

Supplementary information

Design, Synthesis and Evaluation of the COX-2 Inhibitory Activities of New 1, 3-dihydro-2*H*-indolin-2-one Derivatives

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Relevant spectroscopic data (^1H , ^{13}C and HRMS Spectra)

(Z)-1-acetyl-6-(trifluoromethyl)-3-(3-(trifluoromethyl)benzylidene)indolin-2-one (4a)

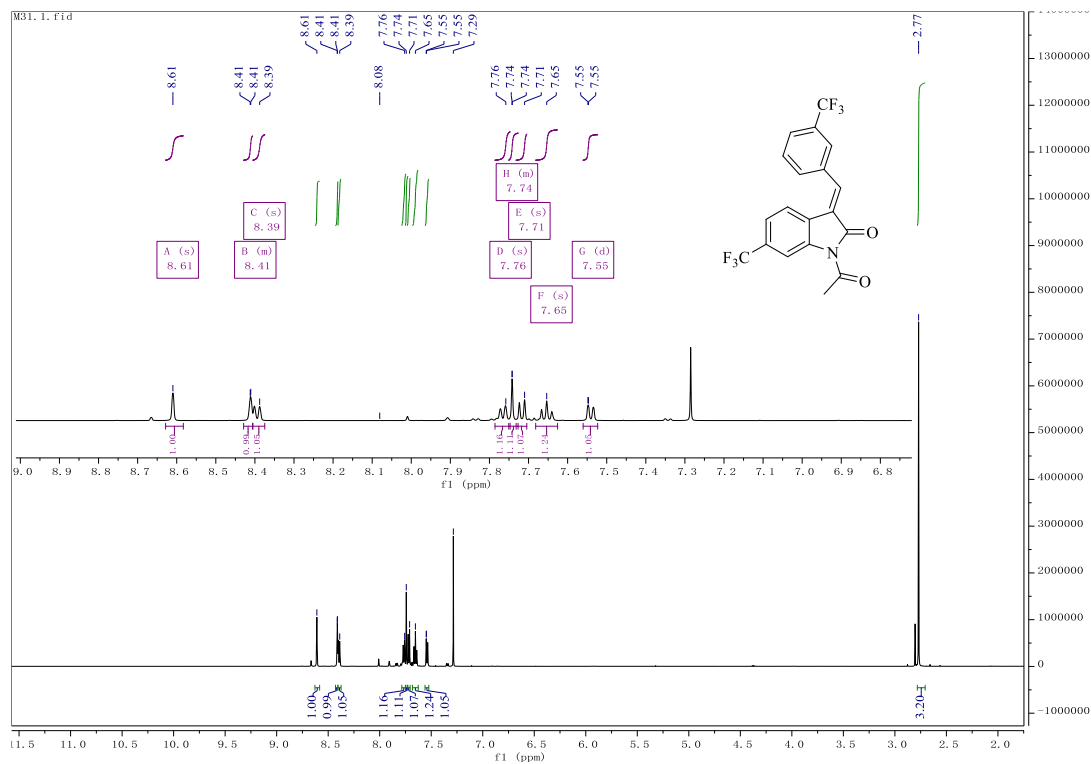


Figure S1-1. ^1H NMR spectrum (600 Hz, CDCl_3) of compound 4a

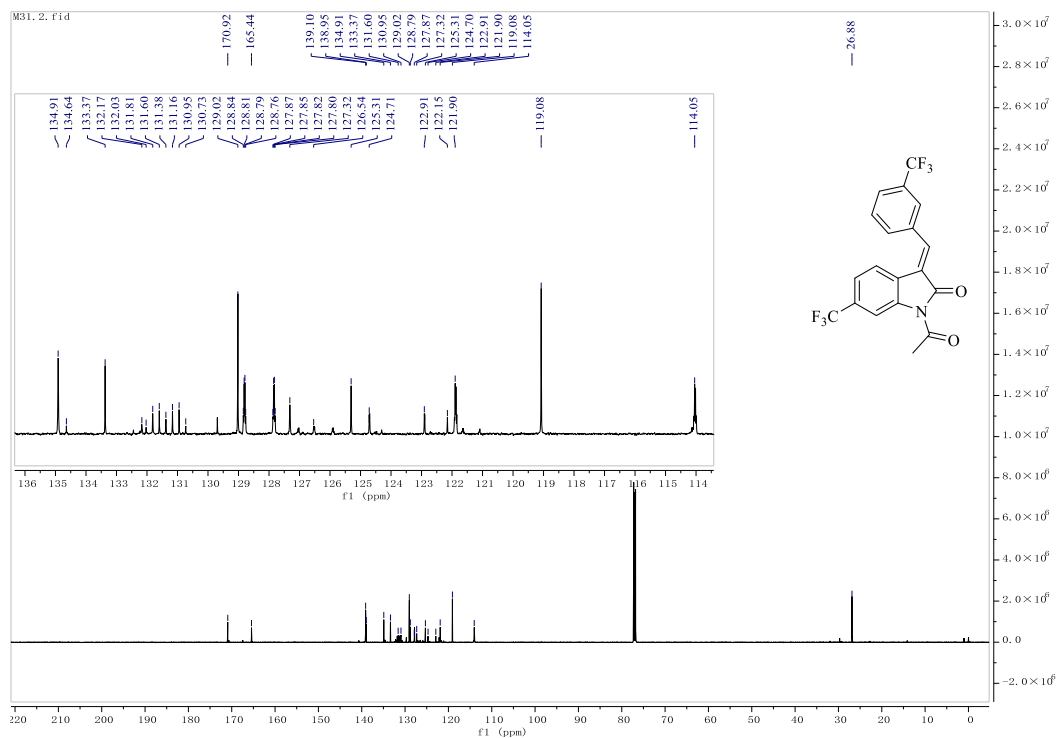


Figure S1-2. ^{13}C NMR spectrum (150 Hz, CDCl_3) of compound 4a

M31 #23 RT: 0.10 AV: 1 NL: 8.40E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

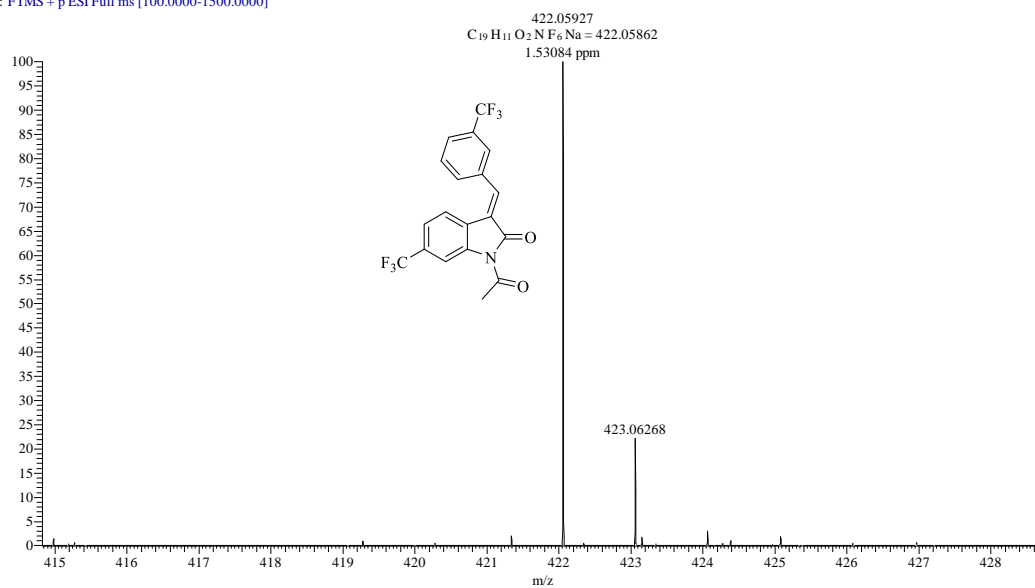


Figure S1-3. HRMS of compound 4a

(E)-1-acetyl-6-(trifluoromethyl)-3-(3-(trifluoromethyl)benzylidene)indolin-2-one (4b)

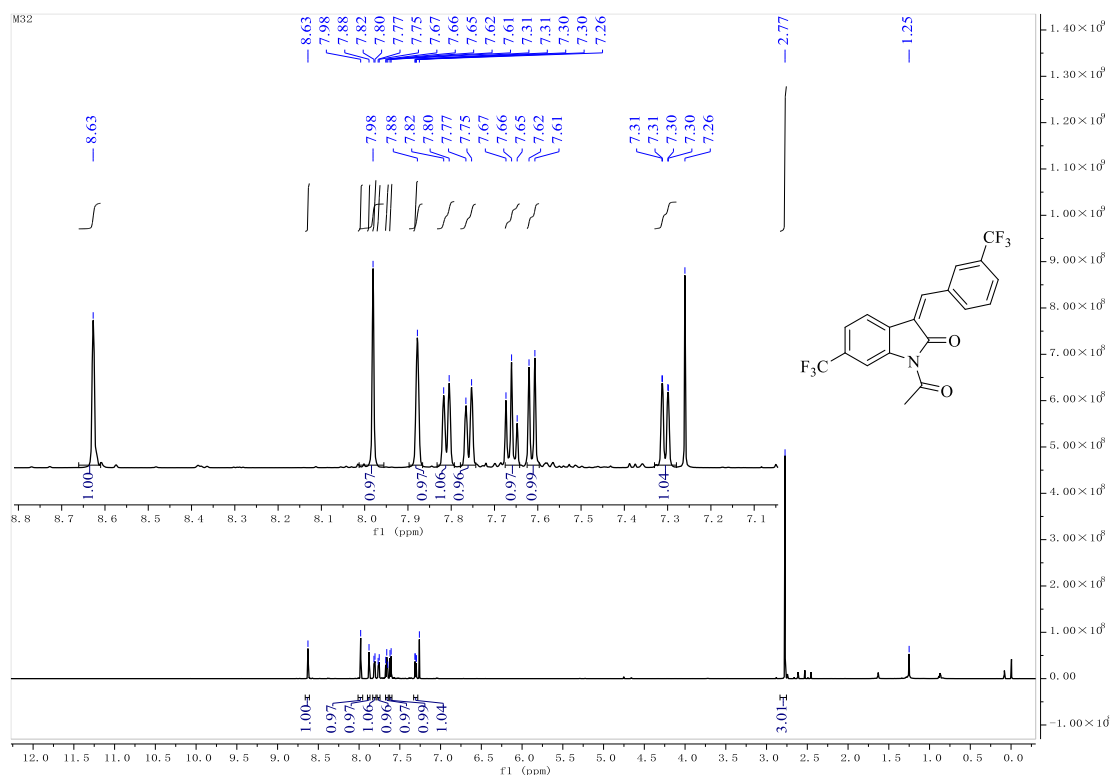


Figure S2-1. ¹H NMR spectrum (600 Hz, CDCl₃) of compound **4b**

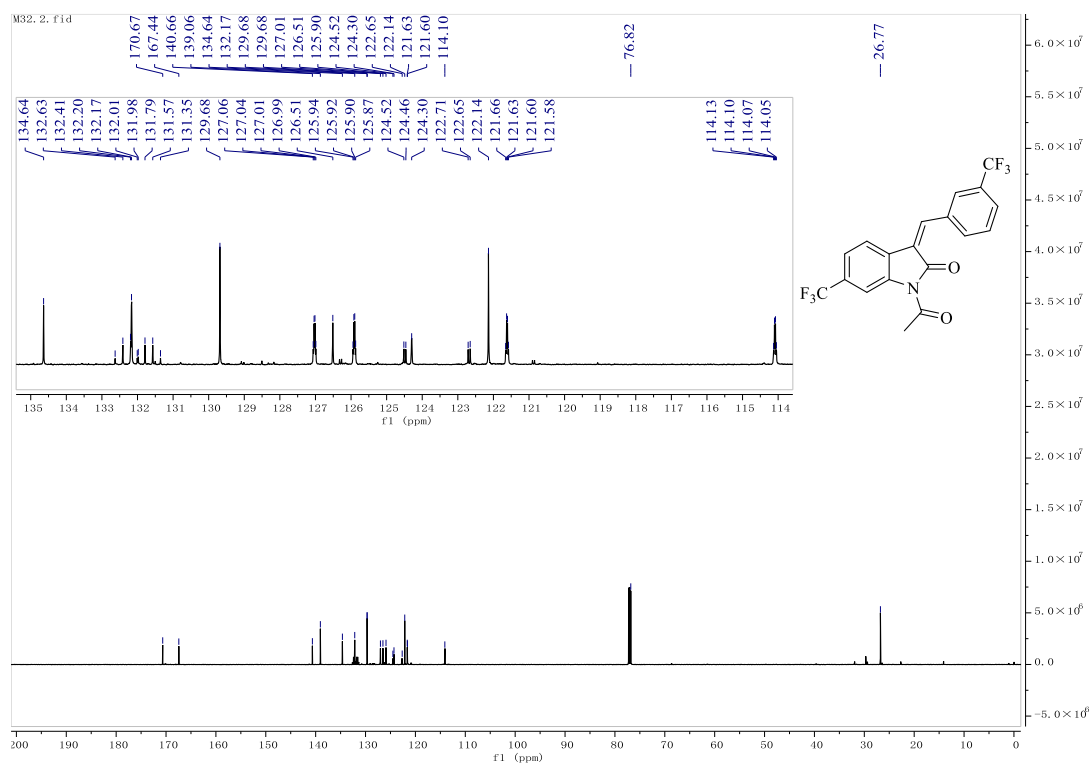


Figure S2-2. ¹³C NMR spectrum (150 Hz, CDCl₃) of compound **4b**

M32 #23 RT: 0.10 AV: 1 NL: 4.67E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

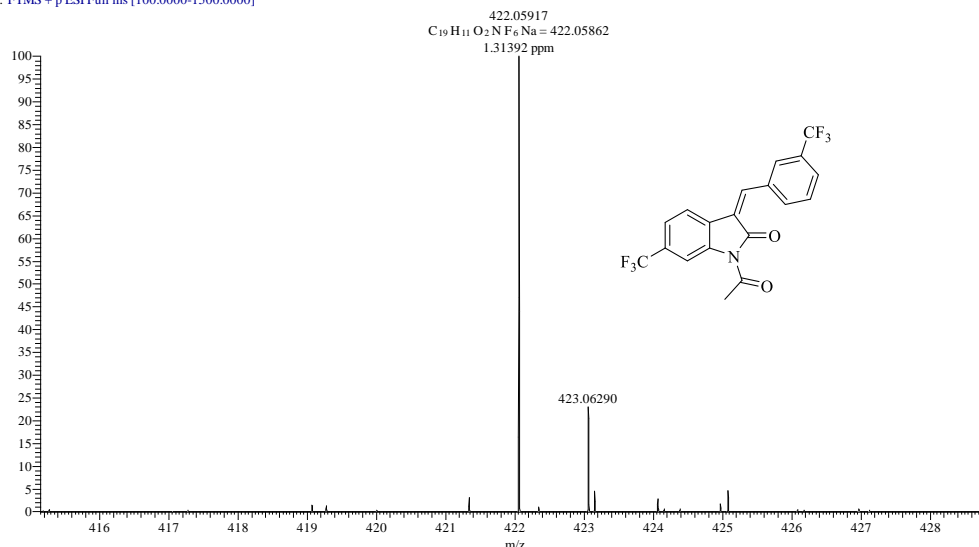


Figure S2-3. HRMS of compound **4b**

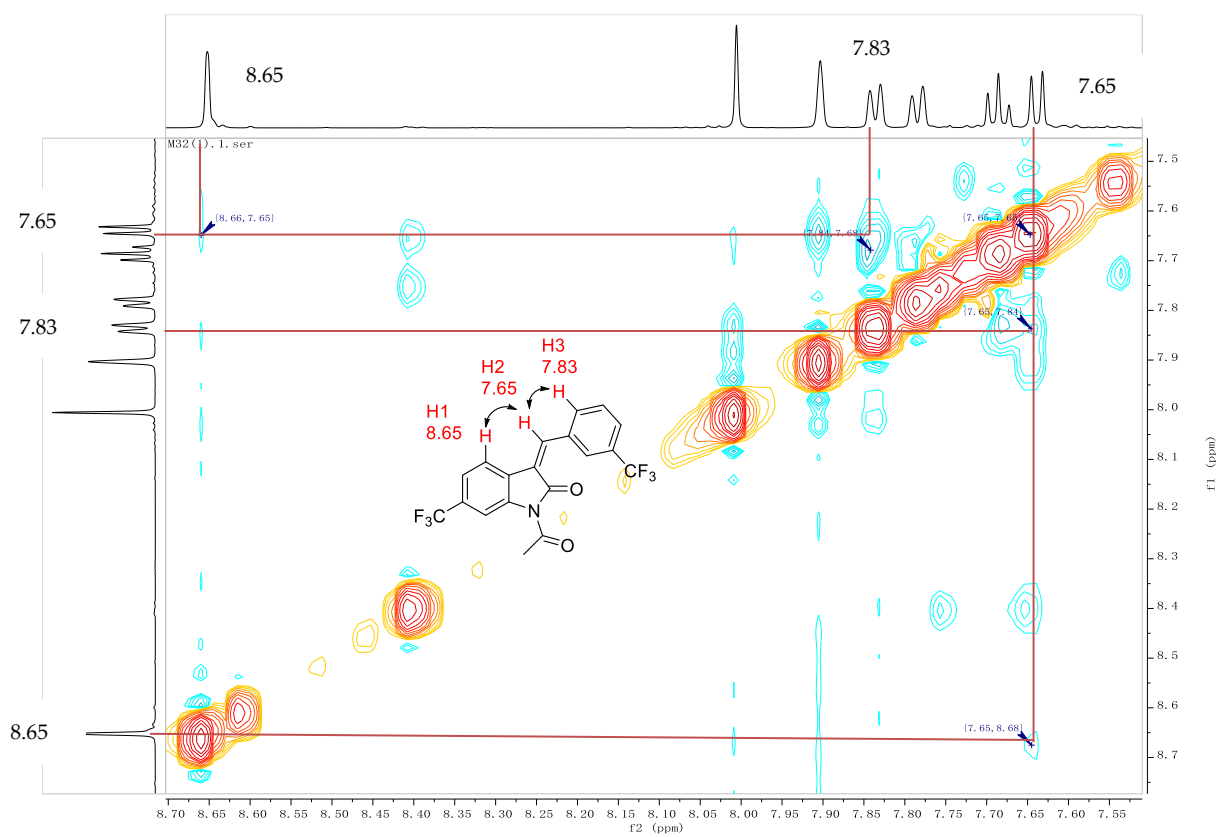


Figure S3-4. 2D-NOEY spectrum (600 Hz, CDCl_3) of compound **4b**

1-Acetyl-5-chloro-3-(3-(trifluoromethyl)benzylidene)indolin-2-one(4c)

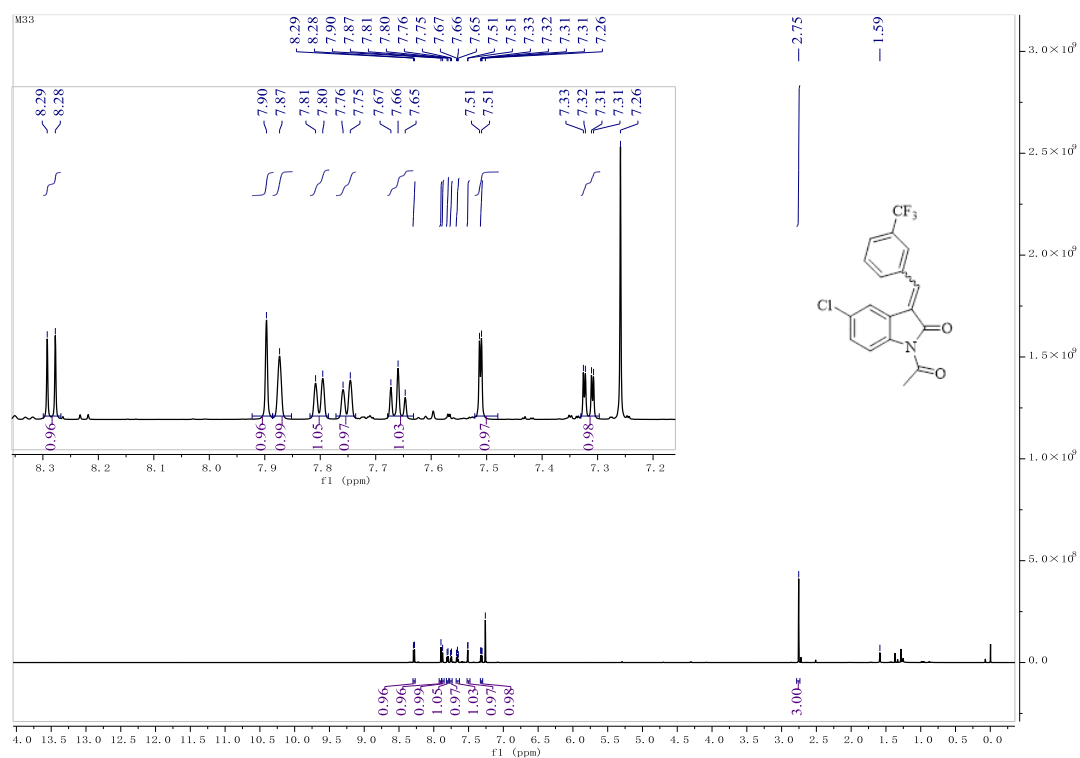


Figure S3-1. ¹H, NMR spectrum (600 Hz, CDCl₃) of compound 4c

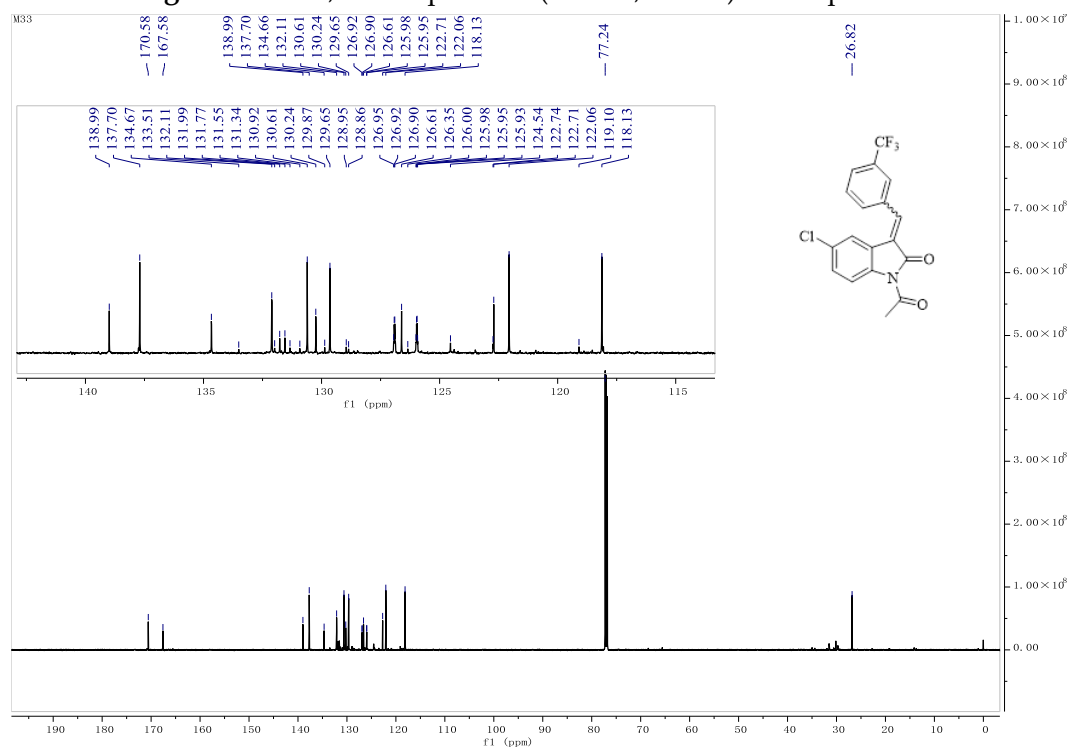


Figure S3-2. ¹³C NMR spectrum (150 Hz, CDCl₃) of compound 4c

M33 #32 RT: 0.14 AV: 1 NL: 4.86E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

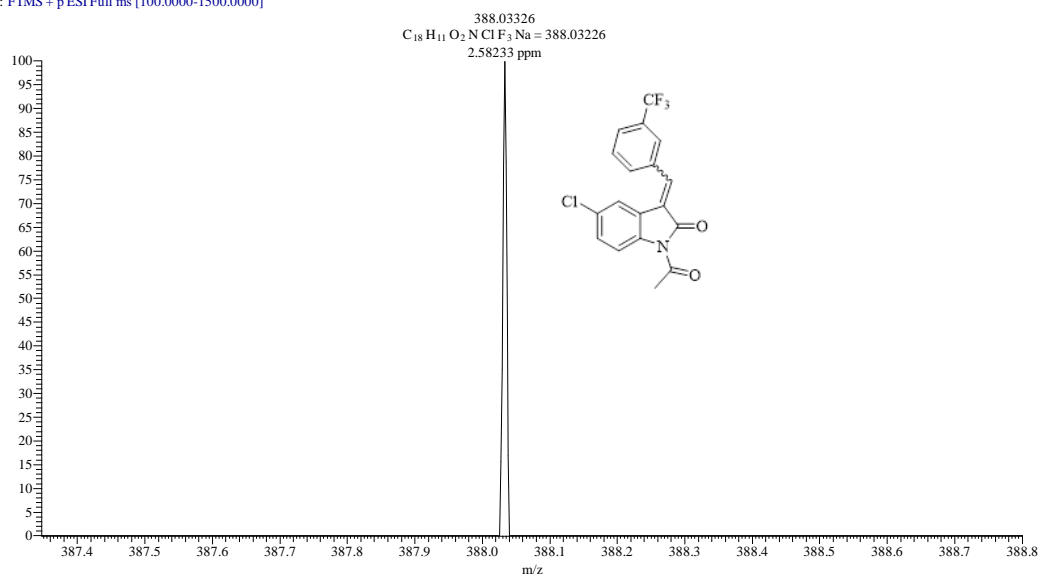


Figure S3-3. HRMS of compound 4c

1-Acetyl-3-(3, 5-bis(trifluoromethyl)benzylidene)-6-chloroindolin-2-one (4d)

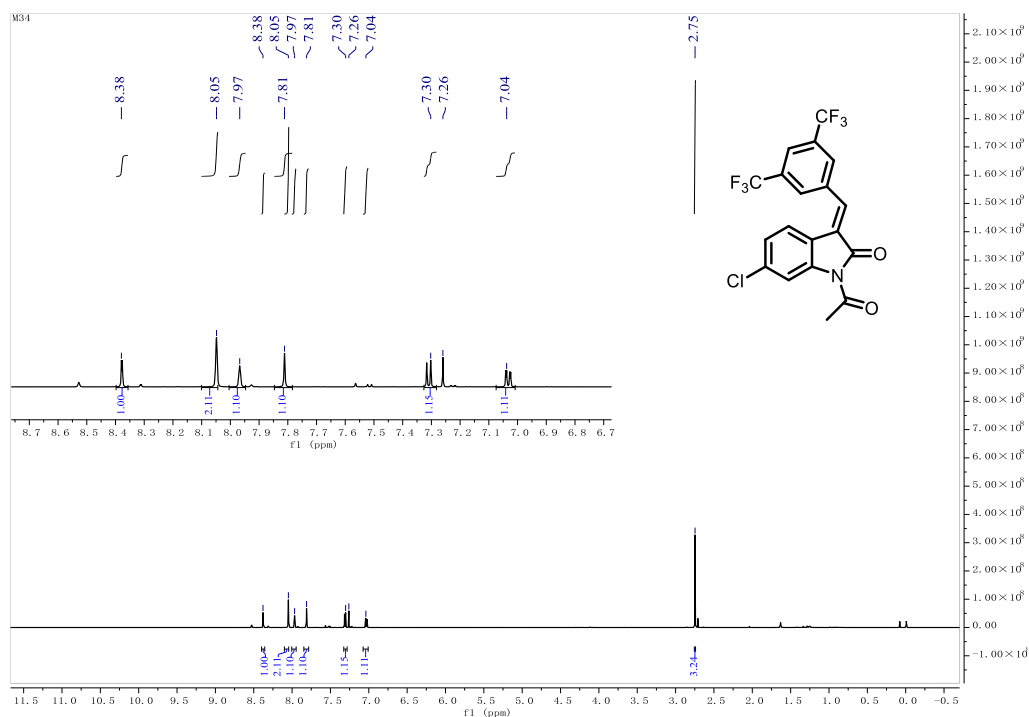


Figure S4-1. ¹H, NMR spectrum (600 Hz, CDCl₃) of compound **4d**

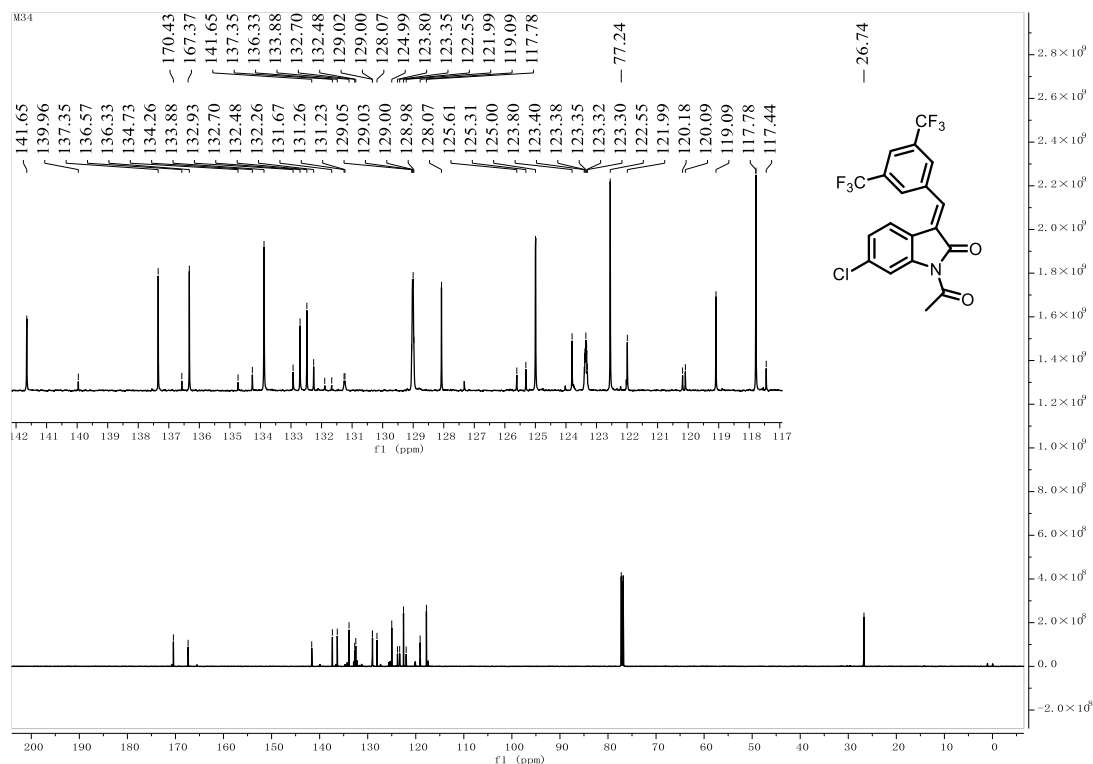


Figure S4-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **4d**

M34 #22 RT: 0.10 AV: 1 NL: 1.53E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

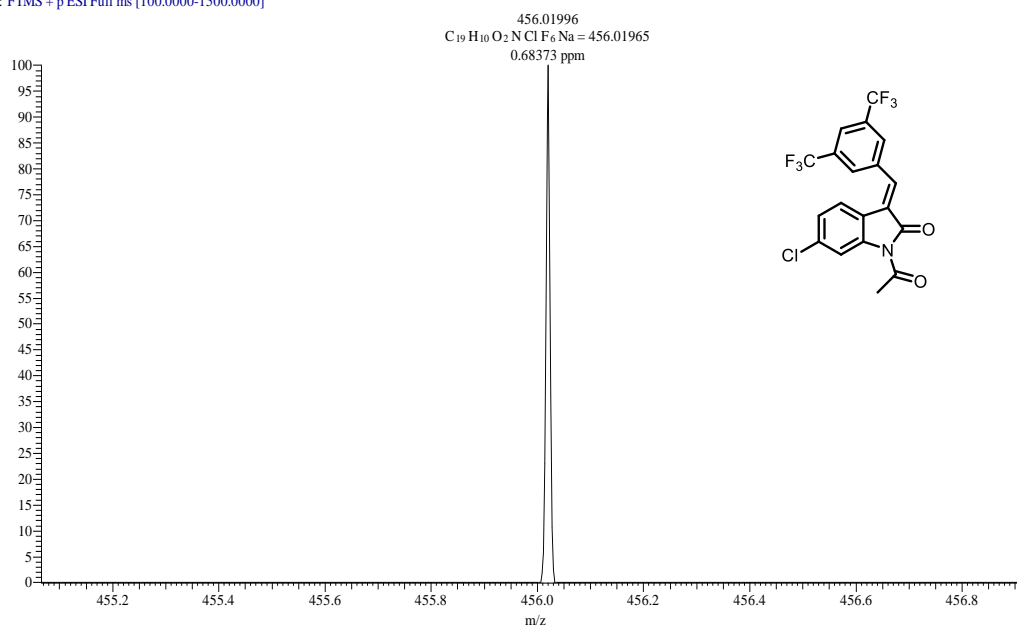


Figure S4-3. HRMS of compound 4d

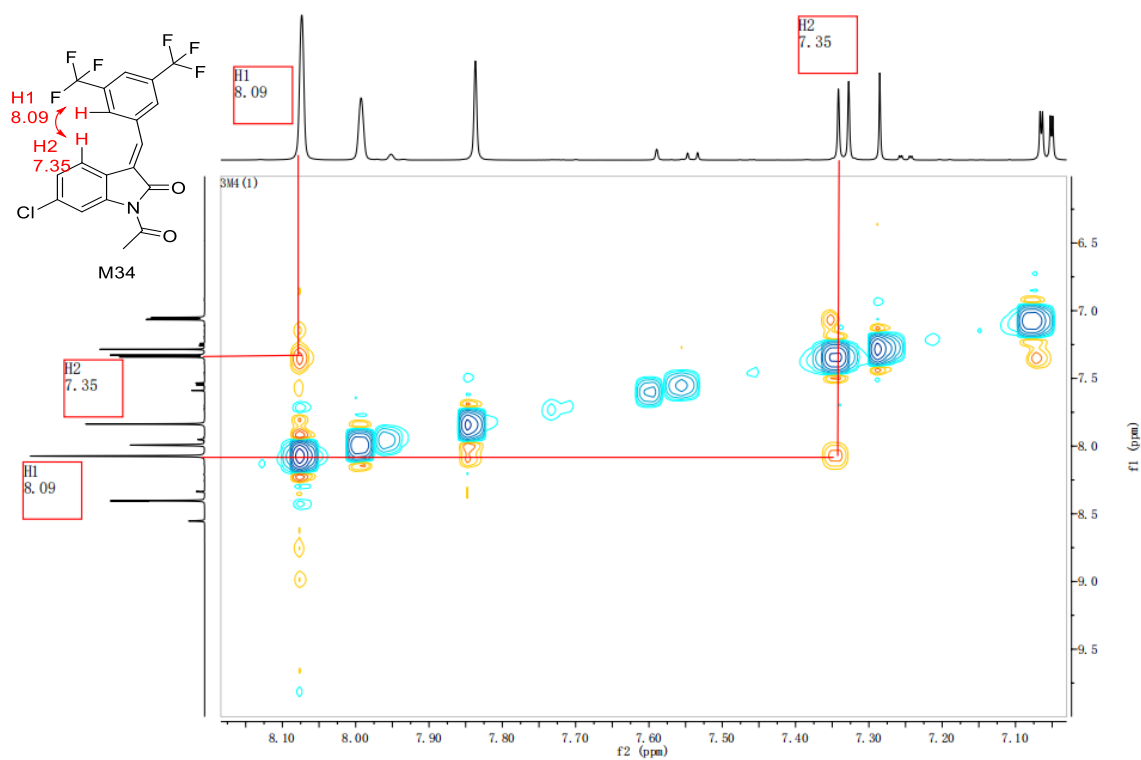


Figure S4-4. 2D-NOEY spectrum (600 Hz, $CDCl_3$) of compound 4d

(E)-1-acetyl-5-amino-3-(3-(trifluoromethyl)benzylidene)indolin-2-one (4e)

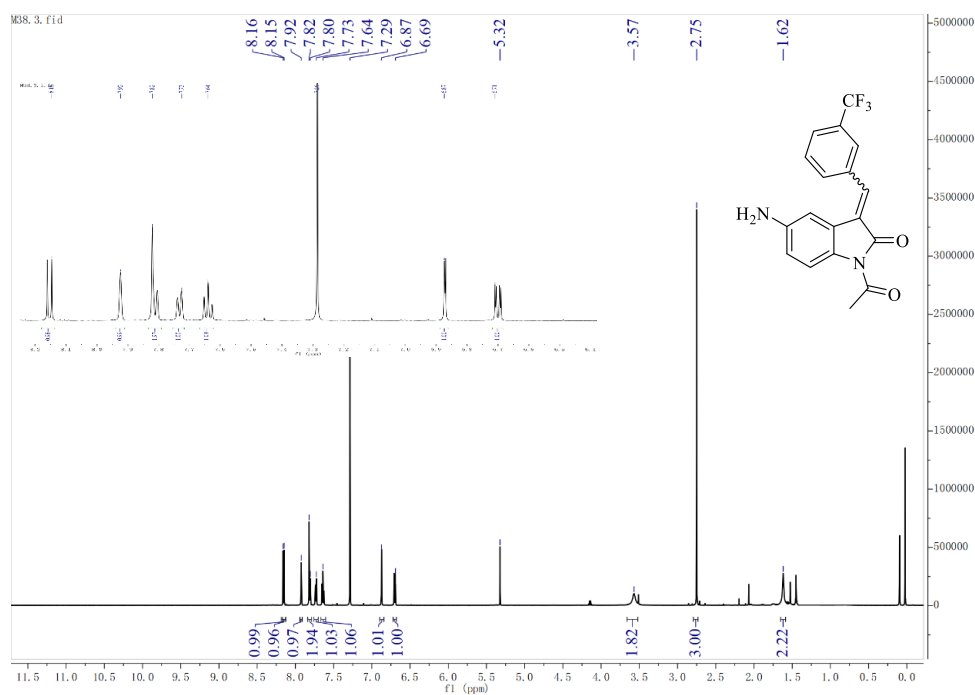


Figure S5-1. ¹H NMR spectrum (600 Hz, CDCl₃) of compound **4e**

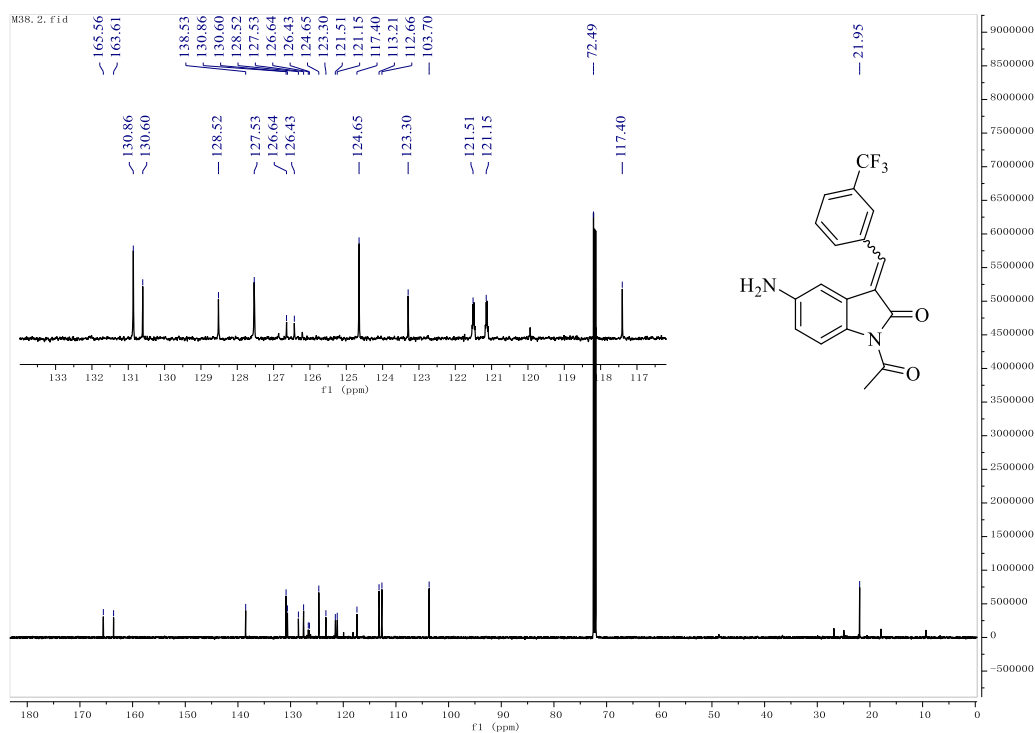


Figure S5-2. ¹H, ¹³C NMR spectrum (150 Hz, DMSO) of compound **4e**

M38 #22 RT: 0.10 AV: 1 NL: 5.99E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

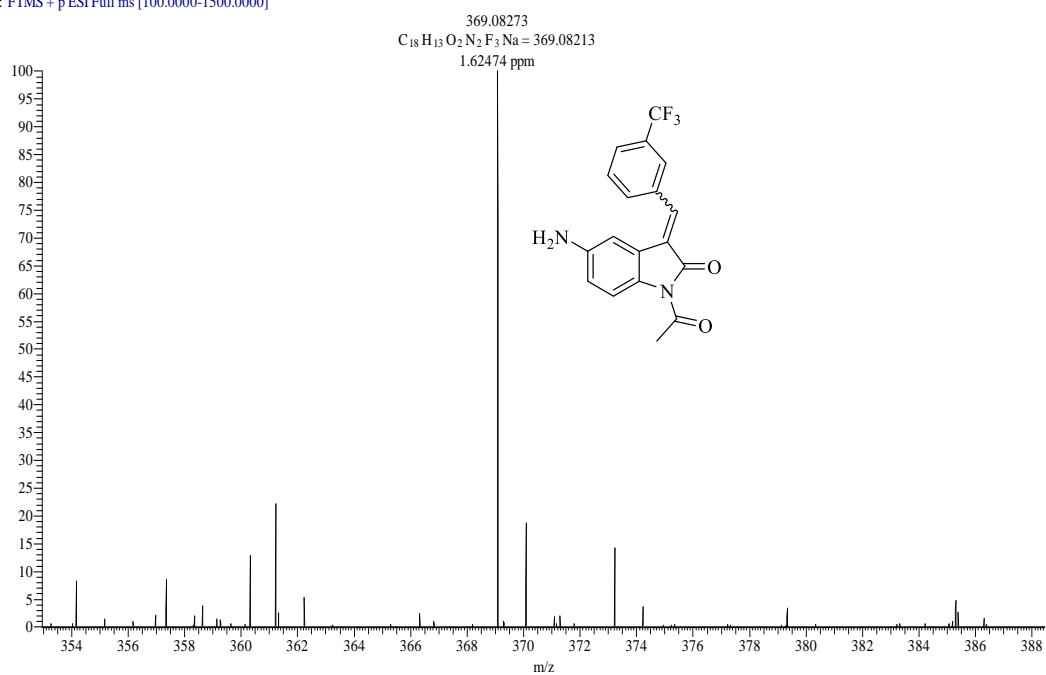


Figure S5-3. HRMS of compound 4e

(Z)-1-acetyl-3-(3,5-bis(trifluoromethyl)benzylidene)-6-chloroindolin-2-one(4f)

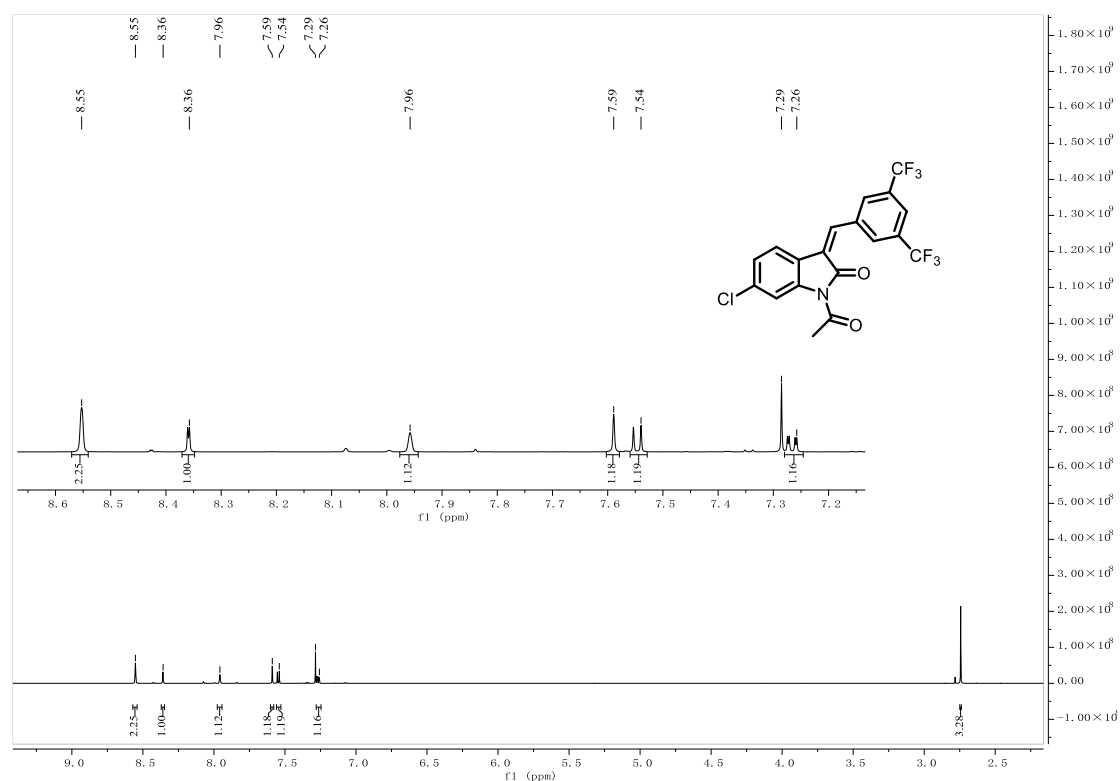


Figure S6-1. ¹H NMR spectrum (600 Hz, CDCl₃) of compound 4f

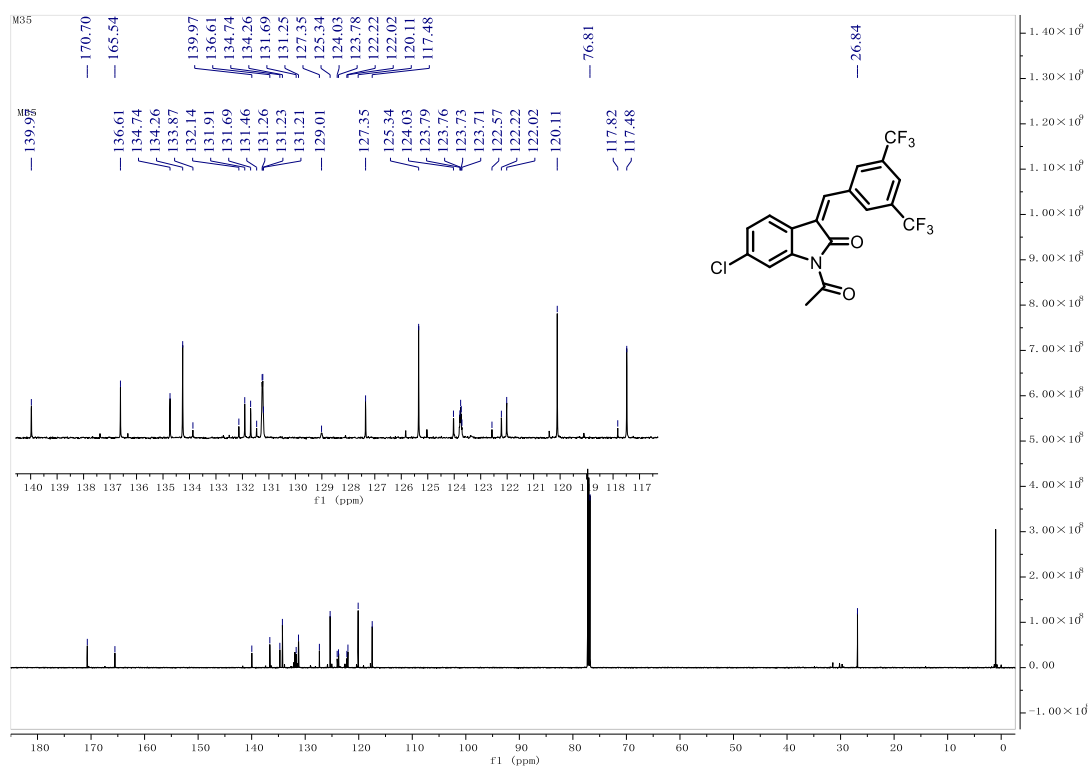


Figure S6-2. ¹H, ¹³C NMR spectrum (600 Hz, 150 Hz, CDCl₃) of compound 4f

M35 #25 RT: 0.11 AV: 1 NL: 3.18E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

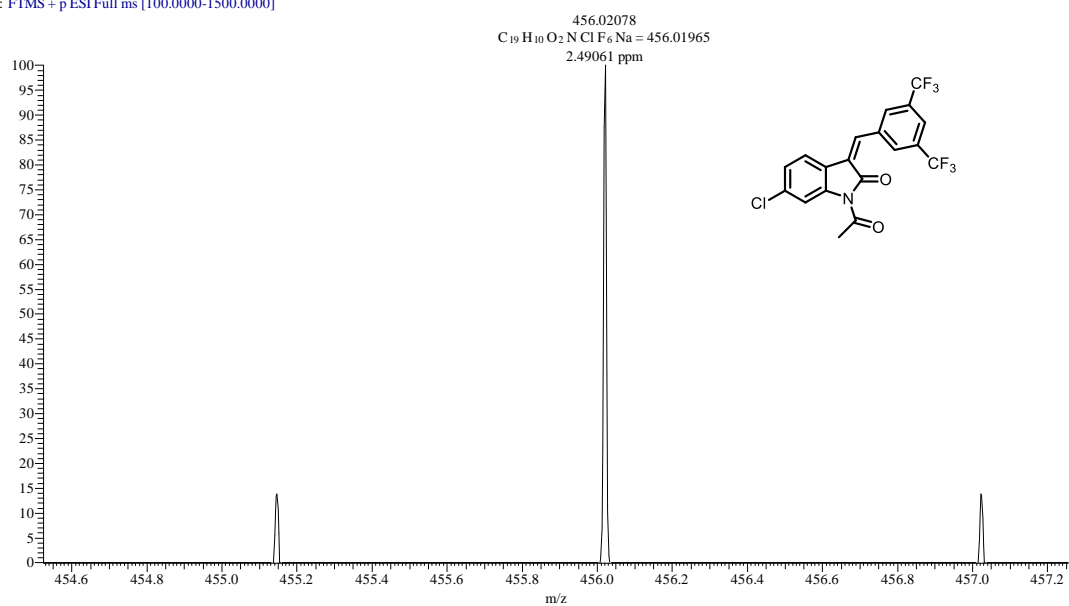


Figure S6-3. HRMS of compound 4f

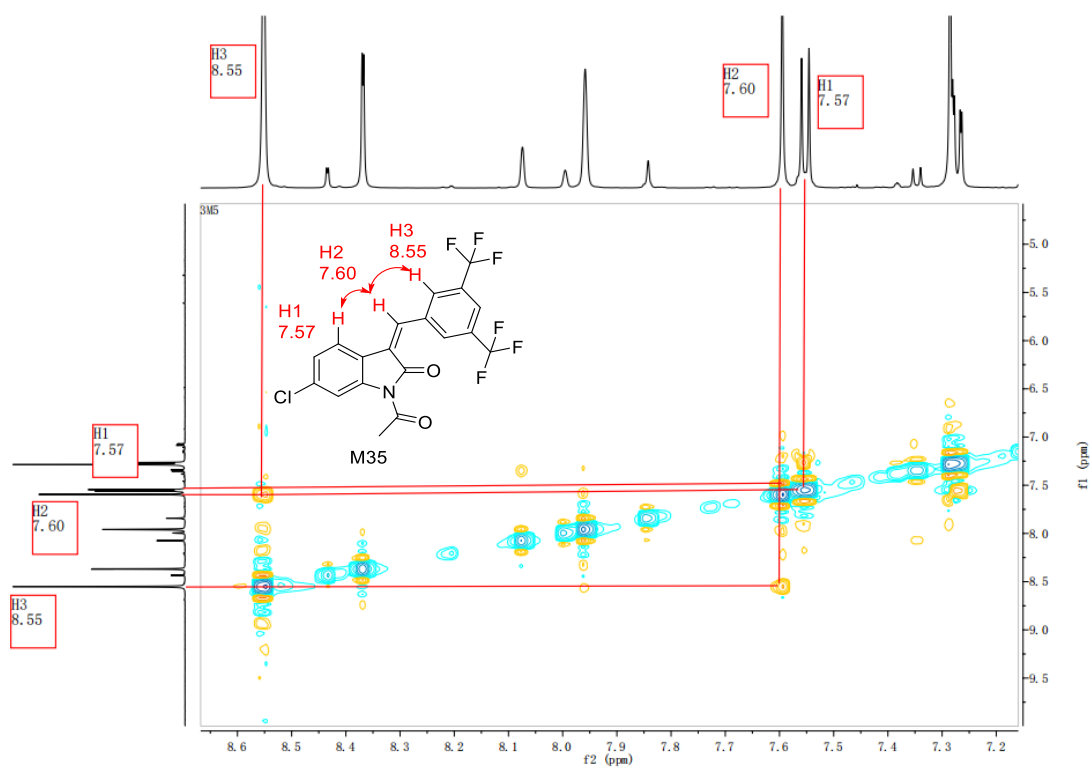


Figure S6-4. 2D-NOESY spectrum (600 Hz, CDCl₃) of compound 4f

1-Acetyl-3-benzylideneindolin-2-one (4g)

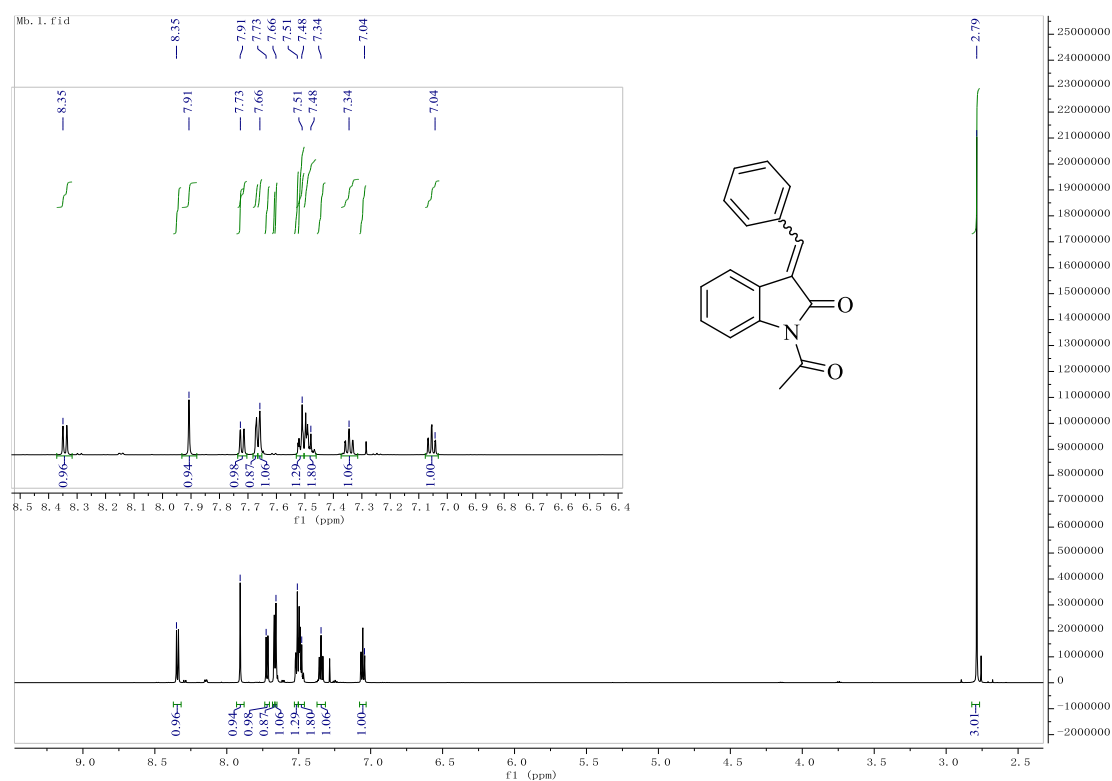


Figure S7-1. ^1H NMR spectrum (600 Hz, CDCl_3) of compound 4g

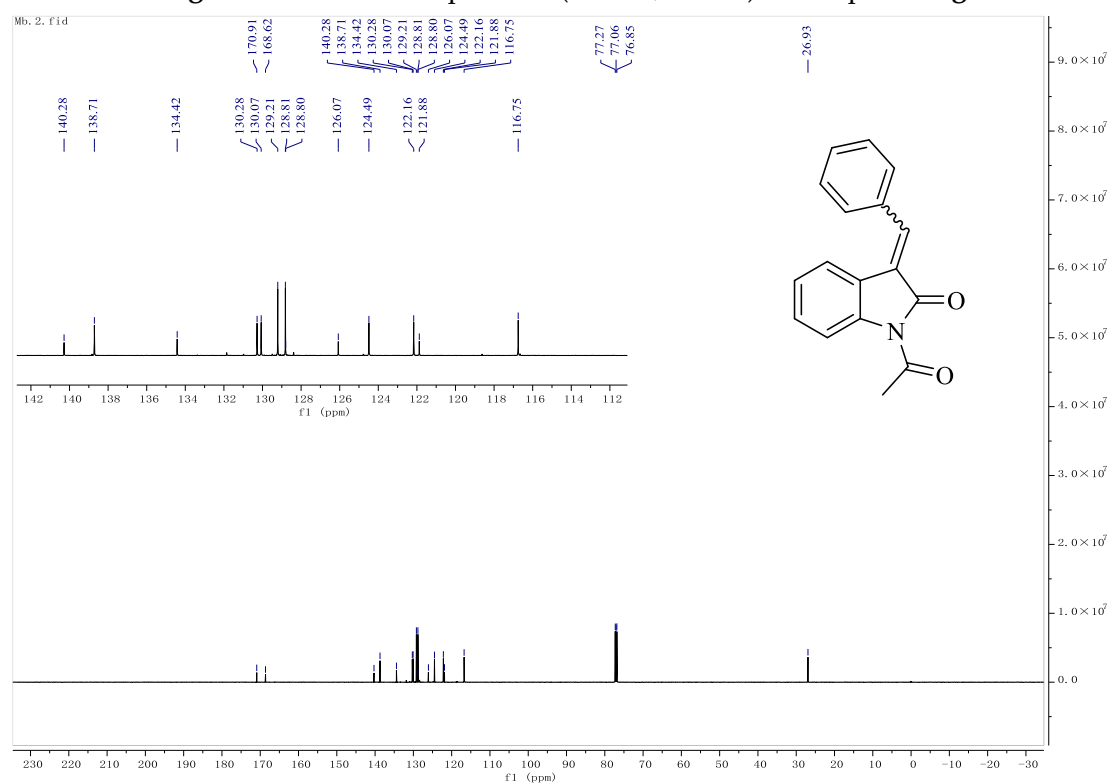


Figure S7-2. ^{13}C NMR spectrum (150 Hz, CDCl_3) of compound 4g

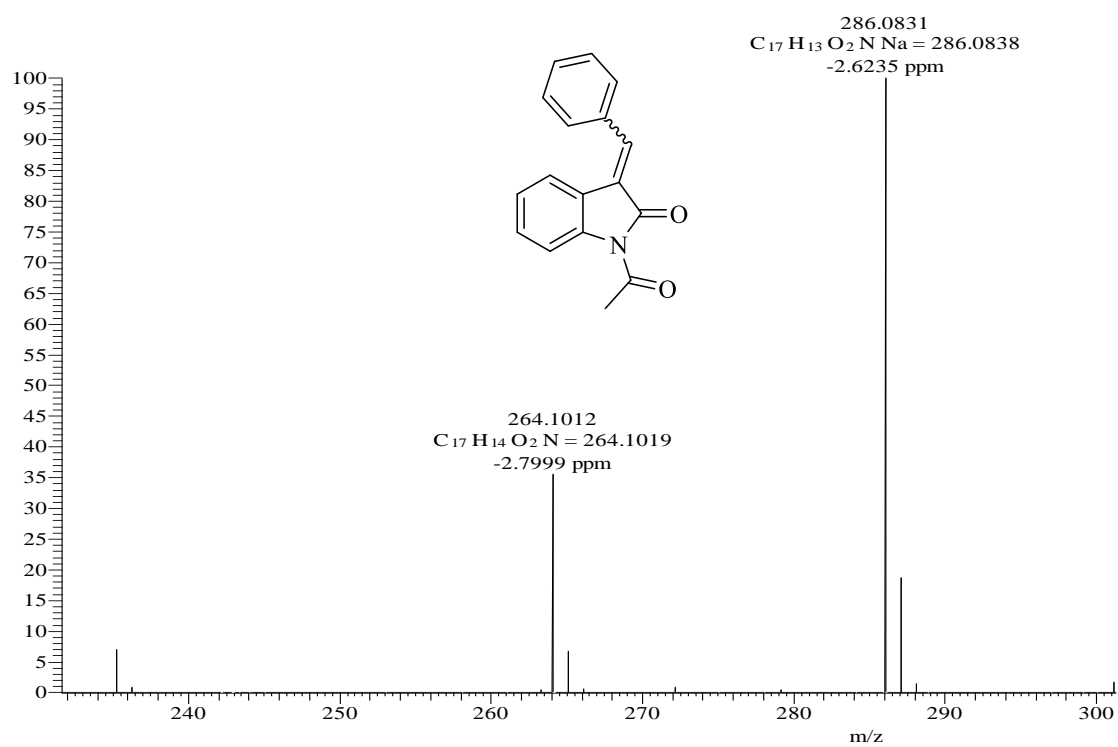


Figure S7-3. HRMS of compound 4g

1-Acetyl-6-chloro-3-(3-(trifluoromethyl)benzylidene)indolin-2-one(4h)

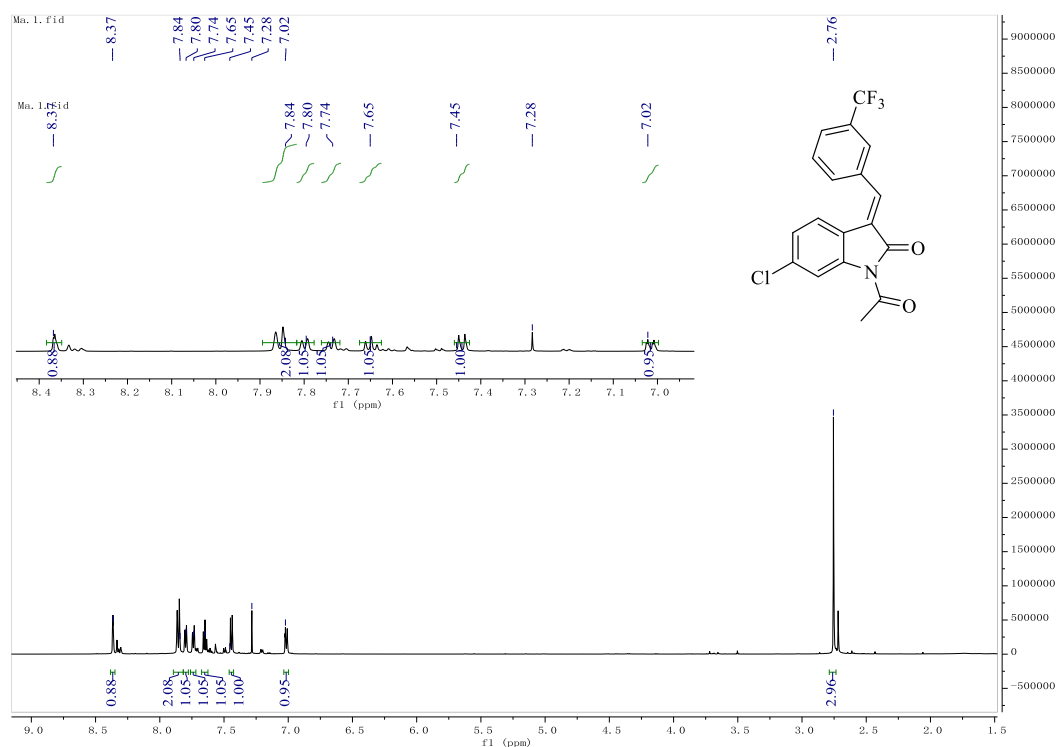


Figure S8-1. ¹H NMR spectrum (600 Hz, CDCl₃) of compound 4h

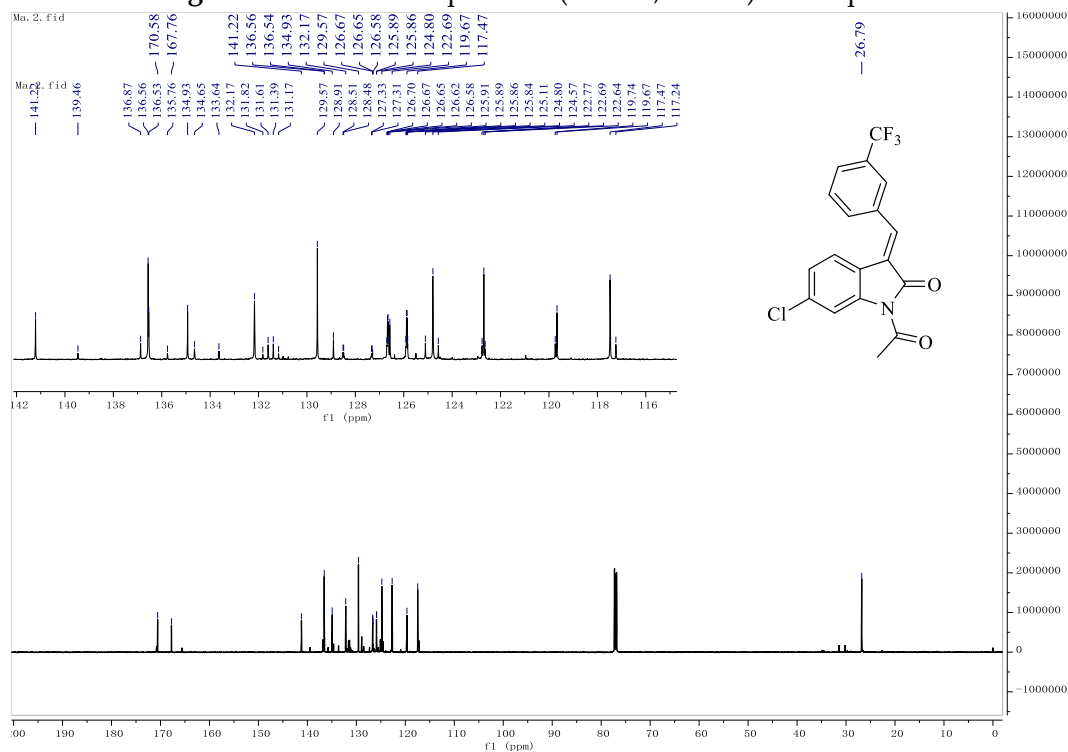


Figure S8-1. ¹³C NMR spectrum (150 Hz, CDCl₃) of compound 4h

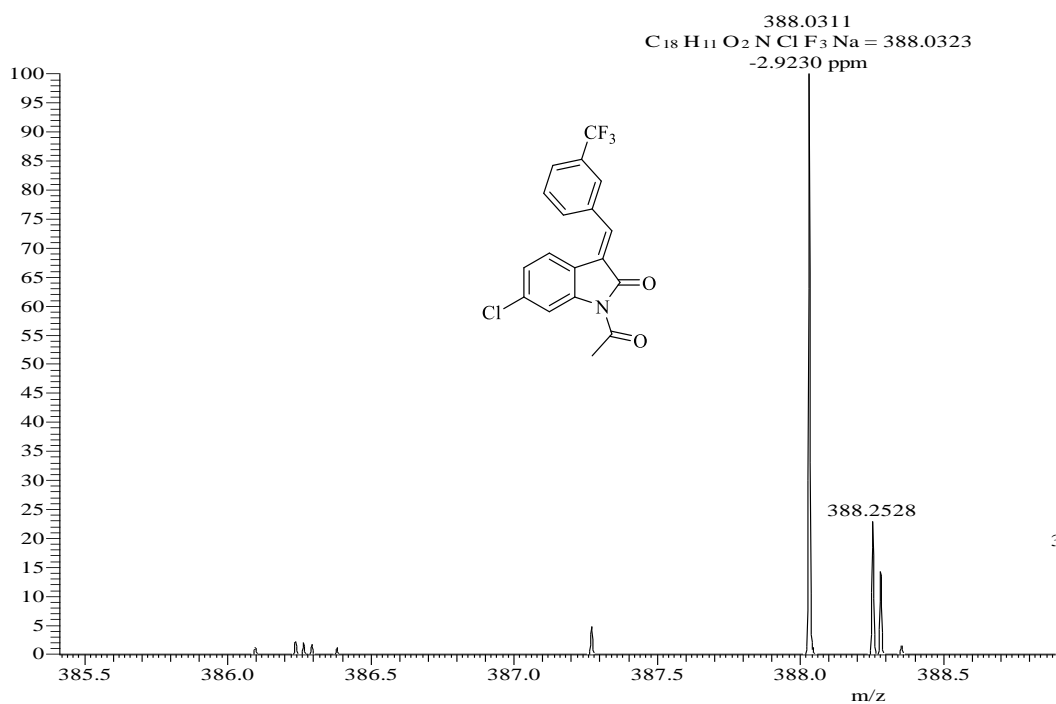


Figure S8-3. HRMS of compound 4h

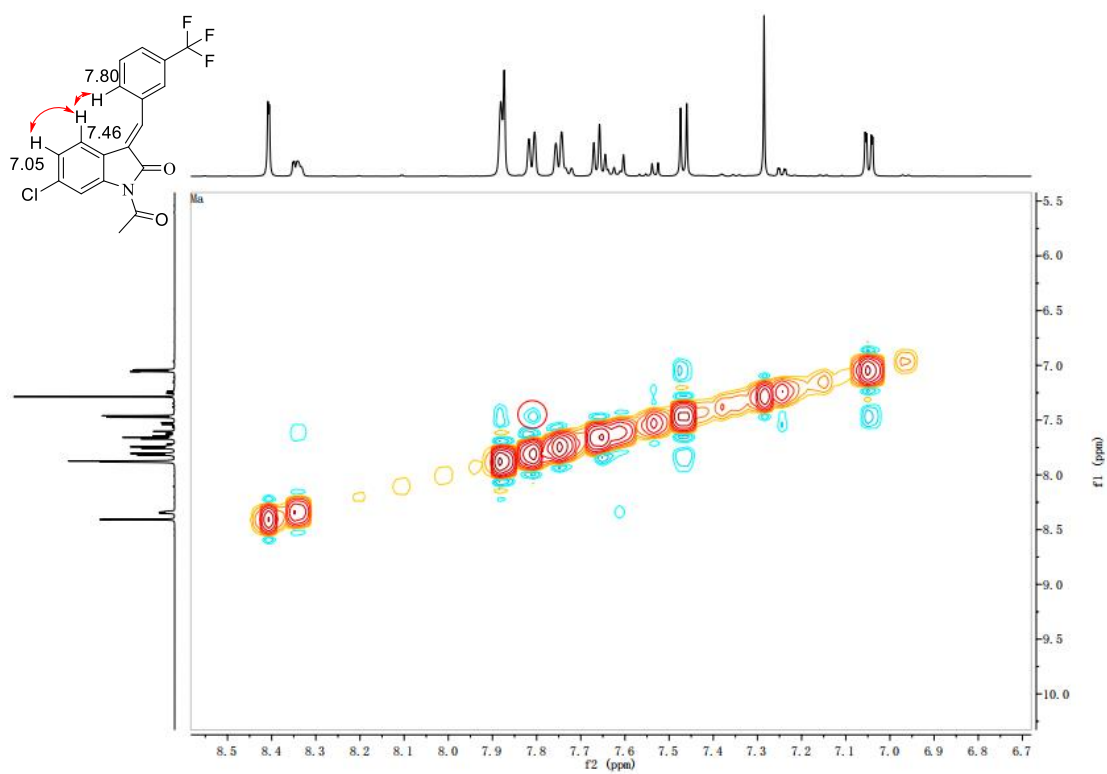


Figure S8-4. 2D-NOEY spectrum (600 Hz, CDCl₃) of compound 4h

1-Acetyl-6-chloro-3-(4-(trifluoromethyl)benzylidene)indolin-2-one(4i)

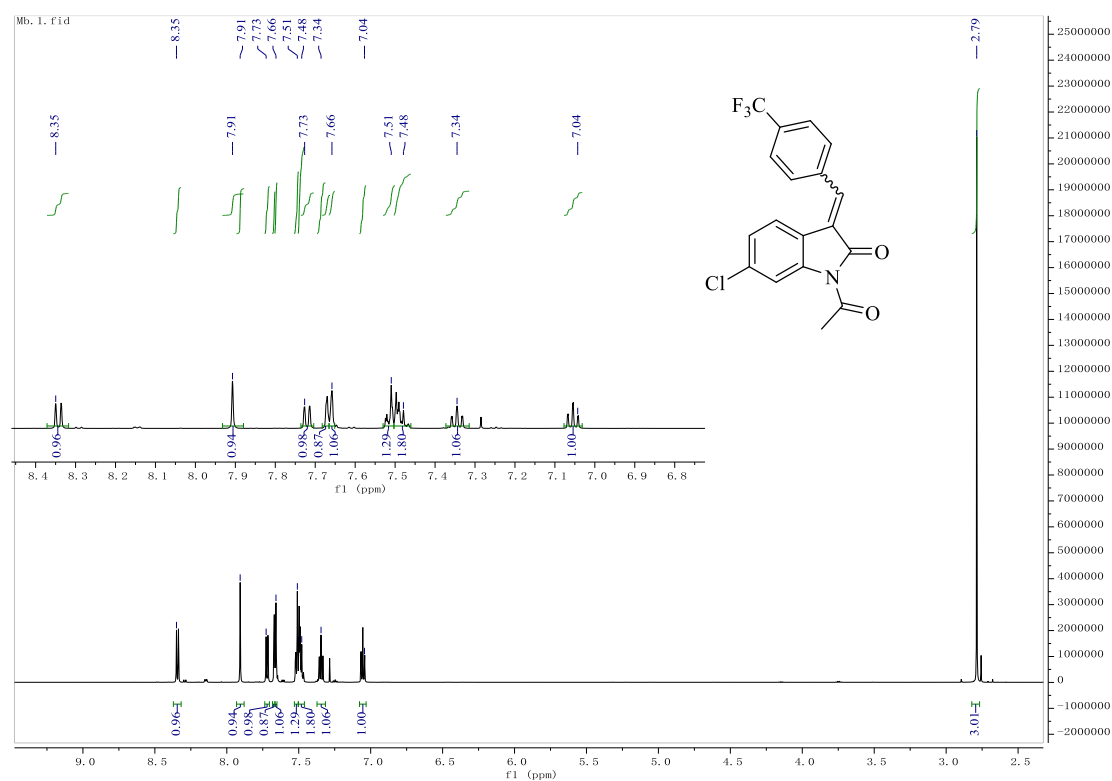


Figure S9-1. ¹H NMR spectrum (600 MHz, CDCl₃) of compound **4i**

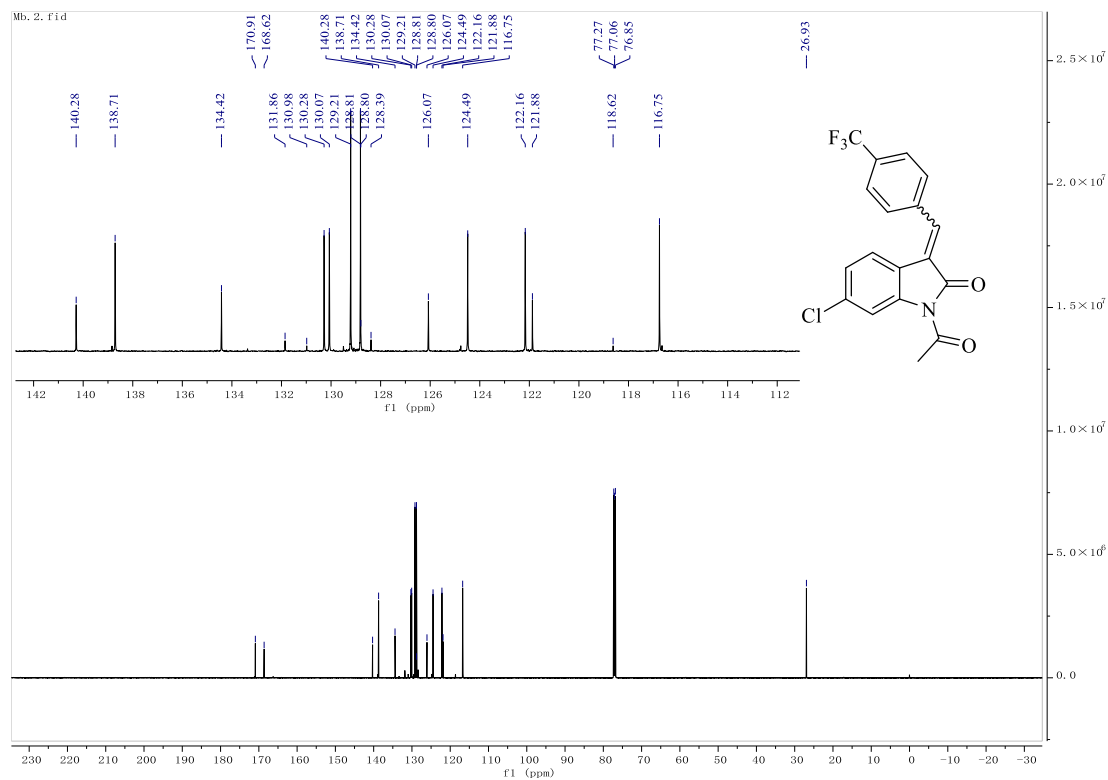


Figure S9-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **4i**

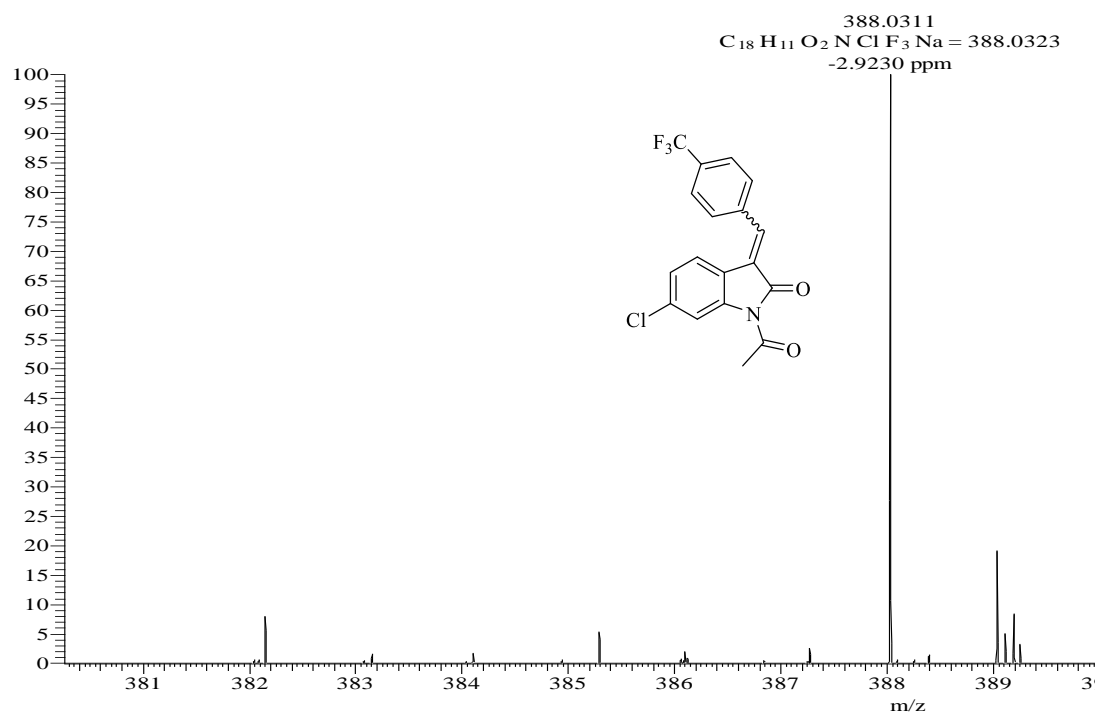


Figure S9-3. HRMS of compound **4i**

1-Acetyl-3-(3-(trifluoromethyl)benzylidene)indolin-2-one(4j)

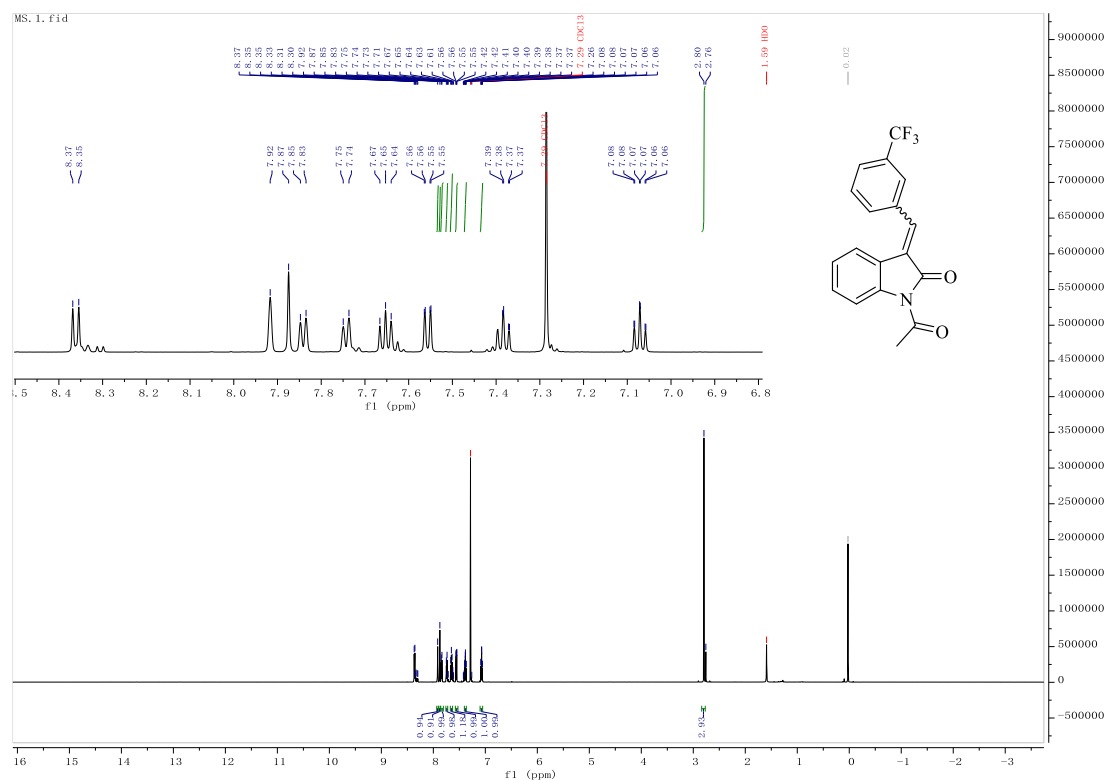


Figure S10-1. ^1H NMR spectrum (600 Hz, CDCl_3) of compound **4j**

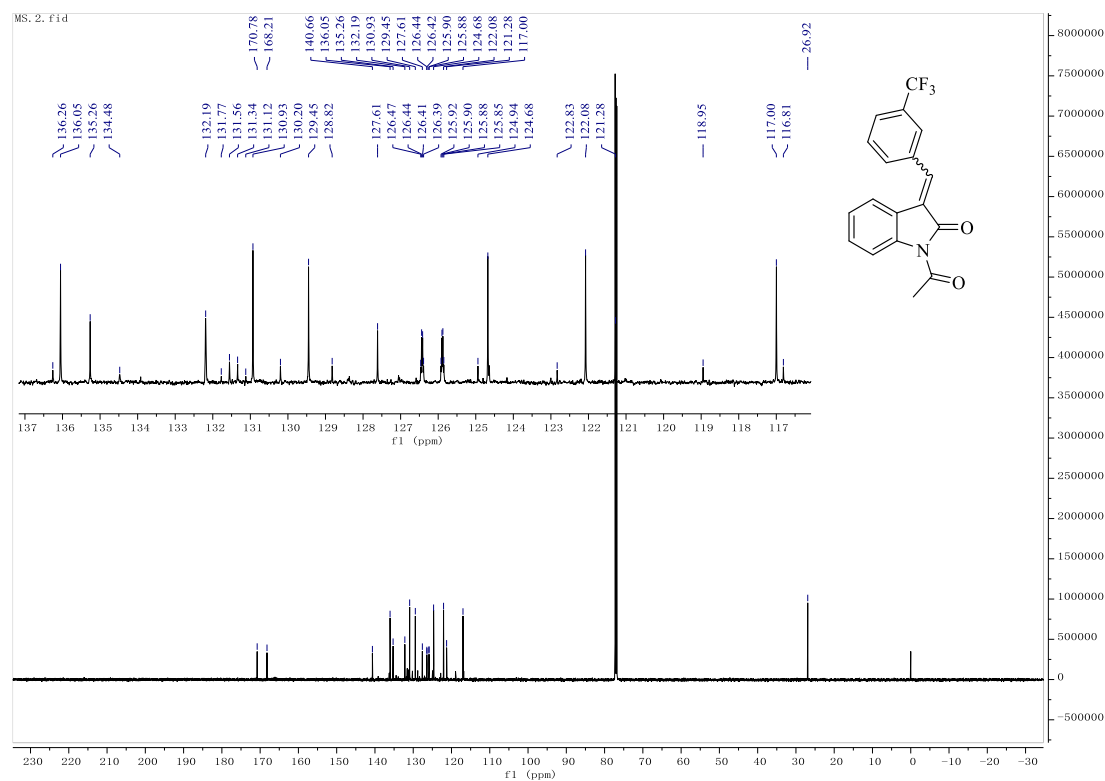


Figure S10-2. ^{13}C NMR spectrum (150 Hz, CDCl_3) of compound **4j**

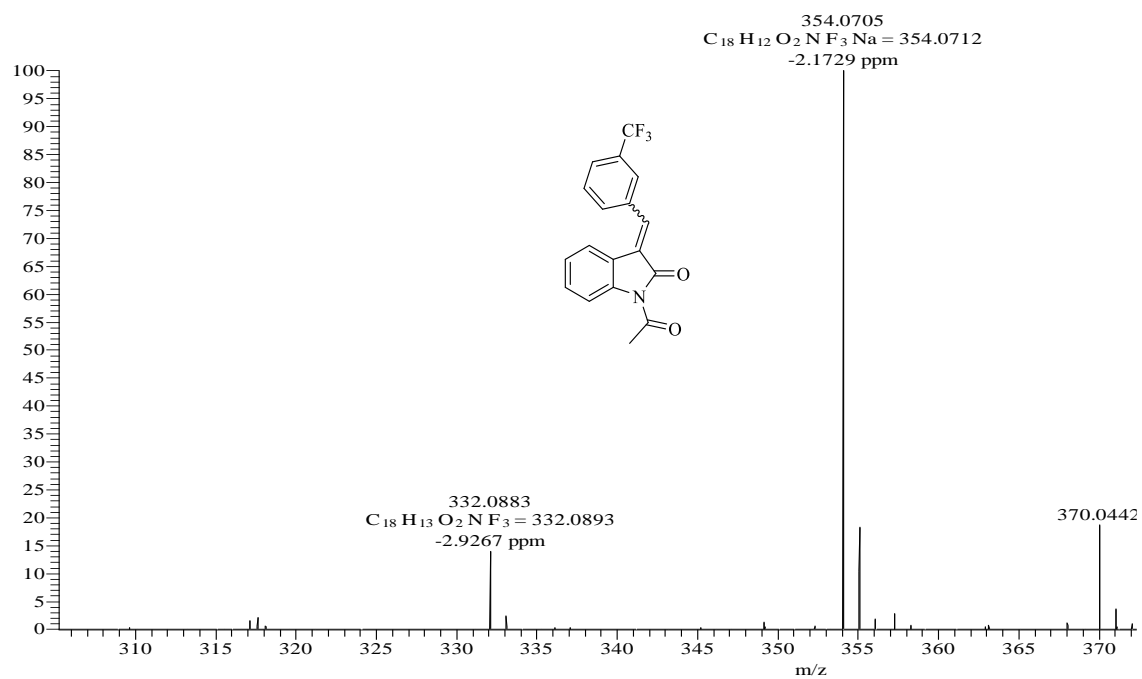


Figure S10-3. HRMS of compound **4j**

1-Acetyl-6-chloro-3-(2-(trifluoromethyl)benzylidene)indolin-2-one(4k)

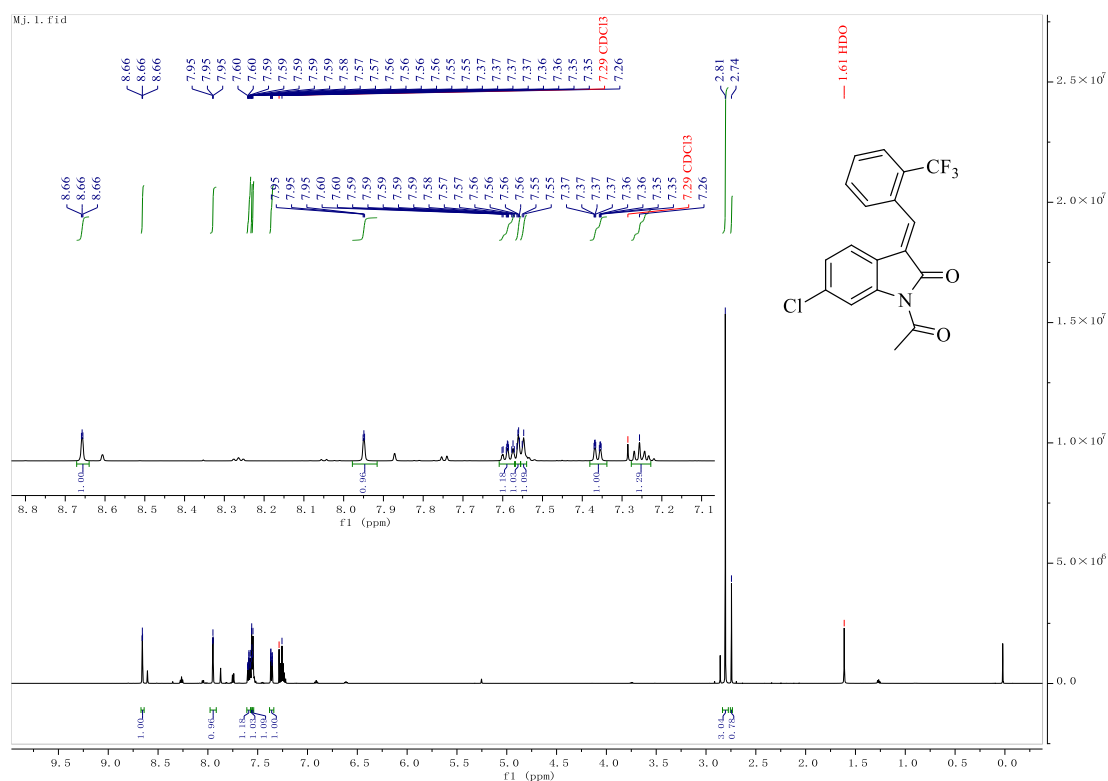


Figure S11-1. ¹H NMR spectrum (600 Hz, CDCl₃) of compound 4k

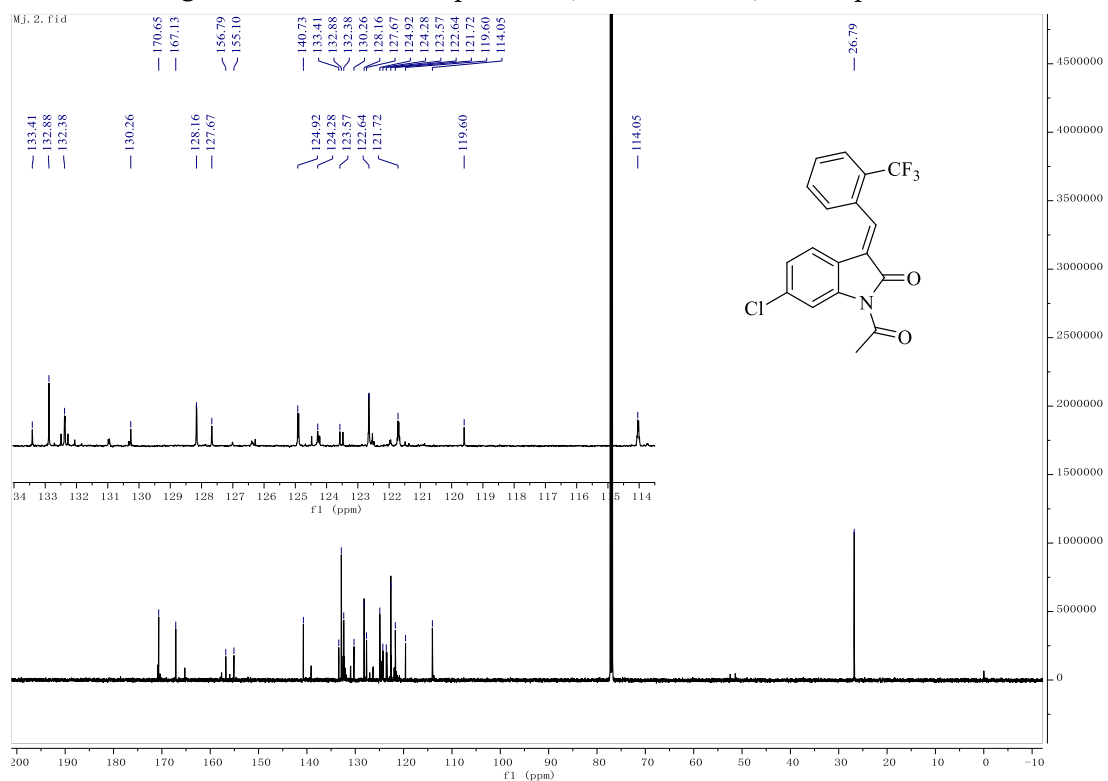


Figure S11-2. ¹³C NMR spectrum (150 Hz, CDCl₃) of compound 4k

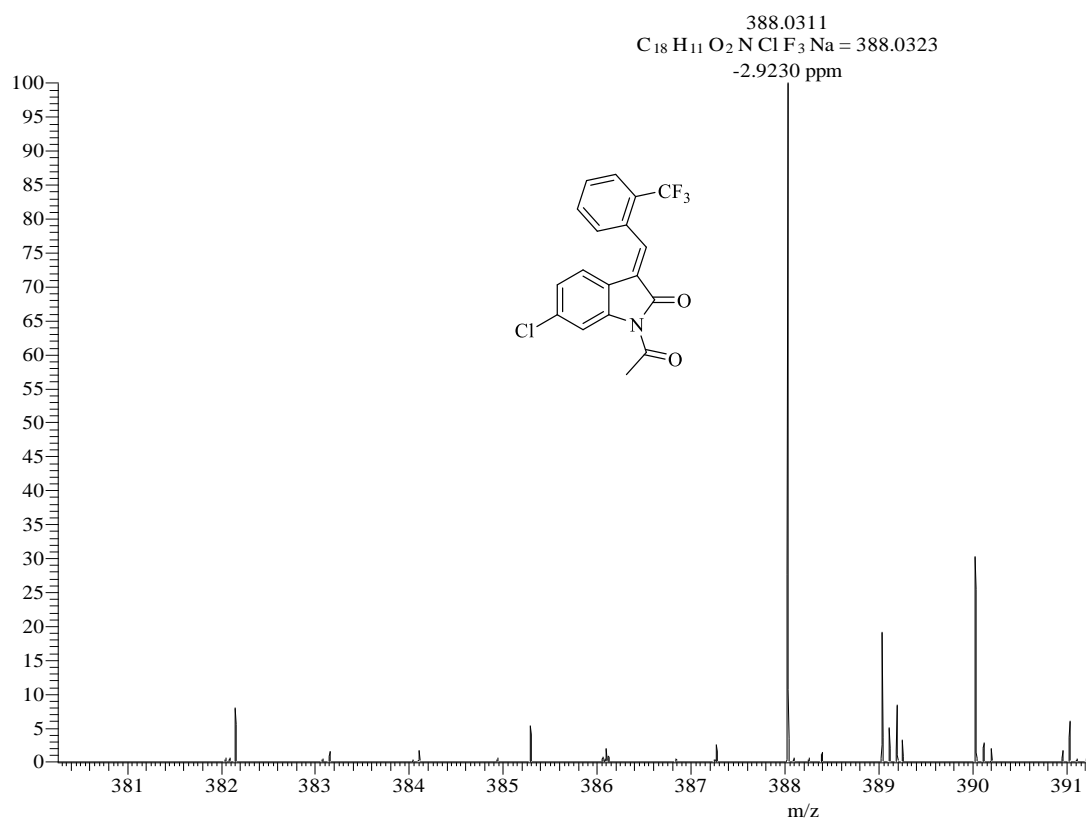
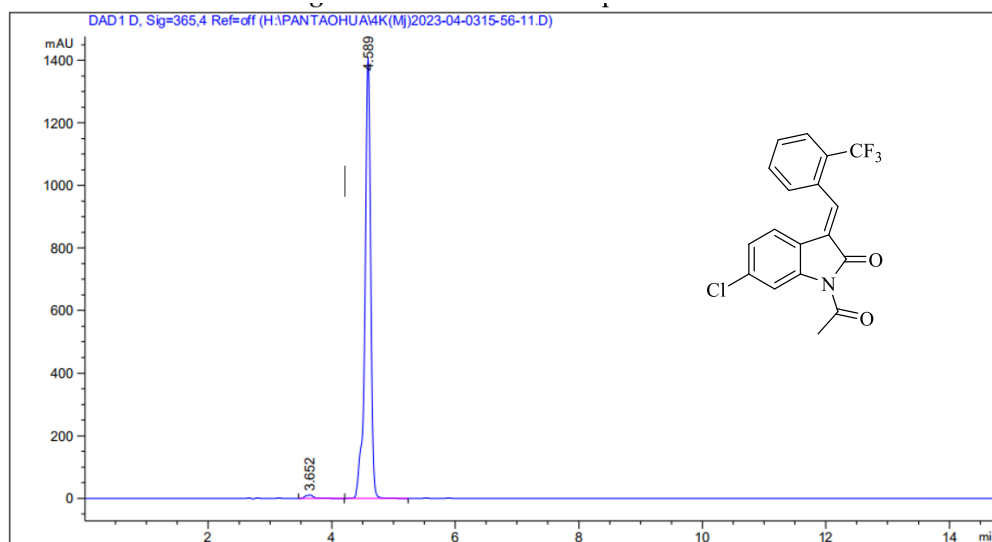


Figure S11-3. HRMS of compound 4k



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.652	BV R	0.1241	92.01453	9.92733	1.0192
2	4.589	BB	0.0961	8936.00000	1406.58325	98.9808

Totals : 9028.01453 1416.51058

Figure S11-4. HPLC of compound 4k

1-Acetyl-6-chloro-3-(4-chloro-3-(trifluoromethyl)benzylidene)indolin-2-one(4l)

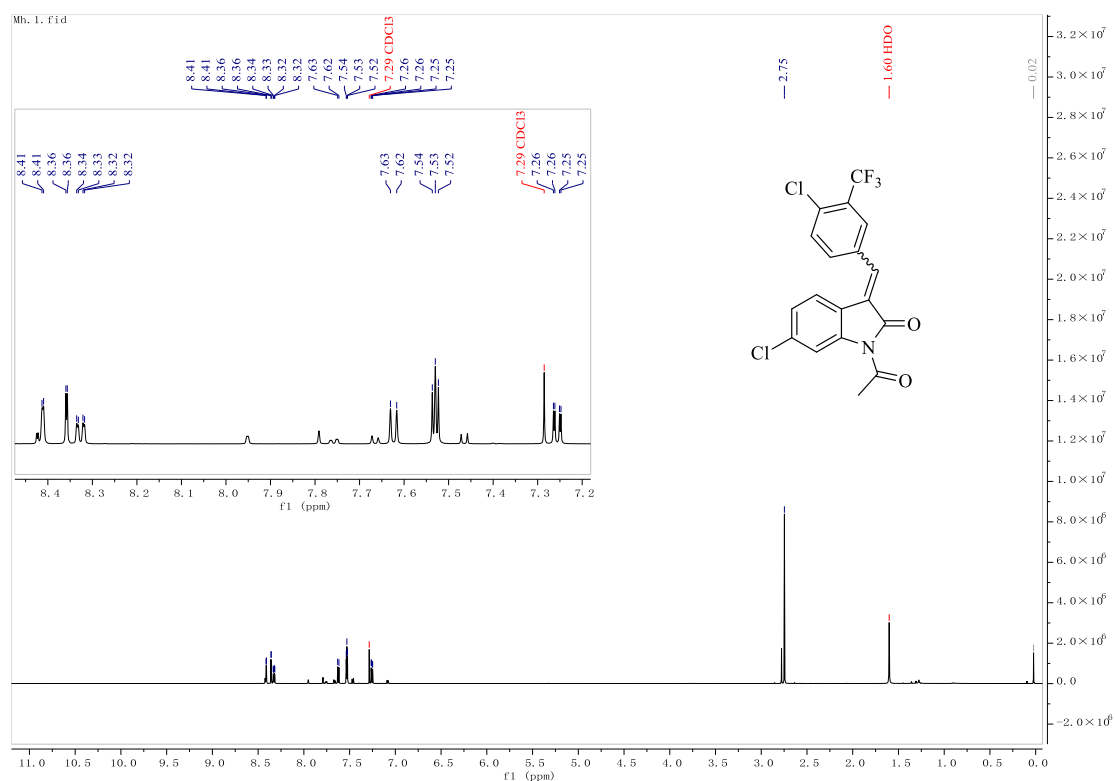


Figure S12-1. ^1H , NMR spectrum (600 Hz, CDCl_3) of compound 4l

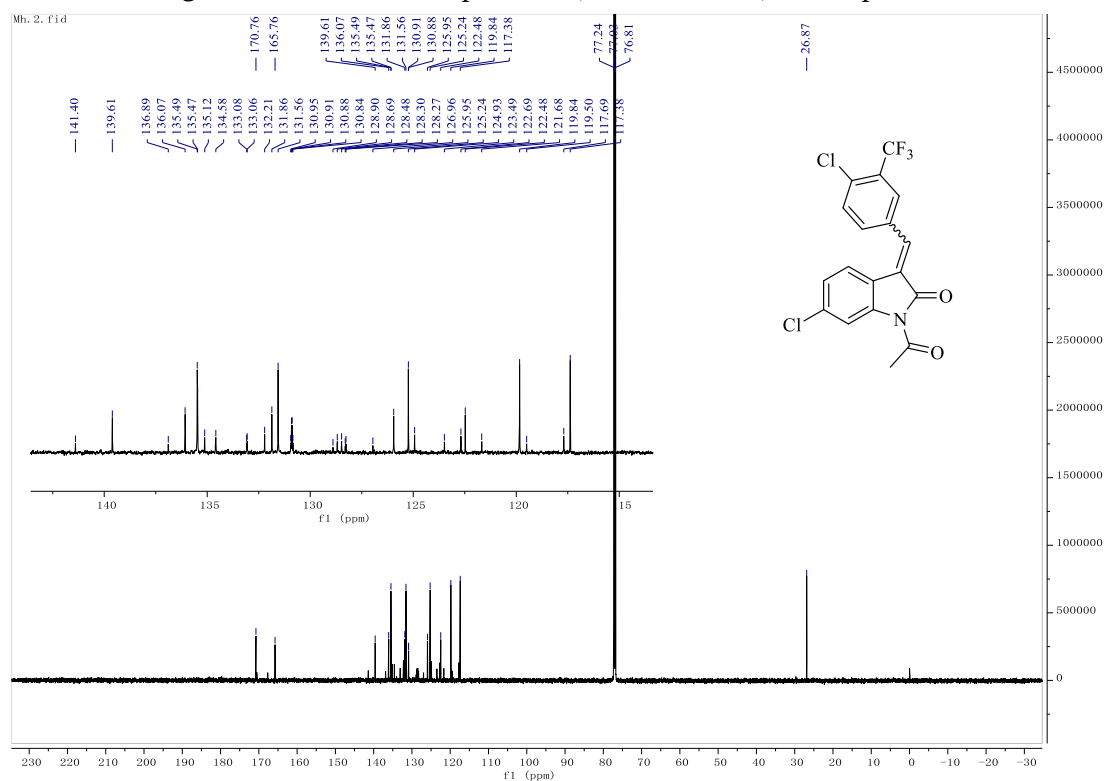


Figure S12-2. ^{13}C NMR spectrum (150 Hz, CDCl_3) of compound 4l

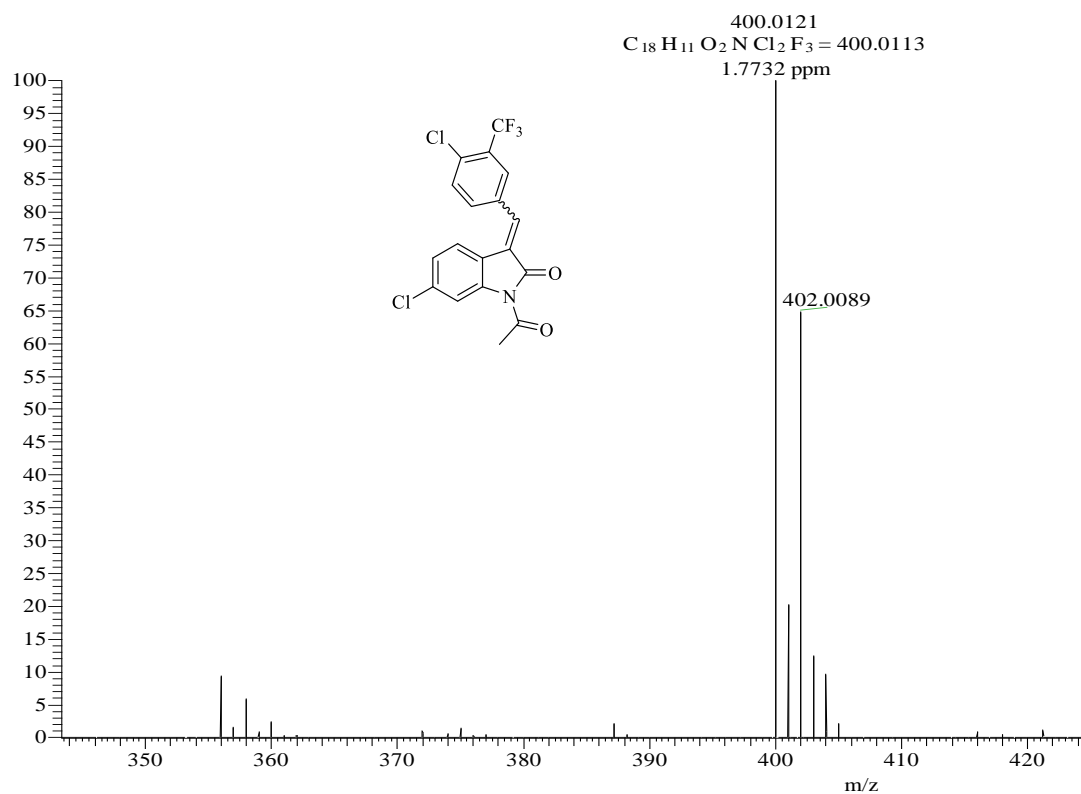


Figure S12-3. HRMS of compound 4l

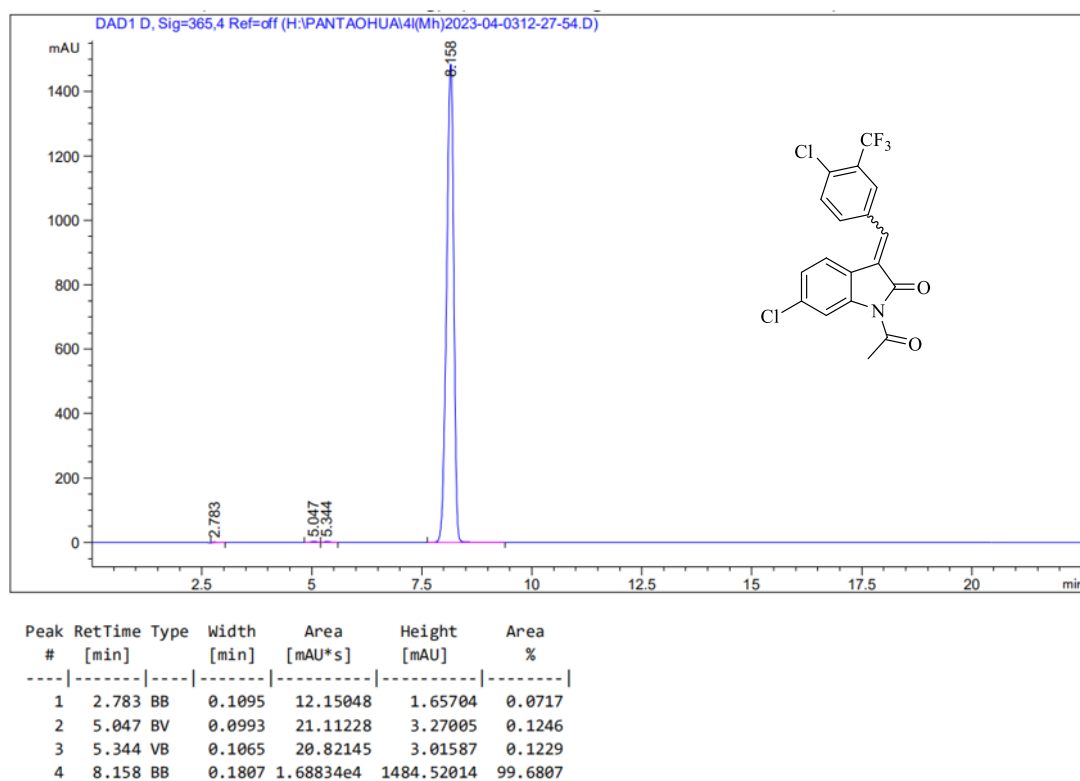


Figure S12-4. HPLC of compound 4l

1-Acetyl-6-chloro-3-(4-chloro-3-fluorobenzylidene)indolin-2-one(4m)

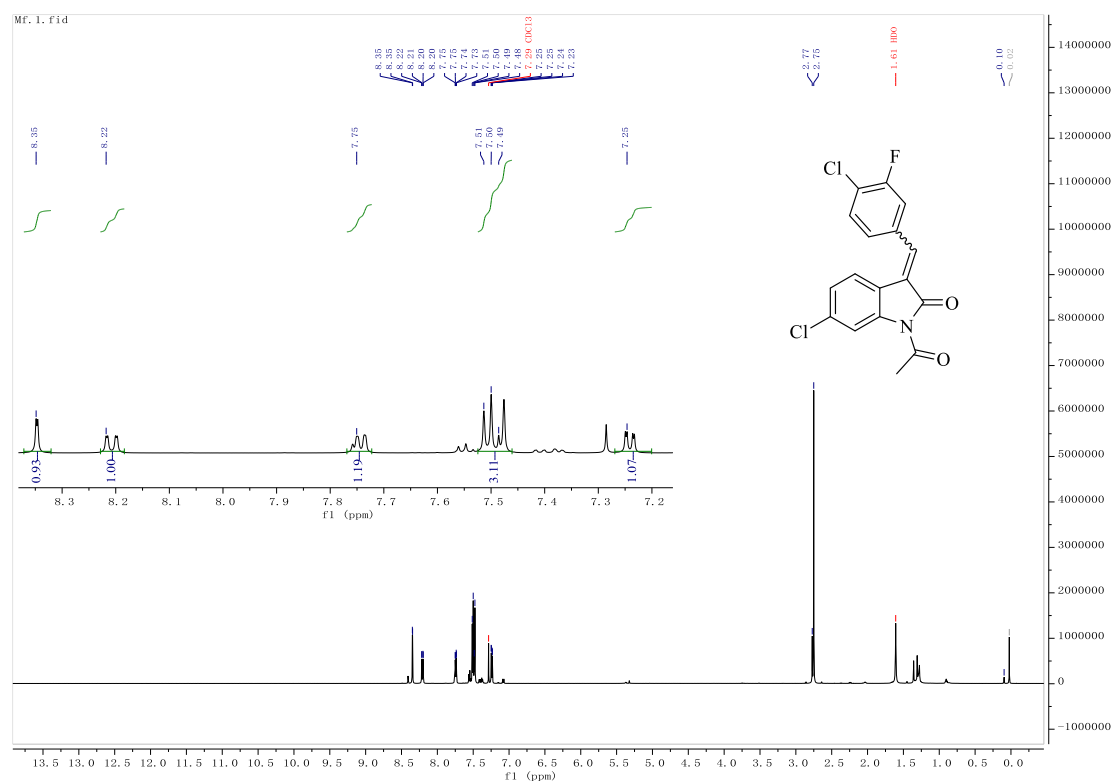


Figure S13-1. ¹H NMR spectrum (600 MHz CDCl₃) of compound **4m**

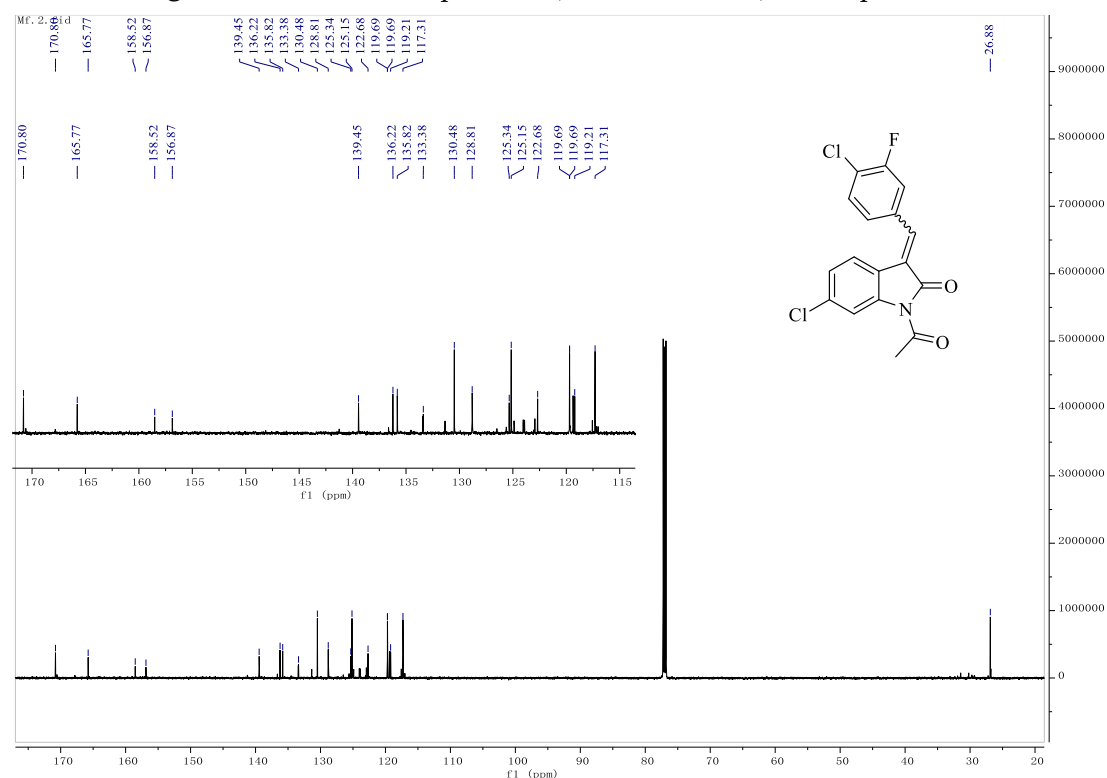


Figure S13-2. ¹³C NMR spectrum (150 MHz CDCl₃) of compound **4m**

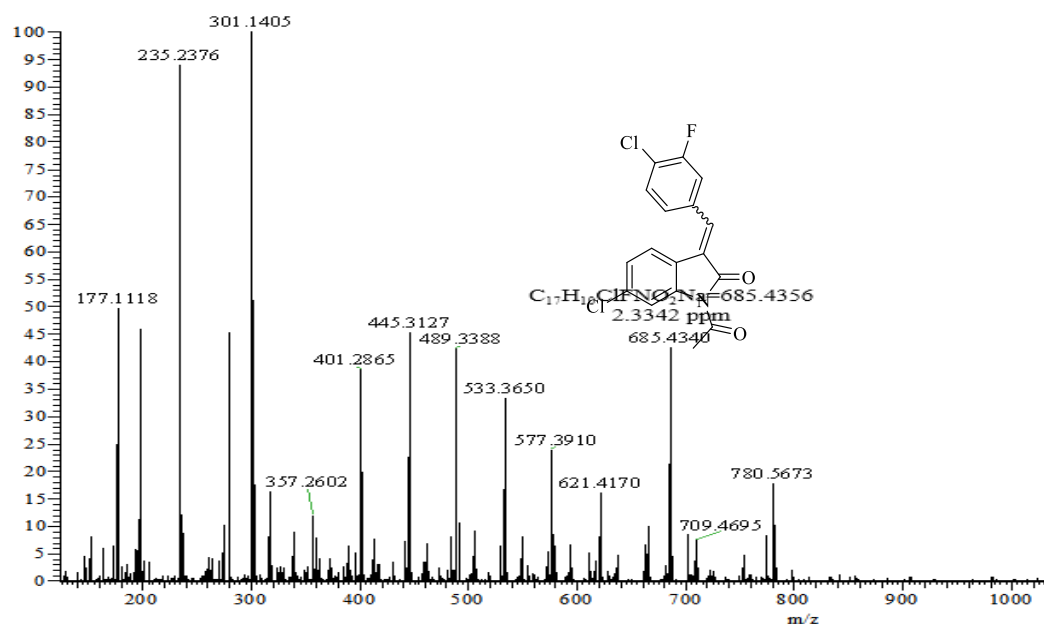


Figure S13-3. HRMS of compound 4m

1-Acetyl-6-chloro-3-(2,3-difluorobenzylidene)indolin-2-one(4n)

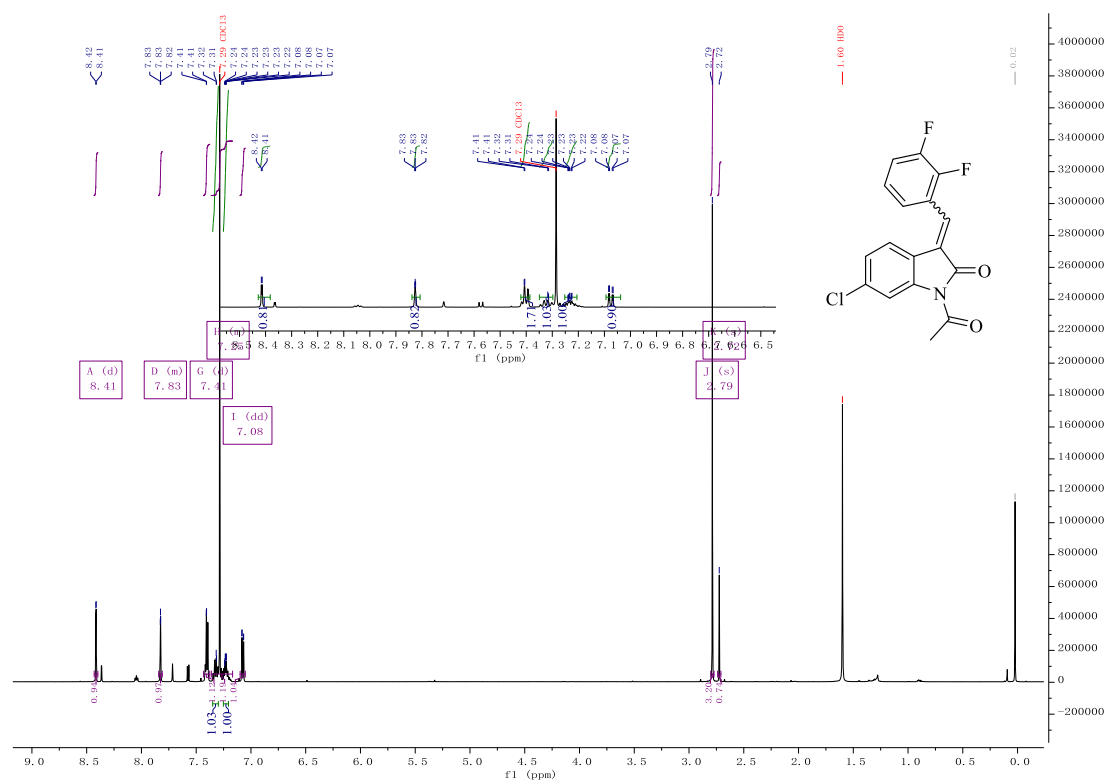


Figure S14-1. ¹H NMR spectrum (600 MHz, CDCl₃) of compound 4n

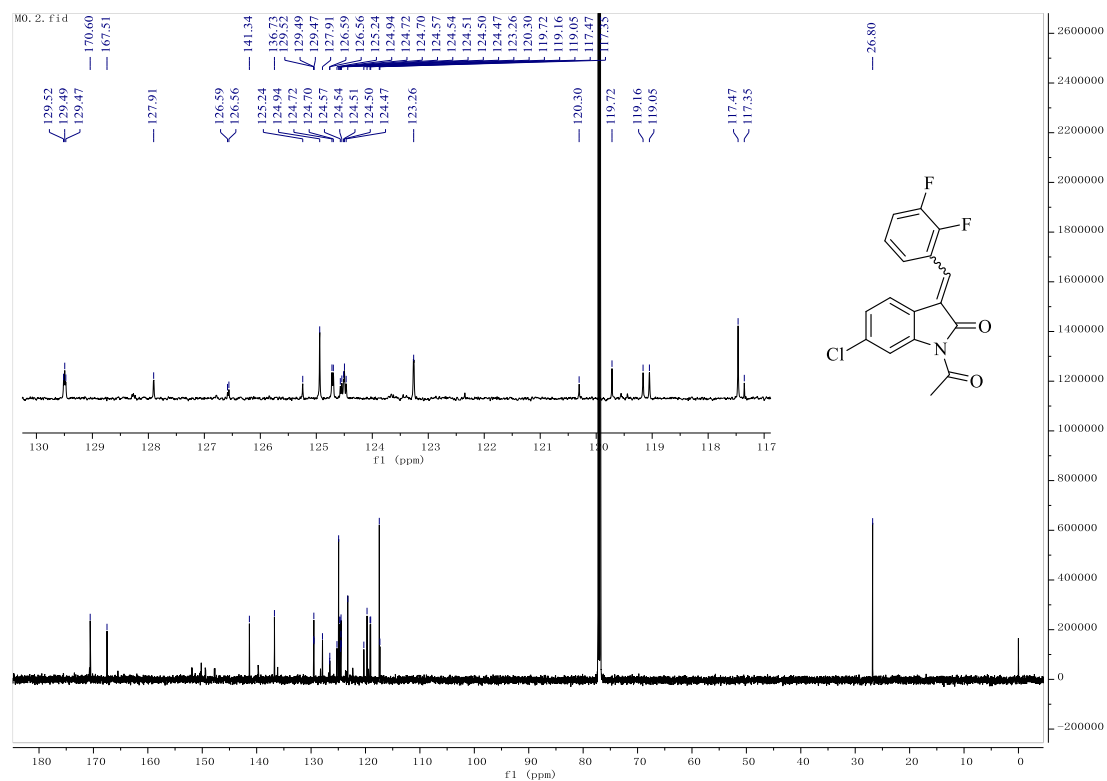


Figure S14-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4n

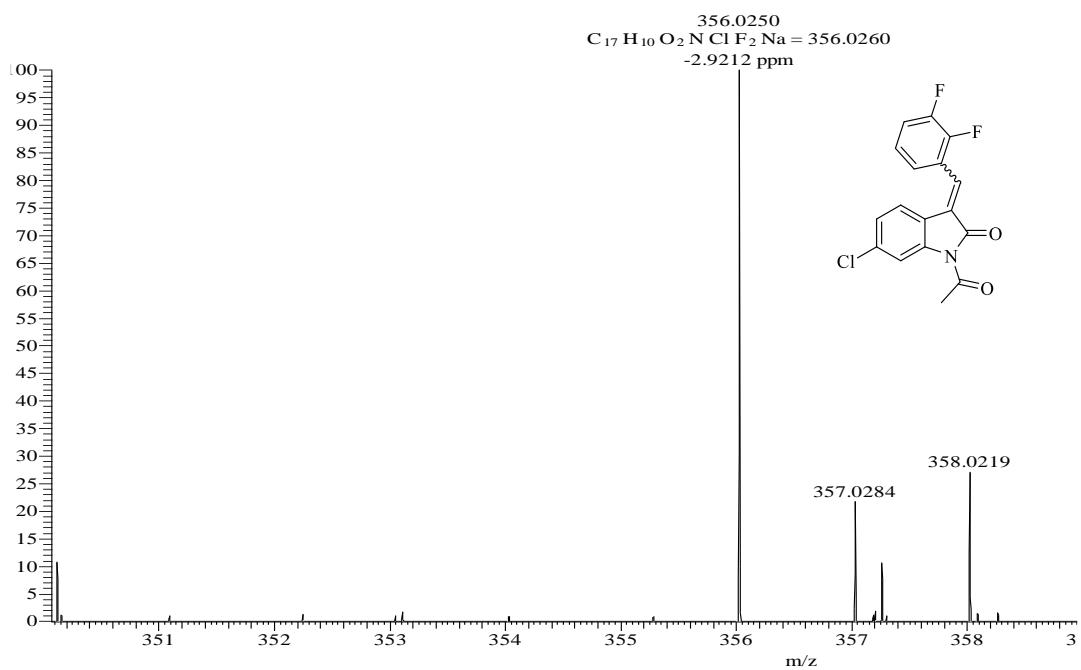


Figure S14-3. HRMS of compound **4n**

¹H NMR Spectrum (CDCl₃)

Chemical Structure: 1-(2-chlorophenyl)-2-(2-chlorophenyl)-1H-imidazole-3-carboxamide

Peak Data:

Chemical Shift (ppm)	Integration
8.40	0.90
7.82	0.96
7.53	2.07
7.38	1.02
7.36	1.02
7.34	1.37
7.29	1.00
7.28	1.00
7.27	1.00
7.26	1.00
7.25	1.00
7.24	1.00
7.23	1.00
7.22	1.00
7.21	1.00
7.20	1.00
7.19	1.00
7.18	1.00
7.17	1.00
7.16	1.00
7.15	1.00
7.14	1.00
7.13	1.00
7.12	1.00
7.11	1.00
7.10	1.00
7.09	1.00
7.08	1.00
7.07	1.00
7.06	1.00
7.05	1.00
7.04	1.00
7.03	1.00
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6.57	1.00
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6.55	1.00
6.54	1.00
6.53	1.00
6.52	1.00
6.51	1.00
6.50	1.00
6.49	1.00
6.48	1.00
6.47	1.00
6.46	1.00
6.45	1.00
6.44	1.00
6.43	1.00
6.42	1.00
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6.37	1.00
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6.35	1.00
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6.33	1.00
6.32	1.00
6.31	1.00
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6.08	1.00
6.07	1.00
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6.05	1.00
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6.03	1.00
6.02	1.00
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5.92	1.00
5.91	1.00
5.90	1.00
5.89	1.00
5.88	1.00
5.87	1.00
5.86	1.00
5.85	1.00
5.84	1.00
5.83	1.00
5.82	1.00
5.81	1.00
5.80	1.00
5.79	1.00
5.78	1.00
5.77	1.00
5.76	1.00
5.75	1.00
5.74	1.00
5.73	1.00
5.72	1.00
5.71	1.00
5.70	1.00
5.69	1.00
5.68	1.00
5.67	1.00
5.66	1.00
5.65	1.00
5.64	1.00
5.63	1.00
5.62	1.00
5.61	1.00
5.60	1.00
5.59	1.00</

¹H NMR (400 MHz, CDCl₃)

Chemical Shift (ppm)	Integration
8.18	0.10
8.15	0.10
8.12	0.10
8.08	0.10
8.05	0.10
8.02	0.10
7.98	0.10
7.95	0.10
7.92	0.10
7.88	0.10
7.85	0.10
7.82	0.10
7.78	0.10
7.75	0.10
7.72	0.10
7.68	0.10
7.65	0.10
7.62	0.10
7.58	0.10
7.55	0.10
7.52	0.10
7.48	0.10
7.45	0.10
7.42	0.10
7.38	0.10
7.35	0.10
7.32	0.10
7.28	0.10
7.25	0.10
7.22	0.10
7.18	0.10
7.15	0.10
7.12	0.10
7.08	0.10
7.05	0.10
7.02	0.10
6.98	0.10
6.95	0.10
6.92	0.10
6.88	0.10
6.85	0.10
6.82	0.10
6.78	0.10
6.75	0.10
6.72	0.10
6.68	0.10
6.65	0.10
6.62	0.10
6.58	0.10
6.55	0.10
6.52	0.10
6.48	0.10
6.45	0.10
6.42	0.10
6.38	0.10
6.35	0.10
6.32	0.10
6.28	0.10
6.25	0.10
6.22	0.10
6.18	0.10
6.15	0.10
6.12	0.10
6.08	0.10
6.05	0.10
6.02	0.10
5.98	0.10
5.95	0.10
5.92	0.10
5.88	0.10
5.85	0.10
5.82	0.10
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5.22	0.10
5.18	0.10
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5.12	0.10
5.08	0.10
5.05	0.10
5.02	0.10
4.98	0.10
4.95	0.10
4.92	0.10
4.88	0.10
4.85	0.10
4.82	0.10
4.78	0.10
4.75	0.10
4.72	0.10
4.68	0.10
4.65	0.10
4.62	0.10
4.58	0.10
4.55	0.10
4.52	0.10
4.48	0.10
4.45	0.10
4.42	0.10
4.38	0.10
4.35	0.10
4.32	0.10
4.28	0.10
4.25	0.10
4.22	0.10
4.18	0.10
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4.12	0.10
4.08	0.10
4.05	0.10
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3.95	0.10
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3.52	0.10
3.48	0.10
3.45	0.10
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3.35	0.10
3.32	0.10
3.28	0.10
3.25	0.10
3.22	0.10
3.18	0.10
3.15	0.10
3.12	0.10
3.08	0.10
3.05	0.10
3.02	0.10
2.98	0.10
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2.88	0.10
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2.82	0.10
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2.75	0.10
2.72	0.10
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2.62	0.10
2.58	0.10
2.55	0.10
2.52	0.10
2.48	0.10
2.45	0.10
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2.25	0.10

31

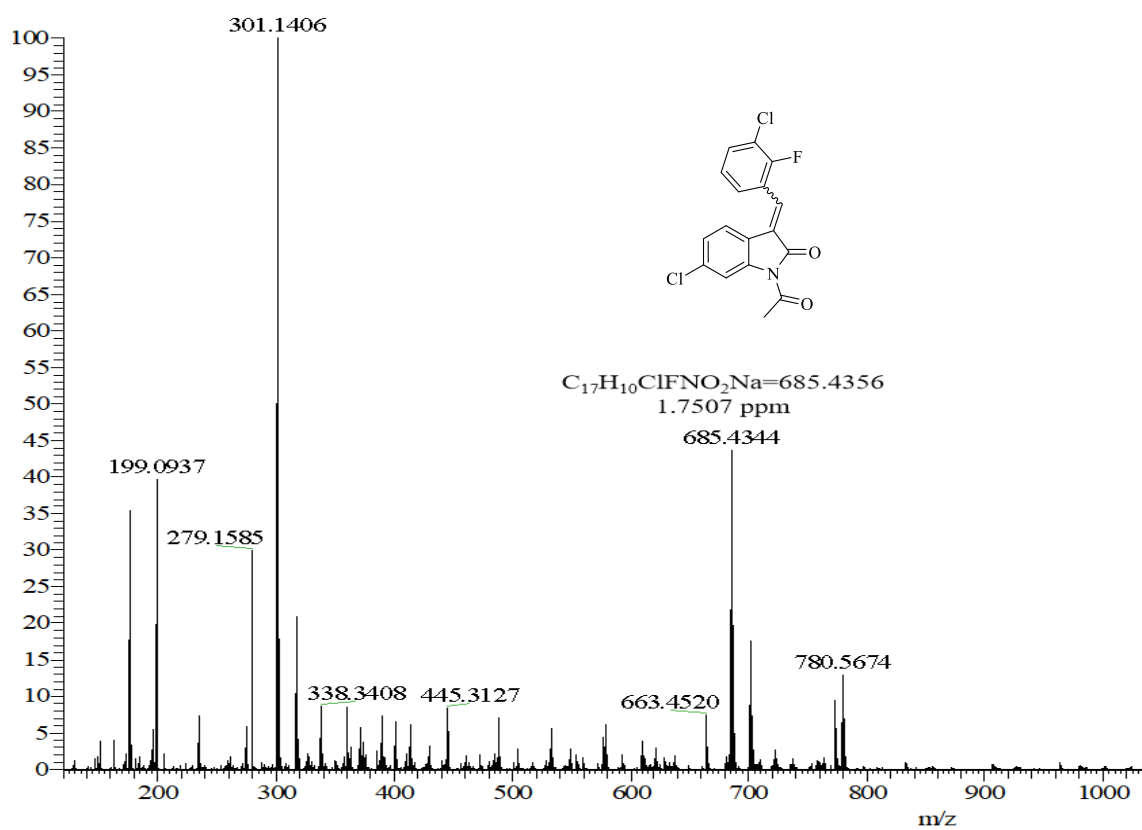


Figure S15-3. HRMS of compound 4o

1-Acetyl-3-(3-chloro-2-fluorobenzylidene)-6-(trifluoromethyl)indolin-2-one (4p)

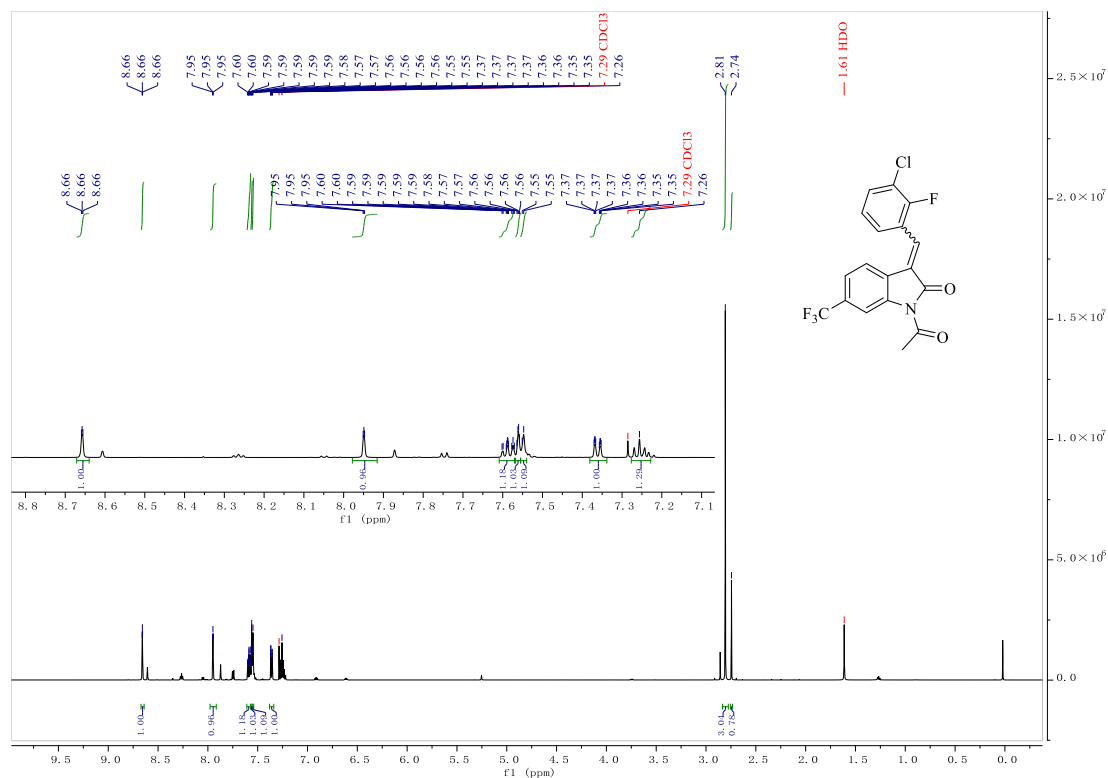


Figure S16-1. ¹H NMR spectrum (600 MHz, CDCl₃) of compound 4p

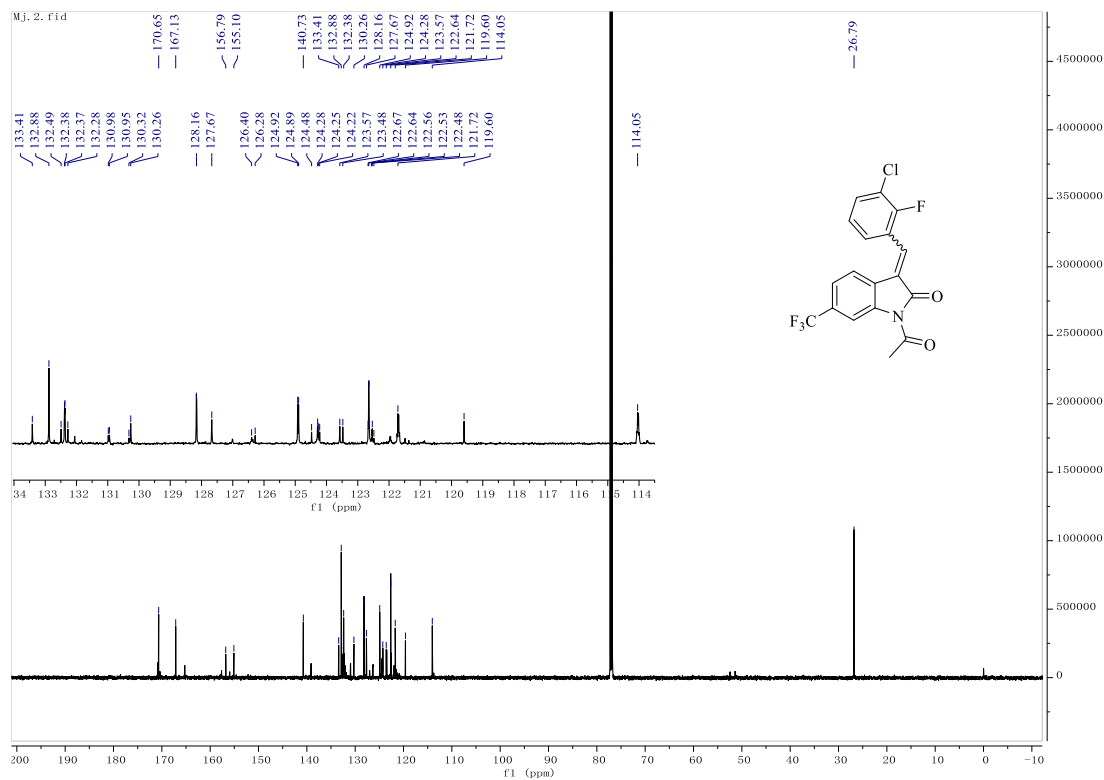


Figure S16-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4p

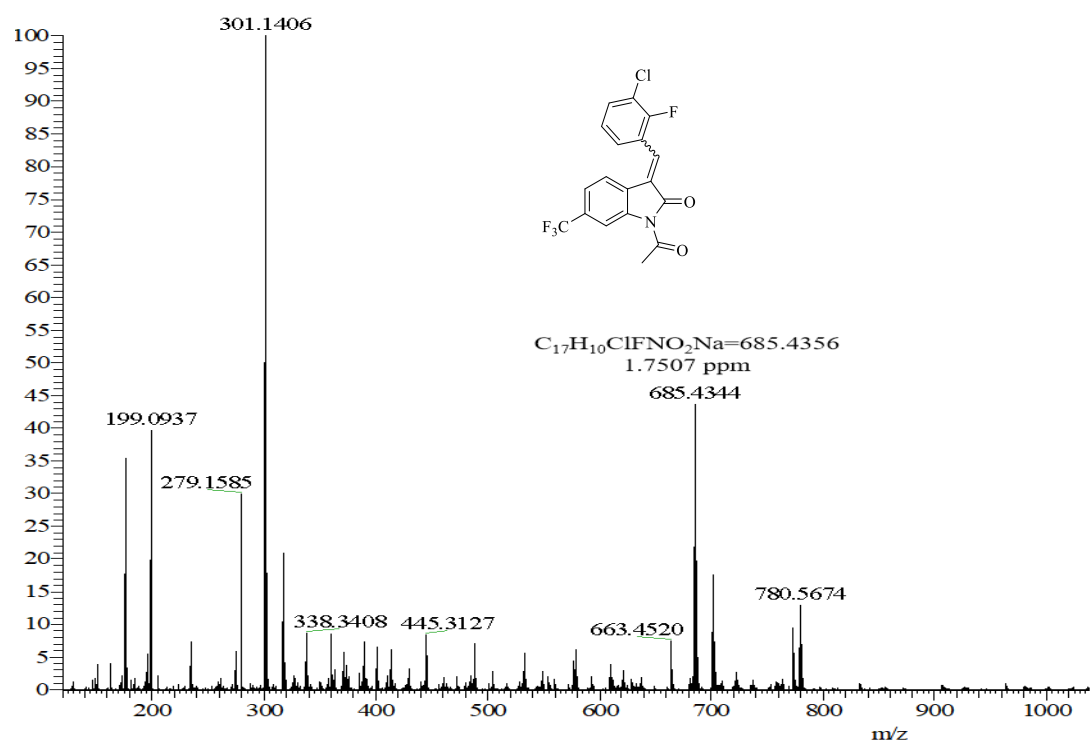


Figure S16-3. HRMS of compound 4p

35

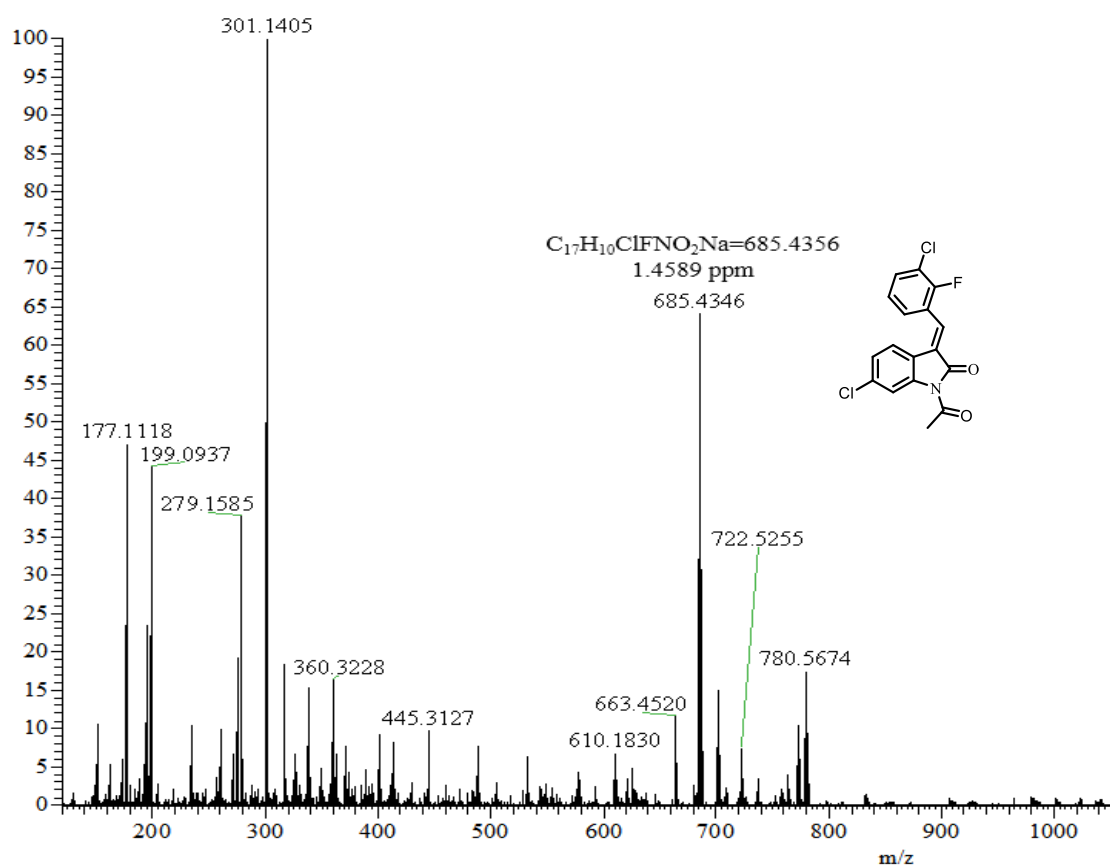


Figure S17-3. HRMS of compound 4q

Chemical structure of compound 10:

COc1ccc(cc1C(=O)N2C(=O)c3ccc(Cl)cc32)C4=CC=C(C=C4)C(F)(F)F

¹H NMR spectrum (CDCl₃):

- Chemical shift range:** 0.0 to 11.0 ppm.
- Integration values:** 3.24, 3.11, 1.00, 1.06, 1.91, 1.19, 1.91, 1.10.
- Peak assignments:**
 - ~0.9 ppm (t, 3H, 3.24)
 - ~1.6 ppm (d, 3H, 3.11)
 - 7.0-7.5 ppm (m, 1.10, 1.19, 1.91, 1.91, 1.06)
 - ~7.3 ppm (s, 1H, 1.91)
 - 8.3-8.4 ppm (m, 1.00)
- Solvent peaks:** CDCl₃ (7.26, 7.29), H₂O (1.64, 1.63).

37

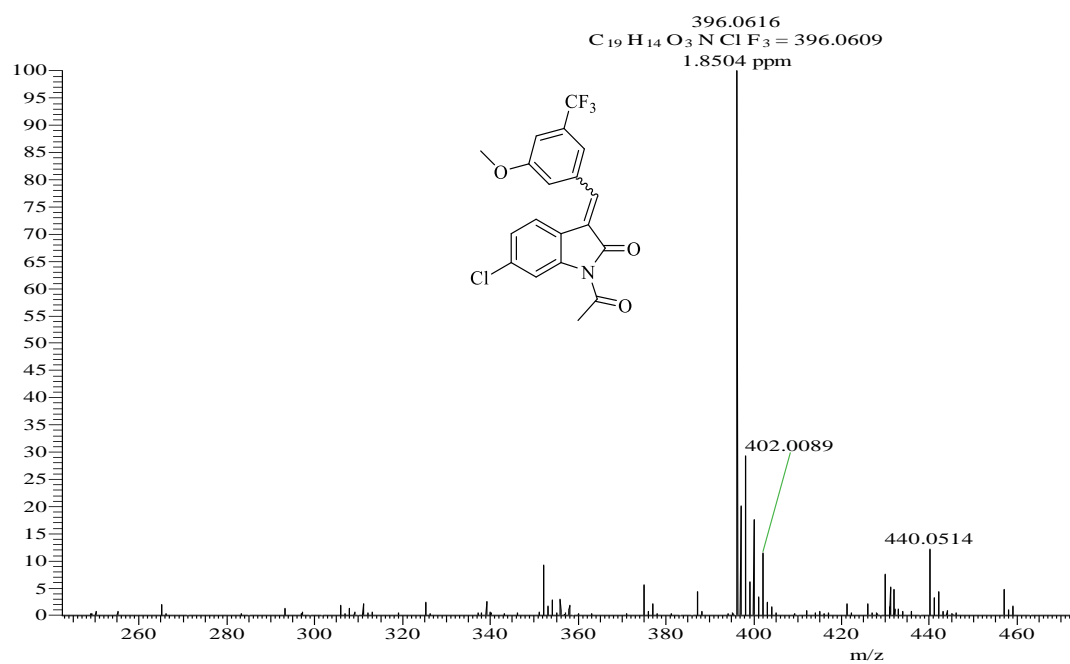


Figure S18-3. HRMS of compound **4r**

1-Acetyl-6-chloro-3-(3-methoxybenzylidene)indolin-2-one(4s)

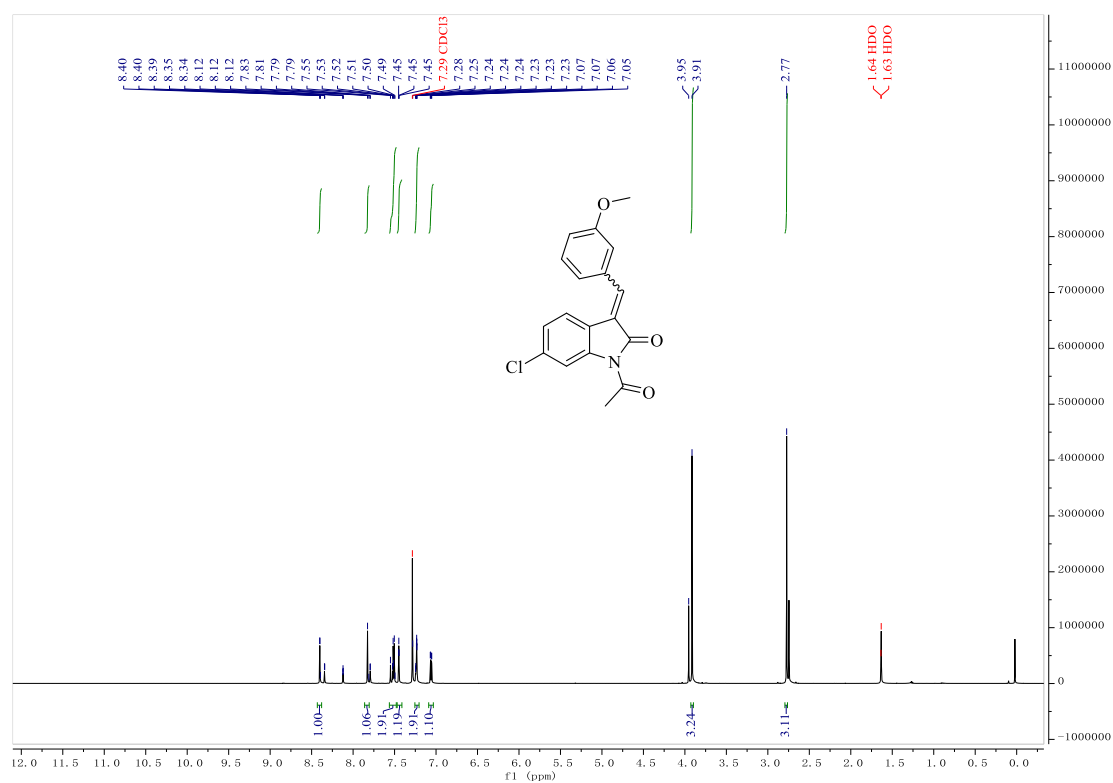


Figure S19-1. ¹H NMR spectrum (600 MHz, 150 MHz, CDCl₃) of compound 4s

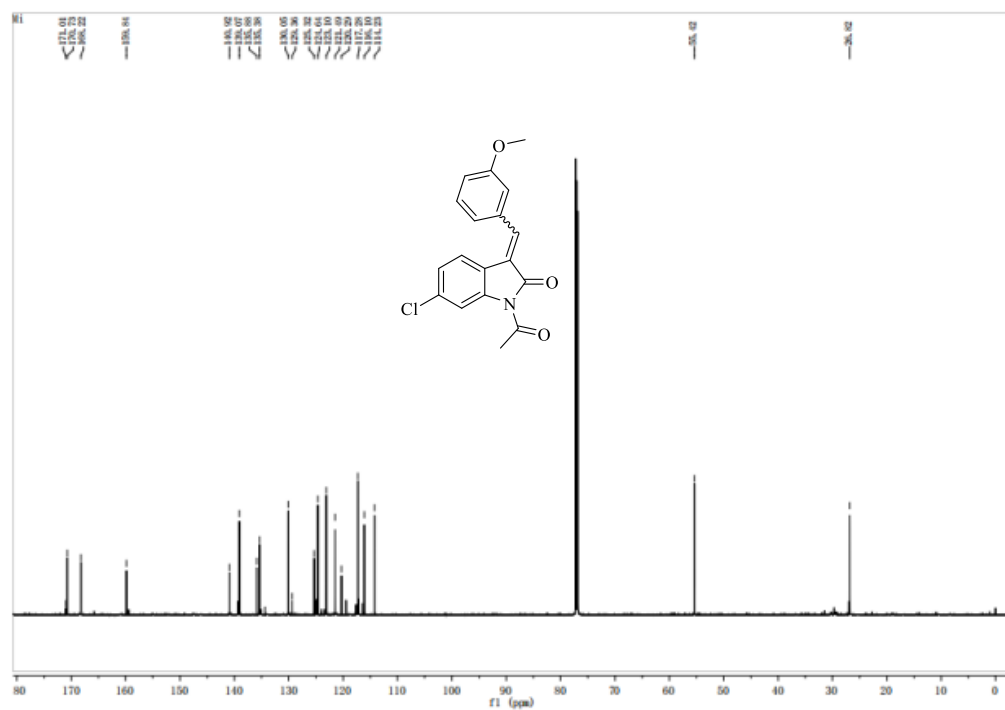


Figure S19-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4s

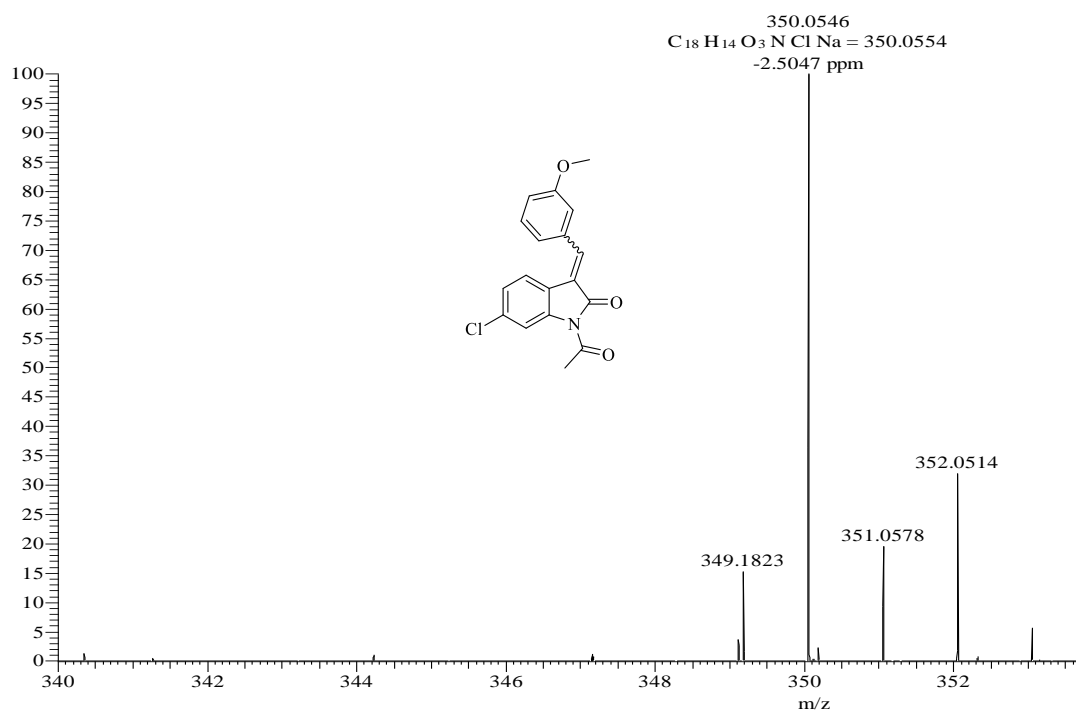


Figure S19-3. HRMS of compound 4s

Tert-butyl-6-chloro-2-oxo-3-(3-(trifluoromethyl)benzylidene)indoline-1-carboxylate(4t)

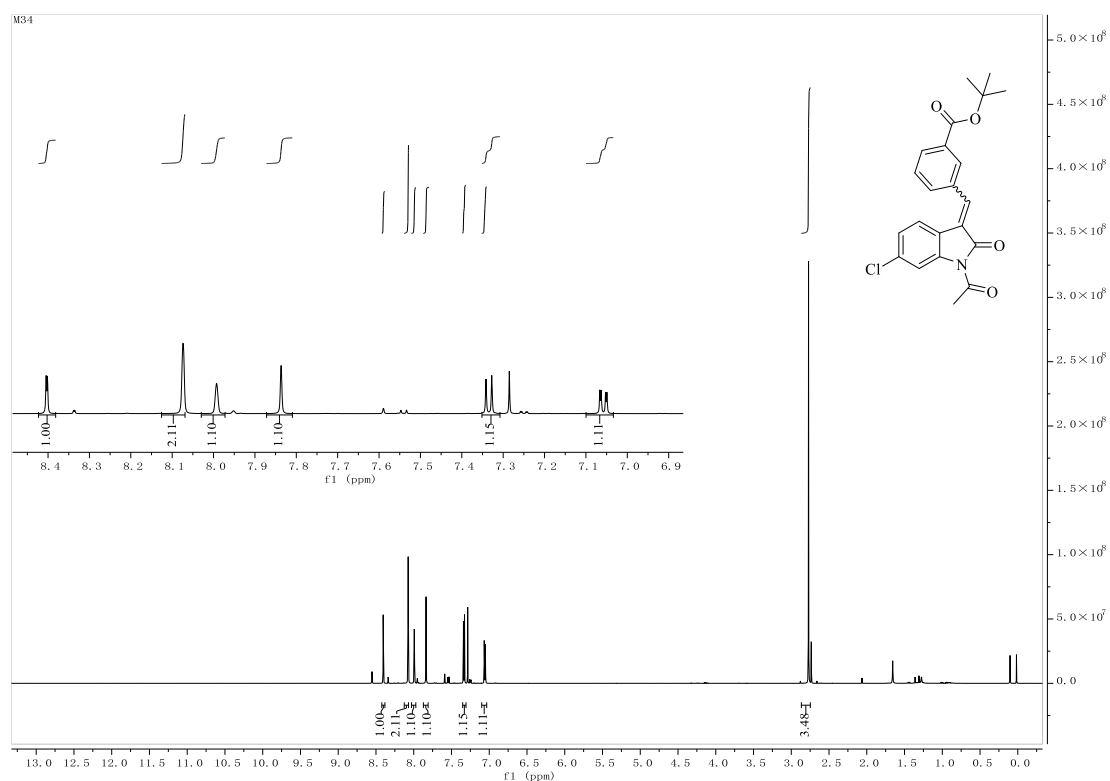


Figure S20-1. ¹H NMR spectrum (600 MHz, CDCl₃) of compound 4t

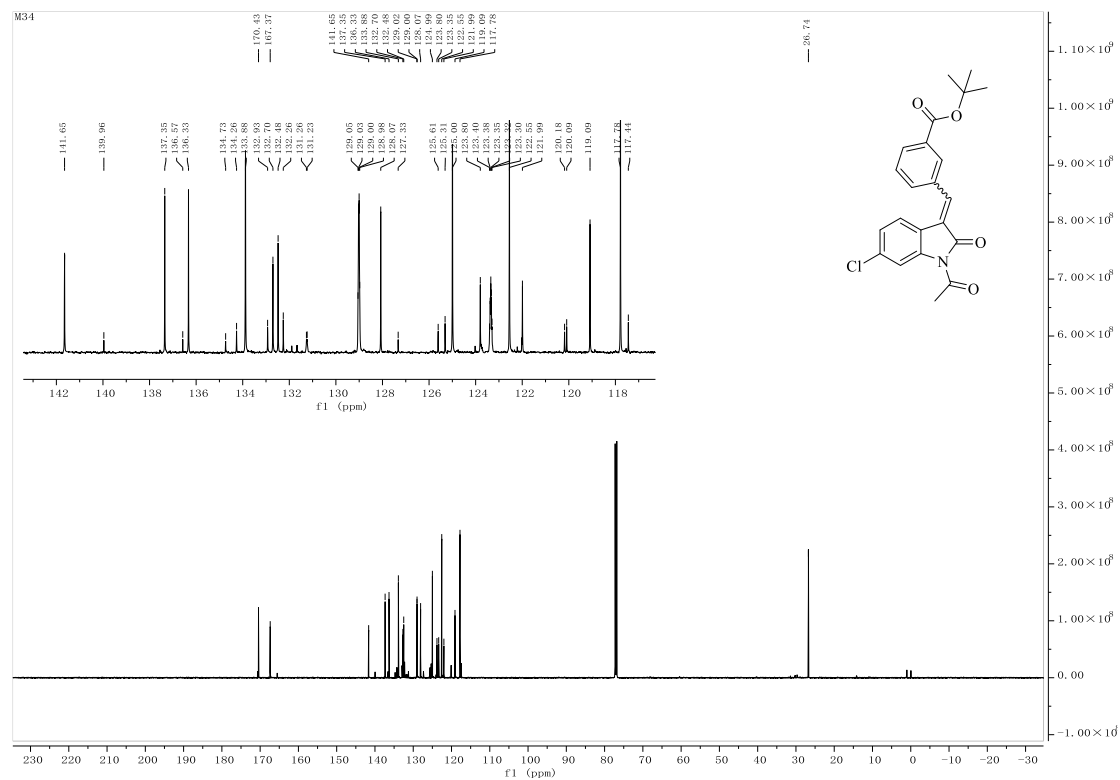


Figure S20-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4t

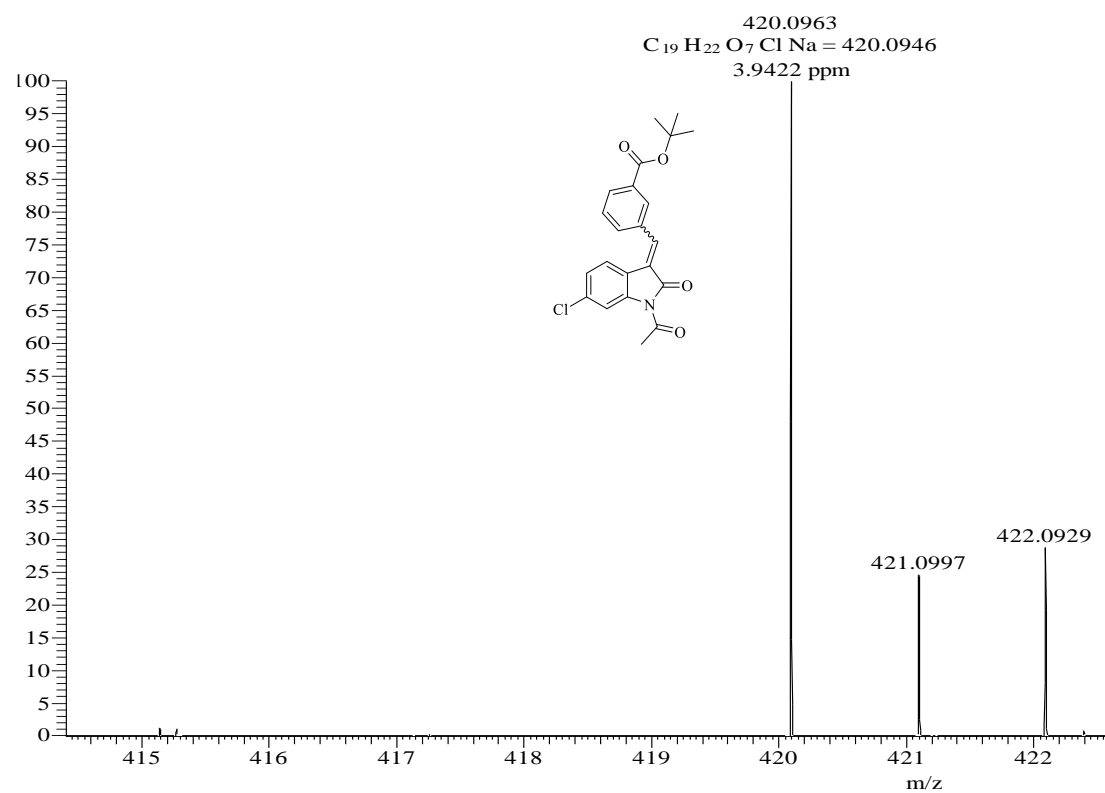


Figure S20-2. HRMS of compound **4t**

MP: 1, f1d

Chemical structure of compound 10: CC(=O)N1C(=O)C(=C(c2ccc(OC(F)(F)F)cc2))c3ccc(Cl)cc31

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from 0 to 8.5. The y-axis represents the intensity, ranging from -1,000,000 to 14,000,000. The spectrum shows several peaks, with integration values provided for some of them: 1.00, 1.11, 1.05, 1.28, 0.80, 1.04, 1.33, 1.53, 3.26, and 0.73. The chemical structure of compound 10 is shown as an inset.

MP, 2. f1d

141.22 139.49 136.95 136.58 136.53 136.12 135.77 134.88 130.60 130.19 129.72 127.48 126.50 124.81 123.87 123.77 123.61 122.94 122.73 122.53 121.28 170.61 167.89 141.22 136.58 136.54 136.12 130.60 127.48 126.50 124.81 122.94 122.53 121.28 119.53 117.49 26.80

f1 (ppm)

f1 (ppm)

Chemical structure of compound 10b: COc1ccc(cc1C(=O)N2C(=O)c3cc(Cl)ccc3N2C(=O)c4ccccc4OC(F)(F)F)OC(F)(F)F

43

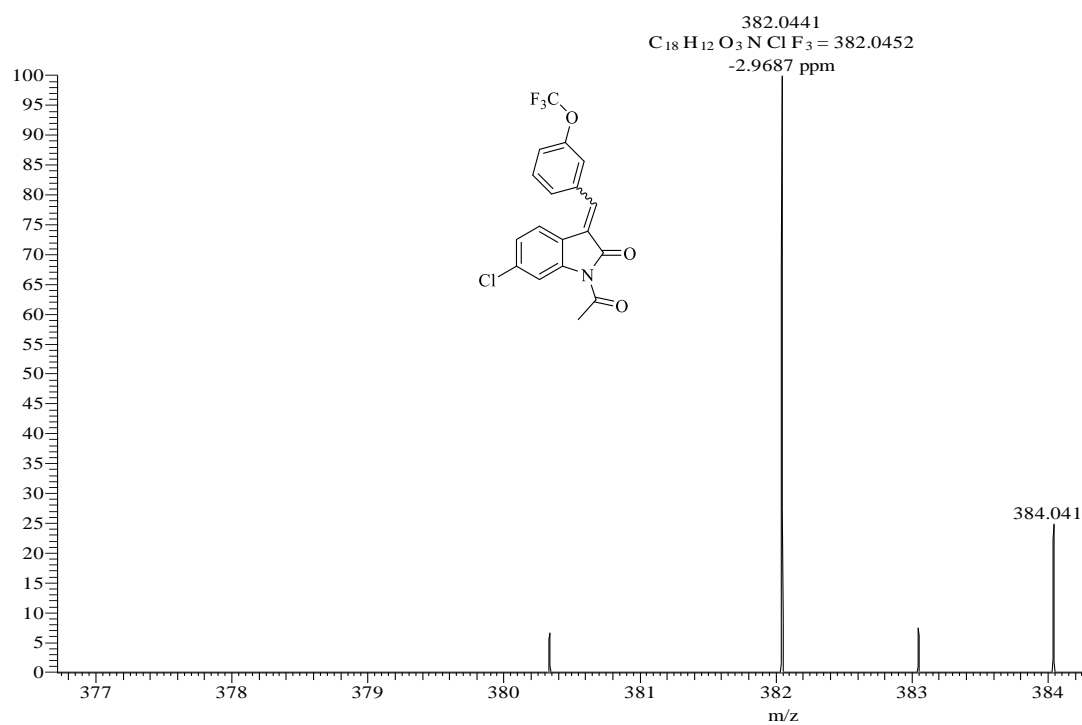


Figure S21-3. HRMS of compound **4u**

1-Acetyl-6-chloro-3-(pyridin-4-ylmethylene)indolin-2-one(4v)

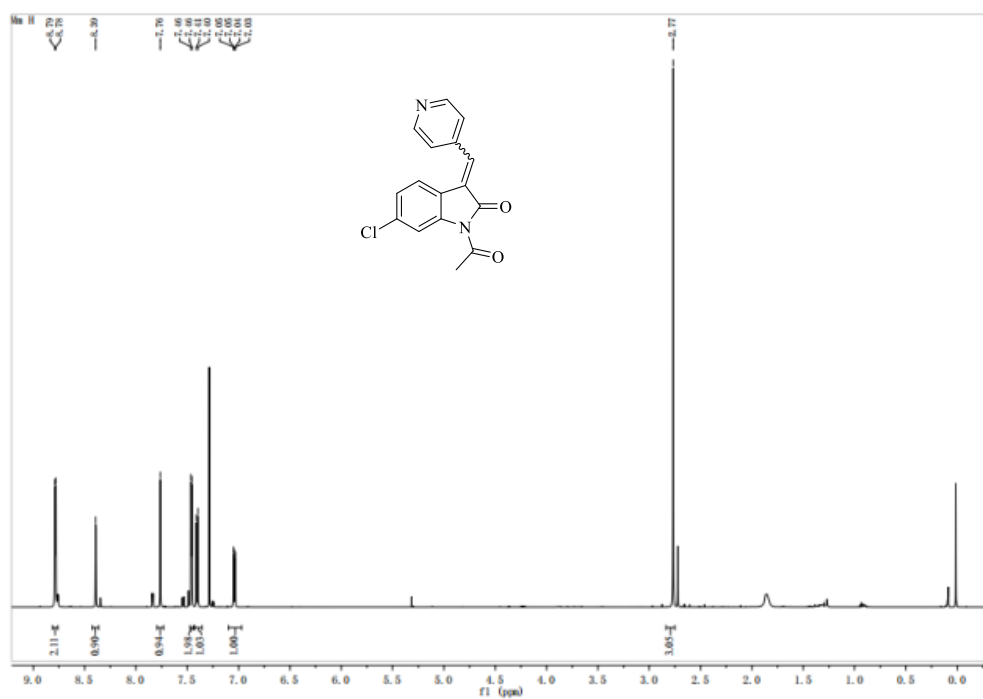


Figure S22-1. ¹H NMR spectrum (600 MHz, CDCl₃) of compound 4v

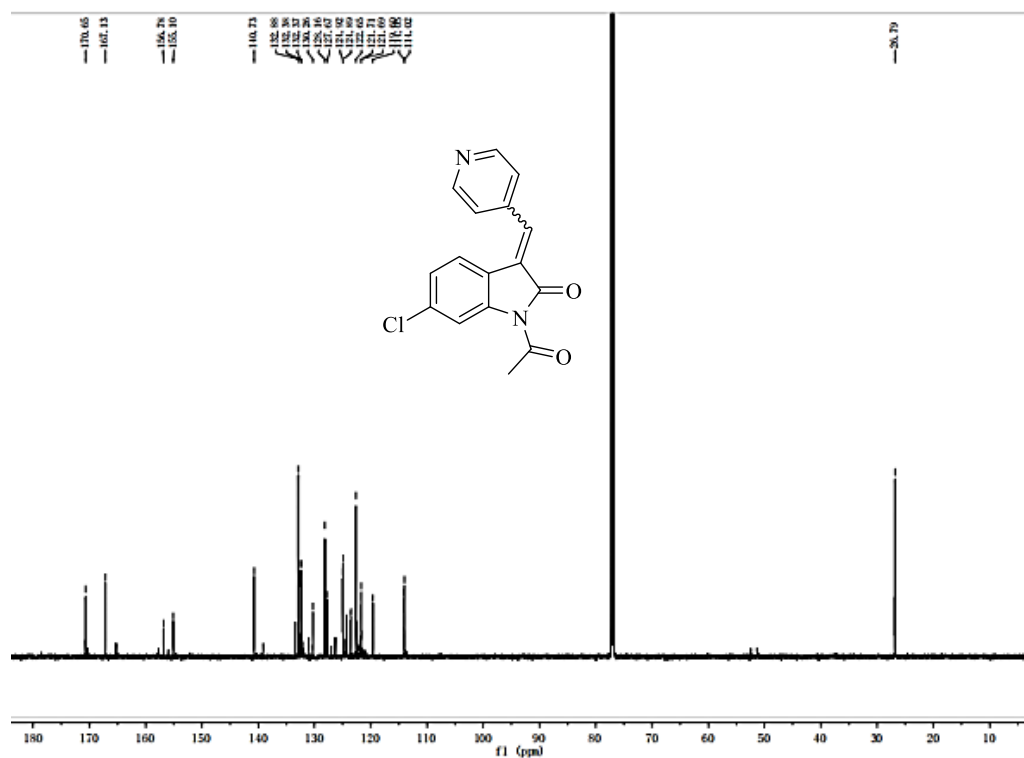


Figure S22-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4v

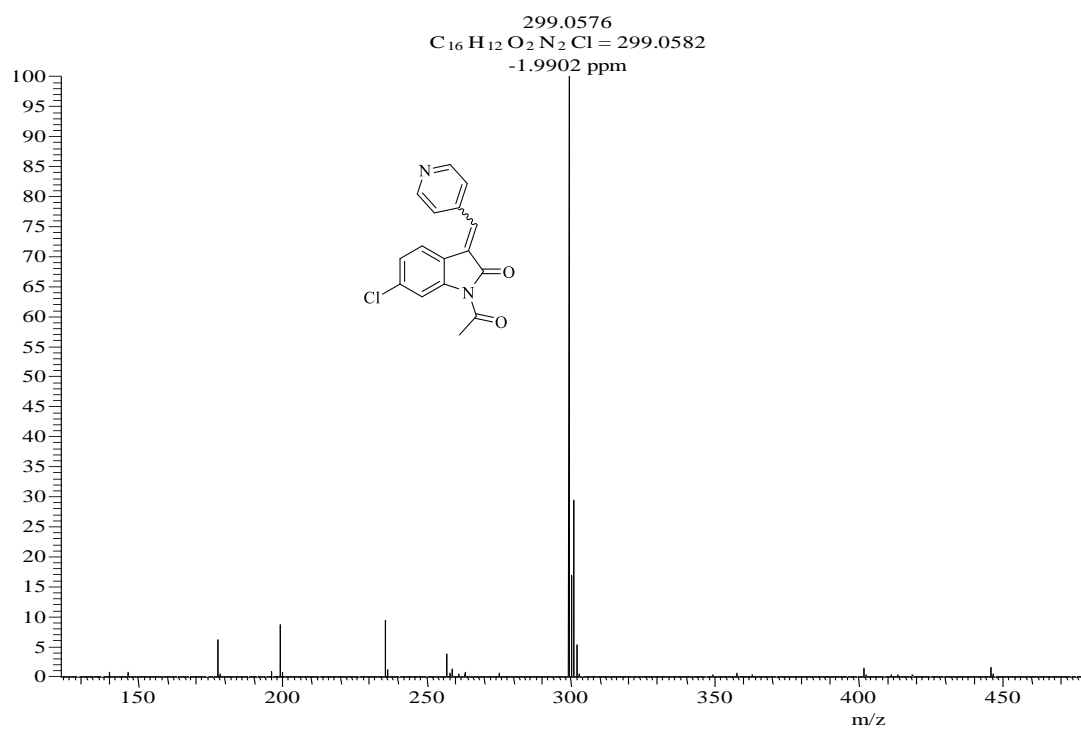


Figure S22-3. HRMS of compound **4v**

1H NMR spectrum of compound 10 in CDCl₃.

Chemical structure of compound 10: CC(=O)N1C(=O)C=Cc2ccc(C(F)(F)F)cn2c1

1H NMR data (ppm):

- 8.35 (d, 0.91H)
- 8.22 (d, 1.00H)
- 7.76 (d, 1.12H)
- 7.50 (d, 1.05H)
- 7.29 (s, 1.05H)
- 7.24 (s, 1.05H)
- 7.23 (s, 1.05H)
- 7.22 (s, 1.05H)
- 7.21 (s, 1.05H)
- 7.20 (s, 1.05H)
- 7.19 (s, 1.05H)
- 7.18 (s, 1.05H)
- 7.17 (s, 1.05H)
- 7.16 (s, 1.05H)
- 7.15 (s, 1.05H)
- 7.14 (s, 1.05H)
- 7.13 (s, 1.05H)
- 7.12 (s, 1.05H)
- 7.11 (s, 1.05H)
- 7.10 (s, 1.05H)
- 7.09 (s, 1.05H)
- 7.08 (s, 1.05H)
- 7.07 (s, 1.05H)
- 7.06 (s, 1.05H)
- 7.05 (s, 1.05H)
- 7.04 (s, 1.05H)
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- 7.02 (s, 1.05H)
- 7.01 (s, 1.05H)
- 7.00 (s, 1.05H)
- 6.99 (s, 1.05H)
- 6.98 (s, 1.05H)
- 6.97 (s, 1.05H)
- 6.96 (s, 1.05H)
- 6.95 (s, 1.05H)
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- 6.89 (s, 1.05H)
- 6.88 (s, 1.05H)
- 6.87 (s, 1.05H)
- 6.86 (s, 1.05H)
- 6.85 (s, 1.05H)
- 6.84 (s, 1.05H)
- 6.83 (s, 1.05H)
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- 6.81 (s, 1.05H)
- 6.80 (s, 1.05H)
- 6.79 (s, 1.05H)
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- 5.11 (s, 1.05H)
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Mr. 2. f1d

139.45, 136.24, 135.82, 133.43, 133.38, 131.35, 130.48, 128.81, 128.81, 128.81, 125.34, 125.15, 124.83, 124.63, 123.91, 123.68, 122.94, 122.68, 119.69, 119.36, 119.21, 117.56, 117.31, 117.15, 117.01, 170.80, 165.77, 158.52, 156.87, 26.88, 26.80

CF₃

Cl

13C NMR (ppm): 139.45, 136.24, 135.82, 133.43, 133.38, 131.35, 130.48, 128.81, 125.34, 125.15, 124.83, 124.63, 123.91, 123.68, 122.94, 122.68, 119.69, 119.36, 119.21, 117.56, 117.31, 117.15, 117.01, 170.80, 165.77, 158.52, 156.87, 26.88, 26.80

Chemical structure: 2-chloro-3-(4-(trifluoromethyl)phenyl)indolizin-5(1H)-one

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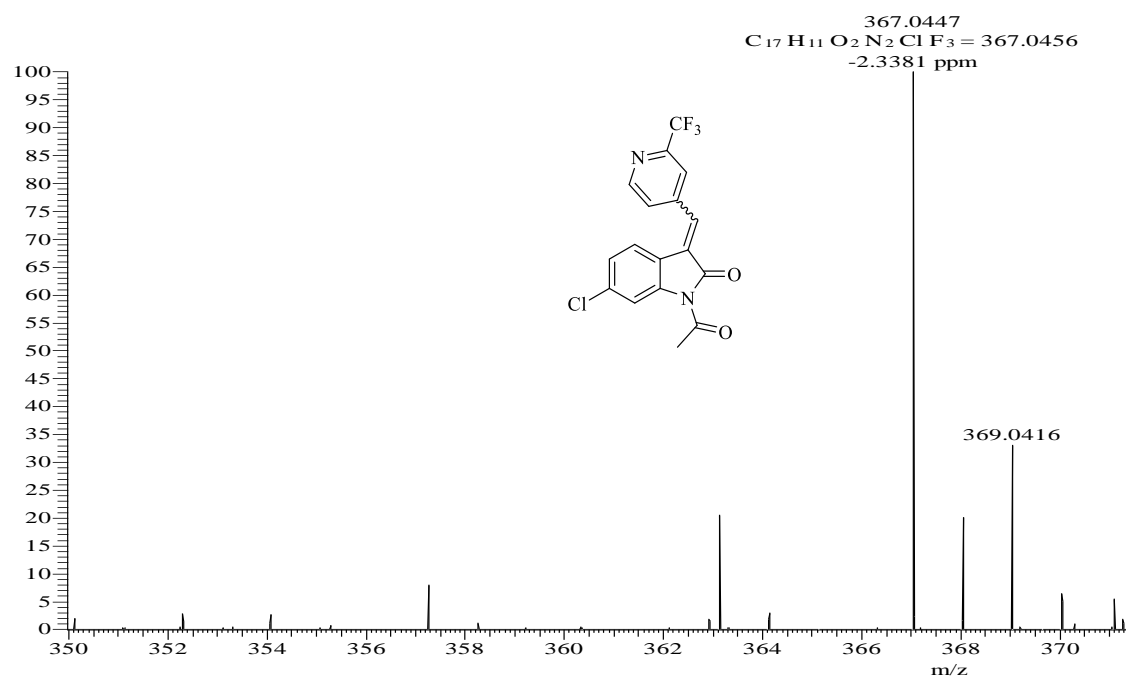


Figure S23-3. HRMS of compound 4w

***Tert*-butyl 4-((1-acetyl-6-chloro-2-oxoindolin-3-ylidene)methyl)benzoate(4x)**

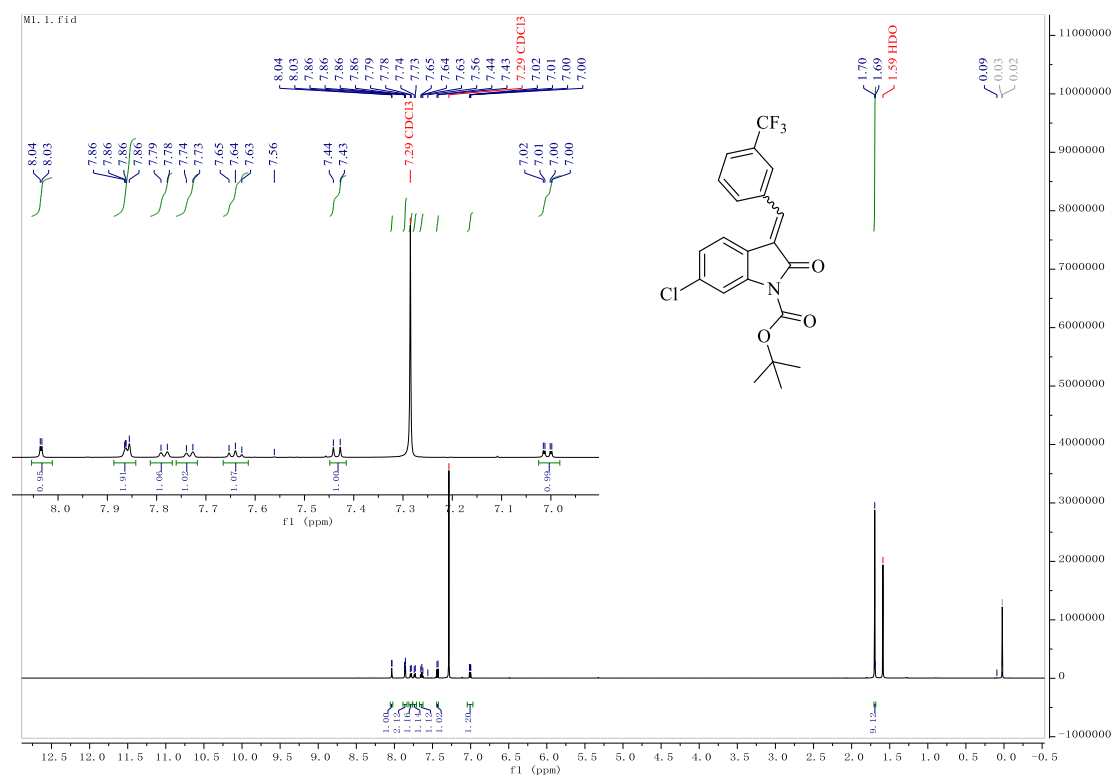


Figure S24-1. ¹H NMR spectrum (600 MHz, CDCl₃) of compound 4x

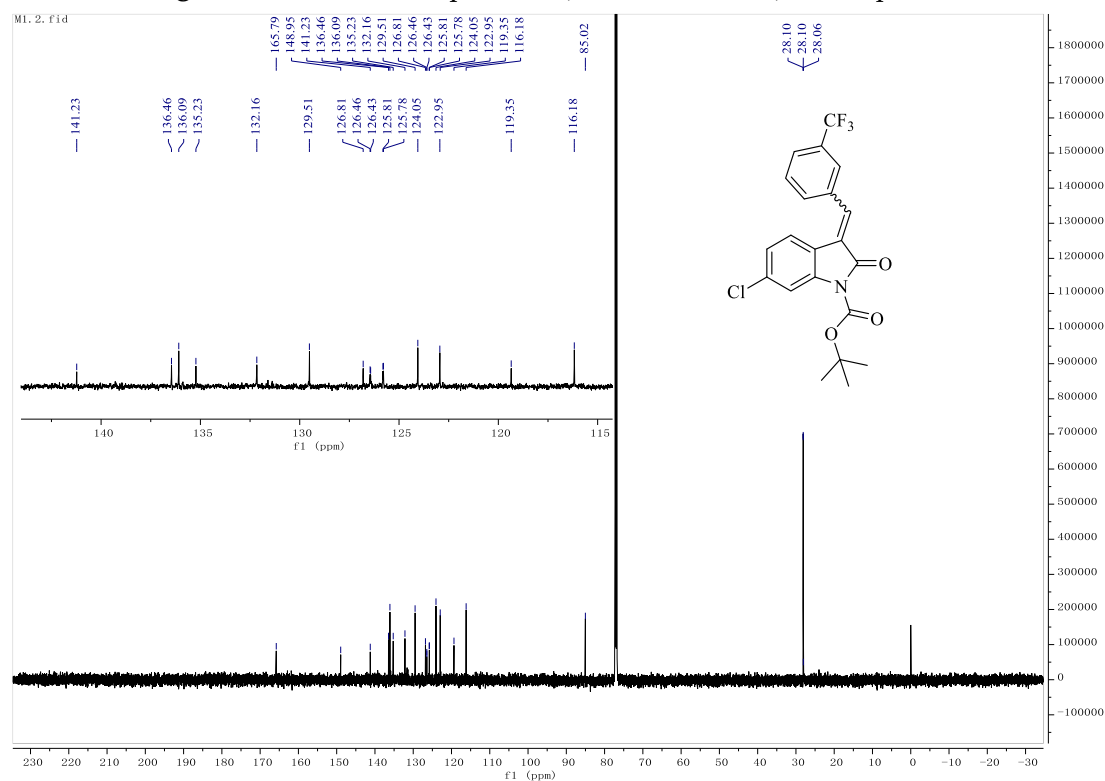


Figure S24-2. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 4x

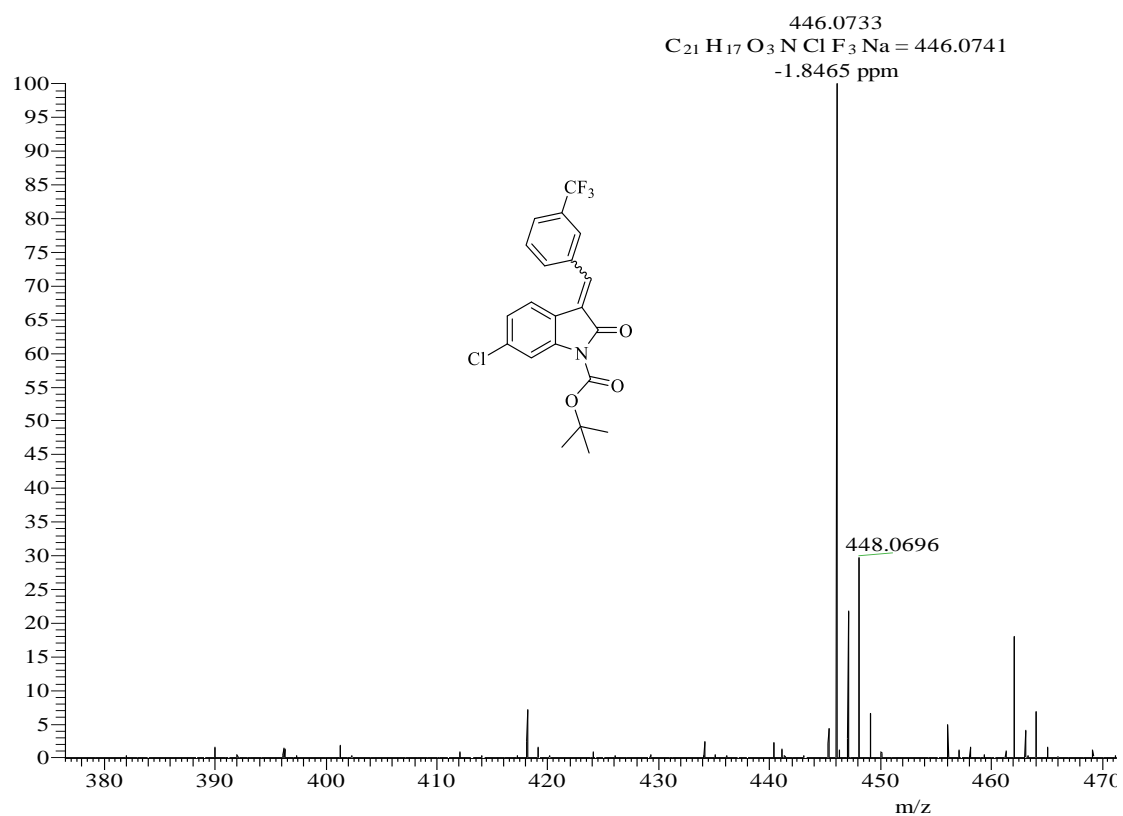


Figure S24-3. HRMS of compound 4x

4-Nitro-N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)benzenesulfonamide (9d)

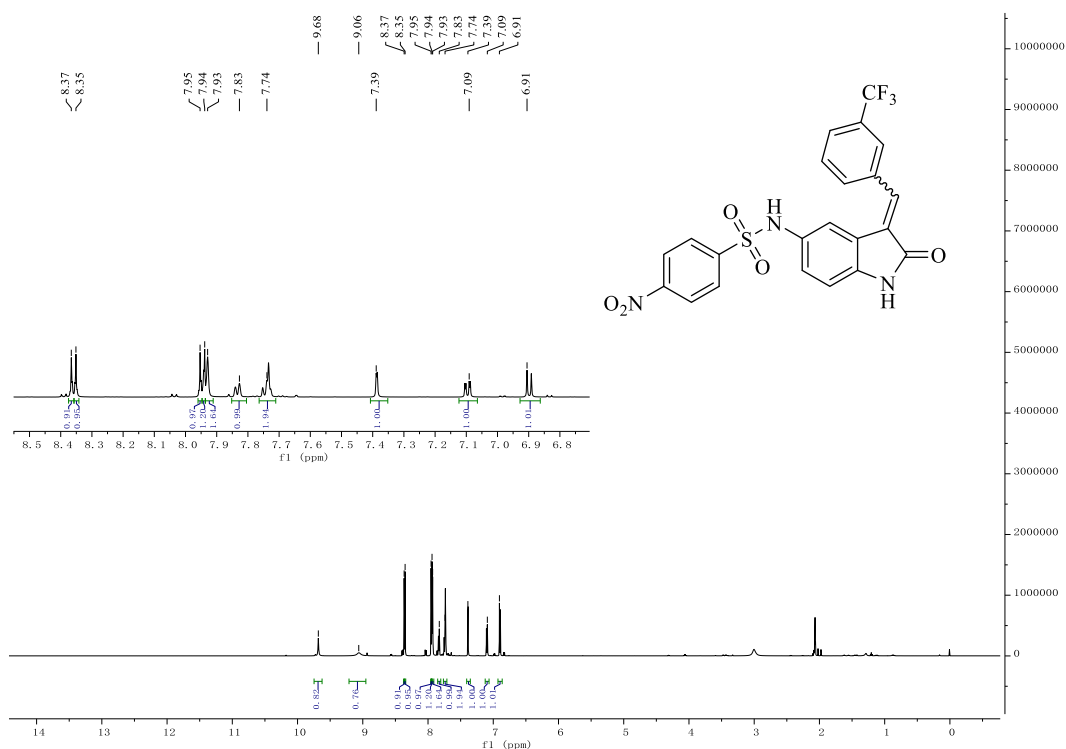


Figure S25-1. ¹H NMR spectrum (600 Hz, Acetone) of compound 9d

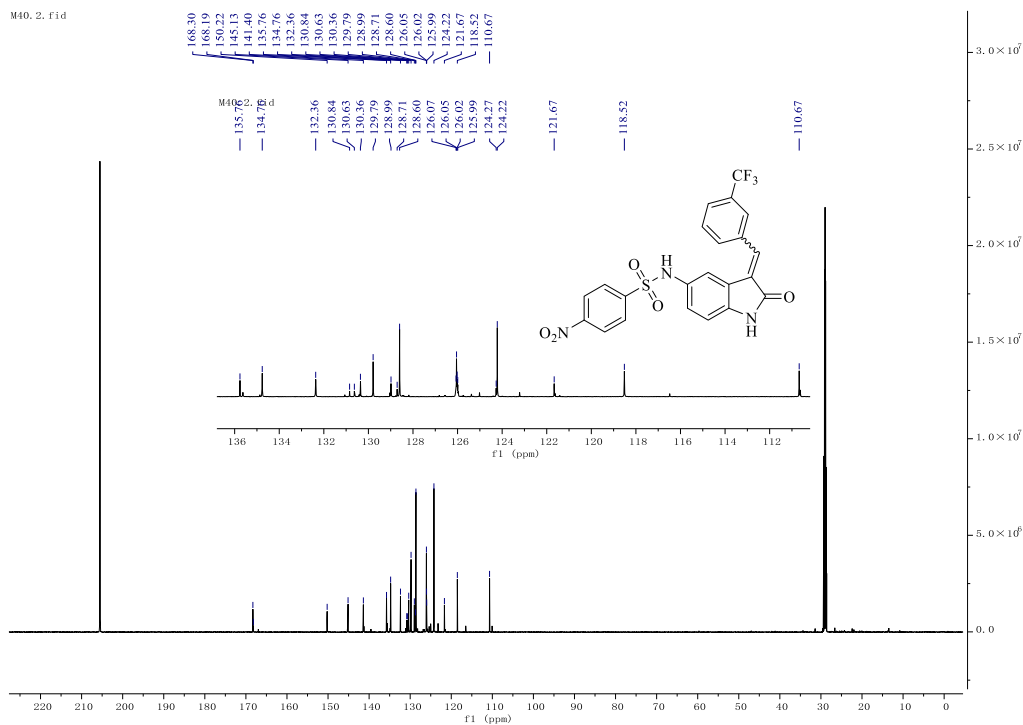


Figure S25-2. ¹³C NMR spectrum (150 Hz, Acetone) of compound 9d

M40 #20 RT: 0.09 AV: 1 NL: 6.14E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

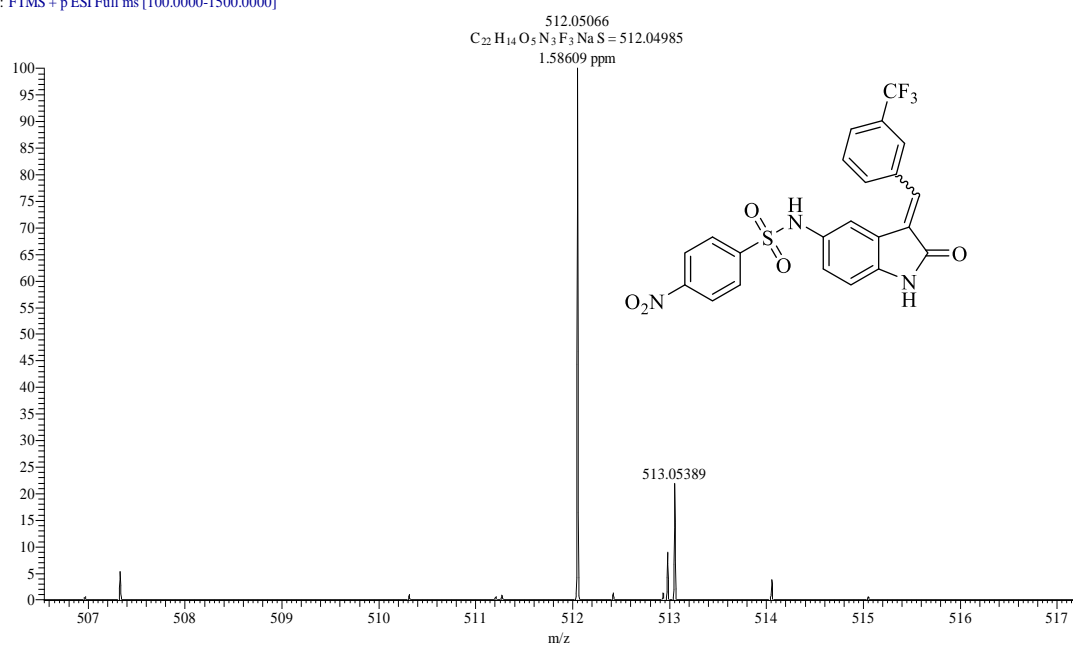


Figure S25-3. HRMS of compound 9d

nitro-N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)benzenesulfonamide(**9a**)

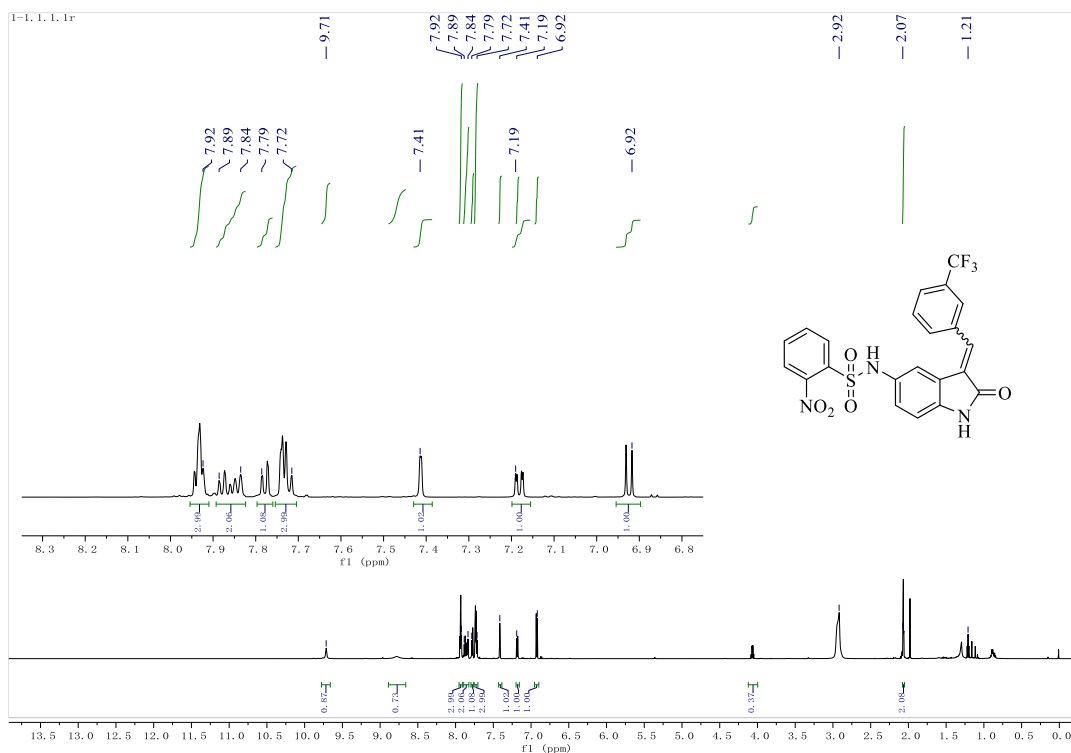


Figure S26-1. ¹H NMR spectrum (600 Hz, CD₃COCD₃) of compound **9a**

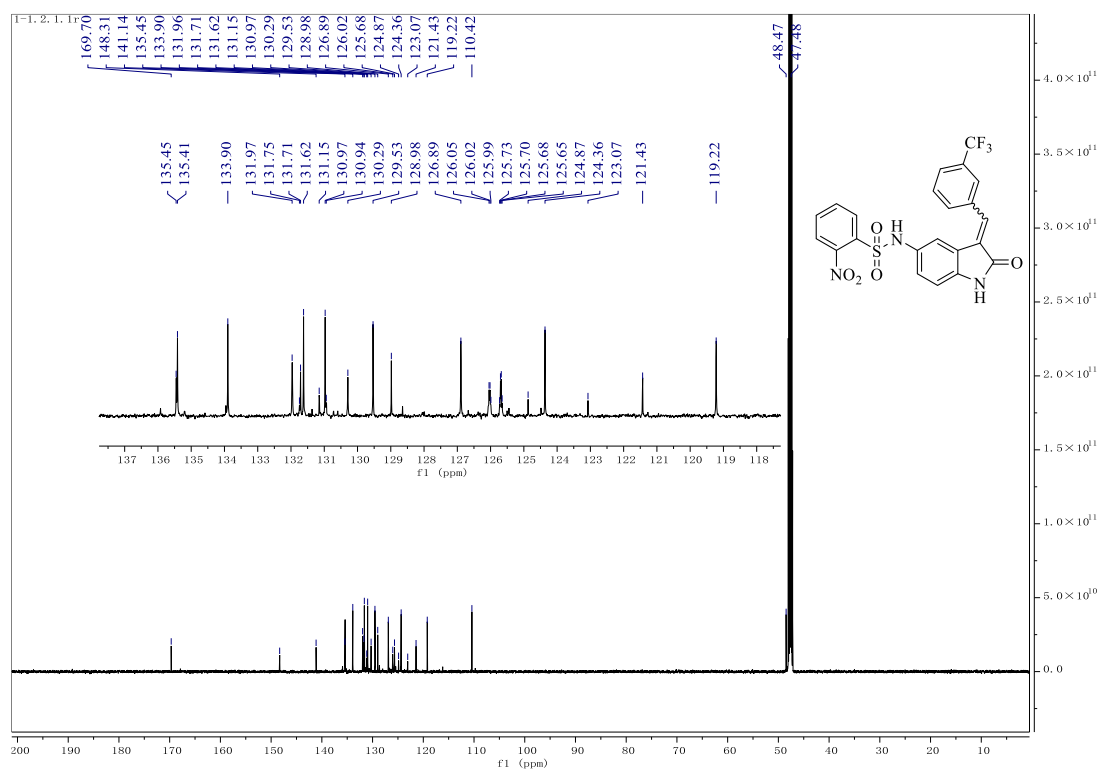


Figure S26-2. ¹³C NMR spectrum (150 Hz, CD₃OD) of compound **9a**

1-1 #22 RT: 0.10 AV: 1 NL: 5.14E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

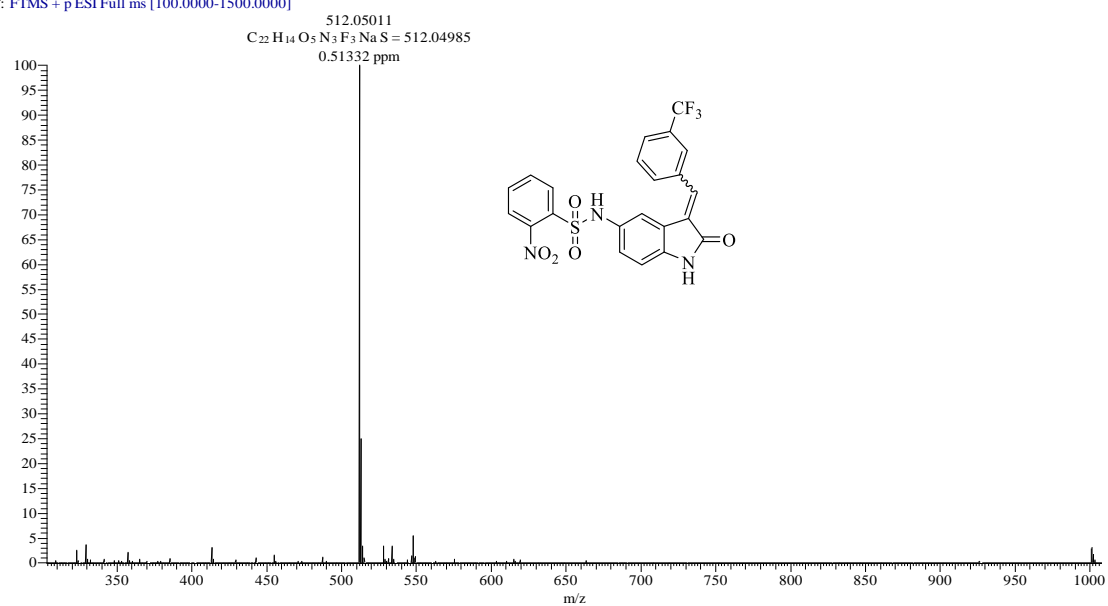


Figure S26-3. HRMS of compound **9a**

2,4-Difluoro-N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)benzenesulfonamide (9b)

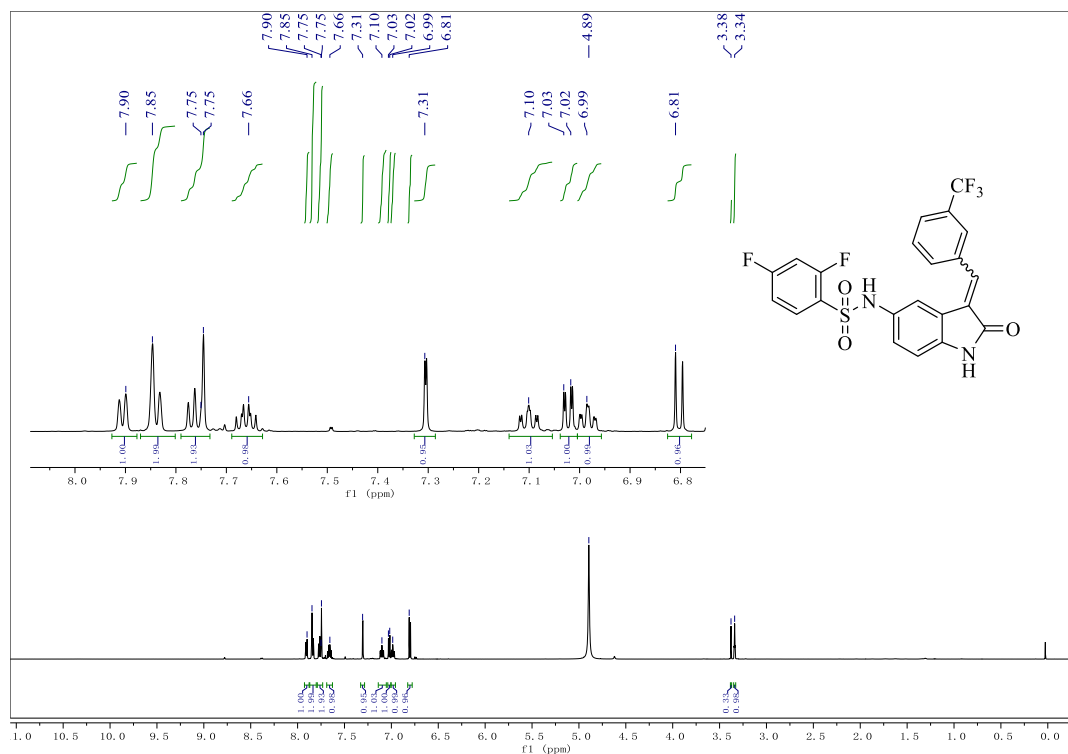


Figure S27-1. ¹H, NMR spectrum (150 Hz, CD₃OD) of compound **9b**

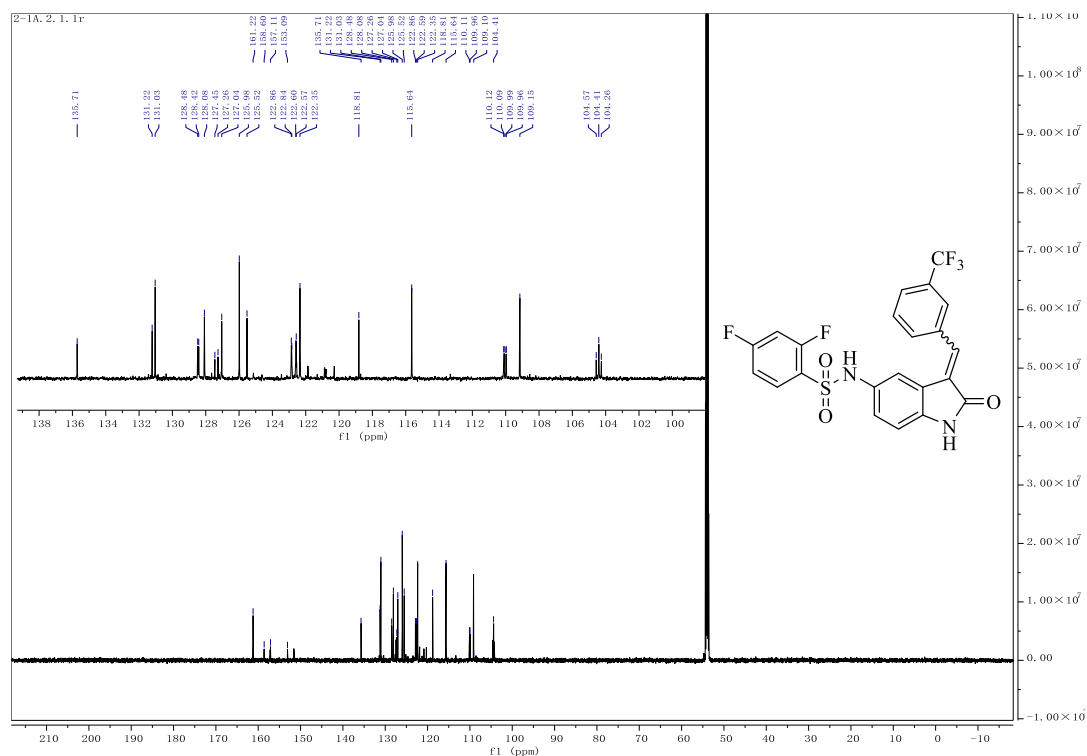


Figure S27-2. ¹³C NMR spectrum (150 Hz, CD₃OD) of compound **9b**

2-1-A #22 RT: 0.10 AV: 1 NL: 9.62E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

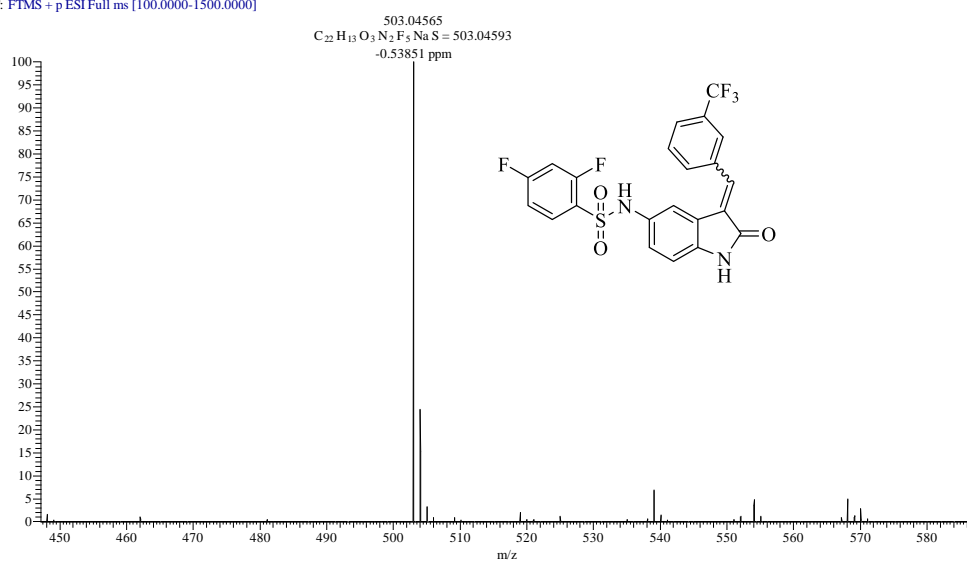


Figure S27-3. HRMS of compound **9b**

N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)ethanesulfonamide (9c)

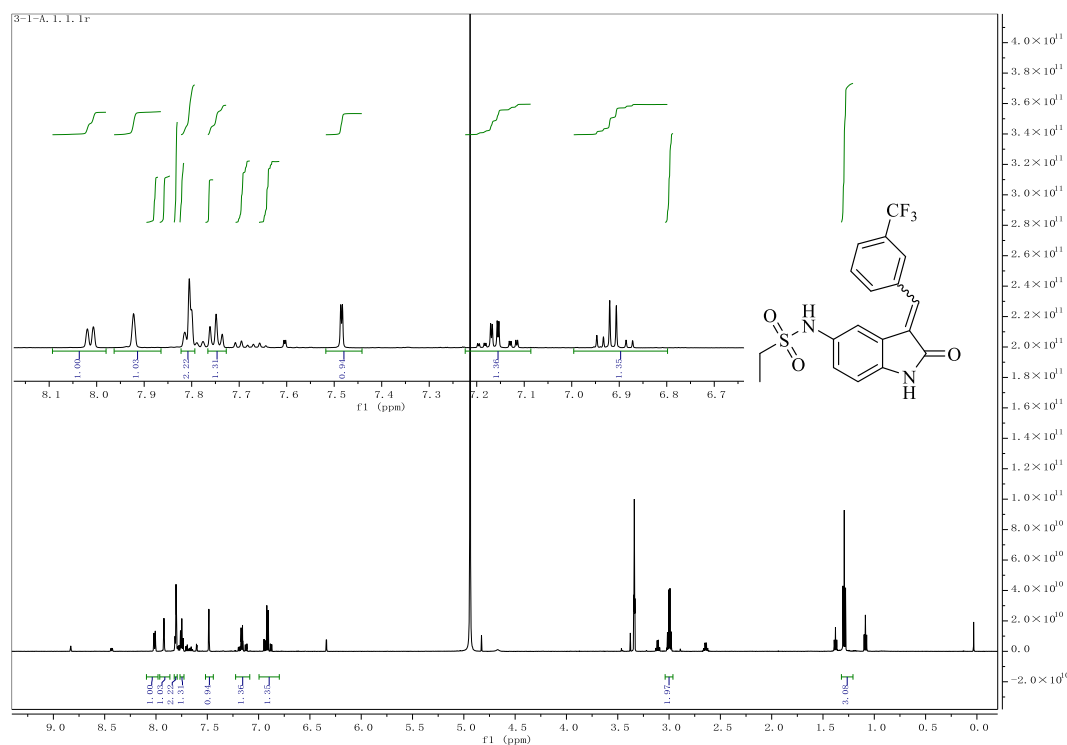


Figure S28-1. ¹H NMR spectrum (600 MHz, CD₃OCD₃) of compound 9c

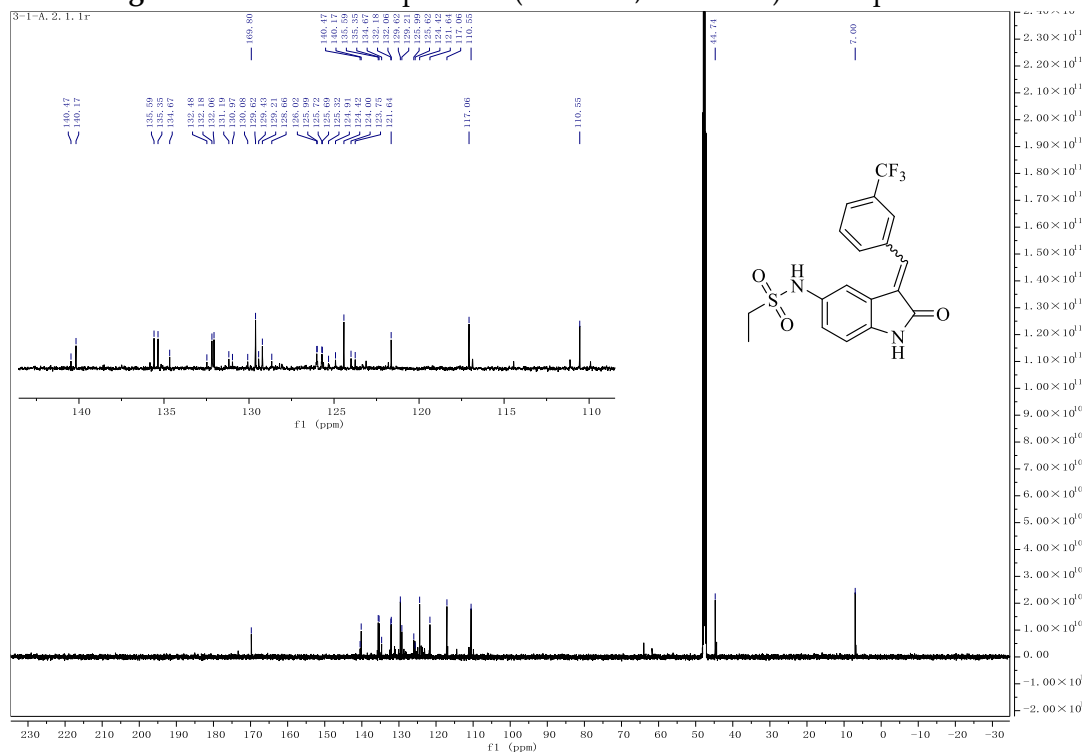


Figure S28-2. ¹³C NMR spectrum (150 MHz, CD₃OCD₃) of compound 9c

3-1-A#23 RT: 0.10 AV: 1 NL: 6.18E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

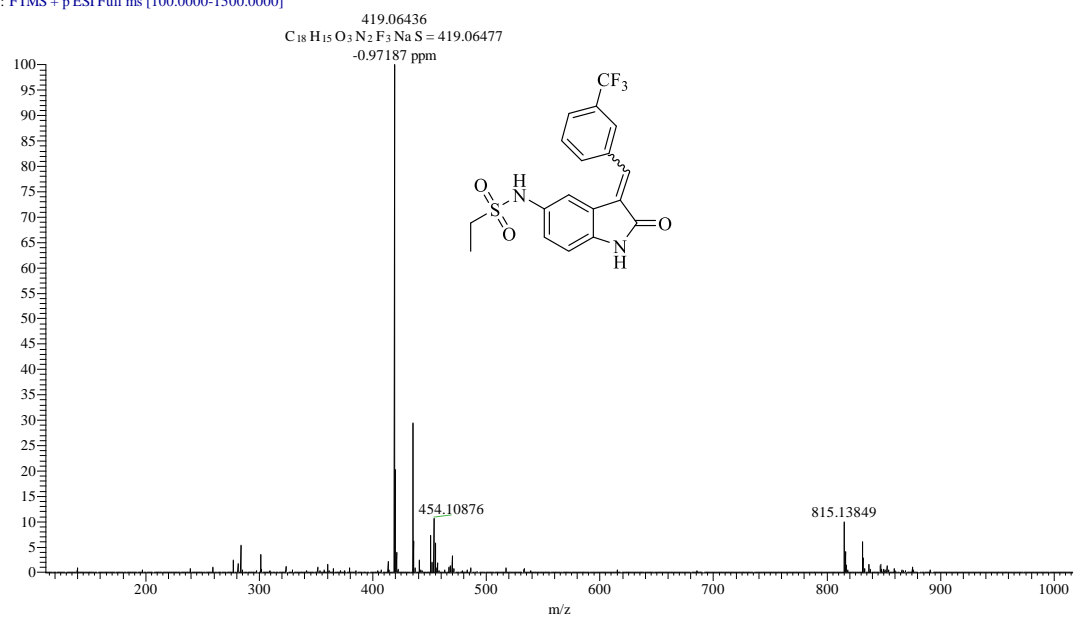


Figure S28-3. HRMS of compound 9c

N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)-1-phenylmethanesulfonamide
(9e)

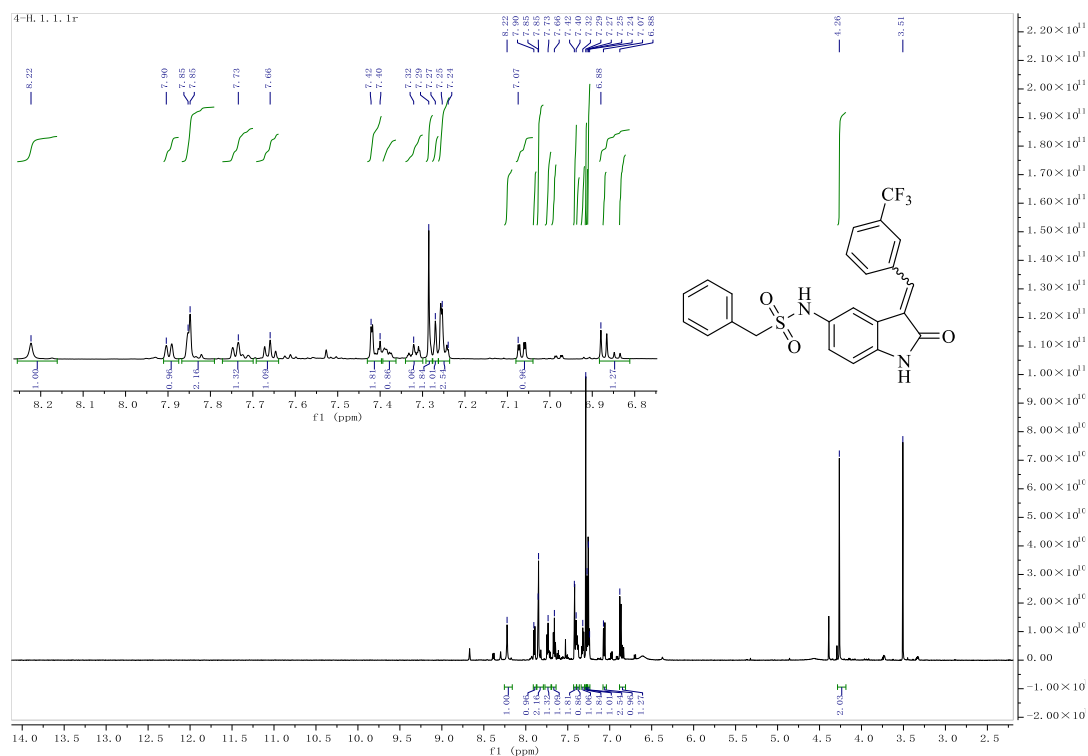


Figure S29-1. ¹H NMR spectrum (600 Hz, CDCl₃) of compound 9e

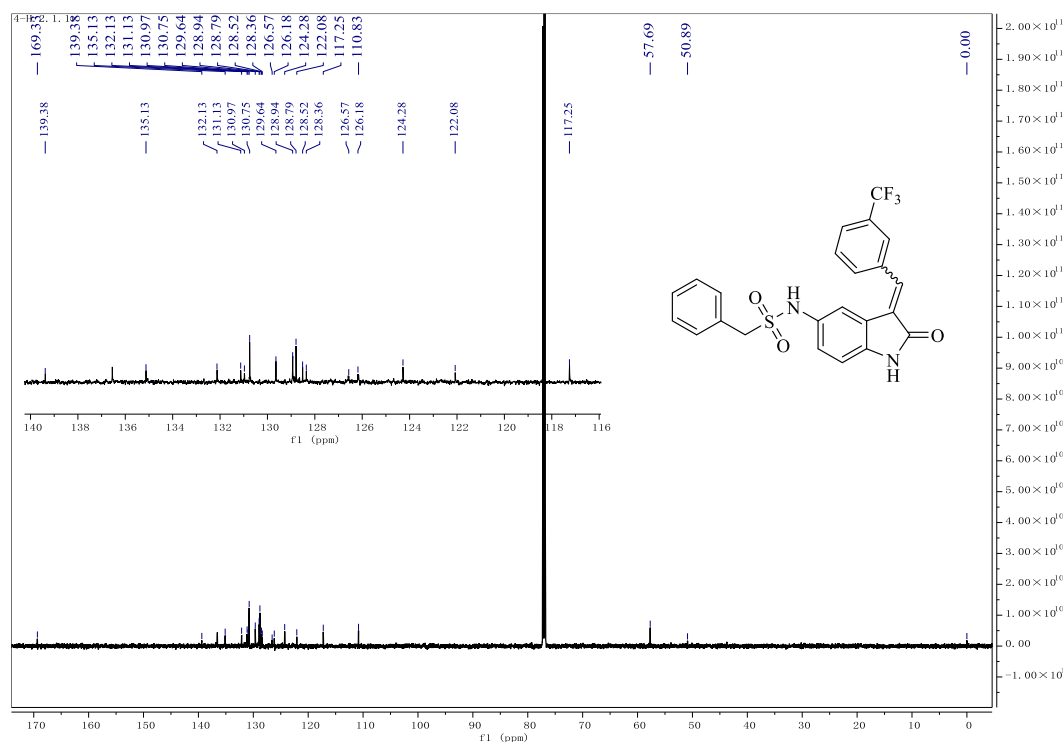


Figure S29-2. ¹³C NMR spectrum (150 Hz, CDCl₃) of compound 9e

4-1-1 #22 RT: 0.10 AV: 1 NL: 1.47E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

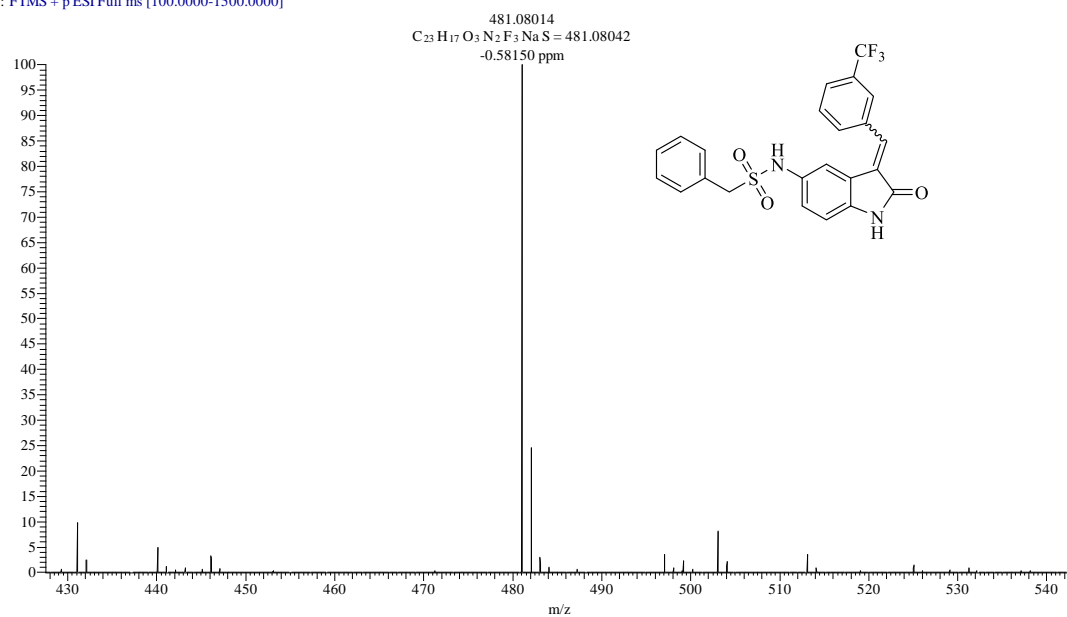


Figure S29-2. HRMS of compound **9e**

(Z)-4-methyl-N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)benzenesulfonamide (9f)

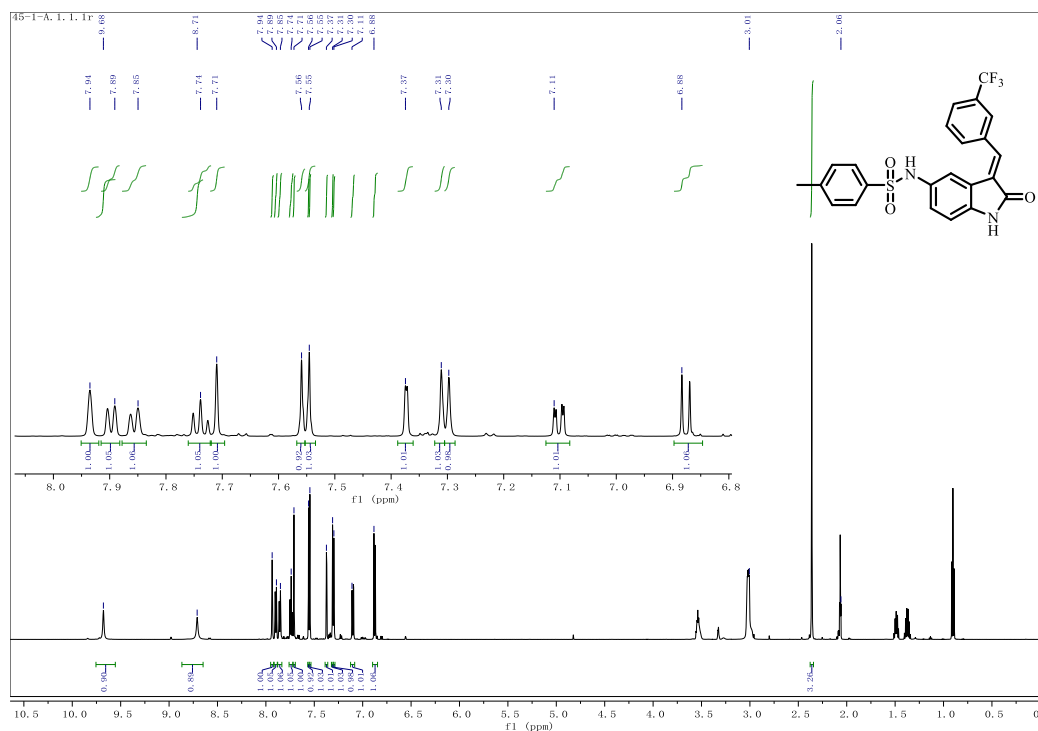


Figure S30-1. ¹H NMR spectrum (600 Hz, CD₃OCD₃) of compound 9f

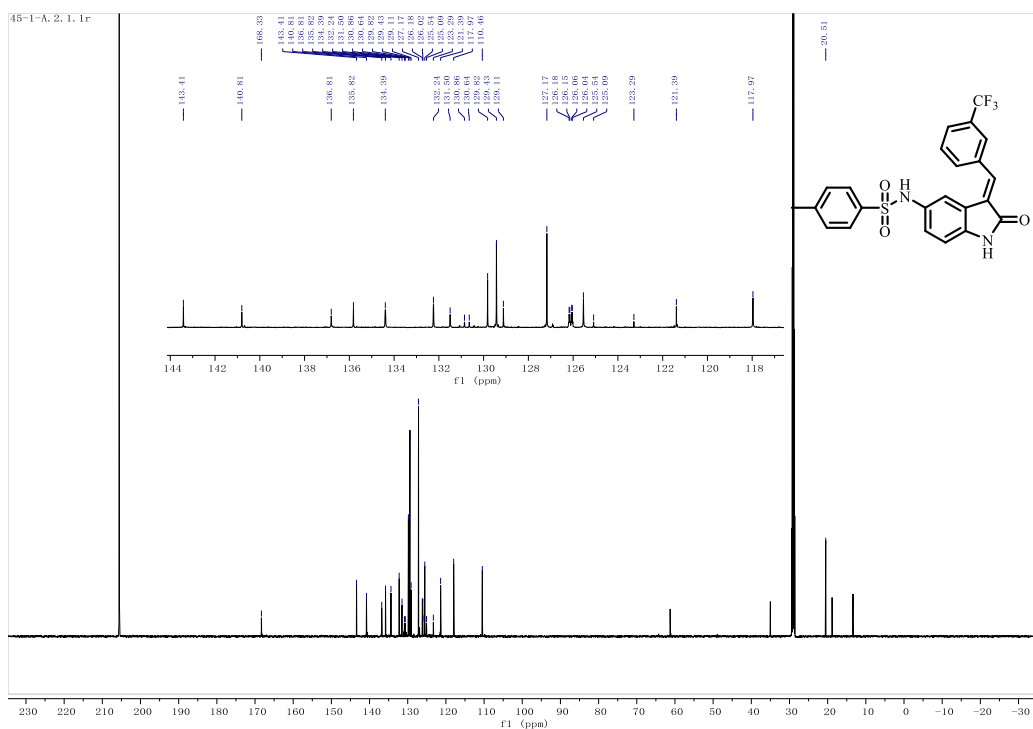


Figure S30-2. ¹³C NMR spectrum (150 Hz, CD₃OCD₃) of compound 9f

45-1 #23 RT: 0.10 AV: 1 NL: 3.71E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

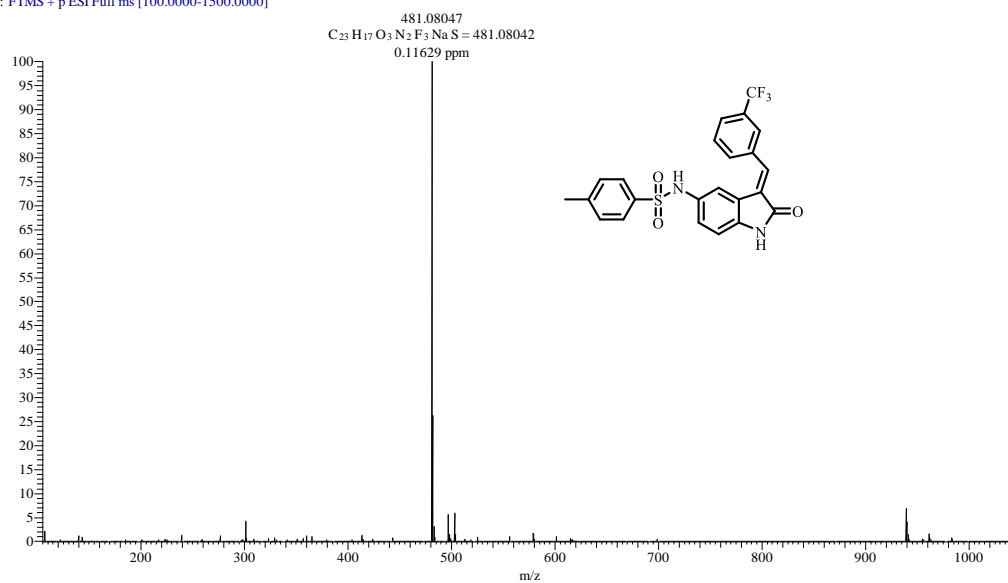


Figure S30-2. HRMS of compound **9f**

(*E*)-4-methyl-N-(2-oxo-3-(3-(trifluoromethyl)benzylidene)indolin-5-yl)benzenesulfonamide (**9g**).

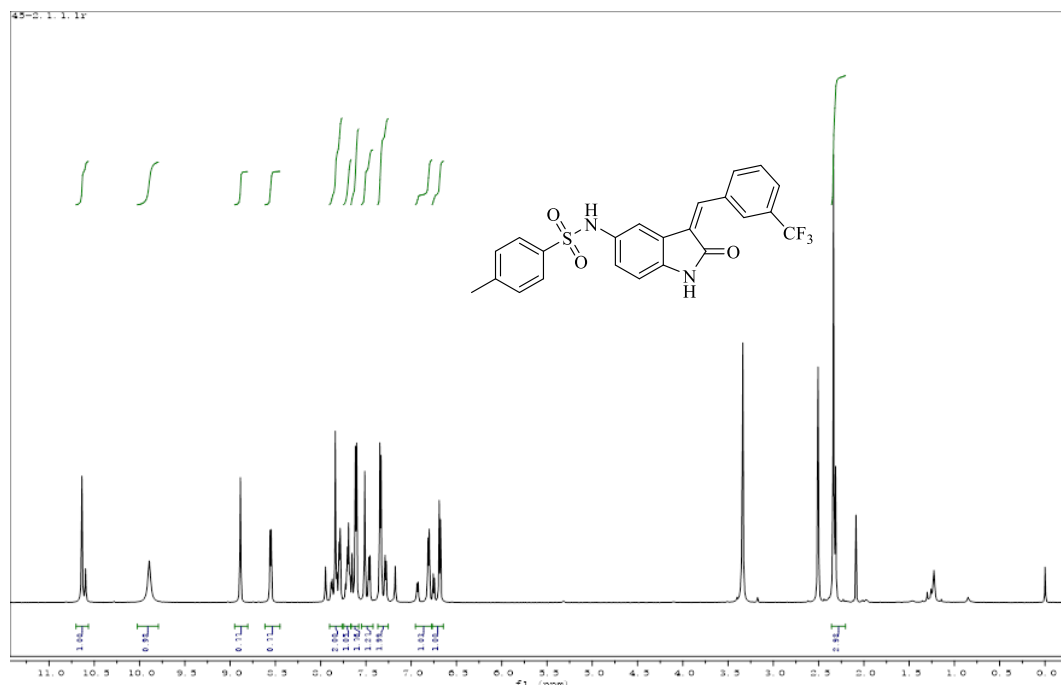


Figure S31-1. ¹H NMR spectrum (600 Hz, DMSO) of compound **9g**

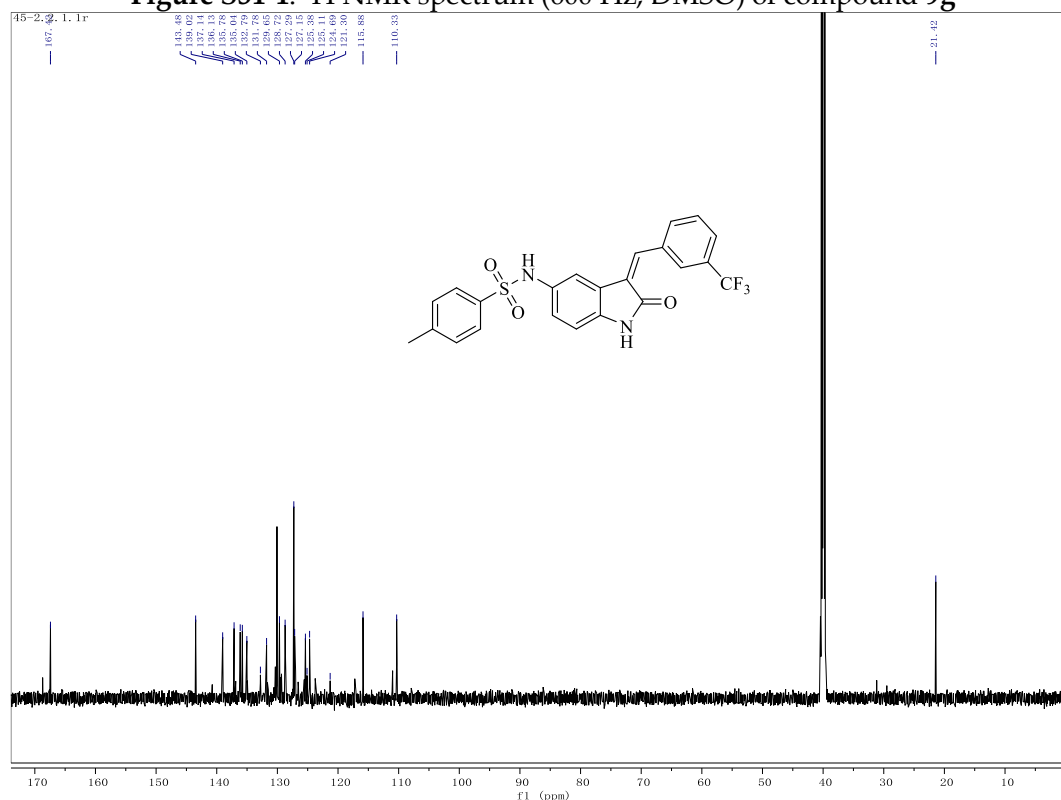


Figure S31-2. ¹³C NMR spectrum (150 Hz, DMSO) of compound **9g**

45-2 #21 RT: 0.09 AV: 1 NL: 2.71E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

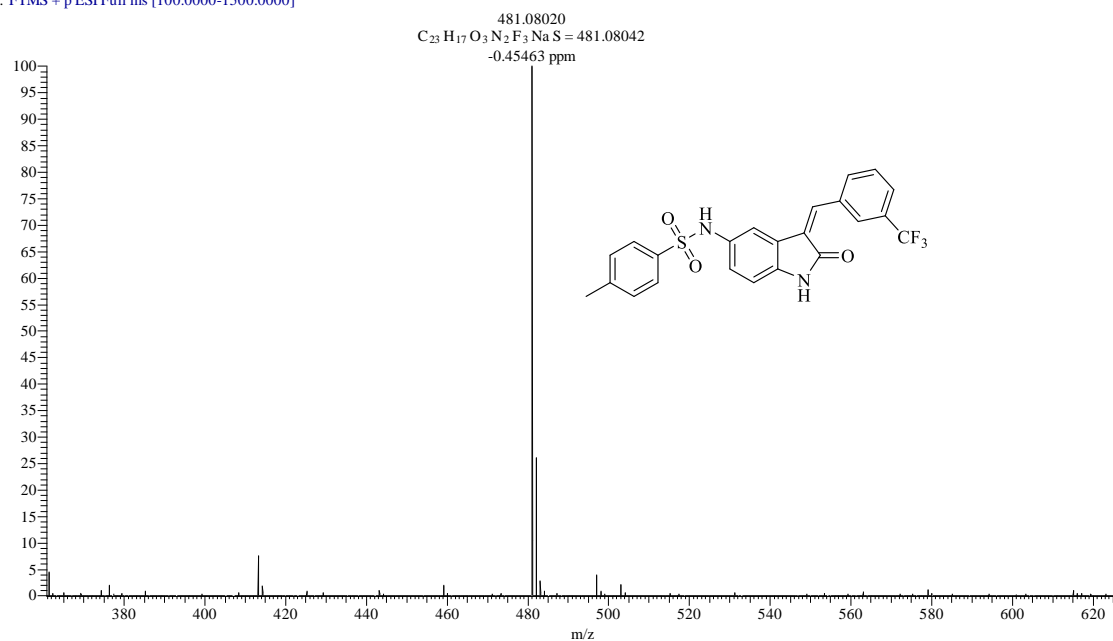


Figure S31-2. HRMS of compound **9g**

5-((3,5-bis(trifluoromethyl)benzylidene)amino)indolin-2-one (9i)

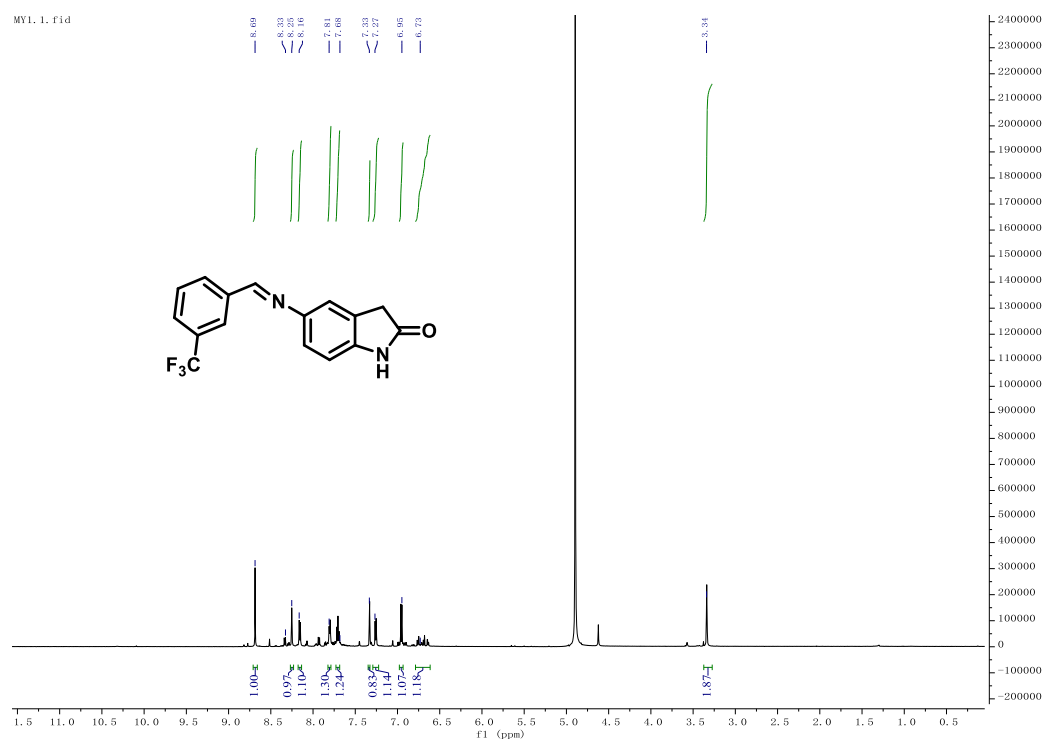


Figure S32-1. ^1H NMR spectrum (600 Hz, CD_3OD) of compound 9h

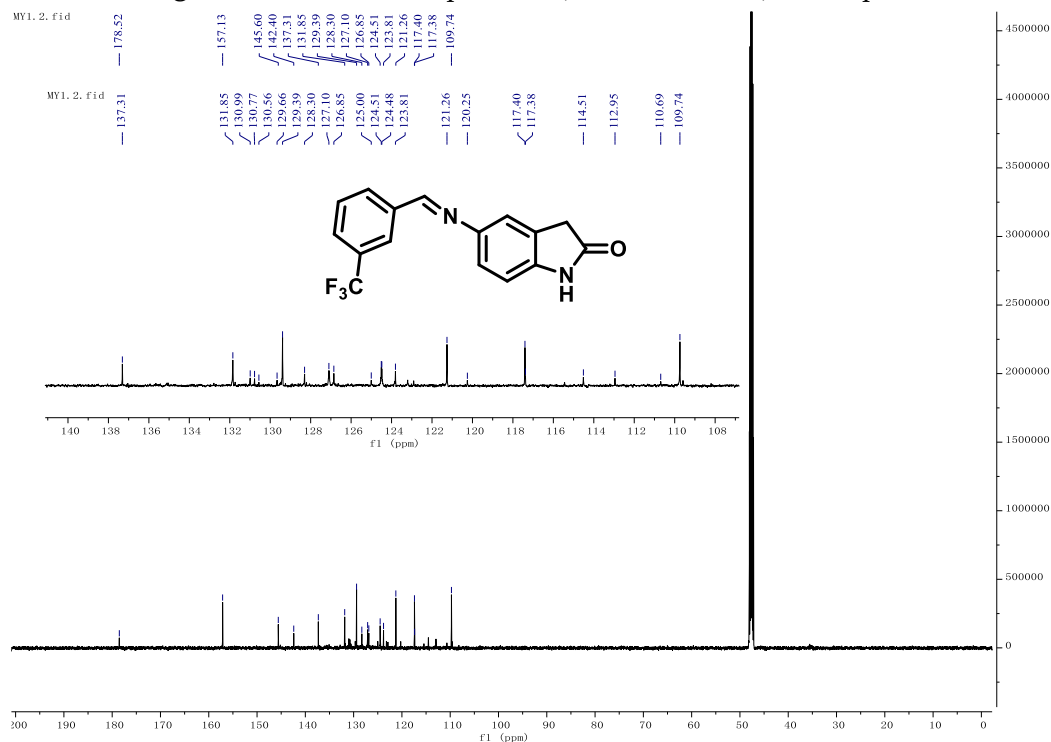


Figure S32-2. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 9h

MY1 #25 RT: 0.11 AV: 1 NL: 6.51E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

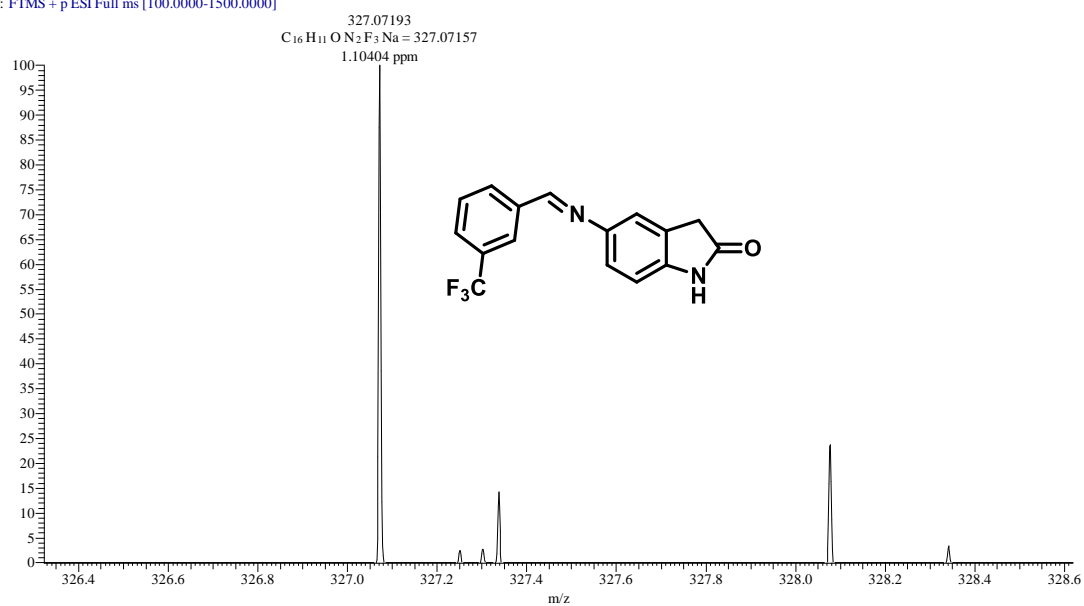


Figure S32-3. HRMS of compound **9h**

5-((3,5-bis(trifluoromethyl)benzylidene)amino)indolin-2-one (9i)

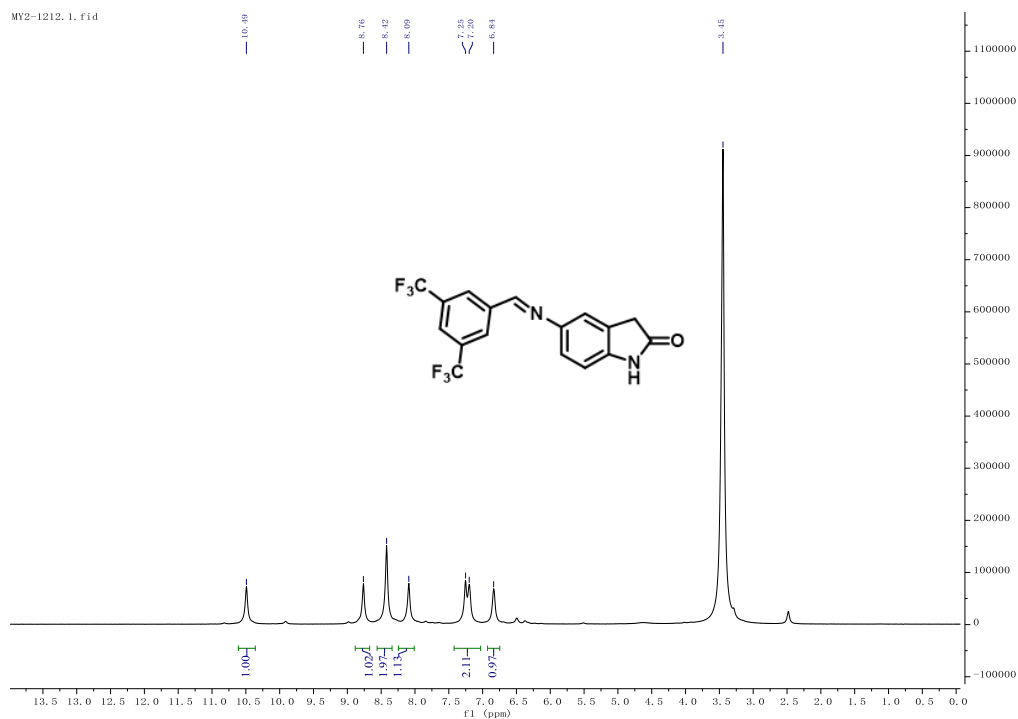


Figure S33-1. ¹H NMR spectrum (600 Hz, DMSO) of compound 9i

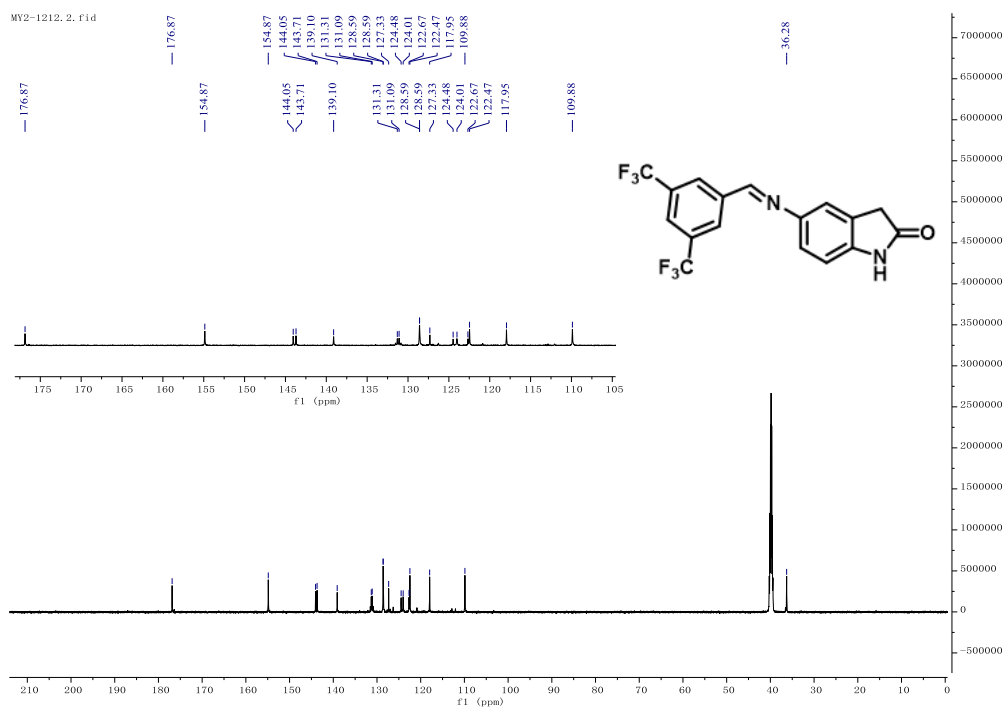


Figure S33-2. ¹³C NMR spectrum (150 Hz, DMSO) of compound 9i

MY2 #24 RT: 0.10 AV: 1 NL: 3.75E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

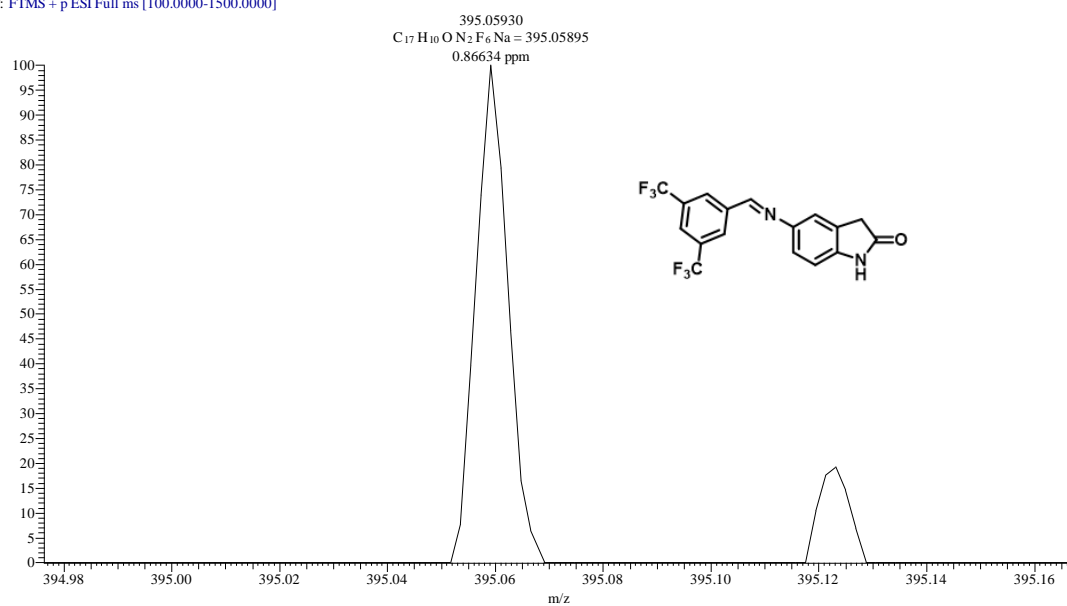


Figure S33-3. HRMS of compound 9i