Supporting Information

Identification of probe-quality degraders for Poly (ADP-ribose) polymerase-1 (PARP-1)

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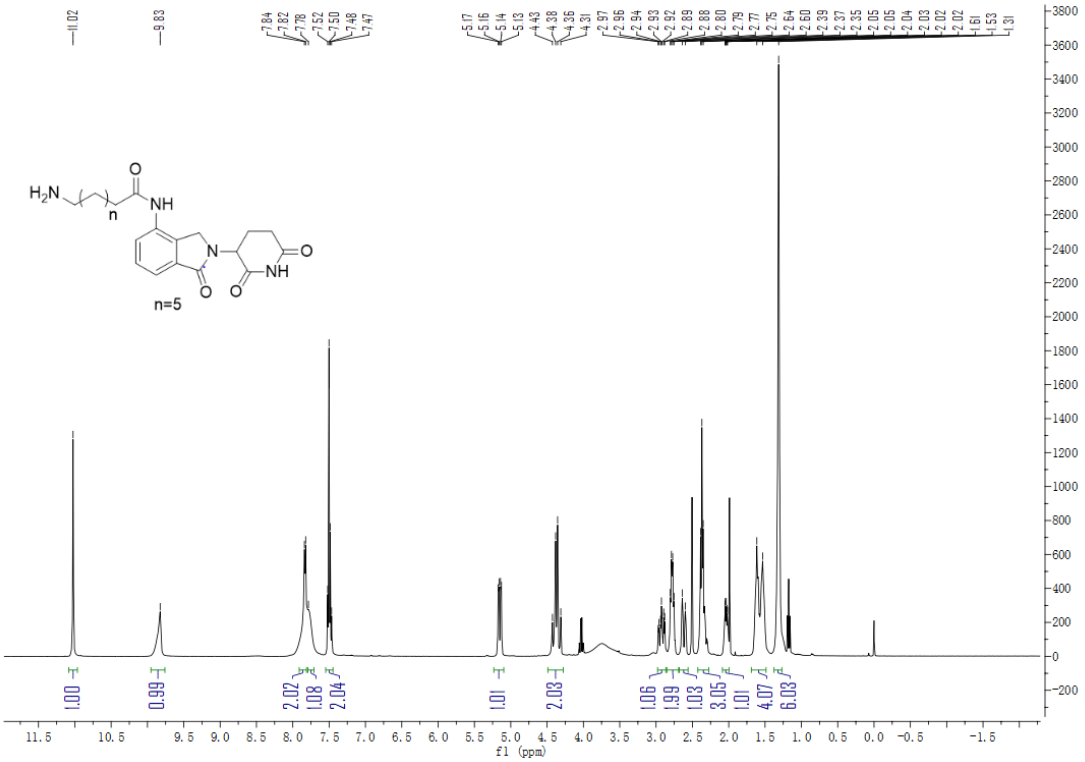
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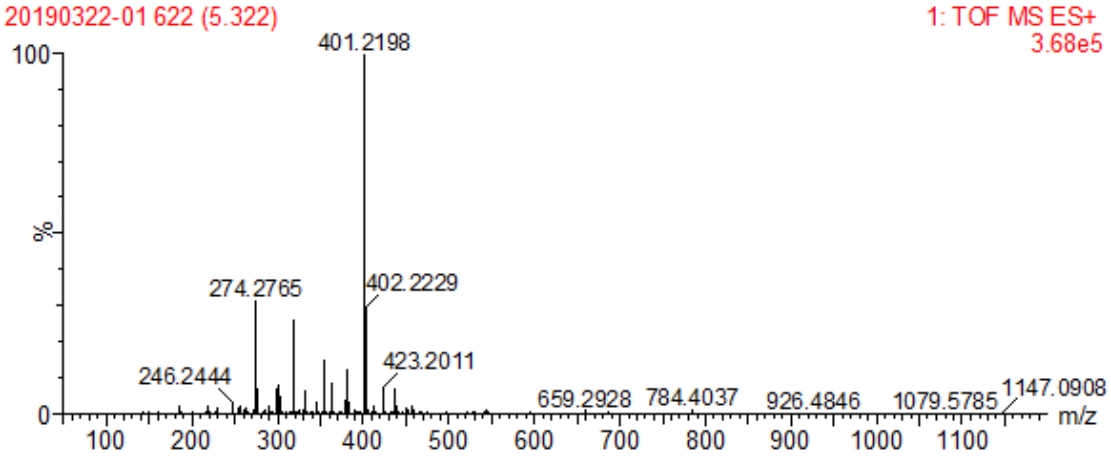
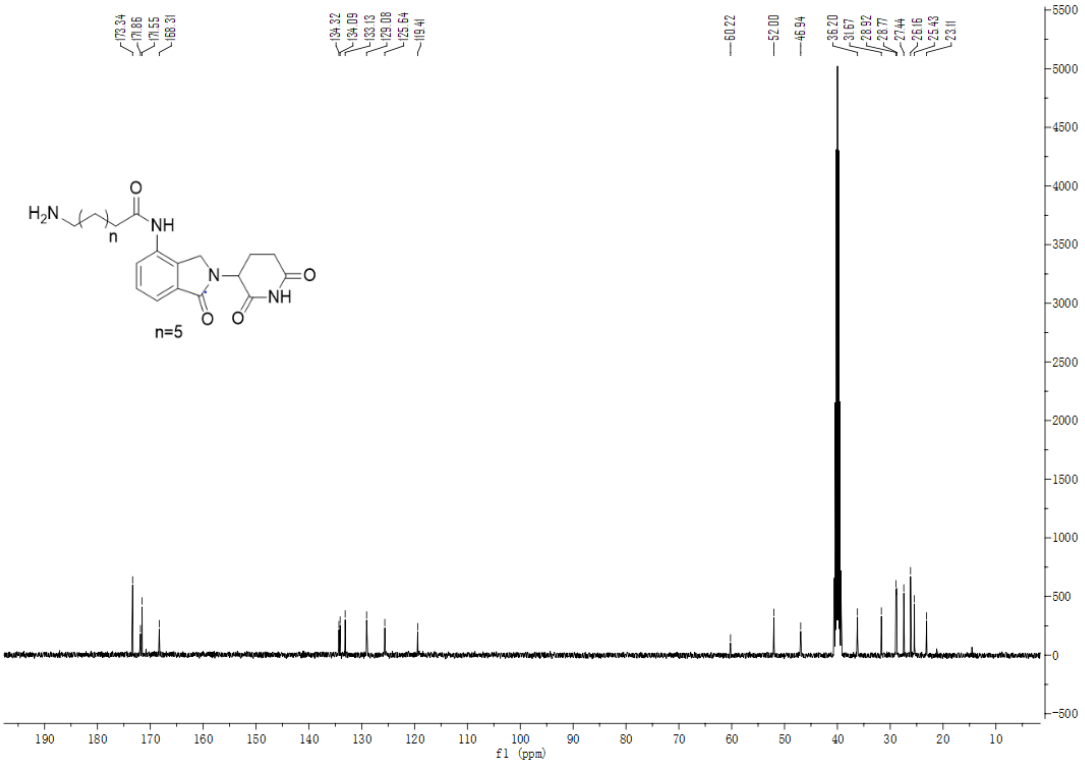

20190322-01 622 (5.322)
1: TOF MS ES+
3.68e5
401.2198
274.2765
402.2229
423.2011
246.2444
659.2928
784.4037
926.4846
1079.5785
1147.0908
m/z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171.86
171.55
168.31
134.32
134.09
133.13
129.08
125.64
119.41
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31.67
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28.77
27.44
26.16
25.43
23.11
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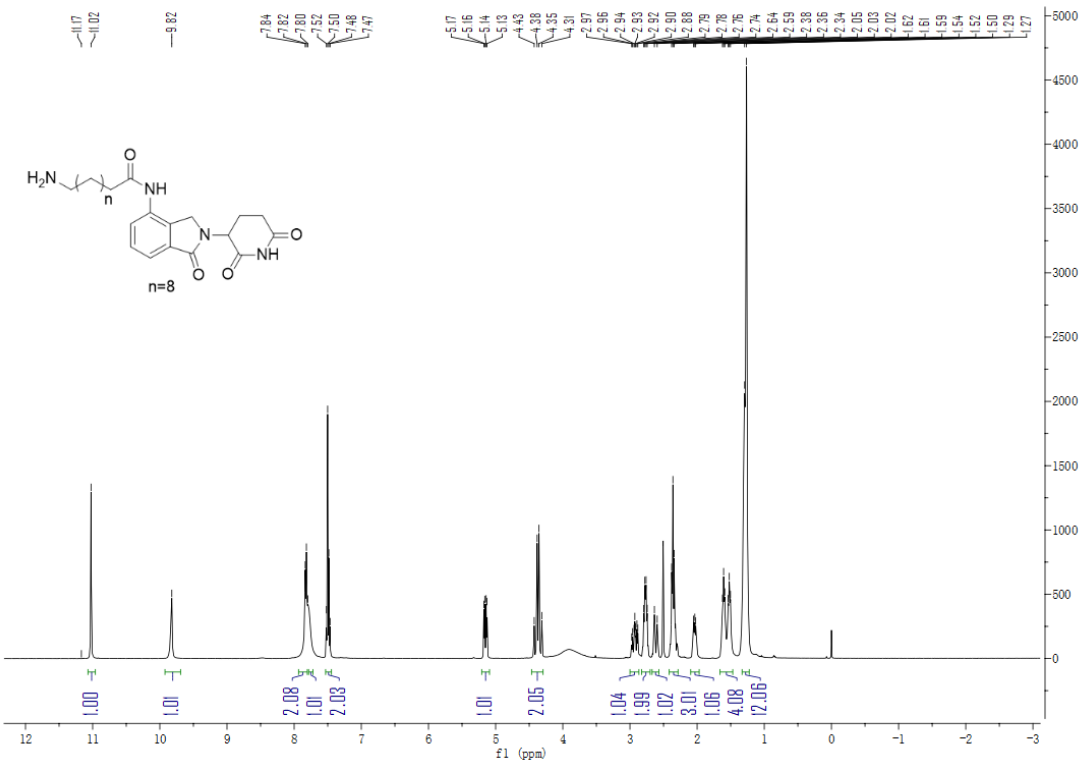
f1 (ppm)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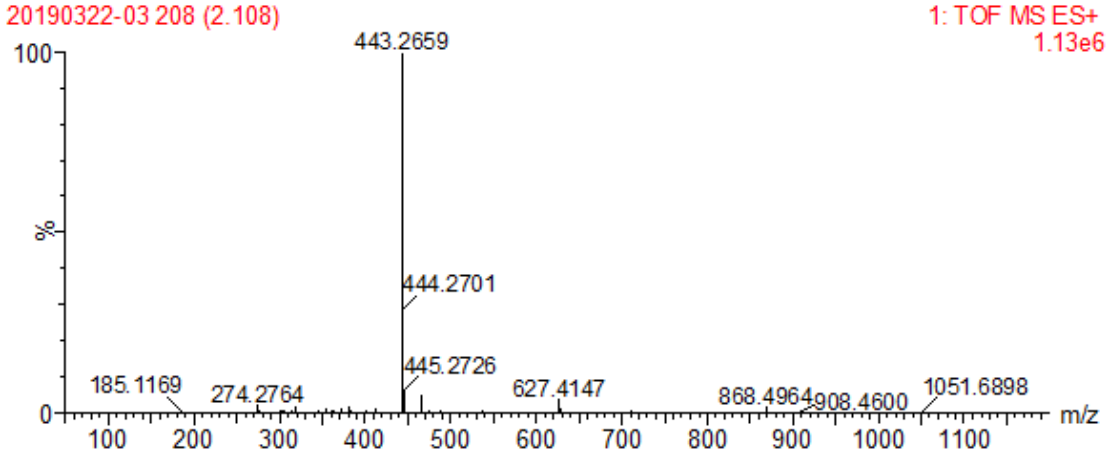
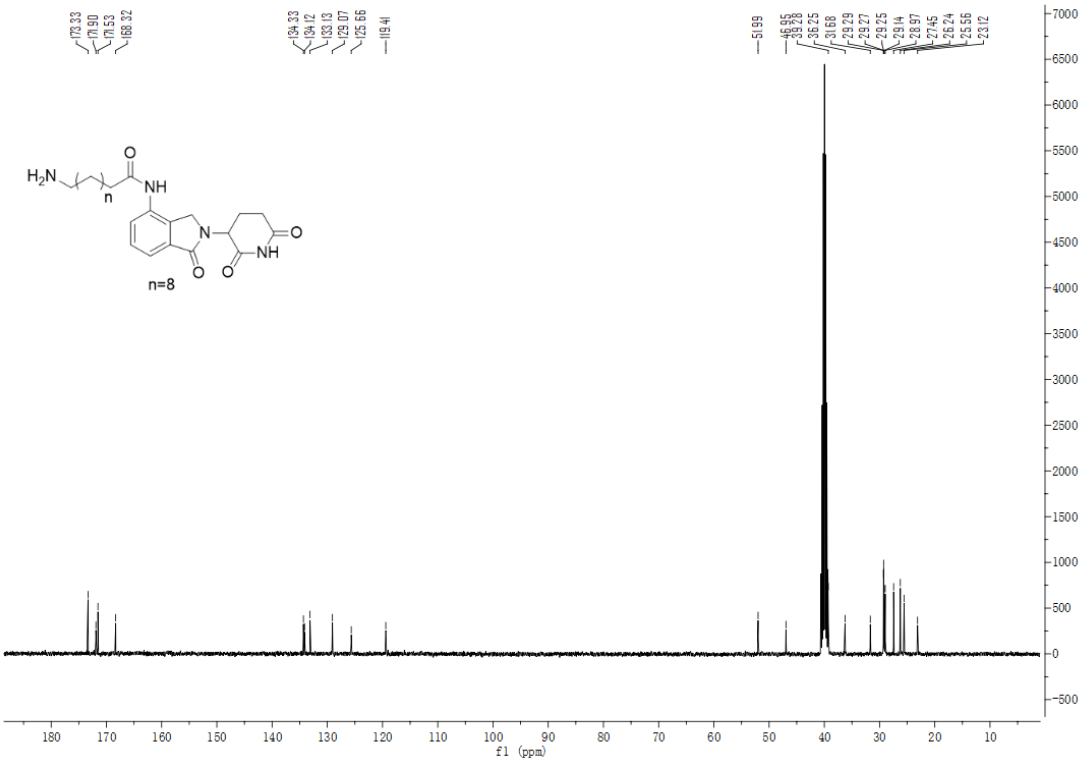
f1 (ppm)


20190322-03 208 (2.108)
1: TOF MS ES+
1.13e6
443.2659
444.2701
445.2726
185.1169
274.2764
627.4147
868.4964
908.4600
1051.6898
m/z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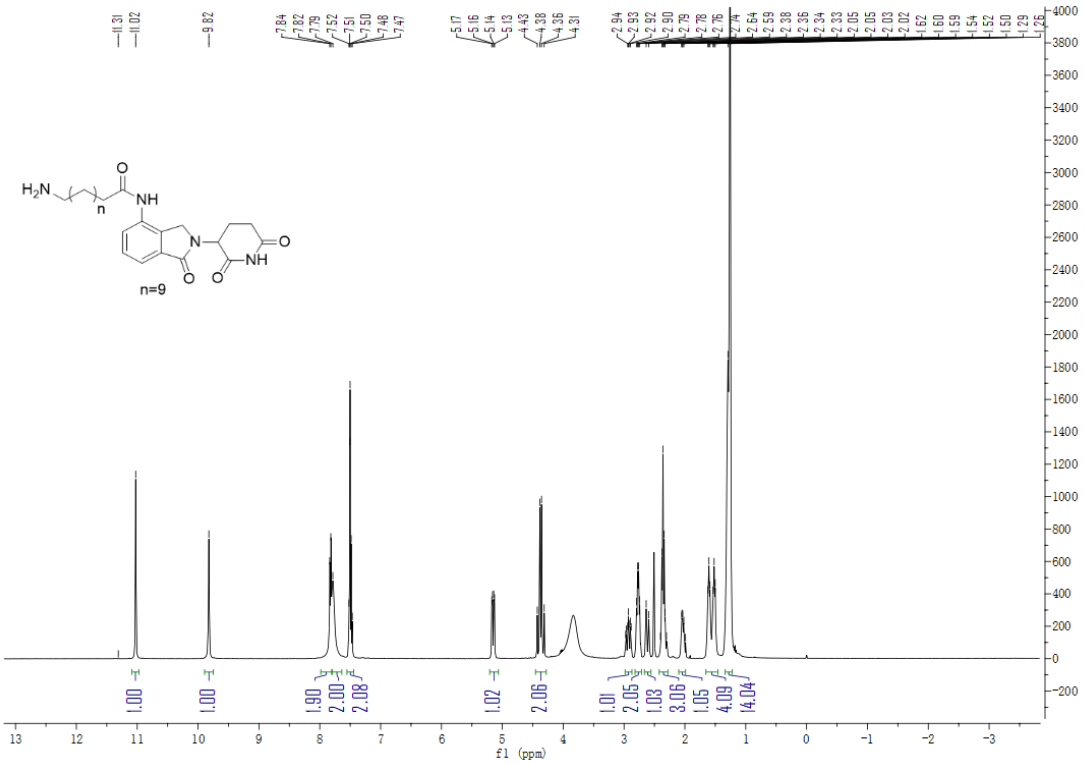
171.90
171.53
168.32
134.33
134.12
132.13
129.07
125.66
119.41
51.99
46.55
39.28
36.25
31.68
29.29
29.27
29.25
29.14
28.97
27.45
26.24
25.56
23.12
H2N
n
O
NH
N
O
NH
O
O
n=8
f1 (ppm)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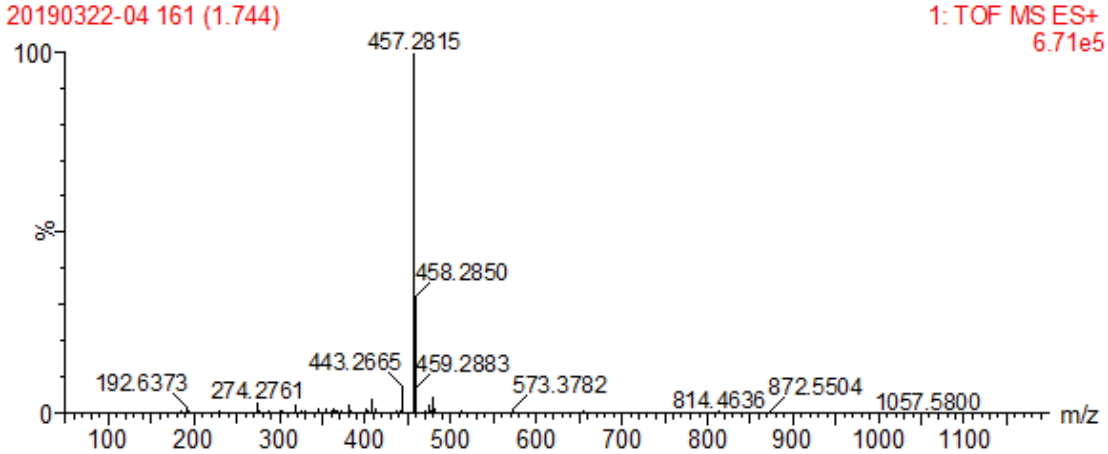
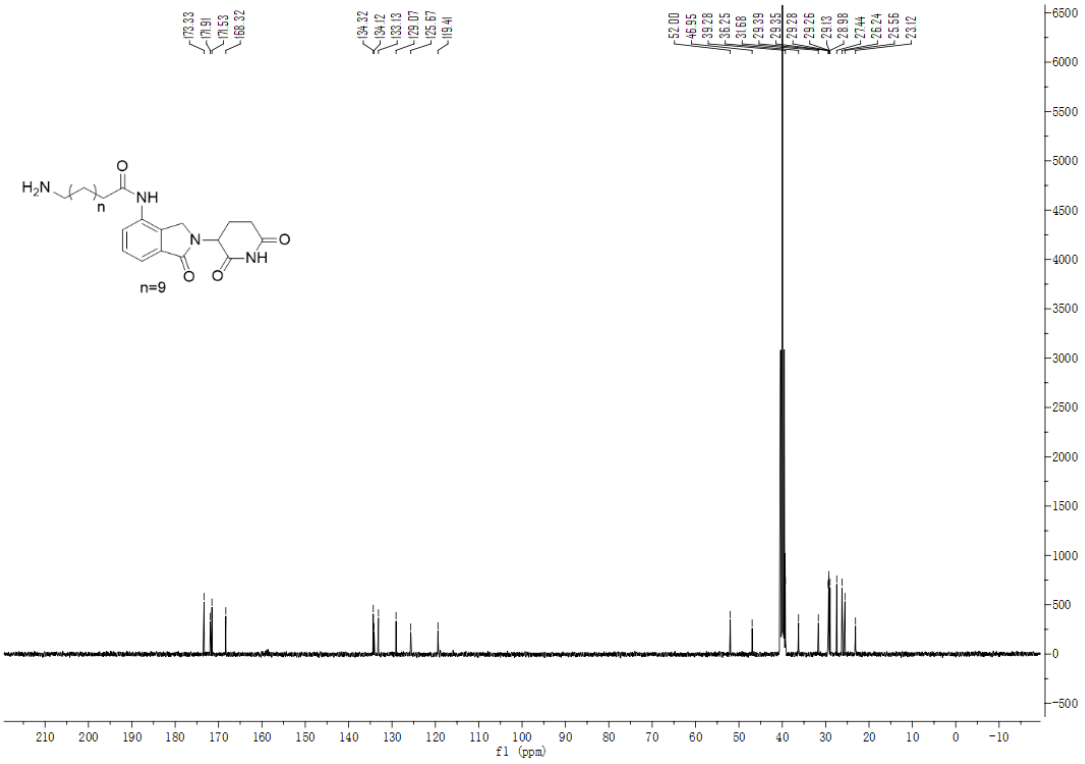

20190322-04 161 (1.744)
1: TOF MS ES+
6.71e5
457.2815
458.2850
443.2665
459.2883
192.6373
274.2761
573.3782
814.4636
872.5504
1057.5800
%
m/z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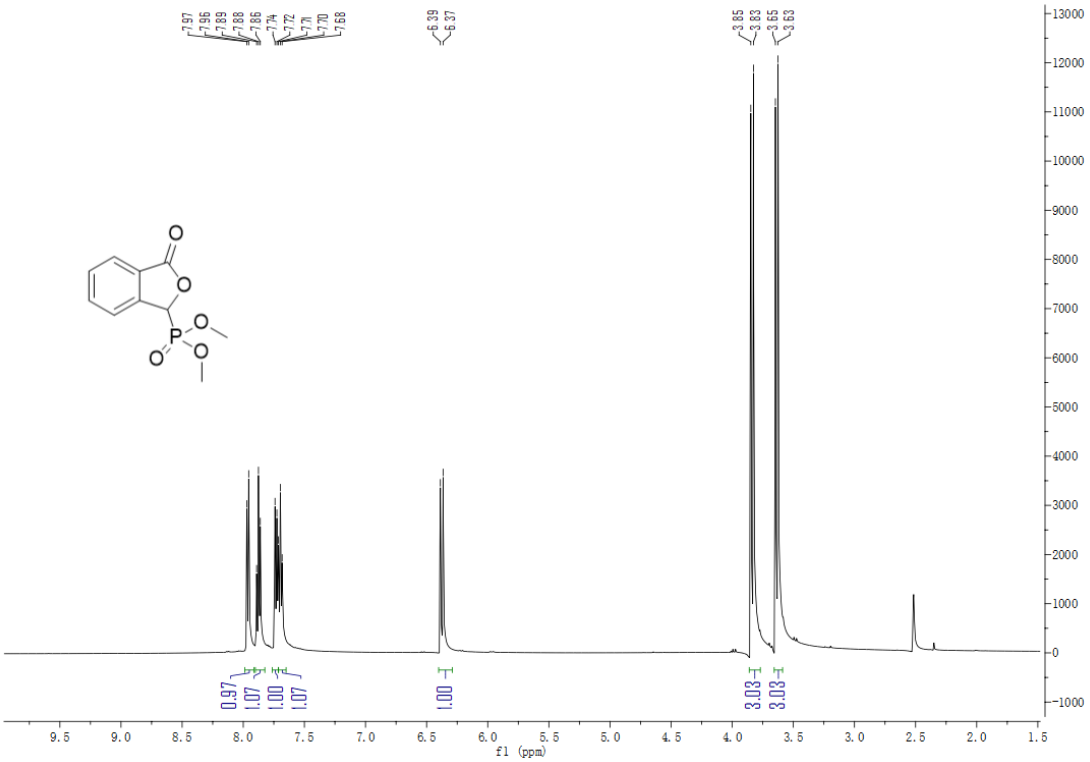
171.91
171.53
168.32
134.32
134.12
133.13
129.07
125.67
119.41
52.00
46.85
39.28
36.25
31.68
29.39
29.35
29.28
29.26
29.13
28.98
27.44
26.24
25.56
23.12
n=9
f1 (ppm)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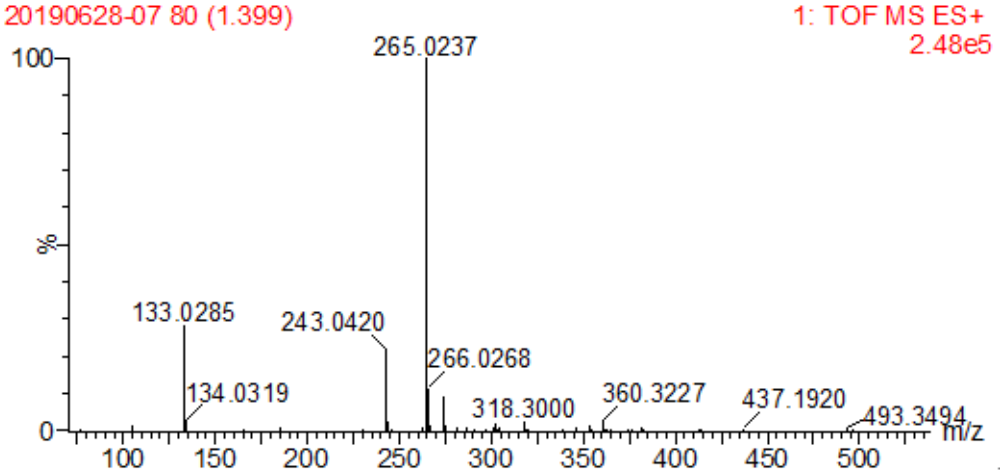
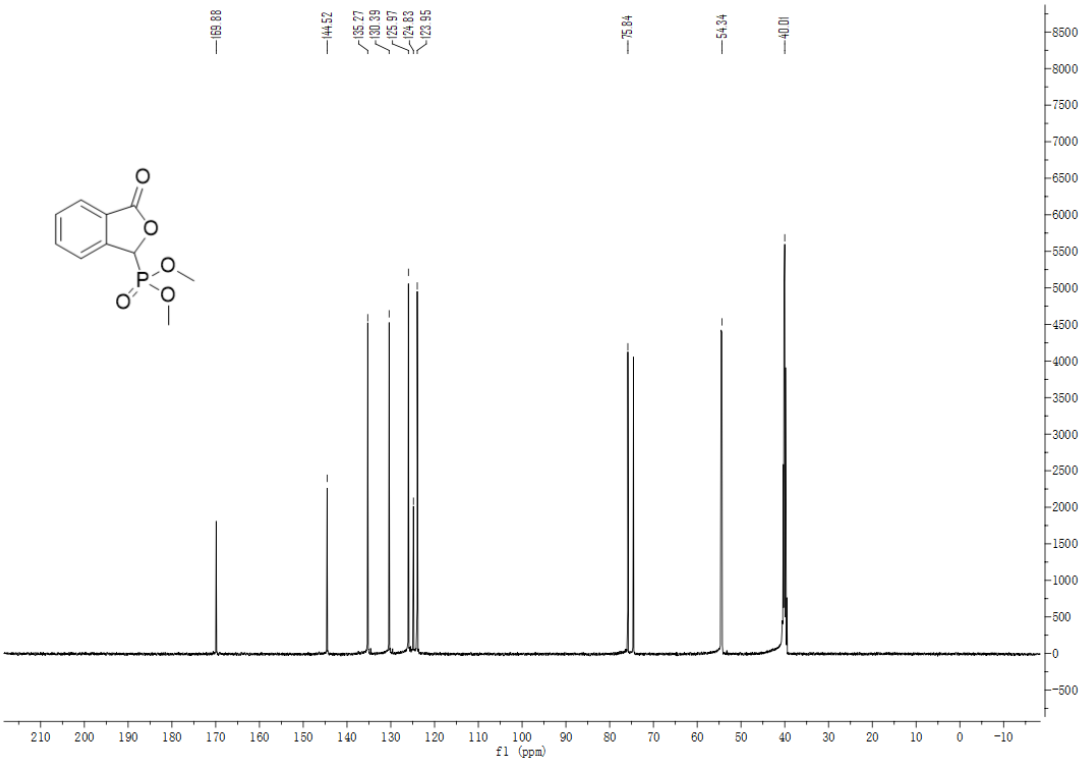
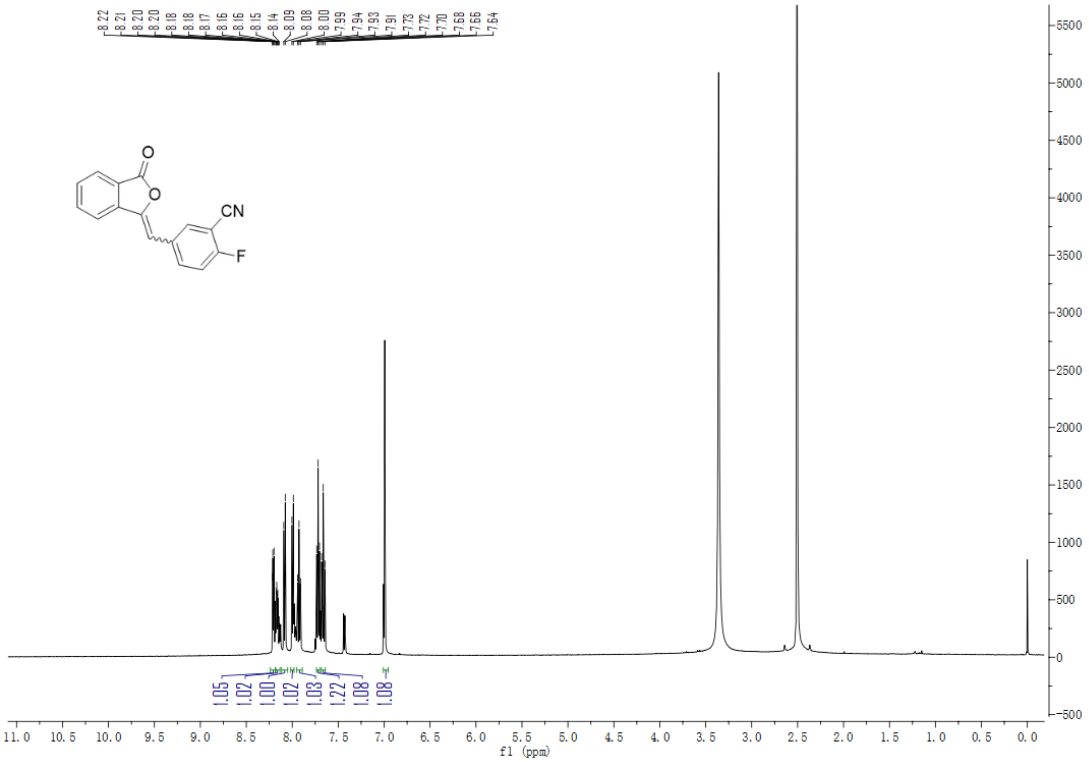
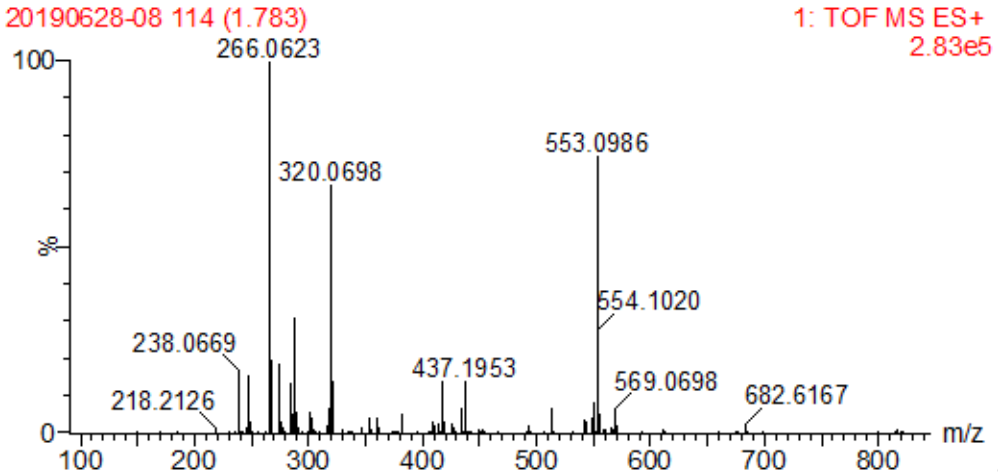
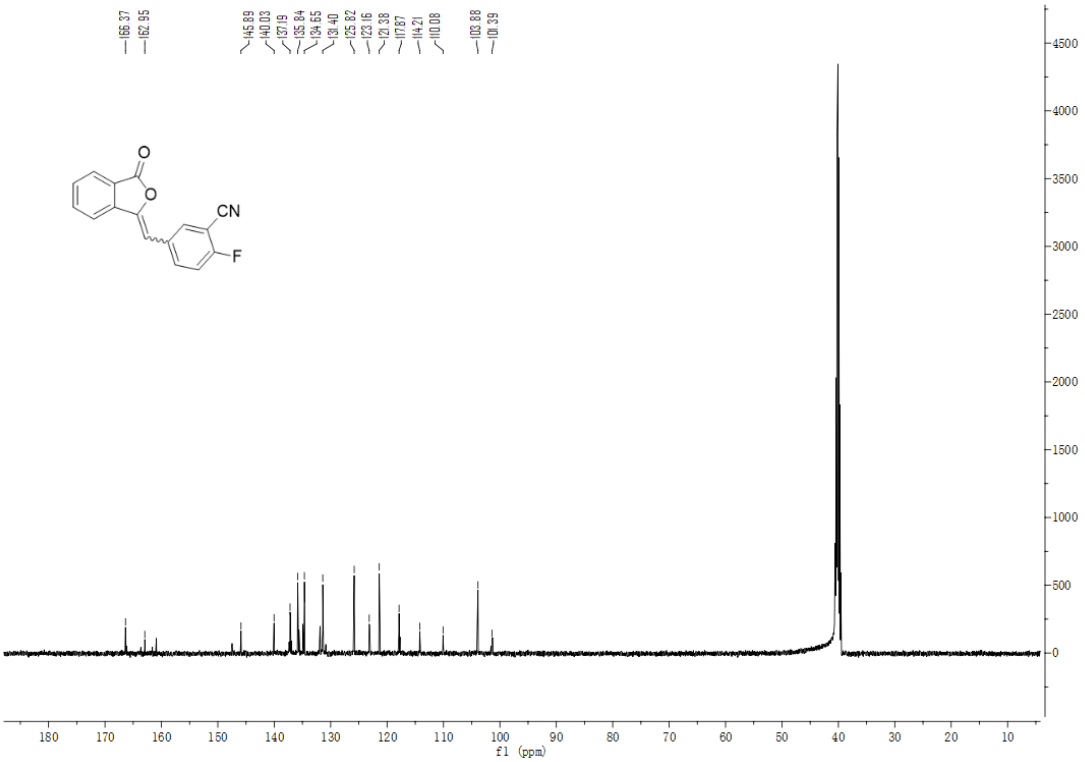
7.96
7.89
7.88
7.86
7.74
7.72
7.71
7.70
7.68
6.39
6.37
3.85
3.83
3.65
3.63
0.97
1.07
1.00
1.07
1.00
3.03
3.03
f1 (ppm)

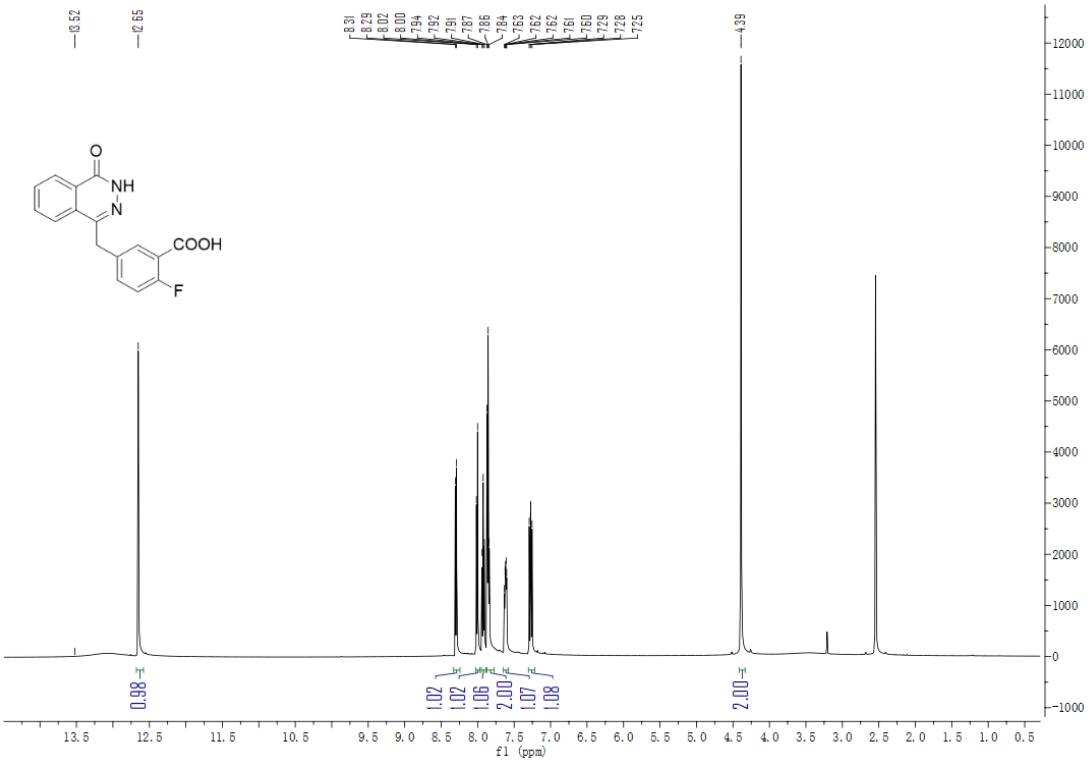

20190628-07 80 (1.399)
1: TOF MS ES+
2.48e5
265.0237
133.0285
243.0420
266.0268
134.0319
318.3000
360.3227
437.1920
493.3494
m/z
%


169.88
144.52
135.27
130.39
125.97
124.83
123.95
75.84
54.34
40.01
f1 (ppm)


O
O
CN
F
1.05
1.02
1.00
1.02
1.03
1.22
1.08
1.08
f1 (ppm)


20190628-08 114 (1.783)
1: TOF MS ES+
2.83e5
266.0623
320.0698
553.0986
554.1020
238.0669
218.2126
437.1953
569.0698
682.6167
%
m/z


166.37
162.95
145.89
140.03
137.19
135.84
134.65
131.40
125.82
123.16
121.38
117.87
114.21
110.08
103.88
101.39
O
O
CN
F
f1 (ppm)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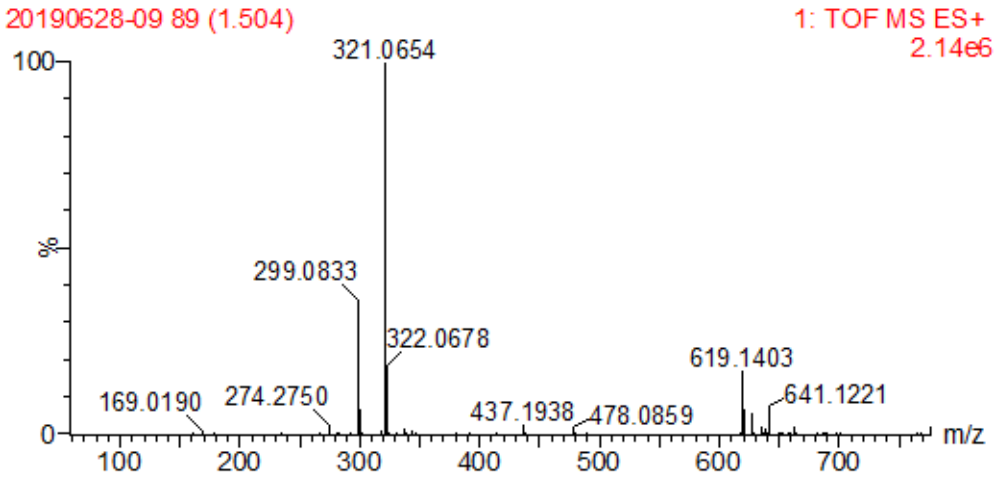
12.65
8.31
8.29
8.02
8.00
7.94
7.92
7.91
7.87
7.86
7.84
7.63
7.62
7.62
7.61
7.60
7.29
7.28
7.25
4.39
O
NH
N
COOH
F
0.98
1.02
1.02
1.06
2.00
1.07
1.08
2.00
f1 (ppm)


20190628-09 89 (1.504)
1: TOF MS ES+
2.14e6
321.0654
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322.0678
619.1403
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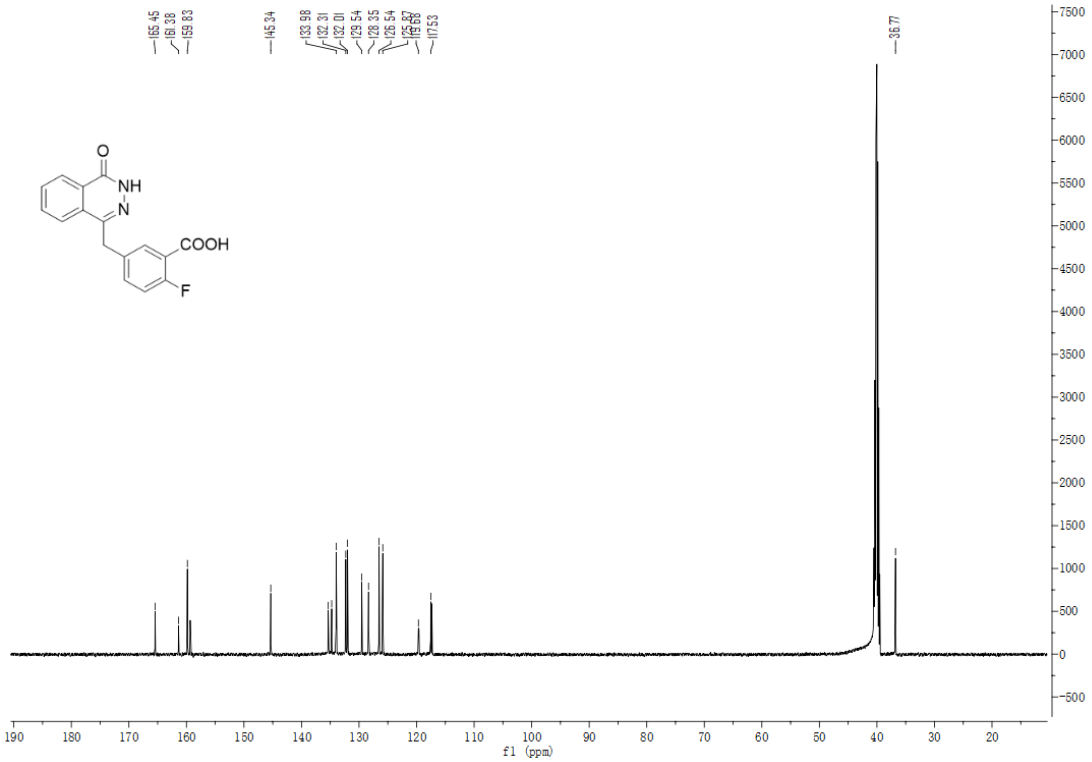
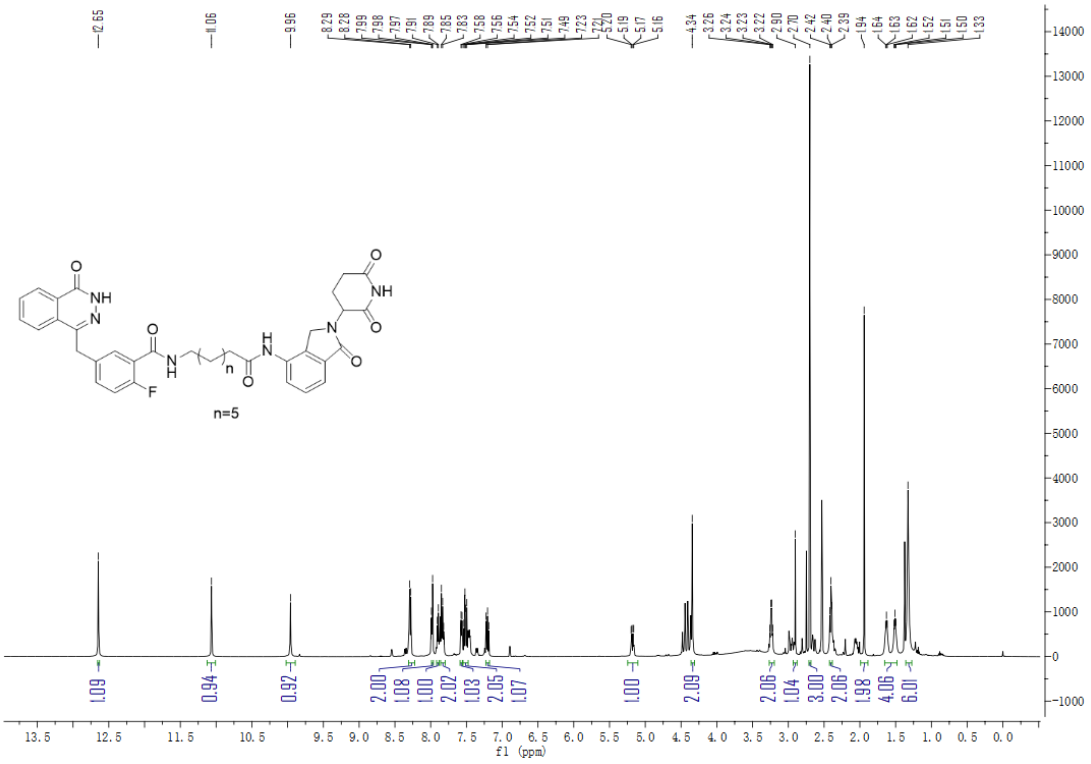
169.0190
274.2750
437.1938
478.0859
%
m/z


165.45
161.38
159.83
145.34
133.98
132.31
132.01
129.54
128.35
126.54
126.57
126.55
117.53
36.77
O
NH
N
COOH
F
f1 (ppm)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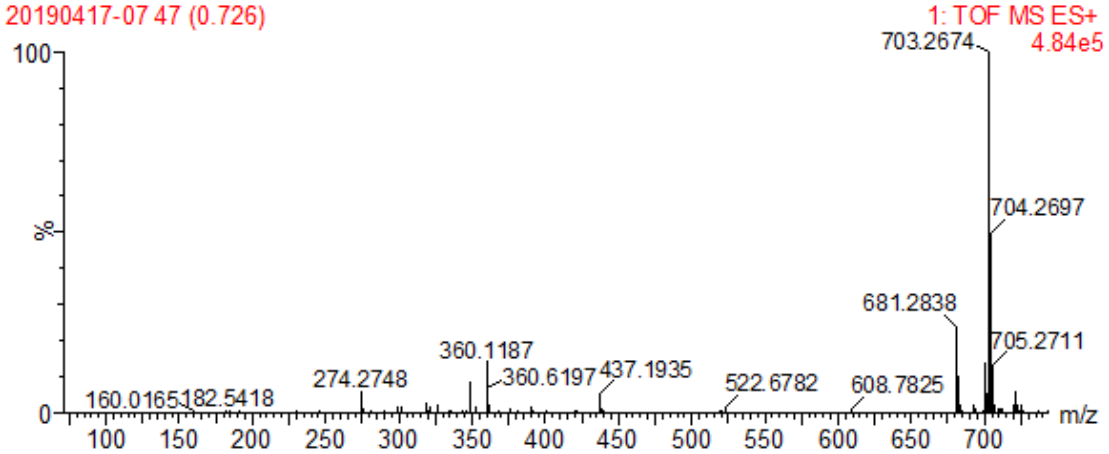
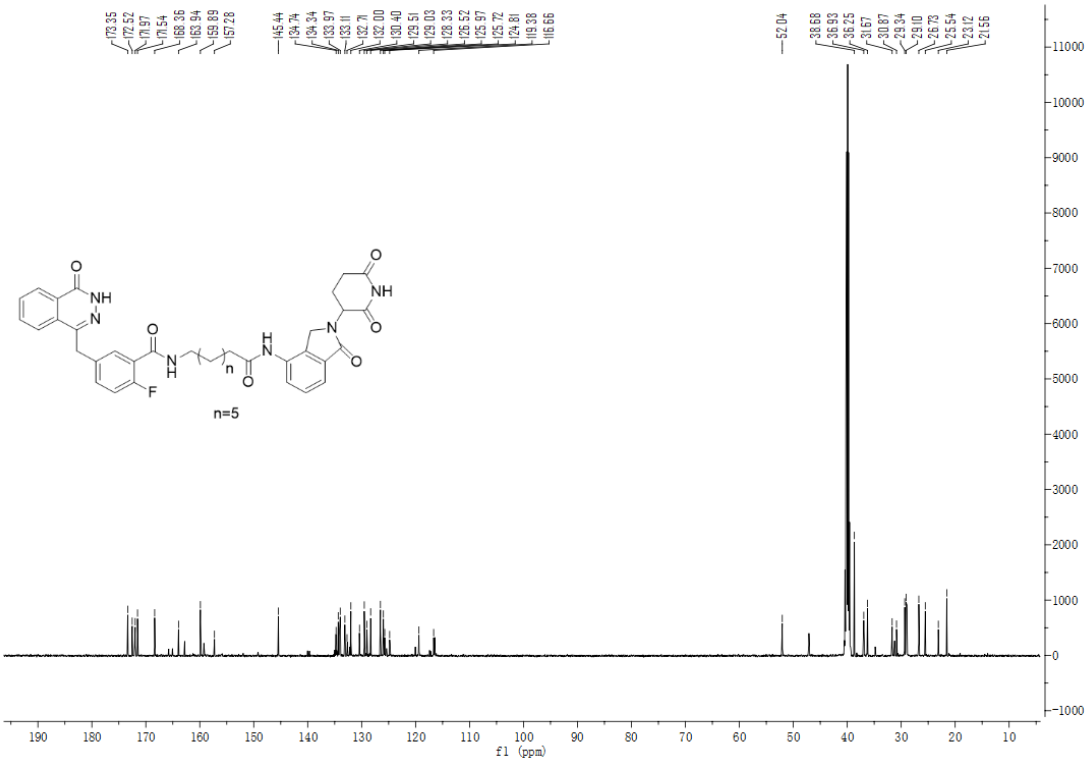
f1 (ppm)


20190417-07 47 (0.726)
1: TOF MS ES+
4.84e5
703.2674
704.2697
681.2838
705.2711
360.1187
360.6197
437.1935
274.2748
522.6782
608.7825
160.0165
182.5418
%
m/z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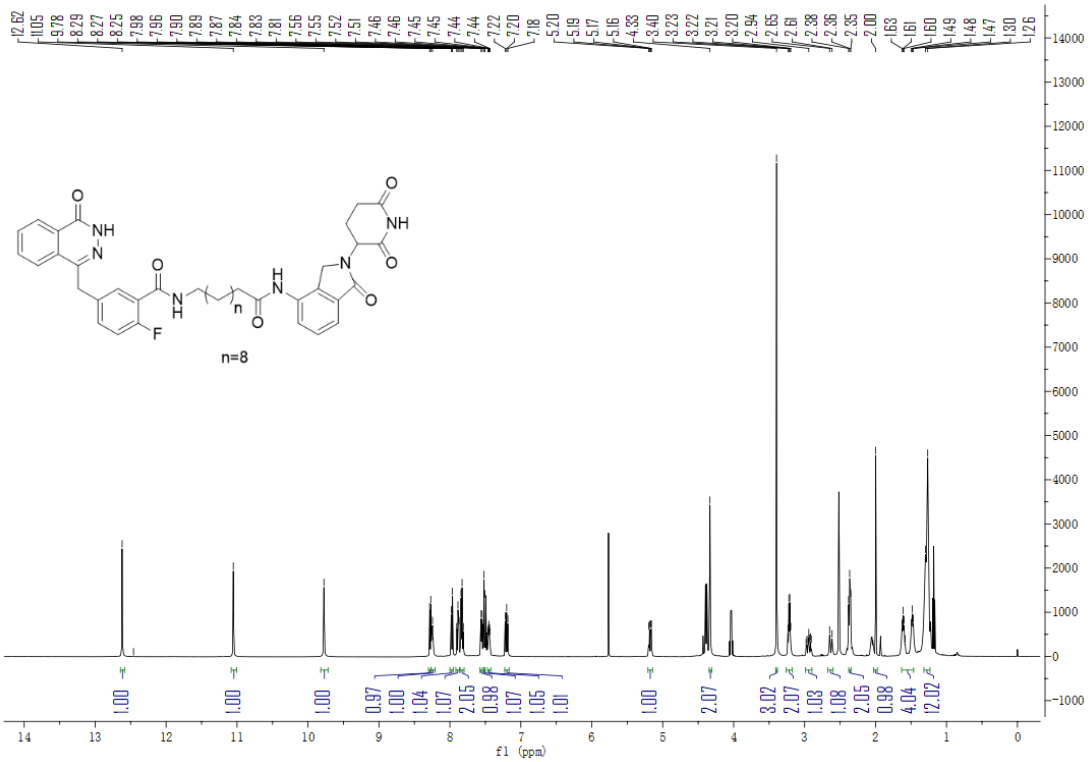
f1 (ppm)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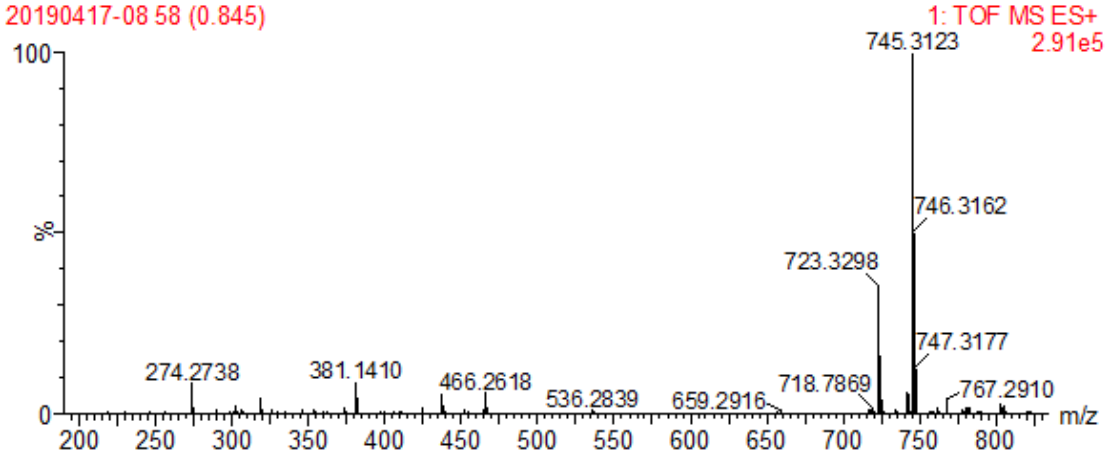
f1 (ppm)


20190417-08 58 (0.845)
1: TOF MS ES+
2.91e5
745.3123
746.3162
723.3298
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274.2738
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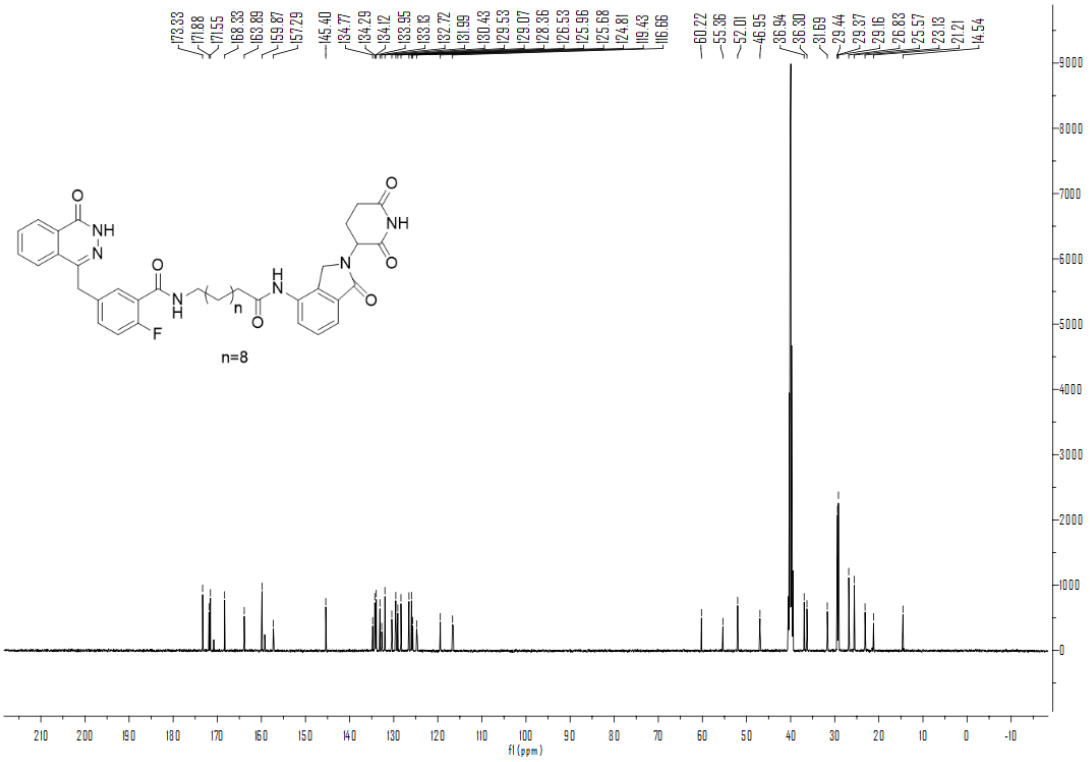
466.2618
536.2839
659.2916
718.7869
767.2910
m/z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145.40
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125.68
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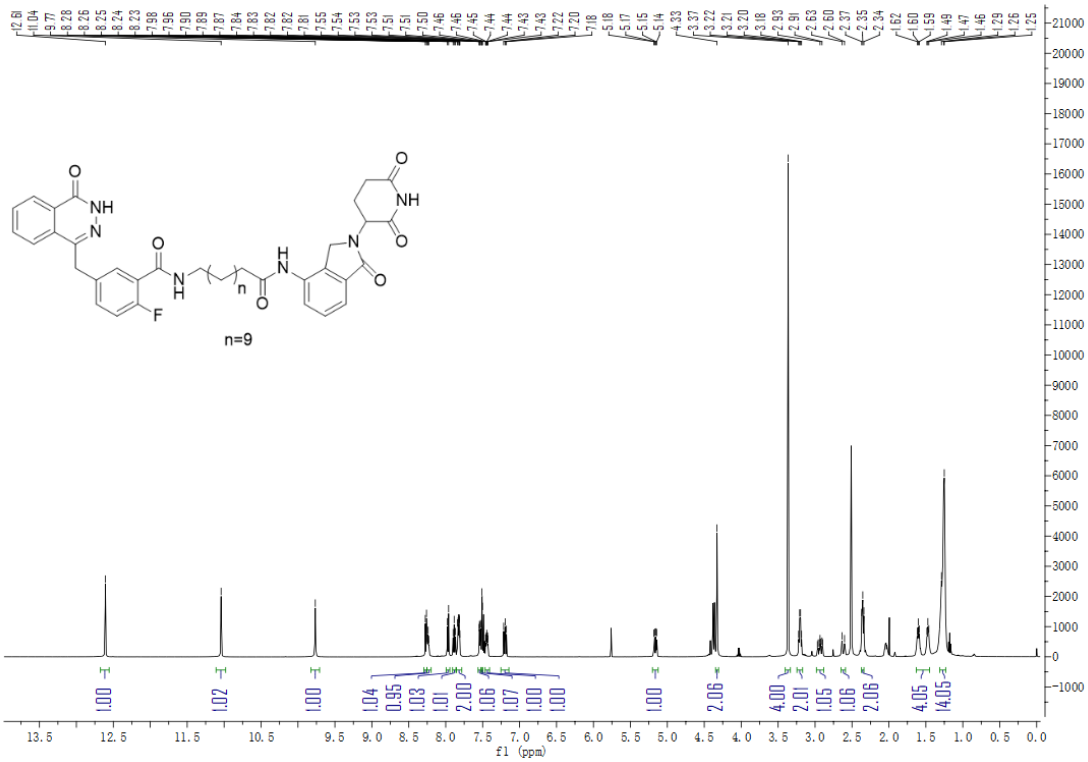
f1 (ppm)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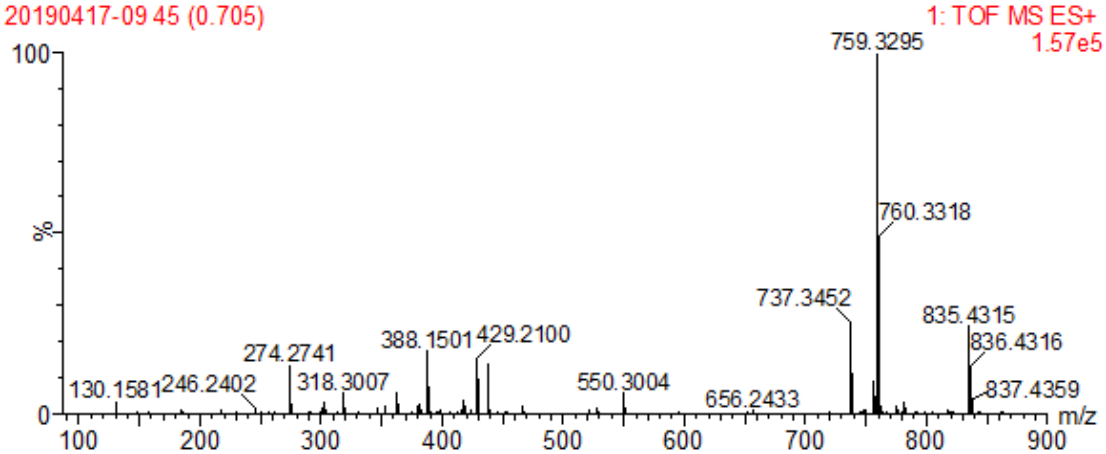
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759.3295
760.3318
737.3452
835.4315
836.4316
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429.2100
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246.2402
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656.2433
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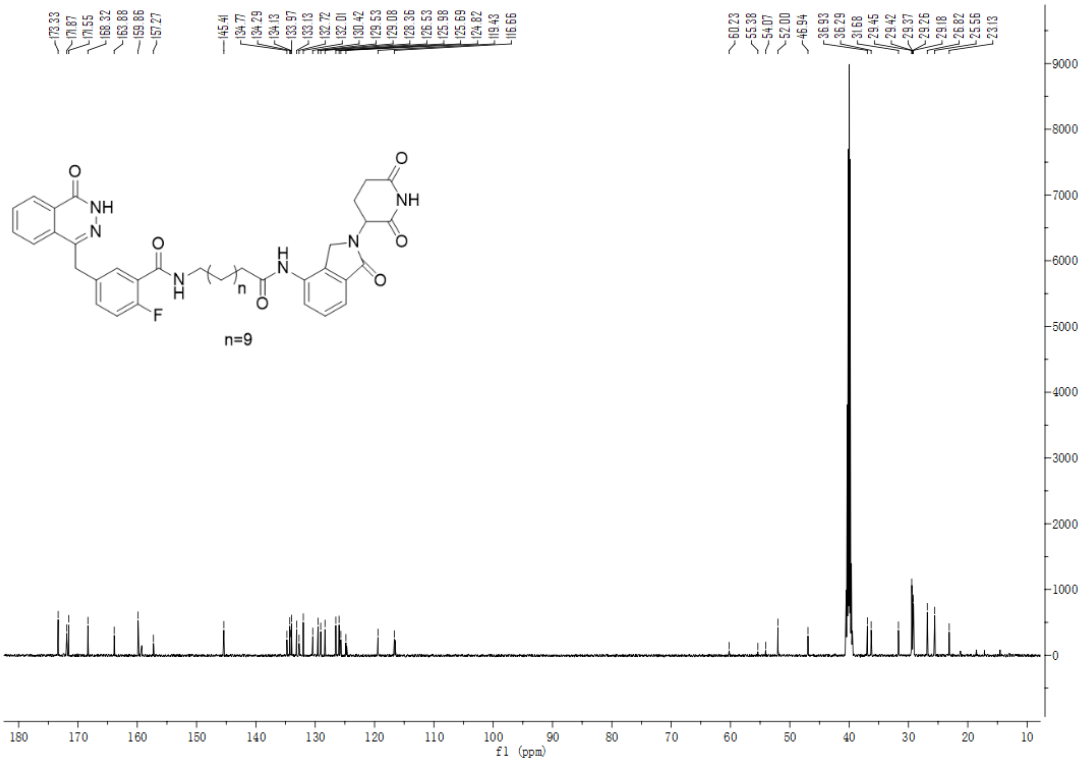
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171.55
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145.41
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133.13
132.72
132.01
130.42
129.53
129.08
128.36
126.53
125.98
125.69
124.82
119.43
116.66
60.23
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54.07
52.00
46.94
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36.29
31.68
29.45
29.42
29.37
29.26
29.18
26.82
25.56
23.13
n=9
f1 (ppm)