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Supporting Information

LiO*t*Bu-Promoted Synthesis of Bis(3-indolyl)methanes by the Alkylation of Indoles with Alcohols under Air

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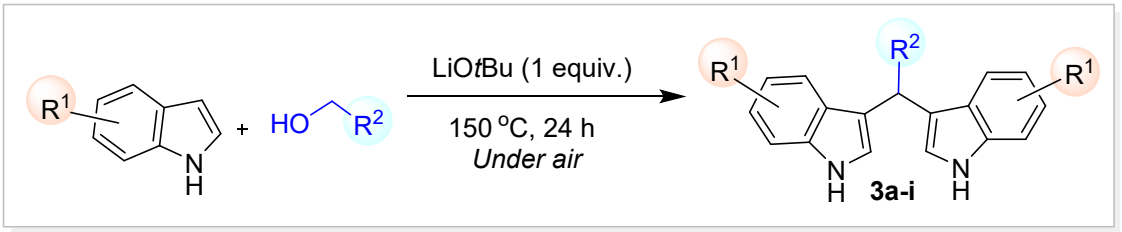
# Both authors contributed equally to this work.

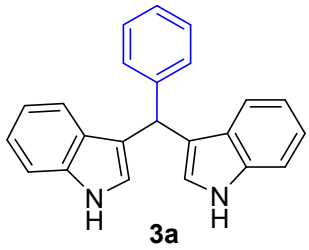
CONTENTS:

1. General information

All chemicals were purchased from Sigma-Aldrich, Ak-Sci and used without further purification. Mass spectra were obtained with a Hewlett–Packard HPGC–MS 5890/5972 instrument (EI, 70 eV) by using a GC inlet or with an MX-1321 instrument (EI, 70 eV) by using a direct inlet. Column chromatography was performed on silica gel (200 mesh, Merck), and silica gel Merck 60 F254 plates were used for TLC. Commercially available solvents were distilled for column chromatography. All other solvents were purified and dried by standard methods.

2. Experimental section

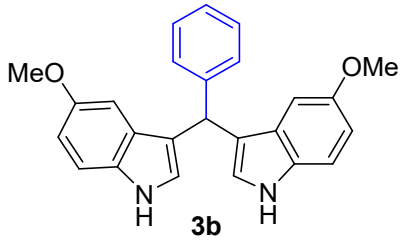




3a

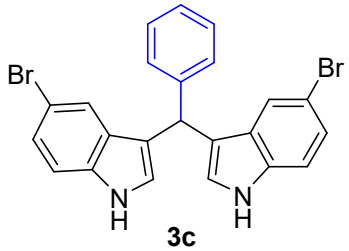
3,3'-(phenylmethylene)bis(1H-indole)[1]: Indole (35.1 mg, 0.3 mmol, 1eq) was added to a pressure tube that was charged with benzyl alcohol (130 mg, 1.2 mmol, 4eq)), LiOtBu (24 mg, 0,3 mmol, 1eq) under air. The reaction mixture was stirred with a magnetic stirrer and heated at 150°C for 24 hours. After cooling, the reaction mixture was filtered through a pad of Celite, which was washed three times with hot water (200 mL) to eliminate benzyl alcohol and three times with EtOAc to have the final filtrate. The filtrate was concentrated in vacuo. The crude product was further purified on Silica gel column chromatography with a 5:1 elution system of hexane/ ethyl acetate to yield **3a** (38.6 mg, 80%) as pale-yellow solid; mp = 86-87 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (s, 2H), 7.42 – 7.32 (m, 6H), 7.28 (dd, J = 8.4, 6.8 Hz, 2H), 7.25 – 7.14 (m, 3H), 7.01 (ddd, J = 8.0, 7.0, 1.0 Hz, 2H), 6.65 (dd, J = 2.4, 1.0 Hz, 2H), 5.90 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.03, 136.72, 128.74, 128.22, 127.12, 126.14, 123.61, 121.94, 119.96, 119.77, 119.25, 111.02, 77.24, 77.03, 76.82, 40.23.

[1] N. K. Nguyen, D. L. Tran, T. Q. Hung, T. M. Le, N. T. Son, Q. T. Trinh, T. T. Dang, P. Langer, *Tetrahedron Lett.* **2021**, *68*, 152936.



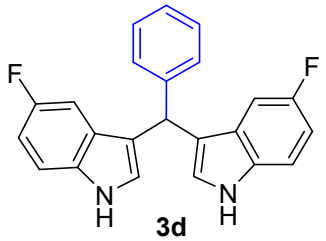
3b

3,3'-(phenylmethylene)bis(5-methoxy-1H-indole):[1] Following the general procedure and using compound **2** (130 mg, 1.2 mmol) and 5-methoxy indole (44 mg, 0.3 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3b** (47.2 mg, 82%) as pale-yellow solid; mp = 215-216 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.65 (s, 2H), 7.40 – 7.36 (m, 2H), 7.30 – 7.24 (m, 5H), 7.20 – 7.15 (m, 1H), 6.84 (t, J = 2.3 Hz, 2H), 6.76 (t, J = 2.3 Hz, 3H), 6.72 (dt, J = 8.7, 2.1 Hz, 2H), 5.77 (s, 1H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 152.67, 145.02, 131.80, 128.31, 127.97, 127.02, 125.70, 124.28, 117.68, 111.99, 110.55, 101.47, 55.24, 40.01, 39.84, 39.67, 39.51, 39.34, 39.17, 39.01.



3c

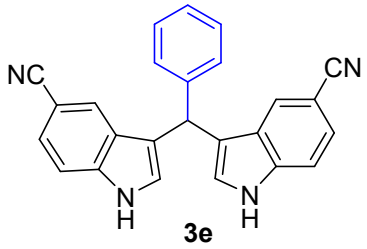
3,3'-(phenylmethylene)bis(5-bromo-1H-indole):[2] Following the general procedure and using compound **2** (130 mg, 1.2 mmol) and 5-bromoindole (59 mg, 0.3 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane/ ethyl acetate, 30:1) to yield **3c** (51.8 mg, 72%) as pale-yellow solid; mp = 230-232 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (s, 4H), 7.50 – 7.39 (m, 3H), 7.28 – 7.25 (m, 6H), 7.24 – 7.20 (m, 7H), 6.61 (dd, J = 2.5, 1.1 Hz, 3H), 5.72 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.07, 135.37, 128.70, 128.54, 128.43, 126.53, 124.99, 124.76, 122.30, 119.10, 112.70, 112.57, 77.22, 77.01, 76.80, 39.92.



3d

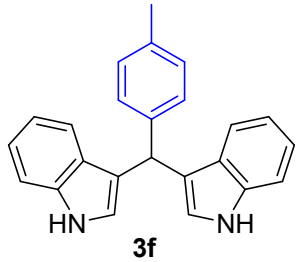
3,3'-(phenylmethylene)bis(5-fluoro-1H-indole):[1] Following the general procedure and using compound **2** (130 mg, 1.2 mmol) and 5-fluoroindole (41 mg, 0.3 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3d** (25.5 mg, 48%) as pale-yellow solid; mp = 169-171 °C;. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.97 (d, J = 2.6 Hz, 2H), 7.42 – 7.35 (m, 4H), 7.29 (t, J = 7.7 Hz, 2H), 7.21 – 7.14 (m, 1H), 7.02 – 6.96 (m, 4H), 6.90 (td, J = 9.1, 2.6 Hz, 2H), 5.82 (s, 1H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 156.43 (d, J =

231.1 Hz), 144.46, 133.27, 128.25, 128.14, 126.80 (d, J = 9.9 Hz), 125.95, 125.64, 118.04 (d, J = 4.7 Hz), 112.45 (d, J = 9.7 Hz), 109.05 (d, J = 26.1 Hz), 103.63 (d, J = 23.2 Hz).



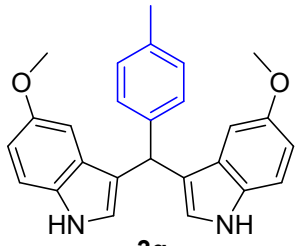
3e

3,3'-(phenylmethylene)bis(1H-indole-5-carbonitrile):[2] Following the general procedure and using compound **2** (130 mg, 1.2 mmol) and 5-cyanodindole (47 mg, 0.3 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3e** (42.5 mg, 76%) as pale-yellow solid; mp = 240-242 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 11.47 (s, 1H), 7.89 (d, J = 1.5 Hz, 2H), 7.41 (d, J = 8.3 Hz, 2H), 7.34 (d, J = 7.3 Hz, 2H), 7.28 (t, J = 7.6 Hz, 2H), 7.24 – 7.14 (m, 6H), 5.96 (s, 1H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 143.84, 135.41, 129.45, 128.34, 128.23, 128.21, 126.23, 121.07, 120.67, 120.09, 118.69, 116.55, 102.46, 79.16, 40.01, 39.84, 39.67, 39.51, 39.34, 39.17, 39.01.



3f

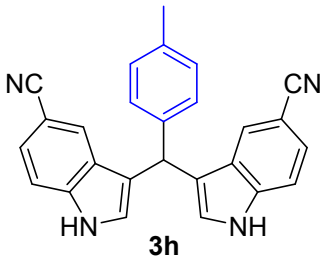
3,3'-((4-methylphenyl)methylene)bis(1H-indole):[1] Following the general procedure and using compound **1** (35 mg, 0.3 mmol) and 4-methylbenzyl alcohol (146 mg, 1.2 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3f** (42.9 mg, 85%) as pale-yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (s, 2H), 7.40 (dq, J = 7.9, 0.9 Hz, 2H), 7.34 (dt, J = 8.1, 0.9 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.16 (ddd, J = 8.2, 7.0, 1.2 Hz, 2H), 7.11 – 7.07 (m, 2H), 7.00 (ddd, J = 8.0, 7.1, 1.0 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.02, 136.73, 135.47, 128.91, 128.58, 127.14, 123.54, 121.87, 119.98, 119.94, 119.19, 110.99, 77.24, 77.03, 76.82, 39.80.



3g

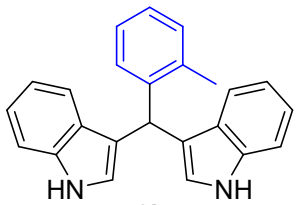
[2] N. Biswas, R. Sharma, D. Srimani, *Adv. Synth. Catal.* **2020**, *362*, 2902–2910.

3,3'-(p-tolylmethylene)bis(5-methoxy-1H-indole):[3] Following the general procedure and using 5-methoxy indole (44 mg, 0.3 mmol) and 4-methylbenzyl alcohol (146 mg, 1.2 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3g** (26.8 mg, 45%) as pale-yellow solid. ^{1}H NMR (600 MHz, Acetone-d_6) δ 9.79 (s, 2H), 7.29 (dd, J = 10.9, 8.3 Hz, 4H), 7.09 (d, J = 7.8 Hz, 2H), 6.86 (d, J = 2.4 Hz, 2H), 6.82 (d, J = 2.5 Hz, 2H), 6.75 (dd, J = 8.8, 2.4 Hz, 2H), 5.81 (s, 1H), 3.63 (s, 6H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, Acetone-d_6) δ 154.33, 142.89, 135.76, 133.24, 129.41, 129.40, 128.50, 125.23, 119.62, 112.64, 111.86, 102.61, 55.74, 40.78, 21.02.



3h

3,3'-(p-tolylmethylene)bis(1H-indole-5-carbonitrile):[4] Following the general procedure and using 5-cyanodindole (47 mg, 0.3 mmol) and 4-methylbenzyl alcohol (146 mg, 1.2 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3h** (20.1 mg, 36%) as pale-yellow solid. ^{1}H NMR (500 MHz, Acetone-d_6) δ 10.63 (s, 2H), 7.79 (s, 2H), 7.59 (d, J = 8.3 Hz, 2H), 7.39 (d, J = 8.5 Hz, 2H), 7.31 (d, J = 7.6 Hz, 2H), 7.13 (d, J = 7.6 Hz, 2H), 7.07 (s, 2H), 6.05 (s, 1H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, Acetone-d_6) δ 141.59, 139.71, 136.61, 129.85, 129.24, 127.73, 127.17, 125.72, 124.92, 121.18, 120.56, 113.58, 102.51, 40.01, 21.00.



3i

3,3'-((2-methylphenyl)methylene)bis(1H-indole):[1] Following the general procedure and using compound **1** (35 mg, 0.3 mmol) and 2-methylbenzyl alcohol (146 mg, 1.2 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3i** (41.4 mg, 82%) as pale-yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (s, 2H), 7.36 (ddd, J = 13.6, 8.1, 1.0 Hz, 3H), 7.24 – 7.09 (m, 5H), 7.08 – 6.99 (m, 3H), 6.54 (dd, J = 2.5, 1.0 Hz, 2H), 6.04 (s, 1H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 207.07, 142.11, 136.77, 136.08, 130.20, 128.43, 127.23, 126.09, 125.84, 123.89, 121.90, 119.80, 119.21, 119.16, 111.06, 77.27, 77.05, 76.84, 36.25.

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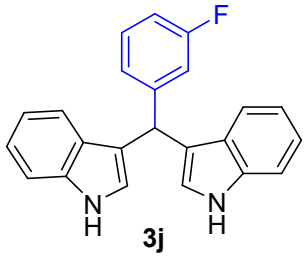
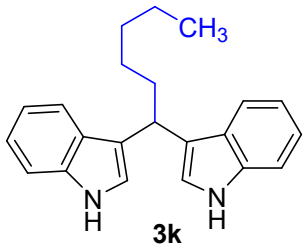
[3] S. S. Gogula, D. V. Prasanna, V. Thumma, S. Misra, C. A. Lincoln, P. M. Reddy, A. Hu and B. V. Subbareddy, *ACS Omega*, **2023**, *8*, 36401-36411.

[4] V. Yadav, E. Balaraman, S. B. Mhaske, *Adv. Synth. Catal.,* **2021**, *363*, 4430.



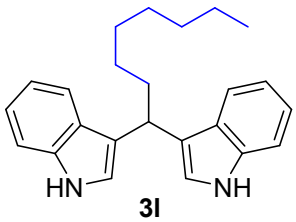
3j

3,3'-((3-fluorophenyl)methylene)bis(1H-indole):[1] Following the general procedure and using compound **1** (35 mg, 0.3 mmol) and 3-fluorobenzyl alcohol (151 mg, 1.2 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3j** (40,2 mg, 79%) as pale-yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (s, 2H), 7.43 – 7.33 (m, 4H), 7.30 – 7.22 (m, 2H), 7.22 – 7.12 (m, 3H), 7.08 – 6.98 (m, 3H), 6.91 (tdd, J = 8.4, 2.6, 1.0 Hz, 1H), 6.66 (dd, J = 2.5, 1.0 Hz, 2H), 5.89 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.84, 162.21, 146.86, 146.81, 136.72, 129.60, 129.55, 126.95, 124.43, 124.41, 123.58, 122.09, 119.80, 119.38, 119.10, 115.67, 115.52, 113.16, 113.02, 111.11, 77.24, 77.03, 76.82, 29.72.



3k

3,3'-(hexane-1,1-diyl)bis(1H-indole):[1] Following general procedure and using compound **1** (35 mg, 0.3 mmol) and n-hexanol (123 mg, 1.2 mmol) gave a crude product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3k** (35.6 mg, 75%) as pale-yellow solid; mp = 67-69 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 8.1 Hz, 1H), 7.16 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 7.10 – 7.01 (m, 1H), 6.98 (d, J = 2.4 Hz, 1H), 4.49 (s, 1H), 2.23 (qd, J = 7.4, 1.4 Hz, 1H), 1.44 (ddd, J = 15.2, 8.3, 6.4 Hz, 1H), 1.36 (dddd, J = 13.4, 7.7, 6.4, 2.9 Hz, 1H), 1.33 – 1.26 (m, 1H), 0.87 (t, J = 7.2 Hz, 1H).^{13}C NMR (151 MHz, $CDCl_3$) δ 136.64, 127.23, 121.72, 121.38, 120.64, 119.70, 119.00, 111.04, 77.24, 77.03, 76.82, 35.84, 34.04, 32.04, 28.04, 22.68, 14.13.



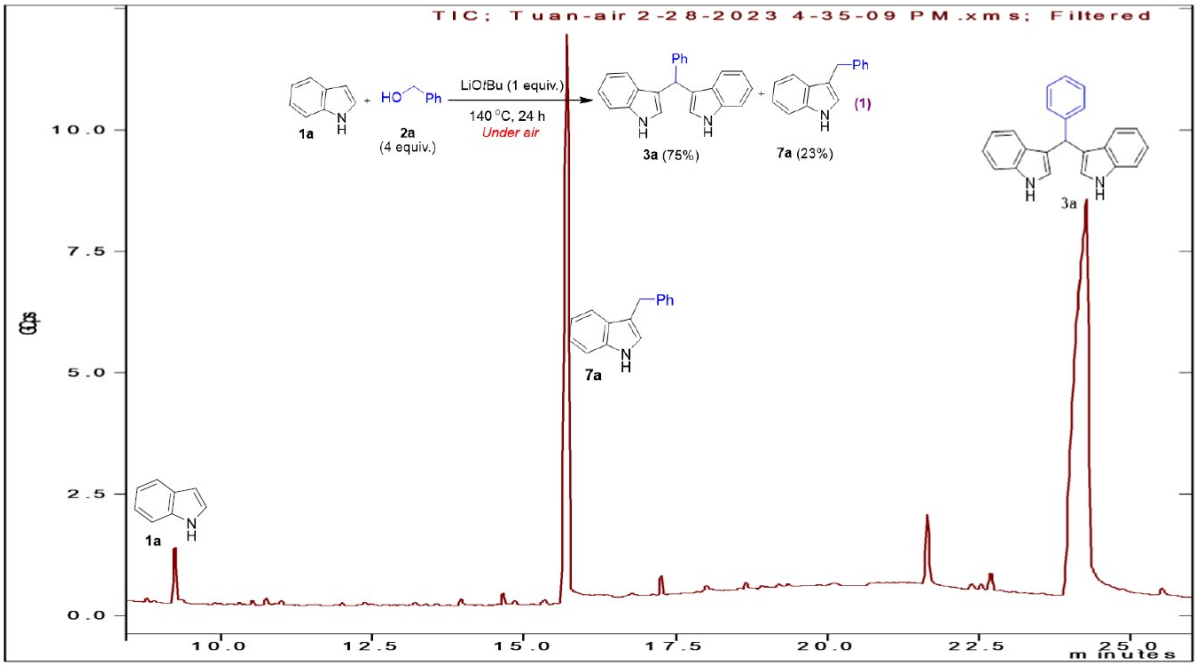
3l

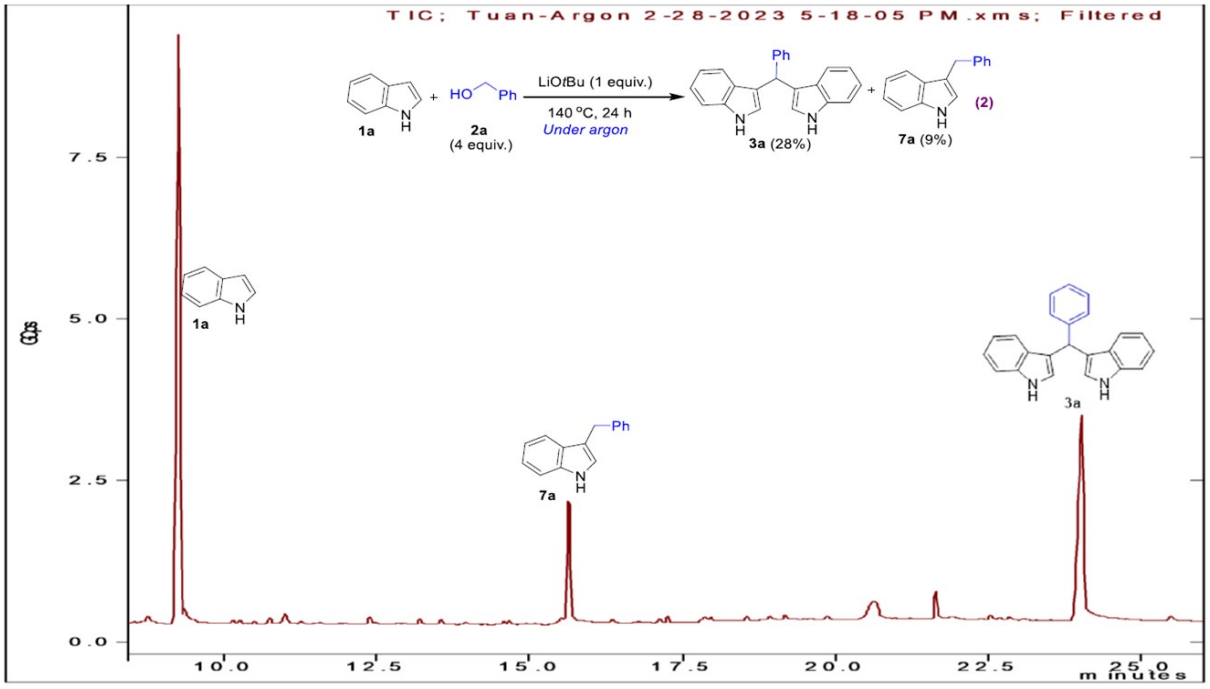
3,3'-(octane-1,1-diyl)bis(1H-indole):[5] Following general procedure and using compound **1** (35 mg, 0.3 mmol) and n-octanol (156.28 mg, 1.2 mmol) gave a pale-yellow semisolid product, which was purified by preparative thin-layer chromatography (silica gel; hexane) to yield **3l** (31.0 mg,

[5] A. Gogoi, G. Basumatary and G. Bez, *Synthesis*, **2022**, *55*, 786-798.

60%) as pale-yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 2H), 7.60 (dd, *J* = 8.0, 1.1 Hz, 2H), 7.33 (dt, *J* = 8.1, 1.0 Hz, 2H), 7.15 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 2H), 7.04 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 2H), 7.01 – 6.97 (m, 2H), 4.48 (t, *J* = 7.4 Hz, 1H), 2.22 (q, *J* = 7.5 Hz, 2H), 1.46 – 1.39 (m, 2H), 1.39 – 1.31 (m, 2H), 1.24 – 1.20 (m, 4H), 0.89 – 0.82 (m, 5H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.63, 127.23, 121.71, 121.37, 120.65, 119.70, 118.99, 111.02, 35.87, 34.04, 31.93, 29.78, 29.31, 28.35, 22.67, 14.10.

3. Results of control experiments were analyzed by GC MS method.

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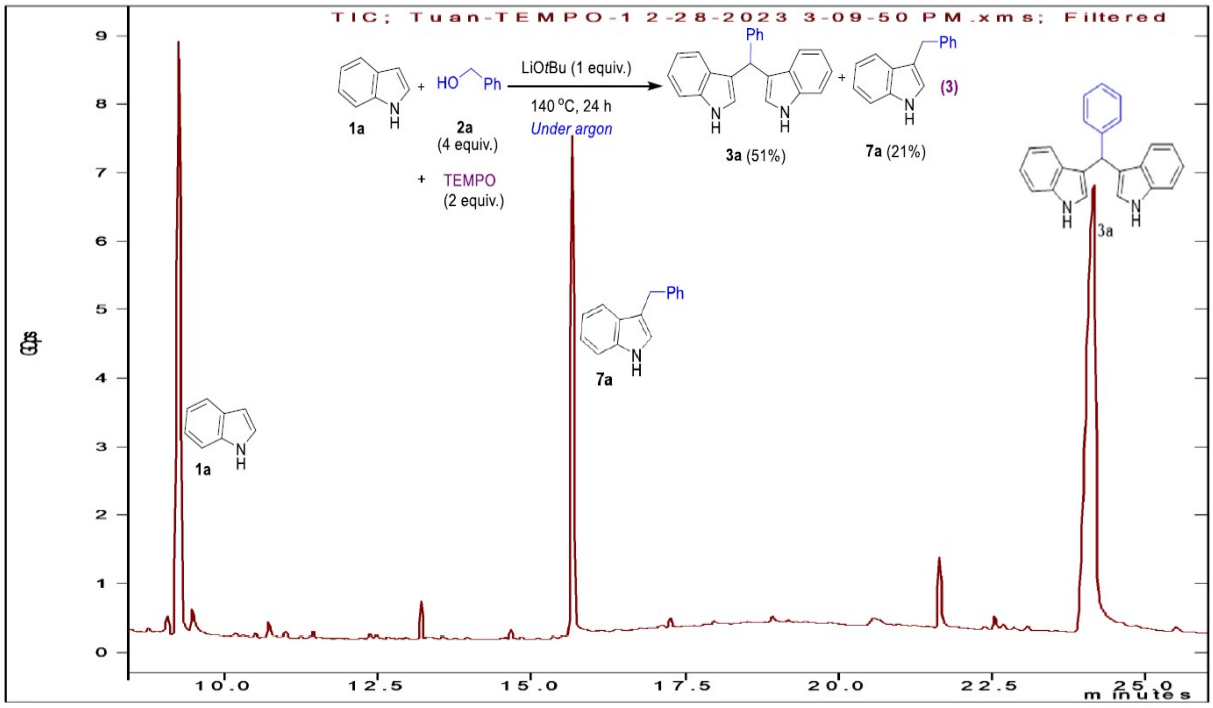
7a (9%)
(2)
Cps
minutes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2a
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+ TEMPO
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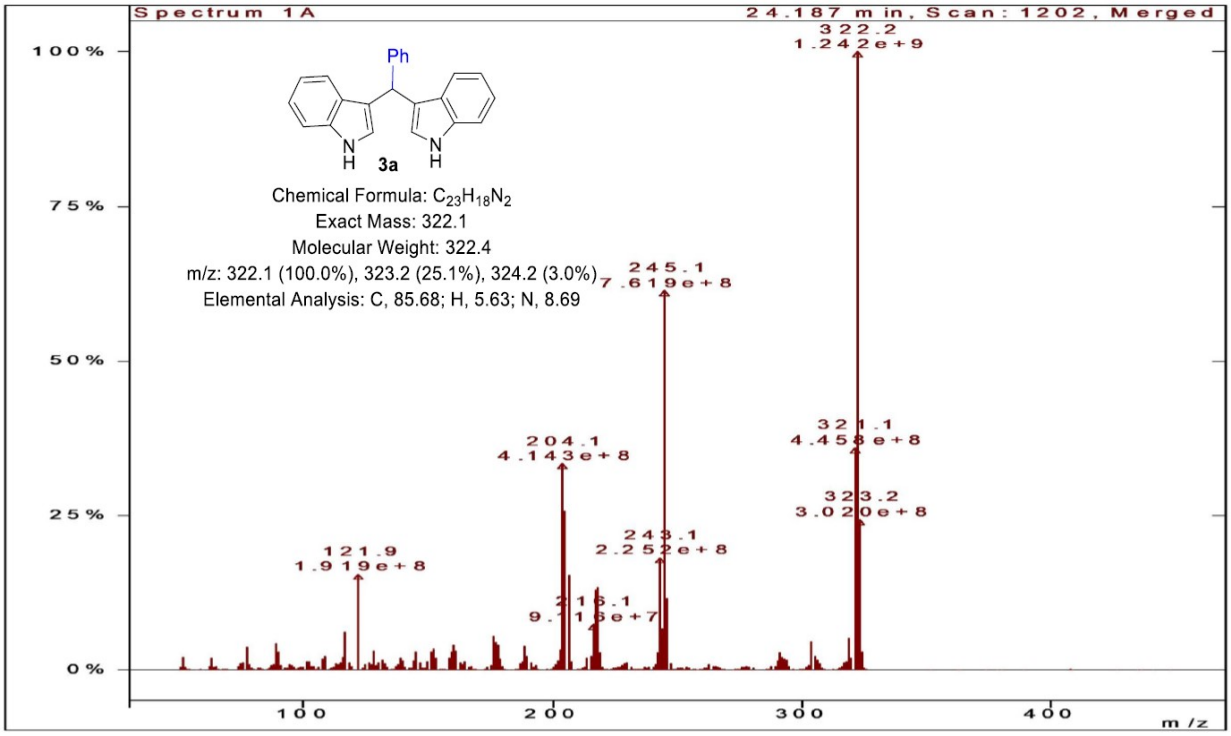
140 °C, 24 h
Under argon
3a (51%)
7a (21%)
(3)
Cps
minutes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3a
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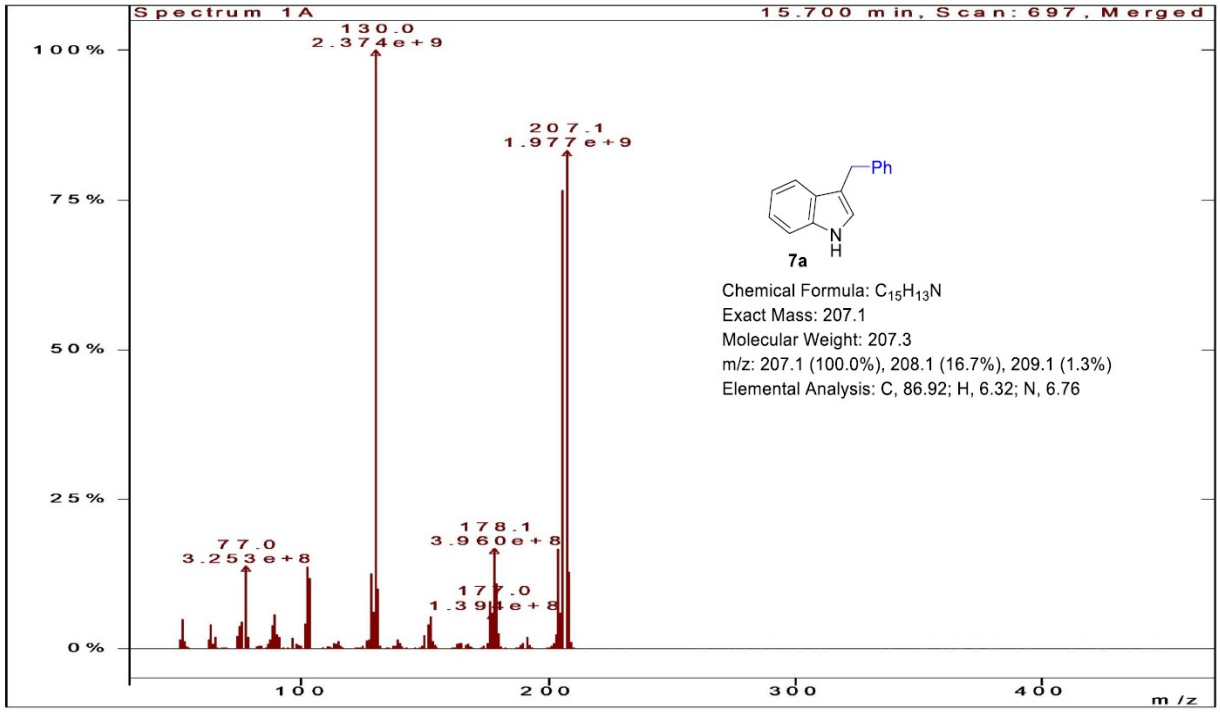
m/z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m/z: 207.1 (100.0%), 208.1 (16.7%), 209.1 (1.3%)
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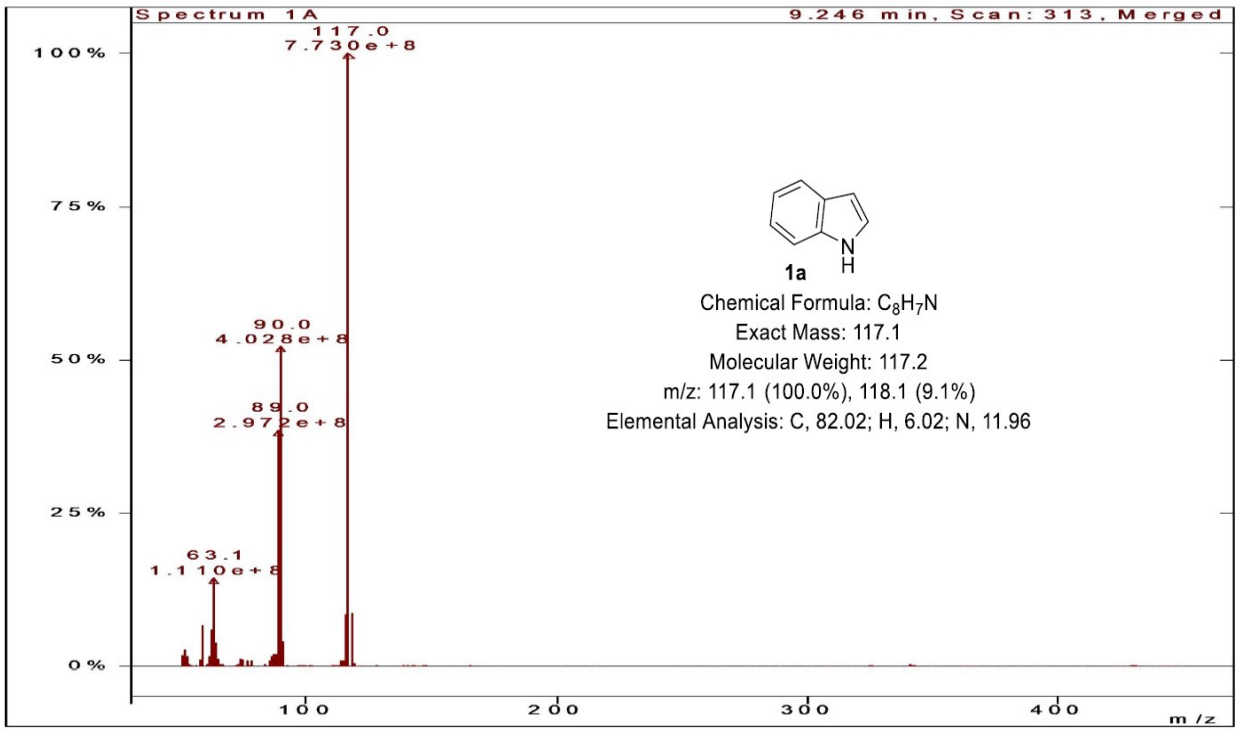
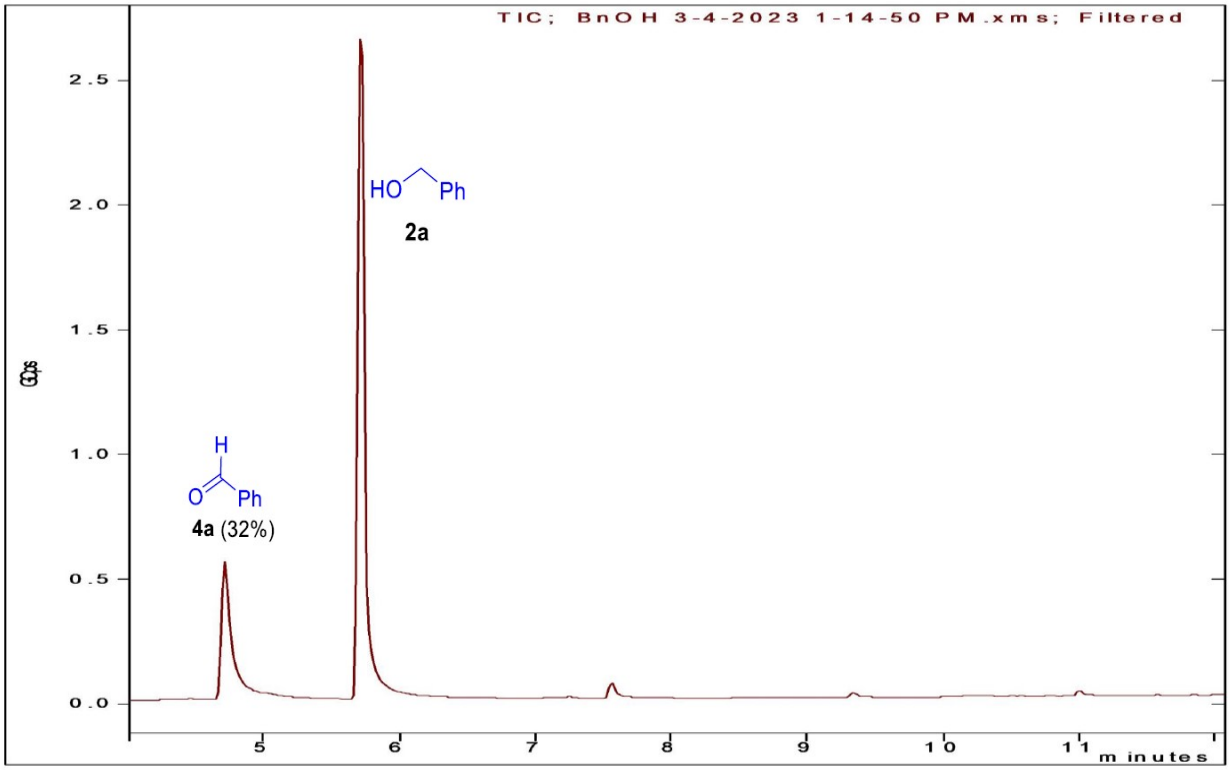
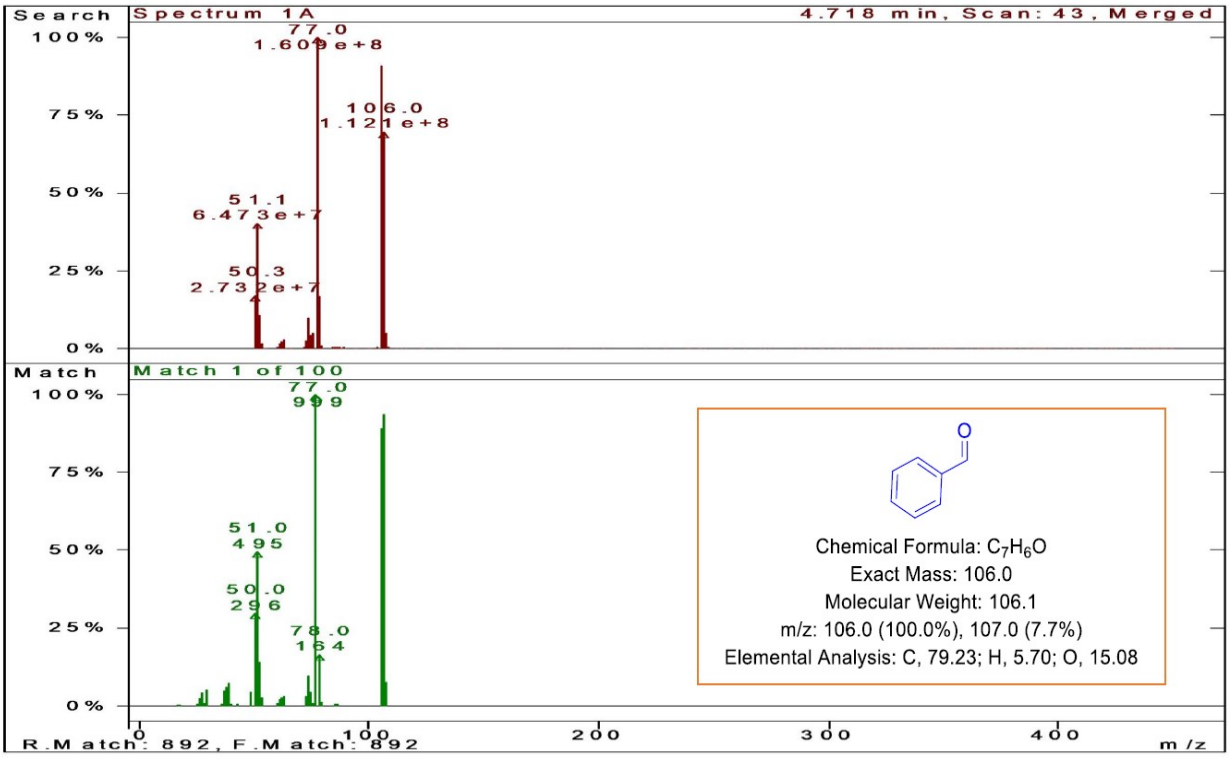
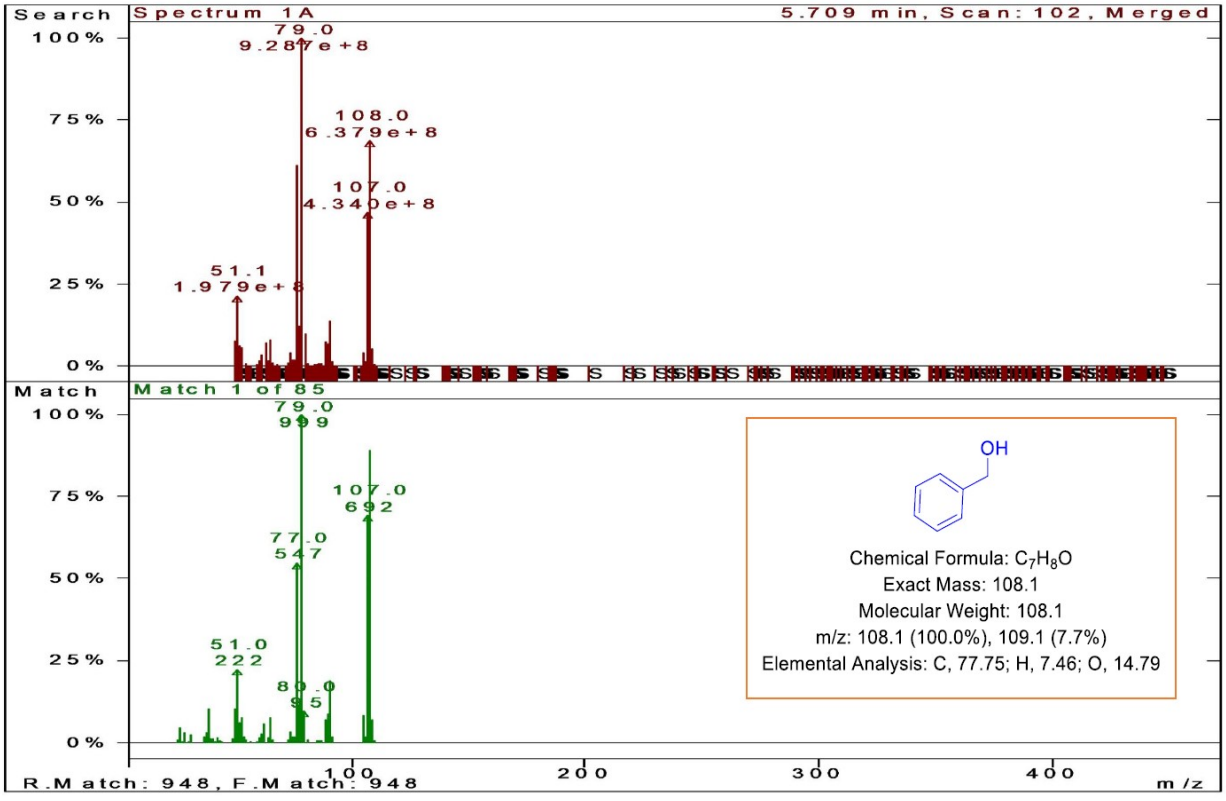
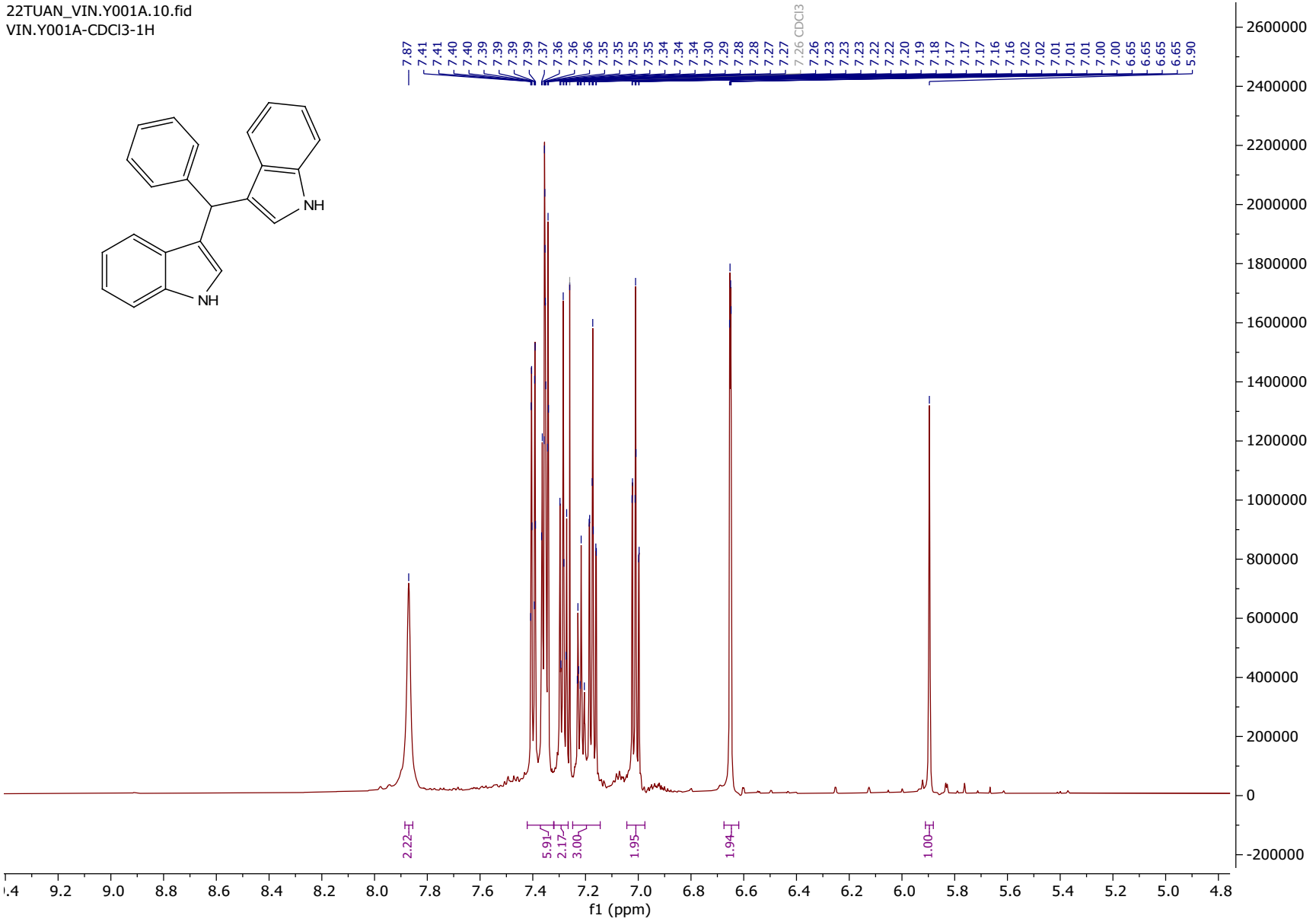
75%
50%
25%
0%
100
200
300
400
m/z

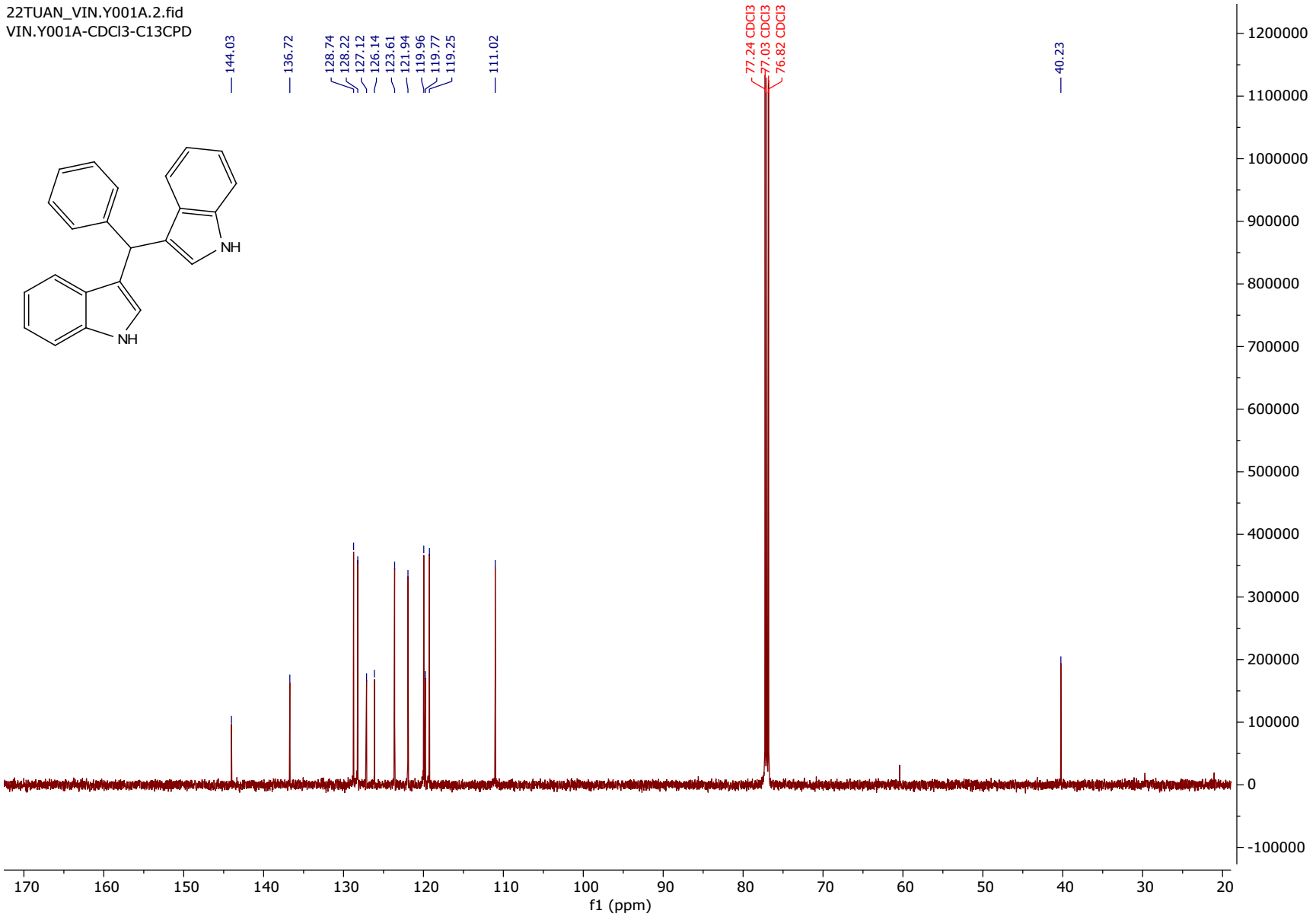

Spectrum 1A
9.246 min, Scan: 313, Merged
117.0
7.730e+8
90.0
4.028e+8
89.0
2.972e+8
63.1
1.110e+8
100%
75%
50%
25%
0%
100
200
300
400
m/z
1a
Chemical Formula: C8H7N
Exact Mass: 117.1
Molecular Weight: 117.2
m/z: 117.1 (100.0%), 118.1 (9.1%)
Elemental Analysis: C, 82.02; H, 6.02; N, 11.96

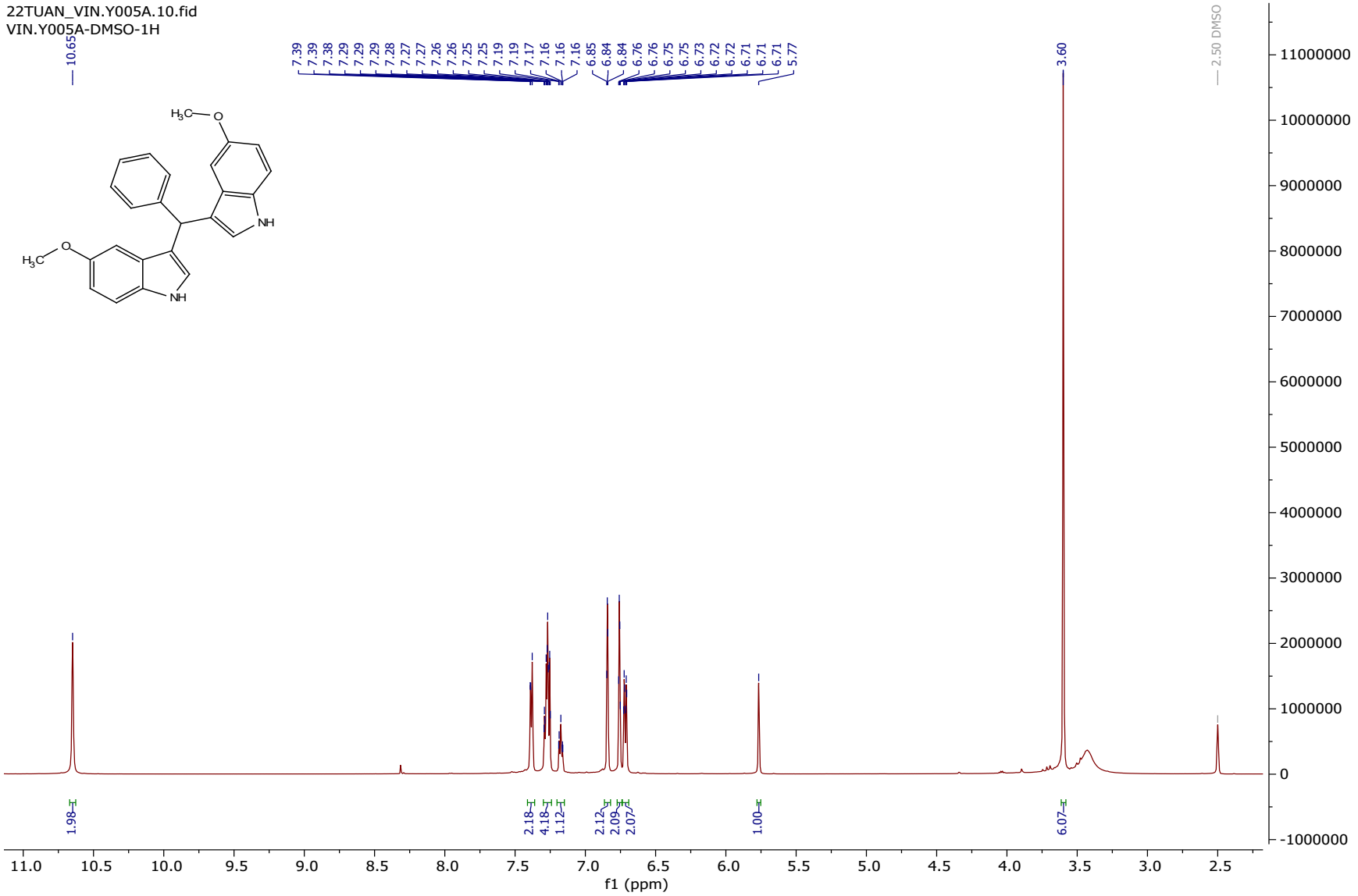

TIC; BnOH 3-4-2023 1-14-50 PM.xms; Filtered
2.5
2.0
1.5
1.0
0.5
0.0
5
6
7
8
9
10
11
minutes
HO
Ph
2a
H
O
Ph
4a (32%)

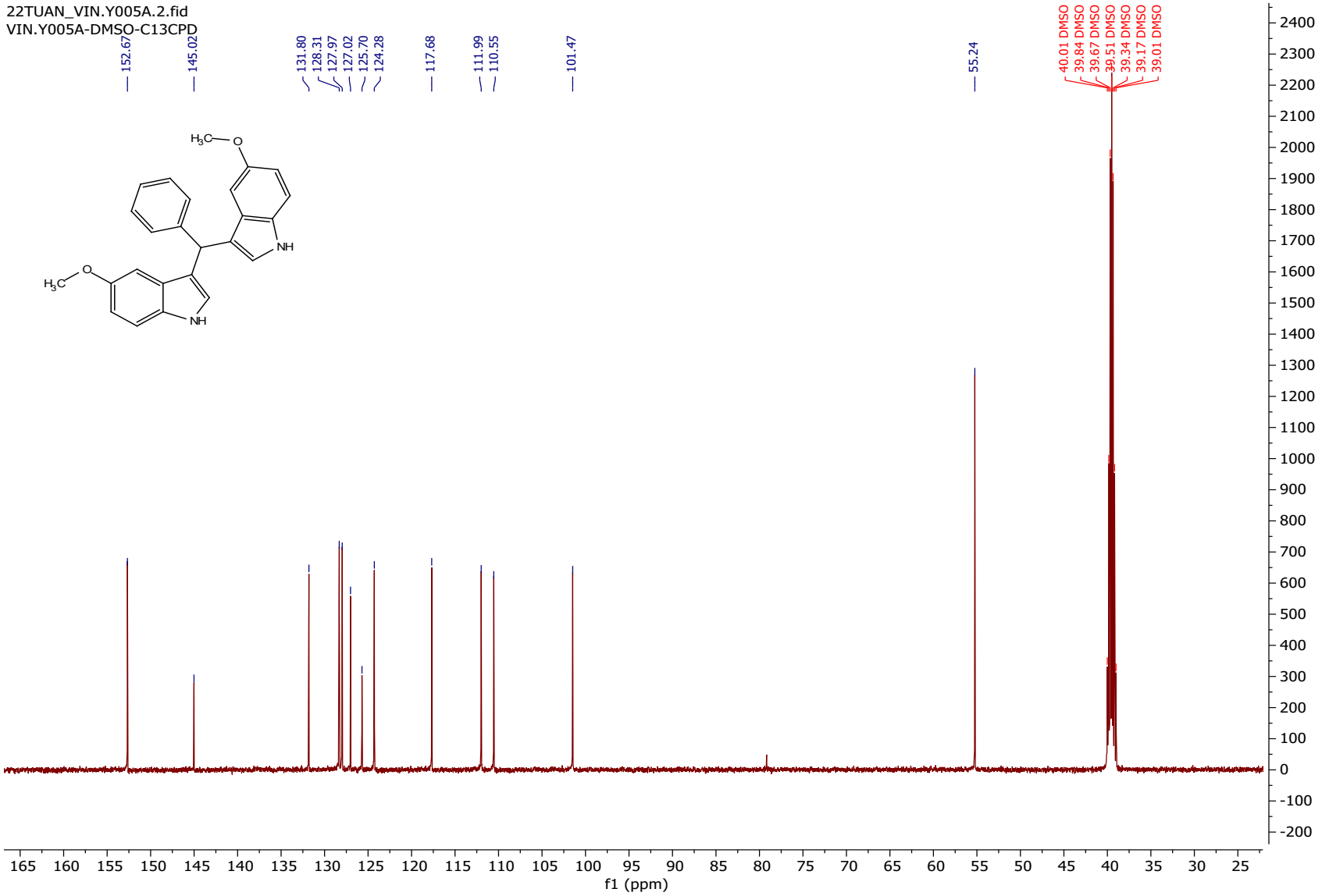

Search
Spectrum 1A
4.718 min, Scan: 43, Merged
100%
75%
50%
25%
0%
77.0
1.609e+8
106.0
1.121e+8
51.1
6.473e+7
50.3
2.732e+7
Match
Match 1 of 100
77.0
999
51.0
495
50.0
296
78.0
164
O
Chemical Formula: C7H6O
Exact Mass: 106.0
Molecular Weight: 106.1
m/z: 106.0 (100.0%), 107.0 (7.7%)
Elemental Analysis: C, 79.23; H, 5.70; O, 15.08
0
100
200
300
400
m/z
R.Match: 892, F.Match: 892

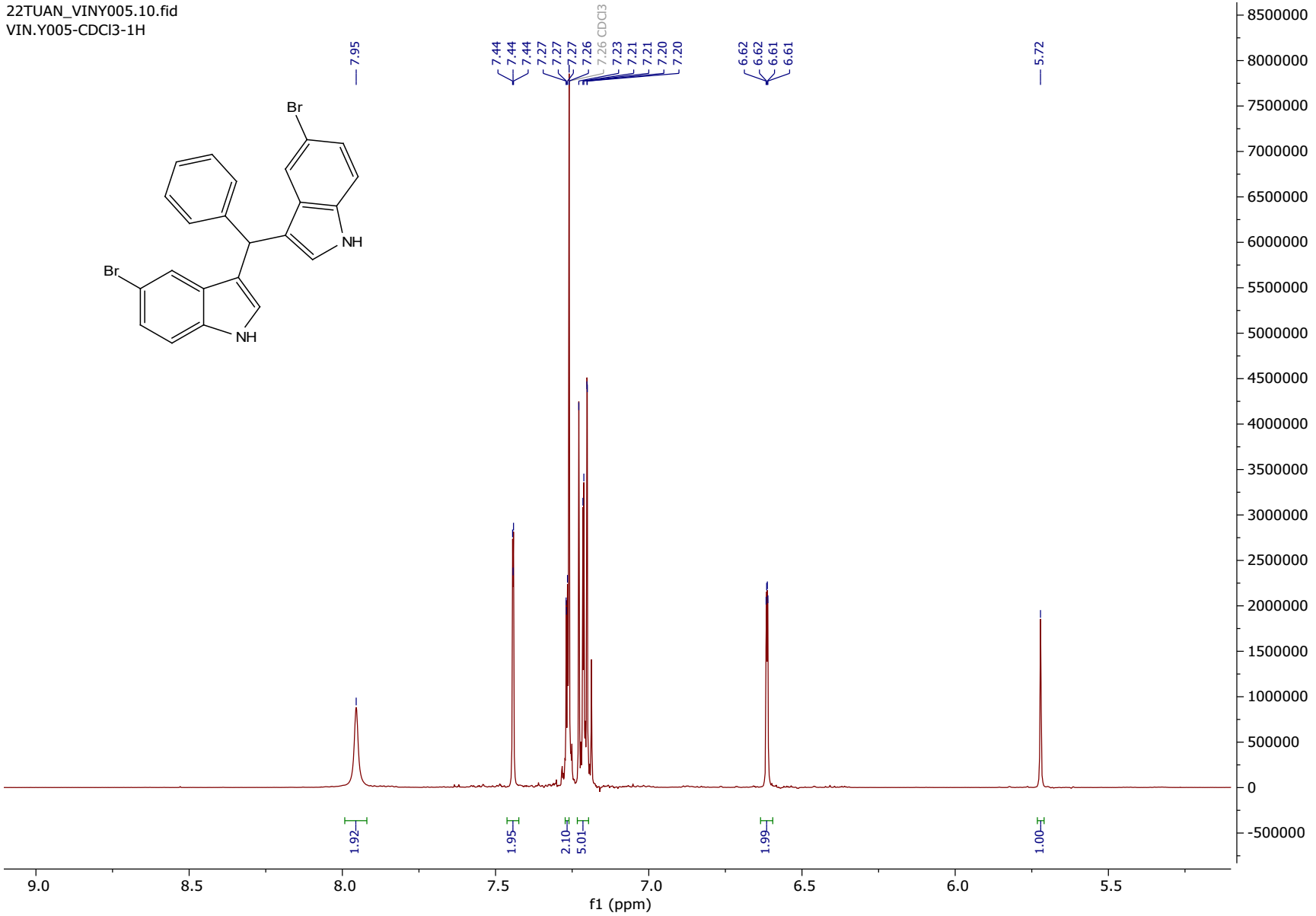

Search
Spectrum 1A
5.709 min, Scan: 102, Merged
100%
75%
50%
25%
0%
79.0
9.287e+8
108.0
6.379e+8
107.0
4.340e+8
51.1
1.979e+8
Match
Match 1 of 85
79.0
999
107.0
692
77.0
547
51.0
222
80.0
95
OH
Chemical Formula: C7H8O
Exact Mass: 108.1
Molecular Weight: 108.1
m/z: 108.1 (100.0%), 109.1 (7.7%)
Elemental Analysis: C, 77.75; H, 7.46; O, 14.79
0
100
200
300
400
m/z
R.Match: 948, F.Match: 948

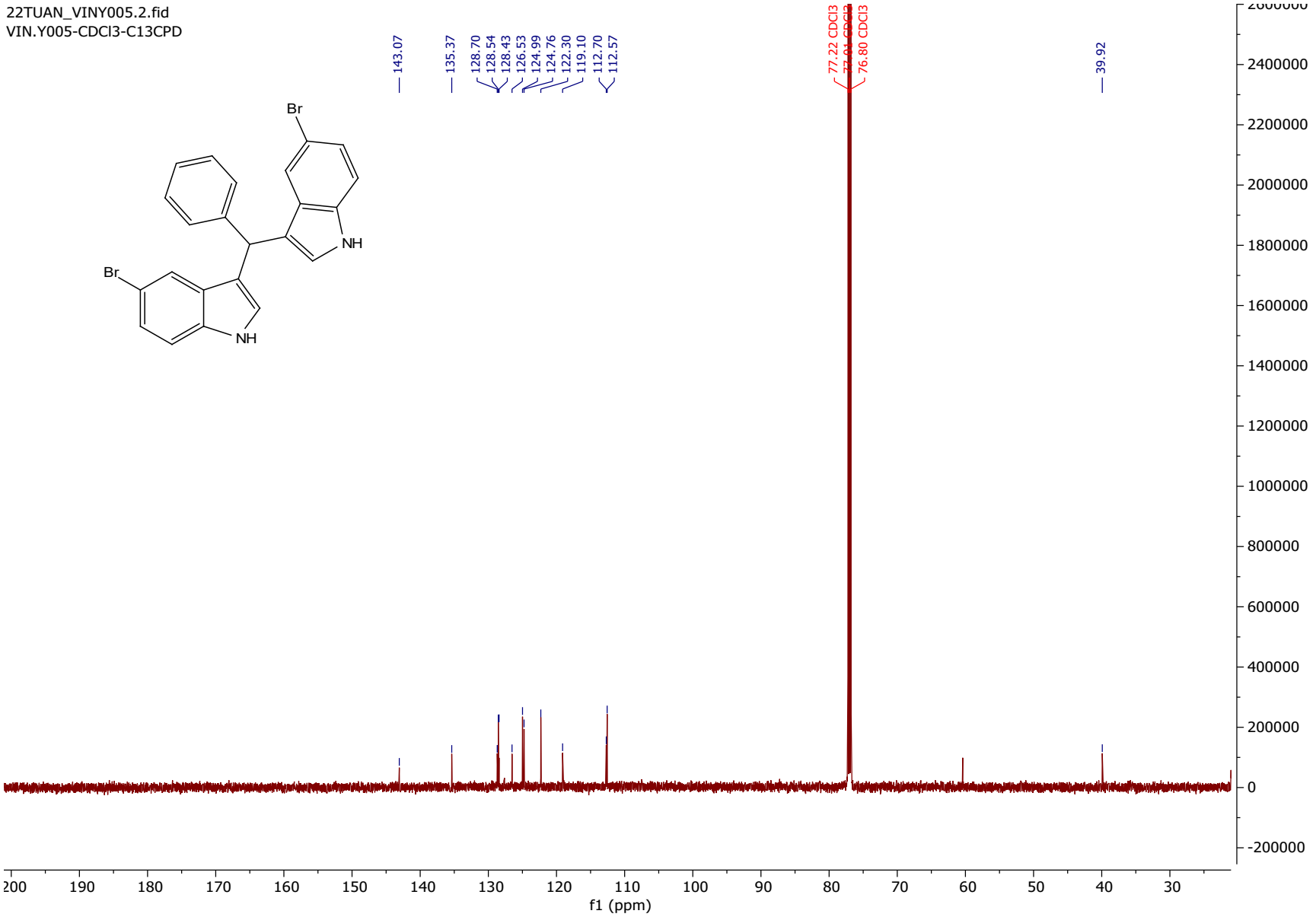

22TUAN_VIN.Y001A.10.fid
VIN.Y001A-CDCl3-1H
NH
NH
7.87 7.41 7.41 7.40 7.40 7.39 7.39 7.39 7.39 7.37 7.36 7.36 7.36 7.35 7.35 7.35 7.35 7.34 7.34 7.34 7.30 7.29 7.28 7.28 7.27 7.27 7.26 CDCl3 7.26 7.23 7.23 7.23 7.22 7.22 7.20 7.19 7.18 7.17 7.17 7.17 7.16 7.16 7.02 7.02 7.01 7.01 7.01 7.00 7.00 6.65 6.65 6.65 5.90
2.22
5.91
2.17
3.00
1.95
1.94
1.00
f1 (ppm)

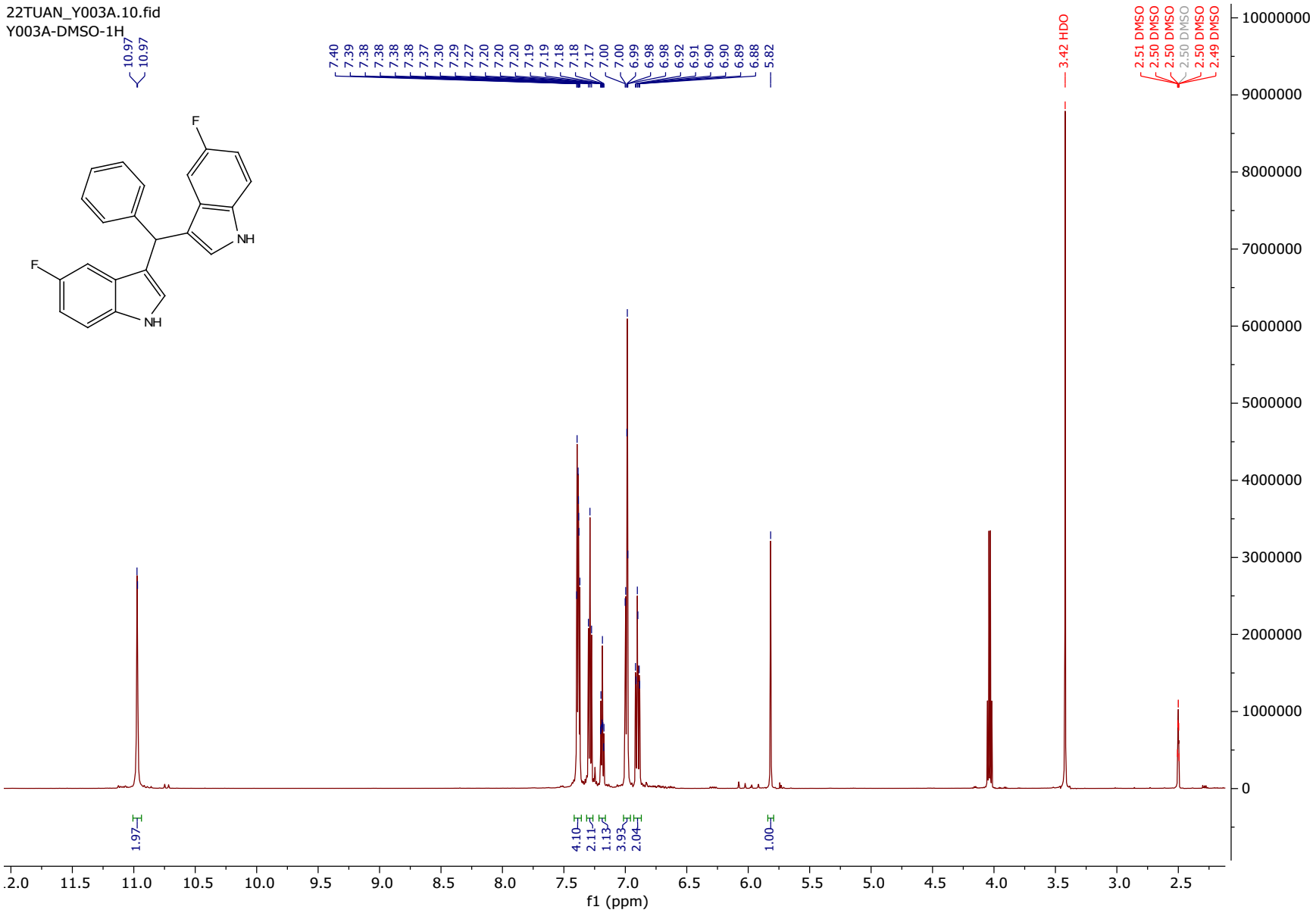

22TUAN_VIN.Y001A.2.fid
VIN.Y001A-CDCl3-C13CPD
144.03
136.72
128.74
128.22
127.12
126.14
123.61
121.94
119.96
119.77
119.25
111.02
77.24 CDCl3
77.03 CDCl3
76.82 CDCl3
40.23
NH
NH
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

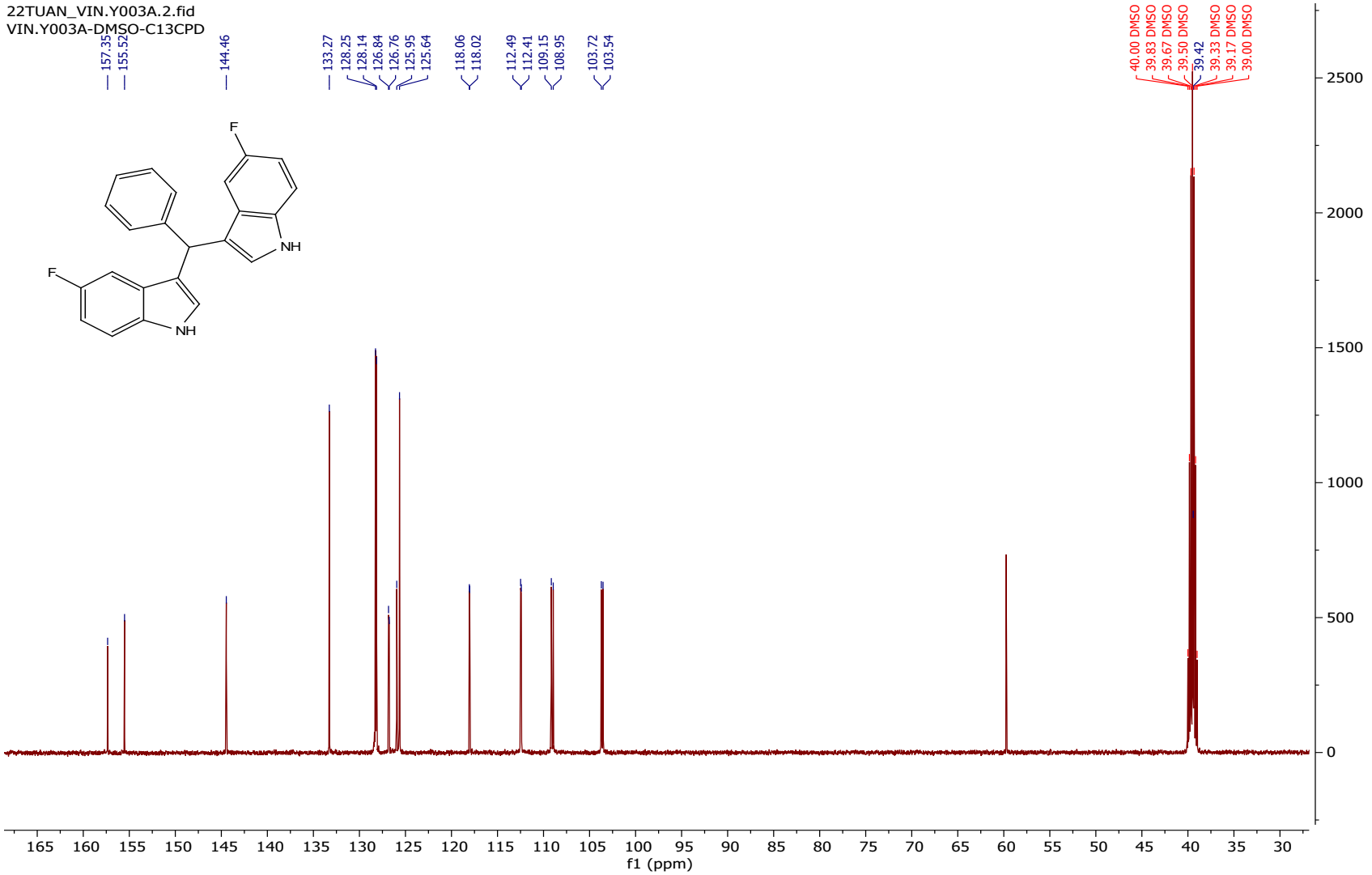

22TUAN_VIN.Y005A.10.fid
VIN.Y005A-DMSO-1H
10.65
7.39 7.39 7.38 7.29 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.19 7.19 7.17 7.16 7.16 7.16
6.85 6.84 6.84 6.76 6.76 6.75 6.75 6.73 6.72 6.72 6.71 6.71 6.71 5.77
3.60
2.50 DMSO
H3C O
NH
H3C O
NH
1.98
2.18 4.18 1.12 2.12 2.09 2.07
1.00
6.07
11.0 10.5 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
f1 (ppm)
11000000 10000000 9000000 8000000 7000000 6000000 5000000 4000000 3000000 2000000 1000000 0 -1000000

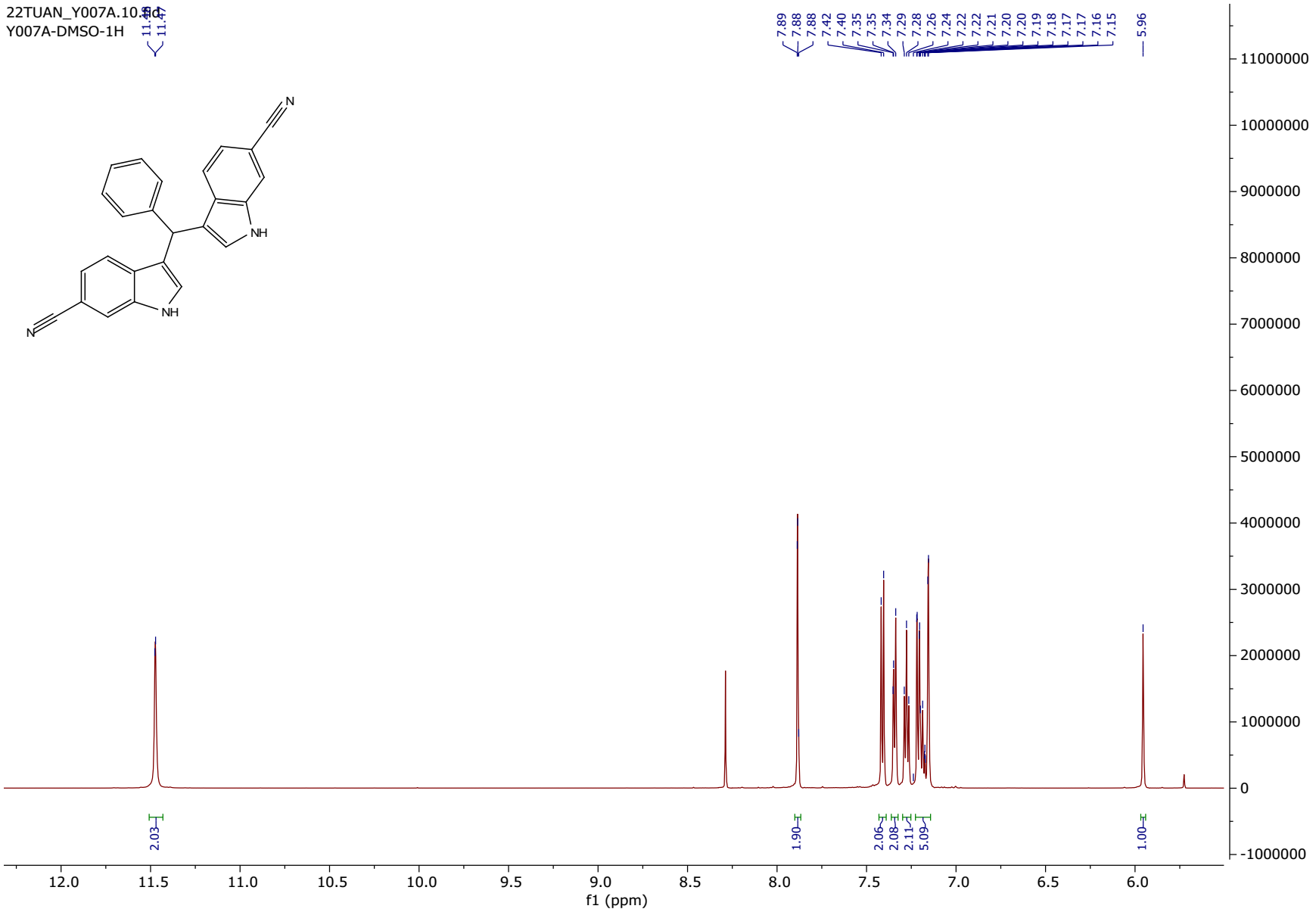

22TUAN_VIN.Y005A.2.fid
VIN.Y005A-DMSO-C13CPD
152.67
145.02
131.80
128.31
127.97
127.02
125.70
124.28
117.68
111.99
110.55
101.47
55.24
40.01 DMSO
39.84 DMSO
39.67 DMSO
39.51 DMSO
39.34 DMSO
39.17 DMSO
39.01 DMSO
H3C
O
NH
f1 (ppm)

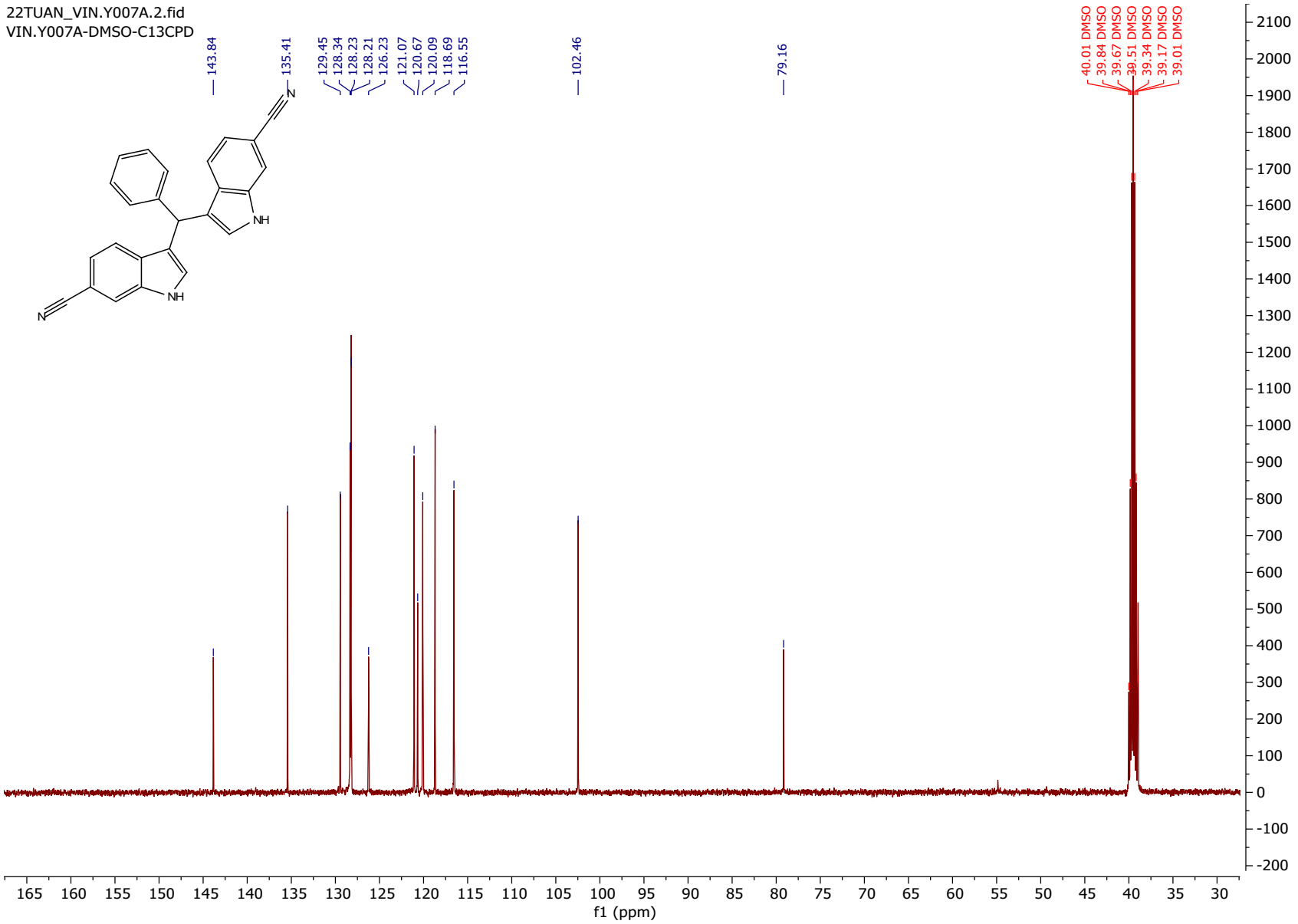

22TUAN_VINY005.10.fid
VIN.Y005-CDCl3-1H
Br
NH
Br
NH
7.95
7.44
7.44
7.44
7.27
7.27
7.27
7.26
7.26 CDCl3
7.23
7.21
7.21
7.20
7.20
6.62
6.62
6.61
6.61
5.72
1.92
1.95
2.10
5.01
1.99
1.00
f1 (ppm)

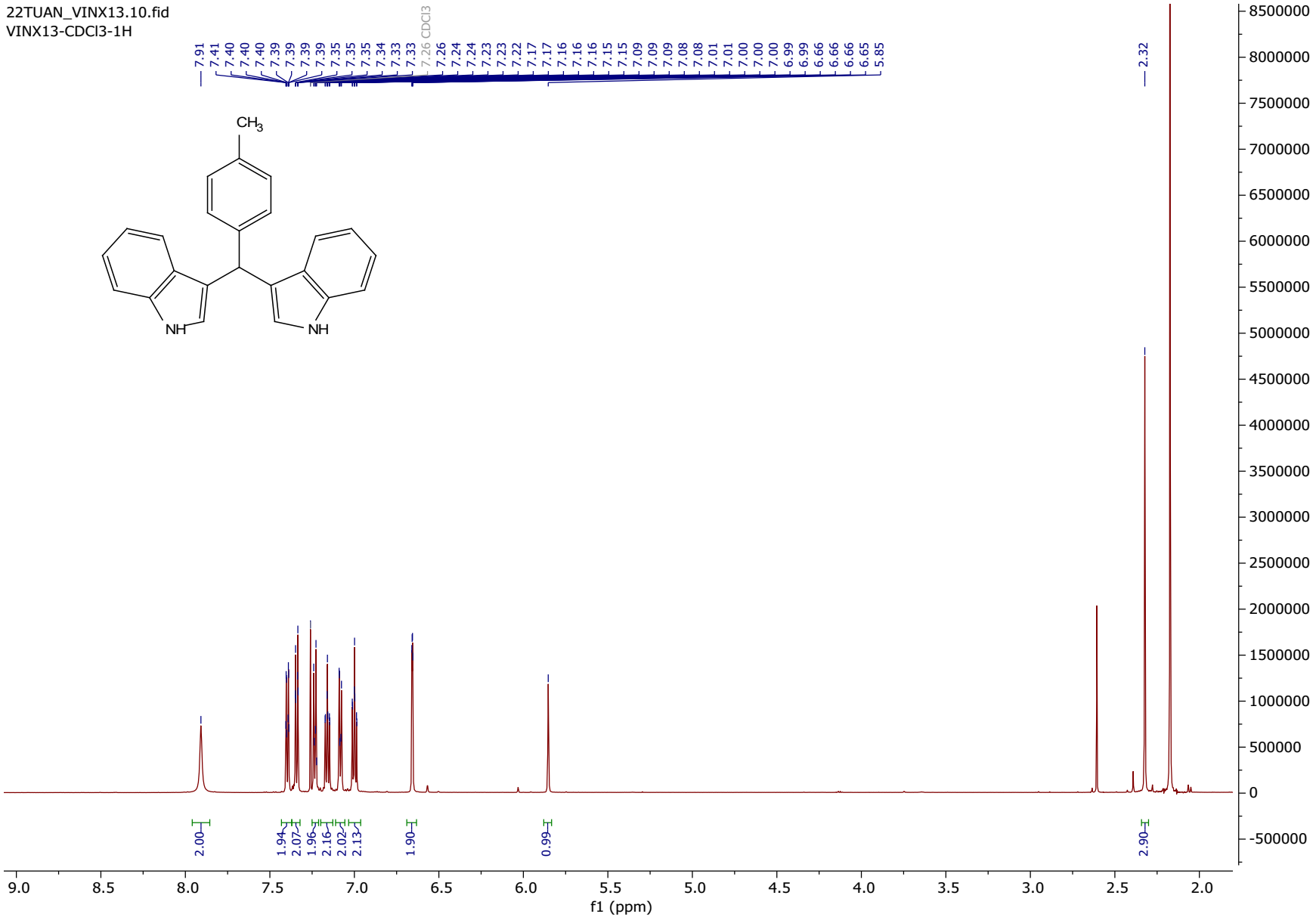

22TUAN_VINY005.2.fid
VIN.Y005-CDCl3-C13CPD
143.07
135.37
128.70
128.54
128.43
126.53
124.99
124.76
122.30
119.10
112.70
112.57
77.22 CDCl3
77.01 CDCl3
76.80 CDCl3
39.92
Br
NH
Br
NH
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
-200000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

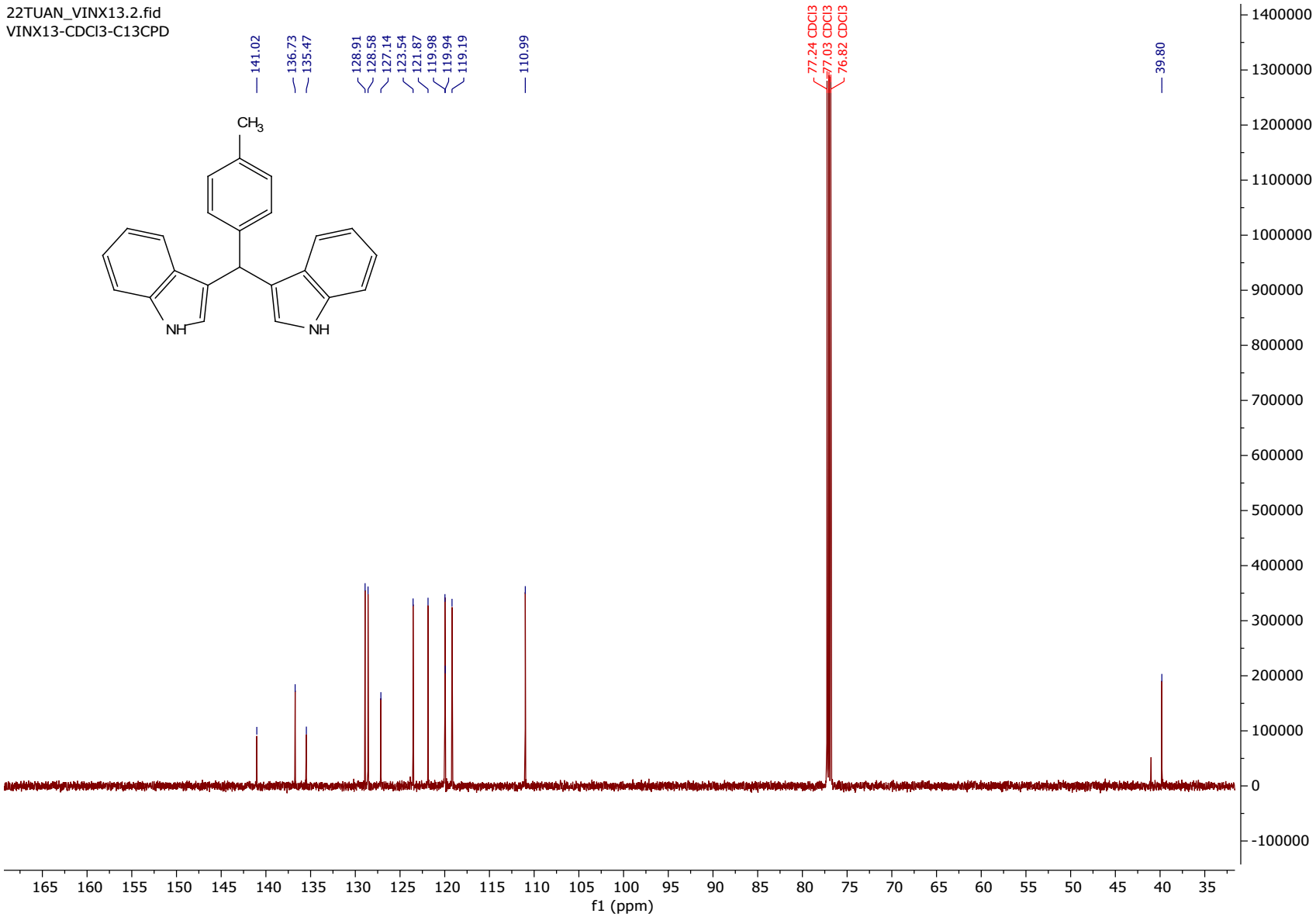

22TUAN_Y003A.10.fid
Y003A-DMSO-1H
10.97
10.97
7.40
7.39
7.38
7.38
7.38
7.38
7.37
7.30
7.29
7.27
7.20
7.20
7.20
7.19
7.19
7.18
7.18
7.17
7.00
7.00
6.99
6.98
6.98
6.92
6.91
6.90
6.90
6.89
6.88
5.82
3.42 HDO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO
2.49 DMSO
F
NH
F
NH
1.97
4.10
2.11
1.13
3.93
2.04
1.00
f1 (ppm)

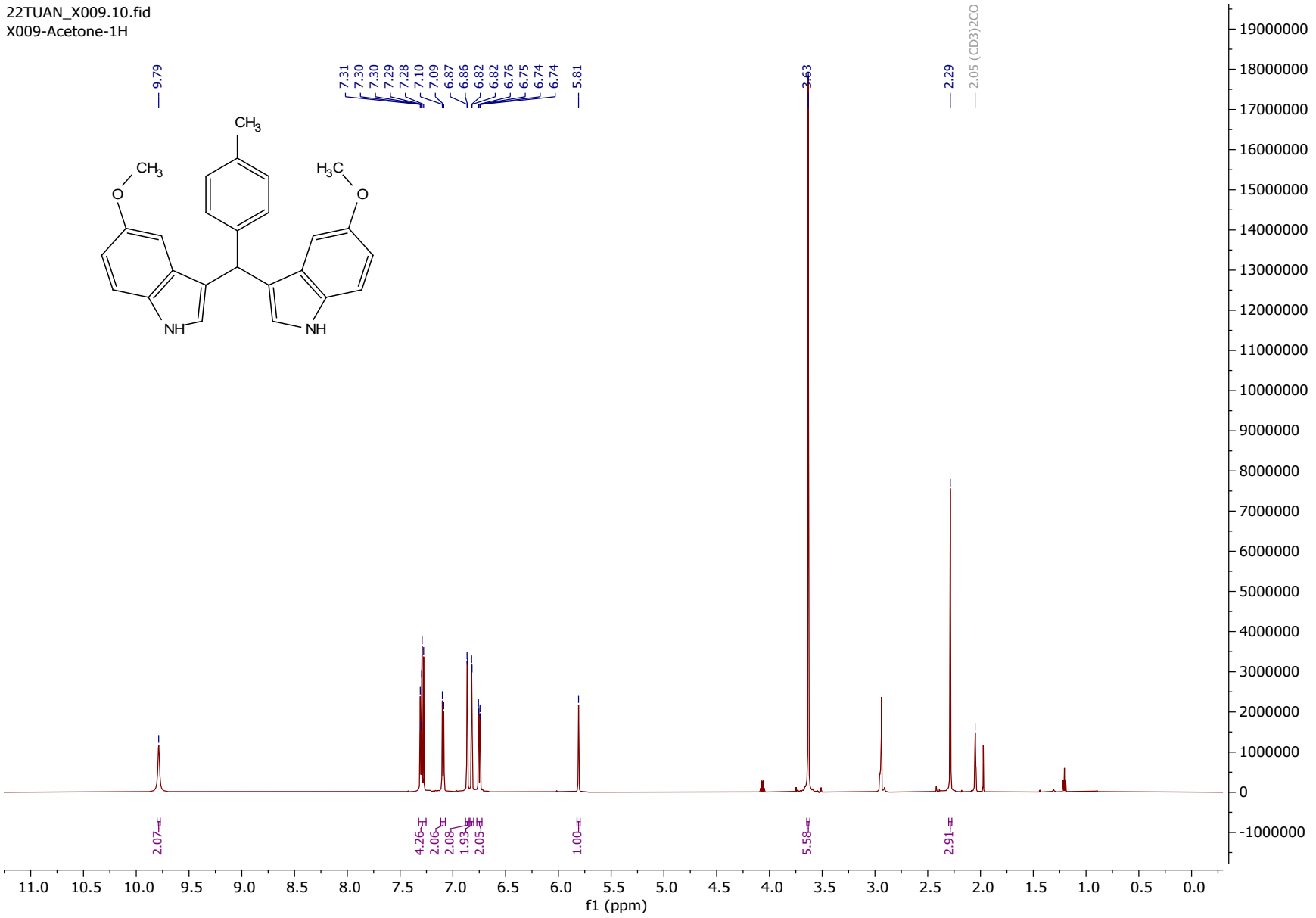

22TUAN_VIN.Y003A.2.fid
VIN.Y003A-DMSO-C13CPD
157.35
155.52
144.46
133.27
128.25
128.14
126.84
126.76
125.95
125.64
118.06
118.02
112.49
112.41
109.15
108.95
103.72
103.54
40.00 DMSO
39.83 DMSO
39.67 DMSO
39.50 DMSO
39.42
39.33 DMSO
39.17 DMSO
39.00 DMSO
F
NH
F
NH
2500
2000
1500
1000
500
0
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)

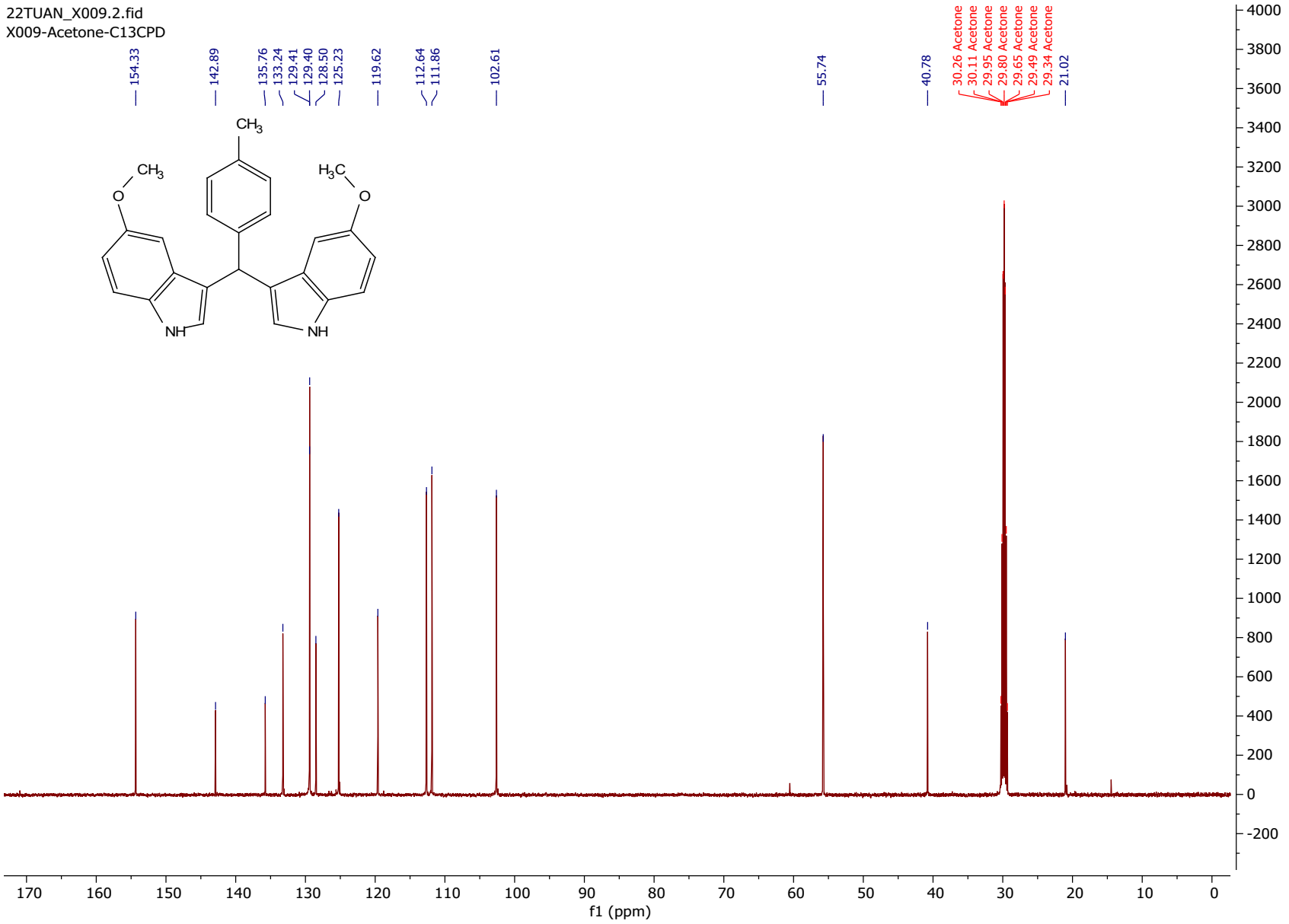

22TUAN_Y007A.10.fid
Y007A-DMSO-1H
11.47
11.47
7.89
7.88
7.88
7.42
7.40
7.35
7.35
7.34
7.29
7.28
7.26
7.24
7.22
7.22
7.21
7.20
7.20
7.19
7.18
7.17
7.17
7.16
7.15
5.96
N
NH
NH
N
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
2.03
1.90
2.06
2.08
2.11
5.09
1.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
f1 (ppm)

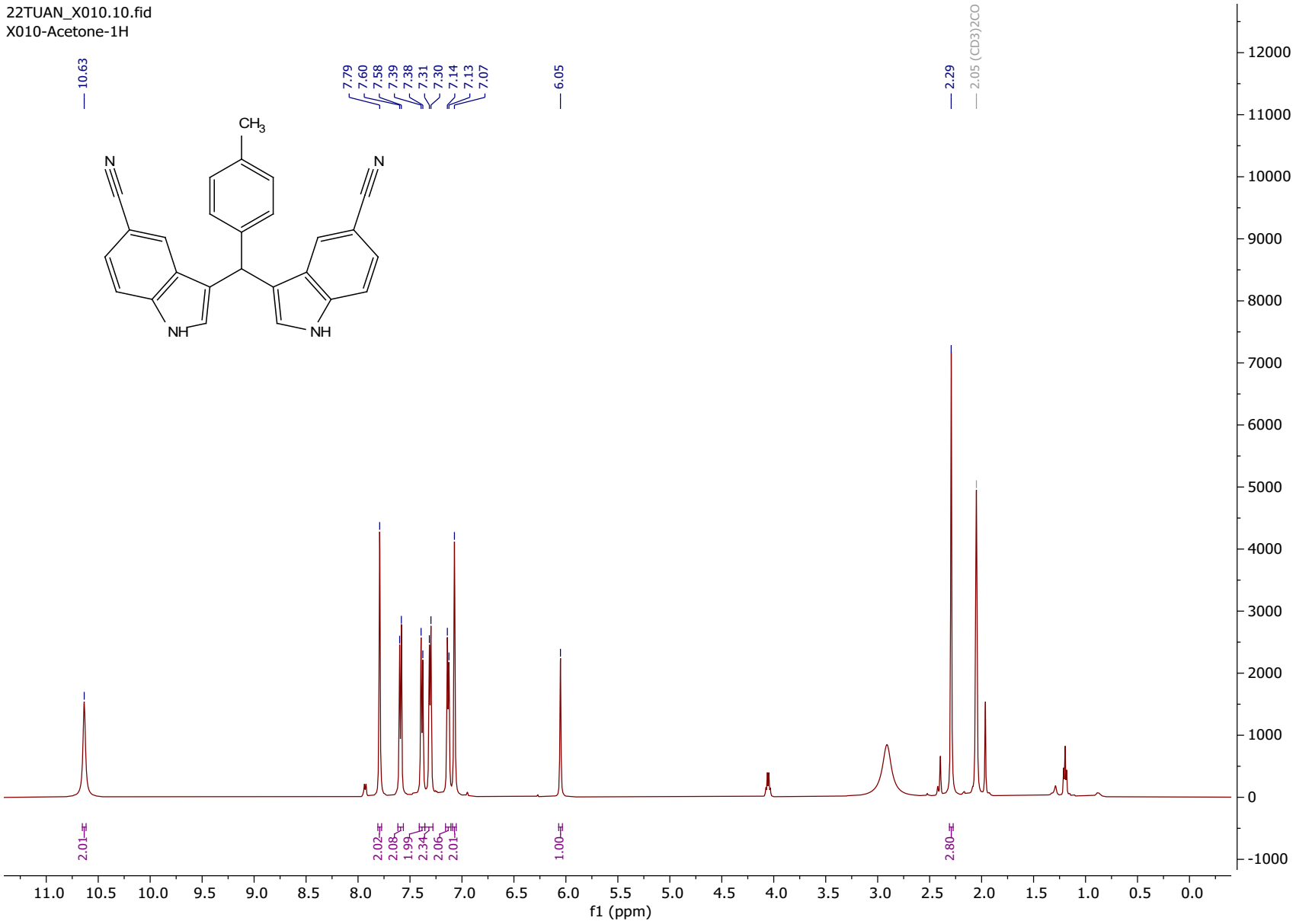

22TUAN_VIN.Y007A.2.fid
VIN.Y007A-DMSO-C13CPD
143.84
135.41
129.45
128.34
128.23
128.21
126.23
121.07
120.67
120.09
118.69
116.55
102.46
79.16
40.01 DMSO
39.84 DMSO
39.67 DMSO
39.51 DMSO
39.34 DMSO
39.17 DMSO
39.01 DMSO
NH
NH
N
N
f1 (ppm)

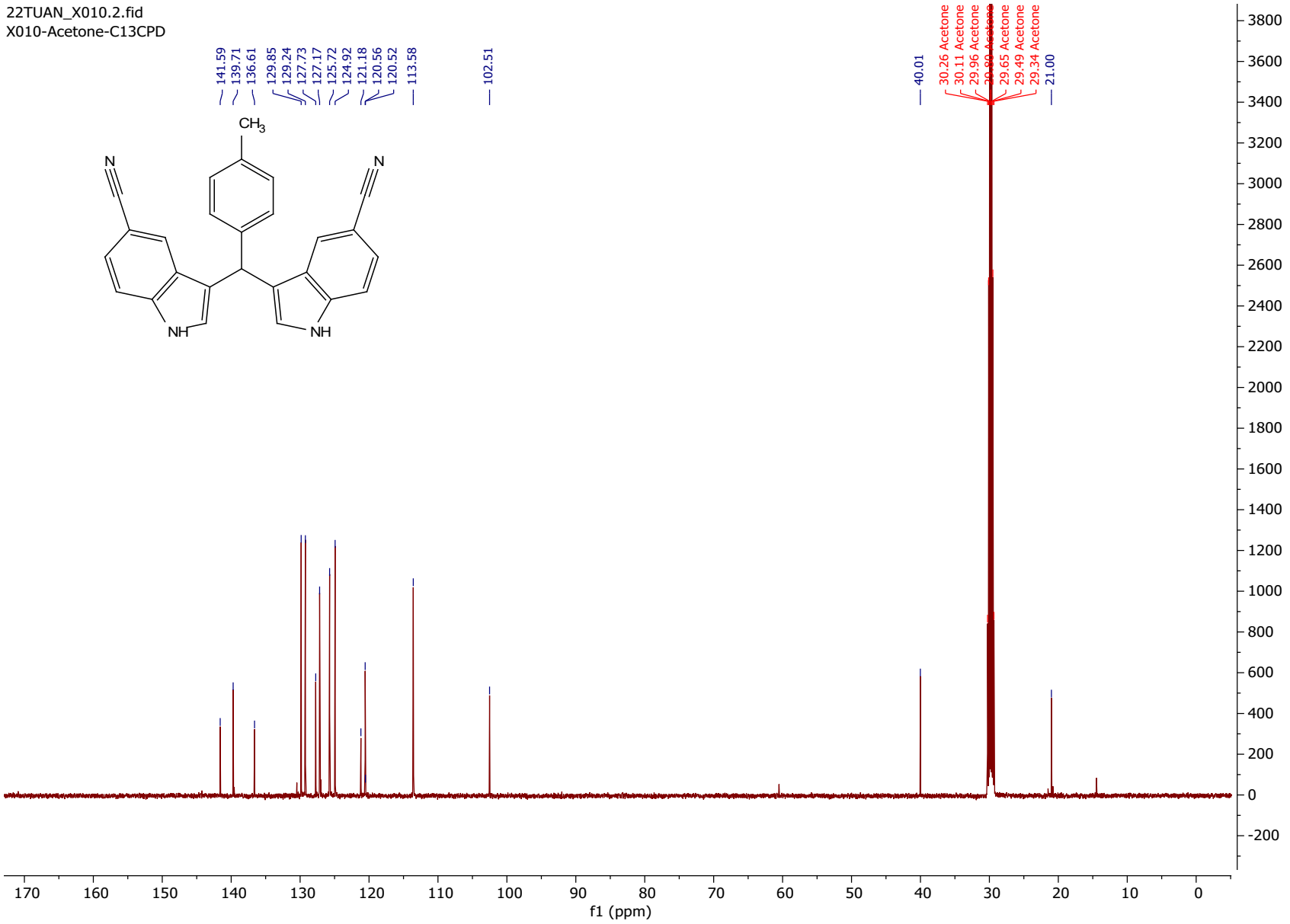

22TUAN_VINX13.10.fid
VINX13-CDCl3-1H
7.91 7.41 7.40 7.40 7.40 7.39 7.39 7.39 7.39 7.35 7.35 7.35 7.34 7.33 7.33 7.26 CDCl3 7.26 7.24 7.23 7.23 7.22 7.17 7.17 7.16 7.16 7.16 7.15 7.15 7.09 7.09 7.09 7.08 7.08 7.01 7.01 7.00 7.00 7.00 6.99 6.99 6.66 6.66 6.66 6.65 5.85
2.32
CH3
NH
NH
2.00 1.94 2.07 1.96 2.16 2.02 2.13 1.90 0.99 2.90
f1 (ppm)

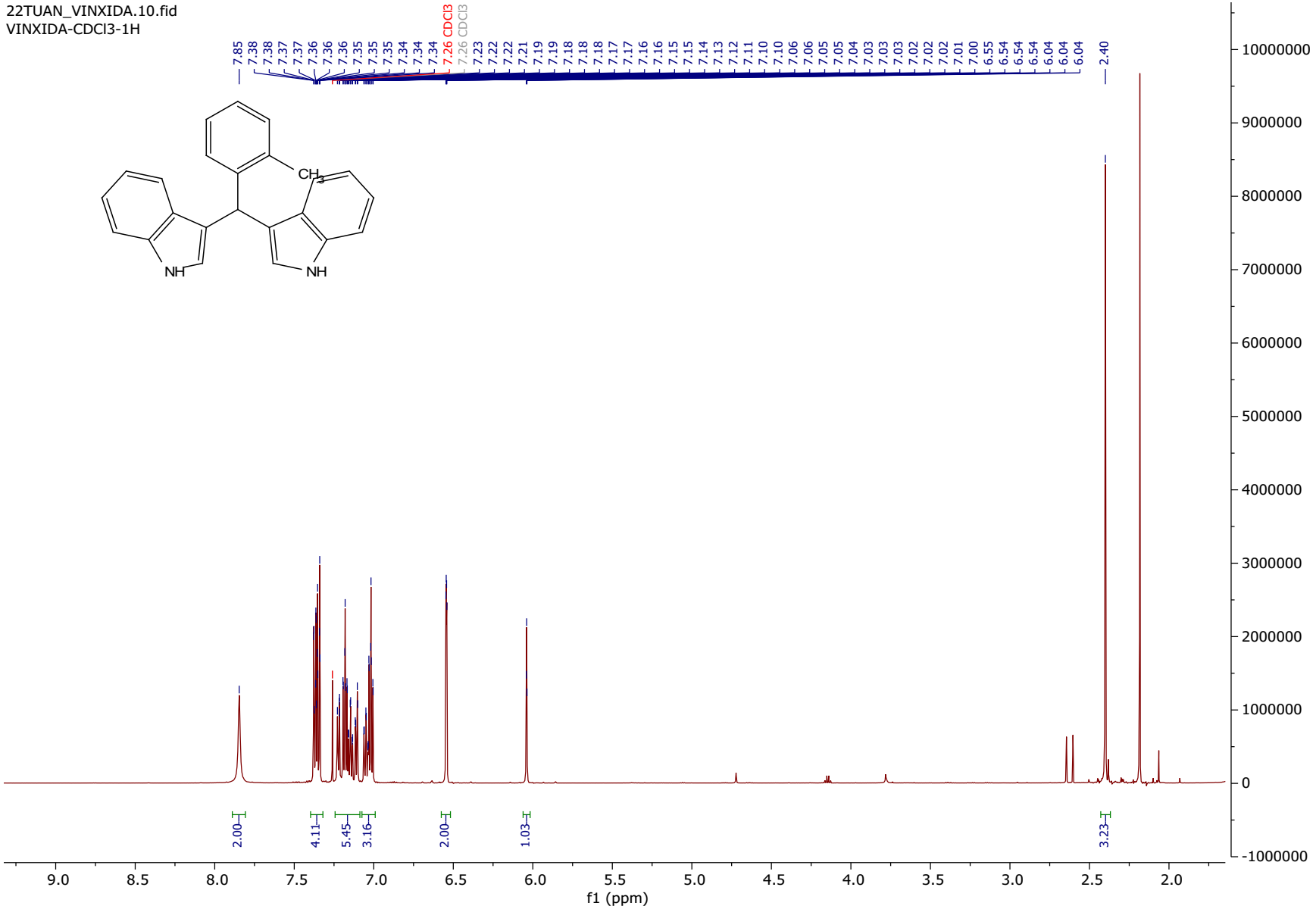

22TUAN_VINX13.2.fid
VINX13-CDCl3-C13CPD
141.02
136.73
135.47
128.91
128.58
127.14
123.54
121.87
119.98
119.94
119.19
110.99
77.24 CDCl3
77.03 CDCl3
76.82 CDCl3
39.80
CH3
NH
NH
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

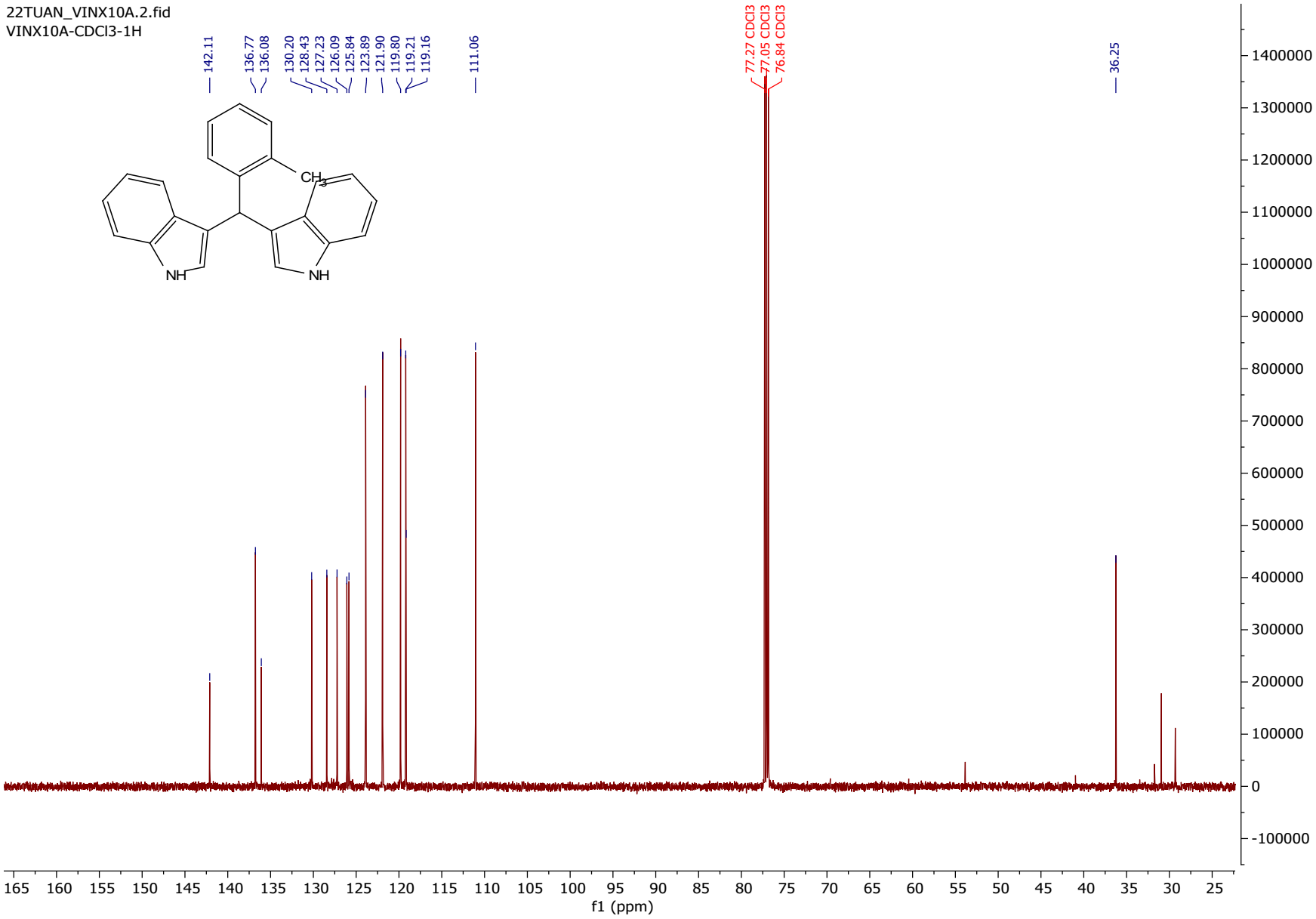

22TUAN_X009.10.fid
X009-Acetone-1H
9.79
7.31
7.30
7.30
7.29
7.28
7.10
7.09
6.87
6.86
6.82
6.82
6.76
6.75
6.74
6.74
5.81
3.63
2.29
2.05 (CD3)2CO
CH3
CH3
O
H3C
O
NH
NH
2.07
4.26
2.06
2.08
1.93
2.05
1.00
5.58
2.91
f1 (ppm)

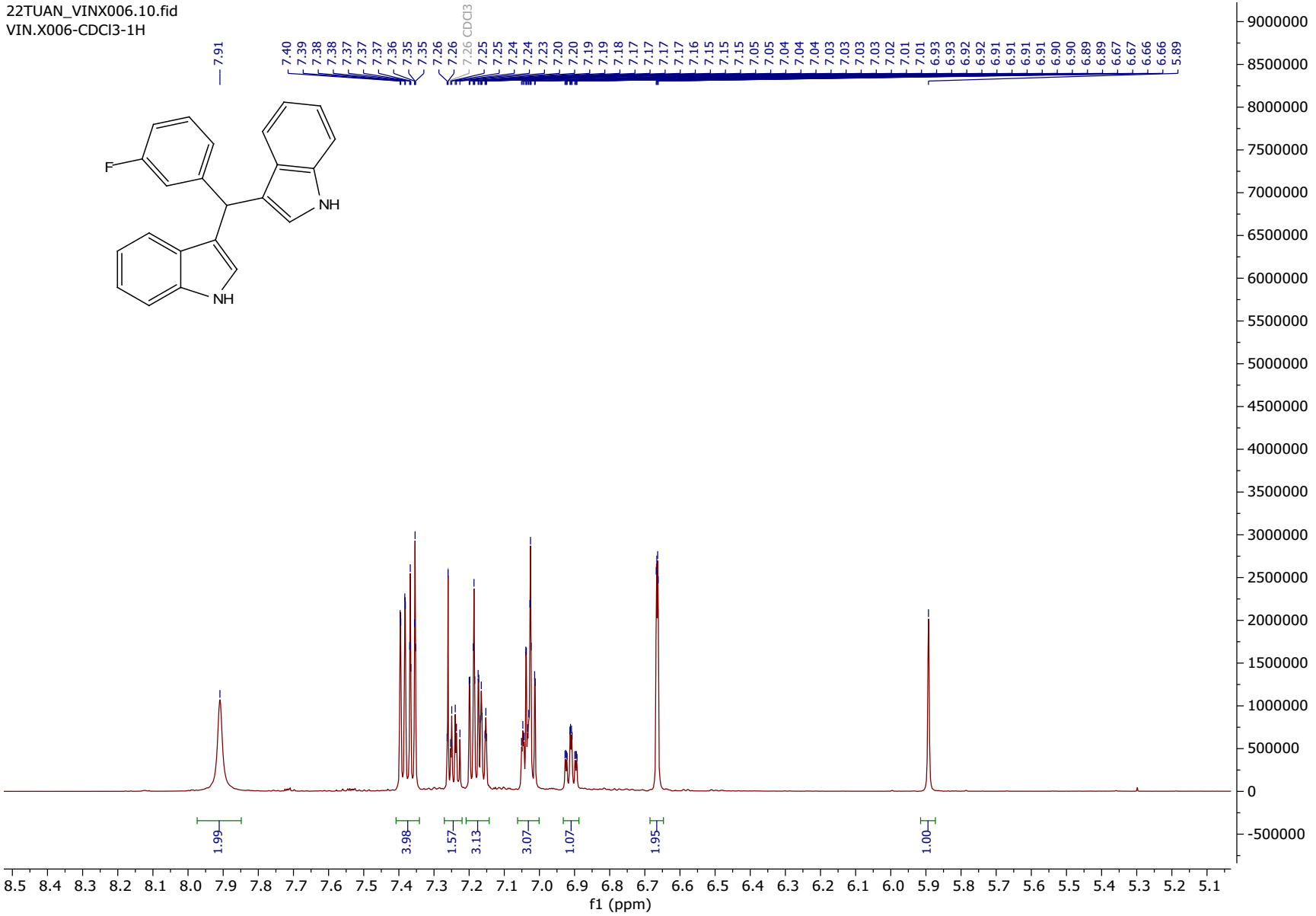

22TUAN_X009.2.fid
X009-Acetone-C13CPD
154.33
142.89
135.76
133.24
129.41
129.40
128.50
125.23
119.62
112.64
111.86
102.61
55.74
40.78
30.26 Acetone
30.11 Acetone
29.95 Acetone
29.80 Acetone
29.65 Acetone
29.49 Acetone
29.34 Acetone
21.02
CH3
CH3
O
H3C
O
NH
NH
f1 (ppm)

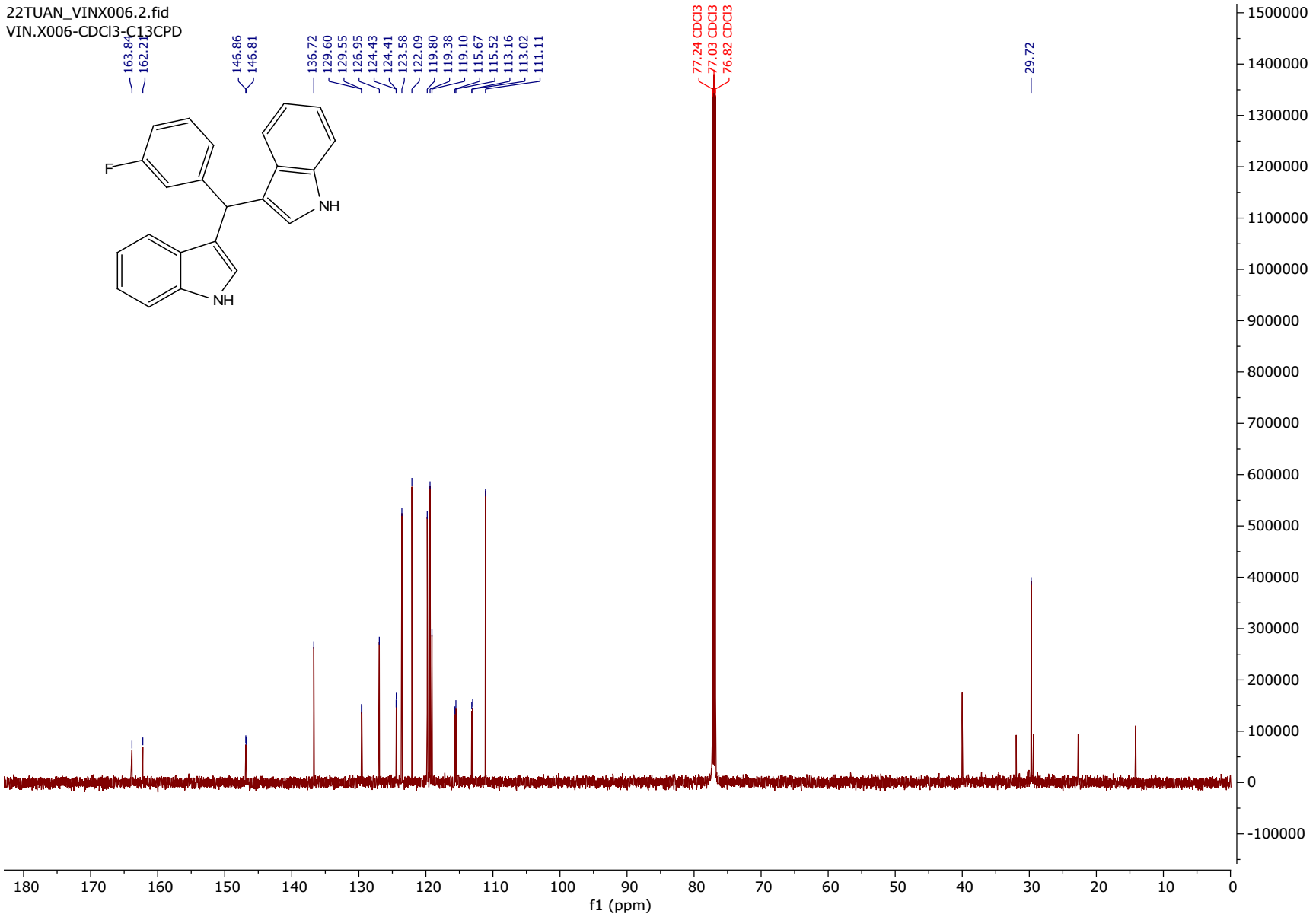

22TUAN_X010.10.fid
X010-Acetone-1H
10.63
7.79
7.60
7.58
7.39
7.38
7.31
7.30
7.14
7.13
7.07
6.05
2.29
2.05 (CD3)2CO
CH3
N
N
NH
NH
2.01
2.02
2.08
1.99
2.34
2.06
2.01
1.00
2.80
f1 (ppm)

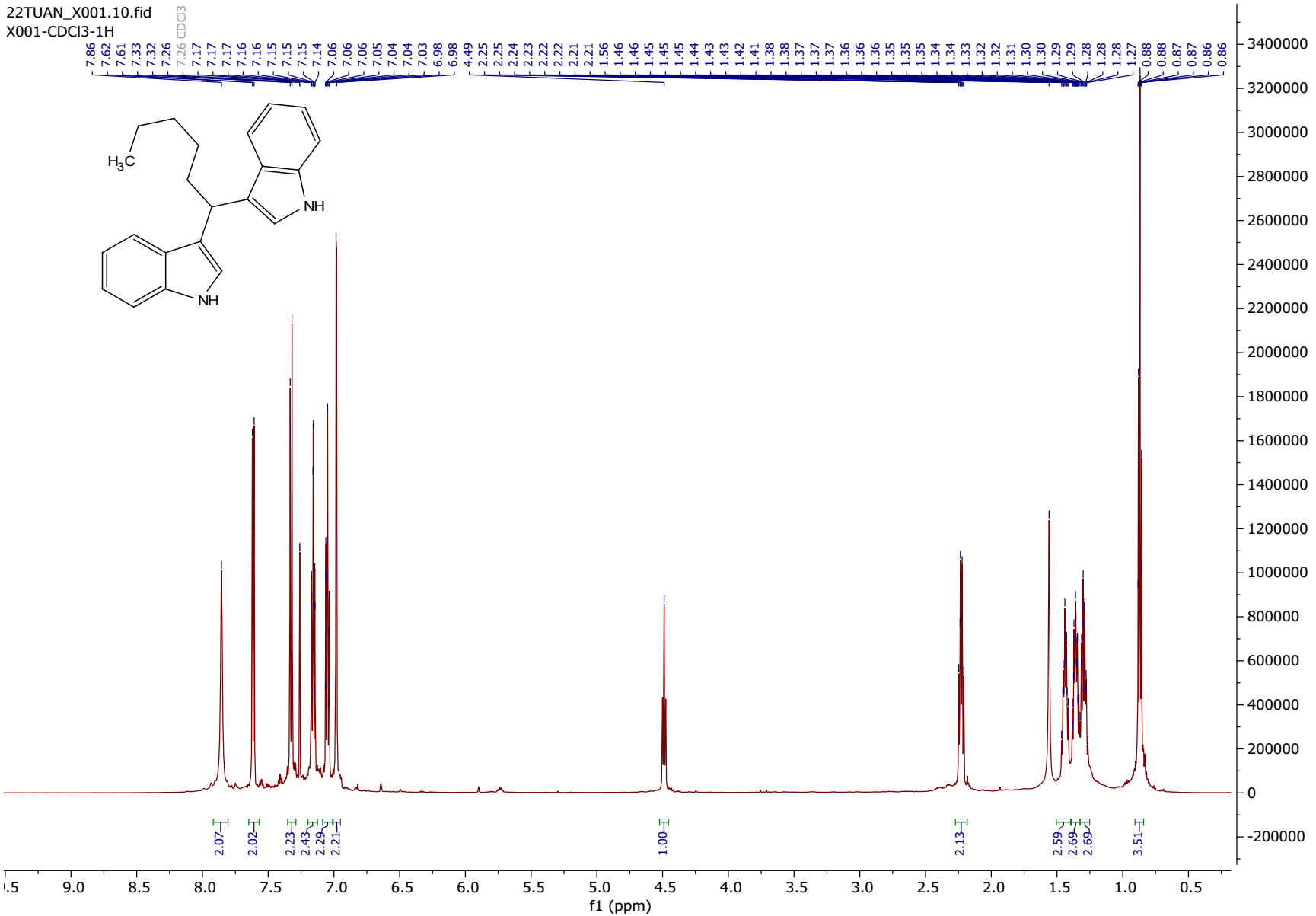

22TUAN_X010.2.fid
X010-Acetone-C13CPD
141.59
139.71
136.61
129.85
129.24
127.73
127.17
125.72
124.92
121.18
120.56
120.52
113.58
102.51
40.01
30.26 Acetone
30.11 Acetone
29.96 Acetone
29.65 Acetone
29.49 Acetone
29.34 Acetone
21.00
CH3
N
N
NH
NH
f1 (ppm)

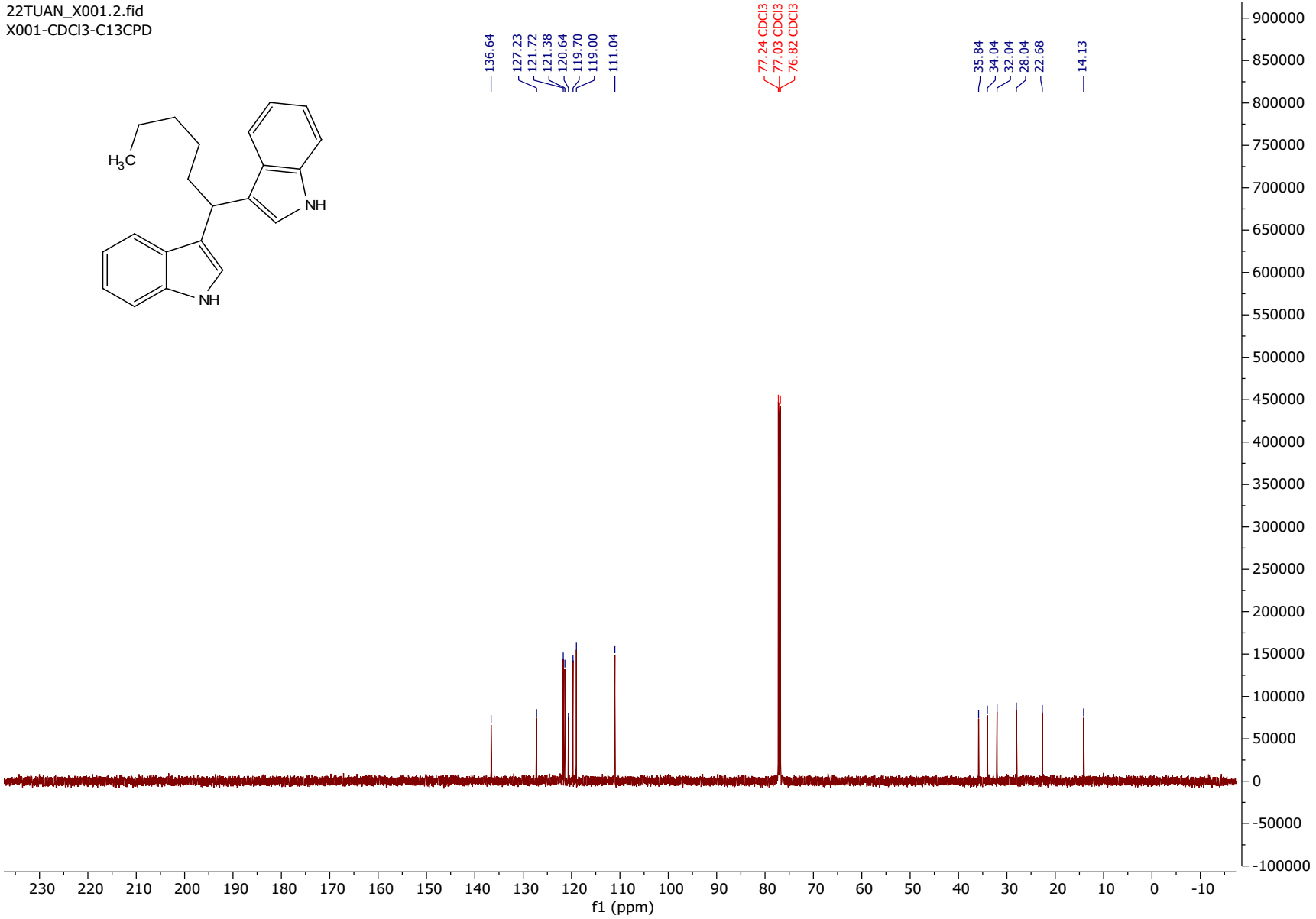

22TUAN_VINXIDA.10.fid
VINXIDA-CDCl3-1H
CH3
NH
NH
f1 (ppm)

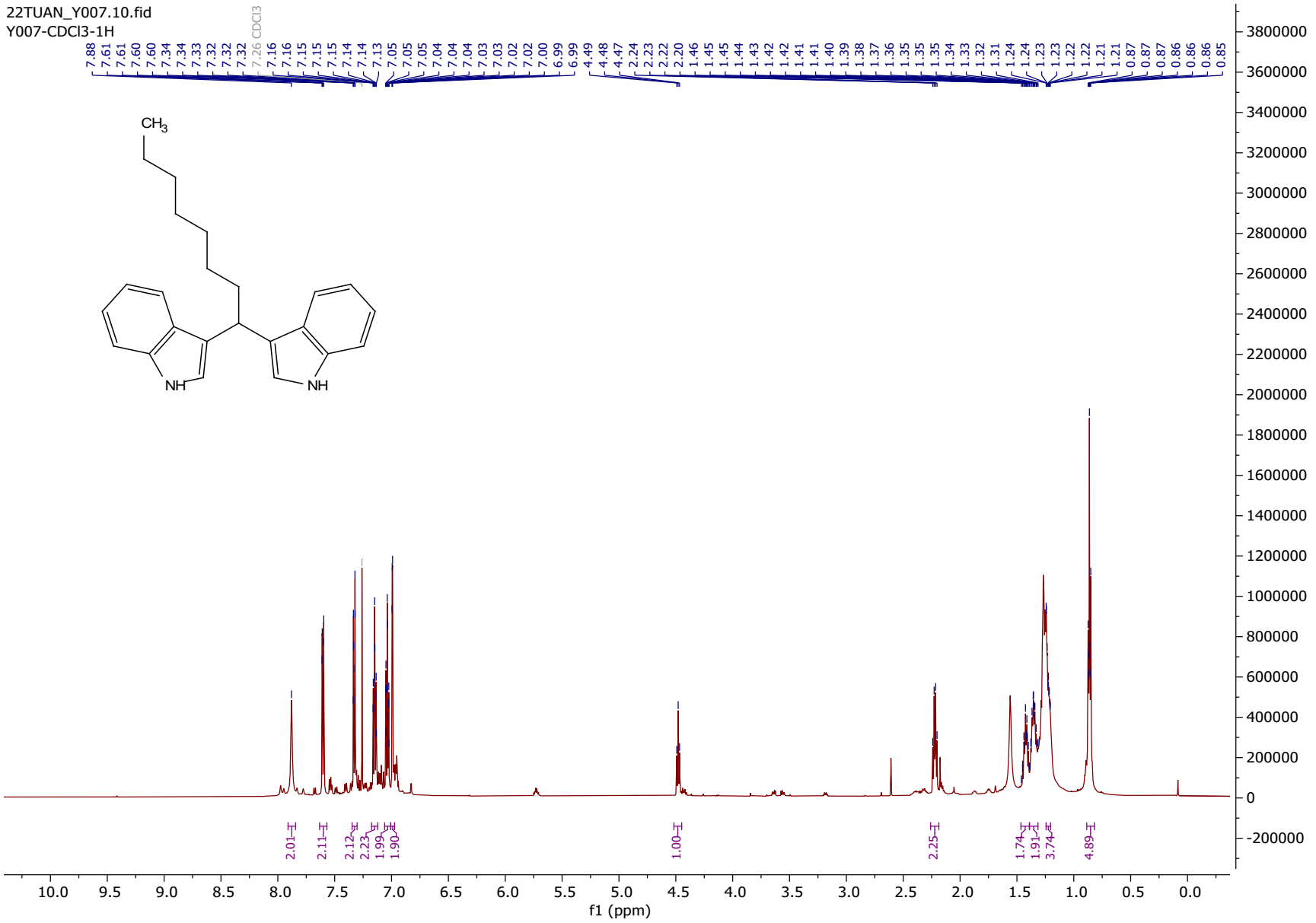

22TUAN_VINX10A.2.fid
VINX10A-CDCl3-1H
142.11
136.77
136.08
130.20
128.43
127.23
126.09
125.84
123.89
121.90
119.80
119.21
119.16
111.06
77.27 CDCl3
77.05 CDCl3
76.84 CDCl3
36.25
CH3
NH
NH
f1 (ppm)

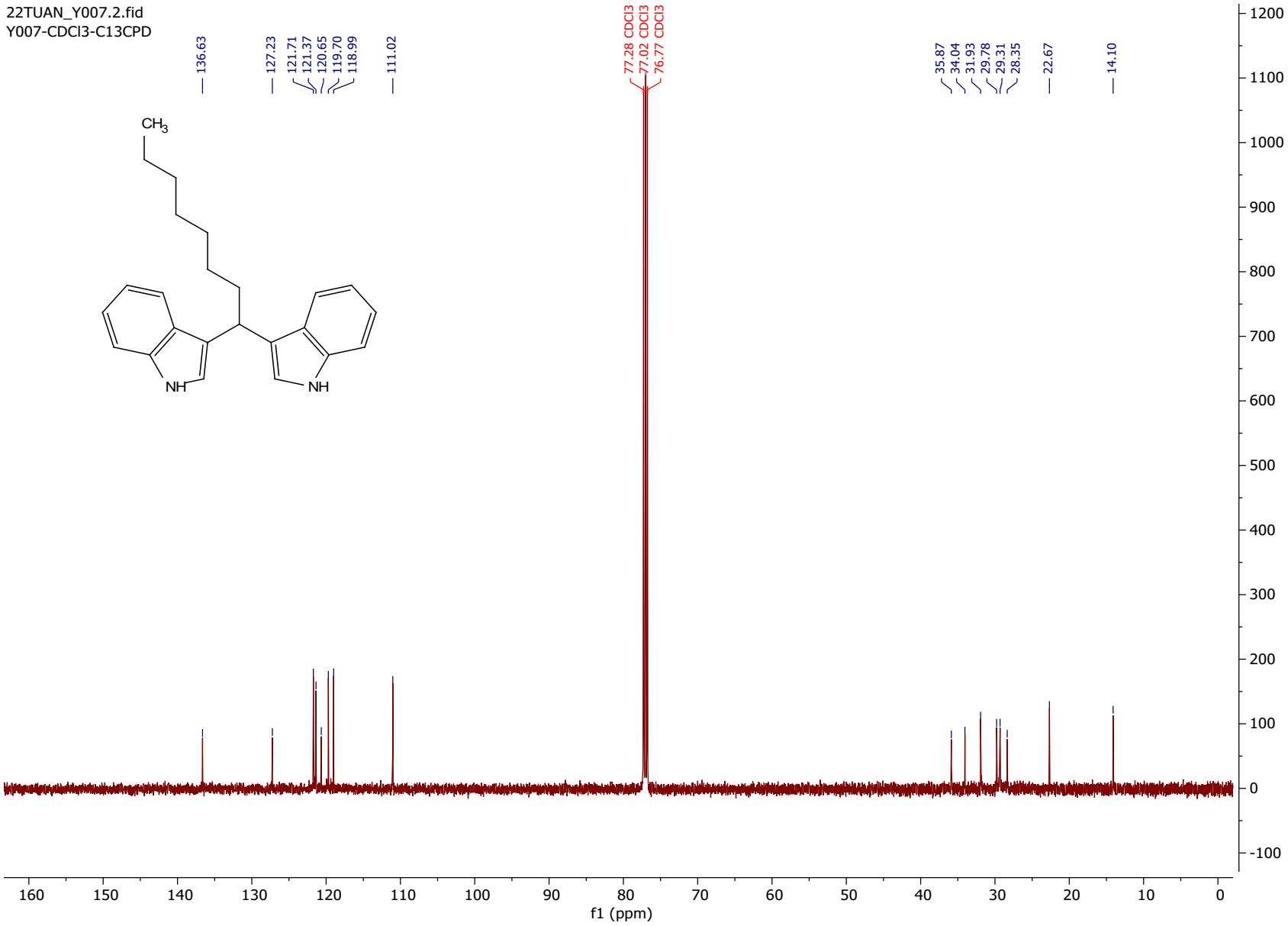

22TUAN_VINX006.10.fid
VIN.X006-CDCl3-1H
F
NH
NH
f1 (ppm)


22TUAN_VINX006.2.fid
VIN.X006-CDCl3-C13CPD
163.84
162.21
146.86
146.81
136.72
129.60
129.55
126.95
124.43
124.41
123.58
122.09
119.80
119.38
119.10
115.67
115.52
113.16
113.02
111.11
77.24 CDCl3
77.03 CDCl3
76.82 CDCl3
29.72
F
NH
NH
f1 (ppm)


22TUAN_X001.10.fid
X001-CDCl3-1H
7.26 CDCl3
H3C
NH
NH
f1 (ppm)


22TUAN_X001.2.fid
X001-CDCl3-C13CPD
136.64
127.23
121.72
121.38
120.64
119.70
119.00
111.04
77.24 CDCl3
77.03 CDCl3
76.82 CDCl3
35.84
34.04
32.04
28.04
22.68
14.13
H3C
NH
NH
f1 (ppm)


22TUAN_Y007.10.fid
Y007-CDCl3-1H
CH3
NH
NH
f1 (ppm)


22TUAN_Y007.2.fid
Y007-CDCl3-C13CPD
136.63
127.23
121.71
121.37
120.65
119.70
118.99
111.02
77.28 CDCl3
77.02 CDCl3
76.77 CDCl3
35.87
34.04
31.93
29.78
29.31
28.35
22.67
14.10
CH3
NH
NH
f1 (ppm)