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New Journal of Chemistry

Synthesis and *in vitro* phototoxicity of novel π-extension derivatives of chlorin e6

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[b]*State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024, P.R. China*

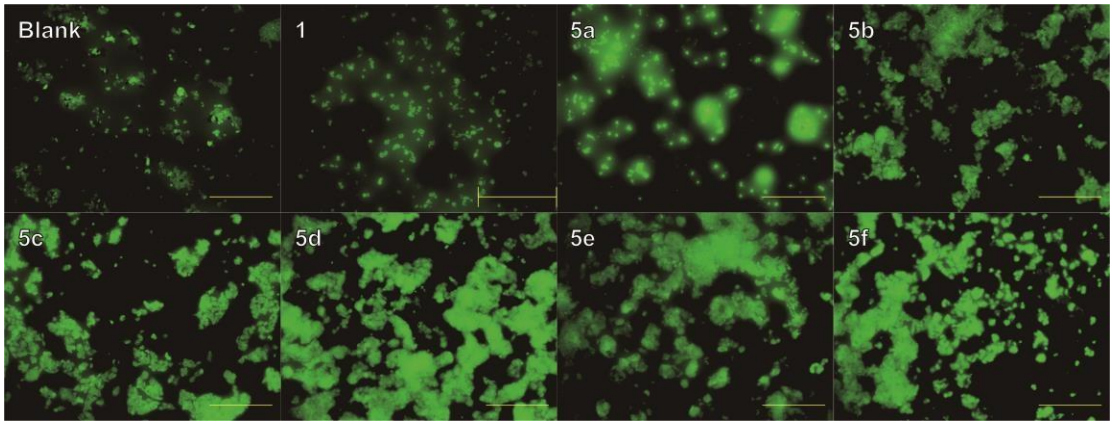


Figure S1. Fluorescent images of HepG2 cells stained by DCF.

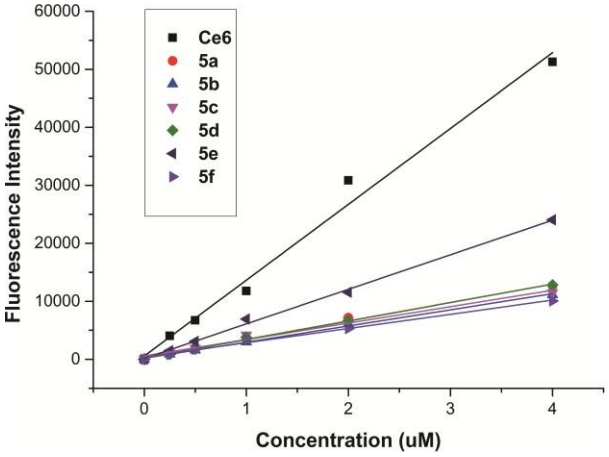


Figure S2. The standard curve of fluorescence intensity versus concentration of chlorins **1** and **5a-5f** in the present of HepG2 cells.

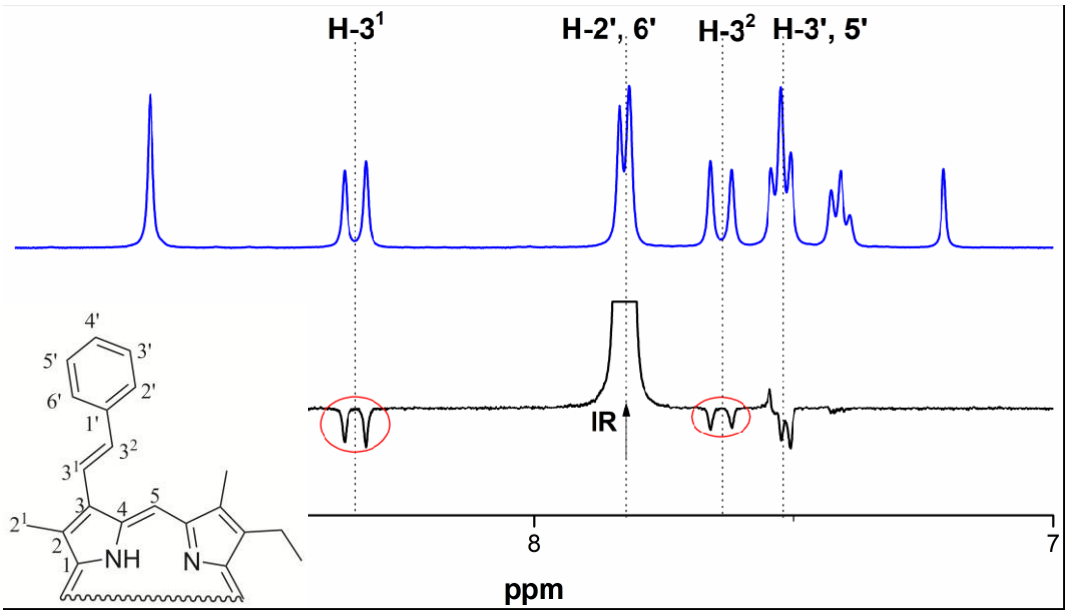
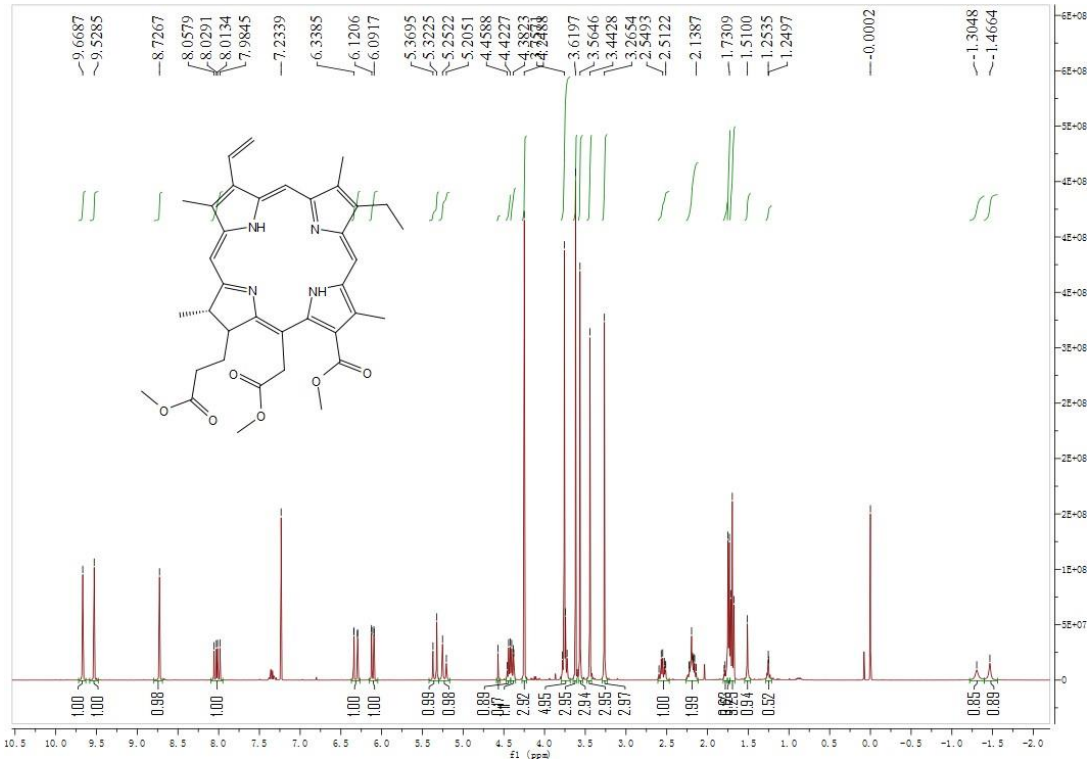
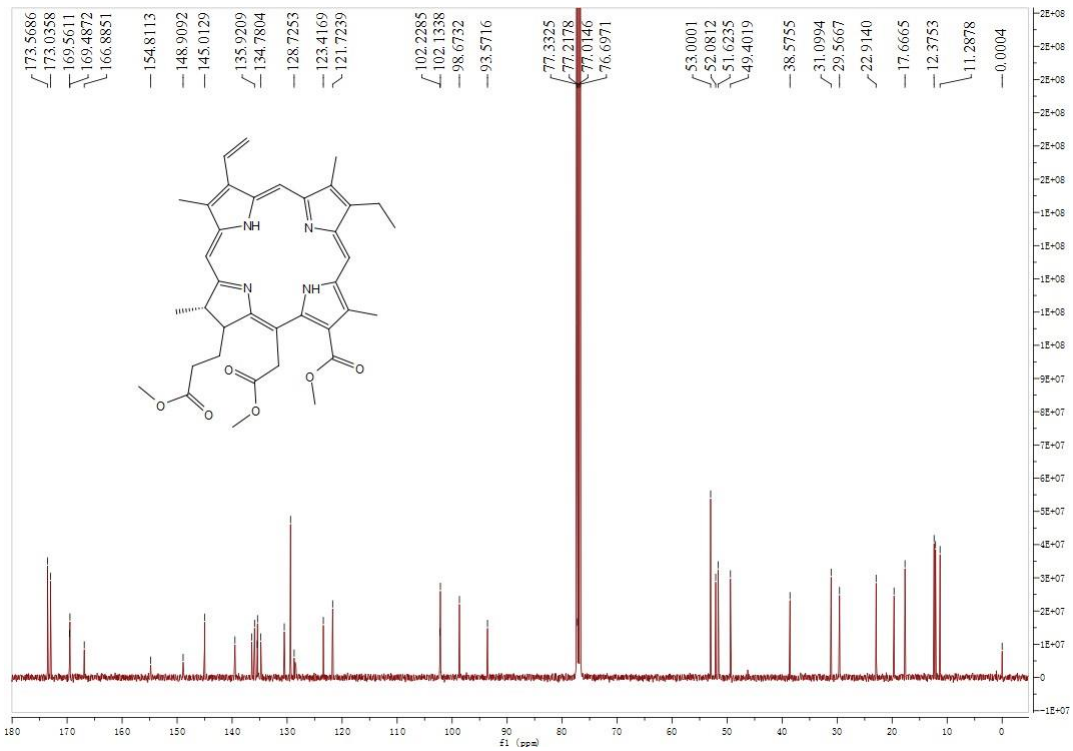


Figure S3. Selective NOE spectrum of compound **4a.** When selectively irradiating the Ar- Hα, the NOE signal of H-3^1 was obviously stronger than that of H-3^2.

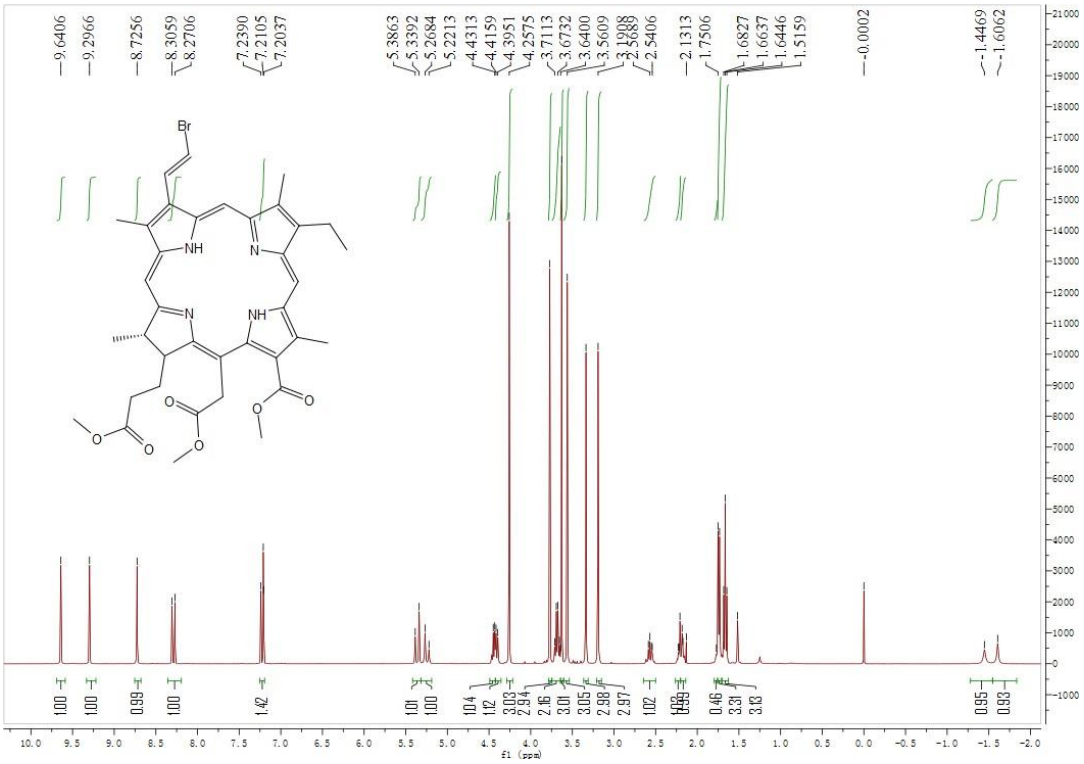
^{1}H NMR and ^{13}CNMR spectrum of products

Compound **2**





Compound **3a**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5.2684
5.2213
4.4313
4.4159
4.3951
4.2575
3.7113
3.6732
3.6400
3.5609
3.1908
3.1688
2.5406
2.1313
1.7506
1.6827
1.6637
1.6446
1.5159
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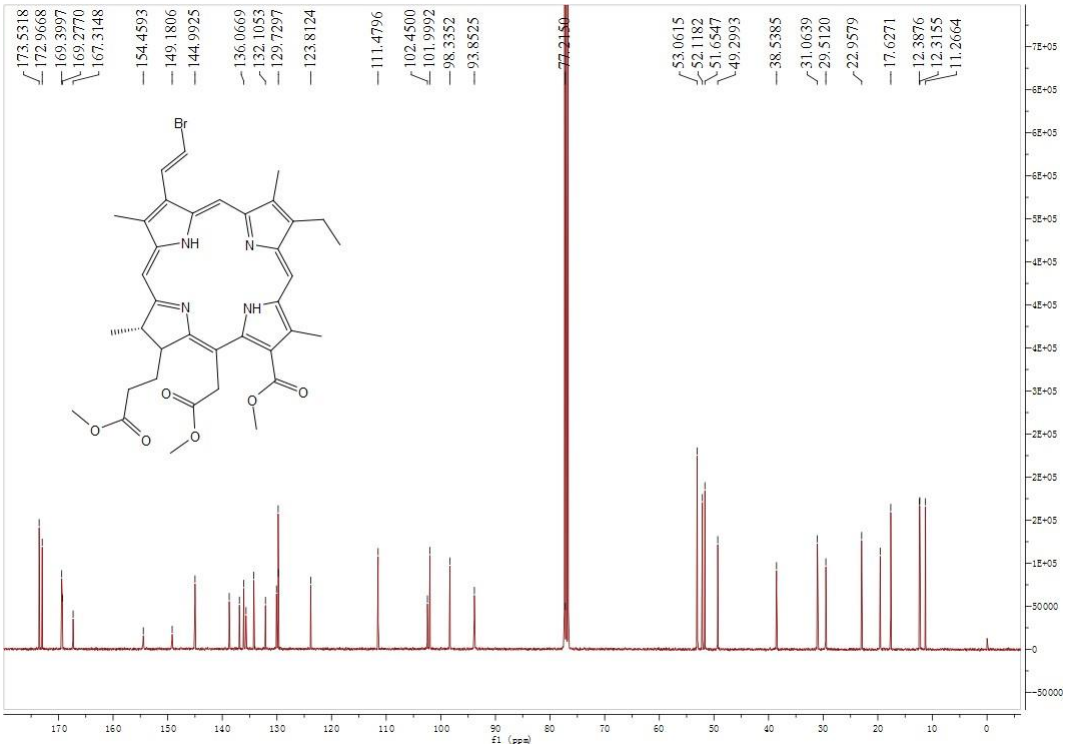
-1.6062
Br
NH
N
N
NH
O
O
O
O
O
O
f1 (ppm)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167.3148
154.4593
149.1806
144.9925
136.0669
132.1053
129.7297
123.8124
111.4796
102.4500
101.9992
98.3352
93.8525
77.2150
53.0615
52.1182
51.6547
49.2993
38.5385
31.0639
29.5120
22.9579
17.6271
12.3876
12.3155
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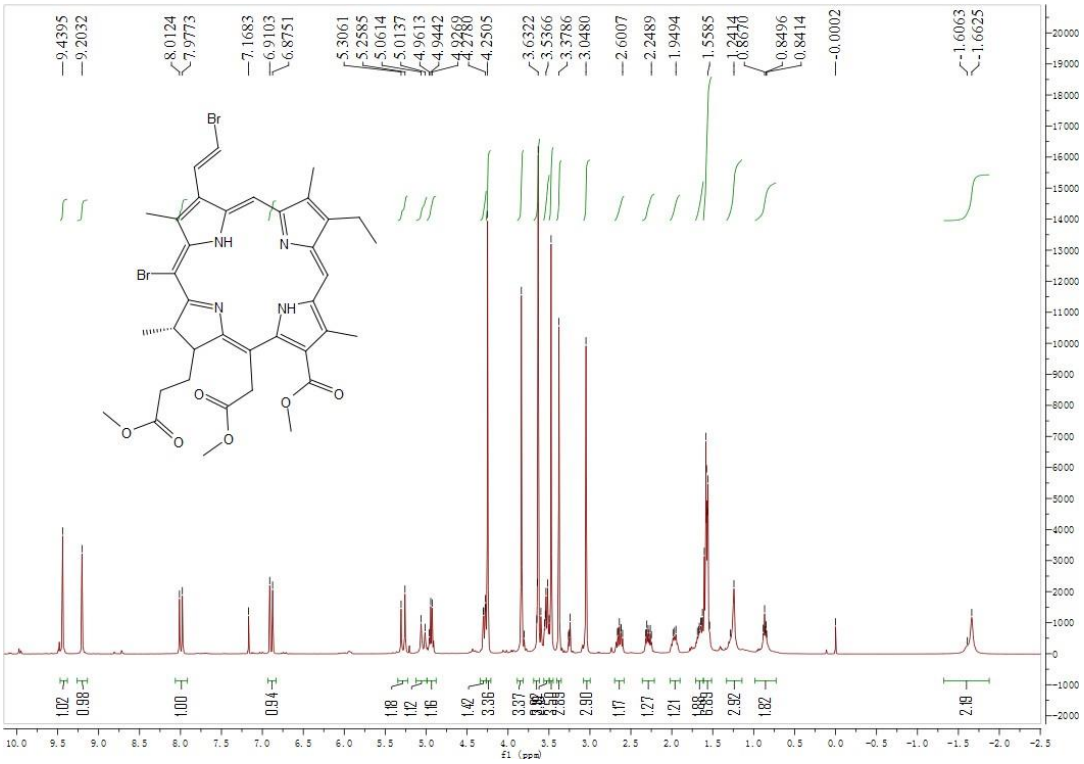
Br
NH
N
N
NH
O
O
O
O
O
O
f1 (ppm)

Compound **3b**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5.0614
5.0137
4.9613
4.9442
4.2505
3.6322
3.5366
3.3786
3.0480
2.6007
2.2489
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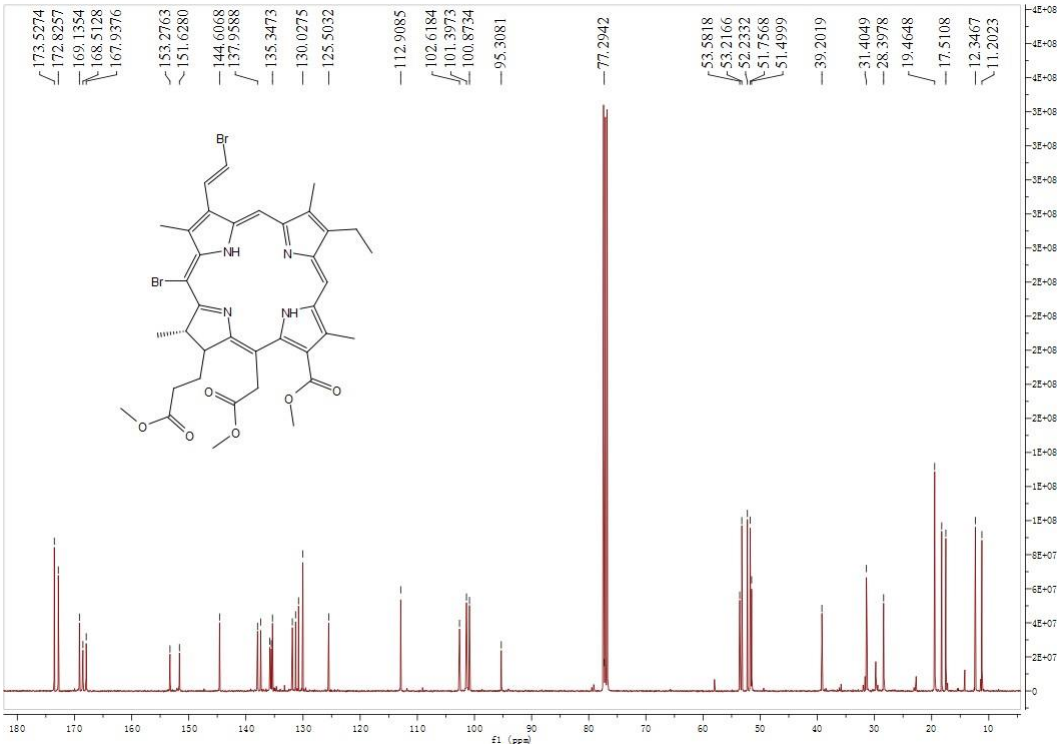
-1.6625
Br
NH
N
O
f1 (ppm)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125.5032
112.9085
102.6184
101.3973
100.8734
95.3081
77.2942
53.5818
53.2166
52.2332
51.7568
51.4999
39.2019
31.4049
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17.5108
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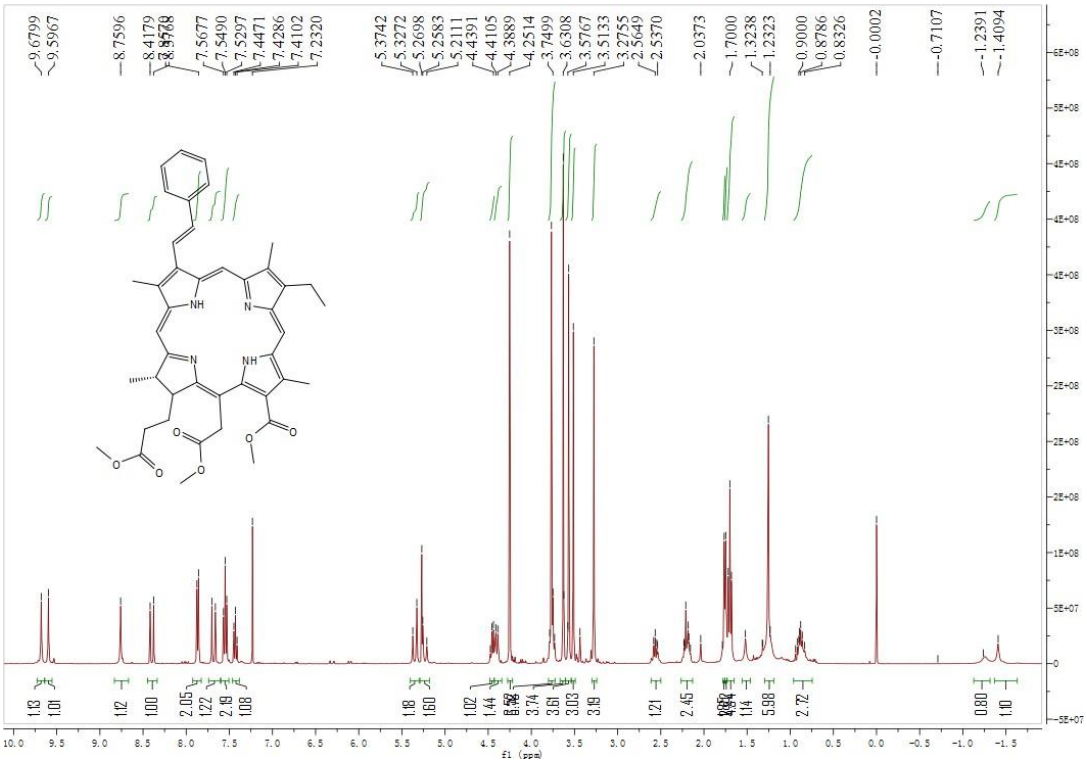
11.2023
Br
NH
N
O
f1 (ppm)

Compound **4a**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7.2320
5.3742
5.3272
5.2698
5.2583
5.2111
4.4391
4.4105
4.3889
4.2514
3.7499
3.6308
3.5767
3.5133
3.2755
2.5649
2.5370
2.0373
1.7000
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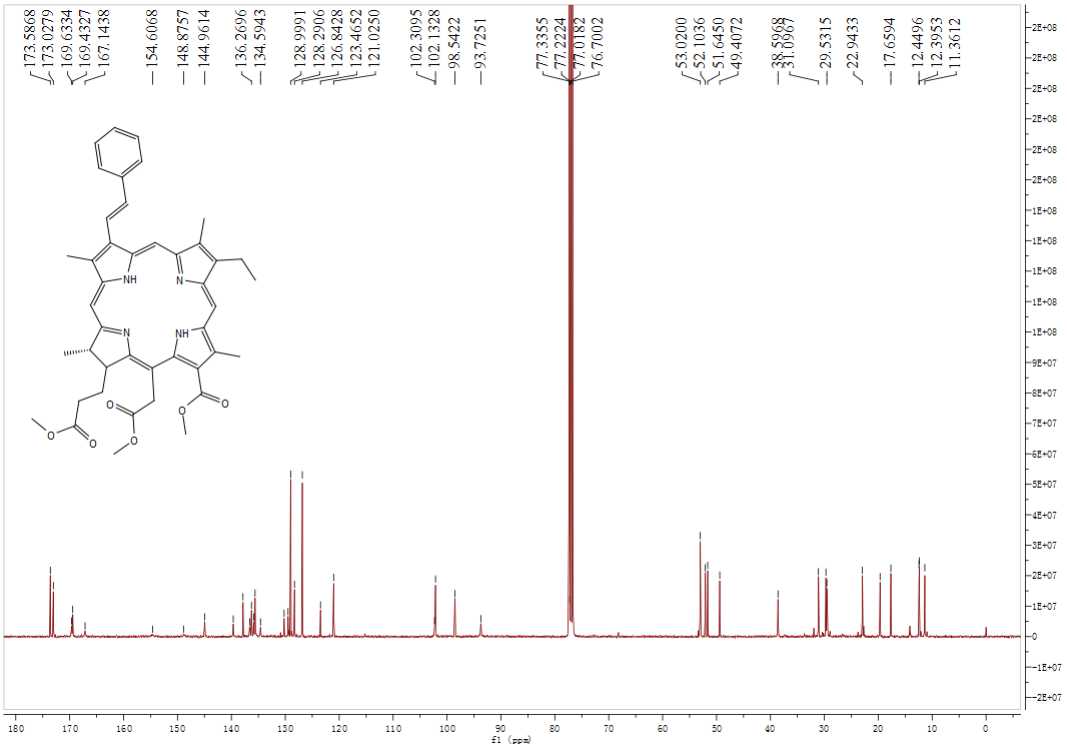
f1 (ppm)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128.2906
126.8428
123.4652
121.0250
102.3095
102.1328
98.5422
93.7251
77.3355
77.2224
77.0182
76.7002
53.0200
52.1036
51.6450
49.4072
38.5968
31.0967
29.5315
22.9433
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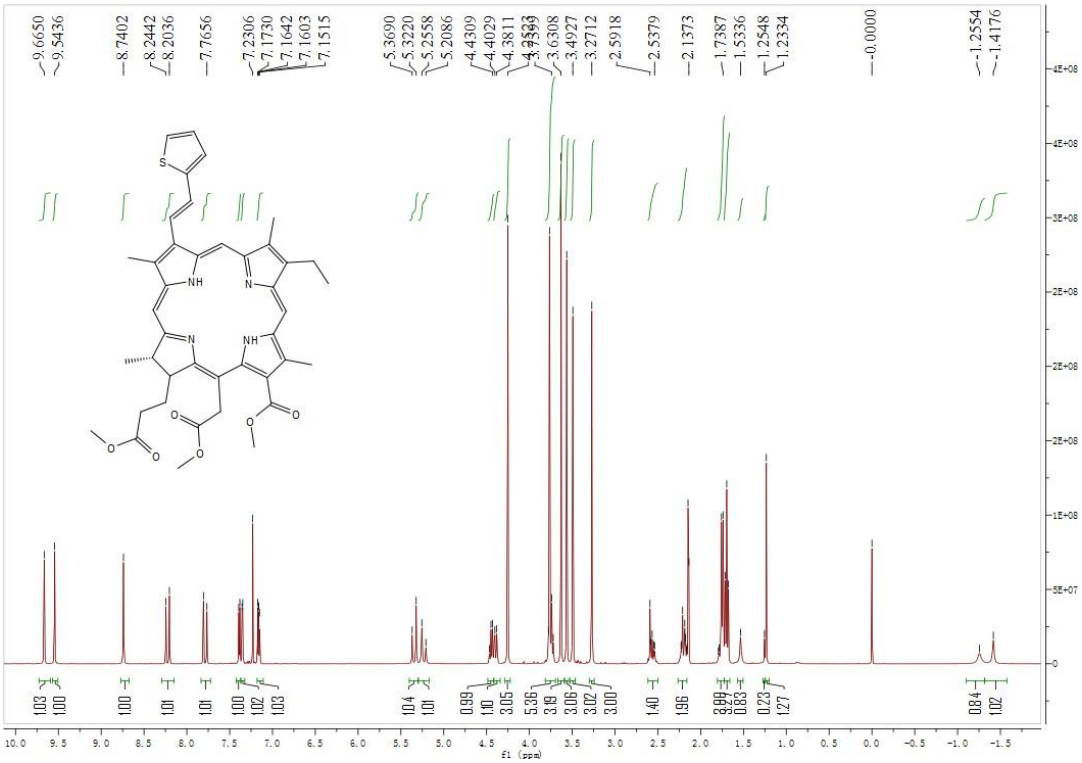
12.3953
11.3612
f1 (ppm)

Compound **4b**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8.2442
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7.2306
7.1730
7.1642
7.1603
7.1515
5.3690
5.3220
5.2558
5.2086
4.4309
4.4029
4.3811
3.6308
3.4927
3.2712
2.5918
2.5379
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1.5336
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1.2334
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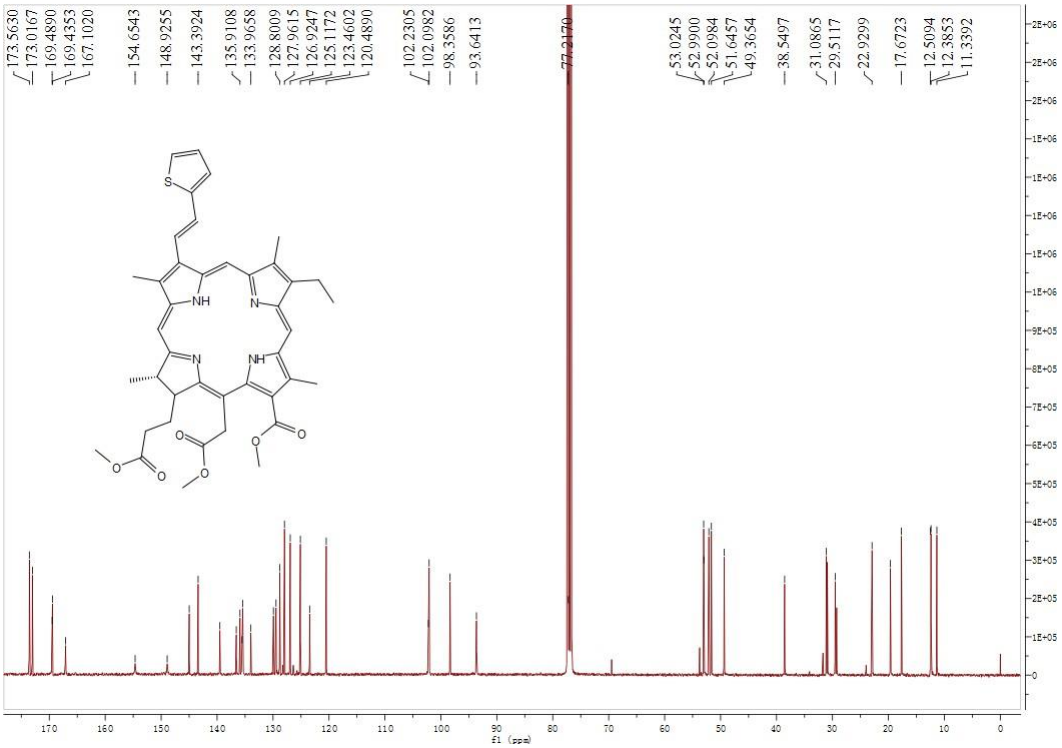
f1 (ppm)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127.9615
126.9247
125.1172
123.4602
120.4890
102.2305
102.0982
98.3586
93.6413
77.2170
53.0245
52.9900
52.0984
51.6457
49.3654
38.5497
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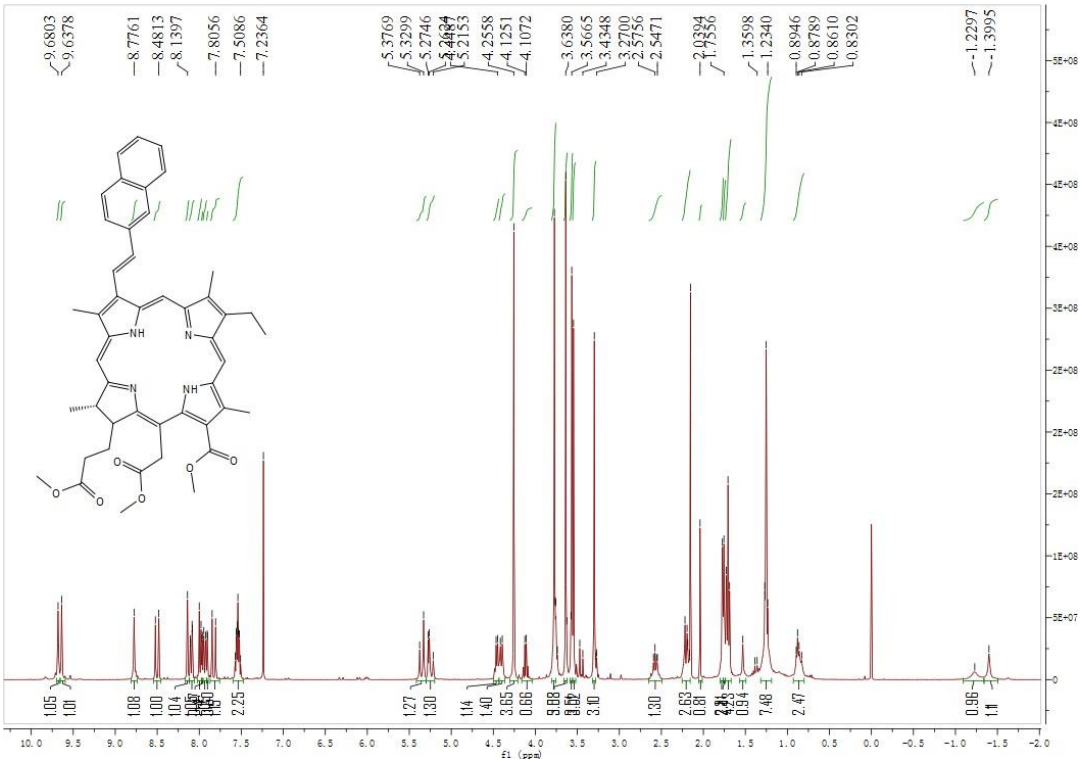
11.3392
f1 (ppm)

Compound **4c**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5.2153
4.2558
4.1251
4.1072
3.6380
3.5665
3.4348
3.2700
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2.5471
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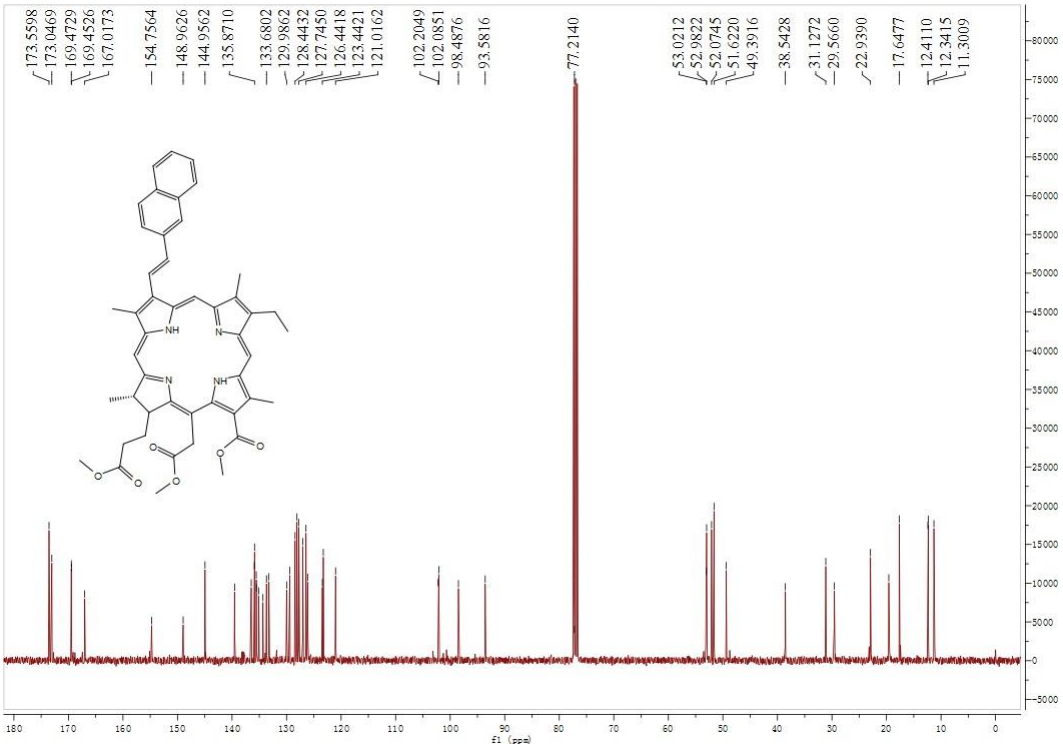
f1 (ppm)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128.4432
127.7450
126.4418
123.4421
121.0162
102.2049
102.0851
98.4876
93.5816
77.2140
53.0212
52.9822
52.0745
51.6220
49.3916
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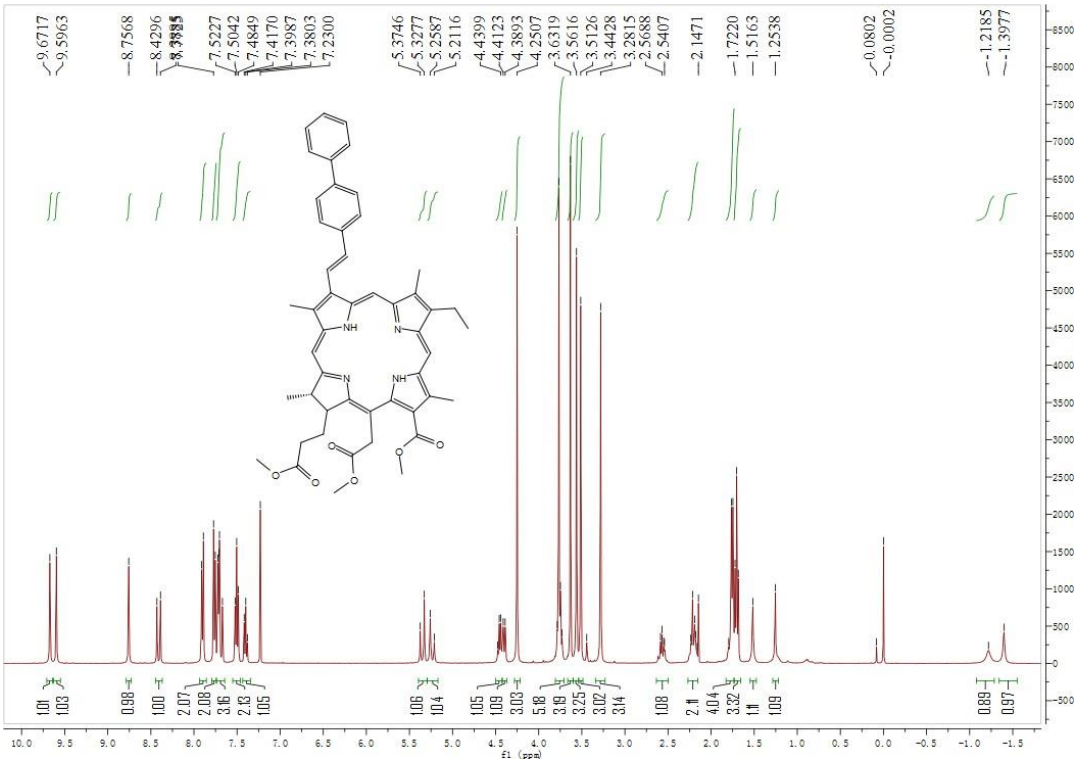
17.6477
12.4110
12.3415
11.3009
f1 (ppm)

Compound **4d**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5.3746
5.3277
5.2587
5.2116
4.4399
4.4123
4.3893
4.2507
3.6319
3.5616
3.5126
3.4428
3.2815
2.5688
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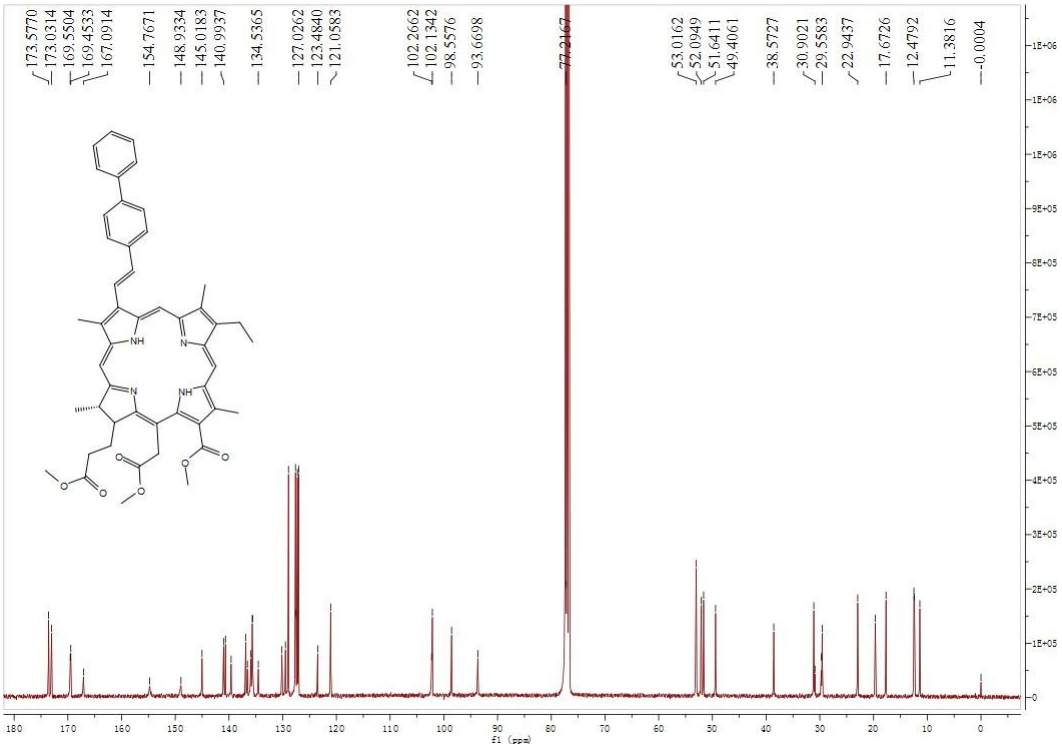
f1 (ppm)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123.4840
121.0583
102.2662
102.1342
98.5576
93.6698
77.2167
53.0162
52.0949
51.6411
49.4061
38.5727
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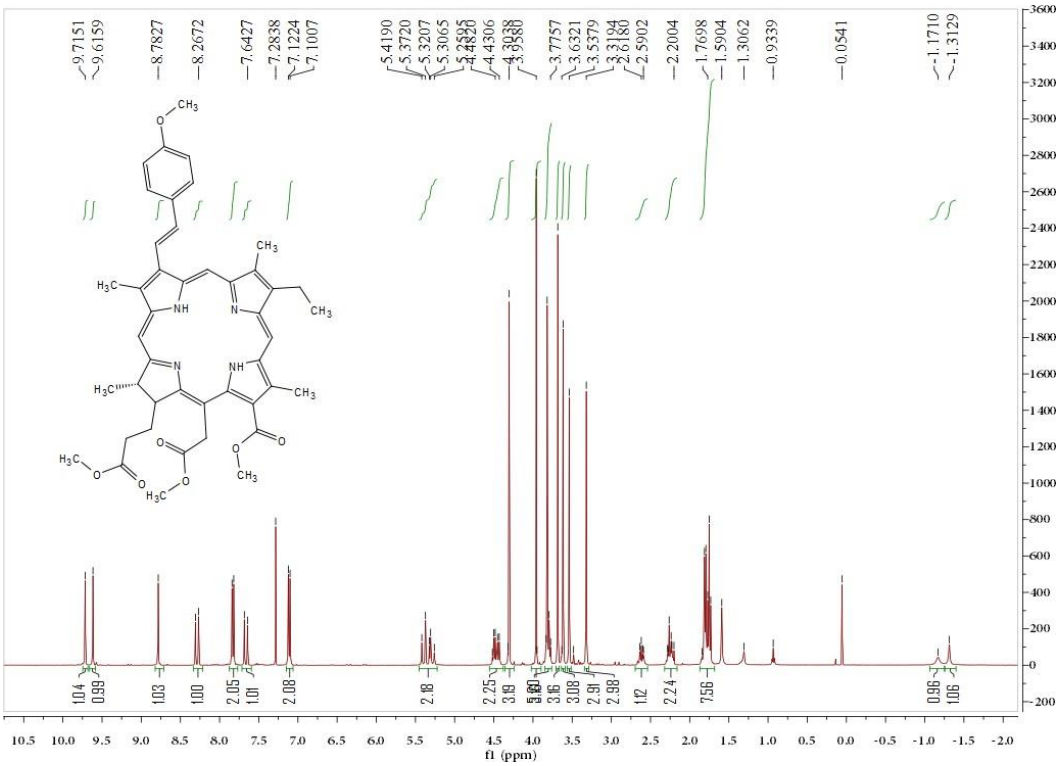
f1 (ppm)

Compound **4e**



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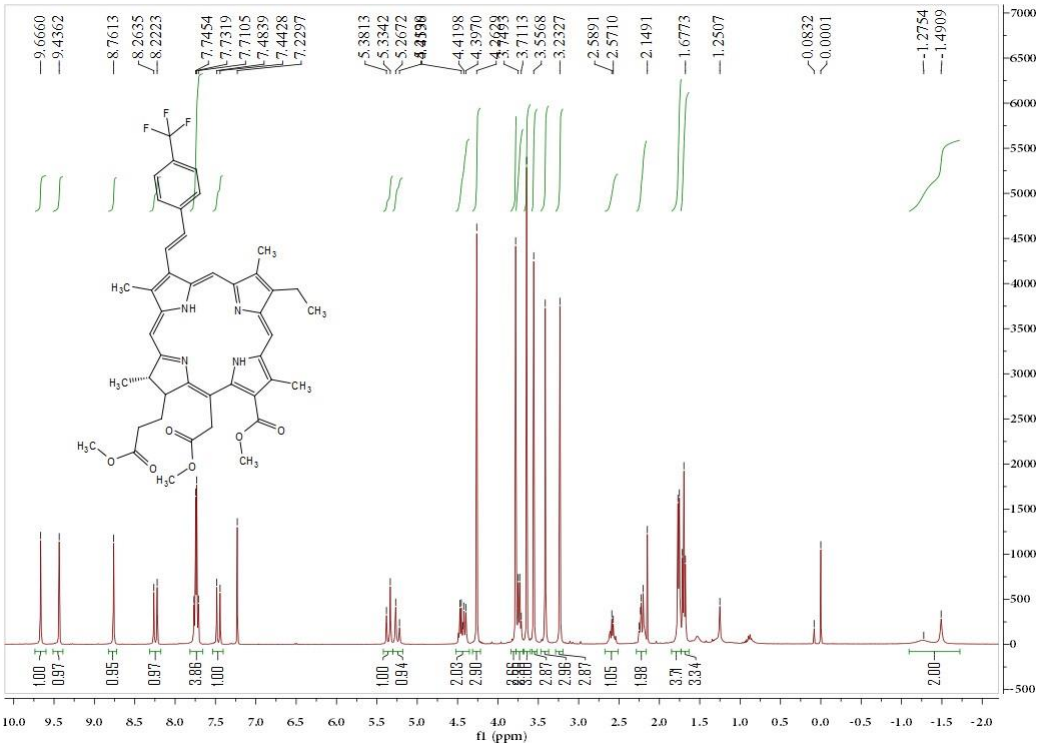

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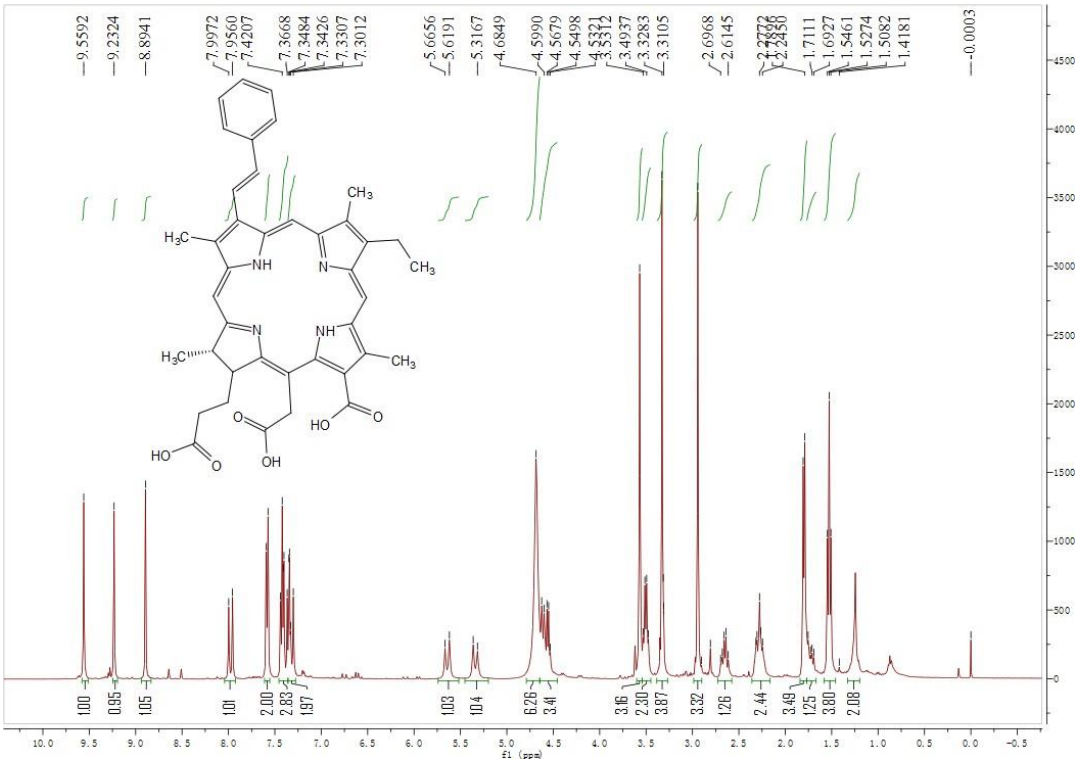
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7.3012
5.6656
5.6191
5.3167
4.6849
4.5990
4.5679
4.5498
4.5321
4.5312
3.4937
3.3283
3.3105
2.6968
2.6145
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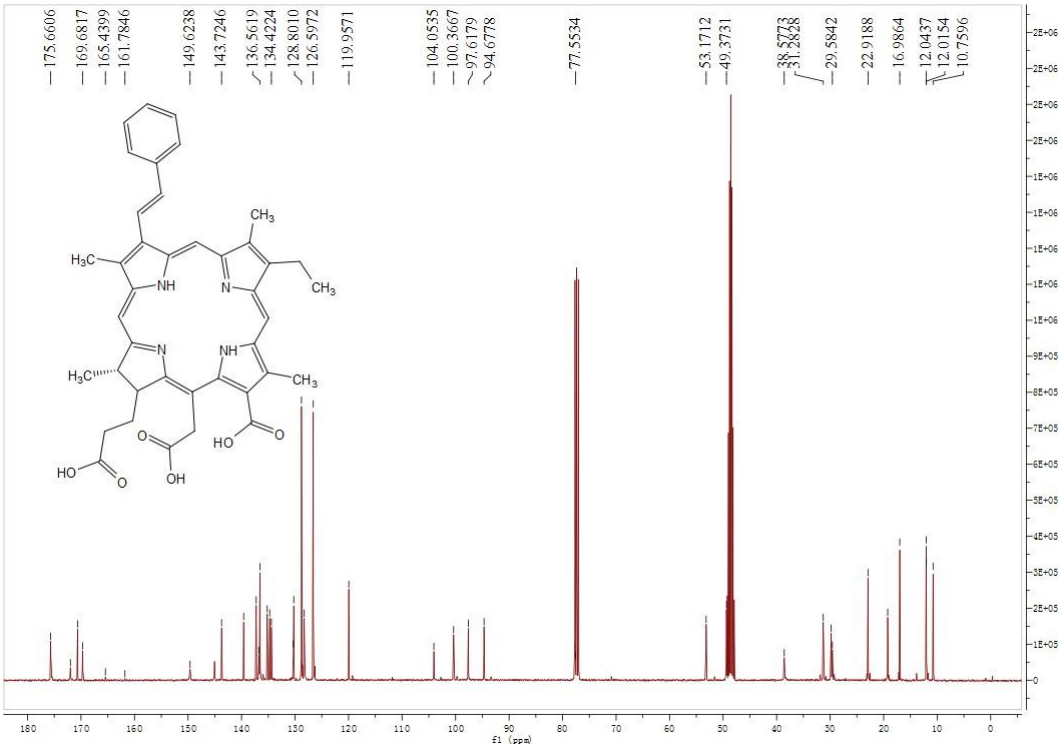
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119.9571
104.0535
100.3667
97.6179
94.6778
77.5534
53.1712
49.3731
38.5773
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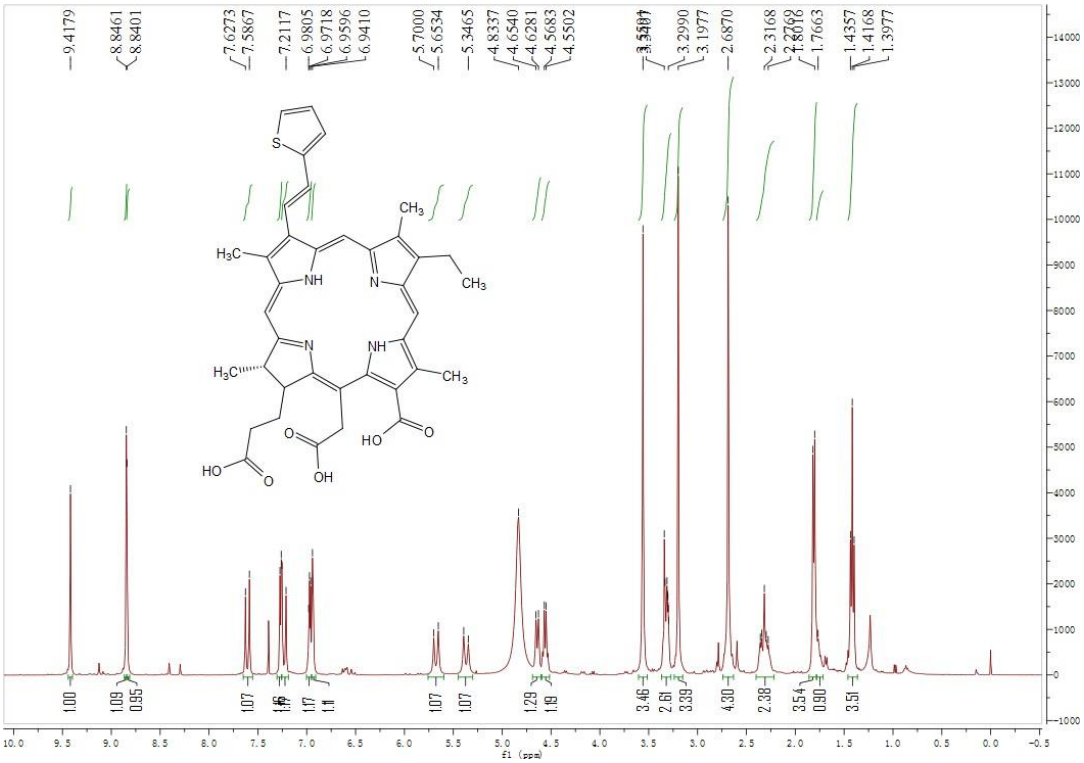
f1 (ppm)

Compound **5b**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6.9596
6.9410
5.7000
5.6534
5.3465
4.8337
4.6540
4.6281
4.5683
4.5502
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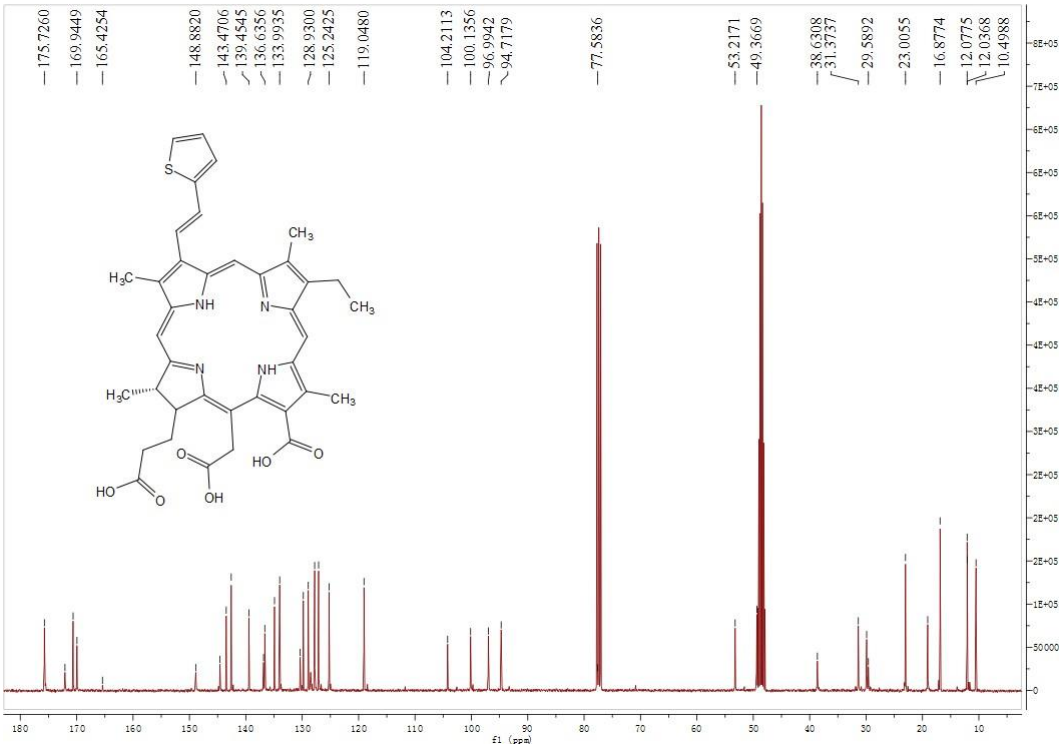
1.4168
1.3977
f1 (ppm)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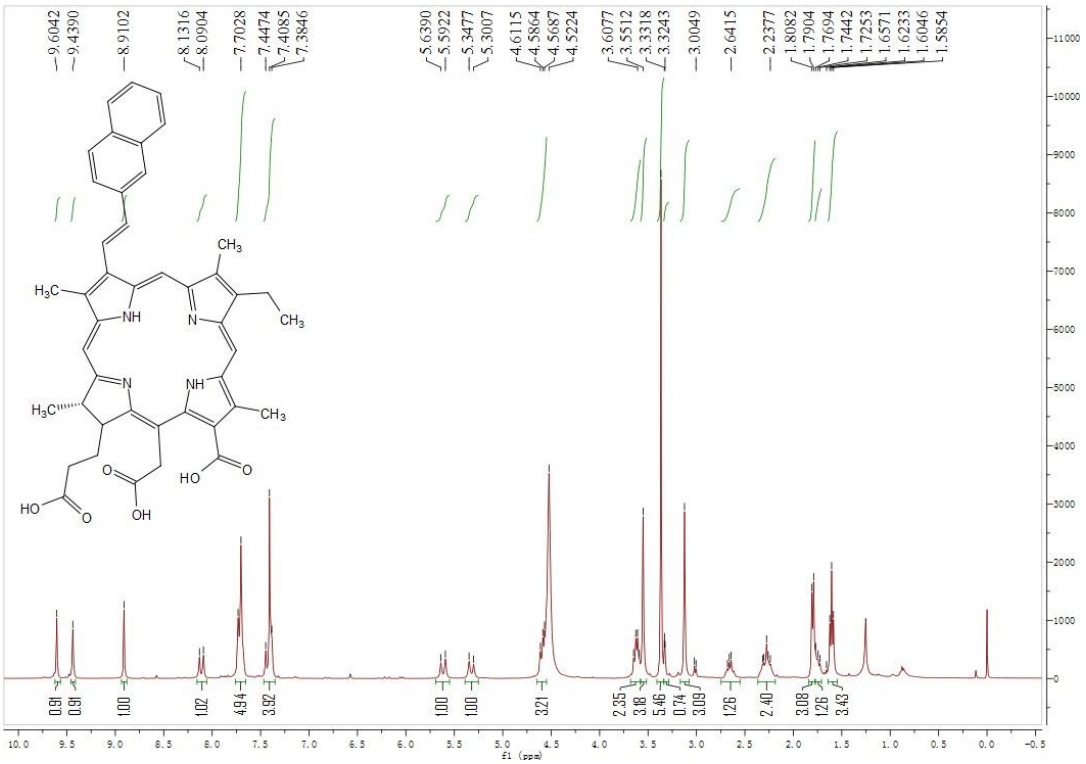
143.4706
139.4545
136.6356
133.9935
128.9300
125.2425
119.0480
104.2113
100.1356
96.9942
94.7179
77.5836
53.2171
49.3669
38.6308
31.3737
29.5892
23.0055
16.8774
12.0775
12.0368
10.4988
f1 (ppm)

Compound **5c**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7.3846
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5.5922
5.3477
5.3007
4.6115
4.5864
4.5687
4.5224
3.6077
3.5512
3.3318
3.3243
3.0049
2.6415
2.2377
1.8082
1.7904
1.7694
1.7442
1.7253
1.6571
1.6233
1.6046
1.5854
0.91
0.91
1.00
1.02
4.94
3.92
1.00
1.00
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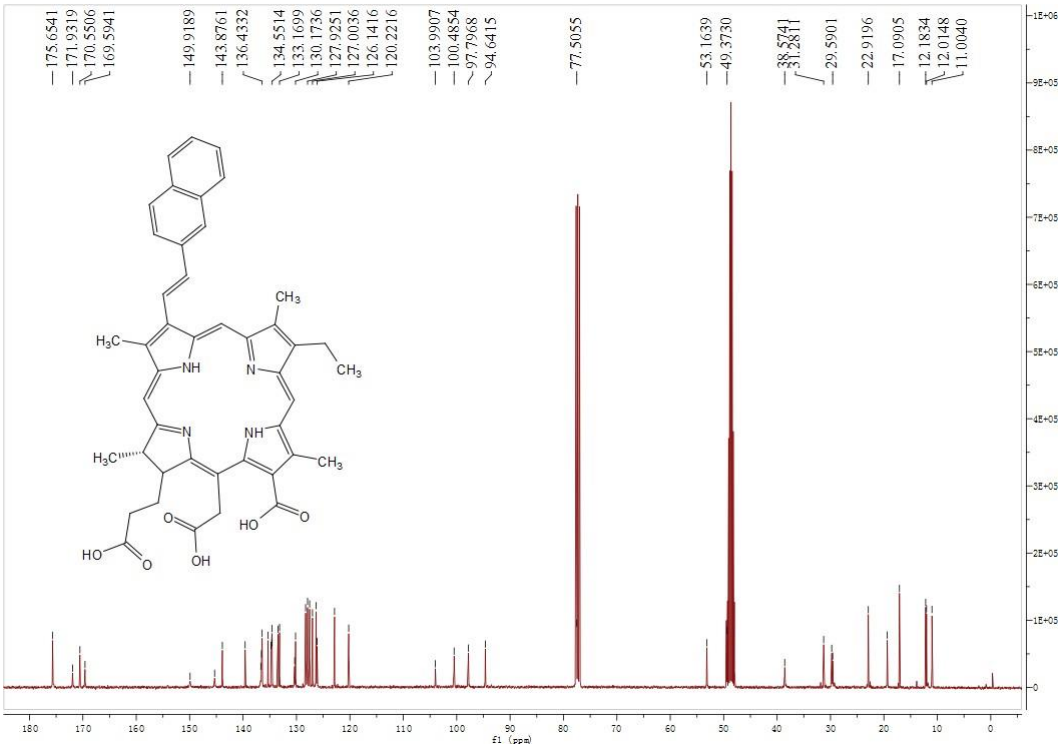
3.08
1.26
3.43
f1 (ppm)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127.0036
126.1416
120.2216
103.9907
100.4854
97.7968
94.6415
77.5055
53.1639
49.3730
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22.9196
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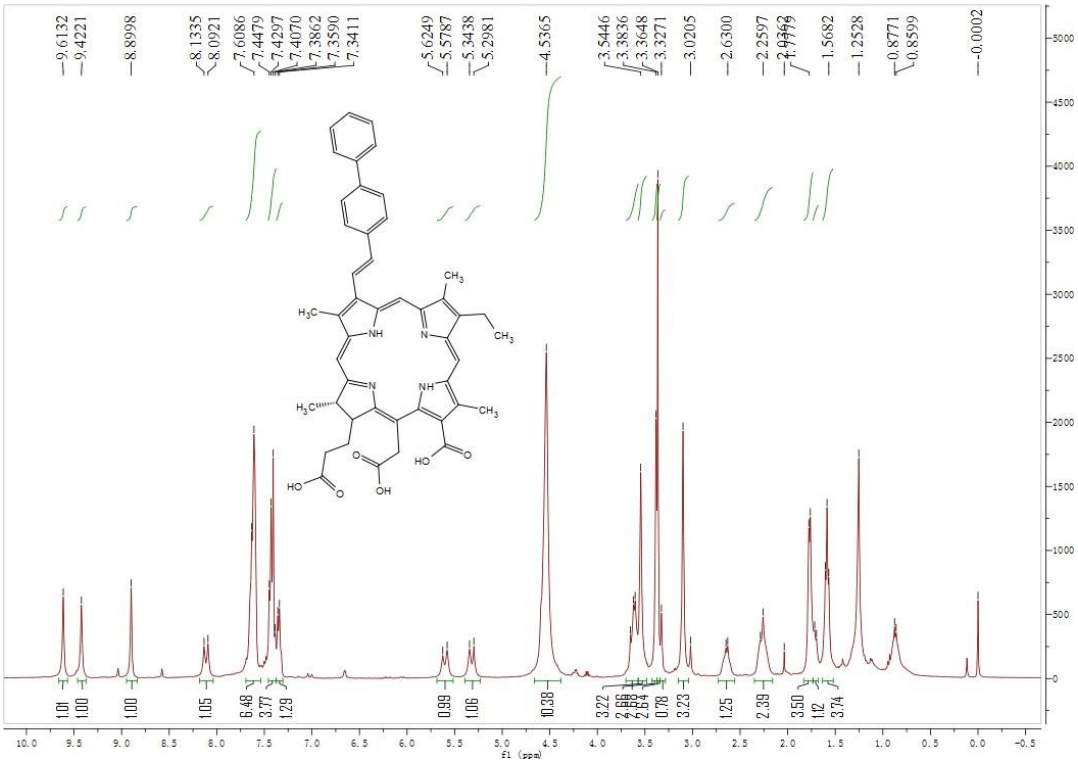
12.1834
12.0148
11.0040
f1 (ppm)

Compound **5d**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7.4479
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7.3862
7.3590
7.3411
5.6249
5.5787
5.3438
5.2981
4.5365
3.5446
3.3836
3.3648
3.3271
3.0205
2.6300
2.2597
1.5682
1.2528
0.8771
0.8599
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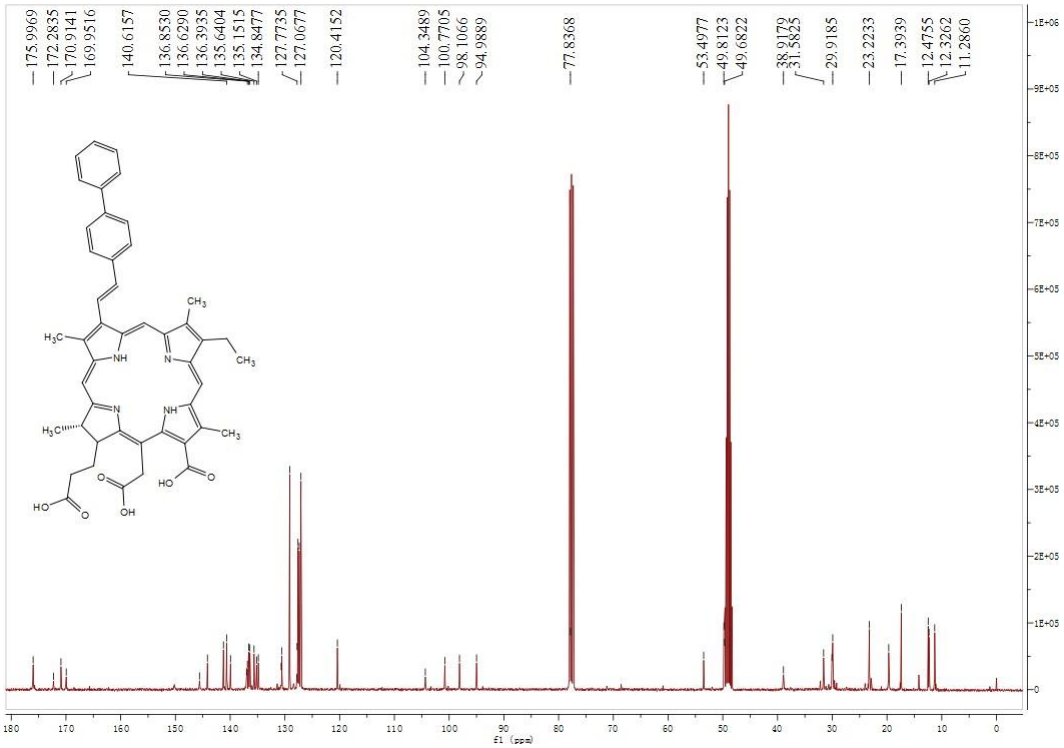
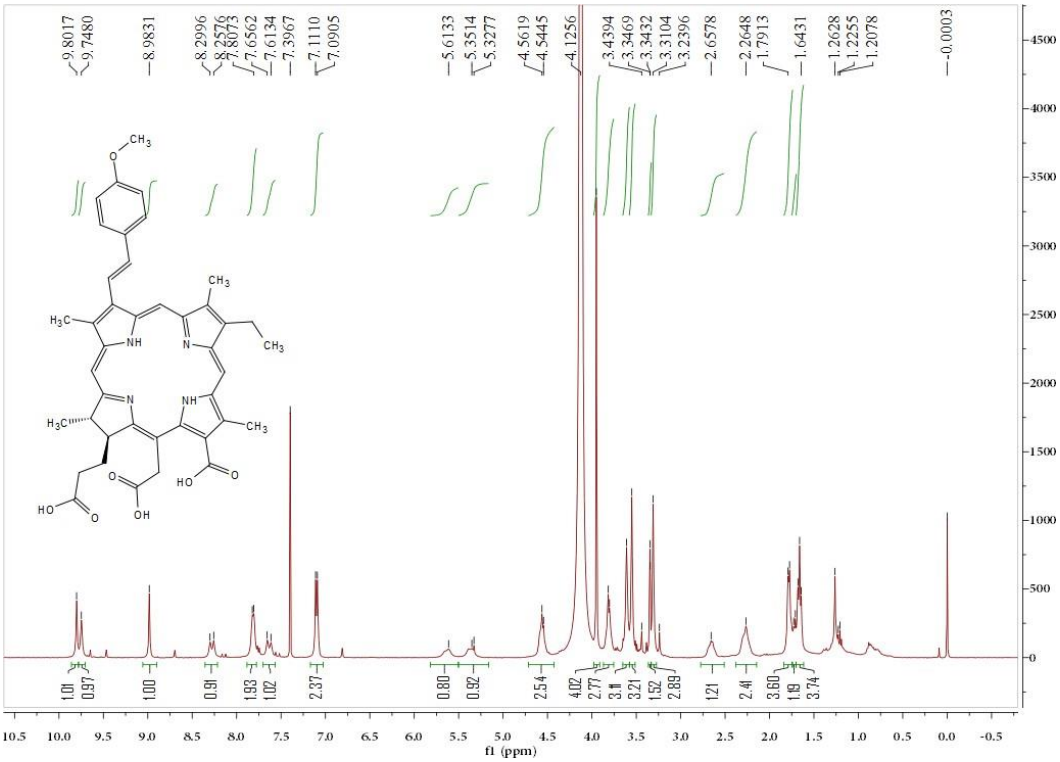
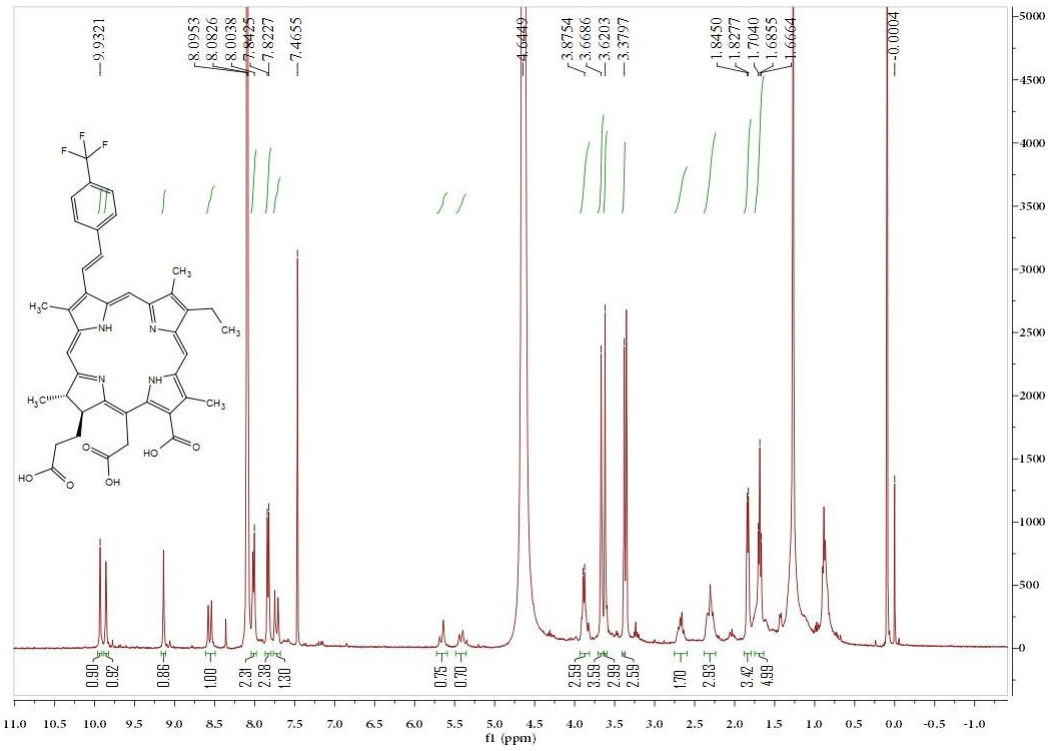
1.01
1.00
1.00
1.05
6.48
3.77
1.29
0.99
1.06
10.38
3.22
0.78
3.23
1.25
2.39
3.50
1.12
3.74
f1 (ppm)


175.9969
172.2835
170.9141
169.9516
140.6157
136.8530
136.6290
136.3935
135.6404
135.1515
134.8477
127.7735
127.0677
120.4152
104.3489
100.7705
98.1066
94.9889
77.8368
53.4977
49.8123
49.6822
38.9179
31.5825
29.9185
23.2233
17.3939
12.4755
12.3262
11.2860
f1 (ppm)

Compound **5e**



Compound **5f**