

Design, synthesis and bioactivity studies of flavonol bio-containing β -amino alcohols

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^1H NMR, ^{13}C NMR, ^{19}F NMR and HRMS spectrum of target compounds Y1-Y21

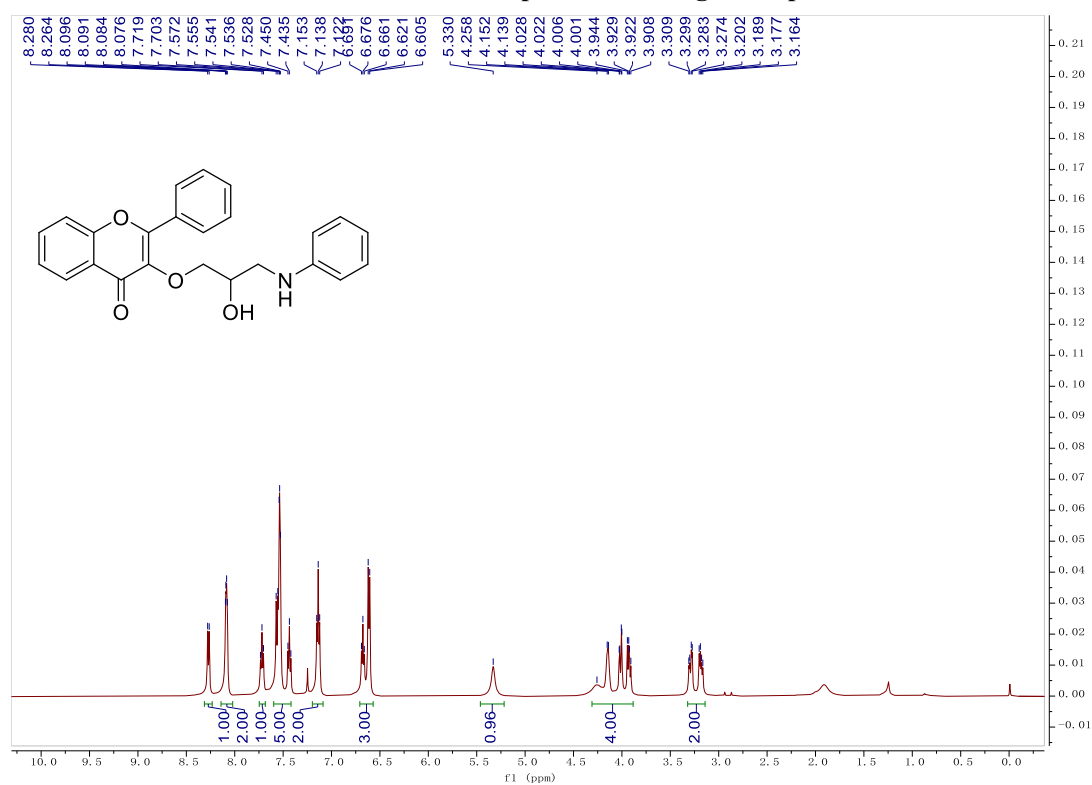


Fig. 1 ^1H NMR spectrum of title compound Y1

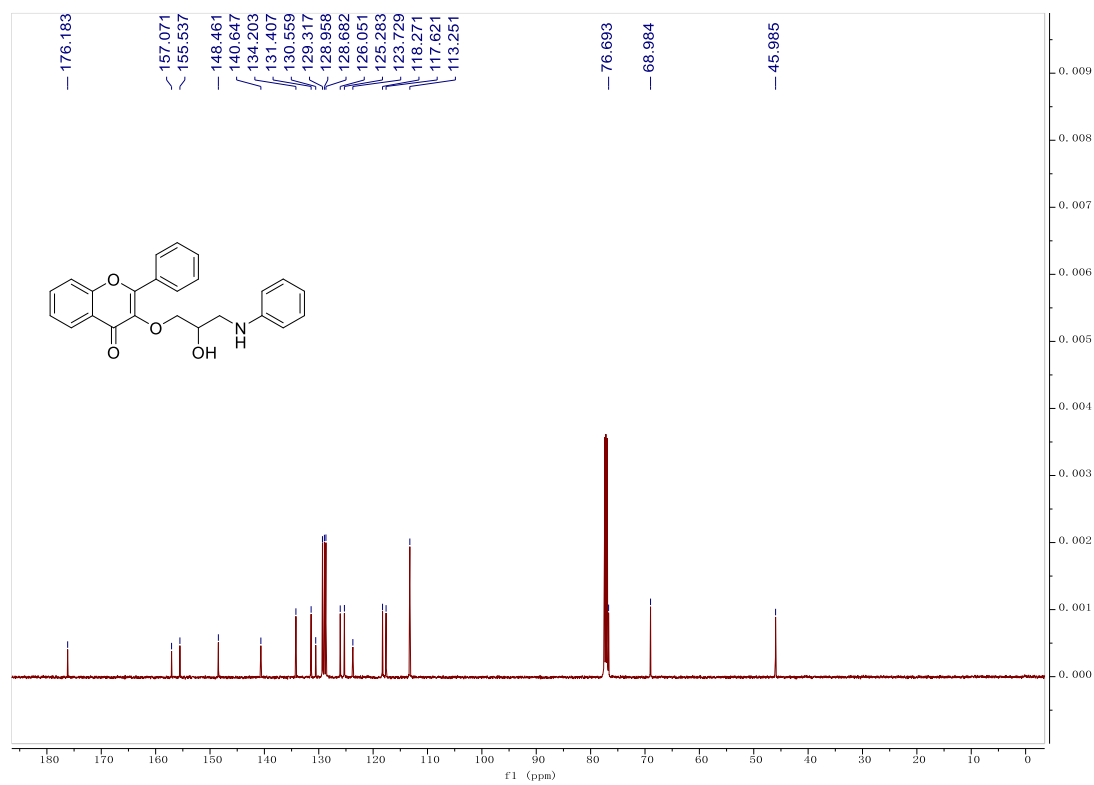


Fig. 2 ^{13}C NMR spectrum of title compound Y1

Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) and the y-axis represents the relative abundance. The base peak is at m/z 388.15308. The chemical formula is $C_{24}H_{22}O_4N$ with a molecular weight of 388.15433. The peak at 388.15308 is labeled with a value of -3.24 ppm.

m/z	Relative Abundance (approx.)
387.14117	2
387.56586	2
387.89996	10
388.15308	100
388.25281	5
388.71262	2
389.15643	28
389.25613	5

Chemical structure: OCC(Nc1ccccc1)COc2cc(Br)ccc2C3=CC=CC=C3C4=CC=CC=C4O4=O

¹H NMR spectrum (ppm):

- 8.270, 8.267, 8.254, 8.251, 8.010, 7.994, 7.981, 7.977, 7.968, 7.963, 7.951, 7.934, 7.741, 7.738, 7.727, 7.723, 7.720, 7.710, 7.706, 7.689, 7.672, 7.659, 7.655, 7.646, 7.642, 7.630, 7.560, 7.543, 7.455, 7.439, 6.699, 6.684, 6.669, 6.642, 6.629, 6.613, 4.157, 4.152, 4.147, 4.143, 4.029, 4.023, 4.007, 4.002, 3.955, 3.940, 3.933, 3.919, 3.923, 3.913, 3.297, 3.288, 3.216, 3.203, 3.191, 3.178

Integration values (from left to right): 1.00, 2.00, 2.00, 2.00, 1.00, 2.00, 0.96, 1.00, 1.00, 1.00, 1.00, 1.00.

Fig. 4 ^1H NMR spectrum of title compound **Y2**

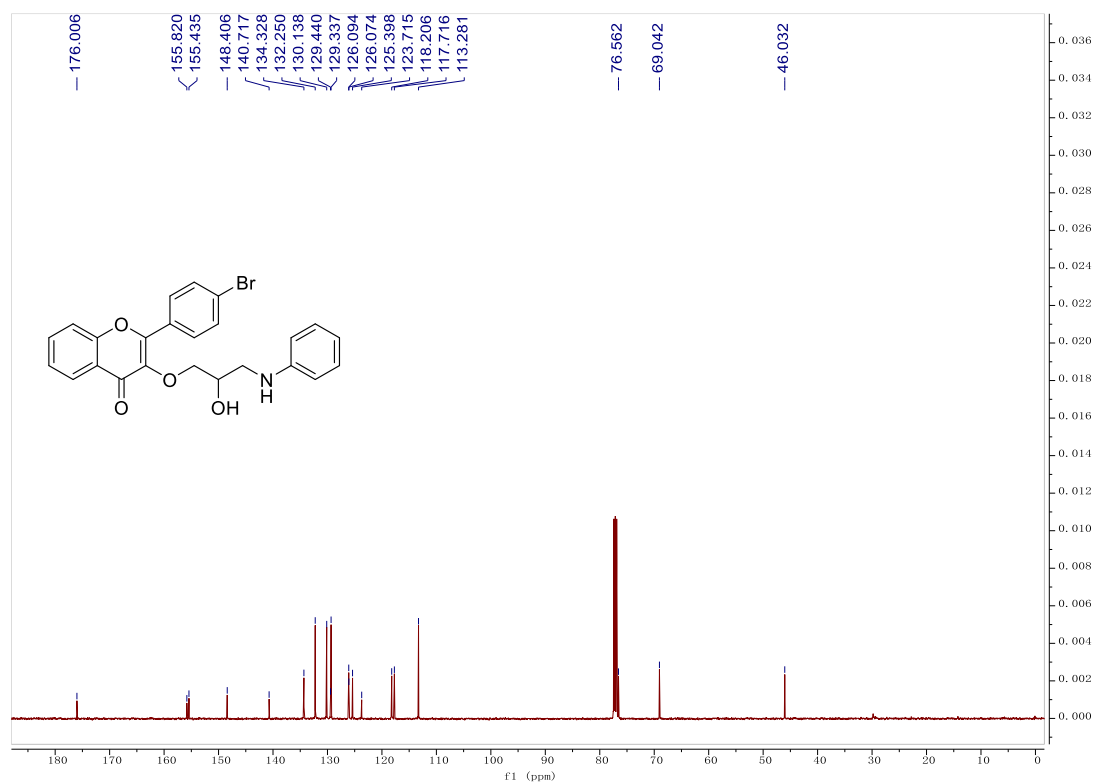


Fig. 5 ¹³C NMR spectrum of title compound Y2

42 #53 RT: 0.52 AV: 1 NL: 2.52E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

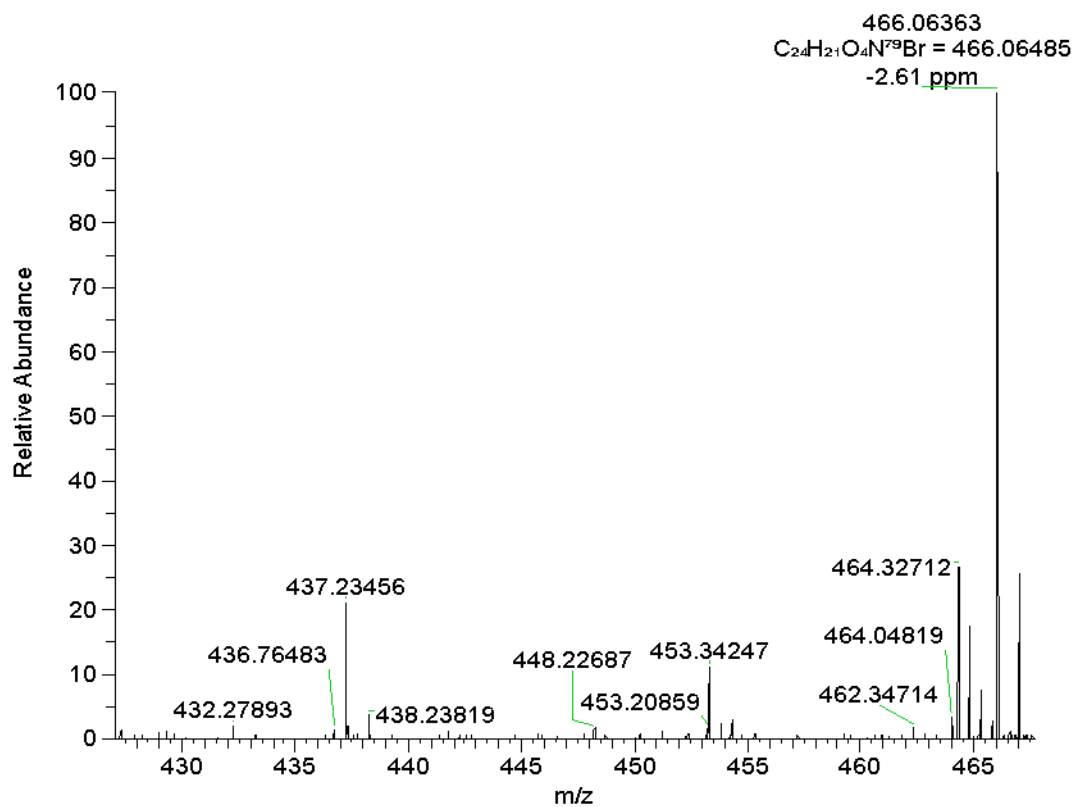


Fig. 6 HRMS spectrum of title compound Y2

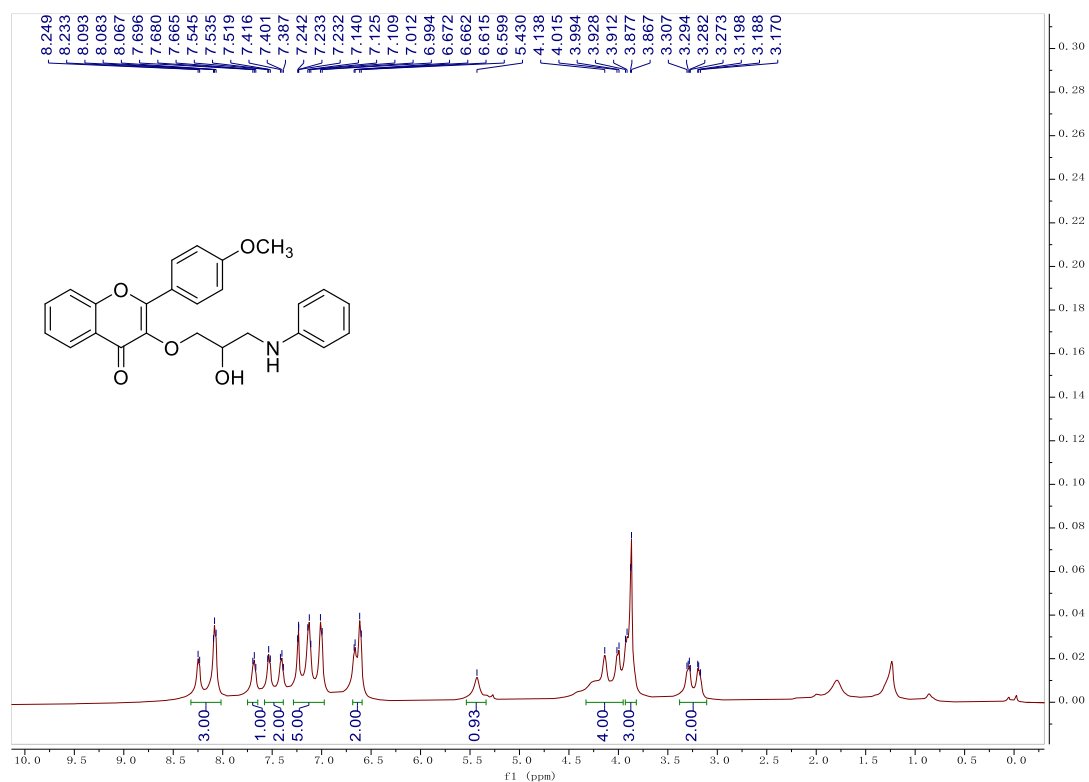


Fig. 7 ¹H NMR spectrum of title compound Y3

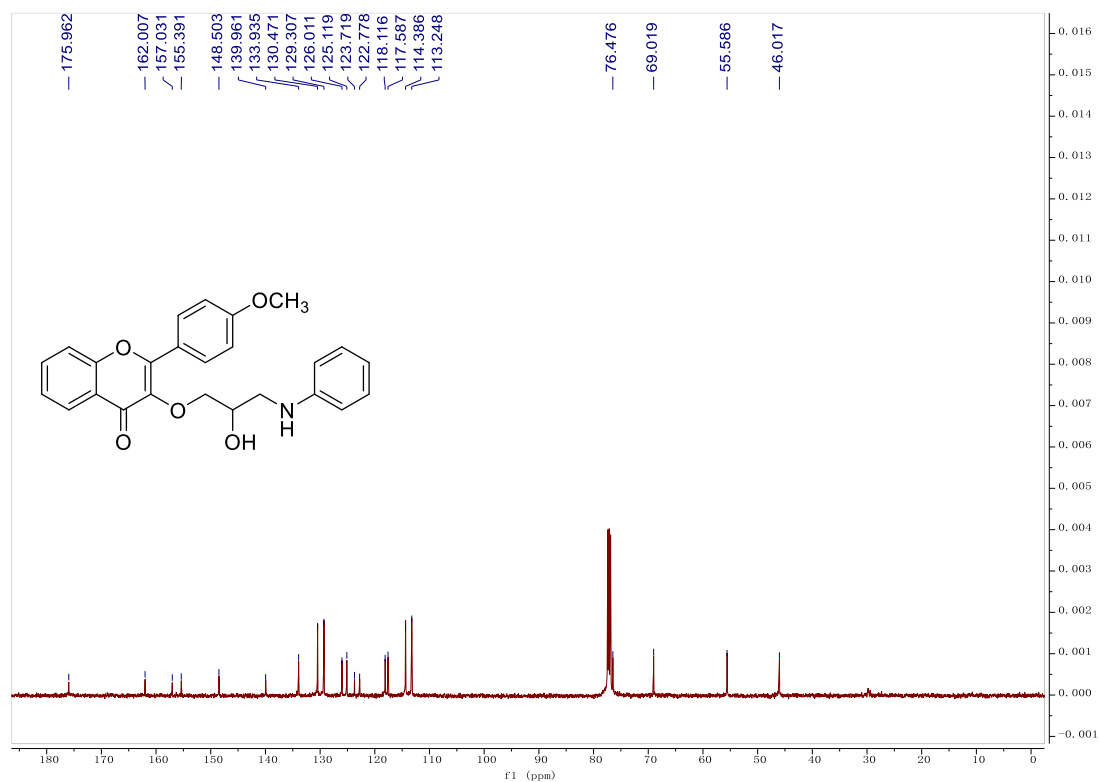


Fig. 8 ¹³C NMR spectrum of title compound Y3

43 #45 RT: 0.44 AV: 1 NL: 7.72E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

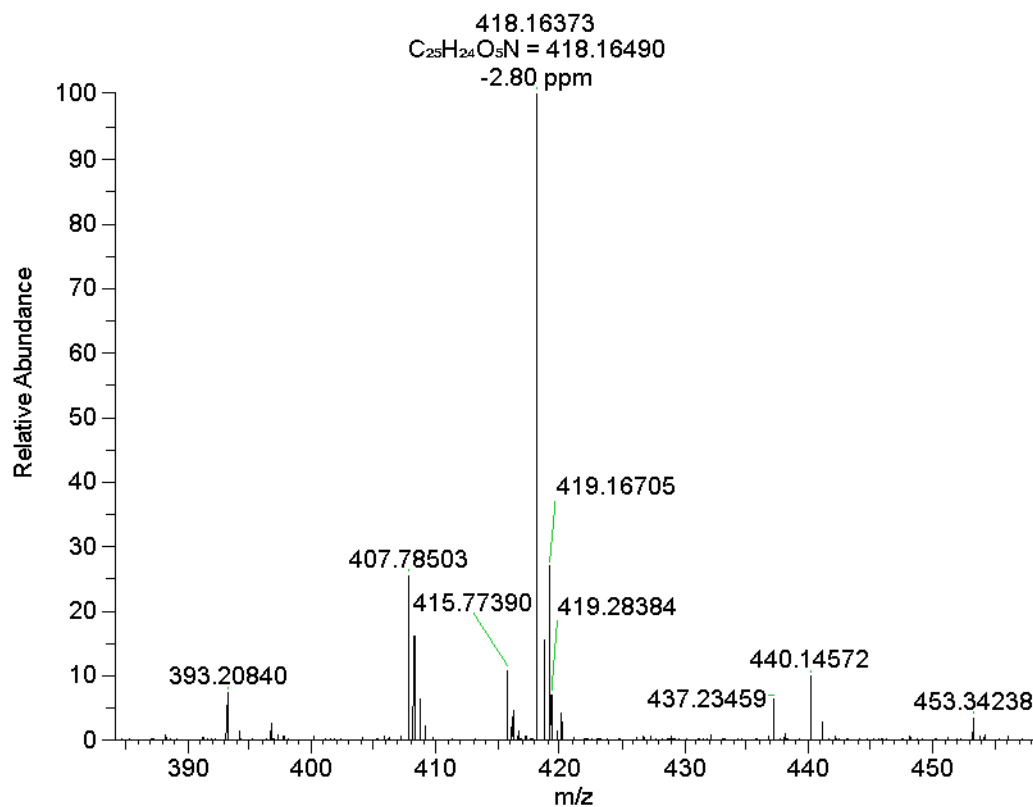


Fig. 9 HRMS spectrum of title compound Y3

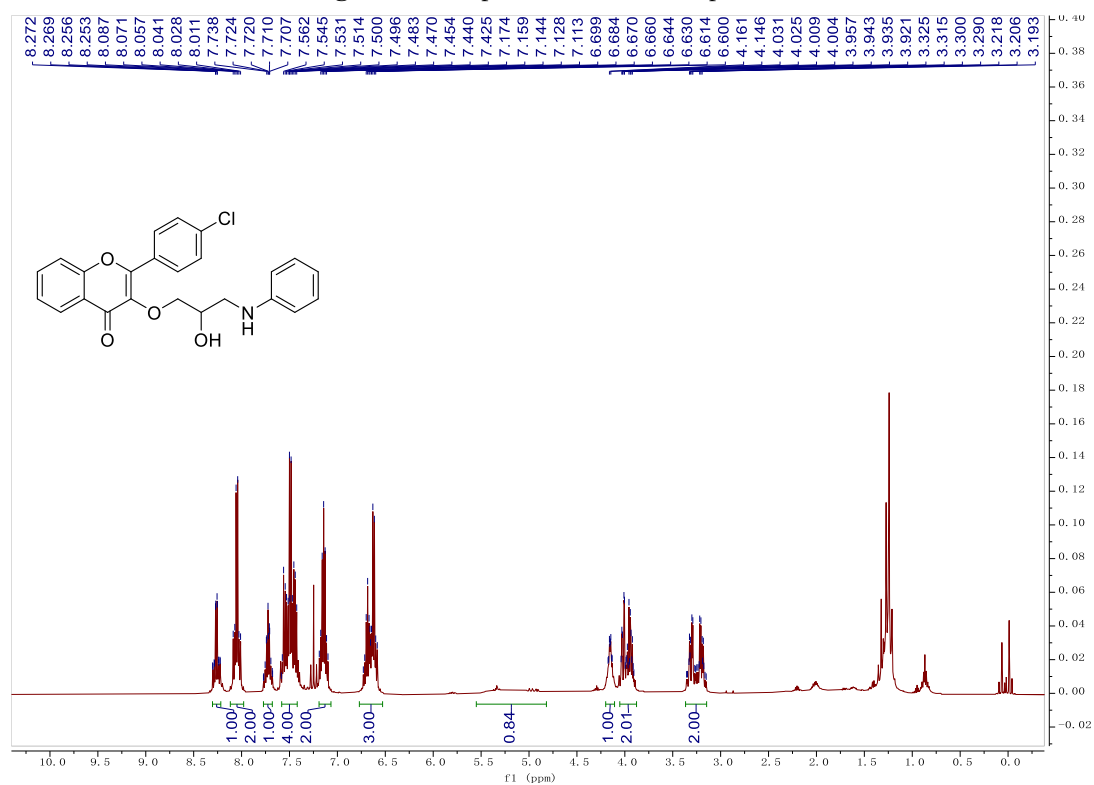


Fig. 10 1H NMR spectrum of title compound Y4

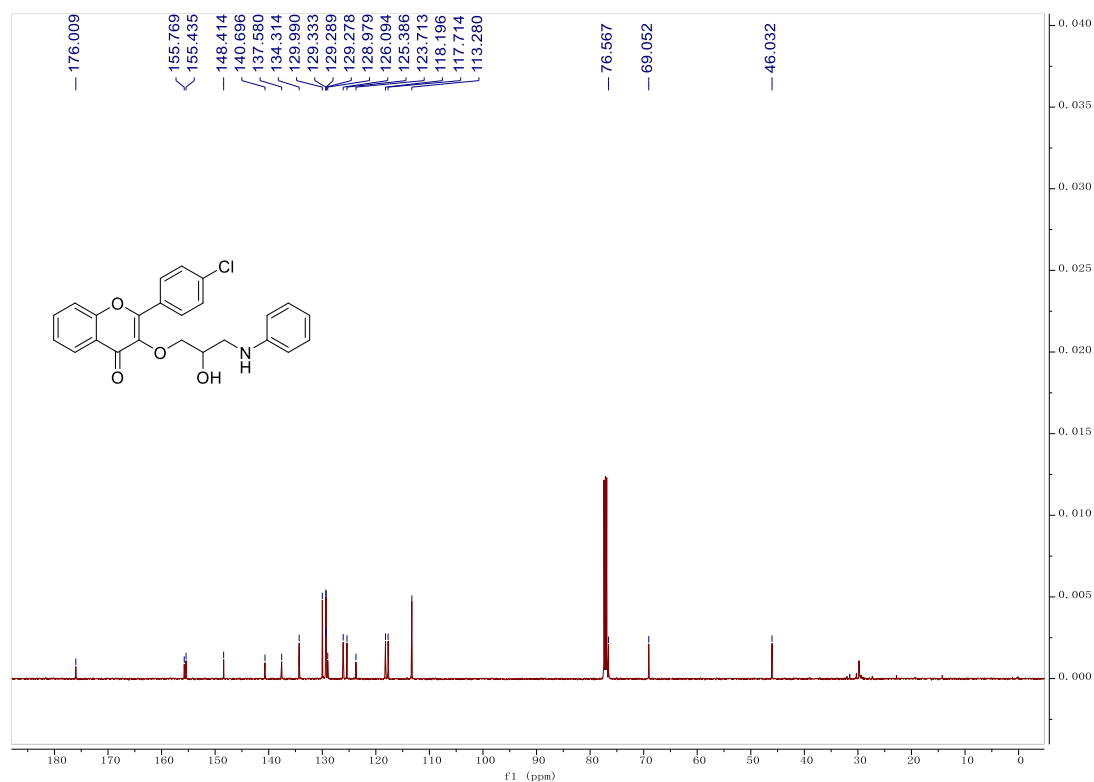


Fig. 11 ¹³C NMR spectrum of title compound Y4

44 #51 RT: 0.49 AV: 1 NL: 2.11E+006
T: FTMS + p ESI Full ms [100.0000-1300.0000]

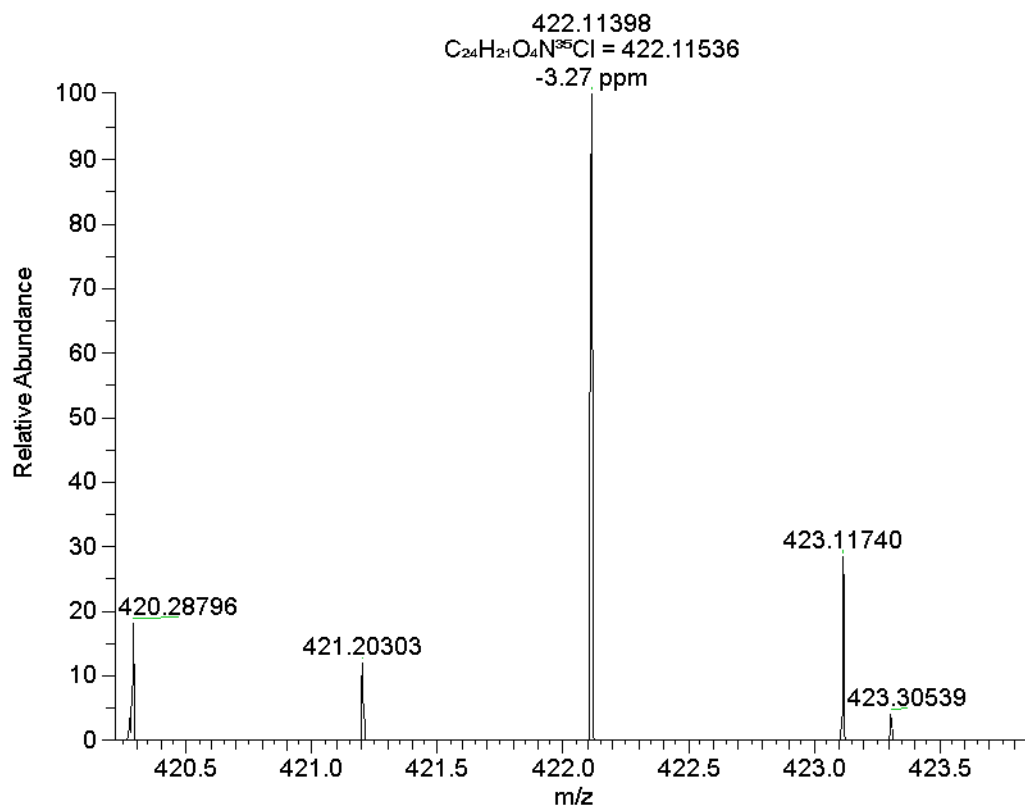


Fig. 12 HRMS spectrum of title compound Y4

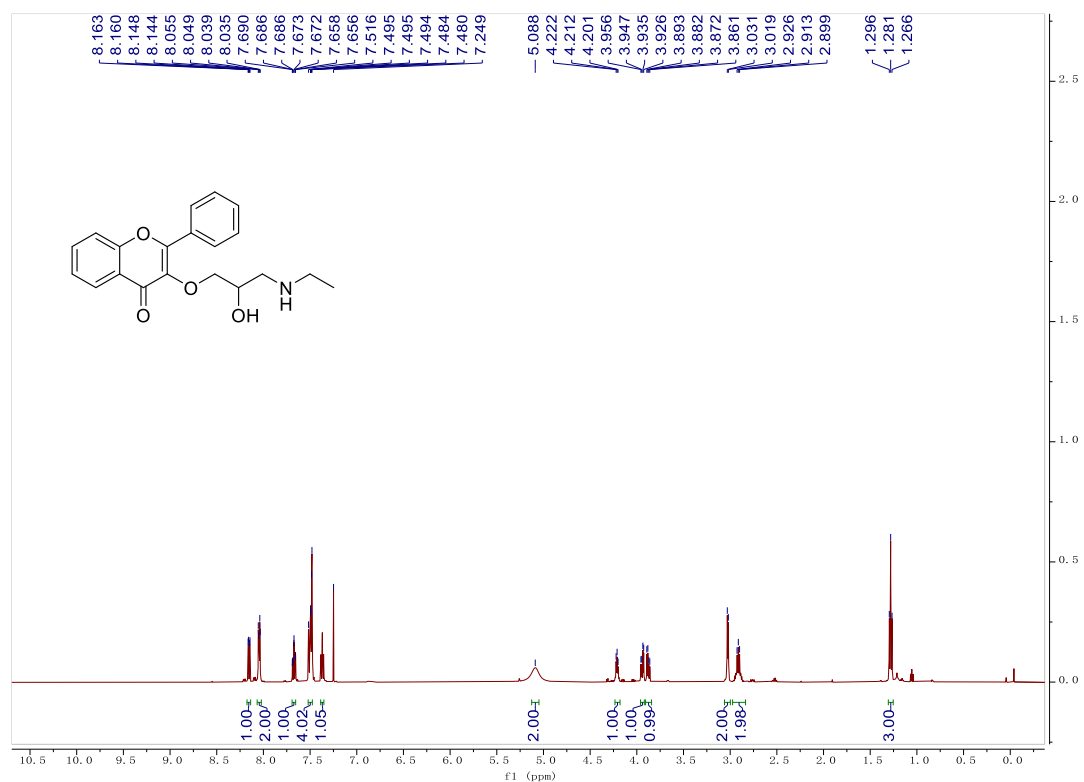


Fig. 13 ¹H NMR spectrum of title compound **Y5**

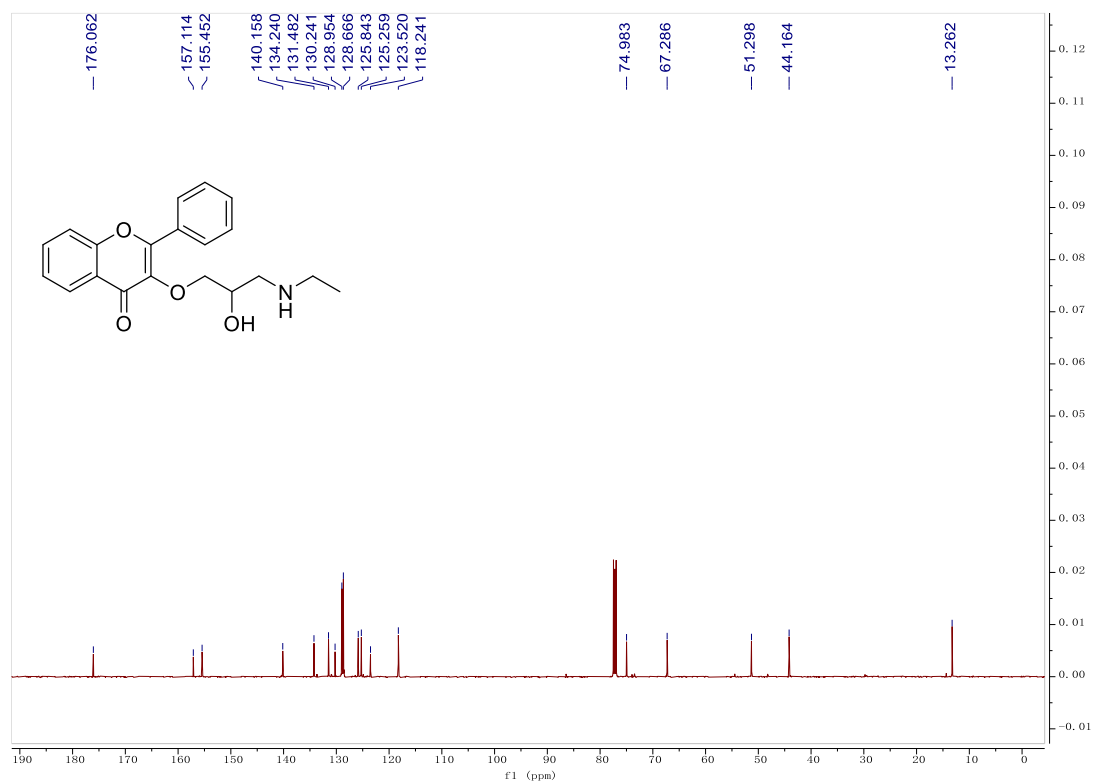


Fig. 14 ¹³C NMR spectrum of title compound **Y5**

Mass spectrum of compound 10 ($C_{20}H_{22}O_4N$). The x-axis represents the mass-to-charge ratio (m/z) and the y-axis represents the relative abundance. The base peak is at m/z 340.15411.

m/z	Relative Abundance (approx.)
118.05218	5
158.01247	10
309.27853	10
340.15411	100
396.80139	25
453.34332	20
588.40930	25
679.51135	20
701.49323	25

Chemical structure: Cc1ccc(cc1)Oc2c(=O)c3ccccc3oc2C(O)CNc4ccccc4

¹H NMR spectrum (ppm):

Chemical Shift (ppm)	Integration
8.270	1.00
8.267	2.00
8.254	1.00
8.251	1.00
8.010	2.00
7.993	3.00
7.701	4.00
7.698	1.00
7.695	1.00
7.684	2.00
7.556	3.00
7.539	4.00
7.429	1.00
7.415	1.00
7.413	2.00
7.411	3.00
7.399	4.00
7.339	1.00
7.323	1.00
7.164	2.00
7.150	3.00
7.147	4.00
7.145	1.00
7.133	1.00
6.703	2.00
6.688	3.00
6.687	4.00
6.686	1.00
6.673	1.00
6.671	2.00
6.669	3.00
6.636	4.00
6.634	1.00
6.618	1.00
4.168	3.00
4.163	4.00
4.154	1.00
4.034	1.00
4.029	2.00
4.013	3.00
4.007	4.00
3.948	1.00
3.933	1.00
3.926	2.00
3.912	3.00
3.319	4.00
3.309	1.00
3.294	2.00
3.284	3.00
3.215	4.00
3.202	1.00
3.190	2.00
3.177	3.00
2.443	4.00

Fig. 16 ^1H NMR spectrum of title compound **Y6**

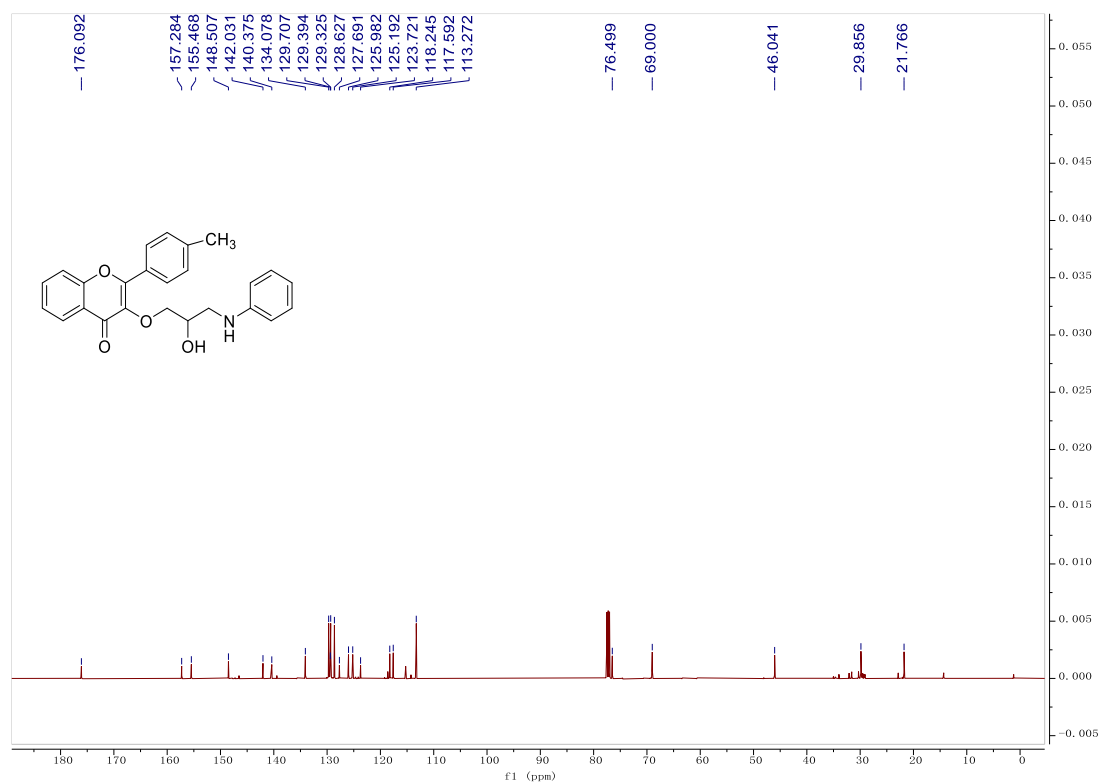


Fig. 17 ¹³C NMR spectrum of title compound Y6

46 #51 RT: 0.50 AV: 1 NL: 2.16E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

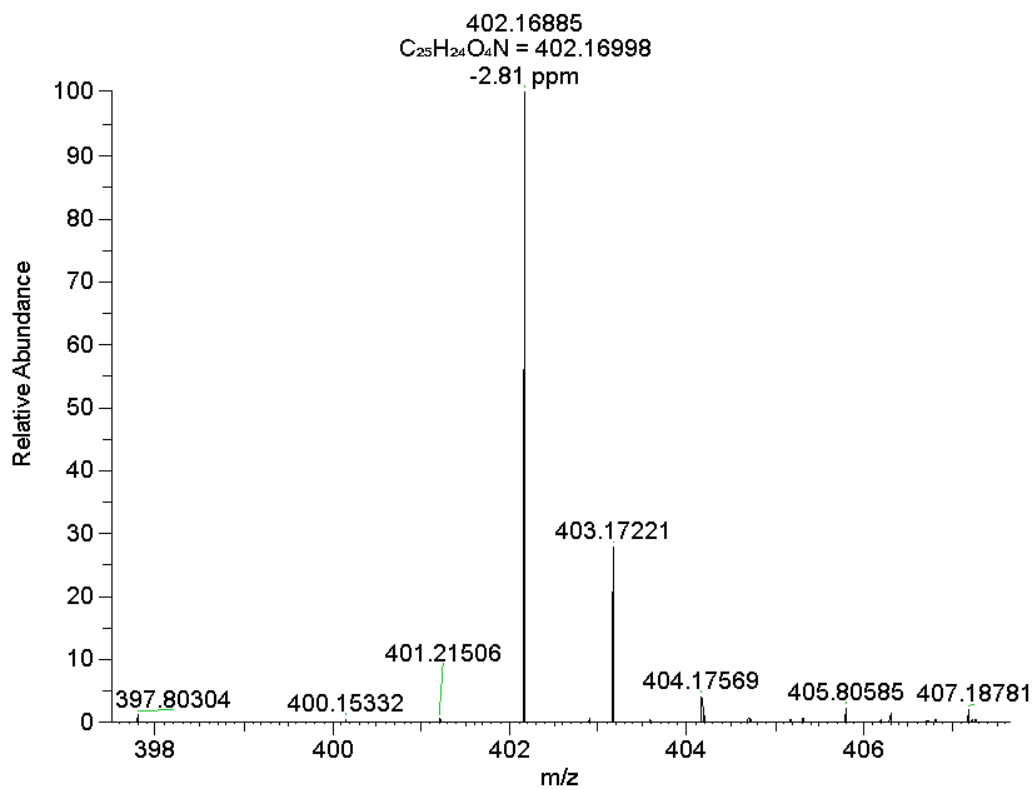


Fig. 18 HRMS spectrum of title compound Y6

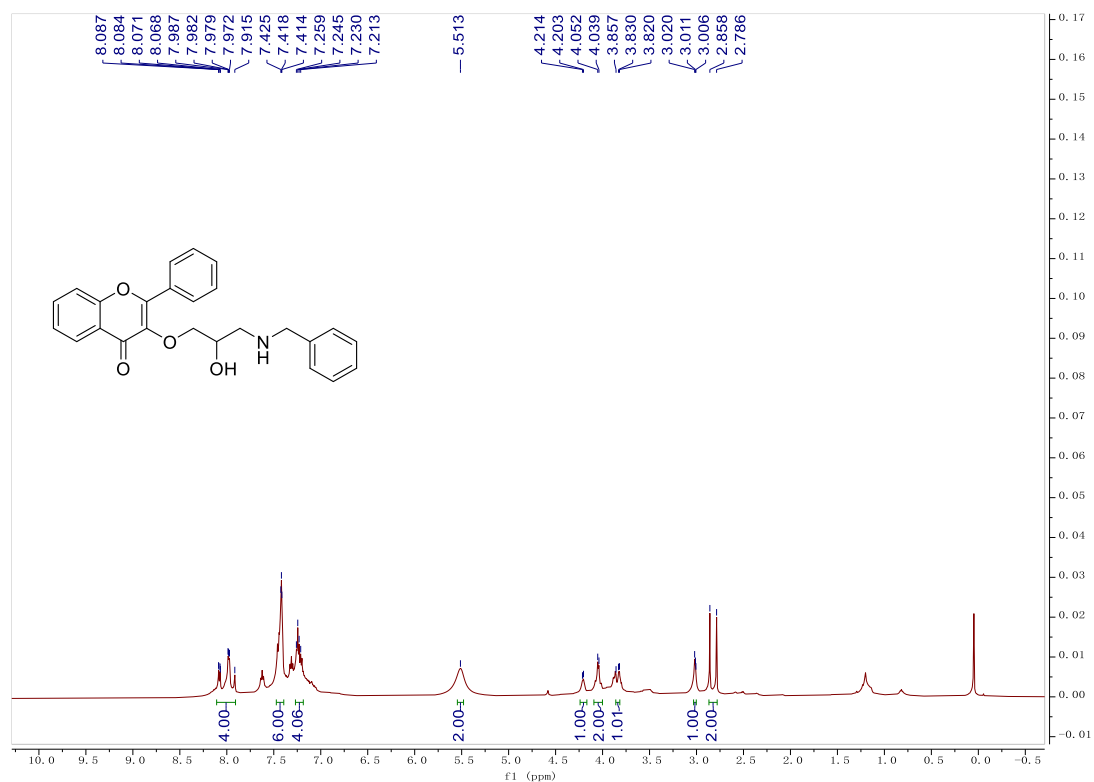


Fig. 19 ¹H NMR spectrum of title compound Y7

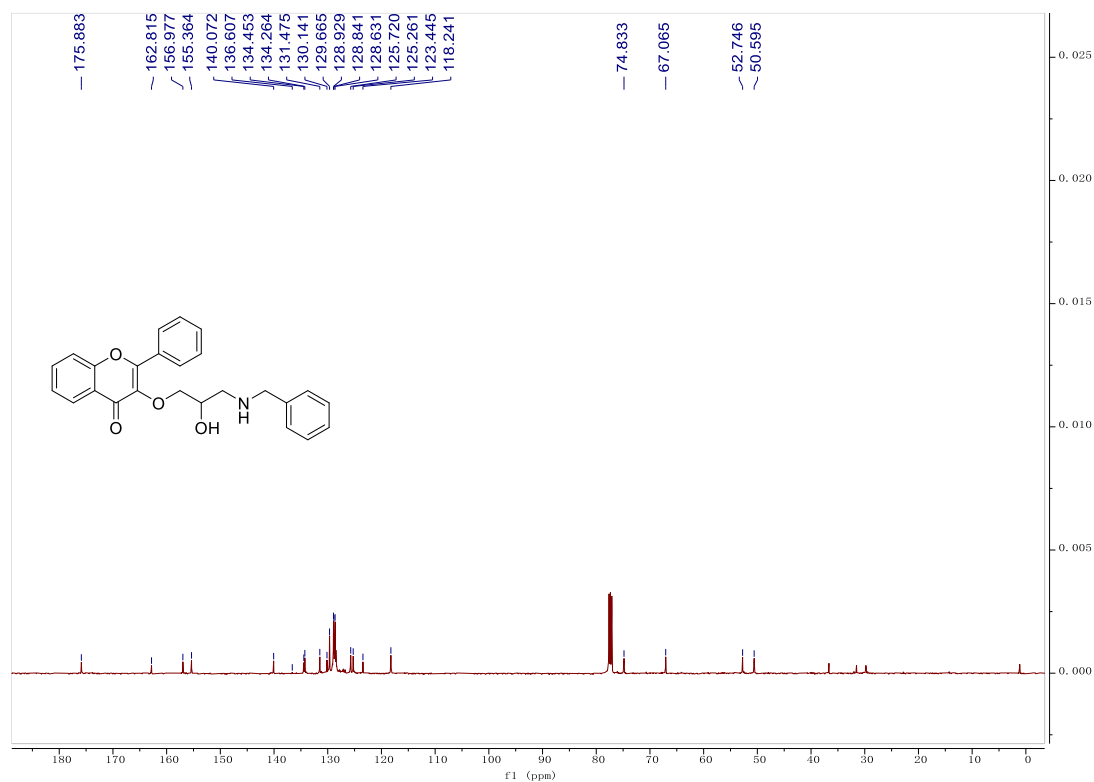


Fig. 20 ¹³C NMR spectrum of title compound Y7

Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 398 to 407. The y-axis represents the relative abundance from 0 to 100. The base peak is at m/z 402.16879. Other labeled peaks include m/z 398.28510, 400.15356, 401.15613, 403.17203, 404.17508, and 405.17773. The chemical formula $C_{25}H_{24}O_4N = 402.16998$ and a shift of -2.96 ppm are noted.

m/z	Relative Abundance (%)
398.28510	~1
400.15356	~1
401.15613	~10
402.16879	100
403.17203	~25
404.17508	~2
405.17773	~1

Chemical structure of compound 10: CC(C)(C)c1ccc(cc1)C2=CC(=O)C(=C(c3ccccc3)OC(CO)CNc4ccccc4)O2

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 10.0. The y-axis represents intensity, ranging from -1000 to 24000. The spectrum shows several peaks, with integration values indicated below the baseline.

Integration values (from left to right): 1.01, 2.00, 1.02, 3.00, 1.00, 2.01, 3.00, 1.00, 2.03, 1.09, 1.06, 1.00, 1.00, 9.00.

Chemical shift values (ppm) labeled above the peaks (from left to right): 8.300, 8.296, 8.280, 8.276, 8.068, 7.726, 7.581, 7.566, 7.560, 7.545, 7.486, 7.447, 7.175, 7.157, 7.154, 7.138, 6.692, 6.674, 6.646, 6.626, 5.412, 4.273, 4.179, 4.163, 4.071, 4.064, 4.044, 4.037, 3.978, 3.960, 3.951, 3.933, 3.347, 3.335, 3.316, 3.304, 3.235, 3.219, 3.204, 3.188, 1.384.

Fig. 22 ^1H NMR spectrum of title compound **Y8**

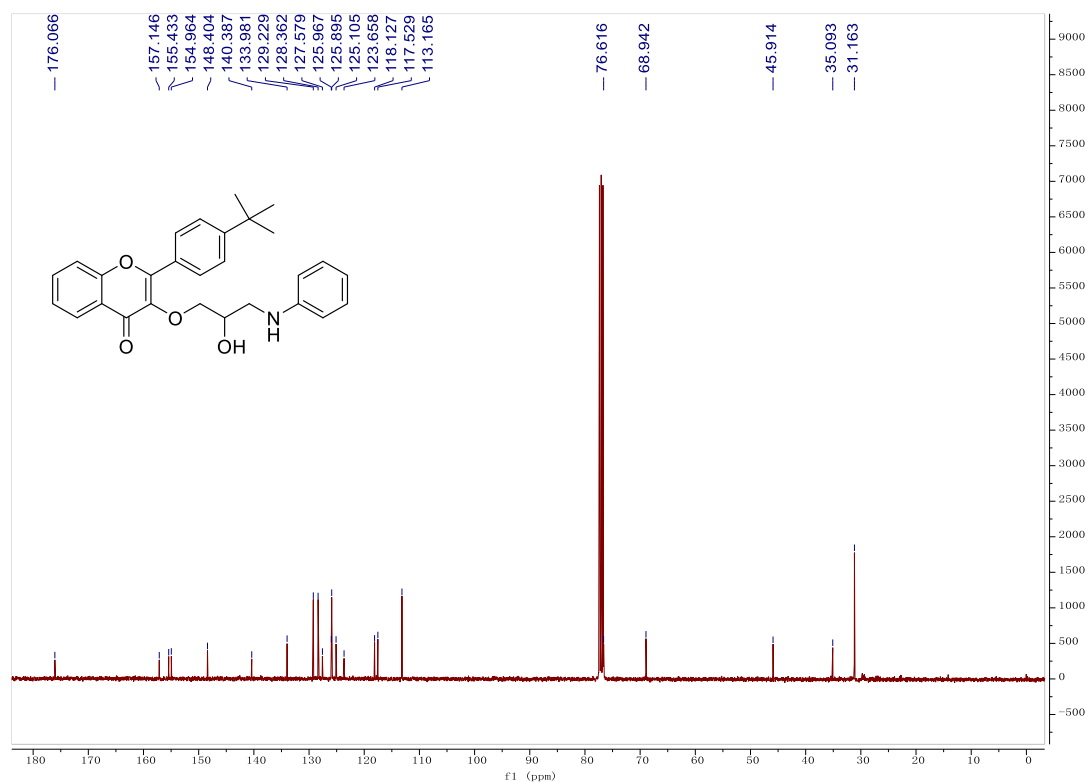


Fig. 23 ¹³C NMR spectrum of title compound Y8

48 #131 RT: 1.27 AV: 1 NL: 1.50E+006
T: FTMS + p ESI Full ms [100.0000-1300.0000]

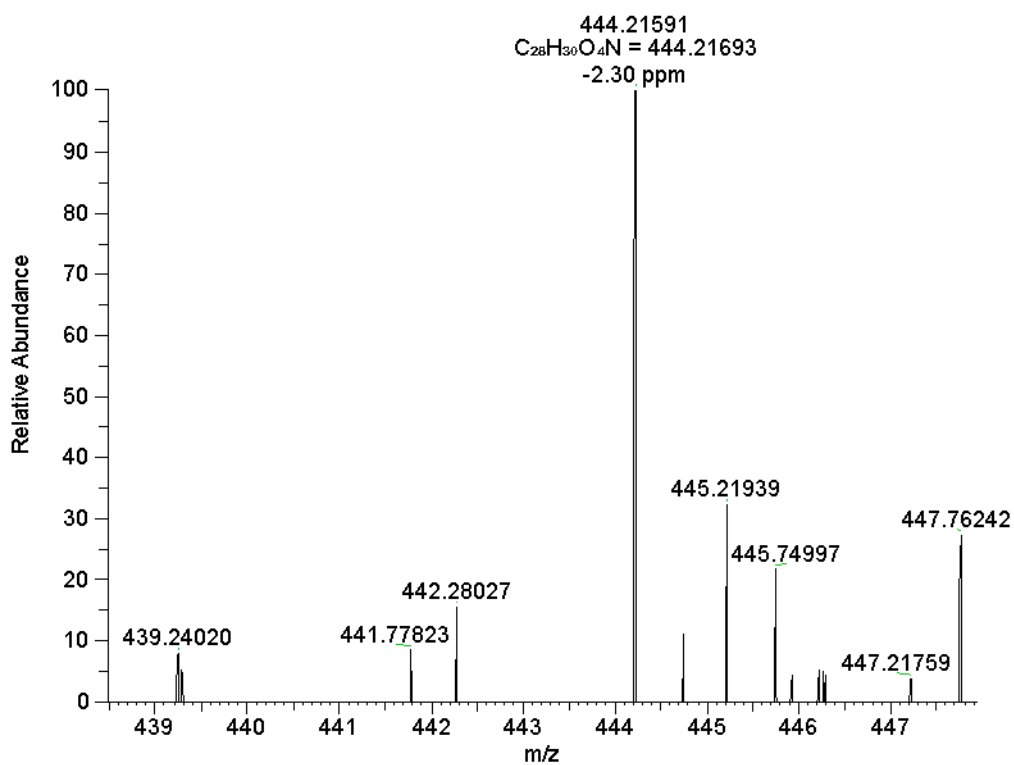


Fig. 24 HRMS spectrum of title compound Y8

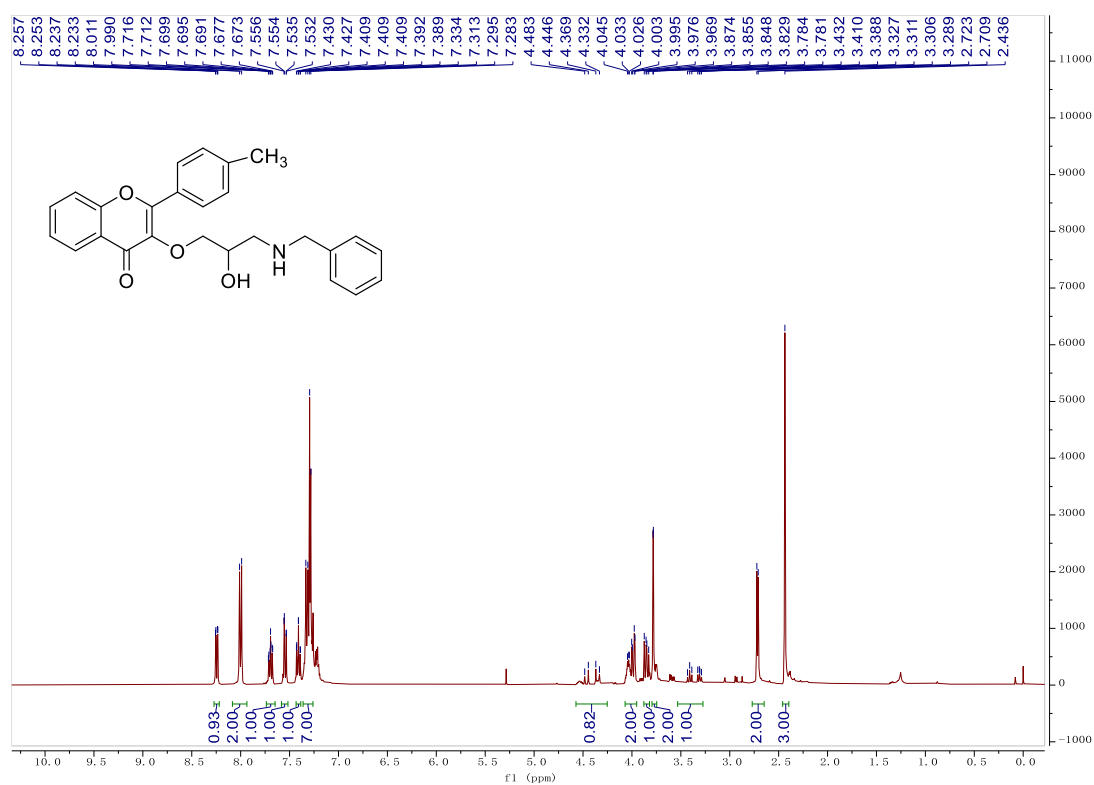


Fig. 25 ¹H NMR spectrum of title compound Y9

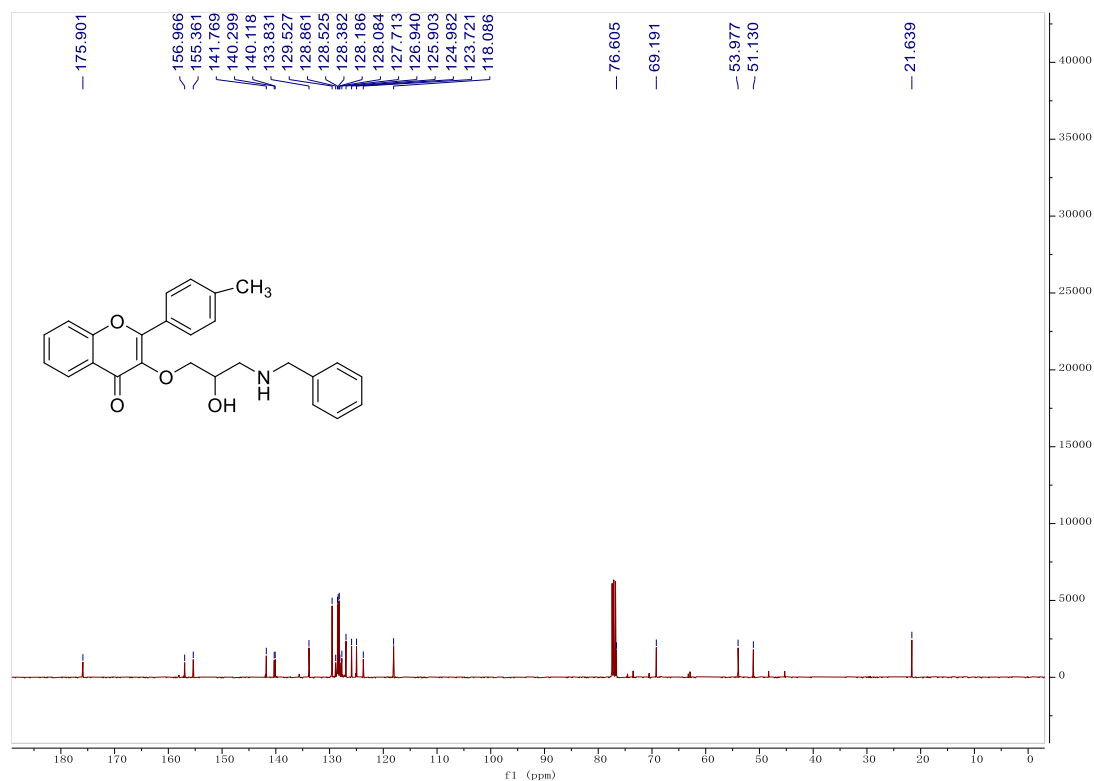


Fig. 26 ¹³C NMR spectrum of title compound Y9

49 #79 RT: 0.77 AV: 1 NL: 1.85E+009
T: FTMS + p ESI Full ms [100.0000-1300.0000]

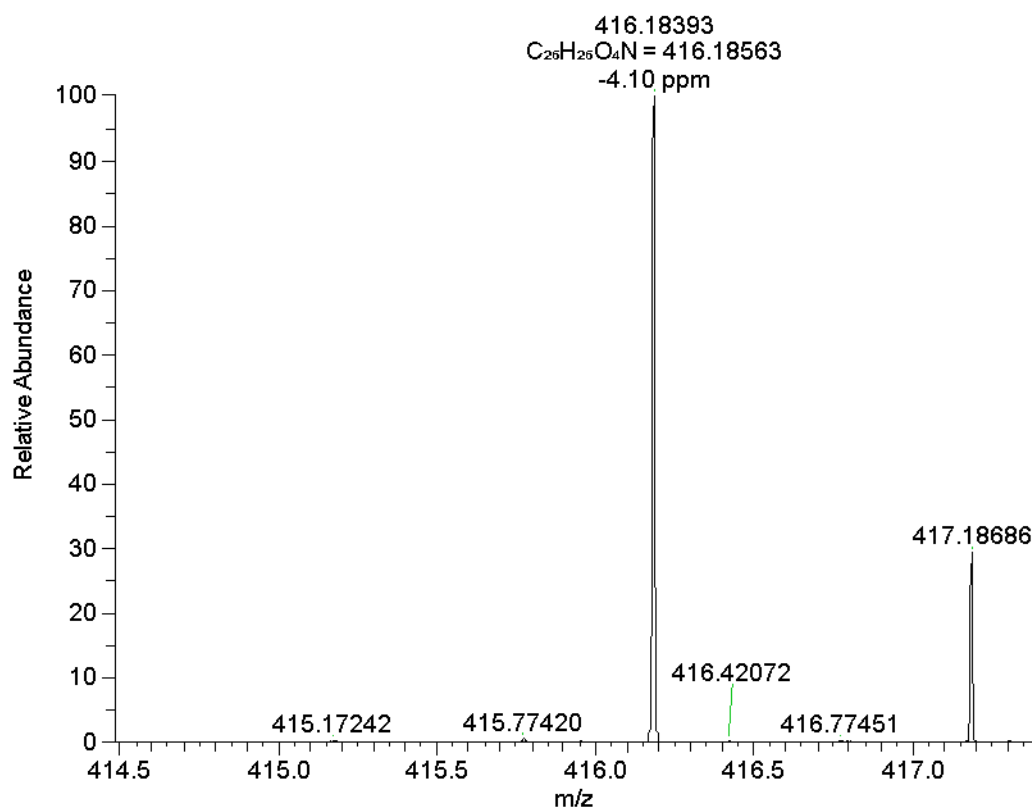


Fig. 27 HRMS spectrum of title compound Y9

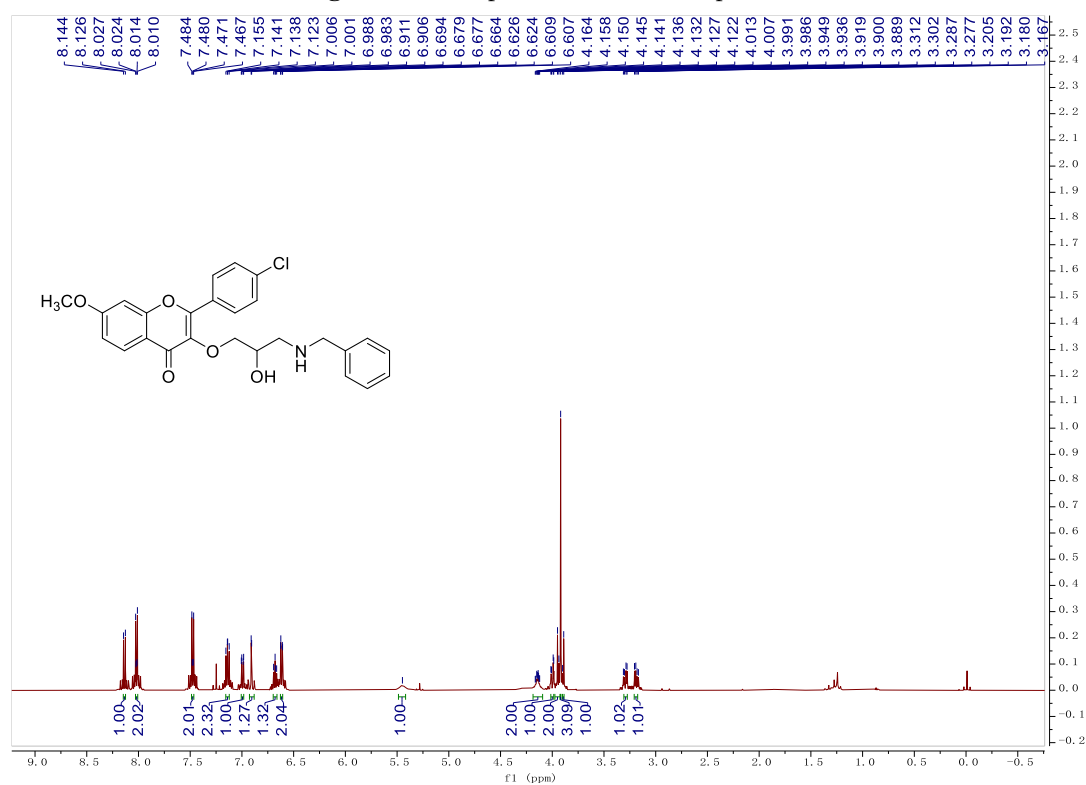


Fig. 28 1H NMR spectrum of title compound Y10

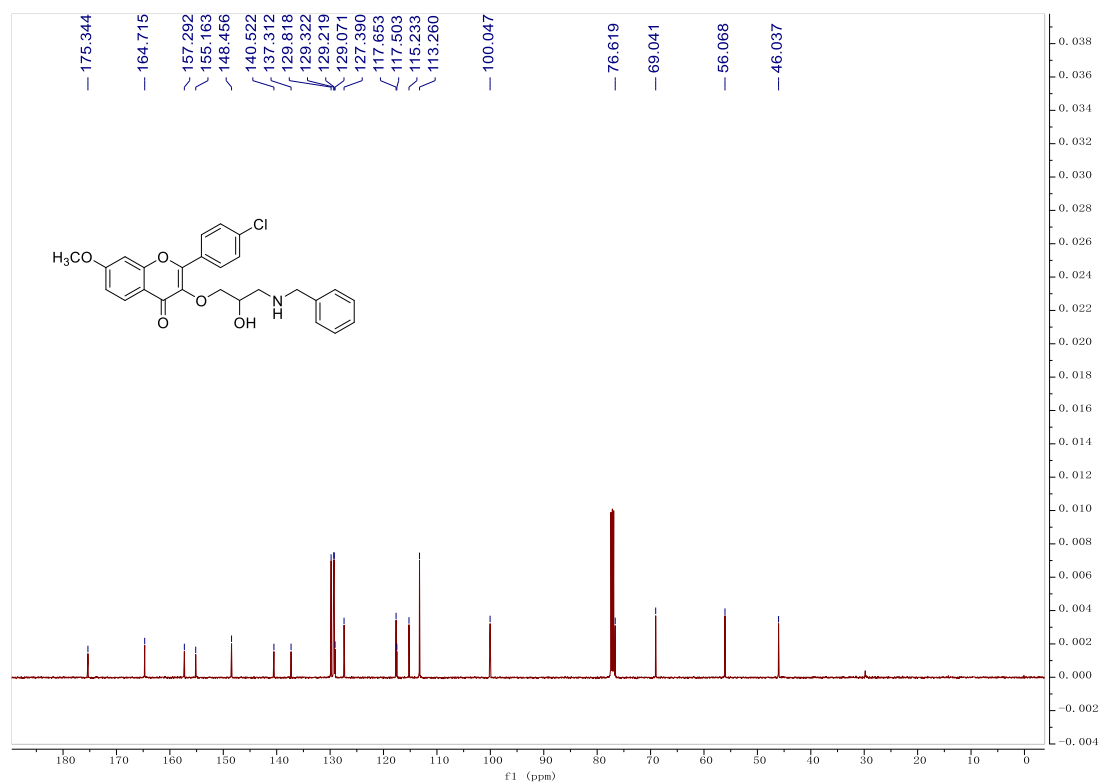


Fig. 29 ¹³C NMR spectrum of title compound Y10

50 #63 RT: 0.61 AV: 1 NL: 1.97E+005
T: FTMS + p ESI Full ms [100.0000-1300.0000]

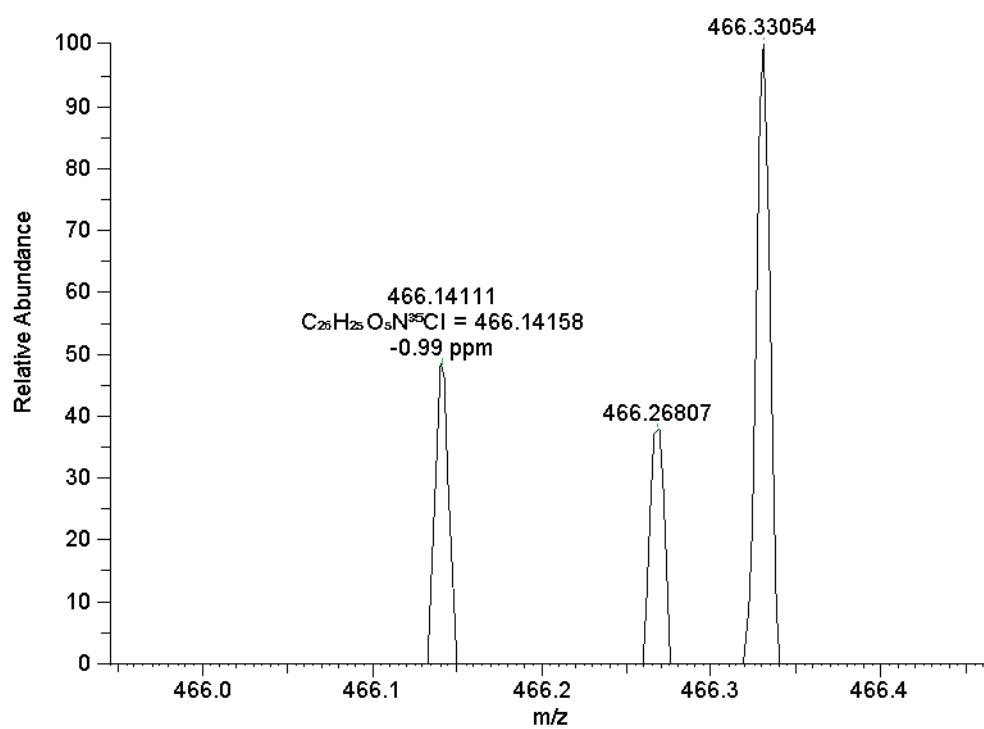


Fig. 30 HRMS spectrum of title compound Y10

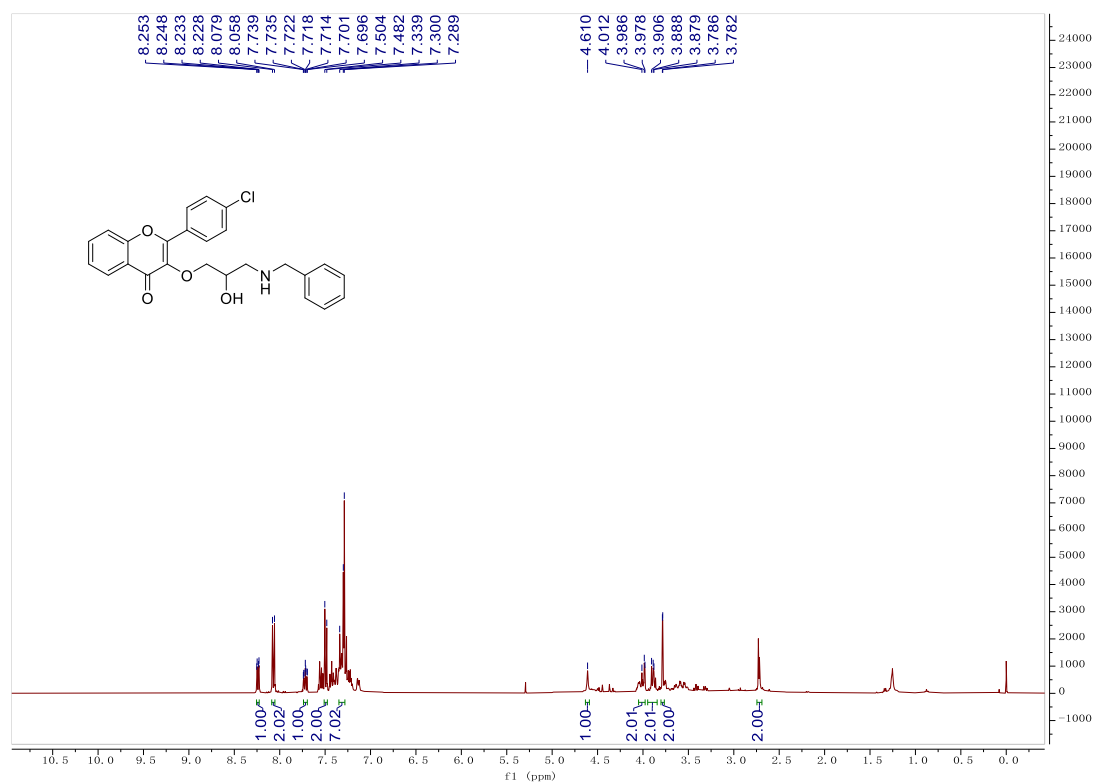


Fig. 31 ¹H NMR spectrum of title compound Y11

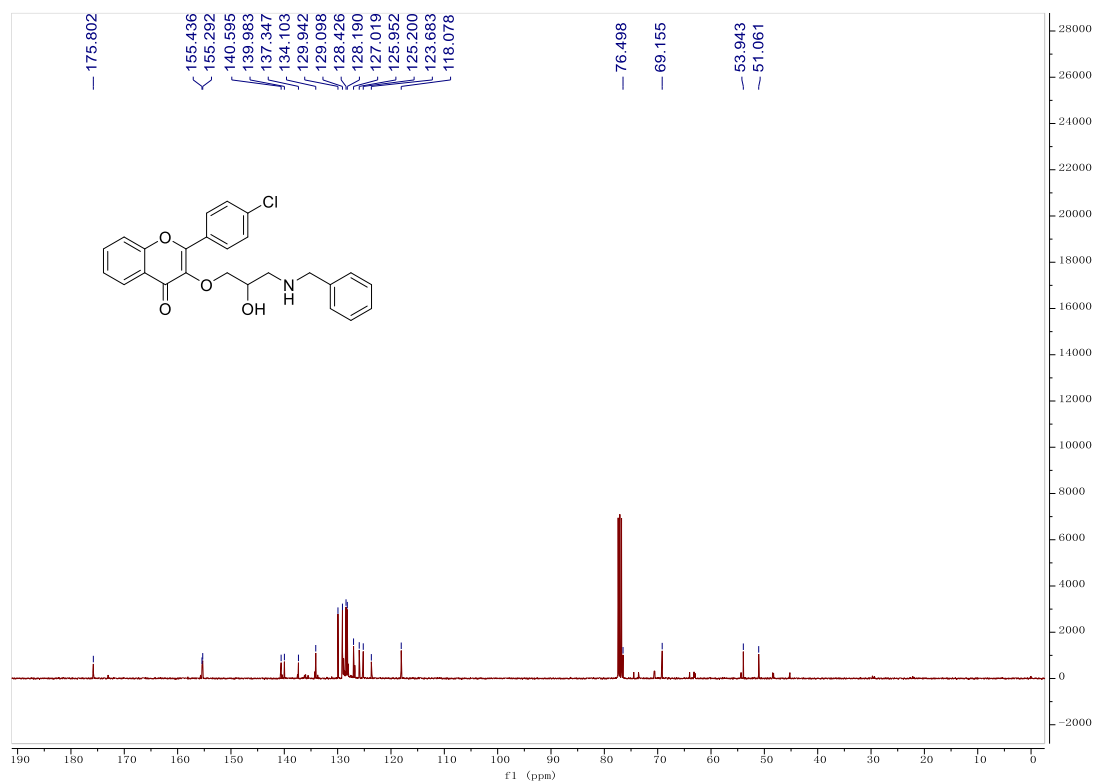


Fig. 32 ¹³C NMR spectrum of title compound Y11

51 #79 RT: 0.77 AV: 1 NL: 1.73E+006
T: FTMS + p ESI Full ms [100.0000-1300.0000]

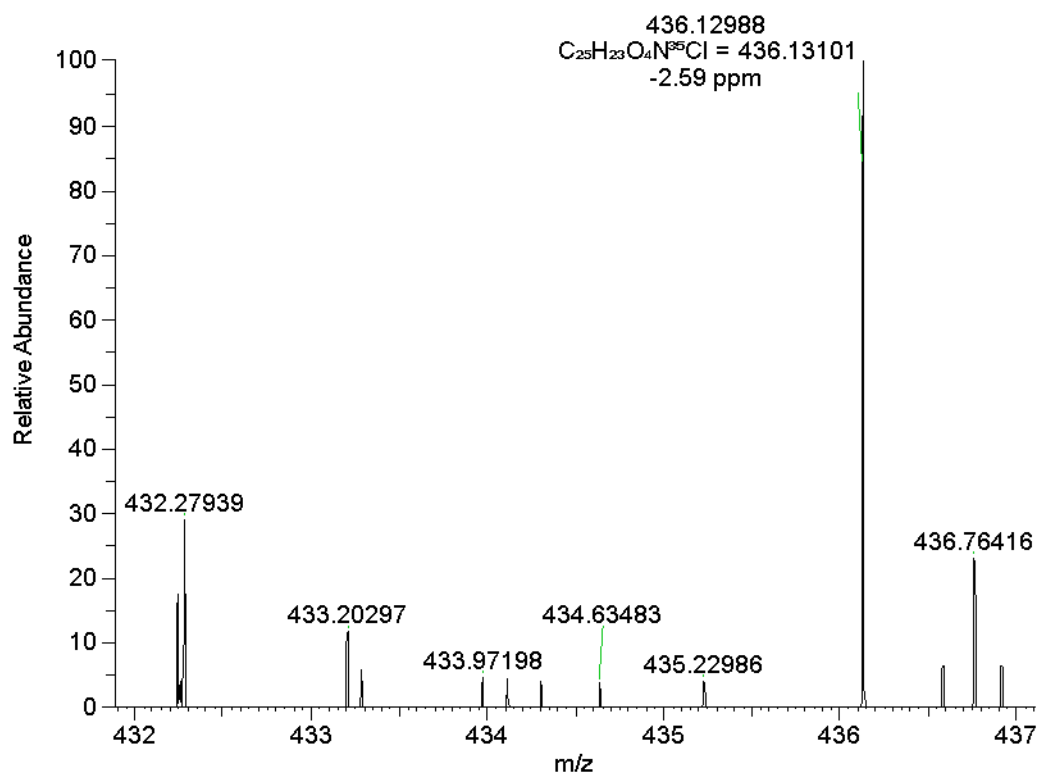


Fig. 33 HRMS spectrum of title compound Y11

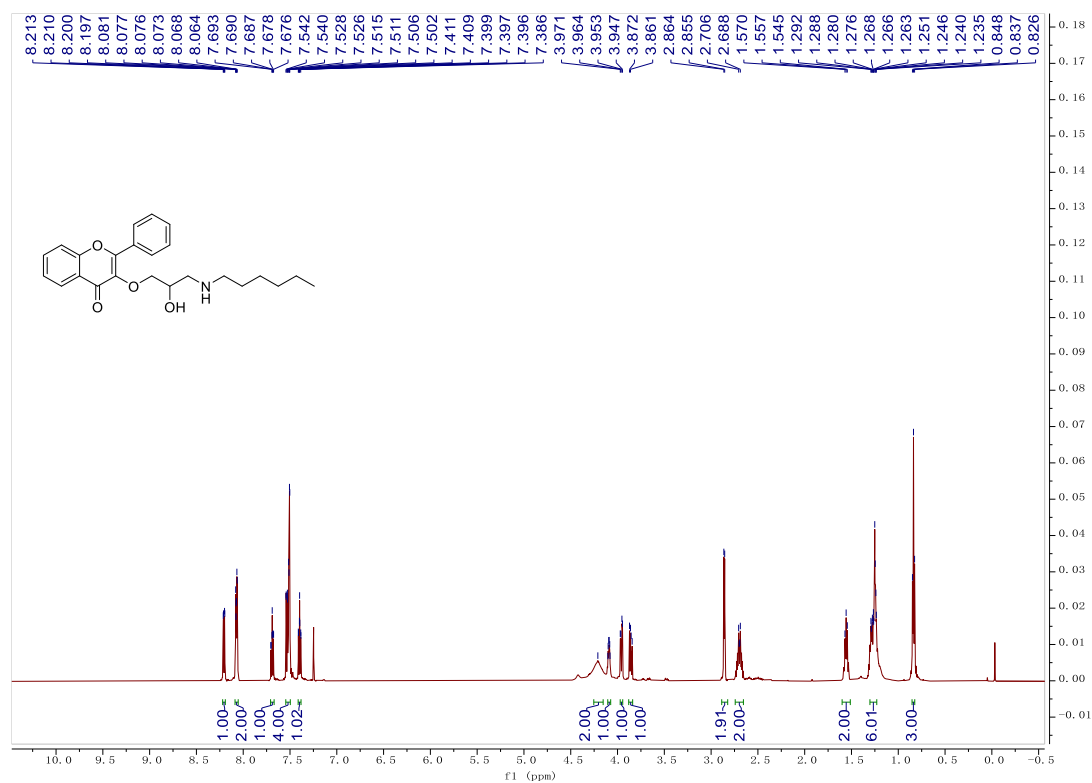


Fig. 34 1H NMR spectrum of title compound Y12

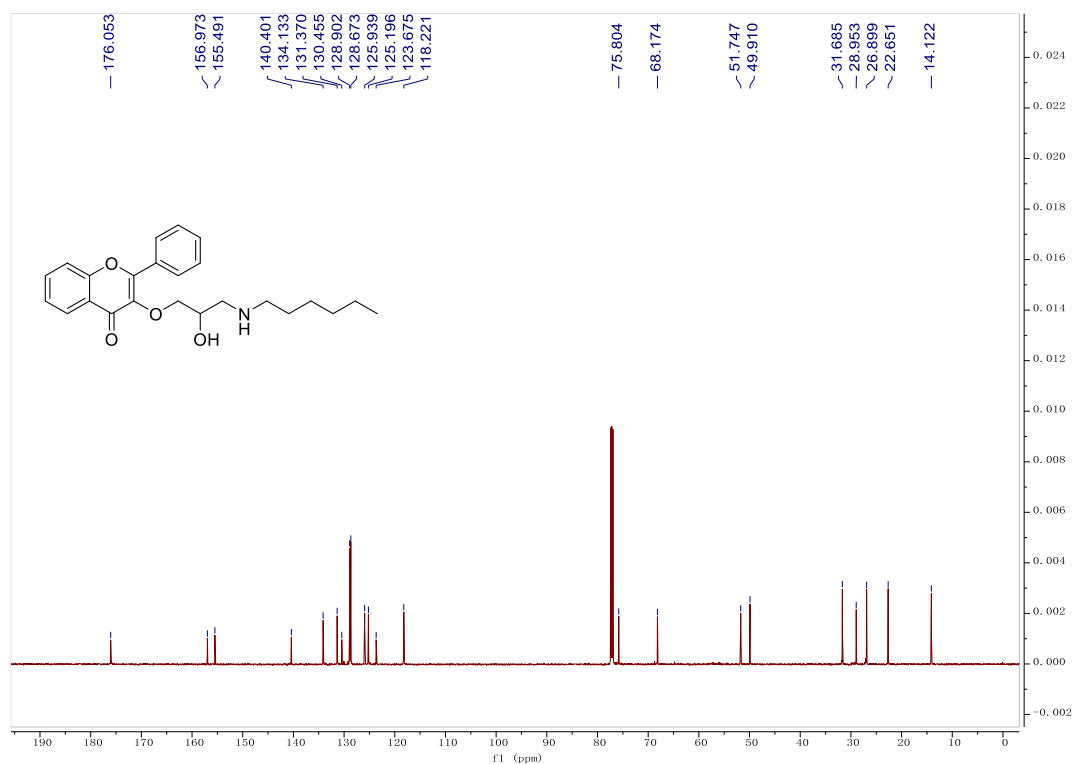


Fig. 35 ¹³C NMR spectrum of title compound Y12

52 #97 RT: 0.93 AV: 1 NL: 9.03E+008

T: FTMS + p ESI Full ms [100.0000-1300.0000]

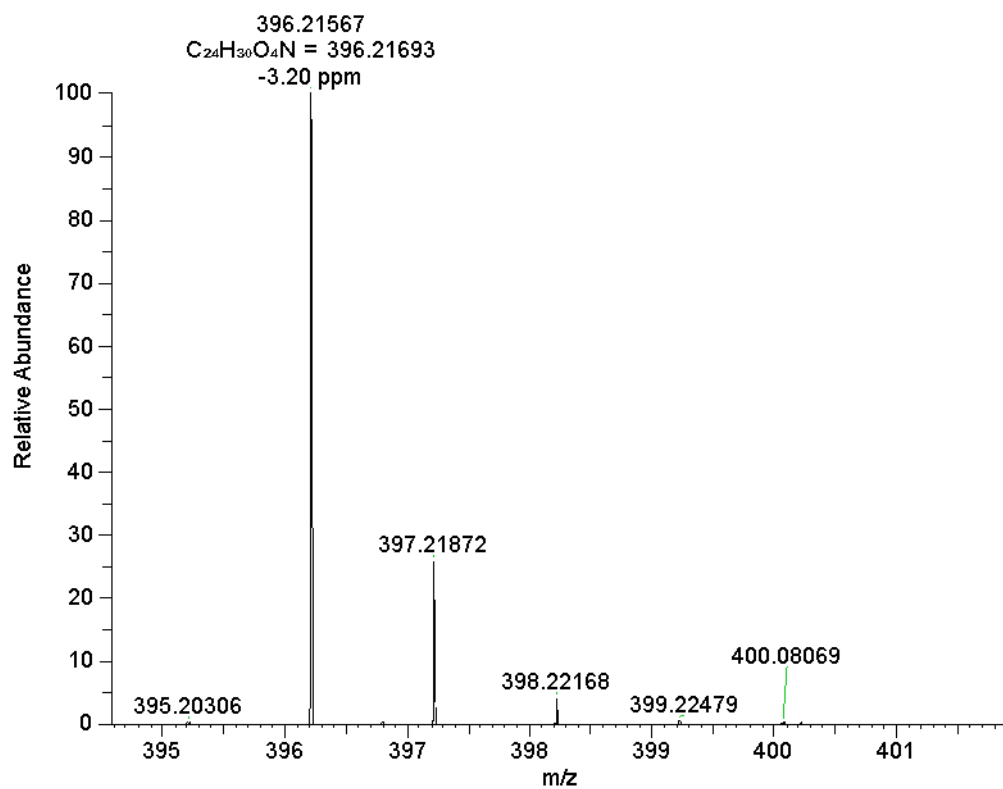


Fig. 36 HRMS spectrum of title compound Y12

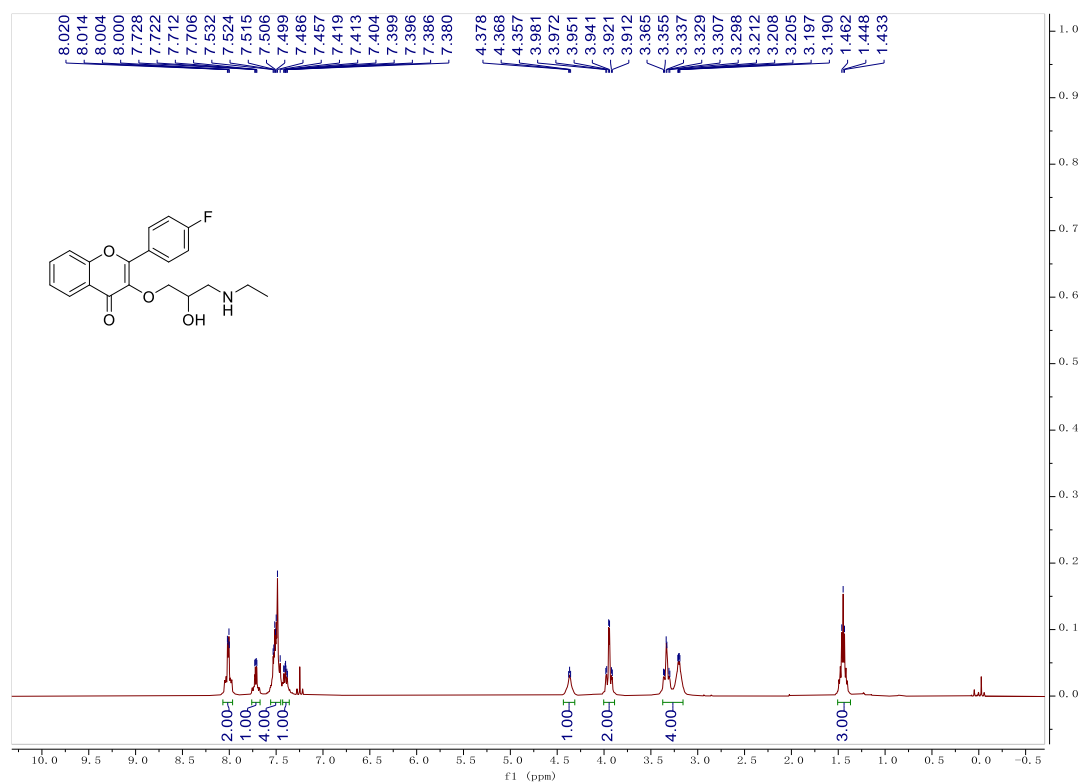


Fig. 37 ¹H NMR spectrum of title compound Y13

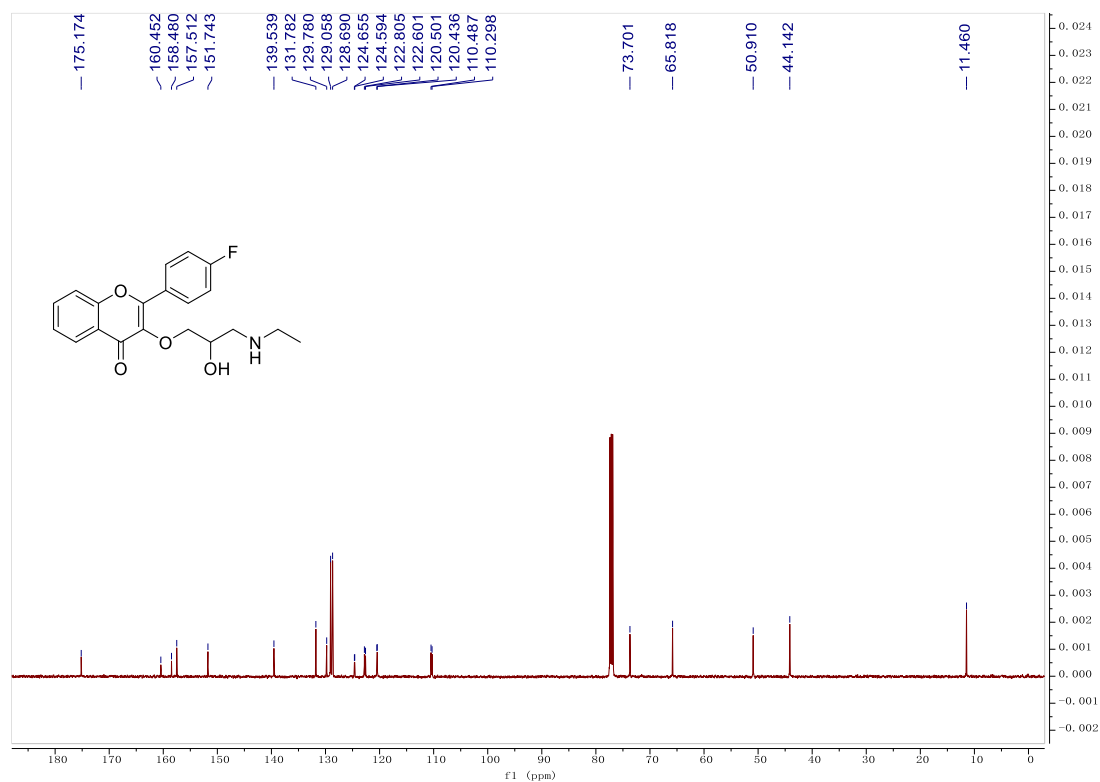


Fig. 38 ¹³C NMR spectrum of title compound Y13

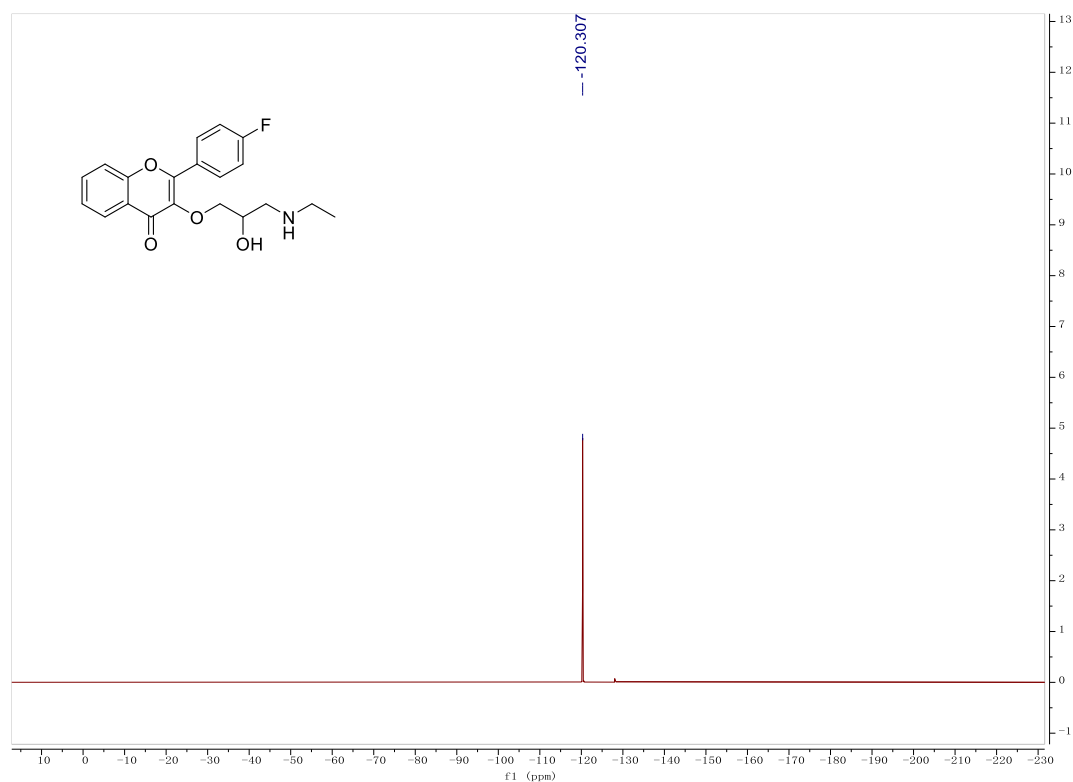


Fig. 39 ¹⁹F NMR spectrum of title compound Y13

64 #73 RT: 0.71 AV: 1 NL: 2.66E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

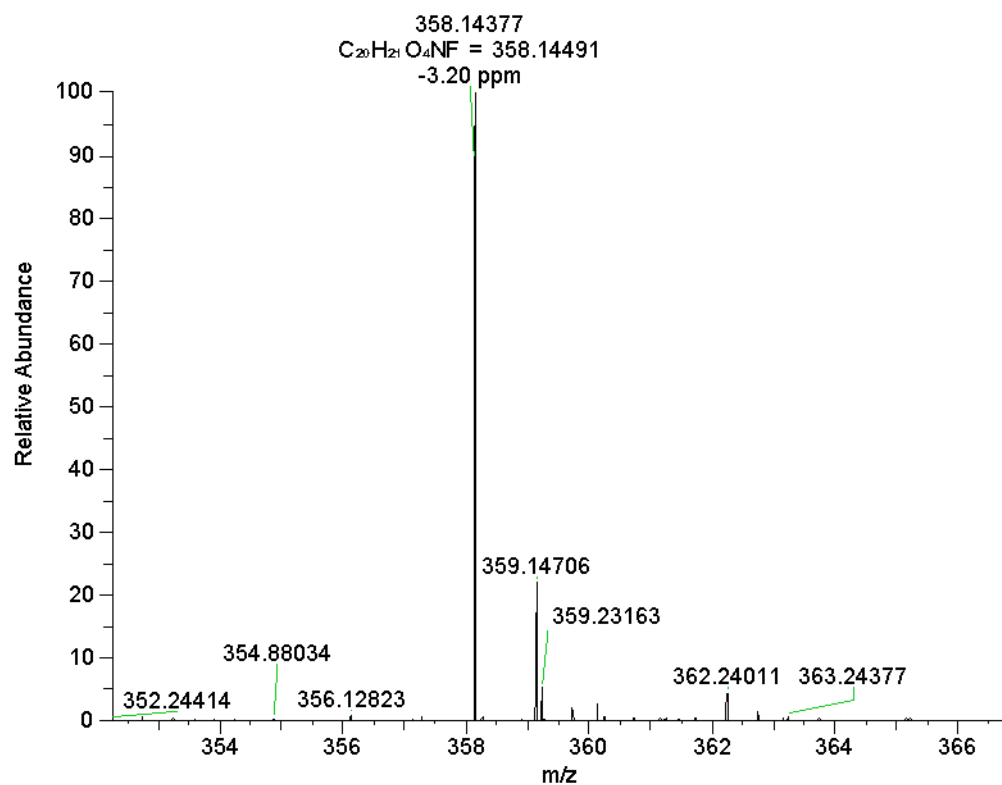


Fig. 40 HRMS spectrum of title compound Y13

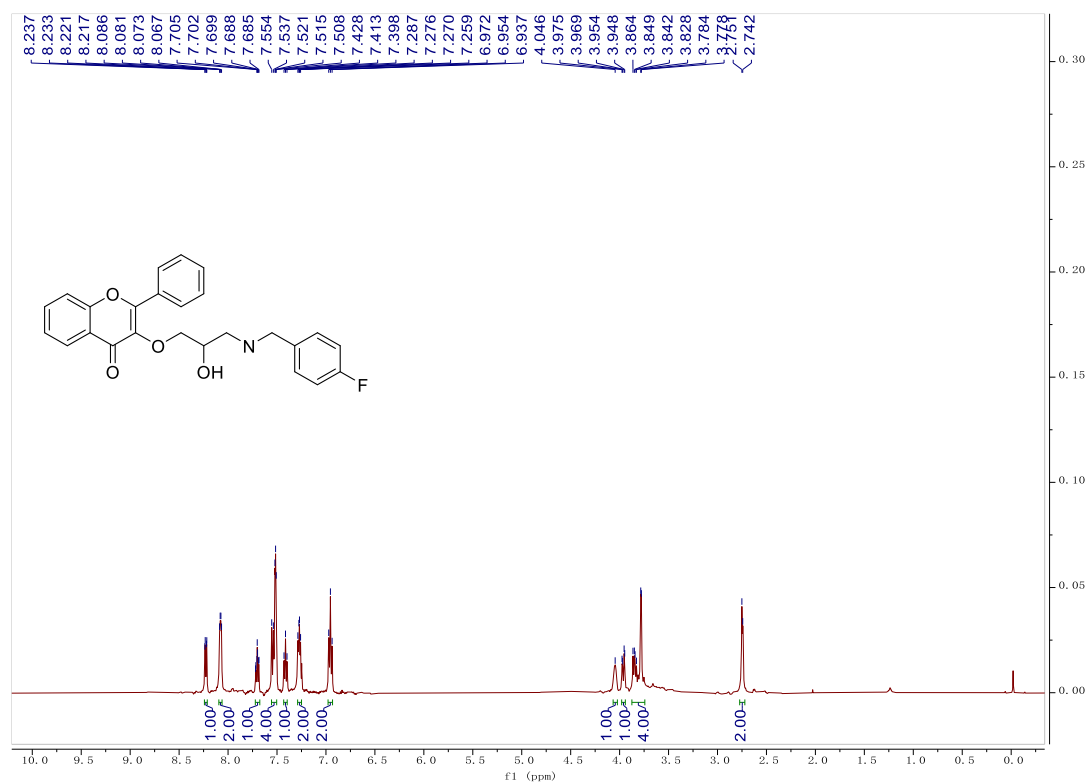


Fig. 41 ¹H NMR spectrum of title compound Y14

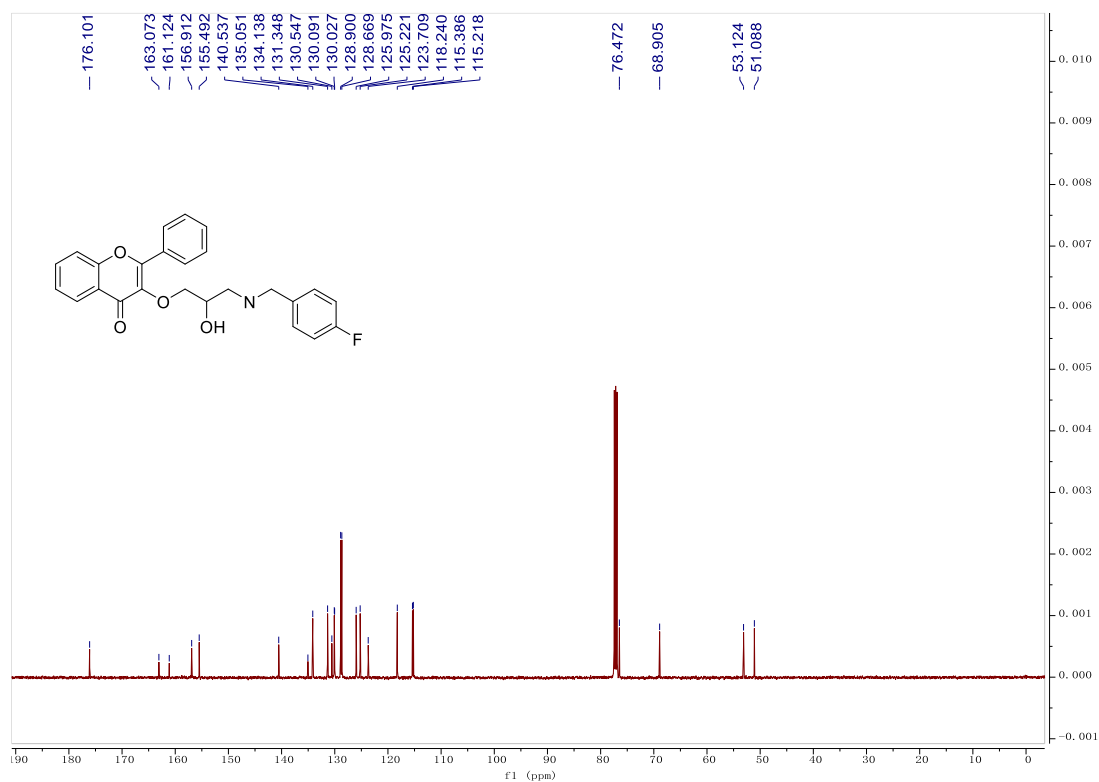


Fig. 42 ¹³C NMR spectrum of title compound Y14

54 #71 RT: 0.69 AV: 1 NL: 1.09E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

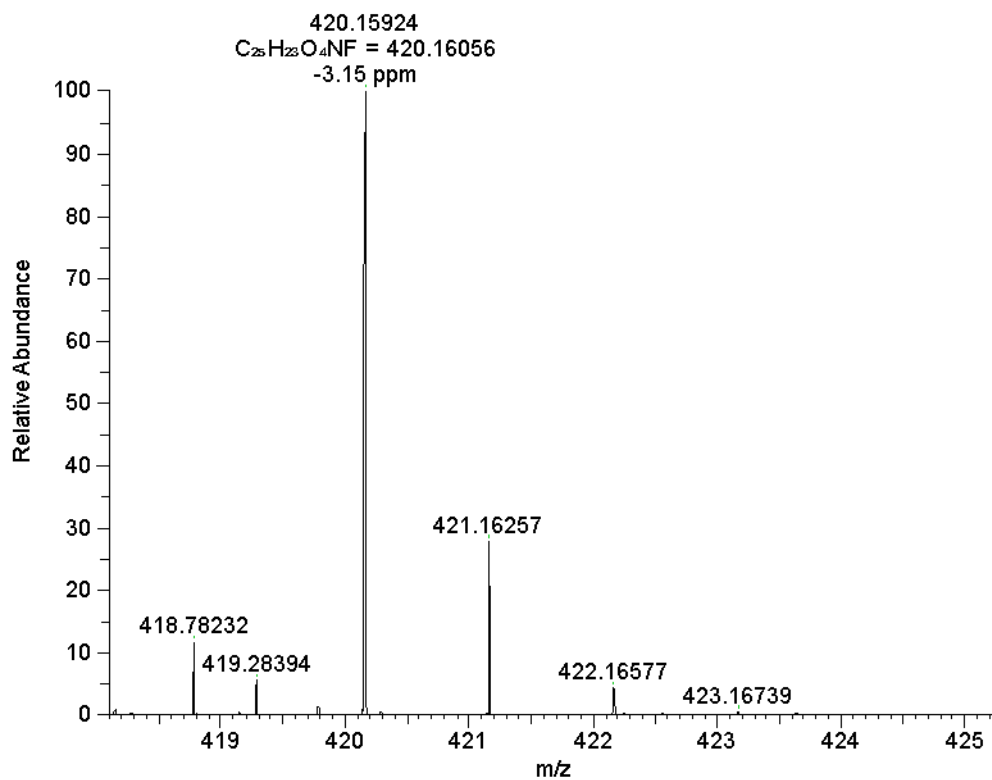


Fig. 43 HRMS spectrum of title compound Y14

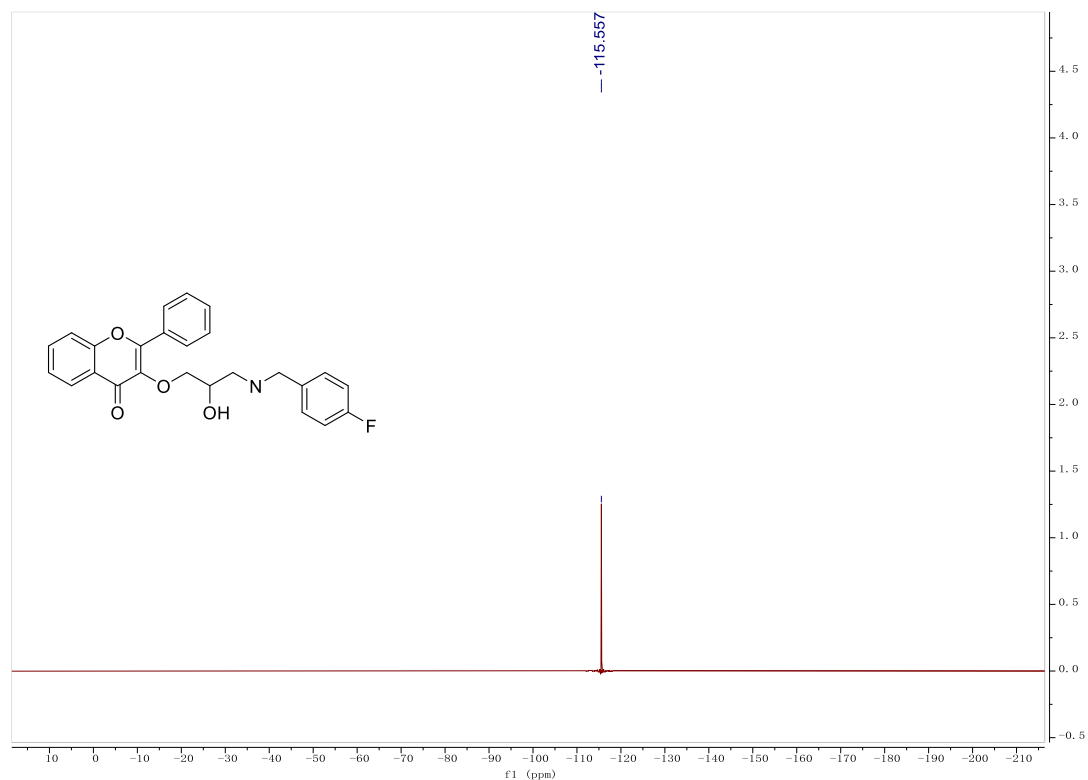


Fig. 44 ^{19}F NMR spectrum of title compound Y14

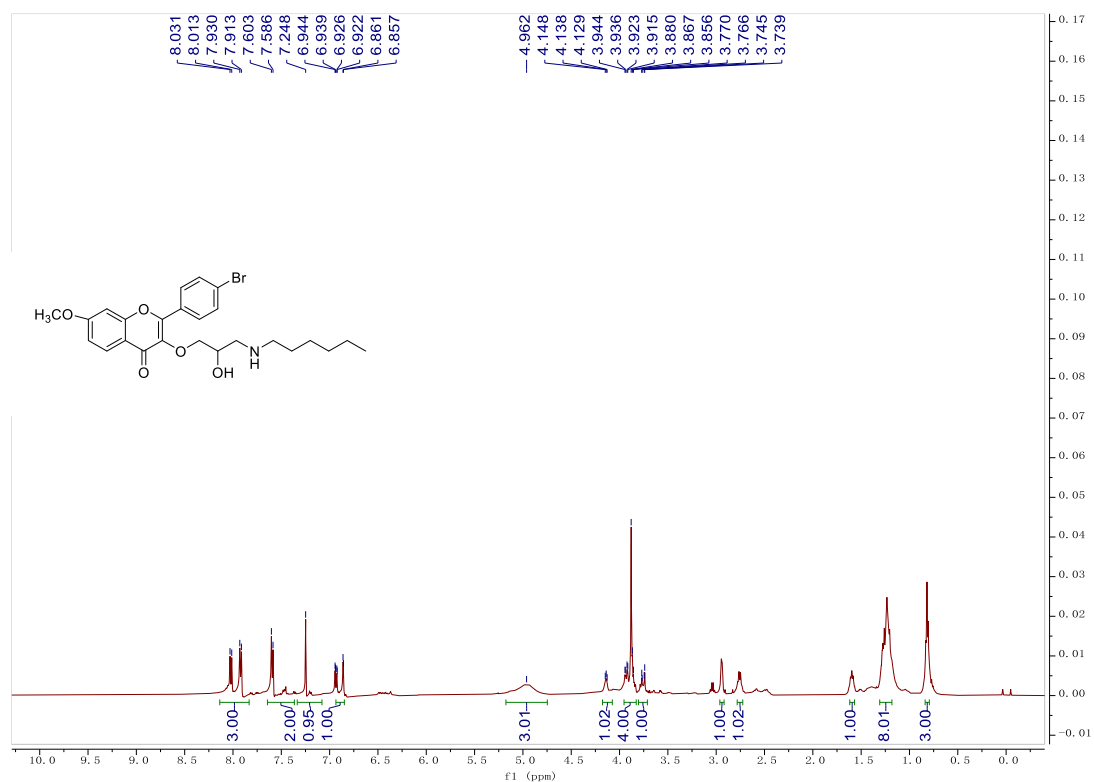


Fig. 45 ¹H NMR spectrum of title compound Y15

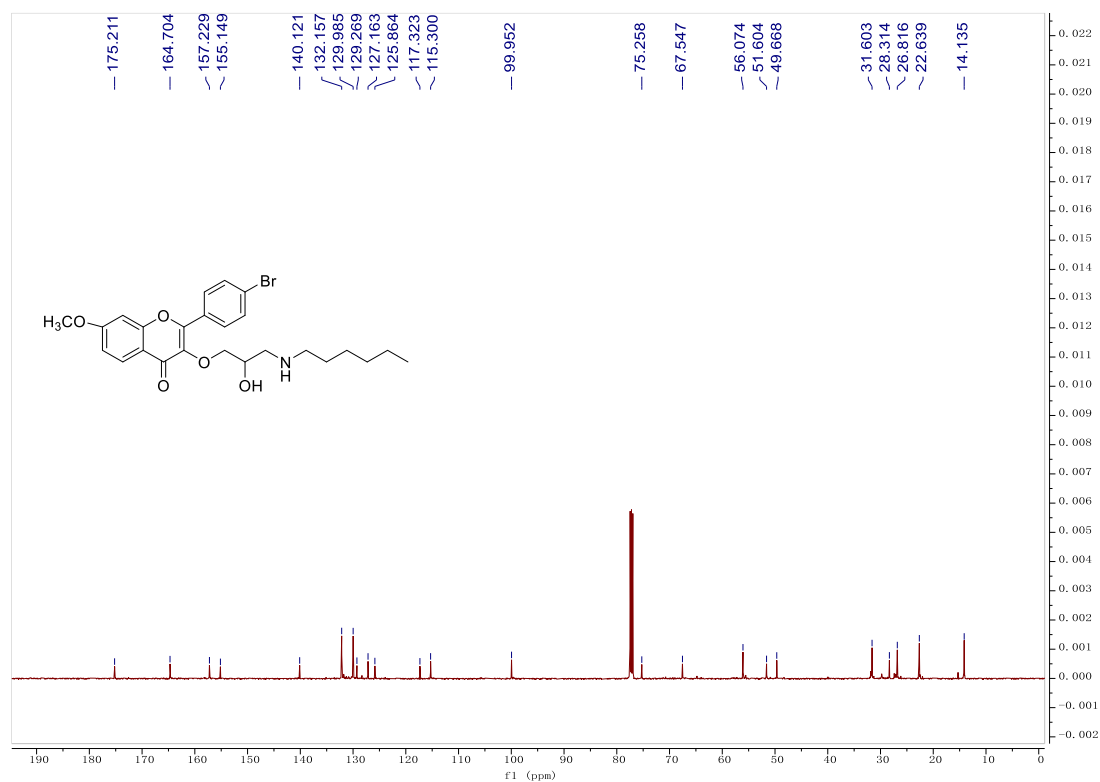


Fig. 46 ¹³C NMR spectrum of title compound Y15

55 #139 RT: 1.34 AV: 1 NL: 1.83E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

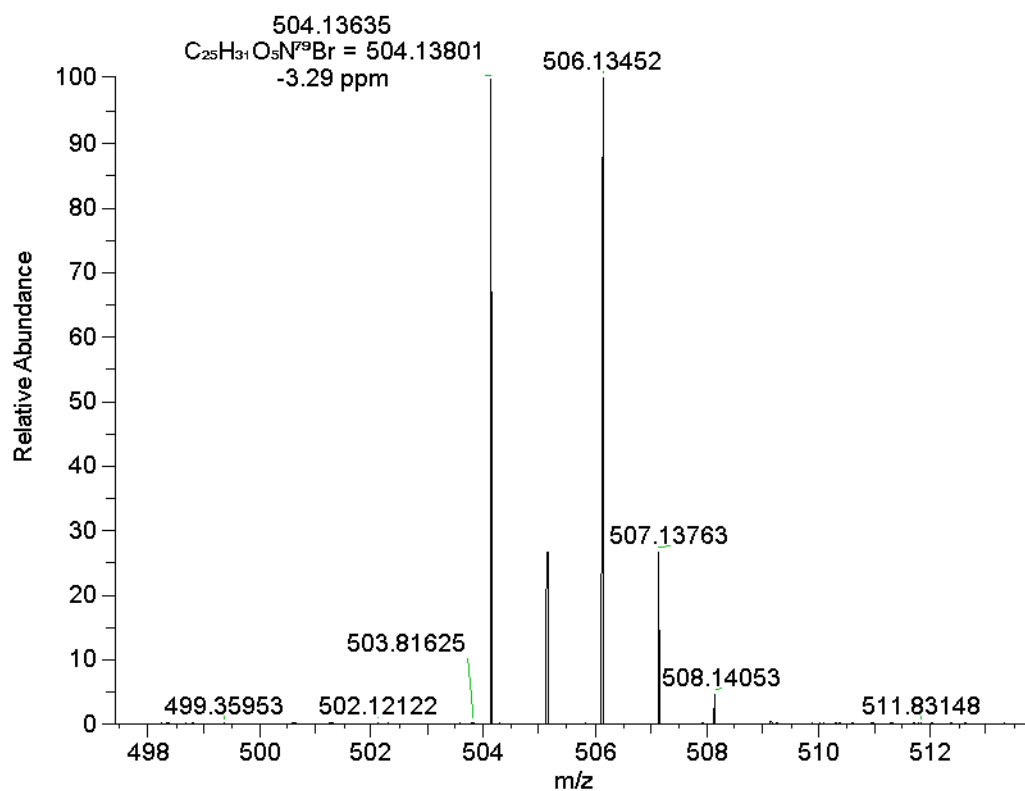


Fig. 47 HRMS spectrum of title compound Y15

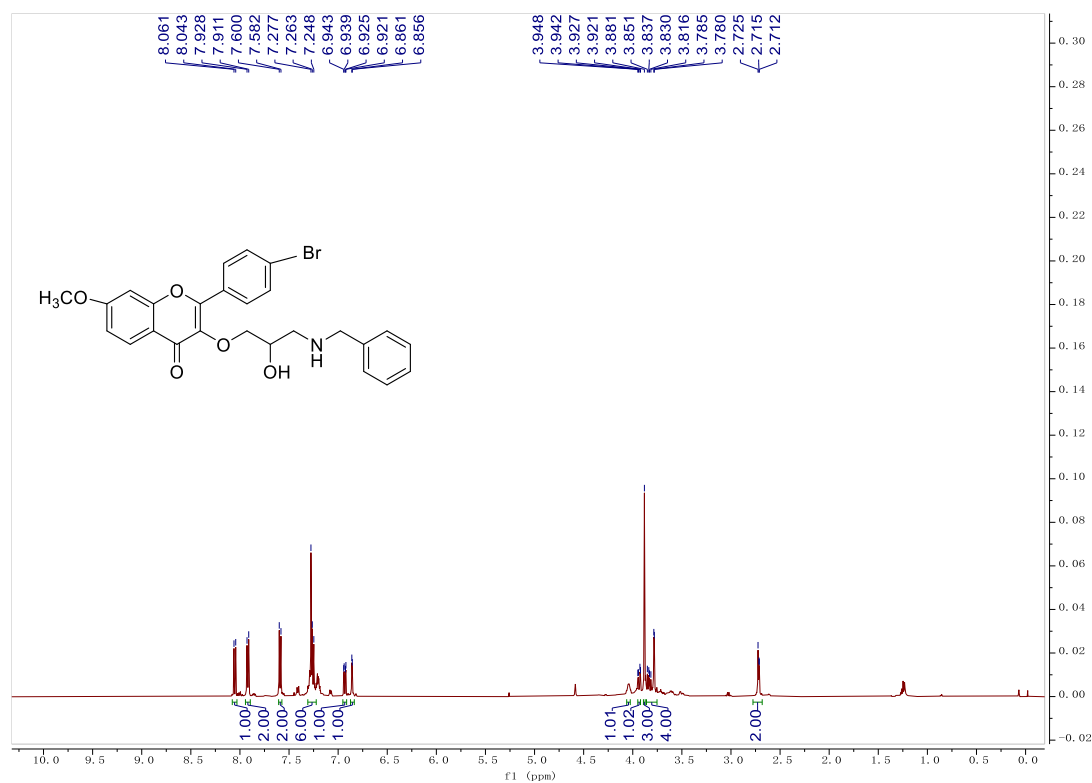


Fig. 48 ¹H NMR spectrum of title compound Y16

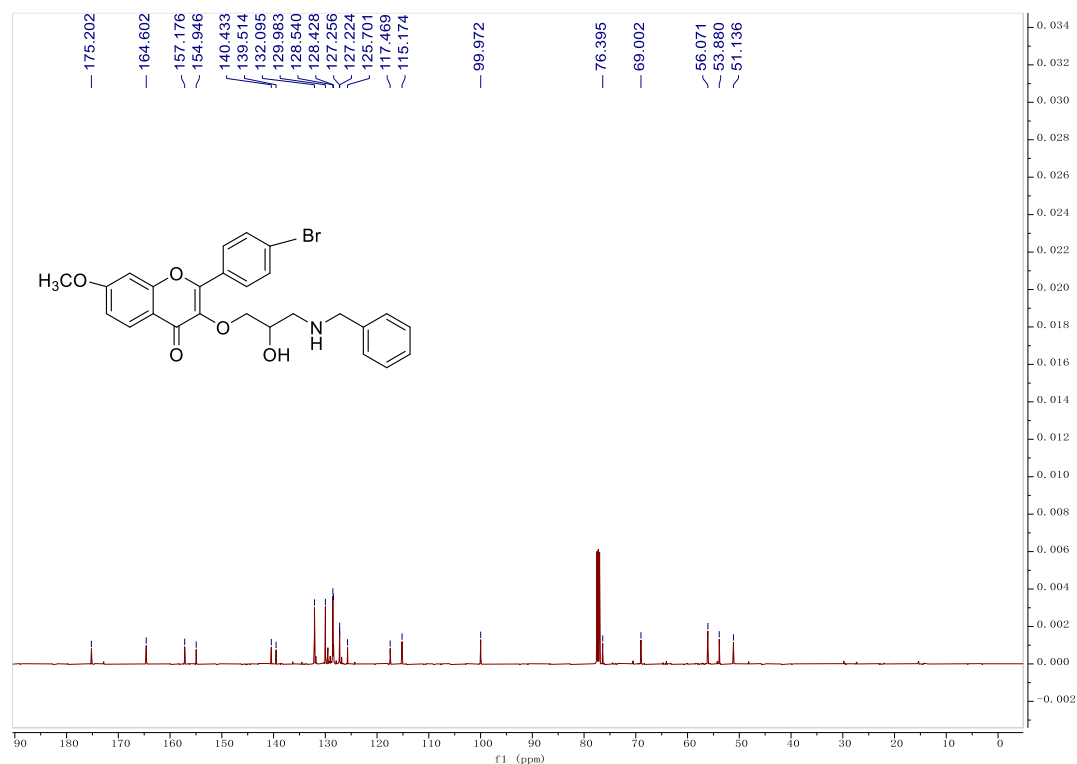


Fig. 49 ¹³C NMR spectrum of title compound Y16

56 #95 RT: 0.92 AV: 1 NL: 7.92E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

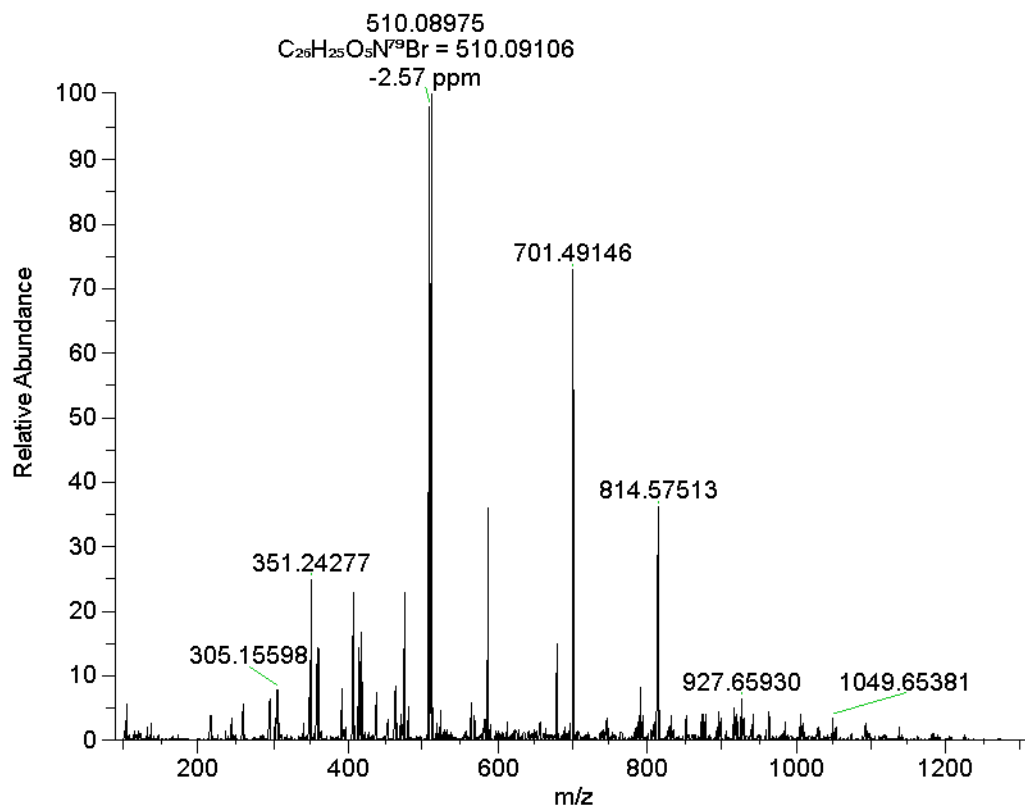


Fig. 50 HRMS spectrum of title compound Y16

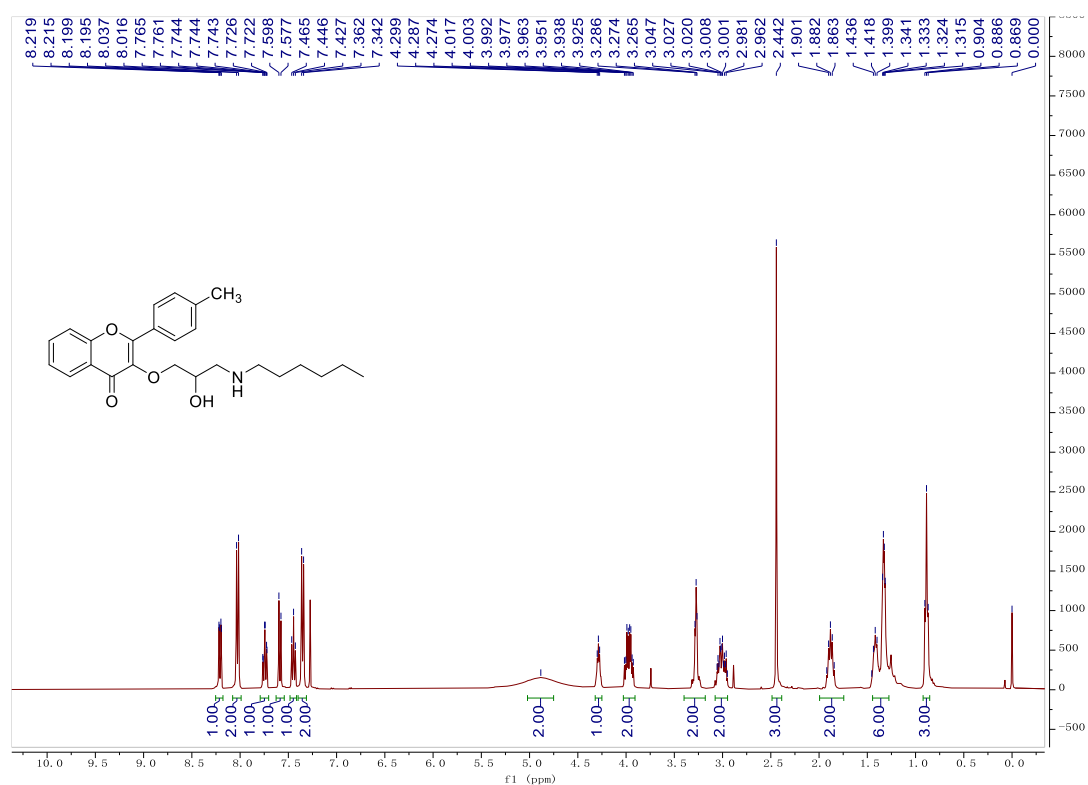


Fig. S1 ¹H NMR spectrum of title compound Y17

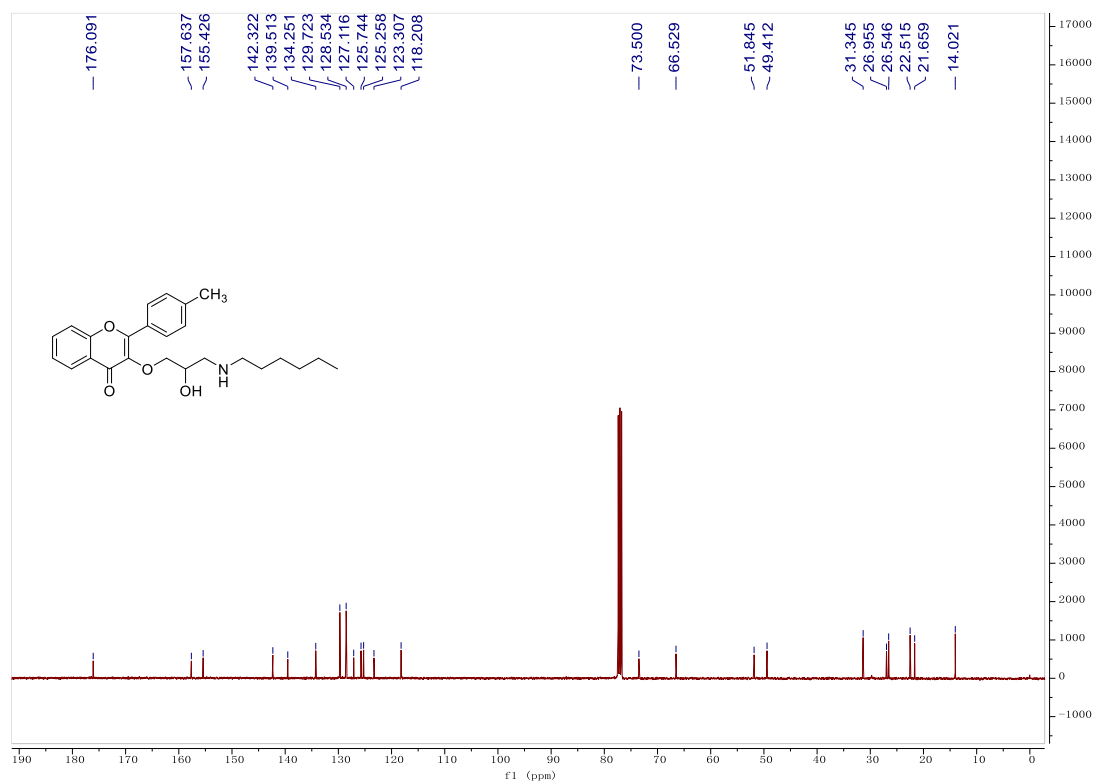


Fig. S2 ¹³C NMR spectrum of title compound Y17

57 #107 RT: 1.04 AV: 1 NL: 4.61E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

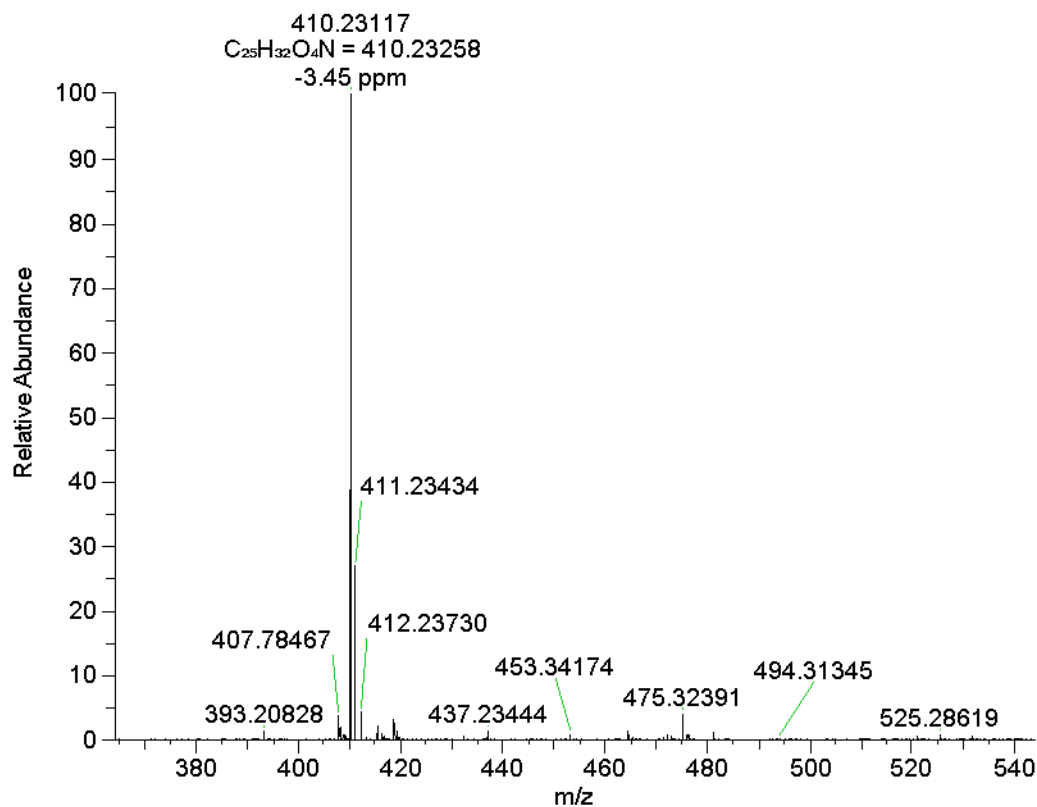


Fig. 53 HRMS spectrum of title compound Y17

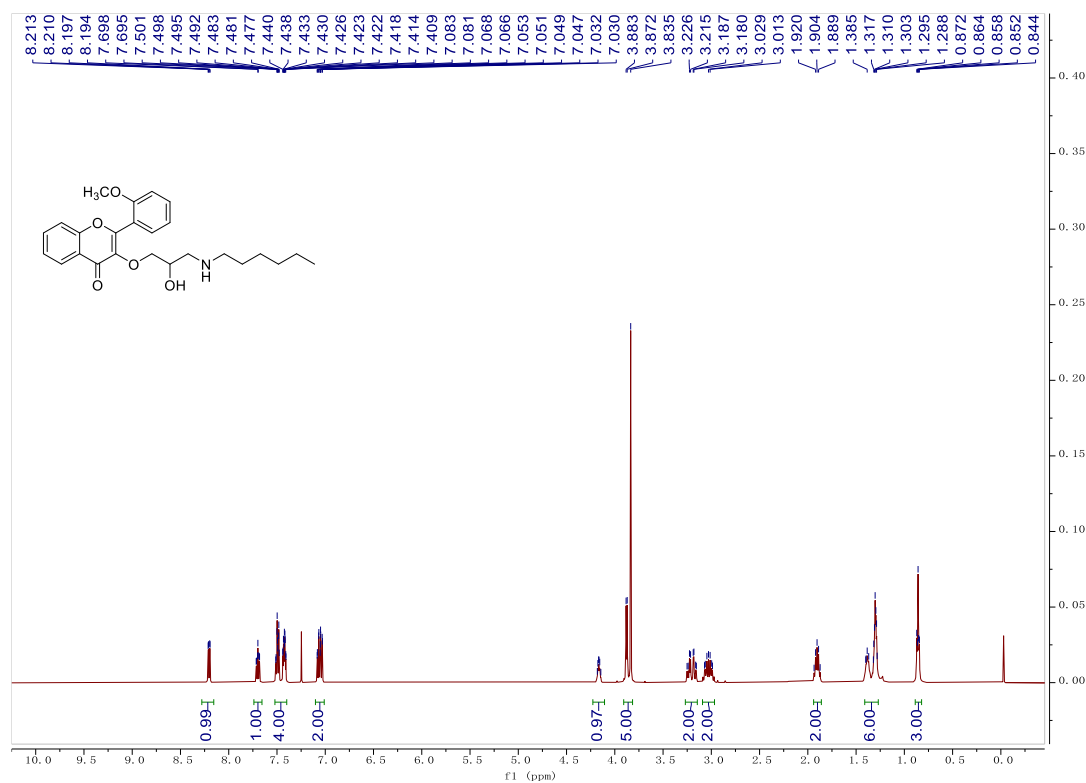


Fig. 54 1H NMR spectrum of title compound Y18

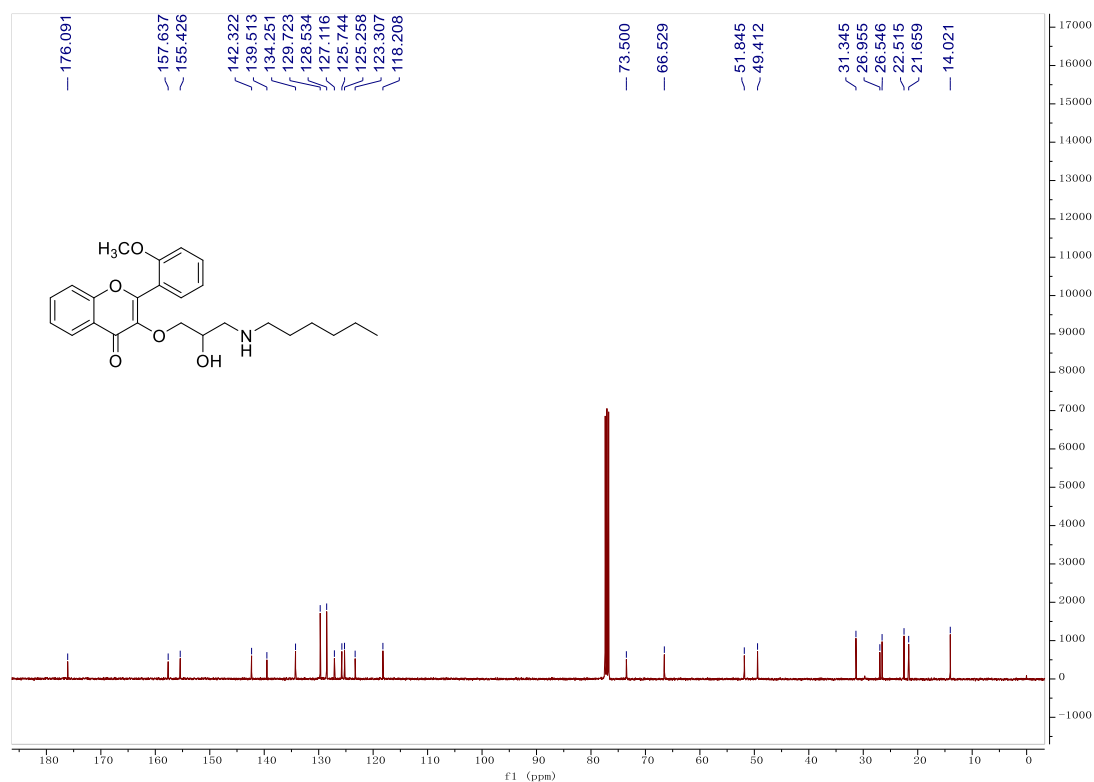


Fig. 55 ¹³C NMR spectrum of title compound Y18

58 #87 RT: 0.85 AV: 1 NL: 4.35E+008

T: FTMS + p ESI Full ms [100.0000-1300.0000]

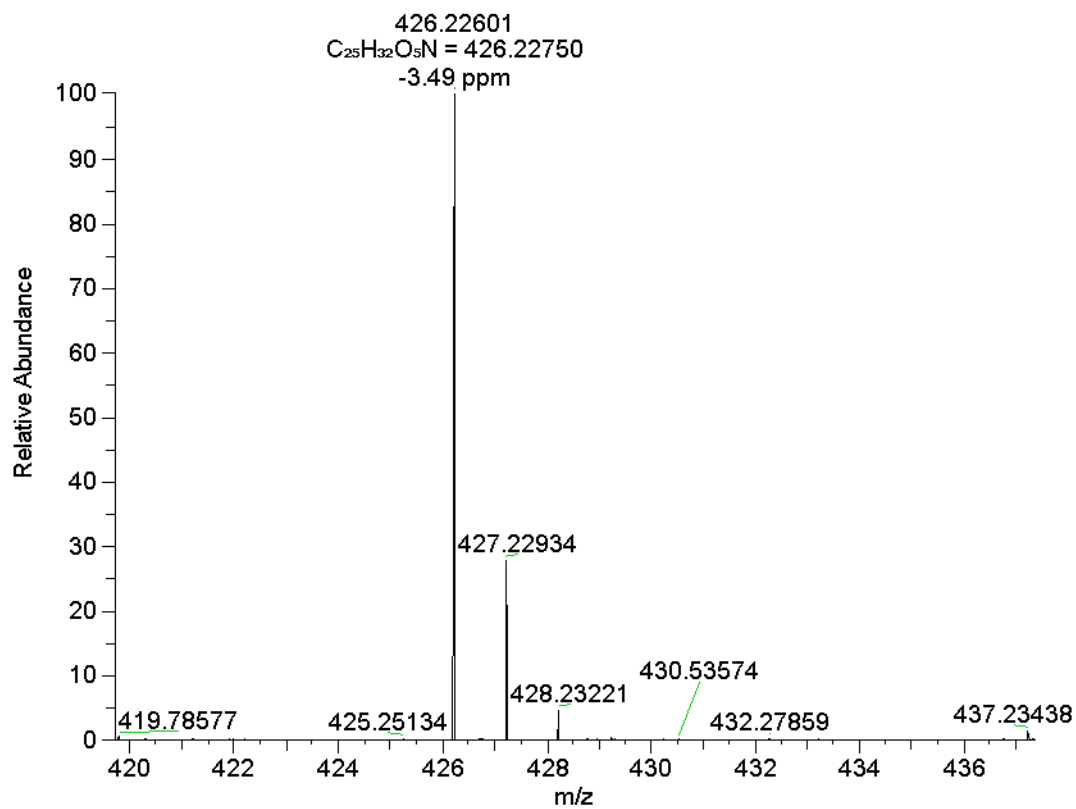


Fig. 56 HRMS spectrum of title compound Y18

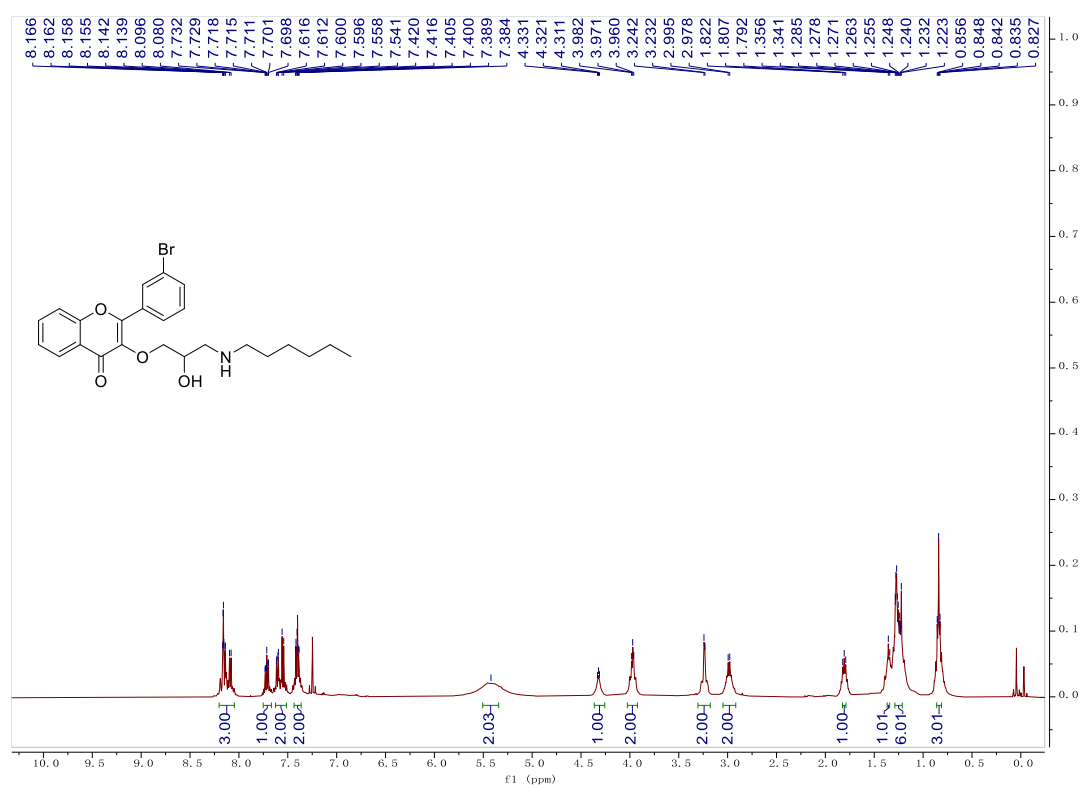


Fig. 57 ¹H NMR spectrum of title compound **Y19**

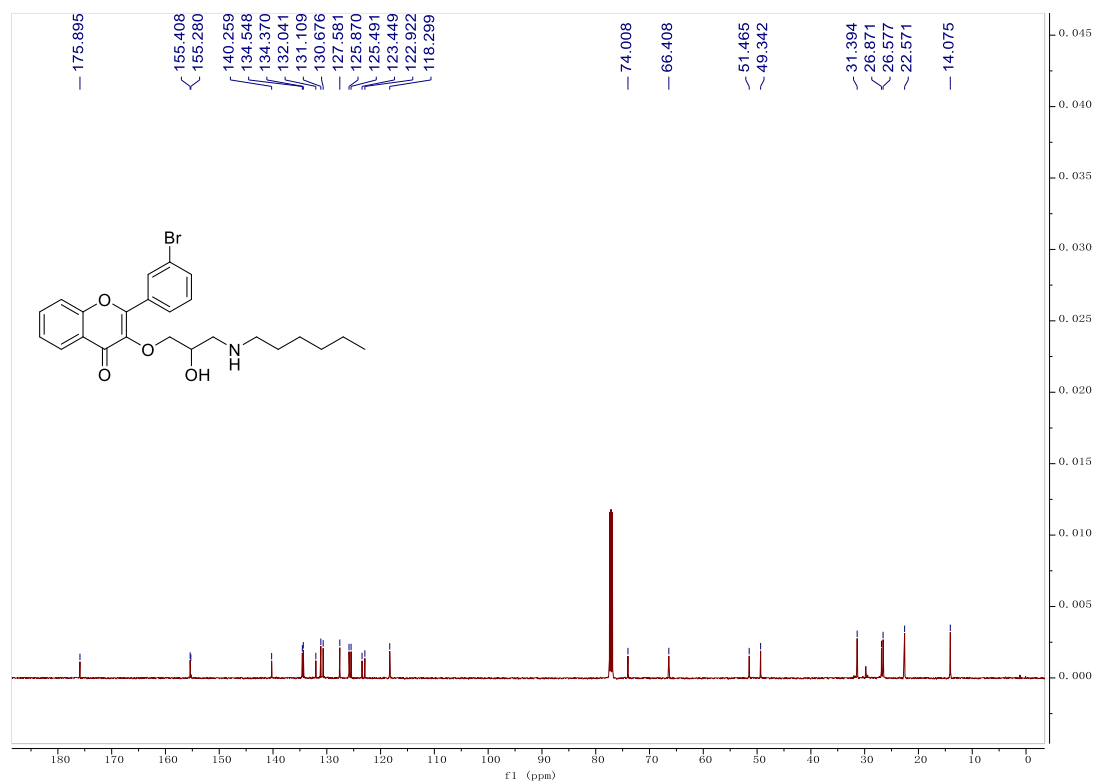


Fig. 58 ¹³C NMR spectrum of title compound **Y19**

59 #119 RT: 1.15 AV: 1 NL: 1.40E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

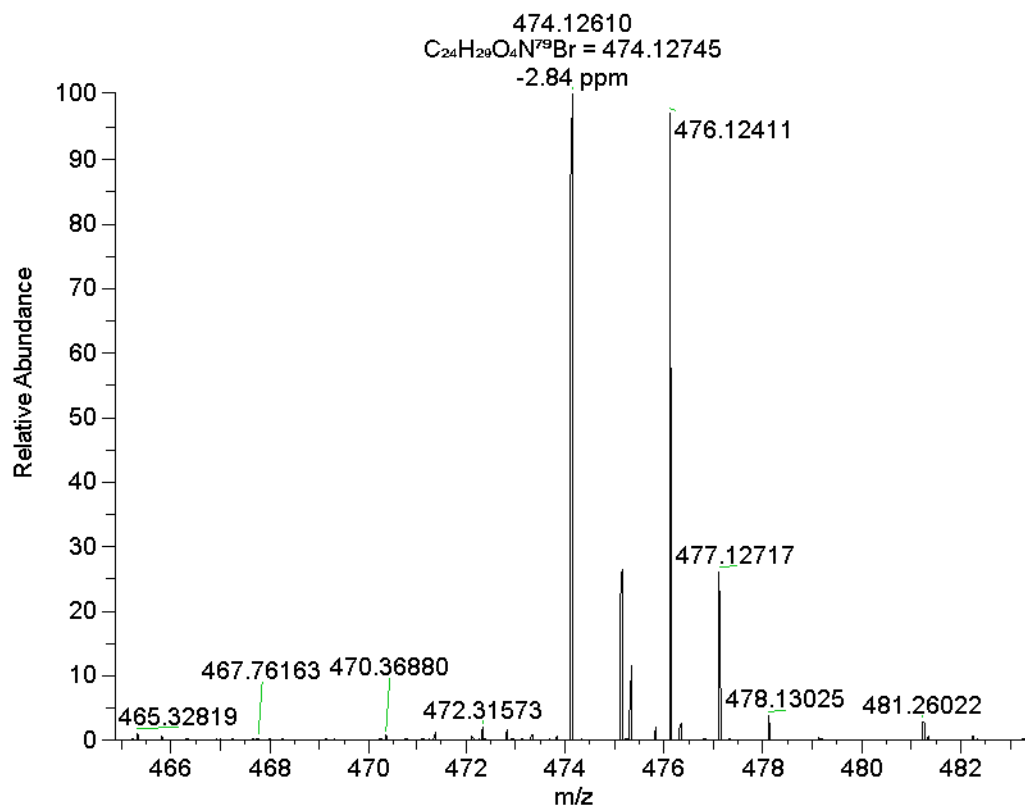


Fig. 59 HRMS spectrum of title compound Y19

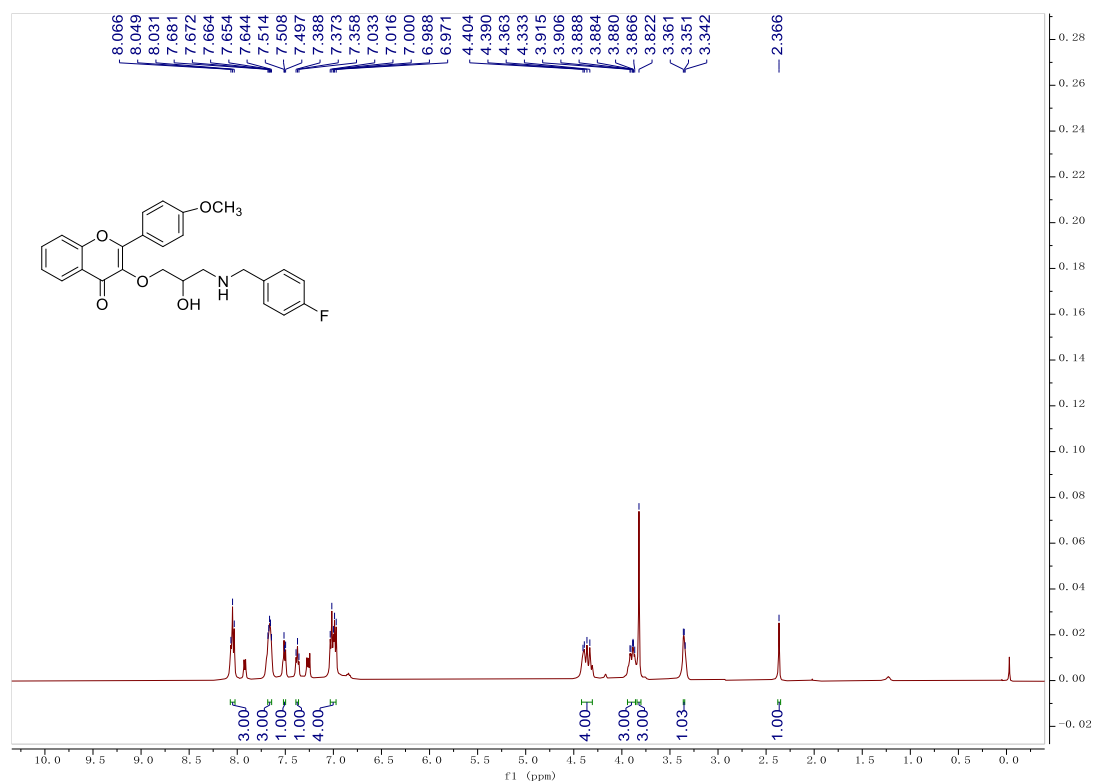


Fig. 60 ¹H NMR spectrum of title compound Y20

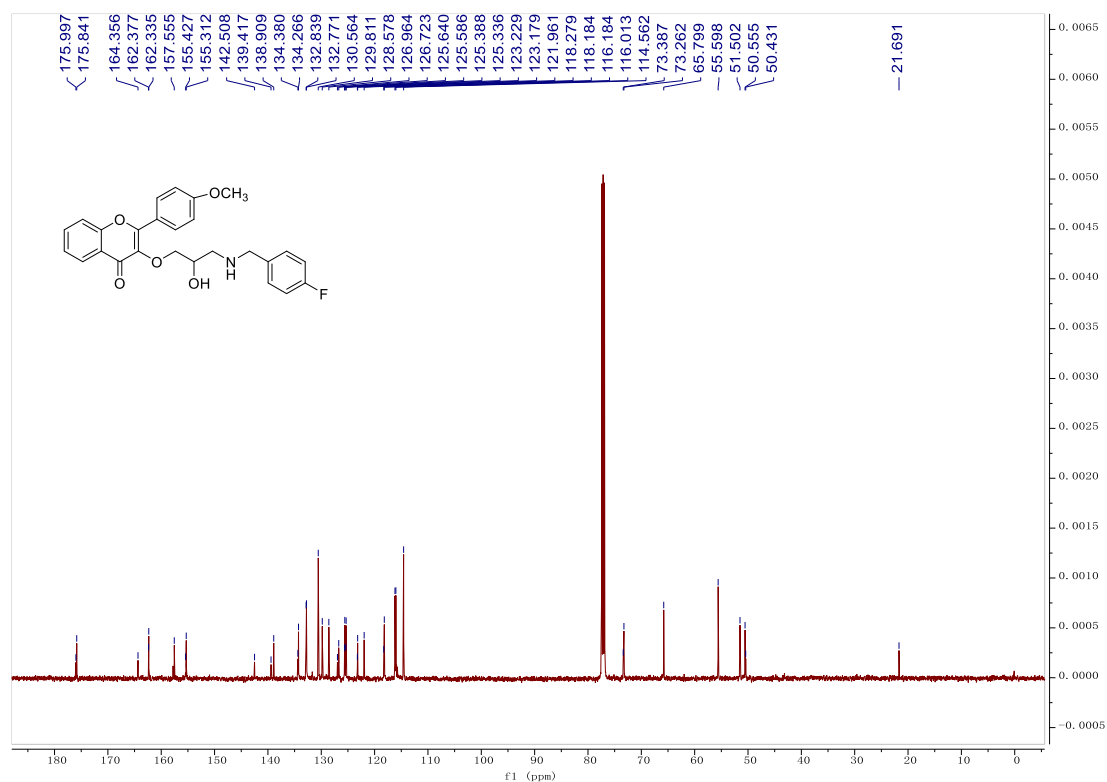


Fig. 61 ¹³C NMR spectrum of title compound Y20

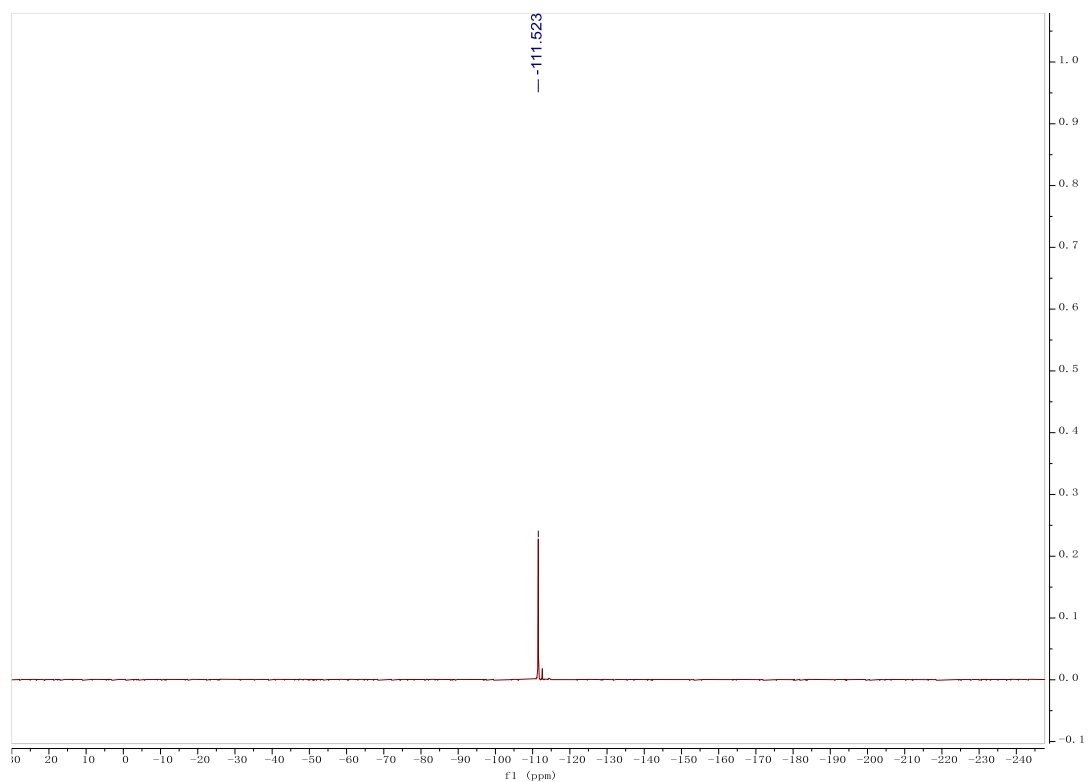


Fig. 62 ¹⁹F NMR spectrum of title compound Y20

60 #71 RT: 0.69 AV: 1 NL: 2.44E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

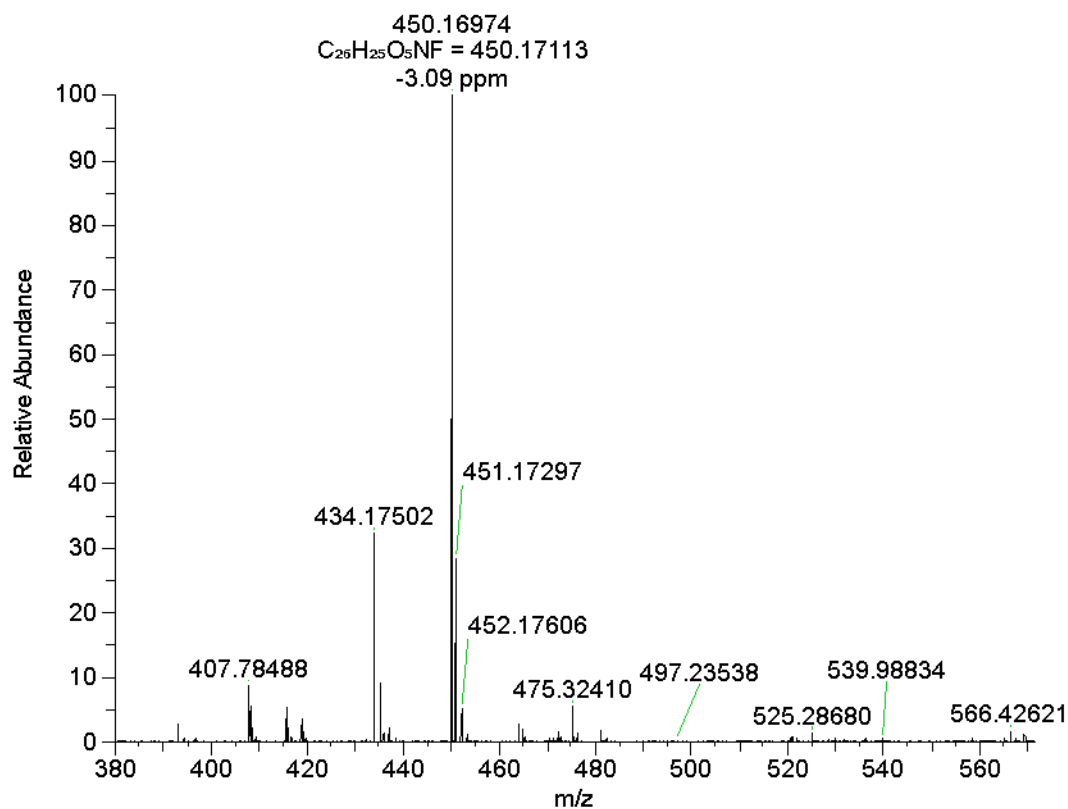


Fig. 63 HRMS spectrum of title compound Y20

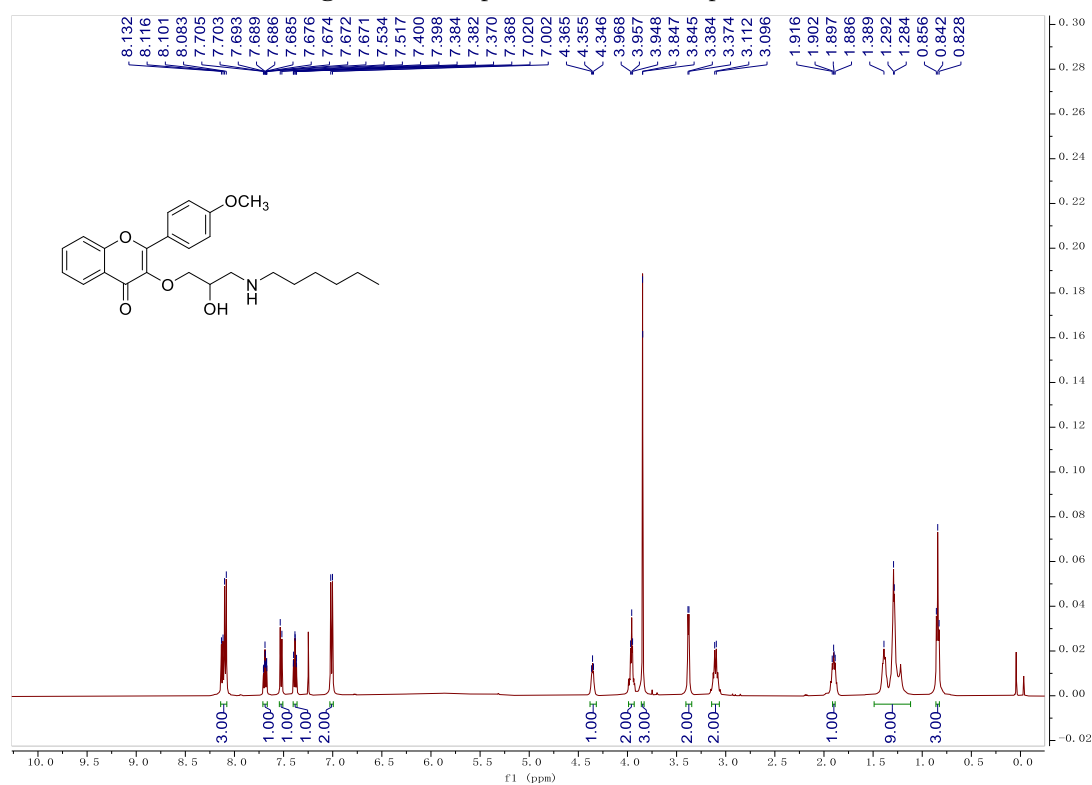


Fig. 64 ¹H NMR spectrum of title compound Y21

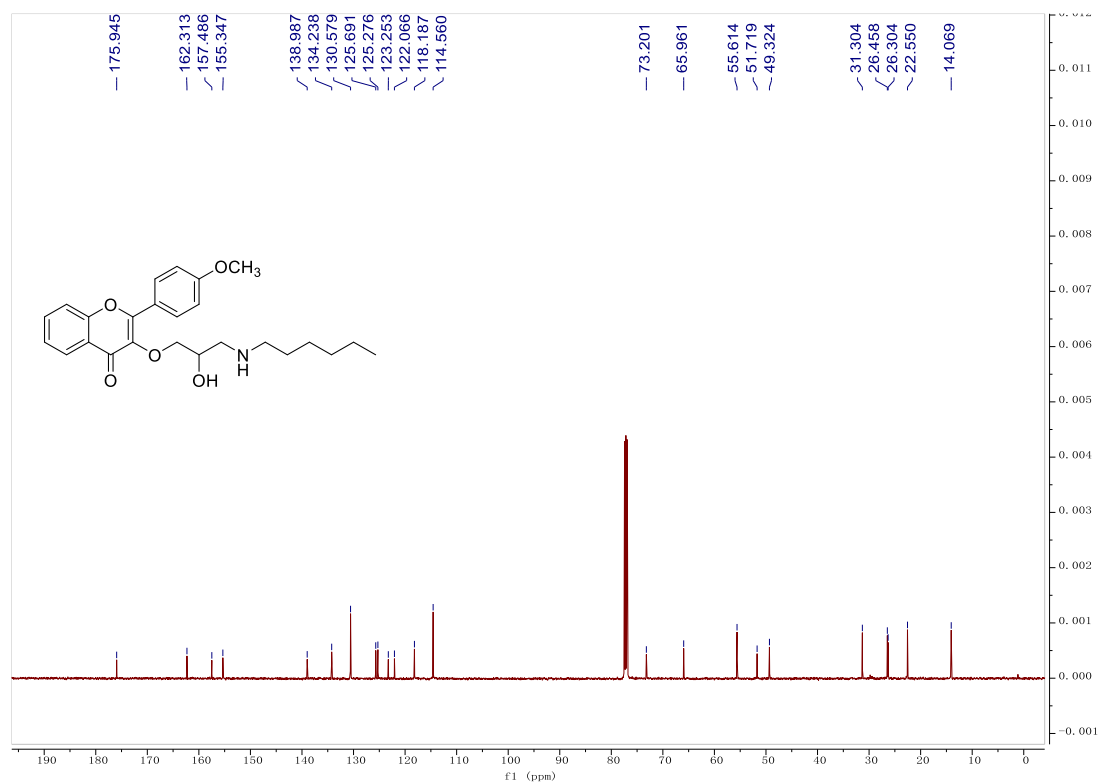


Fig. 65 ¹³C NMR spectrum of title compound Y21

61 #101 RT: 0.98 AV: 1 NL: 5.37E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

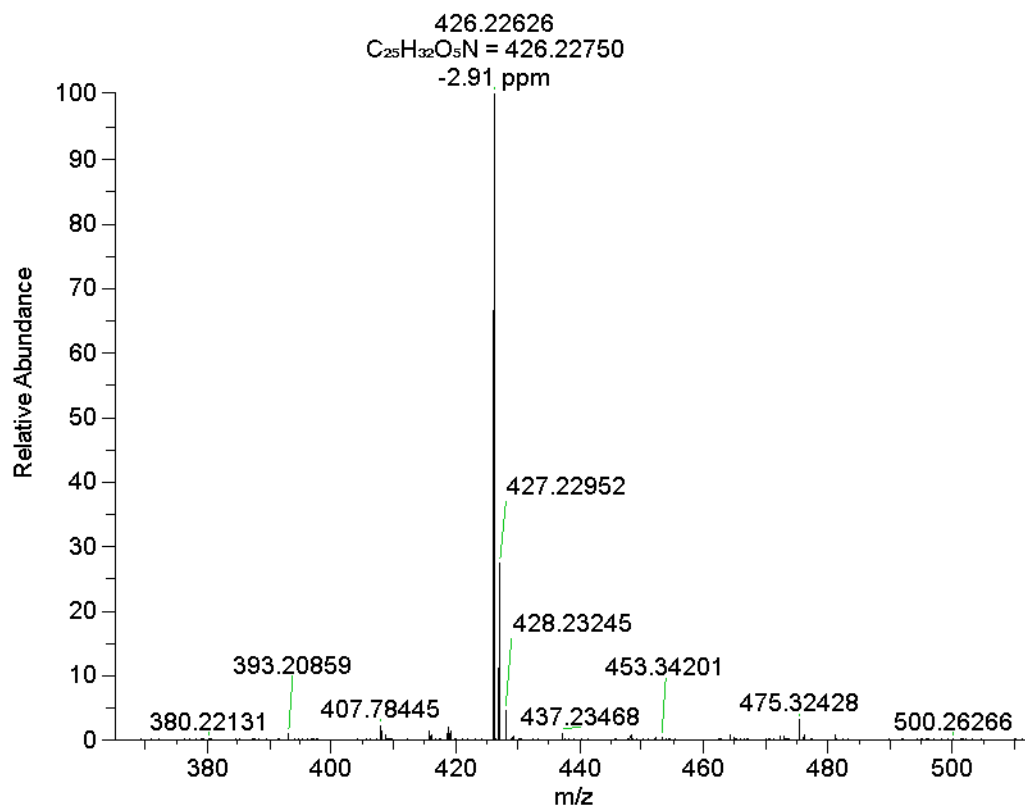


Fig. 66 HRMS spectrum of title compound Y21

