Supporting Information

Cu-Catalyzed Oxidative Dual Arylation of Active Alkenes: Preparation of Cyanoarylated Oxindoles Through Denitrogenation of 3-Aminoindazoles

Qiao-Lin Wang,[†ab] Quan-Zhou,[†a] Jia Liao,[c] Zan Chen,[a] Bi-Quan Xiong,[a] Guo-Jun Deng,*[b] Ke-Wen Tang,[a] Yu Liu*[ab]

[a] Department of Chemistry and Chemical Engineering, Hunan Institute of Science and Technology, Yueyang 414006, P. R. China

[b] Key Laboratory of Environmentally Friendly Chemistry and Application of Ministry of Education, College of Chemistry, Xiangtan University, Xiangtan, 411105, China

[c] Technical Center of Gongbei Customs, No. 501, Yinhua Road, Xiangzhou District, Zhuhai, Guangdong 519000, China

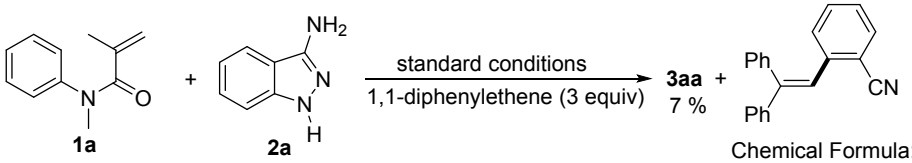
Fax: (+86)-730-8640-122; phone: (+86)-730-8640-122; email: lyxtmj_613@163.com and email: gjdeng@xtu.edu.cn

[†] These authors contributed equally to this work

List of Contents

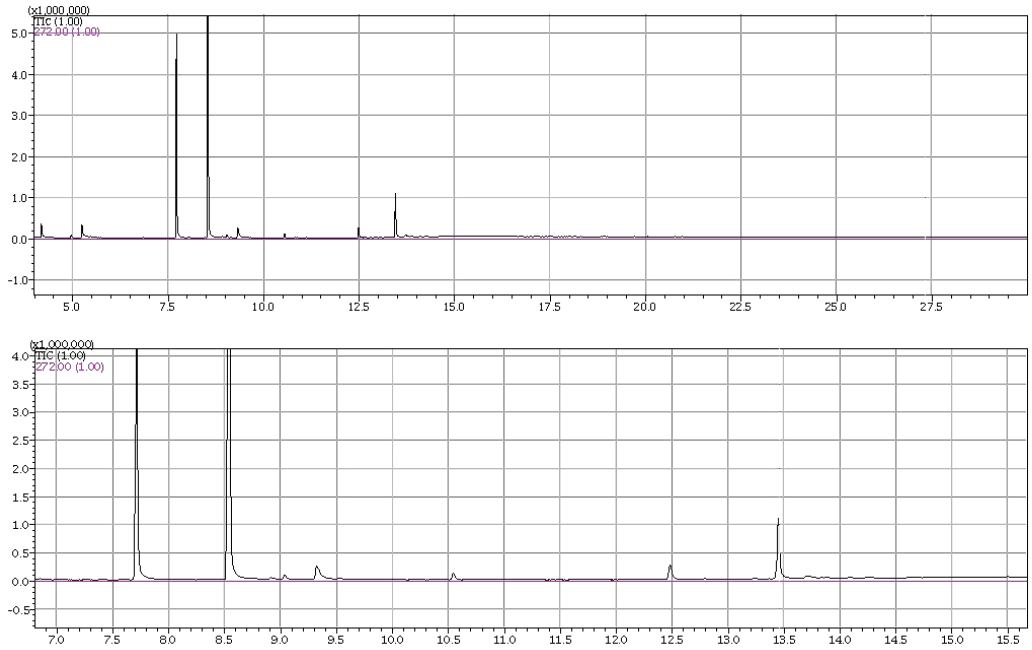
1. **GC-MS Analysis of Raw Reaction Mixture by Using 1,1-Diphenylethene as Radical Inhibitor** **S1-S3**
2. **^{1}H and ^{13}C spectra** **S4-S83**

1. GC-MS Analysis of Raw Reaction Mixture by Using 1,1-Diphenylethene as Radical Inhibitor

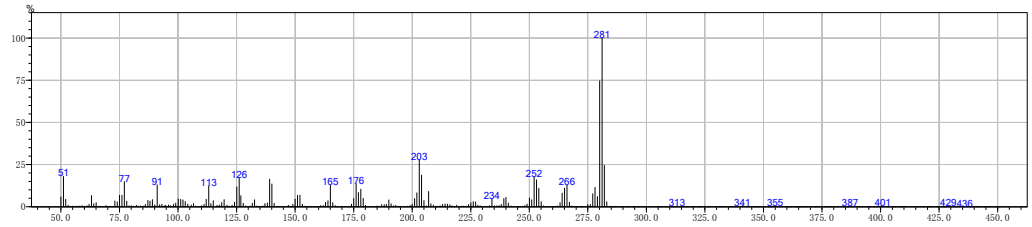


Chemical Formula: $C_{21}H_{15}N$
Exact Mass: 281.1204
Molecular Weight: 281.3580
4, detected by GC-MS

GC Spectra of Raw Reaction Mixture by Using 1,1-Diphenylethene as Radical Inhibitor



MS Analysis of the peak at 13.5 min



[MS Spectrum]
# of Peaks399
Raw Spectrum 13.460 (scan : 1893)
Background No Background Spectrum
Base Peakm/z 281.10 (Inten : 70,201)
Event# 1
m/z Absolute Intensity Relative Intensity

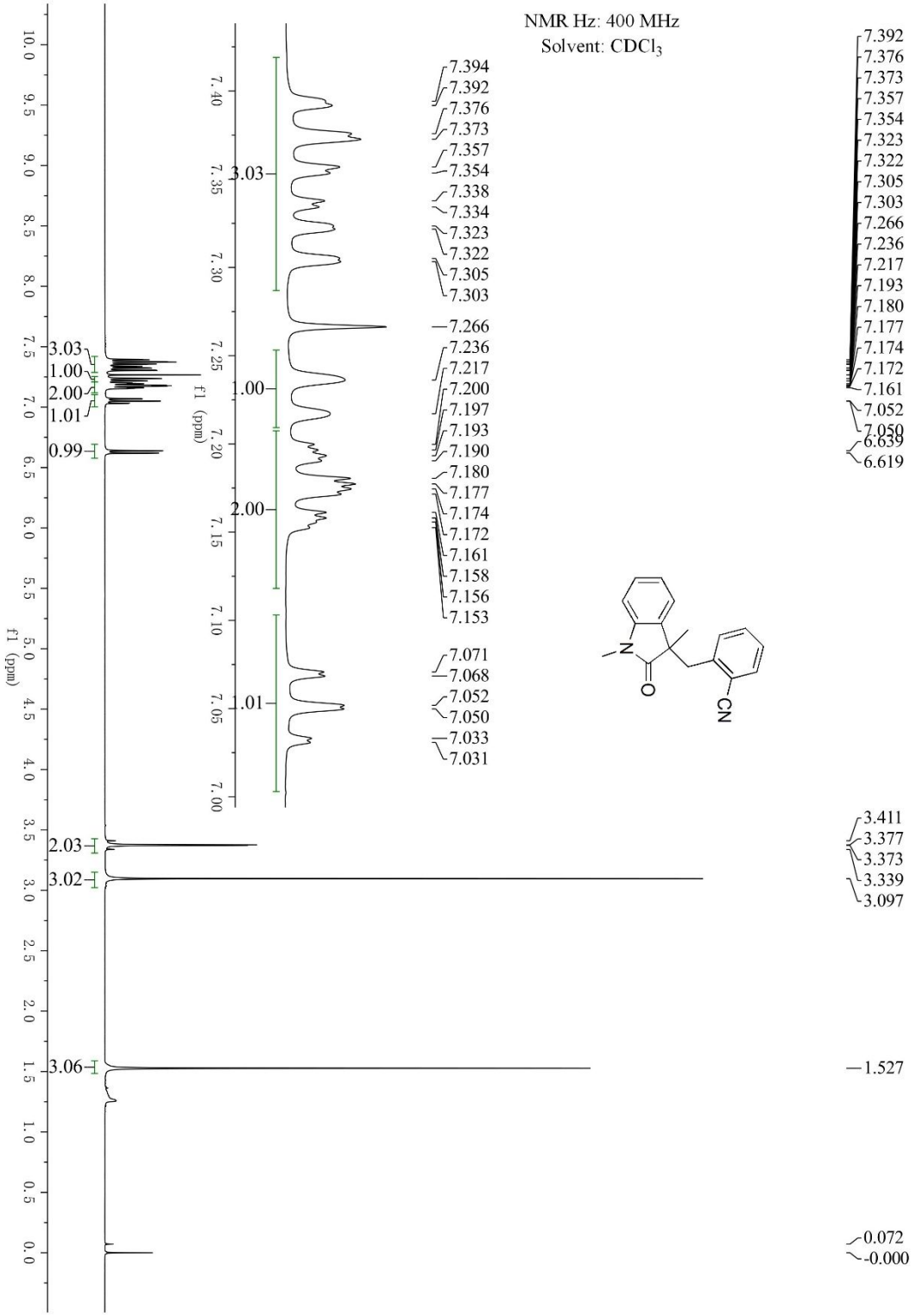
50.00	4068	5.79
51.05	12599	17.95
52.05	3042	4.33
53.10	553	0.79
54.10	118	0.17
55.10	252	0.36
56.10	161	0.23
57.10	162	0.23
58.00	282	0.40
59.00	414	0.59
60.00	172	0.25
61.15	407	0.58
62.05	1023	1.46
63.05	4646	6.62
64.00	1282	1.83
65.05	1687	2.40
66.10	215	0.31
67.10	135	0.19
68.10	92	0.13
69.20	473	0.67
70.20	103	0.15
71.20	137	0.20
72.10	54	0.08
73.05	2356	3.36
74.05	2025	2.88
75.05	4774	6.80
76.05	4774	6.80
77.05	10394	14.81
78.10	2322	3.31
79.10	396	0.56
80.10	390	0.56
81.10	188	0.27
82.20	535	0.76
83.20	230	0.33
84.05	316	0.45
85.10	228	0.32
86.05	967	1.38
87.10	2657	3.78
88.05	2303	3.28
89.05	2941	4.19
90.05	754	1.07
91.10	9087	12.94
92.15	833	1.19
93.10	1010	1.44
94.05	364	0.52
94.70	586	0.83
95.95	766	1.09
96.85	421	0.60
98.15	1022	1.46
99.05	1519	2.16
100.10	3182	4.53
101.15	2993	4.26
102.10	2831	4.03
103.05	2162	3.08
104.15	1059	1.51
105.65	708	1.01
106.60	1310	1.87
107.55	298	0.42
108.60	121	0.17
110.10	462	0.66
111.10	986	1.40
112.05	3054	4.35
113.10	8713	12.41
114.05	1250	1.78
115.05	2536	3.61
116.65	541	0.77
117.65	747	1.06
118.65	1682	2.40
119.65	2974	4.24
120.90	647	0.92
121.90	212	0.30
123.10	623	0.89
124.15	1809	2.58
125.10	8214	11.70
126.10	11937	17.00
126.85	4588	6.54
127.85	1420	2.02
128.80	310	0.44
129.80	38	0.05
130.75	251	0.36
131.70	1433	2.04
132.70	2890	4.12
133.65	311	0.44
134.70	153	0.22
136.15	330	0.47
137.10	1348	1.92
138.15	1561	2.22
139.10	11478	16.35
140.05	9470	13.49
141.05	1400	1.99
142.10	111	0.16
143.10	74	0.11
144.10	94	0.13
145.10	105	0.15
146.10	65	0.09
147.10	534	0.76
148.00	169	0.24
149.05	1001	1.43
150.00	3161	4.50
151.00	4673	6.66
152.05	4844	6.90
153.10	1090	1.55
154.10	199	0.28
155.10	124	0.18
156.10	30	0.04
157.10	41	0.06
158.10	22	0.03
159.10	137	0.20
160.10	137	0.20
160.95	527	0.75
162.00	522	0.74
163.00	1836	2.62
164.05	2502	3.56
165.05	8843	12.60
166.05	1685	2.40
167.20	455	0.65
168.20	71	0.10
169.20	114	0.16
170.20	66	0.09
171.20	33	0.05
172.20	145	0.21
173.10	143	0.20
174.05	1042	1.48
175.05	3392	4.83
176.05	9533	13.58
177.05	5872	8.36
178.05	7304	10.40
179.05	3478	4.95
180.05	533	0.76
181.00	97	0.14
182.00	124	0.18
183.00	70	0.10

184.00	42	0.06
185.00	290	0.41
185.90	94	0.13
186.90	854	1.22
188.00	820	1.17
188.95	1028	1.46
190.00	2828	4.03
191.00	1217	1.73
192.05	397	0.57
193.00	591	0.84
194.00	156	0.22
195.00	103	0.15
196.00	41	0.06
197.00	63	0.09
198.00	191	0.27
199.10	516	0.74
200.00	1017	1.45
201.00	3410	4.86
202.00	5758	8.20
203.05	19471	27.74
204.00	13198	18.80
205.00	2569	3.66
205.95	358	0.51
207.00	6346	9.04
207.95	1199	1.71
209.10	684	0.97
210.10	188	0.27
210.90	218	0.31
211.90	358	0.51
213.00	916	1.30
214.05	1158	1.65
215.05	1050	1.50
216.10	796	1.13
217.00	372	0.53
218.00	108	0.15
219.00	620	0.88
220.00	135	0.19
221.00	247	0.35
222.00	233	0.33
223.00	281	0.40
224.05	875	1.25
225.00	1617	2.30
226.05	2149	3.06
227.10	1924	2.74
228.05	617	0.88
229.05	381	0.54
230.00	86	0.12
231.00	39	0.06
232.00	95	0.14
233.00	466	0.66
234.05	3313	4.72
235.00	420	0.60
236.00	310	0.44
237.05	487	0.69
238.05	943	1.34
239.10	3415	4.86
240.05	3901	5.56
241.05	1529	2.18
242.15	325	0.46
243.10	71	0.10
244.10	49	0.07
245.10	22	0.03
246.10	41	0.06
247.10	135	0.19
248.10	498	0.71
249.05	1152	1.64
250.05	3608	5.14
251.05	2885	4.11
252.05	12420	17.69
253.10	11140	15.87
254.05	7714	10.99
255.10	2073	2.95
256.05	336	0.48
257.10	62	0.09
258.10	34	0.05
259.10	42	0.06
260.10	21	0.03
261.10	146	0.21
262.10	294	0.42
263.15	1718	2.45
264.05	5625	8.01
265.05	7691	10.96
266.10	9055	12.90
267.10	1886	2.69
268.10	295	0.42
269.10	89	0.13
270.10	11	0.02
271.10	55	0.08
272.10	21	0.03
273.10	34	0.05
274.00	70	0.10
275.00	921	1.31
276.05	948	1.35
277.10	5415	7.71
278.05	8097	11.53
279.10	4183	5.96
280.05	**52392**	**74.63**
281.10	**70201**	**100.00**
282.05	**17218**	**24.53**
283.10	2071	2.95
284.10	185	0.26
285.10	34	0.05
286.10	14	0.02
287.10	66	0.09
288.10	39	0.06
289.10	27	0.04
290.10	47	0.07
291.10	65	0.09
292.10	18	0.03
293.10	44	0.06
294.10	10	0.01
295.10	114	0.16
296.10	16	0.02
297.10	108	0.15
298.10	58	0.08
299.10	26	0.04
300.10	38	0.05
301.10	24	0.01
302.10	34	0.02
303.10	22	0.01
304.10	13	0.01
305.10	33	0.02
306.10	33	0.02
307.10	18	0.01
308.10	76	0.04
309.10	24	0.01
310.10	29	0.02
311.10	24	0.01
312.10	29	0.02
313.10	49	0.03
314.10	27	0.02
315.10	16	0.01

316.10	174	0.10	317.10	50	0.03

2. Spectra

2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3aa)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Solvent: $CDCl_3$
f1 (ppm)
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1.00
2.00
1.01
0.99
2.03
3.02
3.06
7.394
7.392
7.376
7.373
7.357
7.354
7.338
7.334
7.323
7.322
7.305
7.303
7.266
7.236
7.217
7.200
7.197
7.193
7.190
7.180
7.177
7.174
7.172
7.161
7.158
7.156
7.153
7.071
7.068
7.052
7.050
7.033
7.031
7.392
7.376
7.373
7.357
7.354
7.323
7.322
7.305
7.303
7.266
7.236
7.217
7.193
7.180
7.177
7.174
7.172
7.161
7.052
7.050
6.639
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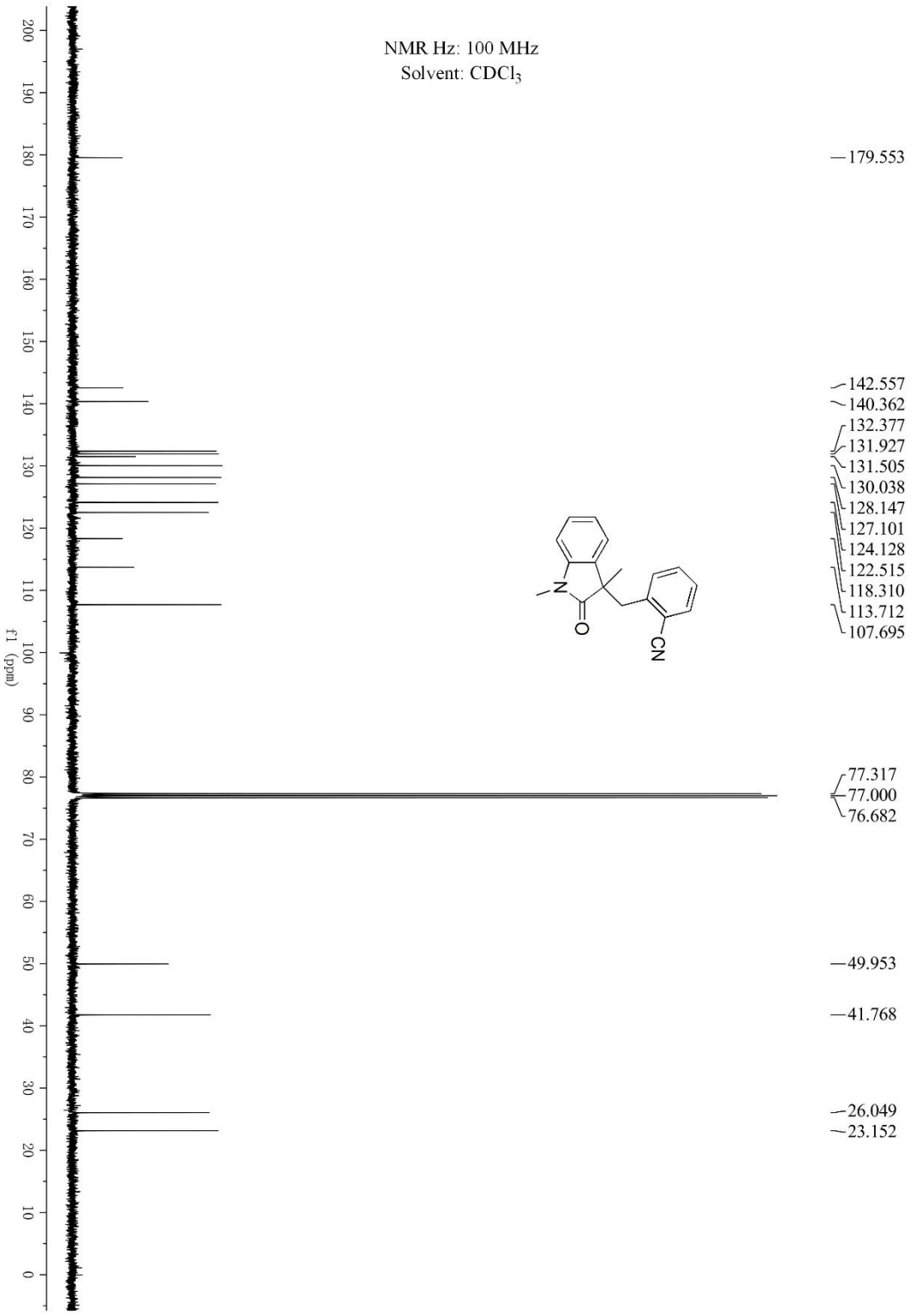
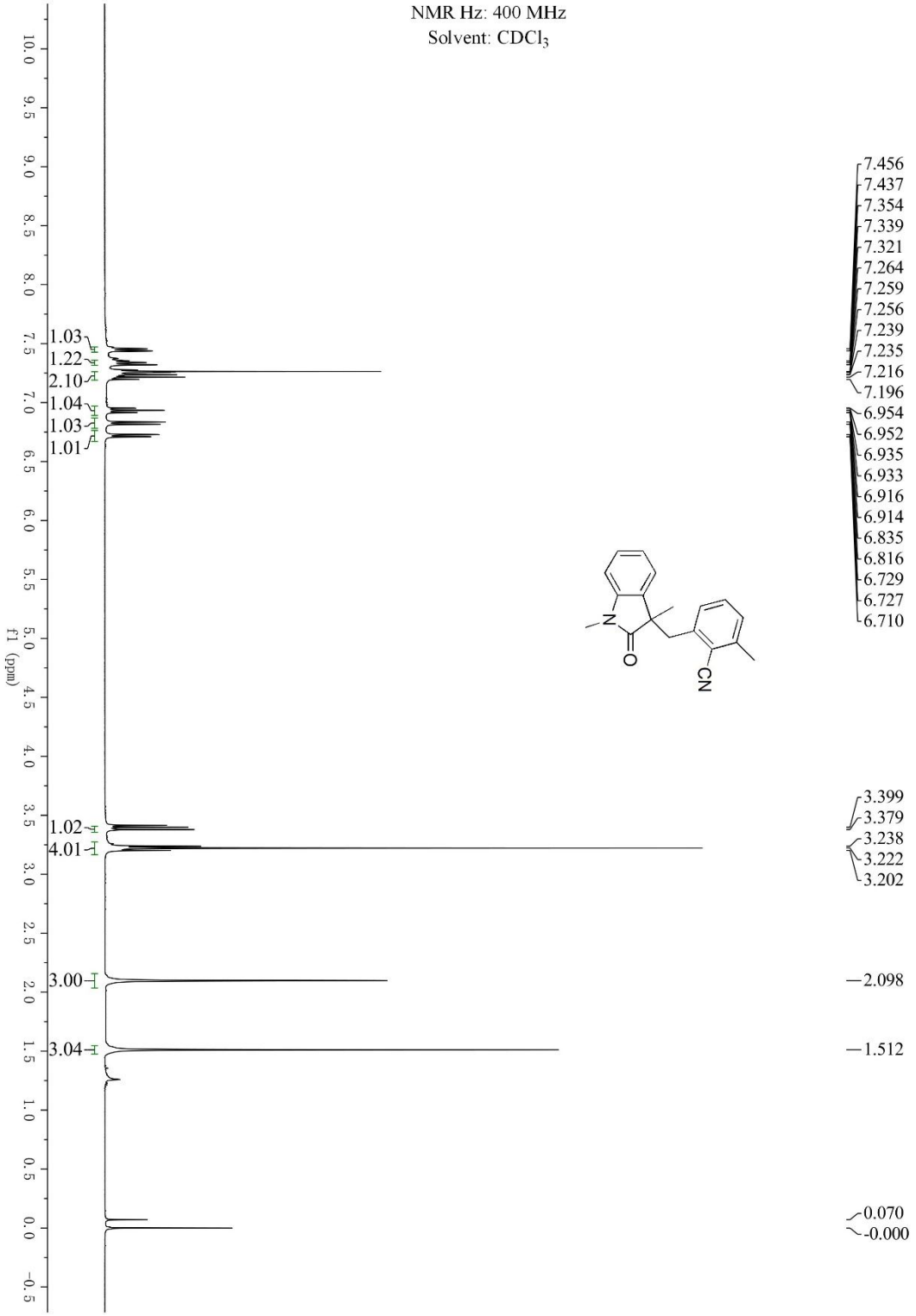
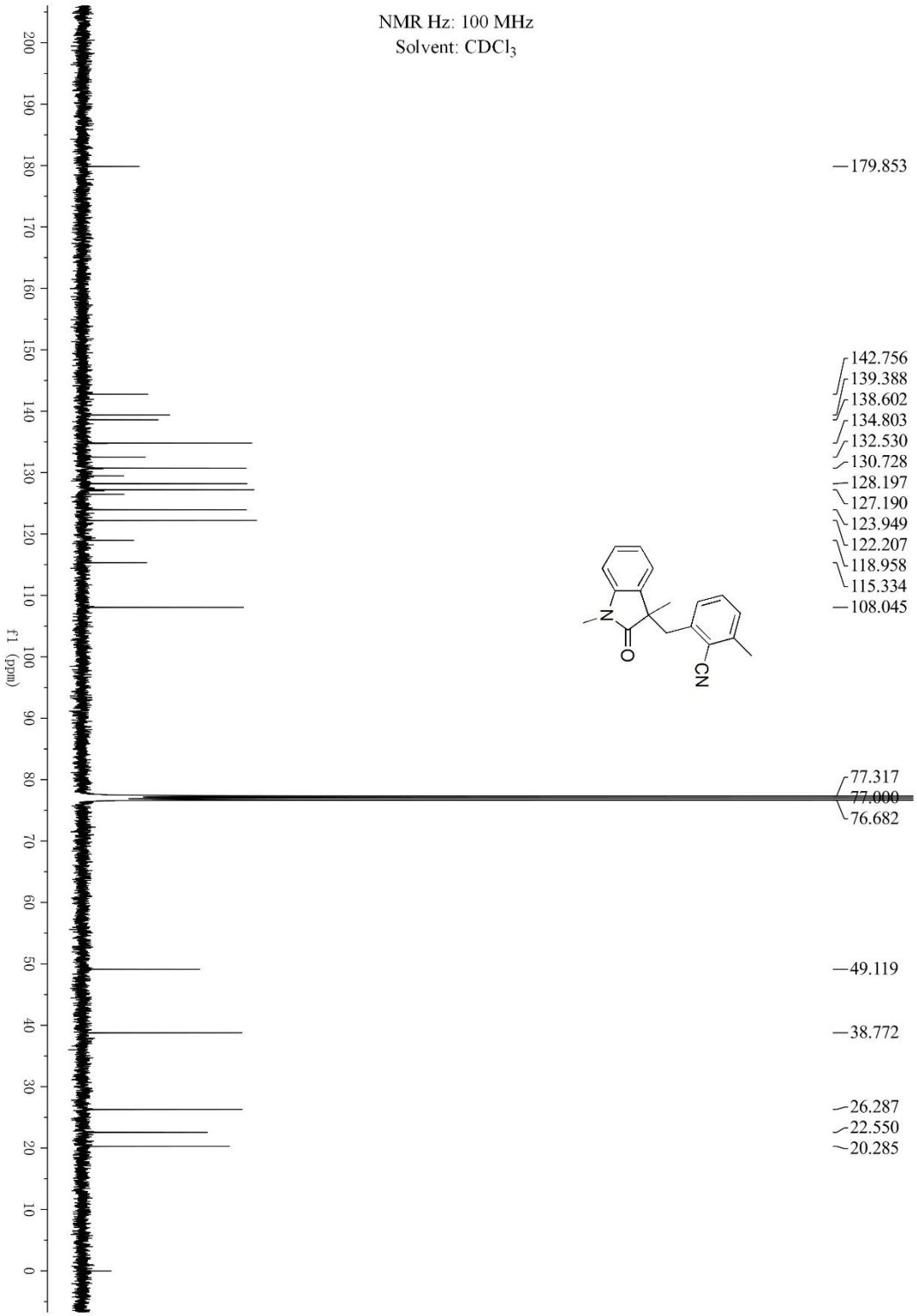
N
O
CN

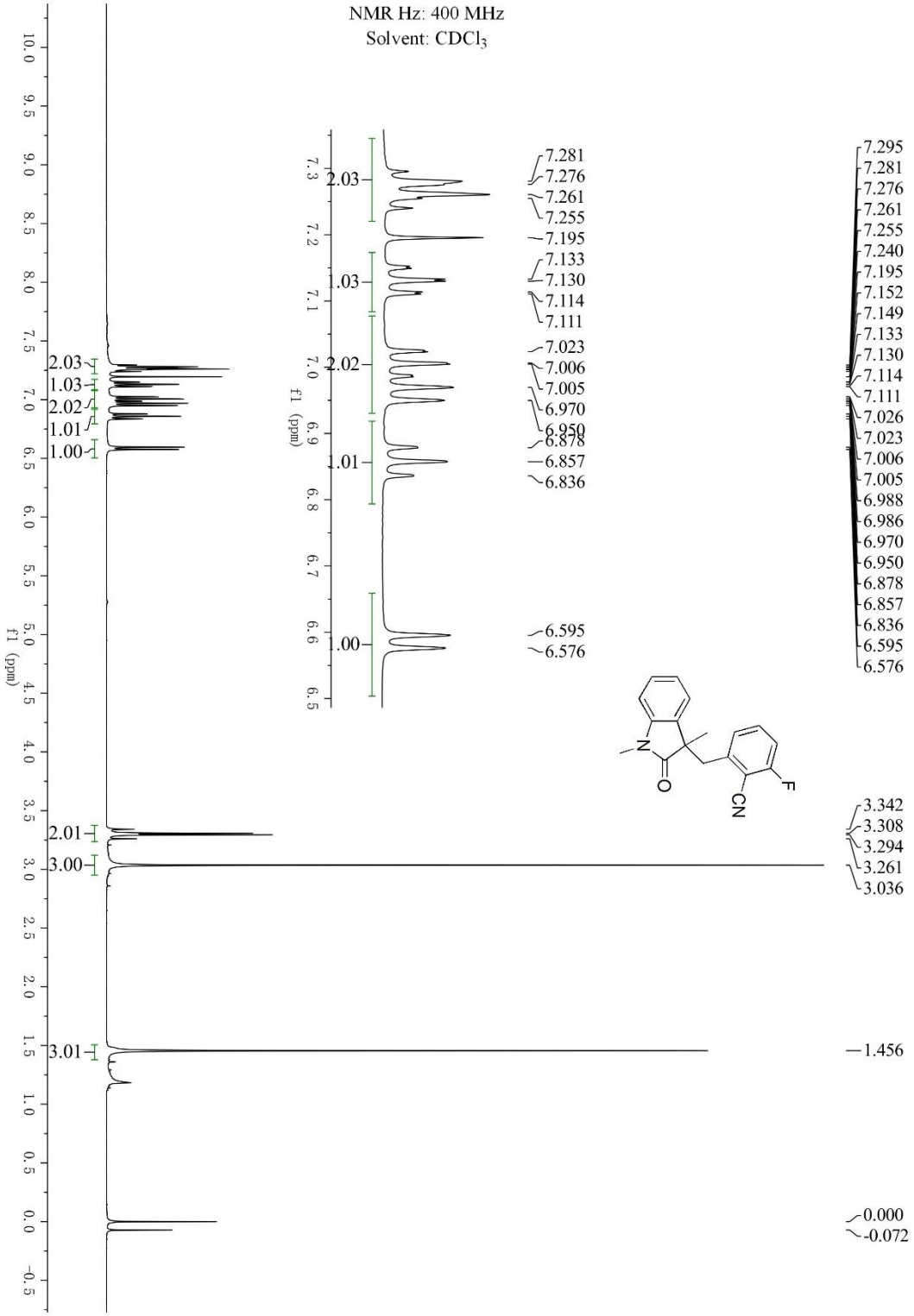

NMR Hz: 100 MHz
Solvent: CDCl3
179.553
142.557
140.362
132.377
131.927
131.505
130.038
128.147
127.101
124.128
122.515
118.310
113.712
107.695
77.317
77.000
76.682
49.953
41.768
26.049
23.152
f1 (ppm)
N
O
CN

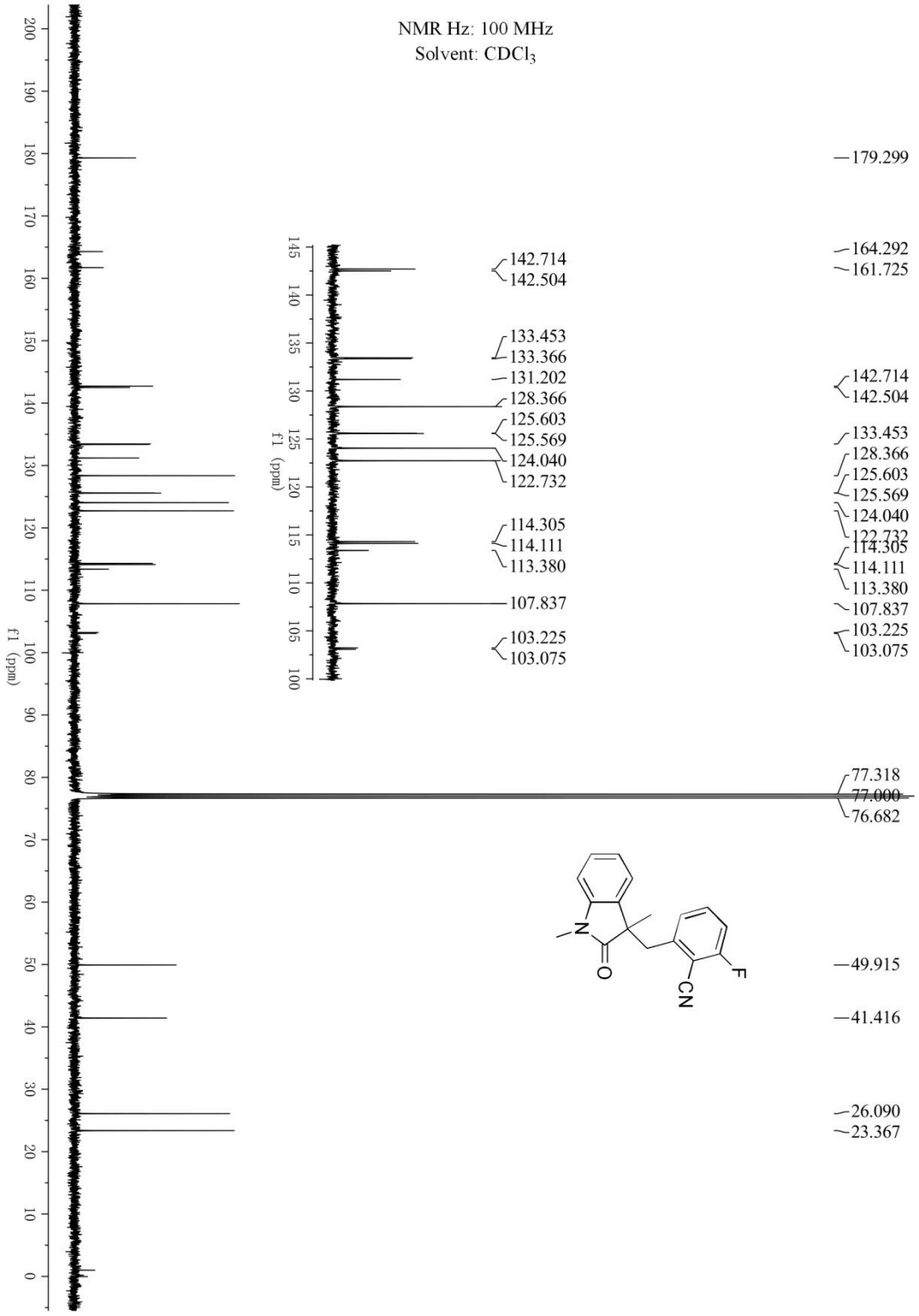
2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-6-methylbenzonitrile (3ab)

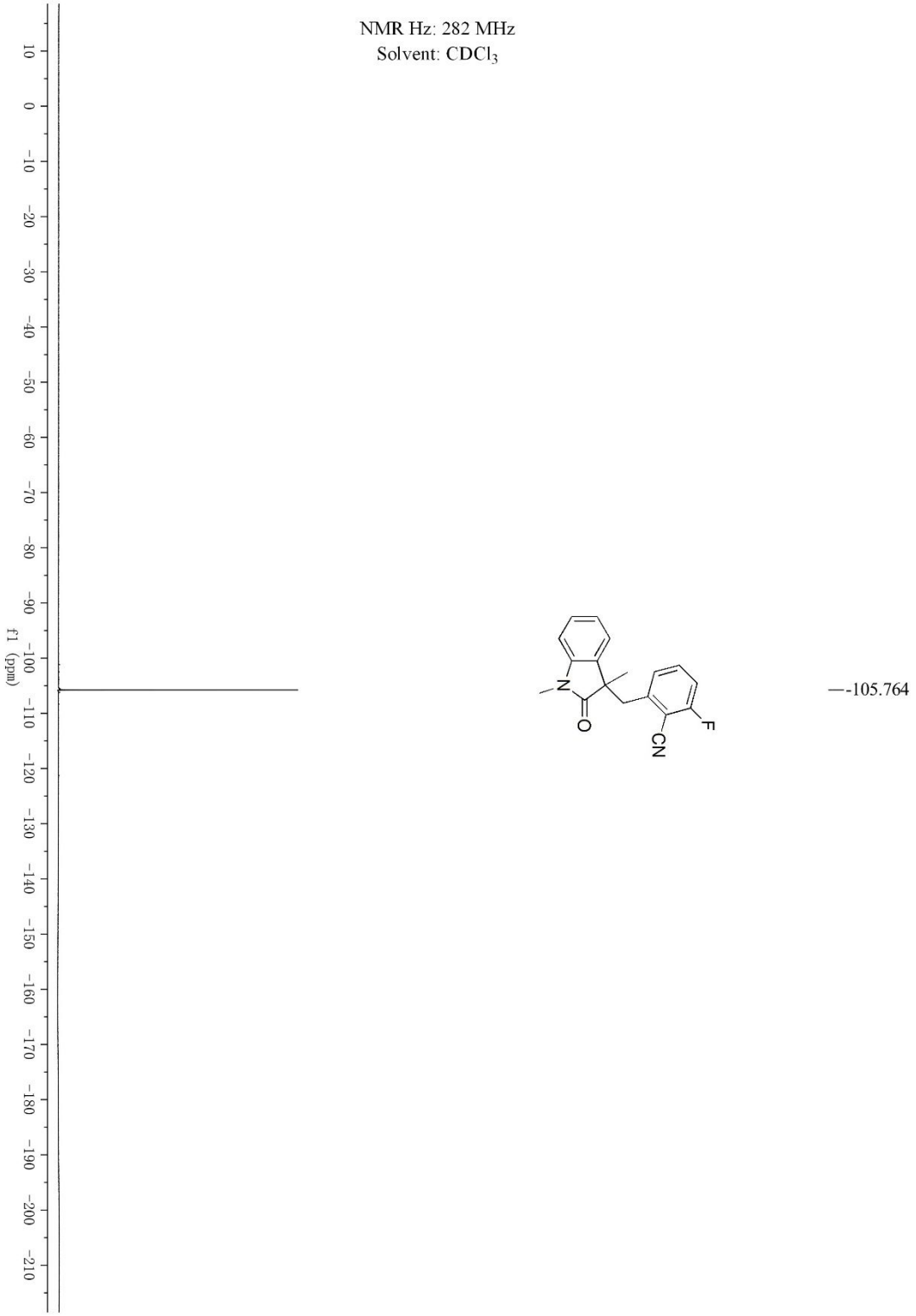



NMR Hz: 100 MHz
Solvent: CDCl3
179.853
142.756
139.388
138.602
134.803
132.530
130.728
128.197
127.190
123.949
122.207
118.958
115.334
108.045
77.317
77.000
76.682
49.119
38.772
26.287
22.550
20.285
f1 (ppm)
N
O
CN

2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-6-fluorobenzonitrile (3ac)




NMR Hz: 100 MHz
Solvent: CDCl3
179.299
164.292
161.725
142.714
142.504
133.453
133.366
131.202
128.366
125.603
125.569
124.040
122.732
114.305
114.111
113.380
107.837
103.225
103.075
77.318
77.000
76.682
49.915
41.416
26.090
23.367
f1 (ppm)
N
O
CN
F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Solvent: $CDCl_3$
f1 (ppm)
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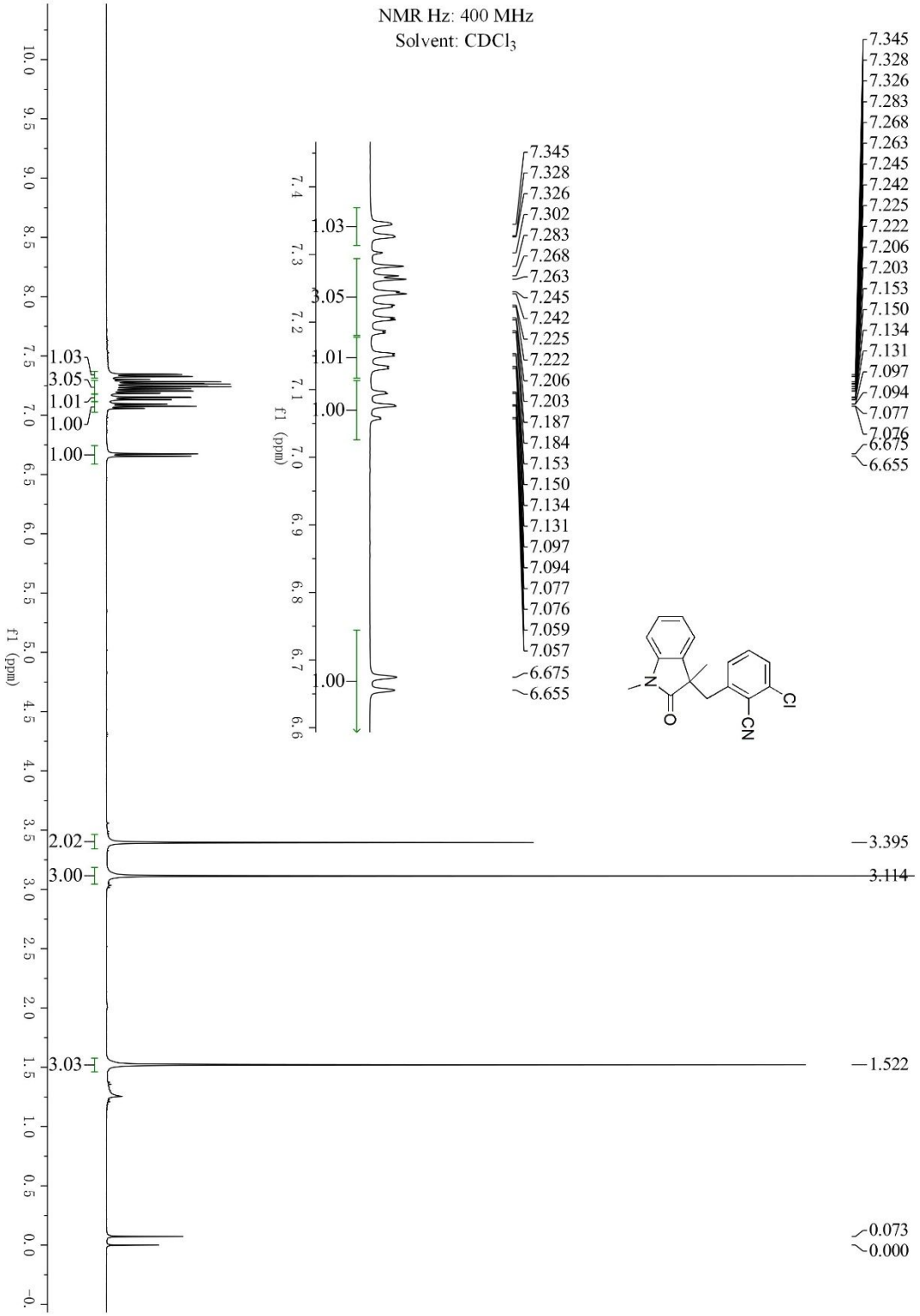
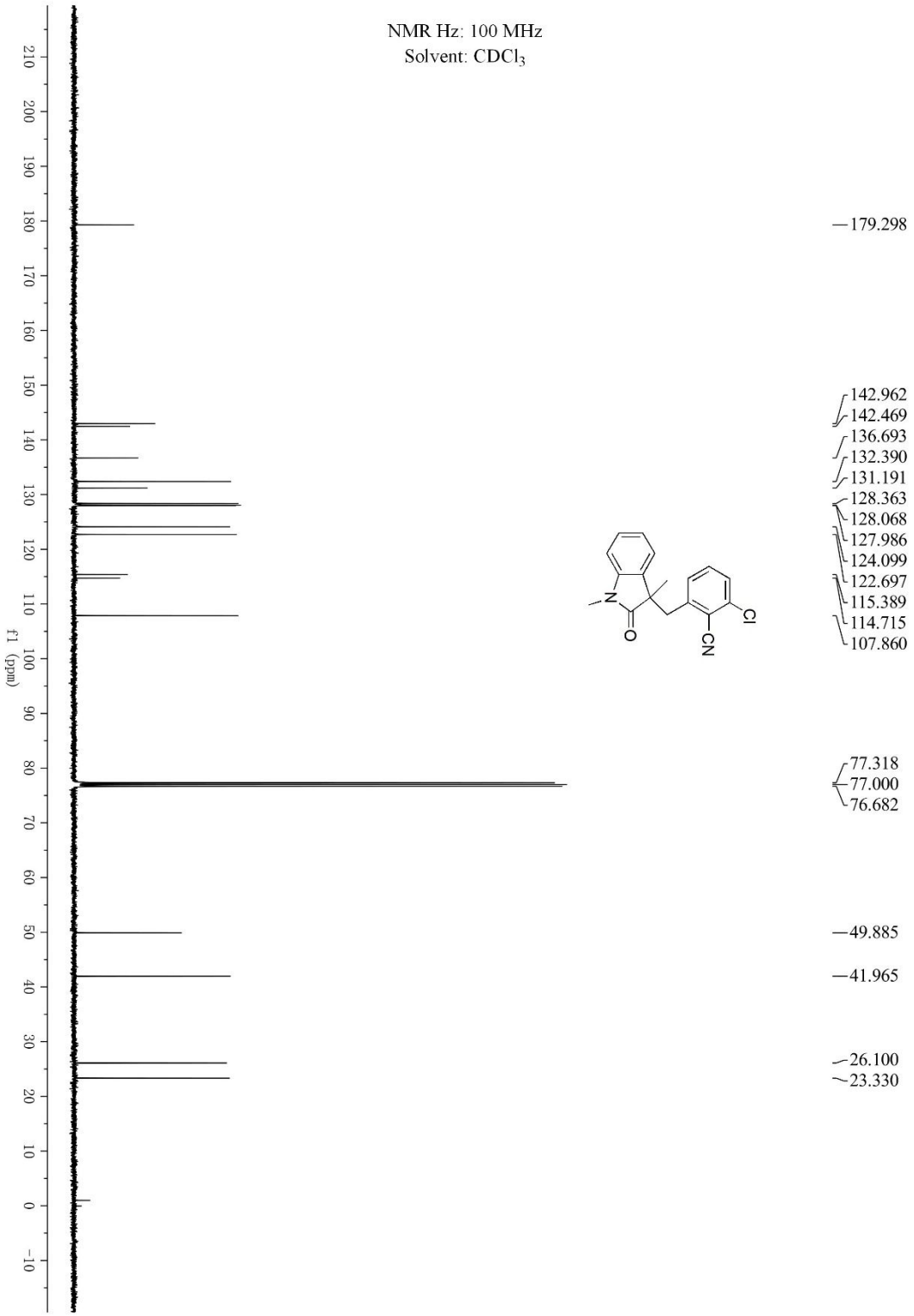
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
N
O
CN
F
—-105.764

2-Chloro-6-((1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ad)

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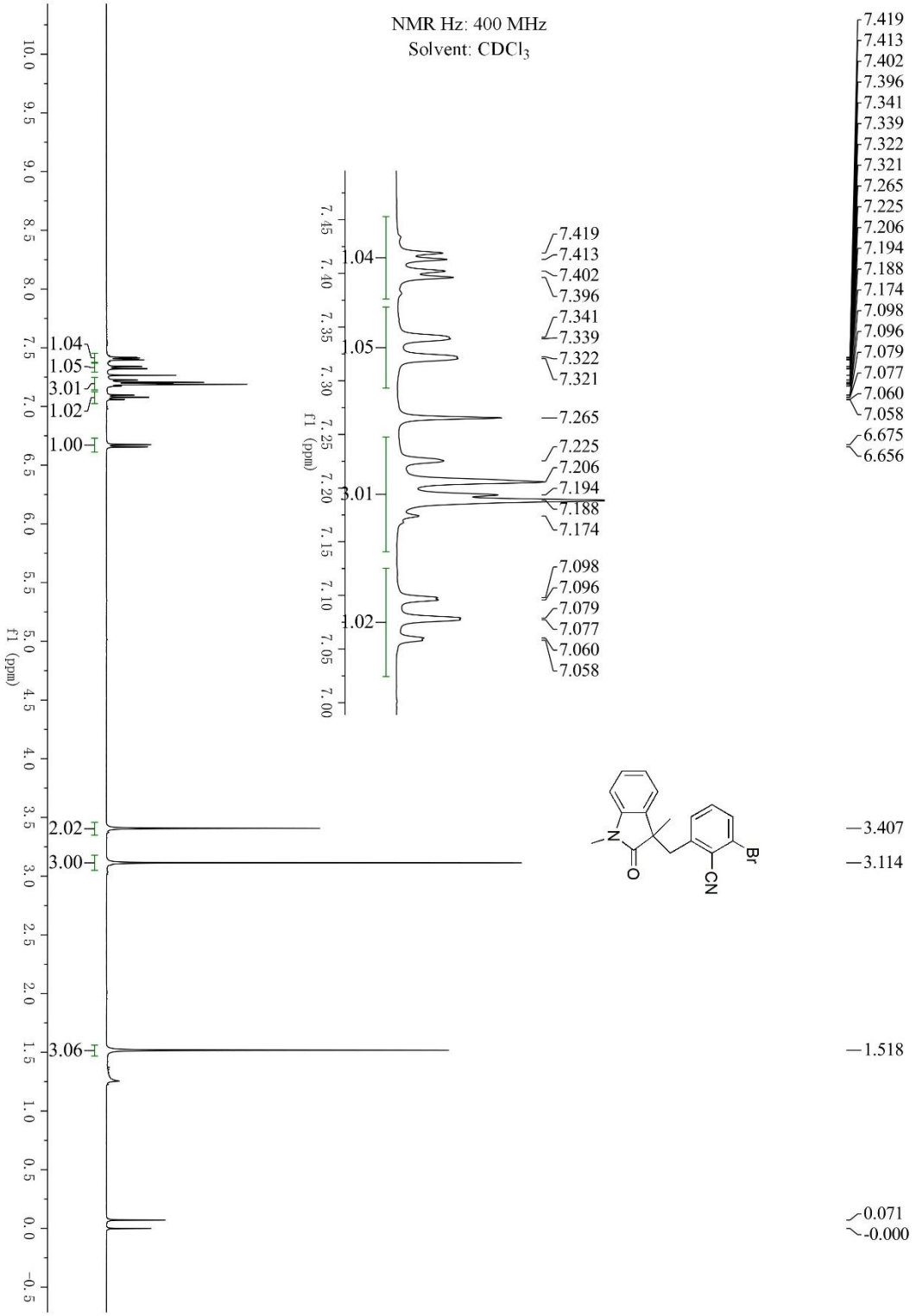
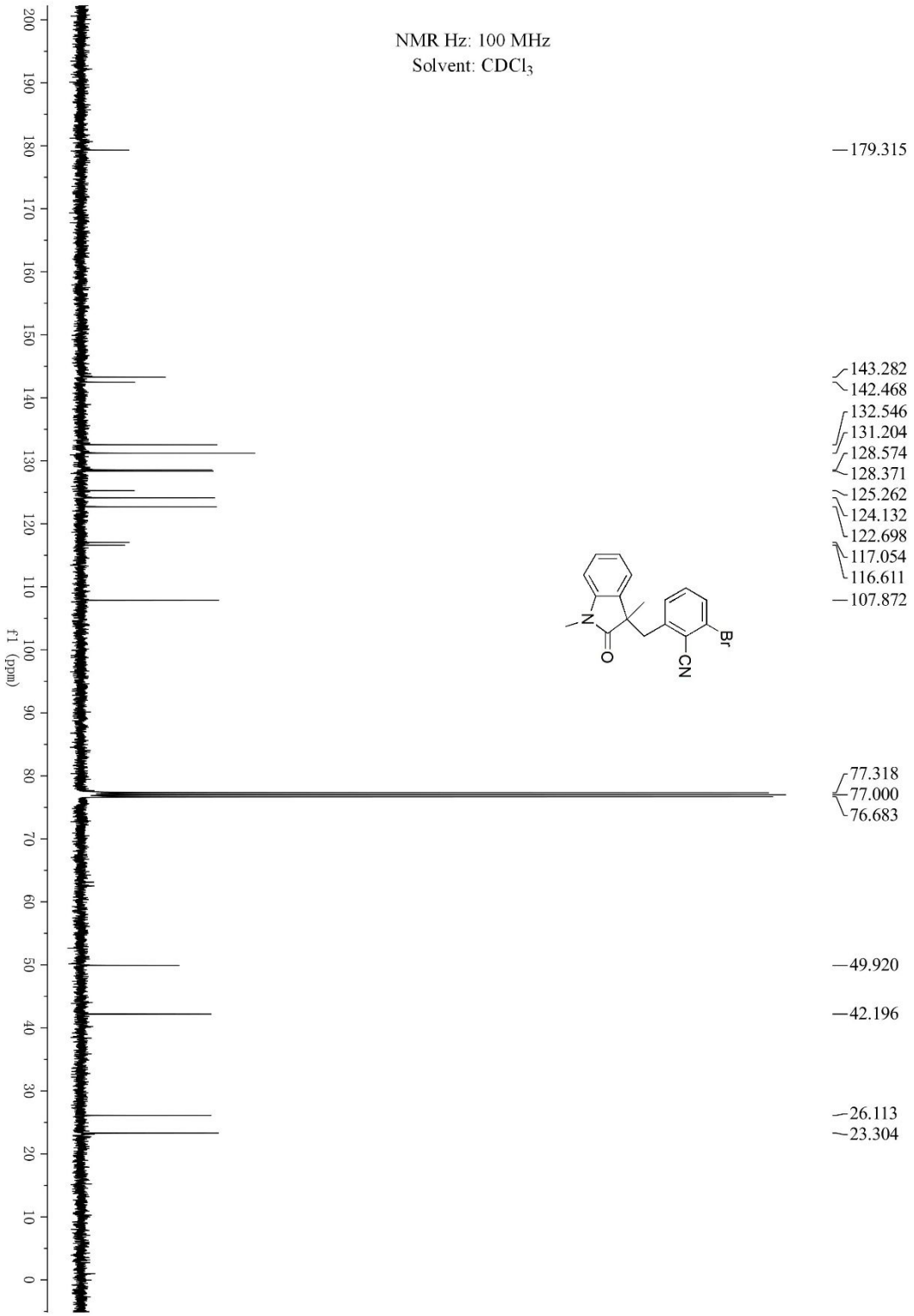
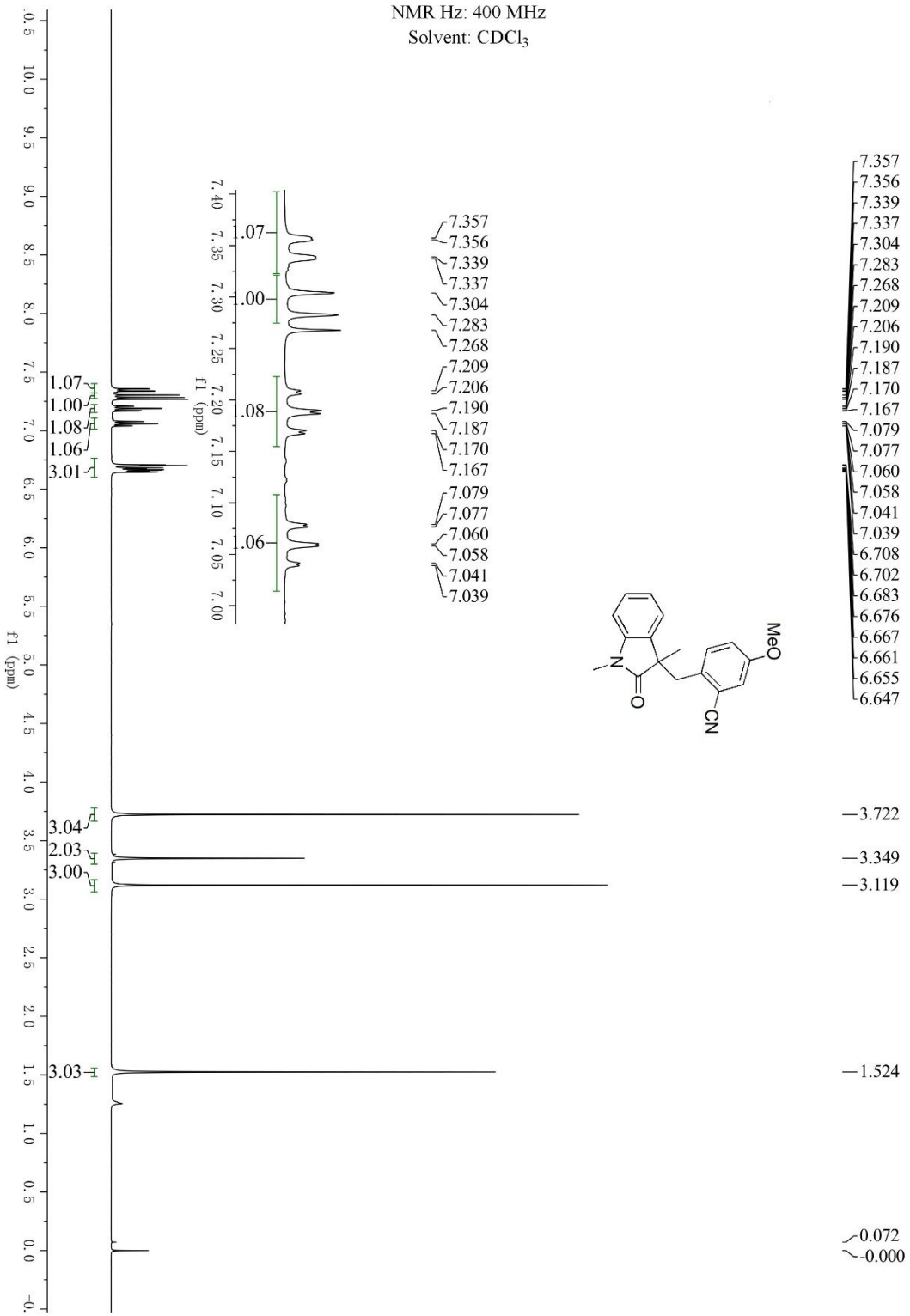
Solvent: CDCl3
f1 (ppm)
179.298
142.962
142.469
136.693
132.390
131.191
128.363
128.068
127.986
124.099
122.697
115.389
114.715
107.860
77.318
77.000
76.682
49.885
41.965
26.100
23.330
N
O
Cl
CN

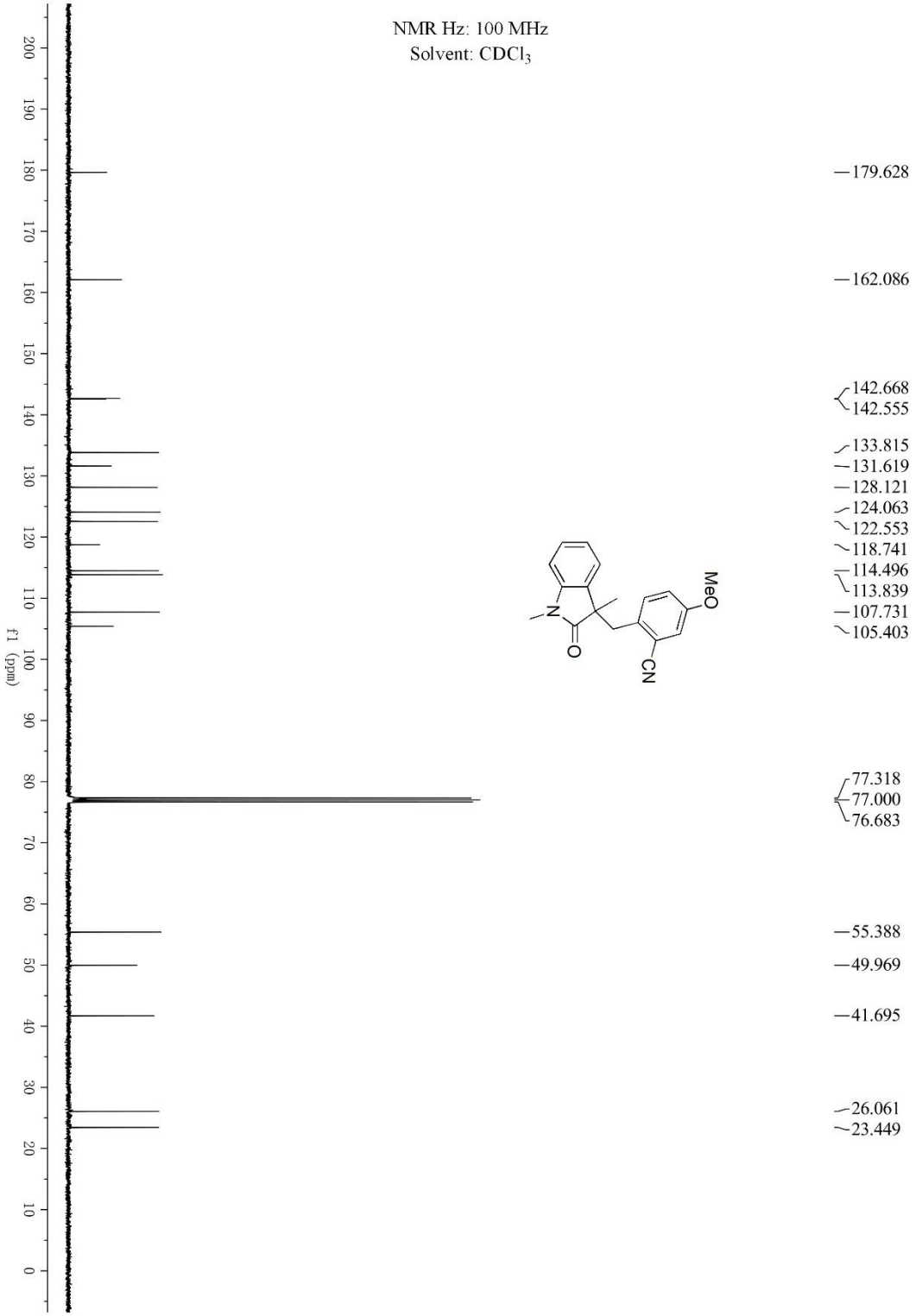
2-Bromo-6-((1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ae)




NMR Hz: 100 MHz
Solvent: CDCl3
179.315
143.282
142.468
132.546
131.204
128.574
128.371
125.262
124.132
122.698
117.054
116.611
107.872
77.318
77.000
76.683
49.920
42.196
26.113
23.304
f1 (ppm)
Br
CN
N
O

2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-5-methoxybenzonitrile (3af)




NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
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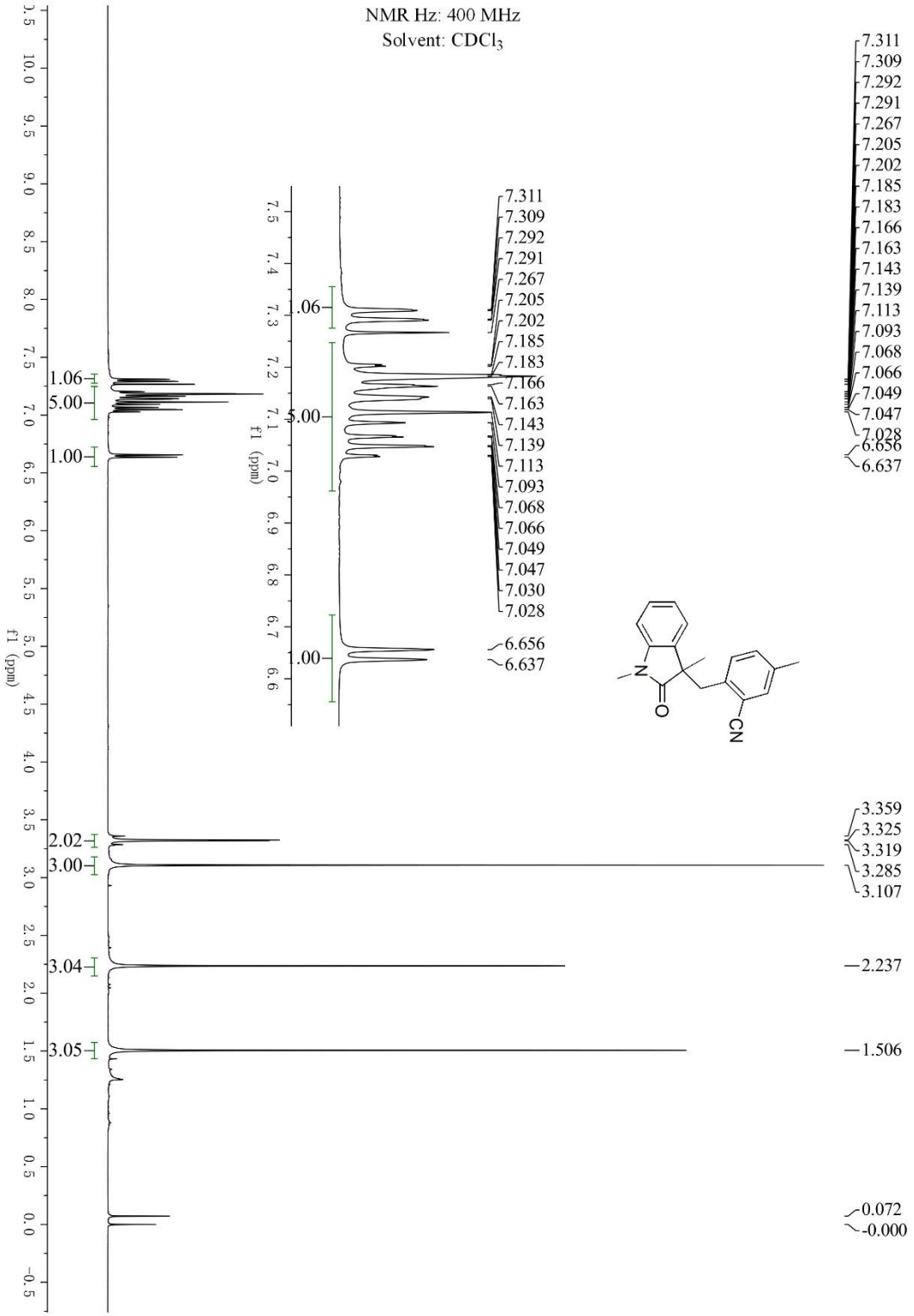
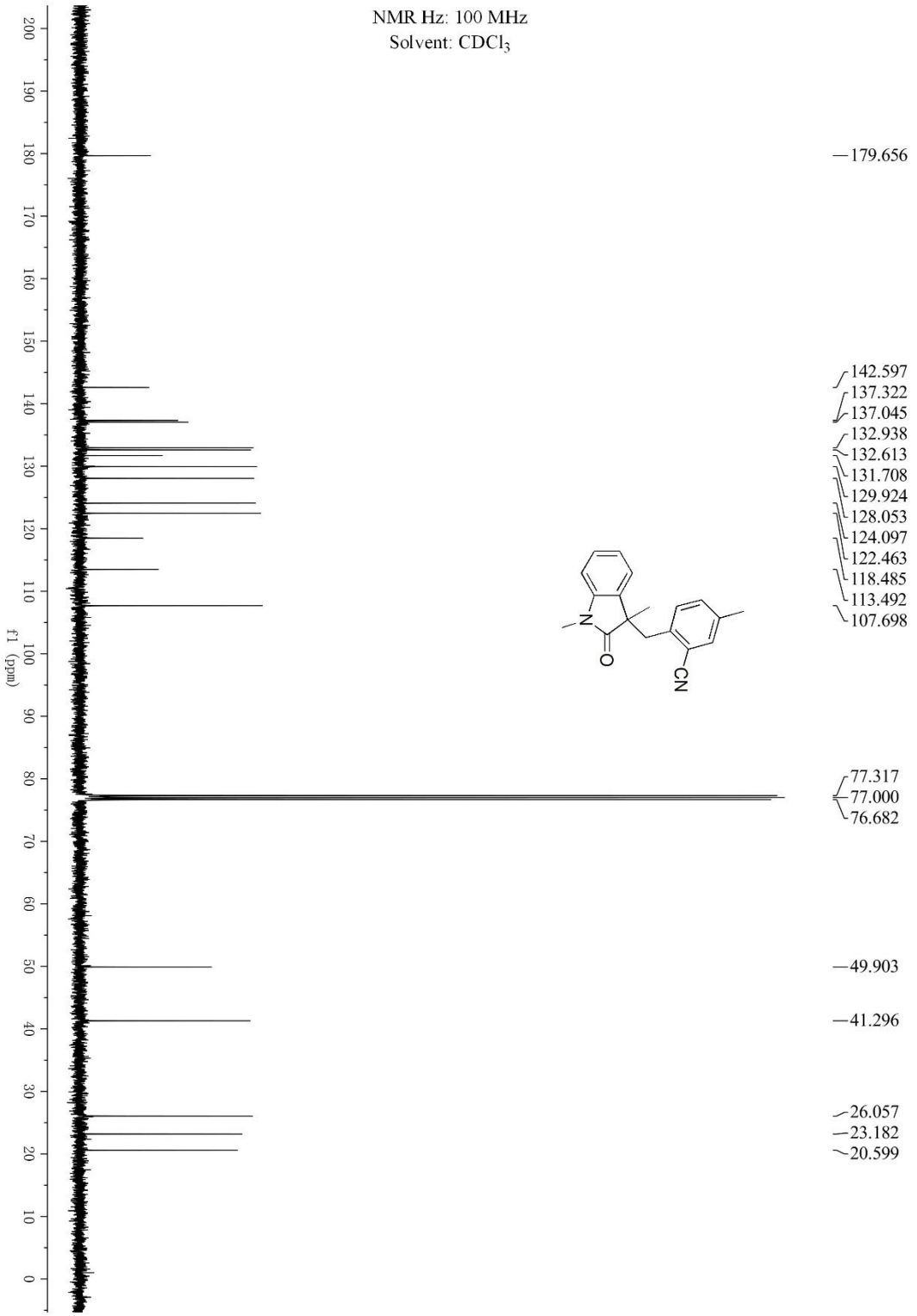
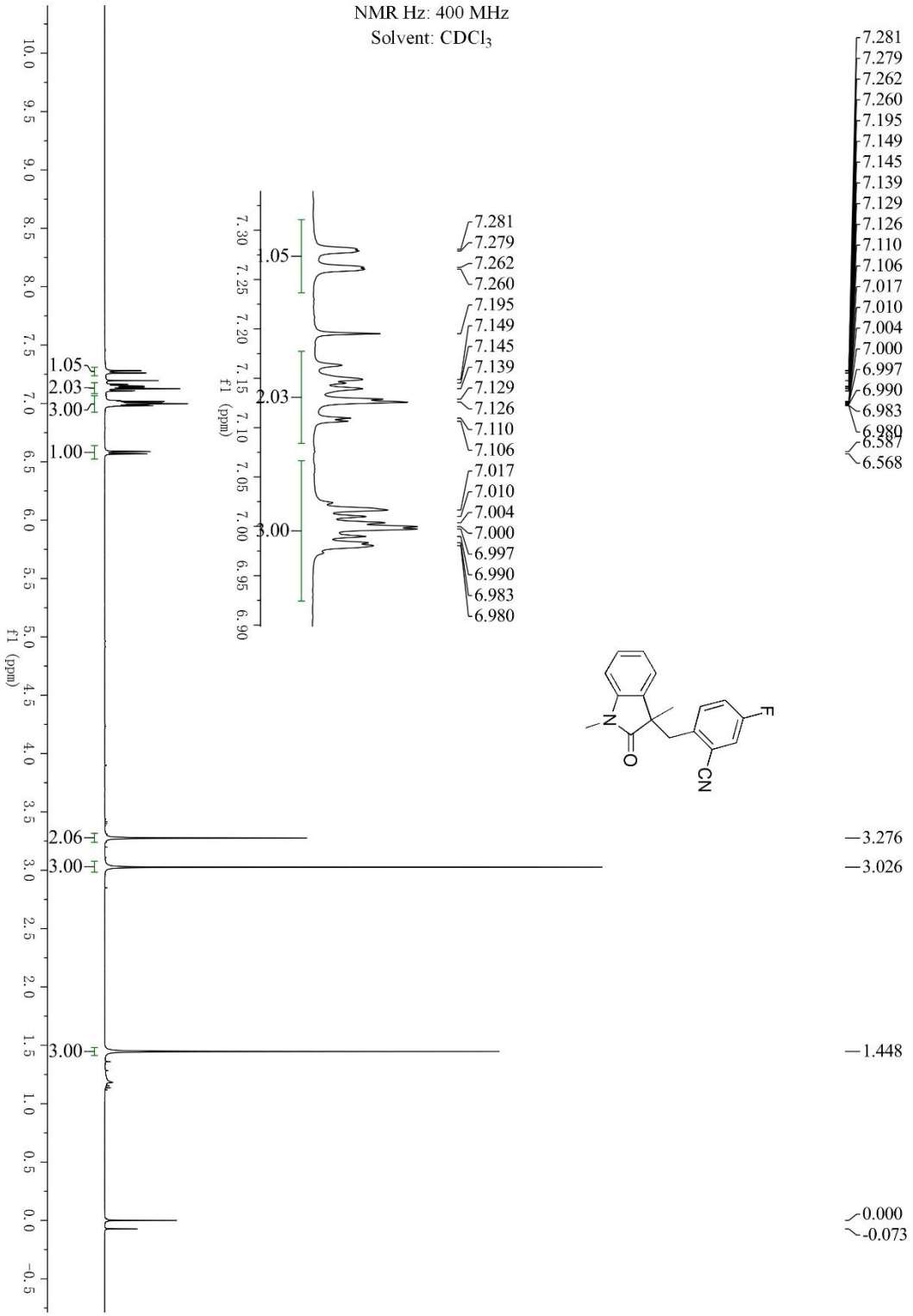
142.668
142.555
133.815
131.619
128.121
124.063
122.553
118.741
114.496
113.839
107.731
105.403
77.318
77.000
76.683
55.388
49.969
41.695
26.061
23.449
MeO
CN
N
O

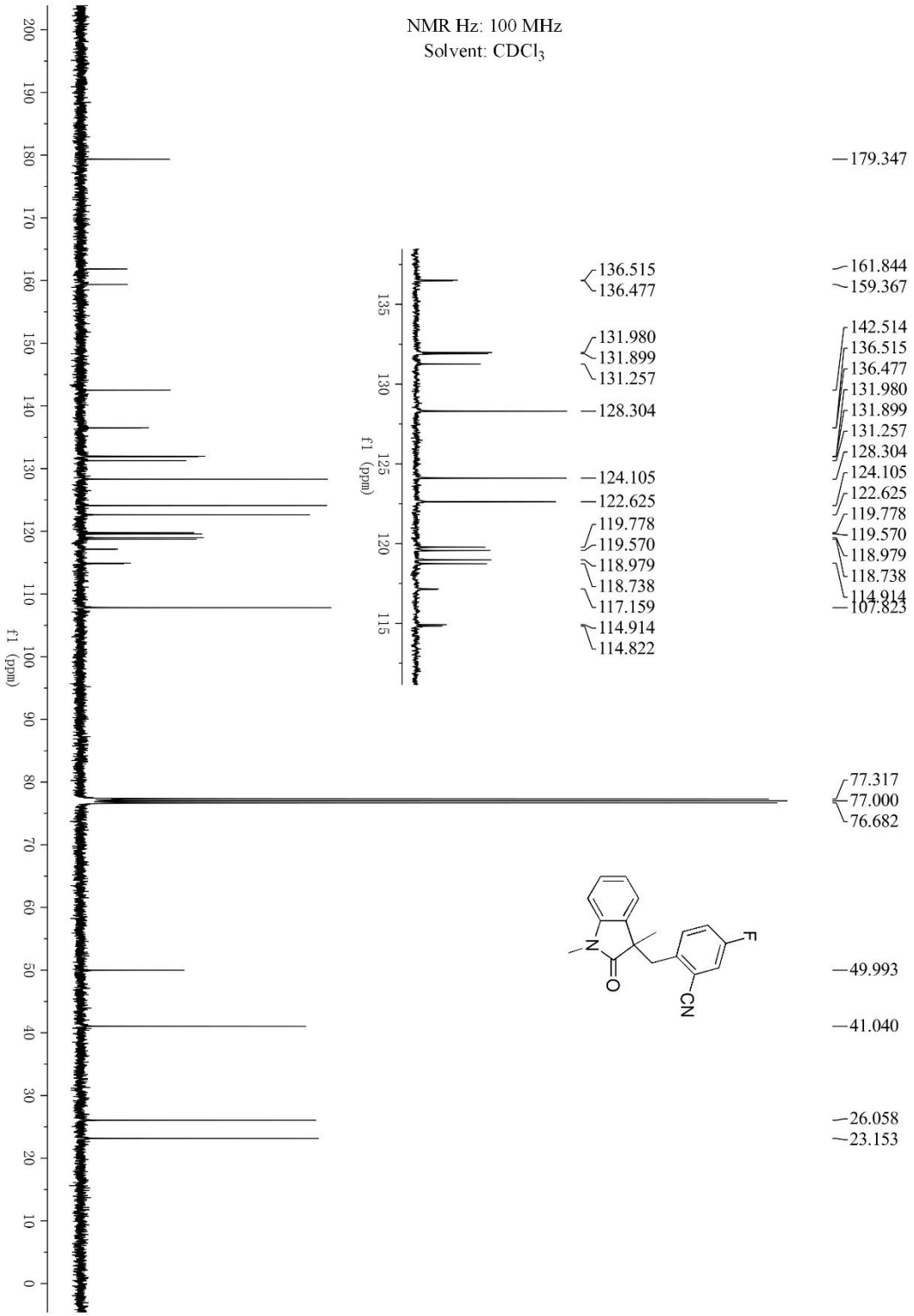
2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-5-methylbenzonitrile (3ag)

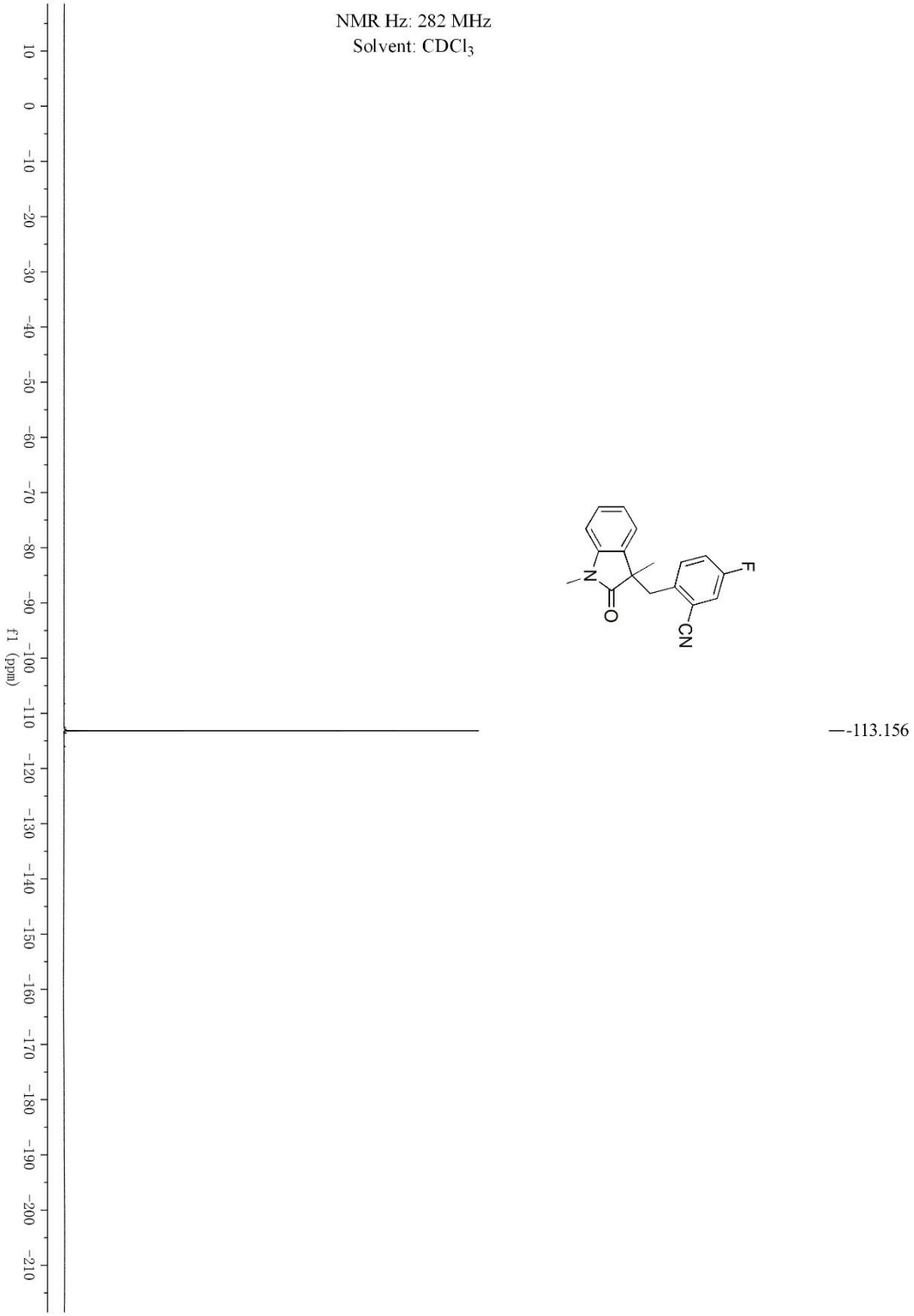



NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.656
142.597
137.322
137.045
132.938
132.613
131.708
129.924
128.053
124.097
122.463
118.485
113.492
107.698
77.317
77.000
76.682
49.903
41.296
26.057
23.182
20.599
N
O
CN

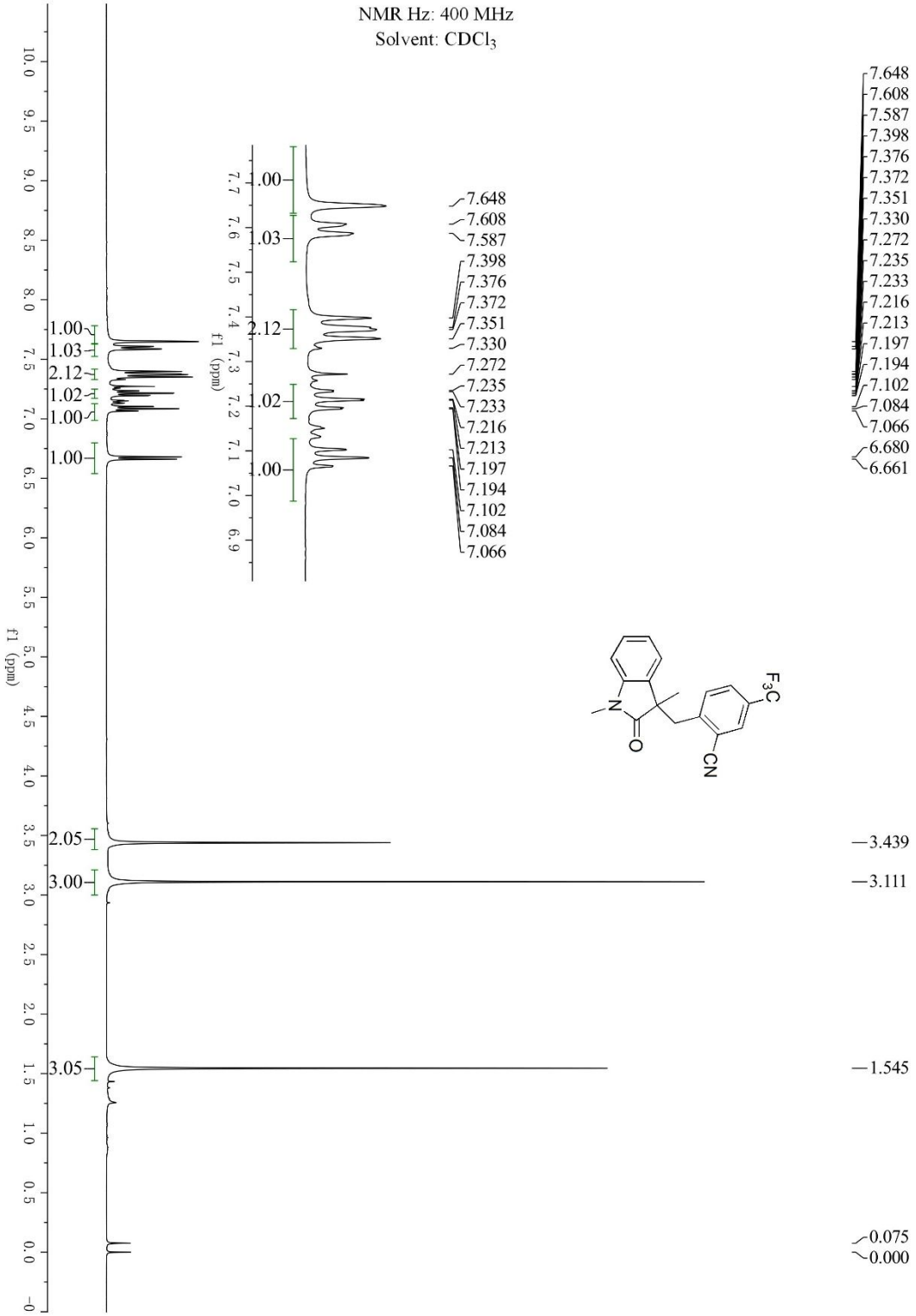
2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-5-fluorobenzonitrile (3ah)

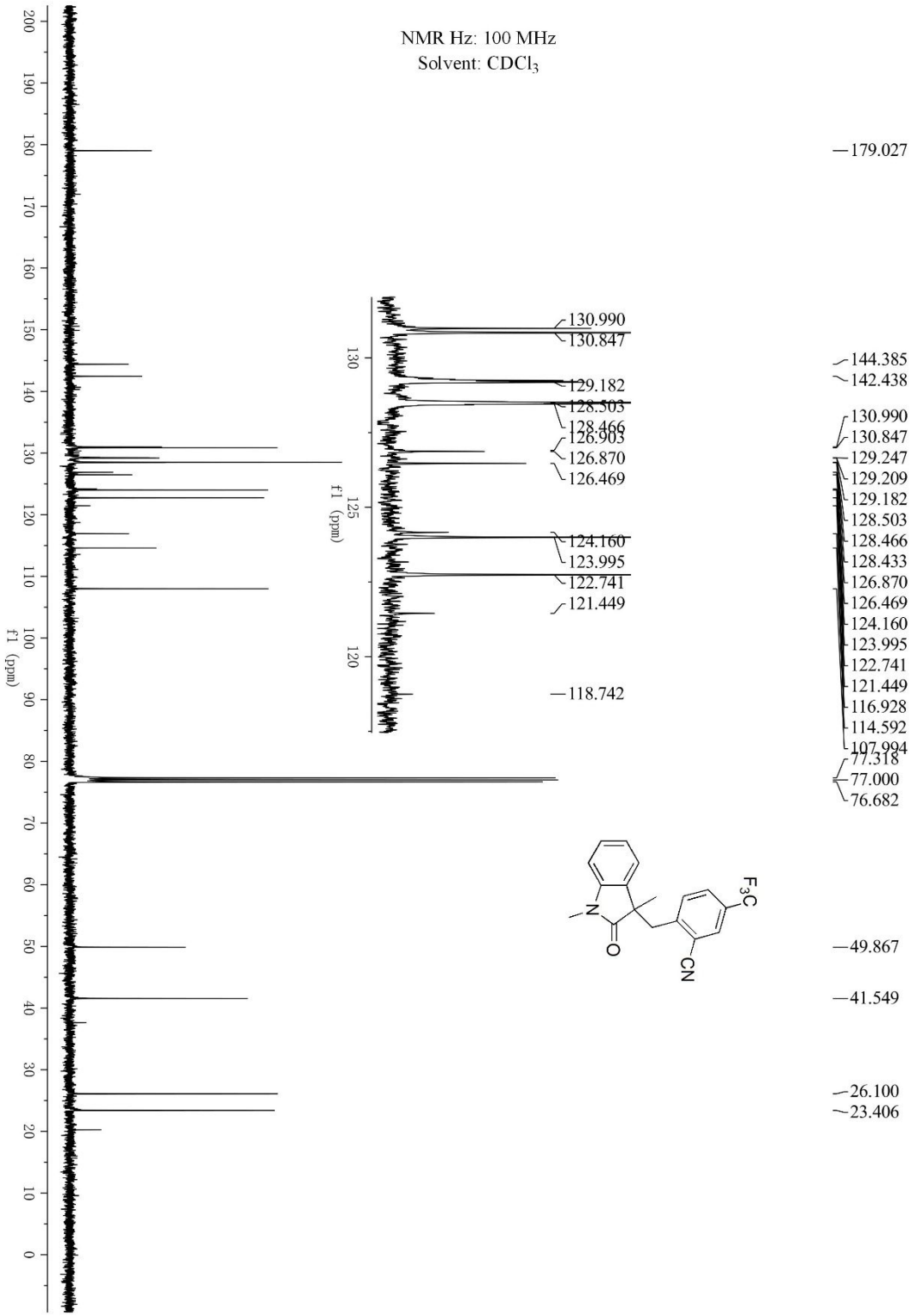


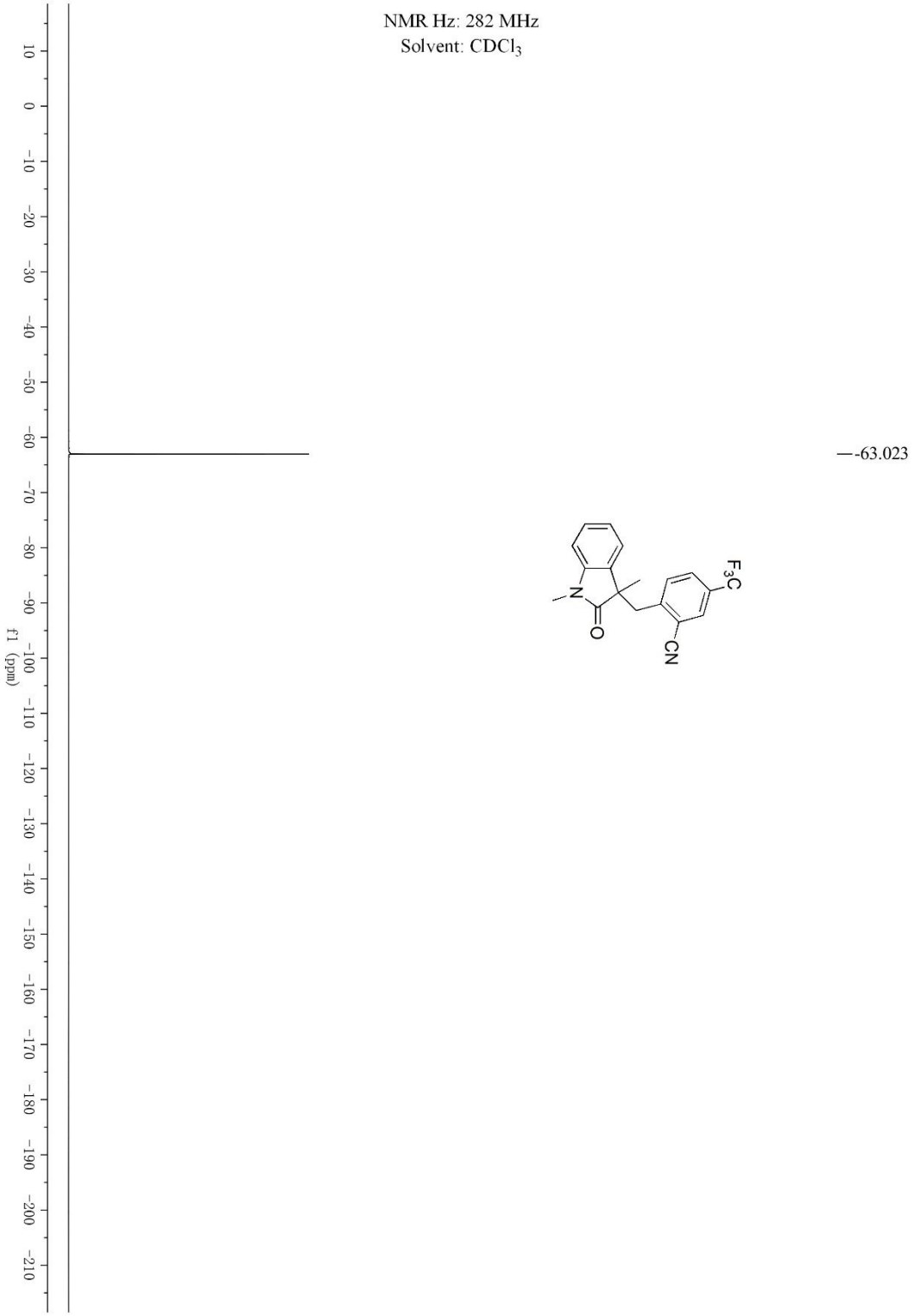

NMR Hz: 100 MHz
Solvent: $CDCl_3$
179.347
161.844
159.367
142.514
136.515
136.477
131.980
131.899
131.257
128.304
124.105
122.625
119.778
119.570
118.979
118.738
114.914
107.823
77.317
77.000
76.682
49.993
41.040
26.058
23.153
136.515
136.477
131.980
131.899
131.257
128.304
124.105
122.625
119.778
119.570
118.979
118.738
117.159
114.914
114.822
f1 (ppm)
N
O
F
CN


NMR Hz: 282 MHz
Solvent: CDCl3
-113.156
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
N
O
CN
F

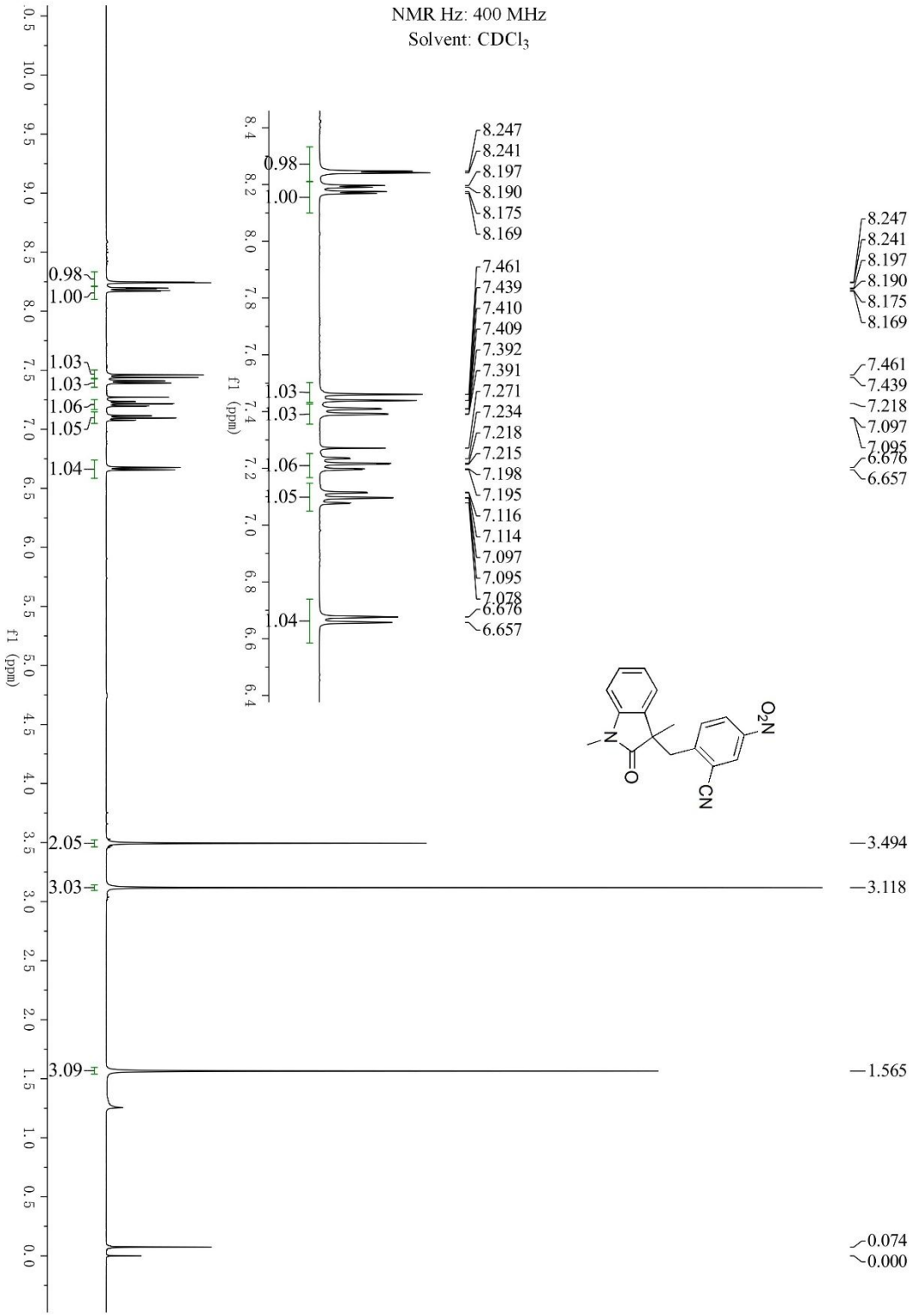
2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-5-(trifluoromethyl)benzonitrile (3ai)

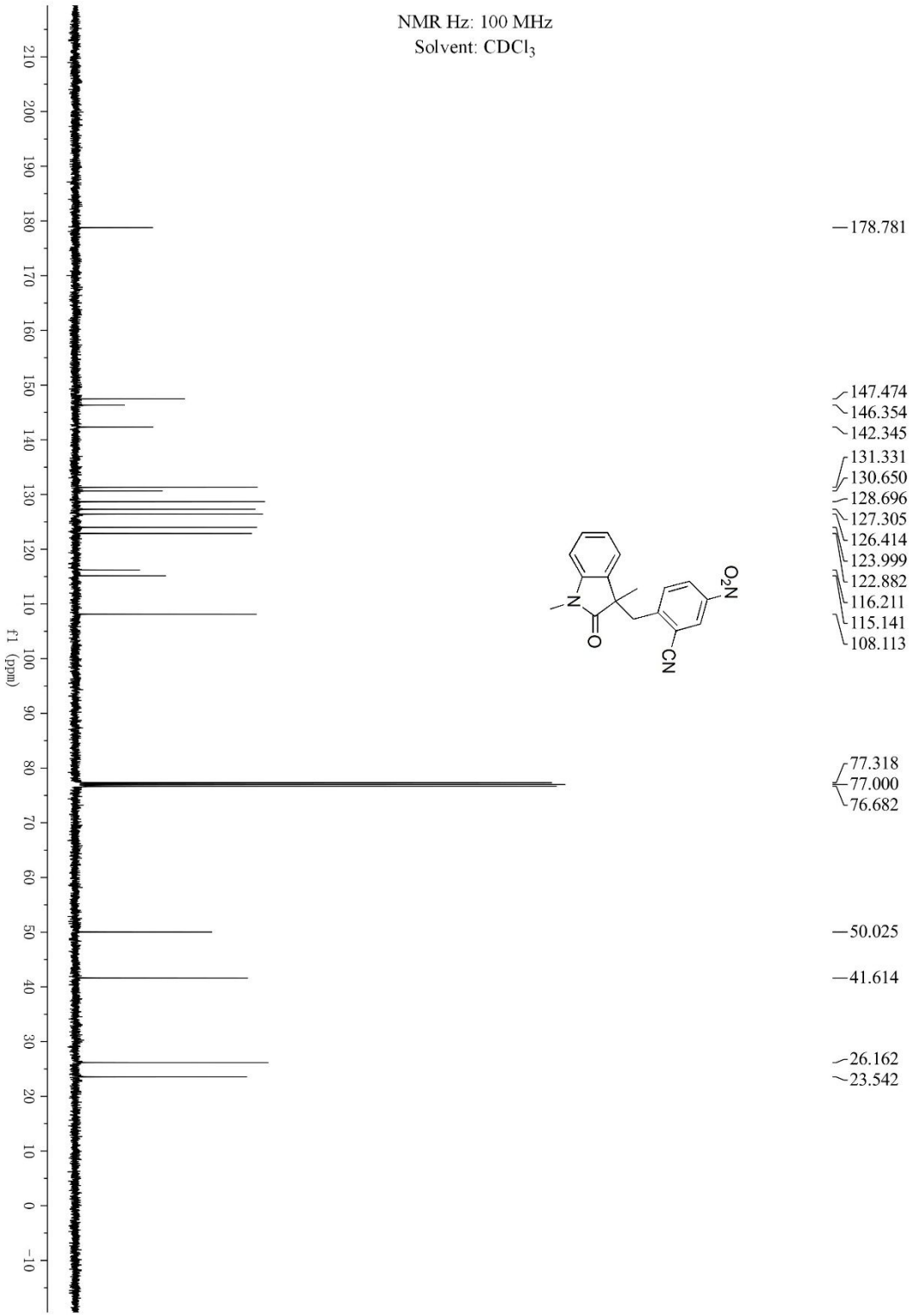



NMR Hz: 100 MHz
Solvent: CDCl3
179.027
144.385
142.438
130.990
130.847
129.247
129.209
129.182
128.503
128.466
128.433
126.870
126.469
124.160
123.995
122.741
121.449
116.928
114.592
107.994
77.318
77.000
76.682
49.867
41.549
26.100
23.406
130.990
130.847
129.182
128.503
128.466
126.903
126.870
126.469
124.160
123.995
122.741
121.449
118.742
f1 (ppm)
F3C
CN
N
O

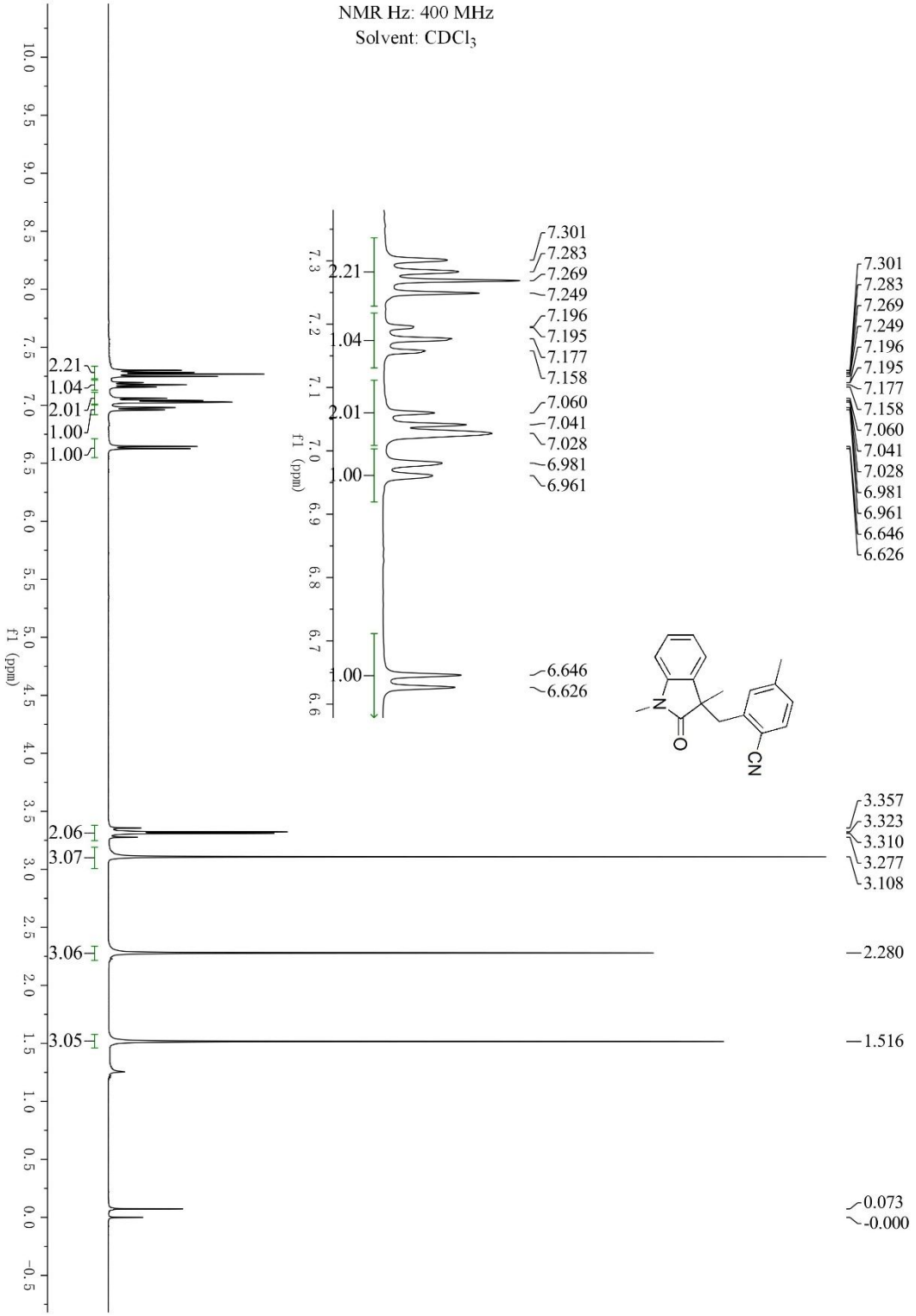

NMR Hz: 282 MHz
Solvent: CDCl3
-63.023
F3C
CN
N
O
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210

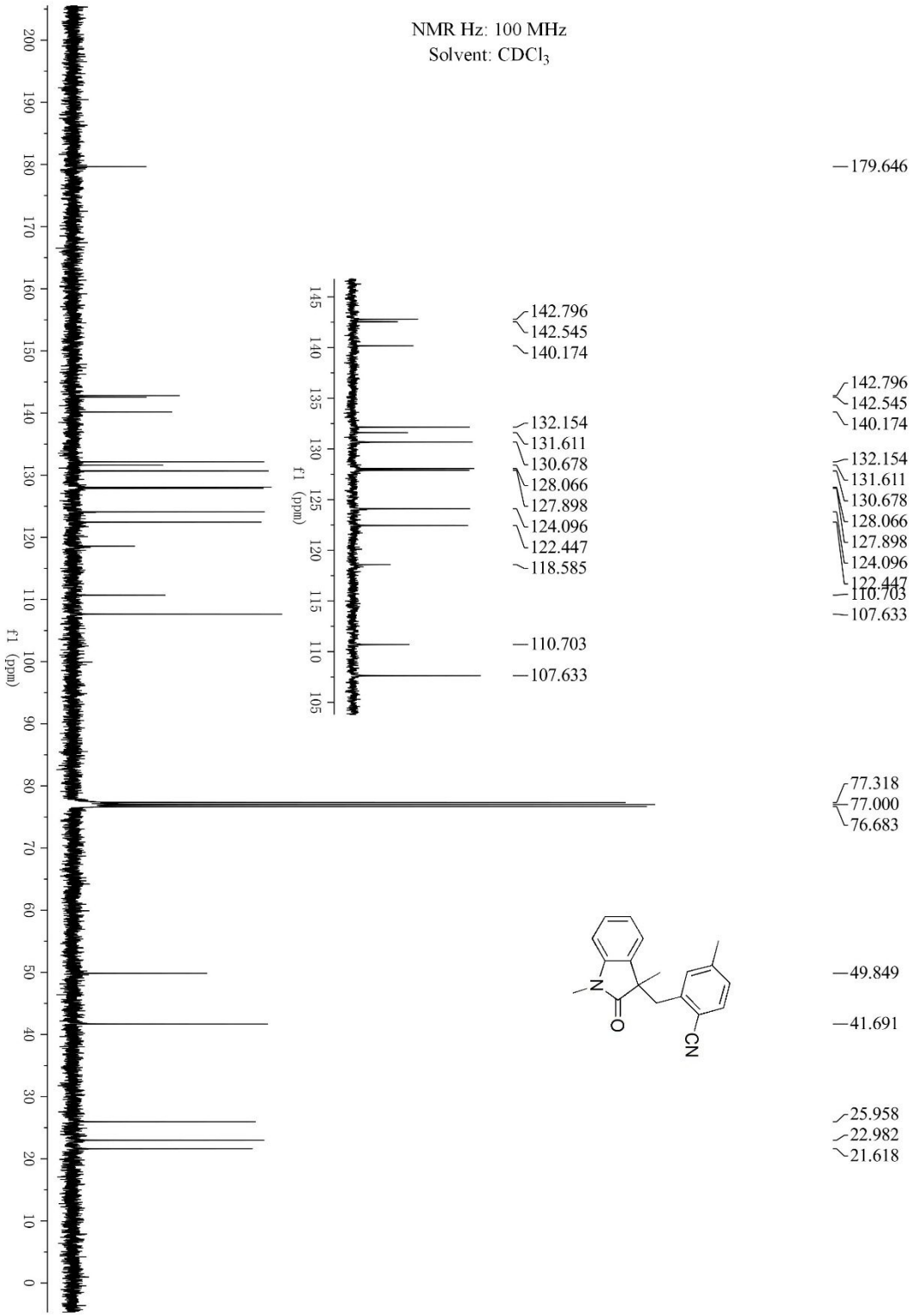
2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-5-nitrobenzonitrile (3aj)



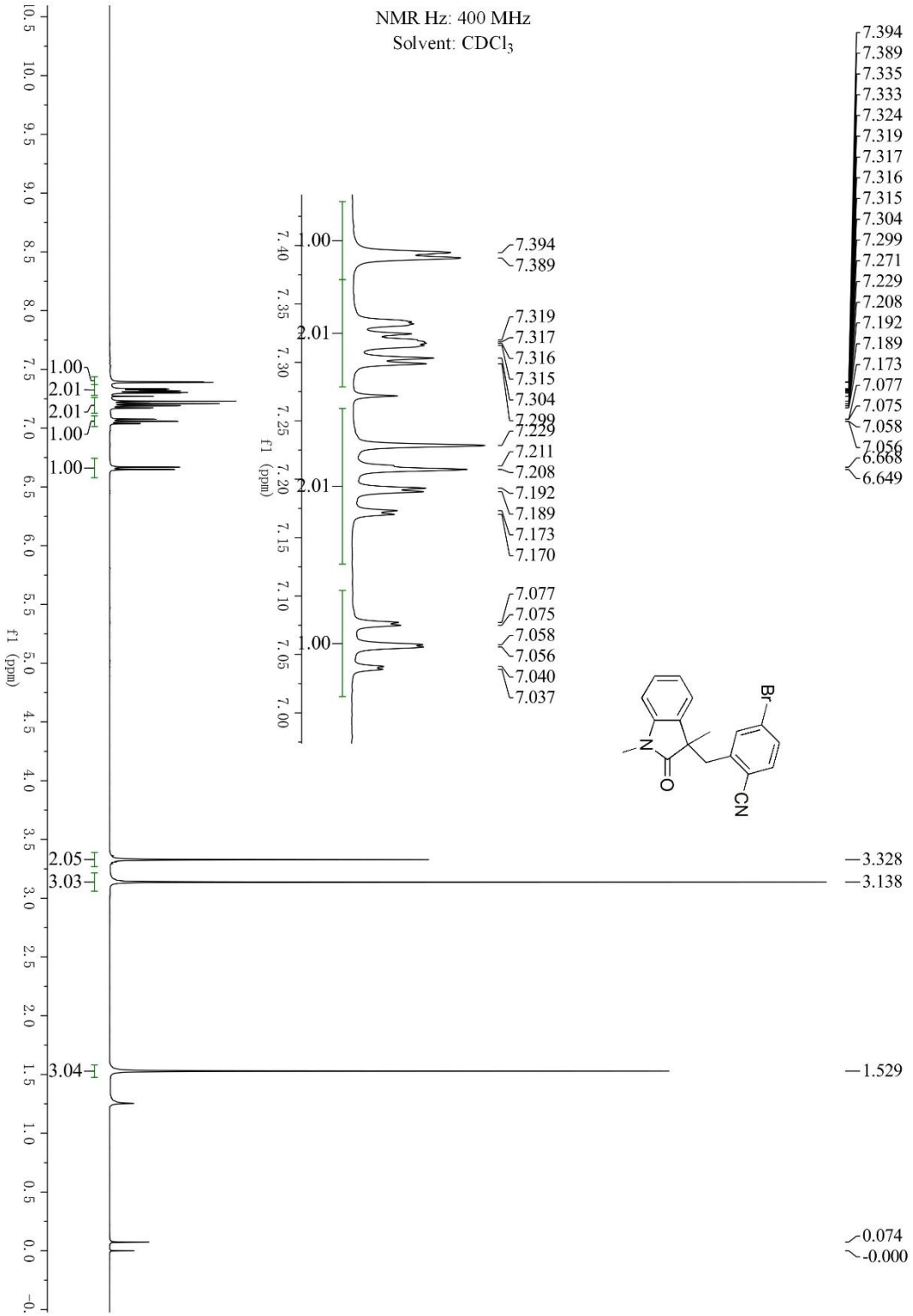

NMR Hz: 100 MHz
Solvent: CDCl3
178.781
147.474
146.354
142.345
131.331
130.650
128.696
127.305
126.414
123.999
122.882
116.211
115.141
108.113
77.318
77.000
76.682
50.025
41.614
26.162
23.542
f1 (ppm)

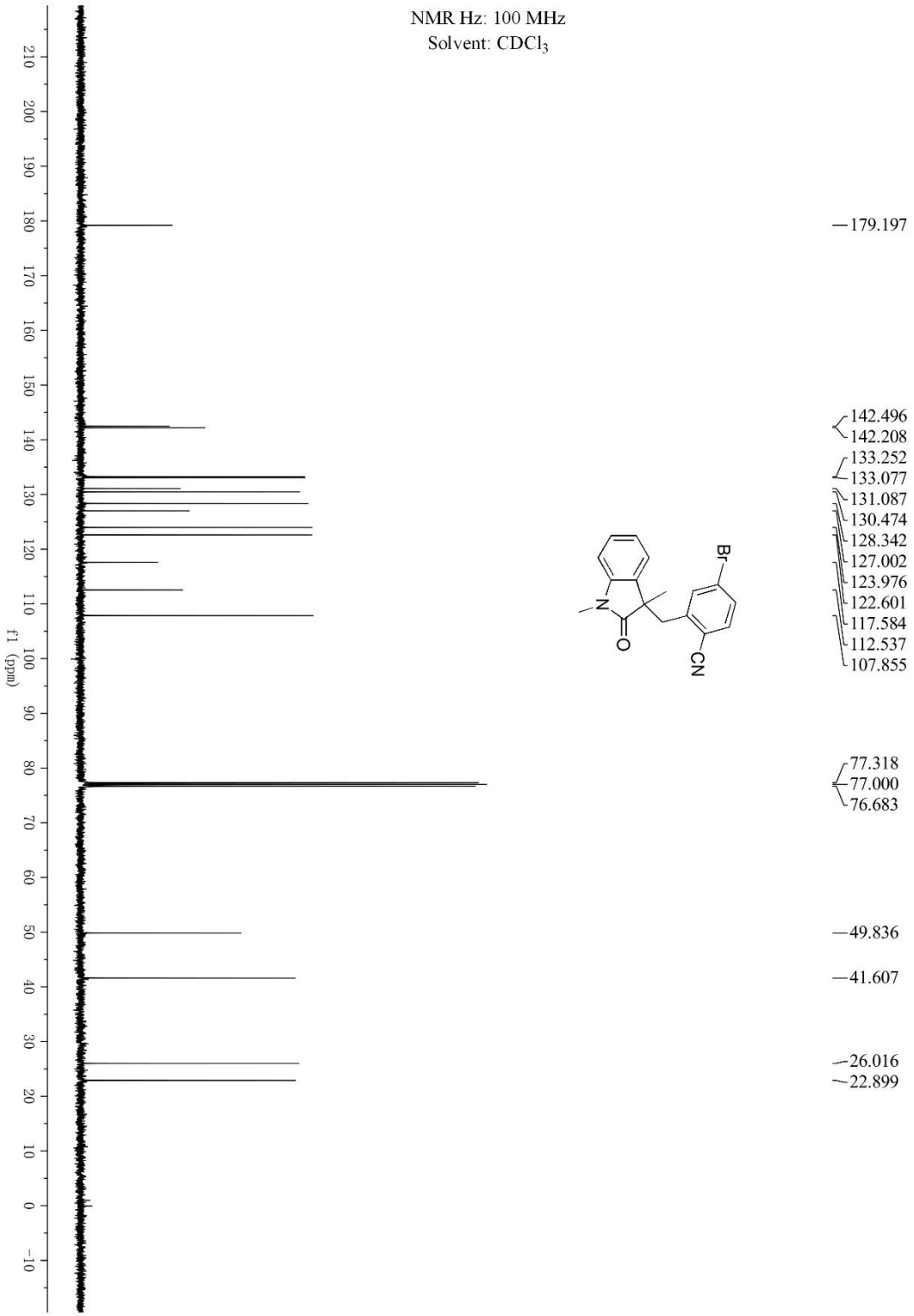
2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)-4-methylbenzonitrile (3ak)



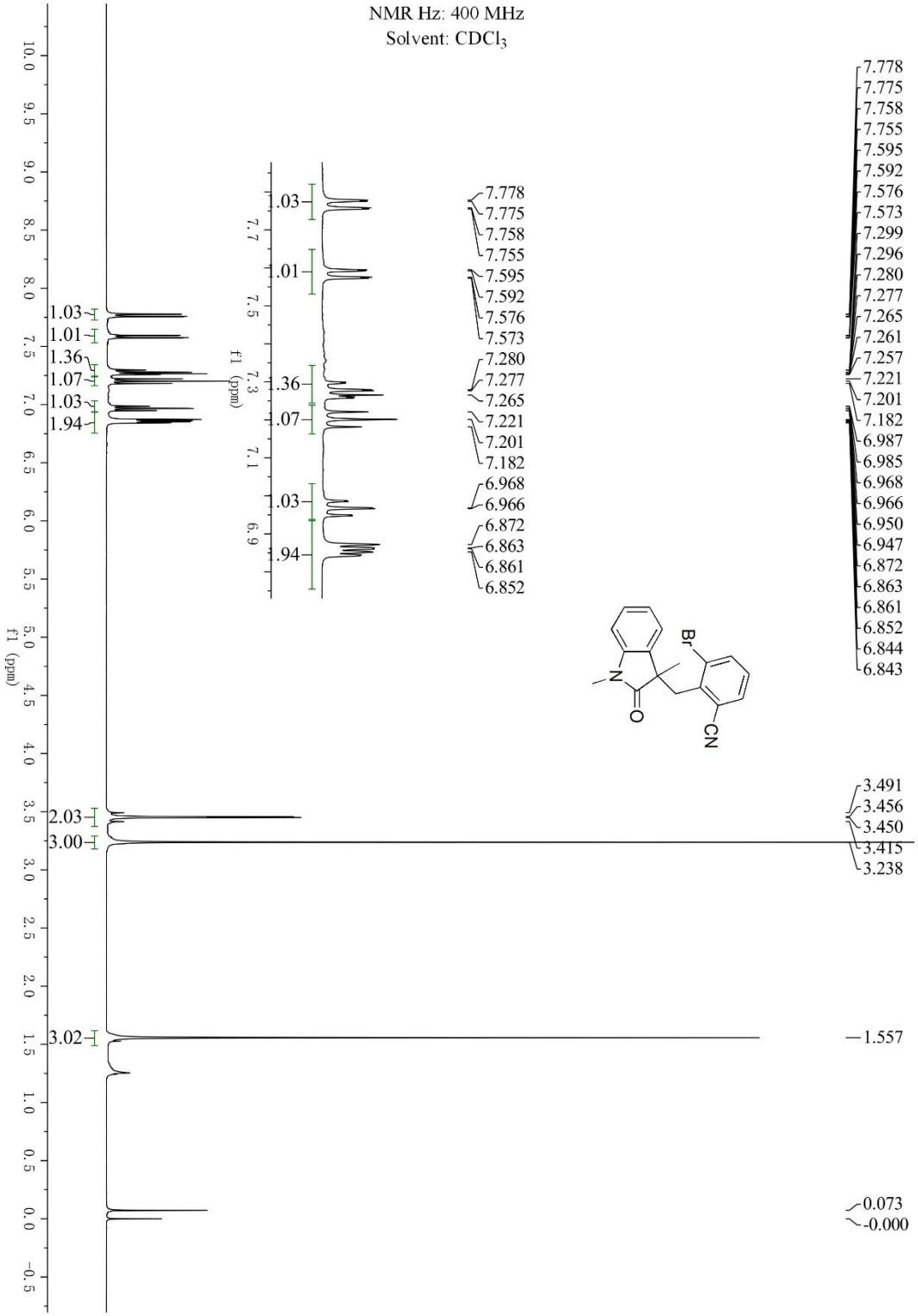

NMR Hz: 100 MHz
Solvent: CDCl3
179.646
142.796
142.545
140.174
132.154
131.611
130.678
128.066
127.898
124.096
122.447
118.585
110.703
107.633
77.318
77.000
76.683
49.849
41.691
25.958
22.982
21.618
f1 (ppm)
N
O
CN

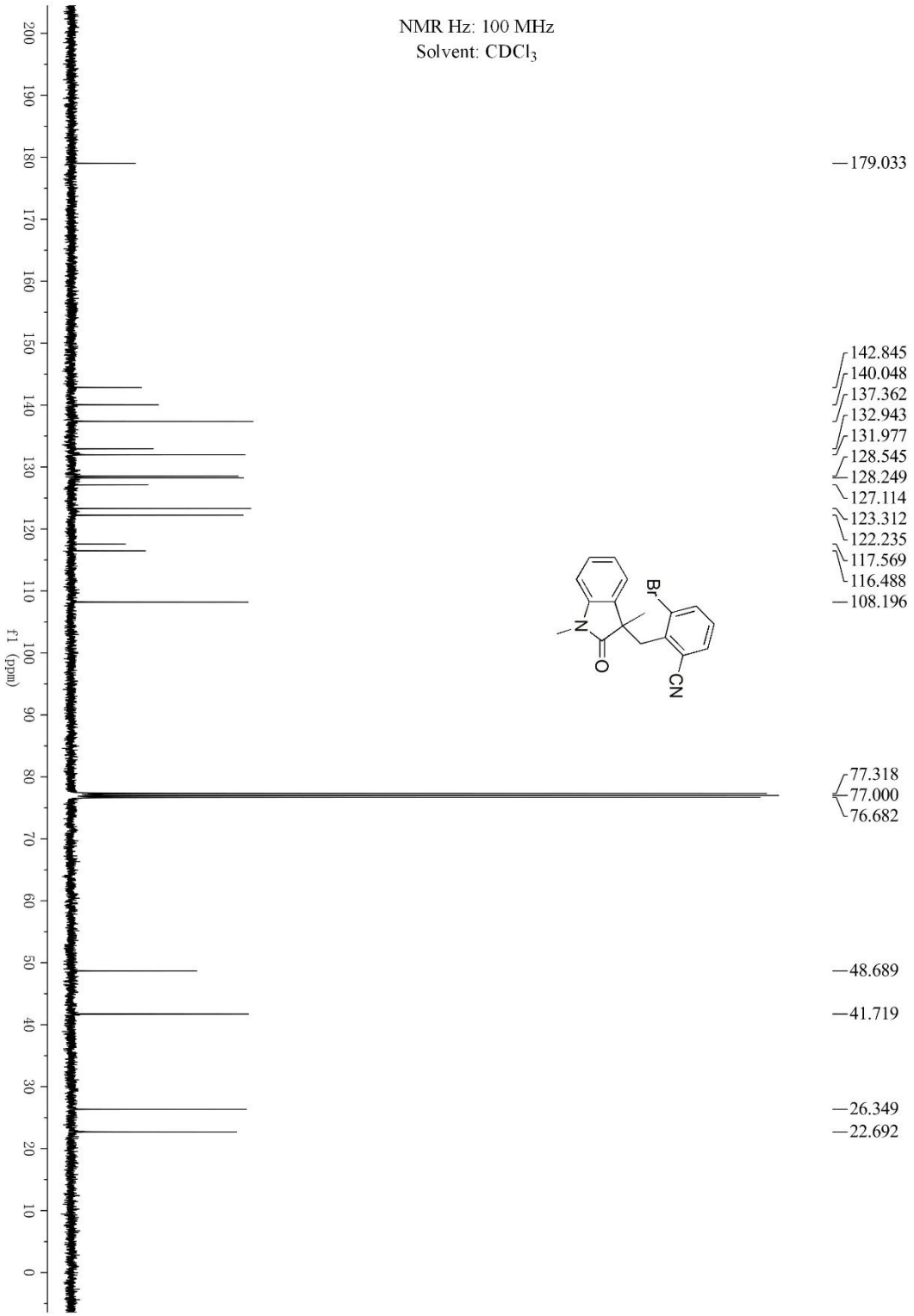
4-Bromo-2-((1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3al)



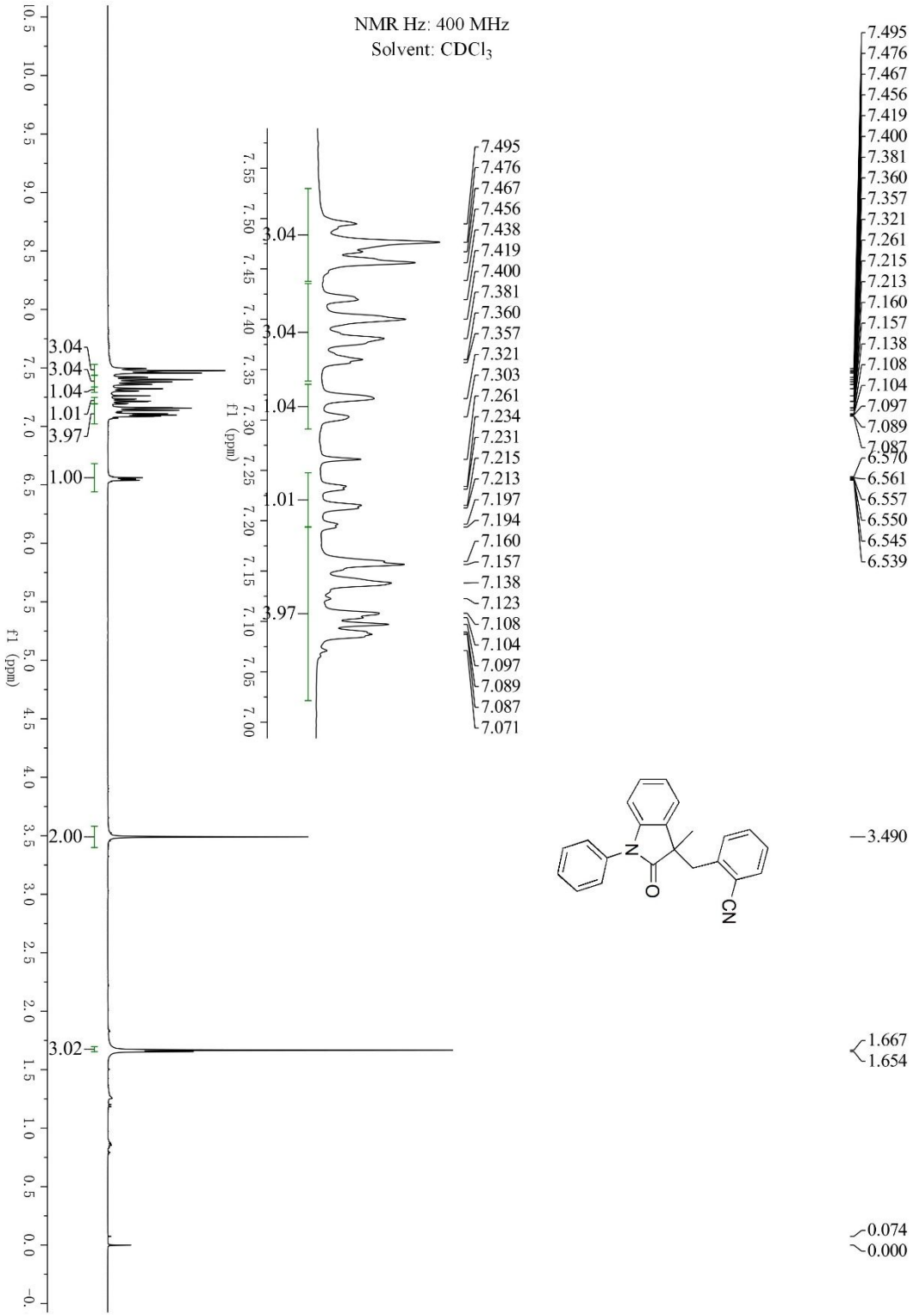

NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.197
142.496
142.208
133.252
133.077
131.087
130.474
128.342
127.002
123.976
122.601
117.584
112.537
107.855
77.318
77.000
76.683
49.836
41.607
26.016
22.899
Br
CN
N
O

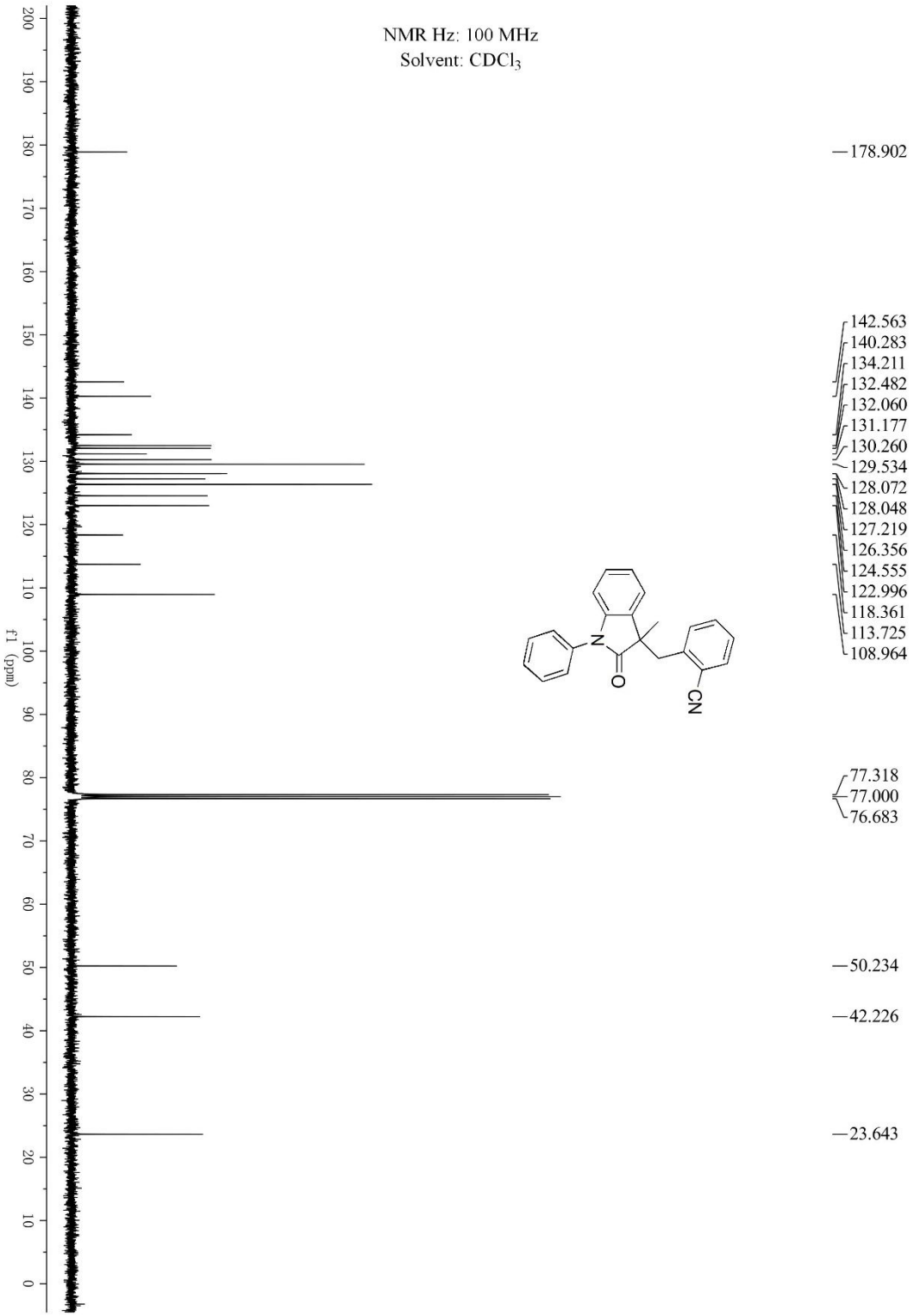
3-Bromo-2-((1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3am)



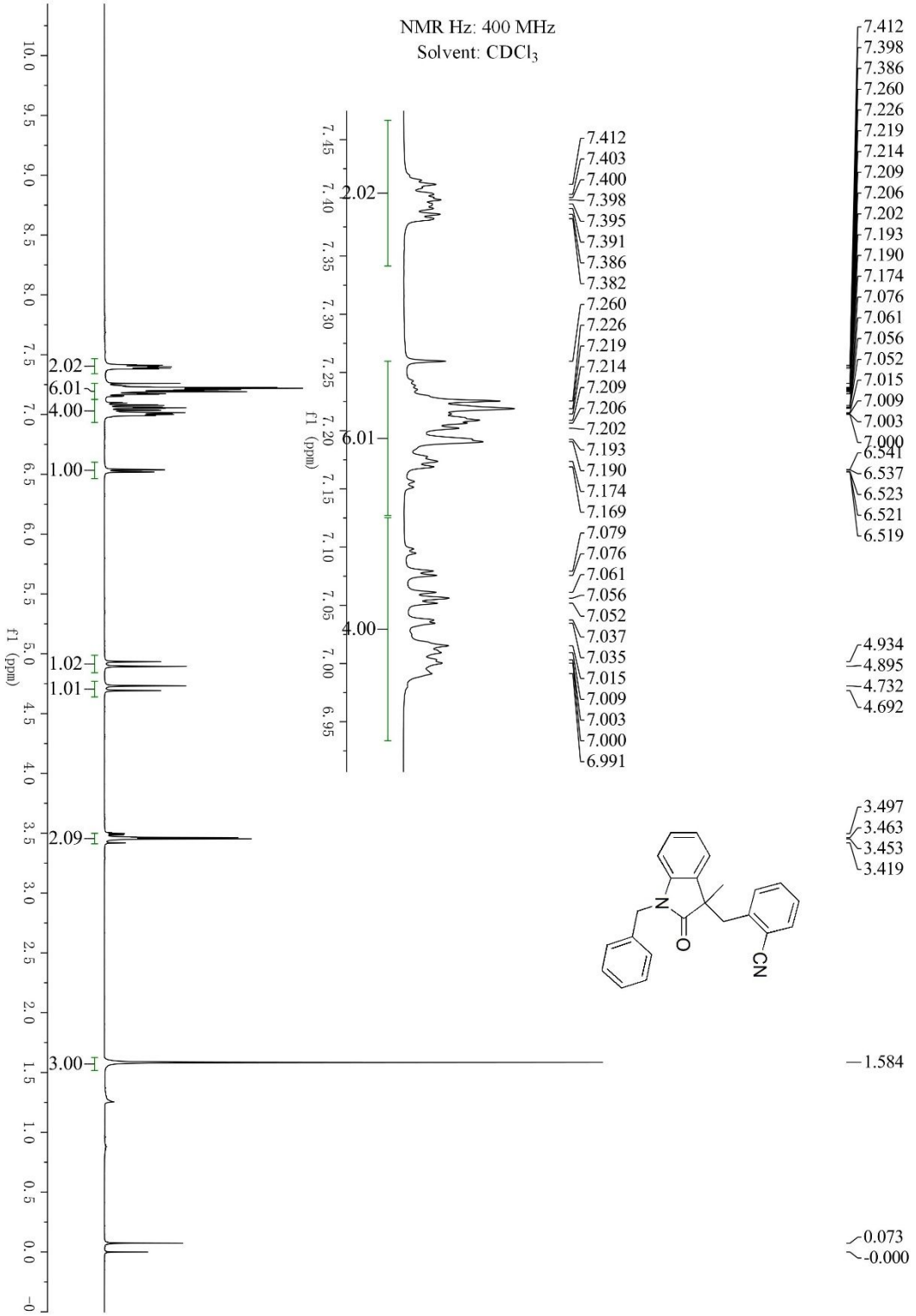

NMR Hz: 100 MHz
Solvent: CDCl3
179.033
142.845
140.048
137.362
132.943
131.977
128.545
128.249
127.114
123.312
122.235
117.569
116.488
108.196
77.318
77.000
76.682
48.689
41.719
26.349
22.692
f1 (ppm)
Br
N
O
CN

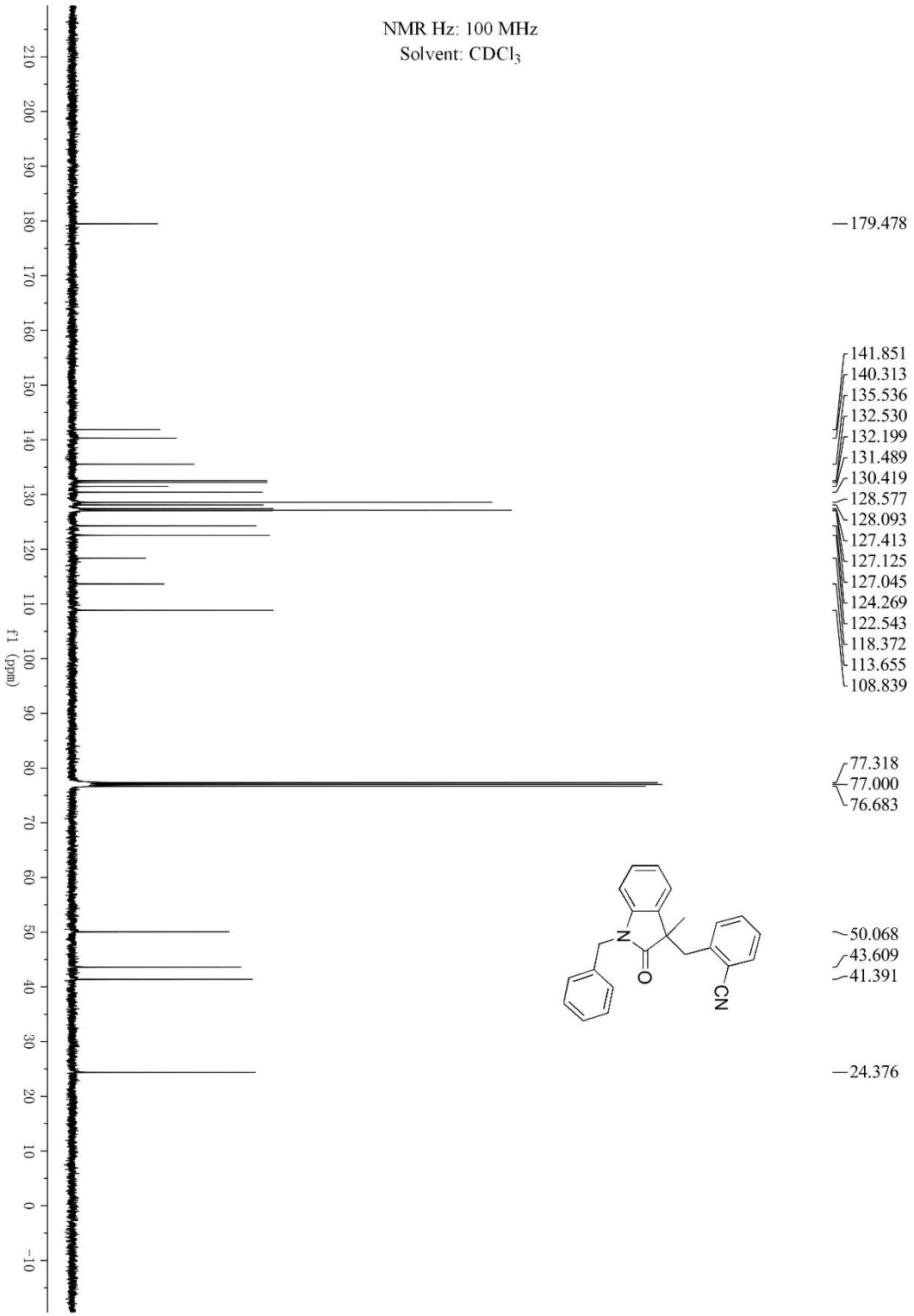
2-((3-Methyl-2-oxo-1-phenylindolin-3-yl)methyl)benzonitrile (3ba)



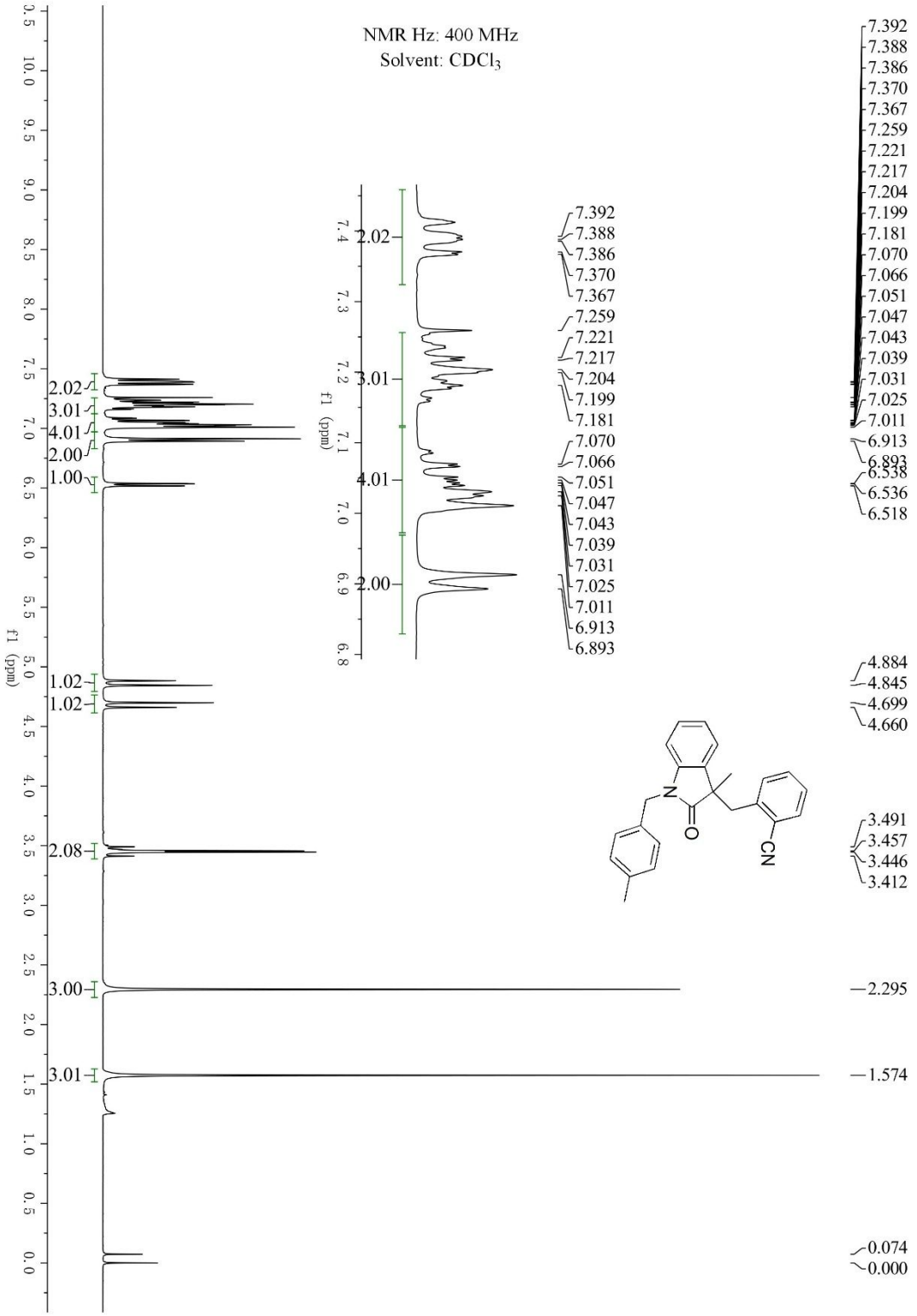

NMR Hz: 100 MHz
Solvent: $CDCl_3$
f1 (ppm)
178.902
142.563
140.283
134.211
132.482
132.060
131.177
130.260
129.534
128.072
128.048
127.219
126.356
124.555
122.996
118.361
113.725
108.964
77.318
77.000
76.683
50.234
42.226
23.643
N
O
CN

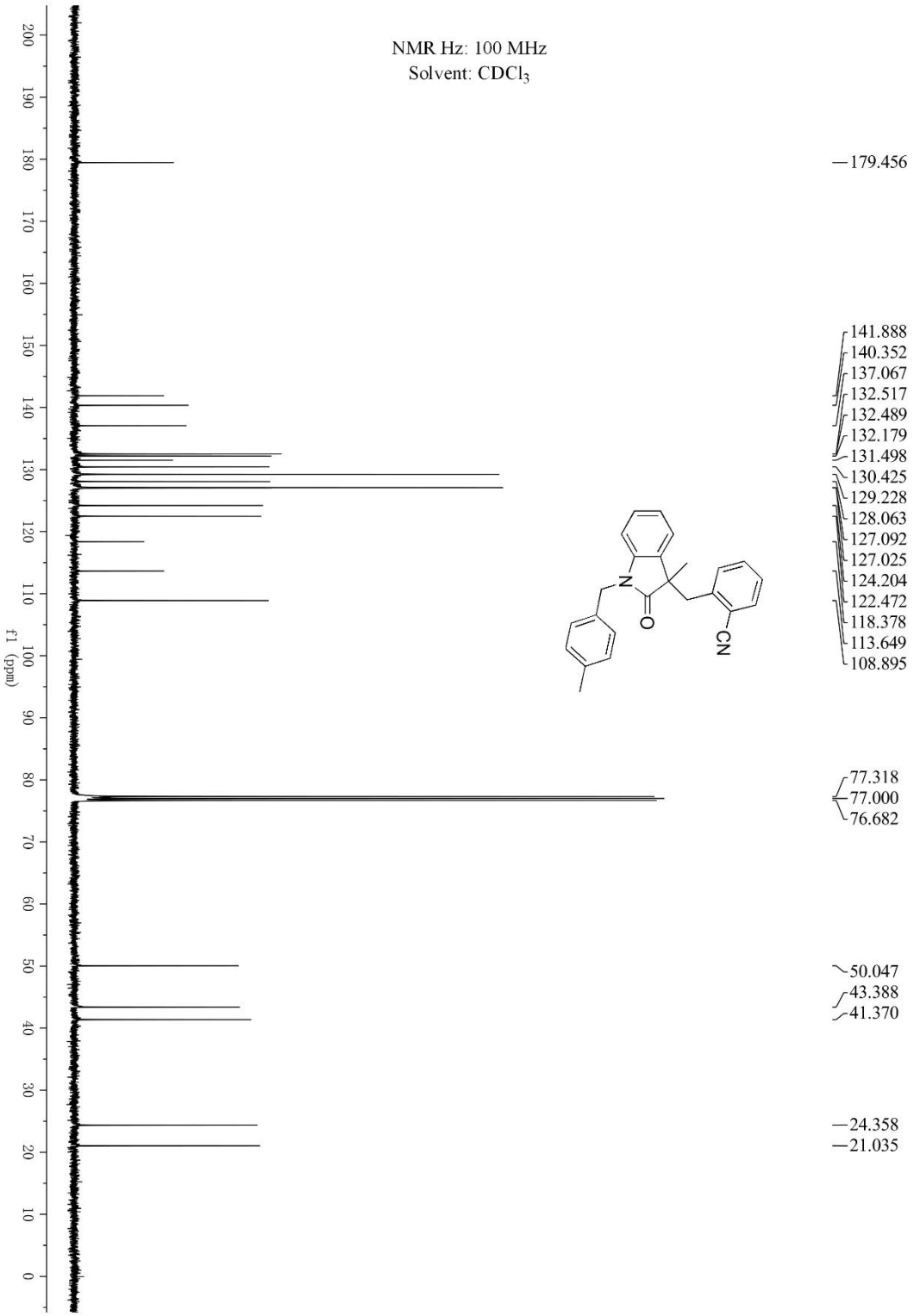
2-((1-Benzyl-3-methyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ca)



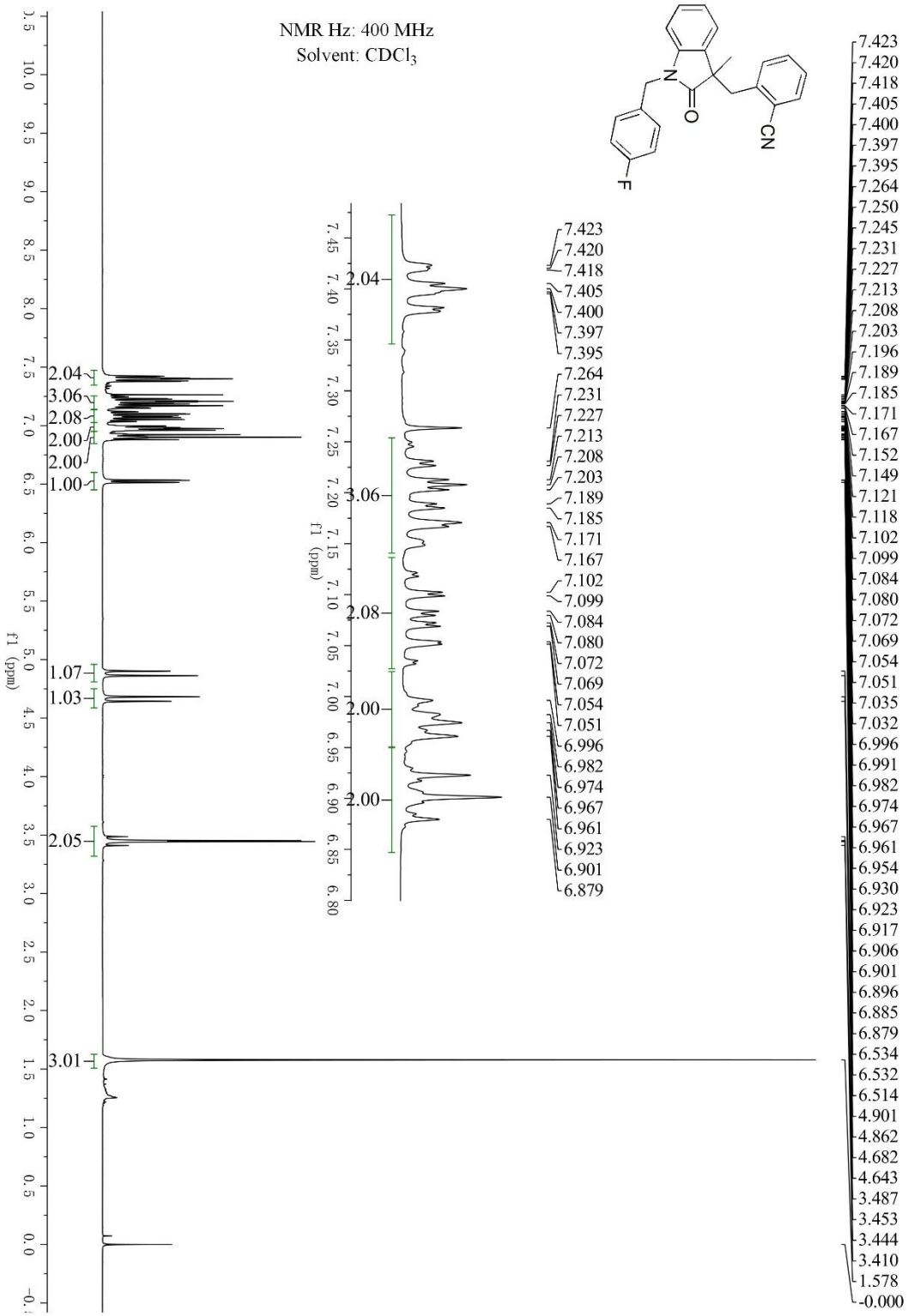

NMR Hz: 100 MHz
Solvent: $CDCl_3$
f1 (ppm)
179.478
141.851
140.313
135.536
132.530
132.199
131.489
130.419
128.577
128.093
127.413
127.125
127.045
124.269
122.543
118.372
113.655
108.839
77.318
77.000
76.683
50.068
43.609
41.391
24.376
N
O
CN

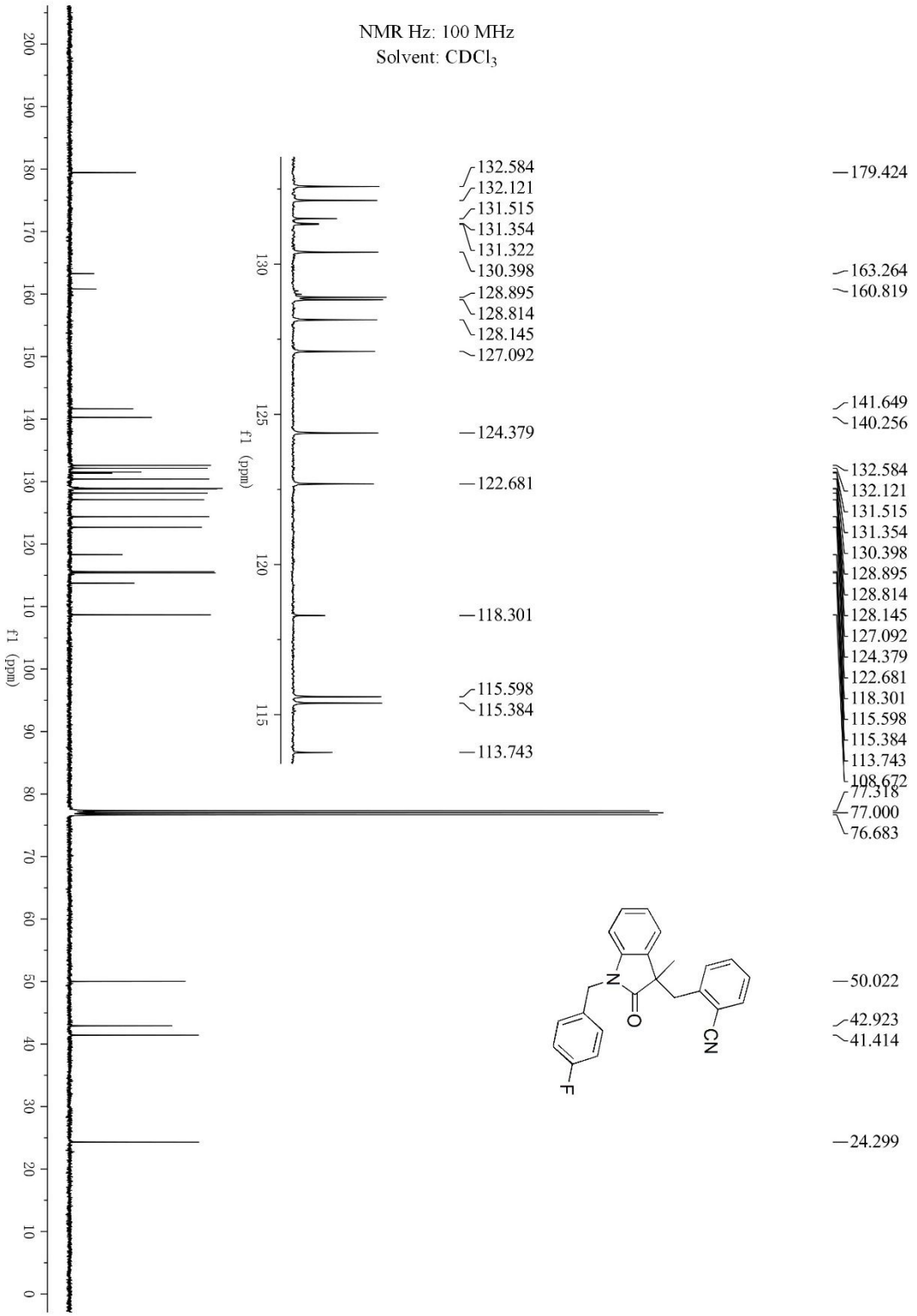
2-((3-Methyl-1-(4-methylbenzyl)-2-oxoindolin-3-yl)methyl)benzonitrile (3da)

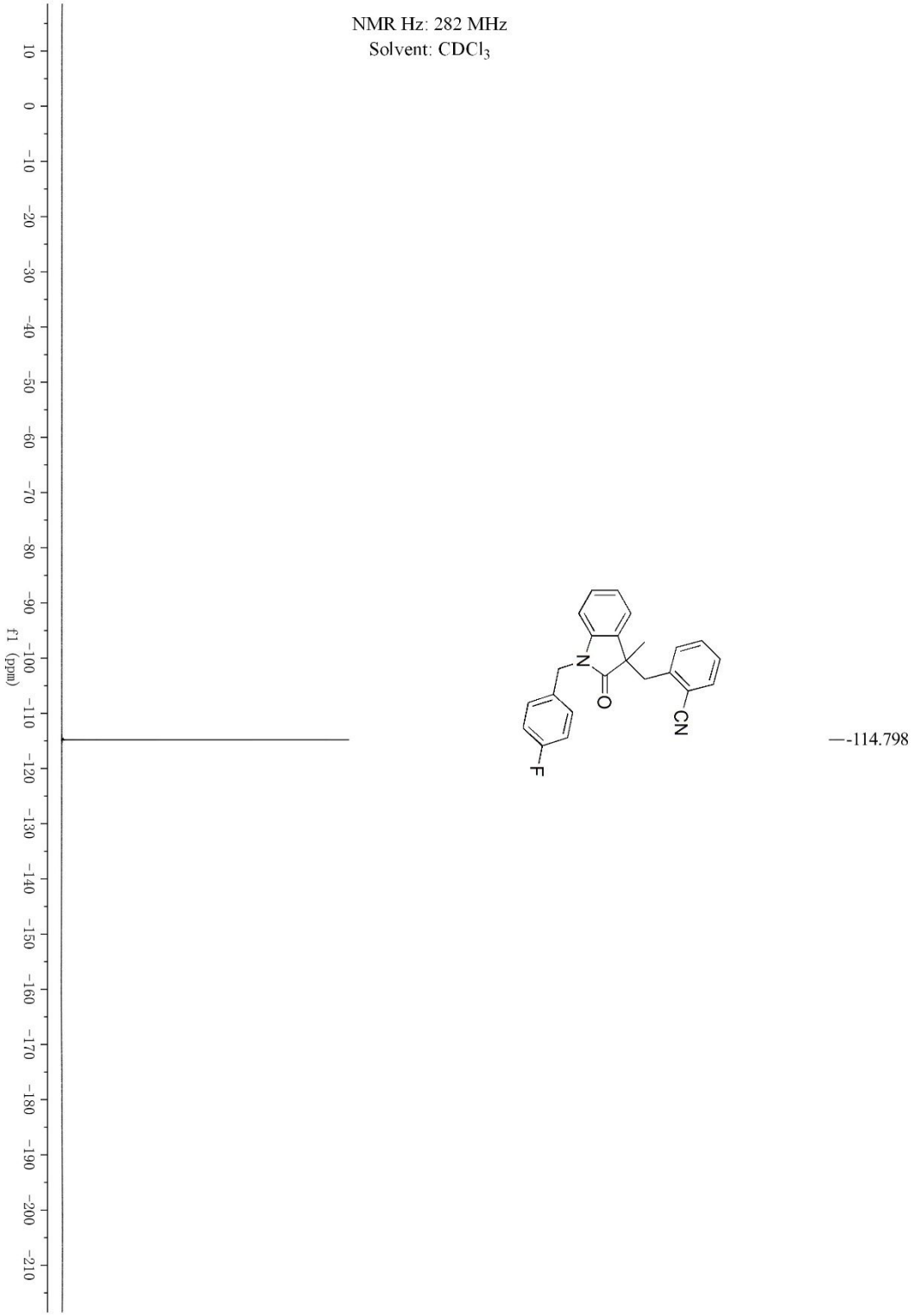



NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.456
141.888
140.352
137.067
132.517
132.489
132.179
131.498
130.425
129.228
128.063
127.092
127.025
124.204
122.472
118.378
113.649
108.895
77.318
77.000
76.682
50.047
43.388
41.370
24.358
21.035
N
O
CN

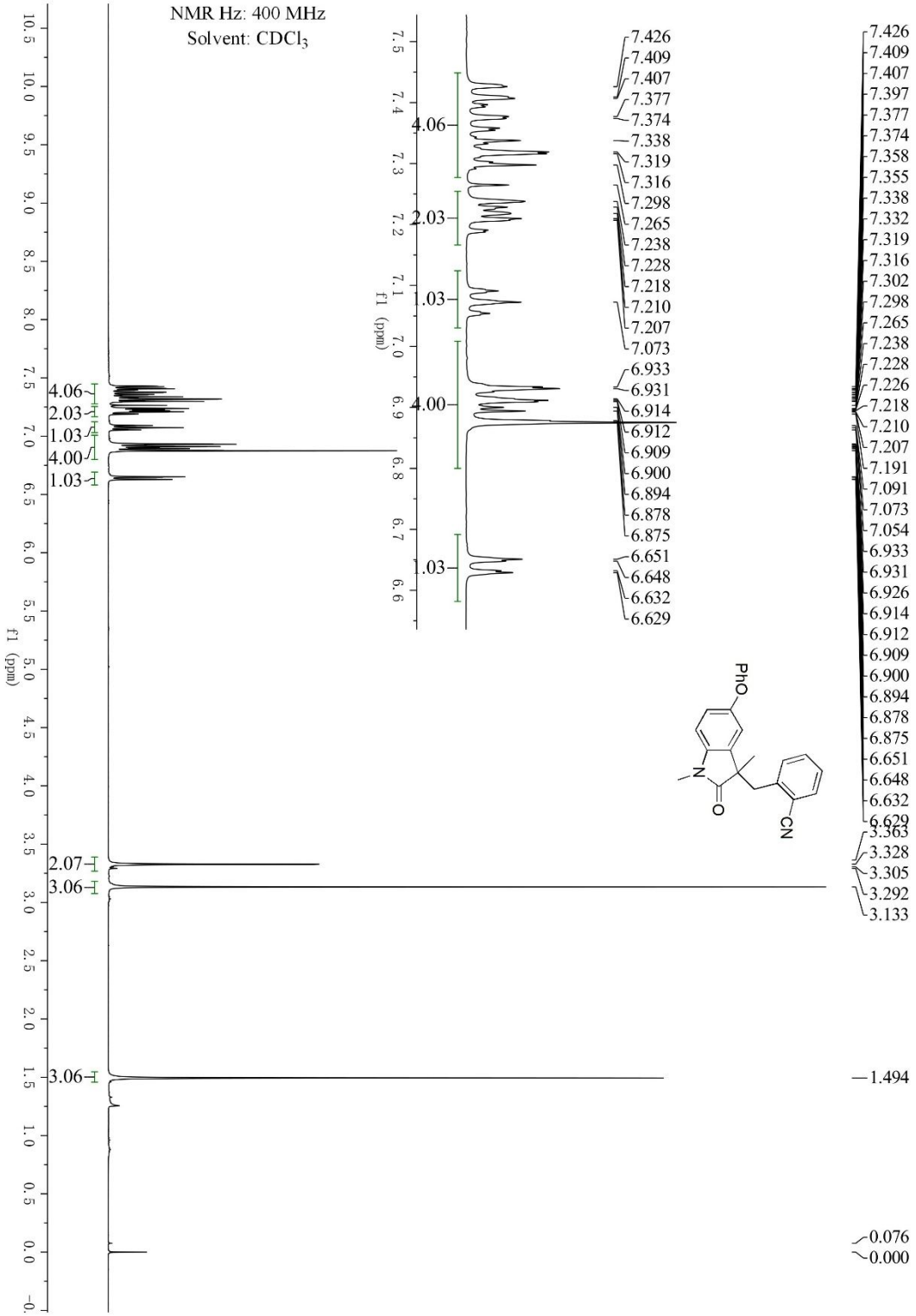
2-((1-(4-Fluorobenzyl)-3-methyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ea)

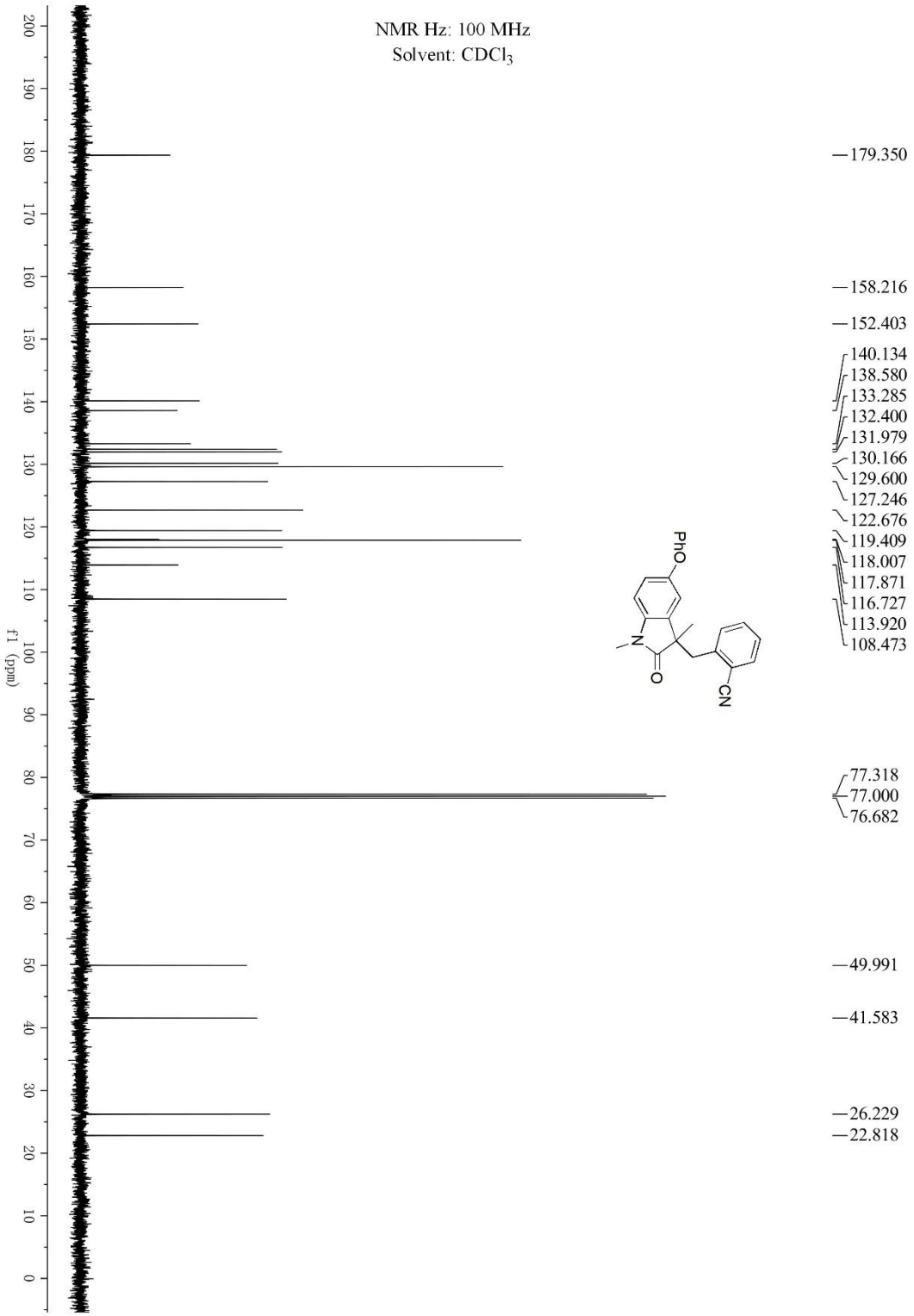



NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.424
163.264
160.819
141.649
140.256
132.584
132.121
131.515
131.354
130.398
128.895
128.814
128.145
127.092
124.379
122.681
118.301
115.598
115.384
113.743
108.672
77.318
77.000
76.683
50.022
42.923
41.414
24.299
N
O
CN
F

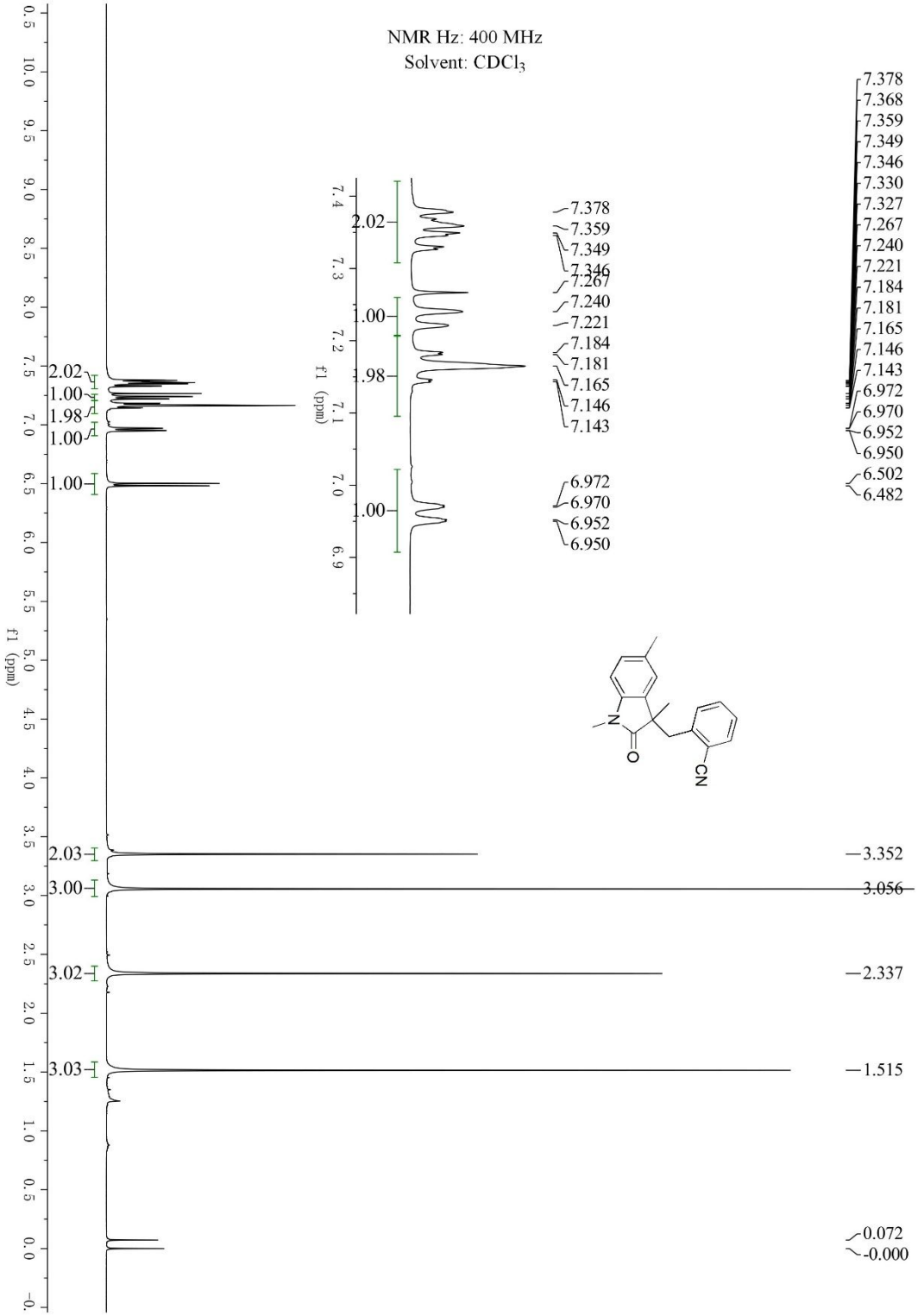

NMR Hz: 282 MHz
Solvent: CDCl3
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-114.798
F
N
O
CN

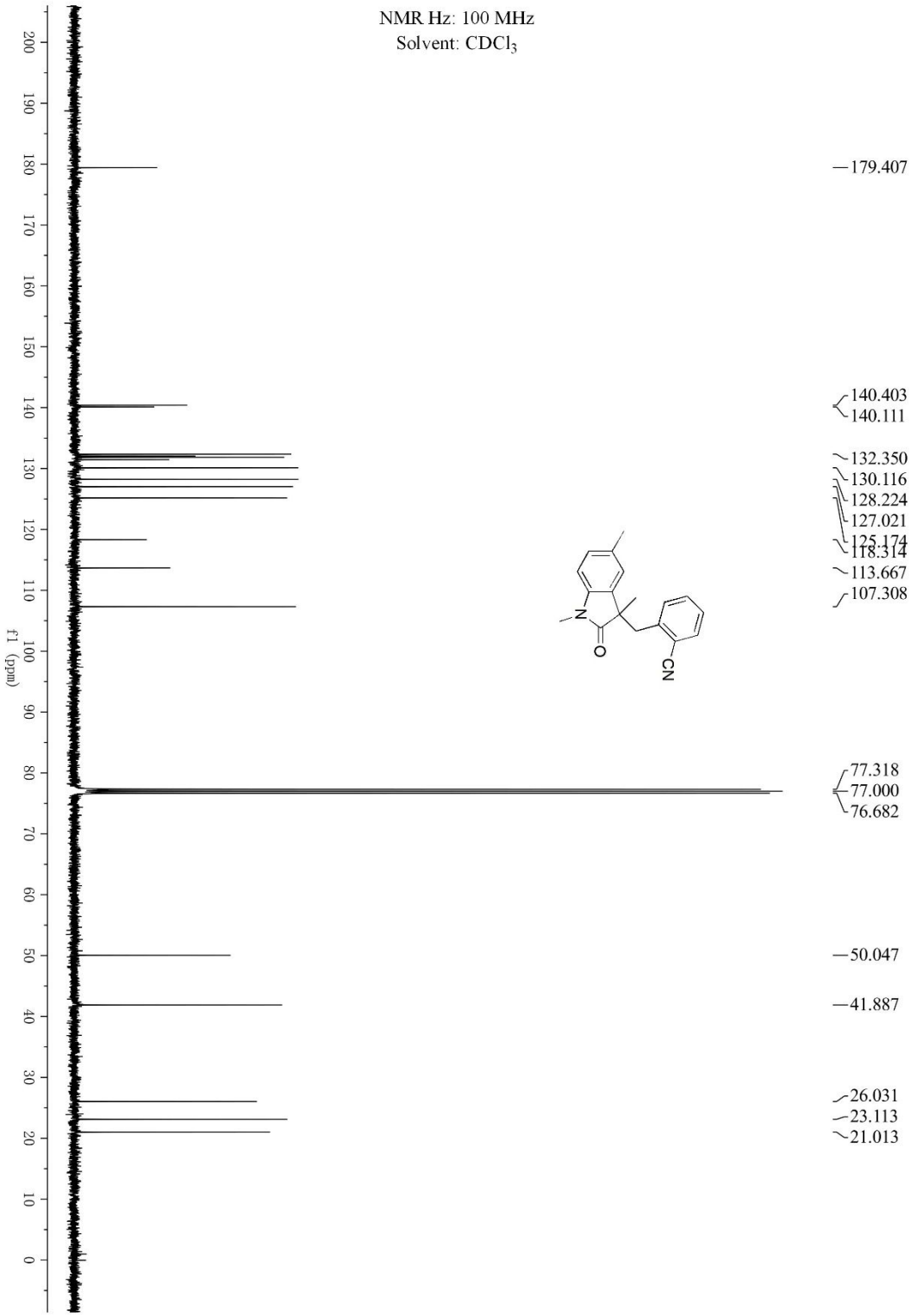
2-((1,3-Dimethyl-2-oxo-5-phenoxyindolin-3-yl)methyl)benzonitrile (3ga)



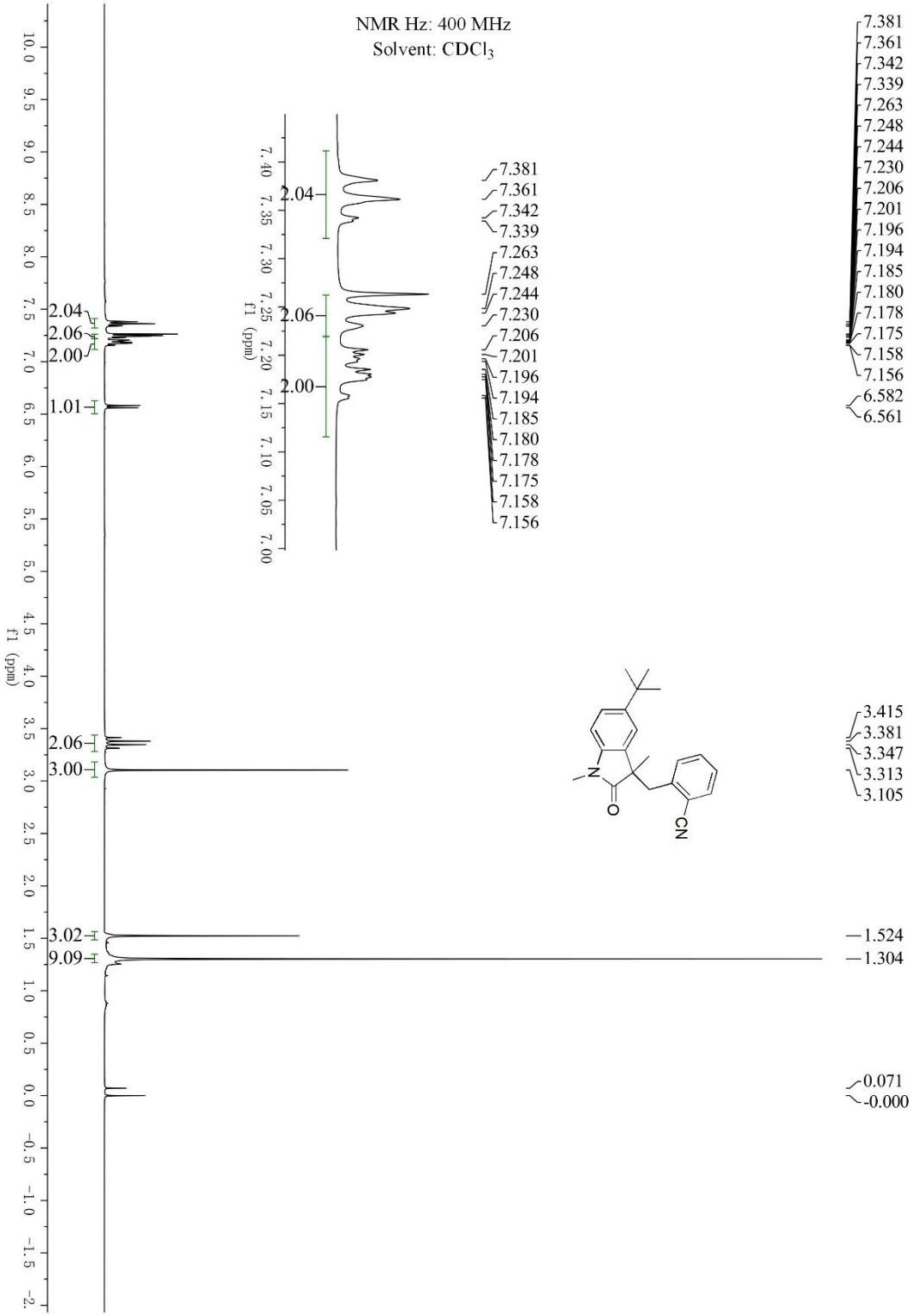

NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.350
158.216
152.403
140.134
138.580
133.285
132.400
131.979
130.166
129.600
127.246
122.676
119.409
118.007
117.871
116.727
113.920
108.473
77.318
77.000
76.682
49.991
41.583
26.229
22.818
PhO
N
O
CN

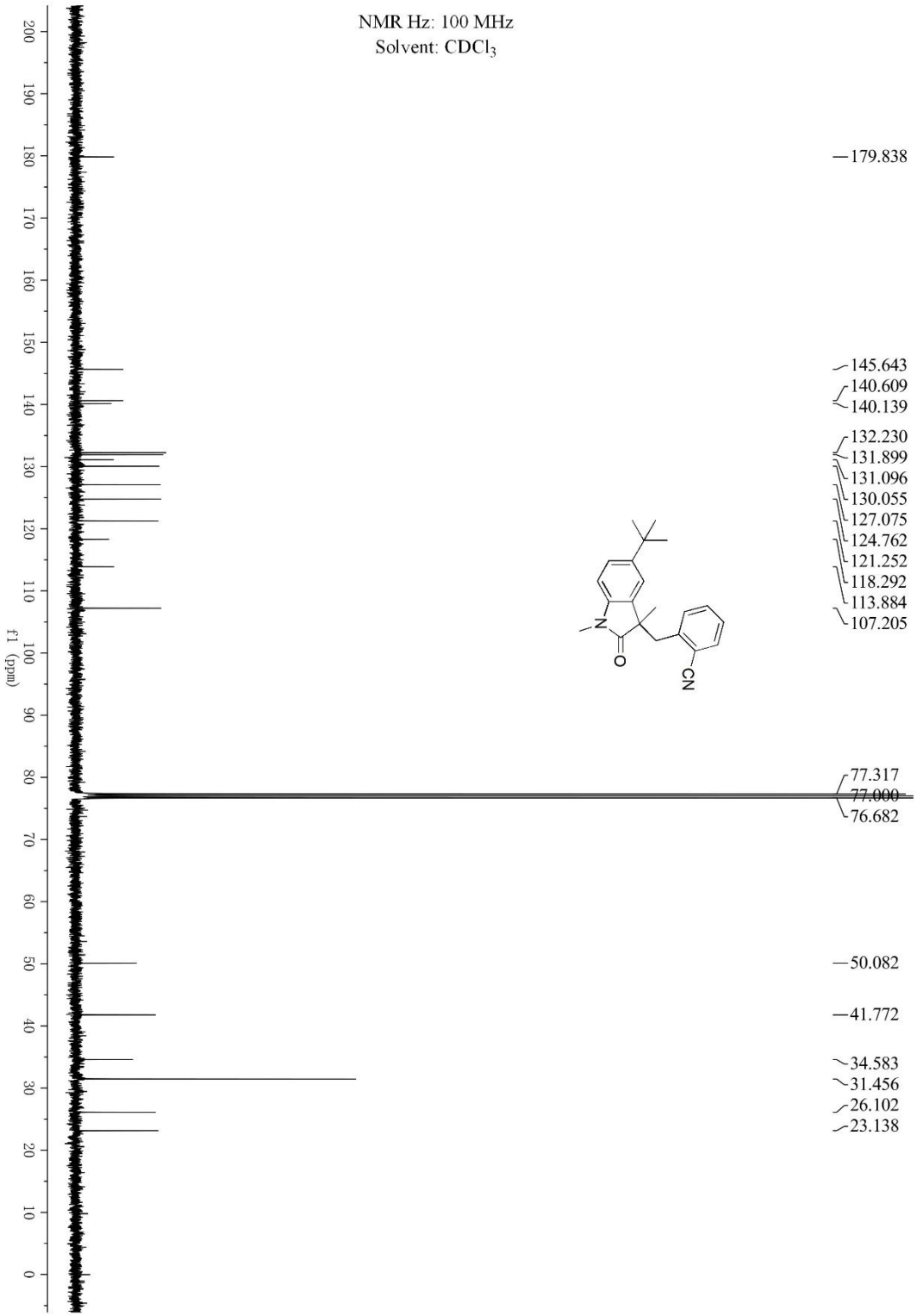
2-((1,3,5-Trimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ha)



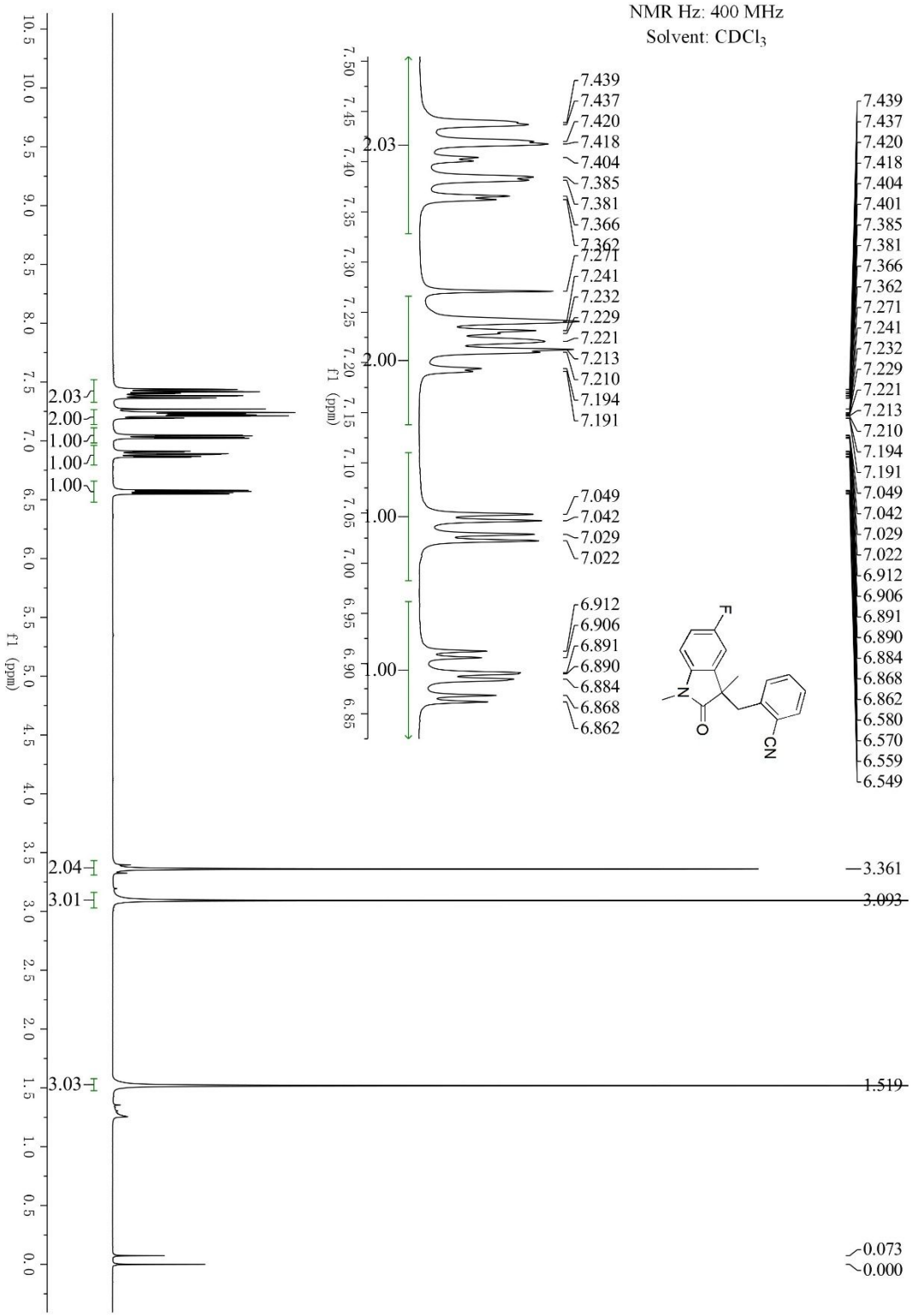

NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.407
140.403
140.111
132.350
130.116
128.224
127.021
125.174
118.314
113.667
107.308
77.318
77.000
76.682
50.047
41.887
26.031
23.113
21.013
N
O
CN

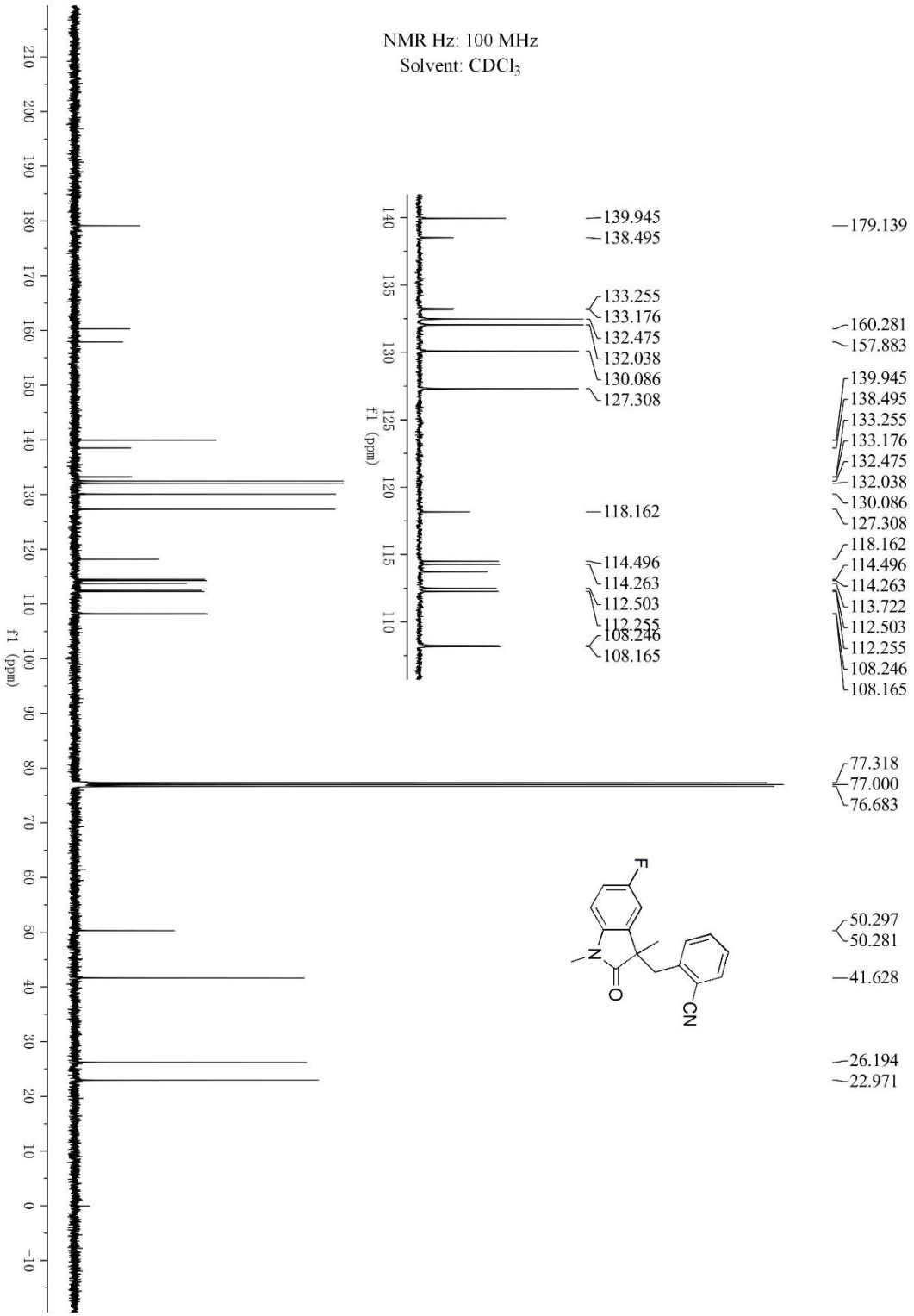
2-((5-(*tert*-Butyl)-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ia)

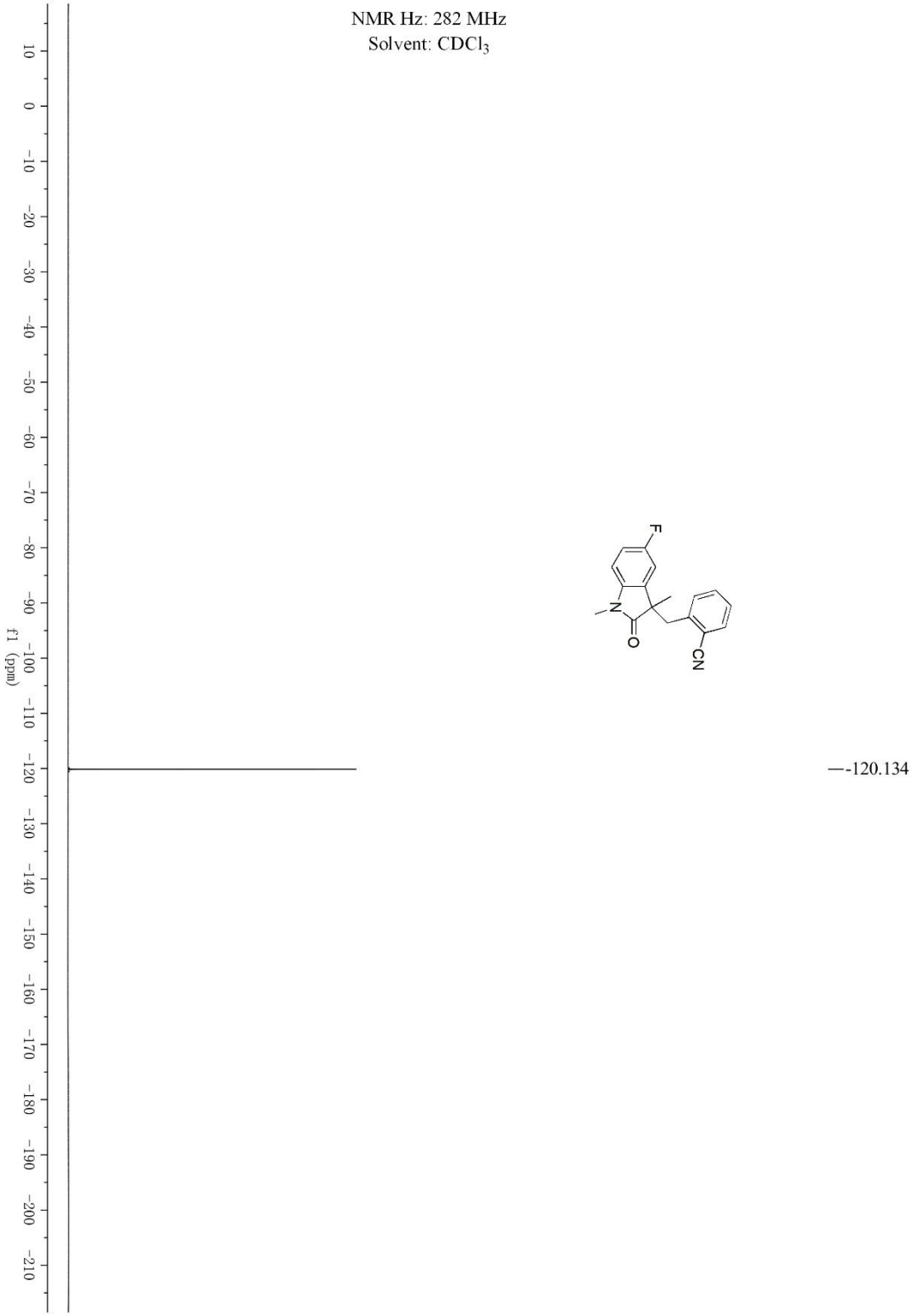



NMR Hz: 100 MHz
Solvent: $CDCl_3$
f1 (ppm)
179.838
145.643
140.609
140.139
132.230
131.899
131.096
130.055
127.075
124.762
121.252
118.292
113.884
107.205
77.317
77.000
76.682
50.082
41.772
34.583
31.456
26.102
23.138
N
O
CN

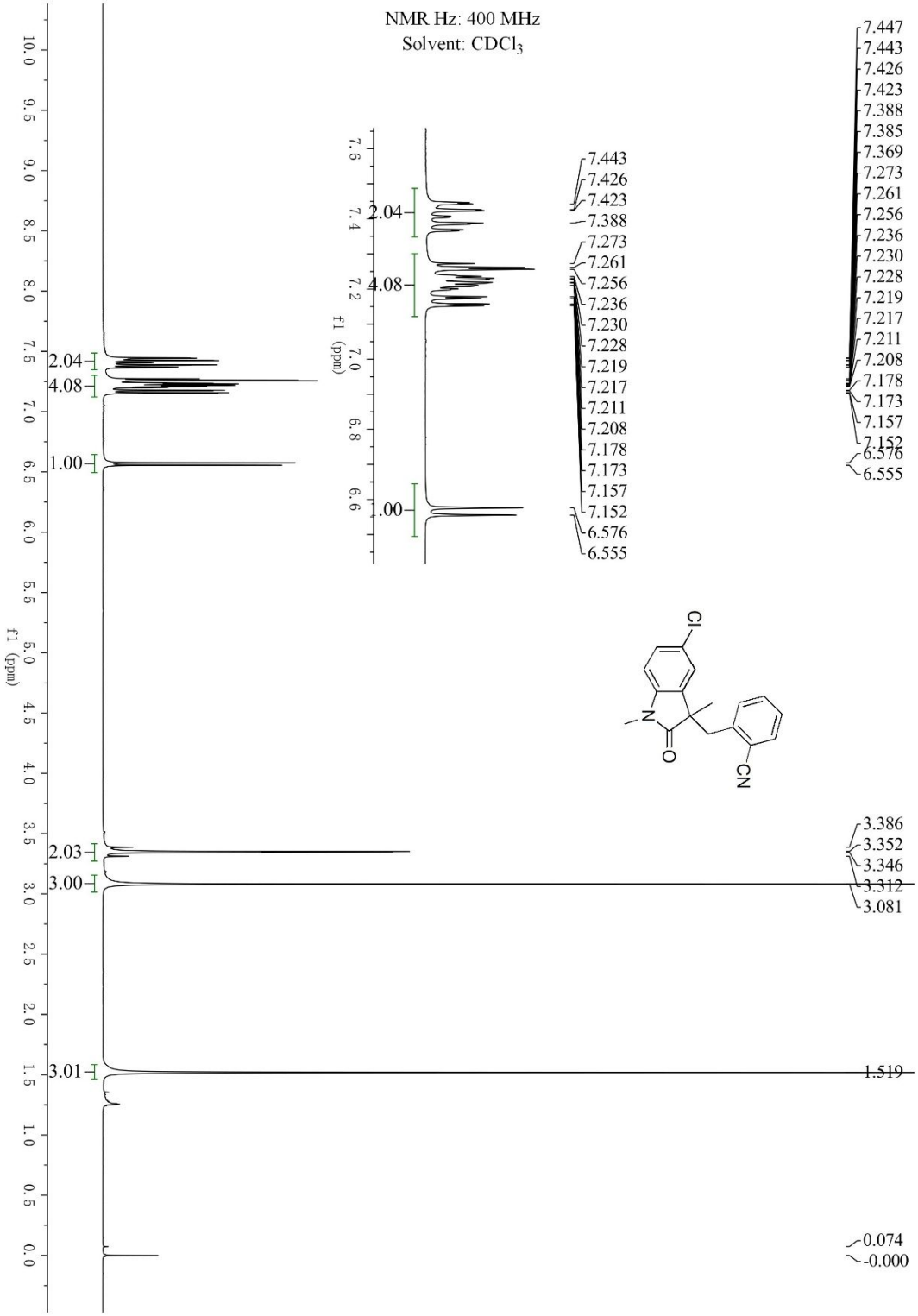
2-((5-Fluoro-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ja)

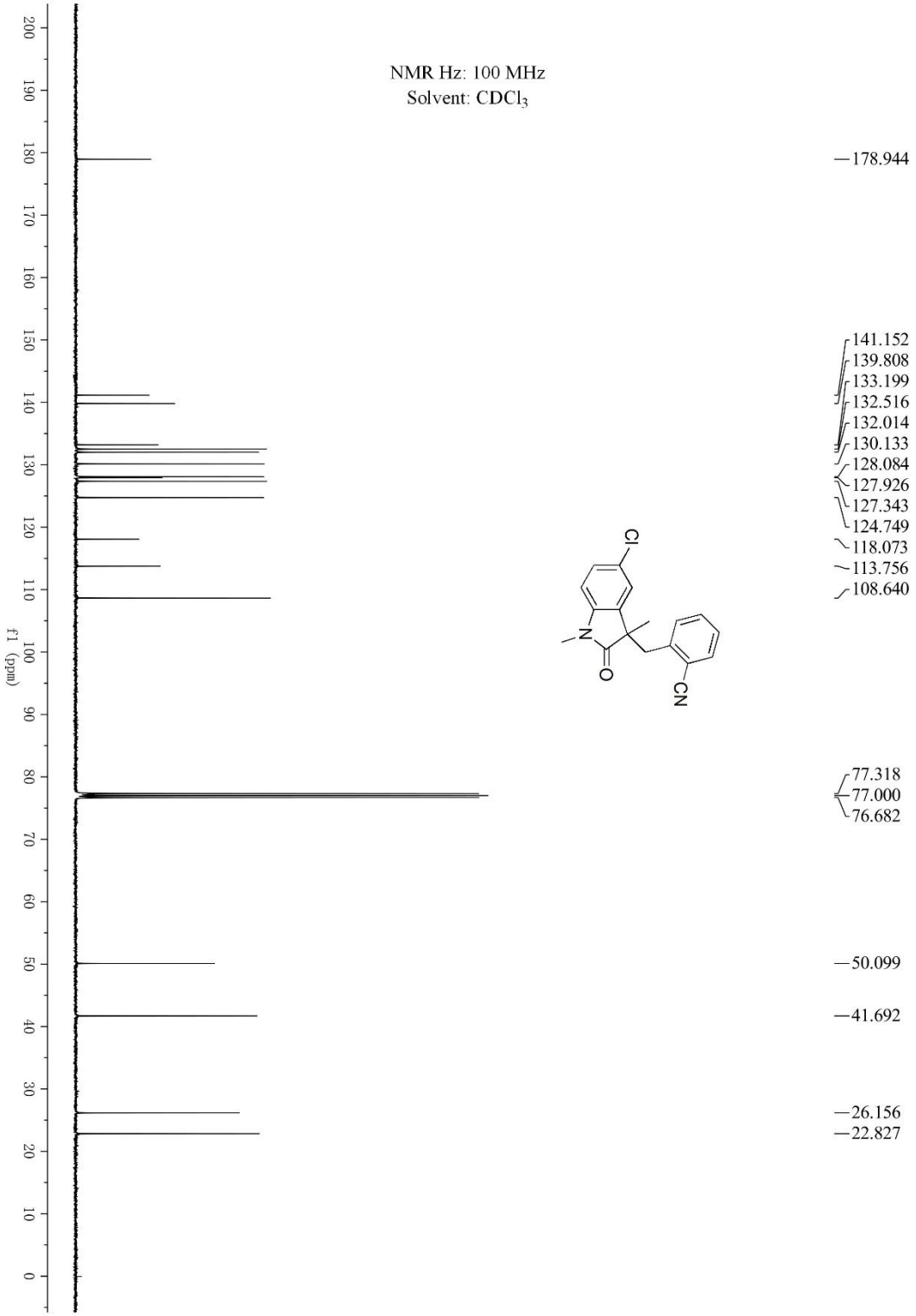



NMR Hz: 100 MHz
Solvent: $CDCl_3$
f1 (ppm)
139.945
138.495
133.255
133.176
132.475
132.038
130.086
127.308
118.162
114.496
114.263
112.503
112.255
108.246
108.165
179.139
160.281
157.883
139.945
138.495
133.255
133.176
132.475
132.038
130.086
127.308
118.162
114.496
114.263
113.722
112.503
112.255
108.246
108.165
77.318
77.000
76.683
50.297
50.281
41.628
26.194
22.971
F
N
O
CN

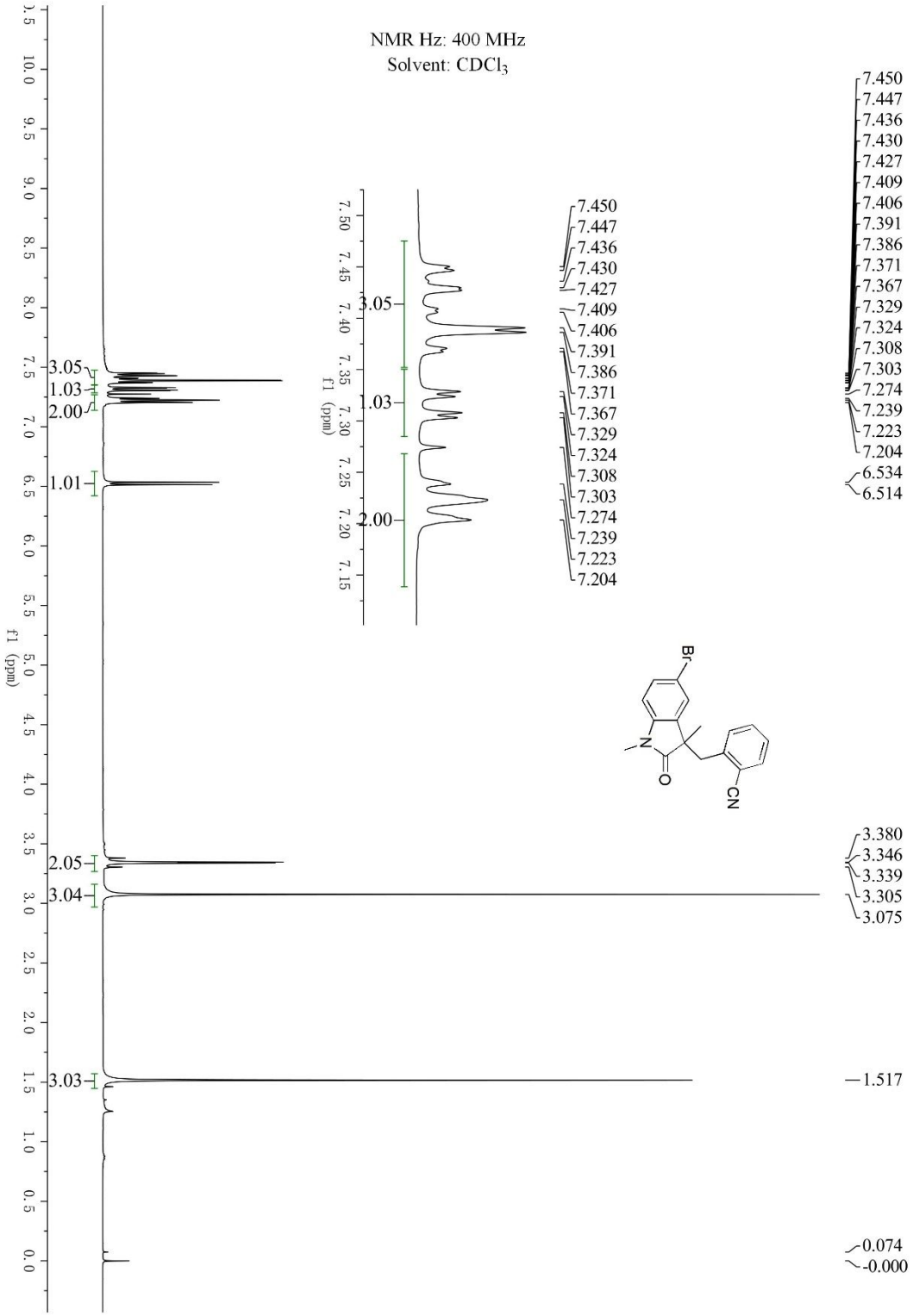

NMR Hz: 282 MHz
Solvent: CDCl3
F
N
O
CN
-120.134
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210

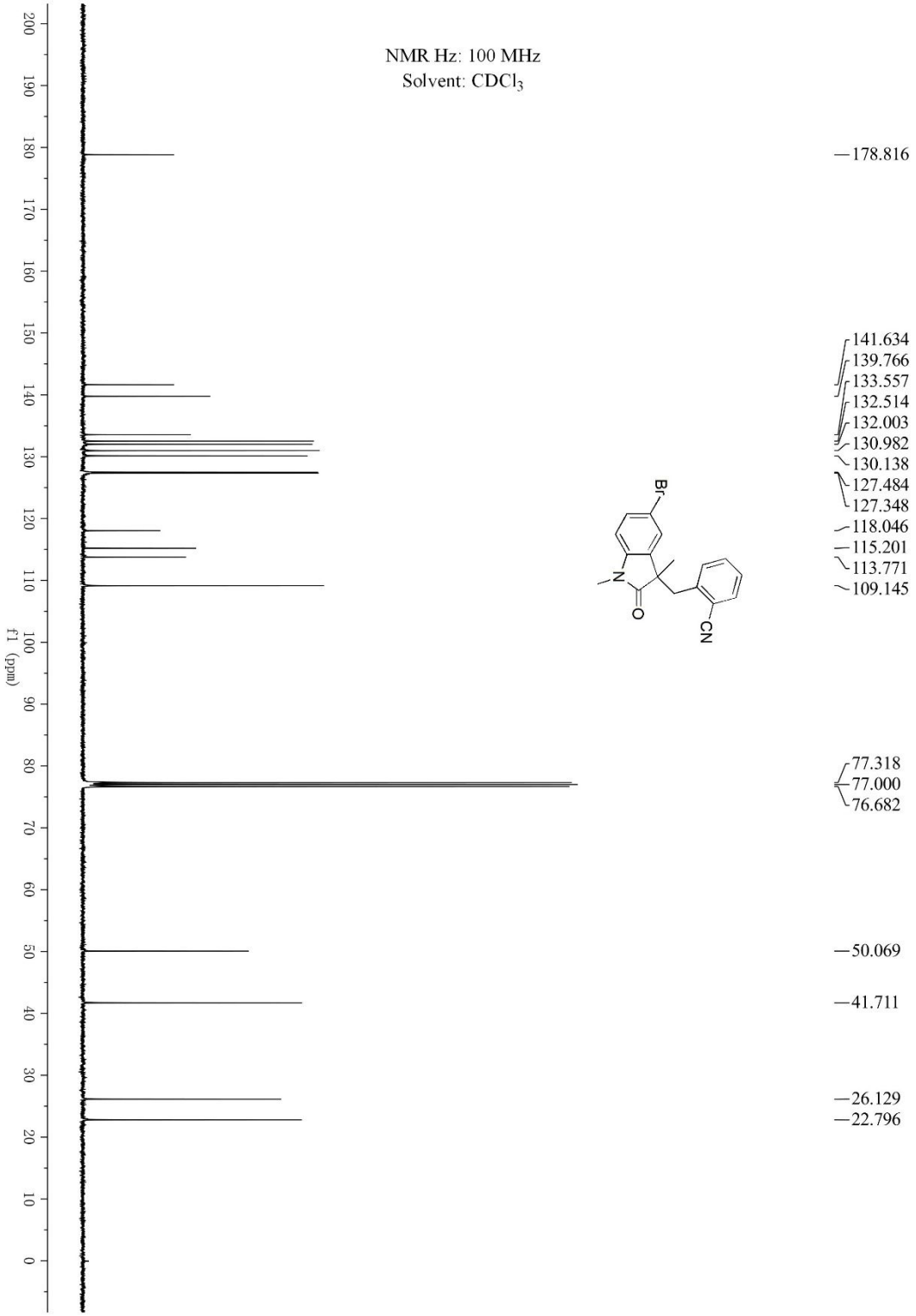
2-((5-Chloro-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ka)



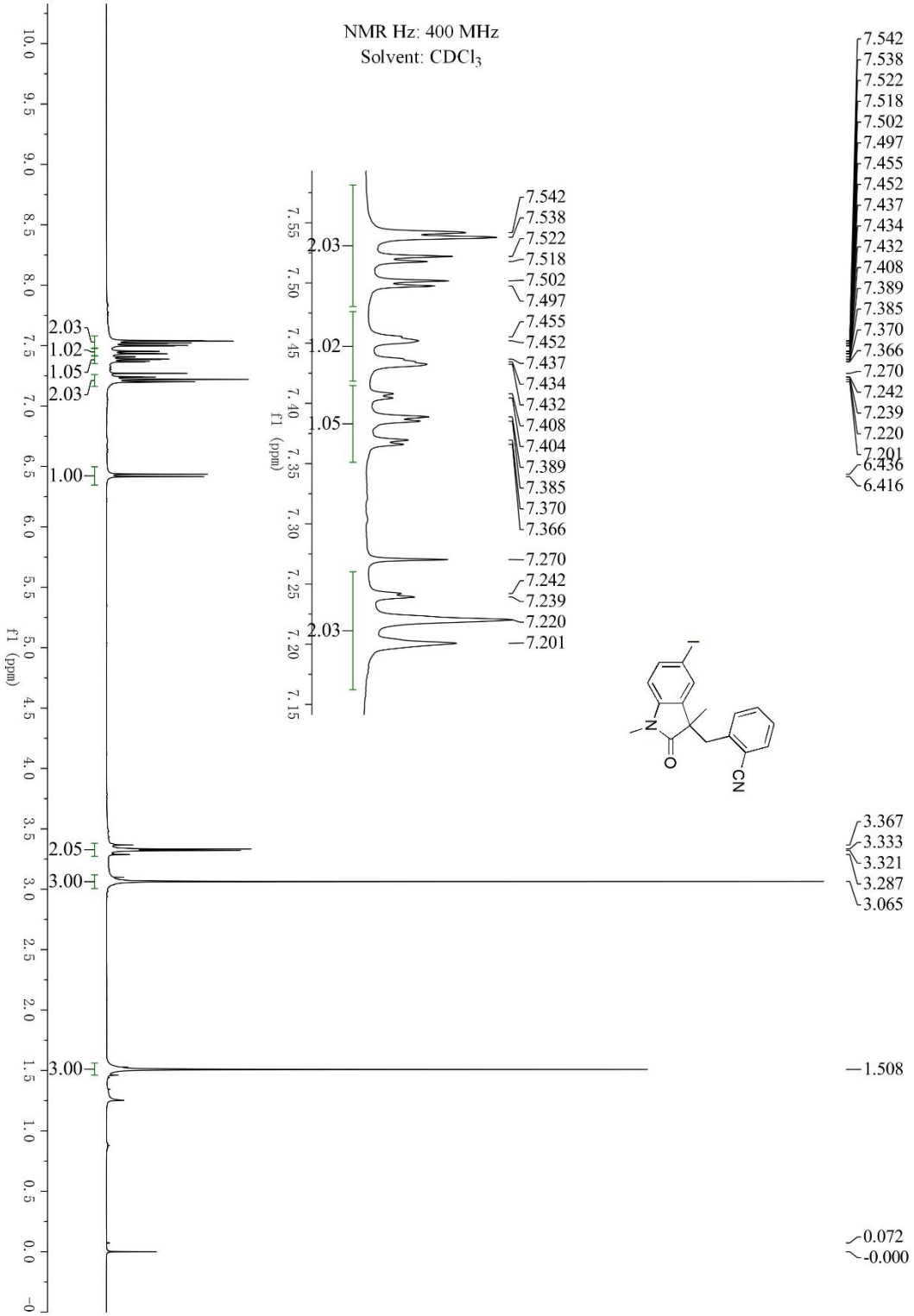

NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
178.944
141.152
139.808
133.199
132.516
132.014
130.133
128.084
127.926
127.343
124.749
118.073
113.756
108.640
77.318
77.000
76.682
50.099
41.692
26.156
22.827
Cl
N
O
CN

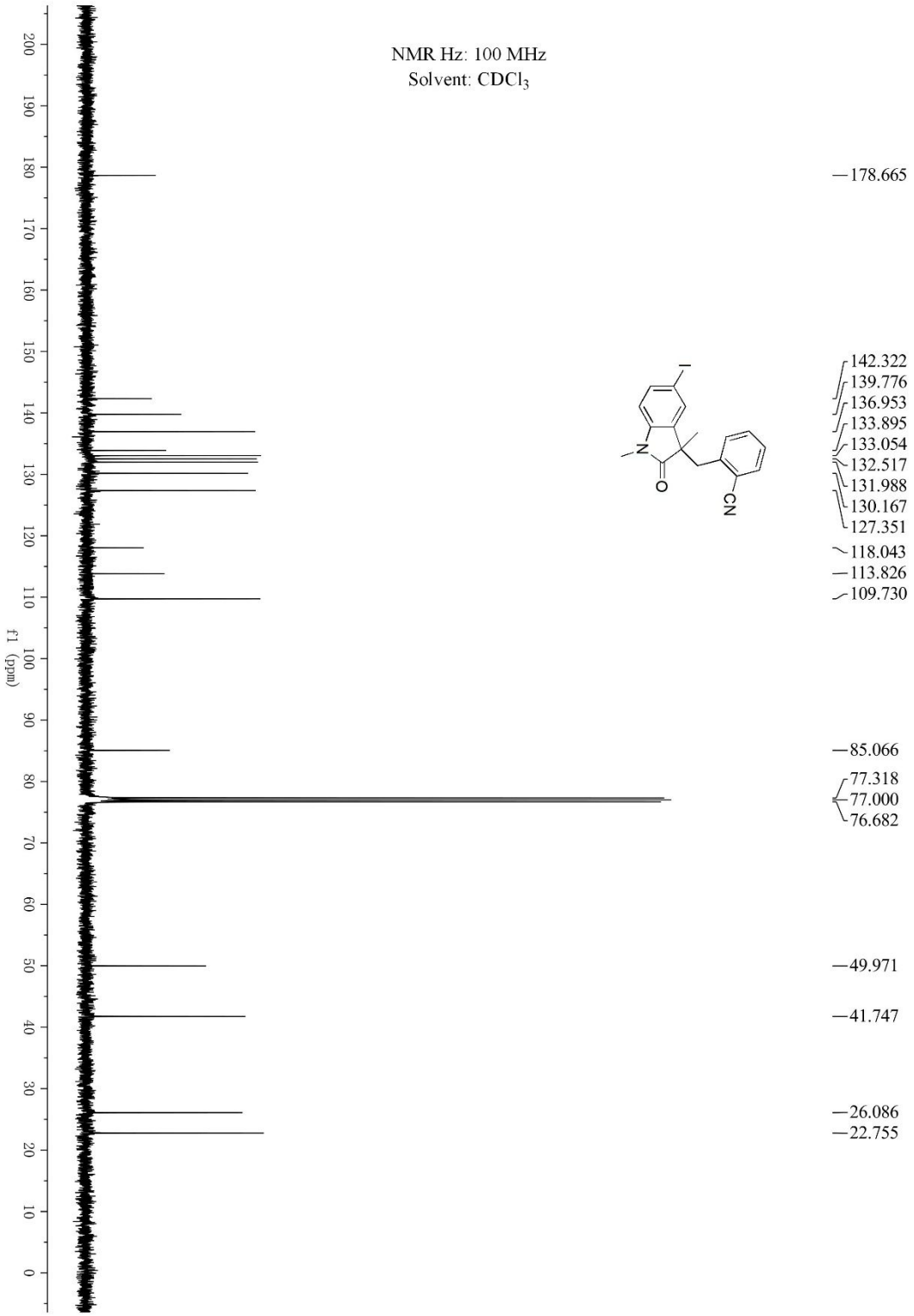
2-((5-Bromo-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3la)



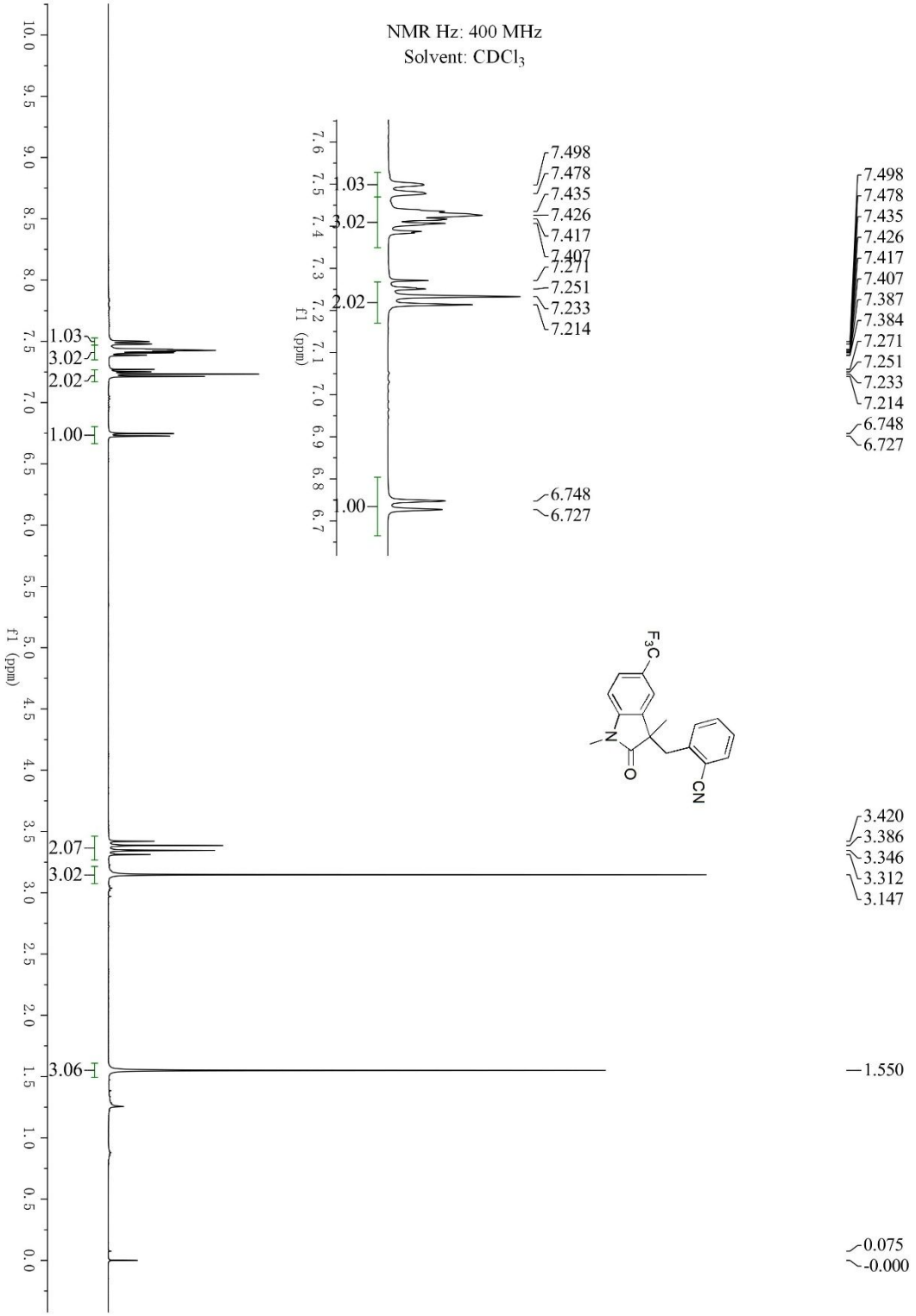

NMR Hz: 100 MHz
Solvent: CDCl3
178.816
141.634
139.766
133.557
132.514
132.003
130.982
130.138
127.484
127.348
118.046
115.201
113.771
109.145
77.318
77.000
76.682
50.069
41.711
26.129
22.796
Br
N
O
CN
f1 (ppm)

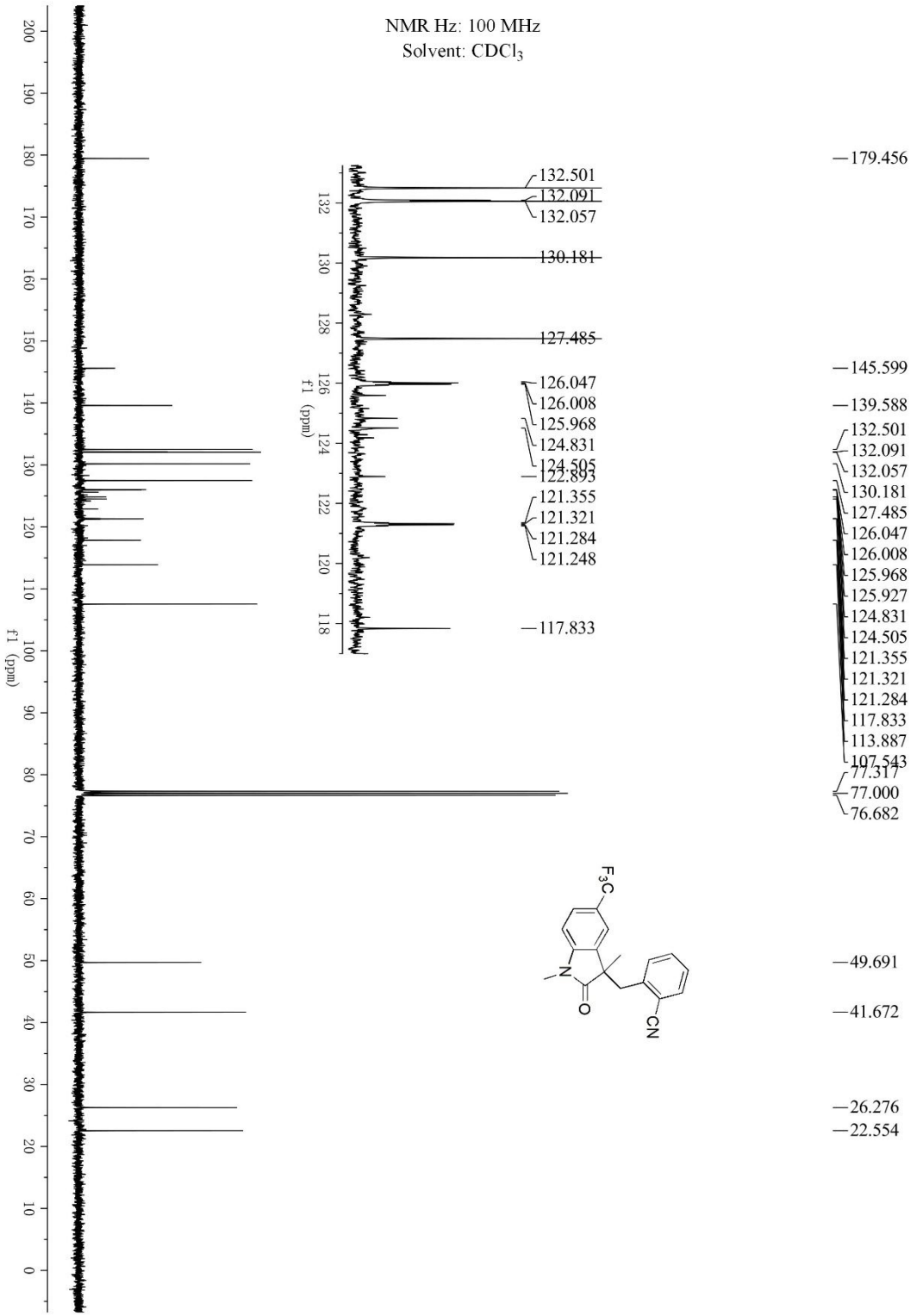
2-((5-Iodo-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ma)

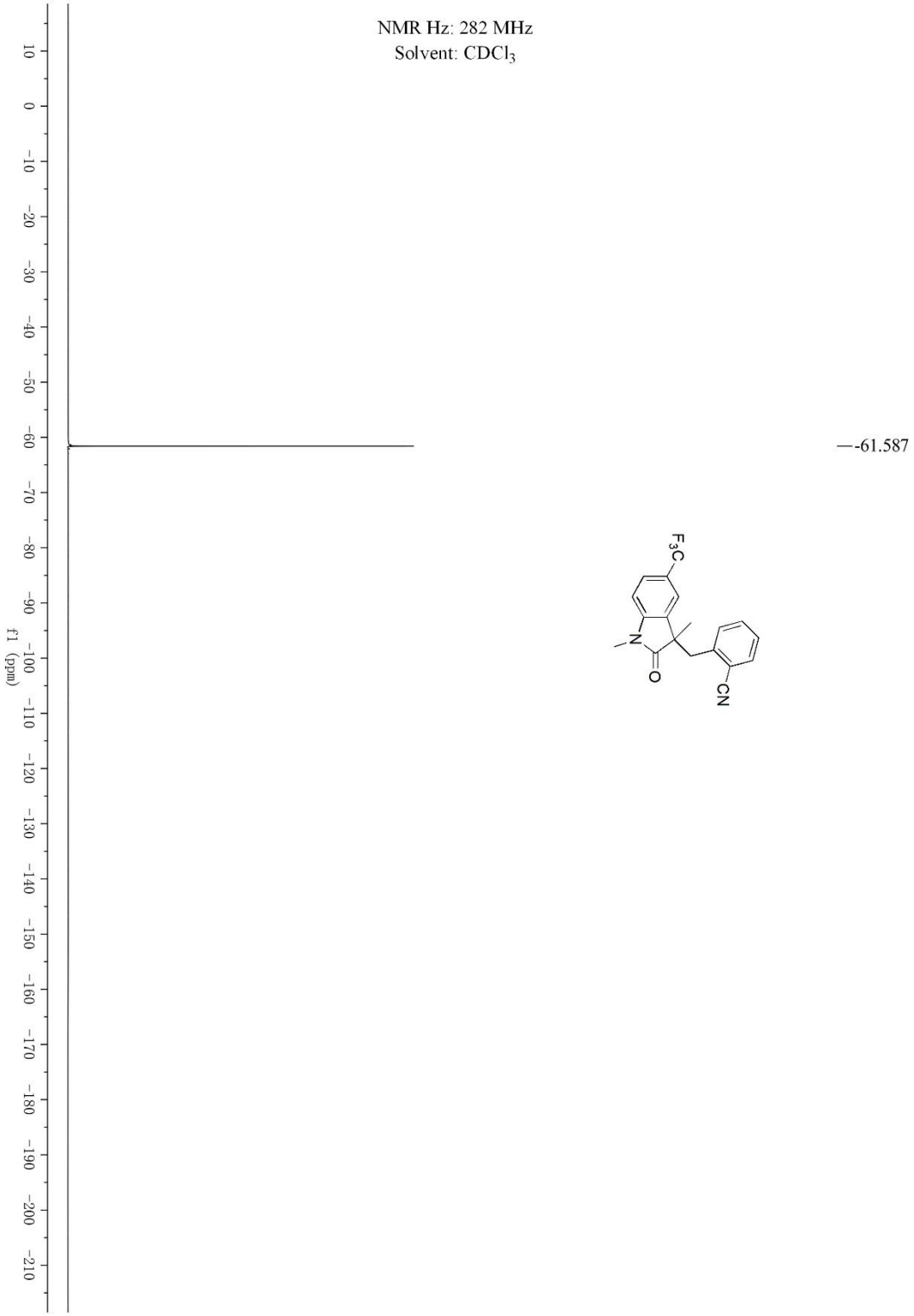



NMR Hz: 100 MHz
Solvent: CDCl3
178.665
142.322
139.776
136.953
133.895
133.054
132.517
131.988
130.167
127.351
118.043
113.826
109.730
85.066
77.318
77.000
76.682
49.971
41.747
26.086
22.755
f1 (ppm)

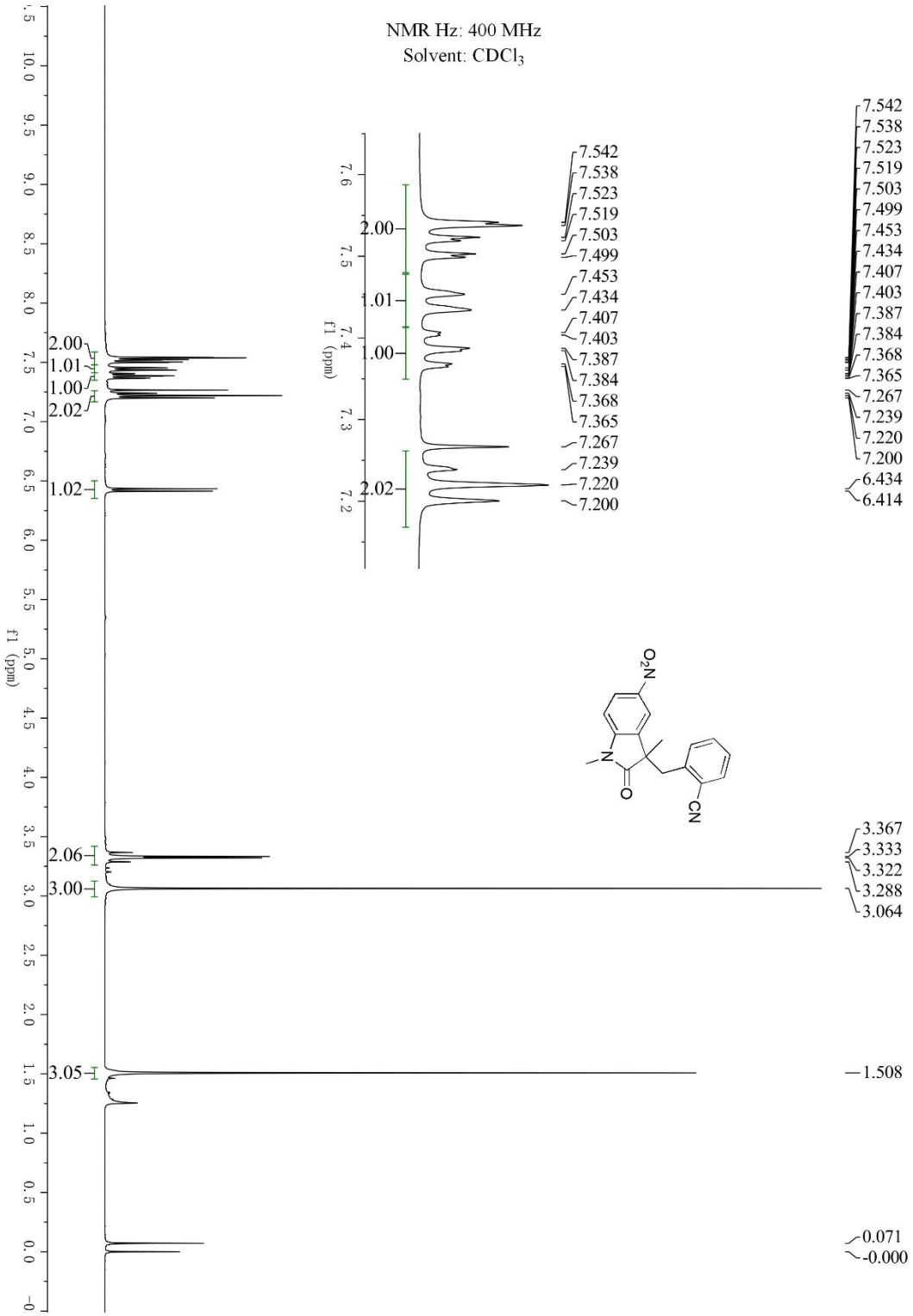
2-((1,3-Dimethyl-2-oxo-5-(trifluoromethyl)indolin-3-yl)methyl)benzonitrile (3na)

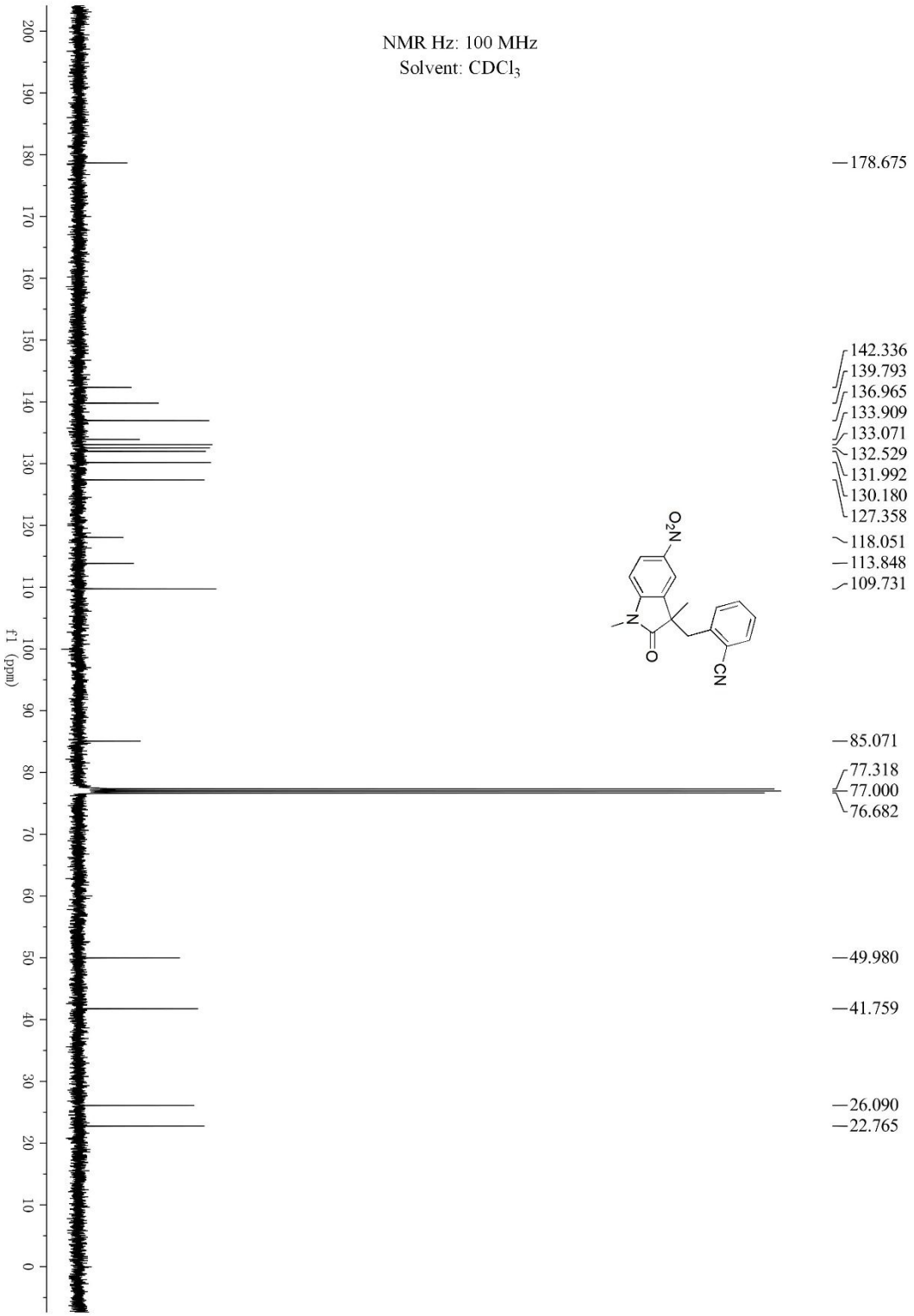



NMR Hz: 100 MHz
Solvent: $CDCl_3$
f1 (ppm)
179.456
145.599
139.588
132.501
132.091
132.057
130.181
127.485
126.047
126.008
125.968
125.927
124.831
124.505
121.355
121.321
121.284
121.248
117.833
113.887
107.543
77.317
77.000
76.682
49.691
41.672
26.276
22.554
F_3C
N
O
CN

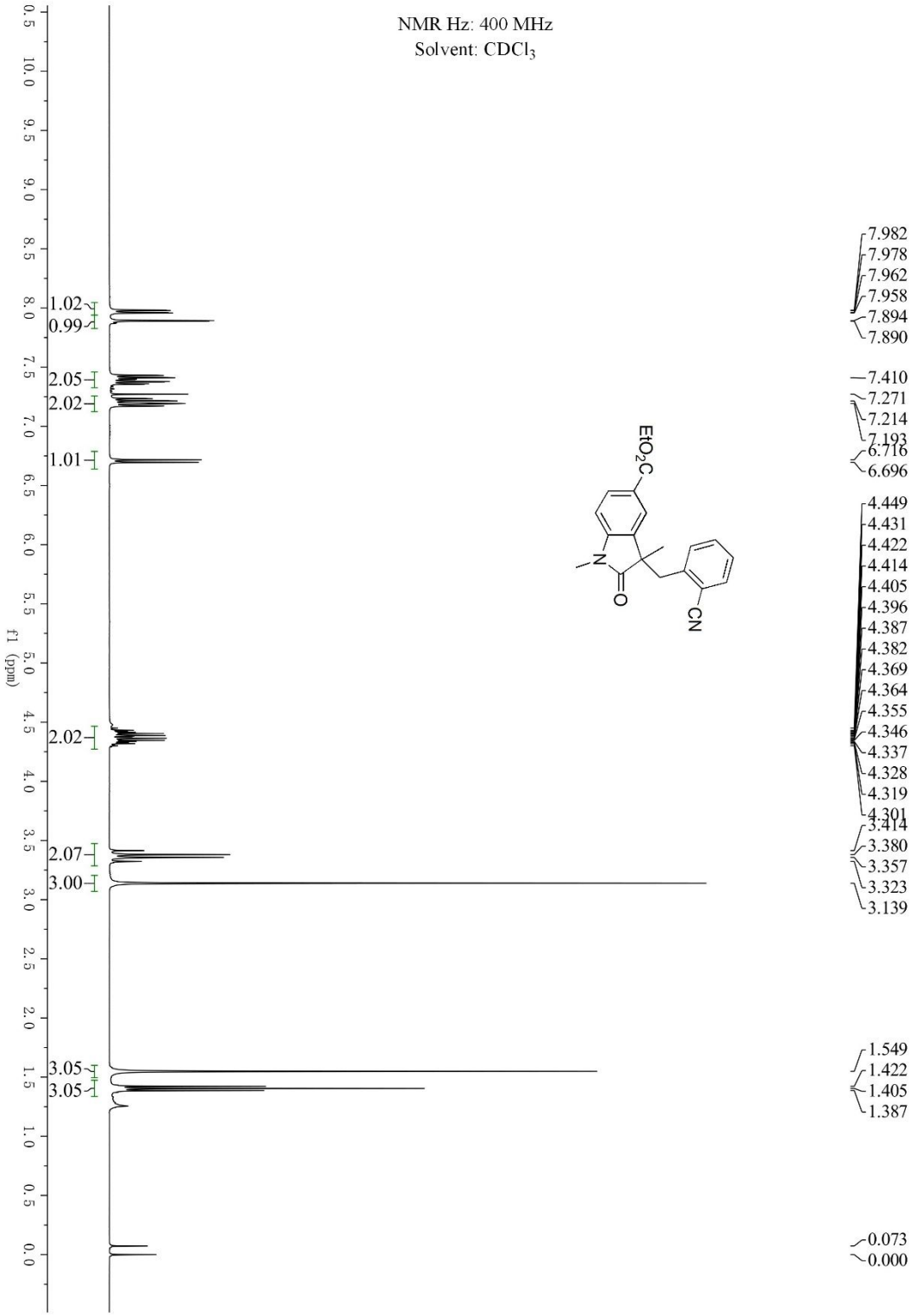

NMR Hz: 282 MHz
Solvent: CDCl3
-61.587
F3C
N
O
CN
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210

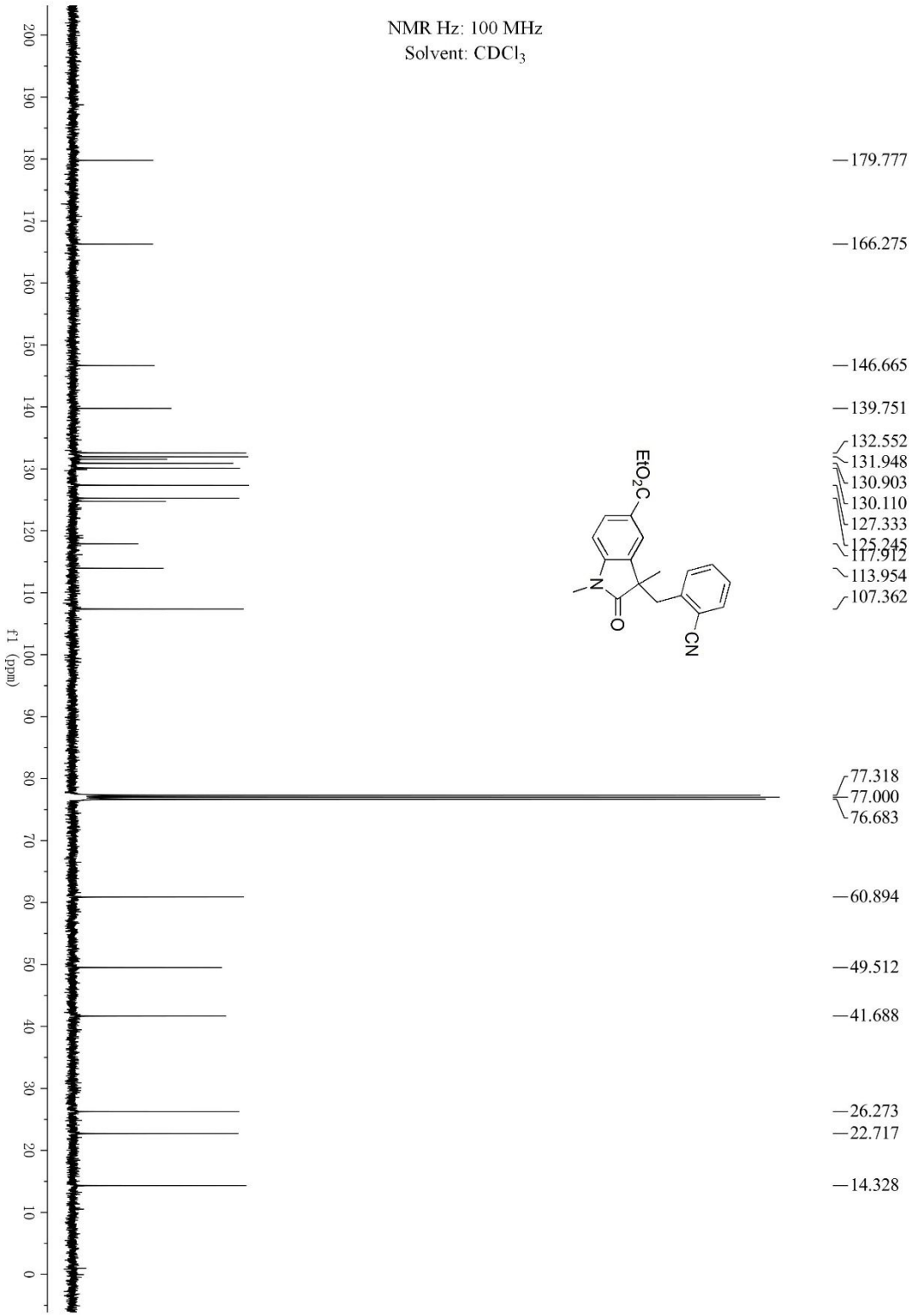
2-((1,3-Dimethyl-5-nitro-2-oxoindolin-3-yl)methyl)benzonitrile (3oa)



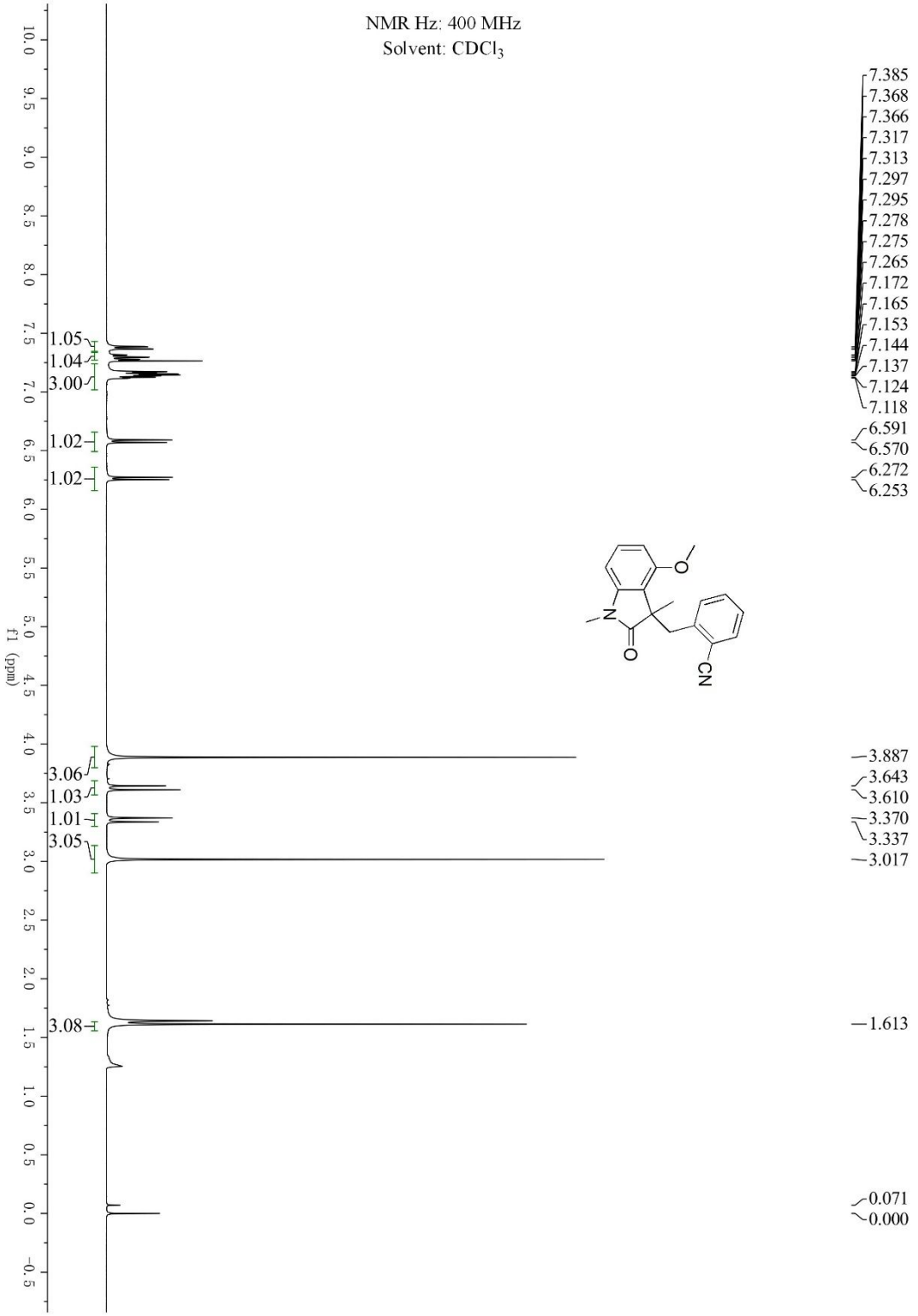

NMR Hz: 100 MHz
Solvent: CDCl3
178.675
142.336
139.793
136.965
133.909
133.071
132.529
131.992
130.180
127.358
118.051
113.848
109.731
85.071
77.318
77.000
76.682
49.980
41.759
26.090
22.765
f1 (ppm)

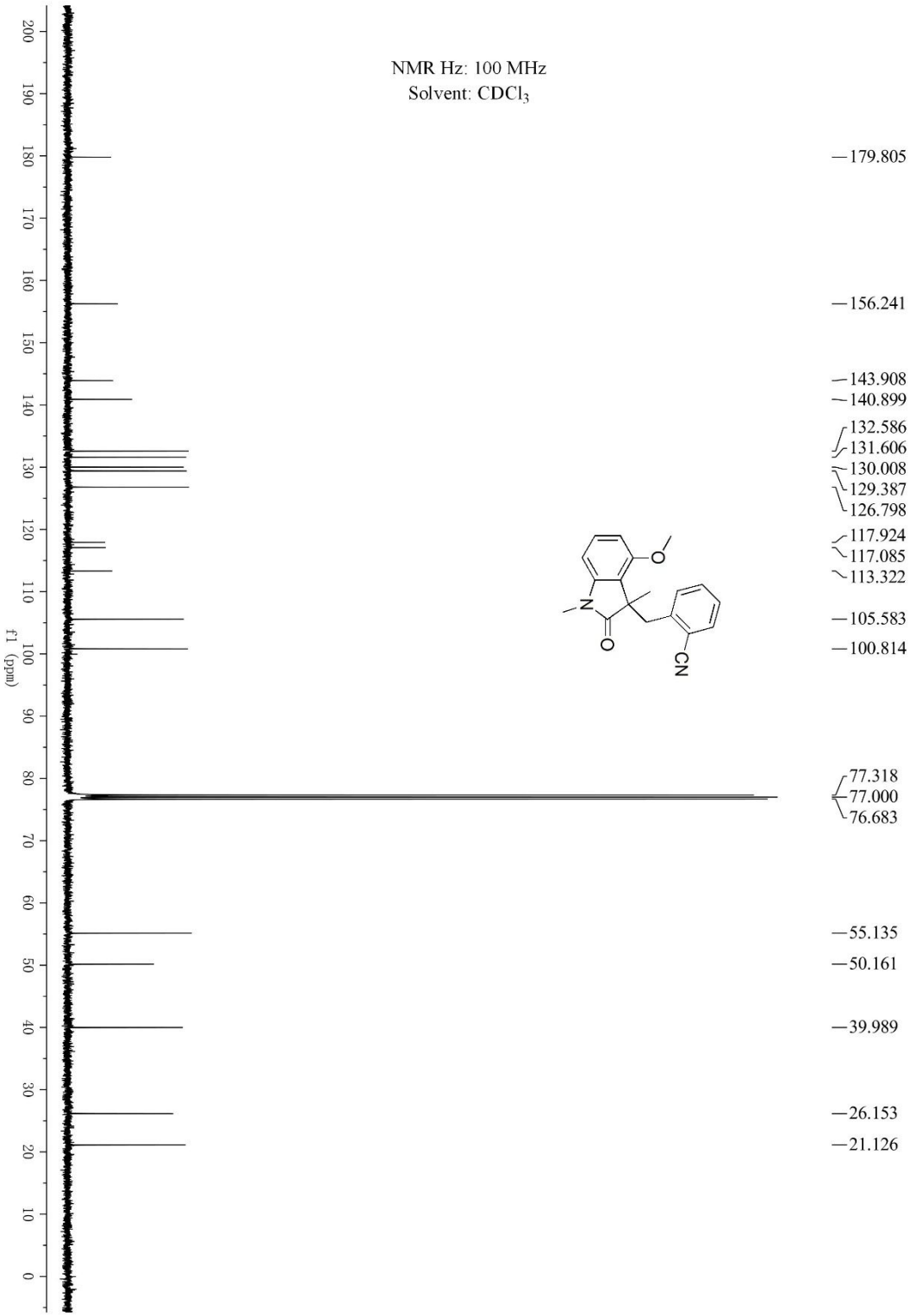
Ethyl 3-(2-cyanobenzyl)-1,3-dimethyl-2-oxoindoline-5-carboxylate (3pa)



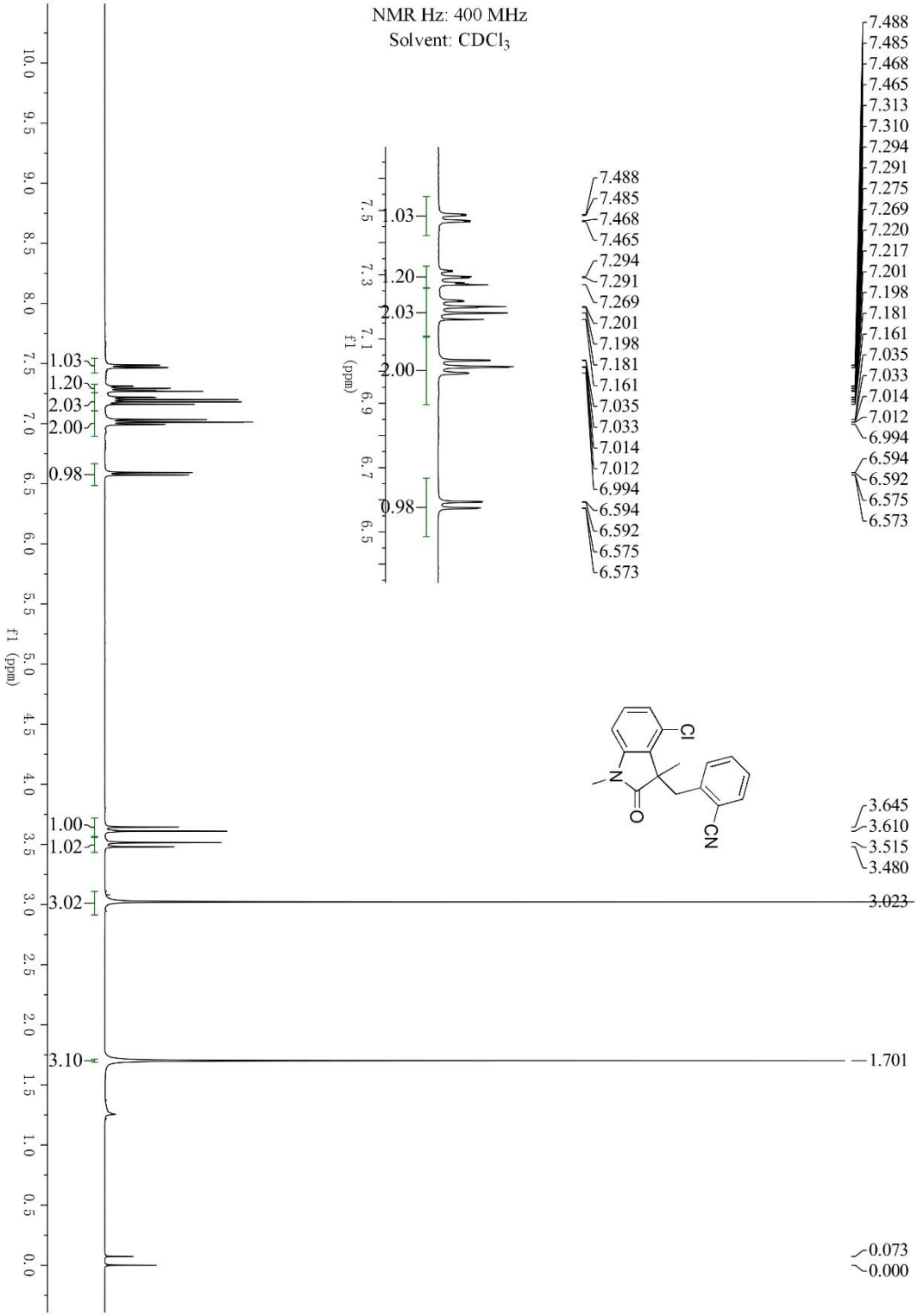

NMR Hz: 100 MHz
Solvent: CDCl3
179.777
166.275
146.665
139.751
132.552
131.948
130.903
130.110
127.333
125.245
117.912
113.954
107.362
77.318
77.000
76.683
60.894
49.512
41.688
26.273
22.717
14.328
f1 (ppm)
EtO2C
N
O
CN

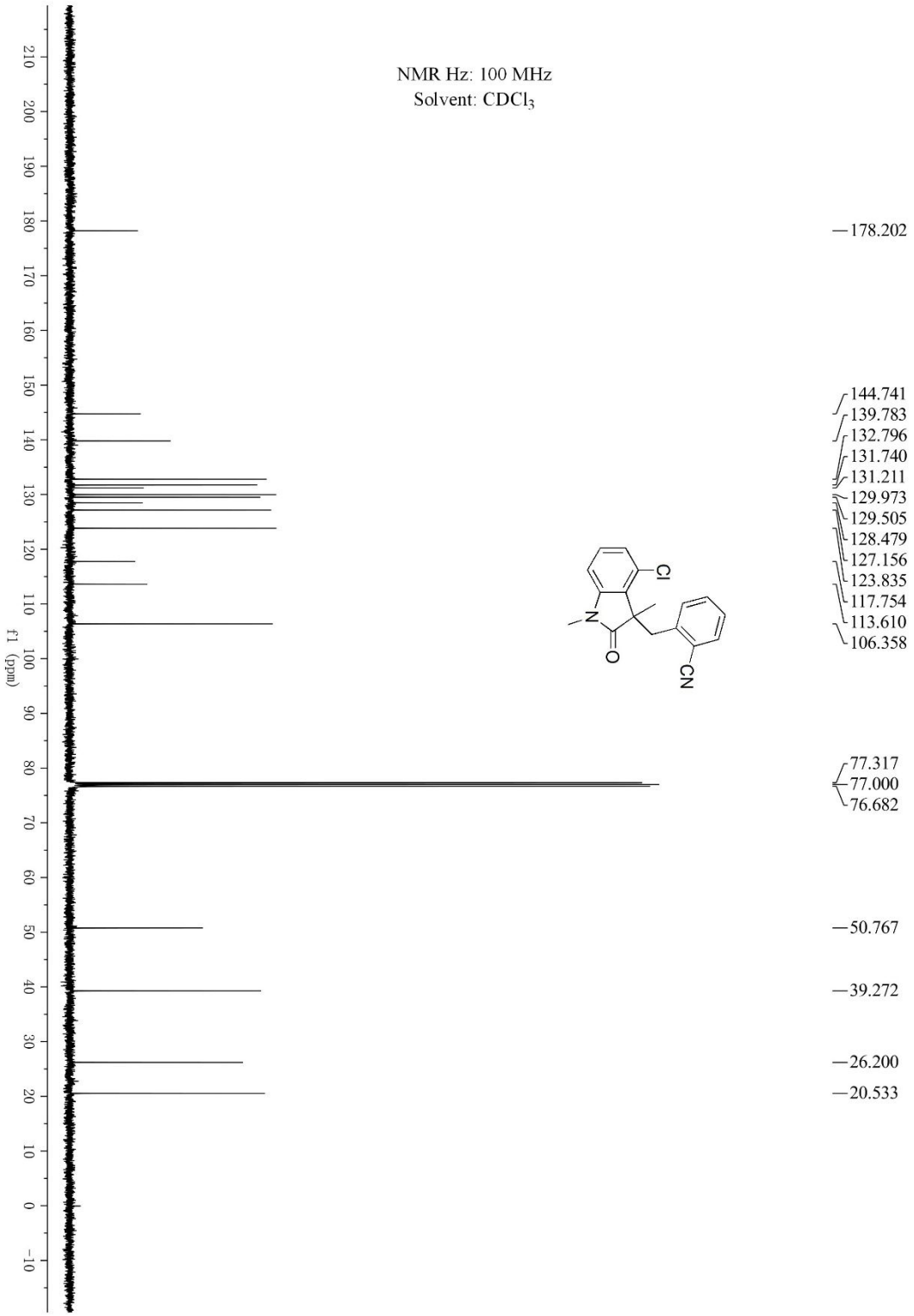
2-((4-methoxy-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3qa)



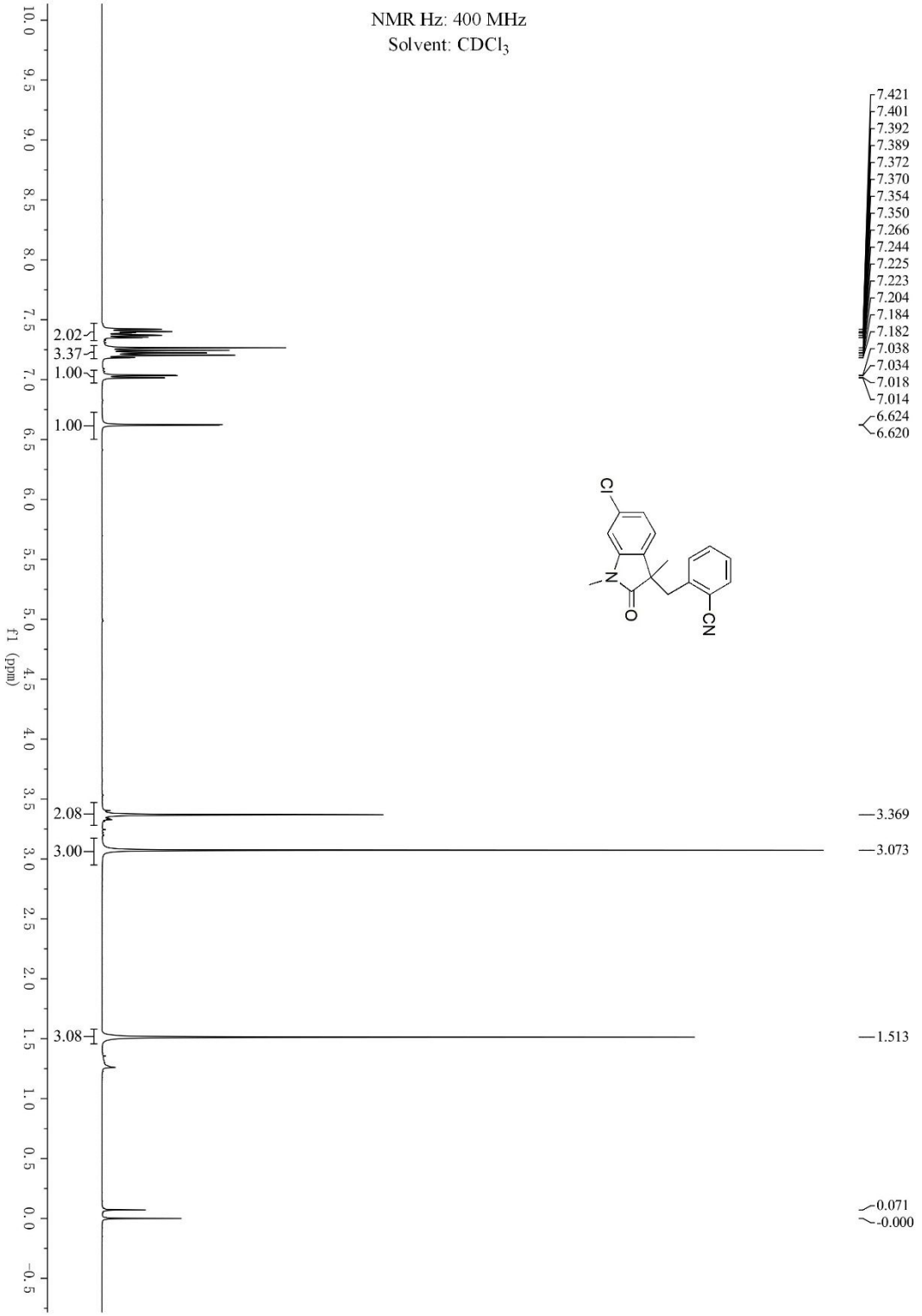

NMR Hz: 100 MHz
Solvent: CDCl3
179.805
156.241
143.908
140.899
132.586
131.606
130.008
129.387
126.798
117.924
117.085
113.322
105.583
100.814
77.318
77.000
76.683
55.135
50.161
39.989
26.153
21.126
f1 (ppm)

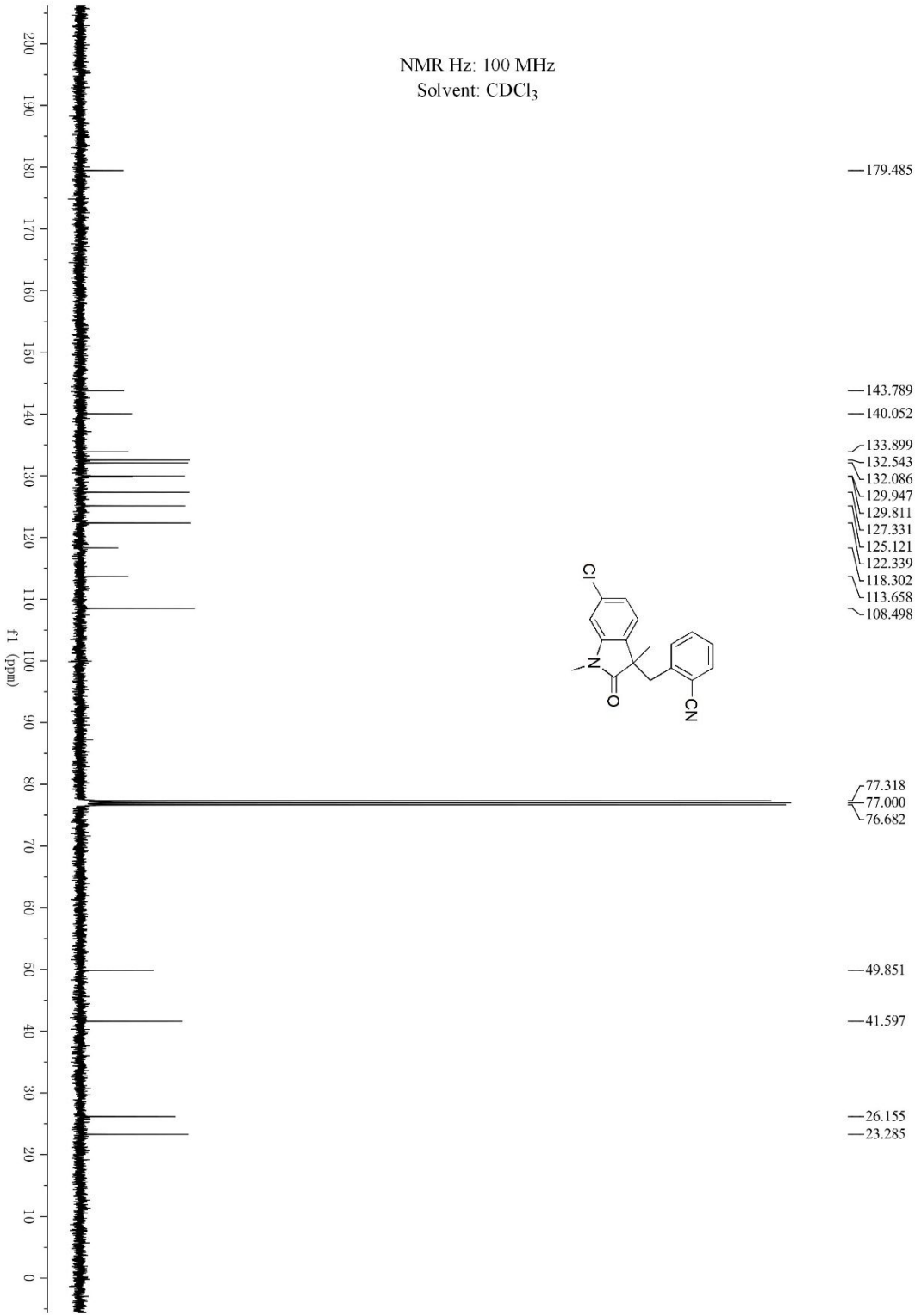
2-((4-Chloro-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ra)



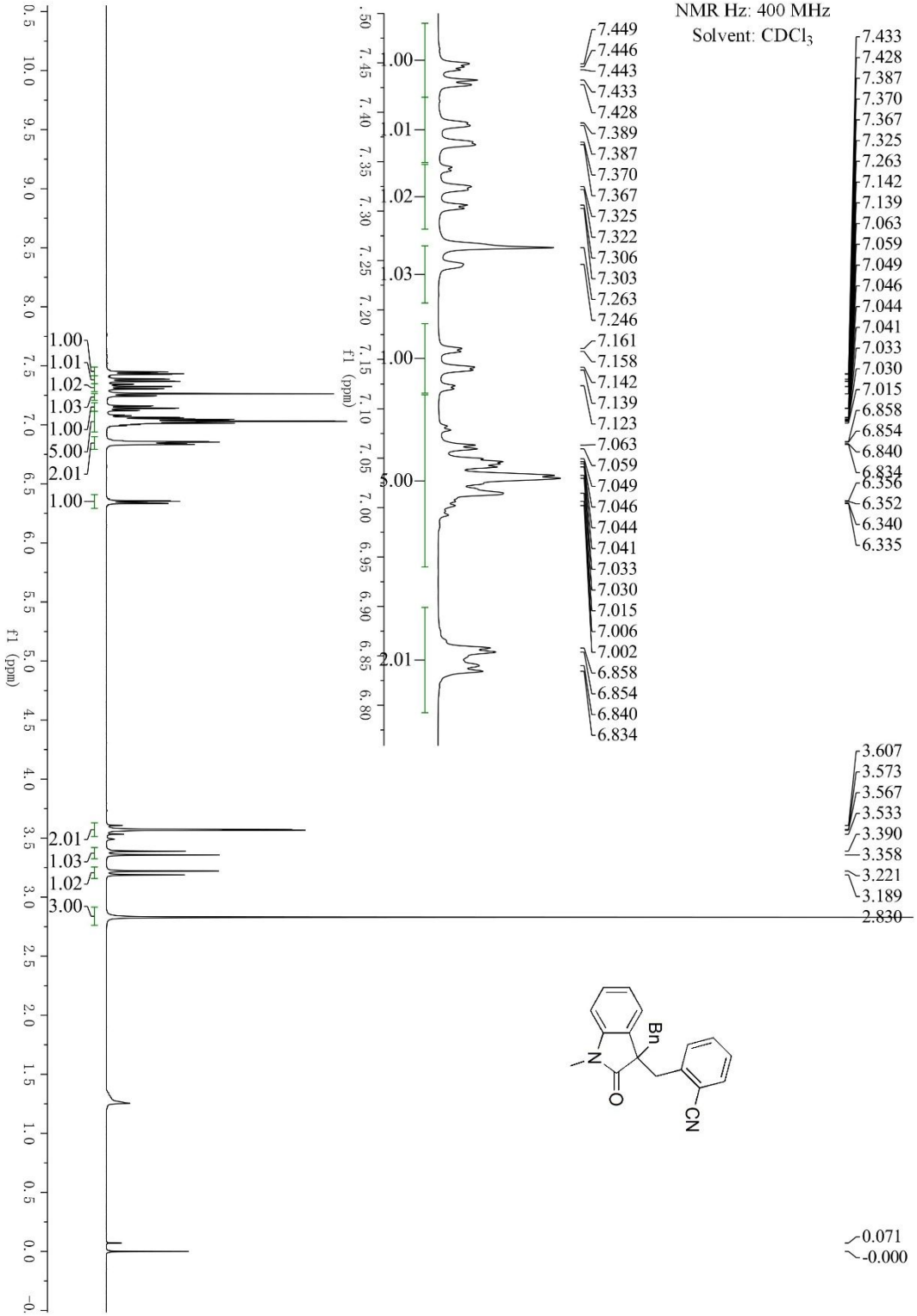

NMR Hz: 100 MHz
Solvent: CDCl3
178.202
144.741
139.783
132.796
131.740
131.211
129.973
129.505
128.479
127.156
123.835
117.754
113.610
106.358
77.317
77.000
76.682
50.767
39.272
26.200
20.533
f1 (ppm)
Cl
N
O
CN

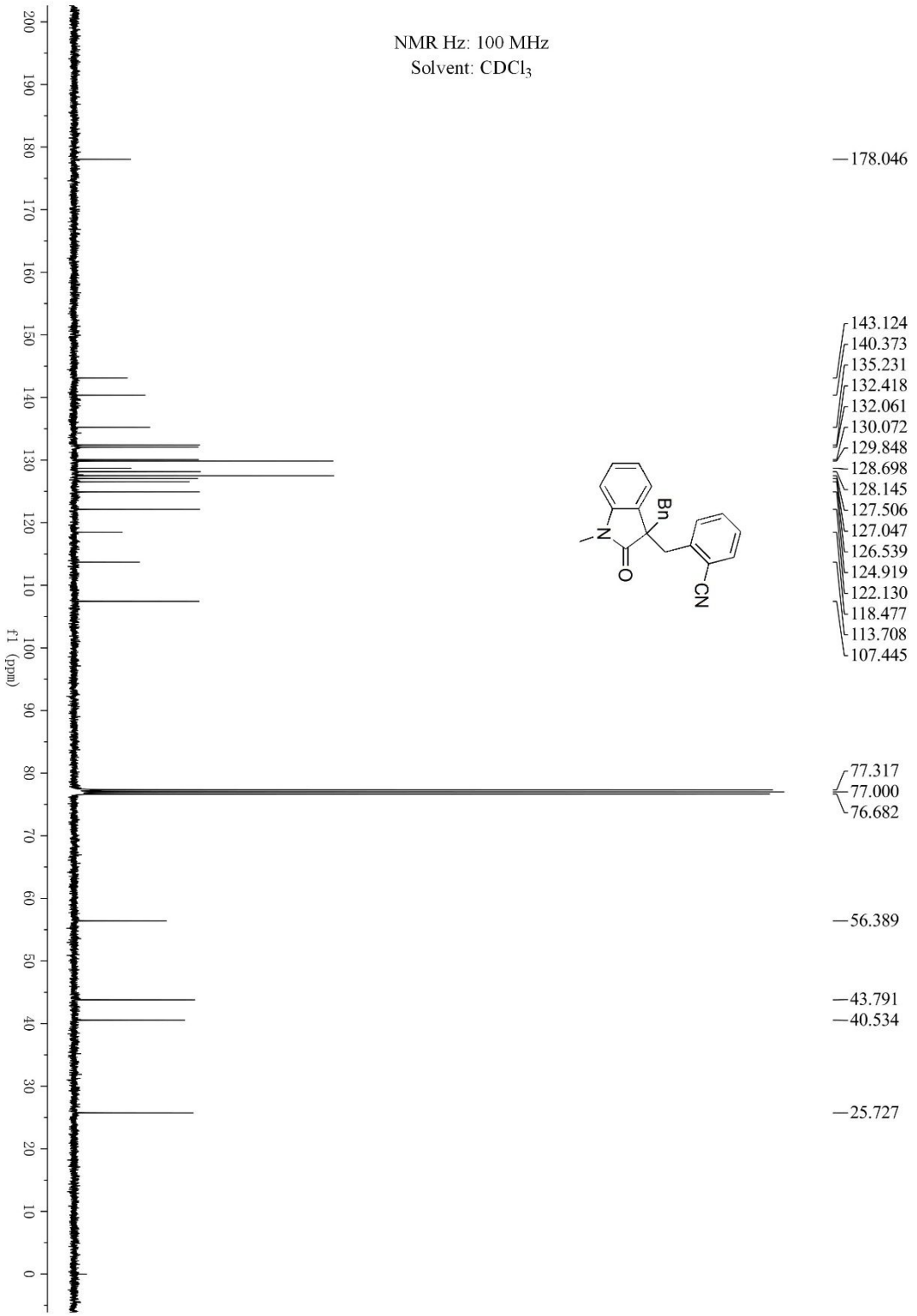
2-((6-chloro-1,3-dimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3ra')



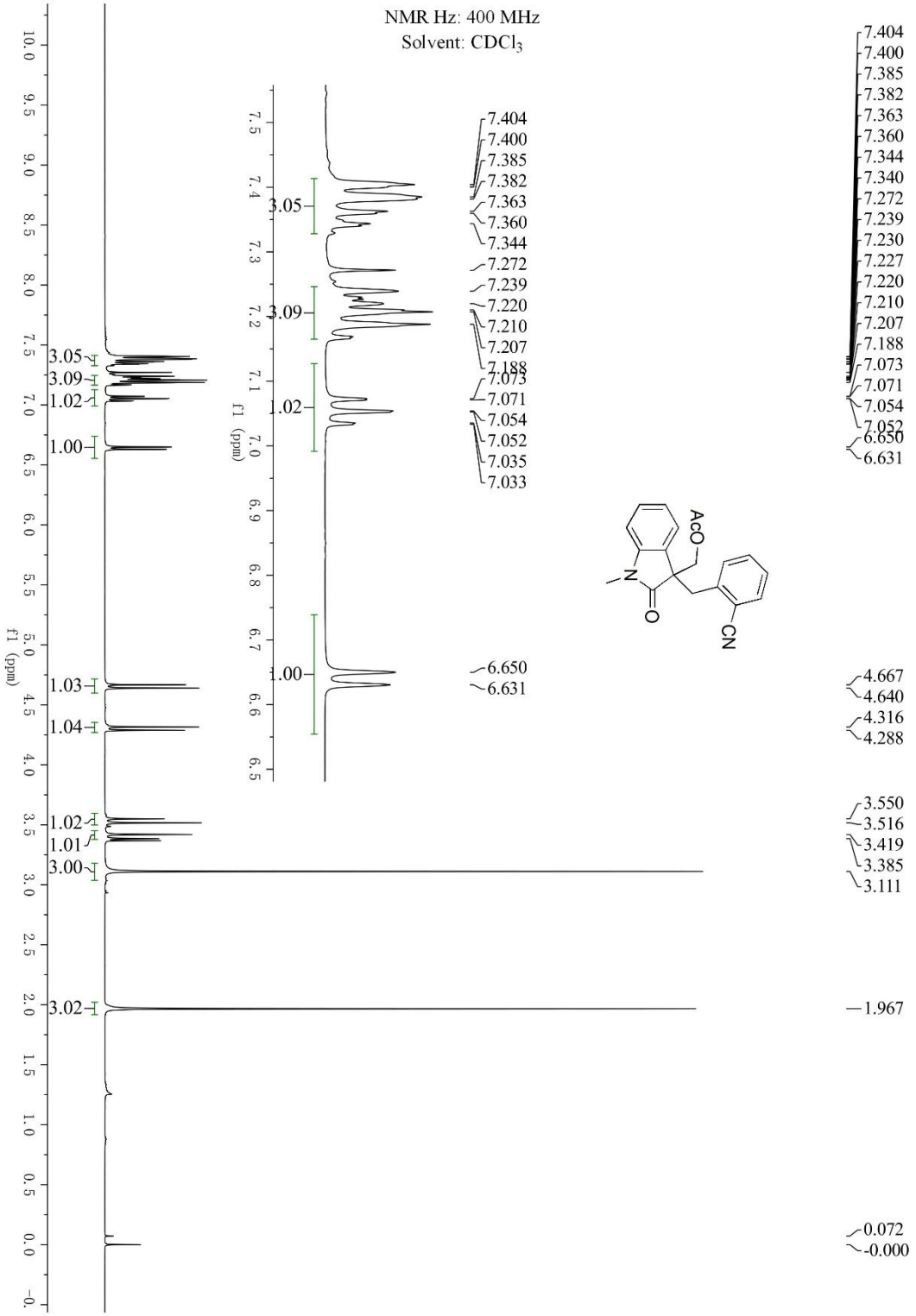

NMR Hz: 100 MHz
Solvent: CDCl3
179.485
143.789
140.052
133.899
132.543
132.086
129.947
129.811
127.331
125.121
122.339
118.302
113.658
108.498
77.318
77.000
76.682
49.851
41.597
26.155
23.285
f1 (ppm)
Cl
N
O
CN

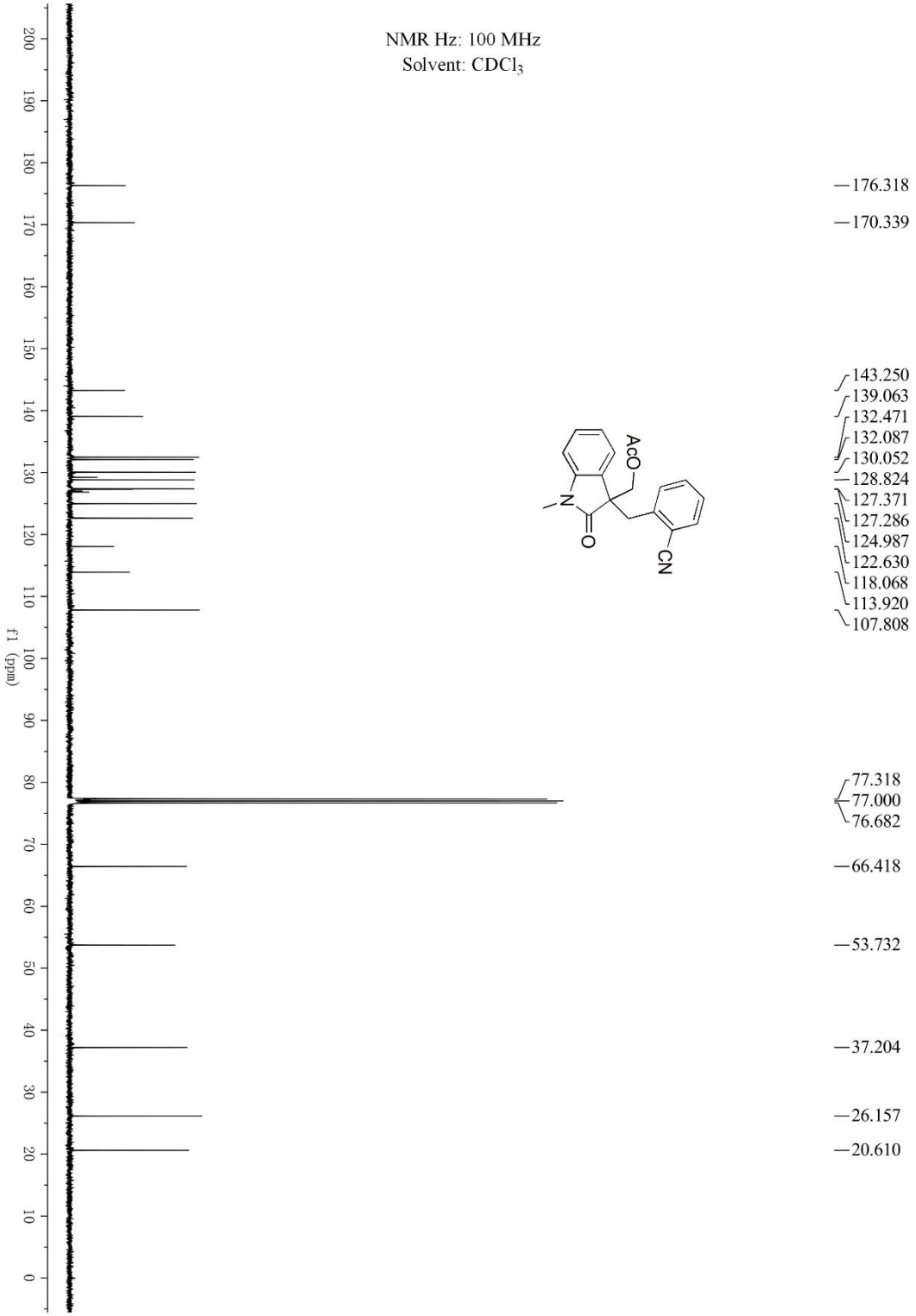
2-((3-Benzyl-1-methyl-2-oxoindolin-3-yl)methyl)benzonitrile (3sa)



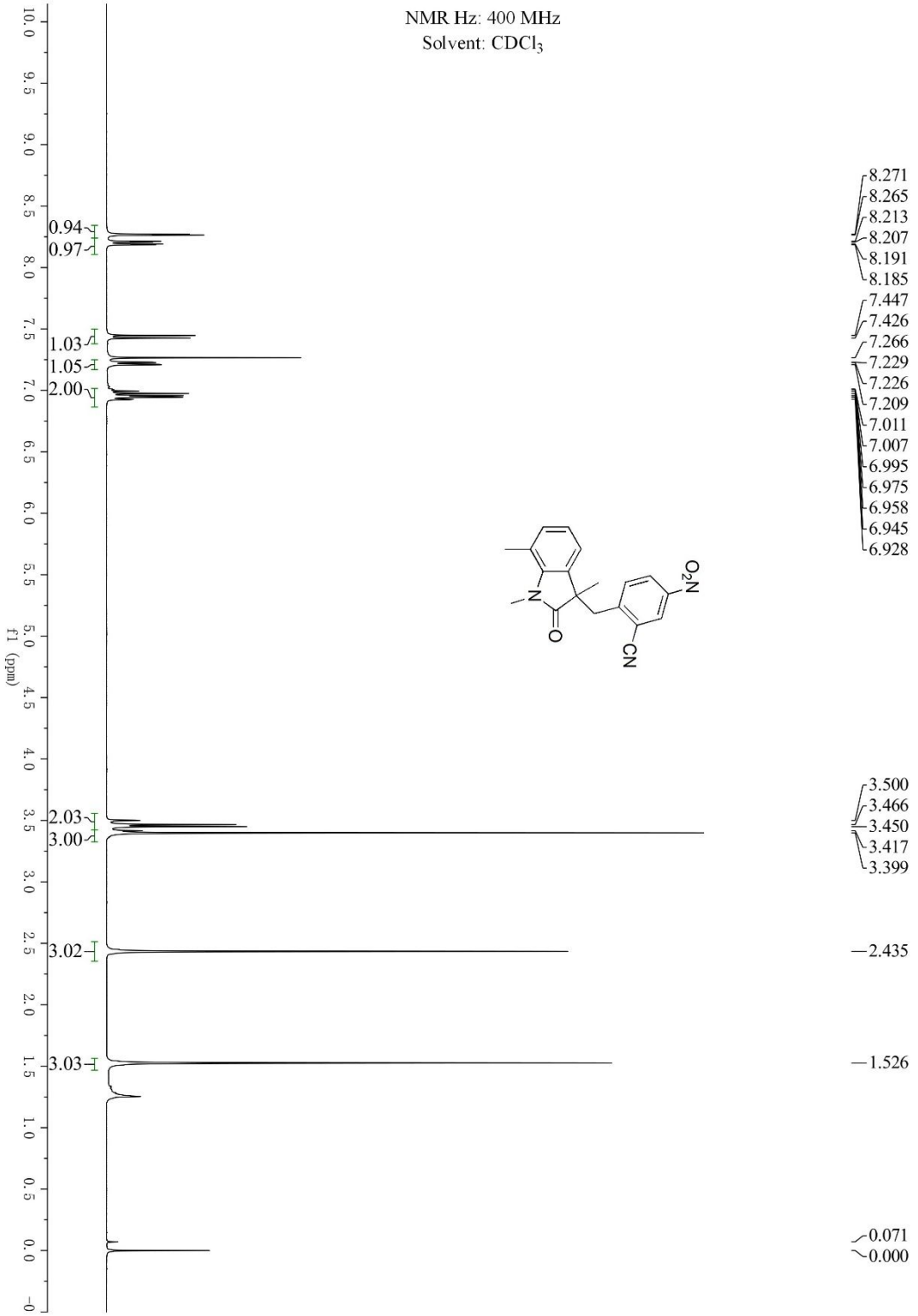

NMR Hz: 100 MHz
Solvent: CDCl3
178.046
143.124
140.373
135.231
132.418
132.061
130.072
129.848
128.698
128.145
127.506
127.047
126.539
124.919
122.130
118.477
113.708
107.445
77.317
77.000
76.682
56.389
43.791
40.534
25.727
Bn
N
O
CN
f1 (ppm)

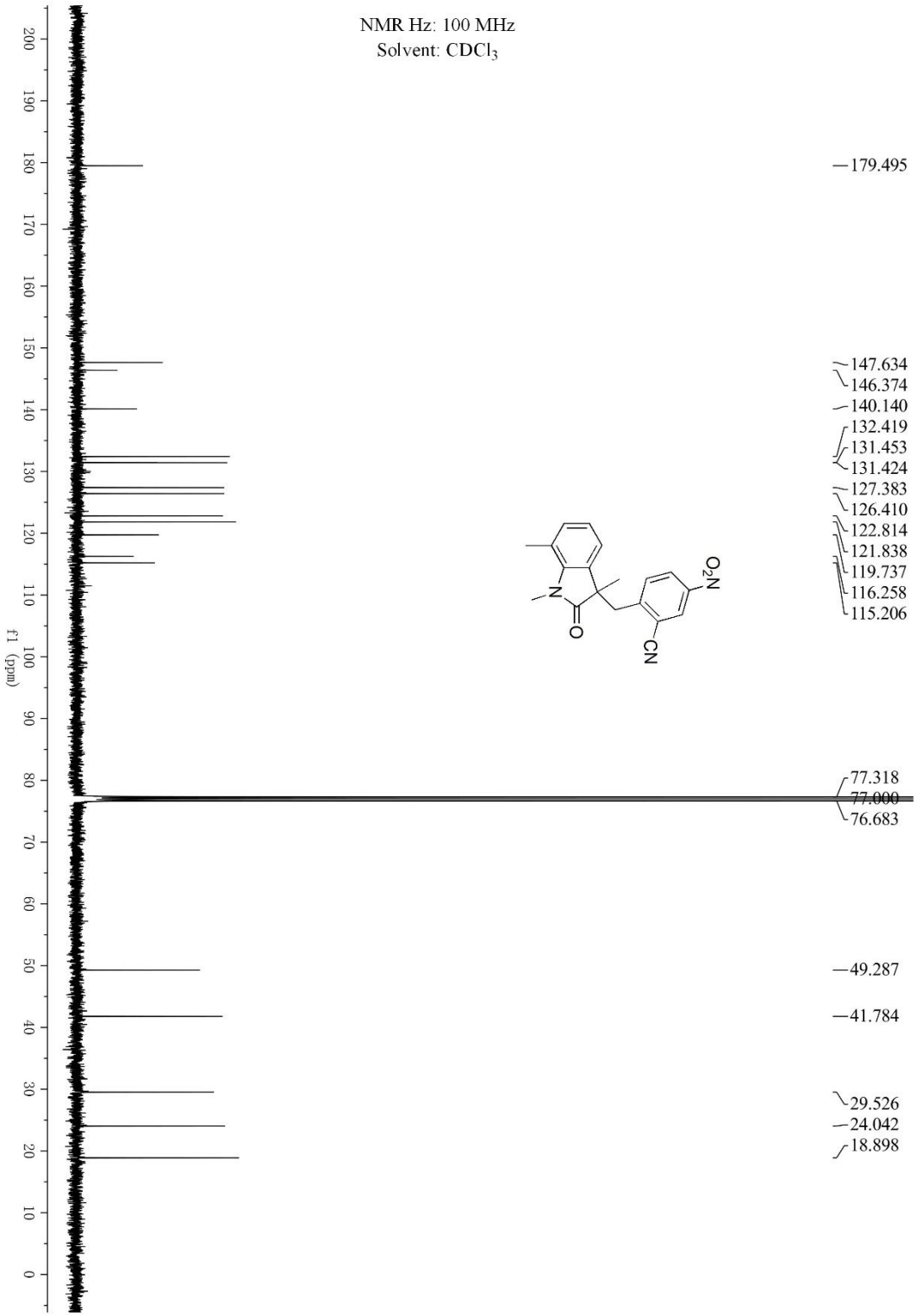
(3-(2-Cyanobenzyl)-1-methyl-2-oxoindolin-3-yl)methyl acetate (3ta)



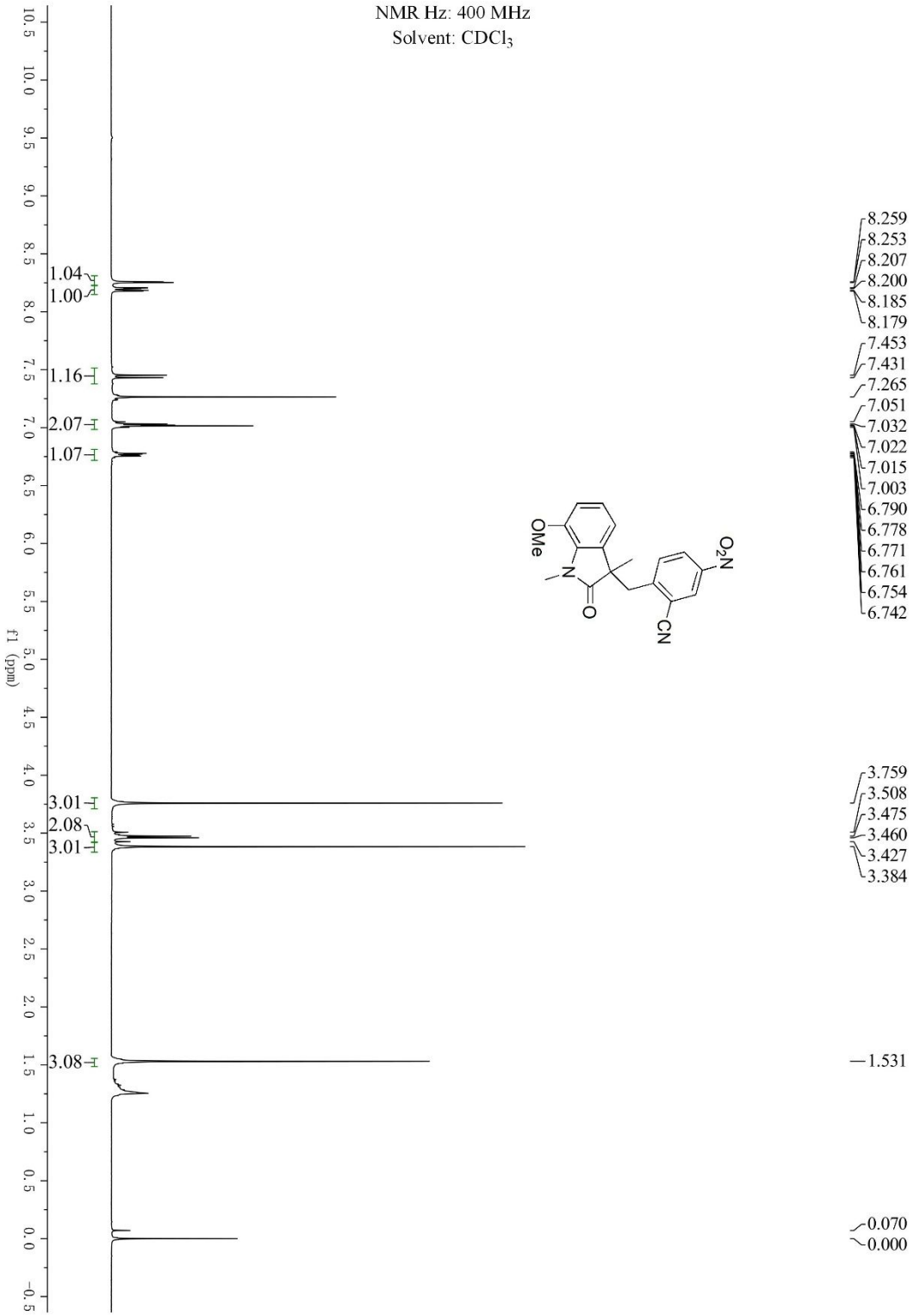

NMR Hz: 100 MHz
Solvent: $CDCl_3$
f1 (ppm)
176.318
170.339
143.250
139.063
132.471
132.087
130.052
128.824
127.371
127.286
124.987
122.630
118.068
113.920
107.808
77.318
77.000
76.682
66.418
53.732
37.204
26.157
20.610
AcO
N
O
CN

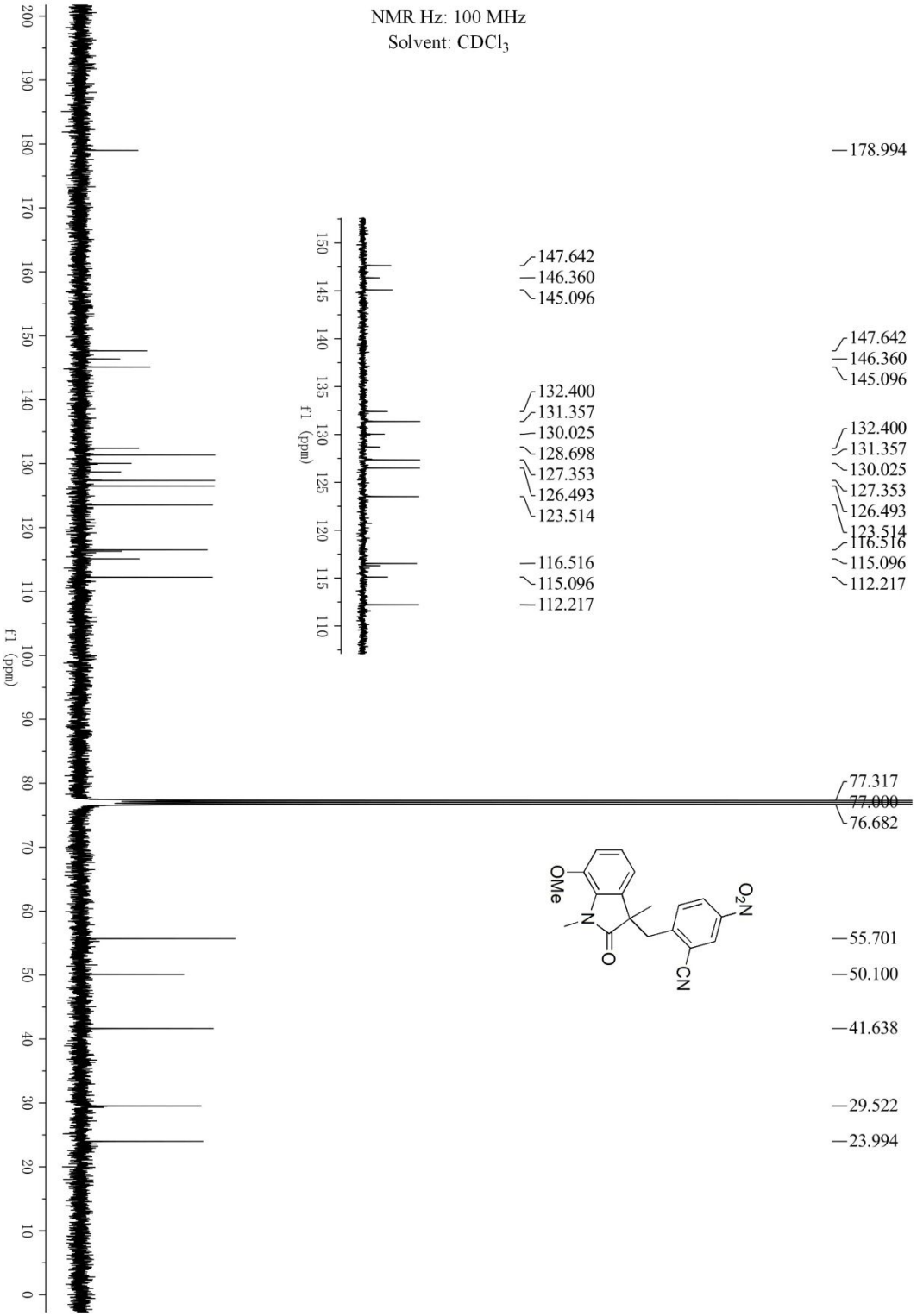
5-Nitro-2-((1,3,7-trimethyl-2-oxoindolin-3-yl)methyl)benzonitrile (3wj)



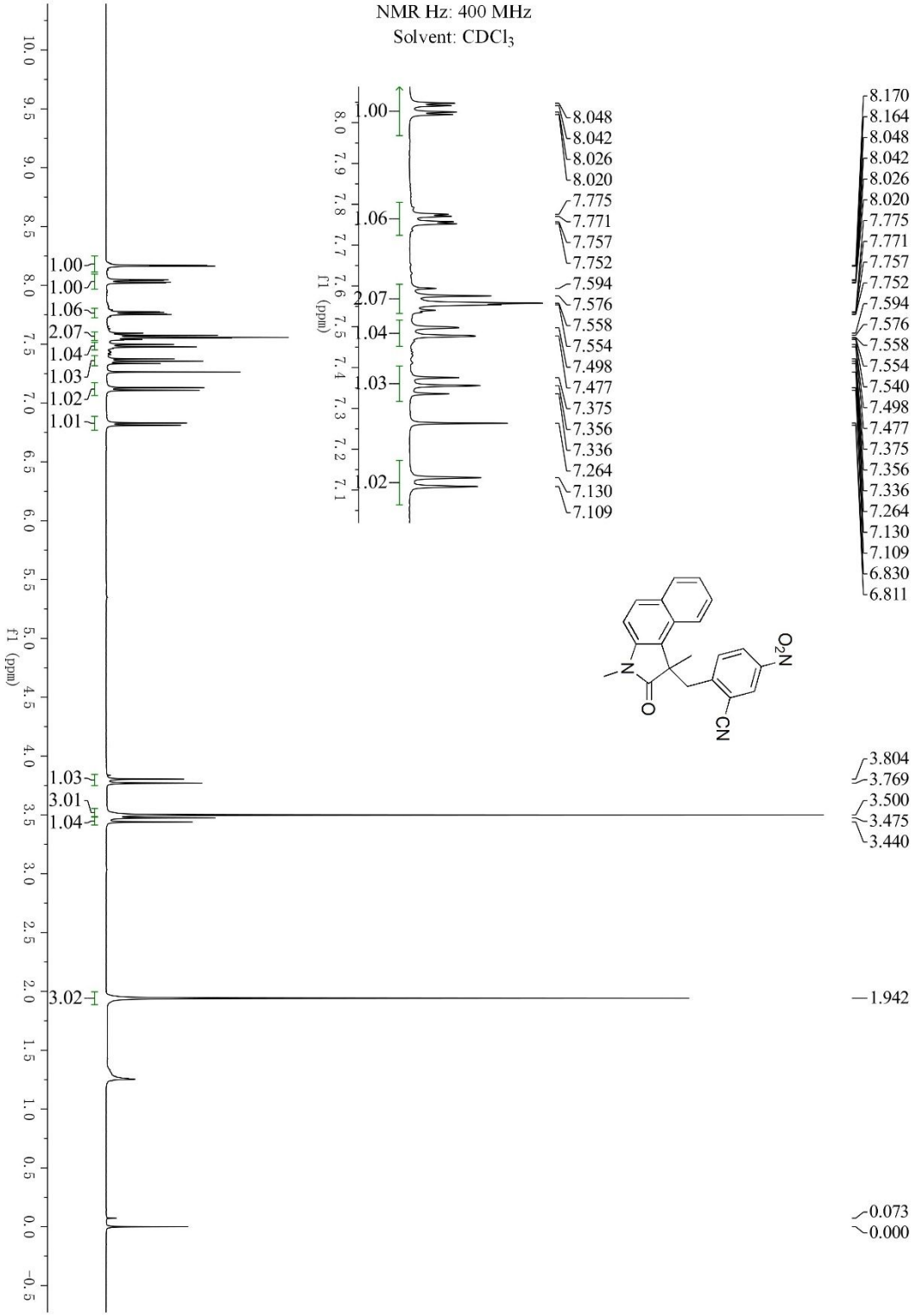

NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
179.495
147.634
146.374
140.140
132.419
131.453
131.424
127.383
126.410
122.814
121.838
119.737
116.258
115.206
77.318
77.000
76.683
49.287
41.784
29.526
24.042
18.898
O2N
CN
N
O

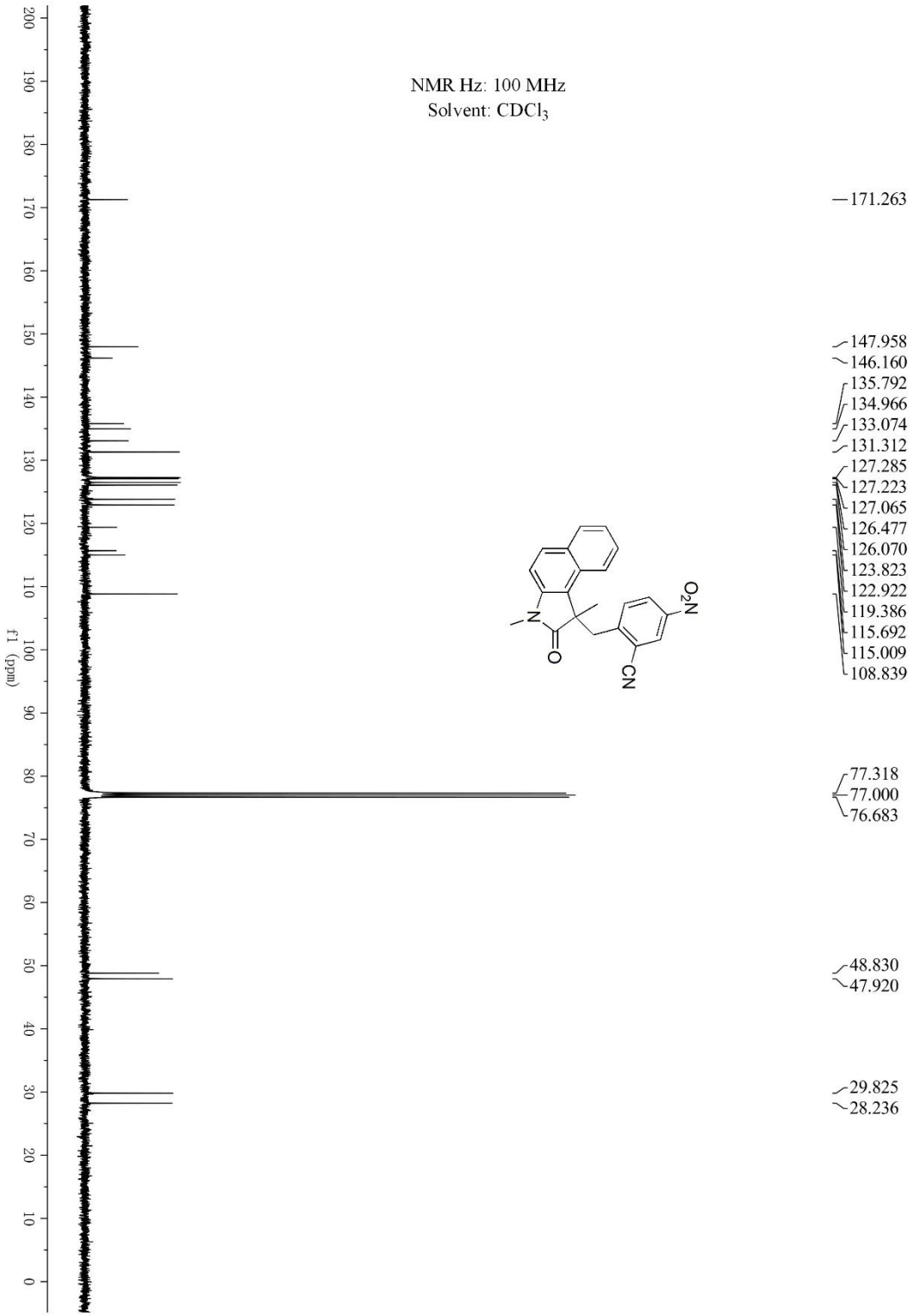
2-((7-Methoxy-1,3-dimethyl-2-oxoindolin-3-yl)methyl)-5-nitrobenzonitrile (3xj)



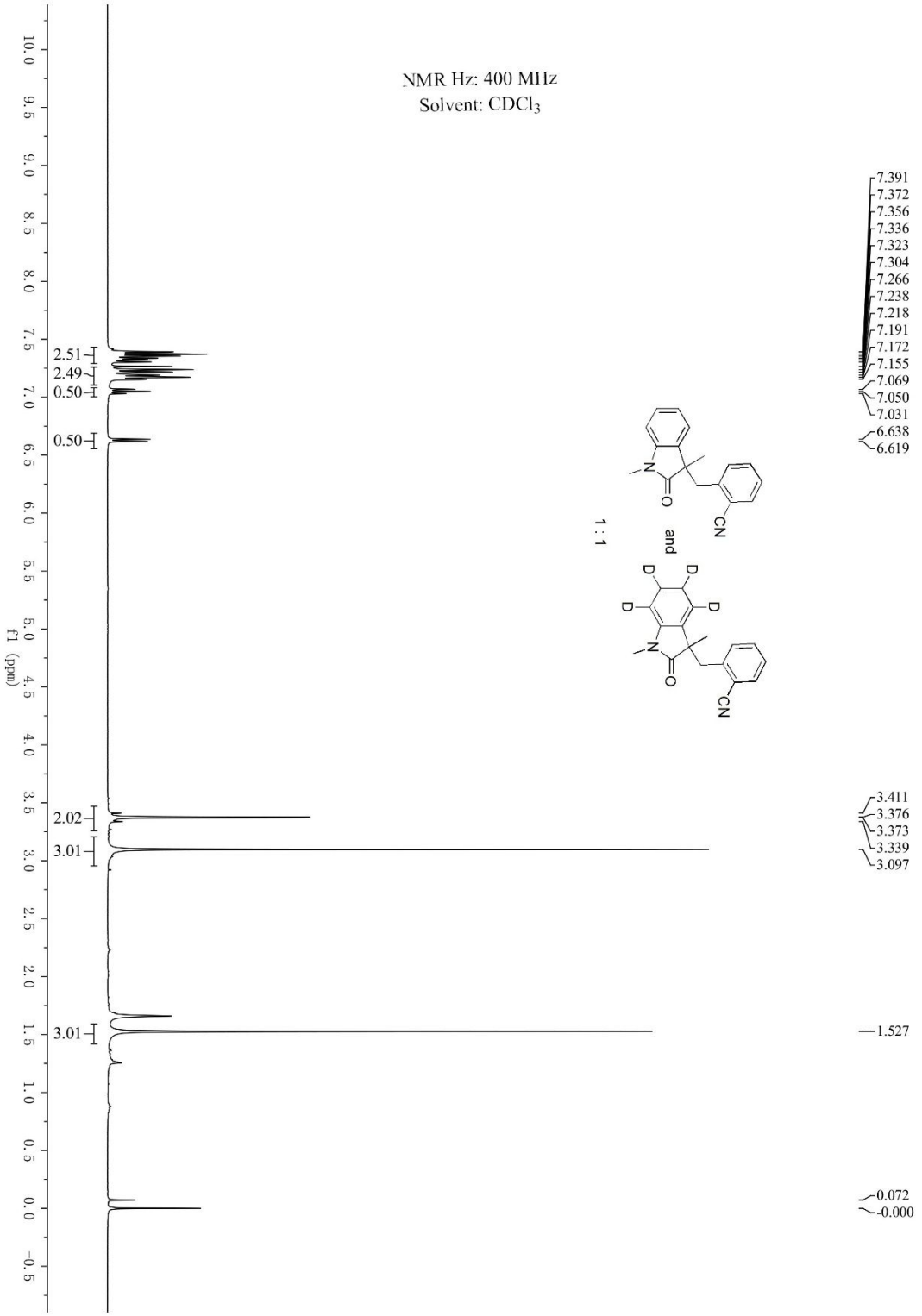

NMR Hz: 100 MHz
Solvent: CDCl3
178.994
147.642
146.360
145.096
132.400
131.357
130.025
128.698
127.353
126.493
123.514
116.516
115.096
112.217
77.317
77.000
76.682
55.701
50.100
41.638
29.522
23.994
OMe
N
O
O2N
CN
f1 (ppm)

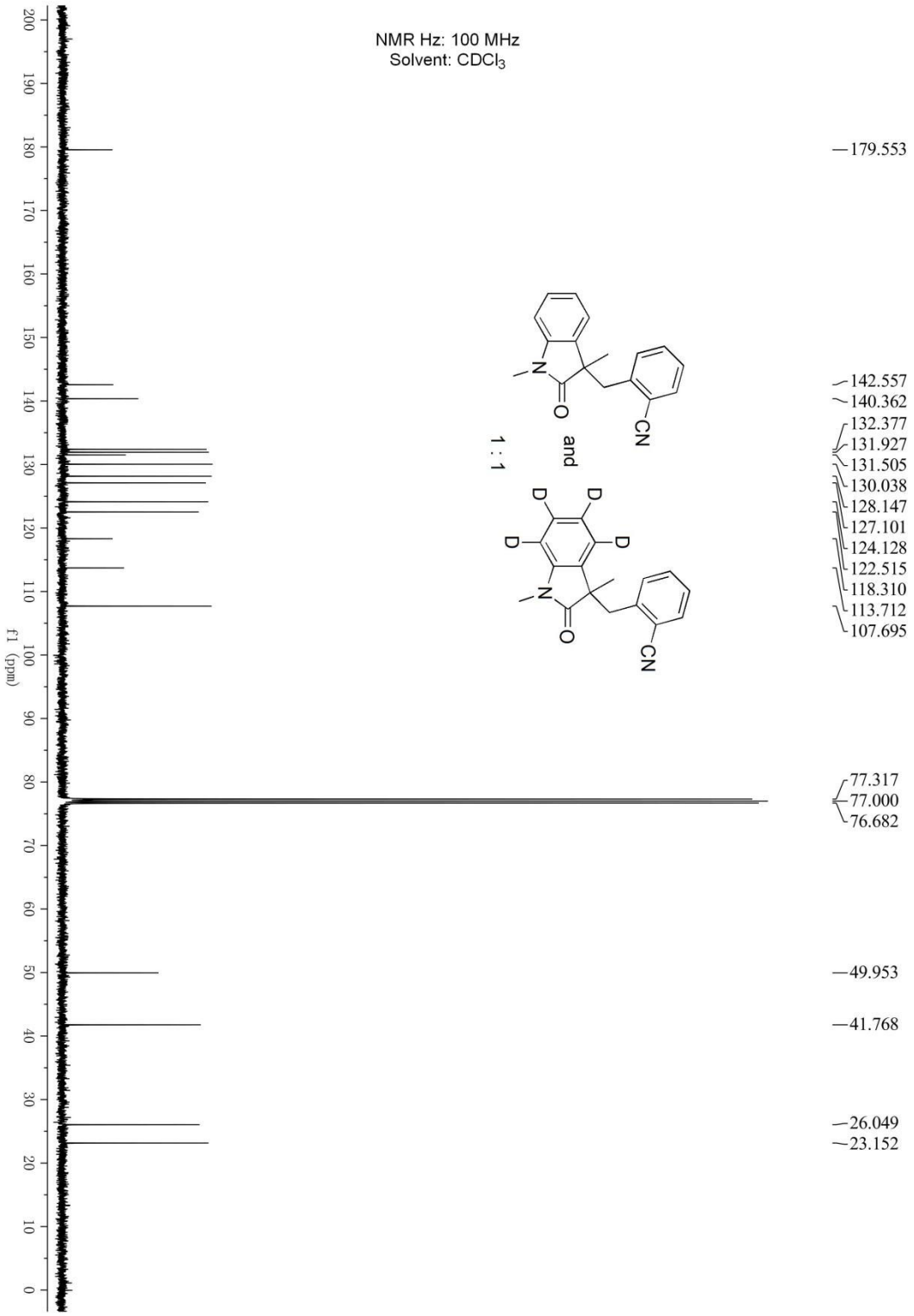
2-((1,3-Dmethyl-2-oxo-2,3-dihydro-1*H*-benzo[*f*]indol-3-yl)methyl)-5-nitrobenzonitrile (3yj)



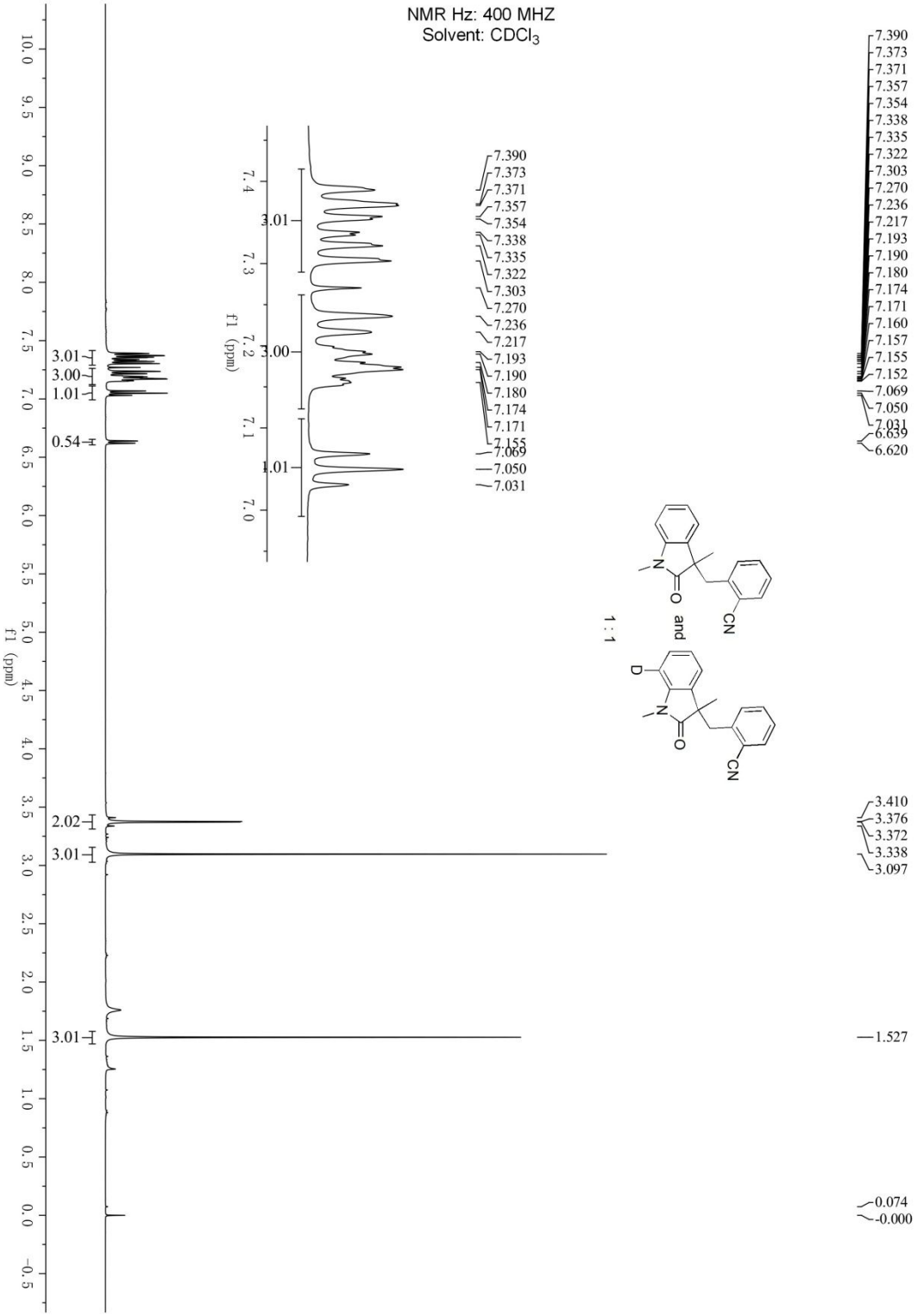

NMR Hz: 100 MHz
Solvent: CDCl3
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
171.263
147.958
146.160
135.792
134.966
133.074
131.312
127.285
127.223
127.065
126.477
126.070
123.823
122.922
119.386
115.692
115.009
108.839
77.318
77.000
76.683
48.830
47.920
29.825
28.236
N
O
O2N
CN

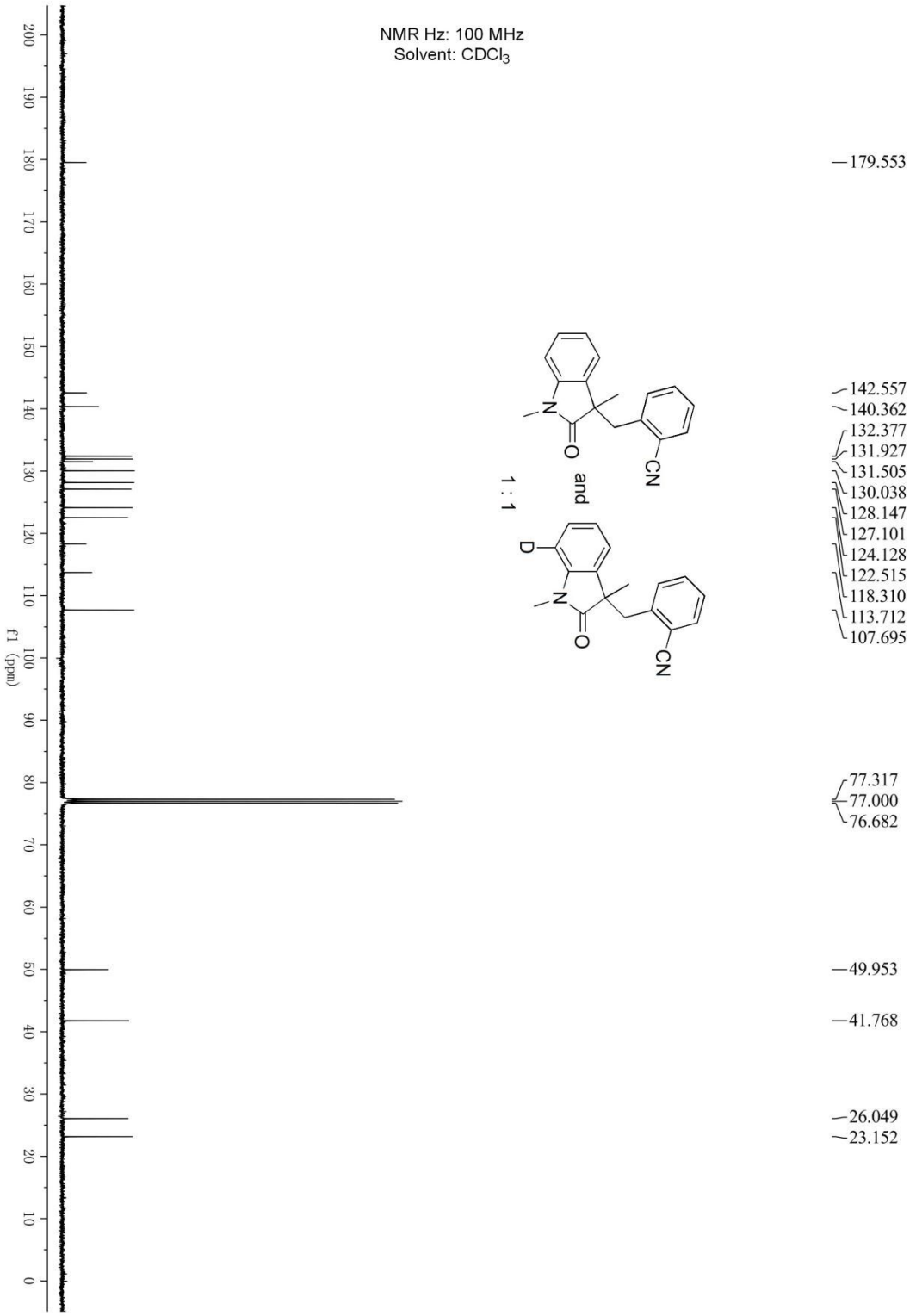
Product 3aa and 3aa-D_4




NMR Hz: 100 MHz
Solvent: CDCl3
179.553
142.557
140.362
132.377
131.927
131.505
130.038
128.147
127.101
124.128
122.515
118.310
113.712
107.695
77.317
77.000
76.682
49.953
41.768
26.049
23.152
f1 (ppm)
CN
and
1 : 1
D

Product 3aa and 3aa-D_1




NMR Hz: 100 MHz
Solvent: CDCl3
179.553
142.557
140.362
132.377
131.927
131.505
130.038
128.147
127.101
124.128
122.515
118.310
113.712
107.695
77.317
77.000
76.682
49.953
41.768
26.049
23.152
f1 (ppm)
CN
N
O
and
1 : 1
D
CN
N
O