

Supporting Information

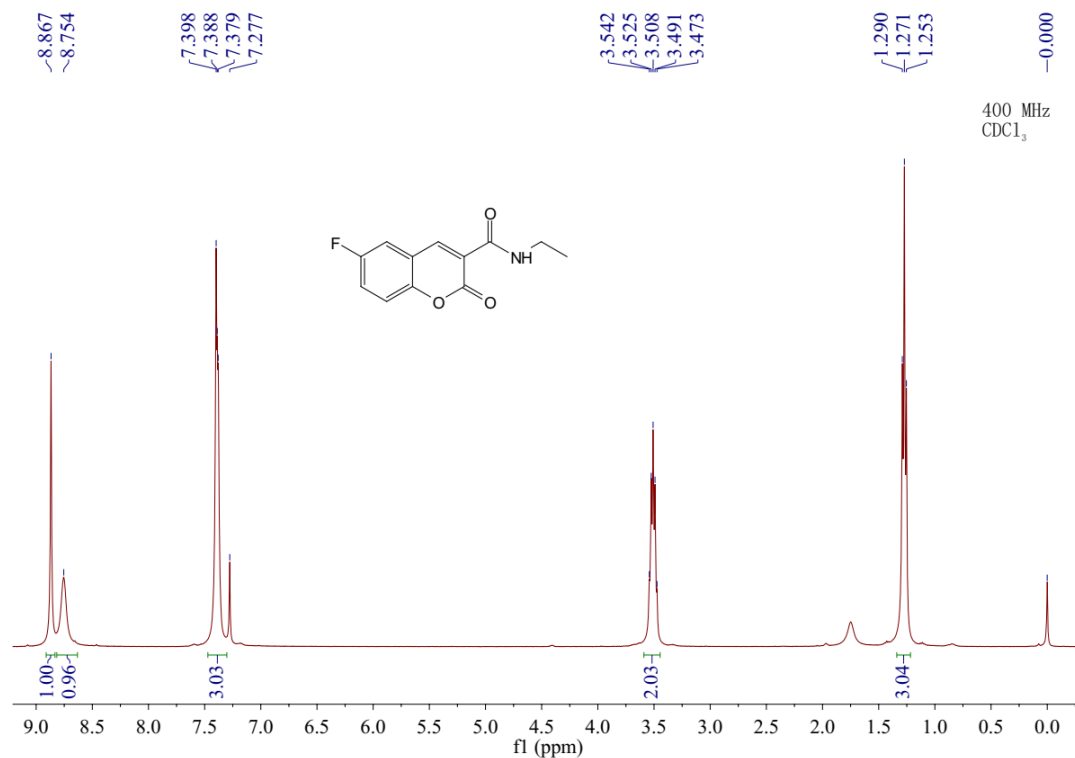


Figure S1. ¹H NMR spectrum of compound A1

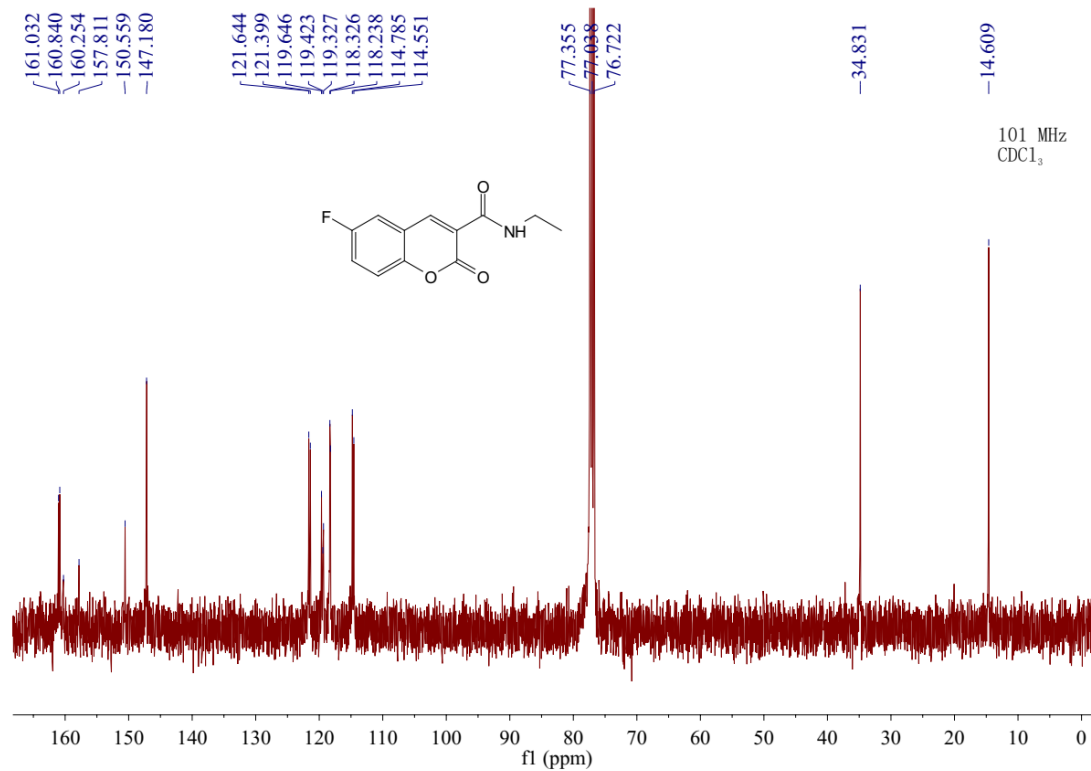


Figure S2. ¹³C NMR spectrum of compound A1

C1 #31 RT: 0.31 AV: 1 NL: 3.11E8
T: FTMS + p ESIFull.ms [100.0000-1300.0000]

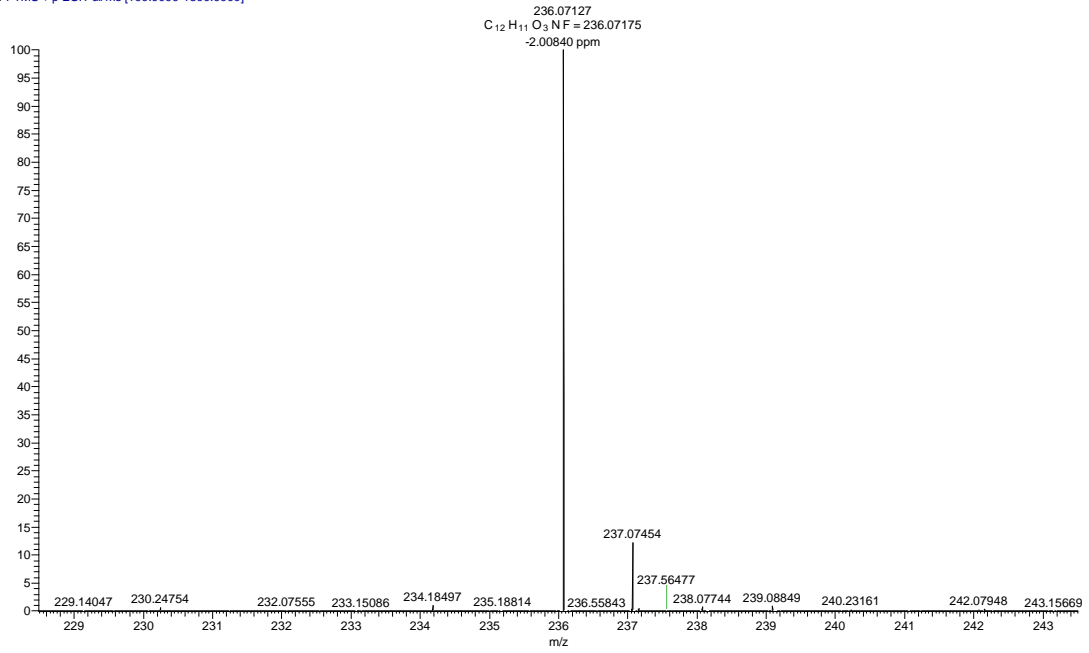


Figure S3. HRMS spectrum of compound A1

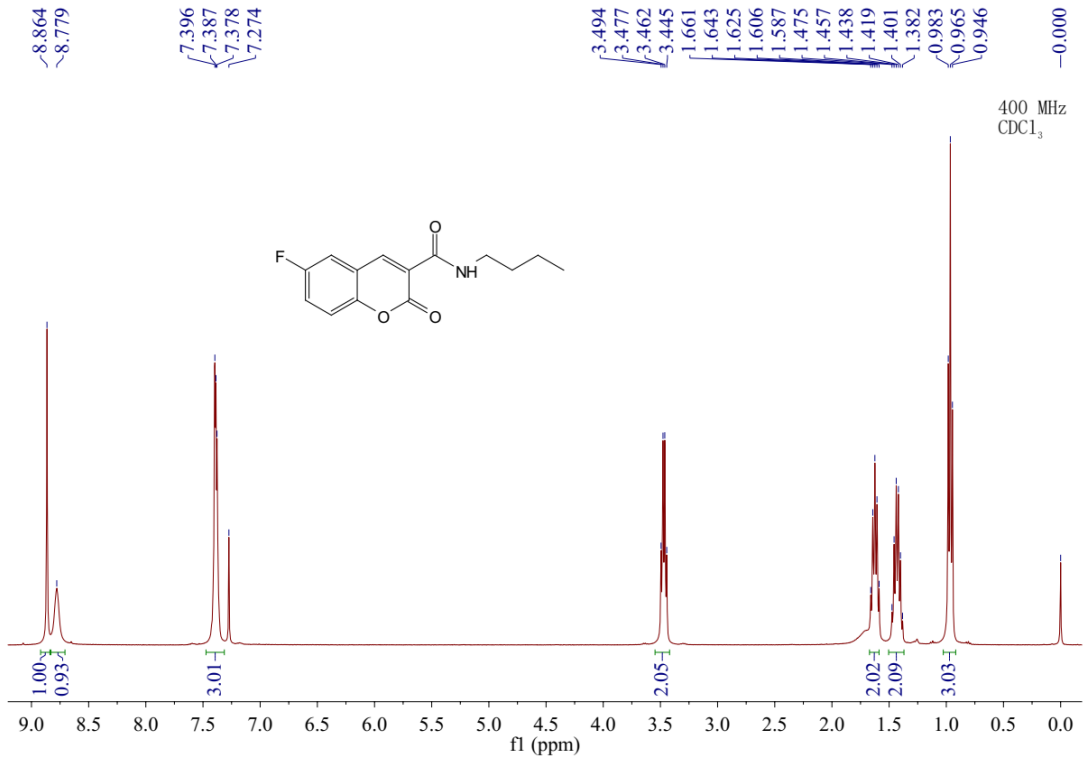


Figure S4. ¹H NMR spectrum of compound A2

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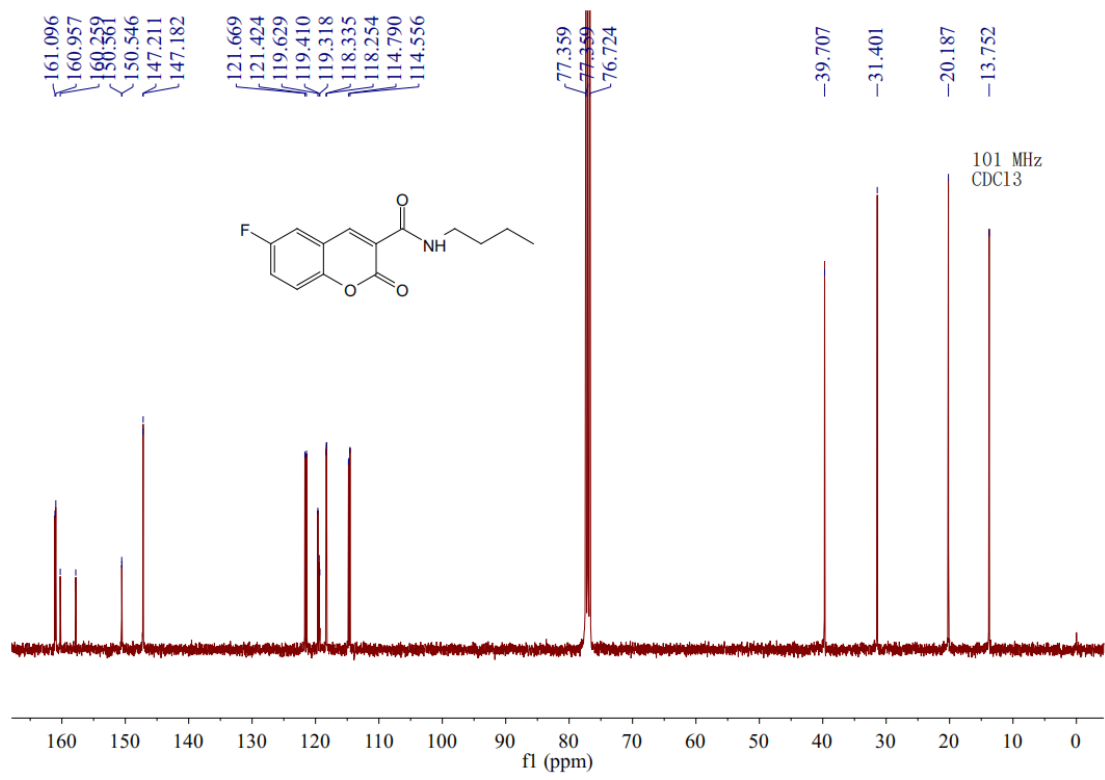


Figure S5. ¹³C NMR spectrum of compound A2

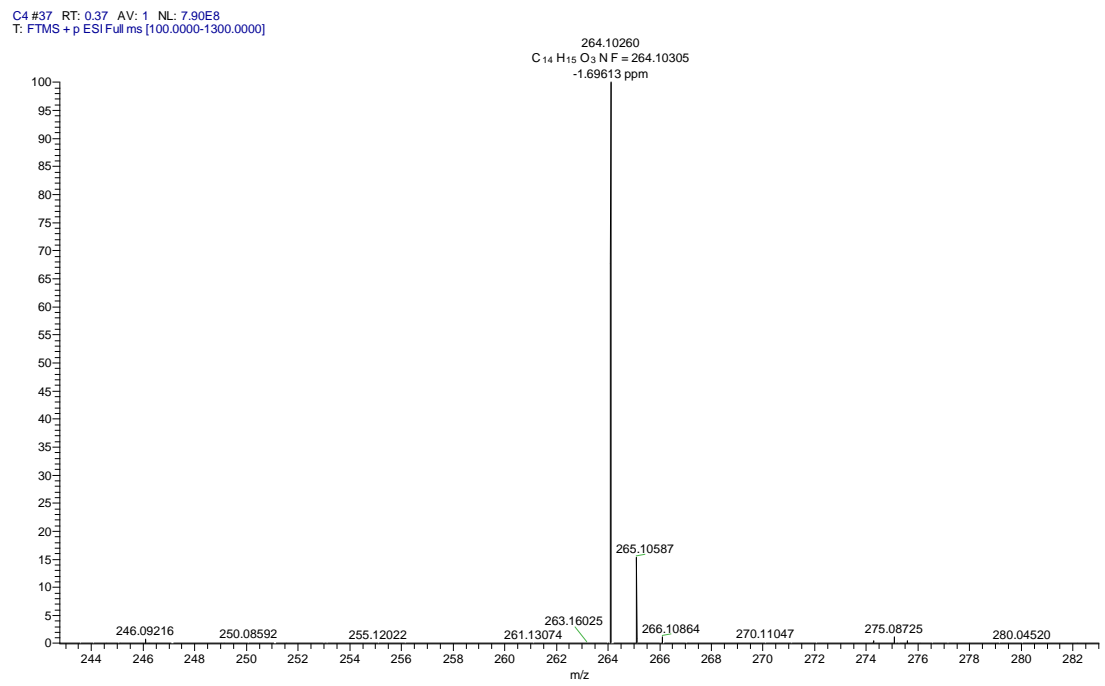
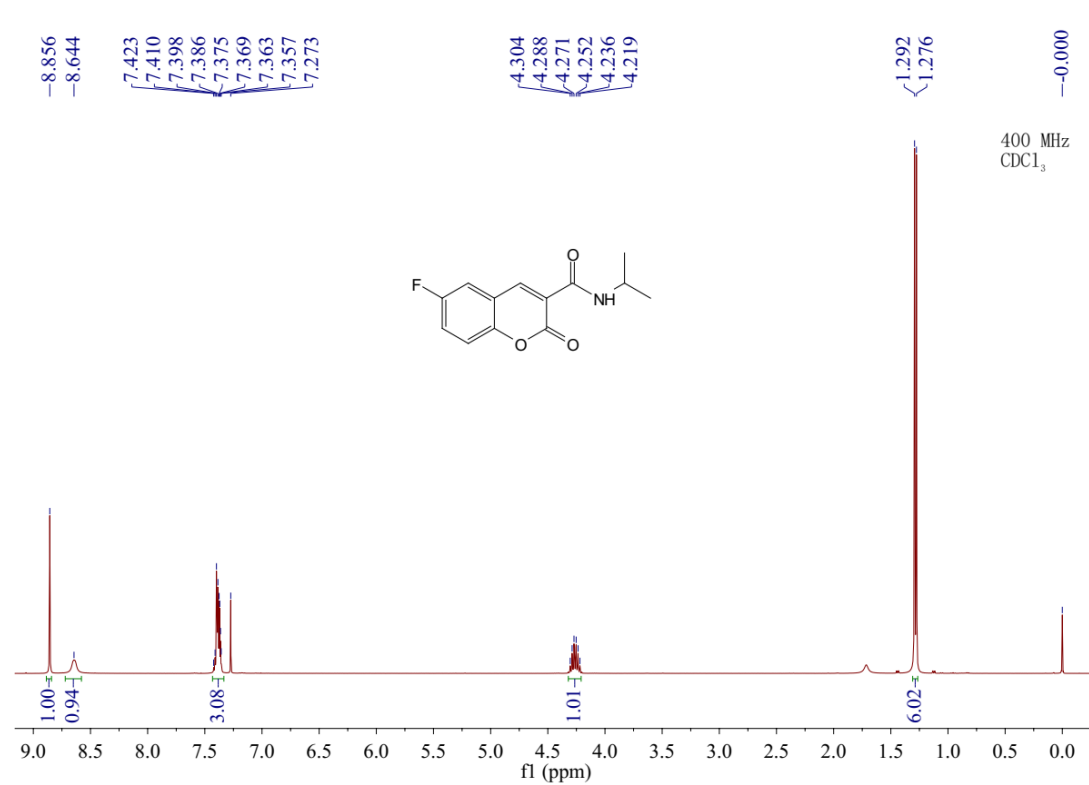


Figure S6. HRMS spectrum of compound A2



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Figure S7. ¹H NMR spectrum of compound A3

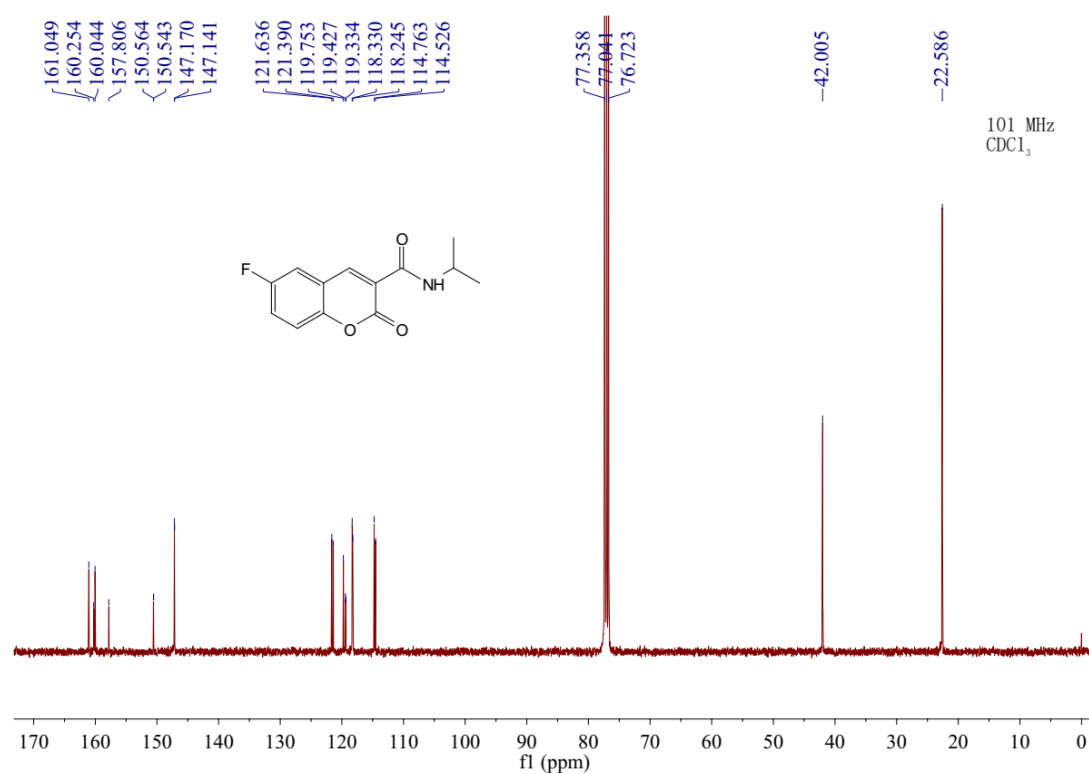


Figure S8. ¹³C NMR spectrum of compound A3

C3 #35 RT: 0.35 AV: 1 NL: 3.50E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

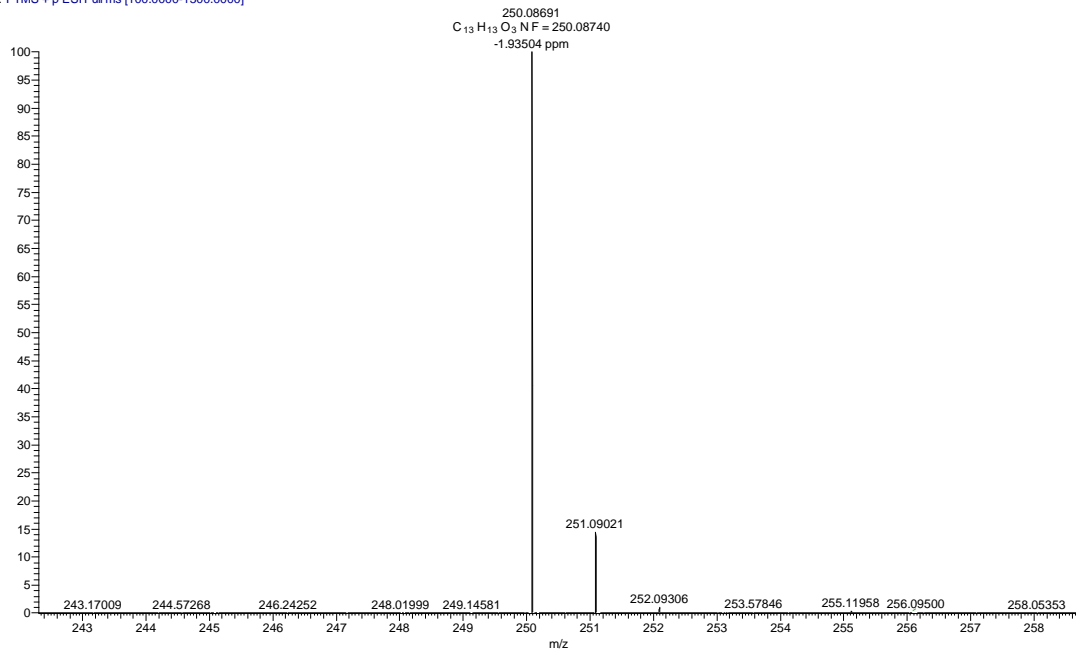


Figure S9. HRMS spectrum of compound A3

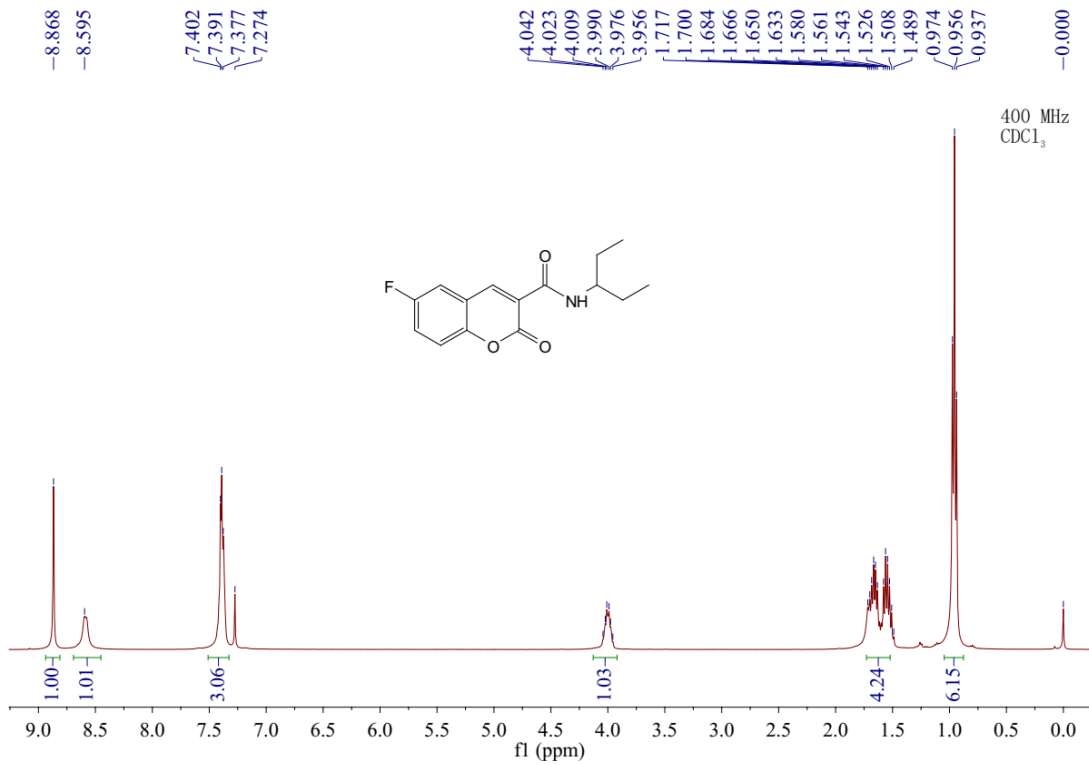


Figure S10. ¹H NMR spectrum of compound A4

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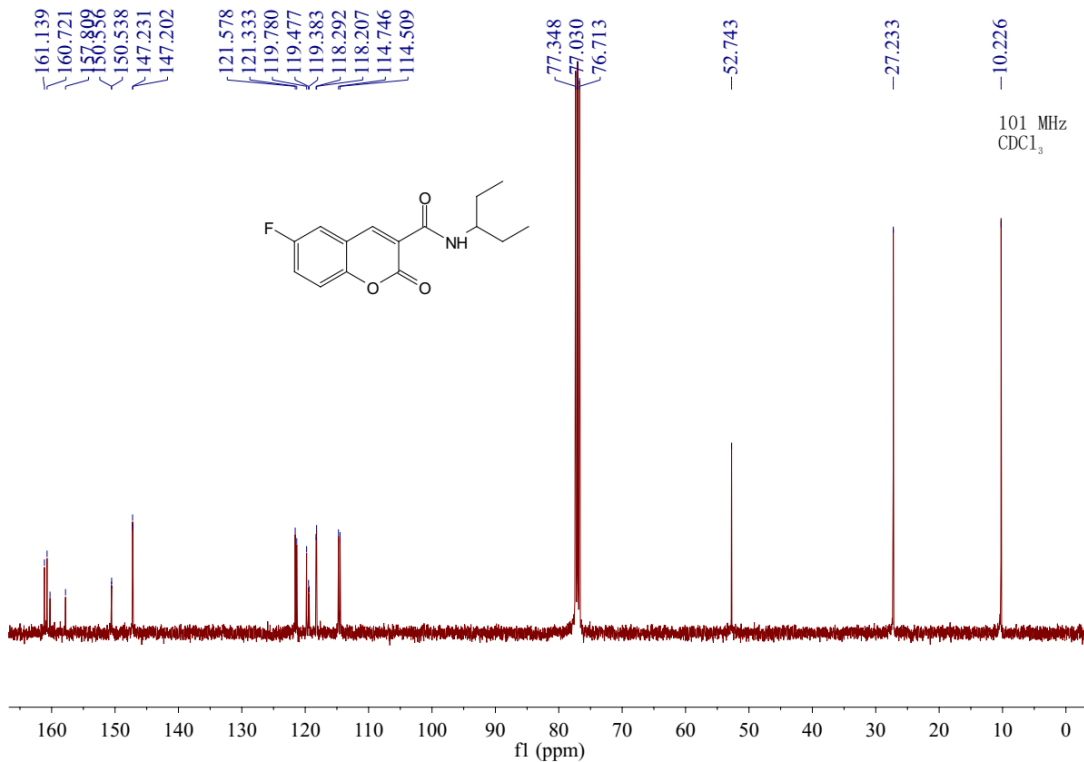


Figure S11. ¹³C NMR spectrum of compound A4

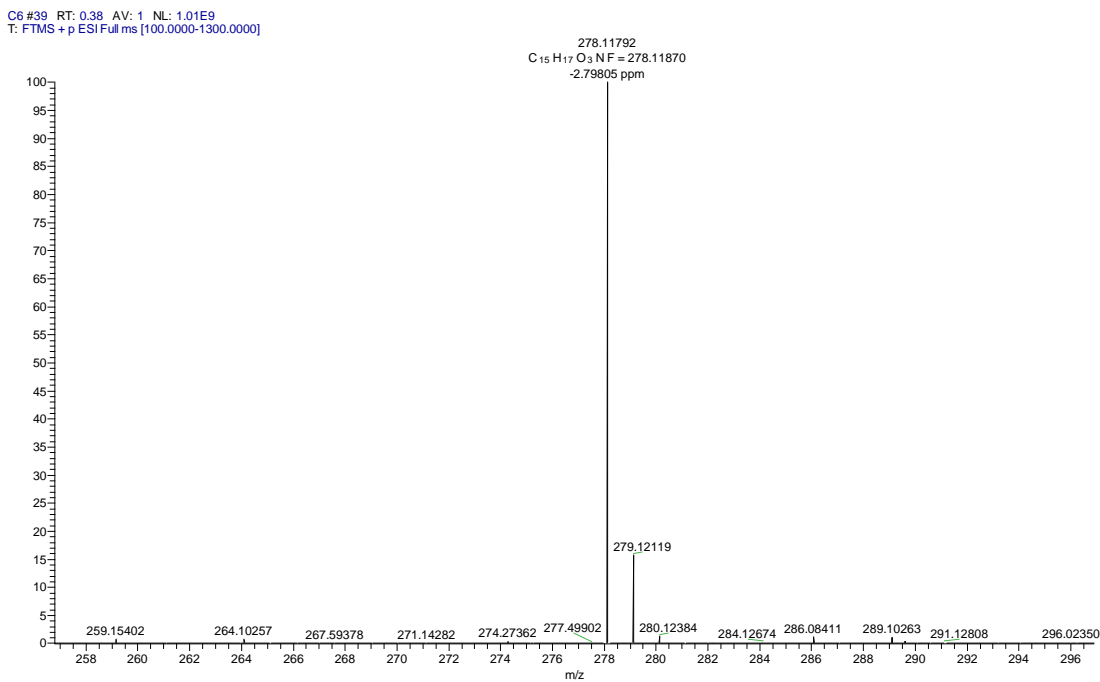


Figure S12. HRMS spectrum of compound A4

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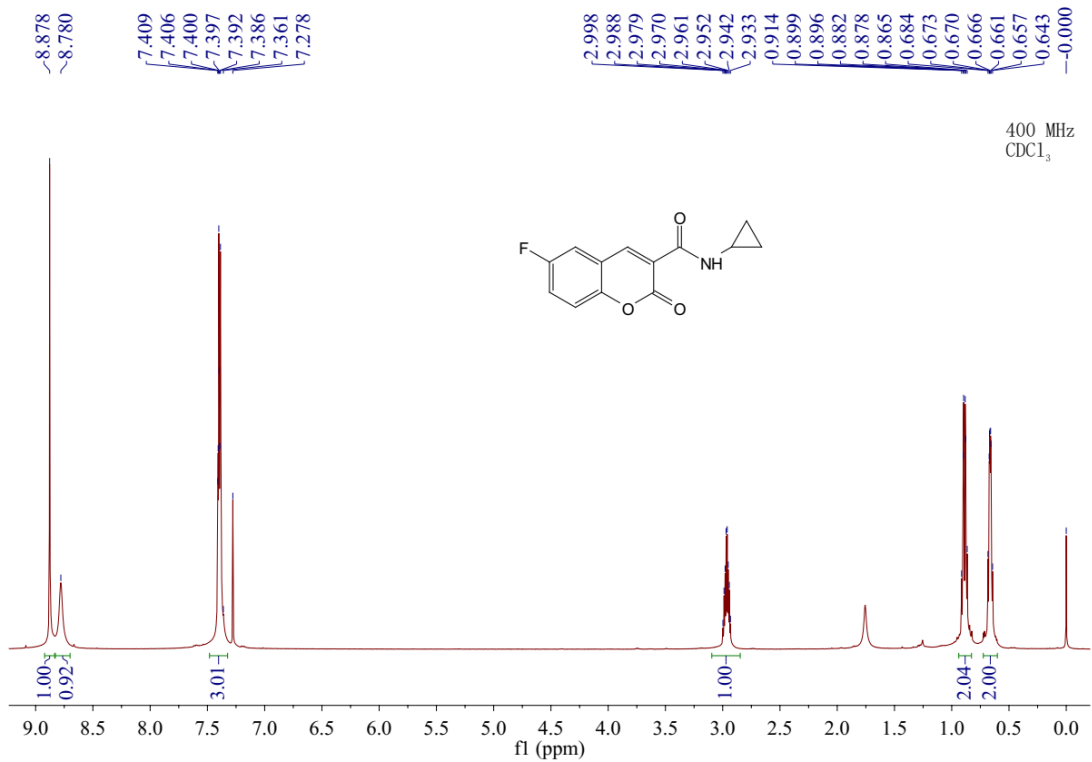


Figure S13. ¹H NMR spectrum of compound A5

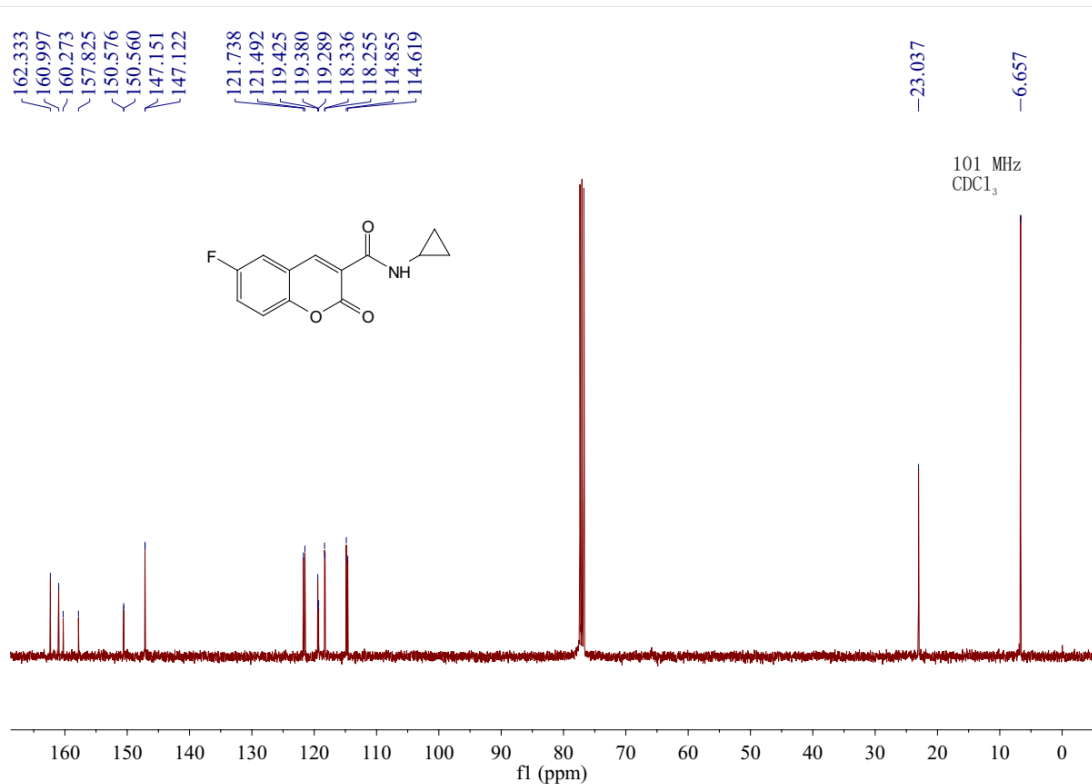


Figure S14. ¹³C NMR spectrum of compound A5

C2 #35 RT: 0.35 AV: 1 NL: 3.49E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

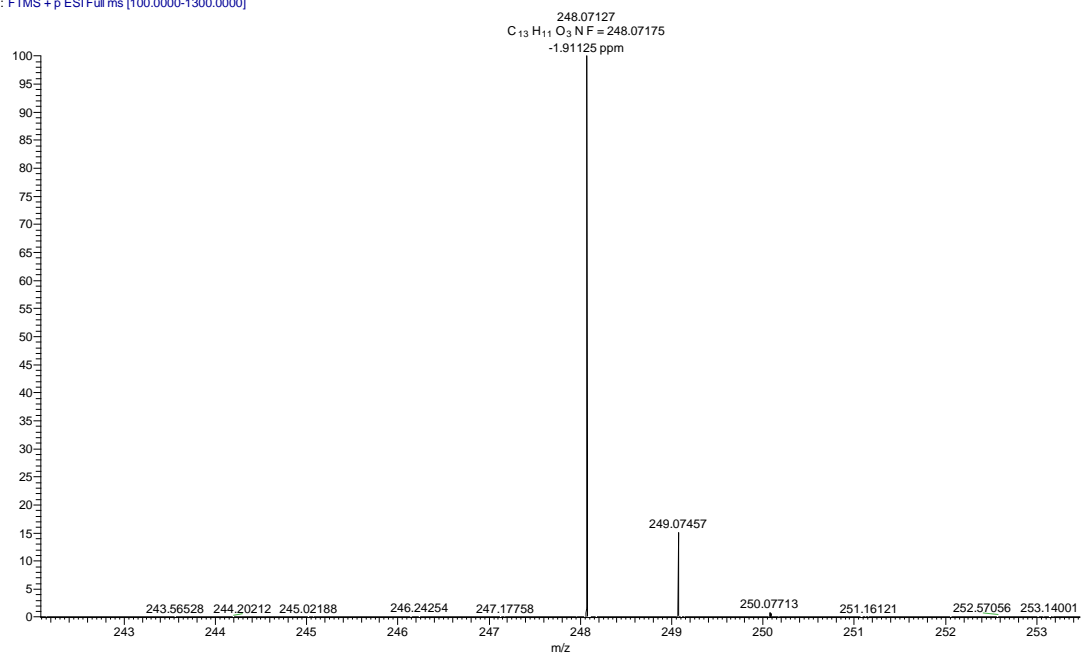


Figure S15. HRMS spectrum of compound A5

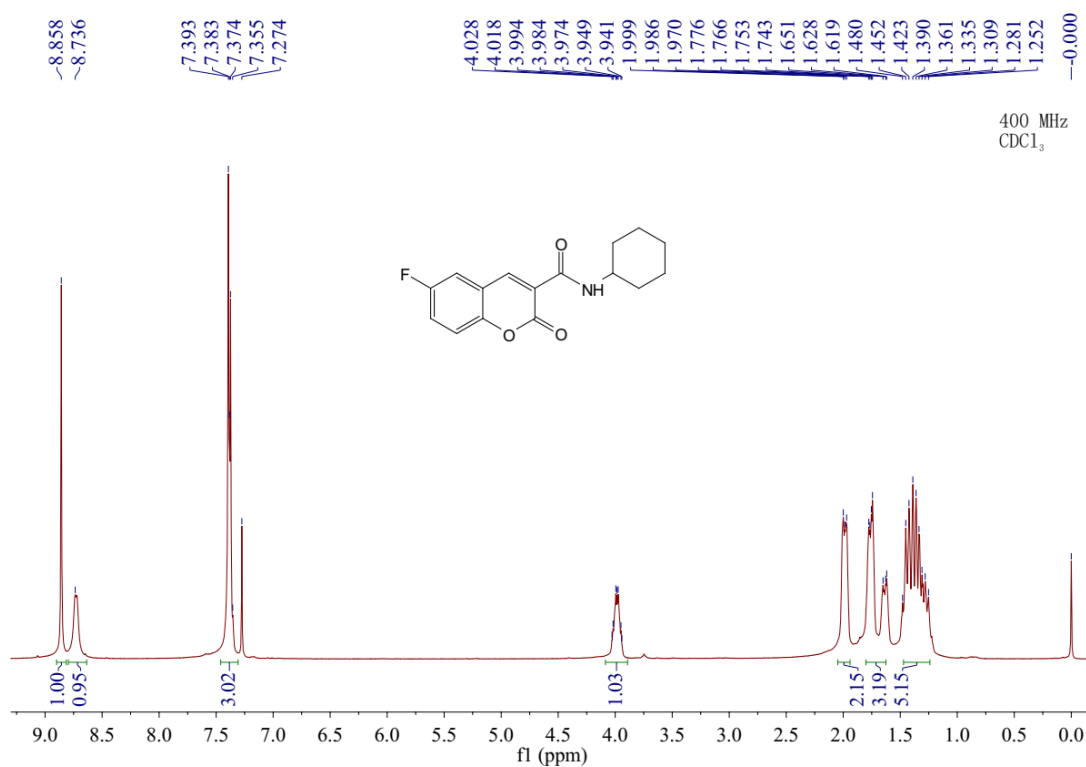


Figure S16. ¹H NMR spectrum of compound A6

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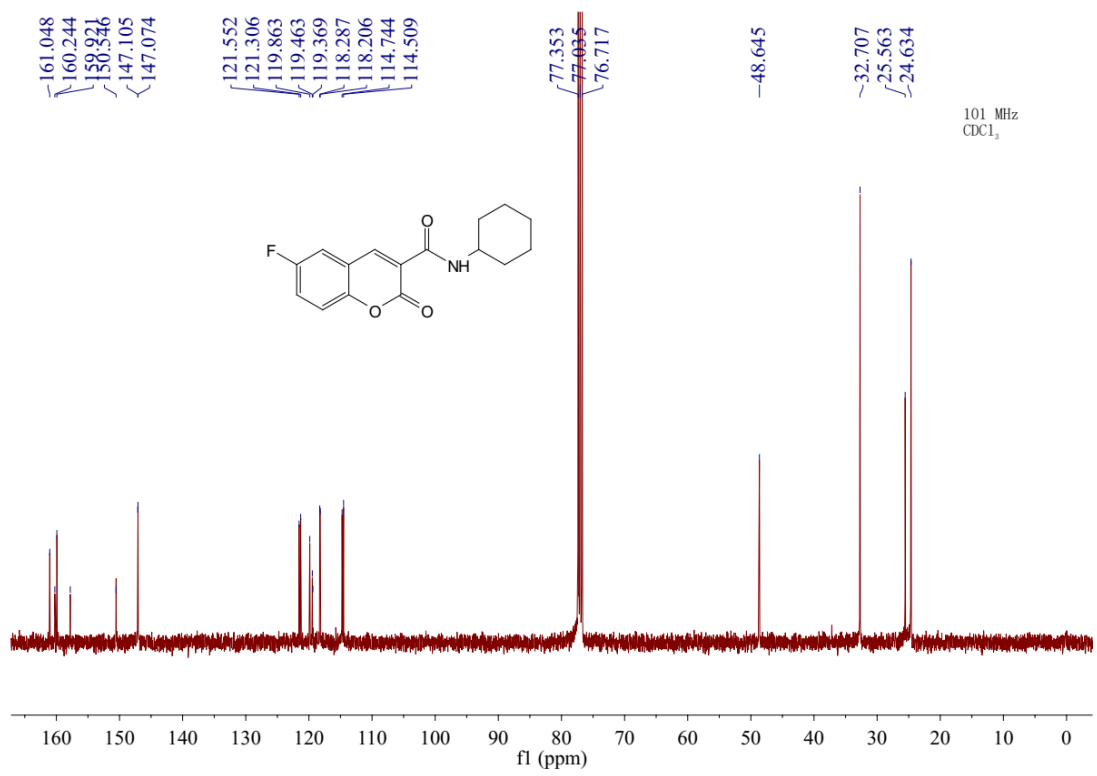


Figure S17. ¹³C NMR spectrum of compound A6

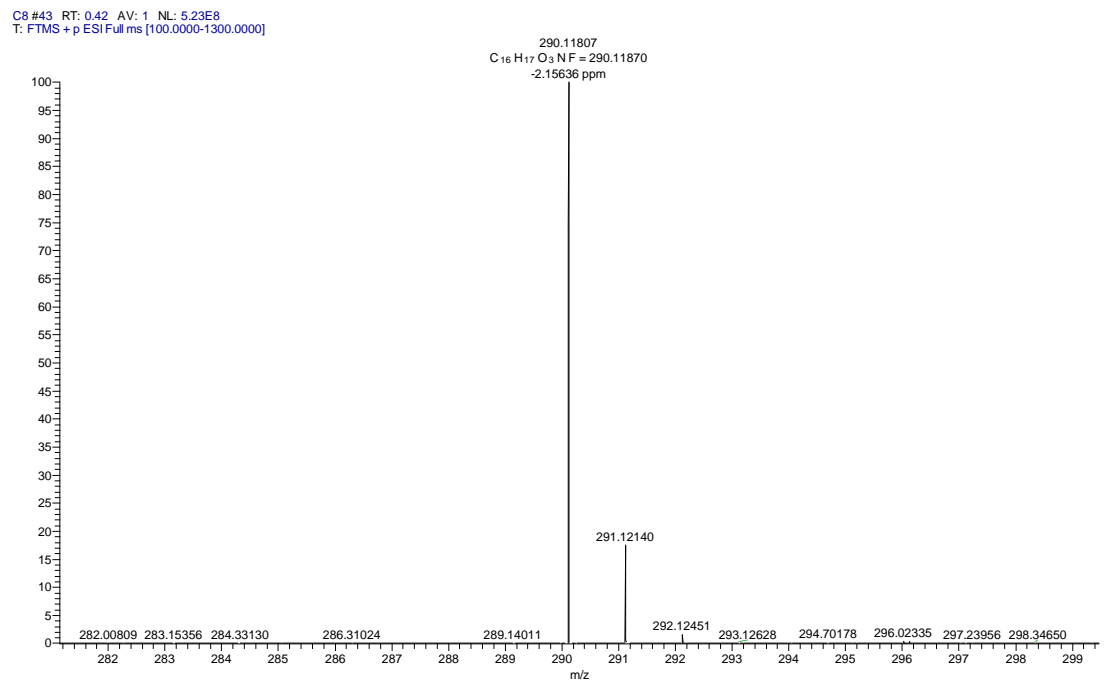
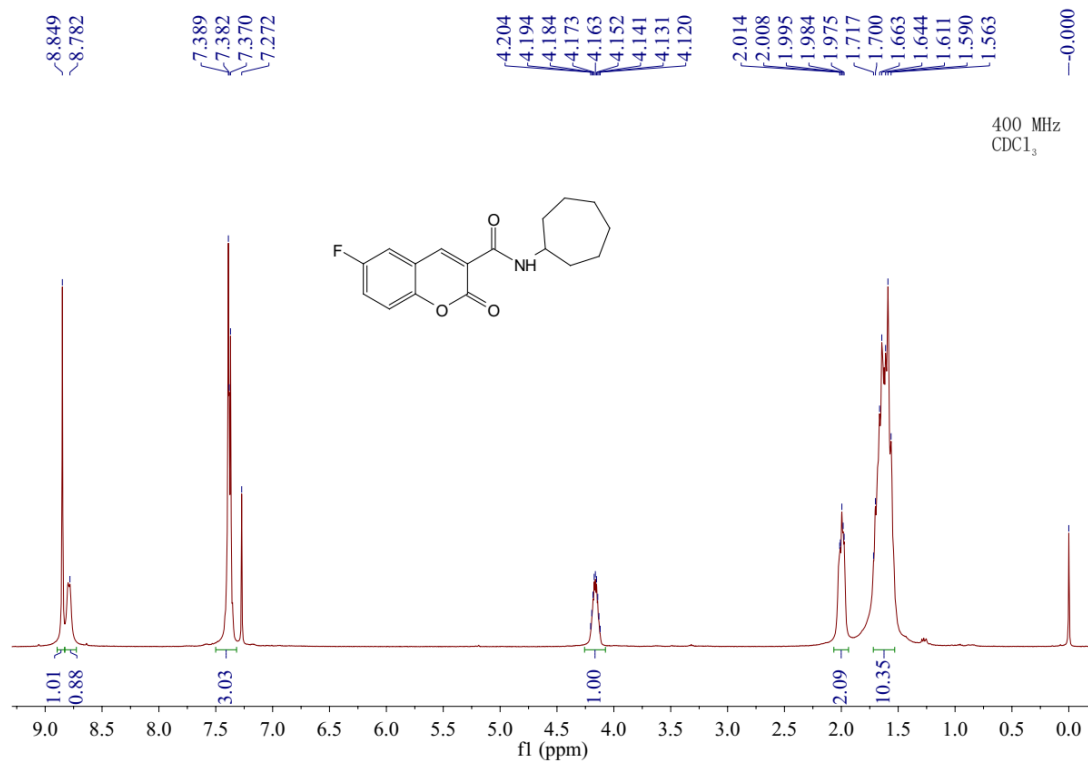
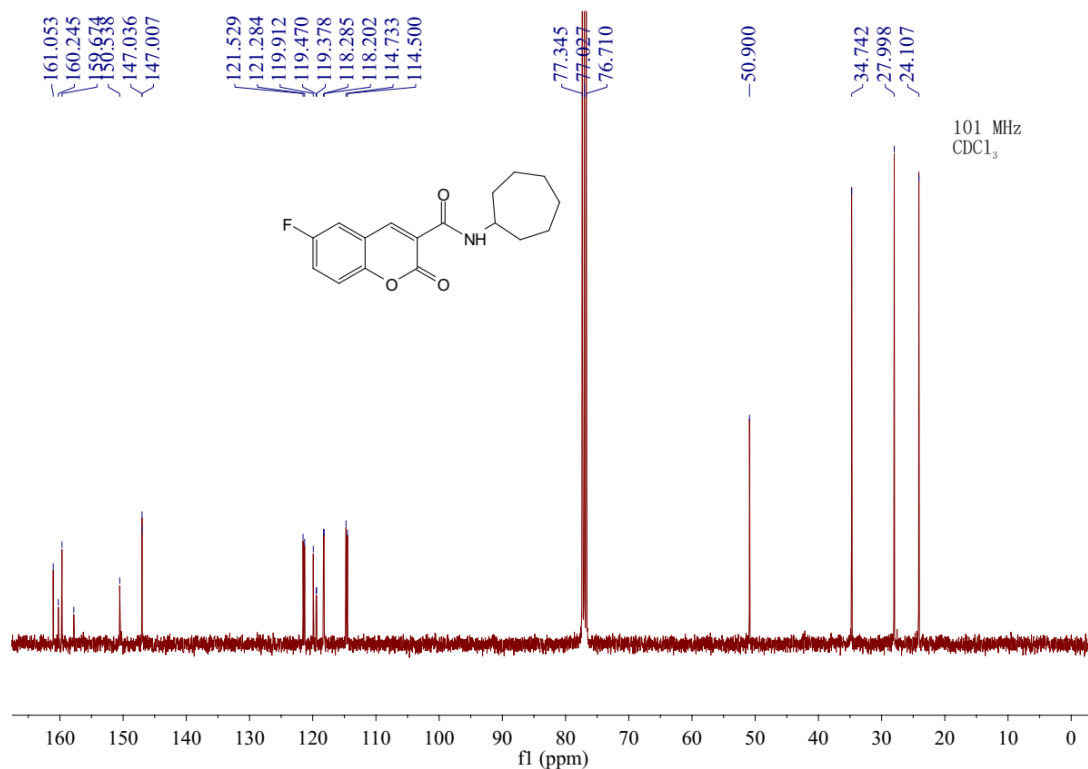


Figure S18. HRMS spectrum of compound A6



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Figure S19. ¹H NMR spectrum of compound A7



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Figure S20. ¹³C NMR spectrum of compound A7

C9 #49 RT: 0.48 AV: 1 NL: 3.73E8
T: FTMS + p ESIFull.ms [100.0000-1300.0000]

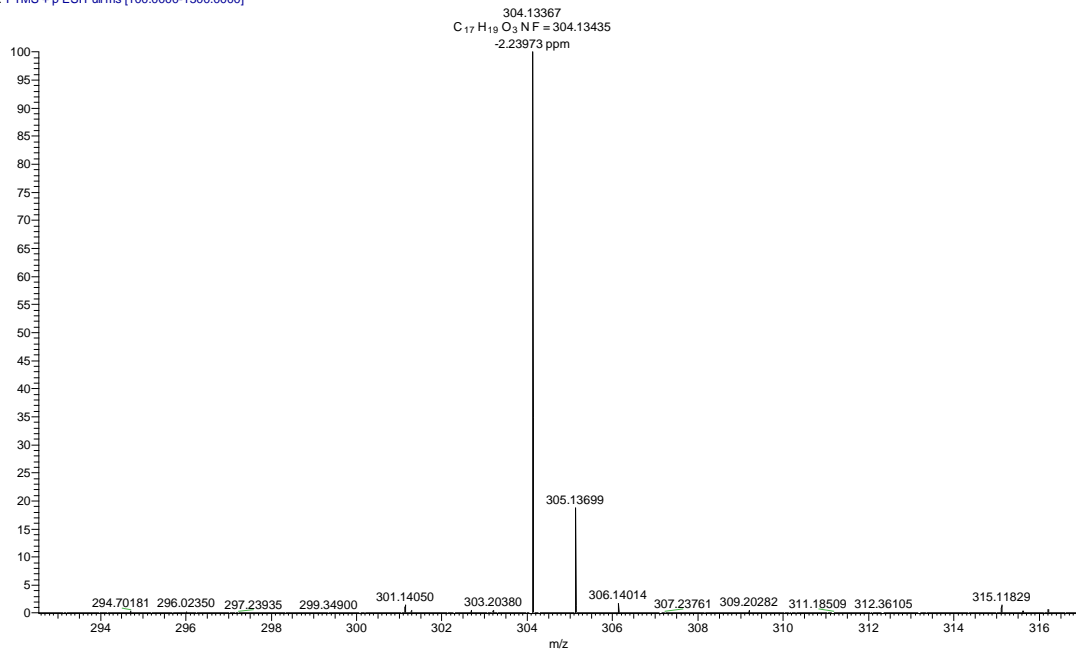


Figure S21. HRMS spectrum of compound A7

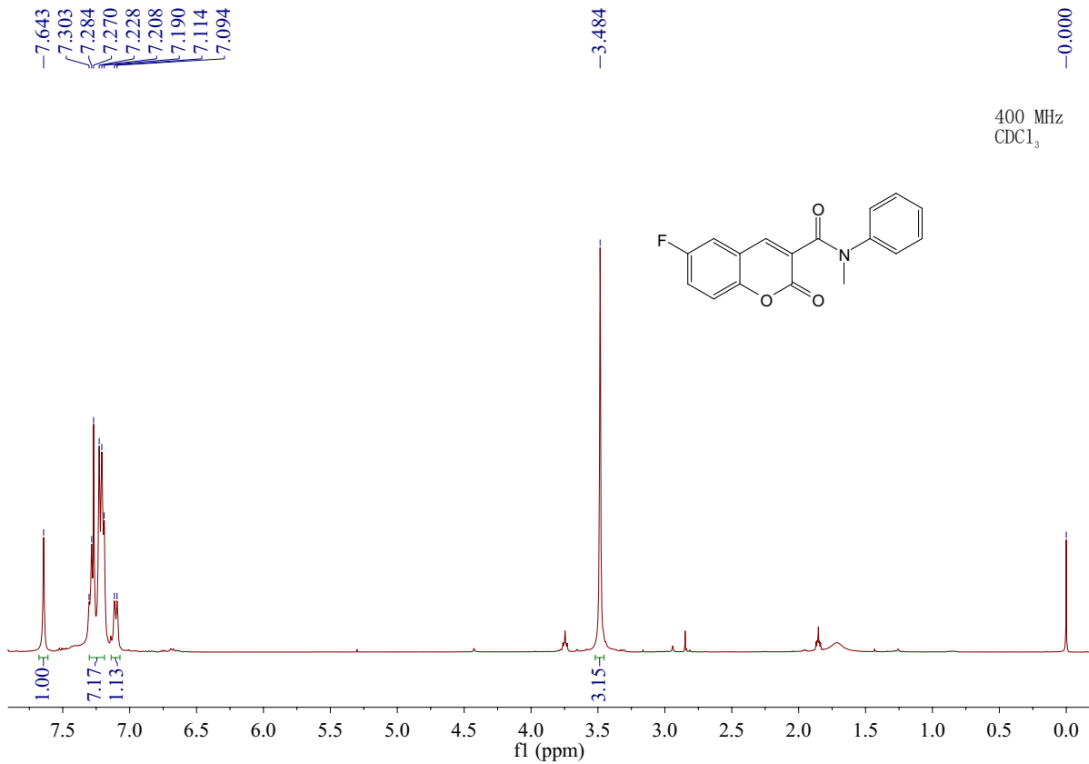


Figure S22. ¹H NMR spectrum of compound A8

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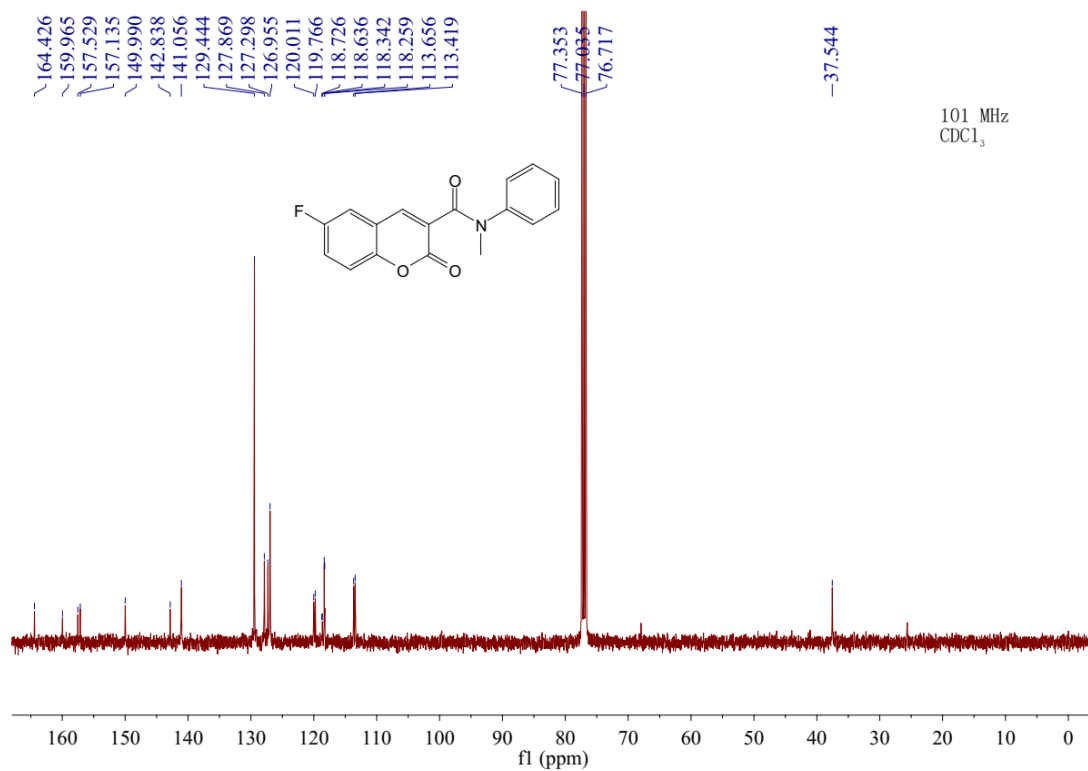


Figure S23. ¹³C NMR spectrum of compound A8

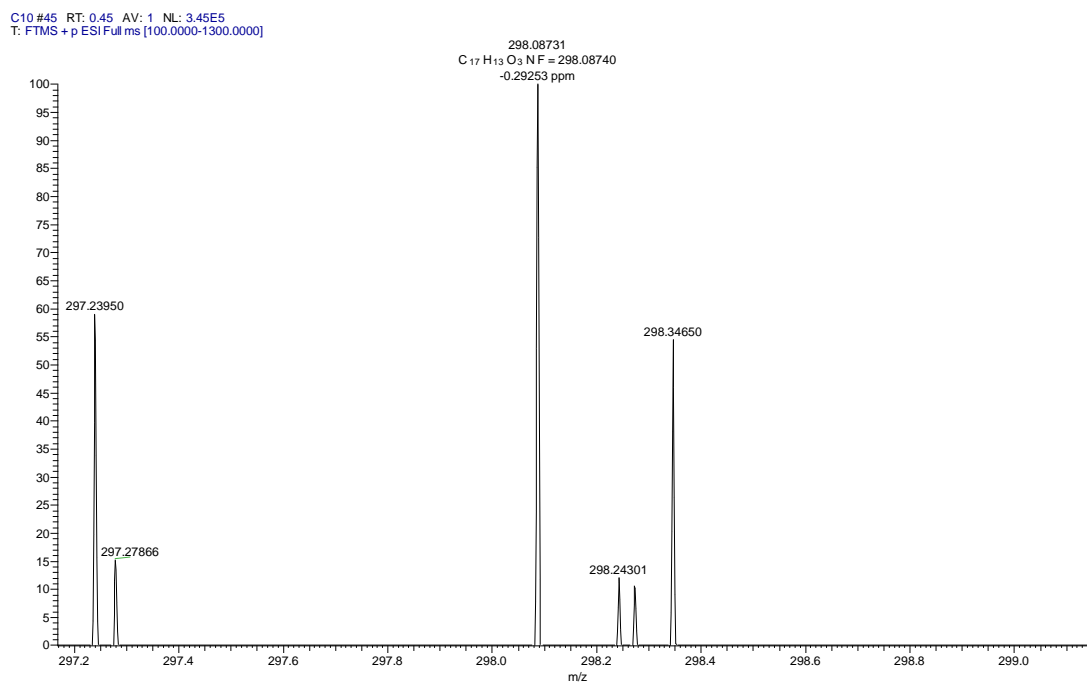


Figure S24. HRMS spectrum of compound A8

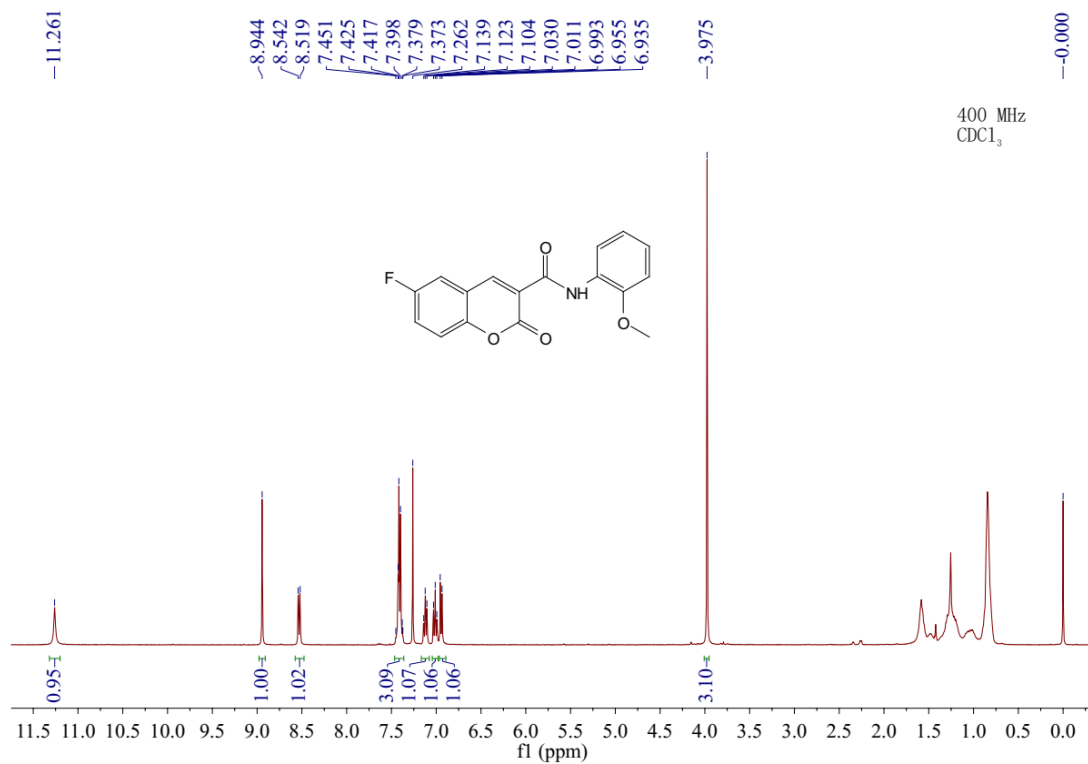


Figure S25. ¹H NMR spectrum of compound A9

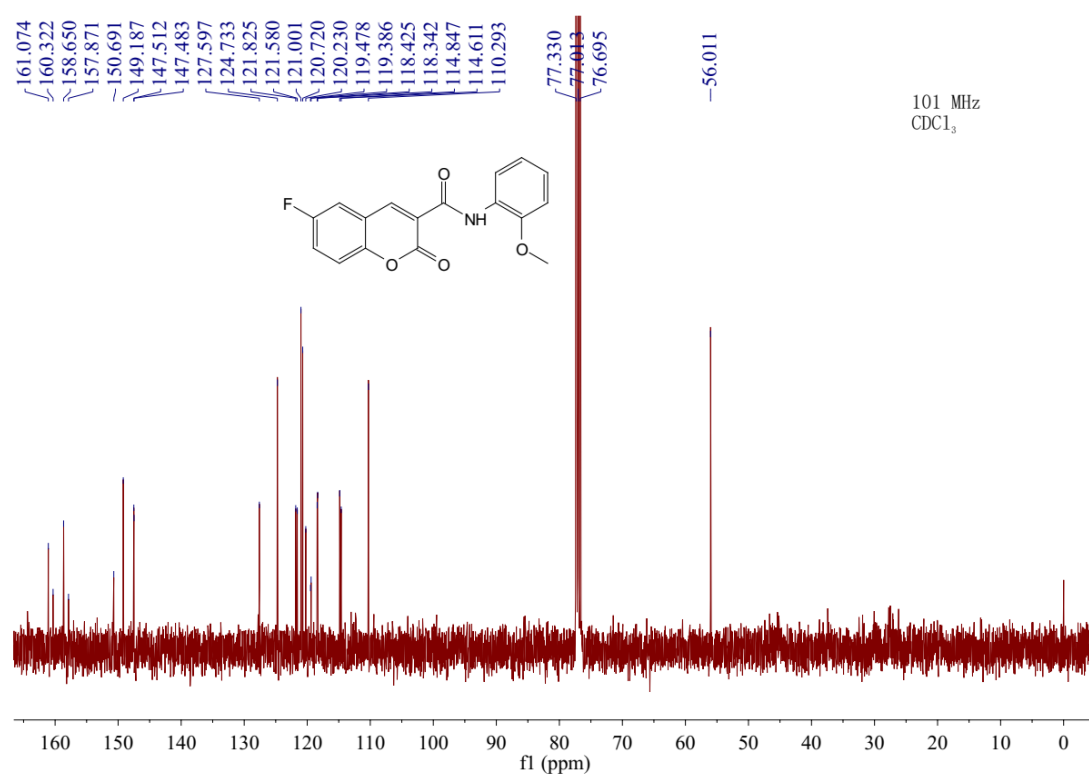


Figure S26. ¹³C NMR spectrum of compound A9

C11 #41 RT: 0.41 AV: 1 NL: 1.22E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

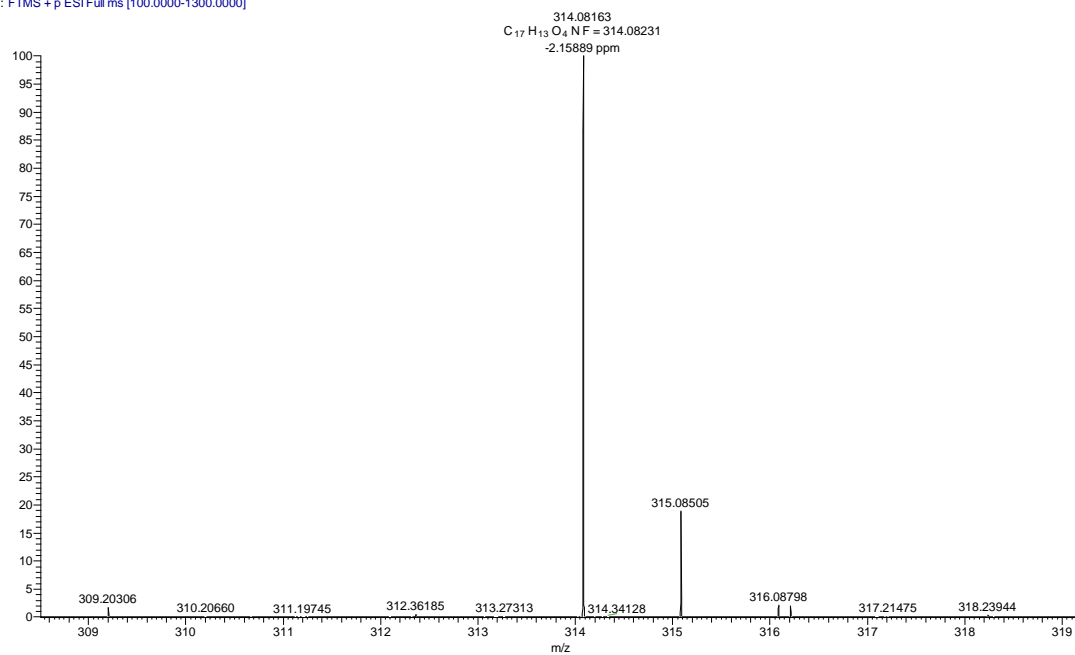


Figure S27. HRMS spectrum of compound A9

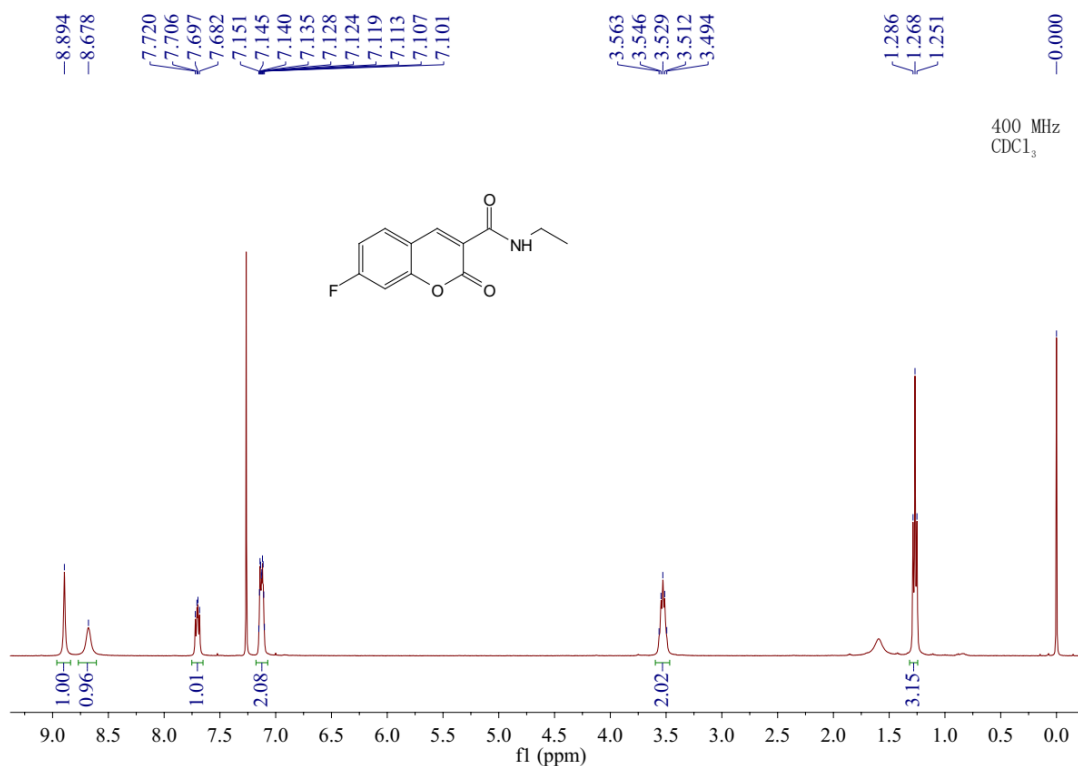


Figure S28. ¹H NMR spectrum of compound B1

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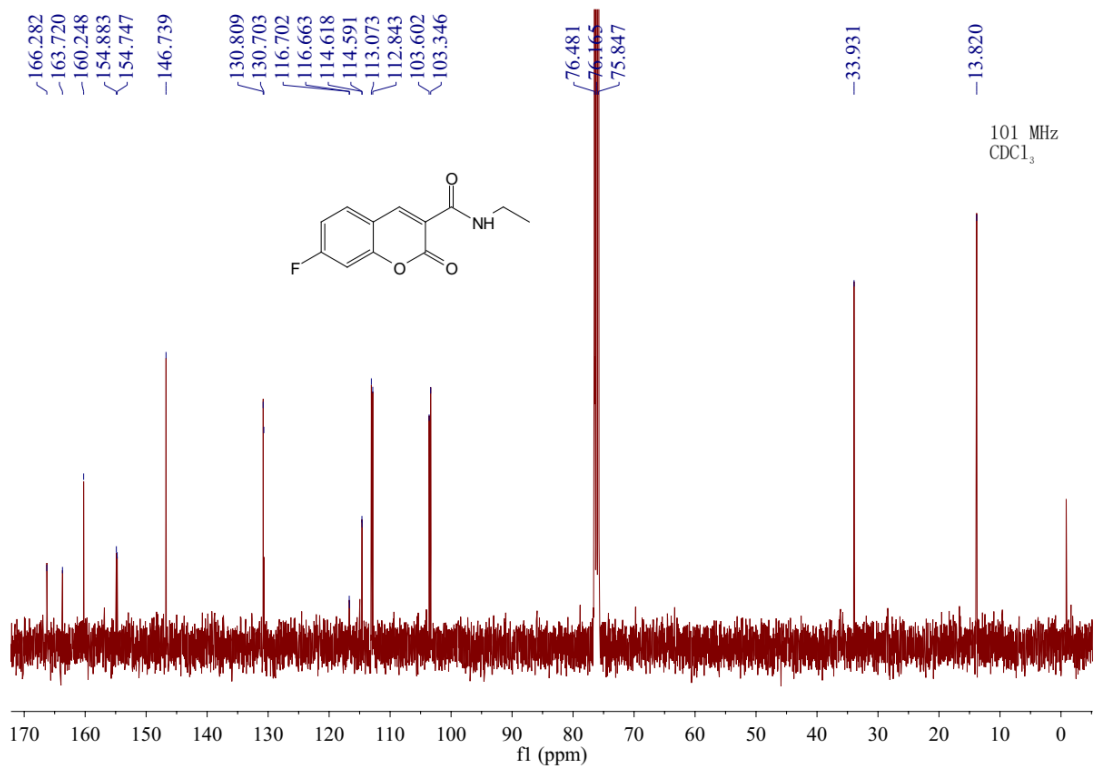


Figure S29. ¹³C NMR spectrum of compound B1

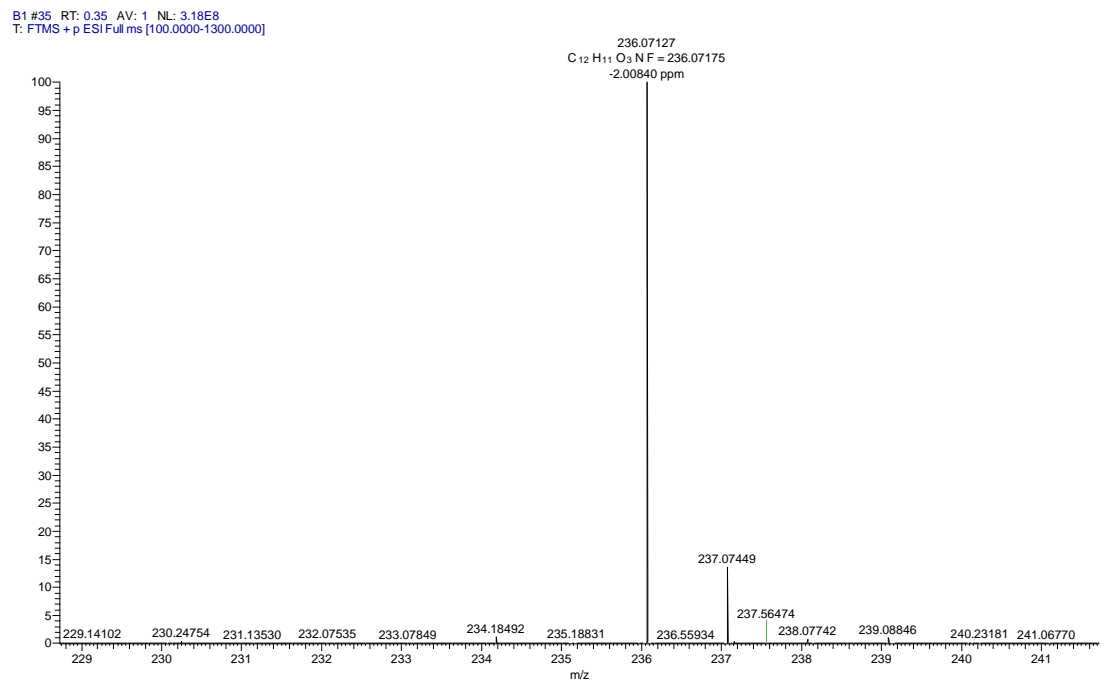


Figure S30. HRMS spectrum of compound B1

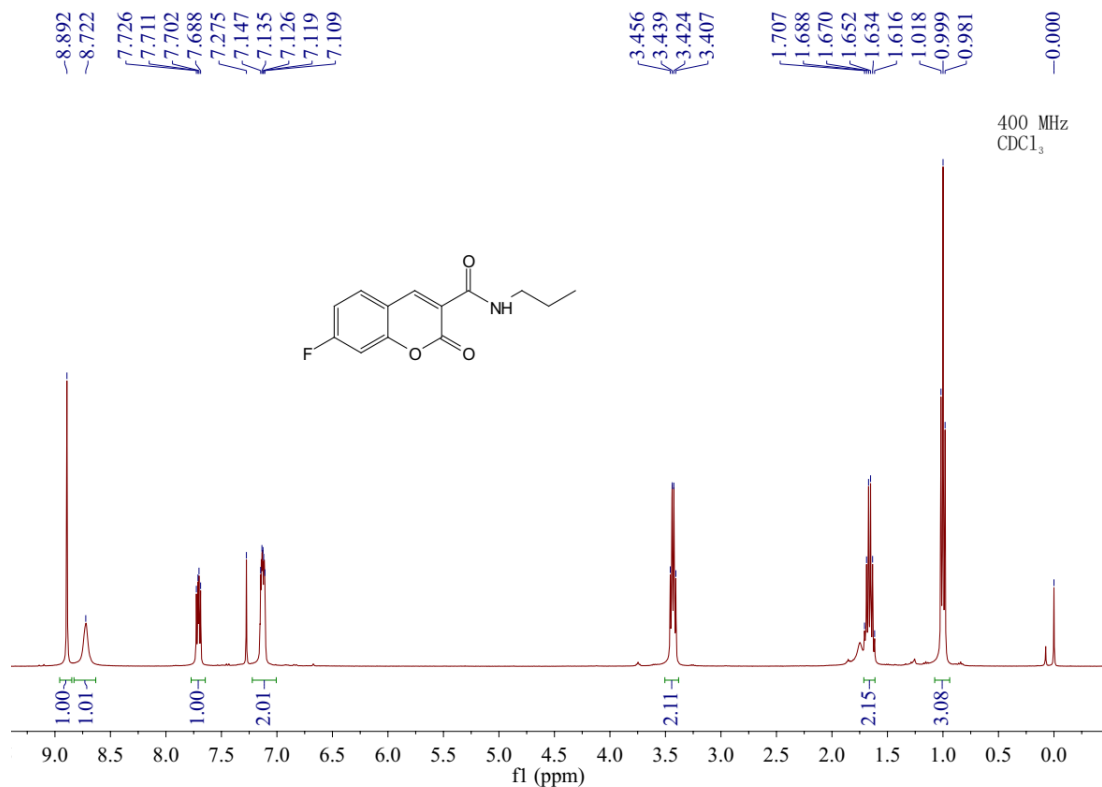


Figure S31. ¹H NMR spectrum of compound B2

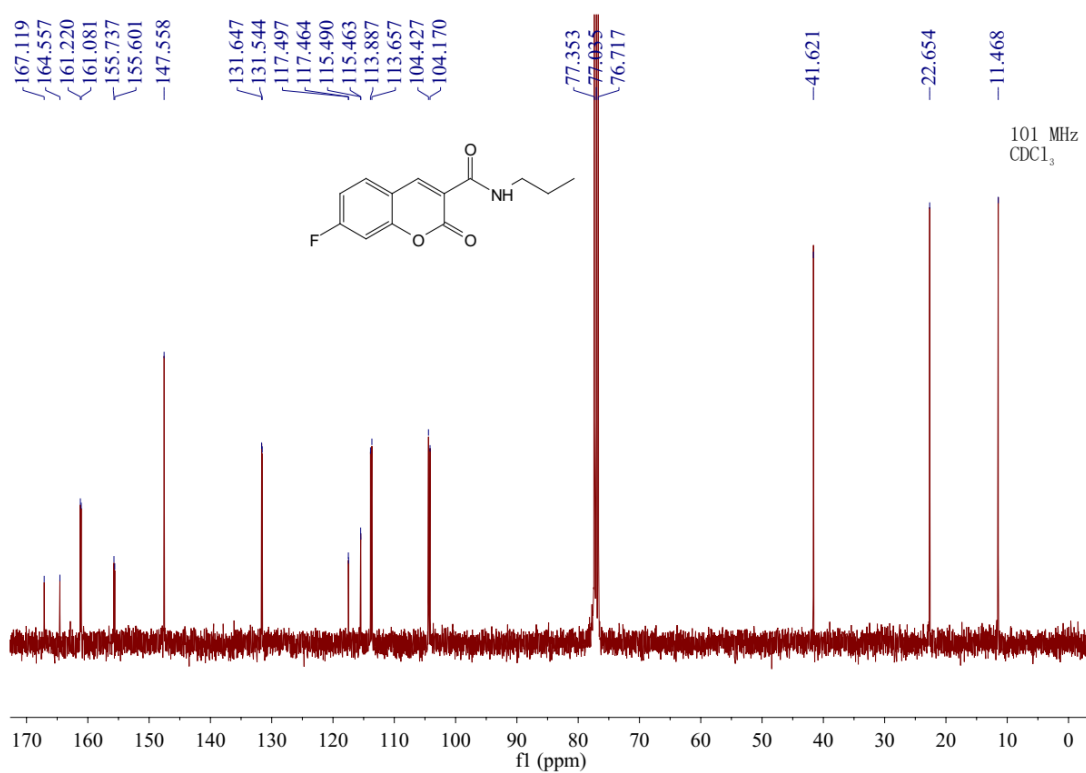


Figure S32. ¹³C NMR spectrum of compound B2

B2 #35 RT: 0.35 AV: 1 NL: 8.23E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

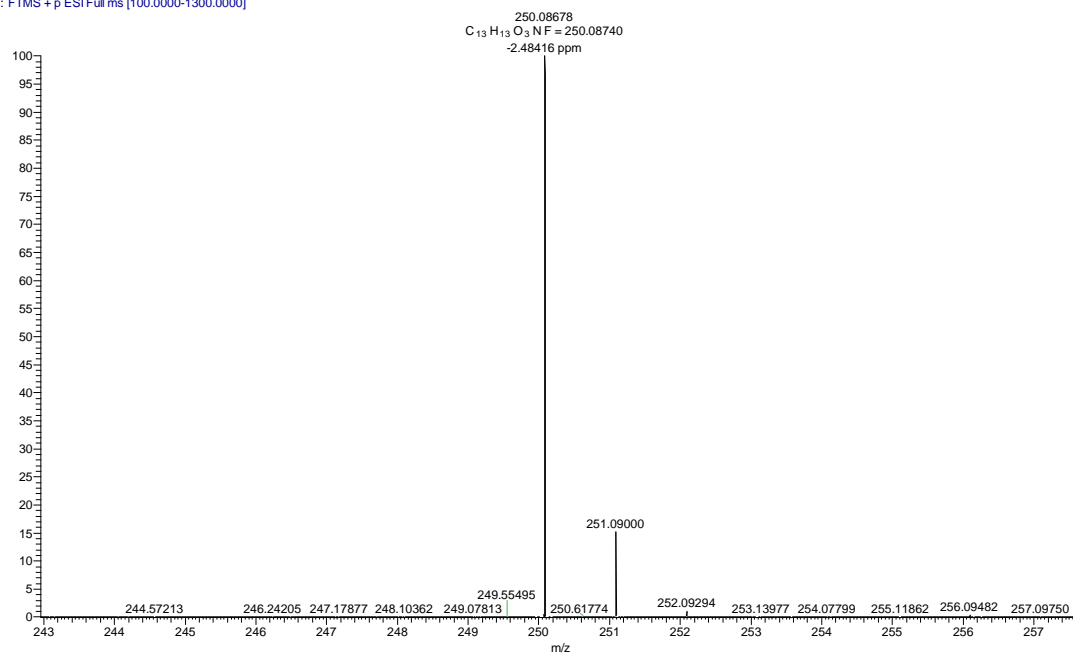


Figure S33. HRMS spectrum of compound B2

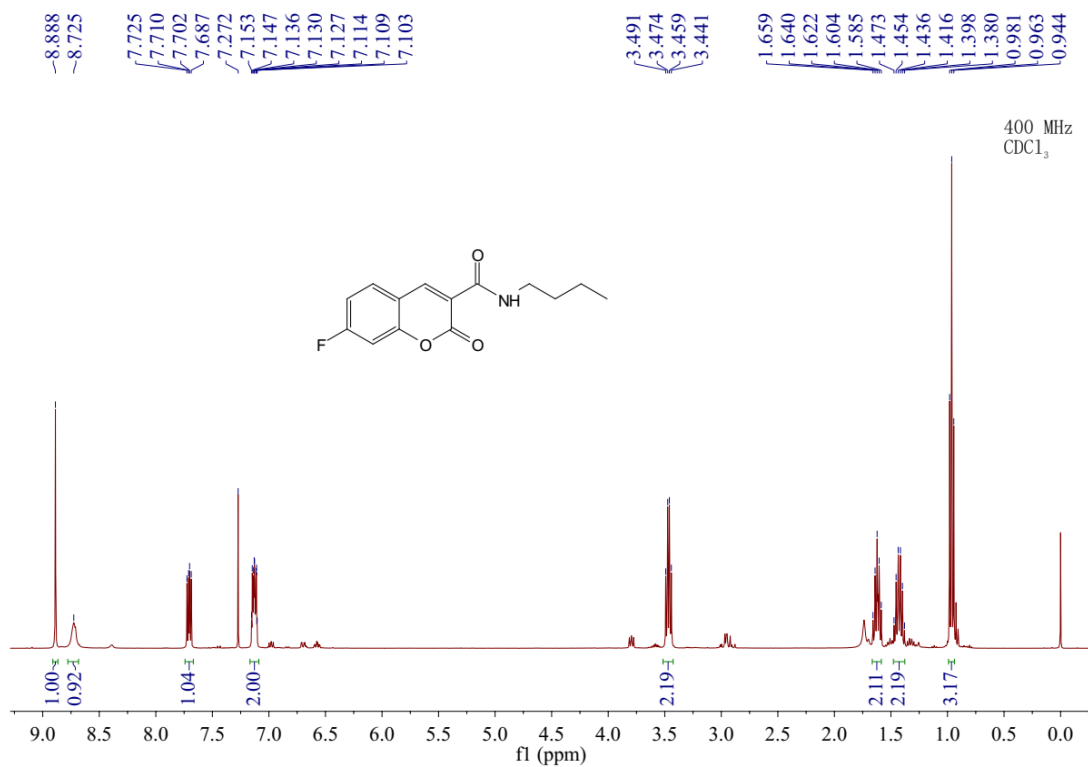


Figure S34 ¹H NMR spectrum of compound B3

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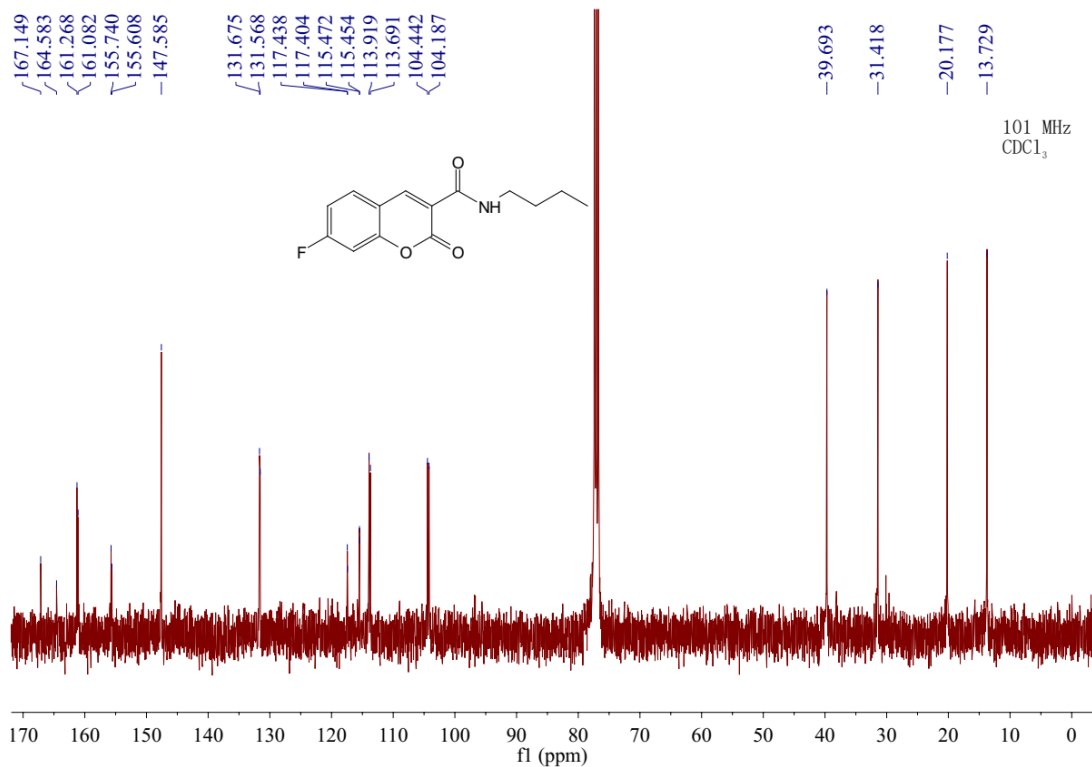


Figure S35. ¹³C NMR spectrum of compound B3

B5 #37 RT: 0.36 AV: 1 NL: 6.46E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

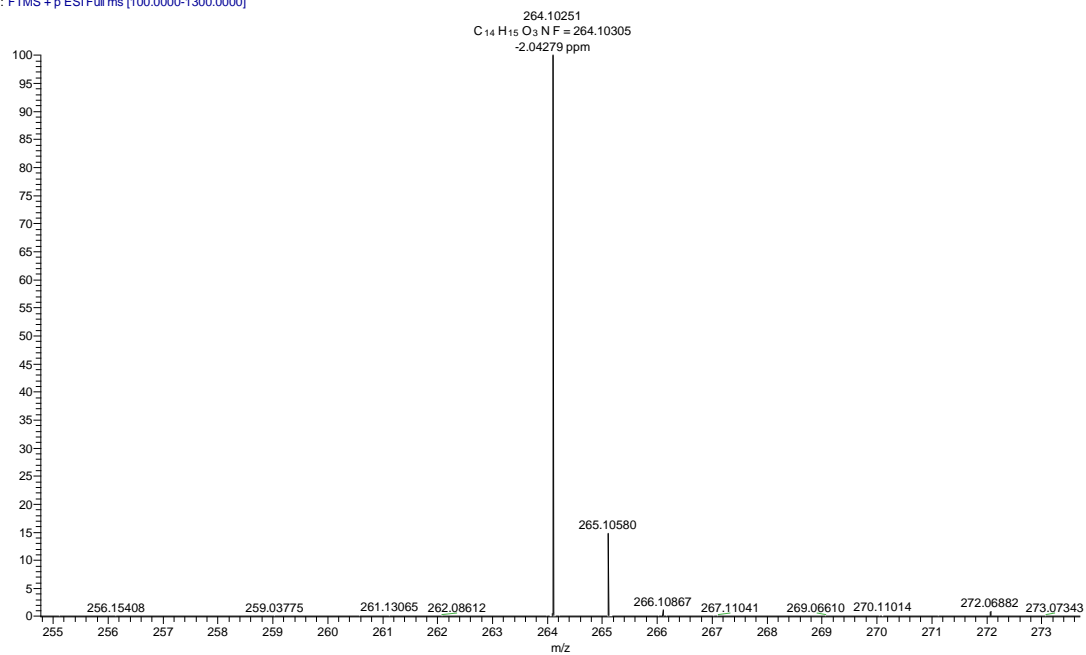
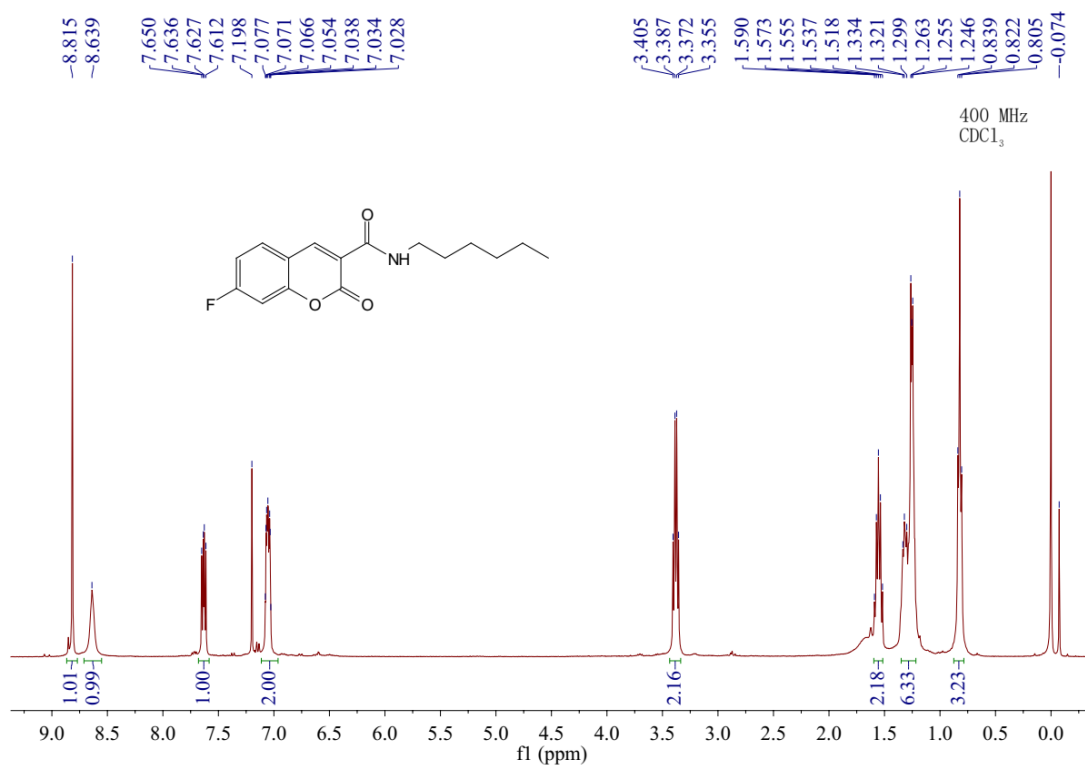


Figure S36. HRMS spectrum of compound B3



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Figure S37 ¹H NMR spectrum of compound B4

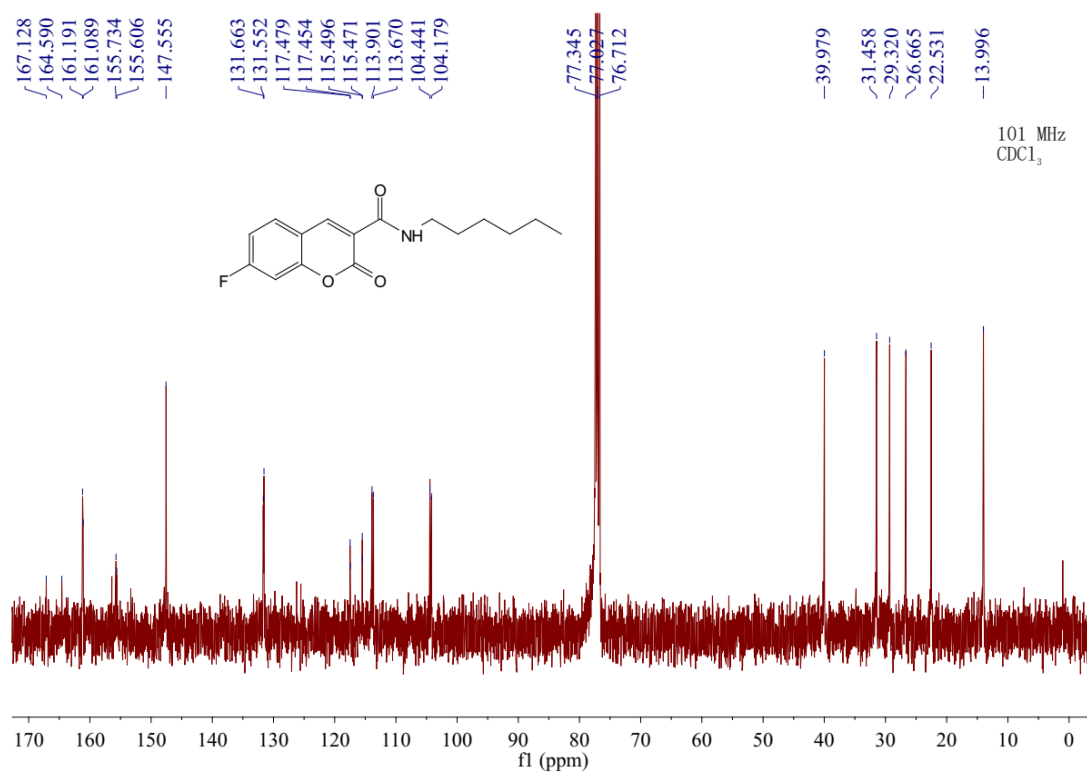


Figure S38. ¹³C NMR spectrum of compound B4

B9 #49 RT: 0.48 AV: 1 NL: 8.03E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

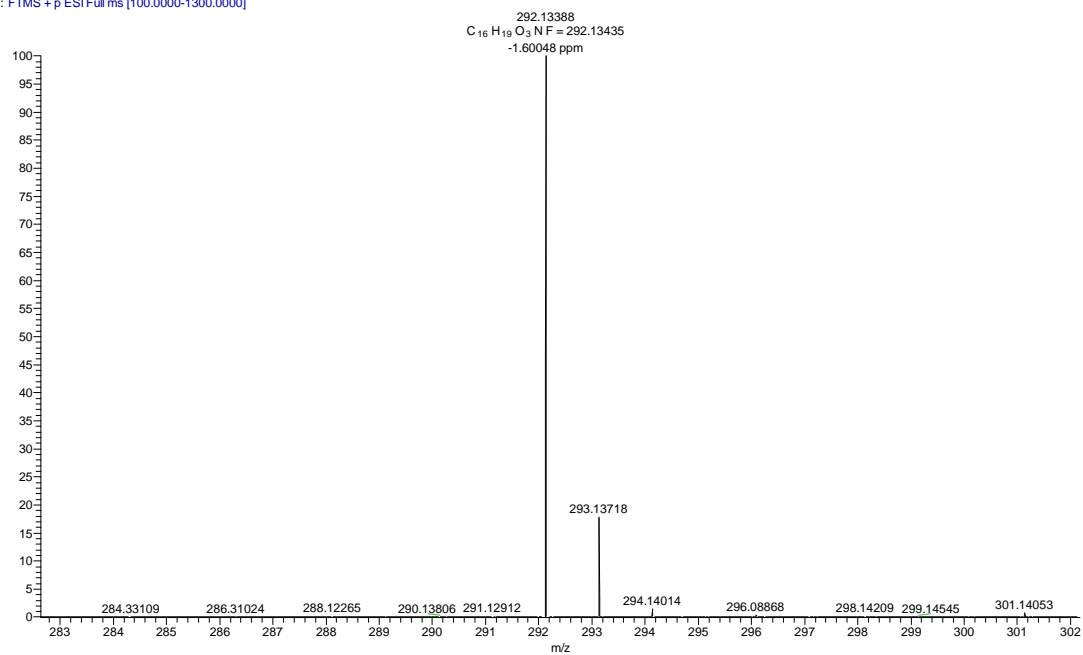


Figure S39. HRMS spectrum of compound B4

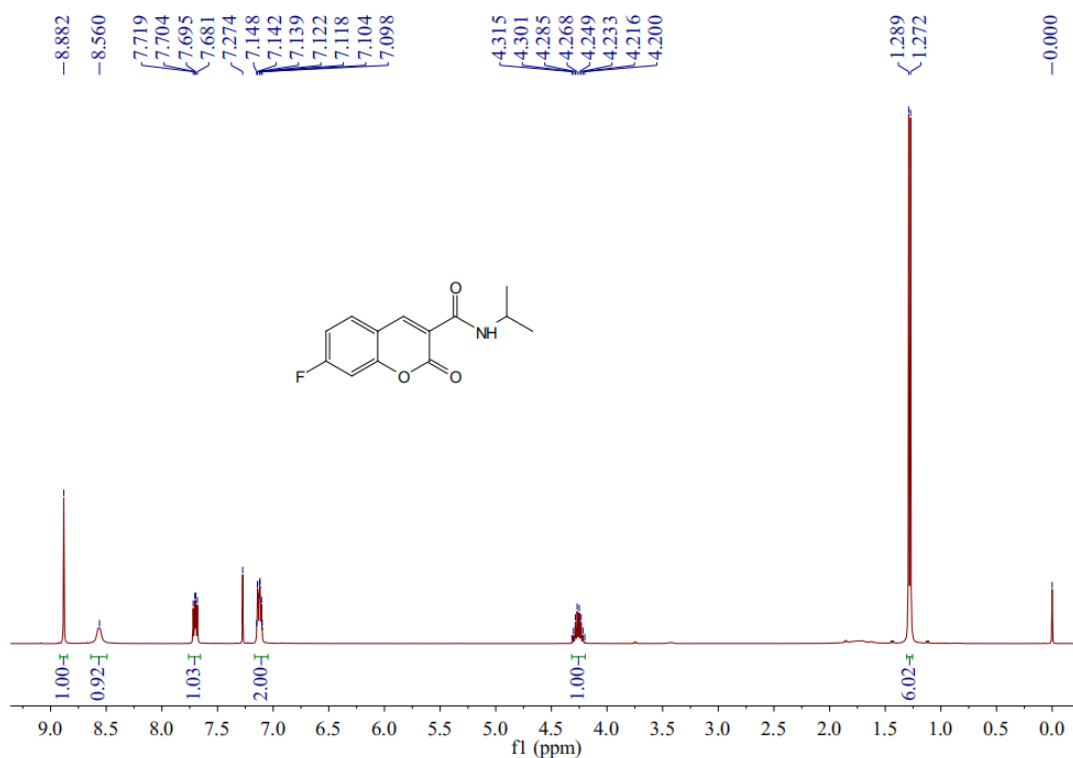


Figure S40 ¹H NMR spectrum of compound B5

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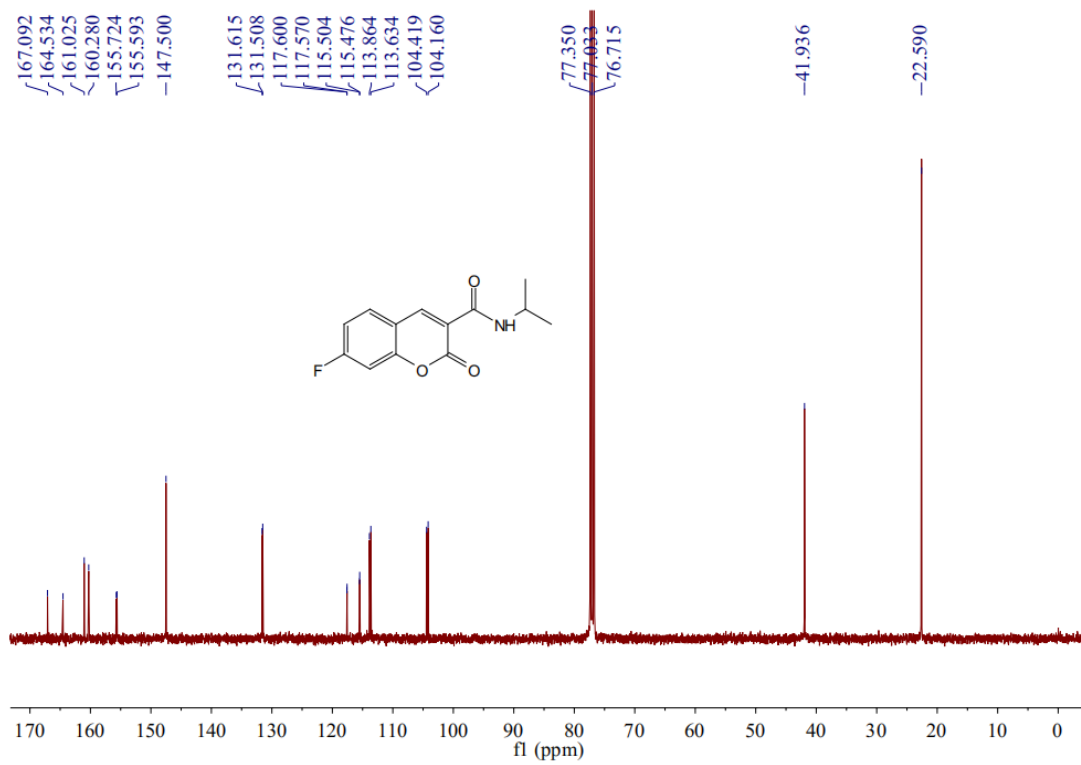


Figure S41. ¹³C NMR spectrum of compound B5

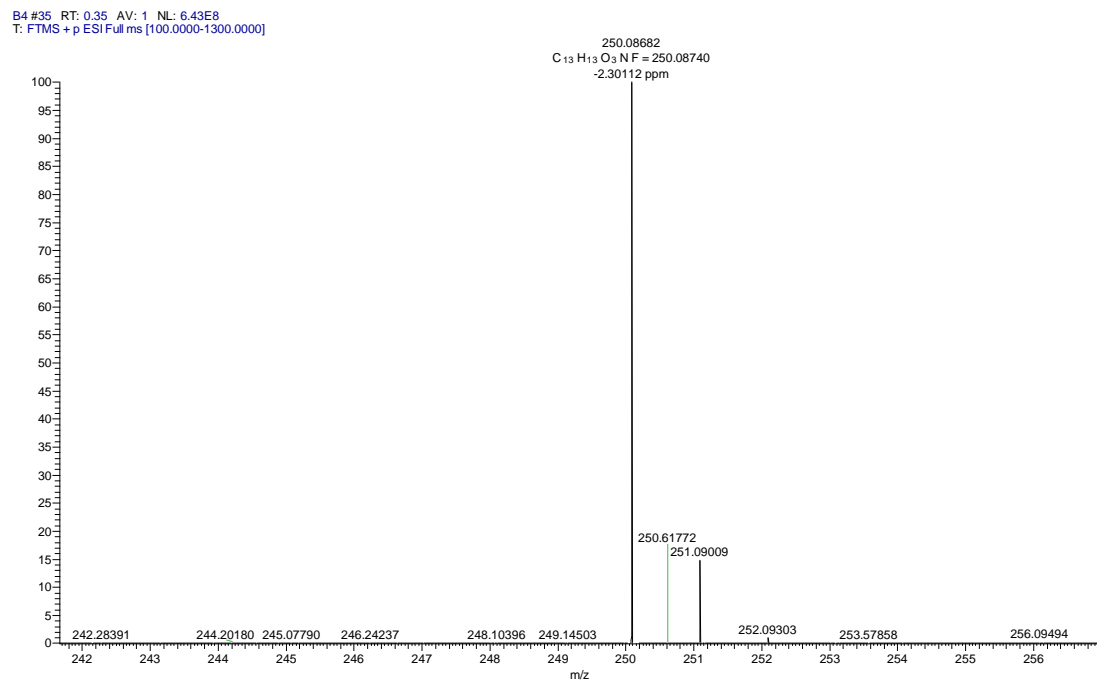
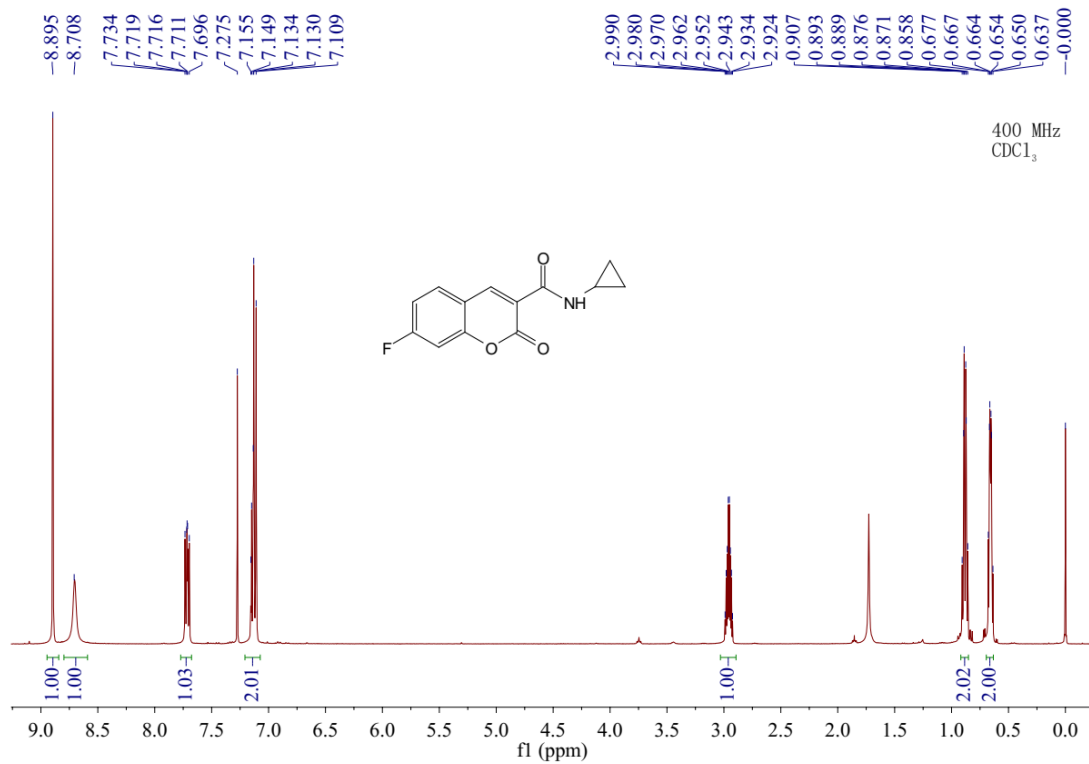
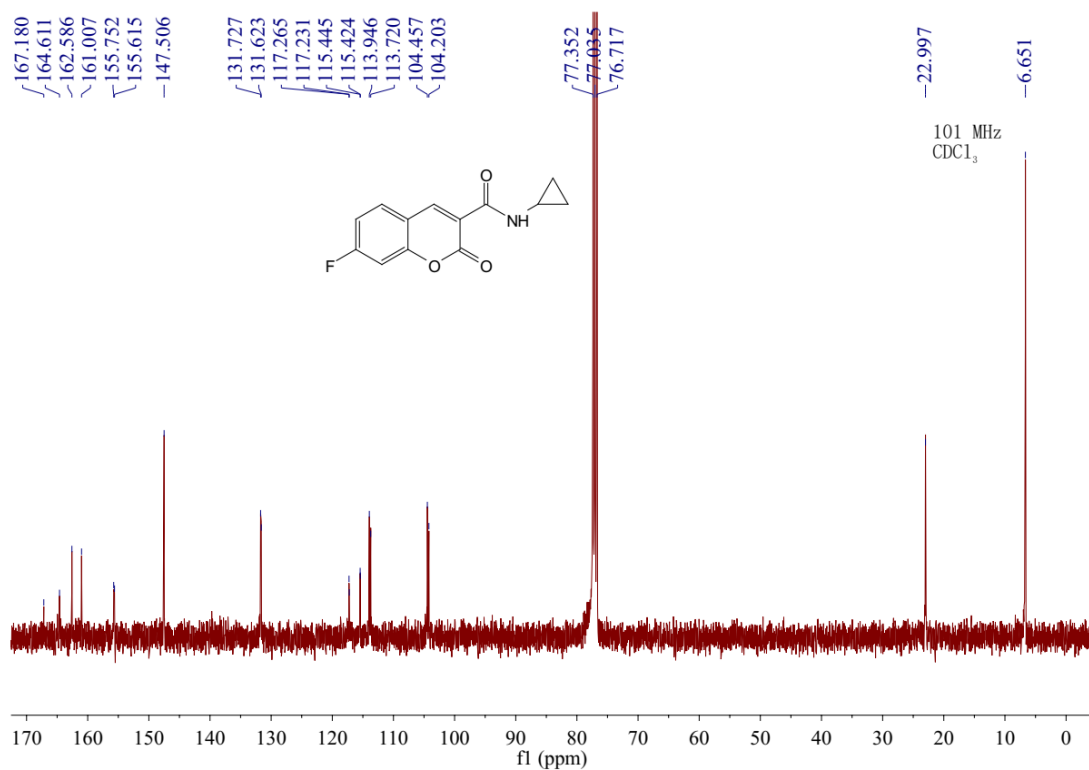


Figure S42. HRMS spectrum of compound B5



26 **Figure S43.** ¹H NMR spectrum of compound B6



55 **Figure S44.** ¹³C NMR spectrum of compound B6

B3 #33 RT: 0.33 AV: 1 NL: 4.24E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

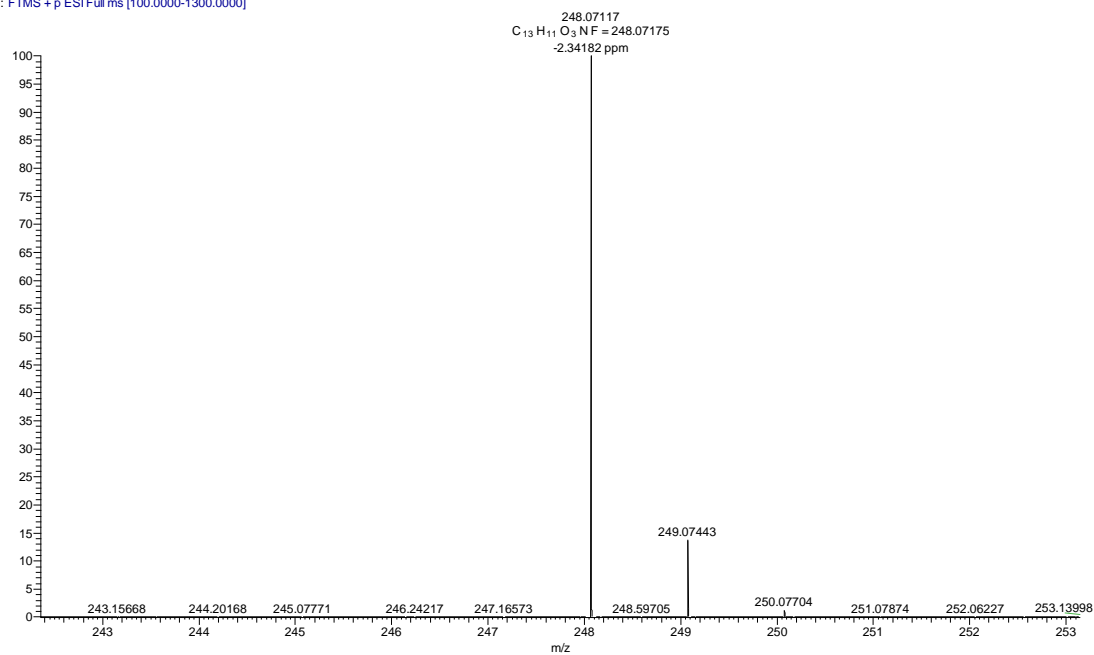


Figure S45. HRMS spectrum of compound B6

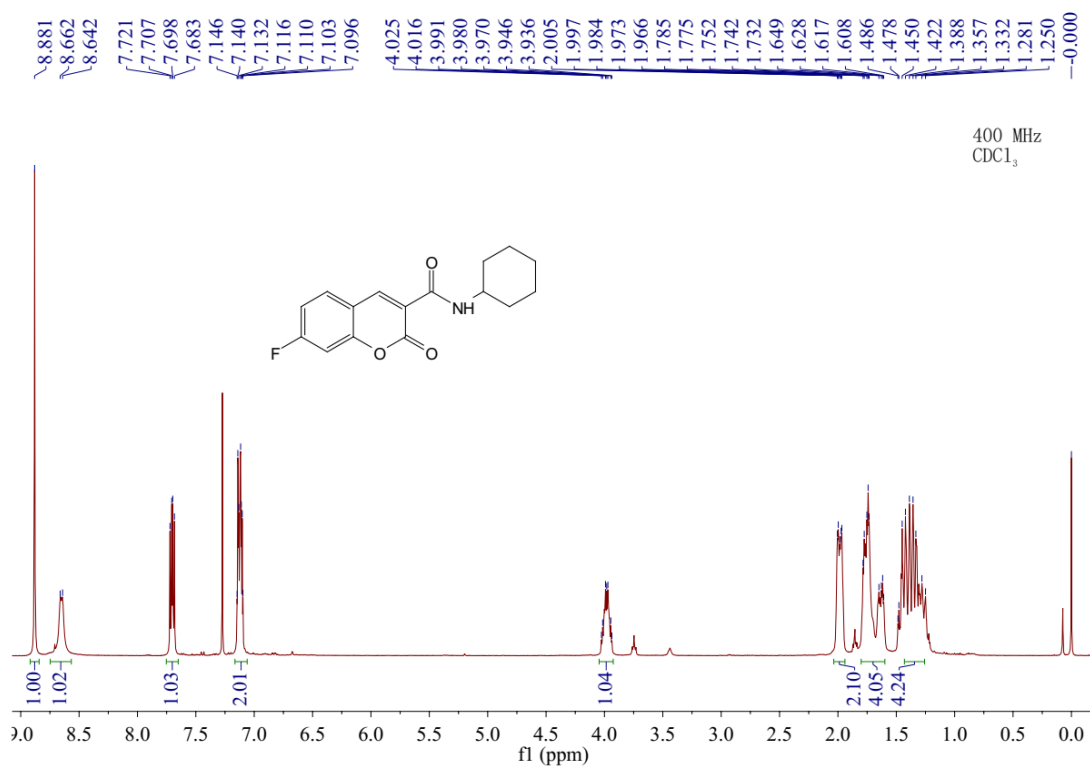


Figure S46. ¹H NMR spectrum of compound B7

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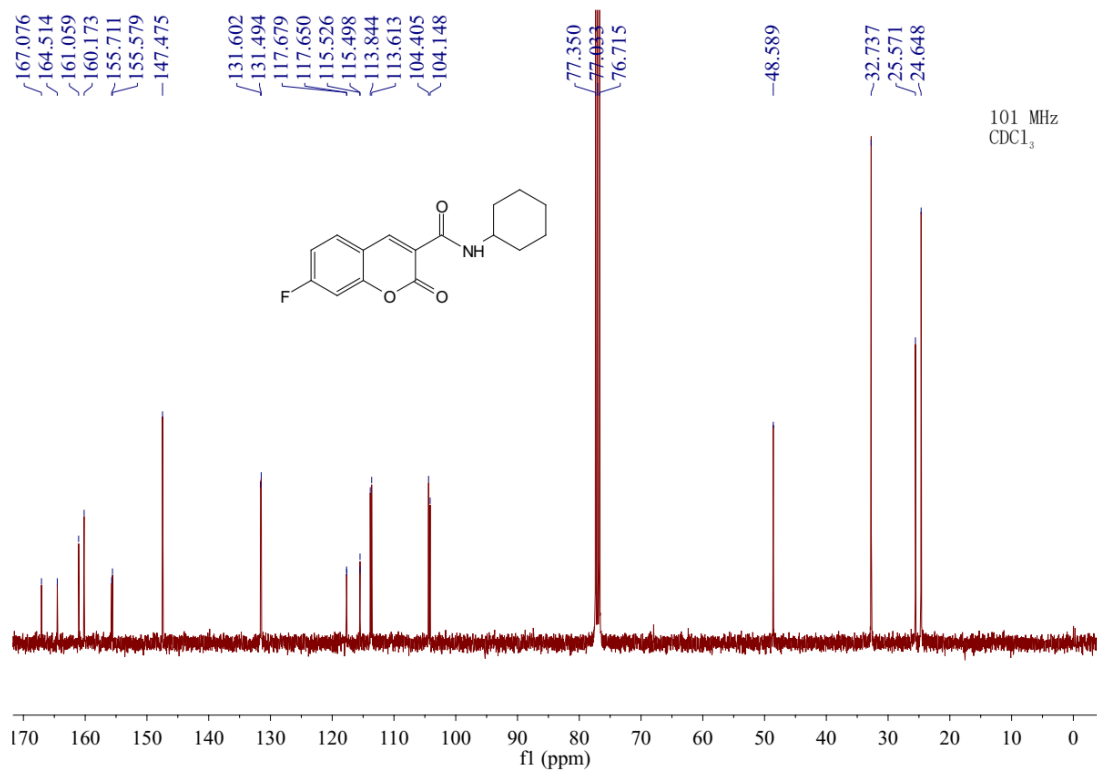


Figure S47. ¹³C NMR spectrum of compound B7

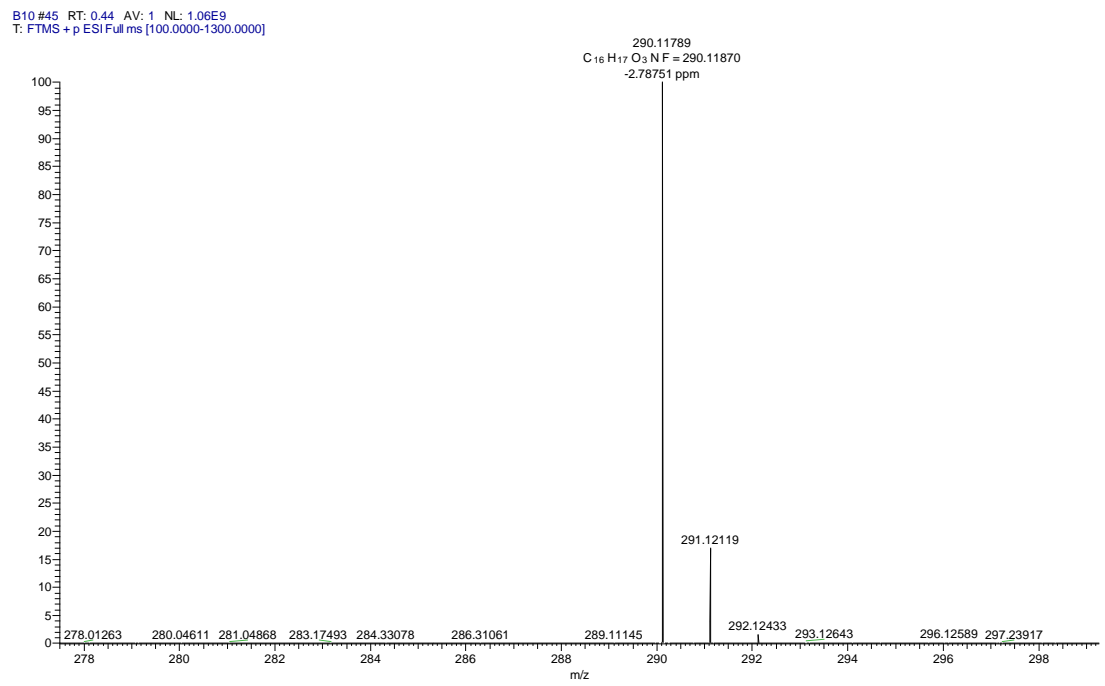


Figure S48. HRMS spectrum of compound B7

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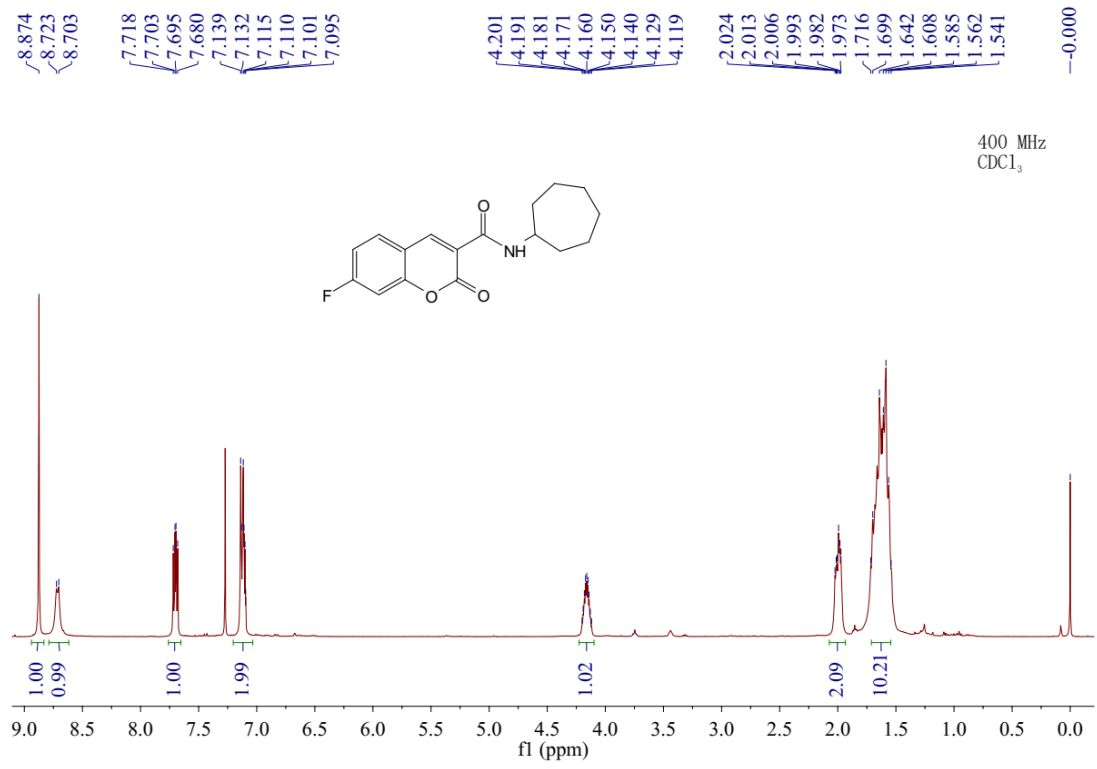


Figure S49. ¹H NMR spectrum of compound B8

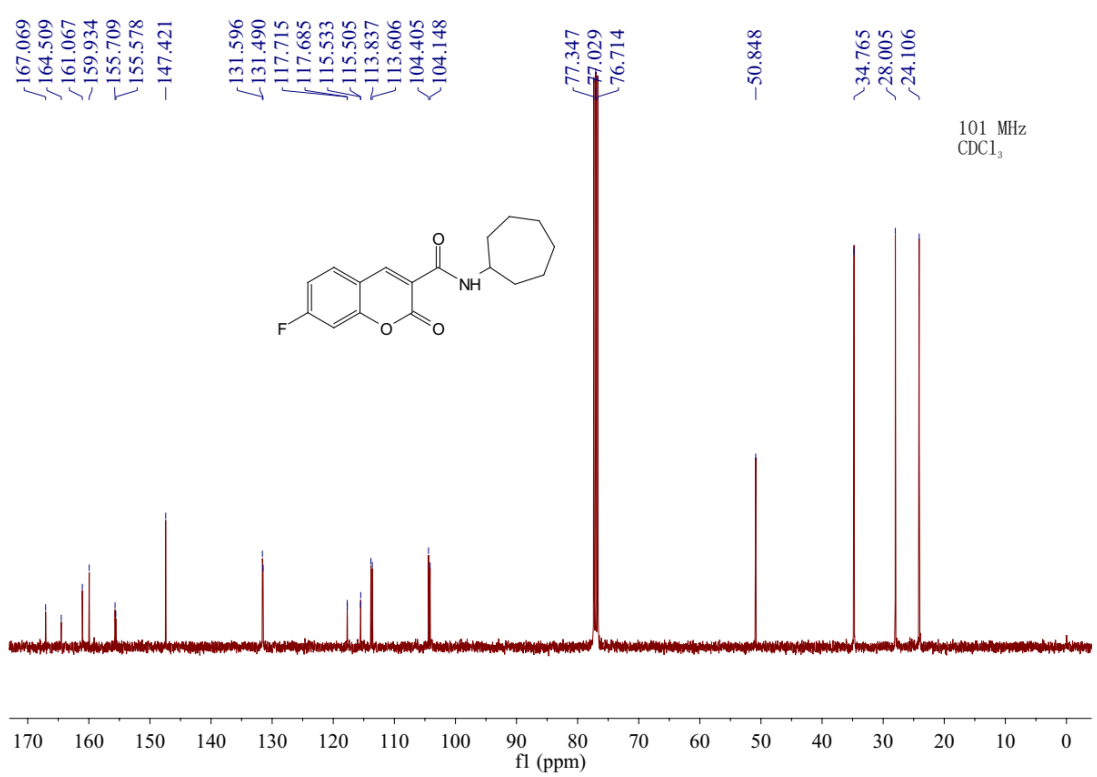


Figure S50. ¹³C NMR spectrum of compound B8

B11 #53 RT: 0.52 AV: 1 NL: 4.59E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

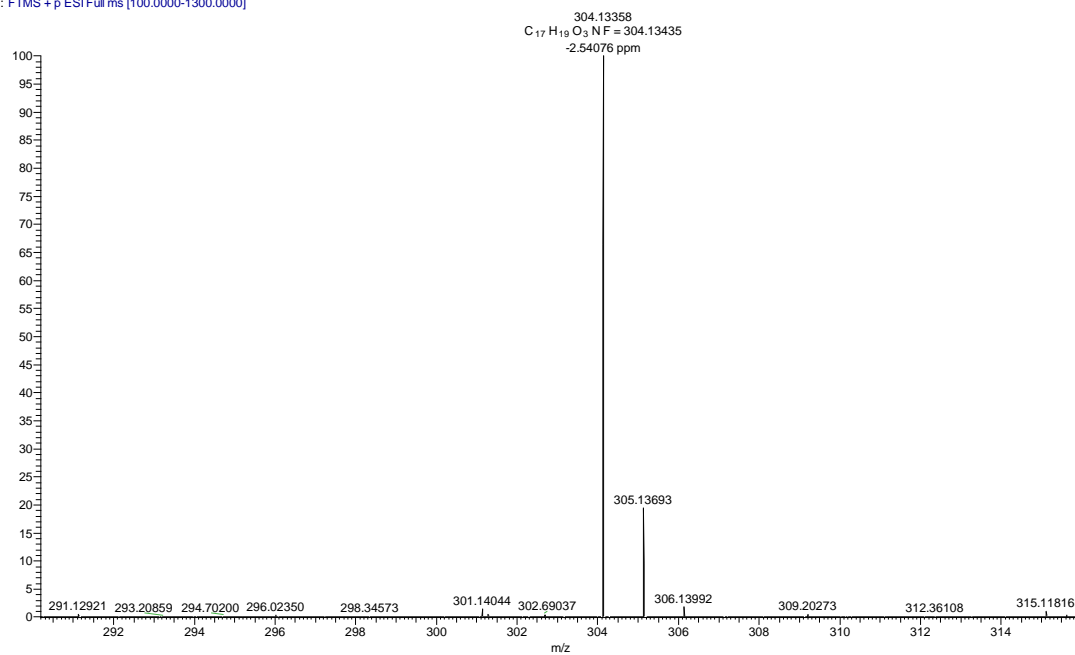


Figure S51. HRMS spectrum of compound B8

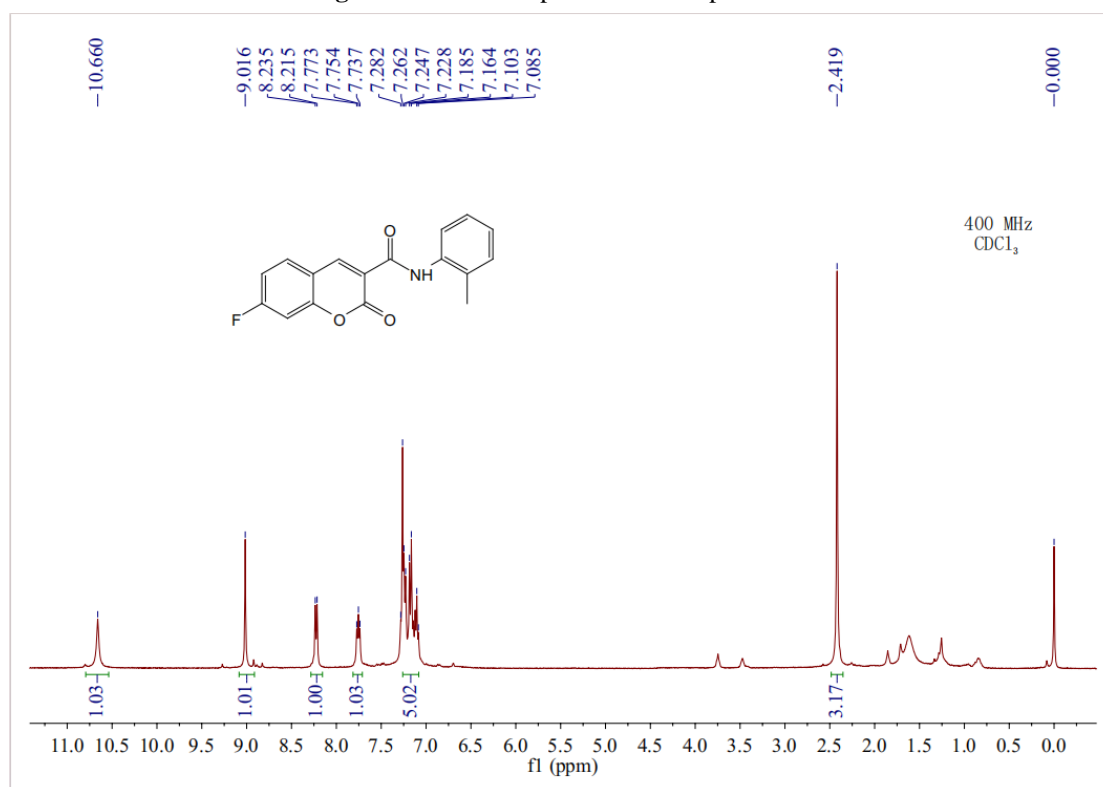


Figure S52. ¹H NMR spectrum of compound B9

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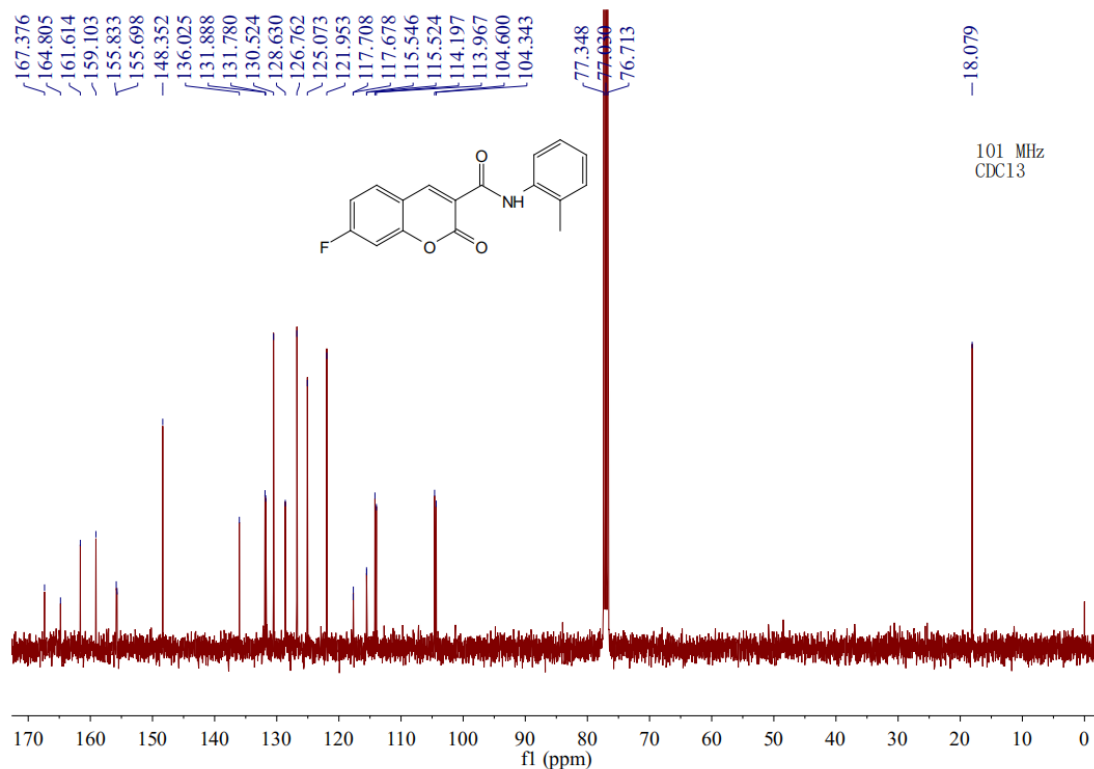


Figure S53. ^{13}C NMR spectrum of compound B9

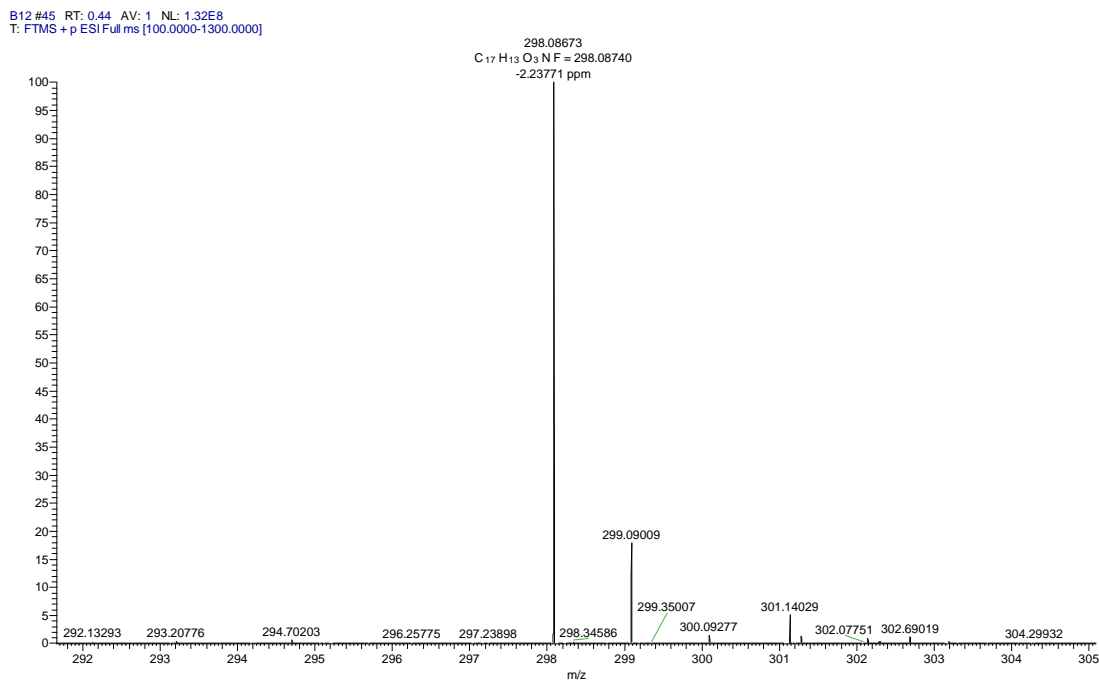
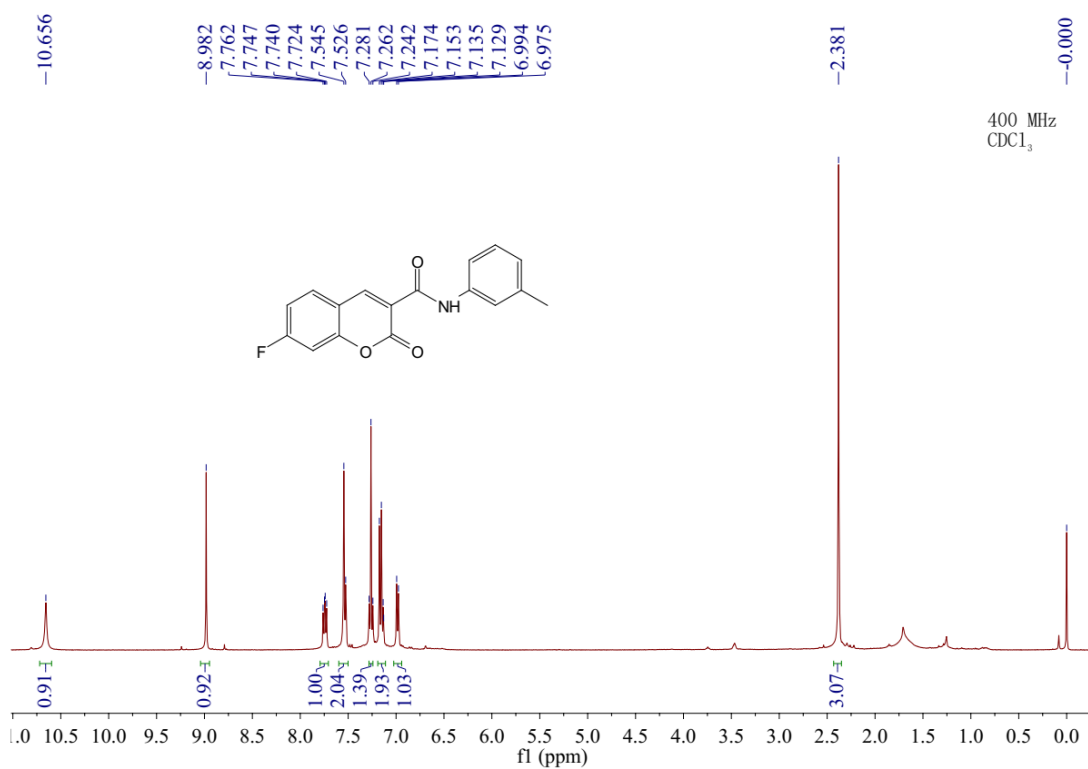
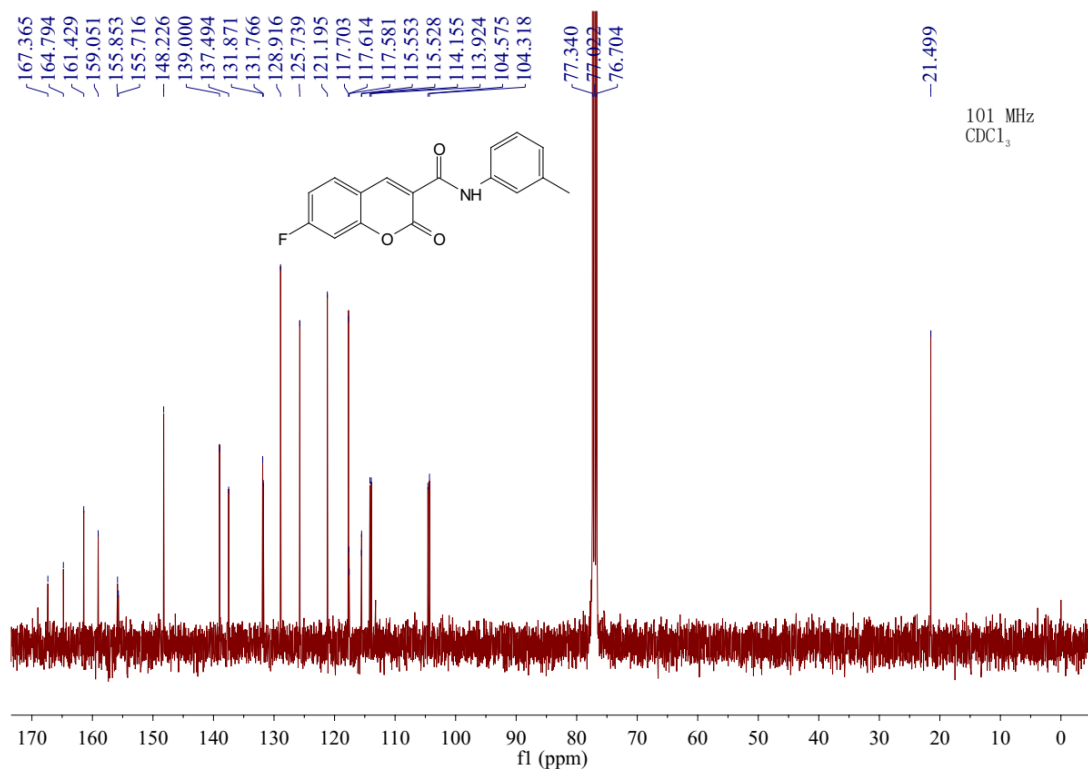


Figure S54. HRMS spectrum of compound B9



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Figure S55. ¹H NMR spectrum of compound B10



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Figure S56. ¹³C NMR spectrum of compound B10

B13 #45 RT: 0.44 AV: 1 NL: 9.39E7
T: FTMS + p ESI Full ms [100.0000-1300.0000]

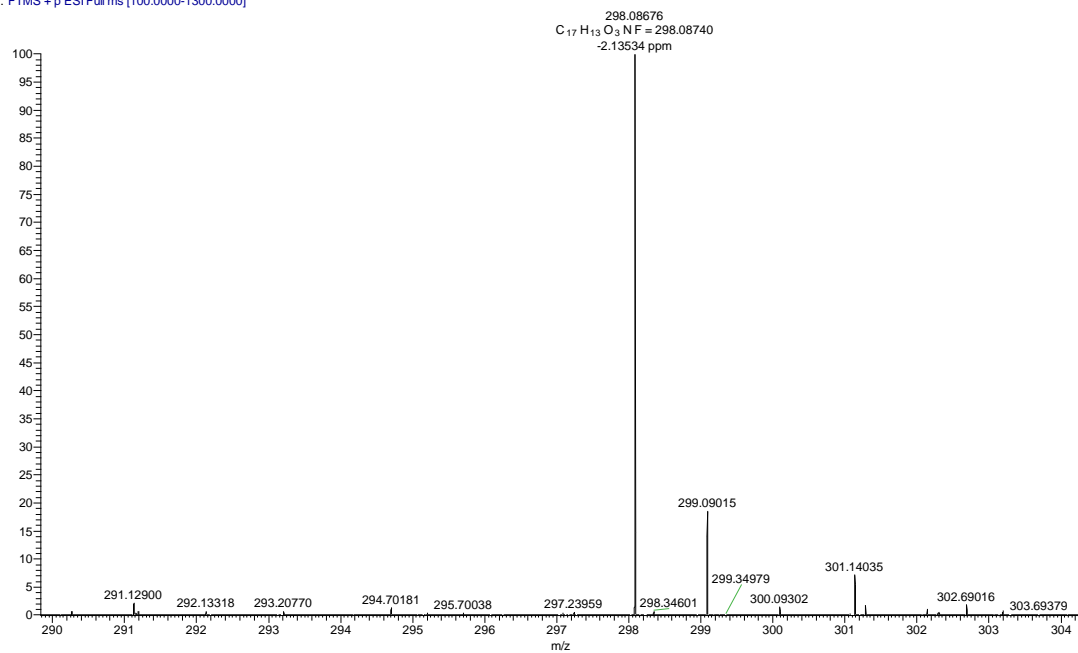


Figure S57. HRMS spectrum of compound B10

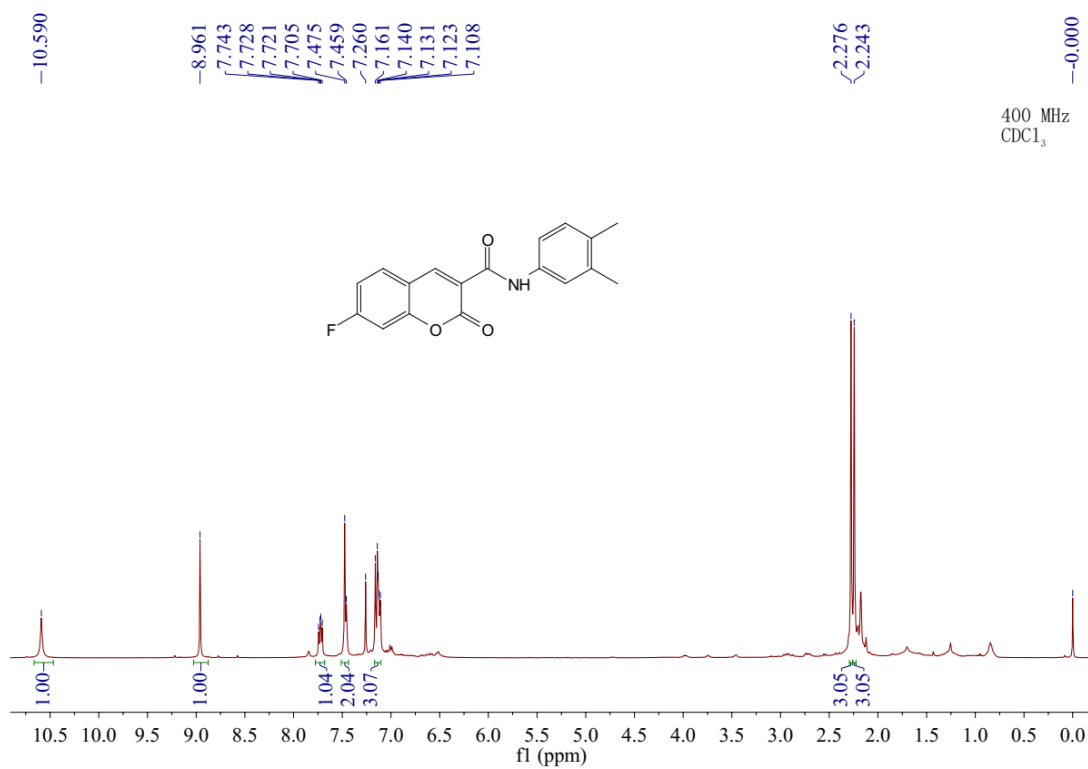


Figure S58. ¹H NMR spectrum of compound B11

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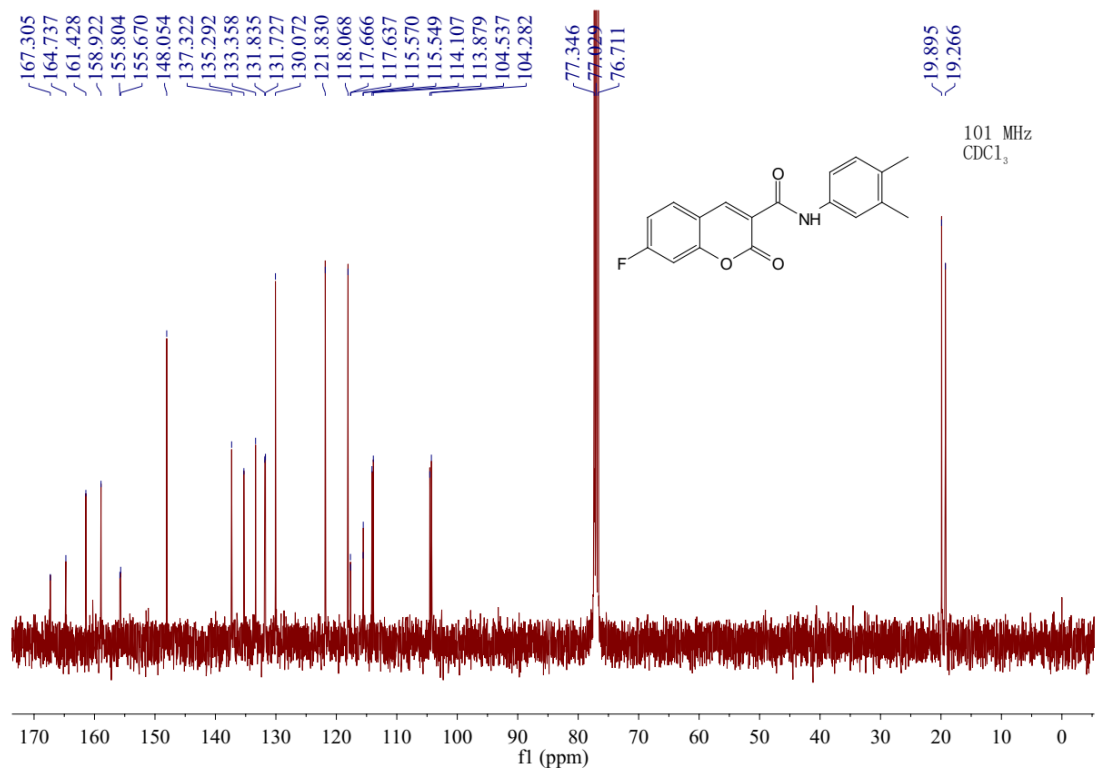


Figure S59. ¹³C NMR spectrum of compound B11

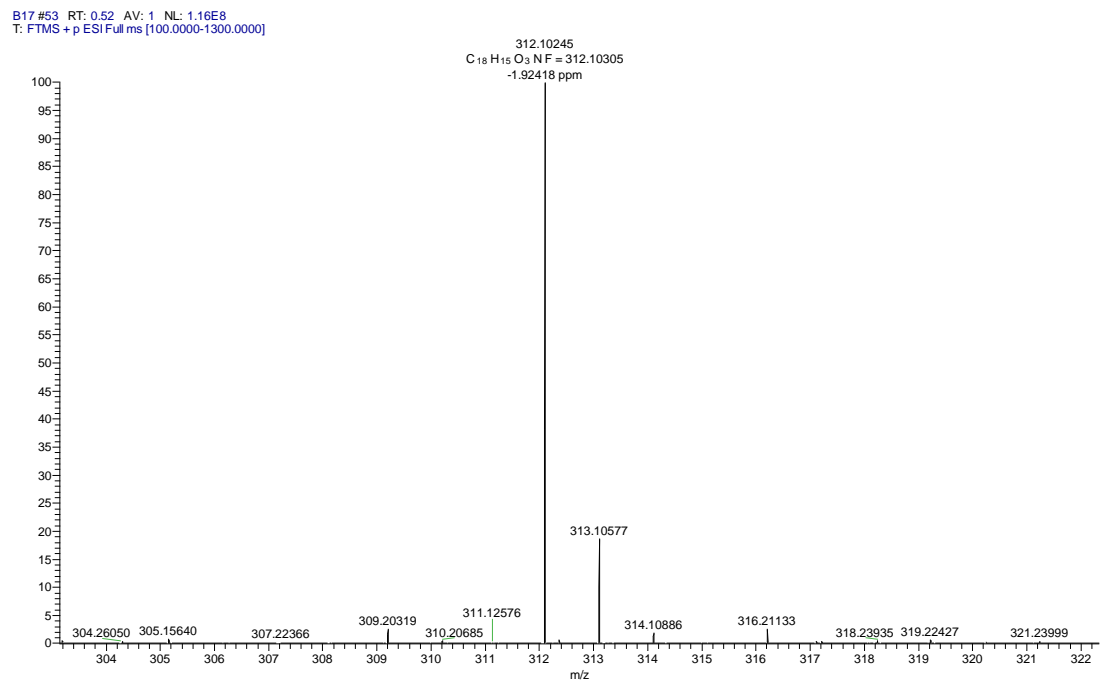
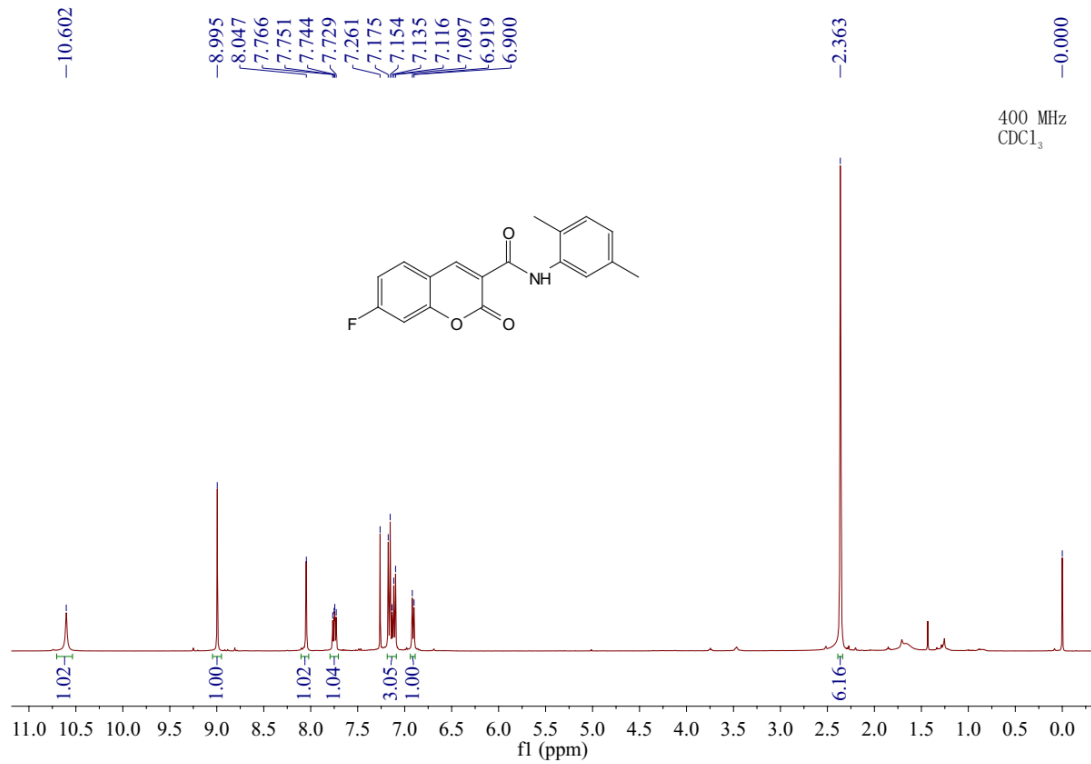
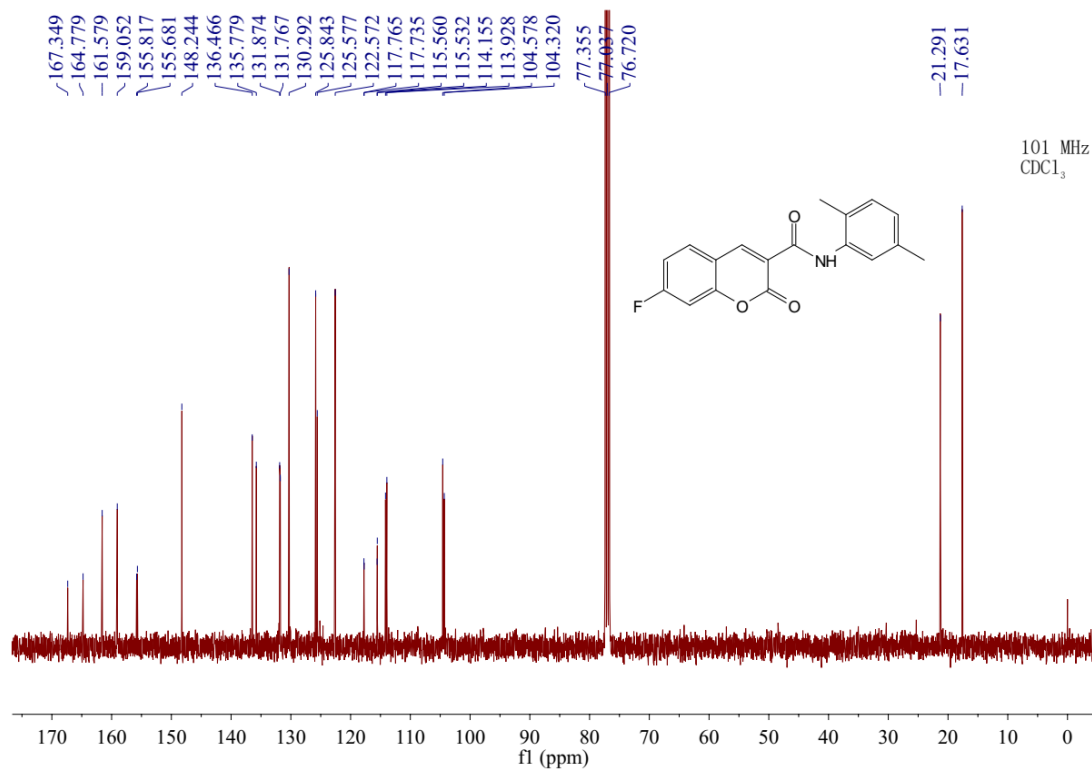


Figure S60. HRMS spectrum of compound B11



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Figure S61. ¹H NMR spectrum of compound B12



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Figure S62. ¹³C NMR spectrum of compound B12

B16 #51 RT: 0.50 AV: 1 NL: 2.82E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

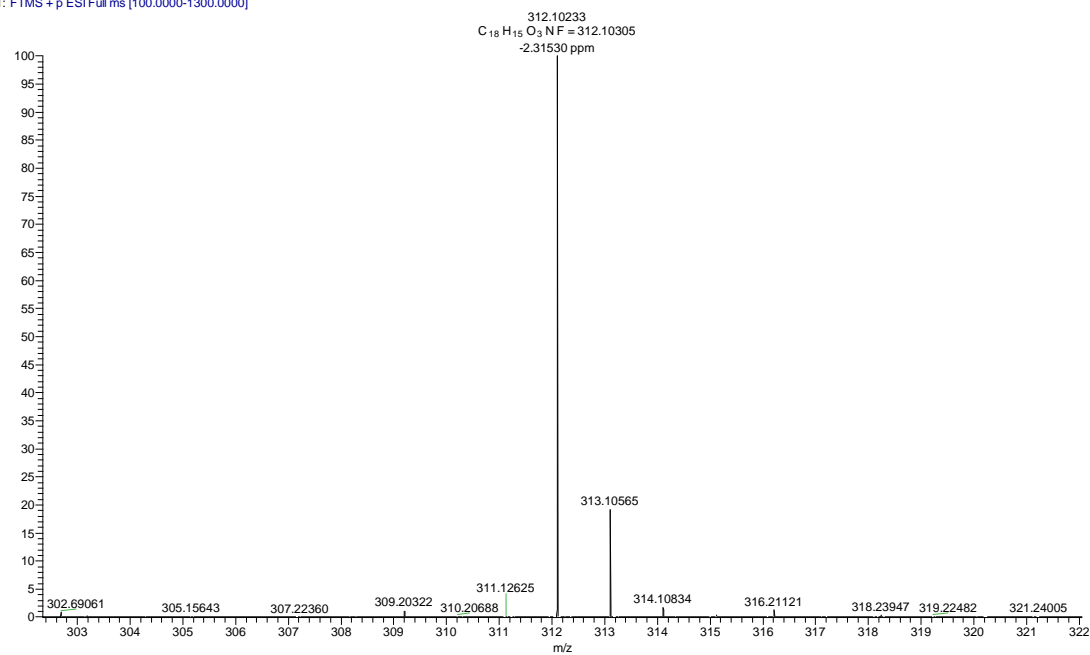


Figure S63. HRMS spectrum of compound B12

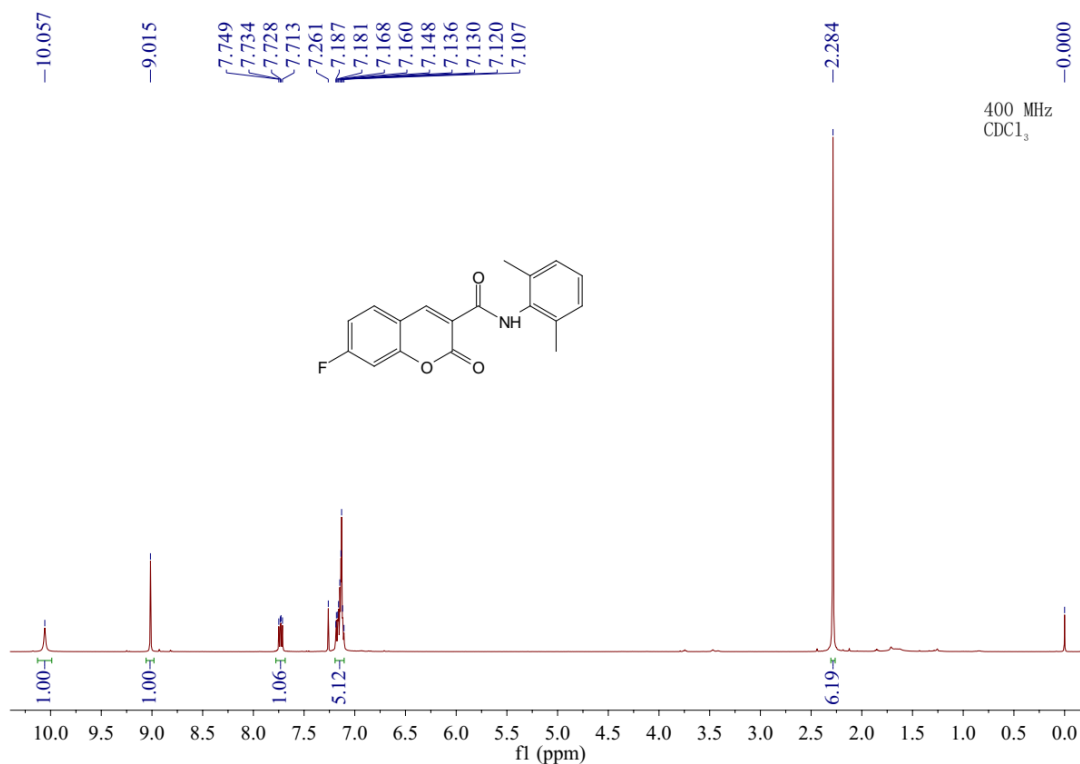


Figure S64. ¹H NMR spectrum of compound B13

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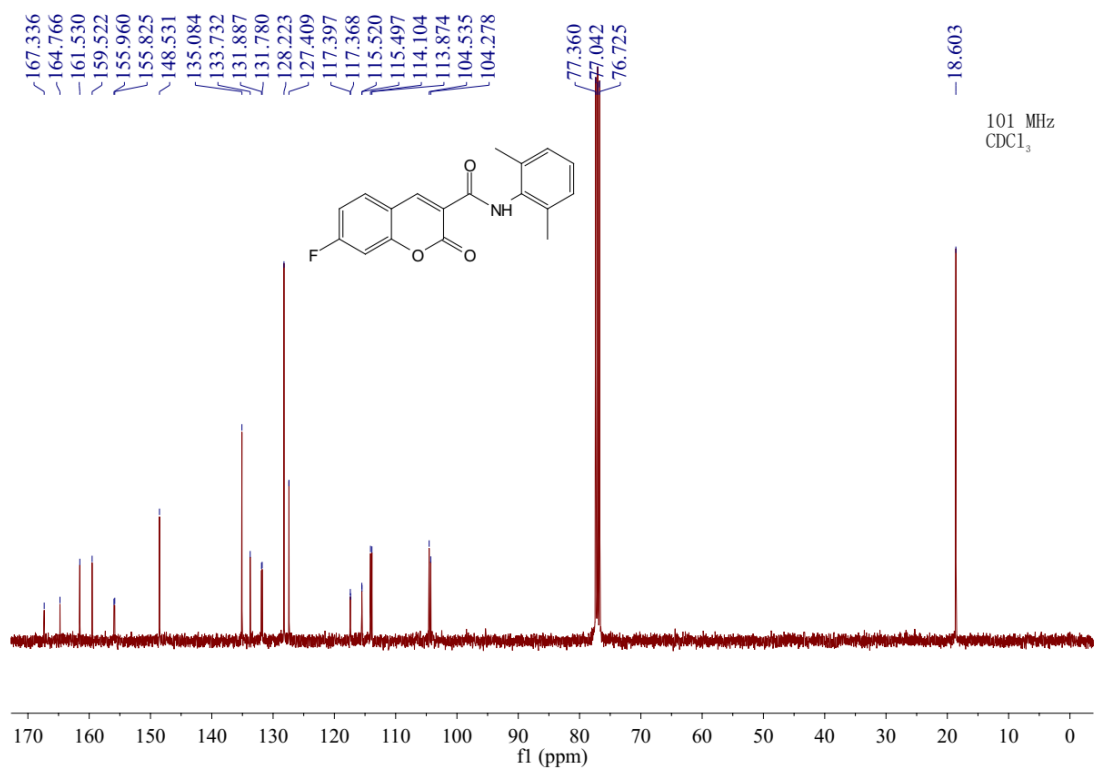


Figure S65. ¹³C NMR spectrum of compound B13

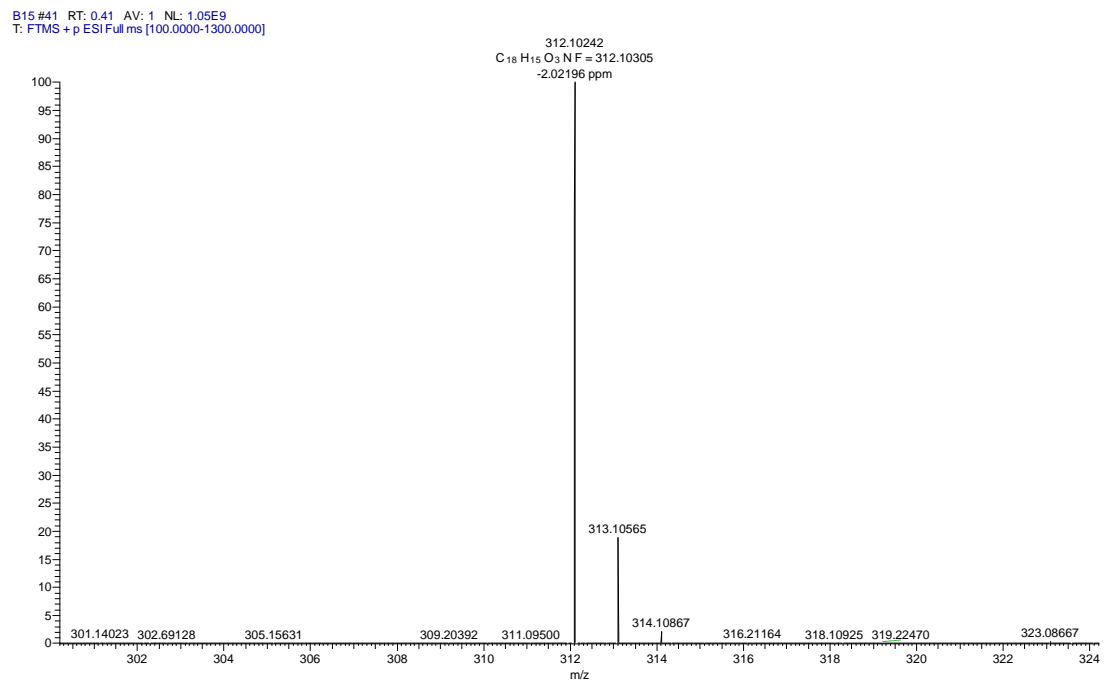
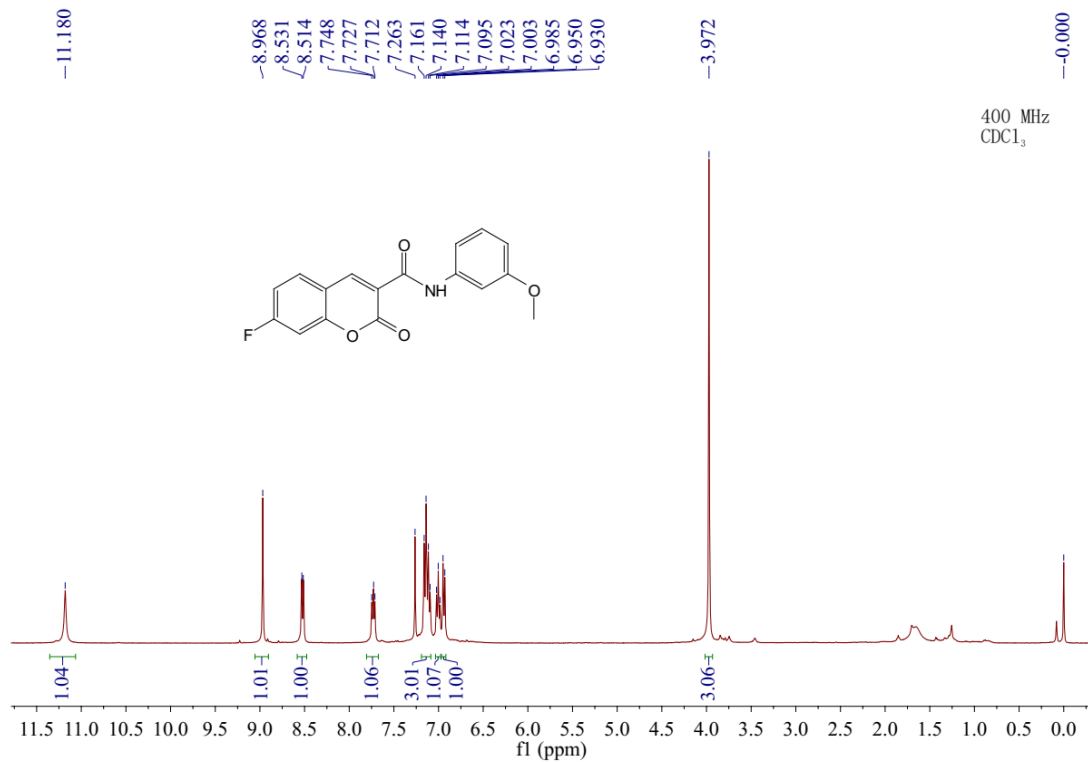
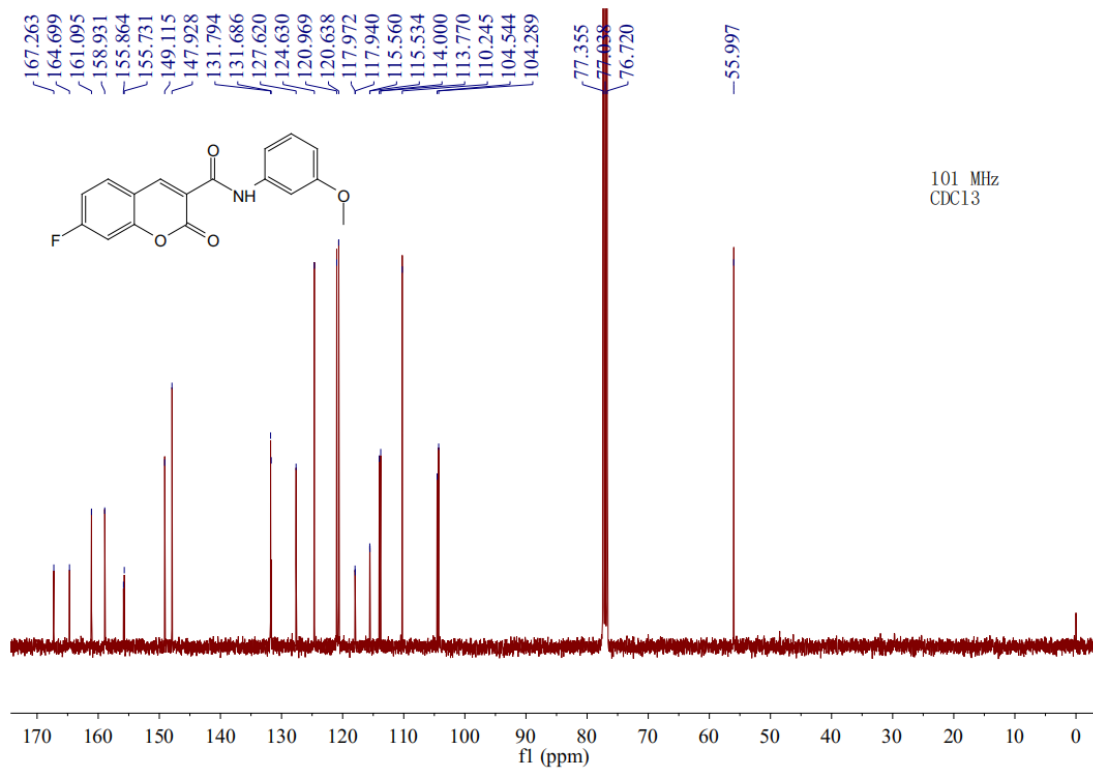


Figure S66. HRMS spectrum of compound B13



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Figure S67. ¹H NMR spectrum of compound B14



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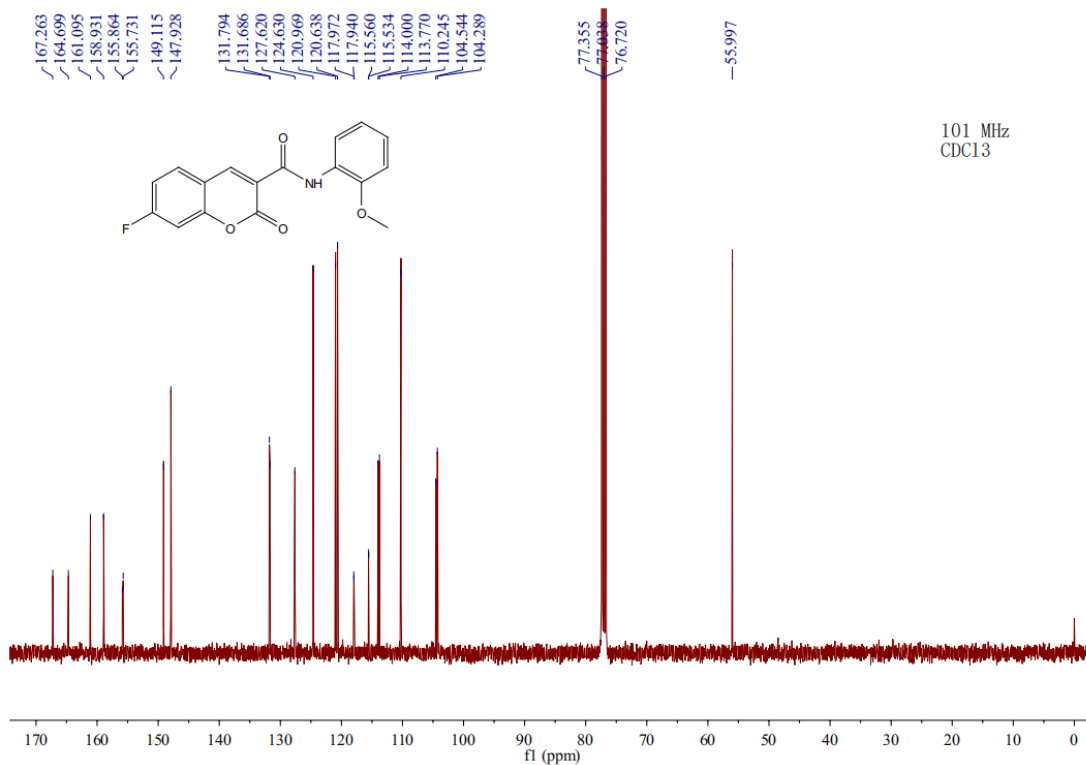


Figure S68. ¹³C NMR spectrum of compound B14

B14 #43 RT: 0.42 AV: 1 NL: 1.75E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

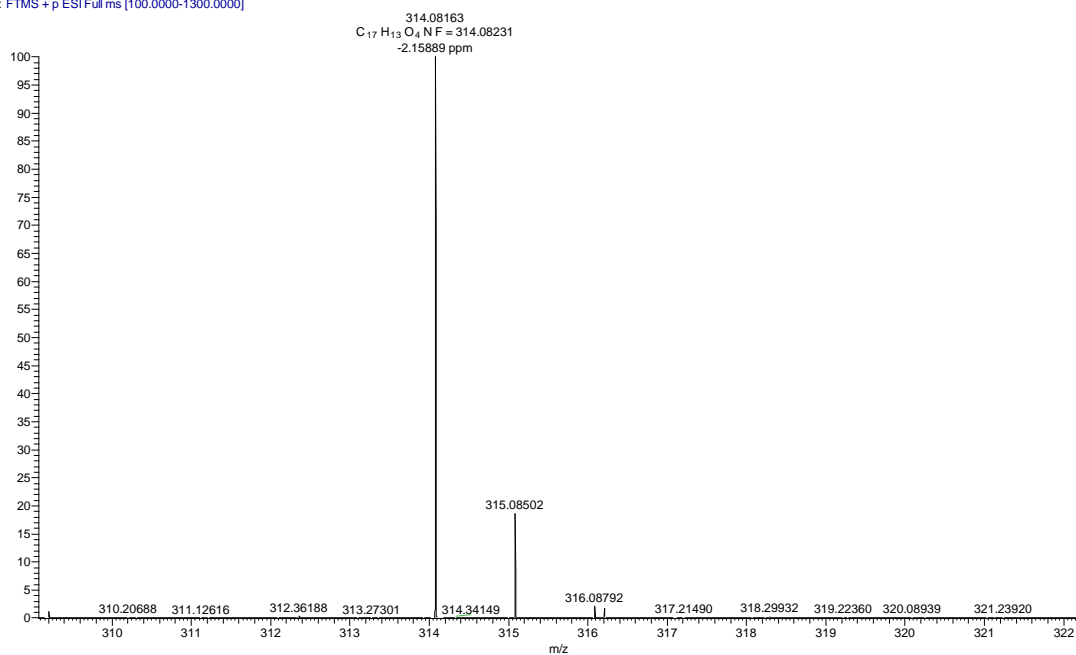
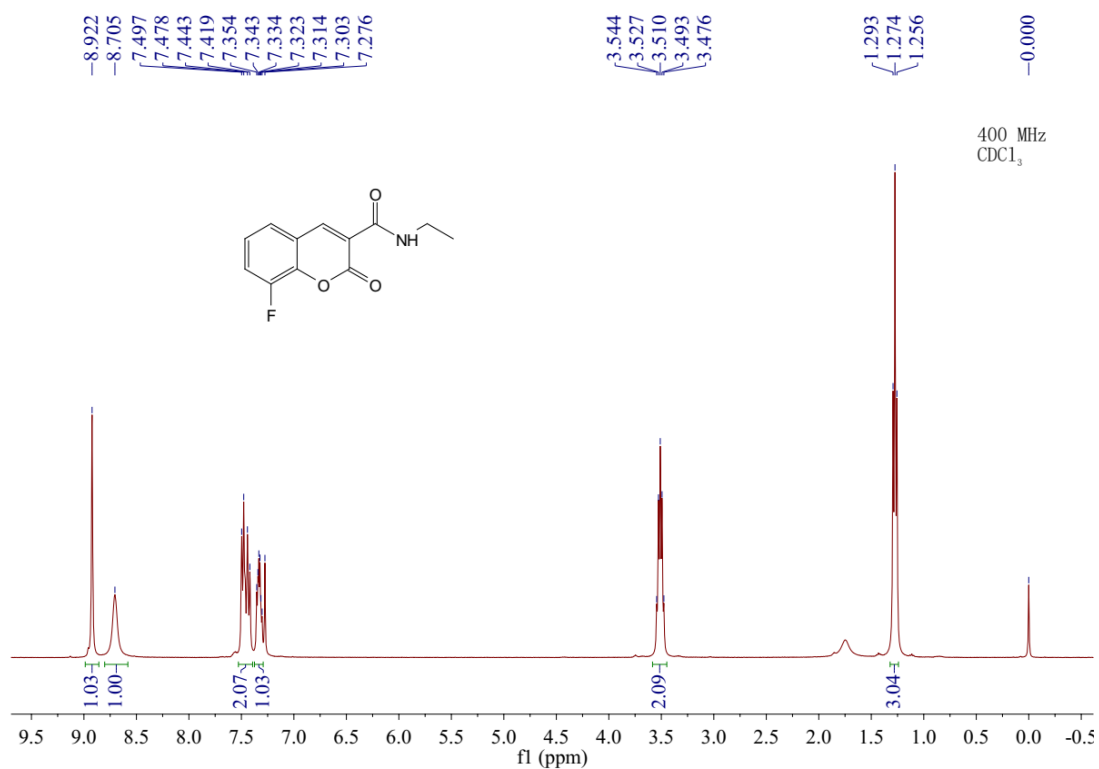


Figure S69. HRMS spectrum of compound B14



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Figure S70. ¹H NMR spectrum of compound C1

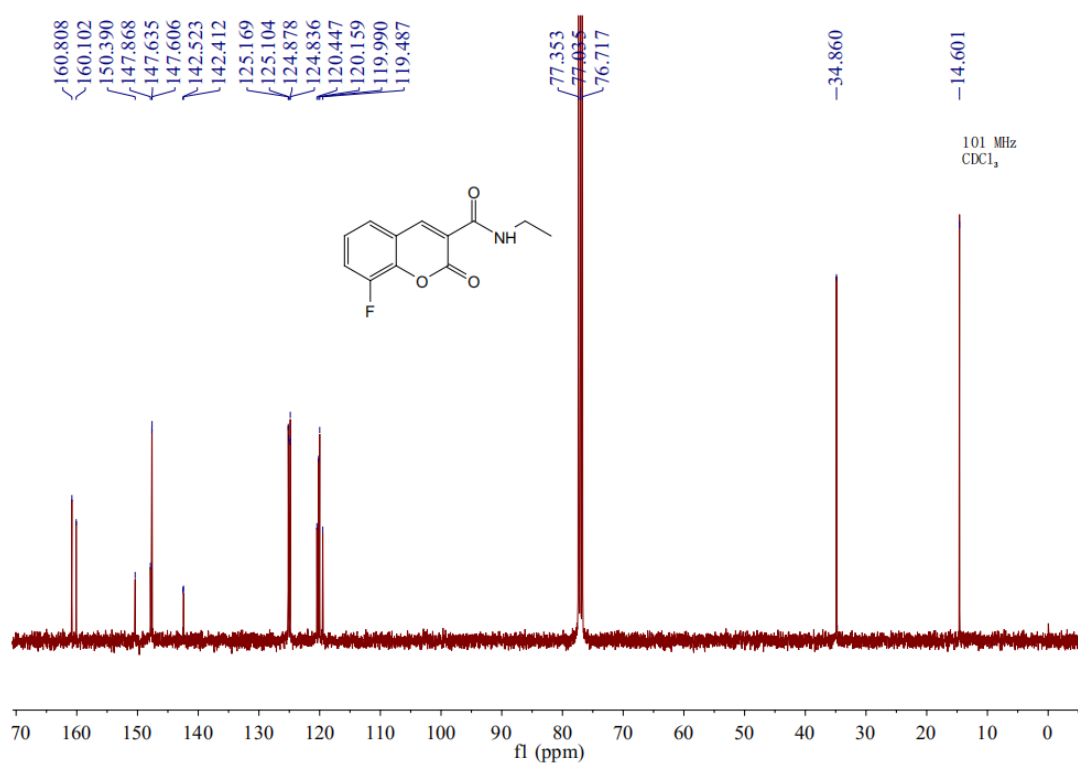


Figure S71. ¹³C NMR spectrum of compound C1

A1 #35 RT: 0.34 AV: 1 NL: 2.16E8
T: FTMS + p ESIFull.ms [100.0000-1300.0000]

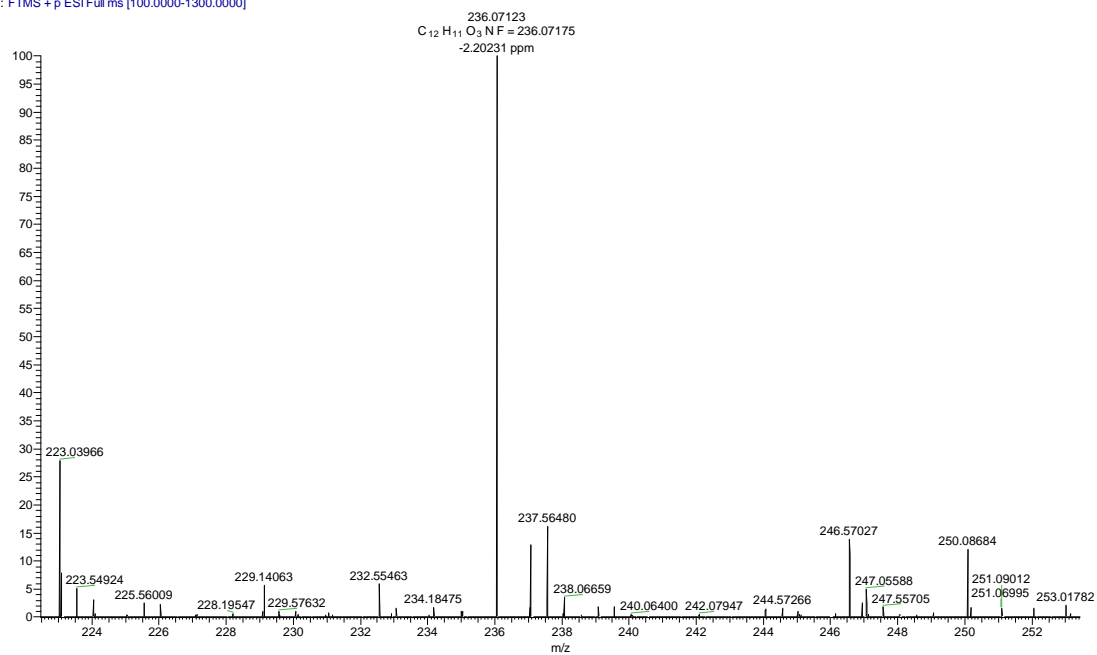


Figure S72. HRMS spectrum of compound C1

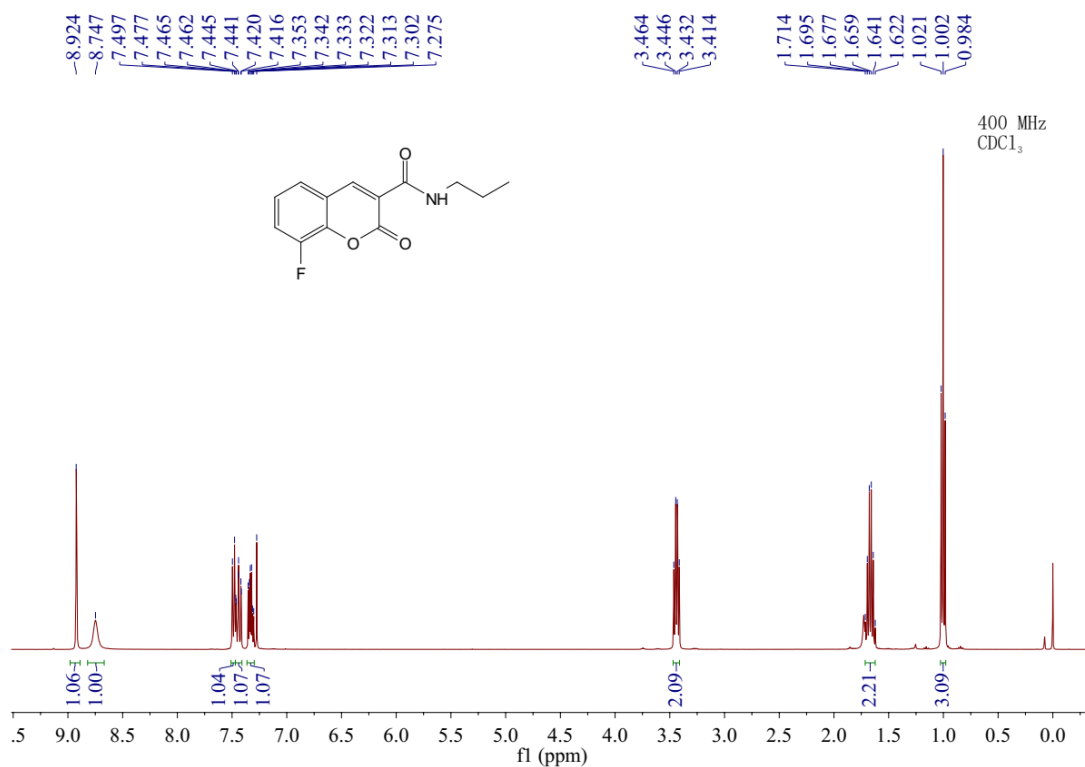


Figure S73. ¹H NMR spectrum of compound C2

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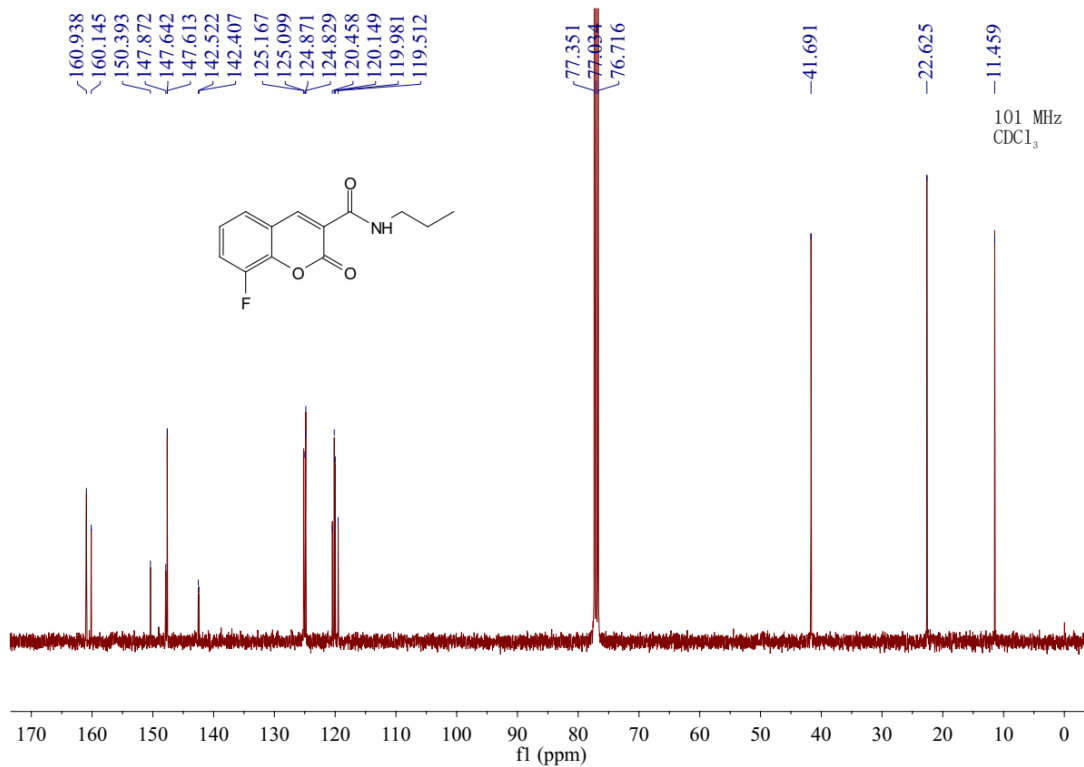


Figure S74. ¹³C NMR spectrum of compound C2

A2 #69 RT: 0.67 AV: 1 NL: 9.08E6
T: FTMS + p ESI Full ms [100.0000-1300.0000]

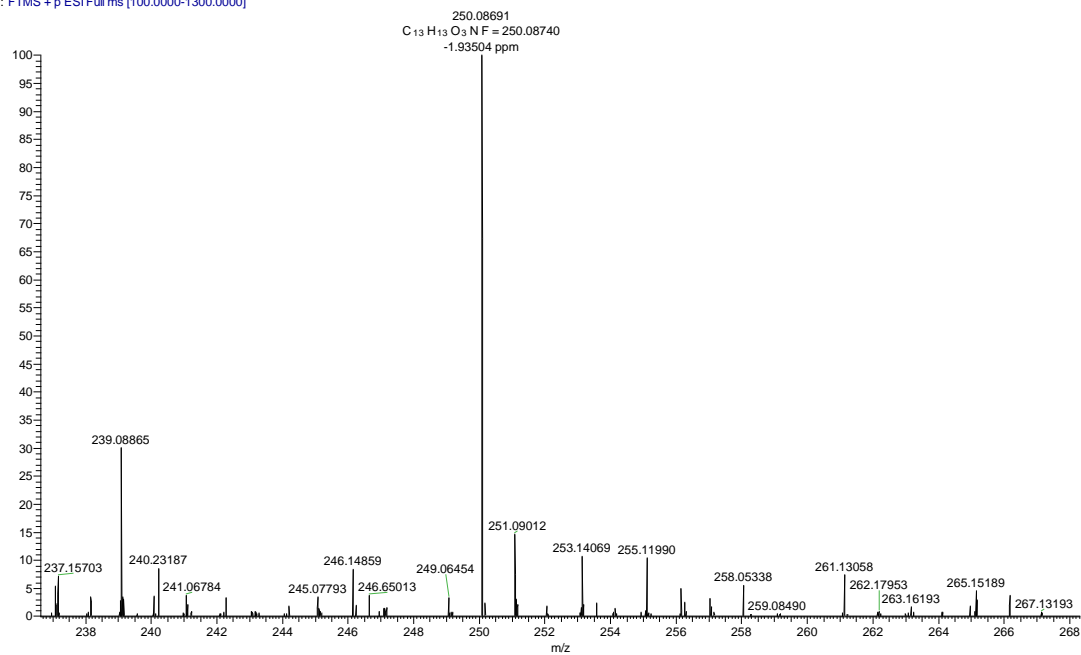
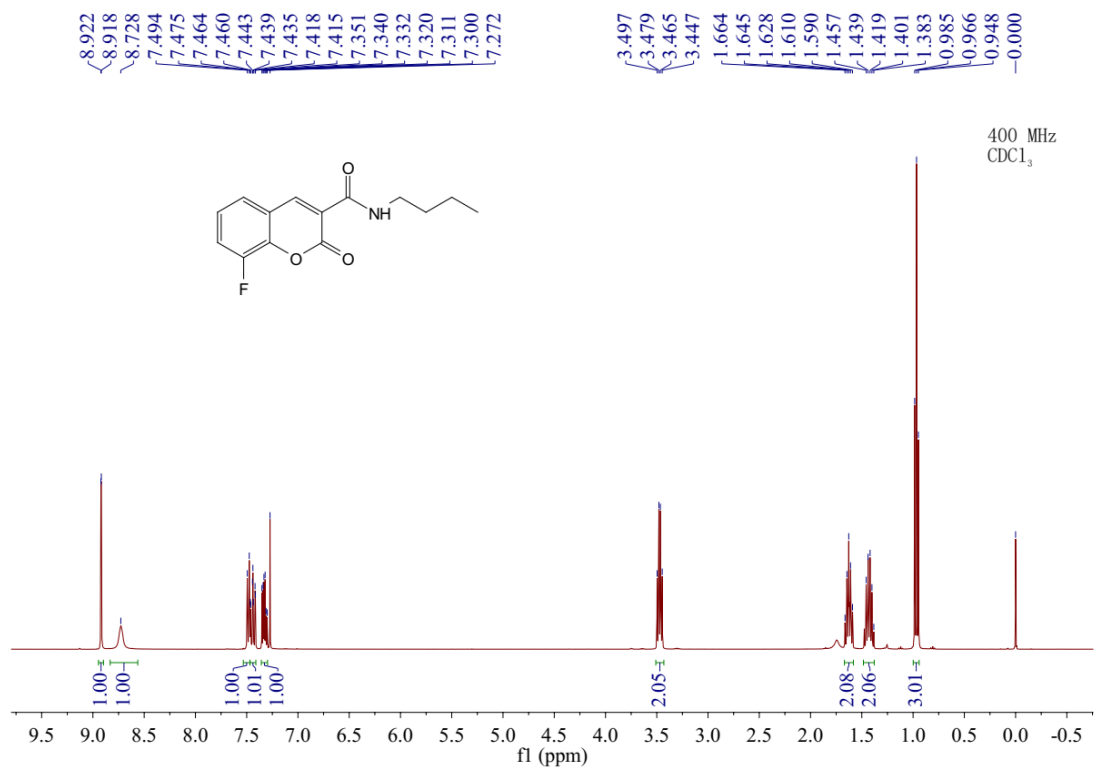


Figure S75. HRMS spectrum of compound C2



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Figure S76. ¹H NMR spectrum of compound C3

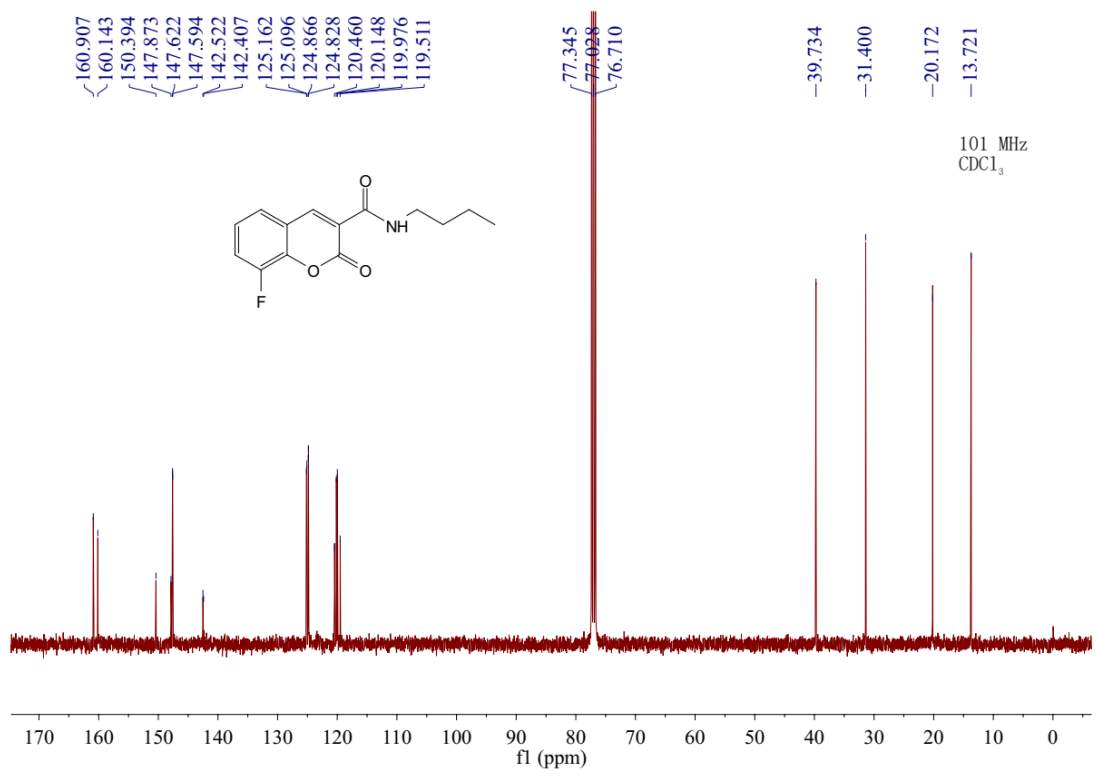


Figure S77. ¹³C NMR spectrum of compound C3

A5 #39 RT: 0.38 AV: 1 NL: 7.12E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

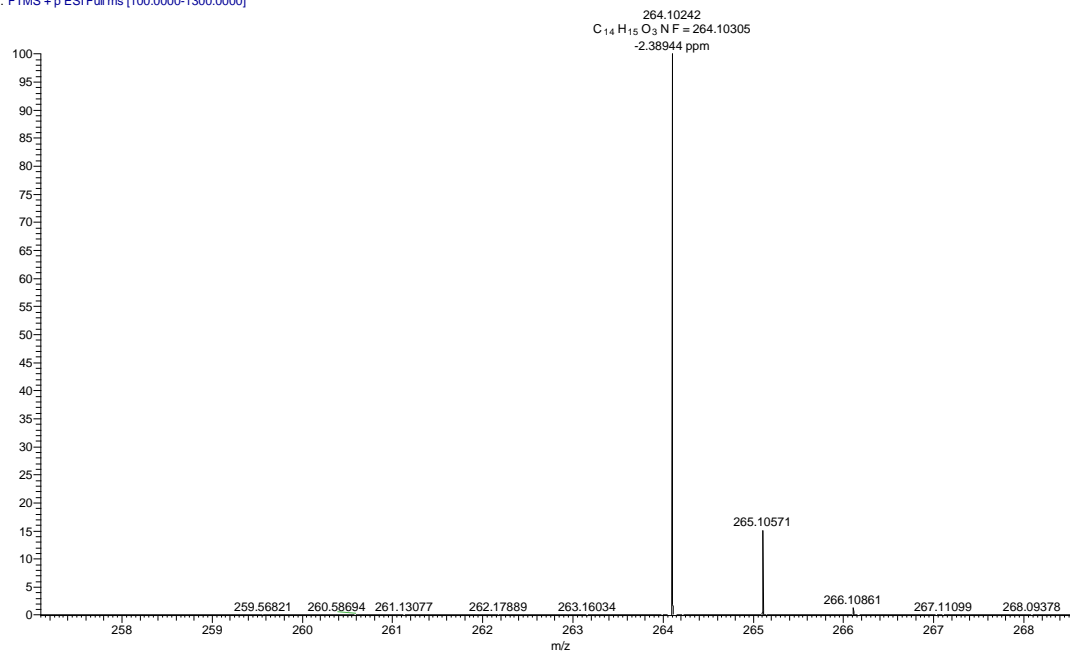


Figure S78. HRMS spectrum of compound C3

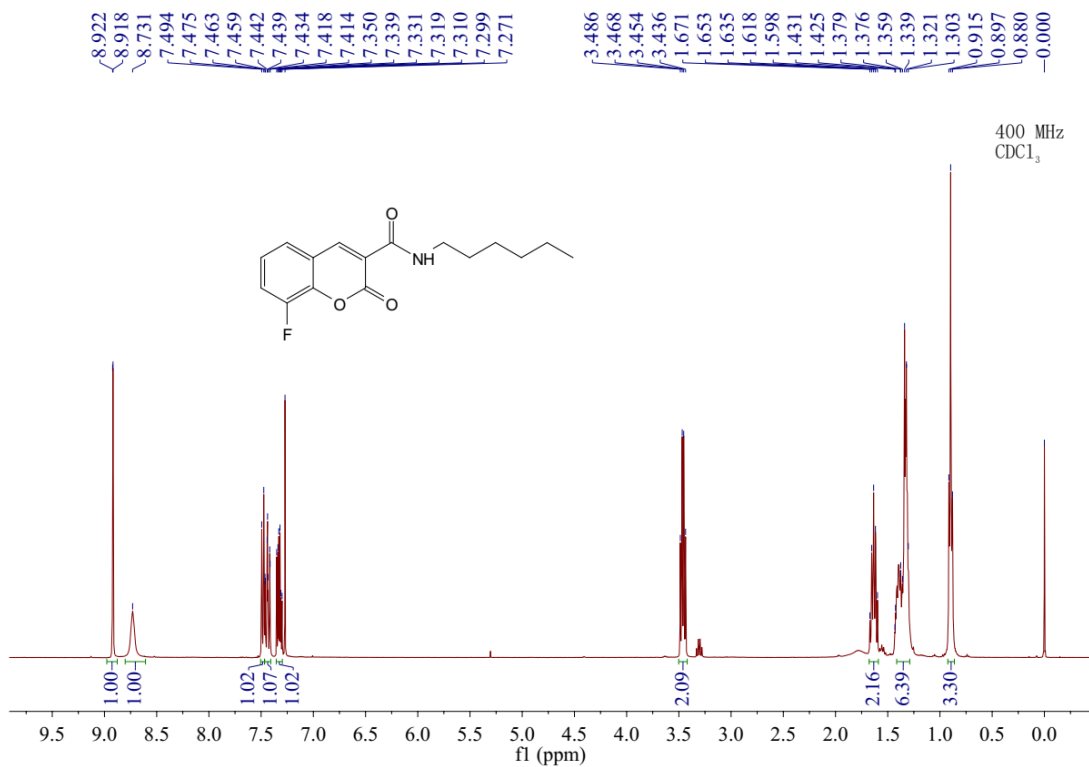
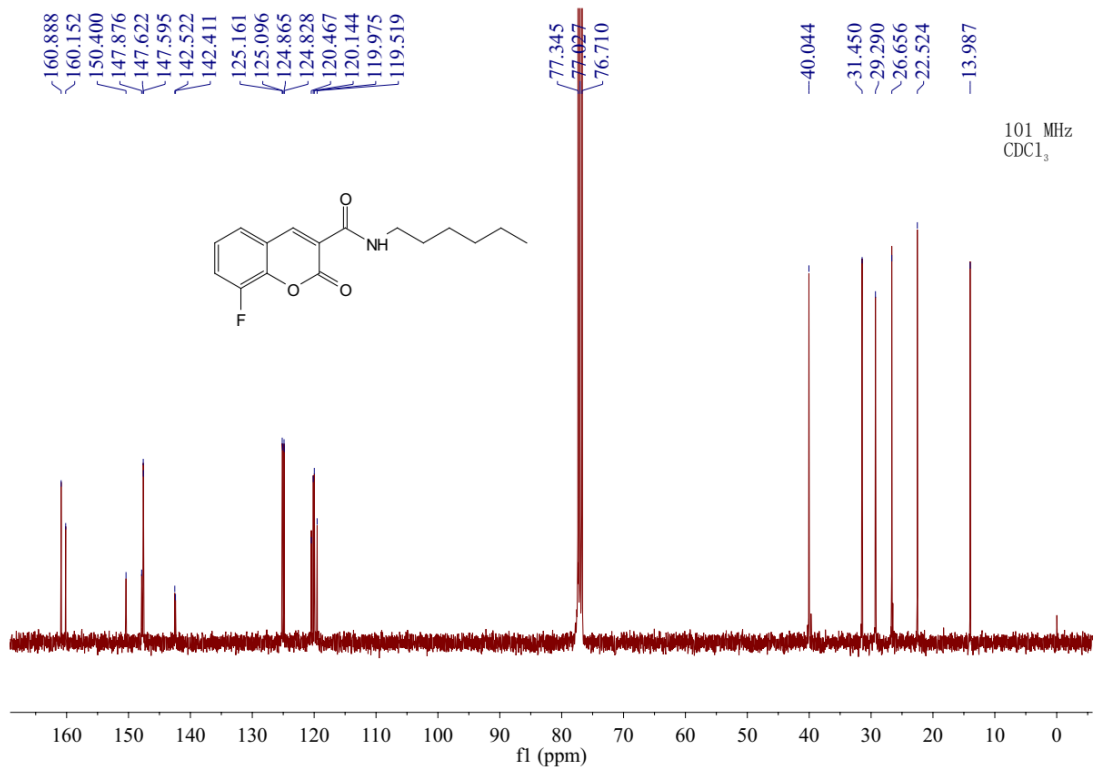
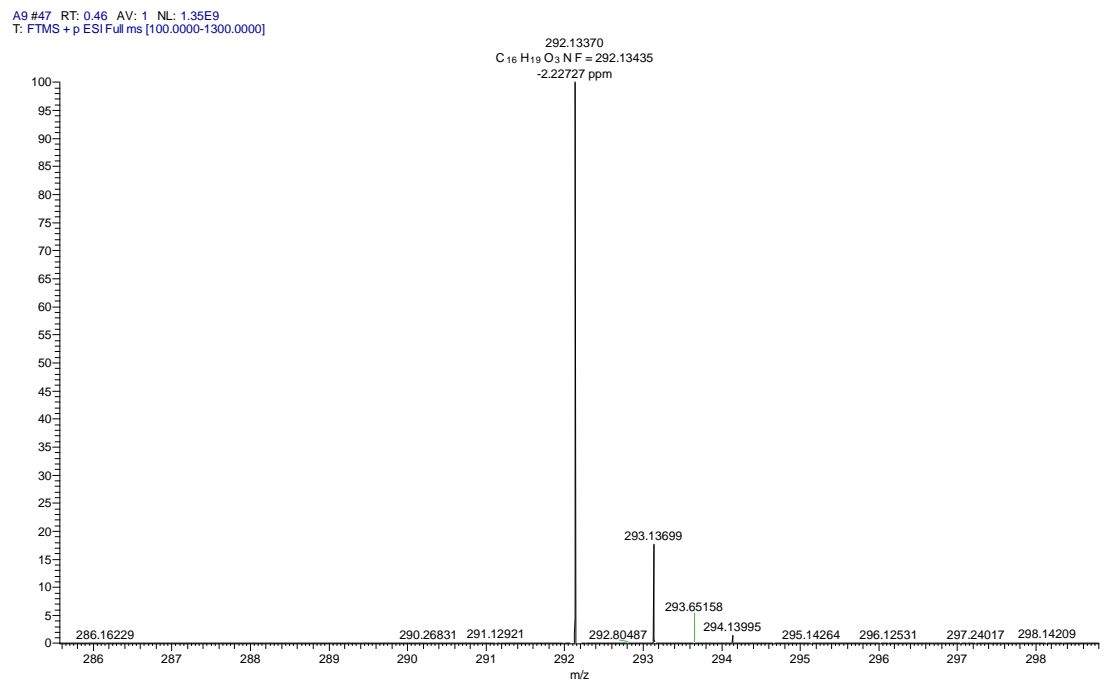


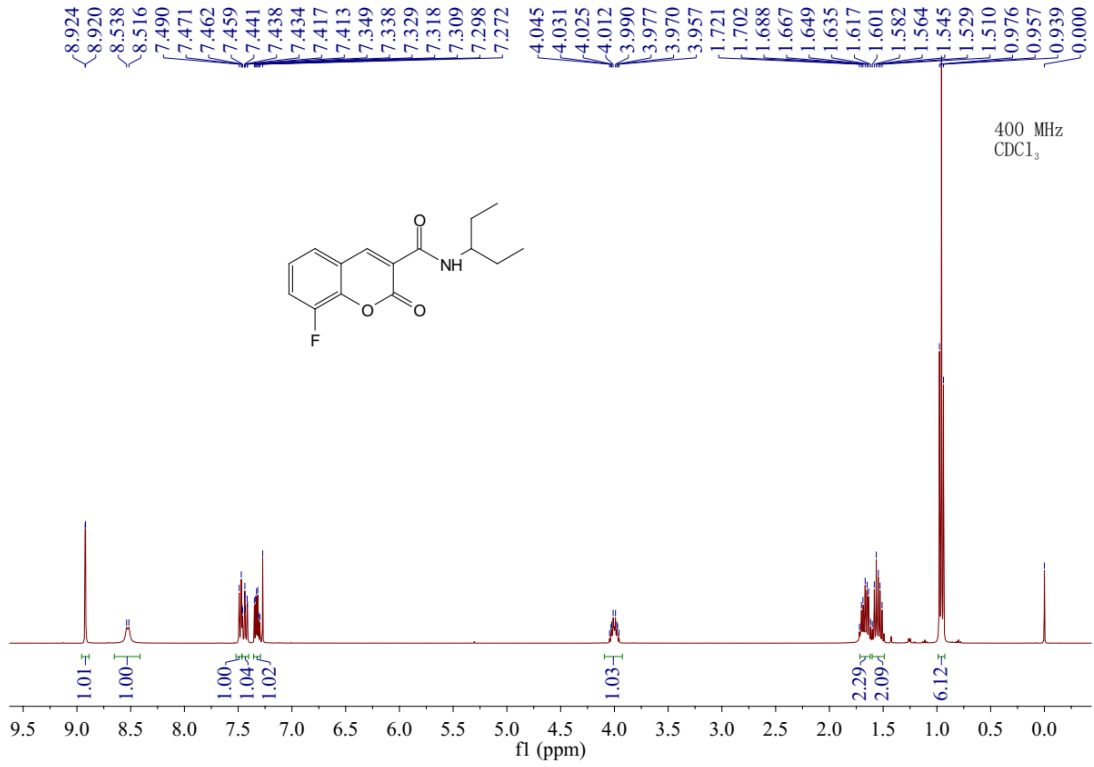
Figure S79. ¹H NMR spectrum of compound C4



26 **Figure S80.** ¹³C NMR spectrum of compound C4

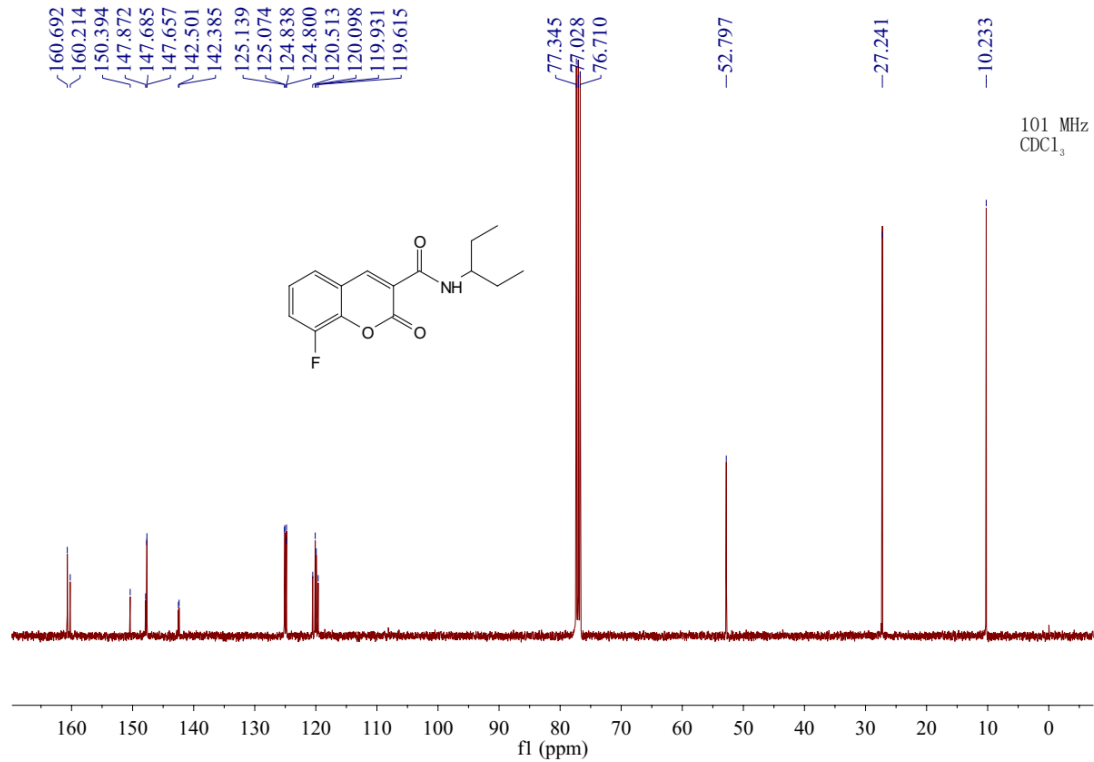


59 **Figure S81.** HRMS spectrum of compound C4



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Figure S82. ¹H NMR spectrum of compound C5



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Figure S83. ¹³C NMR spectrum of compound C5

A8 #39 RT: 0.38 AV: 1 NL: 1.41E9
T: FTMS + p ESI Full ms [100.0000-1300.0000]

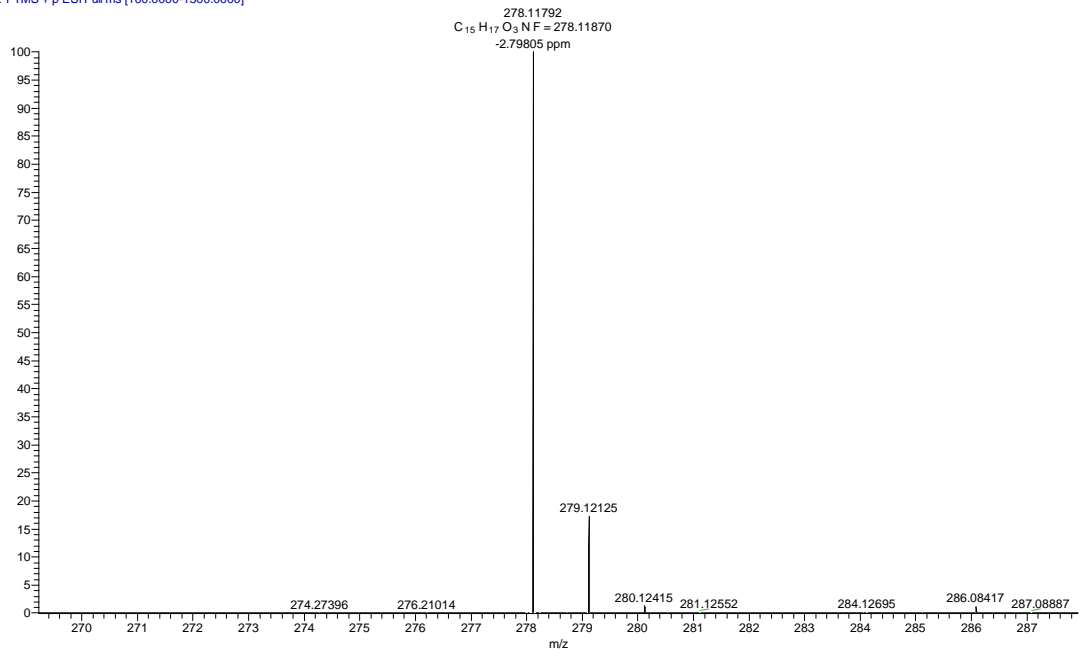


Figure S84. HRMS spectrum of compound C5

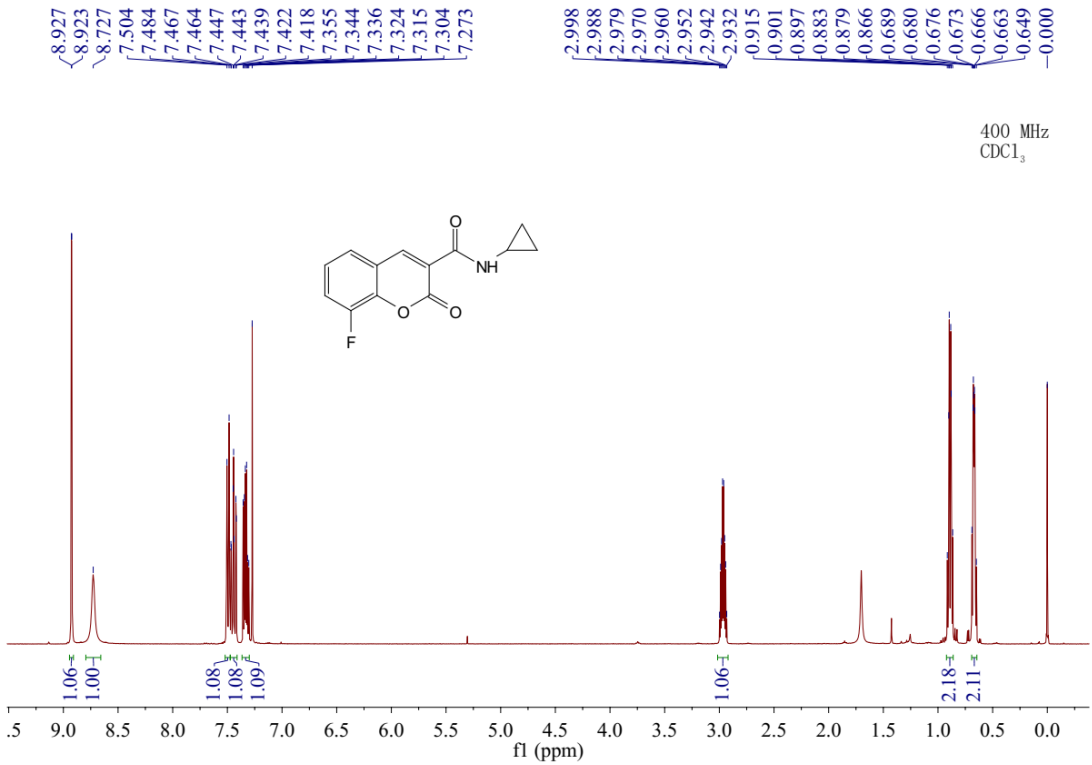


Figure S85. ¹H NMR spectrum of compound C6

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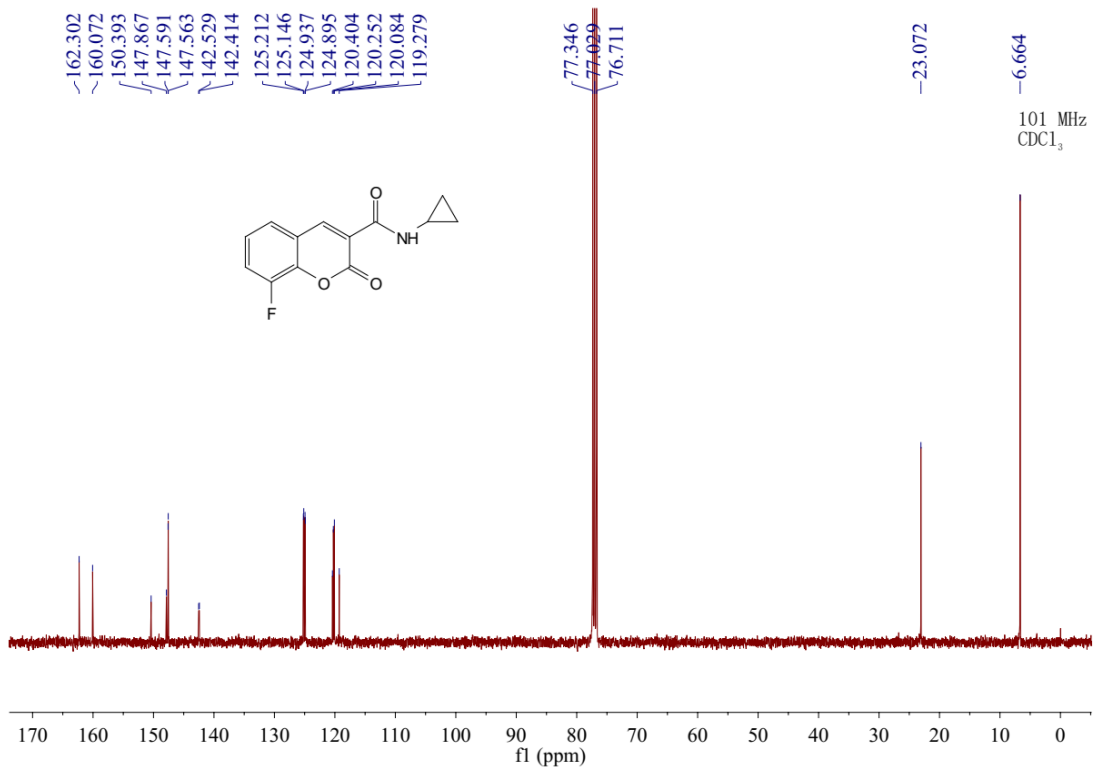


Figure S86. ¹³C NMR spectrum of compound C6

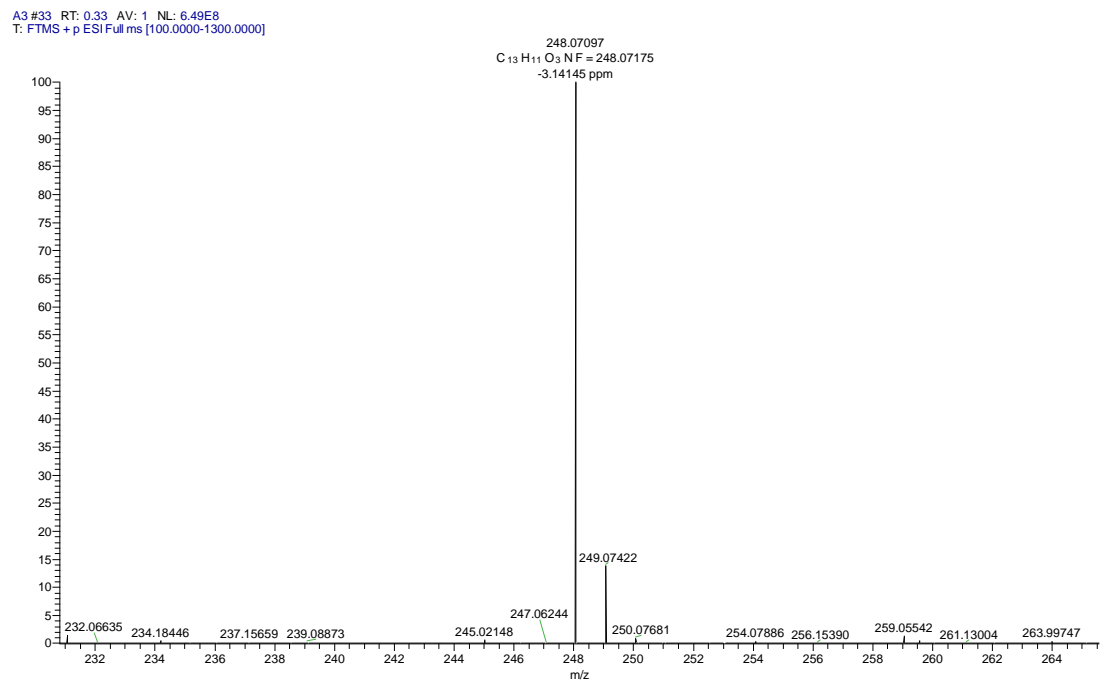
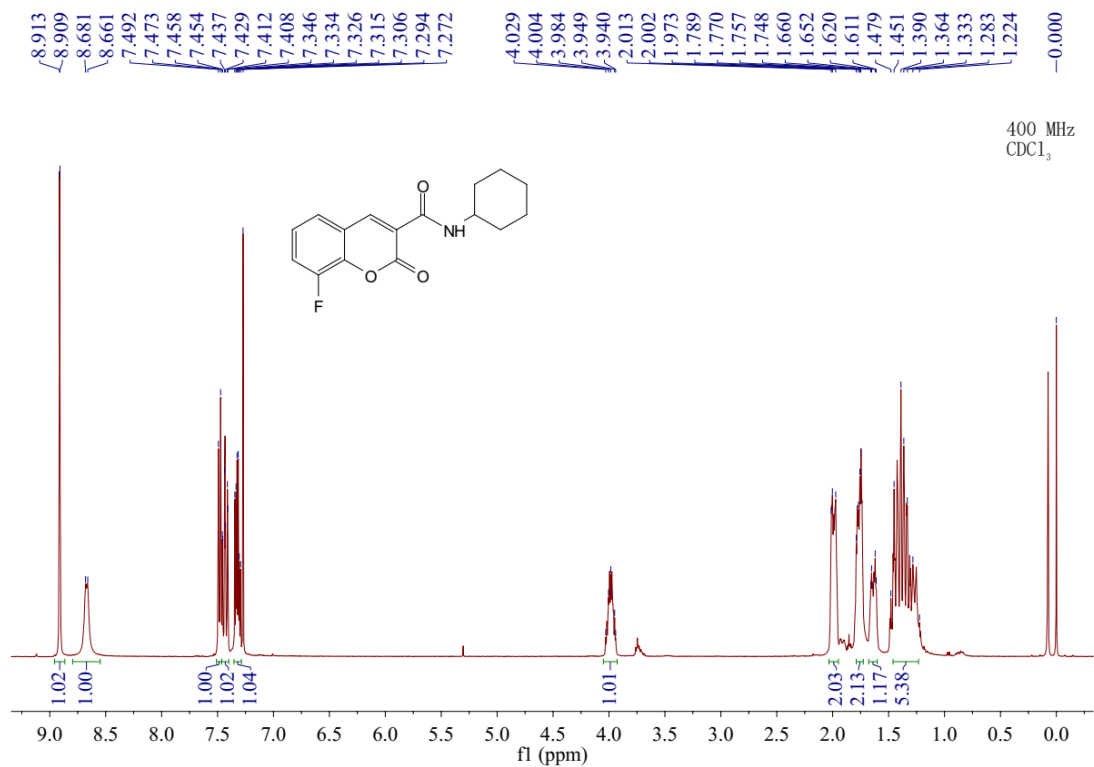
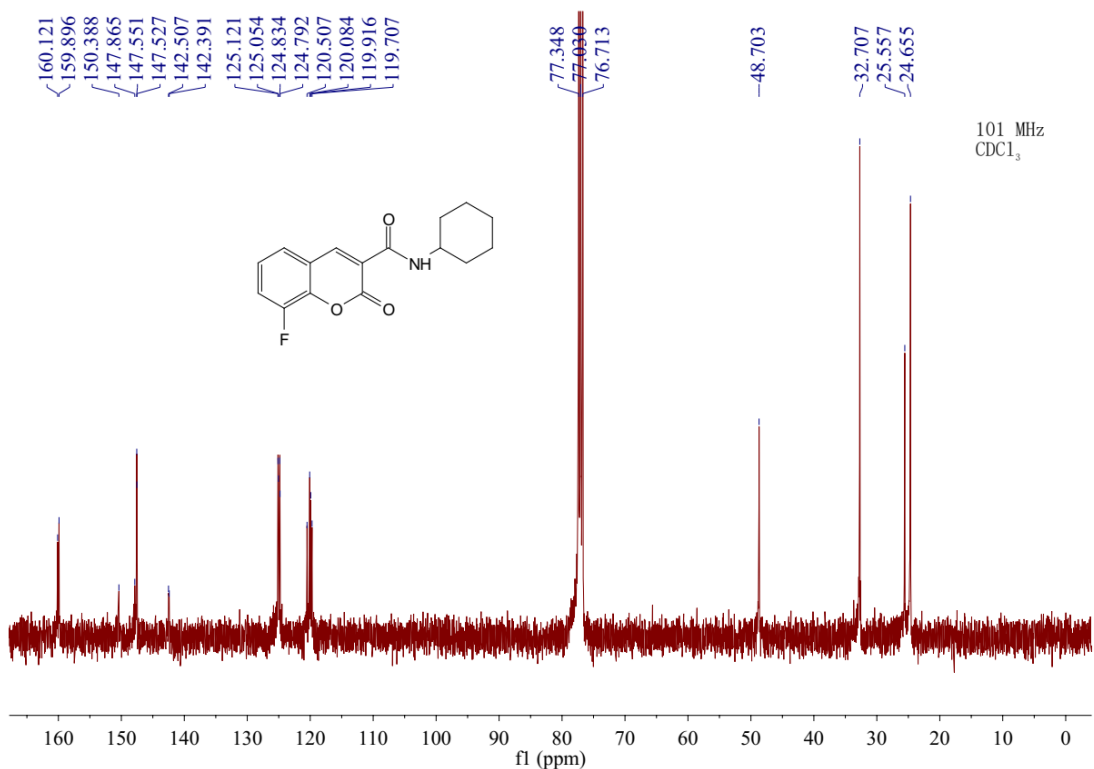


Figure S87. HRMS spectrum of compound C6



26 **Figure S88.** ¹H NMR spectrum of compound C7



56 **Figure S89.** ¹³C NMR spectrum of compound C7

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A10 #43 RT: 0.42 AV: 1 NL: 6.84E8
T: FTMS + p ESI Full ms [100.0000-1300.0000]

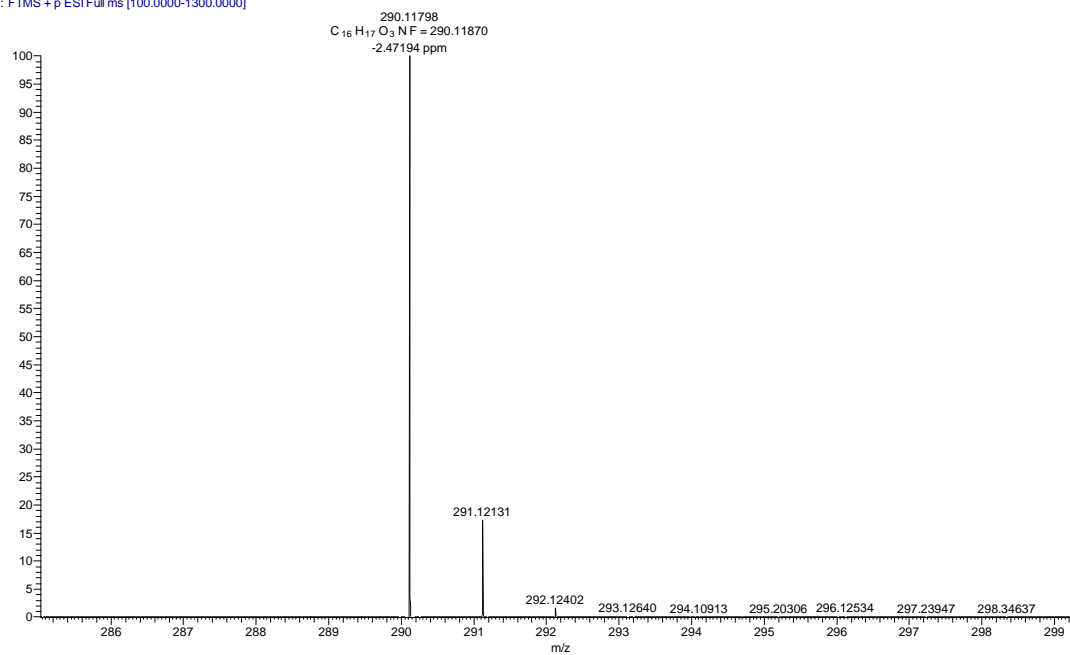


Figure S90. HRMS spectrum of compound C7

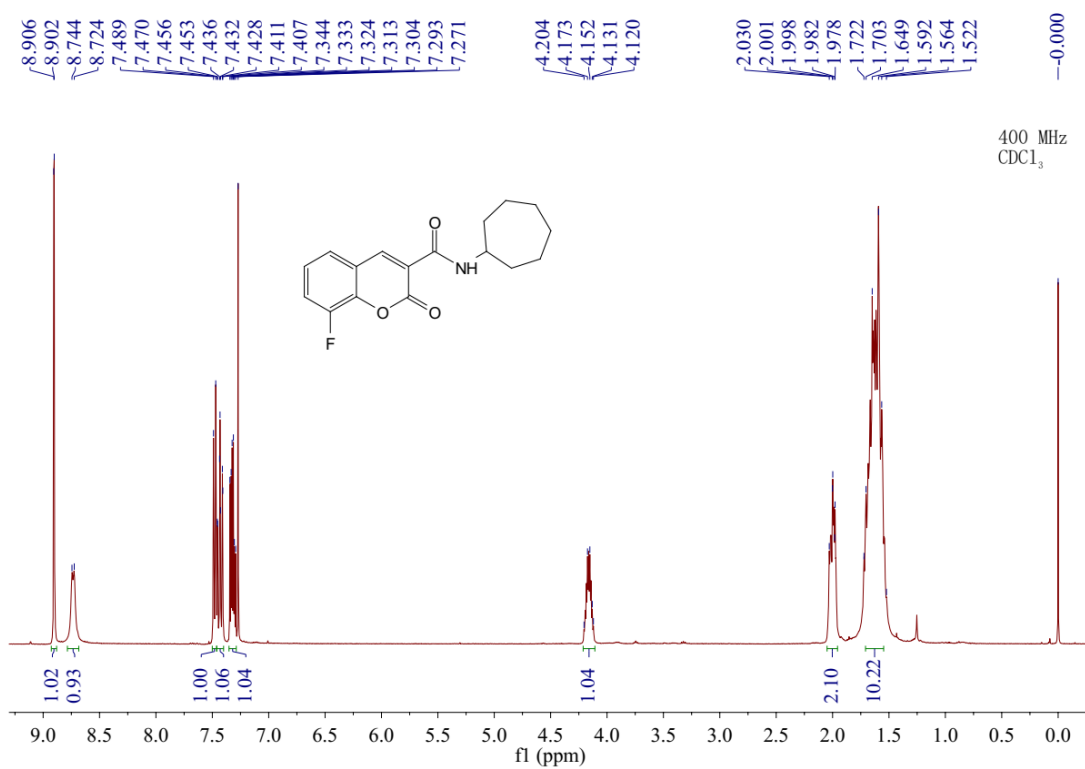


Figure S91. ¹H NMR spectrum of compound C8

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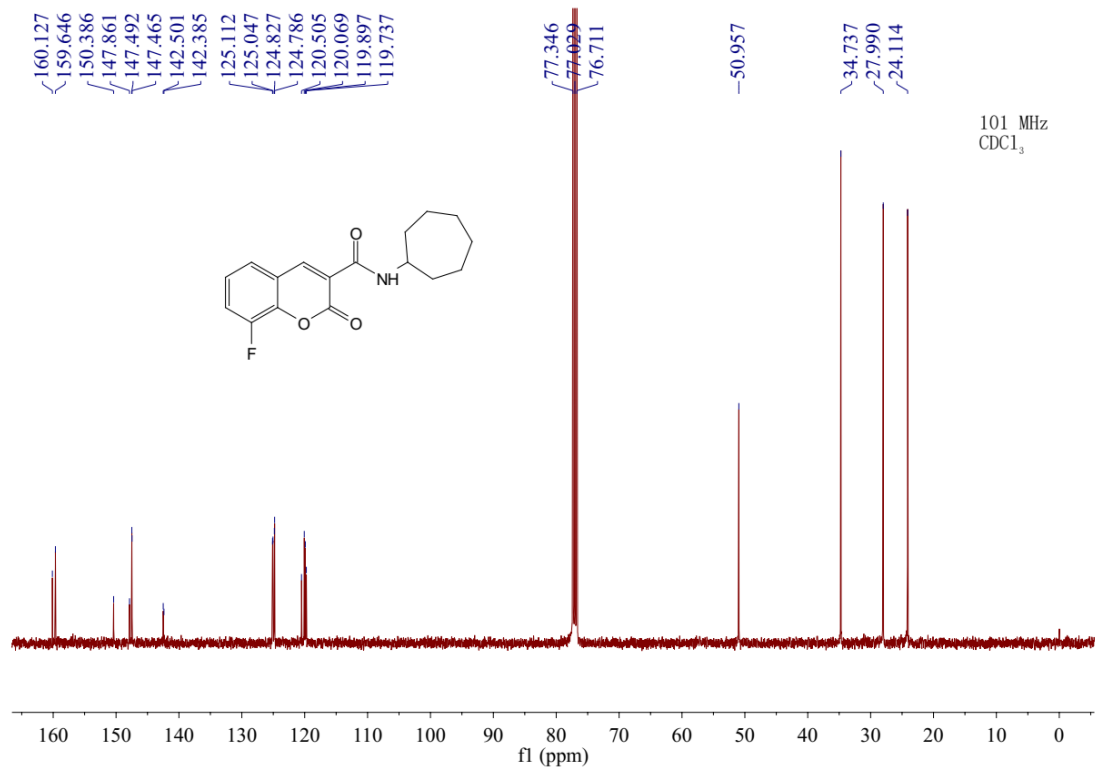


Figure S92. ¹³C NMR spectrum of compound C8

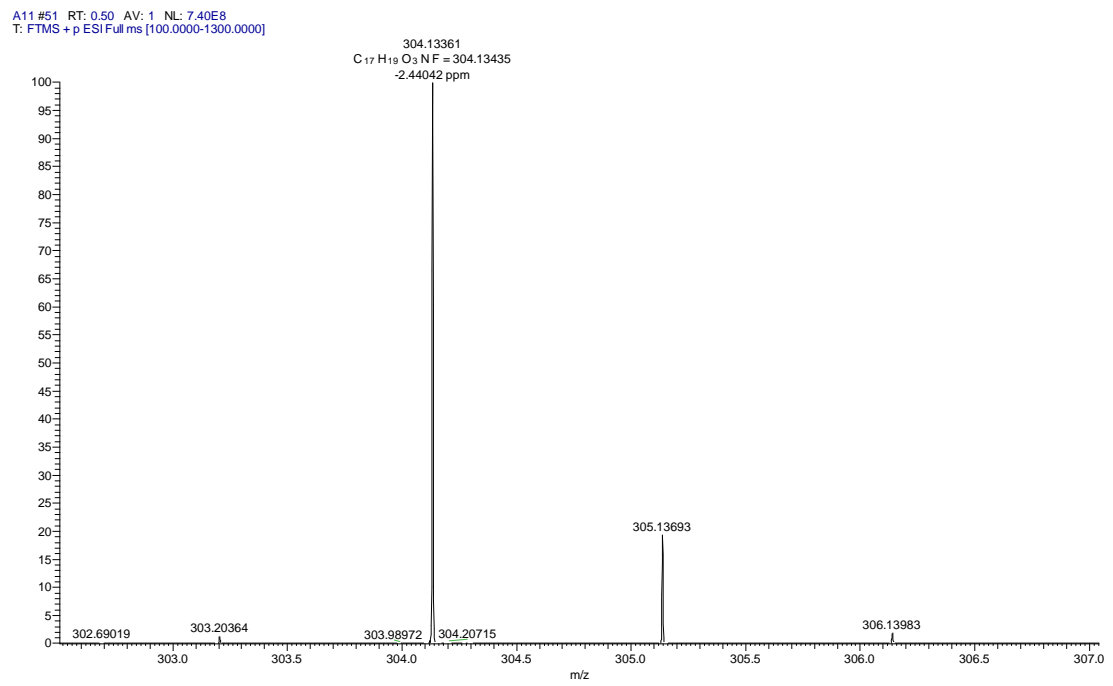


Figure S93. HRMS spectrum of compound C8

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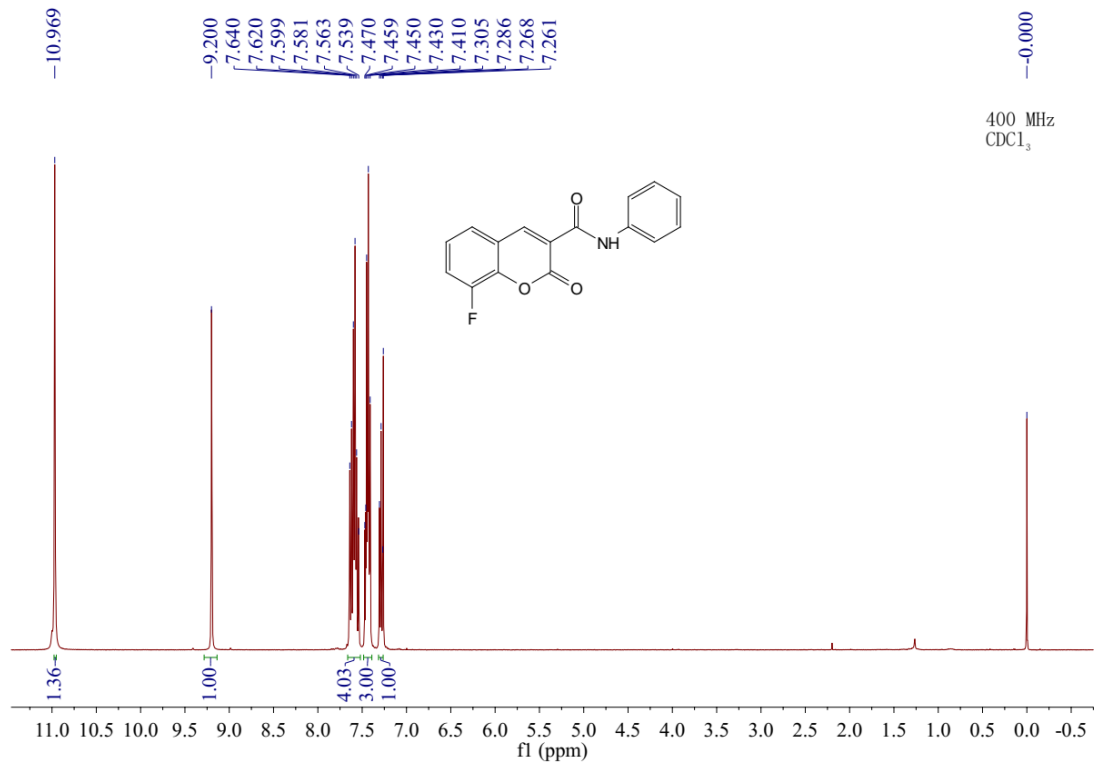


Figure S94. ¹H NMR spectrum of compound C9

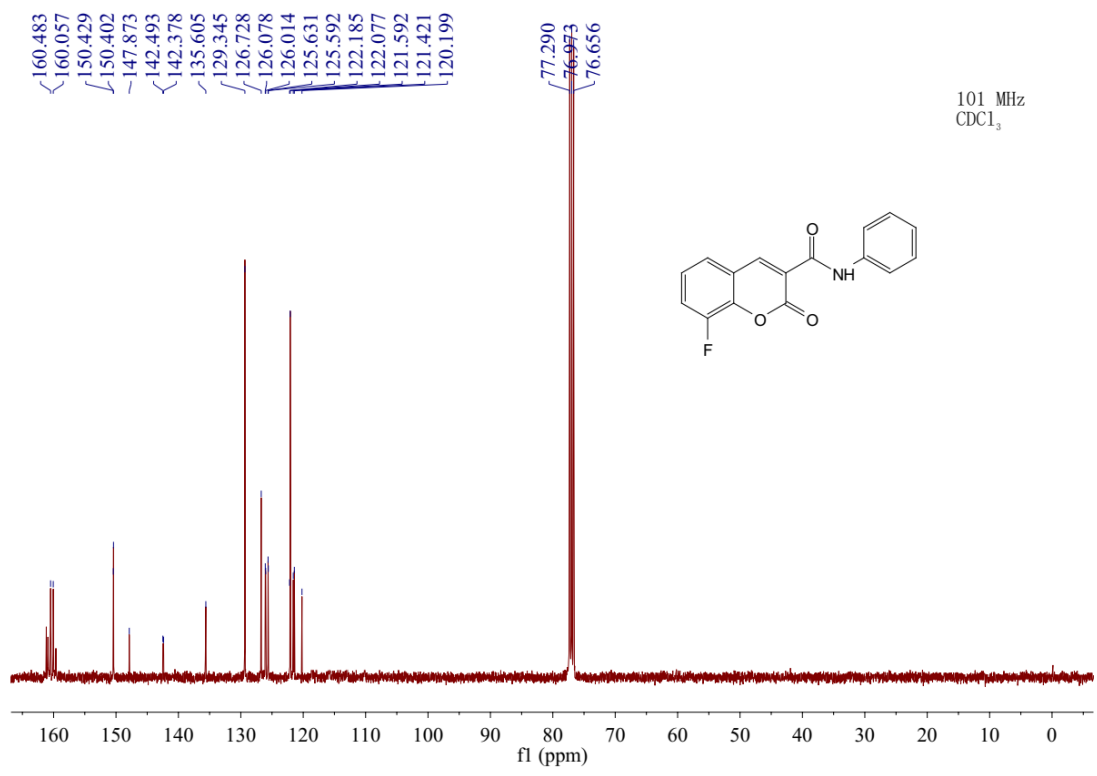


Figure S95. ¹³C NMR spectrum of compound C9

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A12 #41 RT: 0.40 AV: 1 NL: 8.81E7
T: FTMS + p ESI Full ms [100.0000-1300.0000]

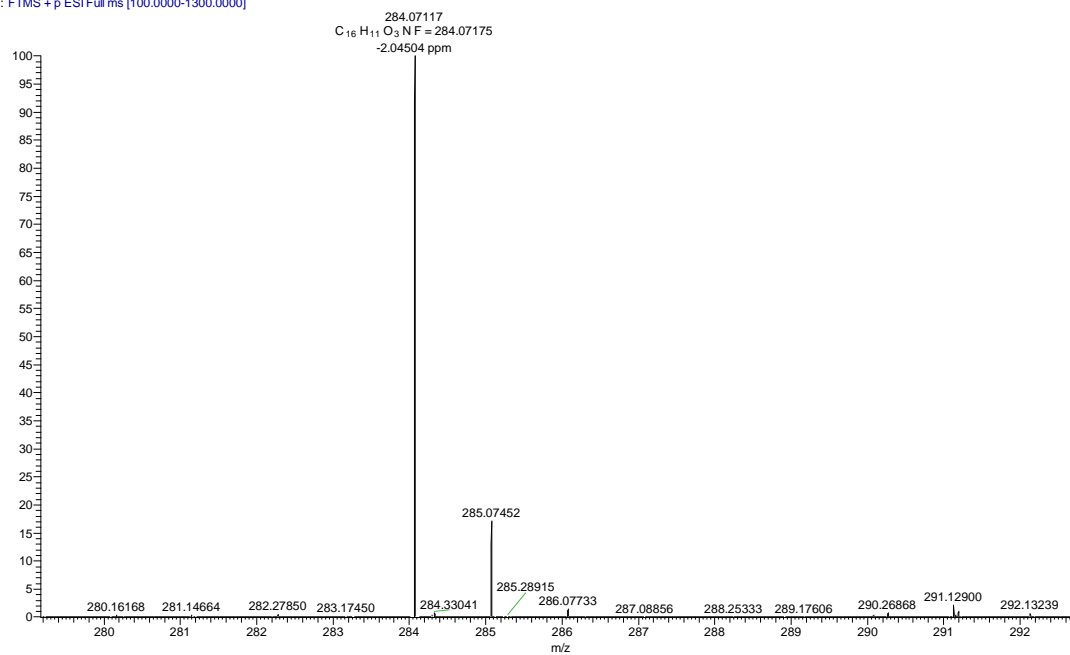


Figure S96. HRMS spectrum of compound C9

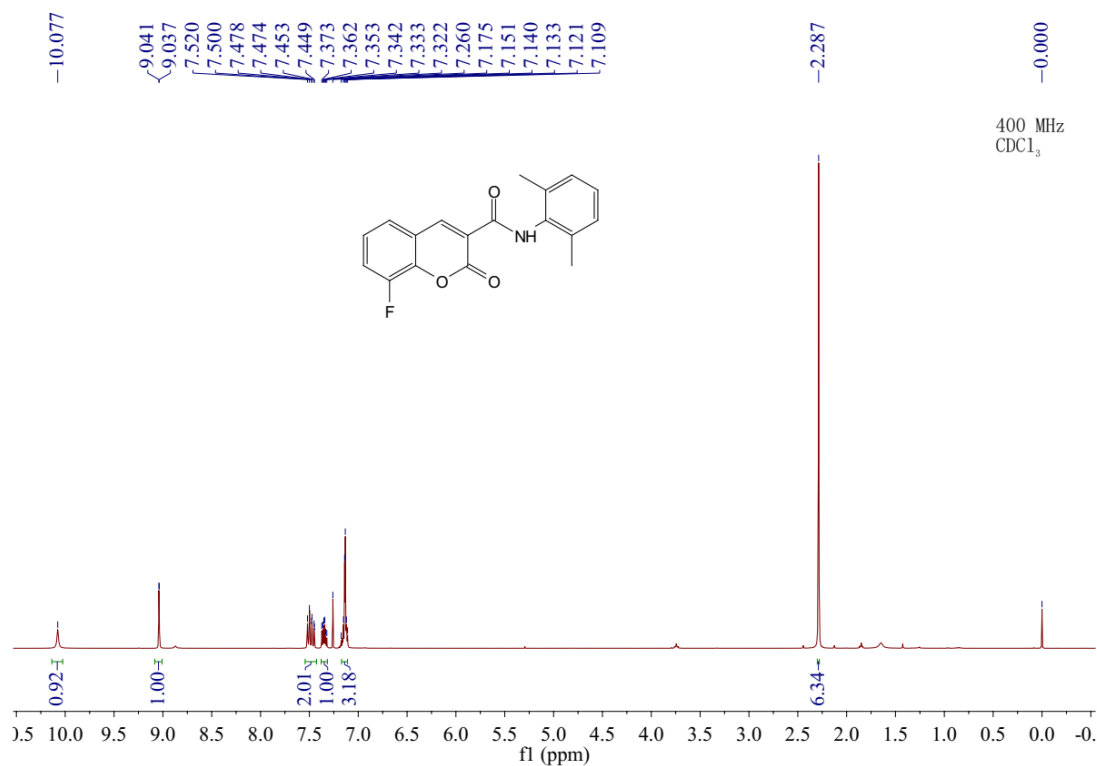


Figure S97. ¹H NMR spectrum of compound C10

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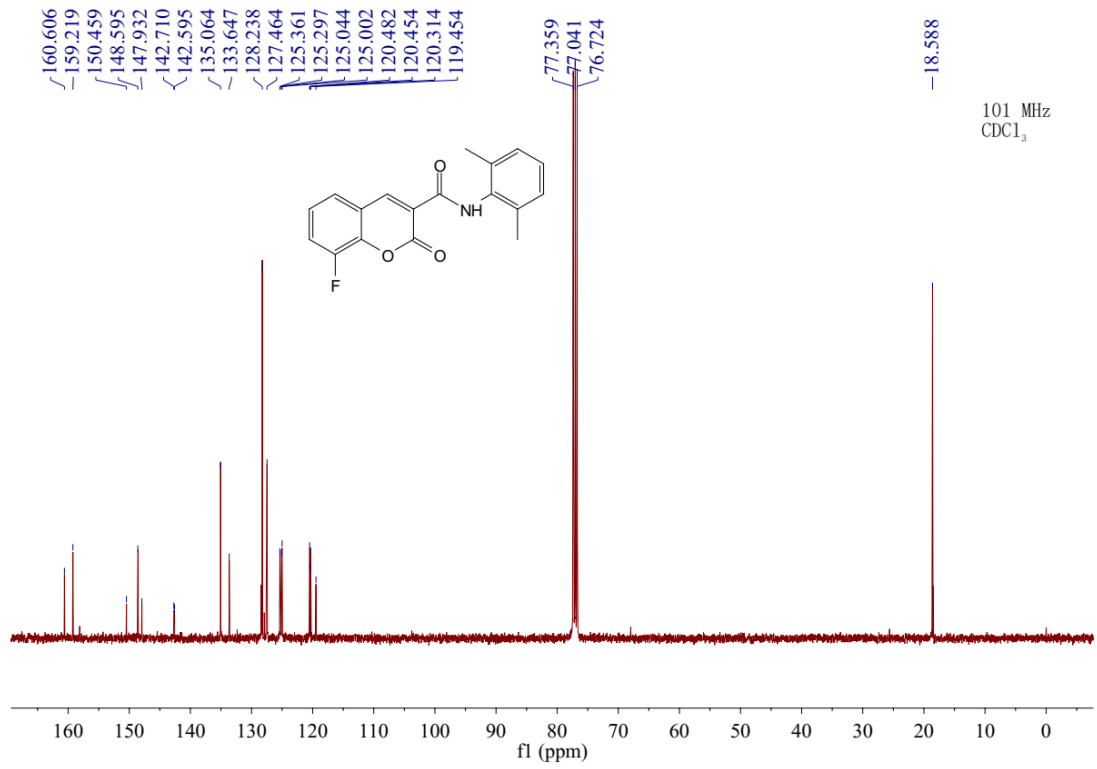


Figure S98. ¹³C NMR spectrum of compound C10

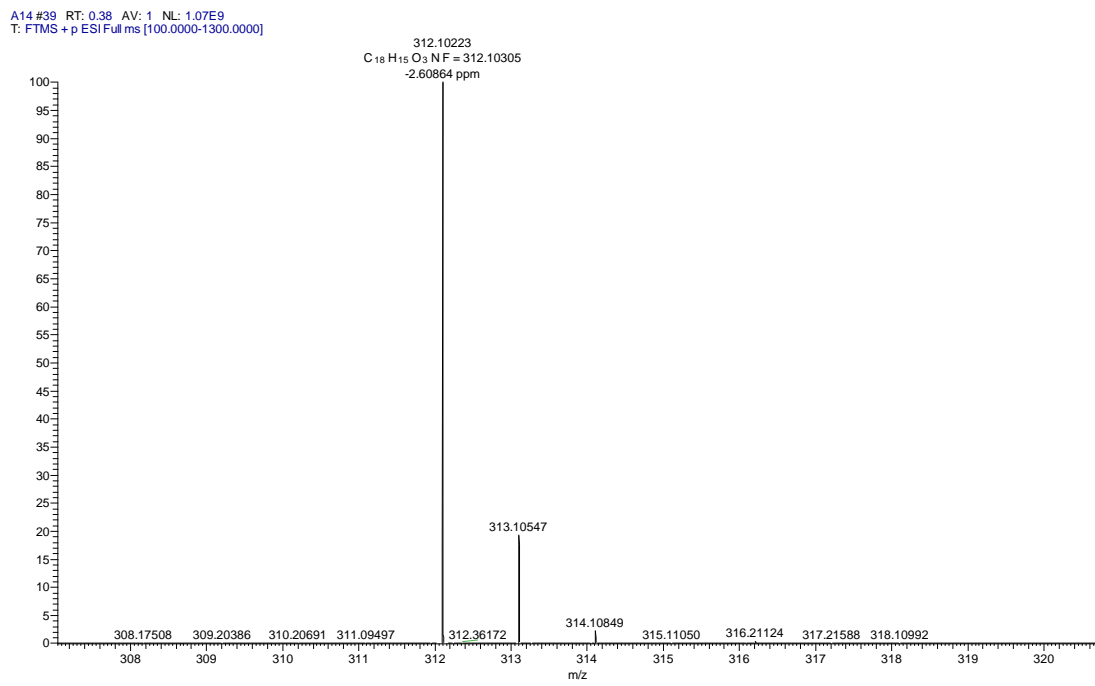
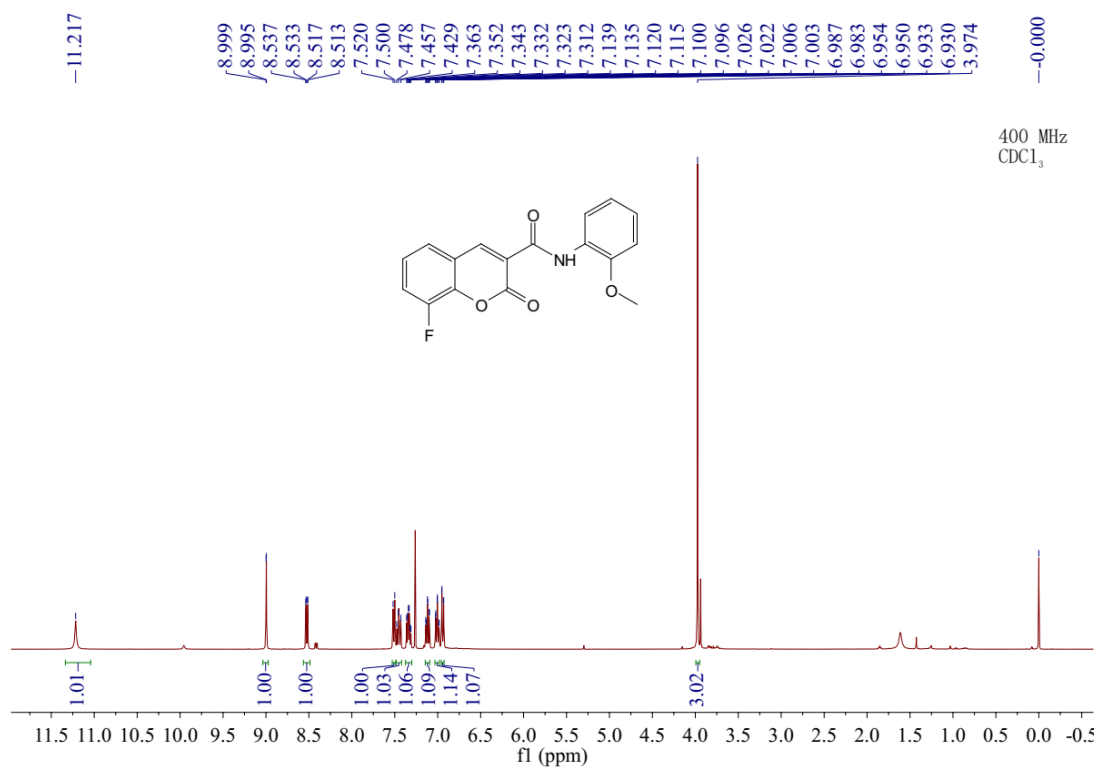
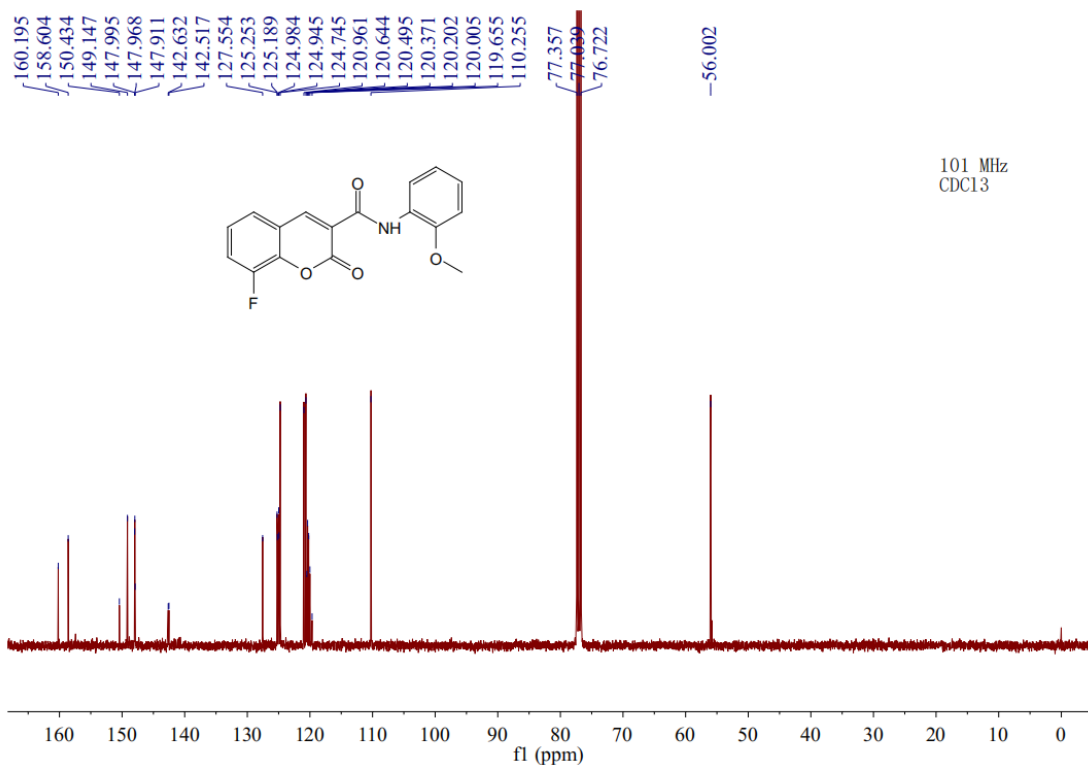


Figure S99. HRMS spectrum of compound C10



26 **Figure S100.** ¹H NMR spectrum of compound C11



54 **Figure S101.** ¹³C NMR spectrum of compound C11

A13 #43 RT: 0.42 AV: 1 NL: 1.85E8
T: FTMS + p ESIFull ms [100.0000-1300.0000]

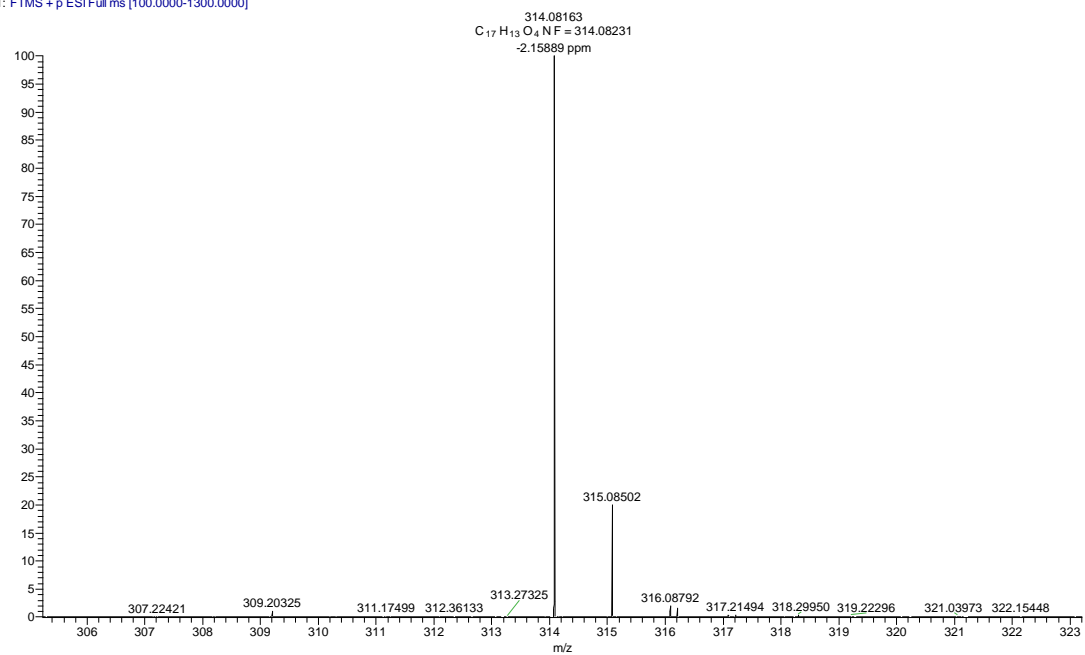


Figure S102. HRMS spectrum of compound C11

Table S1. The single crystal XRD data of **A6**

compounds	A6
Chemical formula	C ₁₆ H ₁₆ FNO ₃
Formula weight	289.30
Temperature (K)	273.15
Wavelength	1.54178
Crystal system	triclinic
Space group	<i>P</i> -1
a (Å)	6.2002(2)
b (Å)	9.7846(4)
c (Å)	12.3705(4)
α (°)	92.156(2)
β (°)	99.798(2)
γ (°)	106.066(2)
Volume (Å ³)	707.79(2)
Cell formula units Z	2
Density (calculated)(g/cm ³)	1.357
Absorption coefficient μ (mm ⁻¹)	0.857
F(000)	304.0
Crystal size (mm ³)	0.22 × 0.2 × 0.18
Radiation	$\lambda = 1.54178$
Theta range for data collection	9.444 to 133.124
Reflections collected	6906
Independent reflections	2024[$R_{(int)} = 0.0509$, $R_{(sigma)} = 0.0540$]
Data / restraints / parameters	2404/0/190
Goodness-of-fit on F ²	1.080
Final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0609$, $wR_2 = 0.1603$
Final <i>R</i> indices [all data]	$R_1 = 0.0666$, $wR_2 = 0.1664$

Table S2. The single crystal XRD data of **B11**

compounds	B11
Chemical formula	C ₁₈ H ₁₄ FNO ₃
Formula weight	311.30
Temperature (K)	273.15
Wavelength	1.54178
Crystal system	triclinic
Space group	<i>P</i> -1
a (Å)	7.140
b (Å)	8.000
c (Å)	14.400
α (°)	98.00
β (°)	96.27
γ (°)	113.48
Volume (Å ³)	734.7
Cell formula units Z	2
Density (calculated)(g/cm ³)	1.407
Absorption coefficient μ (mm ⁻¹)	0.874
F(000)	324.0
Crystal size (mm ³)	0.22 × 0.2 × 0.18
Radiation	$\lambda = 1.54178$
Theta range for data collection	12.312 to 134.224
Reflections collected	2588
Independent reflections	2588 [$R_{(int)} = 0$, $R_{(sigma)} = 0.0274$]
Data / restraints / parameters	2588/0/210
Goodness-of-fit on F ²	1.212
Final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0842$, $wR_2 = 0.2641$
Final <i>R</i> indices [all data]	$R_1 = 0.0963$, $wR_2 = 0.2844$

Table S3. The single crystal XRD data of **C2**

compounds	C2
Chemical formula	C ₁₃ H ₁₂ FNO ₃
Formula weight	249.24
Temperature (K)	296
Wavelength	0.71073
Crystal system	triclinic
Space group	<i>P</i> -1
a (Å)	5.140(3)
b (Å)	10.708(6)
c (Å)	11.455(6)
α (°)	109.331(13)
β (°)	95.618(12)
γ (°)	99.899(11)
Volume (Å ³)	577.9(5)
Cell formula units Z	2
Density (calculated)(g/cm ³)	1.432
Absorption coefficient μ (mm ⁻¹)	0.113
F(000)	260.0
Crystal size (mm ³)	0.22 × 0.2 × 0.18
Radiation	$\lambda = 0.71073$
Theta range for data collection	3.274 to 24.977
Reflections collected	11135
Independent reflections	1944 [$R_{\text{int}} = 0.1163$, $R_{\text{sigma}} = 0.1183$]
Data / restraints / parameters	1944/0/152
Goodness-of-fit on F ²	1.005
Final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.1278$, $wR_2 = 0.2157$
Final <i>R</i> indices [all data]	$R_1 = 0.2408$, $wR_2 = 0.2538$

Table S4. The single crystal XRD data of **C7**

compounds	C7
Chemical formula	C ₁₆ H ₁₆ FNO ₃
Formula weight	289.30
Temperature (K)	273.15
Wavelength	1.54178
Crystal system	monoclinic
Space group	<i>C2/c</i>
a (Å)	24.9849(4)
b (Å)	5.50780(10)
c (Å)	20.0851(3)
α (°)	90
β (°)	96.2800(10)
γ (°)	90
Volume (Å ³)	2747.36(8)
Cell formula units Z	8
Density (calculated)(g/cm ³)	1.399
Absorption coefficient μ (mm ⁻¹)	0.883
F(000)	1216.0
Crystal size (mm ³)	0.22 × 0.2 × 0.18
Radiation	$\lambda = 1.54178$
Theta range for data collection	7.118 to 144.282
Reflections collected	12021
Independent reflections	2660 [$R_{\text{(int)}} = 0.0556$, $R_{\text{(sigma)}} = 0.0568$]
Data / restraints / parameters	2660/0/191
Goodness-of-fit on F ²	1.321
Final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0865$, $wR_2 = 0.2795$
Final <i>R</i> indices [all data]	$R_1 = 0.0902$, $wR_2 = 0.2872$