Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2020

Stereoselective synthesis of trifluoroethyl 3,2'-spriooxindole γ-lactam through organocatalytic cascade reaction of 3-((2,2,2-trifluoroethyl)amino)indolin-2-one†

Shuai-Jiang Liu,‡[a] Qing Mao,‡[a] Gu Zhan,*[a] Rui Qin,[a] Ben-Hong Chen,[a] Jing Xue,[a] Meng-Lan Luo,[a] Qian Zhao*[a] and Bo Han*[a]

[a] School of Basic Medical Sciences, School of Pharmacy, State Key Laboratory of Southwestern Chinese Medicine Resources, Chengdu University of Traditional Chinese Medicine, Chengdu 611137, China. Email: zhangu@cdutcm.edu.cn; Email: zhaoq584@sina.cn; Email: hanbo@cdutcm.edu.cn

‡ These authors contributed equally.

Supporting information

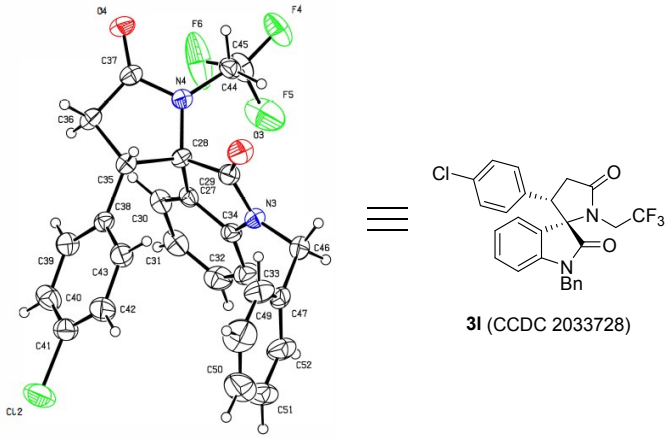
1. X-Ray Diffraction Data for Compound 3l 2

2. General procedure for the synthesis of compound 1 3

3. NMR of compound 1 9

4. NMR and HPLC spectra of intermediate I (3k') and compound 3 19

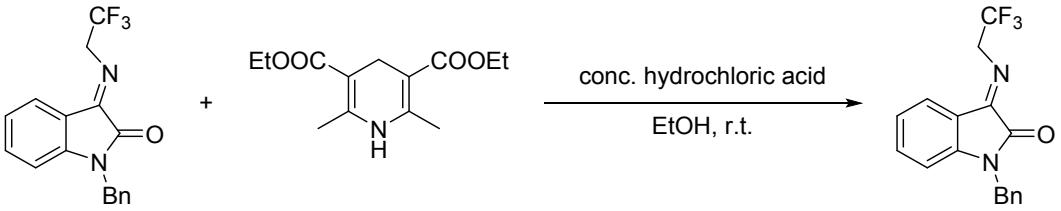
1. X-Ray Diffraction Data for Compound 3l



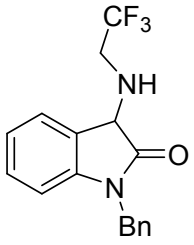
3l (CCDC 2033728)

Identification code	3l
Empirical formula	$C_{26}H_{20}ClF_3N_2O_2$
Formula weight	484.89
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	8.1617(4)
b/Å	24.6313(11)
c/Å	11.5178(7)
α/°	90
β/°	91.993(5)
γ/°	90
Volume/Å^3	2314.1(2)
Z	4
ρcalcg/cm^3	1.392
μ/mm^{-1}	0.216
F(000)	1000.0
Crystal size/mm3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.99 to 58.82
Index ranges	$-6 \le h \le 11$, $-19 \le k \le 31$, $-15 \le l \le 14$
Reflections collected	10939
Independent reflections	7552 [Rint = 0.0171, Rsigma = 0.0438]
Data/restraints/parameters	7552/1/613
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0505, wR_2 = 0.1091
Final R indexes [all data]	R_1 = 0.0763, wR_2 = 0.1220
Largest diff. peak/hole / e Å^{-3}	0.18/-0.29
Flack parameter	0.01(4)

2. General procedure for the synthesis of 3-((2,2,2-trifluoroethyl)amino)indoles 1

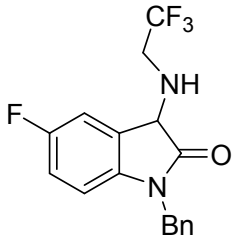


The reaction was carried out with *N*-2, 2, 2 trifluoroethyl isatin ketamines (5.0 mmol), Hantzsch ester (1.27 g, 5.0 mmol) in the presence of conc. hydrochloric acid (0.1 mL) in EtOH (35 ml) at room temperture. The reaction was monitored by TLC. The mixture was purified by flash chromatography (silica gel, hexane/ethyl acetate) to give the products **1**.



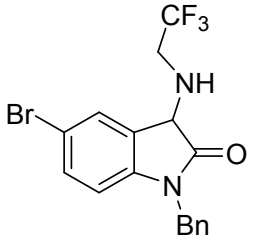
1a

1-benzyl-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1a). White solid, 1.42 g, 89% yield, m.p. 124–126 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.43 (d, *J* = 7.2 Hz, 1H), 7.35–7.27 (m, 5H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.08 (td, *J* = 7.2, 0.6 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 4.92 (d, *J* = 15.6 Hz, 1H), 4.84 (d, *J* = 15.6 Hz, 1H), 4.50 (s, 1H), 3.41–3.34 (m, 1H), 3.08–3.00 (m, 1H), 2.36 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 176.4, 143.4, 135.5, 129.5, 128.9, 127.8, 127.3, 125.1 (d, *J* = 274.5 Hz), 125.3, 125.2, 123.2, 109.4, 77.3, 77.0, 76.8, 59.3, 46.3 (q, *J* = 33.0 Hz), 43.9 ppm. ESI HRMS: calcd for $C_{17}H_{15}F_3N_2O + Na^+$ 343.1029, found 343.1034.



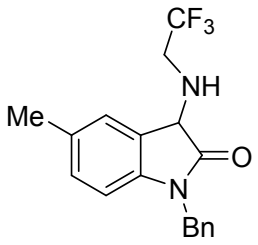
1b

1-benzyl-5-fluoro-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1b). White solid, 1.44 g, 85% yield, m.p. 130–132 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.34–7.27 (m, 5H), 7.20–7.18 (m, 1H), 6.94 – 6.90 (m, 1H), 6.64 (dd, *J* = 8.6, 4.2 Hz, 1H), 4.91 (d, *J* = 15.6 Hz, 1H), 4.83 (d, *J* = 15.6 Hz, 1H), 4.49 (s, 1H), 3.43–3.36 (m, 1H), 3.07–3.00 (m, 1H), 2.33 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 176.1, 159.5 (d, *J* = 240.0 Hz), 139.2, 135.2, 129.0, 128.0, 127.3, 127.1 (d, *J* = 9.0 Hz), 124.9, 115.9 (d, *J* = 24.0 Hz), 113.4 (d, *J* = 25.5 Hz), 110.1 (d, *J* = 7.5 Hz), 59.6, 45.5 (q, *J* = 31.5 Hz), 44.0 ppm. ESI HRMS: calcd for $C_{17}H_{14}F_4N_2O + Na^+$ 361.0934, found 361.0944.



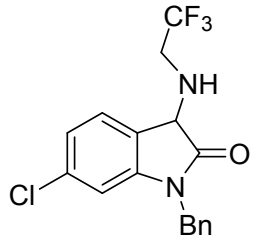
1d

1-benzyl-5-bromo-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1d). White solid, 1.79 g, 89% yield, m.p. 166–168 °C.^{1}H NMR (600 MHz, d_6-DMSO): δ = 7.47 (d, *J* = 1.2 Hz, 1H), 7.43–7.41 (m, 1H), 7.33–7.32 (m, 4H), 7.29–7.25 (m, 1H), 6.81 (d, *J* = 8.4 Hz, 1H), 4.88 (d, *J* = 15.6 Hz, 1H), 4.83 (d, *J* = 15.6*J* Hz, 1H), 4.61 (d, *J* = 7.8 Hz, 1H), 3.74–3.70 (m, 1H), 3.52–3.45 (m, 1H), 3.41–3.37 (m, 1H) ppm; ^{13}C NMR (150 MHz, d_6-DMSO): δ = 176.35, 142.68, 136.45, 131.77, 130.32, 129.08, 127.90, 127.81, 127.69, 126.17 (d, *J* = 275 Hz), 114.61, 111.50, 59.46, 47.20 (q, *J* = 30.0 Hz), 43.09 ppm. ESI HRMS: calcd for $C_{17}H_{14}BrF_3N_2O + Na^+$ 421.0134, found 421.0134.



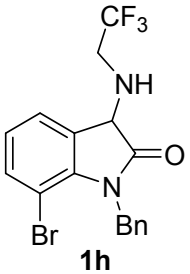
1e

1-benzyl-5-methyl-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1e). White solid, 1.47 g, 88% yield, m.p. 145–147 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.35–7.27 (m, 5H), 7.25 (s, 1H), 7.03–7.01 (m, 1H), 6.62 (d, *J* = 7.8 Hz, 1H), 4.90 (d, *J* = 15.6 Hz, 1H), 4.83 (d, 15.6 Hz, 1H), 4.46 (s, 1H), 3.41–3.34 (m, 1H), 3.10–3.03 (m, 1H), 2.31 (s, 3H), 1.67 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 176.3, 140.9, 135.6, 132.9, 129.7, 128.9, 126.9 (d, *J* = 267.0 Hz), 127.3, 125.3, 124.2, 109.2, 59.4, 46.4 (q, *J* = 31.5 Hz), 43.9, 21.0 ppm. ESI HRMS: calcd for $C_{18}H_{17}F_3N_2O$ + Na^+ 357.1185, found 357.1193.



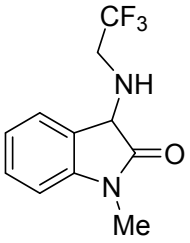
1f

1-benzyl-6-chloro-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1f). White solid, 1.42 g, 80% yield, m.p. 140–142 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.36–7.33 (m, 3H), 7.30–7.26 (m, 3H), 7.06 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.73 (d, *J* = 1.8 Hz, 1H), 4.89 (d, *J* = 15.6 Hz, 1H), 4.81 (d, *J* = 15.6 Hz, 1H), 4.46 (s, 1H), 3.41–3.34 (m, 1H), 3.06–3.00 (m, 1H), 2.33 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 176.37, 144.52, 135.35, 134.98, 129.04, 128.07, 127.30, 126.21, 124.94 (d, *J* = 274.5 Hz), 123.65, 123.13, 110.02, 58.95, 46.33 (q, *J* = 33.0 Hz), 43.99 ppm. ESI HRMS: calcd for $C_{17}H_{14}ClF_3N_2O$ + Na^+ 377.0639, found 377.0645.



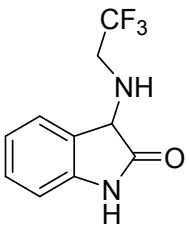
1h

1-benzyl-7-bromo-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1h). White solid, 1.58 g, 79% yield, m.p. 112–114 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.42–7.40 (m, 2H), 7.33–7.26 (m, 3H), 7.25–7.20 (m, 3H), 6.97 (dd, *J* = 7.8, 7.2 Hz, 1H), 5.38 (s, 2H), 4.48 (s, 1H), 3.40–3.33 (m, 1H), 3.07–3.00 (m, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 177.2, 140.8, 137.1, 135.5, 128.7, 128.6, 127.3, 126.4, 125.0 (d, *J* = 274.5 Hz), 124.5, 124.4, 124.0, 102.8, 58.8, 46.4 (q, *J* = 33.0 Hz), 44.6 ppm. ESI HRMS: calcd for $C_{17}H_{14}BrF_3N_2O$ + Na^+ 421.0134, found 421.0134.



1i

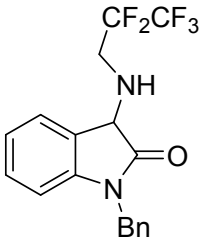
1-methyl-3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1i). White solid, 1.00 g, 82% yield, m.p. 80–82 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.43 (d, *J* = 7.2 Hz, 1H), 7.36–7.33 (m, 1H), 7.12 (td, *J* = 7.2, 0.6 Hz, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 4.40 (s, 1H), 3.37–3.30 (m, 1H), 3.20 (s, 3H), 3.06–3.00 (m, 1H), 2.18 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 176.3, 144.3, 129.6, 126.0 (d, *J* = 276.0 Hz), 125.3, 125.1, 123.1, 108.4, 59.3, 46.4 (q, *J* = 31.5 Hz), 26.2 ppm. ESI HRMS: calcd for $C_{11}H_{11}F_3N_2O$ + Na^+ 267.0716, found 267.0727.



1j

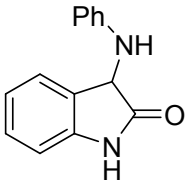
3-((2,2,2-trifluoroethyl)amino)indolin-2-one (1j). White solid, 0.98 g, 85% yield,

m.p. 118–120 °C. ^{1}H NMR (600 MHz, d_6-DMSO): δ = 10.33 (s, 1H), 7.29 (d, J = 7.2 Hz, 1H), 7.22–7.19 (m, 1H), 6.97 (td, J = 7.8, 0.6 Hz, 1H), 6.80 (d, J = 7.2 Hz, 1H), 4.31 (d, J = 6.0 Hz, 1H), 3.49–3.46 (m, 1H), 3.44–3.39 (m, 1H), 3.29–3.22 (m, 1H) ppm; ^{13}C NMR (150 MHz, d_6-DMSO): δ = 178.50, 142.96, 129.17, 128.14, 126.22 (d, J = 276.0 Hz), 125.23, 121.96, 109.94, 59.73, 46.93 (q, J = 30.0 Hz) ppm. ESI HRMS: calcd for $C_{10}H_{19}F_3N_2O$ + Na^+ 253.0559, found 253.0564.



1w

1-benzyl-3-((2,2,3,3,3-pentafluoropropyl)amino)indolin-2-one (1w). White solid, 1.52 g, 82% yield, m.p. 49–51 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.41 (d, J = 7.2 Hz, 1H), 7.34 – 7.28 (m, 5H), 7.23 (t, J = 7.8 Hz, 1H), 7.08 (t, J = 7.8 Hz, 1H), 6.75 (d, J = 7.8 Hz, 1H), 4.94 (d, J = 15.6 Hz, 1H), 4.84 (d, J = 15.6 Hz, 1H), 4.50 (s, 1H), 3.41 (q, J = 13.8 Hz, 1H), 3.09 (m, 1H), 2.28 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 176.4, 143.4, 135.5, 129.6, 128.9, 127.9, 127.3, 125.2, 125.2, 123.2, 119.9 (t, J = 3.6 Hz), 118.0 (t, J = 3.6 Hz), 115.7 (d, J = 3.6 Hz), 114.0 (d, J = 3.6 Hz), 109.4, 59.5, 44.5 (t, J = 2.4 Hz), 43.9 ppm. ESI HRMS: calcd for $C_{18}H_{15}F_5N_2O$ + Na^+ 393.0997, found 393.0995.

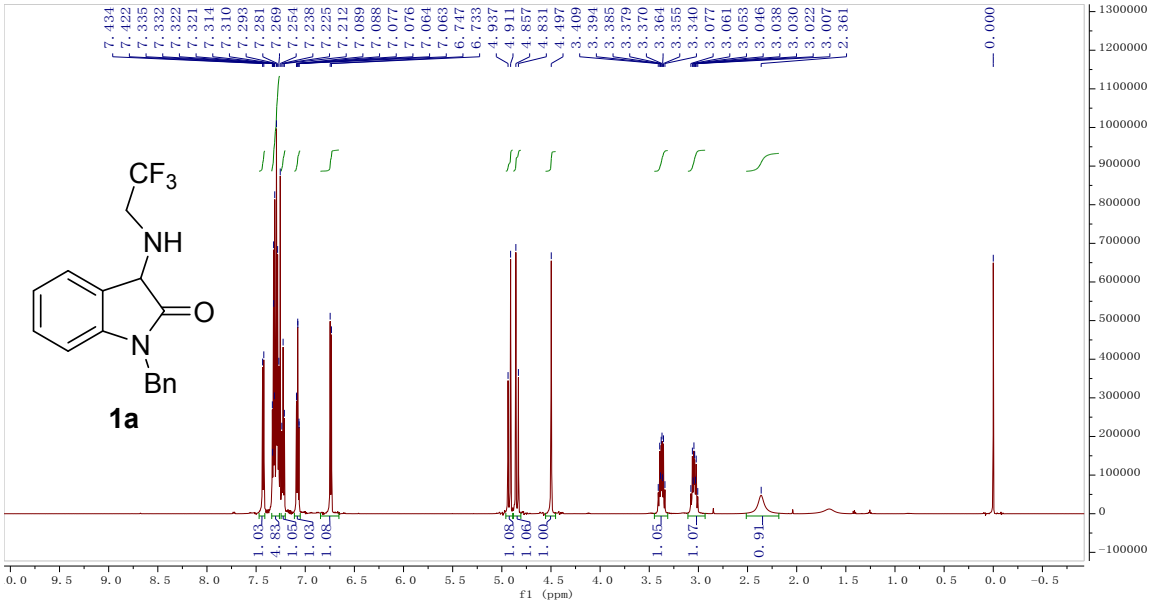


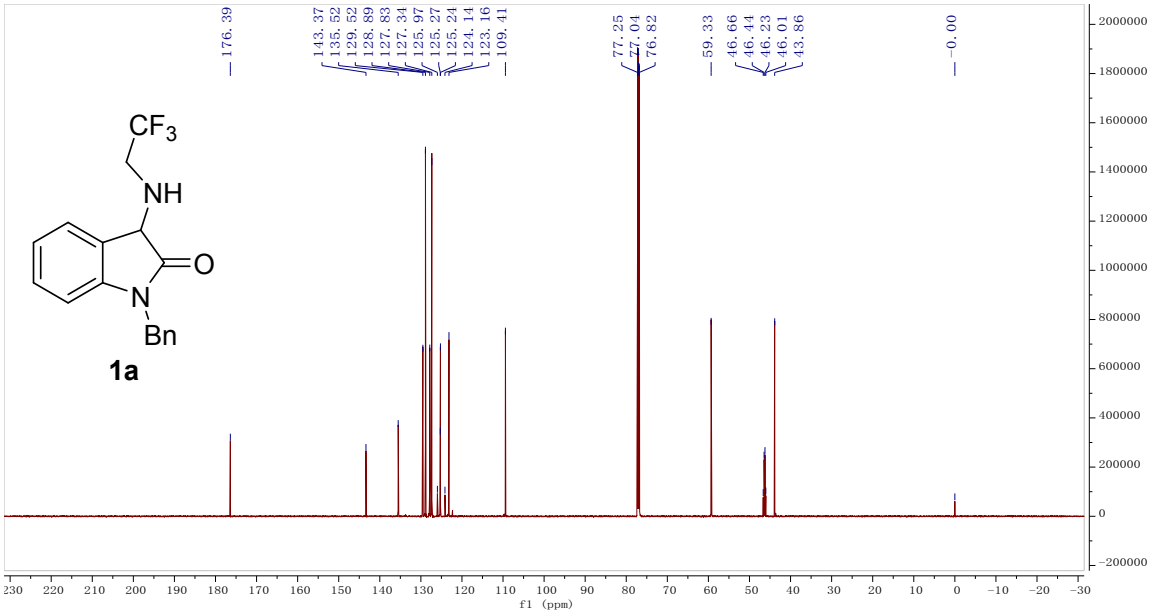
1x

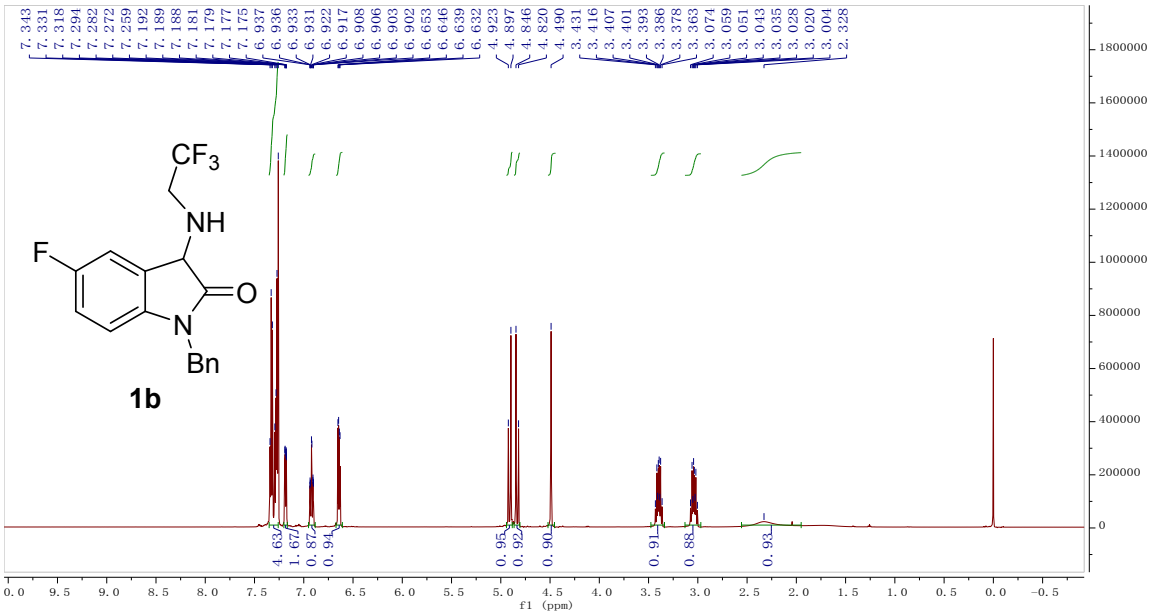
3-(phenylamino)indolin-2-one (1x). Pale yellow solid, 0.89 g, 79% yield, m.p. 150–152 °C. ^{1}H NMR (600 MHz, d_6-DMSO): δ = 10.51 (s, 1H), 7.22 (t, J = 7.2 Hz, 1H), 7.18 (d, J = 7.2 Hz, 1H), 7.02 – 6.99 (m, 2H), 6.94 (t, J = 7.2 Hz, 1H), 6.87 (d, J = 7.8 Hz, 1H), 6.53 (t, J = 7.2 Hz, 1H), 6.48 (m, 3H), 5.07 (d, J = 8.4 Hz, 1H) ppm; ^{13}C NMR (150 MHz, d_6-DMSO): δ = 177.52, 147.97, 142.42, 129.23, 129.03, 128.66, 124.54, 122.05, 116.83, 113.14, 110.14, 56.34 ppm. ESI HRMS: calcd for $C_{14}H_{12}N_2O$ + Na^+

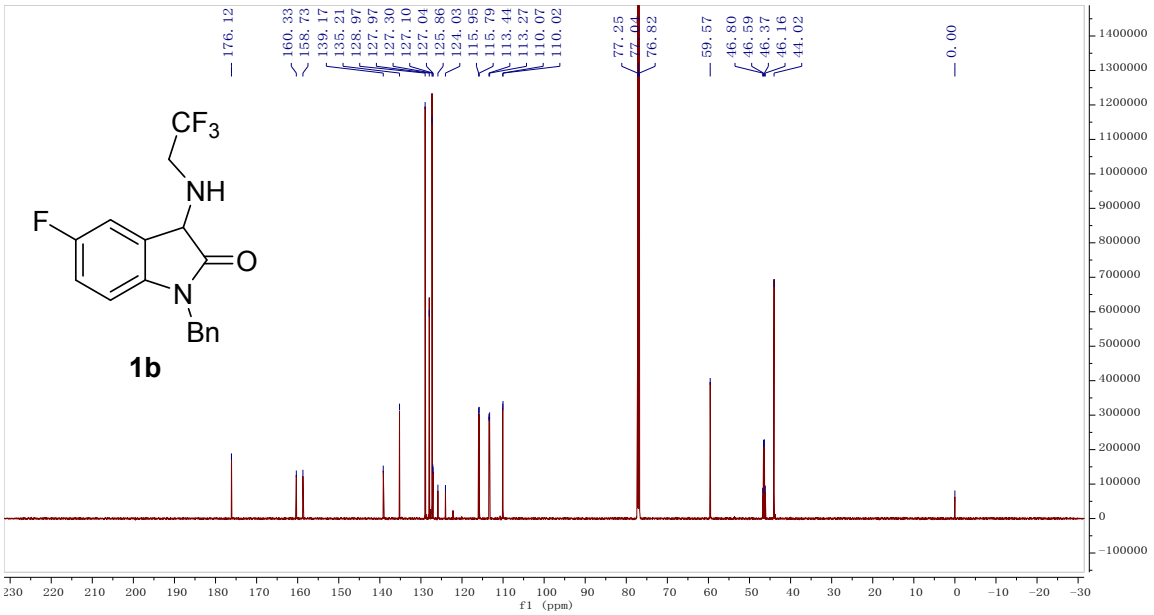
247.0842, found 247.0839.

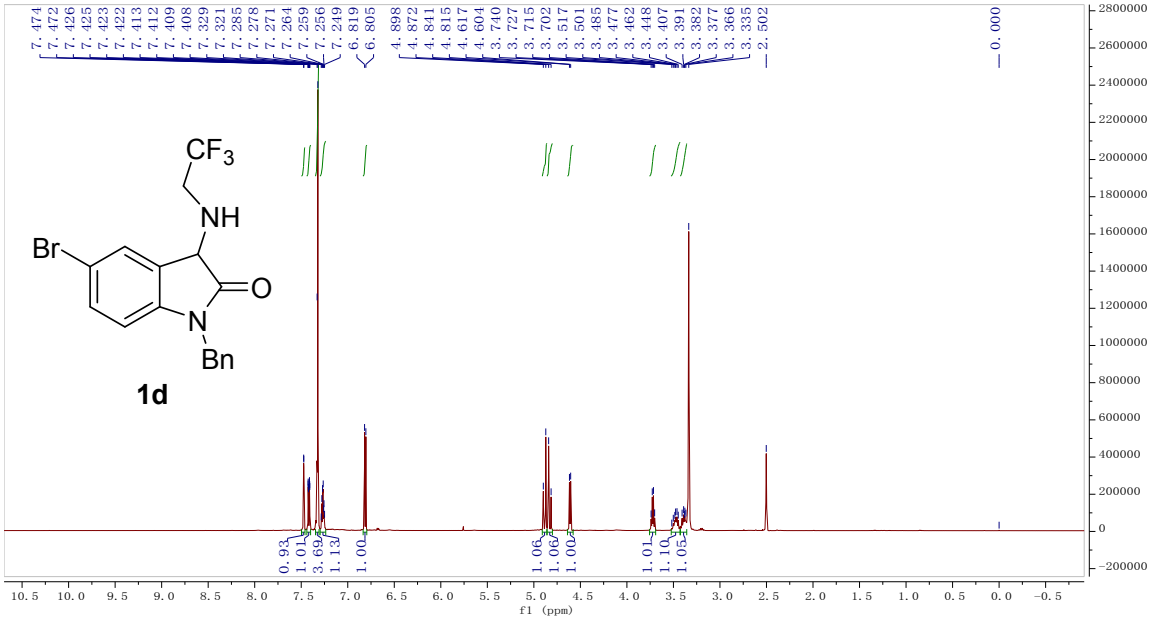
3. NMR of compound 1

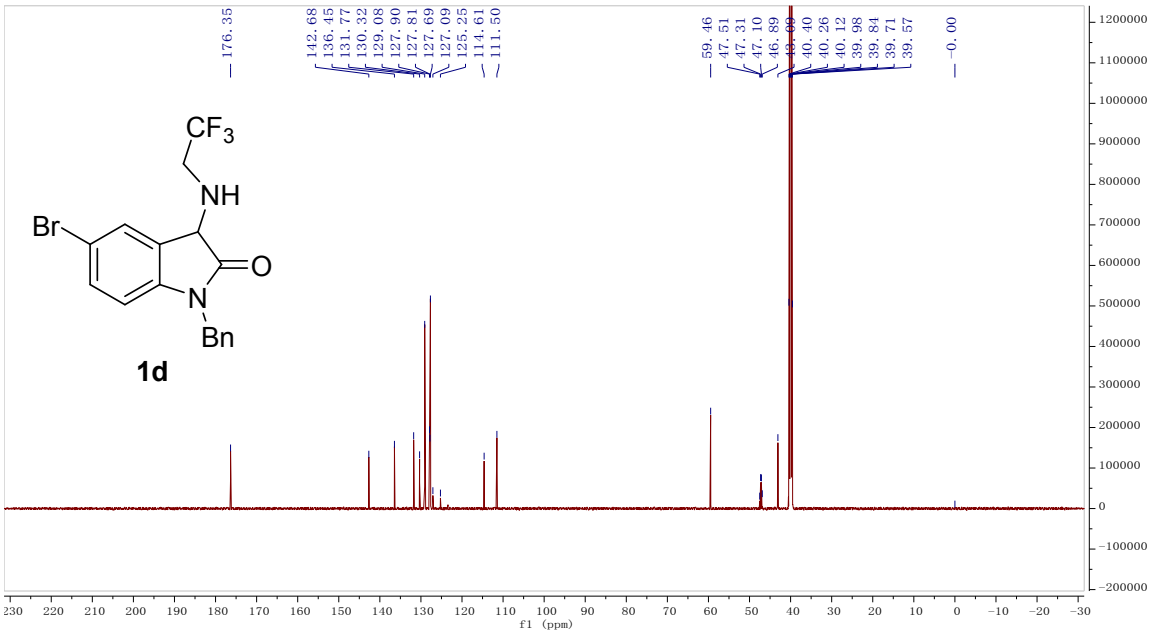


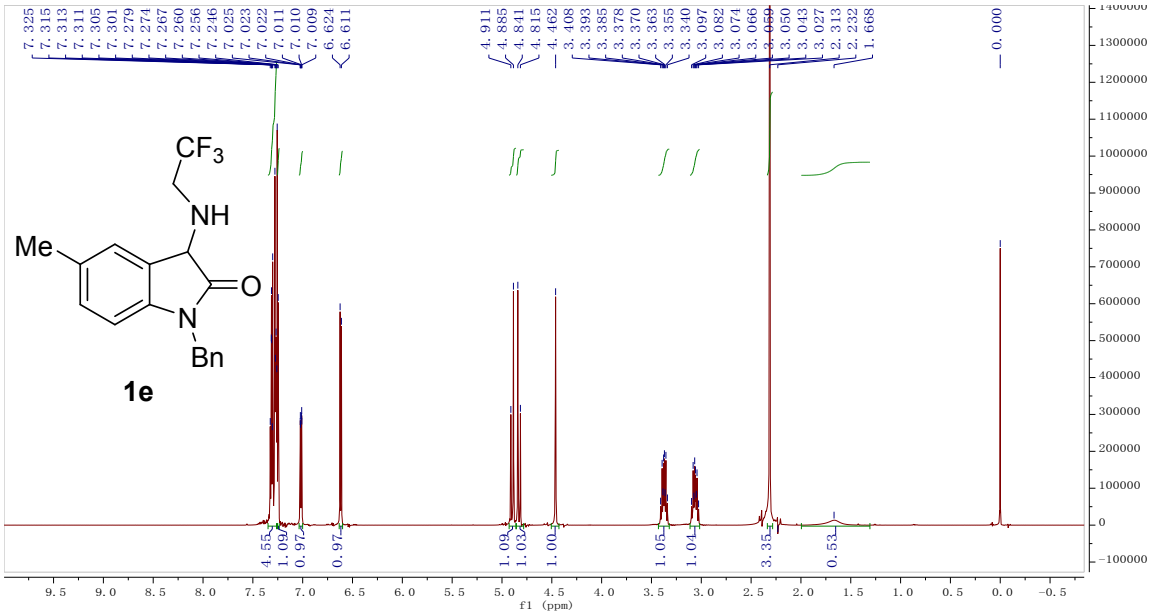


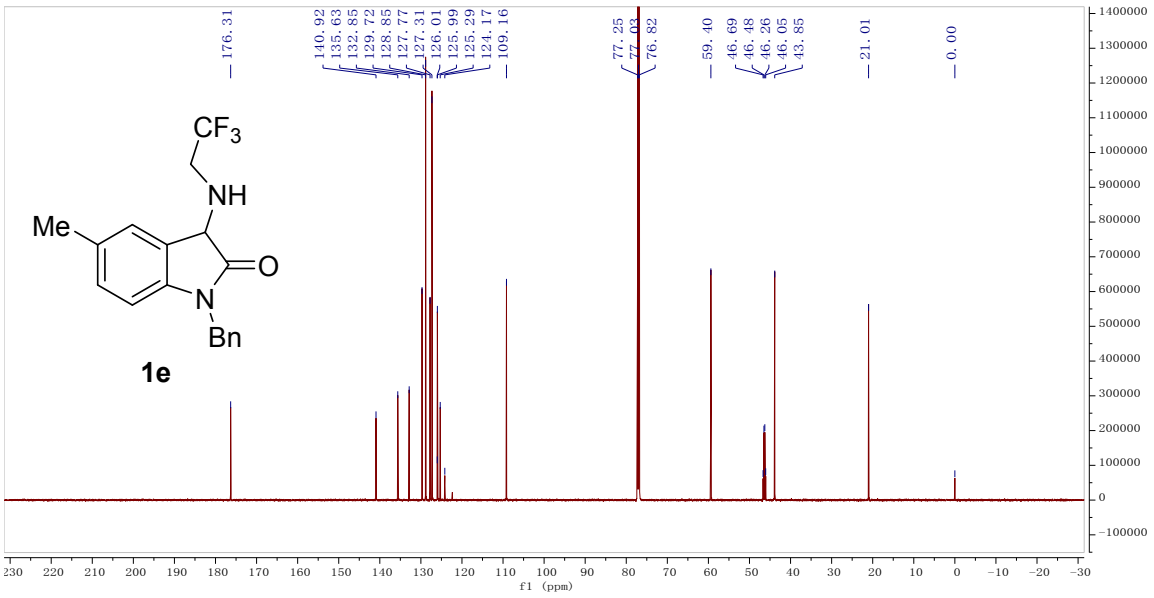

7.343
7.331
7.318
7.294
7.282
7.272
7.259
7.192
7.189
7.188
7.181
7.179
7.177
7.175
6.937
6.936
6.933
6.931
6.922
6.917
6.908
6.906
6.903
6.902
6.653
6.646
6.639
6.632
4.923
4.897
4.846
4.820
4.490
3.431
3.416
3.407
3.401
3.393
3.386
3.378
3.363
3.074
3.059
3.051
3.043
3.035
3.028
3.020
3.004
2.328
CF3
NH
F
O
N
Bn
1b
4.63
1.67
0.87
0.94
0.95
0.92
0.90
0.91
0.88
0.93
f1 (ppm)

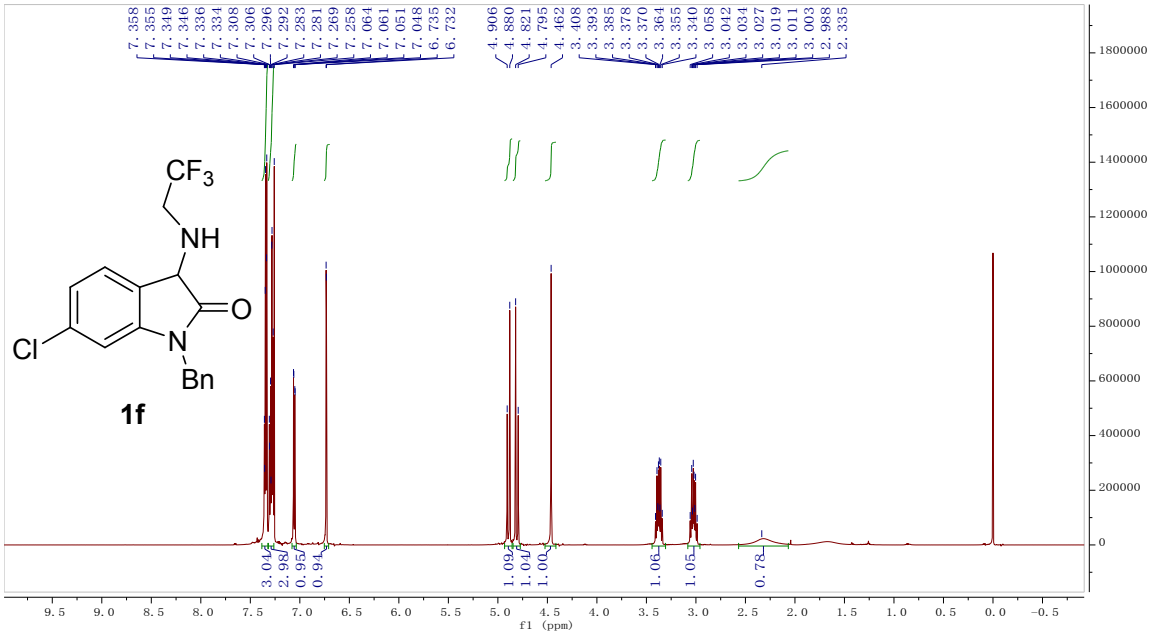

176.12
160.33
158.73
139.17
135.21
128.97
127.97
127.30
127.10
127.04
125.86
124.03
115.95
115.79
113.44
113.27
110.07
110.02
77.25
77.04
76.82
59.57
46.80
46.59
46.37
46.16
44.02
0.00
CF3
NH
F
O
N
Bn
1b
f1 (ppm)

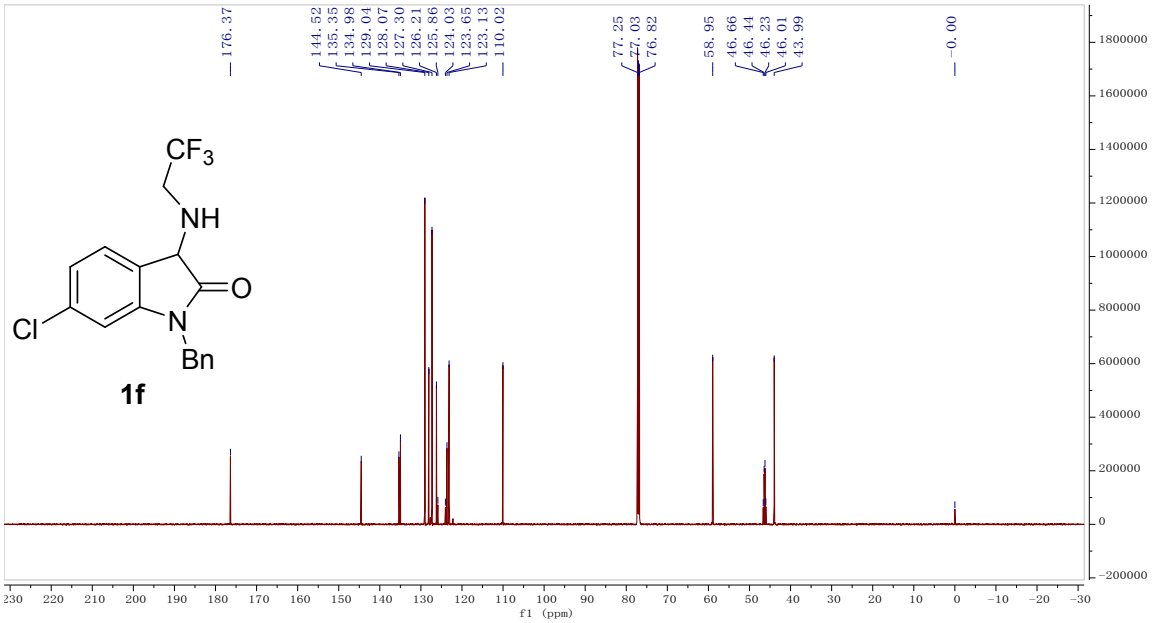

7.474
7.472
7.426
7.425
7.423
7.422
7.413
7.412
7.409
7.408
7.329
7.321
7.285
7.278
7.271
7.264
7.259
7.256
7.249
6.819
6.805
4.898
4.872
4.841
4.815
4.617
4.604
4.740
3.727
3.715
3.702
3.517
3.501
3.485
3.477
3.462
3.448
3.407
3.391
3.382
3.377
3.366
3.335
2.502
0.000
CF3
NH
Br
O
N
Bn
1d
0.93
1.01
3.69
1.13
1.00
1.06
1.06
1.00
1.01
1.10
1.05
f1 (ppm)

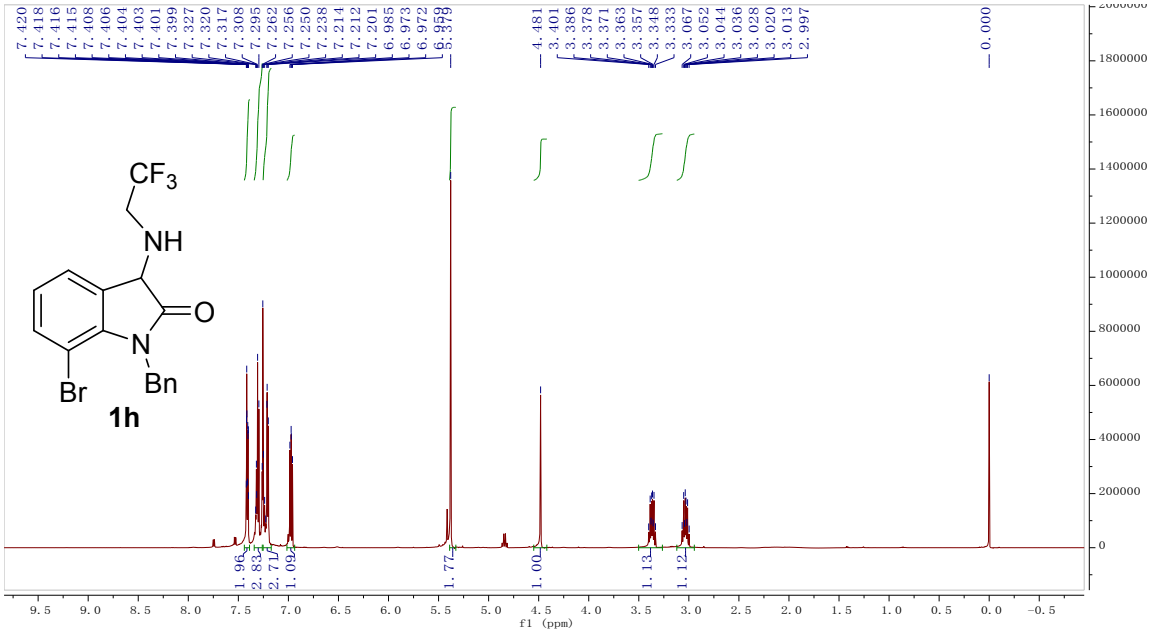

176.35
142.68
136.45
131.77
130.32
129.08
127.90
127.81
127.69
127.09
125.25
114.61
111.50
59.46
47.51
47.31
47.10
46.89
40.40
40.26
40.12
39.98
39.84
39.71
39.57
0.00
CF3
NH
Br
O
N
Bn
1d
f1 (ppm)

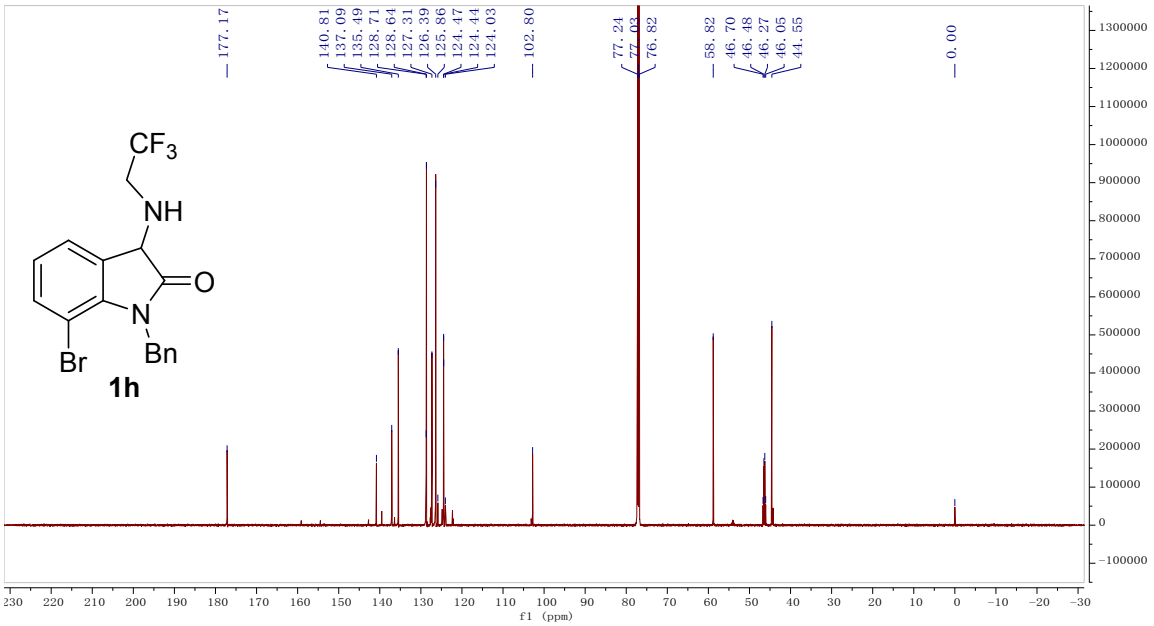

7.325
7.315
7.313
7.311
7.305
7.301
7.279
7.274
7.267
7.260
7.256
7.246
7.025
7.023
7.022
7.011
7.010
7.009
6.624
6.611
4.911
4.885
4.841
4.815
4.462
3.408
3.393
3.385
3.378
3.370
3.363
3.355
3.340
3.097
3.082
3.074
3.066
3.050
3.043
3.027
2.313
2.232
1.668
0.000
CF3
NH
Me
O
N
Bn
1e
4.55
1.09
0.97
0.97
1.09
1.03
1.00
1.05
1.04
3.35
0.53
f1 (ppm)

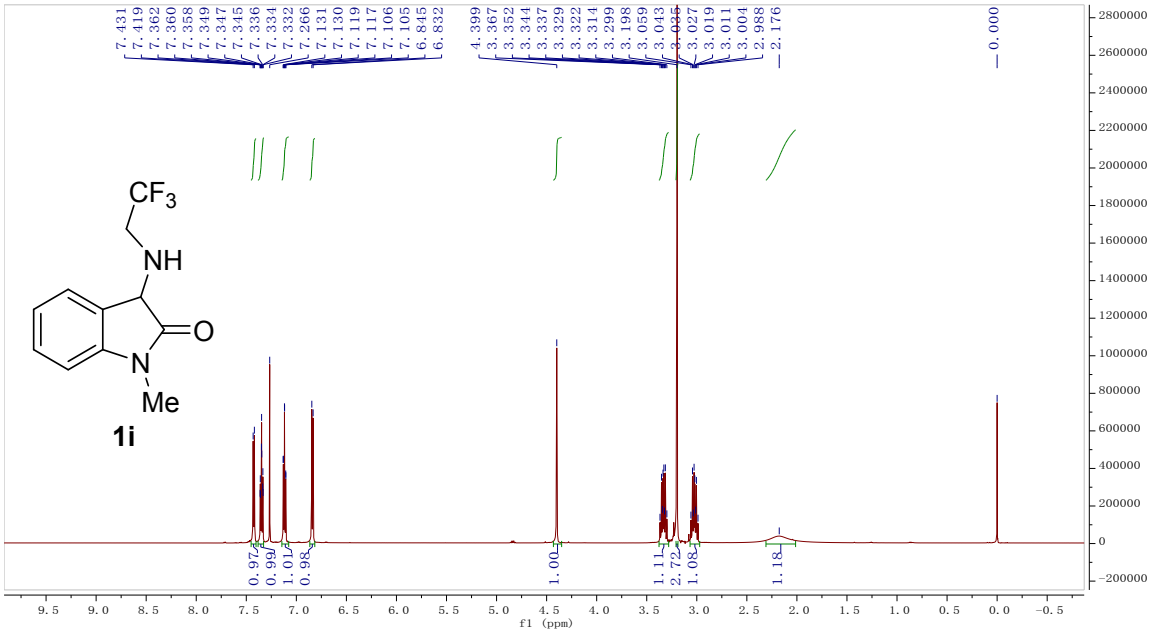

176.31
140.92
135.63
132.85
129.72
128.85
127.77
127.31
126.01
125.99
125.29
124.17
109.16
77.25
77.03
76.82
59.40
46.69
46.48
46.26
46.05
43.85
21.01
0.00
CF3
NH
Me
O
N
Bn
1e
f1 (ppm)

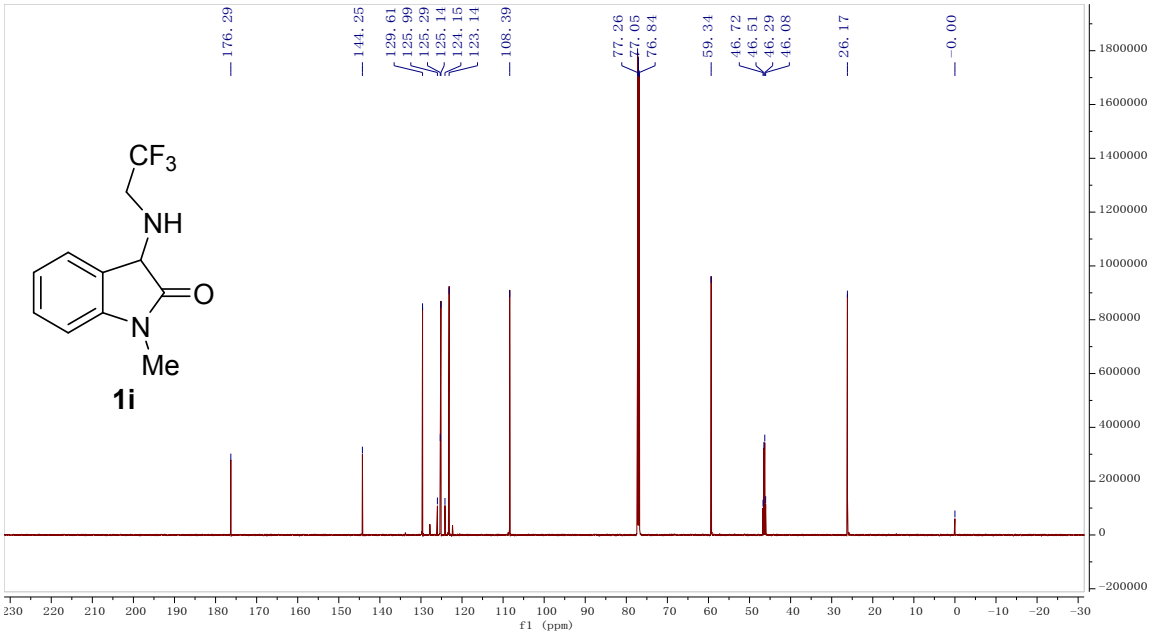

7.358
7.355
7.349
7.346
7.336
7.334
7.308
7.306
7.296
7.292
7.283
7.281
7.269
7.258
7.064
7.061
7.051
7.048
6.735
6.732
4.906
4.880
4.821
4.795
4.462
4.408
3.393
3.385
3.378
3.370
3.364
3.355
3.340
3.058
3.042
3.034
3.027
3.019
3.011
3.003
2.988
2.335
CF3
NH
O
Cl
N
Bn
1f
3.04
2.95
0.95
0.94
1.03
1.04
1.00
1.06
1.05
0.78
f1 (ppm)

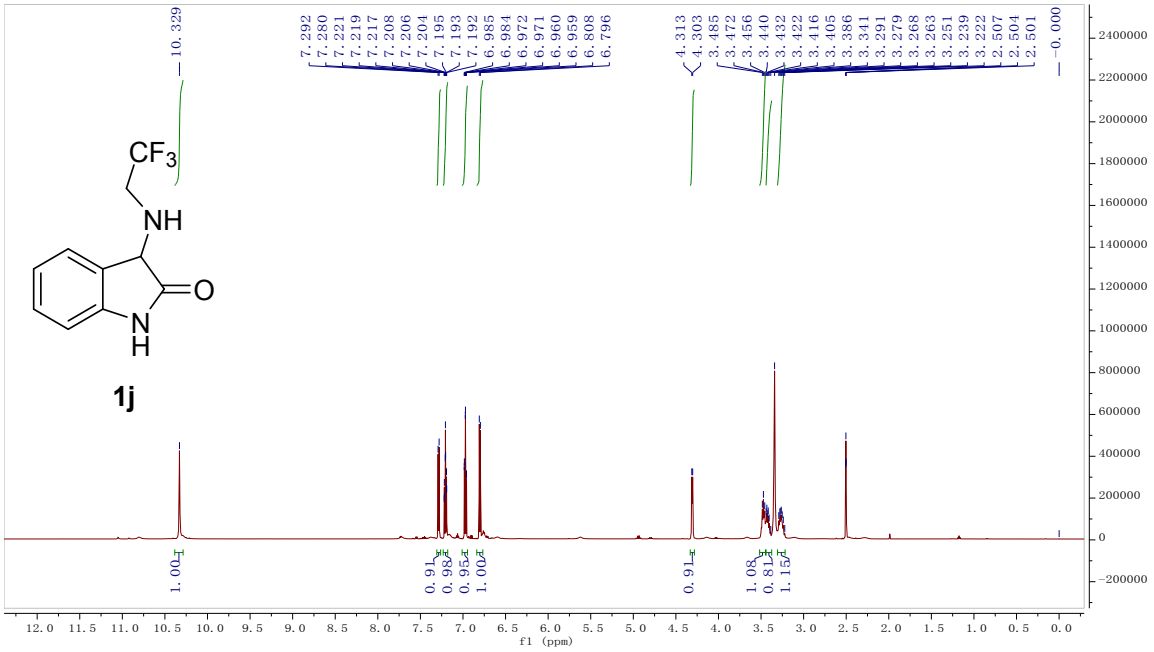

176.37
144.52
135.35
134.98
129.04
128.07
127.30
126.21
125.86
124.03
123.65
123.13
110.02
77.25
77.03
76.82
58.95
46.66
46.44
46.23
46.01
43.99
0.00
CF3
NH
O
Cl
N
Bn
1f
f1 (ppm)

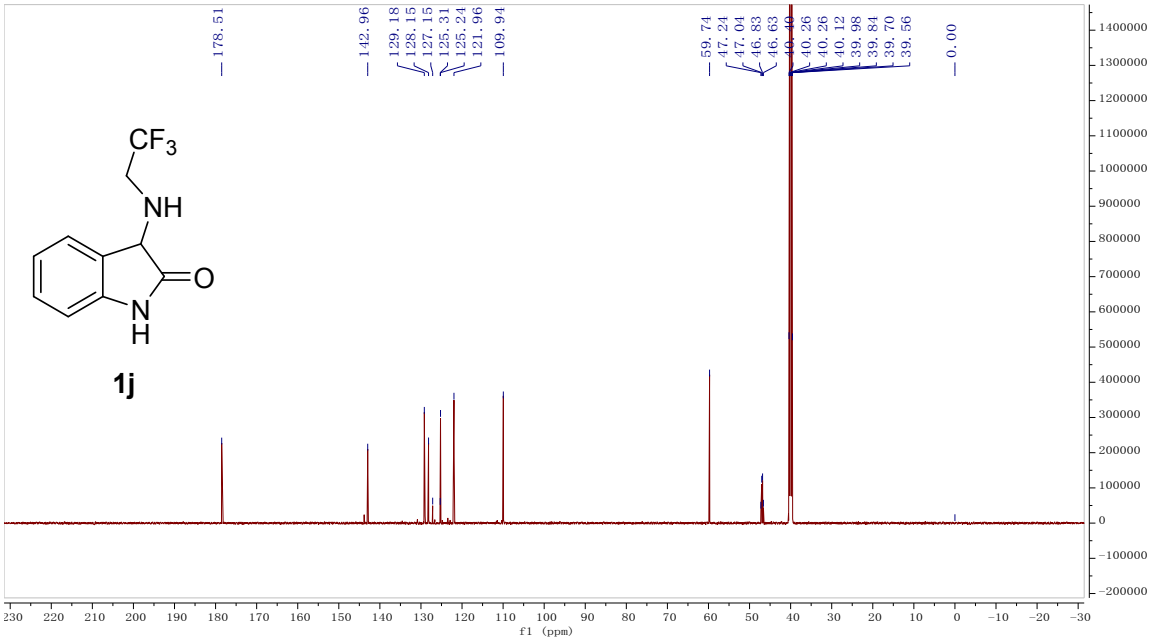

7.420
7.418
7.416
7.415
7.408
7.406
7.404
7.403
7.401
7.399
7.327
7.320
7.317
7.308
7.295
7.262
7.256
7.250
7.238
7.214
7.212
7.201
6.985
6.973
6.972
3.579
4.481
3.401
3.386
3.378
3.371
3.363
3.357
3.348
3.333
3.067
3.052
3.044
3.036
3.028
3.020
3.013
2.997
0.000
CF3
NH
O
N
Bn
Br
1h
1.96
2.83
2.71
1.09
1.77
1.00
1.13
1.12
f1 (ppm)

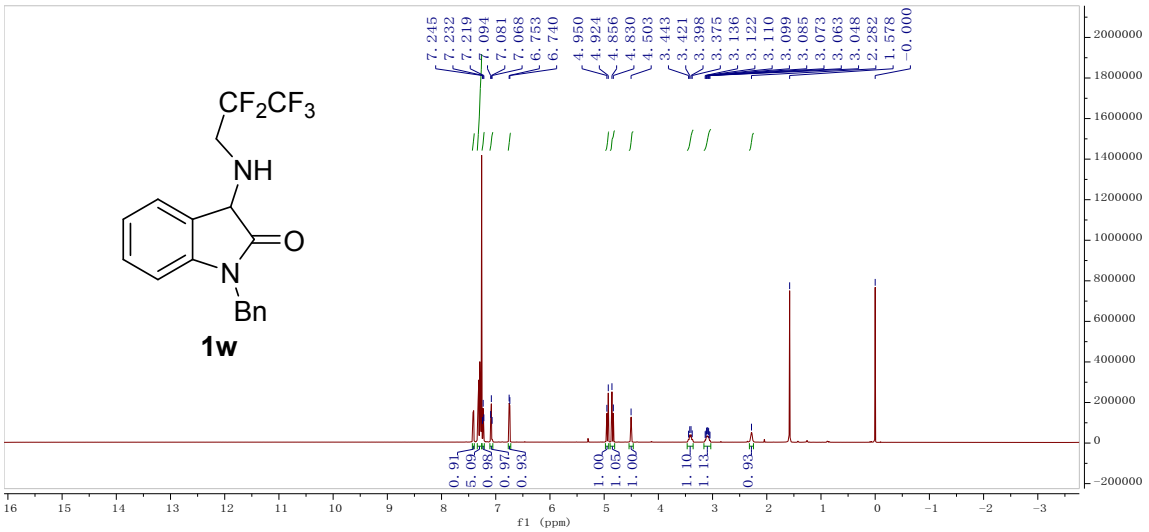

177.17
140.81
137.09
135.49
128.71
128.64
127.31
126.39
125.86
124.47
124.44
124.03
102.80
77.24
77.03
76.82
58.82
46.70
46.48
46.27
46.05
44.55
0.00
CF3
NH
O
N
Bn
Br
1h
f1 (ppm)

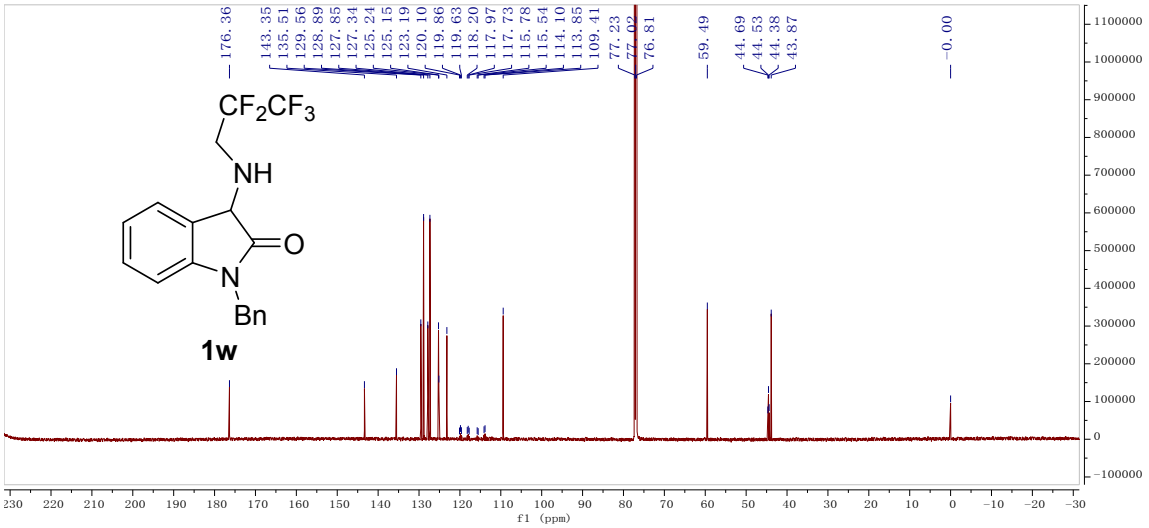

7.431
7.419
7.362
7.360
7.358
7.349
7.347
7.345
7.336
7.334
7.332
7.266
7.131
7.130
7.119
7.117
7.106
7.105
6.845
6.832
4.399
3.367
3.352
3.344
3.337
3.329
3.322
3.314
3.299
3.198
3.059
3.043
3.027
3.019
3.011
3.004
2.988
2.176
0.000
0.97
0.99
1.01
0.98
1.00
1.11
2.72
1.08
1.18
CF3
NH
O
N
Me
1i
f1 (ppm)

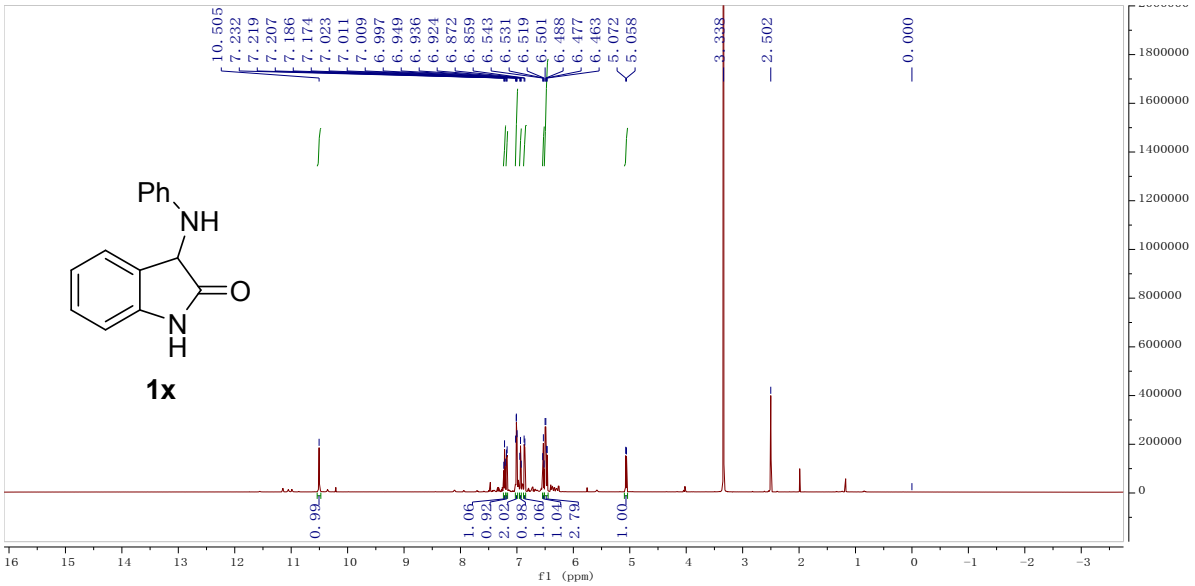

176.29
144.25
129.61
125.99
125.29
125.14
124.15
123.14
108.39
77.26
77.05
76.84
59.34
46.72
46.51
46.29
46.08
26.17
-0.00
CF3
NH
O
N
Me
1i
f1 (ppm)

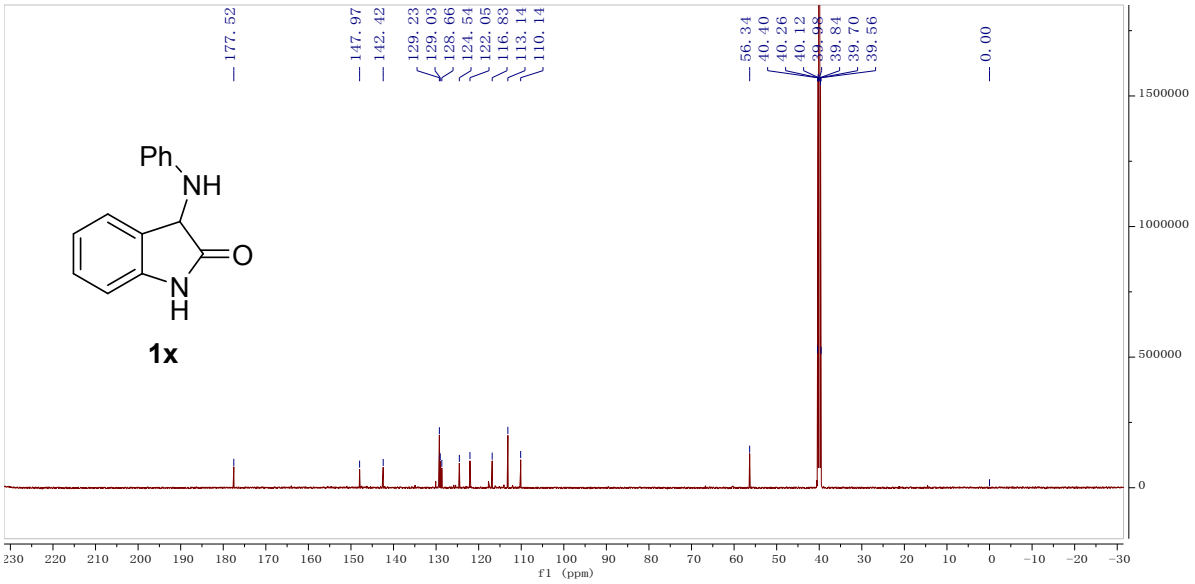

10.329
7.292
7.280
7.221
7.219
7.217
7.208
7.206
7.204
7.195
7.193
7.192
6.985
6.984
6.972
6.971
6.960
6.959
6.808
6.796
4.313
4.303
3.485
3.472
3.456
3.440
3.432
3.422
3.416
3.405
3.386
3.341
3.291
3.279
3.268
3.263
3.251
3.239
3.222
2.507
2.504
2.501
0.000
CF3
NH
O
N
H
1j
1.00
0.91
0.98
0.95
1.00
0.91
1.08
0.81
1.15
f1 (ppm)


178.51
142.96
129.18
128.15
127.15
125.31
125.24
121.96
109.94
59.74
47.24
47.04
46.83
46.63
40.40
40.26
40.26
40.12
39.98
39.84
39.70
39.56
0.00
CF3
NH
O
N
H
1j
f1 (ppm)

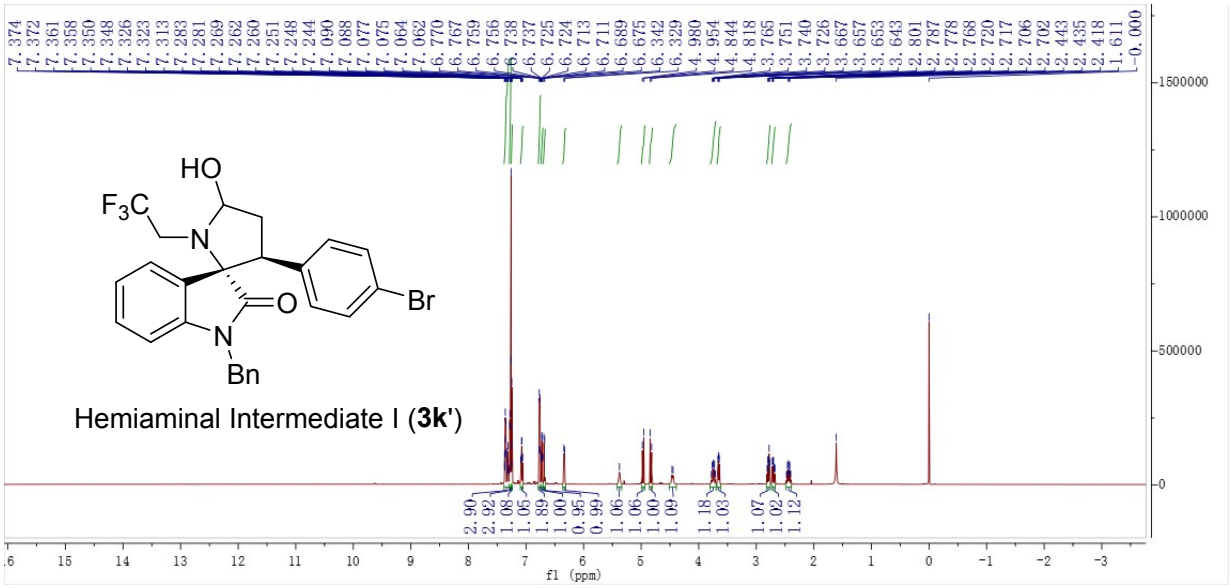

7.245
7.232
7.219
7.094
7.081
7.068
6.753
6.740
4.950
4.924
4.856
4.830
4.503
3.443
3.421
3.398
3.375
3.136
3.122
3.110
3.099
3.085
3.073
3.063
3.048
2.282
1.578
-0.000
0.91
5.09
0.98
0.97
0.93
1.00
1.05
1.00
1.10
1.13
0.93
CF2CF3
NH
O
N
Bn
1w
f1 (ppm)

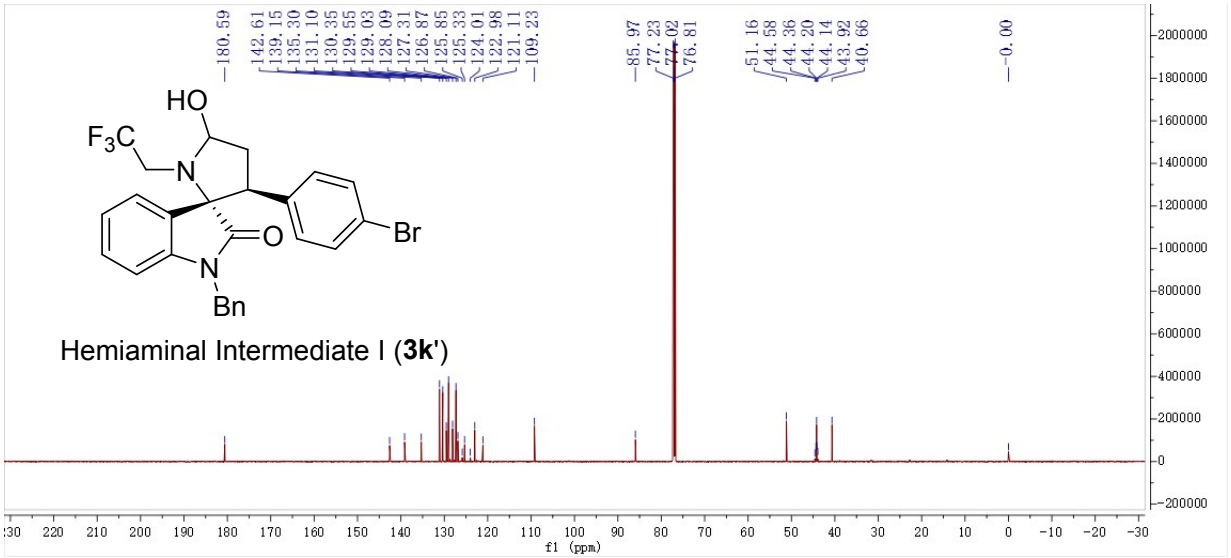

176.36
143.35
135.51
129.56
128.89
127.85
127.34
125.24
125.15
123.19
120.10
119.86
119.63
118.20
117.97
117.73
115.78
115.54
114.10
113.85
109.41
77.23
77.02
76.81
59.49
44.69
44.53
44.38
43.87
-0.00
CF2CF3
NH
O
N
Bn
1w
f1 (ppm)


10.505
7.232
7.219
7.207
7.186
7.174
7.023
7.011
7.009
6.997
6.949
6.936
6.924
6.872
6.859
6.543
6.531
6.519
6.501
6.488
6.477
6.463
5.072
5.058
3.338
2.502
0.000
Ph
NH
O
N
H
1x
0.99
1.06
0.92
2.02
0.98
1.06
1.04
2.79
1.00
f1 (ppm)

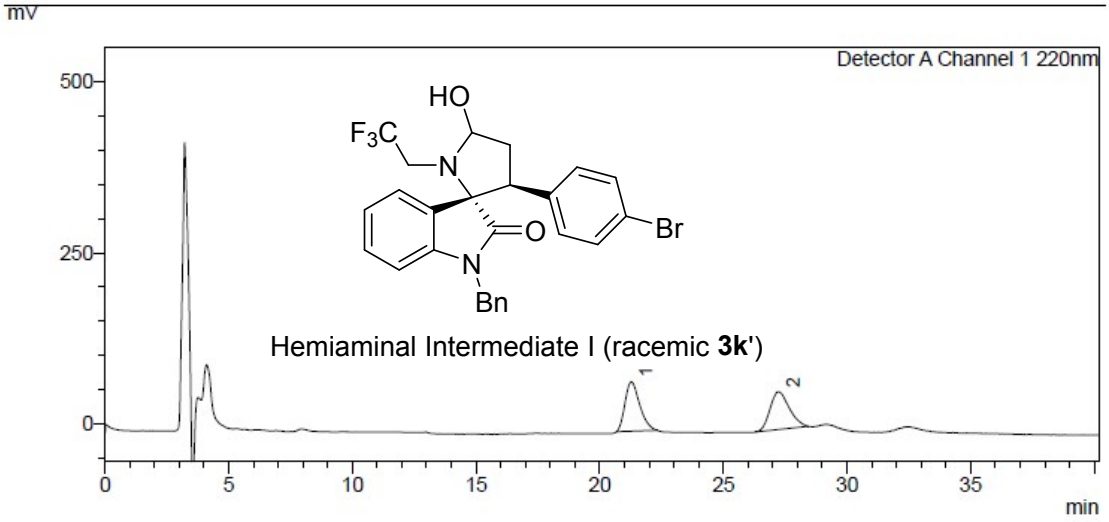

177.52
147.97
142.42
129.23
129.03
128.66
124.54
122.05
116.83
113.14
110.14
56.34
40.40
40.26
40.12
39.98
39.84
39.70
39.56
0.00
Ph
NH
O
N
H
1x
f1 (ppm)

4. NMR and HPLC spectra of intermediate I (3k') and compound 3





<Chromatogram>

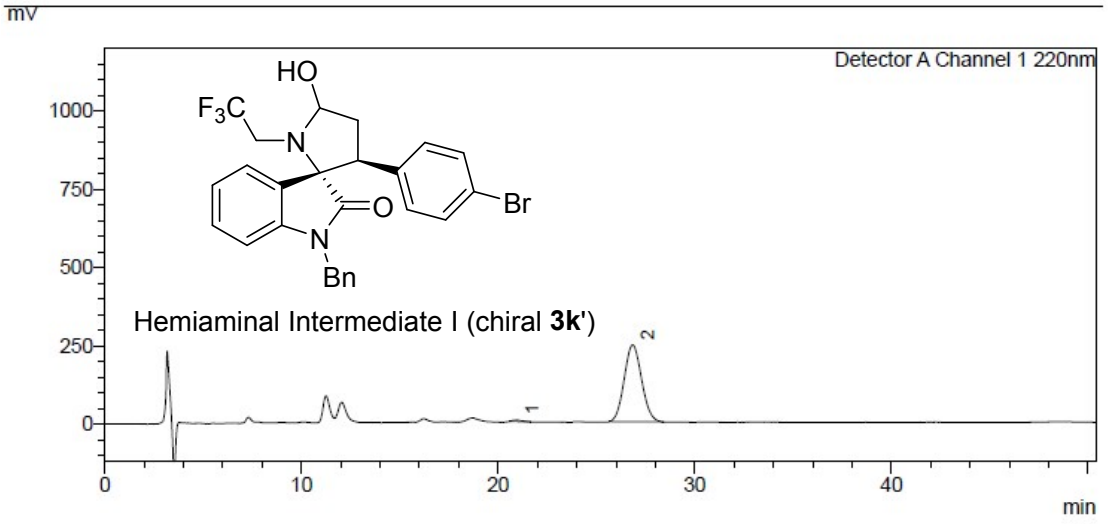


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	21.277	2970276	72321	50.097	50.097
2	27.233	2958732	54948	49.903	49.903
Total		5929008	127269		100.000

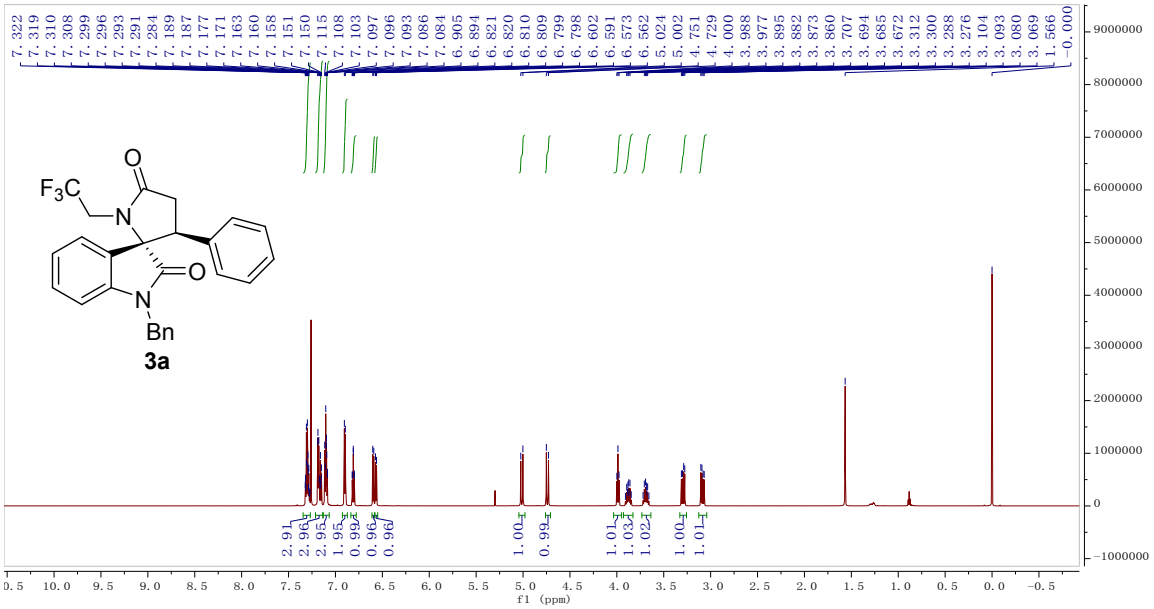
<Chromatogram>

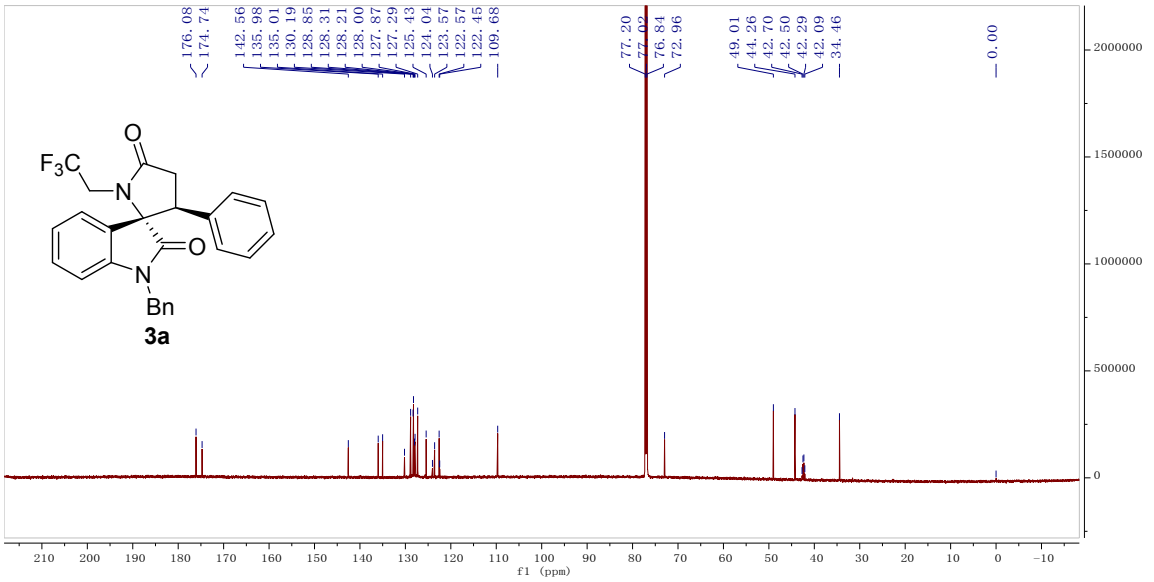


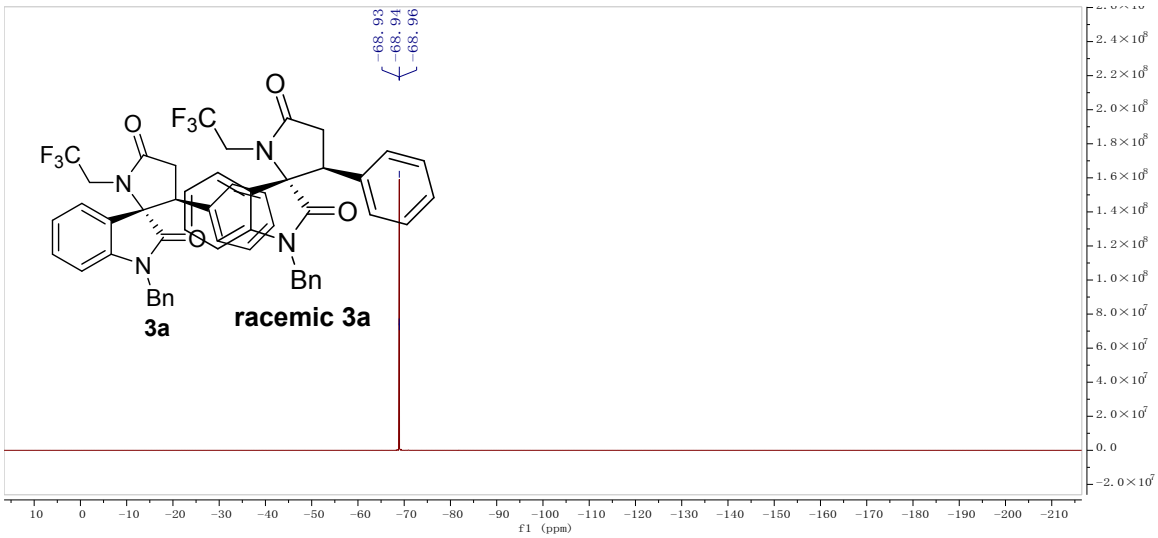
<Peak Table>

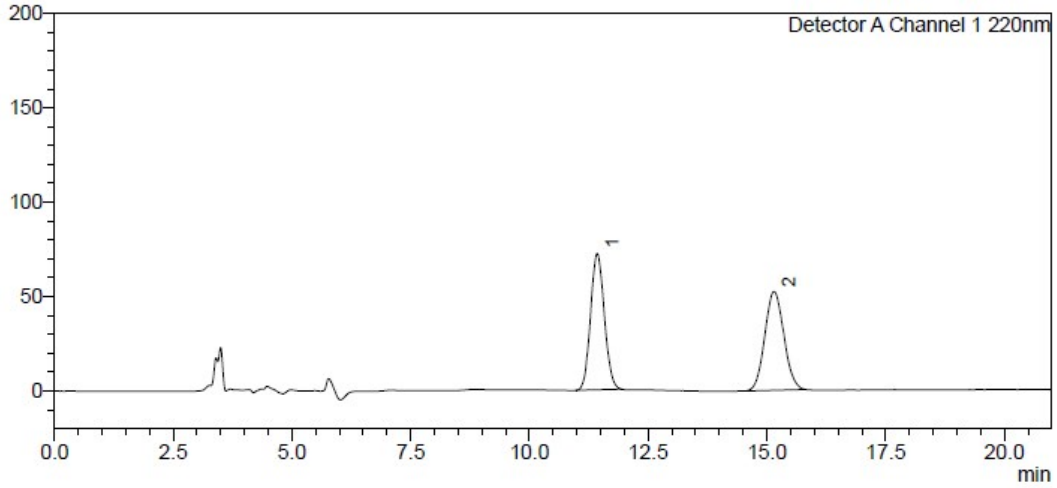
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	21.493	143409	4787	0.809	0.809
2	27.305	17573388	227824	99.191	99.191
Total		17716797	232611		100.000


3a


3a

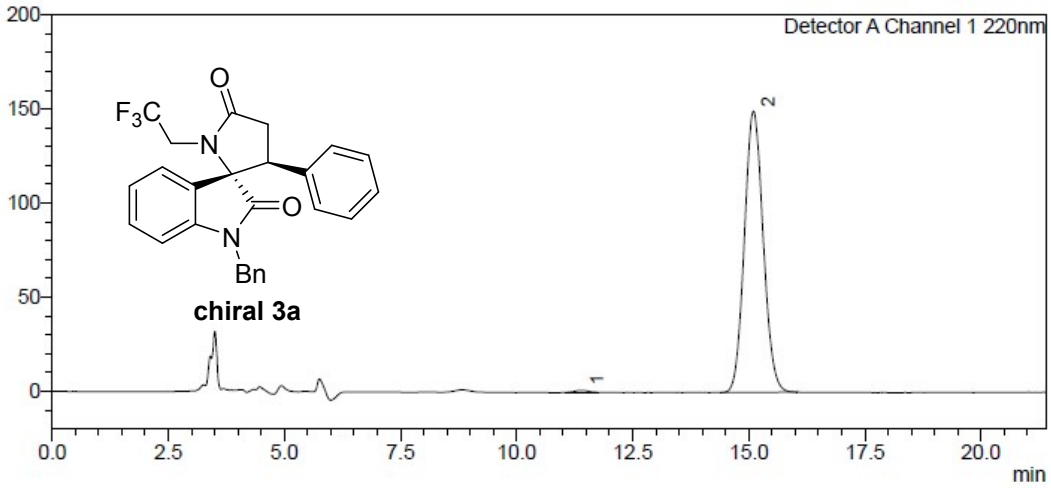




<Peak Table>

Detector A Channel 1 220nm

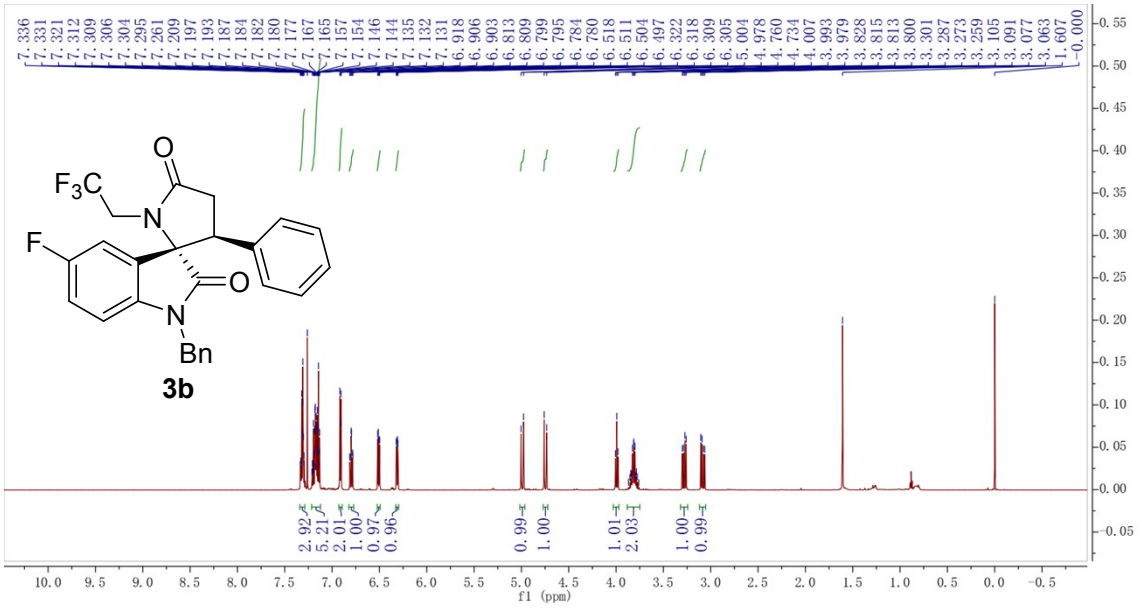
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.429	1455013	72196	49.892	49.892
2	15.153	1461320	52357	50.108	50.108
Total		2916333	124552		100.000

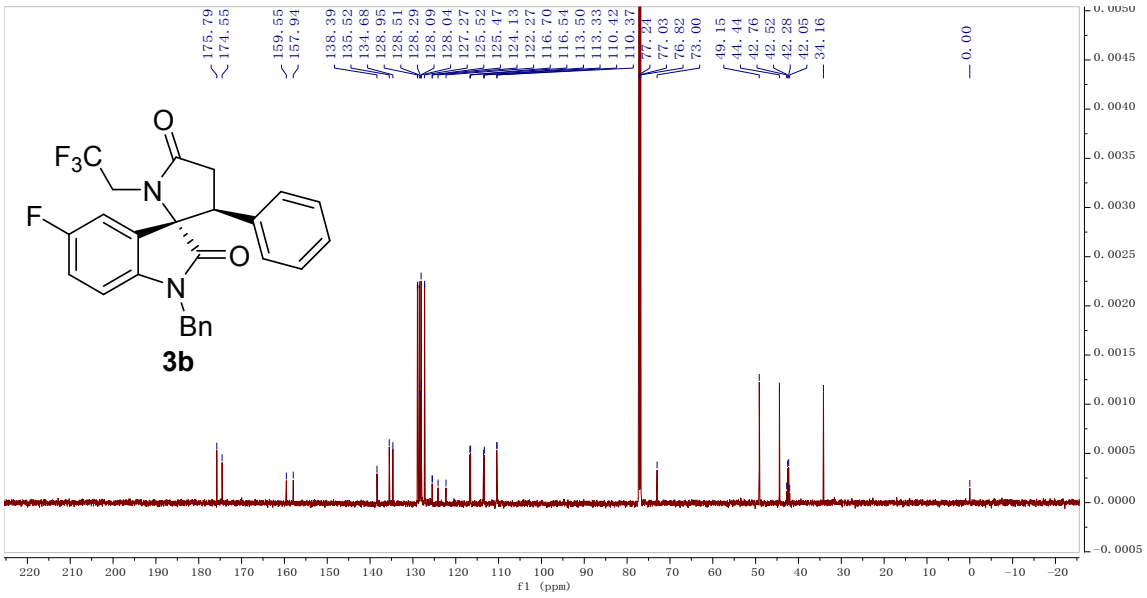


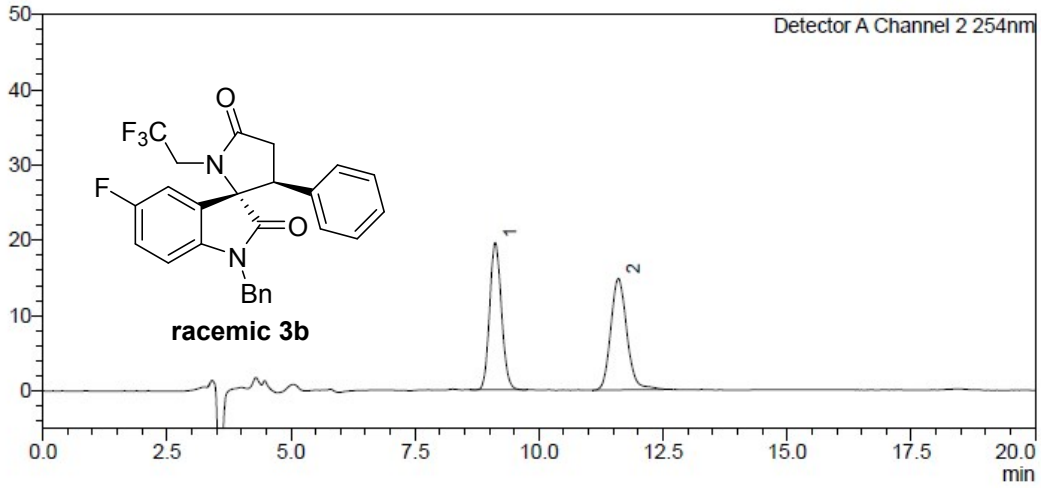
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.405	21543	1090	0.509	0.509
2	15.102	4209138	149398	99.491	99.491
Total		4230681	150488		100.000


3b
f1 (ppm)

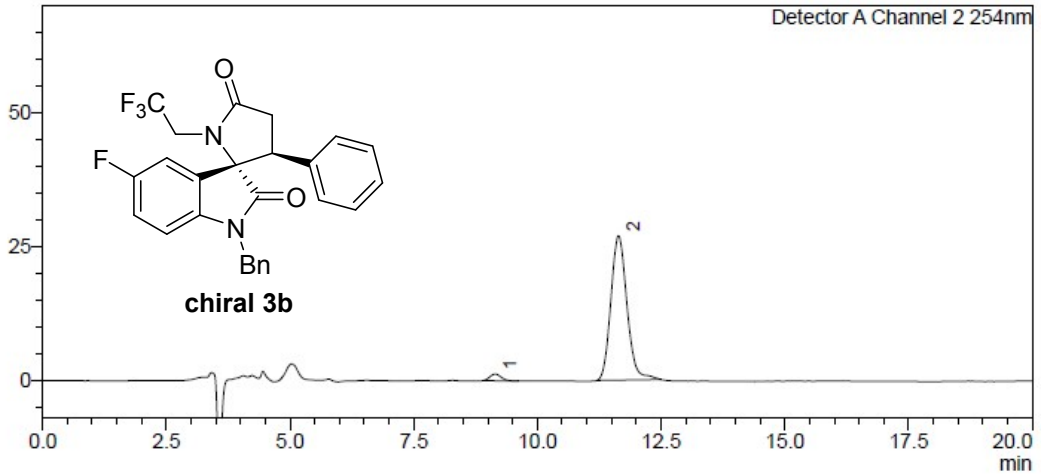

3b
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

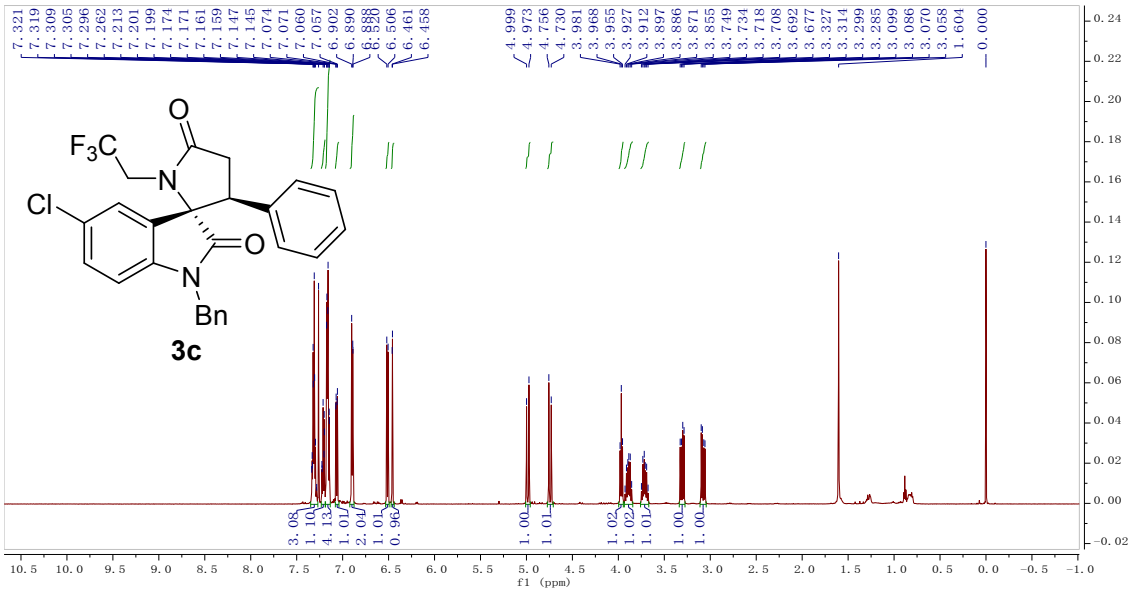
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.118	323771	19576	49.090	49.090
2	11.598	335777	14817	50.910	50.910
Total		659548	34392		100.000

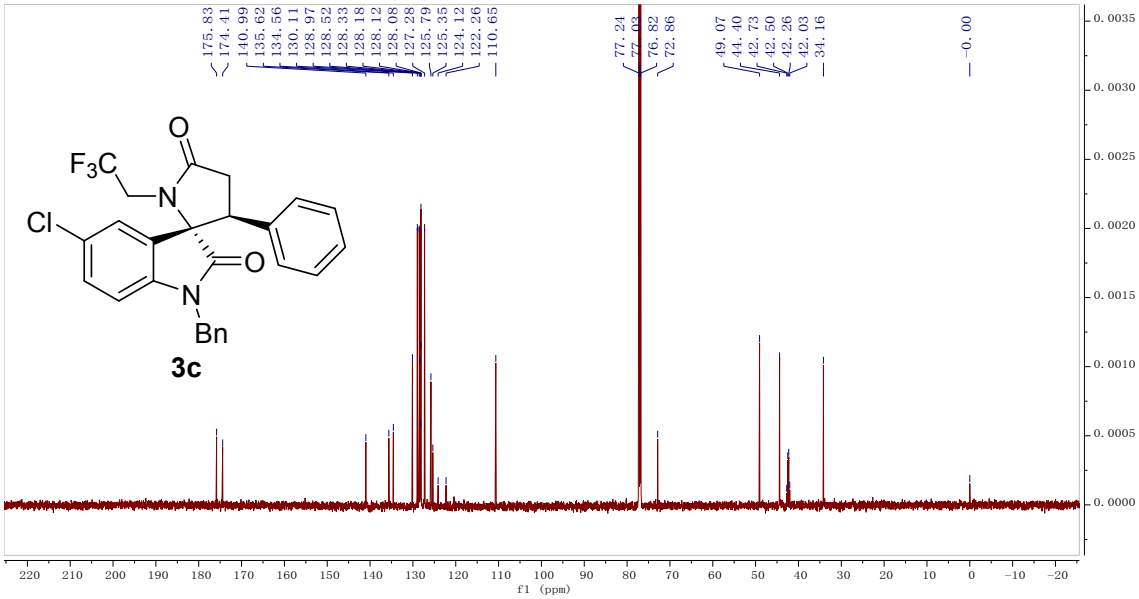


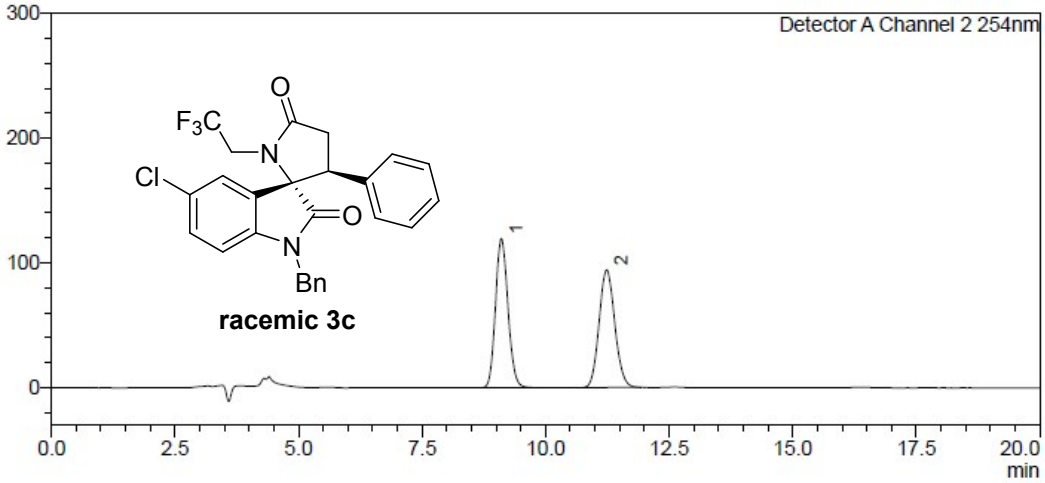
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.146	20575	1271	3.262	3.262
2	11.638	610164	26960	96.738	96.738
Total		630739	28231		100.000


7.321 7.319 7.309 7.305 7.296 7.262 7.213 7.201 7.199 7.174 7.171 7.161 7.159 7.147 7.145 7.074 7.071 7.060 7.057 6.902 6.890 6.506 6.461 6.458
4.999 4.973 4.756 4.730 3.981 3.968 3.955 3.927 3.912 3.897 3.886 3.871 3.855 3.749 3.734 3.718 3.708 3.692 3.677 3.327 3.314 3.299 3.285 3.099 3.086 3.070 3.058 1.604 0.000
3.08 1.10 4.13 1.01 2.04 1.01 0.96 1.00 1.01 1.02 1.02 1.01 1.00 1.00
O
F3C
N
Cl
O
N
Bn
3c
f1 (ppm)

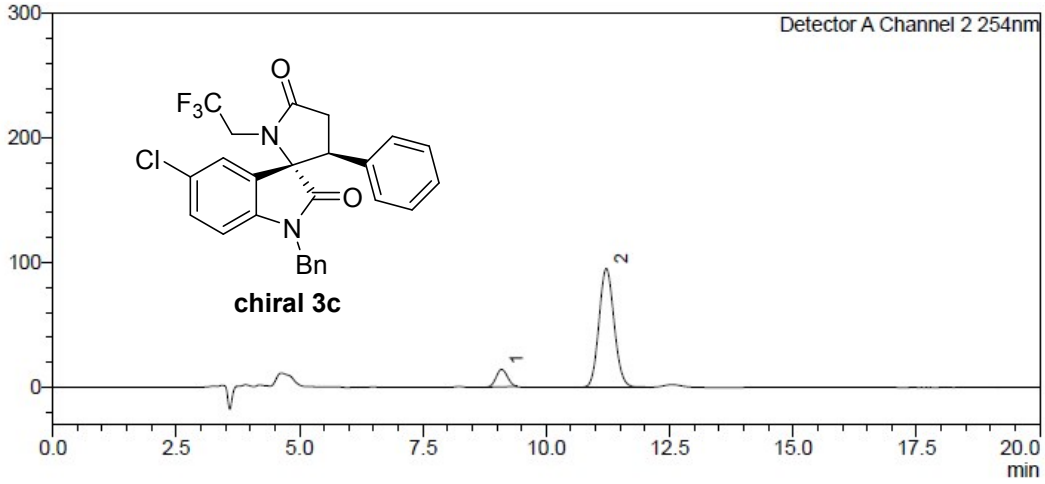

175.83 174.41 140.99 135.62 134.56 130.11 128.97 128.52 128.33 128.18 128.12 128.08 127.28 125.79 125.35 124.12 122.26 110.65
77.24 77.03 76.82 72.86
49.07 44.40 42.73 42.50 42.26 42.03 34.16
0.00
O
F3C
N
Cl
O
N
Bn
3c
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

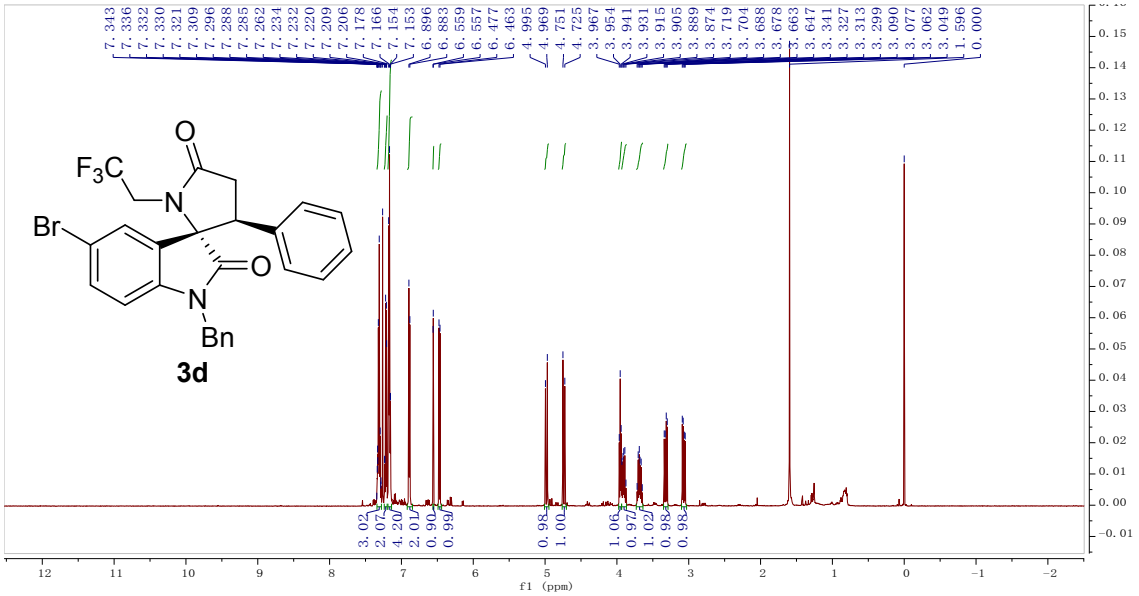
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.105	2096127	119430	50.156	50.156
2	11.236	2082021	94269	49.818	49.818
3	28.924	1069	64	0.026	0.026
Total		4179218	213763		100.000

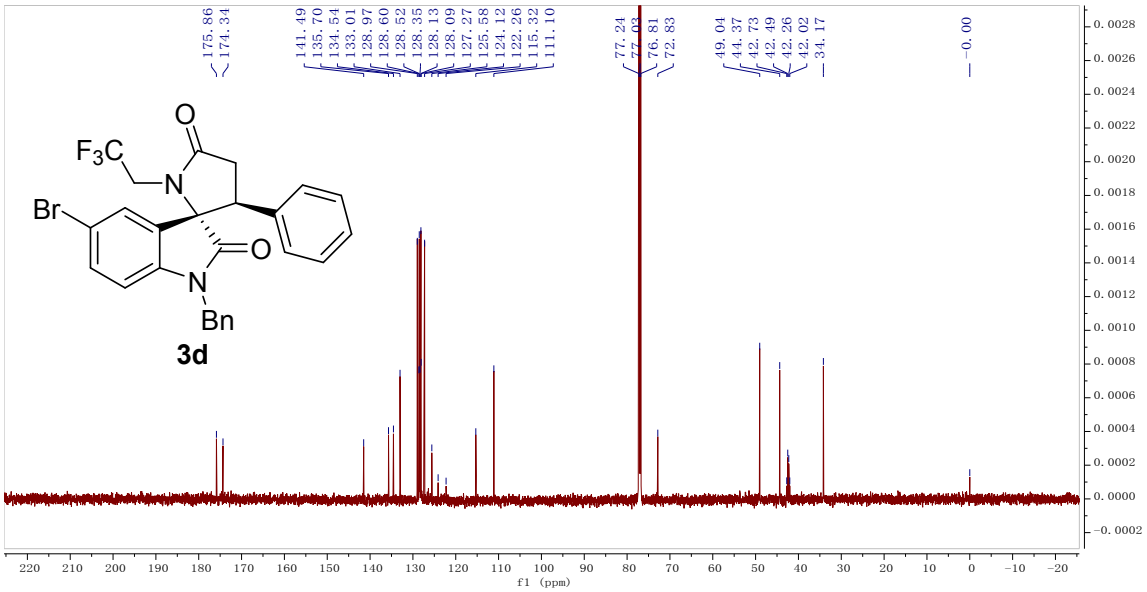


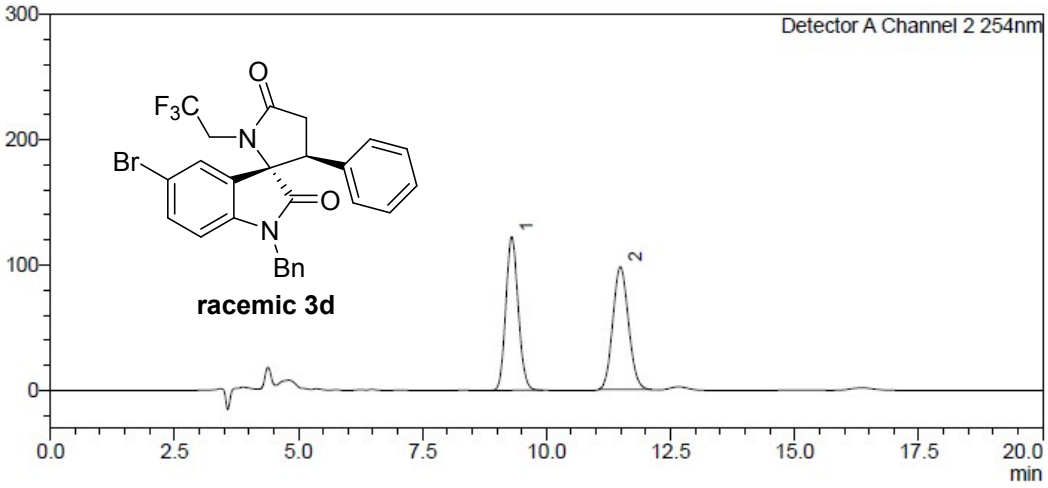
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.097	222867	13989	9.876	9.876
2	11.216	2033727	95279	90.124	90.124
Total		2256594	109268		100.000


7.343
7.336
7.332
7.330
7.321
7.309
7.296
7.288
7.285
7.262
7.234
7.232
7.220
7.209
7.206
7.178
7.166
7.154
7.153
6.896
6.883
6.559
6.557
6.477
6.463
4.995
4.969
4.751
4.725
3.967
3.954
3.941
3.931
3.915
3.905
3.889
3.874
3.719
3.704
3.688
3.678
3.663
3.647
3.341
3.327
3.313
3.299
3.090
3.077
3.062
3.049
1.596
0.000
3.02
2.07
4.20
2.01
0.90
0.99
0.98
1.00
1.06
0.97
1.02
0.98
0.98
F3C
N
O
Br
O
N
Bn
3d
f1 (ppm)

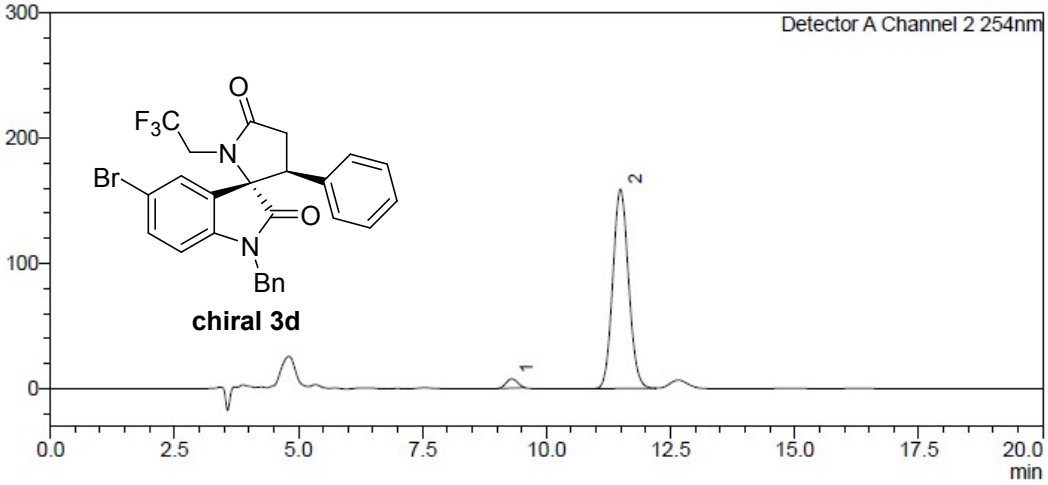

175.86
174.34
141.49
135.70
134.54
133.01
128.97
128.60
128.52
128.35
128.13
128.09
127.27
125.58
124.12
122.26
115.32
111.10
77.24
77.03
76.81
72.83
49.04
44.37
42.73
42.49
42.26
42.02
34.17
-0.00
F3C
N
O
Br
O
N
Bn
3d
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

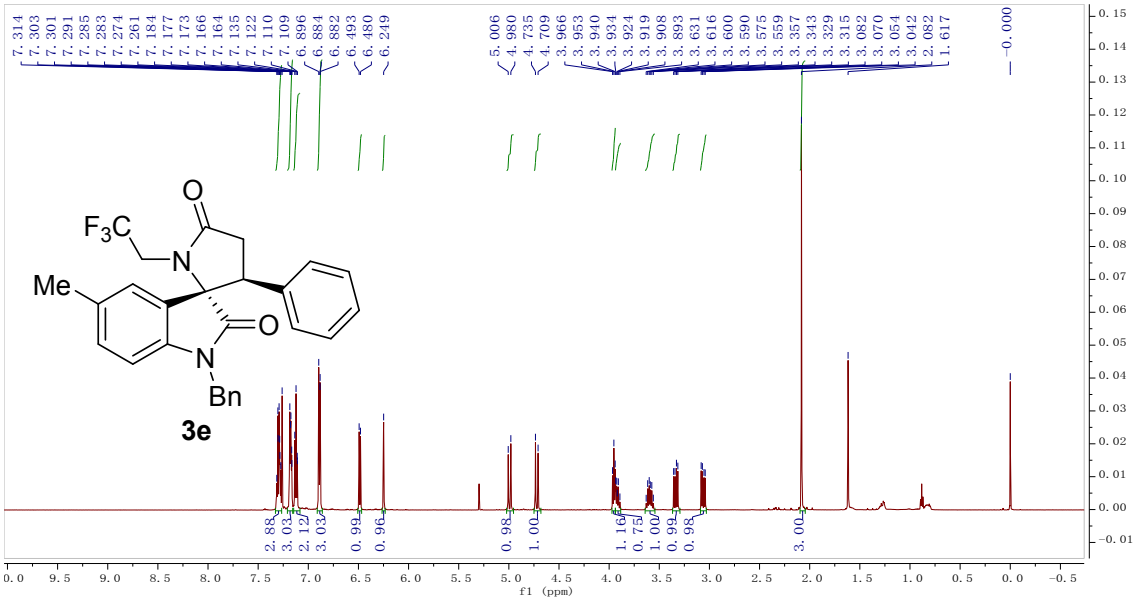
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.298	2136081	122696	49.830	49.830
2	11.488	2150695	97845	50.170	50.170
Total		4286776	220541		100.000

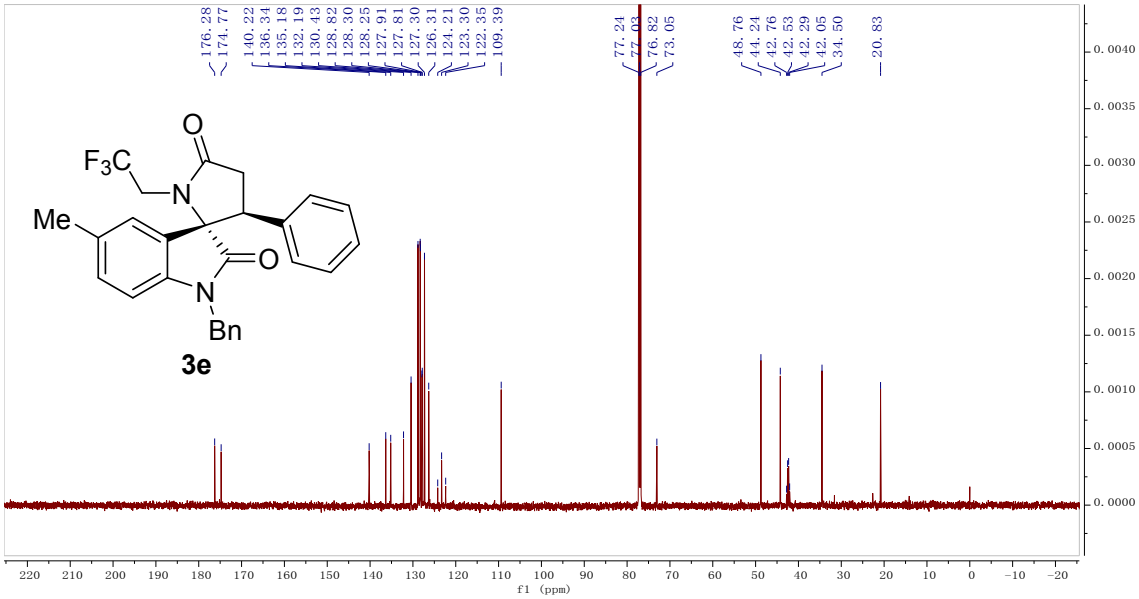


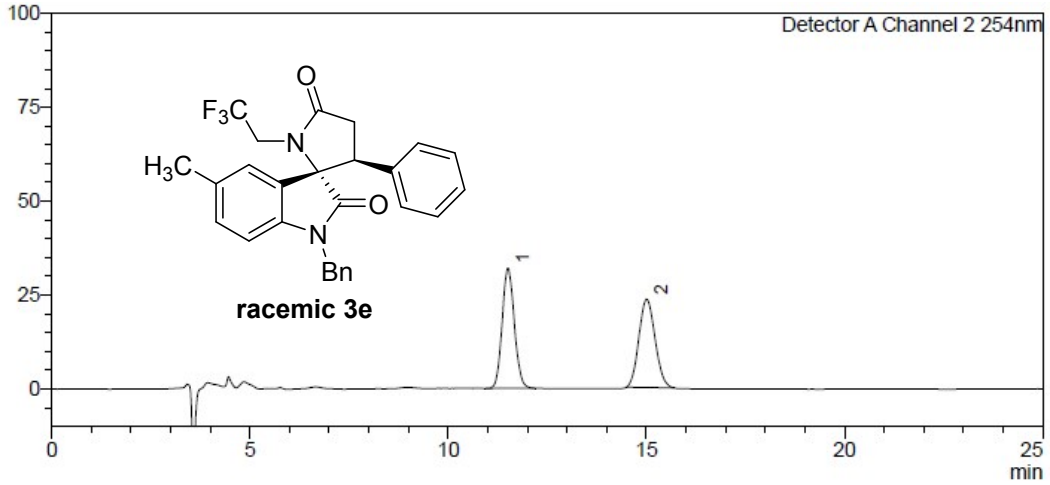
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.301	118382	7535	3.261	3.261
2	11.489	3511840	159015	96.739	96.739
Total		3630222	166550		100.000


7.314
7.303
7.301
7.291
7.285
7.283
7.274
7.261
7.184
7.177
7.173
7.166
7.164
7.135
7.122
7.110
7.109
6.896
6.884
6.882
6.493
6.480
6.249
5.006
4.980
4.735
4.709
3.966
3.953
3.940
3.934
3.924
3.919
3.908
3.893
3.631
3.616
3.600
3.590
3.575
3.559
3.357
3.343
3.329
3.315
3.082
3.070
3.054
3.042
2.082
1.617
-0.000
F3C
N
O
Me
O
N
Bn
3e
f1 (ppm)

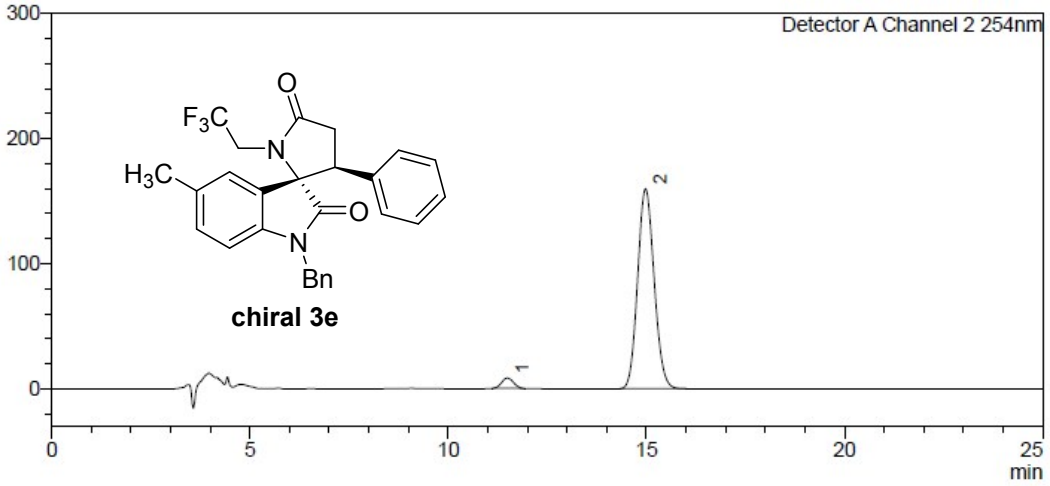

176.28
174.77
140.22
136.34
135.18
132.19
130.43
128.82
128.30
128.25
127.91
127.81
127.30
126.31
124.21
123.30
122.35
109.39
77.24
77.03
76.82
73.05
48.76
44.24
42.76
42.53
42.29
42.05
34.50
20.83
F3C
N
O
Me
O
N
Bn
3e
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

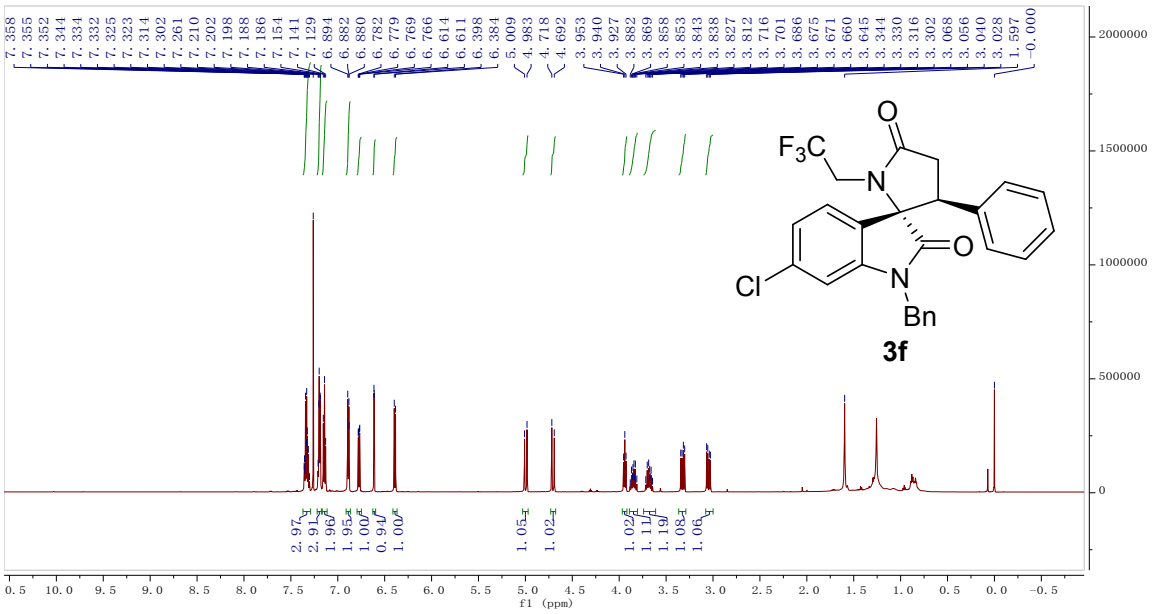
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.510	685046	31998	50.695	50.695
2	15.008	666254	23490	49.305	49.305
Total		1351301	55488		100.000

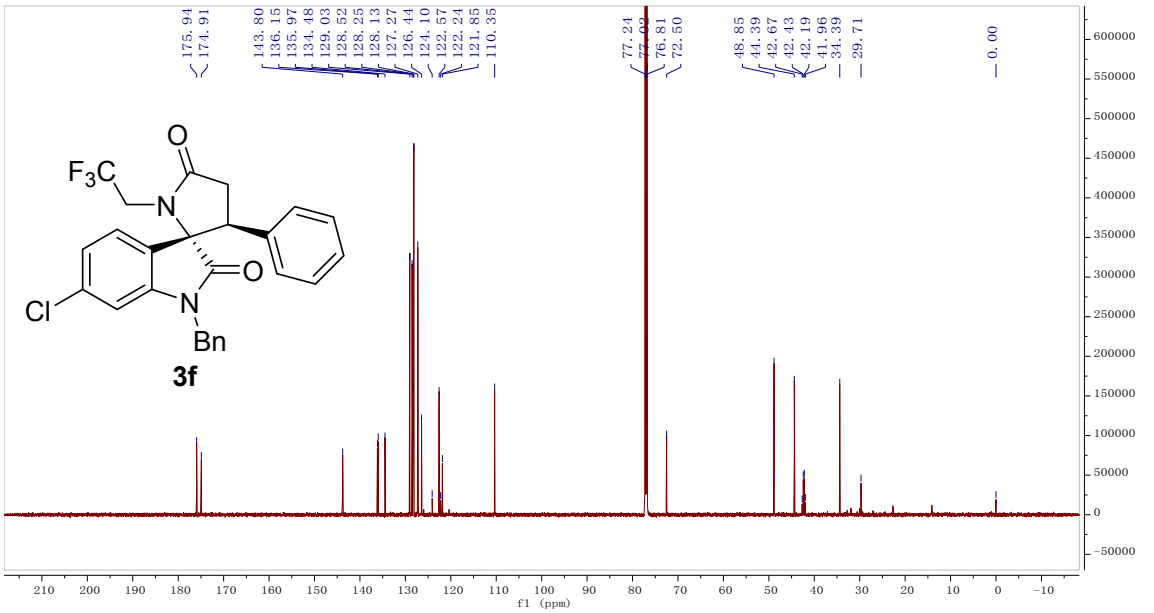


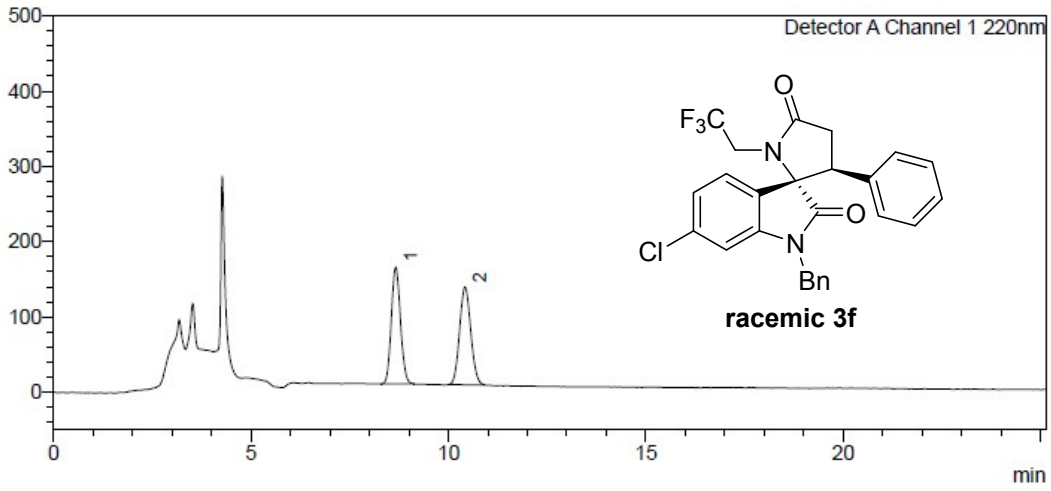
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.496	173152	8454	3.613	3.613
2	14.980	4618683	159636	96.387	96.387
Total		4791835	168090		100.000


7.358
7.355
7.352
7.344
7.334
7.332
7.325
7.323
7.314
7.302
7.261
7.210
7.202
7.198
7.188
7.186
7.154
7.141
7.129
6.894
6.882
6.880
6.782
6.779
6.769
6.766
6.614
6.611
6.398
6.384
5.009
4.983
4.718
4.692
3.953
3.940
3.927
3.882
3.869
3.858
3.853
3.843
3.838
3.827
3.812
3.716
3.701
3.686
3.675
3.671
3.660
3.645
3.344
3.330
3.316
3.302
3.068
3.056
3.040
3.028
1.597
0.000
2.97
2.91
1.96
1.95
1.00
0.94
1.00
1.05
1.02
1.02
1.11
1.19
1.08
1.06
f1 (ppm)
F3C
N
O
O
N
Cl
Bn
3f


175.94
174.91
143.80
136.15
135.97
134.48
129.03
128.52
128.25
128.13
127.27
126.44
124.10
122.57
122.24
121.85
110.35
77.24
77.02
76.81
72.50
48.85
44.39
42.67
42.43
42.19
41.96
34.39
29.71
0.00
f1 (ppm)
F3C
N
O
O
N
Cl
Bn
3f

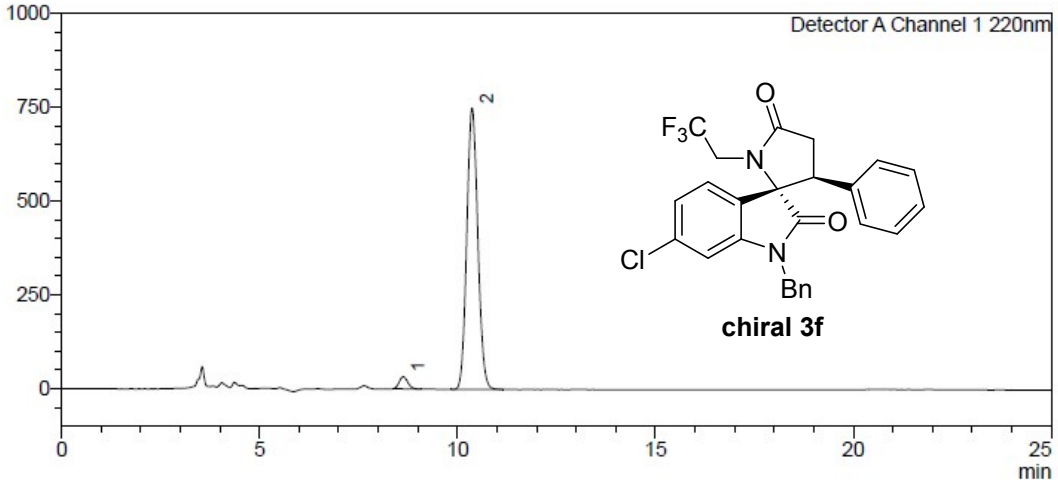


racemic 3f

<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.667	2495640	155327	49.404	49.404
2	10.421	2555818	130033	50.596	50.596
Total		5051458	285360		100.000

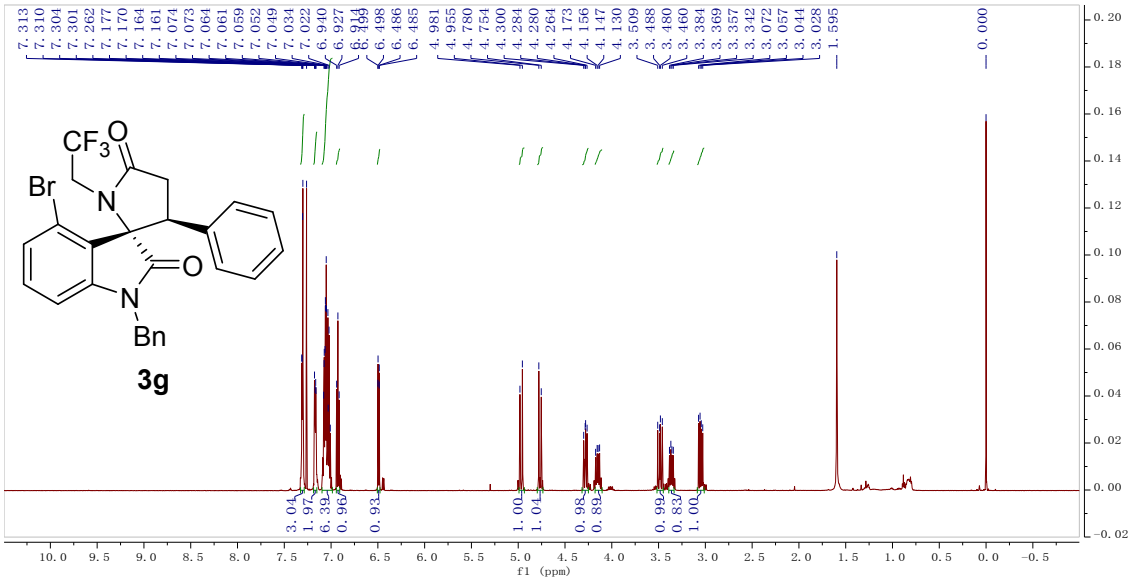


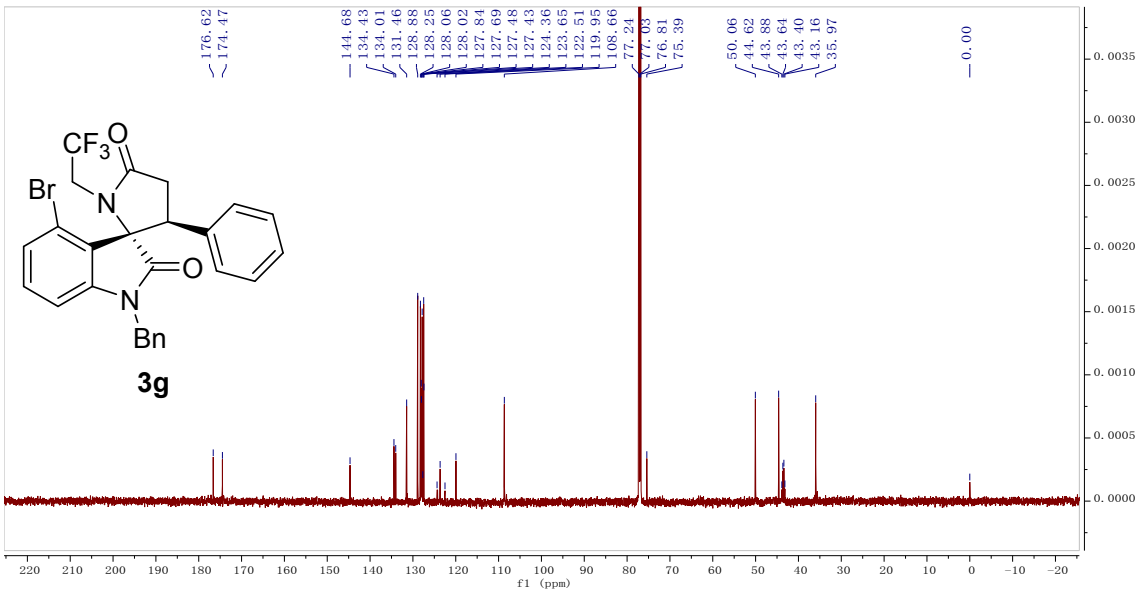
chiral 3f

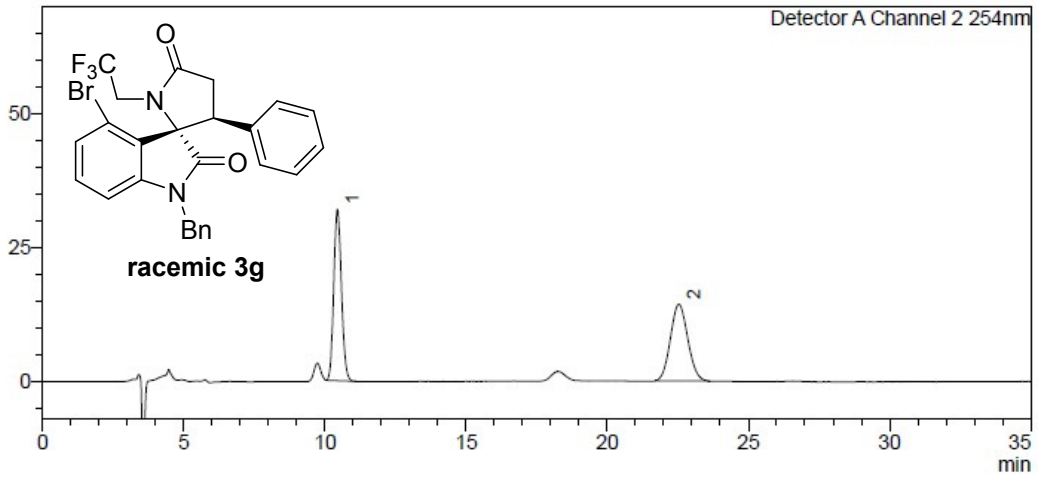
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.630	492651	32264	3.282	3.282
2	10.370	14519440	749884	96.718	96.718
Total		15012091	782148		100.000


7.313 7.310 7.304 7.301 7.262 7.177 7.170 7.164 7.161 7.074 7.073 7.064 7.061 7.059 7.052 7.049 7.034 7.022 6.940 6.927 6.498 6.486 6.485 4.981 4.955 4.780 4.754 4.300 4.284 4.280 4.264 4.173 4.156 4.147 4.130 3.509 3.488 3.480 3.460 3.384 3.369 3.357 3.342 3.072 3.057 3.044 3.028 1.595 0.000
3.04 1.97 6.39 0.96 0.93 1.00 1.04 0.98 0.89 0.99 0.83 1.00
f1 (ppm)
Br
CF3
O
N
O
N
Bn
3g

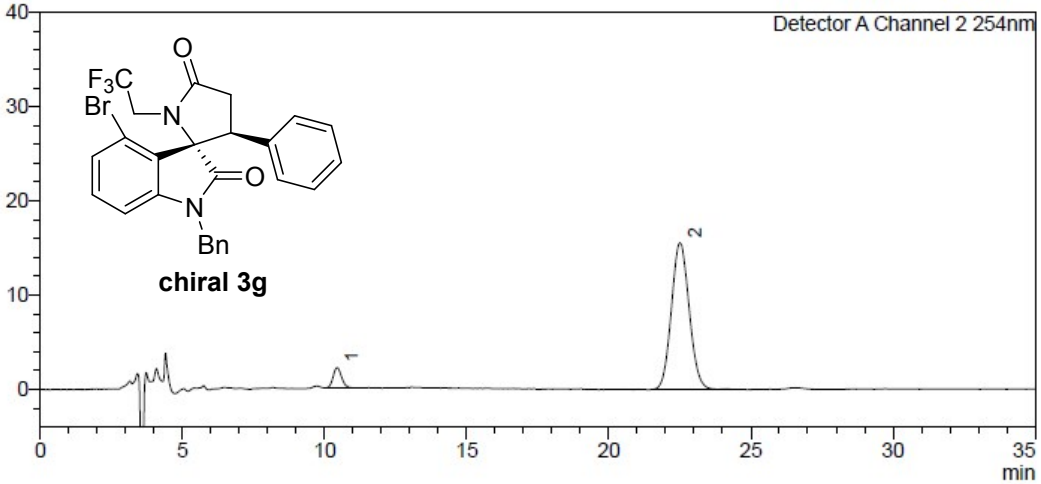

176.62 174.47 144.68 134.43 134.01 131.46 128.88 128.25 128.06 128.02 127.84 127.69 127.48 127.43 124.36 123.65 122.51 119.95 108.66 77.24 77.03 76.81 75.39 50.06 44.62 43.88 43.64 43.40 43.16 35.97 0.00
f1 (ppm)
Br
CF3
O
N
O
N
Bn
3g



<Peak Table>

Detector A Channel 2 254nm

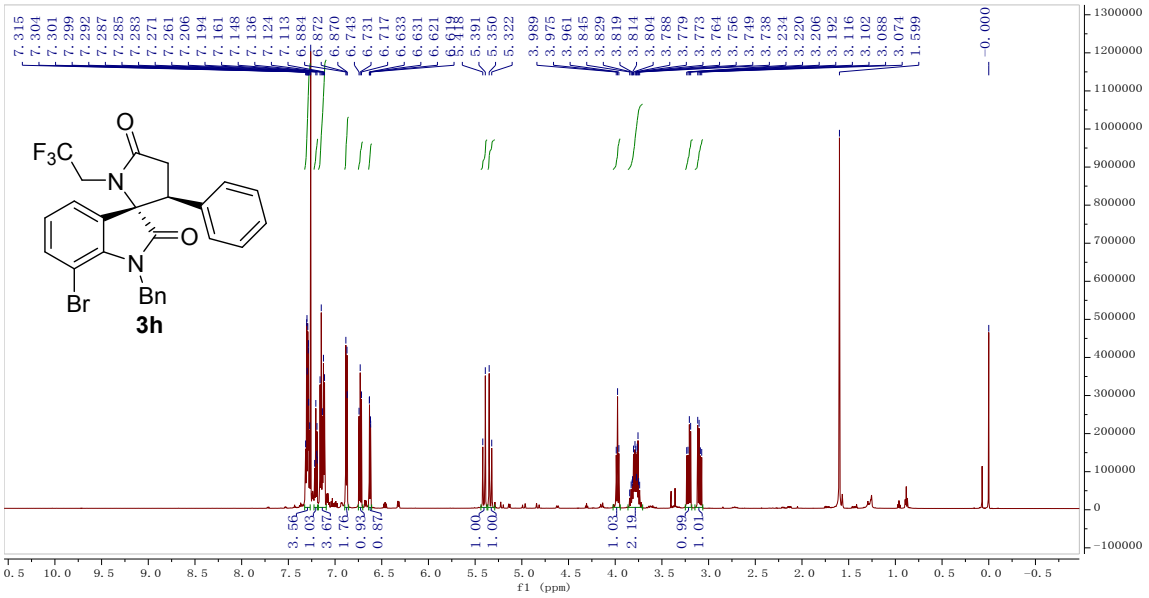
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.445	607340	32023	49.904	49.904
2	22.542	609677	14308	50.096	50.096
Total		1217017	46331		100.000

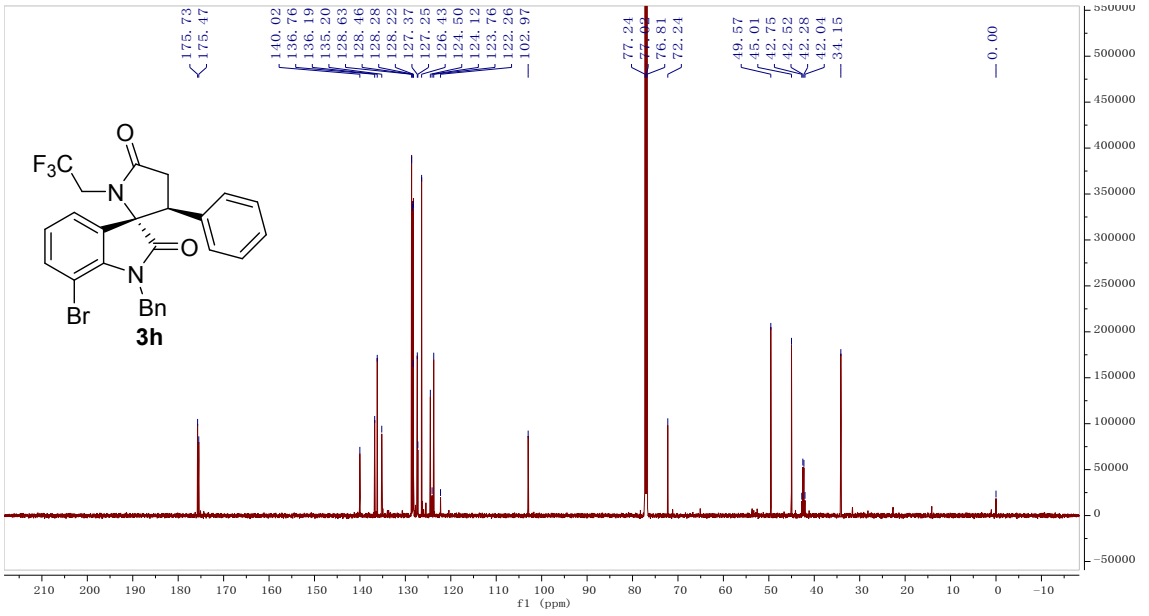


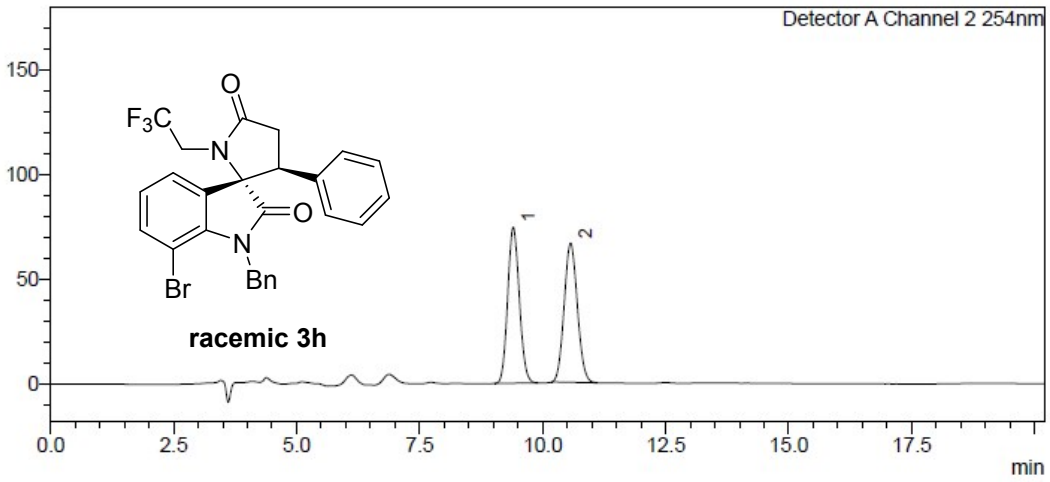
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.437	44467	2177	6.171	6.171
2	22.509	676111	15577	93.829	93.829
Total		720578	17754		100.000


7.315
7.304
7.301
7.299
7.292
7.287
7.285
7.283
7.271
7.261
7.206
7.194
7.161
7.148
7.136
7.124
7.113
6.884
6.872
6.870
6.743
6.731
6.717
6.633
6.631
6.621
6.618
5.391
5.350
5.322
3.989
3.975
3.961
3.845
3.829
3.819
3.814
3.804
3.788
3.779
3.773
3.764
3.756
3.749
3.738
3.234
3.220
3.206
3.192
3.116
3.102
3.088
3.074
1.599
0.000
3.56
1.02
3.67
1.76
0.93
0.87
1.00
1.00
1.03
2.19
0.99
1.01
F3C
N
O
O
N
Bn
Br
3h
f1 (ppm)

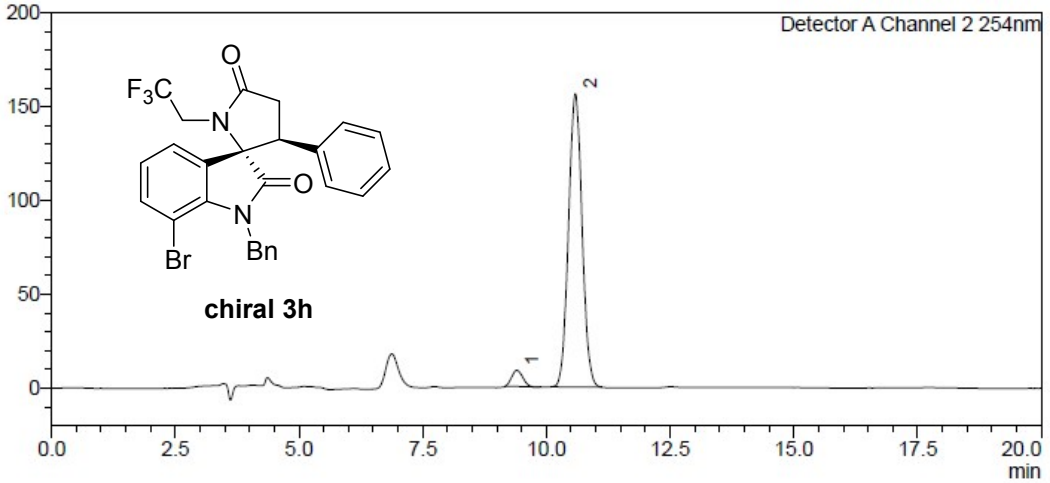

175.73
175.47
140.02
136.76
136.19
135.20
128.63
128.46
128.28
128.22
127.37
127.25
126.43
124.50
124.12
123.76
122.26
102.97
77.24
77.02
76.81
72.24
49.57
45.01
42.75
42.52
42.28
42.04
34.15
0.00
F3C
N
O
O
N
Bn
Br
3h
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

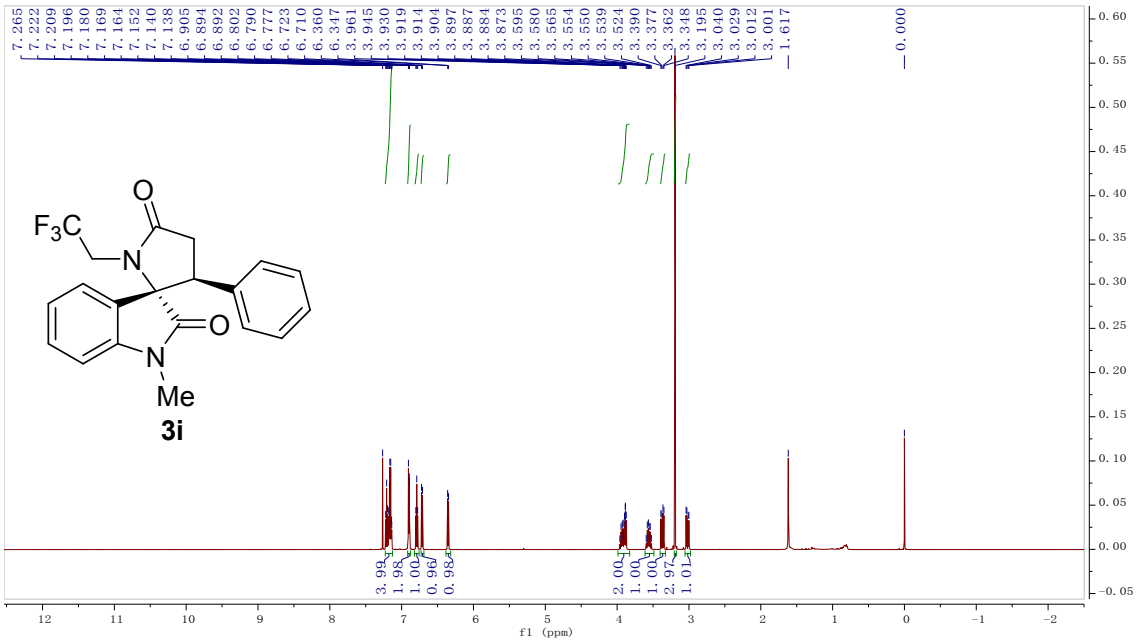
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.402	1222916	74523	49.678	49.678
2	10.568	1238762	66482	50.322	50.322
Total		2461679	141005		100.000

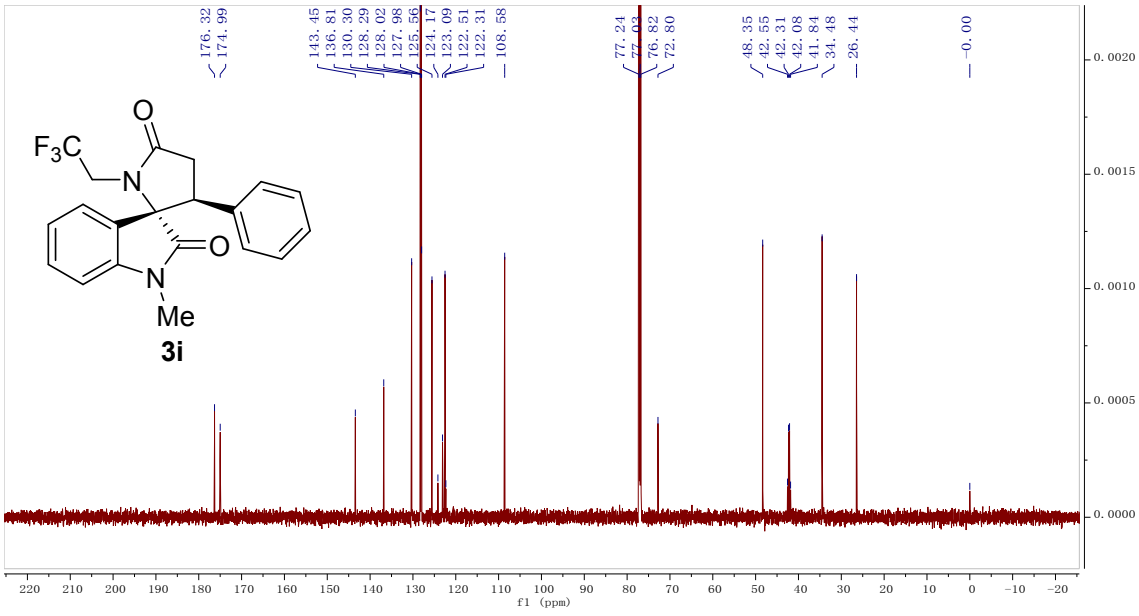


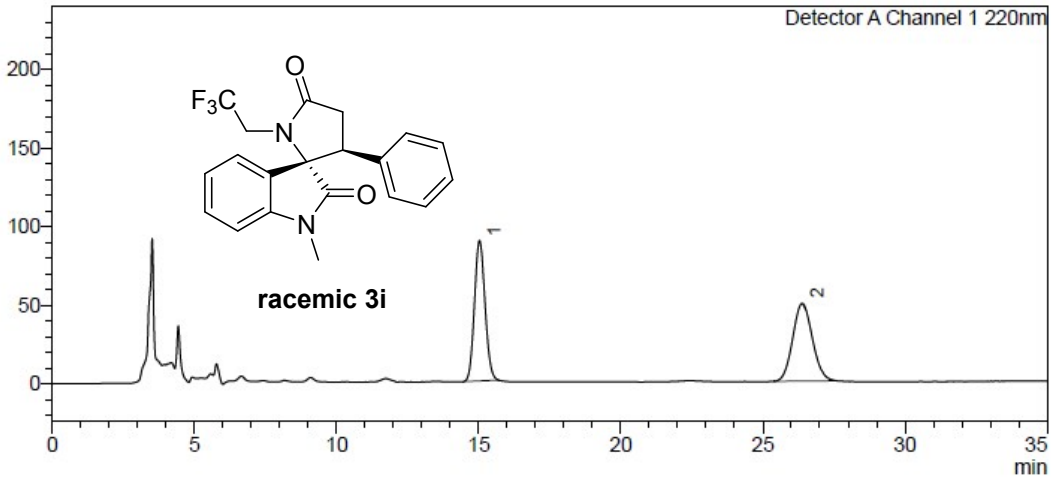
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.404	130889	8571	4.217	4.217
2	10.584	2972670	156216	95.783	95.783
Total		3103559	164787		100.000


7.265
7.222
7.209
7.196
7.180
7.169
7.164
7.152
7.140
7.138
6.905
6.894
6.892
6.802
6.790
6.777
6.723
6.710
6.360
6.347
3.961
3.945
3.930
3.919
3.914
3.904
3.897
3.887
3.884
3.873
3.595
3.580
3.565
3.554
3.550
3.539
3.524
3.390
3.377
3.362
3.348
3.195
3.040
3.029
3.012
3.001
1.617
0.000
3.99
1.98
1.00
0.96
0.98
2.00
1.00
1.00
2.97
1.01
f1 (ppm)
F3C
N
O
O
N
Me
3i

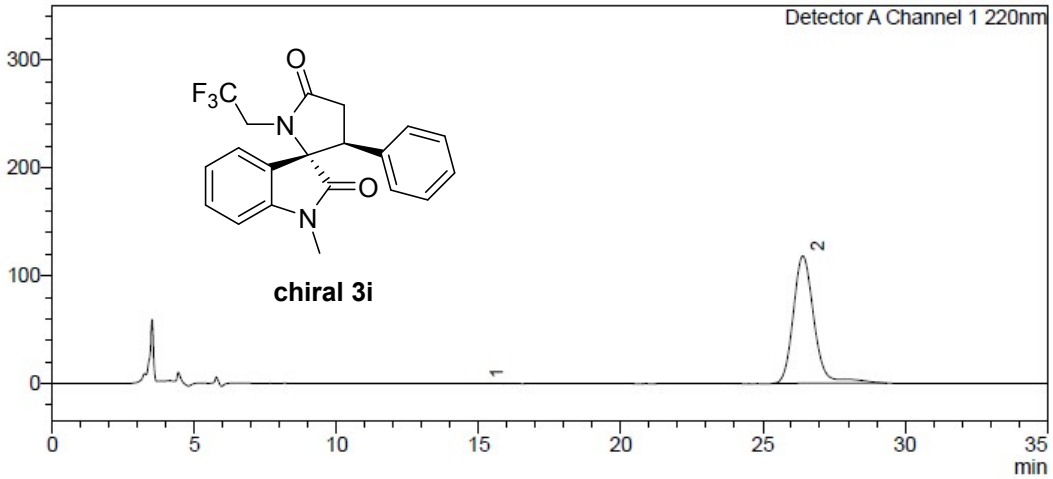

176.32
174.99
143.45
136.81
130.30
128.29
128.02
127.98
125.56
124.17
123.09
122.51
122.31
108.58
77.24
77.03
76.82
72.80
48.35
42.55
42.31
42.08
41.84
34.48
26.44
0.00
f1 (ppm)
F3C
N
O
O
N
Me
3i



<Peak Table>

Detector A Channel 1 220nm

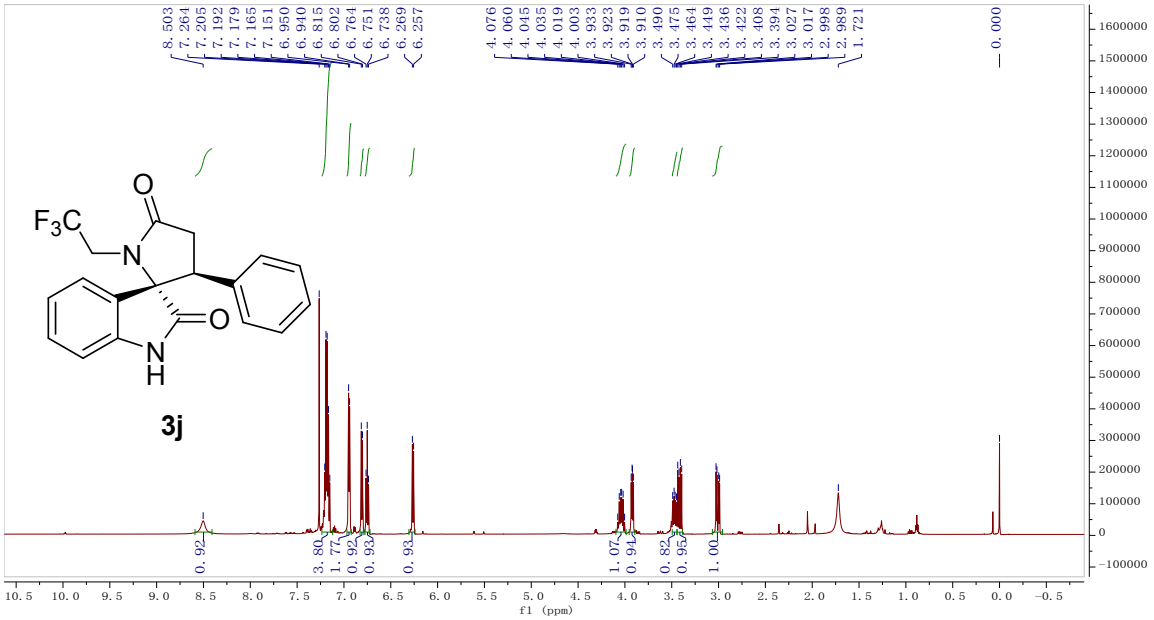
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	15.033	2302562	89304	49.308	49.308
2	26.384	2367228	49442	50.692	50.692
Total		4669790	138746		100.000

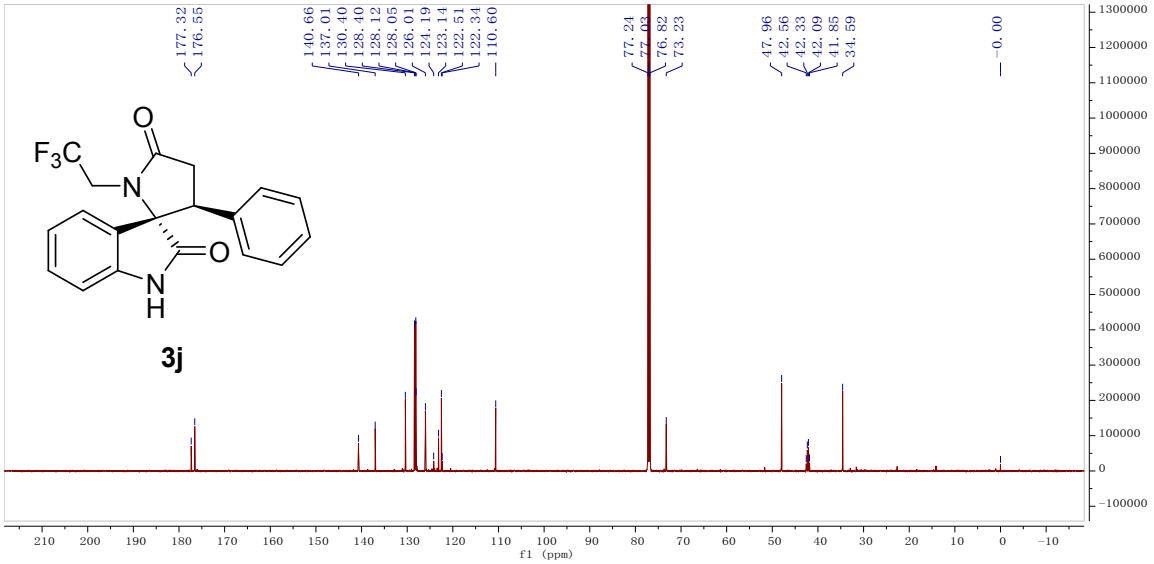


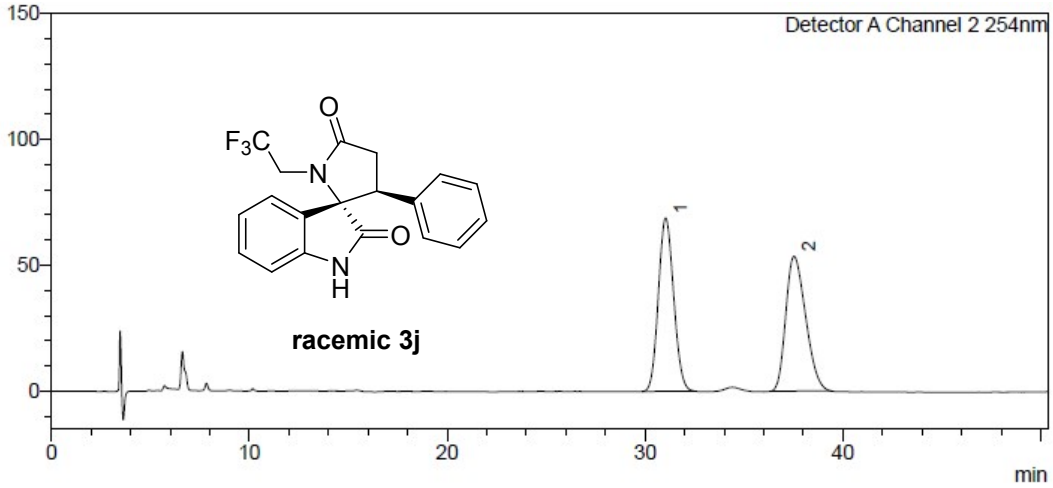
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	15.105	803	149	0.013	0.013
2	26.406	5997234	117964	99.987	99.987
Total		5998037	118113		100.000


8.503
7.264
7.205
7.192
7.179
7.165
7.151
6.950
6.940
6.815
6.802
6.764
6.751
6.738
6.269
6.257
4.076
4.060
4.045
4.035
4.019
4.003
3.933
3.923
3.919
3.910
3.490
3.475
3.464
3.449
3.436
3.422
3.408
3.394
3.027
3.017
2.998
2.989
1.721
0.000
F3C
N
O
O
N
H
3j
0.92
3.80
1.77
0.92
0.93
0.93
1.07
0.94
0.82
0.95
1.00
f1 (ppm)

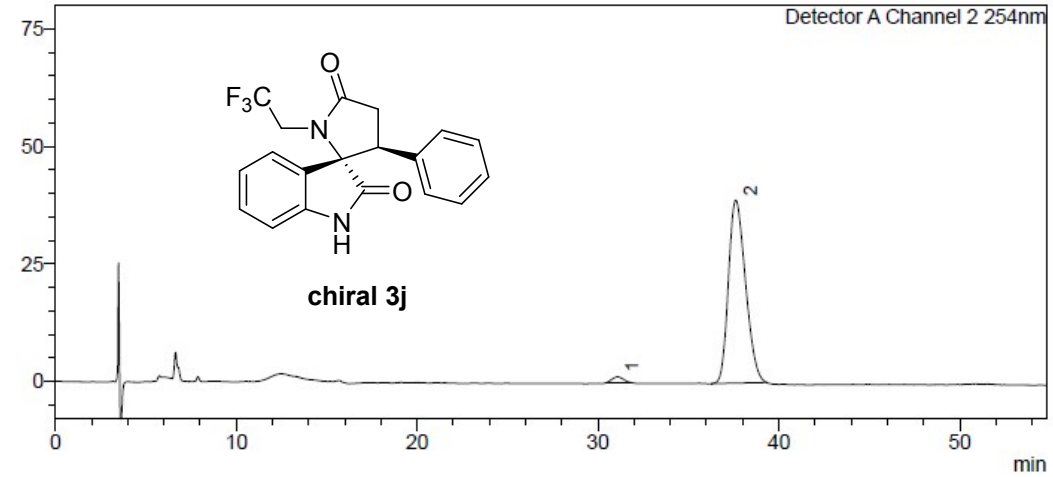

177.32
176.55
140.66
137.01
130.40
128.40
128.12
128.05
126.01
124.19
123.14
122.51
122.34
110.60
77.24
77.03
76.82
73.23
47.96
42.56
42.33
42.09
41.85
34.59
-0.00
F3C
N
O
O
N
H
3j
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

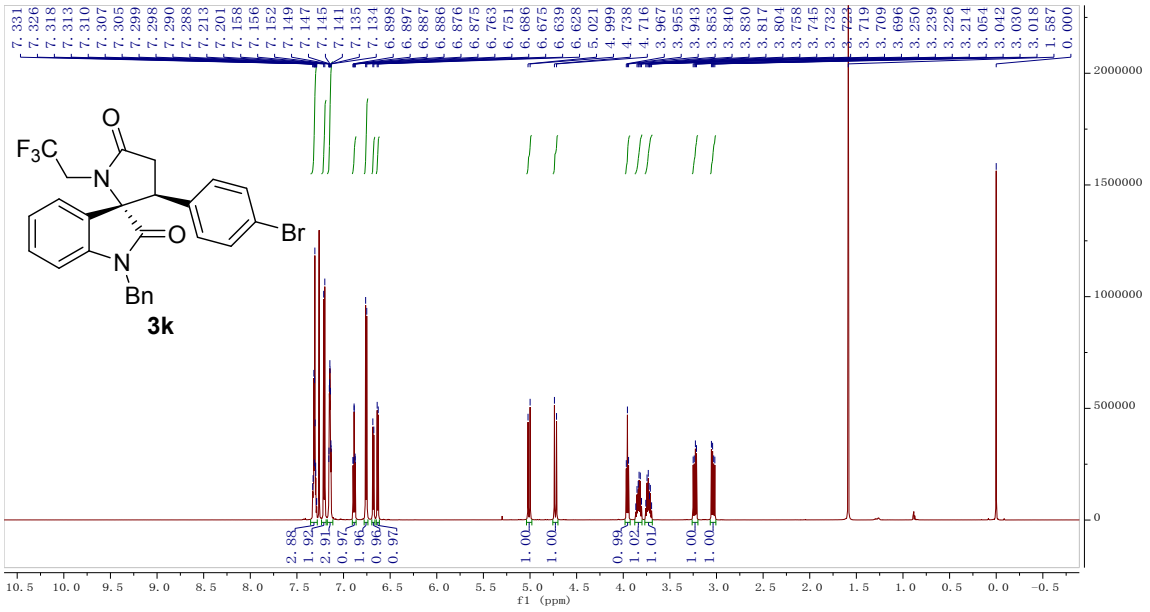
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	31.039	3690610	68776	49.721	49.721
2	37.528	3731956	53496	50.279	50.279
Total		7422566	122271		100.000

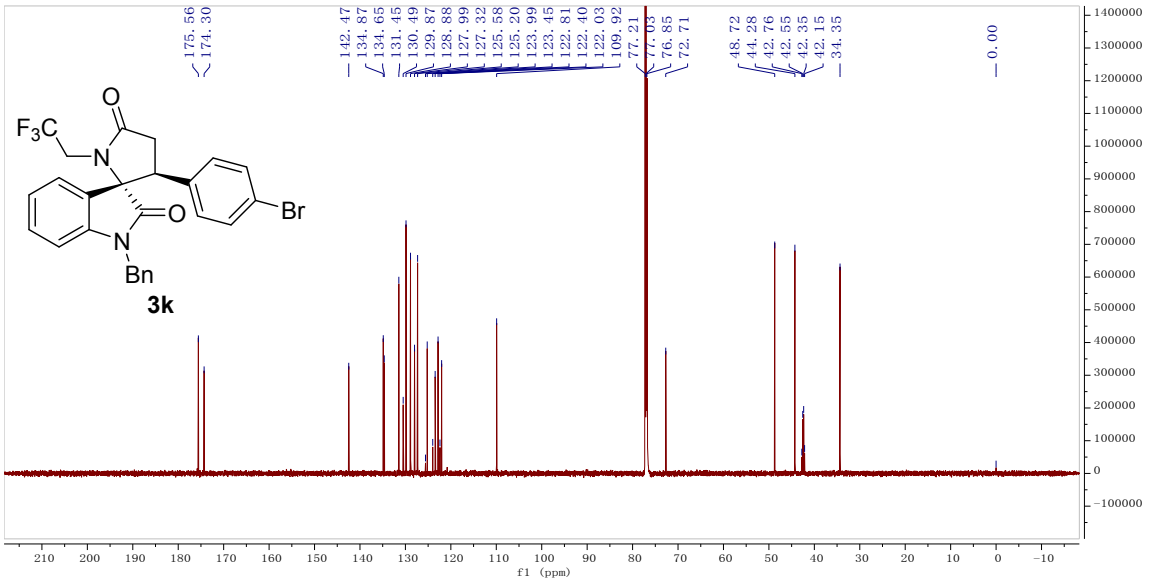


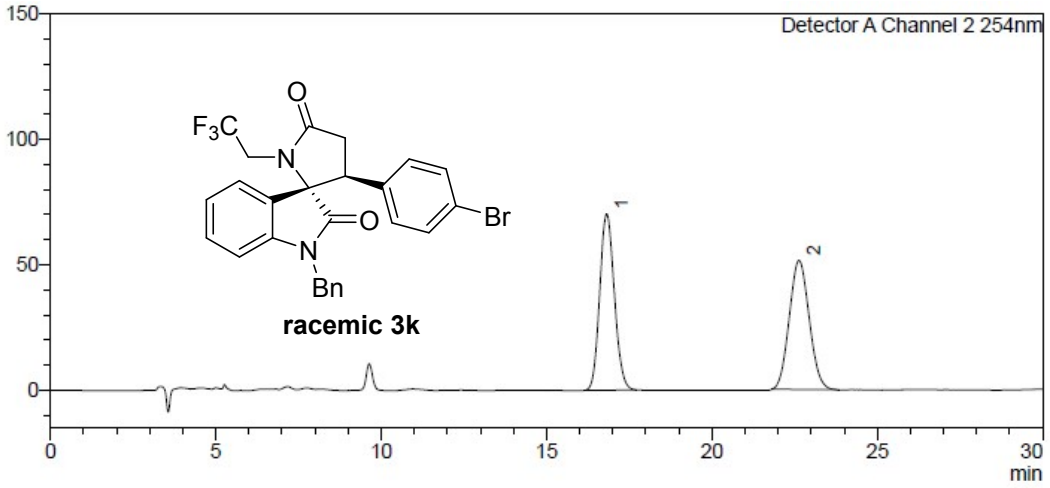
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	31.076	56087	1286	2.149	2.149
2	37.620	2553259	38927	97.851	97.851
Total		2609346	40213		100.000


3k
f1 (ppm)

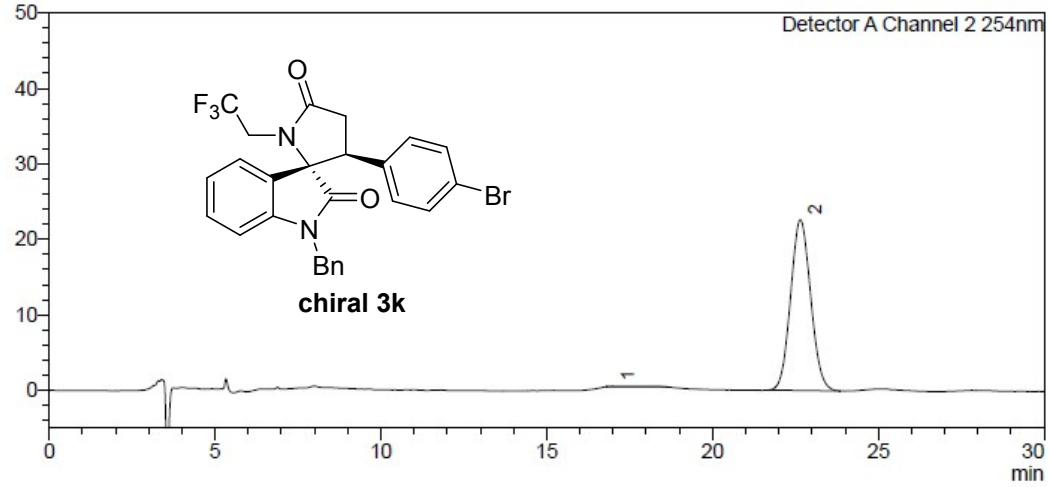

3k
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

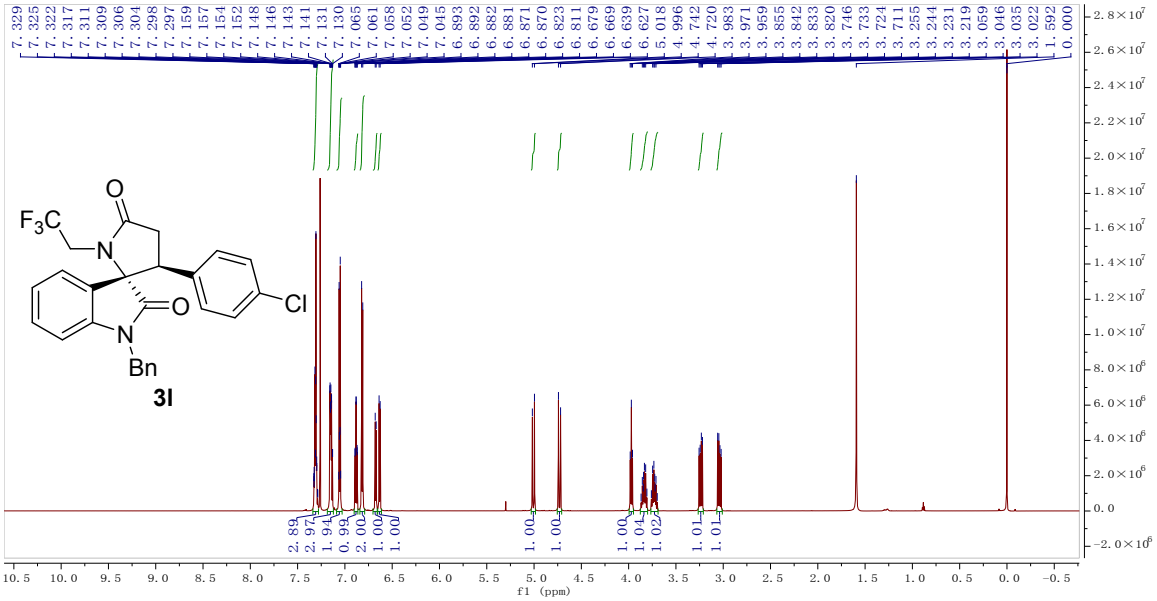
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	16.817	2161316	70297	50.094	50.094
2	22.634	2153216	51422	49.906	49.906
Total		4314532	121719		100.000

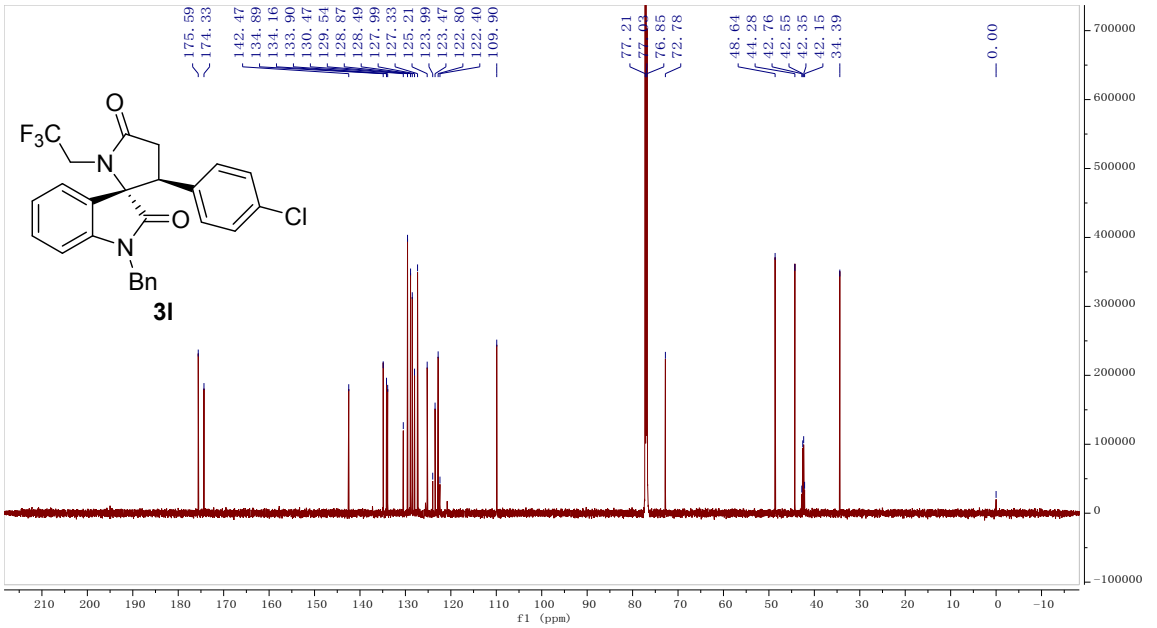


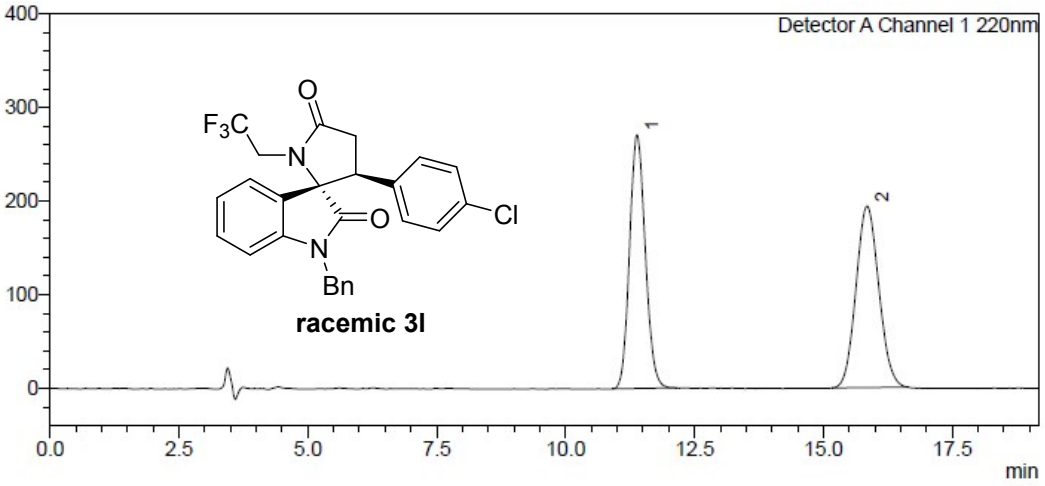
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	16.990	3916	53	0.409	0.409
2	22.648	952441	22638	99.591	99.591
Total		956357	22691		100.000


7.329 7.325 7.322 7.317 7.311 7.309 7.306 7.304 7.298 7.297 7.159 7.157 7.154 7.152 7.148 7.146 7.143 7.141 7.131 7.130 7.065 7.061 7.058 7.052 7.049 7.045 6.893 6.892 6.882 6.881 6.871 6.870 6.823 6.811 6.679 6.669 6.639 6.627 5.018 4.996 4.742 4.720 3.983 3.971 3.959 3.855 3.842 3.833 3.820 3.746 3.733 3.724 3.711 3.255 3.244 3.231 3.219 3.059 3.046 3.035 3.022 1.592 0.000
2.89 2.97 1.94 0.99 2.00 1.00 1.00 1.00 1.00 1.00 1.04 1.02 1.01 1.01
F3C N O O N Bn Cl
3l
f1 (ppm)


175.59 174.33 142.47 134.89 134.16 133.90 130.47 129.54 128.87 128.49 127.99 127.33 125.21 123.99 123.47 122.80 122.40 109.90
77.21 77.03 76.85 72.78
48.64 44.28 42.76 42.55 42.35 42.15 34.39
0.00
F3C N O O N Bn Cl
3l
f1 (ppm)

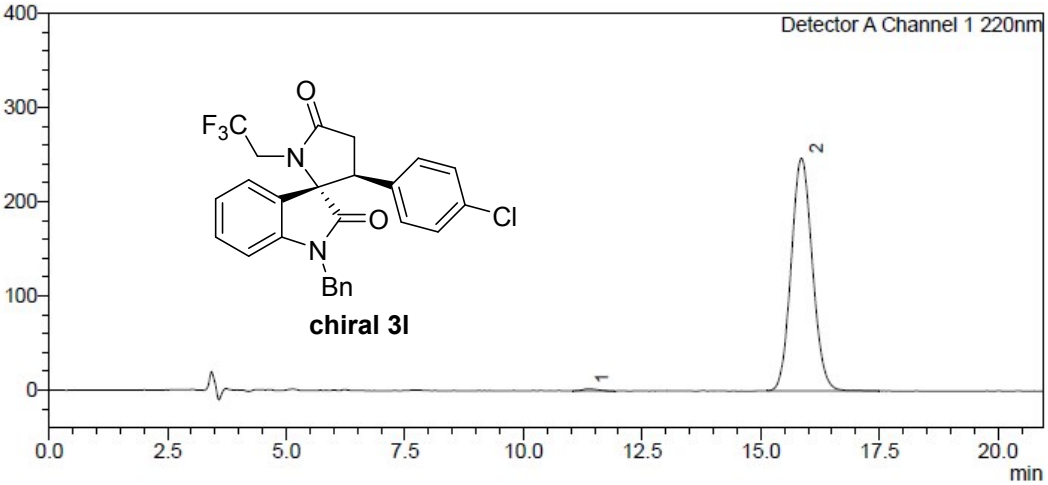


racemic 3l

<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.384	5757039	270946	49.139	49.139
2	15.846	5958807	193730	50.861	50.861
Total		11715846	464676		100.000

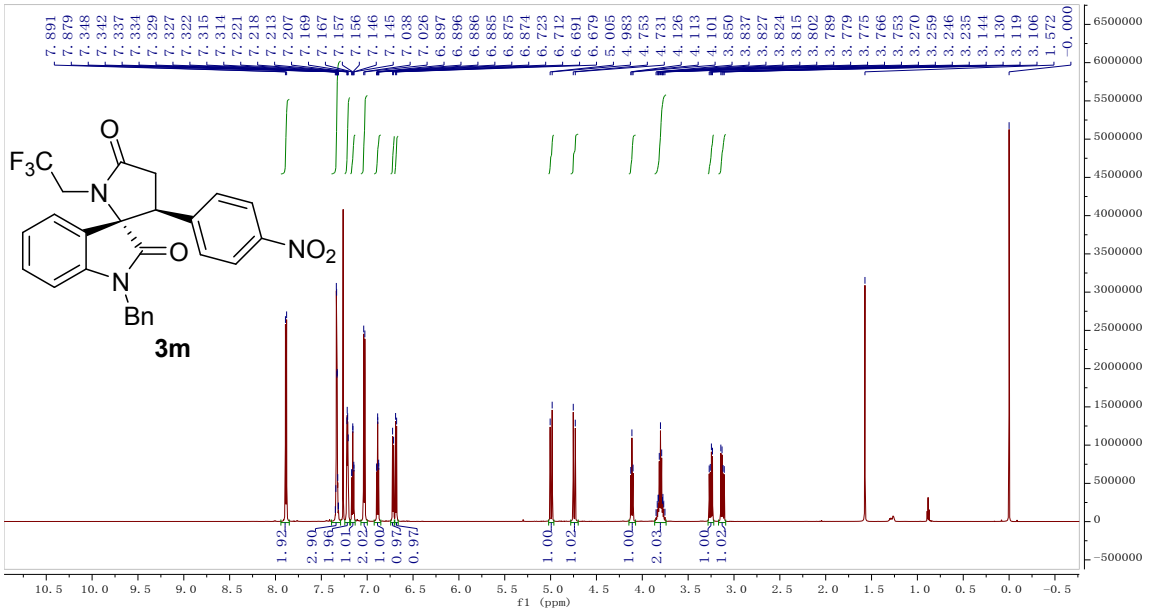


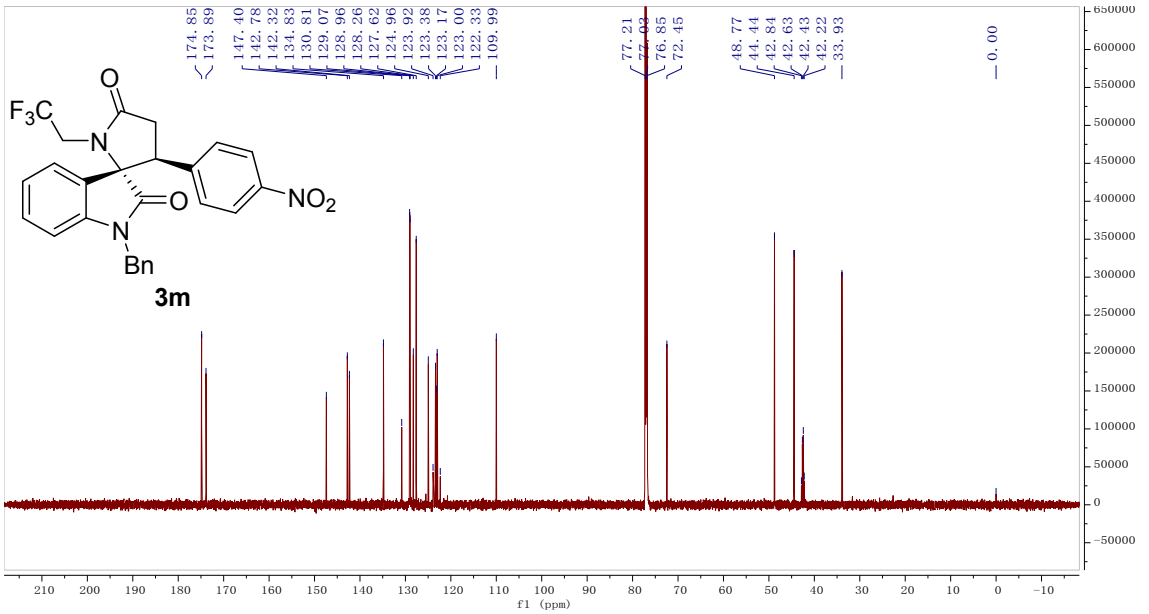
chiral 3l

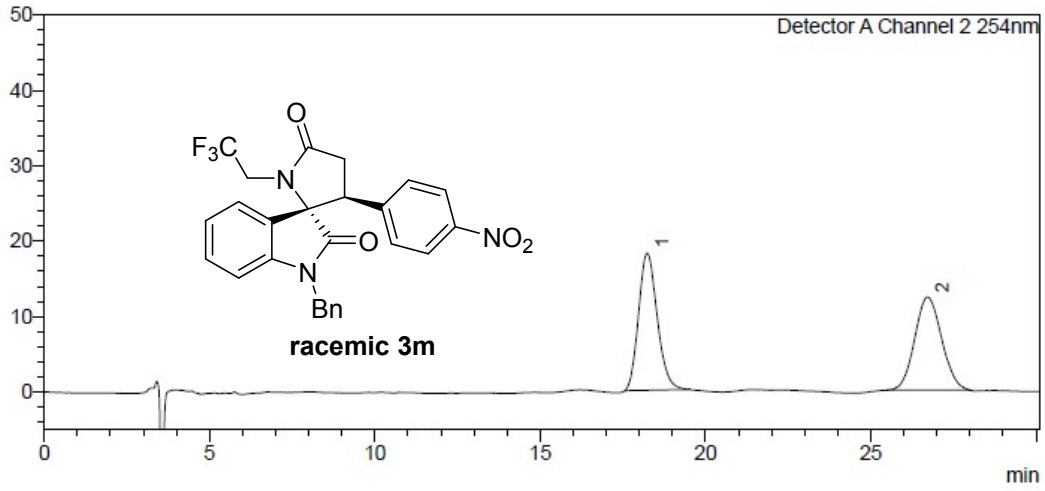
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.338	50953	2220	0.660	0.660
2	15.857	7667700	247096	99.340	99.340
Total		7718654	249316		100.000


7.891
7.879
7.348
7.342
7.337
7.334
7.329
7.327
7.322
7.315
7.314
7.221
7.218
7.213
7.207
7.169
7.167
7.157
7.156
7.146
7.145
7.038
7.026
6.897
6.896
6.886
6.885
6.875
6.874
6.723
6.712
6.691
6.679
5.005
4.983
4.753
4.731
4.126
4.113
4.101
3.850
3.837
3.827
3.824
3.815
3.802
3.789
3.779
3.775
3.766
3.753
3.270
3.259
3.246
3.235
3.144
3.130
3.119
3.106
1.572
-0.000
F3C
N
O
O
N
Bn
NO2
3m
1.92
2.90
1.96
1.01
2.02
1.00
0.97
0.97
1.00
1.02
1.00
2.03
1.00
1.02
f1 (ppm)

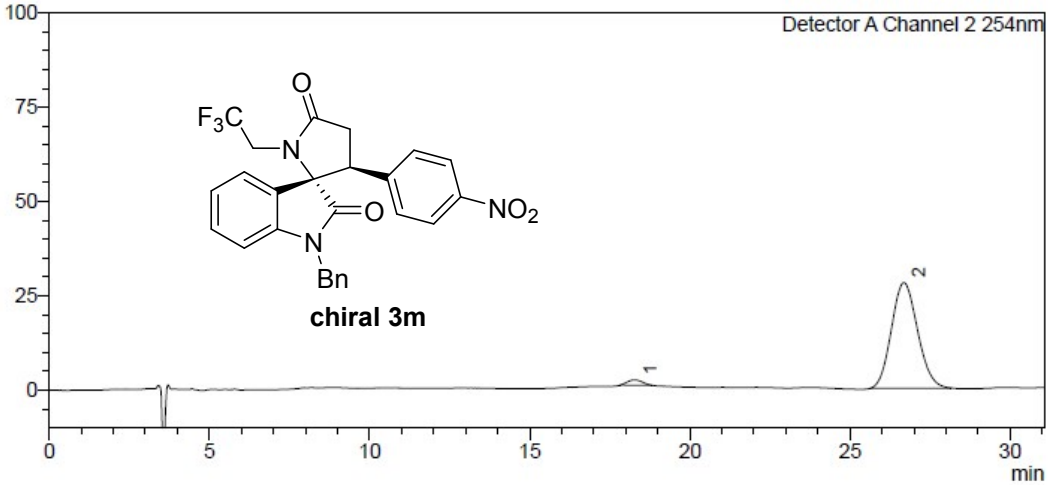

174.85
173.89
147.40
142.78
142.32
134.83
130.81
129.07
128.96
128.26
127.62
124.96
123.92
123.38
123.17
123.00
122.33
109.99
77.21
77.03
76.85
72.45
48.77
44.44
42.84
42.63
42.43
42.22
33.93
0.00
F3C
N
O
O
N
Bn
NO2
3m
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

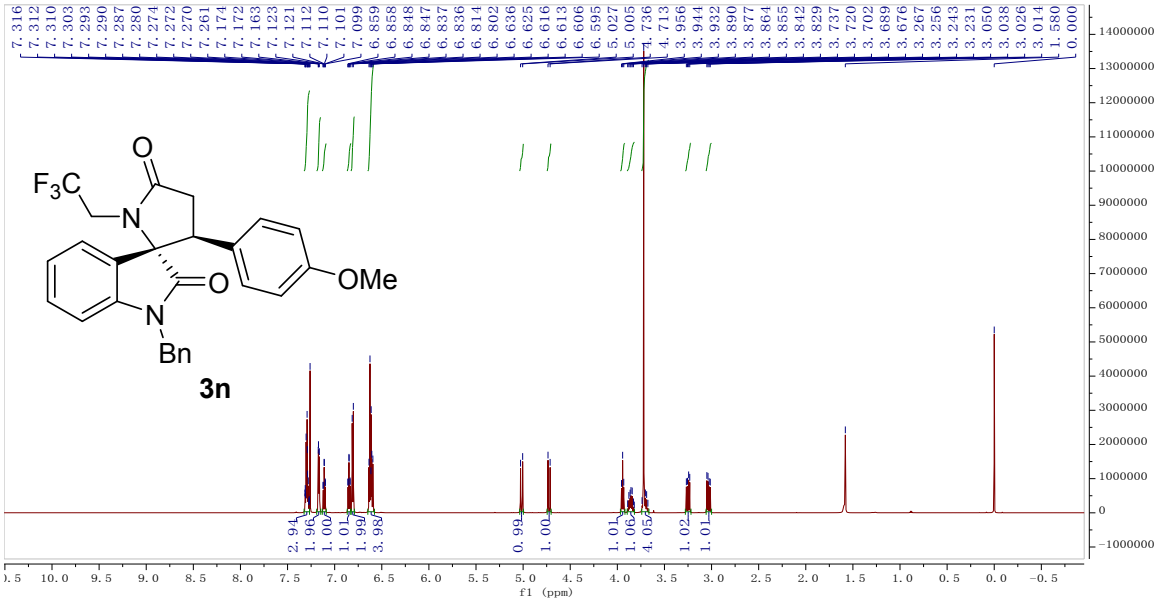
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	18.239	713863	18183	50.537	50.537
2	26.716	698683	12332	49.463	49.463
Total		1412546	30515		100.000

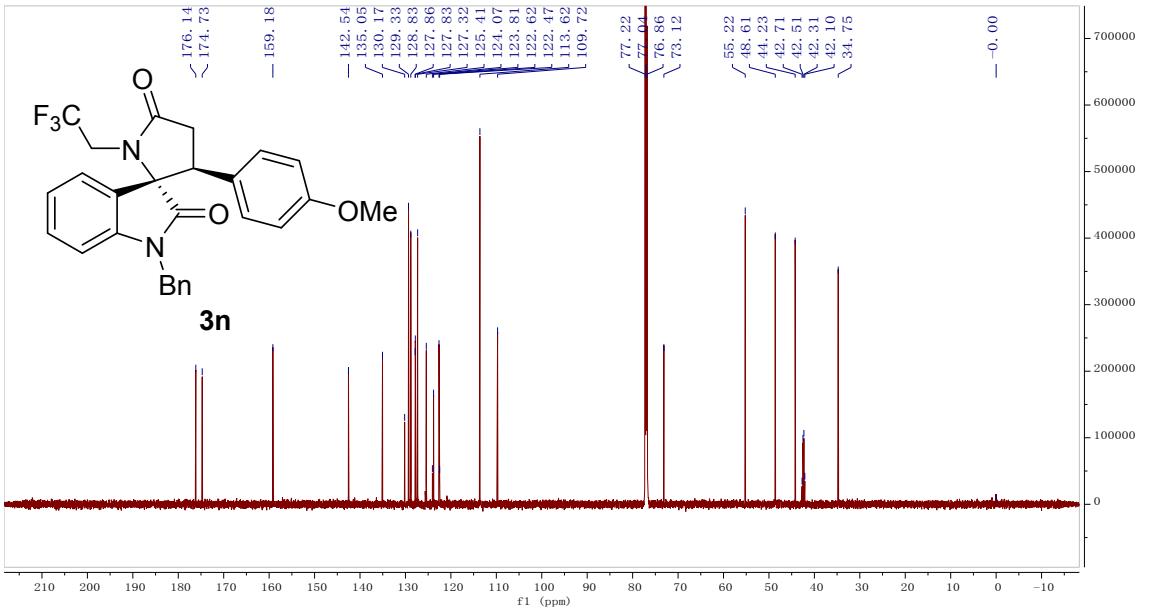


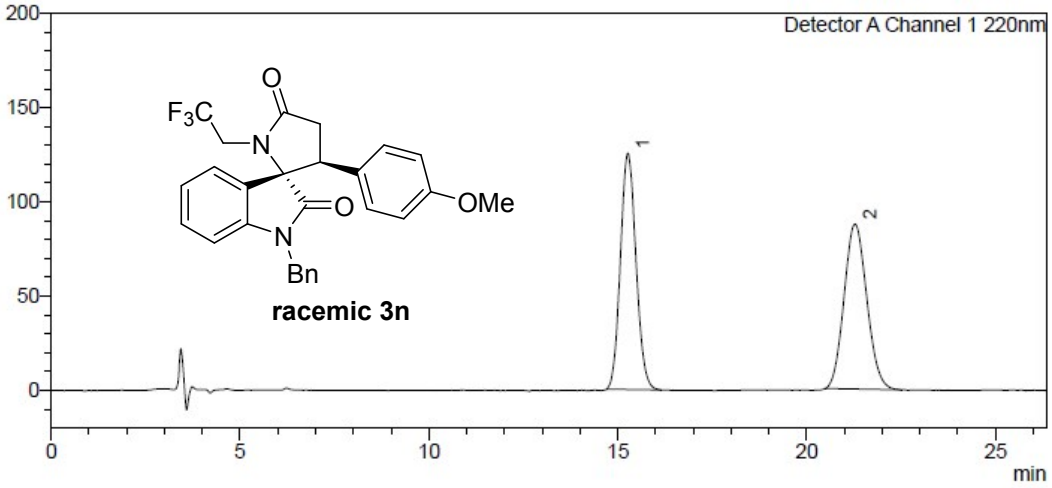
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	18.288	43895	1383	2.693	2.693
2	26.678	1585998	27973	97.307	97.307
Total		1629893	29356		100.000


7.316
7.312
7.310
7.303
7.293
7.290
7.287
7.280
7.274
7.272
7.270
7.261
7.174
7.172
7.163
7.123
7.121
7.112
7.110
7.101
7.099
6.859
6.858
6.848
6.847
6.837
6.836
6.814
6.802
6.636
6.625
6.616
6.613
6.606
6.595
5.027
5.005
4.736
4.713
3.956
3.944
3.932
3.890
3.877
3.864
3.855
3.842
3.829
3.737
3.720
3.702
3.689
3.676
3.267
3.256
3.243
3.231
3.050
3.038
3.026
3.014
1.580
0.000
O
F3C
N
O
OMe
N
Bn
3n
2.94
1.96
1.00
1.01
1.99
3.98
0.99
1.00
1.01
1.06
4.05
1.02
1.01
f1 (ppm)

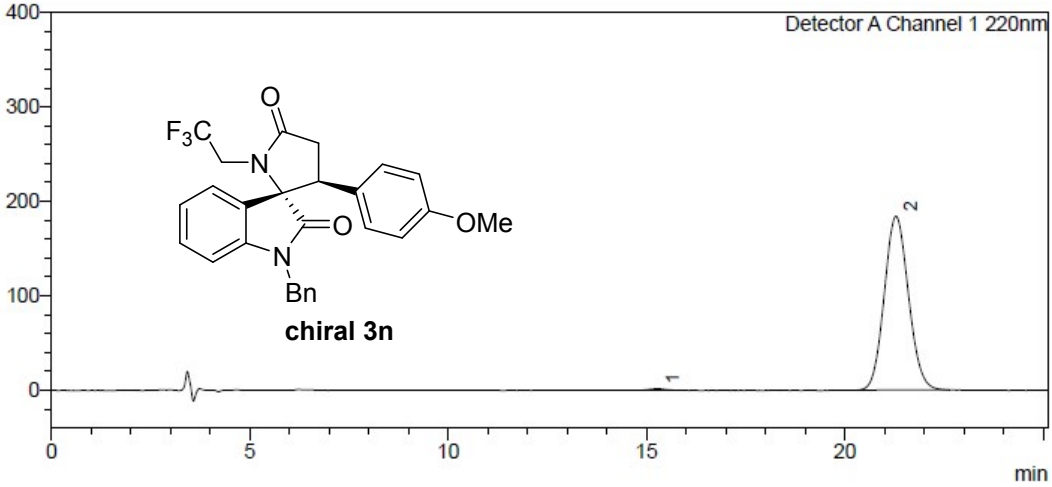

176.14
174.73
159.18
142.54
135.05
130.17
129.33
128.83
127.86
127.83
127.32
125.41
124.07
123.81
122.62
122.47
113.62
109.72
77.22
77.01
76.86
73.12
55.22
48.61
44.23
42.71
42.51
42.31
42.10
34.75
-0.00
O
F3C
N
O
OMe
N
Bn
3n
f1 (ppm)



<Peak Table>

Detector A Channel 1 220nm

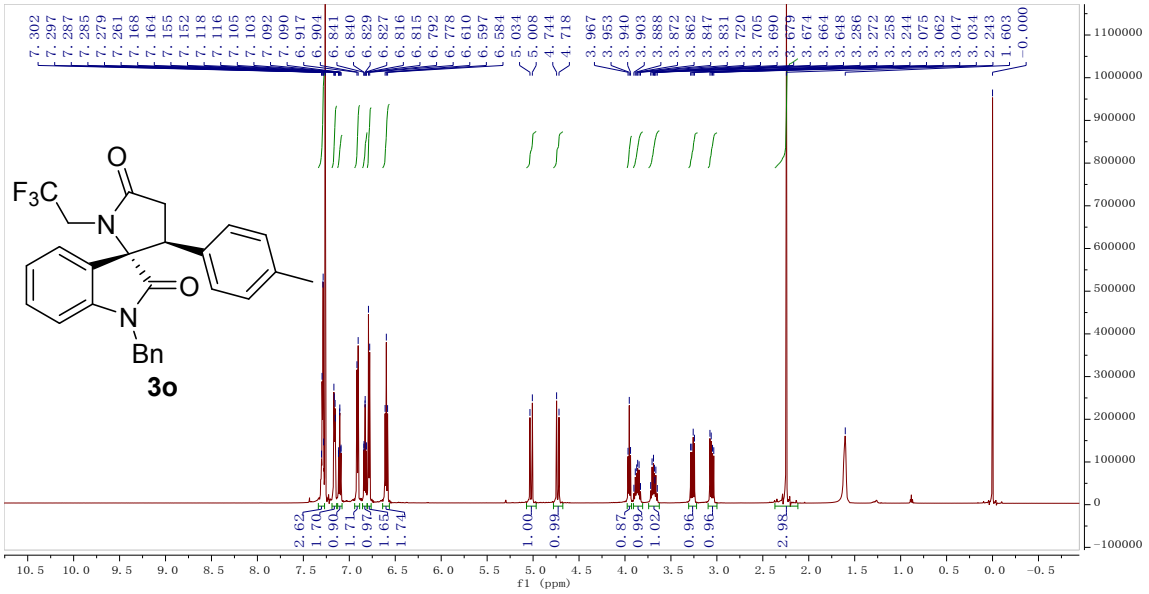
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	15.268	3599229	125383	49.559	49.559
2	21.280	3663275	87588	50.441	50.441
Total		7262503	212971		100.000

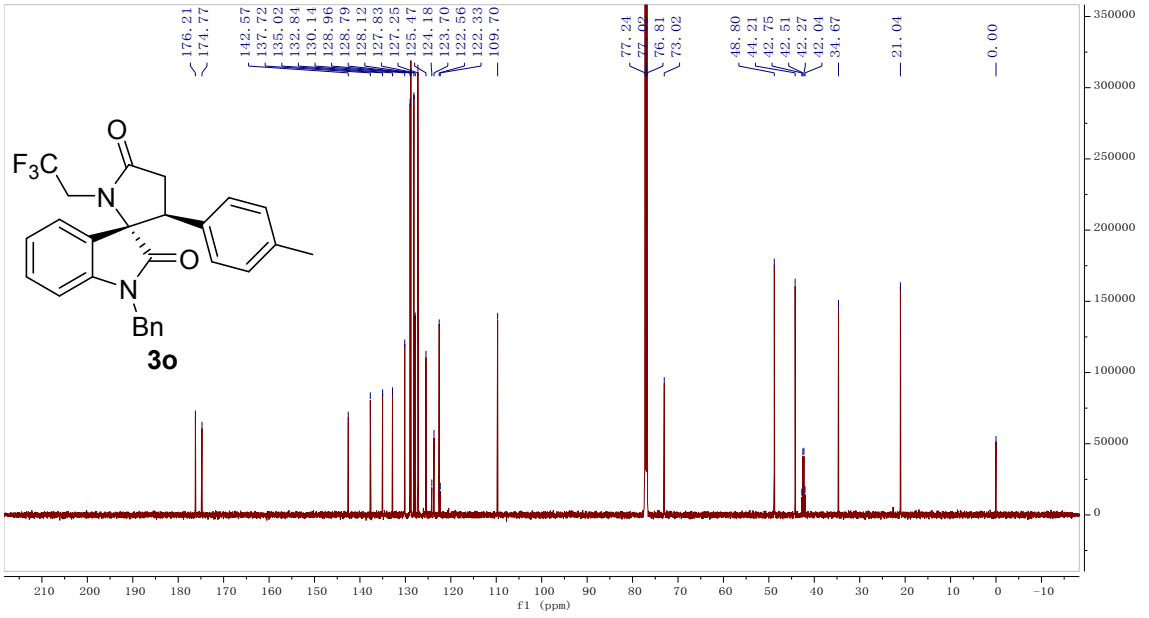


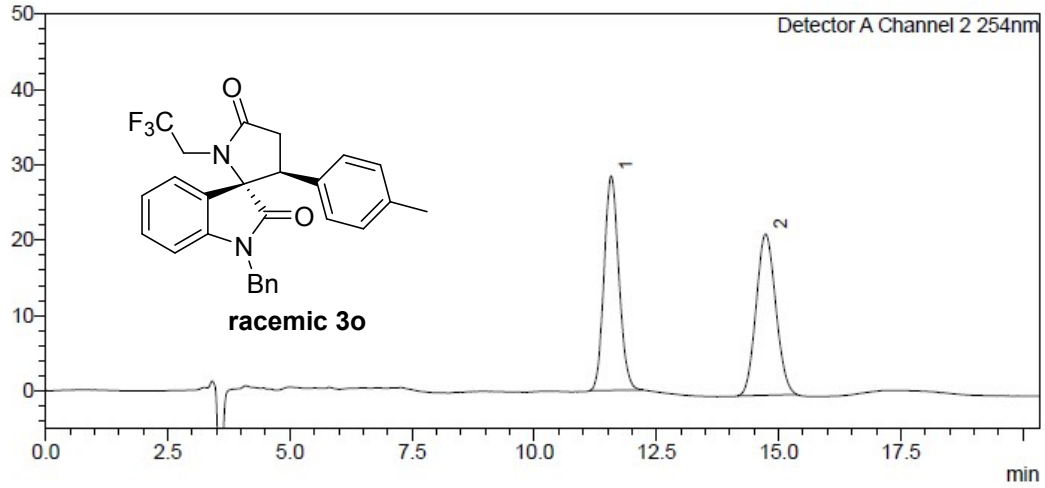
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	15.291	38613	1478	0.493	0.493
2	21.292	7795744	184013	99.507	99.507
Total		7834357	185491		100.000


7.302
7.297
7.287
7.285
7.279
7.261
7.168
7.164
7.155
7.152
7.118
7.116
7.105
7.103
7.092
7.090
6.917
6.904
6.841
6.840
6.829
6.827
6.816
6.815
6.792
6.778
6.610
6.597
6.584
5.034
5.008
4.744
4.718
3.967
3.953
3.940
3.903
3.888
3.872
3.862
3.847
3.831
3.720
3.705
3.690
3.679
3.674
3.664
3.648
3.286
3.272
3.258
3.244
3.075
3.062
3.047
3.034
2.243
1.603
0.000
2.62
1.70
0.90
1.71
0.97
1.65
1.74
1.00
0.99
0.87
0.99
1.02
0.96
0.96
2.98
F3C
N
O
O
N
Bn
3o
f1 (ppm)

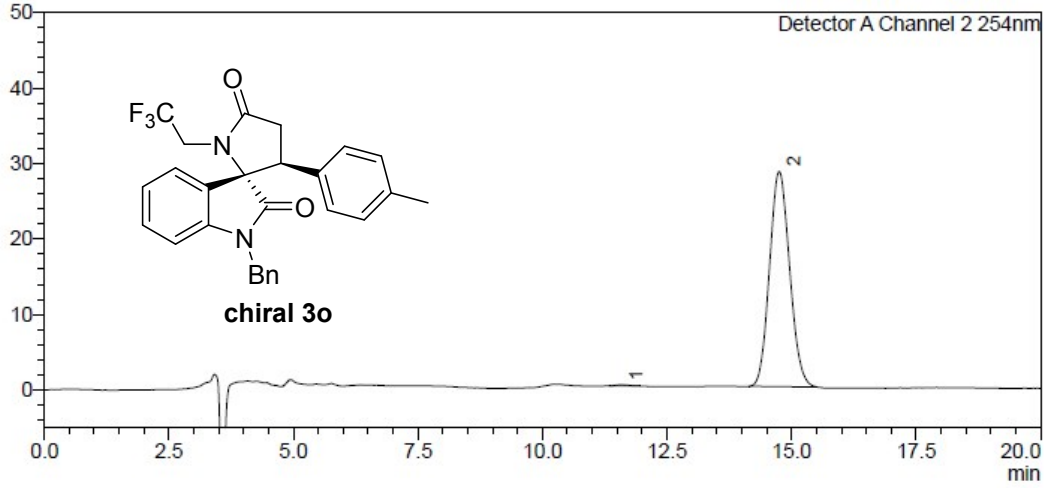

176.21
174.77
142.57
137.72
135.02
132.84
130.14
128.96
128.79
128.12
127.83
127.25
125.47
124.18
123.70
122.56
122.33
109.70
77.24
77.02
76.81
73.02
48.80
44.21
42.75
42.51
42.27
42.04
34.67
21.04
0.00
F3C
N
O
O
N
Bn
3o
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

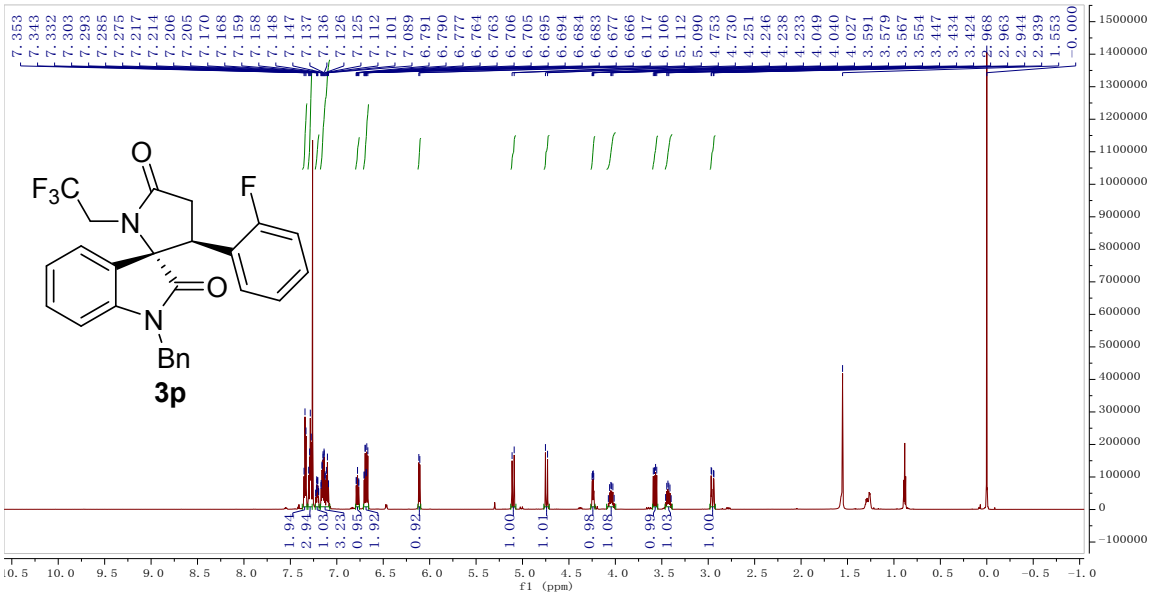
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.574	598122	28446	50.057	50.057
2	14.735	596752	21387	49.943	49.943
Total		1194874	49834		100.000

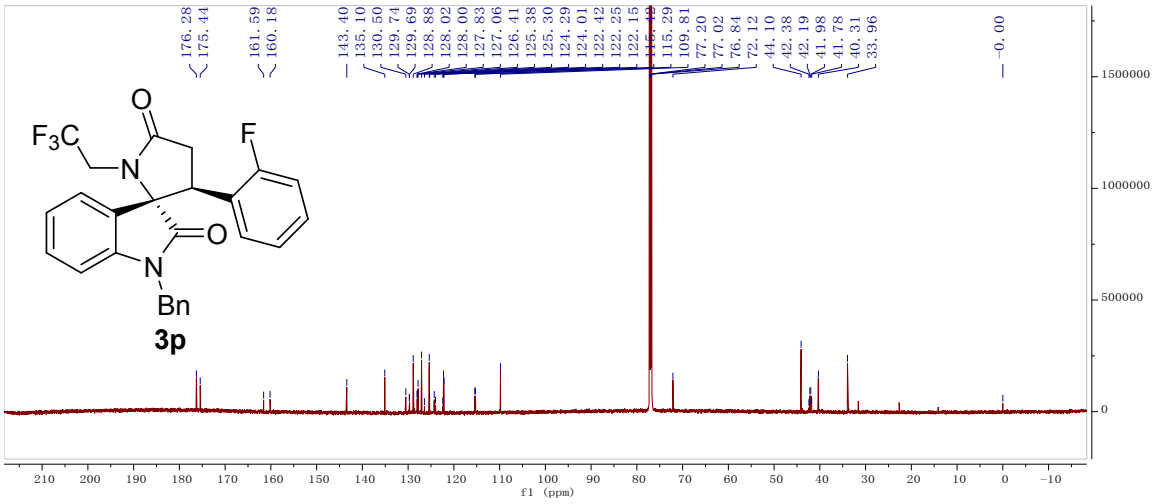


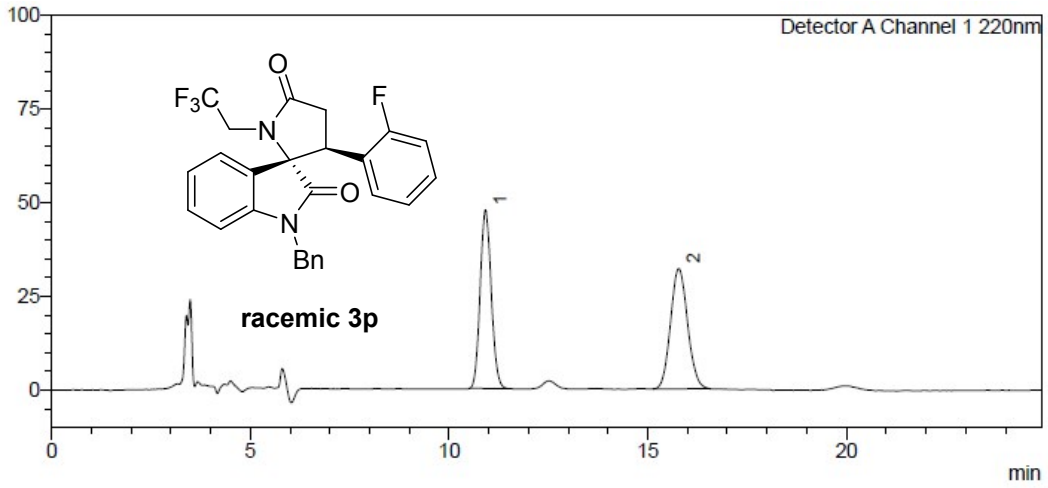
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.577	2558	138	0.319	0.319
2	14.751	799658	28505	99.681	99.681
Total		802215	28643		100.000


7.353
7.343
7.332
7.303
7.293
7.285
7.275
7.217
7.214
7.206
7.205
7.170
7.168
7.159
7.158
7.148
7.147
7.137
7.136
7.126
7.125
7.112
7.101
7.089
6.791
6.790
6.777
6.764
6.763
6.706
6.705
6.695
6.694
6.684
6.683
6.677
6.666
6.117
6.106
5.112
5.090
4.753
4.730
4.251
4.246
4.238
4.233
4.049
4.040
4.027
3.591
3.579
3.567
3.554
3.447
3.434
3.424
2.968
2.963
2.944
2.939
1.553
0.000
1.94
2.94
1.03
3.23
0.95
1.92
0.92
1.00
1.01
0.98
1.08
0.99
1.03
1.00
F3C
F
N
O
O
N
Bn
3p
f1 (ppm)

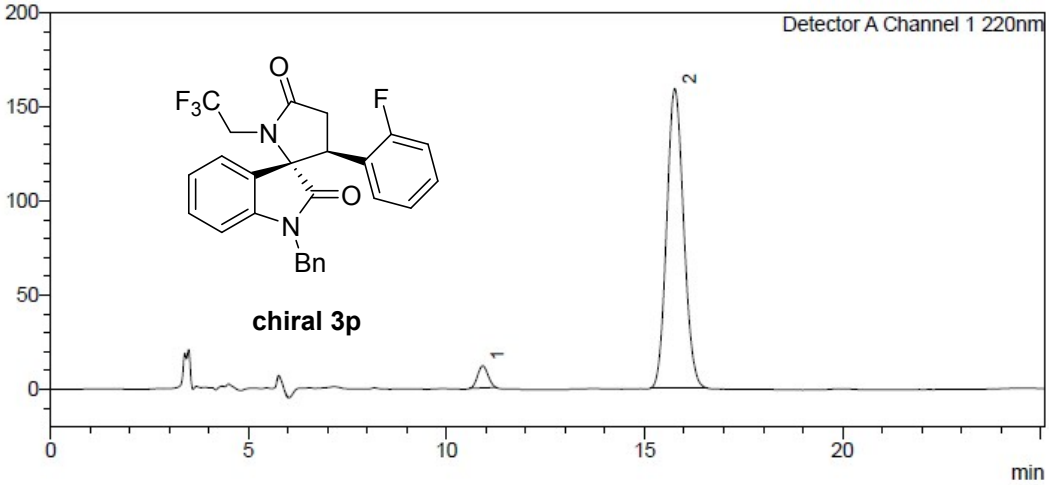

176.28
175.44
161.59
160.18
143.40
135.10
130.50
129.74
129.69
128.88
128.02
128.00
127.83
127.06
126.41
125.38
125.30
124.29
124.01
122.42
122.25
122.15
115.29
109.81
77.20
77.02
76.84
72.12
44.10
42.38
42.19
41.98
41.78
40.31
33.96
0.00
F3C
F
N
O
O
N
Bn
3p
f1 (ppm)



<Peak Table>

Detector A Channel 1 220nm

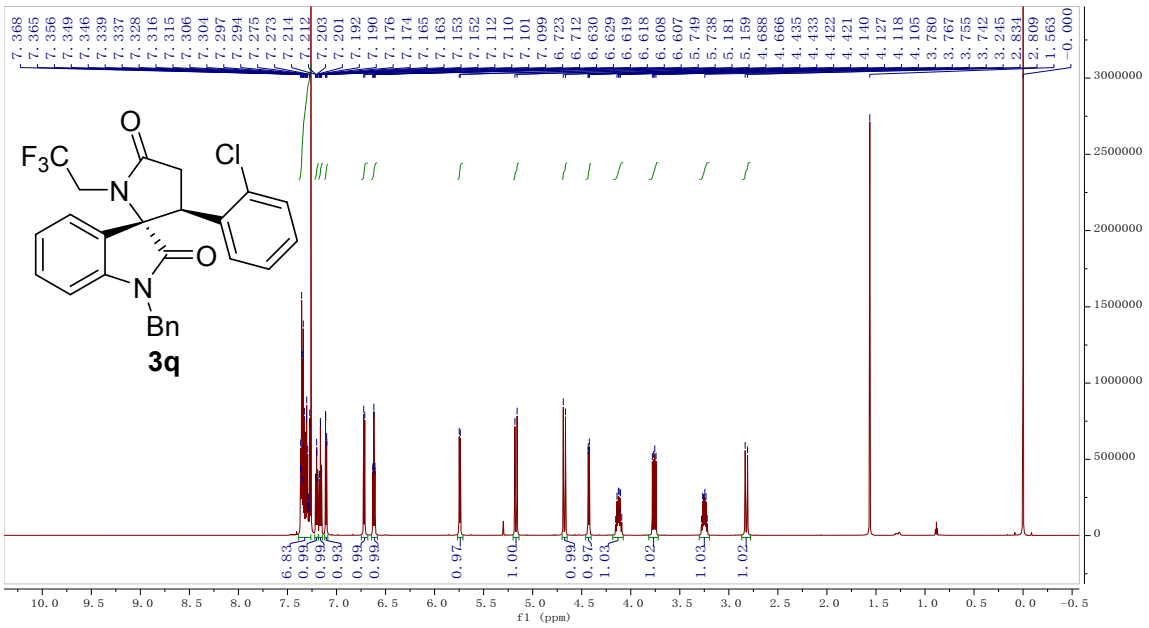
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.916	925223	47686	49.183	49.183
2	15.779	955956	32098	50.817	50.817
Total		1881179	79785		100.000

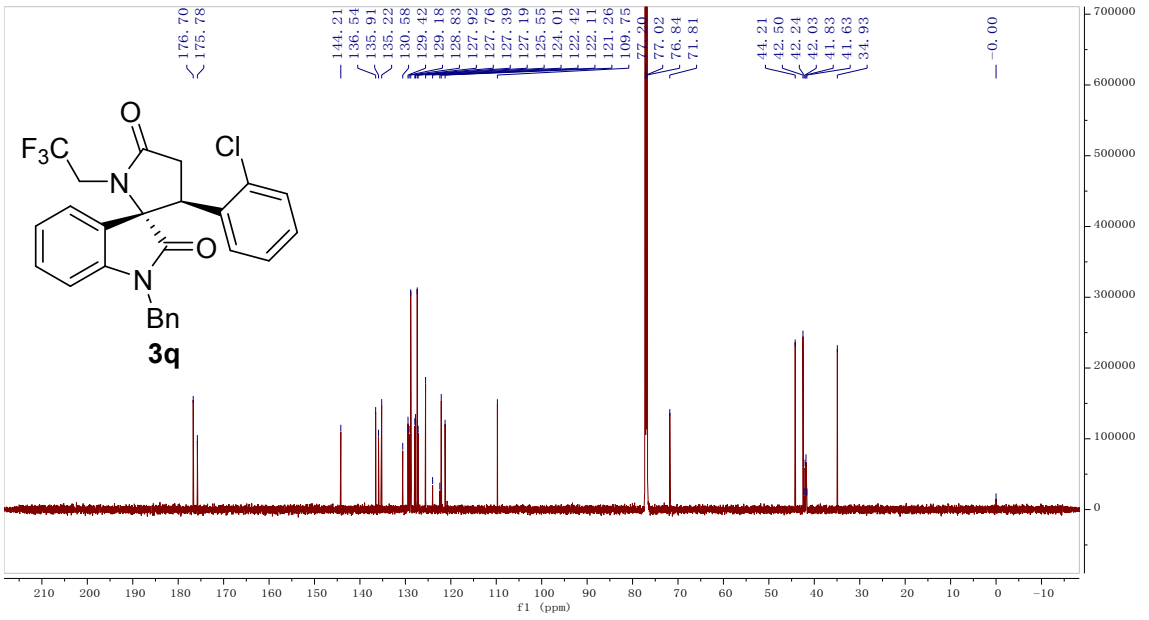


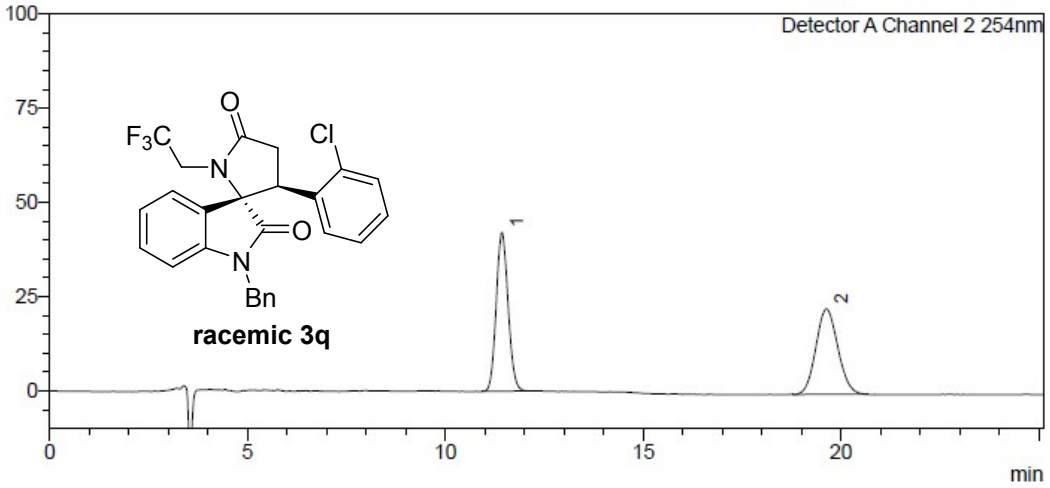
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.915	213084	11709	4.301	4.301
2	15.765	4741611	159220	95.699	95.699
Total		4954695	170929		100.000


7.368
7.365
7.356
7.349
7.346
7.339
7.337
7.328
7.316
7.315
7.306
7.304
7.297
7.294
7.275
7.273
7.214
7.212
7.203
7.201
7.192
7.190
7.176
7.174
7.165
7.163
7.153
7.152
7.112
7.110
7.101
7.099
6.723
6.712
6.630
6.629
6.619
6.618
6.608
6.607
5.749
5.738
5.181
5.159
4.688
4.666
4.435
4.433
4.422
4.421
4.140
4.127
4.118
4.105
3.780
3.767
3.755
3.742
3.245
2.834
2.809
1.563
-0.000
O
F3C
N
Cl
O
N
Bn
3q
6.83
0.99
0.99
0.93
0.99
0.99
0.97
1.00
0.99
0.97
1.03
1.02
1.03
1.02
3000000
2500000
2000000
1500000
1000000
500000
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

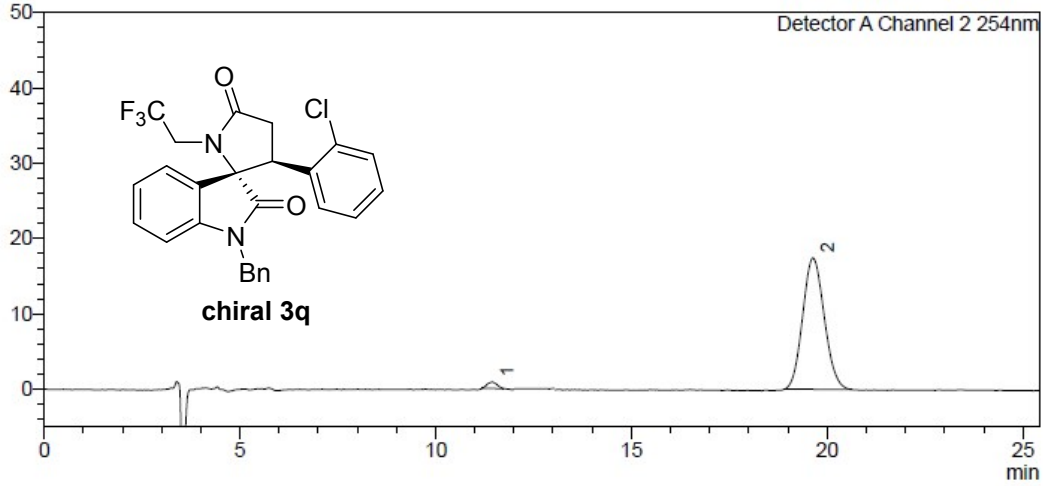

176.70
175.78
144.21
136.54
135.91
135.22
130.58
129.42
129.18
128.83
127.92
127.76
127.39
127.19
125.55
124.01
122.42
122.11
121.26
109.75
77.20
77.02
76.84
71.81
44.21
42.50
42.24
42.03
41.83
41.63
34.93
-0.00
O
F3C
N
Cl
O
N
Bn
3q
700000
600000
500000
400000
300000
200000
100000
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

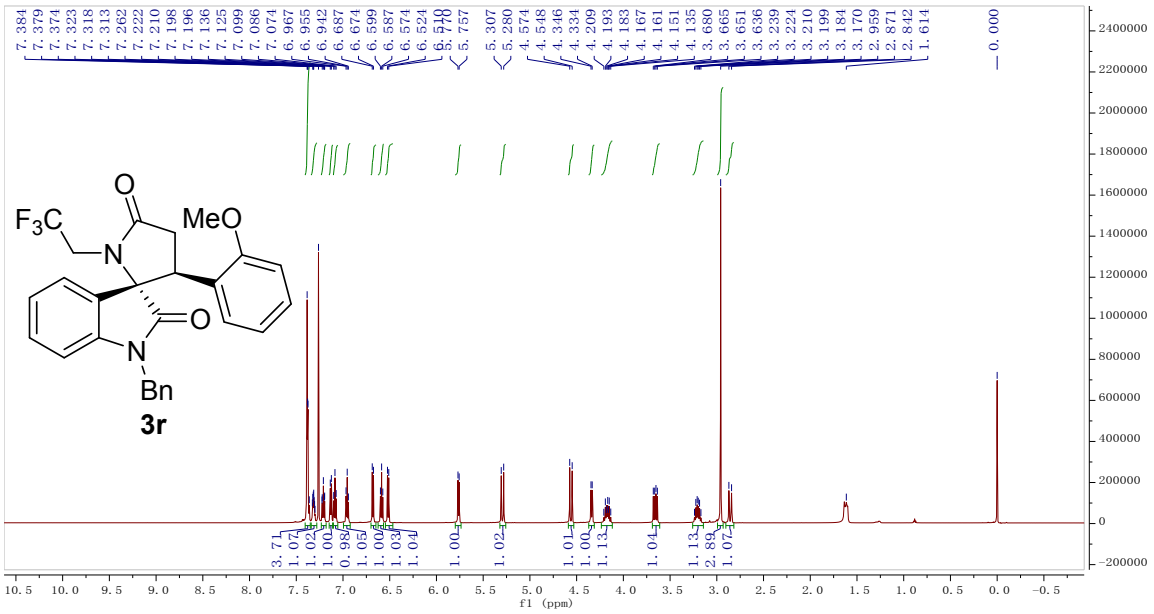
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.431	879504	42118	50.191	50.191
2	19.631	872804	22696	49.809	49.809
Total		1752308	64815		100.000

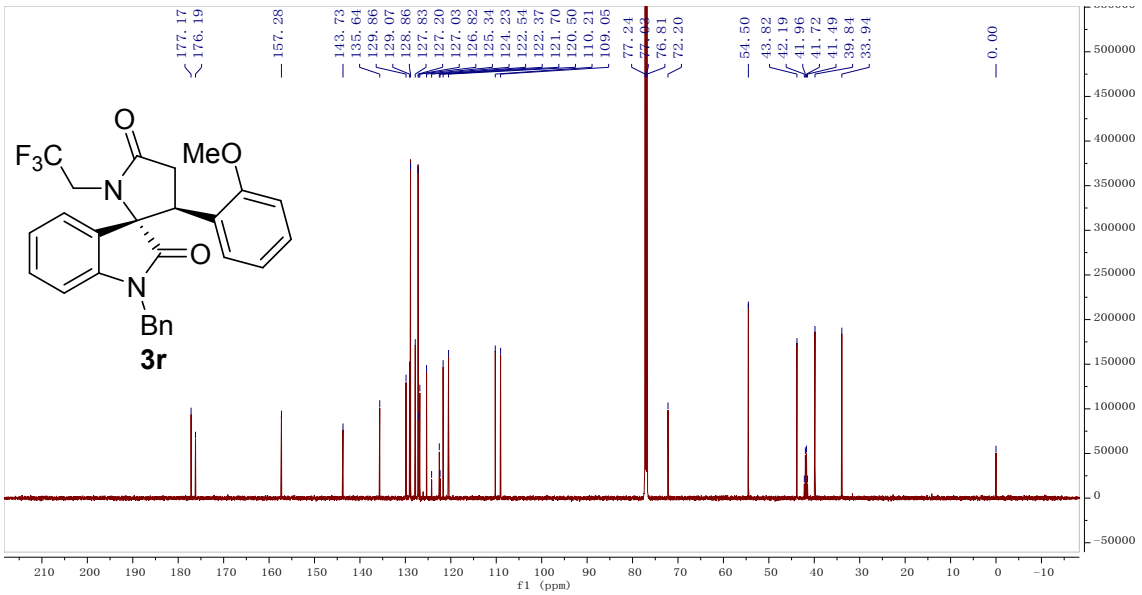


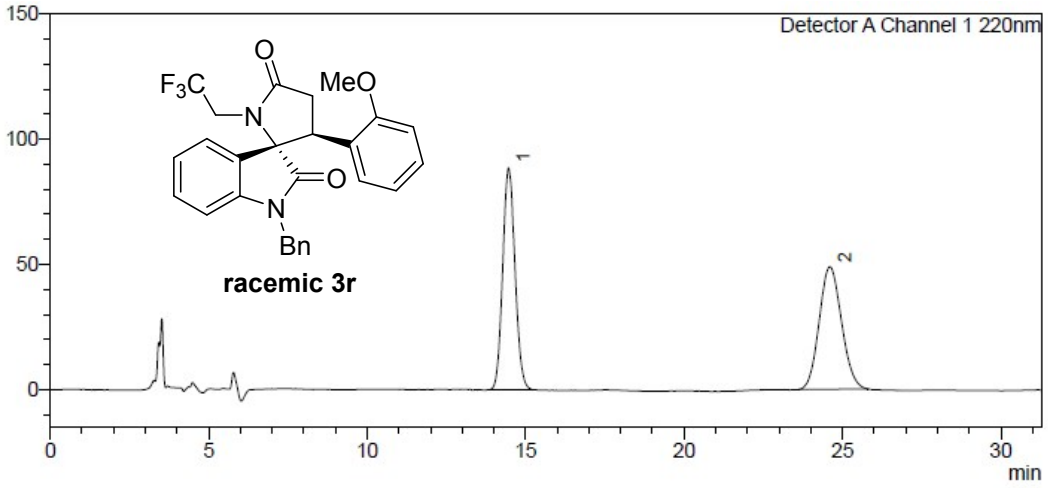
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.445	14908	843	2.180	2.180
2	19.639	668826	17438	97.820	97.820
Total		683734	18281		100.000


F3C
MeO
O
N
O
N
Bn
3r
f1 (ppm)

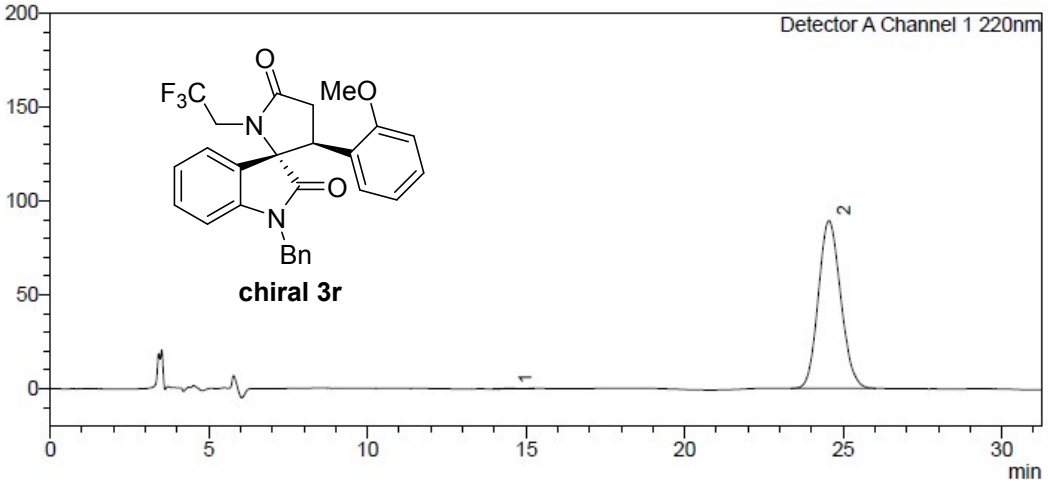

F3C
MeO
O
N
O
N
Bn
3r
f1 (ppm)



<Peak Table>

Detector A Channel 1 220nm

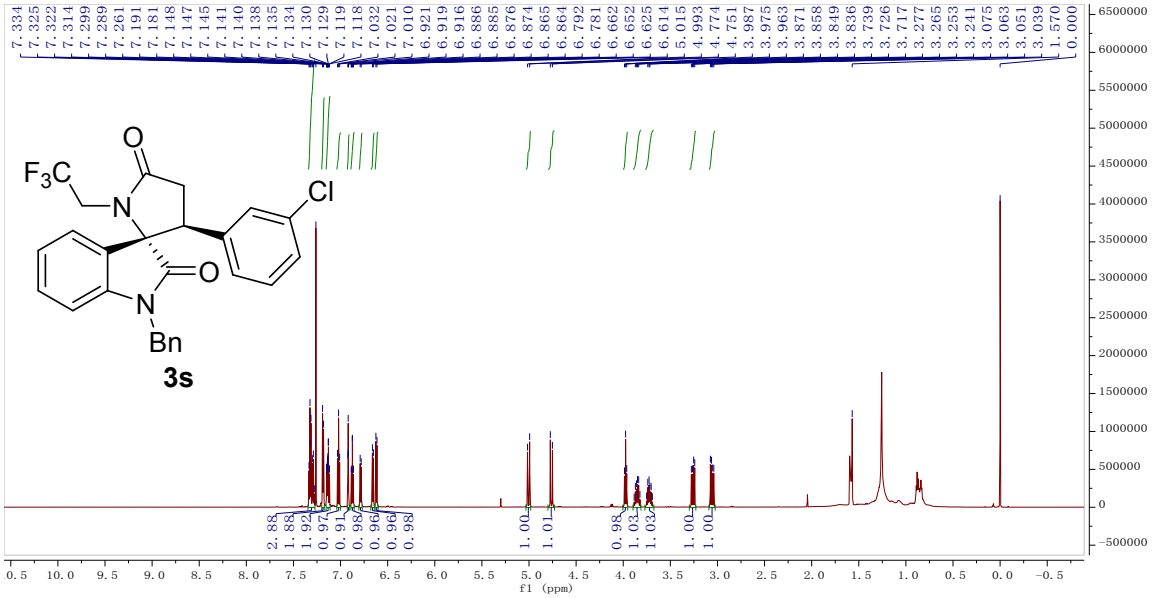
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	14.467	2388321	88535	49.946	49.946
2	24.607	2393464	48852	50.054	50.054
Total		4781785	137387		100.000

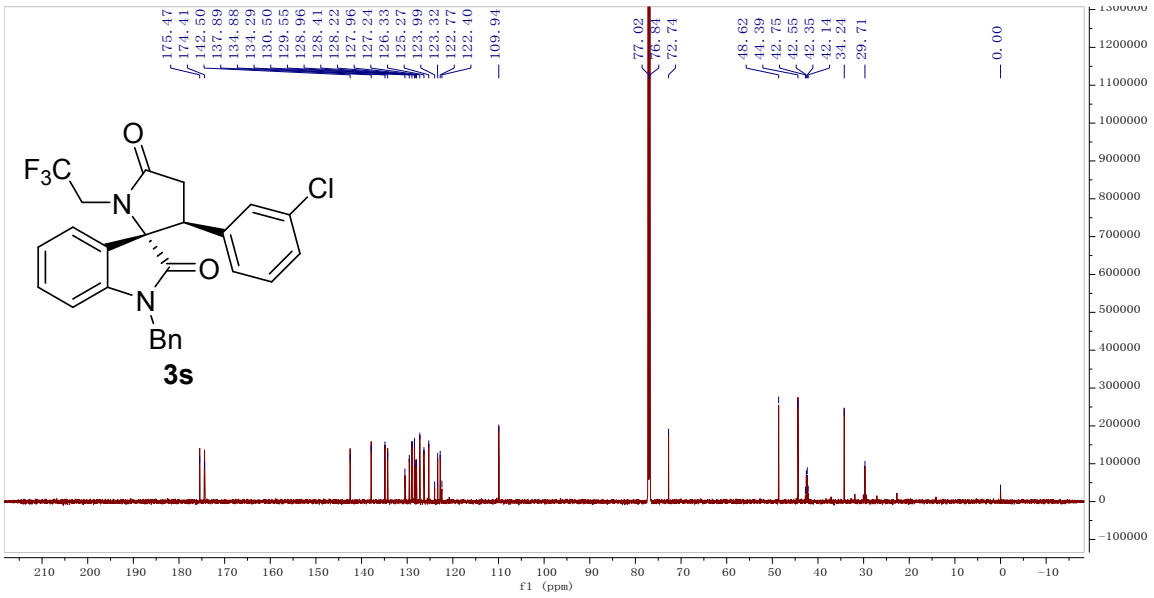


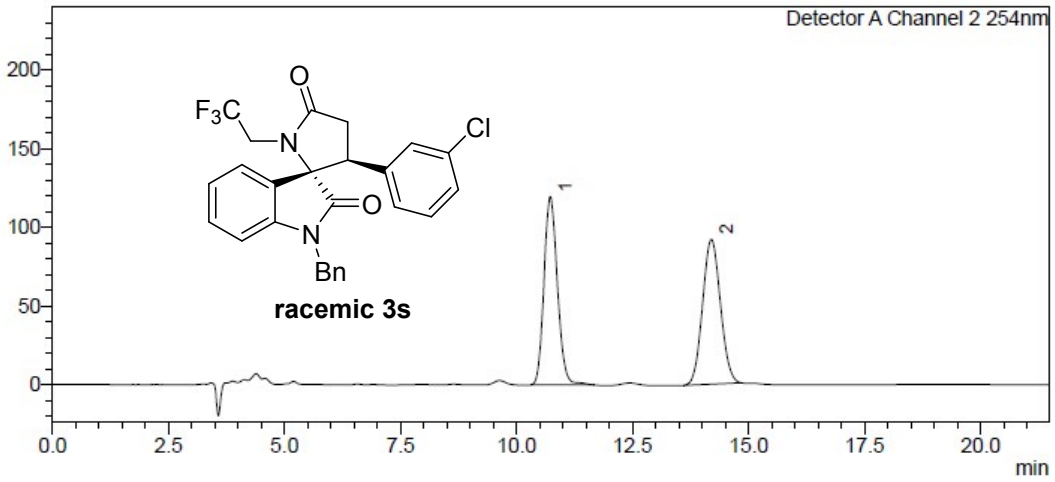
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	14.510	6280	239	0.144	0.144
2	24.550	4364780	89284	99.856	99.856
Total		4371060	89522		100.000


7.334
7.325
7.322
7.314
7.299
7.289
7.261
7.191
7.181
7.148
7.147
7.145
7.141
7.140
7.138
7.135
7.134
7.130
7.129
7.119
7.118
7.032
7.021
7.010
6.921
6.919
6.916
6.886
6.885
6.876
6.874
6.865
6.864
6.792
6.781
6.662
6.652
6.625
6.614
5.015
4.993
4.774
4.751
3.987
3.975
3.963
3.871
3.858
3.849
3.836
3.739
3.726
3.717
3.277
3.265
3.253
3.241
3.075
3.063
3.051
3.039
1.570
0.000
O
F3C
N
Cl
O
N
Bn
3s
2.88
1.88
1.92
0.97
0.91
0.98
0.96
0.96
0.98
1.00
1.01
0.98
1.03
1.03
1.00
1.00
f1 (ppm)

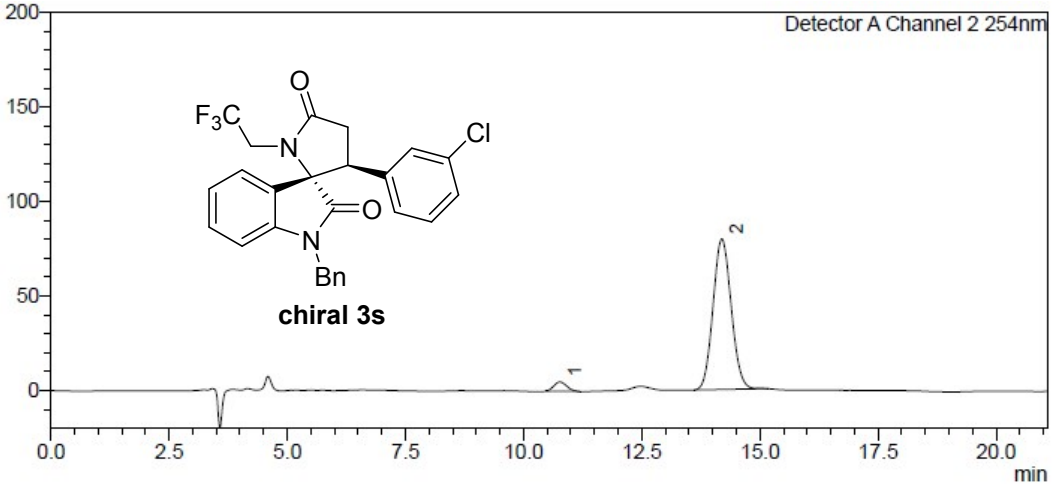

175.47
174.41
142.50
137.89
134.88
134.29
130.50
129.55
128.96
128.41
128.22
127.96
127.24
126.33
125.27
123.99
123.32
122.77
122.40
109.94
77.02
76.81
72.74
48.62
44.39
42.75
42.55
42.35
42.14
34.24
29.71
0.00
O
F3C
N
Cl
O
N
Bn
3s
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

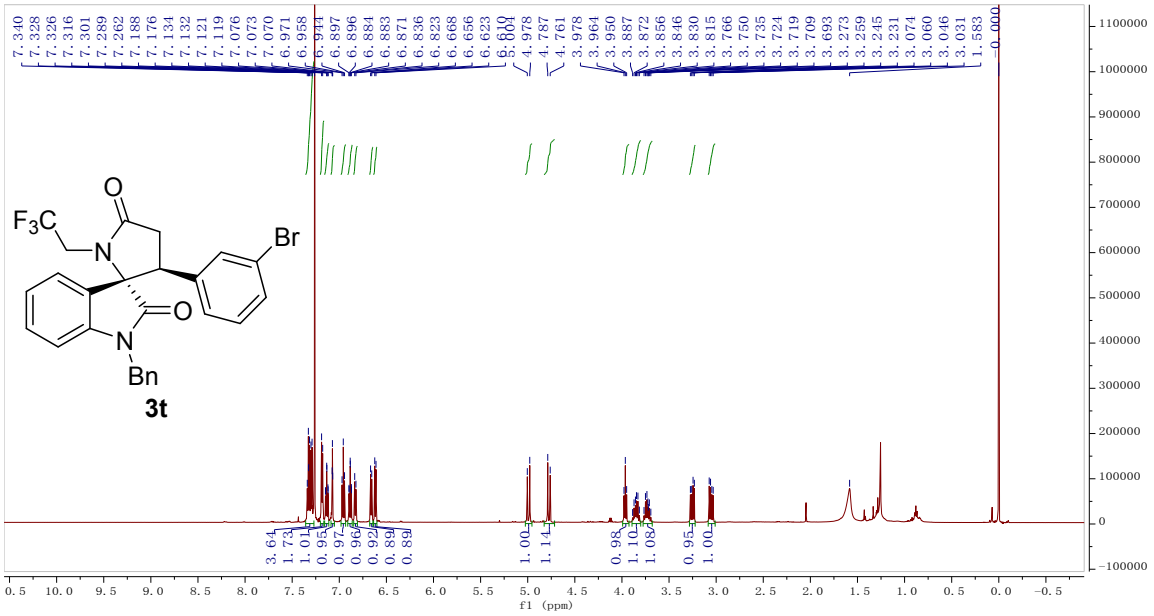
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.728	2411379	119713	49.488	49.488
2	14.199	2461260	92070	50.512	50.512
Total		4872639	211783		100.000

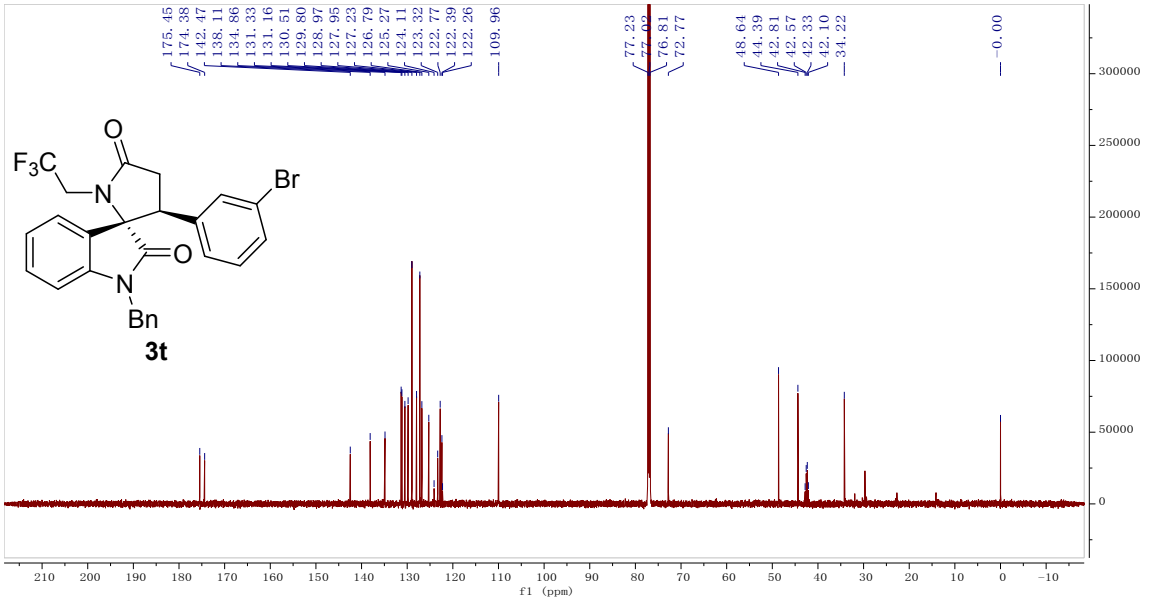


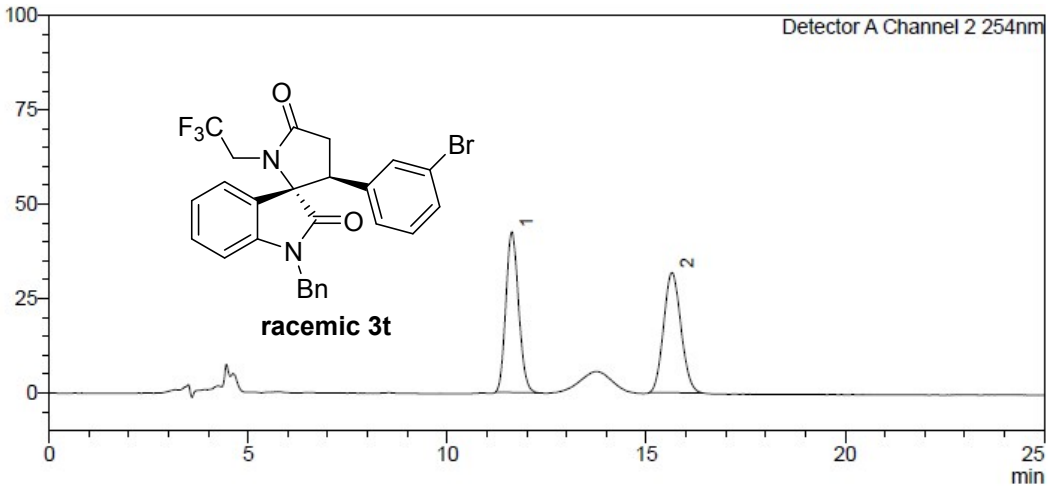
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.768	91288	4893	4.103	4.103
2	14.194	2133865	79689	95.897	95.897
Total		2225153	84581		100.000


7.340
7.328
7.326
7.316
7.301
7.289
7.262
7.188
7.176
7.134
7.132
7.121
7.119
7.076
7.073
7.070
6.971
6.958
6.944
6.897
6.896
6.884
6.883
6.871
6.836
6.823
6.668
6.656
6.623
6.610
5.001
4.978
4.787
4.761
3.978
3.964
3.950
3.887
3.872
3.856
3.846
3.830
3.815
3.766
3.750
3.735
3.724
3.719
3.709
3.693
3.273
3.259
3.245
3.231
3.074
3.060
3.046
3.031
1.583
0.000
3.64
1.73
1.01
0.95
0.97
0.96
0.92
0.89
0.89
1.00
1.14
0.98
1.10
1.08
0.95
1.00
F3C
O
N
Br
O
N
Bn
3t
f1 (ppm)

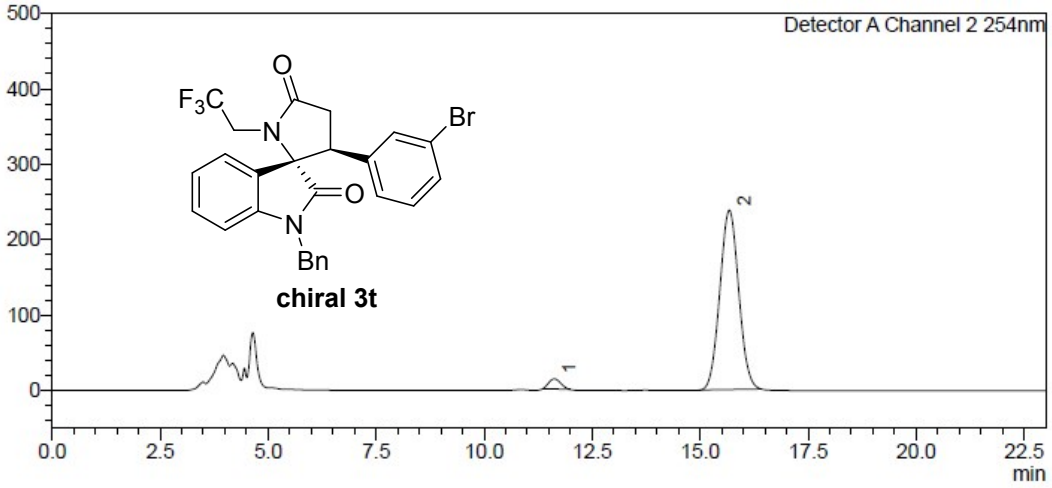

175.45
174.38
142.47
138.11
134.86
131.33
131.16
130.51
129.80
128.97
127.95
127.23
126.79
125.27
124.11
123.32
122.77
122.39
122.26
109.96
77.23
77.02
76.81
72.77
48.64
44.39
42.81
42.57
42.33
42.10
34.22
0.00
F3C
O
N
Br
O
N
Bn
3t
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

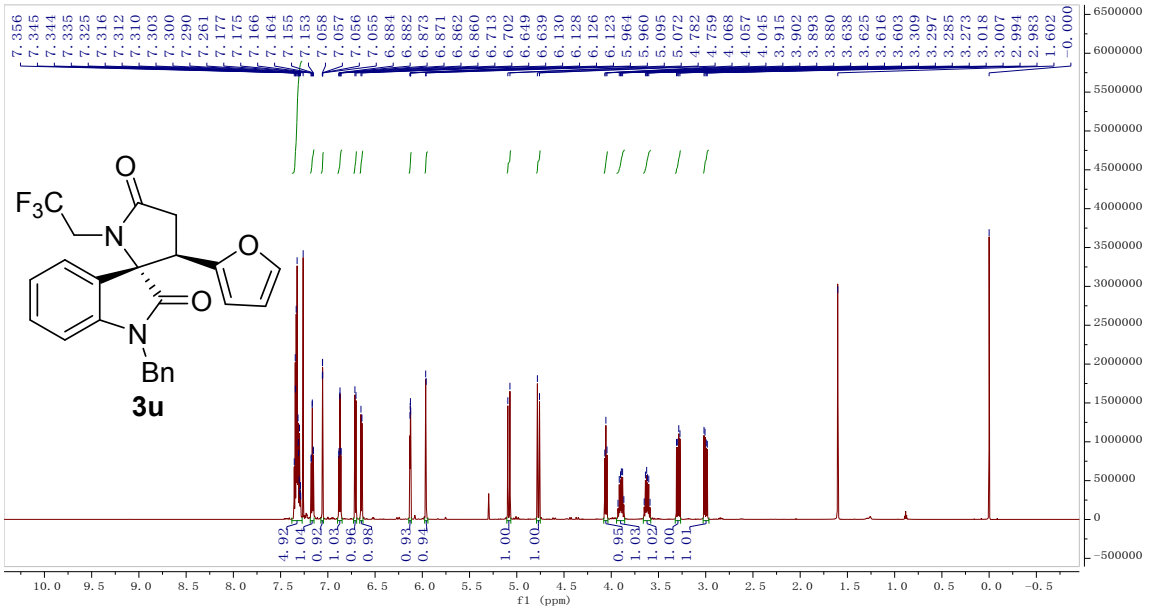
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.625	948078	42527	49.545	49.545
2	15.649	965479	31817	50.455	50.455
Total		1913557	74345		100.000

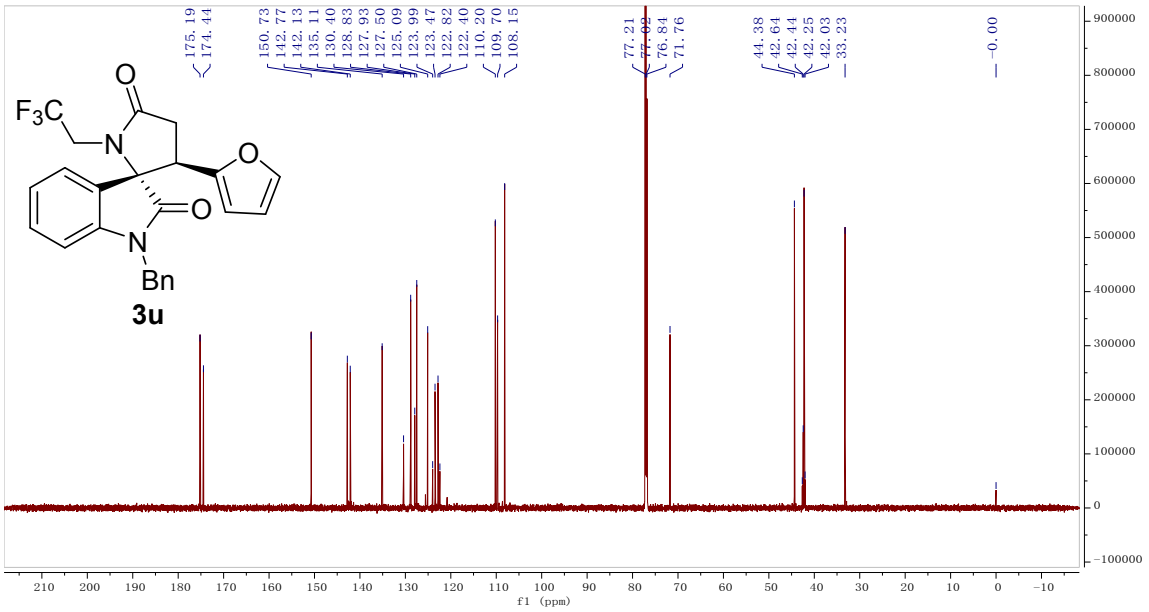


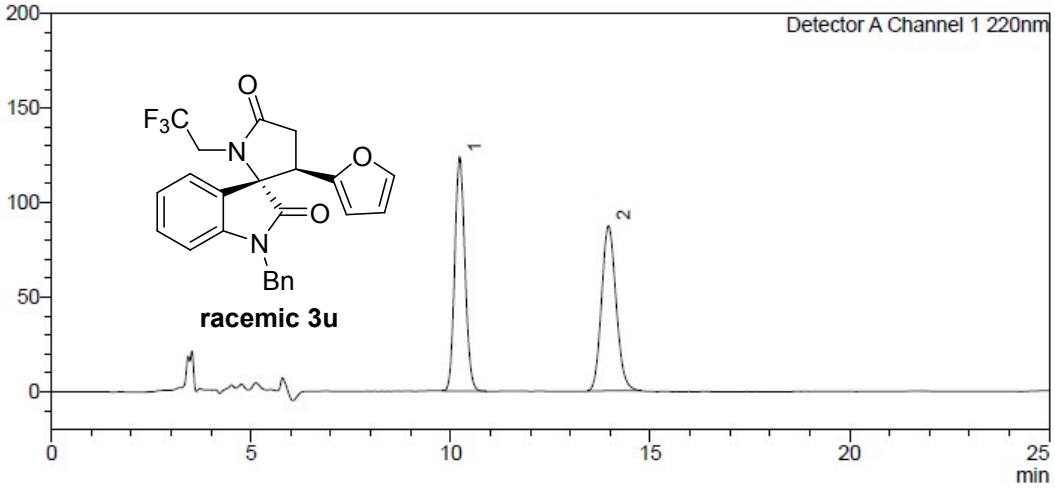
<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.627	257193	13409	3.436	3.436
2	15.677	7228092	237903	96.564	96.564
Total		7485285	251312		100.000


3u

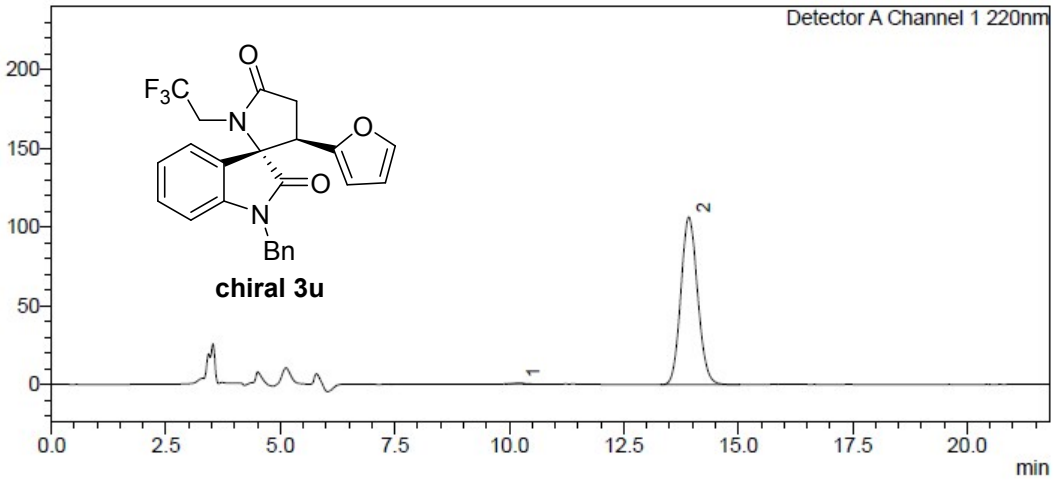

3u



<Peak Table>

Detector A Channel 1 220nm

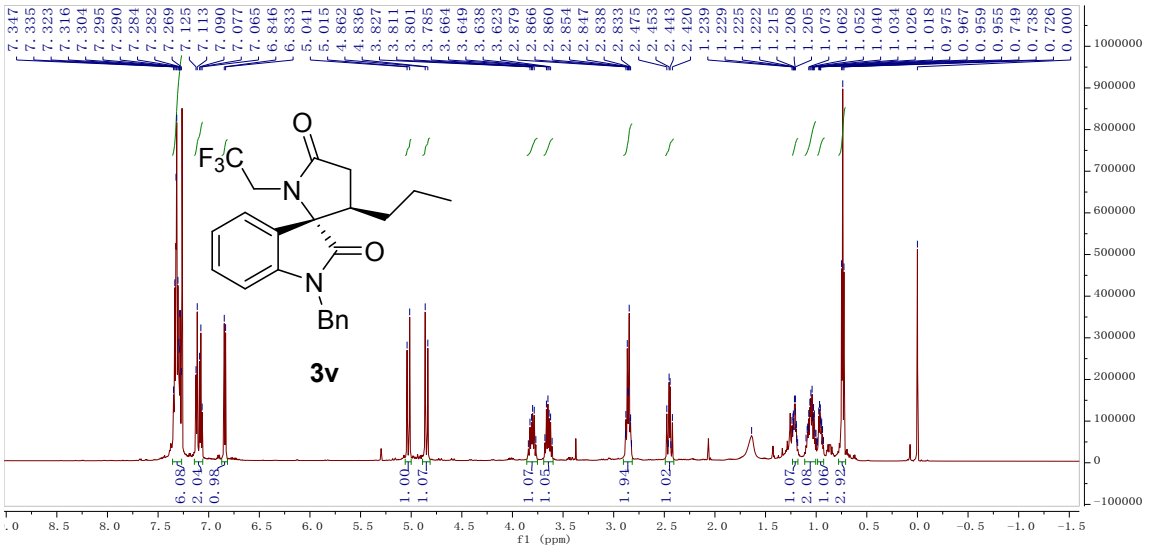
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.227	2206598	123754	49.920	49.920
2	13.957	2213702	87307	50.080	50.080
Total		4420299	211060		100.000

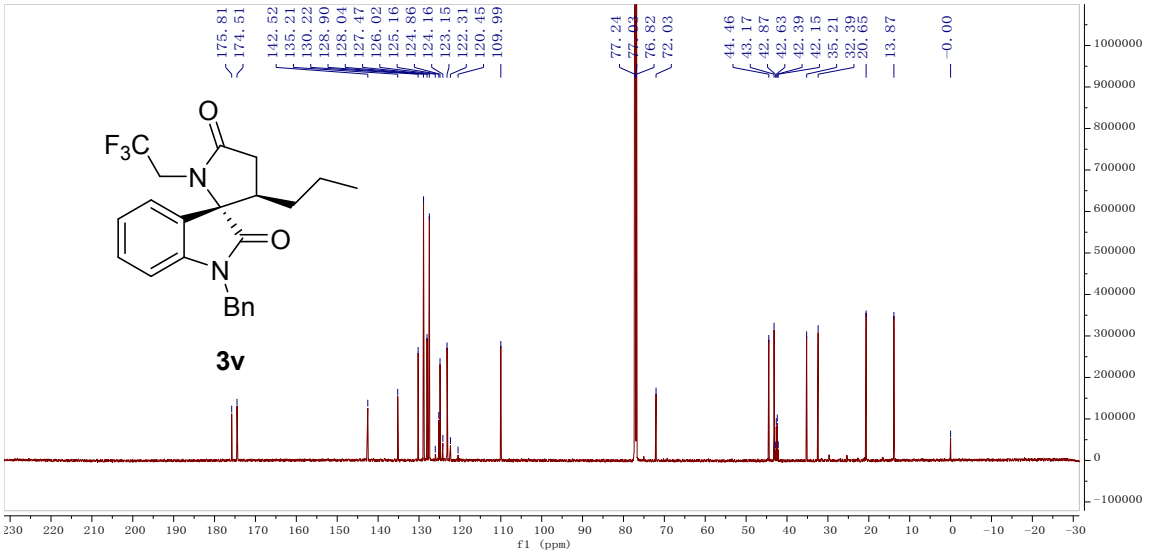


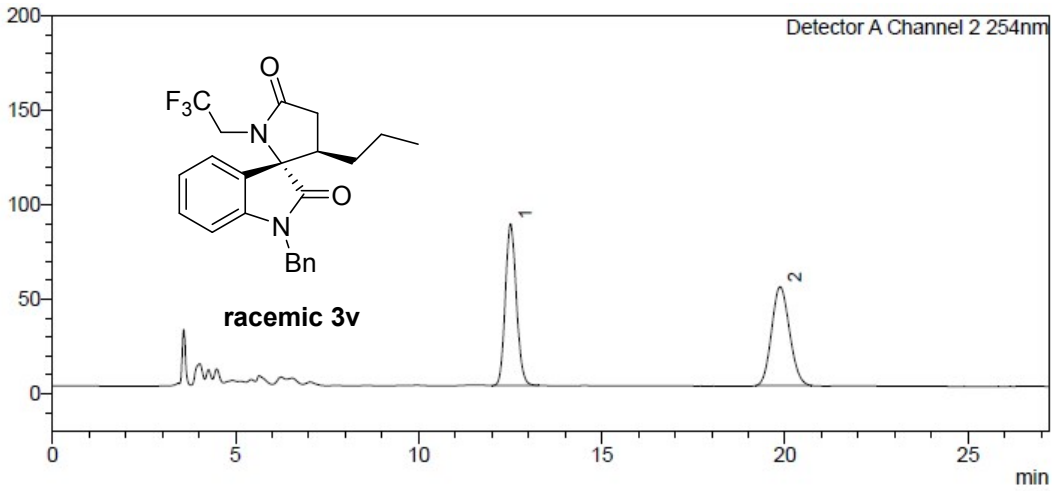
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.194	10931	688	0.400	0.400
2	13.923	2719610	106517	99.600	99.600
Total		2730541	107205		100.000


7.347 7.335 7.323 7.316 7.304 7.295 7.290 7.284 7.282 7.269 7.125 7.113 7.090 7.077 7.065 6.846 6.833 5.041 5.015 4.862 4.836 3.827 3.811 3.801 3.785 3.664 3.649 3.638 3.623 2.879 2.866 2.860 2.854 2.847 2.838 2.833 2.475 2.453 2.443 2.420 1.239 1.229 1.225 1.222 1.215 1.208 1.205 1.073 1.062 1.052 1.040 1.034 1.026 1.018 0.975 0.967 0.959 0.955 0.749 0.738 0.726 0.000
6.08 2.04 0.98 1.00 1.07 1.07 1.05 1.94 1.02 1.07 2.08 1.06 2.92
F3C
N
O
O
N
Bn
3v
f1 (ppm)

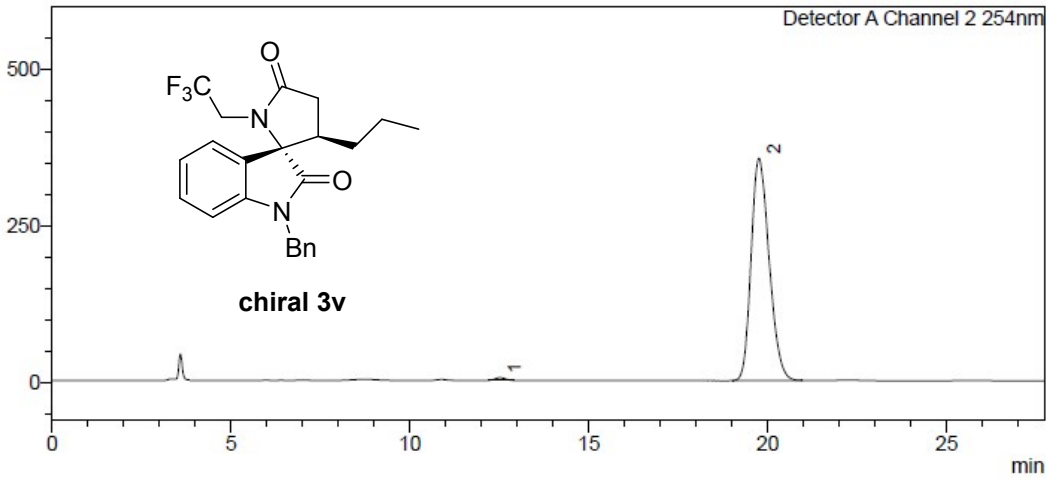

175.81 174.51 142.52 135.21 130.22 128.90 128.04 127.47 126.02 125.16 124.86 124.16 123.15 122.31 120.45 109.99 77.24 77.03 76.82 72.03 44.46 43.17 42.87 42.63 42.39 42.15 35.21 32.39 20.65 13.87 -0.00
F3C
N
O
O
N
Bn
3v
f1 (ppm)



<Peak Table>

Detector A Channel 2 254nm

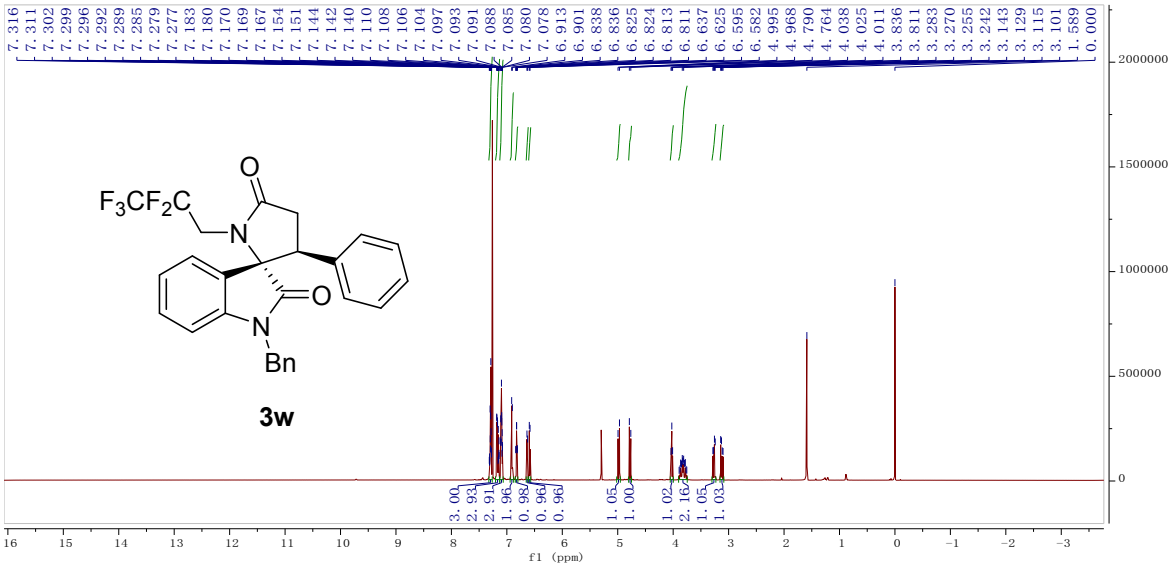
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	12.509	1794200	85571	50.184	50.184
2	19.869	1781028	52336	49.816	49.816
Total		3575228	137907		100.000

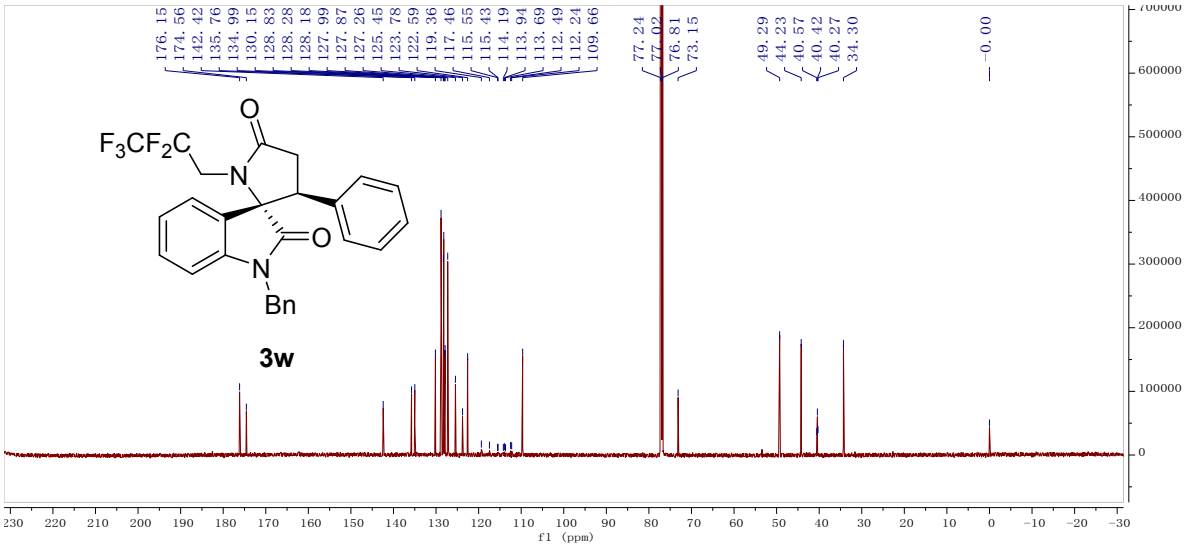


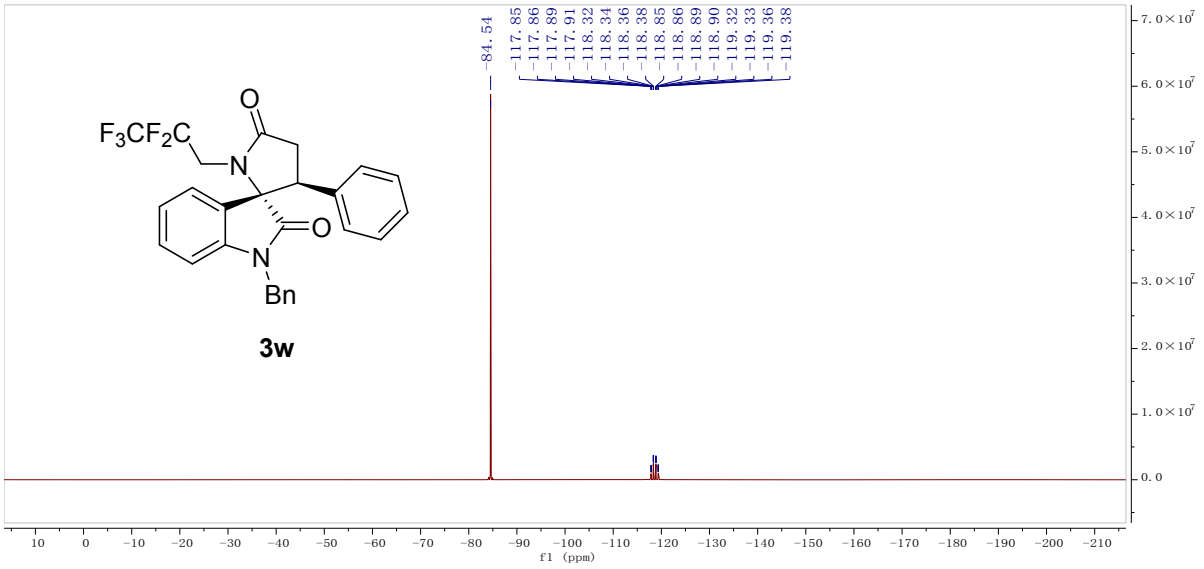
<Peak Table>

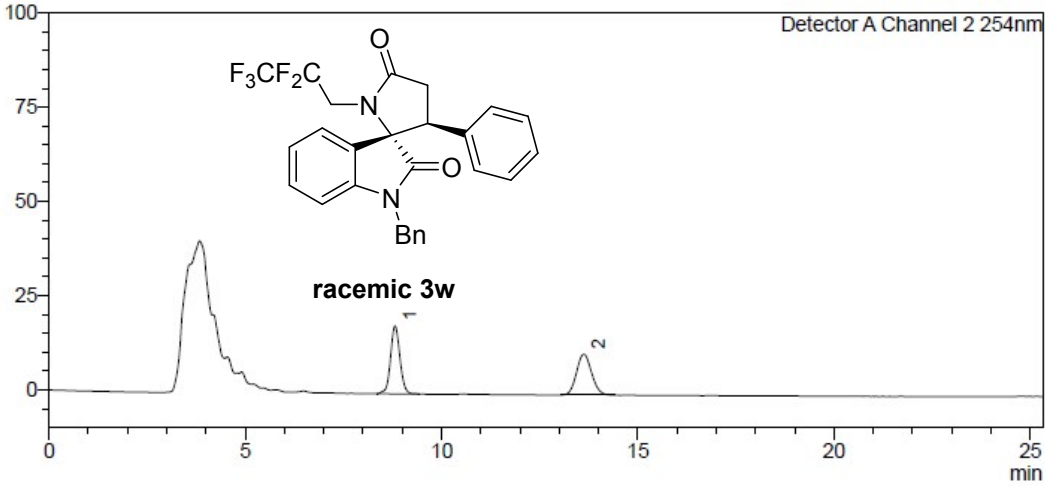
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	12.520	86004	4390	0.688	0.688
2	19.756	12423333	354688	99.312	99.312
Total		12509337	359078		100.000


7.316 7.311 7.302 7.299 7.296 7.292 7.289 7.285 7.279 7.277 7.183 7.180 7.170 7.169 7.167 7.154 7.151 7.144 7.142 7.140 7.110 7.108 7.106 7.104 7.097 7.093 7.091 7.088 7.085 7.080 7.078 6.913 6.901 6.838 6.836 6.825 6.824 6.813 6.811 6.637 6.625 6.595 6.582 4.995 4.968 4.790 4.764 4.038 4.025 4.011 3.836 3.811 3.283 3.270 3.255 3.242 3.143 3.129 3.115 3.101 1.589 0.000
F3CF2C
O
N
O
N
Bn
3w
3.00 2.93 2.91 1.96 0.98 0.96 0.96 0.96
1.05 1.00
1.02 2.16
1.05 1.03
2000000
1500000
1000000
500000
0
f1 (ppm)


176.15 174.56 142.42 135.76 134.99 130.15 128.83 128.28 128.18 127.99 127.87 127.26 125.45 123.78 122.59 119.36 117.46 115.55 115.43 114.19 113.94 113.69 112.49 112.24 109.66
77.24 77.02 76.81 73.15
49.29 44.23 40.57 40.42 40.27 34.30
-0.00
F3CF2C
O
N
O
N
Bn
3w
600000
500000
400000
300000
200000
100000
0
f1 (ppm)

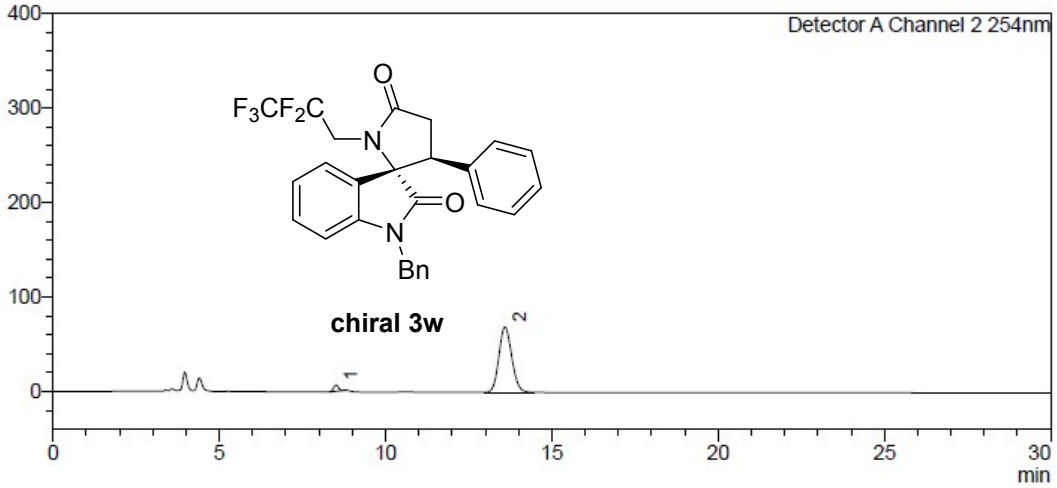




<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.816	299221	18005	50.733	50.733
2	13.625	290572	10879	49.267	49.267
Total		589793	28884		100.000



<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.510	69344	6852	3.602	3.602
2	13.592	1855597	69272	96.398	96.398
Total		1924942	76124		100.000