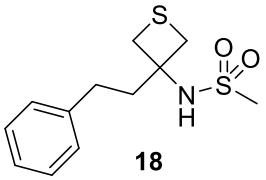



Multiset name: **BL-0667 (Cpd 18)**
Filename:

Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 10.45 ±0.02 (n=50)
RMSD 0.126

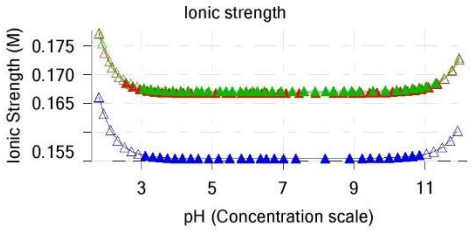


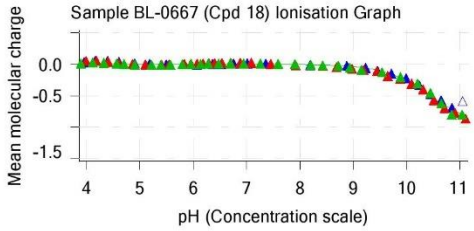

**18**

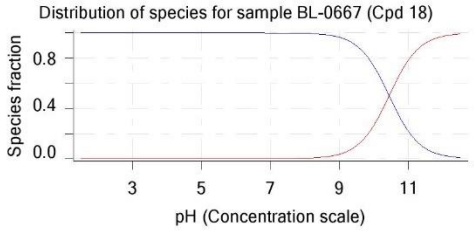
## Warnings and errors

Errors None
Warnings None

## Graphs




## Multiset assays

***Assay 1 of 2***

| | |
|---|---|
| Sample name | pH-metric pKa |
| Assay name | pH-metric pKa |
| Assay ID | 19B-04002 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/5/2019 3:29:09 PM |
| Analyst name | |
| Experiment start time | 2/4/2019 6:02:03 PM |

***Assay 2 of 2***

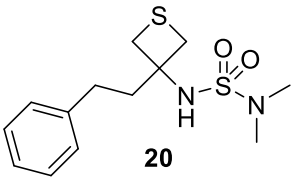
| | |
|---|---|
| Sample name | pH-metric pKa |
| Assay name | pH-metric pKa |
| Assay ID | 19B-07002 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/5/2019 3:29:17 PM |
| Analyst name | |
| Experiment start time | 2/7/2019 10:46:12 AM |

Sample name: **BL-0668 (Cpd 20)**
Assay name: **pH-metric pKa**
Assay ID: **19C-06005**
Filename:

Experiment start time: **3/6/2019 4:28:54 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 11.93 ±0.05 (n=50)
RMSD 0.214

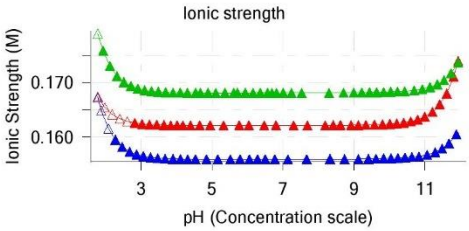


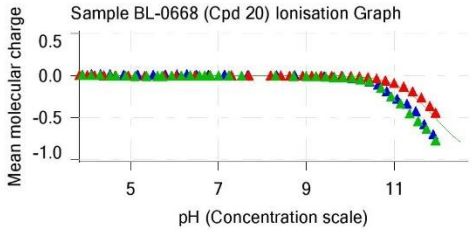

**20**

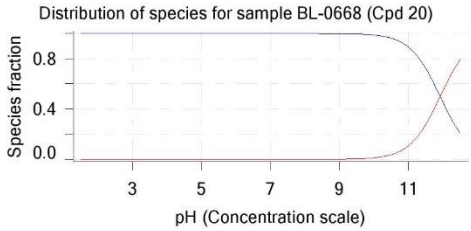
## Warnings and errors

Errors None
Warnings None

## Graphs



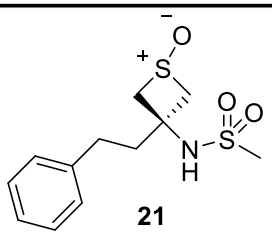



Sample name: **BL-0679 (Cpd 21)**
Assay name: **pH-metric pKa**
Assay ID: **19I-28008**
Filename:

Experiment start time: **9/28/2019 5:22:55 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 9.87 ±0.01 (n=50)
RMSD 0.537

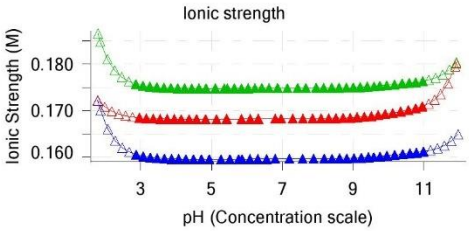


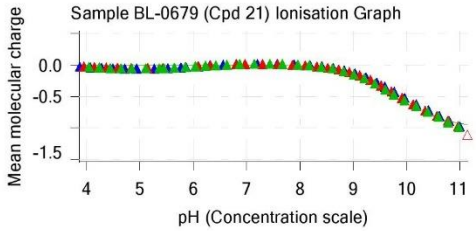
**21**

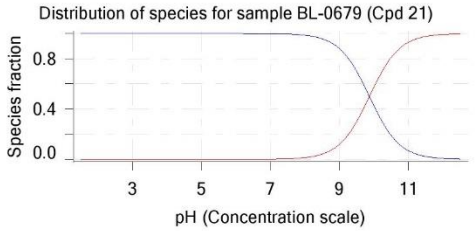
## Warnings and errors

Errors None
Warnings None

## Graphs



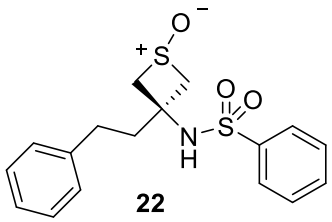



Multiset name: **BL-0688 (Cpd 22)** Instrument ID: **T317135**
Filename:

## pH-metric Result

Acid pKa 1 9.80 ±0.06 (n=50)
RMSD 0.338

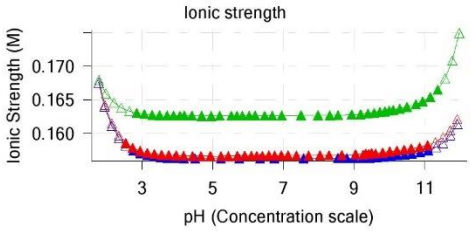


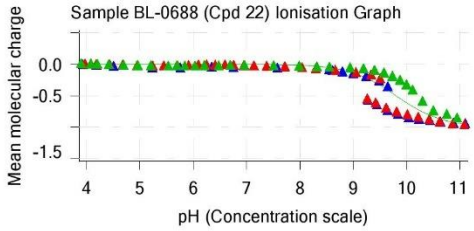

**22**

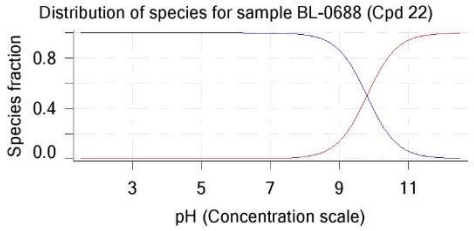
## Warnings and errors

Errors None
Warnings None

## Graphs




## Multiset assays

***Assay 1 of 2***

| | |
|---|---|
| Sample name | pH-metric pKa |
| Assay name | pH-metric pKa |
| Assay ID | 19I-11003 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/5/2019 3:52:40 PM |
| Analyst name | |
| Experiment start time | 9/11/2019 9:26:10 AM |

***Assay 2 of 2***

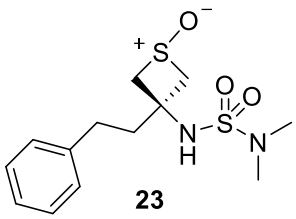
| | |
|---|---|
| Sample name | pH-metric pKa |
| Assay name | pH-metric pKa |
| Assay ID | 19I-11006 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/5/2019 3:52:40 PM |
| Analyst name | |
| Experiment start time | 9/11/2019 12:59:56 PM |

Sample name: **BL-0749 (Cpd 23)**
Assay name: **pH-metric pKa**
Assay ID: **19I-29005**
Filename:

Experiment start time: **9/29/2019 1:25:58 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 10.33 ±0.02 (n=50)
RMSD 0.484

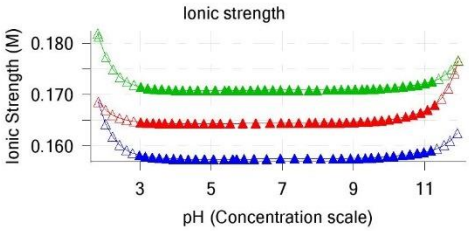


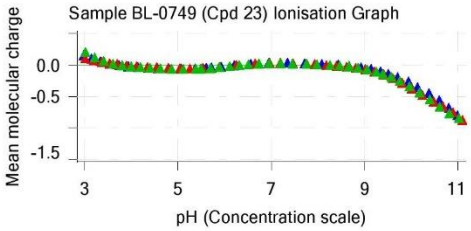
**23**

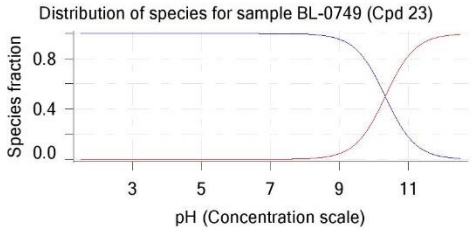
## Warnings and errors

Errors None
Warnings None

## Graphs



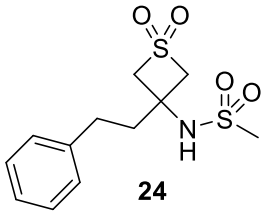



Sample name: **BL-0672 (Cpd 24)**
Assay name: **pH-metric pKa**
Assay ID: **19B-05004**
Filename:

Experiment start time: **2/5/2019 11:59:18 AM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 9.44 ±0.02 (n=50)
RMSD 0.258

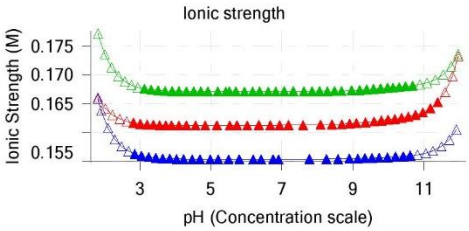


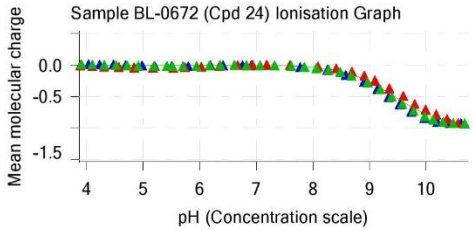

**24**

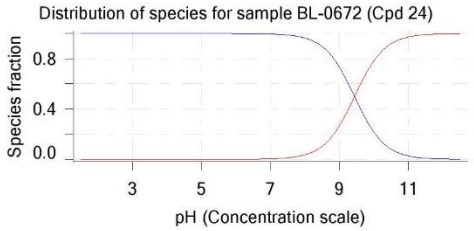
## Warnings and errors

Errors None
Warnings None

## Graphs



# Yasuda-Shedlovsky Result

Multiset name: **BL-0750 (Cpd 25)** Instrument ID: **T317135**
Filename:

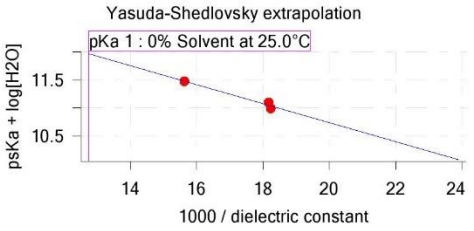
## Yasuda-Shedlovsky result

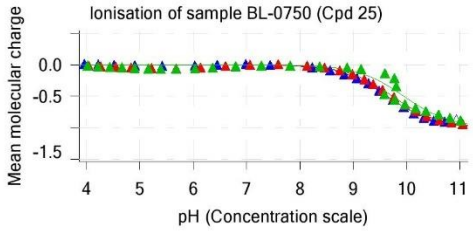
| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 10.22 | ±0.15 | 14.12 | -169.1780 | 0.9673 | 0.158 M | 25.0°C |

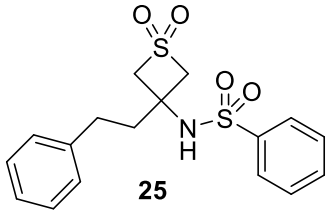
## Warnings and errors

Errors None
Warnings None

## Graphs



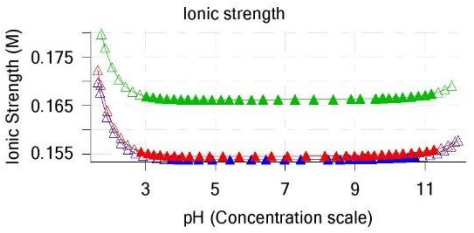

## pH-metric Result

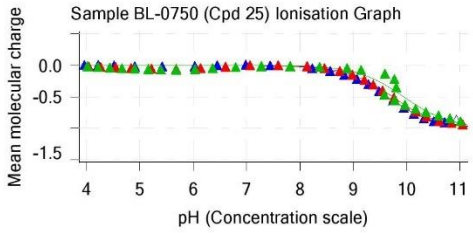
RMSD 0.508

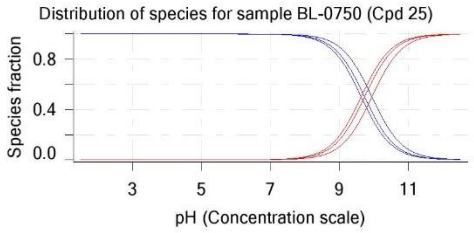
## Warnings and errors

Errors None
Warnings None

## Graphs




## Multiset assays

***Assay 1 of 2***

| | |
|---|---|
| Sample name | 490 pKa |
| Assay name | pH-metric psKa |
| Assay ID | 19I-12005 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/5/2019 3:54:52 PM |
| Analyst name | |
| Experiment start time | 9/12/2019 2:14:23 PM |

***Assay 2 of 2***

| | |
|---|---|
| Sample name | KKF-I-494 pska |
| Assay name | pH-metric psKa |
| Assay ID | 19I-28005 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/5/2019 3:54:52 PM |
| Analyst name | |

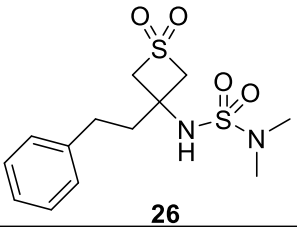
pH-metric Result

Sample name: **BL-0689 (Cpd 26)**
Assay name: **pH-metric pKa**
Assay ID: **19J-05005**
Filename:

Experiment start time: **10/5/2019 12:16:57 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 9.58 ±0.01 (n=50)
RMSD 0.202

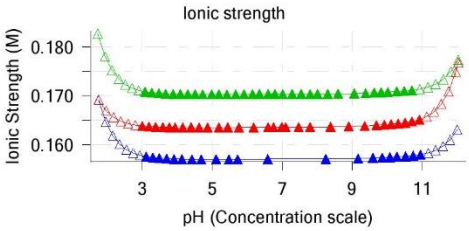


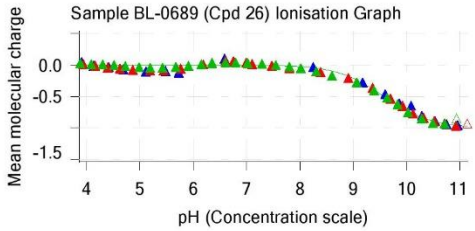
**26**

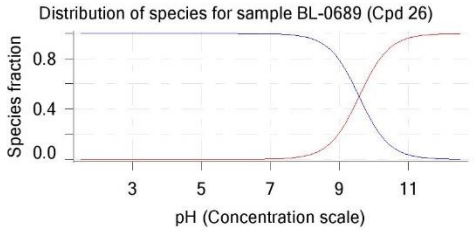
## Warnings and errors

Errors None
Warnings None

## Graphs



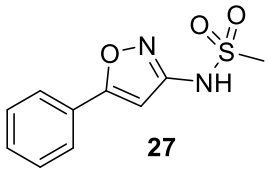



Sample name: **BL-0792 (Cpd 27)**
Assay name: **pH-metric pKa**
Assay ID: **20A-21002**
Filename:

Experiment start time: **1/21/2020 4:32:00 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 5.22 ±0.01 (n=50)
RMSD 0.281

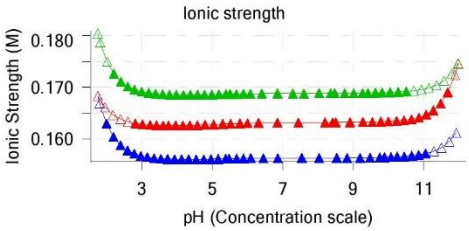


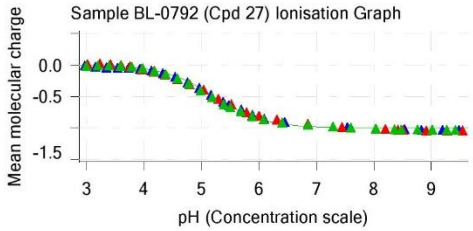

**27**

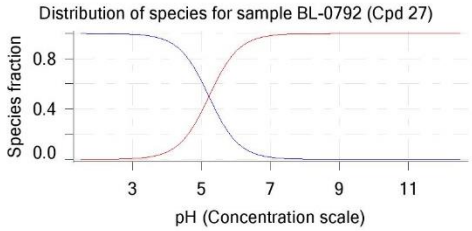
## Warnings and errors

Errors None
Warnings None

## Graphs



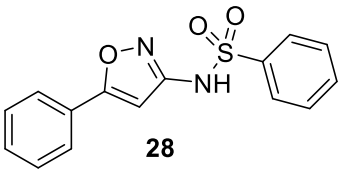



Multiset name: **BL-0793 (Cpd 28)** Instrument ID: **T317135**
Filename:

## pH-metric Result

Acid pKa 1 6.62 ±0.02 (n=50)
RMSD 0.157

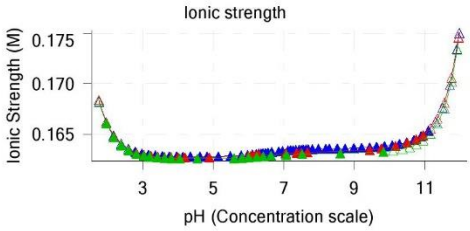


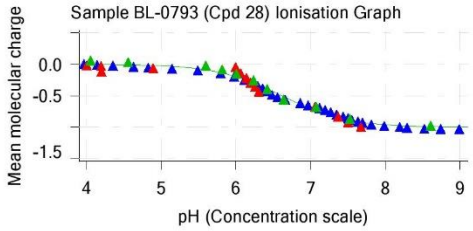

**28**

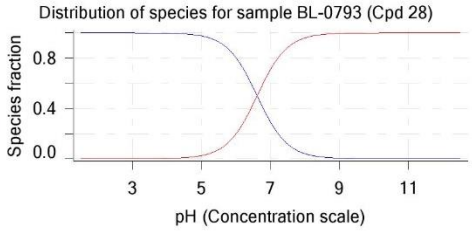
## Warnings and errors

Errors None
Warnings None

## Graphs




## Multiset assays

***Assay 1 of 3***

| | |
|---|---|
| Sample name | KKF-II-028 |
| Assay name | pH-metric pKa |
| Assay ID | 20A-28003 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 1/29/2020 6:18:41 PM |
| Analyst name | |
| Experiment start time | 1/28/2020 10:08:17 AM |

***Assay 2 of 3***

| | |
|---|---|
| Sample name | KKF-II-028 pka |
| Assay name | pH-metric pKa |
| Assay ID | 20A-29002 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 1/29/2020 6:18:44 PM |
| Analyst name | |
| Experiment start time | 1/29/2020 10:41:37 AM |

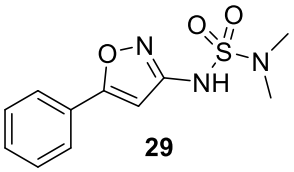
***Assay 3 of 3***

| | |
|---|---|
| Sample name | KKF-II-028 pka |
| Assay name | pH-metric pKa |
| Assay ID | 20A-29005 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 1/29/2020 6:18:45 PM |
| Analyst name | |
| Experiment start time | 1/29/2020 4:45:17 PM |

Multiset name: **BL-0797 (Cpd 29)** Instrument ID: **T317135**
Filename:

## pH-metric Result

Acid pKa 1 5.62 ±0.02 (n=50)
RMSD 0.148

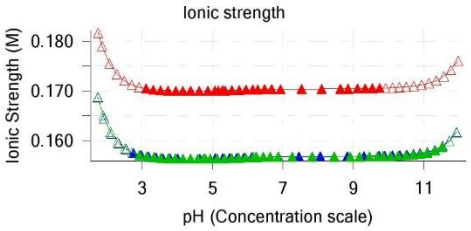


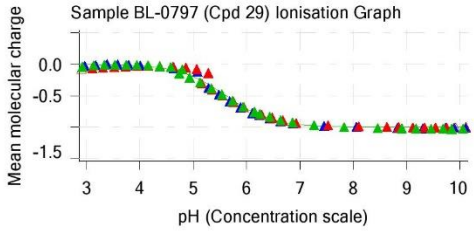

**29**

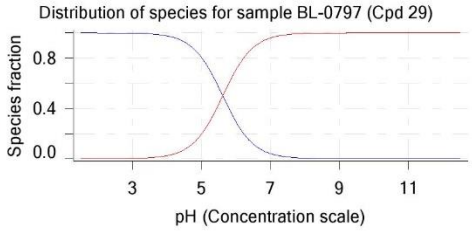
## Warnings and errors

Errors None
Warnings None

## Graphs




## Multiset assays

***Assay 1 of 2***

| | |
|---|---|
| Sample name | KKF-II-031 pka |
| Assay name | pH-metric pKa |
| Assay ID | 20A-27003 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 1/27/2020 5:16:57 PM |
| Analyst name | |
| Experiment start time | 1/27/2020 3:59:26 PM |

***Assay 2 of 2***

| | |
|---|---|
| Sample name | KKF-II-031 pka |
| Assay name | pH-metric pKa |
| Assay ID | 20A-27002 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 1/27/2020 5:17:02 PM |
| Analyst name | |
| Experiment start time | 1/27/2020 3:16:05 PM |

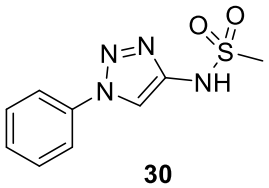
pH-metric Result

Sample name: **BL-0771 (Cpd 30)**
Assay name: **pH-metric pKa**
Assay ID: **19J-25002**
Filename:

Experiment start time: **10/25/2019 2:43:03 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 6.34 ±0.01 (n=50)
RMSD 0.104

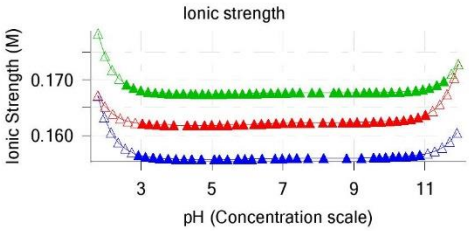


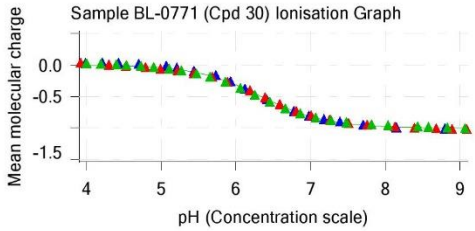
**30**

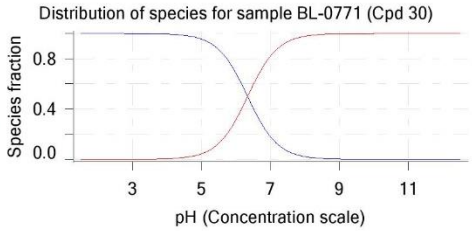
## Warnings and errors

Errors None
Warnings None

## Graphs



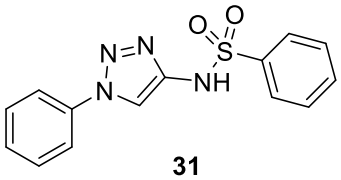



Multiset name: **BL-0772 (Cpd 31)** Instrument ID: **T317135**
Filename:

## pH-metric Result

Acid pKa 1 5.93 ±0.05 (n=50)
RMSD 0.136

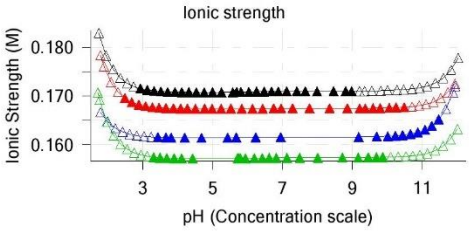


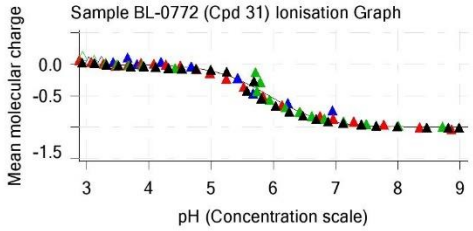
**31**

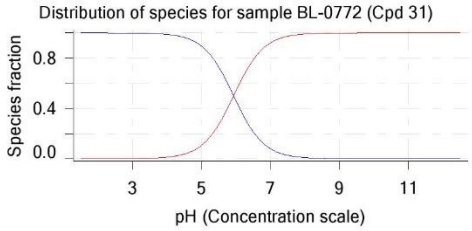
## Warnings and errors

Errors None
Warnings None

## Graphs




## Multiset assays

***Assay 1 of 2***

| | |
|---|---|
| Sample name | KKF-I-535 |
| Assay name | pH-metric pKa |
| Assay ID | 19J-26003 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/26/2019 12:47:21 PM |
| Analyst name | |
| Experiment start time | 10/26/2019 11:57:30 AM |

***Assay 2 of 2***

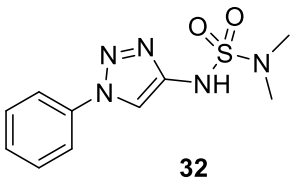
| | |
|---|---|
| Sample name | KKF-I-535 |
| Assay name | pH-metric pKa |
| Assay ID | 19J-19005 |
| Instrument ID | T317135 |
| Imported from | |
| Imported on | 10/26/2019 12:47:33 PM |
| Analyst name | |
| Experiment start time | 10/19/2019 2:00:20 PM |

Sample name: **BL-0773 (Cpd 32)**
Assay name: **pH-metric pKa**
Assay ID: **19J-20005**
Filename:

Experiment start time: **10/20/2019 12:36:44 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

Acid pKa 1 6.42 ±0.01 (n=50)
RMSD 0.174

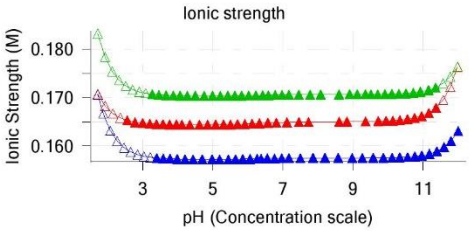


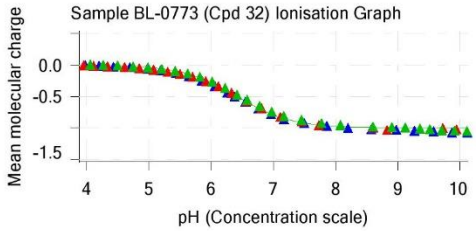
**32**

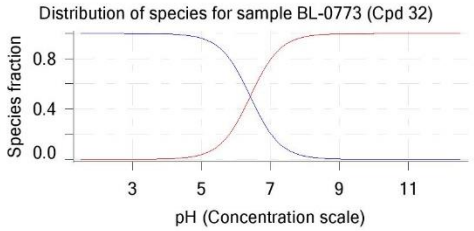
## Warnings and errors

Errors None
Warnings None

## Graphs



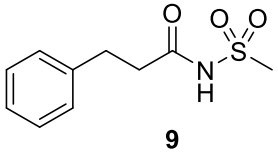
# pH-metric Result

Sample name: **BL-0393 (Cpd 9)**
Assay name: **pH-metric medium logP**
Assay ID: **20D-21010**
Filename:

Experiment start time: **4/21/2020 3:53:14 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.10 | ±0.01 (n=50) |
| logP (X -) | -0.69 | ±0.08 (n=50) |
| RMSD | 0.199 | |



**9**

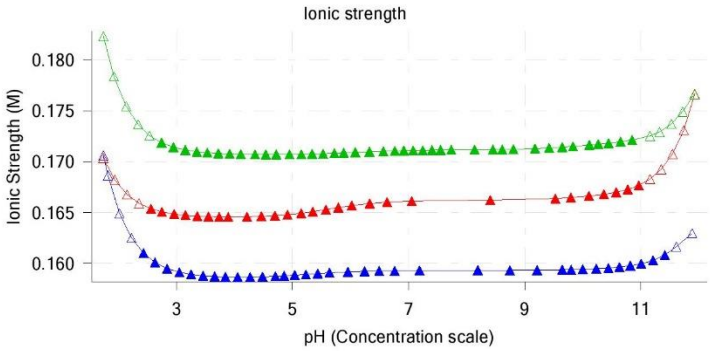
## Warnings and errors

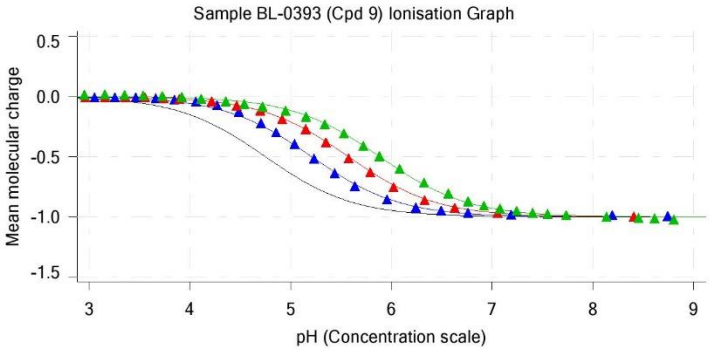
Errors None
Warnings None

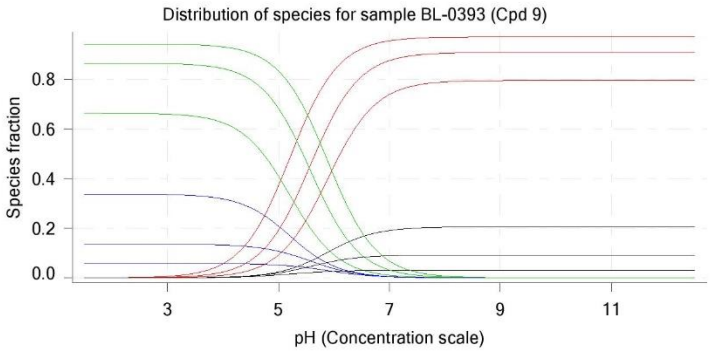
## Sample logD values

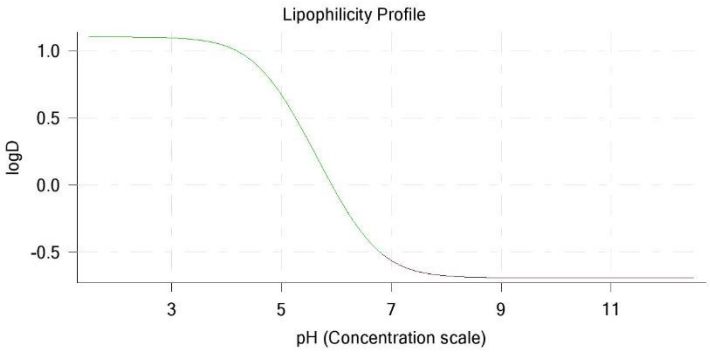
| pH | BL-0393 (Cpd 9) logD | Comment |
|---|---|---|
| 1.000 | 1.10 | |
| 1.200 | 1.10 | Stomach pH |
| 2.000 | 1.10 | |
| 3.000 | 1.10 | |
| 4.000 | 1.03 | |
| 5.000 | 0.67 | |
| 6.000 | -0.06 | |
| 6.500 | -0.38 | |
| 7.000 | -0.56 | |
| 7.400 | -0.64 | Blood pH |
| 8.000 | -0.68 | |
| 9.000 | -0.69 | |
| 10.000 | -0.69 | |
| 11.000 | -0.69 | |
| 12.000 | -0.69 | |

## Graphs



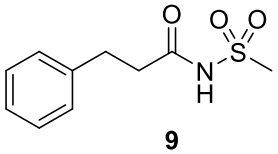



Multiset name: **BL-0393 (Cpd 9) CYCLOHEXANE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | -1.03 | ±0.03 (n=50) |
| logP (X -) | -8.96 | ±0.92 (n=50) |
| RMSD | 0.112 | |



**9**

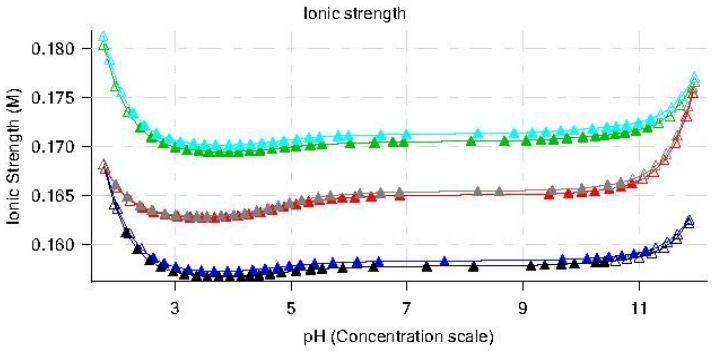
## Warnings and errors

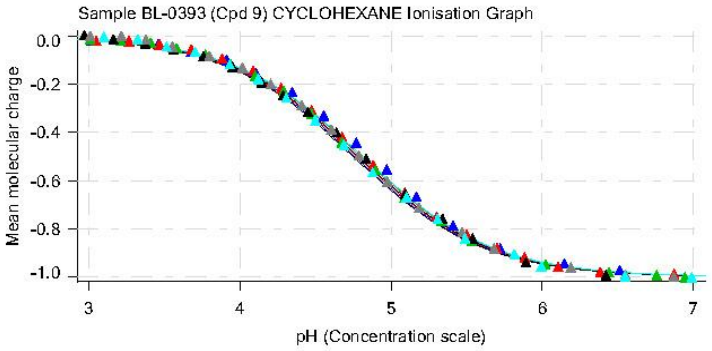
Errors None
Warnings None

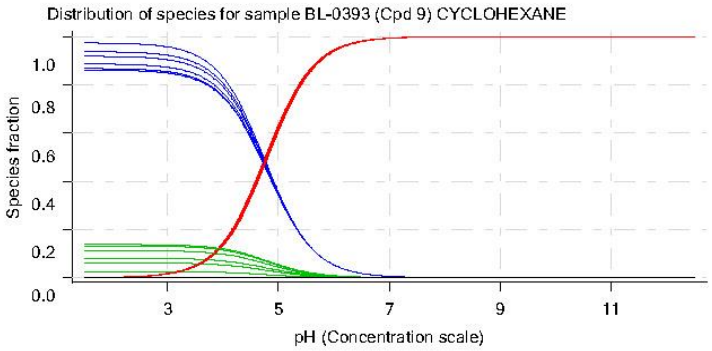
## Sample logD values

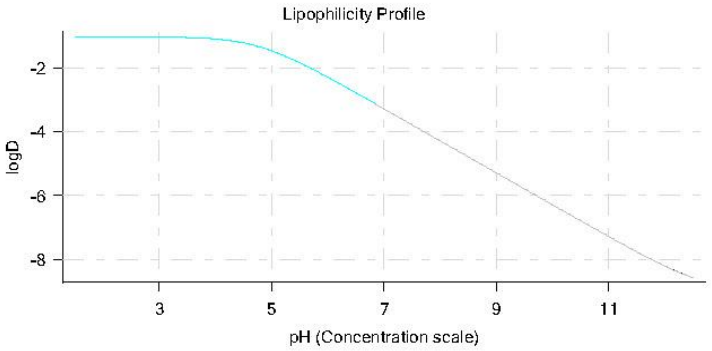
| pH | BL-0393 (Cpd 9) logD | Comment |
|---|---|---|
| 1.000 | -1.03 | |
| 1.200 | -1.03 | Stomach pH |
| 2.000 | -1.03 | |
| 3.000 | -1.04 | |
| 4.000 | -1.10 | |
| 5.000 | -1.47 | |
| 6.000 | -2.30 | |
| 6.500 | -2.79 | |
| 7.000 | -3.28 | |
| 7.400 | -3.68 | Blood pH |
| 8.000 | -4.28 | |
| 9.000 | -5.28 | |
| 10.000 | -6.28 | |
| 11.000 | -7.27 | |
| 12.000 | -8.20 | |

## Graphs



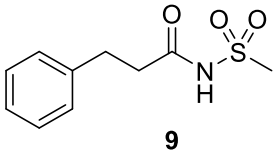



Multiset name: **BL-0393 (Cpd 9) HEPTANE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

logP (neutral XH) -0.53 ±0.04 (n=50)
logP (X -) -7.93 ±0.72 (n=50)
RMSD 0.319



**9**

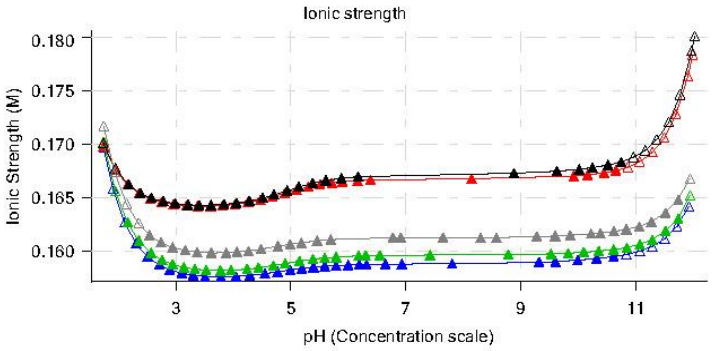
## Warnings and errors

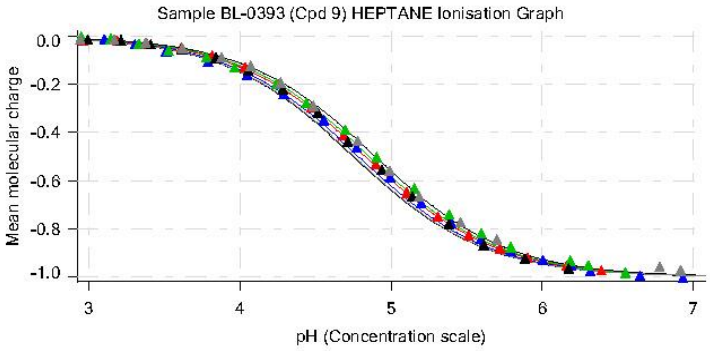
Errors None
Warnings None

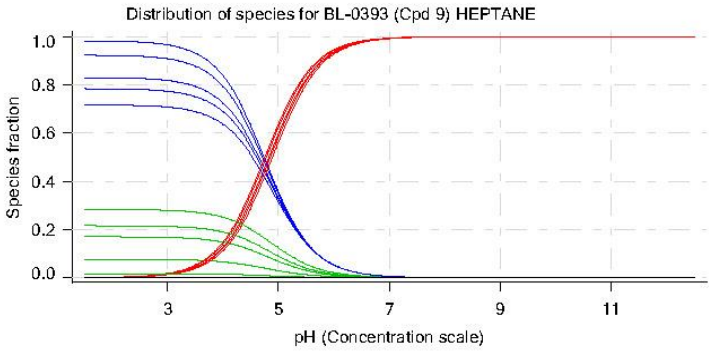
## Sample logD values

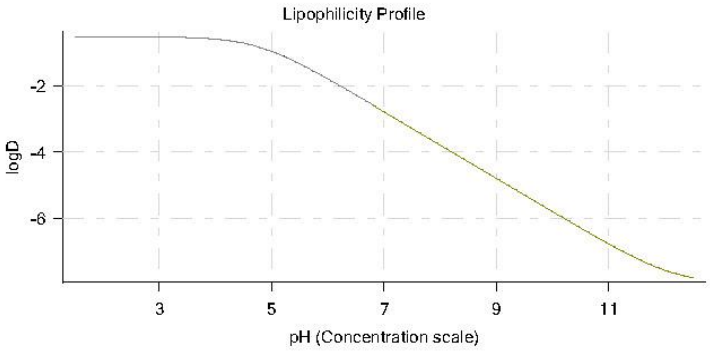
| pH | BL-0393 (Cpd 9) logD | Comment |
|---|---|---|
| 1.000 | -0.53 | |
| 1.200 | -0.53 | Stomach pH |
| 2.000 | -0.53 | |
| 3.000 | -0.54 | |
| 4.000 | -0.60 | |
| 5.000 | -0.97 | |
| 6.000 | -1.80 | |
| 6.500 | -2.29 | |
| 7.000 | -2.78 | |
| 7.400 | -3.18 | Blood pH |
| 8.000 | -3.78 | |
| 9.000 | -4.78 | |
| 10.000 | -5.78 | |
| 11.000 | -6.75 | |
| 12.000 | -7.55 | |

## Graphs



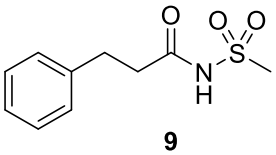
pH-metric Result

Sample name: **BL-0393 (Cpd 9) TOLUENE**
Assay name: **pH-metric medium logP**
Assay ID: **20J-27003**
Filename:

Experiment start time: **10/27/2020 8:21:42 AM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 0.21 | ±0.02 (n=50) |
| logP (X -) | -0.81 | ±0.08 (n=50) |
| RMSD | 0.249 | |



**9**

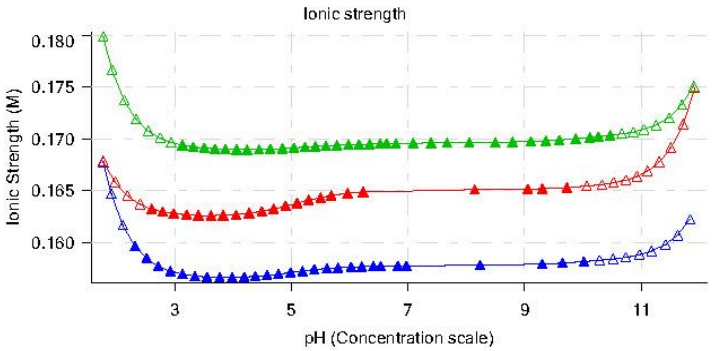
## Warnings and errors

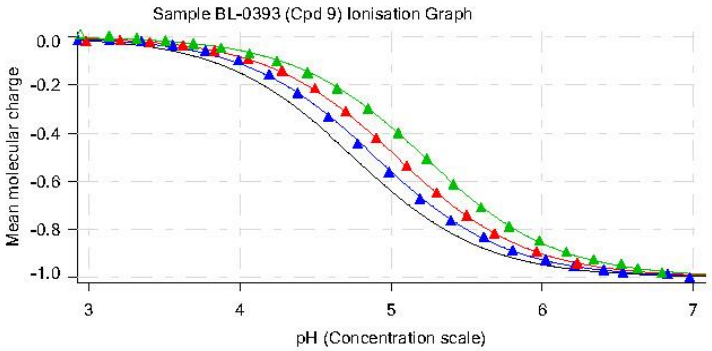
Errors None
Warnings None

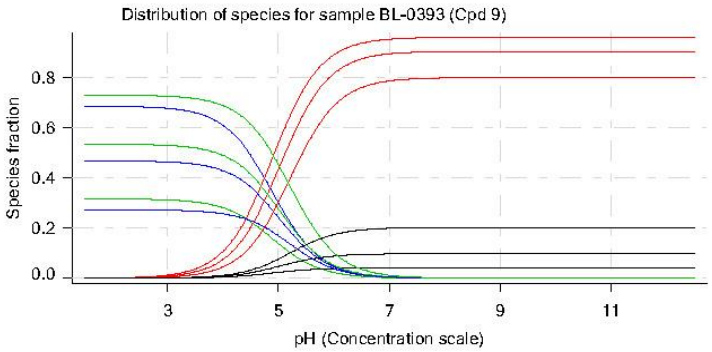
## Sample logD values

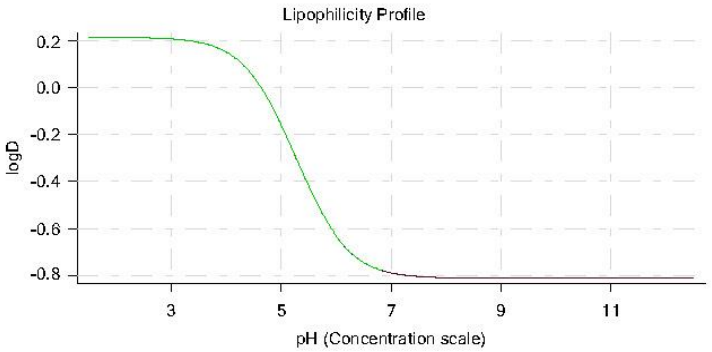
| pH | BL-0393 (Cpd 9) logD | Comment |
|---|---|---|
| 1.000 | 0.21 | |
| 1.200 | 0.21 | Stomach pH |
| 2.000 | 0.21 | |
| 3.000 | 0.21 | |
| 4.000 | 0.15 | |
| 5.000 | -0.16 | |
| 6.000 | -0.63 | |
| 6.500 | -0.74 | |
| 7.000 | -0.79 | |
| 7.400 | -0.80 | Blood pH |
| 8.000 | -0.81 | |
| 9.000 | -0.81 | |
| 10.000 | -0.81 | |
| 11.000 | -0.81 | |
| 12.000 | -0.81 | |

## Graphs




Report by: Carlo Ballatore 11/19/2020 10:57:29 AM

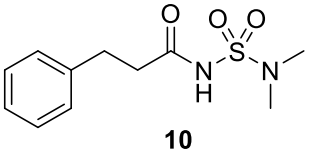
pH-metric Result

Multiset name: **BL-0344 (Cpd 10)**
Quality: **Good**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.66 | ±0.02 (n=50) |
| logP (X -) | -0.66 | ±0.09 (n=50) |
| RMSD | 0.129 | |



**10**

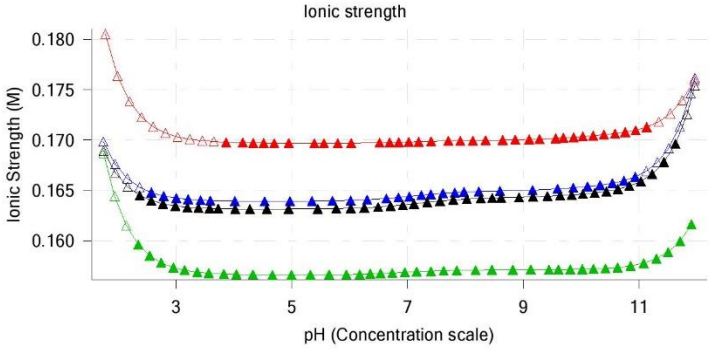
## Warnings and errors

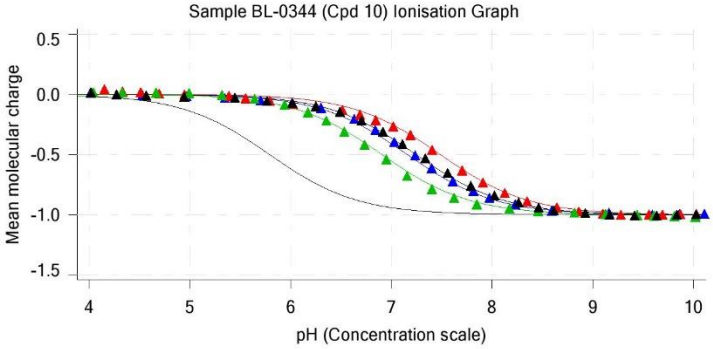
Errors None
Warnings None

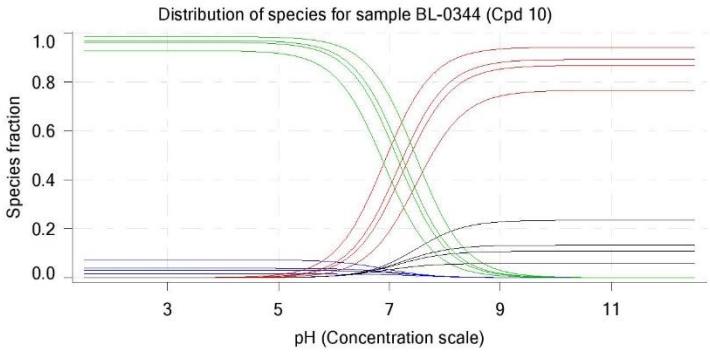
## Sample logD values

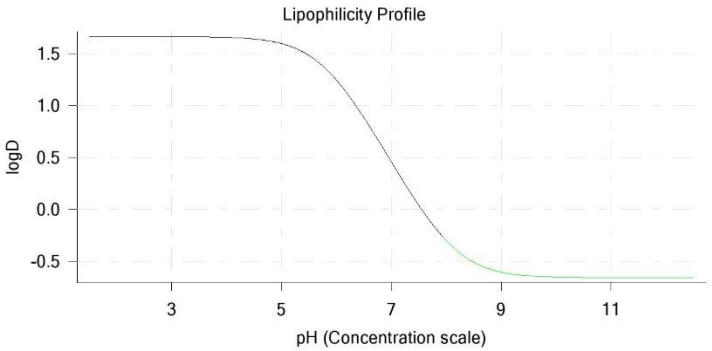
| pH | BL-0344 (Cpd 10) logD | Comment |
|---|---|---|
| 1.000 | 1.66 | |
| 1.200 | 1.66 | Stomach pH |
| 2.000 | 1.66 | |
| 3.000 | 1.66 | |
| 4.000 | 1.65 | |
| 5.000 | 1.60 | |
| 6.000 | 1.25 | |
| 6.500 | 0.88 | |
| 7.000 | 0.46 | |
| 7.400 | 0.12 | Blood pH |
| 8.000 | -0.30 | |
| 9.000 | -0.61 | |
| 10.000 | -0.65 | |
| 11.000 | -0.66 | |
| 12.000 | -0.66 | |

## Graphs



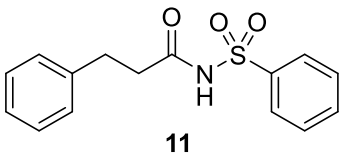
pH-metric Result

Sample name: **BL-0664 (Cpd 11)**
Assay name: **pH-metric high logP**
Assay ID: **19B-21007**
Filename:

Experiment start time: **2/21/2019 1:38:13 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 2.67 | ±0.01 (n=50) |
| logP (X -) | -0.61 | ±0.11 (n=50) |
| RMSD | 0.428 | |



**11**

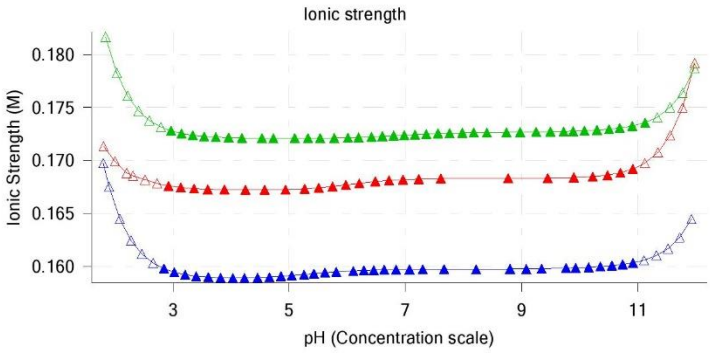
## Warnings and errors

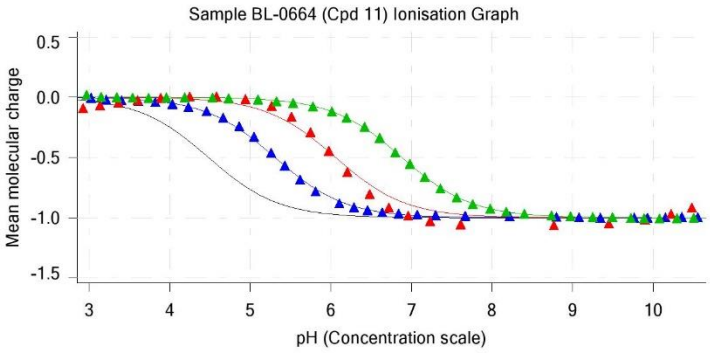
Errors None
Warnings None

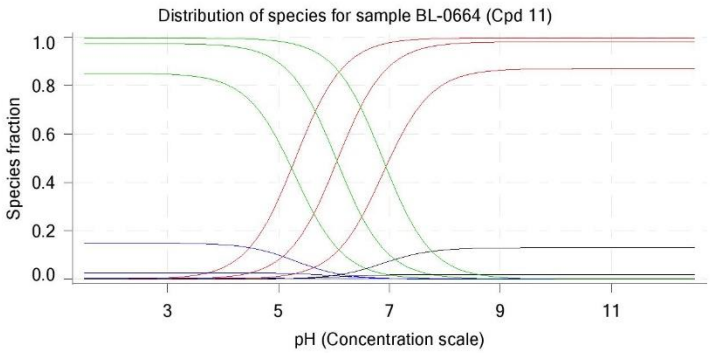
## Sample logD values

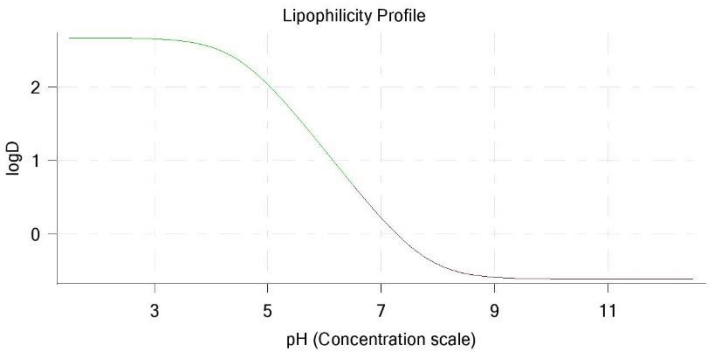
| pH | BL-0664 (Cpd 11) logD | Comment |
|---|---|---|
| 1.000 | 2.67 | |
| 1.200 | 2.67 | Stomach pH |
| 2.000 | 2.67 | |
| 3.000 | 2.66 | |
| 4.000 | 2.55 | |
| 5.000 | 2.04 | |
| 6.000 | 1.15 | |
| 6.500 | 0.67 | |
| 7.000 | 0.22 | |
| 7.400 | -0.09 | Blood pH |
| 8.000 | -0.41 | |
| 9.000 | -0.59 | |
| 10.000 | -0.61 | |
| 11.000 | -0.61 | |
| 12.000 | -0.61 | |

## Graphs



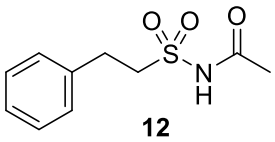
# pH-metric Result

Sample name: **BL-0822 (Cpd 12)**
Assay name: **pH-metric medium logP**
Assay ID: **20C-24004**
Filename:

Experiment start time: **3/24/2020 10:17:38 AM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.04 | ±0.01 (n=50) |
| logP (X -) | -1.00 | ±0.10 (n=50) |
| RMSD | 0.139 | |



**12**

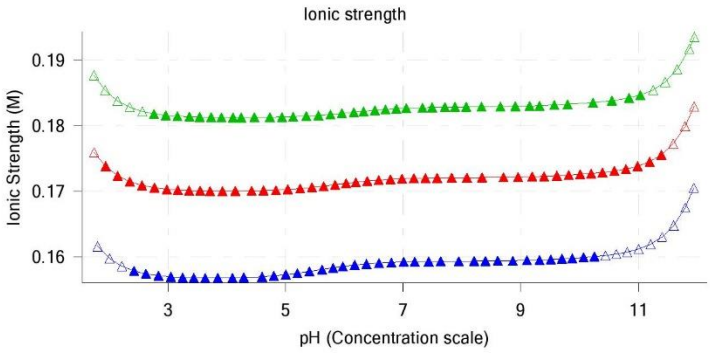
## Warnings and errors

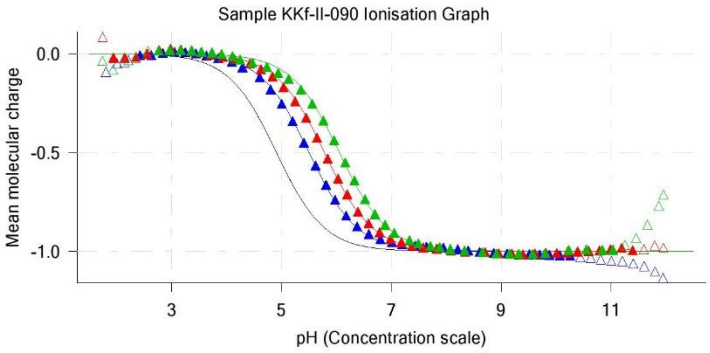
Errors None
Warnings None

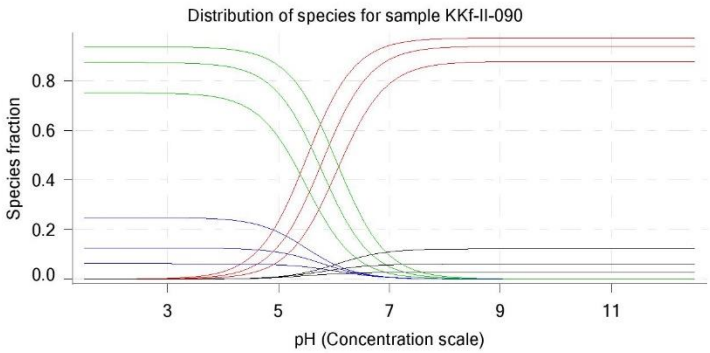
## Sample logD values

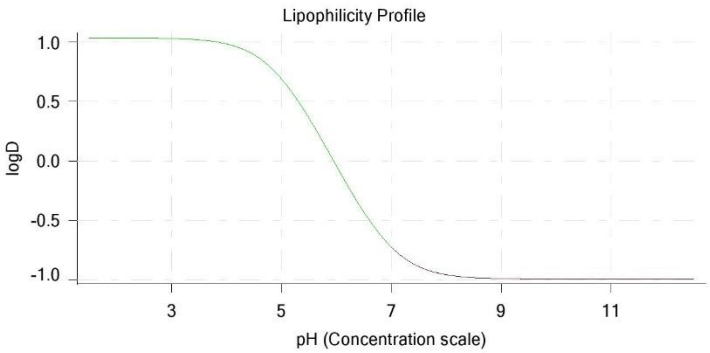
| pH | KKf-II-090 logD | Comment |
|---|---|---|
| 1.000 | 1.04 | |
| 1.200 | 1.04 | Stomach pH |
| 2.000 | 1.03 | |
| 3.000 | 1.03 | |
| 4.000 | 0.99 | |
| 5.000 | 0.69 | |
| 6.000 | -0.04 | |
| 6.500 | -0.43 | |
| 7.000 | -0.73 | |
| 7.400 | -0.87 | Blood pH |
| 8.000 | -0.96 | |
| 9.000 | -0.99 | |
| 10.000 | -1.00 | |
| 11.000 | -1.00 | |
| 12.000 | -1.00 | |

## Graphs



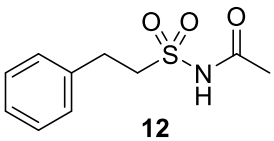



Multiset name: **BL-0822 (Cpd 12) CYCLOHEXANE** Instrument ID: **T317135**
Filename:

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | -0.59 | ±0.04 (n=50) |
| logP (X -) | -8.86 | ±0.80 (n=50) |
| RMSD | 0.217 | |



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### Assay 20J-28007 -

| | |
|---|---|
| **BL-0822 (Cpd 12)** | 0.995 |
| Carbonate | 0.1136 mM |
| Acidity error | 0.05528 mM |

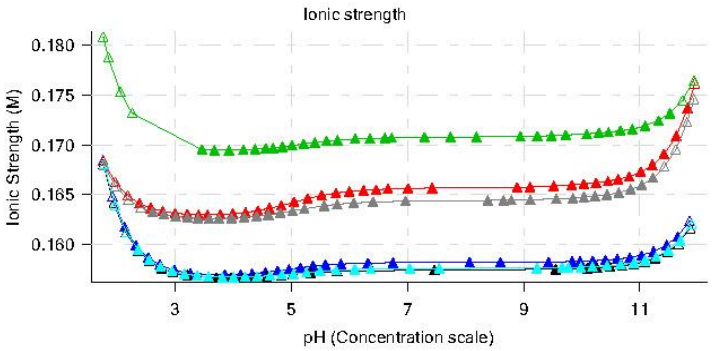
## Warnings and errors

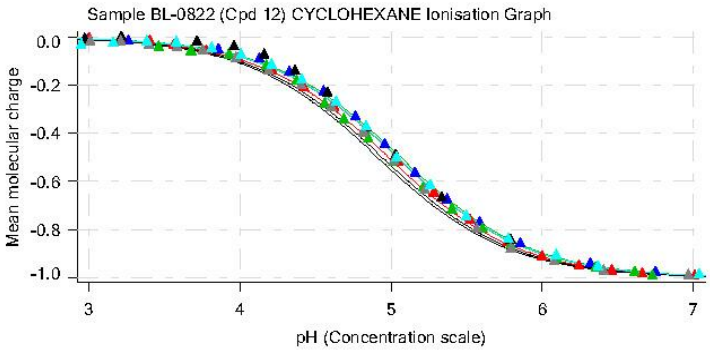
| | |
|---|---|
| Errors | None |
| Warnings | None |

## Sample logD values

| pH | BL-0822 (Cpd 12) logD | Comment |
|---|---|---|
| 1.000 | -0.59 | |
| 1.200 | -0.59 | Stomach pH |
| 2.000 | -0.59 | |
| 3.000 | -0.60 | |
| 4.000 | -0.64 | |
| 5.000 | -0.94 | |
| 6.000 | -1.72 | |
| 6.500 | -2.19 | |
| 7.000 | -2.68 | |
| 7.400 | -3.08 | Blood pH |
| 8.000 | -3.68 | |
| 9.000 | -4.68 | |
| 10.000 | -5.68 | |
| 11.000 | -6.68 | |
| 12.000 | -7.65 | |

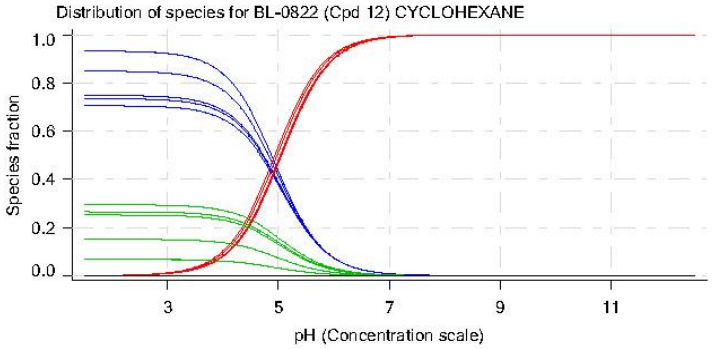
## Graphs

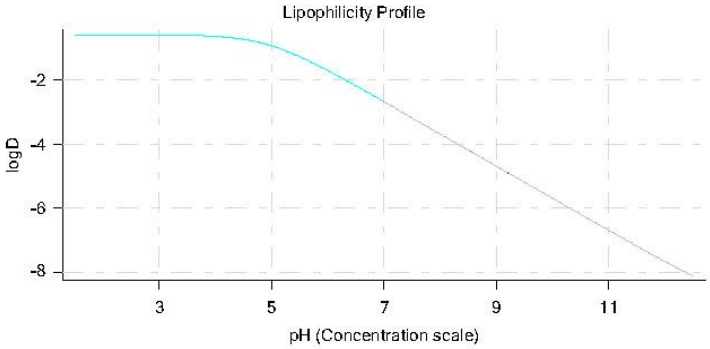


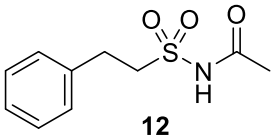



Multiset name: **BL-0822 (Cpd 12) CYCLOHEXANE** Instrument ID: **T317135**
Filename:

## Graphs (continued)



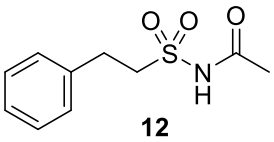

**12**

Multiset name: **BL-0822 (Cpd 12) HEPTANE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | -0.44 | ±0.03 (n=50) |
| logP (X -) | -9.50 | ±0.52 (n=50) |
| RMSD | 0.274 | |




**12**

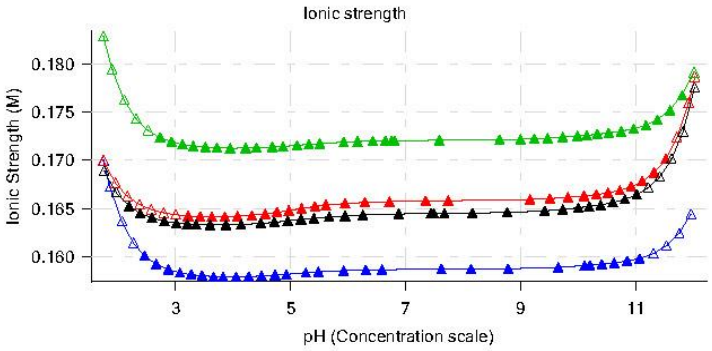
## Warnings and errors

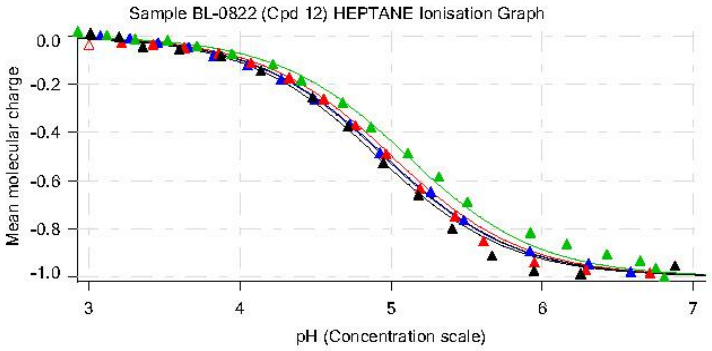
| | |
|---|---|
| Errors | None |
| Warnings | None |

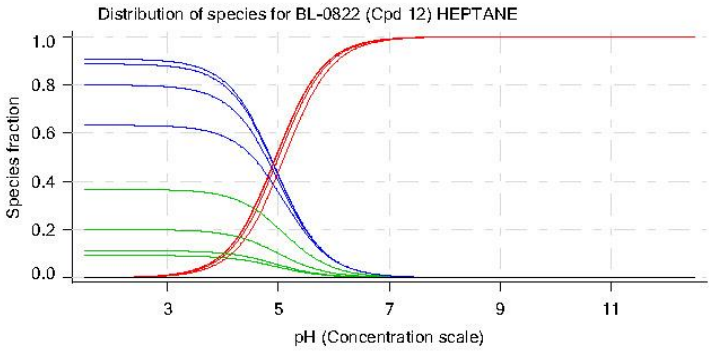
## Sample logD values

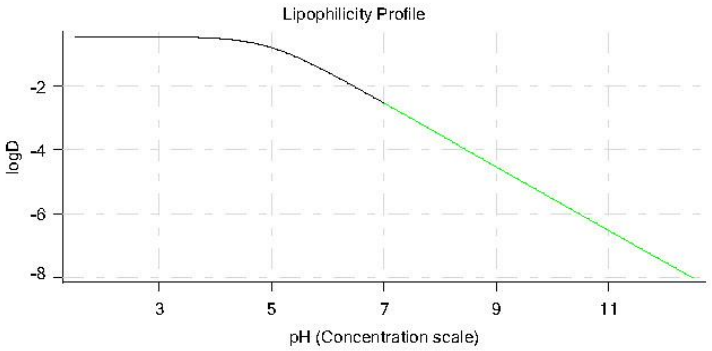
| pH | BL-0822 (Cpd 12) logD | Comment |
|---|---|---|
| 1.000 | -0.44 | |
| 1.200 | -0.44 | Stomach pH |
| 2.000 | -0.44 | |
| 3.000 | -0.44 | |
| 4.000 | -0.49 | |
| 5.000 | -0.79 | |
| 6.000 | -1.56 | |
| 6.500 | -2.04 | |
| 7.000 | -2.53 | |
| 7.400 | -2.93 | Blood pH |
| 8.000 | -3.53 | |
| 9.000 | -4.53 | |
| 10.000 | -5.53 | |
| 11.000 | -6.53 | |
| 12.000 | -7.52 | |

## Graphs



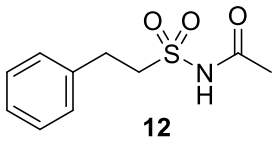



Multiset name: **BL-0822 (Cpd 12) TOLUENE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 0.64 | ±0.05 (n=50) |
| logP (X -) | 0.20 | ±0.07 (n=50) |
| RMSD | 0.073 | |



**12**

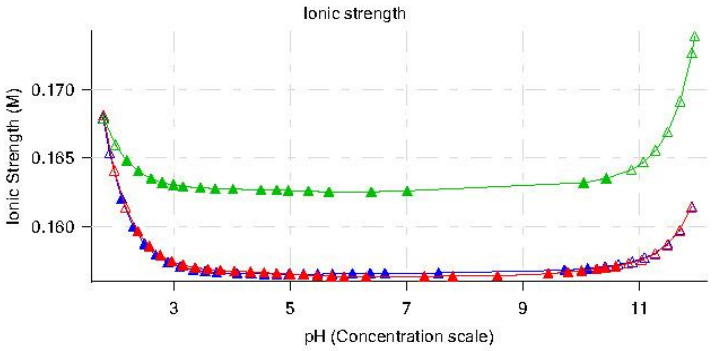
## Warnings and errors

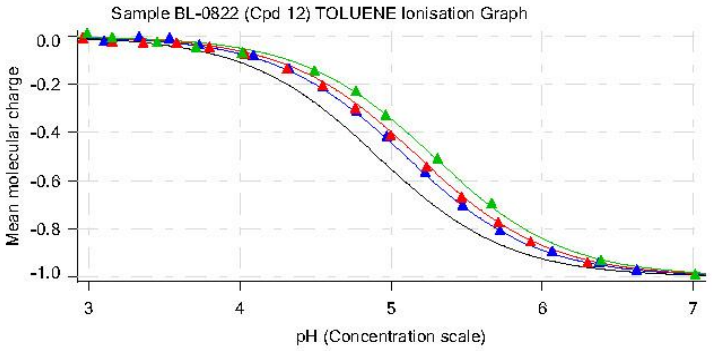
| | |
|---|---|
| Errors | None |
| Warnings | None |

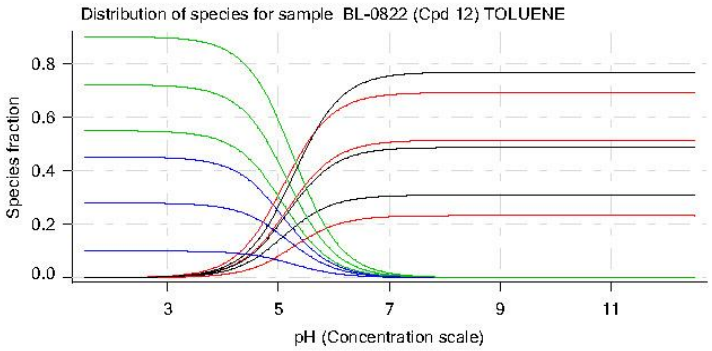
## Sample logD values

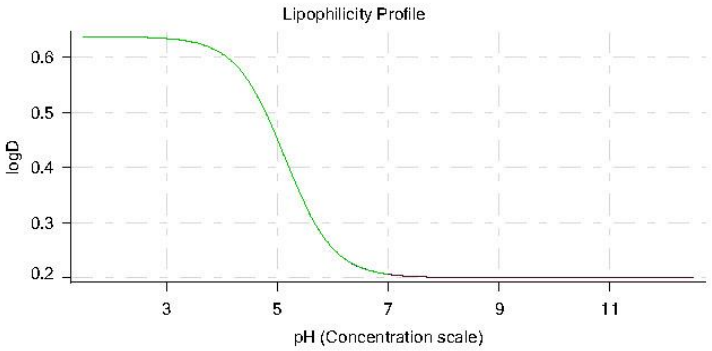
| pH | BL-0822 (Cpd 12) logD | Comment |
|---|---|---|
| 1.000 | 0.64 | |
| 1.200 | 0.64 | Stomach pH |
| 2.000 | 0.64 | |
| 3.000 | 0.63 | |
| 4.000 | 0.61 | |
| 5.000 | 0.45 | |
| 6.000 | 0.25 | |
| 6.500 | 0.22 | |
| 7.000 | 0.21 | |
| 7.400 | 0.20 | Blood pH |
| 8.000 | 0.20 | |
| 9.000 | 0.20 | |
| 10.000 | 0.20 | |
| 11.000 | 0.20 | |
| 12.000 | 0.20 | |

## Graphs



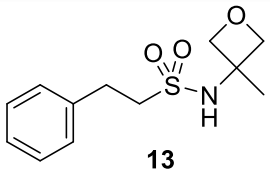
pH-metric Result

Multiset name: **BL-0789 (Cpd 13)**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.58 | ±0.06 (n=50) |
| logP (X -) | 0.65 | ±0.10 (n=50) |
| RMSD | 0.289 | |



**13**

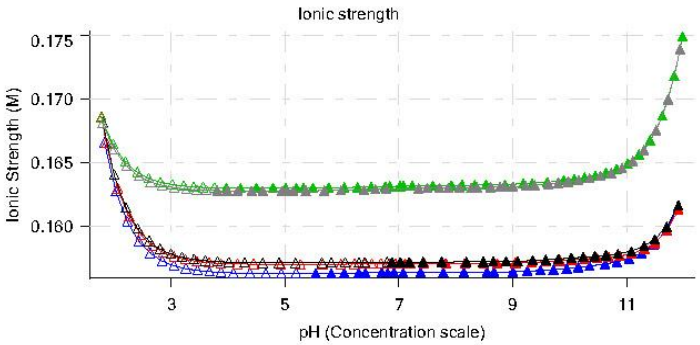
## Warnings and errors

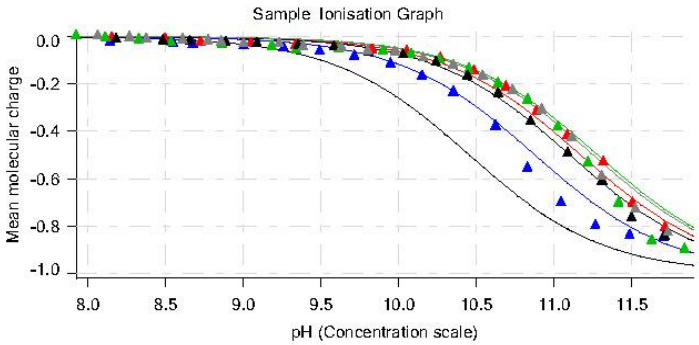
Errors None
Warnings None

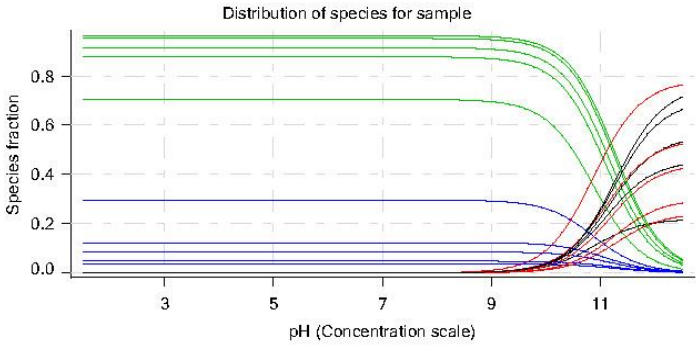
## Sample logD values

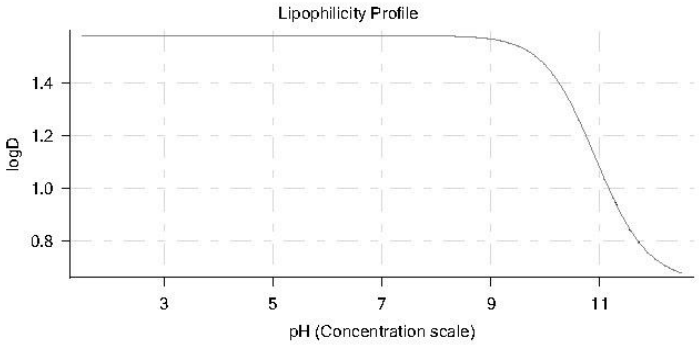
| pH | logD | Comment |
|---|---|---|
| 1.000 | 1.58 | |
| 1.200 | 1.58 | Stomach pH |
| 2.000 | 1.58 | |
| 3.000 | 1.58 | |
| 4.000 | 1.58 | |
| 5.000 | 1.58 | |
| 6.000 | 1.58 | |
| 6.500 | 1.58 | |
| 7.000 | 1.58 | |
| 7.400 | 1.58 | Blood pH |
| 8.000 | 1.58 | |
| 9.000 | 1.57 | |
| 10.000 | 1.47 | |
| 11.000 | 1.07 | |
| 12.000 | 0.73 | |

## Graphs



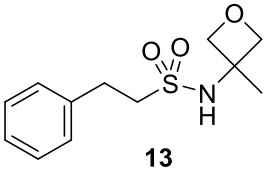



Multiset name: **BL-0789 (Cpd 13) CYCLOHEXANE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | -0.43 | ±0.03 (n=50) |
| logP (X -) | -9.04 | ±0.55 (n=50) |
| RMSD | 0.532 | |



**13**

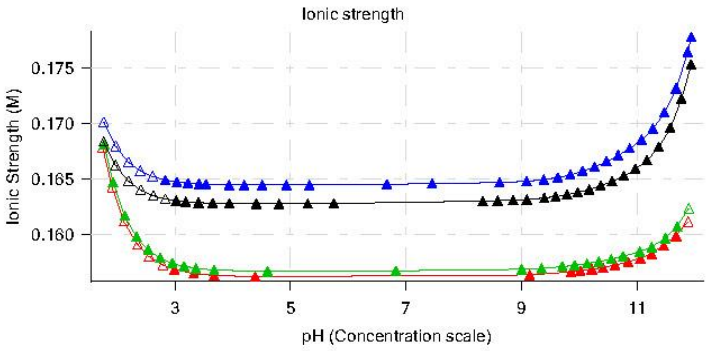
## Warnings and errors

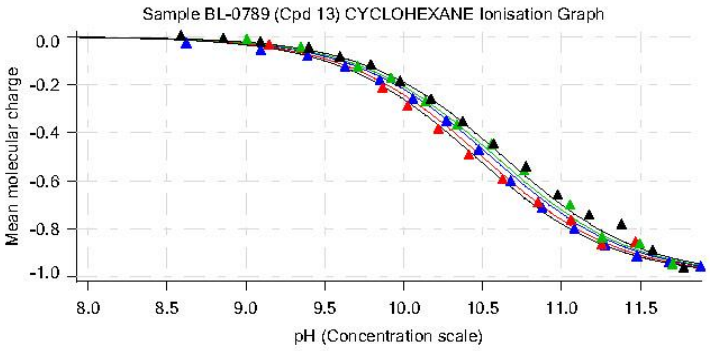
| | |
|---|---|
| Errors | None |
| Warnings | None |

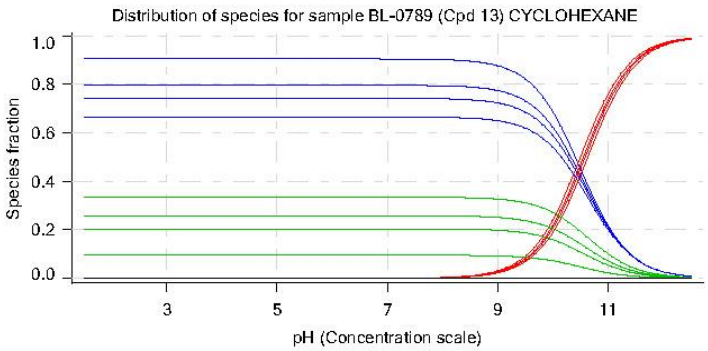
## Sample logD values

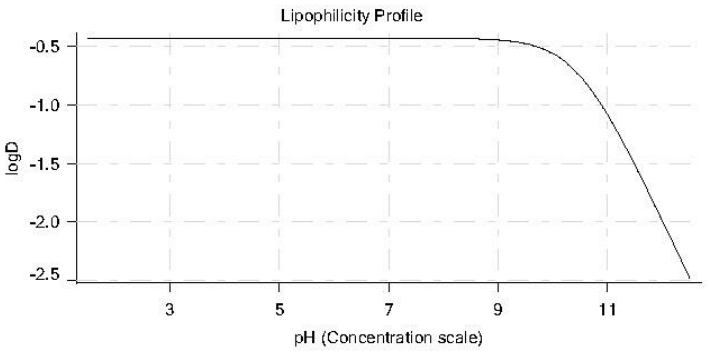
| pH | BL-0789 (Cpd 13) logD | Comment |
|---|---|---|
| 1.000 | -0.43 | |
| 1.200 | -0.43 | Stomach pH |
| 2.000 | -0.43 | |
| 3.000 | -0.43 | |
| 4.000 | -0.43 | |
| 5.000 | -0.43 | |
| 6.000 | -0.43 | |
| 6.500 | -0.43 | |
| 7.000 | -0.43 | |
| 7.400 | -0.43 | Blood pH |
| 8.000 | -0.43 | |
| 9.000 | -0.44 | |
| 10.000 | -0.56 | |
| 11.000 | -1.09 | |
| 12.000 | -1.99 | |

## Graphs



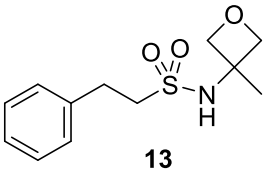



Multiset name: **BL-0789 (Cpd 13) HEPTANE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | -0.14 | ±0.07 (n=50) |
| logP (X -) | -6.00 | ±0.54 (n=50) |
| RMSD | 0.470 | |



**13**

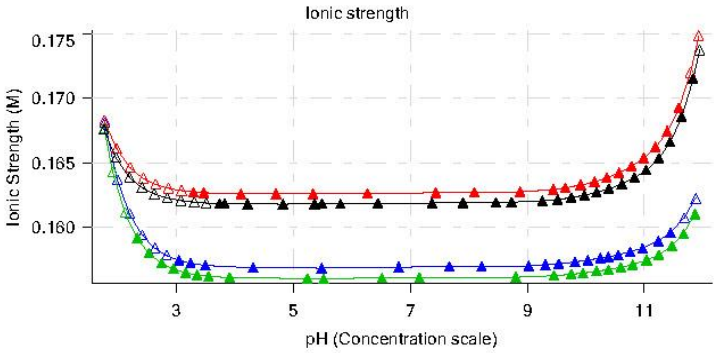
## Warnings and errors

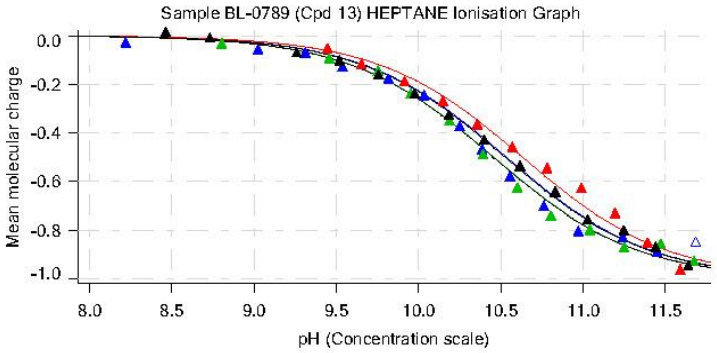
Errors None
Warnings None

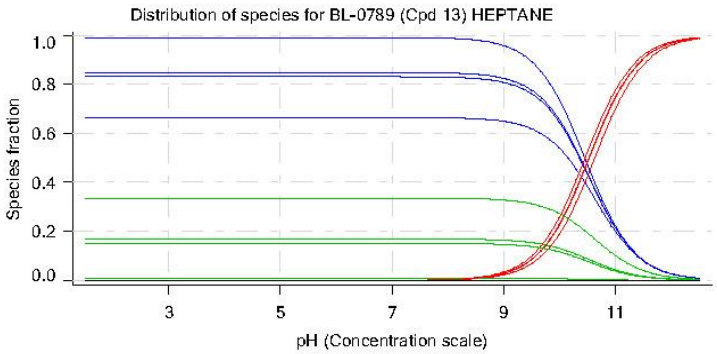
## Sample logD values

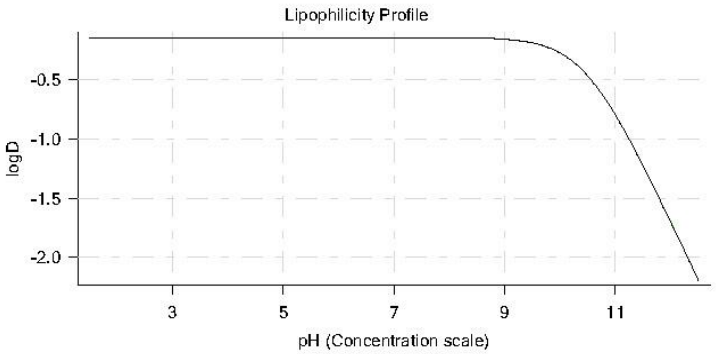
| pH | BL-0789 (Cpd 13) logD | Comment |
|---|---|---|
| 1.000 | -0.14 | |
| 1.200 | -0.14 | Stomach pH |
| 2.000 | -0.14 | |
| 3.000 | -0.14 | |
| 4.000 | -0.14 | |
| 5.000 | -0.14 | |
| 6.000 | -0.14 | |
| 6.500 | -0.14 | |
| 7.000 | -0.14 | |
| 7.400 | -0.14 | Blood pH |
| 8.000 | -0.14 | |
| 9.000 | -0.16 | |
| 10.000 | -0.27 | |
| 11.000 | -0.80 | |
| 12.000 | -1.70 | |

## Graphs



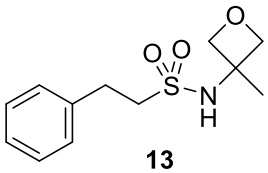



Multiset name: **BL-0789 (Cpd 13) TOLUENE**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.06 | ±0.01 (n=50) |
| logP (X -) | -9.00 | ±0.77 (n=50) |
| RMSD | 0.365 | |



**13**

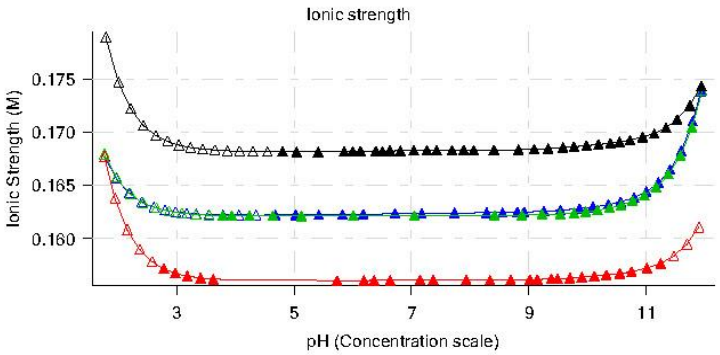
## Warnings and errors

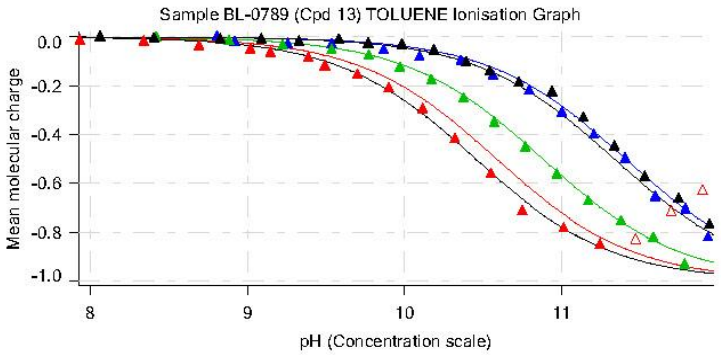
| | |
|---|---|
| Errors | None |
| Warnings | None |

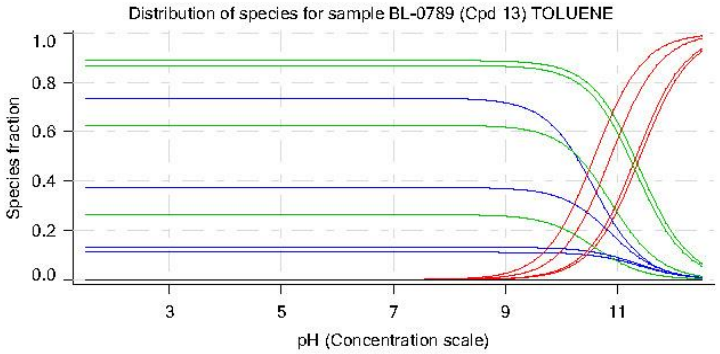
## Sample logD values

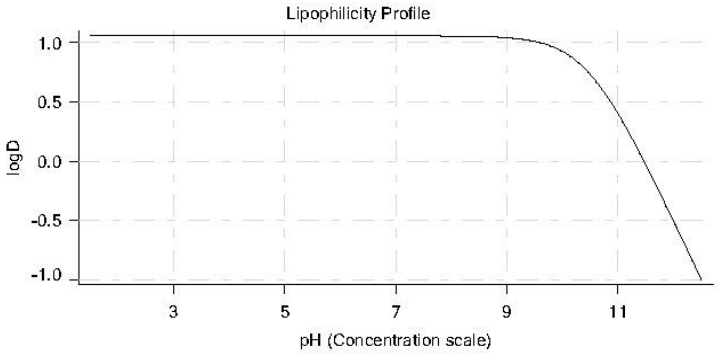
| pH | BL-0789 (Cpd 13) logD | Comment |
|---|---|---|
| 1.000 | 1.06 | |
| 1.200 | 1.06 | Stomach pH |
| 2.000 | 1.06 | |
| 3.000 | 1.06 | |
| 4.000 | 1.06 | |
| 5.000 | 1.06 | |
| 6.000 | 1.06 | |
| 6.500 | 1.06 | |
| 7.000 | 1.06 | |
| 7.400 | 1.06 | Blood pH |
| 8.000 | 1.06 | |
| 9.000 | 1.04 | |
| 10.000 | 0.92 | |
| 11.000 | 0.40 | |
| 12.000 | -0.51 | |

## Graphs



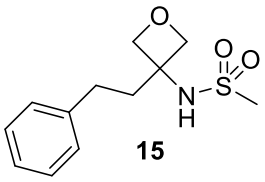
pH-metric Result

Sample name: **BL-0650 (Cpd 15)**
Assay name: **pH-metric high logP**
Assay ID: **18I-12003**
Filename:

Experiment start time: **9/12/2018 5:19:42 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.61 | ±0.03 (n=50) |
| logP (X -) | -4.54 | ±1.16 (n=50) |
| RMSD | 56.408 | |



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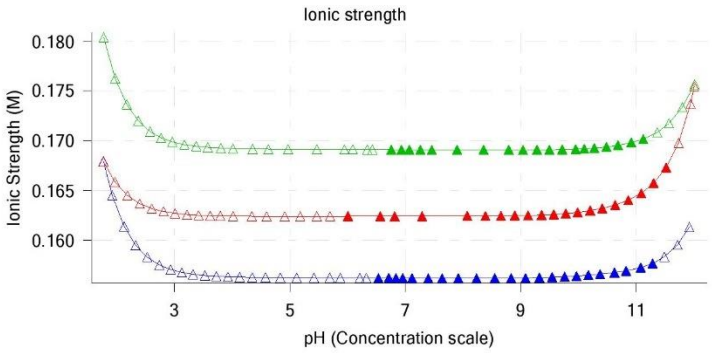
## Warnings and errors

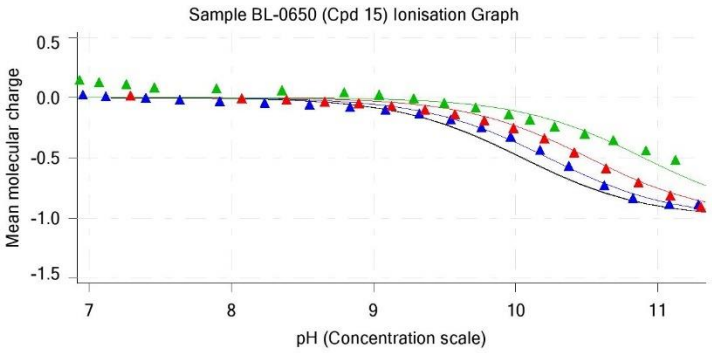
Errors None
Warnings None

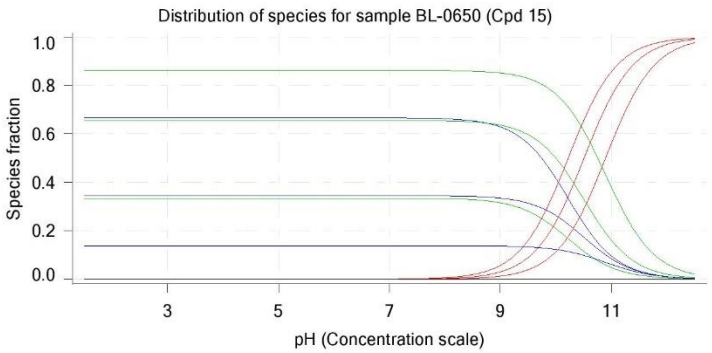
## Sample logD values

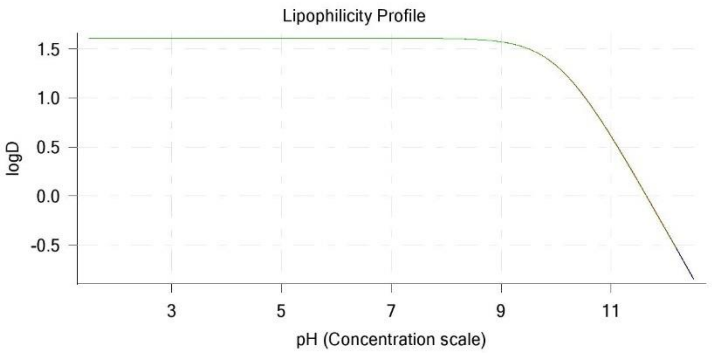
| pH | BL-0650 (Cpd 15) logD | Comment |
|---|---|---|
| 1.000 | 1.61 | |
| 1.200 | 1.61 | Stomach pH |
| 2.000 | 1.61 | |
| 3.000 | 1.61 | |
| 4.000 | 1.61 | |
| 5.000 | 1.61 | |
| 6.000 | 1.61 | |
| 6.500 | 1.61 | |
| 7.000 | 1.61 | |
| 7.400 | 1.61 | Blood pH |
| 8.000 | 1.61 | |
| 9.000 | 1.57 | |
| 10.000 | 1.33 | |
| 11.000 | 0.61 | |
| 12.000 | -0.34 | |

## Graphs



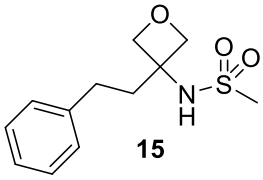



Multiset name: **BL-0650 (Cpd 15) CYCLOHEXANE** Instrument ID: **T317135**
Filename:

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | -0.26 | ±0.01 (n=48) |
| logP (X -) | -7.76 | ±0.99 (n=48) |
| RMSD | 0.346 | |



**15**

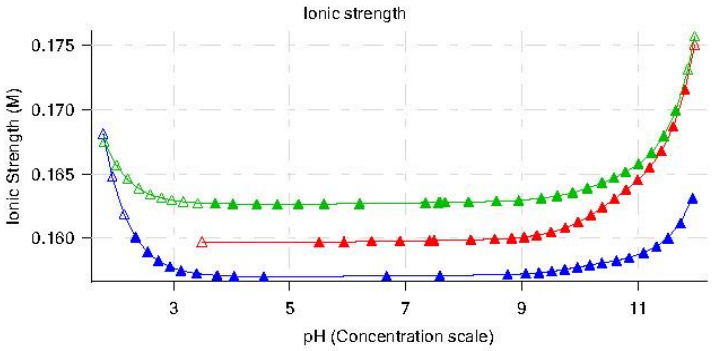
## Warnings and errors

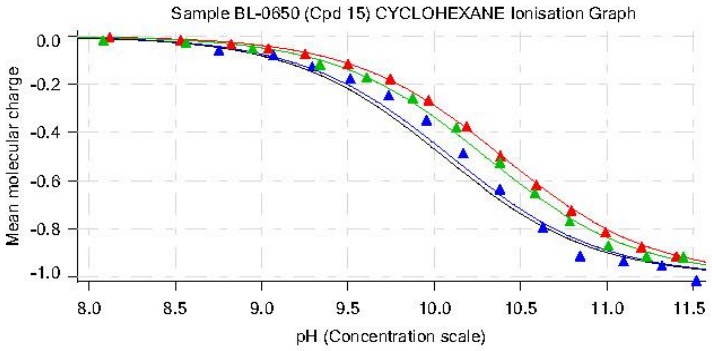
Errors None
Warnings None

## Sample logD values

| pH | BL-0650 (Cpd 15) CYCLOHEXANE logD | Comment |
|---|---|---|
| 1.000 | -0.26 | |
| 1.200 | -0.26 | Stomach pH |
| 2.000 | -0.26 | |
| 3.000 | -0.26 | |
| 4.000 | -0.26 | |
| 5.000 | -0.26 | |
| 6.000 | -0.26 | |
| 6.500 | -0.26 | |
| 7.000 | -0.26 | |
| 7.400 | -0.26 | Blood pH |
| 8.000 | -0.26 | |
| 9.000 | -0.30 | |
| 10.000 | -0.54 | |
| 11.000 | -1.26 | |
| 12.000 | -2.22 | |

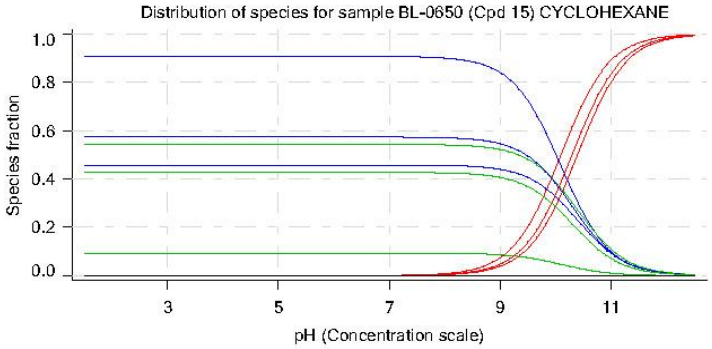
## Graphs

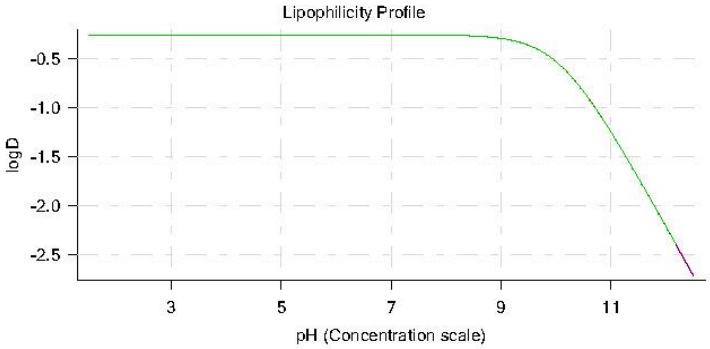


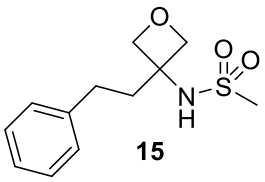



Multiset name: **BL-0650 (Cpd 15) CYCLOHEXANE** Instrument ID: **T317135**
Filename:

## Graphs (continued)



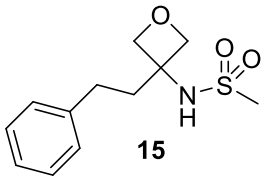




**15**

Multiset name: **BL-0650 (Cpd 15) HEPTANE** Instrument ID: **T317135**
Filename:

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 0.01 | ±0.02 (n=50) |
| logP (X -) | -8.00 | ±0.92 (n=50) |
| RMSD | 0.260 | |




**15**

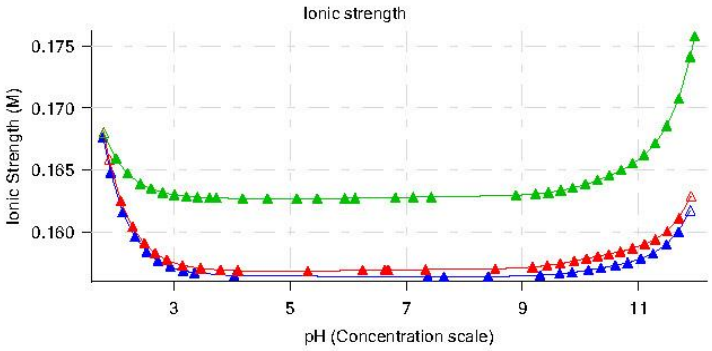
## Warnings and errors

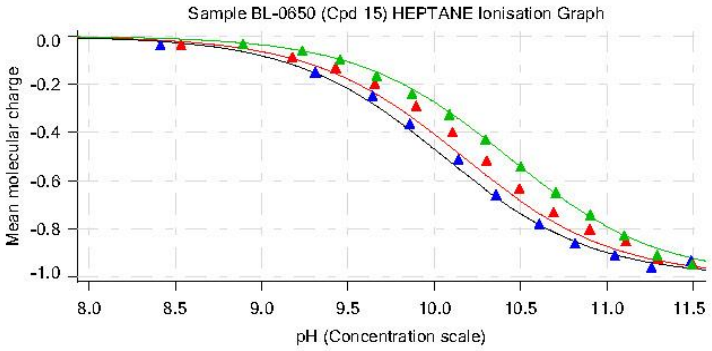
| | |
|---|---|
| Errors | None |
| Warnings | None |

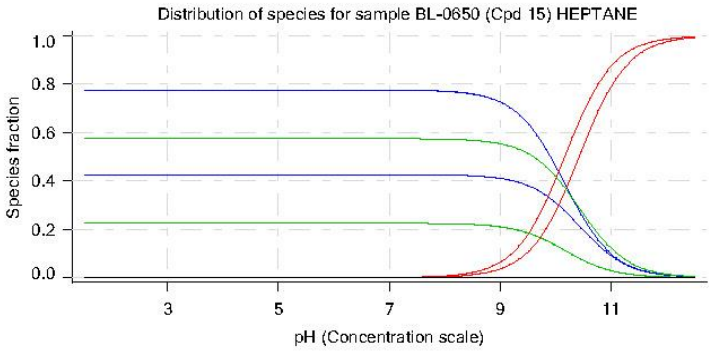
## Sample logD values

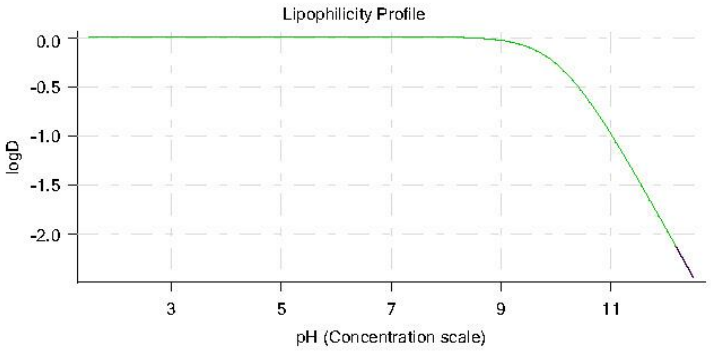
| pH | BL-0650 (Cpd 15) HEPTANE logD | Comment |
|---|---|---|
| 1.000 | 0.01 | |
| 1.200 | 0.01 | Stomach pH |
| 2.000 | 0.01 | |
| 3.000 | 0.01 | |
| 4.000 | 0.01 | |
| 5.000 | 0.01 | |
| 6.000 | 0.01 | |
| 6.500 | 0.01 | |
| 7.000 | 0.01 | |
| 7.400 | 0.01 | Blood pH |
| 8.000 | 0.01 | |
| 9.000 | -0.02 | |
| 10.000 | -0.26 | |
| 11.000 | -0.98 | |
| 12.000 | -1.94 | |

## Graphs



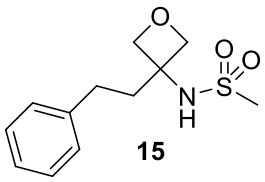
pH-metric Result

Sample name: **BL-0650 (Cpd 15) TOLUENE**
Assay name: **pH-metric medium logP**
Assay ID: **20K-10004**
Filename:

Experiment start time: **11/10/2020 9:32:21 AM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.18 | ±0.01 (n=50) |
| logP (X -) | -9.50 | ±0.89 (n=50) |
| RMSD | 0.401 | |



**15**

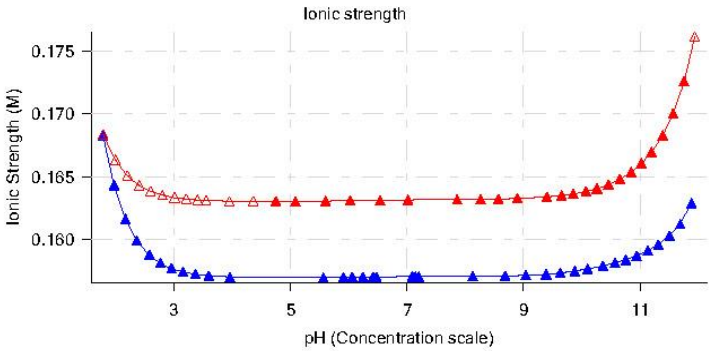
## Warnings and errors

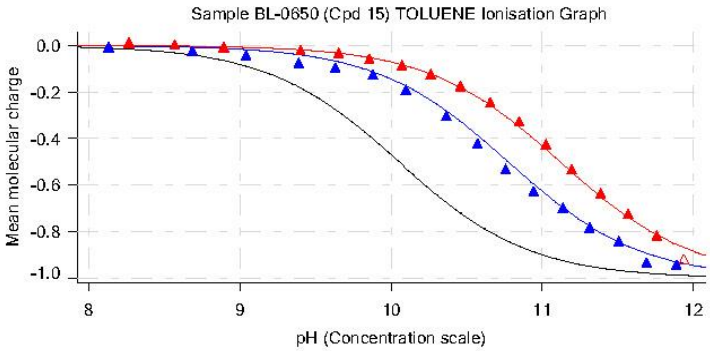
Errors None
Warnings None

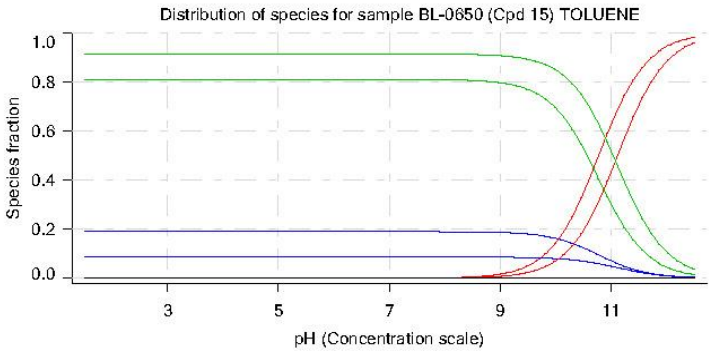
## Sample logD values

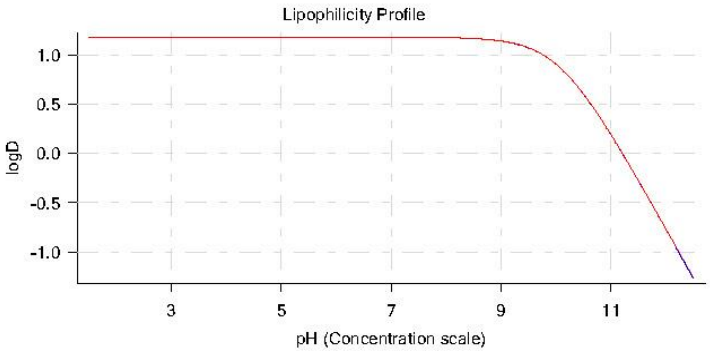
| pH | BL-0650 (Cpd 15) TOLUENE logD | Comment |
|---|---|---|
| 1.000 | 1.18 | |
| 1.200 | 1.18 | Stomach pH |
| 2.000 | 1.18 | |
| 3.000 | 1.18 | |
| 4.000 | 1.18 | |
| 5.000 | 1.18 | |
| 6.000 | 1.18 | |
| 6.500 | 1.18 | |
| 7.000 | 1.18 | |
| 7.400 | 1.18 | Blood pH |
| 8.000 | 1.18 | |
| 9.000 | 1.15 | |
| 10.000 | 0.91 | |
| 11.000 | 0.19 | |
| 12.000 | -0.77 | |

## Graphs




Report by: Carlo Ballatore 11/19/2020 9:54:10 AM

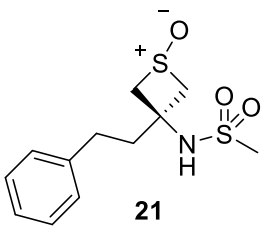
# pH-metric Result

Sample name: **BL-0679 (Cpd 21)**
Assay name: **pH-metric medium logP**
Assay ID: **19I-28009**
Filename:

Experiment start time: **9/28/2019 6:43:19 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 0.88 | ±0.02 (n=50) |
| logP (X -) | -5.73 | ±2.18 (n=50) |
| RMSD | 0.870 | |



**21**

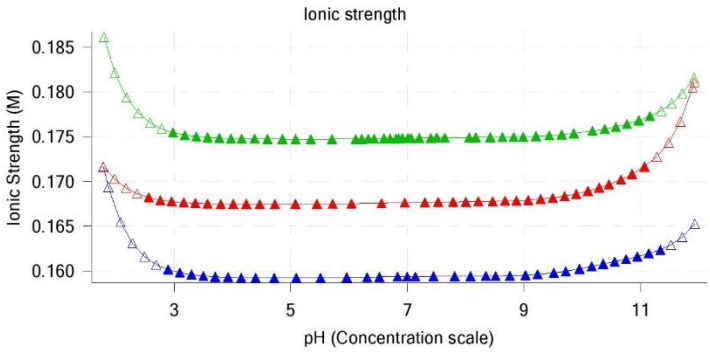
## Warnings and errors

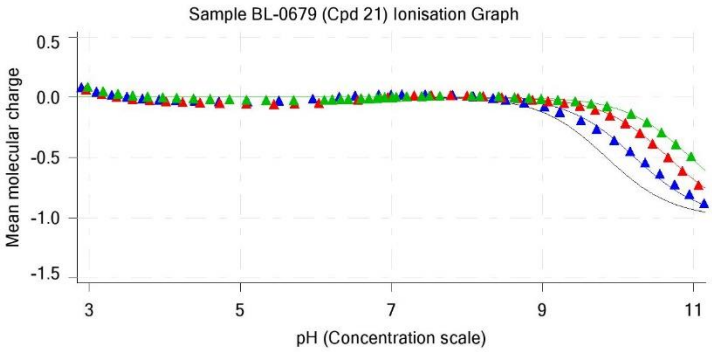
Errors None
Warnings None

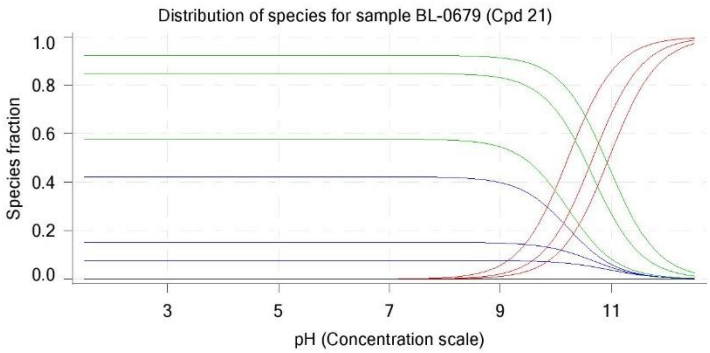
## Sample logD values

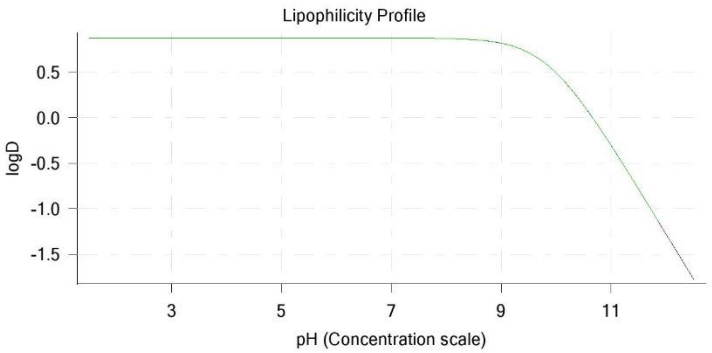
| pH | BL-0679 (Cpd 21) logD | Comment |
|---|---|---|
| 1.000 | 0.88 | |
| 1.200 | 0.88 | Stomach pH |
| 2.000 | 0.88 | |
| 3.000 | 0.88 | |
| 4.000 | 0.88 | |
| 5.000 | 0.88 | |
| 6.000 | 0.88 | |
| 6.500 | 0.88 | |
| 7.000 | 0.88 | |
| 7.400 | 0.87 | Blood pH |
| 8.000 | 0.87 | |
| 9.000 | 0.82 | |
| 10.000 | 0.49 | |
| 11.000 | -0.30 | |
| 12.000 | -1.28 | |

## Graphs




Report by: Carlo Ballatore 4/20/2020 2:54:52 PM

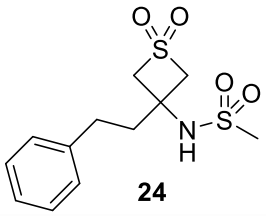
pH-metric Result

Multiset name: **BL-0672 (Cpd 24)**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.03 | ±0.01 (n=50) |
| logP (X -) | -8.50 | ±1.54 (n=50) |
| RMSD | 0.429 | |



**24**

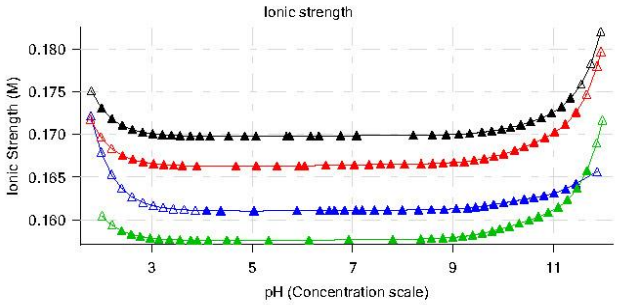
## Warnings and errors

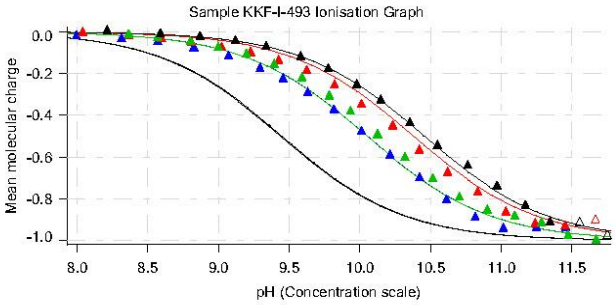
| | |
|---|---|
| Errors | None |
| Warnings | None |

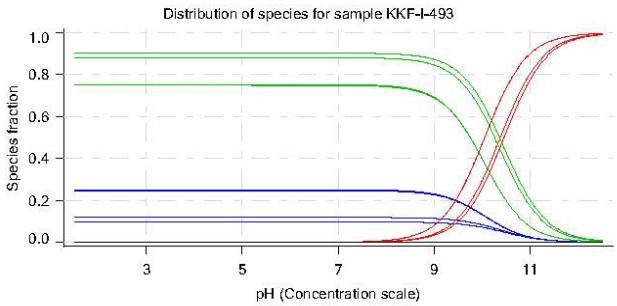
## Sample logD values

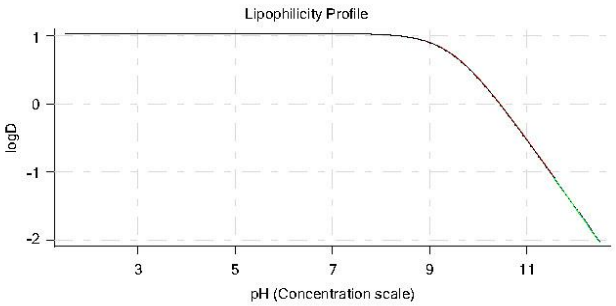
| pH | KKF-I-493 logD | Comment |
|---|---|---|
| 1.000 | 1.03 | |
| 1.200 | 1.03 | Stomach pH |
| 2.000 | 1.03 | |
| 3.000 | 1.03 | |
| 4.000 | 1.03 | |
| 5.000 | 1.03 | |
| 6.000 | 1.03 | |
| 6.500 | 1.03 | |
| 7.000 | 1.03 | |
| 7.400 | 1.03 | Blood pH |
| 8.000 | 1.02 | |
| 9.000 | 0.90 | |
| 10.000 | 0.37 | |
| 11.000 | -0.53 | |
| 12.000 | -1.52 | |

## Graphs




Report by: Carlo Ballatore 12/14/2020 4:29:42 PM

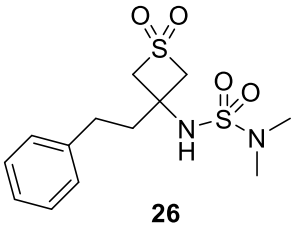
Page 1 of 1

Multiset name: **BL-0689 (Cpd 26)**
Filename:

Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.83 | ±0.05 (n=50) |
| logP (X -) | -8.49 | ±0.69 (n=50) |
| RMSD | 0.456 | |



**26**

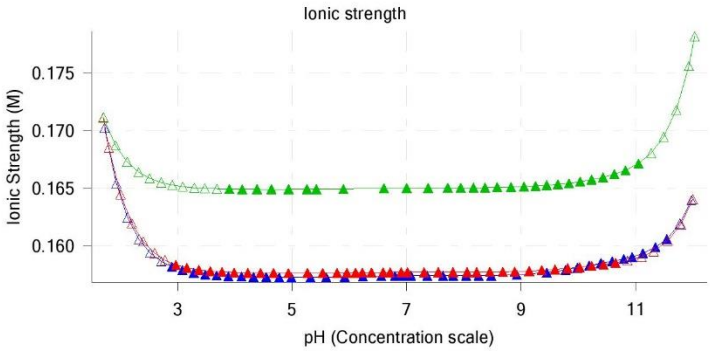
## Warnings and errors

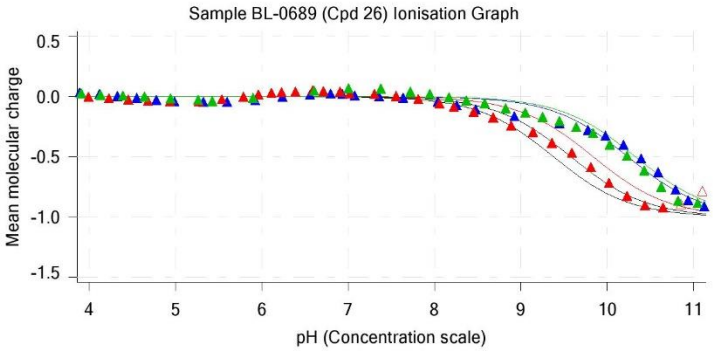
| | |
|---|---|
| Errors | None |
| Warnings | None |

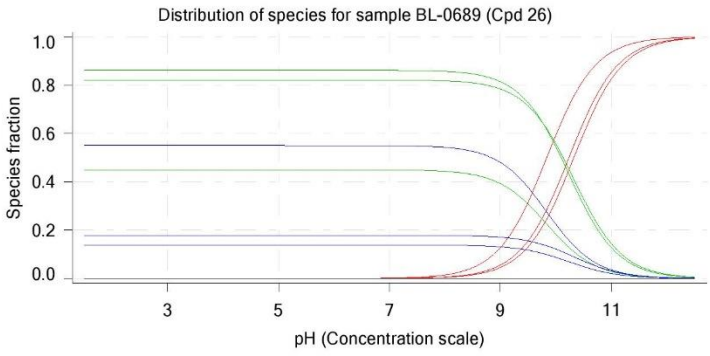
## Sample logD values

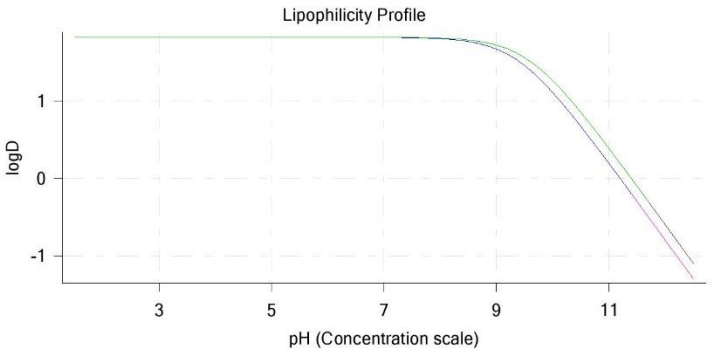
| pH | BL-0689 (Cpd 26) logD | Comment |
|---|---|---|
| 1.000 | 1.83 | |
| 1.200 | 1.83 | Stomach pH |
| 2.000 | 1.83 | |
| 3.000 | 1.83 | |
| 4.000 | 1.83 | |
| 5.000 | 1.83 | |
| 6.000 | 1.83 | |
| 6.500 | 1.83 | |
| 7.000 | 1.83 | |
| 7.400 | 1.82 | Blood pH |
| 8.000 | 1.81 | |
| 9.000 | 1.71 | |
| 10.000 | 1.21 | |
| 11.000 | 0.31 | |
| 12.000 | -0.67 | |

## Graphs



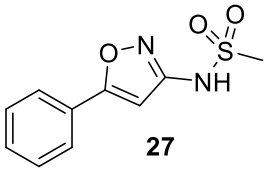
# pH-metric Result

Sample name: **BL-0792 (Cpd 27)**
Assay name: **pH-metric medium logP**
Assay ID: **20A-21003**
Filename:

Experiment start time: **1/21/2020 5:35:07 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 0.58 | ±0.02 (n=50) |
| logP (X -) | -9.45 | ±0.85 (n=50) |
| RMSD | 0.155 | |




**27**

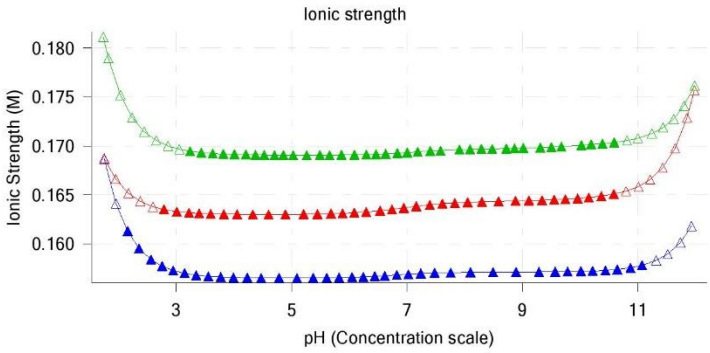
## Warnings and errors

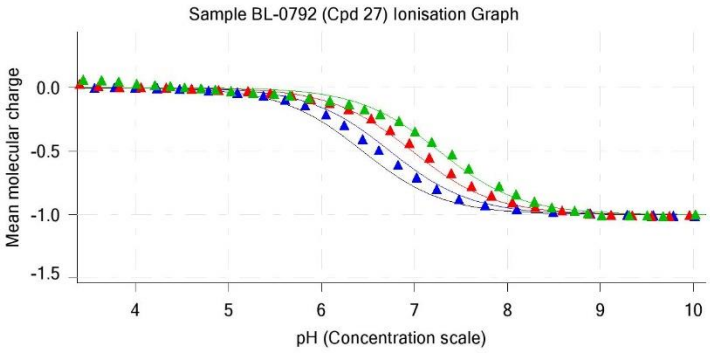
Errors None
Warnings None

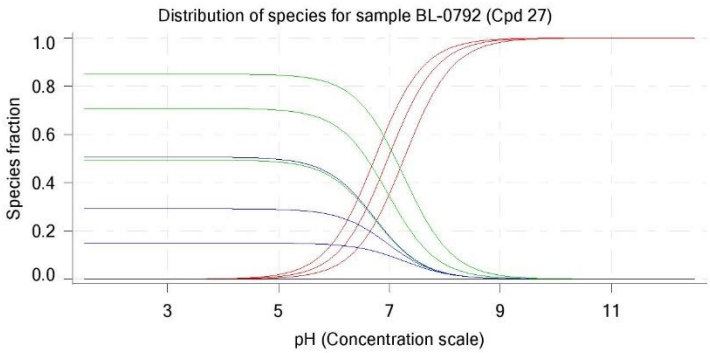
## Sample logD values

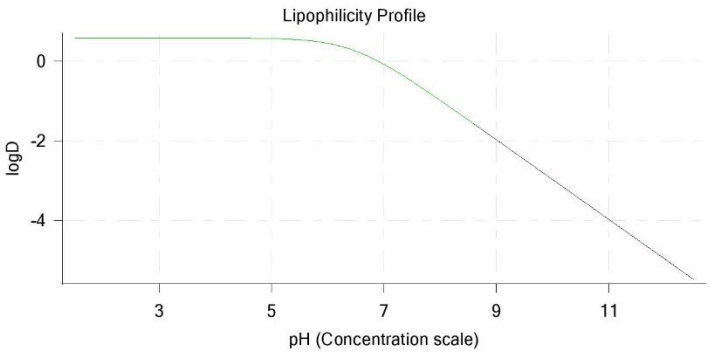
| pH | BL-0792 (Cpd 27) logD | Comment |
|---|---|---|
| 1.000 | 0.58 | |
| 1.200 | 0.58 | Stomach pH |
| 2.000 | 0.58 | |
| 3.000 | 0.58 | |
| 4.000 | 0.58 | |
| 5.000 | 0.57 | |
| 6.000 | 0.45 | |
| 6.500 | 0.25 | |
| 7.000 | -0.08 | |
| 7.400 | -0.42 | Blood pH |
| 8.000 | -0.99 | |
| 9.000 | -1.98 | |
| 10.000 | -2.98 | |
| 11.000 | -3.98 | |
| 12.000 | -4.98 | |

## Graphs



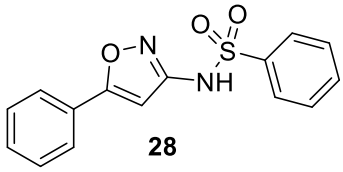
# pH-metric Result

Sample name: **BL-0793 (Cpd 28)**
Assay name: **pH-metric medium logP**
Assay ID: **20A-29003**
Filename:

Experiment start time: **1/29/2020 12:17:42 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.76 | ±0.03 (n=50) |
| logP (X -) | 0.26 | ±0.06 (n=50) |
| RMSD | 0.211 | |




**28**

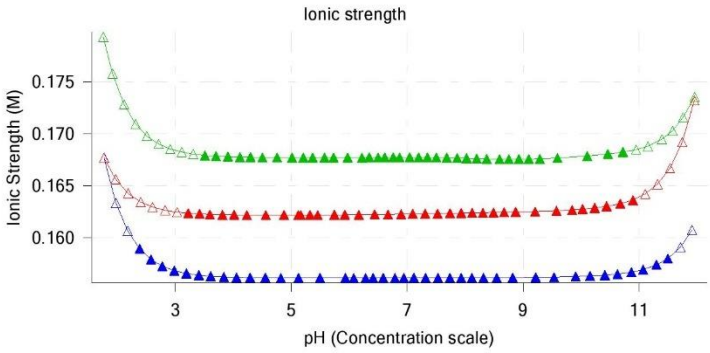
## Warnings and errors

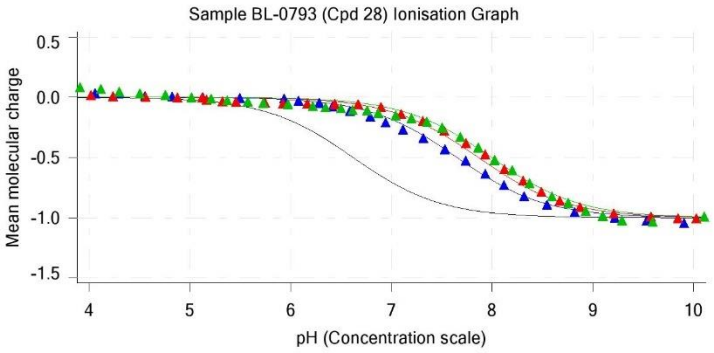
Errors None
Warnings None

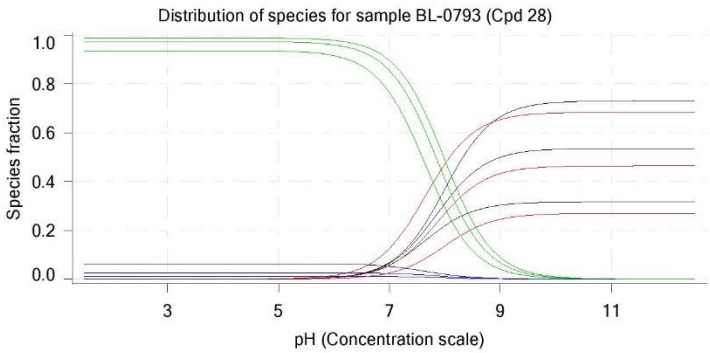
## Sample logD values

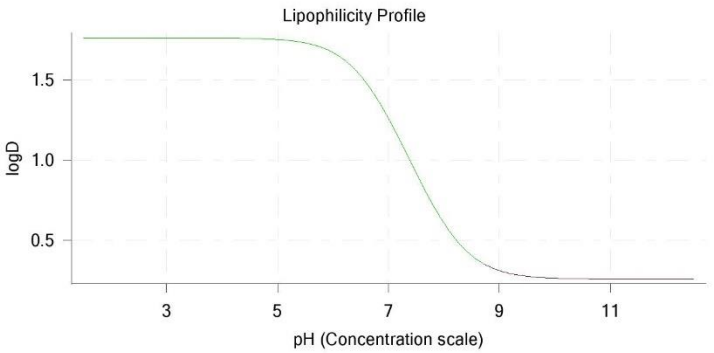
| pH | BL-0793 (Cpd 28) logD | Comment |
|---|---|---|
| 1.000 | 1.76 | |
| 1.200 | 1.76 | Stomach pH |
| 2.000 | 1.76 | |
| 3.000 | 1.76 | |
| 4.000 | 1.76 | |
| 5.000 | 1.75 | |
| 6.000 | 1.67 | |
| 6.500 | 1.52 | |
| 7.000 | 1.26 | |
| 7.400 | 0.99 | Blood pH |
| 8.000 | 0.60 | |
| 9.000 | 0.31 | |
| 10.000 | 0.26 | |
| 11.000 | 0.26 | |
| 12.000 | 0.26 | |

## Graphs




Report by: Carlo Ballatore 4/20/2020 3:13:14 PM

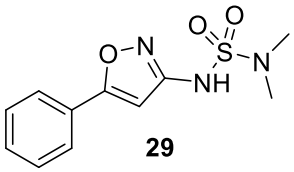
# pH-metric Result

Sample name: **BL-0797 (Cpd 29)**
Assay name: **pH-metric medium logP**
Assay ID: **20A-27004**
Filename:

Experiment start time: **1/27/2020 5:30:43 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 0.85 | ±0.01 (n=50) |
| logP (X -) | -9.98 | ±0.71 (n=50) |
| RMSD | 0.176 | |




**29**

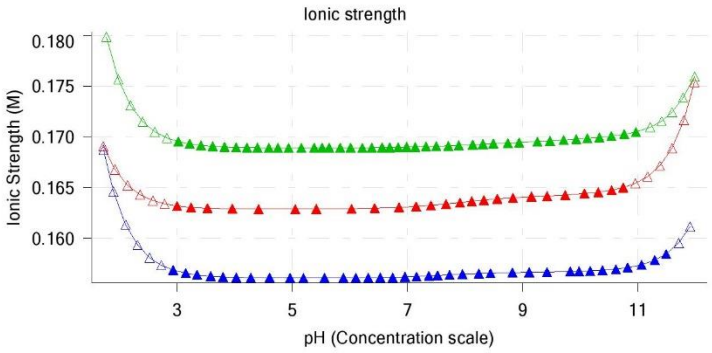
## Warnings and errors

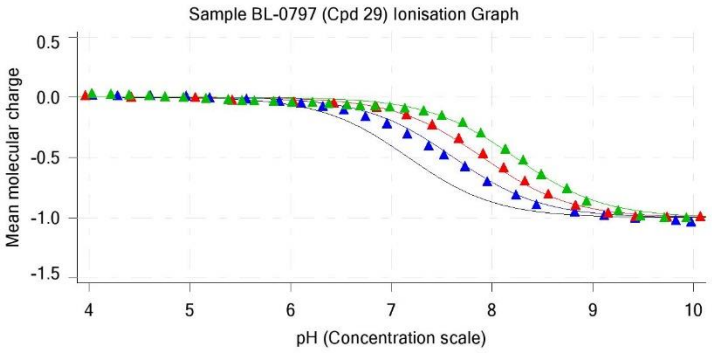
Errors None
Warnings None

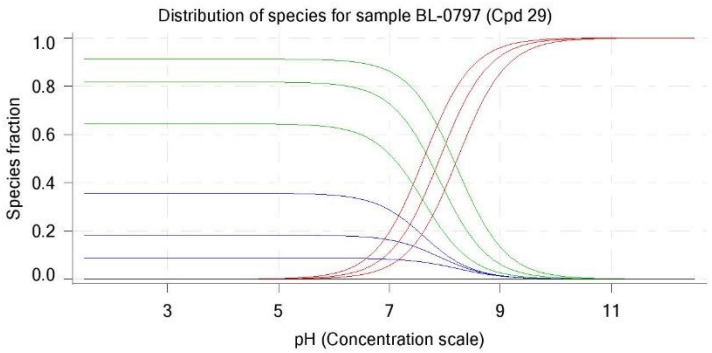
## Sample logD values

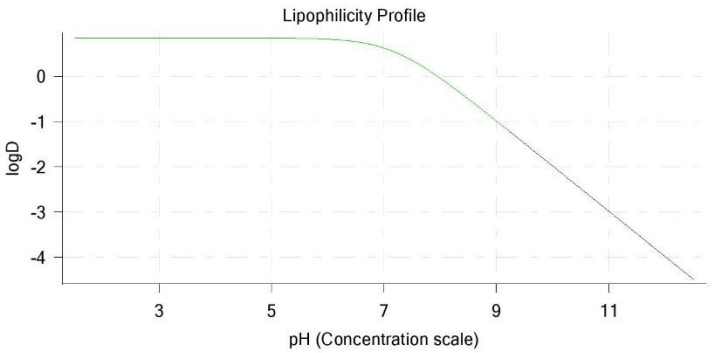
| pH | BL-0797 (Cpd 29) logD | Comment |
|---|---|---|
| 1.000 | 0.85 | |
| 1.200 | 0.85 | Stomach pH |
| 2.000 | 0.85 | |
| 3.000 | 0.85 | |
| 4.000 | 0.85 | |
| 5.000 | 0.84 | |
| 6.000 | 0.82 | |
| 6.500 | 0.76 | |
| 7.000 | 0.62 | |
| 7.400 | 0.42 | Blood pH |
| 8.000 | -0.04 | |
| 9.000 | -0.99 | |
| 10.000 | -1.98 | |
| 11.000 | -2.98 | |
| 12.000 | -3.98 | |

## Graphs



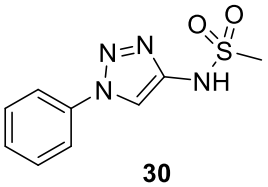
# pH-metric Result

Sample name: **BL-0771 (Cpd 30)**
Assay name: **pH-metric medium logP**
Assay ID: **19J-25003**
Filename:

Experiment start time: **10/25/2019 4:14:54 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.16 | ±0.03 (n=50) |
| logP (X -) | -10.00 | ±0.61 (n=50) |
| RMSD | 0.141 | |



**30**

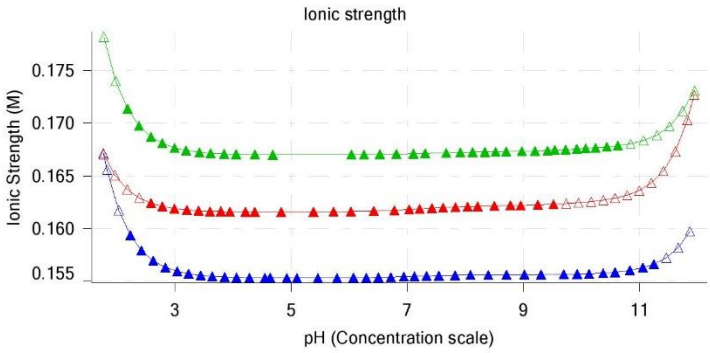
## Warnings and errors

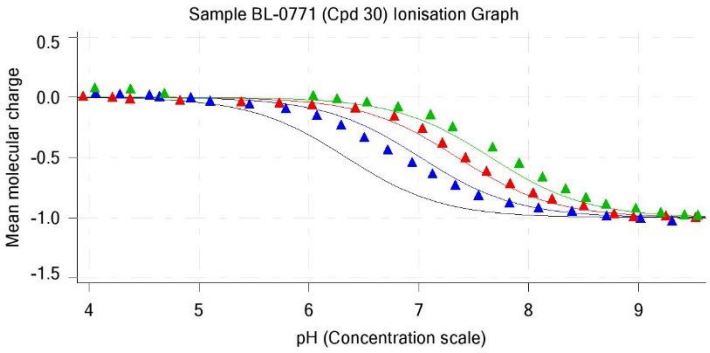
Errors None
Warnings None

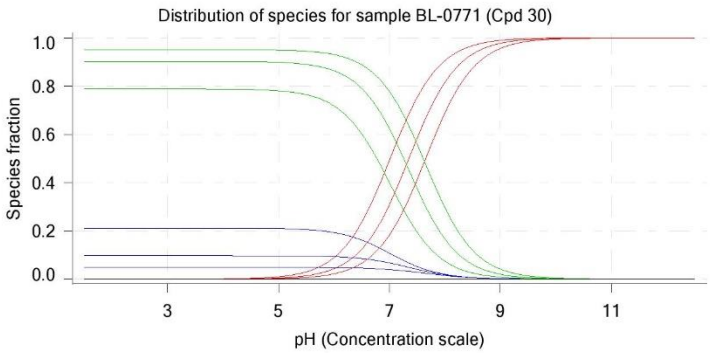
## Sample logD values

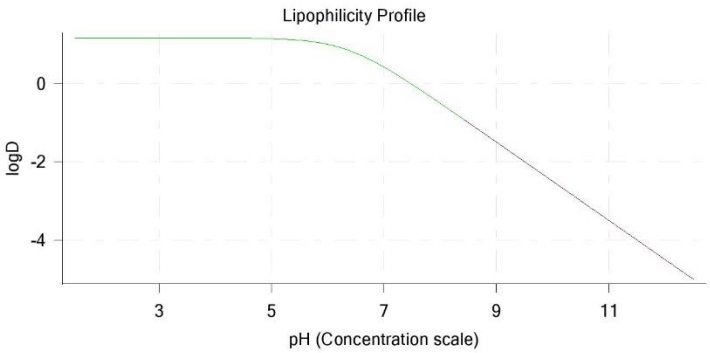
| pH | BL-0771 (Cpd 30) logD | Comment |
|---|---|---|
| 1.000 | 1.16 | |
| 1.200 | 1.16 | Stomach pH |
| 2.000 | 1.16 | |
| 3.000 | 1.16 | |
| 4.000 | 1.16 | |
| 5.000 | 1.14 | |
| 6.000 | 1.00 | |
| 6.500 | 0.77 | |
| 7.000 | 0.41 | |
| 7.400 | 0.06 | Blood pH |
| 8.000 | -0.51 | |
| 9.000 | -1.50 | |
| 10.000 | -2.50 | |
| 11.000 | -3.50 | |
| 12.000 | -4.50 | |

## Graphs



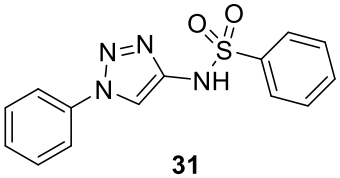
# pH-metric Result

Sample name: **BL-0772 (Cpd 31)**
Assay name: **pH-metric medium logP**
Assay ID: **19J-19006**
Filename:

Experiment start time: **10/19/2019 3:18:57 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 2.55 | ±0.04 (n=50) |
| logP (X -) | -8.00 | ±3.75 (n=50) |
| RMSD | 0.133 | |



**31**

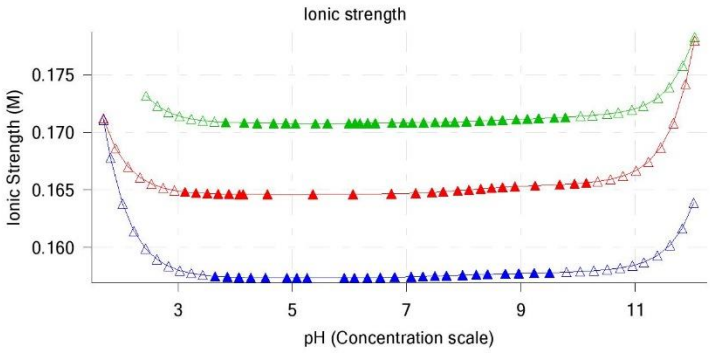
## Warnings and errors

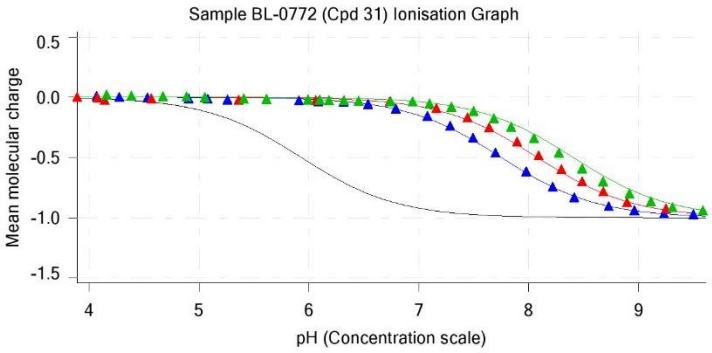
Errors None
Warnings None

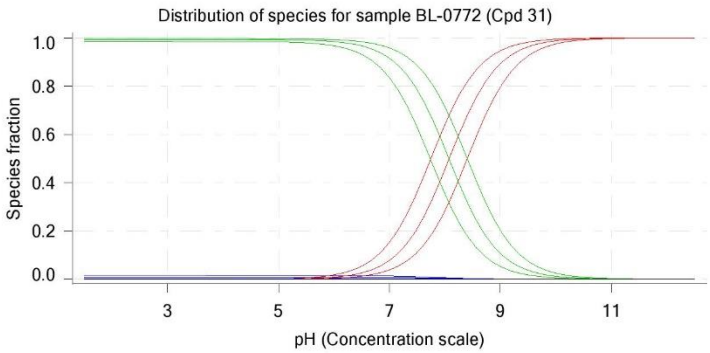
## Sample logD values

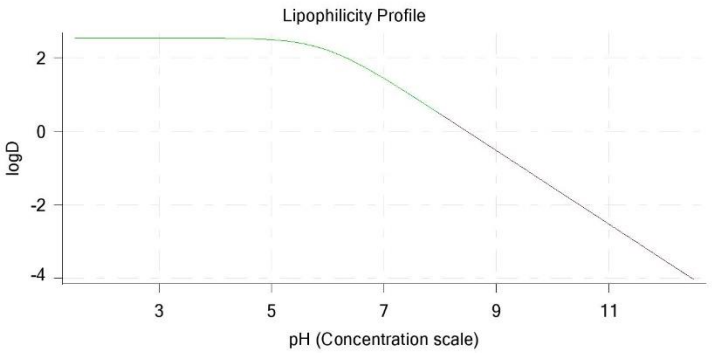
| pH | BL-0772 (Cpd 31) logD | Comment |
|---|---|---|
| 1.000 | 2.55 | |
| 1.200 | 2.55 | Stomach pH |
| 2.000 | 2.55 | |
| 3.000 | 2.54 | |
| 4.000 | 2.54 | |
| 5.000 | 2.50 | |
| 6.000 | 2.21 | |
| 6.500 | 1.87 | |
| 7.000 | 1.44 | |
| 7.400 | 1.06 | Blood pH |
| 8.000 | 0.47 | |
| 9.000 | -0.53 | |
| 10.000 | -1.52 | |
| 11.000 | -2.52 | |
| 12.000 | -3.52 | |

## Graphs



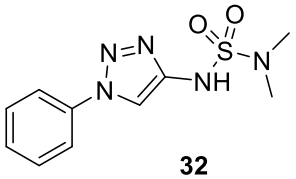
pH-metric Result

Sample name: **BL-0773 (Cpd 32)**
Assay name: **pH-metric medium logP**
Assay ID: **19J-20006**
Filename:

Experiment start time: **10/20/2019 1:32:14 PM**
Analyst:
Instrument ID: **T317135**

## pH-metric Result

| | | |
|---|---|---|
| logP (neutral XH) | 1.72 | ±0.01 (n=49) |
| logP (X -) | -9.50 | ±0.59 (n=49) |
| RMSD | 0.216 | |



**32**

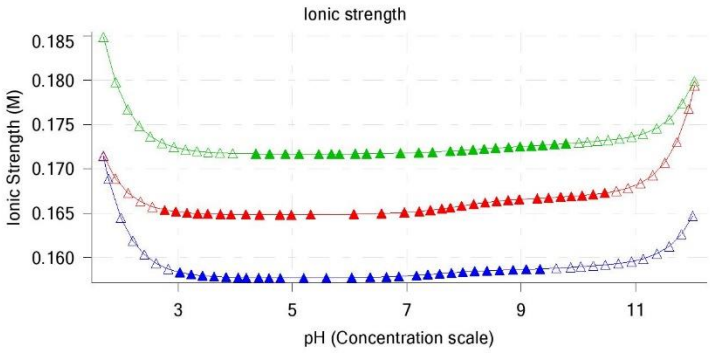
## Warnings and errors

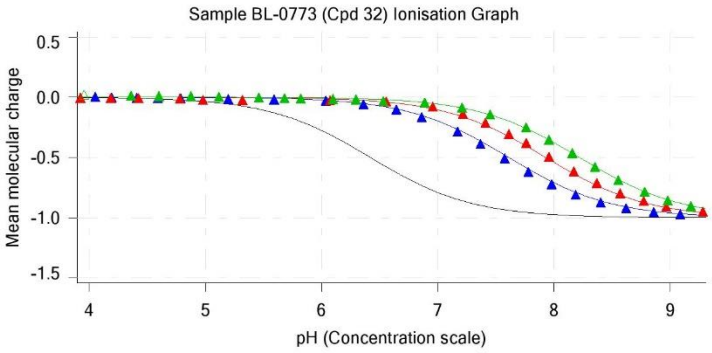
Errors None
Warnings None

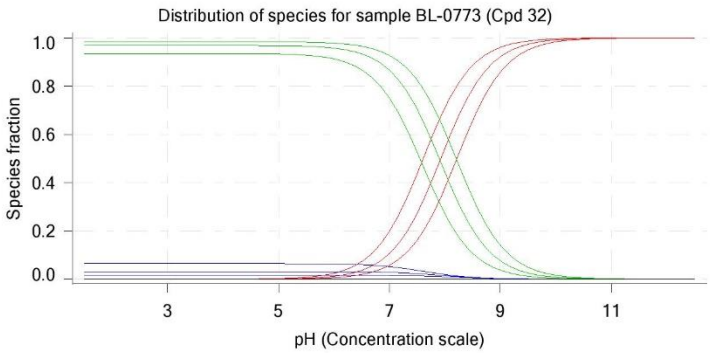
## Sample logD values

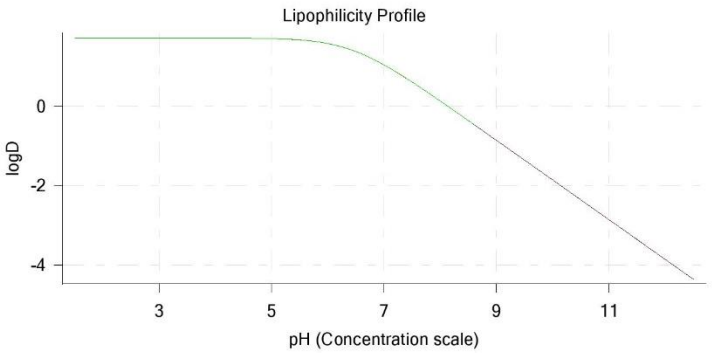
| pH | BL-0773 (Cpd 32) logD | Comment |
|---|---|---|
| 1.000 | 1.72 | |
| 1.200 | 1.72 | Stomach pH |
| 2.000 | 1.72 | |
| 3.000 | 1.72 | |
| 4.000 | 1.72 | |
| 5.000 | 1.70 | |
| 6.000 | 1.58 | |
| 6.500 | 1.38 | |
| 7.000 | 1.04 | |
| 7.400 | 0.69 | Blood pH |
| 8.000 | 0.13 | |
| 9.000 | -0.86 | |
| 10.000 | -1.86 | |
| 11.000 | -2.86 | |
| 12.000 | -3.86 | |

## Graphs



**Experimental Details on PAMPA Analysis:** these determinations were carried out by Analiza Inc. (Cleveland, OH).

**Assay Summary:** Parallel Artificial Membrane Permeability Assay (PAMPA) using the Corning GentestTM pre-coated PAMPA plate system with quantitation by HPLC-UV.

**Sample Preparation:** Upon arrival at Analiza samples will be prepared as DMSO stock solutions and sonicated in a 40°C water bath to facilitate dissolution.

**Assay Setup:** Dilutions (50-fold) of the DMSO stocks are prepared in PBS, 7.4 for a dose concentration of 200µM in a volume of 300µL directly in the Donor compartment of the Corning GentestTM Pre-coated PAMPA plate. After preparation of the Donor plate, any precipitation is noted. The Acceptor compartment is filled with 1xPBS (200µL), pH 7.4. After careful assembly of the PAMPA plate, it is left to incubate for five hours in the dark at ambient temperature. A sister plate is created (50x dilution of 10mM test articles are prepared in 1xPBS, pH 7.4) directly in a Millipore solubility filter plate to measure the initial concentration of the sample in buffer (C0). Following incubation, the PAMPA plate is disassembled, and the samples are transferred from the Donor and Acceptor plates to 96-well plates for analysis. The C0 plate is filtered prior to analysis.

1. HPLC-UV: a. The filtrates are injected onto an AQUASIL C18, 50x2.1mM column and eluted using a fast generic gradient program.
    a. A standard calibration curve (STD) is prepared for each compound. The DMSO stock is diluted in DMSO (or other suitable solvent) spanning the concentration range of the assay and instrument
    b. The filtrates are quantified with respect to this calibration curve.
    c. A comments field will contain notes pertinent to the assay of each compound.
    d. Chromatograms are reported for each compound

**Calculation of Results:** The concentration values from the Donor and Acceptor compartment are used in the calculation of the effective permeability (Pe) of the compound. A mass balance equation is used to calculate the amount of compound retained in the membrane (%R). A high %R indicates either that the compound is bound to the PAMPA membrane, or that the compound is precipitating in the donor compartment. The equations for permeability and membrane retention are shown below. Note that we experimentally determine Co, instead of assuming the full solubility of the compound. Pe values less than 1.5E-6 cm/s correlate with human fraction absorbed (%FA) less than 80%, a generally accepted cutoff for low permeability.

PAMPA Effective Permeability

$$P_e = \frac{-\ln\left(1-\frac{C_A(t)}{C_{eq}}\right)}{A*\left(\frac{1}{V_D}+\frac{1}{V_A}\right)*t}$$

Membrane Retention (R)

$$R = 1 - (C_D(t) * V_D + C_A(t) * V_A)/(C_0 * V_D))$$

CA(t) = compound concentration in acceptor well at time t (mM)
CD(t) = compound concentration in acceptor well at time t (mM)
C0 = initial compound concentration in donor well (mM)
VD = donor well volume = 0.3mL
VA = acceptor well volume = 0.2mL
A = filter area = 0.3cm2
t = incubation time = 5hr = 18000s
Ceq = compound concentration at equilibrium

$$= = (C_D(t) * V_D + C_A(t) * V_A)/(V_D * V_A)$$

**Experimental Details on Shake-Flask logD determination:** these determinations were carried out by Analiza Inc. (Cleveland, OH).

**Assay Summary:** Analiza measures LogD directly, using its thermodynamic definition: the partition coefficient in buffer-octanol system in equilibrium using a novel, automated and miniaturized version of the gold standard shake-flask method.

**Partitioning:** For octanol/buffer partitioning, Analiza's standard two phase system plates will be used. Octanol in equilibrium with 1X-PBS, 7.4 is used to prepare partitioning plates for the assay. DMSO stock solutions will be added to each partitioning plate to a final concentration of 10% DMSO. The plates are sealed, vortexed on our specially designed deepwell plate mixer, and centrifuged to aid in phase settling. The assay will be conducted on the ADW workstation using chemiluminescent nitrogen detection.

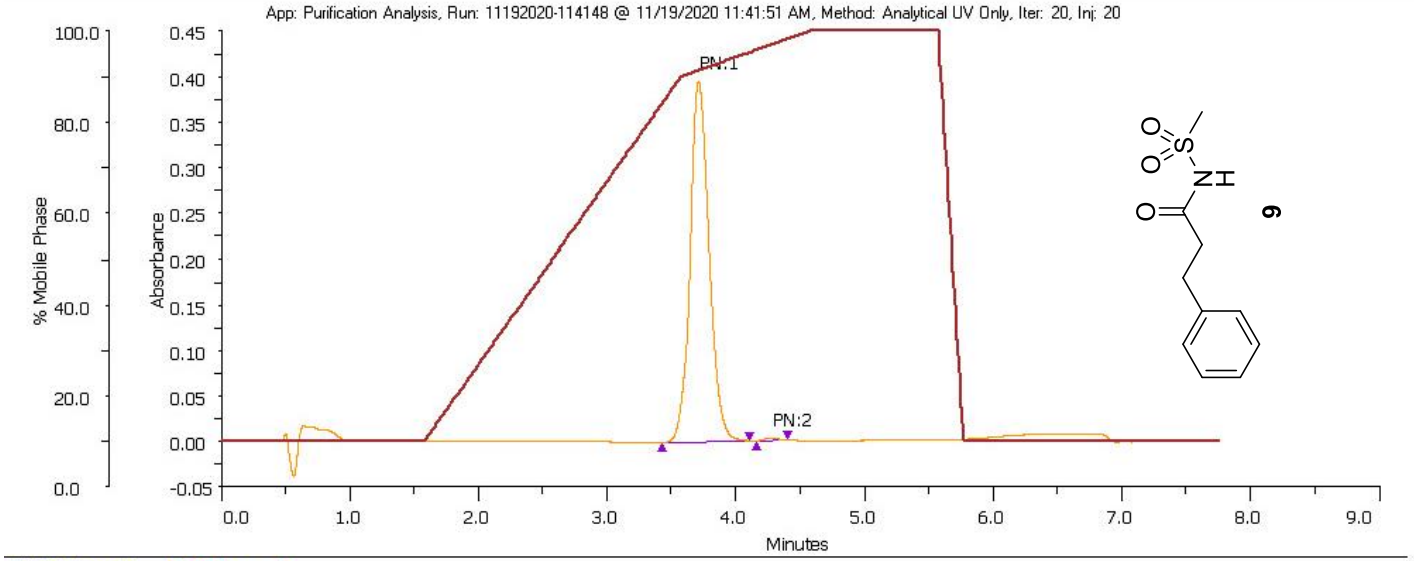
**Calculation of Results:** The equimolar nitrogen response of the detector is calibrated using standards which span the dynamic range of the instrument from 0.08 to 4500 μg/ml nitrogen. Both the top and bottom phases are quantified with respect to this calibration curve and the logarithm of the ratio of the concentration in the top phase to the concentration in the bottom phase is calculated as LogD. In addition to reporting the directly observed LogD value, the observed LogD value will be adjusted to a corrected LogD* based upon our previous work correlating LogD in the presence and absence of DMSO in the partitioning system.

The calculated LogD and LogD* values are corrected for background nitrogen in the DMSO and octanol-buffer 2-phase systems. A comments field contains notes pertinent to the assay of each compound, such as solid residue in the source plate, or aggregation of compound in the two phase system.

**Quality:** Each sample submission includes a series of on-board performance indicating standards (with LogD values spanning the range of the assay) which are prepared and assayed in duplicate in each media. The LogD results for these standards are control charted and monitored.

## Graph

| | |
|---|---|
| Sample Name | Cpd 9 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 20 |





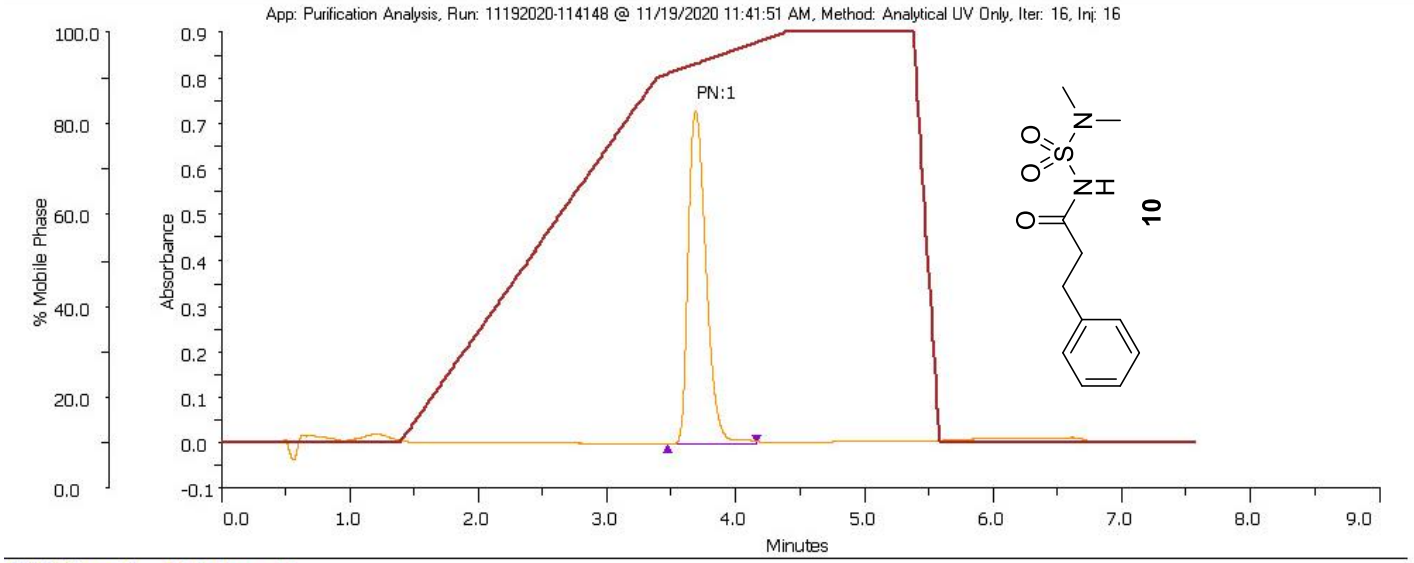

**9**

## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.715 | 6787.1778 | Cpd 9 | 99.536 | | | | | | |
| 4.284 | 31.6639 | Cpd 9 | 0.464 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 10 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 16 |

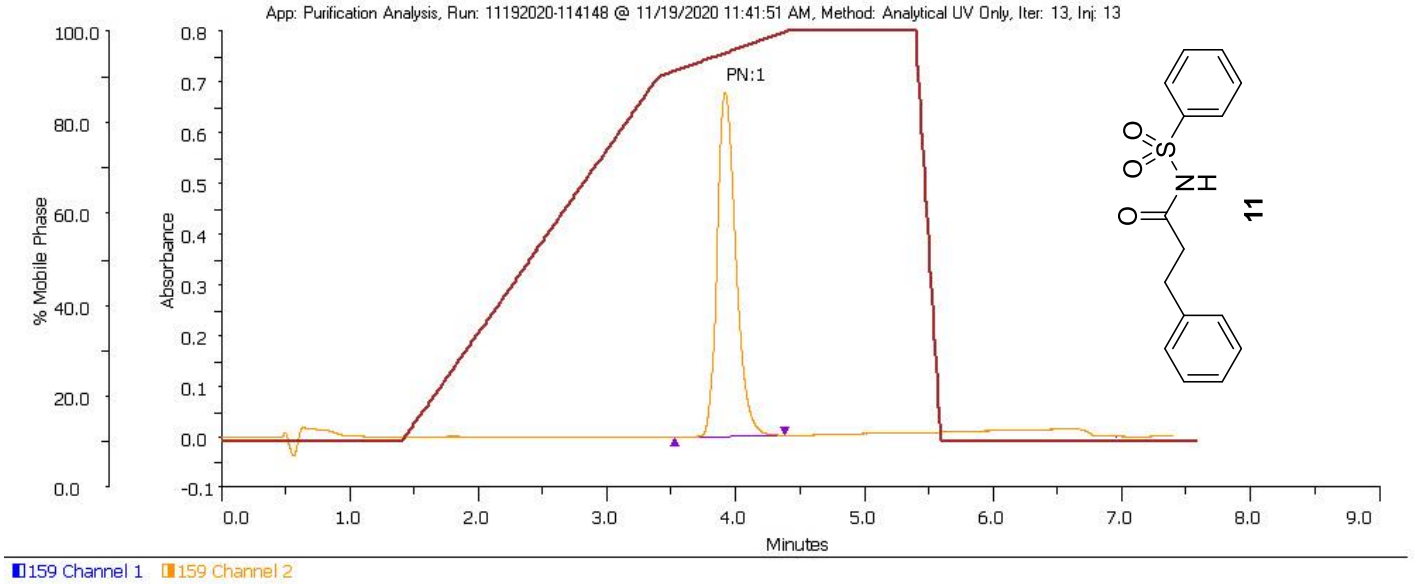



## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.691 | 11757.7444 | Cpd 10 | 100 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 11 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 13 |

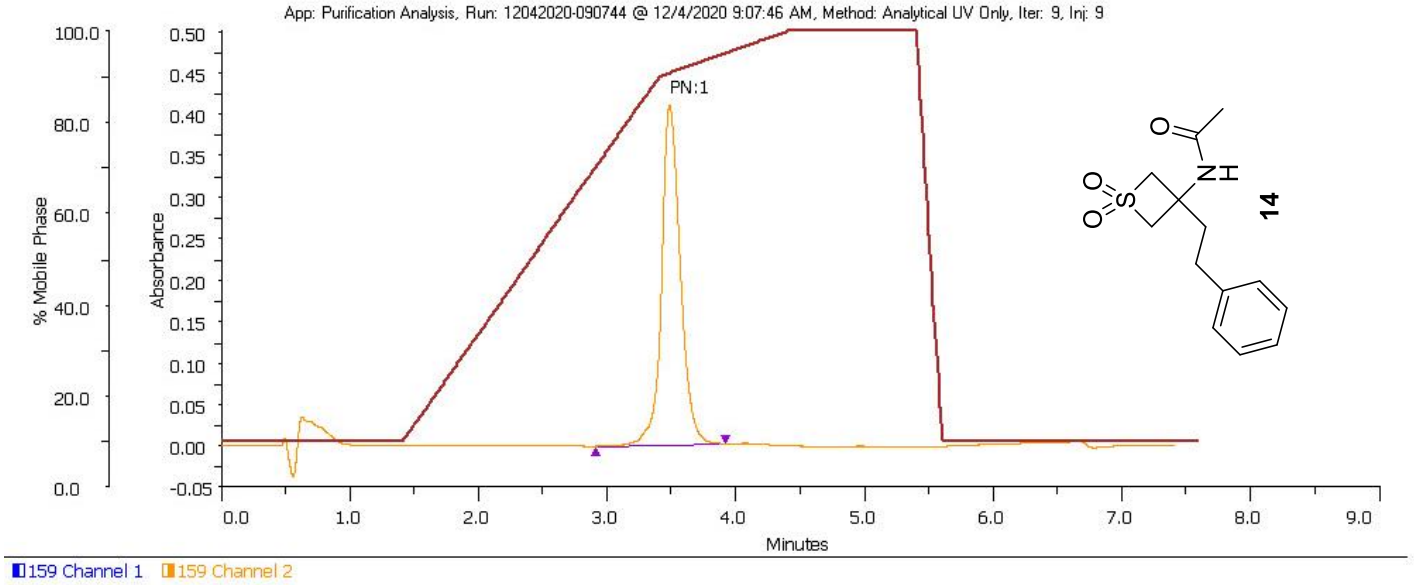



## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.92 | 11454.6342 | Cpd 11 | 100 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 14 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 9 |





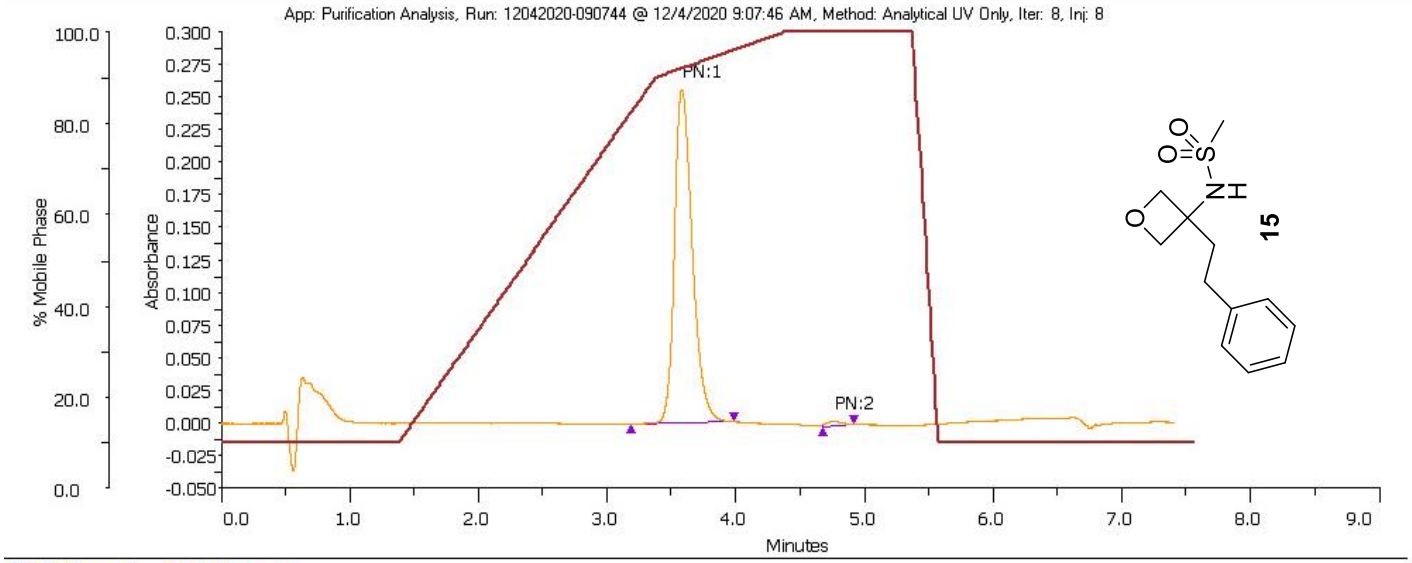


## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.488 | 6947.7902 | Cpd 14 | 100 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 15 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 8 |

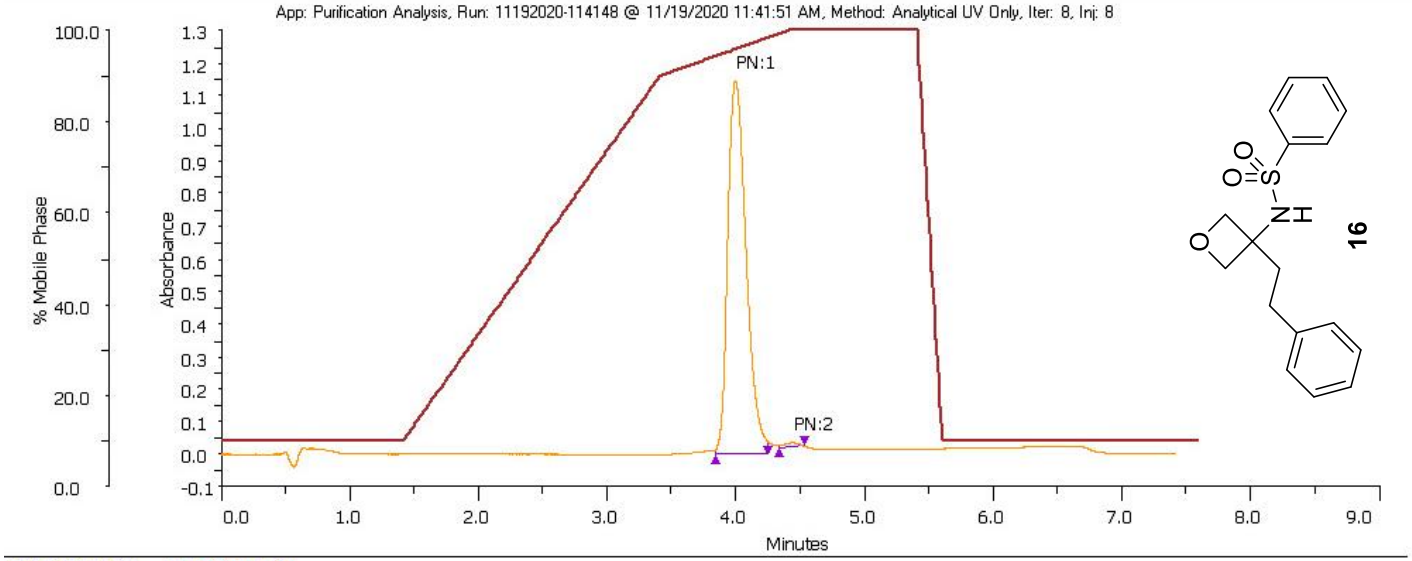



## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.583 | 4131.9665 | Cpd 15 | 98.944 | | | | | | |
| 4.76 | 44.0801 | Cpd 15 | 1.056 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 16 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 8 |





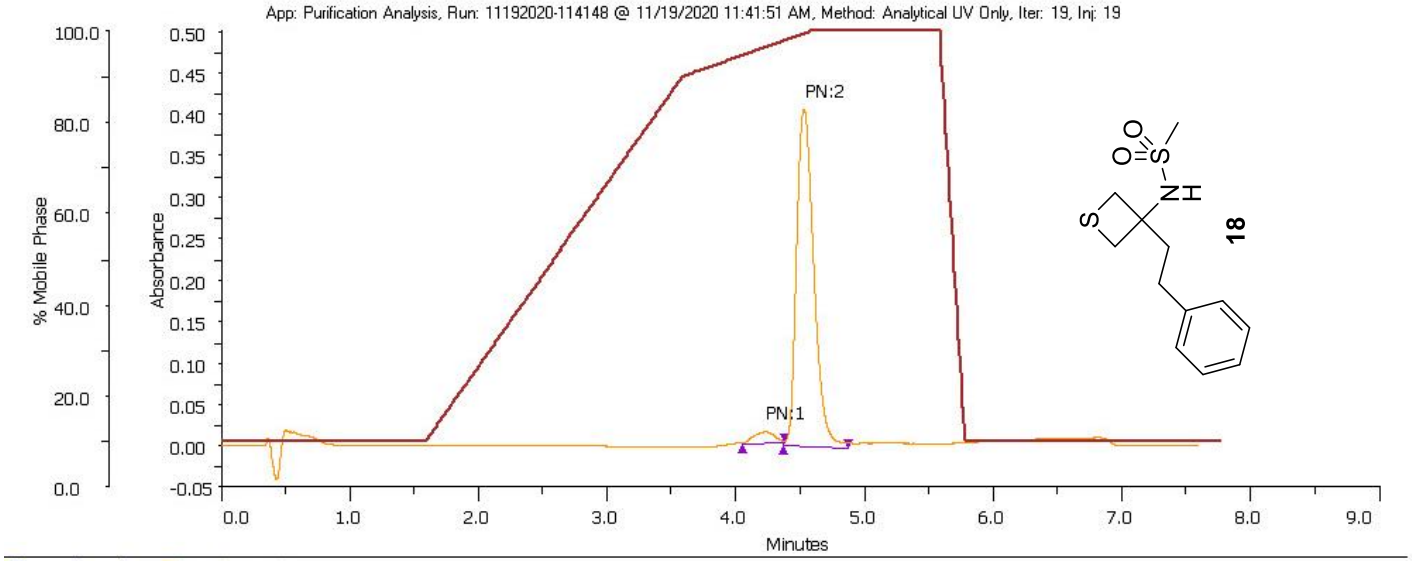


## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4.001 | 19088.5686 | Cpd 16 | 99.124 | | | | | | |
| 4.434 | 168.612 | Cpd 16 | 0.876 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 18 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 19 |

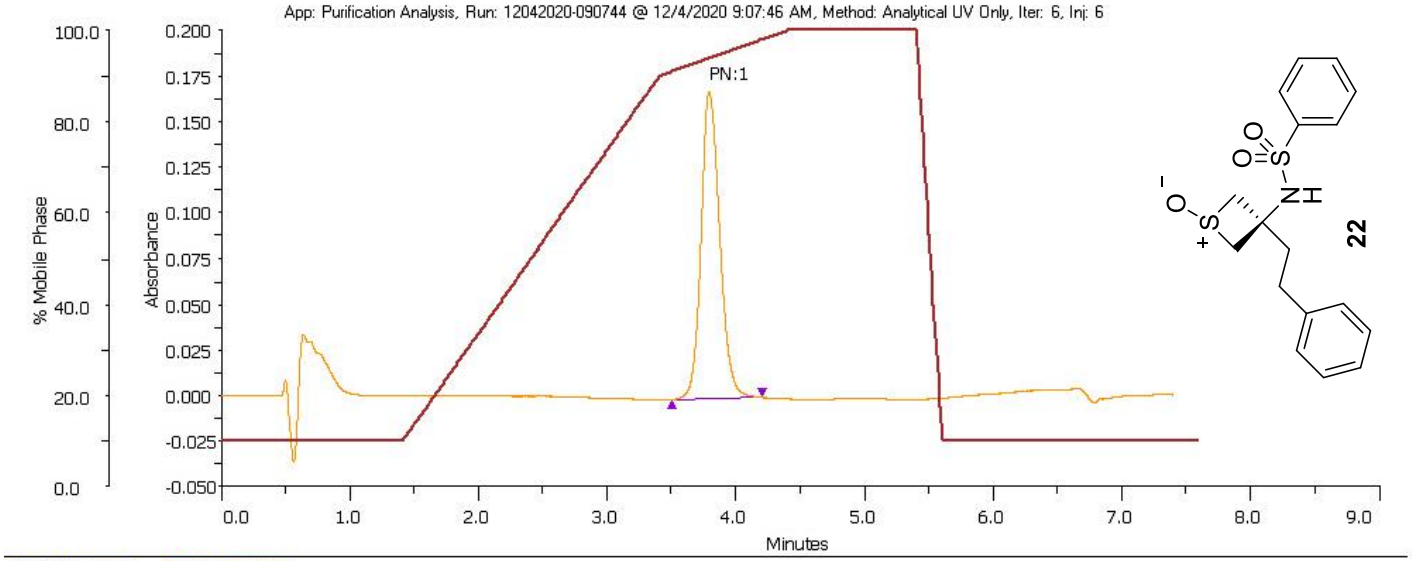



## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4.234 | 248.6748 | Cpd 18 | 3.774 | | | | | | |
| 4.535 | 6341.2665 | Cpd 18 | 96.226 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 22 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 6 |





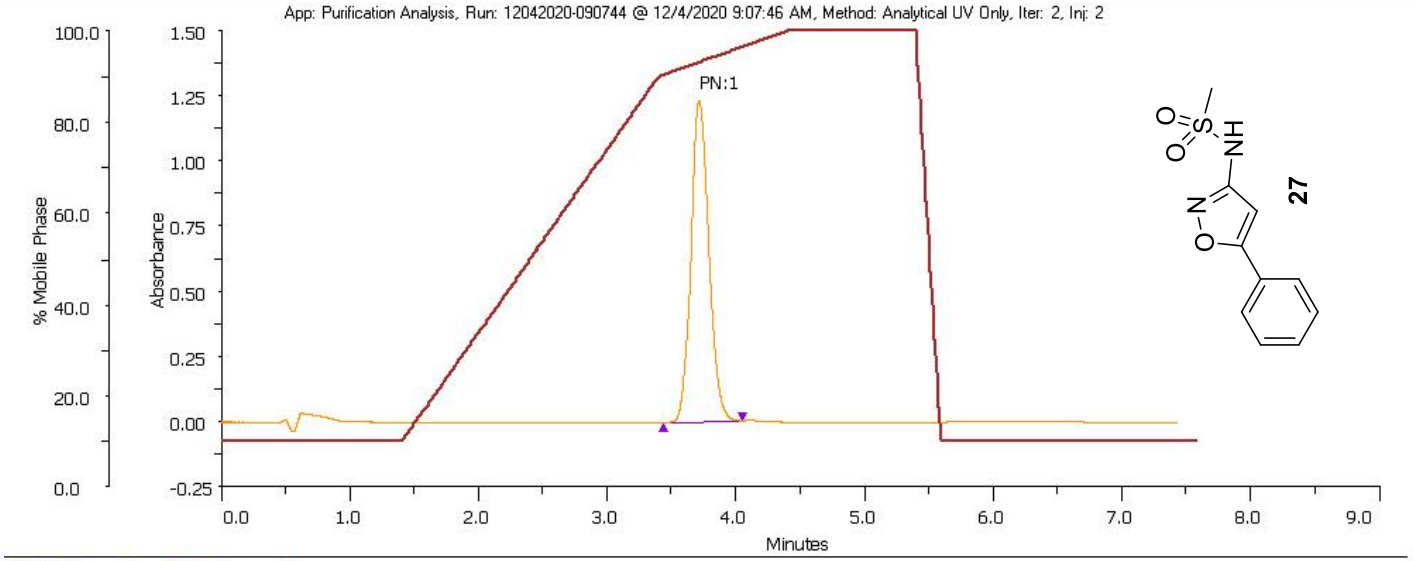


## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.798 | 2846.4563 | Cpd 22 | 100 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 27 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 2 |





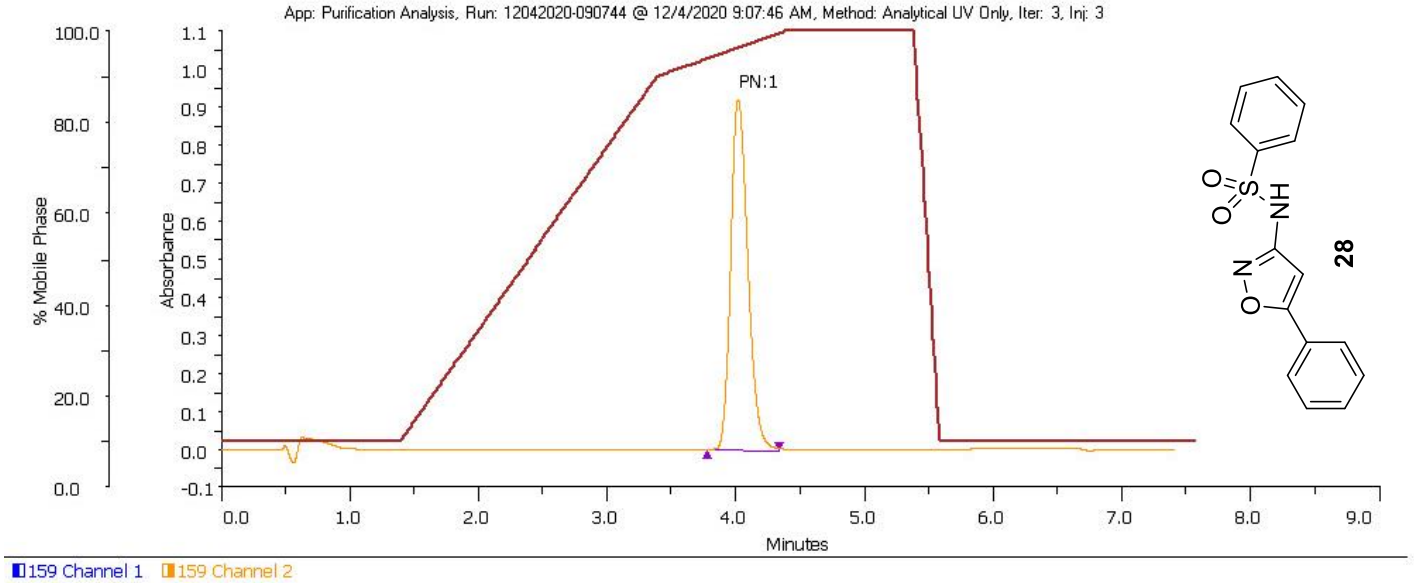


## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 3.719 | 19871.9541 | Cpd 27 | 100 | | | | | | |

## Graph

| | |
|---|---|
| Sample Name | Cpd 28 |
| Application Name | Purification Analysis (Administrator) |
| Method Name | Analytical UV Only |
| Configuration Name | UV Only Config |
| Version | 18 |
| Data Instrument Name | Detector |
| Data Channel Name | 159 Channel 1 |
| Notes | |
| Injection Number | 3 |



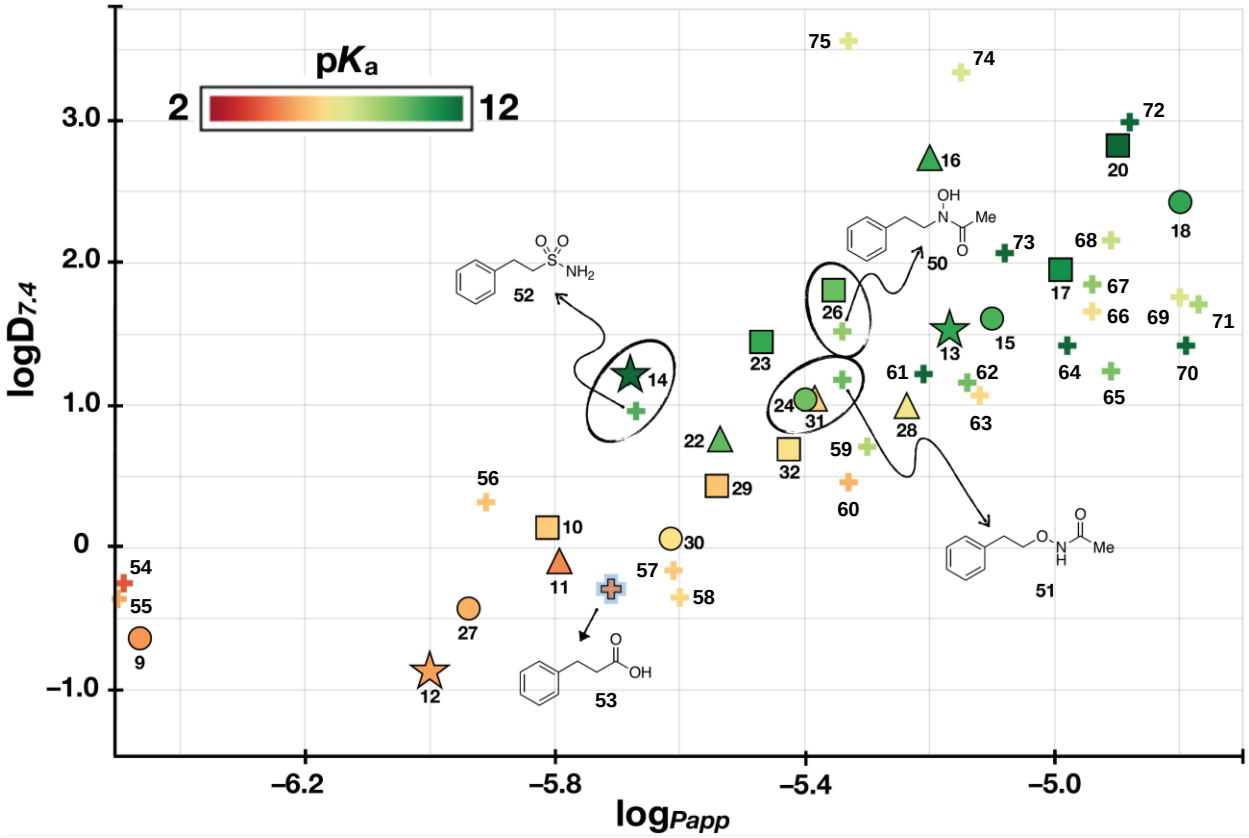


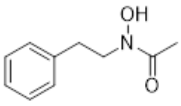
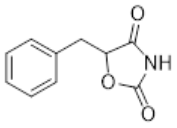
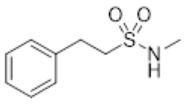
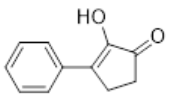
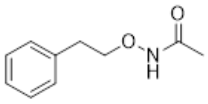
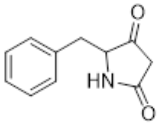
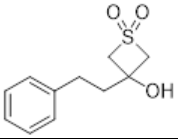
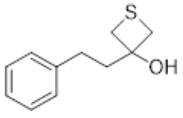
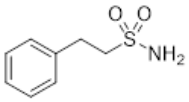
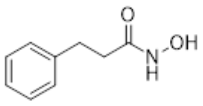
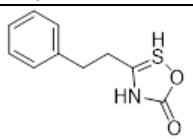
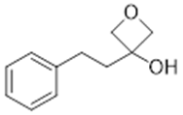
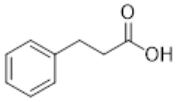
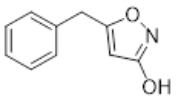
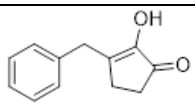
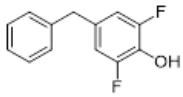
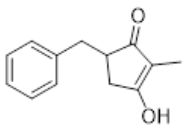
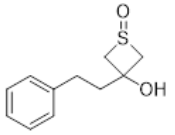
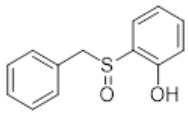
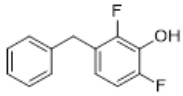
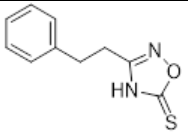
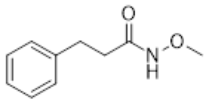
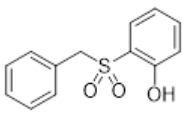
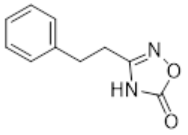
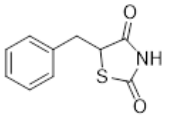
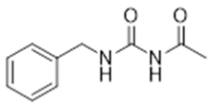


## Sample Table

| Retention Time (min) | Area (mAUmin x100) | Sample Name | Area % | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4.023 | 14366.6859 | Cpd 28 | 100 | | | | | | |

**Figure S4.** Comparison of lipophilicity (i.e., log$D_{7.4}$), acidity (i.e., p$K_a$), and permeability (i.e., log$P_{app}$) of test compounds vs other classes of carboxylic acid bioisosteres (crosses) from Lassalas, P. et. al. *J. Med. Chem*. **2016**, 59, 3183-3203.




| Cpd ID | Structure | Cpd ID | Structure | Cpd ID | Structure | Cpd ID | Structure |
|---|---|---|---|---|---|---|---|
| 50 |  | 57 |  | 64 |  | 71 |  |
| 51 |  | 58 |  | 65 |  | 72 |  |
| 52 |  | 59 |  | 66 |  | 73 |  |
| 53 |  | 60 |  | 67 |  | 74 |  |
| 54 |  | 61 |  | 68 |  | 75 |  |
| 55 |  | 62 |  | 69 |  | | |
| 56 |  | 63 |  | 70 |  | | |

**X-ray Structure Determination for BL-0650 (Cpd 15, CCDC 1998391)**

**Experimental:**

Crystals of BL-0650 (Cpd 15) were grown from dichloromethane/hexanes. The single crystal X-ray diffraction studies were carried out on a Bruker APEX-II CCD diffractometer equipped with with Mo Kα radiation (λ = 0.71073). A 0.20 × 0.06 × 0.04 mm colorless block was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 60 mm with 5.00 s exposure time. A total of 5531 reflections were collected covering the indices $-10 \leq h \leq 10$, $-7 \leq k \leq 7$, $-11 \leq l \leq 16$. 2529 reflections were found to be symmetry independent, with a Rint of 0.0256. The space group was found to be $P2_1$. Crystallographic data are summarized in Table 1.

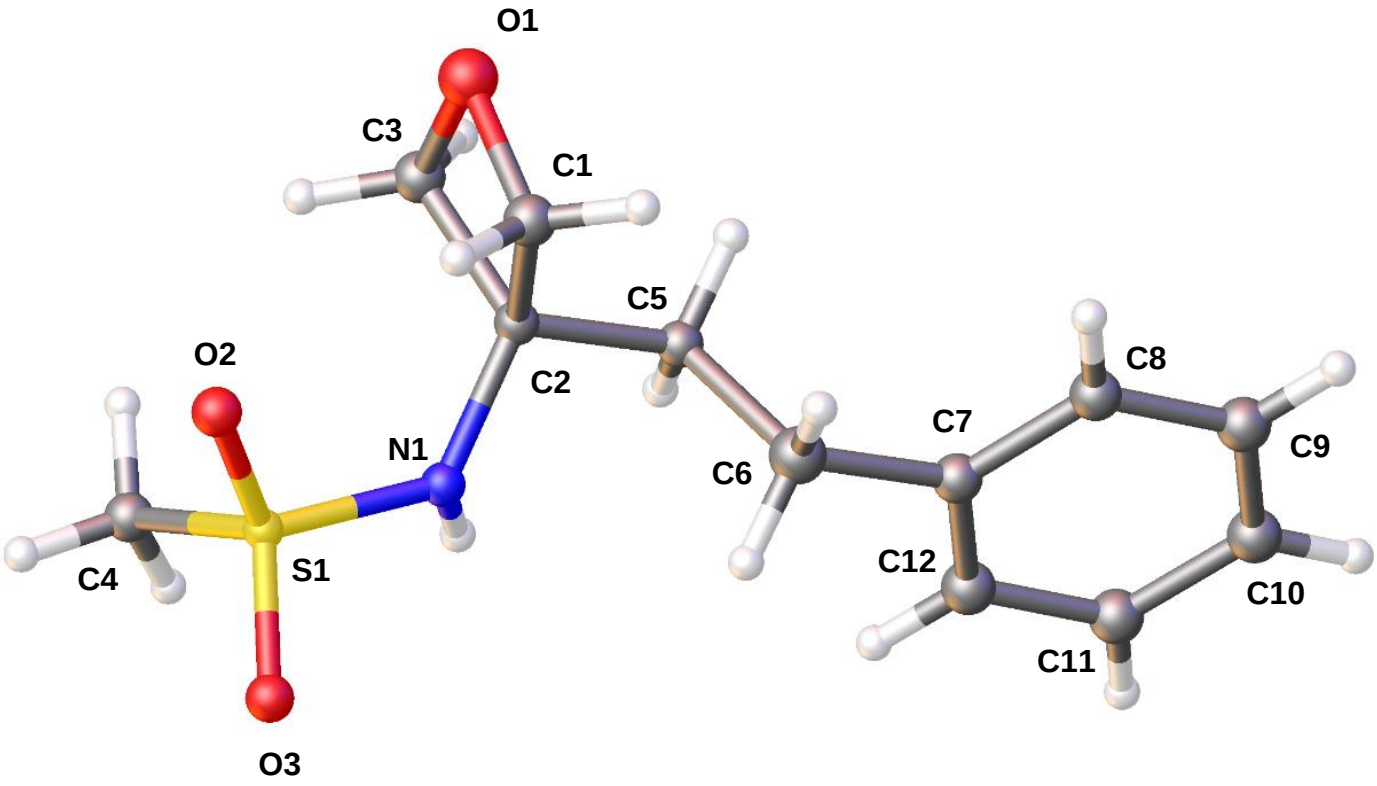


**Table 1 Crystal data and structure refinement for BL-0650 (Cpd 15)**

| | |
|---|---|
| Identification code | BL-0650 |
| Empirical formula | C12H17NO3S |
| Formula weight | 255.32 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | P21 |
| a/Å | 8.0972(6) |
| b/Å | 5.7922(5) |
| c/Å | 13.2864(11) |
| α/° | 90 |
| β/° | 95.043(3) |
| γ/° | 90 |
| Volume/Å3 | 620.73(9) |
| Z | 2 |
| ρcalcg/cm3 | 1.366 |
| μ/mm-1 | 0.257 |
| F(000) | 272.0 |
| Crystal size/mm3 | 0.20 × 0.06 × 0.04 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.078 to 52.784 |
| Index ranges | -10 ≤ h ≤ 10, -7 ≤ k ≤ 7, -11 ≤ l ≤ 16 |
| Reflections collected | 5531 |
| Independent reflections | 2529 [Rint = 0.0256, Rsigma = 0.0302] |
| Data/restraints/parameters | 2529/1/155 |
| Goodness-of-fit on F2 | 1.046 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0269, wR2 = 0.0662 |
| Final R indexes [all data] | R1 = 0.0283, wR2 = 0.0673 |
| Largest diff. peak/hole / e Å-3 | 0.32/-0.24 |

**Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for BL-0650 (Cpd 15) $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| S1 | 3055.3(6) | 5772.7(10) | 5217.6(4) | 12.36(13) |
| N1 | 3619(2) | 5297(3) | 4096.8(14) | 14.6(4) |
| O2 | 1992(2) | 7771(3) | 5180.0(13) | 18.3(4) |
| O3 | 4565.7(17) | 5847(4) | 5884.2(11) | 17.2(3) |
| O1 | 477(2) | 7568(4) | 2550.9(13) | 26.0(4) |
| C2 | 2681(2) | 5818(5) | 3125.0(15) | 15.1(4) |
| C4 | 1930(3) | 3359(4) | 5576.5(19) | 18.1(5) |
| C7 | 6389(3) | 4764(4) | 1474.9(18) | 18.6(5) |
| C6 | 5411(3) | 5824(7) | 2280.8(18) | 24.4(5) |
| C5 | 3669(3) | 4791(4) | 2298.1(17) | 16.2(5) |
| C1 | 2143(3) | 8335(4) | 2909.7(18) | 20.5(5) |
| C8 | 6563(3) | 5908(6) | 571.2(17) | 19.9(5) |
| C10 | 8344(3) | 2885(5) | 41.8(19) | 22.2(5) |
| C12 | 7166(3) | 2636(5) | 1641.0(19) | 21.9(5) |
| C11 | 8143(3) | 1698(5) | 931(2) | 22.4(5) |
| C9 | 7550(3) | 4981(5) | -136.2(18) | 22.4(5) |
| C3 | 808(3) | 5259(4) | 2952.0(19) | 19.9(6) |

**Table 3 Anisotropic Displacement Parameters (Å2×103) for BL-0650 (Cpd 15). The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| S1 | 11.2(2) | 11.7(2) | 14.2(2) | -0.4(2) | 1.52(17) | -0.9(2) |
| N1 | 15.1(9) | 13.0(11) | 15.8(9) | -1.0(7) | 2.7(7) | 3.3(7) |
| O2 | 19.0(8) | 16.5(9) | 19.8(9) | -1.0(7) | 3.8(7) | 3.9(7) |
| O3 | 15.5(7) | 18.5(7) | 17.2(7) | -1.6(9) | -0.9(6) | -3.0(9) |
| O1 | 22.4(9) | 31.6(10) | 23.5(9) | 6.4(8) | -1.0(7) | 8.0(8) |
| C2 | 15.8(9) | 14.6(10) | 14.7(10) | 0.0(12) | 1.2(8) | -1.8(12) |
| C4 | 16.5(11) | 16.8(12) | 20.7(12) | 2.4(10) | 0.7(10) | -5.1(10) |
| C7 | 15.6(10) | 21.4(12) | 19.2(12) | -6.0(10) | 3.6(9) | -7.5(11) |
| C6 | 23.3(11) | 26.7(12) | 24.4(12) | -8.9(14) | 9.5(9) | -9.6(14) |
| C5 | 16.0(10) | 17.0(11) | 15.7(11) | -1.7(9) | 1.5(8) | -0.1(10) |
| C1 | 26.2(13) | 18.9(13) | 16.4(11) | 0.5(10) | 1.1(10) | 4.8(11) |
| C8 | 19.1(10) | 18.4(11) | 22.1(11) | -0.6(12) | 1.5(8) | -0.4(12) |
| C10 | 16.3(11) | 29.5(15) | 21.4(12) | -10.9(11) | 5.1(9) | -3.4(10) |
| C12 | 22.6(12) | 24.4(13) | 18.3(12) | 2.3(11) | 0.4(10) | -6.0(11) |
| C11 | 18.0(12) | 18.7(11) | 29.8(14) | -2.2(11) | -1.1(10) | -0.8(9) |
| C9 | 23.3(12) | 27.9(14) | 16.2(12) | 2.1(10) | 3.4(9) | -5.3(11) |
| C3 | 15.9(11) | 24.2(16) | 19.6(11) | -0.6(10) | 1.3(9) | 2.6(9) |

**Table 4 Bond Lengths for BL-0650 (Cpd 15)**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| S1 | N1 | 1.6189(19) | C2 | C3 | 1.549(3) |
| S1 | O2 | 1.4407(18) | C7 | C6 | 1.516(3) |
| S1 | O3 | 1.4462(14) | C7 | C8 | 1.389(4) |
| S1 | C4 | 1.757(3) | C7 | C12 | 1.393(4) |
| N1 | C2 | 1.471(3) | C6 | C5 | 1.534(3) |
| O1 | C1 | 1.460(3) | C8 | C9 | 1.394(3) |
| O1 | C3 | 1.456(3) | C10 | C11 | 1.390(4) |
| C2 | C5 | 1.534(3) | C10 | C9 | 1.384(4) |
| C2 | C1 | 1.541(4) | C12 | C11 | 1.393(4) |

## Table 5 Bond Angles for BL-0650 (Cpd 15)

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| N1 | S1 | C4 | 107.98(11) | C1 | C2 | C3 | 85.01(17) |
| O2 | S1 | N1 | 108.71(10) | C8 | C7 | C6 | 121.1(3) |
| O2 | S1 | O3 | 117.91(11) | C8 | C7 | C12 | 118.7(2) |
| O2 | S1 | C4 | 109.02(11) | C12 | C7 | C6 | 120.2(2) |
| O3 | S1 | N1 | 106.07(9) | C7 | C6 | C5 | 113.0(2) |
| O3 | S1 | C4 | 106.74(12) | C2 | C5 | C6 | 113.4(2) |
| C2 | N1 | S1 | 127.39(15) | O1 | C1 | C2 | 90.62(18) |
| C3 | O1 | C1 | 91.44(16) | C7 | C8 | C9 | 120.5(3) |
| N1 | C2 | C5 | 106.72(18) | C9 | C10 | C11 | 119.5(2) |
| N1 | C2 | C1 | 118.2(2) | C11 | C12 | C7 | 120.9(2) |
| N1 | C2 | C3 | 120.70(19) | C10 | C11 | C12 | 119.9(2) |
| C5 | C2 | C1 | 113.0(2) | C10 | C9 | C8 | 120.5(2) |
| C5 | C2 | C3 | 112.20(19) | O1 | C3 | C2 | 90.47(19) |

## Table 6 Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for BL-0650 (Cpd 15)

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| H1 | 3975.34 | 3863.72 | 4075.74 | 17 |
| H4a | 899.58 | 3229.13 | 5135.07 | 27 |
| H4b | 1668.27 | 3541.48 | 6278.29 | 27 |
| H4c | 2596.22 | 1961.09 | 5516.36 | 27 |
| H6a | 5312.85 | 7507.57 | 2161.5 | 29 |
| H6b | 6027.9 | 5590.8 | 2949.96 | 29 |
| H5a | 3046.2 | 5052.31 | 1632.69 | 19 |
| H5b | 3767.89 | 3102.99 | 2402.35 | 19 |
| H1a | 2175.38 | 9308.59 | 3523.53 | 25 |
| H1b | 2743.21 | 9086.69 | 2380.57 | 25 |
| H8 | 6005.25 | 7331.04 | 434.43 | 24 |
| H10 | 9021.23 | 2264.15 | -440.46 | 27 |
| H12 | 7028.48 | 1812.38 | 2246.36 | 26 |
| H11 | 8670.29 | 247.78 | 1055.55 | 27 |
| H9 | 7678.68 | 5793.91 | -745.42 | 27 |
| H3a | 547.52 | 4017.24 | 2450.88 | 24 |
| H3b | 283.81 | 4946.04 | 3583.84 | 24 |

**X-ray Structure Determination for BL-0658 (Cpd 16, CCDC 1995771)**

**Experimental:**

Crystals of BL-0658 (Cpd 16) were grown from ethyl acetate. The single crystal X-ray diffraction studies were carried out on a Bruker APEX-II CCD diffractometer equipped with Cu Kα radiation (l = 1.54178). A 0.28 × 0.03 × 0.03 mm colorless needle was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 40 mm with 5.00 s exposure time. A total of 9057 reflections were collected covering the indices $-20 \leq h \leq 21$, $-9 \leq k \leq 9$, $-13 \leq l \leq 12$. 2727 reflections were found to be symmetry independent, with a Rint of 0.0770. The space group was found to be $P2_1/c$. Crystallographic data are summarized in Table 1.

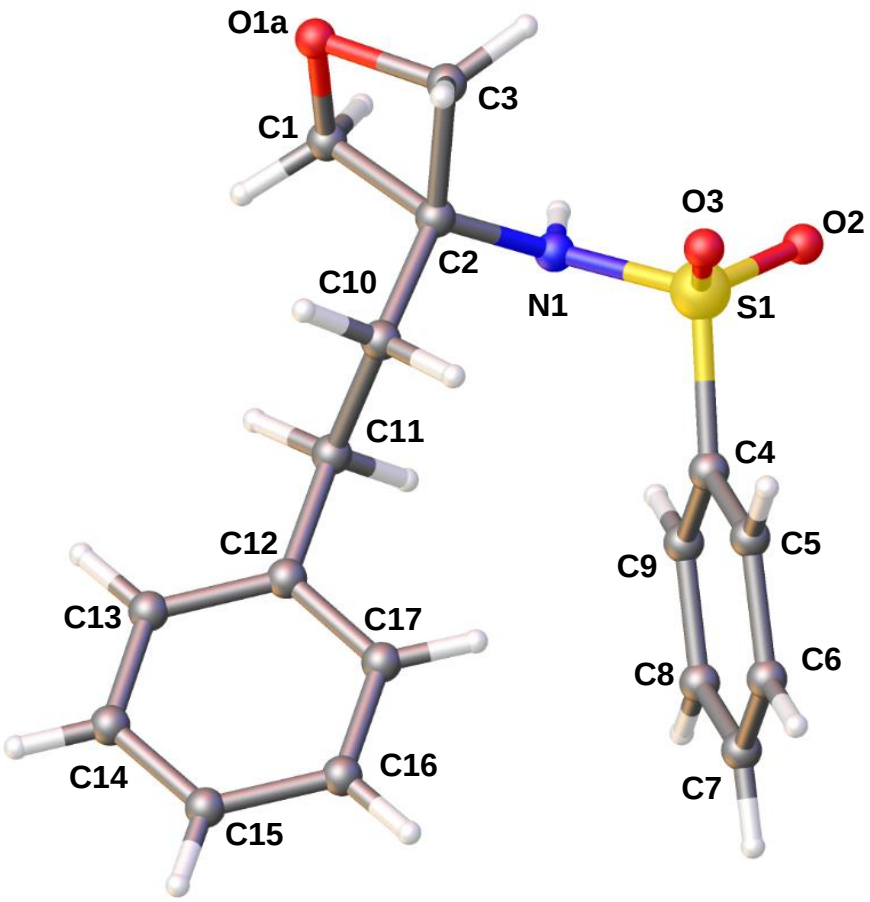


**Table 1 Crystal data and structure refinement for BL-0658 (Cpd 15, CCDC 1995771)**

| | |
|---|---|
| Identification code | BL-0658 |
| Empirical formula | C17H19NO3S |
| Formula weight | 317.41 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 18.180(2) |
| b/Å | 7.6435(12) |
| c/Å | 11.3056(15) |
| α/° | 90 |
| β/° | 96.444(9) |
| γ/° | 90 |
| Volume/Å3 | 1561.1(4) |
| Z | 4 |
| ρcalcg/cm3 | 1.3504 |
| μ/mm-1 | 1.947 |
| F(000) | 675.3 |
| Crystal size/mm3 | 0.28 × 0.03 × 0.03 |
| Radiation | Cu Kα (λ = 1.54178) |
| 2Θ range for data collection/° | 4.9 to 133.16 |
| Index ranges | -20 ≤ h ≤ 21, -9 ≤ k ≤ 9, -13 ≤ l ≤ 12 |
| Reflections collected | 9057 |
| Independent reflections | 2727 [Rint = 0.0770, Rsigma = 0.0822] |
| Data/restraints/parameters | 2727/0/213 |
| Goodness-of-fit on F2 | 1.016 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0632, wR2 = 0.1566 |
| Final R indexes [all data] | R1 = 0.1035, wR2 = 0.1837 |
| Largest diff. peak/hole / e Å-3 | 0.46/-0.58 |

**Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for BL-0658 (Cpd 15) $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| S1 | 3576.2(5) | 6736.0(15) | 5299.9(8) | 39.9(3) |
| O2 | 3998.4(17) | 8268(5) | 5089(3) | 54.4(8) |
| O3 | 3534.4(17) | 5305(4) | 4477(2) | 52.1(8) |
| C4 | 2656(2) | 7464(5) | 5378(3) | 32.5(8) |
| C9 | 2503(2) | 8635(5) | 6254(3) | 39.1(9) |
| C5 | 2110(2) | 6938(5) | 4506(3) | 36.8(9) |
| C12 | 1901(2) | 3742(5) | 7882(3) | 34.6(8) |
| C11 | 2683(2) | 4384(6) | 7914(3) | 37.4(9) |
| C13 | 1687(2) | 2621(5) | 8761(3) | 38.1(9) |
| C17 | 1376(2) | 4229(5) | 6965(3) | 38.9(9) |
| C10 | 3103(2) | 3487(5) | 6986(3) | 34.1(8) |
| C7 | 1242(2) | 8762(6) | 5379(4) | 47.7(11) |
| C8 | 1791(3) | 9275(6) | 6253(4) | 44.0(10) |
| C6 | 1394(2) | 7599(6) | 4505(3) | 41.9(10) |
| C15 | 448(2) | 2525(6) | 7783(4) | 41.9(9) |
| C16 | 657(2) | 3640(6) | 6914(3) | 42.6(10) |
| C14 | 965(2) | 2040(6) | 8704(3) | 41.1(10) |
| N1 | 3872.5(19) | 6056(5) | 6628(3) | 38.8(8) |
| O1a | 4738(8) | 2418(18) | 7526(8) | 46(3) |
| C2 | 3878(2) | 4205(5) | 6950(3) | 37.2(9) |
| C1 | 4404(2) | 3839(6) | 8087(3) | 41.2(10) |
| C3 | 4414(2) | 3045(6) | 6326(3) | 45.6(11) |
| O1b | 4999(11) | 3200(40) | 7337(9) | 53(6) |

**Table 3 Anisotropic Displacement Parameters (Å2×103) for BL-0658 (Cpd 15). The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].**

| Atom | U11 | U22 | U33 | U12 | U13 | U23 |
|---|---|---|---|---|---|---|
| S1 | 35.4(5) | 51.3(6) | 34.2(5) | -0.4(5) | 9.0(4) | 6.7(5) |
| O2 | 39.9(16) | 68(2) | 56.4(18) | -7.9(15) | 9.2(13) | 23.0(17) |
| O3 | 54.5(18) | 69(2) | 34.5(14) | 13.9(16) | 13.6(12) | 1.4(15) |
| C4 | 33.5(19) | 32.6(19) | 32.8(18) | -4.6(16) | 10.1(15) | 6.4(16) |
| C9 | 46(2) | 39(2) | 31.4(18) | -1.5(18) | 0.4(16) | 2.4(17) |
| C5 | 45(2) | 38(2) | 27.5(17) | -3.1(18) | 5.3(15) | 4.6(17) |
| C12 | 41(2) | 33(2) | 31.0(17) | -0.7(16) | 12.4(15) | -2.4(15) |
| C11 | 39(2) | 44(2) | 28.7(17) | -3.5(18) | 3.5(15) | -6.2(17) |
| C13 | 47(2) | 40(2) | 27.8(17) | 0.1(18) | 4.4(16) | 5.0(17) |
| C17 | 44(2) | 41(2) | 34.0(18) | 3.8(18) | 12.6(16) | 9.0(17) |
| C10 | 35.4(19) | 35(2) | 31.8(18) | 0.1(16) | 4.5(15) | -2.0(16) |
| C7 | 43(2) | 54(3) | 46(2) | 9(2) | 7.5(18) | 21(2) |
| C8 | 54(3) | 39(2) | 39(2) | 9(2) | 11.3(18) | 0.7(18) |
| C6 | 41(2) | 49(2) | 34.3(19) | -6.1(19) | -1.2(17) | 10.8(18) |
| C15 | 36(2) | 51(2) | 41(2) | -2.1(19) | 11.8(16) | 3.8(19) |
| C16 | 40(2) | 54(3) | 35.1(19) | 7.6(19) | 7.2(16) | 9.2(19) |
| C14 | 44(2) | 49(2) | 32.8(18) | -4.8(19) | 16.2(16) | 7.9(18) |
| N1 | 30.3(17) | 43(2) | 41.0(18) | -4.0(16) | -2.7(14) | 1.8(16) |
| O1a | 37(5) | 55(5) | 46(3) | 11(4) | 6(3) | 0(4) |
| C2 | 37(2) | 40(2) | 35.2(19) | 2.6(18) | 8.3(16) | -3.6(17) |
| C1 | 48(2) | 42(2) | 33.9(19) | 4.5(19) | 5.9(17) | -7.4(17) |
| C3 | 45(2) | 57(3) | 35(2) | 11(2) | 4.1(17) | -6.2(19) |
| O1b | 42(7) | 92(12) | 26(4) | 25(8) | 5(4) | -12(5) |

## Table 4 Bond Lengths for BL-0658 (Cpd 15)

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| S1 | O2 | 1.434(3) | C17 | C16 | 1.377(6) |
| S1 | O3 | 1.432(3) | C10 | C2 | 1.517(5) |
| S1 | C4 | 1.775(4) | C7 | C8 | 1.381(6) |
| S1 | N1 | 1.622(3) | C7 | C6 | 1.380(6) |
| C4 | C9 | 1.386(5) | C15 | C16 | 1.386(6) |
| C4 | C5 | 1.378(5) | C15 | C14 | 1.373(6) |
| C9 | C8 | 1.384(6) | N1 | C2 | 1.461(5) |
| C5 | C6 | 1.395(6) | O1a | C1 | 1.426(8) |
| C12 | C11 | 1.501(5) | O1a | C3 | 1.496(10) |
| C12 | C13 | 1.400(5) | C2 | C1 | 1.539(5) |
| C12 | C17 | 1.379(6) | C2 | C3 | 1.545(6) |
| C11 | C10 | 1.528(5) | C1 | O1b | 1.527(13) |
| C13 | C14 | 1.380(6) | C3 | O1b | 1.476(12) |

## Table 5 Bond Angles for BL-0658 (Cpd 15)

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O3 | S1 | O2 | 120.3(2) | C2 | C10 | C11 | 113.2(3) |
| C4 | S1 | O2 | 106.10(19) | C6 | C7 | C8 | 120.5(4) |
| C4 | S1 | O3 | 106.87(18) | C7 | C8 | C9 | 120.2(4) |
| N1 | S1 | O2 | 106.67(19) | C7 | C6 | C5 | 119.7(4) |
| N1 | S1 | O3 | 110.16(19) | C14 | C15 | C16 | 119.0(4) |
| N1 | S1 | C4 | 105.75(18) | C15 | C16 | C17 | 120.4(4) |
| C9 | C4 | S1 | 120.2(3) | C15 | C14 | C13 | 121.0(4) |
| C5 | C4 | S1 | 118.7(3) | C2 | N1 | S1 | 122.3(3) |
| C5 | C4 | C9 | 120.9(4) | C3 | O1a | C1 | 90.9(5) |
| C8 | C9 | C4 | 119.3(4) | N1 | C2 | C10 | 112.1(3) |
| C6 | C5 | C4 | 119.4(4) | C1 | C2 | C10 | 113.8(3) |
| C13 | C12 | C11 | 121.4(4) | C1 | C2 | N1 | 111.8(3) |
| C17 | C12 | C11 | 120.3(4) | C3 | C2 | C10 | 116.1(3) |
| C17 | C12 | C13 | 118.4(4) | C3 | C2 | N1 | 115.4(3) |
| C10 | C11 | C12 | 112.4(3) | C3 | C2 | C1 | 85.0(3) |
| C14 | C13 | C12 | 120.1(4) | C3 | O1b | C1 | 87.8(8) |
| C16 | C17 | C12 | 121.1(4) | | | | |

**Table 6 Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for BL-0658 (Cpd 15)**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| H9 | 2884(2) | 8995(5) | 6850(3) | 46.9(11) |
| H5 | 2219(2) | 6131(5) | 3911(3) | 44.1(11) |
| H11a | 2678(2) | 5662(6) | 7772(3) | 44.8(11) |
| H11b | 2946(2) | 4170(6) | 8716(3) | 44.8(11) |
| H13 | 2039(2) | 2260(5) | 9398(3) | 45.7(11) |
| H17 | 1512(2) | 4984(5) | 6359(3) | 46.7(11) |
| H10a | 3136(2) | 2219(5) | 7162(3) | 40.9(10) |
| H10b | 2821(2) | 3631(5) | 6191(3) | 40.9(10) |
| H7 | 755(2) | 9212(6) | 5380(4) | 57.2(13) |
| H8 | 1680(3) | 10068(6) | 6855(4) | 52.8(12) |
| H6 | 1014(2) | 7251(6) | 3906(3) | 50.3(12) |
| H15 | -46(2) | 2102(6) | 7743(4) | 50.2(11) |
| H16 | 303(2) | 3999(6) | 6279(3) | 51.1(12) |
| H14 | 824(2) | 1294(6) | 9311(3) | 49.3(12) |
| H1a | 4145(2) | 3475(6) | 8771(3) | 49.4(12) |
| H1d | 4751(2) | 4812(6) | 8314(3) | 49.4(12) |
| H1b | 4548(2) | 4903(6) | 8557(3) | 49.4(12) |
| H1c | 4223(2) | 2918(6) | 8598(3) | 49.4(12) |
| H3a | 4765(2) | 3713(6) | 5892(3) | 54.8(13) |
| H3d | 4165(2) | 2118(6) | 5817(3) | 54.8(13) |
| H3b | 4233(2) | 1832(6) | 6187(3) | 54.8(13) |
| H3c | 4554(2) | 3563(6) | 5581(3) | 54.8(13) |
| H1 | 4200(20) | 6590(50) | 6940(30) | 17(9) |

**Table 7 Atomic Occupancy for BL-0658 (Cpd 15)**

| Atom | Occupancy | Atom | Occupancy |
|---|---|---|---|
| O1a | 0.56(4) | H1a | 0.56(4) |
| H1b | 0.44(4) | H1c | 0.44(4) |
| H3d | 0.56(4) | H3b | 0.44(4) |
| O1b | 0.44(4) | | |

**X-ray Structure Determination for BL-0667 (Cpd 18, CCDC 1995773)**

**Experimental:**

Crystals of BL-0667 (Cpd 18) were grown from ethyl acetate. The single crystal X-ray diffraction studies were carried out on a Bruker APEX-II CCD diffractometer equipped with Cu Kα radiation (l = 1.54178). A 0.230 × 0.05 × 0.05 mm colorless rod was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 40 mm with 5.00 s exposure time. A total of 5101 reflections were collected covering the indices $-9 \leq h \leq 9$, $-6 \leq k \leq 6$, $-16 \leq l \leq 16$. 2275 reflections were found to be symmetry independent, with a Rint of 0.0334. The space group was found to be $P2_1$. Crystallographic data are summarized in Table 1.

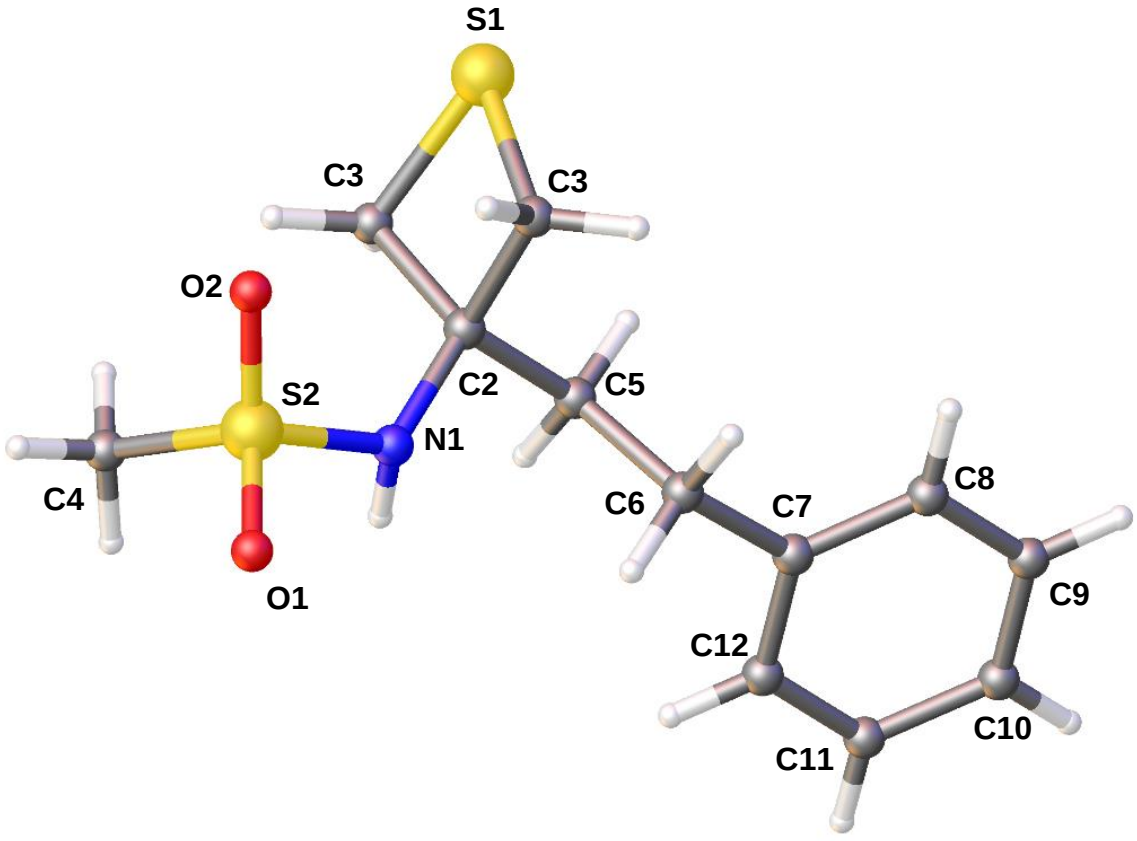


**Table 1 Crystal data and structure refinement for BL-0667 (Cpd 18)**

| | |
|---|---|
| Identification code | BL-0667 |
| Empirical formula | C12H17NO2S2 |
| Formula weight | 271.38 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | P21 |
| a/Å | 8.1251(5) |
| b/Å | 5.7879(4) |
| c/Å | 13.8802(9) |
| α/° | 90 |
| β/° | 95.521(4) |
| γ/° | 90 |
| Volume/Å3 | 649.72(7) |
| Z | 2 |
| ρcalcg/cm3 | 1.387 |
| μ/mm-1 | 3.636 |
| F(000) | 288.0 |
| Crystal size/mm3 | 0.23 × 0.05 × 0.05 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 6.398 to 139.872 |
| Index ranges | -9 ≤ h ≤ 9, -6 ≤ k ≤ 6, -16 ≤ l ≤ 16 |
| Reflections collected | 5101 |
| Independent reflections | 2275 [Rint = 0.0334, Rsigma = 0.0465] |
| Data/restraints/parameters | 2275/1/155 |
| Goodness-of-fit on F2 | 0.719 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0316, wR2 = 0.0827 |
| Final R indexes [all data] | R1 = 0.0324, wR2 = 0.0837 |
| Largest diff. peak/hole / e Å-3 | 0.40/-0.27 |

**Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for BL-0667 (Cpd 18) $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| S2 | 6968.4(7) | 5467.7(10) | 4864.8(4) | 17.55(17) |
| S1 | 9880.4(9) | 7271.9(14) | 7622.6(5) | 30.1(2) |
| O2 | 8185(2) | 7261(4) | 4908.4(14) | 25.2(4) |
| O1 | 5492(2) | 5753(4) | 4210.0(13) | 24.8(4) |
| N1 | 6356(3) | 5140(4) | 5937.2(15) | 19.9(5) |
| C4 | 7864(3) | 2847(5) | 4554.6(19) | 22.0(5) |
| C2 | 7357(3) | 5594(6) | 6860.1(18) | 20.8(5) |
| C1 | 7840(4) | 8141(5) | 7047(2) | 27.3(6) |
| C7 | 3702(4) | 4787(6) | 8491(2) | 26.1(6) |
| C8 | 3622(4) | 6049(6) | 9339(2) | 31.1(7) |
| C12 | 2879(4) | 2693(6) | 8397(2) | 29.7(7) |
| C10 | 1861(4) | 3184(7) | 9950(2) | 32.7(7) |
| C6 | 4626(4) | 5683(8) | 7672(2) | 39.9(8) |
| C11 | 1961(4) | 1890(6) | 9119(2) | 33.2(7) |
| C5 | 6359(4) | 4652(5) | 7662(2) | 24.0(6) |
| C9 | 2698(4) | 5246(7) | 10053(2) | 33.9(7) |
| C3 | 9148(3) | 4626(6) | 6989.8(19) | 24.4(6) |

**Table 3 Anisotropic Displacement Parameters (Å2×103) for BL-0667 (Cpd 18). The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| S2 | 17.4(3) | 15.5(3) | 19.7(3) | 0.7(2) | 1.86(19) | 1.6(2) |
| S1 | 29.9(4) | 37.9(5) | 22.3(3) | -6.8(3) | 1.4(2) | -9.1(3) |
| O2 | 27.6(10) | 23.0(11) | 25.3(9) | 2.1(8) | 4.9(7) | -2.4(8) |
| O1 | 23.1(9) | 25.8(11) | 24.4(8) | 1.2(8) | -2.6(7) | 4.5(8) |
| N1 | 20.9(10) | 17.2(13) | 21.7(10) | 0.0(8) | 2.6(8) | -2.5(8) |
| C4 | 20.5(12) | 20.9(14) | 24.3(12) | -3.9(10) | 1.5(9) | 4.1(10) |
| C2 | 23.6(13) | 16.8(13) | 21.5(11) | 0.3(11) | 0.0(9) | 1.5(12) |
| C1 | 35.6(16) | 22.1(15) | 24.1(13) | -3.3(10) | 2.7(11) | -3.8(12) |
| C7 | 24.1(14) | 28.5(16) | 26.0(13) | 7.9(11) | 4.1(10) | 9.1(11) |
| C8 | 29.6(15) | 23.5(17) | 39.7(16) | -3.1(12) | 0.7(12) | 0.1(11) |
| C12 | 34.3(16) | 29.0(18) | 25.2(12) | -4.8(12) | 0.3(11) | 5.6(13) |
| C10 | 28.7(16) | 41(2) | 29.0(14) | 12.3(13) | 7.8(12) | 4.4(12) |
| C6 | 35.9(17) | 44(2) | 42.2(17) | 21.8(17) | 16.7(13) | 15.9(16) |
| C11 | 29.2(15) | 26.6(17) | 42.7(17) | 3.8(14) | -1.5(12) | -4.0(13) |
| C5 | 26.9(14) | 22.1(14) | 23.2(12) | 4.2(10) | 3.2(10) | 2.8(11) |
| C9 | 38.2(16) | 41(2) | 22.7(12) | -4.0(13) | 2.0(11) | 11.1(16) |
| C3 | 23.6(14) | 25.6(14) | 23.5(12) | -1.5(11) | -0.6(10) | 0.4(11) |

**Table 4 Bond Lengths for BL-0667 (Cpd 18)**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| S2 | O2 | 1.431(2) | C2 | C3 | 1.554(4) |
| S2 | O1 | 1.4432(19) | C7 | C8 | 1.392(5) |
| S2 | N1 | 1.625(2) | C7 | C12 | 1.385(5) |
| S2 | C4 | 1.754(3) | C7 | C6 | 1.513(4) |
| S1 | C1 | 1.840(3) | C8 | C9 | 1.381(5) |
| S1 | C3 | 1.836(3) | C12 | C11 | 1.385(5) |
| N1 | C2 | 1.474(3) | C10 | C11 | 1.384(5) |
| C2 | C1 | 1.541(4) | C10 | C9 | 1.374(6) |
| C2 | C5 | 1.539(4) | C6 | C5 | 1.531(4) |

## Table 5 Bond Angles for BL-0667 (Cpd 18)

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O2 | S2 | O1 | 118.22(13) | C5 | C2 | C3 | 110.0(2) |
| O2 | S2 | N1 | 108.49(12) | C2 | C1 | S1 | 90.89(18) |
| O2 | S2 | C4 | 109.66(13) | C8 | C7 | C6 | 121.5(3) |
| O1 | S2 | N1 | 106.30(11) | C12 | C7 | C8 | 118.5(3) |
| O1 | S2 | C4 | 106.49(13) | C12 | C7 | C6 | 120.0(3) |
| N1 | S2 | C4 | 107.15(13) | C9 | C8 | C7 | 120.2(3) |
| C3 | S1 | C1 | 77.49(13) | C7 | C12 | C11 | 121.0(3) |
| C2 | N1 | S2 | 125.66(18) | C9 | C10 | C11 | 119.3(3) |
| N1 | C2 | C1 | 115.3(2) | C7 | C6 | C5 | 113.3(3) |
| N1 | C2 | C5 | 106.3(2) | C10 | C11 | C12 | 120.0(3) |
| N1 | C2 | C3 | 118.0(2) | C6 | C5 | C2 | 114.7(2) |
| C1 | C2 | C3 | 96.0(2) | C10 | C9 | C8 | 121.0(3) |
| C5 | C2 | C1 | 111.2(2) | C2 | C3 | S1 | 90.64(19) |

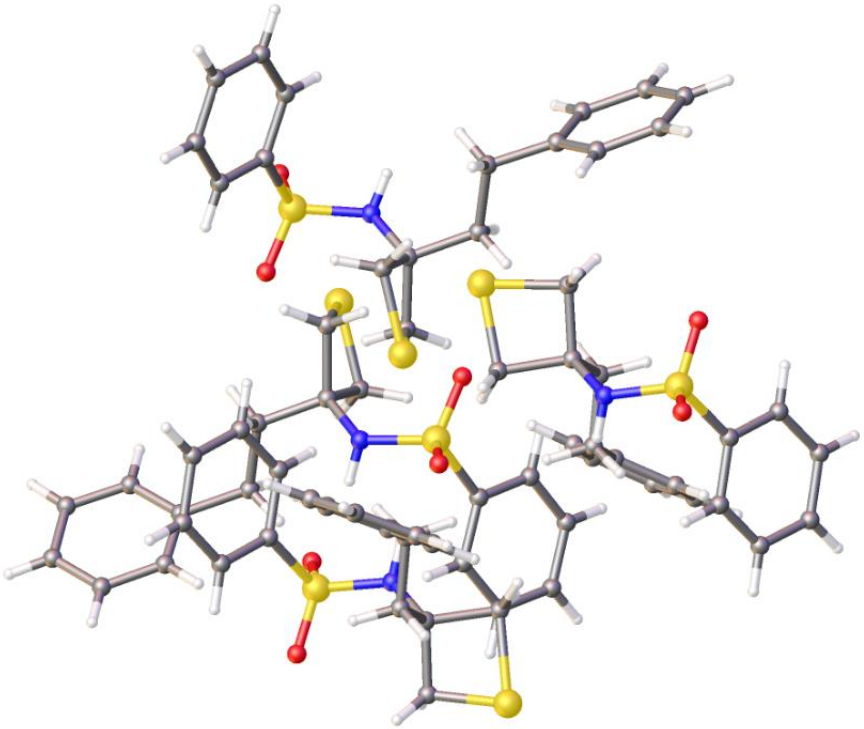
## Table 6 Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for BL-0667 (Cpd 18)

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| H1 | 5890.16 | 3773.2 | 5969.21 | 24 |
| H4A | 8186.19 | 2947.38 | 3893.44 | 33 |
| H4B | 7061.99 | 1593.7 | 4592.77 | 33 |
| H4C | 8843.94 | 2536.35 | 5004.29 | 33 |
| H1A | 7146.52 | 8935.85 | 7492.86 | 33 |
| H1B | 7896.2 | 9049.87 | 6446.36 | 33 |
| H8 | 4206.37 | 7466.98 | 9427.05 | 37 |
| H12 | 2943.93 | 1793.37 | 7829.93 | 36 |
| H10 | 1221.66 | 2651.63 | 10443.28 | 39 |
| H6A | 4719.7 | 7384.57 | 7726.24 | 48 |
| H6B | 3976.92 | 5326.85 | 7048.98 | 48 |
| H11 | 1399.88 | 452.22 | 9043.22 | 40 |
| H5A | 6255.65 | 2956.29 | 7585.61 | 29 |
| H5B | 6986.56 | 4954.35 | 8296.77 | 29 |
| H9 | 2638.46 | 6133.19 | 10624.98 | 41 |
| H3A | 9633.98 | 4375.89 | 6370.81 | 29 |
| H3B | 9265.43 | 3225.04 | 7400.08 | 29 |

**X-ray Structure Determination for BL-0657 (Cpd 19, CCDC 1995772)**

**Experimental:**

Crystals of BL-0657 (Cpd 19) were grown from dichloromethane/hexanes. The single crystal X-ray diffraction studies were carried out on a Bruker APEX-II CCD diffractometer equipped with with Mo Kα radiation (λ = 0.71073). A **0.**18 × 0.05 × 0.04 mm colorless block was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 60 mm with 5.00 s exposure time. A total of 66842 reflections were collected covering the indices -16 ≤ h ≤ 16, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23. 13392 reflections were found to be symmetry independent, with a Rint of 0.0434. The space group was found to be P-1. Crystallographic data are summarized in Table 1.



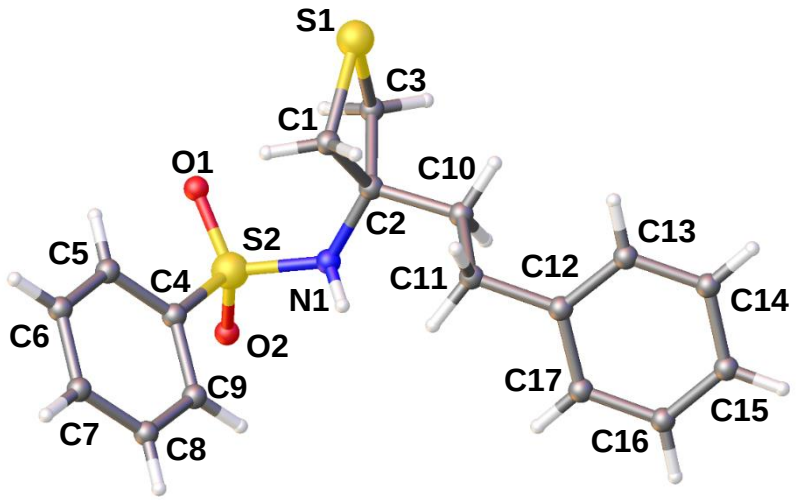


**Table 1 Crystal data and structure refinement for BL-0657 (Cpd 19)**

| | |
|---|---|
| Identification code | BL-0657 |
| Empirical formula | $C_{17}H_{19}NO_2S_2$ |
| Formula weight | 333.46 |
| Temperature/K | 100.0 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 13.0037(7) |
| b/Å | 15.1406(11) |
| c/Å | 18.8773(14) |
| α/° | 100.792(2) |
| β/° | 100.006(2) |
| γ/° | 111.272(2) |
| Volume/Å$^3$ | 3281.4(4) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.347 |
| μ/mm$^{-1}$ | 0.329 |
| F(000) | 1403.0 |
| Crystal size/mm$^3$ | 0.18 × 0.05 × 0.04 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3 to 52.734 |
| Index ranges | $-16 \leq h \leq 16$, $-18 \leq k \leq 18$, $-23 \leq l \leq 23$ |
| Reflections collected | 66842 |
| Independent reflections | 13392 [$R_{int}$ = 0.0434, $R_{sigma}$ = 0.0370] |
| Data/restraints/parameters | 13392/0/355 |
| Goodness-of-fit on F$^2$ | 1.081 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0878, $wR_2$ = 0.2143 |
| Final R indexes [all data] | $R_1$ = 0.1136, $wR_2$ = 0.2382 |
| Largest diff. peak/hole / e Å$^{-3}$ | 3.40/-2.43 |

**Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for BL-0657 (Cpd 19) Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| S2D | 1256.4(9) | 5180.7(7) | 1477.9(6) | 15.5(2) |
| S2A | 1520.4(9) | 2280.2(7) | 992.7(6) | 15.9(2) |
| S2C | -5563.6(9) | 20.7(8) | 3696.4(6) | 17.2(2) |
| S2B | 4024.9(9) | 2880.7(8) | 4232.6(6) | 16.7(2) |
| S1B | 548.9(10) | 2771.3(9) | 3533.6(7) | 25.2(4) |
| S1A | 4953.5(11) | 2228.5(9) | 1383.7(7) | 27.8(3) |
| S1C | -1432.5(13) | 1667.7(11) | 4802.0(8) | 39.4(3) |
| S1D | -2869.4(13) | 3551.4(11) | 276.2(8) | 37.4(5) |
| O2A | 750(3) | 2593(2) | 1330.2(17) | 20.0(6) |
| O1D | 2061(3) | 4877(2) | 1176.7(17) | 20.3(6) |
| O1A | 1712(3) | 1456(2) | 1153.4(17) | 22.1(7) |
| O2D | 976(3) | 5932(2) | 1247.1(17) | 21.6(7) |
| O2C | -6347(3) | 334(2) | 4017.6(17) | 20.3(6) |
| O1B | 3878(3) | 3704(2) | 4032.5(17) | 22.5(7) |
| O1C | -5275(3) | -728(2) | 3922.9(18) | 24.5(7) |
| O2B | 4958(3) | 2652(2) | 4070.0(18) | 24.8(7) |
| N1D | 91(3) | 4196(3) | 1259.1(19) | 16.3(7) |
| N2A | 2727(3) | 3230(3) | 1255.5(19) | 17.2(7) |
| N1B | 2882(3) | 1900(3) | 3801.5(19) | 16.4(7) |
| N1C | -4412(3) | 1002(3) | 3869.3(19) | 17.1(7) |
| C2A | 3881(4) | 3242(3) | 1345(2) | 17.7(8) |
| C4D | 1837(4) | 5591(3) | 2460(2) | 16.1(8) |
| C2B | 1701(4) | 1831(3) | 3646(2) | 16.8(8) |
| C12C | -3185(4) | 743(3) | 1793(2) | 17.9(8) |
| C12D | -1315(4) | 4454(3) | 3261(2) | 17.6(8) |
| C4A | 948(4) | 1992(3) | 13(2) | 16.7(8) |
| C3B | 1372(4) | 2440(3) | 4252(2) | 18.2(9) |
| C9B | 4334(4) | 2360(3) | 5540(2) | 20.2(9) |
| C12A | 5383(4) | 5893(3) | 1151(2) | 21.7(9) |
| C4C | -6201(4) | -413(3) | 2721(2) | 17.8(8) |
| C7D | 2791(4) | 6230(3) | 3988(3) | 22.2(9) |
| C10D | -1223(4) | 4600(3) | 1964(2) | 18.9(9) |
| C5D | 1966(4) | 6514(3) | 2853(2) | 19.1(9) |
| C4B | 4209(4) | 3077(3) | 5209(2) | 18.1(9) |
| C9C | -6375(4) | -1350(3) | 2330(2) | 20.2(9) |
| C2C | -3265(4) | 1028(3) | 3884(2) | 20.6(9) |
| C5C | -6552(4) | 195(3) | 2362(2) | 21.1(9) |
| C10C | -3166(4) | 589(3) | 3110(2) | 20.3(9) |
| C10A | 4710(4) | 4318(3) | 1524(2) | 19.5(9) |
| C17D | -472(4) | 5152(3) | 3879(3) | 24.7(10) |
| C12B | 188(4) | -849(3) | 3807(2) | 19.2(9) |
| C5A | 723(4) | 1067(3) | -427(3) | 24.7(10) |
| C9D | 2181(4) | 4982(3) | 2823(2) | 21.1(9) |

| | | | | |
|---|---|---|---|---|
| C1A | 4071(4) | 2562(3) | 702(2) | 21.9(9) |
| C2D | -1067(4) | 4167(3) | 1207(2) | 20.0(9) |
| C7C | -7272(4) | -1089(3) | 1204(3) | 24.6(10) |
| C8B | 4522(4) | 2539(3) | 6312(3) | 23.5(9) |
| C6D | 2450(4) | 6832(3) | 3623(3) | 21.9(9) |
| C11B | 973(4) | 231(3) | 4055(3) | 22.2(9) |
| C11D | -1007(4) | 4083(3) | 2564(3) | 22.8(9) |
| C11C | -3401(4) | 1124(3) | 2528(3) | 23.6(9) |
| C9A | 668(4) | 2672(3) | -285(3) | 22.5(9) |
| C13D | -2443(4) | 4112(3) | 3300(3) | 24.6(10) |
| C5B | 4275(4) | 3962(3) | 5633(2) | 21.9(9) |
| C17B | 521(4) | -1547(3) | 3450(3) | 23.8(10) |
| C13C | -2080(4) | 1036(4) | 1713(3) | 25.5(10) |
| C17C | -4089(4) | 94(4) | 1186(3) | 25.9(10) |
| C6C | -7086(4) | -146(3) | 1602(3) | 23.2(9) |
| C10B | 910(4) | 733(3) | 3423(2) | 18.7(9) |
| C3A | 4228(4) | 2783(3) | 1966(3) | 21.9(9) |
| C11A | 4652(4) | 4801(3) | 884(3) | 25.1(10) |
| C17A | 4887(4) | 6567(4) | 1228(3) | 26.3(10) |
| C7B | 4593(4) | 3423(4) | 6741(3) | 27.0(10) |
| C8D | 2656(4) | 5305(3) | 3589(3) | 22.8(9) |
| C7A | -94(4) | 1484(4) | -1493(3) | 28.1(10) |
| C8A | 142(4) | 2410(4) | -1044(3) | 25.9(10) |
| C1B | 1415(4) | 2307(3) | 3027(3) | 23.1(9) |
| C8C | -6923(4) | -1690(3) | 1567(3) | 23.6(10) |
| C16D | -756(5) | 5495(4) | 4519(3) | 31.2(11) |
| C14D | -2725(5) | 4448(4) | 3940(3) | 31.6(11) |
| C3C | -2353(4) | 2094(4) | 4233(3) | 25.5(10) |
| C3D | -1472(4) | 4609(4) | 597(3) | 26.1(10) |
| C6B | 4465(4) | 4124(4) | 6404(3) | 27.5(10) |
| C16B | -199(4) | -2542(4) | 3243(3) | 28.3(10) |
| C1C | -2815(4) | 592(4) | 4483(3) | 26.9(10) |
| C13B | -881(4) | -1170(4) | 3947(3) | 28.3(10) |
| C6A | 198(4) | 818(4) | -1189(3) | 29.9(11) |
| C14C | -1885(5) | 697(4) | 1035(3) | 32.7(11) |
| C1D | -1968(4) | 3105(4) | 835(3) | 27.8(10) |
| C15D | -1876(4) | 5142(4) | 4553(3) | 30.7(11) |
| C16A | 5555(5) | 7575(4) | 1471(3) | 33.0(11) |
| C15C | -2793(5) | 52(4) | 433(3) | 31.7(11) |
| C16C | -3899(5) | -258(4) | 509(3) | 33.3(11) |
| C14B | -1591(5) | -2166(4) | 3757(3) | 35.3(12) |
| C15B | -1245(5) | -2857(4) | 3398(3) | 35.3(12) |
| C13A | 6570(5) | 6260(4) | 1347(3) | 38.2(13) |
| C15A | 6726(5) | 7925(4) | 1657(3) | 36.8(12) |
| C14A | 7237(6) | 7265(5) | 1612(4) | 50.7(16) |

## Table 3 Bond Lengths for BL-0657 (Cpd 19)

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| S2D | O1D | 1.445(3) | C12A | C13A | 1.389(7) |
| S2D | O2D | 1.431(3) | C4C | C9C | 1.386(6) |
| S2D | N1D | 1.614(4) | C4C | C5C | 1.395(6) |
| S2D | C4D | 1.770(4) | C7D | C6D | 1.388(6) |
| S2A | O2A | 1.444(3) | C7D | C8D | 1.392(6) |
| S2A | O1A | 1.432(3) | C10D | C2D | 1.536(6) |
| S2A | N2A | 1.613(4) | C10D | C11D | 1.533(6) |
| S2A | C4A | 1.774(4) | C5D | C6D | 1.395(6) |
| S2C | O2C | 1.445(3) | C4B | C5B | 1.390(6) |
| S2C | O1C | 1.430(3) | C9C | C8C | 1.395(6) |
| S2C | N1C | 1.610(4) | C2C | C10C | 1.534(6) |
| S2C | C4C | 1.770(4) | C2C | C3C | 1.546(6) |
| S2B | O1B | 1.435(3) | C2C | C1C | 1.546(6) |
| S2B | O2B | 1.443(3) | C5C | C6C | 1.387(6) |
| S2B | N1B | 1.613(4) | C10C | C11C | 1.534(6) |
| S2B | C4B | 1.770(4) | C10A | C11A | 1.531(6) |
| S1B | C3B | 1.837(4) | C17D | C16D | 1.389(7) |
| S1B | C1B | 1.836(5) | C12B | C11B | 1.507(6) |
| S1A | C1A | 1.838(5) | C12B | C17B | 1.389(6) |
| S1A | C3A | 1.843(5) | C12B | C13B | 1.387(7) |
| S1C | C3C | 1.838(5) | C5A | C6A | 1.395(7) |
| S1C | C1C | 1.838(5) | C9D | C8D | 1.384(6) |
| S1D | C3D | 1.838(5) | C2D | C3D | 1.546(6) |
| S1D | C1D | 1.832(5) | C2D | C1D | 1.541(6) |
| N1D | C2D | 1.475(5) | C7C | C6C | 1.395(6) |
| N2A | C2A | 1.473(5) | C7C | C8C | 1.388(6) |
| N1B | C2B | 1.473(5) | C8B | C7B | 1.390(7) |
| N1C | C2C | 1.472(6) | C11B | C10B | 1.535(6) |
| C2A | C10A | 1.524(6) | C9A | C8A | 1.389(6) |
| C2A | C1A | 1.555(6) | C13D | C14D | 1.383(7) |
| C2A | C3A | 1.552(6) | C5B | C6B | 1.392(7) |
| C4D | C5D | 1.388(6) | C17B | C16B | 1.388(7) |
| C4D | C9D | 1.397(6) | C13C | C14C | 1.388(7) |
| C2B | C3B | 1.551(6) | C17C | C16C | 1.388(7) |
| C2B | C10B | 1.531(6) | C17A | C16A | 1.390(7) |
| C2B | C1B | 1.544(6) | C7B | C6B | 1.379(7) |

| | | | | | |
|---|---|---|---|---|---|
| C12C | C11C | 1.513(6) | C7A | C8A | 1.390(7) |
| C12C | C13C | 1.387(6) | C7A | C6A | 1.381(7) |
| C12C | C17C | 1.389(6) | C16D | C15D | 1.375(7) |
| C12D | C17D | 1.390(6) | C14D | C15D | 1.387(7) |
| C12D | C11D | 1.510(6) | C16B | C15B | 1.373(7) |
| C12D | C13D | 1.387(6) | C13B | C14B | 1.389(7) |
| C4A | C5A | 1.385(6) | C14C | C15C | 1.386(7) |
| C4A | C9A | 1.389(6) | C16A | C15A | 1.371(8) |
| C9B | C4B | 1.394(6) | C15C | C16C | 1.384(7) |
| C9B | C8B | 1.393(6) | C14B | C15B | 1.391(8) |
| C12A | C11A | 1.507(6) | C13A | C14A | 1.387(9) |
| C12A | C17A | 1.391(7) | C15A | C14A | 1.385(9) |

**Table 4 Bond Angles for BL-0657 (Cpd 19)**

| **Atom** | **Atom** | **Atom** | **Angle/°** | **Atom** | **Atom** | **Atom** | **Angle/°** |
|---|---|---|---|---|---|---|---|
| O1D | S2D | N1D | 105.44(18) | C5B | C4B | S2B | 119.2(3) |
| O1D | S2D | C4D | 105.78(19) | C5B | C4B | C9B | 121.5(4) |
| O2D | S2D | O1D | 119.66(19) | C4C | C9C | C8C | 119.2(4) |
| O2D | S2D | N1D | 107.90(19) | N1C | C2C | C10C | 112.8(4) |
| O2D | S2D | C4D | 107.82(19) | N1C | C2C | C3C | 109.8(4) |
| N1D | S2D | C4D | 110.05(19) | N1C | C2C | C1C | 114.0(4) |
| O2A | S2A | N2A | 105.56(18) | C10C | C2C | C3C | 111.3(4) |
| O2A | S2A | C4A | 105.71(19) | C10C | C2C | C1C | 111.9(4) |
| O1A | S2A | O2A | 118.78(18) | C3C | C2C | C1C | 95.9(4) |
| O1A | S2A | N2A | 108.74(19) | C6C | C5C | C4C | 119.3(4) |
| O1A | S2A | C4A | 108.03(19) | C11C | C10C | C2C | 113.7(4) |
| N2A | S2A | C4A | 109.80(19) | C2A | C10A | C11A | 115.7(4) |
| O2C | S2C | N1C | 105.72(18) | C16D | C17D | C12D | 120.5(5) |
| O2C | S2C | C4C | 105.52(19) | C17B | C12B | C11B | 121.2(4) |
| O1C | S2C | O2C | 119.50(19) | C13B | C12B | C11B | 120.4(4) |
| O1C | S2C | N1C | 109.05(19) | C13B | C12B | C17B | 118.4(4) |
| O1C | S2C | C4C | 107.5(2) | C4A | C5A | C6A | 118.7(4) |
| N1C | S2C | C4C | 109.19(19) | C8D | C9D | C4D | 119.2(4) |
| O1B | S2B | O2B | 119.03(19) | C2A | C1A | S1A | 90.7(3) |
| O1B | S2B | N1B | 108.39(19) | N1D | C2D | C10D | 113.0(4) |
| O1B | S2B | C4B | 108.2(2) | N1D | C2D | C3D | 113.9(4) |
| O2B | S2B | N1B | 105.41(19) | N1D | C2D | C1D | 109.8(4) |
| O2B | S2B | C4B | 106.3(2) | C10D | C2D | C3D | 111.6(4) |
| N1B | S2B | C4B | 109.24(19) | C10D | C2D | C1D | 111.7(4) |
| C1B | S1B | C3B | 77.3(2) | C1D | C2D | C3D | 95.6(4) |
| C1A | S1A | C3A | 77.7(2) | C8C | C7C | C6C | 120.2(4) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C3C | S1C | C1C | 77.3(2) | C7B | C8B | C9B | 120.2(4) |
| C1D | S1D | C3D | 77.1(2) | C7D | C6D | C5D | 120.1(4) |
| C2D | N1D | S2D | 125.6(3) | C12B | C11B | C10B | 112.5(4) |
| C2A | N2A | S2A | 127.6(3) | C12D | C11D | C10D | 111.7(4) |
| C2B | N1B | S2B | 126.2(3) | C12C | C11C | C10C | 112.7(4) |
| C2C | N1C | S2C | 125.4(3) | C4A | C9A | C8A | 118.7(4) |
| N2A | C2A | C10A | 106.5(3) | C14D | C13D | C12D | 120.9(5) |
| N2A | C2A | C1A | 117.3(4) | C4B | C5B | C6B | 118.7(4) |
| N2A | C2A | C3A | 114.2(3) | C16B | C17B | C12B | 120.6(4) |
| C10A | C2A | C1A | 112.8(4) | C12C | C13C | C14C | 120.4(5) |
| C10A | C2A | C3A | 109.8(4) | C16C | C17C | C12C | 121.1(5) |
| C3A | C2A | C1A | 96.1(3) | C5C | C6C | C7C | 120.1(4) |
| C5D | C4D | S2D | 119.9(3) | C2B | C10B | C11B | 114.4(4) |
| C5D | C4D | C9D | 121.2(4) | C2A | C3A | S1A | 90.6(3) |
| C9D | C4D | S2D | 118.9(3) | C12A | C11A | C10A | 111.2(4) |
| N1B | C2B | C3B | 118.2(3) | C16A | C17A | C12A | 121.1(5) |
| N1B | C2B | C10B | 106.7(3) | C6B | C7B | C8B | 120.3(5) |
| N1B | C2B | C1B | 113.7(3) | C9D | C8D | C7D | 120.1(4) |
| C10B | C2B | C3B | 111.9(3) | C6A | C7A | C8A | 120.3(5) |
| C10B | C2B | C1B | 110.4(3) | C9A | C8A | C7A | 120.2(5) |
| C1B | C2B | C3B | 95.8(3) | C2B | C1B | S1B | 91.1(3) |
| C13C | C12C | C11C | 120.5(4) | C7C | C8C | C9C | 120.1(4) |
| C13C | C12C | C17C | 118.8(4) | C15D | C16D | C17D | 120.4(5) |
| C17C | C12C | C11C | 120.7(4) | C13D | C14D | C15D | 120.0(5) |
| C17D | C12D | C11D | 120.5(4) | C2C | C3C | S1C | 91.2(3) |
| C13D | C12D | C17D | 118.6(4) | C2D | C3D | S1D | 90.5(3) |
| C13D | C12D | C11D | 120.9(4) | C7B | C6B | C5B | 120.6(5) |
| C5A | C4A | S2A | 118.9(3) | C15B | C16B | C17B | 120.8(5) |
| C5A | C4A | C9A | 121.8(4) | C2C | C1C | S1C | 91.1(3) |
| C9A | C4A | S2A | 119.2(3) | C12B | C13B | C14B | 121.1(5) |
| C2B | C3B | S1B | 90.9(3) | C7A | C6A | C5A | 120.2(5) |
| C8B | C9B | C4B | 118.7(4) | C15C | C14C | C13C | 120.3(5) |
| C17A | C12A | C11A | 120.8(4) | C2D | C1D | S1D | 90.9(3) |
| C13A | C12A | C11A | 121.5(4) | C16D | C15D | C14D | 119.6(5) |
| C13A | C12A | C17A | 117.7(5) | C15A | C16A | C17A | 120.3(5) |
| C9C | C4C | S2C | 120.3(3) | C16C | C15C | C14C | 119.8(5) |
| C9C | C4C | C5C | 121.1(4) | C15C | C16C | C17C | 119.5(5) |
| C5C | C4C | S2C | 118.5(3) | C13B | C14B | C15B | 119.8(5) |
| C6D | C7D | C8D | 120.4(4) | C16B | C15B | C14B | 119.3(5) |
| C11D | C10D | C2D | 114.1(4) | C14A | C13A | C12A | 121.2(6) |
| C4D | C5D | C6D | 119.0(4) | C16A | C15A | C14A | 119.4(6) |
| C9B | C4B | S2B | 119.3(3) | C15A | C14A | C13A | 120.2(6) |

**Table 5 Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for BL-0657 (Cpd 19)**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| H1D | 193.67 | 3808.2 | 1532.1 | 20 |
| H2A | 2672.49 | 3633.82 | 985.93 | 21 |
| H1B | 2904.63 | 1425.26 | 4001.72 | 20 |
| H1C | -4541.24 | 1373.4 | 3589.05 | 21 |
| H3BA | 2035.94 | 3012.99 | 4603.32 | 22 |
| H3BB | 896.22 | 2037.92 | 4527.12 | 22 |
| H9B | 4291.85 | 1760.18 | 5244.53 | 24 |
| H7D | 3119.75 | 6449.42 | 4513.42 | 27 |
| H10A | -693.67 | 5305.2 | 2149.41 | 23 |
| H10B | -2013.18 | 4559.43 | 1888.37 | 23 |
| H5D | 1729.12 | 6921.92 | 2599.89 | 23 |
| H9C | -6125.11 | -1754.7 | 2579.18 | 24 |
| H5C | -6426.01 | 835.91 | 2635.58 | 25 |
| H10E | -2385.9 | 611.31 | 3160.17 | 24 |
| H10F | -3713.3 | -111.24 | 2927.05 | 24 |
| H10C | 5498.63 | 4364.69 | 1688.51 | 23 |
| H10D | 4563.38 | 4700.67 | 1951.01 | 23 |
| H17D | 305.43 | 5395.75 | 3862.2 | 30 |
| H5A | 921.48 | 611.11 | -214.01 | 30 |
| H9D | 2090.51 | 4353.12 | 2548.08 | 25 |
| H1AA | 4496.65 | 2920.17 | 384.17 | 26 |
| H1AB | 3358.21 | 1997.83 | 391.67 | 26 |
| H7C | -7639.35 | -1320.83 | 683.98 | 29 |
| H8B | 4601.04 | 2056.38 | 6547.23 | 28 |
| H6D | 2545.27 | 7462.22 | 3899.4 | 26 |
| H11G | 1769.45 | 307.22 | 4238.4 | 27 |
| H11H | 766.13 | 564.73 | 4475.26 | 27 |
| H11A | -1466.42 | 3364.68 | 2360.73 | 27 |
| H11B | -189.36 | 4197.78 | 2692.95 | 27 |
| H11E | -4207.36 | 1043.57 | 2437.44 | 28 |
| H11F | -2907.06 | 1836.55 | 2730.06 | 28 |
| H9A | 831.69 | 3304.69 | 24.93 | 27 |
| H13D | -3030.48 | 3640.9 | 2879.92 | 30 |
| H5B | 4193.3 | 4445.97 | 5400.61 | 26 |
| H17B | 1247.97 | -1342.94 | 3346.09 | 29 |
| H13C | -1452.28 | 1471.45 | 2124.83 | 31 |
| H17C | -4848.86 | -111.99 | 1235.31 | 31 |
| H6C | -7324.8 | 263.64 | 1352.06 | 28 |

| | | | | |
|---|---|---|---|---|
| H10G | 1106.29 | 389.63 | 3001.6 | 22 |
| H10H | 112.3 | 655.24 | 3242.7 | 22 |
| H3AA | 3567.08 | 2292.24 | 2070.53 | 26 |
| H3AB | 4752.42 | 3279.13 | 2434.26 | 26 |
| H11C | 4917.14 | 4494.02 | 483.81 | 30 |
| H11D | 3849.1 | 4687.56 | 670.82 | 30 |
| H17A | 4077.41 | 6333.99 | 1114 | 32 |
| H7B | 4730.55 | 3545.41 | 7268.55 | 32 |
| H8D | 2889.42 | 4896.05 | 3842.28 | 27 |
| H7A | -459.16 | 1306.84 | -2011.02 | 34 |
| H8A | -55.53 | 2866.29 | -1258.02 | 31 |
| H1BA | 966.11 | 1823.38 | 2537.63 | 28 |
| H1BB | 2093.26 | 2836.55 | 2972.72 | 28 |
| H8C | -7056.26 | -2333.37 | 1295.15 | 28 |
| H16D | -173.74 | 5977 | 4936.51 | 37 |
| H14D | -3500.74 | 4203.86 | 3959.2 | 38 |
| H3CA | -2626.49 | 2527.89 | 4533.3 | 31 |
| H3CB | -2006.82 | 2401.92 | 3864.54 | 31 |
| H3DA | -1029.38 | 4664.07 | 217.61 | 31 |
| H3DB | -1515.28 | 5243.05 | 799.58 | 31 |
| H6B | 4505.83 | 4722.76 | 6700.66 | 33 |
| H16B | 34.58 | -3010.32 | 2990.82 | 34 |
| H1CA | -2754.83 | -31.66 | 4270.6 | 32 |
| H1CB | -3244.3 | 517.83 | 4868.76 | 32 |
| H13B | -1132.52 | -700.19 | 4176.76 | 34 |
| H6A | 41.41 | 188.74 | -1499.71 | 36 |
| H14C | -1126.15 | 907.96 | 983.44 | 39 |
| H1DA | -2328.39 | 2776.73 | 1190.17 | 33 |
| H1DB | -1682.4 | 2685.03 | 531.2 | 33 |
| H15D | -2066.78 | 5372.19 | 4994.6 | 37 |
| H16A | 5199.19 | 8023.49 | 1506.68 | 40 |
| H15C | -2657.15 | -176.92 | -30.88 | 38 |
| H16C | -4524.09 | -707.7 | 100.86 | 40 |
| H14B | -2309.95 | -2375.94 | 3871.65 | 42 |
| H15B | -1728.61 | -3539.48 | 3262.11 | 42 |
| H13A | 6930.58 | 5815.94 | 1300.37 | 46 |
| H15A | 7182.23 | 8614.35 | 1817.03 | 44 |
| H14A | 8046.94 | 7501.05 | 1761.27 | 61 |

## Table 6 Atomic Occupancy for BL-0657 (Cpd 19)

| Atom | Occupancy | Atom | Occupancy |
|---|---|---|---|
| S1B | 0.988(6) | S1D | 0.974(6) |
| H3BB | 0.988(6) | H1BA | 0.988(6) |
| H3DA | 0.974(6) | H3DB | 0.974(6) |
| H1DB | 0.974(6) | H15C | 0.25 |

**X-ray Structure Determination for BL-0679 (Cpd 21, CCDC 1995769)**

**Experimental:**

Crystals of BL-0679 (Cpd 21) were grown from ethyl acetate/hexanes. The single crystal X-ray diffraction studies were carried out on a Bruker APEX-II CCD diffractometer equipped with Mo Kα radiation (λ = 0.71073). A 0. 0.20 × 0.13 × 0.08 mm colorless rod was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 60 mm with 5.00 s exposure time. A total of 11306 reflections were collected covering the indices $-8 \leq h \leq 8$, $-13 \leq k \leq 13$, $-23 \leq l \leq 23$. 2780 reflections were found to be symmetry independent, with a Rint of 0. 0431. The space group was found to be $P2_1/c$. Crystallographic data are summarized in Table 1.

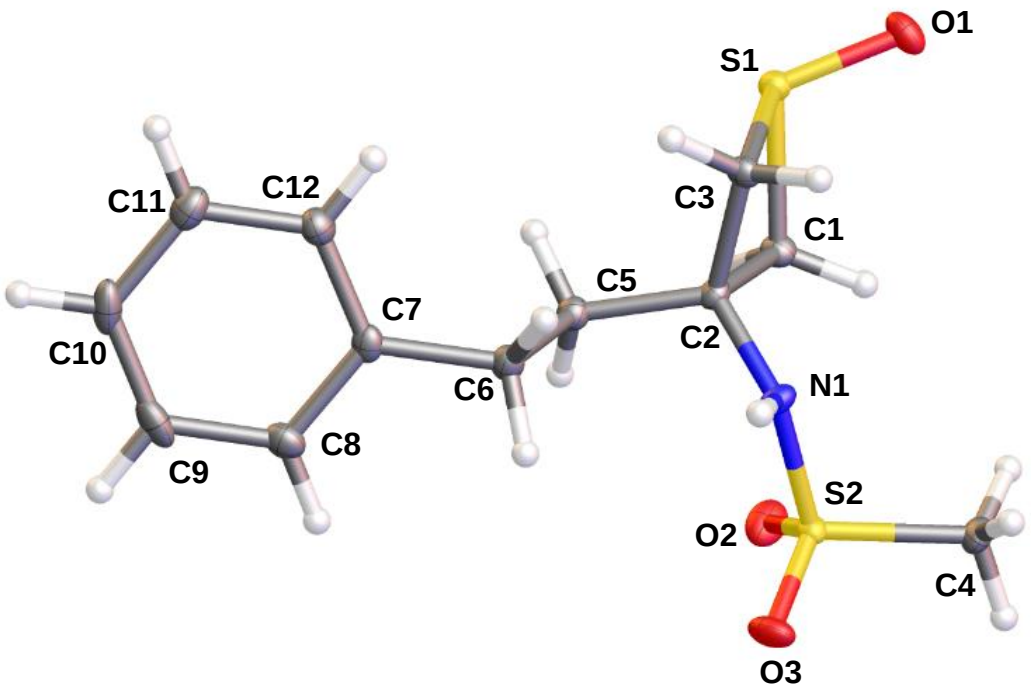


**Table 1 Crystal data and structure refinement for BL-0679 (Cpd 21)**

| | |
|---|---|
| Identification code | BL-0679 |
| Empirical formula | C12H17NO3S2 |
| Formula weight | 287.41 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 6.8795(3) |
| b/Å | 10.5809(4) |
| c/Å | 18.8700(7) |
| α/° | 90 |
| β/° | 99.6090(10) |
| γ/° | 90 |
| Volume/Å3 | 1354.30(9) |
| Z | 4 |
| ρcalcg/cm3 | 1.4095 |
| μ/mm-1 | 0.393 |
| F(000) | 609.3 |
| Crystal size/mm3 | 0.20 × 0.13 × 0.08 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.38 to 52.78 |
| Index ranges | -8 ≤ h ≤ 8, -13 ≤ k ≤ 13, -23 ≤ l ≤ 23 |
| Reflections collected | 11306 |
| Independent reflections | 2780 [Rint = 0.0431, Rsigma = 0.0332] |
| Data/restraints/parameters | 2780/0/79 |
| Goodness-of-fit on F2 | 1.027 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0547, wR2 = 0.1303 |
| Final R indexes [all data] | R1 = 0.0573, wR2 = 0.1326 |
| Largest diff. peak/hole / e Å-3 | 1.04/-0.97 |

**Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for BL-0679 (Cpd 21) $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| S2 | 5913.9(9) | 4941.8(6) | 2456.7(3) | 12.74(18) |
| S1 | 10149.1(10) | 8053.8(6) | 3776.8(4) | 13.2(2) |
| O2 | 5126(3) | 5045.8(19) | 3114.3(11) | 21.6(4) |
| O3 | 5897(3) | 3733.1(19) | 2106.6(11) | 22.7(4) |
| O1 | 9717(3) | 9292.2(18) | 3391.9(10) | 19.6(4) |
| N1 | 8163(3) | 5453(2) | 2607.3(11) | 14.1(4) |
| C12 | 13962(4) | 3479(3) | 4478.5(14) | 17.5(5) |
| C8 | 11426(4) | 1897(3) | 4375.8(14) | 18.5(5) |
| C7 | 12088(4) | 3059(2) | 4161.3(13) | 14.8(5) |
| C5 | 9784(4) | 4953(2) | 3871.3(13) | 14.3(5) |
| C3 | 10864(4) | 6831(2) | 3172.6(13) | 13.9(5) |
| C9 | 12608(4) | 1165(3) | 4889.0(15) | 22.4(6) |
| C11 | 15139(4) | 2748(3) | 4986.8(15) | 20.2(6) |
| C4 | 4615(4) | 6001(3) | 1829.4(14) | 17.9(5) |
| C6 | 10863(4) | 3845(2) | 3583.7(14) | 15.9(5) |
| C10 | 14472(4) | 1588(3) | 5197.1(15) | 21.6(6) |
| C1 | 7963(4) | 7033(2) | 3596.4(14) | 14.5(5) |
| C2 | 9133(4) | 5968(2) | 3298.6(13) | 12.0(5) |
| S1ab | 8898(12) | 8019(8) | 3014(4) | 20(2) |

## Table 3 Bond Lengths for BL-0679 (Cpd 21)

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| S2 | O2 | 1.439(2) | C8 | C9 | 1.391(4) |
| S2 | O3 | 1.439(2) | C7 | C6 | 1.511(3) |
| S2 | N1 | 1.619(2) | C5 | C6 | 1.534(4) |
| S2 | C4 | 1.761(3) | C5 | C2 | 1.536(3) |
| S1 | O1 | 1.504(2) | C3 | C2 | 1.550(3) |
| S1 | C3 | 1.844(3) | C3 | S1ab | 1.833(9) |
| S1 | C1 | 1.837(3) | C9 | C10 | 1.391(4) |
| O1 | S1ab | 1.584(8) | C11 | C10 | 1.392(4) |
| N1 | C2 | 1.467(3) | C1 | C2 | 1.545(3) |
| C12 | C7 | 1.400(4) | C1 | S1ab | 1.717(8) |
| C12 | C11 | 1.383(4) | C2 | S1ab | 2.235(8) |
| C8 | C7 | 1.394(4) | | | |

## Table 4 Bond Angles for BL-0679 (Cpd 21)

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O3 | S2 | O2 | 119.25(12) | C10 | C9 | C8 | 120.2(3) |
| N1 | S2 | O2 | 108.03(11) | C10 | C11 | C12 | 120.5(3) |
| N1 | S2 | O3 | 108.17(12) | C5 | C6 | C7 | 114.2(2) |
| C4 | S2 | O2 | 108.01(12) | C11 | C10 | C9 | 119.3(3) |
| C4 | S2 | O3 | 107.02(12) | C5 | C2 | N1 | 113.7(2) |
| C4 | S2 | N1 | 105.58(12) | C3 | C2 | N1 | 109.25(19) |
| C3 | S1 | O1 | 111.36(11) | C3 | C2 | C5 | 112.3(2) |
| C1 | S1 | O1 | 109.46(11) | C1 | C2 | N1 | 114.0(2) |
| C1 | S1 | C3 | 76.57(11) | C1 | C2 | C5 | 111.3(2) |
| C2 | N1 | S2 | 124.04(17) | C1 | C2 | C3 | 94.93(19) |
| C11 | C12 | C7 | 120.6(3) | C3 | S1ab | O1 | 108.2(5) |
| C9 | C8 | C7 | 120.8(3) | C1 | S1ab | O1 | 111.8(5) |
| C8 | C7 | C12 | 118.6(2) | C1 | S1ab | C3 | 79.9(4) |
| C6 | C7 | C12 | 119.8(2) | C2 | S1ab | O1 | 135.4(5) |
| C6 | C7 | C8 | 121.6(2) | C2 | S1ab | C3 | 43.4(2) |
| C2 | C5 | C6 | 112.7(2) | C2 | S1ab | C1 | 43.6(2) |

**Table 5 Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for BL-0679 (Cpd 21)**

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| H1 | 8894(3) | 5009(2) | 2350.3(11) | 17.0(5) |
| H12 | 14430(4) | 4273(3) | 4343.3(14) | 21.0(6) |
| H8 | 10153(4) | 1602(3) | 4169.2(14) | 22.2(7) |
| H5a | 8609(4) | 4627(2) | 4051.4(13) | 17.2(6) |
| H5b | 10665(4) | 5343(2) | 4281.3(13) | 17.2(6) |
| H3a | 10765(4) | 7118(2) | 2668.5(13) | 16.7(6) |
| H3b | 12177(4) | 6459(2) | 3346.7(13) | 16.7(6) |
| H3c | 11875(4) | 6983(2) | 3603.1(13) | 16.7(6) |
| H3d | 11462(4) | 6614(2) | 2746.2(13) | 16.7(6) |
| H9 | 12140(4) | 374(3) | 5029.4(15) | 26.8(7) |
| H11 | 16413(4) | 3042(3) | 5194.1(15) | 24.2(7) |
| H4a | 3256(9) | 5704(11) | 1688(8) | 26.8(8) |
| H4b | 4610(30) | 6841(5) | 2047(4) | 26.8(8) |
| H4c | 5258(18) | 6045(15) | 1404(5) | 26.8(8) |
| H6a | 11734(4) | 4182(2) | 3260.5(14) | 19.1(6) |
| H6b | 9877(4) | 3290(2) | 3293.9(14) | 19.1(6) |
| H10 | 15283(4) | 1089(3) | 5547.3(15) | 25.9(7) |
| H1a | 7448(4) | 6788(2) | 4036.4(14) | 17.4(6) |
| H1b | 6896(4) | 7387(2) | 3233.3(14) | 17.4(6) |
| H1c | 6514(4) | 6926(2) | 3489.4(14) | 17.4(6) |
| H1d | 8415(4) | 7228(2) | 4110.6(14) | 17.4(6) |

**Table 6 Atomic Occupancy for BL-0679 (Cpd 21)**

| Atom | Occupancy | Atom | Occupancy |
|---|---|---|---|
| S1 | 0.915(3) | H3a | 0.915(3) |
| H3c | 0.085(3) | H3d | 0.085(3) |
| H1b | 0.915(3) | H1c | 0.085(3) |
| S1ab | 0.085(3) | | |