Supporting Information:

Synthesis of Tetrasubstituted Symmetrical Pyridines by Iron-Catalyzed Cyclization of Ketoxime Acetates

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CONTENTS

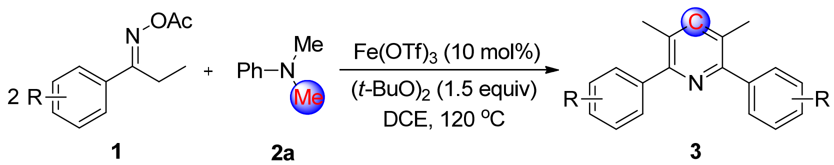
1. General information

Column chromatography was carried out on silica gel. ^{1}H NMR spectra were recorded on 400 MHz in $CDCl_3$ and ^{13}C NMR spectra were recorded on 100 MHz in $CDCl_3$. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. All new products were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Unless otherwise stated, all reagents and solvents were purchased from commercial suppliers and used without further purification.

2. Typical procedure for preparation of ketoxime carboxylates

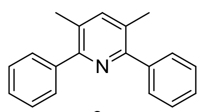
The mixture of ketoxime (3.0 mmol), anhydride (6.0 mmol, 2.0 equiv) was stirred at room temperature to 100 ^{o}C for 3h. After completion of the reaction (detected by TLC), the reaction mixture was cooled to room temperature, diluted with EtOAc (25 mL) and washed with H_2O (20 mL) and brine (10 mL). The organic layers were dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by column chromatography on silica gel to afford the ketoxime carboxylates with hexanes/ethyl acetate as the eluent.

3. Typical procedure for the synthesis of symmetrical pyridines



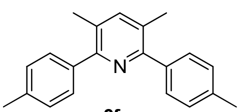
In a 25 mL round bottom flask, the ketoxime acetate **1** (0.4 mmol), *N*,*N*-dimethylaniline **2a** (0.24 mmol, 29.0 mg), (*t*-BuO)$_2$ (0.6 mmol, 87.6 mg) and $Fe(OTf)_3$ (10 mol%, 10.1 mg) was stirred in DCE (3 mL) at 120 °C oil bath. After completion of the reaction (detected by TLC), the reaction mixture was cooled to room temperature, extracted with ethyl acetate (20 mL×3) and washed with brine (20 mL). The organic layer was dried over by anhydrous Na_2SO_4 and evaporated in vacuo. The desired pyridine **3** was obtained after purification by flash chromatography on silica gel with hexanes/ethyl acetate as the eluent.

4. Spectroscopic data for symmetrical pyridines



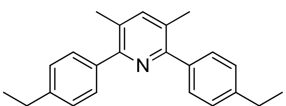
3aa

3aa: Yield 73% (37.7 mg); Yellow solid; mp 118-120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.2 Hz, 4H), 7.48 (s, 1H), 7.44-7.41 (m, 4H), 7.36 (d, *J* = 7.2 Hz, 2H), 2.38 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 141.1, 140.6, 129.2, 129.1, 128.0, 127.6, 19.6. HRMS Calcd (ESI) m/z for $C_{19}H_{18}N$: [M+H] $^+$ 260.1434. Found: 260.1433.



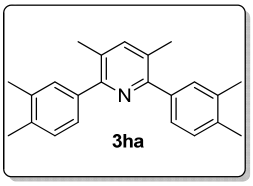
3fa

3fa: Yield 70% (40.0 mg); Yellow solid; mp 100-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.6 Hz, 4H), 7.44 (s, 1H), 7.22 (d, *J* = 7.6 Hz, 4H), 2.38 (s, 6H), 2.37 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 141.1, 137.9, 137.3, 129.1, 128.7, 128.7, 21.2, 19.7. HRMS Calcd (ESI) m/z for $C_{21}H_{22}N$: [M+H] $^+$ 288.1747. Found: 288.1751.

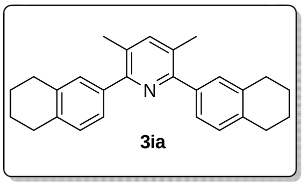


3ga

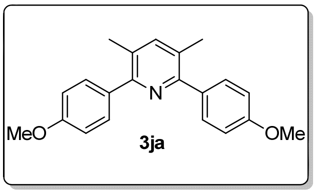
3ga: Yield 72% (53.4 mg); White solid; mp 73-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.4 Hz, 4H), 7.42 (d, *J* = 8.4 Hz, 5H), 2.38 (s, 6H), 1.33 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 150.4, 141.0, 137.9, 128.8, 128.7, 124.9, 34.5, 31.3, 19.7. HRMS Calcd (ESI) m/z for $C_{27}H_{34}N$: [M+H] $^+$ 372.2686. Found: 372.2692.



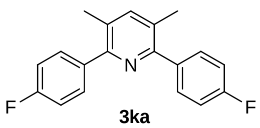
3ha: Yield 75% (47.3 mg); Yellow solid; mp 87-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (s, 1H), 7.37 (s, 2H), 7.29 (d, J = 7.6 Hz, 2H), 7.17 (d, J = 7.6 Hz, 2H), 2.36 (s, 6H), 2.30 (s, 6H), 2.29 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 140.9, 138.3, 136.2, 135.9, 130.5, 129.1, 128.6, 126.5, 19.9, 19.7, 19.6. HRMS Calcd (ESI) m/z for $C_{23}H_{26}N$: $[M+H]^+$ 316.2060. Found: 316.2061.



3ia: Yield 74% (54.3 mg); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.29-7.25 (m, 4H), 7.09 (d, J = 7.6 Hz, 2H), 2.80 (s, 8H), 2.37 (s, 6H), 1.80 (s, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 140.9, 137.9, 136.8, 136.5, 129.9, 128.6, 128.5, 126.2, 29.4, 29.2, 23.2, 19.7. HRMS Calcd (ESI) m/z for $C_{27}H_{30}N$: $[M+H]^+$ 368.2373. Found: 368.2369.

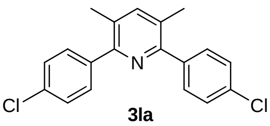


3ja: Yield 64% (40.7 mg); Yellow solid; mp 96-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.8 Hz, 4H), 7.43 (s, 1H), 6.96 (d, J = 8.8 Hz, 4H), 3.84 (s, 6H), 2.37 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 155.2, 141.2, 133.2, 130.4, 128.5, 113.3, 55.3, 19.7. HRMS Calcd (ESI) m/z for $C_{21}H_{22}NO_2$: $[M+H]^+$ 320.1645. Found: 320.1642.



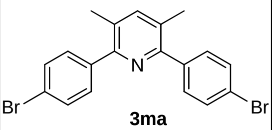
3ka

3ka: Yield 68% (40.2 mg); White solid; mp 89-91 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.53 (m, 4H), 7.48 (s, 1H), 7.14-7.09 (m, 4H), 2.36 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5 (d, J_{CF} = 245.1 Hz), 154.8, 141.3, 136.5, 130.9 (d, J_{CF} = 8.1 Hz), 129.2, 115.0 (d, J_{CF} = 21.3 Hz), 19.6. HRMS Calcd (ESI) m/z for $C_{19}H_{16}F_2N$: $[M+H]^+$ 296.1245. Found: 296.1244.



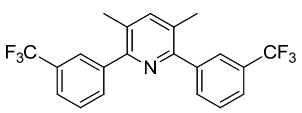
3la

3la: Yield 67% (43.8 mg); White solid; mp 138-139 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 8.4 Hz, 4H), 7.48 (s, 1H), 7.40 (d, J = 8.4 Hz, 4H), 2.37 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 141.4, 138.8, 133.8, 130.5, 129.4, 128.3, 19.6. HRMS Calcd (ESI) m/z for $C_{19}H_{16}Cl_2N$: $[M+H]^+$ 328.0654. Found: 328.0654.



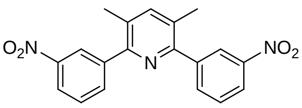
3ma

3ma: Yield 65% (54.0 mg); White solid; mp 145-146 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 8.4 Hz, 4H), 7.48 (s, 1H), 7.45 (d, J = 8.4 Hz, 4H), 2.36 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 141.5, 139.3, 131.2, 130.8, 129.4, 122.0, 19.6. HRMS Calcd (ESI) m/z for $C_{19}H_{16}Br_2N$: $[M+H]^+$ 415.9644. Found: 415.9638.



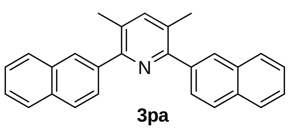
3na

3na: Yield 68% (53.4 mg); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 2H), 7.77 (d, *J* = 7.6 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.59-7.54 (m, 3H), 2.38 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 141.6, 141.0, 132.5, 130.7, 130.4, 130.0, 128.7, 126.0 (q, J_{CF} = 3.9 Hz), 124.6 (q, J_{CF} = 3.7 Hz), 19.4.



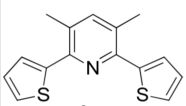
3oa

3oa: Yield 50% (35.0 mg); Yellow solid; mp 173-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 2H), 8.27 (d, *J* = 8.0 Hz, 2H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.67-7.60 (m, 3H), 2.44 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 148.0, 142.0, 141.6, 135.3, 130.5, 129.3, 124.1, 122.9, 19.5.



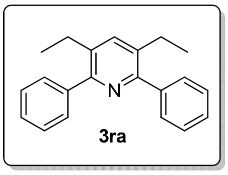
3pa

3pa: Yield 66% (47.3 mg); Yellow solid; mp 73-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 2H), 7.92-7.85 (m, 6H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.55 (s, 1H), 7.50-7.48 (m, 4H), 2.45 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 141.3, 138.0, 133.1, 132.8, 129.5, 128.3, 128.3, 127.7, 127.6, 127.3, 126.0, 126.0, 19.8. HRMS Calcd (ESI) m/z for $C_{27}H_{22}N$: $[M+H]^+$ 360.1747. Found: 360.1741.

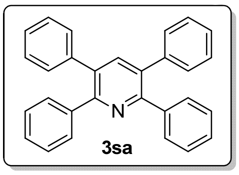


3qa

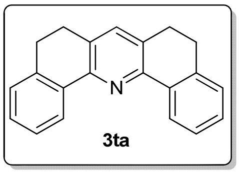
3qa: Yield 60% (32.5 mg); Yellow solid; mp 118-120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 4.8 Hz, 2H), 7.40 (d, *J* = 4.8 Hz, 2H), 7.35 (s, 1H), 7.13-7.11 (m, 2H), 2.54 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 145.7, 142.9, 127.6, 127.3, 127.2, 126.3, 20.8. HRMS Calcd (ESI) m/z for $C_{15}H_{14}NS_2$: $[M+H]^+$ 272.0562. Found: 272.0563.



3ra: Yield 58% (33.2 mg); White solid; mp 130-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.52 (m, 5H), 7.43-7.33 (m, 6H), 2.73-2.68 (m, 4H), 1.21 (t, *J* = 7.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 140.8, 137.4, 135.4, 129.1, 128.0, 127.5, 25.3, 15.3. HRMS Calcd (ESI) m/z for $C_{21}H_{22}N$: $[M+H]^+$ 288.1747. Found: 288.1745.



3sa: Yield 46% (35.2 mg); Yellow solid; mp 197-199 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.49 (s, 4H), 7.29-7.25 (m, 16H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 141.2, 139.9, 139.6, 134.3, 130.1, 129.5, 128.3, 127.8, 127.8, 127.2. HRMS Calcd (ESI) m/z for $C_{29}H_{22}N$: $[M+H]^+$ 384.1747. Found: 384.1747.



3ta: Yield 75% (42.5 mg); Yellow solid; mp 155-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 7.6 Hz, 2H), 7.41-7.37 (m, 2H), 7.31-7.28 (m, 3H), 7.23 (d, *J* = 7.2 Hz, 2H), 2.95 (s, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 137.9, 135.2, 135.0, 130.5, 128.6, 127.7, 127.0, 124.9, 28.2, 27.9. HRMS Calcd (ESI) m/z for $C_{21}H_{18}N$: $[M+H]^+$ 284.1434. Found: 284.1440.

5. General computational calculation details

Calculations were performed with Gaussian 09 program.[1] For all calculations, geometry optimizations of minima and transition states were carried out in the gas phase with the B3LYP[2] functional and the 6-31G(d) basis set for all atoms. Frequency analyses were carried out at the same level to verify all of the stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency) and to evaluate the zero-point vibrational energy and thermal corrections at 298 K.

Cartesian coordinates of optimized structures

acetophenone oxime acetate coordinates with two $FeCl_2$

C	-4.37347500	2.60398200	0.56071000
C	-2.98741100	2.48141900	0.54654600
C	-2.37598500	1.50775100	-0.26138700
C	-3.17982800	0.67656700	-1.07324900
C	-4.56867100	0.81775600	-1.06031700
C	-5.16568300	1.77281800	-0.23723500
H	-4.83836100	3.34628500	1.20208700
H	-2.38344200	3.11368200	1.18880500
H	-2.72067500	-0.01104100	-1.77934300
H	-5.17563400	0.18516400	-1.70040100
H	-6.24629800	1.87767200	-0.22319000
C	-0.91158400	1.31601800	-0.21300300
N	-0.55327000	0.06885600	-0.31909600
C	0.02730900	2.45616800	0.02126600
H	-0.45157700	3.40669900	-0.21593400
H	0.32696000	2.46383300	1.07818300
H	0.95035700	2.35115700	-0.55559800
O	0.87047300	-0.08136300	-0.21645900
C	1.47628000	-0.88057700	-1.11675200
O	2.69123500	-1.01284200	-0.97089000
C	0.70690300	-1.52824300	-2.21587500

H	-0.05015500	-2.21446900	-1.81776100
H	0.17657100	-0.76906900	-2.80051600
H	1.40571600	-2.07016000	-2.85259300
Cl	-2.36917200	-2.98858300	-0.94133500
Cl	-2.34754400	-0.88081900	2.54570600
Fe	-2.04128800	-1.27509800	0.41390300
Fe	4.01373300	0.17882200	0.02507500
Cl	3.65234100	2.18563100	-0.81717600
Cl	5.25349600	-0.80134000	1.51227900

A with $[FeCl_2]^+$

C	-4.54493000	0.05610400	0.00011800
C	-3.41274600	0.86955600	-0.00055600
C	-2.12759500	0.30252900	-0.00039600
C	-2.00550500	-1.09814800	0.00046300
C	-3.13492100	-1.90810200	0.00112000
C	-4.40948300	-1.33253800	0.00095000
H	-5.53230000	0.50874900	-0.00000600
H	-3.53785000	1.94700300	-0.00120500
H	-1.01442200	-1.53952200	0.00059800
H	-3.02416000	-2.98857000	0.00176500
H	-5.29245800	-1.96552400	0.00147400
C	-0.90584100	1.15673600	-0.00109100
N	0.26043300	0.65599400	-0.00081700
C	-1.06094200	2.66868400	-0.00216500
H	-1.61557200	2.99722800	-0.88831400
H	-1.61534100	2.99853000	0.88364300
H	-0.07890900	3.14372600	-0.00262700
Cl	2.90767100	-0.40686000	-1.91372600
Cl	2.90654500	-0.40335700	1.91495100
Fe	1.94838800	-0.00803100	-0.00004200

Fe(OAc)Cl_2

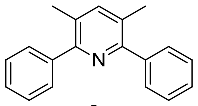
O	-1.23533400	-0.00231000	-1.08492900
C	-1.90991300	-0.00421700	0.00763000
O	-1.23418600	-0.00445500	1.09630000
C	-3.40376100	-0.00147200	-0.00116600
H	-3.75596700	0.90749100	-0.50038400
H	-3.76224200	-0.85541000	-0.58470500
H	-3.79396400	-0.04567100	1.01601000
Fe	0.43864100	0.00005000	-0.00119300
Cl	1.52000500	-1.86361400	-0.00118100
Cl	1.51209500	1.86835300	-0.00056300

Reference

(1) Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

(2) (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652. (b) C. Lee, W. Yang, R. G. Parr, *Physical Review B Condensed Matter and Materials Physics*, 1988, **37**, 785-789.

6. Appendix (copies of ^{1}H and ^{13}C NMR spectra)



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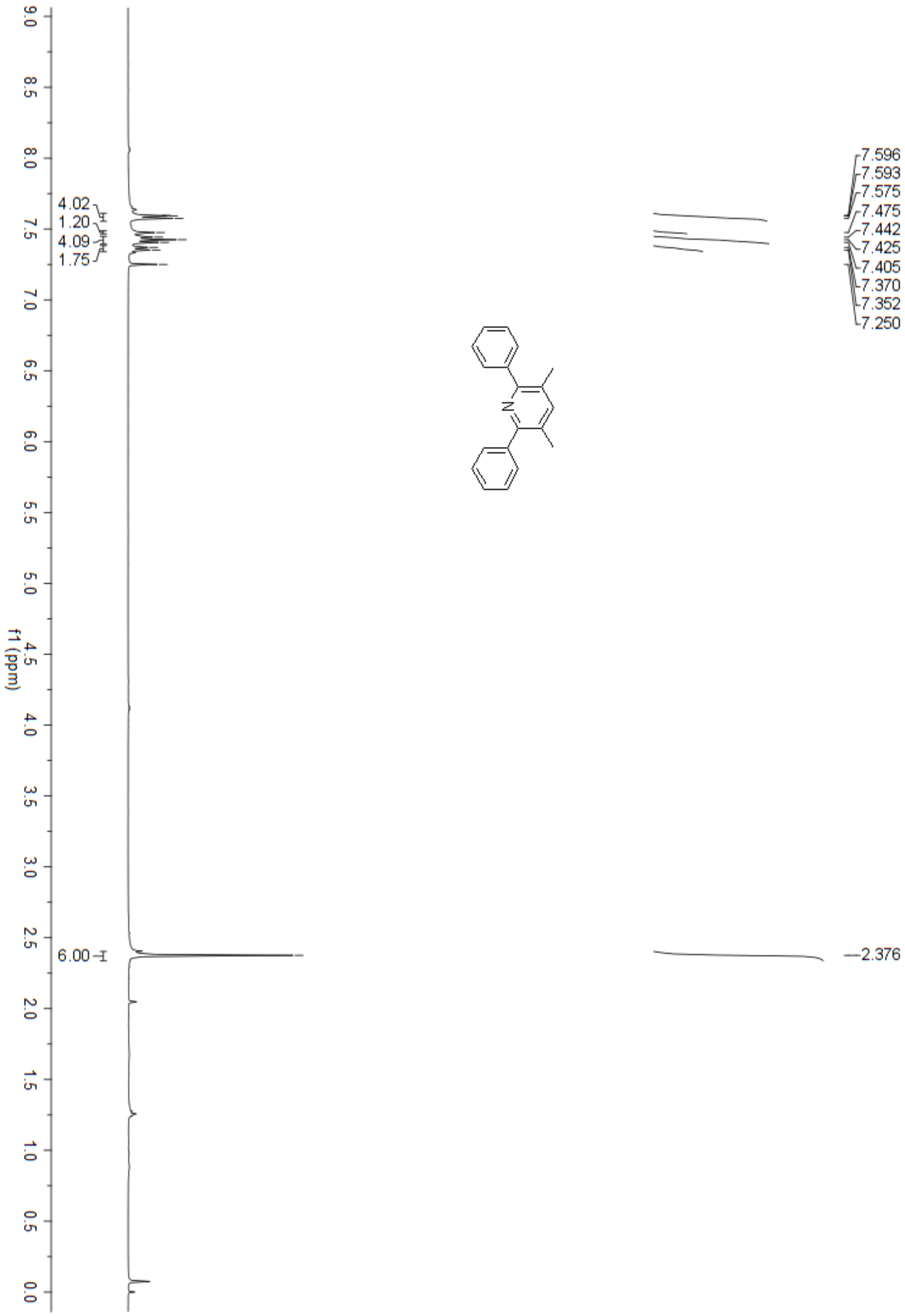
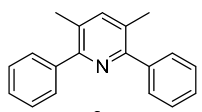
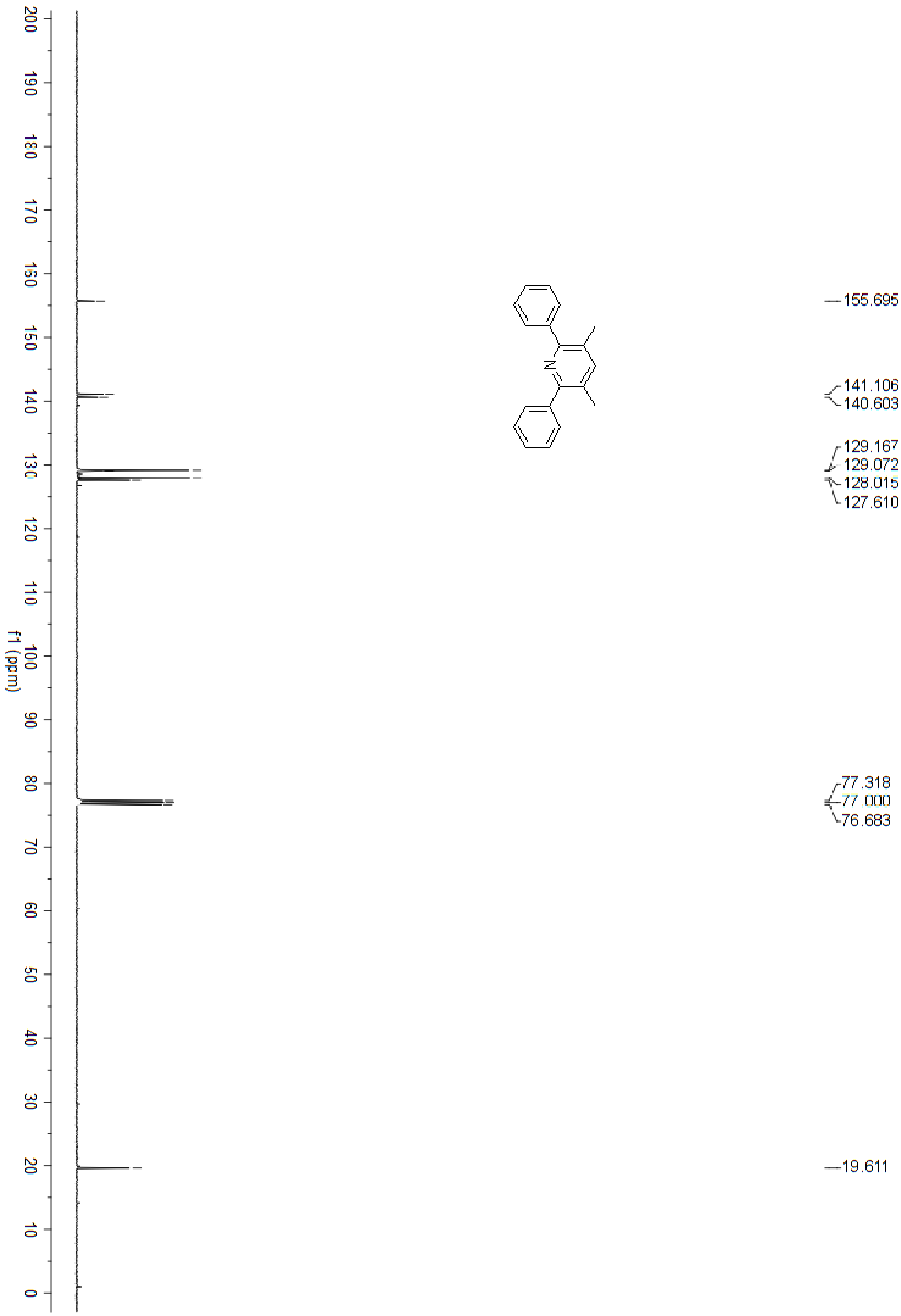
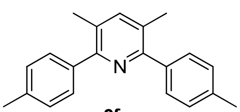


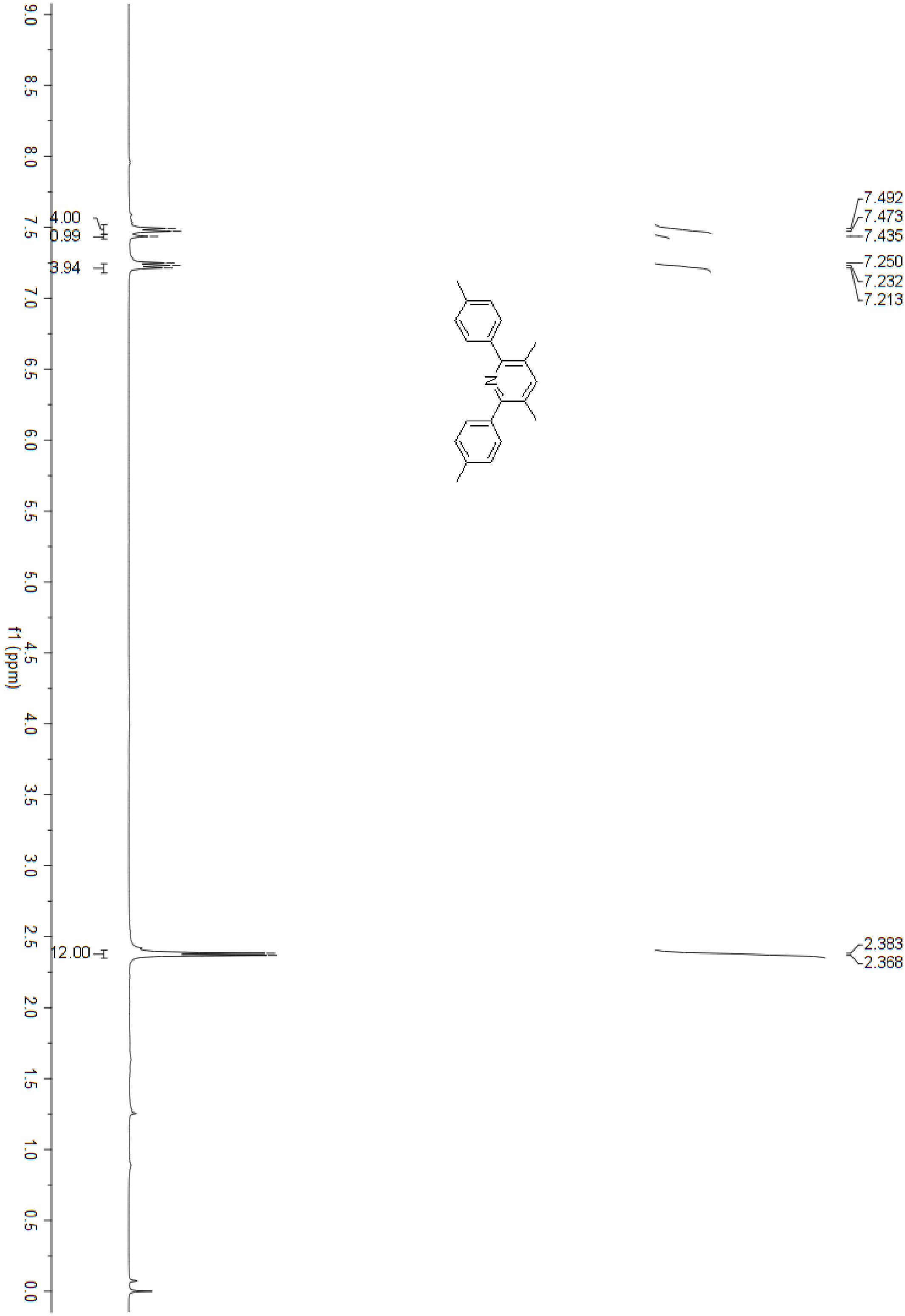


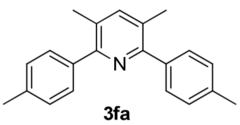
3aa


155.695
141.106
140.603
129.167
129.072
128.015
127.610
77.318
77.000
76.683
19.611
f1 (ppm)

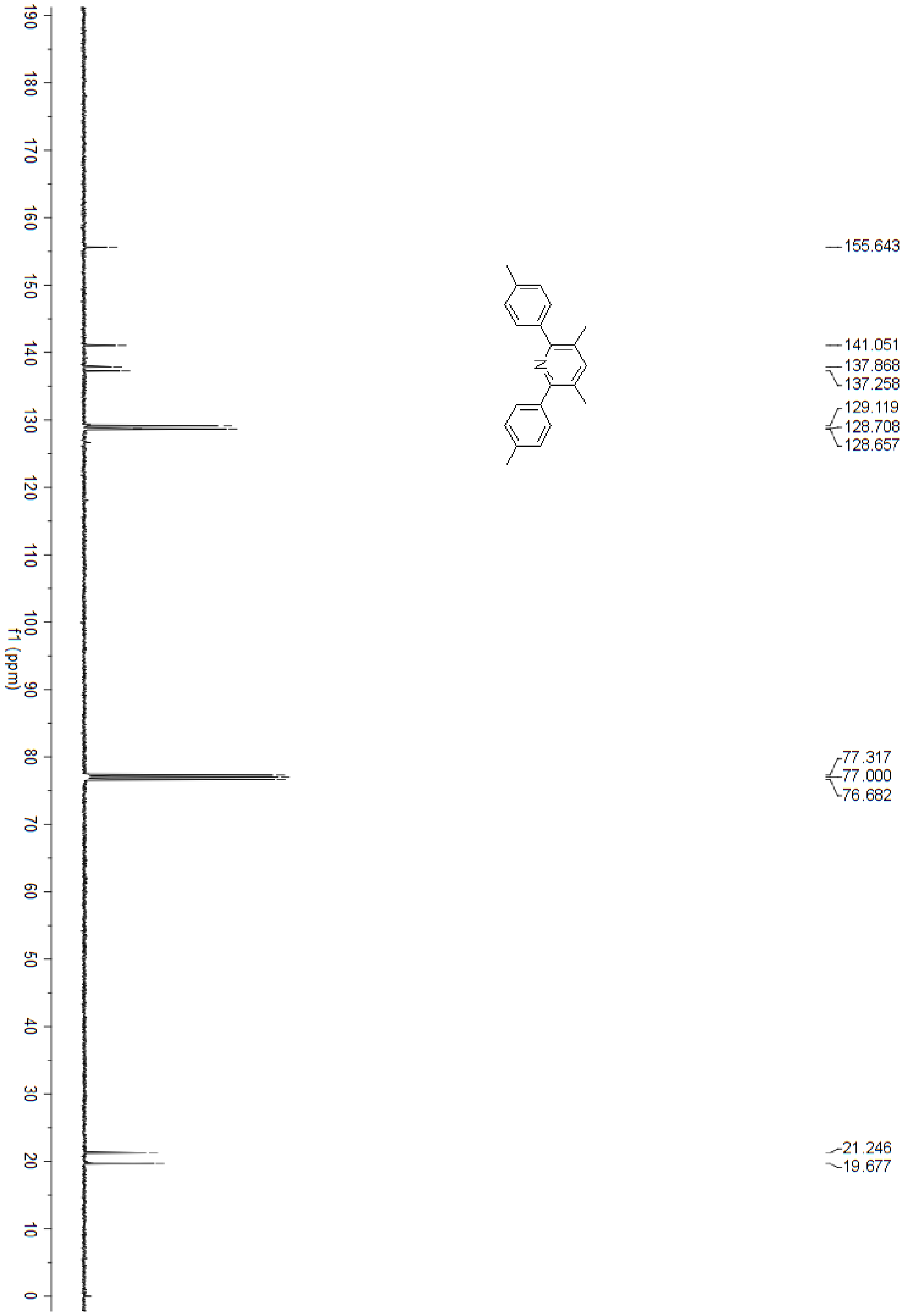


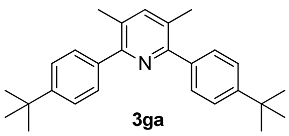
3fa


7.492
7.473
7.435
7.250
7.232
7.213
2.383
2.368
4.00
0.99
3.94
12.00
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
f1 (ppm)
N

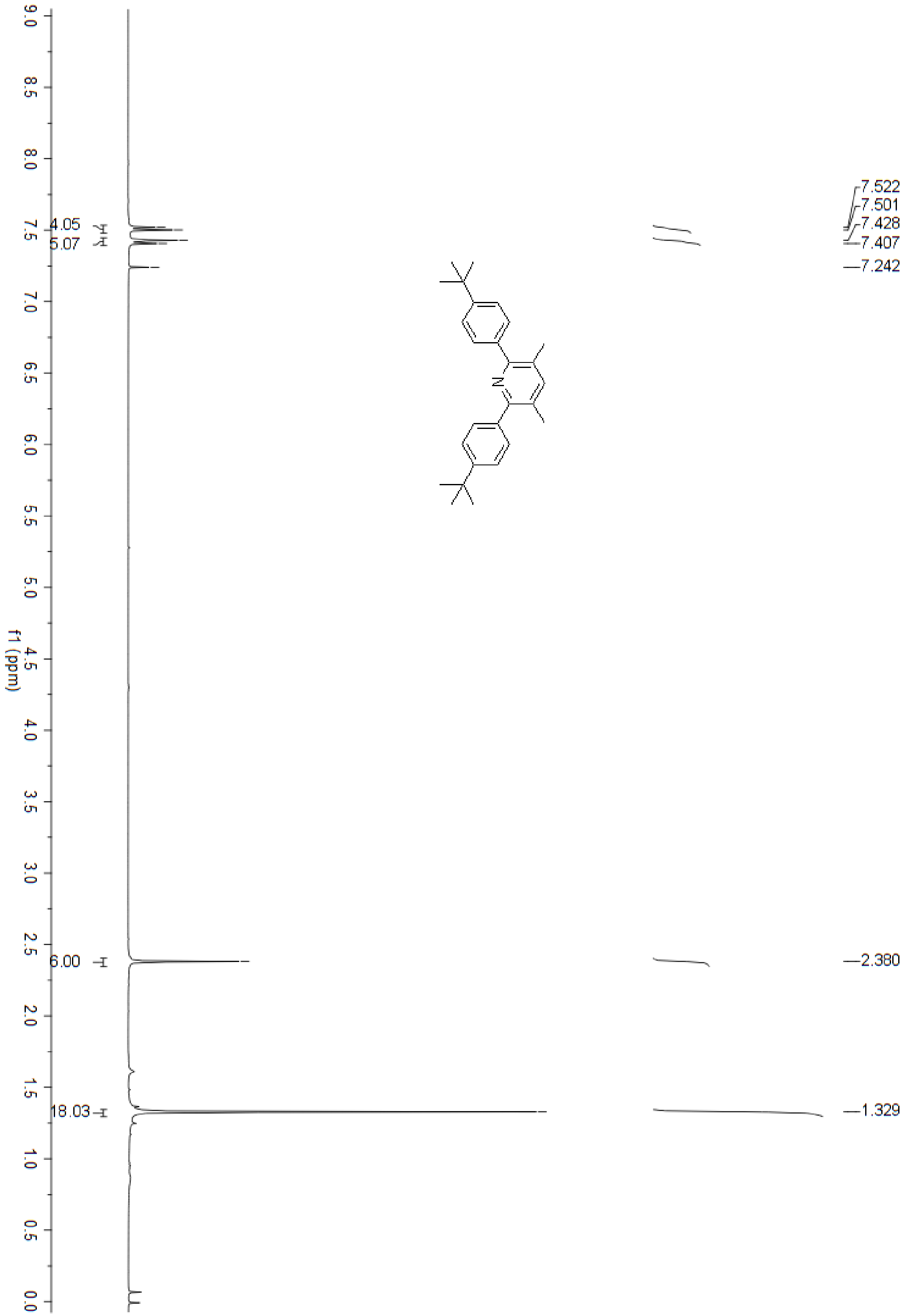


3fa

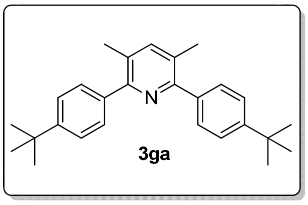

155.643
141.051
137.868
137.258
129.119
128.708
128.657
77.317
77.000
76.682
21.246
19.677
f1 (ppm)



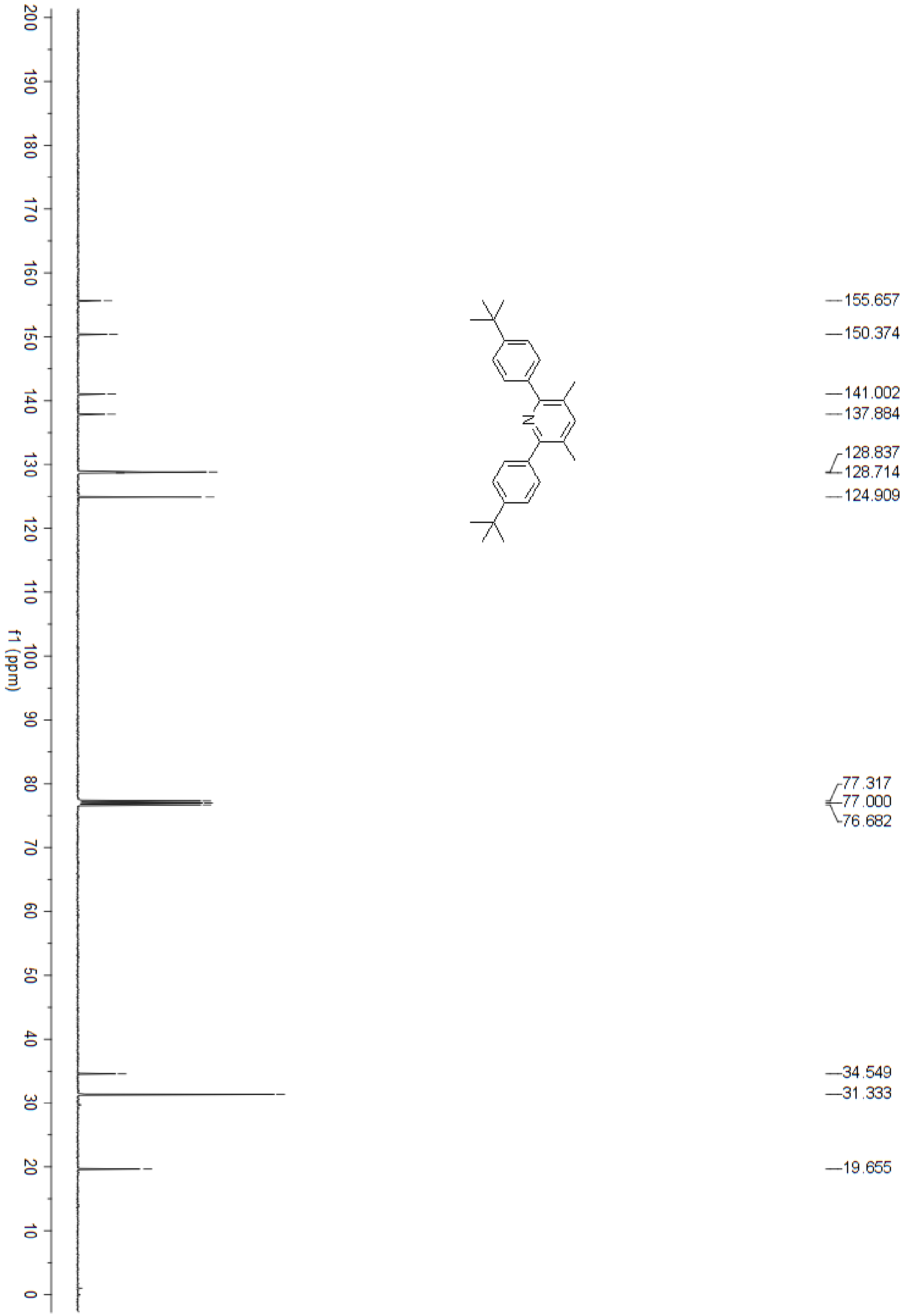
3ga



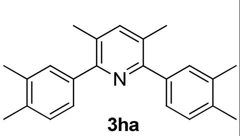
7.522
7.501
7.428
7.407
7.242
2.380
1.329
4.05
5.07
6.00
18.03
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0



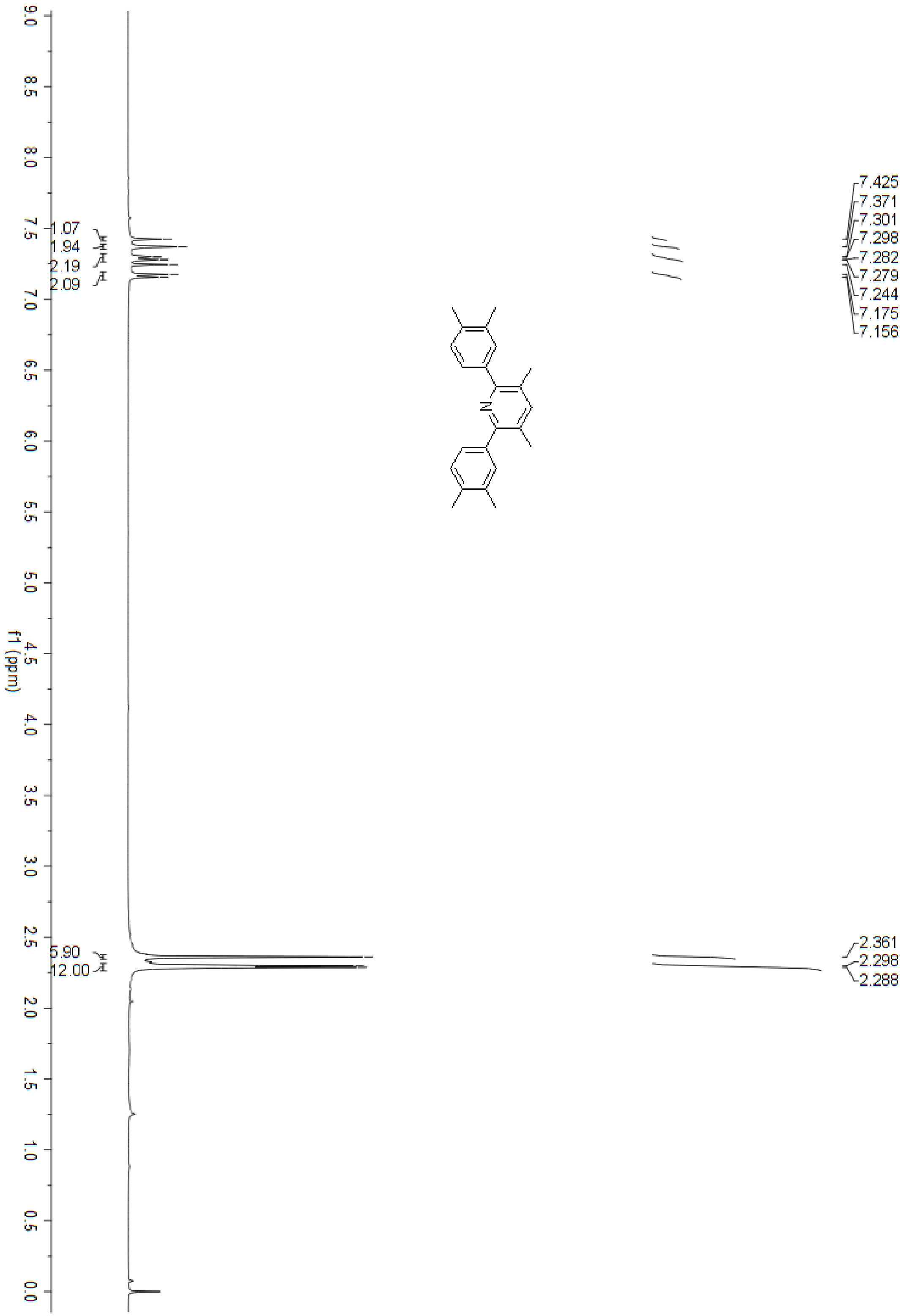
3ga



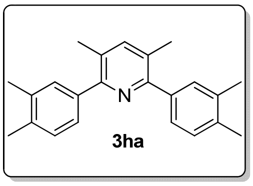
155.657
150.374
141.002
137.884
128.837
128.714
124.909
77.317
77.000
76.682
34.549
31.333
19.655
f1 (ppm)



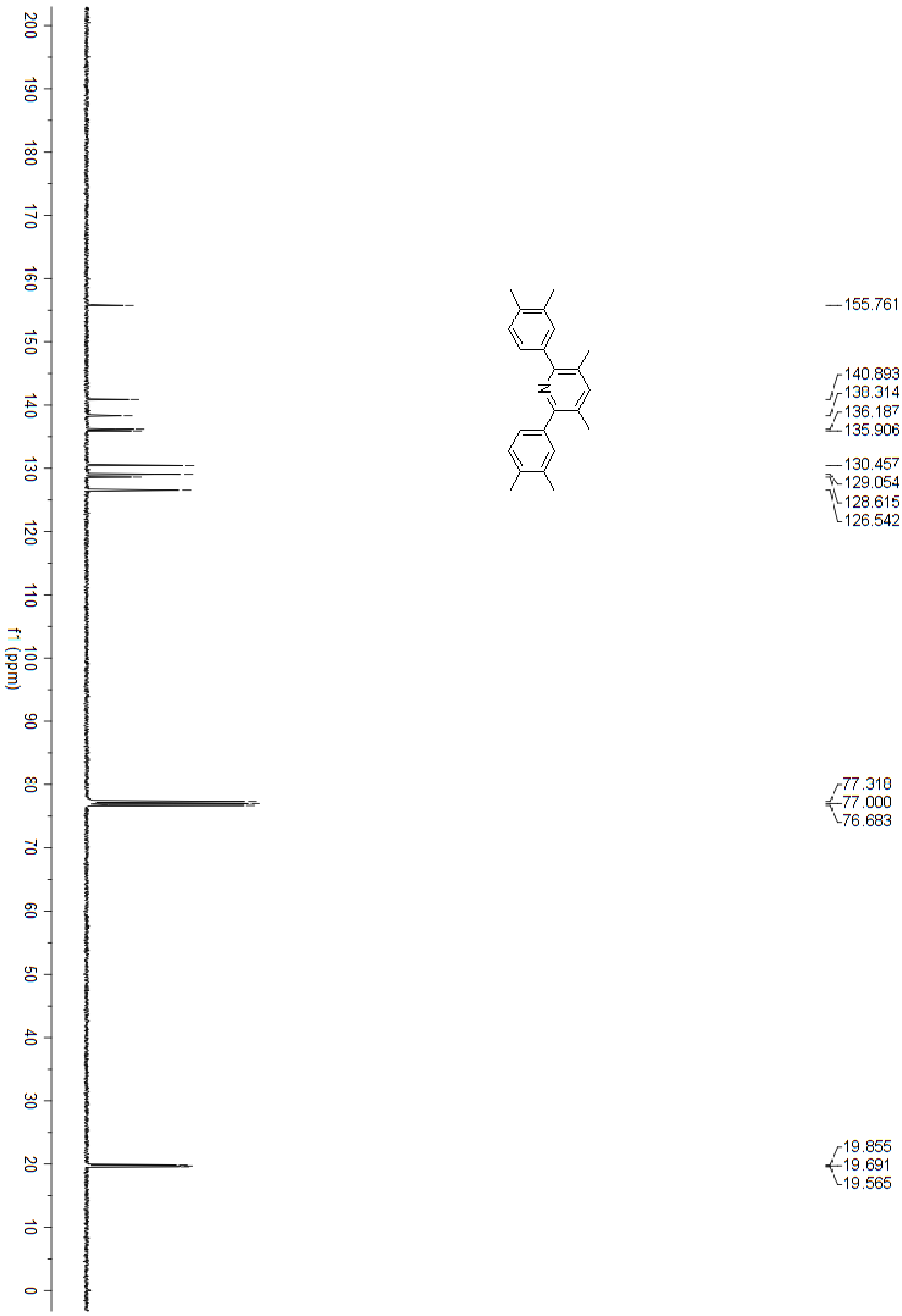
3ha

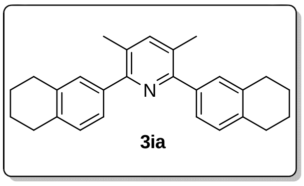


7.425
7.371
7.301
7.298
7.282
7.279
7.244
7.175
7.156
2.361
2.298
2.288
1.07
1.94
2.19
2.09
5.90
12.00
f1 (ppm)

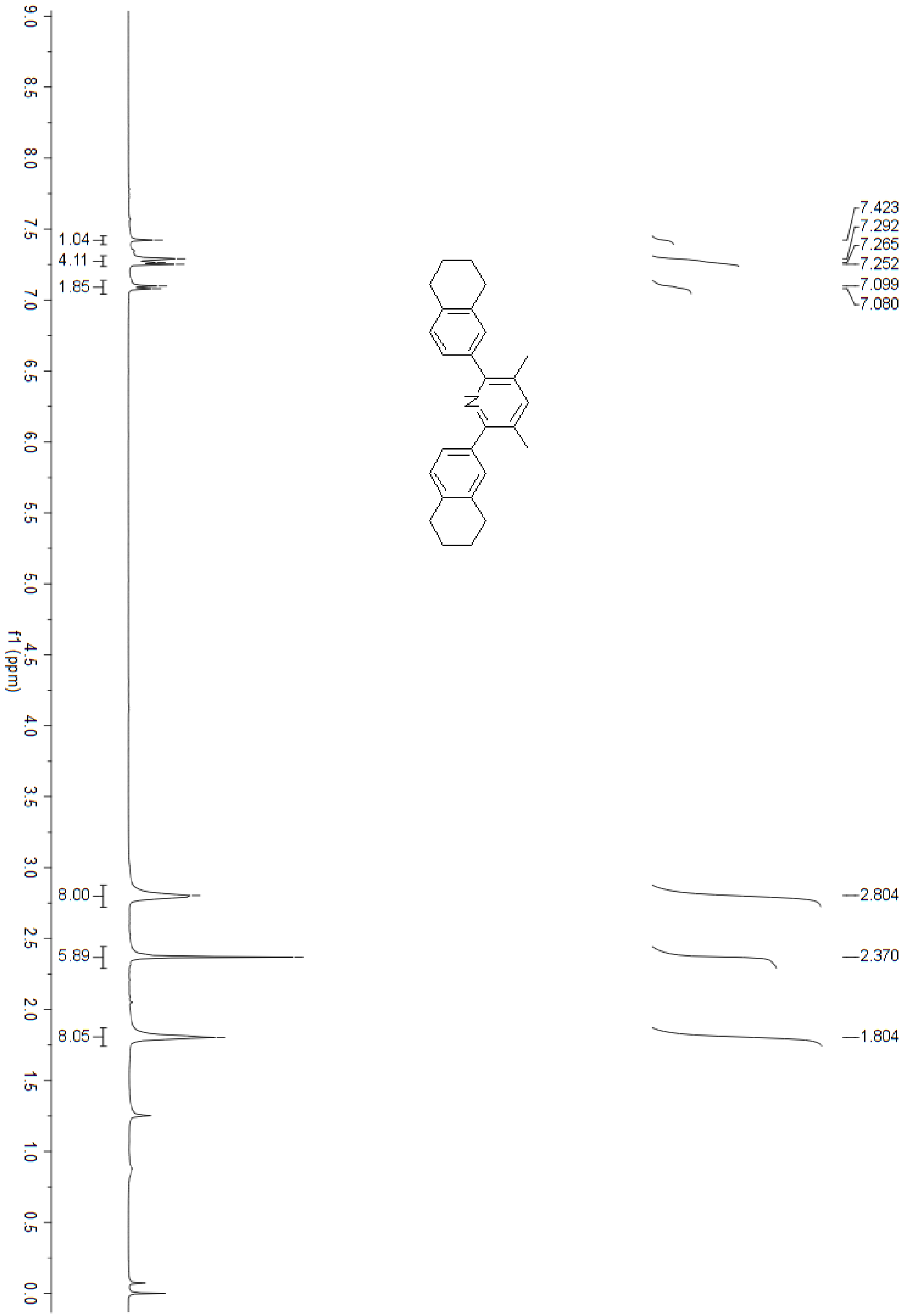

N

3ha

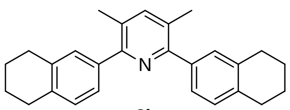

f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
N
155.761
140.893
138.314
136.187
135.906
130.457
129.054
128.615
126.542
77.318
77.000
76.683
19.855
19.691
19.565



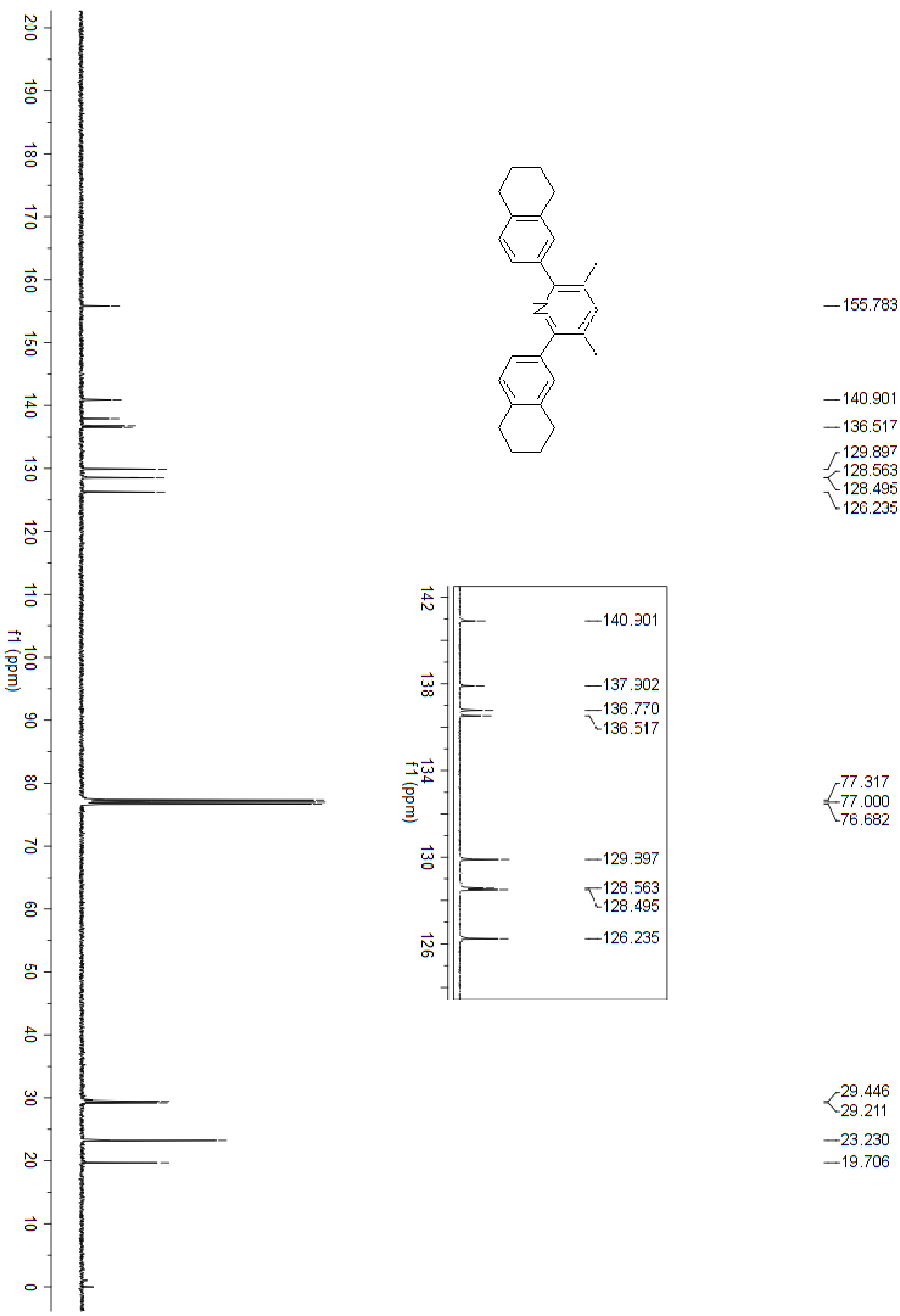
3ia

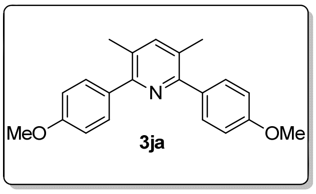


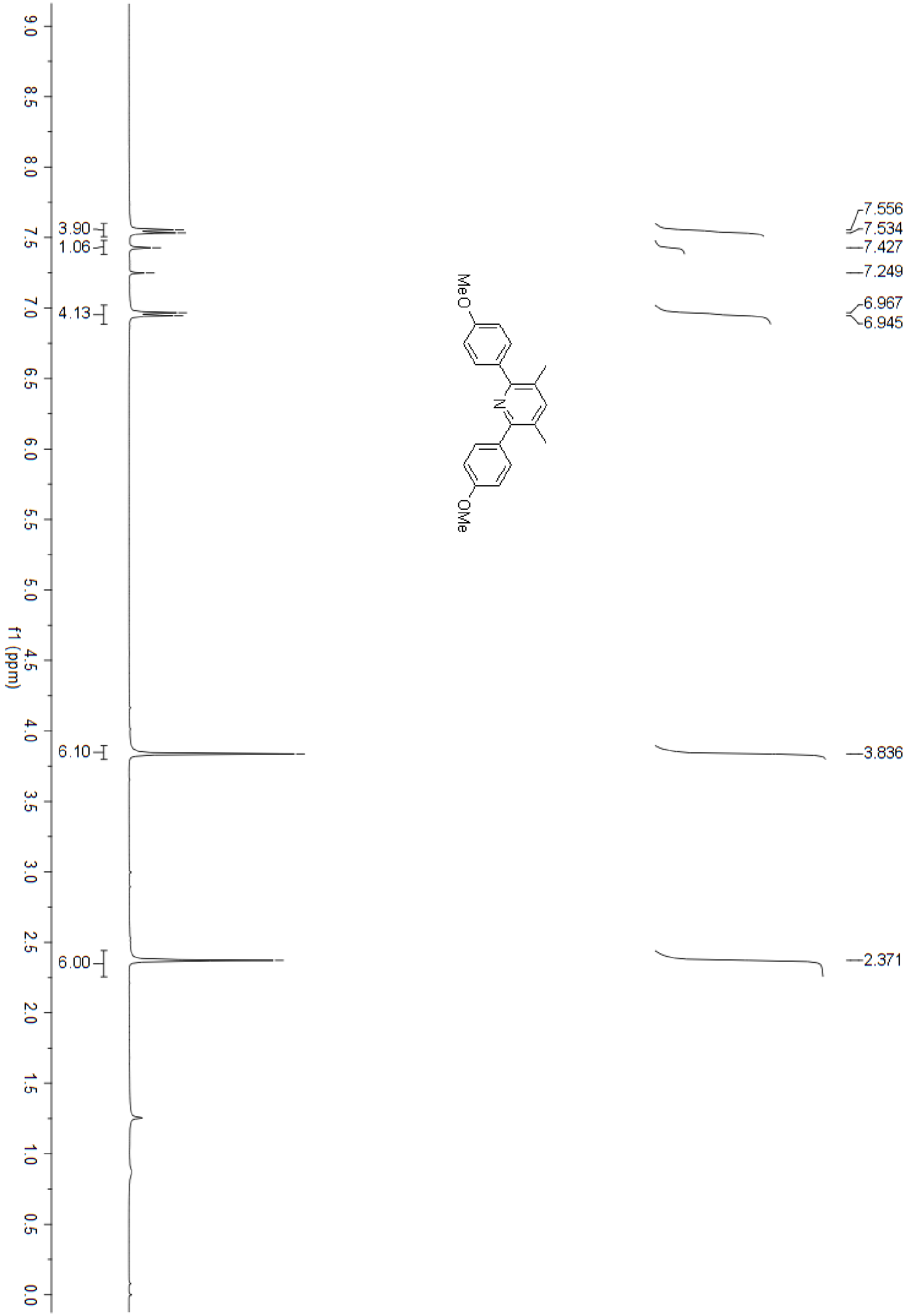
7.423
7.292
7.265
7.252
7.099
7.080
2.804
2.370
1.804
1.04
4.11
1.85
8.00
5.89
8.05
f1 (ppm)

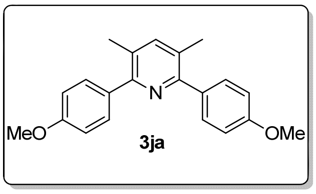


3ia

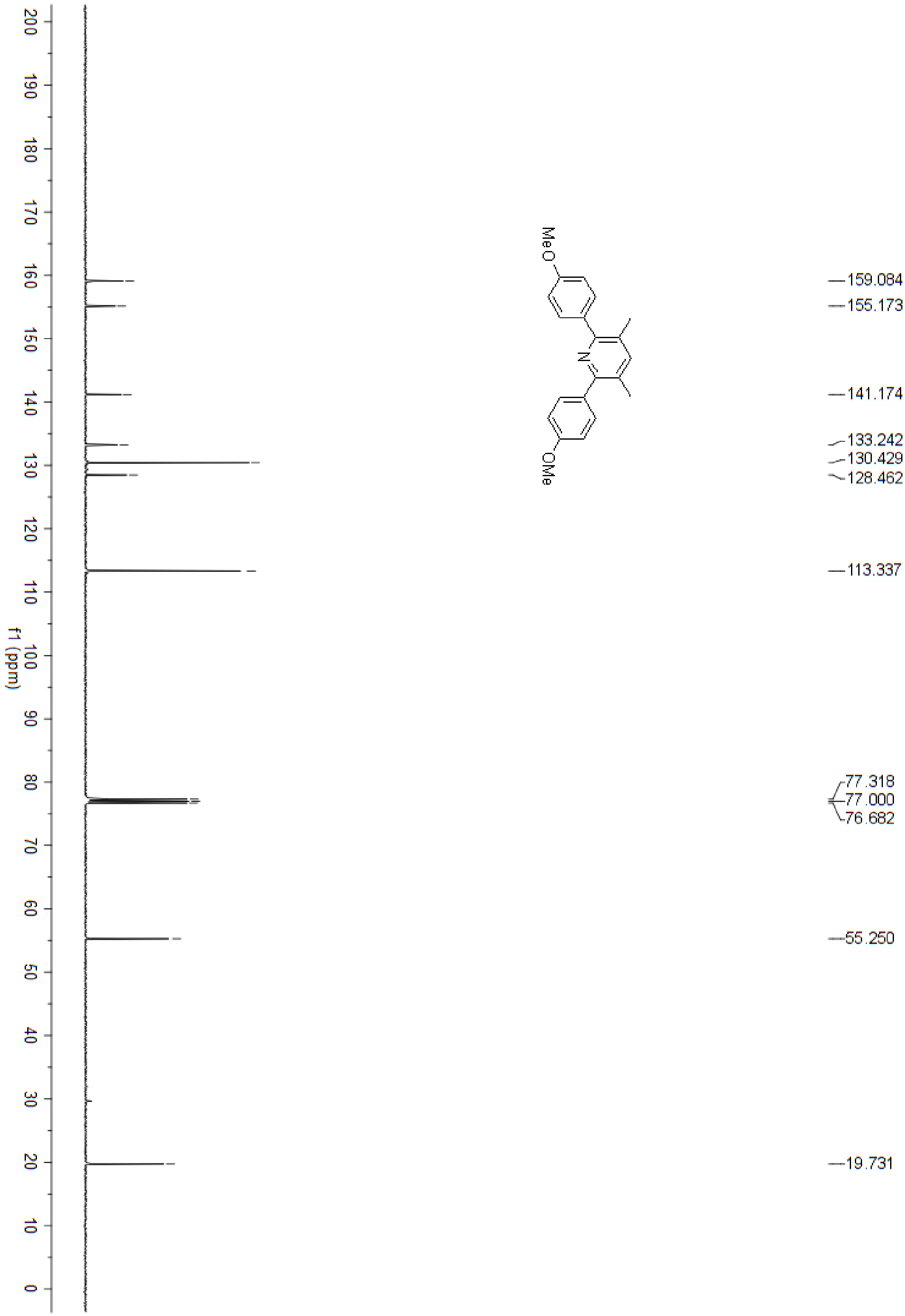

155.783
140.901
136.517
129.897
128.563
128.495
126.235
77.317
77.000
76.682
29.446
29.211
23.230
19.706
140.901
137.902
136.770
136.517
129.897
128.563
128.495
126.235
f1 (ppm)

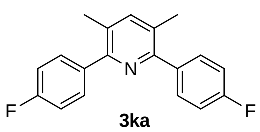

MeO
OMe
N
3ja


7.556
7.534
7.427
7.249
6.967
6.945
3.836
2.371
3.90
1.06
4.13
6.10
6.00
f1 (ppm)
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
MeO
OMe
N

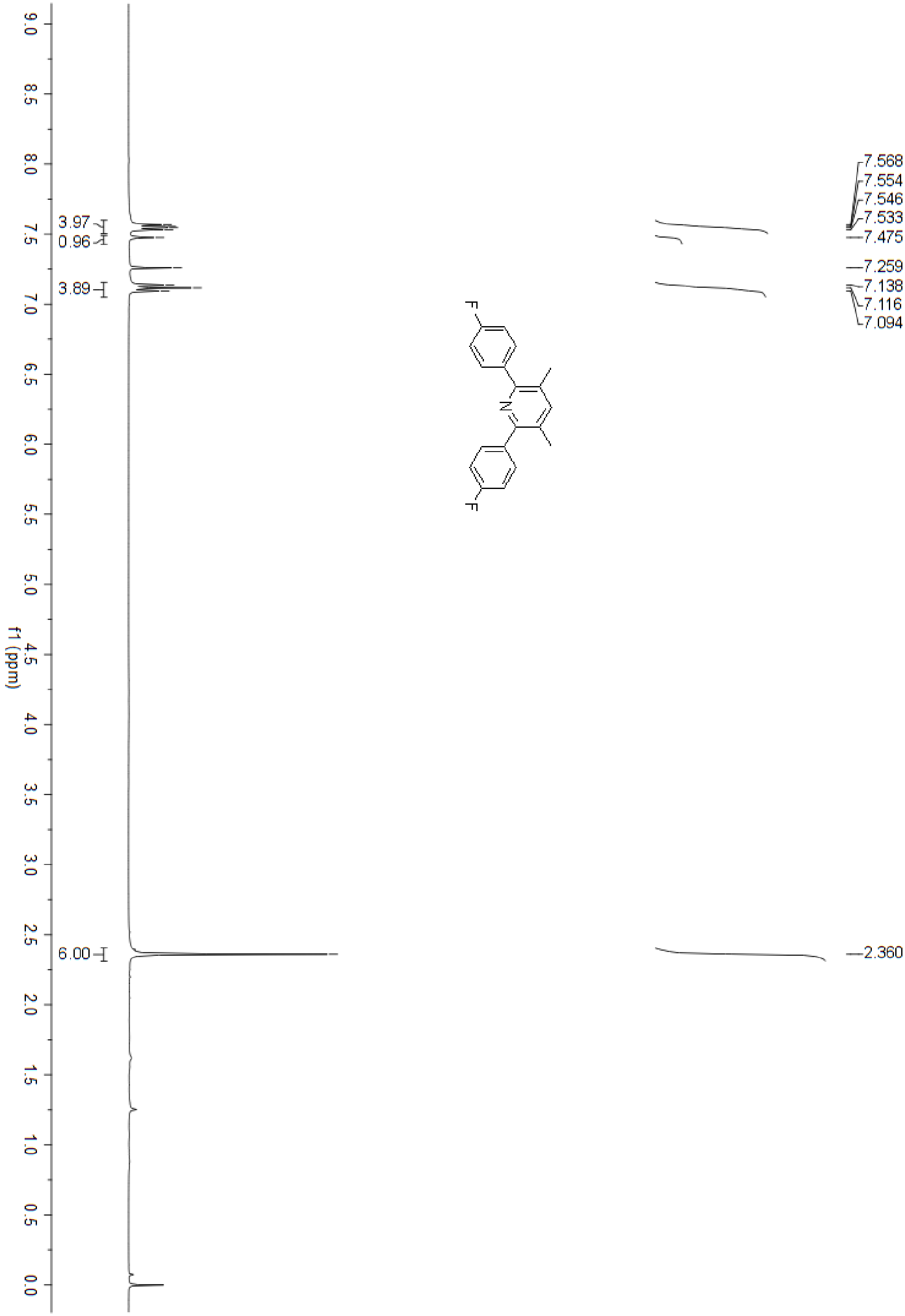

MeO
N
OMe

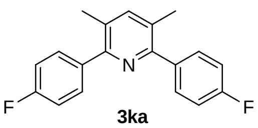
3ja


159.084
155.173
141.174
133.242
130.429
128.462
113.337
77.318
77.000
76.682
55.250
19.731
f1 (ppm)

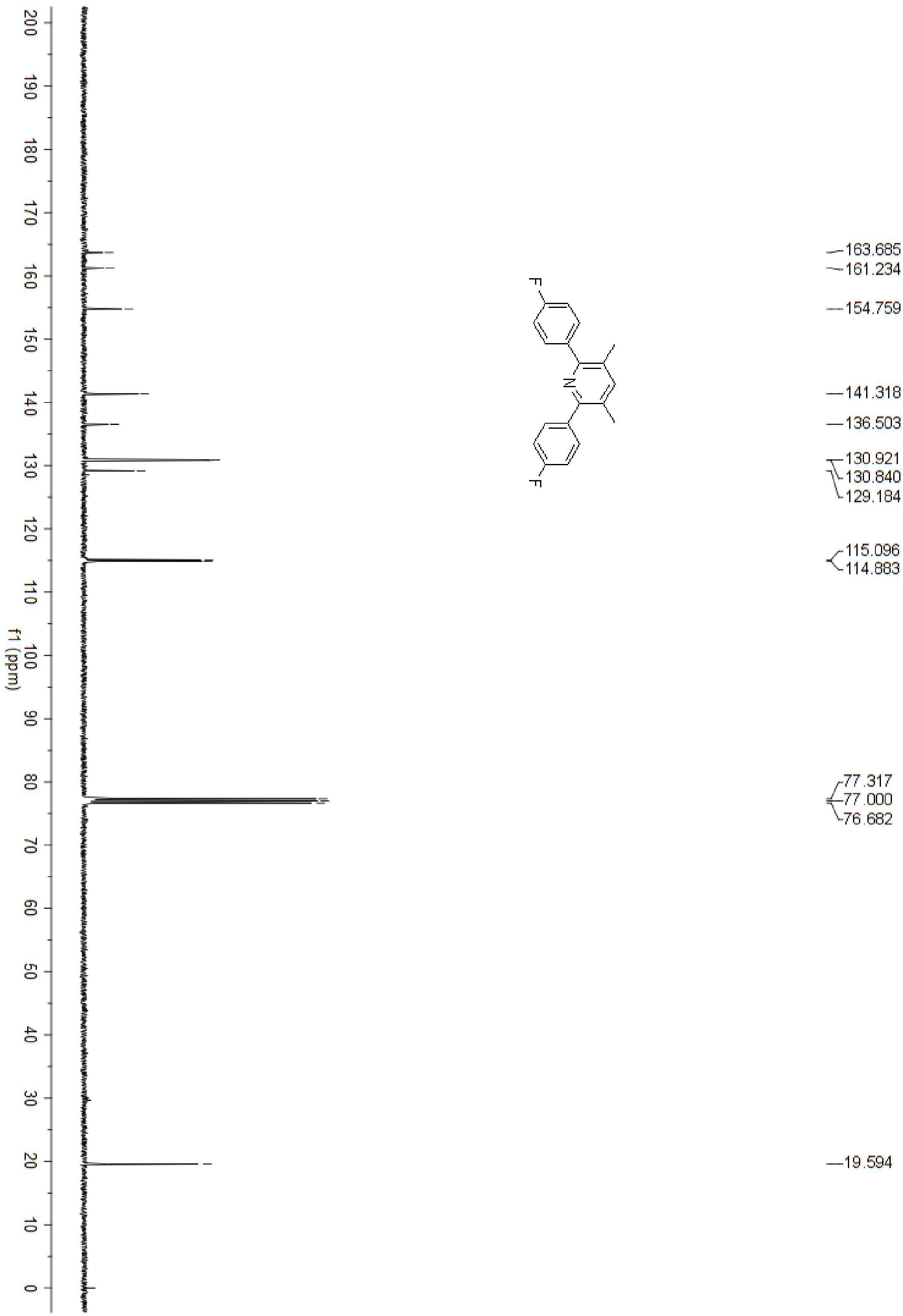

N
F
F

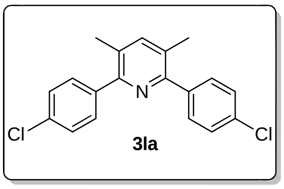
3ka


7.568
7.554
7.546
7.533
7.475
7.259
7.138
7.116
7.094
2.360
3.97
0.96
3.89
6.00
f1 (ppm)

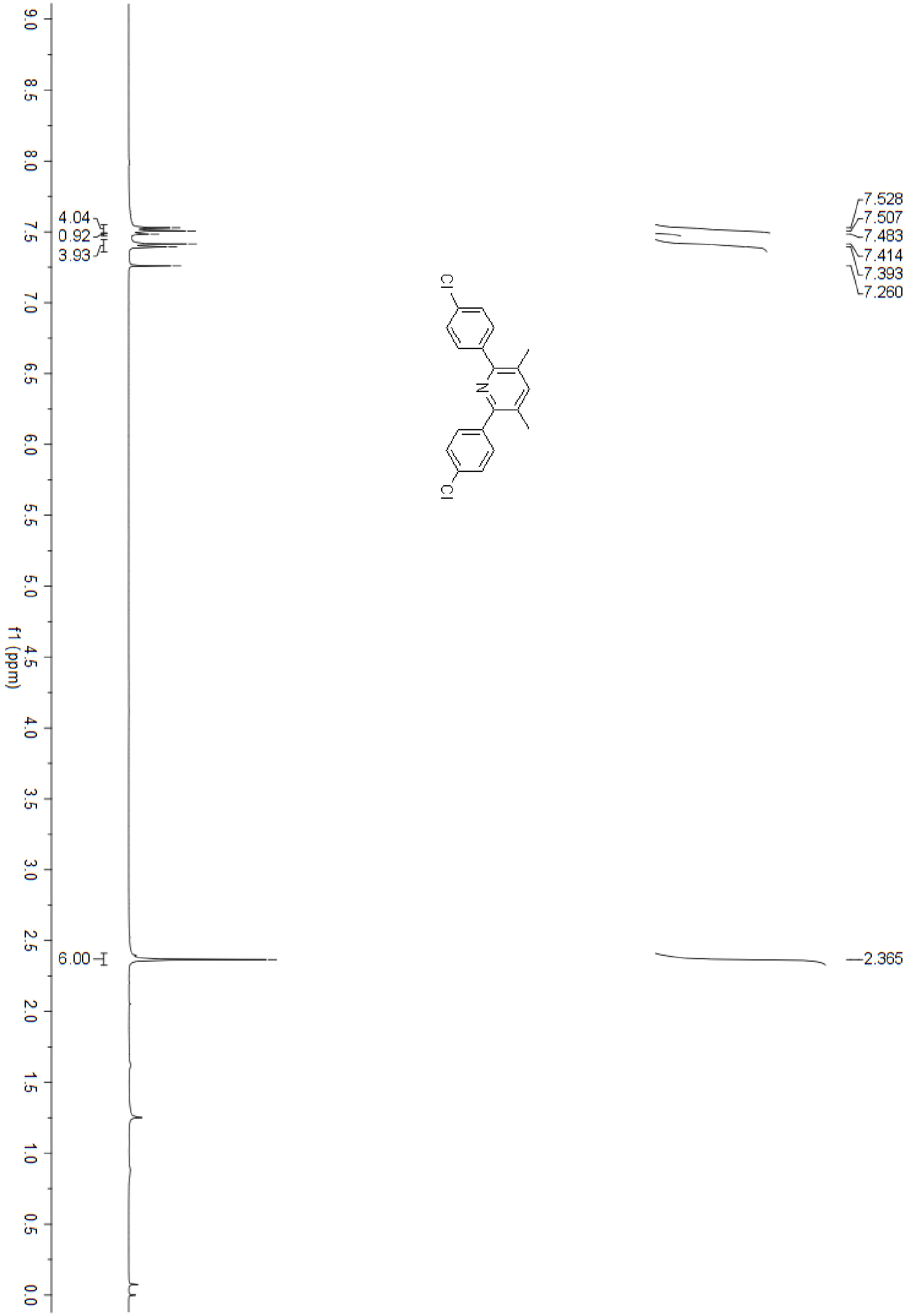


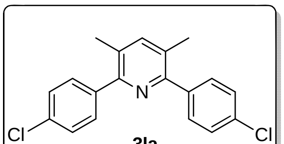
3ka


163.685
161.234
154.759
141.318
136.503
130.921
130.840
129.184
115.096
114.883
77.317
77.000
76.682
19.594
f1 (ppm)


Cl
N
Cl

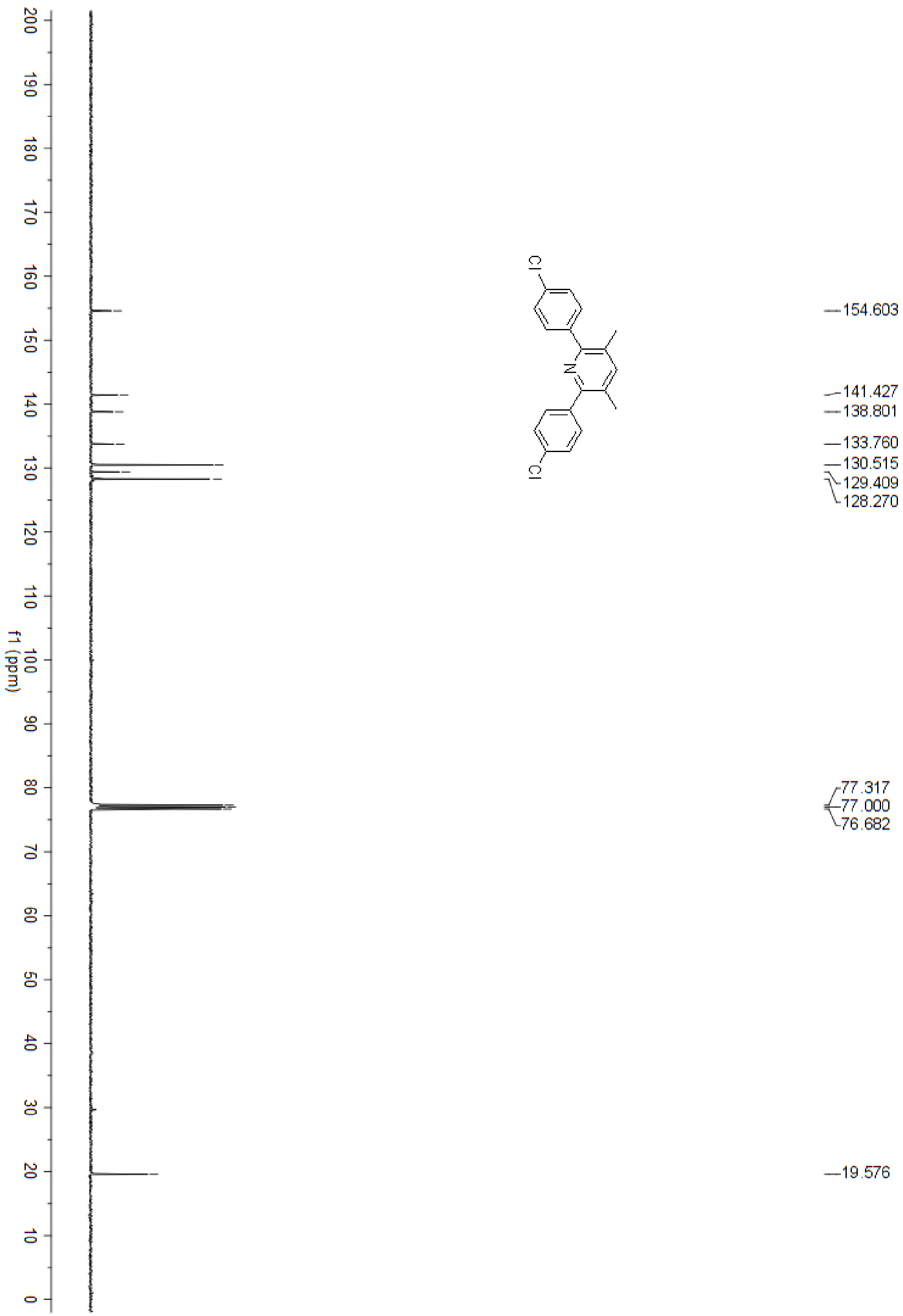
3la


7.528
7.507
7.483
7.414
7.393
7.260
2.365
4.04
0.92
3.93
6.00
f1 (ppm)
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
Cl
N
Cl



N
Cl
Cl

3la



154.603
141.427
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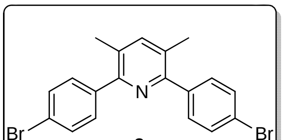
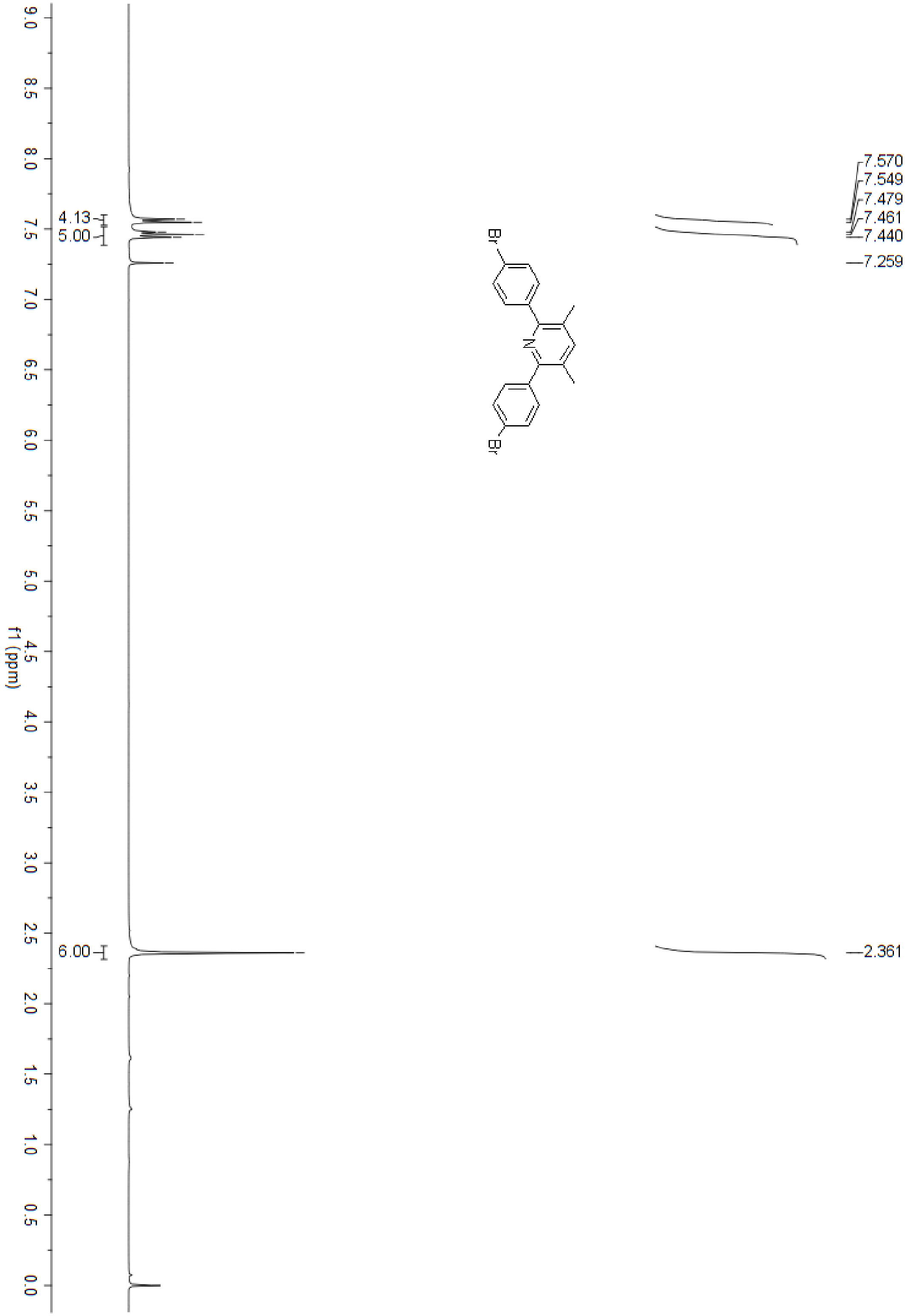
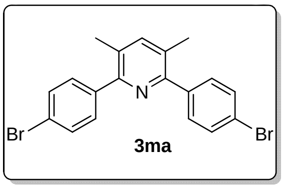
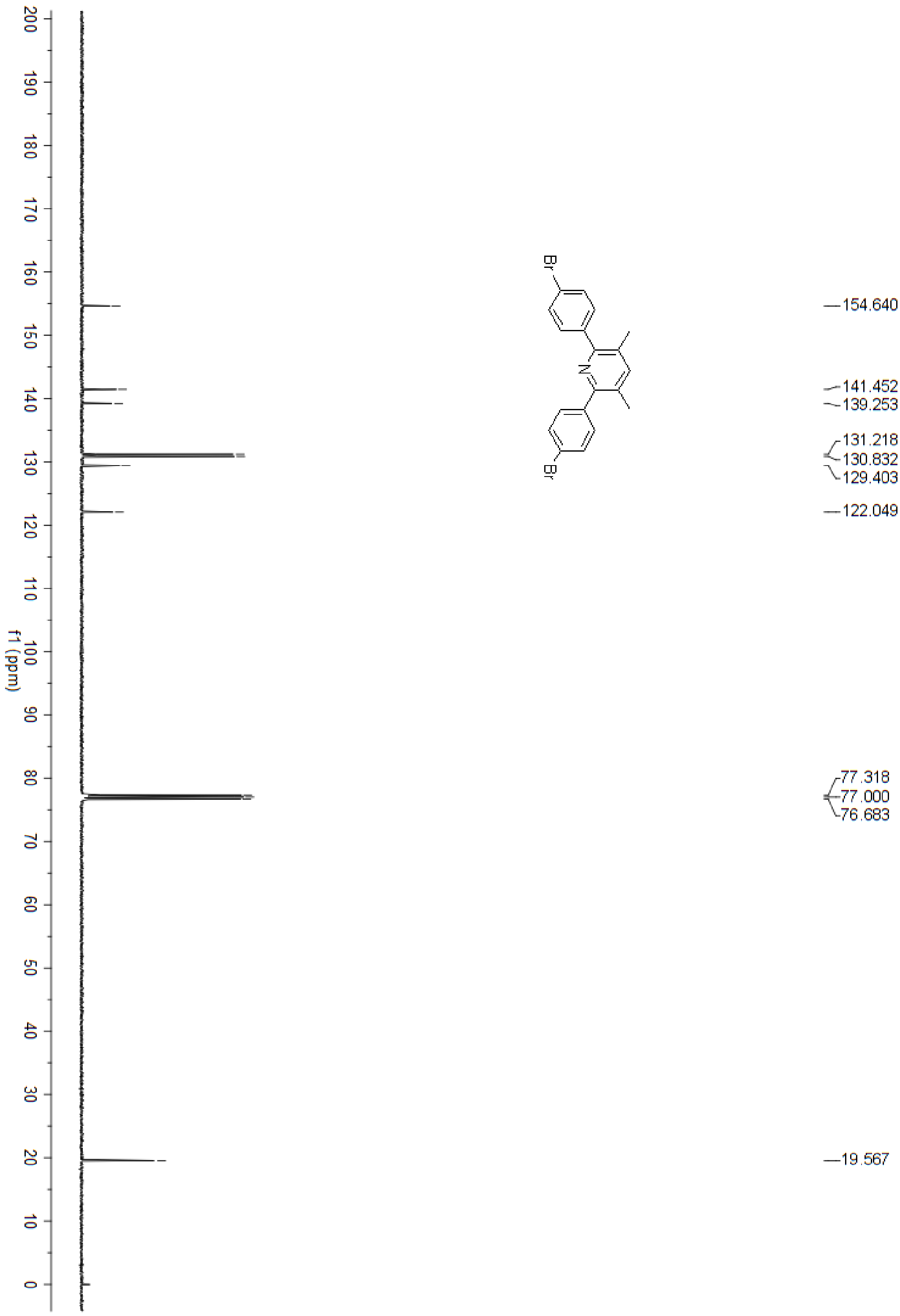
133.760
130.515
129.409
128.270
77.317
77.000
76.682
19.576
f1 (ppm)

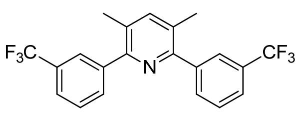

N
Br
Br

3ma

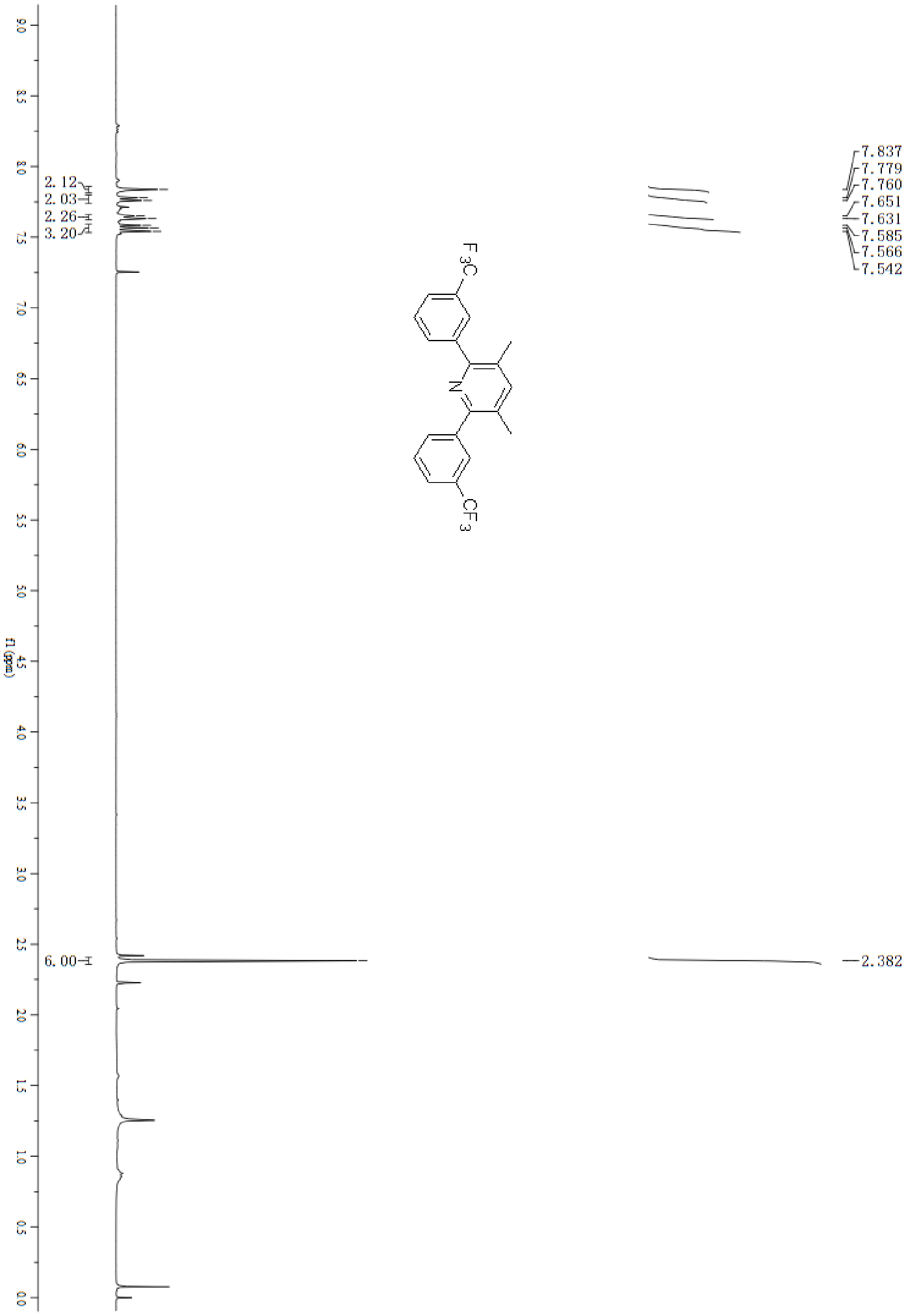

7.570
7.549
7.479
7.461
7.440
7.259
2.361
4.13
5.00
6.00
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

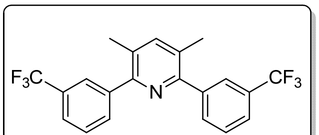

N
Br
Br
3ma


200
190
180
170
160
150
140
130
120
110
100
f1 (ppm)
90
80
70
60
50
40
30
20
10
0
Br
N
Br
154.640
141.452
139.253
131.218
130.832
129.403
122.049
77.318
77.000
76.683
19.567

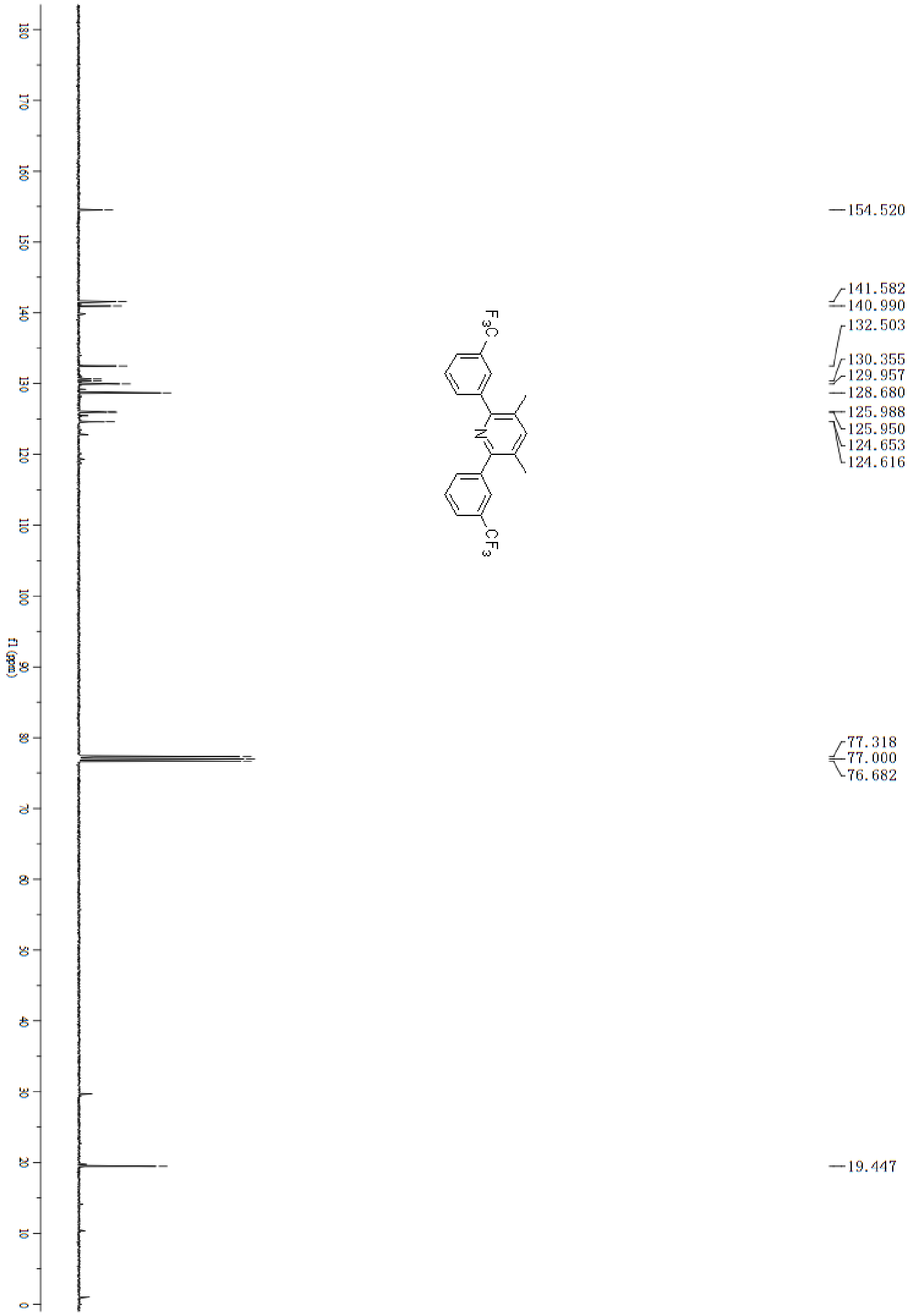

F3C
N
CF3

3na


7.837
7.779
7.760
7.651
7.631
7.585
7.566
7.542
2.382
2.12
2.03
2.26
3.20
6.00
f1 (ppm)


F3C
N
CF3

3na


154.520
141.582
140.990
132.503
130.355
129.957
128.680
125.988
125.950
124.653
124.616
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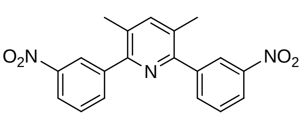
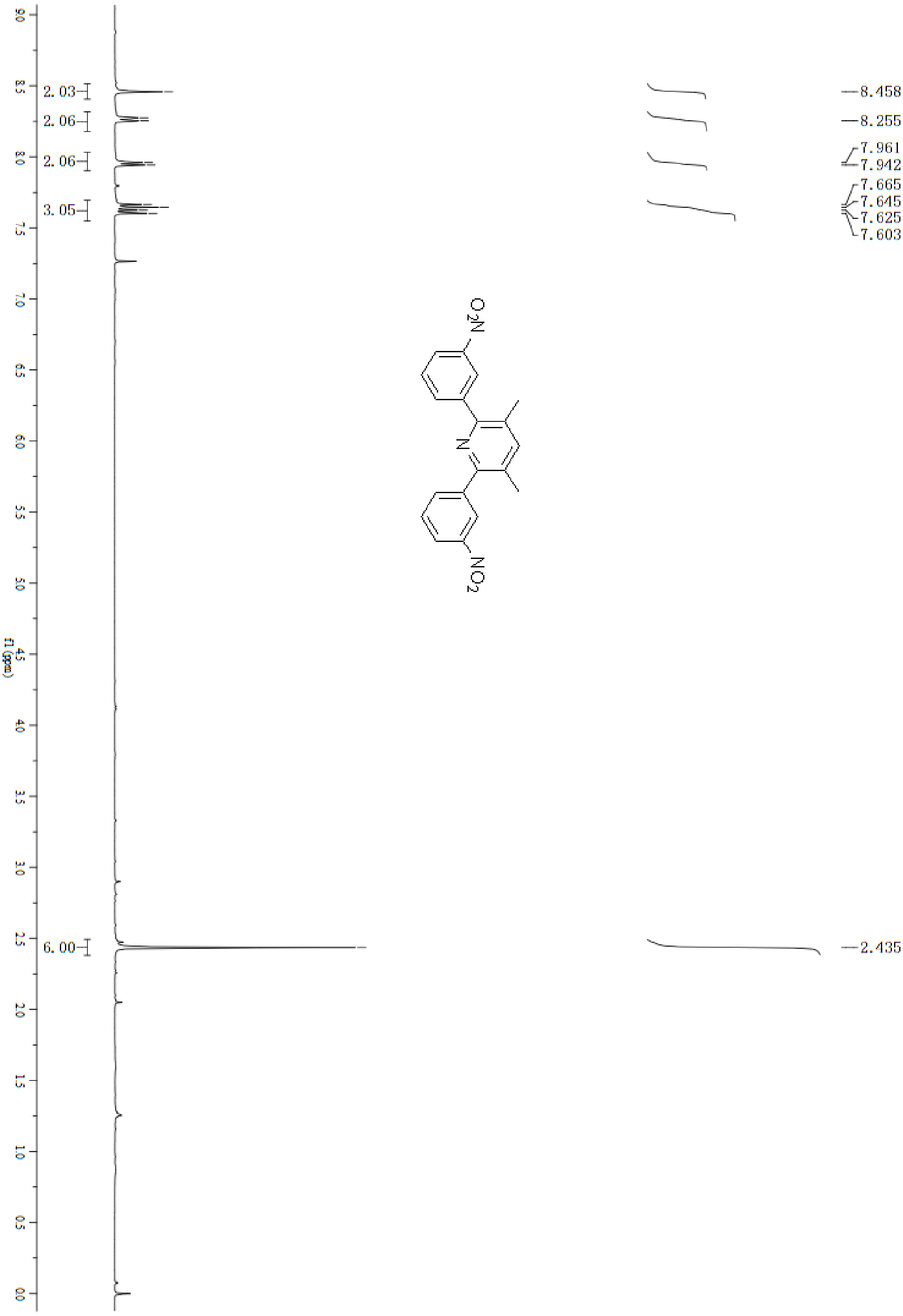
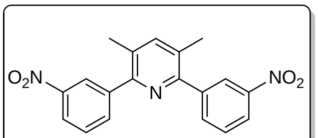
77.000
76.682
19.447
f1 (ppm)

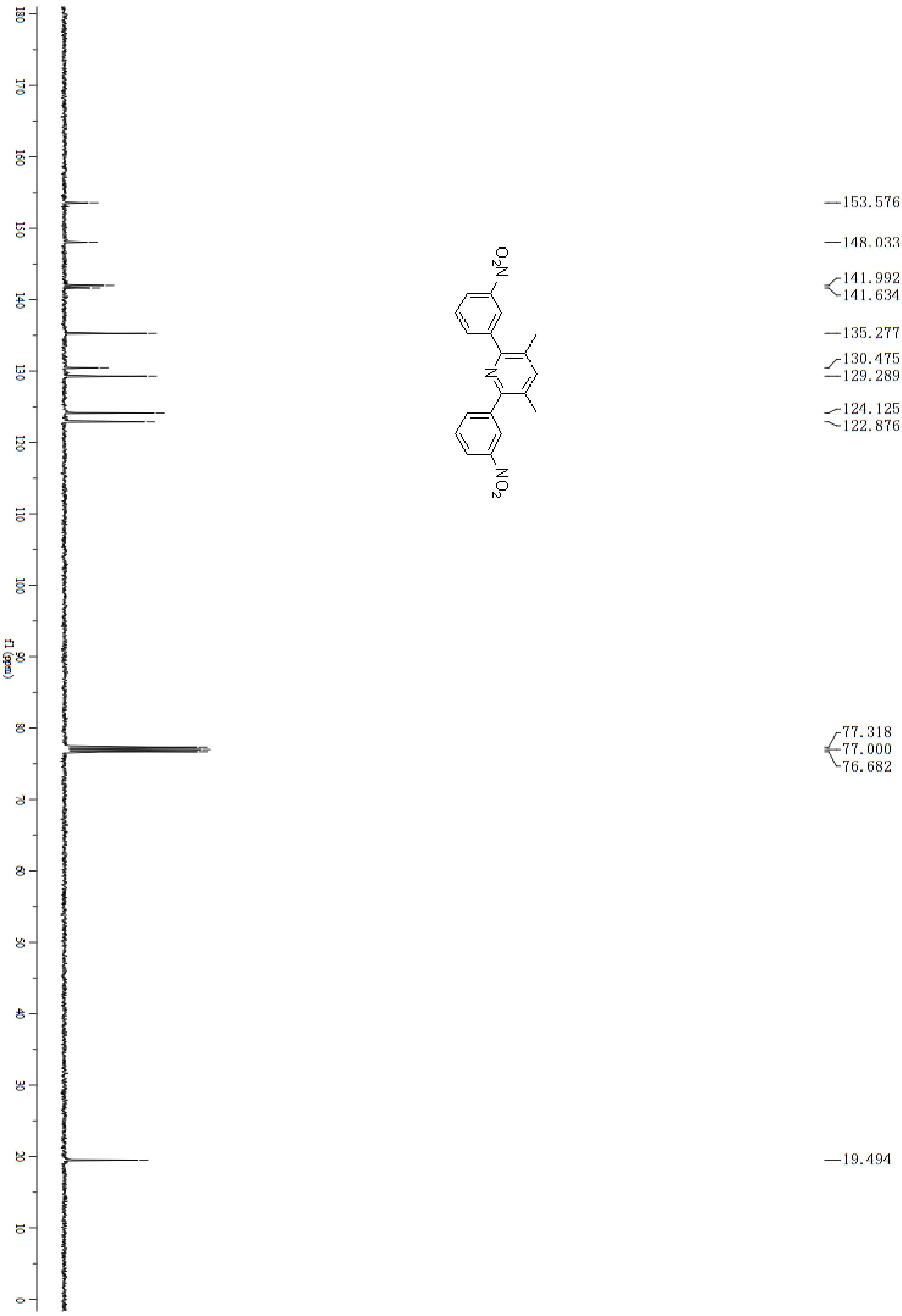

O2N
NO2
N

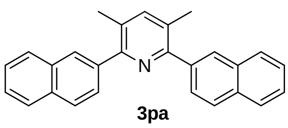
3oa


8.458
8.255
7.961
7.942
7.665
7.645
7.625
7.603
2.435
2.03
2.06
2.06
3.05
6.00
f1 (ppm)
O2N
NO2
N

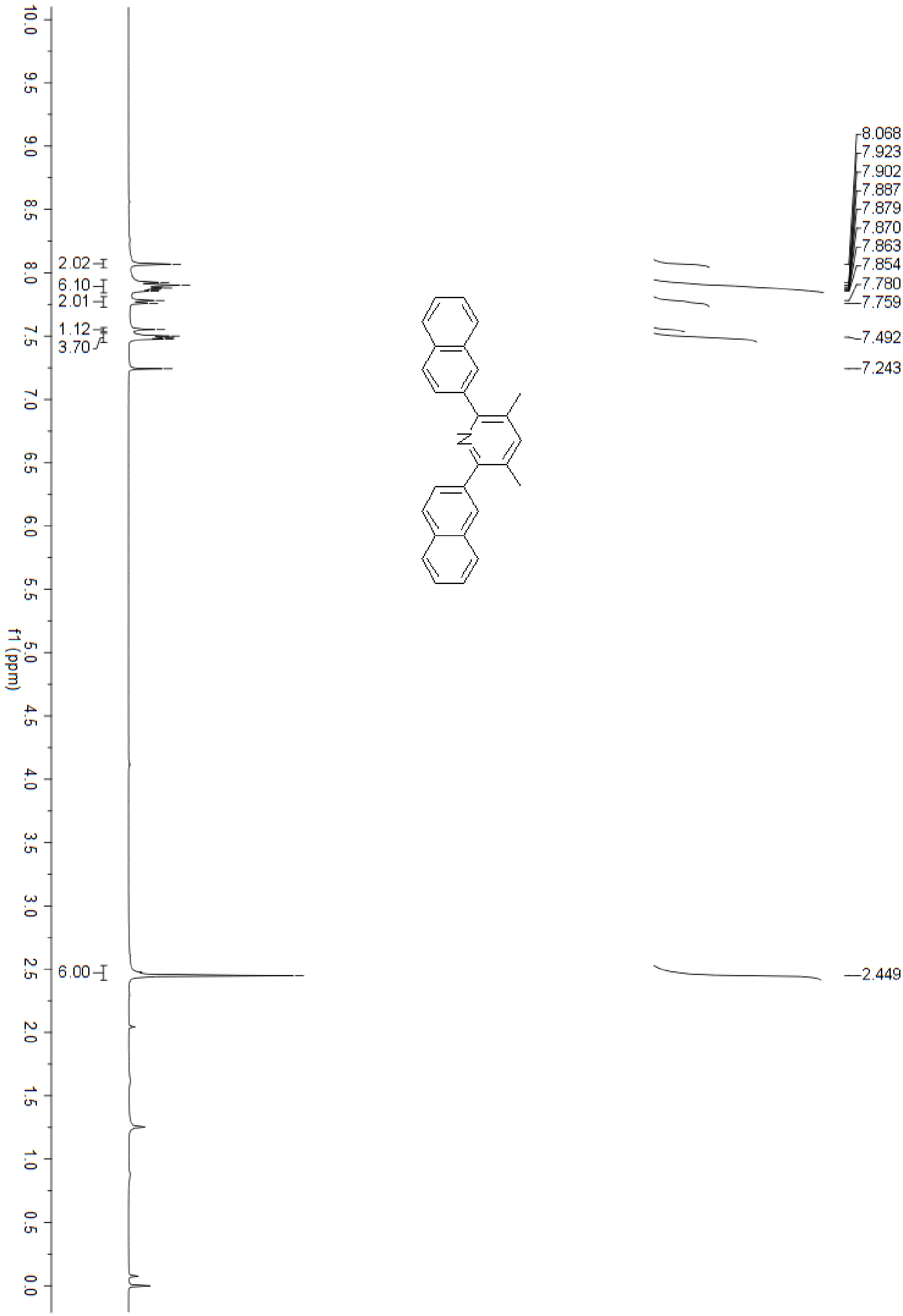

O2N
N
NO2

3oa

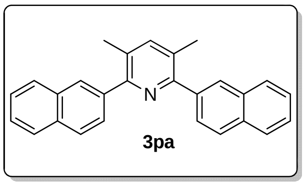

153.576
148.033
141.992
141.634
135.277
130.475
129.289
124.125
122.876
77.318
77.000
76.682
19.494
f1 (ppm)

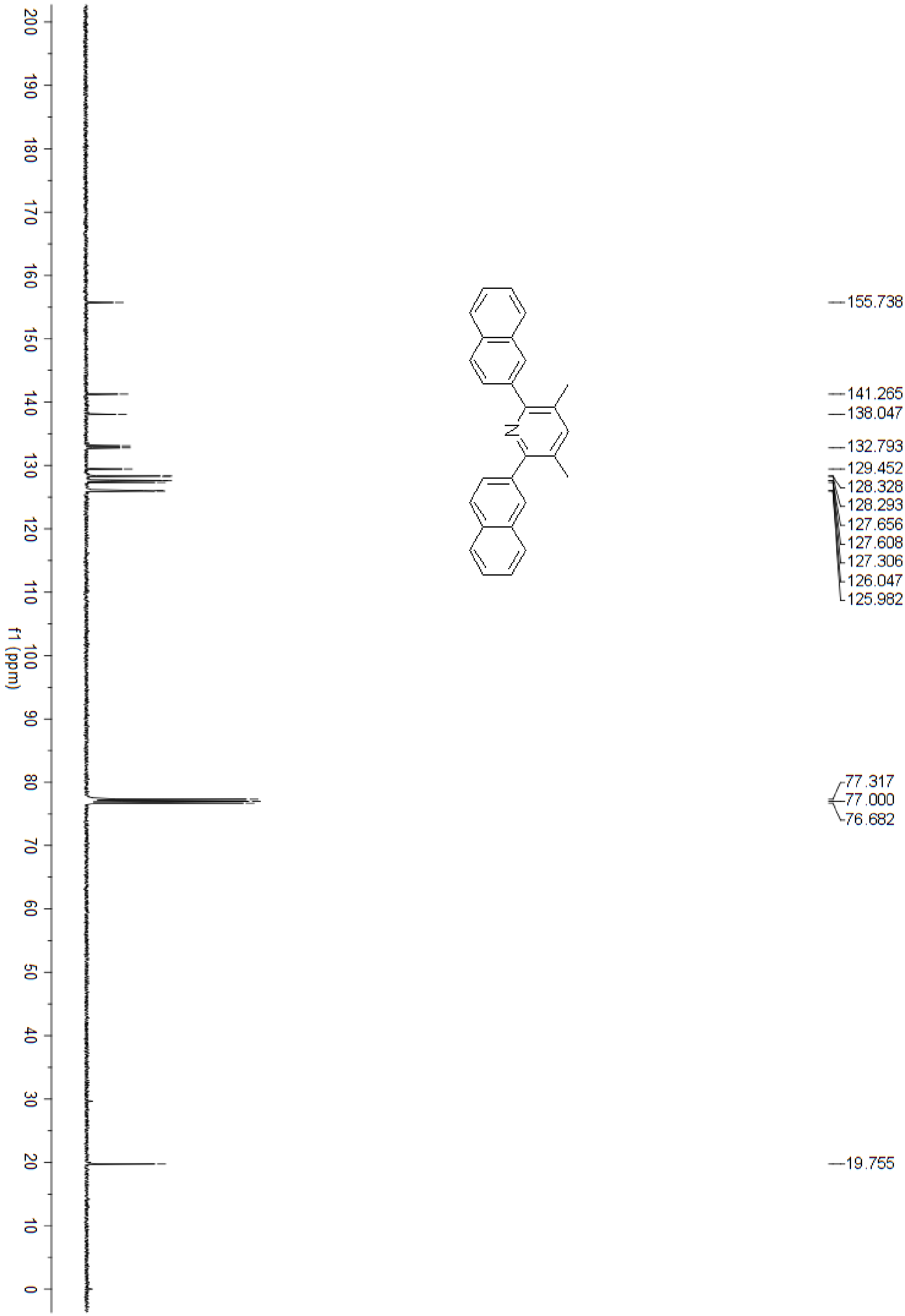


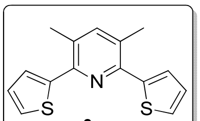
3pa



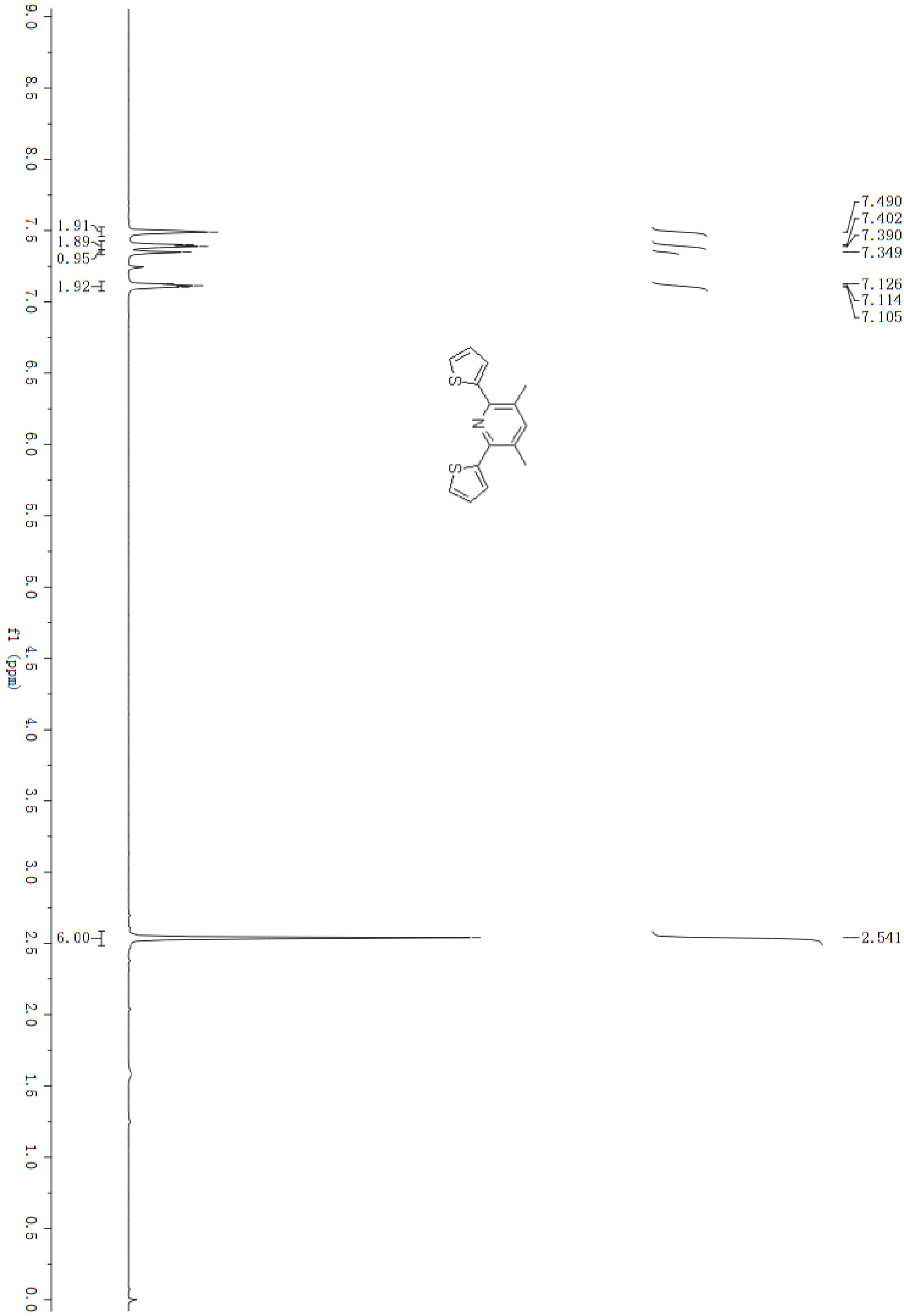
8.068
7.923
7.902
7.887
7.879
7.870
7.863
7.854
7.780
7.759
7.492
7.243
2.449
2.02
6.10
2.01
1.12
3.70
6.00
f1 (ppm)


N
3pa

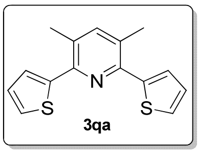

155.738
141.265
138.047
132.793
129.452
128.328
128.293
127.656
127.608
127.306
126.047
125.982
77.317
77.000
76.682
19.755
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
N



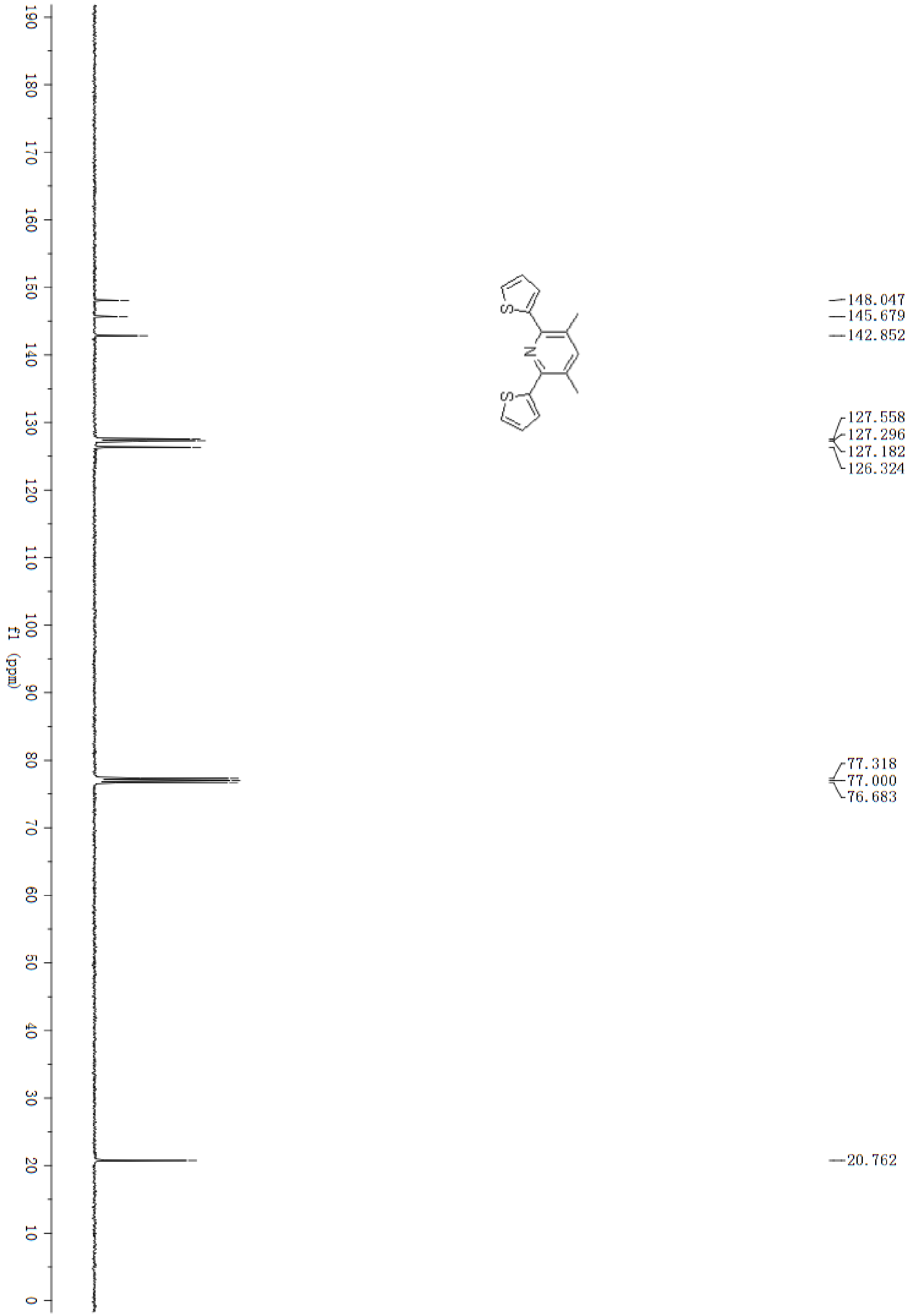
3qa



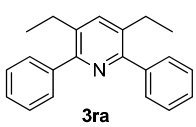
7.490
7.402
7.390
7.349
7.126
7.114
7.105
2.541
1.91
1.89
0.95
1.92
6.00
f1 (ppm)



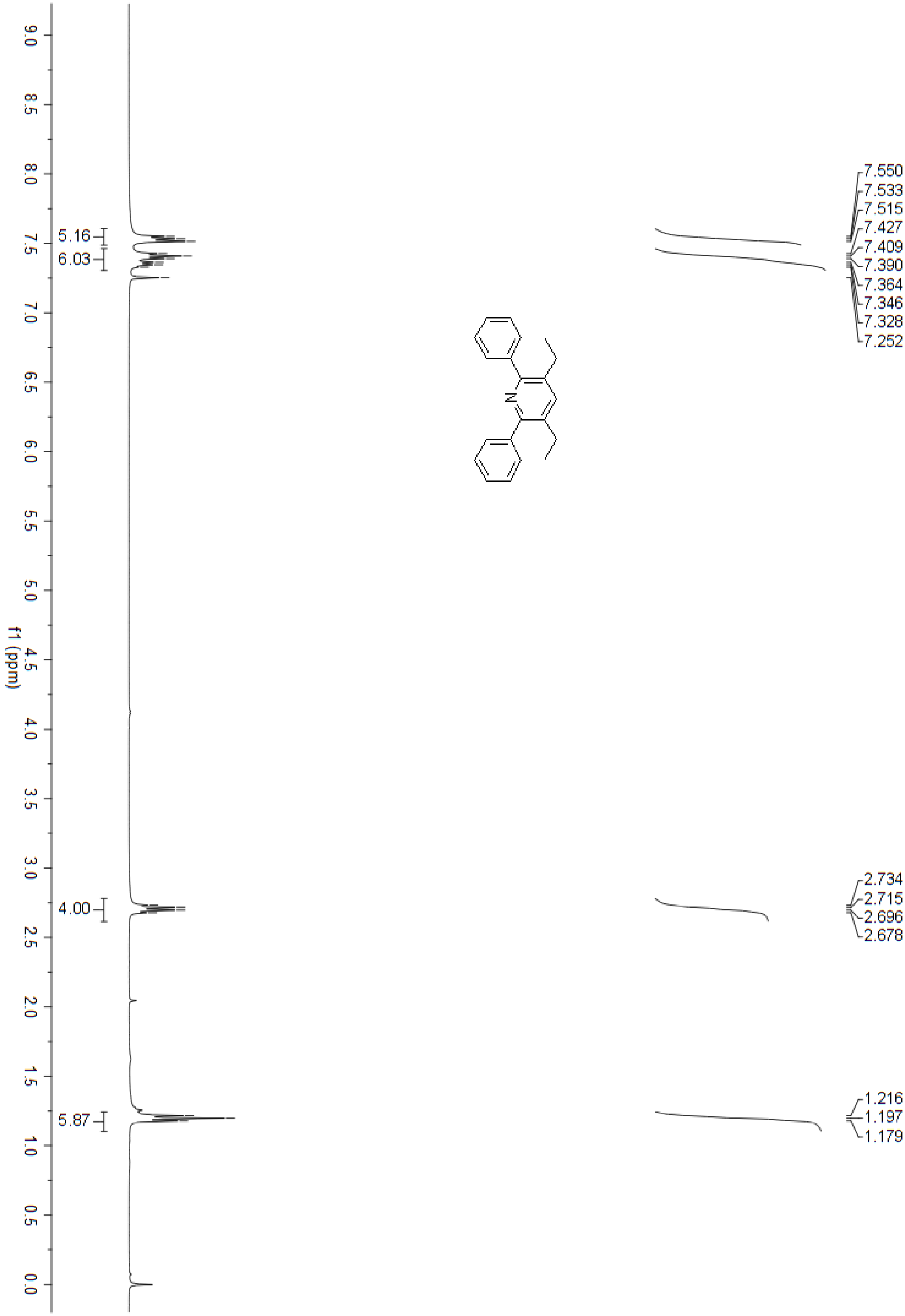
N
S
S
3qa



f1 (ppm)
148.047
145.679
142.852
127.558
127.296
127.182
126.324
77.318
77.000
76.683
20.762



3ra



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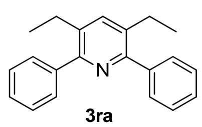
7.533
7.515
7.427
7.409
7.390
7.364
7.346
7.328
7.252
2.734
2.715
2.696
2.678
1.216
1.197
1.179
5.16
6.03
4.00
5.87
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



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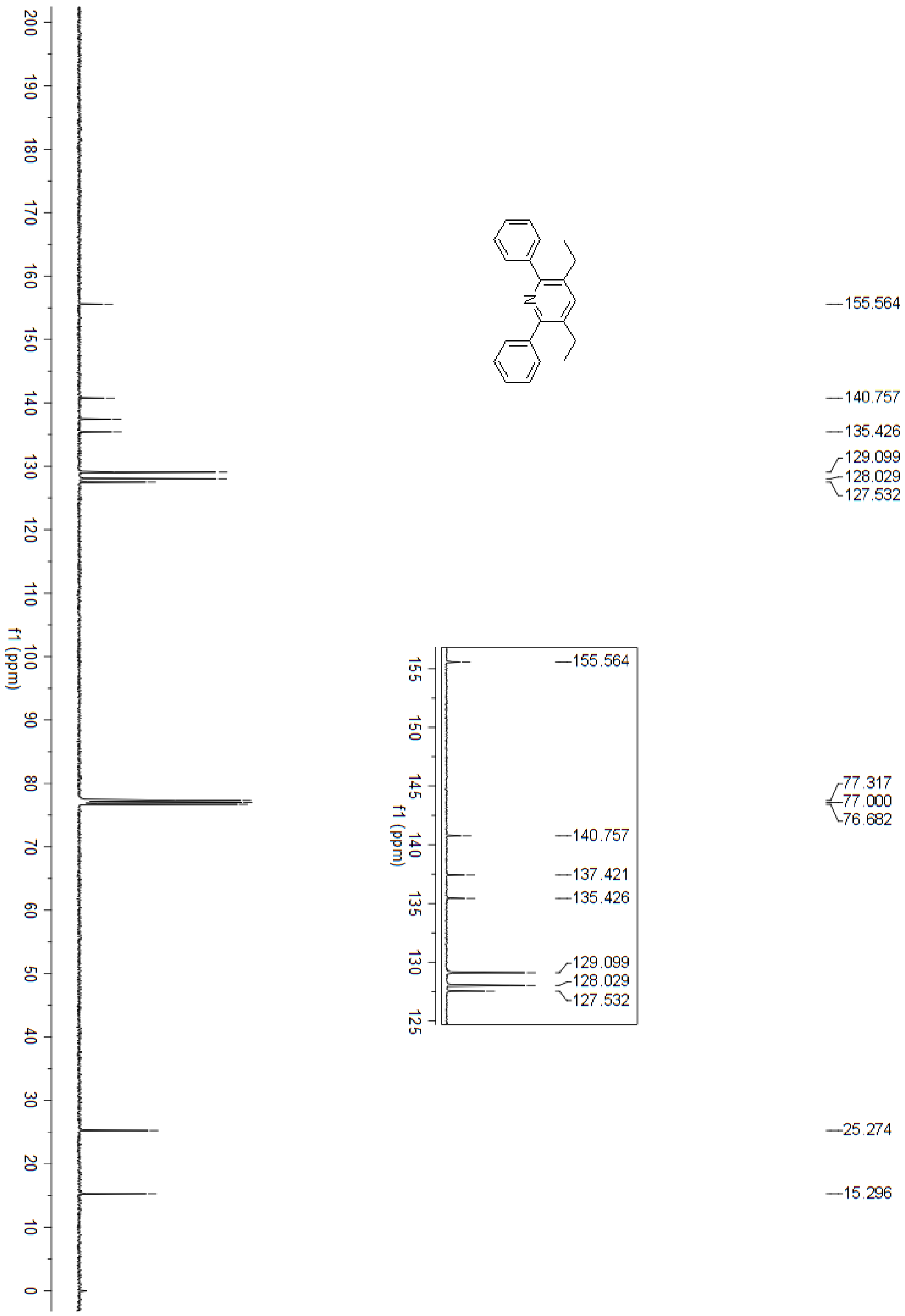
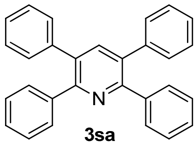
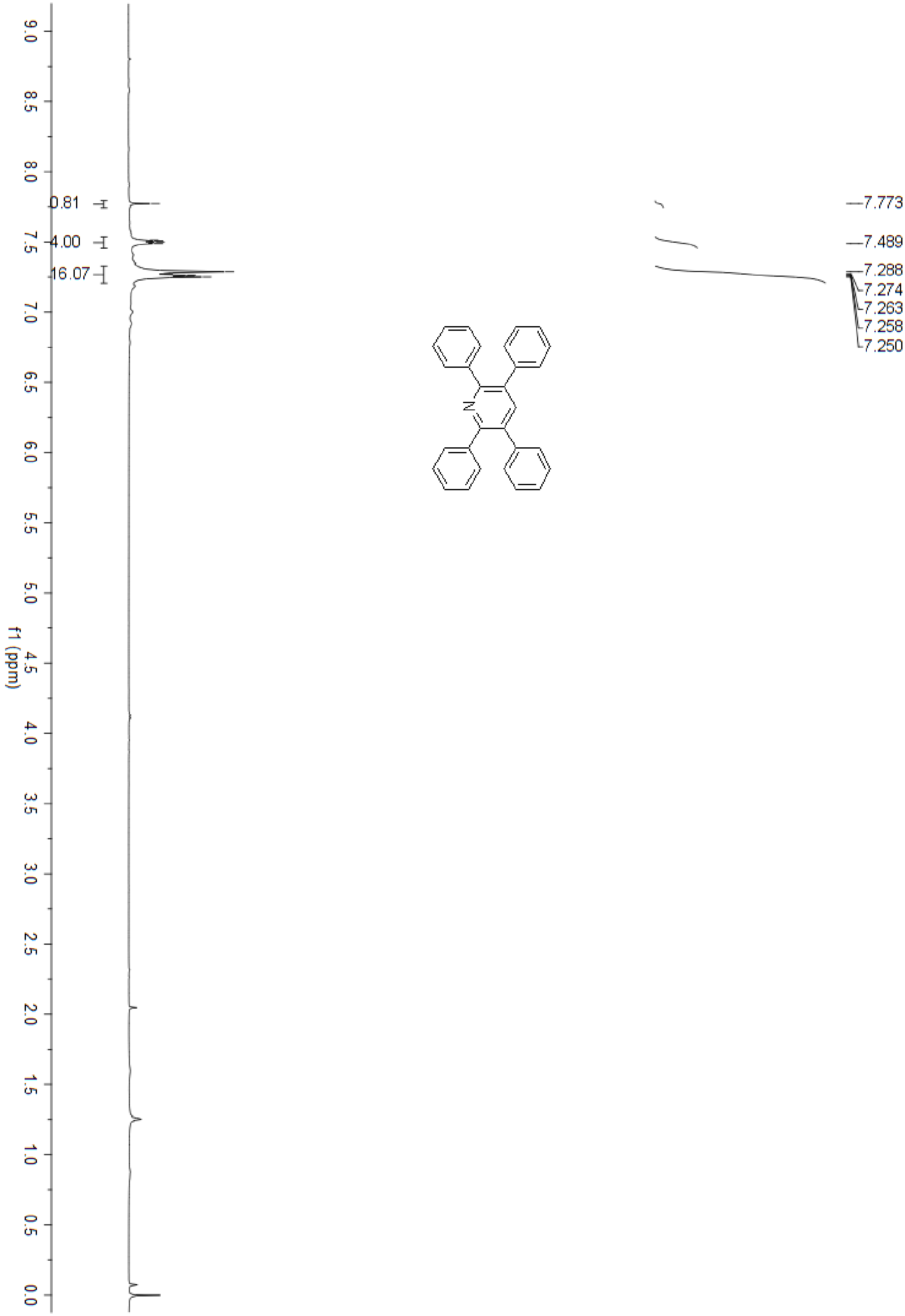
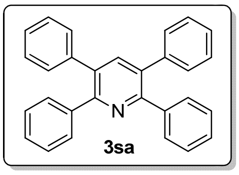

155.564
140.757
135.426
129.099
128.029
127.532
77.317
77.000
76.682
25.274
15.296
f1 (ppm)
155.564
140.757
137.421
135.426
129.099
128.029
127.532
f1 (ppm)



3sa



0.81
4.00
16.07
7.773
7.489
7.288
7.274
7.263
7.258
7.250
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
f1 (ppm)



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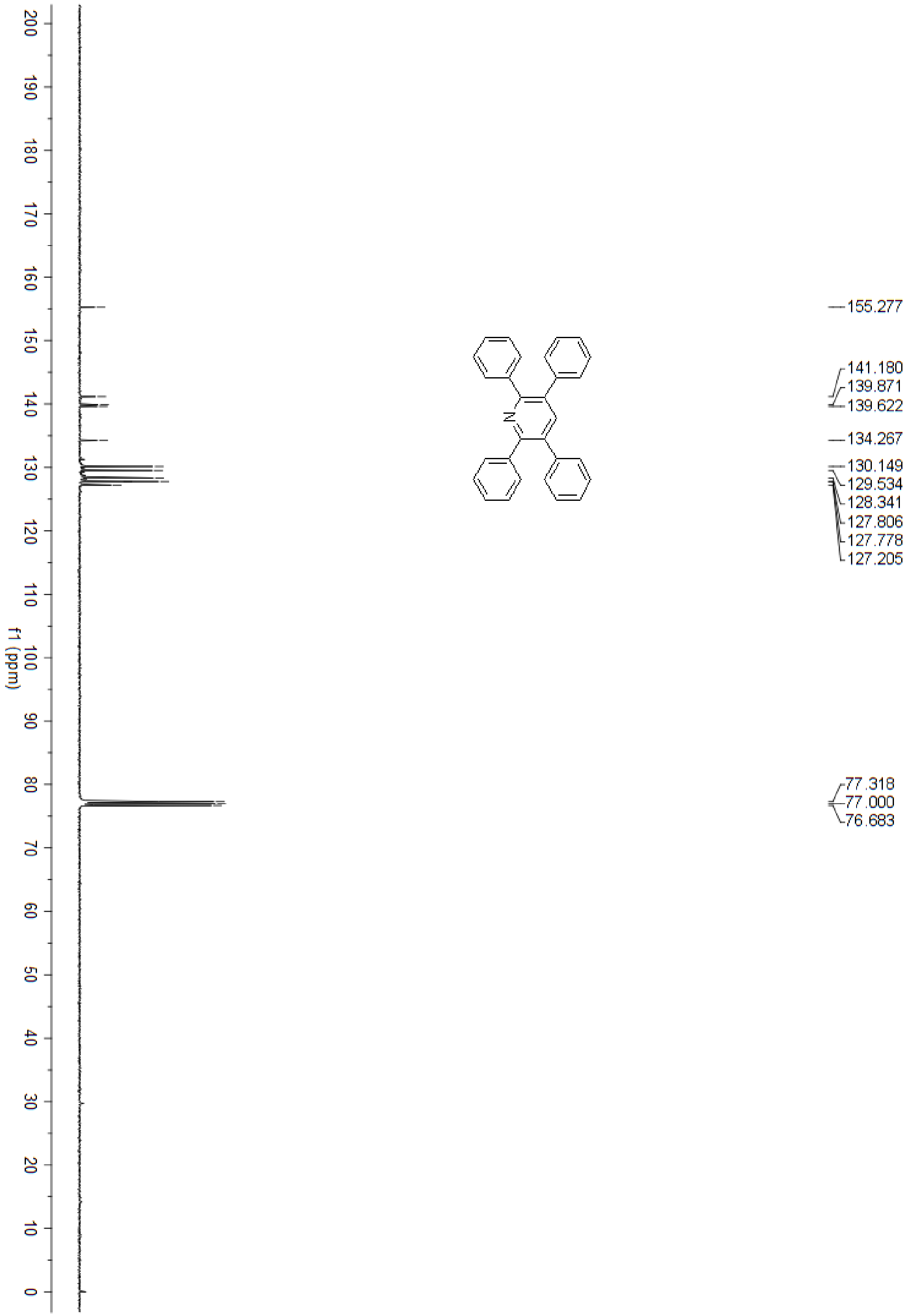
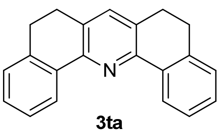


155.277
141.180
139.871
139.622
134.267
130.149
129.534
128.341
127.806
127.778
127.205
77.318
77.000
76.683
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
N



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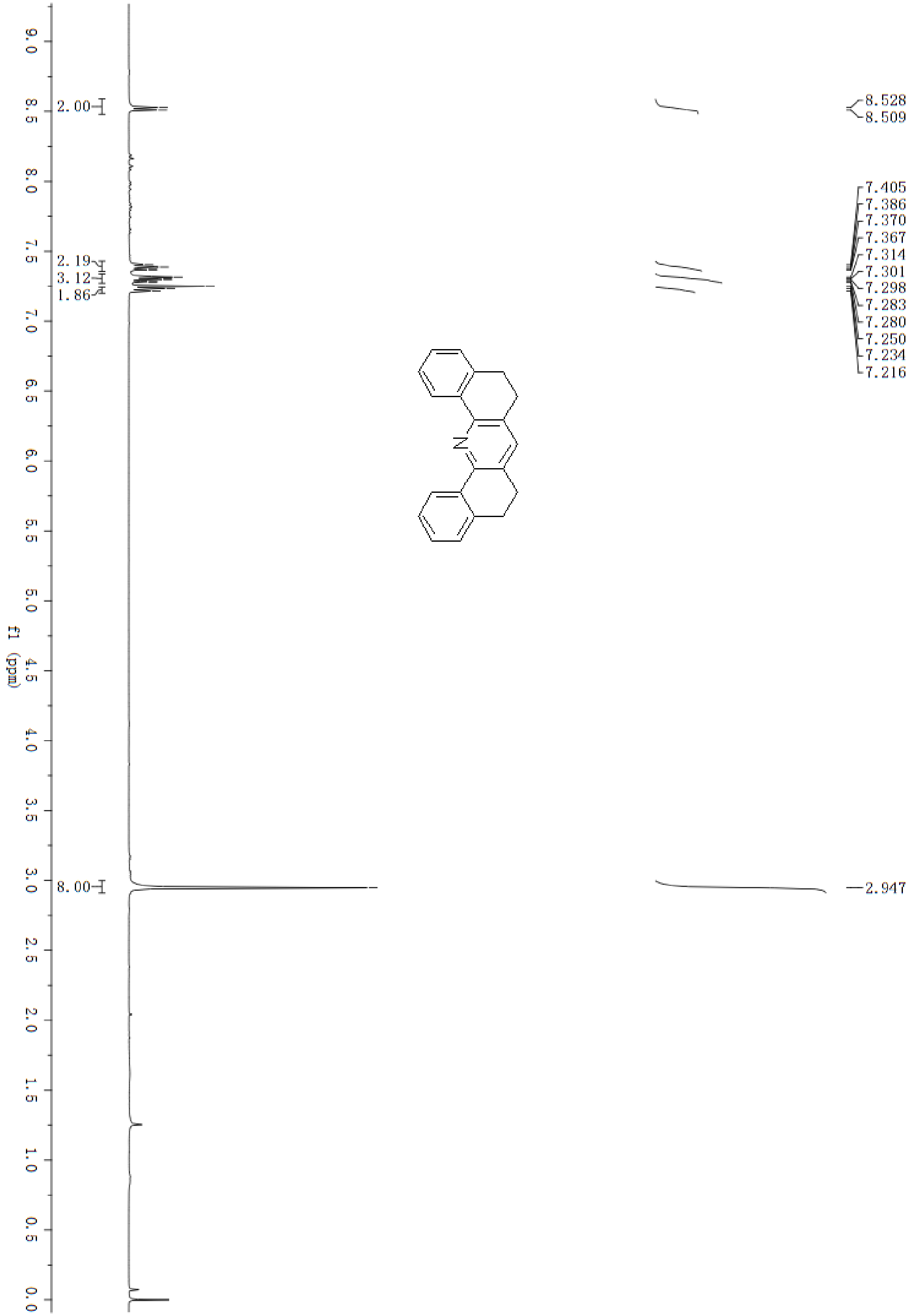
8.528
8.509
7.405
7.386
7.370
7.367
7.314
7.301
7.298
7.283
7.280
7.250
7.234
7.216
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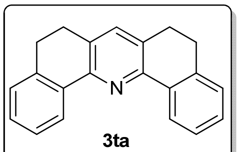
1.86
8.00
f1 (ppm)



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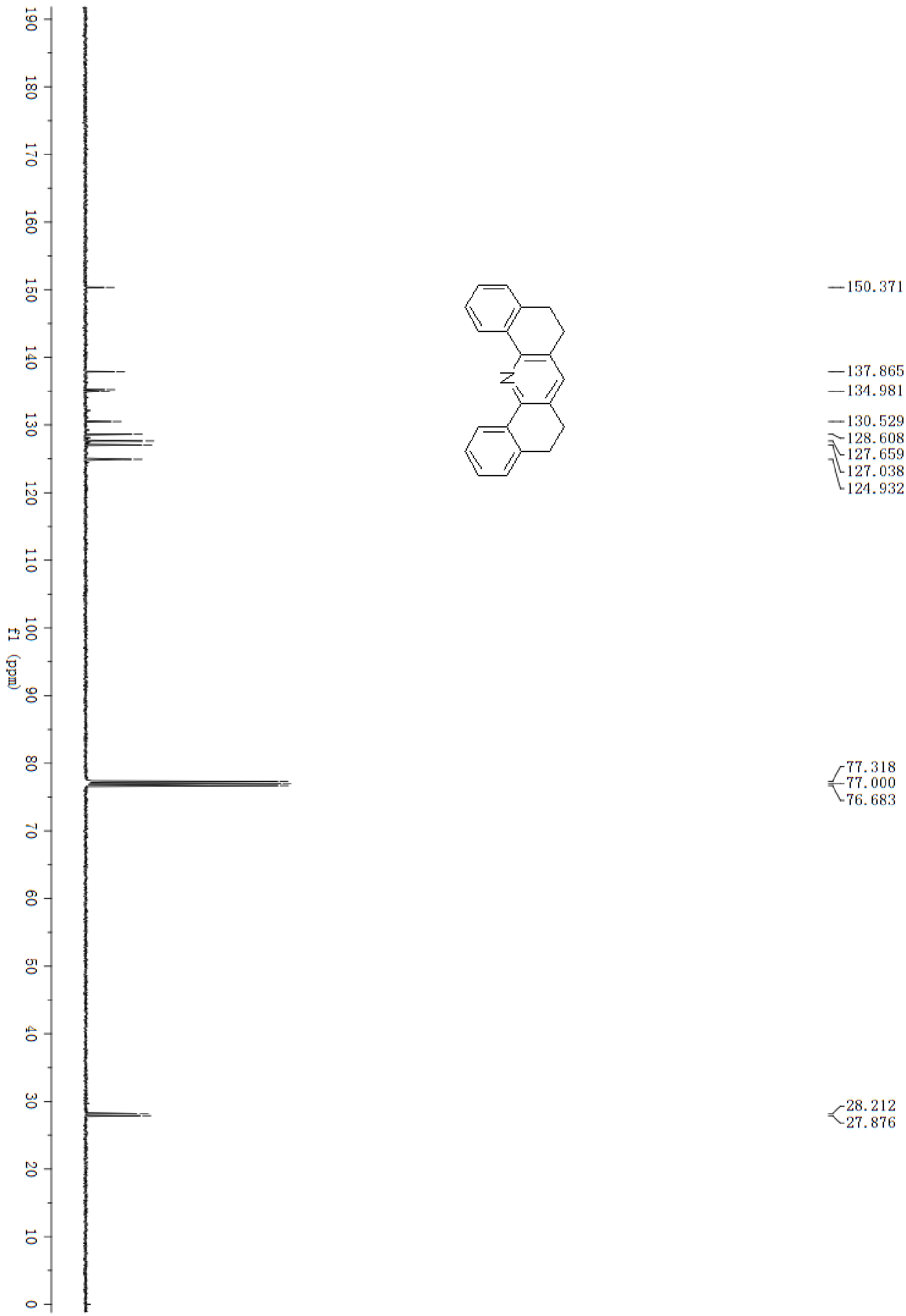
150.371
137.865
134.981
130.529
128.608
127.659
127.038
124.932
77.318
77.000
76.683
28.212
27.876
f1 (ppm)