Supporting Information

Discovery of 3-(1-Amino-2-phenoxyethylidene)-6-methyl-2*H*-pyran-2,4(3*H*)-dione Derivatives as Novel Herbicidal Leads

Chao-Chao Wang[1], Ke Chen[2], Na Li[1], Xue-Kun Wang[1], Shi-Ben Wang[1], Pan Li[1], Xue-Wen Hua[3], Kang Lei*[,1] and Lu-Sha Ji[1]

[1] School of Pharmaceutical Sciences, Liaocheng University, Liaocheng 252000, China

[2] Department of Bioscience and Biotechnology, The University of Suwon, Whasung 18323, Korea

[3] College of Agricultural Science and Engineering, Liaocheng University, Liaocheng 252000, China

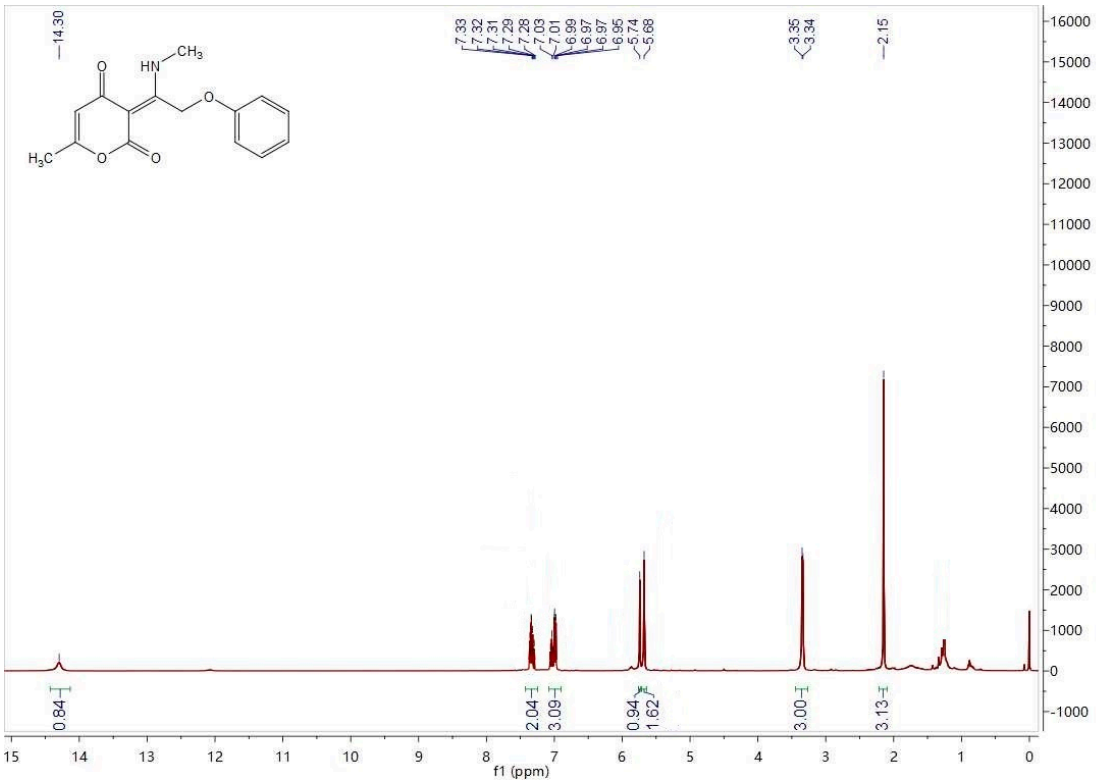
* Correspondence to: Kang Lei, E-mail: leikang@lcu.edu.cn

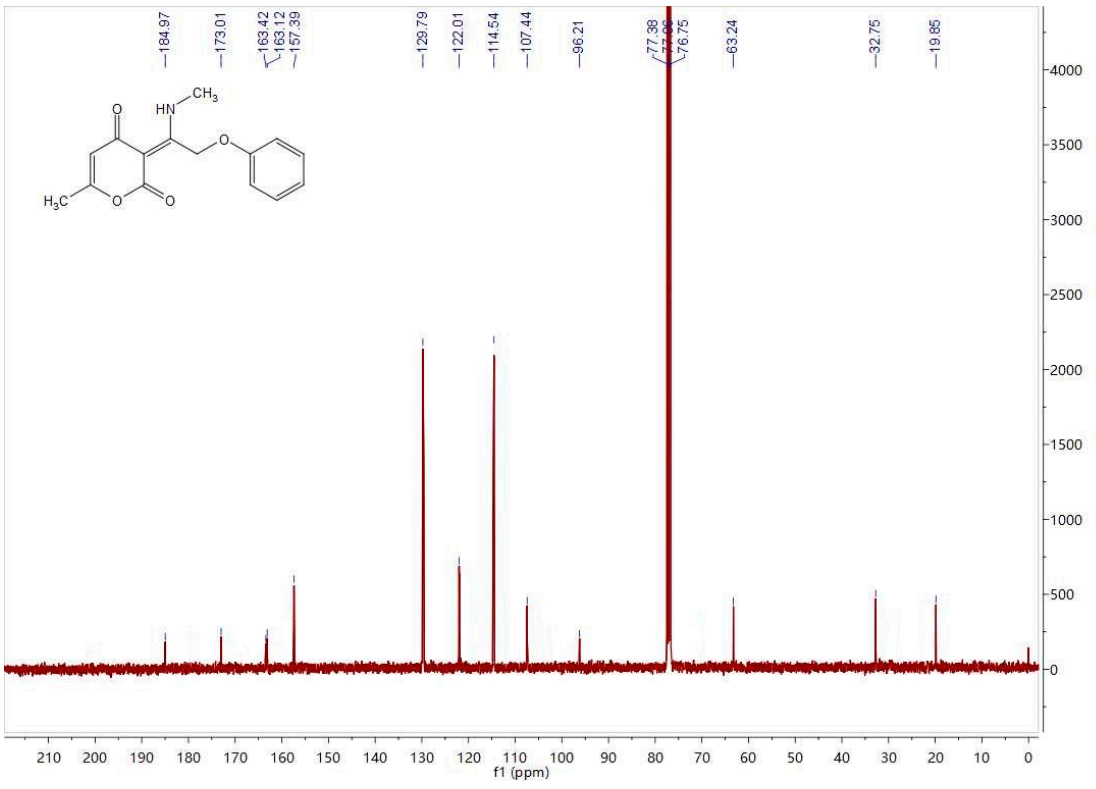
Greenhouse Tests

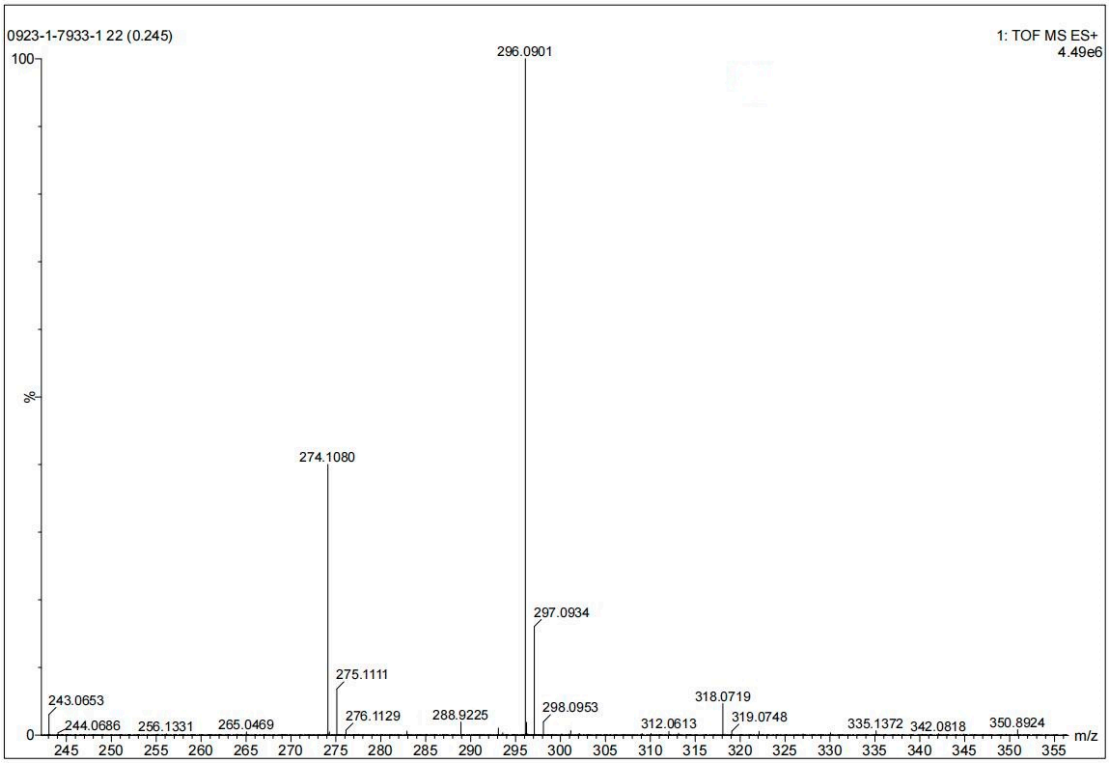
Two dicotyledonous species *Abutilon theophrasti Medicus* (AM) and *Amaranthus retroflexus L.* (AR), and two monocotyledonous species *Echinochloa crus-galli* (EC) and *Digitaria sanguinalis (L.) Scop.* (DS) were used to test the herbicidal activities of the target compounds. For pre-emergence tests, sandy clay (100 g) in a 7-cm-diameter test pot was wetted by water. Then 15 sprouting seeds of the weed were planted to 0.6 cm depth and placed in a greenhouse. All the tested compounds were dissolved in 100 % DMF and then diluted with Tween-80 (concentration: 100 g/L). The resulting solutions were diluted with water to the appropriate concentrations before use. The solutions of the compounds evaluated were sprayed immediately after seed planting. The mixture of same amount of water, *N, N*-dimethylformamide and Tween 80 was sprayed as the control. After 14 days, the fresh weight of the above-ground tissues in each pot was weighed and the percentage of inhibition calculated. For post-emergence tests, the same solution of the compounds was applied at the same rate as for the pre-emergence tests. Compounds were sprayed immediately after the expansion of the first true leaf. After 21 days, the fresh weight of the above-ground tissues in each pot was weighed and the percentage of inhibition calculated. Each treatment was done in triplicate, all the experiments were performed under natural light conditions at 22-28 °C. Additionally, adverse weather lighting was provided using sodium vapour lamps with a 12 : 12 h light : dark photo period.

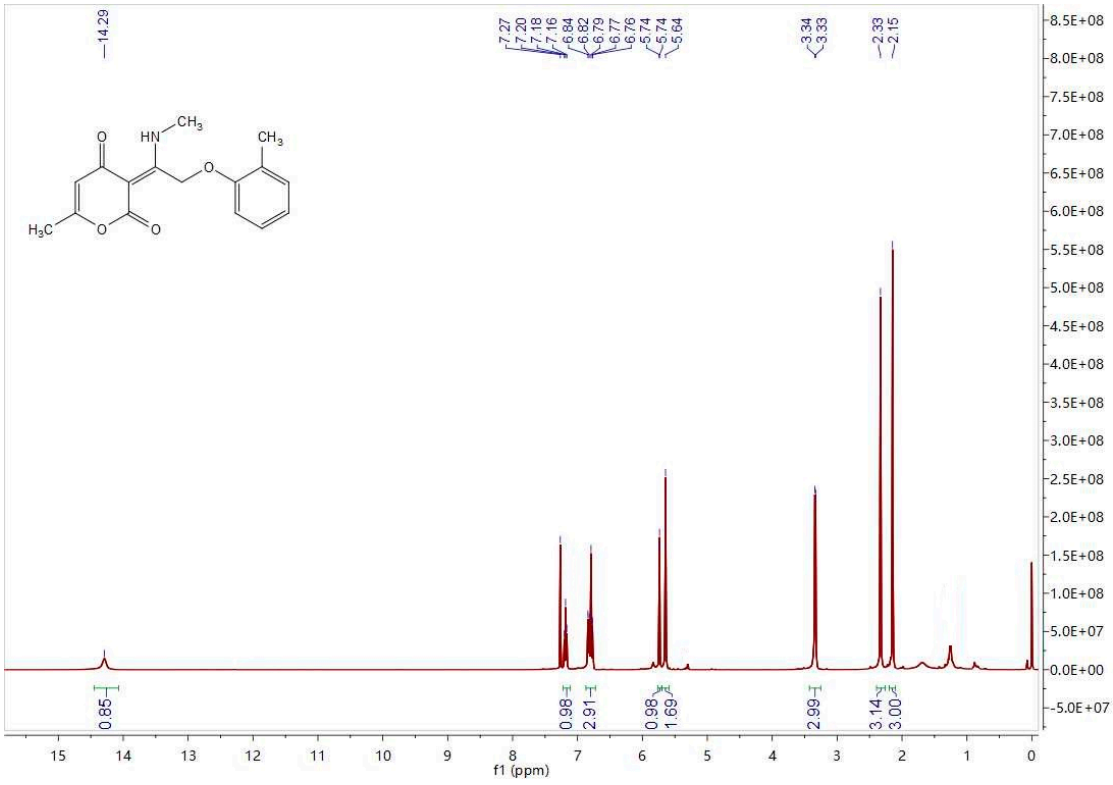
Formulas used in these tests are as follows: Control effect (%) = (the weight of live weeds in the control pots − the weight of live weeds in the treated pots)/the weight of live weeds in the control pots × 100%. The data represented the percent displaying herbicidal damage as compared to the control, where complete control of the target is 100 and no control is 0.

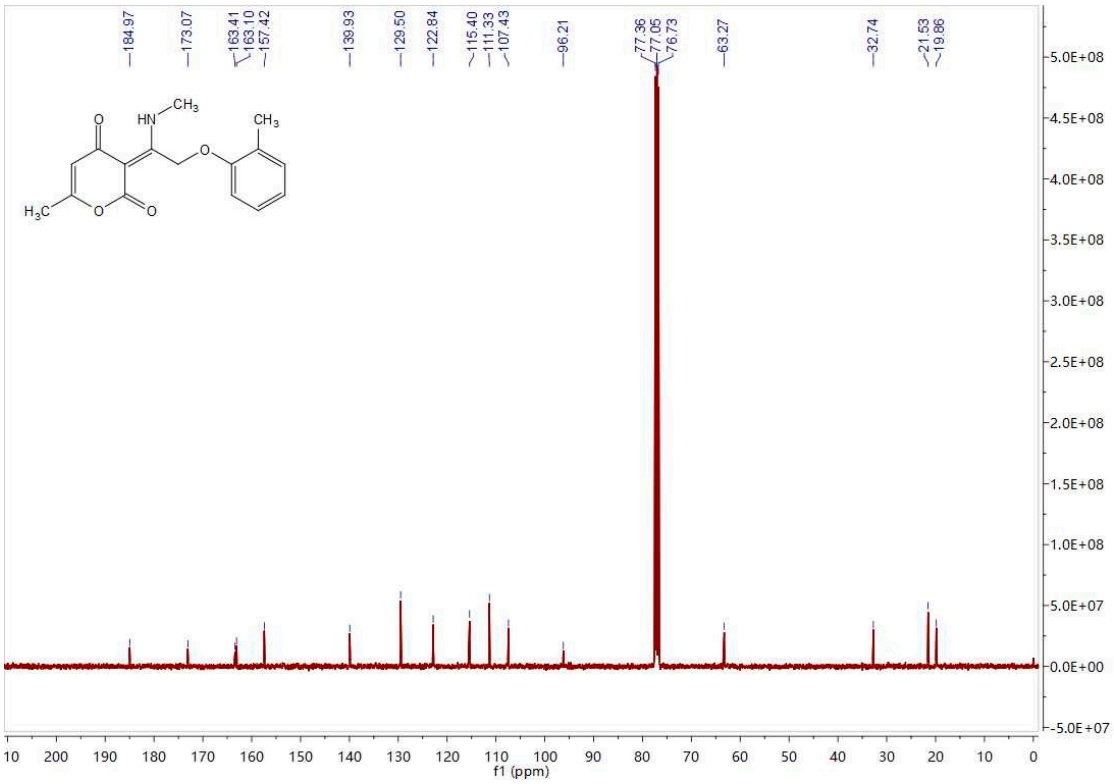
The ^{1}H NMR, ^{13}C NMR and HRMS Spectrum of Target Compounds APD-I and APD-II

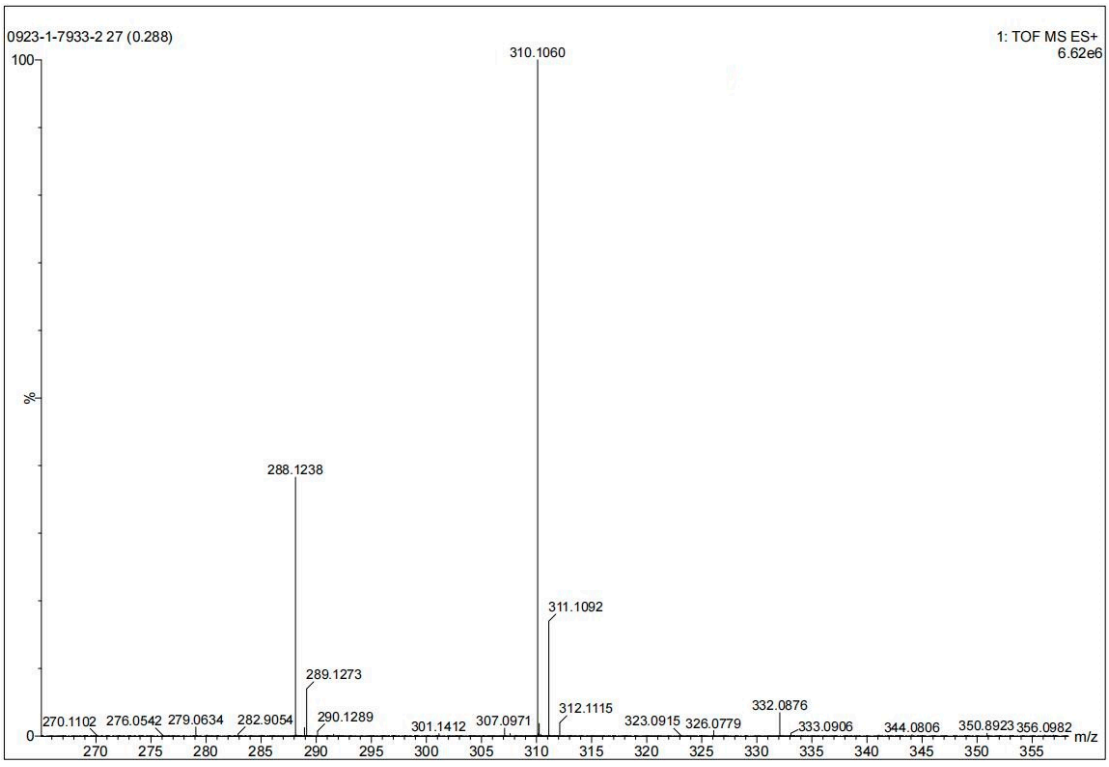

14.30
7.33
7.32
7.31
7.29
7.28
7.03
7.01
6.99
6.97
6.97
5.95
5.74
5.68
3.35
3.34
2.15
HN
CH3
O
O
O
O
H3C
0.84
2.04
3.09
0.94
1.62
3.00
3.13
f1 (ppm)

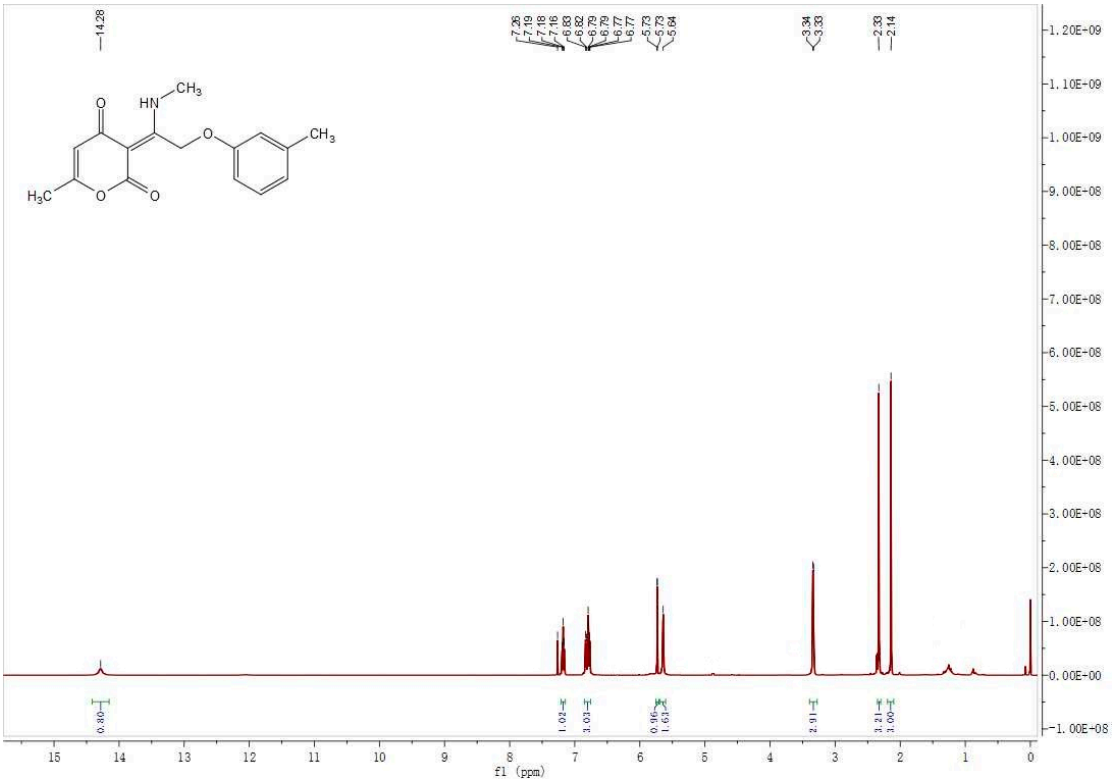

184.97
173.01
163.42
163.12
157.39
129.79
122.01
114.54
107.44
96.21
77.38
77.06
76.75
63.24
32.75
19.85
HN
CH3
O
O
O
O
H3C
f1 (ppm)

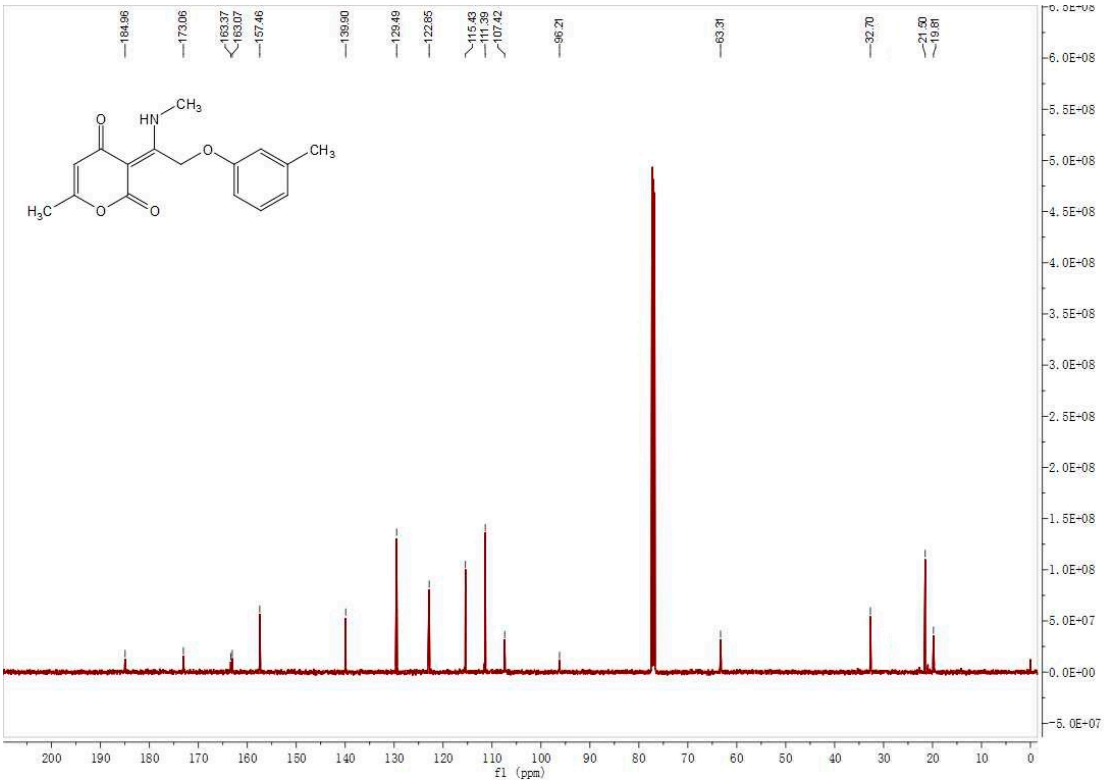

0923-1-7933-1 22 (0.245)
1: TOF MS ES+
4.49e6
100
%
0
296.0901
274.1080
297.0934
275.1111
243.0653
318.0719
244.0686
256.1331
265.0469
276.1129
288.9225
298.0953
312.0613
319.0748
335.1372
342.0818
350.8924
m/z
245 250 255 260 265 270 275 280 285 290 295 300 305 310 315 320 325 330 335 340 345 350 355

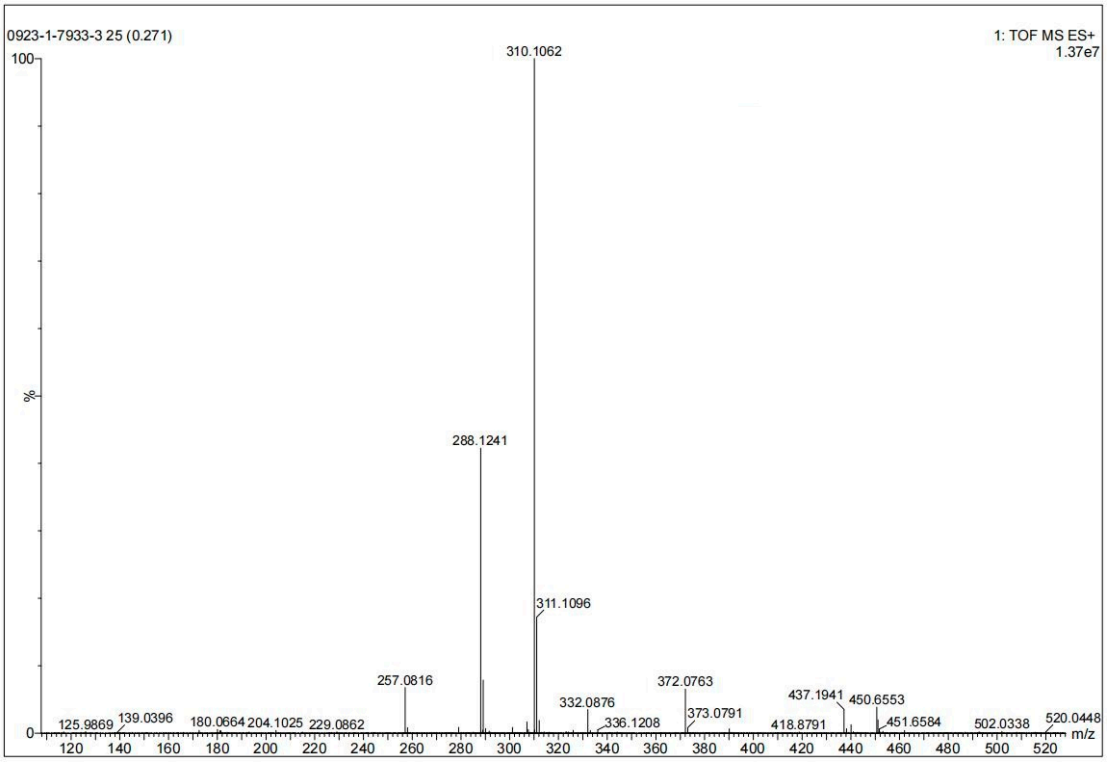

14.29
7.27
7.20
7.18
7.16
6.84
6.82
6.79
6.77
6.76
5.74
5.74
5.64
3.34
3.33
2.33
2.15
HN
CH3
CH3
O
O
O
O
H3C
8.5E+08
8.0E+08
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0.85
0.98
2.91
0.98
1.69
2.99
3.14
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

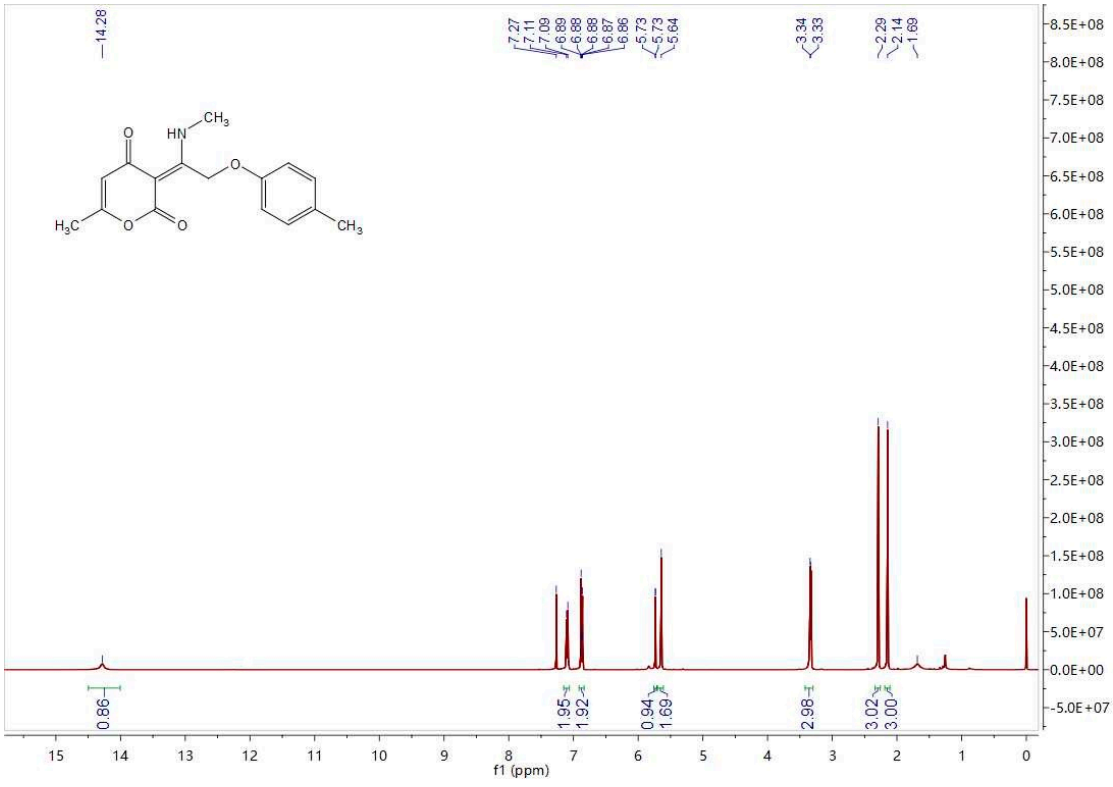

184.97
173.07
163.41
163.10
157.42
139.93
129.50
122.84
115.40
111.33
107.43
96.21
77.36
77.05
76.73
63.27
32.74
21.53
19.86
HN
CH3
CH3
O
O
O
O
H3C
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
f1 (ppm)

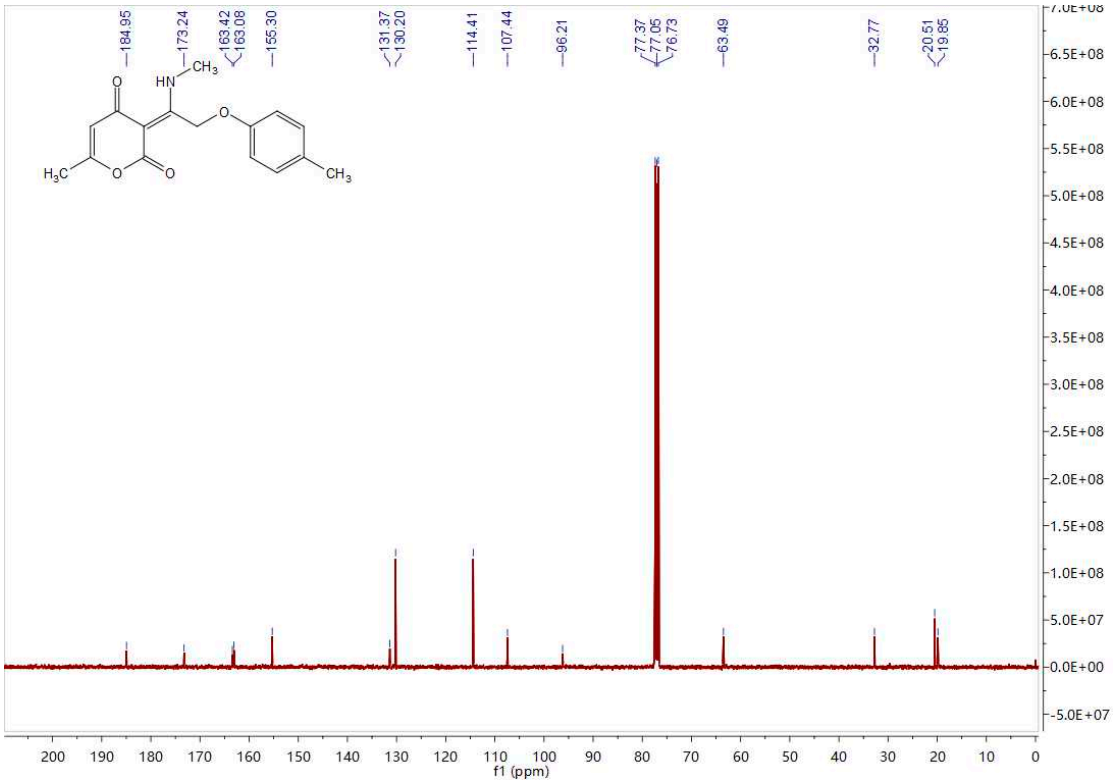

0923-1-7933-2 27 (0.288)
1: TOF MS ES+
6.62e6
100
%
0
310.1060
288.1238
311.1092
289.1273
312.1115
270.1102
276.0542
279.0634
282.9054
290.1289
301.1412
307.0971
323.0915
326.0779
332.0876
333.0906
344.0806
350.8923
356.0982
m/z

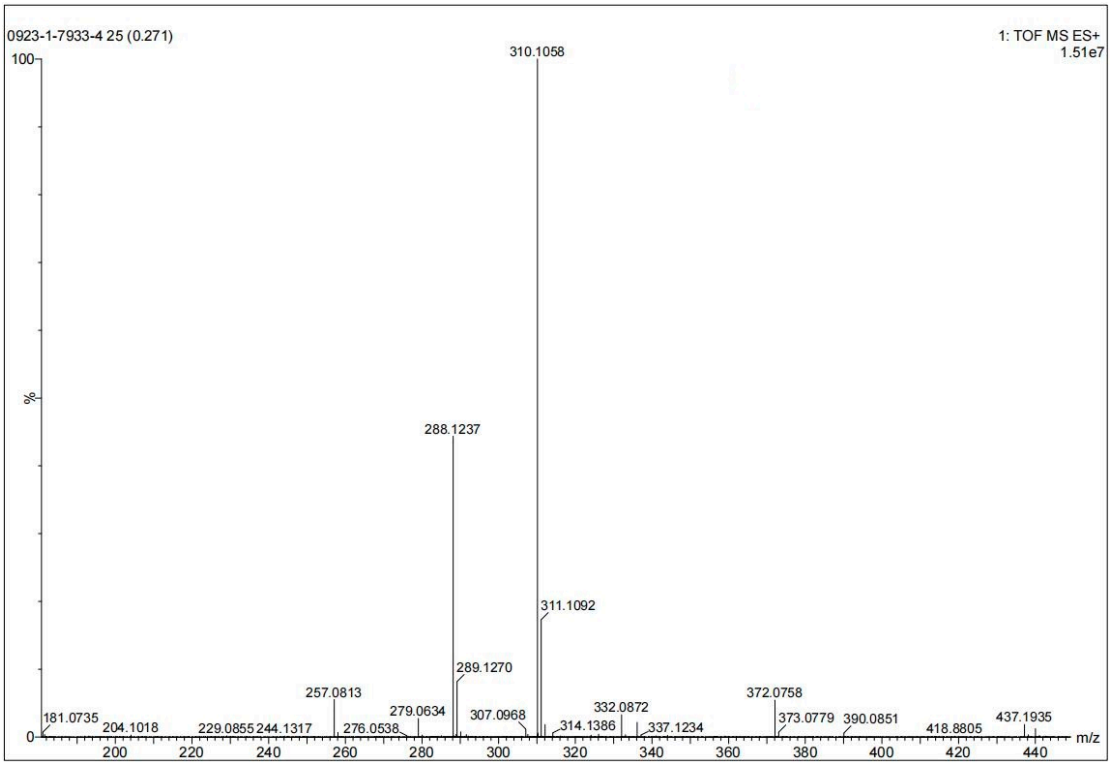

14.28
7.20
7.19
7.18
7.16
6.83
6.82
6.79
6.79
6.77
6.77
5.73
5.73
5.64
3.34
3.33
2.33
2.14
HN
CH3
O
O
CH3
H3C
O
O
0.80
1.03
3.03
0.96
1.63
2.91
3.21
3.00
f1 (ppm)

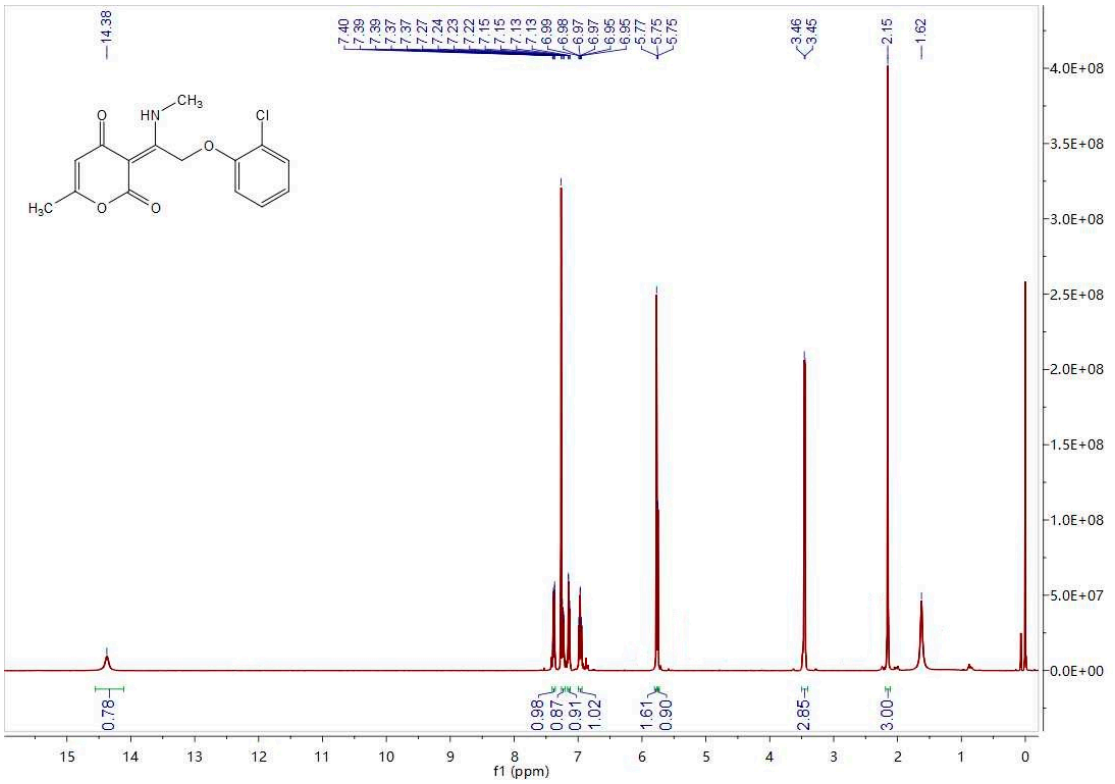

184.96
173.06
163.37
163.07
157.46
139.90
129.49
122.85
115.43
111.39
107.42
96.21
63.31
32.70
21.90
19.61
HN
CH3
O
O
CH3
H3C
O
O
f1 (ppm)

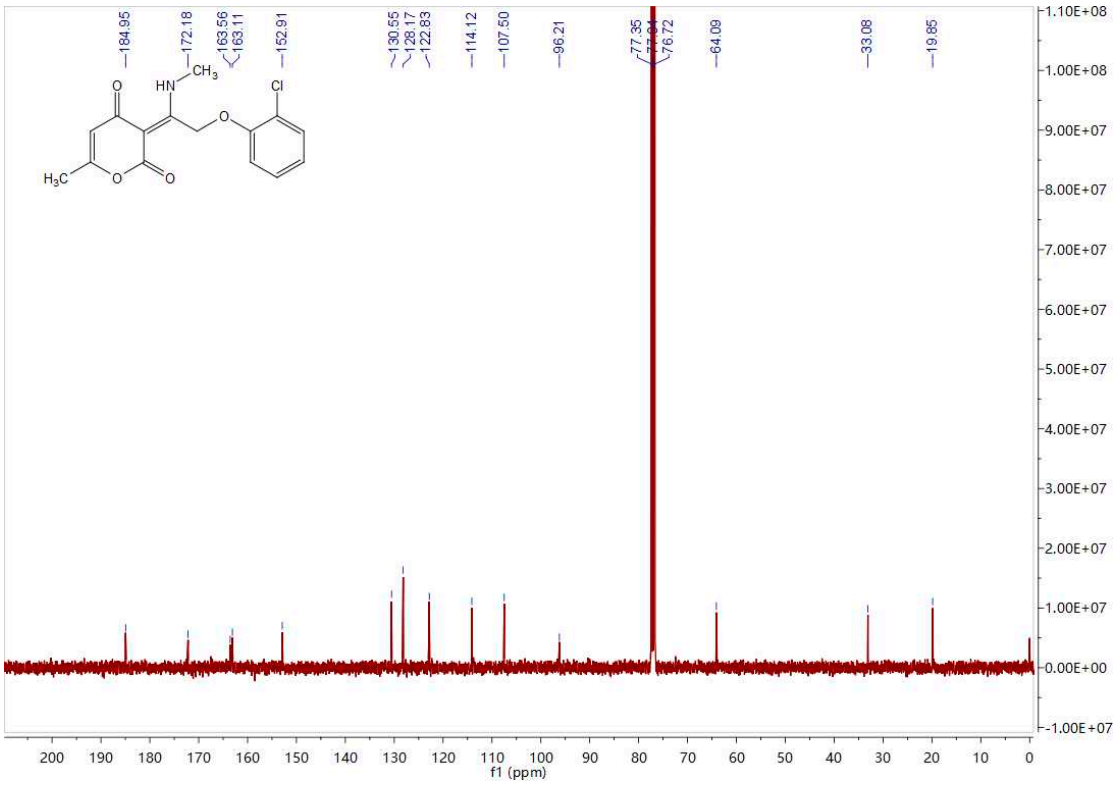

0923-1-7933-3 25 (0.271)
1: TOF MS ES+
1.37e7
100
%
0
310.1062
288.1241
311.1096
257.0816
372.0763
332.0876
373.0791
437.1941
450.6553
125.9869
139.0396
180.0664
204.1025
229.0862
336.1208
418.8791
451.6584
502.0338
520.0448
m/z

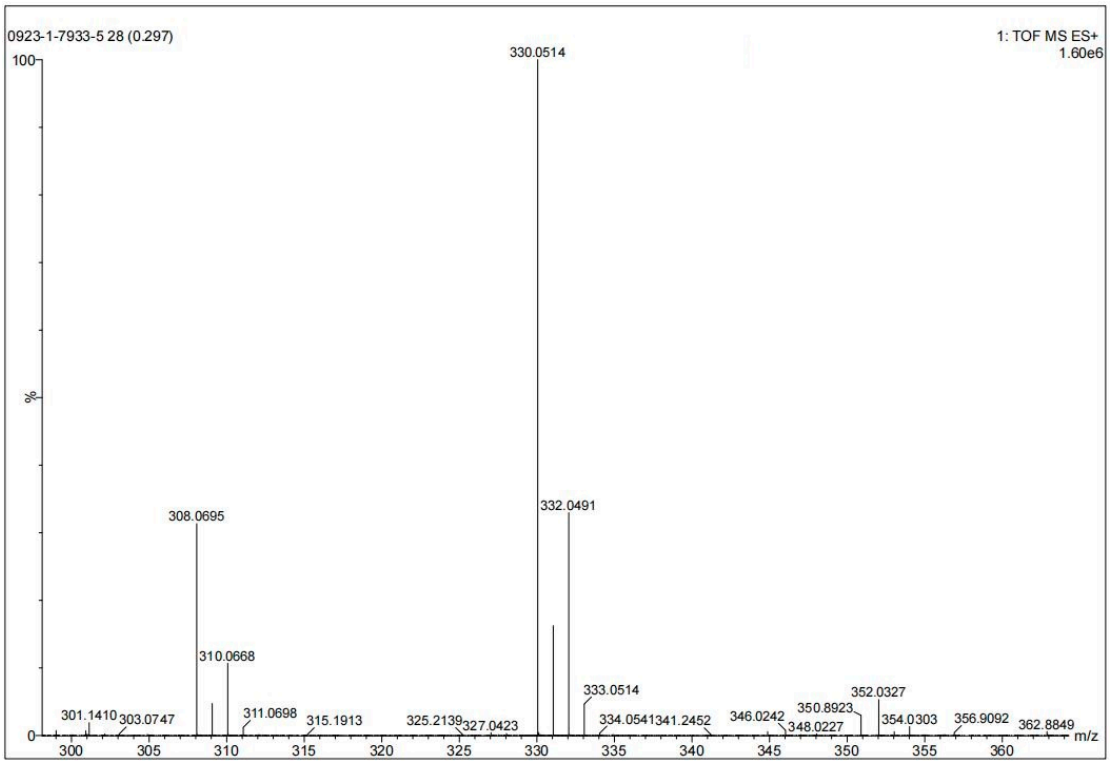

14.28
7.27
7.11
7.09
6.89
6.88
6.88
6.87
6.86
5.73
5.73
5.64
3.34
3.33
2.29
2.14
1.69
HN
CH3
O
O
O
O
H3C
CH3
0.86
1.95
1.92
0.94
1.69
2.98
3.02
3.00
f1 (ppm)

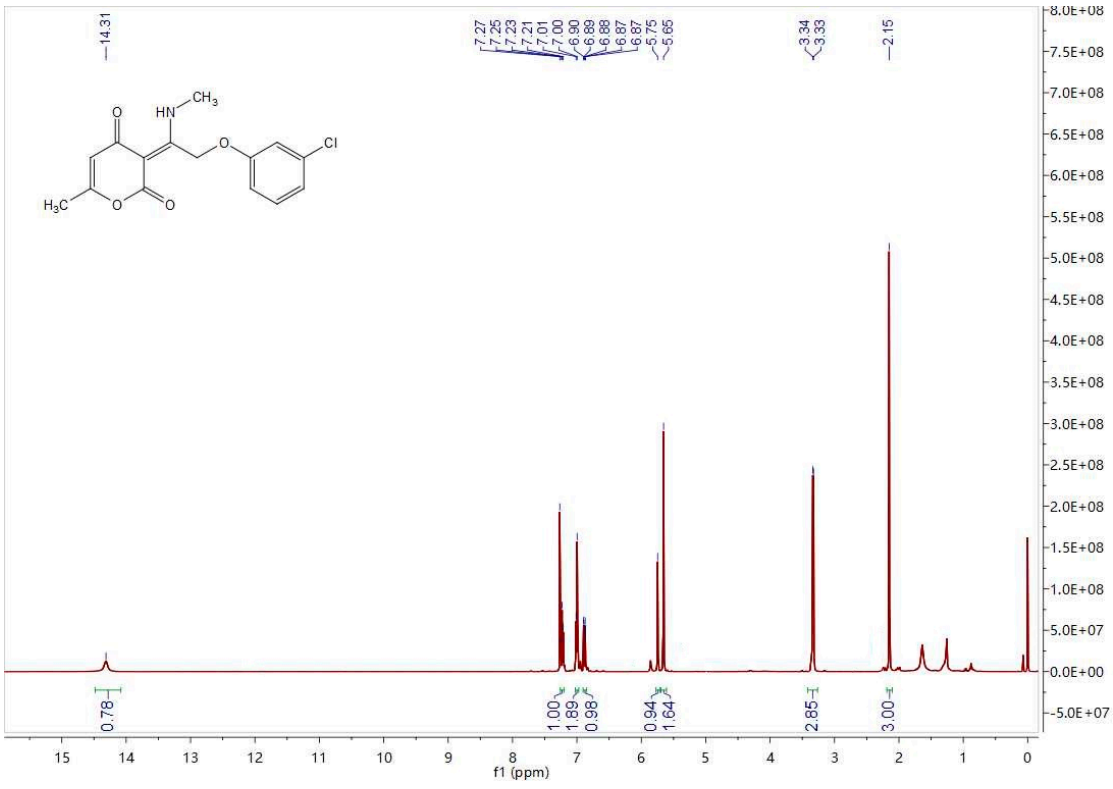

184.95
173.24
163.42
163.08
155.30
131.37
130.20
114.41
107.44
96.21
77.37
77.05
76.73
63.49
32.77
20.51
19.85
HN
CH3
O
O
O
O
H3C
CH3
f1 (ppm)

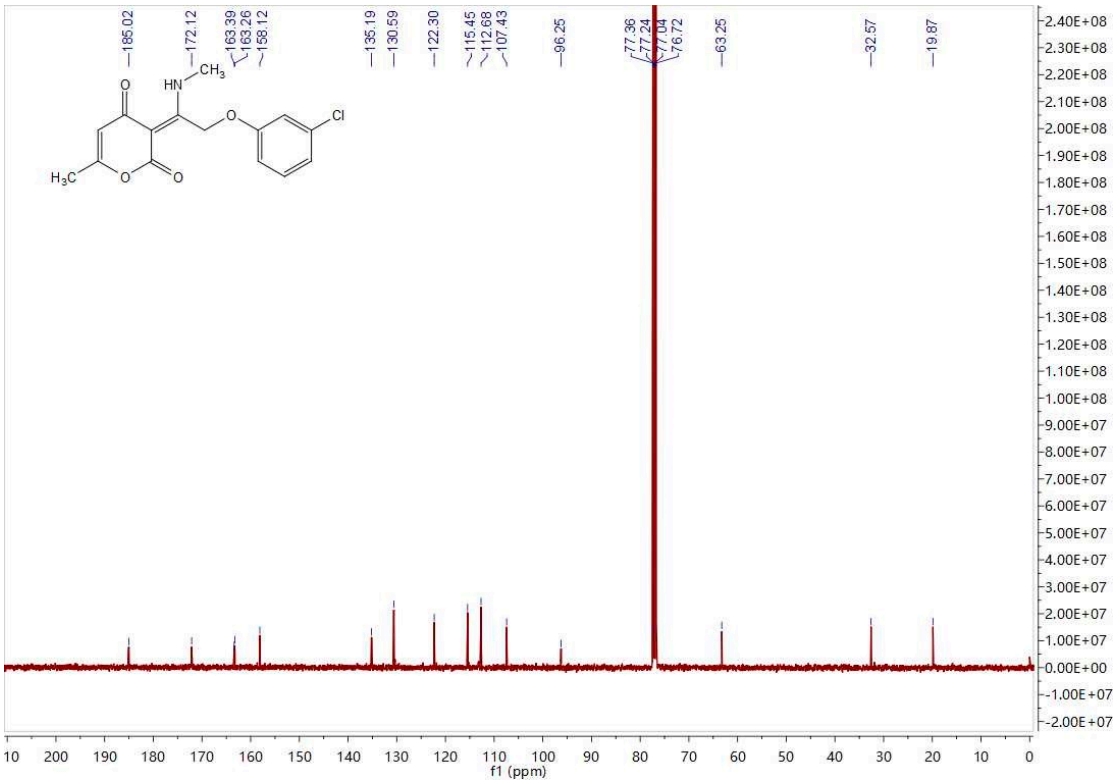

0923-1-7933-4 25 (0.271)
1: TOF MS ES+
1.51e7
100
%
0
310.1058
288.1237
311.1092
289.1270
257.0813
279.0634
307.0968
332.0872
372.0758
181.0735
204.1018
229.0855
244.1317
276.0538
314.1386
337.1234
373.0779
390.0851
418.8805
437.1935
m/z

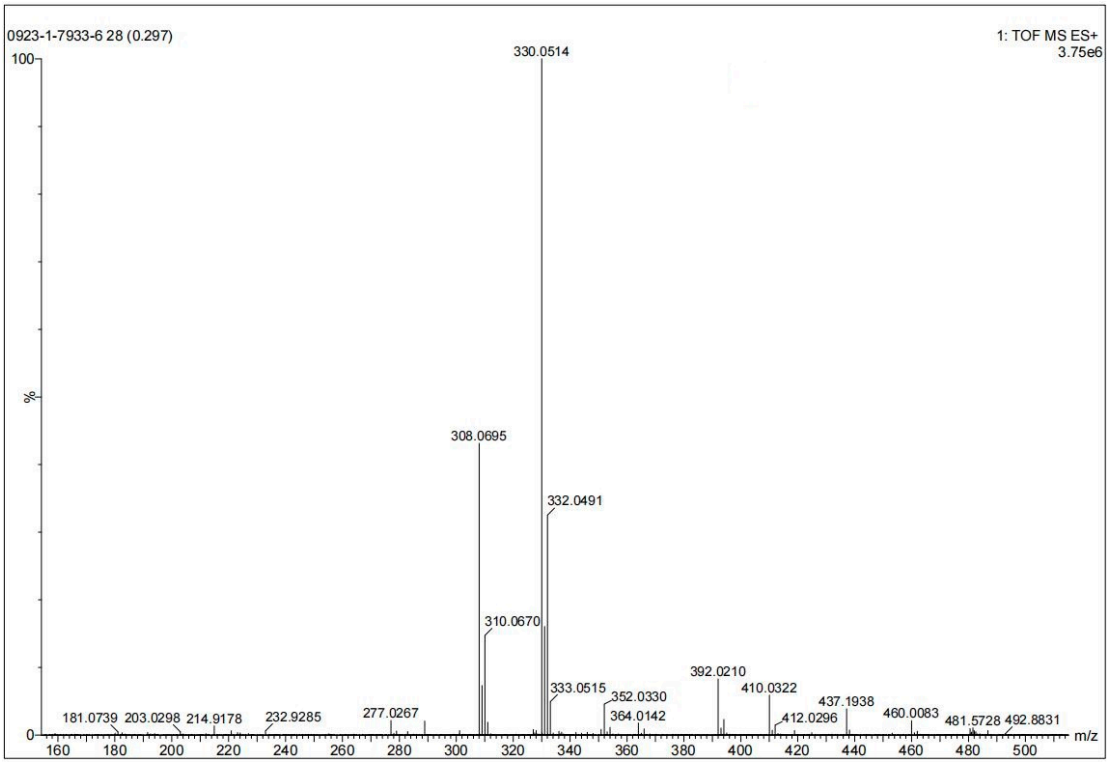

14.38
7.40
7.39
7.39
7.37
7.37
7.27
7.24
7.23
7.22
7.15
7.15
7.13
7.13
6.99
6.98
6.97
6.97
6.95
6.95
5.77
5.75
5.75
3.46
3.45
2.15
1.62
HN
CH3
O
Cl
H3C
0.78
0.98
0.87
0.91
1.02
1.61
0.90
2.85
3.00
f1 (ppm)

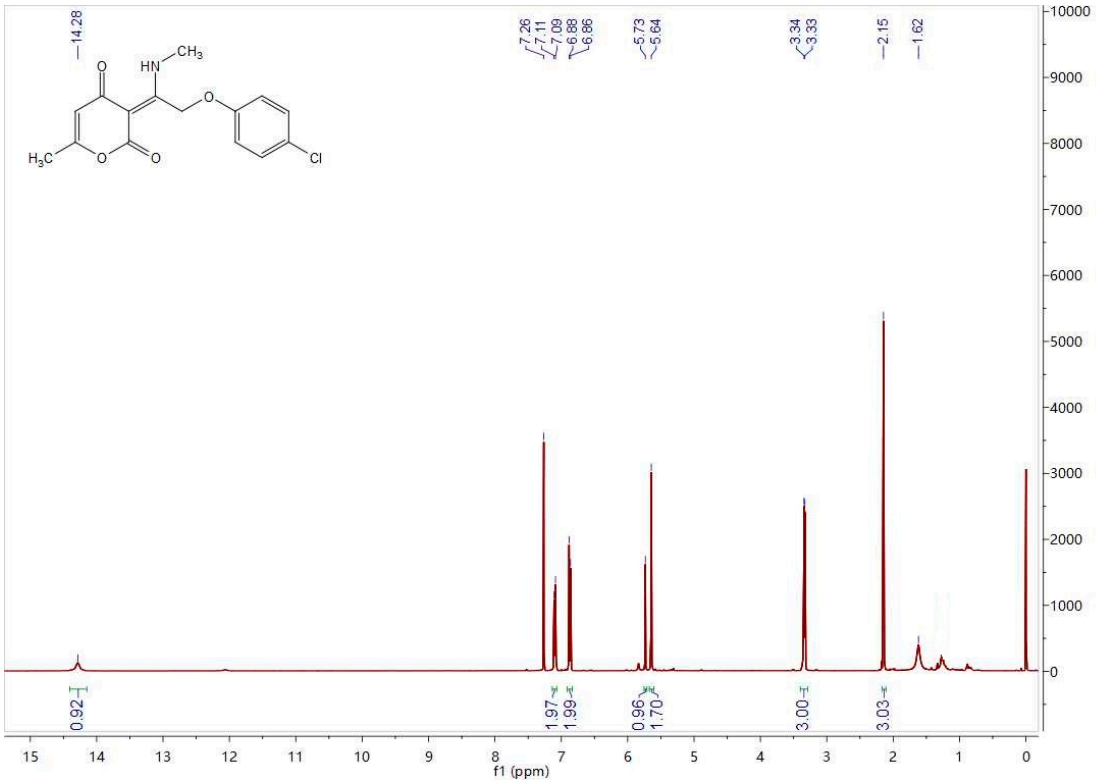

184.95
172.18
163.56
163.11
152.91
130.55
128.17
122.83
114.12
107.50
96.21
77.35
77.04
76.72
64.09
33.08
19.85
HN
CH3
O
Cl
H3C
f1 (ppm)

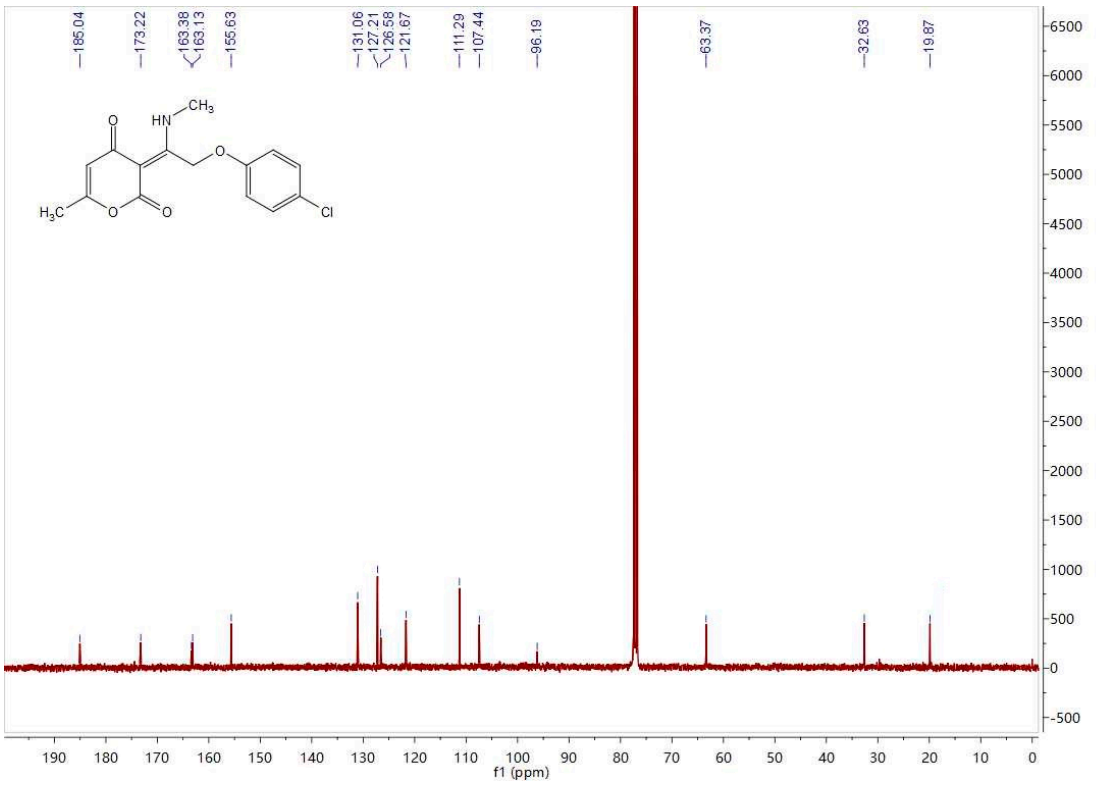

0923-1-7933-5 28 (0.297)
1: TOF MS ES+
1.60e6
100
%
0
330.0514
332.0491
308.0695
310.0668
333.0514
352.0327
301.1410
303.0747
311.0698
315.1913
325.2139
327.0423
334.0541
341.2452
346.0242
348.0227
350.8923
354.0303
356.9092
362.8849
m/z
300
305
310
315
320
325
330
335
340
345
350
355
360

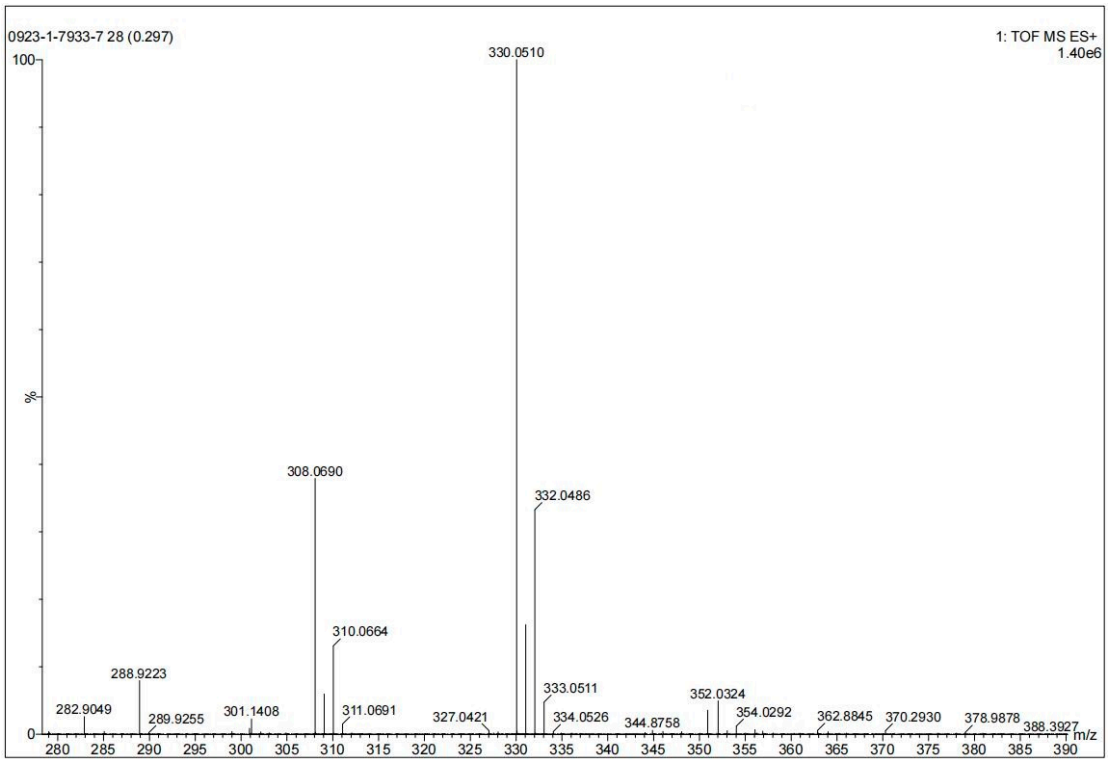

14.31
7.27
7.25
7.23
7.21
7.01
7.00
6.90
6.89
6.88
6.87
6.87
5.75
5.65
3.34
3.33
2.15
HN
CH3
O
O
Cl
H3C
O
O
8.0E+08
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0.78
1.00
1.89
0.98
0.94
1.64
2.85
3.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

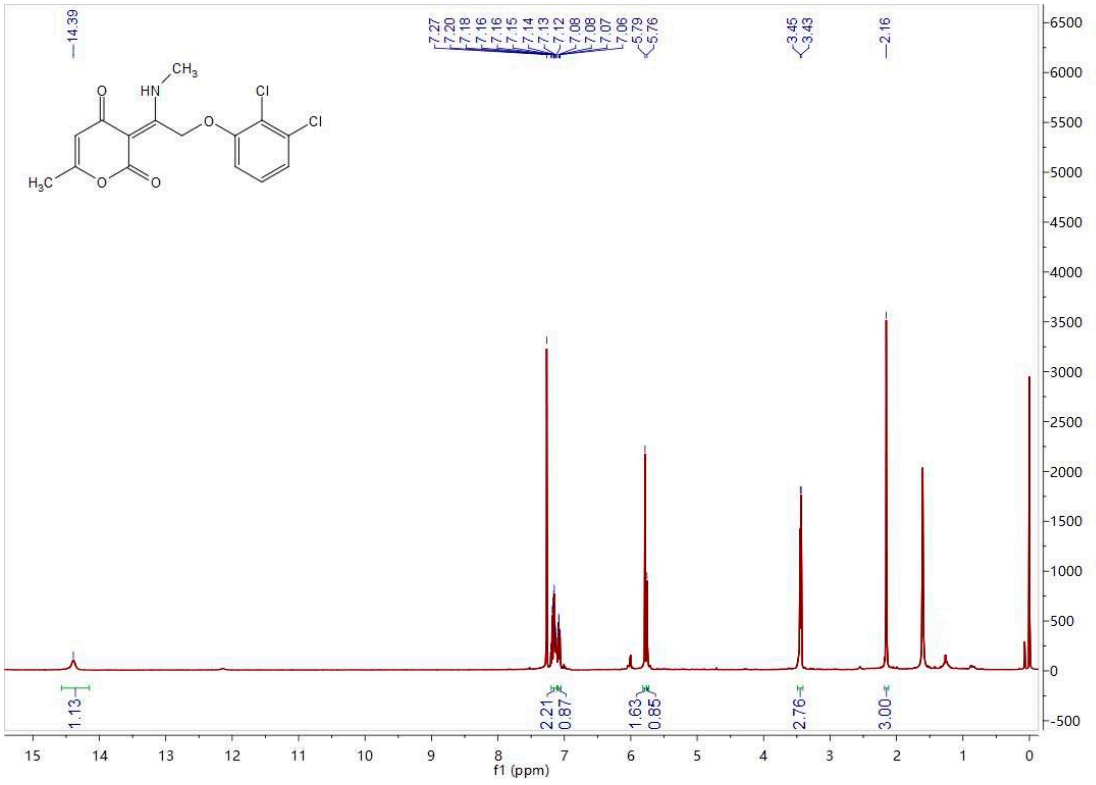

185.02
172.12
163.39
163.26
158.12
135.19
130.59
122.30
115.45
112.68
107.43
96.25
77.36
77.24
77.04
76.72
63.25
32.57
19.87
HN
CH3
O
O
O
O
H3C
Cl
f1 (ppm)

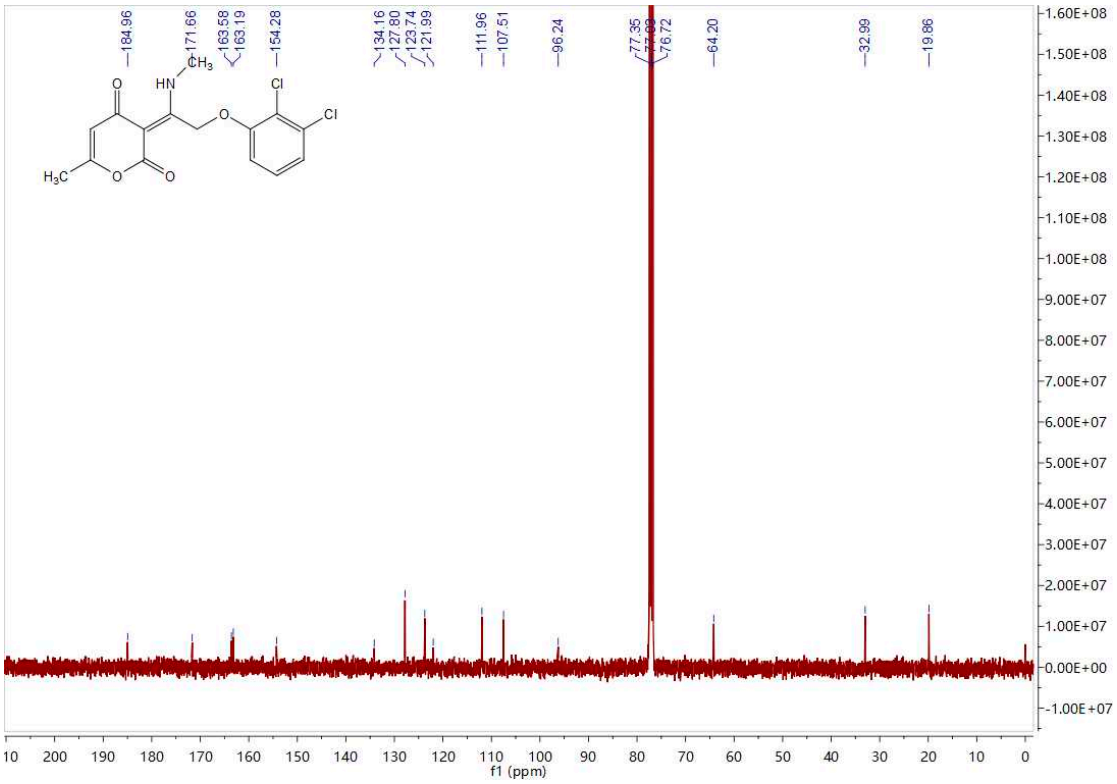

0923-1-7933-6 28 (0.297)
1: TOF MS ES+
3.75e6
100
%
0
330.0514
308.0695
332.0491
310.0670
333.0515
352.0330
364.0142
392.0210
410.0322
412.0296
437.1938
460.0083
481.5728
492.8831
181.0739
203.0298
214.9178
232.9285
277.0267
m/z

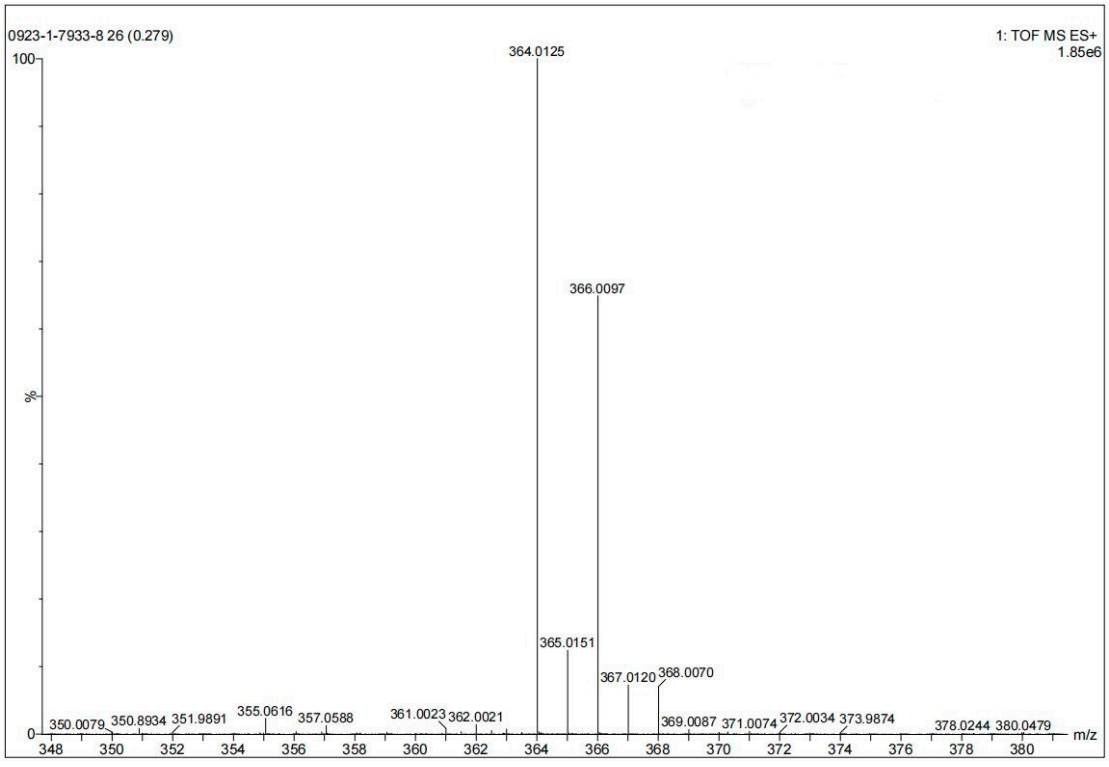

14.28
7.26
7.11
7.09
6.88
6.86
5.73
5.64
3.34
3.33
2.15
1.62
HN
CH3
O
O
O
O
H3C
Cl
0.92
1.97
1.99
0.96
1.70
3.00
3.03
f1 (ppm)

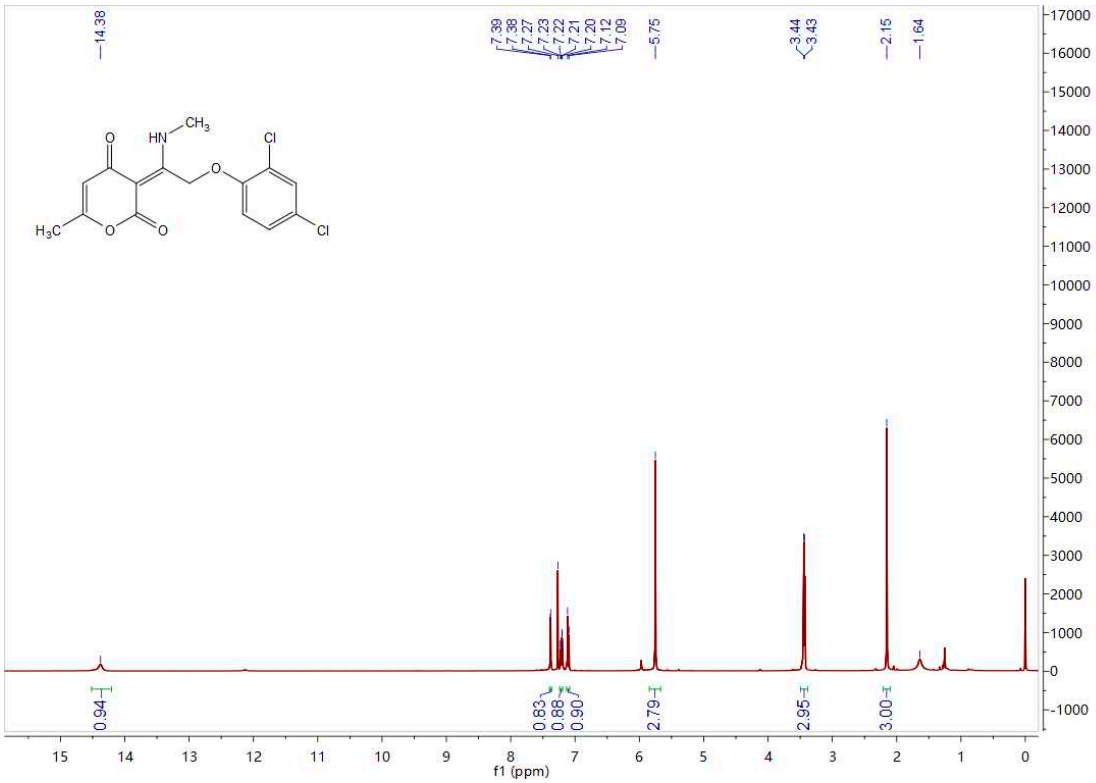

185.04
173.22
163.38
163.13
155.63
131.06
127.21
126.58
121.67
111.29
107.44
96.19
63.37
32.63
19.87
HN
CH3
O
O
O
O
H3C
Cl
f1 (ppm)

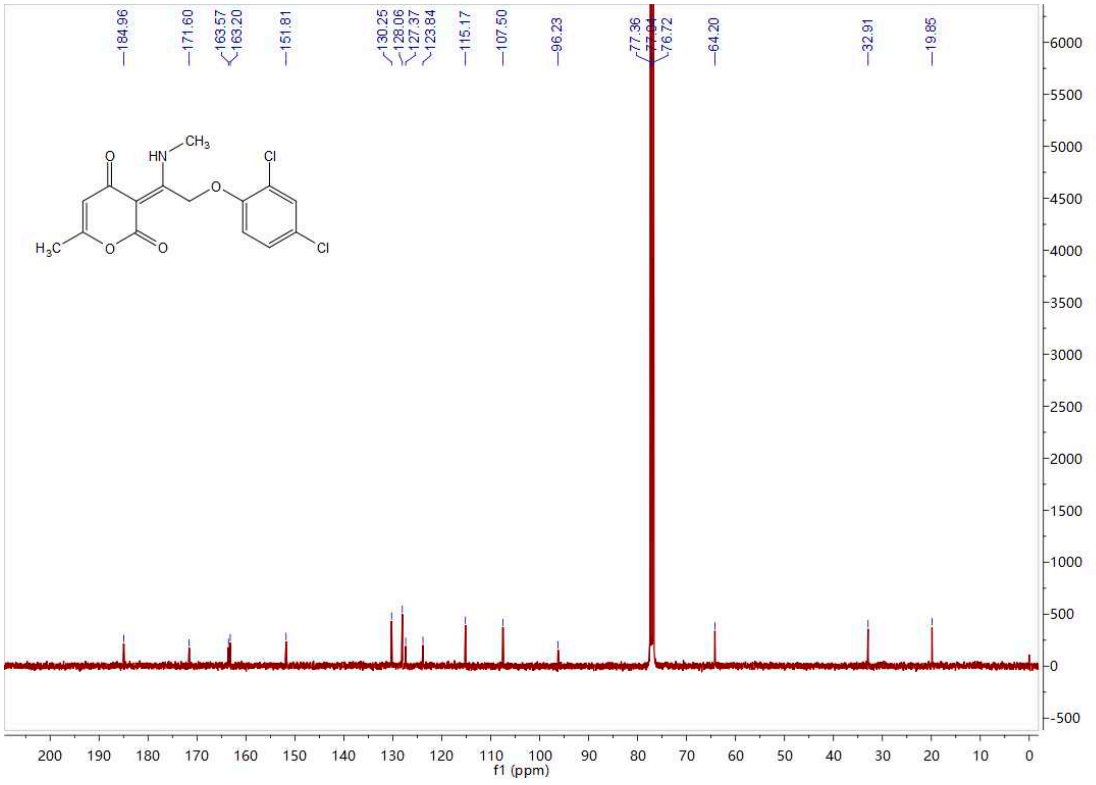

0923-1-7933-7 28 (0.297)
1: TOF MS ES+
1.40e6
100
%
0
330.0510
308.0690
332.0486
310.0664
288.9223
333.0511
352.0324
282.9049
289.9255
301.1408
311.0691
327.0421
334.0526
344.8758
354.0292
362.8845
370.2930
378.9878
388.3927
m/z
280 285 290 295 300 305 310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390

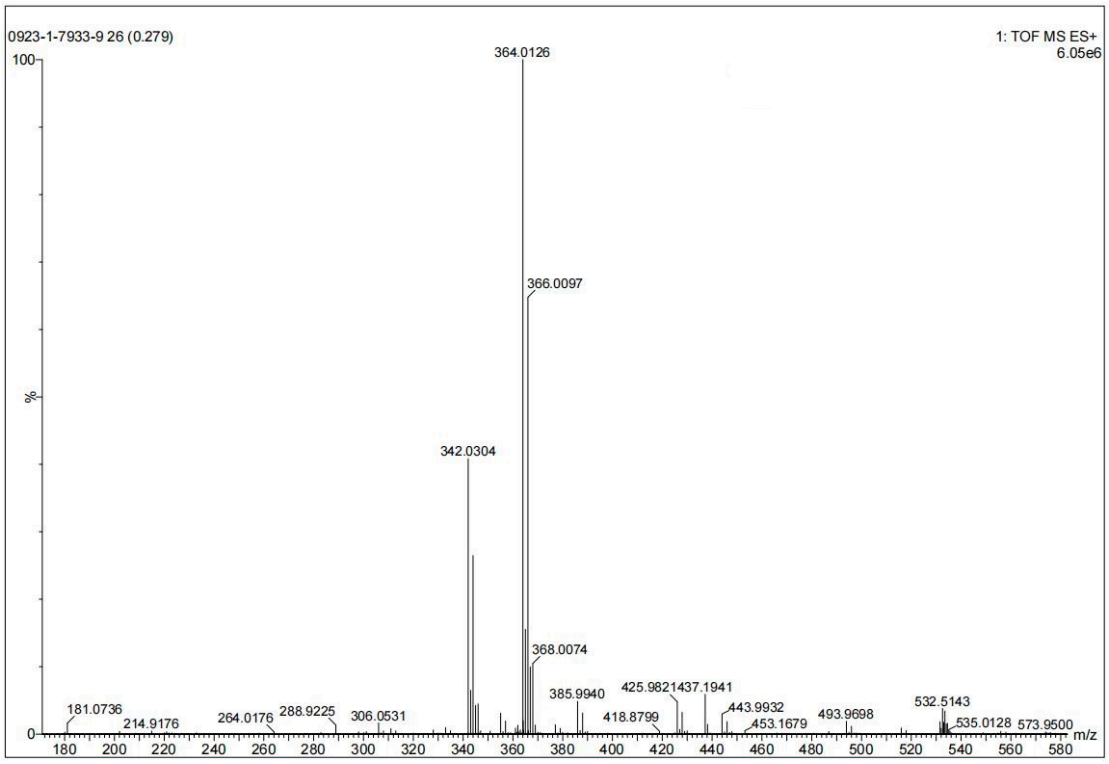

14.39
7.27
7.20
7.18
7.16
7.16
7.15
7.14
7.13
7.12
7.08
7.08
7.07
7.06
5.79
5.76
3.45
3.43
2.16
CH3
HN
O
O
Cl
Cl
O
H3C
O
O
1.13
2.21
0.87
1.63
0.85
2.76
3.00
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

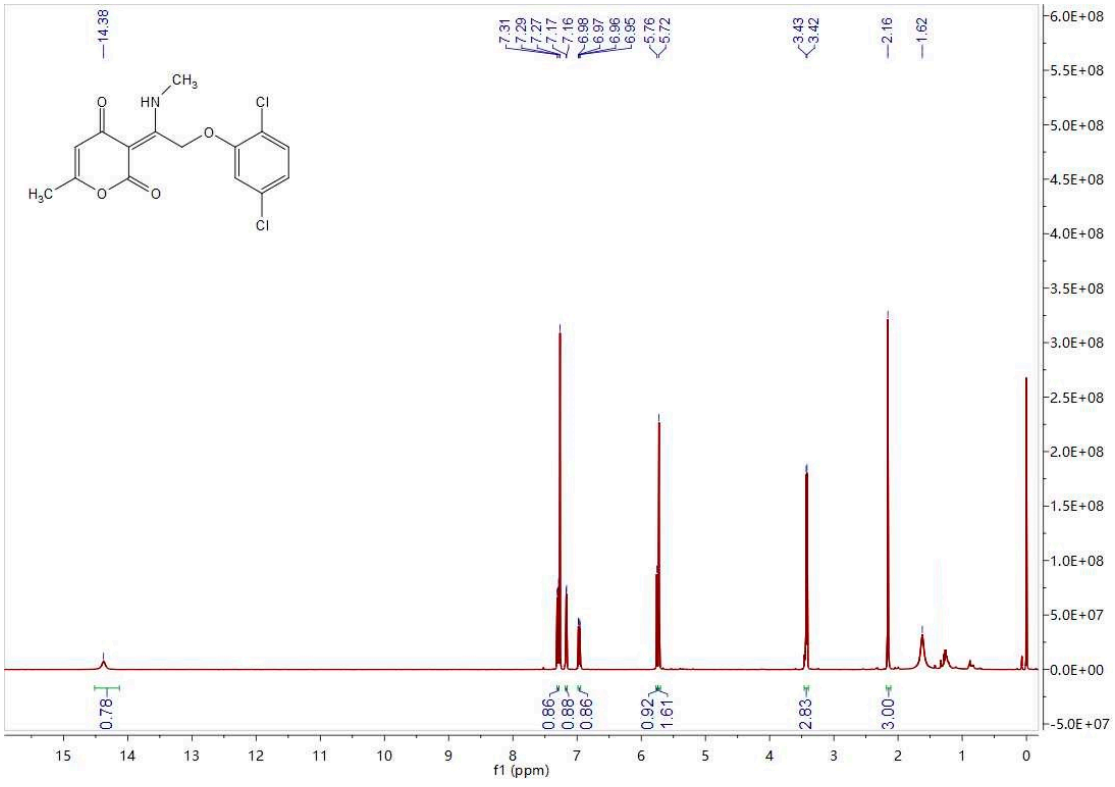

184.96
171.66
163.58
163.19
154.28
134.16
127.80
123.74
121.99
111.96
107.51
96.24
77.35
77.03
76.72
64.20
32.99
19.86
HN
CH3
O
Cl
Cl
O
H3C
O
O
1.60E+08
1.50E+08
1.40E+08
1.30E+08
1.20E+08
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

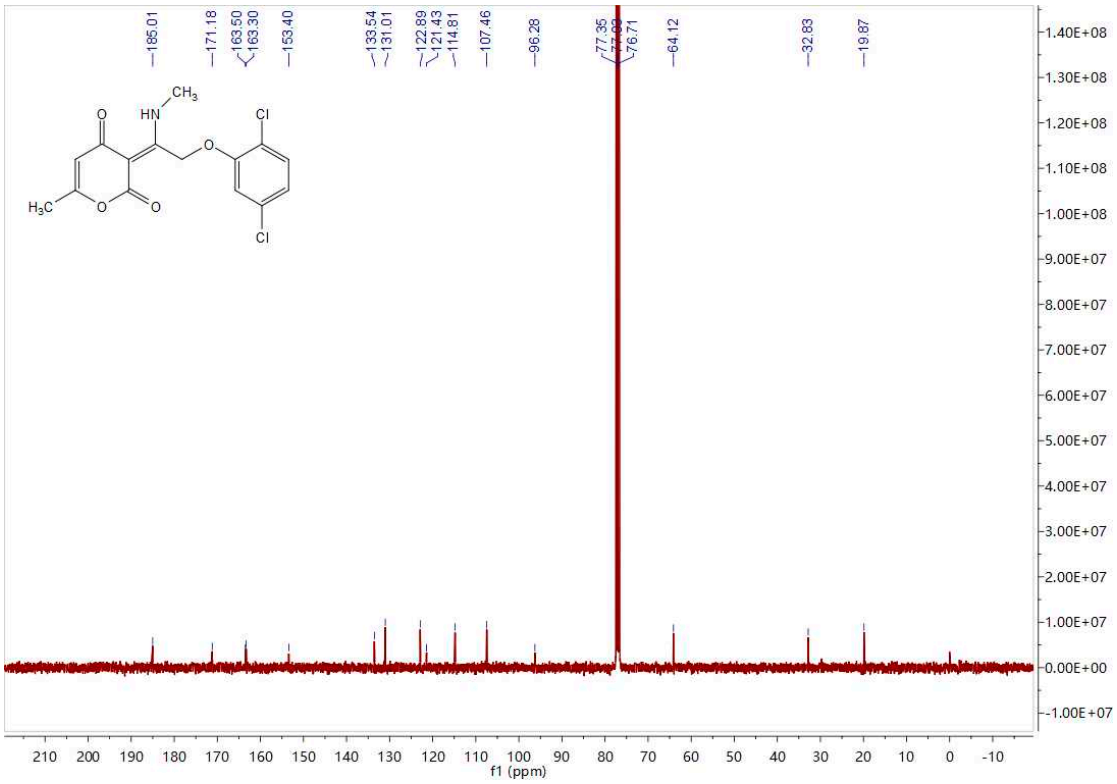

0923-1-7933-8 26 (0.279)
1: TOF MS ES+
1.85e6
100
%
0
364.0125
366.0097
365.0151
367.0120
368.0070
350.0079
350.8934
351.9891
355.0616
357.0588
361.0023
362.0021
369.0087
371.0074
372.0034
373.9874
378.0244
380.0479
m/z
348 350 352 354 356 358 360 362 364 366 368 370 372 374 376 378 380

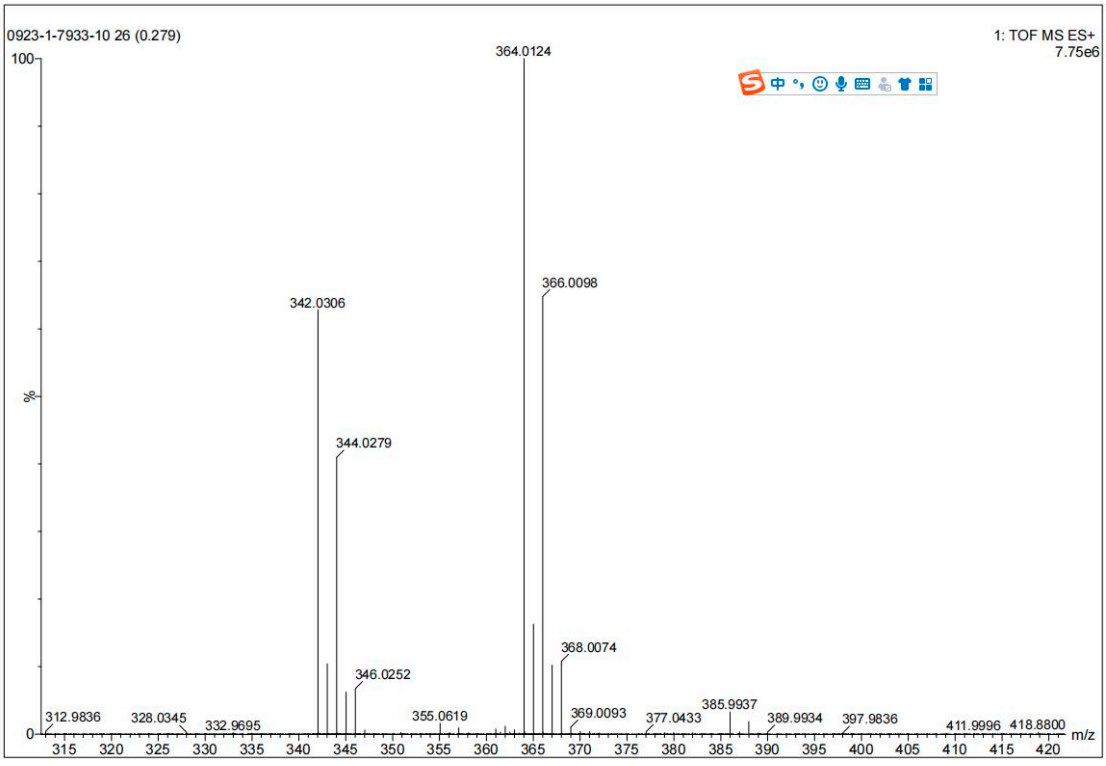

14.38
7.39
7.38
7.27
7.23
7.22
7.21
7.20
7.12
7.09
5.75
3.44
3.43
2.15
1.64
HN
CH3
O
Cl
H3C
0.94
0.83
0.88
0.90
2.79
2.95
3.00
f1 (ppm)

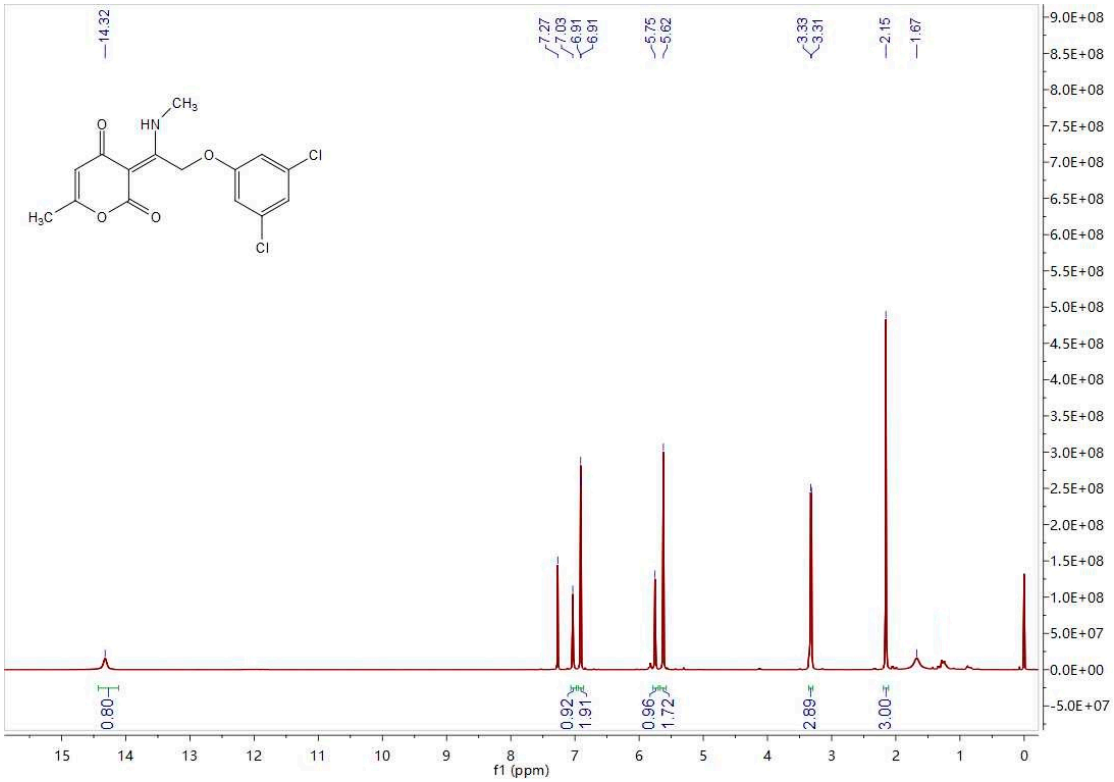

184.96
171.60
163.57
163.20
151.81
130.25
128.06
127.37
123.84
115.17
107.50
96.23
77.36
77.04
76.72
64.20
32.91
19.85
HN
CH3
O
Cl
H3C
f1 (ppm)

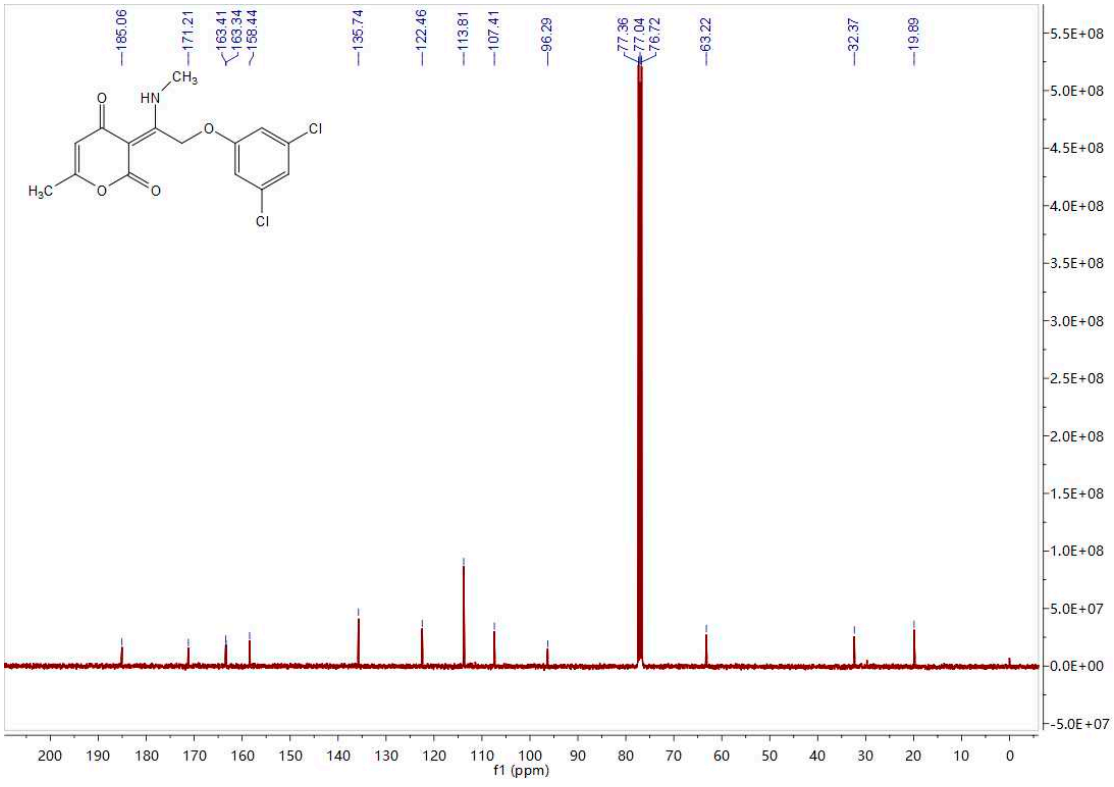

0923-1-7933-9 26 (0.279)
1: TOF MS ES+
6.05e6
100
%
0
364.0126
366.0097
342.0304
368.0074
385.9940
425.9821437.1941
443.9932
453.1679
418.8799
493.9698
532.5143
535.0128
573.9500
181.0736
214.9176
264.0176
288.9225
306.0531
m/z
180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580

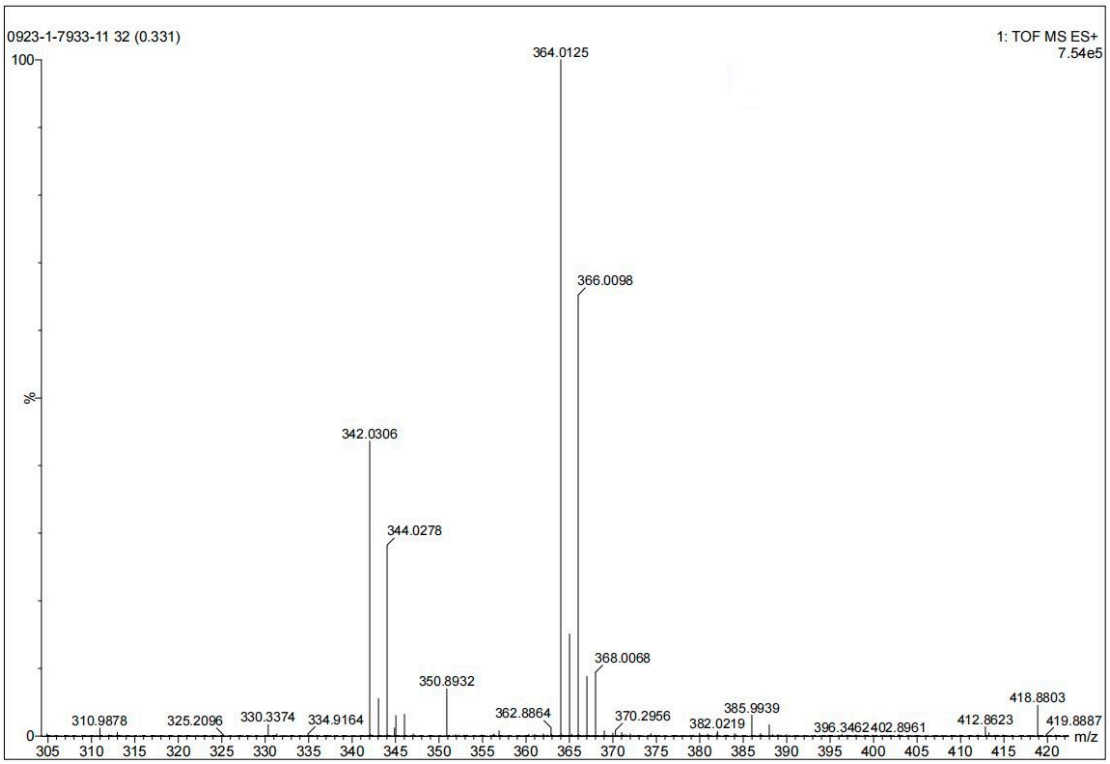

14.38
7.31
7.29
7.27
7.17
7.16
6.98
6.97
6.96
6.95
5.76
5.72
3.43
3.42
2.16
1.62
HN
CH3
O
Cl
H3C
Cl
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0.78
0.86
0.88
0.86
0.92
1.61
2.83
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

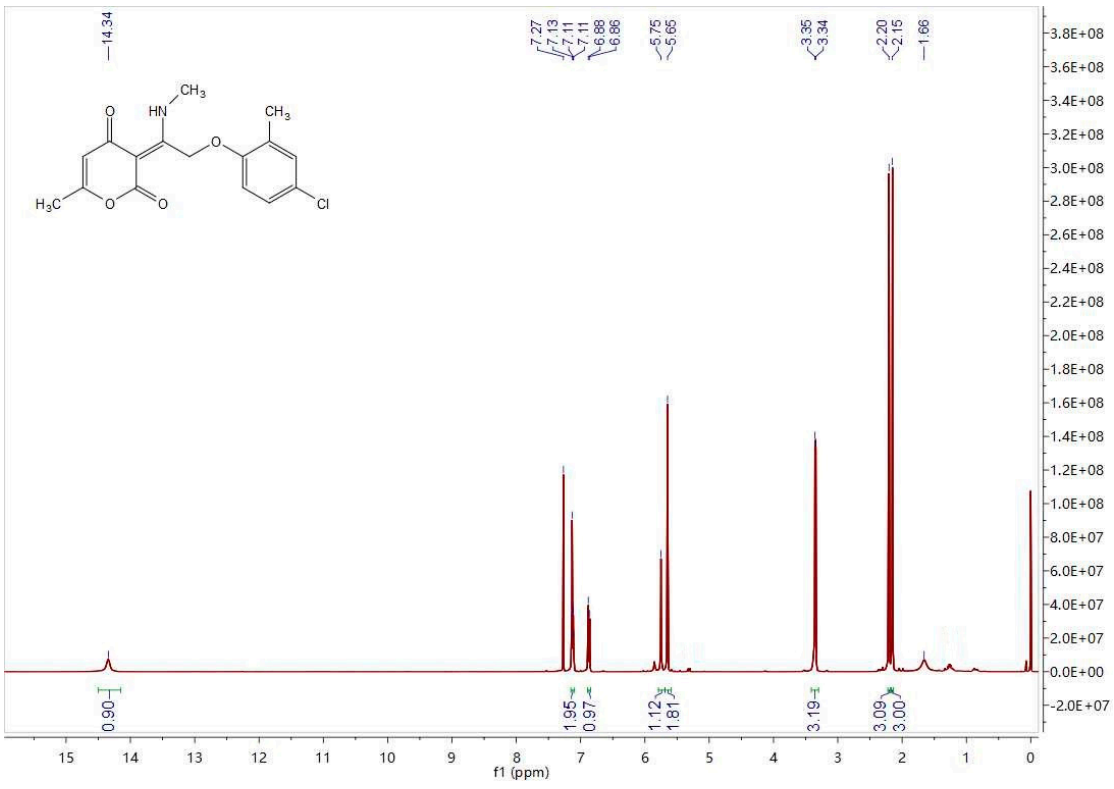

185.01
171.18
163.50
163.30
153.40
133.54
131.01
122.89
121.43
114.81
107.46
96.28
77.35
77.00
76.71
64.12
32.83
19.87
CH3
HN
O
O
O
O
H3C
Cl
Cl
1.40E+08
1.30E+08
1.20E+08
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

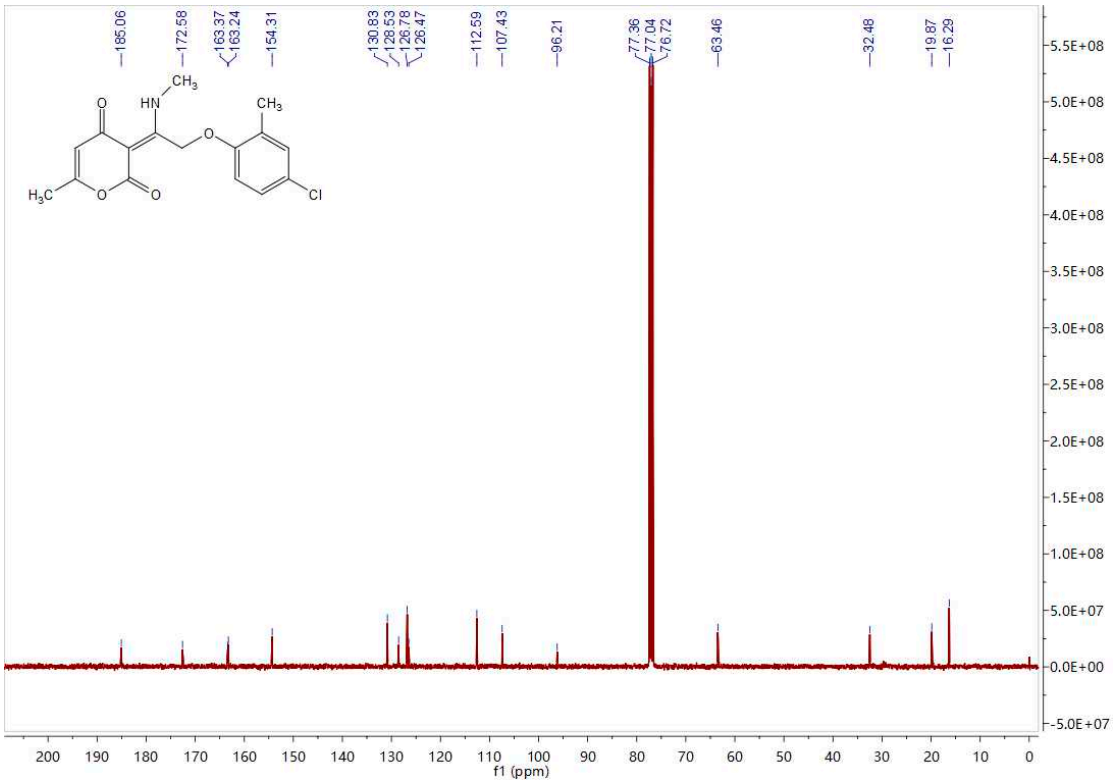

0923-1-7933-10 26 (0.279)
1: TOF MS ES+
7.75e6
100
%
0
364.0124
366.0098
342.0306
344.0279
368.0074
346.0252
312.9836
328.0345
332.9695
355.0619
369.0093
377.0433
385.9937
389.9934
397.9836
411.9996
418.8800
315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420
m/z

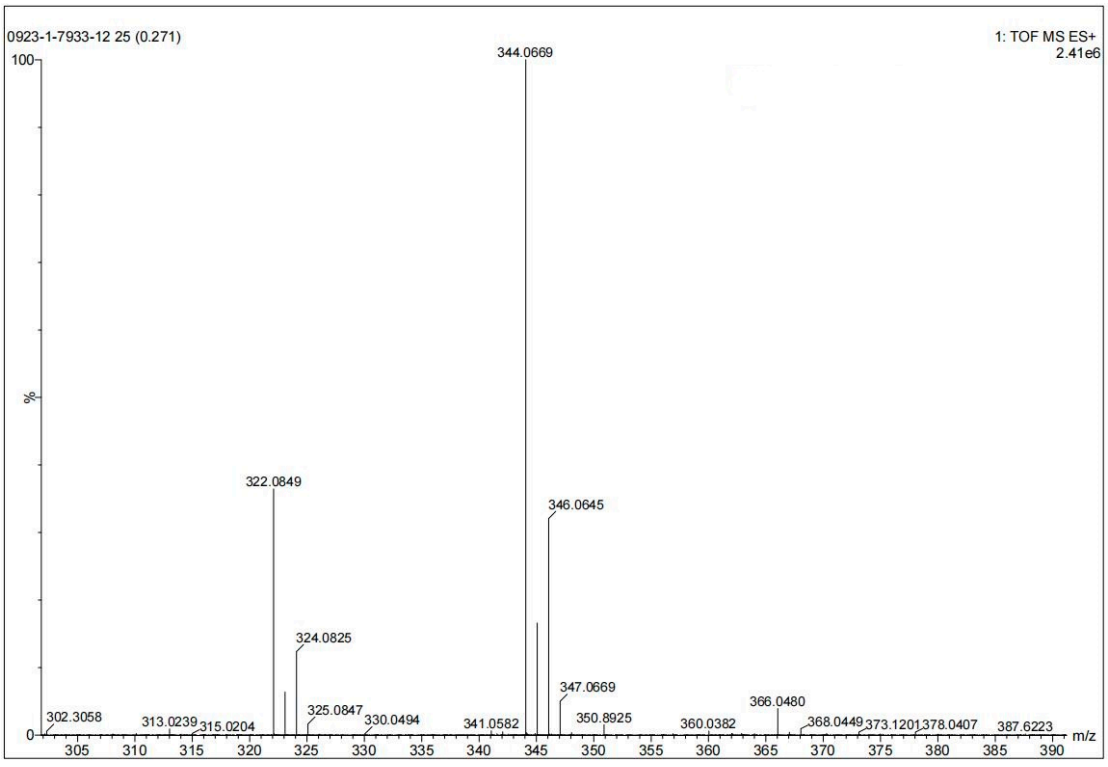

14.32
7.27
7.03
6.91
6.91
5.75
5.62
3.33
3.31
2.15
1.67
HN
CH3
O
O
O
O
H3C
Cl
Cl
0.80
0.92
1.91
0.96
1.72
2.89
3.00
f1 (ppm)

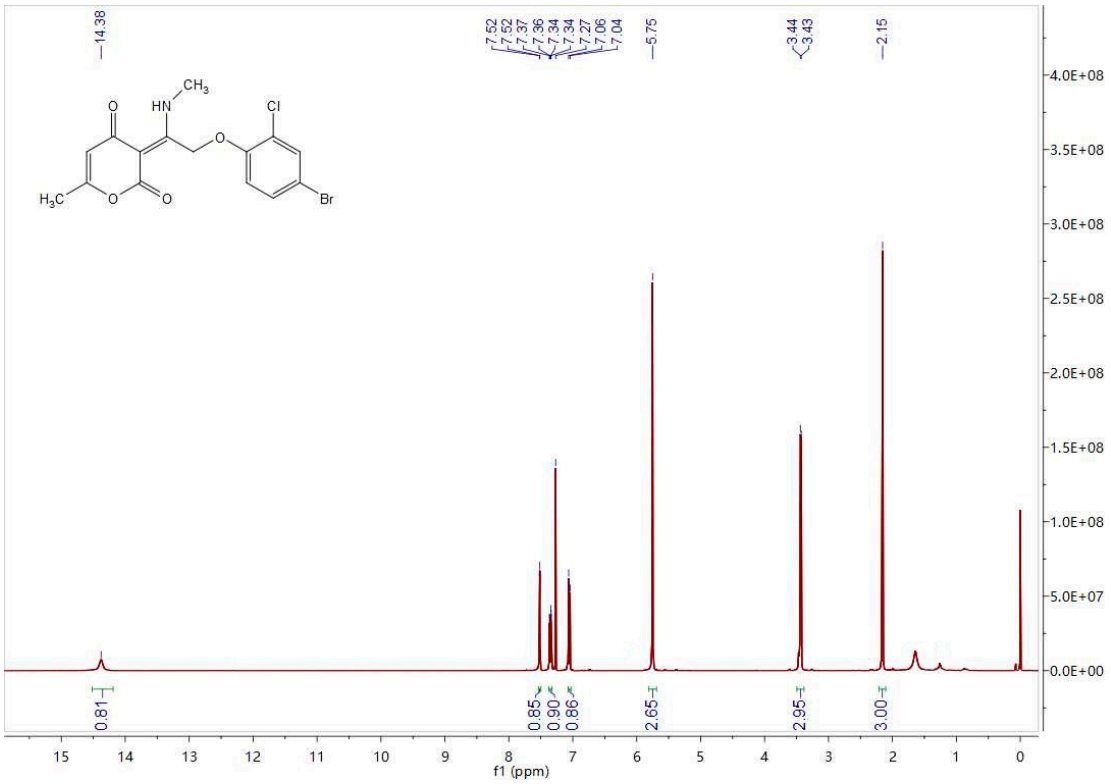

185.06
171.21
163.41
163.34
158.44
135.74
122.46
113.81
107.41
96.29
77.36
77.04
76.72
63.22
32.37
19.89
HN
CH3
O
O
O
O
H3C
Cl
Cl
f1 (ppm)

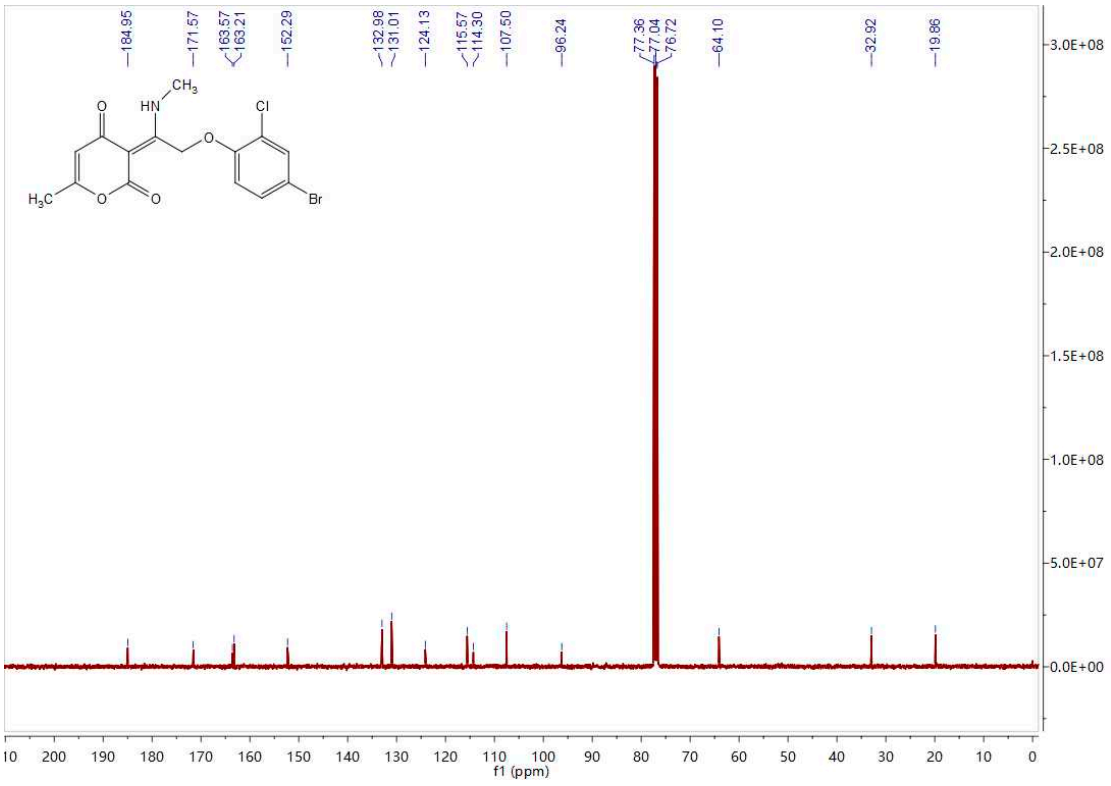

0923-1-7933-11 32 (0.331)
1: TOF MS ES+
7.54e5
100
%
0
364.0125
366.0098
342.0306
344.0278
368.0068
350.8932
310.9878
325.2096
330.3374
334.9164
362.8864
370.2956
382.0219
385.9939
396.3462
402.8961
412.8623
418.8803
419.8887
m/z
305 310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420

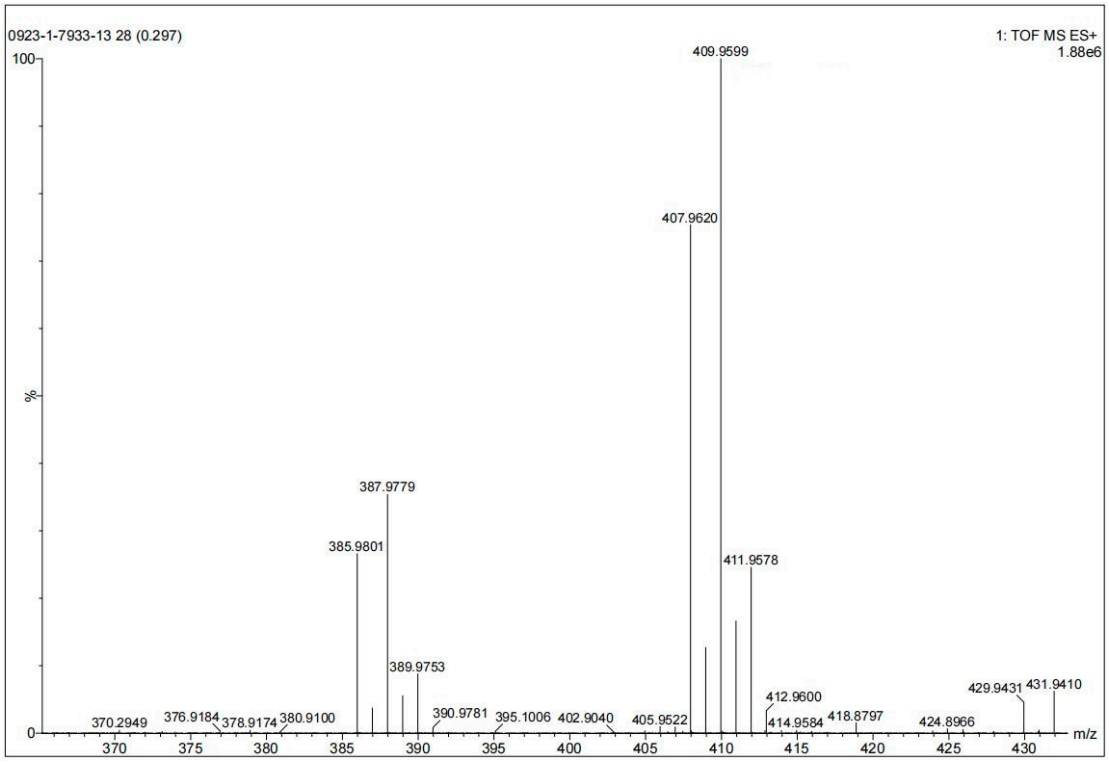

14.34
7.27
7.13
7.11
7.11
6.88
6.86
5.75
5.65
3.35
3.34
2.20
2.15
1.66
CH3
HN
O
O
CH3
O
H3C
O
O
Cl
3.8E+08
3.6E+08
3.4E+08
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
0.90
1.95
0.97
1.12
1.81
3.19
3.09
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

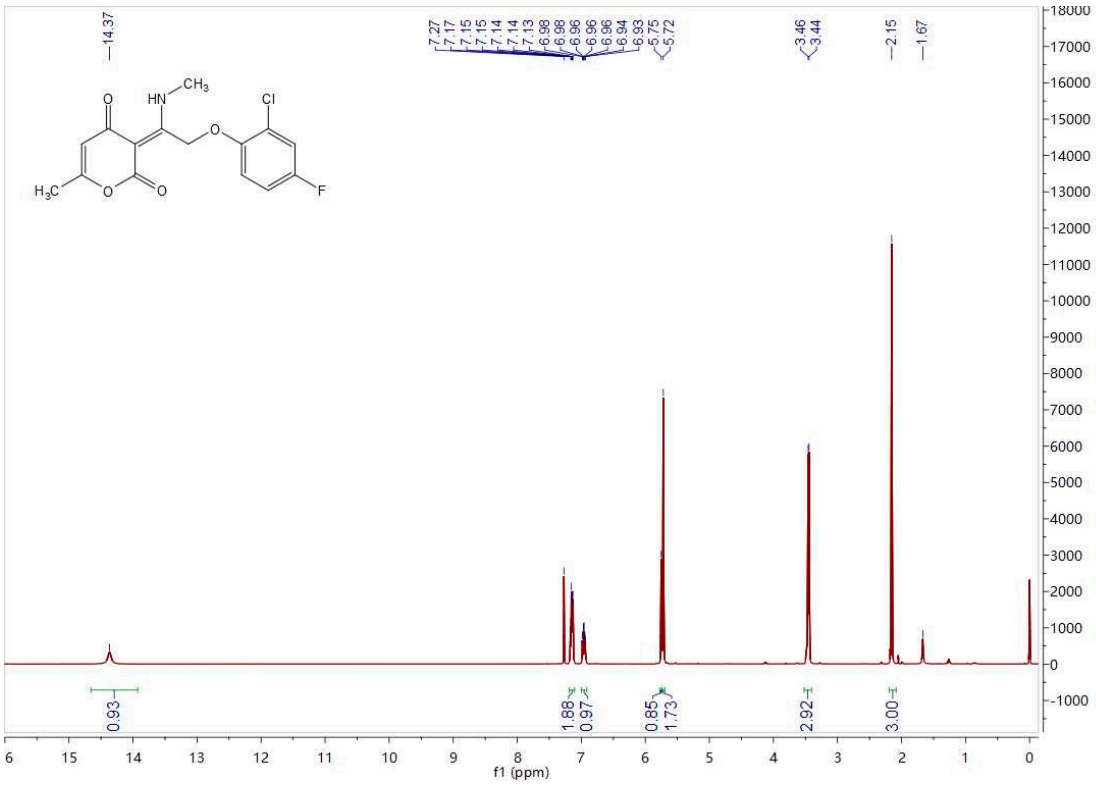

185.06
172.58
163.37
163.24
154.31
130.83
128.53
126.78
126.47
112.59
107.43
96.21
77.36
77.04
76.72
63.46
32.48
19.87
16.29
HN
CH3
O
CH3
O
H3C
O
O
Cl
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

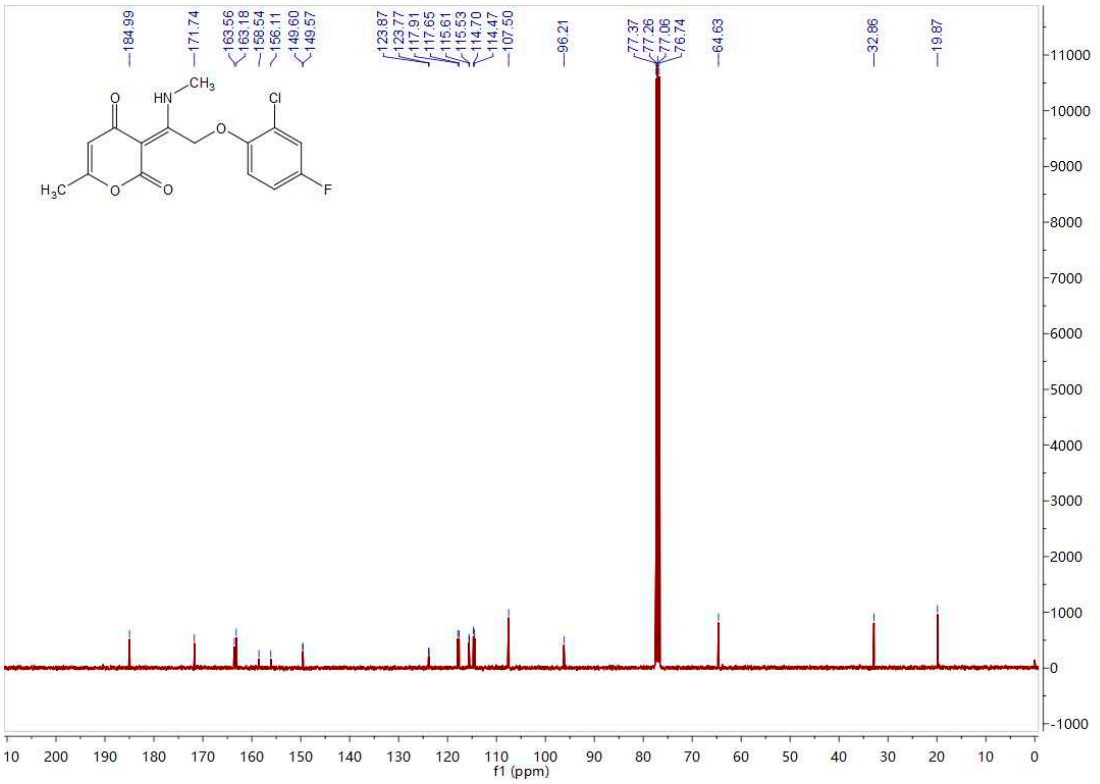

0923-1-7933-12 25 (0.271)
1: TOF MS ES+
2.41e6
100
%
0
344.0669
322.0849
346.0645
324.0825
347.0669
325.0847
366.0480
302.3058
313.0239
315.0204
330.0494
341.0582
350.8925
360.0382
368.0449
373.1201
378.0407
387.6223
m/z
305 310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390

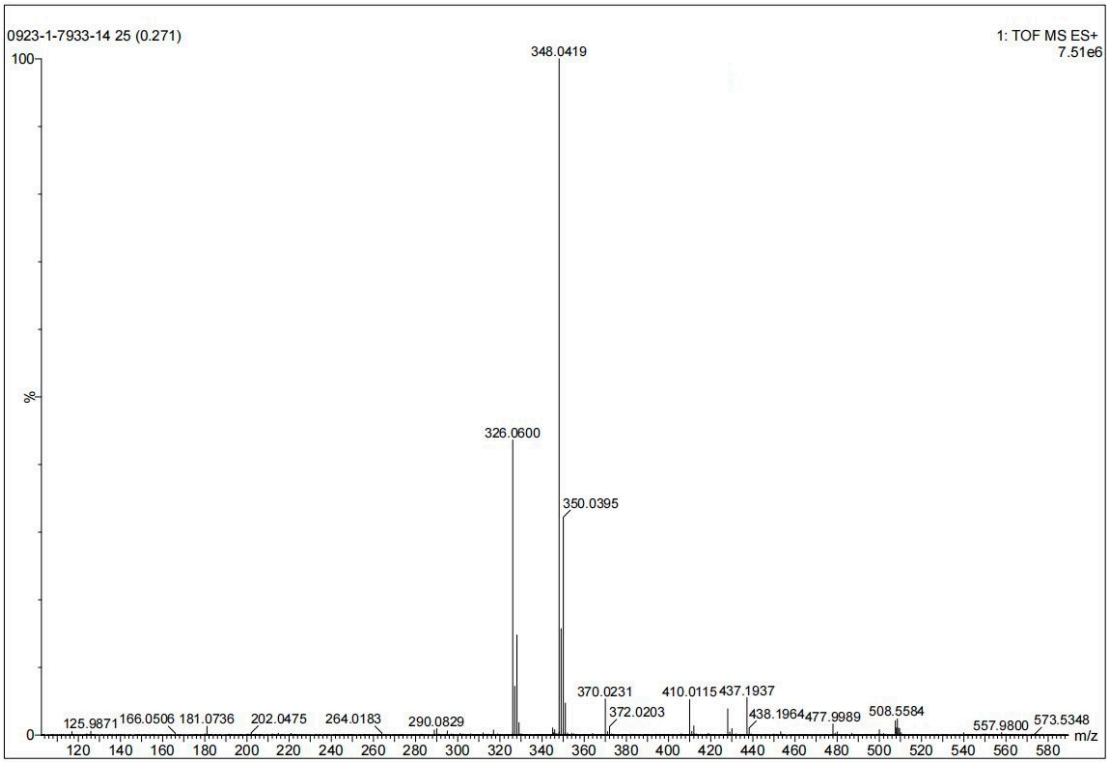

14.38
7.52
7.52
7.37
7.36
7.34
7.34
7.27
7.06
7.04
5.75
3.44
3.43
2.15
0.81
0.85
0.90
0.86
2.65
2.95
3.00
f1 (ppm)

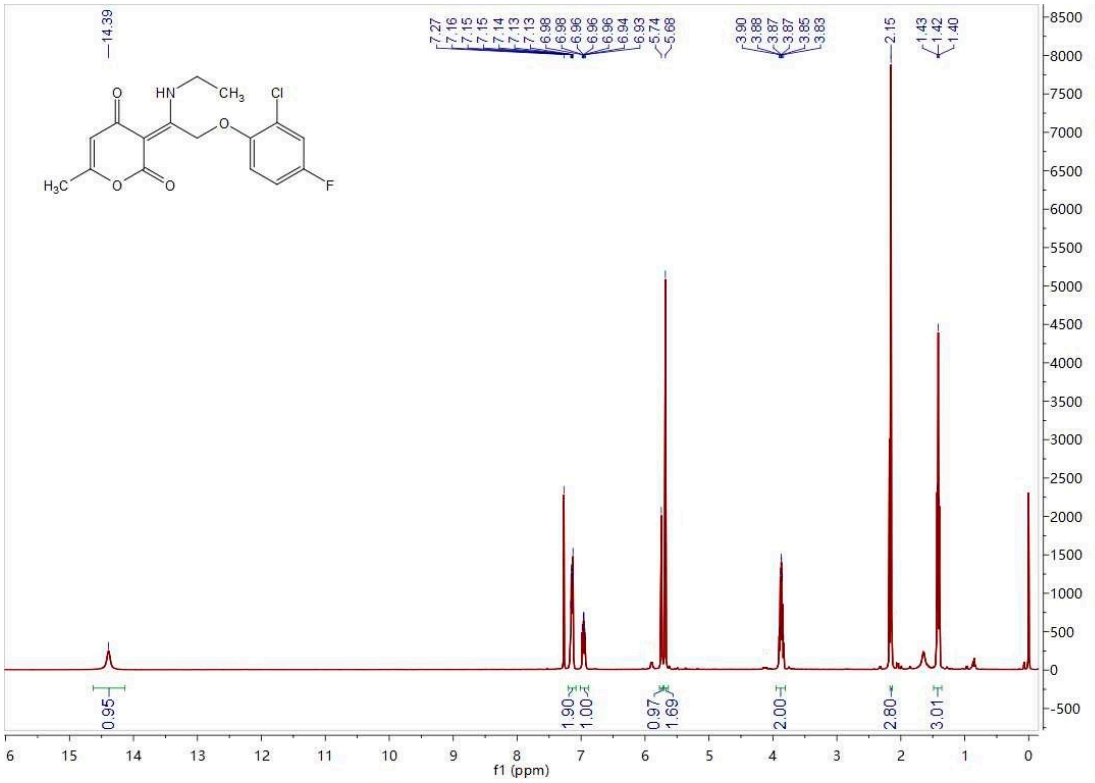

184.95
171.57
163.57
163.21
152.29
132.98
131.01
124.13
115.57
114.30
107.50
96.24
77.36
77.04
76.72
64.10
32.92
19.86
f1 (ppm)

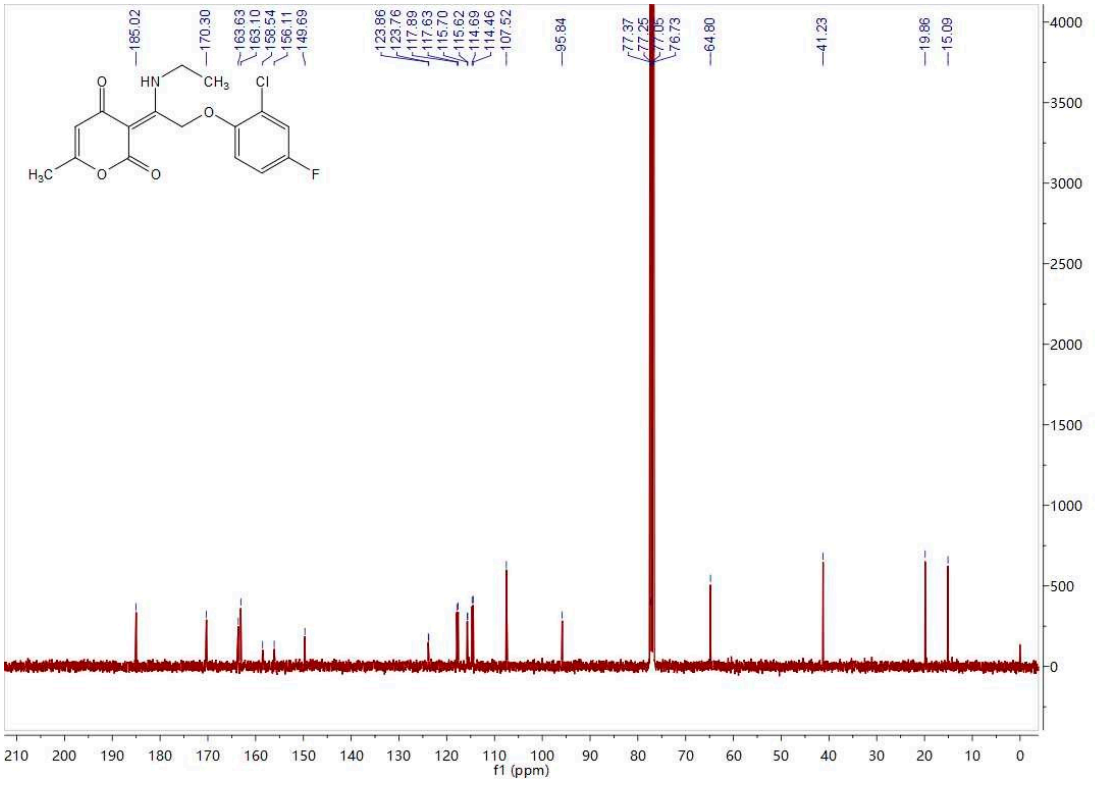

0923-1-7933-13 28 (0.297)
1: TOF MS ES+
1.88e6
100
%
0
409.9599
407.9620
387.9779
385.9801
411.9578
389.9753
412.9600
429.9431
431.9410
370.2949
376.9184
378.9174
380.9100
390.9781
395.1006
402.9040
405.9522
414.9584
418.8797
424.8966
m/z
370
375
380
385
390
395
400
405
410
415
420
425
430

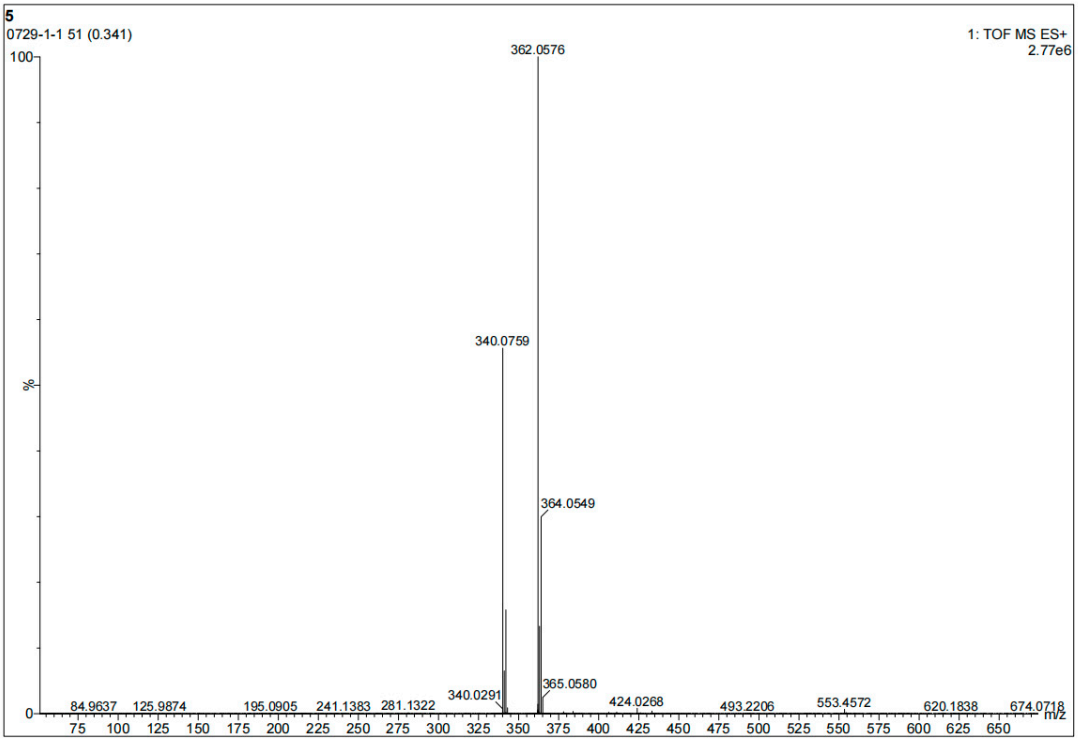

14.37
7.27
7.17
7.15
7.14
7.13
6.98
6.96
6.94
6.93
5.75
5.72
3.46
3.44
2.15
1.67
HN
CH3
O
Cl
O
O
H3C
O
F
0.93
1.88
0.97
0.85
1.73
2.92
3.00
f1 (ppm)

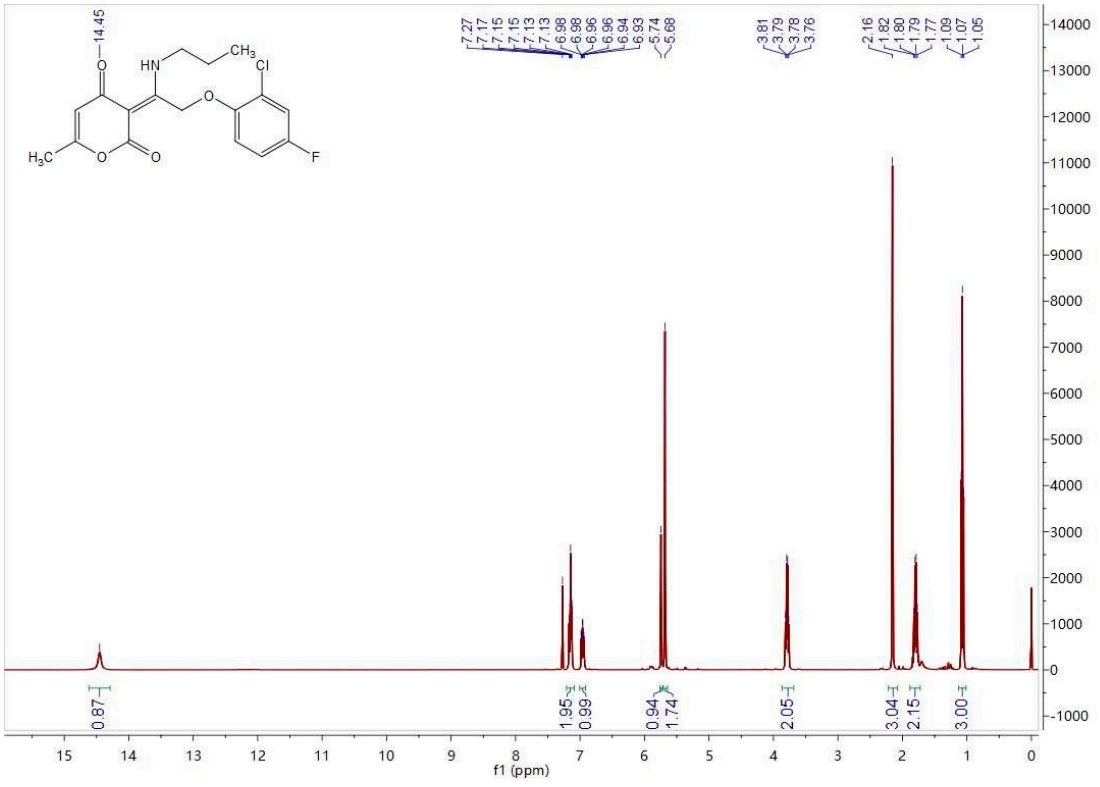

184.99
171.74
163.56
163.18
158.54
156.11
149.60
149.57
123.87
123.77
117.91
117.65
115.61
115.53
114.70
114.47
107.50
96.21
77.37
77.26
77.06
76.74
64.63
32.86
19.87
HN
CH3
O
Cl
F
H3C
f1 (ppm)

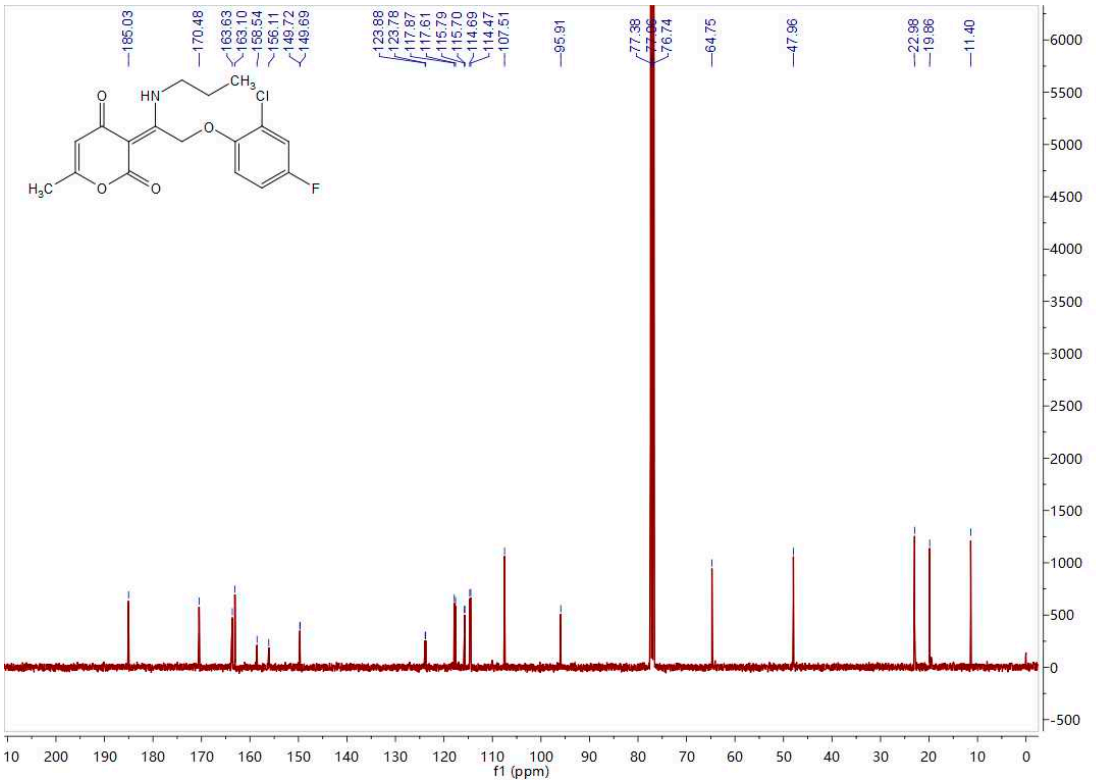

0923-1-7933-14 25 (0.271)
1: TOF MS ES+
7.51e6
348.0419
326.0600
350.0395
370.0231
372.0203
410.0115
437.1937
438.1964
477.9989
508.5584
557.9800
573.5348
125.9871
166.0506
181.0736
202.0475
264.0183
290.0829
%
m/z

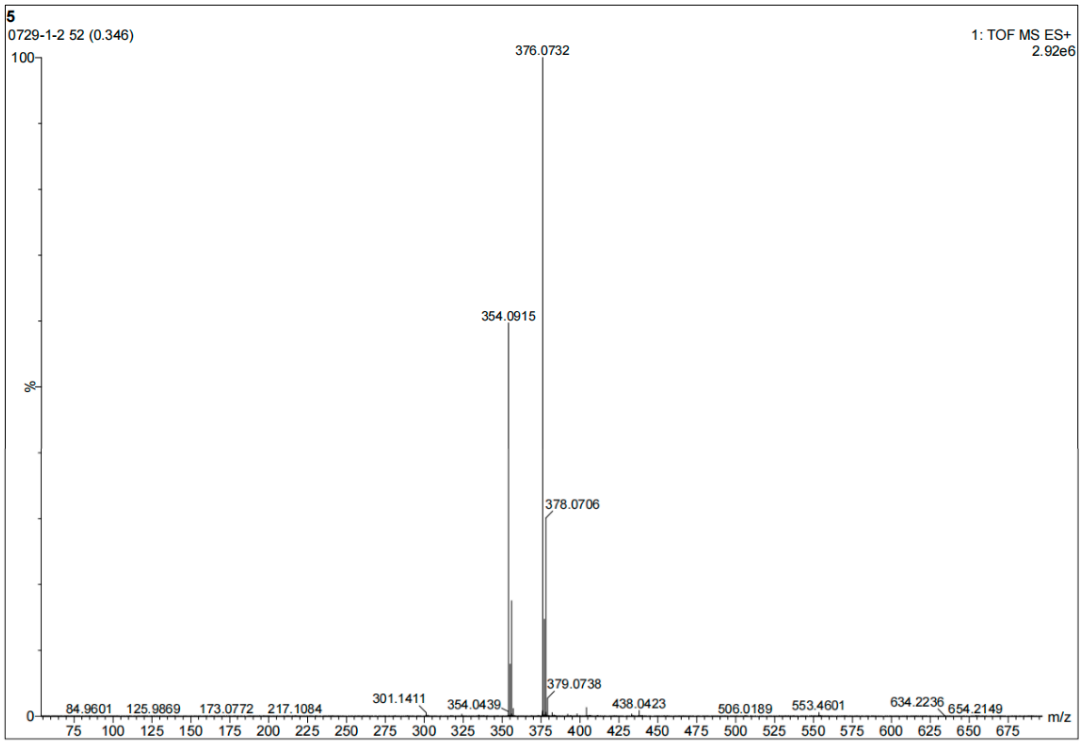

14.39
7.27
7.16
7.15
7.15
7.14
7.13
7.13
6.98
6.98
6.96
6.96
6.96
6.94
6.93
5.74
5.68
3.90
3.88
3.87
3.87
3.85
3.83
2.15
1.43
1.42
1.40
HN
CH3
Cl
O
O
O
O
H3C
F
0.95
1.90
1.00
0.97
1.69
2.00
2.80
3.01
f1 (ppm)

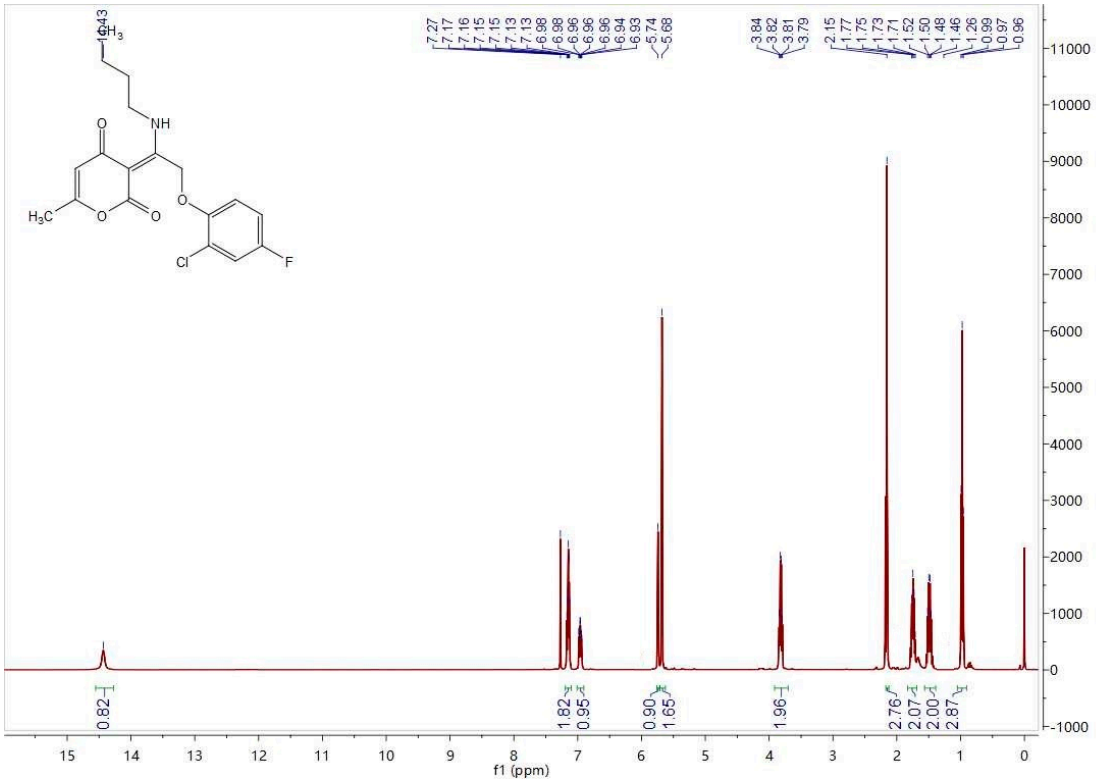

185.02
170.30
163.63
163.10
158.54
156.11
149.69
123.86
123.76
117.89
117.63
115.70
115.62
114.69
114.46
107.52
95.84
77.37
77.25
77.05
76.73
64.80
41.23
19.86
15.09
HN
CH3
Cl
O
O
O
O
H3C
F
f1 (ppm)

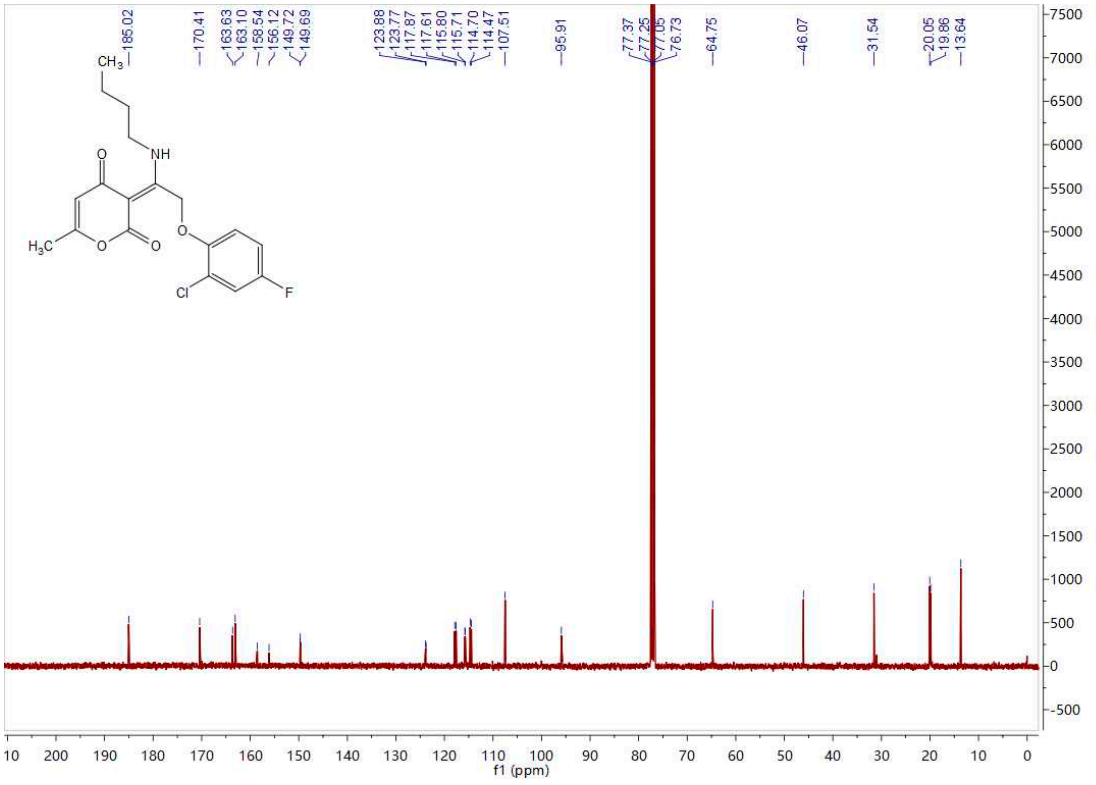

5
0729-1-1 51 (0.341)
1: TOF MS ES+
2.77e6
100
%
0
362.0576
340.0759
364.0549
365.0580
340.0291
84.9637
125.9874
195.0905
241.1383
281.1322
424.0268
493.2206
553.4572
620.1838
674.0718
m/z

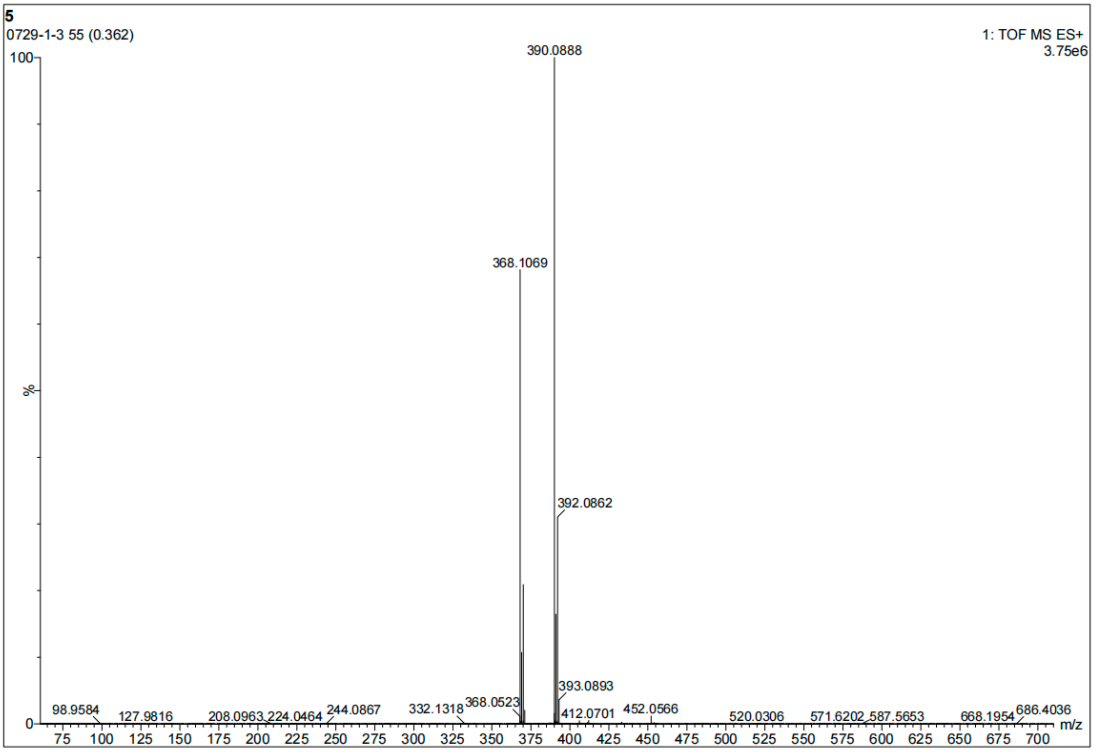

14.45
HN
CH3
Cl
O
F
H3C
7.27
7.17
7.15
7.13
6.98
6.96
6.94
6.93
5.74
5.68
3.81
3.79
3.78
3.76
2.16
1.82
1.80
1.79
1.77
1.09
1.07
1.05
0.87
1.95
0.99
0.94
1.74
2.05
3.04
2.15
3.00
f1 (ppm)

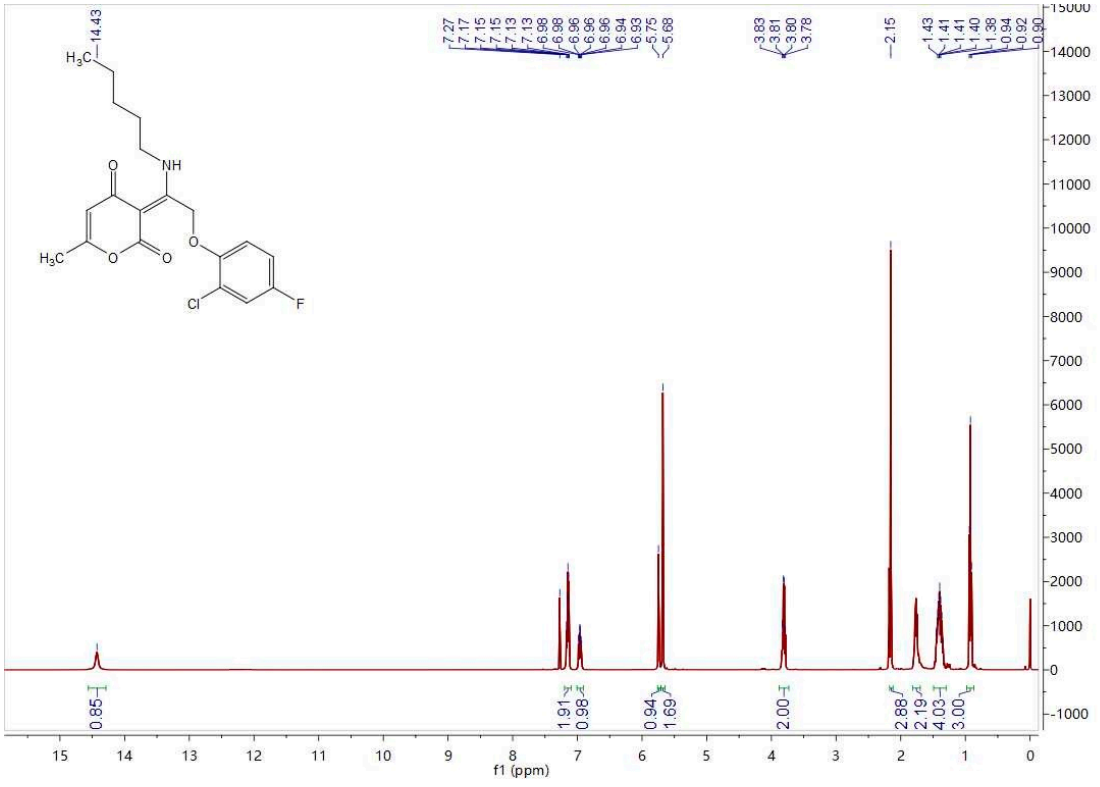

185.03
170.48
163.63
163.10
158.54
156.11
149.72
149.69
123.88
123.78
117.87
117.61
115.79
115.70
114.69
114.47
107.51
95.91
77.38
77.06
76.74
64.75
47.96
22.98
19.86
11.40
HN
CH3
Cl
O
O
O
O
H3C
F
f1 (ppm)

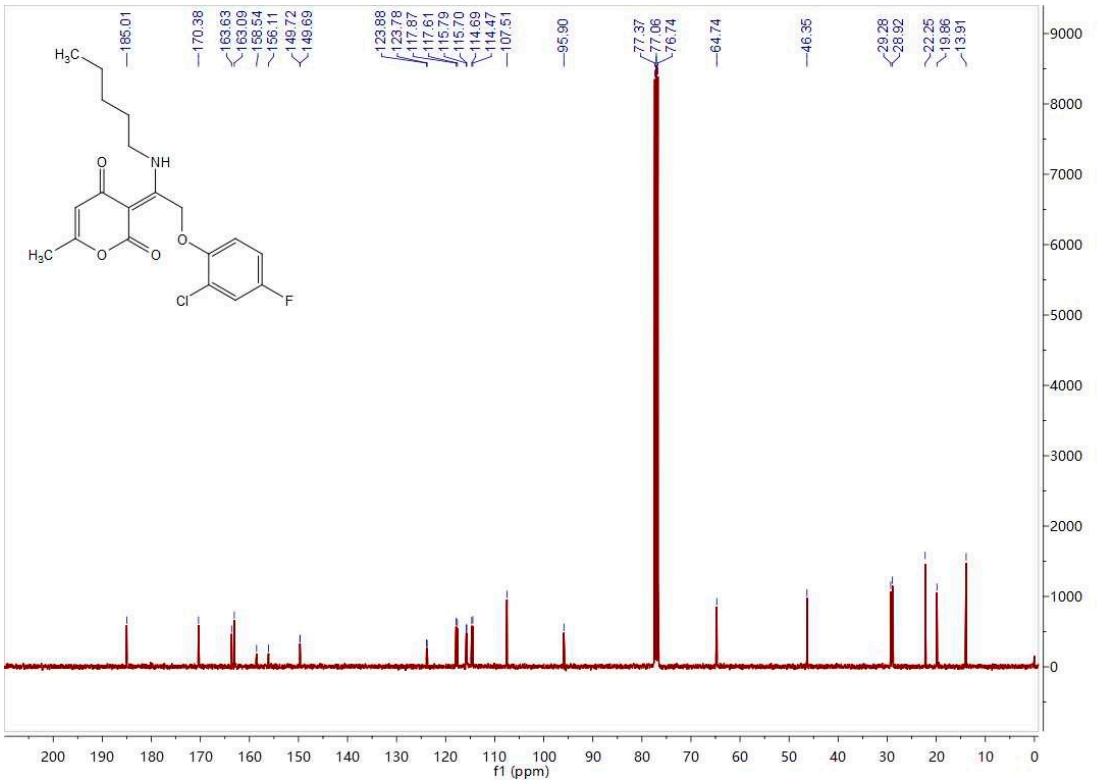

5
0729-1-2 52 (0.346)
1: TOF MS ES+
2.92e6
376.0732
354.0915
378.0706
379.0738
301.1411
354.0439
84.9601
125.9869
173.0772
217.1084
438.0423
506.0189
553.4601
634.2236
654.2149
%
m/z

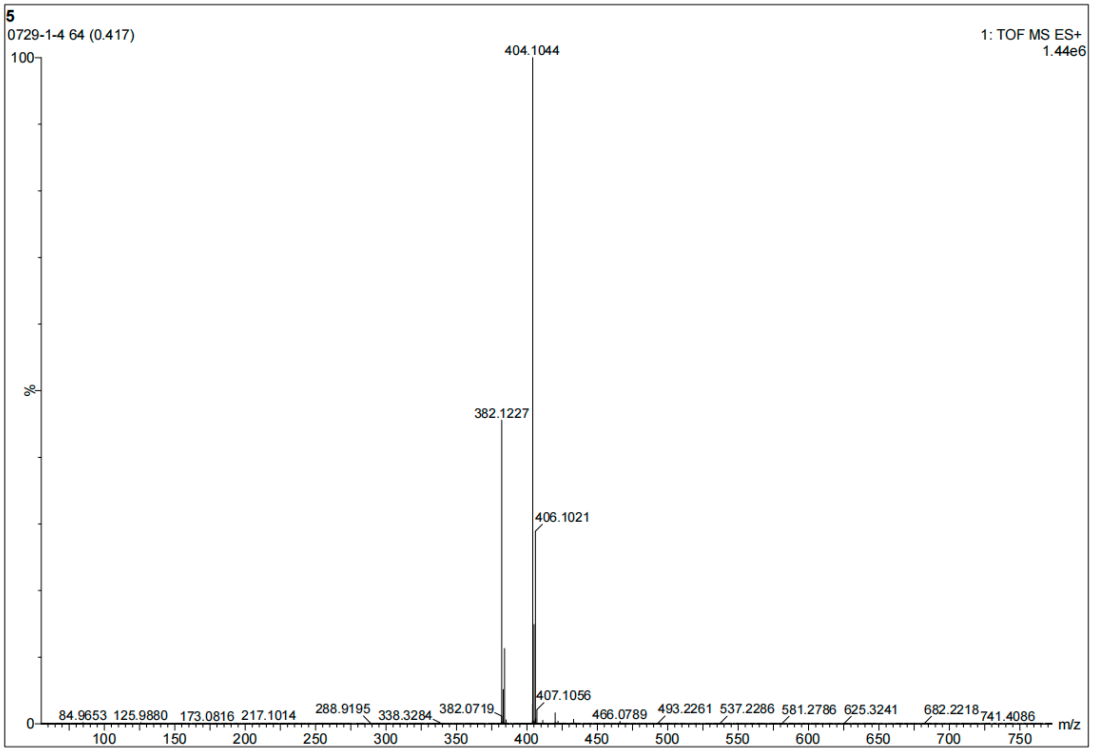

7.27
7.17
7.16
7.15
7.15
7.13
6.98
6.98
6.96
6.96
6.96
6.94
6.93
5.74
5.68
3.84
3.82
3.81
3.79
2.15
1.77
1.75
1.73
1.71
1.52
1.50
1.48
1.46
1.26
0.99
0.97
0.96
1.43
CH3
NH
O
O
O
H3C
O
Cl
F
0.82
1.82
0.95
0.90
1.65
1.96
2.76
2.07
2.00
2.87
f1 (ppm)

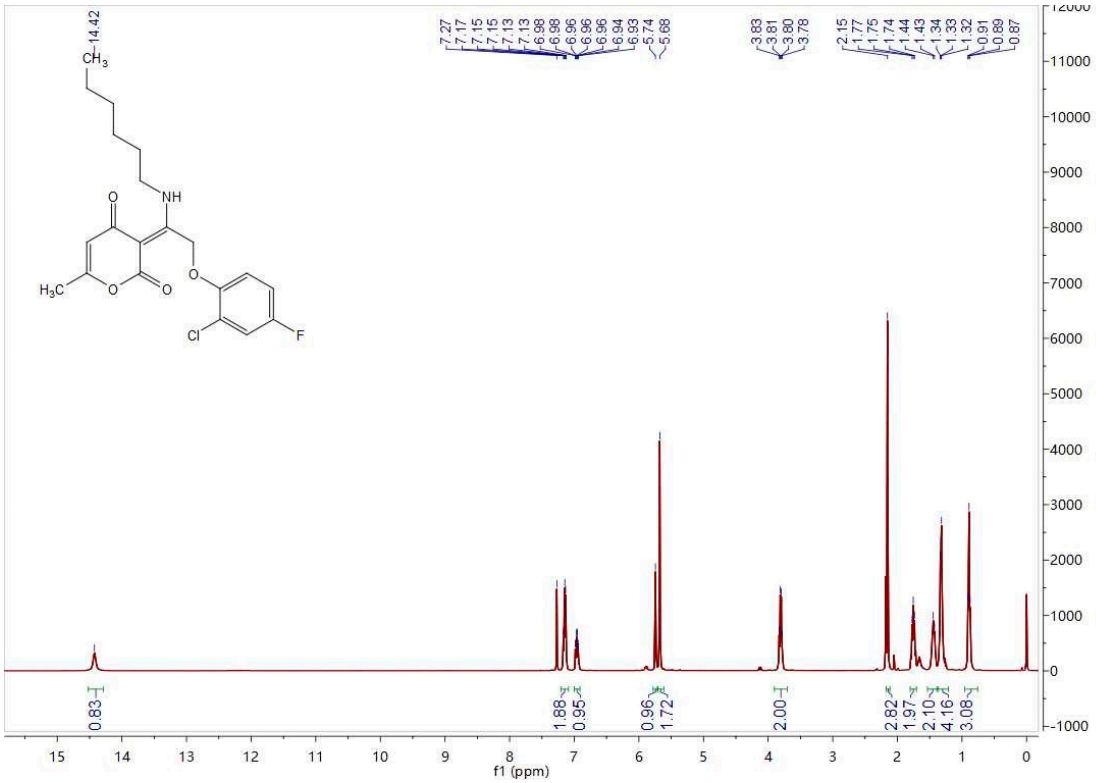

185.02
170.41
163.63
163.10
158.54
156.12
149.72
149.69
123.88
123.77
117.87
117.61
115.80
115.71
114.70
114.47
107.51
95.91
77.37
77.25
77.05
76.73
64.75
46.07
31.54
20.05
19.86
13.64
CH3
NH
O
O
O
H3C
O
Cl
F
f1 (ppm)

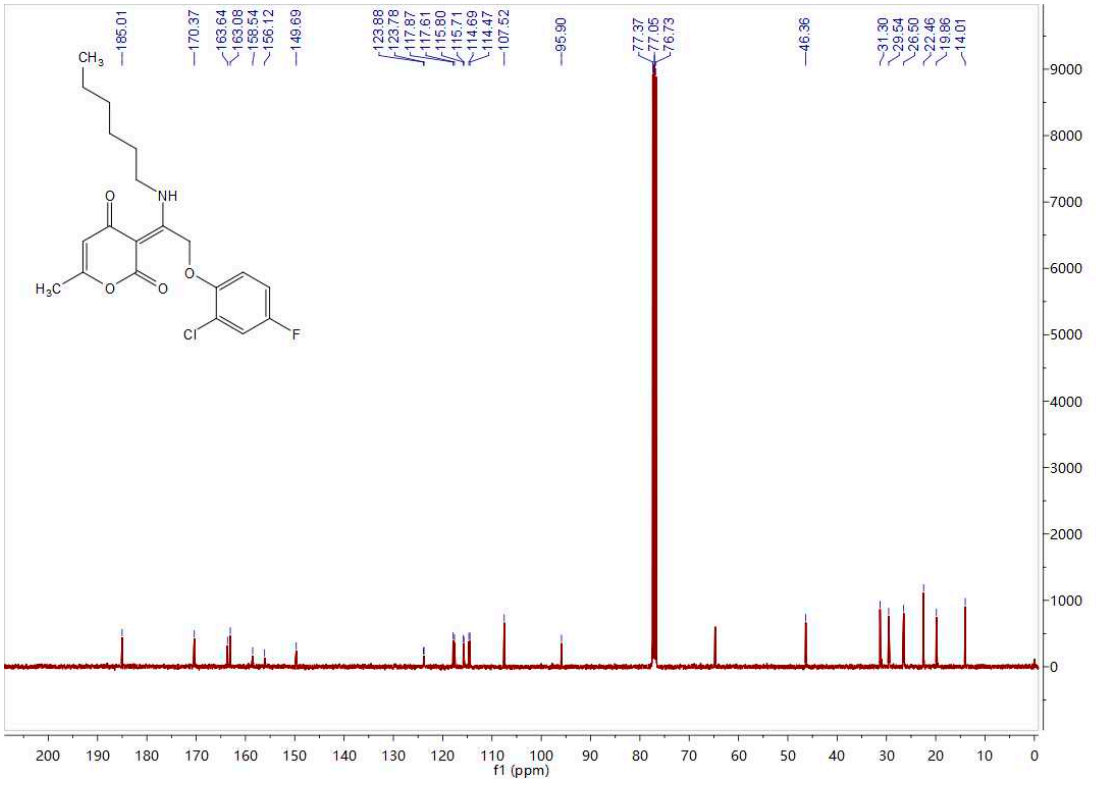

5
0729-1-3 55 (0.362)
1: TOF MS ES+
3.75e6
100
%
0
390.0888
368.1069
392.0862
393.0893
98.9584
127.9816
208.0963
224.0464
244.0867
332.1318
368.0523
412.0701
452.0566
520.0306
571.6202
587.5653
668.1954
686.4036
m/z
75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700

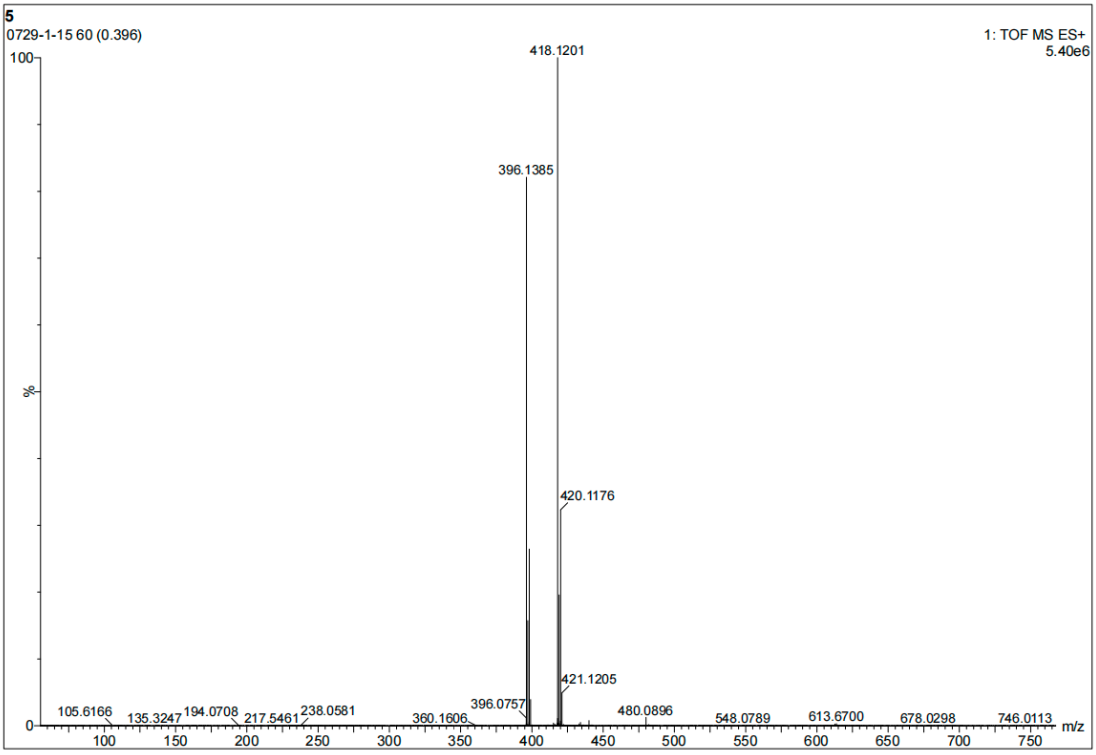

14.43
H3C
NH
O
O
O
H3C
O
Cl
F
7.27
7.17
7.15
7.13
6.98
6.96
6.96
6.94
6.93
5.75
5.68
3.83
3.81
3.80
3.78
2.15
1.43
1.41
1.41
1.40
1.38
0.94
0.92
0.90
0.85
1.91
0.98
0.94
1.69
2.00
2.88
2.19
4.03
3.00
f1 (ppm)

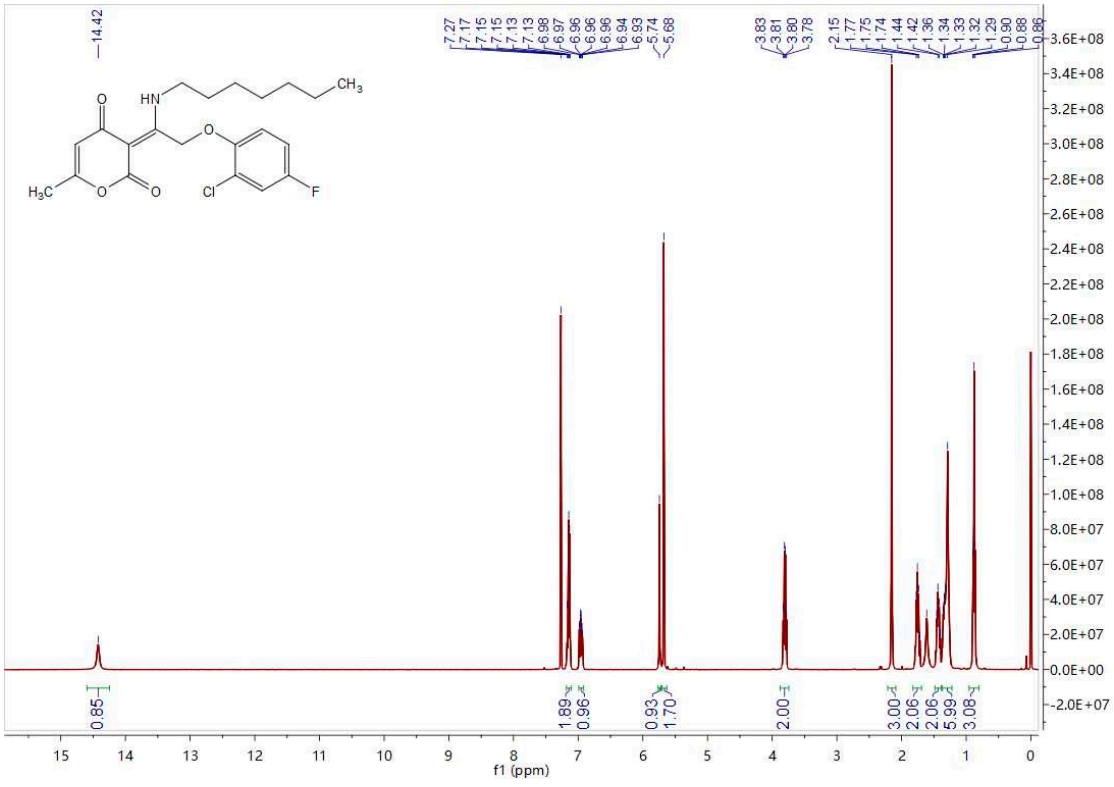

185.01
170.38
163.63
163.09
158.54
156.11
149.72
149.69
123.88
123.78
117.87
117.61
115.79
115.70
114.69
114.47
107.51
95.90
77.37
77.06
76.74
64.74
46.35
29.28
28.92
22.25
19.86
13.91
H3C
NH
O
O
O
H3C
O
Cl
F
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

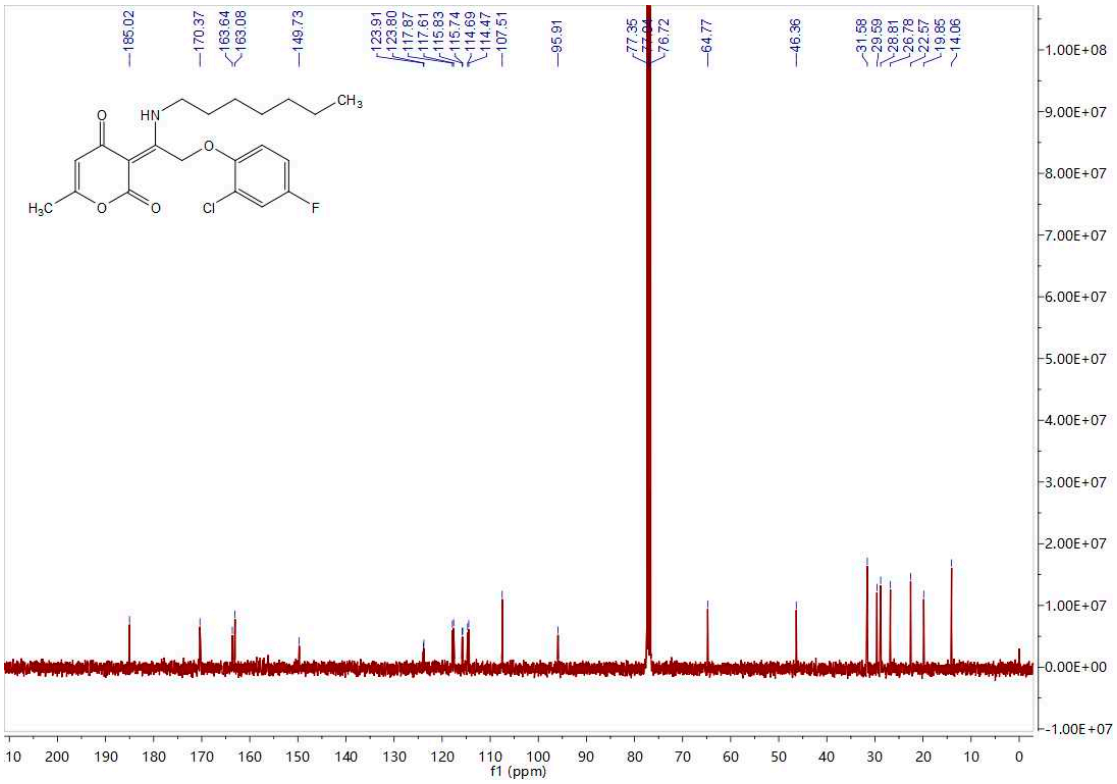

5
0729-1-4 64 (0.417)
1: TOF MS ES+
1.44e6
100
%
0
404.1044
382.1227
406.1021
407.1056
84.9653
125.9880
173.0816
217.1014
288.9195
338.3284
382.0719
466.0789
493.2261
537.2286
581.2786
625.3241
682.2218
741.4086
100 150 200 250 300 350 400 450 500 550 600 650 700 750
m/z

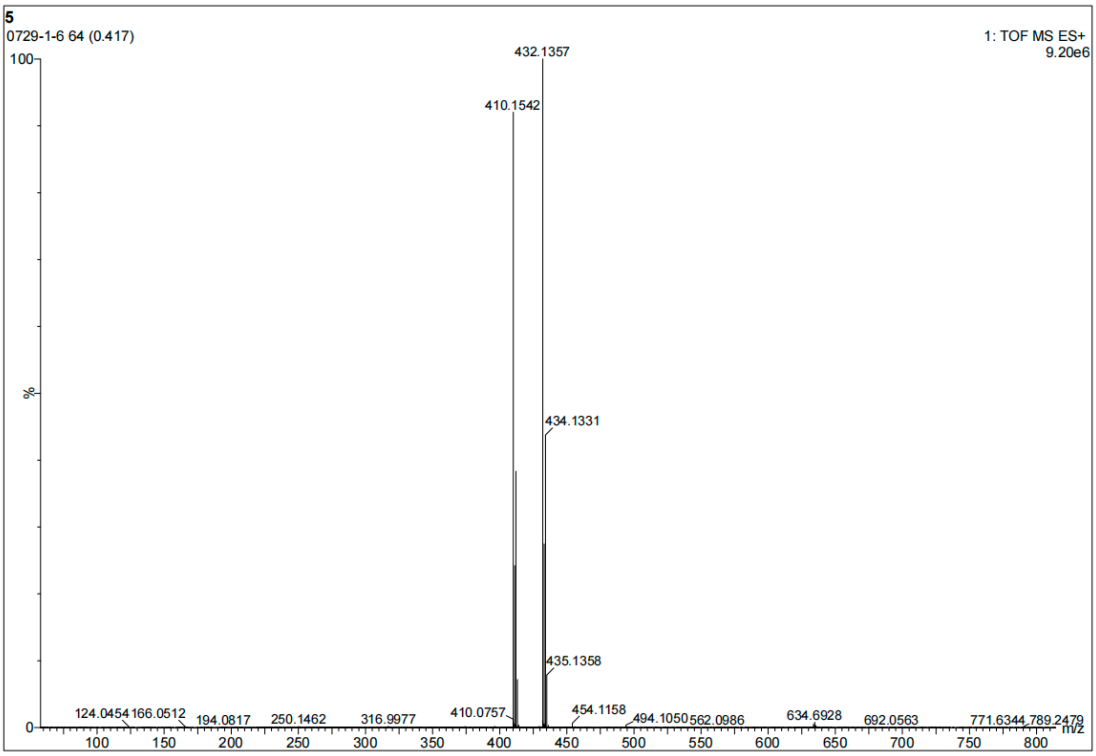

14.42
CH3
NH
O
O
H3C
O
O
Cl
F
7.27
7.17
7.15
7.15
7.13
6.98
6.98
6.96
6.96
6.96
6.94
6.93
5.74
5.68
3.83
3.81
3.80
3.78
2.15
1.77
1.75
1.74
1.44
1.43
1.34
1.33
1.32
0.91
0.89
0.87
0.83
1.88
0.95
0.96
1.72
2.00
2.82
1.97
2.10
4.16
3.08
f1 (ppm)

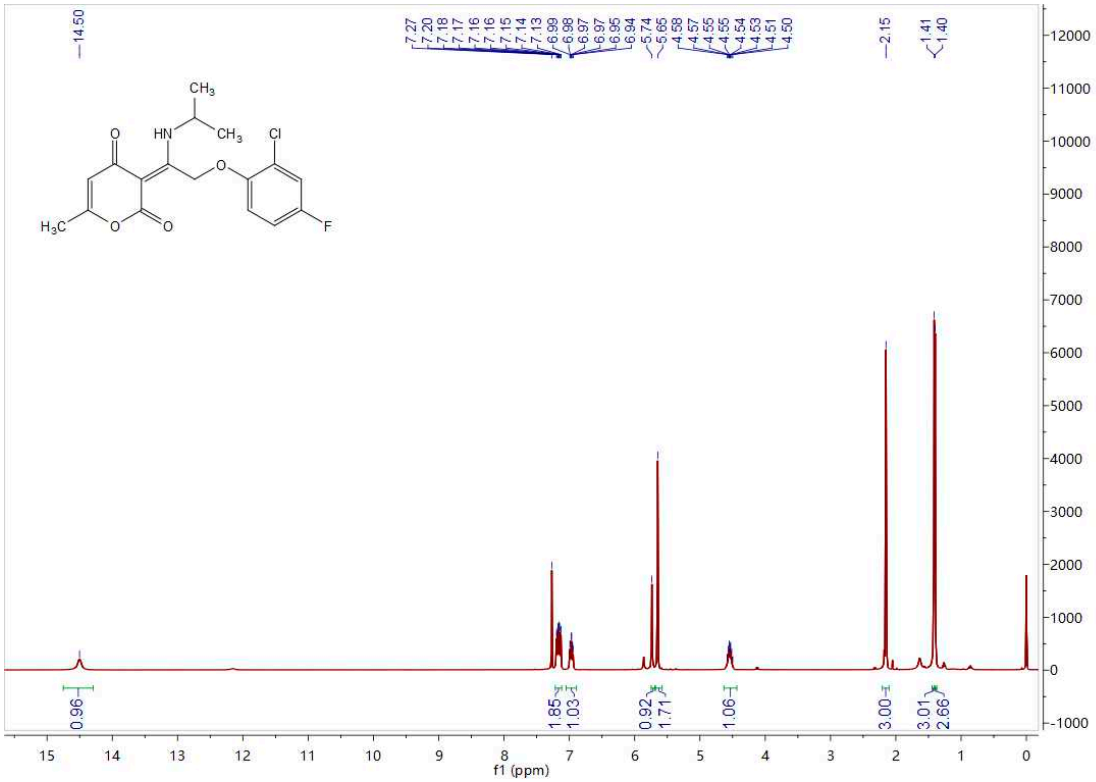

185.01
170.37
163.64
163.08
158.54
156.12
149.69
123.88
123.78
117.87
117.61
115.80
115.71
114.69
114.47
107.52
95.90
77.37
77.05
76.73
46.36
31.30
29.54
26.50
22.46
19.86
14.01
CH3
NH
O
O
H3C
O
O
Cl
F
f1 (ppm)

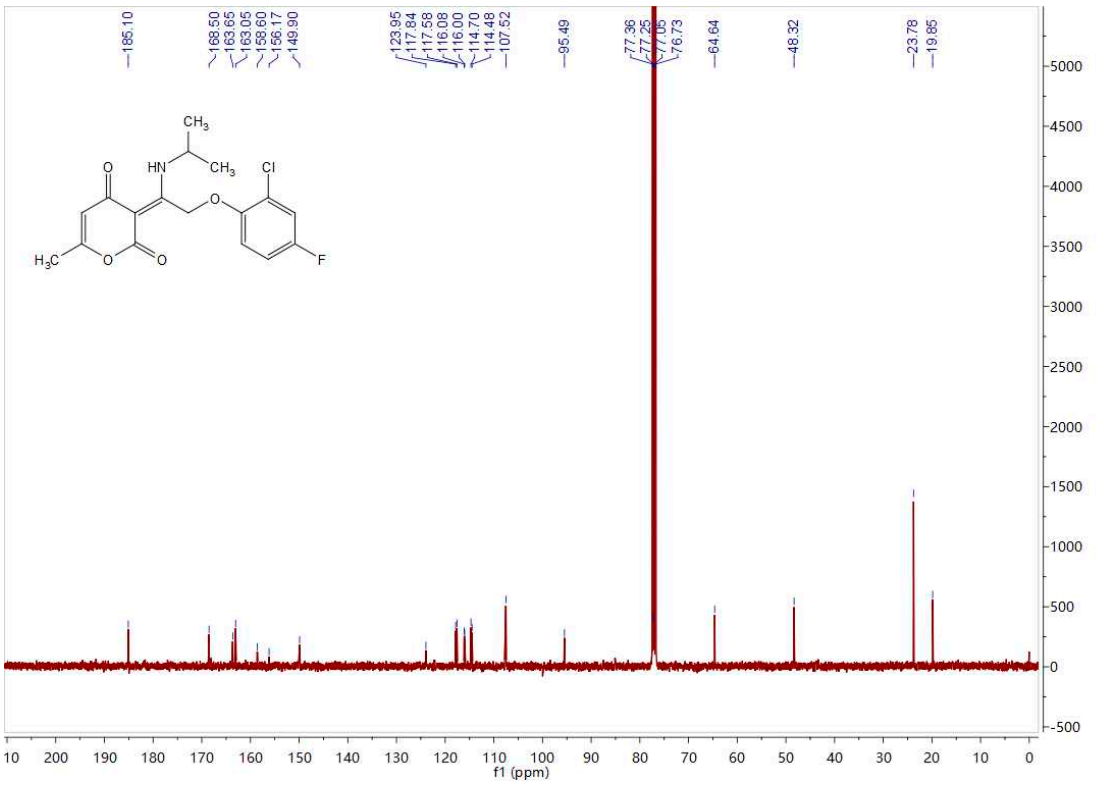

5
0729-1-15 60 (0.396)
1: TOF MS ES+
5.40e6
100
%
0
418.1201
396.1385
420.1176
421.1205
396.0757
105.6166
135.3247
194.0708
217.5461
238.0581
360.1606
480.0896
548.0789
613.6700
678.0298
746.0113
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750

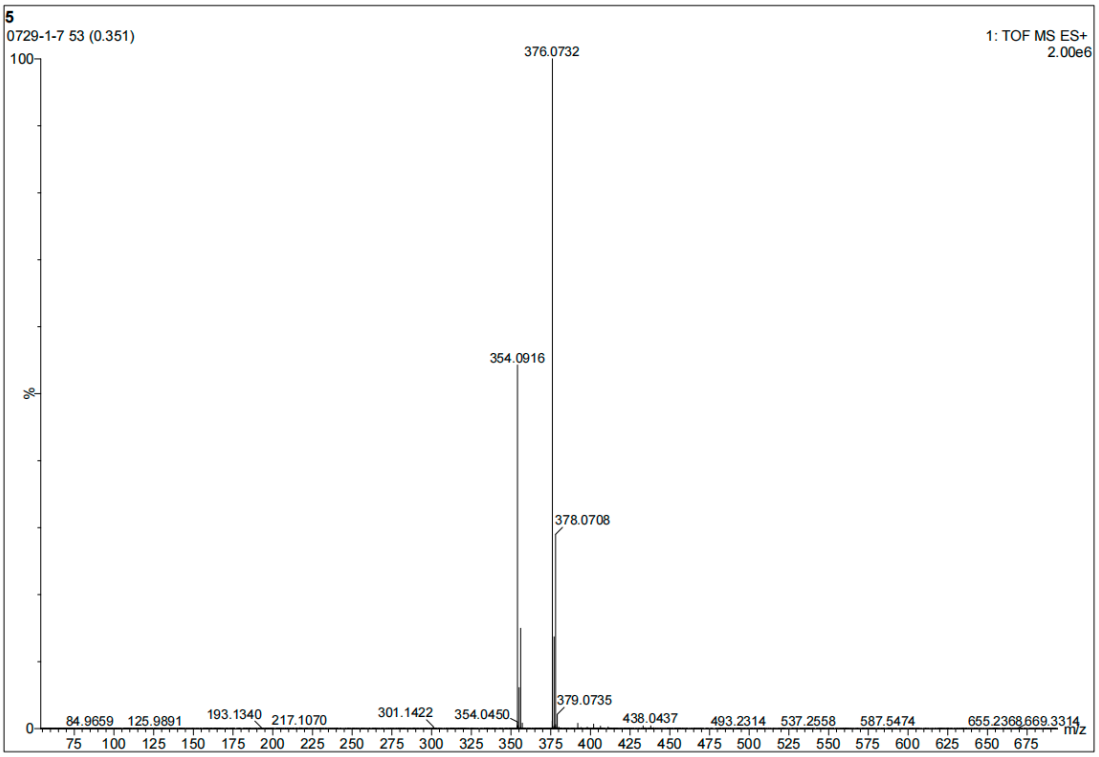

14.42
HN
CH3
O
O
O
H3C
O
Cl
F
7.27
7.17
7.15
7.15
7.13
6.98
6.97
6.96
6.96
6.96
6.94
6.93
5.74
5.68
3.83
3.81
3.80
3.78
2.15
1.77
1.75
1.74
1.44
1.42
1.36
1.34
1.33
1.32
1.29
0.90
0.88
0.86
3.6E+08
3.4E+08
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
0.85
1.89
0.96
0.93
1.70
2.00
3.00
2.06
2.06
5.99
3.08
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

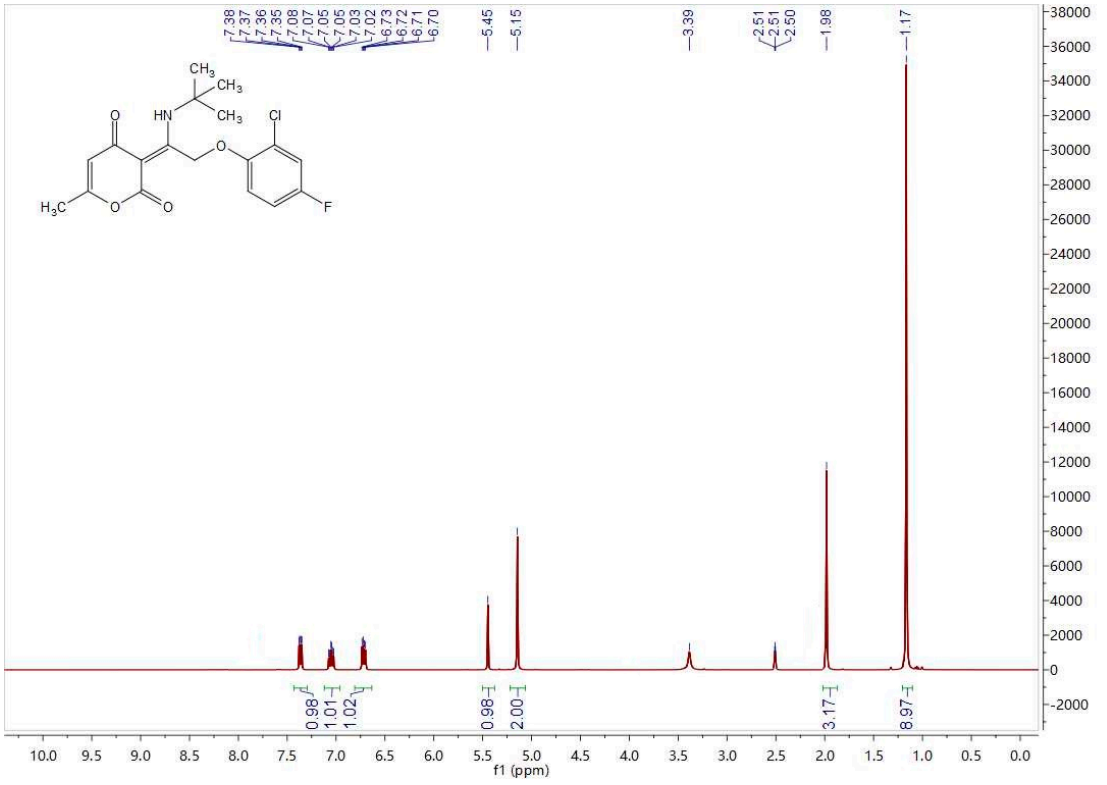

185.02
170.37
163.64
163.08
149.73
123.91
123.80
117.87
117.61
115.83
115.74
114.69
114.47
107.51
95.91
77.35
77.04
76.72
64.77
46.36
31.58
29.59
28.81
26.78
22.57
19.85
14.06
HN
CH3
O
O
O
H3C
O
Cl
F
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
f1 (ppm)

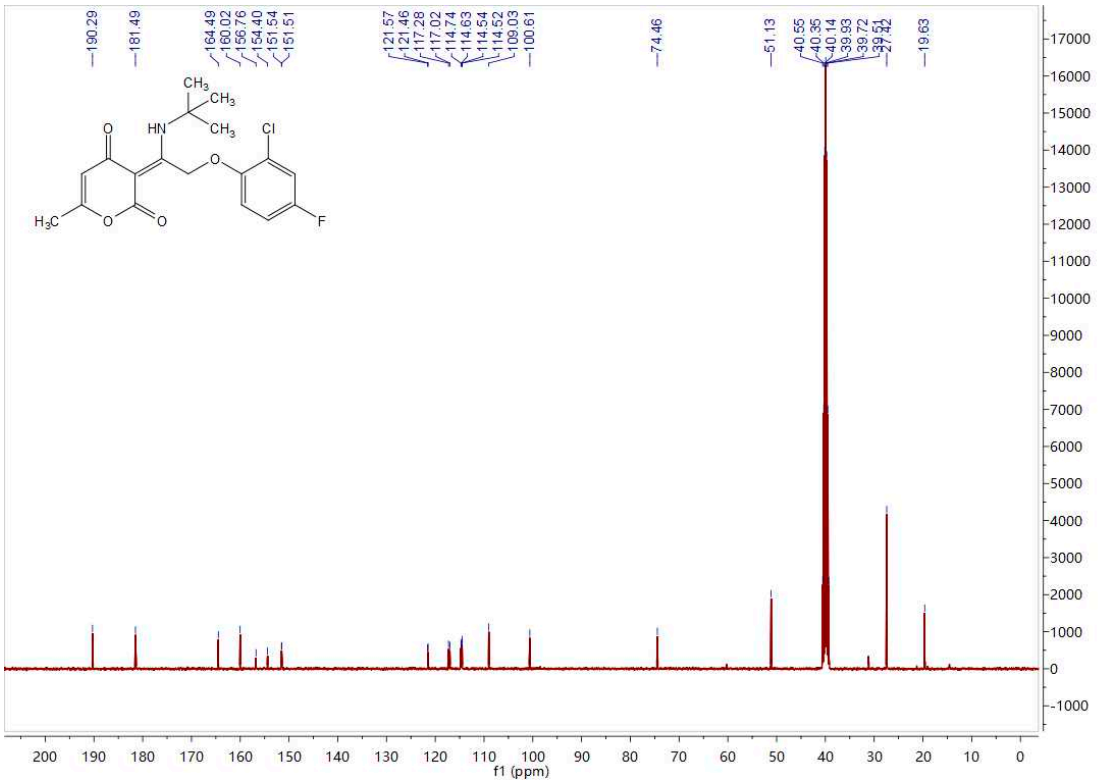

5
0729-1-6 64 (0.417)
1: TOF MS ES+
9.20e6
100
%
0
432.1357
410.1542
434.1331
435.1358
124.0454
166.0512
194.0817
250.1462
316.9977
410.0757
454.1158
494.1050
562.0986
634.6928
692.0563
771.6344
789.2479
m/z

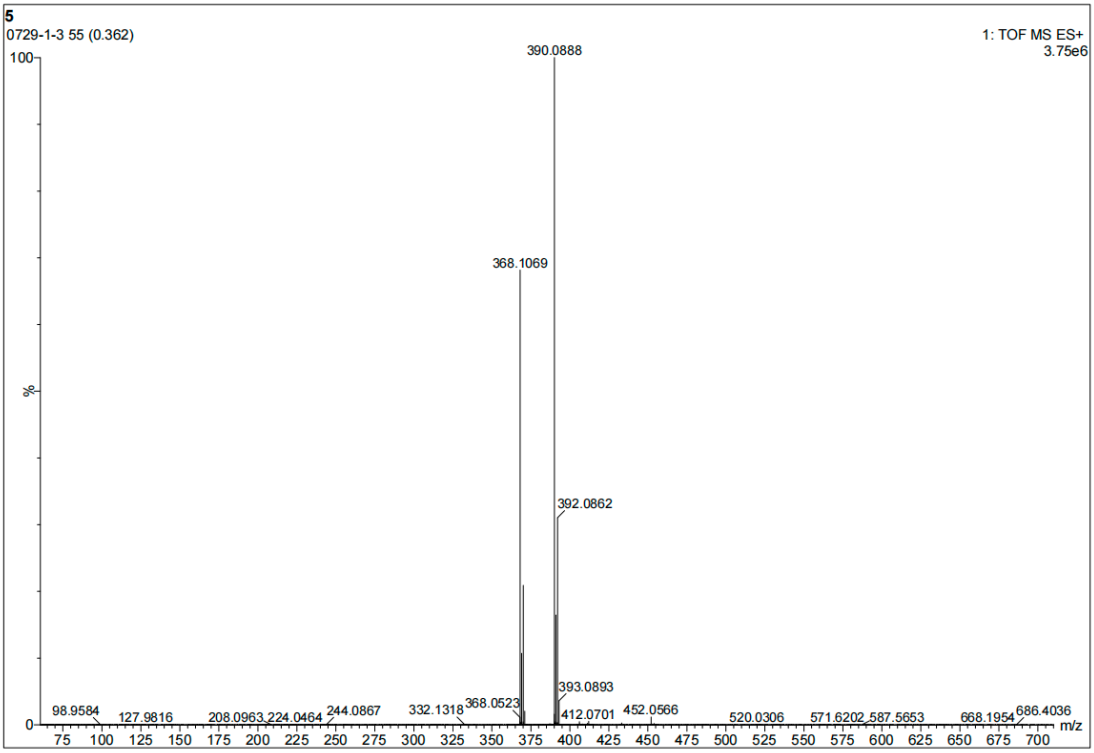

14.50
7.27
7.20
7.18
7.17
7.16
7.16
7.15
7.14
7.13
6.99
6.98
6.97
6.97
6.95
6.94
5.74
5.65
4.58
4.57
4.55
4.55
4.54
4.53
4.51
4.50
2.15
1.41
1.40
CH3
HN
CH3
Cl
O
O
O
H3C
O
O
F
0.96
1.85
1.03
0.92
1.71
1.06
3.00
3.01
2.66
f1 (ppm)

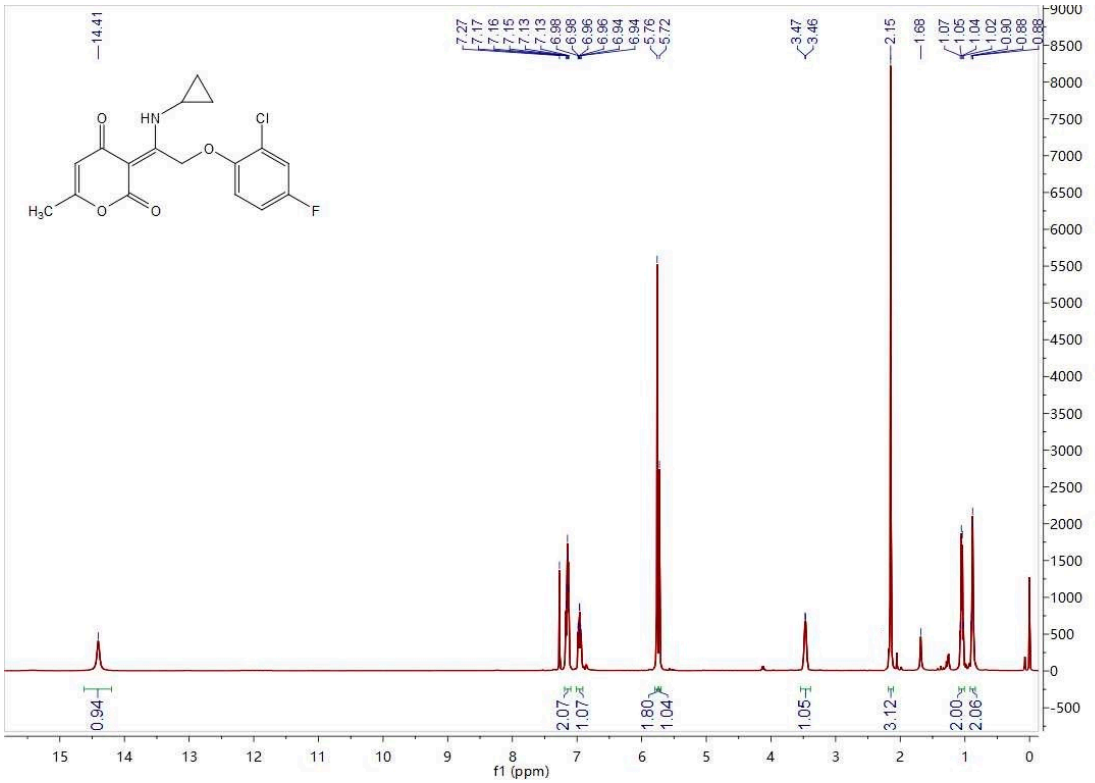

185.10
168.50
163.65
163.05
158.60
156.17
149.90
123.95
117.84
117.58
116.08
116.00
114.70
114.48
107.52
95.49
77.36
77.26
77.05
76.73
64.64
48.32
23.78
19.85
CH3
HN
CH3
Cl
O
O
O
H3C
O
O
F
f1 (ppm)

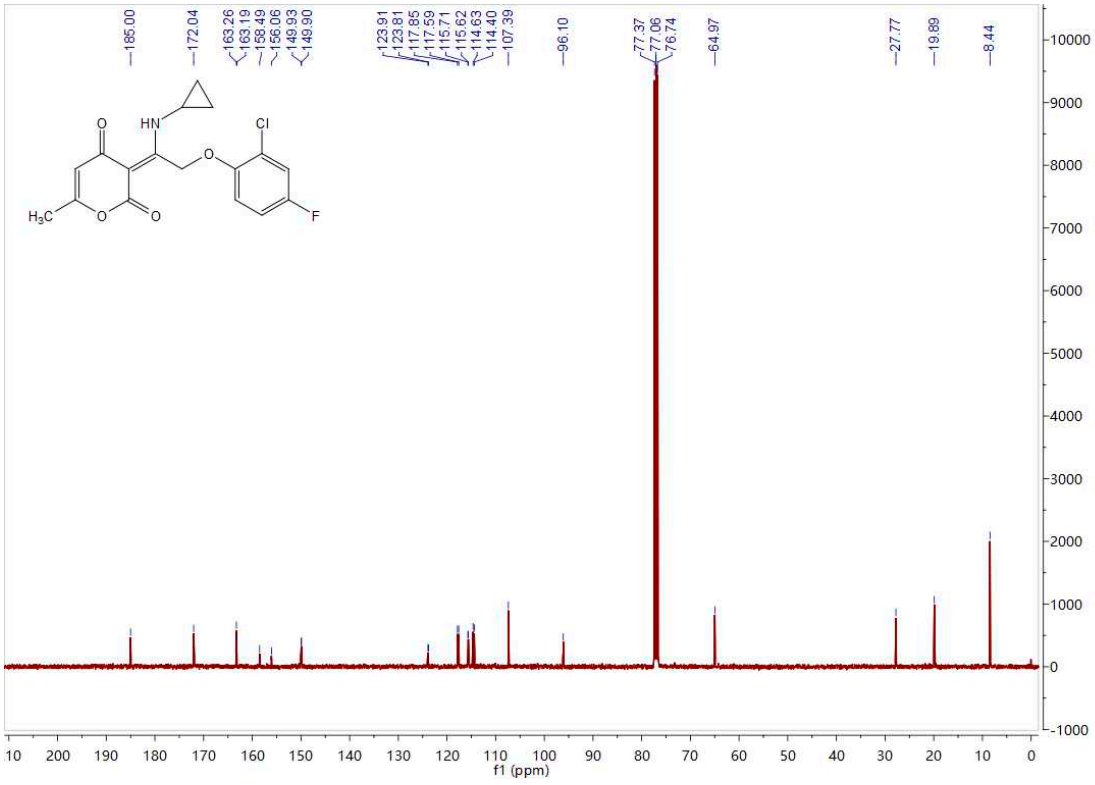

5
0729-1-7 53 (0.351)
1: TOF MS ES+
2.00e6
100
%
0
376.0732
354.0916
378.0708
379.0735
84.9659
125.9891
193.1340
217.1070
301.1422
354.0450
438.0437
493.2314
537.2558
587.5474
655.2368
669.3314
m/z
75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675

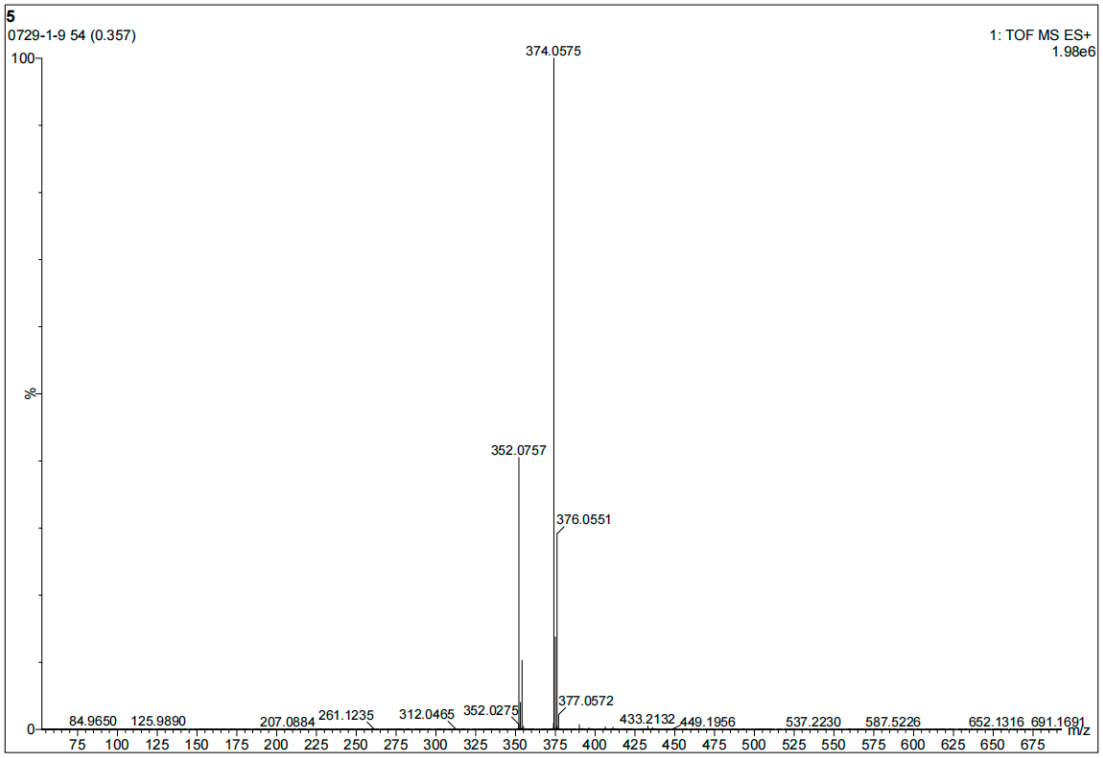

7.38
7.37
7.36
7.35
7.08
7.07
7.05
7.05
7.03
7.02
6.73
6.72
6.71
6.70
5.45
5.15
3.39
2.51
2.51
2.50
1.98
1.17
CH3
CH3
CH3
HN
O
Cl
O
O
H3C
O
O
F
0.98
1.01
1.02
0.98
2.00
3.17
8.97
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
10.0 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)

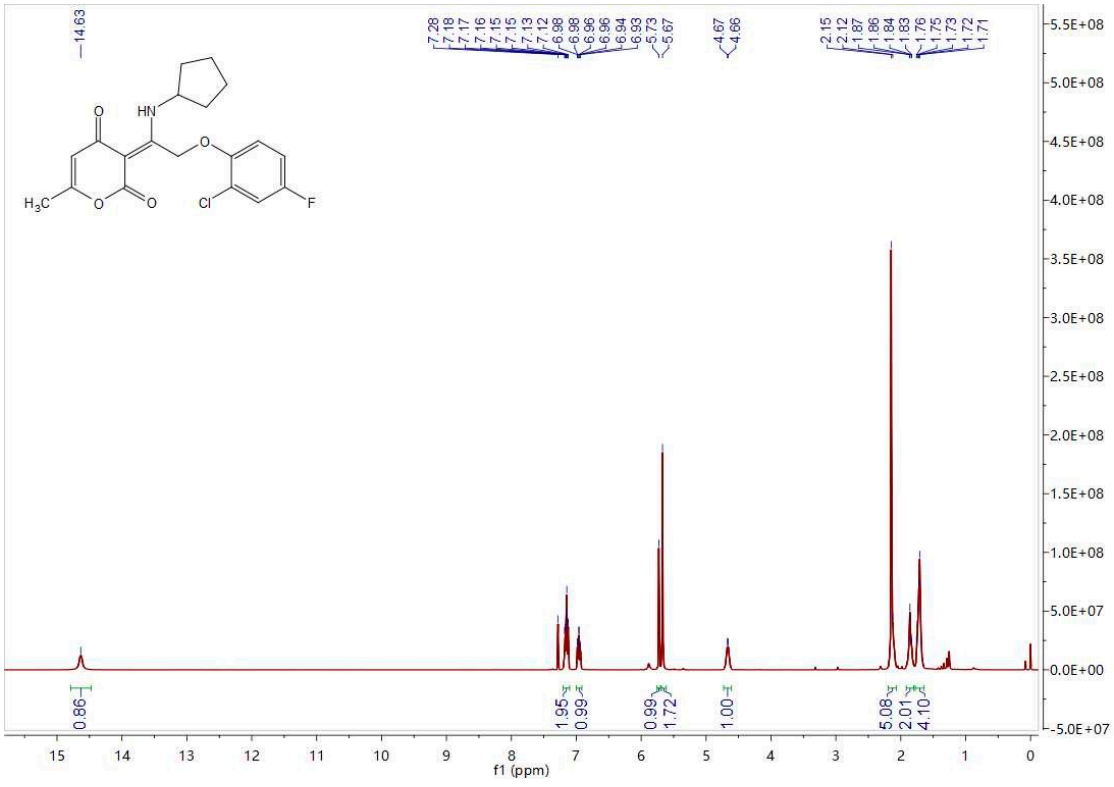

190.29
181.49
164.49
160.02
156.76
154.40
151.54
151.51
121.57
121.46
117.28
117.02
114.74
114.63
114.54
114.52
109.03
100.61
74.46
51.13
40.55
40.35
40.14
39.93
39.72
39.51
27.42
19.63
CH3
CH3
CH3
HN
O
O
O
O
Cl
F
H3C
f1 (ppm)

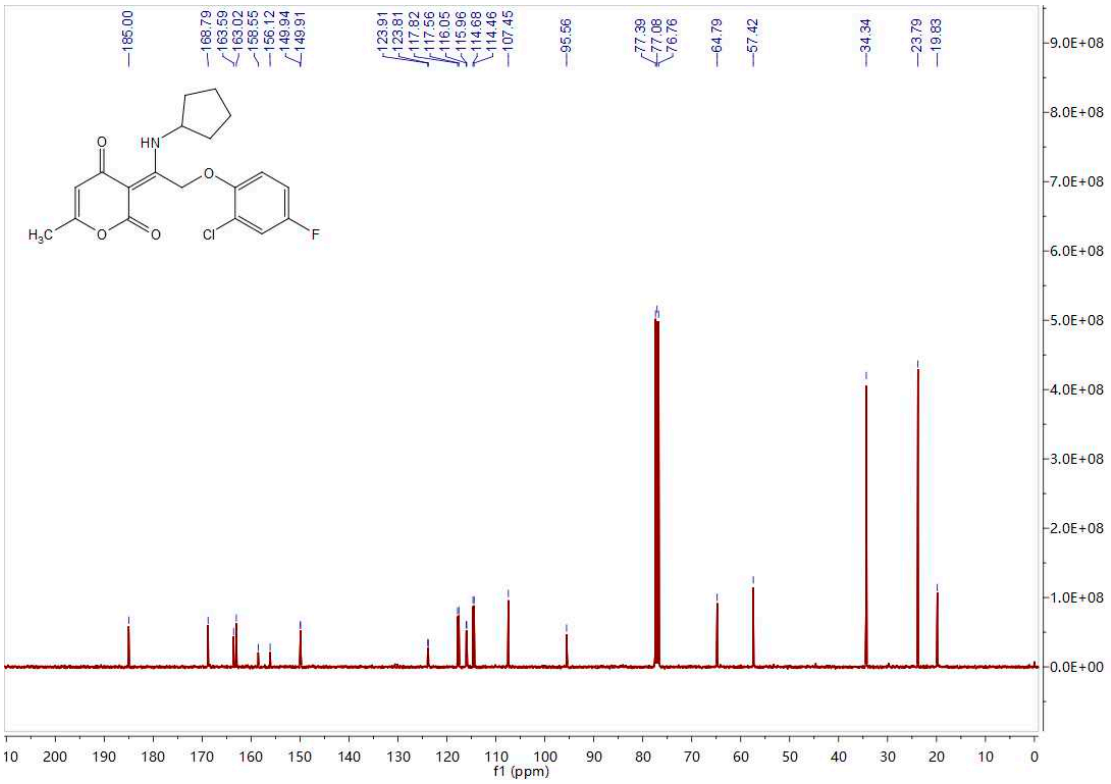

5
0729-1-3 55 (0.362)
1: TOF MS ES+
3.75e6
100
%
0
390.0888
368.1069
392.0862
393.0893
98.9584
127.9816
208.0963
224.0464
244.0867
332.1318
368.0523
412.0701
452.0566
520.0306
571.6202
587.5653
668.1954
686.4036
m/z

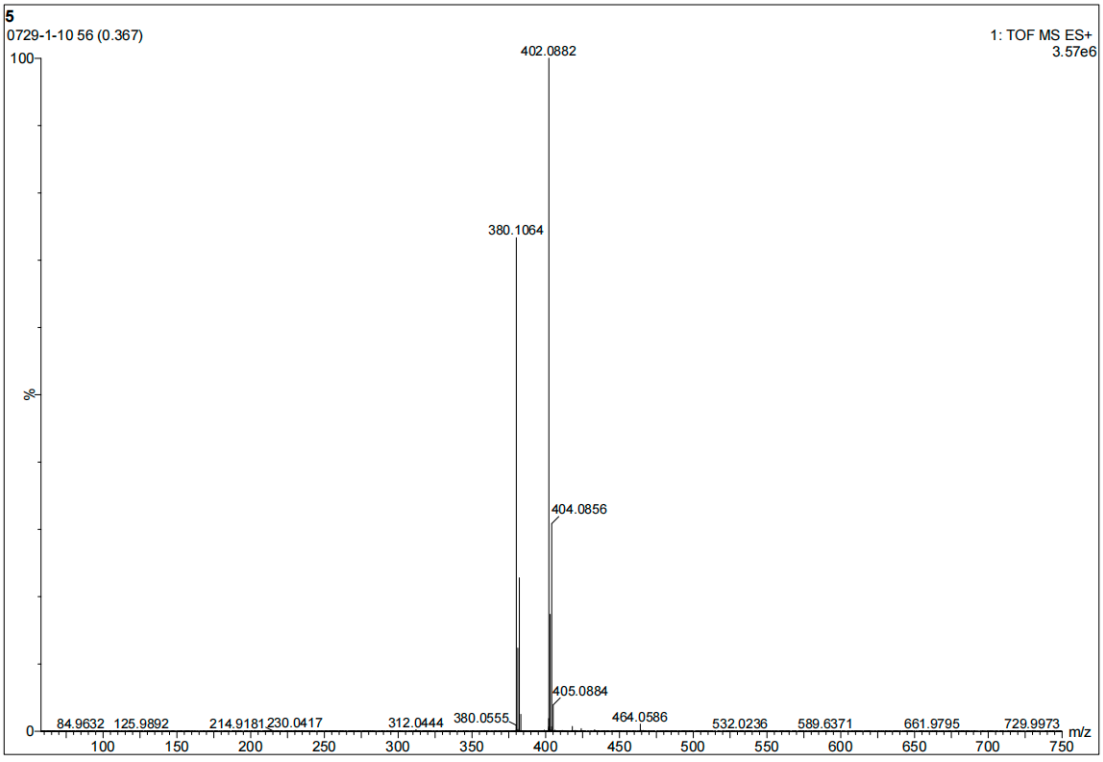

14.41
7.27
7.17
7.16
7.15
7.13
6.98
6.96
6.94
5.76
5.72
3.47
3.46
2.15
1.68
1.07
1.05
1.04
1.02
0.90
0.88
0.94
2.07
1.07
1.80
1.04
1.05
3.12
2.00
2.06
f1 (ppm)

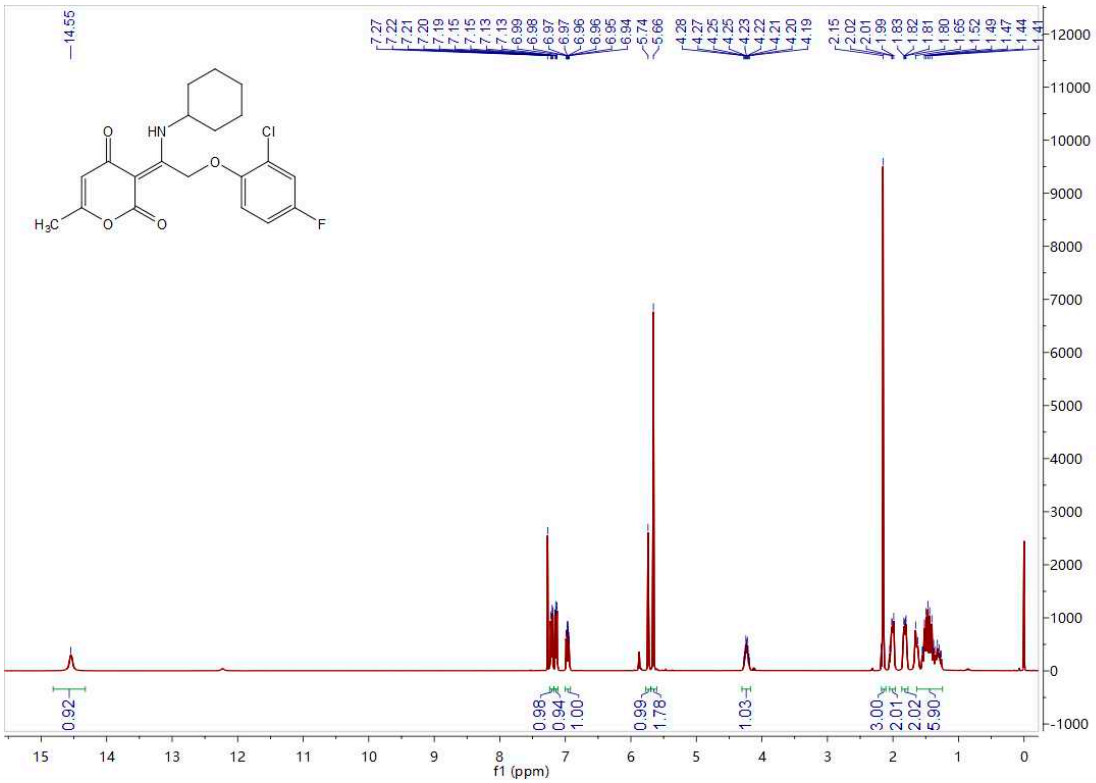

185.00
172.04
163.26
163.19
158.49
156.06
149.93
149.90
123.91
123.81
117.85
117.59
115.71
115.62
114.63
114.40
107.39
96.10
77.37
77.06
76.74
64.97
27.77
19.89
8.44
f1 (ppm)

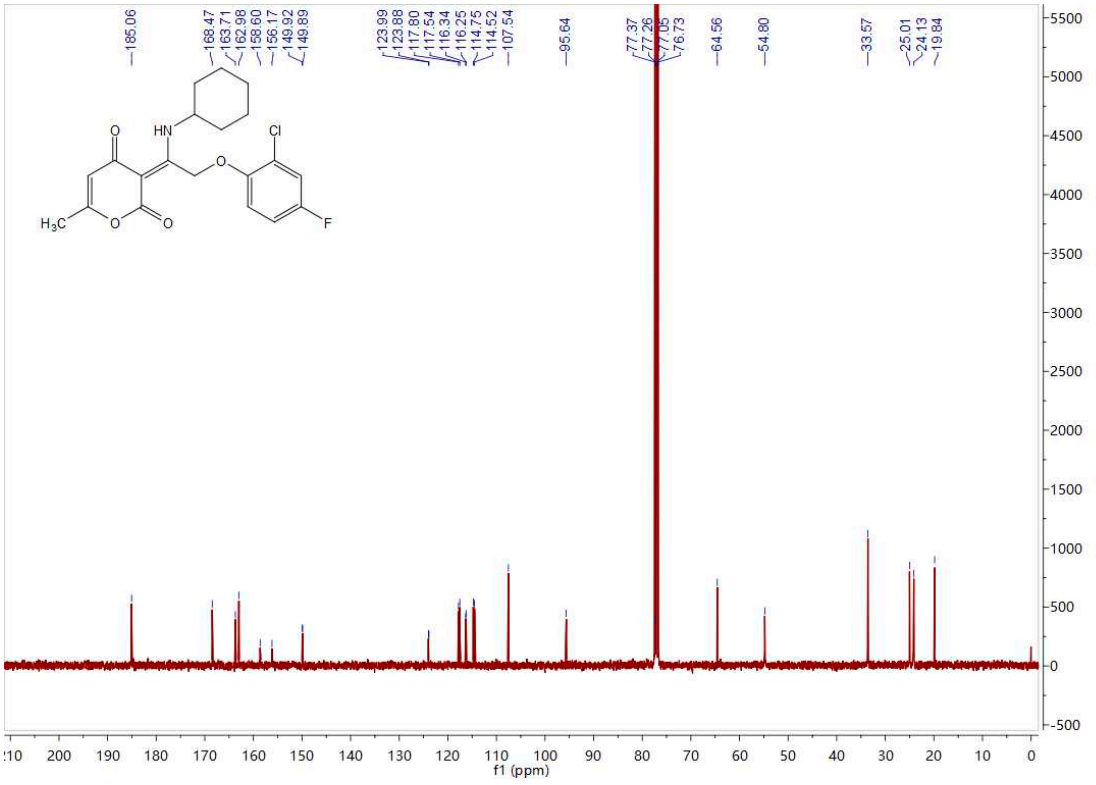

5
0729-1-9 54 (0.357)
1: TOF MS ES+
1.98e6
100
%
0
374.0575
352.0757
376.0551
377.0572
84.9650
125.9890
207.0884
261.1235
312.0465
352.0275
433.2132
449.1956
537.2230
587.5226
652.1316
691.1691
m/z

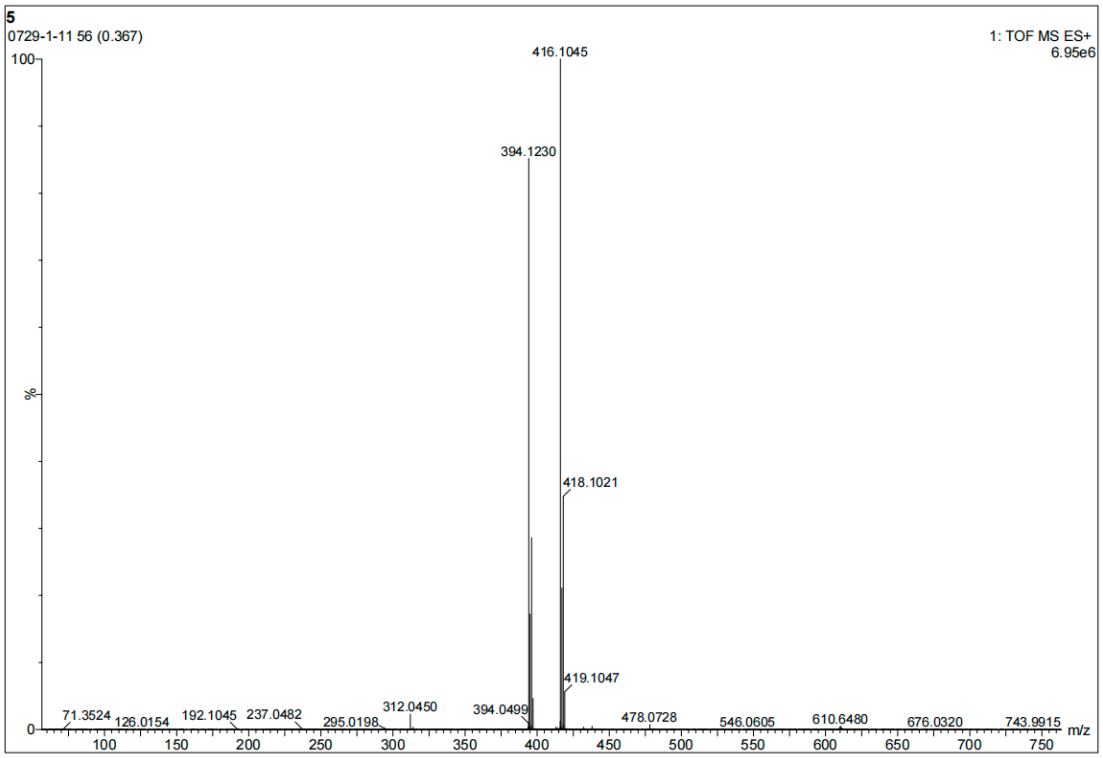

14.63
7.28
7.18
7.17
7.16
7.15
7.15
7.13
7.12
6.98
6.98
6.96
6.96
6.94
6.93
5.73
5.67
4.67
4.66
2.15
2.12
1.87
1.86
1.84
1.83
1.76
1.75
1.73
1.72
1.71
HN
O
O
O
O
O
H3C
Cl
F
0.86
1.95
0.99
0.99
1.72
1.00
5.08
2.01
4.10
f1 (ppm)

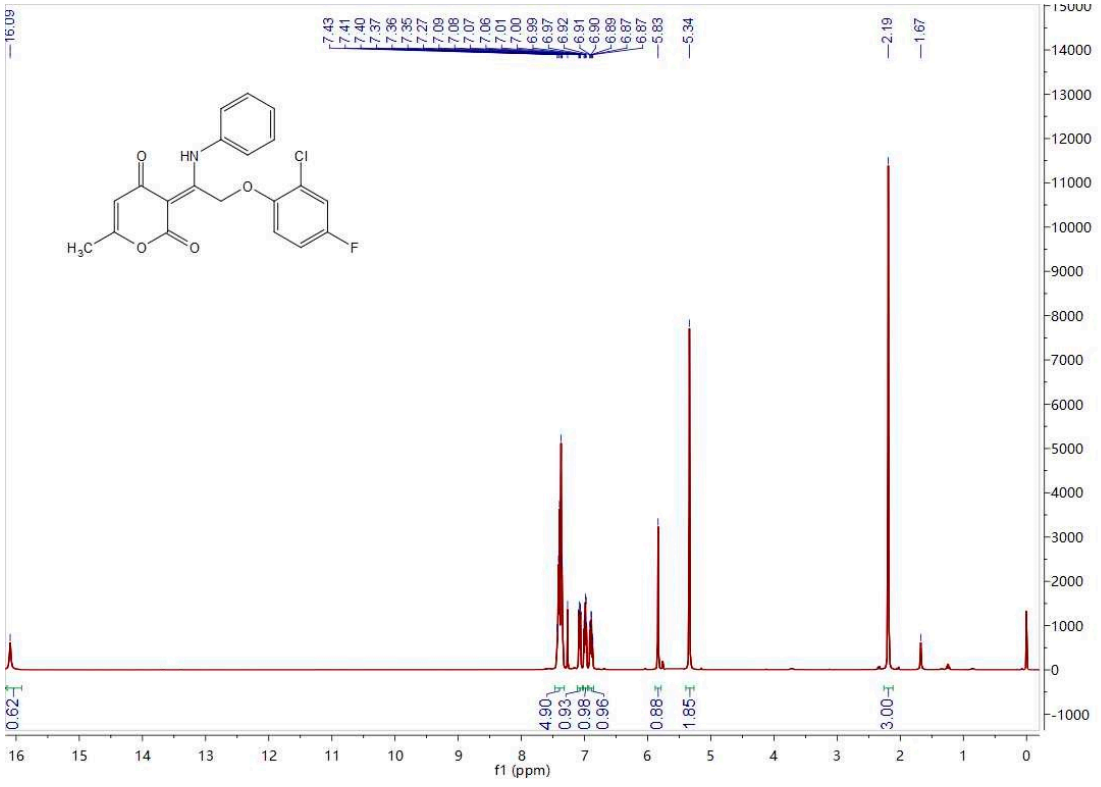

185.00
168.79
163.59
163.02
158.55
156.12
149.94
149.91
123.91
123.81
117.82
117.56
116.05
115.96
114.68
114.46
107.45
95.56
77.39
77.08
76.76
64.79
57.42
34.34
23.79
19.83
HN
O
O
O
O
H3C
Cl
F
9.0E+08
8.0E+08
7.0E+08
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
f1 (ppm)

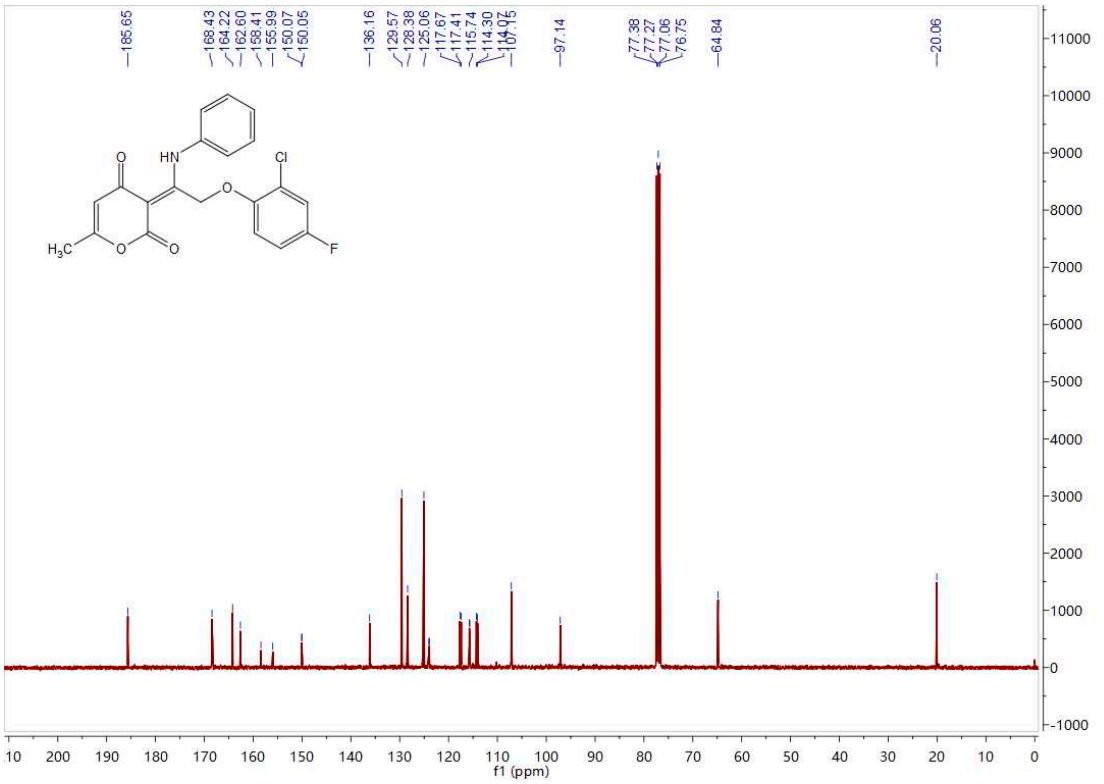

5
0729-1-10 56 (0.367)
1: TOF MS ES+
3.57e6
100
%
0
402.0882
380.1064
404.0856
405.0884
84.9632
125.9892
214.9181
230.0417
312.0444
380.0555
464.0586
532.0236
589.6371
661.9795
729.9973
m/z

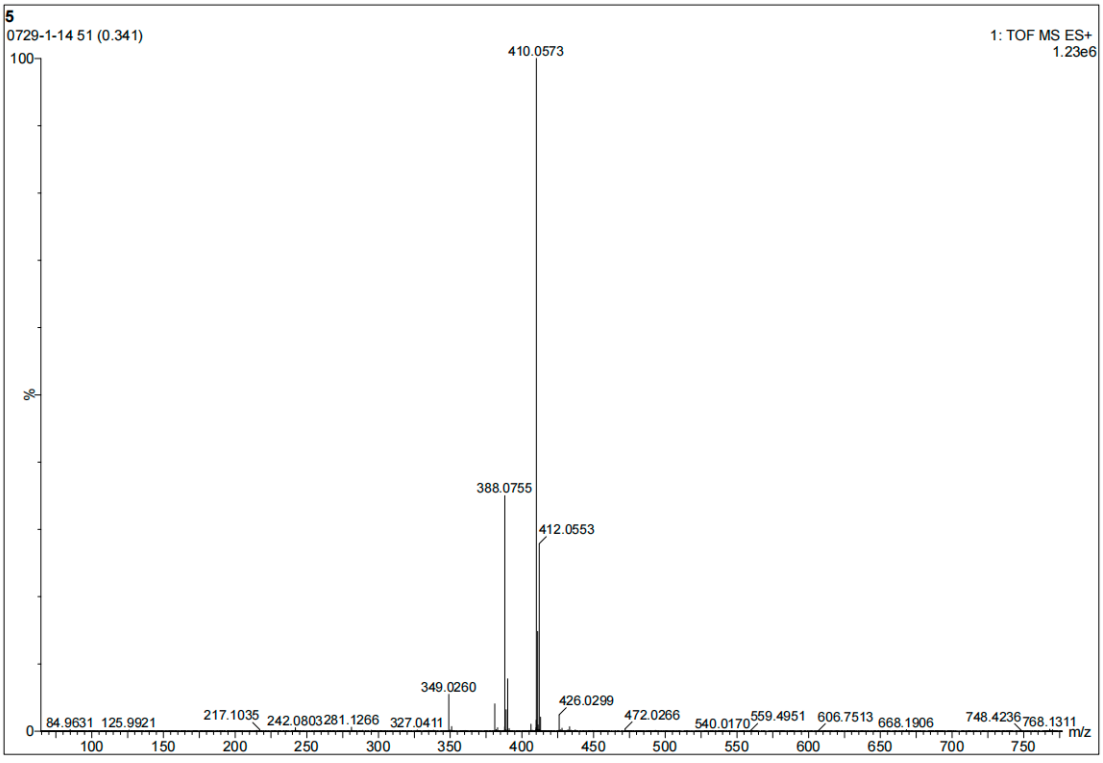

14.55
7.27
7.22
7.21
7.20
7.19
7.15
7.15
7.13
7.13
6.99
6.98
6.97
6.97
6.96
6.96
6.95
6.94
5.74
5.66
4.28
4.27
4.25
4.25
4.23
4.22
4.21
4.20
4.19
2.15
2.02
2.01
1.99
1.83
1.82
1.81
1.80
1.65
1.52
1.49
1.47
1.44
1.41
HN
O
O
O
O
Cl
F
H3C
0.92
0.98
0.94
1.00
0.99
1.78
1.03
3.00
2.01
2.02
5.90
f1 (ppm)

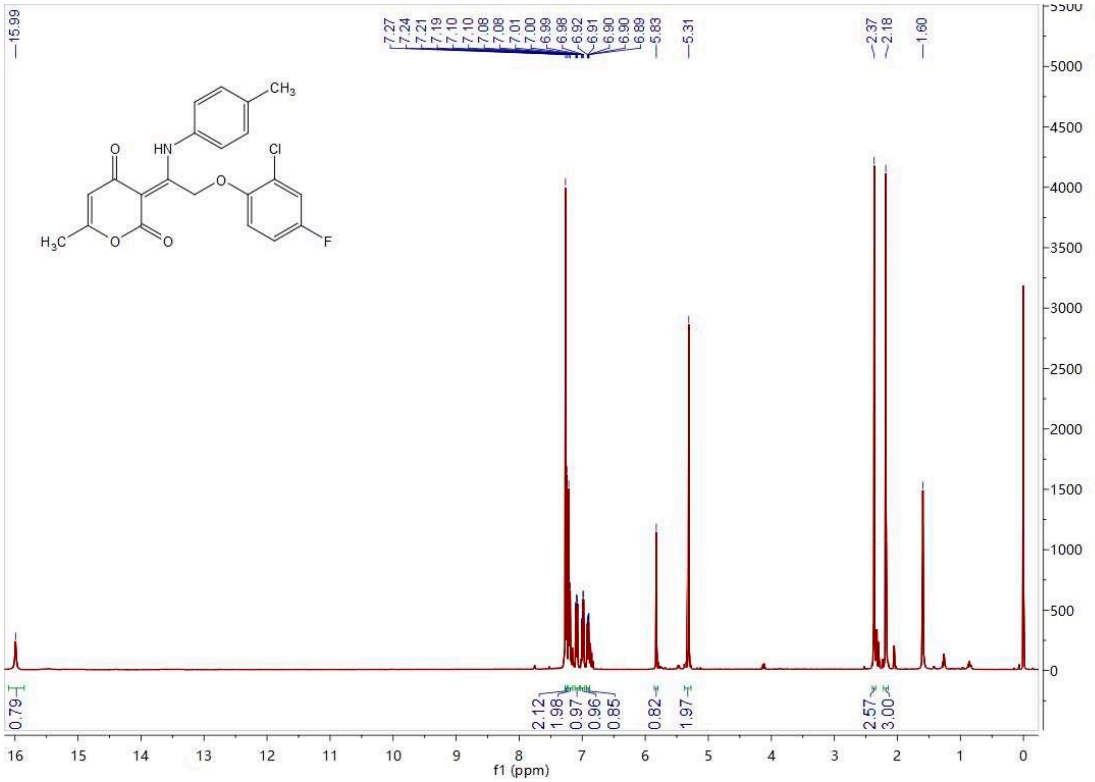

185.06
168.47
163.71
162.98
158.60
156.17
149.92
149.89
123.99
123.88
117.80
117.54
116.34
116.25
114.75
114.52
107.54
95.64
77.37
77.26
77.05
76.73
64.56
54.80
33.57
25.01
24.13
19.84
HN
O
O
O
O
Cl
F
H3C
f1 (ppm)

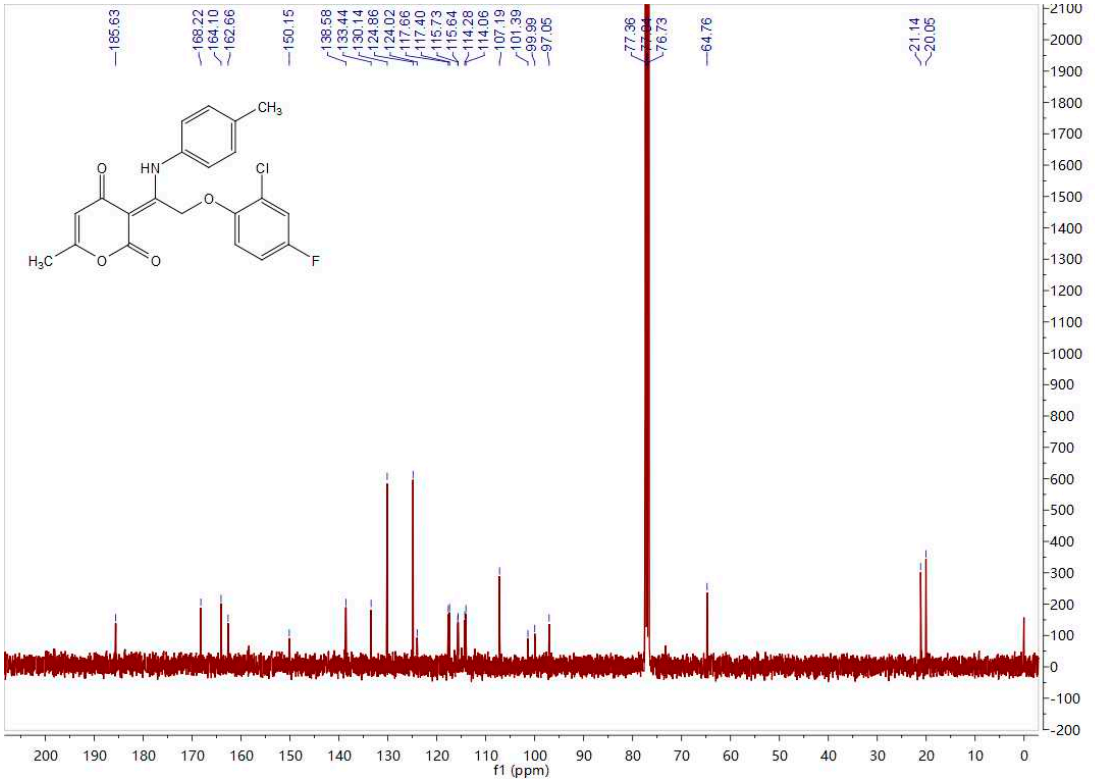

5
0729-1-11 56 (0.367)
1: TOF MS ES+
6.95e6
100
%
0
416.1045
394.1230
418.1021
419.1047
71.3524
126.0154
192.1045
237.0482
295.0198
312.0450
394.0499
478.0728
546.0605
610.6480
676.0320
743.9915
m/z

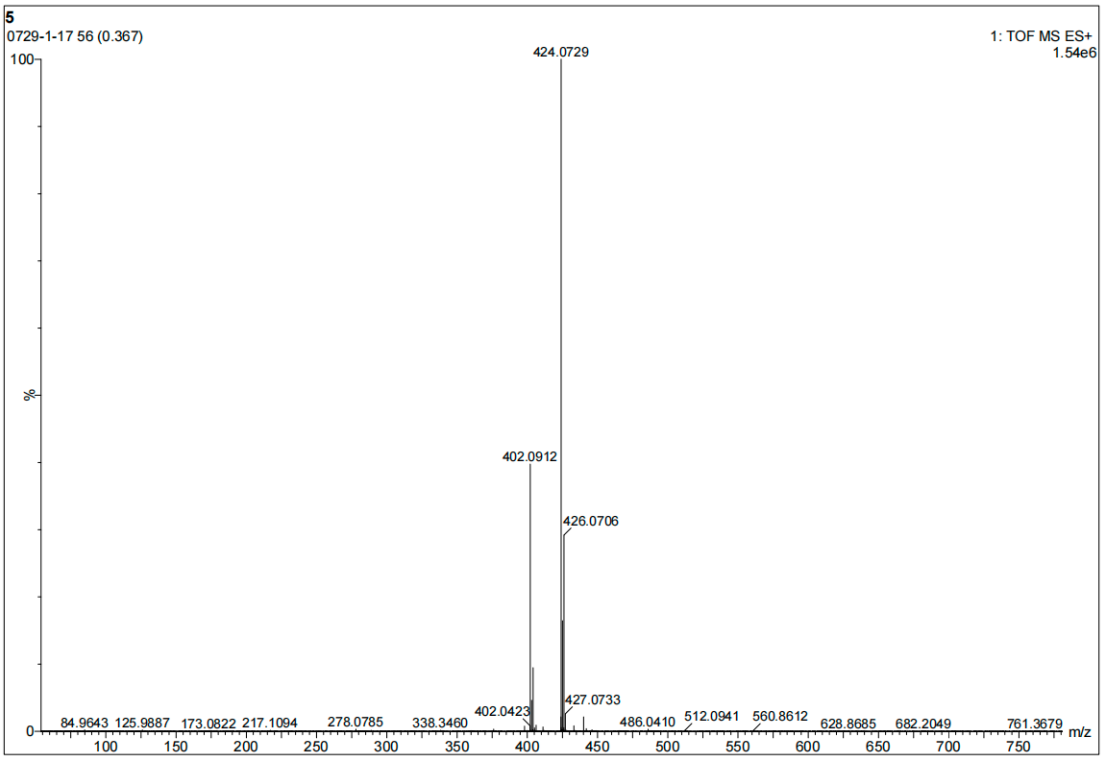

16.09
7.43
7.41
7.40
7.37
7.36
7.35
7.27
7.09
7.08
7.07
7.06
7.01
7.00
6.99
6.97
6.92
6.91
6.90
6.89
6.87
6.87
5.83
5.34
2.19
1.67
O
HN
Cl
O
H3C
O
O
F
0.62
4.90
0.93
0.98
0.96
0.88
1.85
3.00
f1 (ppm)

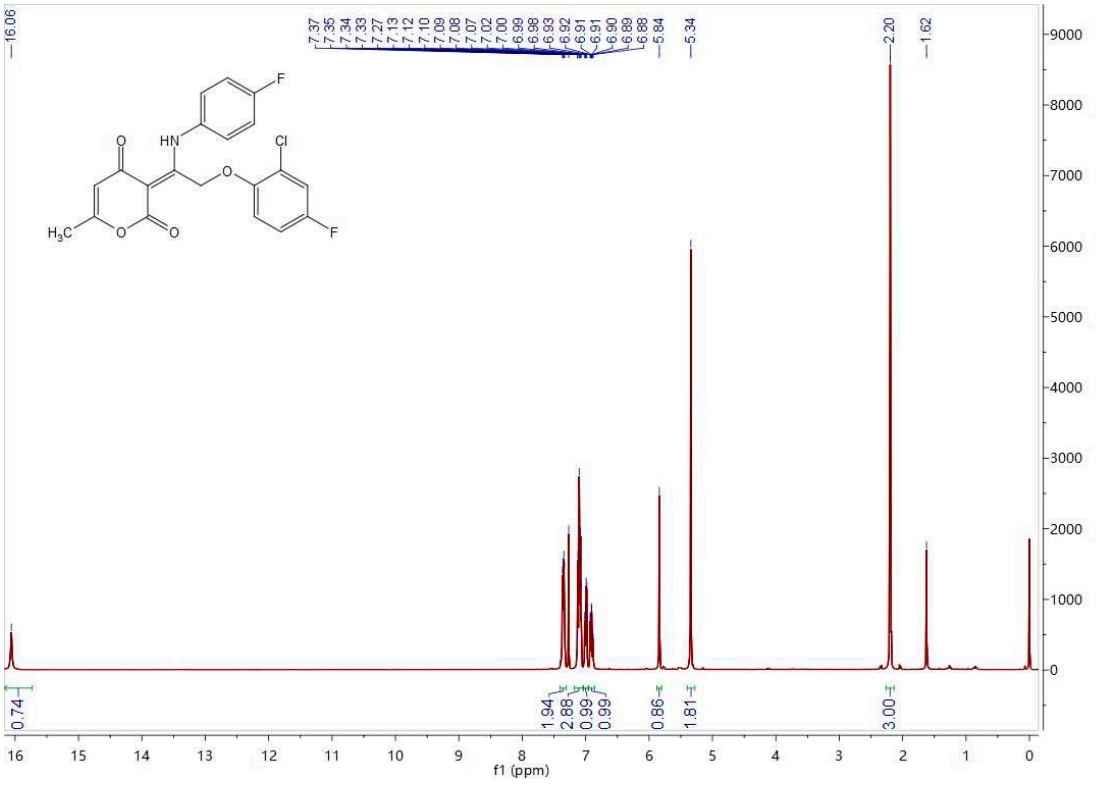

185.65
168.43
164.22
162.60
158.41
155.99
150.07
150.05
136.16
129.57
128.38
125.06
117.67
117.41
115.74
114.30
97.14
77.38
77.27
77.06
76.75
64.84
20.06
HN
Cl
O
O
O
O
H_3C
F
f1 (ppm)

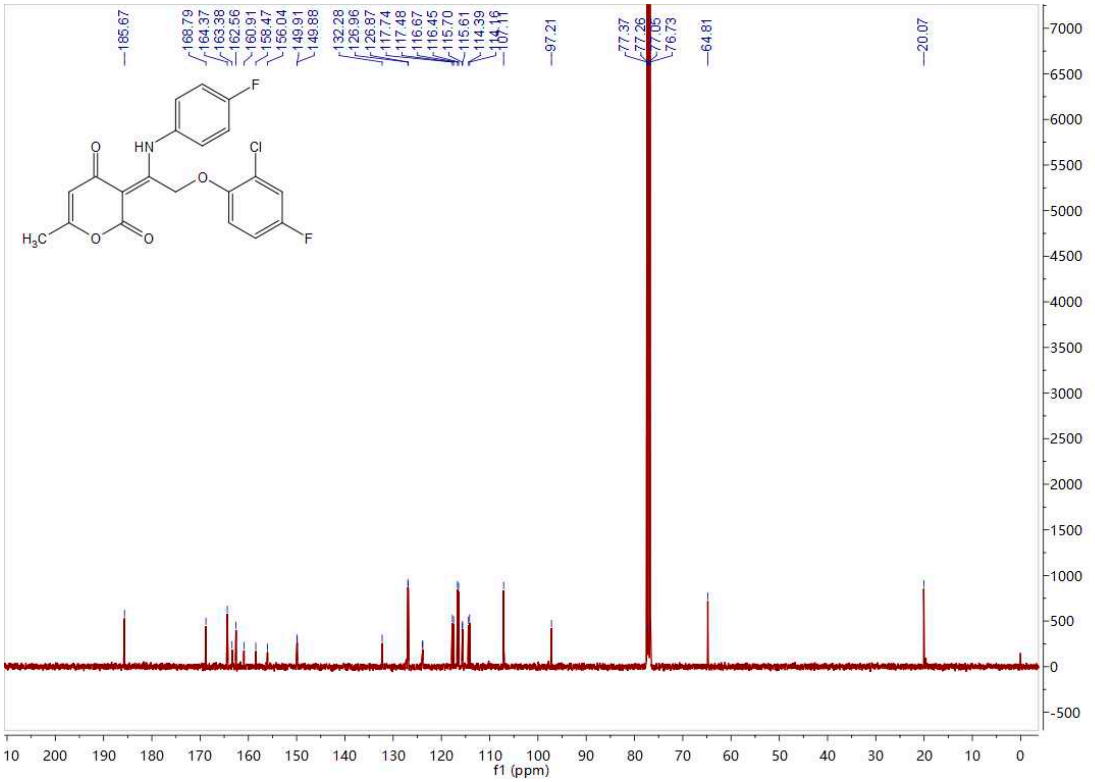

5
0729-1-14 51 (0.341)
1: TOF MS ES+
1.23e6
410.0573
388.0755
412.0553
349.0260
426.0299
472.0266
84.9631
125.9921
217.1035
242.0803
281.1266
327.0411
540.0170
559.4951
606.7513
668.1906
748.4236
768.1311
%
m/z

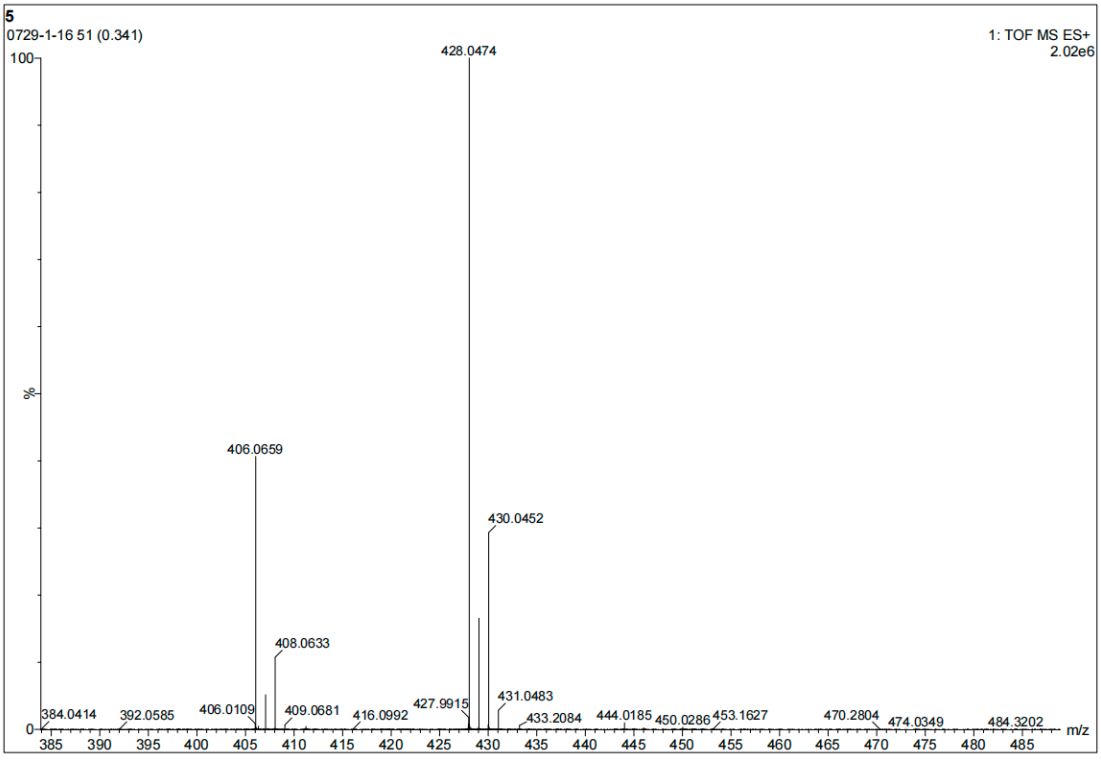

15.99
7.27
7.24
7.21
7.19
7.10
7.10
7.08
7.08
7.01
7.00
6.99
6.98
6.92
6.91
6.90
6.90
6.89
5.83
5.31
2.37
2.18
1.60
CH3
HN
Cl
O
O
O
H3C
O
O
F
0.79
2.12
1.98
0.97
0.96
0.85
0.82
1.97
2.57
3.00
f1 (ppm)

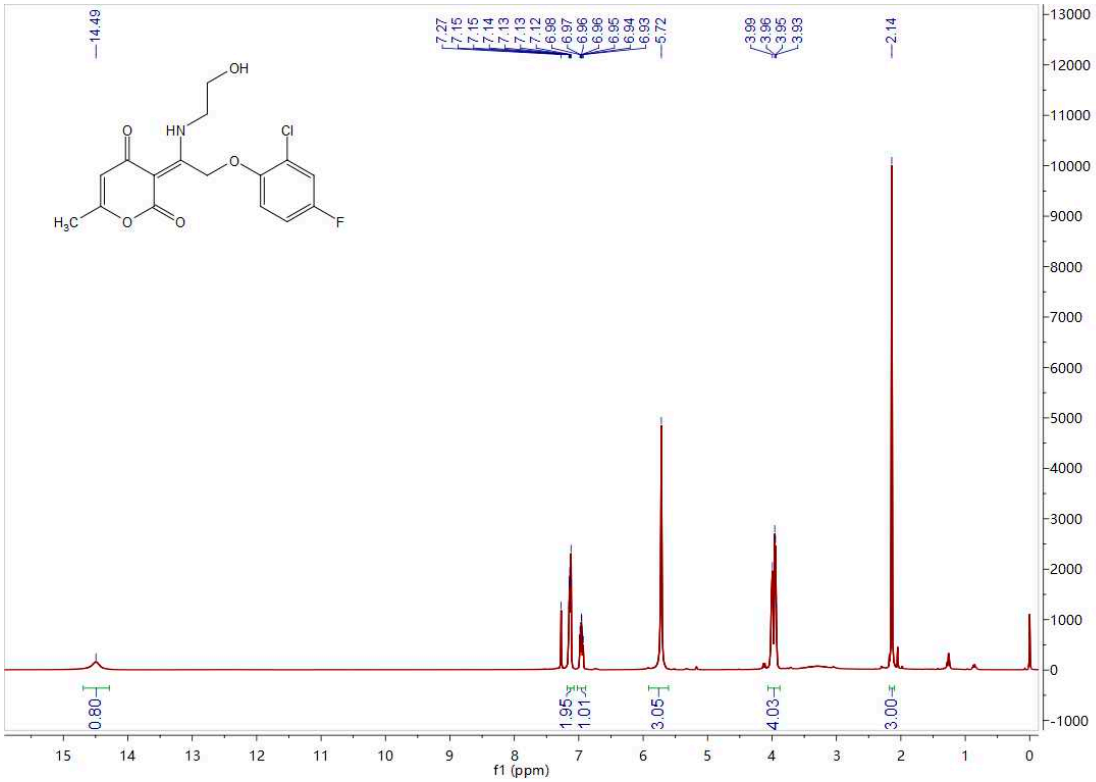

185.63
168.22
164.10
162.66
150.15
138.58
133.44
130.14
124.86
124.02
117.66
117.40
115.73
115.64
114.28
114.06
107.19
101.39
99.99
97.05
77.36
77.04
76.73
64.76
21.14
20.05
CH3
HN
Cl
O
O
O
H3C
O
O
F
f1 (ppm)

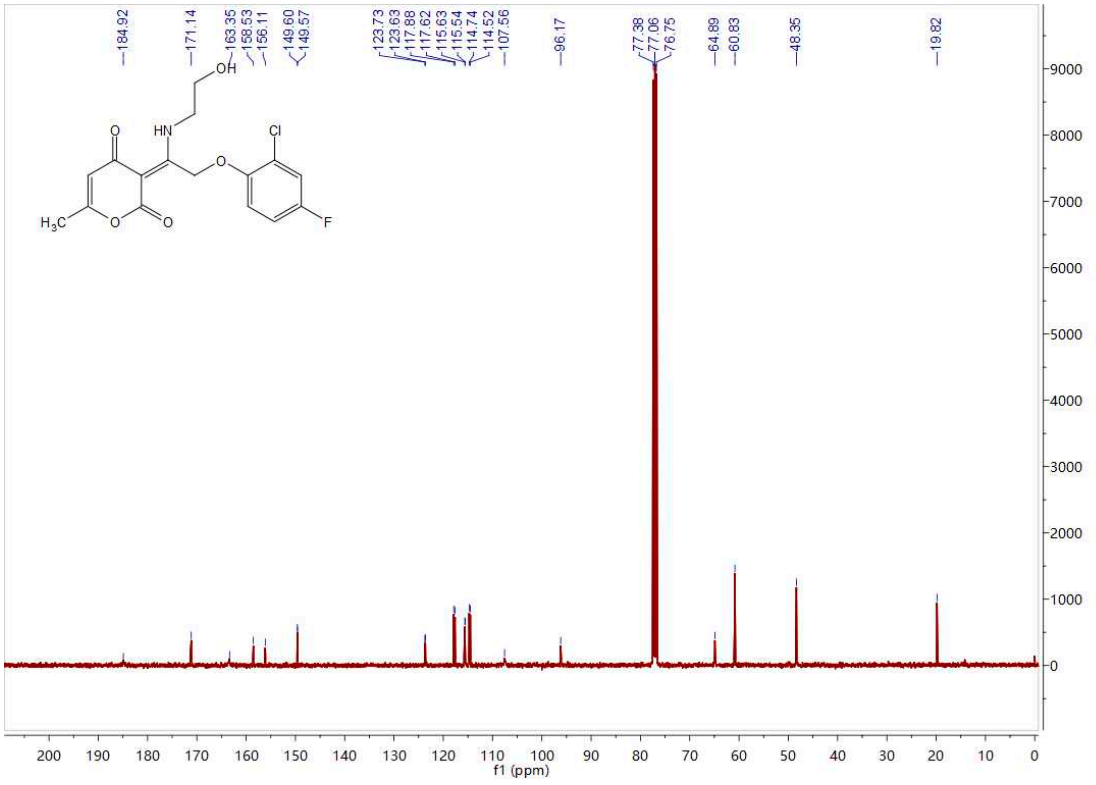

5
0729-1-17 56 (0.367)
1: TOF MS ES+
1.54e6
100
%
0
424.0729
402.0912
426.0706
427.0733
402.0423
84.9643 125.9887 173.0822 217.1094 278.0785 338.3460 486.0410 512.0941 560.8612 628.8685 682.2049 761.3679
100 150 200 250 300 350 400 450 500 550 600 650 700 750
m/z

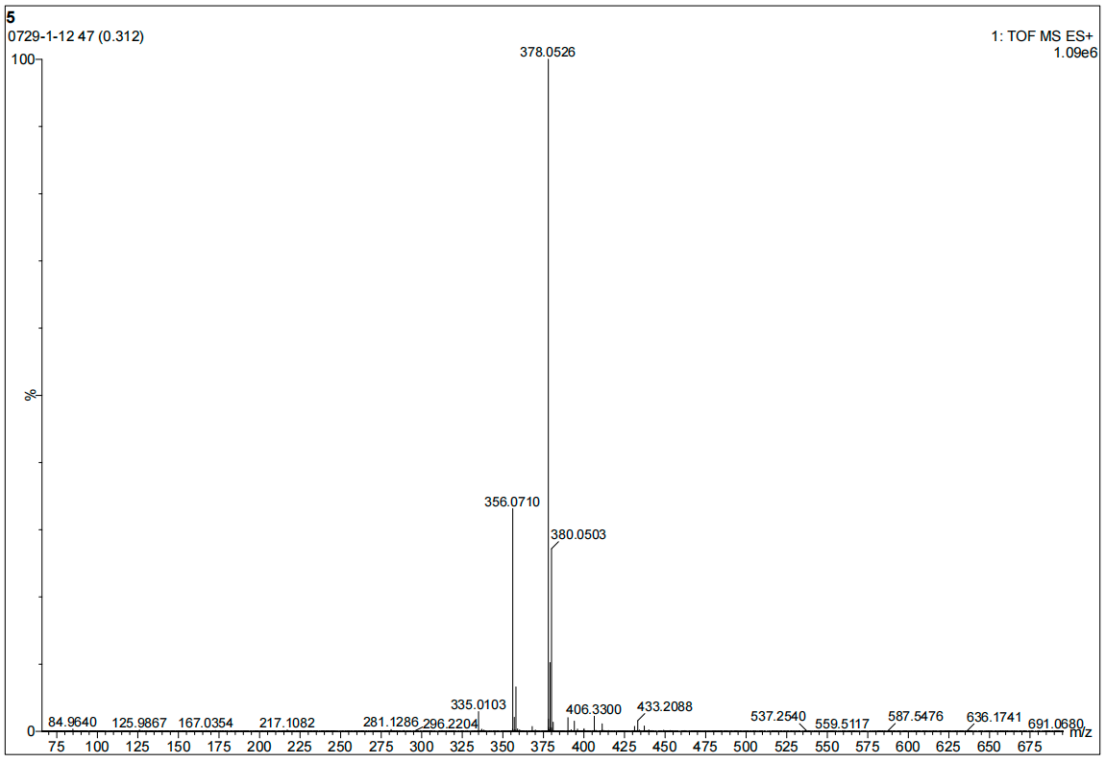

16.06
7.37 7.35 7.34 7.33 7.27 7.13 7.12 7.10 7.09 7.08 7.07 7.02 7.00 6.99 6.98 6.93 6.92 6.91 6.91 6.90 6.89 6.88
5.84
5.34
2.20
1.62
F
HN
O
Cl
O
O
H3C
O
O
F
9000 8000 7000 6000 5000 4000 3000 2000 1000 0
0.74
1.94
2.88
0.99
0.99
0.86
1.81
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

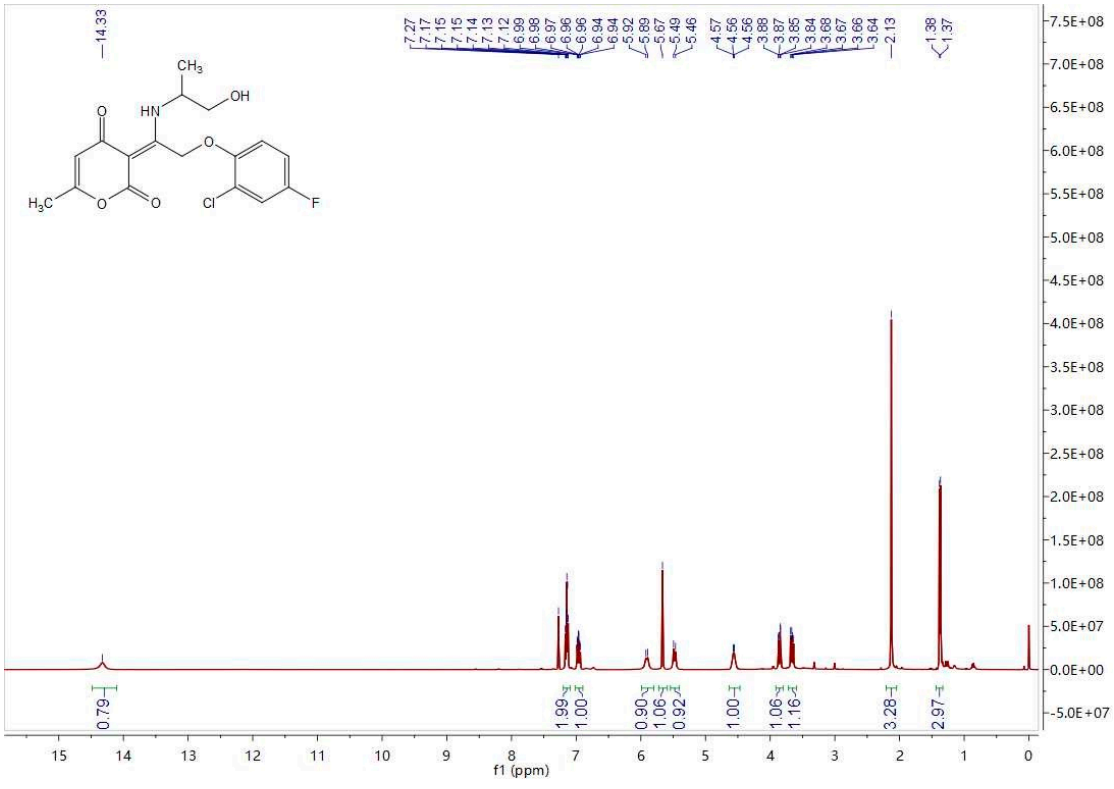

185.67
168.79
164.37
163.38
162.56
160.91
158.47
156.04
149.91
149.88
132.28
126.96
126.87
117.74
117.48
116.67
116.45
115.70
115.61
114.39
97.21
77.37
77.26
77.05
76.73
64.81
20.07
F
HN
Cl
O
O
O
O
O
H3C
F
f1 (ppm)

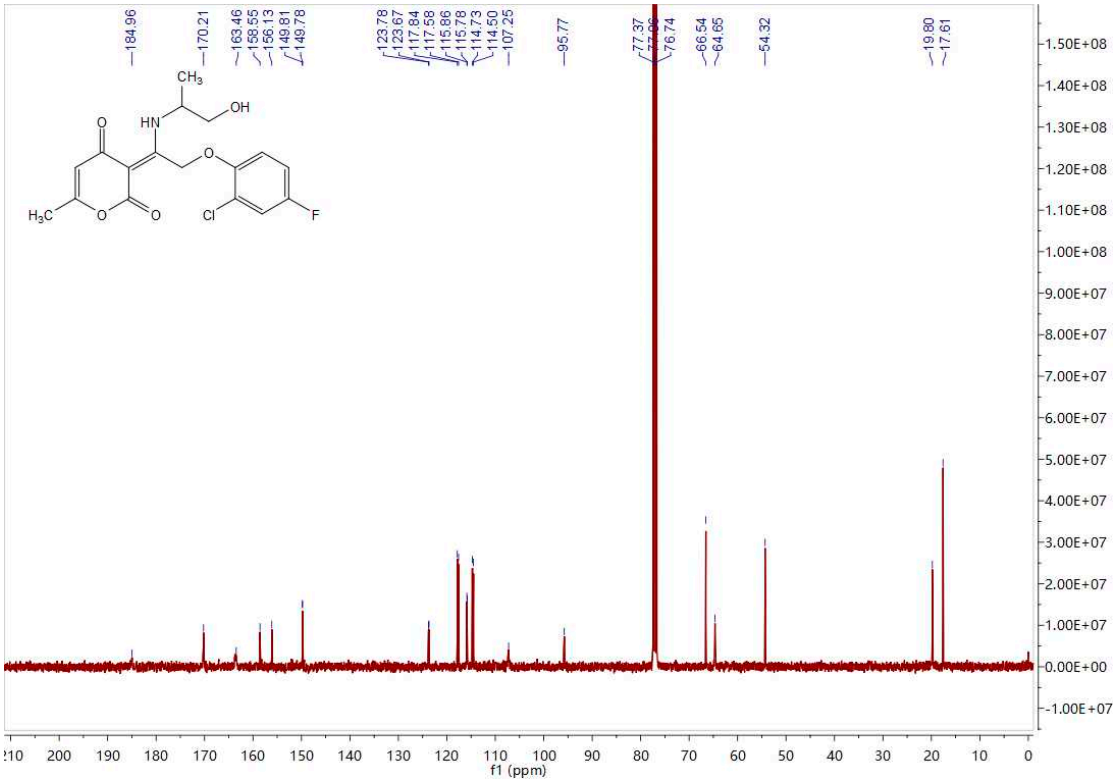

5
0729-1-16 51 (0.341)
1: TOF MS ES+
2.02e6
100
%
0
428.0474
406.0659
430.0452
408.0633
431.0483
384.0414
392.0585
406.0109
409.0681
416.0992
427.9915
433.2084
444.0185
450.0286
453.1627
470.2804
474.0349
484.3202
m/z

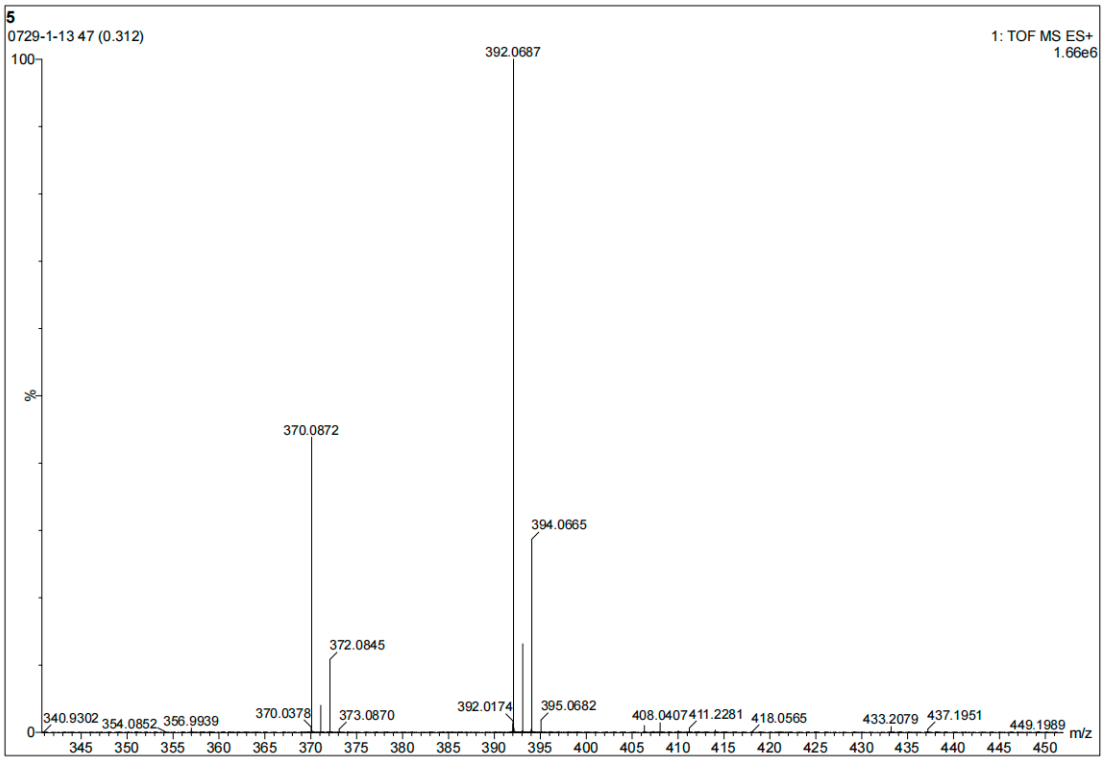

14.49
7.27
7.15
7.15
7.14
7.13
7.13
7.12
6.98
6.97
6.96
6.96
6.95
6.94
6.93
5.72
3.99
3.96
3.95
3.93
2.14
OH
HN
O
Cl
O
H3C
O
O
F
0.80
1.95
1.01
3.05
4.03
3.00
f1 (ppm)

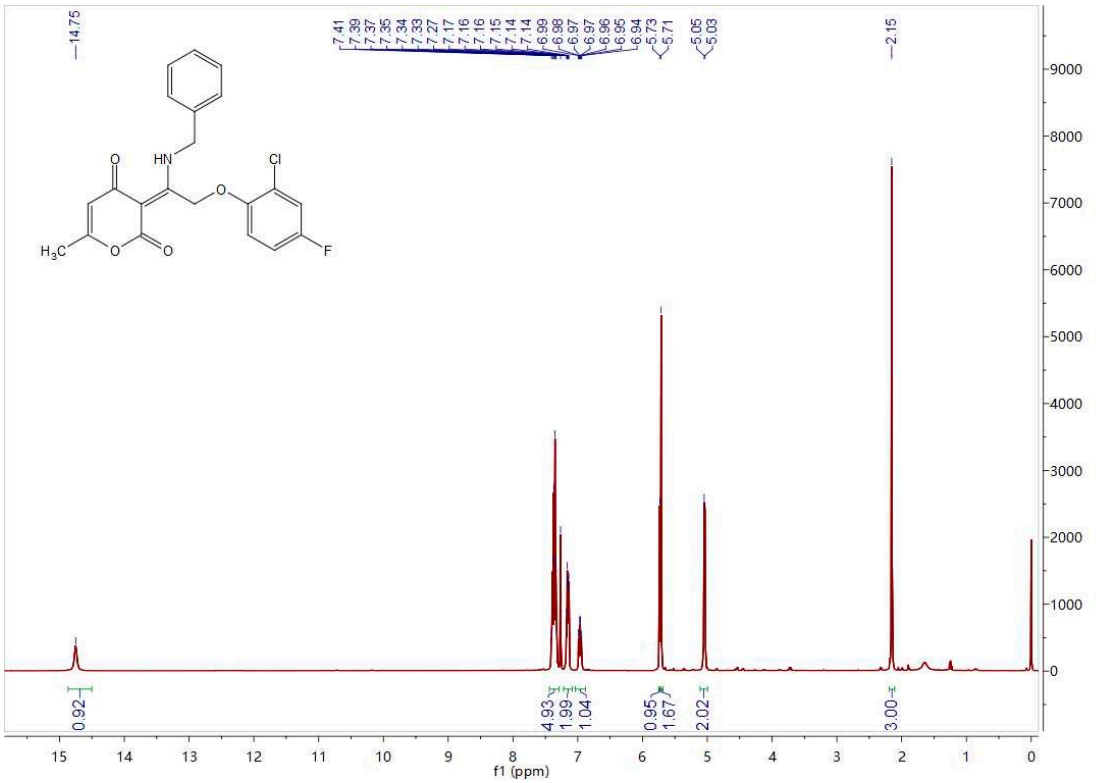

184.92
171.14
163.35
158.53
156.11
149.60
149.57
123.73
123.63
117.88
117.62
115.63
115.54
114.74
114.52
107.56
96.17
77.38
77.06
76.75
64.89
60.83
48.35
19.82
OH
HN
O
Cl
O
H3C
O
O
F
f1 (ppm)

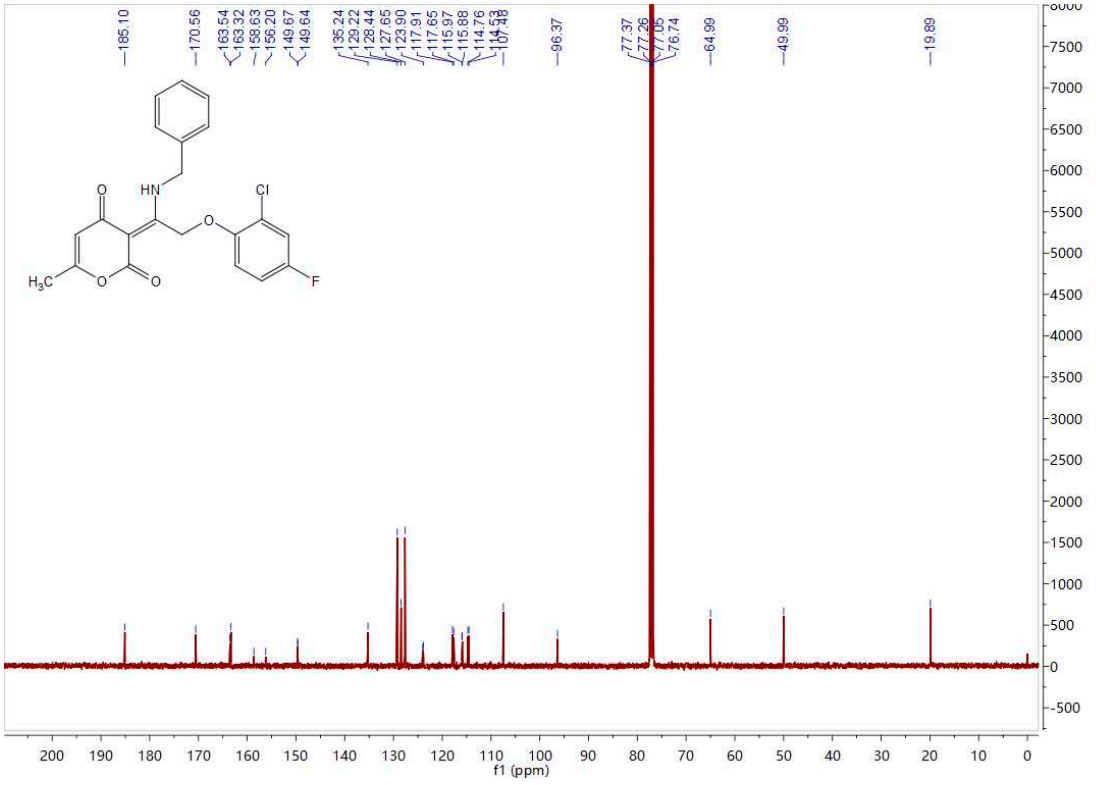

5
0729-1-12 47 (0.312)
1: TOF MS ES+
1.09e6
100
%
0
378.0526
356.0710
380.0503
335.0103
406.3300
433.2088
84.9640
125.9867
167.0354
217.1082
281.1286
296.2204
537.2540
559.5117
587.5476
636.1741
691.0680
m/z

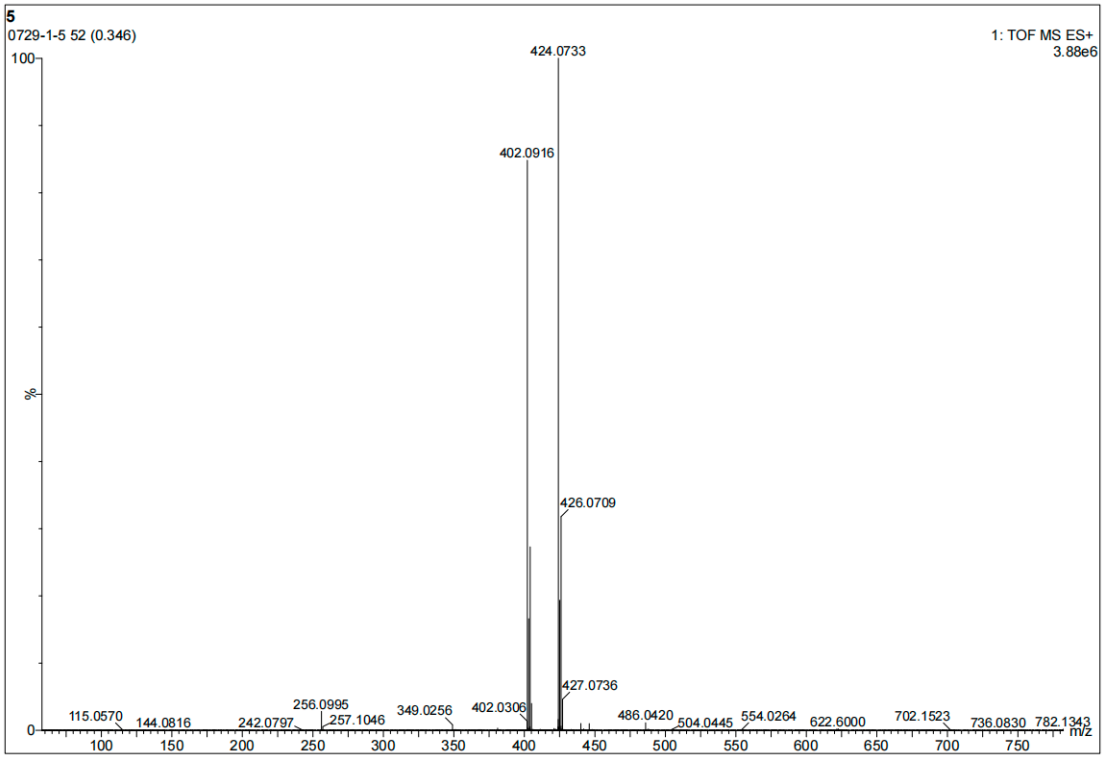

14.33
7.27
7.17
7.15
7.14
7.13
7.12
6.99
6.98
6.97
6.96
6.96
6.94
6.94
5.92
5.89
5.67
5.49
5.46
4.57
4.56
4.56
3.88
3.87
3.85
3.84
3.68
3.67
3.66
3.64
2.13
1.38
1.37
CH3
OH
HN
O
O
O
H3C
O
O
Cl
F
0.79
1.99
1.00
0.90
1.06
0.92
1.00
1.06
1.16
3.28
2.97
f1 (ppm)

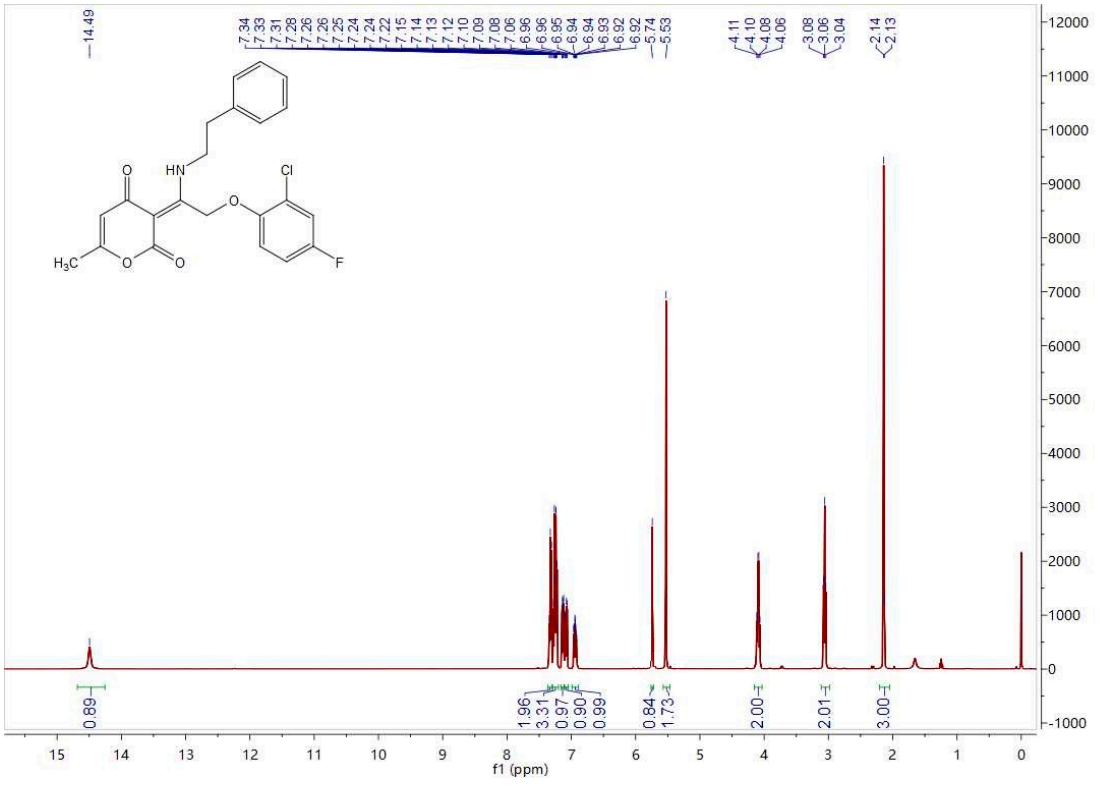

184.96
170.21
163.46
158.55
156.13
149.81
149.78
123.78
123.67
117.84
117.58
115.86
115.78
114.73
114.50
107.25
95.77
77.37
77.06
76.74
66.54
64.65
54.32
19.80
17.61
CH3
HN
OH
O
O
O
H3C
O
O
Cl
F
1.50E+08
1.40E+08
1.30E+08
1.20E+08
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

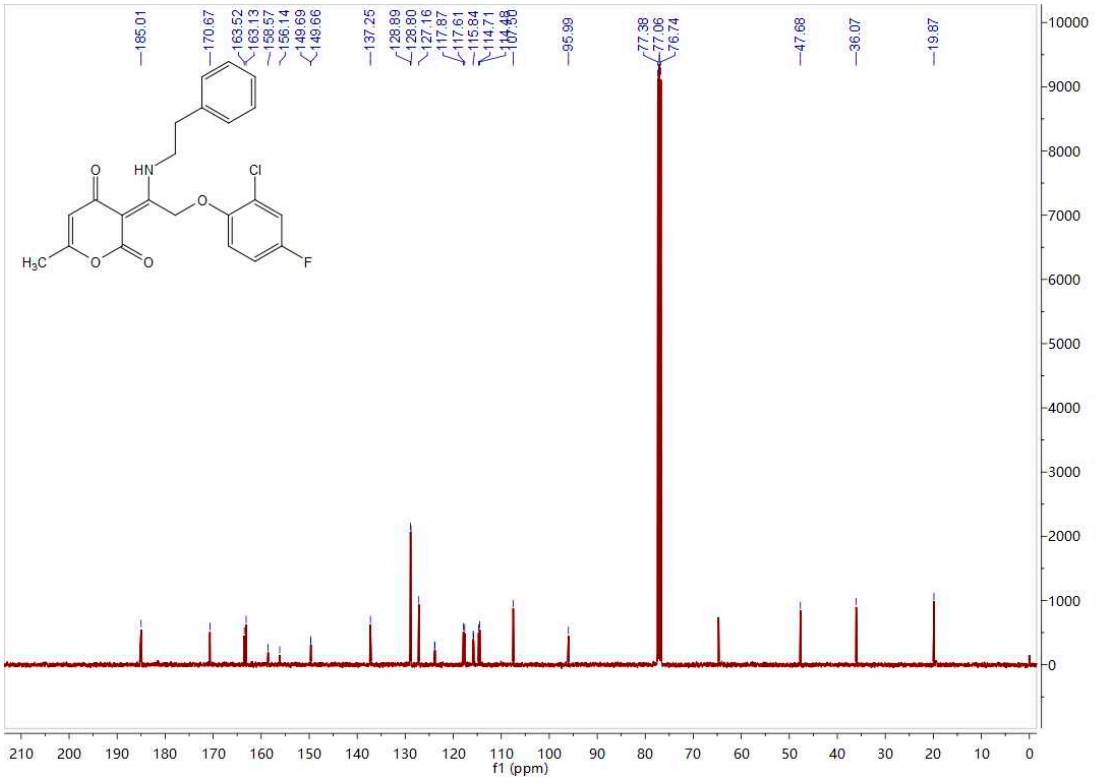

5
0729-1-13 47 (0.312)
1: TOF MS ES+
1.66e6
100
%
0
392.0687
370.0872
394.0665
372.0845
340.9302
354.0852
356.9939
370.0378
373.0870
392.0174
395.0682
408.0407
411.2281
418.0565
433.2079
437.1951
449.1989
m/z
345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440 445 450

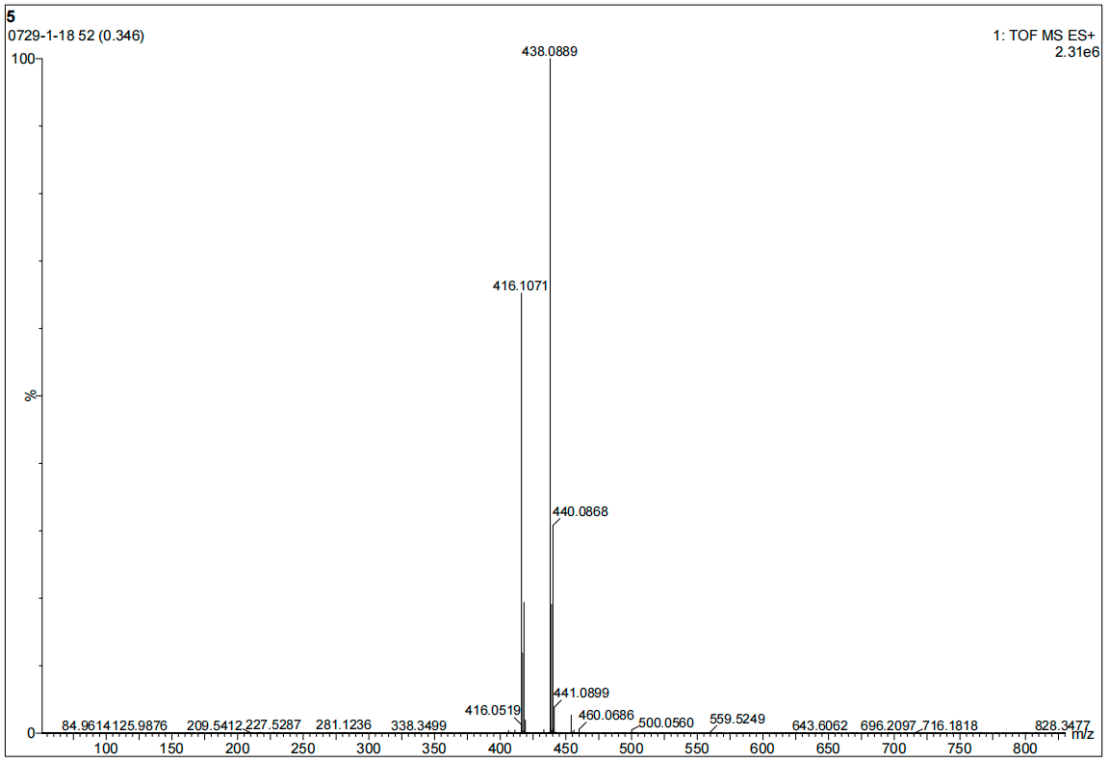

14.75
7.41
7.39
7.37
7.35
7.34
7.33
7.27
7.17
7.16
7.16
7.15
7.14
7.14
6.99
6.98
6.97
6.97
6.96
6.95
6.94
5.73
5.71
5.05
5.03
2.15
O
HN
Cl
O
H3C
O
O
F
0.92
4.93
1.99
1.04
0.95
1.67
2.02
3.00
f1 (ppm)

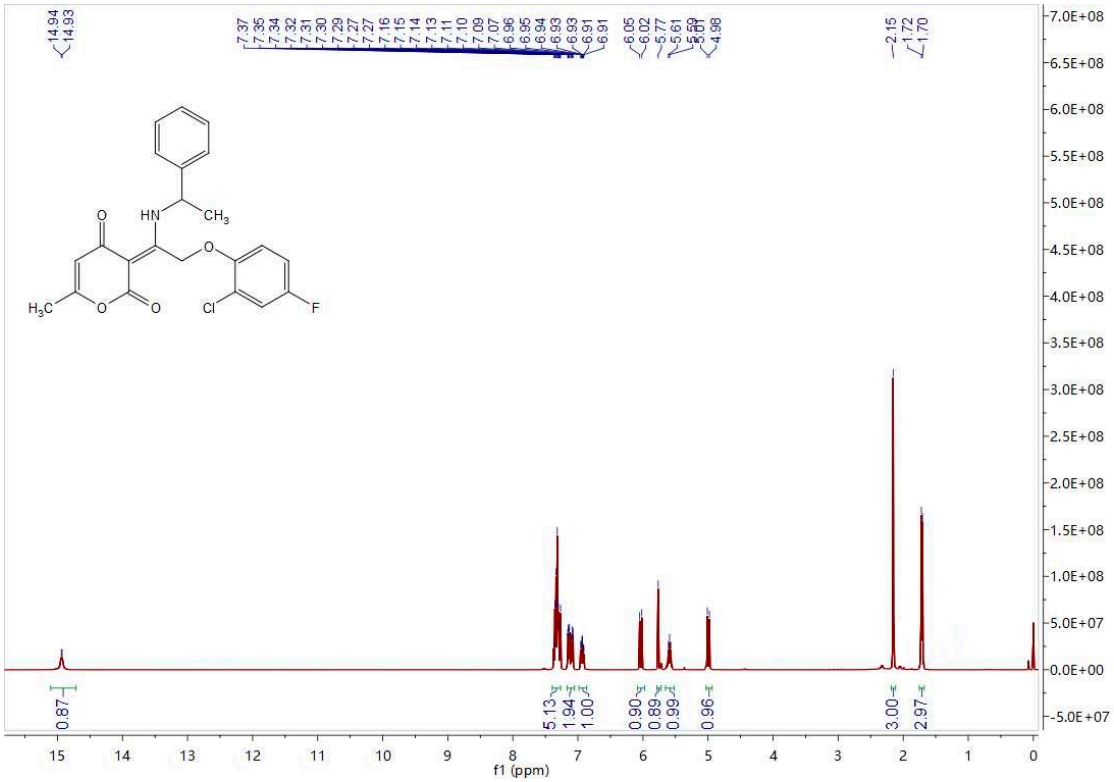

185.10
170.56
163.54
163.32
158.83
156.20
149.67
149.64
135.24
129.22
128.44
127.65
123.90
117.91
117.65
115.97
115.88
114.76
96.37
77.37
77.26
77.05
76.74
64.99
49.99
19.89
O
HN
Cl
O
H3C
O
O
F
f1 (ppm)

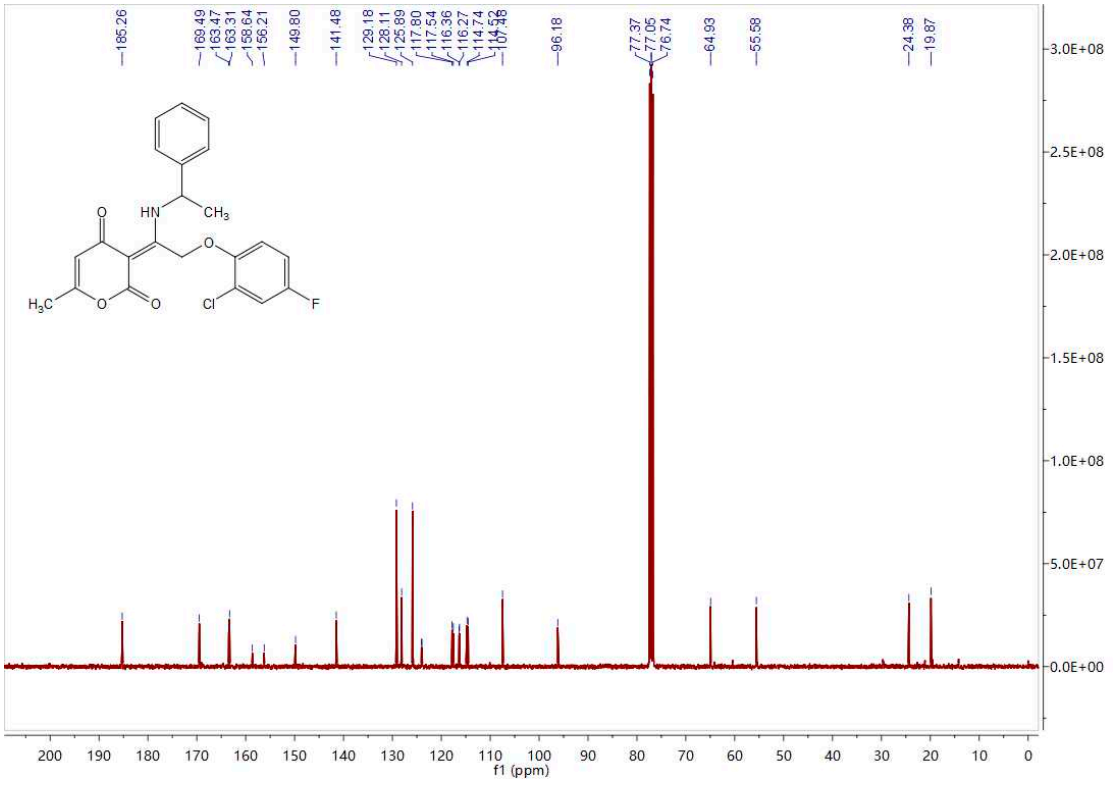

5
0729-1-5 52 (0.346)
1: TOF MS ES+
3.88e6
100
%
0
424.0733
402.0916
426.0709
427.0736
115.0570
144.0816
242.0797
256.0995
257.1046
349.0256
402.0306
486.0420
504.0445
554.0264
622.6000
702.1523
736.0830
782.1343
m/z


14.49
7.34
7.33
7.31
7.28
7.26
7.25
7.24
7.22
7.15
7.14
7.13
7.12
7.10
7.09
7.08
7.06
6.96
6.95
6.94
6.93
6.92
5.74
5.53
4.11
4.10
4.08
4.06
3.08
3.06
3.04
2.14
2.13
HN
O
Cl
F
H3C
0.89
1.96
3.31
0.97
0.90
0.99
0.84
1.73
2.00
2.01
3.00
f1 (ppm)


185.01
170.67
163.52
163.13
158.57
156.14
149.69
149.66
137.25
128.89
128.80
127.16
117.87
117.61
115.84
114.71
114.48
107.50
95.99
77.38
77.06
76.74
47.68
36.07
19.87
HN
Cl
O
O
O
O
H3C
F
f1 (ppm)


5
0729-1-18 52 (0.346)
1: TOF MS ES+
2.31e6
438.0889
416.1071
440.0868
441.1899
416.0519
460.0686
500.0560
559.5249
643.6062
696.2097
716.1818
828.3477
84.9614
125.9876
209.5412
227.5287
281.1236
338.3499
%
m/z


14.94
14.93
7.37
7.35
7.34
7.32
7.31
7.30
7.29
7.27
7.27
7.16
7.15
7.14
7.13
7.11
7.10
7.09
7.07
6.96
6.95
6.94
6.93
6.93
6.91
6.91
6.05
6.02
5.77
5.61
5.59
5.57
4.98
2.15
1.72
1.70
HN
CH3
O
O
O
O
H3C
Cl
F
0.87
5.13
1.94
1.00
0.90
0.89
0.99
0.96
3.00
2.97
f1 (ppm)


185.26
169.49
163.47
163.31
158.64
156.21
149.80
141.48
129.18
128.11
125.89
117.80
117.54
116.36
116.27
114.74
114.52
104.48
96.18
77.37
77.05
76.74
64.93
55.58
24.38
19.87
HN
CH3
O
O
O
O
H3C
Cl
F
f1 (ppm)

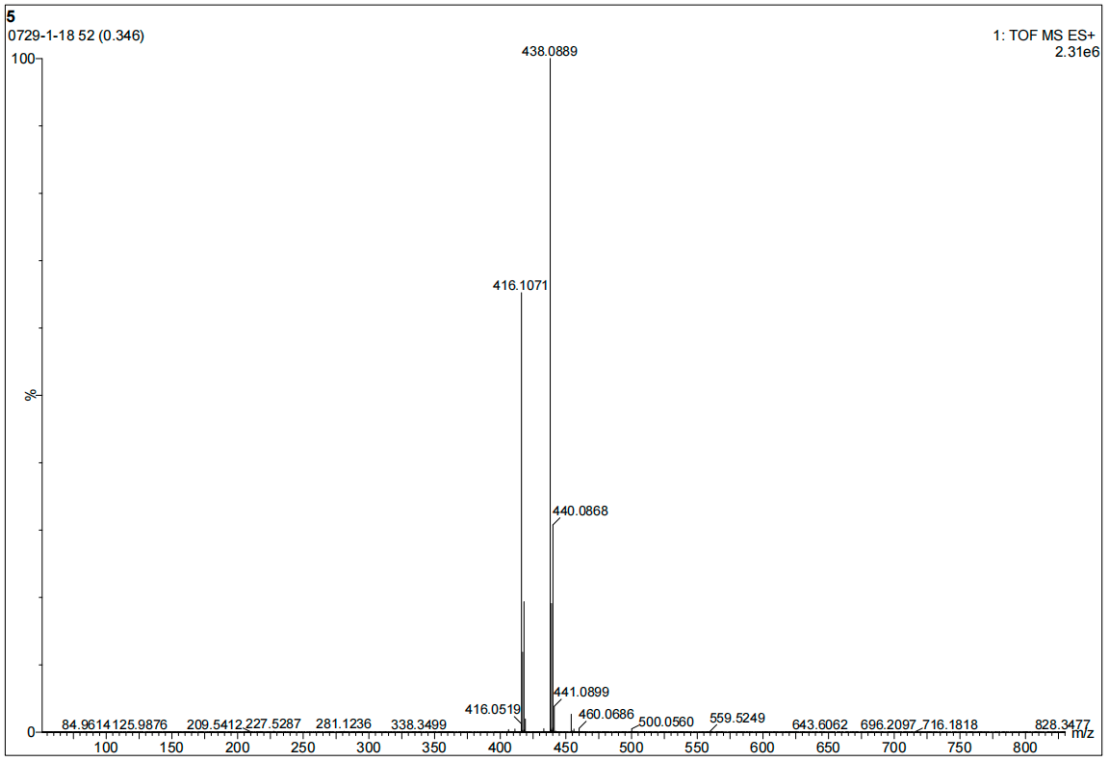


Table S1 Effects (% inhibition) of target compounds **APD-I-1**–**APD-I-14** on loss of plant weight at a dosage of 1500 g ha^{-1} after treatment 14 days (Pre) and 21 days (Post).[a]

Comp.	AM		AR		EC		DS	
	Pre	Post	Pre	Post	Pre	Post	Pre	Post
APD-I-1	0	30.7±3.1	0	27.2±3.9	8.3±1.8	0	0	6.7±0.4
APD-I-2	25.7±1.4	41.2±1.6	56.3±3.2	0	27.5±2.7	0	29.1±1.2	12.4±0.7
APD-I-3	8.7±1.3	24.1±0.6	0	8.3±2.2	22.5±4.4	0	0	11.8±0.7
APD-I-4	19.4±2.1	4.3±0.9	0	20.1±6.6	10.8±2.4	0	8.6±2.4	8.2±1.0
APD-I-5	14.4±2.6	47.0±0.7	10.0±2.4	49.5±2.1	0	0	0	19.0±0.7
APD-I-6	13.7±3.8	27.7±1.2	13.3±2.4	54.2±1.6	23.0±4.3	0	8.1±2.4	27.0±0.7
APD-I-7	60.2±1.8	39.4±1.5	71.4±4.6	26.6±3.9	47.1±2.6	0	17.5±0.4	22.3±0.6
APD-I-8	7.7±3.0	3.0±0.8	26.7±4.8	33.3±2.5	16.2±2.1	7.8±2.5	0	0
APD-I-9	71.4±1.7	21.4±0.8	81.3±2.3	12.4±1.8	25.5±2.3	24.9±2.5	78.8±0.8	17.7±2.7
APD-I-10	70.4±1.6	22.7±0.8	77.3±2.4	17.3±1.9	37.4±3.3	7.0±1.3	51.7±1.2	11.2±0.8
APD-I-11	14.4±2.7	5.2±1.0	0	0	7.4±3.5	0	0	0
APD-I-12	58.4±2.6	36.2±1.0	81.3±1.0	20.8±2.3	23.0±1.2	26.9±1.2	71.0±0.6	15.3±1.3
APD-I-13	39.9±1.6	31.7±1.0	53.3±1.9	37.7±2.3	32.4±3.2	6.9±1.7	42.8±1.8	23.3±0.9
APD-I-14	100	76.8±0.7	99.7±0.2	65.3±1.0	71.5±2.5	43.7±2.9	99.1±0.6	37.4±1.9
AZ	100	100	100	100	82.1±0.8	100	100	86.0±2.4

[a] Each value represents the mean ± SD of three experiments; *Abutilon theophrasti Medicus (AM), Amaranthus retroflexus L. (AR), Echinochloa crus-galli (EC) Digitaria sanguinalis (L.) Scop. (DS).*

Table S2 Effects (% inhibition) of target compounds **APD-I-14**, **APD-II-1**–**APD-II-19** on loss of plant weight at a dosage of 1500 g ha^{-1} after treatment 14 days (Pre) and 21 days (Post).[a]

Comp.	AM		AR		EC		DS	
	Pre	Post	Pre	Post	Pre	Post	Pre	Post

APD-I-14	97.4±1.7	70.8±3.0	100	61.6±2.3	67.4±1.3	40.0±3.6	100	35.4±2.1
APD-II-1	92.6±0.4	68.6±2.2	99.7±0.1	100	71.1±1.6	46.9±4.1	98.5±0.2	33.7±0.4
APD-II-2	97.7±1.4	62.9±1.2	99.6±0.5	86.4±1.0	75.3±0.4	8.8±1.7	99.7±0.3	34.0±2.8
APD-II-3	96.9±0.7	56.1±0.5	99.4±0.8	100	76.4±1.5	43.8±3.2	96.0±0.7	23.0±0.9
APD-II-4	100	64.2±1.8	100	66.0±4.1	77.7±1.3	42.3±2.3	99.2±0.8	36.1±2.1
APD-II-5	100	82.2±0.6	98.6±1.0	46.2±1.0	61.1±1.6	22.4±2.6	98.0±0.3	24.7±1.1
APD-II-6	84.9±3.8	72.2±0.4	96.2±0.9	59.4±3.3	69.0±2.3	21.3±1.8	90.5±0.2	52.3±2.4
APD-II-7	100	66.9±0.4	99.7±0.3	96.0±1.9	60.0±0.8	40.9±1.6	98.9±0.8	35.7±1.9
APD-II-8	99.6±0.3	62.2±1.8	98.3±1.3	100	59.8±1.3	62.7±1.0	98.4±1.2	48.5±1.4
APD-II-9	92.6±1.8	77.4±0.6	98.3±0.4	95.1±3.9	68.6±2.7	42.5±0.9	98.9±0.9	40.7±0.8
APD-II-10	94.2±1.0	70.4±0.6	99.1±0.7	98.4±2.2	52.5±1.6	35.8±3.0	99.3±0.6	33.5±1.5
APD-II-11	83.7±3.9	60.2±3.1	99.7±0.4	3.6±3.5	41.2±1.2	31.3±2.6	98.7±1.0	41.4±1.4
APD-II-12	88.0±1.7	56.9±1.9	93.8±1.4	40.4±1.9	31.6±3.3	21.8±1.8	87.6±0.6	24.3±1.8
APD-II-13	100	59.0±0.9	98.0±0.7	75.3±1.6	59.1±1.1	35.8±2.0	82.8±0.8	11.7±1.2
APD-II-14	91.8±1.1	55.6±0.8	98.6±0.5	80.5±1.9	44.4±0.9	10.3±2.7	80.9±0.3	0
APD-II-15	100	76.3±0.3	100	92.2±2.6	98.2±0.7	41.7±1.2	99.9±0.1	49.6±1.6
APD-II-16	100	74.7±0.5	99.6±0.3	48.3±2.3	95.7±1.0	22.7±2.2	99.5±0.3	25.9±1.7
APD-II-17	100	46.0±1.1	90.5±1.7	53.1±4.0	60.3±0.5	12.8±2.1	81.3±0.8	15.9±2.1
APD-II-18	100	69.5±1.5	98.3±0.2	92.2±2.5	40.8±1.2	24.1±3.0	95.7±0.4	13.6±1.5
APD-II-19	91.1±0.3	74.2±1.1	99.6±0.4	85.9±1.6	33.3±1.2	30.3±1.0	88.1±0.8	25.2±0.5
AZ	100	100	100	100	89.6±0.7	98.0±0.7	100	87.6±1.0

[a] Each value represents the mean ± SD of three experiments; *Abutilon theophrasti Medicus (AM), Amaranthus retroflexus L. (AR), Echinochloa crus-galli (EC) Digitaria sanguinalis (L.) Scop. (DS).*

Table S3 Effects (% inhibition) of target compounds **APD-I-14**, **APD-II-1**–**APD-II-19** on loss of plant weight at a dosage of 750 g ha^{-1}, 375 g ha^{-1}, 187.5 g ha^{-1} after treatment 14 days under pre-emergence conditions.[a]

Comp.	Dosage (g ha^{-1})	AM	AR	EC	DS
APD-I-14	750	91.3±0.8	94.9±4.5	41.5±4.0	98.8±0.8
	375	73.0±1.0	89.1±1.5	0	98.2±0.4
	187.5	16.5±1.0	74.5±0.7	0	61.3±1.6
APD-II-1	750	81.4±2.9	97.8±0.9	30.0±3.6	97.7±1.0
	375	41.7±4.1	90.5±0.6	0	87.4±1.4
	187.5	13.8±1.9	84.0±0.8	0	73.1±0.8
APD-II-2	750	89.8±0.3	98.9±0.9	40.5±5.0	95.9±0.7
	375	81.8±2.3	94.9±1.2	45.5±5.2	91.8±1.9
	187.5	21.3±1.6	89.1±2.4	14.0±1.1	71.6±1.3
APD-II-3	750	83.2±1.5	99.3±1.0	47.5±2.7	90.1±0.6
	375	57.7±2.1	94.9±0.8	5.5±2.1	95.3±1.2
	187.5	34.4±2.9	77.5±1.1	0	63.6±1.0
APD-II-4	750	76.7±1.4	99.3±1.0	33.0±2.1	99.7±0.4
	375	57.1±3.3	97.1±1.9	15.5±3.0	89.8±1.8
	187.5	16.9±2.0	84.0±1.1	0	58.0±1.9
APD-II-5	750	70.0±1.7	96.3±0.7	30.2±4.1	99.0±0.8
	375	60.0±2.2	96.3±0.7	20.0±1.7	59.0±2.9

	187.5	16.9±2.8	69.0±2.4	5.3±0.2	24.1±2.6
	750	72.5±2.3	95.6±0.7	37.0±2.7	97.1±0.7
APD-II-6	375	64.5±1.0	86.9±3.1	41.5±2.1	38.1±1.4
	187.5	25.6±2.4	59.3±1.5	7.0±2.7	11.2±1.6
	750	59.5±2.7	96.4±3.8	32.5±1.9	97.7±0.4
APD-II-7	375	58.4±2.1	94.9±1.0	52.0±2.5	86.6±0.9
	187.5	6.0±1.5	70.9±1.6	1.0±0.3	69.1±2.1
	750	65.4±1.8	96.4±0.4	26.0±2.6	99.1±1.2
APD-II-8	375	49.7±3.1	92.7±1.5	0	84.5±1.4
	187.5	24.9±2.8	67.3±1.0	0	50.0±0.9
	750	90.6±1.4	94.3±4.4	68.0±2.0	96.4±0.6
APD-II-9	375	87.0±1.5	84.3±2.2	69.2±1.3	86.4±1.1
	187.5	81.0±0.7	61.3±1.5	30.7±2.0	32.0±1.4
	750	90.4±2.2	98.2±0.5	33.5±2.2	90.1±1.6
APD-II-10	375	68.5±2.5	92.7±2.9	10.5±1.7	88.6±0.5
	187.5	37.0±1.8	75.5±1.8	0	23.6±0.8
	750	75.2±2.9	96.4±3.0	23.0±2.3	99.7±0.2
APD-II-11	375	37.3±2.7	91.3±2.7	0	84.2±0.7
	187.5	27.1±2.5	69.5±1.9	0	27.6±0.2
	750	46.1±3.4	92.7±0.5	14.0±2.2	52.7±2.0
APD-II-12	375	36.6±2.5	82.5±2.6	0	41.9±1.2
	187.5	11.8±2.3	41.8±4.1	0	0
	750	98.2±0.8	98.9±0.9	41.5±2.1	88.0±3.0
APD-II-13	375	62.0±1.0	90.5±1.6	35.5±2.1	55.6±1.2
	187.5	23.7±3.7	69.1±1.8	0	15.8±2.3
	750	65.0±1.9	96.4±0.7	32.0±1.5	83.9±1.9
APD-II-14	375	19.1±1.5	75.3±2.4	22.5±2.6	46.9±2.0
	187.5	6.0±1.3	52.0±3.9	12.0±2.6	0
	750	100	95.5±0.9	94.9±1.9	95.3±1.6
APD-II-15	375	100	98.3±0.5	96.5±0.6	70.0±0.5
	187.5	95.8±3.6	76.5±2.7	67.9±3.5	30.7±2.0
	750	100	94.2±0.5	92.6±0.5	84.2±1.3
APD-II-16	375	97.1±2.1	92.4±1.5	64.8±2.1	82.2±1.0
	187.5	97.3±0.2	67.7±0.9	9.3±2.0	25.5±1.9
	750	97.0±0.8	87.1±1.9	20.5±4.2	73.4±3.4
APD-II-17	375	74.9±1.6	83.3±1.4	45.5±2.9	62.9±2.2
	187.5	29.8±1.2	51.8±2.3	0	0
	750	100	95.6±0.3	17.5±0.7	88.5±1.3
APD-II-18	375	84.0±3.6	89.8±1.3	15.0±1.3	71.4±0.6
	187.5	43.1±1.3	73.1±1.1	4.5±3.0	20.1±1.3
	750	87.4±0.8	97.1±0.6	40.0±1.2	80.3±0.9
APD-II-19	375	62.1±2.0	85.5±3.5	11.0±1.7	42.5±2.0
	187.5	15.3±1.1	55.6±2.5	0	0
AZ	750	96.0±0.5	100	79.0±1.2	97.2±0.5

	375	81.6±0.5	100	62.3±3.4	96.0±0.6
	187.5	74.3±2.9	80.2±3.3	24.7±3.3	53.6±3.7

[a] Each value represents the mean ± SD of three experiments; *Abutilon theophrasti Medicus (AM), Amaranthus retroflexus L. (AR), Echinochloa crus-galli (EC) Digitaria sanguinalis (L.) Scop. (DS).*