Supporting Information

Cobalt- and Iron- Catalyzed Redox Condensation of *o*-Substituted Nitrobenzenes with Alkylamines: A Step- and Redox- Economical Synthesis of Diazaheterocycles

Thanh Binh Nguyen, Julie Le Bescont, Ludmila Ermolenko, and Ali Al-Mourabit*

General information

Reagents were obtained from commercial supplier and used without further purification. Analytical thinlayer chromatography (TLC) was purchased from Merck KGaA (silica gel 60 F254). Visualization of the chromatogram was performed by UV light (254 nm) or phosphomolybdic acid or vanilline stains. Flash column chromatography was carried out using kieselgel 35-70 μm particle sized silica gel (230-400 mesh). NMR Chemical shifts are reported in (δ) ppm relative to tetramethylsilane (TMS) with the residual solvent as internal reference ($CDCl_3$, δ 7.26 ppm for ^1H and δ 77.0 ppm for ^{13}C; DMSO-d6, δ 2.50 ppm for ^1H and δ 39.5 ppm for ^{13}C; CD_3OD, δ 3.31 ppm for ^1H and δ 49.0 ppm for ^{13}C). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. We note that some quaternary carbon signals are not observable in some cases of NH-benzimidazoles possibly due to tautomerism.

General procedures

Metal-catalyzed redox condensation reaction

A mixture of *o*-substituted nitrobenzene **1** (5 mmol), amine **2** (15 mmol) and metal salt (2-5 mol %, see Tables 1-4 of the Manuscript) and sulfur (20 mol %, 1 mmol, 32.1 mg for examples given in Table 4 of the Manuscript) was stirred in a 20-mL tube under an argon atmosphere for 24 h at indicated temperatures (See Tables 1-4 of the Manuscript). The crude

mixture was stirred vigorously with CH_2Cl_2 (5-10 mL) then filtered. Other portions of CH_2Cl_2 could be used to remove thoroughly all the CH_2Cl_2 soluble materials from the solid residue.

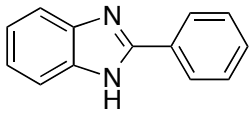
(i) The combined filtrate was purified by column chromatography on silica gel (heptane:EtOAc or CH_2Cl_2:MeOH) to afford a portion of the desired product **3**.

(ii) The solid residue was dissolved in MeOH, then filtered through a short pad of Celite (5 cm). The filtrate thus obtained was concentrated to afford another portion of the desired product **3**.

In the cases of **3ha**, **3ia** and **3ka**, due to their higher solubilities in CH_2Cl_2, the crude mixtures were totally soluble when treated with CH_2Cl_2.

Characterizations of Products

2-Phenylbenzimidazole (3aa)[1]



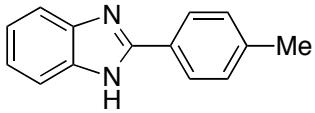
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 99:1.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.09-8.07 (m, 2H), 7.63-7.60 (m, 2H), 7.54-7.47 (m, 3H), 7.28-7.22 (m, 2H).

^{13}C NMR (75 MHz, CD_3OD) δ 153.5, 140.3, 131.5, 131.1, 130.2, 127.9, 124.0, 116.0.

2-(*p*-Tolyl)benzimidazole (3ab)[1]



Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 99:1.

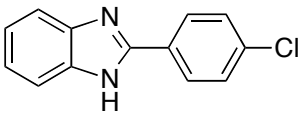
Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 7.96 (d, J = 8.1 Hz, 2H), 7.60-7.56 (m, 2H), 7.34 (d, J = 8.1 Hz, 2H), 7.26-7.21 (m, 2H), 2.41 (s, 3H).

^{13}C NMR (75 MHz, CD_3OD) δ 153.8, 142.0, 130.9, 128.5, 127.9, 123.9, 118.6, 113.1, 21.6.

2-(4-Chlorophenyl)benzimidazole (3ac)[1]

[1] Nguyen, T. B., Ermolenko, L.; Dean, W. A. Al-Mourabit, A. *Org. Lett.* **2012**, *14*, 5948.



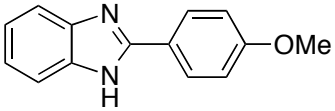
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.07-8.03 (m, 2H), 7.62-7.57 (m, 2H), 7.55-7.51 (m, 2H), 7.29-7.25 (m, 2H).

^{13}C NMR (75 MHz, CD_3OD) δ 152.2, 137.3, 130.3, 129.7, 129.3, 124.2, 115.3.

2-(4-Methoxyphenyl)benzimidazole (3ad)[1]



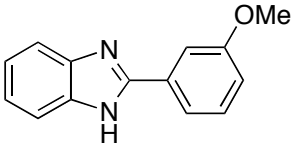
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.03-8.00 (m, 2H), 7.58-7.55 (m, 2H), 7.22-7.20 (m, 2H), 7.08-7.05 (m, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, CD_3OD) δ 163.1, 153.6, 129.5, 123.7, 123.5, 115.8, 56.0.

2-(3-Methoxyphenyl)benzimidazole (3ae)[2]



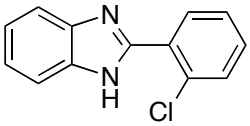
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 7.68-7.58 (m, 4H), 7.45-7.39 (m, 1H), 7.26-7.23 (m, 2H), 7.06-7.03 (m, 1H), 3.88 (s, 3H).

^{13}C NMR (75 MHz, CD_3OD) δ 161.8, 153.4, 132.3, 131.4, 124.1, 120.1, 117.5, 113.0, 56.0

2-(2-Chlorophenyl)benzimidazole (3af)[3]



[2] Savall, B. M.; Fontimayor, J. R. *Tetrahedron Lett*. **2008**, *49*, 6667.
[3] Nguyen, T. B.; Ermolenko, L.; Al-Mourabit, A. *Green Chem*. **2013**, *15*, 2713.

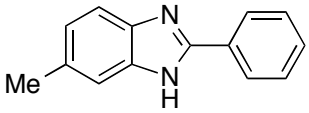
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 98:2.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 7.84-7.80 (m, 1H), 7.68-7.42 (m, 5H), 7.32-7.26 (m, 2H).

^{13}C NMR (75 MHz, CD_3OD) δ 151.2, 139.9, 134.0, 133.2, 132.6, 131.6, 131.1, 128.5, 124.2, 116.2.

6-Methyl-2-phenylbenzimidazole (3ba)[1]

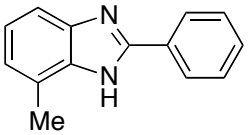


Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 99:1.

^{1}H NMR (300 MHz, CD_3OD) δ 8.07-8.04 (m, 2H), 7.54-7.46 (m, 4H), 7.38 (d, J = 1.5 Hz, 1H), 7.08 (dd, J = 8.2, 1.5 Hz, 1H), 2.45 (s, 3H).

^{13}C NMR (75 MHz, CD_3OD) δ 153.2, 134.0, 131.3, 130.2, 127.8, 125.6, 114.9, 21.9.

7-Methyl-2-phenylbenzimidazole (3ca)[4]



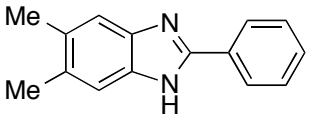
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 98:2.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.13-8.10 (m, 2H), 7.56-7.48 (m, 3H), 7.43 (d, J = 7.4 Hz, 1H), 7.14 (t, J = 7.4 Hz, 1H), 7.03 (t, J = 7.4 Hz, 1H), 2.62 (s, 3H).

^{13}C NMR (75 MHz, CD_3OD) δ 153.3, 131.3, 130.2, 128.1, 124.6, 124.1, 113.8, 113.7, 113.7, 17.3.

5,6-Dimethyl-2-phenylbenzimidazole (3da)[1]



Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

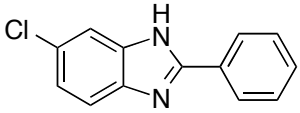
Pale yellow solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.04-8.01 (m, 2H), 7.53-7.43 (m, 3H), 7.34 (s, 2H), 2.34 (s, 5H).

[4] Kim, J.; Kim, J.; Lee, H.; Kim, Byeong H.; Lee, B. M. *Tetrahedron* **2011**, *67*, 8027.

^{13}C NMR (75 MHz, CD_3OD) δ 152.4, 138.5, 133.4, 131.3, 131.0, 130.2, 127.7, 115.9, 20.6.

6-Chloro-2-phenylbenzimidazole (3ea)[1]



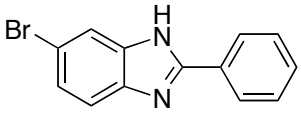
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 98:2.

Gray solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.07-8.02 (m, 2H), 7.57-7.49 (m, 5H), 7.21 (dd, J = 8.6, 2.0 Hz, 1H).

^{13}C NMR (75 MHz, CD_3OD) δ 154.8, 131.8, 130.8, 130.3, 129.8, 129.5, 128.4, 128.0, 124.4, 116.8, 115.9.

6-Bromo-2-phenylbenzimidazole (3fa)[3]



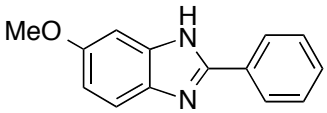
Eluent for column chromatography: CH_2Cl_2.

Yellow solid.

^{1}H NMR (300 MHz, CD_3OD) δ 8.07-8.02 (m, 2H), 7.72 (d, J = 1.7 Hz, 1H), 7.55-7.47 (m, 4H), 7.32 (dd, J = 8.6, 1.7 Hz, 1H).

^{13}C NMR (75 MHz, CD_3OD) δ 154.6, 131.8, 130.7, 130.3, 128.0, 127.1, 119.3, 116.8.

6-Methoxy-2-phenylbenzimidazole (3ga)[5]



Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

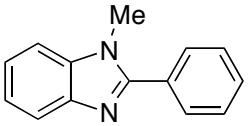
Yellow solid.

^{1}H NMR (300 MHz, MeOD) δ 8.05-8.02 (m, 2H), 7.53-7.46 (m, 4H), 7.08 (broad peak, 1H), 6.89 (dd, J = 8.7, 2.3 Hz, 1H), 3.84 (s, 3H).

^{13}C NMR (75 MHz, MeOD) δ some characteristic signals 158.4, 131.3, 131.2, 130.2, 127.6, 113.8, 56.3.

[5] Diao, X.; Wang, Y.; Jiang, Y.; Ma, D. *J. Org. Chem*. **2009**, *74*, 7974.

1-Methyl-2-phenylbenzimidazole (3ha)[1]



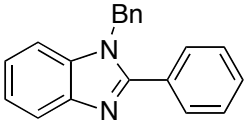
Eluent for column chromatography: heptane:EtOAc 4:1 to 2:1.

Pale yellow solid.

^{1}H NMR (500 MHz, MeOD) δ 7.77-7.75 (m, 2H), 7.69-7.68 (m, 1H), 7.58-7.56 (m, 3H), 7.54-7.52 (m, 1H), 7.35-7.30 (m, 2H), 3.85 (s, 3H).

^{13}C NMR (125 MHz, MeOD) δ 155.2, 143.2, 137.6, 131.3, 131.0, 130.6, 129.9, 124.3, 123.9, 119.6, 111.4, 32.1.

1-Benzyl-2-phenylbenzimidazole (3ia)[6]

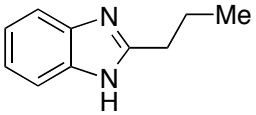


Eluent for column chromatography: heptane:EtOAc 5:1.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91-7.88 (m, 1H), 7.73-7.69 (m, 2H), 7.50-7.43 (m, 3H), 7.38-7.21 (m, 6H), 7.14-7.11 (m, 2H), 5.48 (s, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 153.9, 154.4, 143.4, 136.6, 136.2, 130.3, 130.1, 129.4, 129.2, 128.9, 128.0, 126.2, 123.2, 122.9, 120.2, 110.7, 48.6.

2-Propylbenzimidazole (3ah)[1]



Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

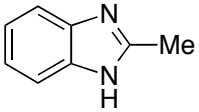
Brown solid.

^{1}H NMR (300 MHz, MeOD) δ 7.49-7.46 (m, 2H), 7.20-7.14 (m, 2H), 2.85 (t, J = 7.3 Hz, 2H), 1.85 (sextet, J = 7.3 Hz, 2H), 0.99 (t, J = 7.3 Hz, 3H).

^{13}C NMR (75 MHz, MeOD) δ 156.9, 123.2, 114.8, 31.8, 22.8, 14.2. One quaternary carbon signals was not observed possibly due to tautomerism.

2-Methylbenzimidazole (3ai)[1]

[6] Sadig, J. E. R.; Foster, R.; Willis, M. C.; Wakenhut, F. *J. Org. Chem*. **2012**, 77, 9473.



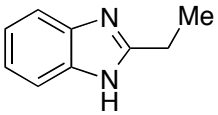
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

Brown solid.

^{1}H NMR (300 MHz, MeOD) δ 7.49-7.46 (m, 2H), 7.20-7.14 (m, 2H), 2.55 (s, 3H).

^{13}C NMR (75 MHz, MeOD) δ 152.9, 139.2, 123.0, 115.3, 14.2.

2-Ethylbenzimidazole (3aj)[1]



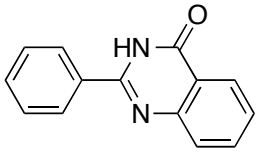
Eluent for column chromatography: CH_2Cl_2 to CH_2Cl_2:MeOH 95:5.

Brown solid.

^{1}H NMR (300 MHz, MeOD) δ 7.49-7.46 (m, 2H), 7.20-7.14 (m, 2H), 2.91 (q, J = 7.6 Hz, 2H), 1.40 (t, J = 7.6 Hz, 3H).

^{13}C NMR (75 MHz, MeOD) δ 123.2, 115.0, 23.3, 12.9. Two quaternary carbon signals were not observed possibly due to tautomerism.

2-Phenylquinazolin-4(3*H*)-one (3ja)[3]



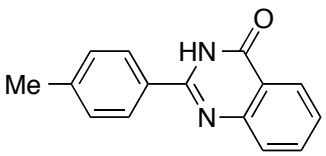
Eluent for column chromatography: CH_2Cl_2:EtOAc 99:1 to 95:5.

Pale yellow solid.

^{1}H NMR (300 MHz, CD_3SOCD_3) δ 11.51 (s, 1H), 8.19-8.15 (m, 3H), 7.87-7.73 (m, 2H), 7.61-7.50 (m, 4H).

^{13}C NMR (75 MHz, CD_3SOCD_3) δ 162.2, 152.4, 148.6, 134.6, 132.7, 131.4, 128.6, 127.8, 127.4, 126.6, 125.8, 120.9.

2-(*p*-Tolyl)quinazolin-4(3*H*)-one (3jb)[3]



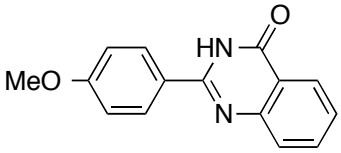
Eluent for column chromatography: CH_2Cl_2:EtOAc 99:1 to 95:5.

Pale yellow solid.

^{1}H NMR (300 MHz, CD_3SOCD_3) δ 12.48 (s, 1H), 8.16-8.09 (m 3H), 7.84-7.79 (m, 1H), 7.72 (d, J = 7.9 Hz, 1H), 7.53-7.48 (m, 1H), 7.35 (d, J = 8.1 Hz, 2H), 2.39 (s, 3H).

^{13}C NMR (75 MHz, CD_3SOCD_3) δ 162.1, 152.2, 148.8, 141.4, 134.6, 129.9, 129.2, 127.7, 127.4, 126.4, 125.8, 120.9, 21.0.

2-(*p*-Methoxyphenyl)quinazolin-4(3*H*)-one (3jd)[3]



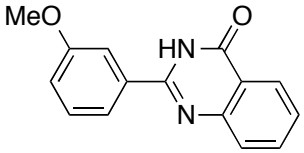
Eluent for column chromatography: CH_2Cl_2:EtOAc 99:1 to 95:5.

Gray solid.

^{1}H NMR (500 MHz, CD_3SOCD_3) δ 12.35 (broad s, 1H), 8.19 (d, J = 7.6 Hz, 2H), 8.13-8.11 (m, 1H), 7.81-7.78 (m, 1H), 7.70-7.69 (m, 1H), 7.48-7.45 (m, 1H), 7.07 (d, J = 7.6 Hz, 2H), 3.83 (s, 3H).

^{13}C NMR (75 MHz, CD_3SOCD_3) δ 162.3, 161.9, 151.8, 148.9, 134.5, 129.5, 127.3, 126.1, 125.8, 124.8, 120.7, 114.0, 55.5.

2-(*m*-Methoxyphenyl)quinazolin-4(3*H*)-one (3je)[7]



Eluent for column chromatography: CH_2Cl_2:EtOAc 99:1 to 95:5.

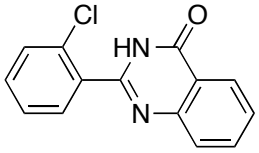
Gray solid.

^{1}H NMR (300 MHz, CD_3SOCD_3) δ 8.15-8.12 (m, 1H), 7.80-7.68 (m, 4H), 7.49-7.38 (m, 2H), 7.11-7.08 (m, 1H), 3.83 (s, 3H).

^{13}C NMR (75 MHz, CD_3SOCD_3) δ 162, 162.3, 159.3, 152.1, 148.6, 134.6, 134.0, 129.8, 127.5, 126.6,125.9, 121.0, 120.1, 117.6, 112.5, 55.4.

2-(*o*-Chlorophenyl)quinazolin-4(3*H*)-one (3jf)[3]

[7] Lopez, S. E.; Romero, A. H.; Salazar, J. *Synthesis*, **2013**, *45*, 2043.



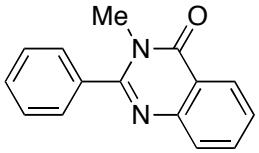
Eluent for column chromatography: CH_2Cl_2:EtOAc 99:1 to 95:5.

Gray solid.

^{1}H NMR (300 MHz, CD_3SOCD_3) δ 12.65 (s, 1H), 8.20-8.17 (m, 1H), 7.88-7.82 (m, 1H), 7.73-7.47 (m, 6H).

^{13}C NMR (75 MHz, CD_3SOCD_3) δ 162, 161.4, 152.2, 148.6, 134.6, 133.8, 131.6, 131.5, 130.9, 129.6, 127.5, 127.2, 127.1, 125.8, 121.2.

3-Methyl-2-phenylquinazolin-4(3*H*)-one (3ka)[8]



Eluent for column chromatography: heptane:EtOAc 4:1.

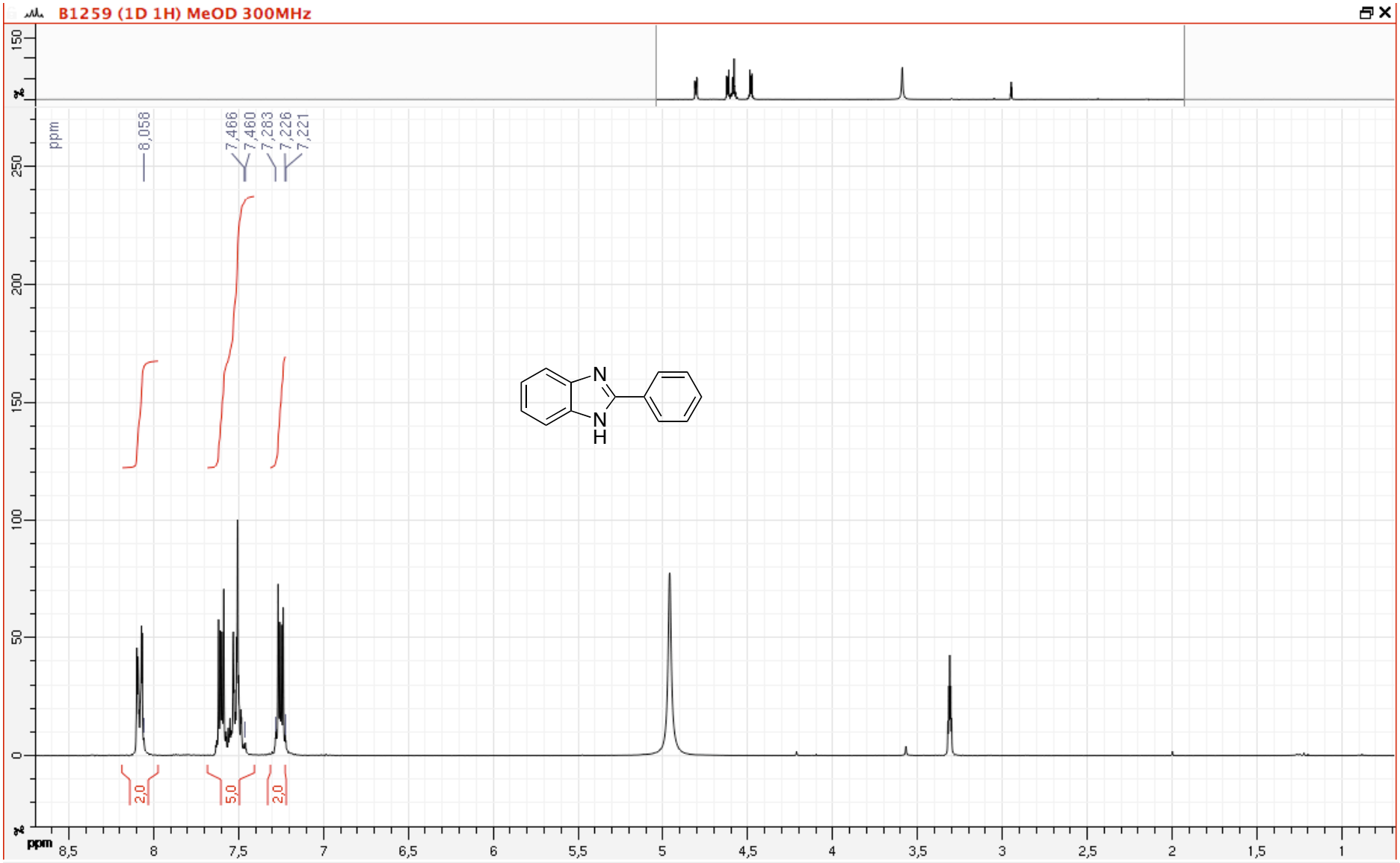
Gray solid.

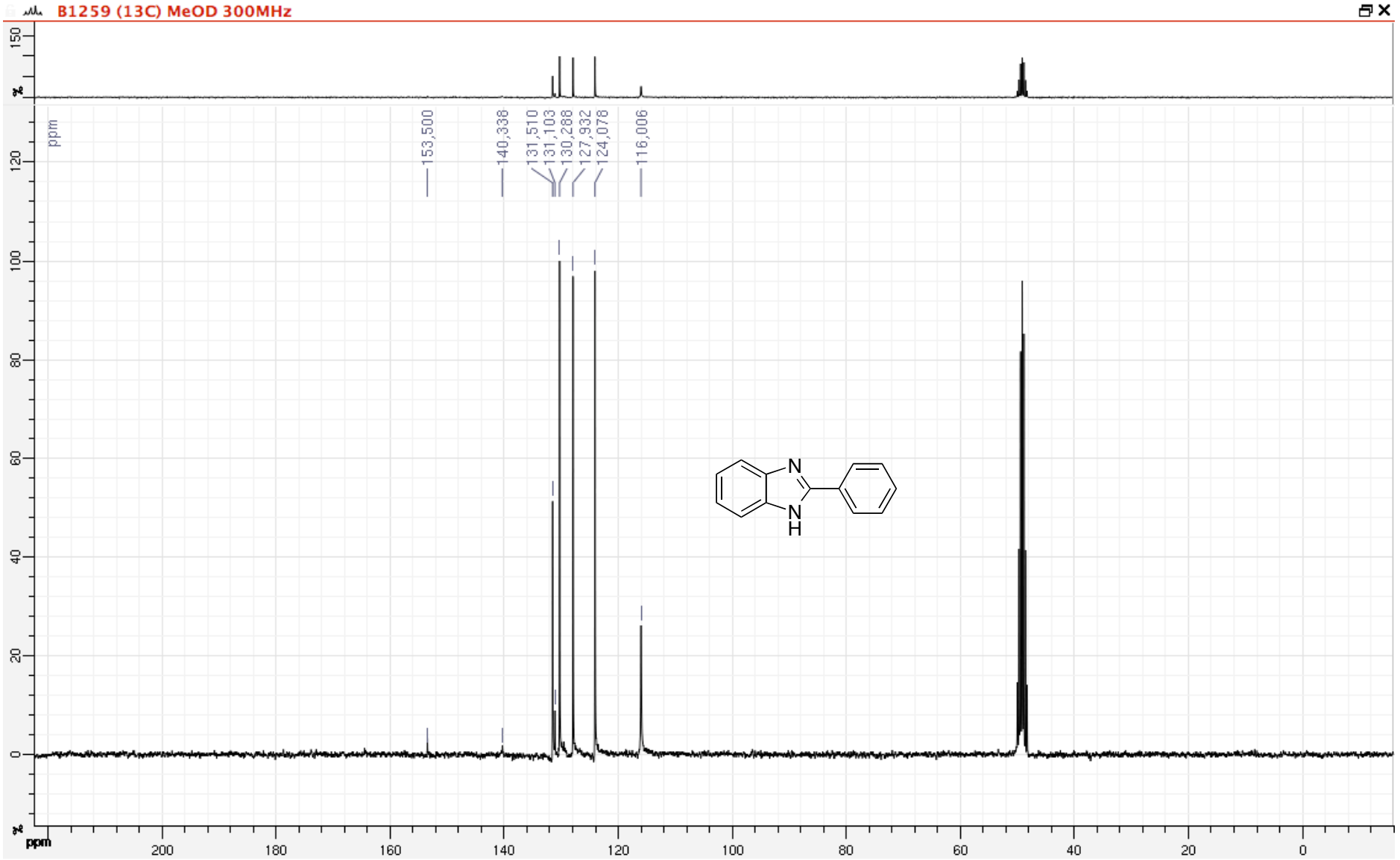
^{1}H NMR (300 MHz, CD_3SOCD_3) δ 8.18 (dd, J = 8.1, 1.5 Hz, 1H), 7.86-7.80 (m, 1H), 7.69-7.66 (m, 3H), 7.58-7.53 (m, 4H), 3.36 (s, 3H).

^{13}C NMR (75 MHz, CD_3SOCD_3) δ 161.6, 156.1, 147.0, 135.4, 134.3, 129.8, 128.4, 128.3, 127.2, 126.9, 126.1, 120.1, 33.9.

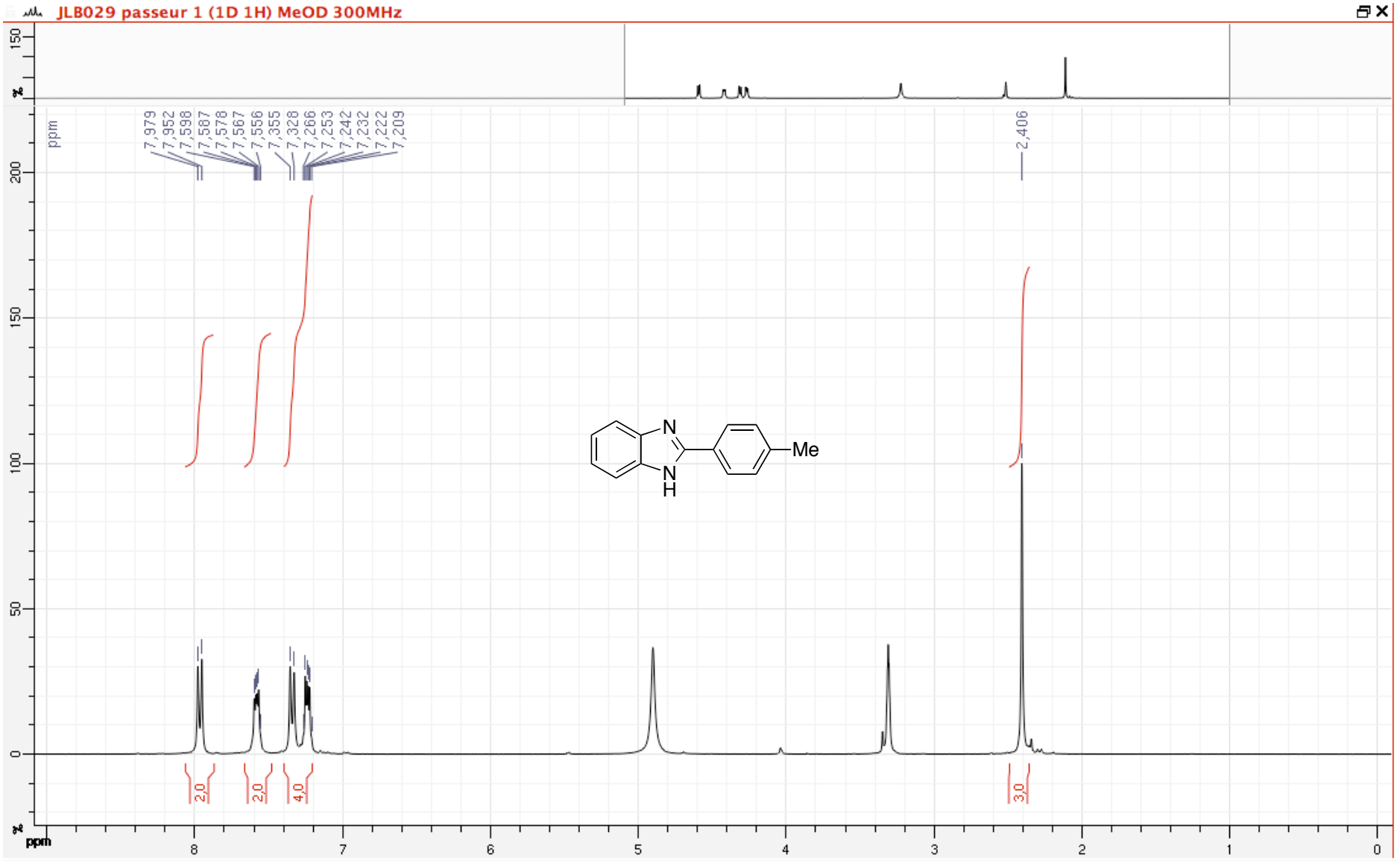
[8] Hikawa, H.; Ino, Y.; Suzuki, H.; Yokoyama, Y. *J. Org. Chem*. **2012**, *77*, 7046.

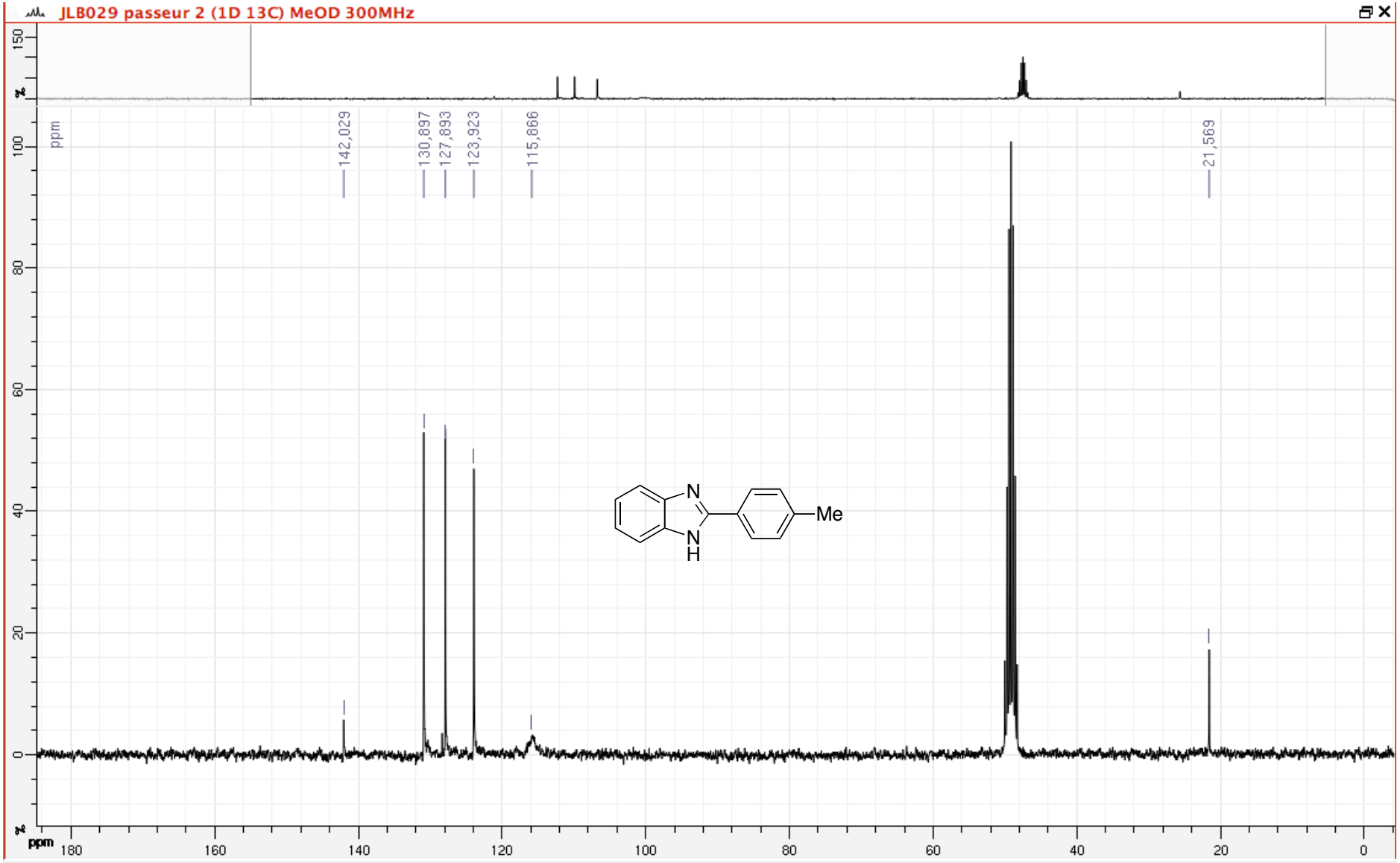
2-Phenylbenzimidazole (3aa)



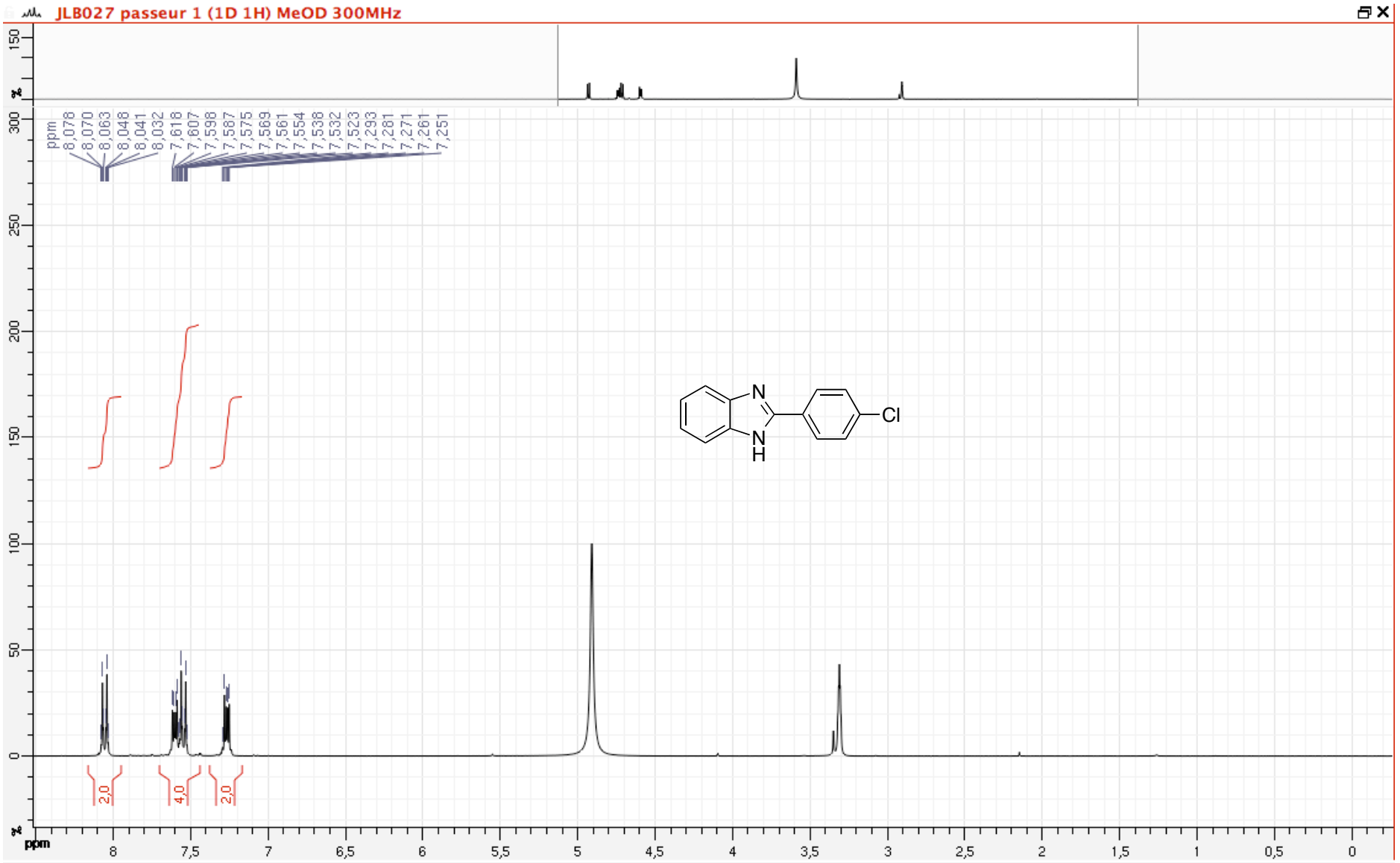

B1259 (13C) MeOD 300MHz
ppm
153,500
140,338
131,510
131,103
130,288
127,932
124,078
116,006
N
N
H

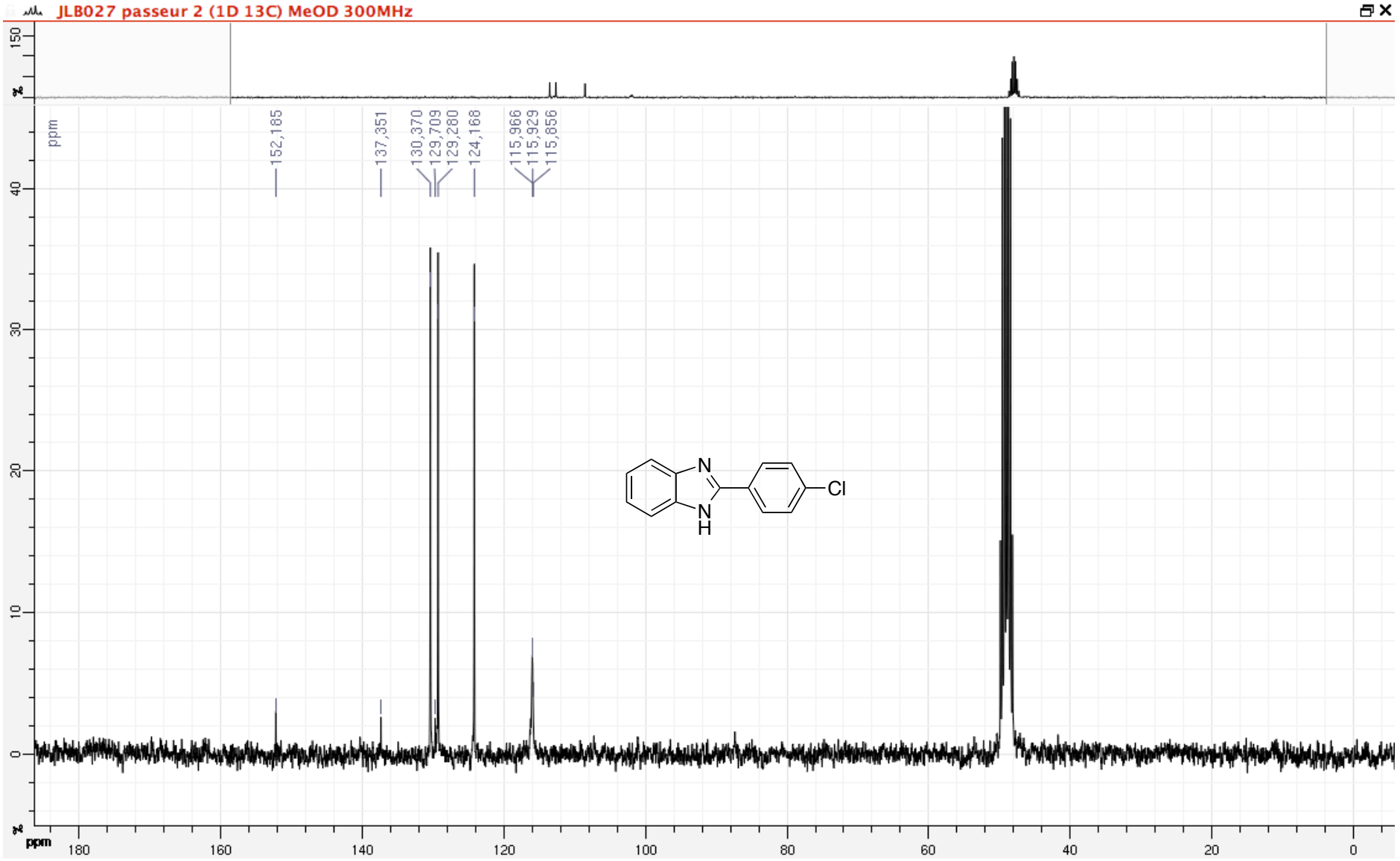
2-(*p*-Tolyl)benzimidazole (3ab)



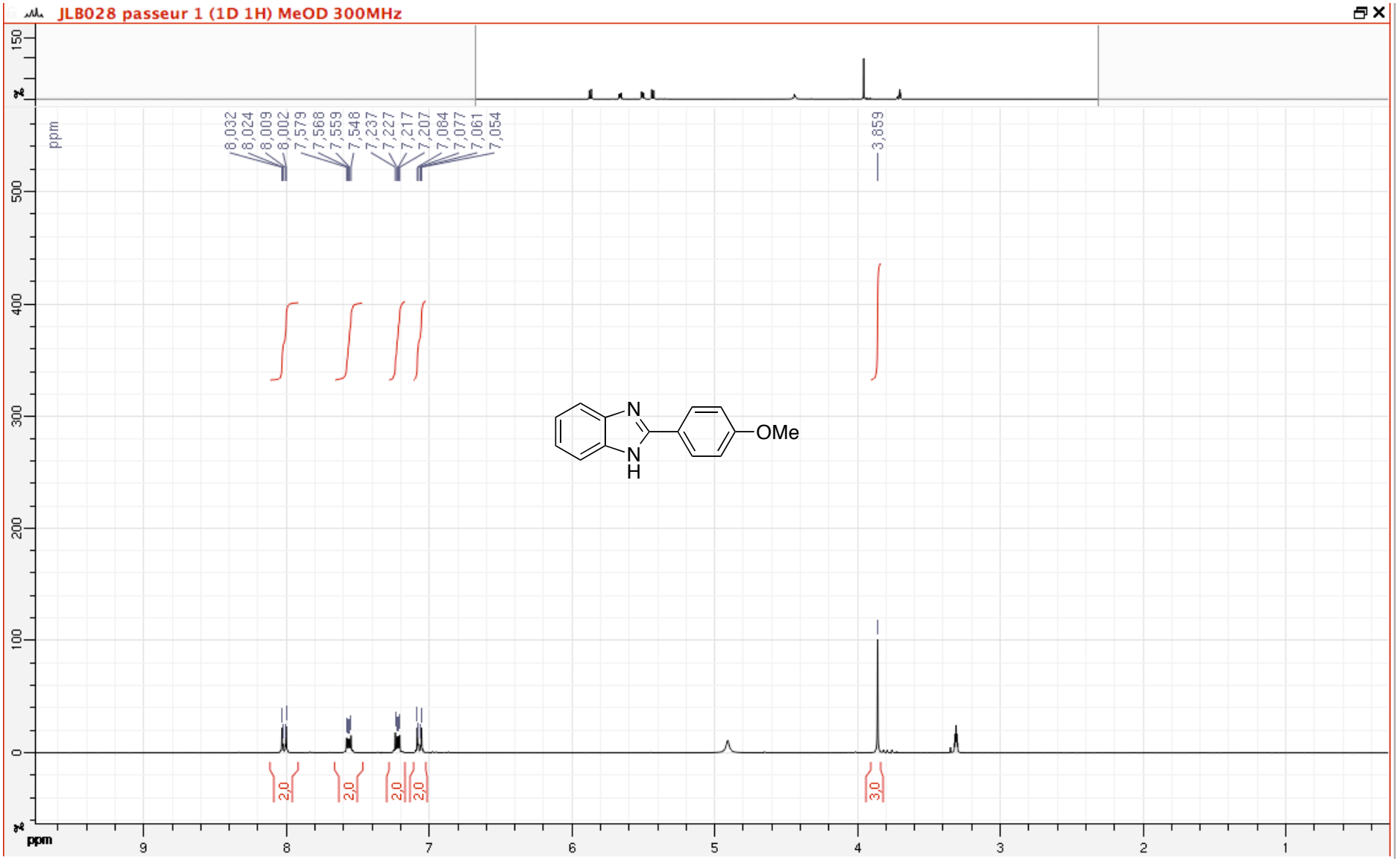

JLB029 passeur 2 (1D 13C) MeOD 300MHz
142,029
130,897
127,893
123,923
115,866
21,569
ppm
N
N
H
Me

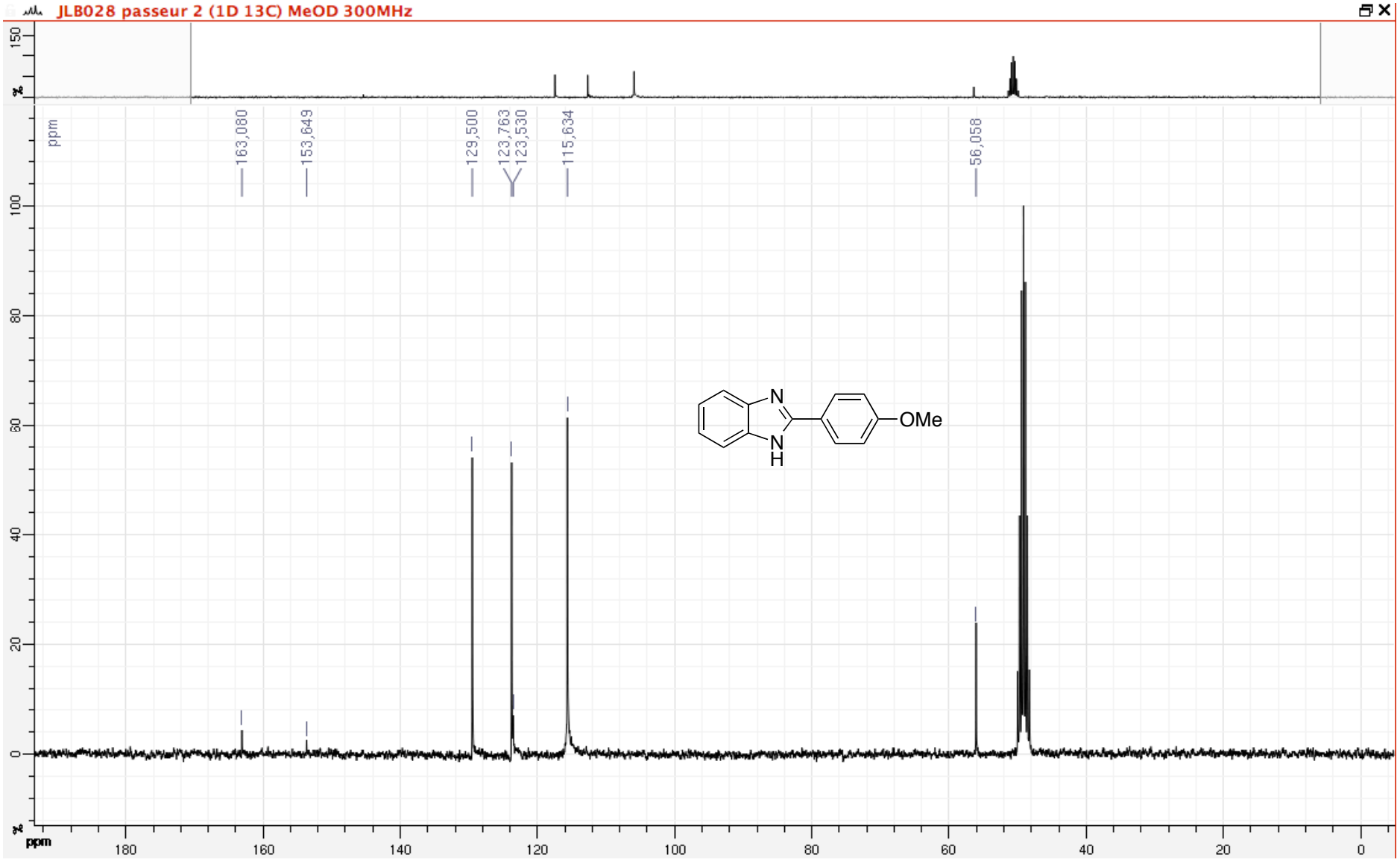
2-(4-Chlorophenyl)benzimidazole (3ac)



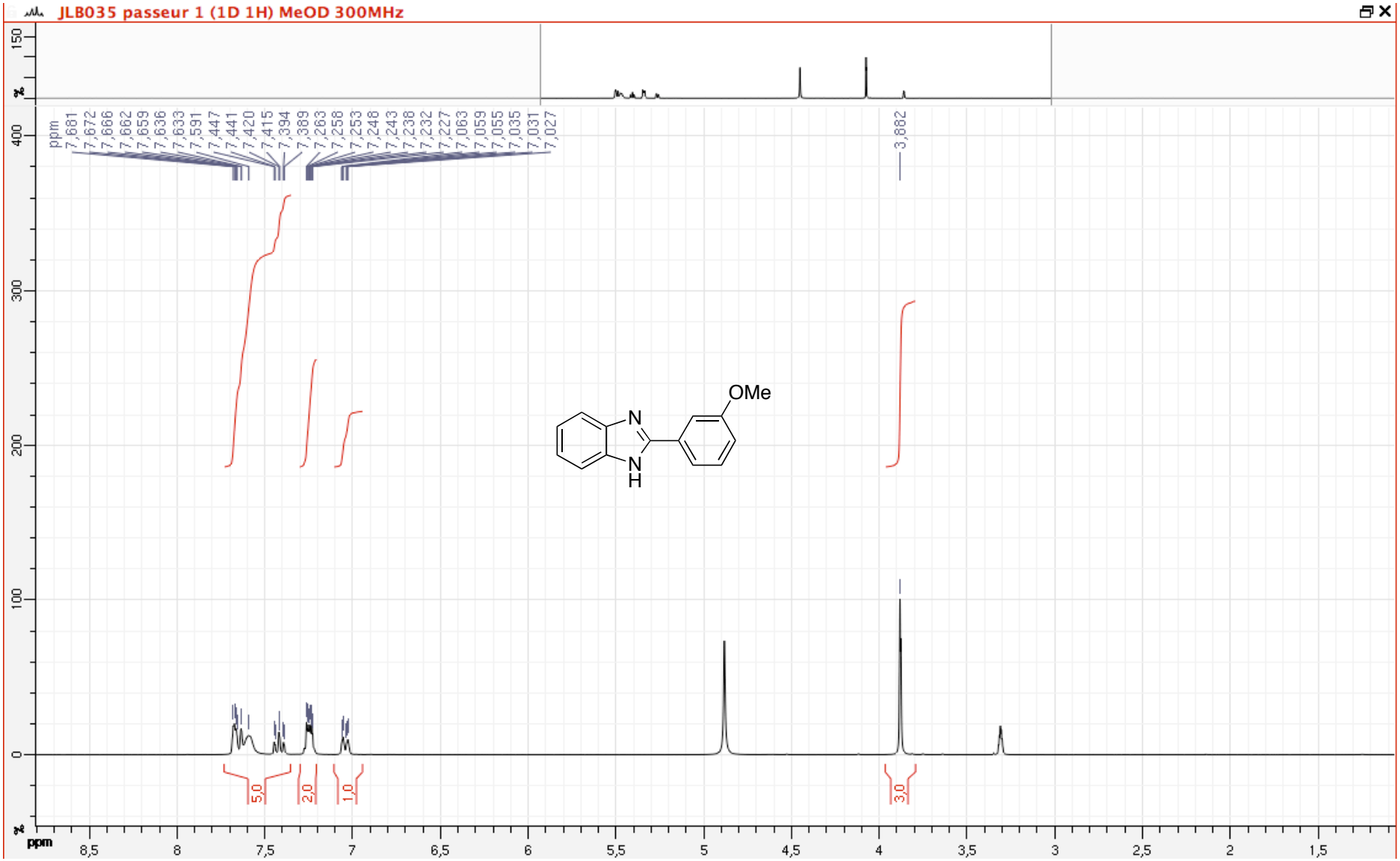

JLB027 passeur 2 (1D 13C) MeOD 300MHz
ppm
152,185
137,351
130,370
129,709
129,280
124,168
115,966
115,929
115,856
N
N
H
Cl
180
160
140
120
100
80
60
40
20
0

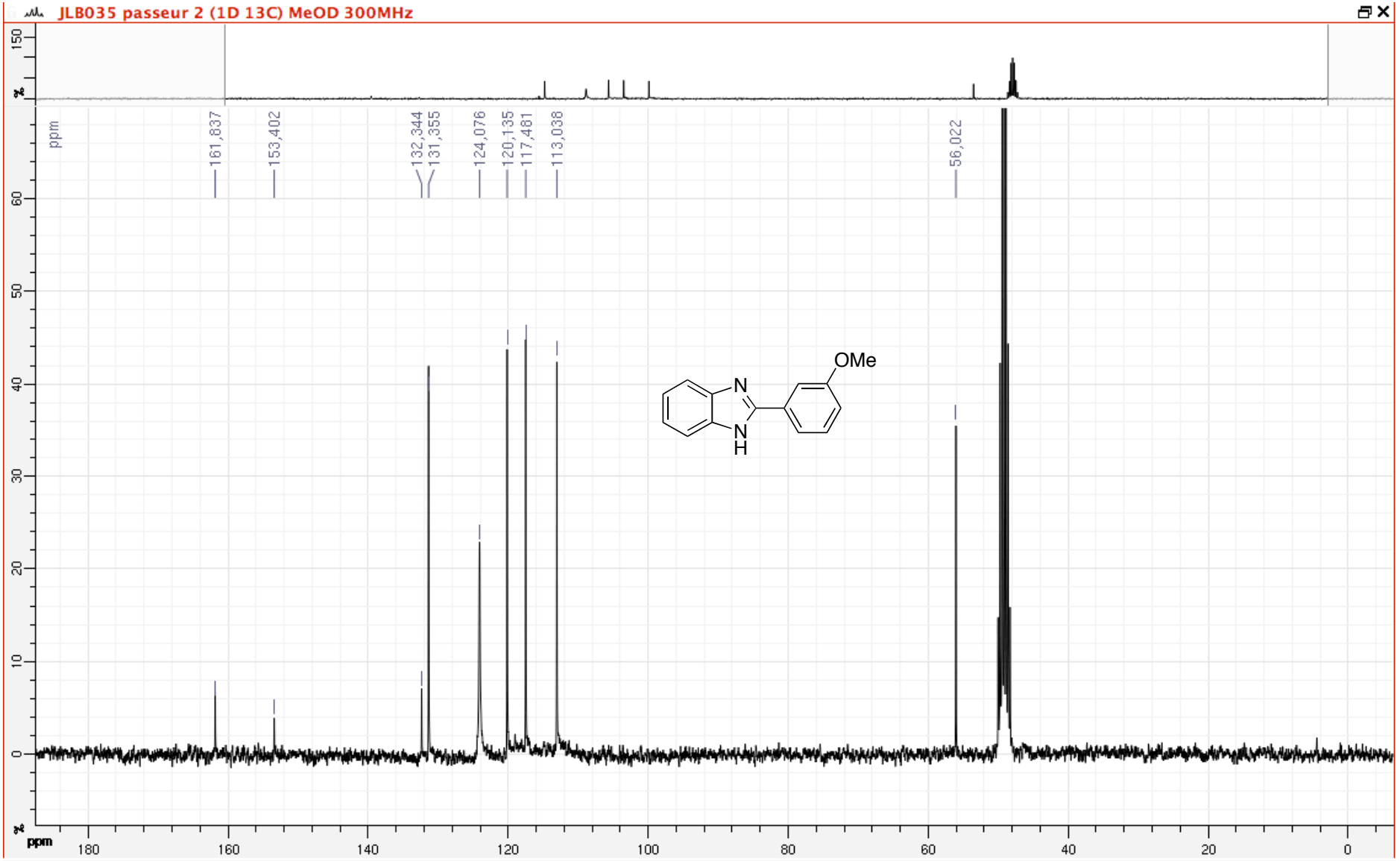
2-(4-Methoxyphenyl)benzimidazole (3ad)



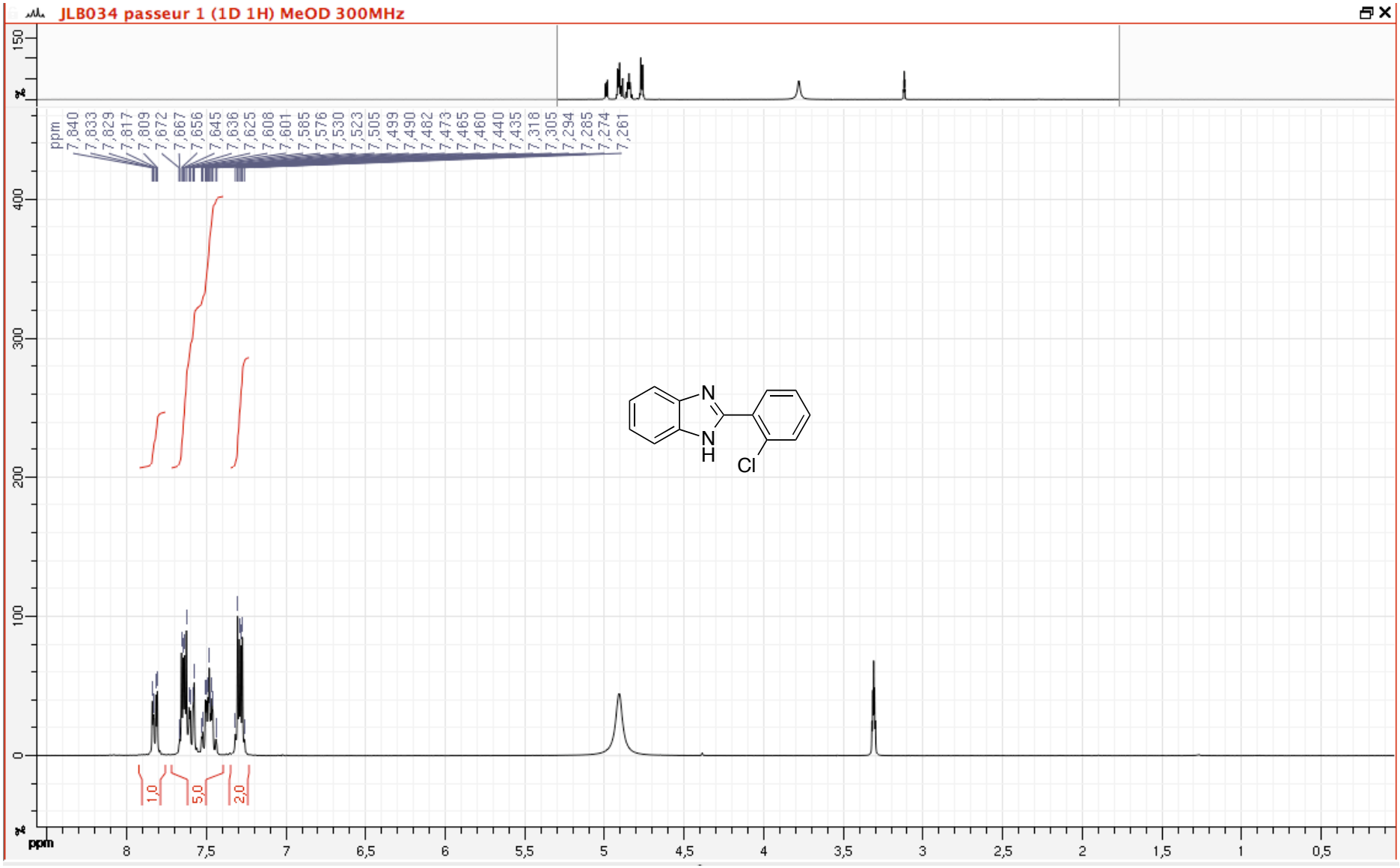

JLB028 passeur 2 (1D 13C) MeOD 300MHz
ppm
163,080
153,649
129,500
123,763
123,530
115,634
56,058
N
N
H
OMe
180
160
140
120
100
80
60
40
20
0

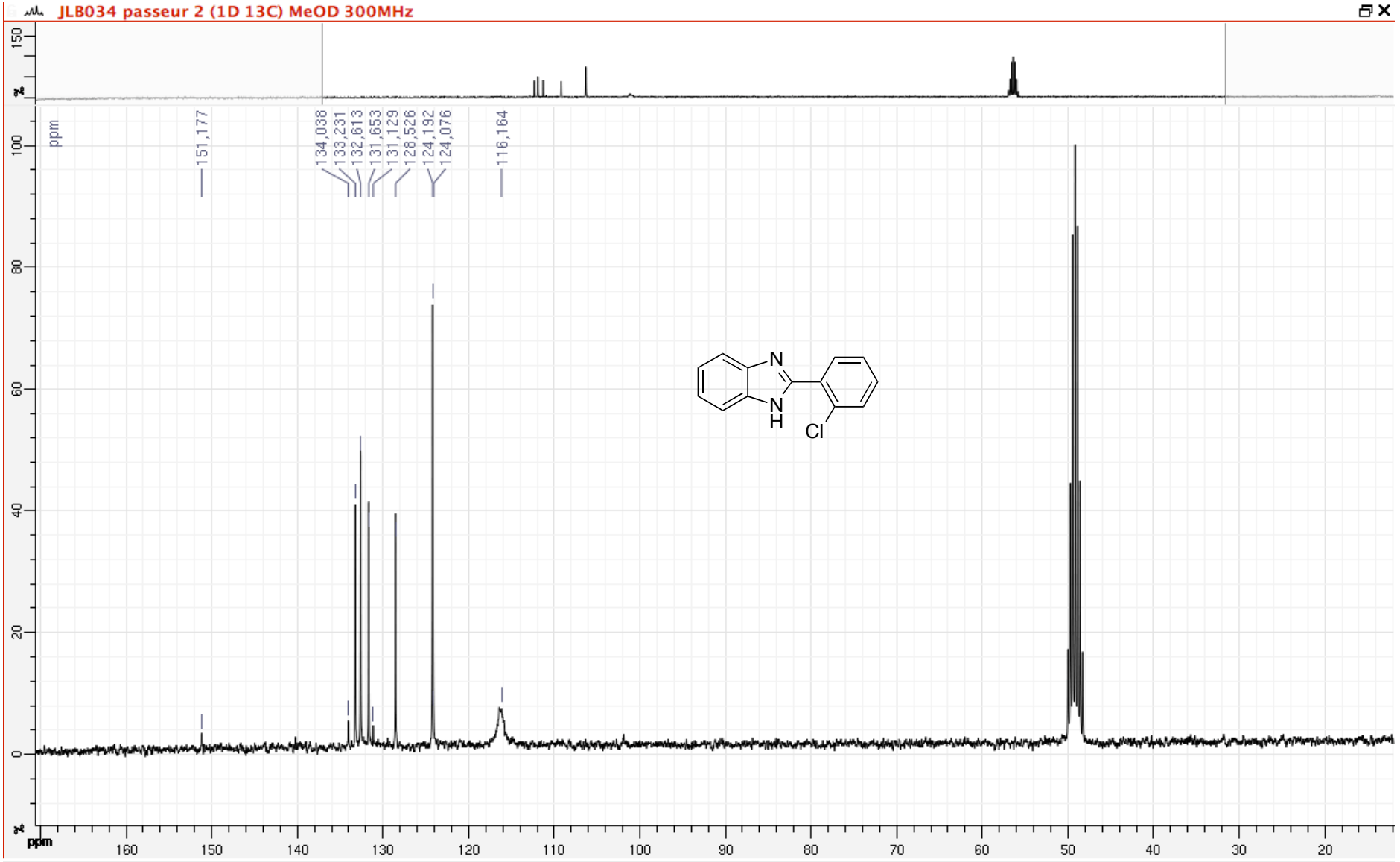
2-(3-Methoxyphenyl)benzimidazole (3ae)



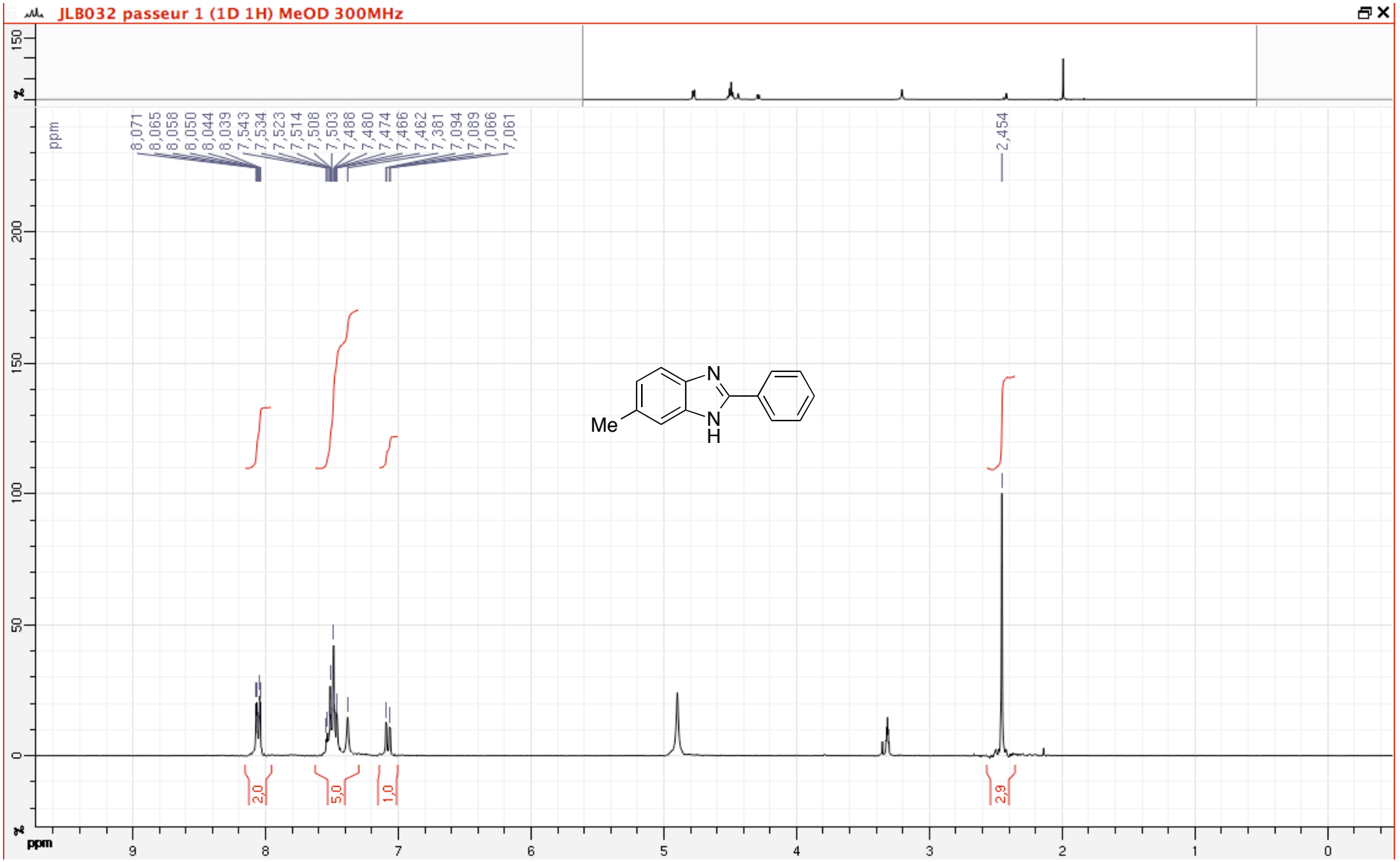

JLB035 passeur 2 (1D 13C) MeOD 300MHz
ppm
161,837
153,402
132,344
131,355
124,076
120,135
117,481
113,038
56,022
OMe
N
N
H
180
160
140
120
100
80
60
40
20
0

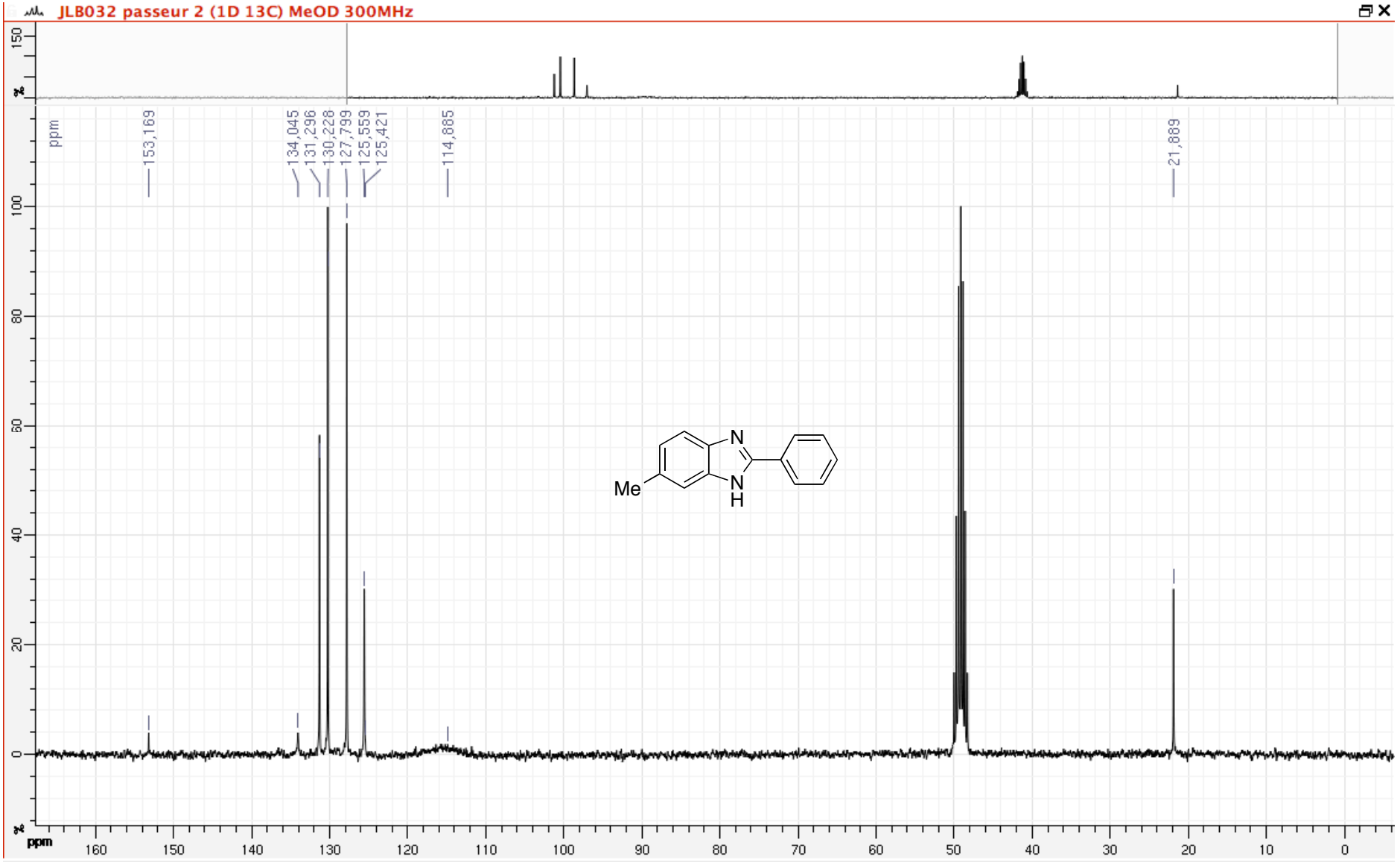
2-(2-Chlorophenyl)benzimidazole (3af)



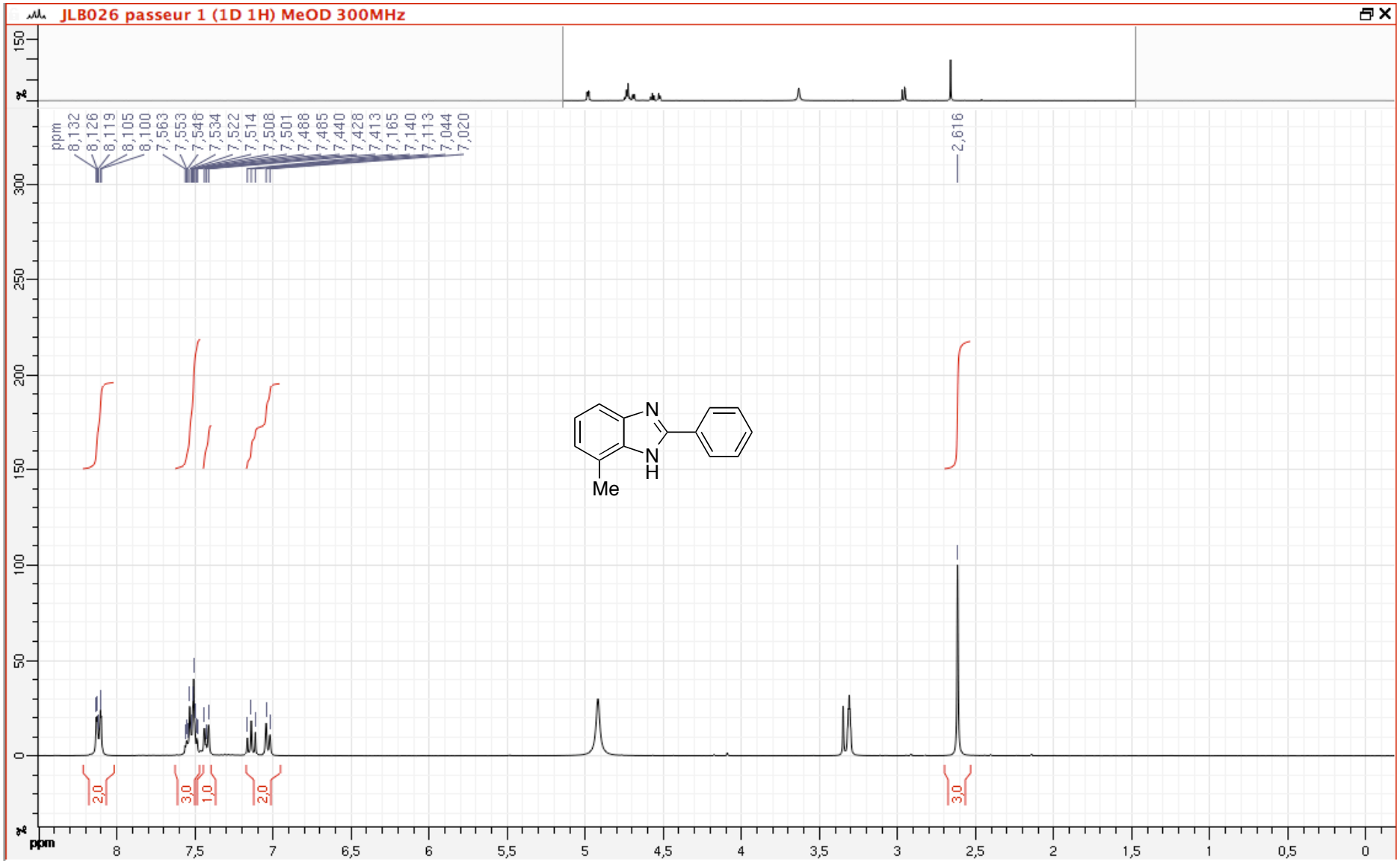

JLB034 passeur 2 (1D 13C) MeOD 300MHz
ppm
151,177
134,038
133,231
132,613
131,653
131,129
128,526
124,192
124,076
116,164
N
N
H
Cl

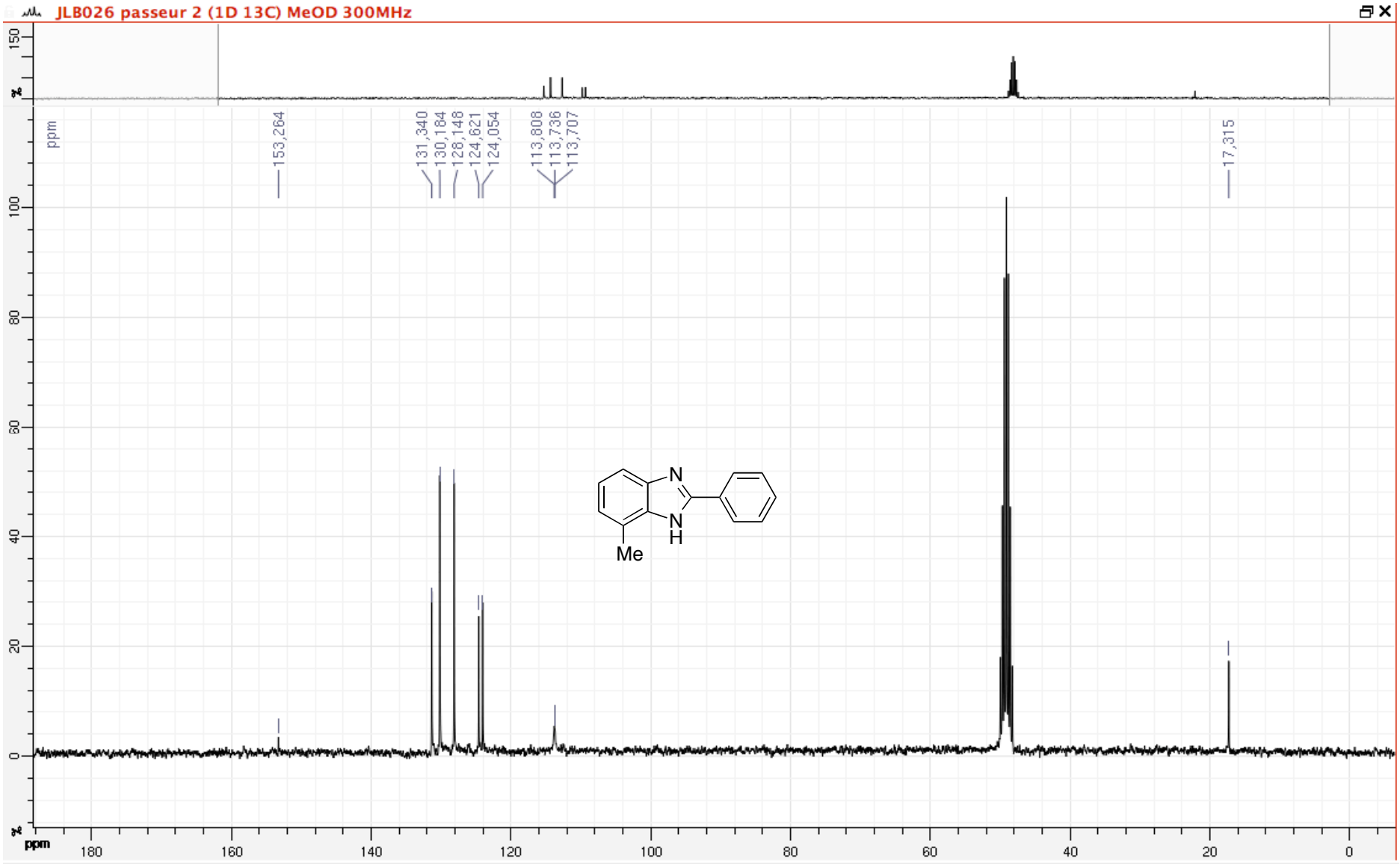
6-Methyl-2-phenylbenzimidazole (3ba)



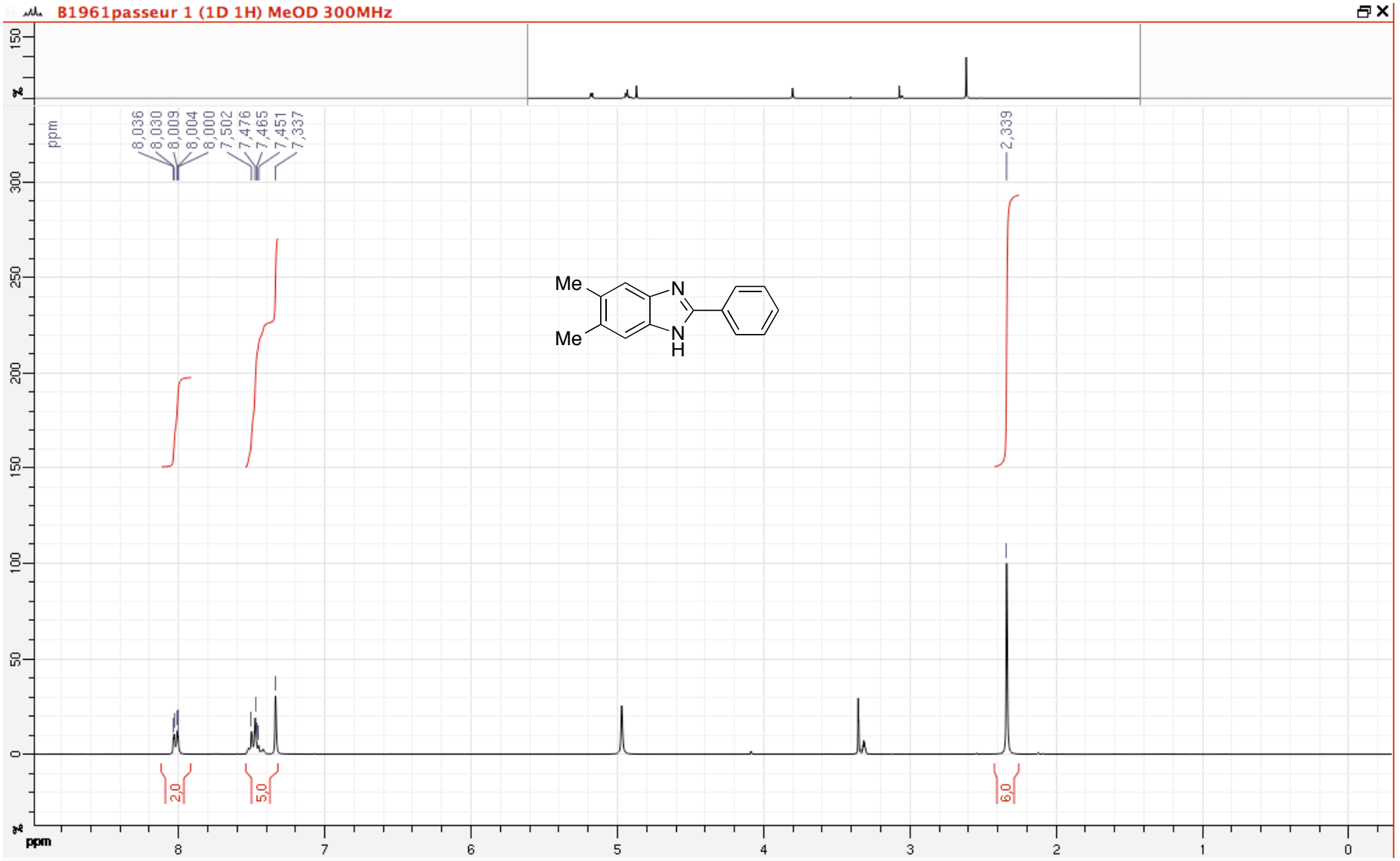

JLB032 passeur 2 (1D 13C) MeOD 300MHz
ppm
153,169
134,045
131,296
130,228
127,799
125,559
125,421
114,885
21,889
Me
N
N
H

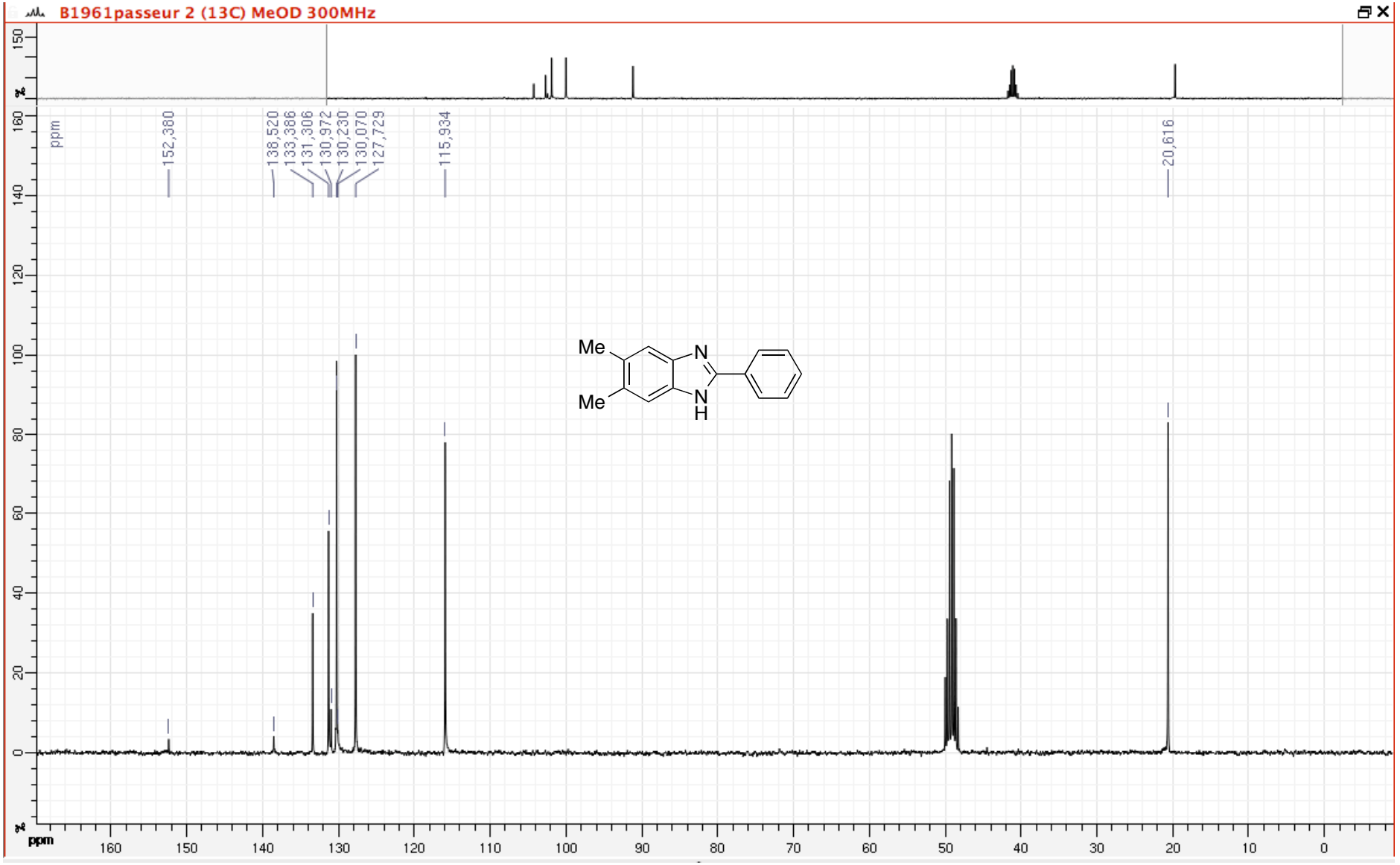
7-Methyl-2-phenylbenzimidazole (3ca)



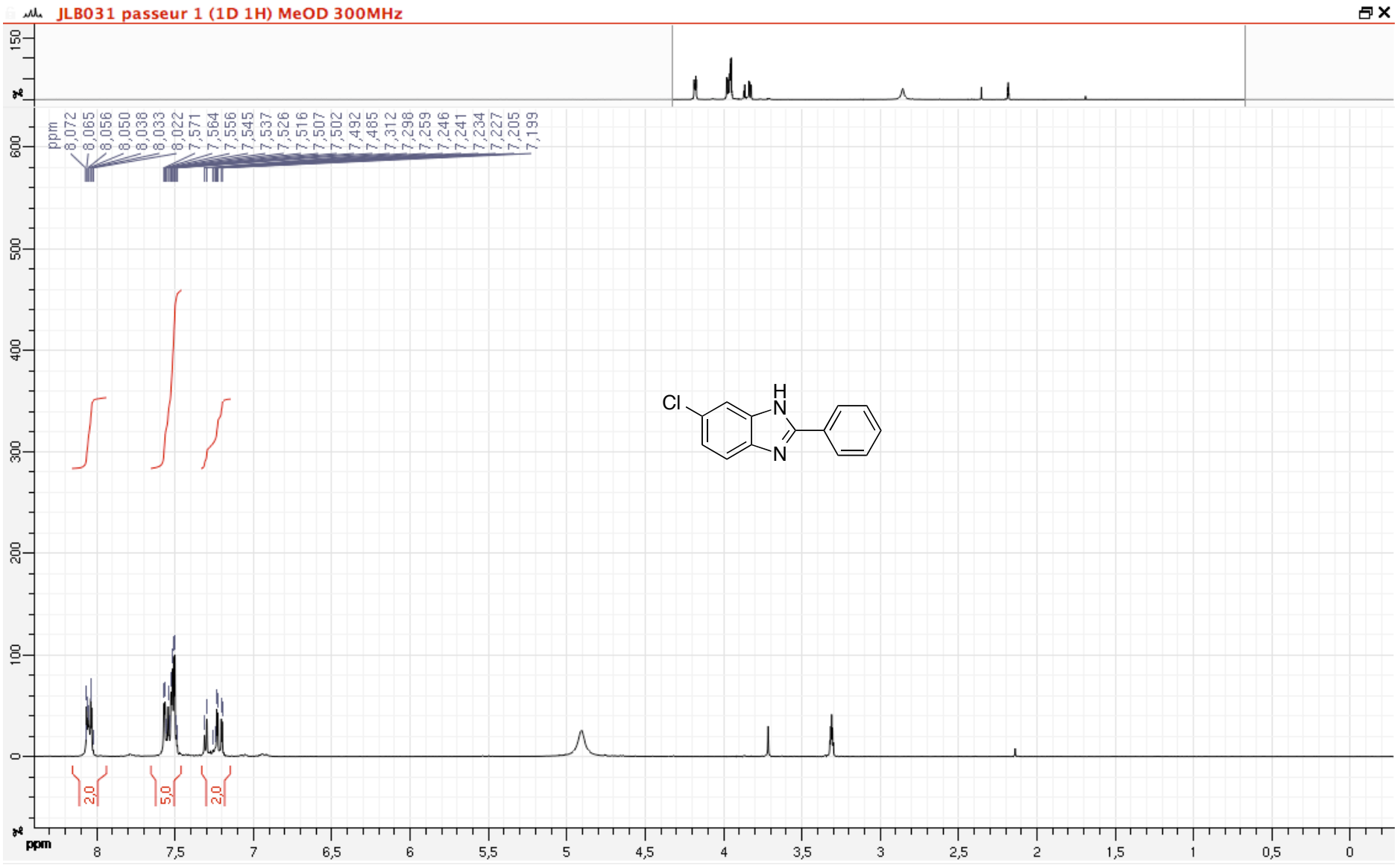

JLB026 passeur 2 (1D 13C) MeOD 300MHz
ppm
153,264
131,340
130,184
128,148
124,621
124,054
113,808
113,736
113,707
17,315
N
N
H
Me

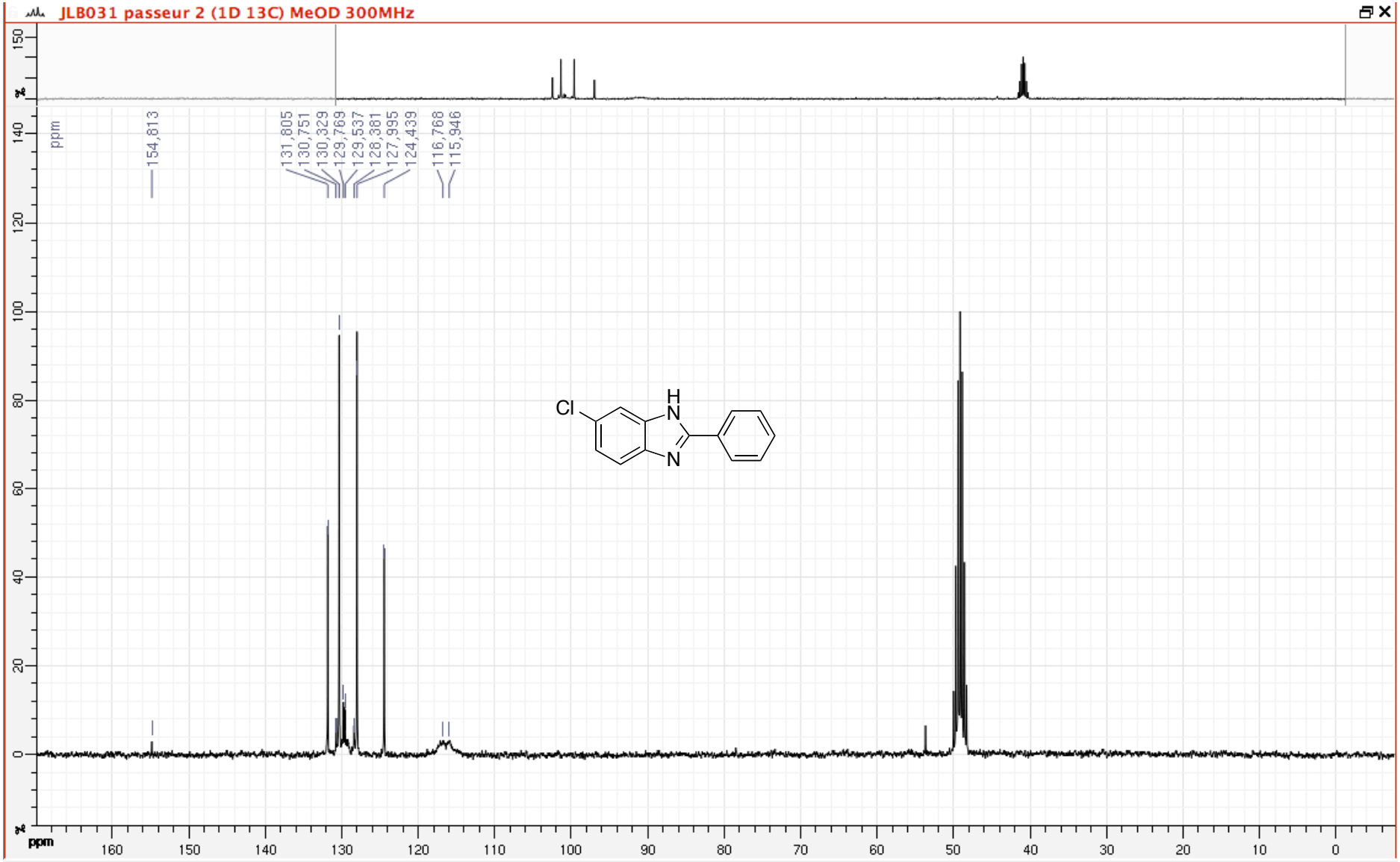
5,6-Dimethyl-2-phenylbenzimidazole (3da)



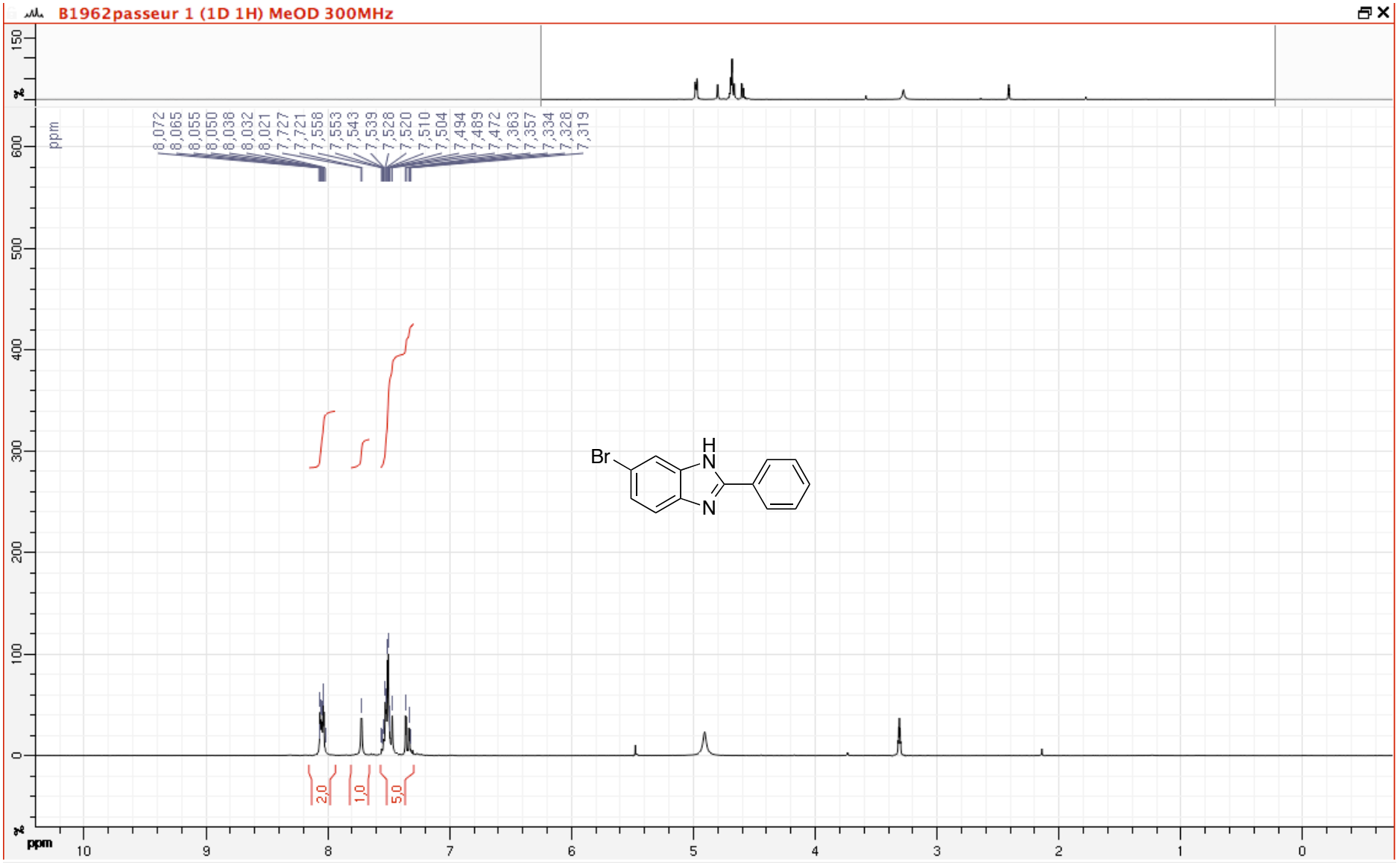

B1961passeur 2 (13C) MeOD 300MHz
ppm
152,380
138,520
133,386
131,306
130,972
130,230
130,070
127,729
115,934
20,616
Me
Me
N
N
H

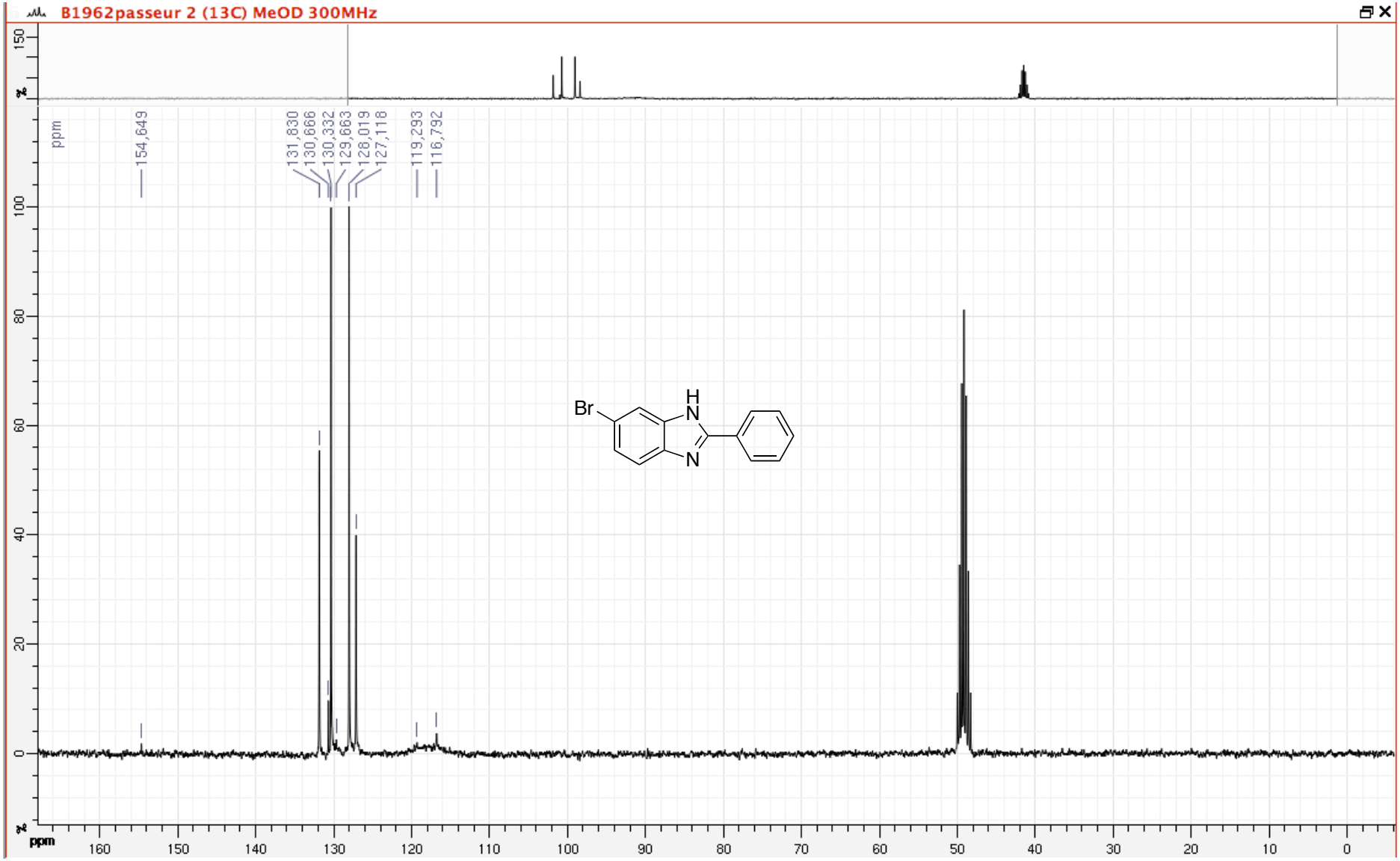
6-Chloro-2-phenylbenzimidazole (3ea)



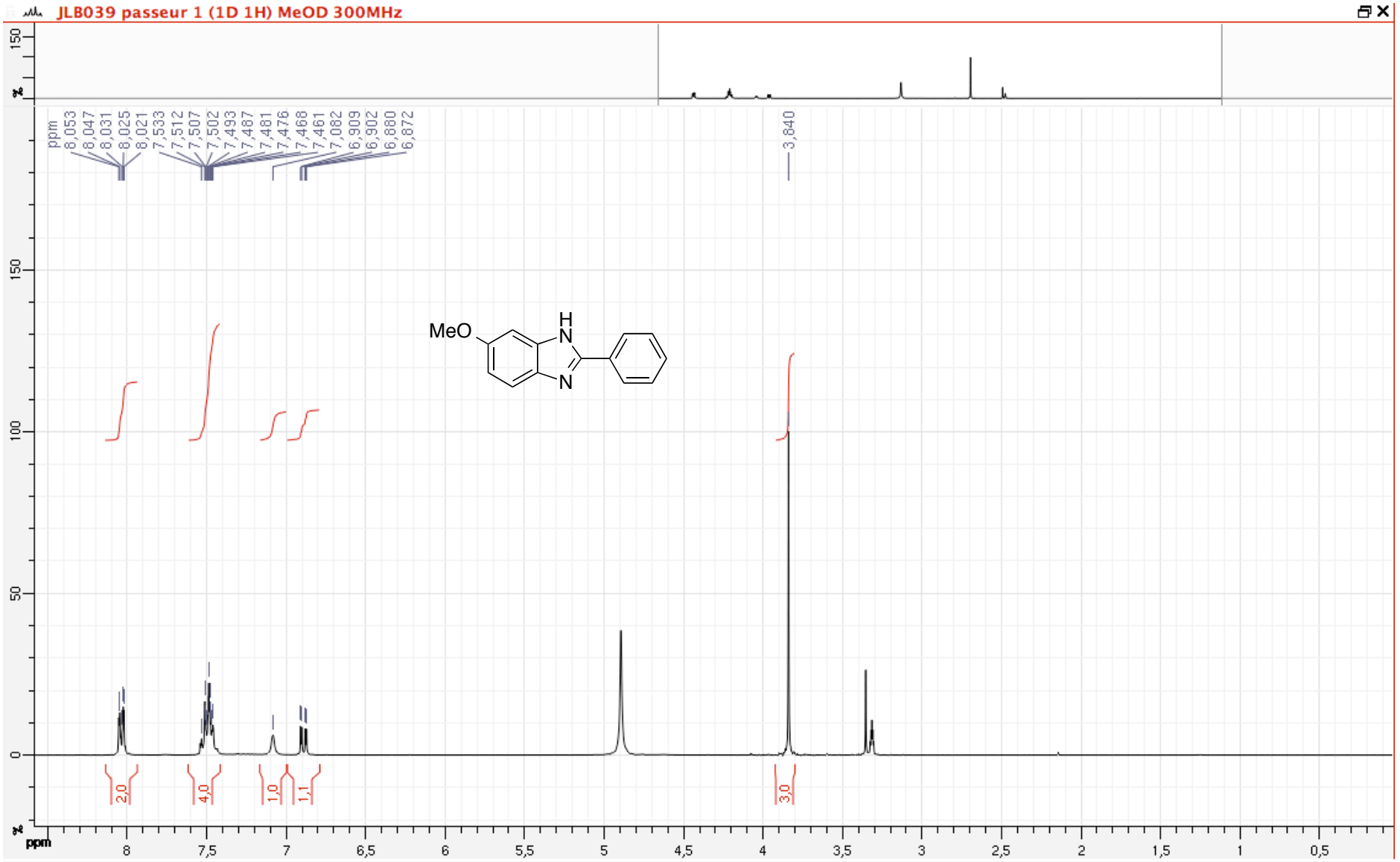

JLB031 passeur 2 (1D 13C) MeOD 300MHz
ppm
154,813
131,605
130,751
130,329
129,769
129,537
128,381
127,995
124,439
116,768
115,946
Cl
H
N
N
ppm

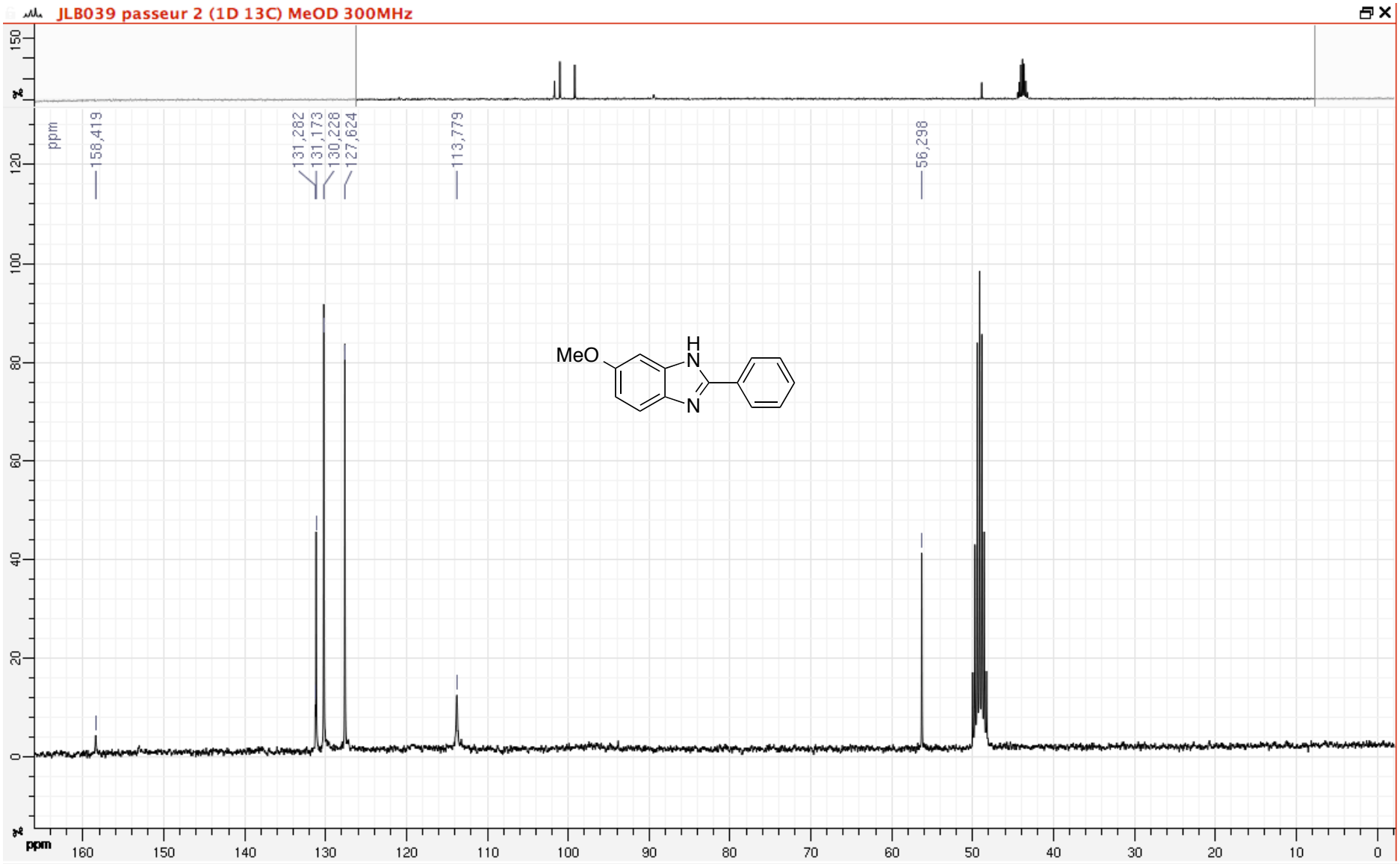
6-Bromo-2-phenylbenzimidazole (3fa)



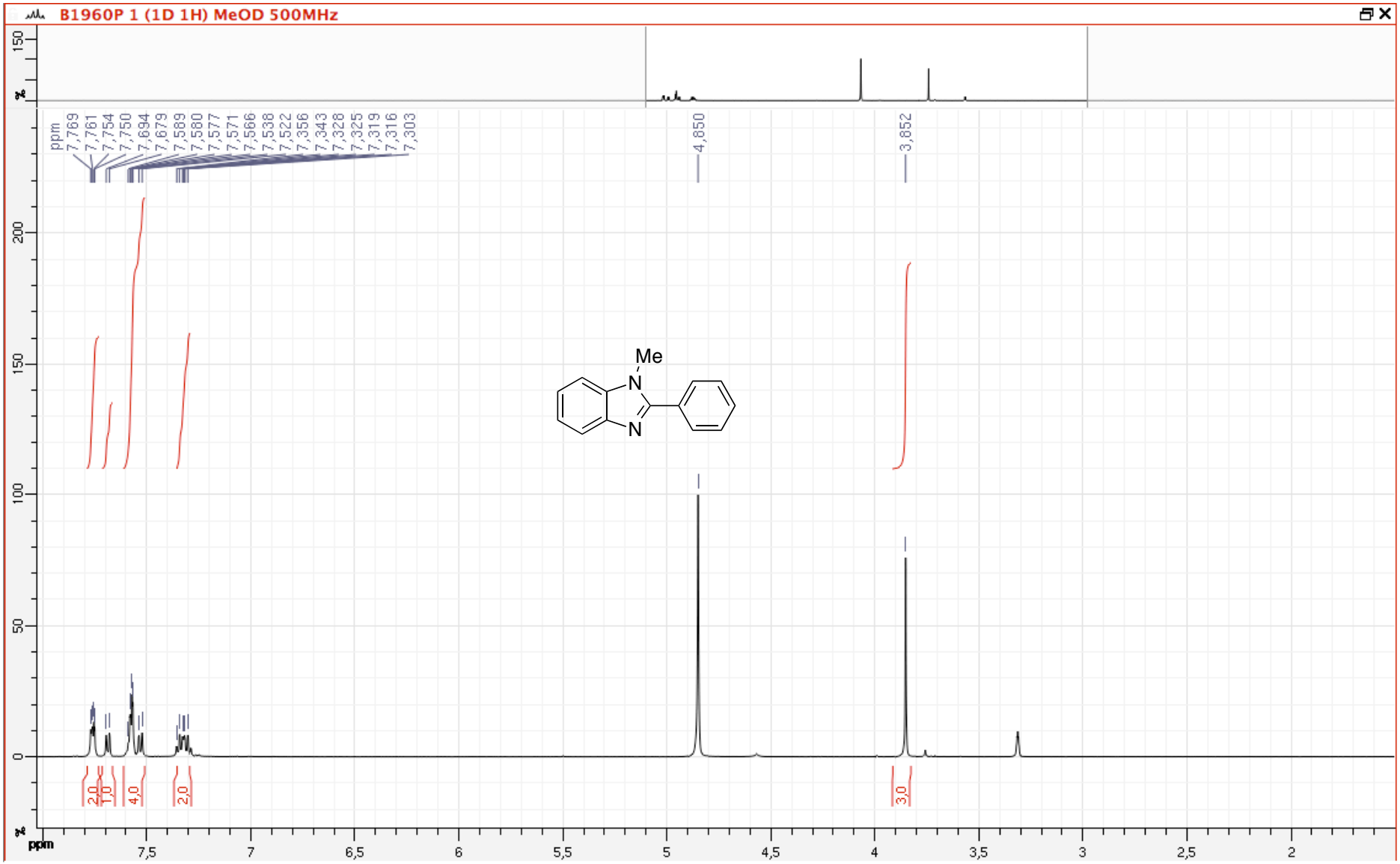

B1962passeur 2 (13C) MeOD 300MHz
ppm
154,649
131,830
130,666
130,332
129,663
128,019
127,118
119,293
116,792
Br
H
N
N

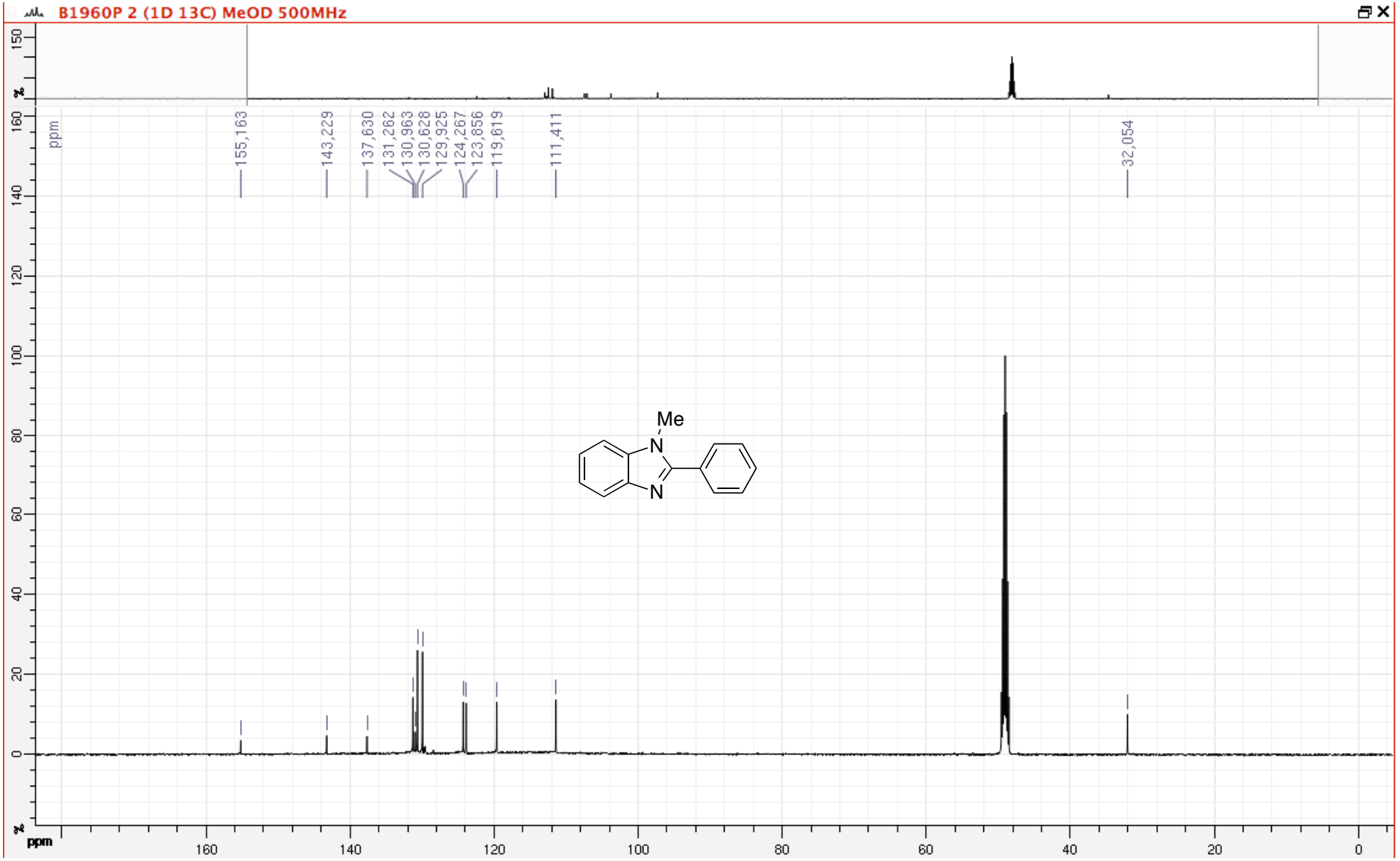
6-Methoxy-2-phenylbenzimidazole (3ga)



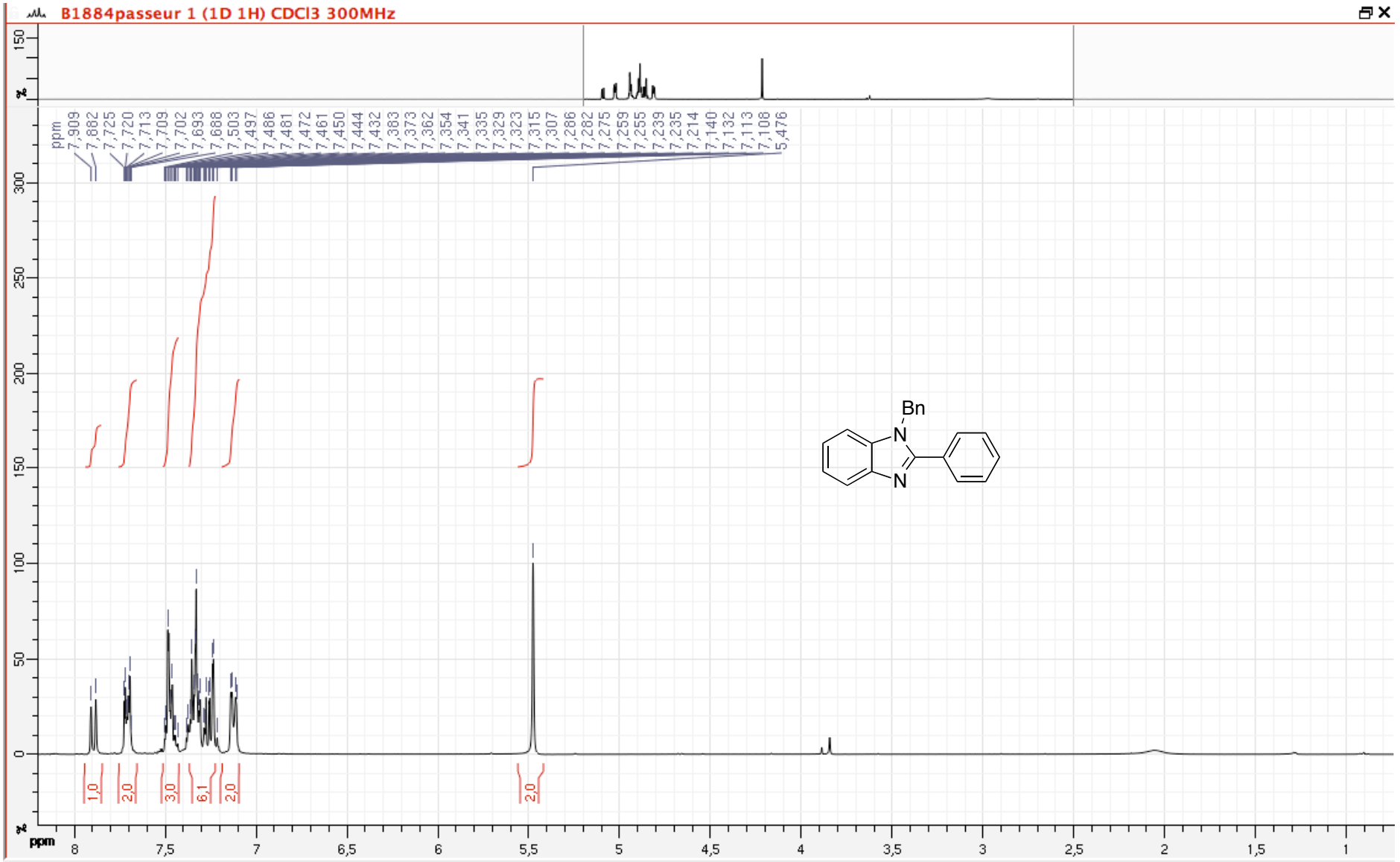

JLB039 passeur 2 (1D 13C) MeOD 300MHz
ppm
158,419
131,282
131,173
130,228
127,624
113,779
56,298
MeO
H
N
N

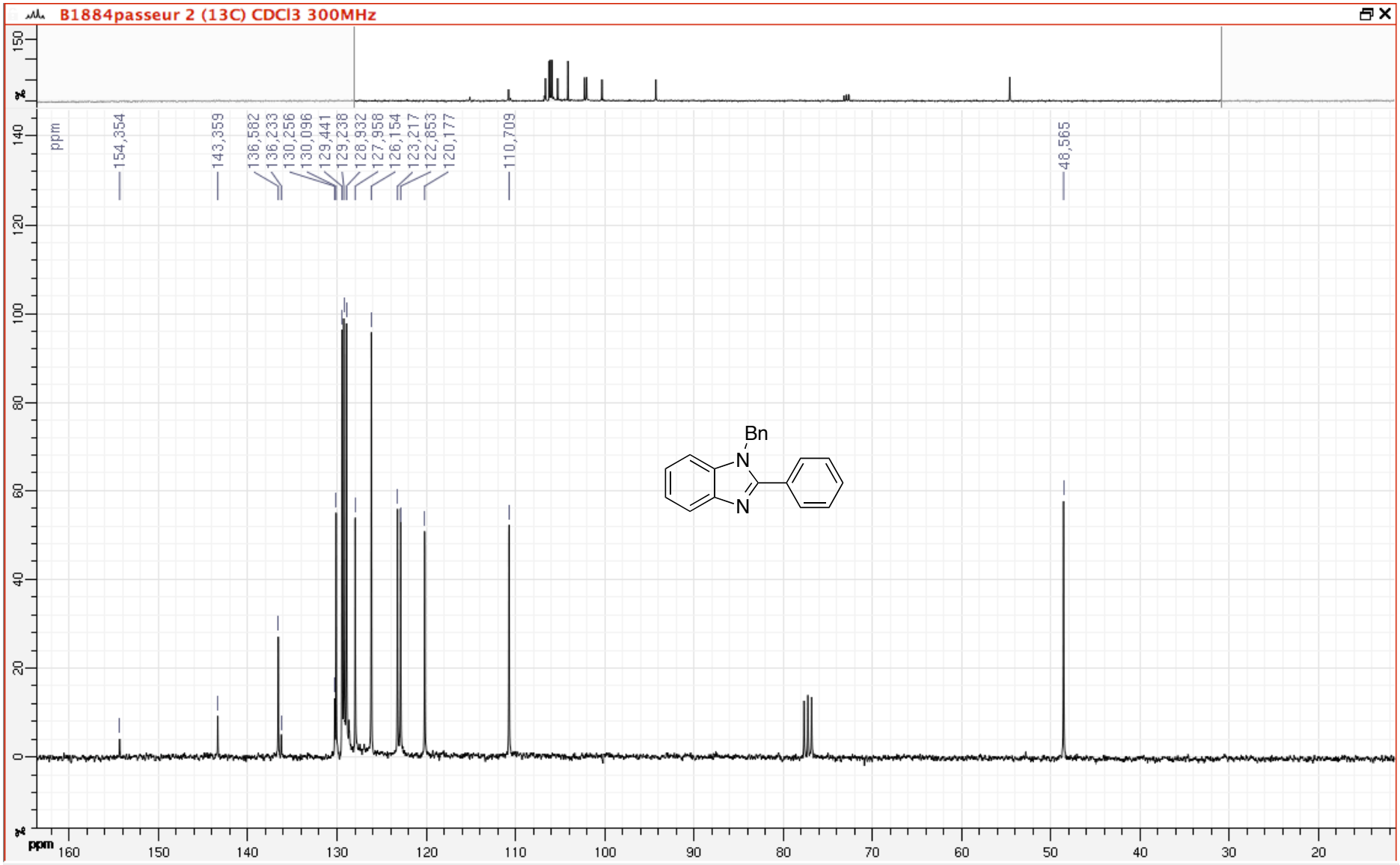
1-Methyl-2-phenylbenzimidazole (3ha)



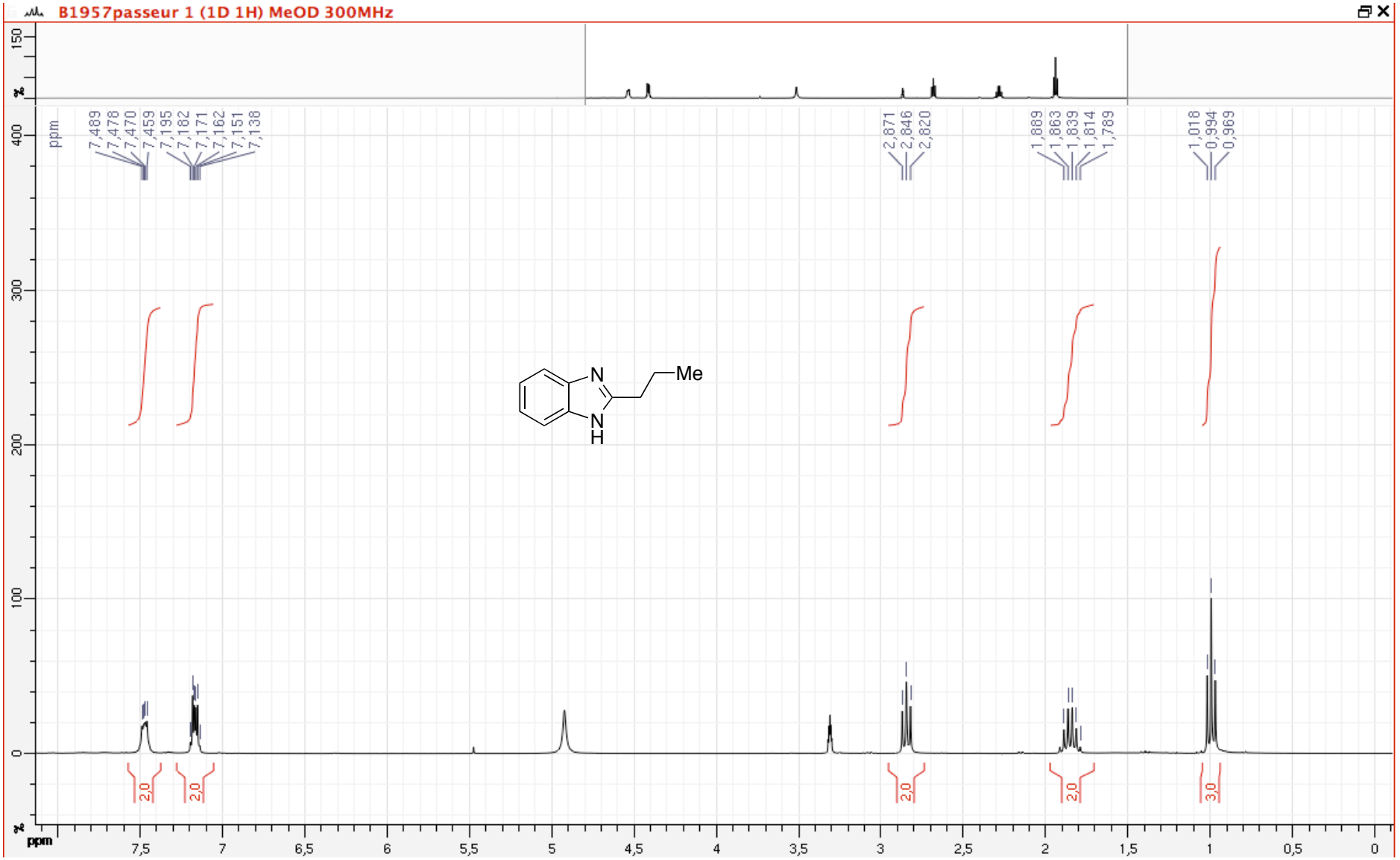

B1960P 2 (1D 13C) MeOD 500MHz
ppm
155,163
143,229
137,630
131,262
130,963
130,628
129,925
124,267
123,856
119,619
111,411
32,054
Me
N
N

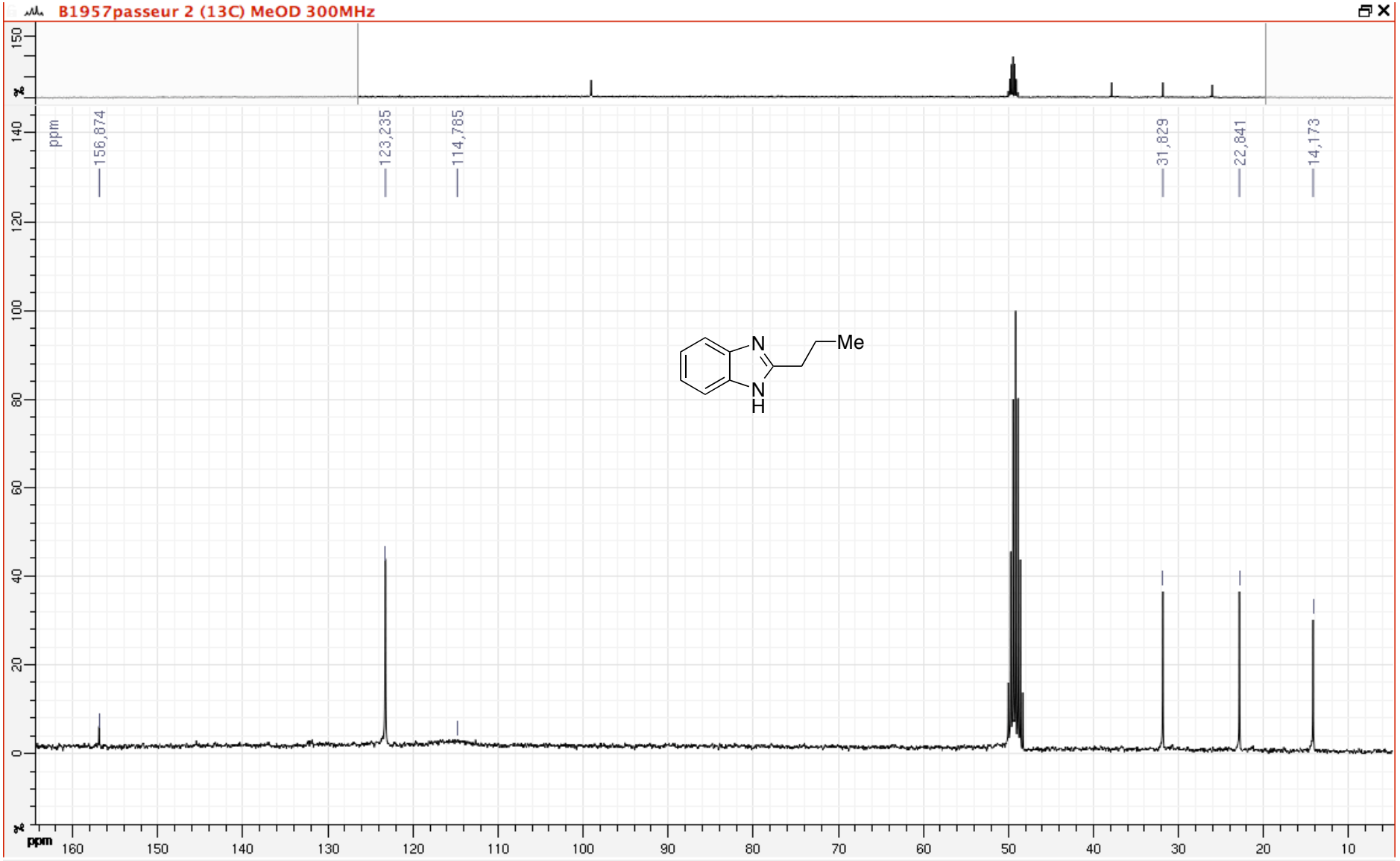
1-Benzyl-2-phenylbenzimidazole (3ia)



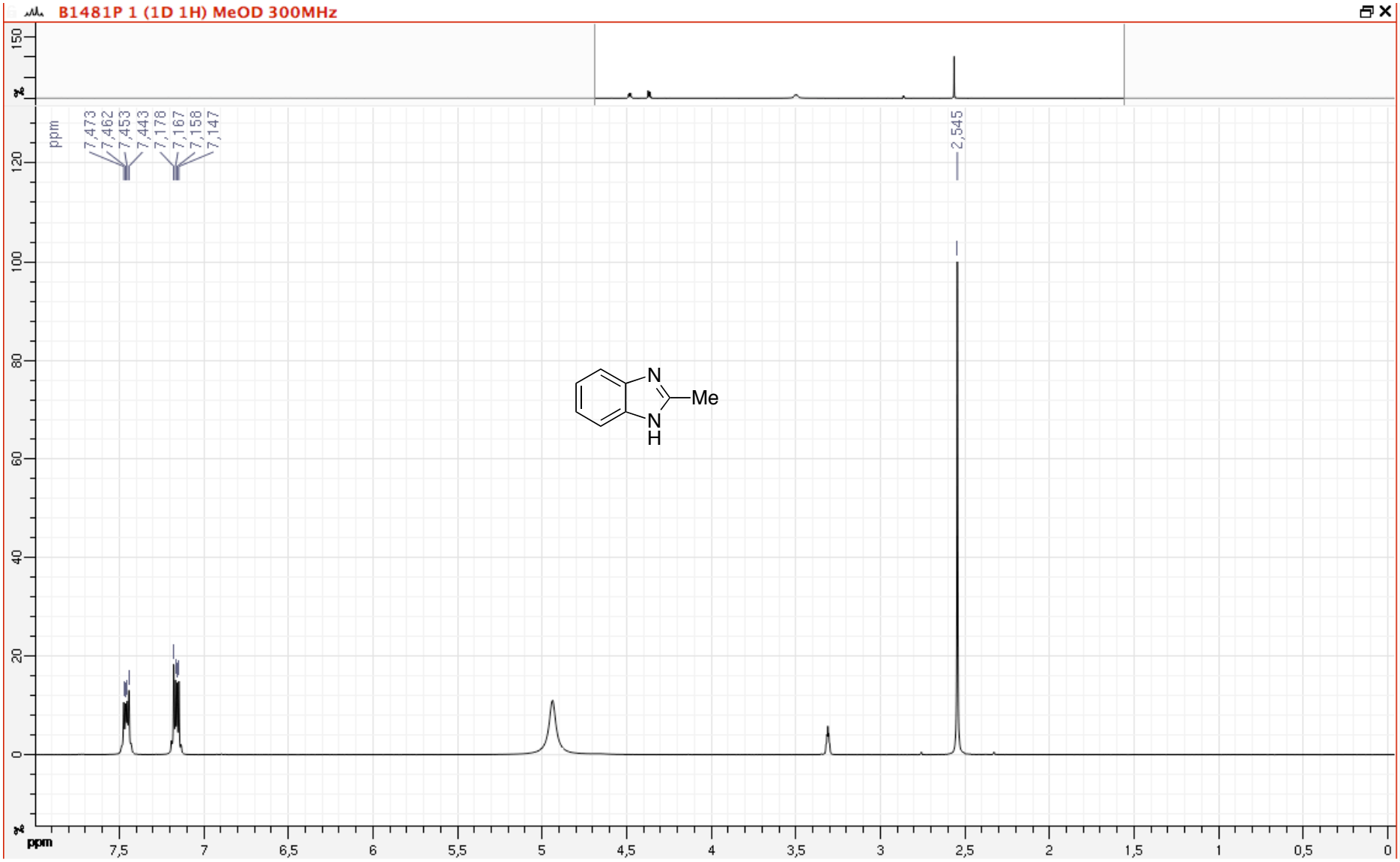

B1884passeur 2 (13C) CDCl3 300MHz
ppm
154,354
143,359
136,582
136,233
130,256
130,096
129,441
129,238
128,932
127,956
126,154
123,217
122,853
120,177
110,709
48,565
Bn
N
N

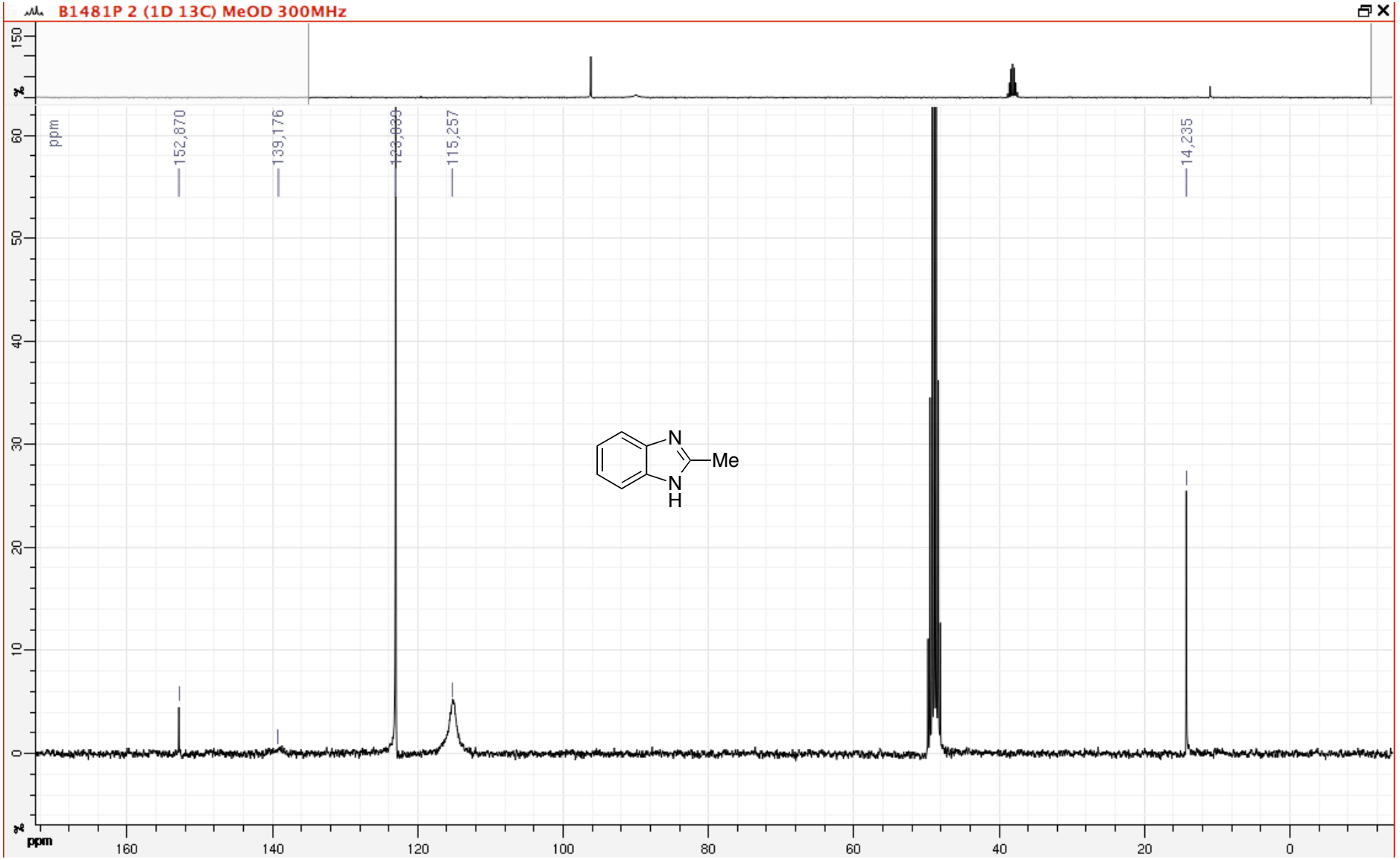
2-Propylbenzimidazole (3ah)



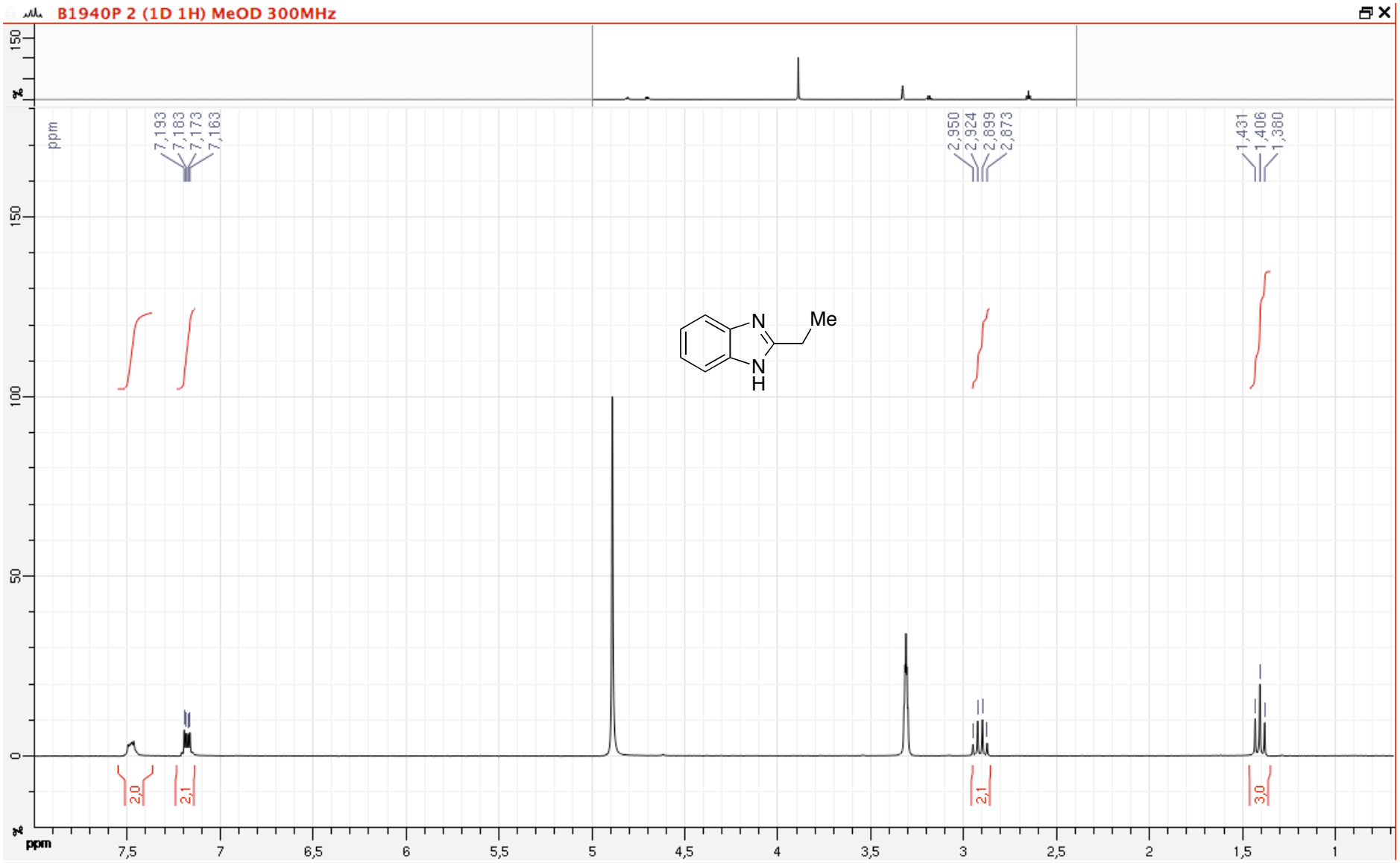

B1957passeur 2 (13C) MeOD 300MHz
ppm
156,874
123,235
114,785
31,829
22,841
14,173
N
N
H
Me

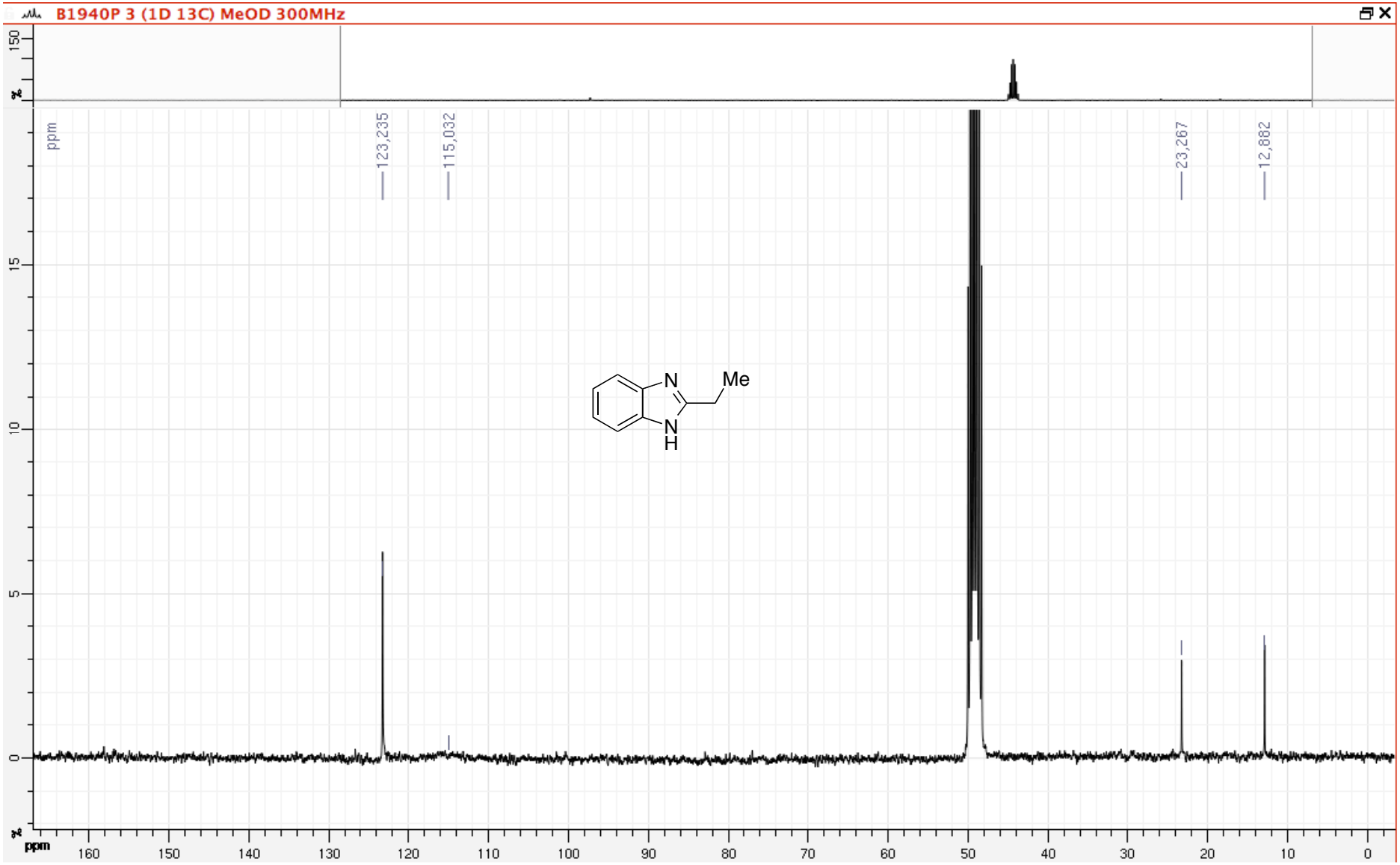
2-Methylbenzimidazole (3ai)



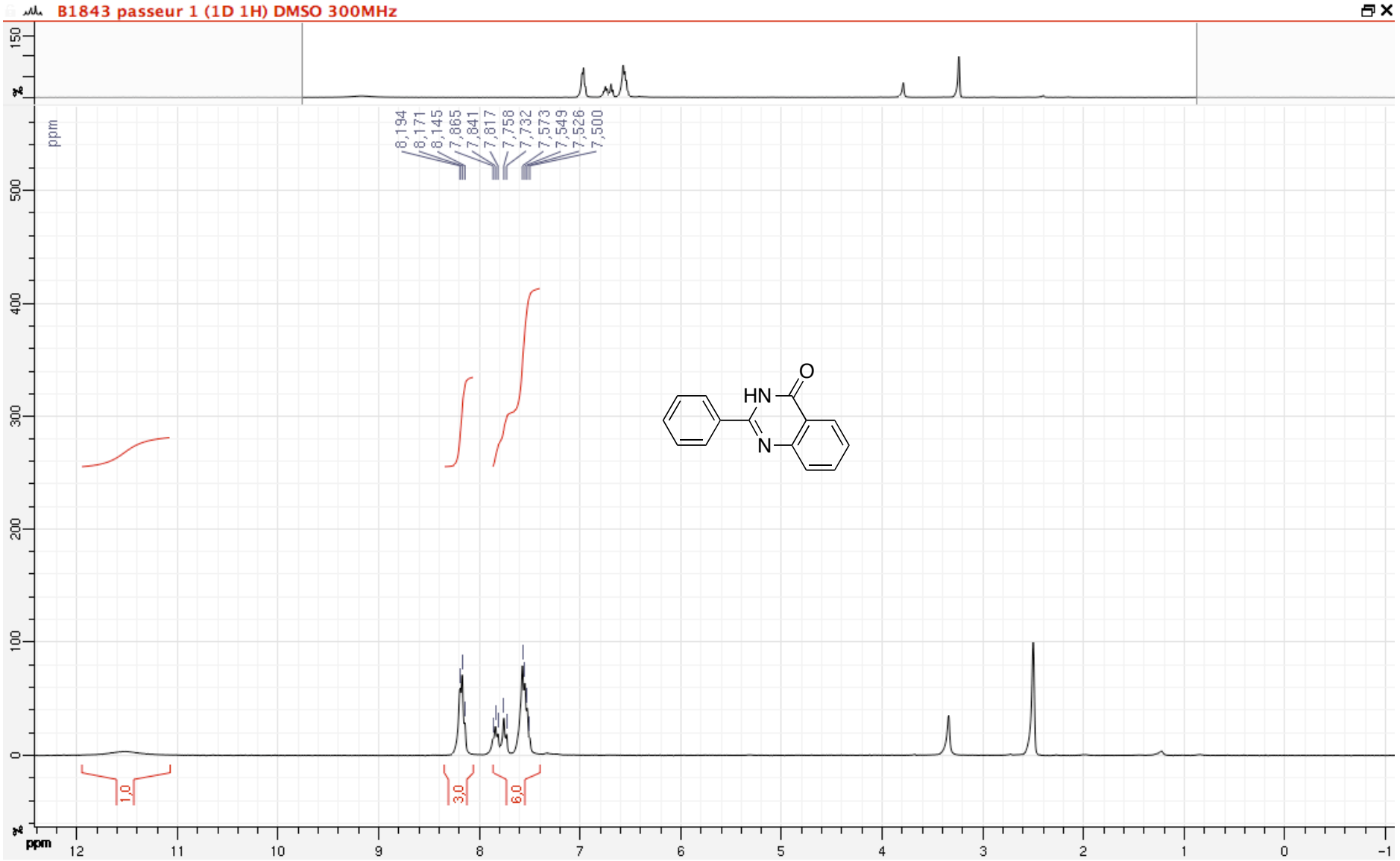

B1481P 2 (1D 13C) MeOD 300MHz
ppm
152,870
139,176
123,030
115,257
14,235
N
Me
N
H
160
140
120
100
80
60
40
20
0

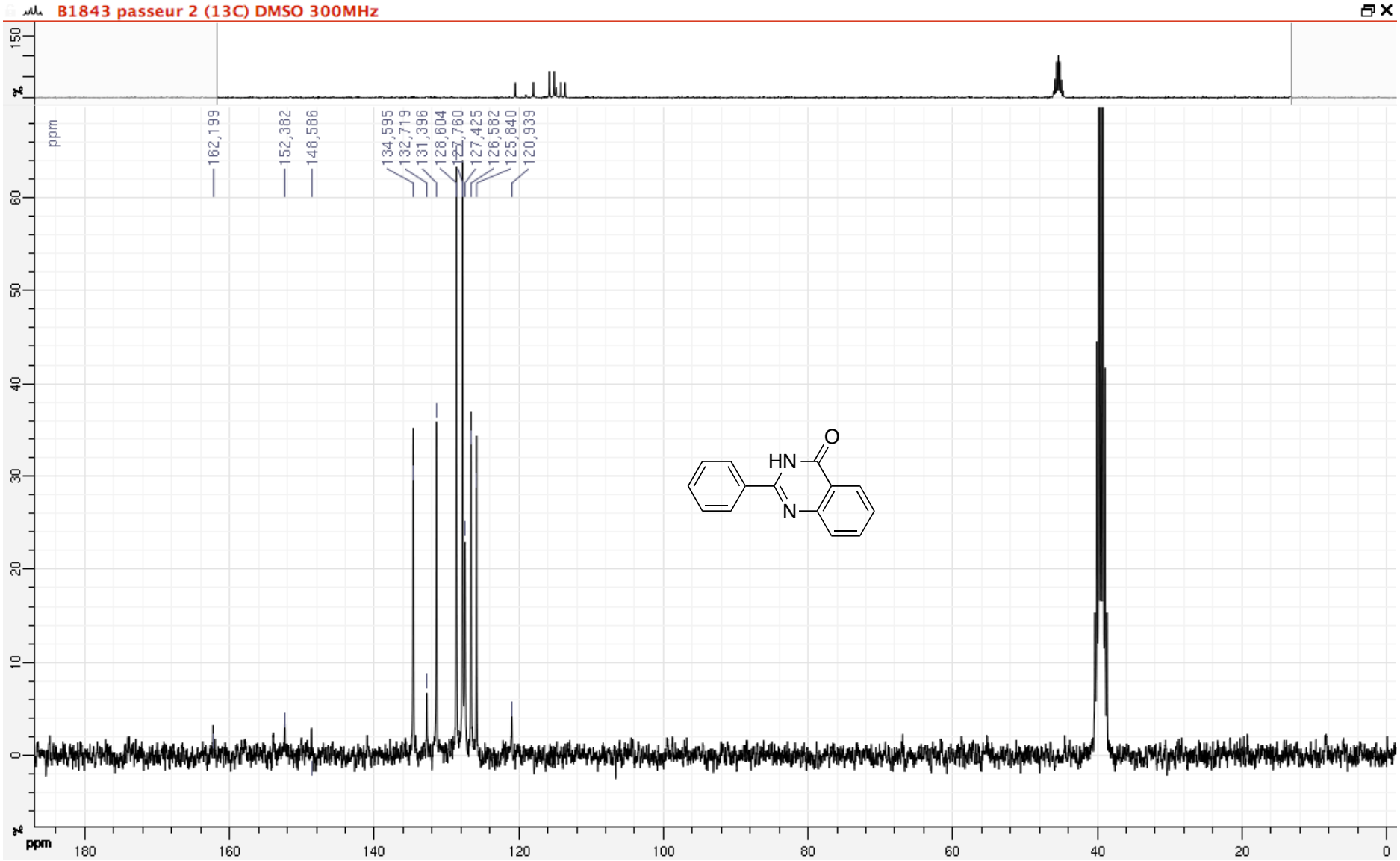
2-Methylbenzimidazole (3aj)



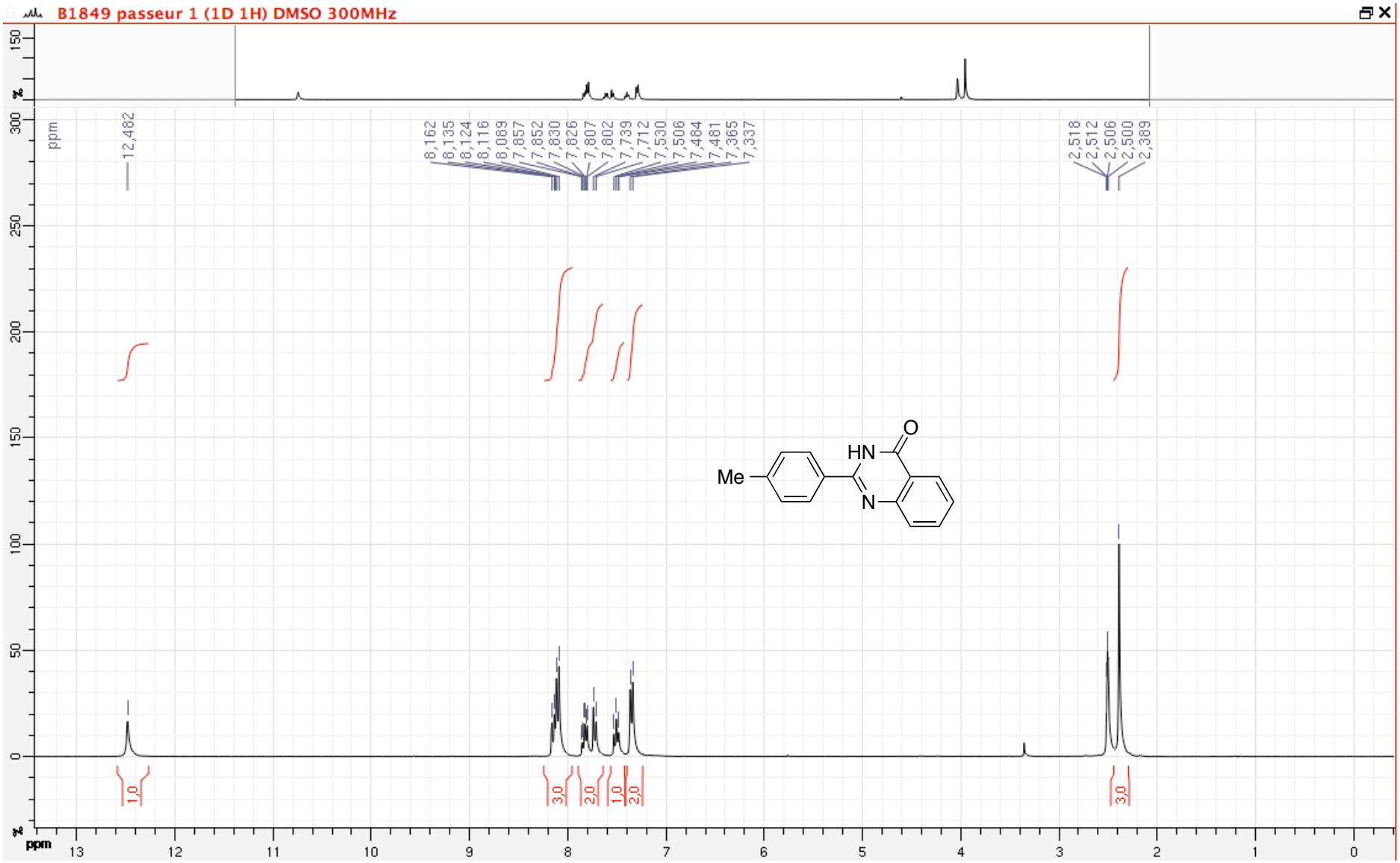

B1940P 3 (1D 13C) MeOD 300MHz
ppm
123,235
115,032
23,267
12,882
N
Me
N
H
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

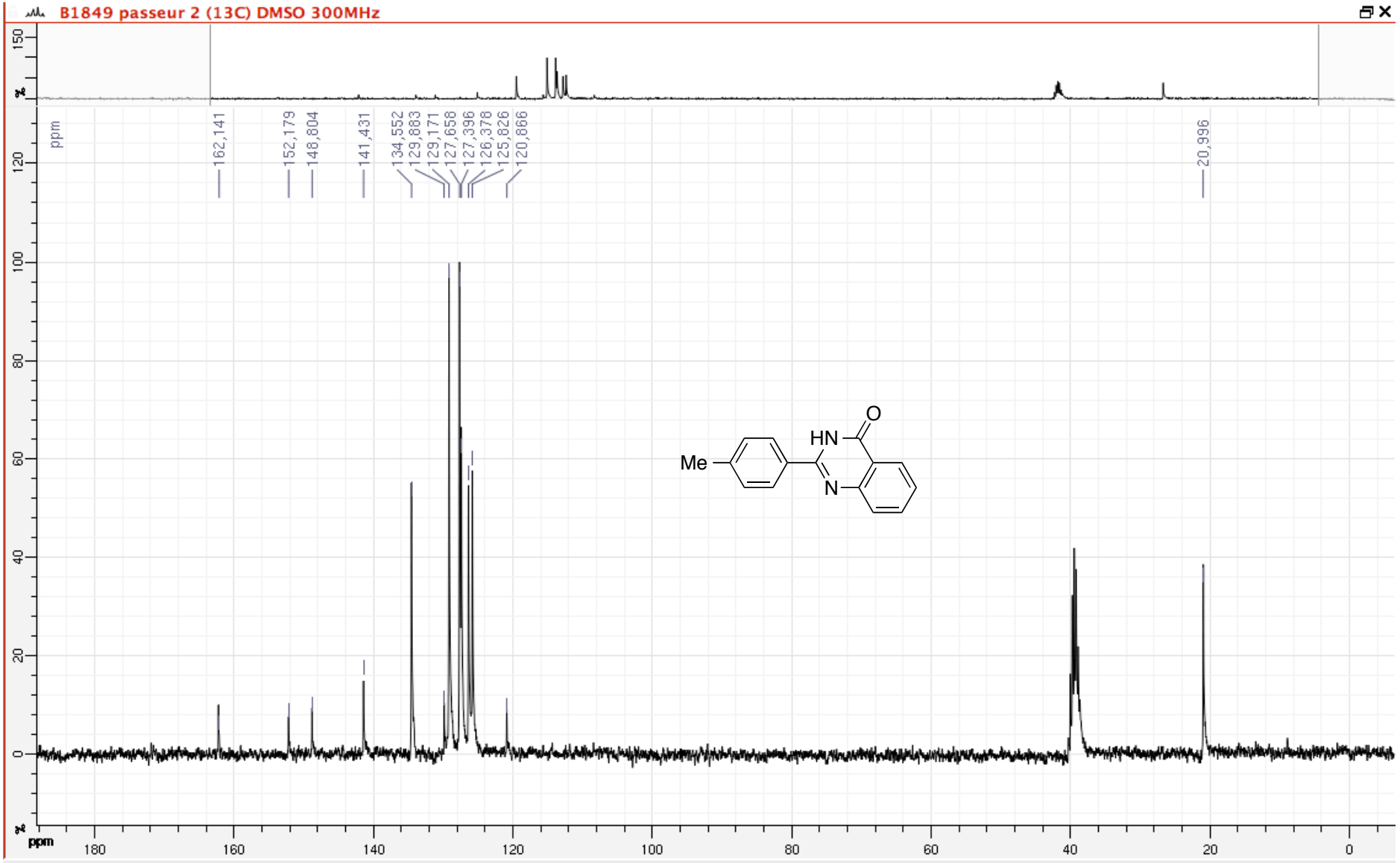
2-Phenylquinazolin-4(3*H*)-one (3ja)



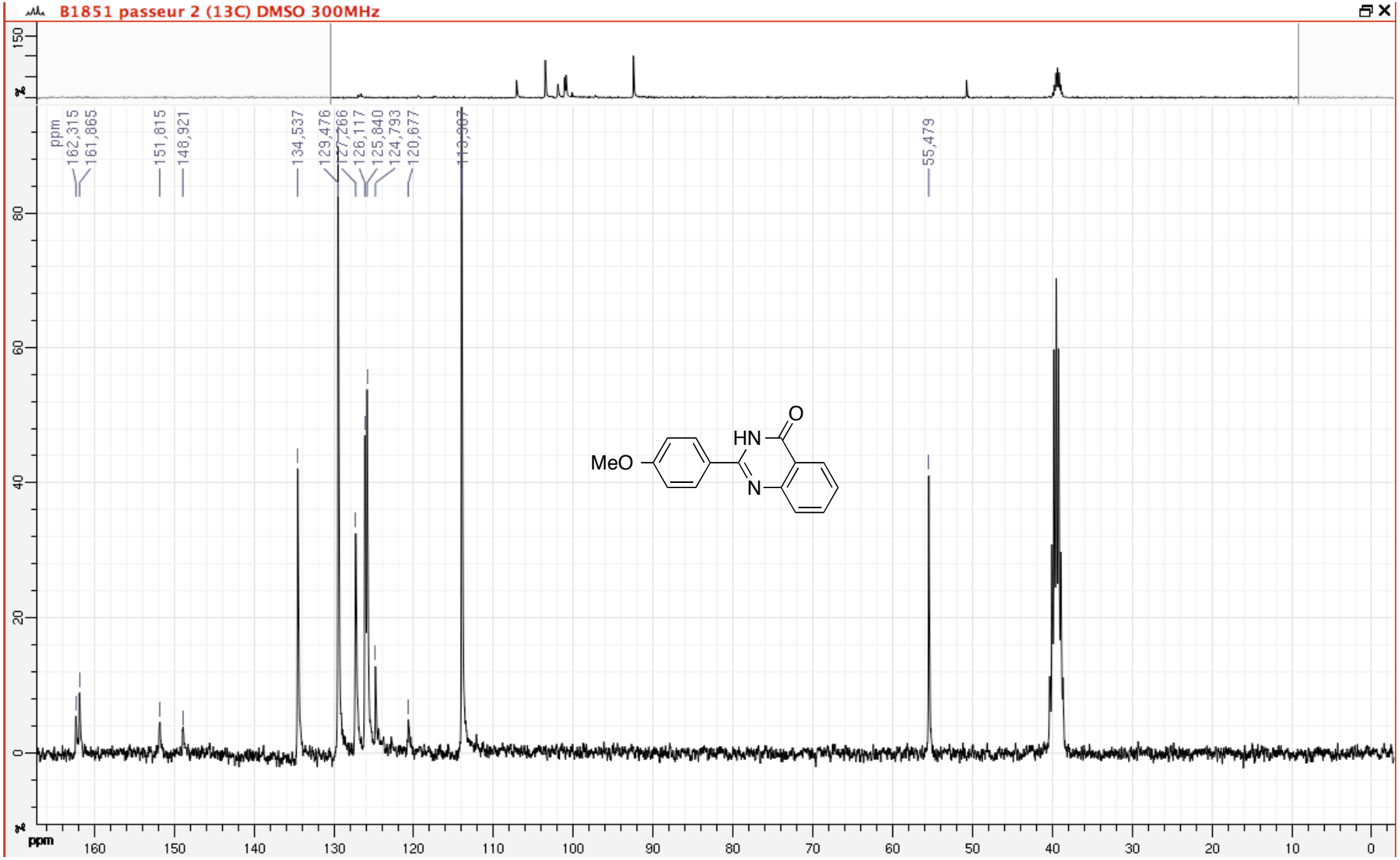

B1843 passeur 2 (13C) DMSO 300MHz
ppm
162,199
152,382
148,586
134,595
132,719
131,396
128,604
127,760
127,425
126,582
125,840
120,939
HN
O
N
180
160
140
120
100
80
60
40
20
0

2-(*p*-Tolyl)quinazolin-4(3*H*)-one (3jb)

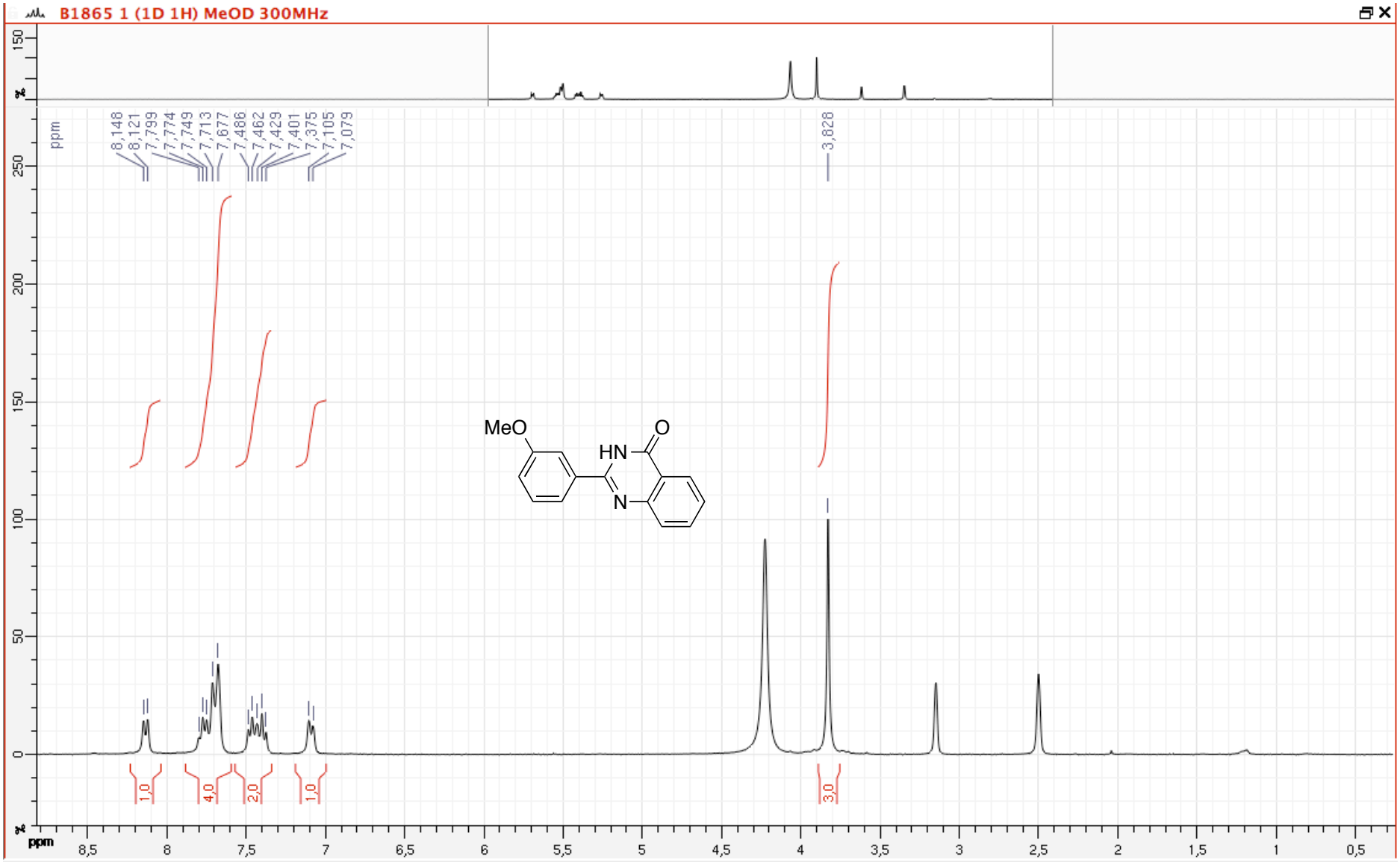


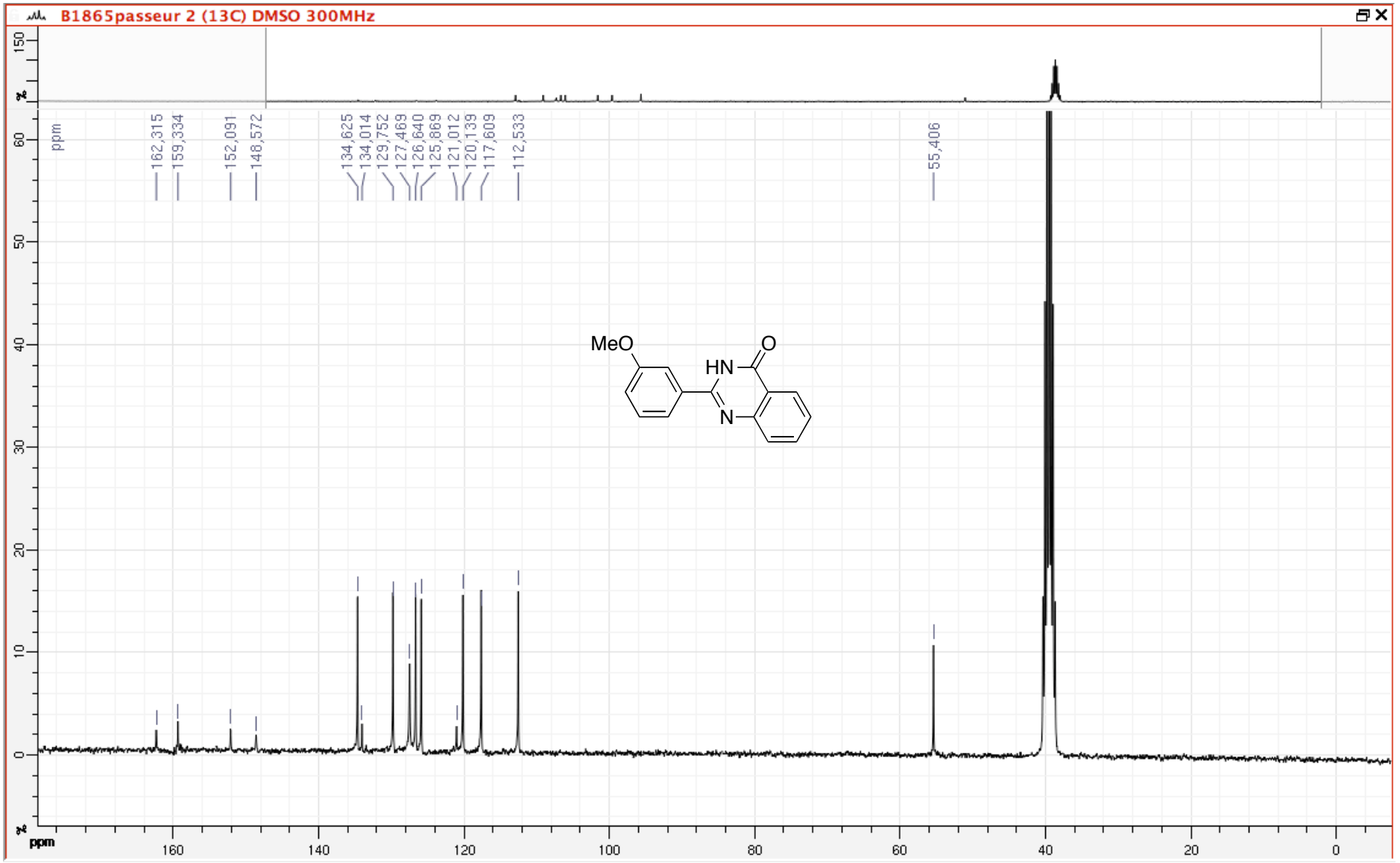

B1849 passeur 2 (13C) DMSO 300MHz
ppm
162,141
152,179
148,804
141,431
134,552
129,883
129,171
127,658
127,396
126,378
125,826
120,866
20,996
Me
HN
O
N
ppm
180
160
140
120
100
80
60
40
20
0

2-(*p*-Methoxyphenyl)quinazolin-4(3*H*)-one (3jd)

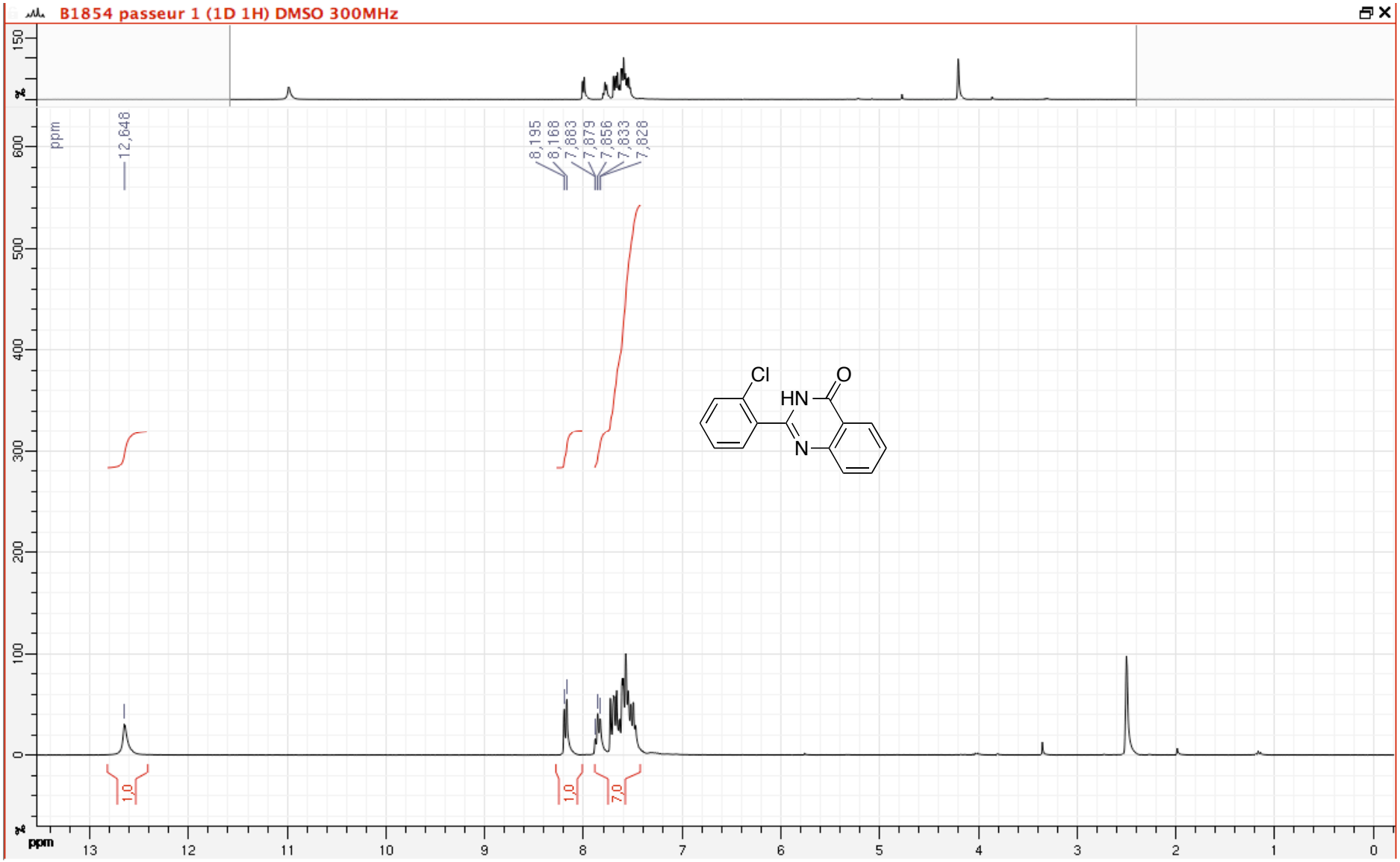

B1851 passeur 2 (13C) DMSO 300MHz
ppm
162,315
161,865
151,815
148,921
134,537
129,476
127,266
126,117
125,840
124,793
120,677
113,987
55,479
MeO
HN
O
N

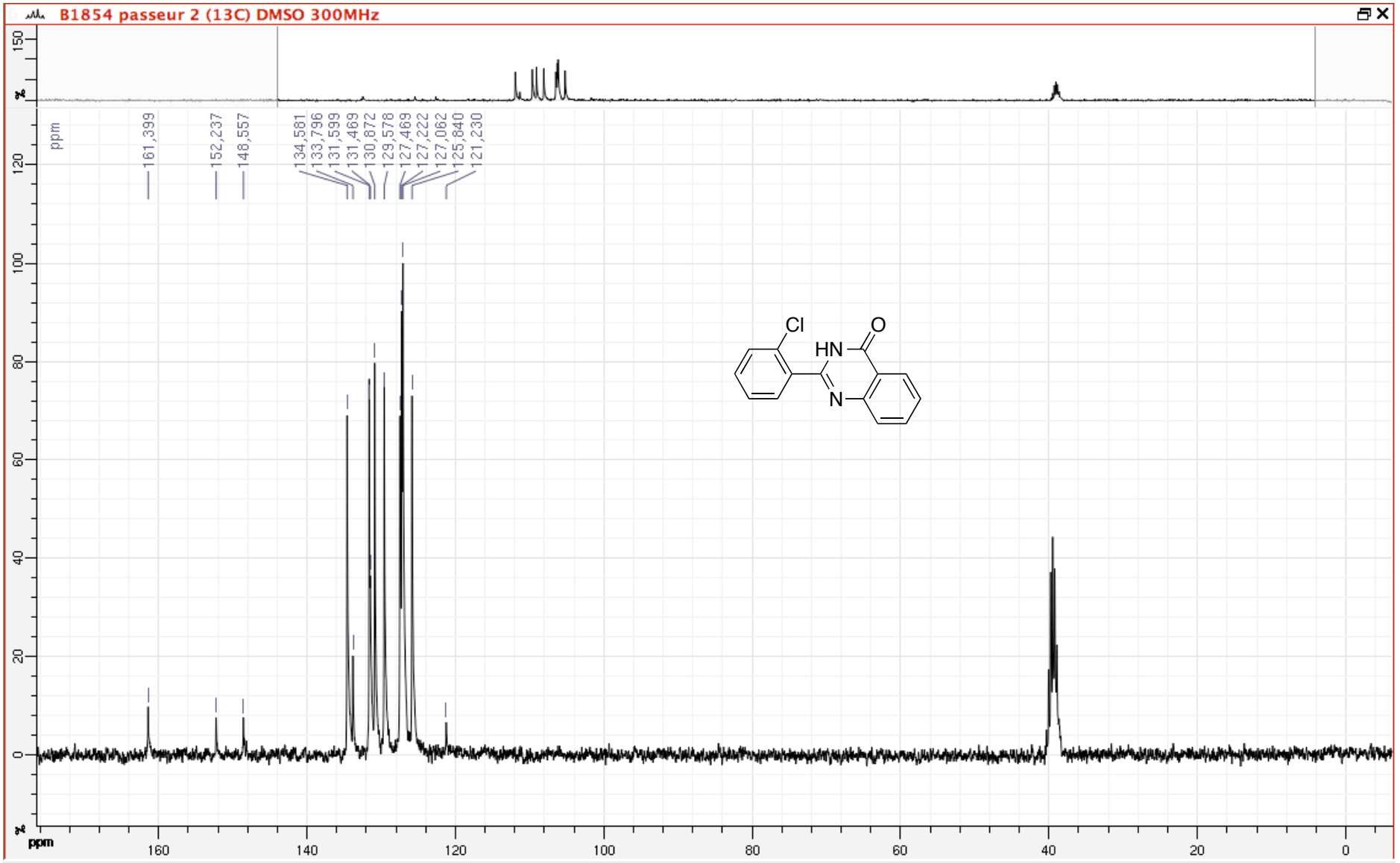
2-(*m*-Methoxyphenyl)quinazolin-4(3*H*)-one (3je)



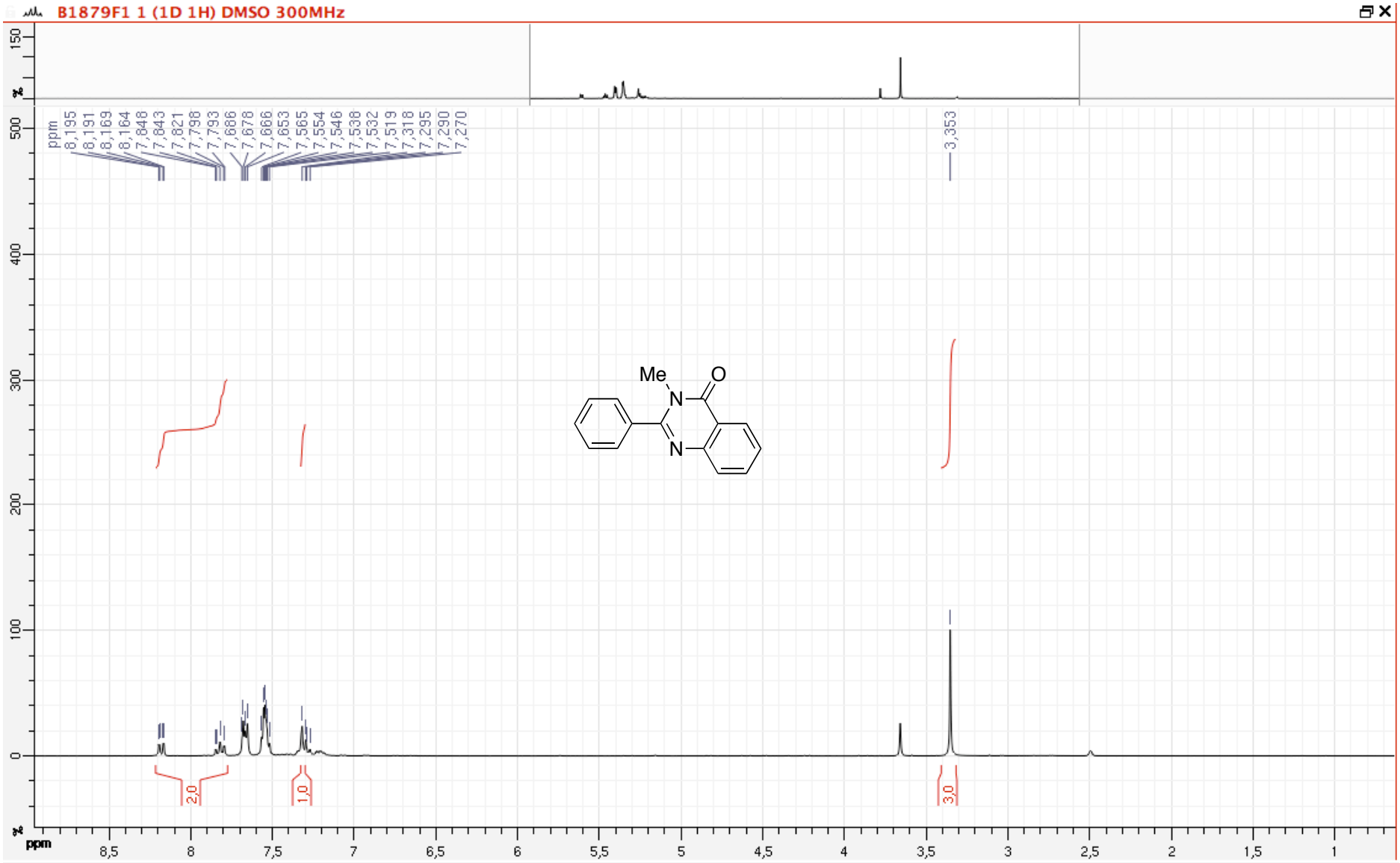

B1865passeur 2 (13C) DMSO 300MHz
ppm
162,315
159,334
152,091
148,572
134,625
134,014
129,752
127,469
126,640
125,869
121,012
120,139
117,609
112,533
55,406
MeO
HN
O
N
160
140
120
100
80
60
40
20
0

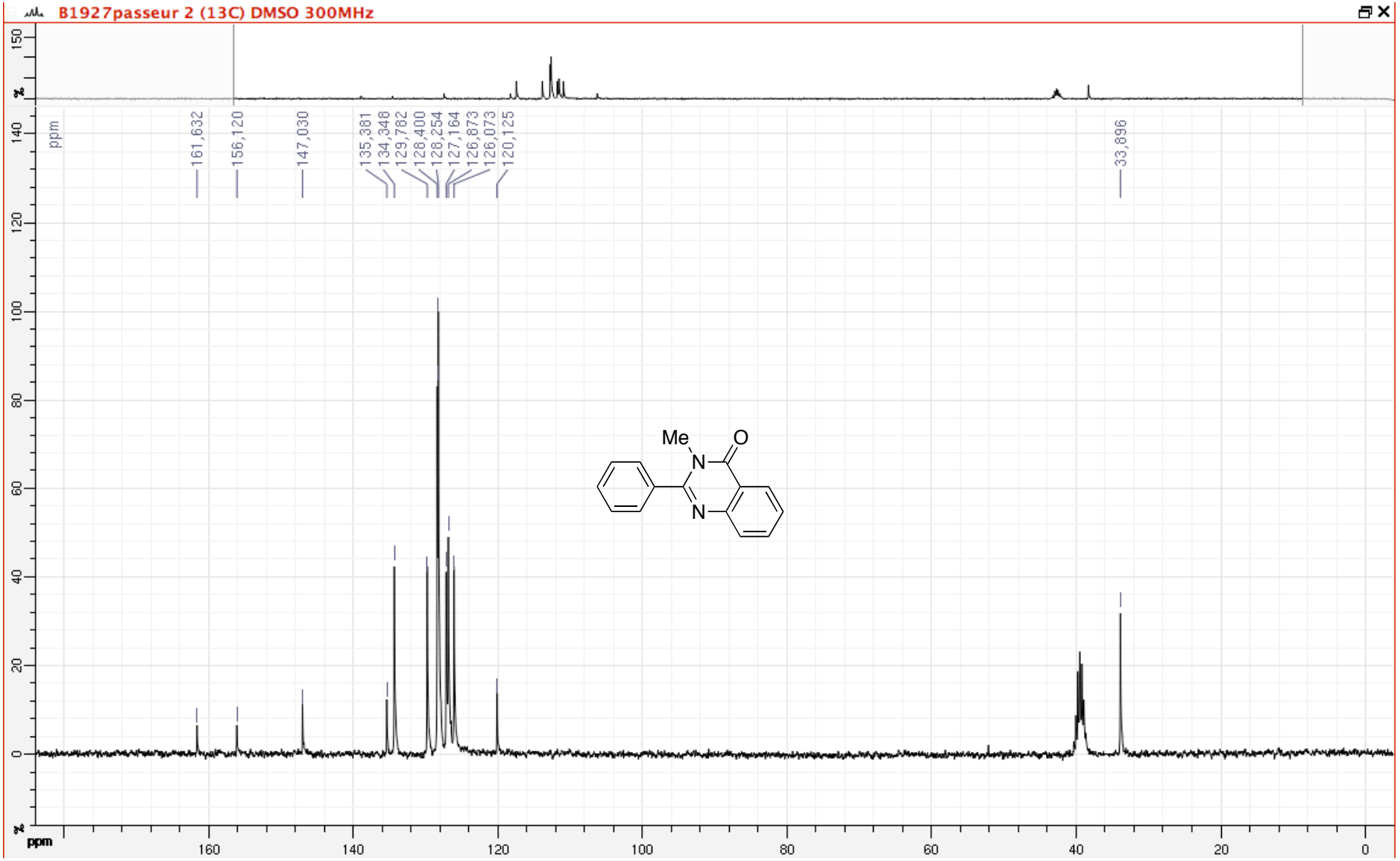
2-(*o*-Chlorophenyl)quinazolin-4(3*H*)-one (3jf)




B1854 passeur 2 (13C) DMSO 300MHz
ppm
161,399
152,237
148,557
134,581
133,796
131,599
131,469
130,872
129,578
127,469
127,222
127,062
125,840
121,230
Cl
O
HN
N

3-Methyl-2-phenylquinazolin-4(3*H*)-one (3ka)




B1927passeur 2 (13C) DMSO 300MHz
ppm
161,632
156,120
147,030
135,381
134,348
129,782
128,400
128,254
127,164
126,873
126,073
120,125
33,896
Me
N
O
N
ppm
160
140
120
100
80
60
40
20
0