Supporting Information

Copper-Catalyzed *N*-Arylation of Azoles and Diazoles using Highly Functionalized Trivalent Organobismuth Reagents

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1. General information

Unless otherwise indicated, all reactions were run under argon in non-flame dried glassware. For reactions performed under oxygen, 99.6% extra dry oxygen was used. Unless otherwise stated, commercial reagents were used without further purification. Grignard reagents were prepared by conventional methods using metallic magnesium or via Knochel's procedure.[1] Triphenylbismuth was prepared according to Barton *et al.*[2] Triarylbismuthanes were prepared according to procedures that we previously reported.[3,4] Anhydrous solvents were obtained using a MBRAUN (model MB-SPS 800) encapsulated solvent purification system. The evolution of reactions was monitored by analytical thin-layer chromatography using silica gel 60 F254 precoated plates. Flash chromatography was performed employing 230-400 mesh silica (Silicycle) using the indicated solvent system according to standard techniques.[5] Melting points were taken on an Electrothermal Mel-TEMP and are uncorrected. Nuclear magnetic resonance spectra (^{1}H, ^{13}C) were recorded on a Bruker Avance-III 300MHz spectrometer. Chemical shifts for ^{1}H-NMR spectra are recorded in parts per million from tetramethylsilane with the solvent resonance as the internal standard (chloroform, δ 7.27 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qt = quintuplet, dd = doublet of doublet, m = multiplet), coupling constant *J* in Hz and integration. Chemical shifts for ^{13}C spectra are recorded in parts per million from tetramethylsilane using the central peak of deuterochloroform (δ 77.16 ppm) as the internal standard. IR spectra were recorded on a Thermo Scientific Nicolet 6700 PT-IR from thin films and are reported in reciprocal centimeters (cm^{-1}). HRMS were performed at Université du Québec à Montréal (nanoQAM center) on Agilent Technologies, LC 1200 Series / 6210 TOF LCMS analyzer using the electrospray (ESI) mode.

2. Triarylbismuthanes used in the *N*-arylation reaction of azoles and diazoles

The organobismuthanes used in this publication are illustrated in **Figure S1**.

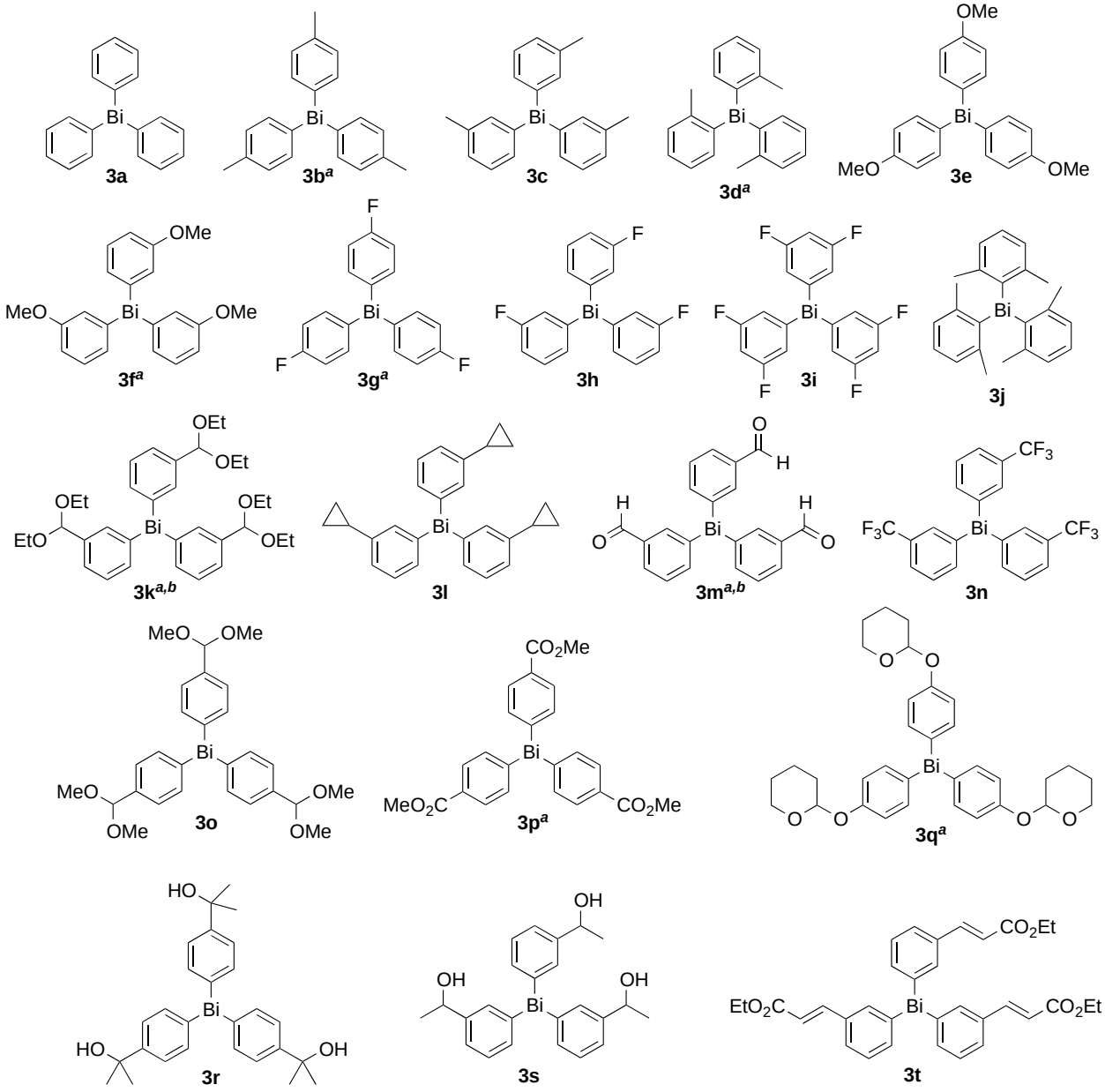
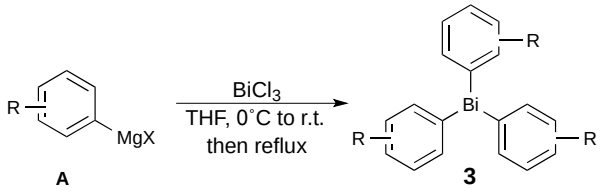


Figure S1. Functionalized organobismuthanes used in this publication. [a] The synthesis of these organobismuthanes has been reported in P. Petiot and A. Gagnon, *Eur. J. Org. Chem.*, 2013, 5282; [b] The synthesis of these organobismuthanes has been reported in C. Crifar, P. Petiot, T. Ahmad and A. Gagnon, *Chem. Eur. J.* **2014**, 2755.

3. Synthesis of triarylbismuthanes

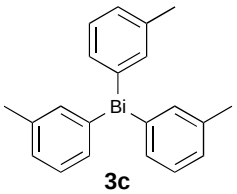
Triphenylbismuth was synthesized according to Barton *et al*. (D. H. R. Barton, N. Y. Bhatnagar, J.-P. Finet and W. B. Motherwell, *Tetrahedron*, 1986, **42**, 3111). Triarylbismuthanes **3b**, **3d**, **3f**, **3g**, **3k**, **3m**, **3p** and **3q** were synthesized according to P. Petiot and A. Gagnon (*Eur. J. Org. Chem.*, **2013**, 5282) and C. Crifar, P. Petiot, T. Ahmad and A. Gagnon (*Chem. Eur. J.*, **2014**, 2755). The procedure for the preparation of organobismuthanes **3c**, **3e**, **3h**, **3i**, **3j**, **3l**, **3n**, **3o**, **3r**, **3s**, and **3t** is described below.

a) General procedure for the synthesis of substituted triarylbismuthanes



In a flask equipped with a magnetic stir bar and a condenser, bismuth chloride (500 mg, 1.6 mmol) was dissolved in anhydrous THF (23 mL) under argon and was cooled to –10°C (ice/acetone bath). The organomagnesium reagent **A** (5.23 mmol) was slowly added dropwise under argon. The reaction mixture was stirred at room temperature for one hour and heated at 65°C for 30 minutes. After cooling to r.t., the solution was diluted with sat. aq. $NaHCO_3$ (100 mL) and extracted with EtOAc (2 x 100 mL). The combined organic phases were washed with sat. aq. $NaHCO_3$ (2 x 100 mL), sat. aq. NaCl (2 x 100 mL), dried over $Na_2S_2O_4$, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using the indicated solvent system to afford the desired triarylbismuthane **3**.

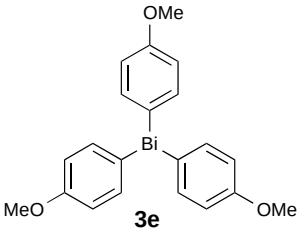
Tris(3-methylphenyl)bismuthine (3c)



3c

The general procedure was followed on a 2.4 mmol scale starting from bismuth chloride and 3-tolylmagnesium bromide. The crude material was purified on silica gel (5% EtOAc/hexanes) to afford tris(3-methylphenyl)bismuthine (**3c**) as a white solid (1.0 g, 87%); m.p. 64-66°C. Spectral data was identical to literature compound[6]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.31-7.29 (m, 1H), 7.13 (d, *J* = 7.4 Hz, 1H), 2.31 (s, 3H).

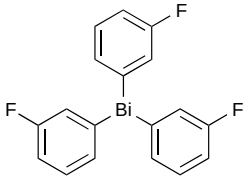
Tris(4-methoxyphenyl)bismuthine (3e)



3e

The general procedure was followed on a 4.4 mmol scale starting from bismuth chloride and 4-methoxyphenylmagnesium bromide. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford tris(4-methoxyphenyl)bismuthine (**3e**) as a white solid (1.8 g, 78%): m.p. 70-74°C. Spectral data was identical to literature compound[6]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2H), 6.92 (d, *J* = 8.5 Hz, 2H), 3.79 (s, 3H).

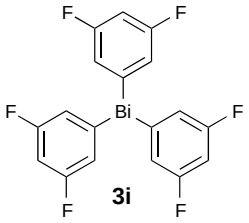
Tris(3-fluorophenyl)bismuthine (3h)



3h

The general procedure was followed on a 2.5 mmol scale starting from bismuth chloride and 3-fluorophenylmagnesium bromide. The crude material was purified on silica gel (5% EtOAc/hexanes) to afford tris(3-fluorophenyl)bismuthine (**3h**) as a white solid (1.0 g, 81%); m.p. 69-73°C. Spectral data was identical to literature compound[7]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.50-7.39 (m, 3H), 7.06-6.99 (m, 1H).

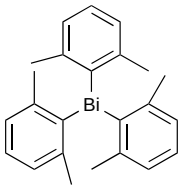
Tris(3,5-difluorophenyl)bismuthine (3i)



3i

The general procedure was followed on a 2.7 mmol scale starting from bismuth chloride and 3,5-difluorophenylmagnesium bromide. The crude material was purified on silica gel (5% EtOAc/hexanes) to afford tris(3,5-difluorophenyl)bismuthine (**3i**) as a yellow solid (1.1 g, 74%): m.p. 100-104°C; R_f 0.68 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.57-7.52 (m, 2H), 7.10-7.03 (m, 1H); ^{13}C-NMR (75 MHz, CDCl3) δ 167.5 (d, *J* = 9.8 Hz), 164.2 (d, *J* = 9.8 Hz), 119.7 (dd, *J* = 15.9, 6.4 Hz), 104.6 (t, *J* = 24.8 Hz); IR (neat) 3088, 1582, 1410, 1263, 1116; HRMS (ESI) calcd for $C_{18}H_9BiF_6$: 548.0412, found 593.0395 (M+HCO_2).

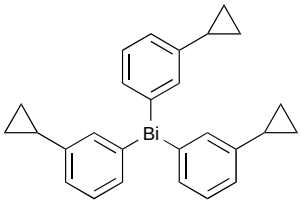
Tris(2,6-dimethylphenyl)bismuthine (3j)



3j

The general procedure was followed on a 2.5 mmol scale starting from bismuth chloride and 2,6-dimethylphenylmagnesium bromide. The crude material was purified on silica gel (5% EtOAc/hexanes) to afford tris(2,6-dimethylphenyl)bismuthine (**3j**) as a white solid (1.1 g, 84%): m.p. 128-130°C; R_f 0.80 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.14-7.10 (m, 3H), 2.34 (s, 6H); ^{13}C-NMR (75 MHz, CDCl3) δ 159.4, 146.0, 128.3, 127.9, 28.1; IR (neat) 3045, 2960, 2918, 1442, 763.

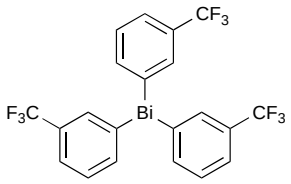
Tris(3-cyclopropylphenyl)bismuthine (3l)



3l

The general procedure was followed on a 0.31 mmol scale starting from bismuth chloride and 3-cyclopropylphenylmagnesium bromide. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford tris(3-cyclopropylphenyl)bismuthine (**3l**) as a colorless oil (151 mg, 87%): R_f 0.71 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.53-7.47 (m, 2H), 7.30-7.25 (m, 2H), 7.01 (d, *J* = 7.9 Hz, 1H), 1.87-1.81 (m, 1H), 0.95-0.88 (m, 2H), 0.65-0.61 (m, 2H); ^{13}C-NMR (75 MHz, CDCl3) δ 155.1, 145.8, 135.0, 134.8, 130.4, 125.1, 15.6, 9.5; IR (neat) 3078, 3039, 3001, 1589, 1560.

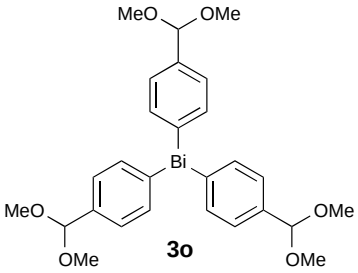
Tris(3-trifluoromethylphenyl)bismuthine (3n)



3n

The general procedure was followed on a 4.4 mmol scale starting from bismuth chloride and 3-trifluoromethylphenylmagnesium bromide. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford tris(3-trifluoromethylphenyl)bismuthine (**3n**) as a yellow oil (2.7 g, 95%): R_f 0.56 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.90 (d, *J* = 7.3 Hz, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.58-7.53 (m, 1H); ^{13}C-NMR (75 MHz, CDCl3) δ 156.2, 140.8 (d, *J* = 1.2 Hz), 133.9 (q, *J* = 3.8 Hz), 132.8 (q, *J* = 31.8 Hz), 131.2, 125.3 (q, *J* = 3.8 Hz), 122.5; IR (neat) 3051, 2959, 1592, 1319, 1308, 1114, 1070; HRMS (ESI) calcd for $C_{21}H_{12}BiF_9$: 644.0599, found 689.0592 ($M+HCO_2$).

Tris(4-(dimethoxymethyl)phenyl)bismuthine (3o)



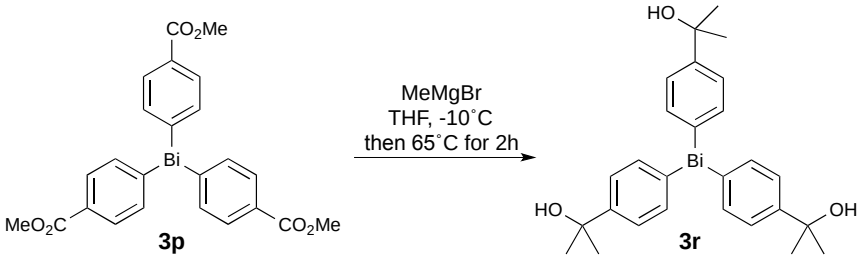
3o

The general procedure was followed on a 3.2 mmol scale starting from bismuth chloride and 4-(dimethoxymethyl)phenylmagnesium bromide. The crude material was purified on silica gel (20% EtOAc/hexanes) to afford tris(4-(dimethoxymethyl)phenyl)-bismuthine (**3o**) as a yellow oil (2.1 g, quant.): R_f 0.32 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 7.8 Hz, 2H), 5.35 (s, 1H), 3.34 (s, 6H); ^{13}C-NMR (75 MHz, CDCl3) δ 155.4,

137.7, 137.5, 128.8, 103.4, 52.9; IR (neat) 2988, 2934, 2903, 2827, 1348, 1207, 1180, 1096, 1048.

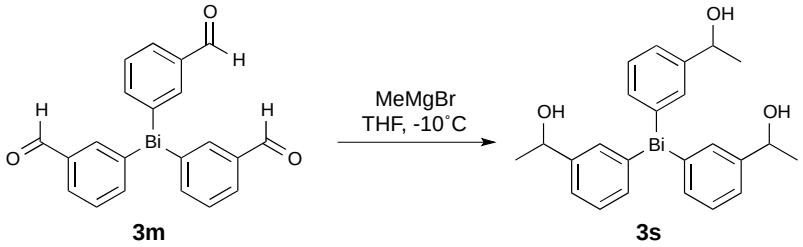
b) Procedures for the synthesis of functionalized organobismuthanes by functional group manipulation

4,4',4''-Bismuthylidyne tris[α,α-dimethylbenzenemethanol] (3r)



A solution of tris(4-carbomethoxyphenyl)bismuthine **3p** (100 mg, 0.2 mmol) in anhydrous THF (5 mL), was cooled to –10°C (acetone/ice bath) and methylmagnesium bromide (0.6 mL, 1.2 mmol, 2M in THF) was added slowly. The reaction mixture was heated at 65°C for 2h, then cooled to r.t., transferred over aq. sat. NH_4Cl (50 mL) and extracted with EtOAc (10 mL). The organic layer was washed with sat. aq. NH_4Cl (10 mL) and sat. aq. NaCl (3 x 10 mL), dried over sodium sulphate, filtered and concentrated under reduced pressure. The crude material was purified on silica gel (20% EtOAc/hexanes) to afford 4,4',4''-bismuthylidyne tris[α,α-dimethylbenzenemethanol] (**3r**) as a colorless oil (103 mg, 84%): R_f 0.53 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 7.7 Hz, 2H), 2.15 (s(br), 1H), 1.56 (s, 6H); ^{13}C-NMR (75 MHz, CDCl3) δ 152.8, 148.7, 137.5, 126.6, 72.6, 31.7; IR (neat) 3375, 3063, 2973, 2925, 2851, 1384, 1169.

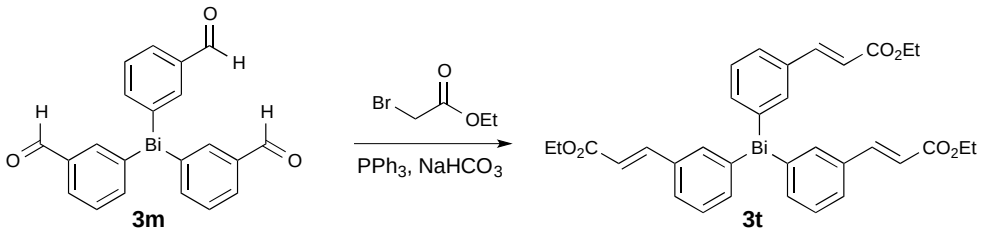
3,3',3''-Bismuthylidyne tris[α-methylbenzenemethanol] (3s)



3m **3s**

A solution of tris(3-formylphenyl)bismuthine **3m** (400 mg, 0.8 mmol) in anhydrous THF (10 mL), was cooled to –10°C (acetone/ice bath) and methylmagnesium bromide (0.83 mL, 2.5 mmol, 3M in THF) was added slowly. After 10 minutes, the reaction mixture was diluted with aq. sat. NH_4Cl (50 mL) and extracted with EtOAc (20 mL). The organic layer was washed with sat. aq. $NaHCO_3$ (15 mL) and sat. aq. NaCl (3 x 15 mL), dried over sodium sulphate, filtered and concentrated under reduced pressure. The crude material was purified on silica gel (40% EtOAc/hexanes) to afford 3,3',3''-bismuthylidyne tris[α-methylbenzenemethanol] (**3s**) as a white solid (384 mg, 84%): m.p. 78-83°C; R_f 0.32 (80% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.40-7.30 (m, 2H), 4.88-4.81 (m, 1H), 1.47-1.43 (m, 3H); ^{13}C-NMR (75 MHz, CDCl3) δ 155.6, 147.6, 136.6, 134.6, 130.4, 125.1, 70.3, 25.1; IR (neat) 3348, 3045, 2972, 2869, 1412, 1264; HRMS (ESI) calcd for $C_{24}H_{27}BiO_3$: 572.1764, found 617.1745 ($M+HCO_2$).

Tris(3-((*E*)-2-propenoic acid ethyl ester)phenyl)bismuthine (3t)

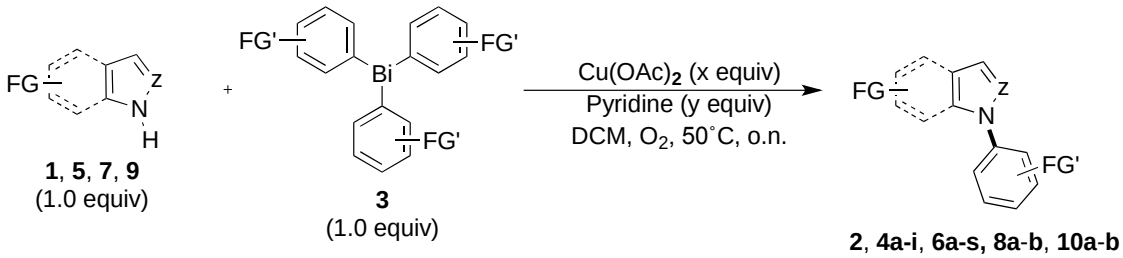


3m **3t**

A solution of PPh_3 (1.1 g, 4.3 mmol) in sat. aq. $NaHCO_3$ (25 mL) was stirred at r.t., then tris(3-formylphenyl)bismuthine **3m** (500 mg, 0.9 mmol) and ethyl bromoacetate (0.58 mL, 5.2 mmol) were added. The reaction mixture was stirred for 2h, acidified with aq. HCl 1M (5 mL) and then diluted with EtOAc (10 mL). The organic layer was washed with sat. aq. NaCl (3 x 10 mL), dried over sodium sulphate, filtered and concentrated under reduced pressure. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford tris(3-((*E*)-2-propenoic acid ethyl ester)phenyl)bismuthine (**3t**) as a yellow oil (519 mg, 79%): R_f 0.21 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 16.1 Hz, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 6.36 (d, *J* = 16.0 Hz, 1H), 4.25 (q, *J* = 7.1 Hz, 2H), 1.32 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (75 MHz, CDCl3) δ 166.8, 156.1, 144.5, 139.3, 137.3, 136.6, 131.2, 127.6, 118.7, 60.5, 14.4; IR (neat) 3042, 2980, 2902, 1703, 1633, 1304, 1164; HRMS (ESI) calcd for $C_{33}H_{33}BiO_6$: 734.2081, found 779.2076 (M+HCO_2).

4. General procedures for the *N*-arylation of azoles and diazoles

Compound **2**, **4a-i**, **6a-s**, **8a**,**b** and **10a**,**b** were prepared according to the following procedures:



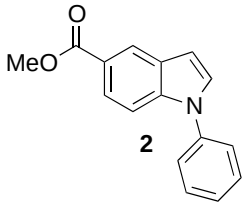
Method	Azole (n equiv)	Ar_3Bi (**5**) (m equiv)	$Cu(OAc)_2$ (x equiv)	Pyridine (y equiv)
A	1.0	1.0	0.1	1.0
B	1.0	1.0	0.1	3.0
C	1.0	1.0	1.0	3.0

Method A: In a sealed tube, triarylbismuthine (1.0 equiv) was added, followed by copper (II) acetate (0.1 equiv) and the azole or diazole (1.0 equiv). The reagents were dissolved in anhydrous dichloromethane (4 mL) and pyridine (1.0 equiv) was added to the mixture. The reaction tube was purged by bubbling dry oxygen in the solution for 30 seconds. The tube was sealed and heated at 50°C overnight. The reaction mixture was cooled to r.t. and transferred in a round bottom flask. Silica gel was added and the mixture was concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel using EtOAc/hexanes as the eluent to give the corresponding product.

Method B: Idem as method **A** except for pyridine (3.0 equiv instead of 1.0 equiv).

Method C: Idem as method **A** except for copper (II) acetate (1.0 equiv instead of 0.1 equiv) and pyridine (3.0 equiv instead of 1.0 equiv).

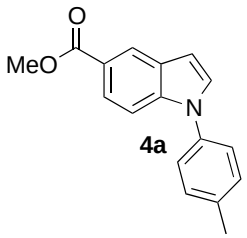
1-Phenyl-1*H*-indole-5-carboxylic acid methyl ester (2)



2

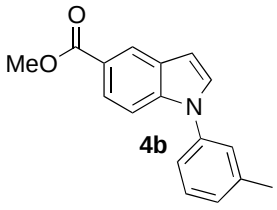
Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3a**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **2** as a yellow oil (70 mg, 96%). Spectral data was identical to literature[8]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.82 (dd, *J* = 10.2, 1.7 Hz, 1H), 7.44-7.36 (m, 5H), 7.31-7.27 (m, 2H), 6.67 (d, *J* = 3.2 Hz, 1H), 3.84 (s, 3H).

1-(4-Methylphenyl)-1*H*-indole-5-carboxylic acid methyl ester (4a)



Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3b**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **4a** as a yellow solid (67 mg, 87%): m.p. 90-92°C; R_f 0.66 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.44 (d, *J* = 1.5 Hz, 1H), 7.90 (dd, *J* = 8.8, 1.7 Hz, 1H), 7.50 (d, *J* = 8.7 Hz, 1H), 7.40-7.32 (m, 5H), 6.75 (d, *J* = 2.8 Hz, 1H), 3.94 (s, 3H), 2.45 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 168.1, 138.5, 137.1, 136.8, 130.4, 129.7, 128.8, 124.5, 124.2, 123.7, 122.3, 110.3, 104.6, 52.0, 21.2; IR (neat) 3105, 2938, 2835, 1721, 1709, 1698, 1606, 1523, 1519, 1514, 1446, 1434, 1335, 1311, 1270, 1228, 1197; HRMS (ESI) calcd for $C_{17}H_{15}NO_2$: 265.1103, found 266.1170 (M+H).

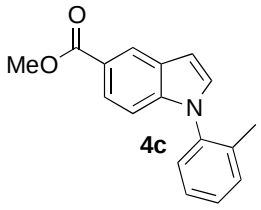
1-(3-Methylphenyl)-1*H*-indole-5-carboxylic acid methyl ester (4b)



Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3c**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **4b** as a yellow oil (67 mg, 87%): R_f 0.52 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.35 (d, *J* = 1.5 Hz, 1H), 7.82 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 1H), 7.33-7.26 (m, 2H), 7.19-7.17 (m, 2H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.65 (d, *J* = 3.3 Hz, 1H), 3.84 (s, 3H), 2.35 (s, 3H); ^{13}C-NMR

(75 MHz, $CDCl_3$) δ 168.1, 139.9, 139.2, 138.4, 129.6, 128.9, 127.9, 125.2, 124.2, 123.7, 122.4, 121.7, 110.3, 104.7, 52.0, 21.5; IR (neat) 3105, 2946, 2835, 1709, 1693, 1605, 1445, 1432, 1334, 1270, 1230, 1191; HRMS (ESI) calcd for $C_{17}H_{15}NO_2$: 265.1103, found 266.1177 (M+H).

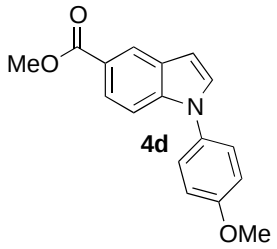
1-(2-Methylphenyl)-1*H*-indole-5-carboxylic acid methyl ester (4c)



4c

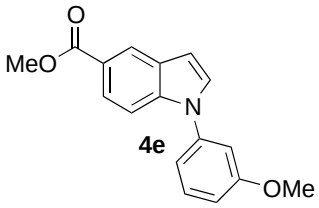
Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3d**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **4c** as a yellow oil (19 mg, 24%): R_f 0.52 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.38 (d, *J* = 1.5 Hz, 1H), 7.78 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.30-7.21 (m, 4H), 7.12 (d, *J* = 3.2 Hz, 1H), 6.93 (d, *J* = 8.7 Hz, 1H), 6.66 (d, *J* = 2.8 Hz, 1H), 3.84 (s, 3H), 1.94 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 168.2, 139.5, 137.8, 135.9, 131.4, 130.2, 128.8, 128.1, 127.9, 127.1, 124.1, 123.6, 122.1, 110.3, 104.0, 52.0, 17.6; IR (neat) 3109, 3027, 2950, 2852, 1720, 1712, 1612, 1513, 1501, 1461, 1445, 1434, 1335, 1300, 1269, 1231, 1196; HRMS (ESI) calcd for $C_{17}H_{15}NO_2$: 265.1103, found 266.1170 (M+H). Compound **3c** was also obtained (59 mg, 78%) following method C on a 0.285 mmole scale starting from methyl 1*H*-indole-5-carboxylate.

1-(4-Methoxyphenyl)-1*H*-indole-5-carboxylic acid methyl ester (4d)



Method A was followed on a 0.28 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3e**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **4d** as a colorless oil (45 mg, 57%): R_f 0.39 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.45 (d, *J* = 1.5 Hz, 1H), 7.91 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.45-7.26 (m, 4H), 7.06-7.03 (m, 2H), 6.74 (dd, *J* = 3.3, 0.7 Hz, 1H), 3.94 (s, 3H), 3.88 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 168.1, 158.7, 138.8, 132.2, 129.8, 128.5, 126.1, 124.1, 123.6, 122.2, 114.9, 110.1, 104.3, 55.6, 51.9; IR (neat) 3106, 2998, 2949, 2837, 1707, 1611, 1513, 1434, 1298.

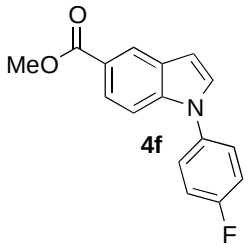
1-(3-Methoxyphenyl)-1*H*-indole-5-carboxylic acid methyl ester (4e)



Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3f**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **4e** as a yellow oil (40 mg, 49%): R_f 0.47 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.44 (d, *J* = 1.5 Hz, 1H), 7.92 (dd, *J* = 8.9, 1.7 Hz, 1H), 7.57 (d, *J* = 8.7 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.41-7.39 (m, 1H), 7.08 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.04 (t, *J* = 2.3 Hz, 1H), 6.94 (dd, *J* = 9.1, 1.0 Hz, 1H), 6.77 (dd, *J* = 3.3, 0.8 Hz, 1H), 3.95 (s, 3H), 3.87 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ

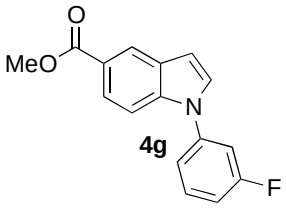
168.0, 160.7, 140.4, 138.3, 130.5, 129.5, 128.9, 124.1, 123.8, 122.5, 116.7, 112.5, 110.5, 110.3, 104.9, 55.6, 51.9; IR (neat) 2998, 2948, 2836, 1708, 1602, 1592, 1493, 1432, 1275; HRMS (ESI) calcd for $C_{17}H_{15}NO_3$: 281.1052, found 282.1128 (M+H).

1-(4-Fluorophenyl)-1*H*-indole-5-carboxylic acid methyl ester (4f)



Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3g**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **4f** as a yellow solid (53 mg, 68%). Spectral data was identical to literature[8]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.35 (d, *J* = 1.8 Hz, 1H), 7.82 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.36-7.31 (m, 3H), 7.22 (d, *J* = 3.3 Hz, 1H), 7.15-7.09 (m, 2H), 6.66 (d, *J* = 3.2 Hz, 1H), 3.84 (s, 3H).

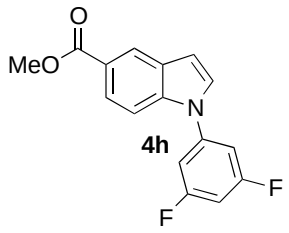
1-(3-Fluorophenyl)-1*H*-indole-5-carboxylic acid methyl ester (4g)



Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3h**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **4g** as a yellow solid (54 mg, 69%): m.p. 95-100°C; R_f 0.41 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.26 (d, *J* = 1.6 Hz, 1H), 7.76 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.35-7.27 (m,

1H), 7.18 (d, *J* = 3.3 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 2H), 7.09 (td, *J* = 11.6, 1.5 Hz, 1H), 6.90 (dt, *J* = 8.5, 2.6 Hz, 1H), 6.59 (d, *J* = 3.3 Hz, 1H), 3.76 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 167.9, 164.9, 161.6, 140.8, 140.6, 138.1, 131.1, 131.0, 129.1, 129.0, 124.2, 124.0, 122.8, 120.0, 119.9, 114.1, 113.8, 111.9, 111.6, 110.1, 105.5, 52.0; IR (neat) 3072, 2955, 1714, 1607, 1301, 1283, 1192; HRMS (ESI) calcd for $C_{16}H_{12}FNO_2$: 269.0852, found 270.0933 (M+H).

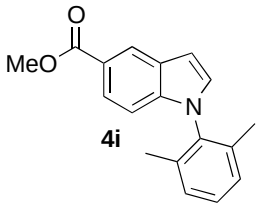
1-(3,5-Difluorophenyl)-1*H*-indole-5-carboxylic acid methyl ester (4h)



4h

Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3i**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **4h** as a yellow solid (43 mg, 52%): m.p. 170-174°C; R_f 0.52 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.44 (d, *J* = 1.7 Hz, 1H), 7.97 (dd, *J* = 8.8, 1.7 Hz, 1H), 7.59 (d, *J* = 8.7 Hz, 1H), 7.36 (d, *J* = 3.4 Hz, 1H), 7.09-7.06 (m, 2H), 6.88-6.79 (m, 2H), 3.96 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 167.7, 165.3, 165.1, 162.0, 161.8, 141.4, 141.2, 137.8, 129.2, 128.7, 124.4, 124.3, 123.2, 110.0, 107.7, 107.6, 107.5, 107.3, 106.1, 102.8, 102.4, 102.1, 52.1; IR (neat) 3099, 2959, 2922, 1708, 1626, 1598, 1283, 1193, 1116; HRMS (ESI) calcd for $C_{16}H_{11}F_2NO_2$: 287.0758, found 288.0834 (M+H).

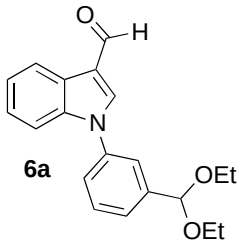
1-(2,6-Dimethylphenyl)-1*H*-indole-5-carboxylic acid methyl ester (4i)



4i

Method A was followed on a 0.29 mmol scale starting from methyl 1*H*-indole-5-carboxylate and **3j**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **4i** as a yellow oil (15 mg, 19%): R_f 0.53 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.47 (d, *J* = 1.6 Hz, 1H), 7.85 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.29-7.04 (m, 4H), 6.88 (d, *J* = 8.6 Hz, 1H), 6.78 (d, *J* = 3.3 Hz, 1H), 3.92 (s, 3H), 1.90 (s, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 168.2, 138.8, 137.1, 136.5, 129.5, 128.8, 128.6, 128.5, 127.7, 124.0, 123.5, 122.0, 109.8, 104.0, 51.9, 17.4; IR (neat) 2948, 2922, 1708, 1611, 1446, 1434, 1295, 1269; HRMS (ESI) calcd for $C_{18}H_{17}NO_2$: 279.1259, found 280.1347 (M+H).

1-((3-Diethoxymethyl)phenyl)-1*H*-indole-3-carboxaldehyde (6a)

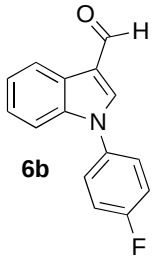


6a

Method A was followed on a 0.34 mmol scale starting from 1*H*-indole-3-carbaldehyde and **3k**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6a** as a yellow oil (101 mg, 92%): R_f 0.18 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.38 (d, *J* = 8.2 Hz, 1H), 7.93 (s, 1H), 7.67 (s, 1H), 7.59-7.54 (m, 2H), 7.49-7.46 (m, 2H), 7.38-7.30 (m, 2H), 5.60 (s, 1H), 3.74-3.55 (m, 4H), 1.28 (t, *J* = 7.0 Hz, 6H); ^{13}C-NMR (75 MHz,

$CDCl_3$) δ 185.0, 141.8, 138.2, 137.5, 129.8, 126.6, 125.6, 124.7, 124.6, 123.5, 123.1, 122.3, 119.8, 111.1, 100.7, 61.4, 15.3; IR (neat) 3117, 3052, 2966, 2868, 2807, 2762, 2725, 1665, 1660, 1605, 1530, 1493, 1480, 1461, 1309; HRMS (ESI) calcd for $C_{20}H_{21}NO_3$: 323.1521, found 324.1584 (M+H).

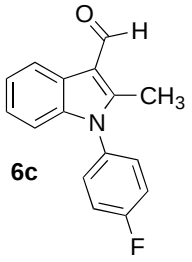
1-(4-Fluorophenyl)-1*H*-indole-3-carboxaldehyde (6b)



6b

Method A was followed on a 0.34 mmol scale starting from 1*H*-indole-3-carbaldehyde and **3g**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6b** as a white solid (43 mg, 52%): m.p. 141-143°C. Spectral data was identical to literature[9]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.29 (dd, *J* = 5.6, 2.0 Hz, 1H), 7.77 (s, 1H), 7.43-7.38 (m, 2H), 7.33-7.16 (m, 5H); HRMS (ESI) calcd for $C_{15}H_{10}FNO$: 239.0746, found 240.0813 (M+H).

1-(4-Fluorophenyl)-2-methyl-1*H*-indole-3-carboxaldehyde (6c)

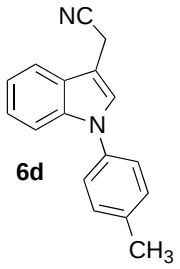


6c

Method A was followed on a 0.31 mmol scale starting from 2-methyl-1*H*-indole-3-carbaldehyde and **3g**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6c** as a

white solid (60 mg, 76%): m.p. 174-176°C; R_f 0.21 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 10.15 (s, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.27-7.17 (m, 5H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.90 (d, *J* = 8.1 Hz, 1H), 2.44 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 184.8, 164.5, 161.2, 147.8, 138.3, 132.0, 130.0, 129.9, 125.7, 123.7, 123.4, 121.0, 117.3, 117.0, 115.3, 110.4, 11.4; IR (neat) 3068, 2929, 2827, 1642, 1511, 1503, 1480, 1461, 1426, 1225, 1218; HRMS (ESI) calcd for $C_{16}H_{12}FNO$: 253.0903, found 254.0981 (M+H).

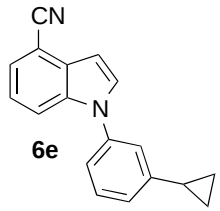
1-(4-Methylphenyl)-1*H*-indole3-acetonitrile (6d)



6d

Method C was followed on a 0.32 mmol scale starting from 1*H*-indole-3-ylacetonitrile and **3b**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **6d** as a red oil (69 mg, 88%): R_f 0.37 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.1 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.24-7.08 (m, 7H), 3.74 (s, 2H), 2.31 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 136.9, 136.7, 136.5, 130.3, 127.2, 126.7, 124.4, 123.2, 120.7, 118.5, 118.1, 111.1, 105.4, 21.1, 14.4; IR (neat) 3040, 2917, 2856, 2251, 1646, 1611, 1518, 1514, 1461, 1454; HRMS (ESI) calcd for $C_{17}H_{14}N_2$: 246.1157, found 247.1223 (M+H).

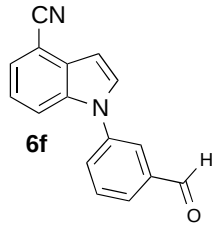
1-(3-Cyclopropylphenyl)-1*H*-indole-4-carbonitrile (6e)



6e

Method C was followed on a 0.27 mmol scale starting from 4-cyanoindole and **3l**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **6e** as a yellow oil (61 mg, 88%): R_f 0.53 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.4 Hz, 1H), 7.43-7.29 (m, 3H), 7.16-7.11 (m, 2H), 7.05-7.01 (m, 2H), 6.78 (d, *J* = 3.1 Hz, 1H), 1.93-1.84 (m, 1H), 0.99-0.93 (m, 2H), 0.70-0.64 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 146.6, 138.8, 135.9, 130.8, 130.5, 129.8, 125.7, 124.9, 122.2, 122.0, 121.8, 118.7, 115.5, 103.6, 102.2, 15.6, 9.8; IR (neat) 3077, 3007, 2917, 2831, 2227, 1587, 1511, 1503, 1494, 1462, 1444, 1428, 1330; HRMS (ESI) calcd for $C_{18}H_{14}N_2$: 258.1157, found 259.1225 (M+H).

1-(3-Formylphenyl)-1*H*-indole-4-carbonitrile (6f)

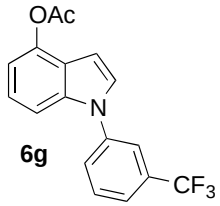


6f

Method A was followed on a 0.35 mmol scale starting from 4-cyanoindole and **3m**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **6f** as a white solid (53 mg, 62%): m.p. 124-127°C; R_f 0.18 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 10.02 (s, 1H), 7.90 (d, *J* = 1.2 Hz, 1H), 7.85 (dt, *J* = 4.6, 1.5 Hz, 1H), 7.68-7.62 (m, 3H), 7.46-7.44 (m, 2H), 7.22-7.17 (m, 1H), 6.84 (dd, *J* = 3.3, 0.5 Hz, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 191.1,

139.8, 138.1, 135.6, 130.9, 130.8, 130.4, 130.2, 129.1, 126.2, 124.6, 122.6, 118.4, 115.1, 104.0, 103.3; IR (neat) 3129, 3105, 2921, 2831, 2733, 2218, 1702, 1692, 1586, 1514, 1492, 1484, 1461, 1432, 1328, 1301, 1184, 1144; HRMS (ESI) calcd for $C_{16}H_{10}N_2O$: 246.0793, found 247.0860 (M+H).

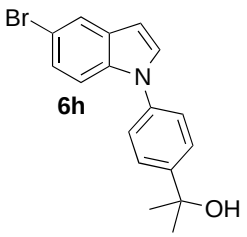
1-(3-Trifluoromethylphenyl)-1*H*-indol-4-ol-4-acetate (6g)



6g

Method C was followed on a 0.29 mmol scale starting from 1*H*-indol-4-yl acetate and **3n**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6g** as a black solid (40 mg, 43%): m.p. 74-76°C; R_f 0.33 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.62-7.54 (m, 3H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.23 (d, *J* = 3.3 Hz, 1H), 7.17-7.12 (m, 1H), 6.86 (d, *J* = 7.7 Hz, 1H), 6.53 (d, *J* = 3.2 Hz, 1H), 2.34 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 169.4, 144.0, 140.2, 137.6, 132.7, 132.3, 130.5, 128.0, 127.7, 123.6, 123.3, 122.9, 121.4, 113.2, 108.4, 101.4, 21.2; IR (neat) 2913, 1765, 1618, 1593, 1493, 1462, 1335, 1323, 1197, 1125; HRMS (ESI) calcd for $C_{17}H_{12}F_3NO_2$: 319.0820, found 320.0891 (M+H).

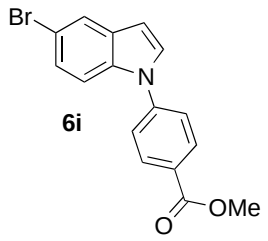
4-(5-Bromo-1*H*-indol-1-yl)-α,α-dimethylbenzenemethanol (6h)



6h

Method C was followed on a 0.063 mmol scale starting from 5-bromoindole and **3r**. The crude product was purified on silica gel (25% EtOAc/hexanes) to afford **6h** as a pink wax (11 mg, 53%): R_f 0.27 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 1.7 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 8.3 Hz, 2H), 7.25-7.18 (m, 3H), 6.53 (d, *J* = 3.1 Hz, 1H), 1.73 (s (br), 1H), 1.58 (s, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 148.0, 138.0, 134.8, 131.1, 129.2, 126.0, 125.3, 124.2, 123.7, 113.6, 112.1, 103.1, 72.5, 32.0; IR (neat) 3379, 2974, 2921, 2844, 1610, 1519, 1514, 1461, 1453; HRMS (ESI) calcd for $C_{17}H_{16}BrNO$: 329.0415, found 312.0373 (M+H)-[H_2O] (^{79}Br), 314.0352 (M+H)-[H_2O] (^{81}Br).

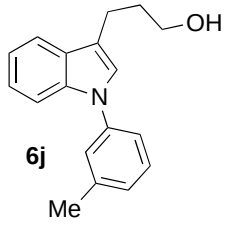
4-(5-Bromo-1*H*-indol-1-yl)benzoic acid methyl ester (6i)



6i

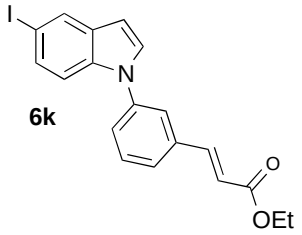
Method C was followed on a 0.24 mmol scale starting from 5-bromoindole and **3p**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **6i** as a pink solid (53 mg, 67%): m.p. 94-98°C; R_f 0.52 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.6 Hz, 2H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.8 Hz, 1H), 7.37 (d, *J* = 3.3 Hz, 1H), 7.33 (dd, *J* = 8.8, 1.7 Hz, 1H), 6.66 (d, *J* = 3.2 Hz, 1H), 3.97 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 166.3, 143.3, 134.3, 131.5, 131.4, 128.7, 128.2, 125.8, 124.0, 123.4, 114.2, 112.1, 104.4, 52.4; IR (neat) 2946, 2840, 1720, 1712, 1666, 1605, 1514, 1450, 1434, 1276; HRMS (ESI) calcd for $C_{16}H_{12}BrNO_2$: 329.0051, found 330.0117 (M+H) (^{79}Br), 332.0100 (M+H) (^{81}Br).

1-(3-Methylphenyl)-1*H*-Indole-3-propanol (6j)



Method C was followed on a 0.29 mmol scale starting from 3-(3-hydroxypropyl)-1*H*-indole and **3c**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6j** as a yellow oil (40 mg, 52%): R_f 0.21 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.2 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 1H), 7.43-7.38 (m, 1H), 7.32-7.15 (m, 5H), 3.79 (t, *J* = 6.4 Hz, 2H), 2.94 (t, *J* = 7.5 Hz, 2H), 2.46 (s, 3H), 2.06 (qt, *J* = 6.4 Hz, 2H), 1.49 (s(br), 1H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 139.9, 139.7, 136.1, 129.4, 128.9, 126.9, 125.3, 124.8, 122.4, 121.2, 119.8, 119.3, 116.9, 110.7, 62.7, 32.9, 21.5, 21.3; IR (neat) 3339 (br), 3047, 2922, 2863, 1605, 1588, 1493, 1477, 1458; HRMS (ESI) calcd for $C_{18}H_{19}NO$: 265.1467, found 266.1544 (M+H), 248.1408 [(M+H)-H_2O].

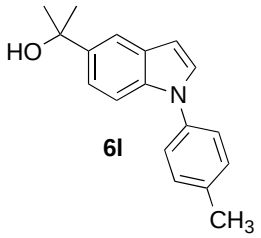
(*E*)-3-(5-Iodo-1*H*-indol-1-yl)phenyl-2-propenoic acid ethyl ester (6k)



Method C was followed on a 0.14 mmol scale starting from 5-iodoindole and **3t**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **6k** as a pink oil (38 mg, 65%): R_f 0.52 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.08 (d, *J* = 1.7 Hz, 1H), 7.78 (d, *J* = 16.1 Hz, 1H), 7.66 (s, 1H), 7.61-7.52 (m, 4H), 7.37-7.32 (m, 2H), 6.68 (d, *J* = 3.4 Hz, 1H), 6.56

(d, *J* = 16.1 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 166.6, 143.3, 139.9, 136.3, 134.9, 131.9, 130.9, 130.4, 130.1, 128.5, 126.4, 125.8, 123.5, 119.9, 112.3, 103.3, 84.1, 60.8, 14.4; IR (neat) 3056, 2978, 1705, 1638, 1582, 1512, 1487, 1456, 1176; HRMS (ESI) calcd for $C_{19}H_{16}INO_2$: 417.0226, found 418.0296 (M+H).

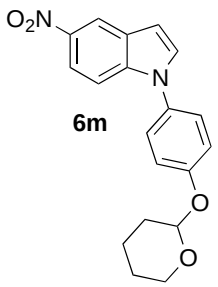
α,α-Dimethyl-1-(4-methylphenyl)-1*H*-indole-5-methanol (6l)



6l

Method A was followed on a 0.28 mmol scale starting from α,α-dimethyl-1*H*-indole-5-methanol and **3b**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6l** as a yellow oil (44 mg, 59%): R_f 0.38 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 1.8 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.43-7.32 (m, 6H), 6.68 (d, *J* = 3.3 Hz, 1H), 2.46 (s, 3H), 1.70 (s, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 141.3, 137.4, 136.3, 134.9, 130.2, 129.0, 128.5, 124.2, 119.6, 116.5, 110.3, 103.5, 72.9, 32.2, 21.1; IR (neat) 3405, 2971, 2923, 1517, 1474, 1334; HRMS (ESI) calcd for $C_{18}H_{19}NO$: 265.1467, found 248.1431 [(M+H)-H_2O].

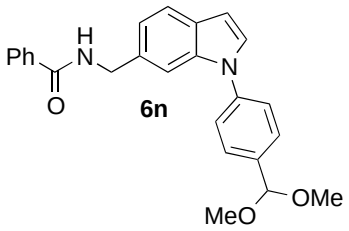
1-[4-(Tetrahydro-2*H*-pyran-2-yl)oxy]phenyl-5-nitro-1*H*-indole (6m)



6m

Method A was followed on a 0.31 mmol scale starting from 5-nitroindole and **3q**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **6m** as a yellow solid (77 mg, 74%): m.p. 99-104°C; R_f 0.36 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$); δ 8.62 (d, *J* = 2.2 Hz, 1H), 8.09 (dd, *J* = 9.1, 2.2 Hz, 1H), 7.46-7.36 (m, 4H), 7.26-7.21 (m, 2H), 6.81 (d, *J* = 3.3 Hz, 1H), 5.50 (t, *J* = 3.3 Hz, 1H), 3.93 (dt, *J* = 9.1, 3.2 Hz, 1H), 3.70-3.64 (m, 1H), 2.12-1.96 (m, 1H), 1.94-1.90 (m, 2H), 1.79-1.62 (m, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 156.6, 142.0, 139.1, 132.2, 131.6, 128.2, 126.1, 118.3, 117.8, 117.6, 110.5, 105.2, 96.6, 62.2, 30.3, 25.2, 18.7; IR (neat) IR 2917, 2852, 1610, 1514, 1468, 1453, 1344, 1329, 1202, 1123, 1069, 966, 920; HRMS (ESI) calcd for $C_{19}H_{18}N_2O_4$: 338.1267, found 339.1333 (M+H).

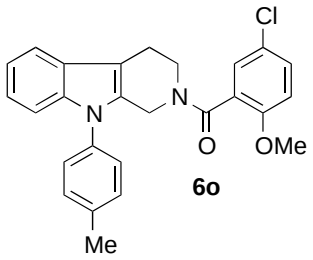
***N*-[4-(dimethoxymethyl)-1*H*-indol-6-yl]methyl benzamide (6n)**



6n

Method C was followed on a 0.20 mmol scale starting from 1*H*-indol-6-yl]methyl benzamide and **3o**. The crude material was purified on silica gel (20% EtOAc/hexanes) to afford **6n** as a pink oil (65 mg, 81%): R_f 0.10 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.77-7.74 (m, 2H), 7.68-7.60 (m, 3H), 7.55 (s, 1H), 7.51-7.48 (m, 3H), 7.42-7.40 (m, 2H), 7.35 (d, *J* = 3.4 Hz, 1H), 7.19 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.68 (d, *J* = 3.2 Hz, 1H), 6.38 (s(br), 1H), 5.46 (s, 1H), 4.72 (d, *J* = 5.4 Hz, 2H), 3.39 (s, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 167.2, 139.6, 136.7, 135.9, 134.6, 132.4, 131.5, 128.9, 128.6, 128.5, 128.2, 127.0, 124.1, 121.6, 120.9, 110.3, 103.7, 102.7, 52.9, 45.0, IR (neat) 3317, 2933, 2829, 1639, 1518, 1450, 1340, 1098; HRMS (ESI) calcd for $C_{25}H_{24}N_2O_3$: 400.1787, found 423.1695 (M+Na).

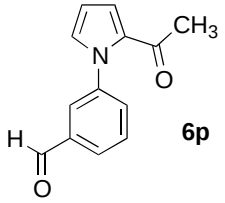
1-(5-Chloro-2-methoxyphenyl)-1-(2-(4-methylphenyl)-1,3,4,9-tetrahydro-2*H*-pyrido[3,4-*b*]indol-2-yl)methanone (6o)



6o

Method C was followed on a 0.15 mmol scale starting from (5-chloro-2-methoxyphenyl)-(1,3,4,9-tetrahydro-2*H*-pyrido[3,4-*b*]indol-2-yl)methanone and **3b**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **6o** as a yellow oil (28 mg, 43%): R_f 0.16 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.53-7.50 (m, 1H), 7.35-7.29 (m, 5H), 7.27-7.23 (m, 2H), 7.22-7.14 (m, 2H), 6.89 (d, *J* = 8.9 Hz, 1H), 4.82 (s, 2H), 3.83 (s, 3H), 3.65-3.60 (m, 2H), 2.88-2.82 (m, 2H), 2.46 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 167.2, 154.2, 137.8, 134.5, 130.4, 130.3, 130.2, 127.8, 127.5, 126.8, 126.6, 126.4, 126.1, 122.0, 120.0, 117.9, 112.4, 110.3, 108.6, 56.0, 45.2, 40.4, 22.1, 21.2; IR (neat) 2925, 2840, 1709, 1659, 1650, 1641, 1632, 1605, 1514, 1493, 1484, 1461, 1440, 1432, 1221; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_2$: 430.1448, found 431.1515 (M+H).

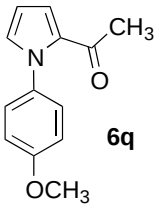
2-Acetyl-N-(3-benzaldehyde)-pyrrole (6p)



6p

Method B was followed on a 0.46 mmol scale starting from 2-acetyl-1*H*-pyrrole and **3m**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **6p** as a beige solid (93 mg, 95%): m.p. 85-87°C; R_f 0.16 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 9.93 (s, 1H), 7.80 (d, *J* = 7.1 Hz, 1H), 7.69 (s, 1H), 7.52-7.43 (m, 2H), 7.05 (d, *J* = 2.7 Hz, 1H), 6.89 (s, 1H), 6.25 (t, *J* = 2.6 Hz, 1H), 2.36 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 191.4, 187.4, 141.8, 137.0, 132.3, 131.6, 131.2, 129.4, 129.1, 126.8, 121.1, 109.9, 27.2; IR (neat) 3117, 3060, 2921, 2827, 2729, 1702, 1692, 1665, 1659, 1650, 1643, 1590, 1461, 1453, 1408; HRMS (ESI) calcd for $C_{13}H_{11}NO_2$: 213.0790, found 214.0859 (M+H).

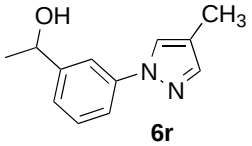
2-Acetyl-*N*-(4-methoxyphenyl)pyrrole (6q)



6q

Method A was followed on a 0.46 mmol scale starting from 2-acetyl-1*H*-pyrrole and **3e**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **6q** as a colorless oil (78 mg, 79%): m.p. 79-82°C. Spectral data was identical to literature[10]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.7 Hz, 2H), 6.97 (d, *J* = 3.8 Hz, 1H), 6.83-6.80 (m, 3H), 6.17 (t, *J* = 3.3 Hz, 1H), 3.74 (s, 3H), 2.31 (s, 3H); HRMS (ESI) calcd for $C_{13}H_{13}NO_2$: 215.0946, found 216.1017 (M+H).

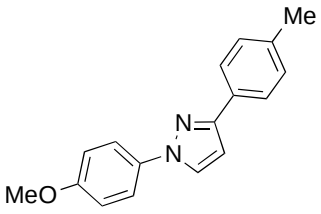
1-[3-(1-Hydroxyethyl)phenyl]-4-methyl-1*H*-pyrazole (6r)



6r

Method C was followed on a 0.50 mmol scale starting from 4-methyl-1*H*-pyrazole and **3s**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **6r** as a colorless oil (70 mg, 69%): R_f 0.12 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.63-7.62 (m, 1H), 7.49-7.45 (m, 2H), 7.34 (t, *J* = 7.7 Hz, 1H), 7.22-7.19 (m, 1H), 4.88 (q, *J* = 6.5 Hz, 1H), 3.02 (s(br), 1H), 2.14 (s, 3H), 1.48 (d, *J* = 6.4 Hz, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 147.7, 141.8, 140.2, 129.4, 125.6, 123.1, 118.2, 117.6, 115.9, 69.9, 25.3, 8.9; IR (neat) 3354, 2971, 2927, 1610, 1593, 1492, 1455, 1390; HRMS (ESI) calcd for $C_{12}H_{14}N_2O$: 202.1106, found [(M+H)-H_2O)] 185.1059, 203.1175 (M+H).

1-(4-Methoxyphenyl)-3-(4-methylphenyl)-1*H*-pyrazole (6s)

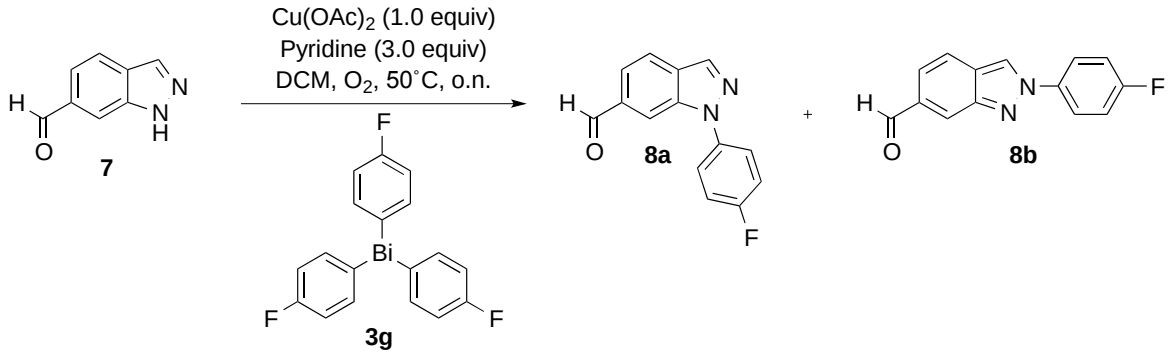


6s

Method C was followed on a 0.32 mmol scale starting from 3-(4-methylphenyl)-1*H*-pyrazole and **3e**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **6s** as a white solid (59 mg, 70%): m.p. 140-143°C; R_f 0.50 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.72-7.69 (m, 3H), 7.55 (d, *J* = 8.7 Hz, 2H), 7.13 (d, *J* = 7.4 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.60 (s, 1H), 3.73 (s, 3H), 2.29 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.2, 152.7, 137.7, 134.2, 130.6, 129.4, 128.0, 125.8, 120.8, 114.6, 104.5, 55.7, 21.4; IR (neat) 3138, 2999,

2909, 2835, 1605, 1524, 1519, 1514, 1503, 1462, 1453, 1434, 1257; HRMS (ESI) calcd for $C_{17}H_{16}N_2O$: 264.1263, found 265.1328 (M+H). The position of the transferred aryl group was determined by nOesy NMR studies.

1-(4-Fluorophenyl)-1*H*-indazole-6-carboxaldehyde (8a) and 2-(4-fluorophenyl)-2*H*-indazole-6-carboxaldehyde (8b)

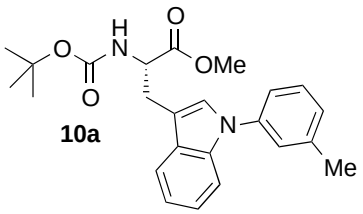


Method C was followed on a 0.34 mmol scale starting from 1*H*-indazole-6-carboxaldehyde **7** and **3g**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **8a** as a yellow solid (41 mg, 50%) and **8b** as an orange solid (6.8 mg, 8%).

Compound **8a**: m.p. 143-145°C; R_f 0.50 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.22 (s, 1H), 8.10 (s, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 1H), 7.66-7.62 (m, 2H), 7.23 (d, *J* = 8.5 Hz, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 192.8, 164.0, 160.7, 139.4, 136.4, 136.2, 136.1, 129.4, 125.7, 125.6, 122.9, 122.1, 117.6, 117.3, 114.2; IR (neat) 2969, 2815, 2725, 1703, 1698, 1692, 1681, 1605, 1519, 1514, 1503, 1493, 1461, 1450, 1434, 1279; HRMS (ESI) calcd for $C_{14}H_9FN_2O$: 240.0699, found 241.0766 (M+H).

Compound **8b**: m.p. 179-183°C; R_f 0.42 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.43 (s, 1H), 8.30 (s, 1H), 7.93-7.89 (m, 2H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.29-7.24 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 192.4, 149.1, 135.9, 126.3, 125.7, 123.2, 123.1, 121.6, 121.3, 119.5, 117.0, 116.7, 29.8; IR (neat) 3121, 2917, 2844, 1687, 1678, 1673, 1666, 1605, 1519, 1514, 1503, 1494, 1468, 1462, 1450, 1432; HRMS (ESI) calcd for $C_{14}H_9FN_2O$: 240.0699, found 241.0767 (M+H). The structure of compound **9** was confirmed by X-ray crystallography; see section **5**: Crystallographic data for compound **9**.

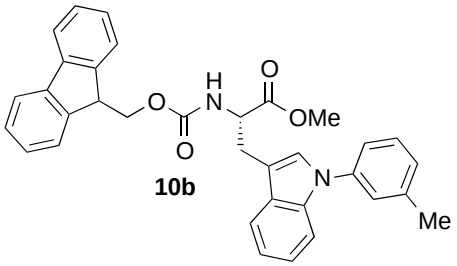
1-(3-Methylphenyl)- ***N-tert*****-butoxycarbonyl-L-tryptophan methyl ester (10a)**



10a

Method C was followed on a 0.16 mmol scale starting from *N-tert*-butoxycarbonyl-L-tryptophan methyl ester and **3c**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **10a** as a yellow oil (57 mg, 87%): R_f 0.33 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.0 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.32-7.27 (m, 1H), 7.19-7.16 (m, 2H), 7.13-7.05 (m, 4H), 5.05 (d, *J* = 8.3 Hz, 1H), 4.62-4.60 (m, 1H), 3.62 (s, 3H), 3.32-3.18 (m, 2H), 2.35 (s, 3H), 1.35 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 172.8, 155.3, 139.7, 139.5, 136.1, 129.4, 129.1, 127.2, 126.6, 124.9, 122.6, 121.3, 120.2, 119.1, 111.2, 110.7, 79.9, 54.1, 52.4, 28.4, 27.9, 21.5; IR (neat) 3433, 3377, 3050, 2976, 2928, 1743, 1709, 1606, 1590, 1494, 1493, 1459, 1365, 1159; HRMS (ESI) calcd for $C_{24}H_{28}N_2O_4$: 408.2049, found 353.1502 (M-C$(CH_3)_3$), 431.1941 (M+Na).

1-(3-Methylphenyl)-Fmoc-D-tryptophan-methyl ester (10b)



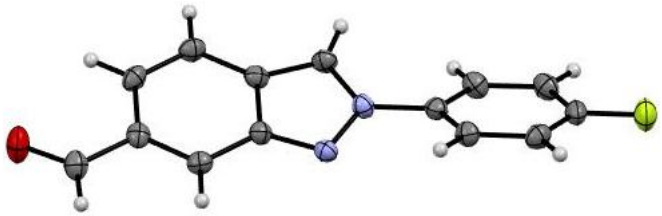
10b

Method C was followed on a 0.11 mmol scale starting from *N*-[(9*H*-fluoren-9-ylmethoxy)carbonyl]-L-tryptophan methyl ester and **3c**. The crude product was purified on silica gel (20% EtOAc/hexanes) to afford **10b** as a yellow oil (47 mg, 80%): R_f 0.29 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.4 Hz, 2H), 7.76-7.66 (m, 5H), 7.55-7.48 (m, 3H), 7.41-7.36 (m, 4H), 7.34-7.26 (m, 3H), 5.56 (d, *J* = 8.3 Hz, 1H), 4.96-4.90 (m, 1H), 4.58-4.49 (m, 2H), 4.36-4.33 (m, 1H), 3.86 (s, 3H), 3.51 (d, *J* = 5.4 Hz, 2H), 2.56 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 172.4, 155.8, 143.9, 143.8, 141.3, 139.7, 139.5, 136.1, 129.5, 127.7, 127.3, 127.1, 126.7, 125.2, 125.0, 122.7, 121.4, 120.3, 120.0, 119.0, 110.8, 67.1, 54.6, 52.5, 47.2, 28.0, 21.5; IR (neat) 3418, 3356, 3049, 2950, 1717, 1606, 1589, 1494, 1459, 1207.

5. Crystallographic data for compound 8b

CCDC-986210 (for **8b**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal Structure Report for compound 8b



A light orange needle-like specimen of $C_{14}H_9FN_2O$, approximate dimensions 0.047 mm x 0.058 mm x 0.268 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. A total of 5856 frames were collected. The total exposure time was 16.27 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 15339 reflections to a maximum θ angle of 68.37° (0.83 Å resolution), of which 1971 were independent (average redundancy 7.782, completeness = 99.8%, R_{int} = 5.15%) and 1661 (84.27%) were greater than $2\sigma(F^2)$. The final cell constants of a = 3.76530(10) Å, b = 17.7911(4) Å, c = 16.0214(3) Å, β = 92.874(2)°, volume = 1071.90(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 9053 reflections above 20 σ(I) with 7.430° < 2θ < 136.7°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.930. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7940 and 0.9590.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P $2_1/c$, with Z = 4 for the formula unit $C_{14}H_9FN_2O$. The final anisotropic full-matrix least-squares refinement on F^2 with 164 variables converged at R_1 = 5.83%, for the observed data and wR_2 = 16.57% for all data. The goodness-of-fit was 1.193. The largest peak in the final difference electron density synthesis was 0.358 $e^-/Å^3$ and the largest hole was -0.276 $e^-/Å^3$ with an RMS deviation of 0.074 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.489 g/cm^3 and F(000) 496 e^-.

Table 1. Sample and crystal data for Pauline1b.

CCDC deposition number	986210	
Chemical formula	$C_{14}H_9FN_2O$	
Formula weight	240.23	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal size	0.047 x 0.058 x 0.268 mm	
Crystal habit	light orange needle	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 3.76530(10) Å	α = 90°
	b = 17.7911(4) Å	β = 92.874(2)°

	c = 16.0214(3) Å	γ = 90°
Volume	1071.90(4) Å^3	
Z	4	
Density (calculated)	1.489 g/cm^3	
Absorption coefficient	0.900 mm^{-1}	
F(000)	496	

Table 2. Data collection and structure refinement for Pauline1b.

Theta range for data collection	3.71 to 68.37°	
Index ranges	-4<=h<=4, -21<=k<=21, -19<=l<=19	
Reflections collected	15339	
Independent reflections	1971 [R(int) = 0.0515]	
Coverage of independent reflections	99.8%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9590 and 0.7940	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2013 (Sheldrick, 2013)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	1971 / 0 / 164	
Goodness-of-fit on F^2	1.193	
Final R indices	1661 data; I>2σ(I)	R_1 = 0.0583, wR_2 = 0.1595
	all data	R_1 = 0.0682, wR_2 = 0.1657
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0789P)^2+0.9563P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0028(8)	
Largest diff. peak and hole	0.358 and -0.276 eÅ^{-3}	
R.M.S. deviation from mean	0.074 eÅ^{-3}	

Atomic coordinates, bond lengths, bond angles, torsion angles, anisotropic atomic displacement parameters are provided in the attached CIF file, which can also be retrieved from the Cambridge Crystallographic Data Centre using deposition number 986210 at the following URL: http://www.ccdc.cam.ac.uk/Community/Requestastructure/Pages/Requestastructure.aspx

checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: I

No errors found in this datablock

```
Bond precision:        C-C = 0.0040 A                Wavelength=1.54178
Cell:        a=3.7653(1)       b=17.7911(4)      c=16.0214(3)
             alpha=90          beta=92.874(2)    gamma=90
Temperature: 150 K
                    Calculated                          Reported
Volume              1071.91(4)                          1071.90(4)
Space group         P 21/c                              P 21/c
Hall group          -P 2ybc                             -P 2ybc
Moiety formula      C14 H9 F N2 O                       C14 H9 F N2 O
Sum formula         C14 H9 F N2 O                       C14 H9 F N2 O
Mr                  240.23                              240.23
Dx,g cm-3           1.489                               1.489
Z                   4                                   4
Mu (mm-1)           0.900                               0.900
F000                496.0                               496.0
F000'               497.66
h,k,lmax            4,21,19                             4,21,19
Nref                1975                                1971
Tmin,Tmax           0.939,0.959
Tmin'               0.786
Correction method= Not given
Data completeness= 0.998          Theta(max)= 68.371
R(reflections)= 0.0583( 1661)         wR2(reflections)= 0.1657( 1971)
S = 1.193               Npar= 164
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checkCIF publication errors

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

0 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

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You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify

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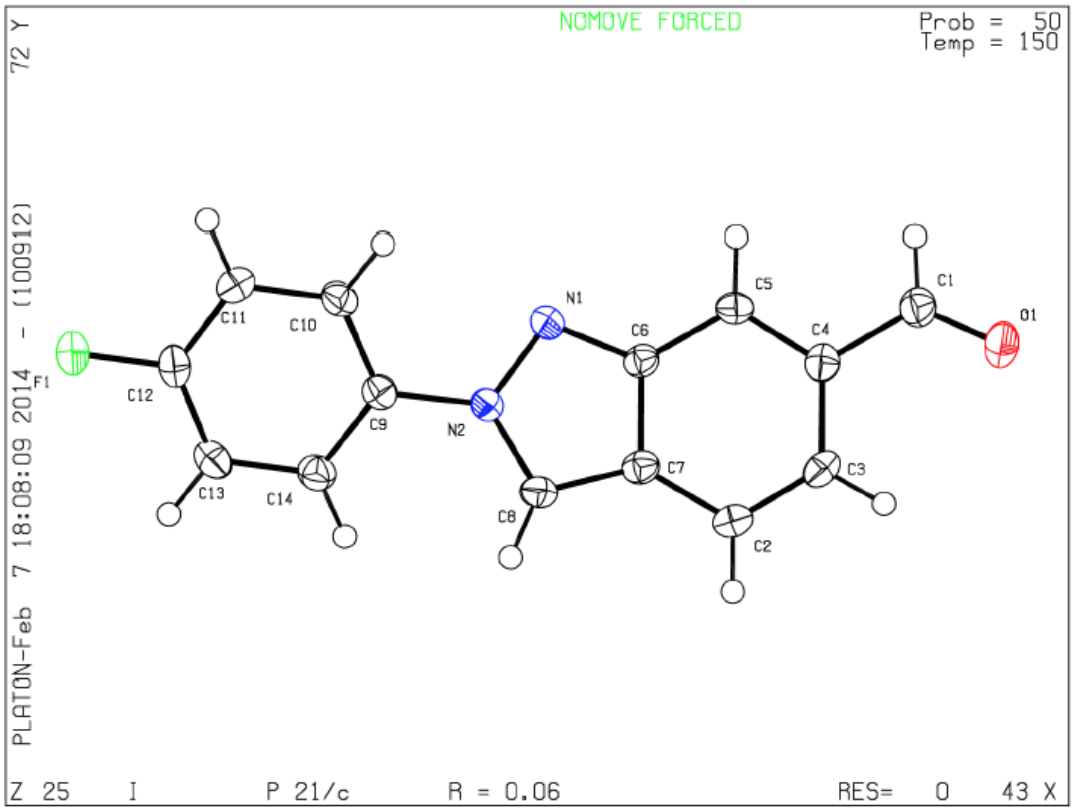
PLATON version of 18/09/2013; check.def file version of 12/09/2013

Datablock I - ellipsoid plot



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6. References

1) W. Dohle, D. M. Lindsay and P. Knochel, *Org. Lett.*, 2001, **18**, 2871.

2) D. H. R. Barton, N. Y. Bhatnagar, J.-P. Finet and W. B. Motherwell, *Tetrahedron*, 1986, **42**, 3111.

3) P. Petiot and A. Gagnon, *Eur. J. Org. Chem.*, 2013, 5282.

4) C. Crifar, P. Petiot, T. Ahmad and A. Gagnon, *Chem. Eur. J.*, 2014, 2755.

5) C. W. Still, M. Kahn and A. Mitra, *J. Org. Chem.*, 1978, **43**, 2923.

6) K. Urgin, C. Aube, M. Pipelier, V. Blot, C. Thobie-Gautier, S. Sengmany, J. Lebreton, E. Leonel, D. Dubreuil and S. Condon, *Eur. J. Org. Chem.*, 2013, 117.

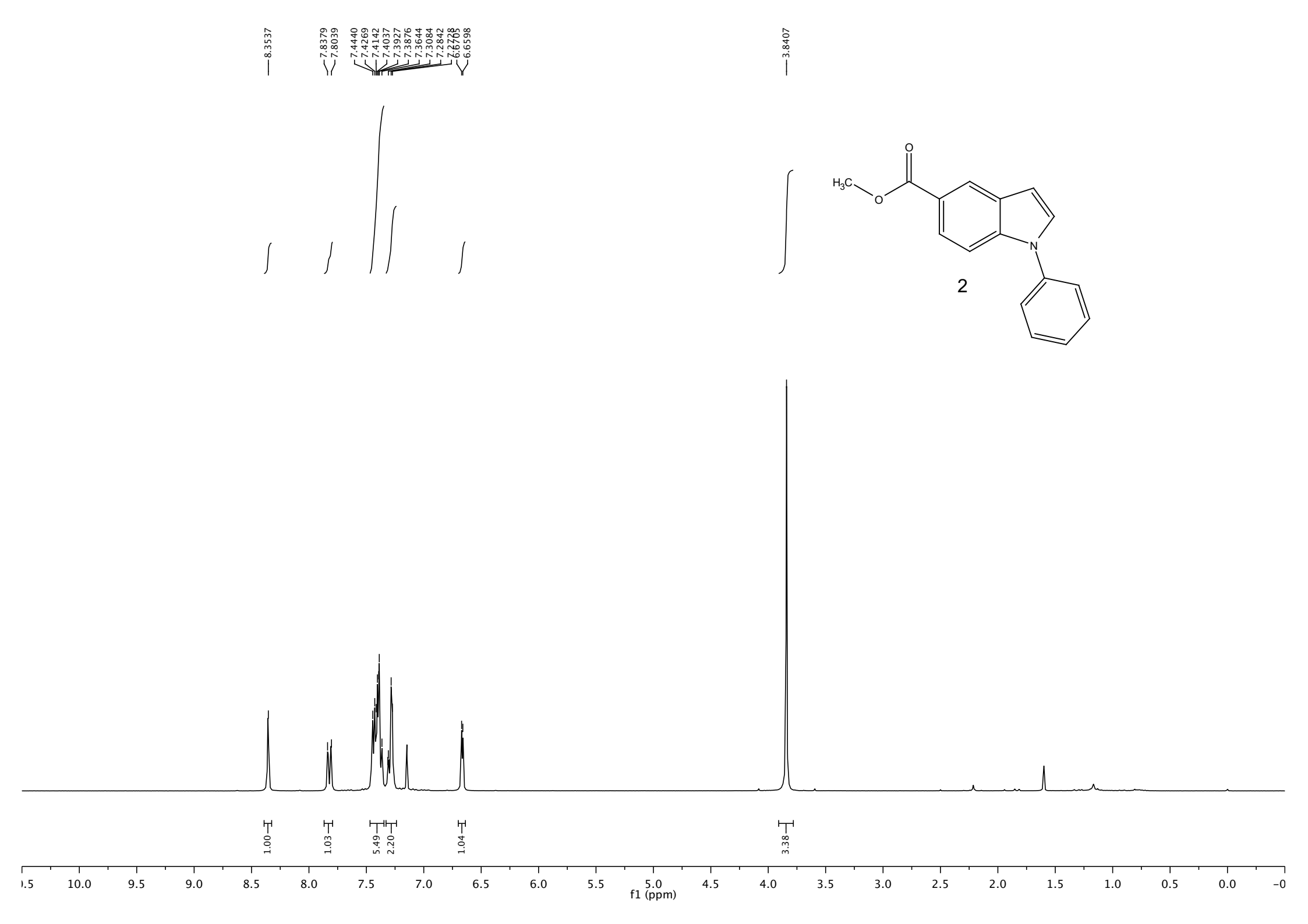
7) R. F. De Ketelaere and G. P. Van der Kelen, *J. Organomet. Chem.*, 1974, **73**, 251-257; M. L. N. Rao and S. Giri, *J. Org. Chem.*, 2012, **24**, 4580.

8) N. E. Faucher, P. Martres and S. Meunier, *PTC Int. Appl.*, 2009, WO2009047240A120090416.

9) Y. M. Na, *Bull. Korean Chem. Soc.*, 2011, **32**, 307.

10) J. C. Antilla, J. M. Baskin, T. E. Barder, S. L. Buchwald, *J. Org. Chem.*, 2004, **69**, 5578.

6. Spectra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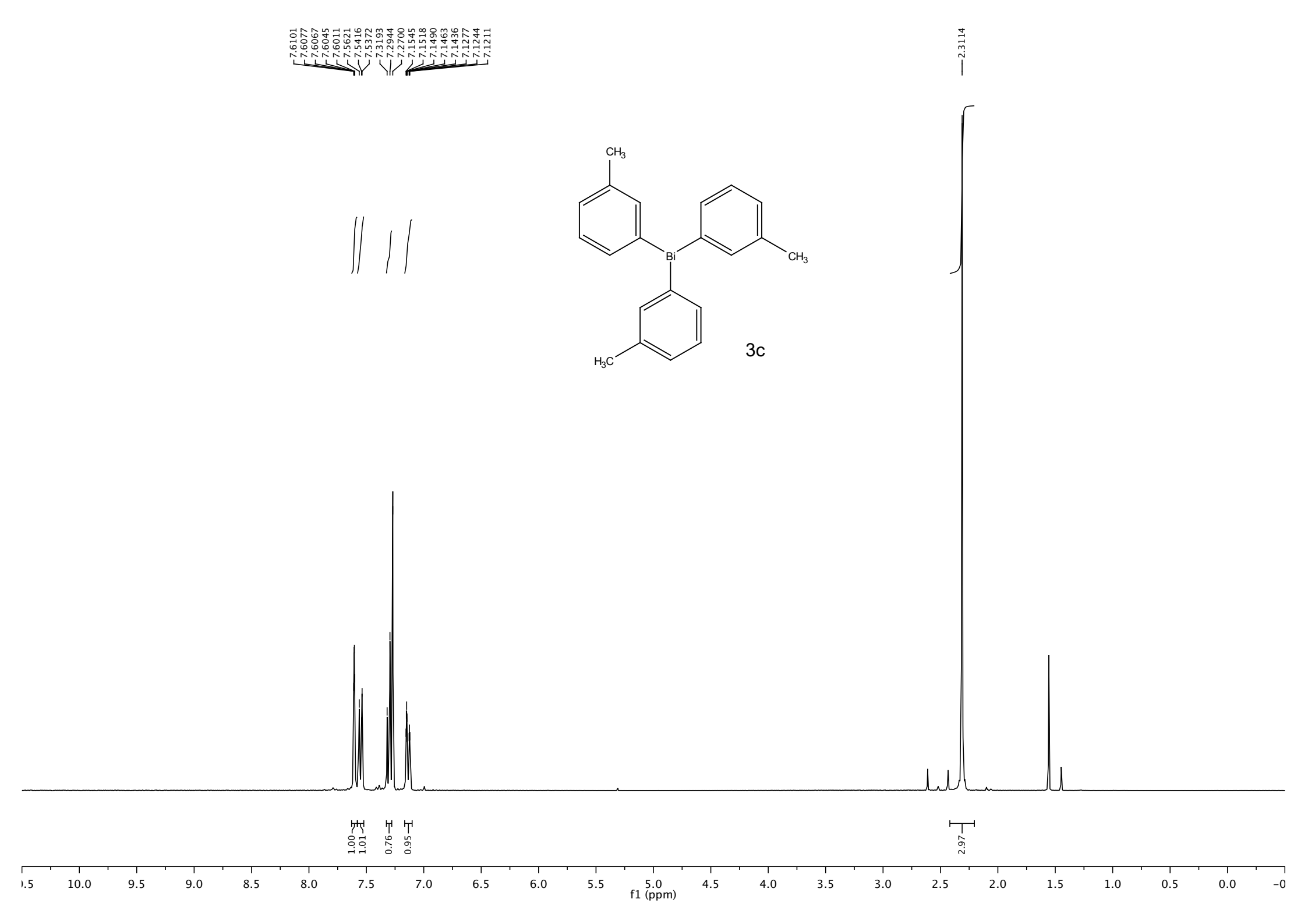
f1 (ppm)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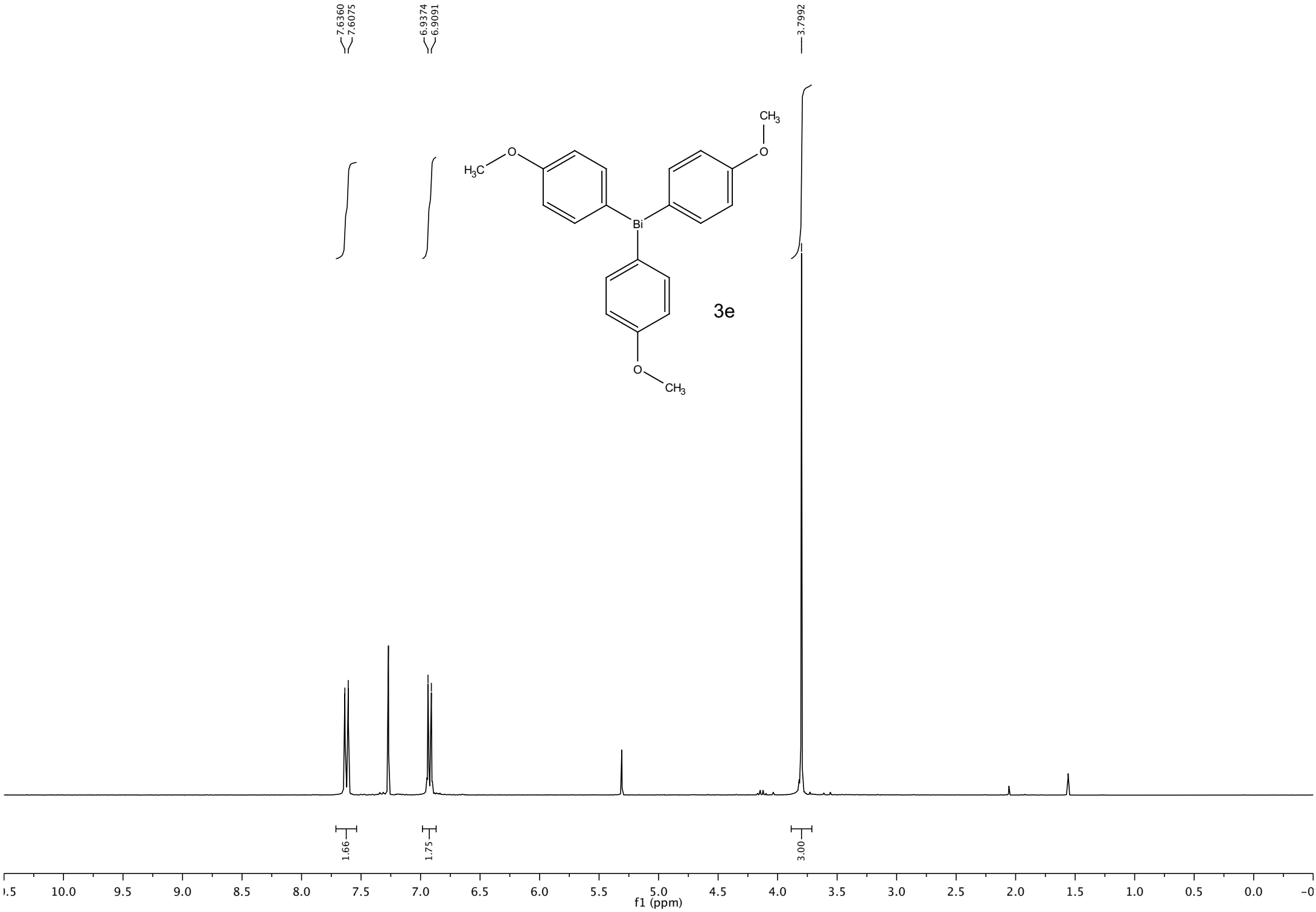
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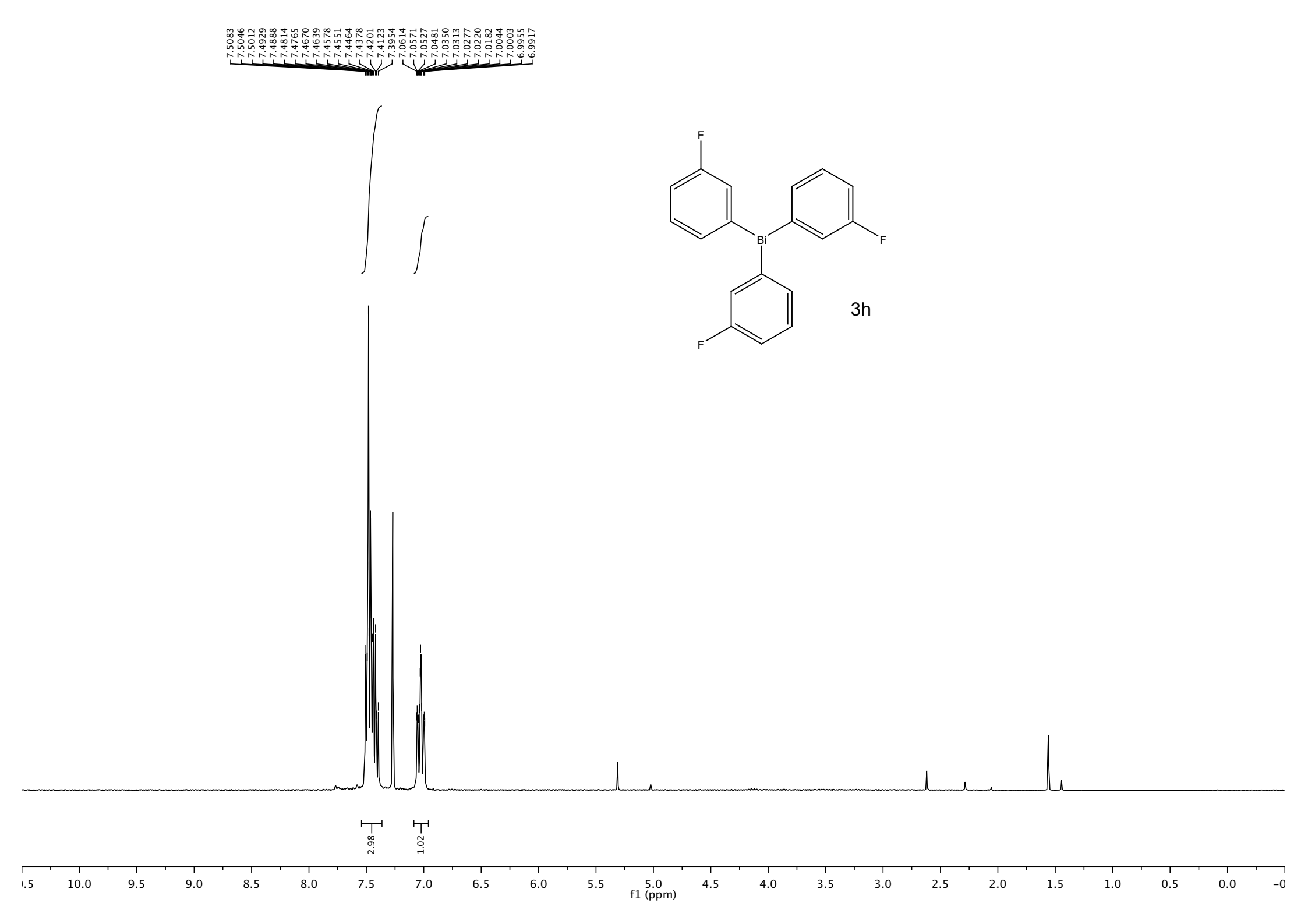
f1 (ppm)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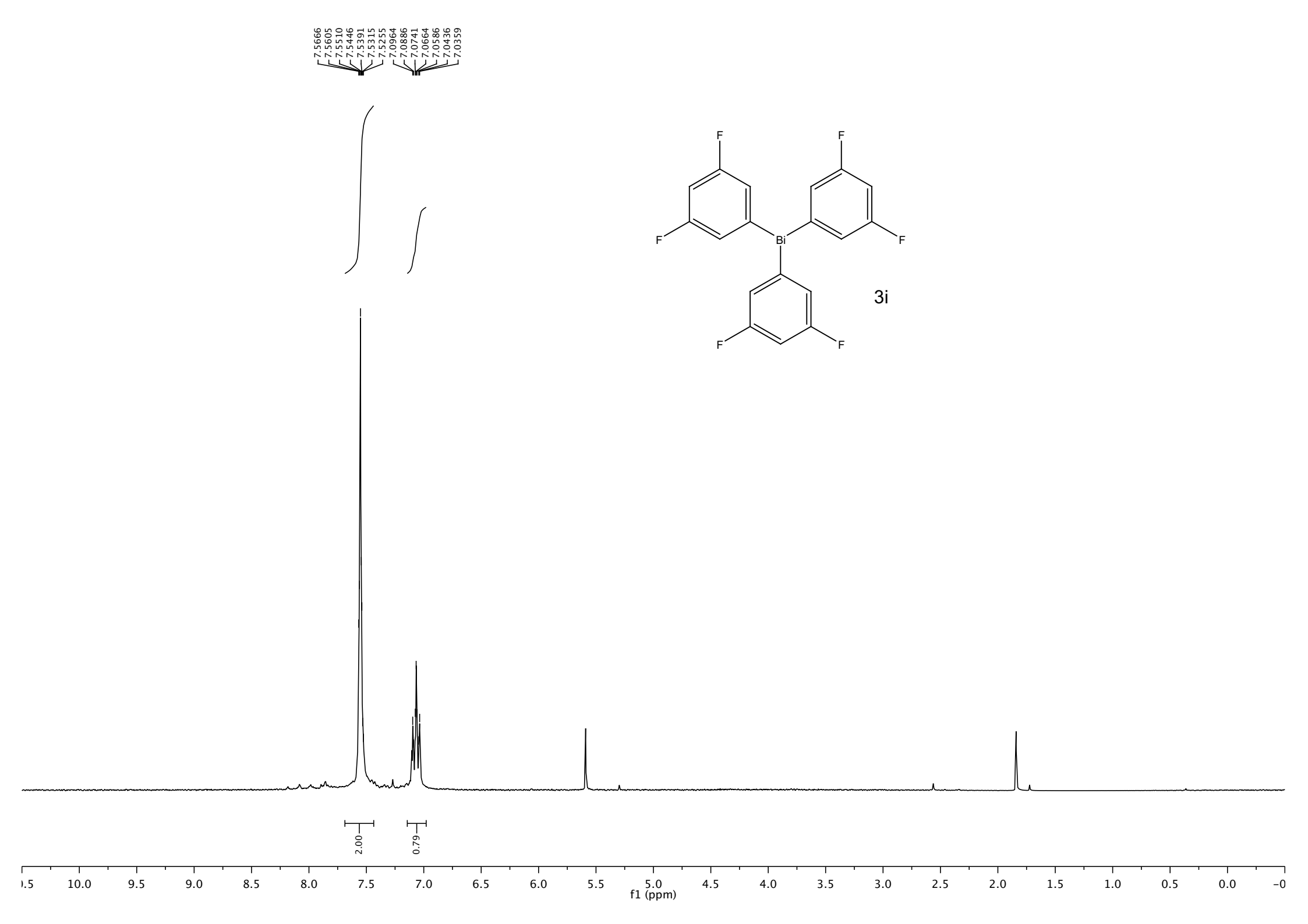
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F
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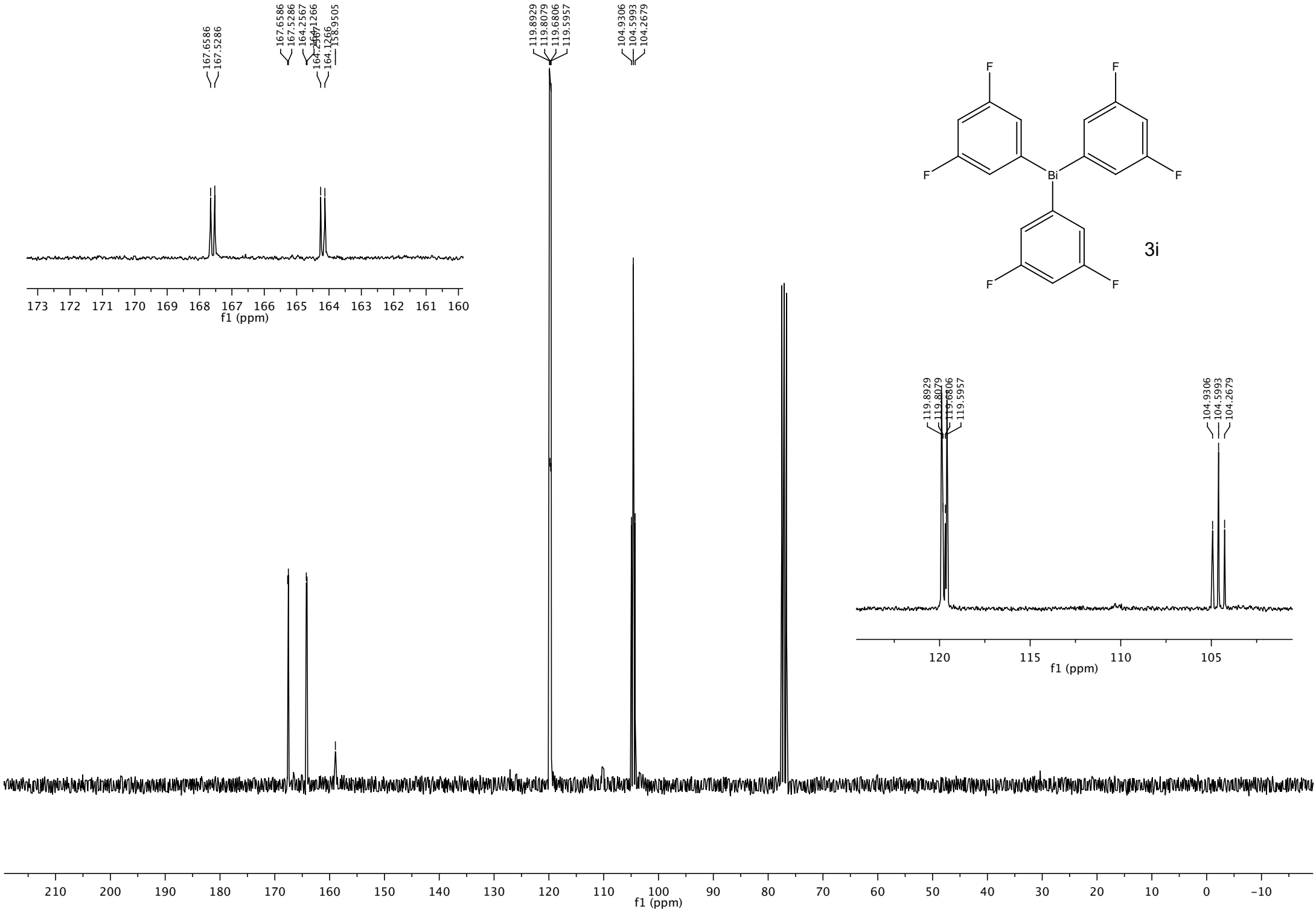
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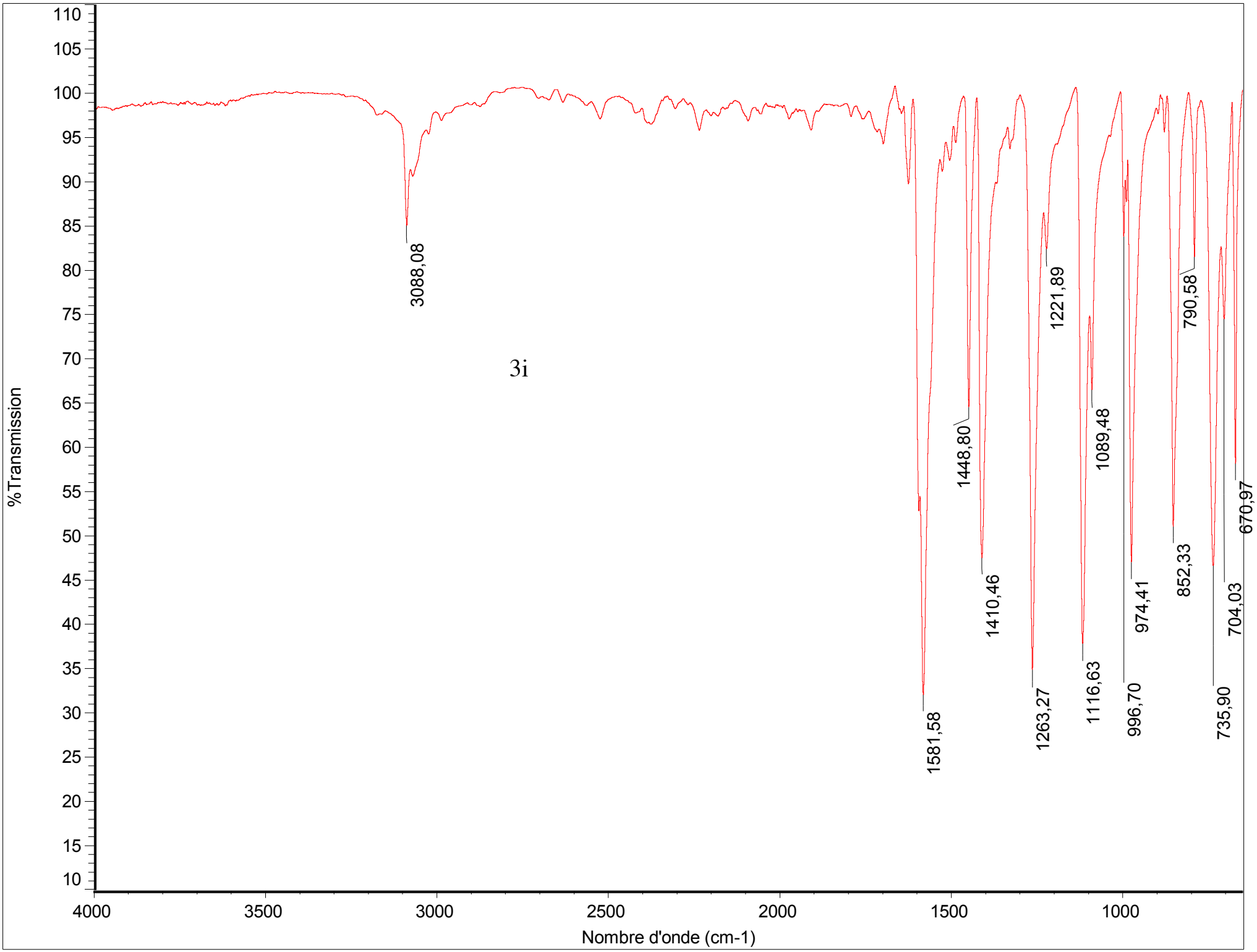
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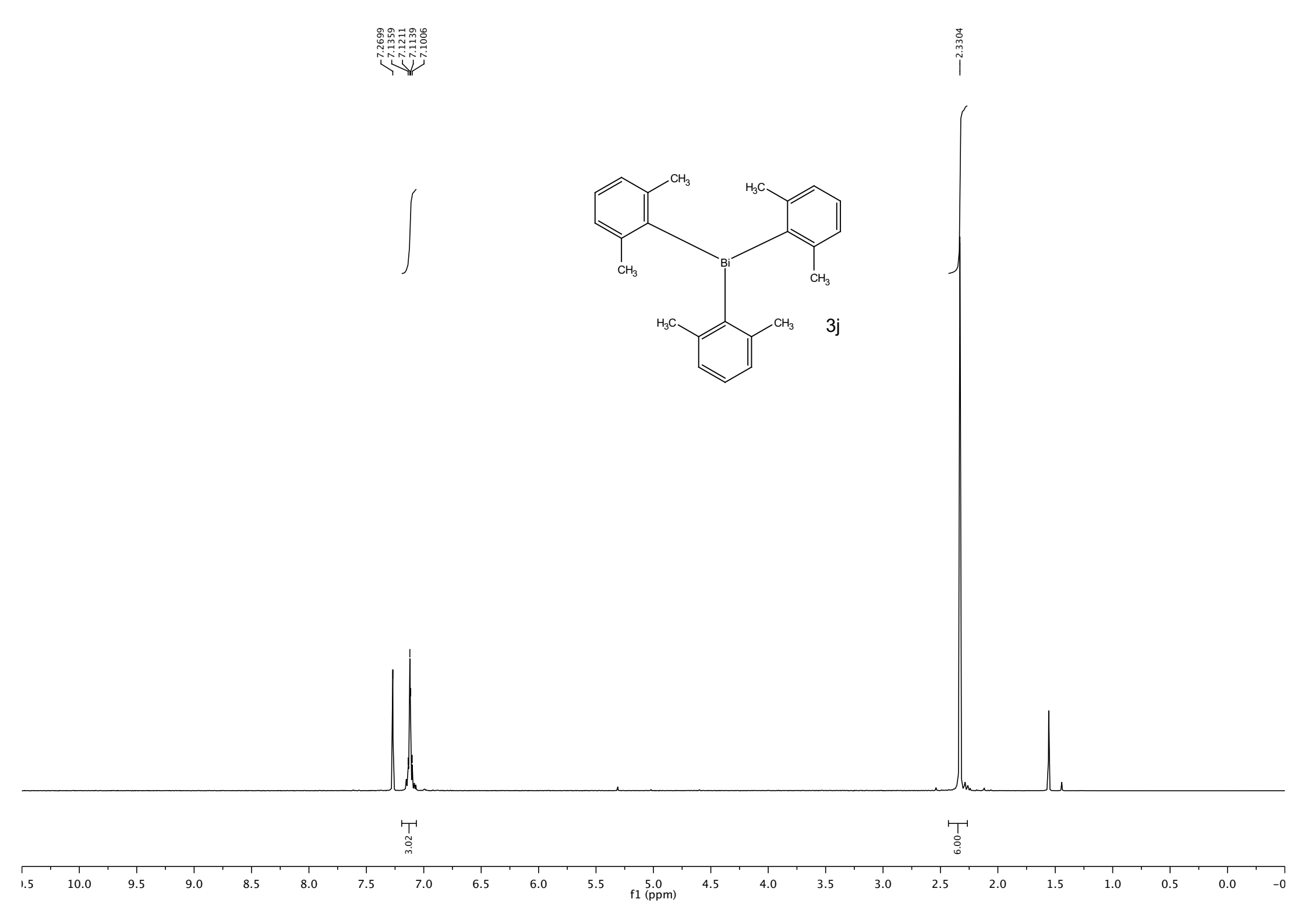
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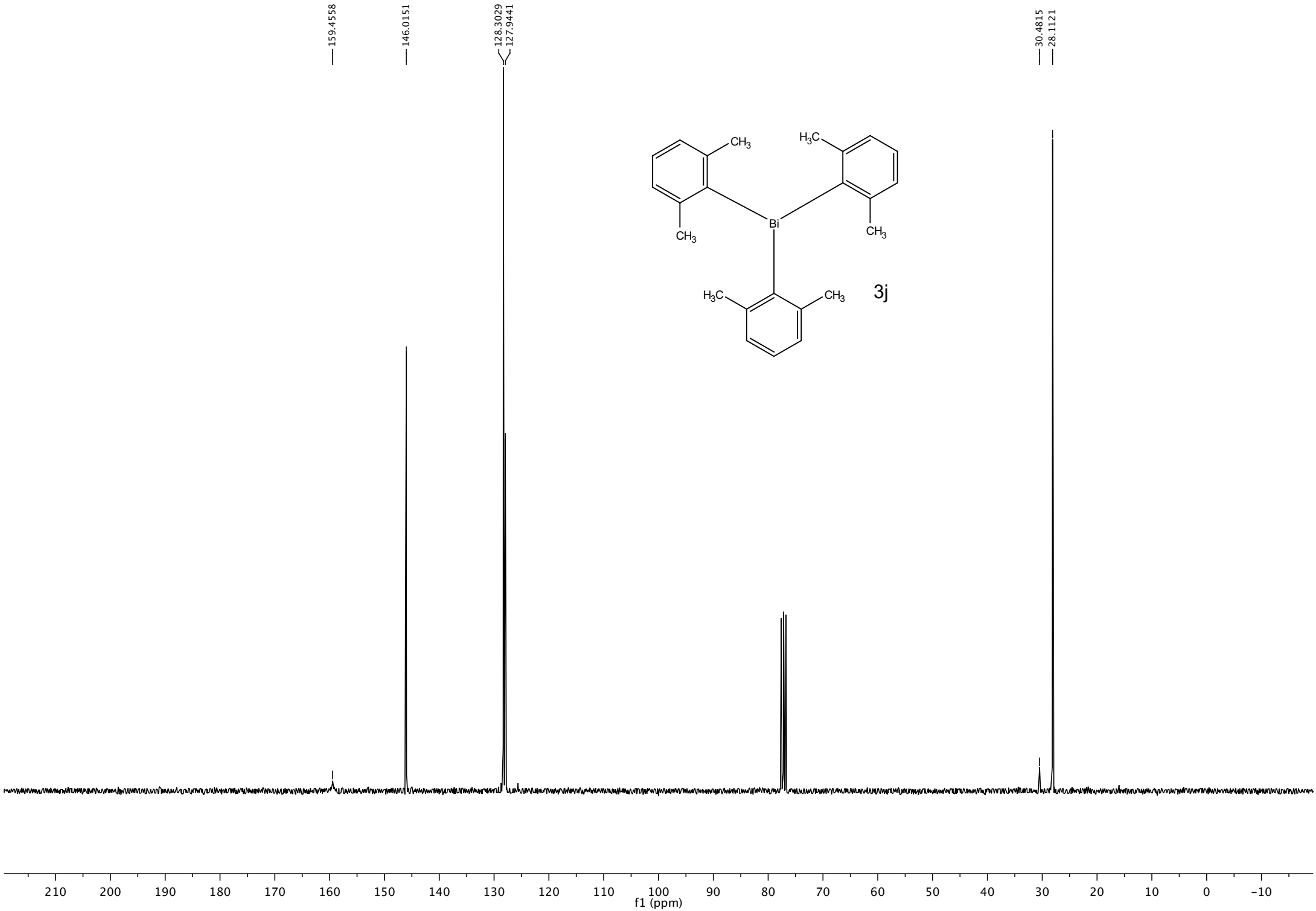
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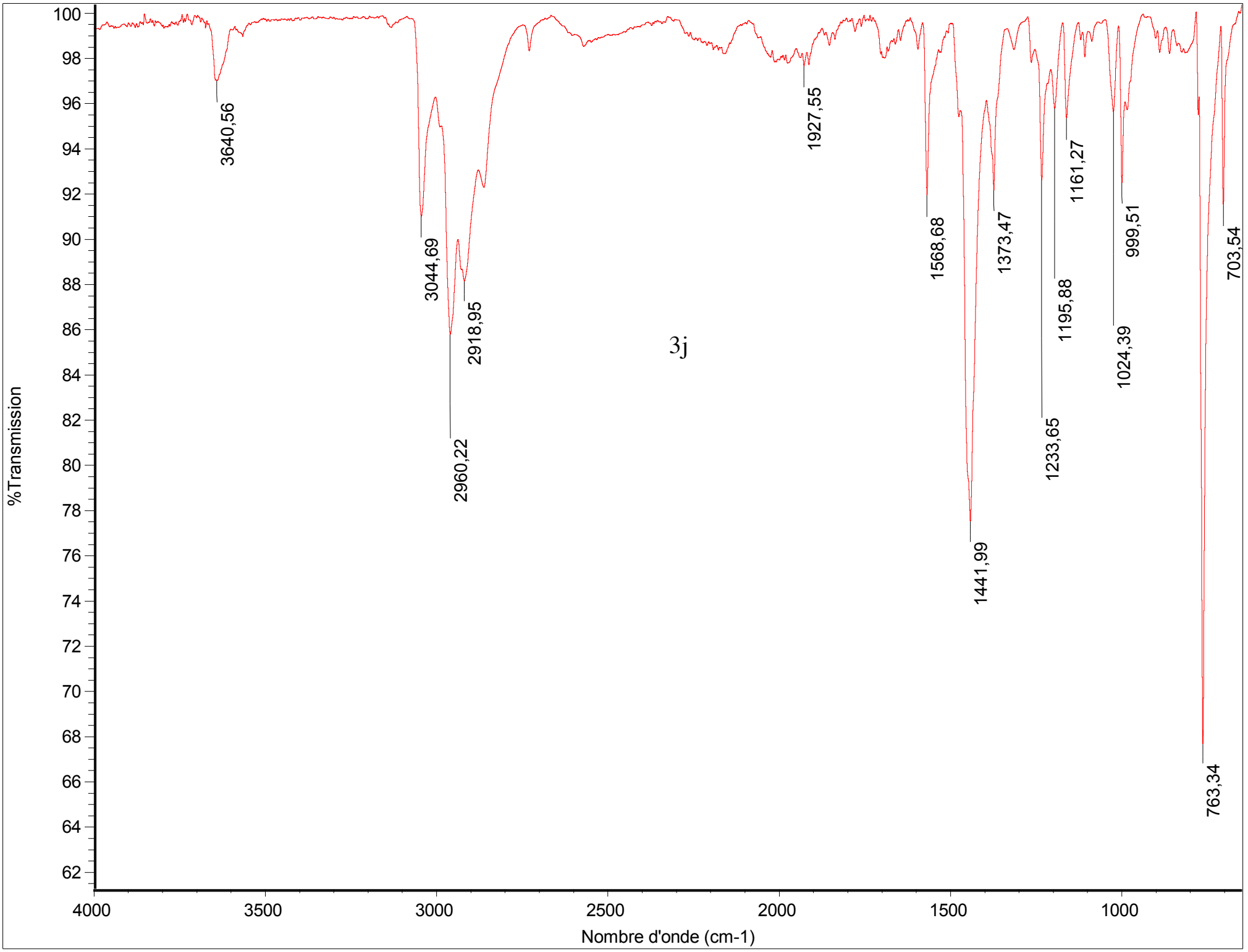
f1 (ppm)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3j
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96
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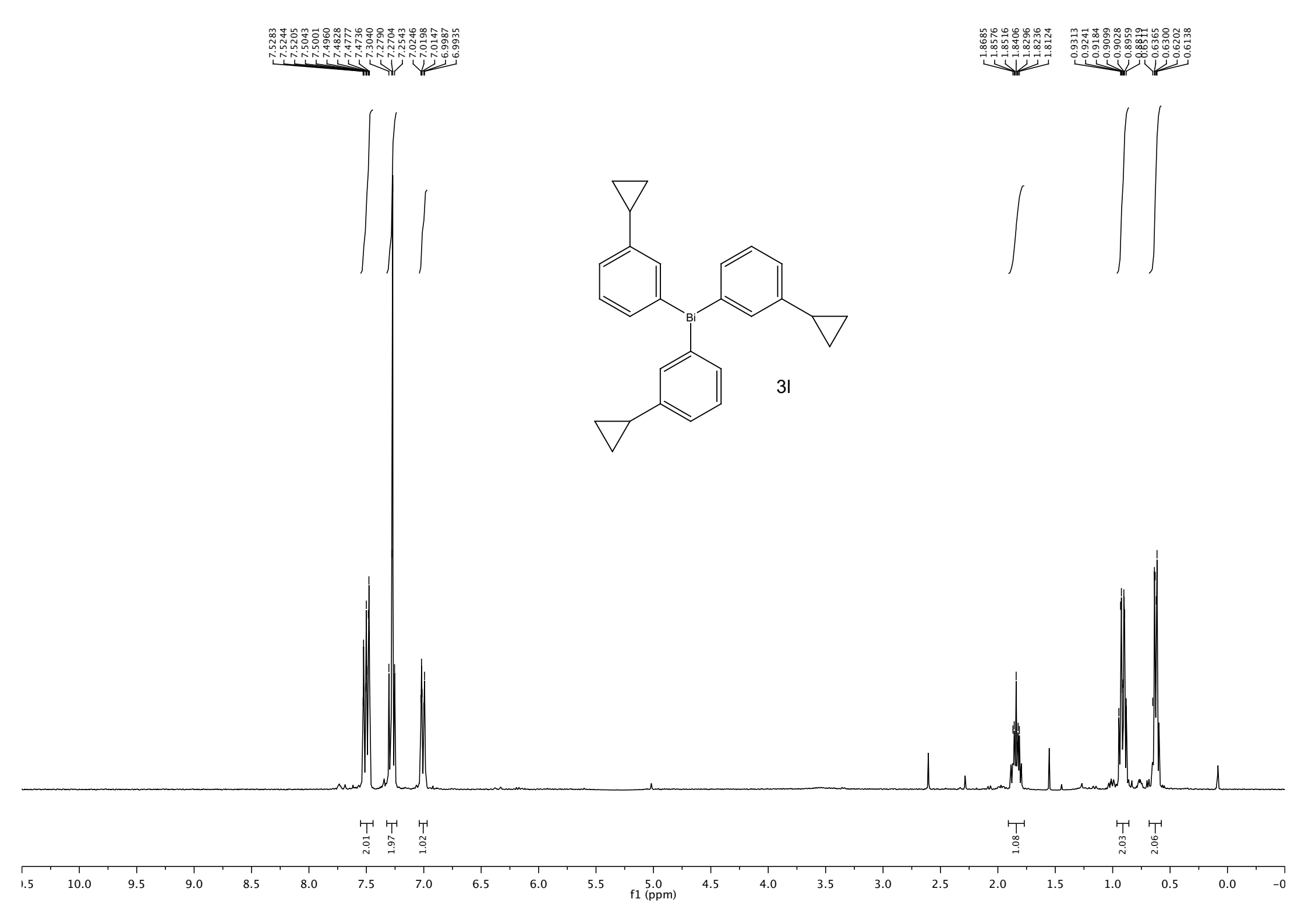
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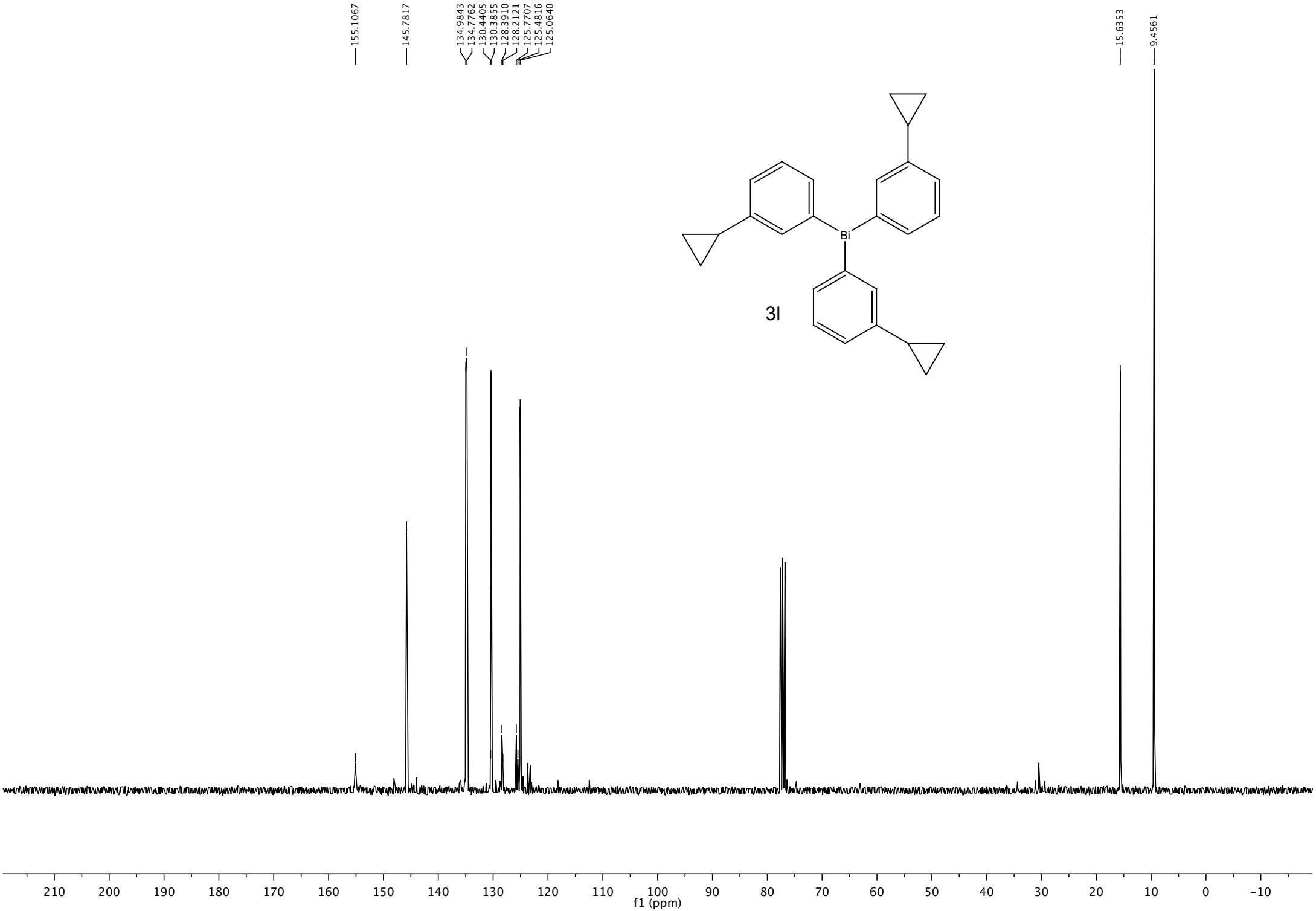
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3l
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180
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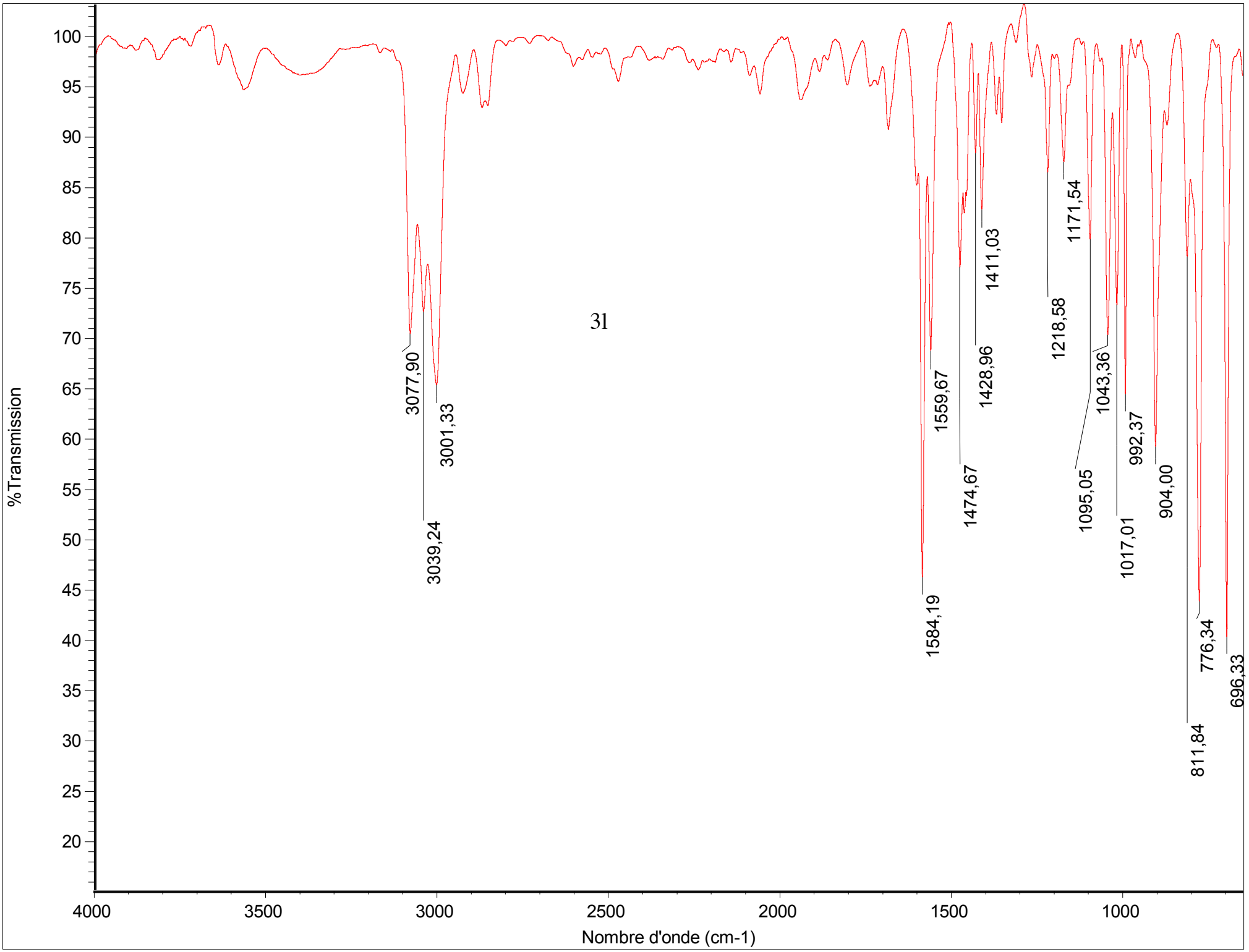
f1 (ppm)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2000
1500
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3001,33
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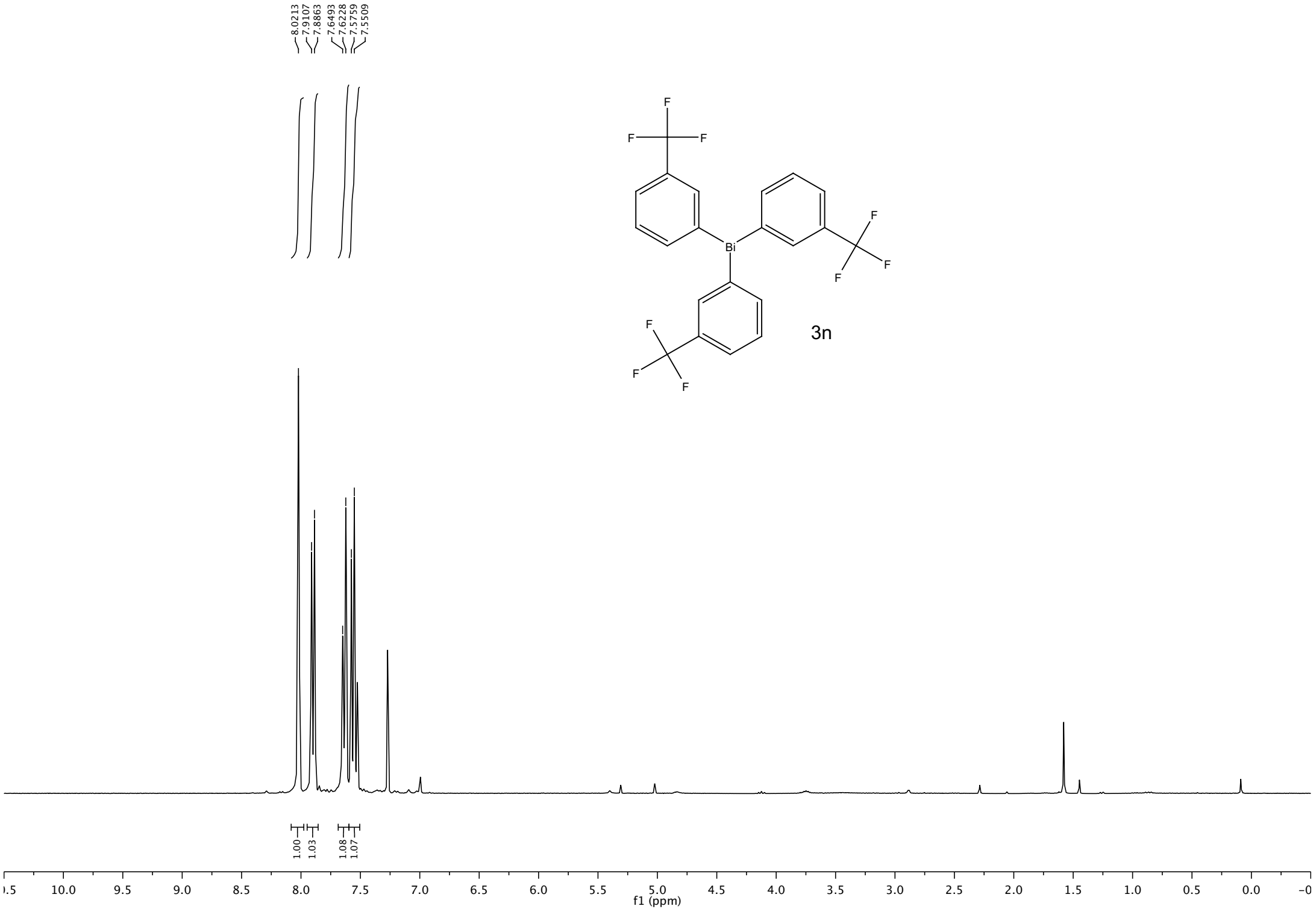
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5.5
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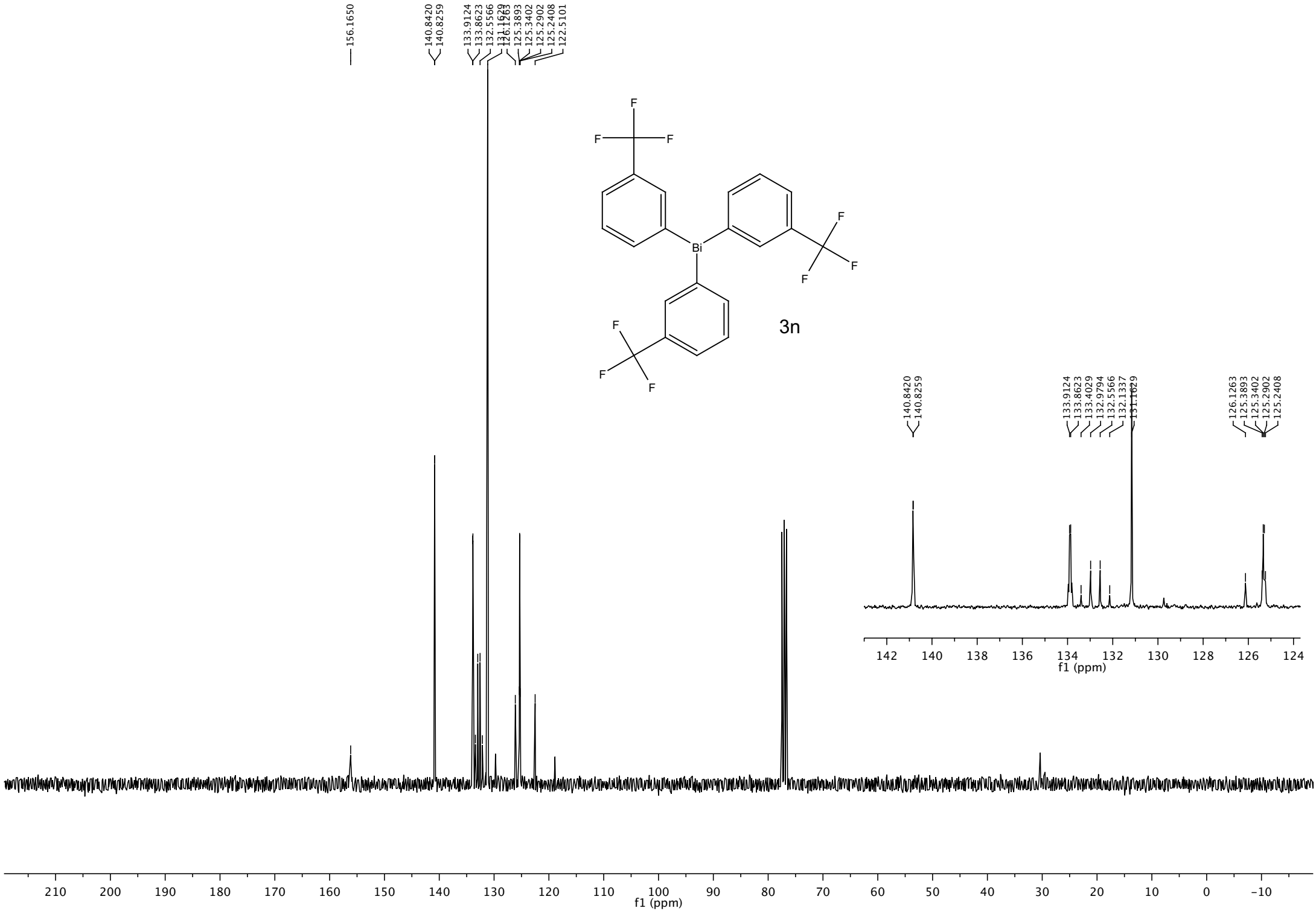
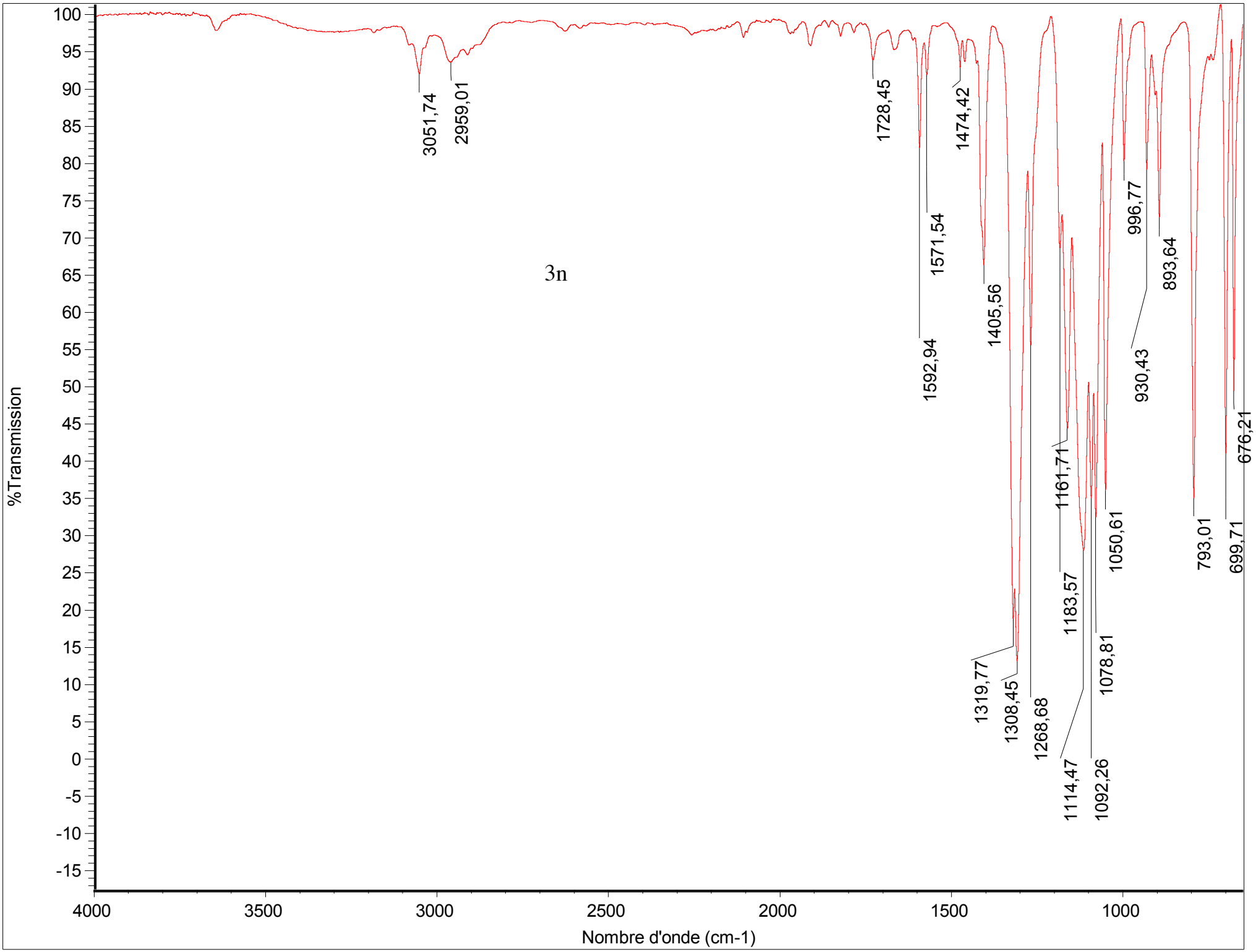
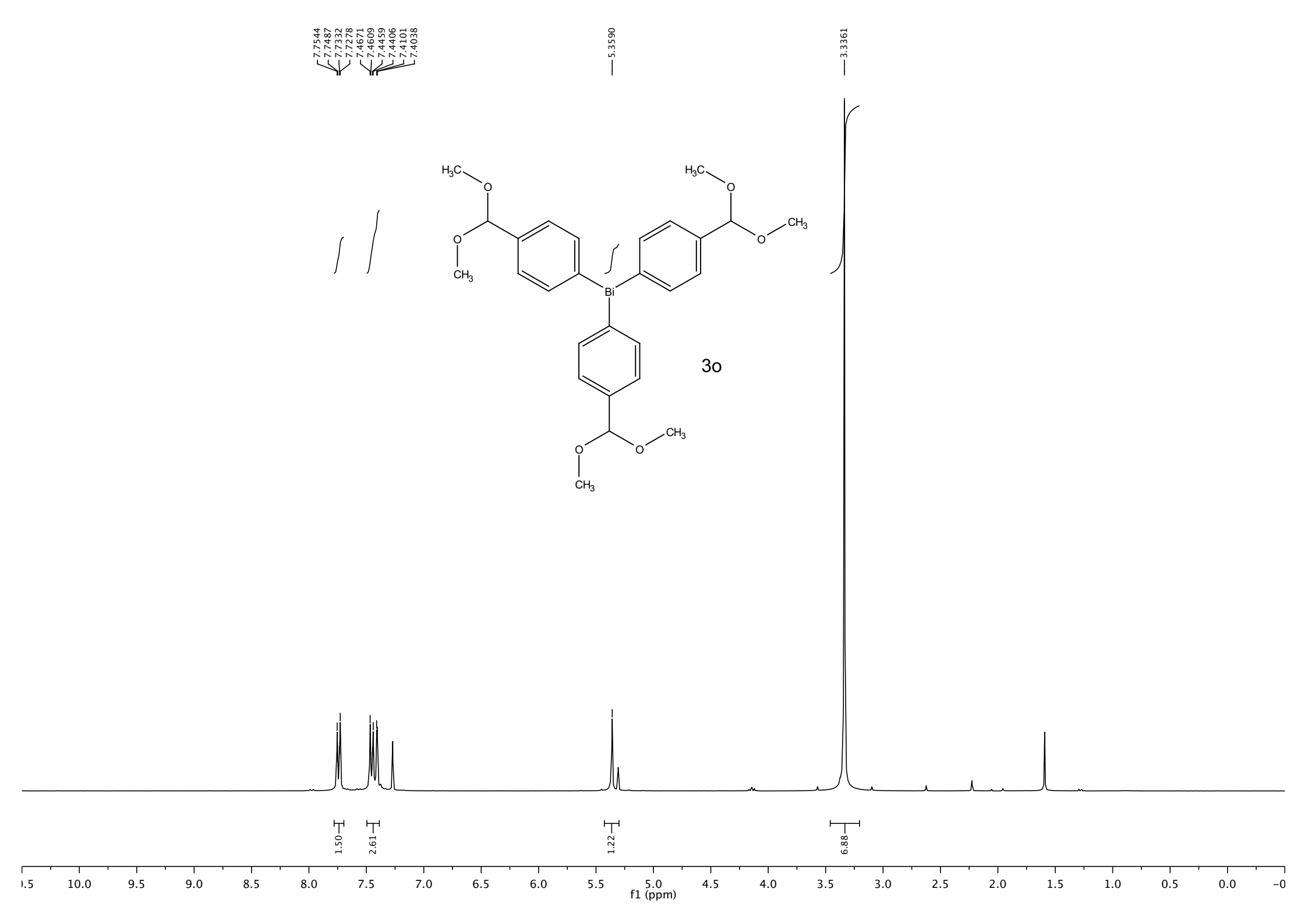
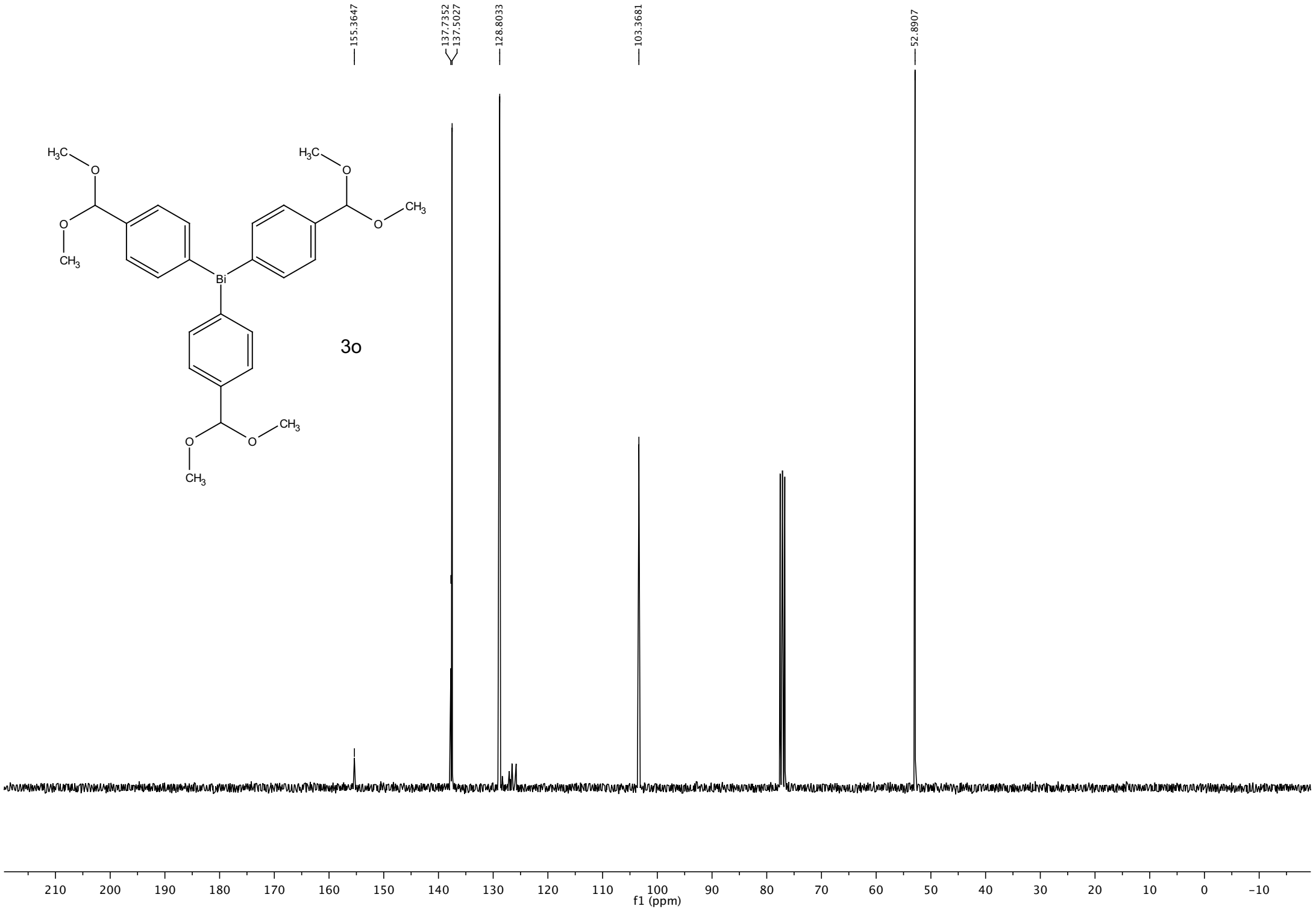
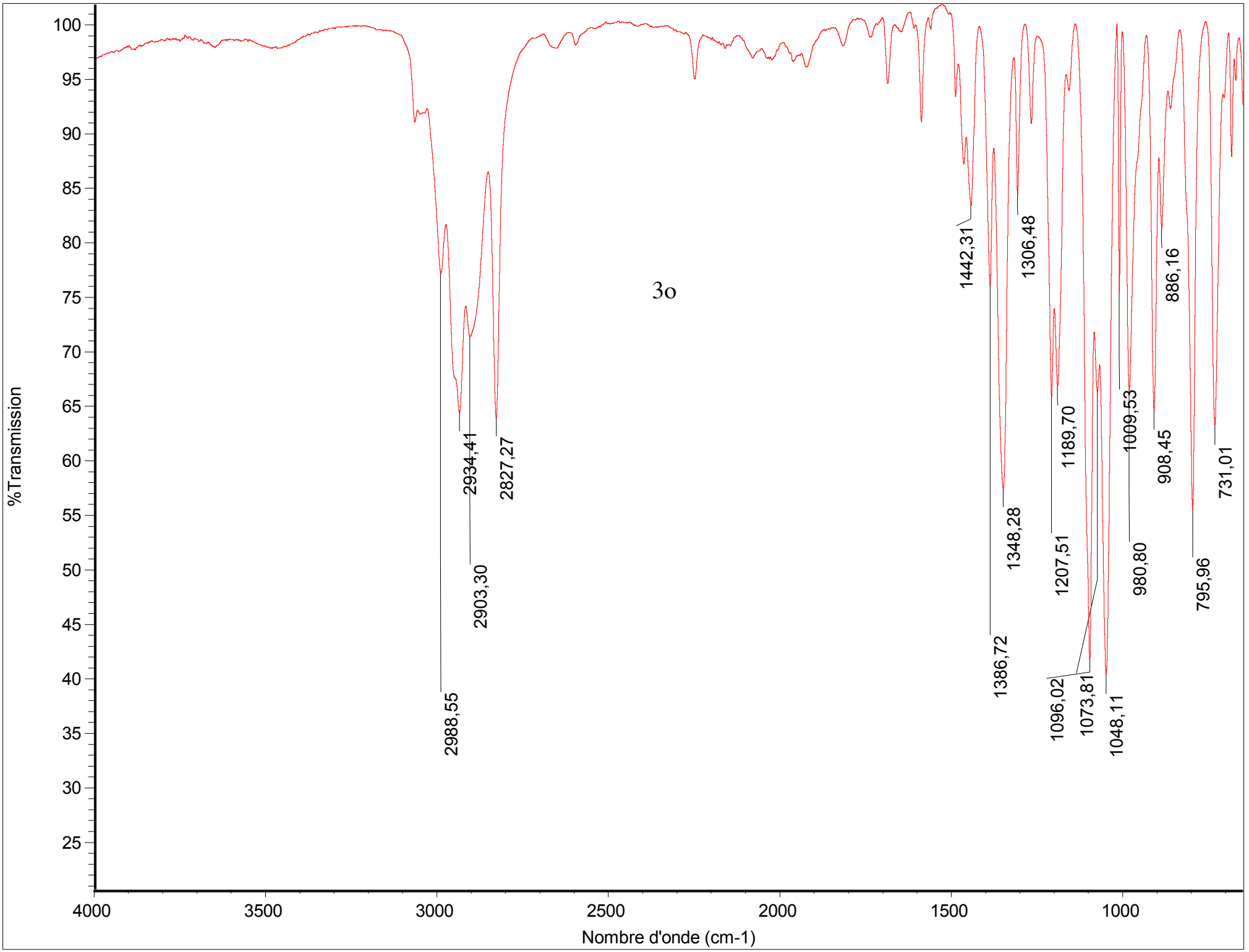
0.0
f1 (ppm)

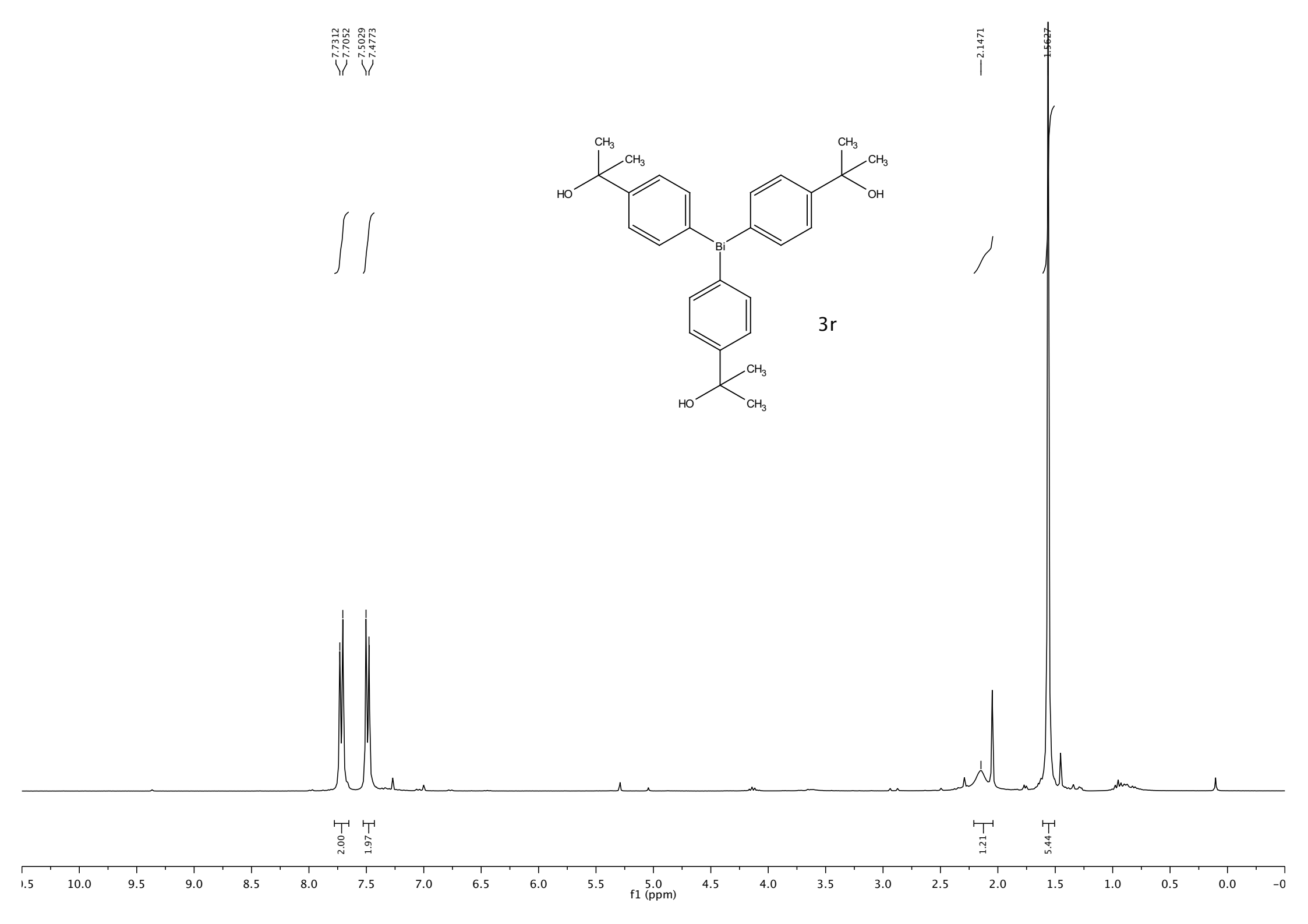

156.1650
140.8420
140.8259
133.9124
133.8623
132.5566
131.1629
126.1263
125.3893
125.3402
125.2902
125.2408
122.5101
F
F
F
Bi
F
F
F
F
F
3n
140.8420
140.8259
133.9124
133.8623
133.4029
132.9794
132.5566
132.1337
131.1629
126.1263
125.3893
125.3402
125.2902
125.2408
142
140
138
136
134
132
130
128
126
124
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

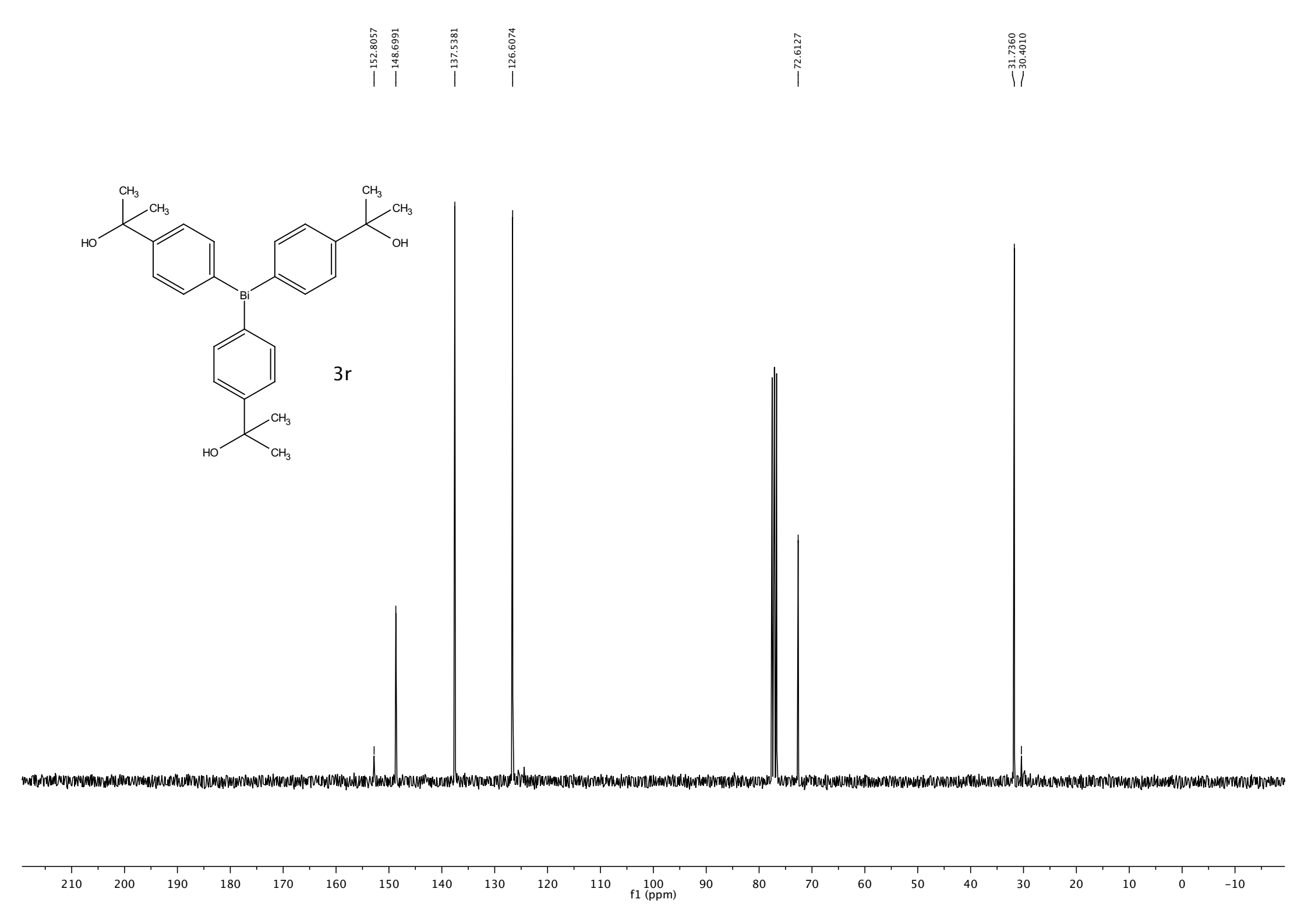

3n
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
4000
3500
3000
2500
2000
1500
1000
3051,74
2959,01
1728,45
1592,94
1571,54
1474,42
1405,56
1319,77
1308,45
1268,68
1183,57
1161,71
1114,47
1092,26
1078,81
1050,61
996,77
930,43
893,64
793,01
699,71
676,21

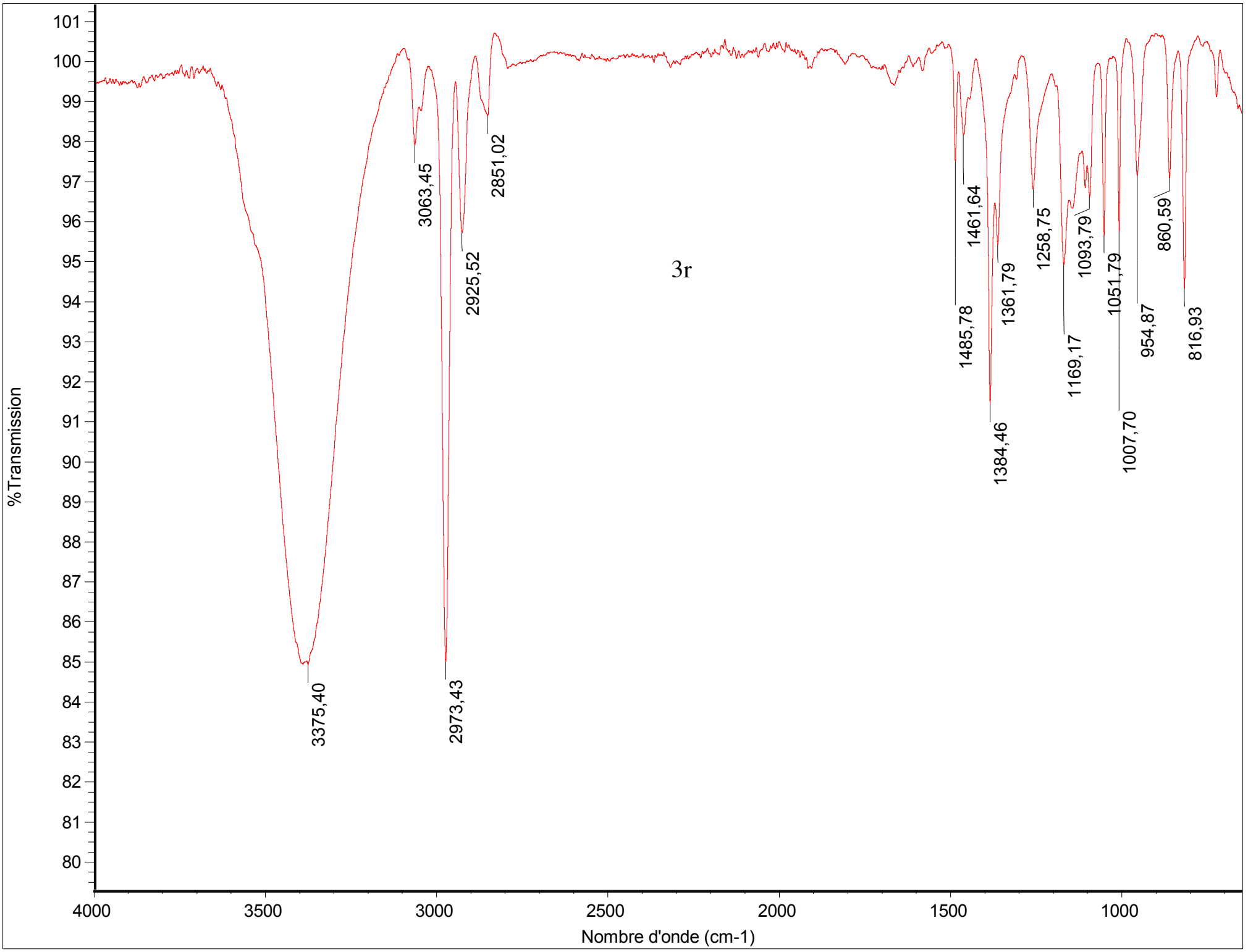

7.7544
7.7487
7.7332
7.7278
7.4671
7.4609
7.4459
7.4406
7.4101
7.4038
5.3590
3.3361
H3C
O
O
CH3
Bi
3o
1.50
2.61
1.22
6.88
f1 (ppm)

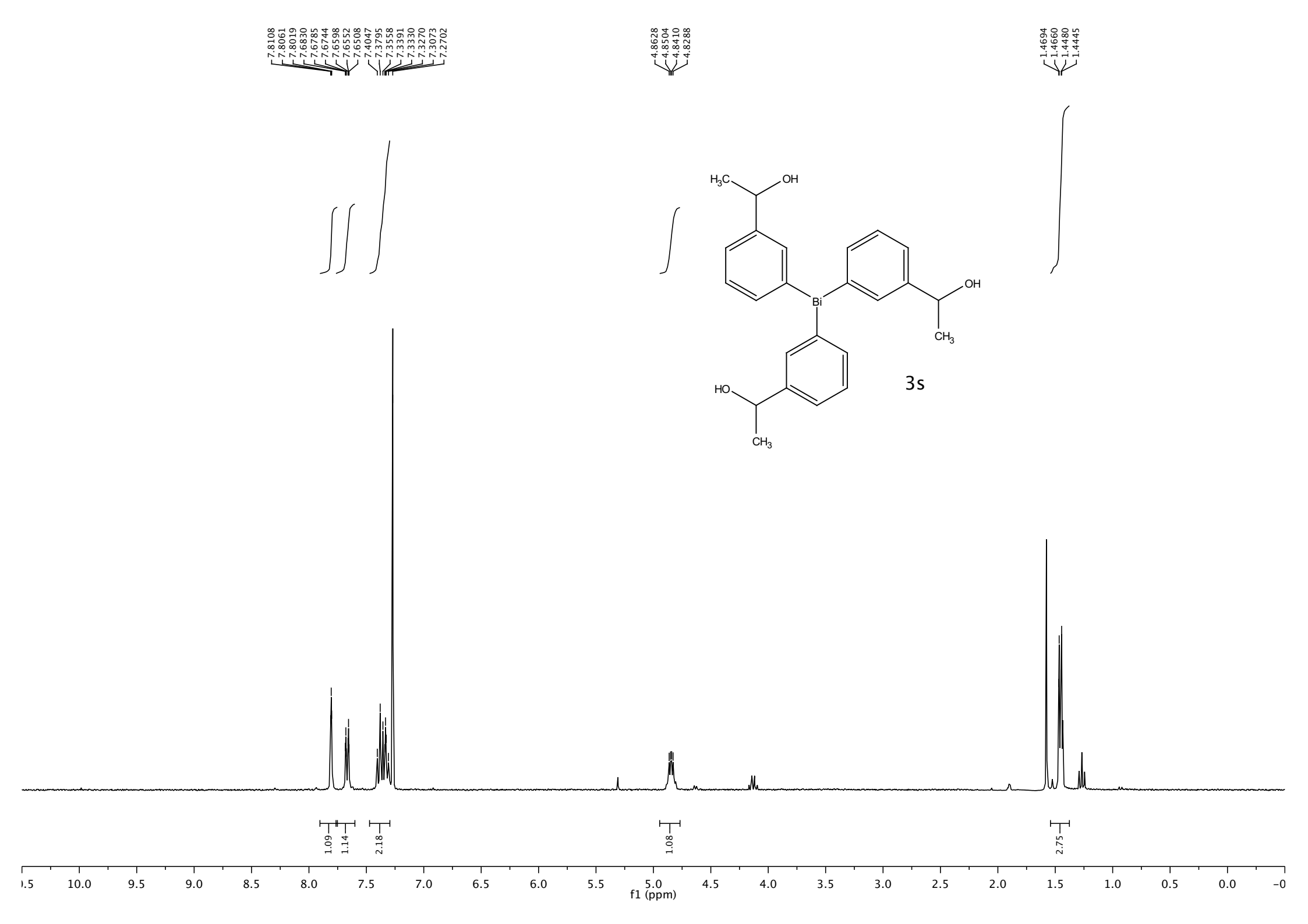

155.3647
137.7352
137.5027
128.8033
103.3681
52.8907
H3C
O
O
CH3
Bi
3o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

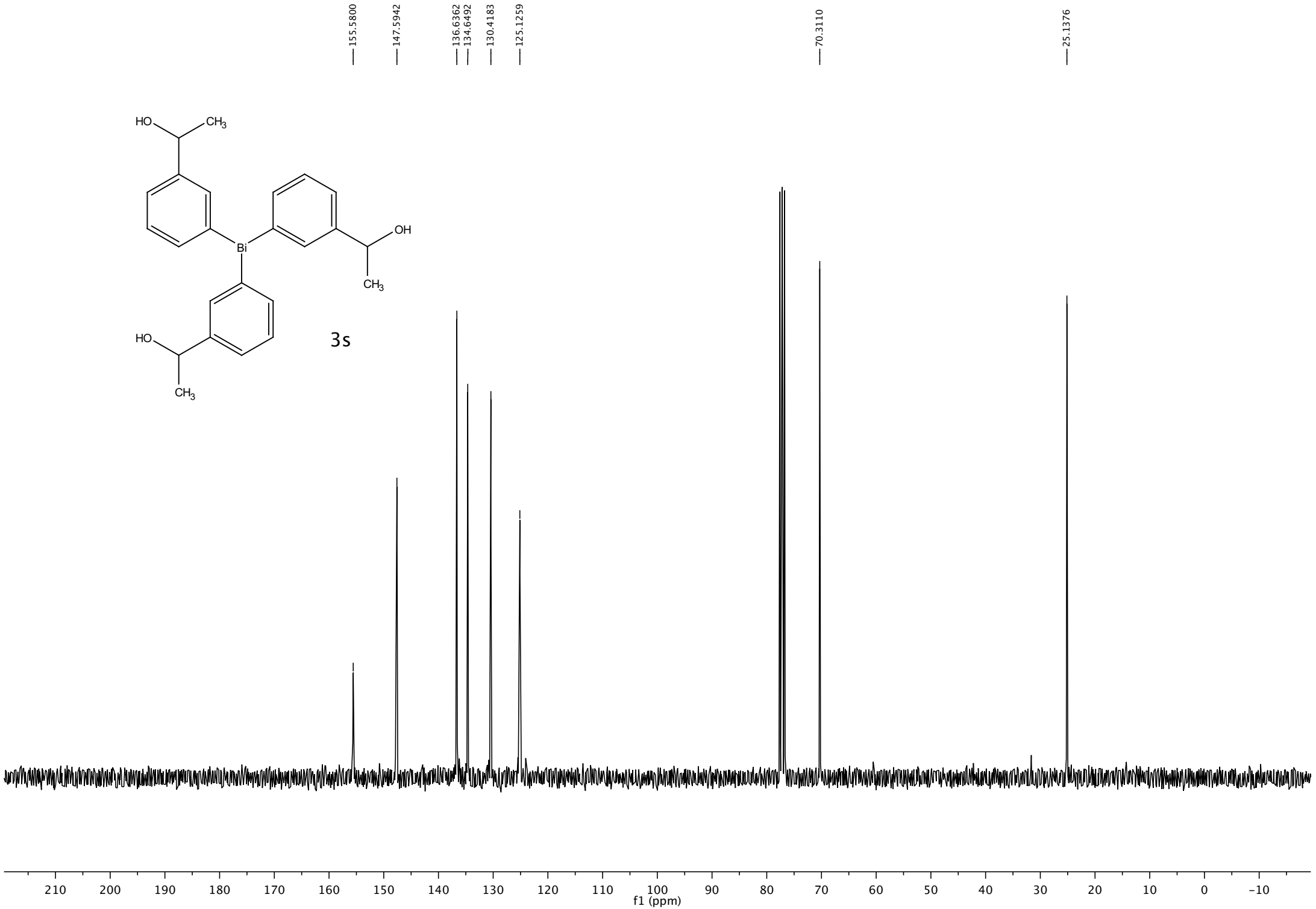

3o
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
4000
3500
3000
2500
2000
1500
1000
2988,55
2934,41
2903,30
2827,27
1442,31
1386,72
1348,28
1306,48
1207,51
1189,70
1096,02
1073,81
1048,11
1009,53
980,80
908,45
886,16
795,96
731,01

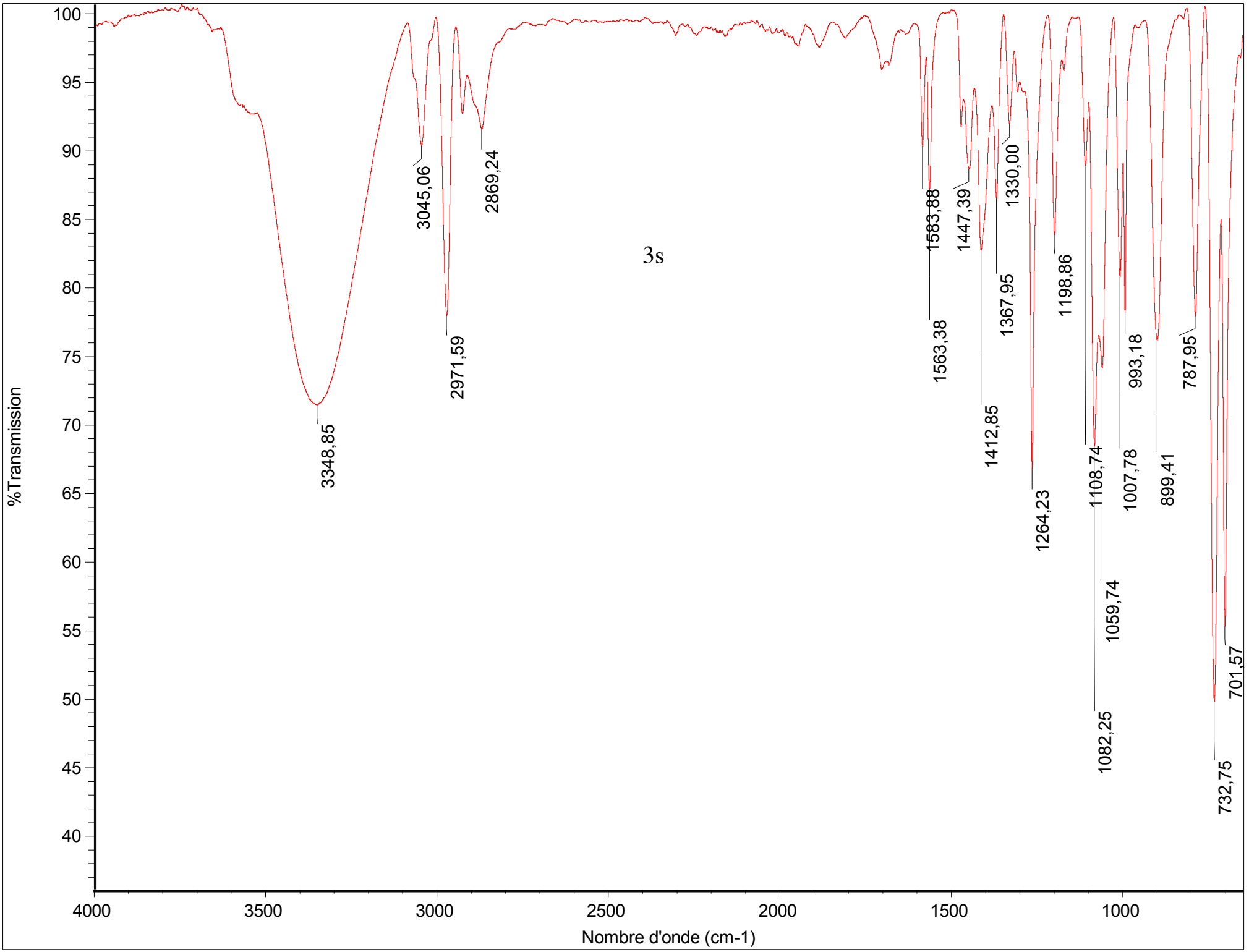

7.7312
7.7052
7.5029
7.4773
2.1471
1.5627
CH3
CH3
HO
CH3
CH3
OH
Bi
CH3
HO
CH3
CH3
3r
2.00
1.97
1.21
5.44
f1 (ppm)

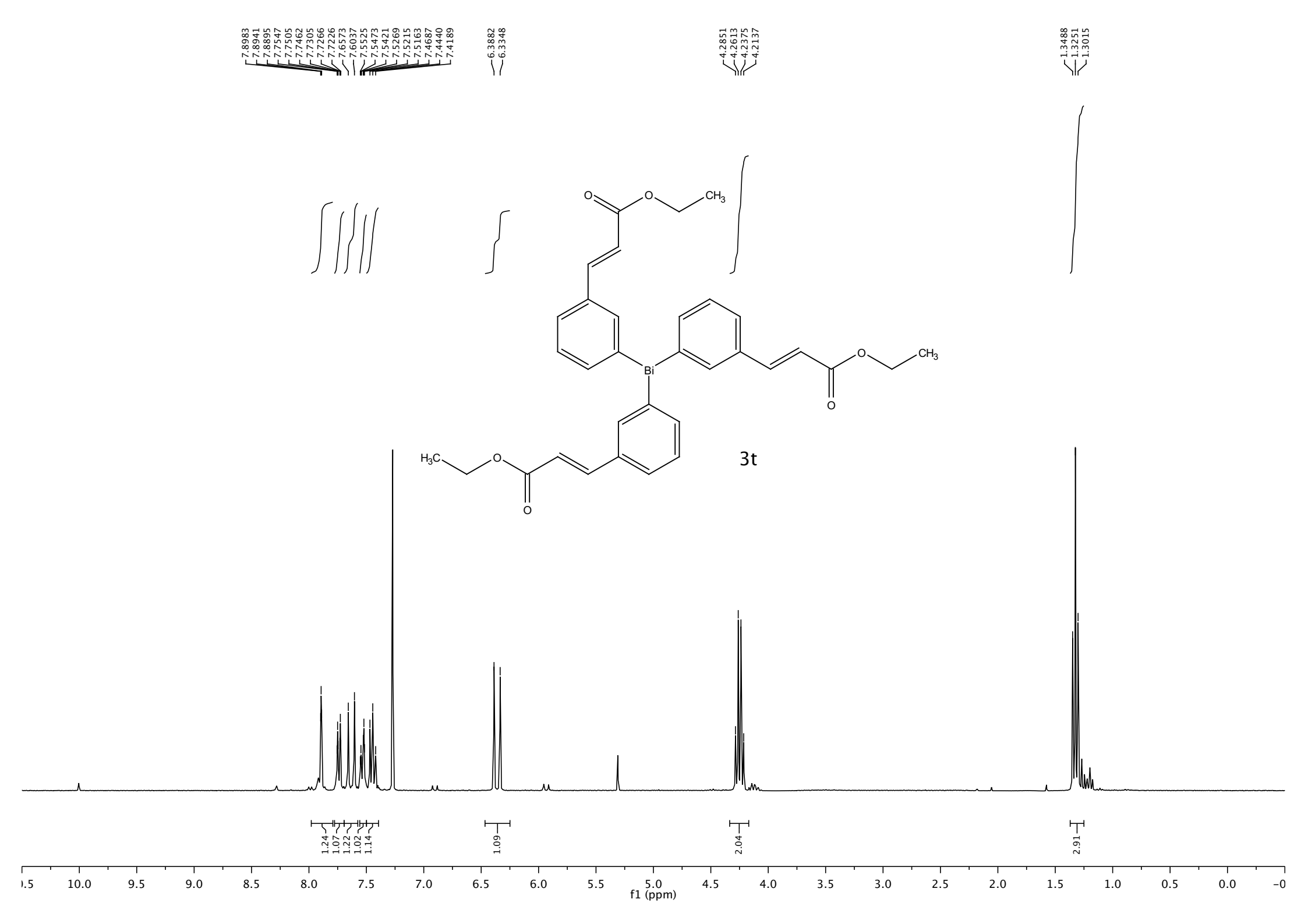

152.8057
148.6991
137.5381
126.6074
72.6127
31.7360
30.4010
CH3
CH3
HO
CH3
CH3
OH
Bi
CH3
CH3
HO
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


3r
%Transmission
Nombre d'onde (cm-1)
101
100
99
98
97
96
95
94
93
92
91
90
89
88
87
86
85
84
83
82
81
80
4000
3500
3000
2500
2000
1500
1000
3375,40
3063,45
2973,43
2925,52
2851,02
1485,78
1461,64
1384,46
1361,79
1258,75
1169,17
1093,79
1051,79
1007,70
954,87
860,59
816,93

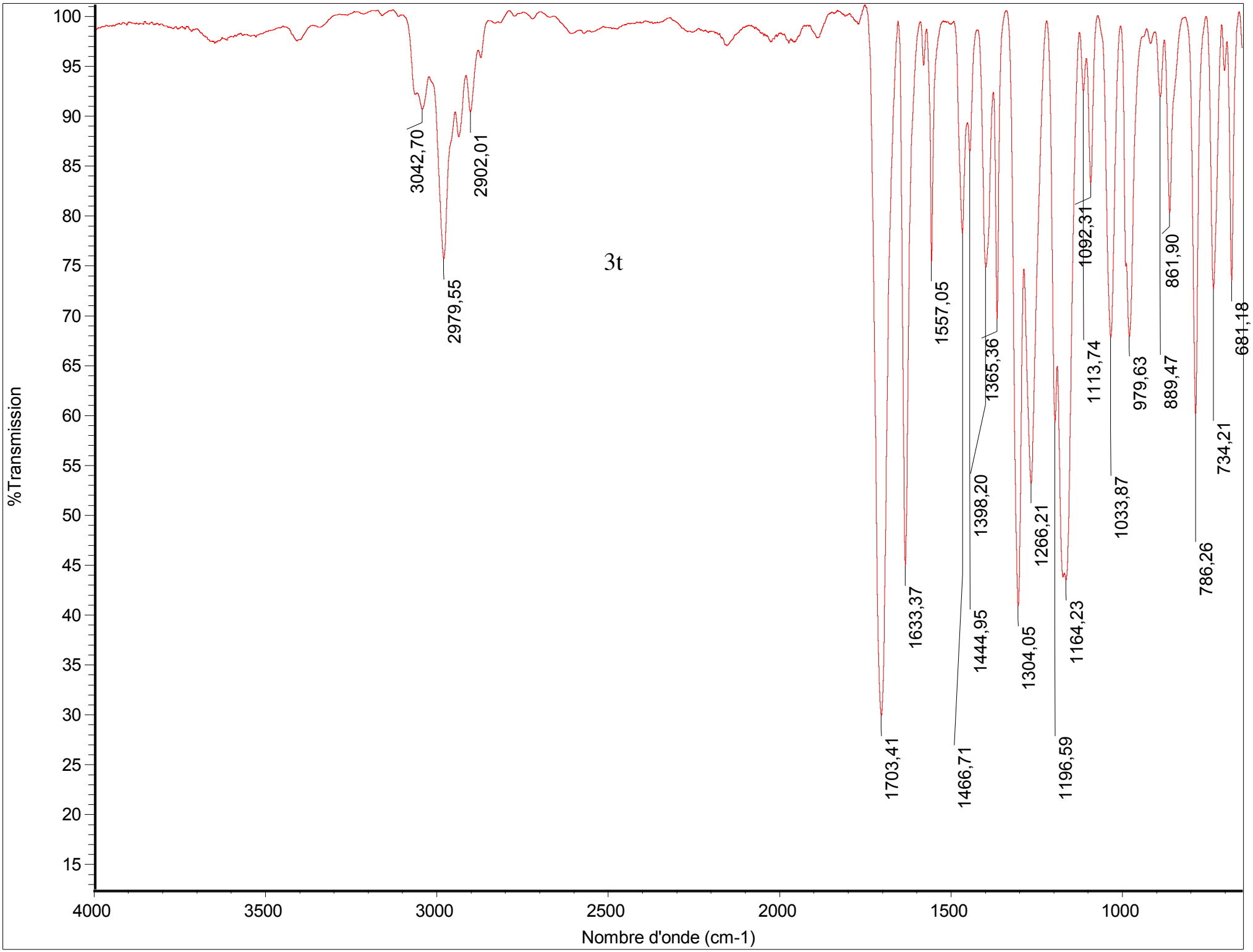

7.8108
7.8061
7.8019
7.6830
7.6785
7.6744
7.6598
7.6552
7.6508
7.4047
7.3795
7.3558
7.3391
7.3330
7.3270
7.3073
7.2702
4.8628
4.8504
4.8410
4.8288
1.4694
1.4660
1.4480
1.4445
H3C
OH
Bi
OH
CH3
HO
CH3
3s
1.09
1.14
2.18
1.08
2.75
f1 (ppm)

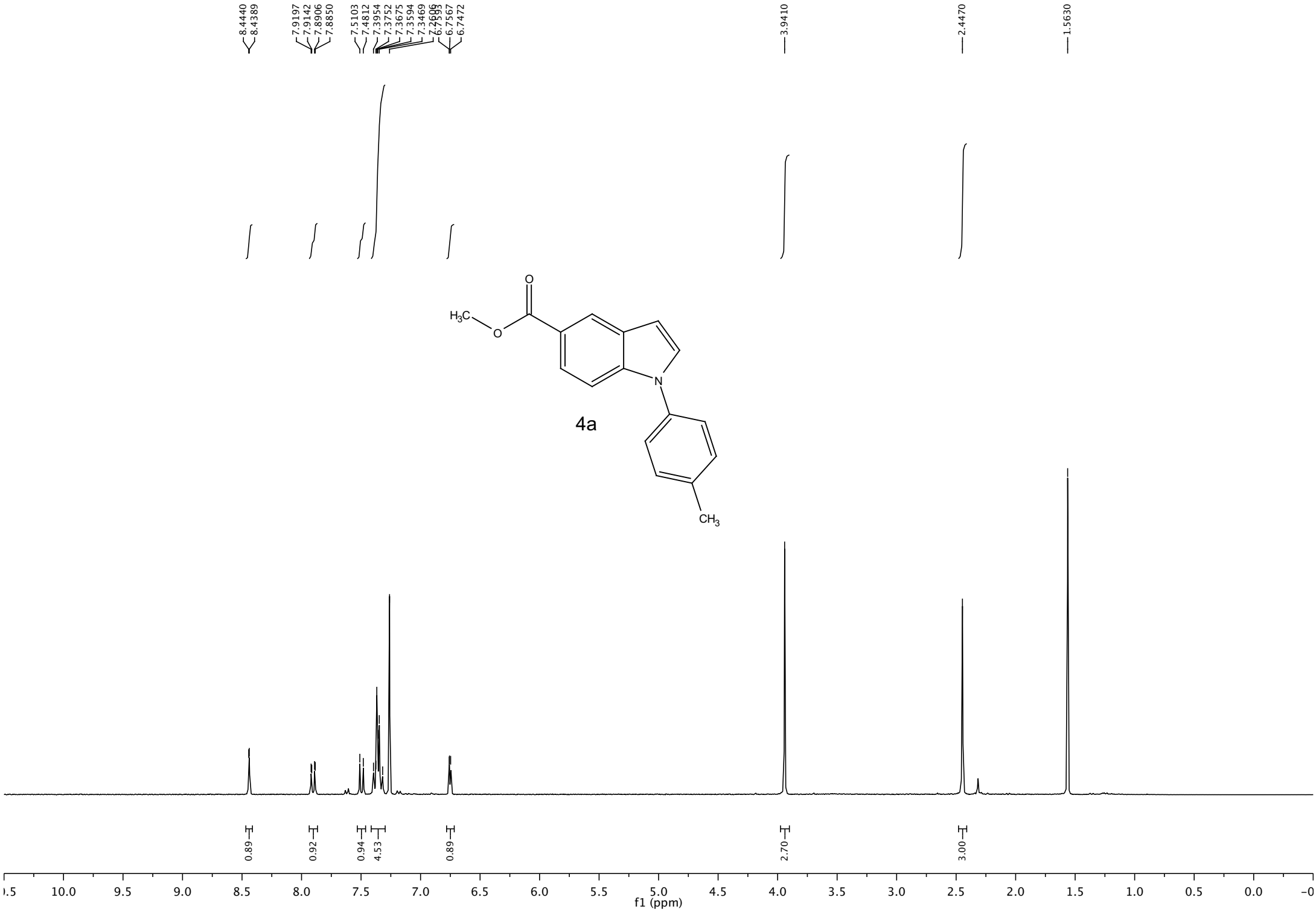

155.5800
147.5942
136.6362
134.6492
130.4183
125.1259
70.3110
25.1376
HO
CH3
Bi
OH
CH3
HO
CH3
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

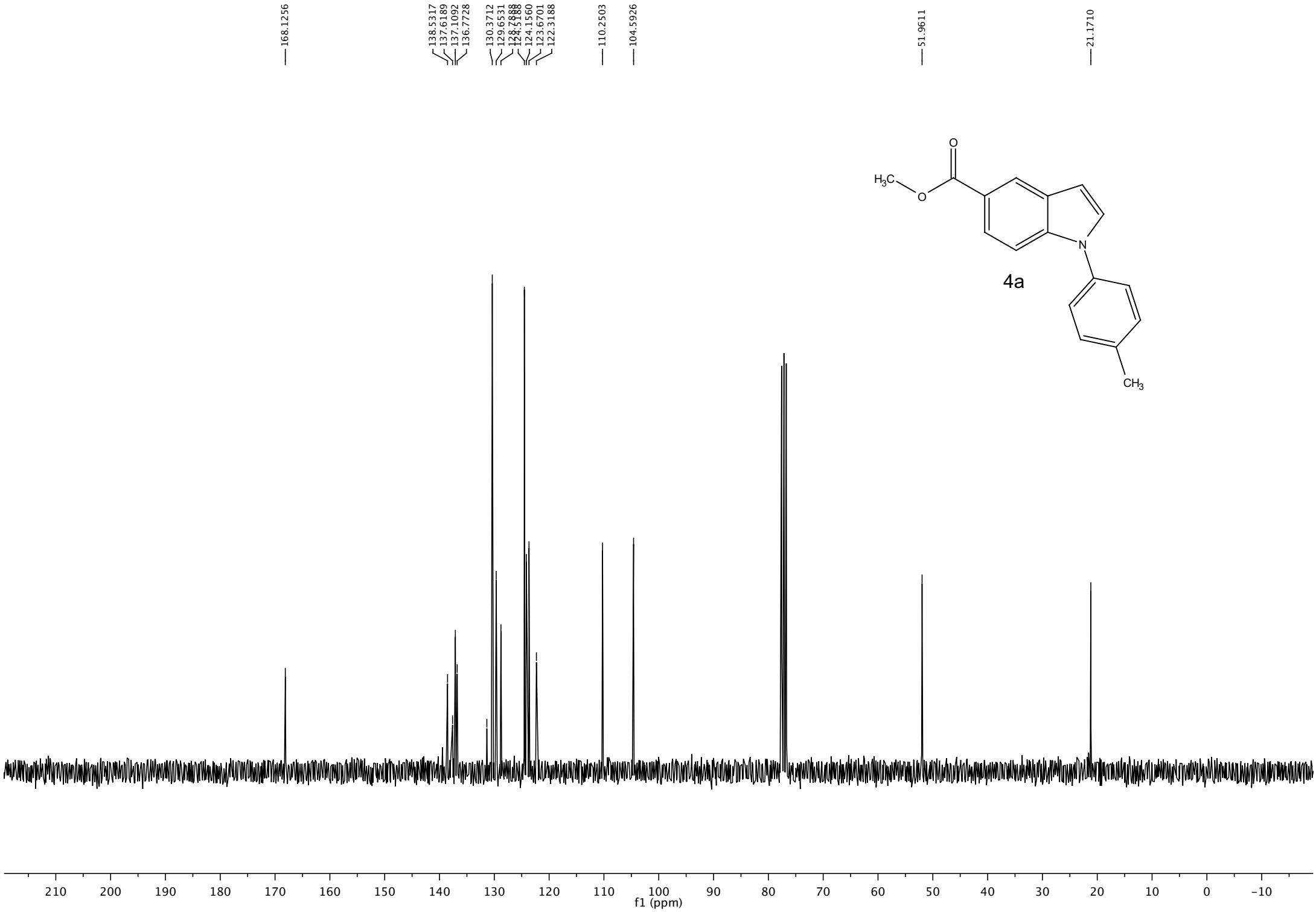

3s
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
4000
3500
3000
2500
2000
1500
1000
3348,85
3045,06
2971,59
2869,24
1583,88
1563,38
1447,39
1412,85
1367,95
1330,00
1264,23
1198,86
1108,74
1082,25
1059,74
1007,78
993,18
899,41
787,95
732,75
701,57

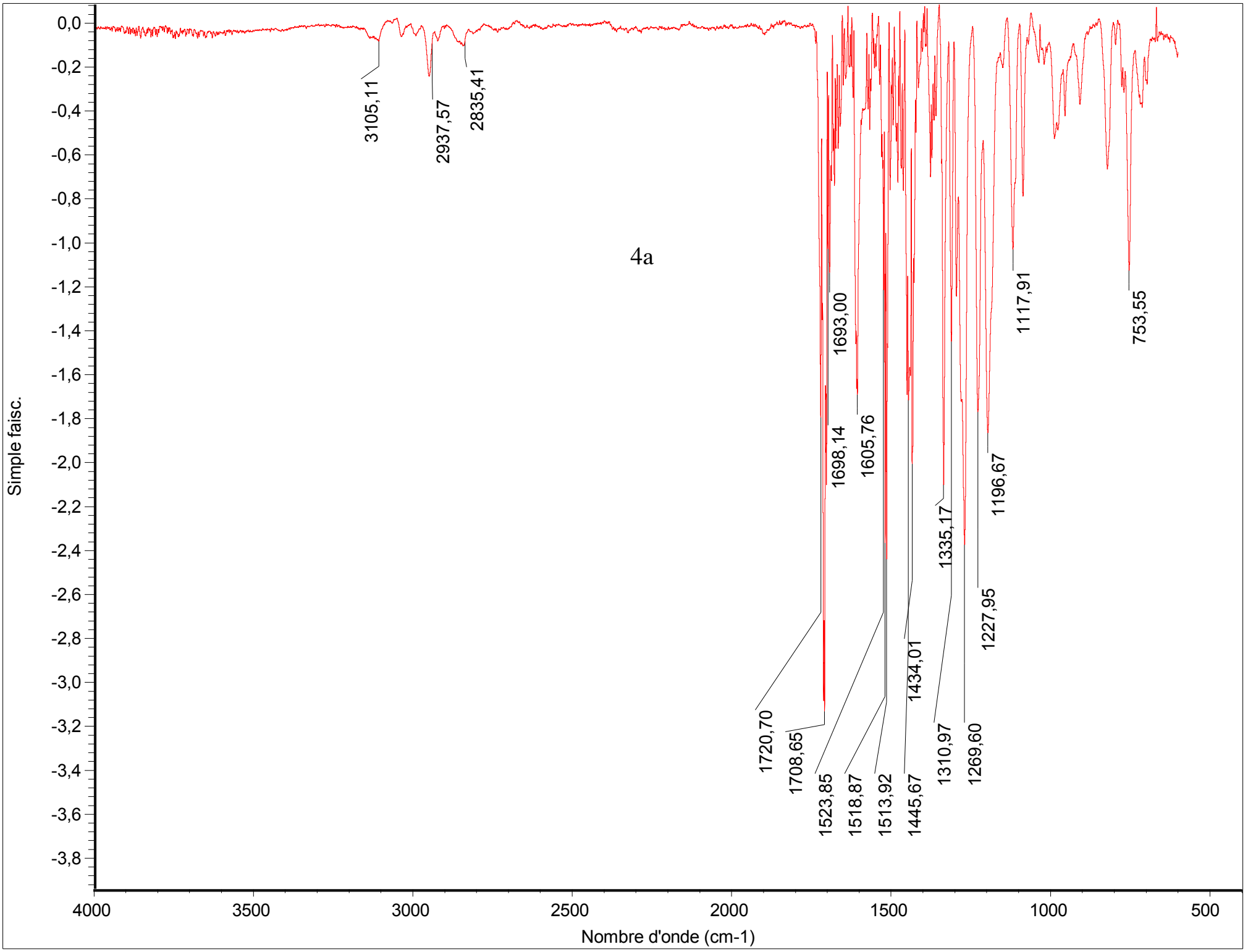

7.8983
7.8941
7.8895
7.7547
7.7505
7.7462
7.7305
7.7266
7.7226
7.6573
7.6037
7.5525
7.5473
7.5421
7.5269
7.5215
7.5163
7.4687
7.4440
7.4189
6.3882
6.3348
4.2851
4.2613
4.2375
4.2137
1.3488
1.3251
1.3015
O
O
CH3
Bi
O
CH3
O
H3C
O
O
3t
1.24
1.07
1.22
1.02
1.14
1.09
2.04
2.91
f1 (ppm)

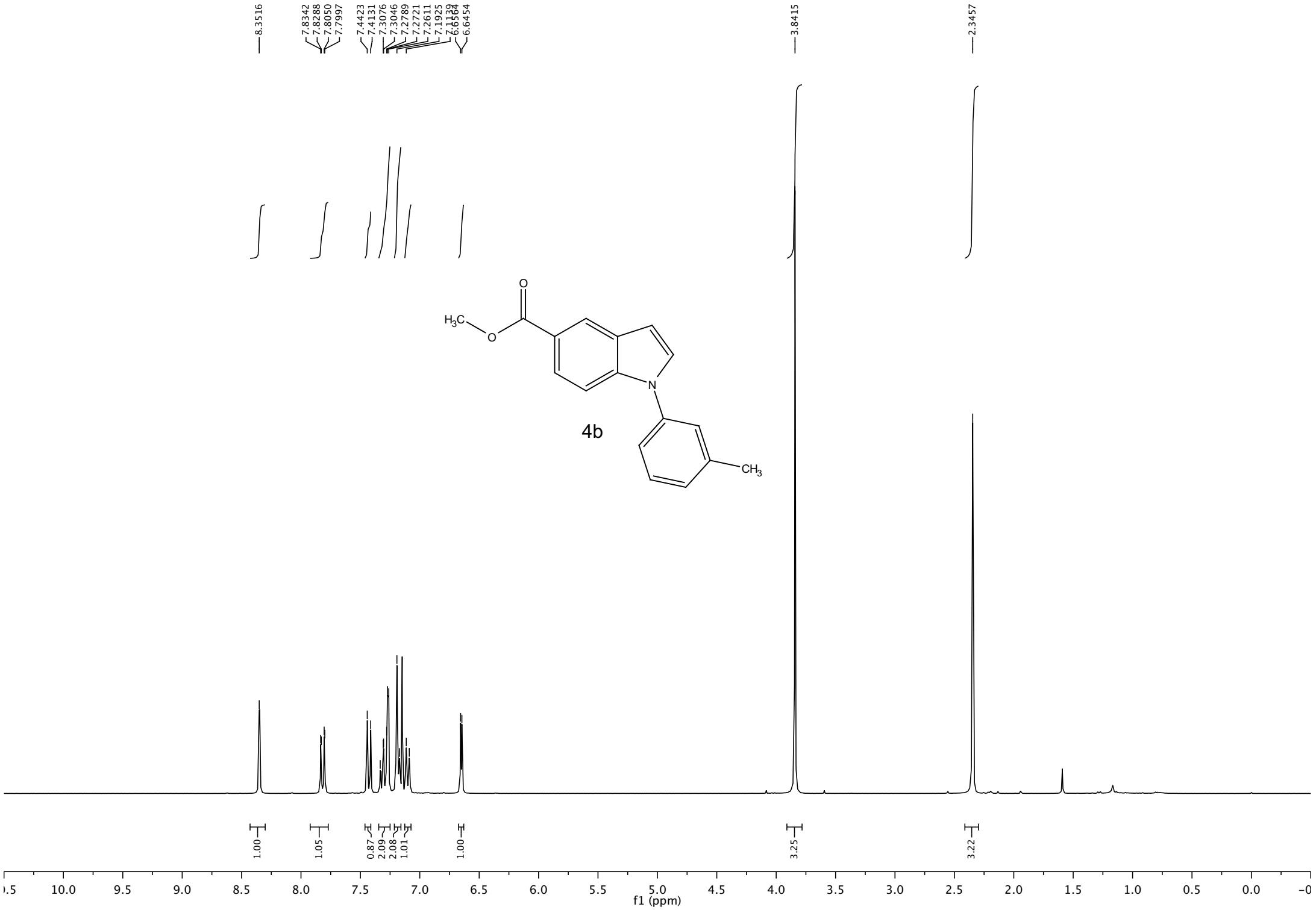

166.8292
156.0675
144.5028
139.3285
137.3010
136.5688
131.1745
127.5505
118.6562
60.5264
14.3943
CH3
O
O
Bi
CH3
O
O
H3C
O
O
3t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

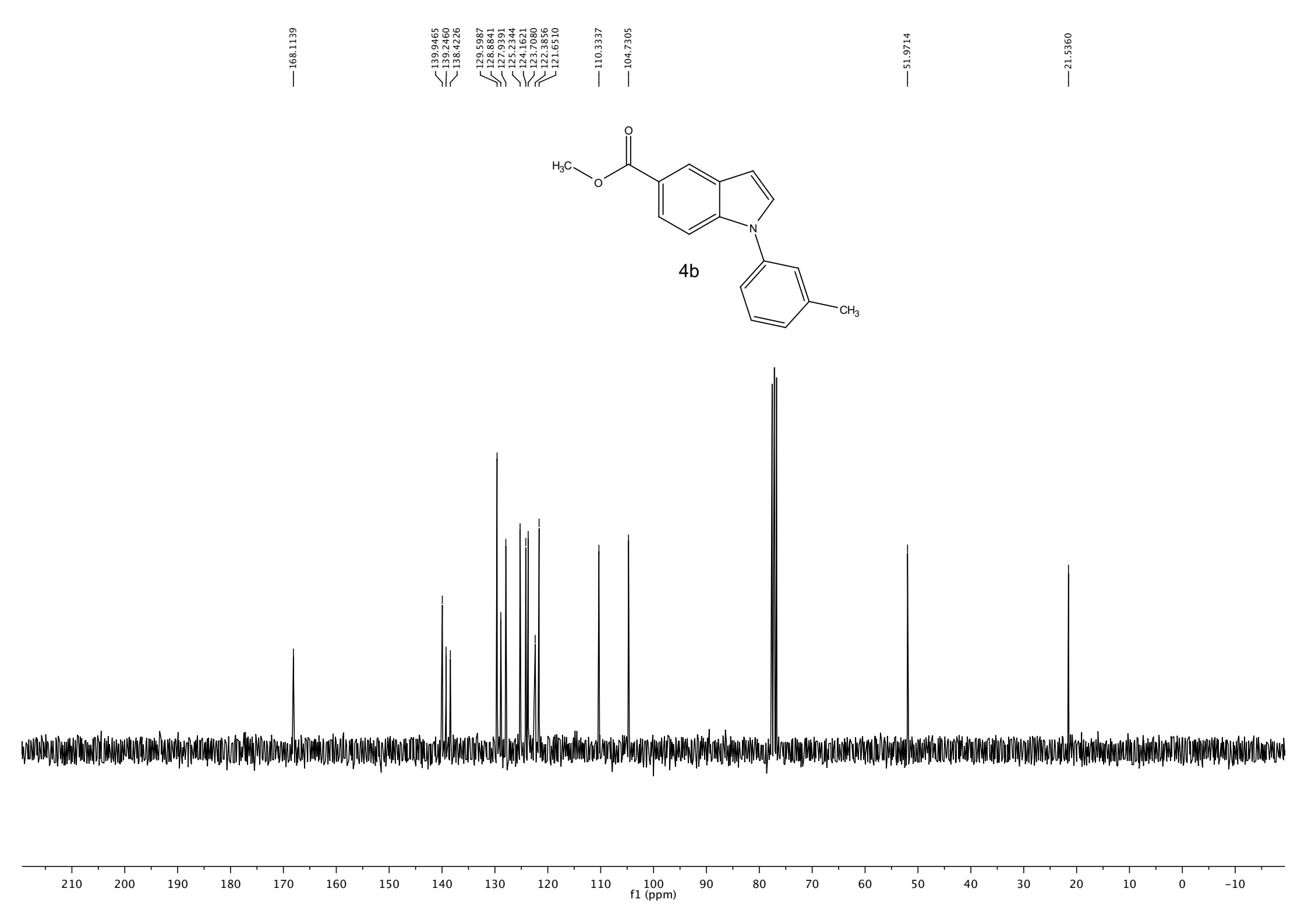

3t
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
4000
3500
3000
2500
2000
1500
1000
3042,70
2979,55
2902,01
1703,41
1633,37
1557,05
1466,71
1444,95
1398,20
1365,36
1304,05
1266,21
1196,59
1164,23
1113,74
1092,31
1033,87
979,63
889,47
861,90
786,26
734,21
681,18

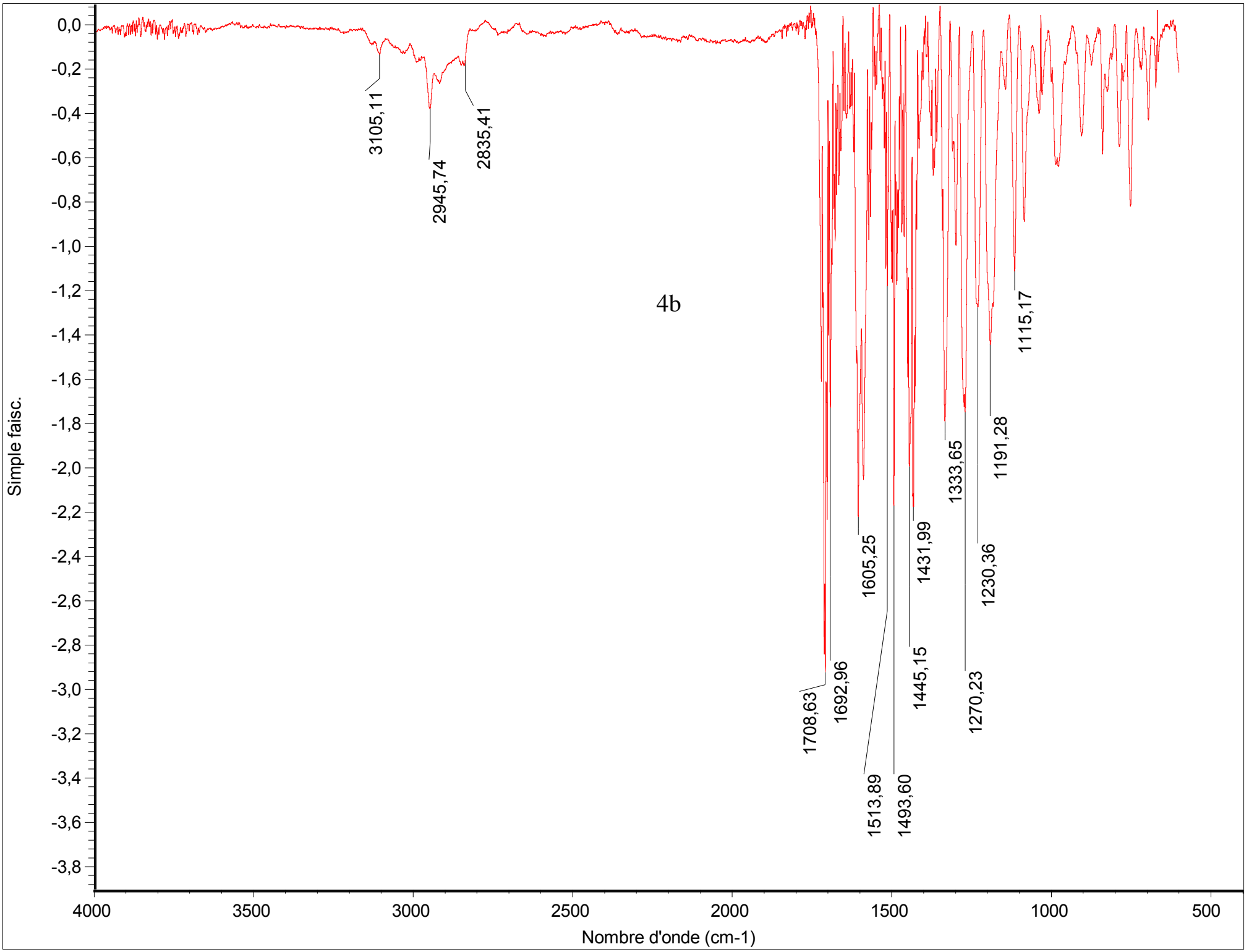

8.4440
8.4389
7.9197
7.9142
7.8906
7.8850
7.5103
7.4812
7.3954
7.3752
7.3675
7.3594
7.3469
7.2606
6.7593
6.7567
6.7472
3.9410
2.4470
1.5630
O
H3C
O
N
CH3
4a
0.89
0.92
0.94
4.53
0.89
2.70
3.00
f1 (ppm)

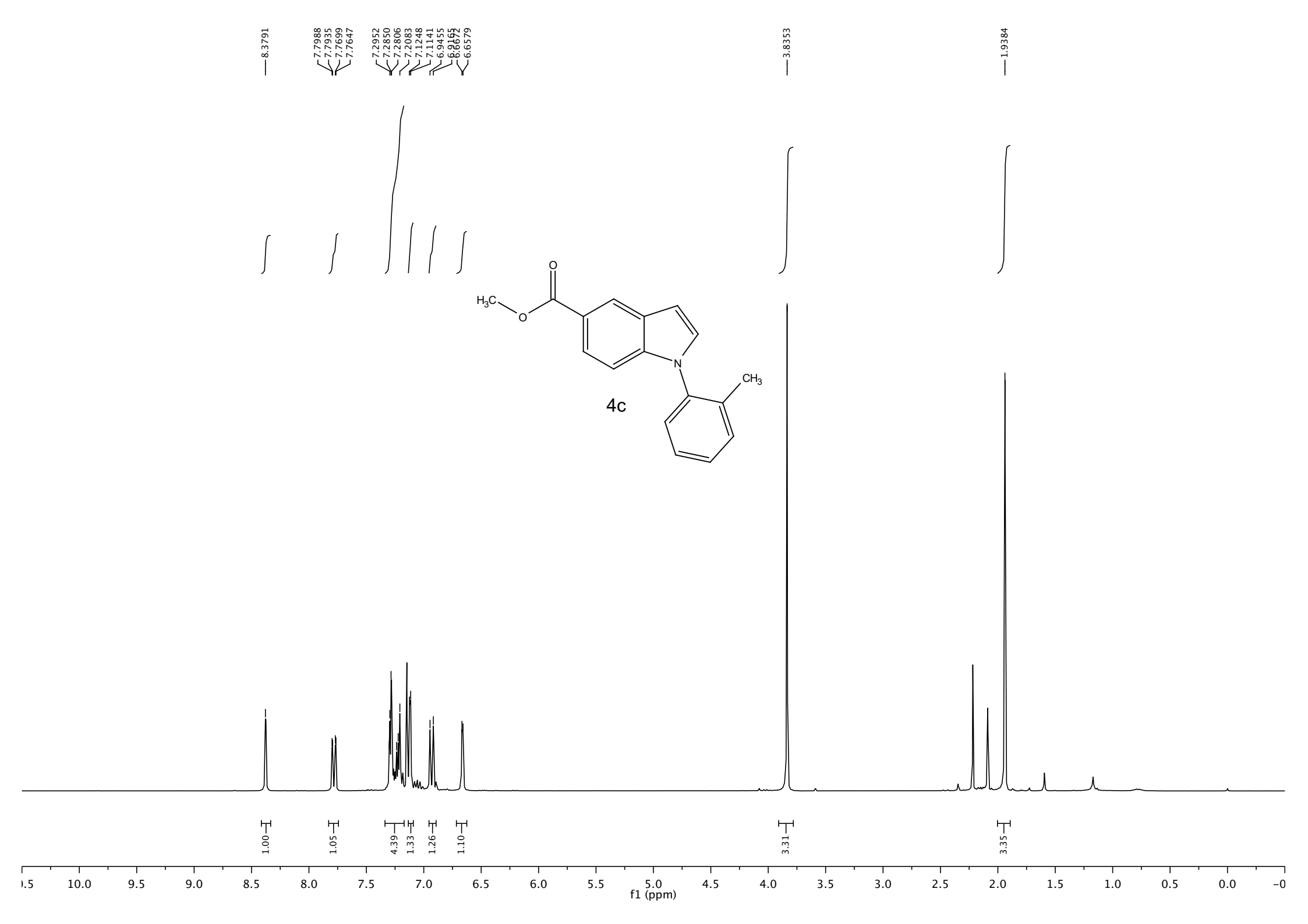

168.1256
138.5317
137.6189
137.1092
136.7728
130.3712
129.6531
124.1560
123.6701
122.3188
110.2503
104.5926
51.9611
21.1710
O
H3C
O
N
CH3
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

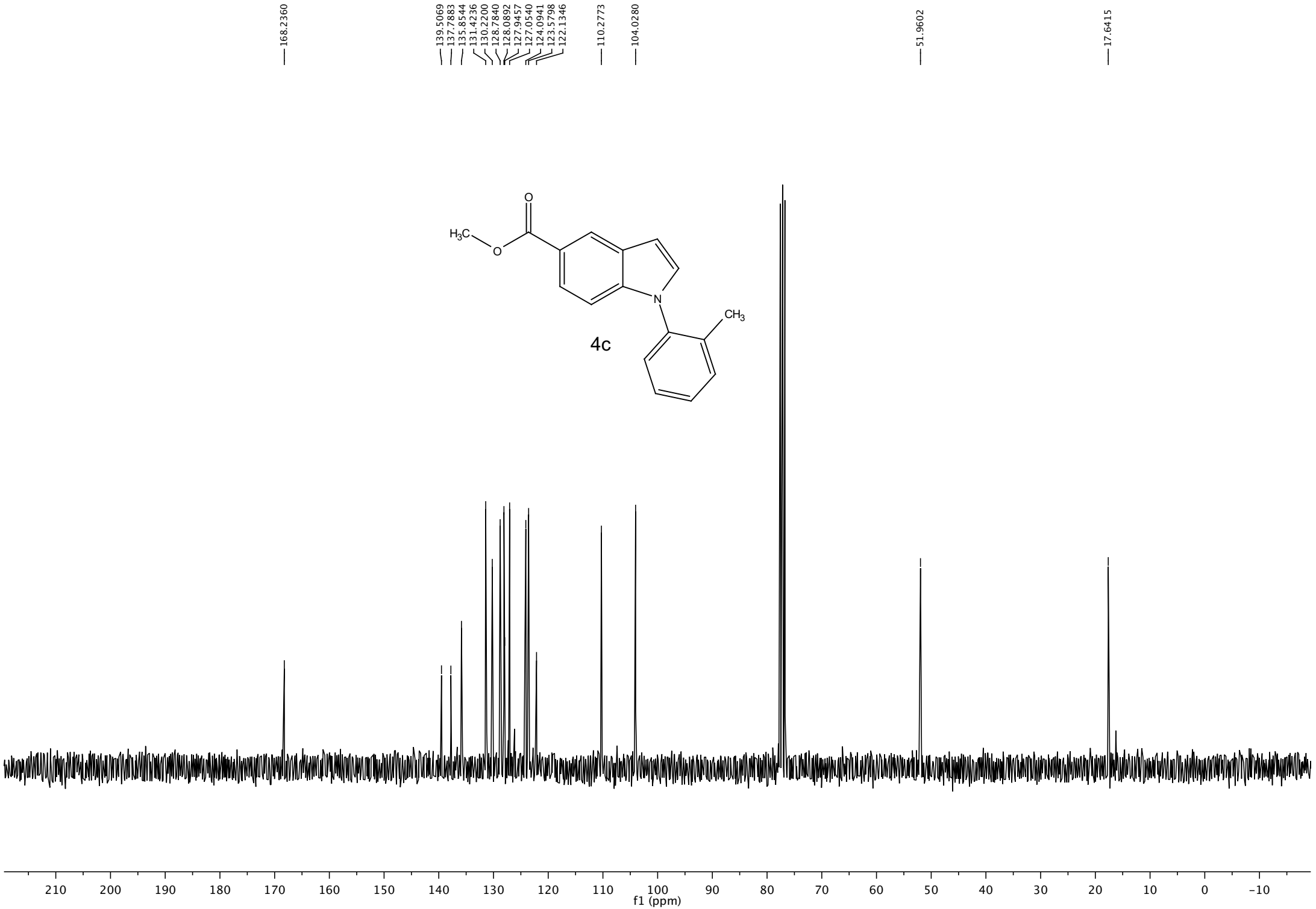

4a
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
-3,8
4000
3500
3000
2500
2000
1500
1000
500
3105,11
2937,57
2835,41
1693,00
1698,14
1605,76
1335,17
1196,67
1117,91
753,55
1227,95
1434,01
1720,70
1708,65
1523,85
1518,87
1513,92
1445,67
1310,97
1269,60

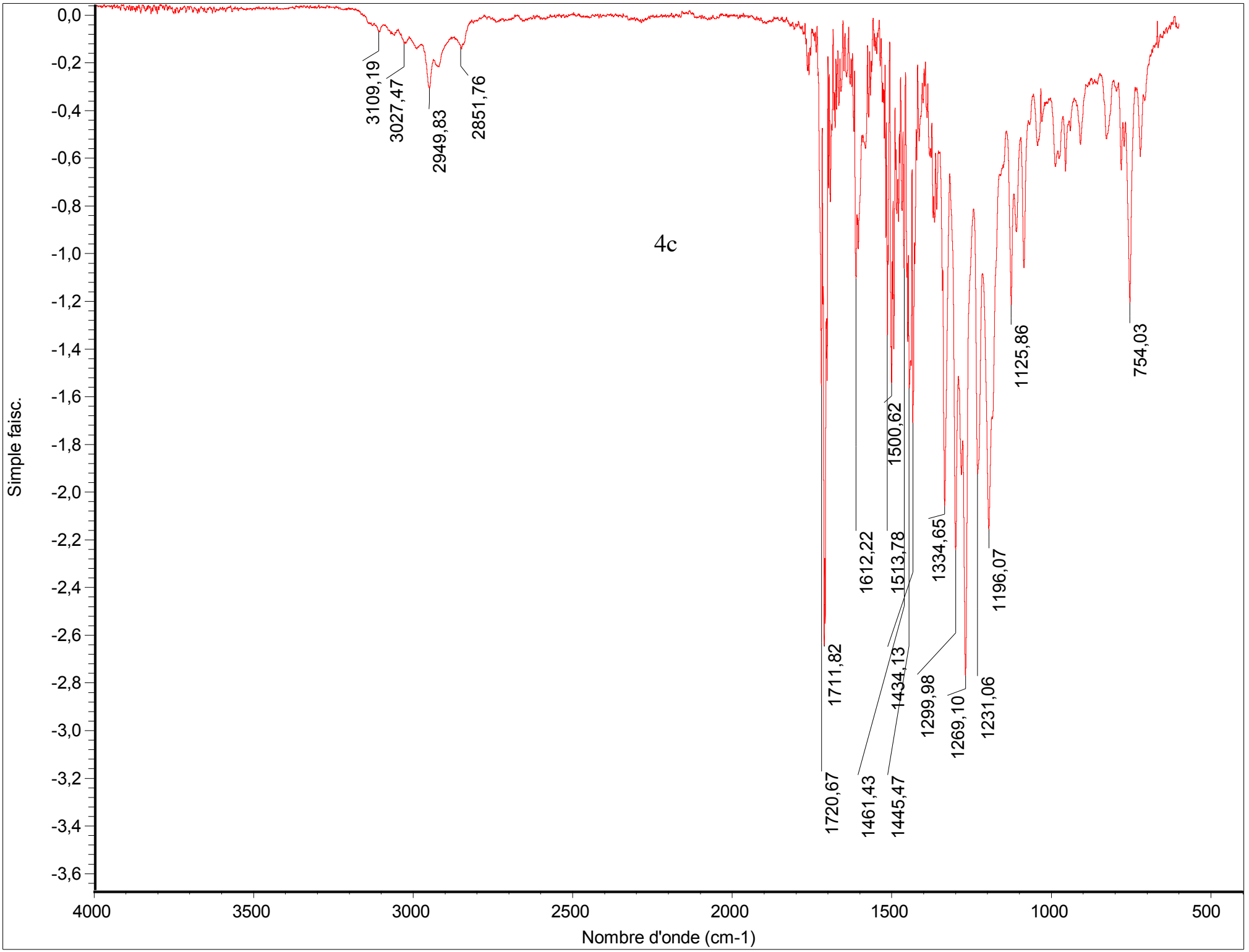

8.3516
7.8342
7.8288
7.8050
7.7997
7.4423
7.4131
7.3076
7.3046
7.2789
7.2721
7.2611
7.1925
7.1139
6.6564
6.6454
3.8415
2.3457
O
H3C
O
N
CH3
4b
1.00
1.05
0.87
2.09
2.08
1.01
1.00
3.25
3.22
f1 (ppm)

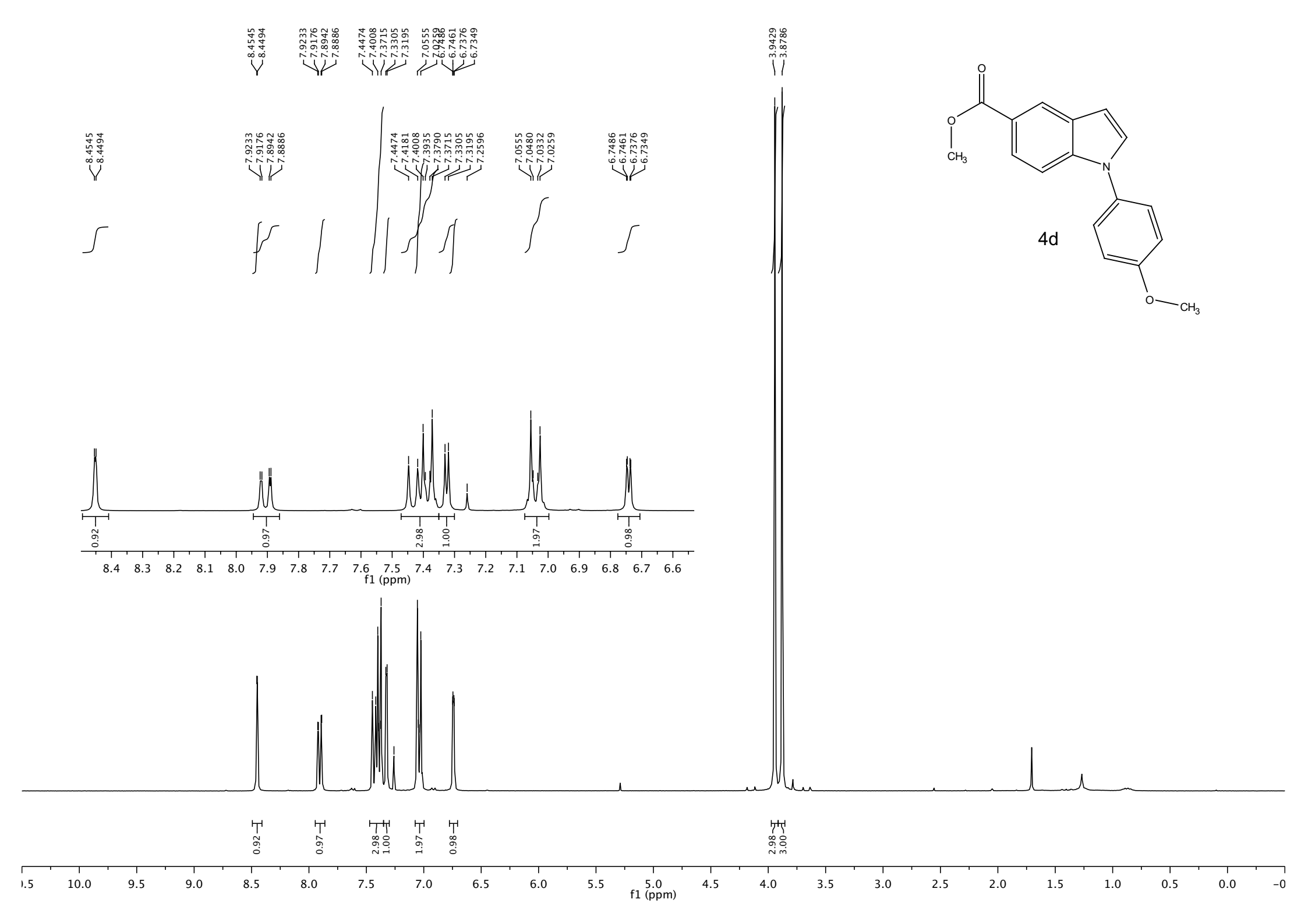

168.1139
139.9465
139.2460
138.4226
129.5987
128.8841
127.9391
125.2344
124.1621
123.7080
122.3856
121.6510
110.3337
104.7305
51.9714
21.5360
O
H3C
O
N
CH3
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

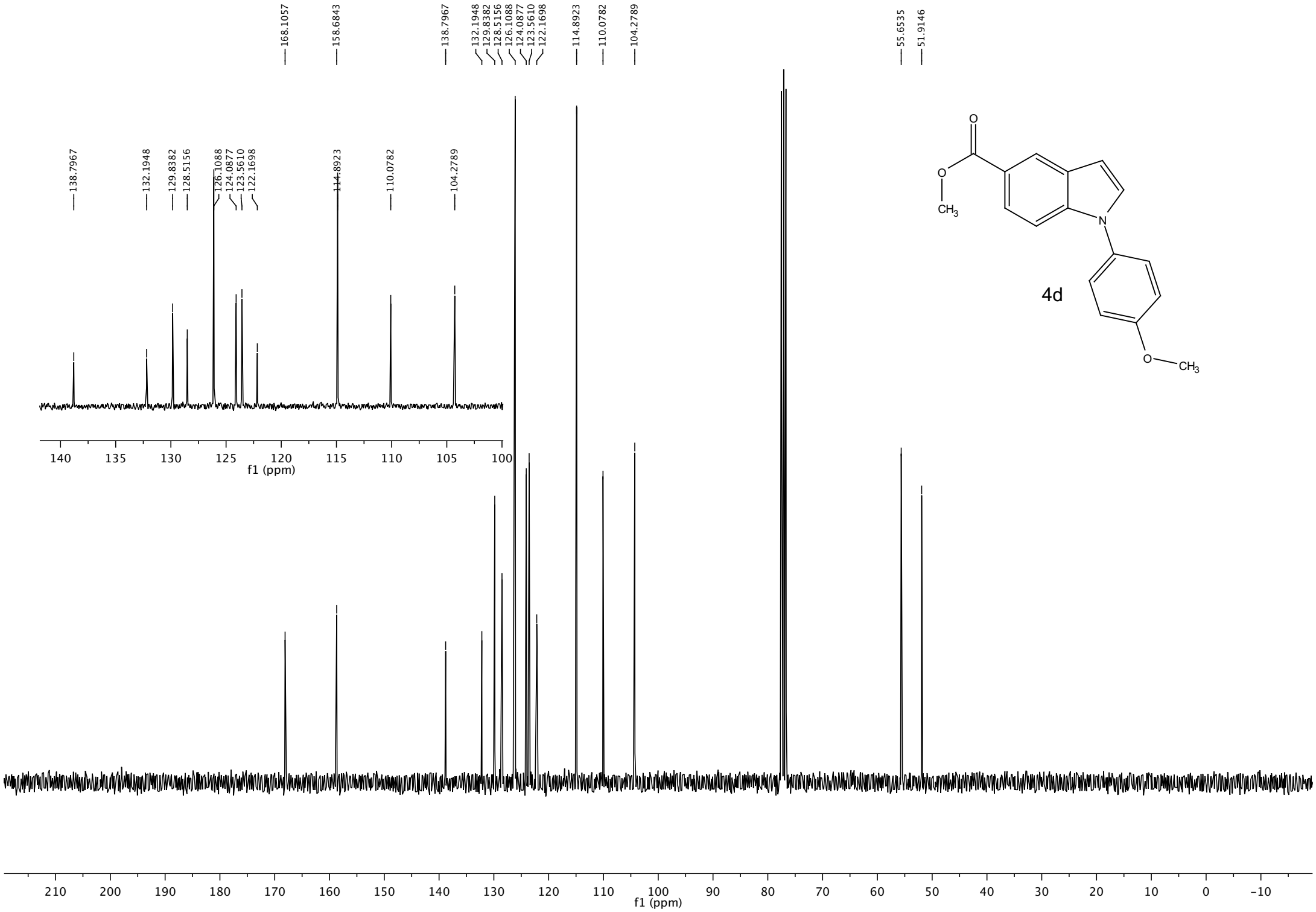

4b
3105,11
2945,74
2835,41
1708,63
1692,96
1605,25
1513,89
1493,60
1445,15
1431,99
1333,65
1270,23
1230,36
1191,28
1115,17
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
-3,8
4000
3500
3000
2500
2000
1500
1000
500

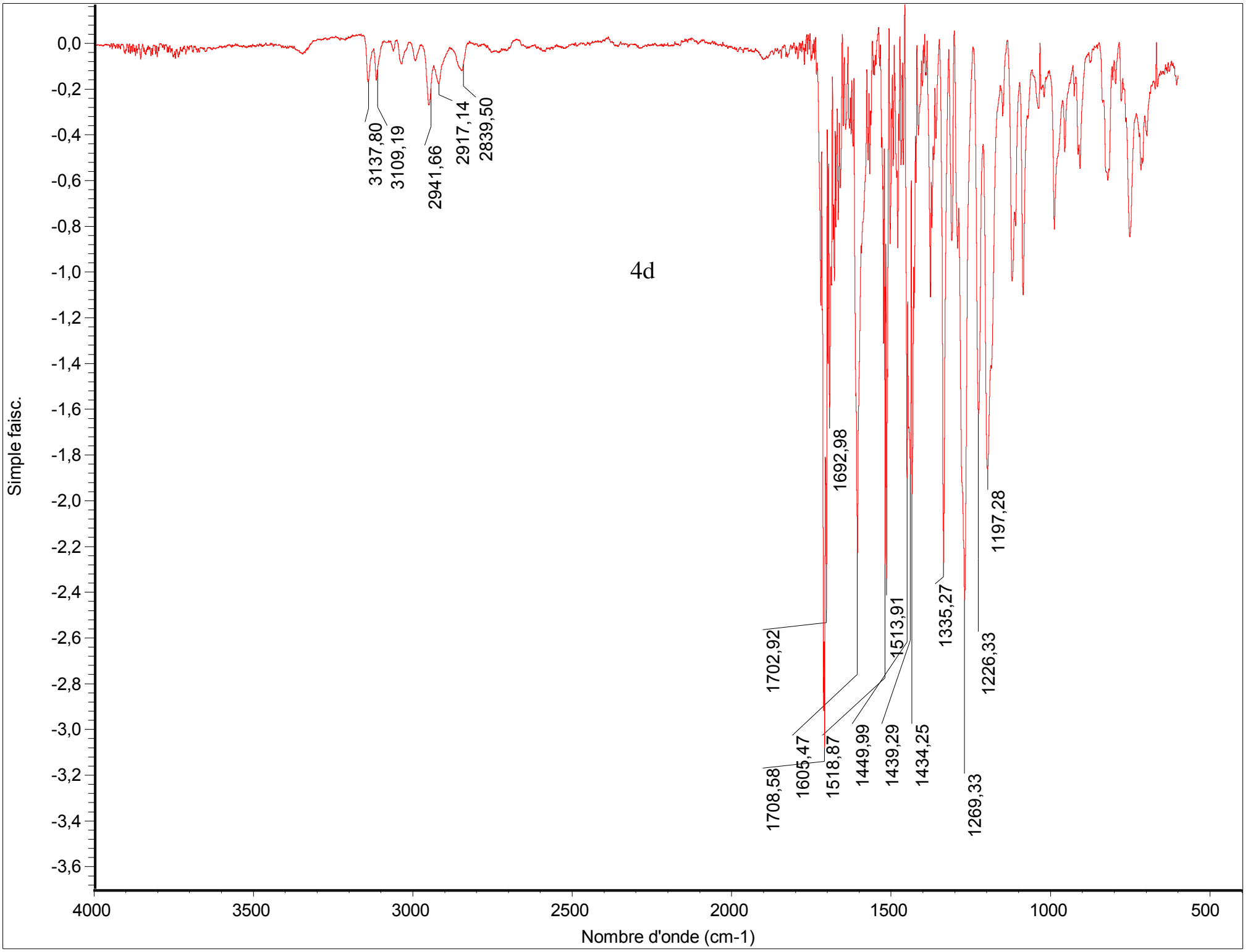

8.3791
7.7988
7.7935
7.7699
7.7647
7.2952
7.2850
7.2806
7.2083
7.1248
7.1141
6.9455
6.6672
6.6579
3.8353
1.9384
O
H3C
O
N
CH3
4c
1.00
1.05
4.39
1.33
1.26
1.10
3.31
3.35
f1 (ppm)

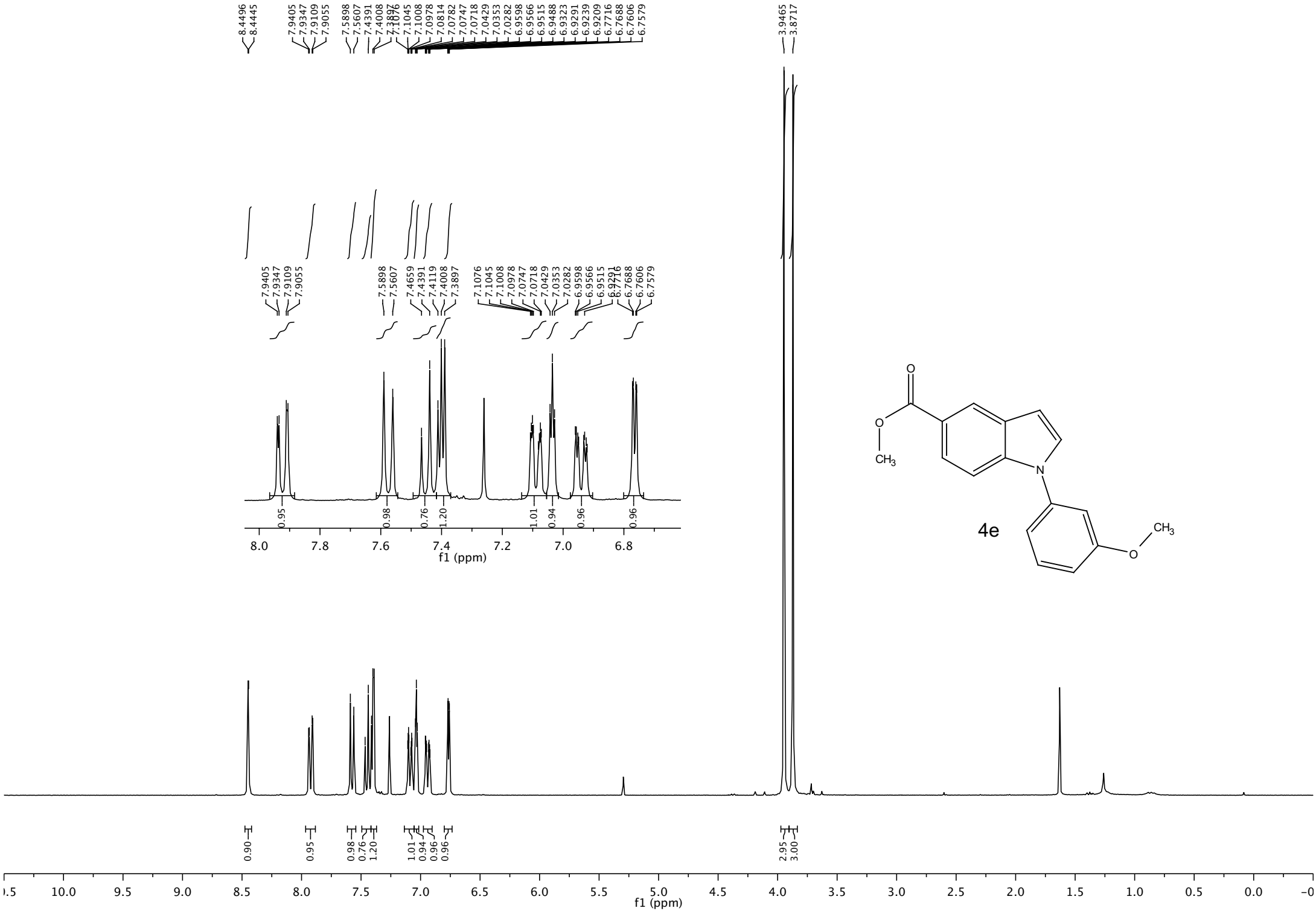

168.2360
139.5069
137.7883
135.8544
131.4236
130.2200
128.7840
128.0892
127.9457
127.0540
124.0941
123.5798
122.1346
110.2773
104.0280
51.9602
17.6415
O
H3C
O
N
CH3
4c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

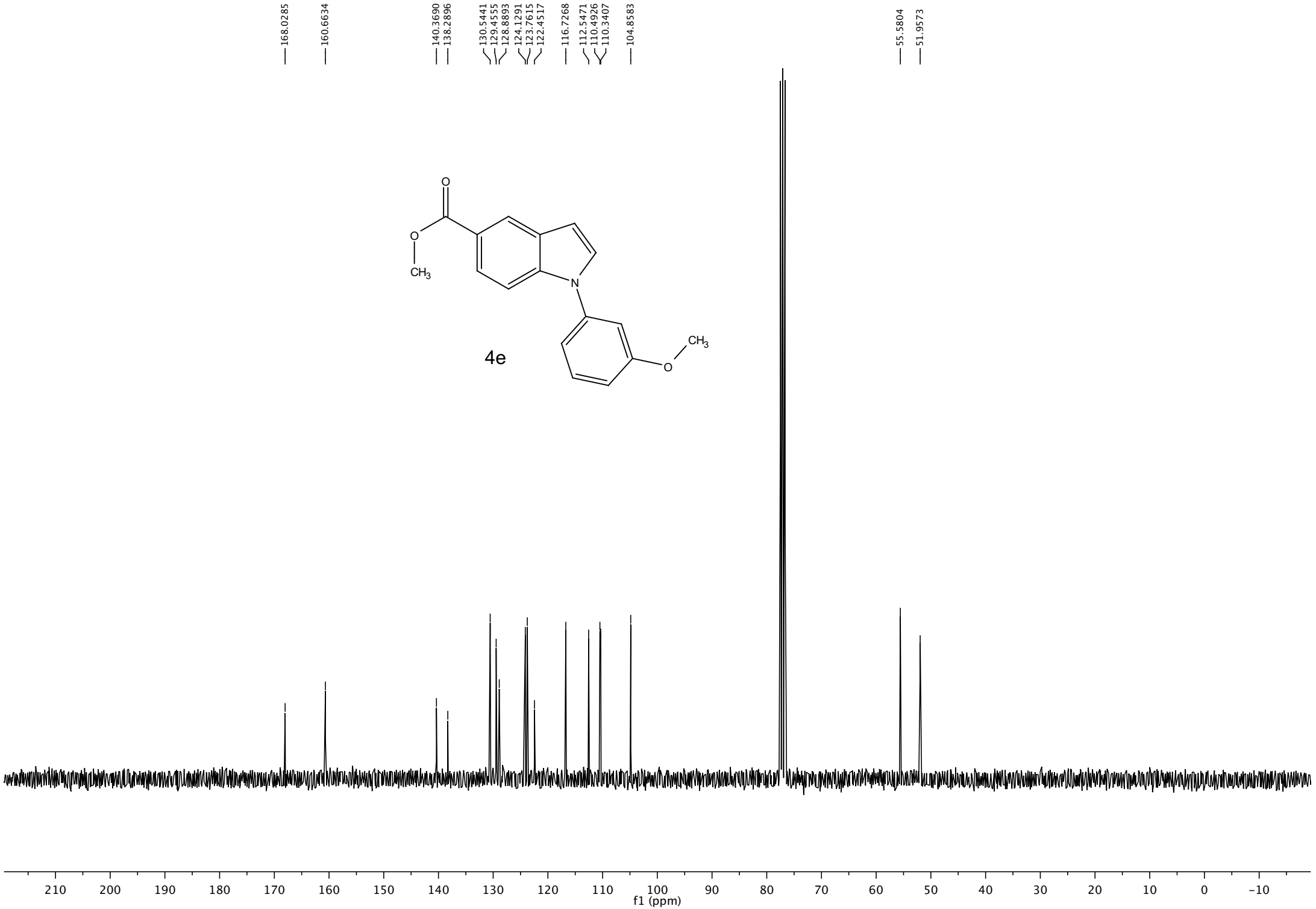

4c
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
4000
3500
3000
2500
2000
1500
1000
500
3109,19
3027,47
2949,83
2851,76
1720,67
1711,82
1612,22
1500,62
1461,43
1445,47
1434,13
1513,78
1334,65
1299,98
1269,10
1231,06
1196,07
1125,86
754,03

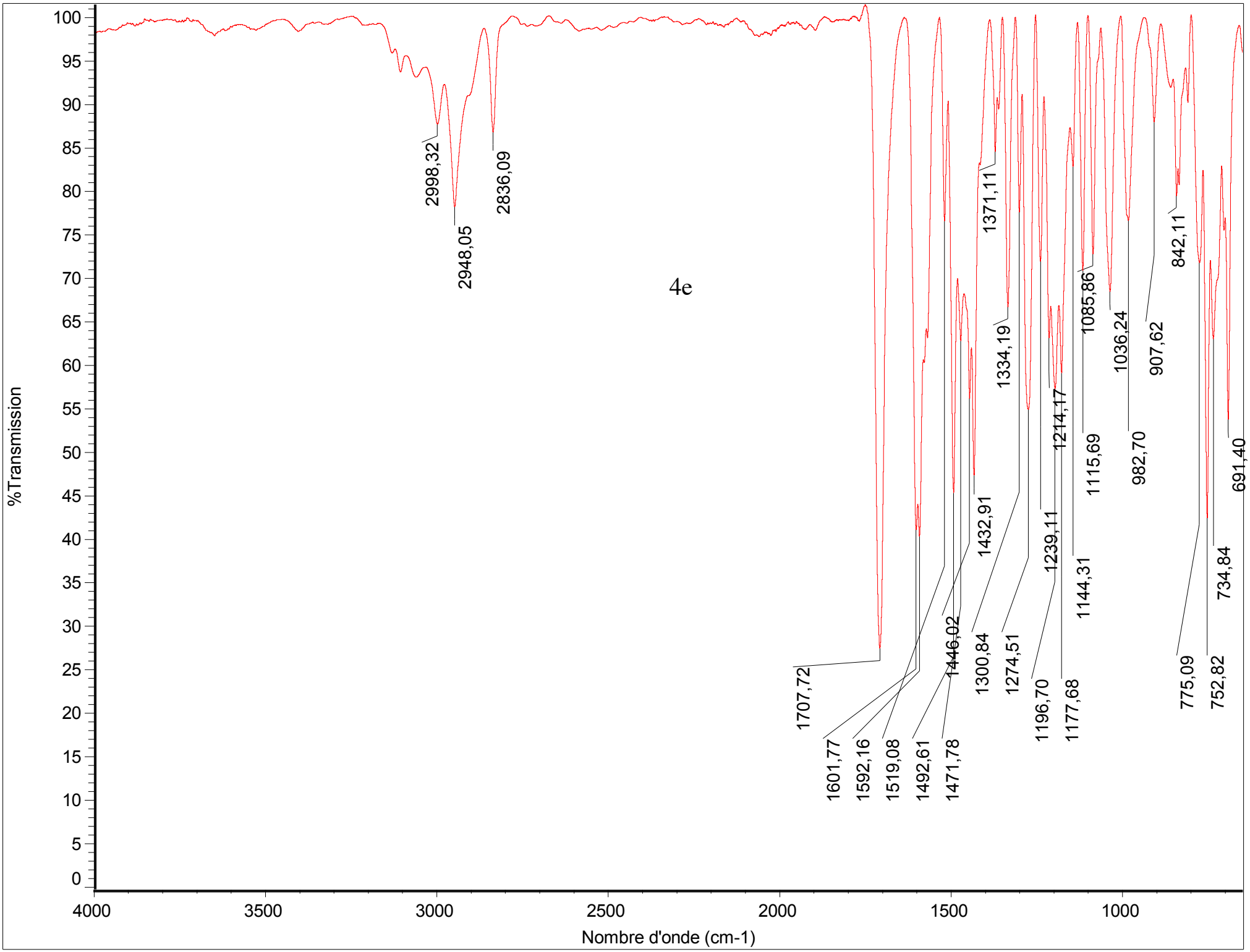

8.4545
8.4494
7.9233
7.9176
7.8942
7.8886
7.4474
7.4008
7.3715
7.3305
7.3195
7.0555
6.7461
6.7376
6.7349
3.9429
3.8786
7.4181
7.3935
7.3790
7.2596
7.0480
7.0332
7.0259
6.7486
0.92
0.97
2.98
1.00
1.97
0.98
3.00
f1 (ppm)
4d
O
CH3
N

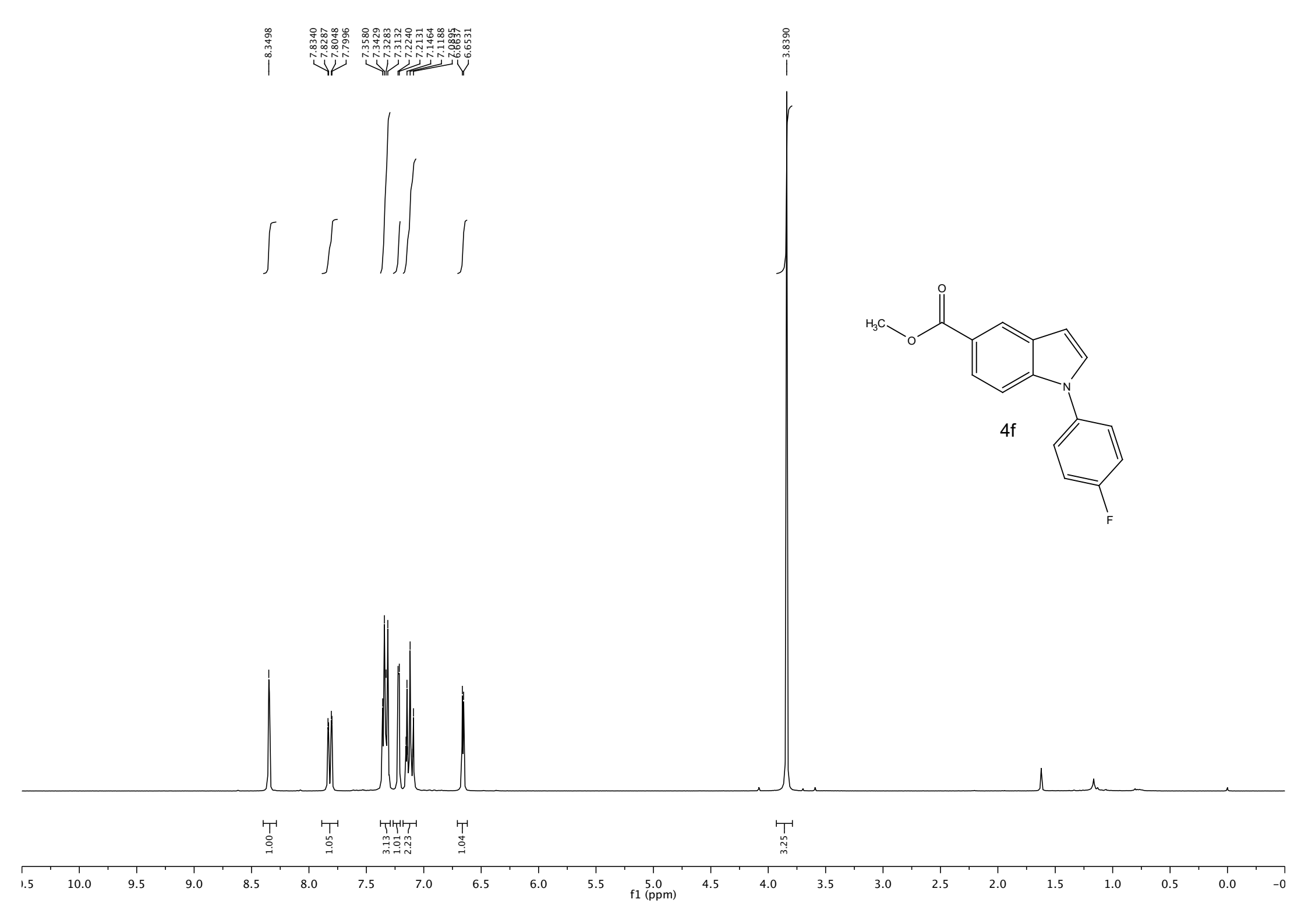

168.1057
158.6843
138.7967
132.1948
129.8382
128.5156
126.1088
124.0877
123.5610
122.1698
114.8923
110.0782
104.2789
55.6535
51.9146
O
O
CH3
N
O
CH3
4d
f1 (ppm)
f1 (ppm)

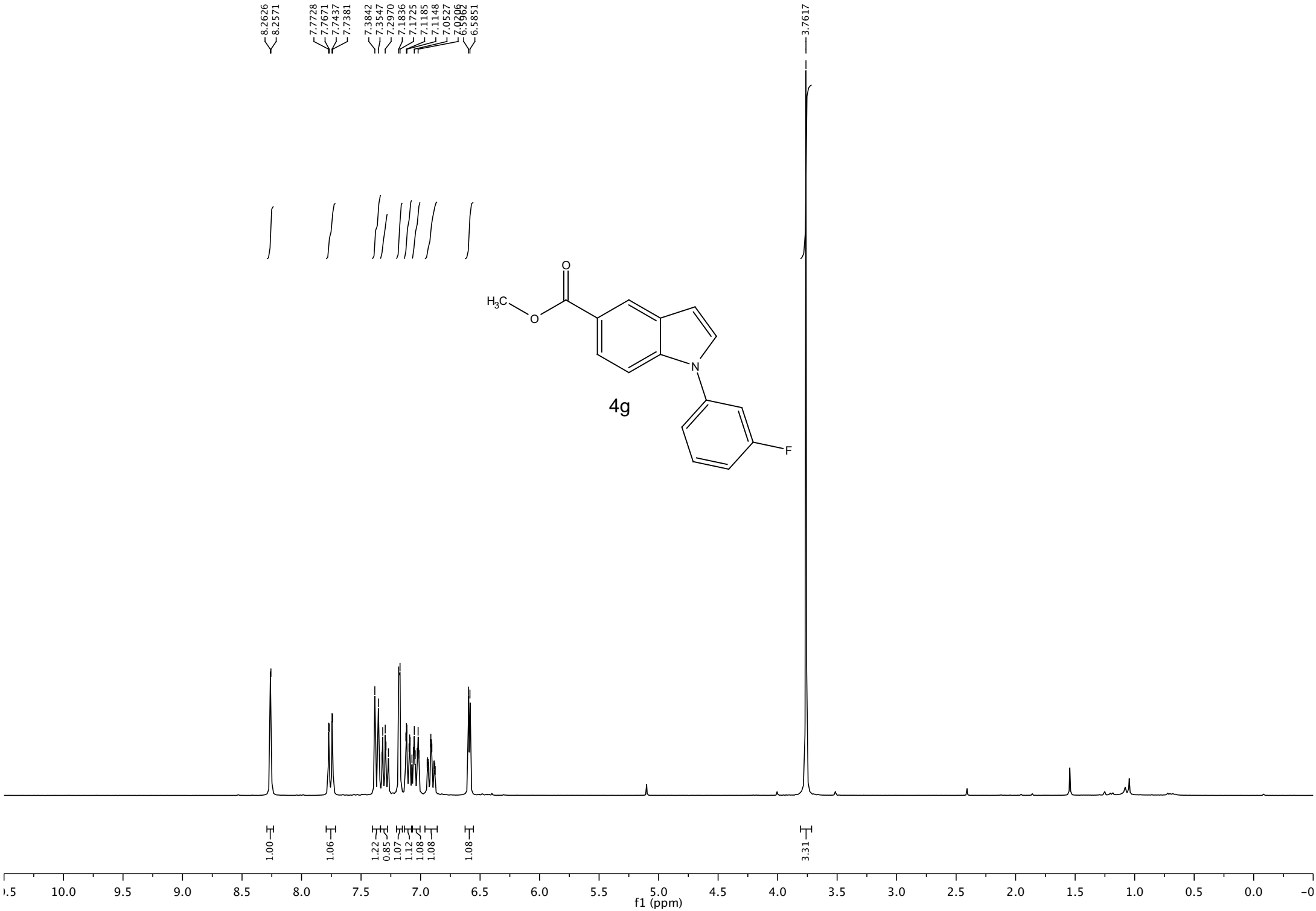

4d
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
4000
3500
3000
2500
2000
1500
1000
500
3137,80
3109,19
2941,66
2917,14
2839,50
1692,98
1702,92
1513,91
1335,27
1197,28
1226,33
1708,58
1605,47
1518,87
1449,99
1439,29
1434,25
1269,33

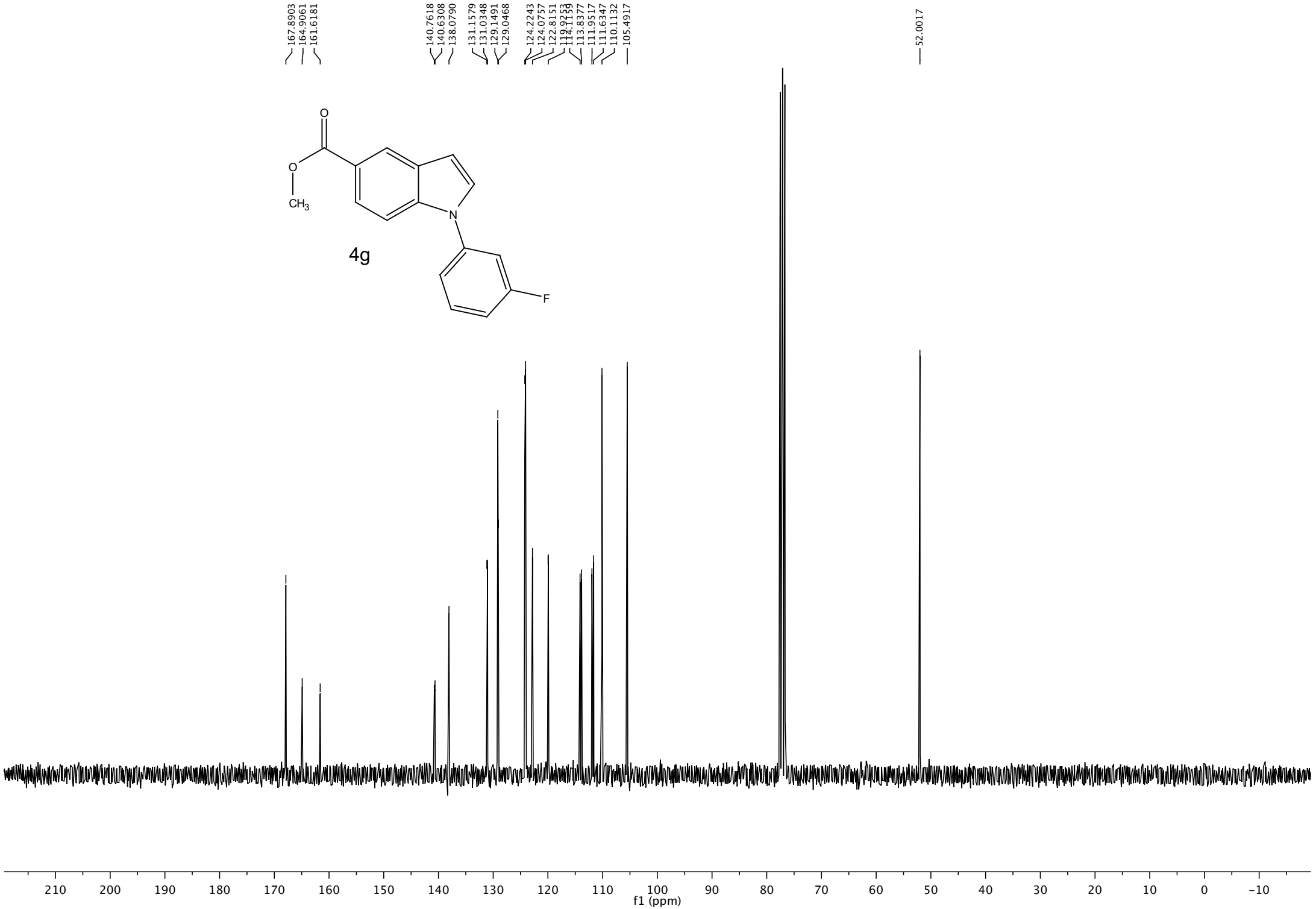

8.4496
8.4445
7.9405
7.9347
7.9109
7.9055
7.5898
7.5607
7.4391
7.4008
7.3897
7.1076
7.1045
7.1008
7.0978
7.0814
7.0782
7.0747
7.0718
7.0429
7.0353
7.0282
6.9598
6.9566
6.9515
6.9488
6.9323
6.9291
6.9239
6.9209
6.7716
6.7688
6.7606
6.7579
3.9465
3.8717
7.4659
7.4119
0.90
0.95
0.98
0.76
1.20
1.01
0.94
0.96
0.96
2.95
3.00
f1 (ppm)
4e
O
O
CH3
N
O
CH3

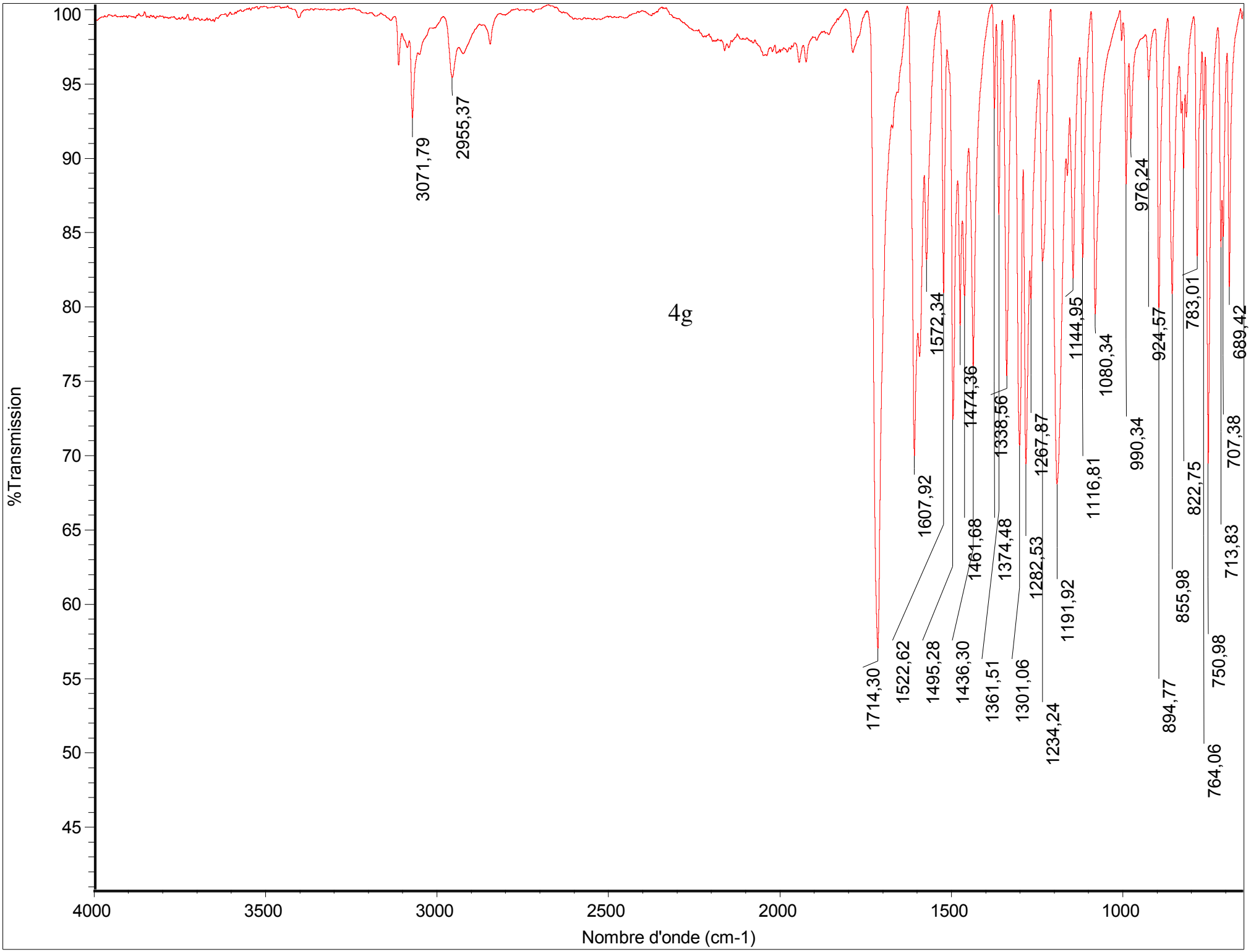

168.0285
160.6634
140.3690
138.2896
130.5441
129.4555
128.8893
124.1291
123.7615
122.4517
116.7268
112.5471
110.4926
110.3407
104.8583
55.5804
51.9573
O
O
CH3
N
CH3
O
4e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

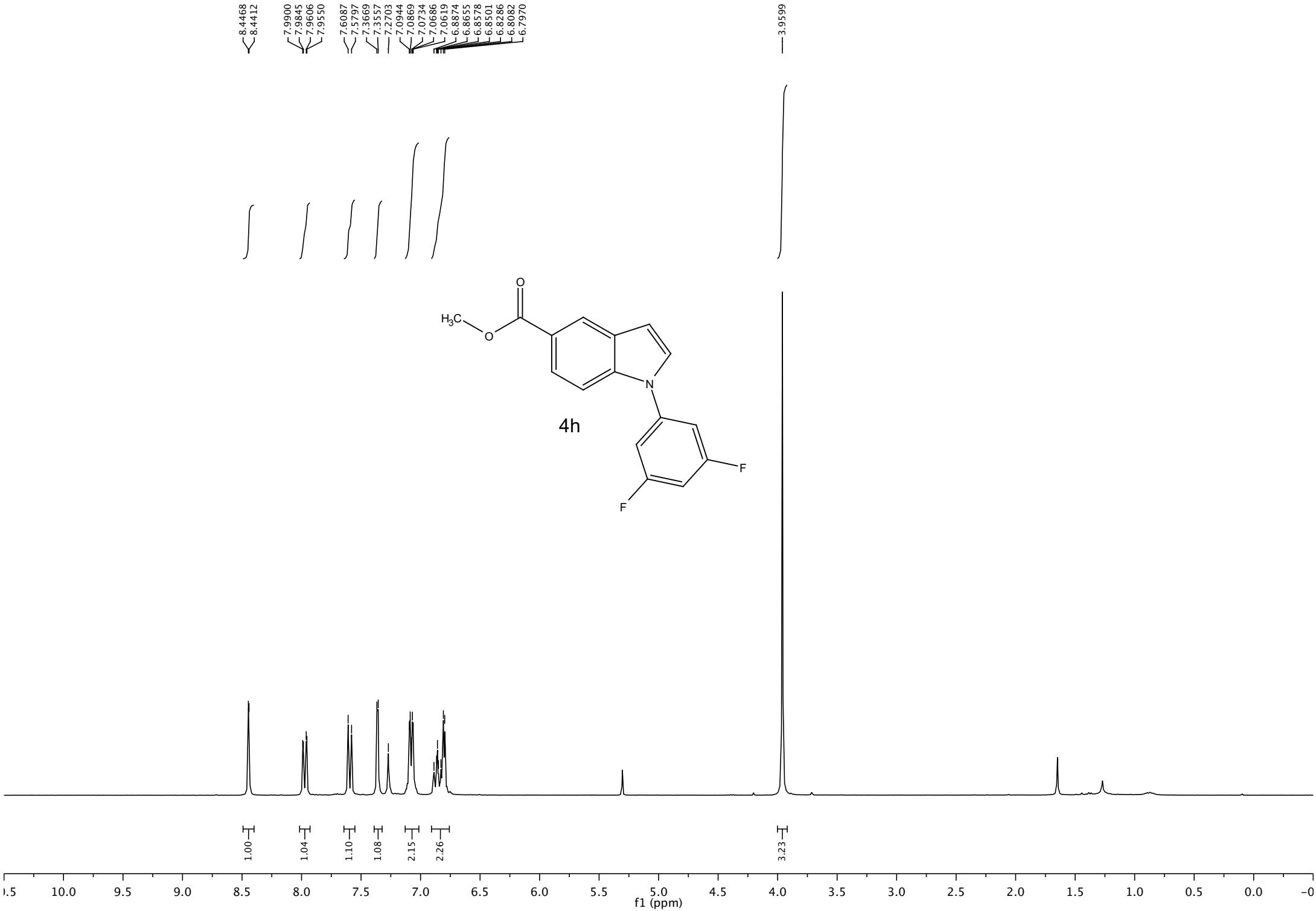

4e
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
4000
3500
3000
2500
2000
1500
1000
2998,32
2948,05
2836,09
1707,72
1601,77
1592,16
1519,08
1492,61
1471,78
1446,02
1432,91
1371,11
1334,19
1300,84
1274,51
1239,11
1214,17
1196,70
1177,68
1144,31
1115,69
1085,86
1036,24
982,70
907,62
842,11
775,09
752,82
734,84
691,40

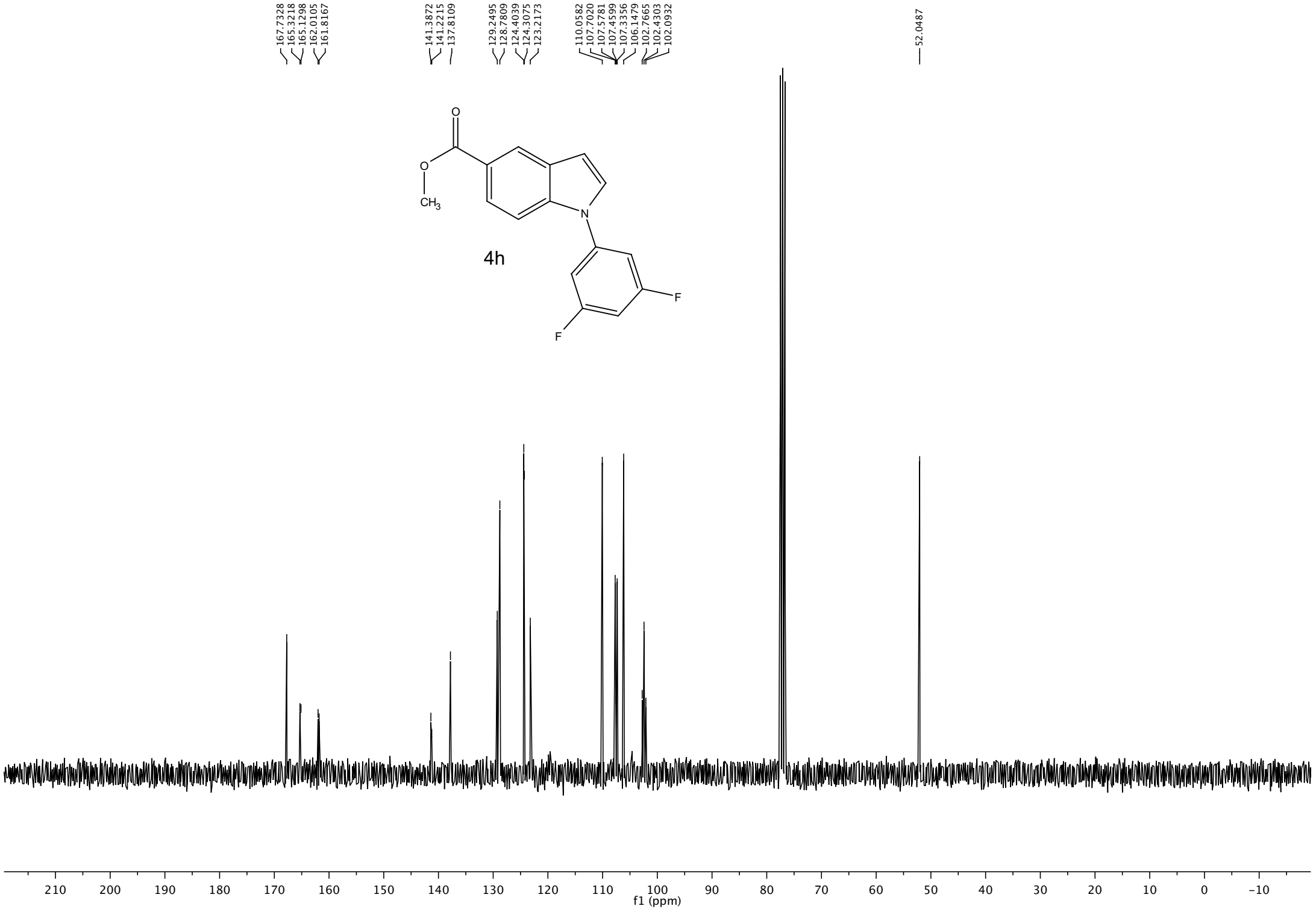

8.3498
7.8340
7.8287
7.8048
7.7996
7.3580
7.3429
7.3283
7.3132
7.2240
7.2131
7.1464
7.1188
7.0895
6.6837
6.6531
3.8390
O
H3C
O
N
F
4f
1.00
1.05
3.13
1.01
2.23
1.04
3.25
f1 (ppm)

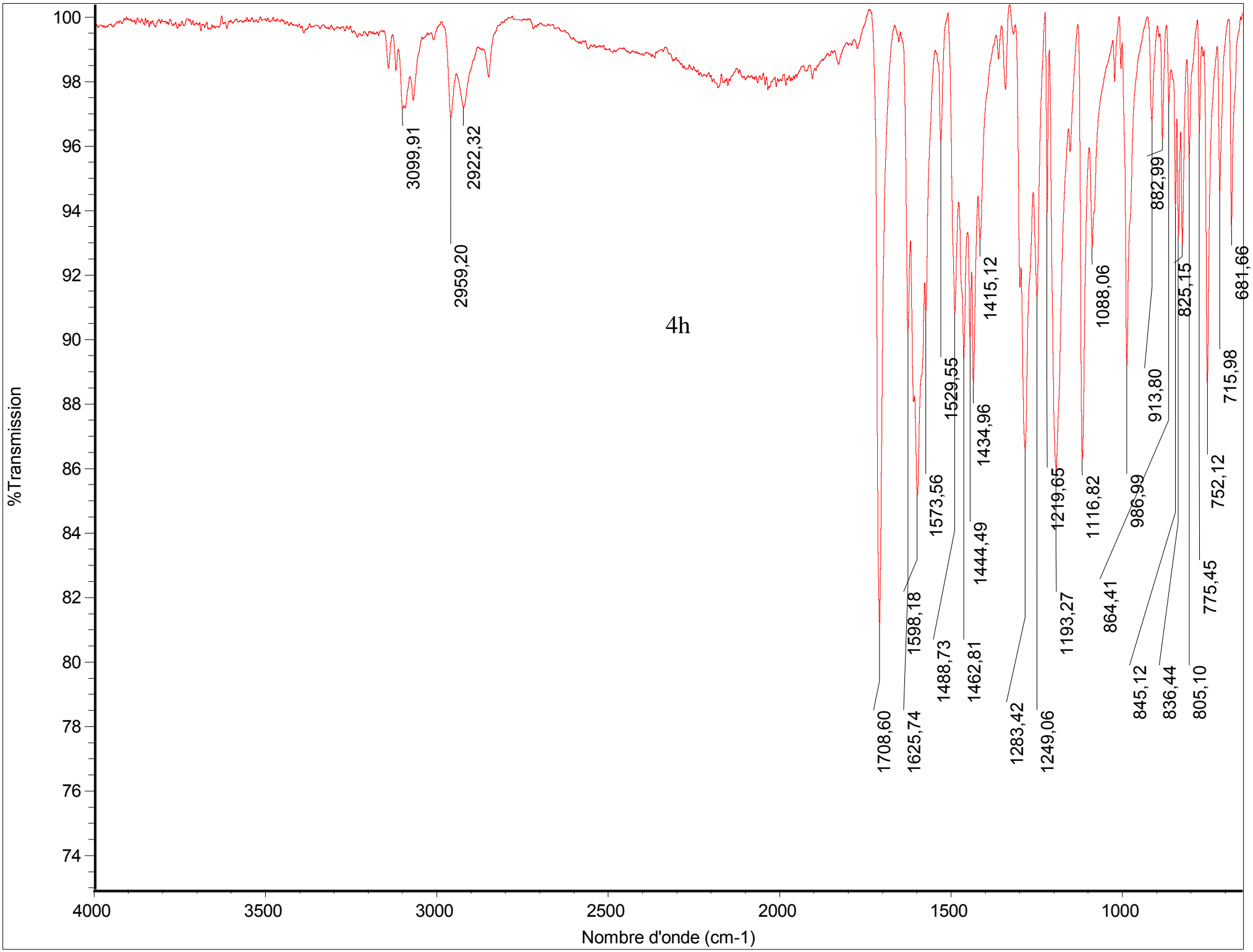

8.2626
8.2571
7.7728
7.7671
7.7437
7.7381
7.3842
7.3547
7.2970
7.1836
7.1725
7.1185
7.1148
7.0527
7.0206
6.9962
6.5851
3.7617
O
H3C
O
N
F
4g
1.00
1.06
1.22
0.85
1.07
1.12
1.08
1.08
1.08
3.31
f1 (ppm)

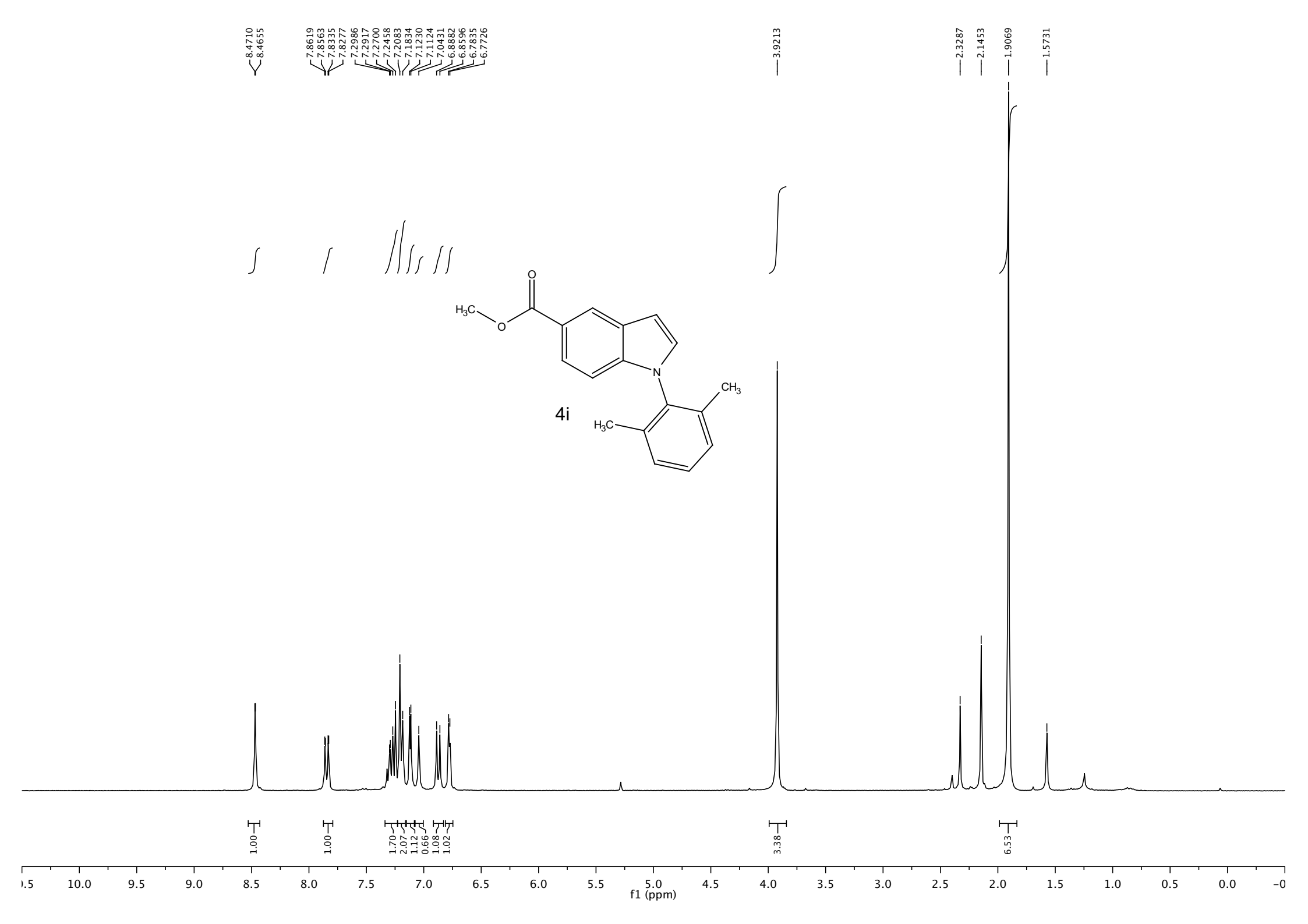

167.8903
164.9061
161.6181
140.7618
140.6308
138.0790
131.1579
131.0348
129.1491
129.0468
124.2243
124.0757
122.8151
113.8377
111.9517
111.6347
110.1132
105.4917
52.0017
O
O
CH3
N
F
4g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

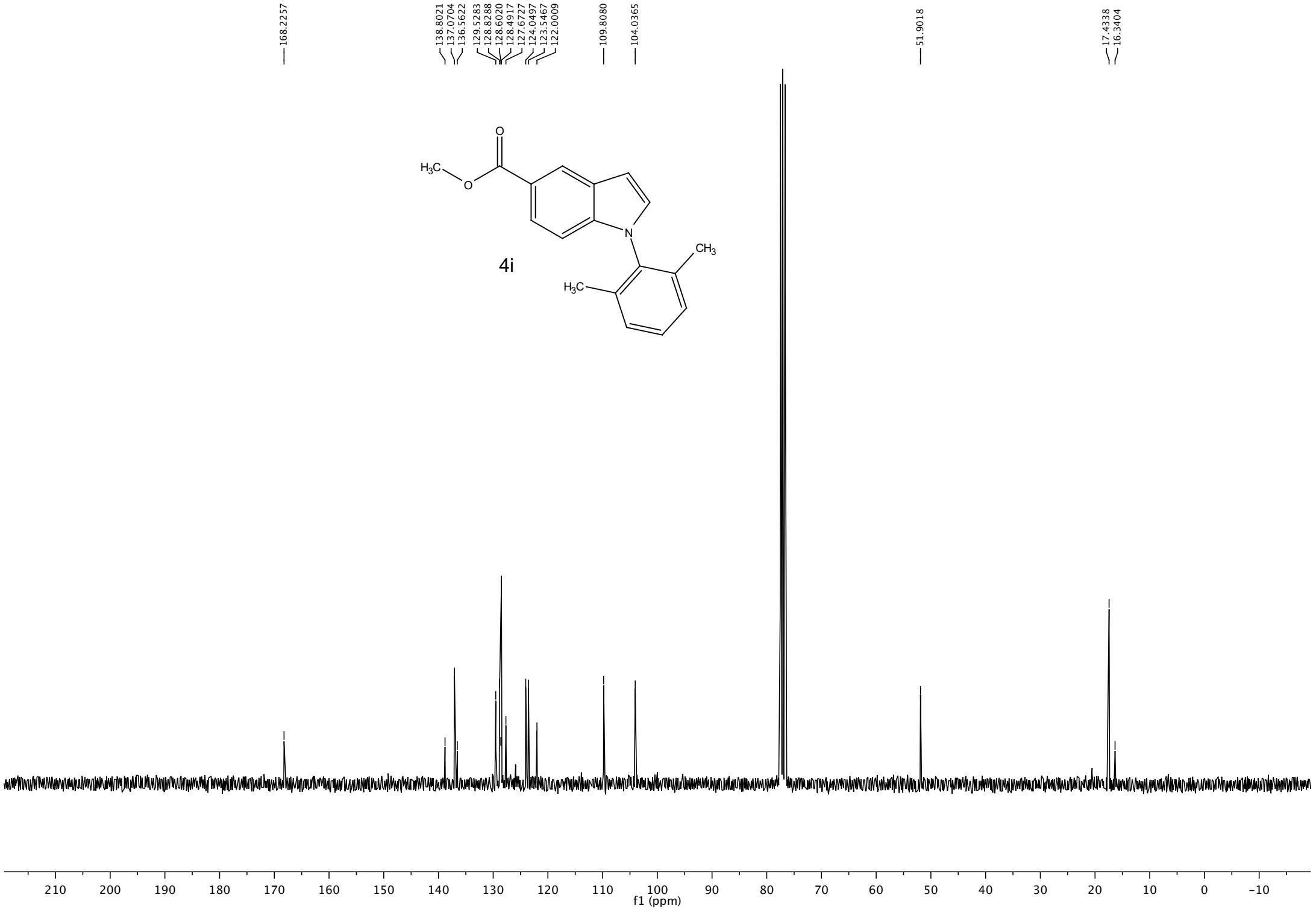

4g
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
4000
3500
3000
2500
2000
1500
1000
3071,79
2955,37
1714,30
1607,92
1572,34
1522,62
1495,28
1474,36
1461,68
1436,30
1374,48
1361,51
1338,56
1301,06
1282,53
1267,87
1234,24
1191,92
1144,95
1116,81
1080,34
990,34
976,24
924,57
894,77
855,98
822,75
783,01
764,06
750,98
713,83
707,38
689,42

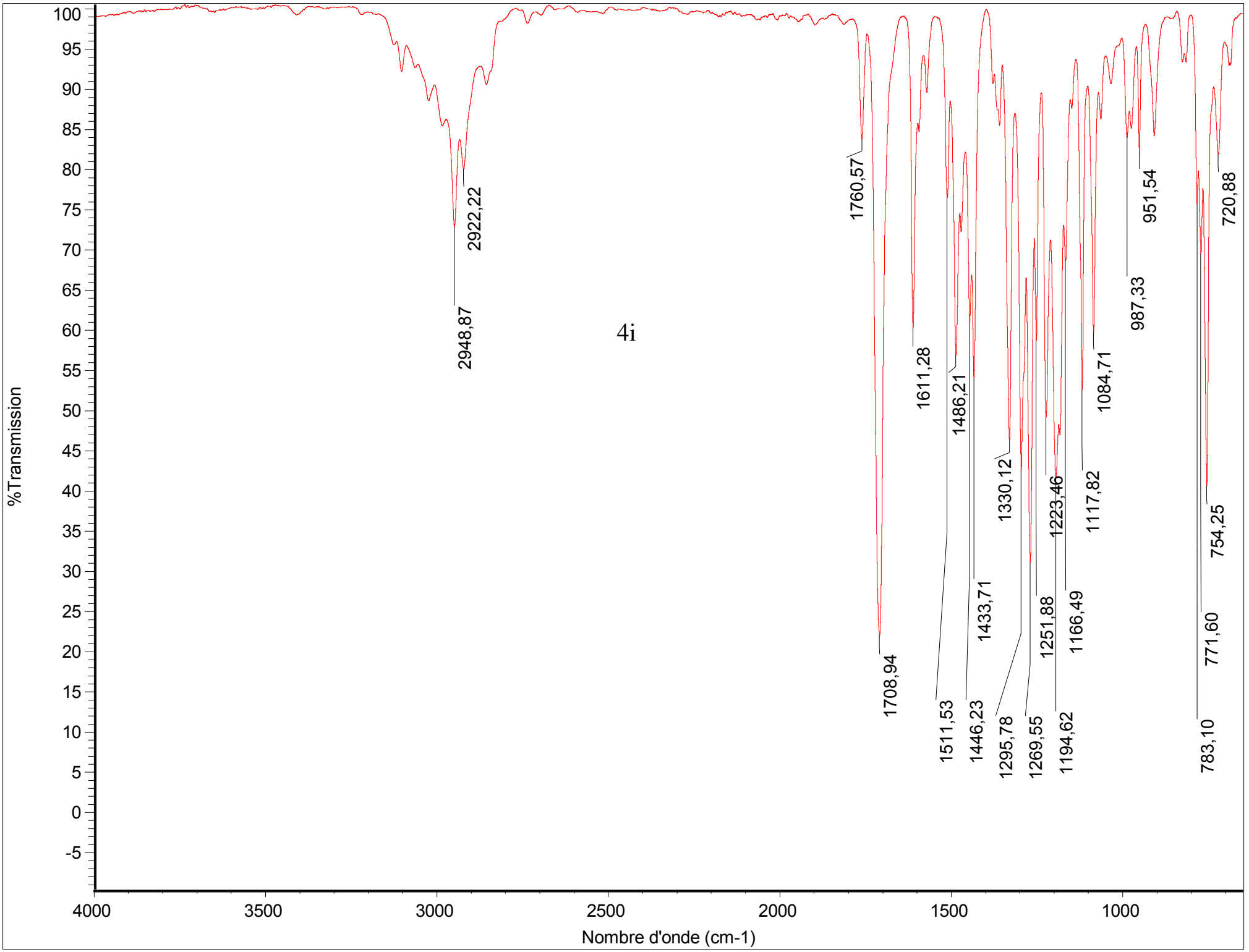

8.4468
8.4412
7.9900
7.9845
7.9606
7.9550
7.6087
7.5797
7.3669
7.3557
7.2703
7.0944
7.0869
7.0734
7.0686
7.0619
6.8874
6.8655
6.8578
6.8501
6.8286
6.8082
6.7970
3.9599
O
H3C
O
N
F
F
4h
1.00
1.04
1.10
1.08
2.15
2.26
3.23
f1 (ppm)

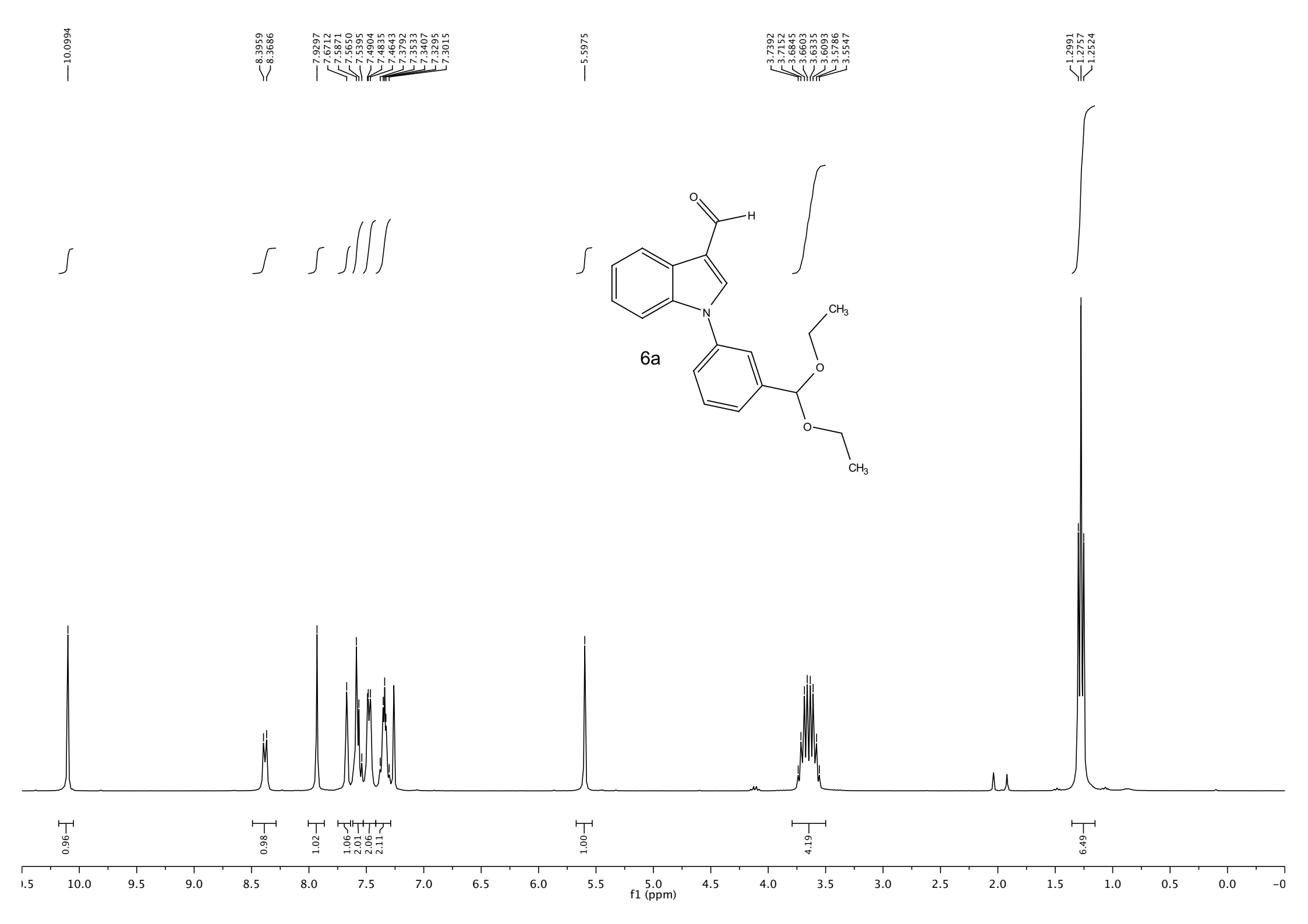

167.7328
165.3218
165.1298
162.0105
161.8167
141.3872
141.2215
137.8109
129.2495
128.7809
124.4039
124.3075
123.2173
110.0582
107.7020
107.5781
107.4599
107.3356
106.1479
102.7665
102.4303
102.0932
52.0487
O
O
CH3
N
F
F
4h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

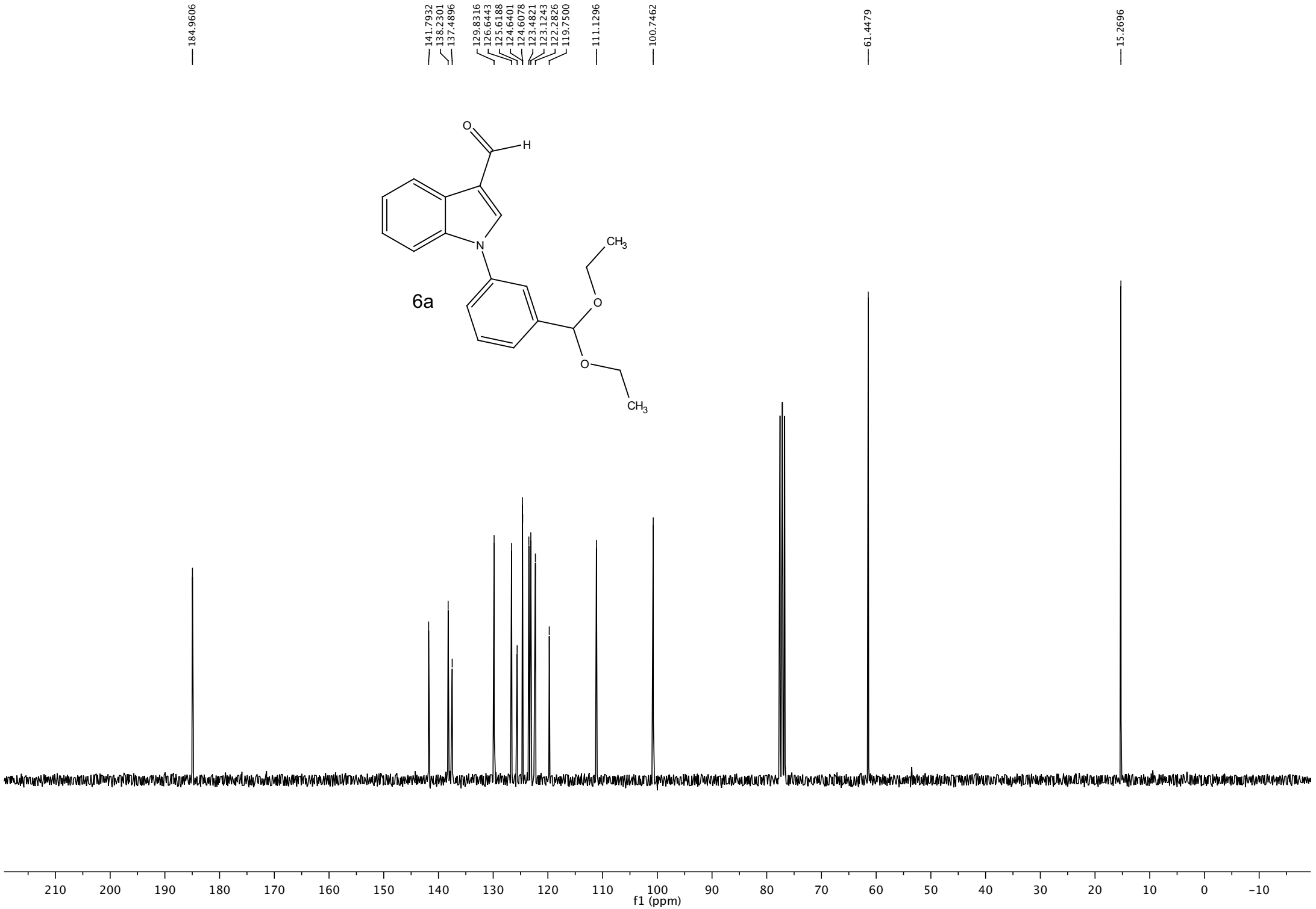

4h
%Transmission
Nombre d'onde (cm-1)
100
98
96
94
92
90
88
86
84
82
80
78
76
74
4000
3500
3000
2500
2000
1500
1000
3099,91
2959,20
2922,32
1708,60
1625,74
1598,18
1573,56
1529,55
1488,73
1462,81
1444,96
1434,49
1415,12
1283,42
1249,06
1219,65
1193,27
1116,82
1088,06
986,99
913,80
882,99
864,41
845,12
836,44
825,15
805,10
775,45
752,12
715,98
681,66

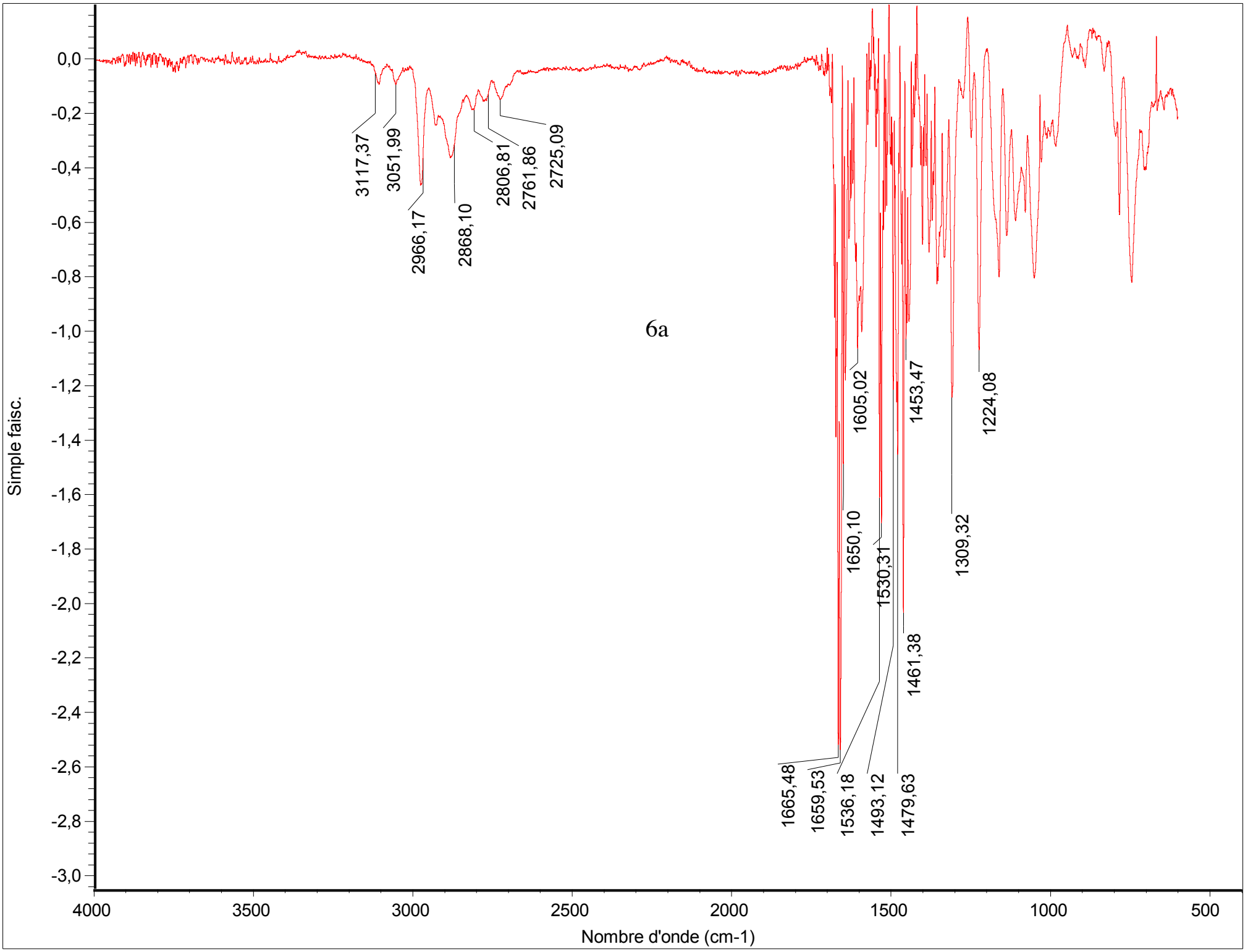

8.4710
8.4655
7.8619
7.8563
7.8335
7.8277
7.2986
7.2917
7.2700
7.2458
7.2083
7.1834
7.1230
7.1124
7.0431
6.8882
6.8596
6.7835
6.7726
3.9213
2.3287
2.1453
1.9069
1.5731
O
H3C
O
N
CH3
H3C
4i
1.00
1.00
1.70
2.07
1.12
0.66
1.08
1.02
3.38
6.53
f1 (ppm)

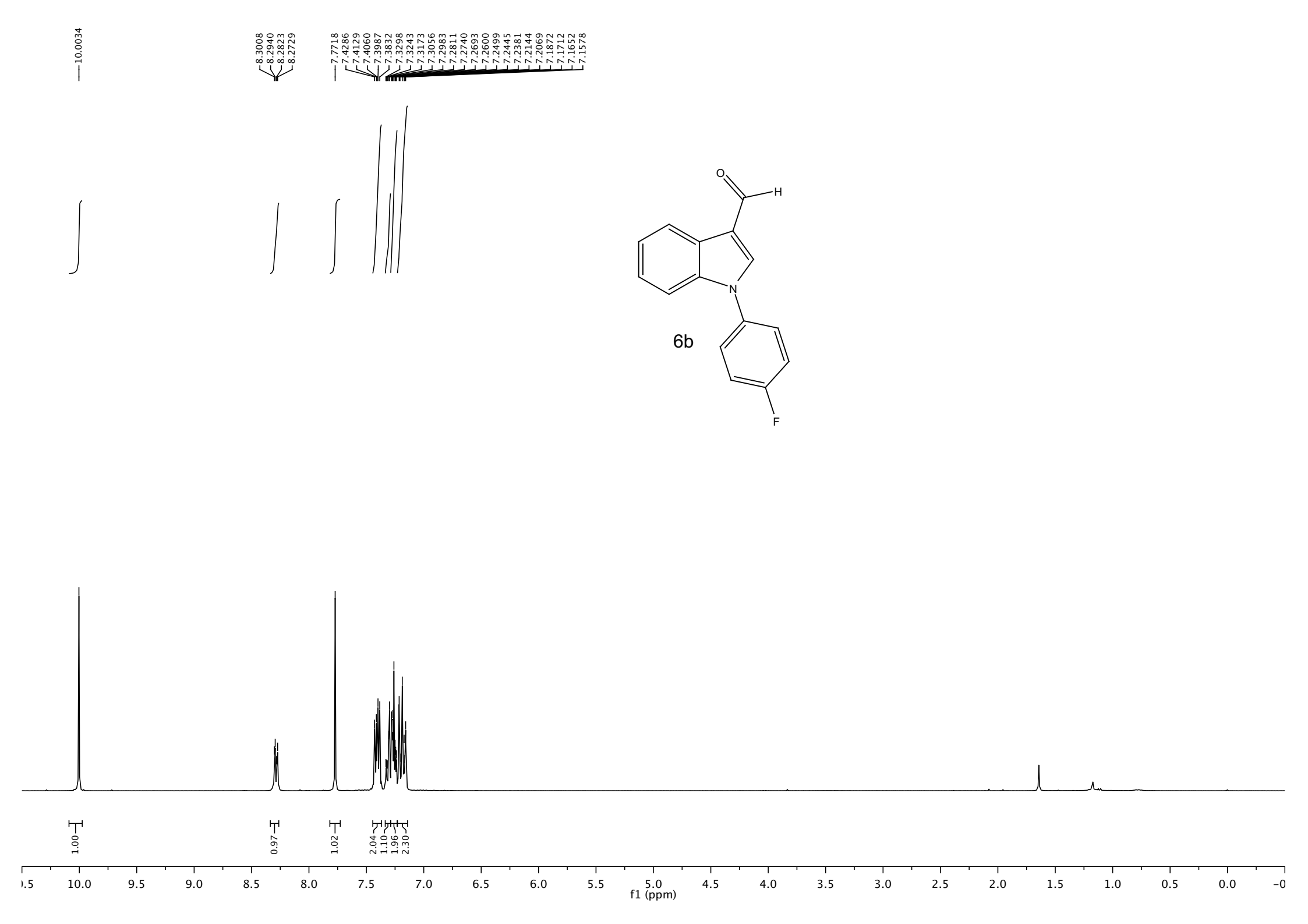

168.2257
138.8021
137.0704
136.5622
129.5283
128.8288
128.6020
128.4917
127.6727
124.0497
123.5467
122.0009
109.8080
104.0365
51.9018
17.4338
16.3404
O
H3C
O
N
CH3
H3C
4i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

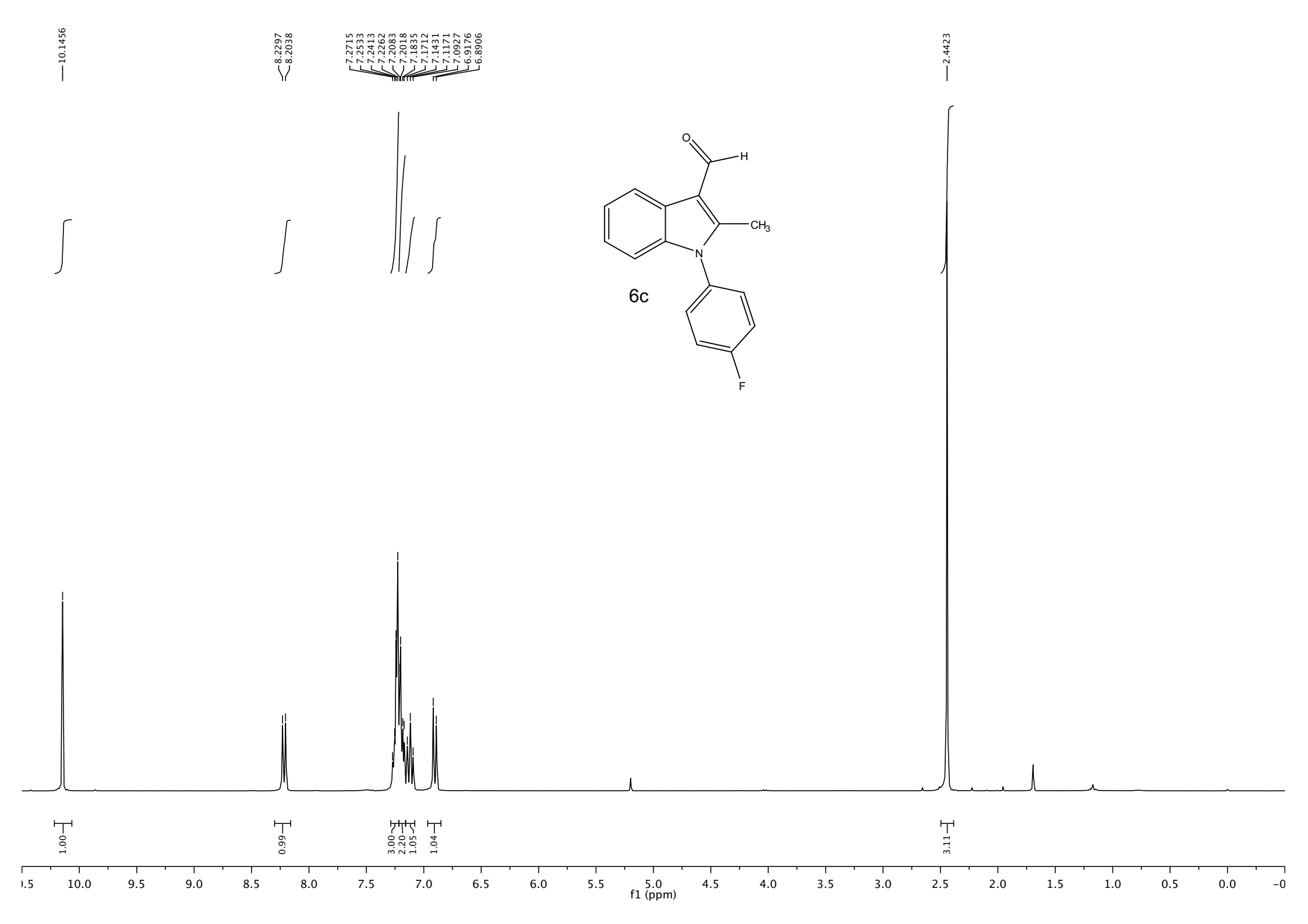

4i
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
4000
3500
3000
2500
2000
1500
1000
2948,87
2922,22
1760,57
1708,94
1611,28
1511,53
1486,21
1446,23
1433,71
1330,12
1295,78
1269,55
1251,88
1223,46
1194,62
1166,49
1117,82
1084,71
987,33
951,54
783,10
771,60
754,25
720,88

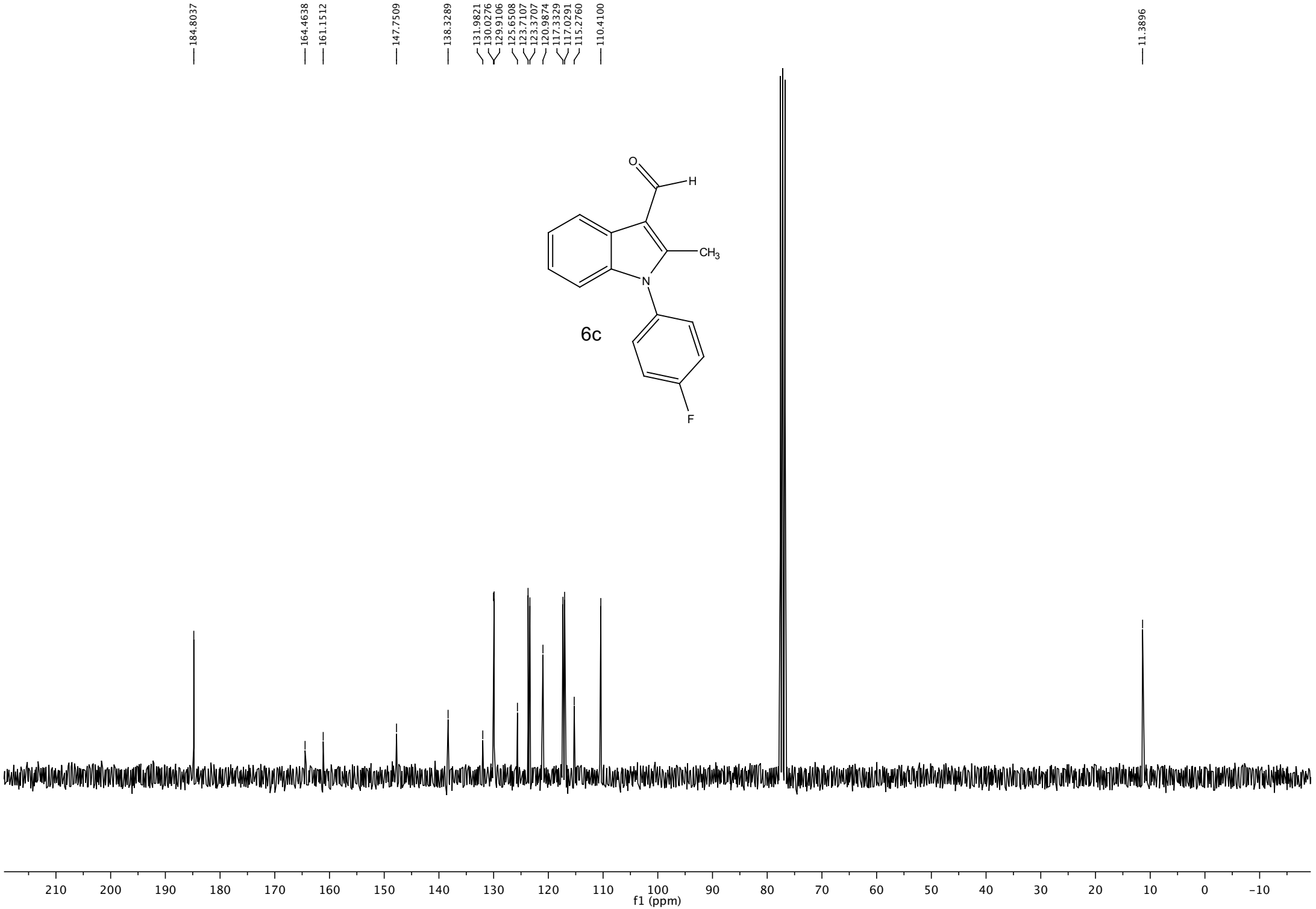

10.0994
8.3959
8.3686
7.9297
7.6712
7.5871
7.5650
7.5395
7.4904
7.4835
7.4643
7.3792
7.3533
7.3407
7.3295
7.3015
5.5975
3.7392
3.7152
3.6845
3.6603
3.6335
3.6093
3.5786
3.5547
1.2991
1.2757
1.2524
O
H
N
CH3
O
O
CH3
6a
0.96
0.98
1.02
1.06
2.01
2.06
2.11
1.00
4.19
6.49
f1 (ppm)

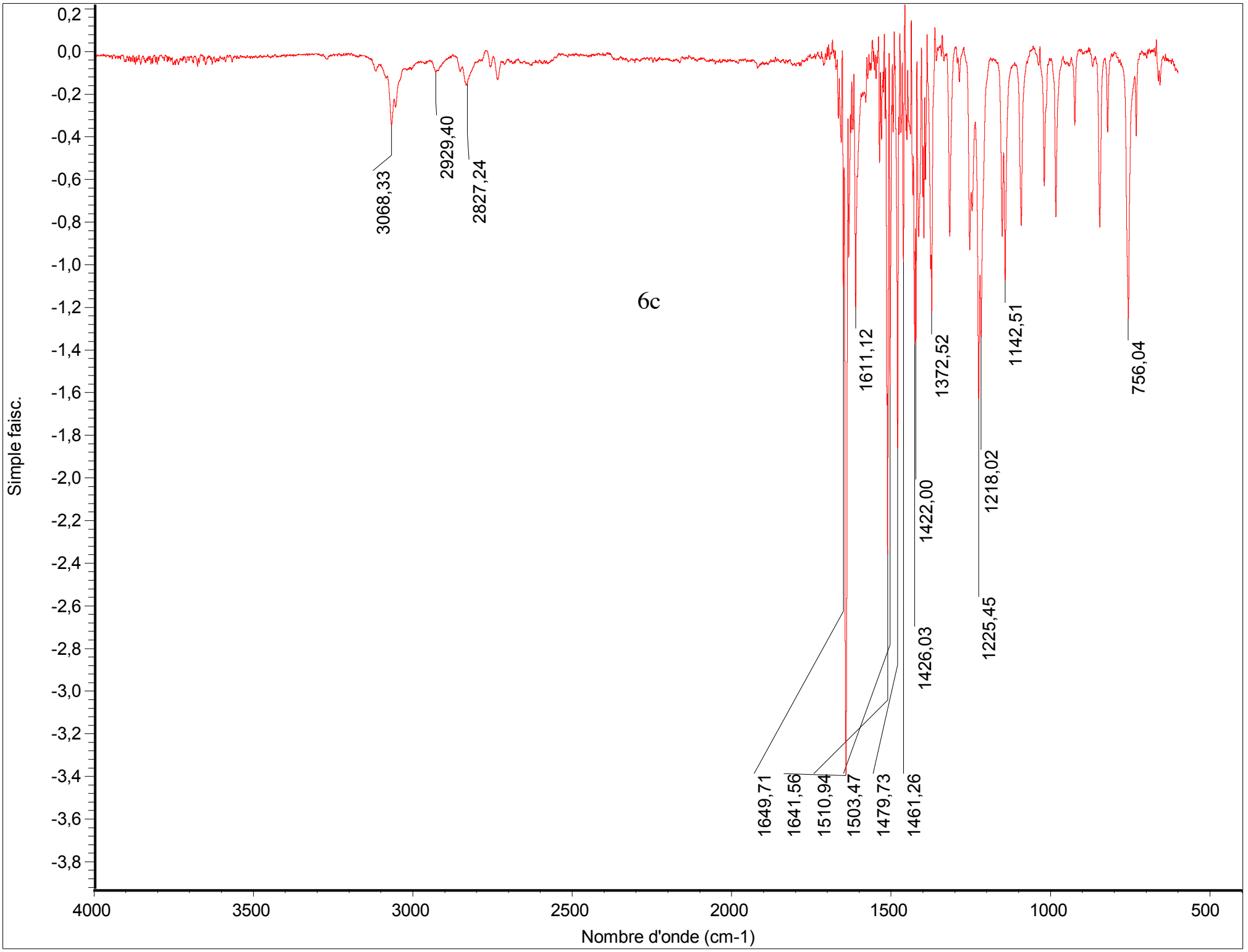

184.9606
141.7932
138.2301
137.4896
129.8316
126.6443
125.6188
124.6401
124.6078
123.4821
123.1243
122.2826
119.7500
111.1296
100.7462
61.4479
15.2696
O
H
N
O
O
CH3
CH3
6a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

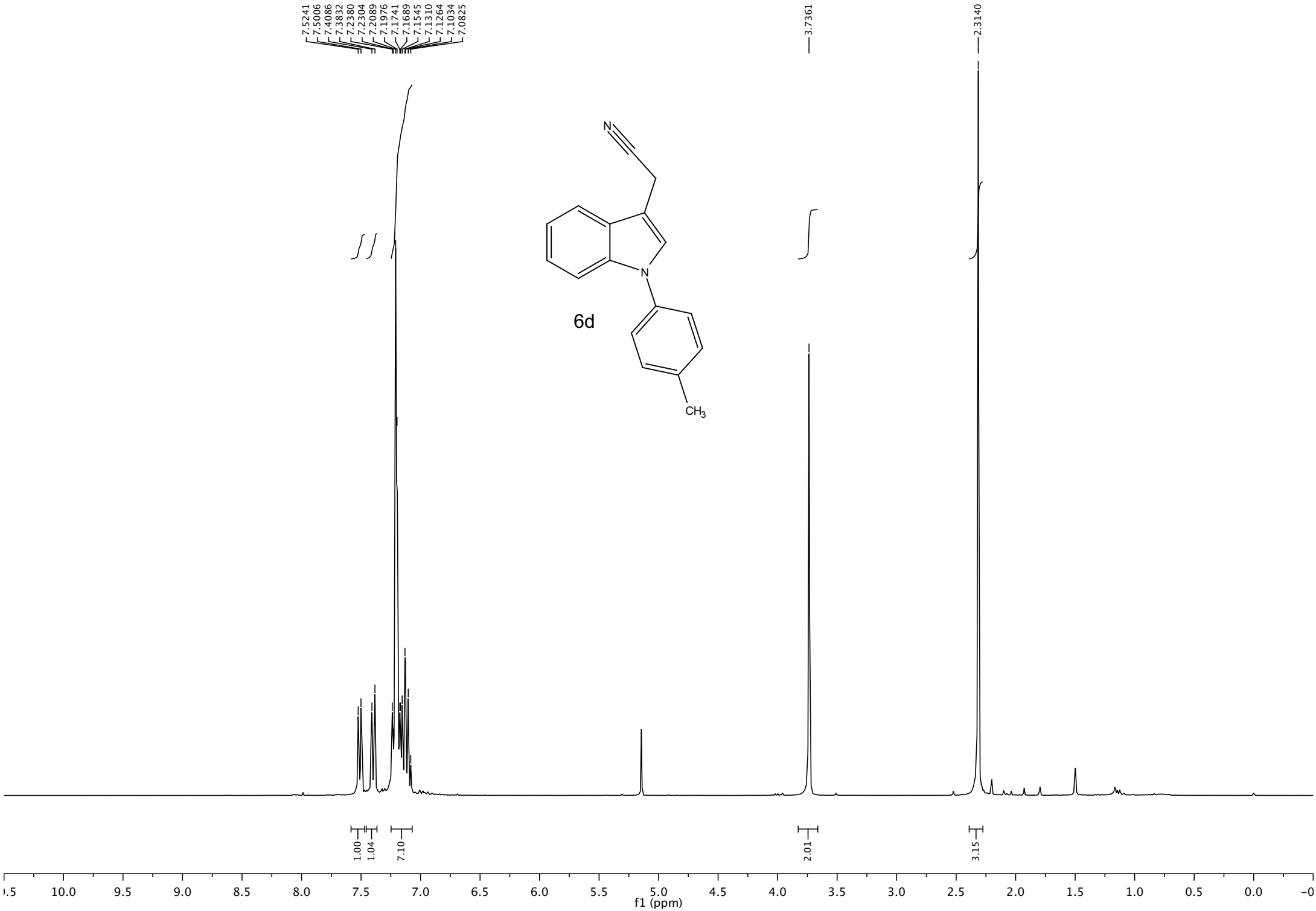

6a
Simple faisc.
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
4000
3500
3000
2500
2000
1500
1000
500
Nombre d'onde (cm-1)
3117,37
3051,99
2966,17
2868,10
2806,81
2761,86
2725,09
1665,48
1659,53
1650,10
1605,02
1536,18
1530,31
1493,12
1479,63
1461,38
1453,47
1309,32
1224,08

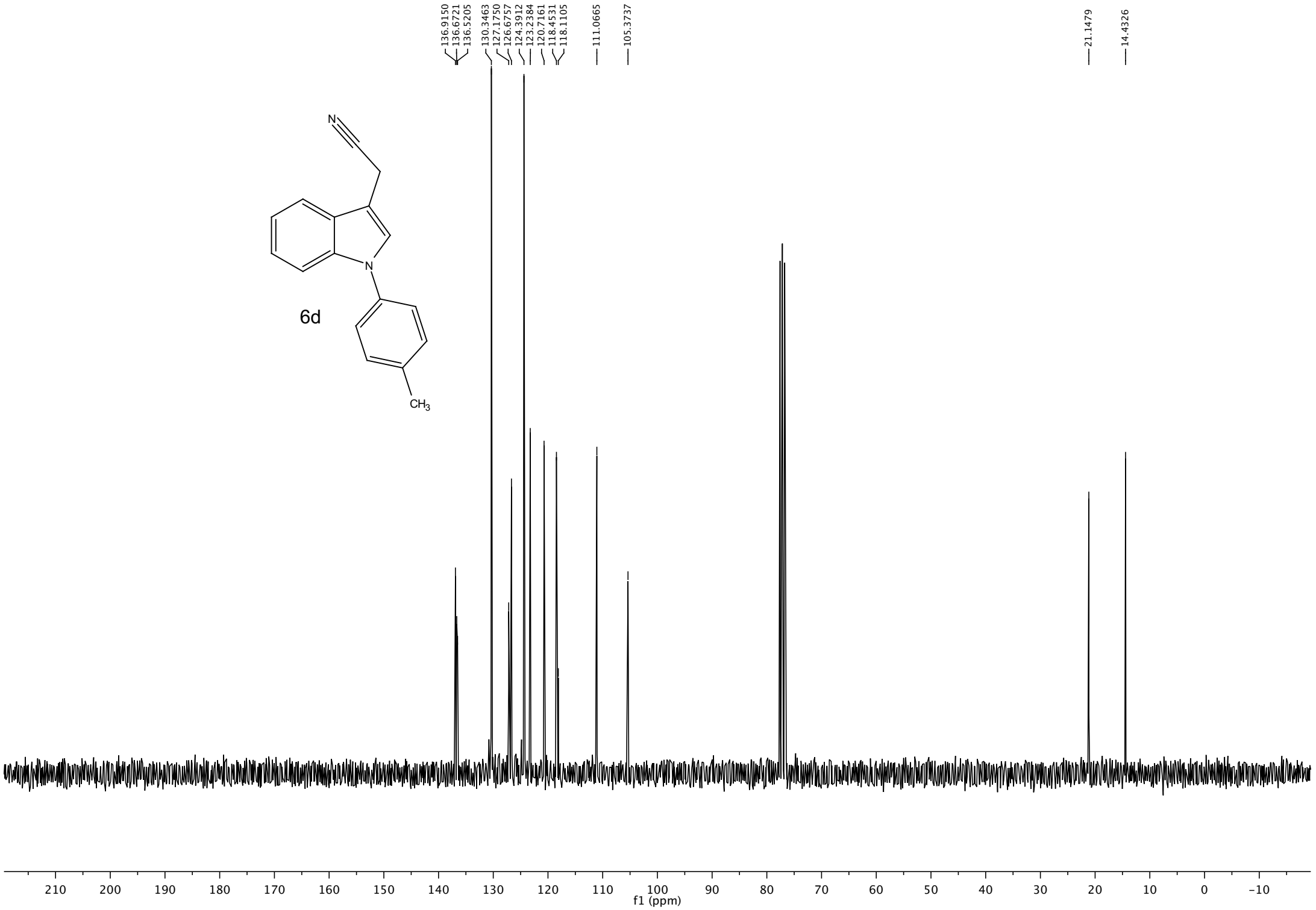

10.0034
8.3008
8.2940
8.2823
8.2729
7.7718
7.4286
7.4129
7.4060
7.3987
7.3832
7.3298
7.3243
7.3173
7.3056
7.2983
7.2811
7.2740
7.2693
7.2600
7.2499
7.2445
7.2381
7.2144
7.2069
7.1872
7.1712
7.1652
7.1578
O
H
N
F
6b
1.00
0.97
1.02
2.04
1.10
1.96
2.30
f1 (ppm)

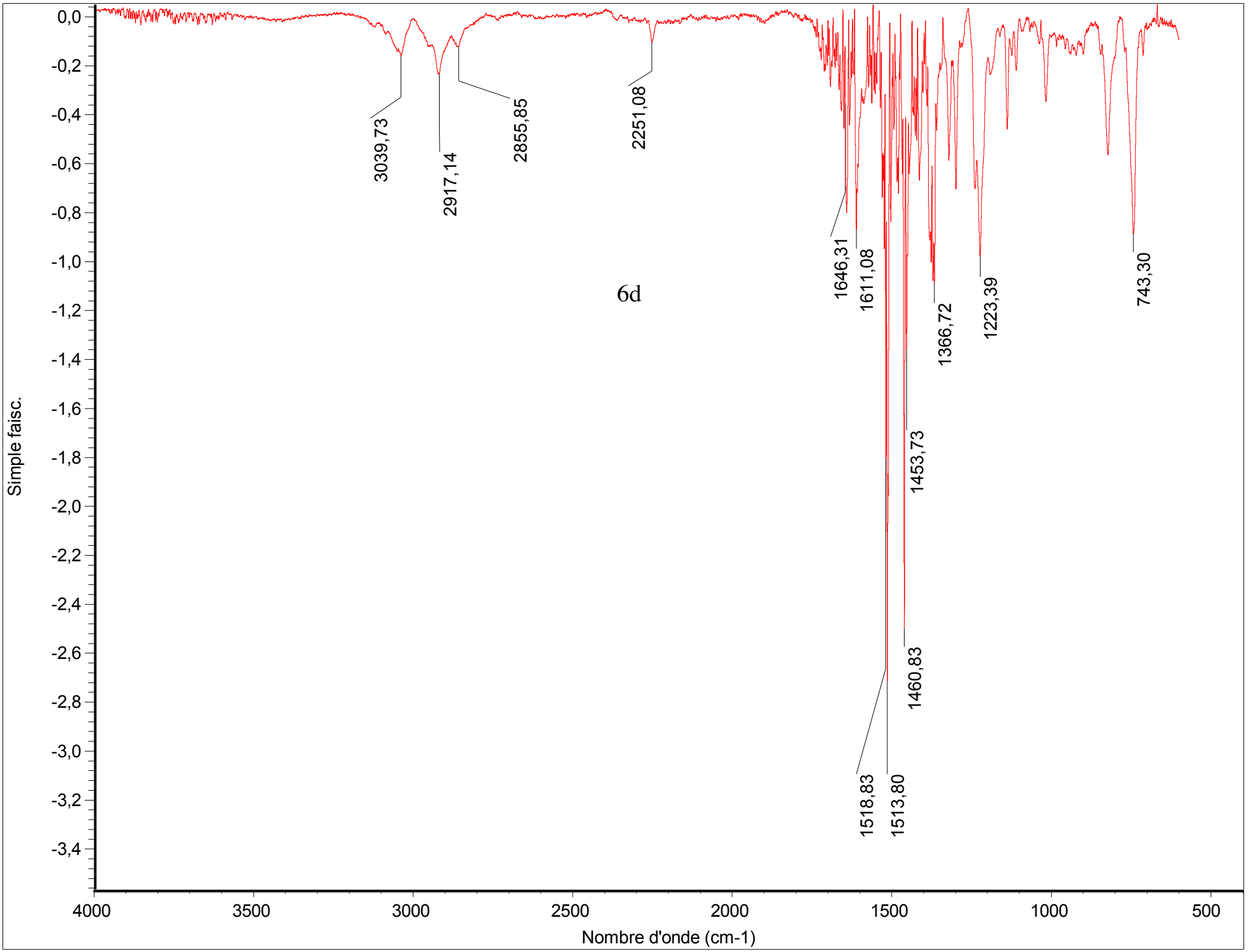

10.1456
8.2297
8.2038
7.2715
7.2533
7.2413
7.2262
7.2083
7.2018
7.1835
7.1712
7.1431
7.1171
7.0927
6.9176
6.8906
2.4423
O
H
CH3
N
F
6c
1.00
0.99
3.00
2.20
1.05
1.04
3.11
f1 (ppm)

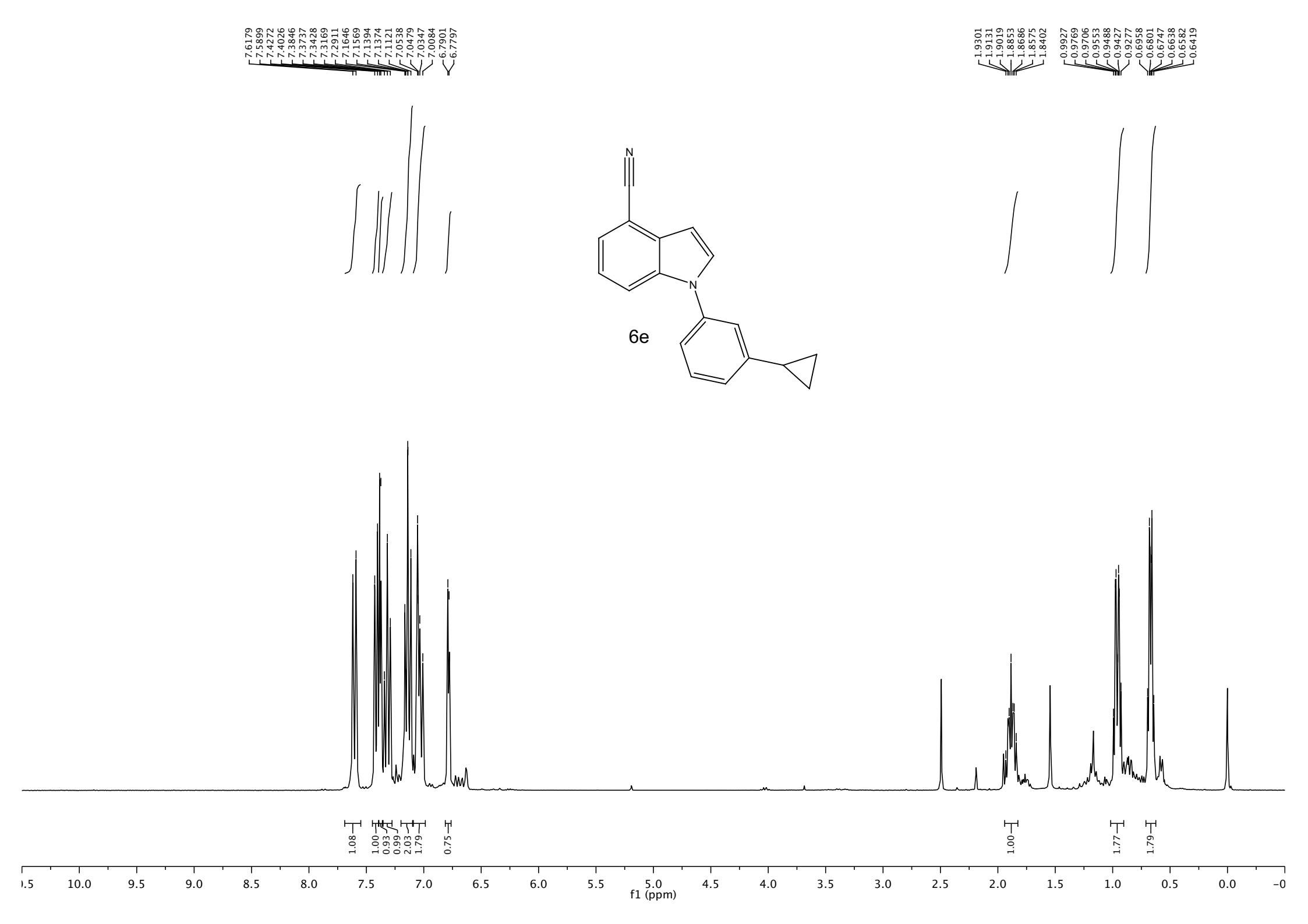

184.8037
164.4638
161.1512
147.7509
138.3289
131.9821
130.0276
129.9106
125.6508
123.7107
123.3707
120.9874
117.3329
117.0291
115.2760
110.4100
11.3896
O
H
CH3
N
F
6c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

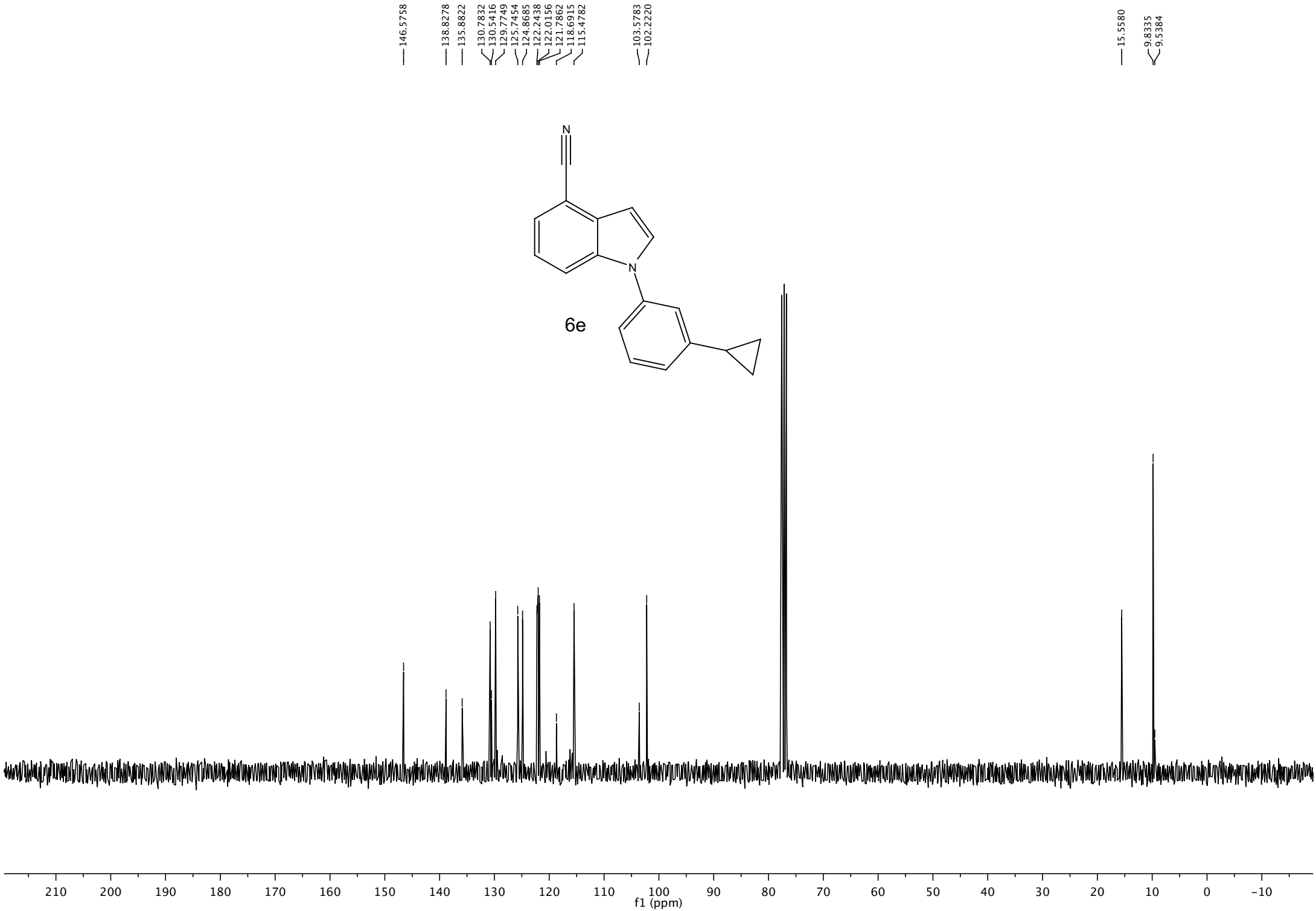

6c
Simple faisc.
Nombre d'onde (cm-1)
0,2
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
-3,8
4000
3500
3000
2500
2000
1500
1000
500
3068,33
2929,40
2827,24
1611,12
1372,52
1142,51
756,04
1218,02
1422,00
1225,45
1426,03
1649,71
1641,56
1510,94
1503,47
1479,73
1461,26

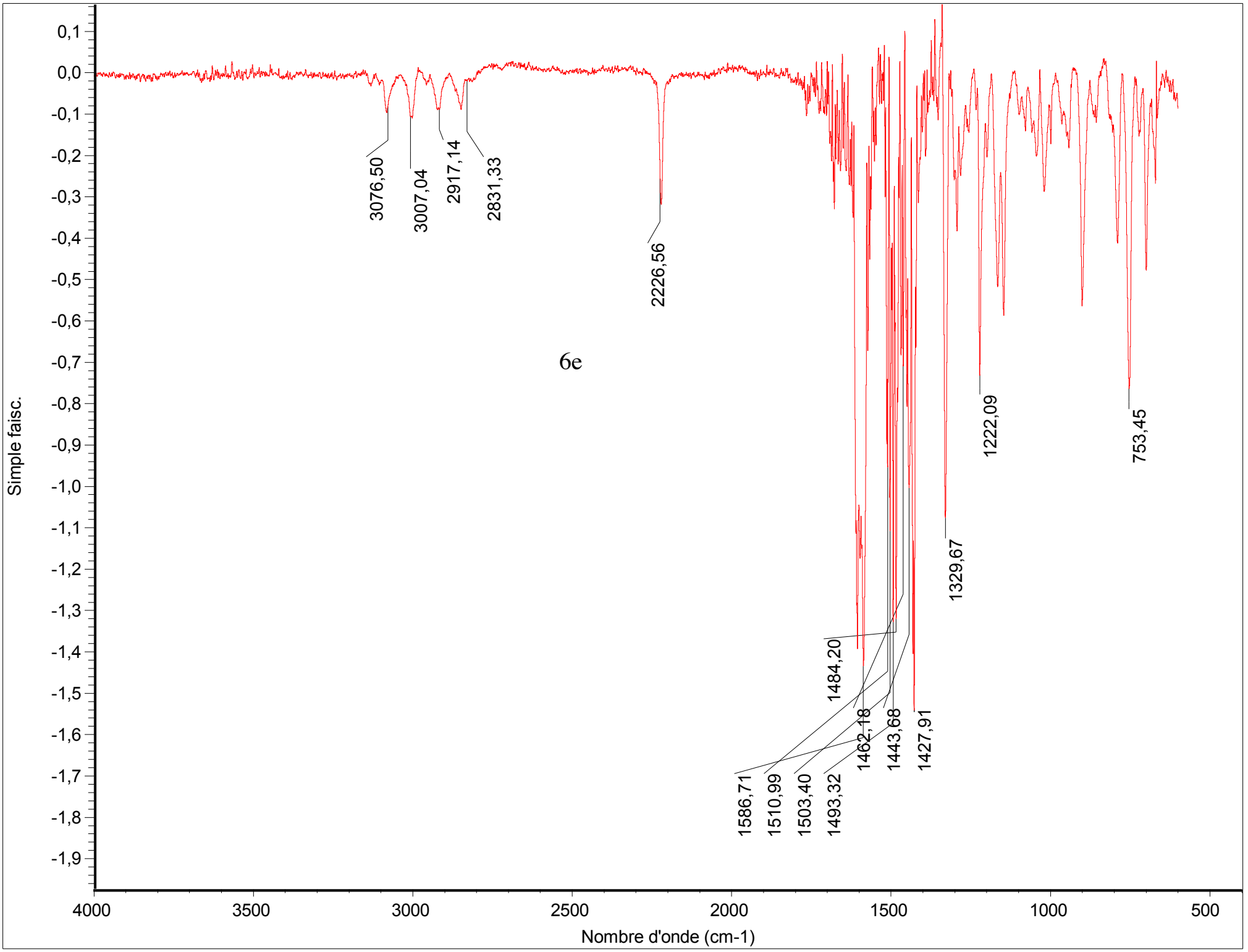

7.5241
7.5006
7.4086
7.3832
7.2380
7.2304
7.2089
7.1976
7.1741
7.1689
7.1545
7.1310
7.1264
7.1034
7.0825
3.7361
2.3140
N
N
CH3
6d
1.00
1.04
7.10
2.01
3.15
f1 (ppm)

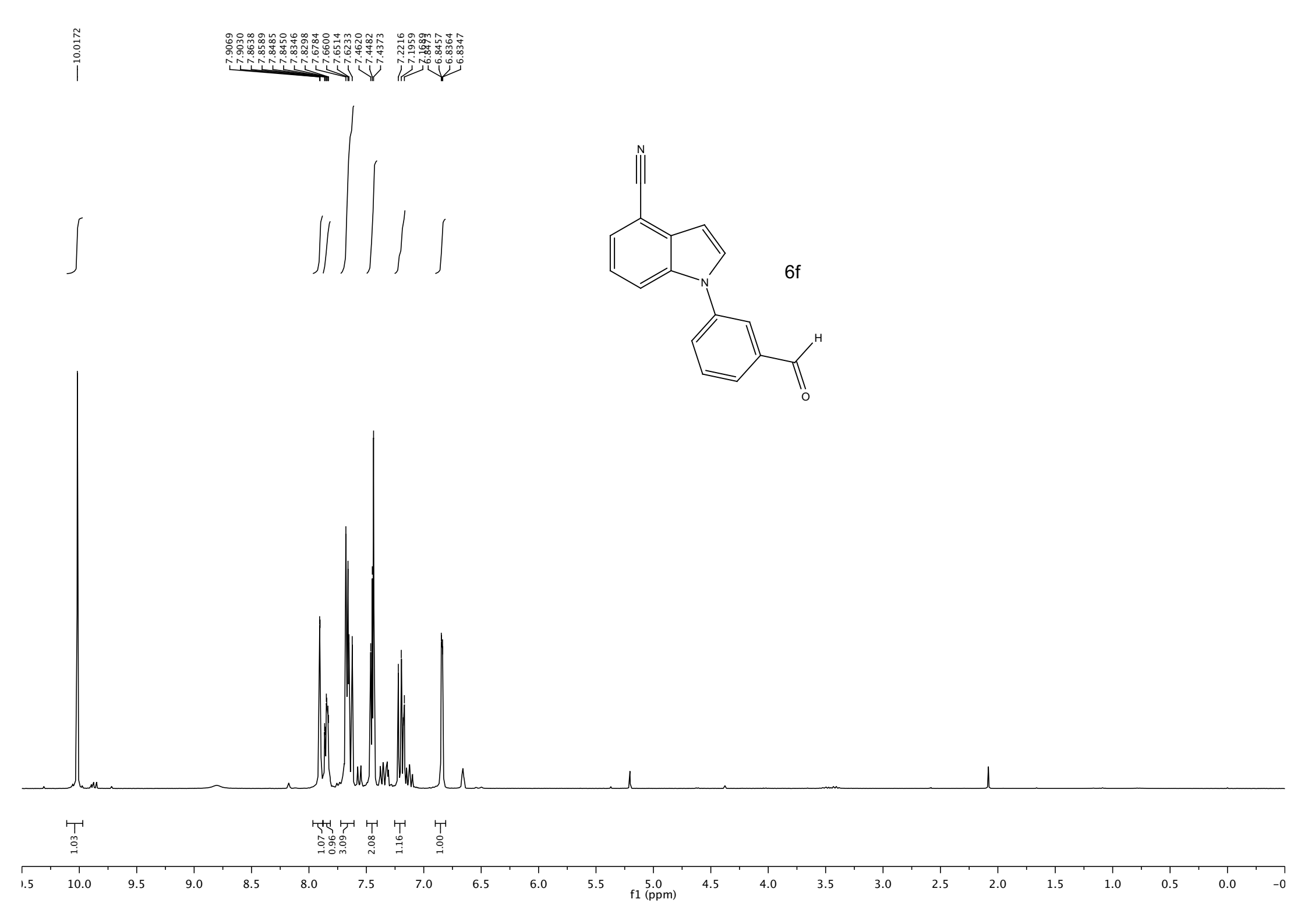

136.9150
136.6721
136.5205
130.3463
127.1750
126.6757
124.3912
123.2384
120.7161
118.4531
118.1105
111.0665
105.3737
21.1479
14.4326
N
N
CH3
6d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

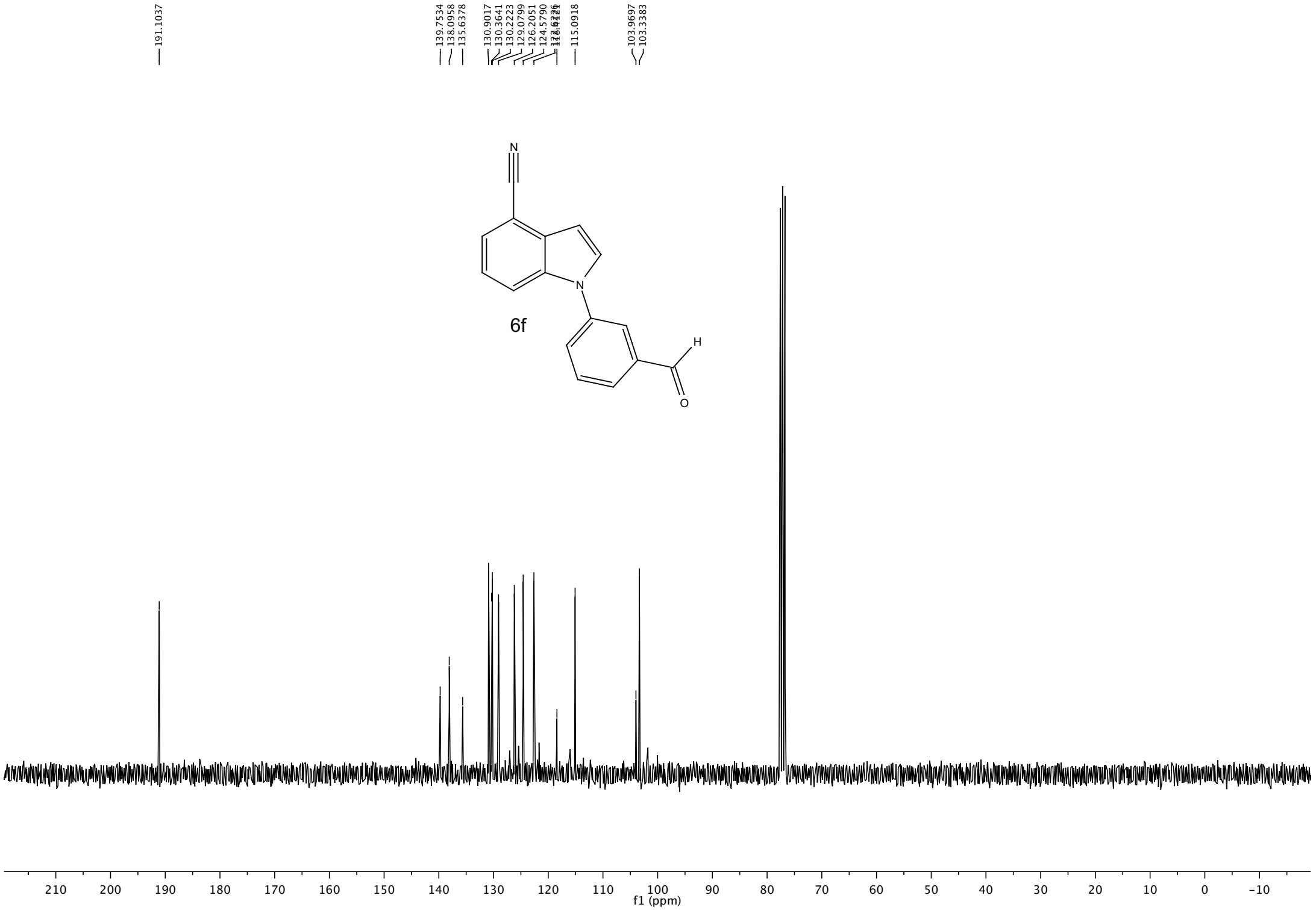

6d
3039,73
2917,14
2855,85
2251,08
1646,31
1611,08
1518,83
1513,80
1460,83
1453,73
1366,72
1223,39
743,30
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
4000
3500
3000
2500
2000
1500
1000
500

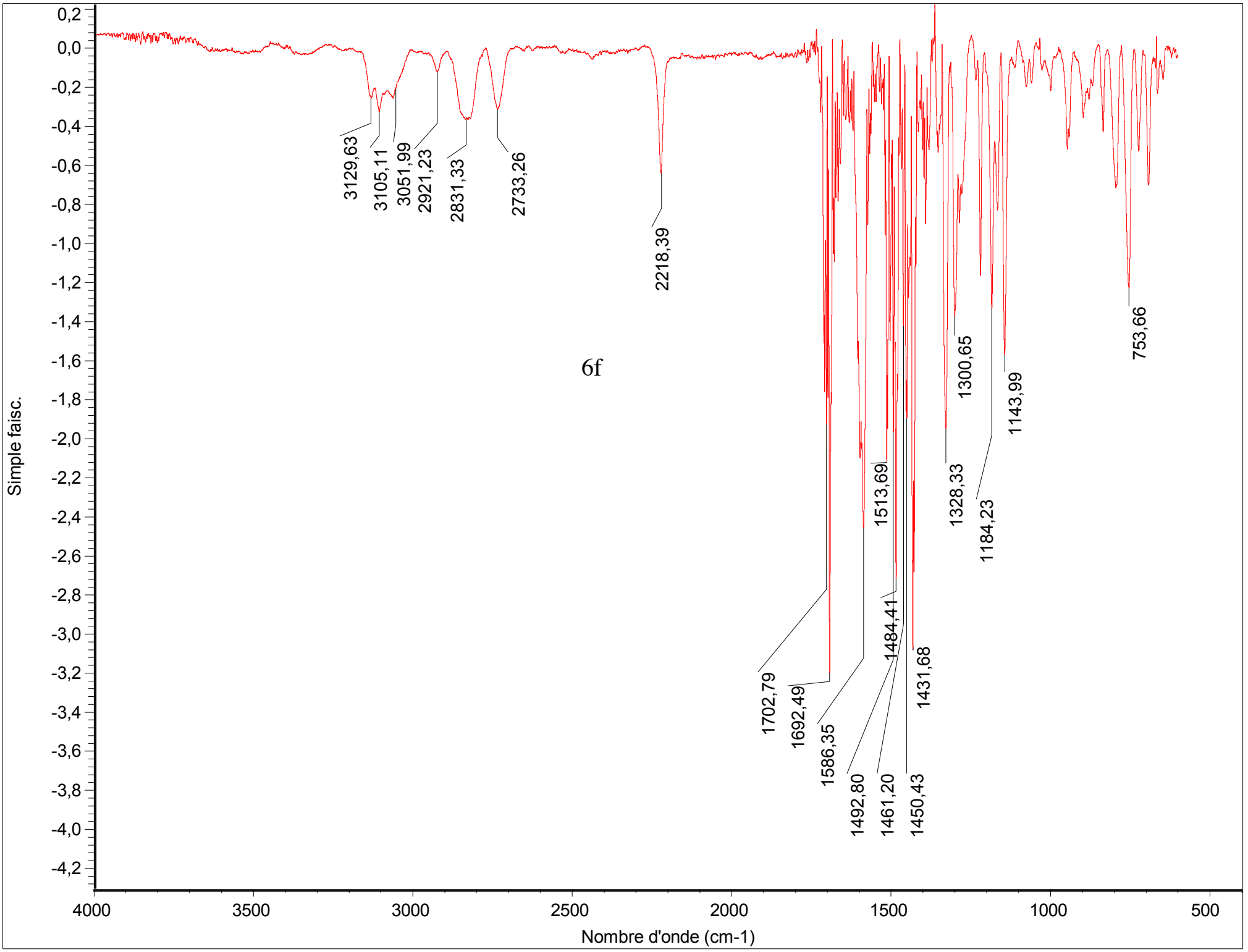

7.6179
7.5899
7.4272
7.4026
7.3846
7.3737
7.3428
7.3169
7.2911
7.1646
7.1569
7.1394
7.1374
7.1121
7.0538
7.0479
7.0347
7.0084
6.7901
6.7797
1.9301
1.9131
1.9019
1.8853
1.8686
1.8575
1.8402
0.9927
0.9769
0.9706
0.9553
0.9488
0.9427
0.9277
0.6958
0.6801
0.6747
0.6638
0.6582
0.6419
N
N
6e
1.08
1.00
0.93
0.99
2.03
1.79
0.75
1.00
1.77
1.79
f1 (ppm)

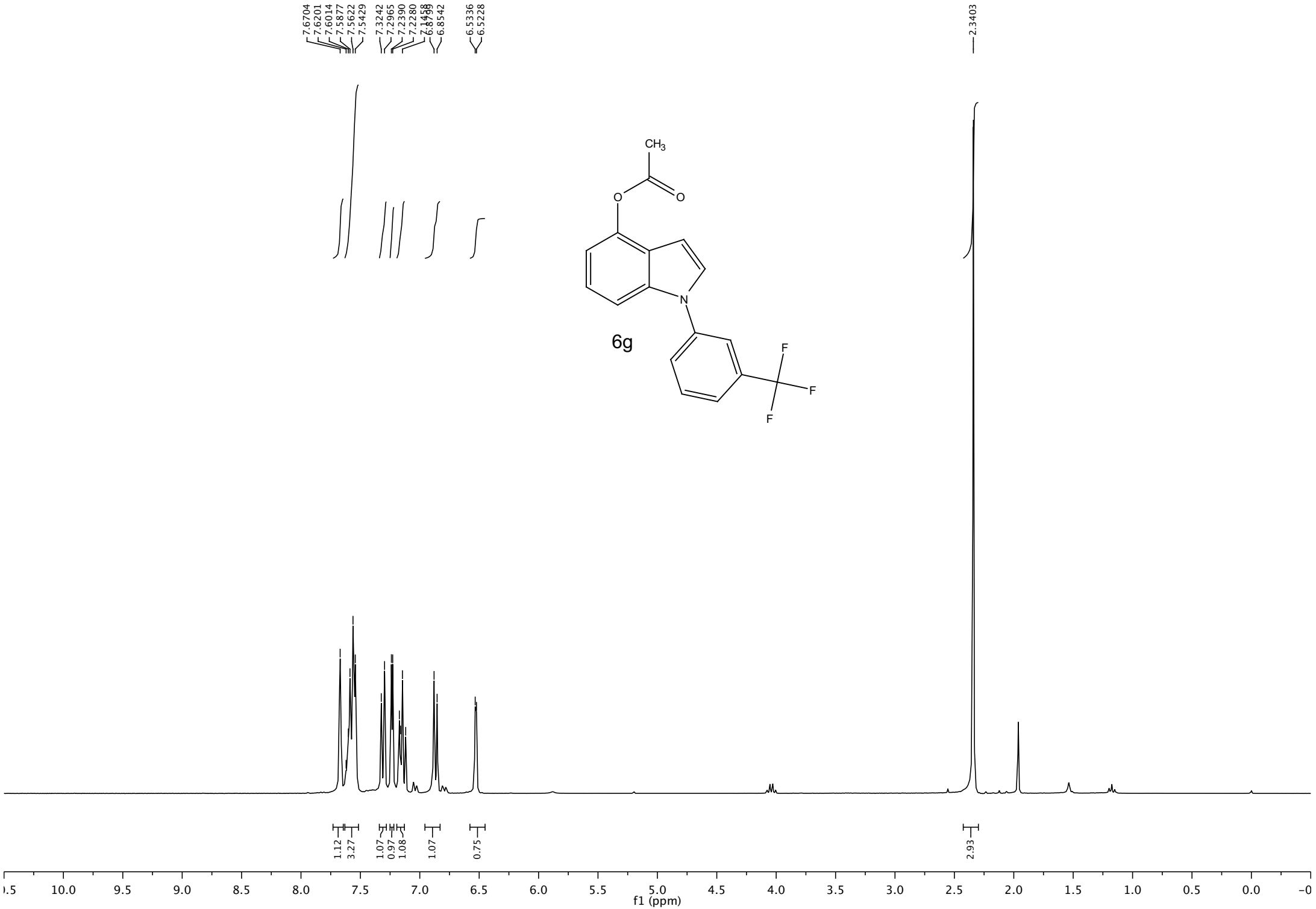

146.5758
138.8278
135.8822
130.7832
130.5416
129.7749
125.7454
124.8685
122.2438
122.0156
121.7862
118.6915
115.4782
103.5783
102.2220
15.5580
9.8335
9.5384
N
N
6e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

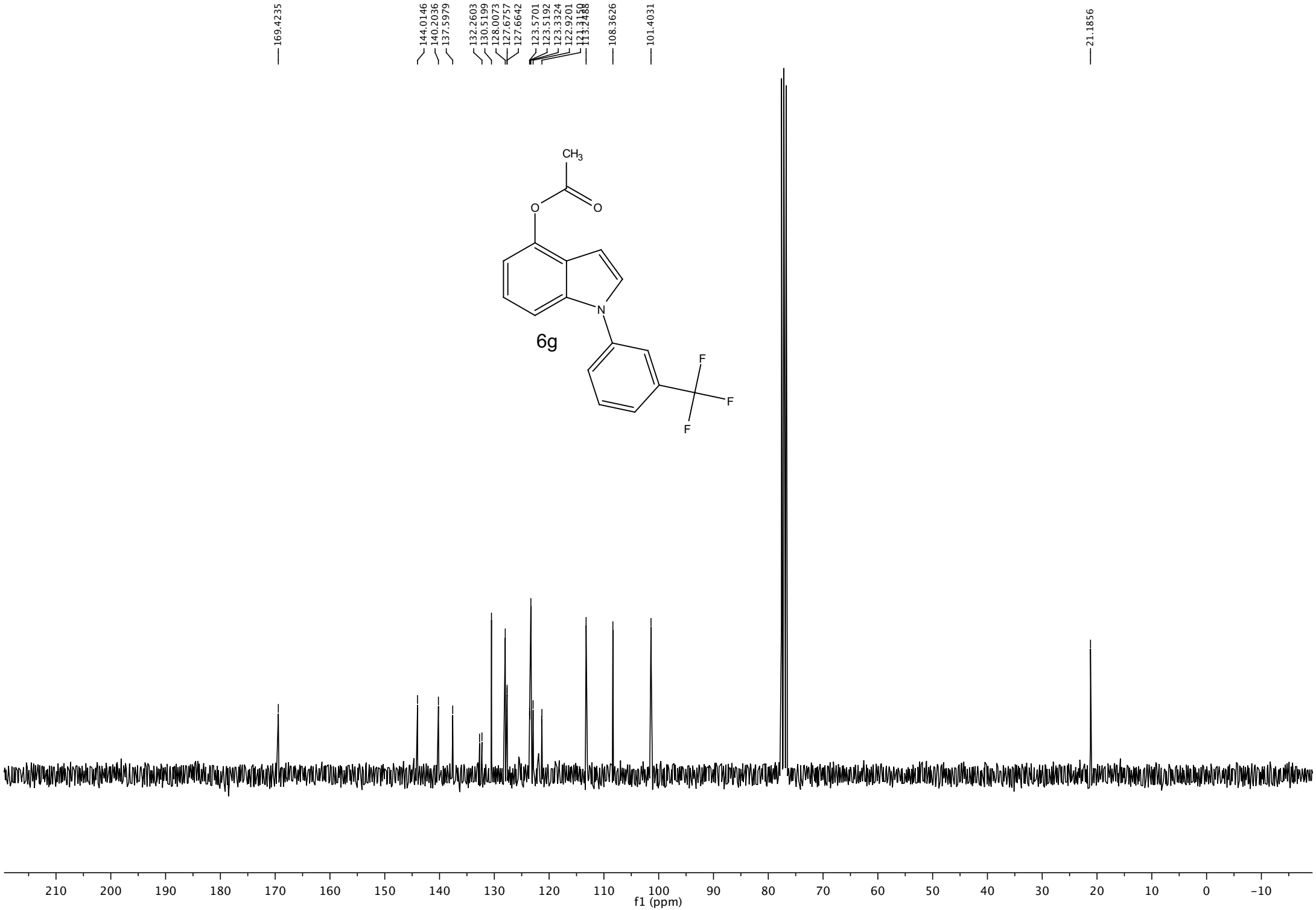

6e
Simple faisc.
Nombre d'onde (cm-1)
0,1
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
-1,3
-1,4
-1,5
-1,6
-1,7
-1,8
-1,9
4000
3500
3000
2500
2000
1500
1000
500
3076,50
3007,04
2917,14
2831,33
2226,56
1586,71
1510,99
1503,40
1493,32
1484,20
1462,18
1443,68
1427,91
1329,67
1222,09
753,45

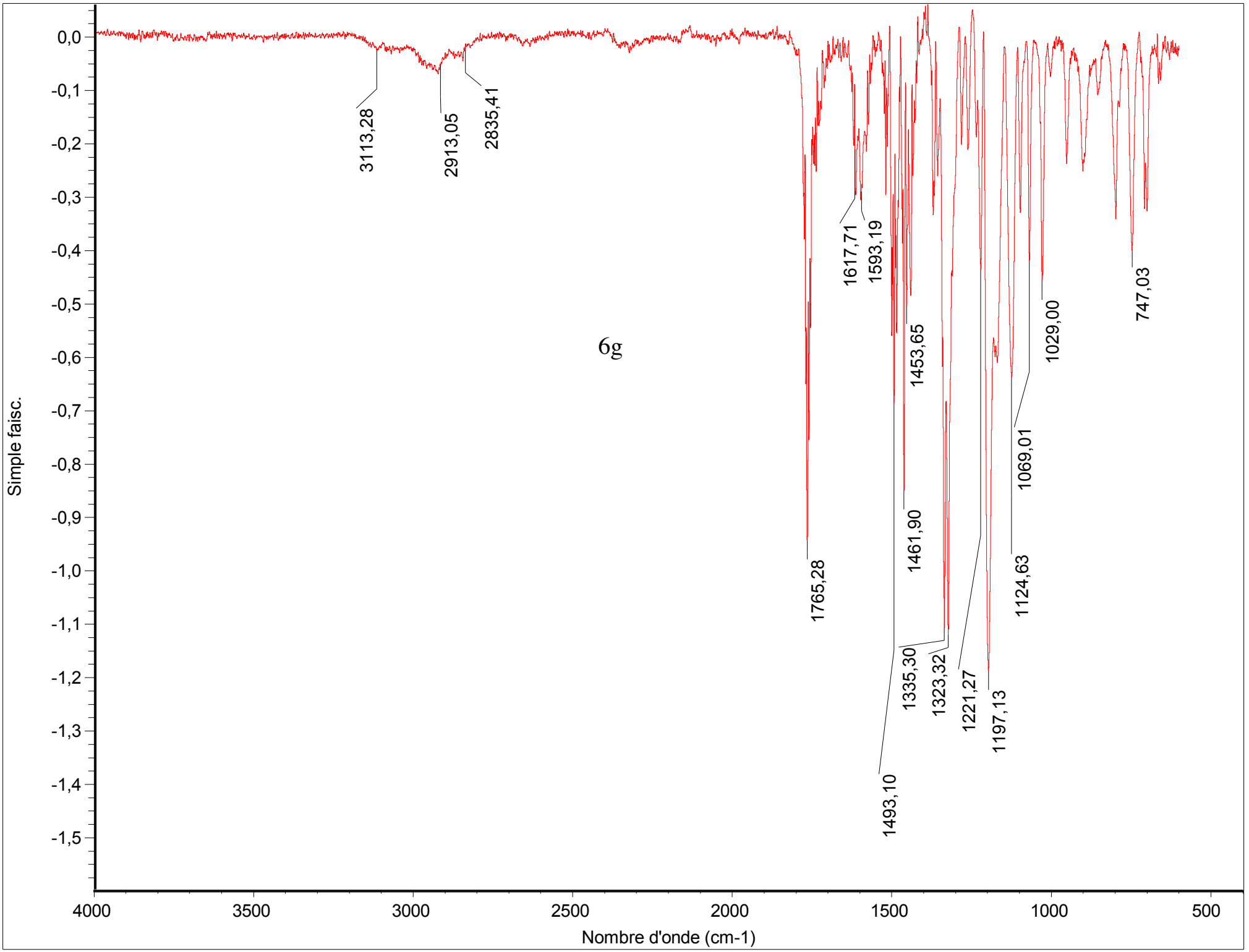

10.0172
7.9069
7.9030
7.8638
7.8589
7.8485
7.8450
7.8346
7.8298
7.6784
7.6600
7.6514
7.6233
7.4620
7.4482
7.4373
7.2216
7.1959
7.1689
6.8473
6.8457
6.8364
6.8347
N
N
H
O
6f
1.03
1.07
0.96
3.09
2.08
1.16
1.00
f1 (ppm)

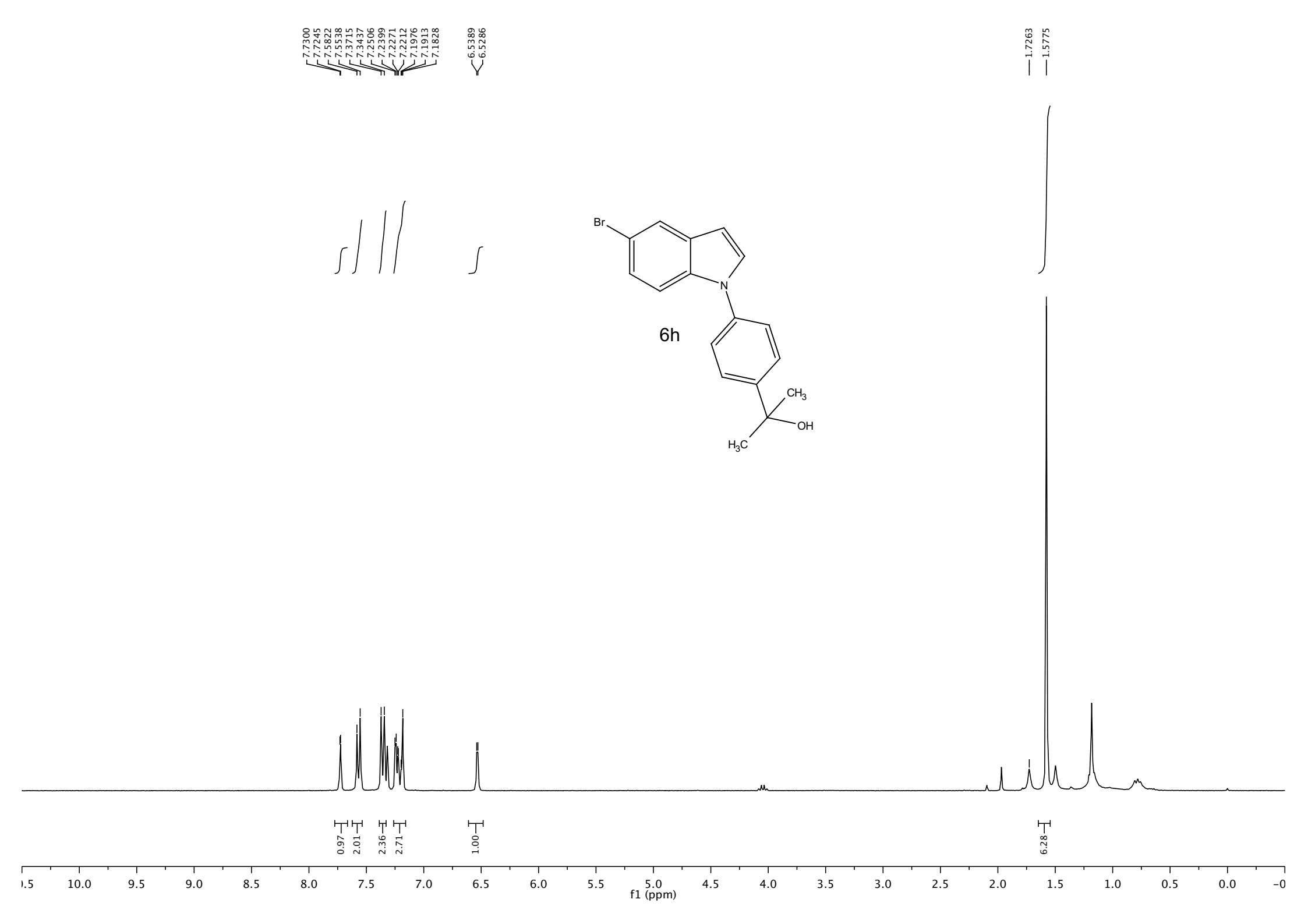

191.1037
139.7534
138.0958
135.6378
130.9017
130.3641
130.2223
129.0799
126.2051
124.5790
115.0918
103.9697
103.3383
N
N
H
O
6f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

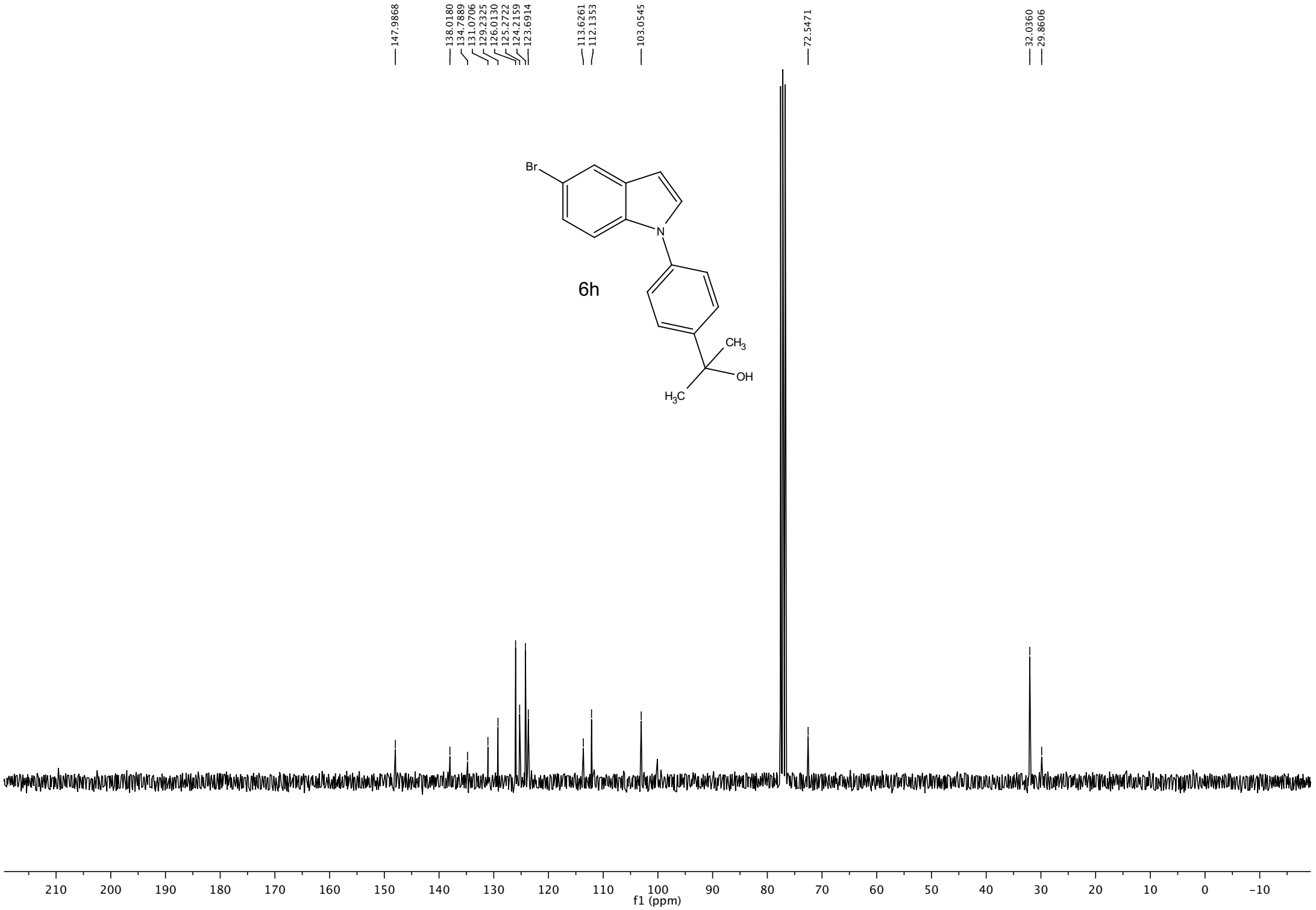

6f
Simple faisc.
Nombre d'onde (cm-1)
0,2
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
-3,8
-4,0
-4,2
4000
3500
3000
2500
2000
1500
1000
500
3129,63
3105,11
3051,99
2921,23
2831,33
2733,26
2218,39
1702,79
1692,49
1586,35
1513,69
1492,80
1484,41
1461,20
1450,43
1431,68
1328,33
1300,65
1184,23
1143,99
753,66

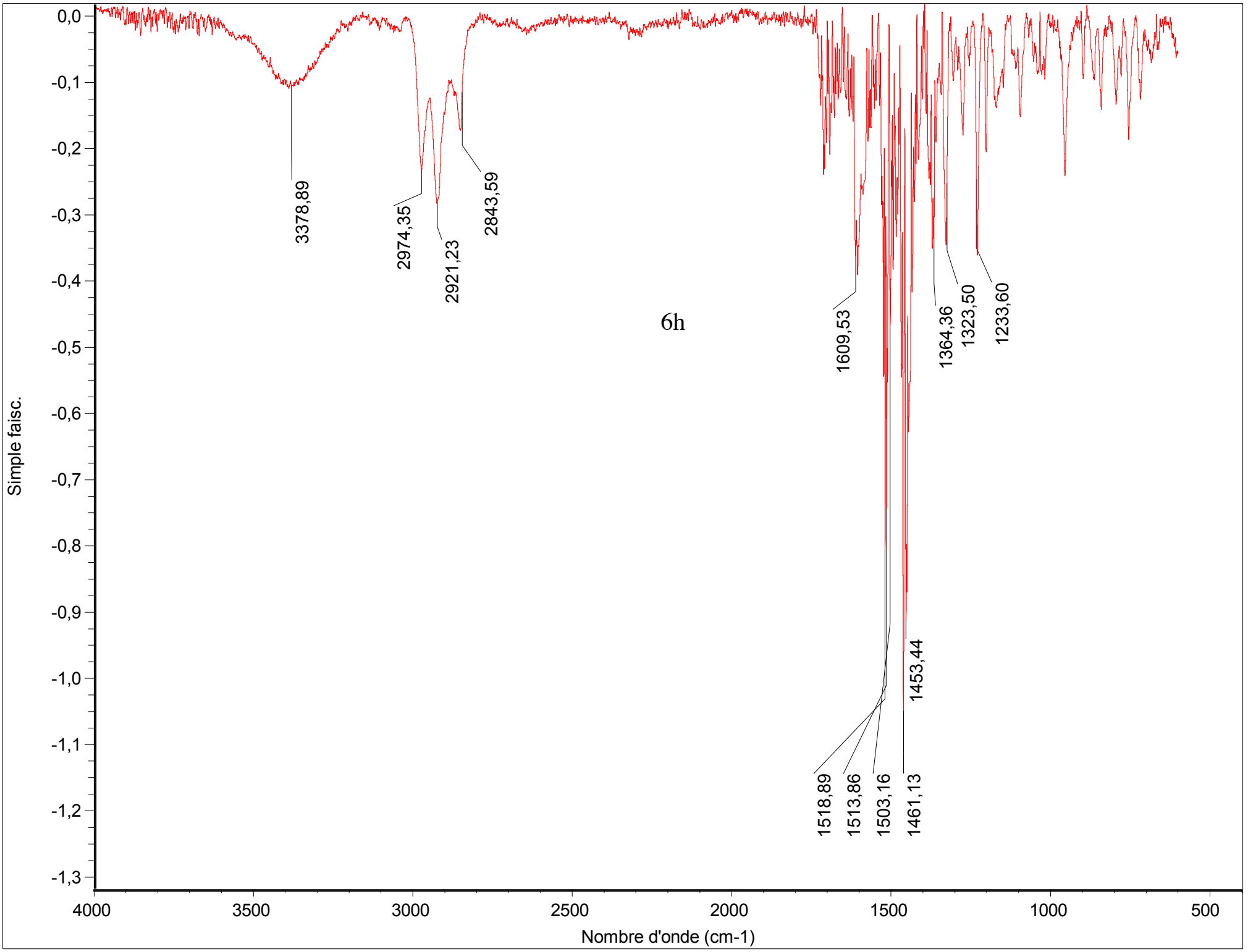

7.6704
7.6201
7.6014
7.5877
7.5622
7.5429
7.3242
7.2965
7.2390
7.2280
7.1458
6.8799
6.8542
6.5336
6.5228
2.3403
CH3
O
O
N
F
F
F
6g
1.12
3.27
1.07
0.97
1.08
1.07
0.75
2.93
f1 (ppm)

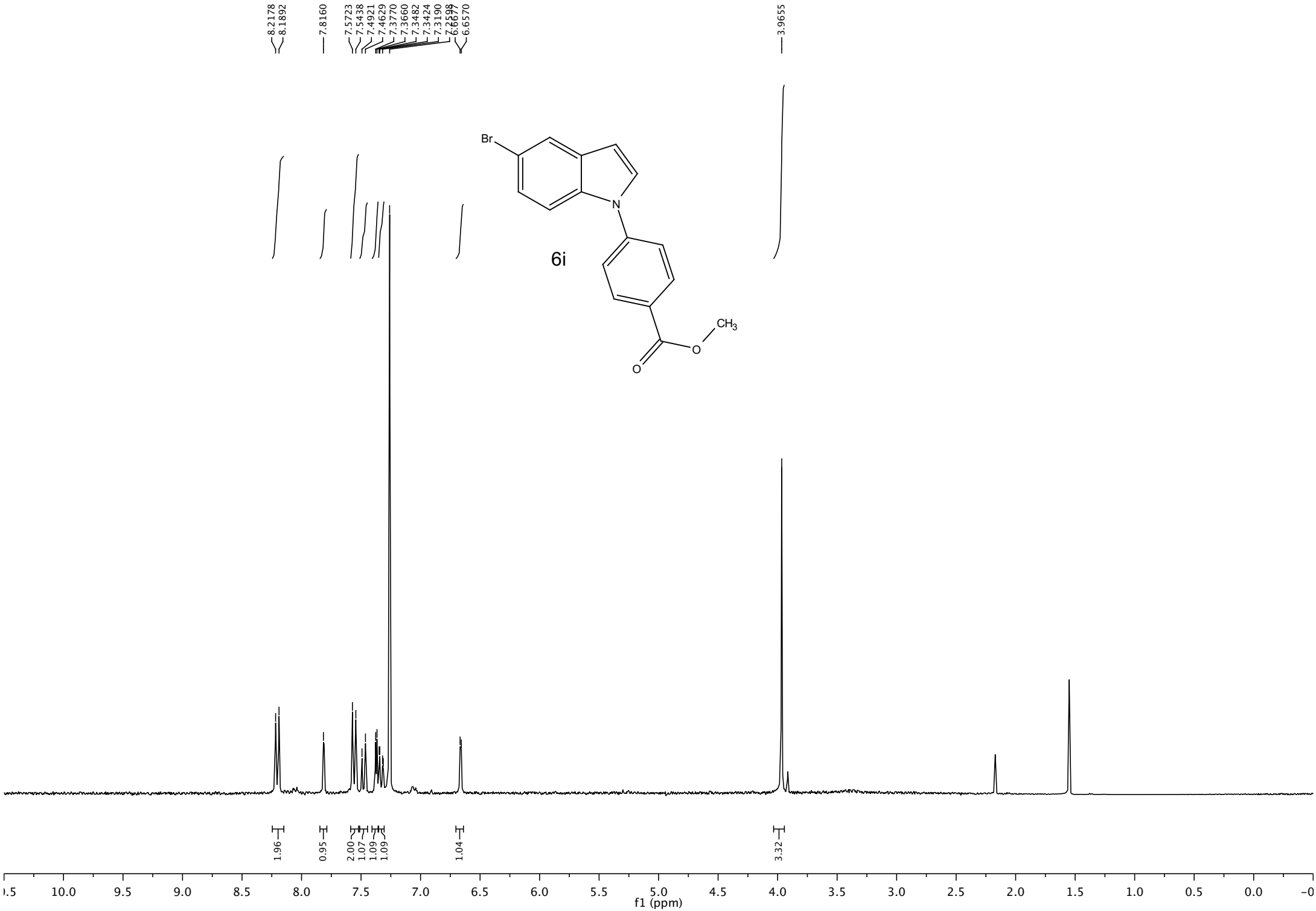

169.4235
144.0146
140.2036
137.5979
132.2603
130.5199
128.0073
127.6757
127.6642
123.5701
123.5192
123.3324
122.9201
121.3150
113.2488
108.3626
101.4031
21.1856
CH3
O
O
N
F
F
F
6g
f1 (ppm)

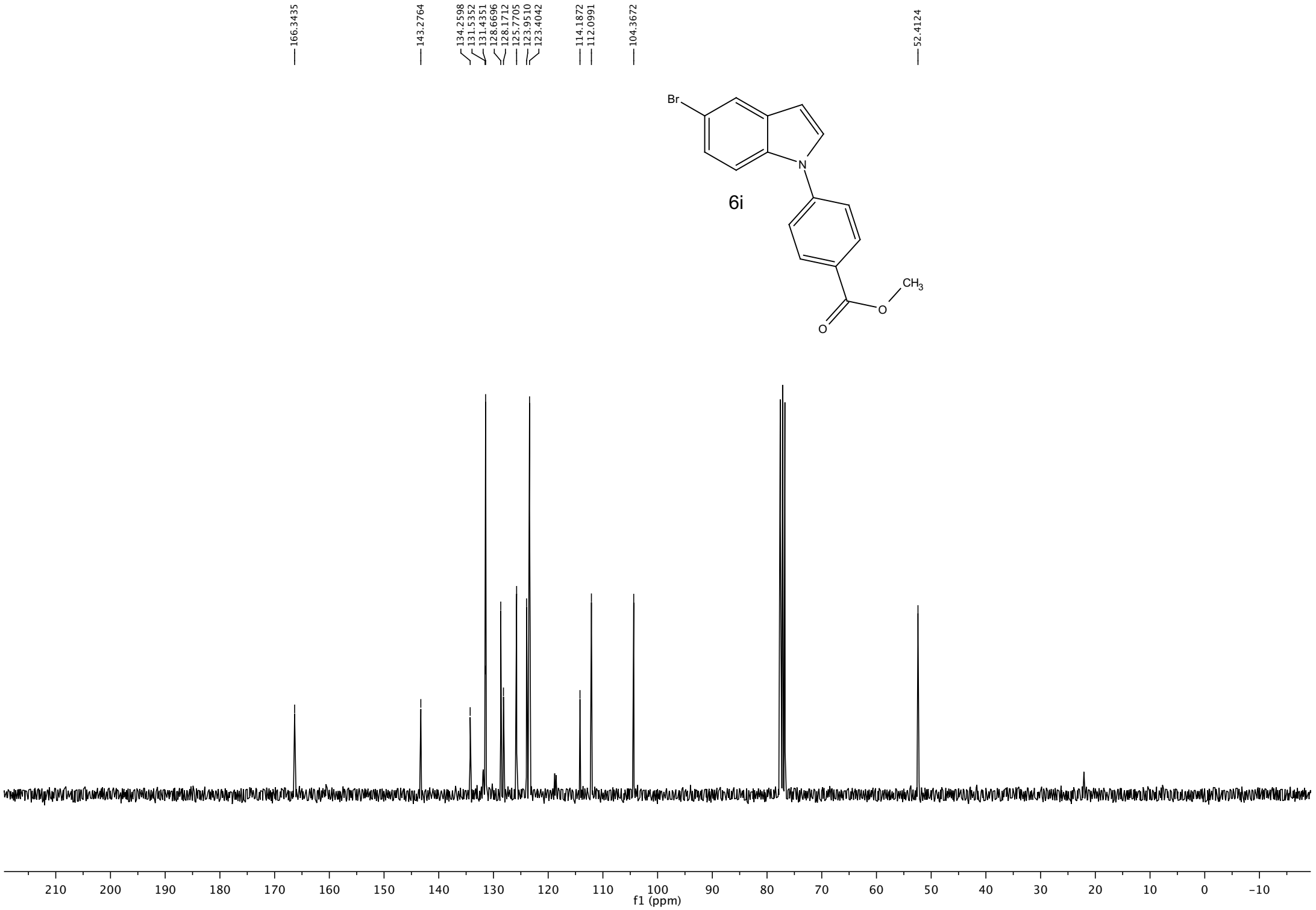

6g
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
-1,3
-1,4
-1,5
4000
3500
3000
2500
2000
1500
1000
500
3113,28
2913,05
2835,41
1765,28
1617,71
1593,19
1493,10
1461,90
1453,65
1335,30
1323,32
1221,27
1197,13
1124,63
1069,01
1029,00
747,03

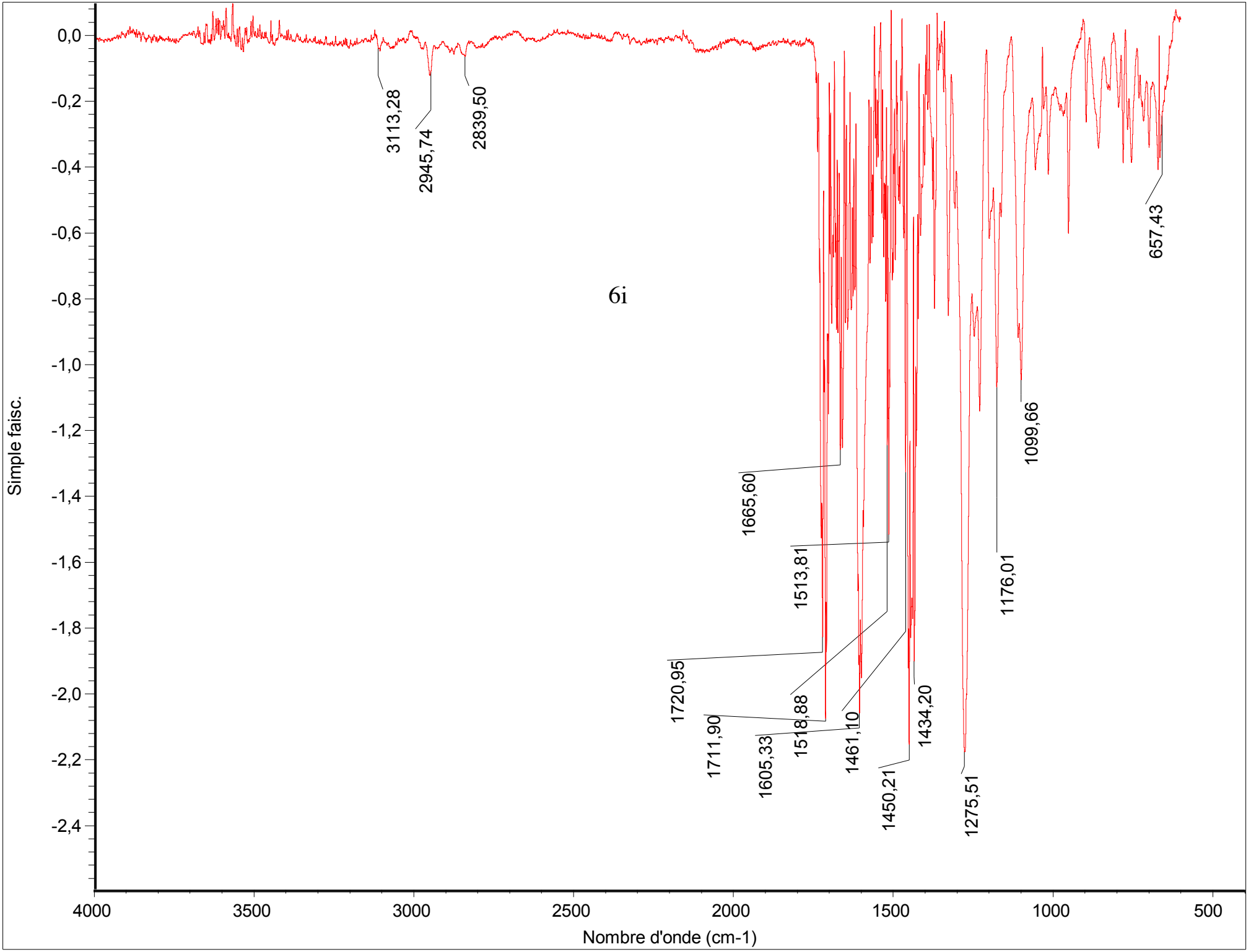

7.7300
7.7245
7.5822
7.5538
7.3715
7.3437
7.2506
7.2399
7.2271
7.2212
7.1976
7.1913
7.1828
6.5389
6.5286
1.7263
1.5775
Br
N
6h
CH3
OH
H3C
0.97
2.01
2.36
2.71
1.00
6.28
f1 (ppm)

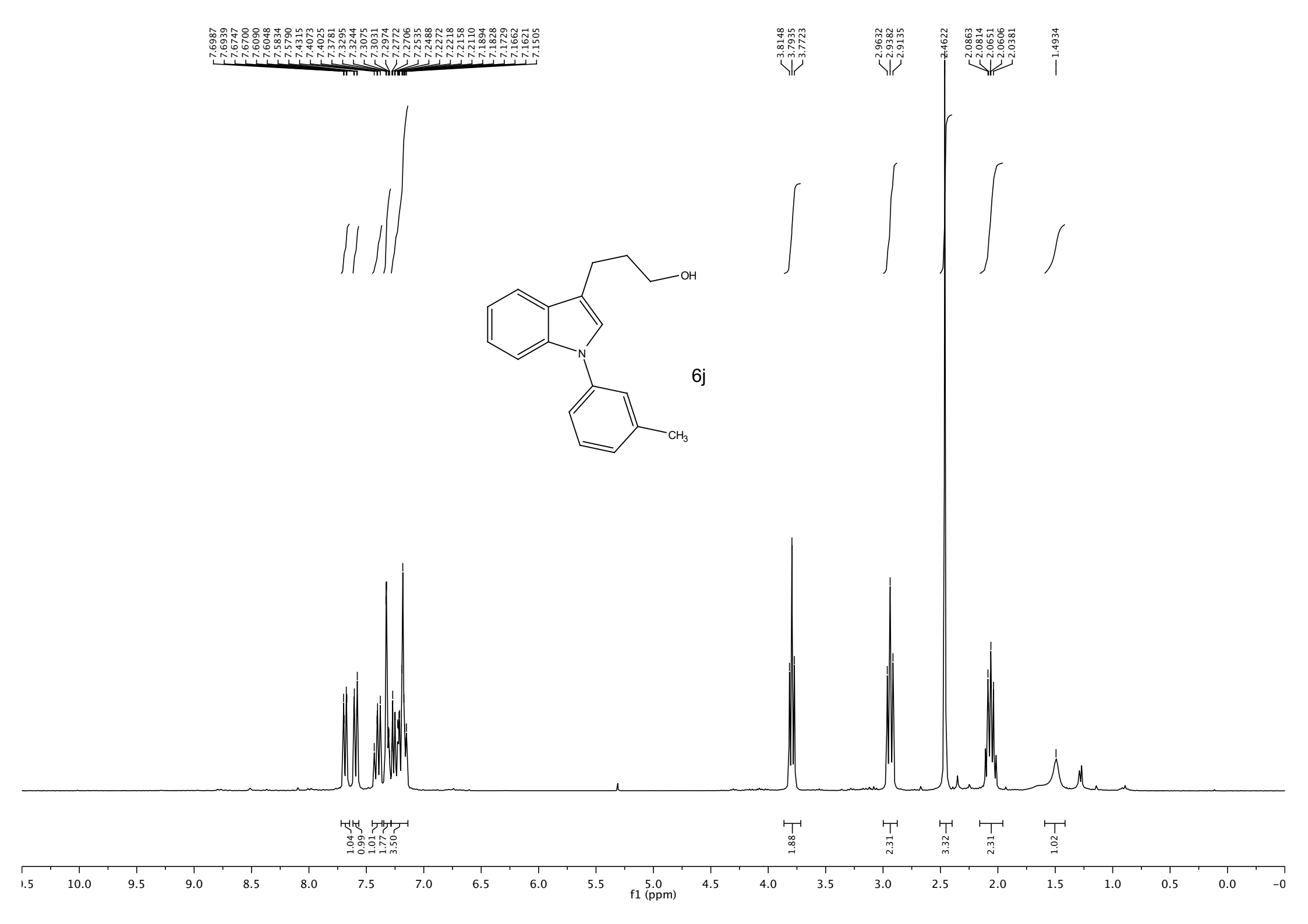

147.9868
138.0180
134.7889
131.0706
129.2325
126.0130
125.2722
124.2159
123.6914
113.6261
112.1353
103.0545
72.5471
32.0360
29.8606
Br
N
6h
CH3
OH
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

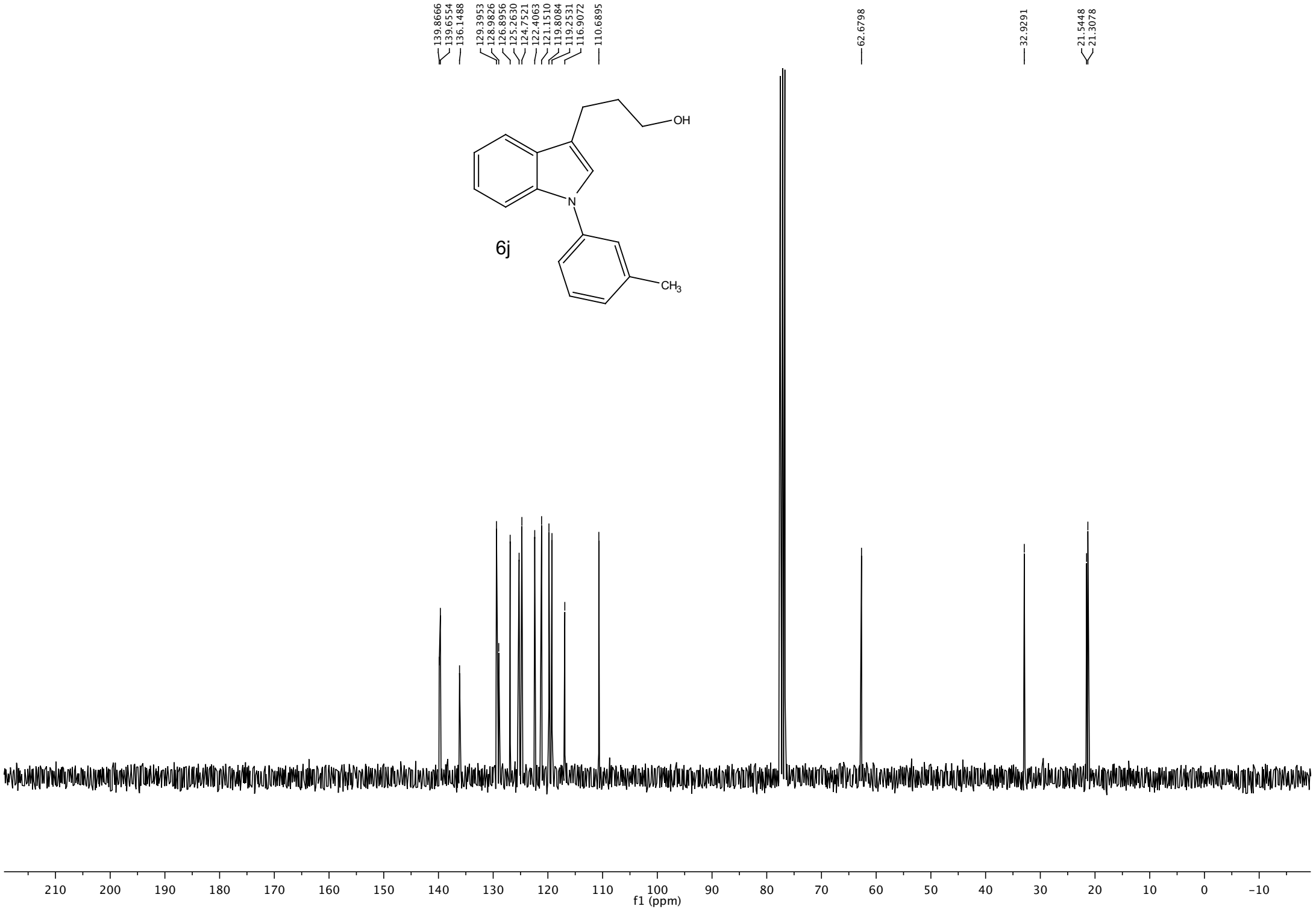

6h
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
-1,3
4000
3500
3000
2500
2000
1500
1000
500
3378,89
2974,35
2921,23
2843,59
1609,53
1364,36
1323,50
1233,60
1453,44
1518,89
1513,86
1503,16
1461,13

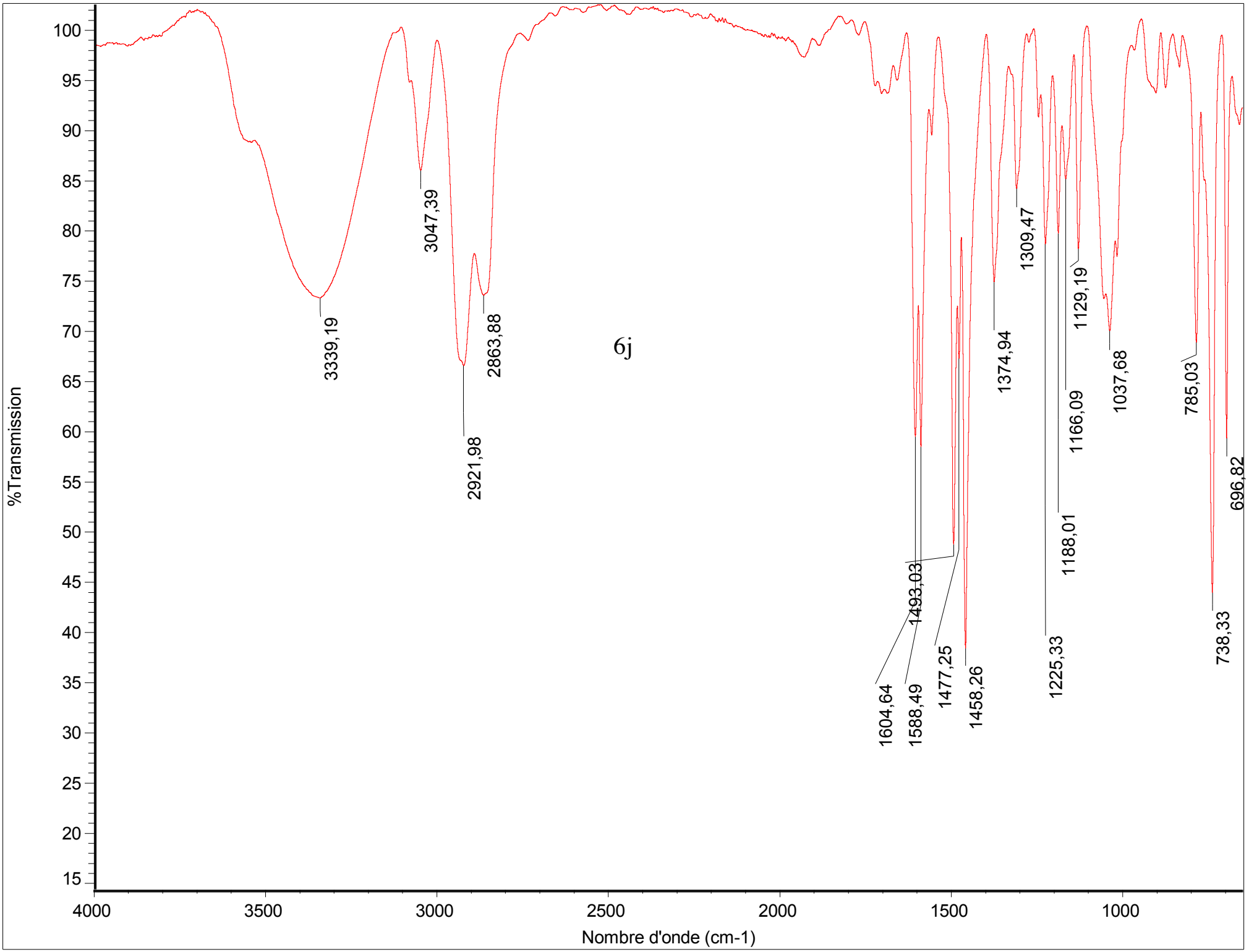

8.2178
8.1892
7.8160
7.5723
7.5438
7.4921
7.4629
7.3770
7.3660
7.3482
7.3424
7.3190
6.6677
6.6570
3.9655
Br
N
6i
CH3
O
O
1.96
0.95
2.00
1.07
1.09
1.09
1.04
3.32
f1 (ppm)

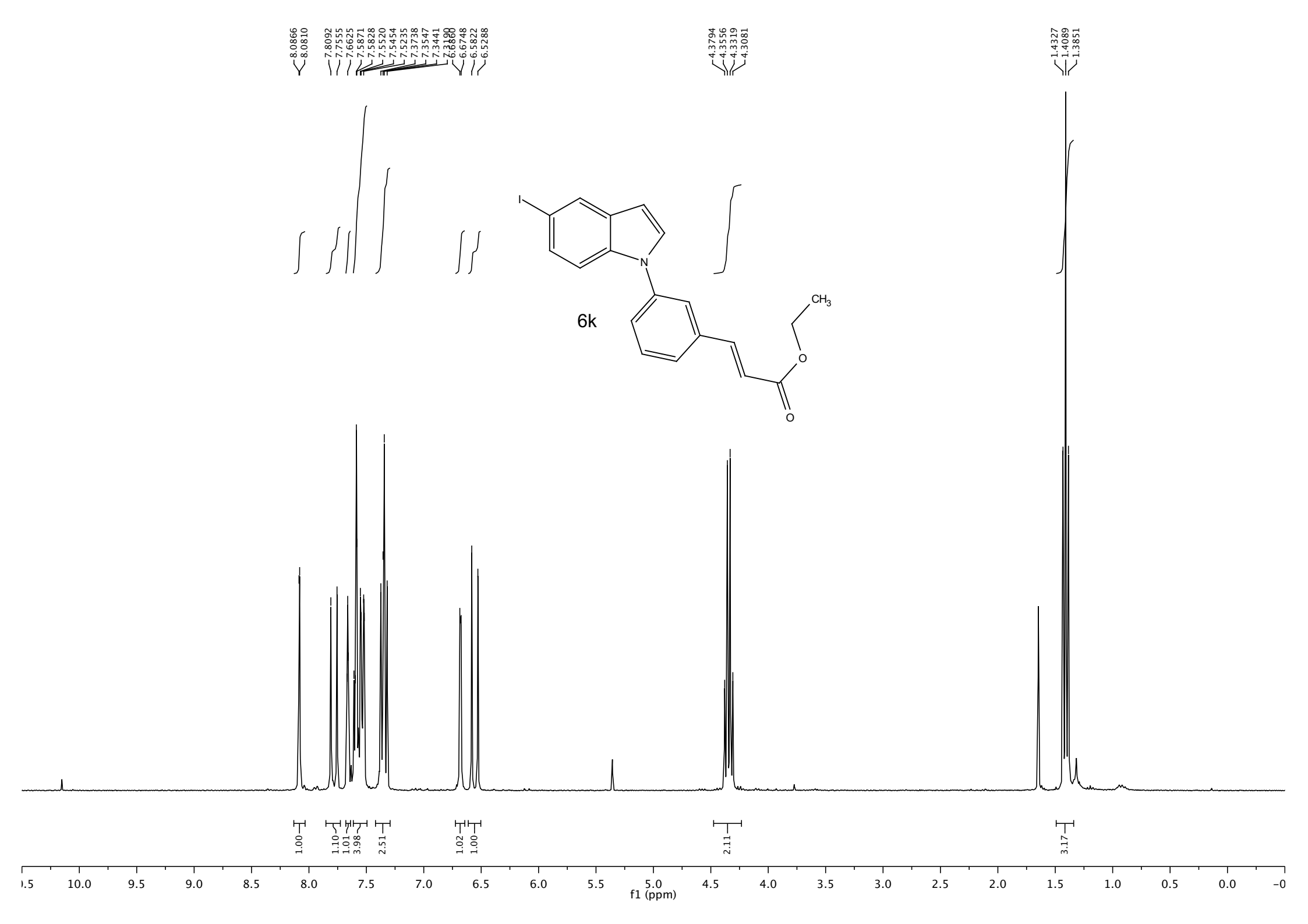

166.3435
143.2764
134.2598
131.5352
131.4351
128.6696
128.1712
125.7705
123.9510
123.4042
114.1872
112.0991
104.3672
52.4124
Br
N
6i
CH3
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

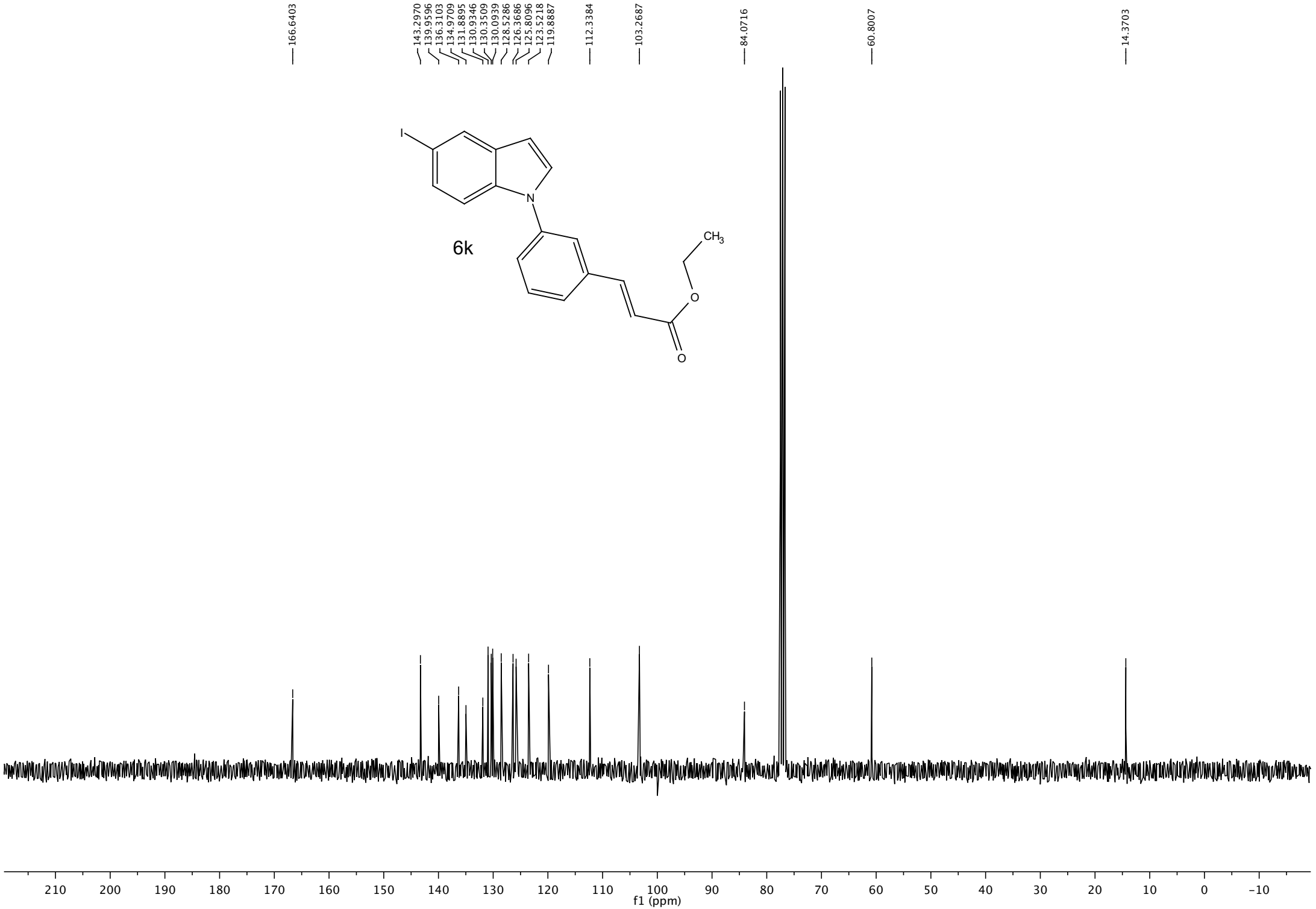

6i
Simple faisc.
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
3113,28
2945,74
2839,50
1665,60
1513,81
1720,95
1711,90
1605,33
1518,88
1461,10
1434,20
1450,21
1275,51
1176,01
1099,66
657,43
4000
3500
3000
2500
2000
1500
1000
500
Nombre d'onde (cm-1)

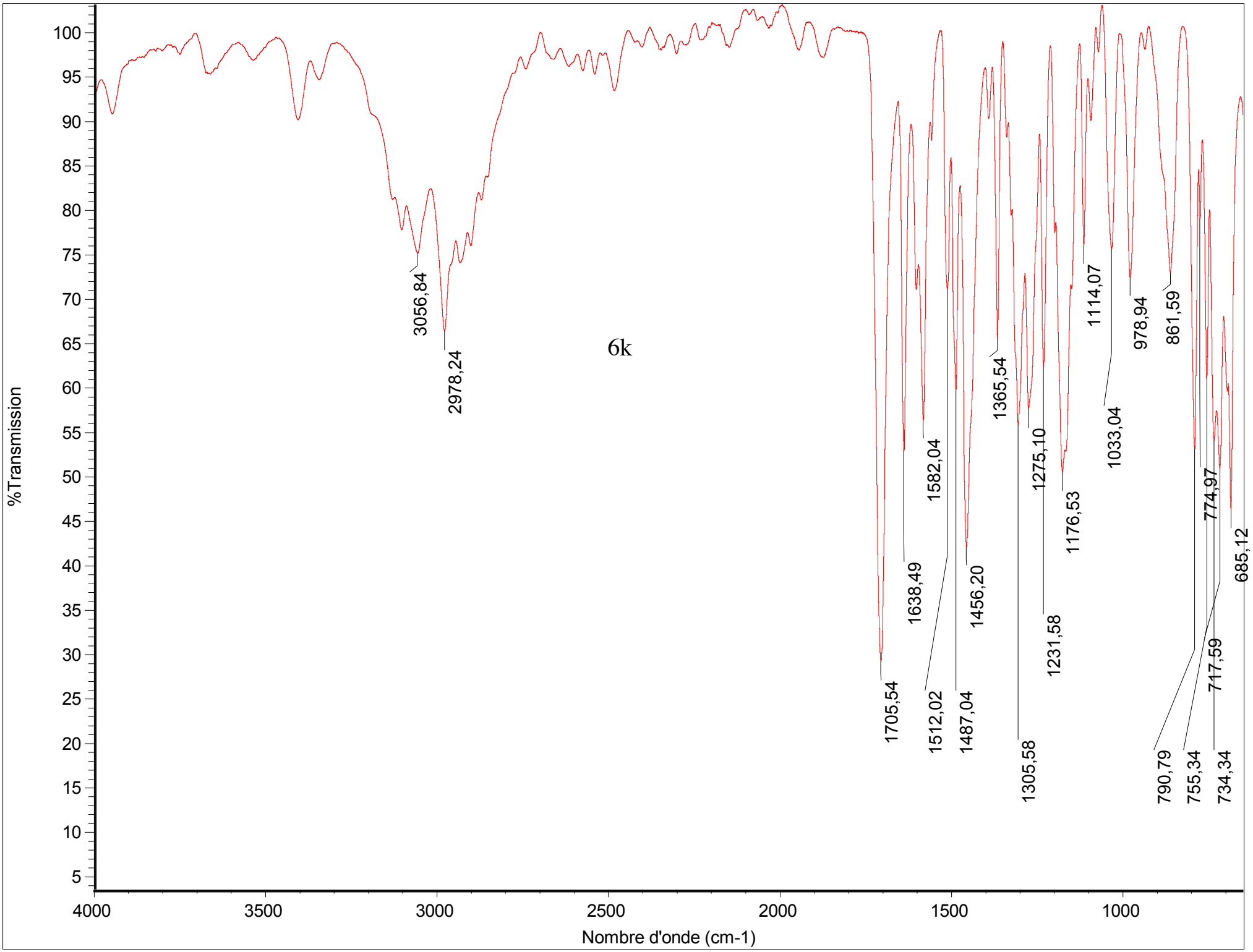

7.6987
7.6939
7.6747
7.6700
7.6090
7.6048
7.5834
7.5790
7.4315
7.4073
7.4025
7.3781
7.3295
7.3244
7.3075
7.3031
7.2974
7.2772
7.2706
7.2535
7.2488
7.2272
7.2218
7.2158
7.2110
7.1894
7.1828
7.1729
7.1662
7.1621
7.1505
3.8148
3.7935
3.7723
2.9632
2.9382
2.9135
2.4622
2.0863
2.0814
2.0651
2.0606
2.0381
1.4934
OH
N
CH3
6j
1.04
0.99
1.01
1.77
3.50
1.88
2.31
3.32
2.31
1.02
f1 (ppm)

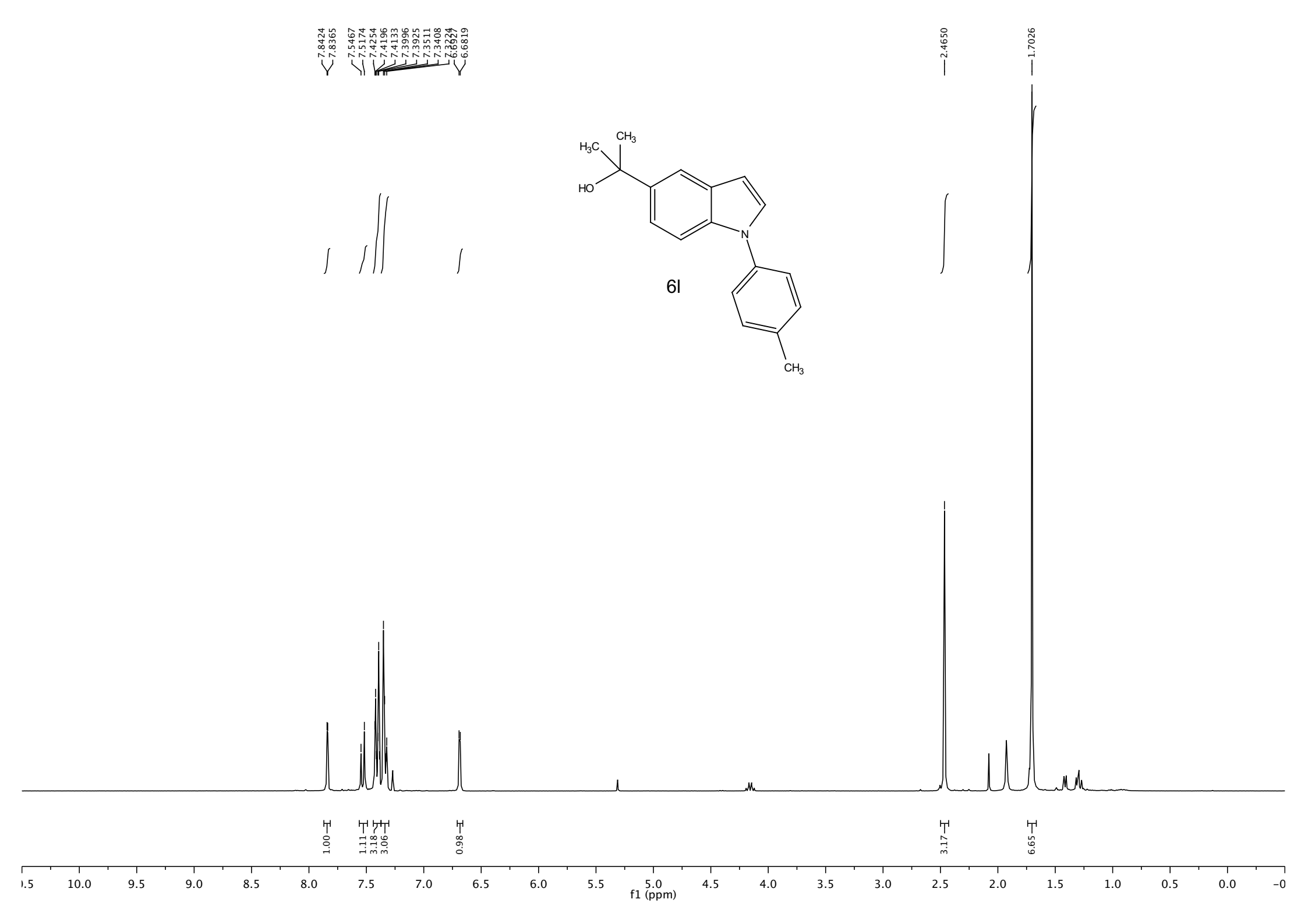

139.8666
139.6554
136.1488
129.3953
128.9826
126.8956
125.2630
124.7521
122.4063
121.1510
119.8084
119.2531
116.9072
110.6895
62.6798
32.9291
21.5448
21.3078
OH
N
CH3
6j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

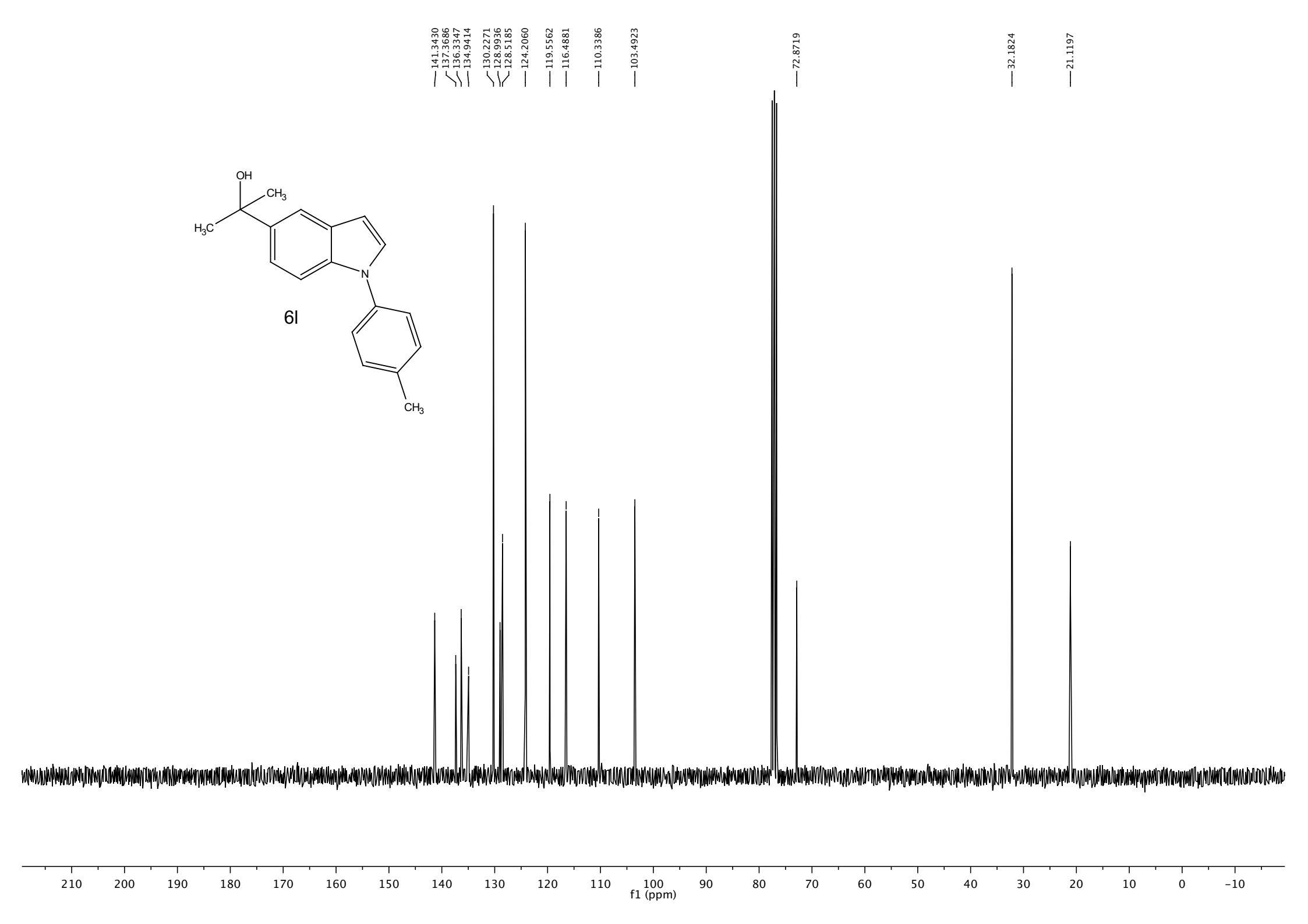

6j
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
4000
3500
3000
2500
2000
1500
1000
3339,19
3047,39
2921,98
2863,88
1604,64
1588,49
1493,03
1477,25
1458,26
1374,94
1309,47
1225,33
1188,01
1166,09
1129,19
1037,68
785,03
738,33
696,82

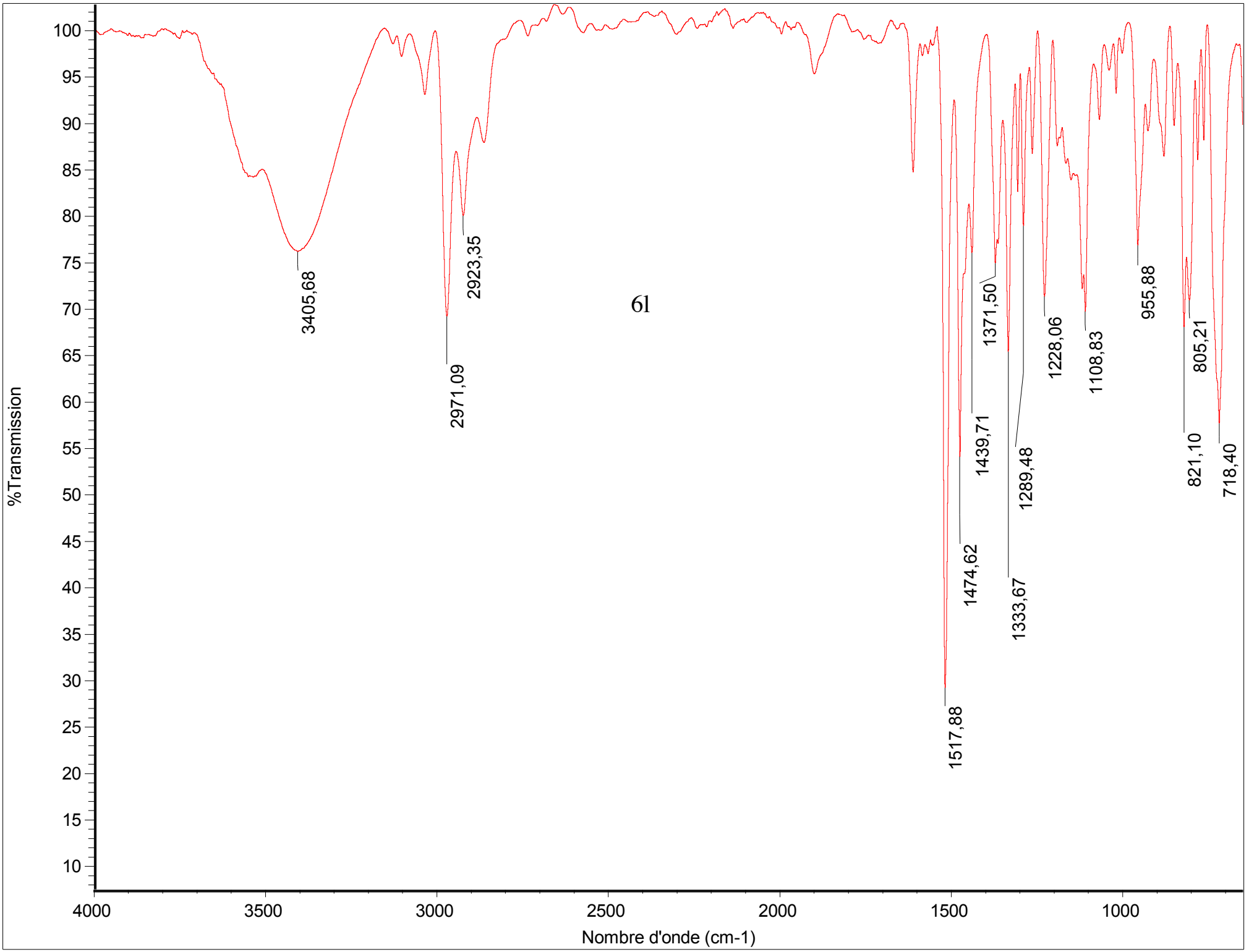

8.0866
8.0810
7.8092
7.7555
7.6625
7.5871
7.5828
7.5520
7.5454
7.5235
7.3738
7.3547
7.3441
7.3190
6.6860
6.6748
6.5822
6.5288
4.3794
4.3556
4.3319
4.3081
1.4327
1.4089
1.3851
I
N
CH3
O
O
6k
1.00
1.10
1.01
3.98
2.51
1.02
1.00
2.11
3.17
f1 (ppm)

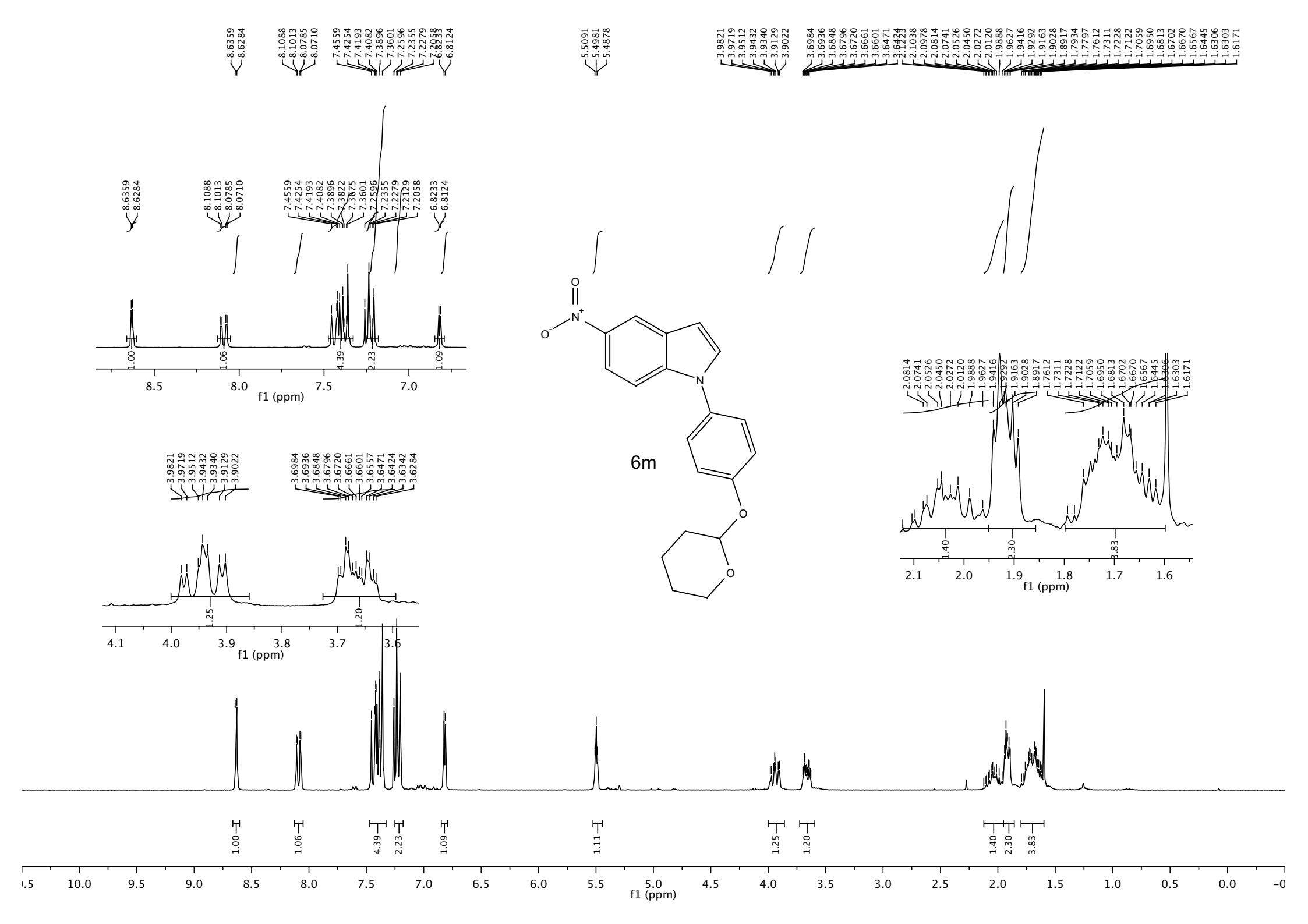

166.6403
143.2970
139.9596
136.3103
134.9709
131.8895
130.9346
130.3509
130.0939
128.5286
126.3686
125.8096
123.5218
119.8887
112.3384
103.2687
84.0716
60.8007
14.3703
I
N
O
O
CH3
6k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

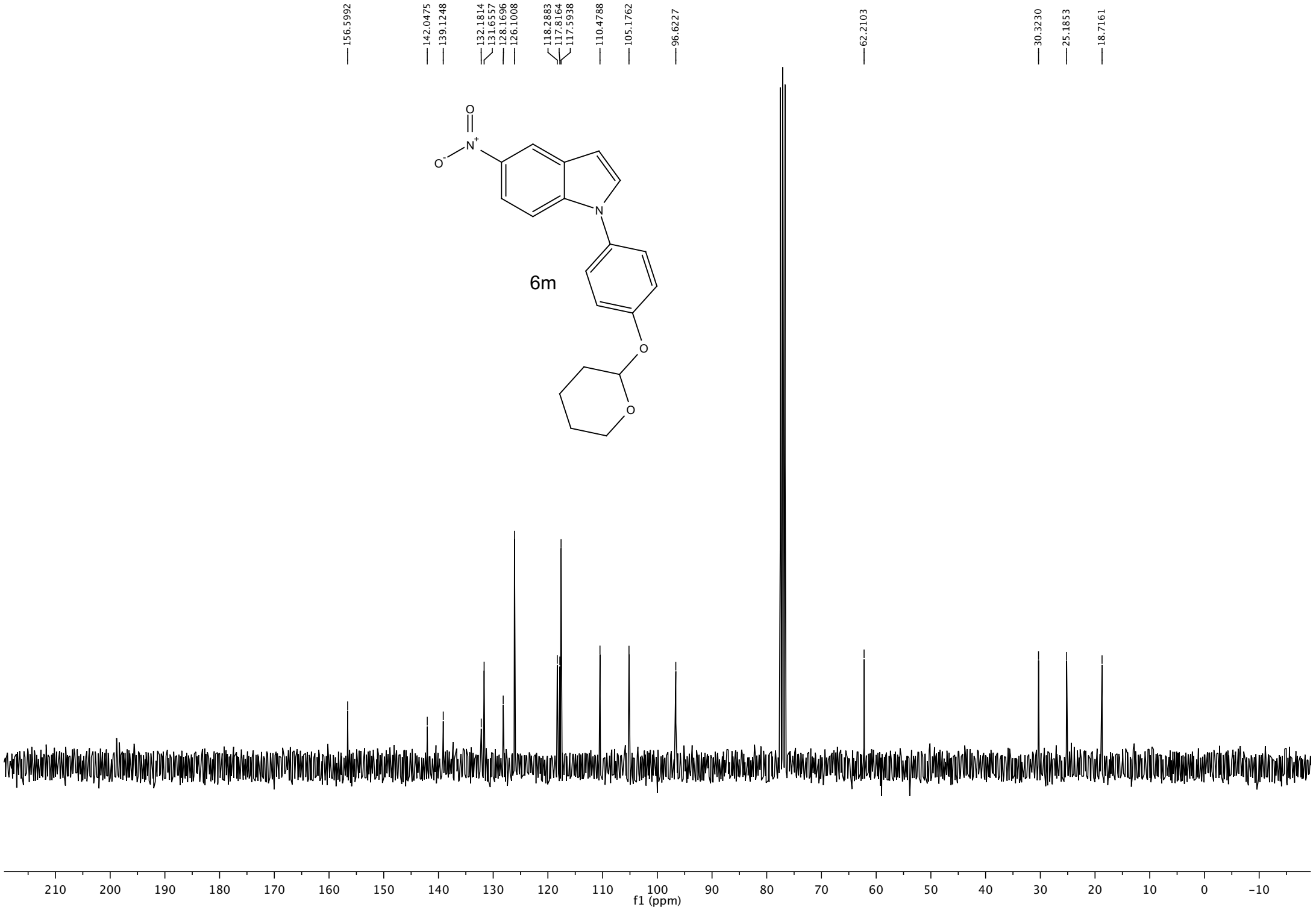

6k
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
4000
3500
3000
2500
2000
1500
1000
3056,84
2978,24
1705,54
1638,49
1582,04
1512,02
1487,04
1456,20
1365,54
1305,58
1275,10
1231,58
1176,53
1114,07
1033,04
978,94
861,59
790,79
755,34
774,97
734,34
717,59
685,12

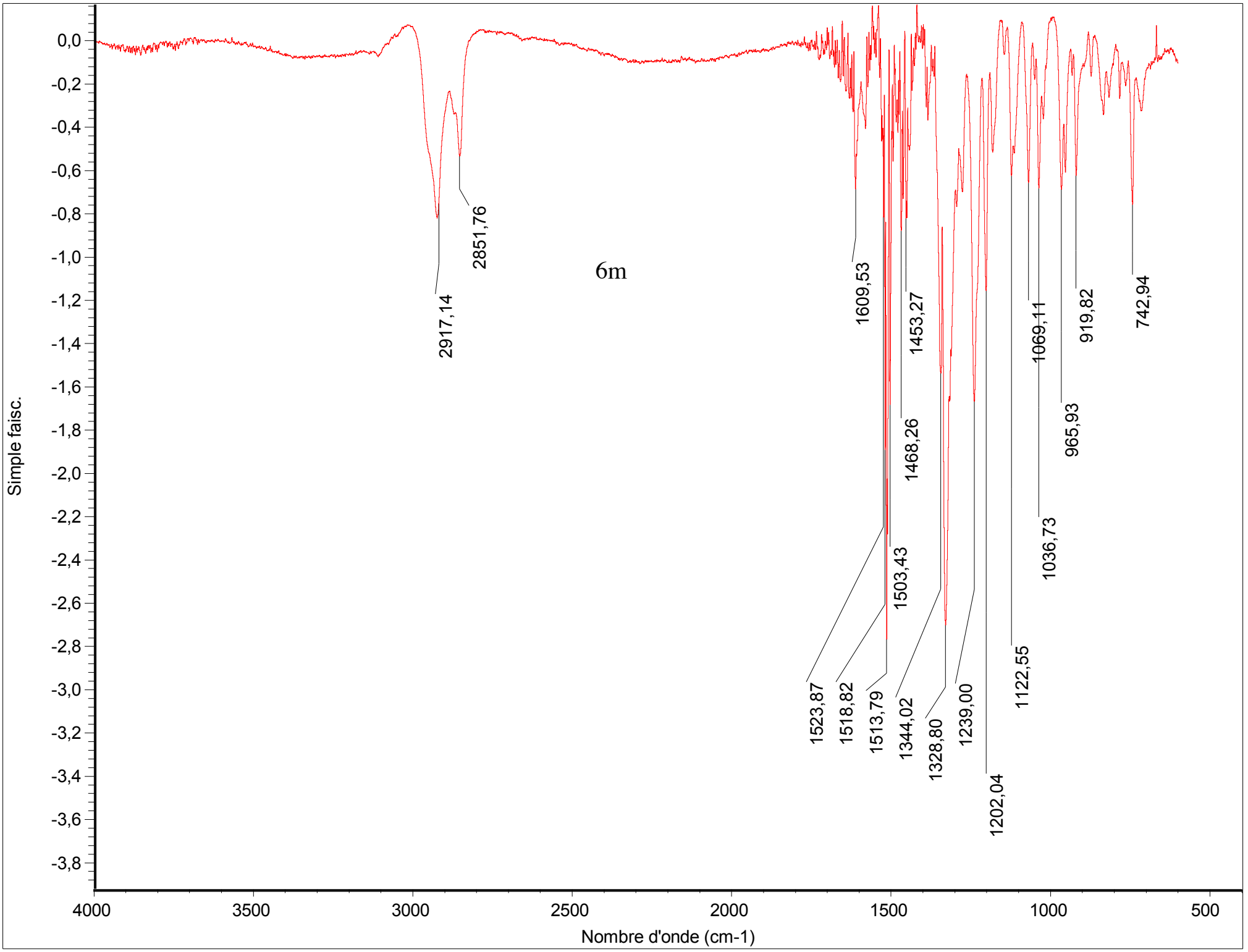

7.8424
7.8365
7.5467
7.5174
7.4254
7.4196
7.4133
7.3996
7.3925
7.3511
7.3408
6.6819
2.4650
1.7026
CH3
H3C
HO
N
CH3
6l
1.00
1.11
3.18
3.06
0.98
3.17
6.65
f1 (ppm)

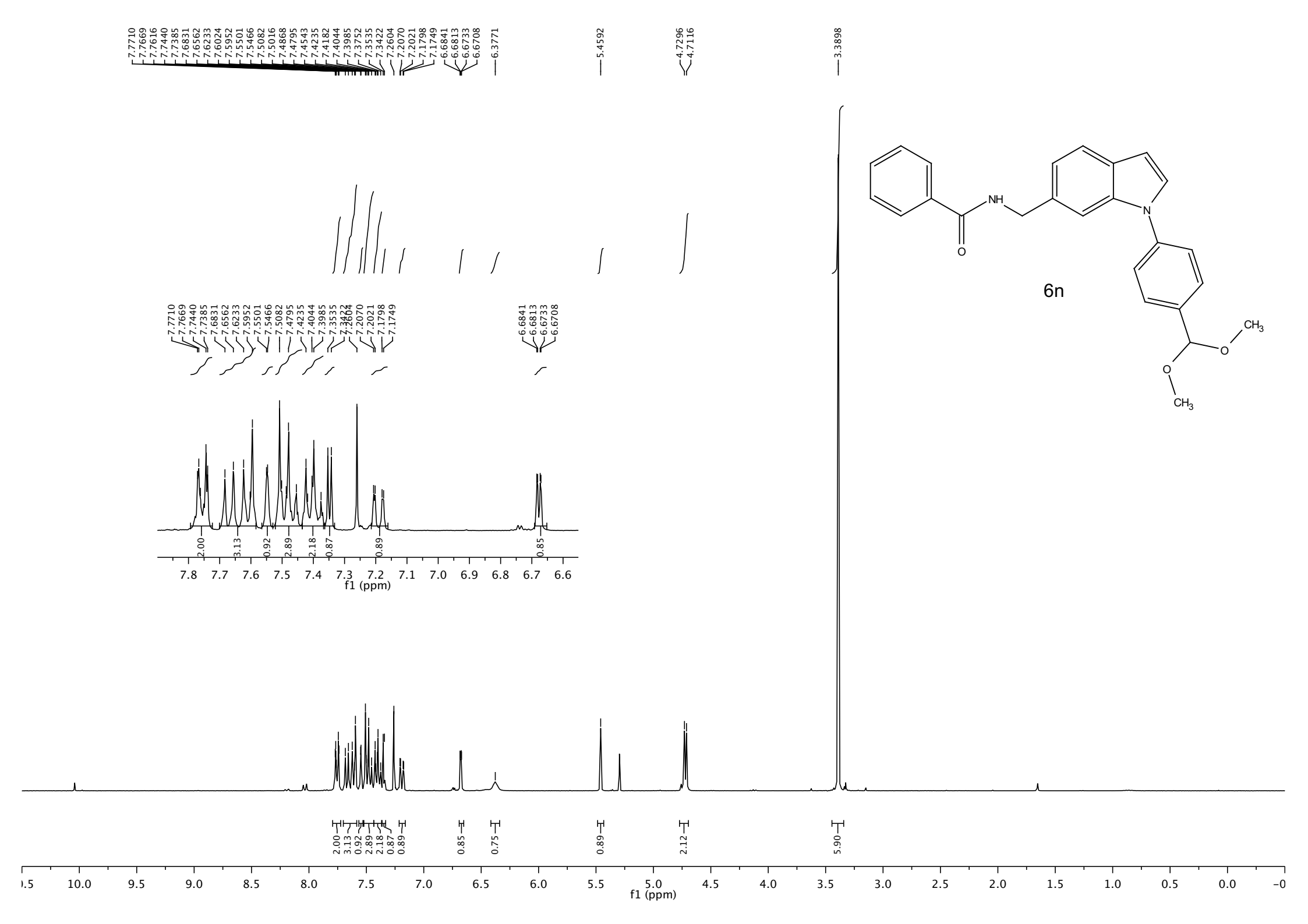

141.3430
137.3686
136.3347
134.9414
130.2271
128.9936
128.5185
124.2060
119.5562
116.4881
110.3386
103.4923
72.8719
32.1824
21.1197
OH
CH3
H3C
N
CH3
6l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

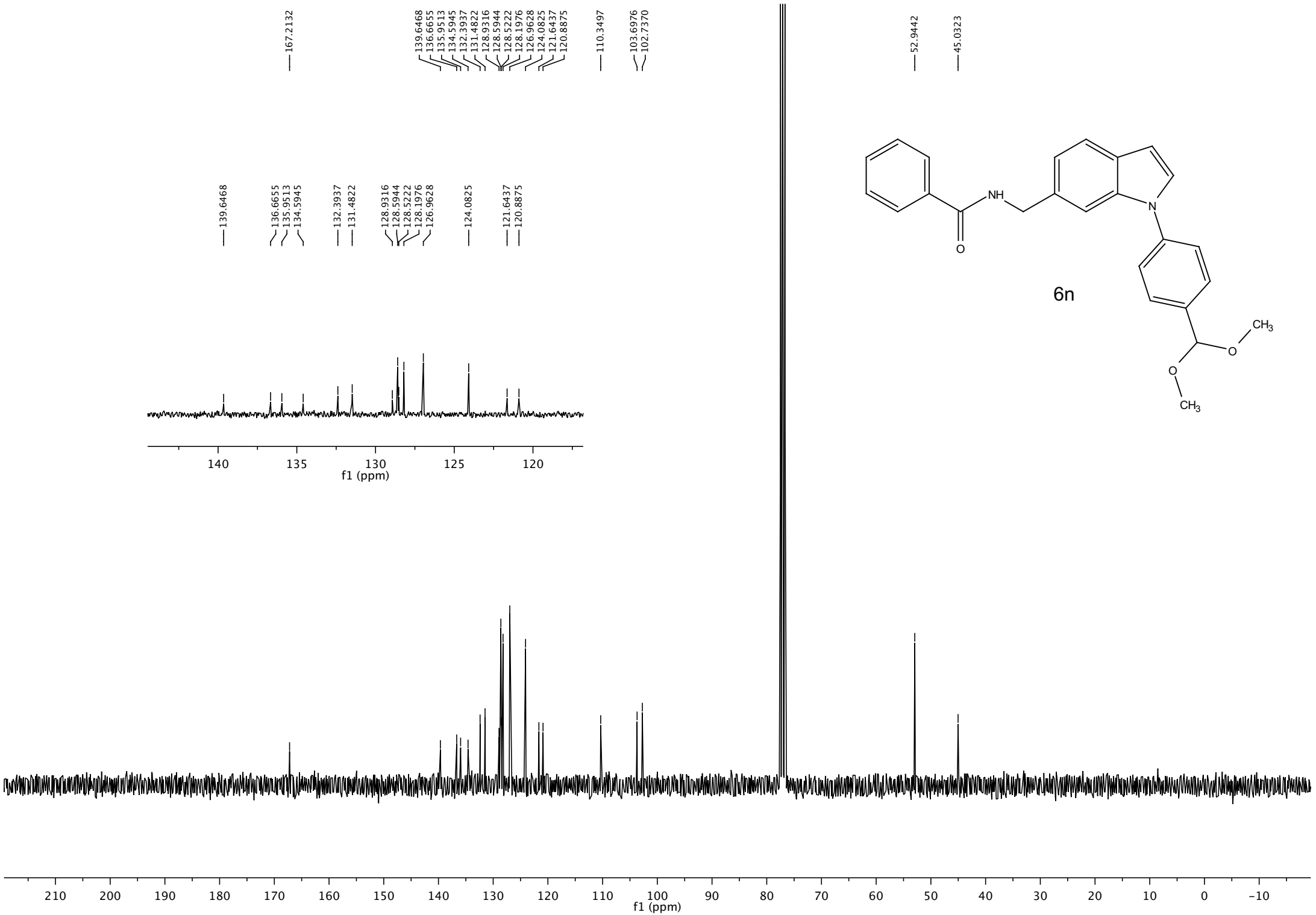

%Transmission
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
4000
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)
3405,68
2971,09
2923,35
1517,88
1474,62
1439,71
1371,50
1333,67
1289,48
1228,06
1108,83
955,88
821,10
805,21
718,40

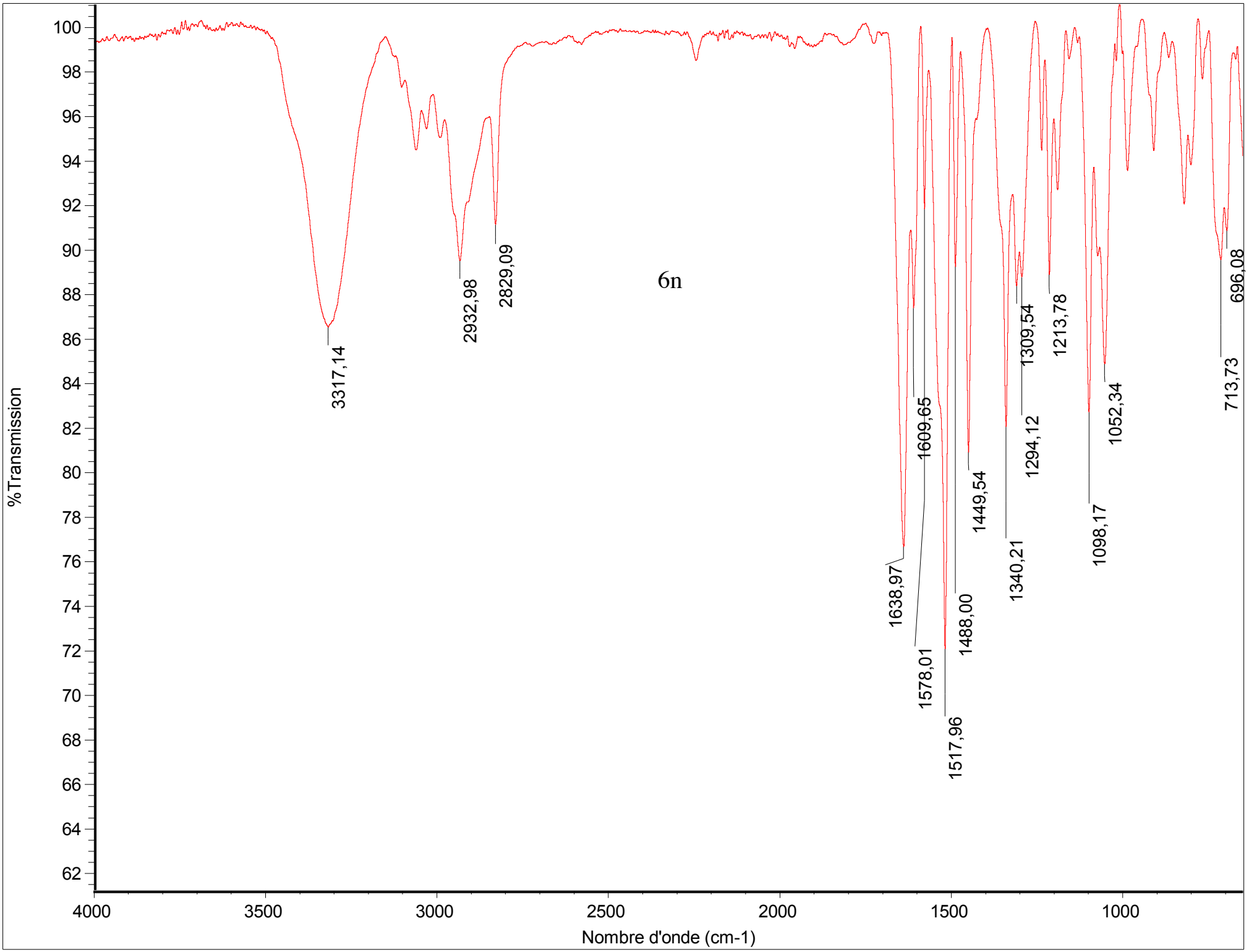

8.6359
8.6284
8.1088
8.1013
8.0785
8.0710
7.4559
7.4254
7.4193
7.4082
7.3896
7.3822
7.3675
7.3601
7.2596
7.2355
7.2279
7.2129
7.2058
6.8233
6.8124
5.5091
5.4981
5.4878
3.9821
3.9719
3.9512
3.9432
3.9340
3.9129
3.9022
3.6984
3.6936
3.6848
3.6796
3.6720
3.6661
3.6601
3.6557
3.6471
3.6424
3.6342
3.6284
2.0814
2.0741
2.0526
2.0450
2.0272
2.0120
1.9888
1.9627
1.9416
1.9292
1.9163
1.9028
1.8917
1.7612
1.7311
1.7228
1.7122
1.7059
1.6950
1.6813
1.6702
1.6670
1.6567
1.6445
1.6306
1.6303
1.6171
6m
f1 (ppm)

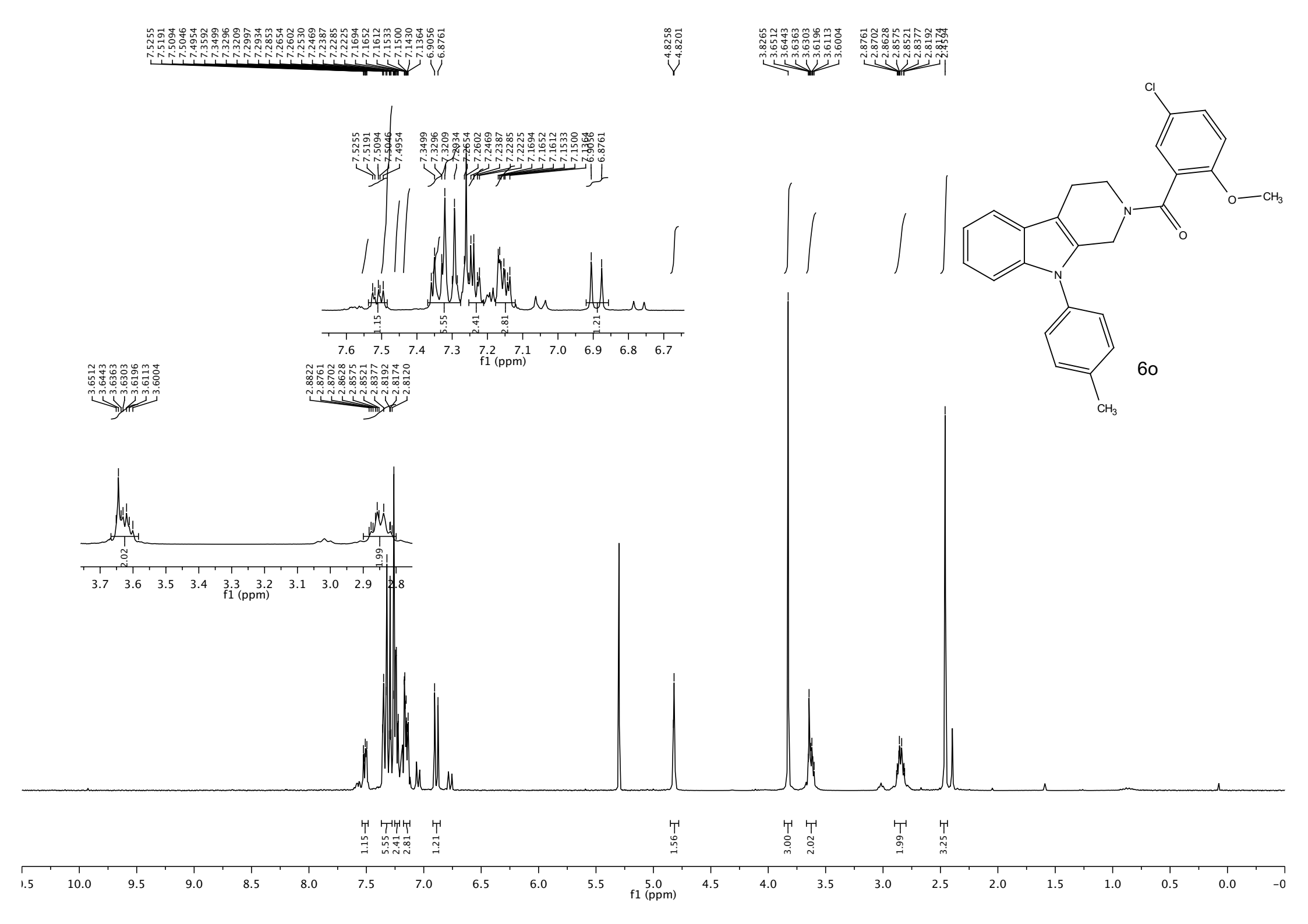

156.5992
142.0475
139.1248
132.1814
131.6557
128.1696
126.1008
118.2883
117.8164
117.5938
110.4788
105.1762
96.6227
62.2103
30.3230
25.1853
18.7161
O
N+
O-
N
O
O
6m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

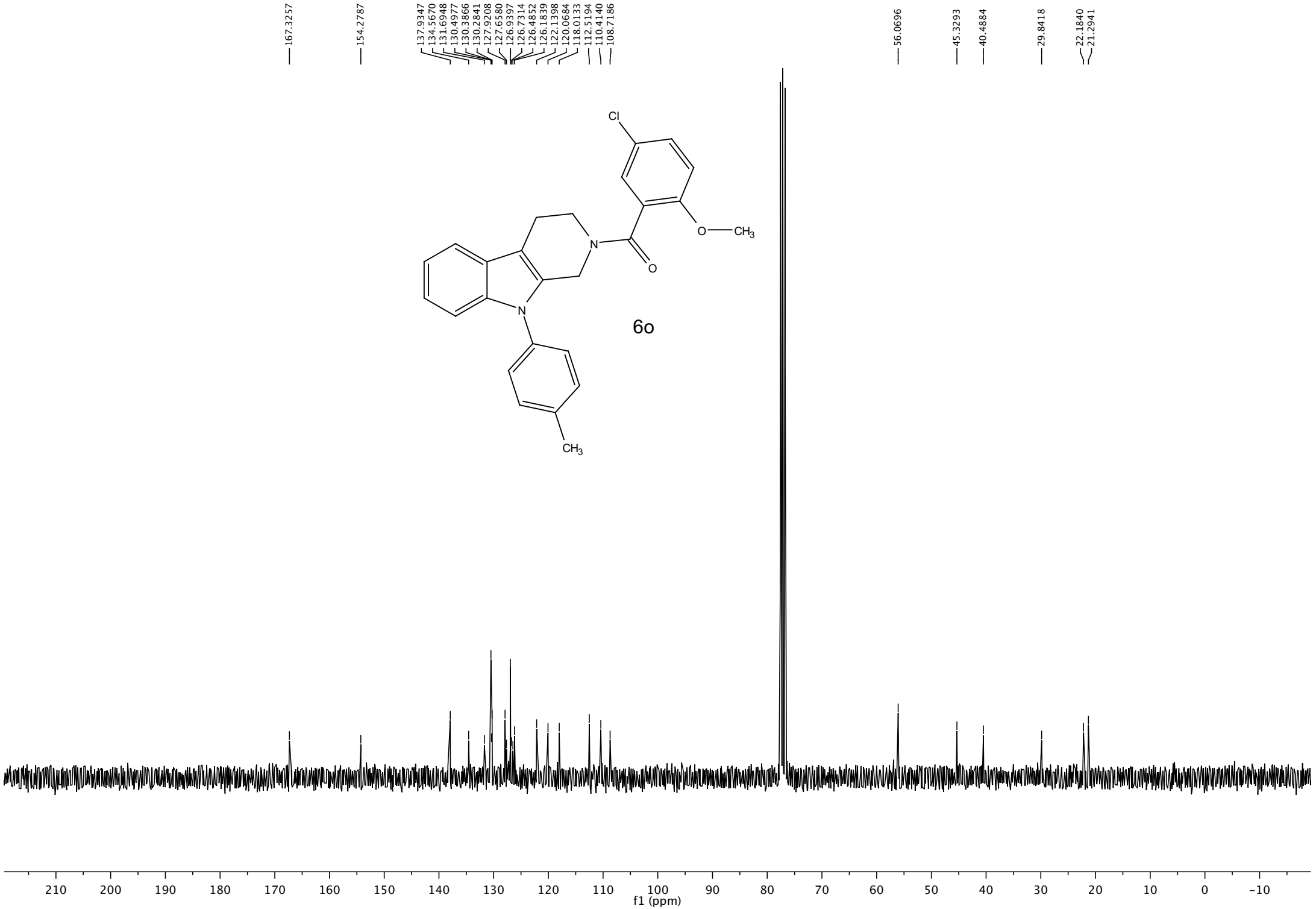

6m
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
-3,2
-3,4
-3,6
-3,8
4000
3500
3000
2500
2000
1500
1000
500
2917,14
2851,76
1609,53
1453,27
1468,26
1503,43
1523,87
1518,82
1513,79
1344,02
1328,80
1239,00
1202,04
1122,55
1069,11
1036,73
965,93
919,82
742,94

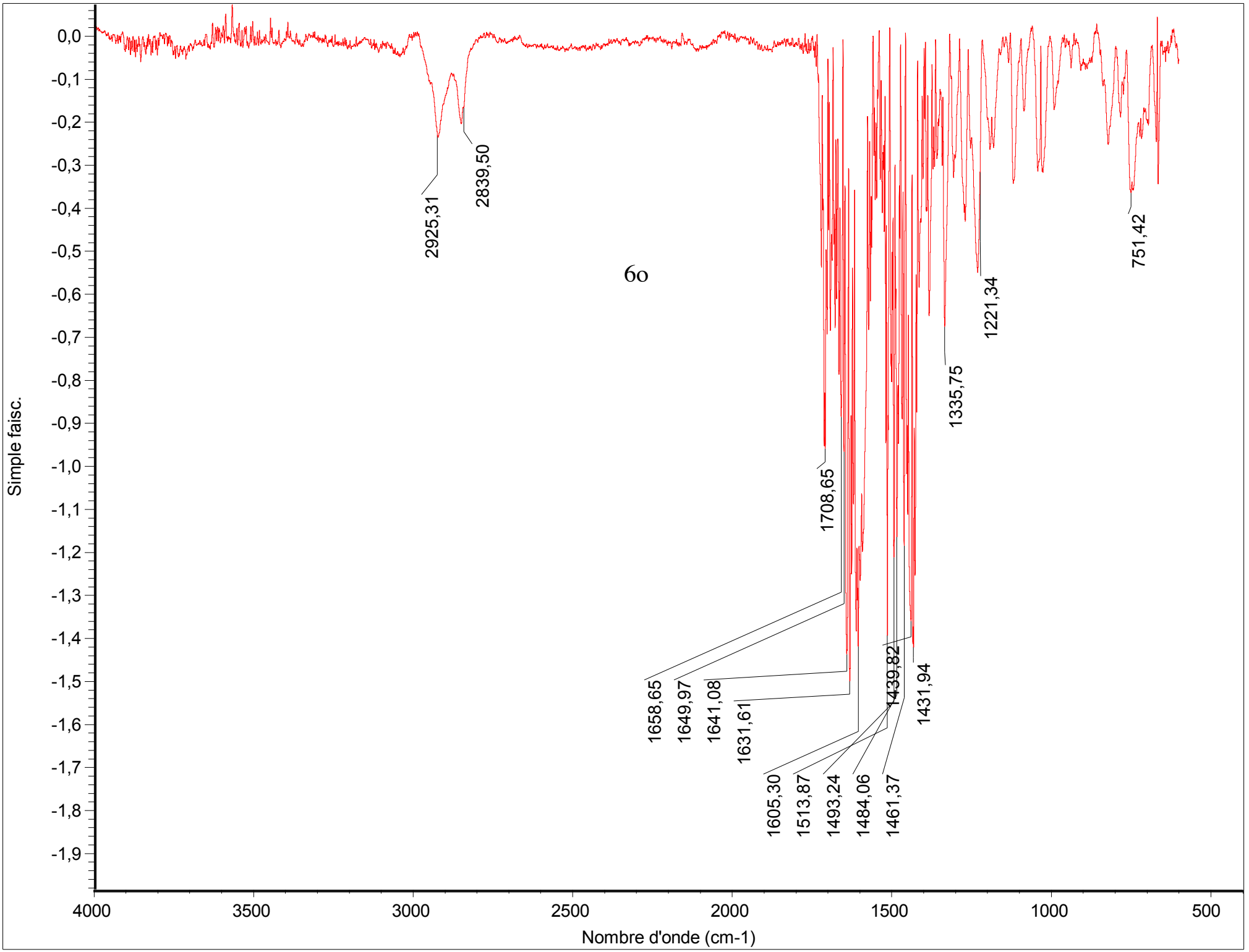

7.7710
7.7669
7.7616
7.7440
7.7385
7.6831
7.6562
7.6233
7.6024
7.5952
7.5501
7.5466
7.5082
7.5016
7.4868
7.4795
7.4543
7.4235
7.4182
7.4044
7.3985
7.3752
7.3535
7.3422
7.2604
7.2070
7.2021
7.1798
7.1749
6.6841
6.6813
6.6733
6.6708
6.3771
5.4592
4.7296
4.7116
3.3898
NH
O
N
O
O
CH3
CH3
6n
2.00
3.13
0.92
2.89
2.18
0.87
0.89
0.85
f1 (ppm)
0.75
0.89
2.12
5.90

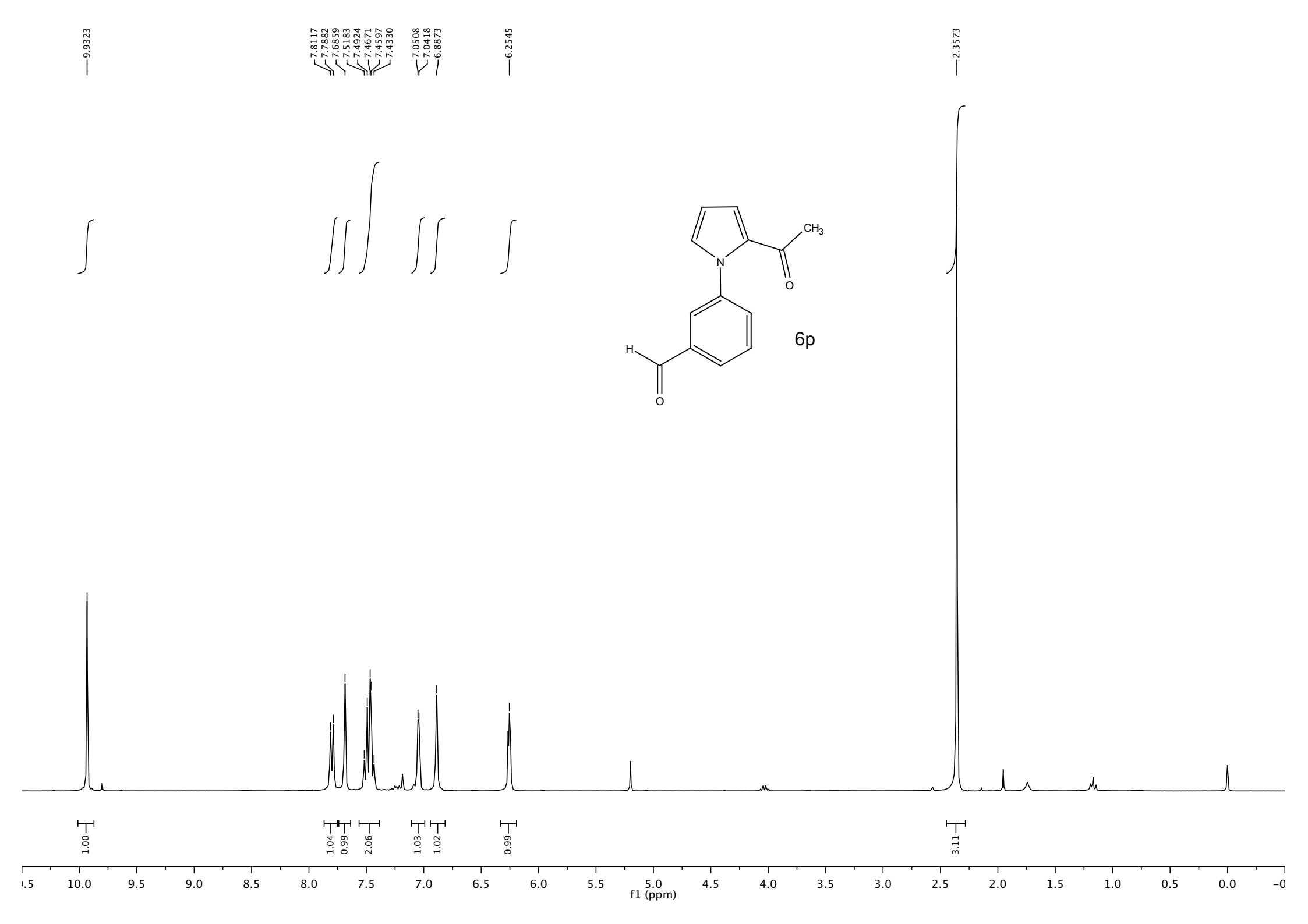

167.2132
139.6468
136.6655
135.9513
134.5945
132.3937
131.4822
128.9316
128.5944
128.5222
128.1976
126.9628
124.0825
121.6437
120.8875
110.3497
103.6976
102.7370
52.9442
45.0323
NH
N
O
O
O
CH3
CH3
6n
f1 (ppm)

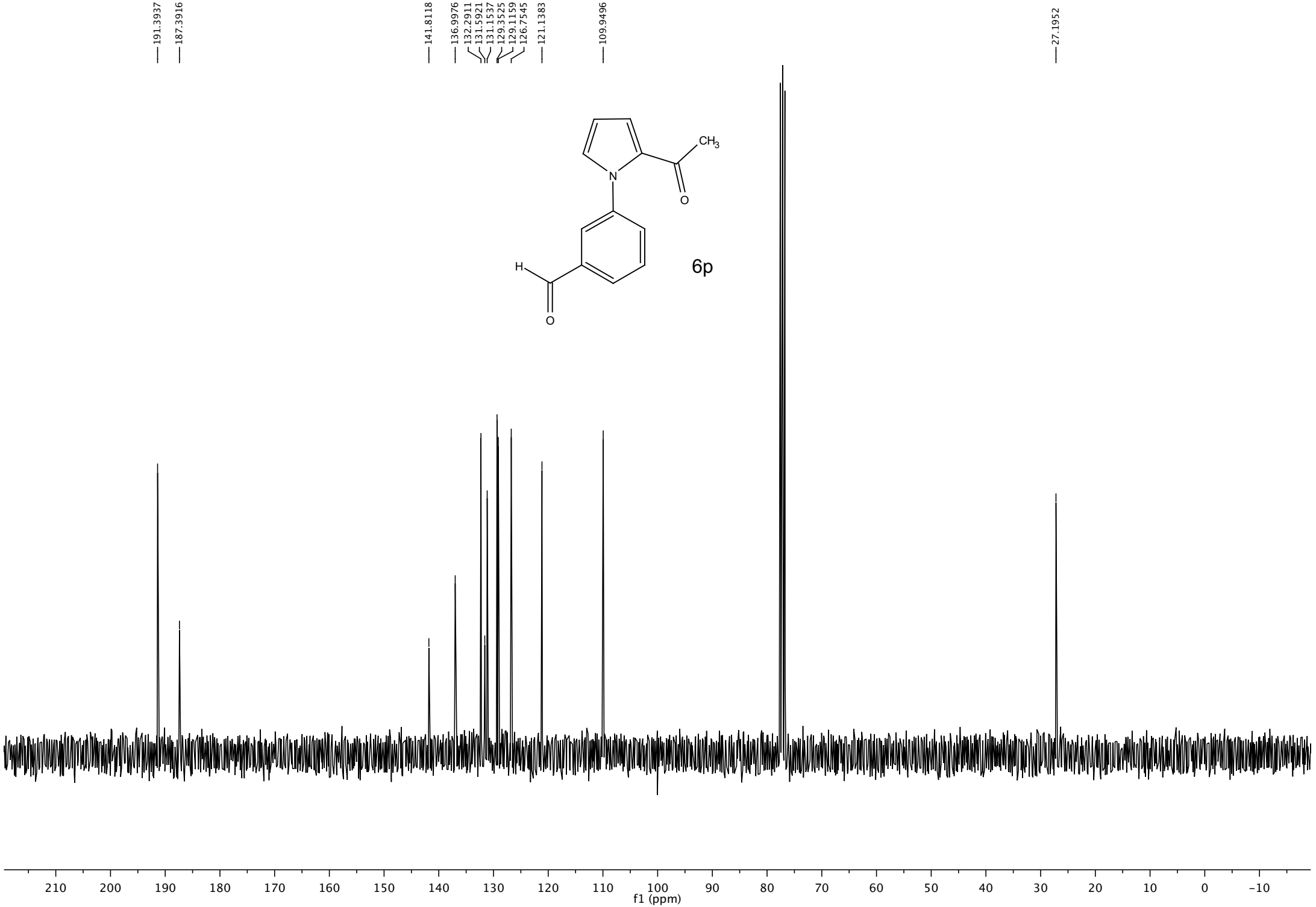

6n
%Transmission
Nombre d'onde (cm-1)
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
4000
3500
3000
2500
2000
1500
1000
3317,14
2932,98
2829,09
1638,97
1609,65
1578,01
1517,96
1488,00
1449,54
1340,21
1309,54
1294,12
1213,78
1098,17
1052,34
713,73
696,08

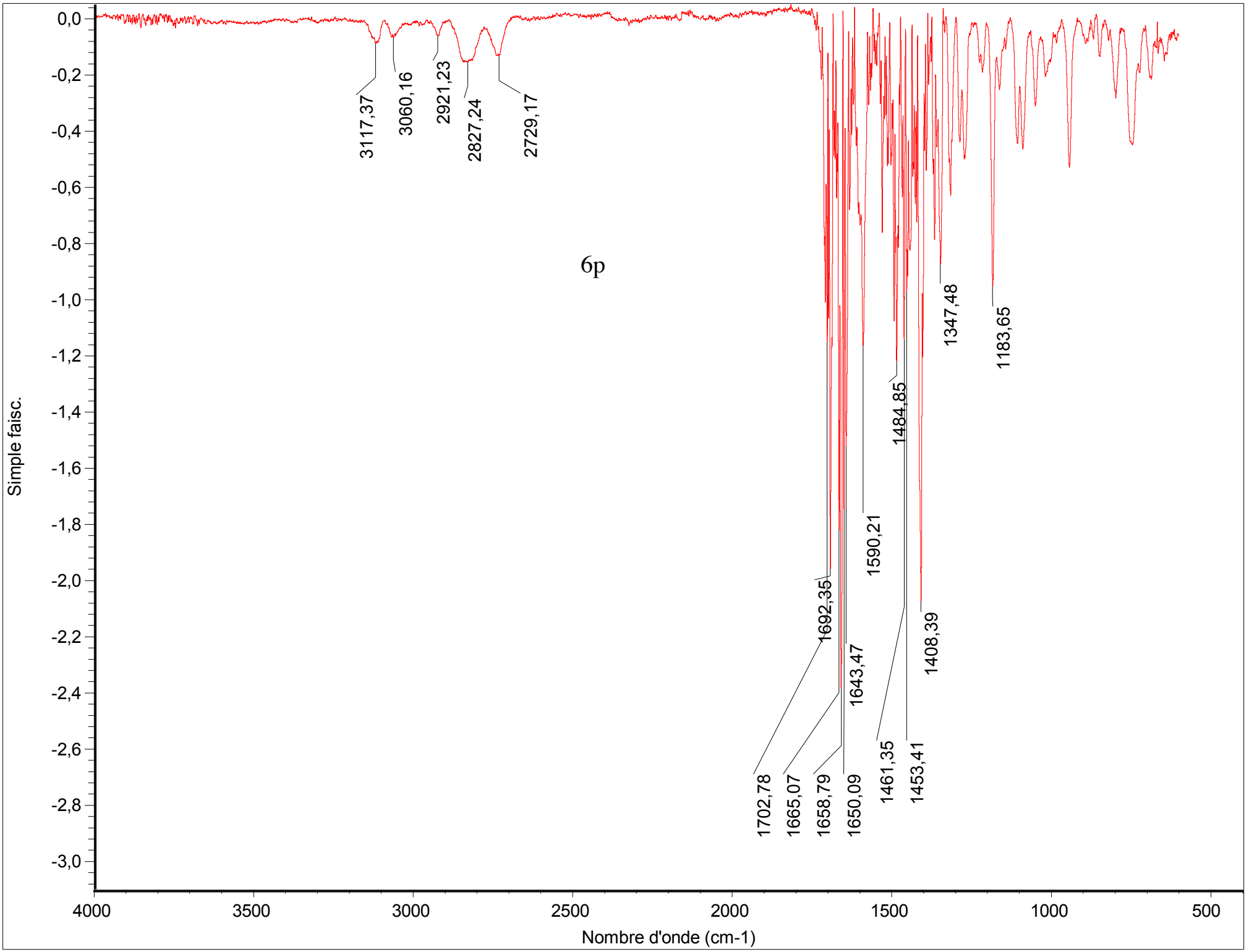

7.5255
7.5191
7.5094
7.5046
7.4954
7.3592
7.3499
7.3296
7.3209
7.2997
7.2934
7.2853
7.2654
7.2602
7.2530
7.2469
7.2387
7.2285
7.2225
7.1694
7.1652
7.1612
7.1533
7.1500
7.1430
7.1364
6.9056
6.8761
4.8258
4.8201
3.8265
3.6512
3.6443
3.6363
3.6303
3.6196
3.6113
3.6004
2.8761
2.8702
2.8628
2.8575
2.8521
2.8377
2.8192
2.8174
2.8120
2.4594
1.15
5.55
2.41
2.81
1.21
1.56
3.00
2.02
1.99
3.25
f1 (ppm)
Cl
O
CH3
N
O
N
CH3
6o

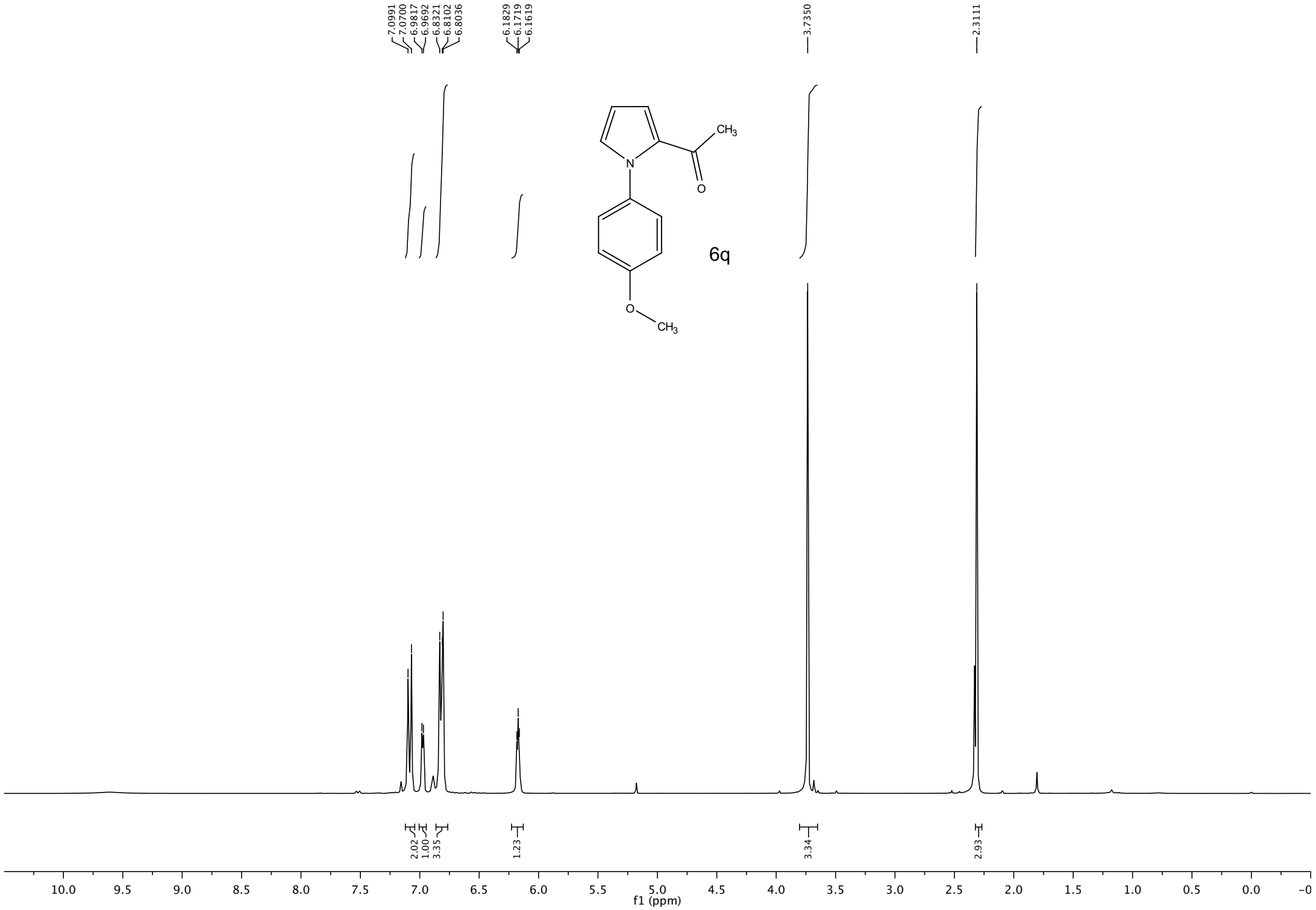

167.3257
154.2787
137.9347
134.5670
131.6948
130.4977
130.3866
130.2841
127.9208
127.6580
126.9397
126.7314
126.4852
126.1839
122.1398
120.0684
118.0133
112.5194
110.4140
108.7186
56.0696
45.3293
40.4884
29.8418
22.1840
21.2941
Cl
O
CH3
N
O
N
CH3
6o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

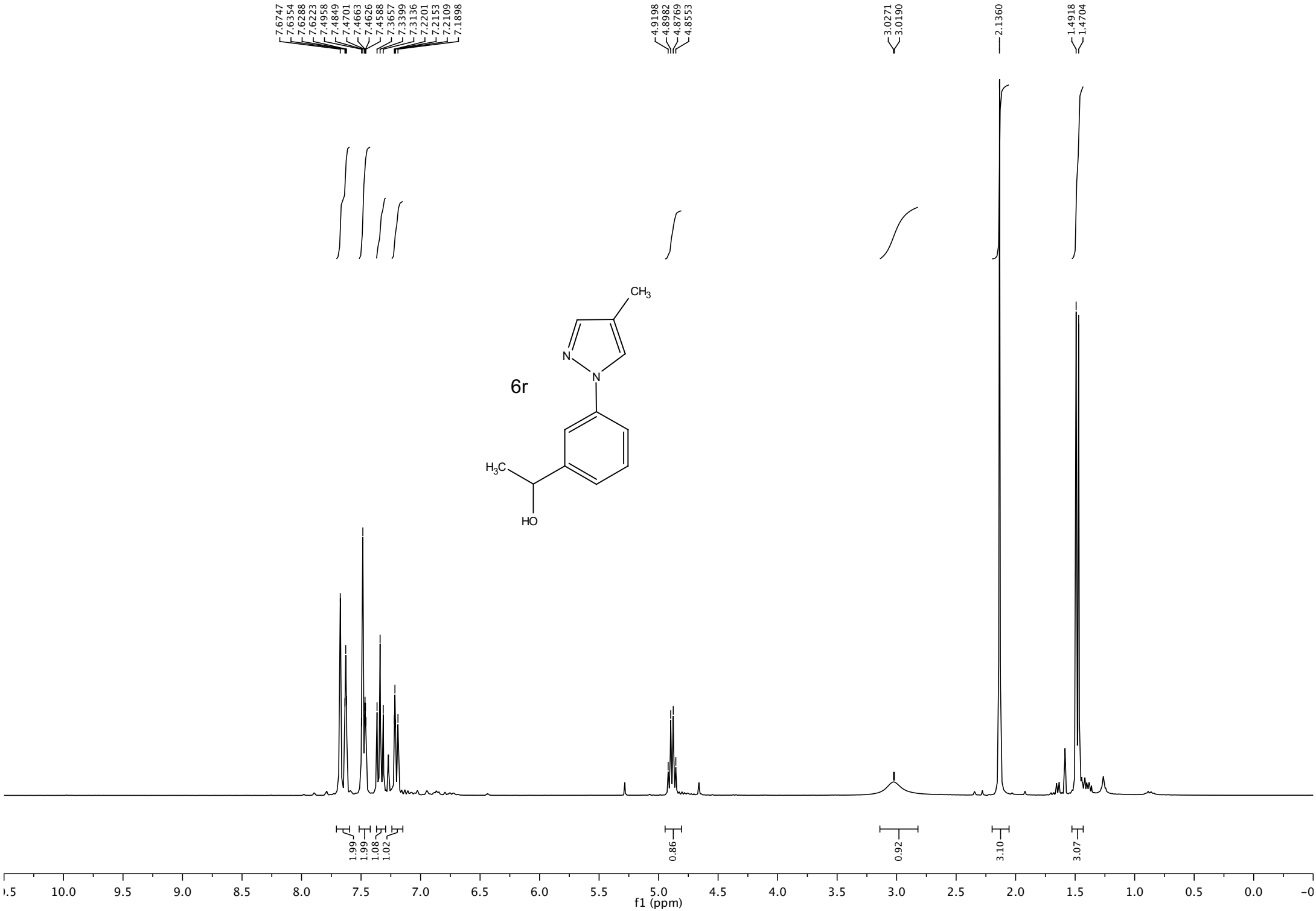

6o
Simple faisc.
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
-1,3
-1,4
-1,5
-1,6
-1,7
-1,8
-1,9
2925,31
2839,50
1708,65
1658,65
1649,97
1641,08
1631,61
1605,30
1513,87
1493,24
1484,06
1461,37
1439,82
1431,94
1335,75
1221,34
751,42
4000
3500
3000
2500
2000
1500
1000
500
Nombre d'onde (cm-1)

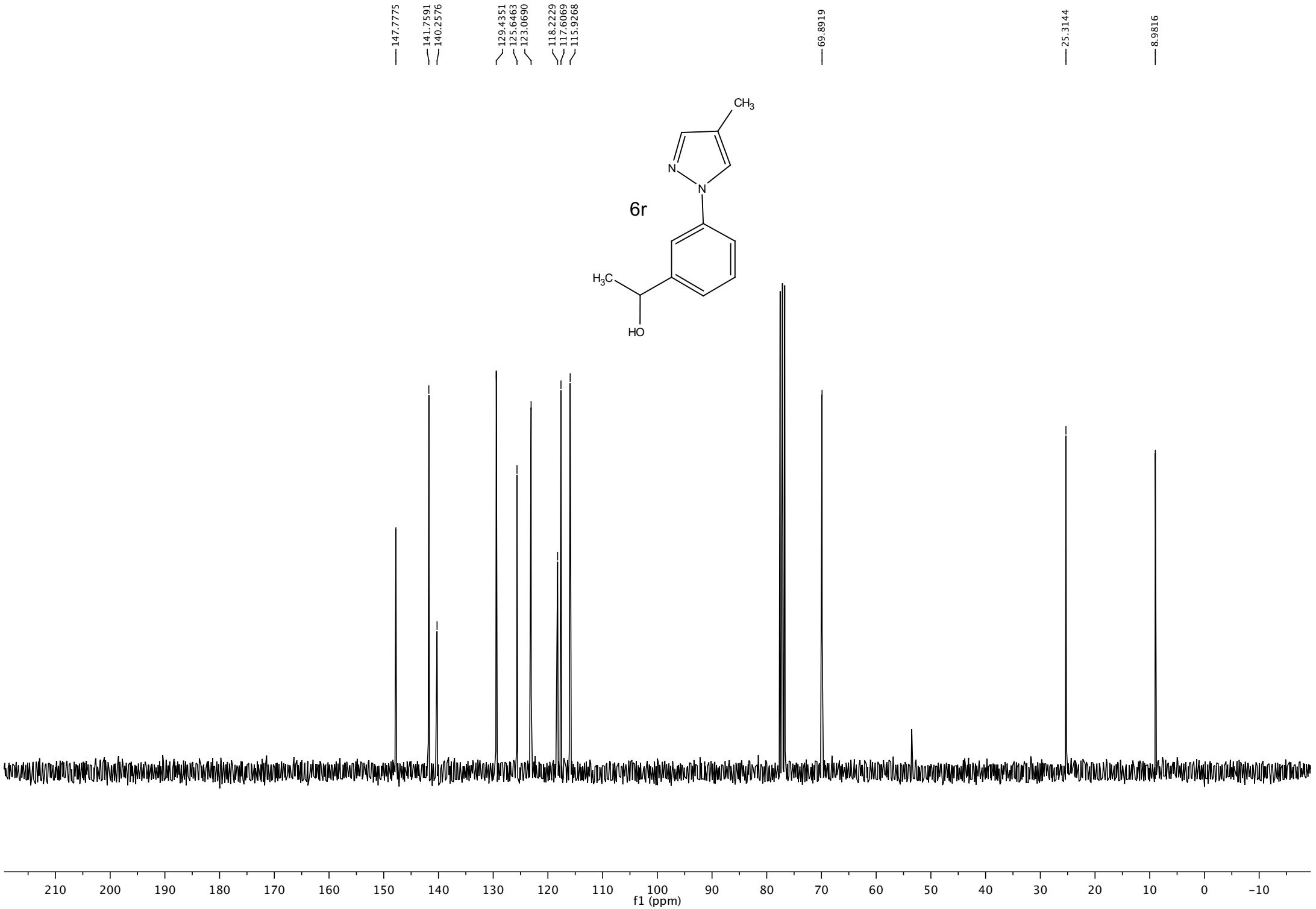

9.9323
7.8117
7.7882
7.6859
7.5183
7.4924
7.4671
7.4597
7.4330
7.0508
7.0418
6.8873
6.2545
2.3573
CH3
N
O
H
O
6p
1.00
1.04
0.99
2.06
1.03
1.02
0.99
3.11
f1 (ppm)

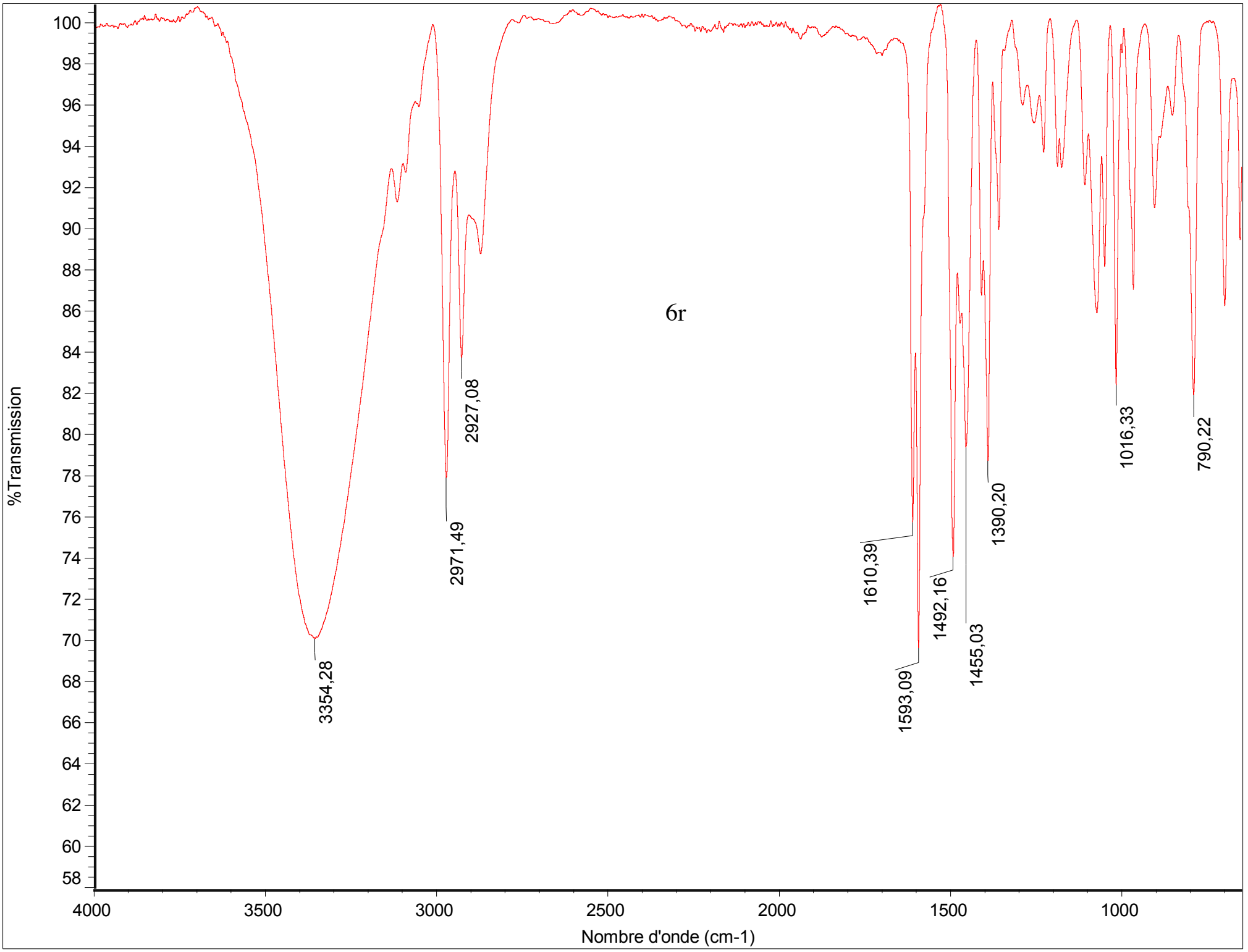

191.3937
187.3916
141.8118
136.9976
132.2911
131.5921
131.1537
129.3525
129.1159
126.7545
121.1383
109.9496
27.1952
CH3
N
O
H
O
6p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

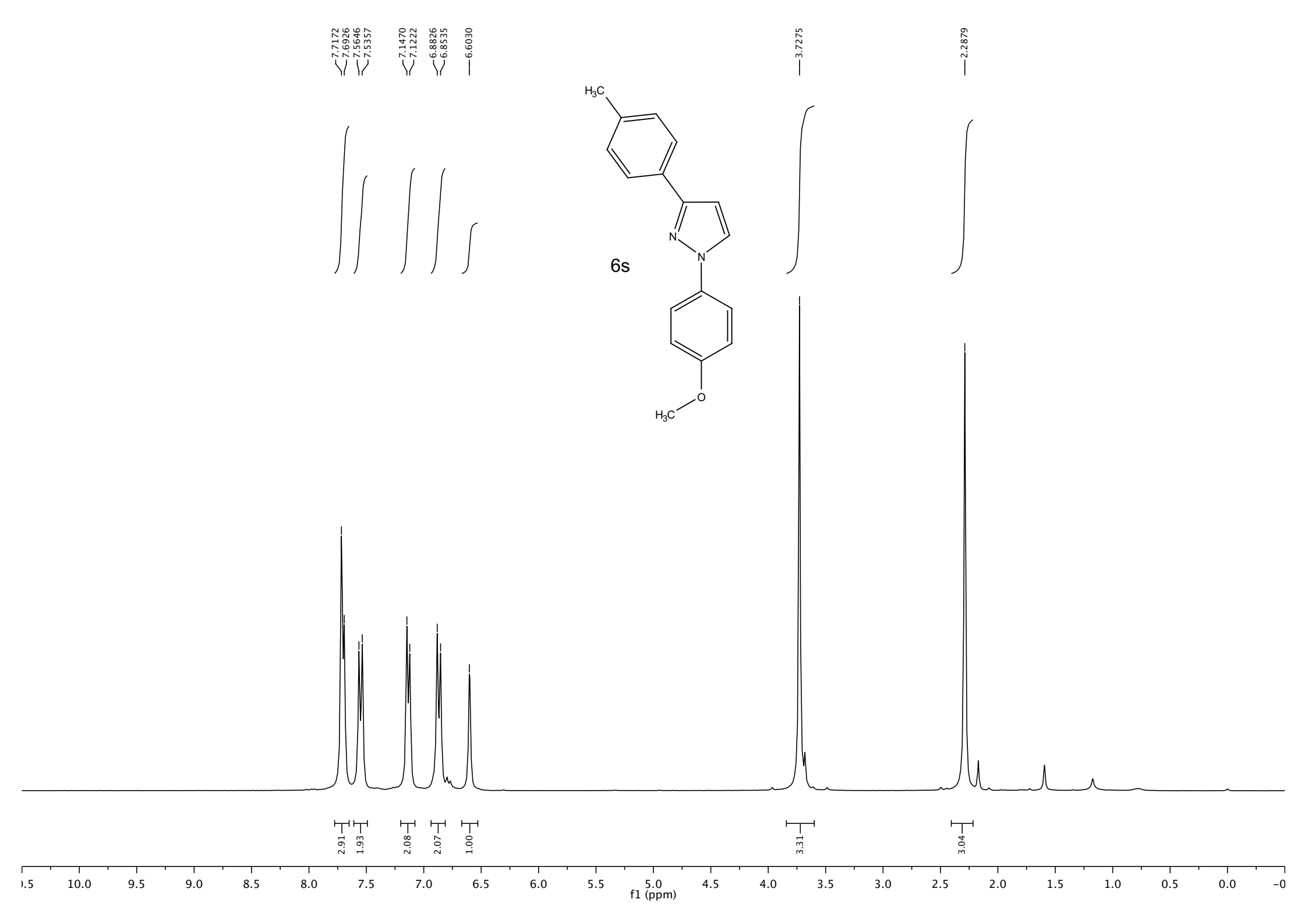

6p
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-1,2
-1,4
-1,6
-1,8
-2,0
-2,2
-2,4
-2,6
-2,8
-3,0
4000
3500
3000
2500
2000
1500
1000
500
3117,37
3060,16
2921,23
2827,24
2729,17
1702,78
1692,35
1665,07
1658,79
1650,09
1643,47
1590,21
1484,85
1461,35
1453,41
1408,39
1347,48
1183,65

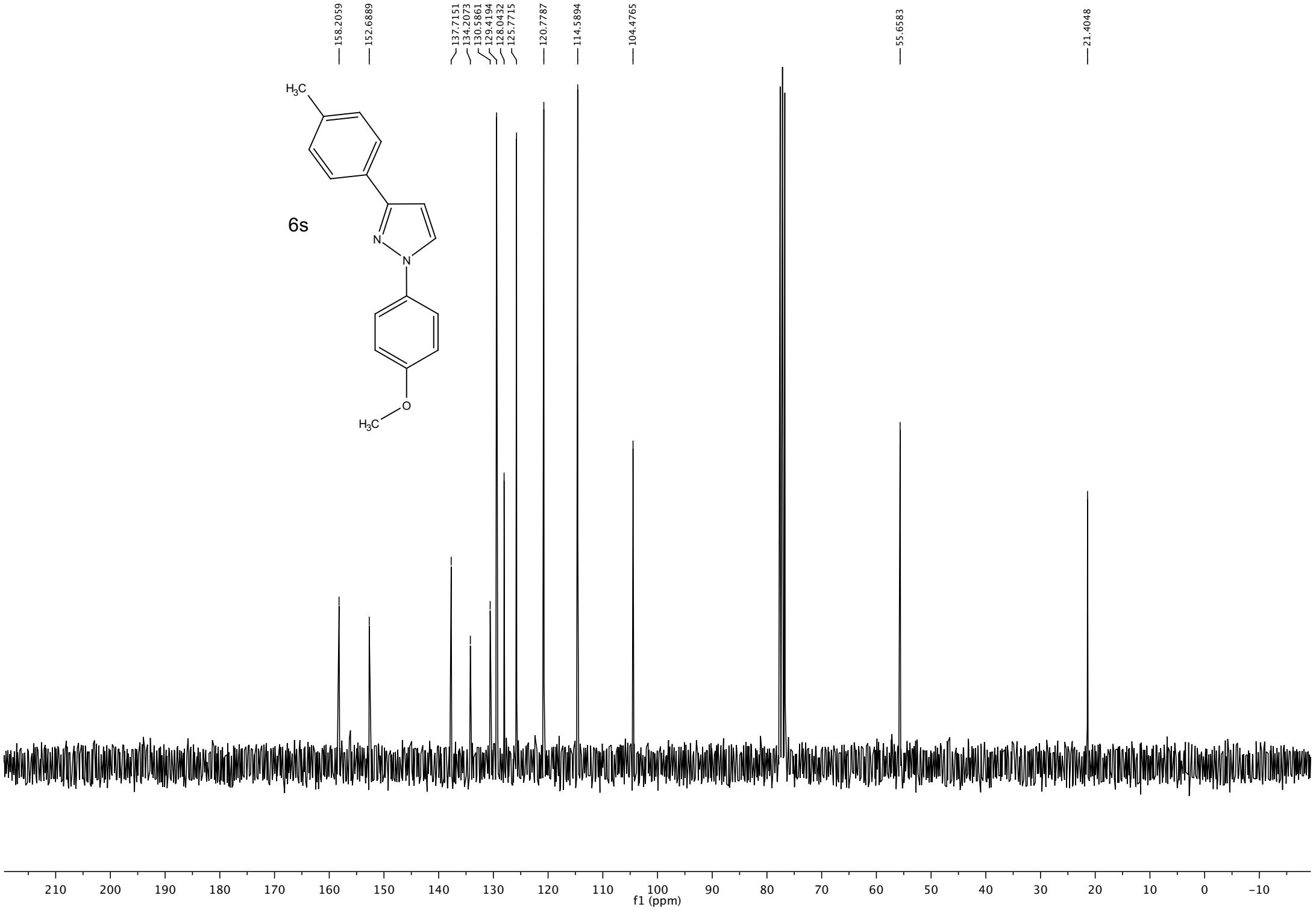

7.0991
7.0700
6.9817
6.9692
6.8321
6.8102
6.8036
6.1829
6.1719
6.1619
3.7350
2.3111
CH3
N
O
6q
O
CH3
2.02
1.00
3.35
1.23
3.34
2.93
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

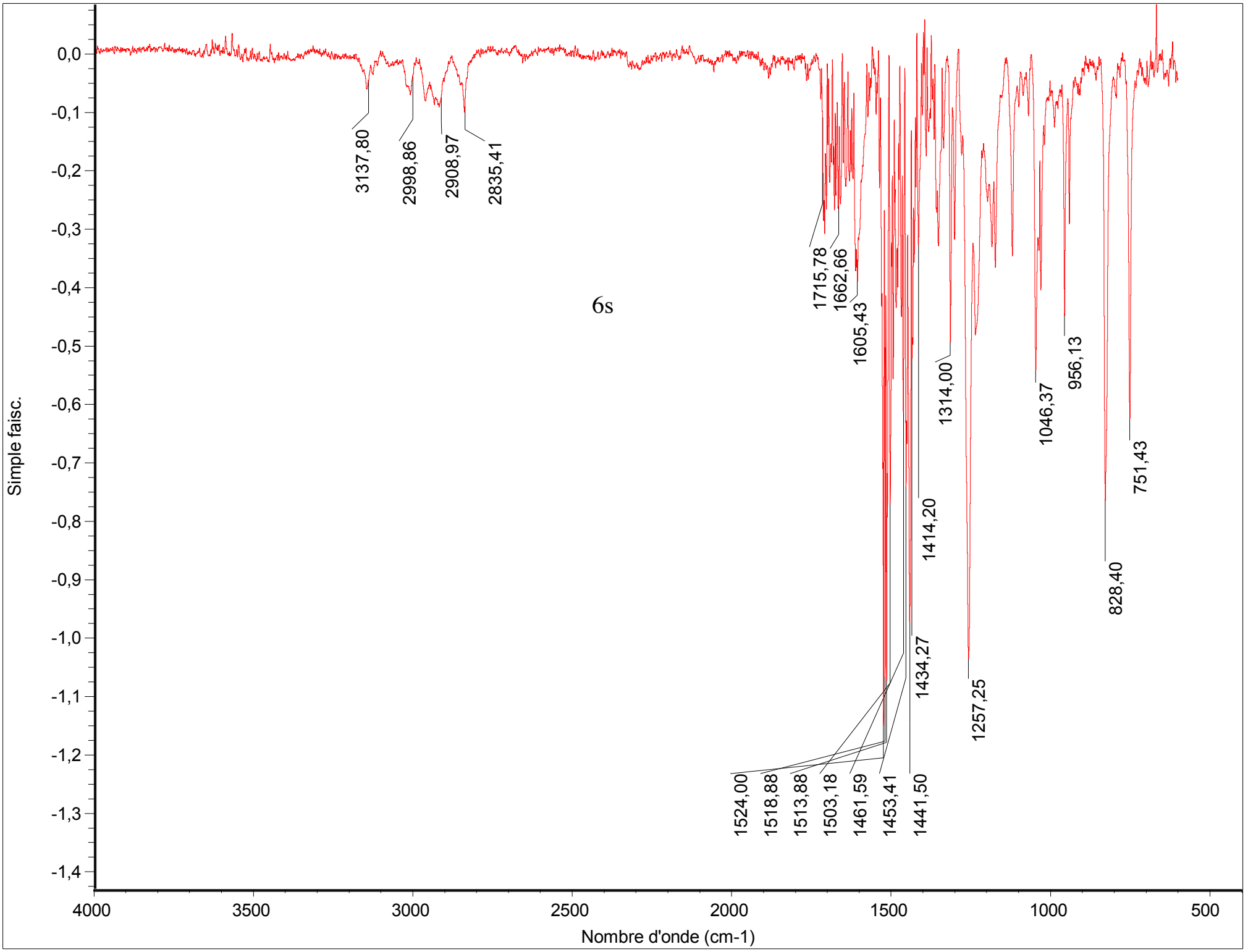

7.6747
7.6354
7.6288
7.6223
7.4958
7.4849
7.4701
7.4663
7.4626
7.4588
7.3657
7.3399
7.3136
7.2201
7.2153
7.2109
7.1898
4.9198
4.8982
4.8769
4.8553
3.0271
3.0190
2.1360
1.4918
1.4704
6r
CH3
N
N
H3C
HO
1.99
1.99
1.08
1.02
0.86
0.92
3.10
3.07
f1 (ppm)

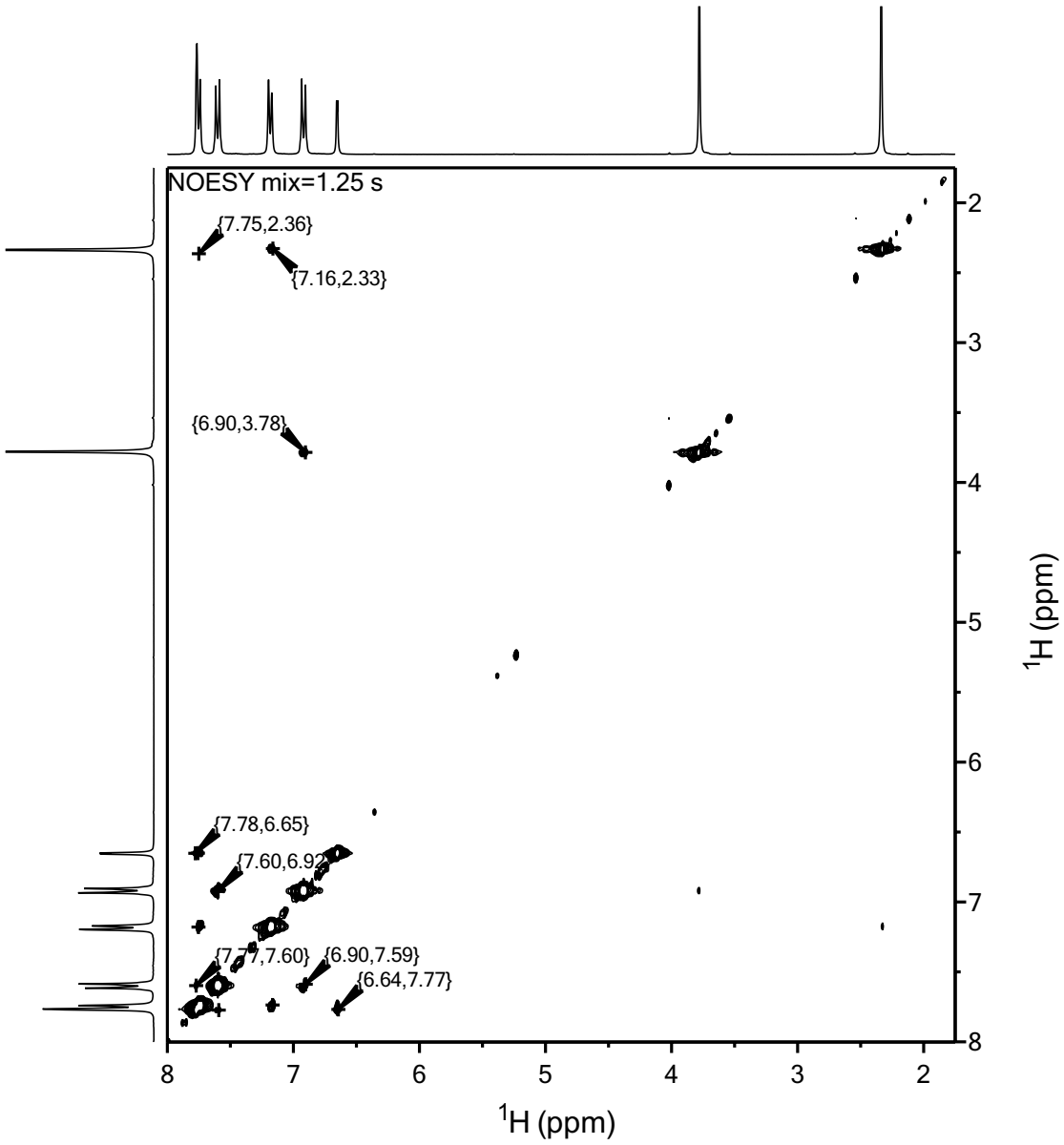

147.7775
141.7591
140.2576
129.4351
125.6463
123.0690
118.2229
117.6069
115.9268
69.8919
25.3144
8.9816
CH3
N
N
6r
H3C
HO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


6r
%Transmission
Nombre d'onde (cm-1)
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
4000
3500
3000
2500
2000
1500
1000
3354,28
2971,49
2927,08
1610,39
1593,09
1492,16
1455,03
1390,20
1016,33
790,22

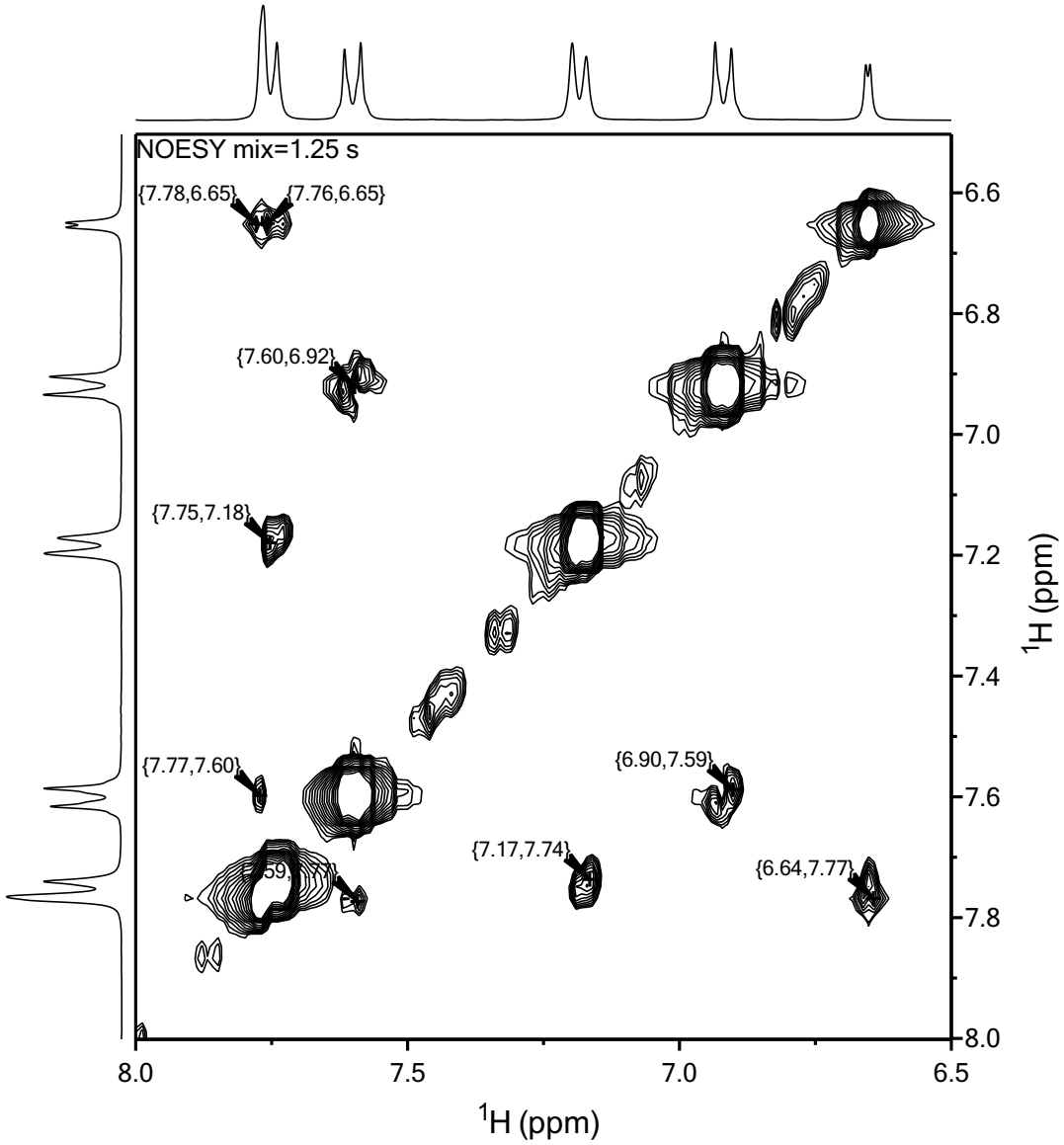

7.7172
7.6926
7.5646
7.5357
7.1470
7.1222
6.8826
6.8535
6.6030
3.7275
2.2879
6s
2.91
1.93
2.08
2.07
1.00
3.31
3.04
f1 (ppm)


158.2059
152.6889
137.7151
134.2073
130.5861
129.4194
128.0432
125.7715
120.7787
114.5894
104.4765
55.6583
21.4048
H3C
6s
N
N
O
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

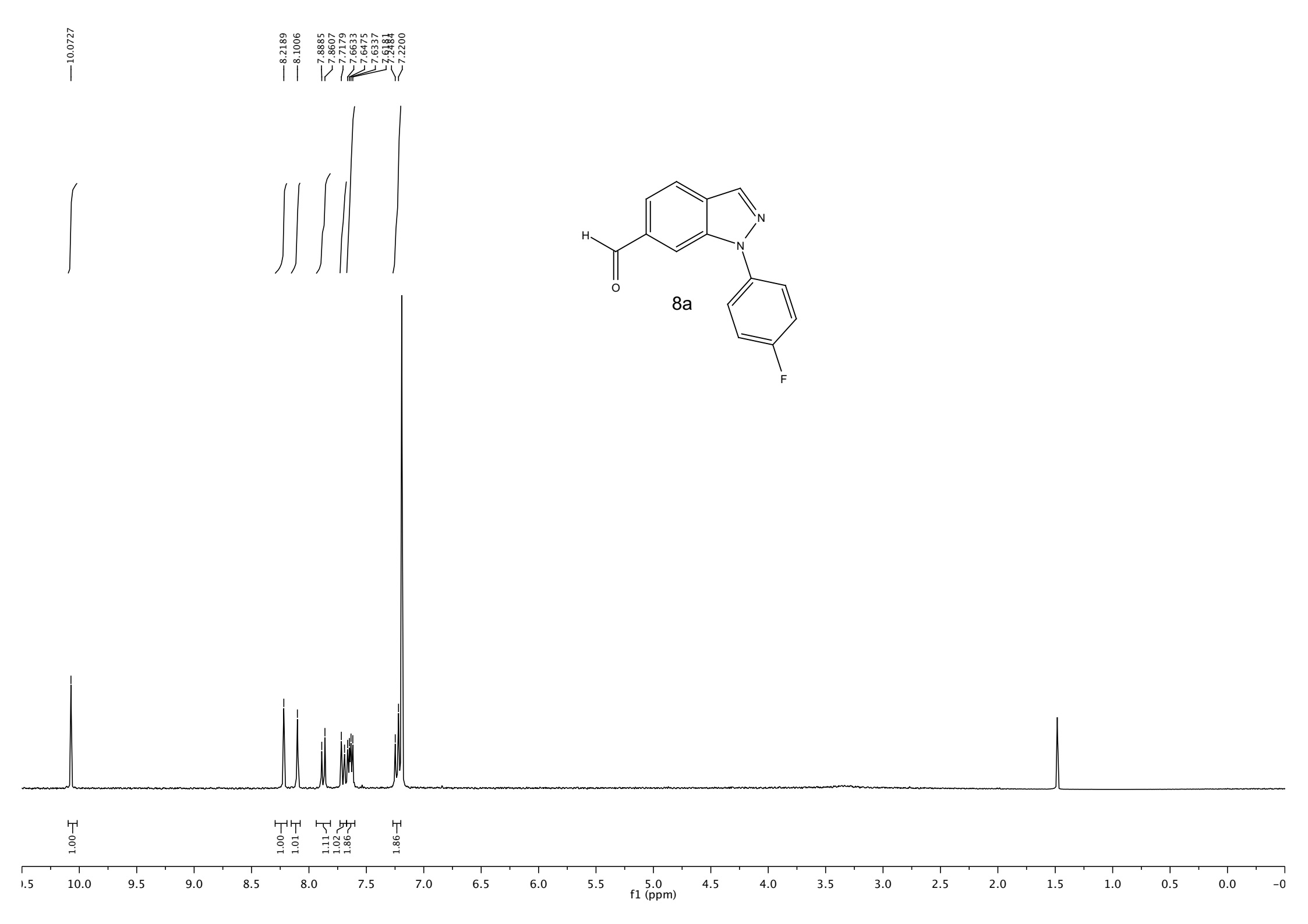

6s
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
-1,3
-1,4
4000
3500
3000
2500
2000
1500
1000
500
3137,80
2998,86
2908,97
2835,41
1715,78
1662,66
1605,43
1524,00
1518,88
1513,88
1503,18
1461,59
1453,41
1441,50
1434,27
1414,20
1314,00
1257,25
1046,37
956,13
828,40
751,43

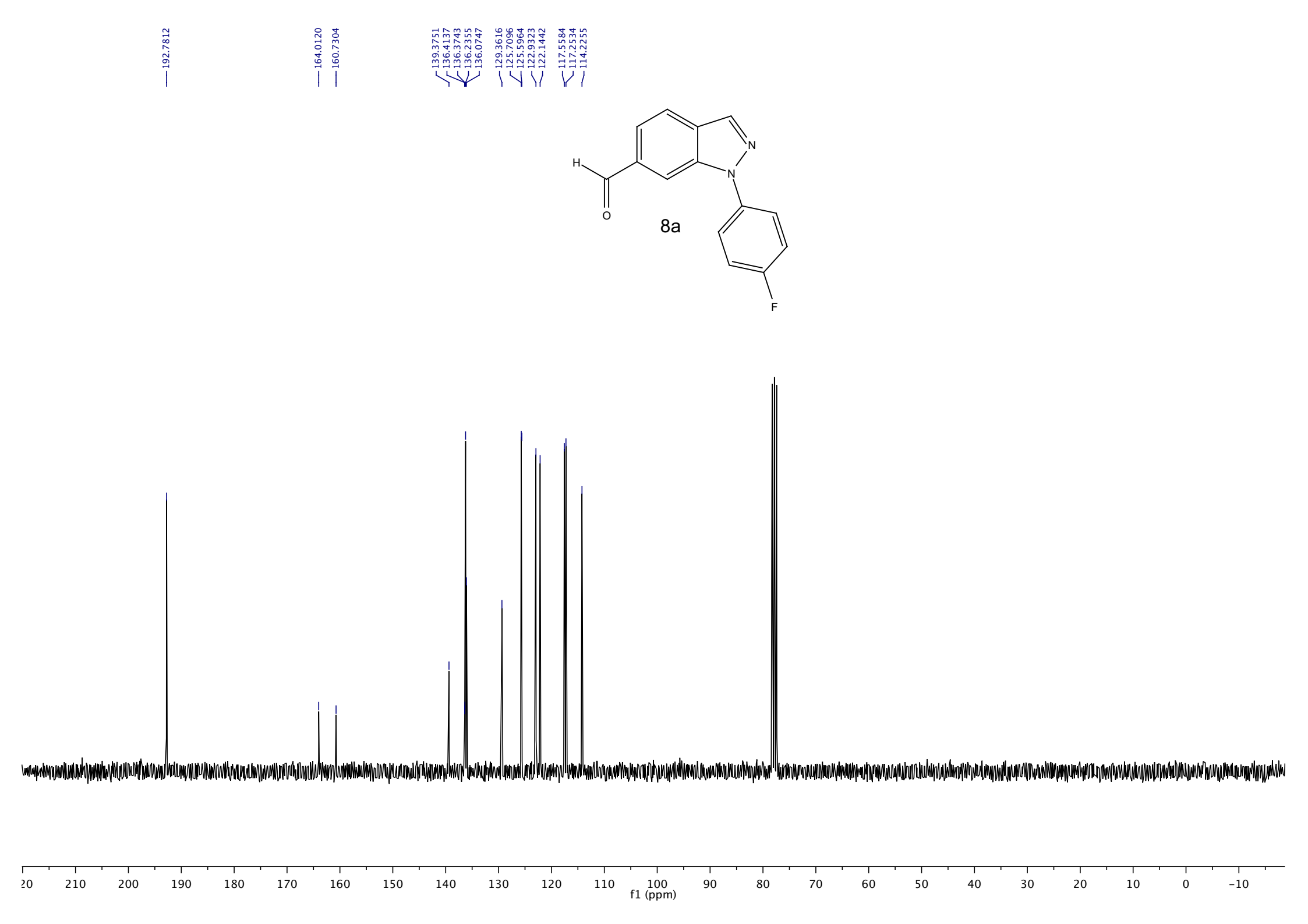

NOESY mix=1.25 s
{7.75,2.36}
{7.16,2.33}
{6.90,3.78}
{7.78,6.65}
{7.60,6.92}
{7.77,7.60}
{6.90,7.59}
{6.64,7.77}
2
3
4
5
6
7
8
1H (ppm)
8
7
6
5
4
3
2
1H (ppm)

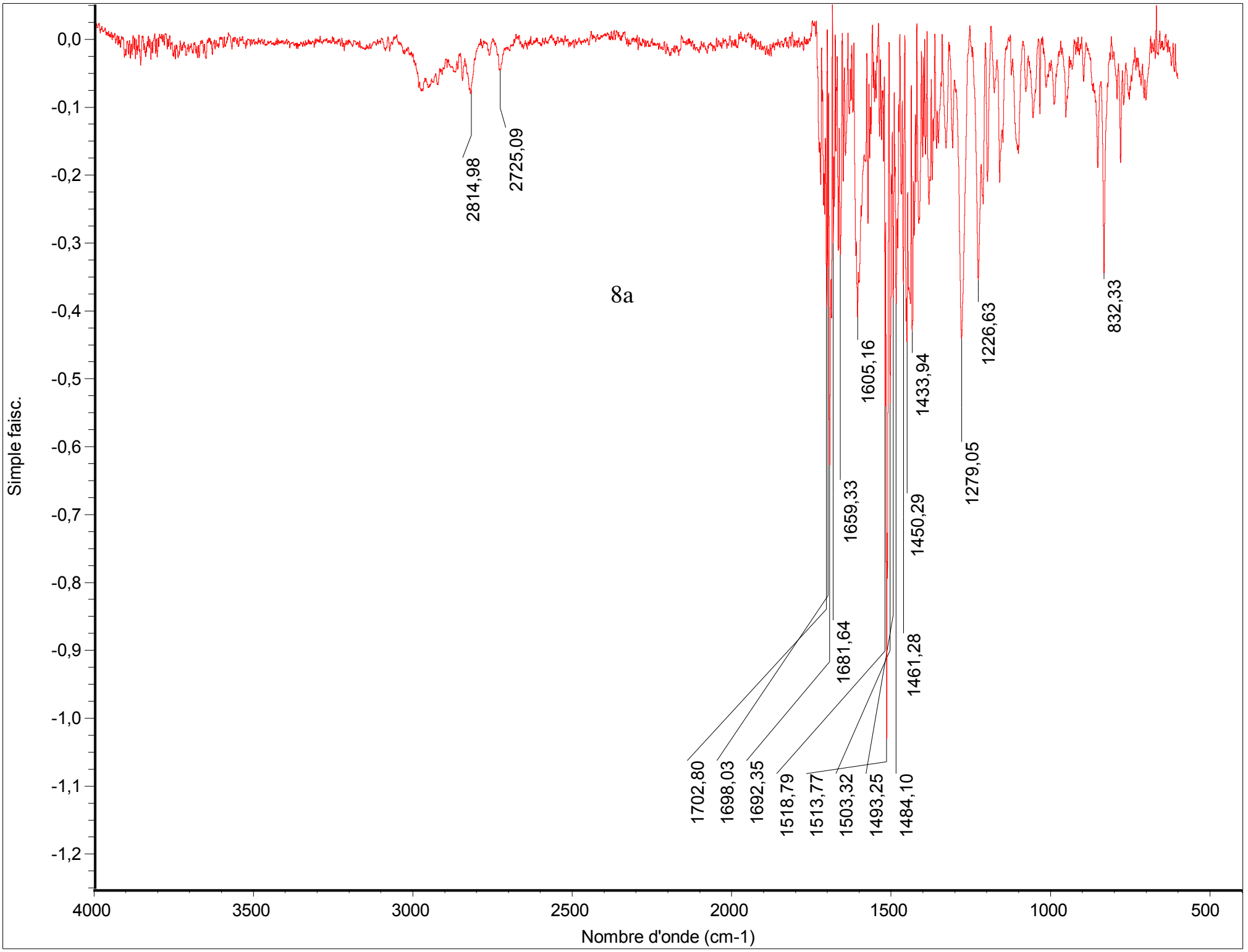
6s

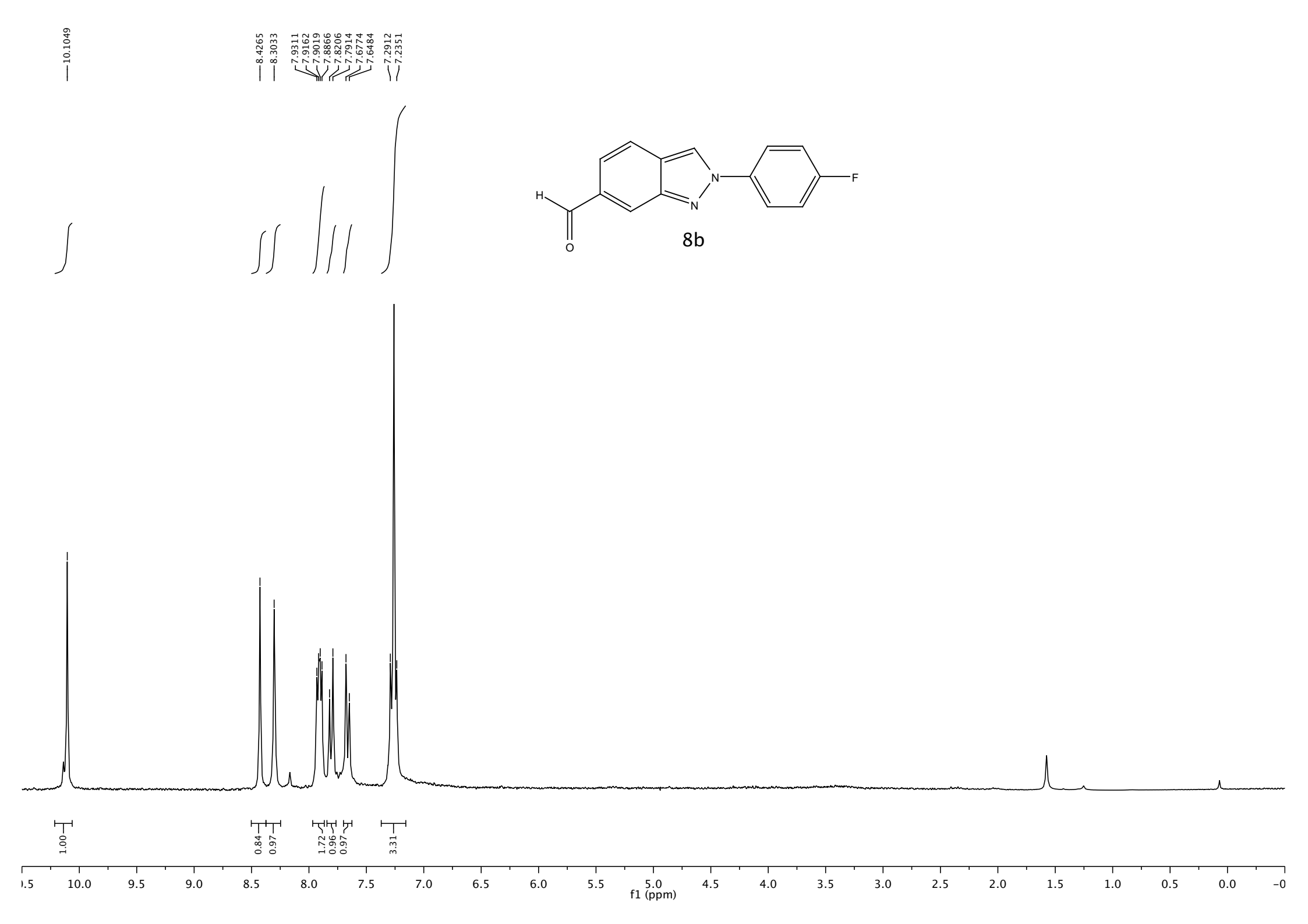

NOESY mix=1.25 s
{7.78,6.65}
{7.76,6.65}
{7.60,6.92}
{7.75,7.18}
{7.77,7.60}
{6.90,7.59}
{7.17,7.74}
{6.64,7.77}
8.0
7.5
7.0
6.5
6.6
6.8
7.0
7.2
7.4
7.6
7.8
8.0
1H (ppm)
1H (ppm)

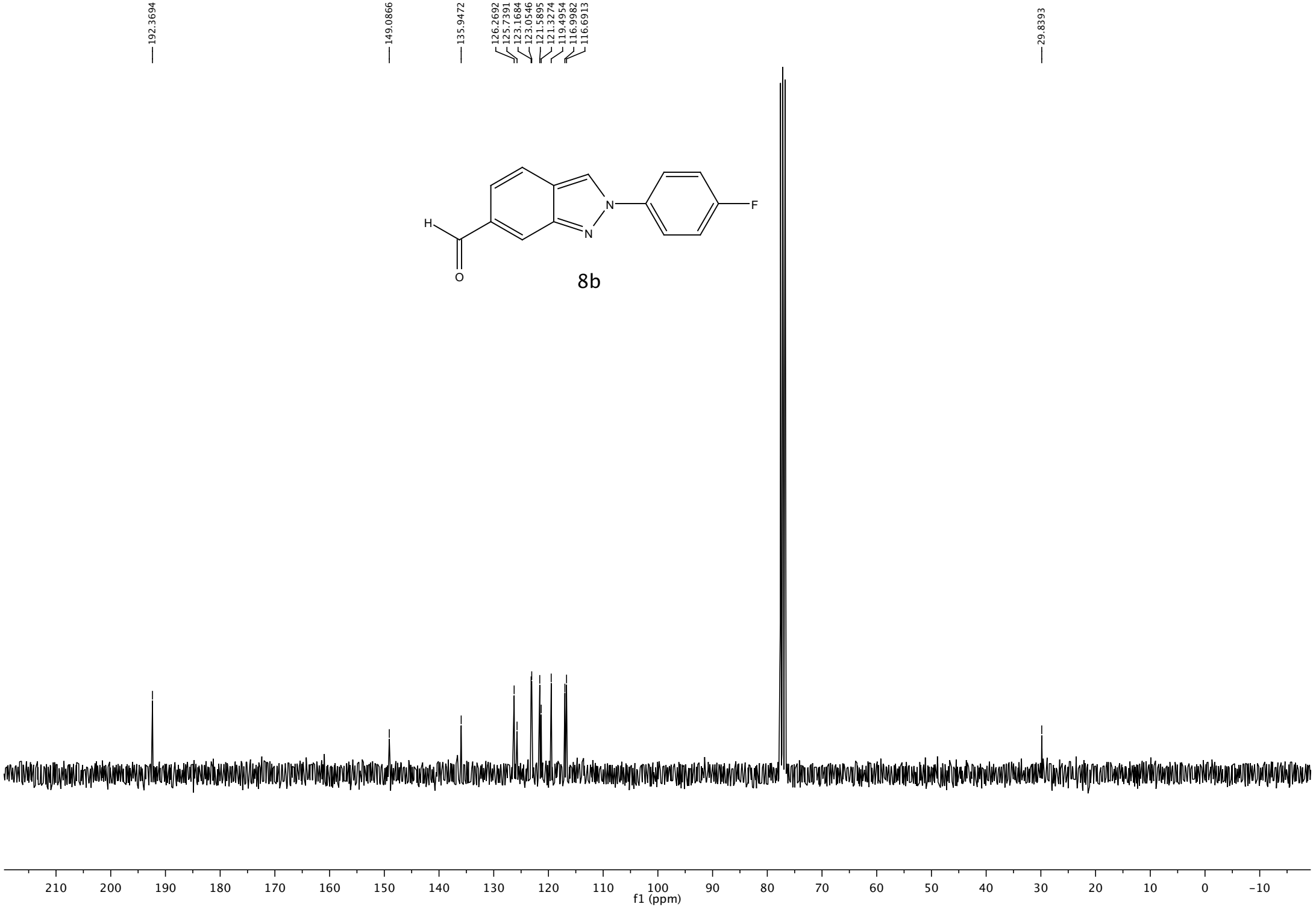
6s

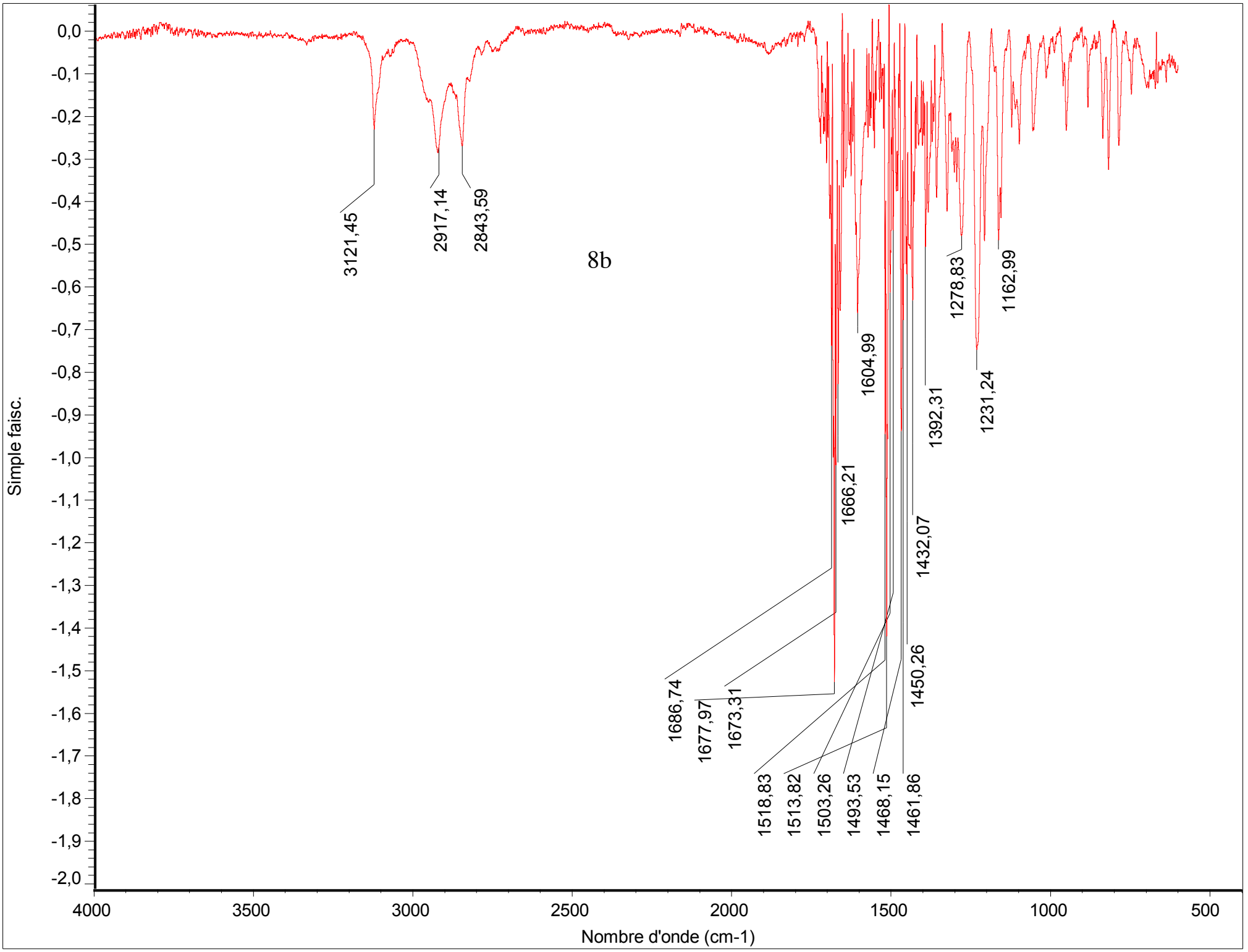

10.0727
8.2189
8.1006
7.8885
7.8607
7.7179
7.6633
7.6475
7.6337
7.2484
7.2200
H
O
N
N
F
8a
1.00
1.00
1.01
1.11
1.02
1.86
1.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

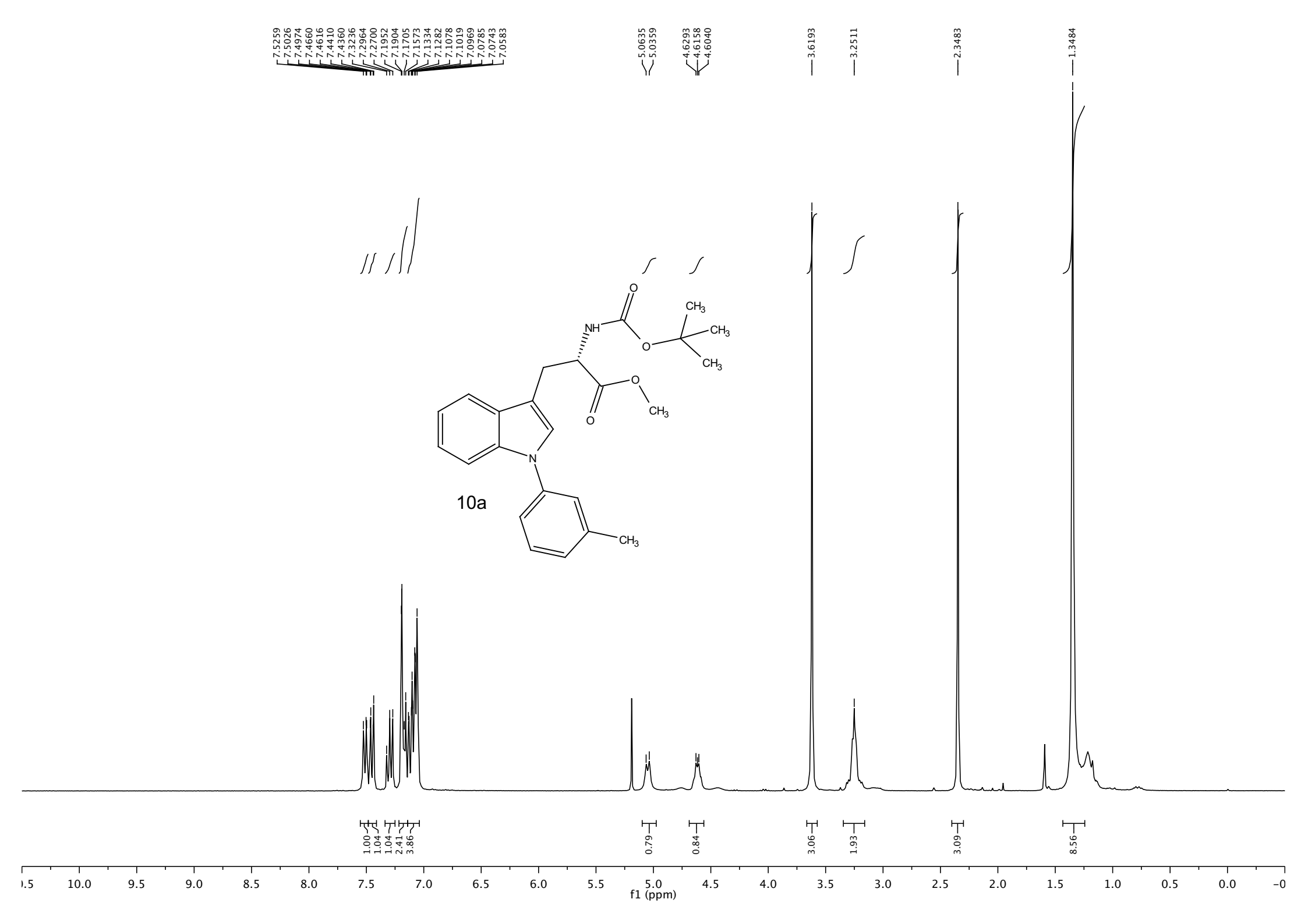

192.7812
164.0120
160.7304
139.3751
136.4137
136.3743
136.2355
136.0747
129.3616
125.7096
125.5964
122.9323
122.1442
117.5584
117.2534
114.2255
H
O
N
N
F
8a
f1 (ppm)

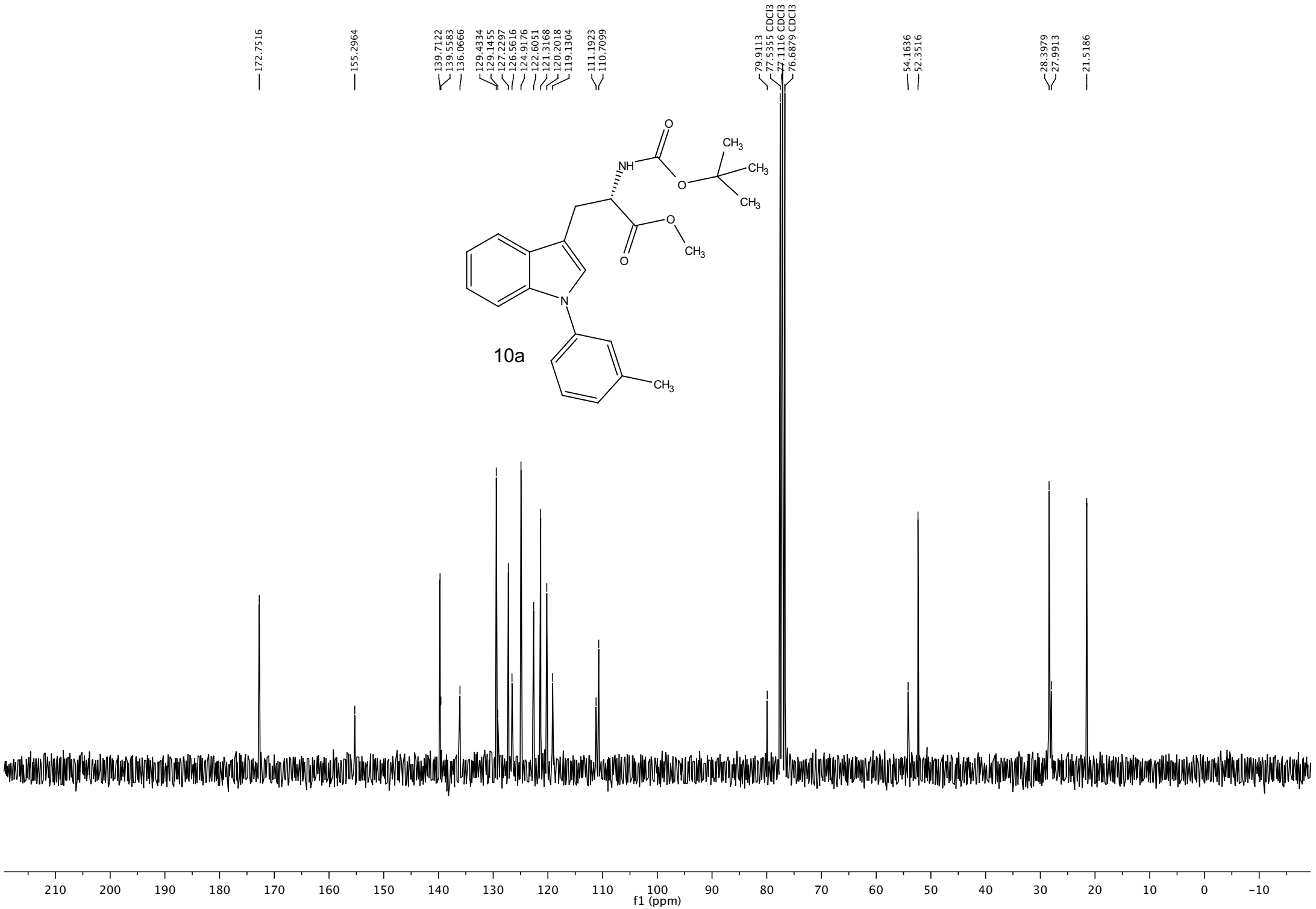

8a
Simple faisc.
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
4000
3500
3000
2500
2000
1500
1000
500
Nombre d'onde (cm-1)
2814,98
2725,09
1702,80
1698,03
1692,35
1681,64
1659,33
1605,16
1518,79
1513,77
1503,32
1493,25
1484,10
1461,28
1450,29
1433,94
1279,05
1226,63
832,33

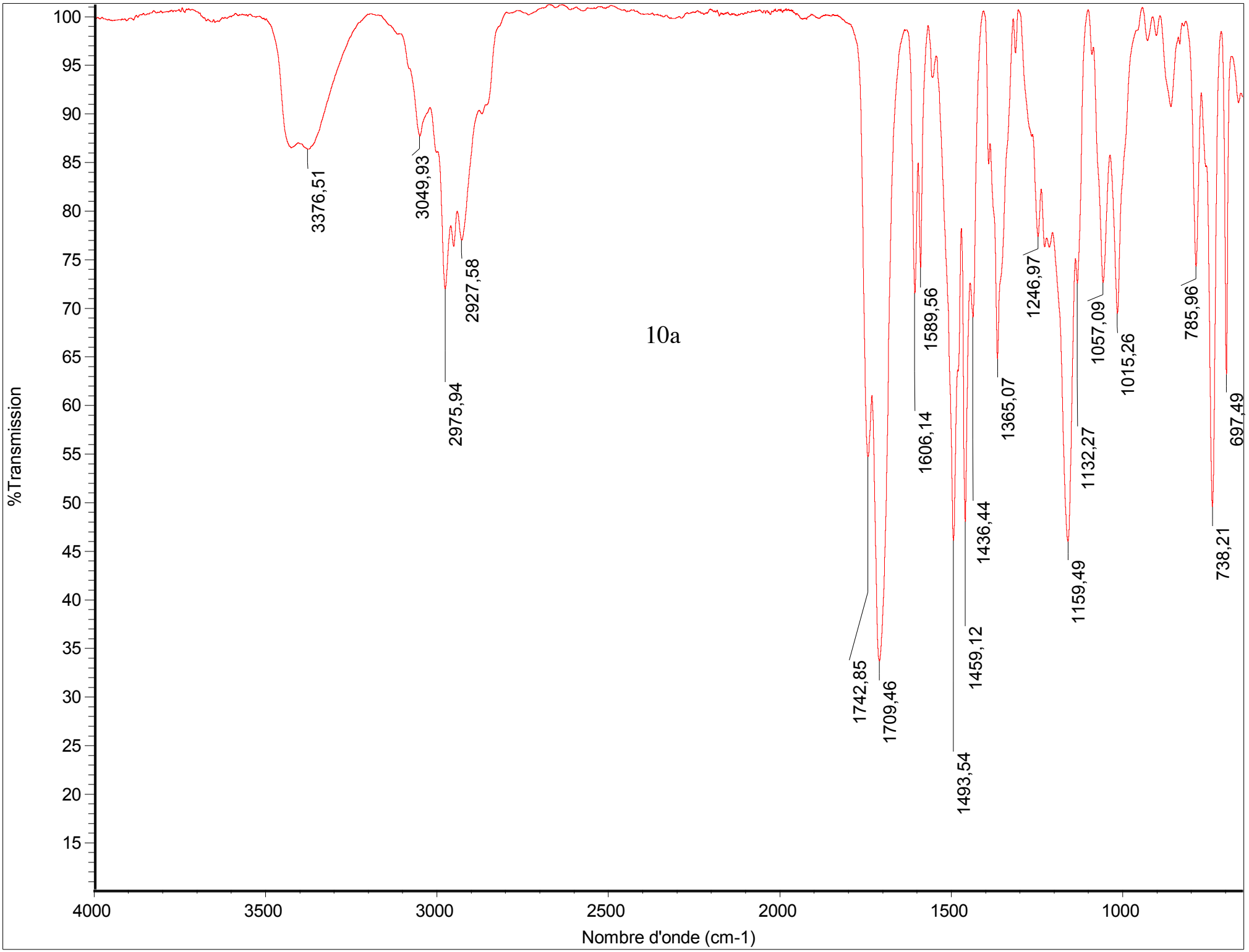

10.1049
8.4265
8.3033
7.9311
7.9162
7.9019
7.8866
7.8206
7.7914
7.6774
7.6484
7.2912
7.2351
H
O
N
N
F
8b
1.00
0.84
0.97
1.72
0.96
0.97
3.31
f1 (ppm)

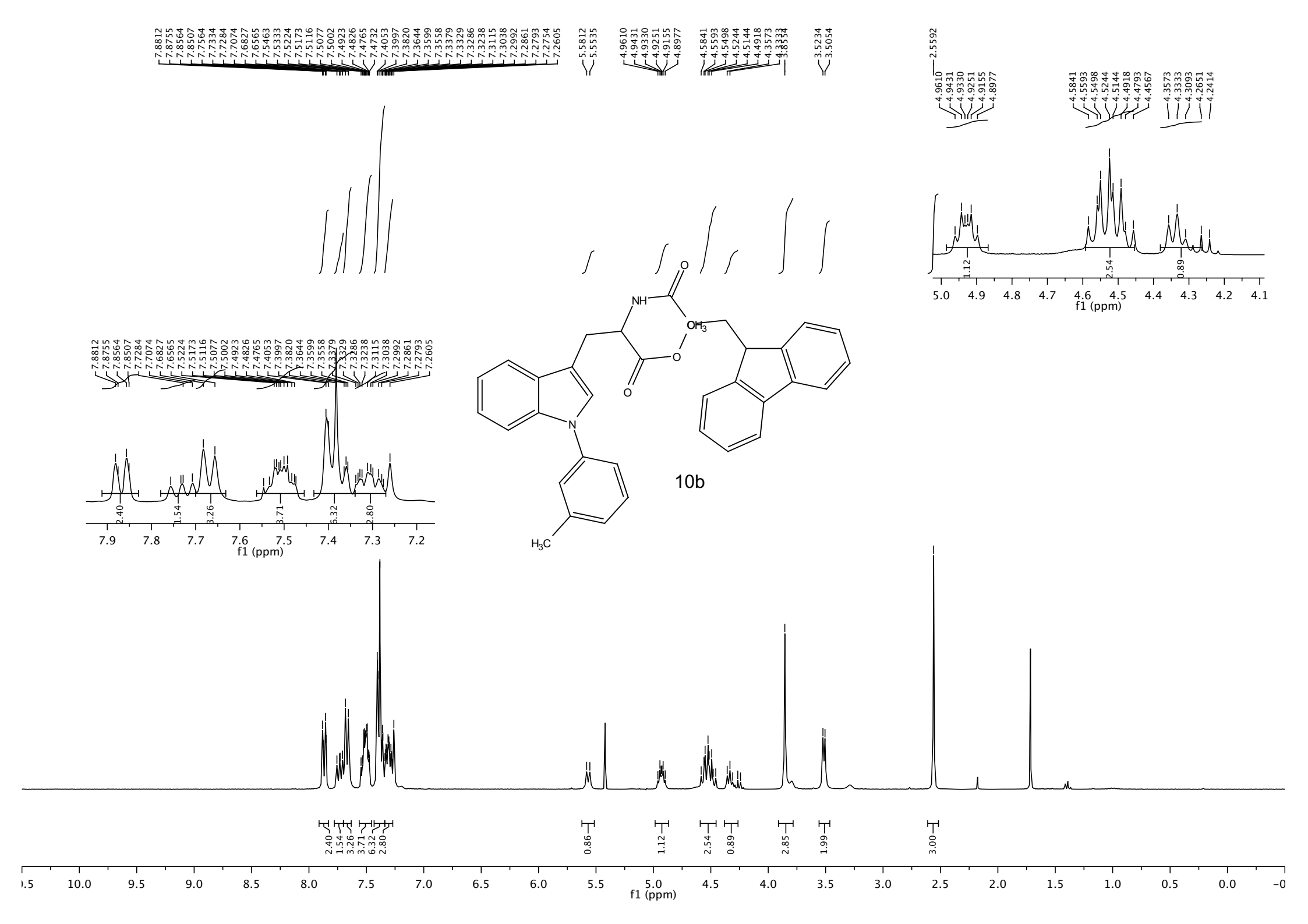

192.3694
149.0866
135.9472
126.2692
125.7391
123.1684
123.0546
121.5895
121.3274
119.4954
116.9982
116.6913
29.8393
H
O
N
N
F
8b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

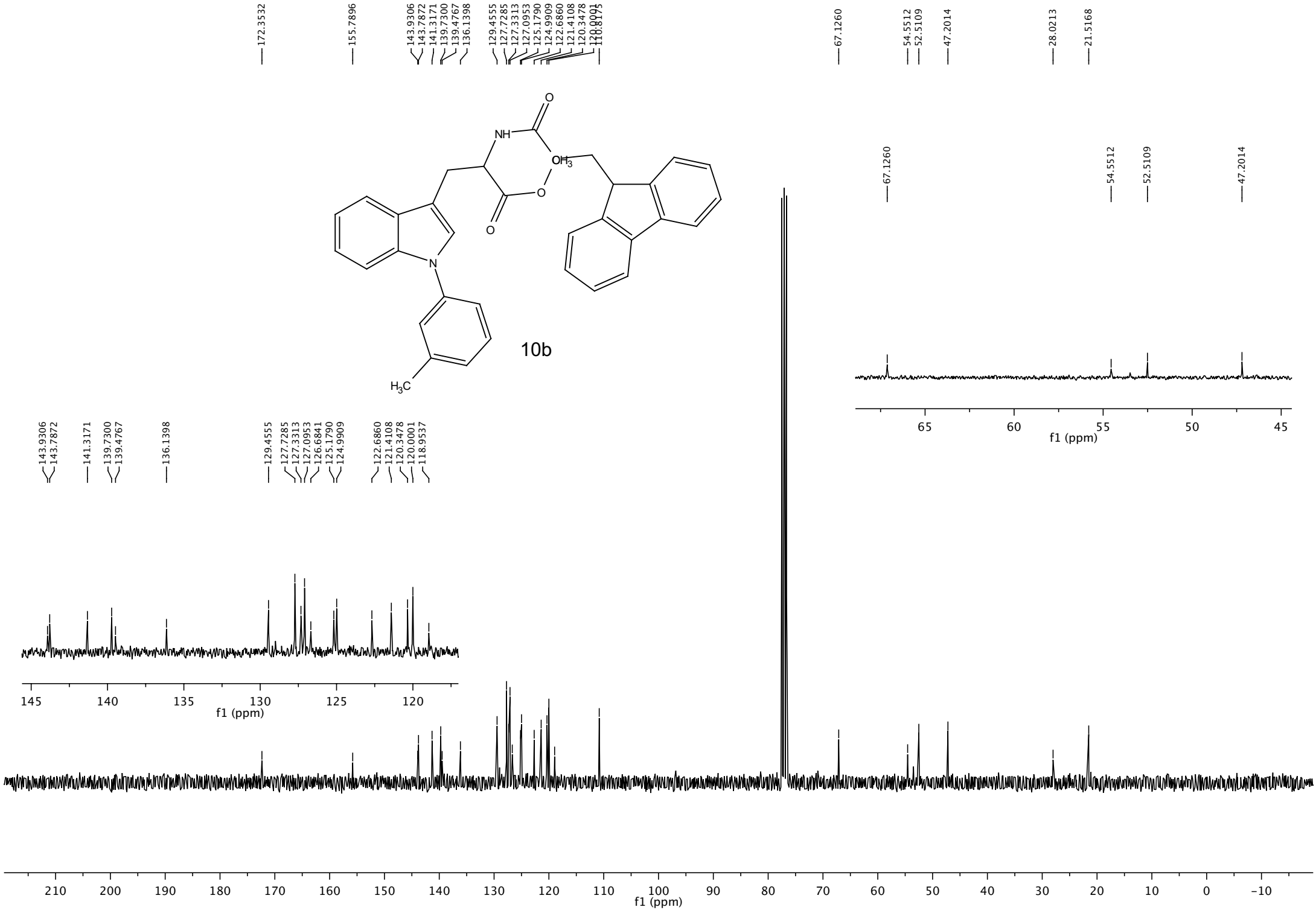

8b
Simple faisc.
Nombre d'onde (cm-1)
0,0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
-0,7
-0,8
-0,9
-1,0
-1,1
-1,2
-1,3
-1,4
-1,5
-1,6
-1,7
-1,8
-1,9
-2,0
4000
3500
3000
2500
2000
1500
1000
500
3121,45
2917,14
2843,59
1686,74
1677,97
1673,31
1666,21
1604,99
1518,83
1513,82
1503,26
1493,53
1468,15
1461,86
1450,26
1432,07
1392,31
1278,83
1231,24
1162,99

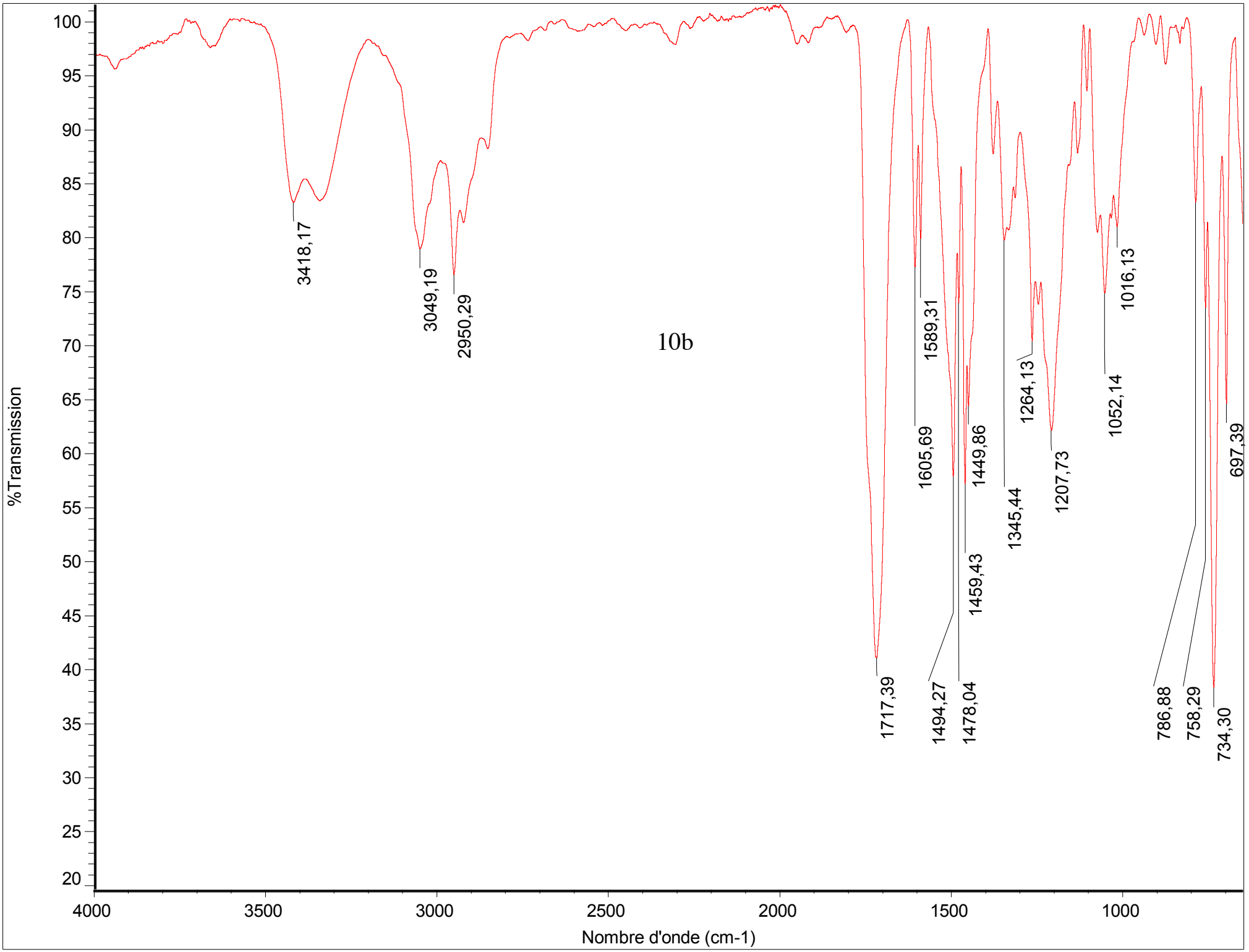

7.5259
7.5026
7.4974
7.4660
7.4616
7.4410
7.4360
7.3236
7.2964
7.2700
7.1952
7.1904
7.1705
7.1573
7.1334
7.1282
7.1078
7.1019
7.0969
7.0785
7.0743
7.0583
5.0635
5.0359
4.6293
4.6158
4.6040
3.6193
3.2511
2.3483
1.3484
NH
O
O
O
O
CH3
CH3
CH3
CH3
N
10a
1.00
1.04
1.04
2.41
3.86
0.79
0.84
3.06
1.93
3.09
8.56
f1 (ppm)


172.7516
155.2964
139.7122
139.5583
136.0666
129.4334
129.1455
127.2297
126.5616
124.9176
122.6051
121.3168
120.2018
119.1304
111.1923
110.7099
79.9113
77.5355 CDCl3
77.1116 CDCl3
76.6879 CDCl3
54.1636
52.3516
28.3979
27.9913
21.5186
NH
O
CH3
N
10a
f1 (ppm)


10a
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
4000
3500
3000
2500
2000
1500
1000
3376,51
3049,93
2975,94
2927,58
1742,85
1709,46
1606,14
1589,56
1493,54
1459,12
1436,44
1365,07
1246,97
1159,49
1132,27
1057,09
1015,26
785,96
738,21
697,49


NH
O
O
O
CH3
N
H3C
10b
f1 (ppm)


172.3532
155.7896
143.9306
143.7872
141.3171
139.7300
139.4767
136.1398
129.4555
127.7285
127.3313
127.0953
125.1790
124.9909
122.6860
121.4108
120.3478
67.1260
54.5512
52.5109
47.2014
28.0213
21.5168
NH
O
O
O
N
OH_3
H_3C
10b
f1 (ppm)


10b
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
4000
3500
3000
2500
2000
1500
1000
3418,17
3049,19
2950,29
1717,39
1605,69
1589,31
1494,27
1478,04
1459,43
1449,86
1345,44
1264,13
1207,73
1052,14
1016,13
786,88
758,29
734,30
697,39