Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Palladium-Catalyzed Geometrically Selective Hydrogenation of (*Z*)-Trifluoromethyl Alkenyl Triflate: An Efficient Approach to (*Z*) or (*E*)-3,3,3-Trifluoropropenyl Derivatives

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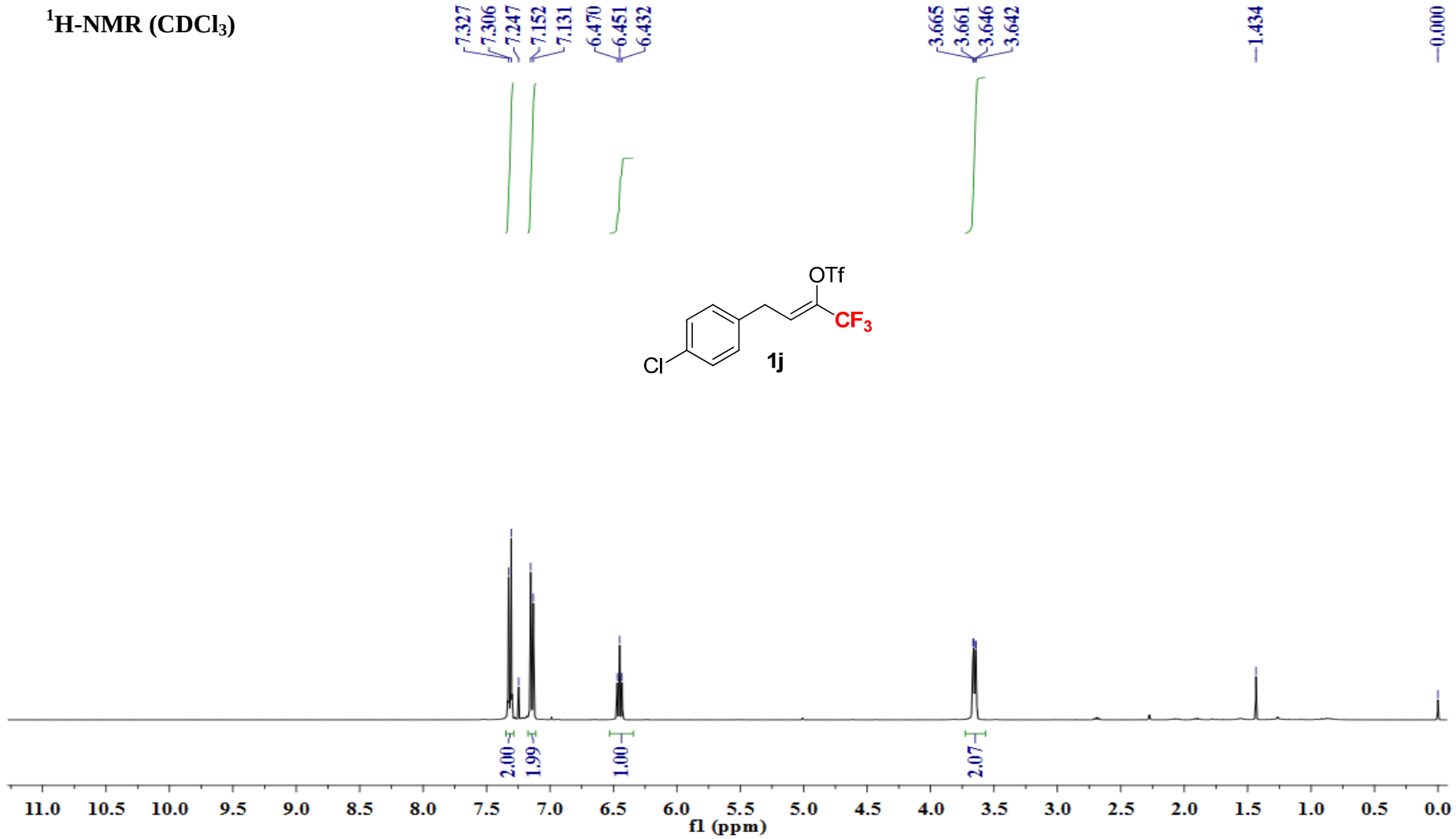
Contents

^{1}H-NMR ($CDCl_3$)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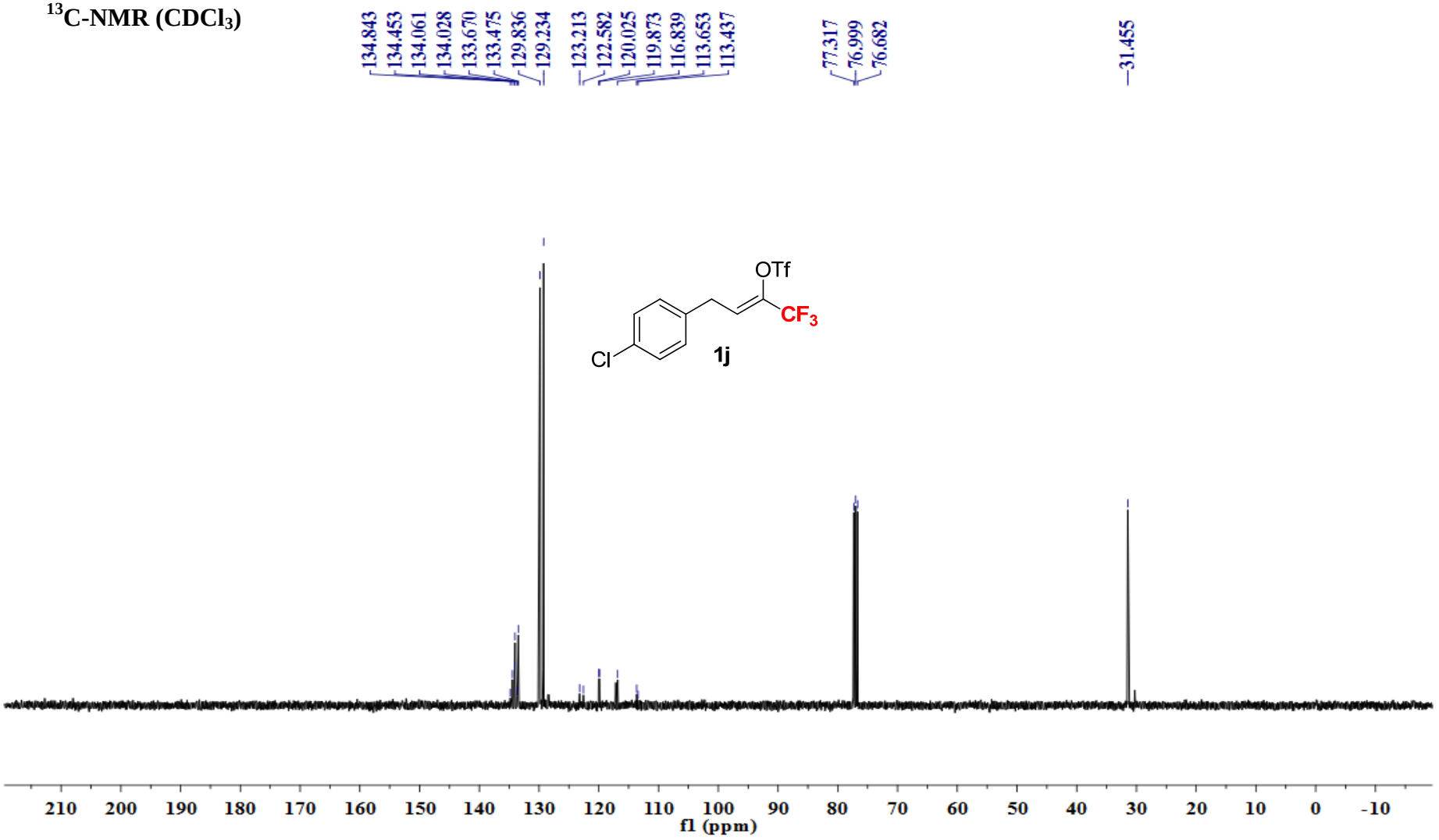
3.661
3.646
3.642
1.434
0.000
OTf
CF3
Cl
1j
2.00
1.99
1.00
2.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

^{13}C-NMR ($CDCl_3$)



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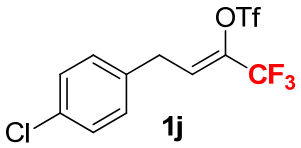

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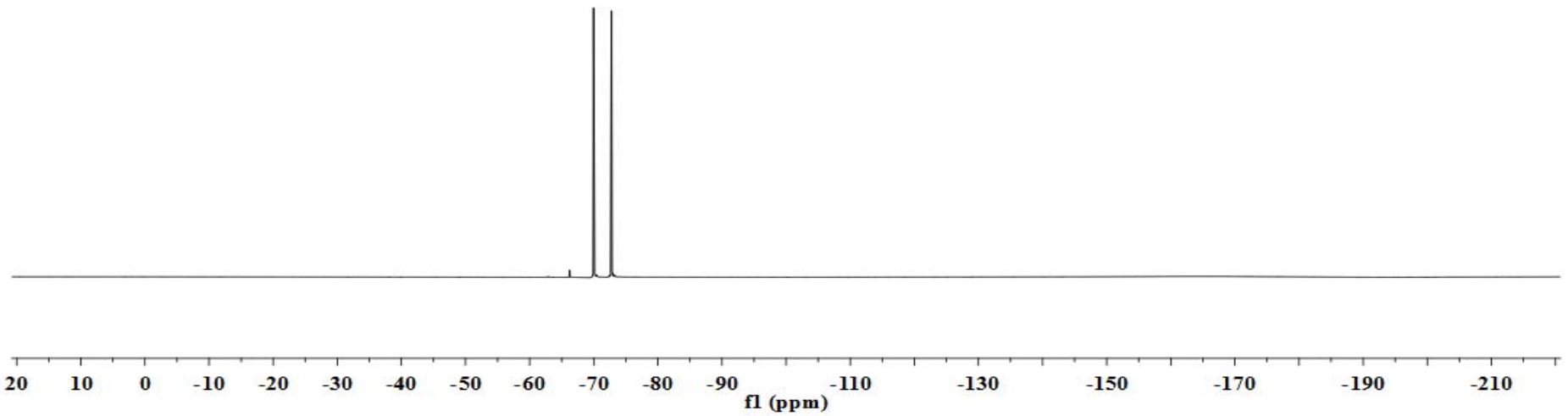

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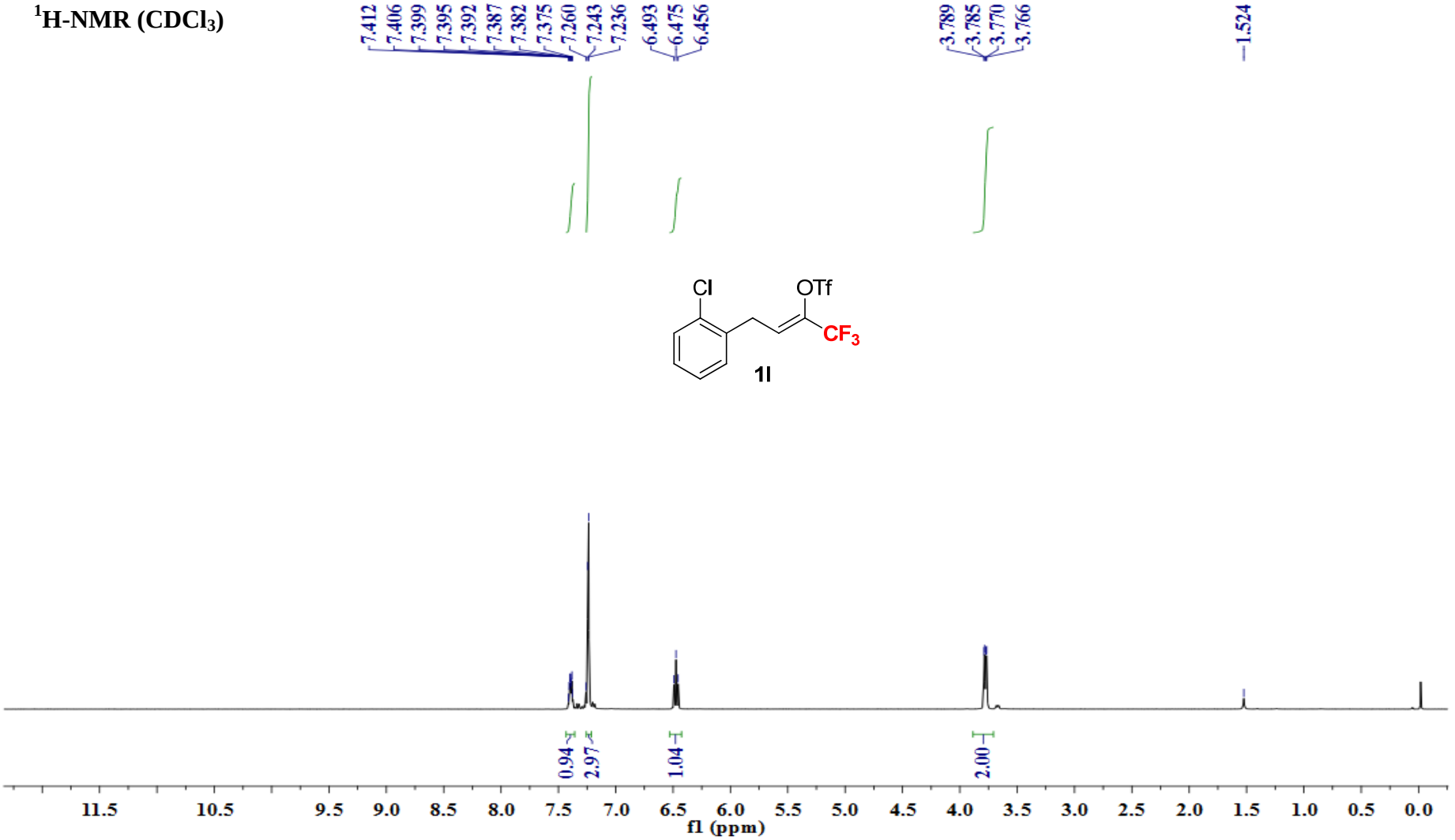
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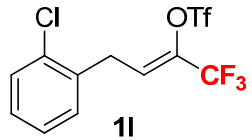
7.406
7.399
7.395
7.392
7.387
7.382
7.375
7.260
7.243
7.236
6.493
6.475
6.456
3.789
3.785
3.770
3.766
1.524
Cl
OTf
CF3
1l
0.94
2.97
1.04
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

^{13}C-NMR ($CDCl_3$)

134.906
134.515
134.124
134.019
133.732
133.484
130.641
129.918
129.126
128.471
128.440
128.407
128.374
120.048
119.918
117.209
116.863
114.501
113.677
77.323
77.005
76.688
30.340



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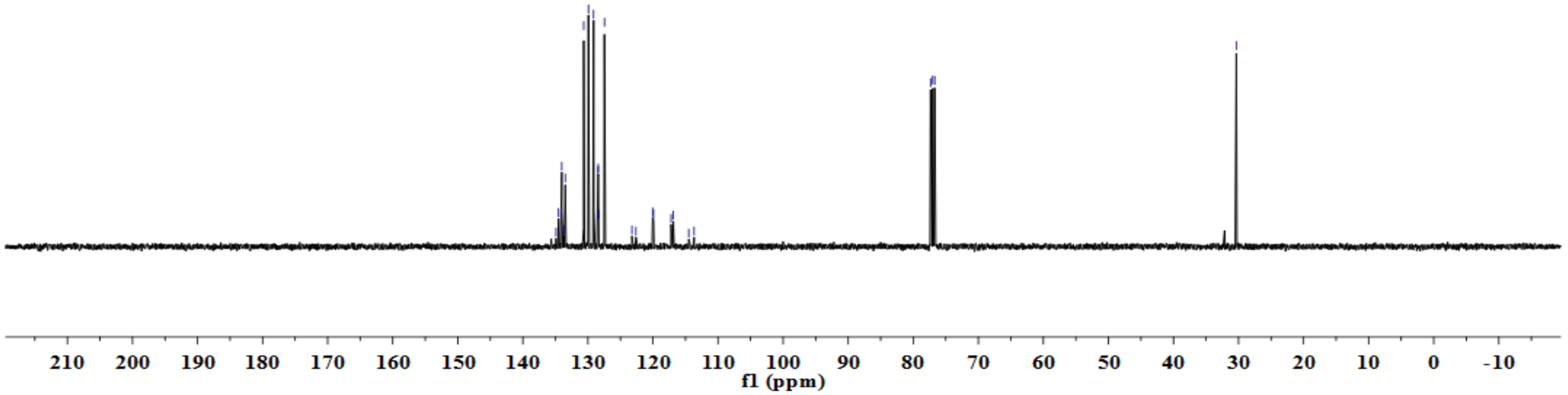

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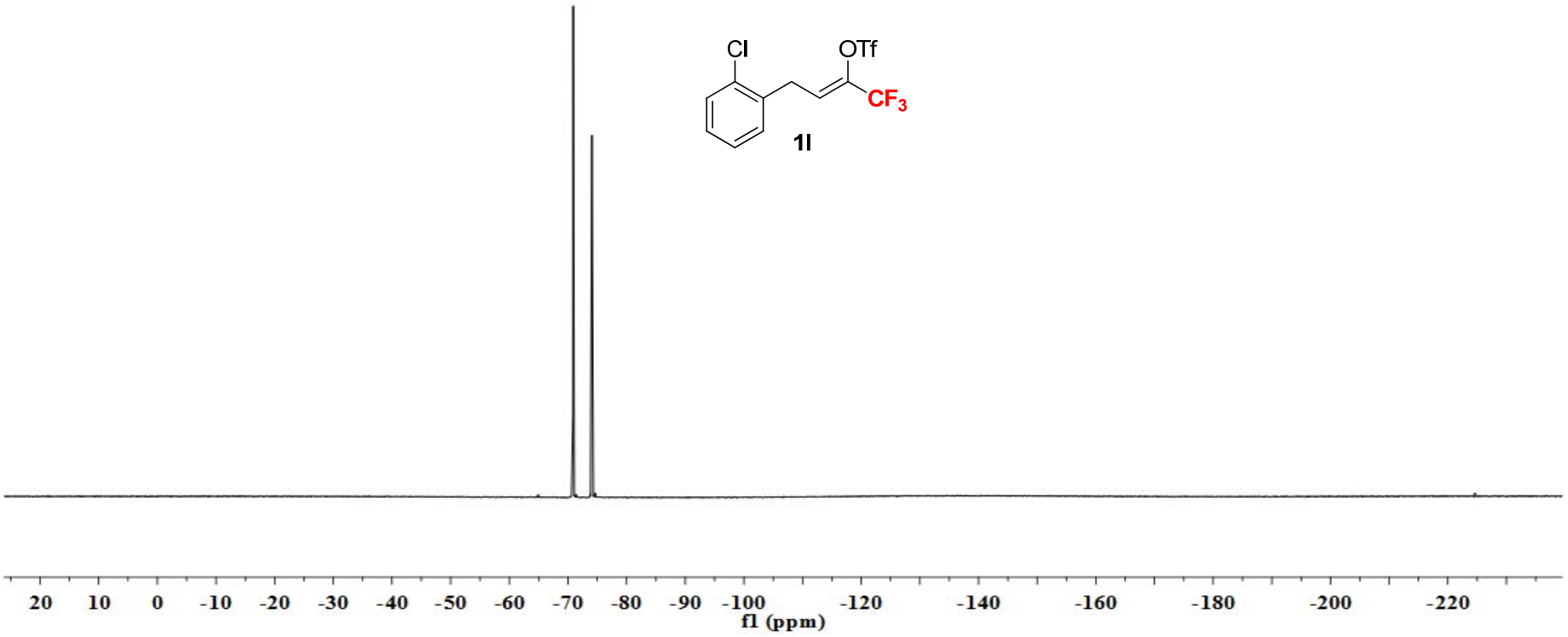

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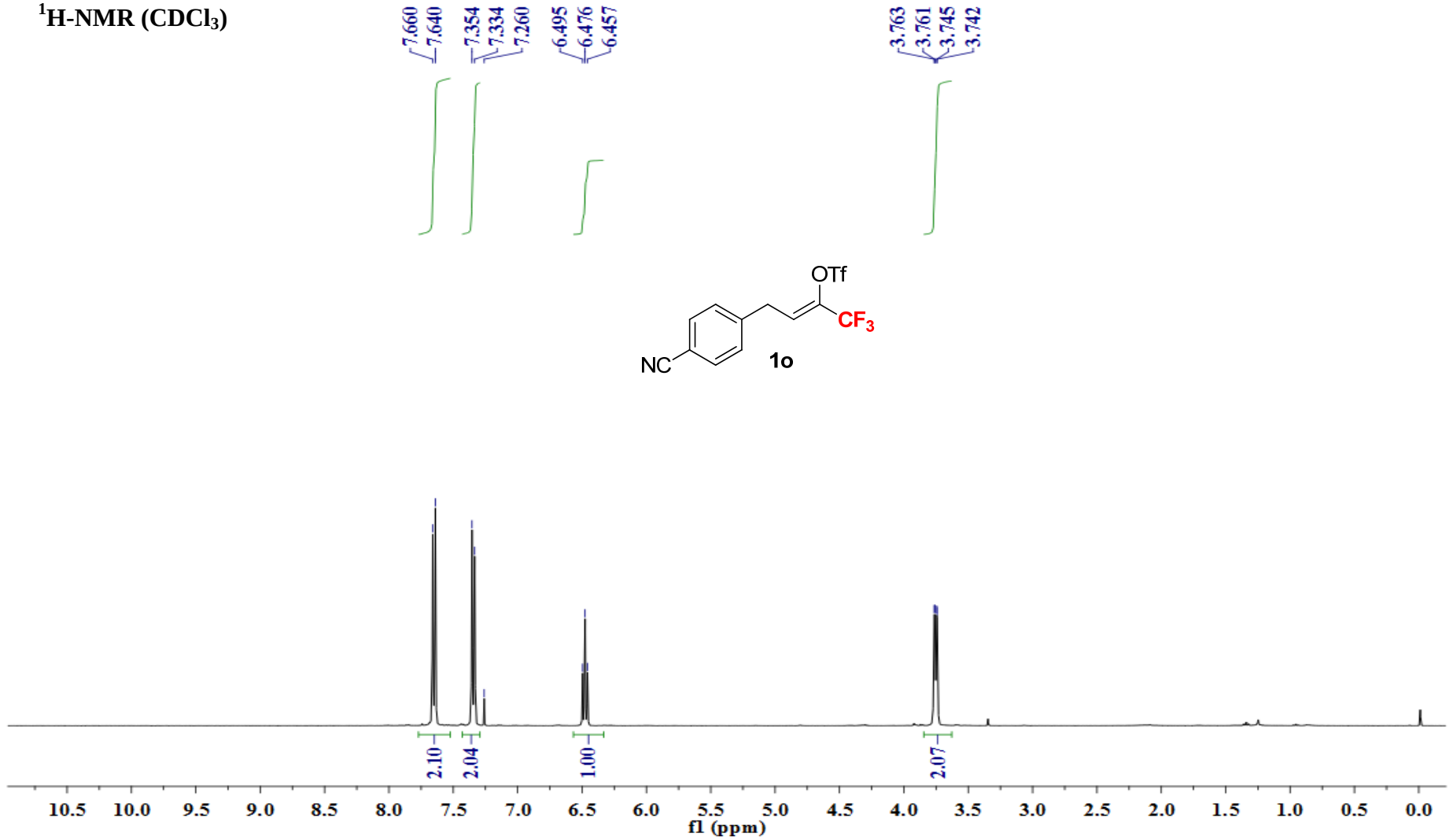
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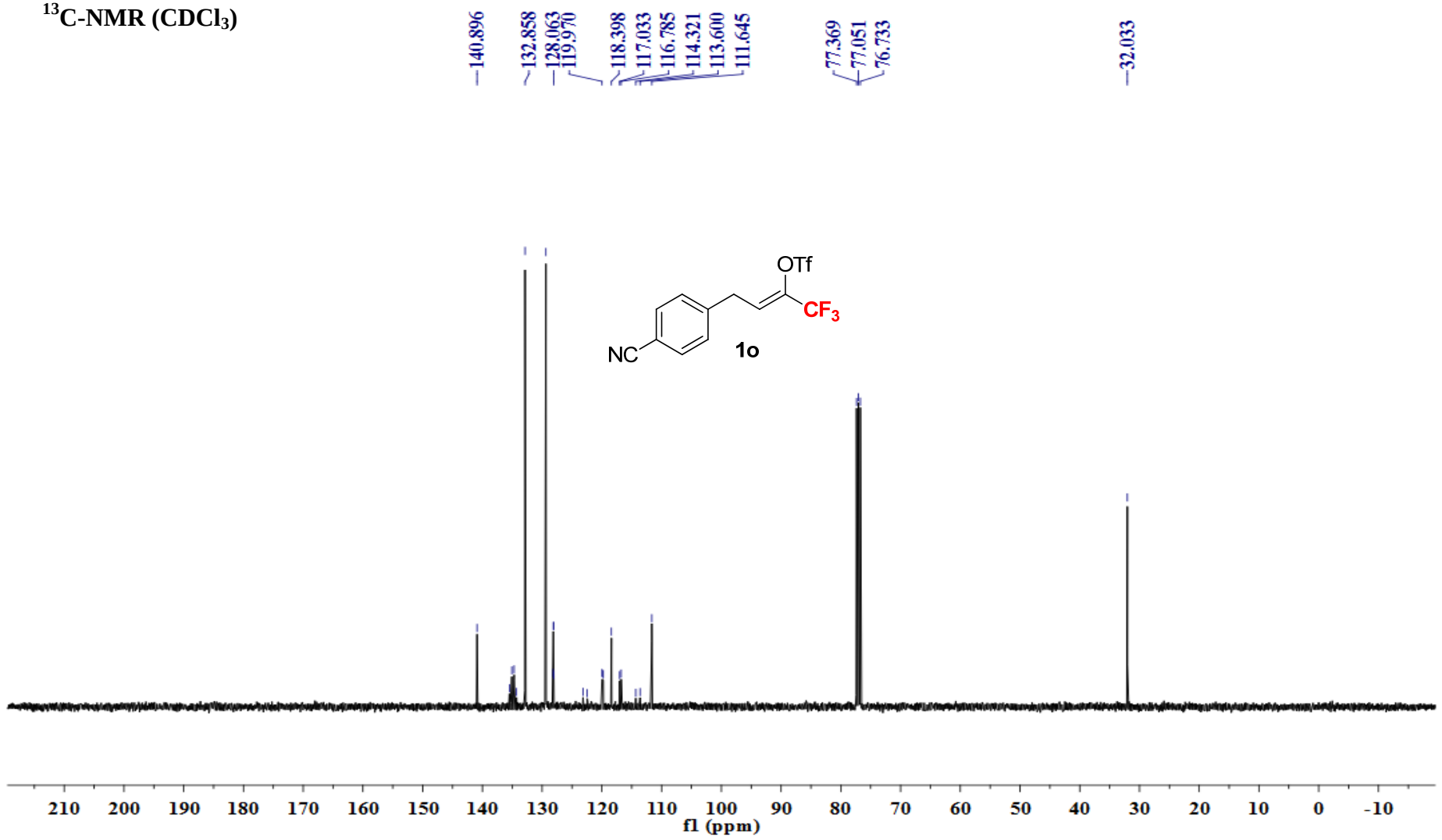
7.640
7.354
7.334
7.260
6.495
6.476
6.457
3.763
3.761
3.745
3.742
OTf
CF3
NC
1o
2.10
2.04
1.00
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

^{13}C-NMR ($CDCl_3$)



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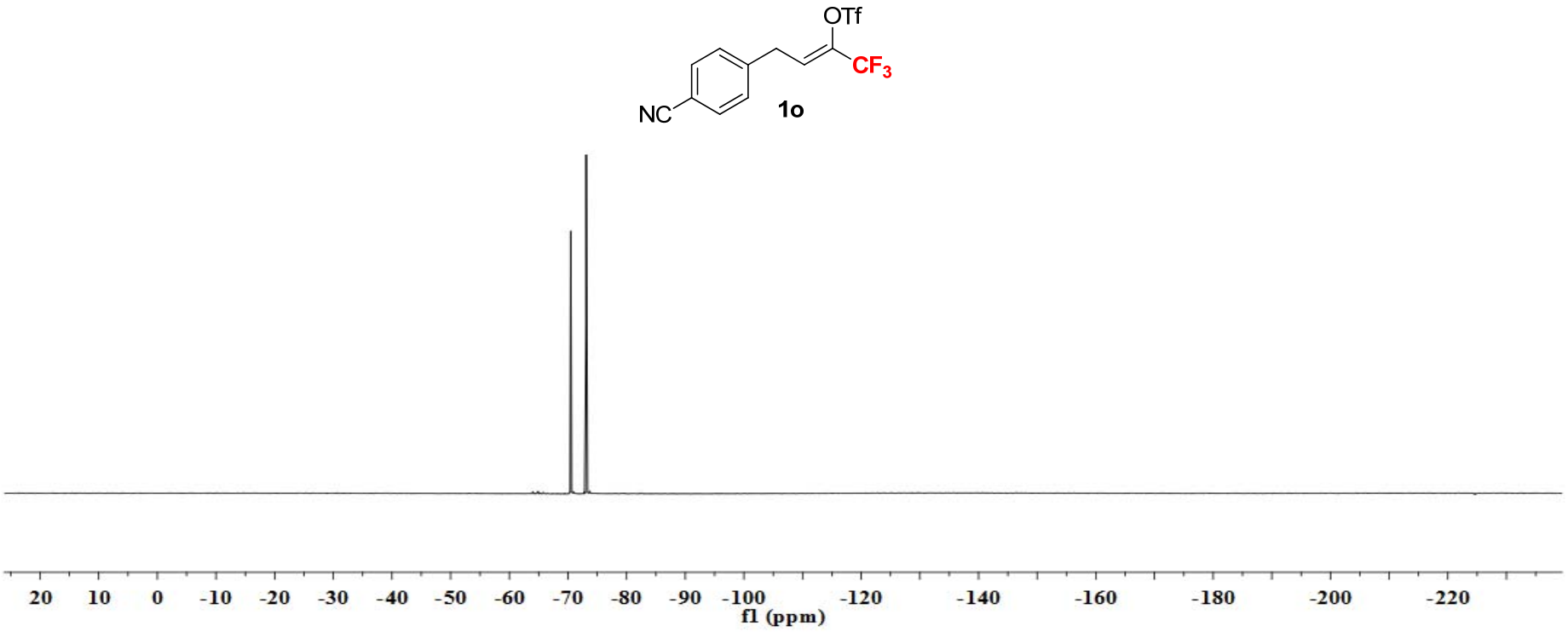

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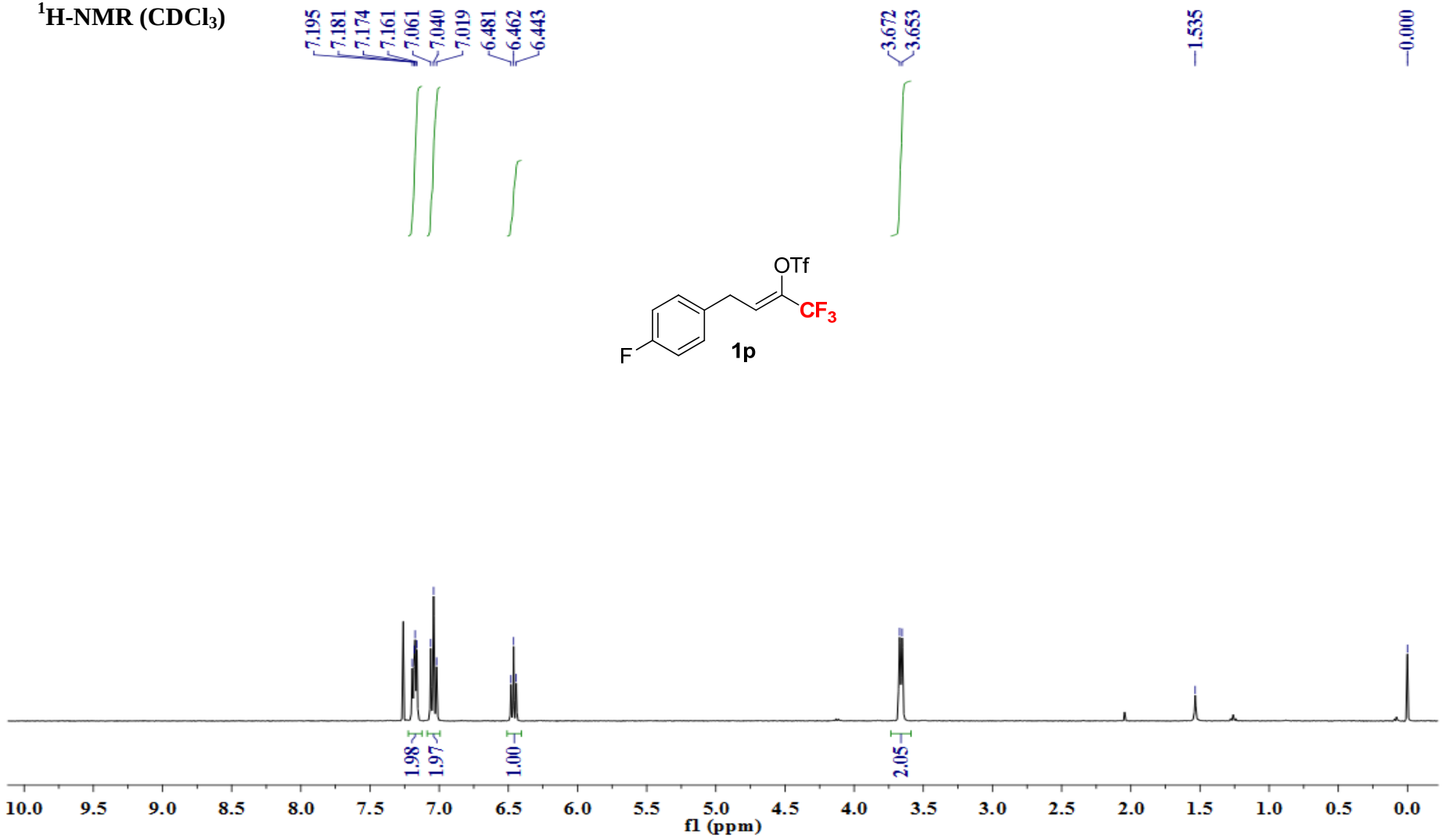
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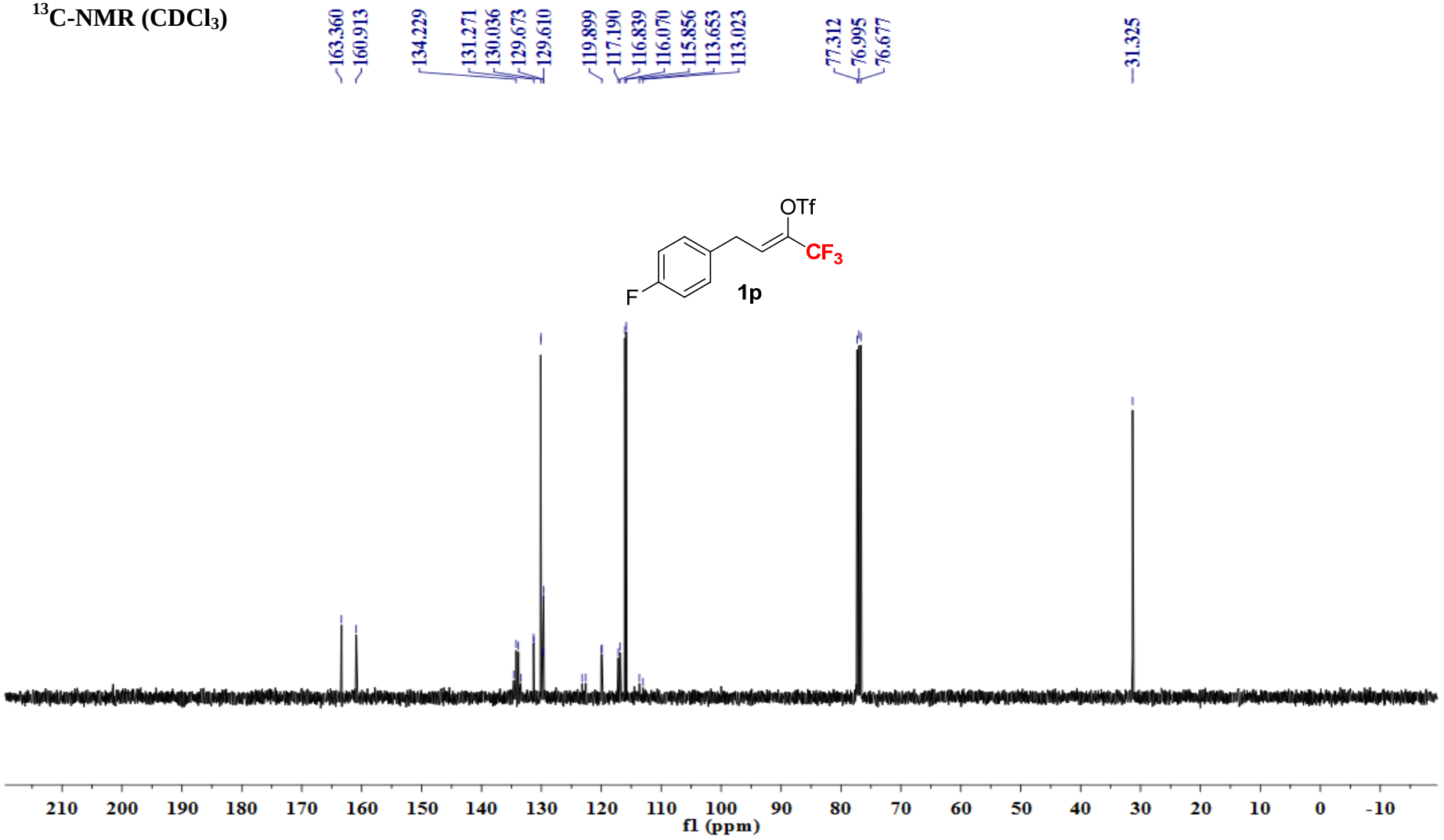
7.181
7.174
7.161
7.061
7.040
7.019
6.481
6.462
6.443
3.672
3.653
1.535
0.000
OTf
CF3
F
1p
1.98
1.97
1.00
2.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

^{13}C-NMR ($CDCl_3$)



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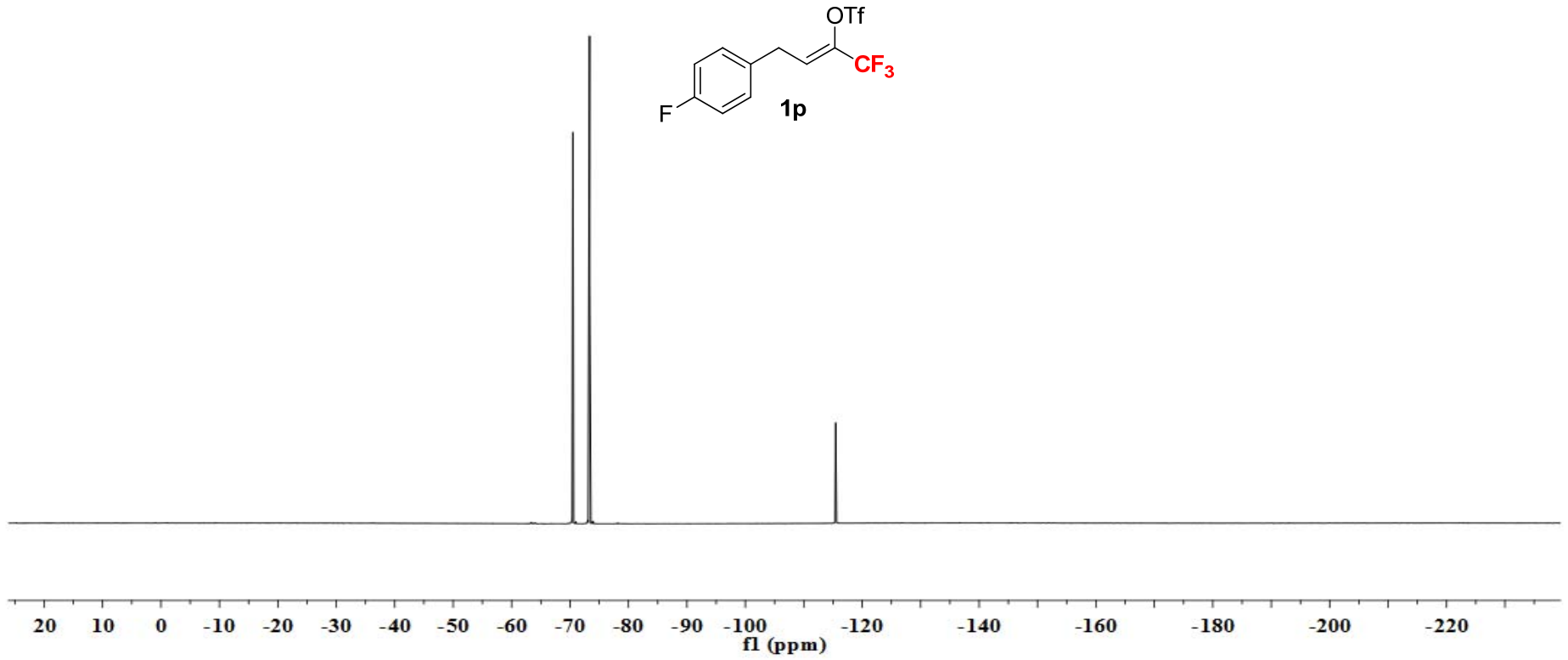

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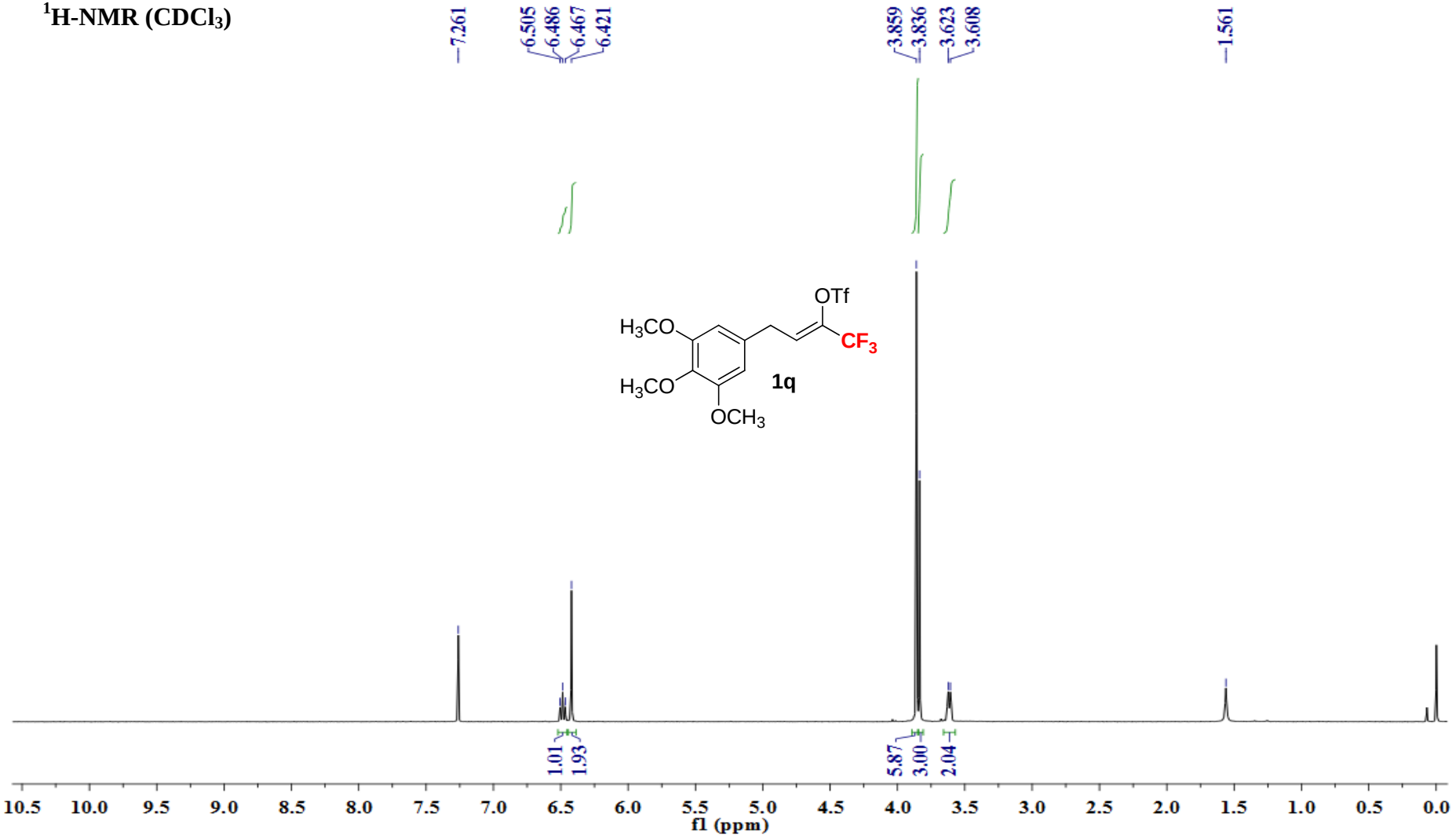
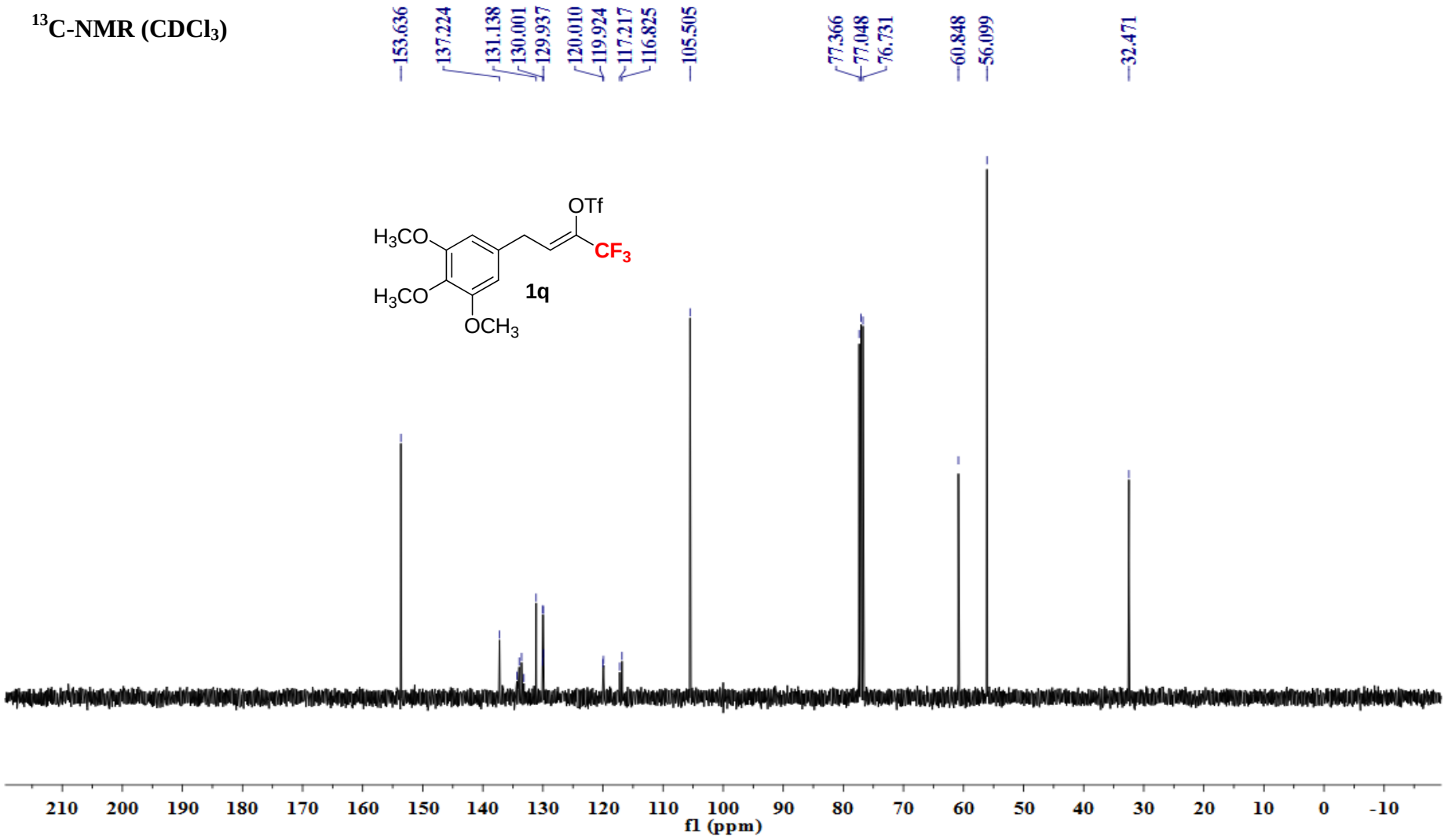

7.261
6.505
6.486
6.467
6.421
3.859
3.836
3.623
3.608
1.561
OTf
H3CO
CF3
H3CO
OCH3
1q
1.01
1.93
5.87
3.00
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

^{13}C-NMR ($CDCl_3$)



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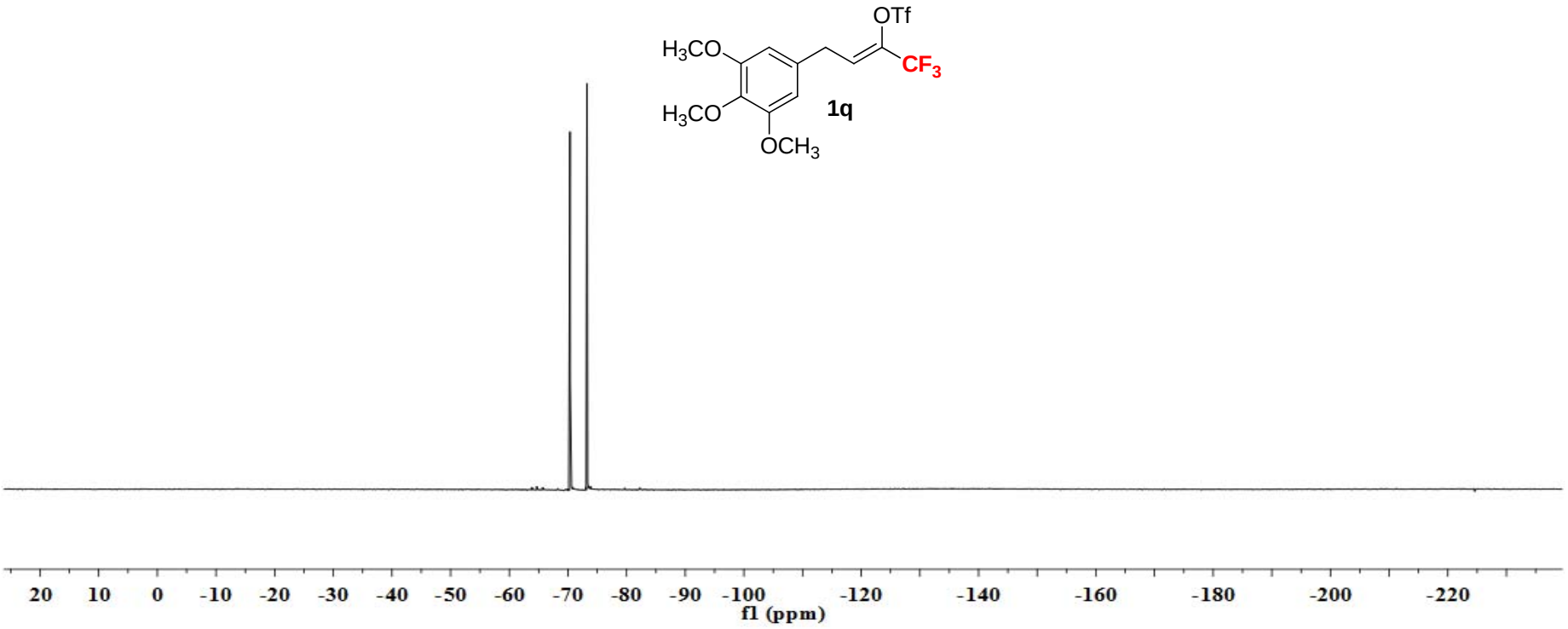

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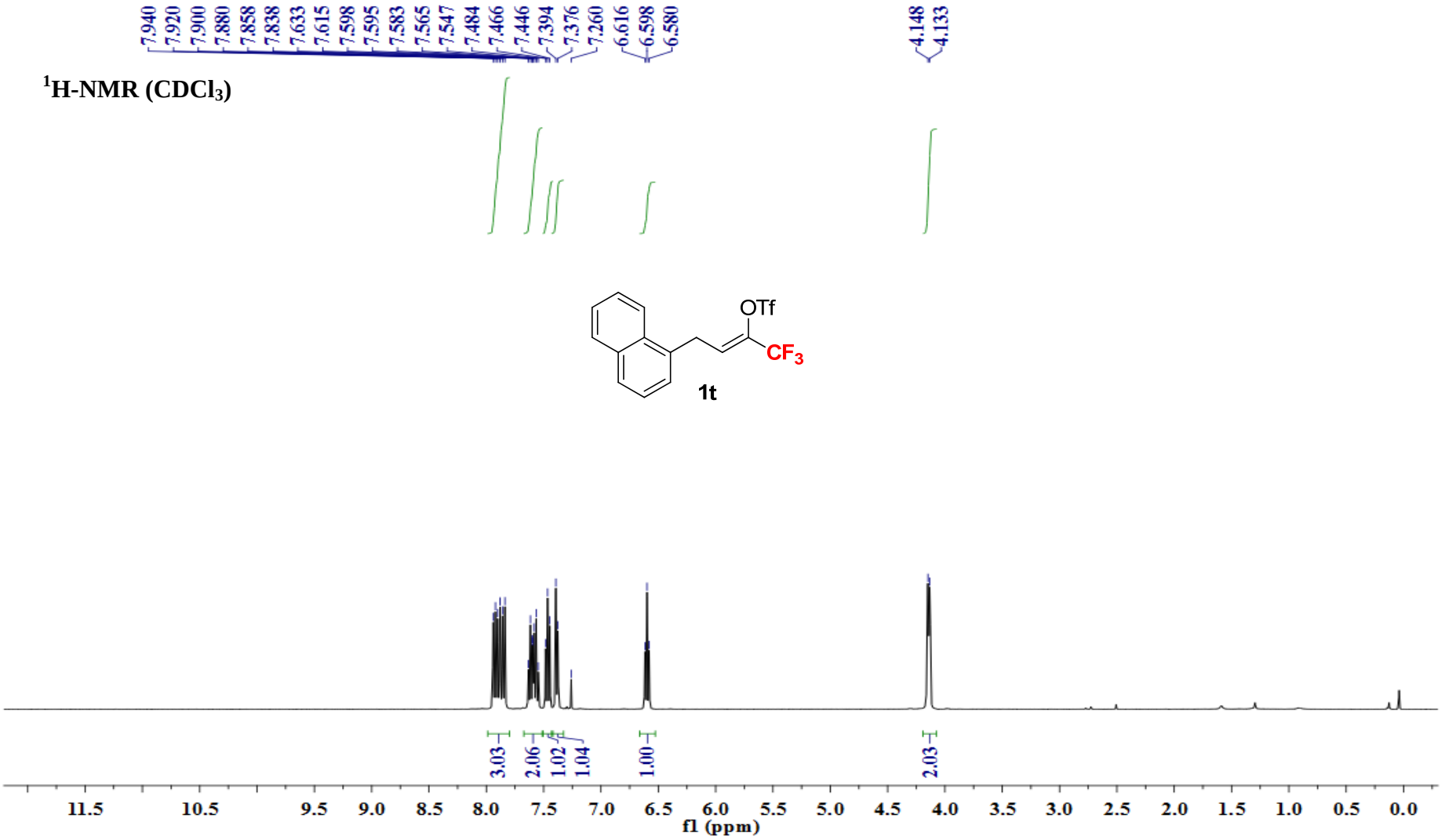
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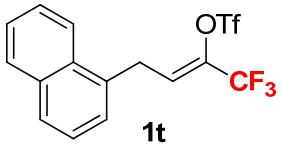
7.920
7.900
7.880
7.858
7.838
7.633
7.615
7.598
7.595
7.583
7.565
7.547
7.484
7.466
7.446
7.394
7.376
7.260
6.616
6.598
6.580
4.148
4.133
OTf
CF3
1t
3.03
2.06
1.02
1.04
1.00
2.03
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

^{13}C-NMR ($CDCl_3$)



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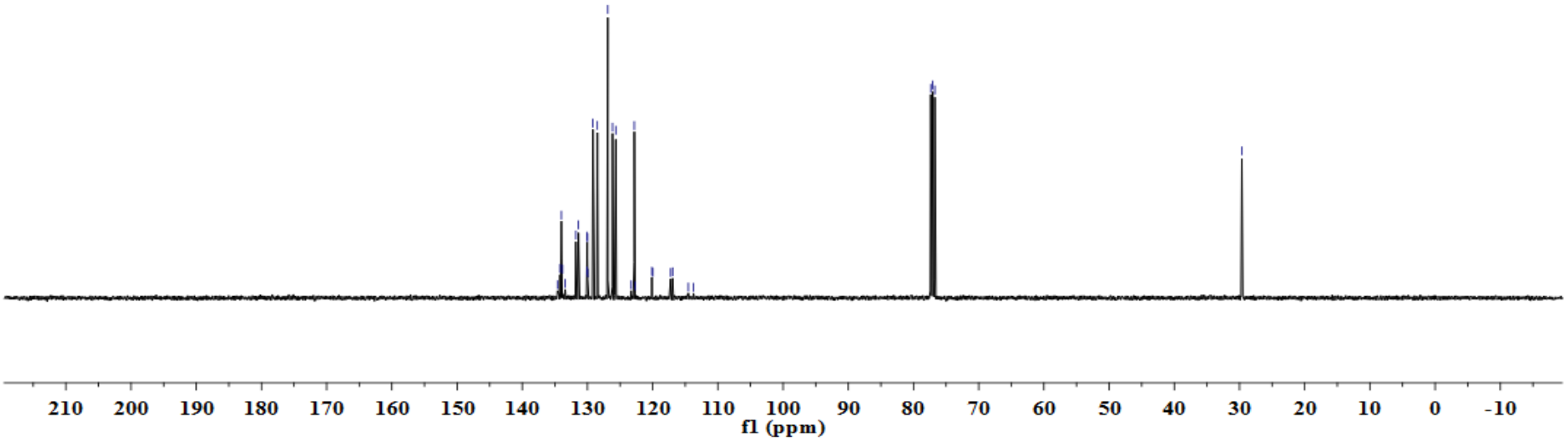
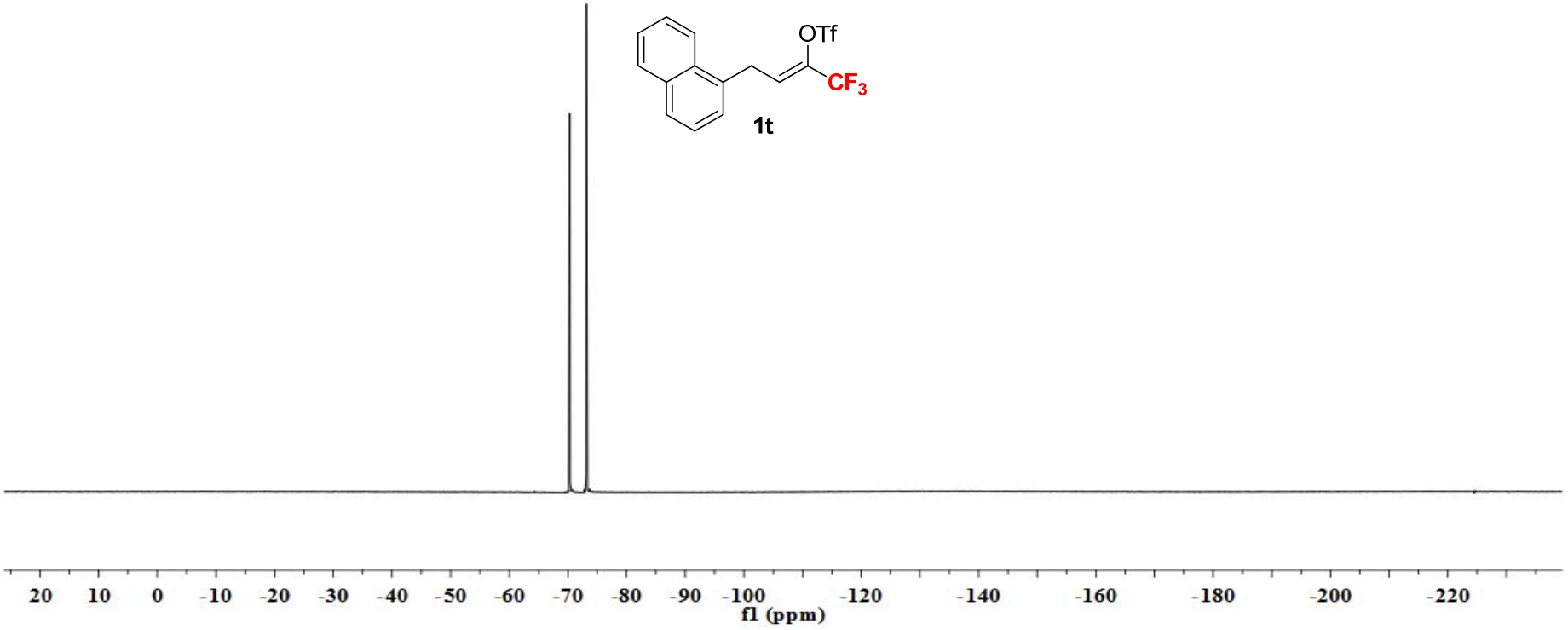
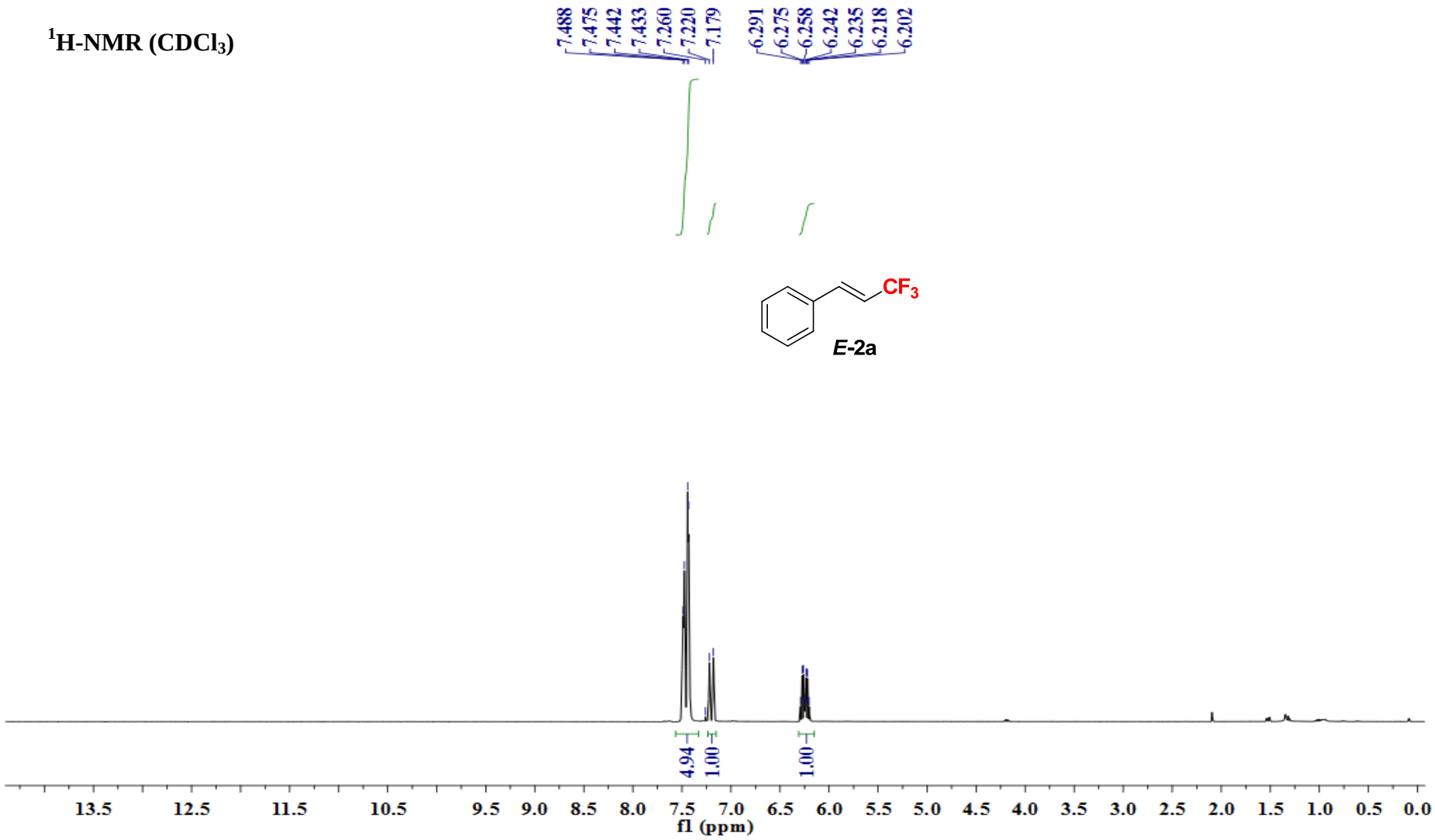


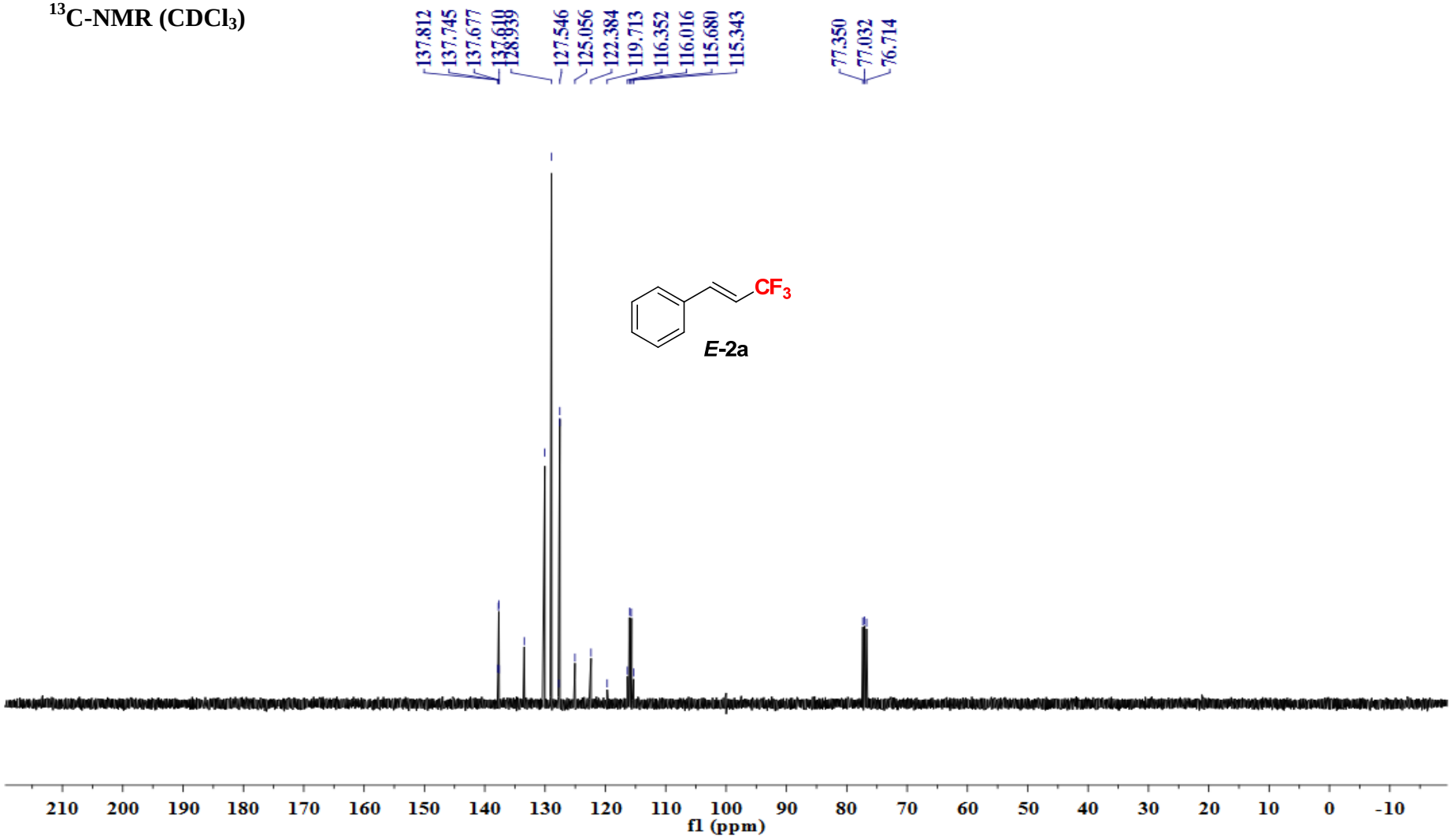
^{19}F-NMR ($CDCl_3$)



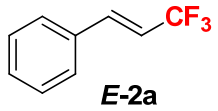
^{1}H-NMR ($CDCl_3$)


7.488
7.475
7.442
7.433
7.260
7.220
7.179
6.291
6.275
6.258
6.242
6.235
6.218
6.202
CF3
E-2a
4.94
1.00
1.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

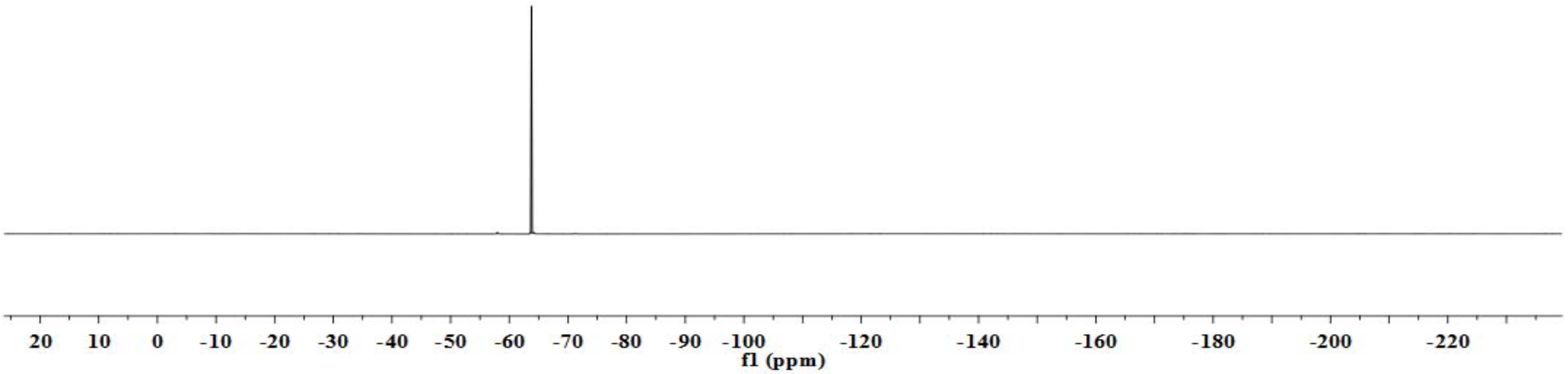
^{13}C-NMR ($CDCl_3$)



^{19}F-NMR ($CDCl_3$)



E-2a



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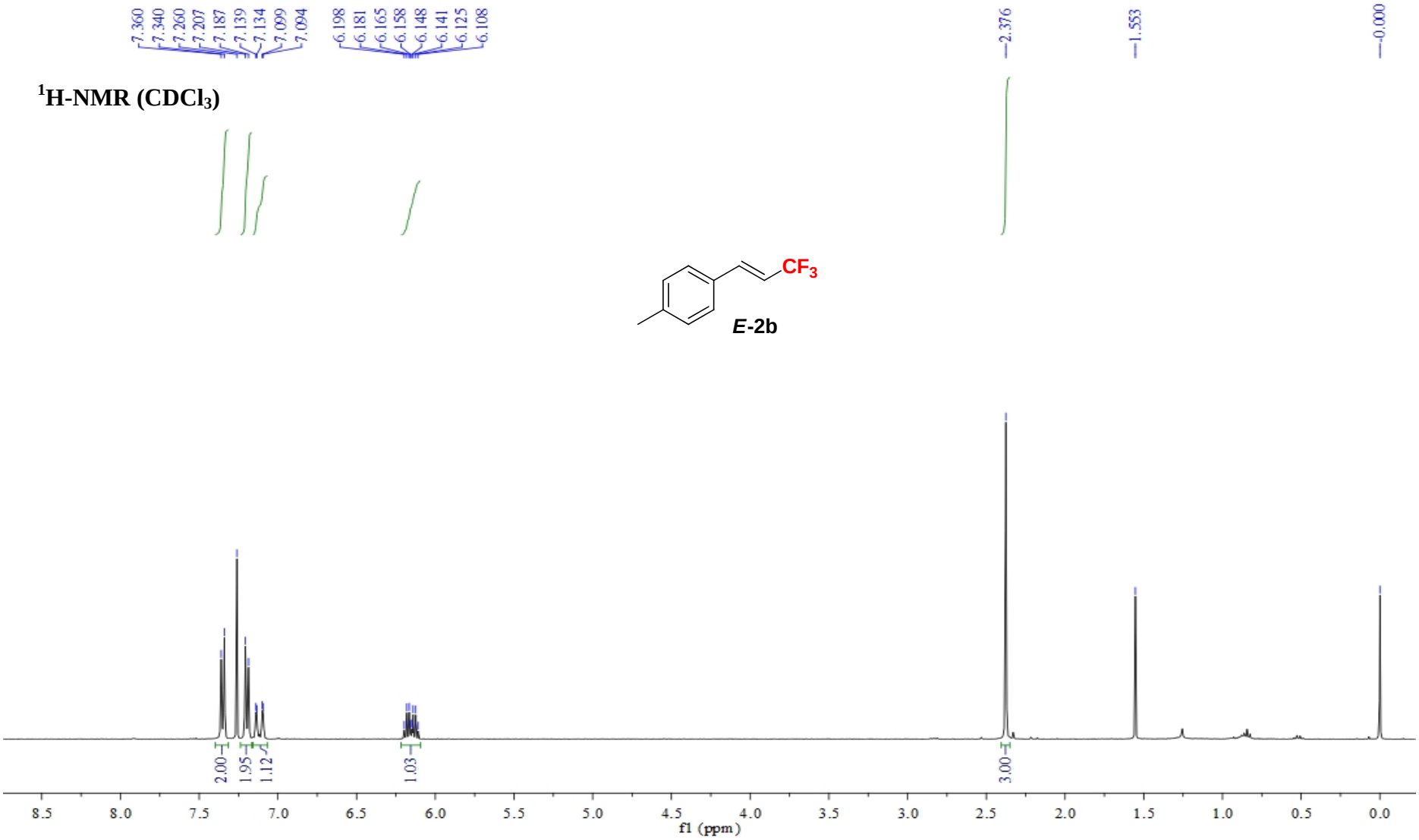

***E*-2b**

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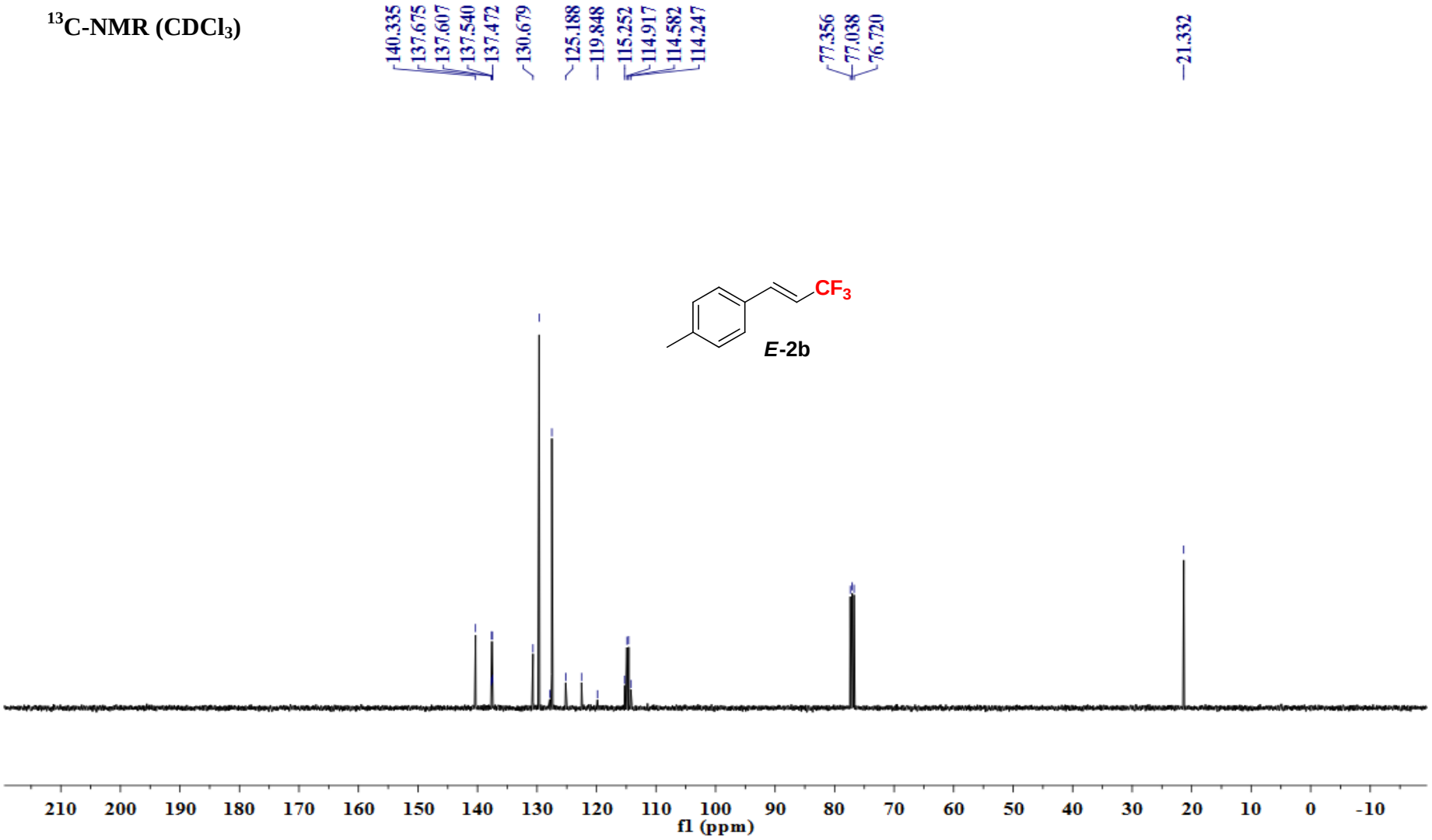

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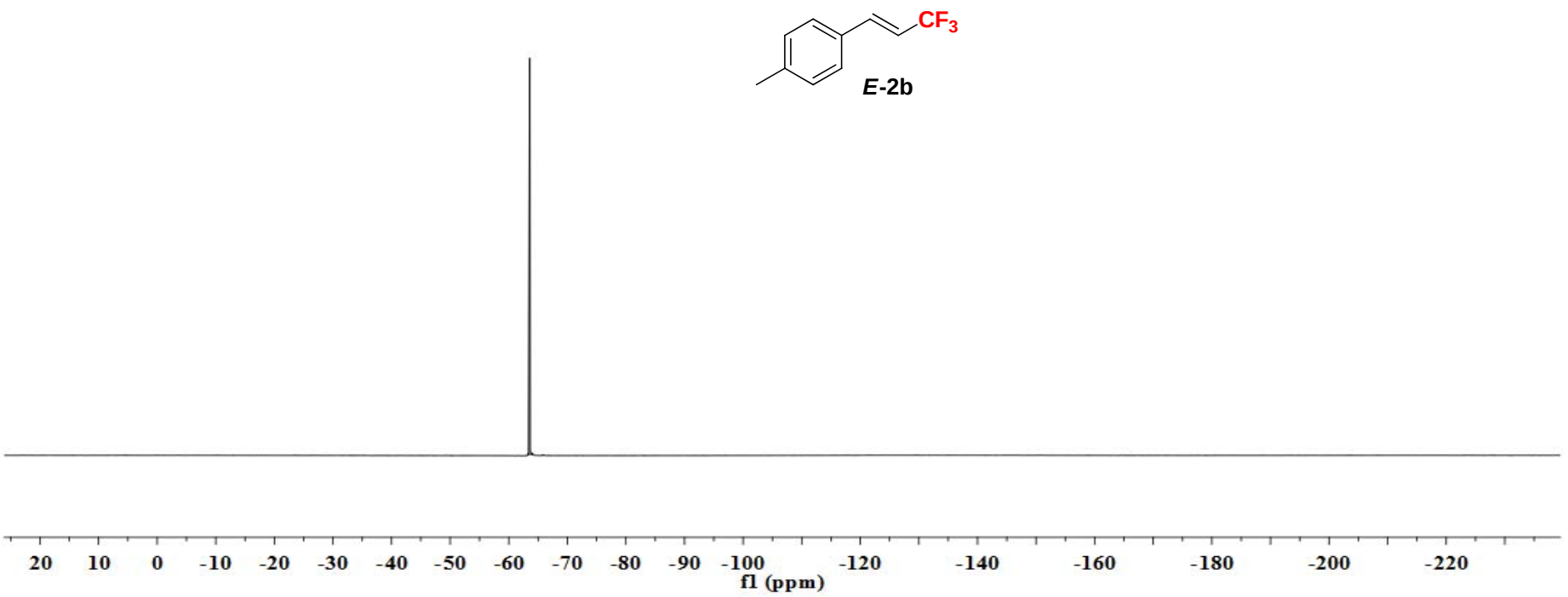

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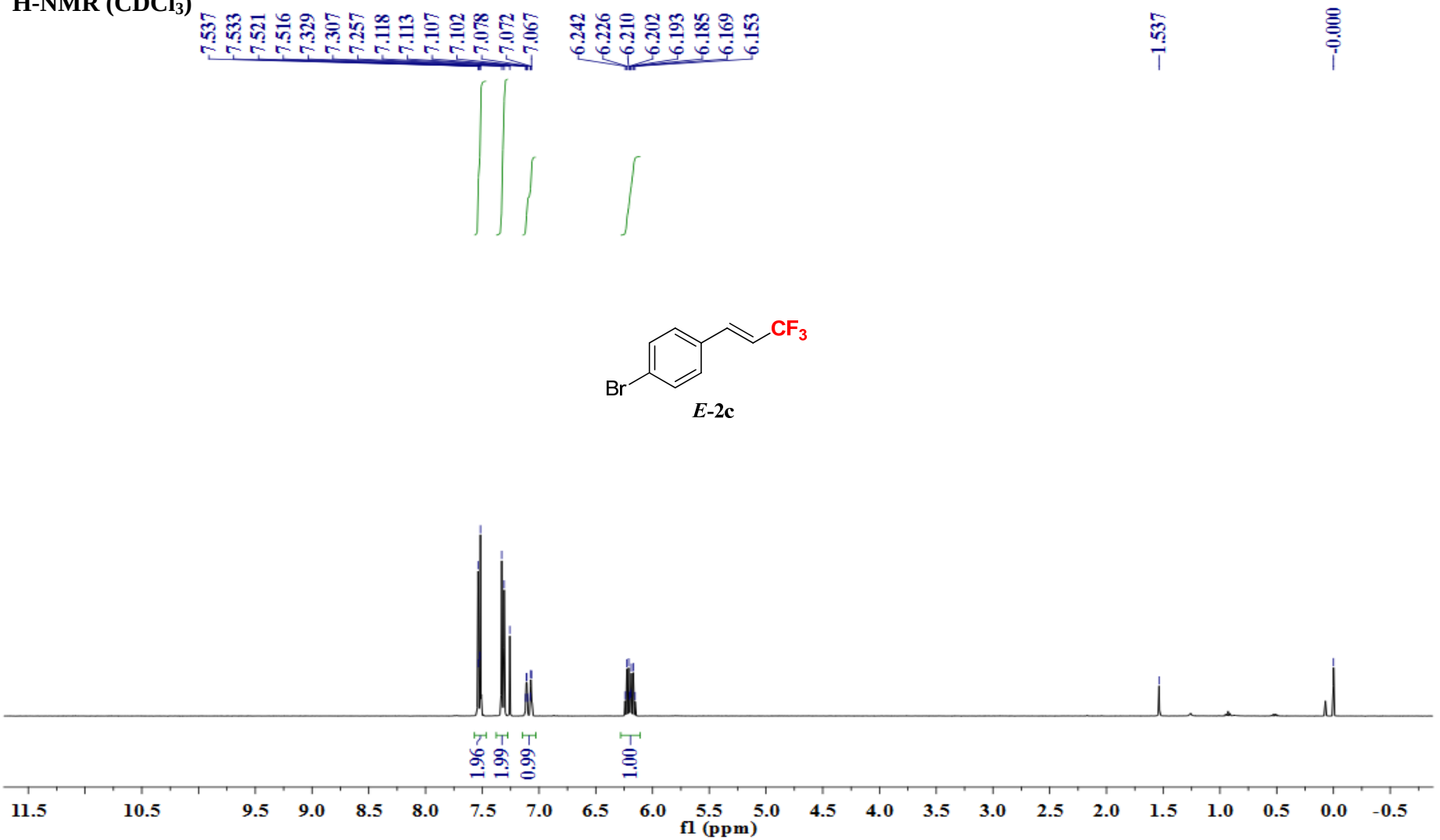
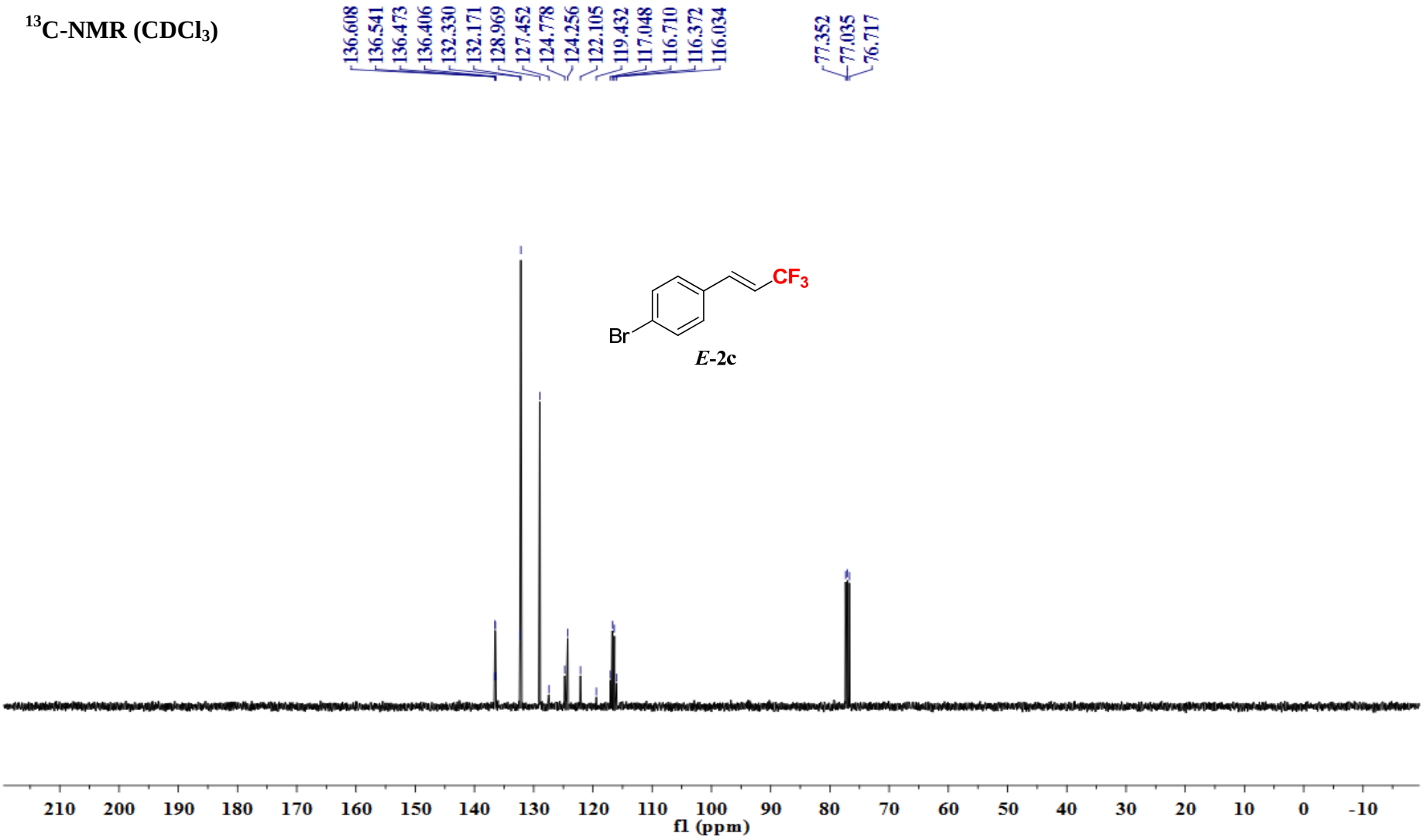
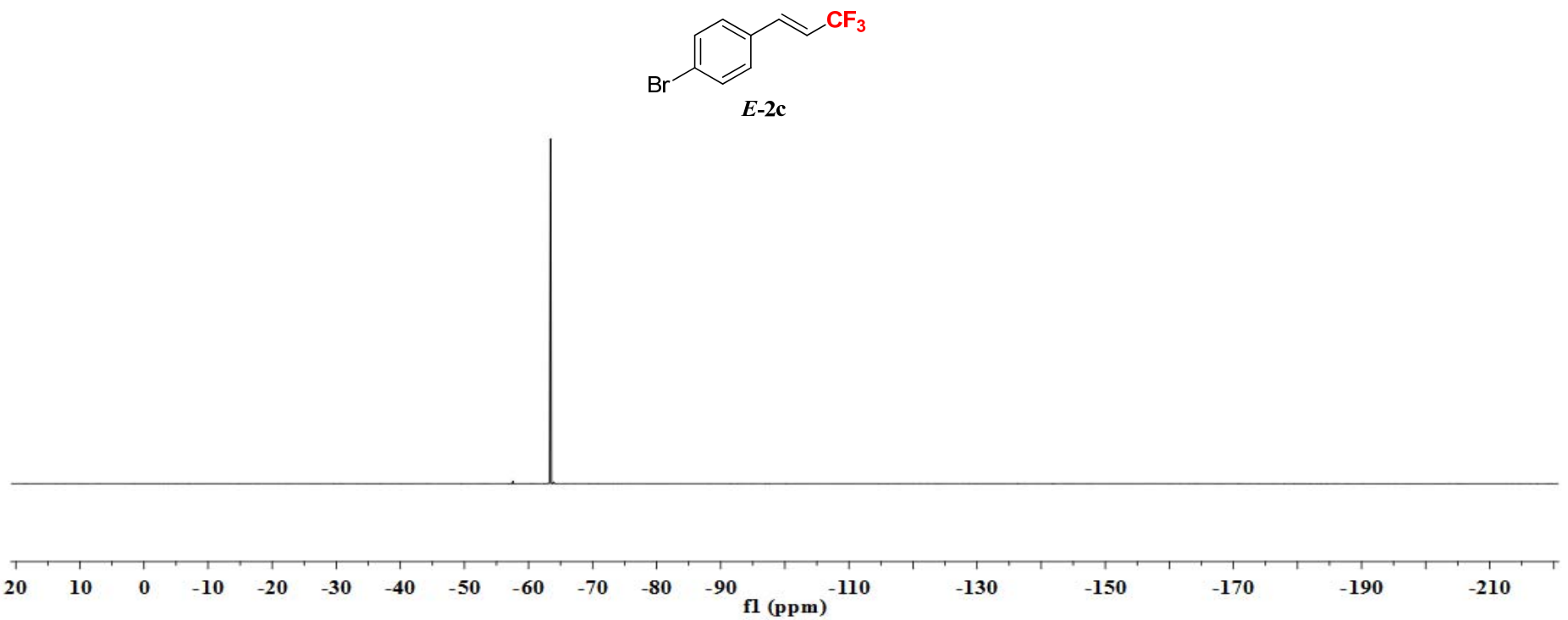


E-2c

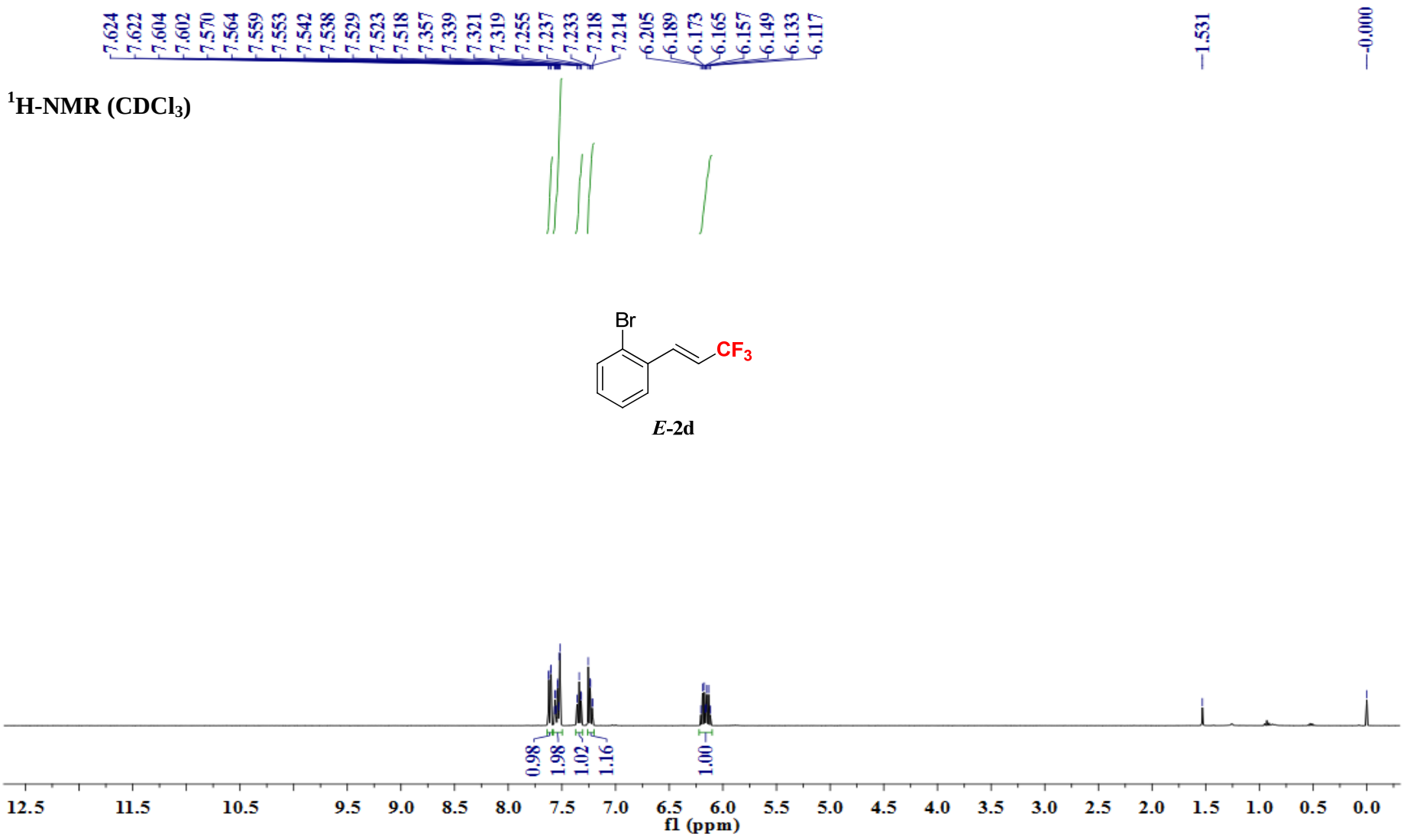
^{13}C-NMR ($CDCl_3$)



^{19}F-NMR ($CDCl_3$)



^{1}H-NMR ($CDCl_3$)



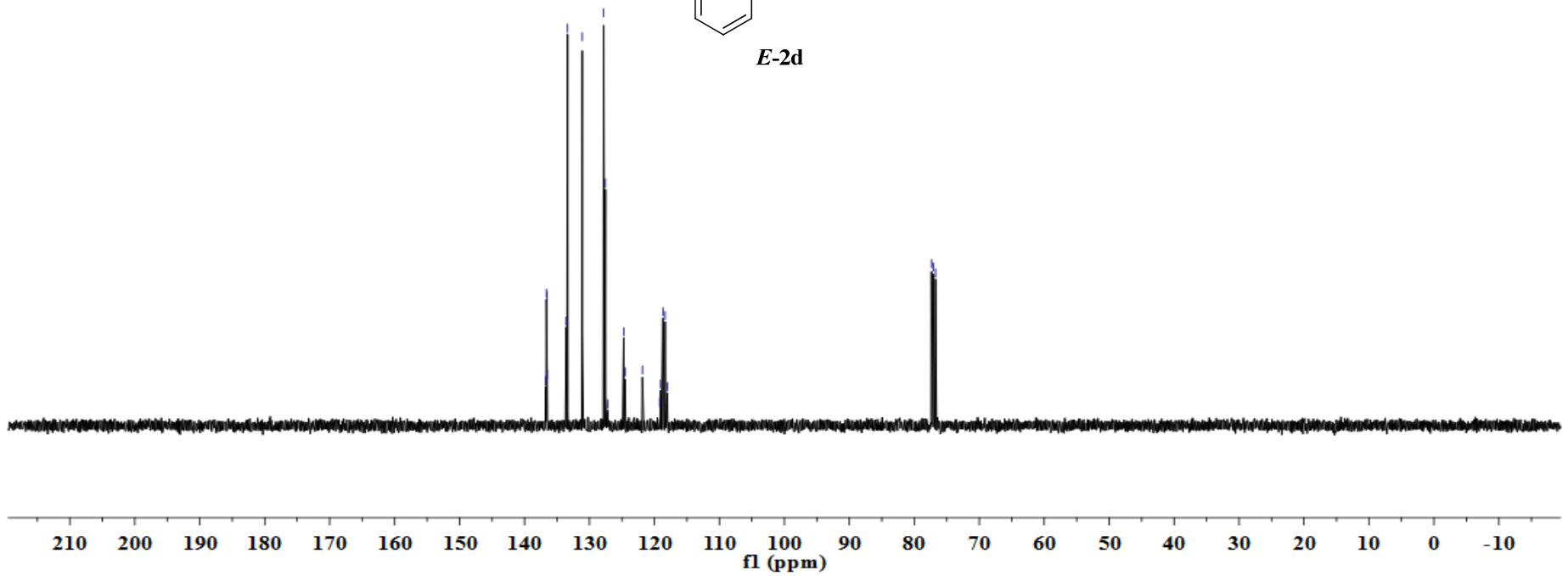
***E*-2d**

^{13}C-NMR ($CDCl_3$)

136.705
136.636
136.567
136.498
133.574
133.384
131.115
127.824
127.552
127.215
124.718
124.539
121.862
119.185
119.037
118.699
118.361
118.022

77.352
77.034
76.716

E-2d



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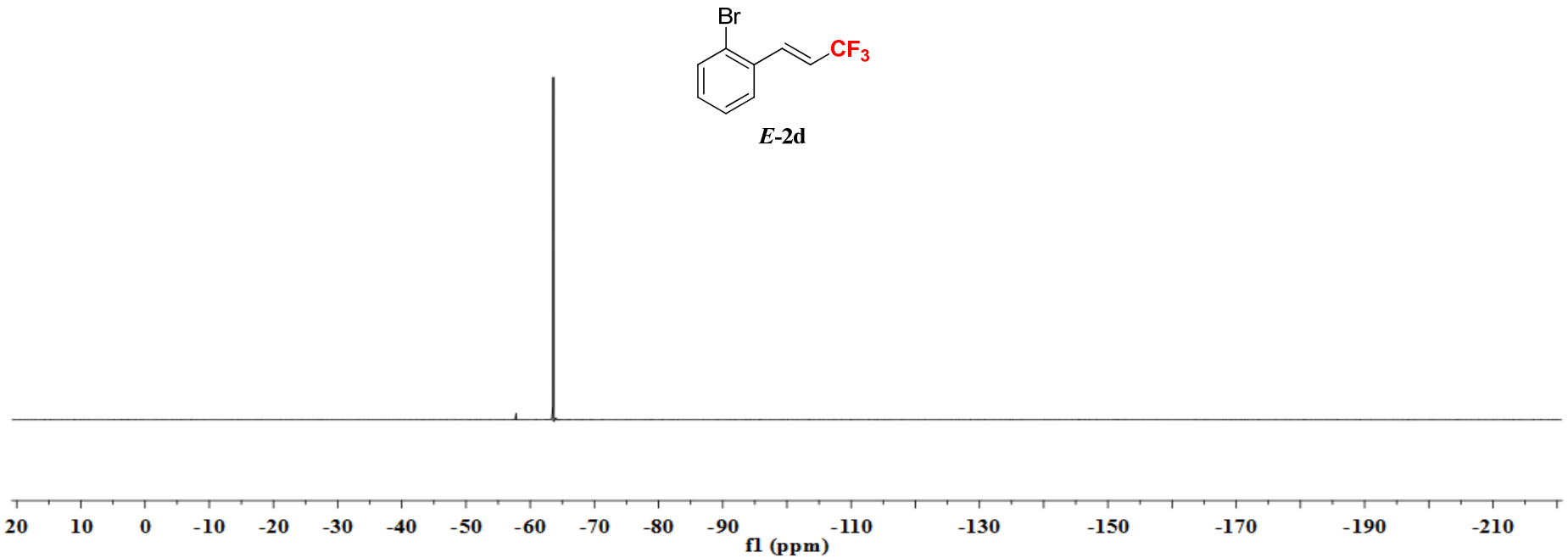
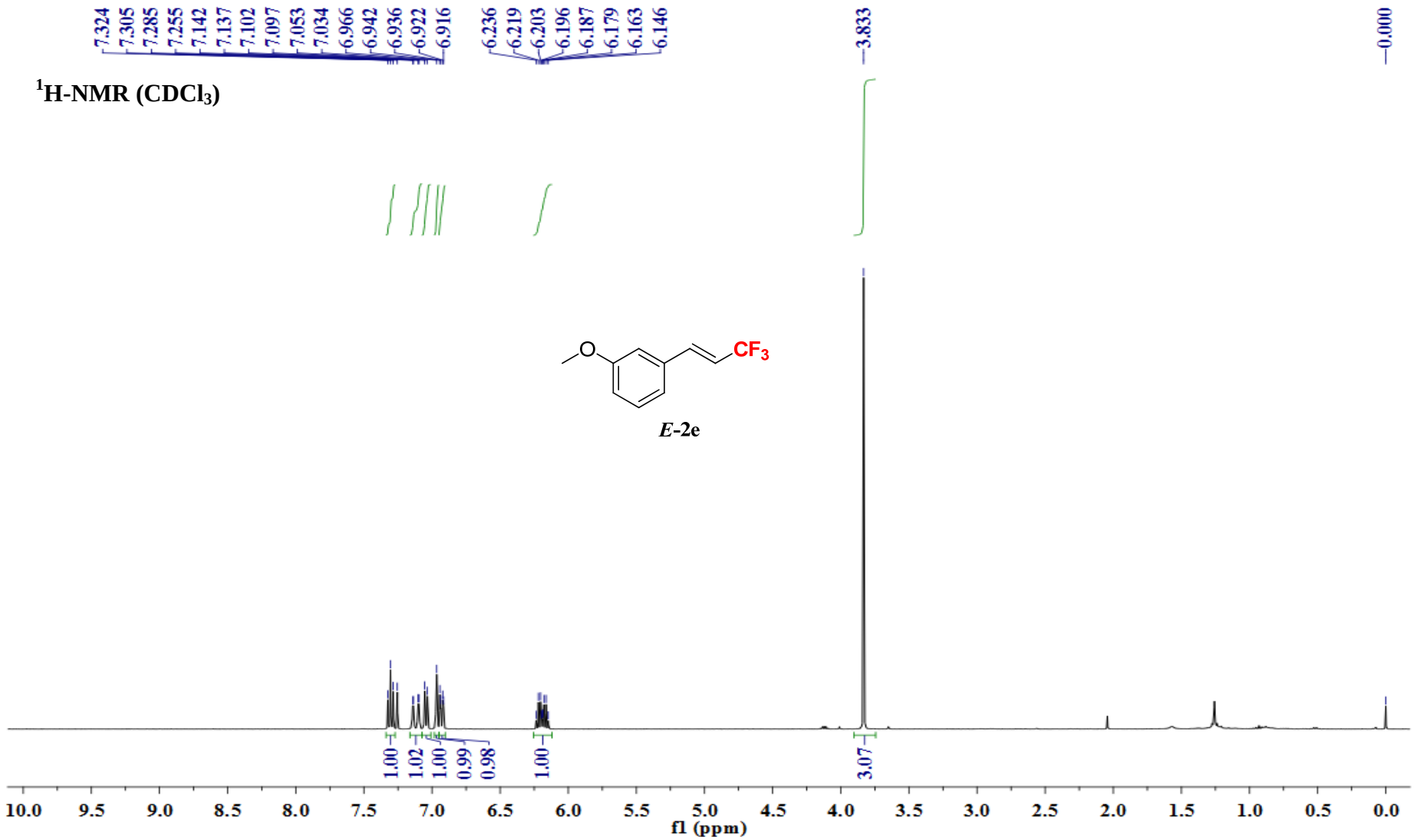


***E*-2d**

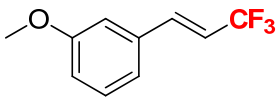
^{1}H-NMR ($CDCl_3$)



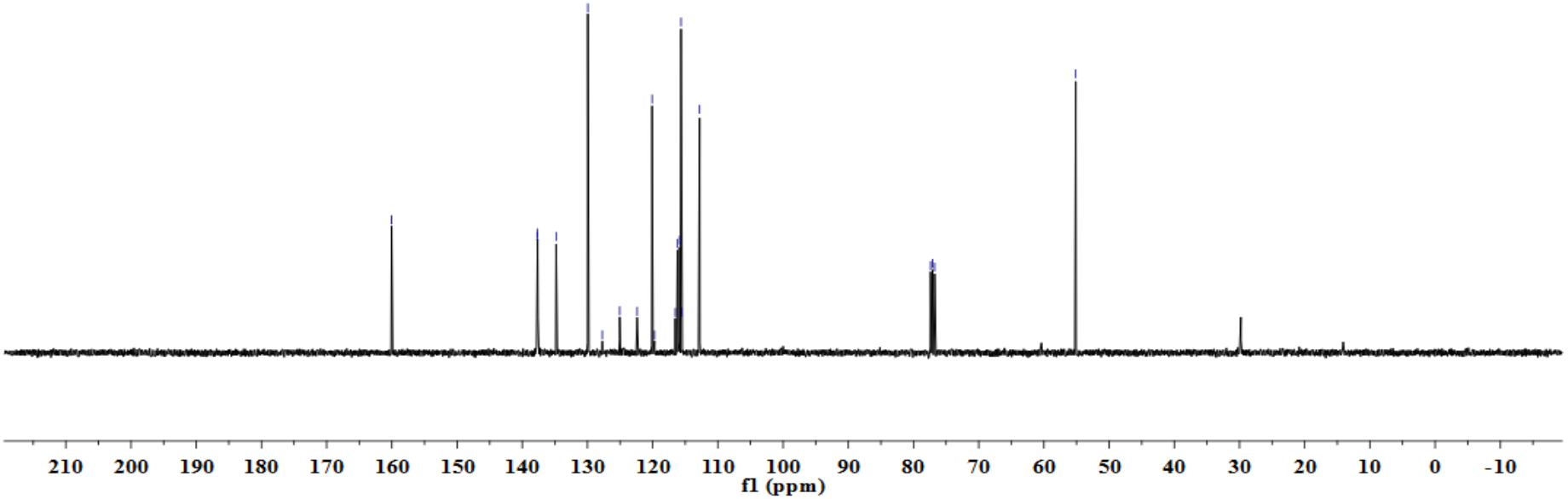
***E*-2e**

^{13}C-NMR ($CDCl_3$)

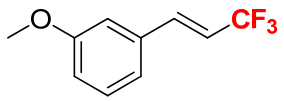
160.034
137.725
137.657
134.797
129.946
119.713
116.537
116.201
115.866
115.651
115.529
112.810
77.383
77.065
76.747
55.121



***E*-2e**



^{19}F-NMR ($CDCl_3$)



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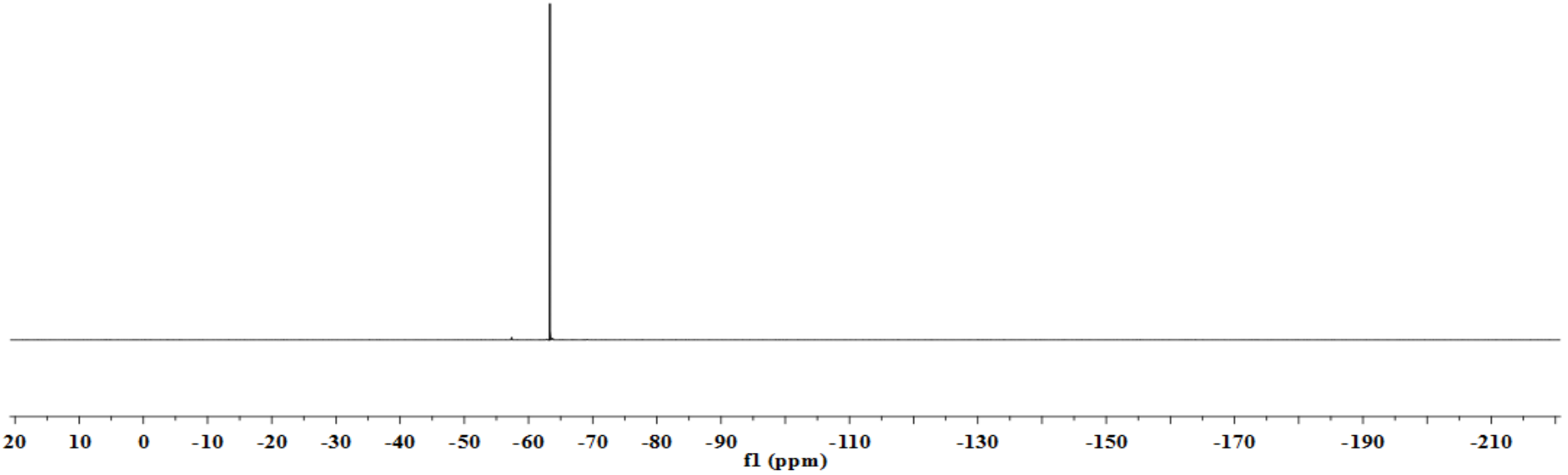

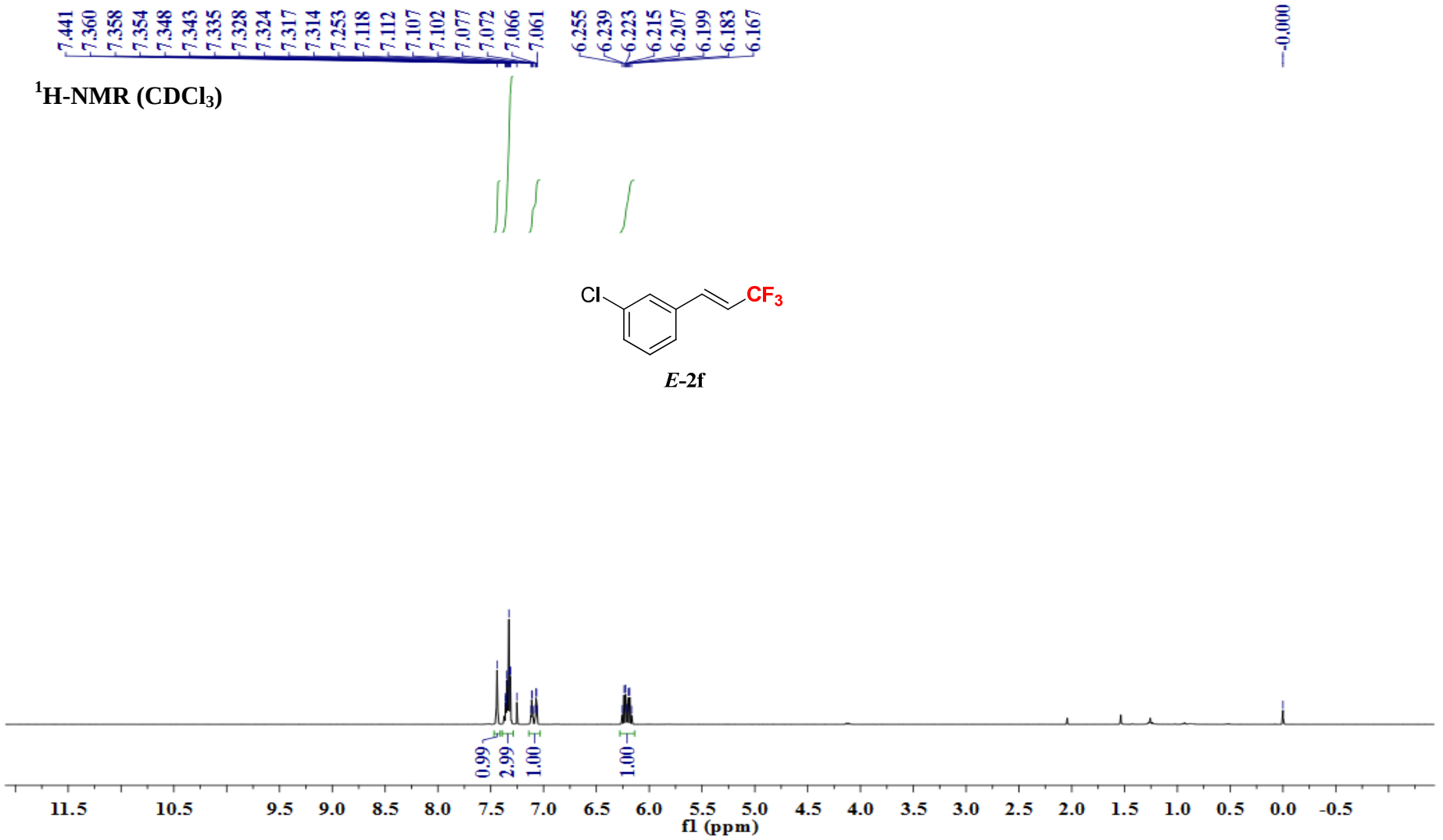

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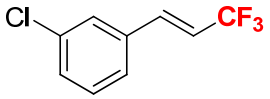
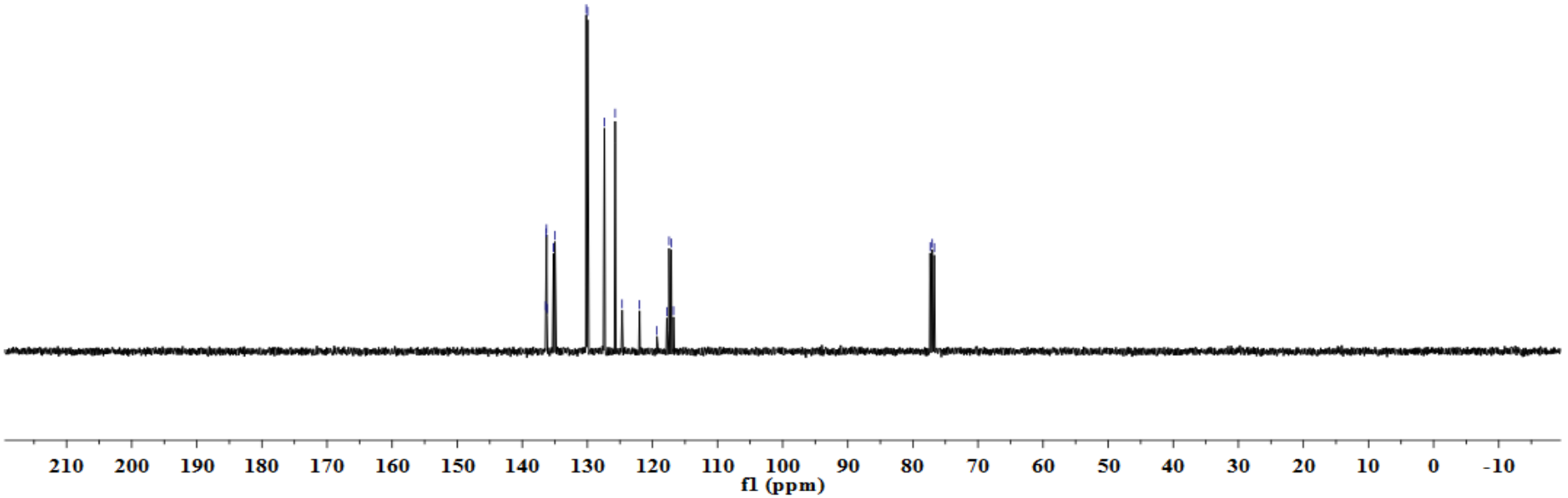
***E*-2f**

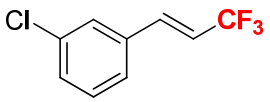
^{13}C-NMR ($CDCl_3$)



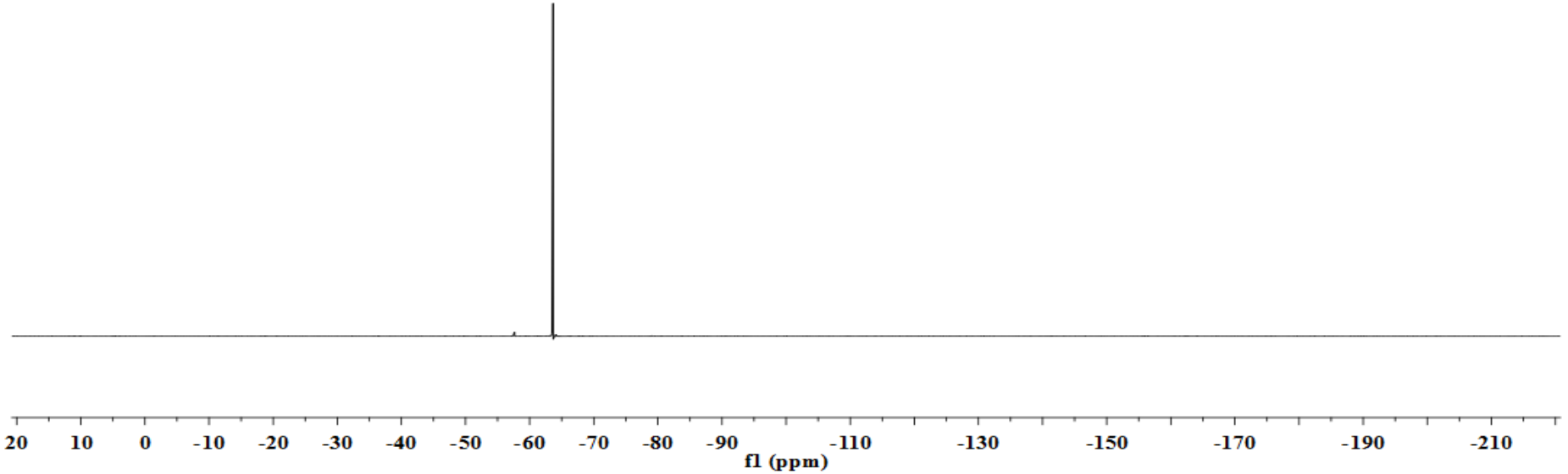
***E*-2f**



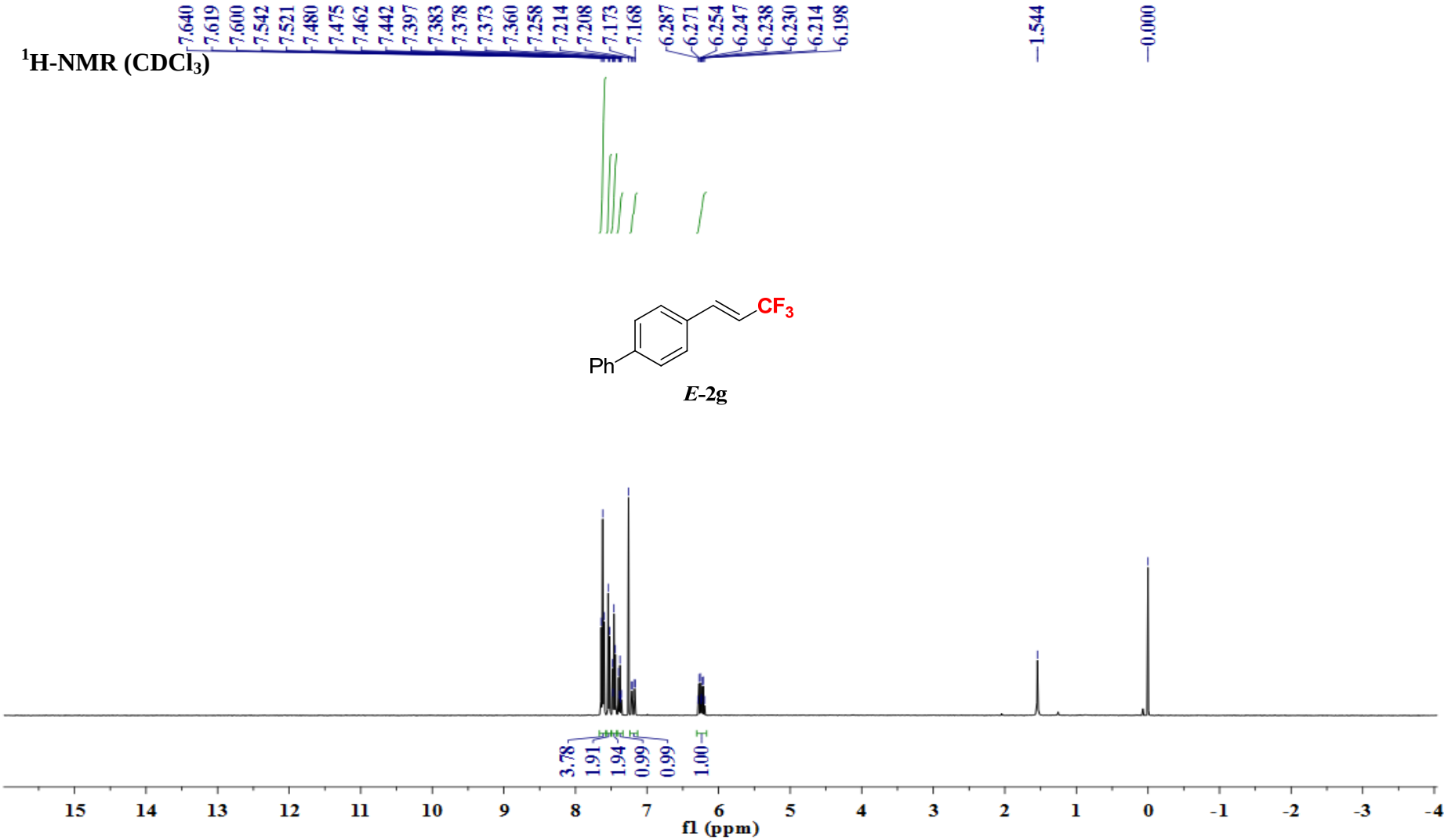
^{19}F-NMR ($CDCl_3$)



***E*-2f**

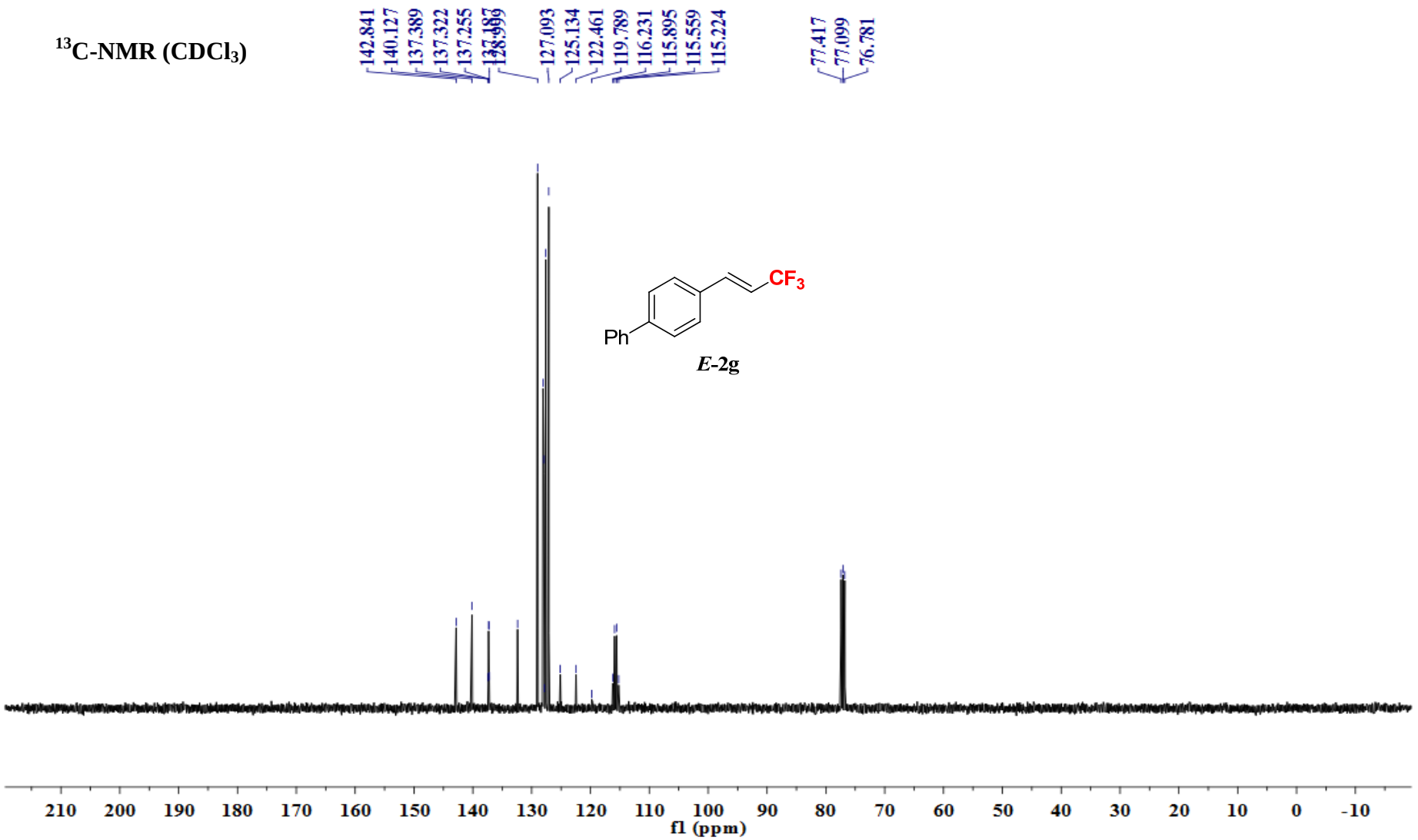


^{1}H-NMR ($CDCl_3$)



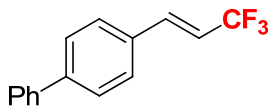
***E*-2g**

^{13}C-NMR ($CDCl_3$)

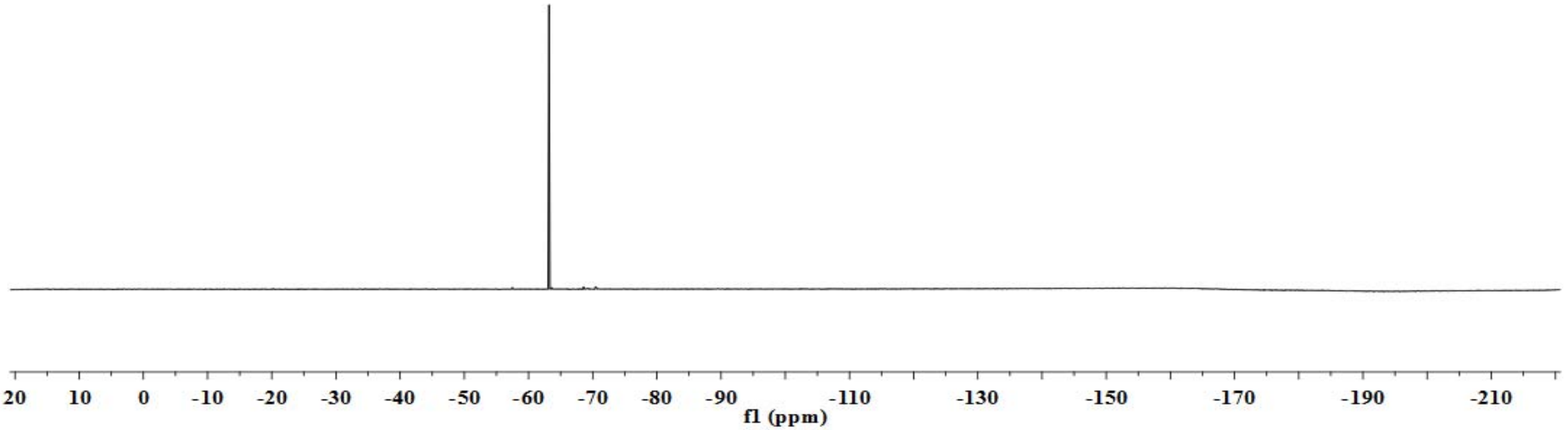


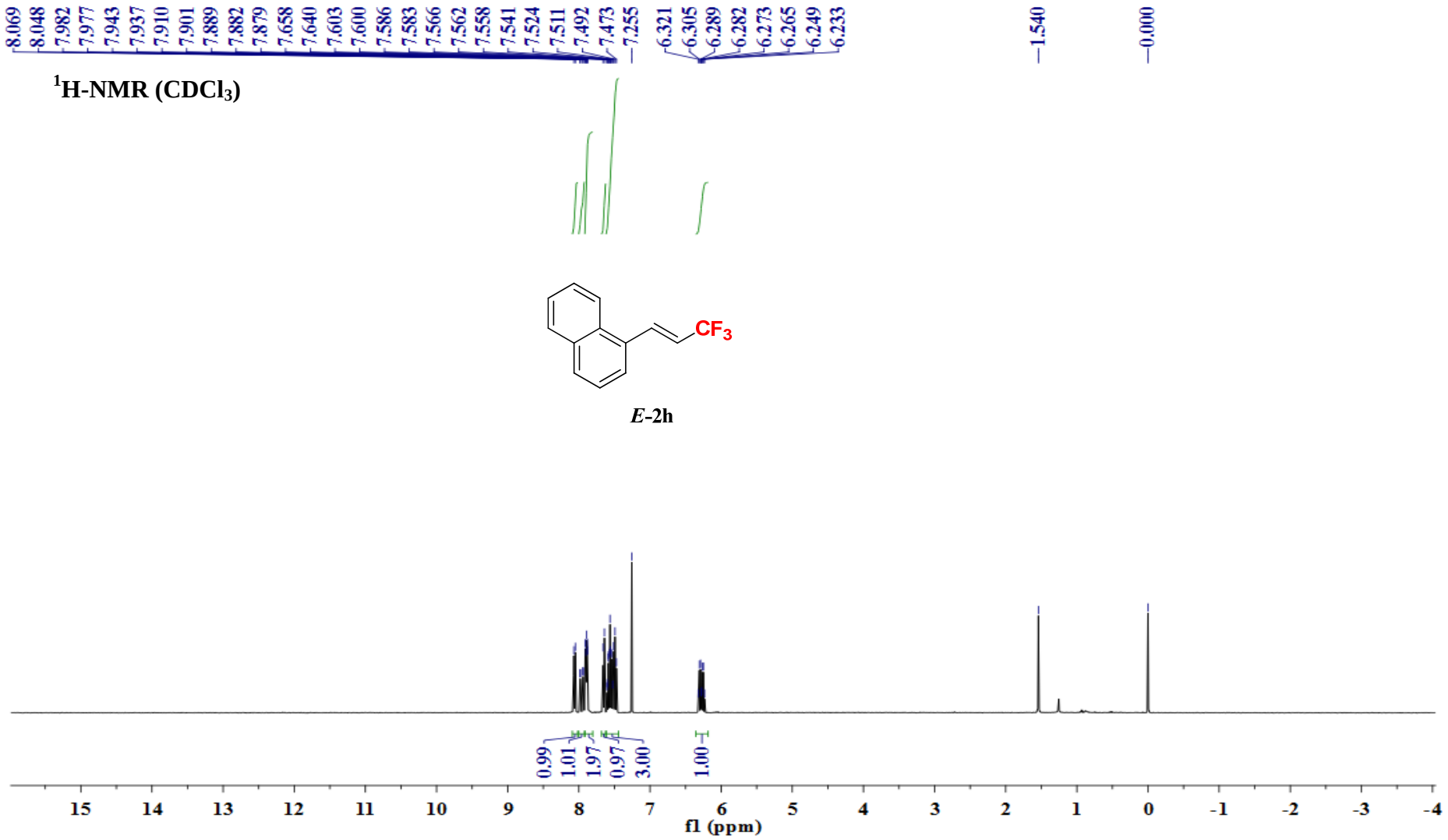
***E*-2g**

^{19}F-NMR ($CDCl_3$)



***E*-2g**

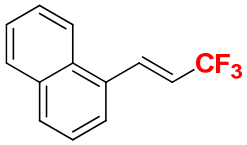




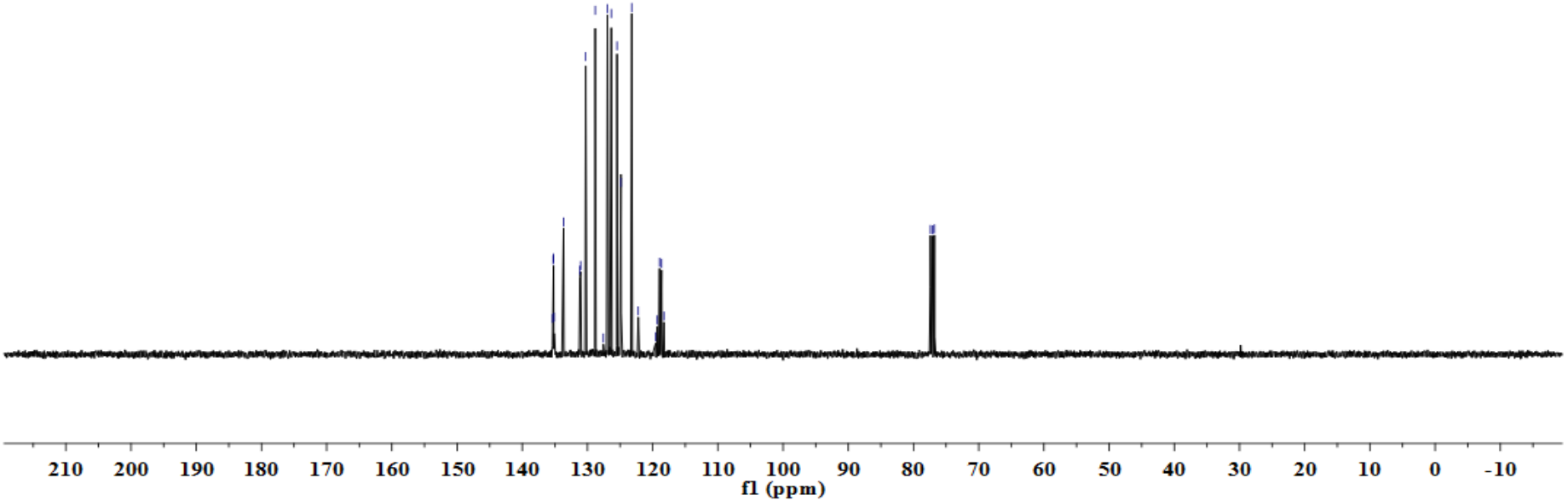
^{1}H-NMR ($CDCl_3$)

***E*-2h**

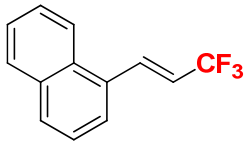
^{13}C-NMR ($CDCl_3$)



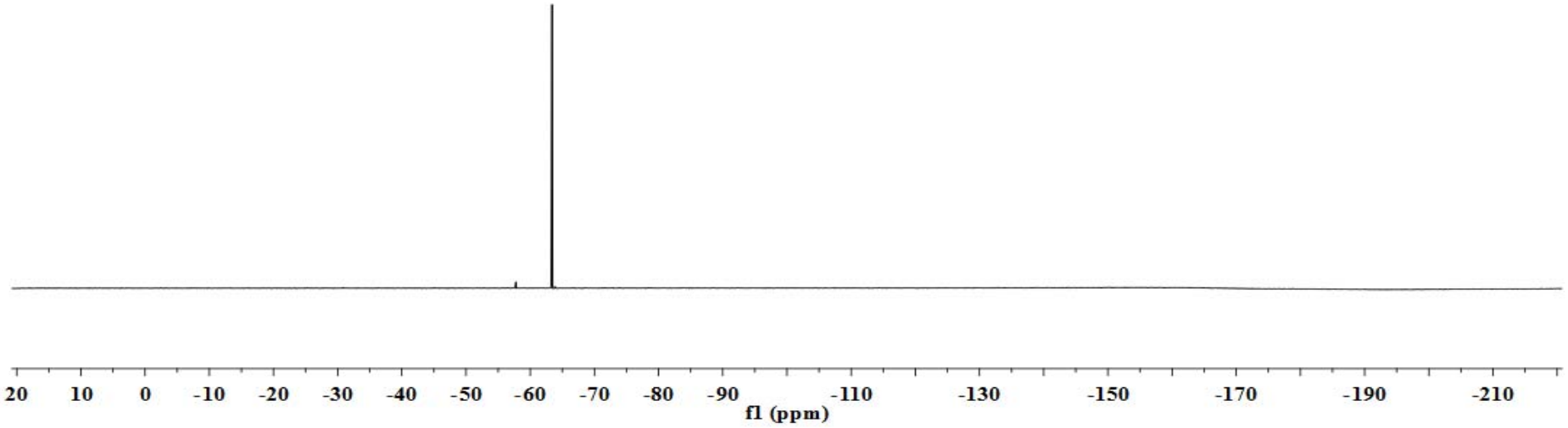
***E*-2h**



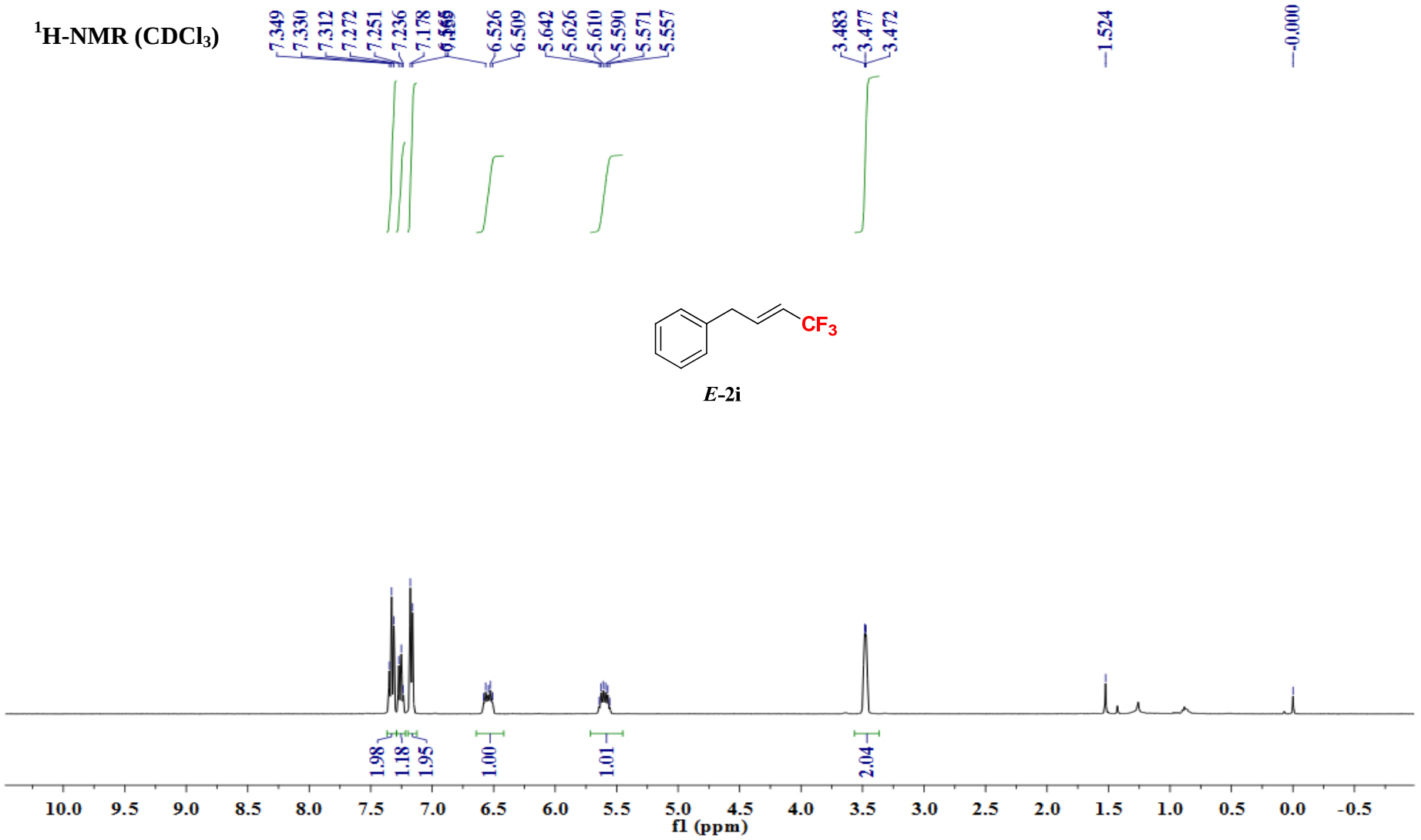
^{19}F-NMR ($CDCl_3$)



***E*-2h**

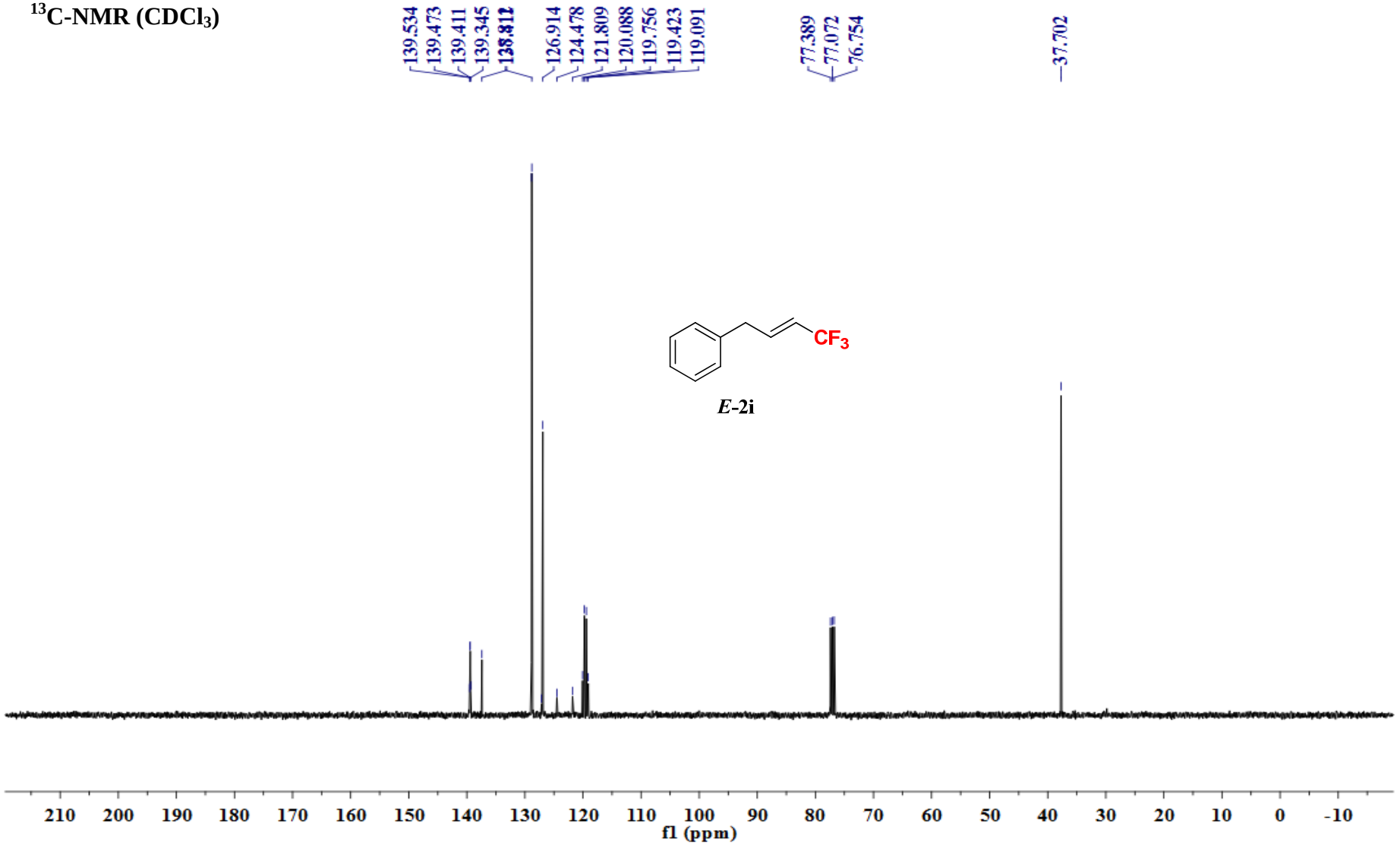


^{1}H-NMR ($CDCl_3$)

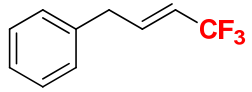


***E*-2i**

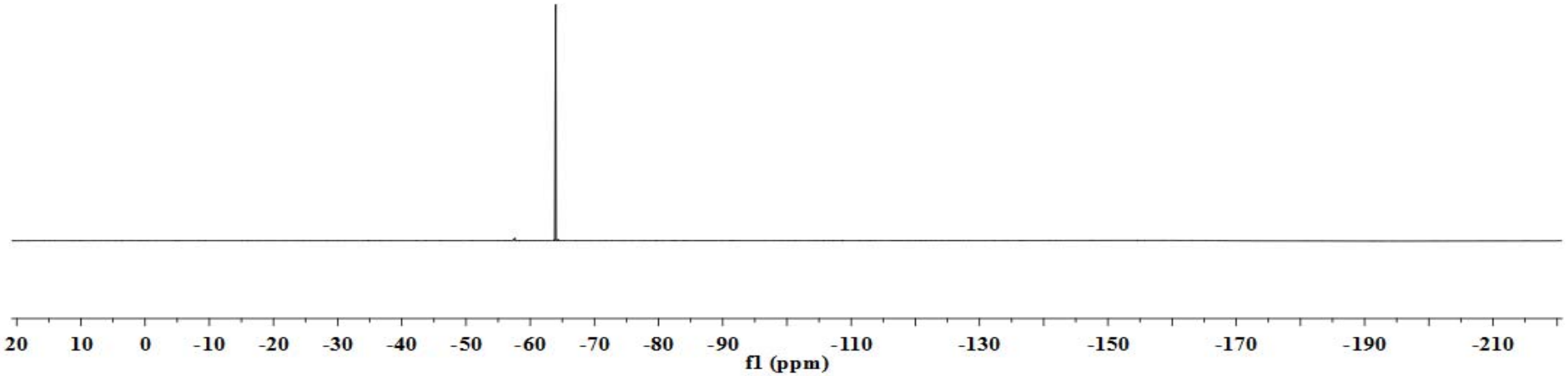
^{13}C-NMR ($CDCl_3$)



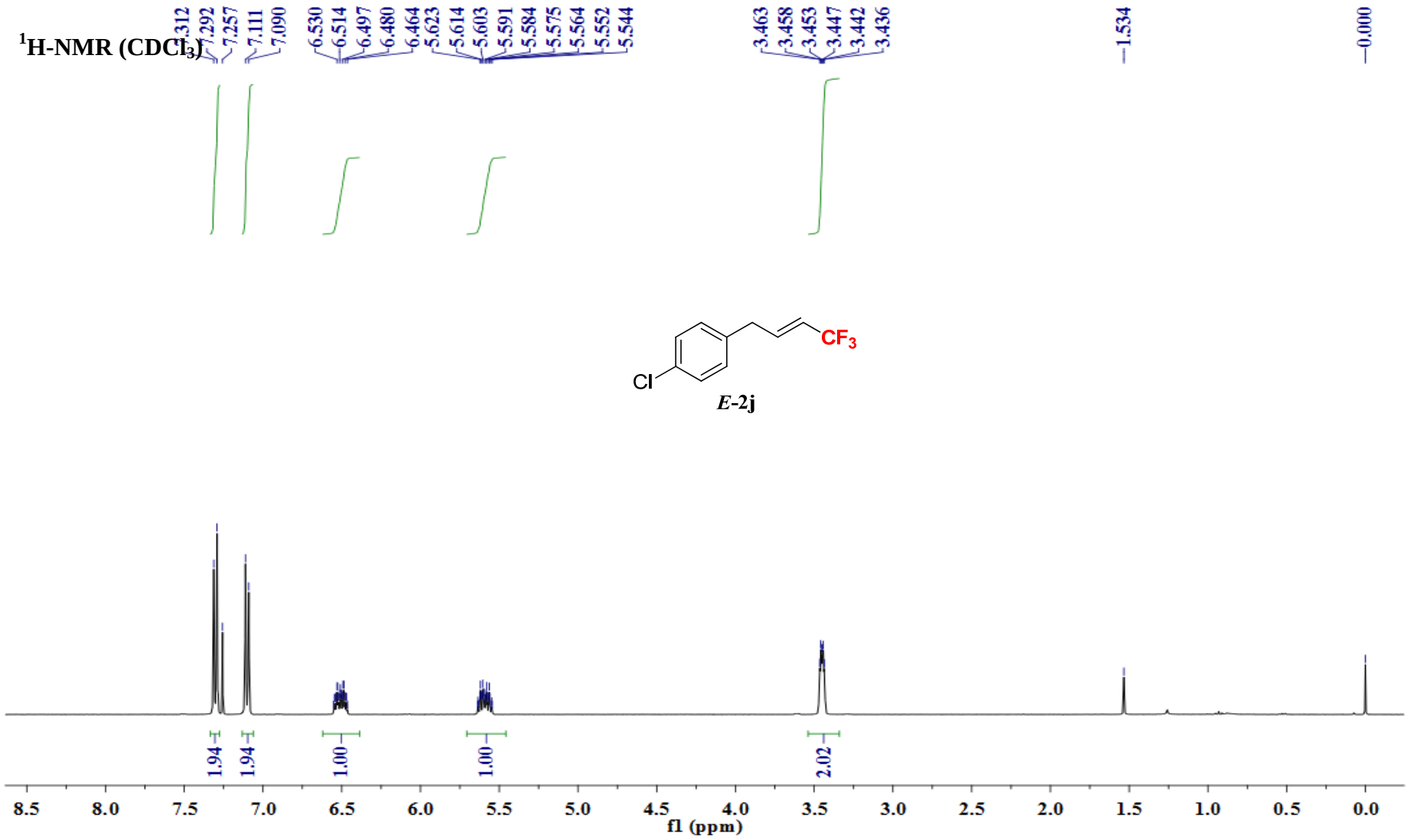
^{19}F-NMR ($CDCl_3$)



***E*-2i**

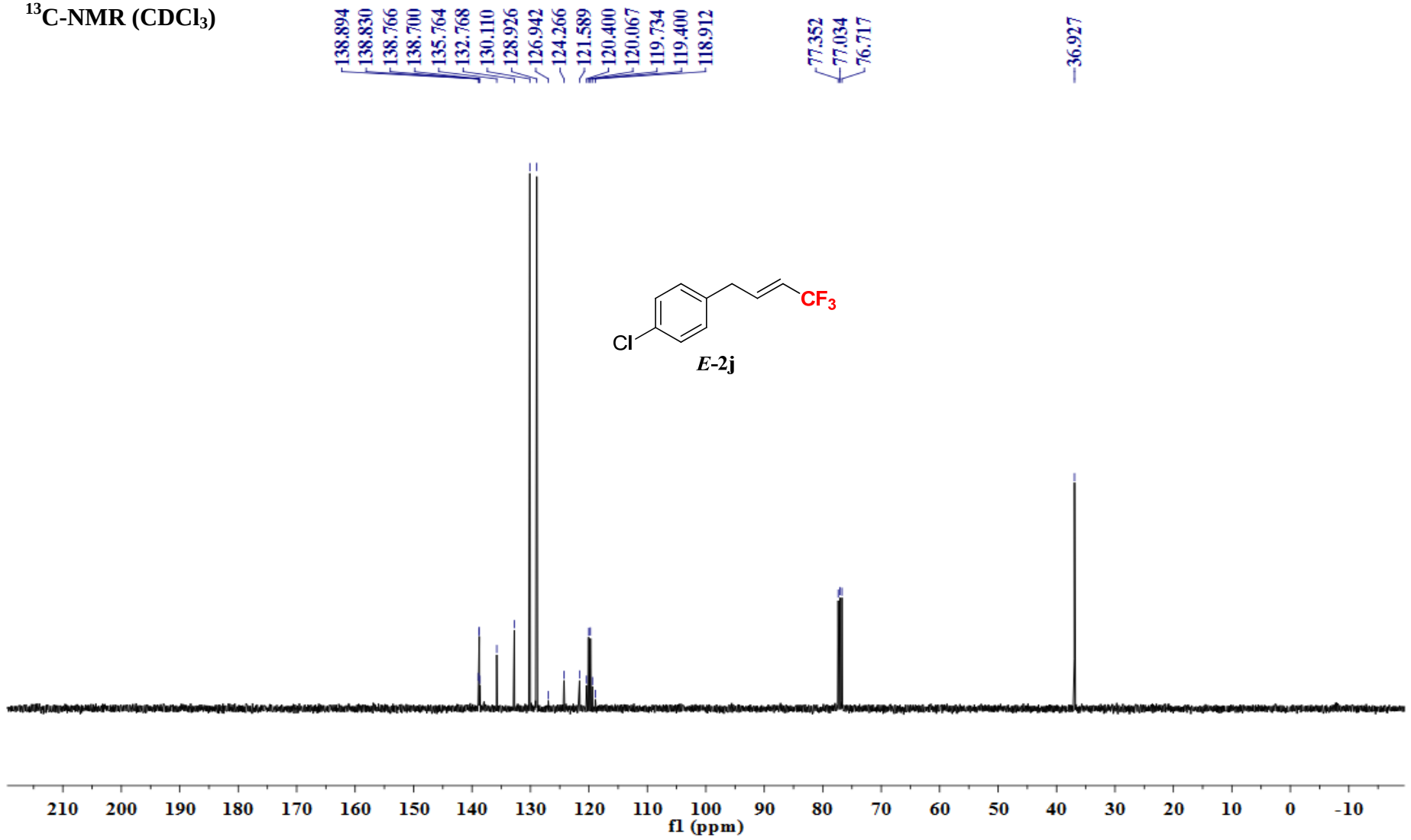


^{1}H-NMR ($CDCl_3$)

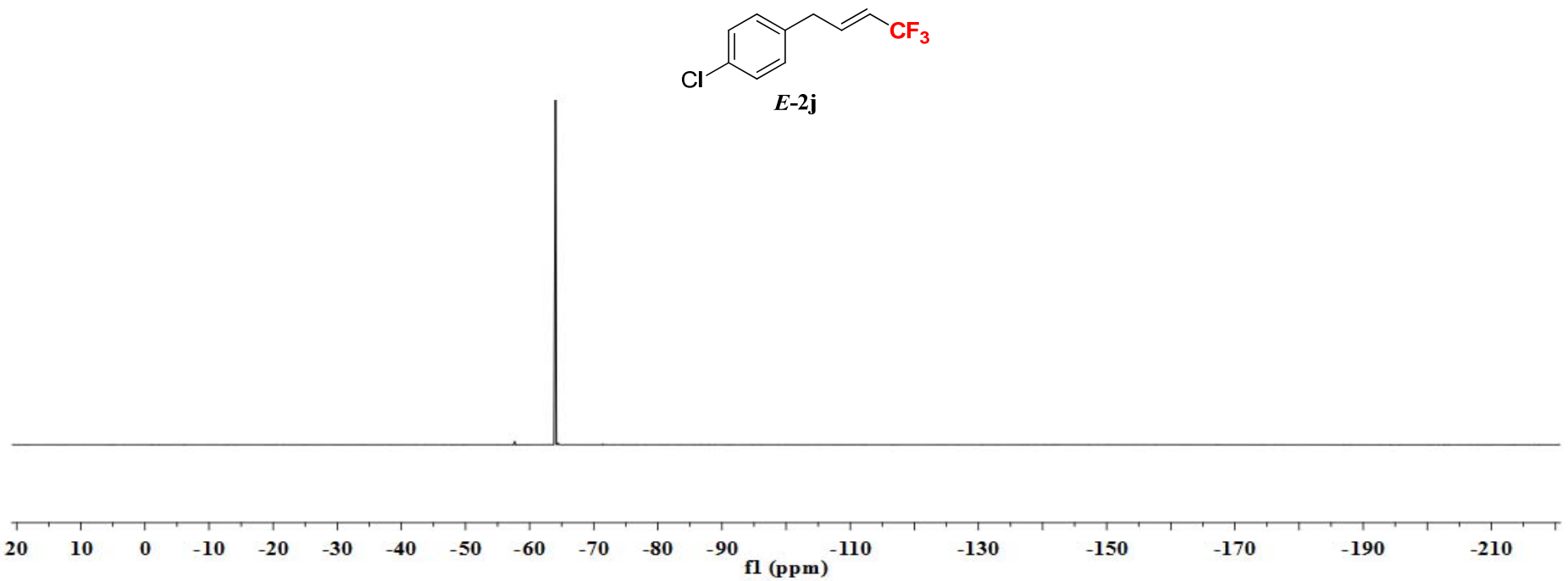


E-2j

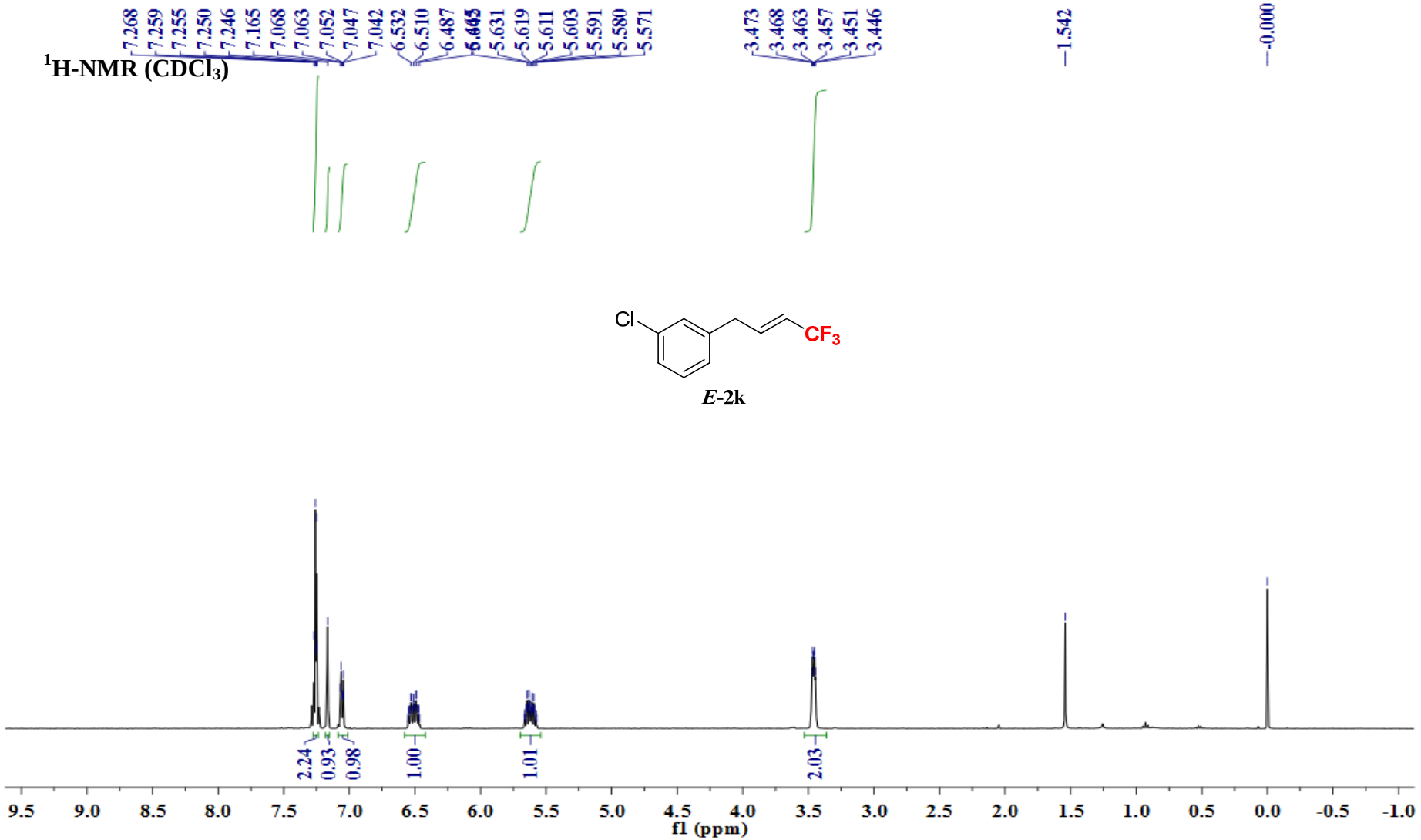
^{13}C-NMR ($CDCl_3$)



^{19}F-NMR ($CDCl_3$)

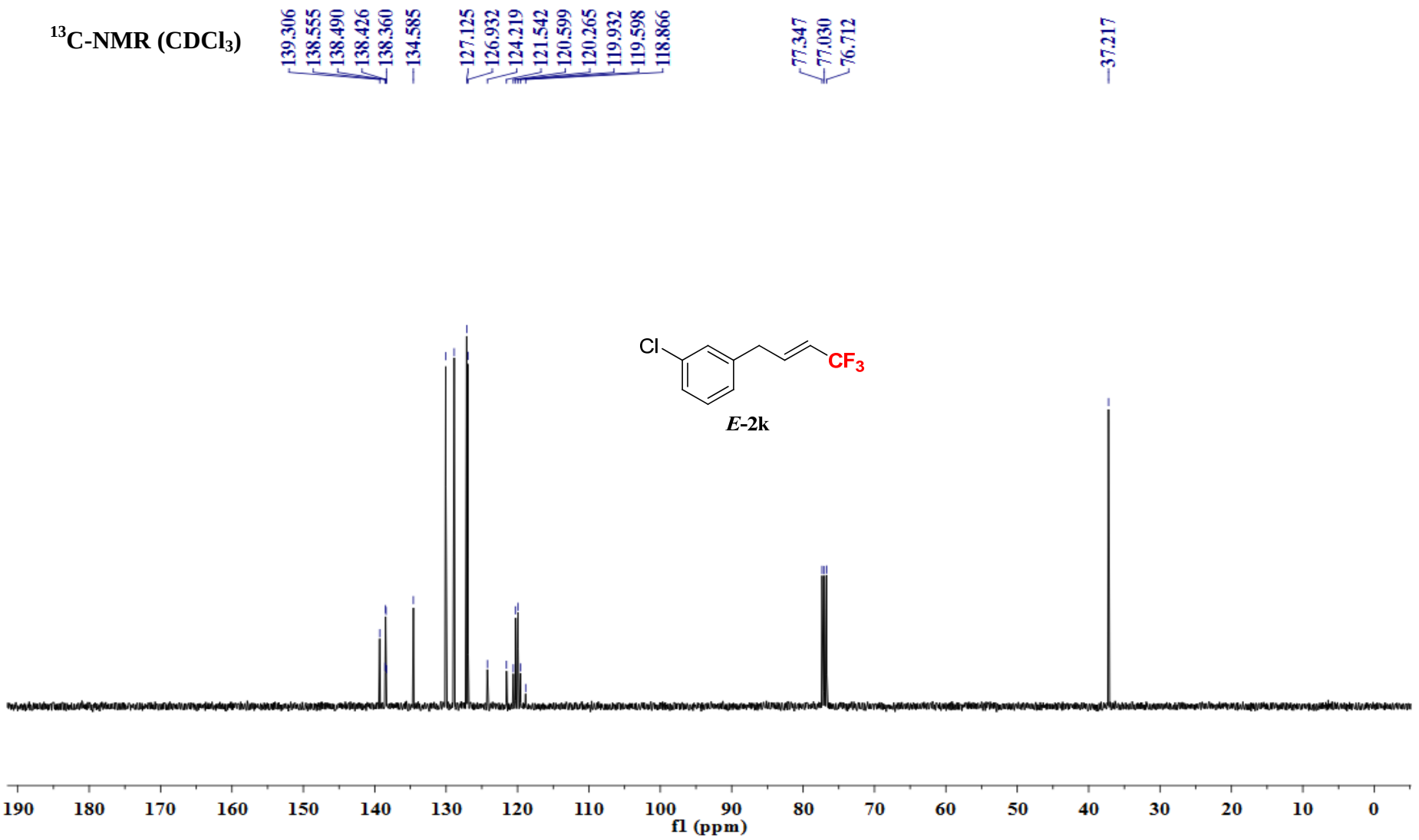


^{1}H-NMR ($CDCl_3$)

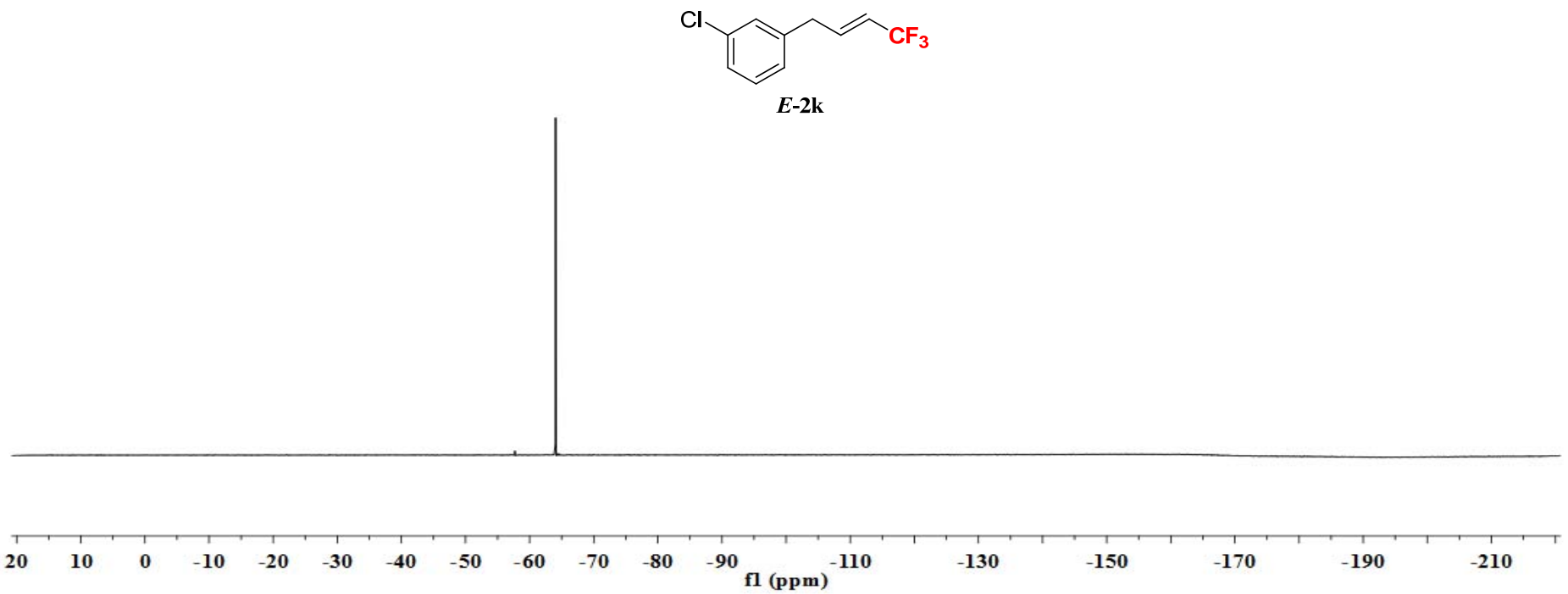


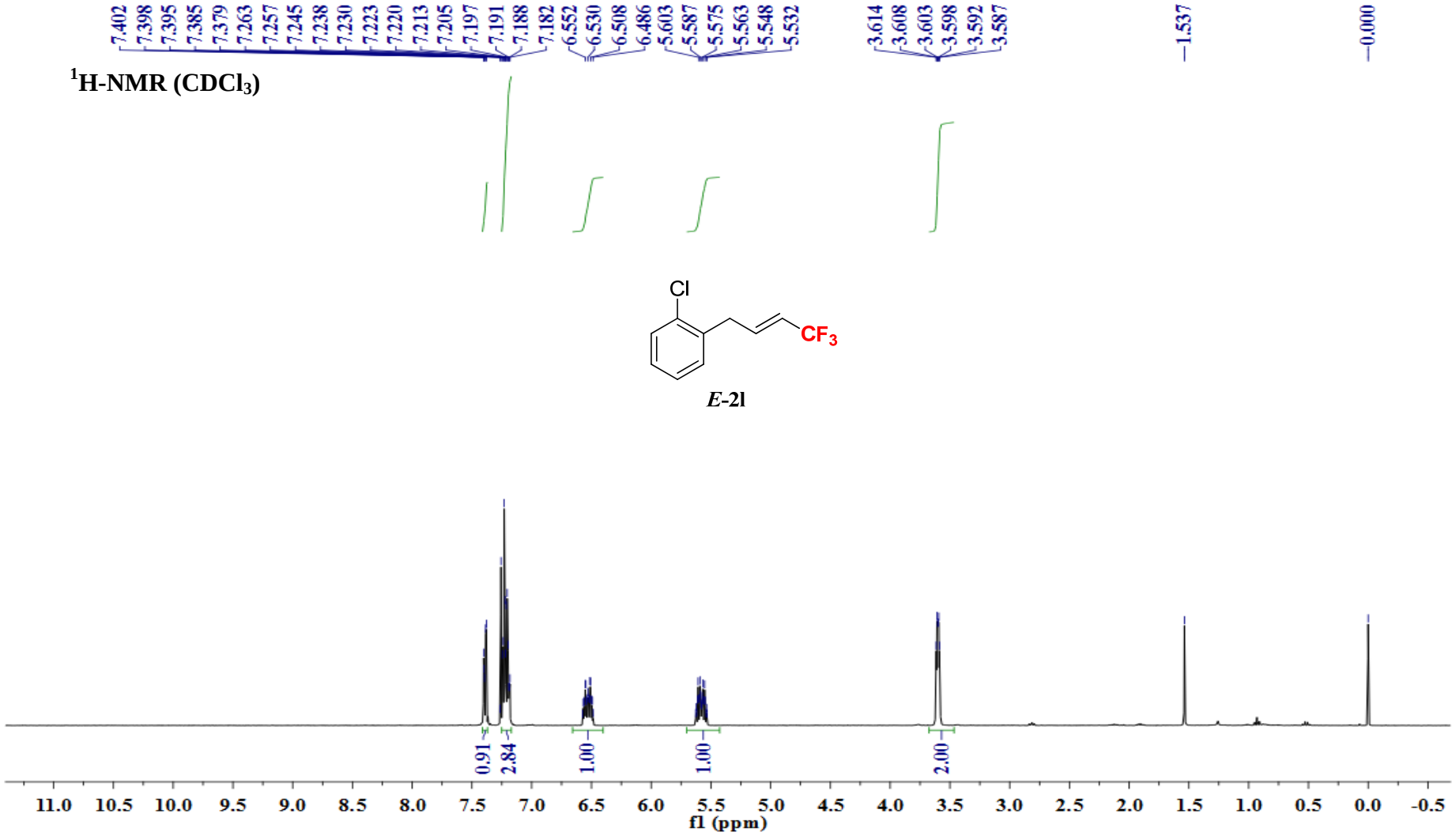
***E*-2k**

^{13}C-NMR ($CDCl_3$)

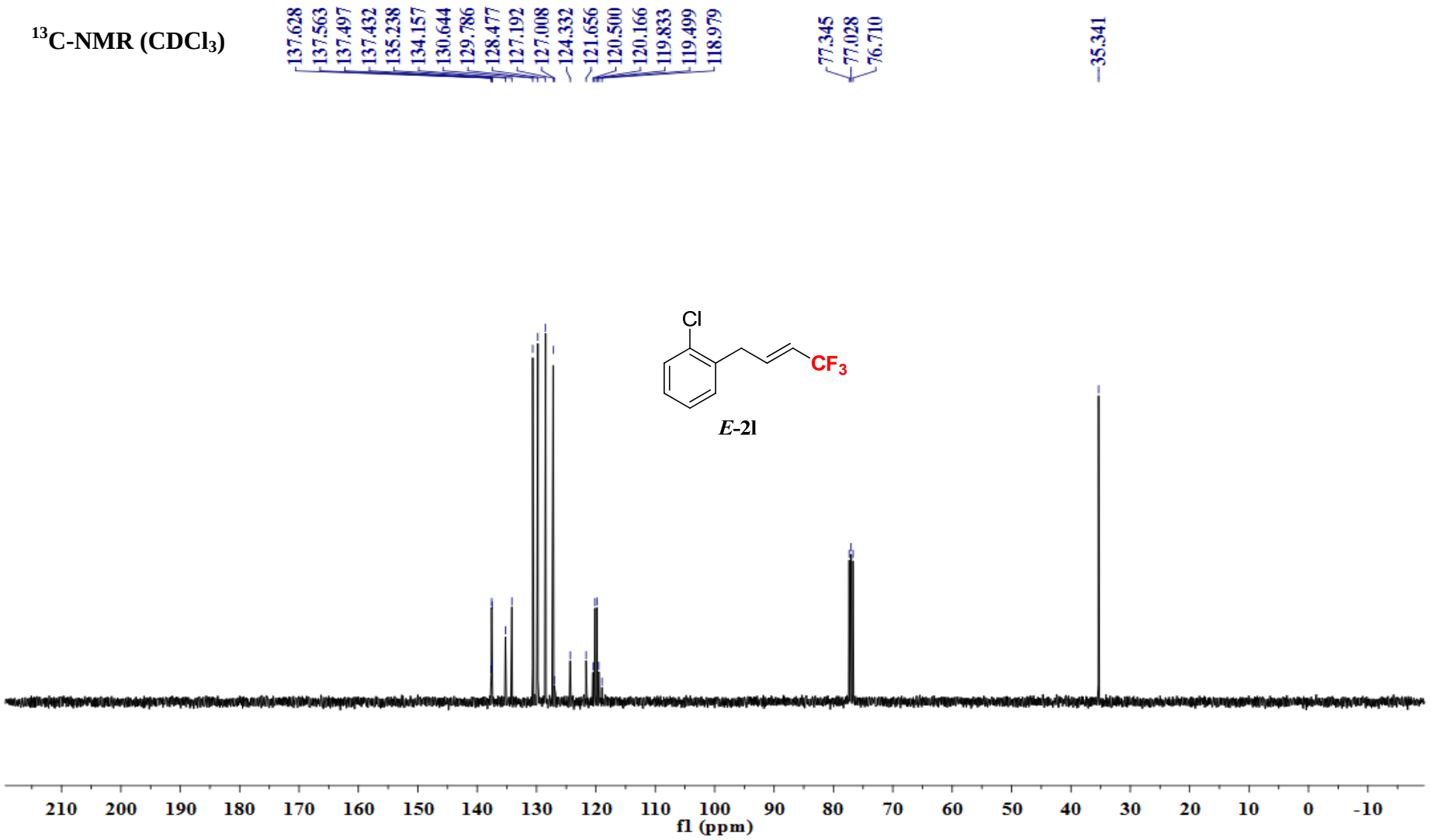


^{19}F-NMR ($CDCl_3$)

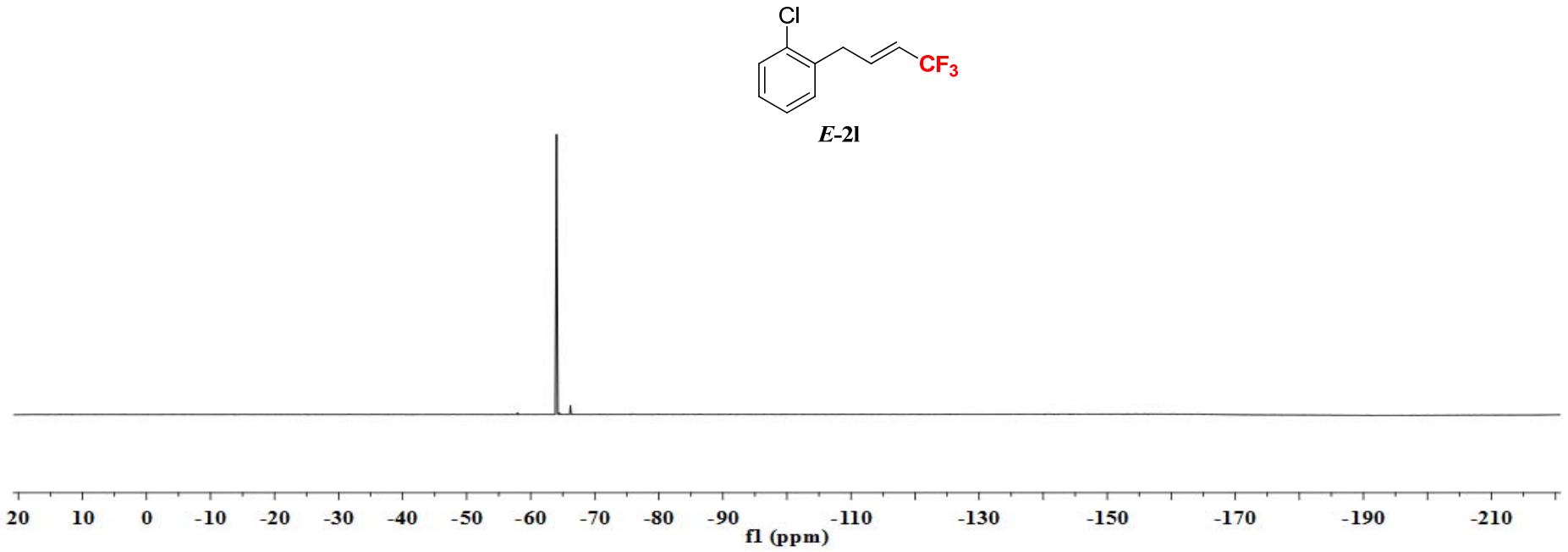



7.402
7.398
7.395
7.385
7.379
7.263
7.257
7.245
7.238
7.230
7.223
7.220
7.213
7.205
7.197
7.191
7.188
7.182
6.552
6.530
6.508
6.486
5.603
5.587
5.575
5.563
5.548
5.532
3.614
3.608
3.603
3.598
3.592
3.587
1.537
0.000
1H-NMR (CDCl3)
Cl
CF3
E-2l
0.91
2.84
1.00
1.00
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

^{13}C-NMR ($CDCl_3$)

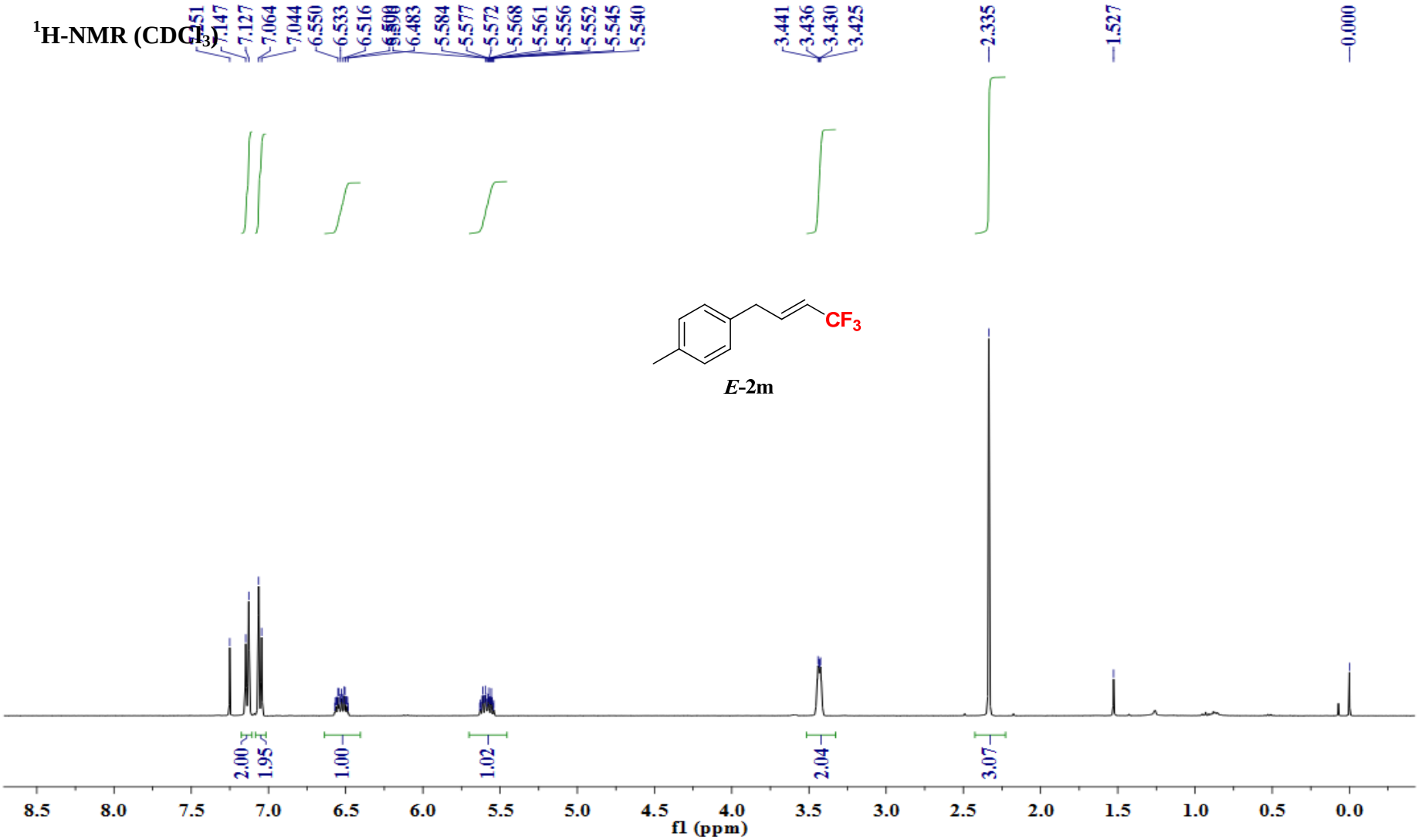


^{19}F-NMR ($CDCl_3$)



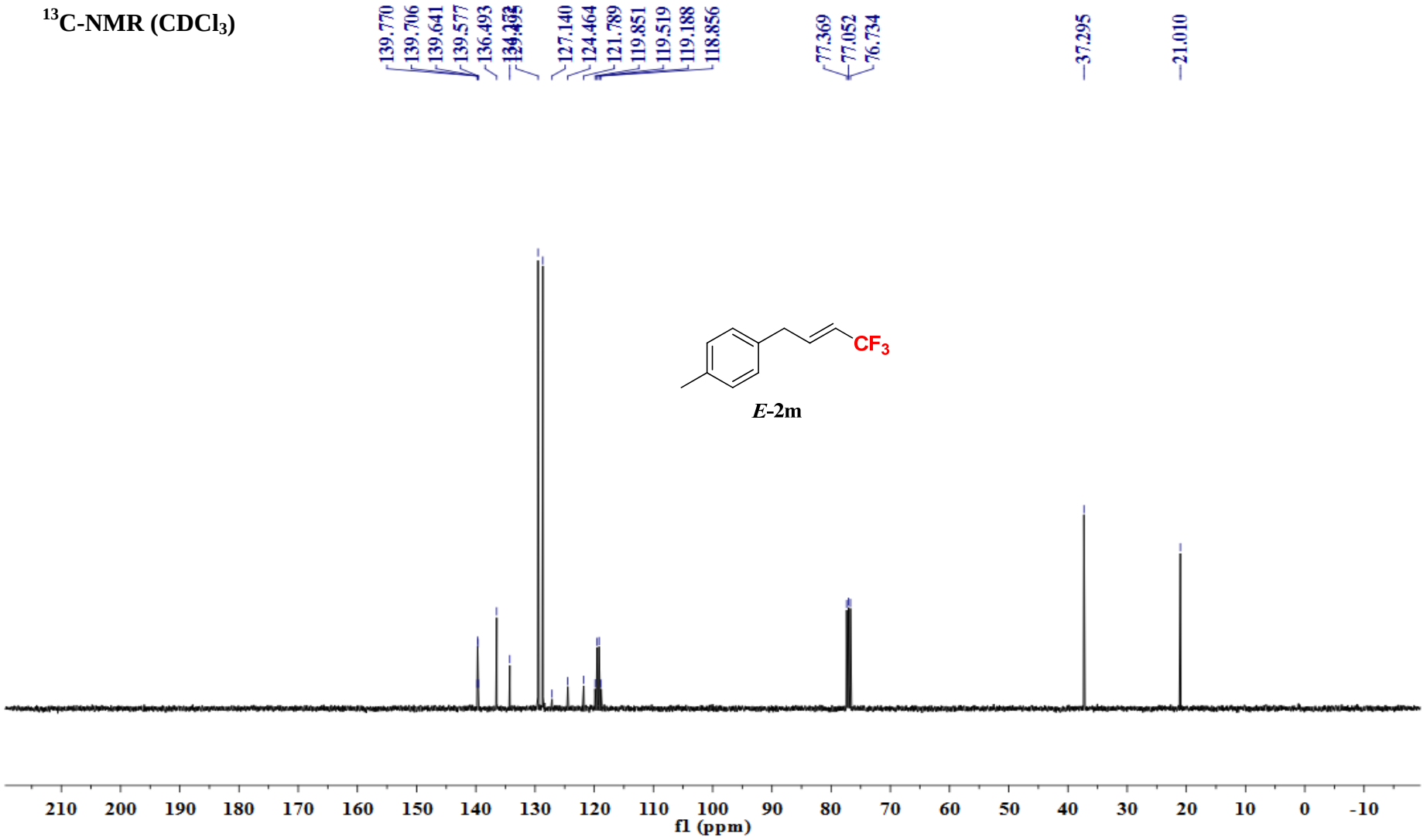
***E*-2l**

^{1}H-NMR ($CDCl_3$)



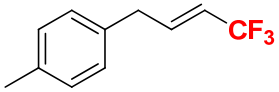
***E*-2m**

^{13}C-NMR ($CDCl_3$)

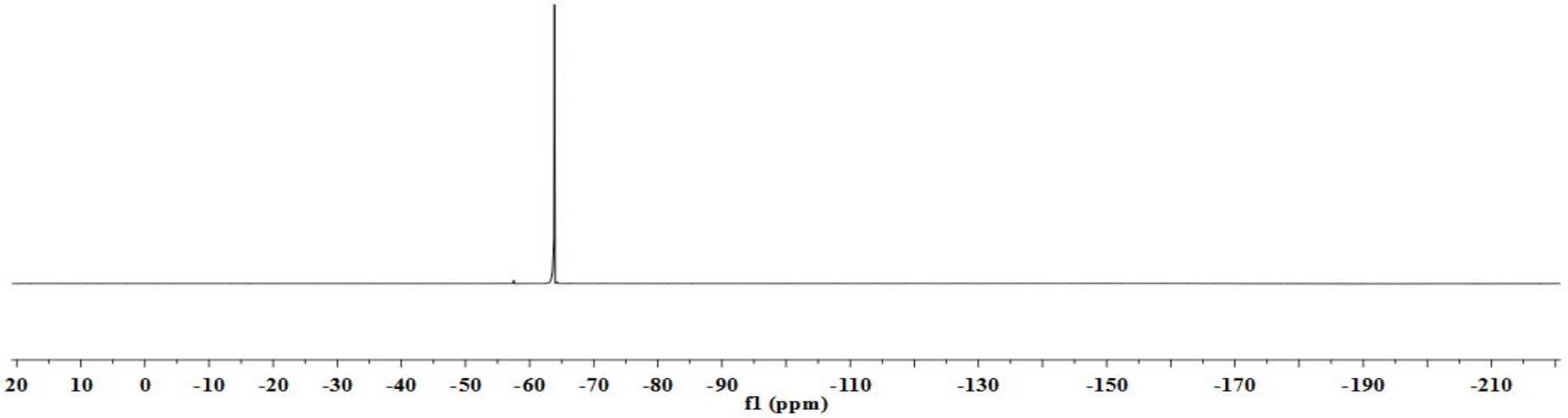


***E*-2m**

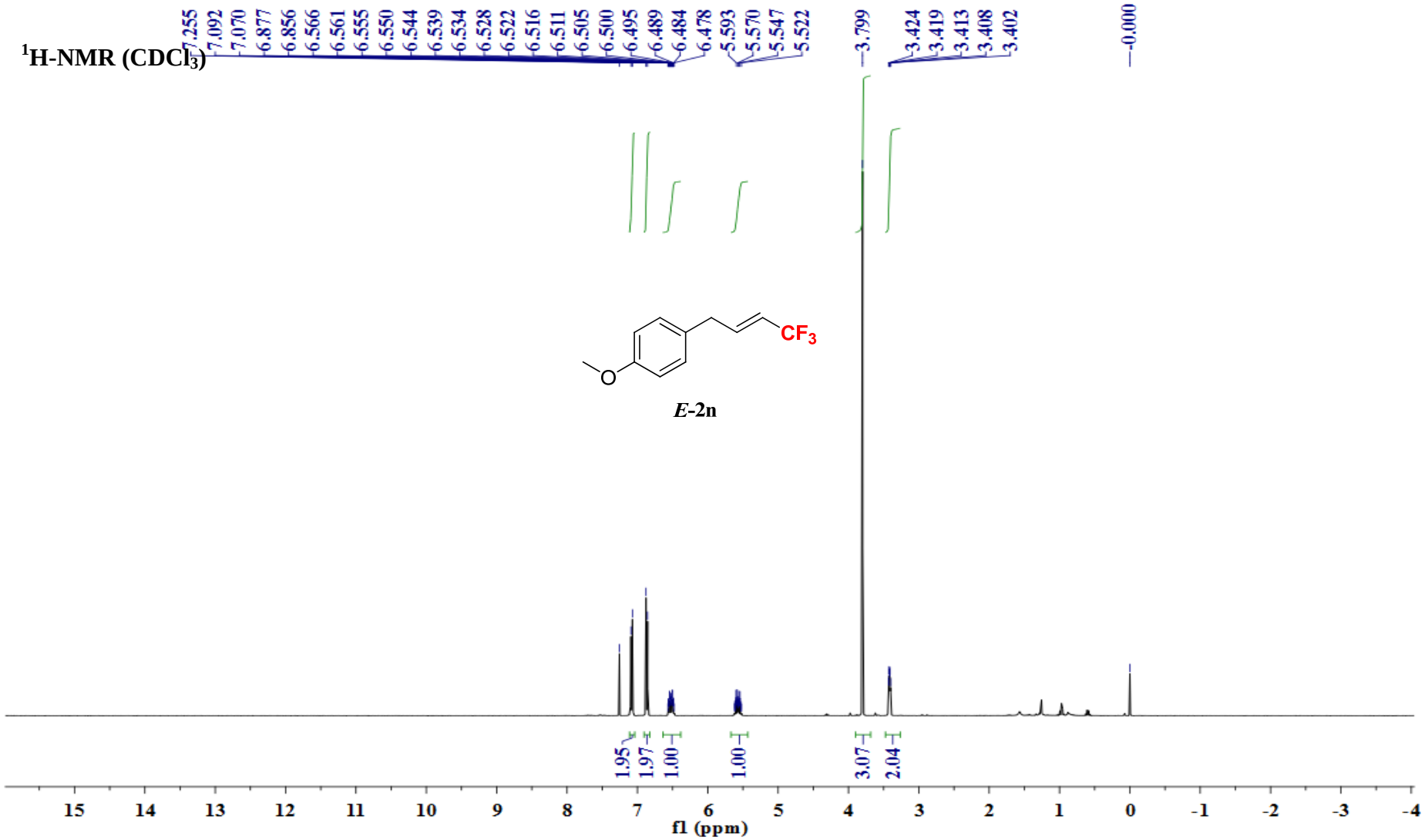
^{19}F-NMR ($CDCl_3$)



***E*-2m**



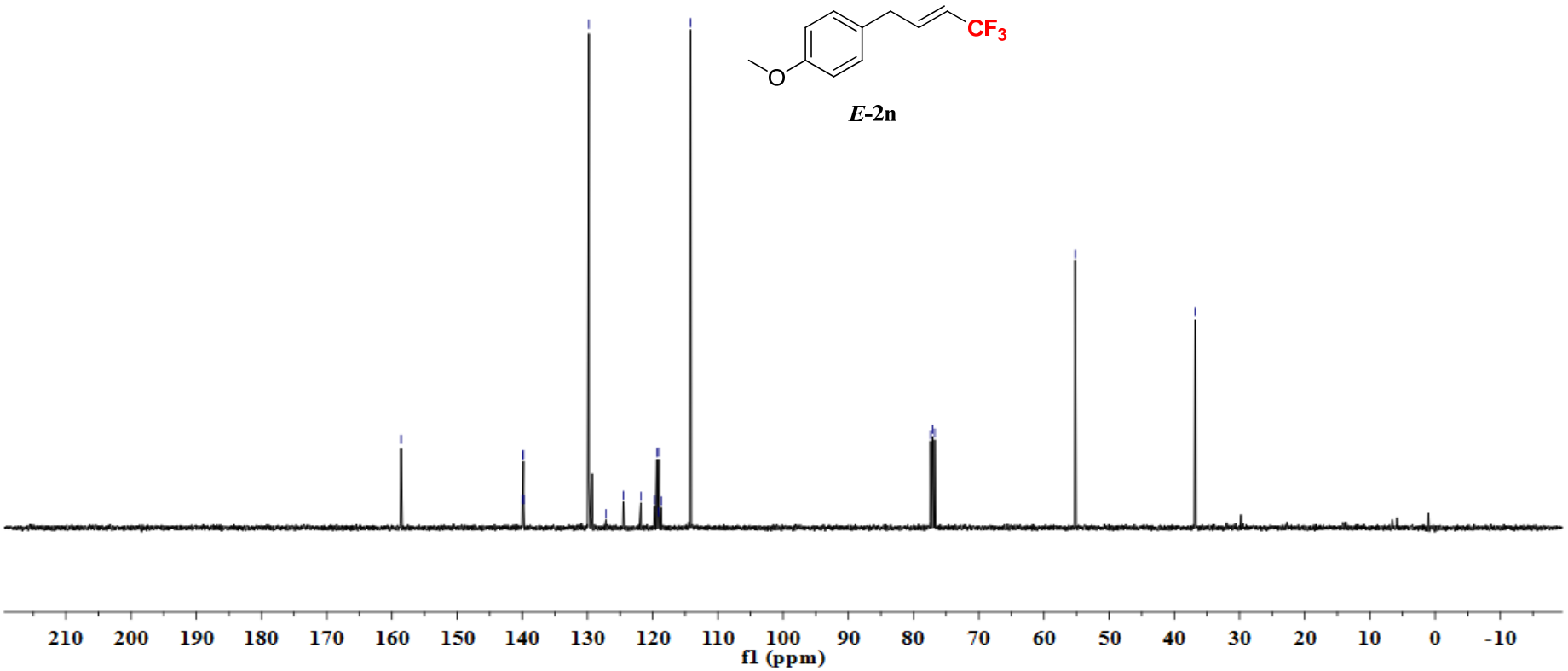
^{1}H-NMR ($CDCl_3$)



***E*-2n**

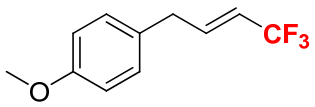
^{13}C-NMR ($CDCl_3$)

158.585
139.900
139.836
139.772
129.779
119.699
119.135
118.705
114.200
77.379
77.061
76.742
55.206
36.804

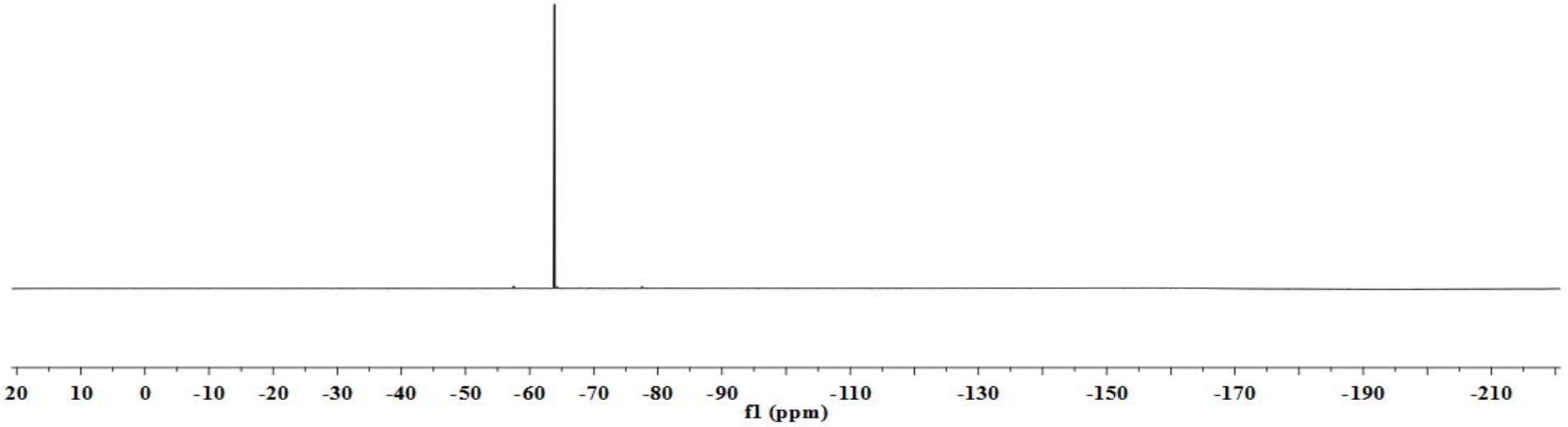


***E*-2n**

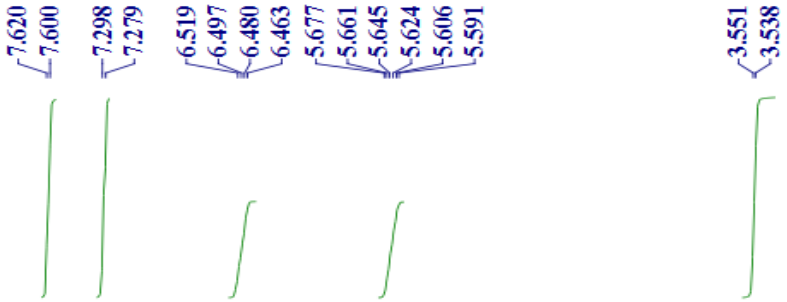
^{19}F-NMR ($CDCl_3$)

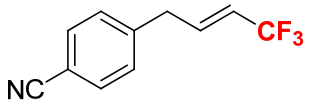


***E*-2n**

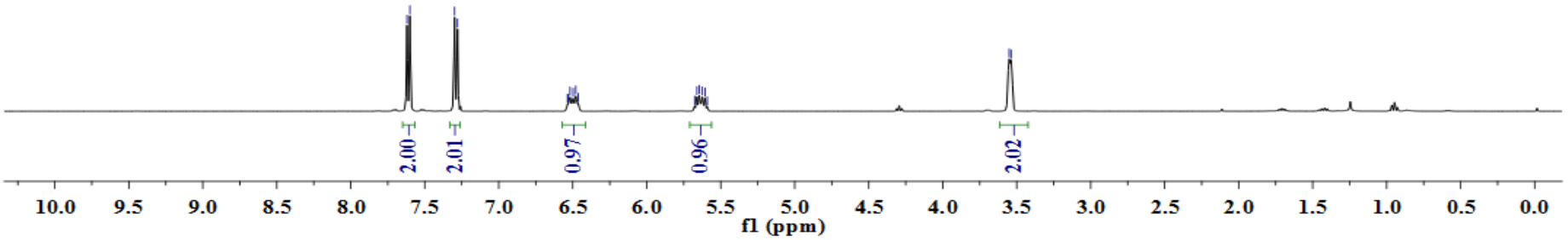


^{1}H-NMR ($CDCl_3$)

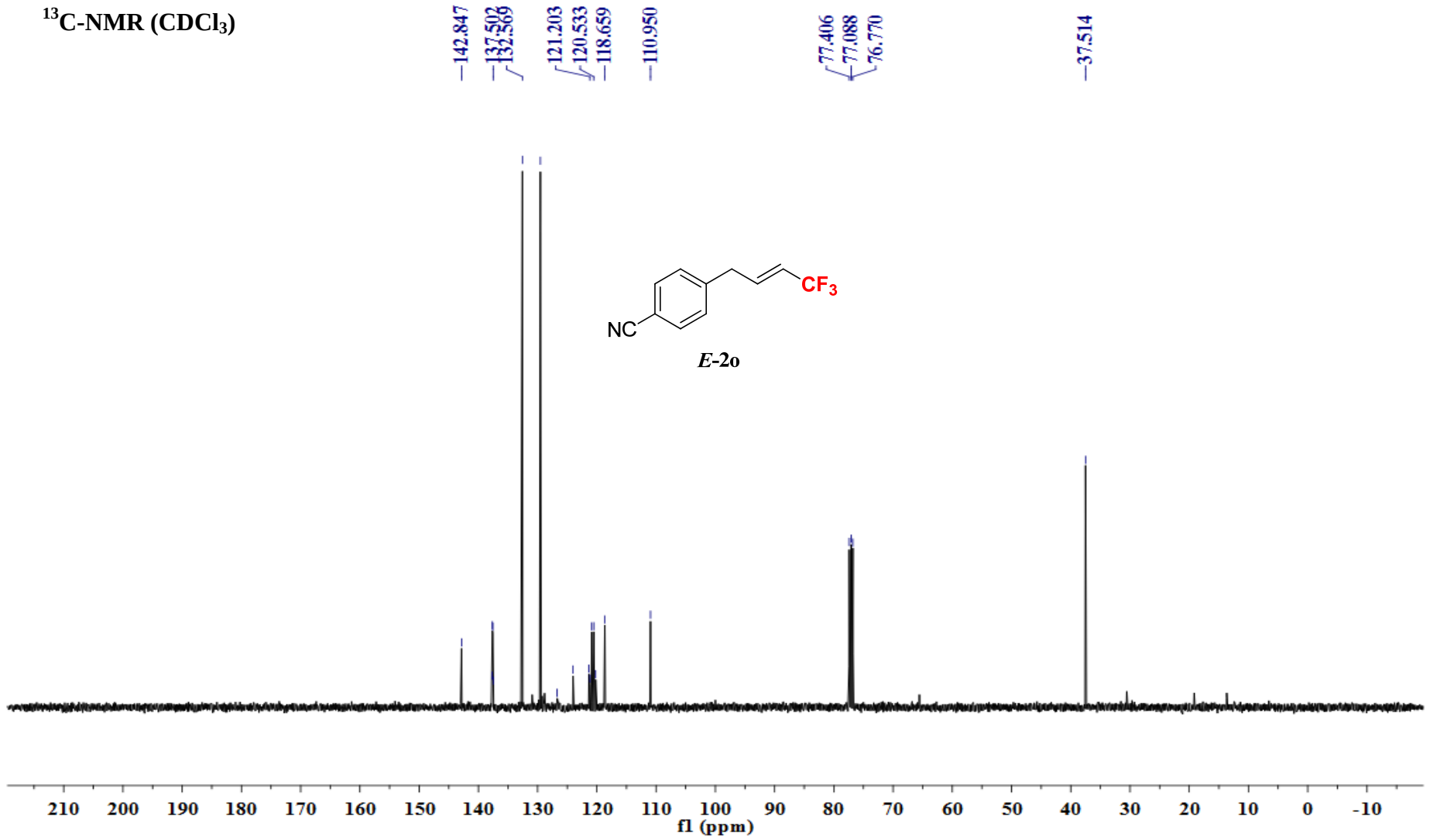




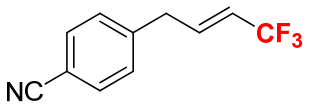
***E*-2o**



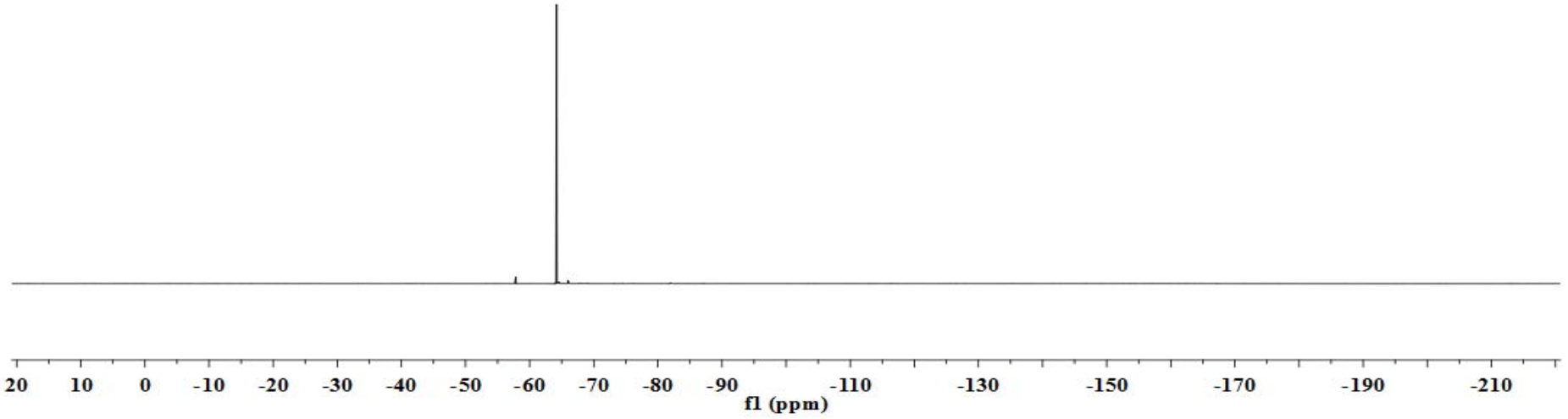
^{13}C-NMR ($CDCl_3$)



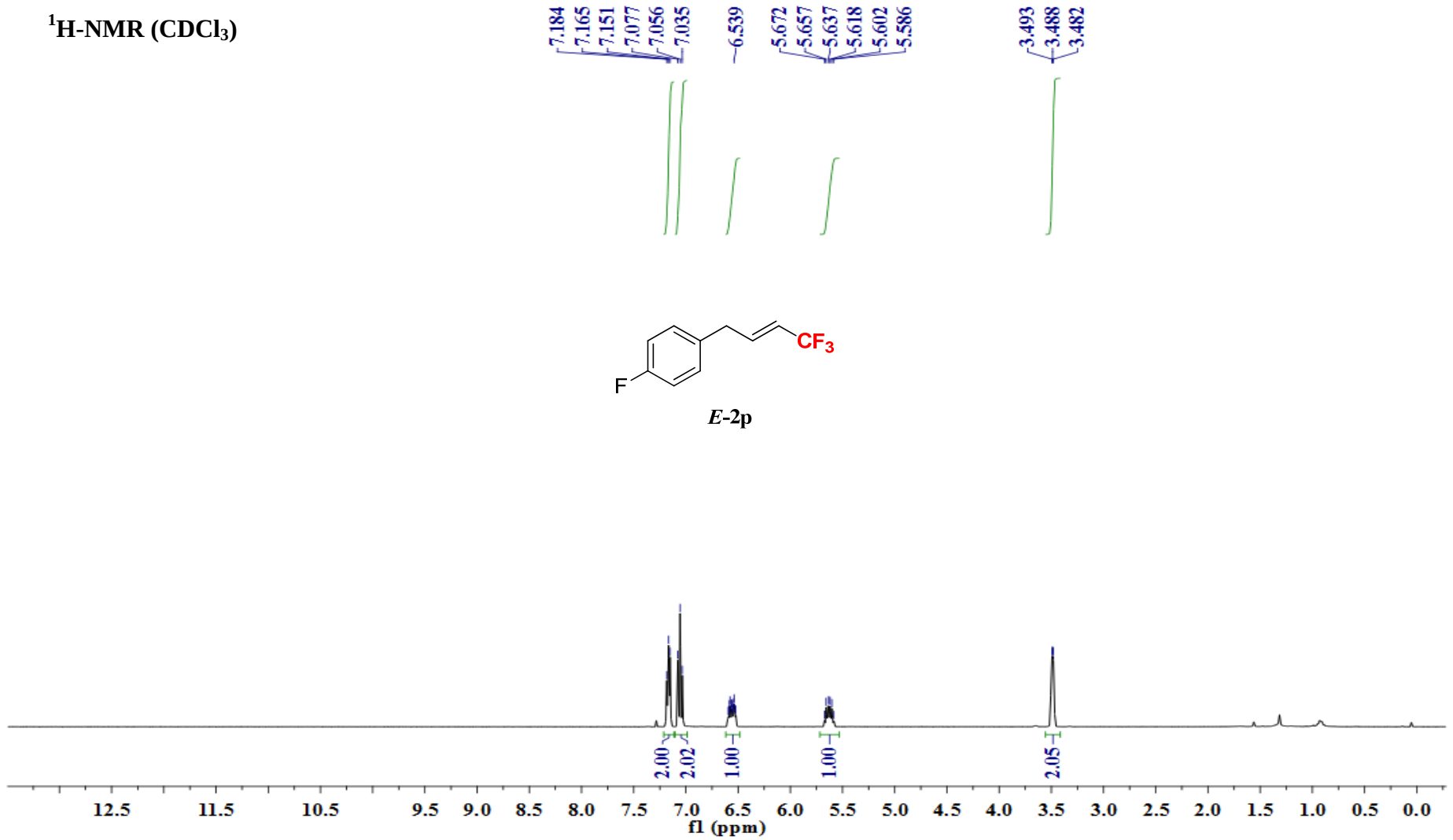
^{19}F-NMR ($CDCl_3$)



***E*-2o**

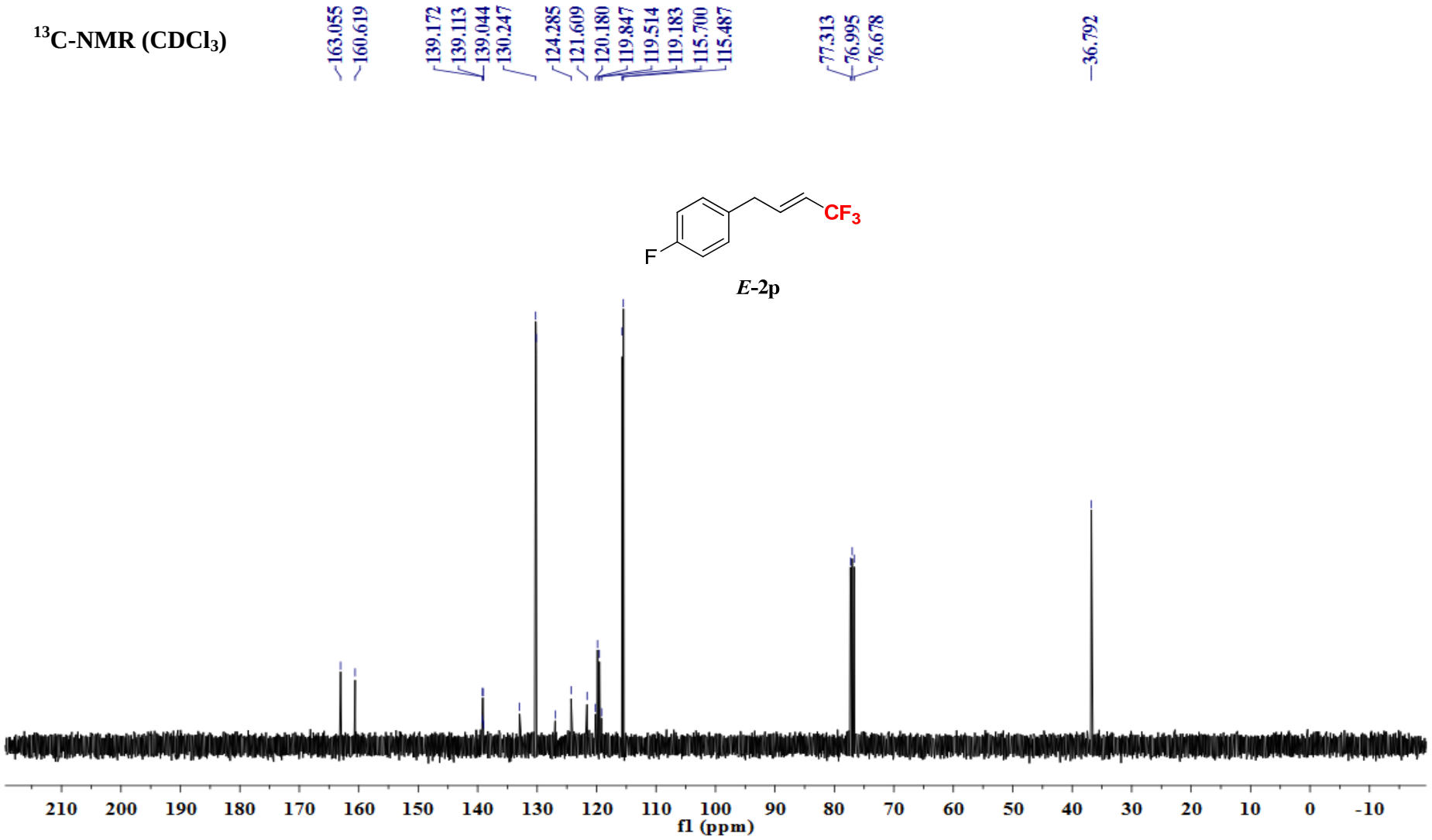


^{1}H-NMR ($CDCl_3$)



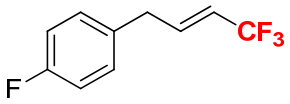
***E*-2p**

^{13}C-NMR ($CDCl_3$)

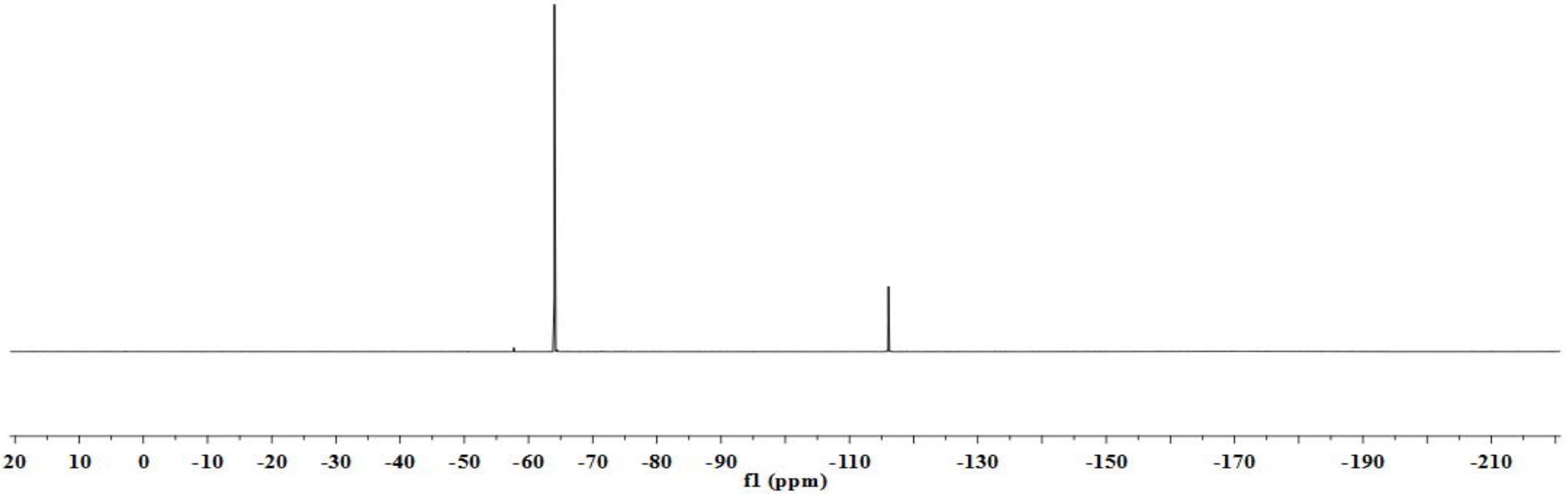


E-2p

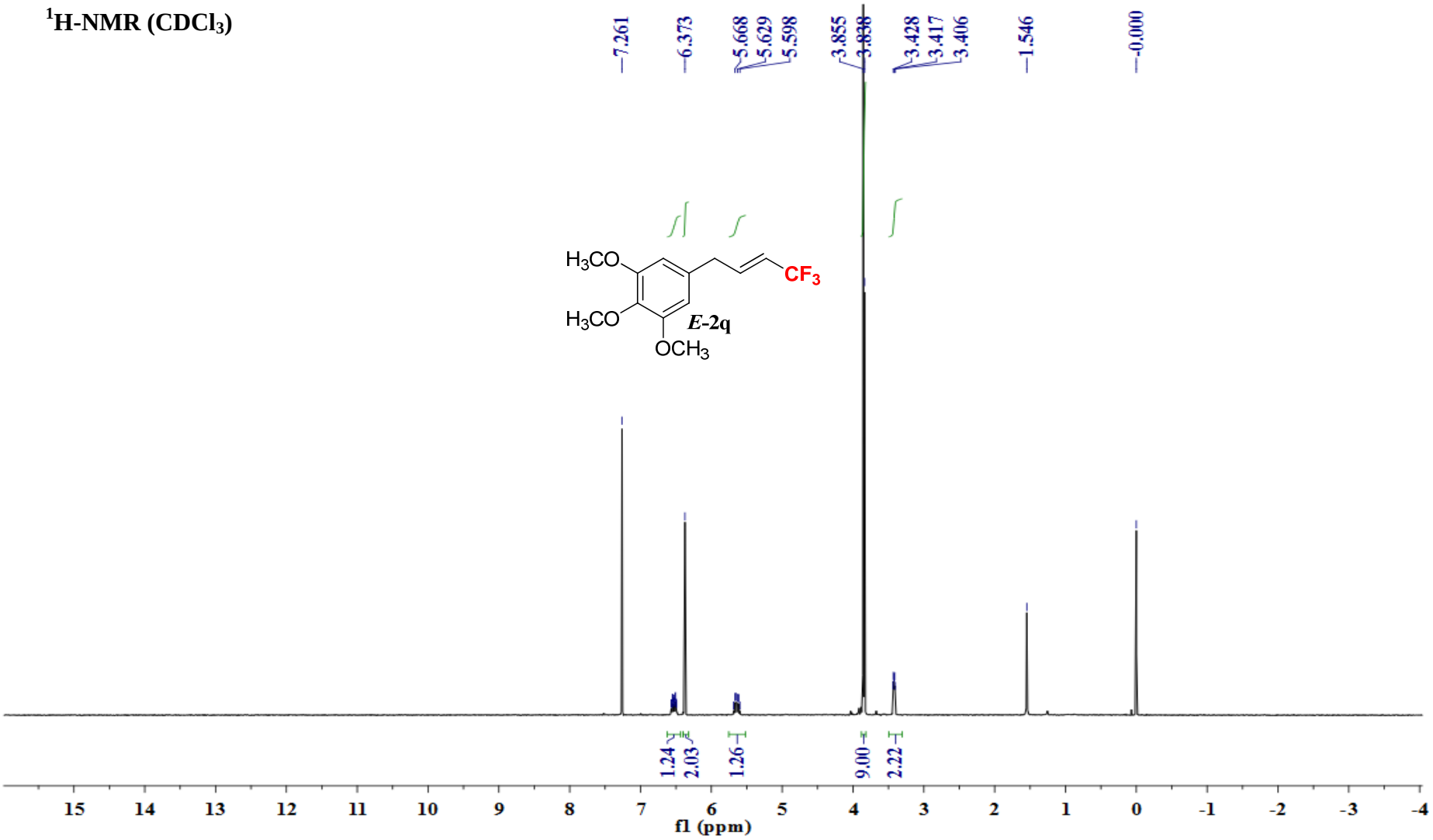
^{19}F-NMR ($CDCl_3$)



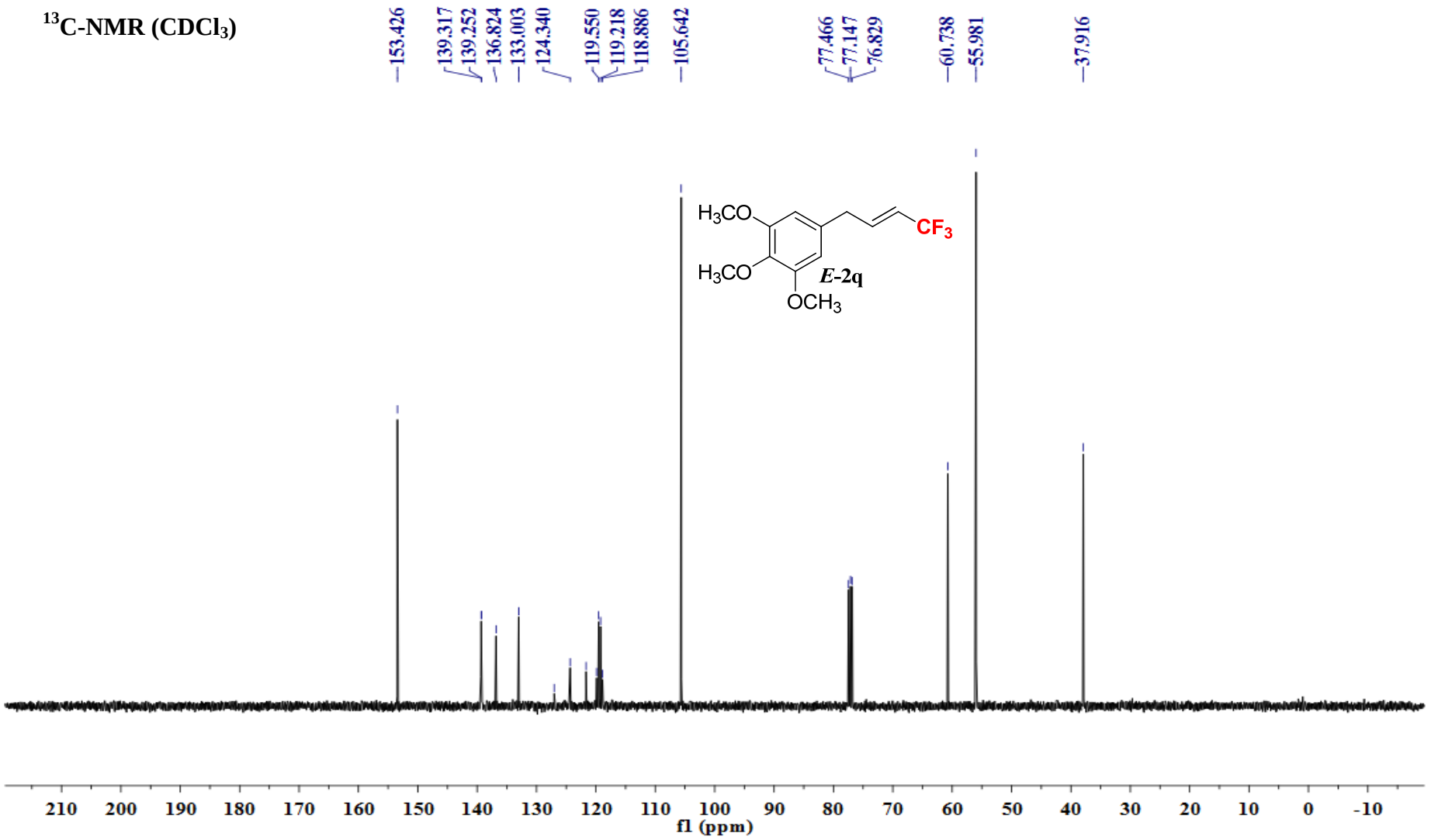
***E*-2p**



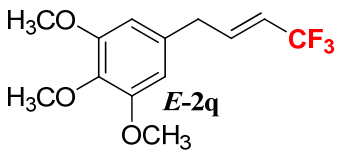
^{1}H-NMR ($CDCl_3$)


7.261
6.373
5.668
5.629
5.598
3.855
3.838
3.428
3.417
3.406
1.546
0.000
H3CO
H3CO
OCH3
CF3
E-2q
1.24
2.03
1.26
9.00
2.22
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

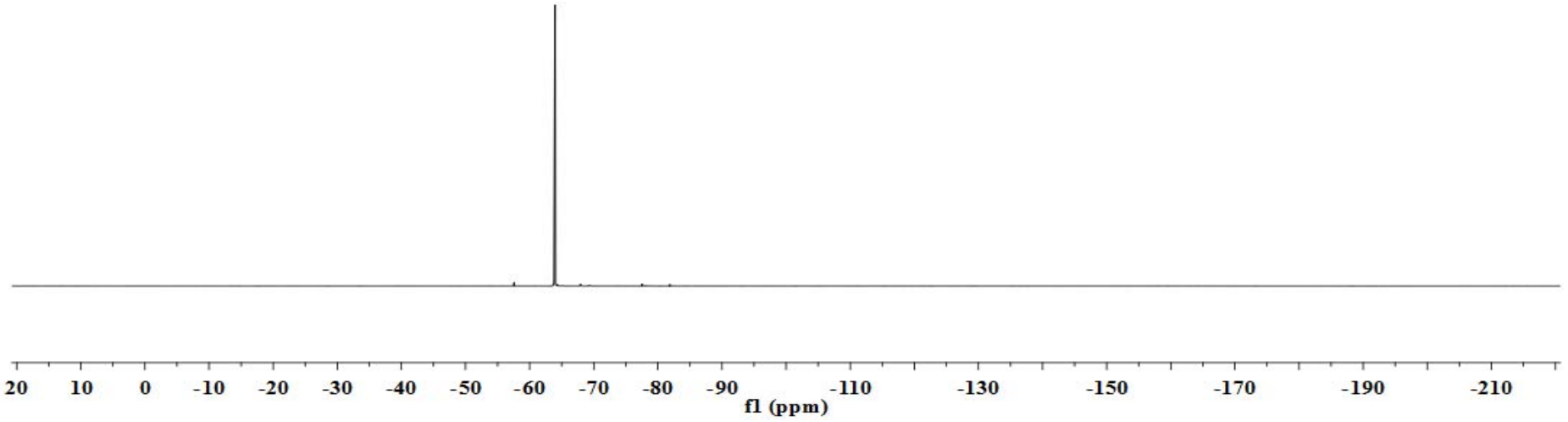
^{13}C-NMR ($CDCl_3$)



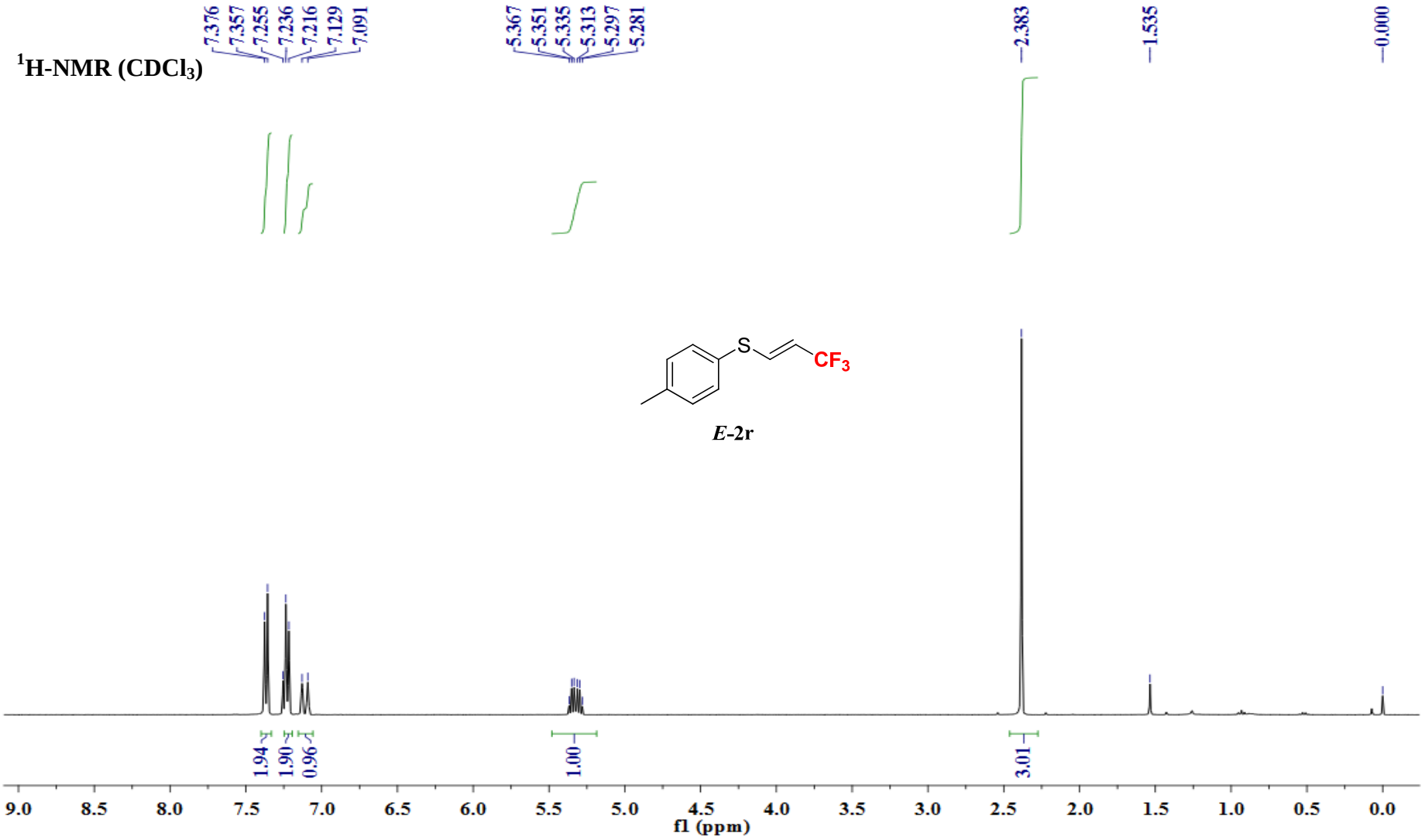
^{19}F-NMR ($CDCl_3$)



***E*-2q**

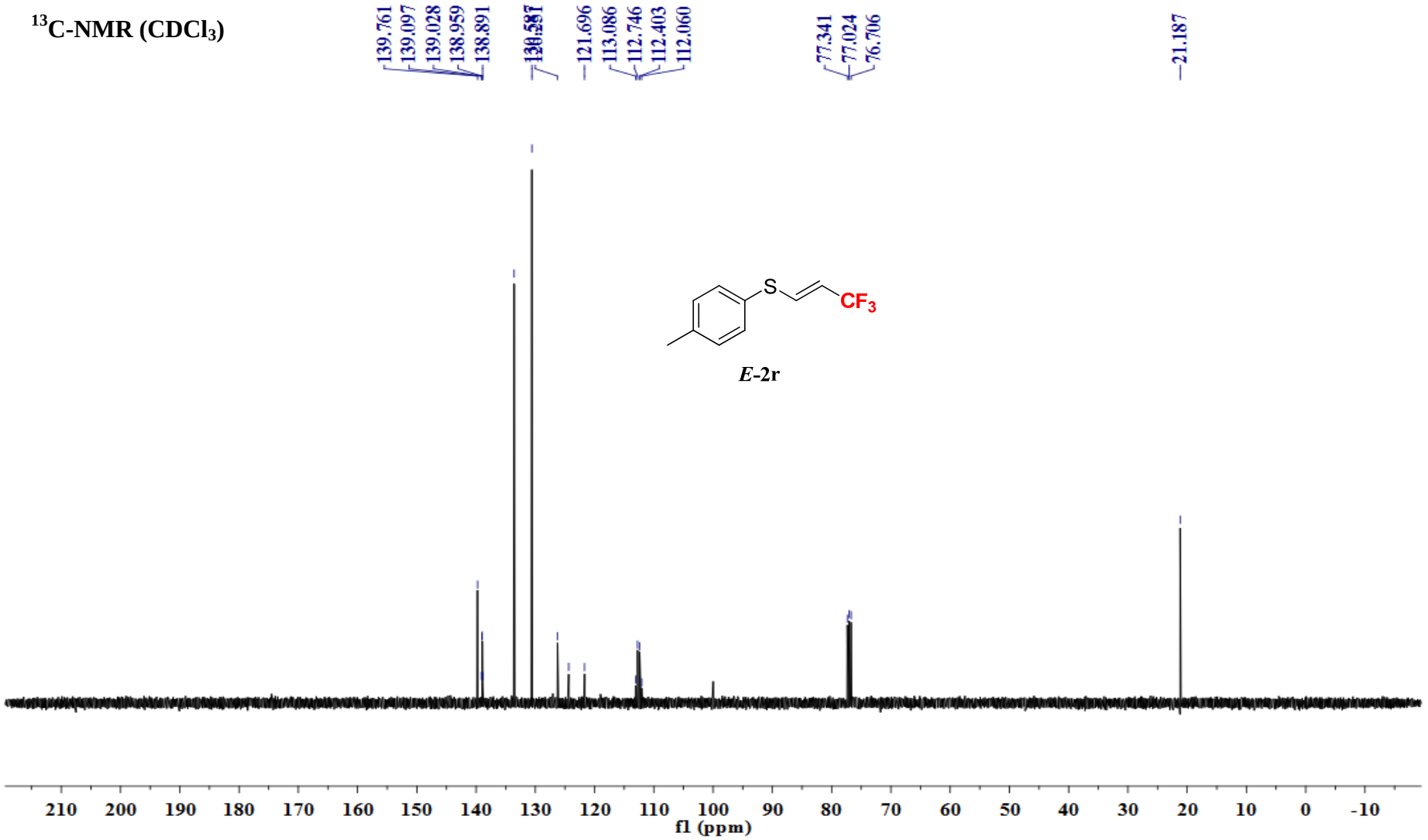


^{1}H-NMR ($CDCl_3$)



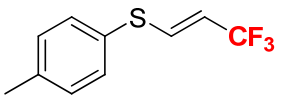
***E*-2r**

^{13}C-NMR ($CDCl_3$)

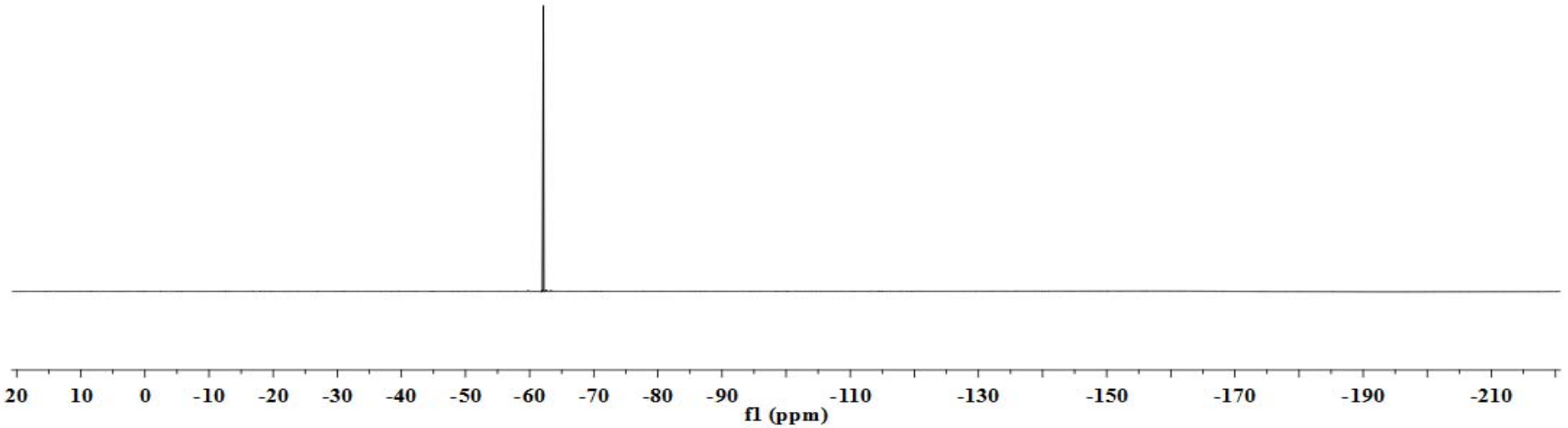


***E*-2r**

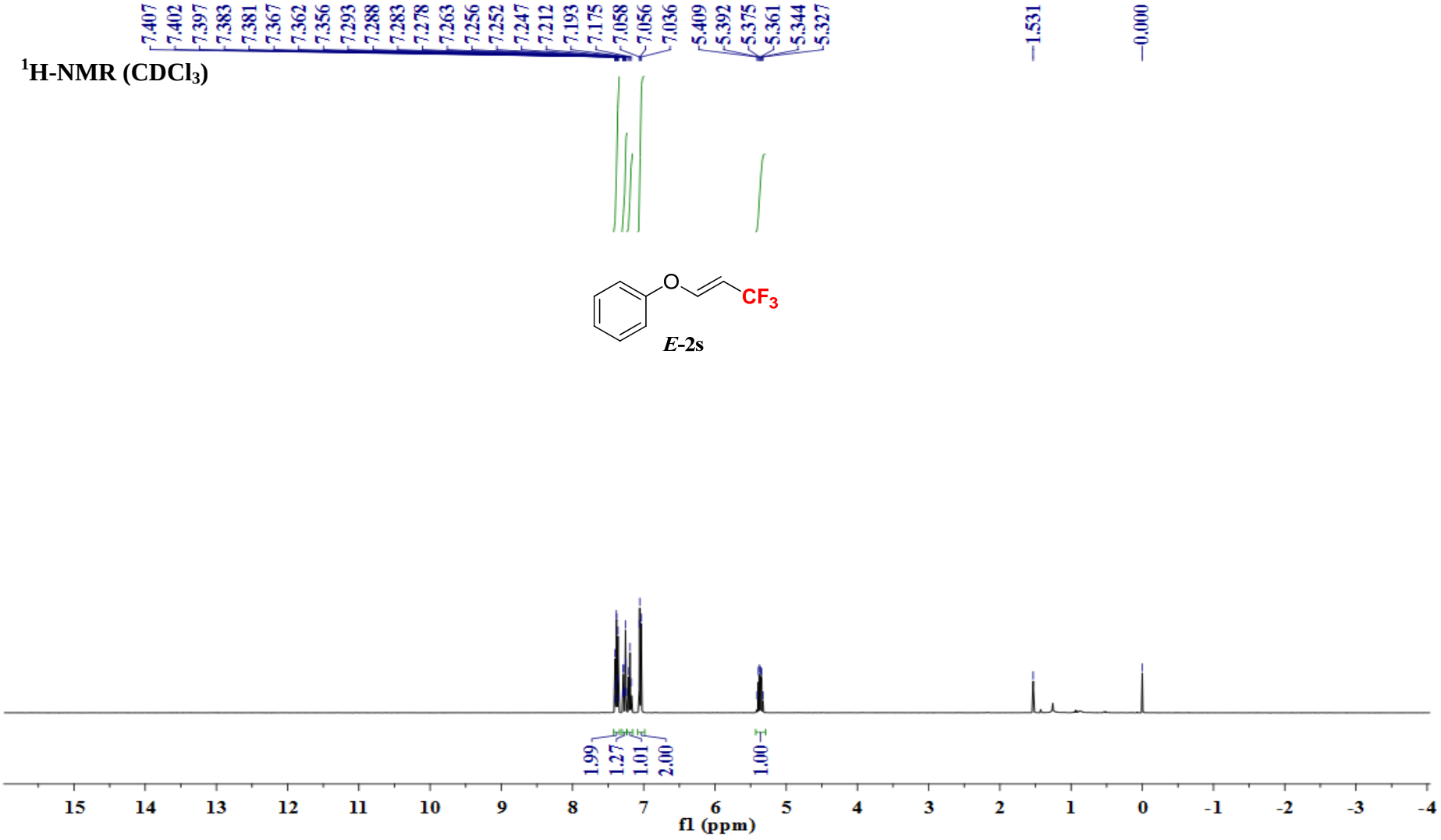
^{19}F-NMR ($CDCl_3$)



***E*-2r**



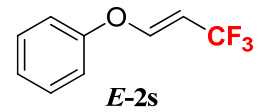
^{1}H-NMR ($CDCl_3$)



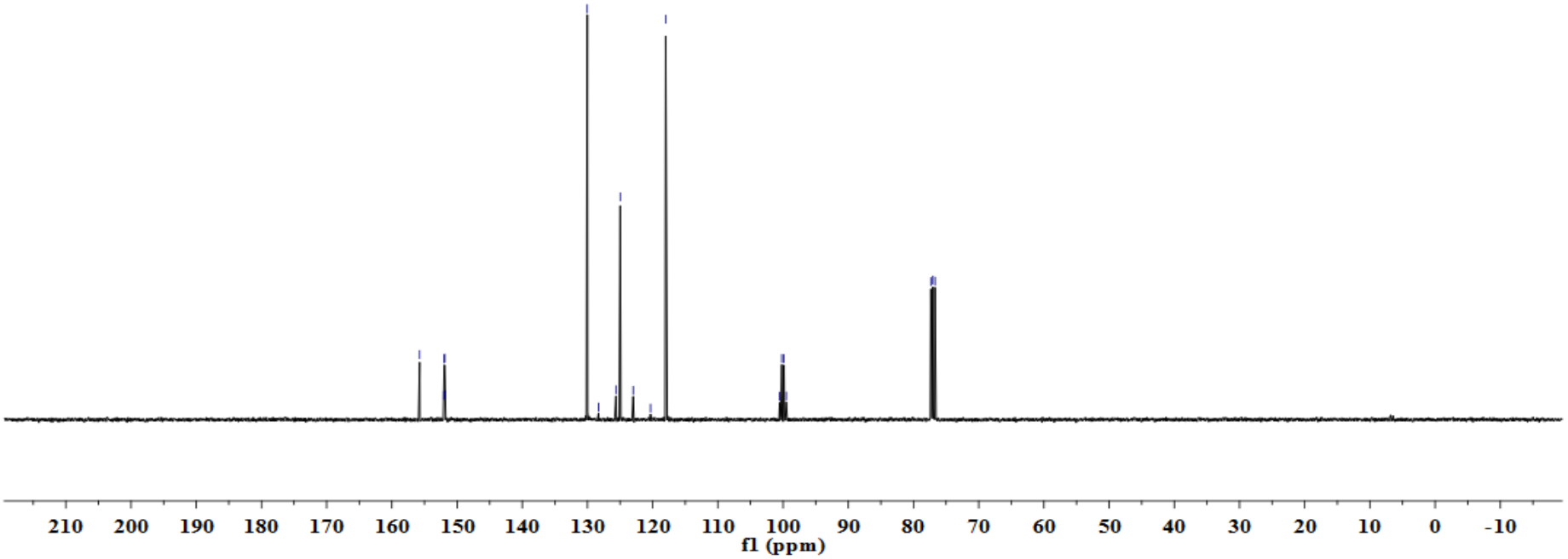
E-2s

^{13}C-NMR ($CDCl_3$)

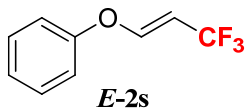
155.742
152.048
151.969
151.891
151.814
130.030
128.291
125.638
124.973
122.986
120.334
118.013
100.535
100.198
99.861
99.524
77.330
77.012
76.694



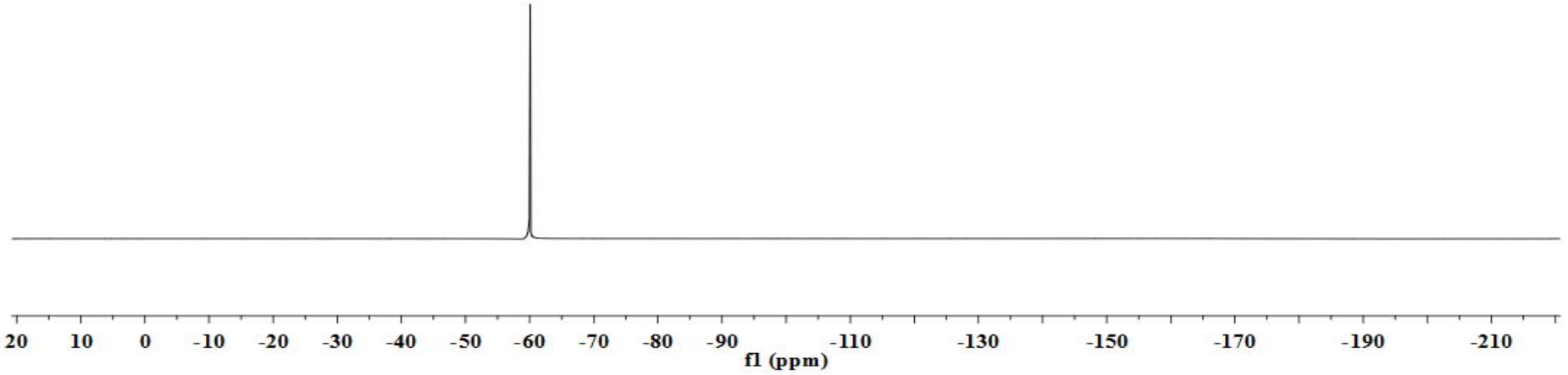
***E*-2s**



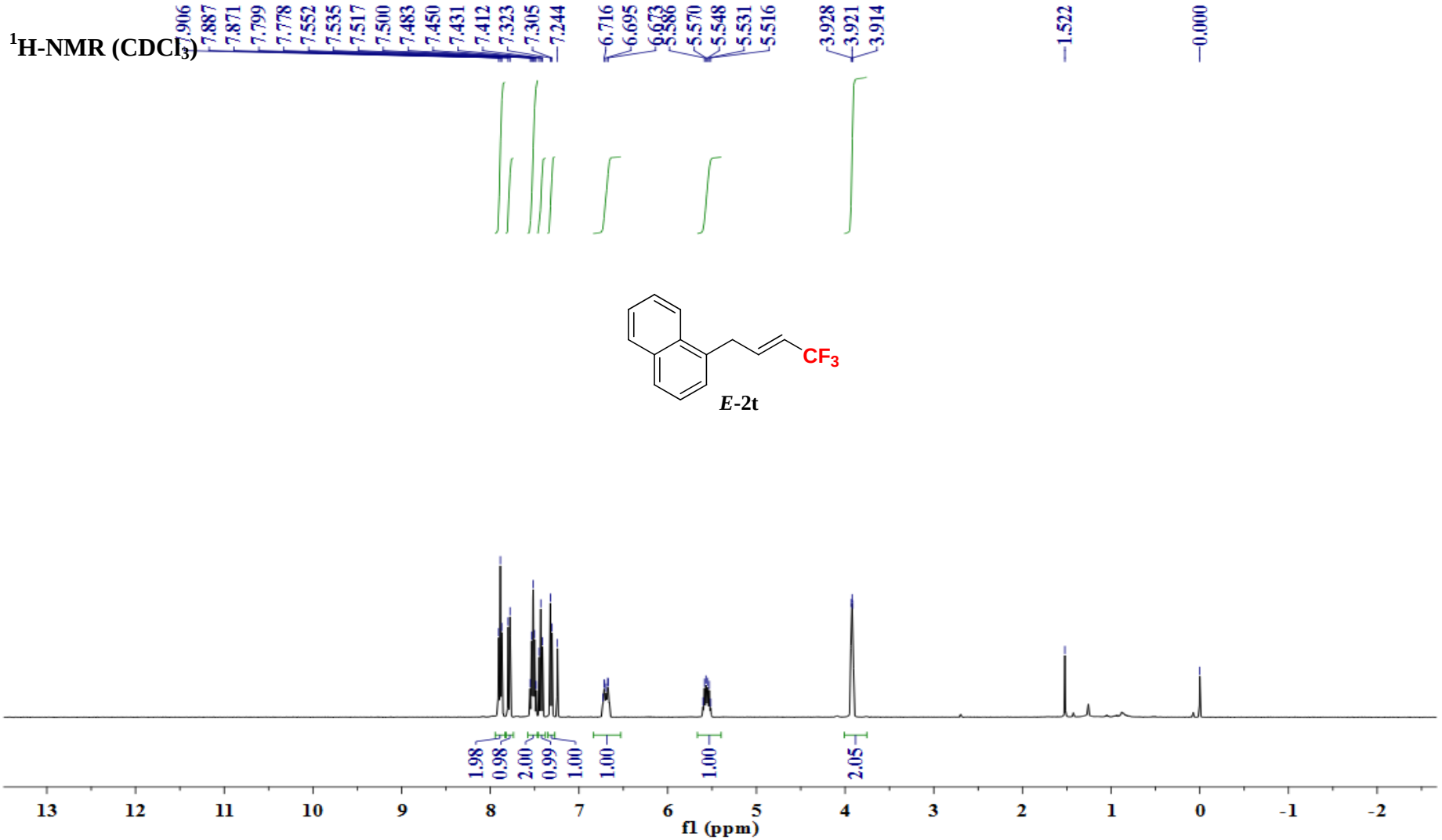
^{19}F-NMR ($CDCl_3$)



***E*-2s**

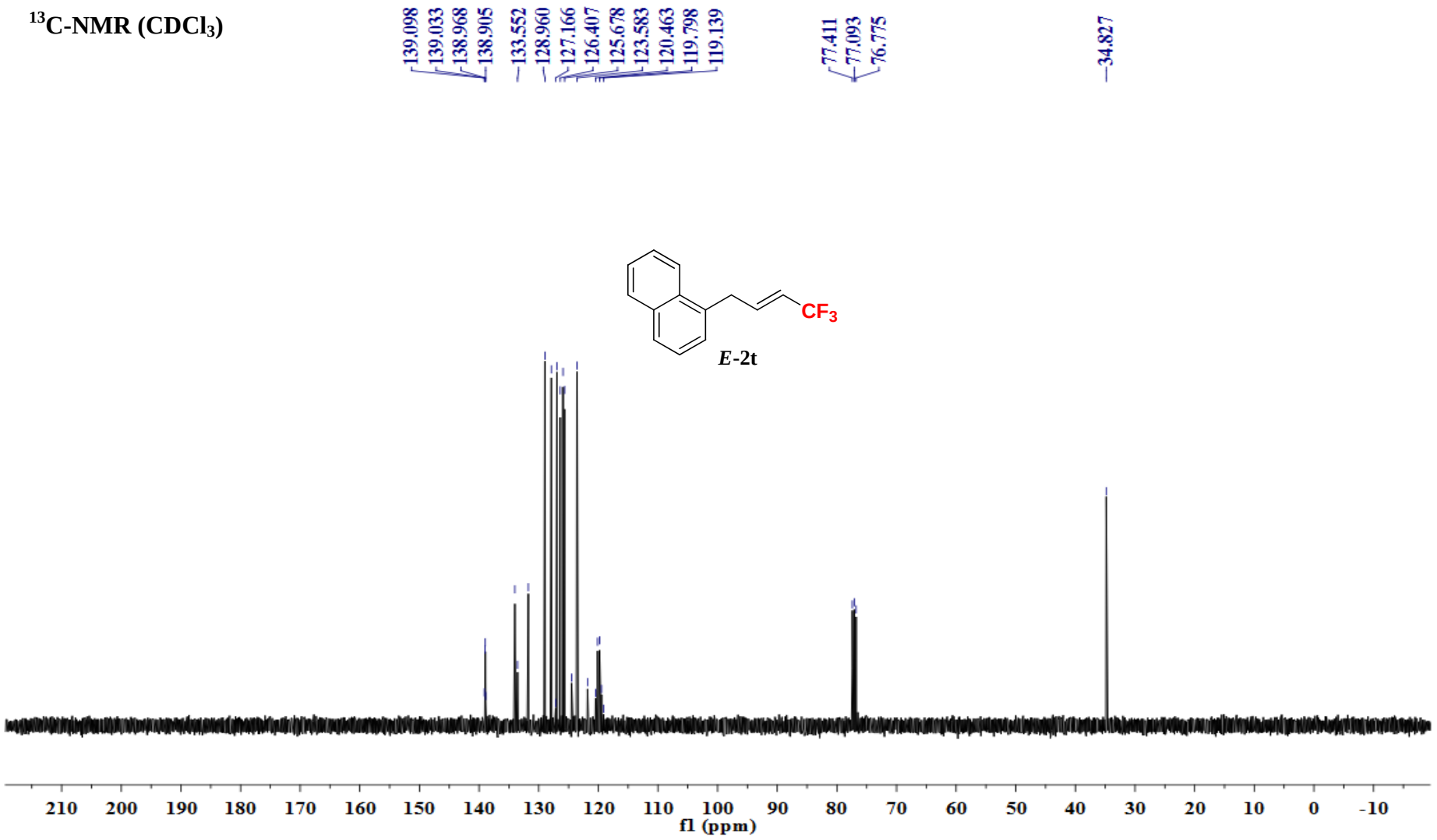


^{1}H-NMR ($CDCl_3$)

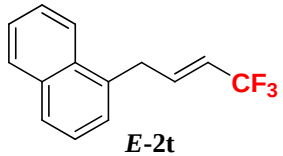


***E*-2t**

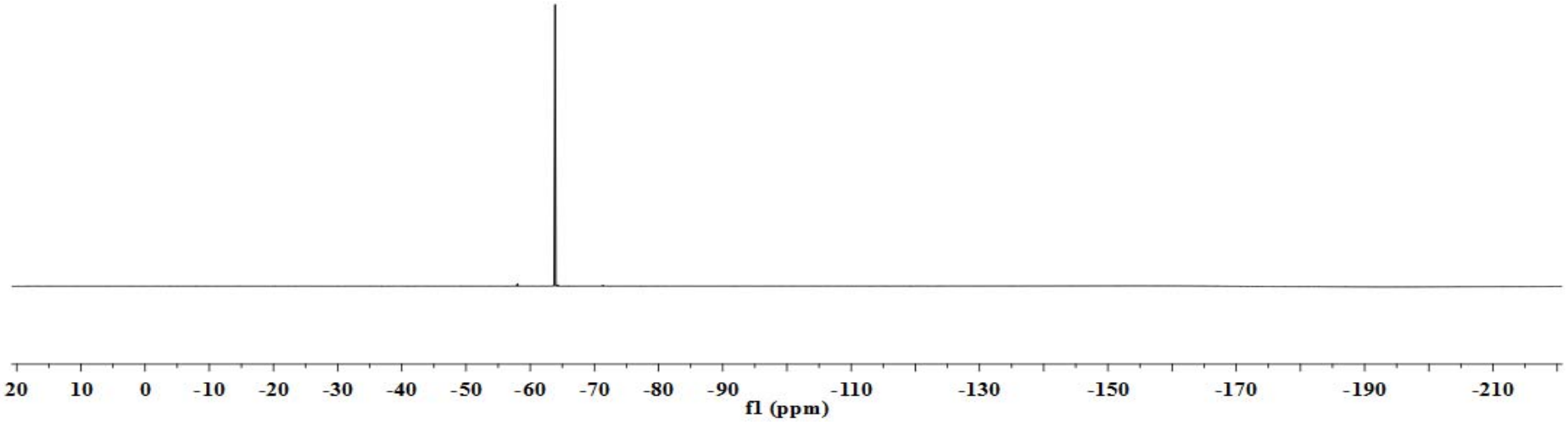
^{13}C-NMR ($CDCl_3$)



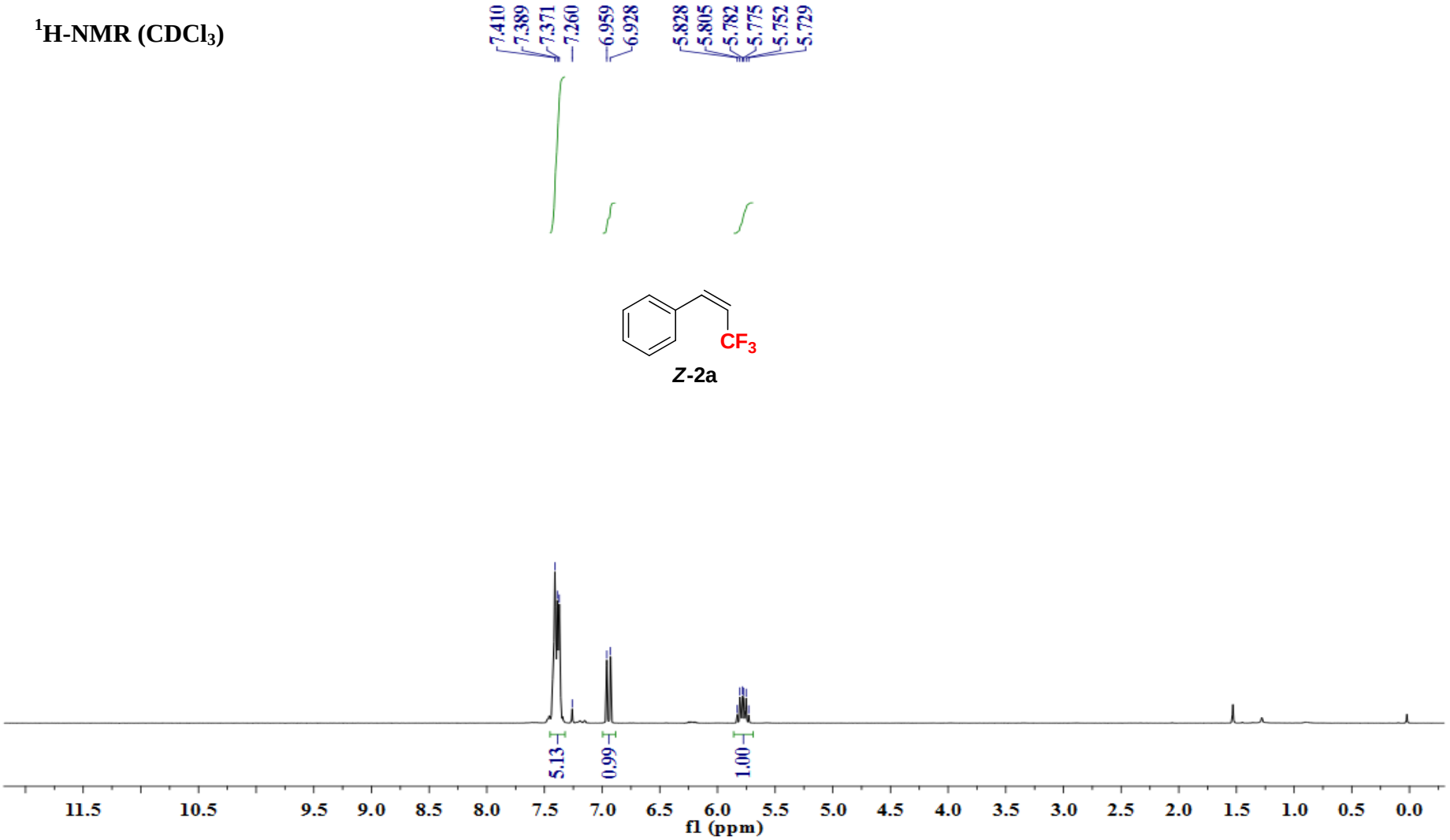
^{19}F-NMR ($CDCl_3$)



***E*-2t**

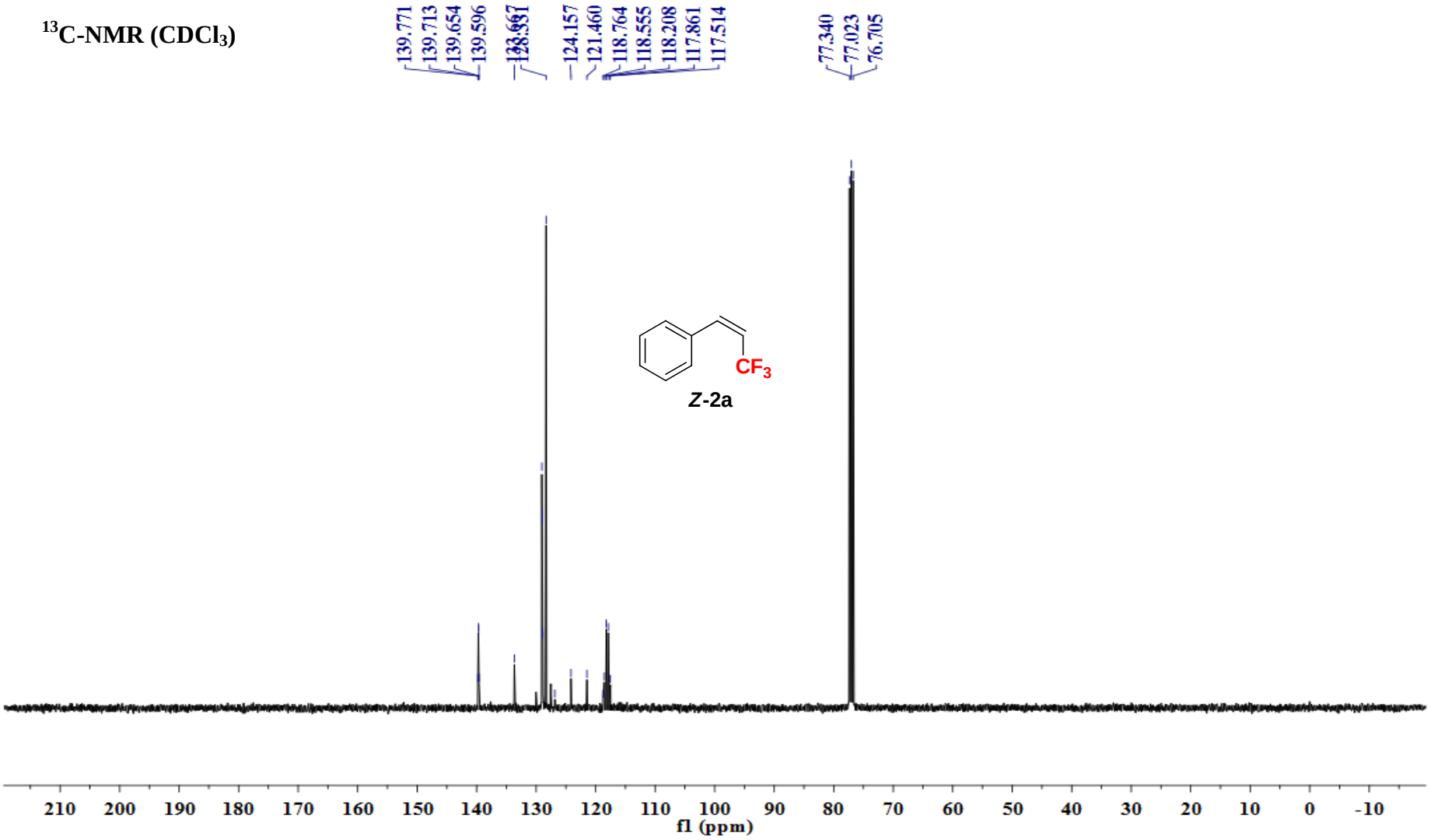


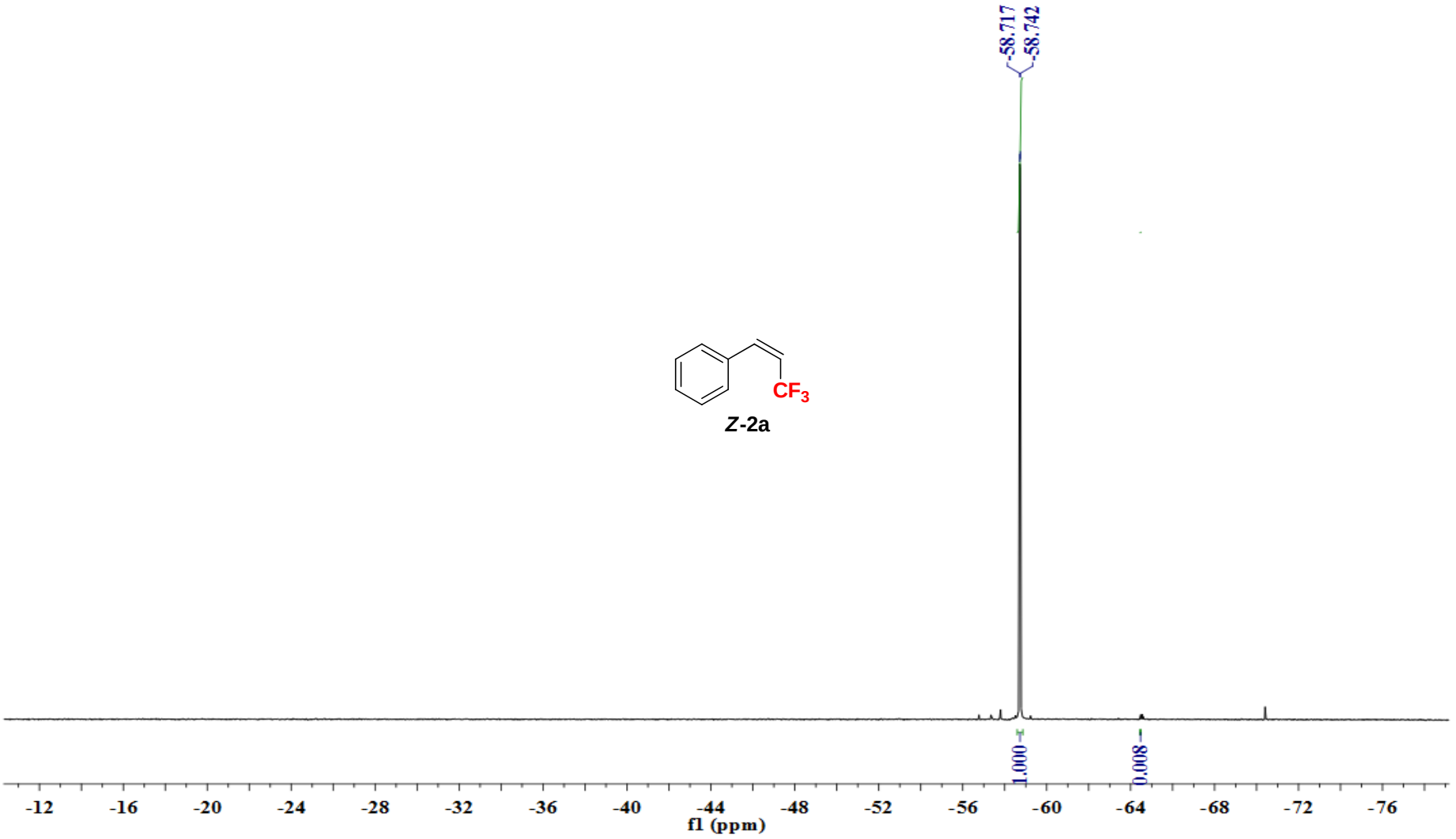
^{1}H-NMR ($CDCl_3$)



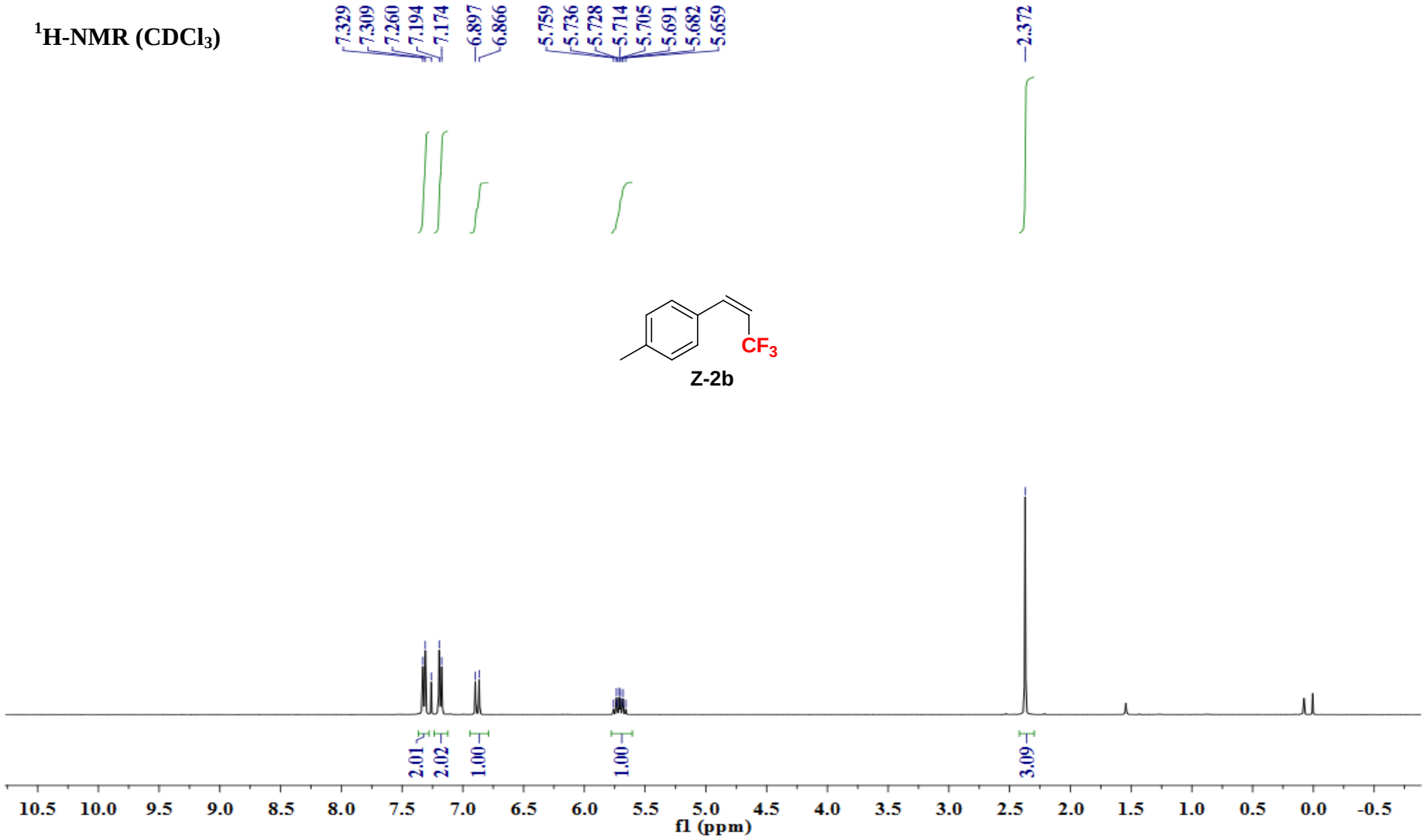
***Z*-2a**

^{13}C-NMR ($CDCl_3$)



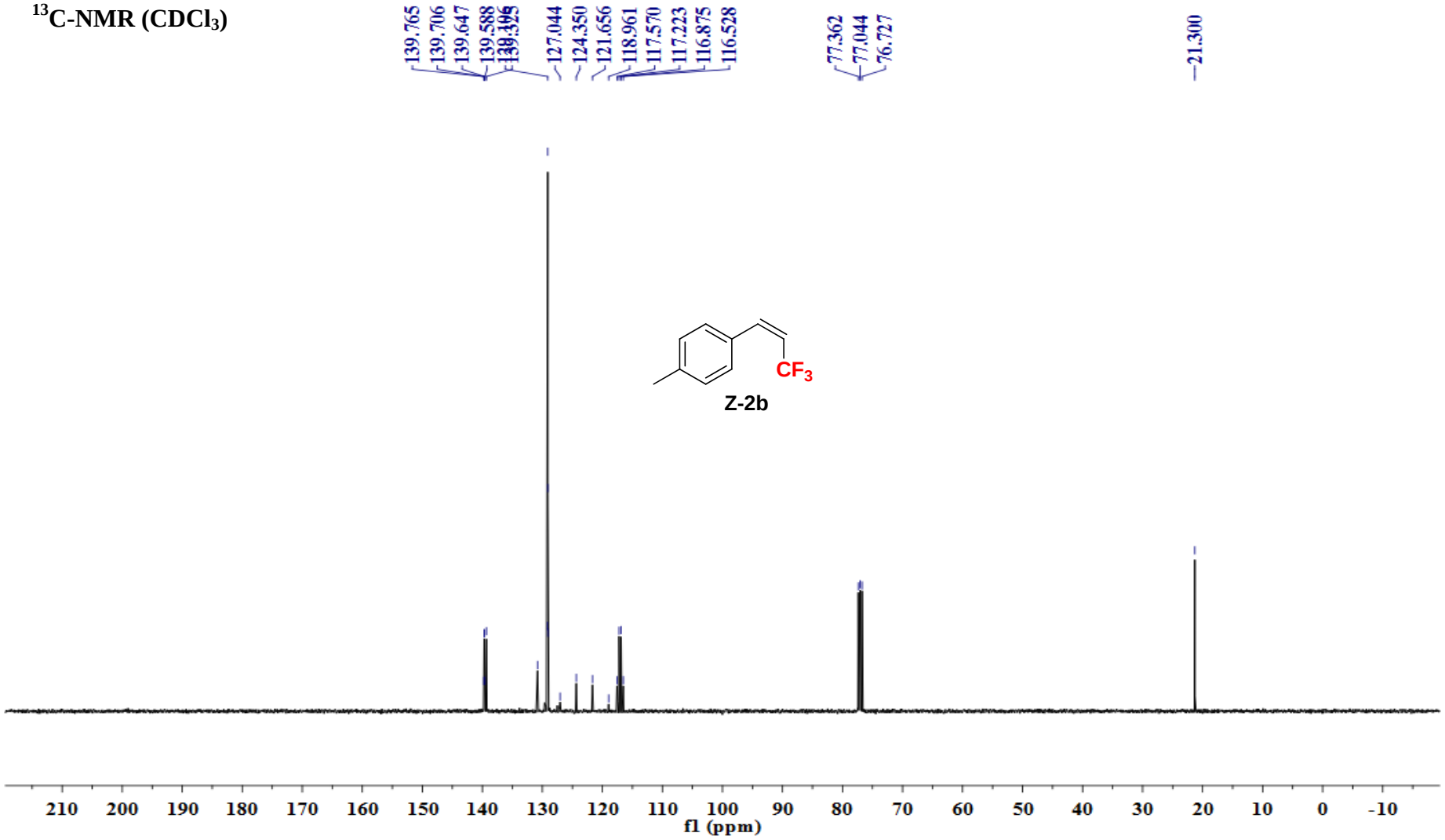

-58.717
-58.742
CF3
Z-2a
1.000
0.008
-12
-16
-20
-24
-28
-32
-36
-40
-44
-48
-52
-56
-60
-64
-68
-72
-76
f1 (ppm)

^{1}H-NMR ($CDCl_3$)

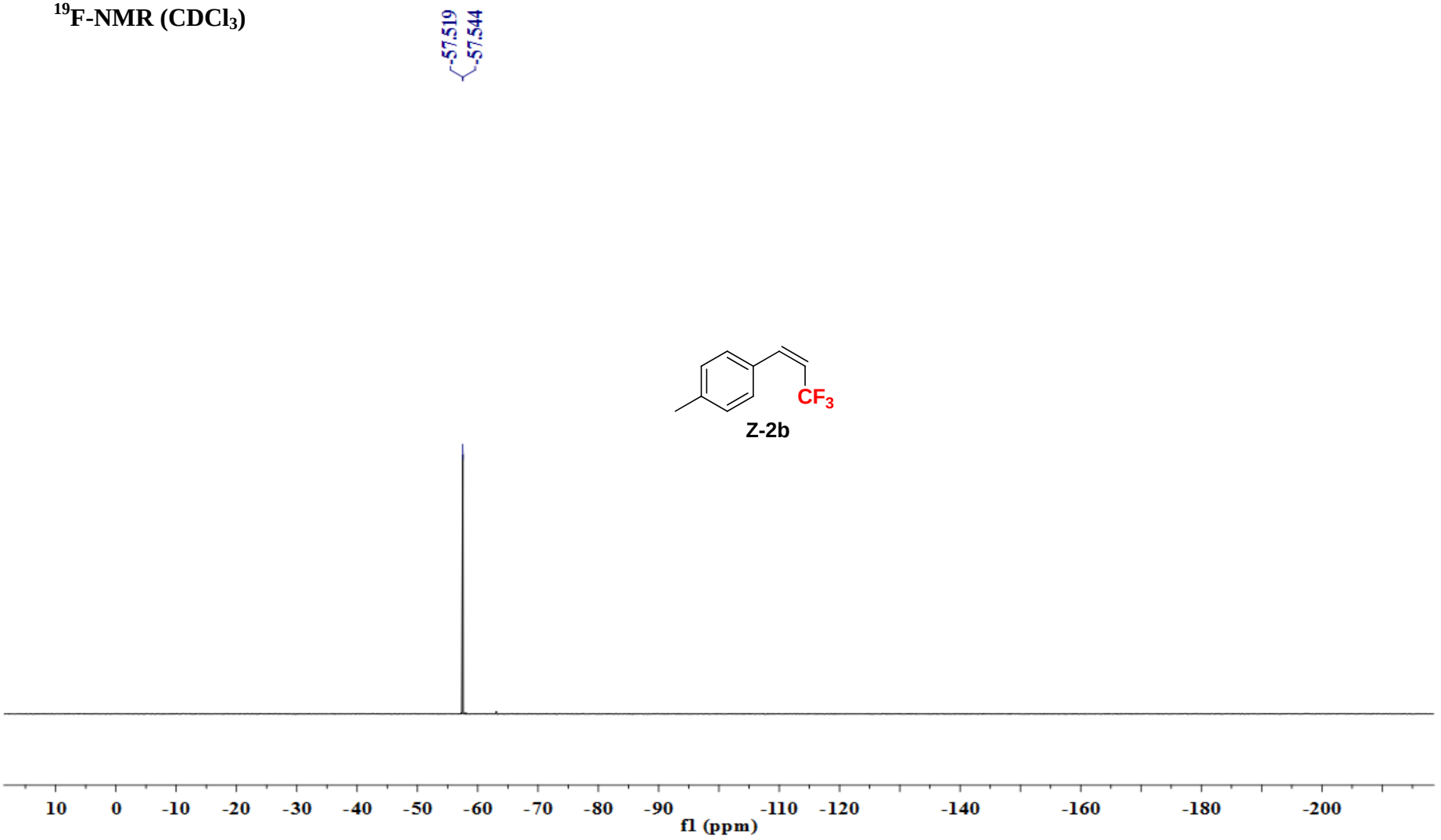


Z-2b

^{13}C-NMR ($CDCl_3$)

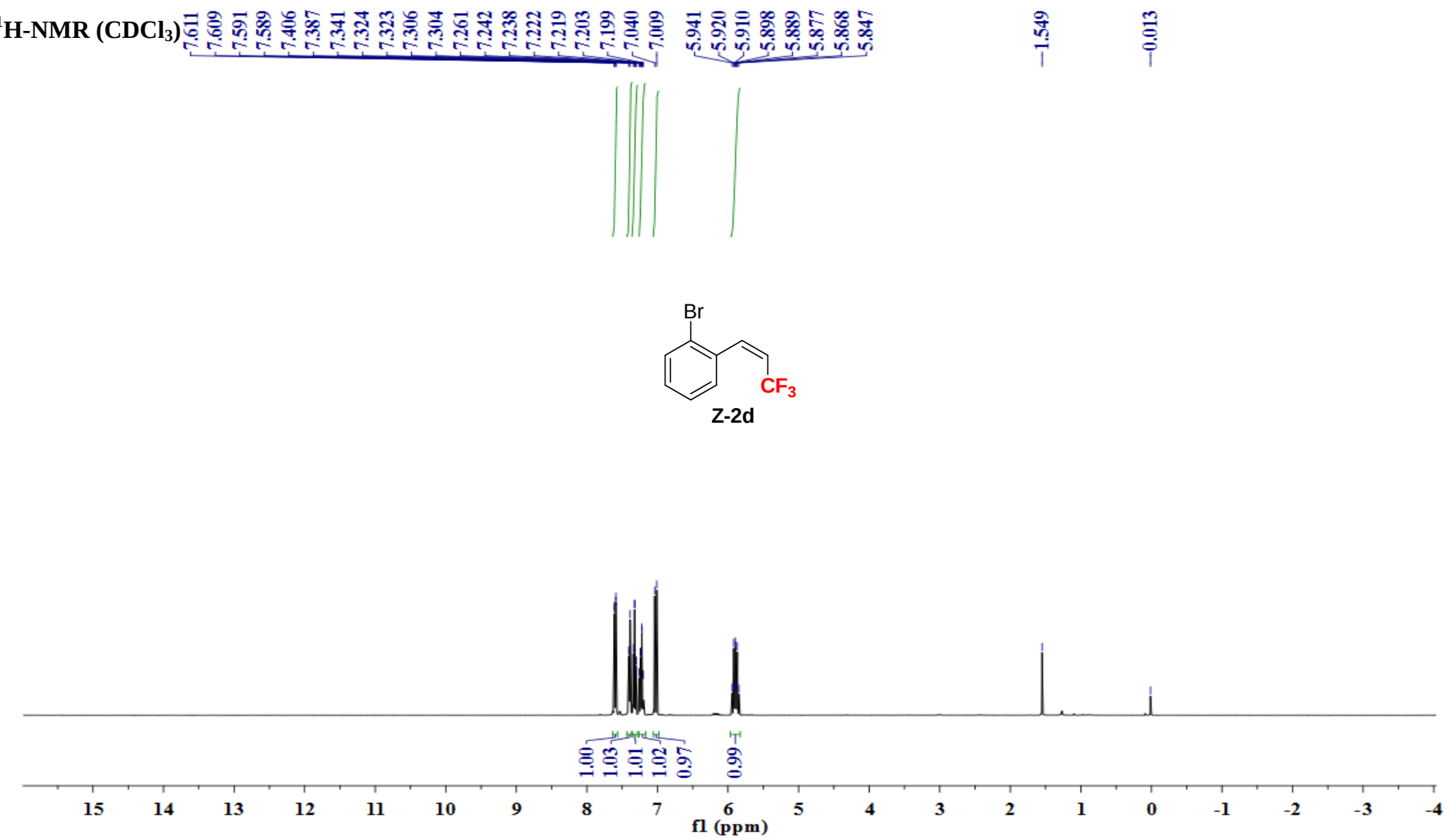


^{19}F-NMR ($CDCl_3$)



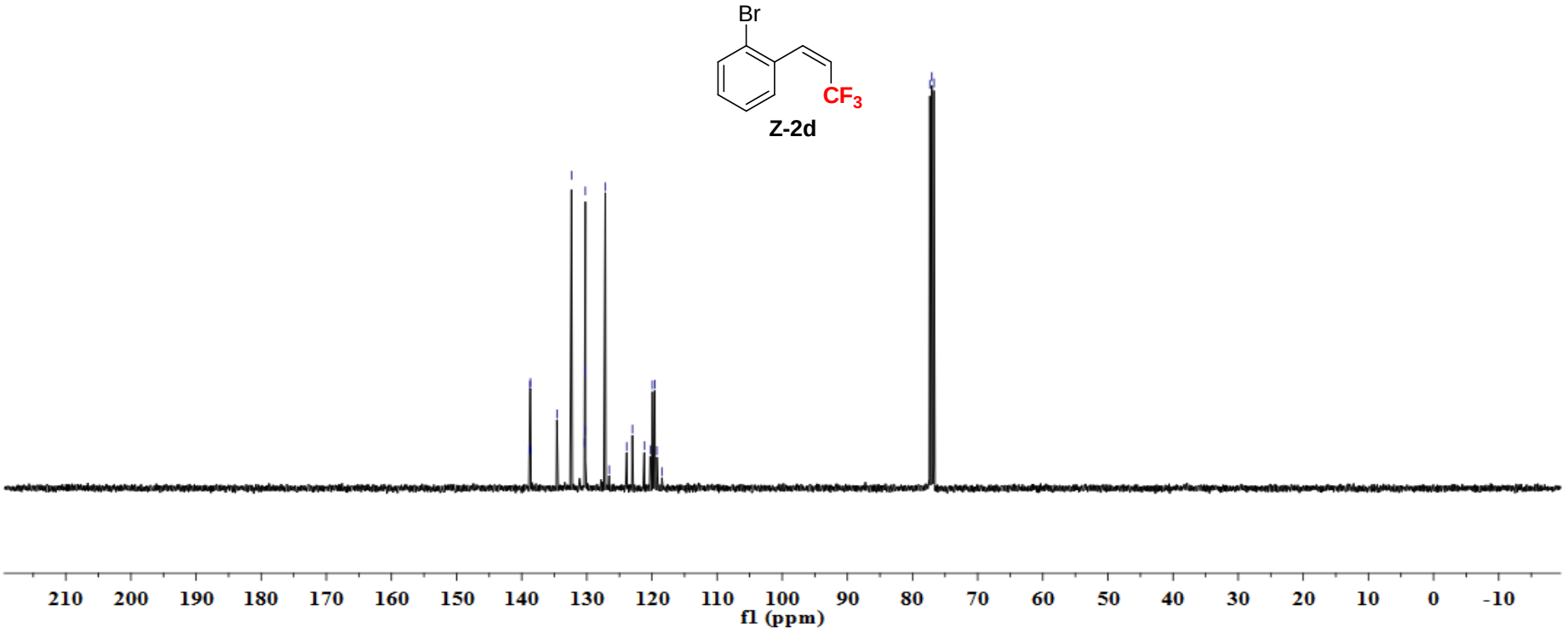
Z-2b

^{1}H-NMR ($CDCl_3$)

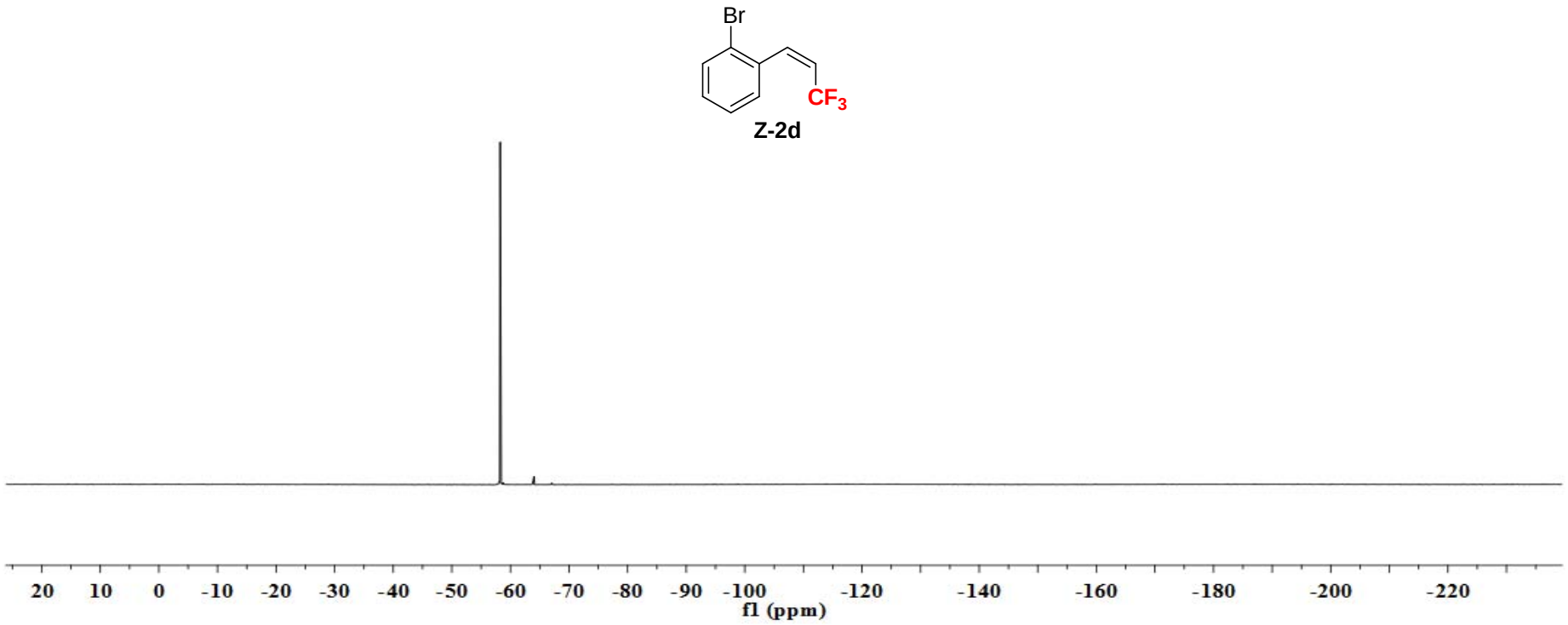


Z-2d

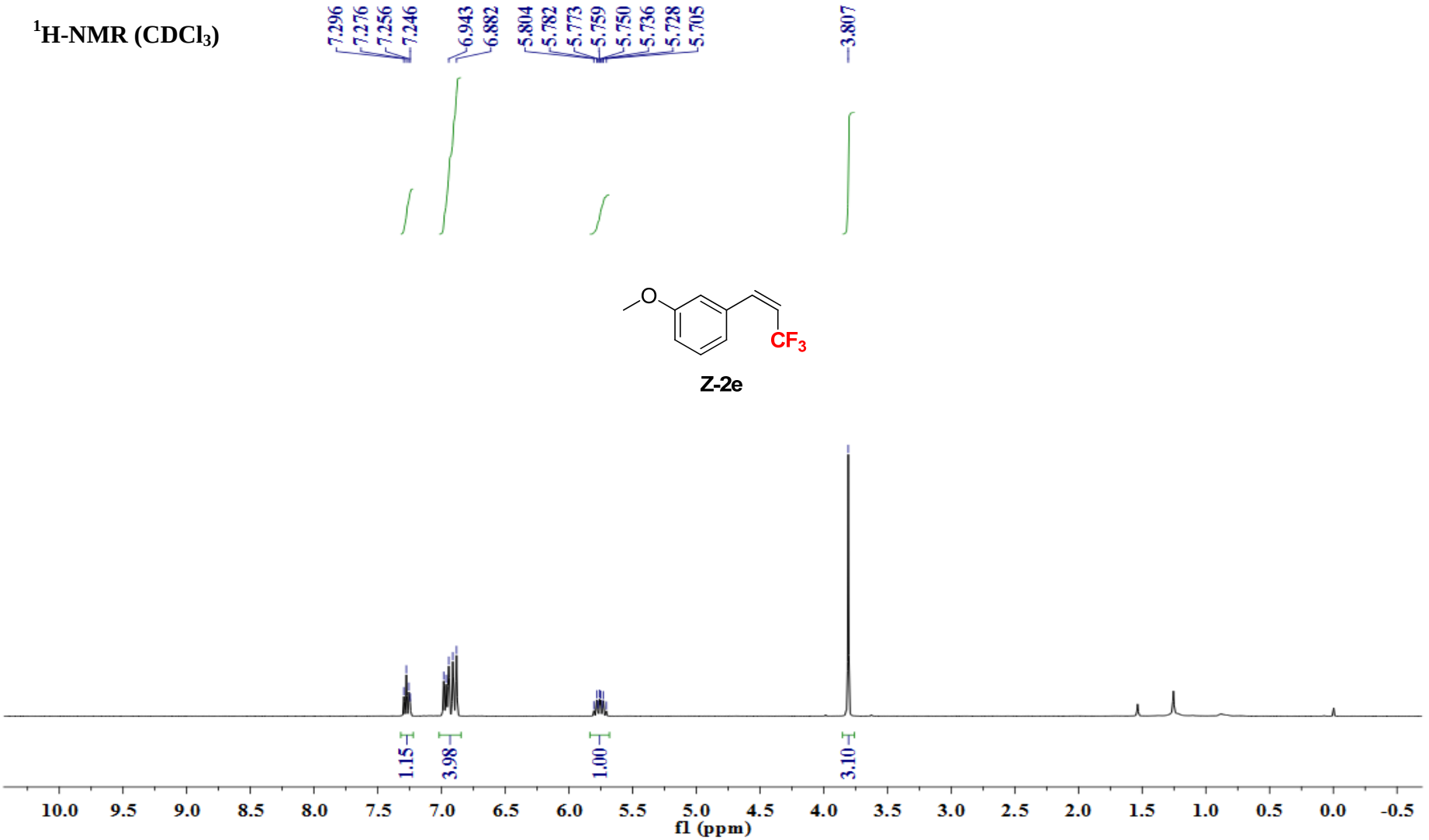
^{13}C-NMR ($CDCl_3$)



^{19}F-NMR ($CDCl_3$)



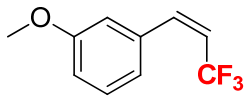
^{1}H-NMR ($CDCl_3$)



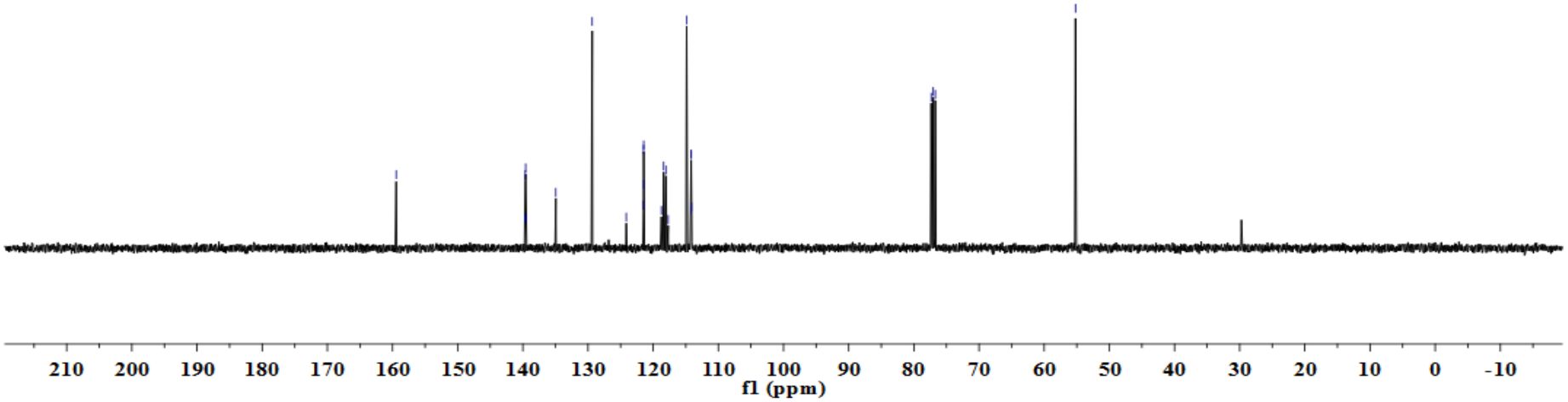
Z-2e

^{13}C-NMR ($CDCl_3$)

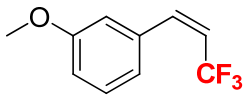
159.438
139.627
139.568
139.511
134.945
129.355
121.500
121.453
118.741
118.047
114.871
114.179
114.126
77.343
77.025
76.708
55.194



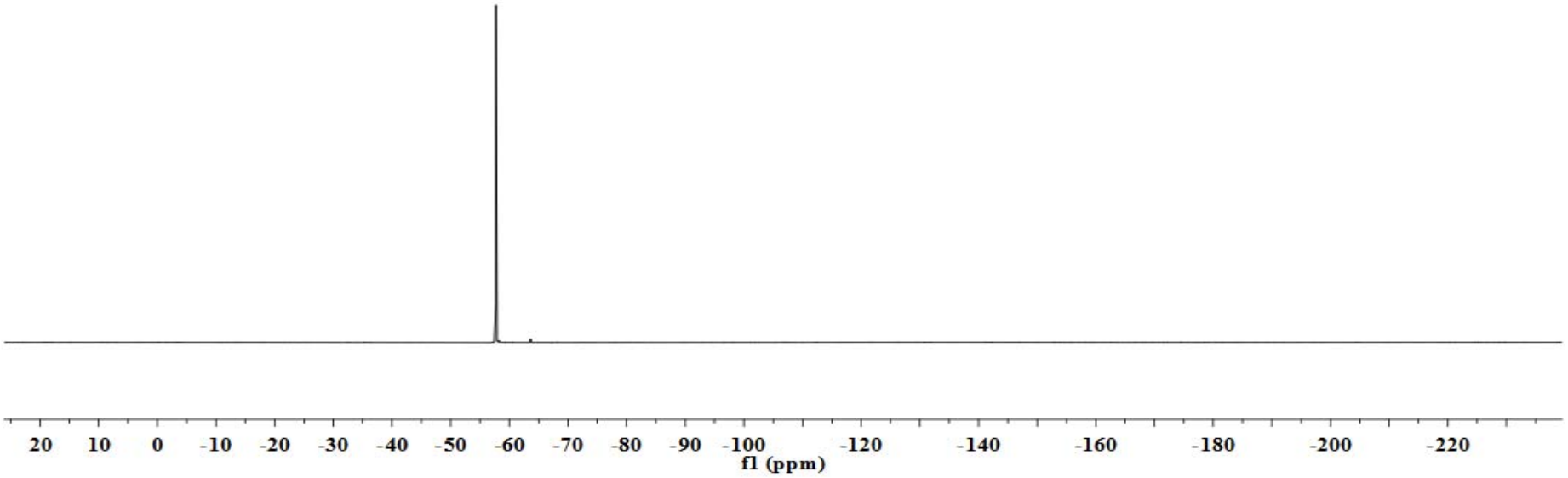
Z-2e



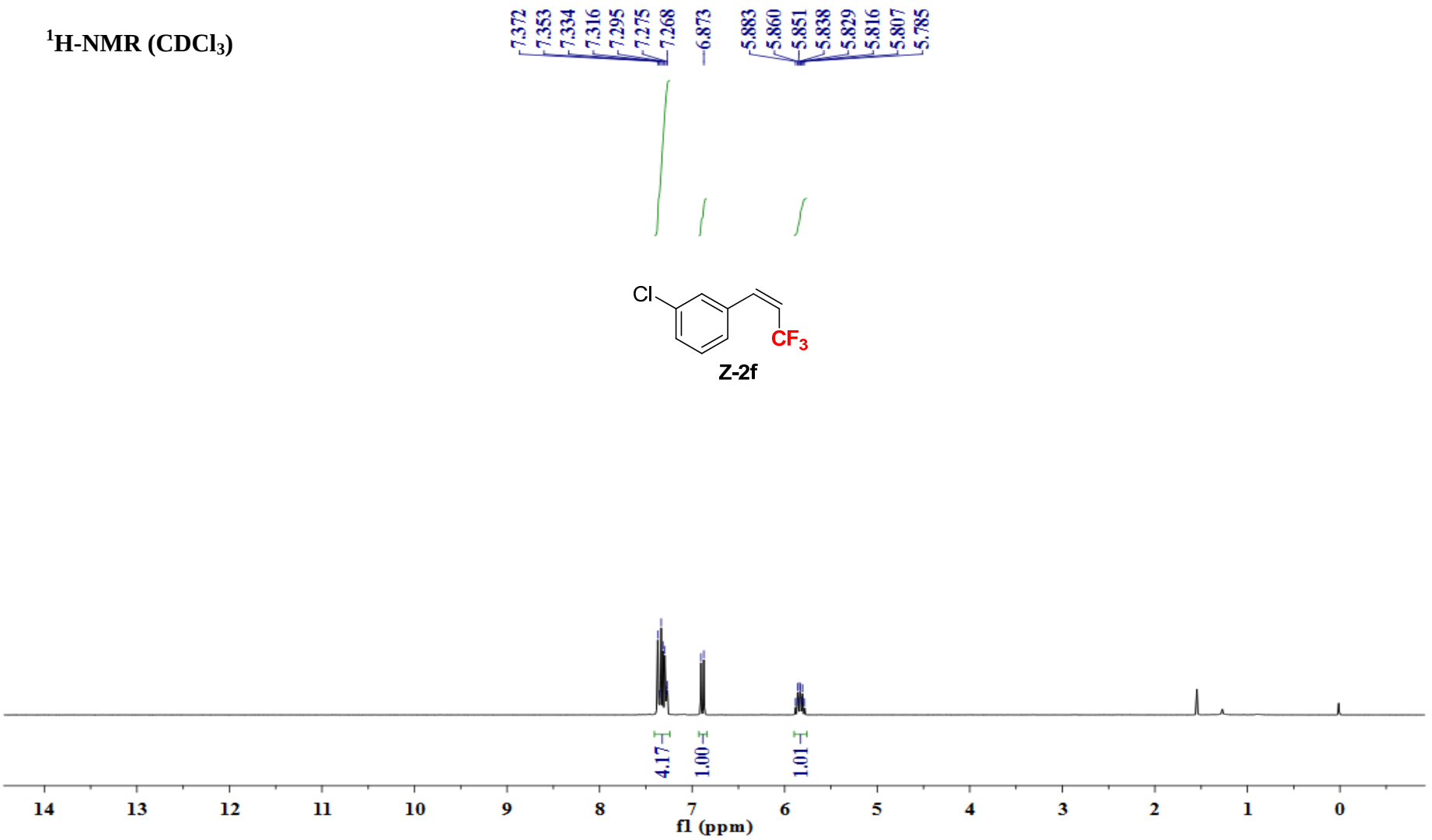
^{19}F-NMR ($CDCl_3$)



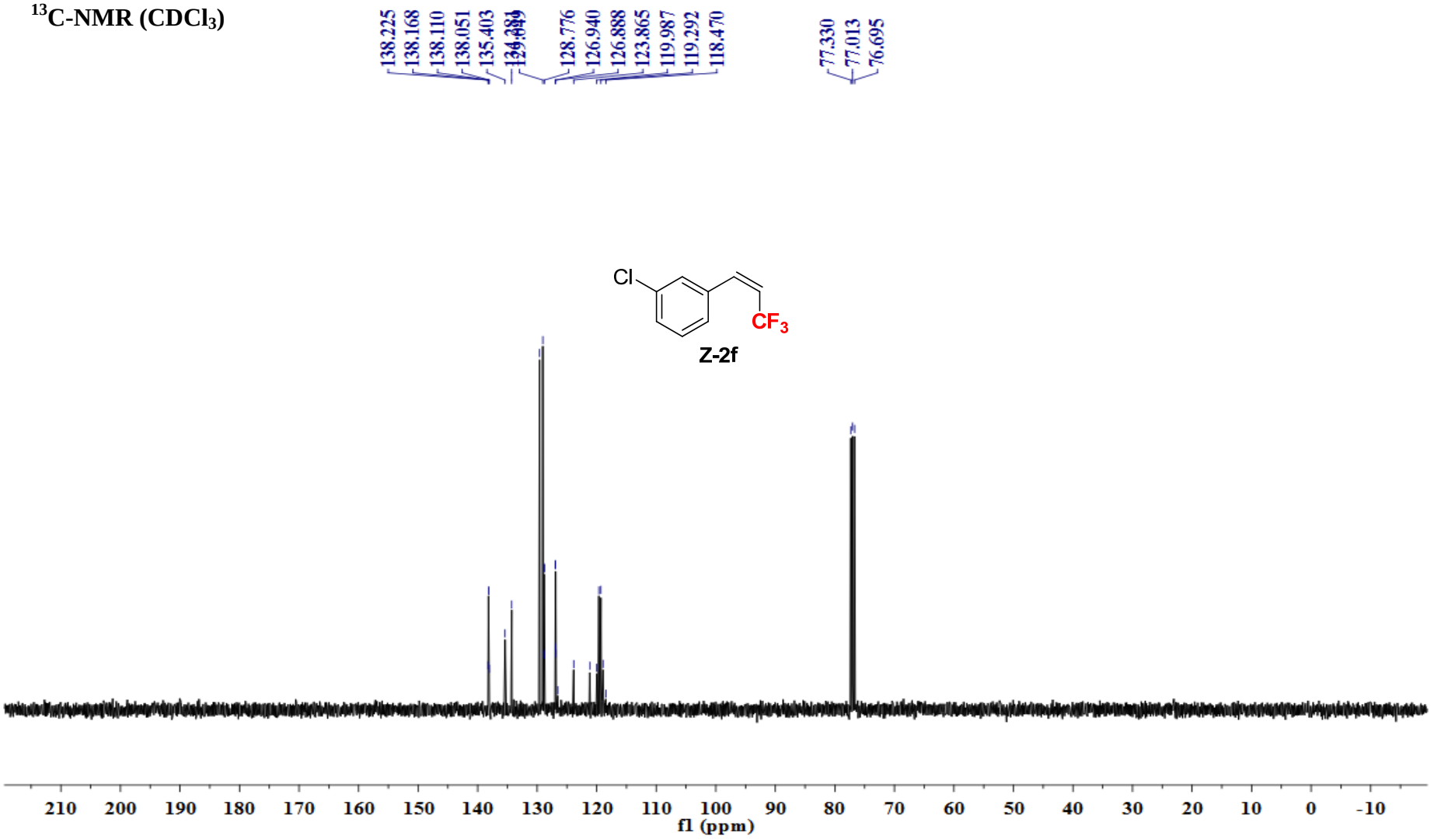
Z-2e



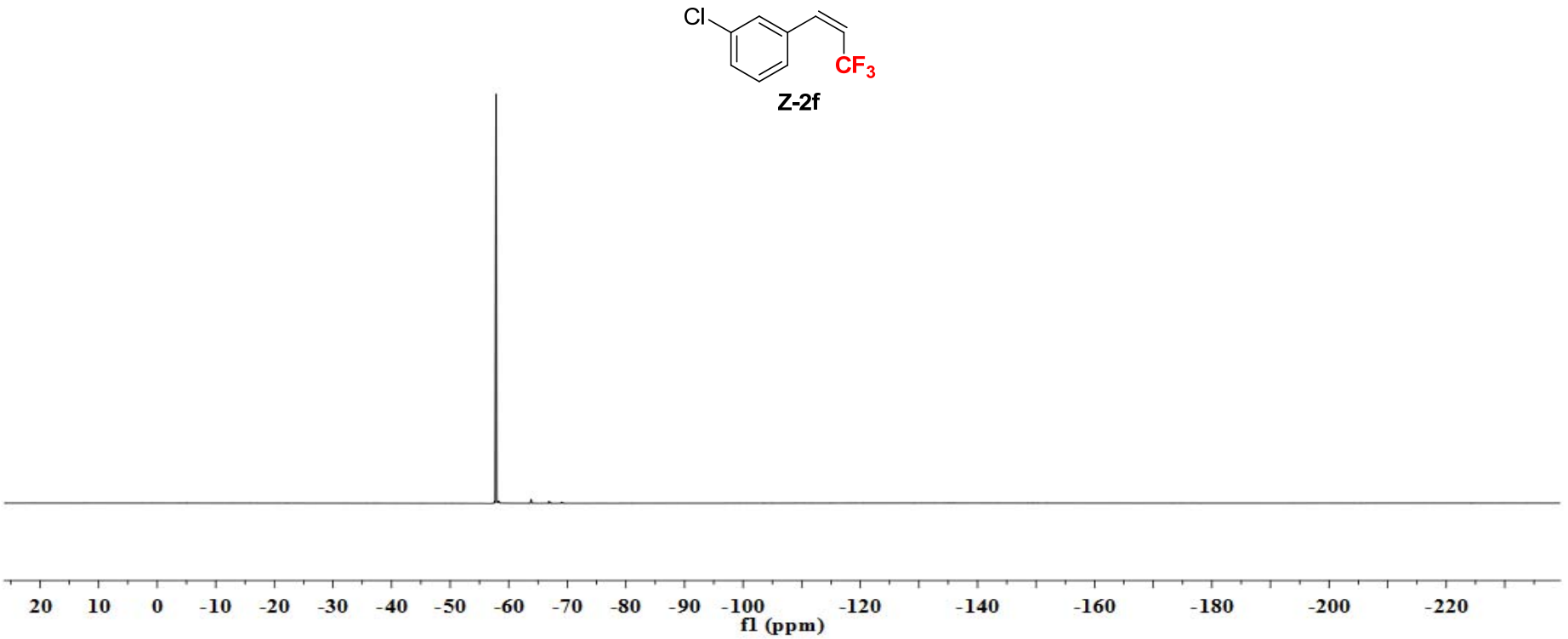
^{1}H-NMR ($CDCl_3$)


7.372
7.353
7.334
7.316
7.295
7.275
7.268
6.873
5.883
5.860
5.851
5.838
5.829
5.816
5.807
5.785
Cl
CF3
Z-2f
4.17
1.00
1.01
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

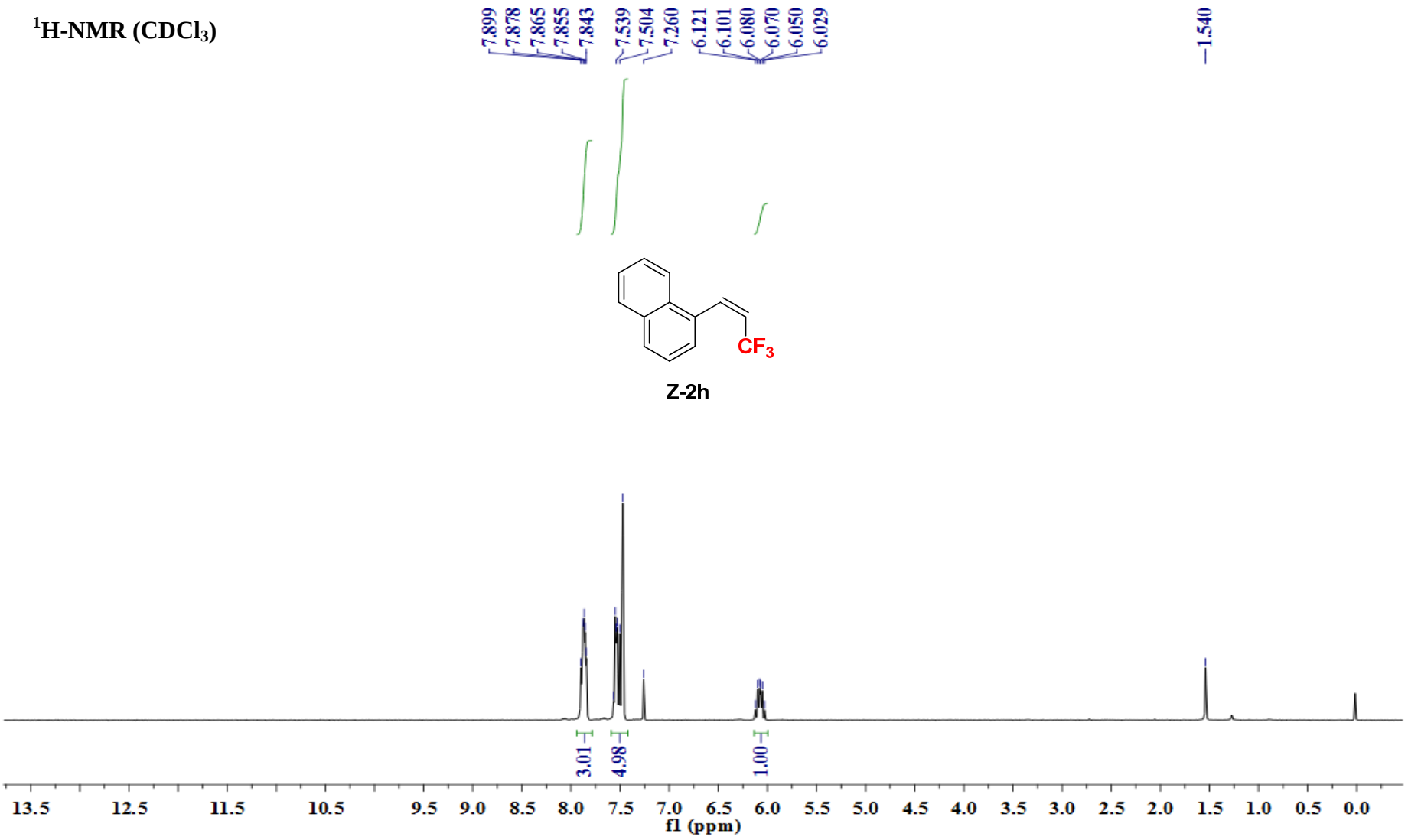
^{13}C-NMR ($CDCl_3$)



^{19}F-NMR ($CDCl_3$)

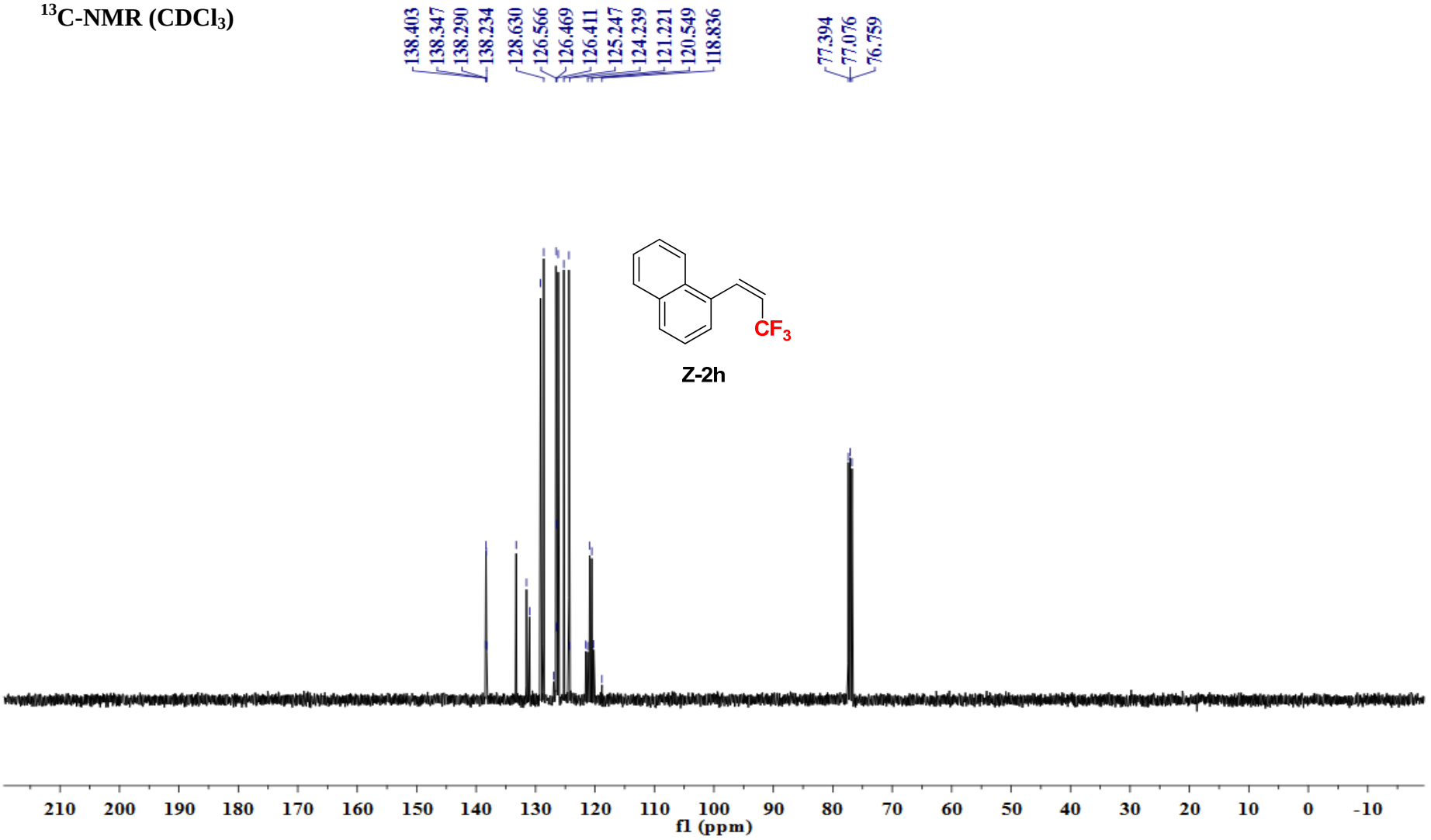


^{1}H-NMR ($CDCl_3$)



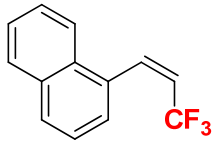
Z-2h

^{13}C-NMR ($CDCl_3$)

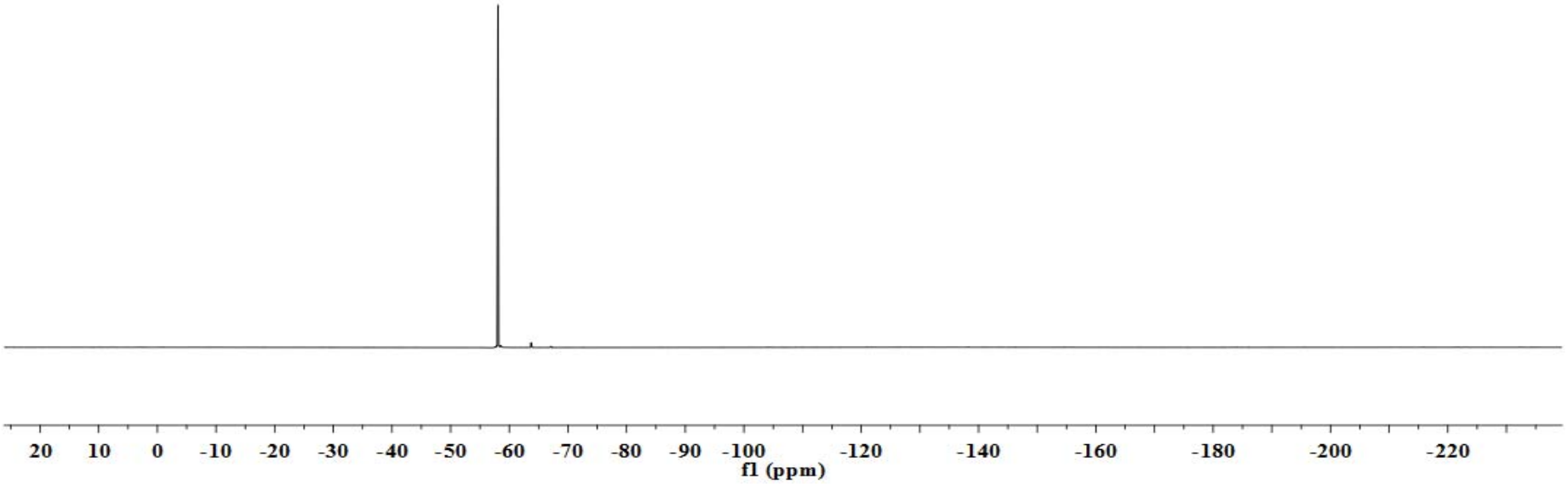


Z-2h

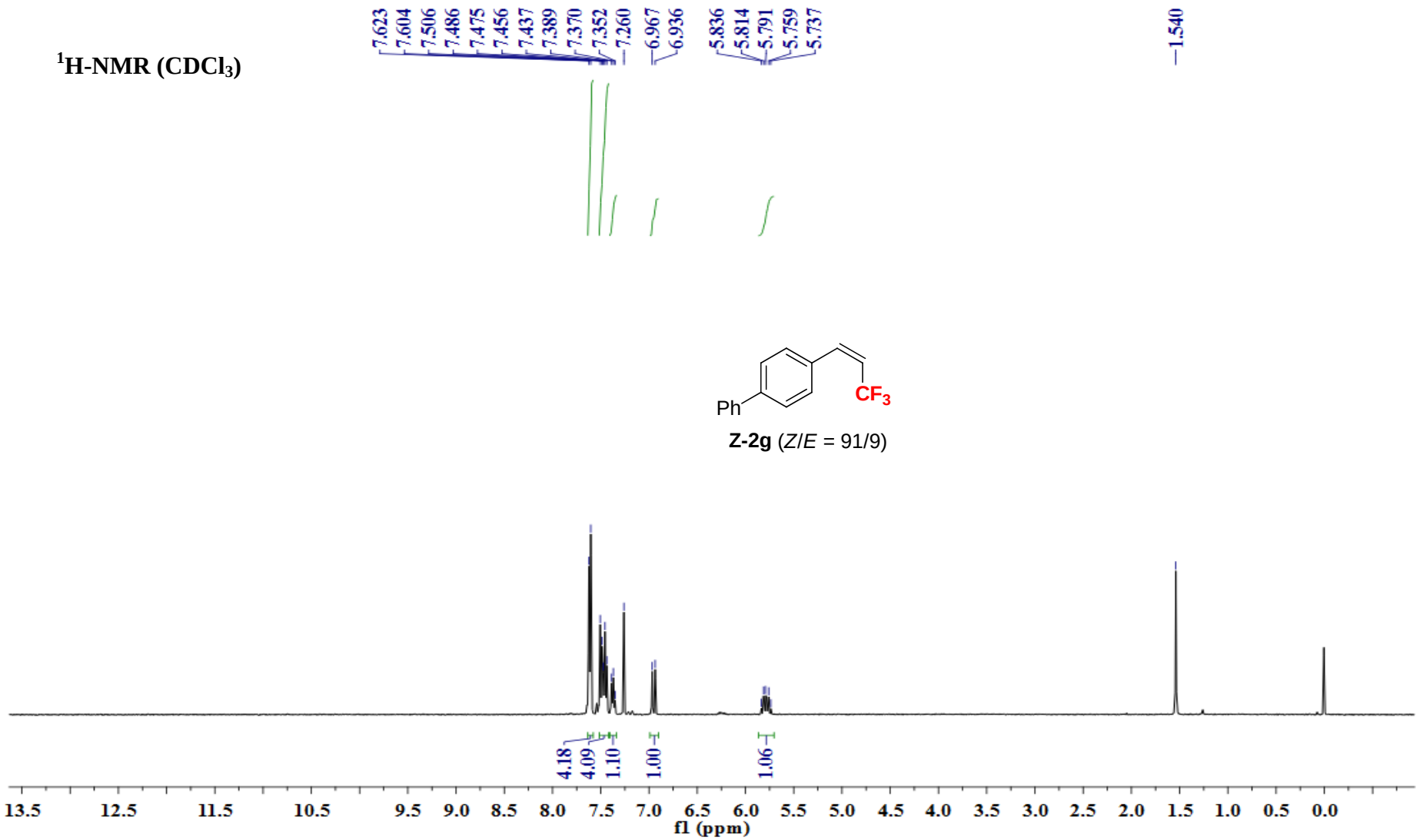
^{19}F-NMR ($CDCl_3$)



Z-2h

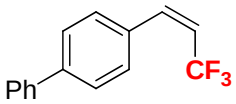


^{1}H-NMR ($CDCl_3$)



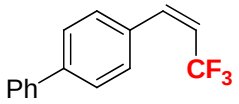
Z-2g (*Z*/*E* = 91/9)

^{13}C-NMR ($CDCl_3$)

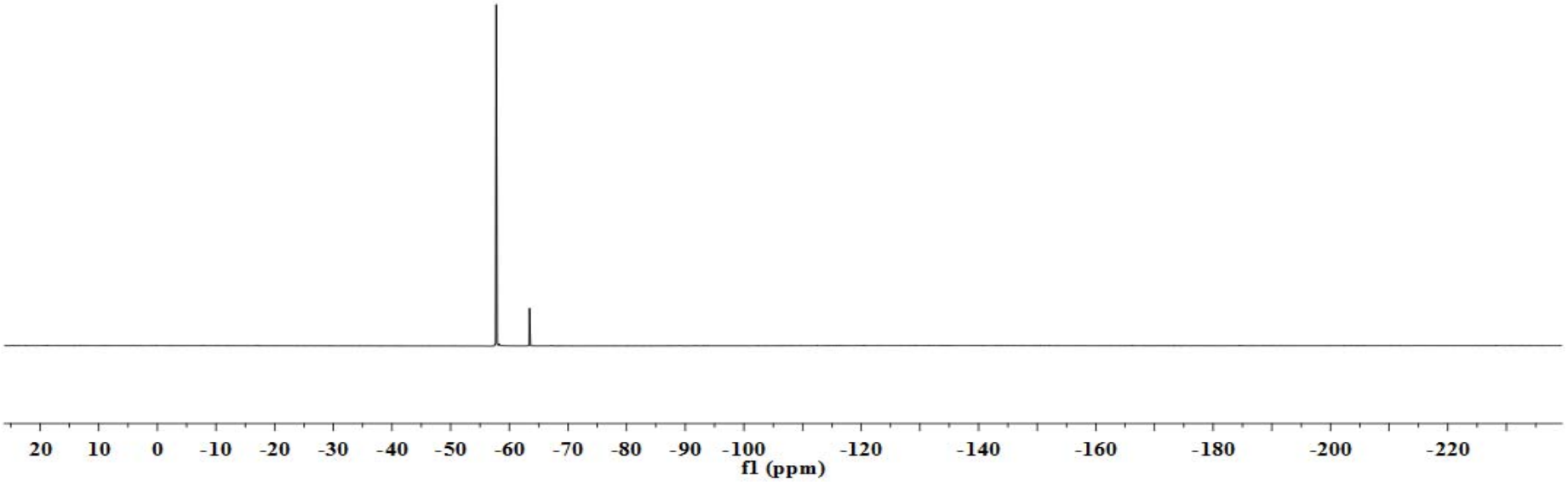


Z-2g (*Z*/*E* = 91/9)

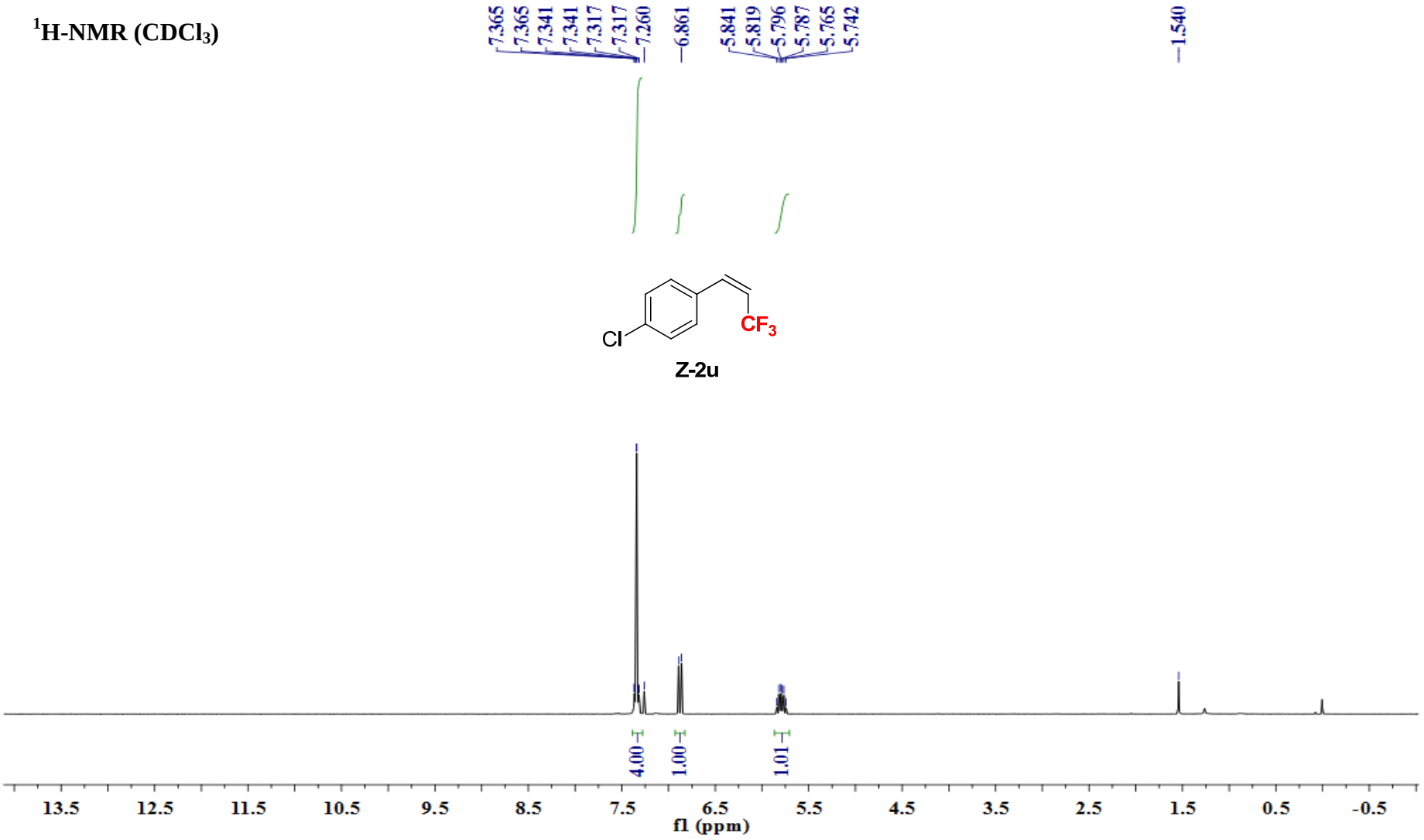
^{19}F-NMR ($CDCl_3$)



Z-2g (*Z*/*E* = 91/9)

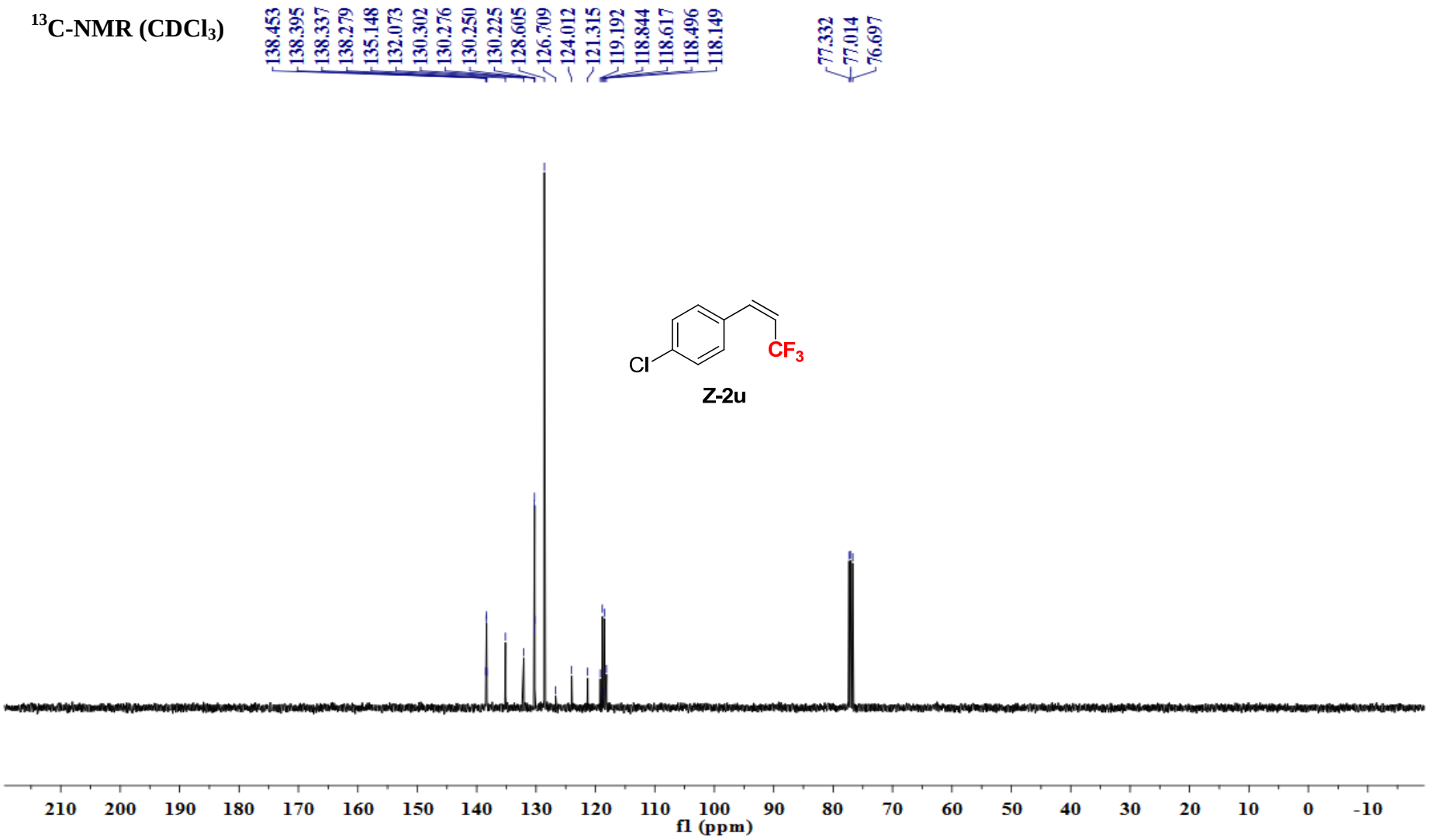


^{1}H-NMR ($CDCl_3$)



Z-2u

^{13}C-NMR ($CDCl_3$)



^{19}F-NMR ($CDCl_3$)