Supporting Information

Copper-Catalyzed *O*-Arylation of *N*-Protected 1,2-Aminoalcohols Using 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 and anhydrous bismuth chloride 99.999% were purchased from Strem Chemicals. Triarylbismuthanes were prepared according to procedures that we previously reported.[2,3,4] 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, s(br) = broad 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 *O*-arylation of *N*-protected 1,2-aminoalcohols

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

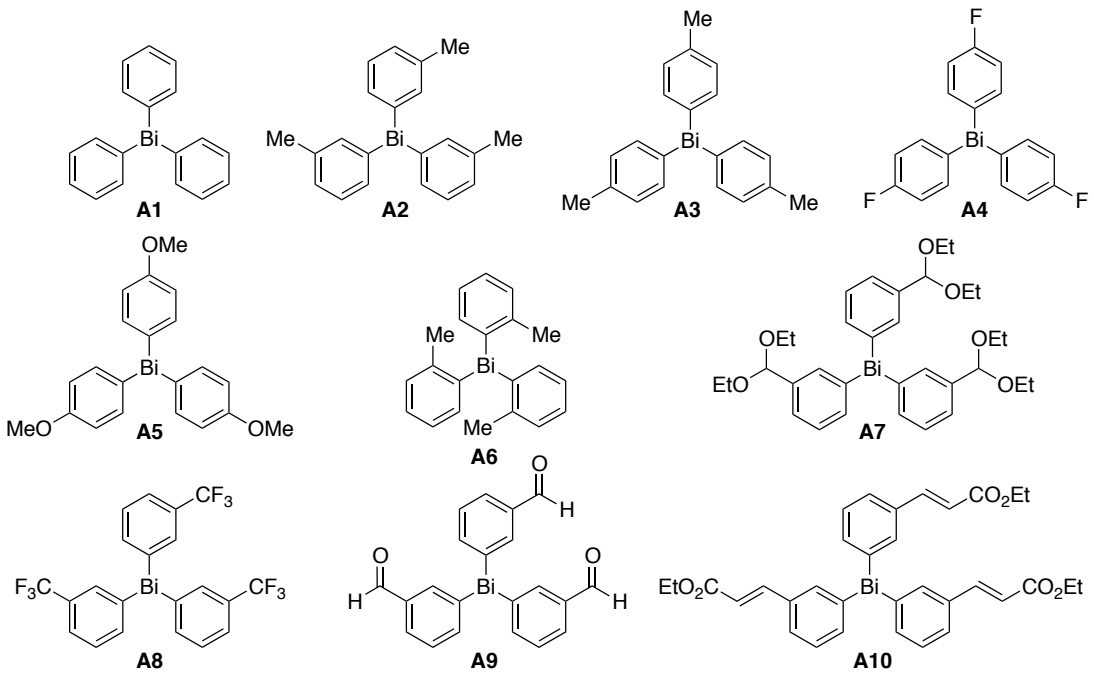


Figure S1. Functionalized organobismuthanes used in this publication. Triphenylbismuth was purchased from Strem. Organobismuthanes **A3**, **A4**, **A6**, **A7**, **A9** were synthesized according to: P. Petiot and A. Gagnon, *Eur. J. Org. Chem.*, **2013**, 5282. Organobismuthanes **A2**, **A5**, **A8**, **A10** were synthesized according to: P. Petiot, J. Dansereau and A. Gagnon, *RSC Adv.*, **2014**, 22255.

3. General procedures for the *O*-arylation of aminoalcohols

Compounds **14**, **16**, **18a-d**, **21a-n**, *cis*-**23**, *trans*-**23**, **25a**,**b**, **27a**,**b**, **29a-c** and **33a-c** were prepared according to the following procedures:

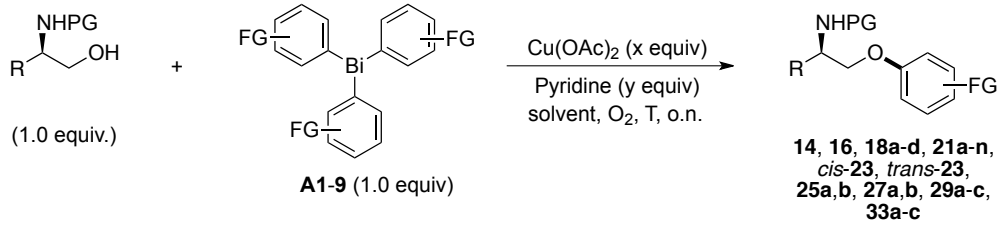


Table S1. Reaction conditions: Method A and B.

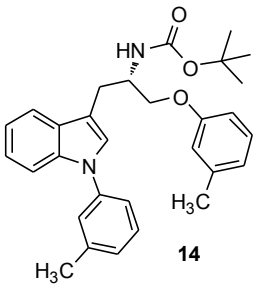
Method	Amino-alcohol (n equiv)	Ar_3Bi (**A**) (m equiv)	$Cu(OAc)_2$ (x equiv)	Pyridine (y equiv)	Solvent	Temperature
A	1.0	1.0	0.3	1.2	toluene	80°C
B	1.0	1.0	1.0	3.0	dichloromethane	50°C

Method A: In a sealed tube, triarylbismuthine **A** (1.0 equiv) was added, followed by copper (II) acetate (0.3 equiv) and the aminoalcohol (1.0 equiv). The reagents were dissolved in anhydrous toluene (4 mL) and pyridine (1.2 equiv) was added to the mixture. The reaction tube was purged with dry oxygen for 30 seconds, sealed and heated at 80°C overnight. The reaction mixture was cooled to r.t., transferred and rinsed with EtOAc 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 the indicated eluent system to give the corresponding product.

Method B: Idem as method **A** except for copper (II) acetate (1.0 equiv instead of 0.3 equiv), pyridine (3.0 equiv instead of 1.2 equiv), in dichloromethane at 50˚C.

4. Characterization of products

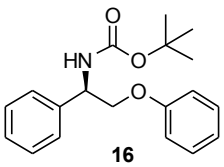
(*S*)-*tert*-Butyl-(1-(1-(*m*-tolyl)-1*H*-indol-3-yl)-3-(*m*-tolyloxy)propan-2-yl)carbamate (**14**)



14

Method B was followed on a 0.17 mmol scale starting from *N*-BOC-tryptophanol **13** and **A2**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **14** as a yellow oil (42 mg, 53%): R_f 0.65 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 8.1 Hz, 1H), 7.26 (t, *J* = 7.7 Hz, 1H), 7.14-7.02 (m, 7H), 6.71-6.62 (m, 3H), 4.98 (d, *J* = 7.8 Hz, 1H), 4.24 (s(br), 1H), 3.86 (qd, *J* = 9.2, 3.3 Hz, 2H), 3.13-3.10 (m, 2H), 2.32 (s, 3H), 2.23 (s, 3H), 1.38 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.9, 155.6, 139.7, 136.1, 129.4, 129.3, 127.0, 126.9, 124.8, 122.6, 122.0, 121.2, 120.2, 119.5, 115.6, 113.0, 111.6, 110.7, 68.1, 50.6, 28.6, 27.3, 21.6, 21.5; IR (neat) 3403, 3048, 2978, 2921, 2860, 1712, 1693, 1605, 1493, 1160; HRMS (ESI) calcd for $C_{30}H_{34}N_2O_3$: 470.2569, found 493.2457 (M+Na).

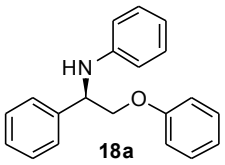
(*R*)-*tert*-Butyl-(2-phenoxy-1-phenylethyl)carbamate (**16**)



16

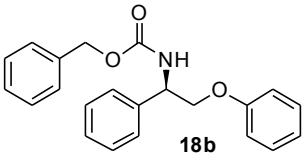
Method B was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A1**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **16** as a yellow solid (48 mg, 73%): m.p. 82°C. Spectral data was identical to literature[6]: ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.34-7.26 (m, 4H), 7.23-7.18 (m, 3H), 6.89 (t, *J* = 7.3 Hz, 1H), 6.82 (d, *J* = 8.1 Hz, 2H), 5.26 (s(br), 1H), 4.99 (s(br), 1H), 4.19-4.08 (m, 2H), 1.36 (s, 9H).

(*R*)-*N*-(2-Phenoxy-1-phenylethyl)aniline (18a)



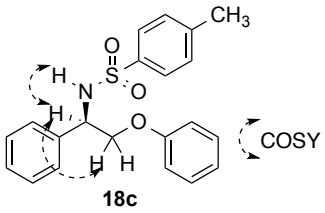
Method B was followed on a 0.36 mmol scale starting from *(R)*-2-phenyl-2-(phenylamino)ethanol **17a** and **A1**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **18a** as a white solid (65 mg, 62%): m.p. 124°C; R_f 0.66 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.52-7.49 (m, 2H), 7.41-7.27 (m, 5H), 7.15-7.09 (m, 2H), 7.05-6.96 (m, 1H), 6.94-6.91 (m, 2H), 6.71 (t, *J* = 7.4 Hz, 1H), 6.60-6.57 (m, 2H), 4.74 (dd, *J* = 8.3, 3.8 Hz, 1H), 4.65 (s(br), 1H), 4.24 (dd, *J* = 9.6, 3.9 Hz, 1H), 4.08 (dd, *J* = 9.6, 8.5 Hz, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.4, 147.5, 140.2, 129.6, 129.2, 128.9, 127.8, 127.0, 121.4, 118.0, 114.8, 114.1, 72.0, 58.2; IR (neat) 3405, 3056, 3026, 2922, 2850, 1598, 1496, 1453, 1234, 1173, 748, 690; HRMS (ESI) calcd for $C_{20}H_{19}NO$: 289.1467, found 290.1548 (M+H). To further confirm the chemoselectivity of the reaction and the structure of the compound, we compared the data with the *N*,*N*-diphenyl isomer from the literature and found the two compounds to be different.[7]

(*R*)-Benzyl (2-phenoxy-1-phenylethyl)carbamate (18b)



Method B was followed on a 0.18 mmol scale starting from *(R)*-benzyl (2-hydroxy-1-phenylethyl)carbamate **17b** and **A1**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **18b** as a white solid (50 mg, 80%): m.p. 84°C; R_f 0.40 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.38-7.21 (m, 12H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.83 (d, *J* = 7.9 Hz, 2H), 5.59 (s(br), 1H), 5.13-5.03 (m, 3H), 4.24-4.14 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.3, 156.0, 139.5, 136.4, 129.6, 128.7, 128.6, 128.3, 127.9, 126.9, 121.4, 114.7, 70.4, 67.1, 54.5; IR (neat) 3403, 3324, 3063, 3032, 2937, 1698, 1599, 1496, 1456, 1239, 1050, 753, 696; HRMS (ESI) calcd for $C_{22}H_{21}NO_3$: 347.1521, found 348.1595 (M+H).

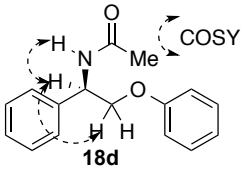
(*R*)-4-Methyl-*N*-(2-phenoxy-1-phenylethyl)benzenesulfonamide (18c)



18c

Method B was followed on a 0.17 mmol scale starting from *(R)-N*-(2-hydroxy-1-phenylethyl)-4-methyl-*S*-methylenebenzenesulfinamide **17c** and **A1**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **18c** as a colorless oil (48 mg, 77%): R_f 0.31 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.31-7.26 (m, 7H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.81-6.79 (m, 2H), 5.37 (d, *J* = 5.5 Hz, 1H), 4.72 (q, *J* = 5.3 Hz, 1H), 4.18-4.06 (m, 2H), 2.42 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 157.8, 143.3, 137.4, 137.2, 129.5, 129.4, 128.6, 128.1, 127.3, 121.5, 114.5, 70.4, 57.1, 21.5; IR (neat) 3305, 3075, 3050, 2983, 2925, 1740, 1373, 1235, 1044, 754, 691; HRMS (ESI) calcd for $C_{21}H_{21}NO_3S$: 367.1242, found 390.1139 (M+Na). The connectivity was further confirmed by COSY-NMR analysis, demonstrating that the *O*-phenyl isomer has been formed.

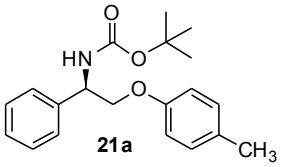
(*R*)-*N*-(2-Phenoxy-1-phenylethyl)acetamide (18d)



18d

Method B was followed on a 0.28 mmol scale starting from *(R)-N*-(2-hydroxy-1-phenylethyl)acetamide **17d** and **A1**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **18d** as a yellow oil (51 mg, 71%): R_f 0.10 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.48-7.41 (m, 3H), 7.39-7.31 (m, 4H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.97-6.94 (m, 2H), 6.45 (d, *J* = 7.6 Hz, 1H), 5.49-5.43 (m, 1H), 4.35-4.26 (m, 2H), 2.10 (s, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 169.7, 158.4, 139.3, 129.6, 128.7, 127.8, 127.1, 121.4, 114.7, 69.9, 52.5, 23.4; IR (neat) 3438, 3285, 3061, 3028, 2920, 2859, 1650, 1599, 1494, 1453, 1238, 751, 690; HRMS (ESI) calcd for $C_{16}H_{17}NO_2$: 255.1259, found 256.1310 (M+H). The connectivity was further confirmed by COSY-NMR analysis, demonstrating that the *O*-phenyl isomer has been formed.

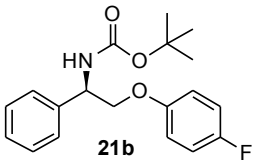
(*R*)-*tert*-Butyl (1-phenyl-2-(*p*-tolyloxy)ethyl)carbamate (**21a**)



21a

Method A was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A3**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **21a** as a colorless oil (47 mg, 68%): R_f 0.55 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.41-7.26 (m, 5H), 7.07 (d, *J* = 8.3 Hz, 2H), 6.78 (d, *J* = 8.6 Hz, 2H), 5.34 (s(br), 1H), 5.05 (s(br), 1H), 4.24-4.12 (m, 2H), 2.29 (s, 3H), 1.44 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 156.3, 155.4, 140.0, 130.5, 130.0, 128.6, 127.6, 126.8, 114.6, 79.8, 70.8, 28.4, 20.5; IR (neat) 3463, 3339, 3081, 3031, 2976, 2926, 2869, 1697, 1509, 1365, 1236, 1164, 1047, 699; HRMS (ESI) calcd for $C_{20}H_{25}NO_3$: 327.1834, found 350.1717 (M+Na).

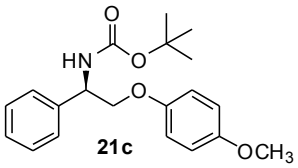
(*R*)-*tert*-Butyl (2-(4-fluorophenoxy)-1-phenylethyl)carbamate (**21b**)



21b

Method B was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A4**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **21b** as a yellow solid (50 mg, 72%): m.p. 86°C; R_f 0.57 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.39-7.26 (m, 5H), 6.98-6.91 (m, 2H), 6.84-6.79 (m, 2H), 5.28 (s(br), 1H), 5.04 (s(br), 1H), 4.22-4.12 (m, 2H), 1.43 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 159.1, 156.0, 155.3, 154.6, 139.7, 128.6, 127.7, 126.8, 116.0, 115.8, 115.7, 79.9, 71.3, 28.4; IR (neat) 3445, 3018, 2979, 2931, 1704, 1506, 1367, 1215, 1165, 907, 751, 731; HRMS (ESI) calcd for $C_{19}H_{22}FNO_3$: 331.1584, found 354.1476 (M+Na).

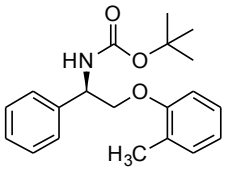
(*R*)-*tert*-Butyl (2-(4-methoxyphenoxy)-1-phenylethyl)carbamate (21c)



21c

Method A was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A5**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **21c** as a yellow oil (38 mg, 53%): R_f 0.43 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.40-7.26 (m, 5H), 6.82 (s, 4H), 5.33 (s(br), 1H), 5.02 (s(br), 1H), 4.21-4.10 (m, 2H), 3.76 (s, 3H), 1.43 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 155.4, 154.2, 152.6, 128.6, 127.6, 126.8, 115.7, 114.7, 79.8, 71.5, 64.9, 55.8, 28.4; IR (neat) 3456, 3345, 3100, 3063, 2975, 2932, 2834, 1701, 1505, 1461, 1227, 1162, 1032, 699; HRMS (ESI) calcd for $C_{20}H_{25}NO_4$: 343.1784, found 366.1665 (M+Na).

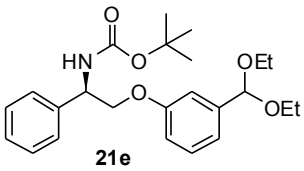
(*R*)-*tert*-Butyl (1-phenyl-2-(*o*-tolyloxy)ethyl)carbamate (21d)



21d

Method A was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A6**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **21d** as a yellow solid (25 mg, 36%): m.p. 100°C; R_f 0.54 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.41-7.26 (m, 5H), 7.15-7.10 (m, 2H), 6.86 (t, *J* = 7.1 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 5.31 (s(br), 1H), 5.11 (s(br), 1H), 4.24 (dd, *J* = 9.3, 4.5 Hz, 1H), 4.16-4.11 (m, 1H), 2.17 (s, 3H), 1.44 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 156.4, 155.4, 139.8, 130.8, 128.5, 127.6, 126.9, 126.8, 120.9, 111.0, 79.8, 70.8, 29.7, 28.4, 16.3; IR (neat) 3341, 3063, 3031, 2976, 2926, 2853, 1703, 1495, 1243, 1169, 750; HRMS (ESI) calcd for $C_{20}H_{25}NO_3$: 327.1834, found 350.1717 (M+Na).

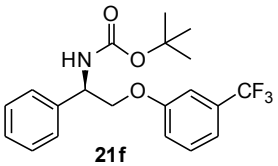
(*R*)-*tert*-Butyl (2-(3-(diethoxymethyl)phenoxy)-1-phenylethyl)carbamate (21e)



21e

Method A was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A7**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **21e** as a colorless oil (50 mg, 57%): R_f 0.29 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.44-7.39 (m, 4H), 7.36-7.29 (m, 2H), 7.10-7.05 (m, 2H), 6.86 (dd, *J* = 7.8, 2.0 Hz, 1H), 5.48 (s, 1H), 5.38 (s, 1H), 5.09 (s(br), 1H), 4.30-4.19 (m, 2H), 3.70-3.51 (m, 4H), 1.47 (s, 9H), 1.26 (t, *J* = 7.1 Hz, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.5, 155.4, 140.9, 129.3, 128.6, 127.6, 126.8, 119.6, 114.6, 112.7, 101.3, 79.8, 70.6, 61.1, 31.6, 28.4, 22.7, 15.2, 14.1, 11.5; IR (neat) 3344, 3078, 3065, 2976, 2931, 2729, 1692, 1597, 1259, 1166, 1050; HRMS (ESI) calcd for $C_{24}H_{33}NO_5$: 415.2359, found 438.2245 (M+Na).

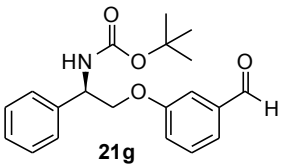
(*R*)-*tert*-Butyl (1-phenyl-2-(3-(trifluoromethyl)phenoxy)ethyl)carbamate (21f)



21f

Method A was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A8**. The crude product was purified on silica gel (10% EtOAc/hexanes) to afford **21f** as a yellow oil (34 mg, 42%): R_f 0.54 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.40-7.30 (m, 6H), 7.21 (d, *J* = 7.7 Hz, 1H), 7.10-7.04 (m, 2H), 5.25 (s(br), 1H), 5.08 (s(br), 1H), 4.30-4.21 (m, 2H), 1.44 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.5, 155.3, 139.4, 132.5, 132.1, 131.7, 131.3, 130.0, 128.7, 127.8, 126.8, 125.7, 122.1, 118.0, 111.6, 80.0, 70.9, 28.3; IR (neat) 3473, 3329, 3079, 3033, 2978, 2931, 1703, 1493, 1452, 1238, 1167, 1126, 698; HRMS (ESI) calcd for $C_{20}H_{22}F_3NO_3$: 381.1552, found 404.1446 (M+Na).

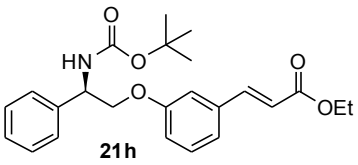
(*R*)-*tert*-Butyl (2-(3-formylphenoxy)-1-phenylethyl)carbamate (21g)



21g

Method B was followed on a 0.21 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A9**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **21g** as a colorless oil (19 mg, 27%): R_f 0.26 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$); δ 9.95 (s, 1H), 7.48-7.26 (m, 8H), 7.15 (dt, *J* = 7.5, 2.1 Hz, 1H), 5.29 (s(br), 1H), 5.08 (s(br), 1H), 4.31-4.19 (m, 2H), 1.43 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 192.0, 159.0, 155.3, 139.4, 137.8, 130.2, 128.7, 127.8, 126.8, 123.9, 121.8, 113.2, 80.0, 70.9, 53.9, 28.4; IR (neat) 3355, 3085, 3056, 2976, 2931, 2740, 1689, 1596, 1585, 1484, 1451, 1251, 1164, 1050; HRMS (ESI) calcd for $C_{20}H_{23}NO_4$: 341.1627, found 364.1529 (M+Na).

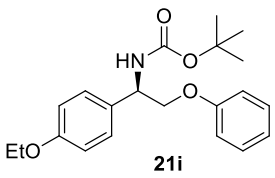
(*R*,*E*)-Ethyl 3-(3-(2-((*tert*-butoxycarbonyl)amino)-2-phenylethoxy)phenyl)acrylate (21h)



21h

Method A was followed on a 0.08 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate **15** and **A10**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **21h** as a colorless oil (23 mg, 70%): R_f 0.30 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$); δ 7.63 (d, *J* = 15.9 Hz, 1H), 7.42-7.26 (m, 6H), 7.12 (d, *J* = 7.7 Hz, 1H), 7.05 (s, 1H), 6.91 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.43 (d, *J* = 15.9 Hz, 1H), 5.31 (s(br), 1H), 5.08 (s(br), 1H), 4.30-4.16 (m, 4H), 1.45 (s, 9H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 166.9, 158.8, 155.3, 144.3, 135.9, 129.9, 128.7, 127.8, 126.8, 121.4, 118.8, 116.7, 113.7, 80.0, 70.7, 60.5, 28.4, 14.3; IR (neat) 3351, 3071, 3048, 2977, 2932, 1700, 1637, 1579, 1492, 1445, 1365, 1245, 1159, 1030; HRMS (ESI) calcd for $C_{24}H_{29}NO_5$: 411.2046, found 434.1941 (M+Na).

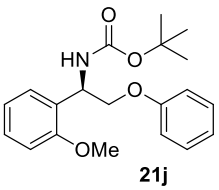
(*R*)-*tert*-Butyl (1-(4-ethoxyphenyl)-2-phenoxyethyl)carbamate (21i)



21i

Method B was followed on a 0.18 mmol scale starting from (*R*)-*tert*-butyl (1-(4-ethoxyphenyl)-2-hydroxyethyl)carbamate and **A1**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford **21i** as a white solid (26 mg, 40%): m.p. 125°C; R_f 0.40 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.34-7.27 (m, 4H), 6.98 (t, *J* = 7.3 Hz, 1H), 6.93-6.87 (m, 4H), 5.29 (s(br), 1H), 5.02 (s(br), 1H), 4.25-4.20 (m, 1H), 4.17-4.15 (m, 1H), 4.04 (q, *J* = 7.0 Hz, 2H), 1.46-1.41 (m, 12H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.4, 155.4, 131.8, 129.5, 128.0, 121.2, 115.4, 114.6, 114.5, 79.8, 70.6, 63.5, 28.4, 14.9; IR (neat) 3350, 3065, 3034, 2977, 2930, 2875, 1694, 1501, 1496, 1238, 1164, 1046, 754; HRMS (ESI) calcd for $C_{21}H_{27}NO_4$: 357.1940, found 380.1837 (M+Na).

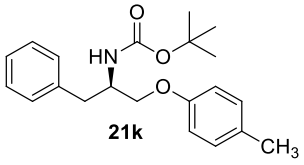
(*R*)-*tert*-Butyl (1-(2-methoxyphenyl)-2-phenoxyethyl)carbamate (21j)



21j

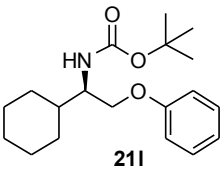
Method B was followed on a 0.13 mmol scale starting from (*R*)-*tert*-butyl (2-hydroxy-1-(2-methoxyphenyl)ethyl)carbamate and **A1**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford **21j** as a white solid (17 mg, 38%): m.p. 104°C; R_f 0.38 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.35-7.22 (m, 4H), 7.00-6.95 (m, 2H), 6.89 (dd, *J* = 8.8, 3.7 Hz, 3H), 5.62 (s(br), 1H), 5.39 (s(br), 1H), 4.24 (dd, *J* = 9.5, 5.1 Hz, 1H), 4.17-4.12 (m, 1H), 3.88 (s, 3H), 1.47 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.6, 156.8, 155.4, 129.6, 129.4, 128.7, 128.5, 120.9, 120.7, 115.3, 114.7, 110.6, 79.6, 69.4, 55.3, 50.8, 28.4; IR (neat) 3444, 3361, 3061, 3038, 2975, 2933, 2837, 1701, 1600, 1492, 1461, 1365, 1240, 1166, 752; HRMS (ESI) calcd for $C_{20}H_{25}NO_4$: 343.1784, found 366.1680 (M+Na).

(*R*)-*tert*-Butyl (1-phenyl-3-(*p*-tolyloxy)propan-2-yl)carbamate (21k)



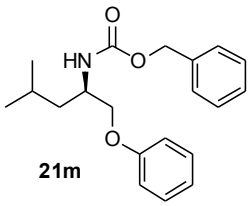
Method A was followed on a 0.20 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)carbamate and **A3**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford **21k** as a yellow solid (33 mg, 48%): m.p. 69°C; R_f 0.54 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.33-7.24 (m, 5H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 5.00 (s(br), 1H), 4.17 (s(br), 1H), 3.92-3.84 (m, 2H), 3.02 (d, *J* = 7.7 Hz, 2H), 2.33 (s, 3H), 1.47 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 156.5, 155.3, 137.9, 130.3, 130.0, 129.5, 128.5, 126.5, 114.4, 79.5, 67.8, 51.4, 37.8, 28.4, 20.5; IR (neat) 3452, 3350, 3061, 3028, 2976, 2925, 2868, 1710, 1510, 1238, 1165, 1039, 700; HRMS (ESI) calcd for $C_{21}H_{27}NO_3$: 341.1991, found 364.1879 (M+Na).

(*R*)-*tert*-Butyl (1-cyclohexyl-2-phenoxyethyl)carbamate (21l)



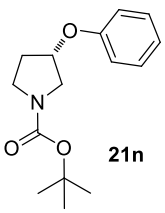
Method A was followed on a 0.20 mmol scale starting from *tert*-butyl (*1R*)-1-cyclohexyl-2-hydroxyethylcarbamate and **A1**. The crude material was purified on silica gel (8% EtOAc/hexanes) to afford **21l** as a white solid (39 mg, 60%): m.p. 130°C; R_f0.31 (10% AcOEt/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.31-7.26 (m, 2H), 6.98-6.93 (m, 1H), 6.91-6.88 (m, 2H), 4.85 (d, *J* = 9.4 Hz, 1H), 4.06 (dd, *J* = 9.4, 3.2 Hz, 1H), 3.95 (dd, *J* = 9.4, 3.8 Hz, 1H), 3.74-3.68 (m, 1H), 1.89-1.66 (m, 6H), 1.45 (s, 9H), 1.26-1.01 (m, 5H); ^{13}C-NMR (300 MHz, $CDCl_3$) δ 158.8, 155.8, 129.5, 120.9, 114.5, 79.2, 67.7, 54.5, 39.0, 29.9, 29.3, 28.4, 26.3, 26.1, 24.7; IR (neat) 3392, 3008, 2965, 2931, 2847, 1686, 1601, 1498, 1467, 1239, 1167, 1152, 753, 692; HRMS (ESI) calcd for $C_{19}H_{29}NO_3$: 319.2147, found 342.2025 (M+Na).

Benzyl (*R*)-(4-methyl-1-phenoxypentan-2-yl)carbamate (21m)



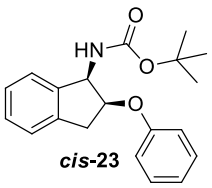
Method A was followed on a 0.20 mmol scale starting from benzyl (*R*)-(1-hydroxy-4-methylpentan-2-yl)carbamate and **A1**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford **21m** as a colorless oil (32 mg, 49%): R_f 0.55 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.41-7.29 (m, 7H), 7.03-6.88 (m, 3H), 5.16 (s, 2H), 5.03 (d, *J* = 8.5 Hz, 1H), 4.19-3.97 (m, 3H), 1.80-1.68 (m, 1H), 1.63-1.54 (m, 2H), 1.00 (d, *J* = 6.5 Hz, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.7, 156.0, 136.5, 129.6, 129.5, 128.6, 128.1, 121.0, 115.3, 114.5, 69.8, 66.8, 48.9, 41.0, 36.7, 24.8, 23.0, 22.3; IR (neat) 3324, 3065, 3038, 2955, 2869, 1695, 1599, 1513, 1496, 1237, 753; HRMS (ESI) calcd for $C_{20}H_{25}NO_3$: 327.1834, found 328.1922 (M+H).

(*S*)-*tert*-Butyl 3-phenoxypyrrolidine-1-carboxylate (21n)



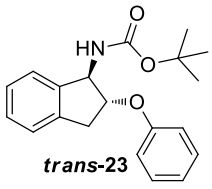
Method B was followed on a 0.27 mmol scale starting from (*S*)-*tert*-butyl 3-hydroxypyrrolidine-1-carboxylate and **A1**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **21n** as a yellow oil (37 mg, 52%): R_f 0.46 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.31-7.28 (m, 2H), 7.00-6.98 (m, 1H), 6.89 (d, *J* = 8.0 Hz, 2H), 4.90 (s, 1H), 3.65-3.55 (m, 4H), 2.18-2.06 (m, 2H), 1.49 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 157.2, 154.6, 129.6, 121.1, 115.6, 79.4, 76.3, 75.5, 51.7, 51.4, 44.1, 43.8, 31.5, 30.8, 28.5; IR (neat) 3069, 3038, 2975, 2881, 1690, 1599, 1587, 1494, 1401, 1364, 1237, 1164, 752; HRMS (ESI) calcd for $C_{15}H_{21}NO_3$: 263.1521, found 286.1420 (M+Na).

***tert*-Butyl ((*1R*,*2S*)-2-phenoxy-2,3-dihydro-*1H*-inden-1-yl)carbamate (*cis*-23)**



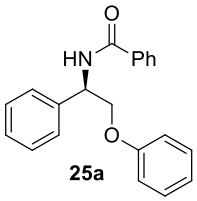
Method B was followed on a 0.20 mmol scale starting from *tert*-butyl ((*1R*,*2S*)-2-hydroxy-2,3-dihydro-*1H*-inden-1-yl)carbamate *cis*-**22** and **A1**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford *cis*-**23** as a yellow solid (34 mg, 52%): m.p. 106°C; R_f 0.57 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.30-7.12 (m, 6H), 6.91-6.81 (m, 3H), 5.40-5.35 (m, 1H), 5.28-5.25 (m, 1H), 5.07 (s(br), 1H), 3.08 (d, *J* = 2.5 Hz, 2H), 1.40 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 157.6, 156.2, 141.7, 139.4, 129.6, 128.0, 127.2, 125.1, 124.1, 121.3, 115.8, 79.7, 78.8, 58.0, 36.9, 28.4; IR (neat) 3471, 3359, 3098, 3061, 2981, 2929, 1695, 1598, 1495, 1243, 1171, 1061; HRMS (ESI) calcd for $C_{20}H_{23}NO_3$: 325.1678, found 348.1578 (M+Na).

***tert*-Butyl ((*1R*,*2R*)-2-phenoxy-2,3-dihydro-*1H*-inden-1-yl)carbamate (*trans*-23)**



Method B was followed on a 0.20 mmol scale starting from *tert*-butyl ((*1R*,*2R*)-2-hydroxy-2,3-dihydro-*1H*-inden-1-yl)carbamate *trans*-**22** and **A1**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford *trans*-**23** as a white solid (45 mg, 69%): m.p. 115°C; R_f 0.46 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.39-7.24 (m, 6H), 7.06-6.98 (m, 3H), 5.32 (s(br), 1H), 4.96-4.91 (m, 1H), 4.84 (s(br), 1H), 3.51 (dd, *J* = 16.4, 6.5 Hz, 1H), 3.04 (dd, *J* = 16.4, 4.8 Hz, 1H), 1.50 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.0, 155.4, 140.6, 139.9, 129.5, 128.6, 127.4, 125.1, 124.6, 121.1, 115.8, 83.8, 79.8, 61.4, 36.9, 28.4; IR (neat) 3338, 3089, 3050, 2974, 2875, 1689, 1519, 1493, 1235, 1166, 1055, 746; HRMS (ESI) calcd for $C_{20}H_{23}NO_3$: 325.1678, found 348.1562 (M+Na).

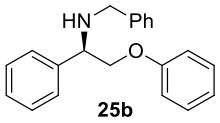
(*R*)-*N*-(2-Phenoxy-1-phenylethyl)benzamide (25a)



25a

Method B was followed on a 0.083 mmol scale starting from *(R)*-*N*-(2-hydroxy-1-phenylethyl)benzamide **24a** and **A1**. The crude product was purified on silica gel (15% EtOAc/hexanes) to afford **25a** as a white solid (18 mg, 68%): m.p. 123°C; R_f 0.25 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.83-7.80 (m, 2H), 7.54-7.26 (m, 9H), 7.01-6.92 (m, 4H), 5.64-5.58 (m, 1H), 4.42-4.33 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 167.1, 158.4, 139.3, 131.7, 129.6, 128.8, 128.7, 127.9, 127.1, 127.0, 121.5, 114.7, 70.0, 52.9; IR (neat) 3446, 3295, 3061, 3030, 2925, 2873, 1634, 1537, 1491, 1239, 1042, 691; HRMS (ESI) calcd for $C_{21}H_{19}NO_2$: 317.1416, found 318.1478 (M+H).

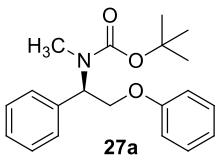
(*R*)-*N*-Benzyl-2-phenoxy-1-phenylethanamine (25b)



25b

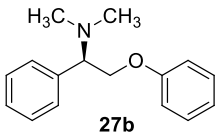
Method B was followed on a 0.22 mmol scale starting from *(R)*-2-(benzylamino)-2-phenylethanol **24b** and **A1**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **25b** as a yellow oil (43 mg, 64%): R_f 0.60 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.55-7.52 (m, 2H), 7.45-7.24 (m, 10H), 6.99-6.88 (m, 3H), 4.21 (dd, *J* = 8.9, 3.8 Hz, 1H), 4.10-3.99 (m, 2H), 3.78 (d, *J* = 13.2 Hz, 1H), 3.65 (d, *J* = 13.3 Hz, 1H), 2.33 (s(br), 1H); ^{1}H-NMR (300 MHz, DMSO-d_6) δ 7.51-7.26 (m, 12H), 6.97-6.92 (m, 3H), 4.10-4.03 (m, 3H), 3.68 (d, *J* = 13.6 Hz, 1H), 3.55 (d, *J* = 13.6 Hz, 1H), 2.76 (s(br), 1H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.6, 140.5, 140.1, 129.5, 128.7, 128.4, 128.1, 127.9, 127.8, 126.9, 121.0, 114.7, 72.8, 61.8, 51.4; IR (neat) 3304, 3057, 3023, 2912, 2848, 1597, 1494, 1448, 1323, 1238, 1144, 752; HRMS (ESI) calcd for $C_{21}H_{21}NO$: 303.1623, found 304.1700 (M+H). To further confirm the chemoselectivity of the reaction and the structure of the compound, we compared the data with the *N*-phenyl isomer from the literature and found the two compounds to be different.[8]

(*R*)-*tert*-Butyl methyl(2-phenoxy-1-phenylethyl)carbamate (27a)



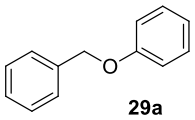
Method B was followed on a 0.20 mmol scale starting from *(R)-tert*-butyl (2-hydroxy-1-phenylethyl)(methyl)carbamate **26a** and **A1**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **27a** as a yellow oil (43 mg, 66%): R_f 0.60 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.40-7.26 (m, 7H), 7.00-6.94 (m, 3H), 5.58 (s, 1H), 4.48-4.36 (m, 2H), 2.76 (s, 3H), 1.46 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.5, 138.0, 129.5, 128.6, 127.6, 127.5, 127.3, 127.2, 121.2, 114.8, 79.9, 67.0, 29.7, 28.4; IR (neat) 3063, 3031, 2975, 2928, 1690, 1599, 1496, 1390, 1243, 1146, 754; HRMS (ESI) calcd for $C_{20}H_{25}NO_3$: 327.1834, found 350.1720 (M+Na).

(*R*)-*N*,*N*-Dimethyl-2-phenoxy-1-phenylethanamine (27b)



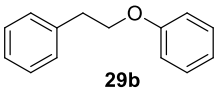
Method B was followed on a 0.24 mmol scale starting from *(R)*-2-(dimethylamino)-2-phenylethanol **26b** and **A1**. The crude product was purified on silica gel (5% EtOAc/hexanes) to afford **27b** as a yellow oil (42 mg, 73%): R_f 0.32 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.33 (d, J = 4.4 Hz, 4H), 7.30-7.21 (m, 3H), 6.93-6.85 (m, 3H), 4.30 (dd, J = 10.0, 6.1 Hz, 1H), 4.18 (dd, J = 10.0, 4.8 Hz, 1H), 3.60 (t, J = 5.2 Hz, 1H), 2.29 (s, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.7, 139.4, 129.4, 128.4, 128.3, 127.6, 120.9, 114.8, 69.9, 69.7, 43.6; IR (neat) 3061, 3029, 2948, 2866, 2821, 2774, 1598, 1586, 1495, 1469, 1454, 1238, 1041, 752, 691; HRMS (ESI) calcd for $C_{16}H_{19}NO$: 241.1467, found 242.1542 (M+H).

Benzyloxybenzene (29a)



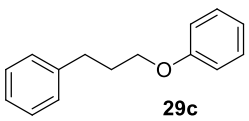
Method B was followed on a 0.46 mmol scale starting from phenylmethanol **28a** and **A1**. The crude material was purified on silica gel (heptane) to afford **29a** as a yellow oil (29 mg, 34%): R_f 0.73 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.48-7.26 (m, 7H), 7.02-6.96 (m, 3H), 5.09 (s, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.8, 137.1, 129.5, 128.6, 128.0, 127.5, 121.0, 114.9, 70.0; IR (neat) 3064, 3032, 2918, 1598, 1495, 1454, 1240, 1029, 752; HRMS (ESI) calcd for $C_{13}H_{12}O$: 184.0888, found 185.0967 (M+H).

Phenethoxybenzene (**29b**)



Method B was followed on a 0.41 mmol scale starting from 2-phenylethanol **28b** and **A1**. The crude material was purified on silica gel (10% EtOAc/hexanes) to afford **29b** as a colorless oil (35 mg, 43%): R_f 0.75 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.39-7.27 (m, 7H), 7.01-6.93 (m, 3H), 4.22 (t, *J* = 7.1 Hz, 2H), 3.15 (t, *J* = 7.1 Hz, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.8, 138.3, 129.5, 129.0, 128.5, 126.5, 120.8, 114.6, 68.6, 35.8; IR (neat) 3063, 3028, 2927, 2870, 1597, 1586, 1497, 1472, 1243, 1037, 752; HRMS (ESI) calcd for $C_{14}H_{14}O$: 198.1045, found 199.1111 (M+H).

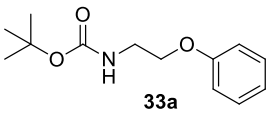
3-Phenoxypropylbenzene 29c



Method B was followed on a 0.37 mmol scale starting from 3-phenylpropan-1-ol **28c** and **A1**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **29c** as a yellow oil (34 mg, 43%): R_f 0.79 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.38-7.23 (m, 7H), 7.03-6.95 (m, 3H), 4.03 (t, *J* = 6.3 Hz, 2H), 2.88 (t, *J* = 7.3 Hz, 2H), 2.22-2.13 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 159.1, 141.6, 129.5, 128.6, 128.5, 126.0, 120.6, 114.6, 66.8, 32.2, 30.9; IR (neat) 3062, 3027, 2927,

2869, 1600, 1586, 1497, 1469, 1245, 1039, 751, 691; HRMS (ESI) calcd for $C_{15}H_{16}O$: 212.1201, found 213.1277 (M+H).

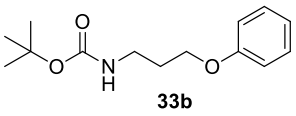
tert-Butyl (2-phenoxyethyl)carbamate 33a



33a

Method A was followed on a 0.31 mmol scale starting from *tert*-butyl (2-hydroxyethyl)carbamate **32a** and **A1**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **33a** as a colorless oil (38 mg, 52%): R_f 0.47 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.34-7.28 (m, 2H), 7.01-6.96 (m, 1H), 6.93-6.90 (m, 2H), 5.07 (s(br), 1H), 4.04 (t, J = 5.1 Hz, 2H), 3.58-3.53 (m, 2H), 1.48 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.6, 156.0, 129.6, 121.1, 115.4, 114.5, 79.6, 67.1, 40.2, 28.4; IR (neat) 3351, 3057, 3038, 2976, 2932, 2875, 1693, 1599, 1587, 1496, 1274, 1241, 1164, 752; HRMS (ESI) calcd for $C_{13}H_{19}NO_3$: 237.1365, found 260.1256 (M+Na).

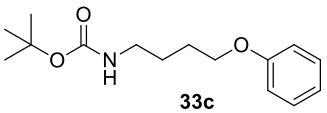
tert-Butyl (3-phenoxypropyl)carbamate 33b



33b

Method A was followed on a 0.28 mmol scale starting from *tert*-butyl (3-hydroxypropyl)carbamate **32b** and **A1**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **33b** as a yellow solid (28 mg, 40%): m.p. 69°C; R_f 0.42 (20% EtOAc/hexanes), ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.30 (dd, J = 8.3, 0.7 Hz, 2H), 6.97-6.90 (m, 3H), 4.82 (s(br), 1H), 4.04 (t, J = 5.9 Hz, 2H), 3.35 (q, J = 6.2 Hz, 2H), 2.07-1.96 (m, 2H), 1.47 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.8, 156.1, 129.5, 120.8, 114.5, 79.2, 65.7, 38.1, 29.5, 28.4; IR (neat) 3351, 3072, 3038, 2976, 2931, 2875, 1689, 1600, 1587, 1497, 1365, 1242, 1169, 753; HRMS (ESI) calcd for $C_{14}H_{21}NO_3$: 251.1521, found 274.1411 (M+Na).

***tert*-Butyl (4-phenoxybutyl)carbamate (33c)**



33c

Method B was followed on a 0.26 mmol scale starting from *tert*-butyl (4-hydroxybutyl)carbamate **32c** and **A1**. The crude material was purified on silica gel (15% EtOAc/hexanes) to afford **33c** as a colorless oil (29 mg, 42%): R_f 0.50 (20% EtOAc/hexanes); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.32-7.27 (m, 2H), 6.98-6.90 (m, 3H), 4.70 (s(br), 1H), 3.99 (t, *J* = 6.1 Hz, 2H), 3.21 (q, *J* = 6.4 Hz, 2H), 1.86-1.79 (m, 2H), 1.74-1.66 (m, 2H), 1.47 (s, 9H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.9, 156.1, 129.5, 120.7, 114.5, 79.1, 67.3, 40.3, 28.4, 26.9, 26.6; IR (neat) 3357, 3065, 3034, 2975, 2933, 2870, 1689, 1600, 1586, 1497, 1473, 1365, 1243, 1168, 753; HRMS (ESI) calcd for $C_{15}H_{23}NO_3$: 265.1678, found 288.1566 (M+Na).

5. Competition studies

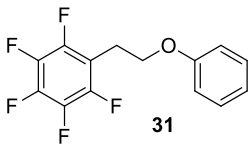
Scheme 8. Competition studies between phenethylalcohol **28b** and (*R*)-*N*-*tert*-butyloxycarbonyl-2-phenylglycinol **15**:

In a sealed tube, triphenylbismuth **A1** (0.41 mmol, 1.0 equiv) was added, followed by copper (II) acetate (1.0 equiv) and alcohol **28b** and **15** (1.0 equiv for each). The reagents were dissolved in anhydrous dichloromethane (5 mL) and pyridine (3.0 equiv) was added to the mixture. The reaction tube was purged with dry oxygen for 30 seconds, sealed and heated at 50°C overnight. The reaction mixture was cooled to r.t., concentrated under reduced pressure, and diluted with EtOAc. The organic layer was washed with aq. ammonium hydroxide (2x20mL), brine (1x20mL), dried over sodium sulfate, filtered and concentrated under reduced pressure. The NMR was taken on the obtained crude oil. The ratio of **29b** and **16** was determined by the integration of signals corresponding to the benzylic C–H of **16**, and the benzylic CH_2 of **29b**, after correction for the number of protons.

Scheme 9. Competition studies between (pentafluorophenyl)ethanol **30** and (*R*)-*N*-*tert*-butyloxycarbonyl-2-phenylglycinol **15**:

In a sealed tube, triphenylbismuth **A1** (0.41 mmol, 1.0 equiv) was added, followed by copper (II) acetate (1.0 equiv) and alcohol **30** and **15** (1.0 equiv for each). The reagents were dissolved in anhydrous dichloromethane (5 mL) and pyridine (3.0 equiv) was added to the mixture. The reaction tube was purged with dry oxygen for 30 seconds, sealed and heated at 50°C overnight. The reaction mixture was cooled to r.t., concentrated under reduced pressure, and diluted with EtOAc. The organic layer was washed with aq. ammonium hydroxide (2x20mL), brine (1x20mL), dried over sodium sulfate, filtered and concentrated under reduced pressure. The NMR was taken on the obtained crude oil. The ratio of **31** and **16** was determined by the integration of signals corresponding to the benzylic C–H of **16** and the benzylic CH_2 of **31**, after correction for the number of protons.

1,2,3,4,5-Pentafluoro-6-(2-phenoxyethyl)benzene (**31**)



31

^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.33-7.26 (m, 2H), 7.00-6.95 (m, 1H), 6.90-6.86 (m, 2H), 4.18 (t, *J* = 6.5 Hz, 2H), 3.22 (t, *J* = 6.5 Hz, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ 158.3, 129.5, 121.2, 114.5, 111.6, 111.5, 111.3, 65.6, 29.7, 22.9; IR (neat) 3706, 3680, 3035, 2967, 2937, 2866, 1657, 1601, 1504, 1242, 1055, 752; HRMS (ESI) calcd for $C_{14}H_9F_5O$: 288.0571, found 289.0644 (M+H).

6. Computational details

All calculations were performed with ORCA 3.0.1 software. The procedure reported by Pulay *et al.* was directly applied to the selected compounds for pK_a determination, using the equation described below.[9] The structures were fully optimized with the OLYP density functional[10] in combination with the 3-21G basis set for all atoms, using the COSMO solvation model for water.[11] Harmonic vibrational frequencies were computed for all optimized structures to verify that they were minima, possessing zero imaginary frequencies. The reported energies, used for pKa calculations, were obtained by single point calculations on the optimized structures using the OLYP density functional with the 6-311+G(d,p) basis set, again using the COSMO solvation model for water.

pK_a prediction equation for alcohols, as reported by Pulay et al.[9]

$pK_a = 0.3333 * \Delta E - 90.447$

Table S2. Computed values for selected compounds.

Compound	E (Eh) anion (A^-)	E (Eh) neutral (HA)	ΔE (kcal/mol)	pK_a
15	-786,696005	-787,204025	318,787856	**15,8**
17b	-899,804801	-900,311973	318,255690	**15,6**
17d	-593,560154	-594,066536	317,759687	**15,5**
24a	-785,273340	-785,779612	317,690598	**15,4**
24b	-711,194933	-711,703171	318,924471	**15,9**
26a	-825,978949	-826,484095	316,984430	**15,2**
26b	-519,463652	-519,971521	318,692688	**15,8**
28b	-385,539151	-386,054130	323,154341	**17,3**
30	-881,759638	-882,266431	318,018046	**15,5**
32a	-555,685213	-556,189037	316,154172	**14,9**
32b	-594,981172	-595,491005	319,925776	**16,2**
32c	-634,276128	-634,786611	320,333426	**16,3**

7. References

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(10) W.-M. Hoe, A. J. Cohen and N. C. Handy, *Chem. Phys. Lett.*, 2001, **341**, 319.

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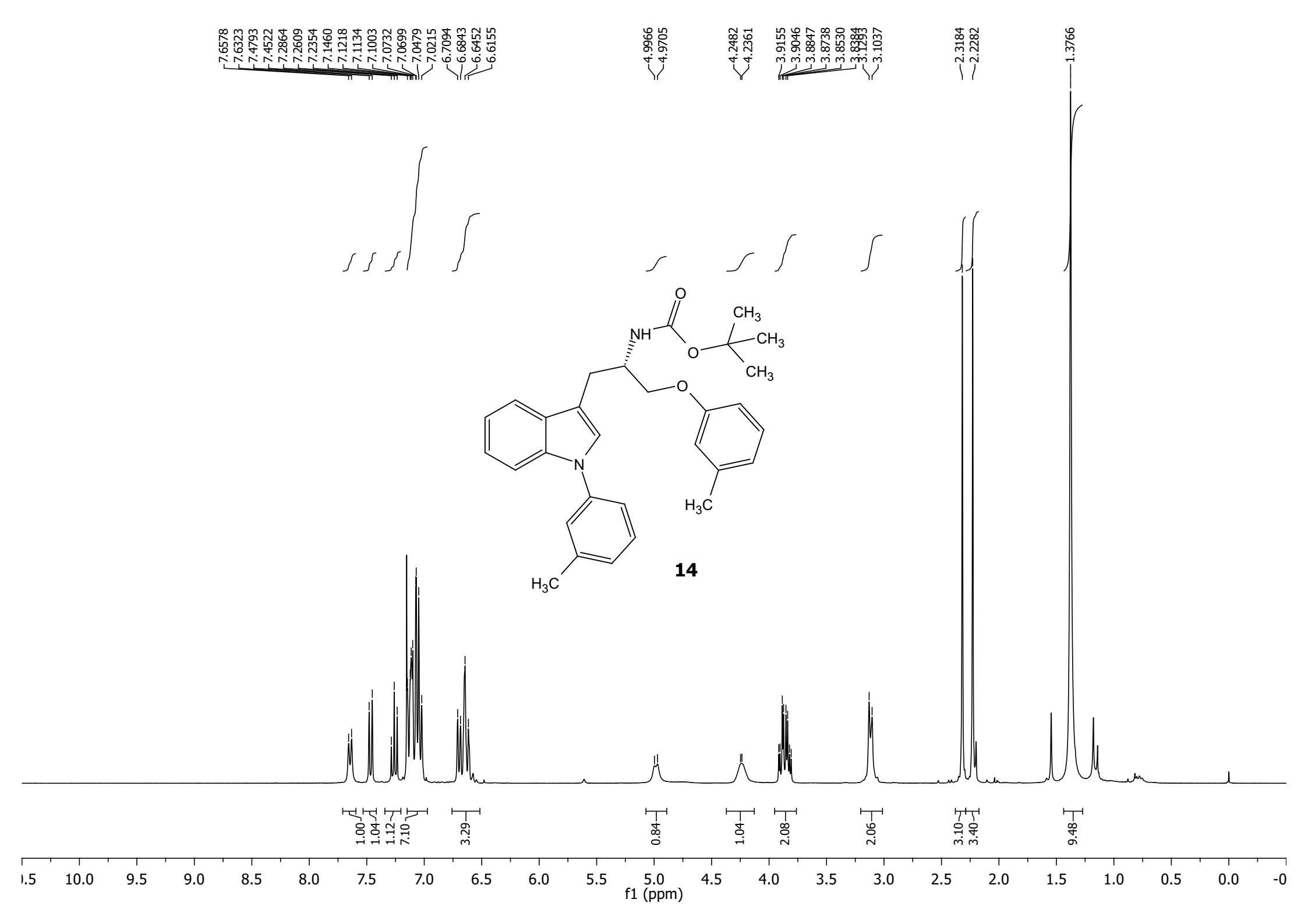
8. Spectra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7.0699
7.0479
7.0215
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CH3
CH3
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H3C
H3C
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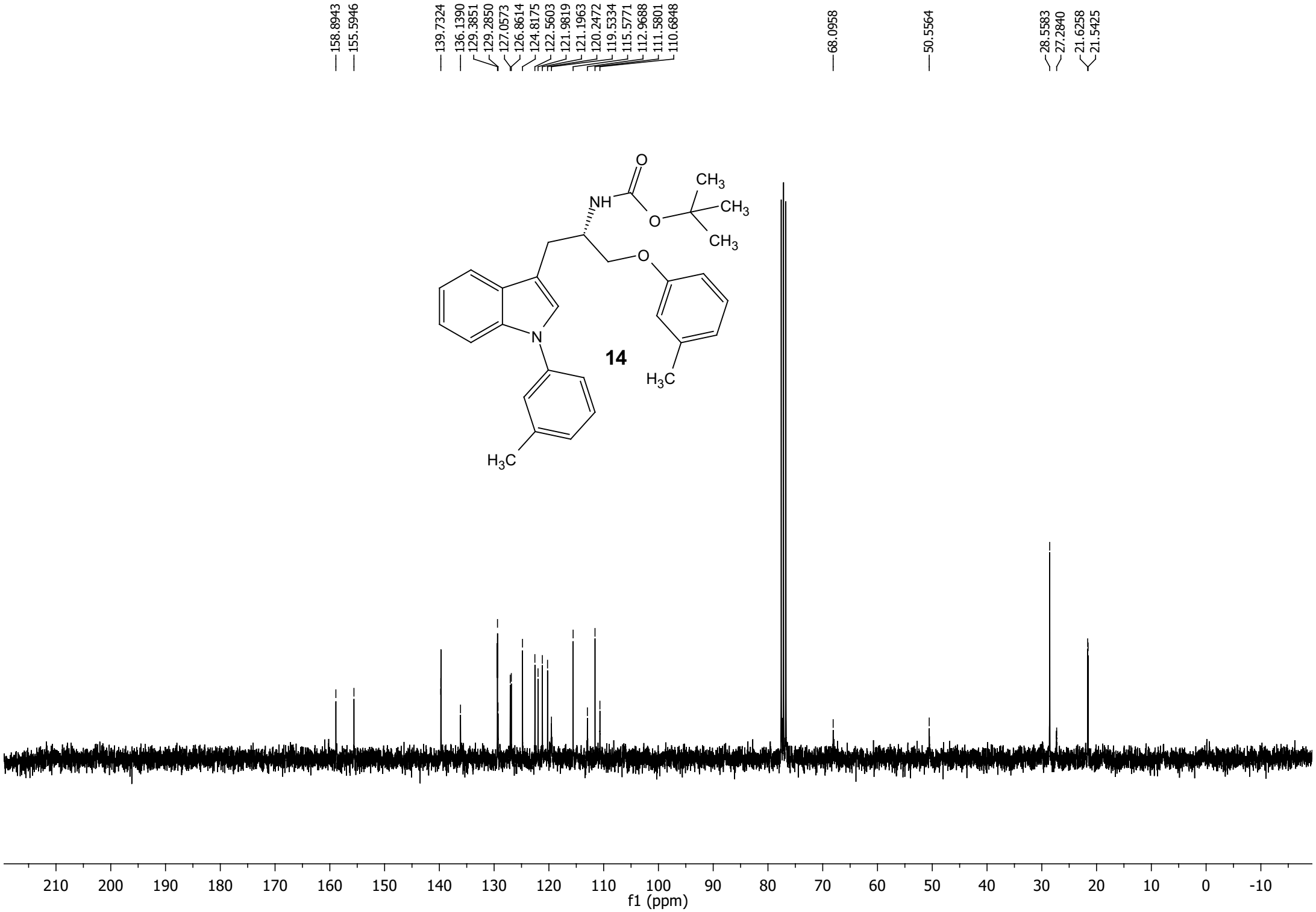
f1 (ppm)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200
190
180
170
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100
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80
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30
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10
0
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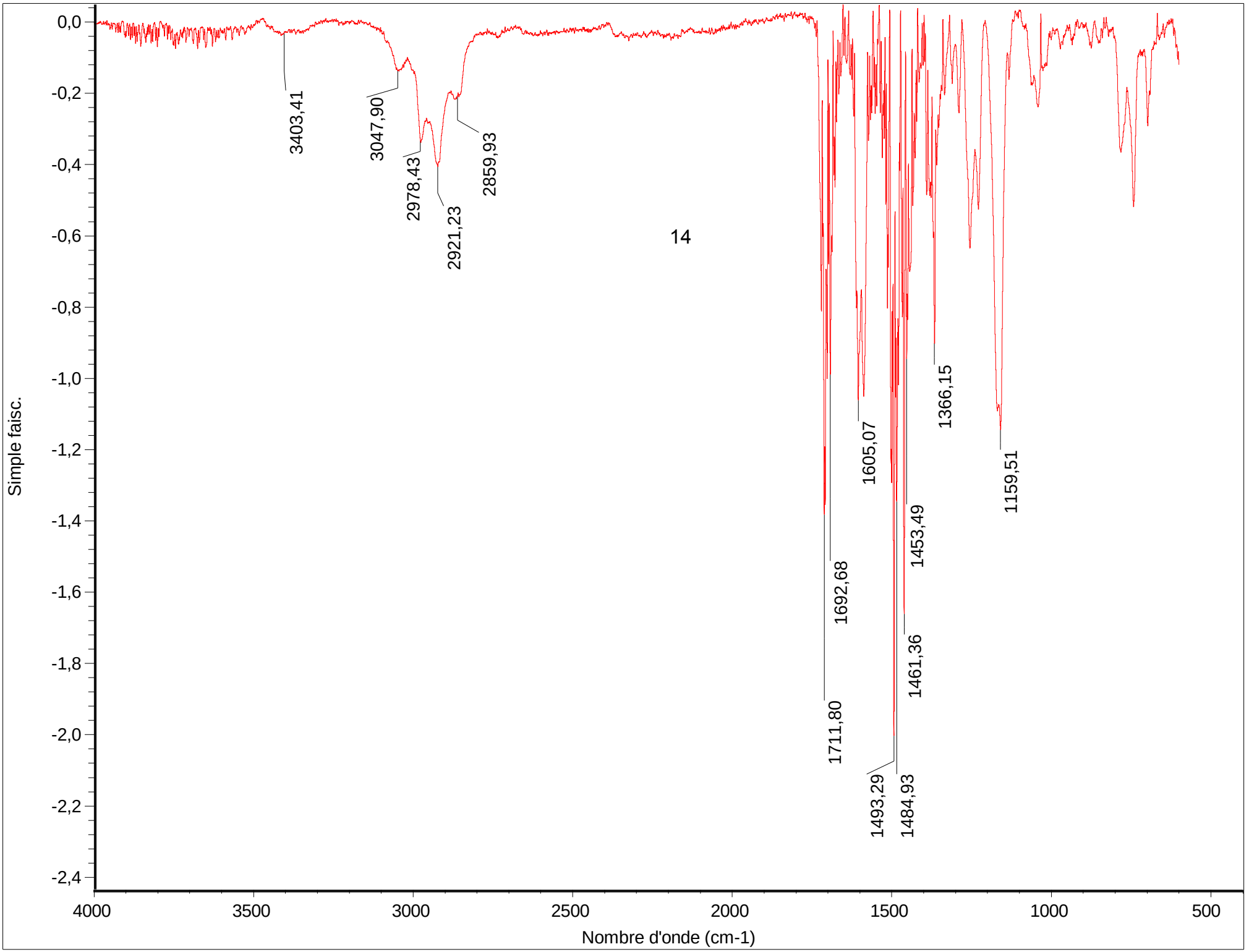
f1 (ppm)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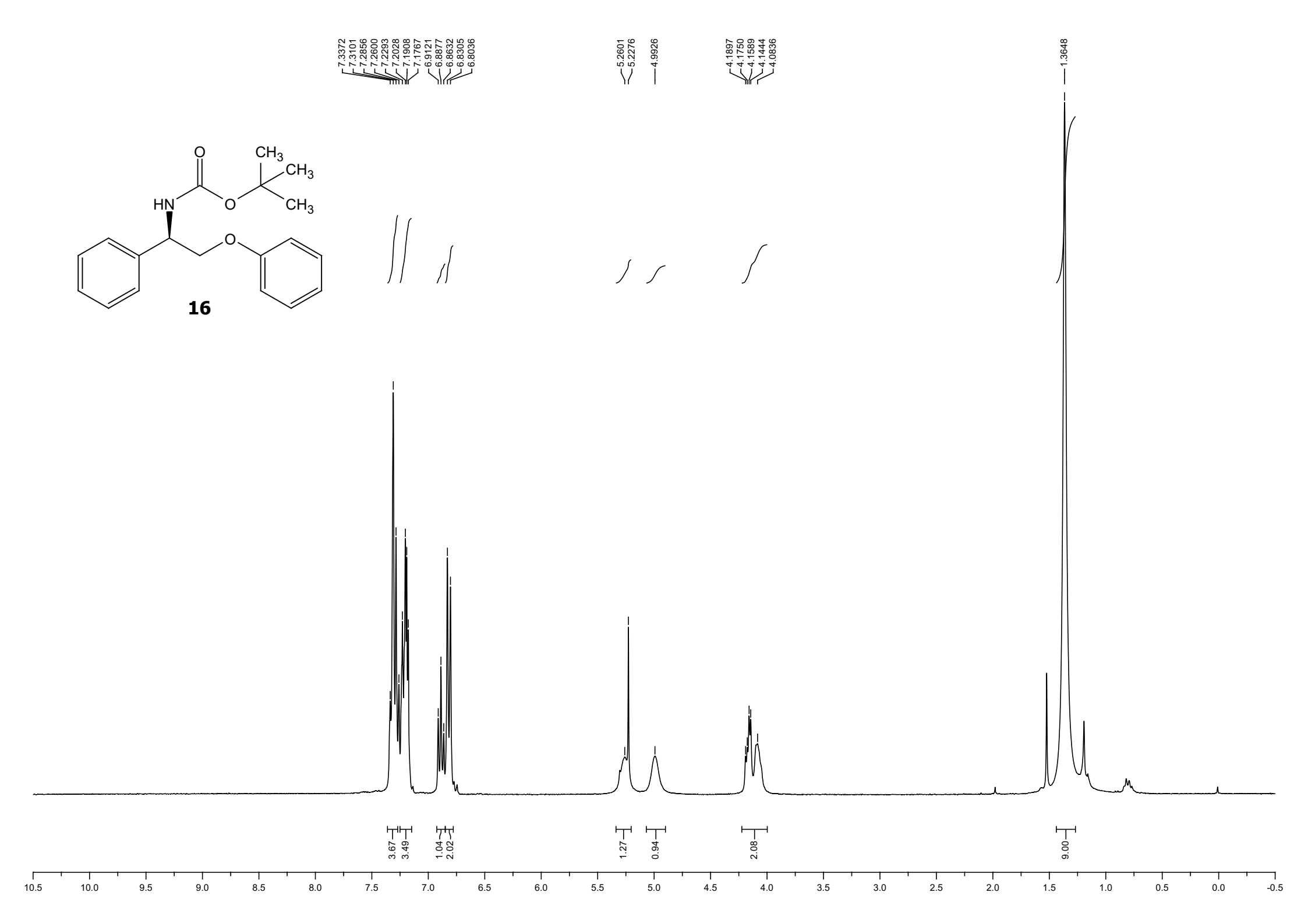
1159,51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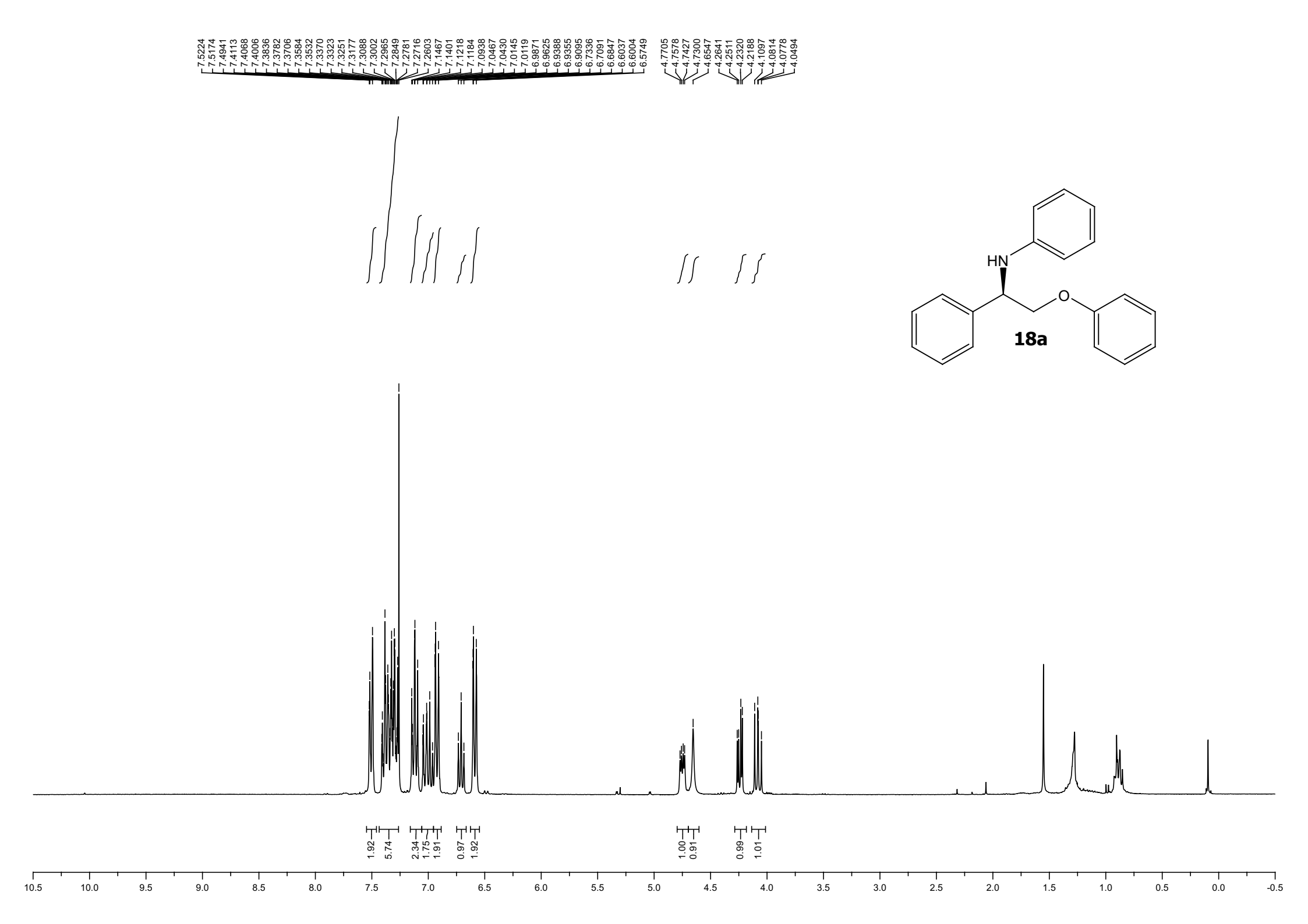
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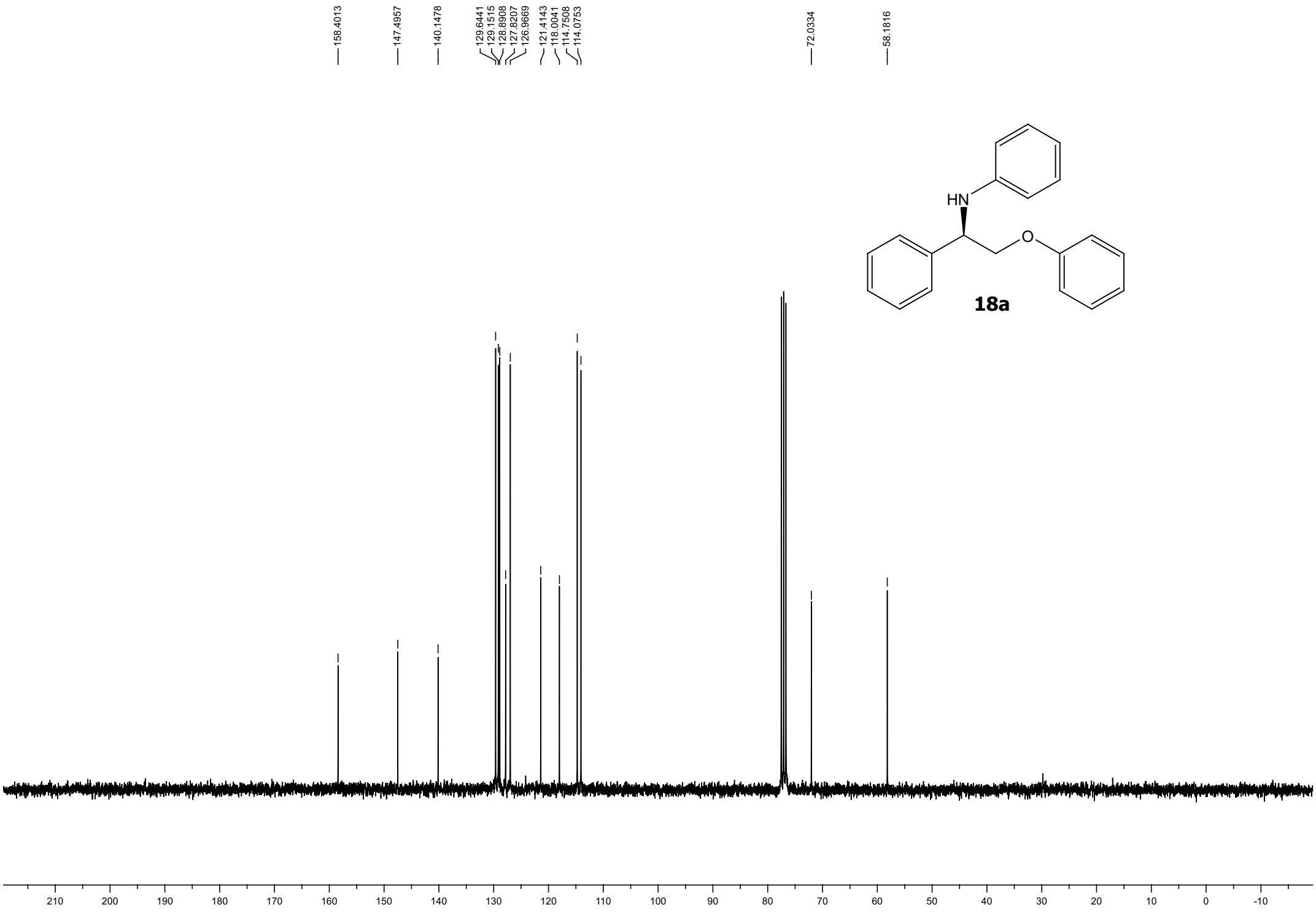
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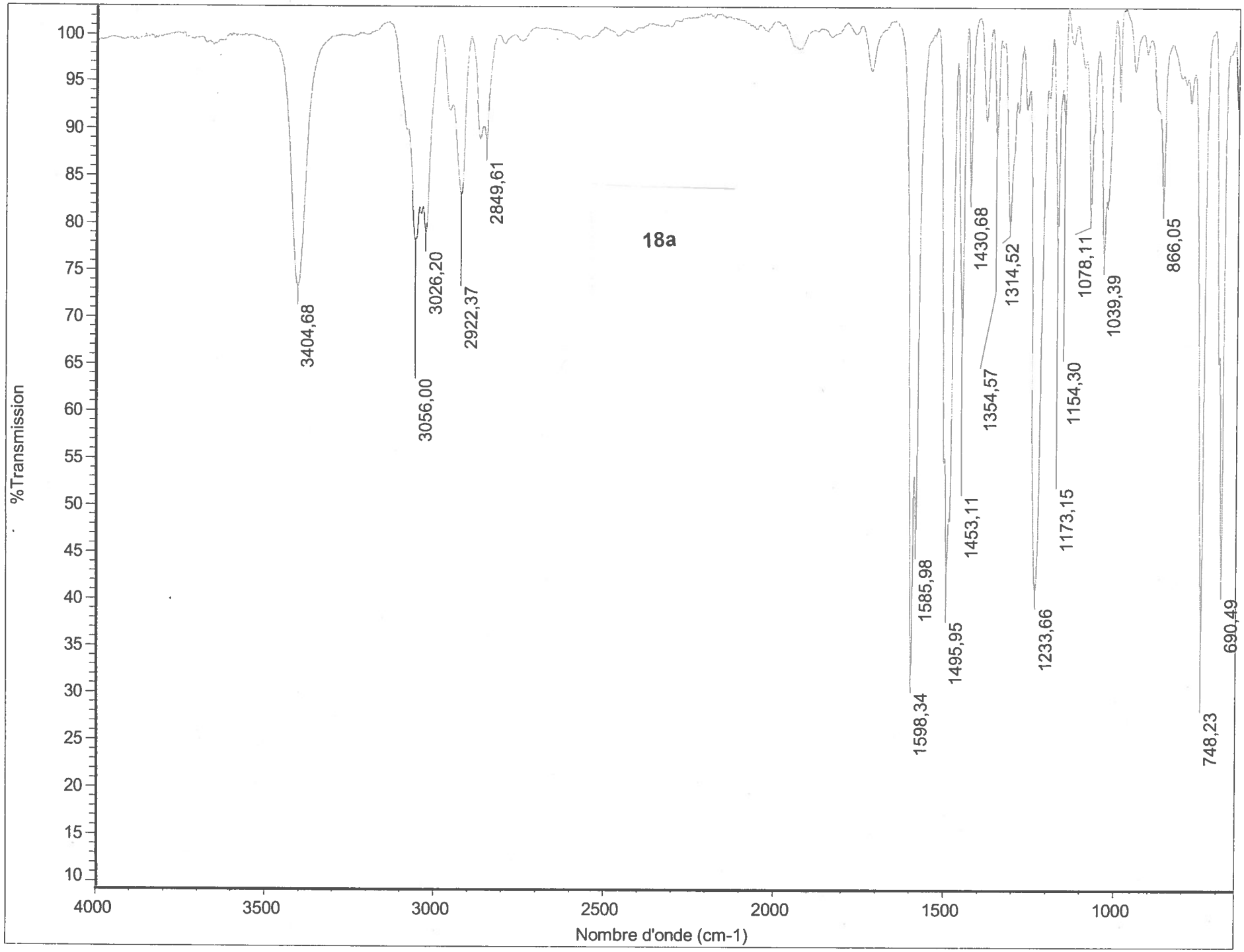
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1495,95
1453,11
1430,68
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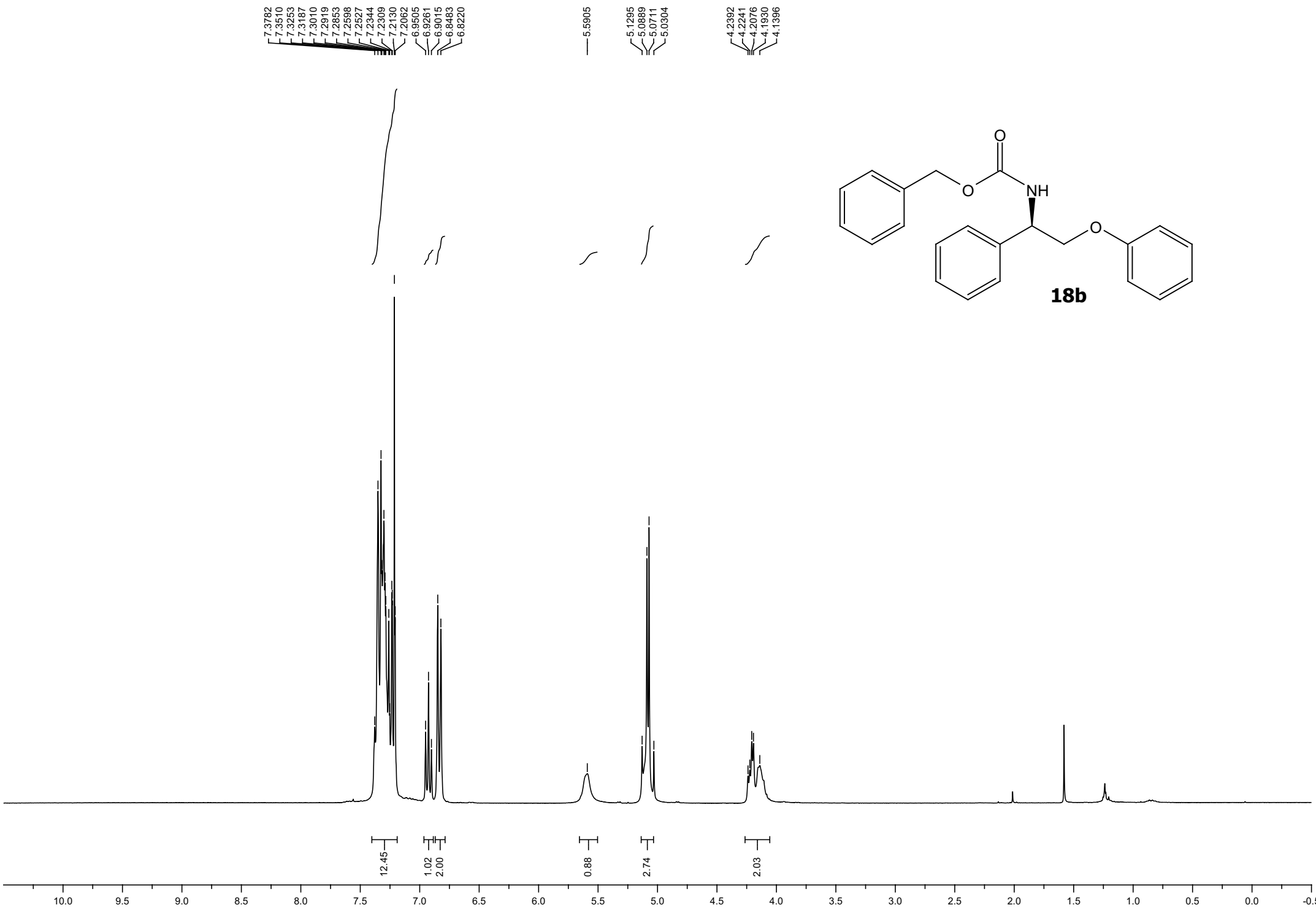
1233,66
1173,15
1154,30
1078,11
1039,39
866,05
748,23
690,49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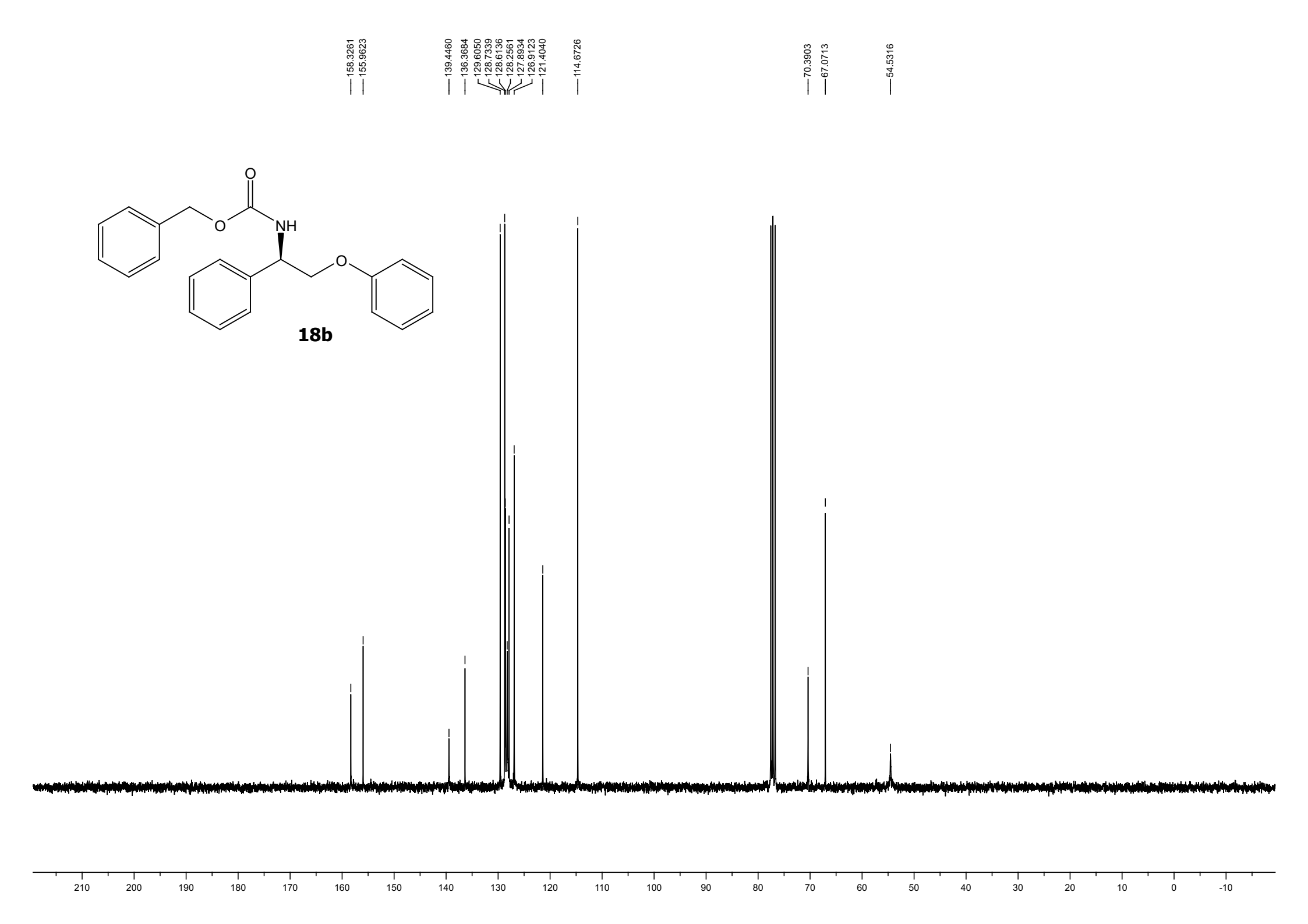
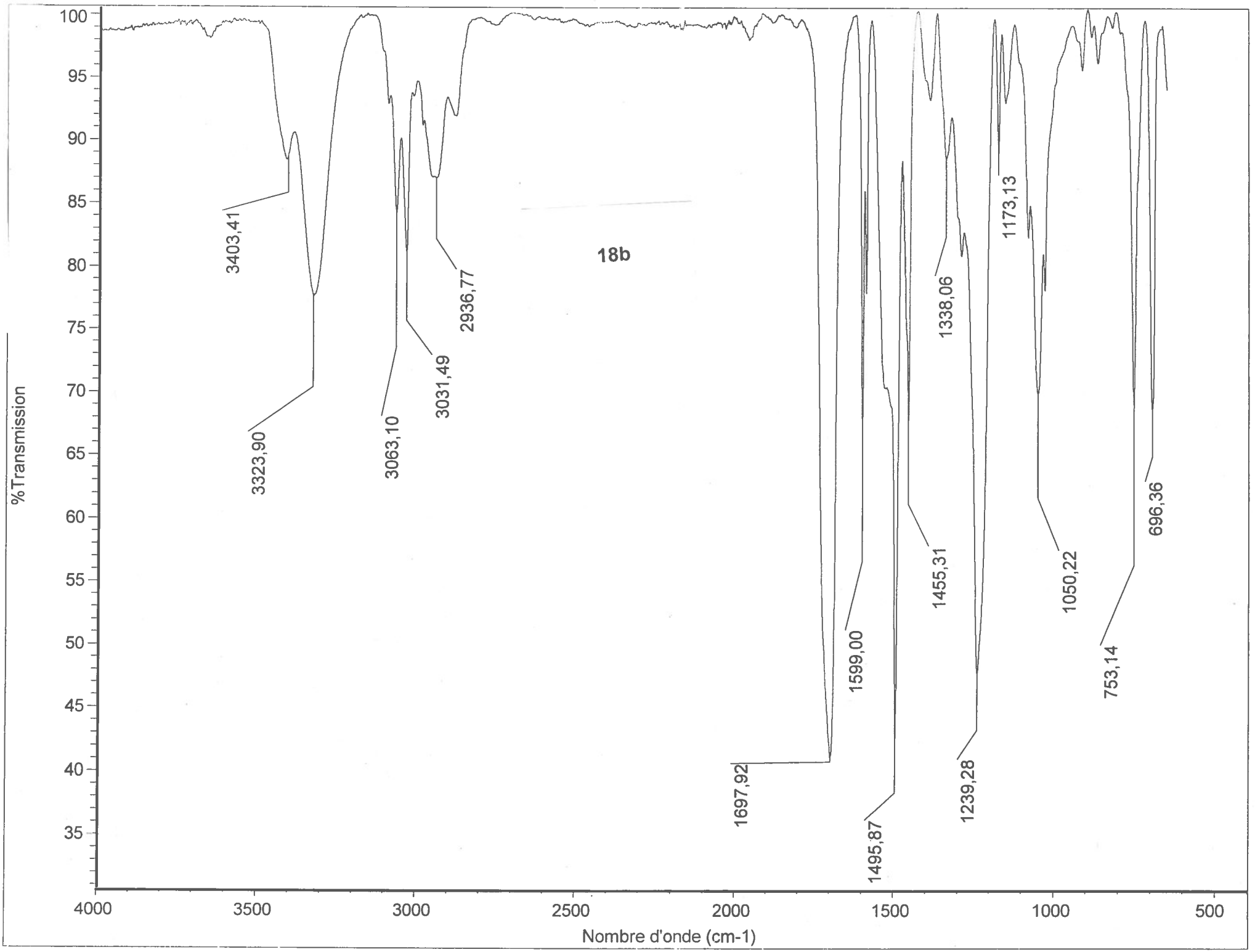
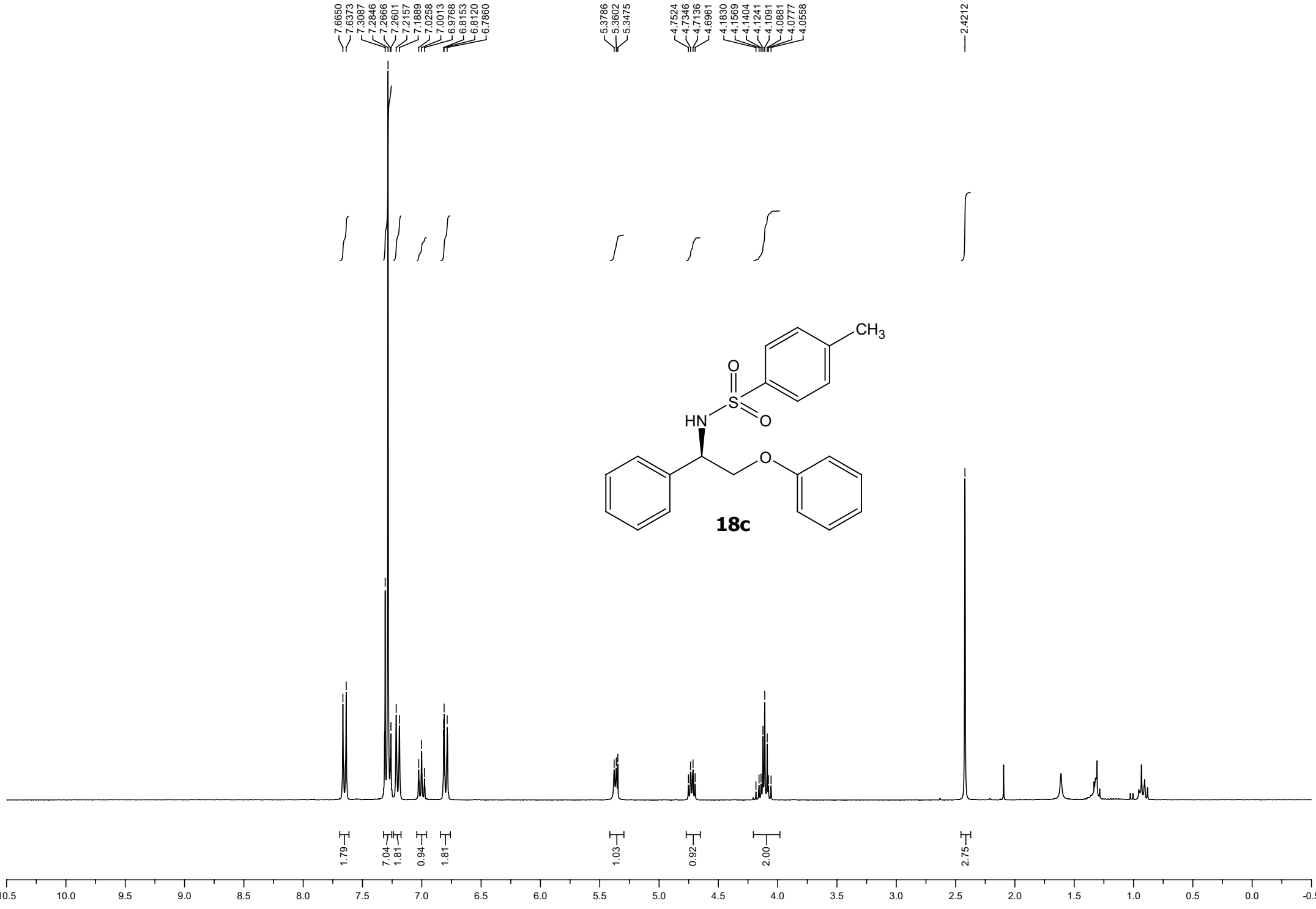
7.3510
7.3253
7.3187
7.3010
7.2919
7.2853
7.2598
7.2527
7.2344
7.2309
7.2130
7.2062
6.9505
6.9261
6.9015
6.8483
6.8220
5.5905
5.1295
5.0889
5.0711
5.0304
4.2392
4.2241
4.2076
4.1930
4.1396
O
O
NH
O
18b
12.45
1.02
2.00
0.88
2.74
2.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


158.3261
155.9623
139.4460
136.3684
129.6050
128.7339
128.6136
128.2561
127.8934
126.9123
121.4040
114.6726
70.3903
67.0713
54.5316
O
O
NH
O
18b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


18b
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
4000
3500
3000
2500
2000
1500
1000
500
3403,41
3323,90
3063,10
3031,49
2936,77
1697,92
1599,00
1495,87
1455,31
1338,06
1239,28
1173,13
1050,22
753,14
696,36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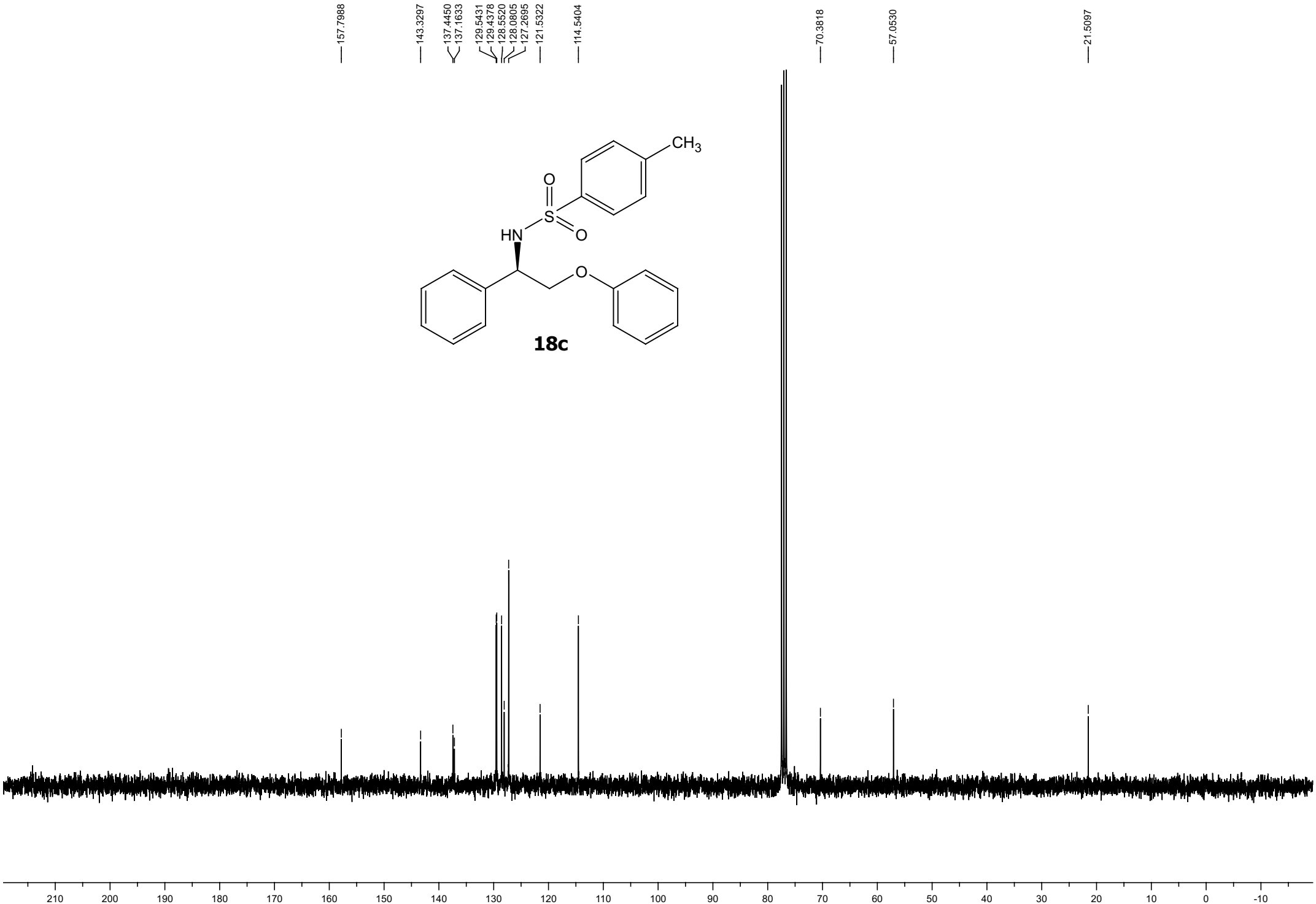
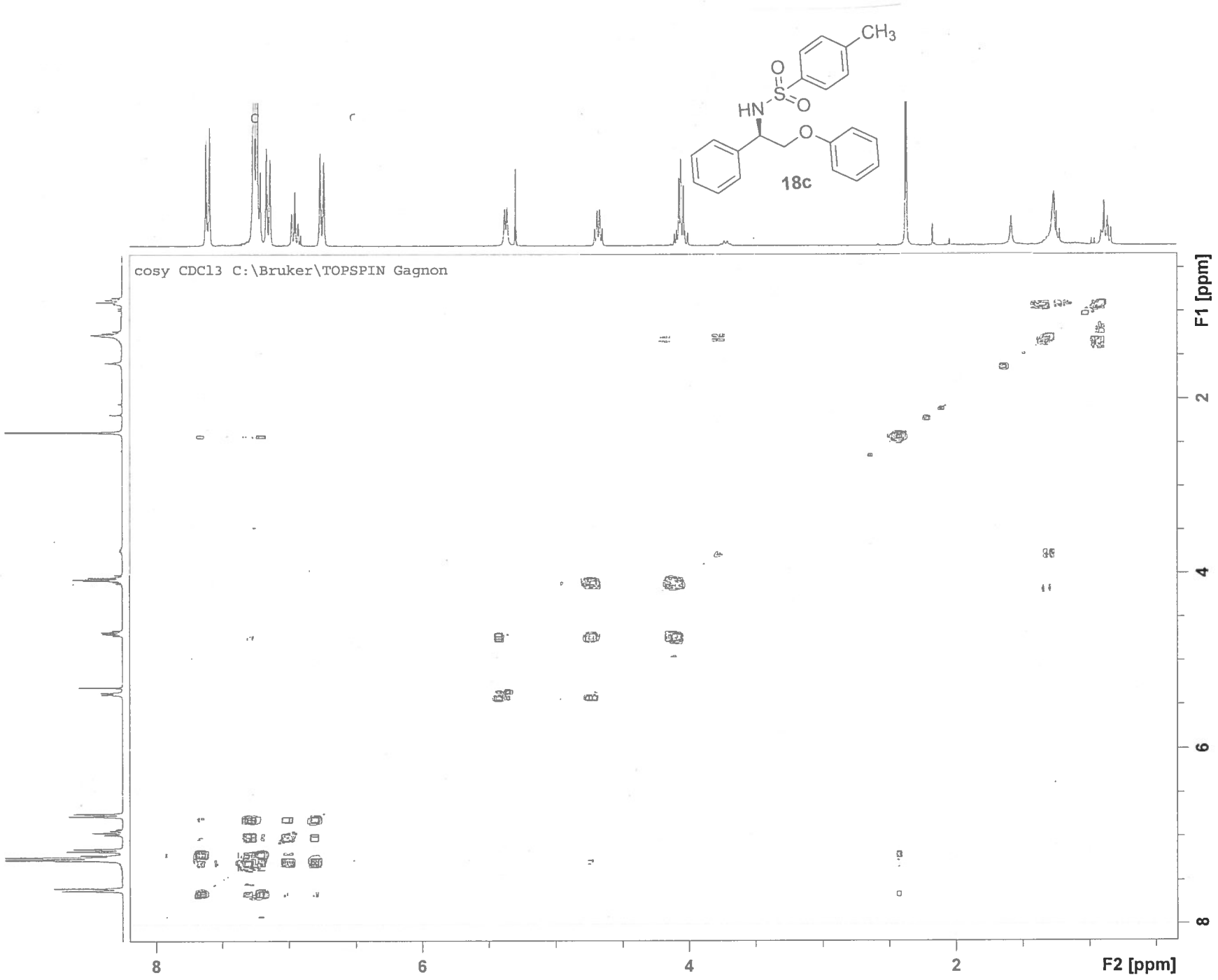
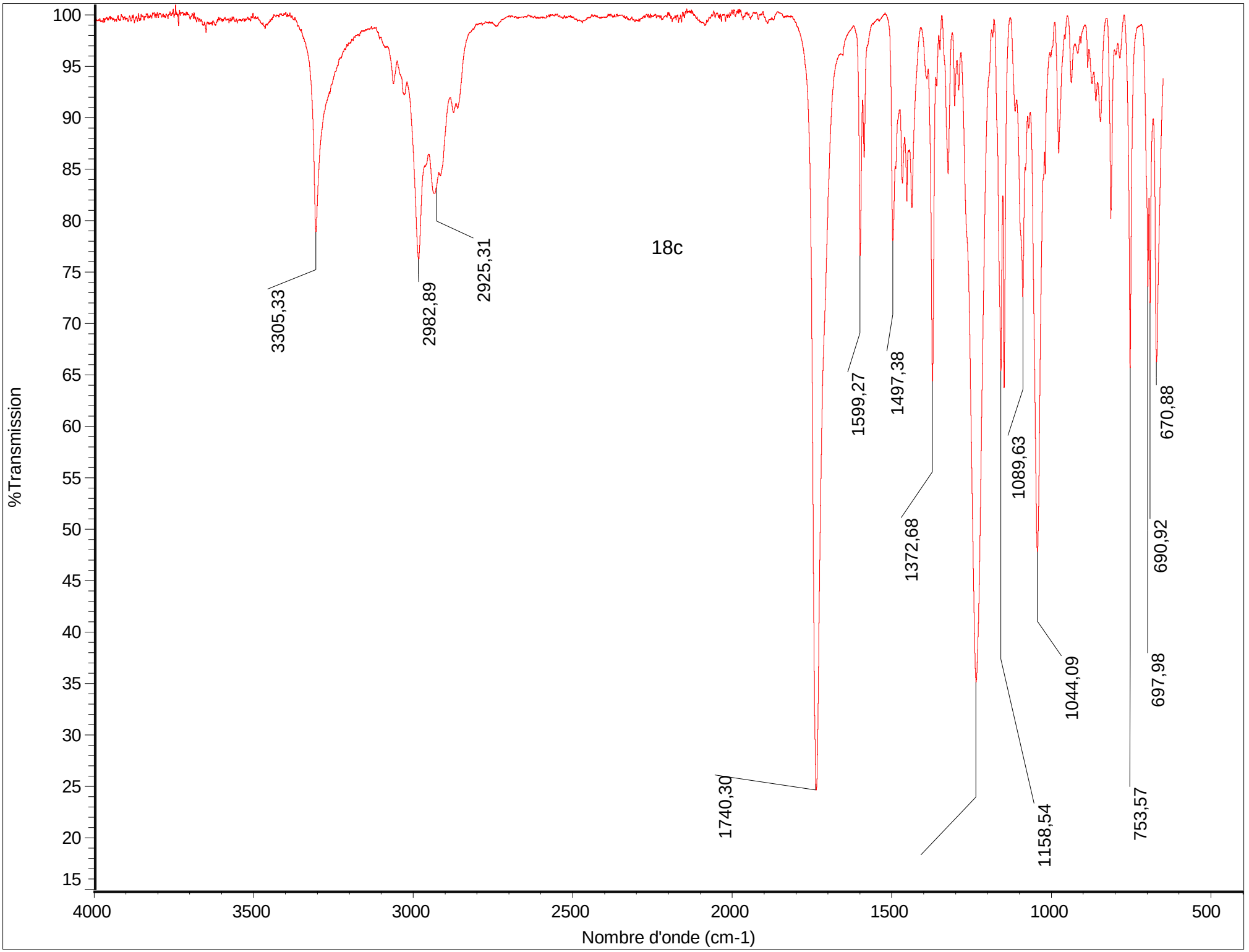
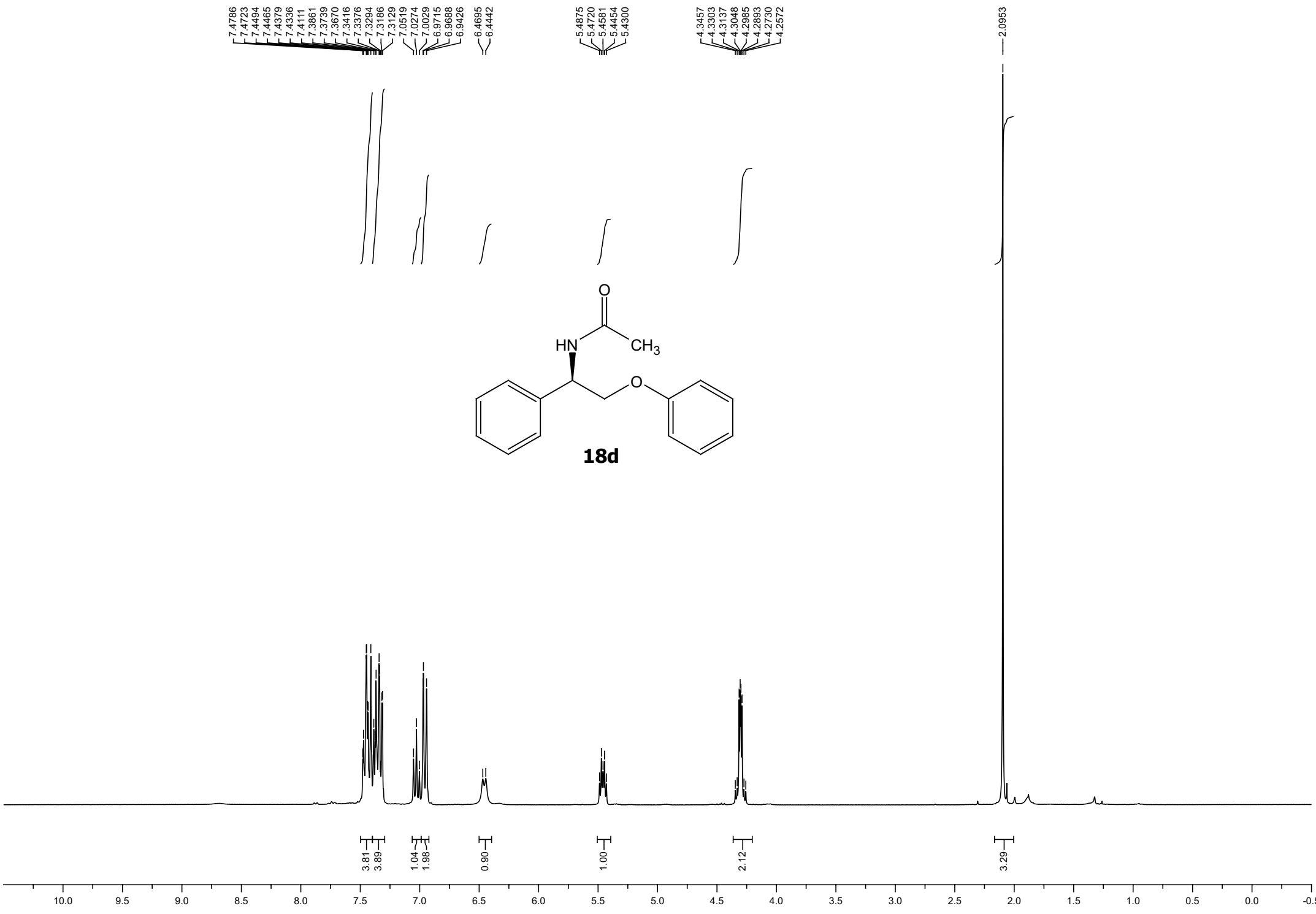
7.6373
7.3087
7.2846
7.2666
7.2601
7.2157
7.1889
7.0258
7.0013
6.9768
6.8153
6.8120
6.7860
5.3786
5.3602
5.3475
4.7524
4.7346
4.7136
4.6961
4.1830
4.1569
4.1404
4.1241
4.1091
4.0881
4.0777
4.0558
2.4212
CH3
O
S
O
HN
O
18c
1.79
7.04
1.81
0.94
1.81
1.03
0.92
2.00
2.75
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


157.7988
143.3297
137.4450
137.1633
129.5431
129.4378
128.5520
128.0805
127.2695
121.5322
114.5404
70.3818
57.0530
21.5097
CH3
O
S
O
HN
O
18c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


cosy CDCl3 C:\Bruker\TOPSPIN Gagnon
CH3
O
S
O
HN
O
18c
F1 [ppm]
F2 [ppm]
2
4
6
8
8
6
4
2


18c
%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
500
3305,33
2982,89
2925,31
1740,30
1599,27
1497,38
1372,68
1158,54
1089,63
1044,09
753,57
697,98
690,92
670,88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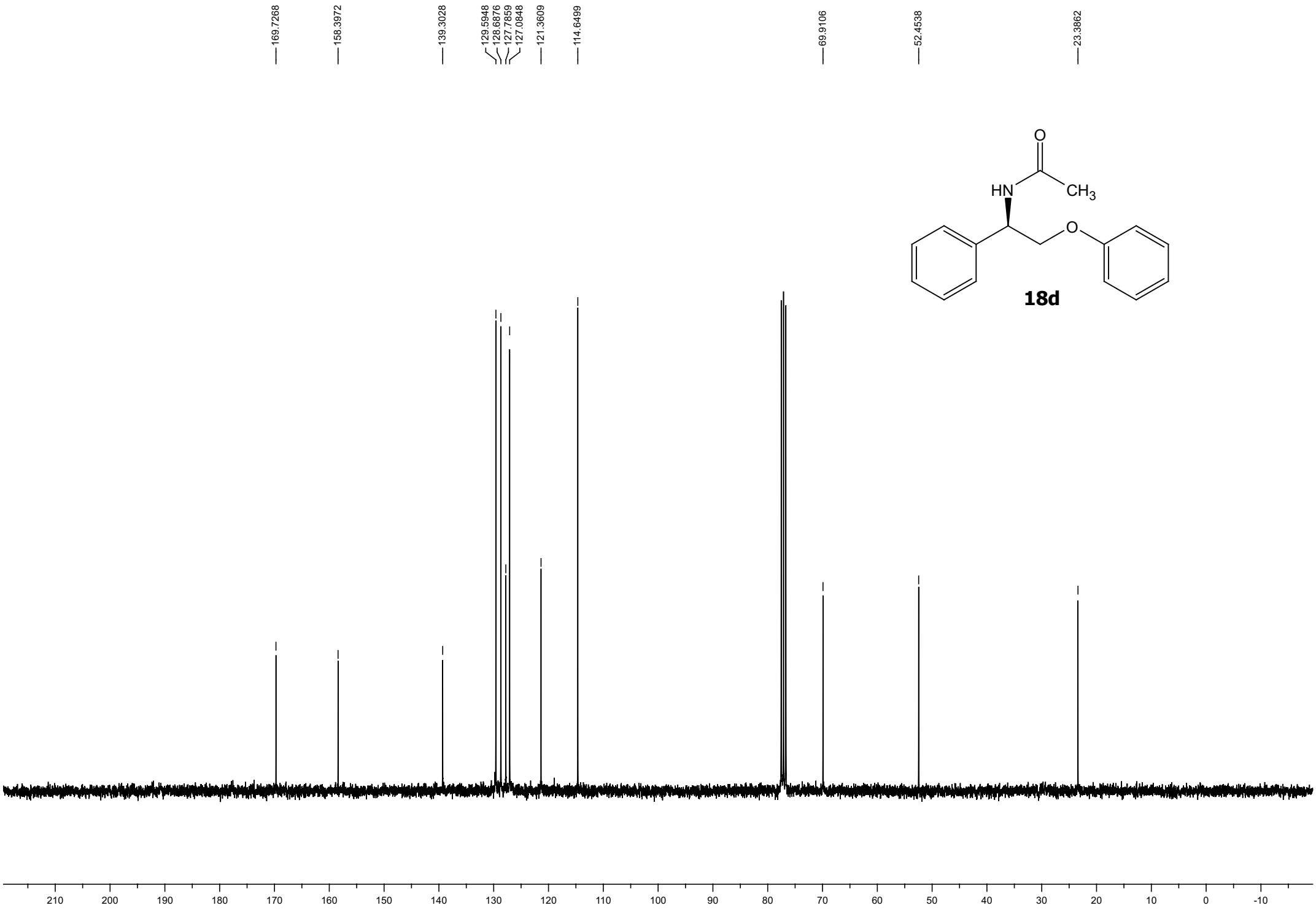
7.4723
7.4494
7.4465
7.4379
7.4336
7.4111
7.3861
7.3739
7.3670
7.3416
7.3376
7.3294
7.3186
7.3129
7.0519
7.0274
7.0029
6.9715
6.9688
6.9426
6.4695
6.4442
5.4875
5.4720
5.4581
5.4454
5.4300
4.3457
4.3303
4.3137
4.3048
4.2985
4.2893
4.2730
4.2572
2.0953
O
HN
CH3
O
18d
3.81
3.89
1.04
1.98
0.90
1.00
2.12
3.29
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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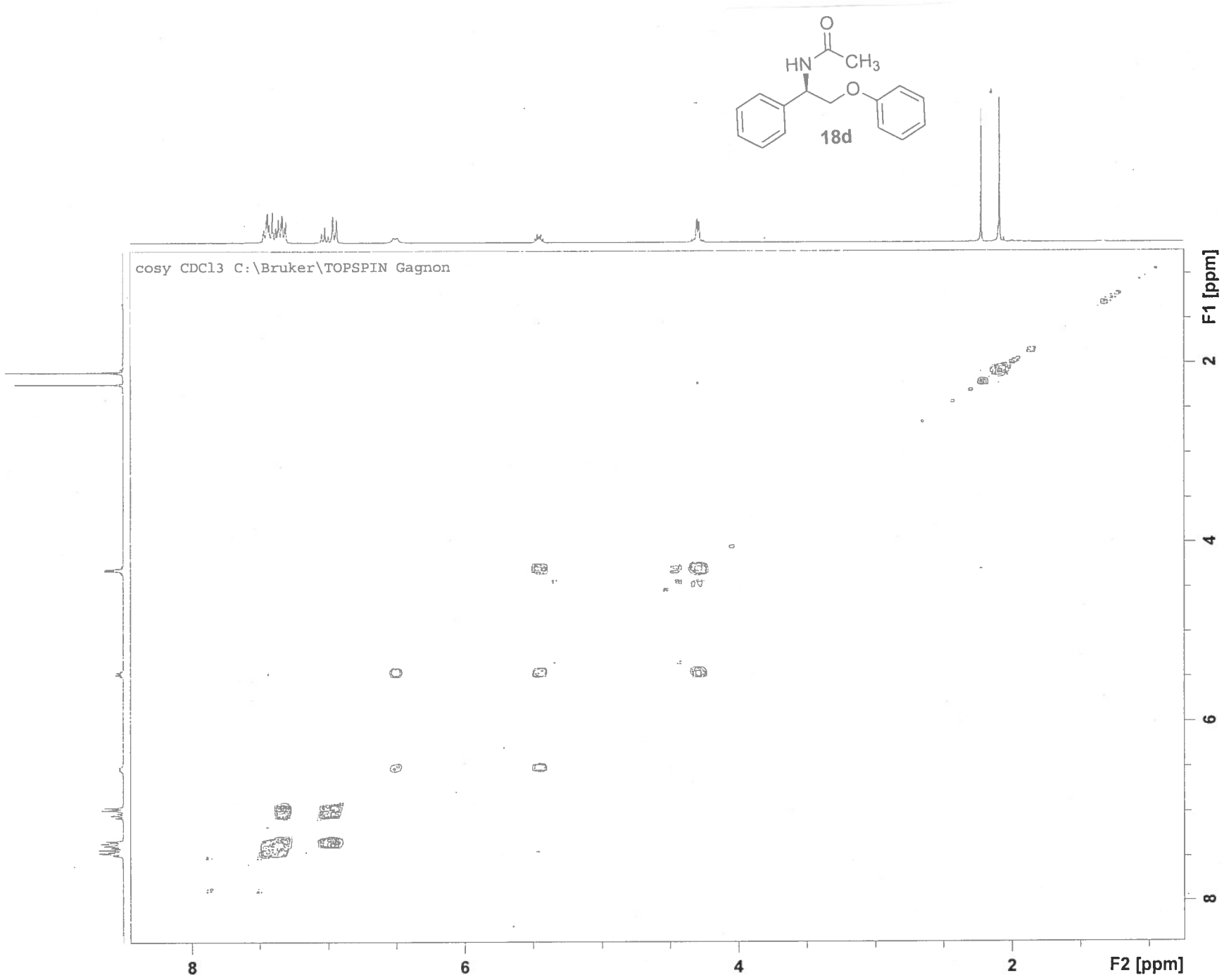
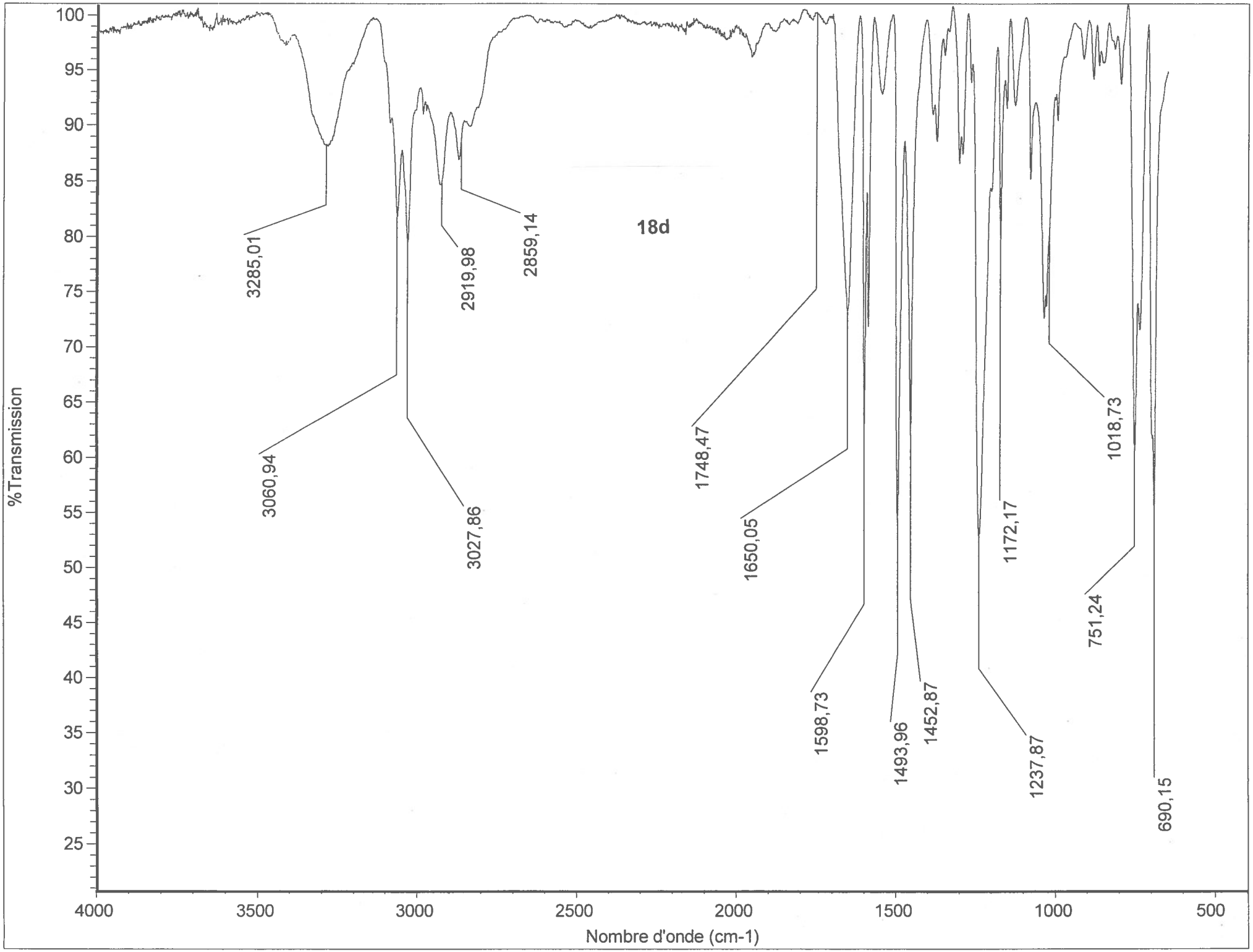
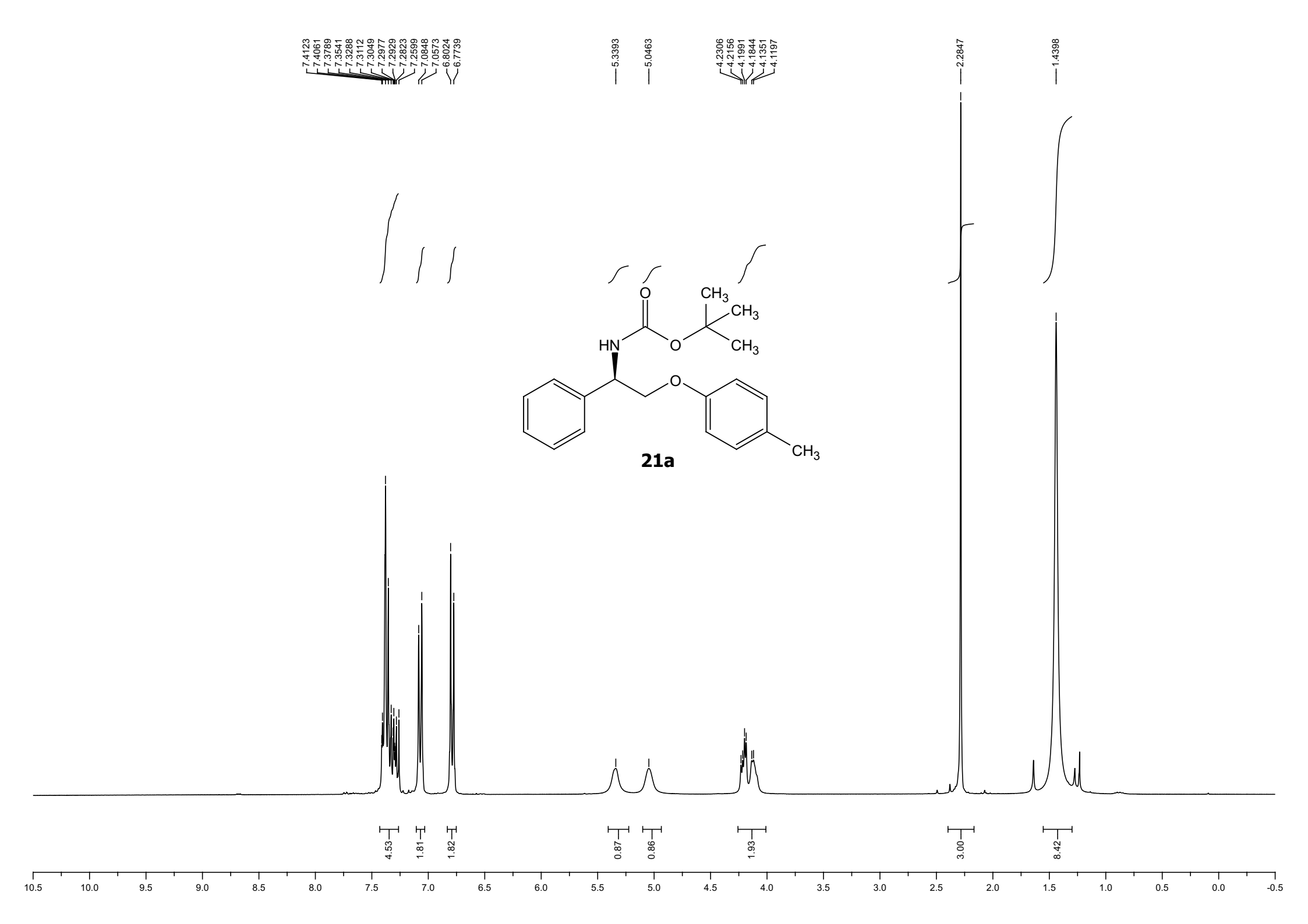
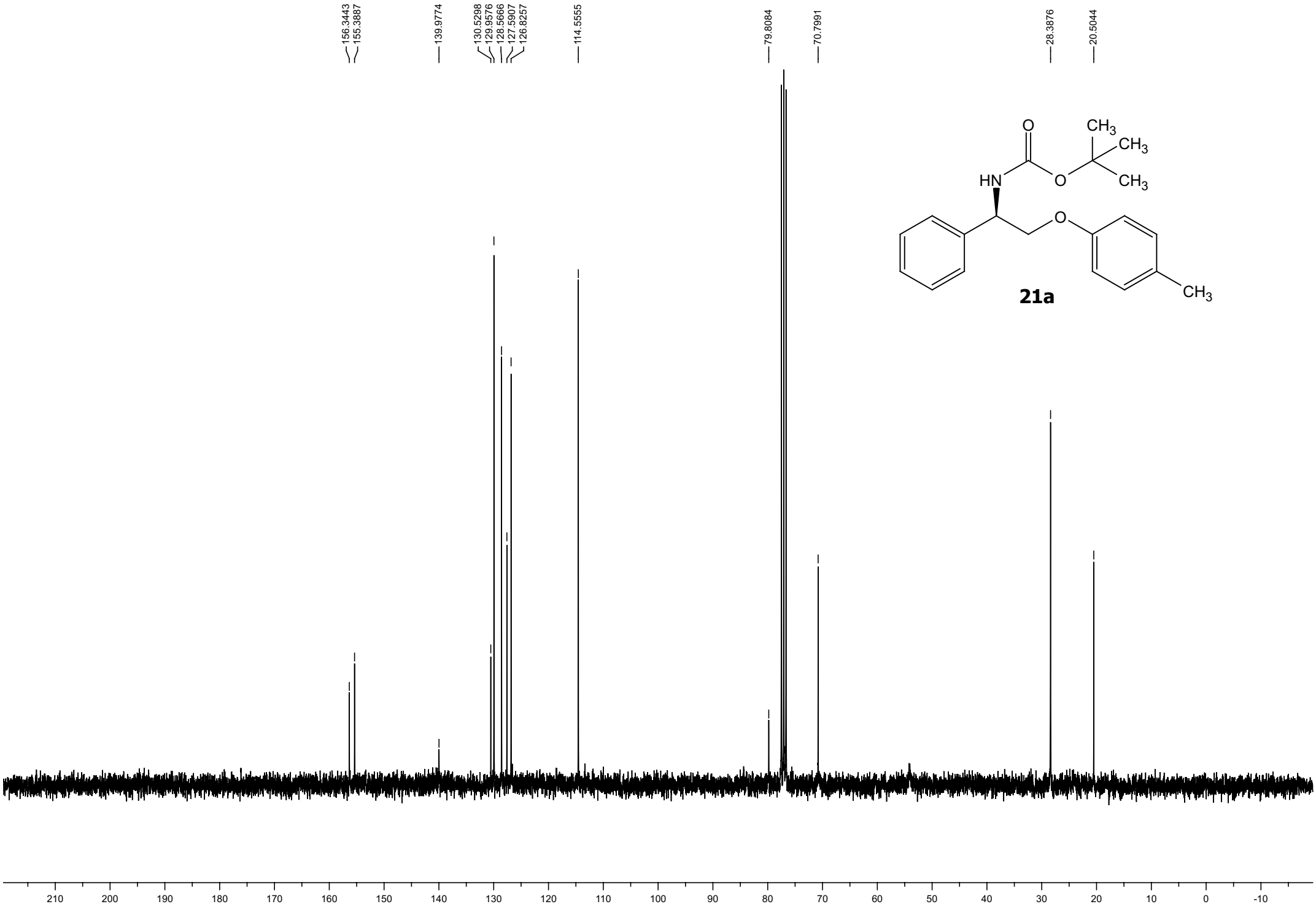
158.3972
139.3028
129.5948
128.6876
127.7859
127.0848
121.3609
114.6499
69.9106
52.4538
23.3862
O
HN
CH3
O
18d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


O
HN
CH3
O
18d
cosy CDCl3 C:\Bruker\TOPSPIN Gagnon
F1 [ppm]
2
4
6
8
8
6
4
2
F2 [ppm]


18d
%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
500
3285,01
3060,94
3027,86
2919,98
2859,14
1748,47
1650,05
1598,73
1493,96
1452,87
1237,87
1172,17
1018,73
751,24
690,15


7.4123
7.4061
7.3789
7.3541
7.3288
7.3112
7.3049
7.2977
7.2929
7.2823
7.2599
7.0848
7.0573
6.8024
6.7739
5.3393
5.0463
4.2306
4.2156
4.1991
4.1844
4.1351
4.1197
2.2847
1.4398
O
CH3
CH3
HN
O
CH3
O
CH3
21a
4.53
1.81
1.82
0.87
0.86
1.93
3.00
8.42
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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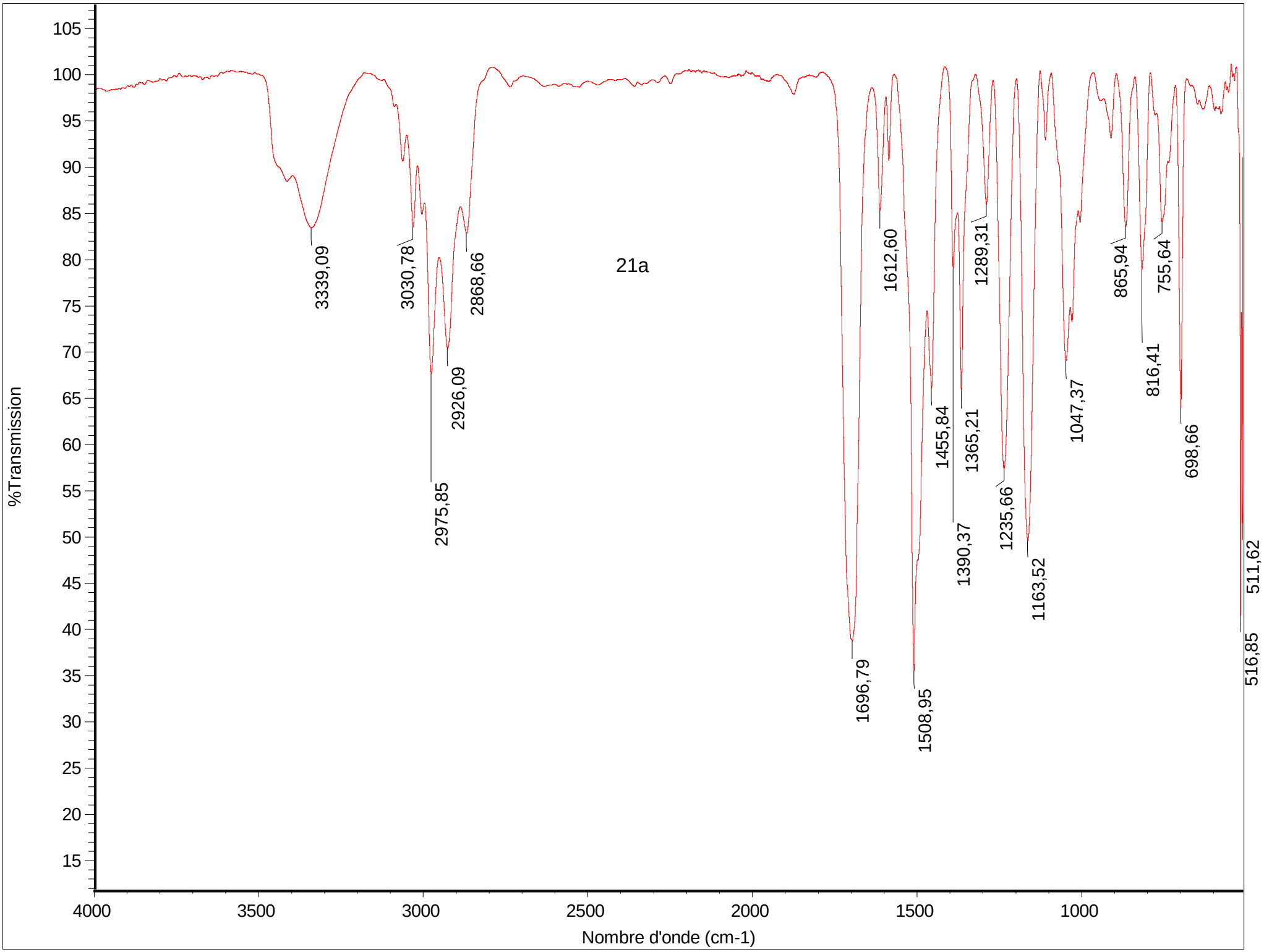
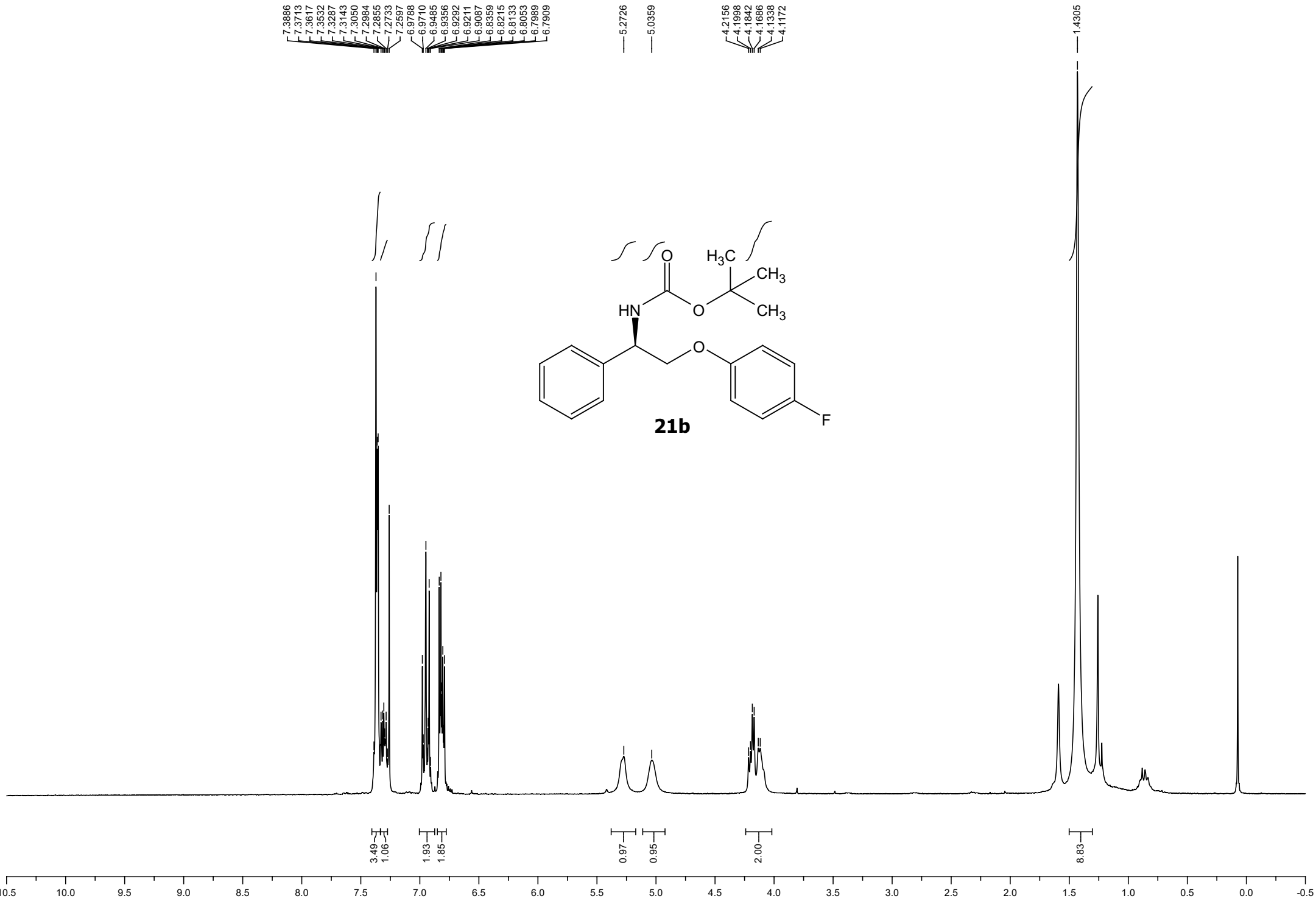
139.9774
130.5298
129.9576
128.5666
127.5907
126.8257
114.5555
79.8084
70.7991
28.3876
20.5044
O
CH3
CH3
HN
O
CH3
O
CH3
21a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


21a
%Transmission
Nombre d'onde (cm-1)
105
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
3339,09
3030,78
2975,85
2926,09
2868,66
1696,79
1612,60
1508,95
1455,84
1390,37
1365,21
1289,31
1235,66
1163,52
1047,37
865,94
816,41
755,64
698,66
516,85
511,62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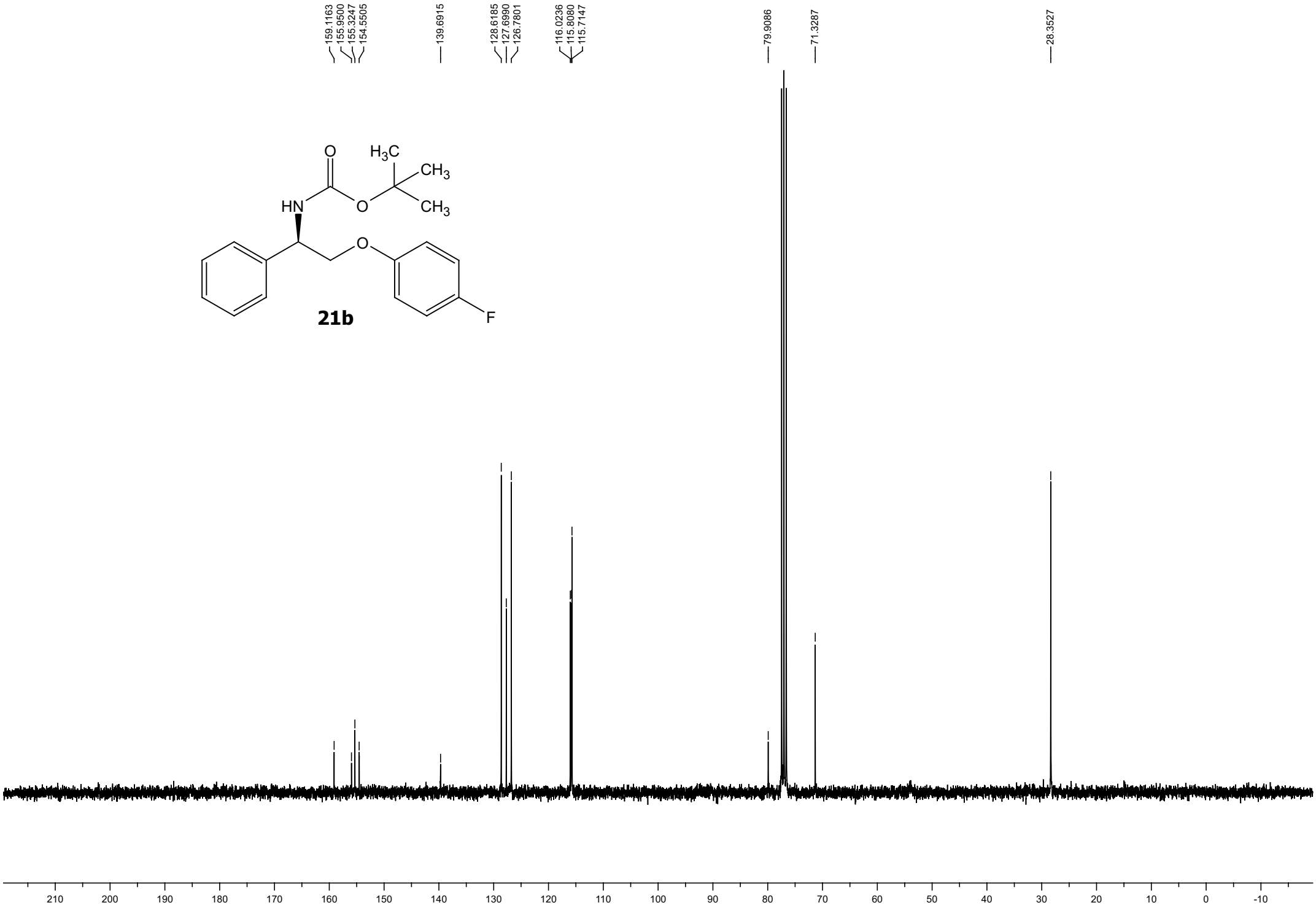
7.3713
7.3617
7.3532
7.3287
7.3143
7.3050
7.2984
7.2855
7.2733
7.2597
6.9788
6.9710
6.9485
6.9356
6.9292
6.9211
6.9087
6.8359
6.8215
6.8133
6.8053
6.7989
6.7909
5.2726
5.0359
4.2156
4.1998
4.1842
4.1686
4.1338
4.1172
1.4305
O
H3C
CH3
HN
O
CH3
O
F
21b
3.49
1.06
1.93
1.85
0.97
0.95
2.00
8.83
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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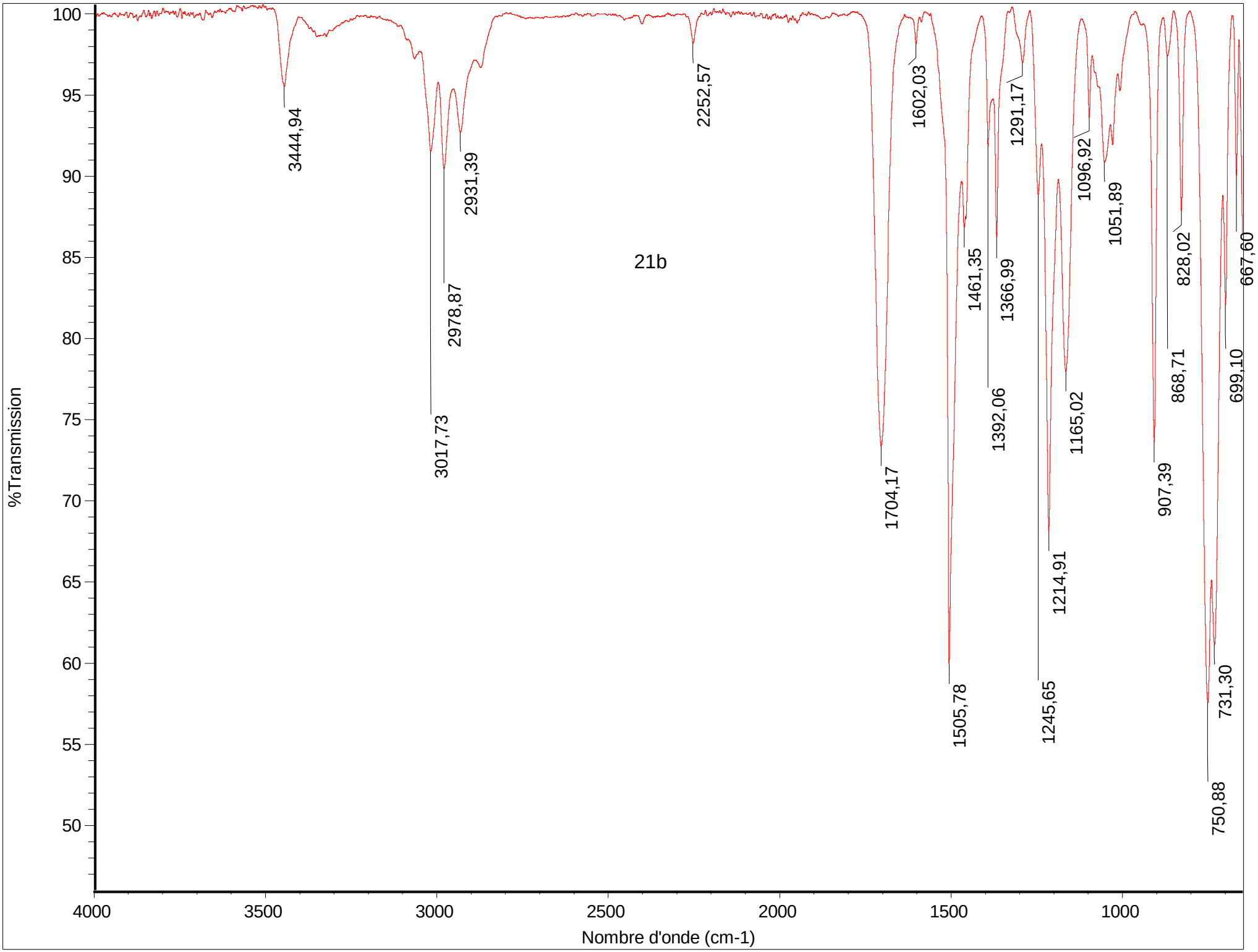
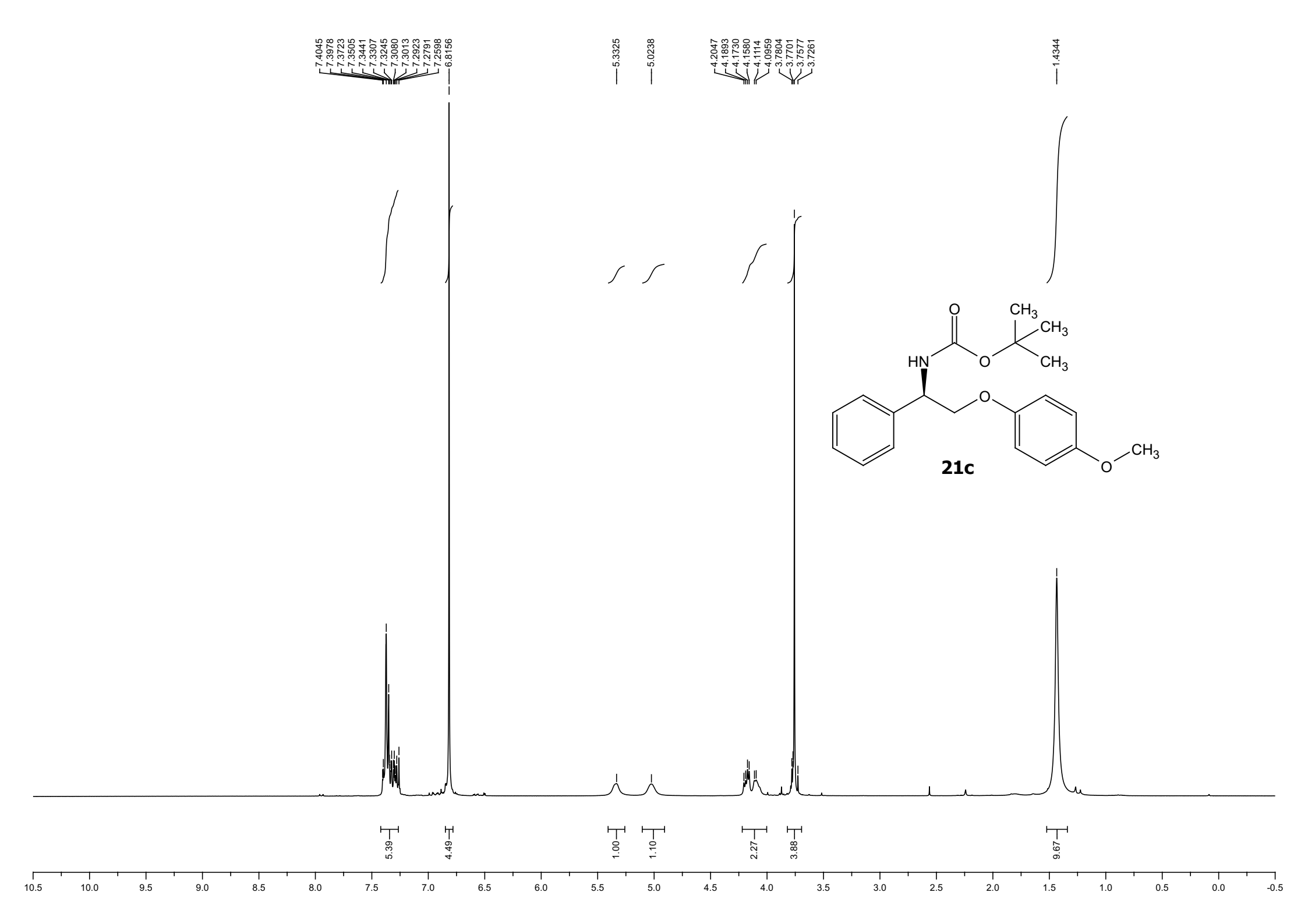
155.9500
155.3247
154.5505
139.6915
128.6185
127.6990
126.7801
116.0236
115.8080
115.7147
79.9086
71.3287
28.3527
O
H3C
CH3
CH3
HN
O
O
F
21b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


21b
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
4000
3500
3000
2500
2000
1500
1000
3444,94
3017,73
2978,87
2931,39
2252,57
1704,17
1602,03
1505,78
1461,35
1392,06
1366,99
1291,17
1245,65
1214,91
1165,02
1096,92
1051,89
907,39
868,71
828,02
750,88
731,30
699,10
667,60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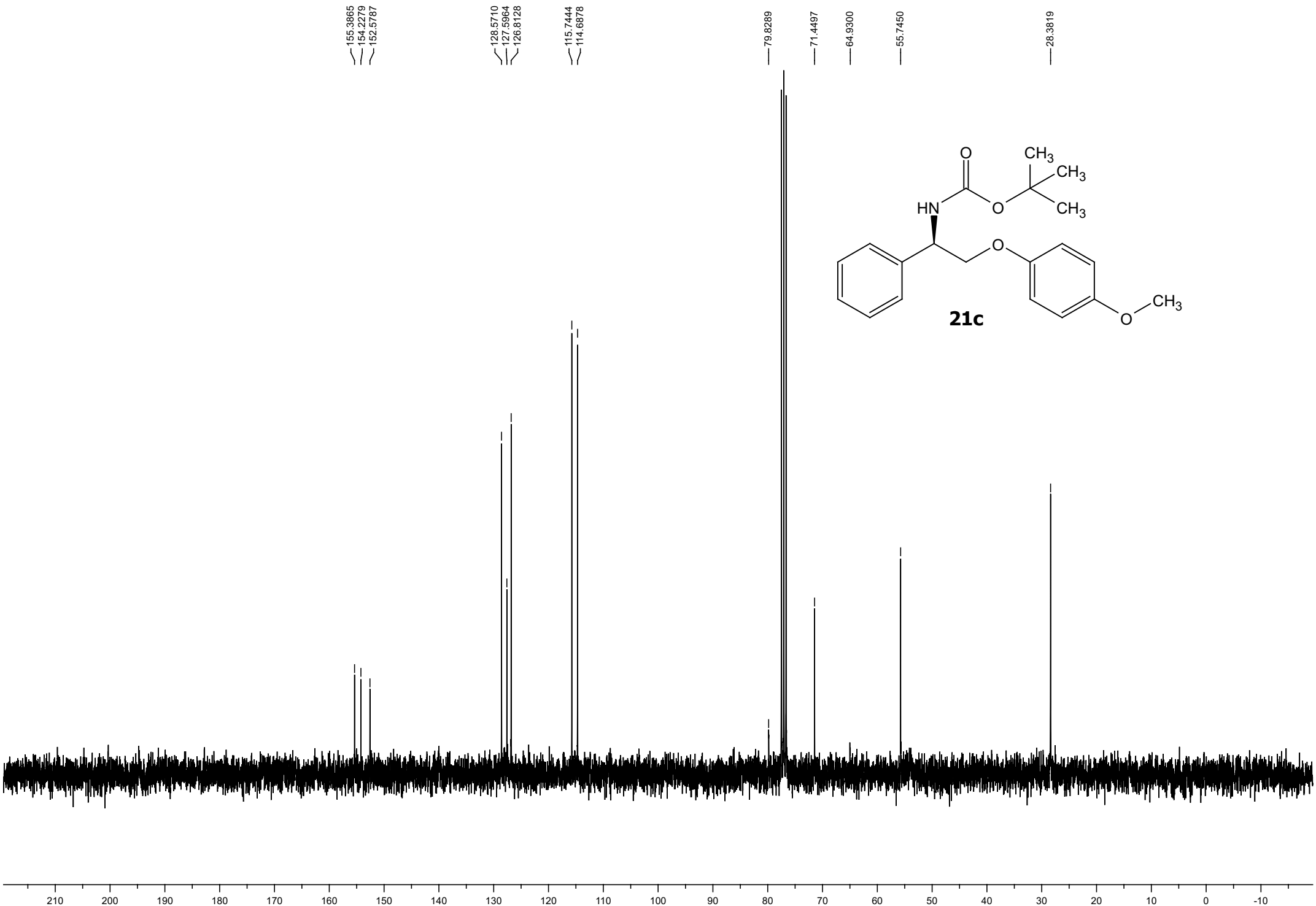
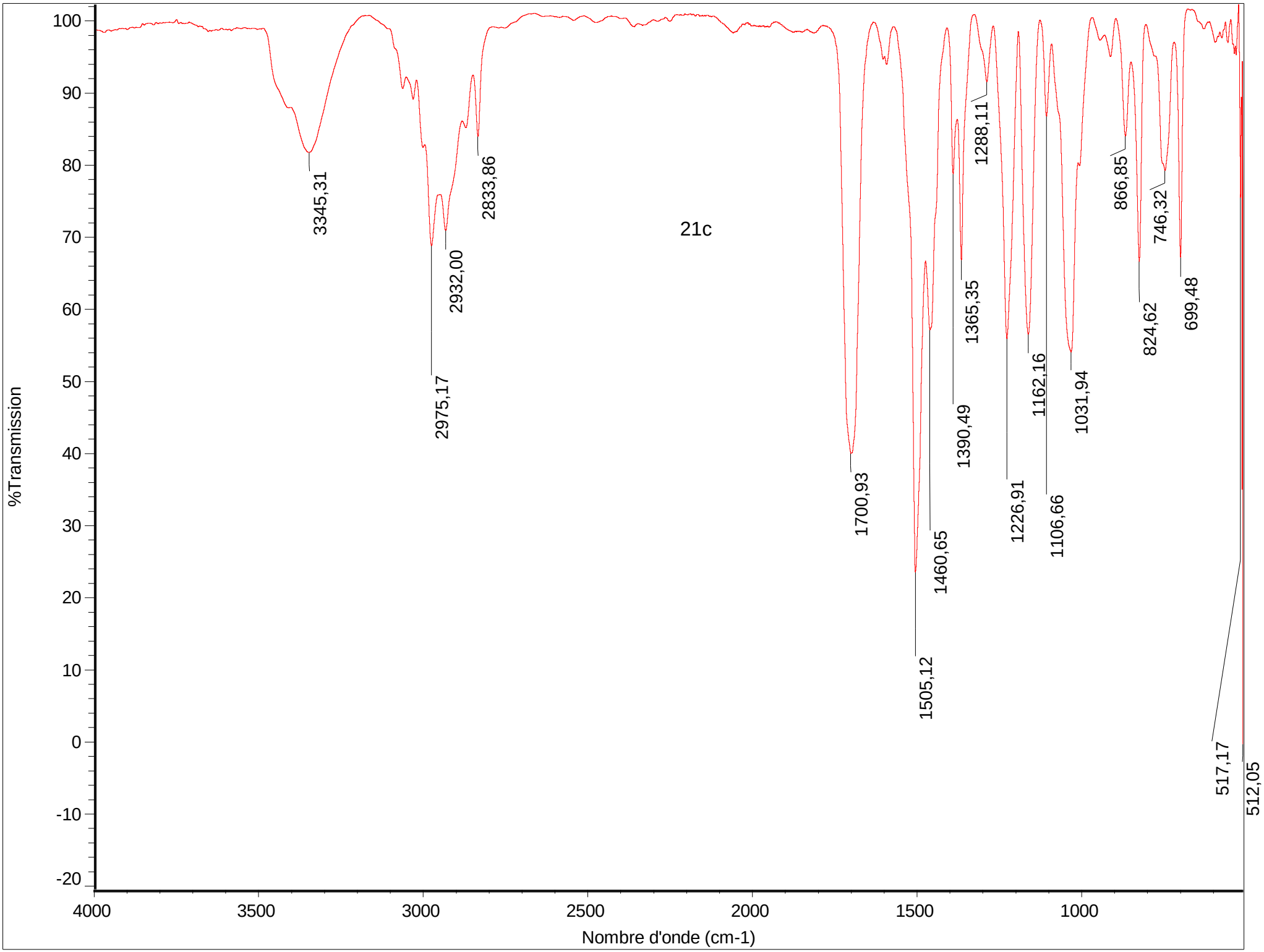
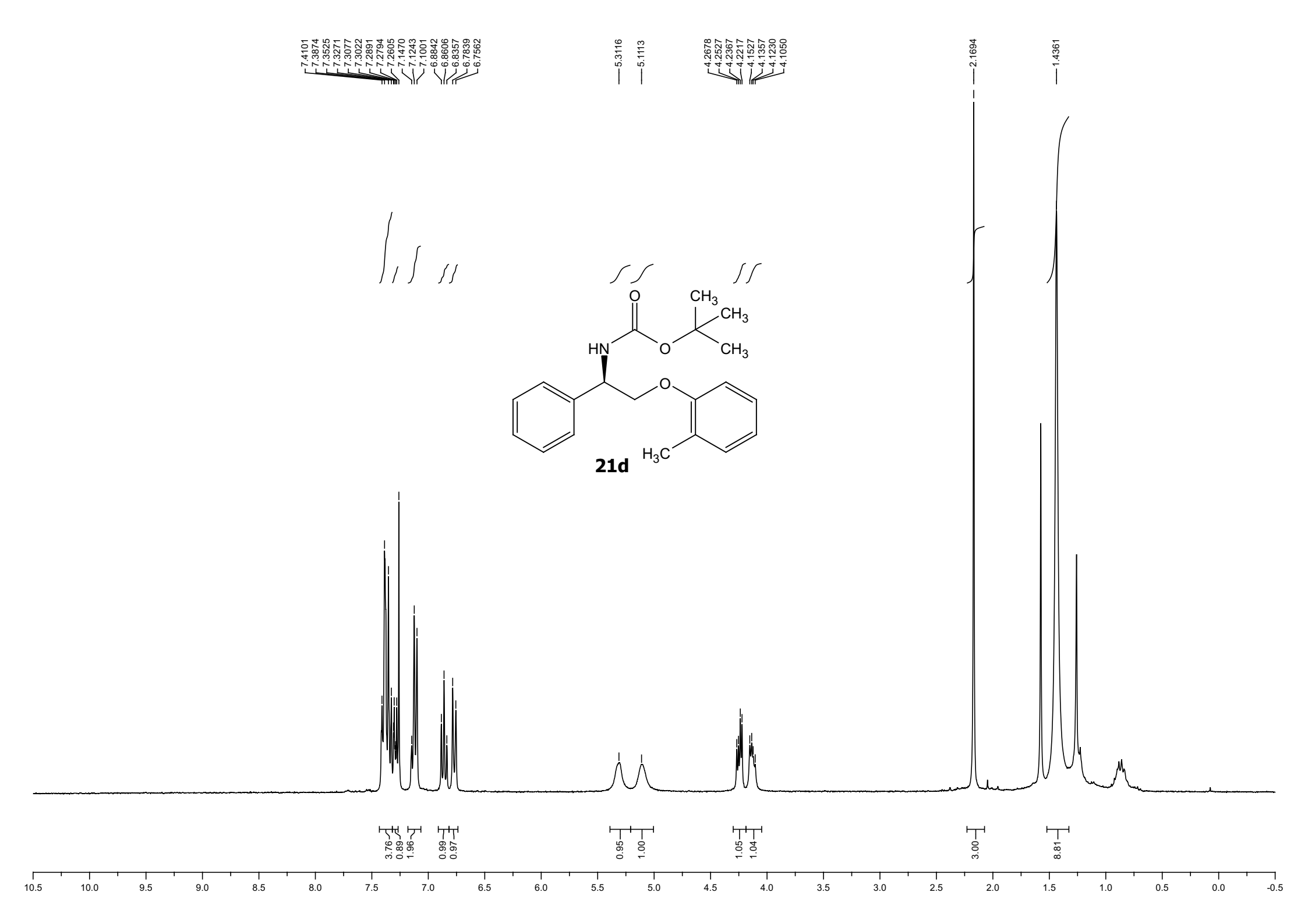
7.3978
7.3723
7.3505
7.3441
7.3307
7.3245
7.3080
7.3013
7.2923
7.2791
7.2598
6.8156
5.3325
5.0238
4.2047
4.1893
4.1730
4.1580
4.1114
4.0959
3.7804
3.7701
3.7577
3.7261
1.4344
O
CH3
CH3
CH3
HN
O
O
O
CH3
21c
5.39
4.49
1.00
1.10
2.27
3.88
9.67
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


155.3865
154.2279
152.5787
128.5710
127.5964
126.8128
115.7444
114.6878
79.8289
71.4497
64.9300
55.7450
28.3819
O
CH3
CH3
CH3
HN
O
O
CH3
O
21c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


21c
%Transmission
Nombre d'onde (cm-1)
100
90
80
70
60
50
40
30
20
10
0
-10
-20
4000
3500
3000
2500
2000
1500
1000
3345,31
2975,17
2932,00
2833,86
1700,93
1505,12
1460,65
1390,49
1365,35
1288,11
1226,91
1162,16
1106,66
1031,94
866,85
824,62
746,32
699,48
517,17
512,05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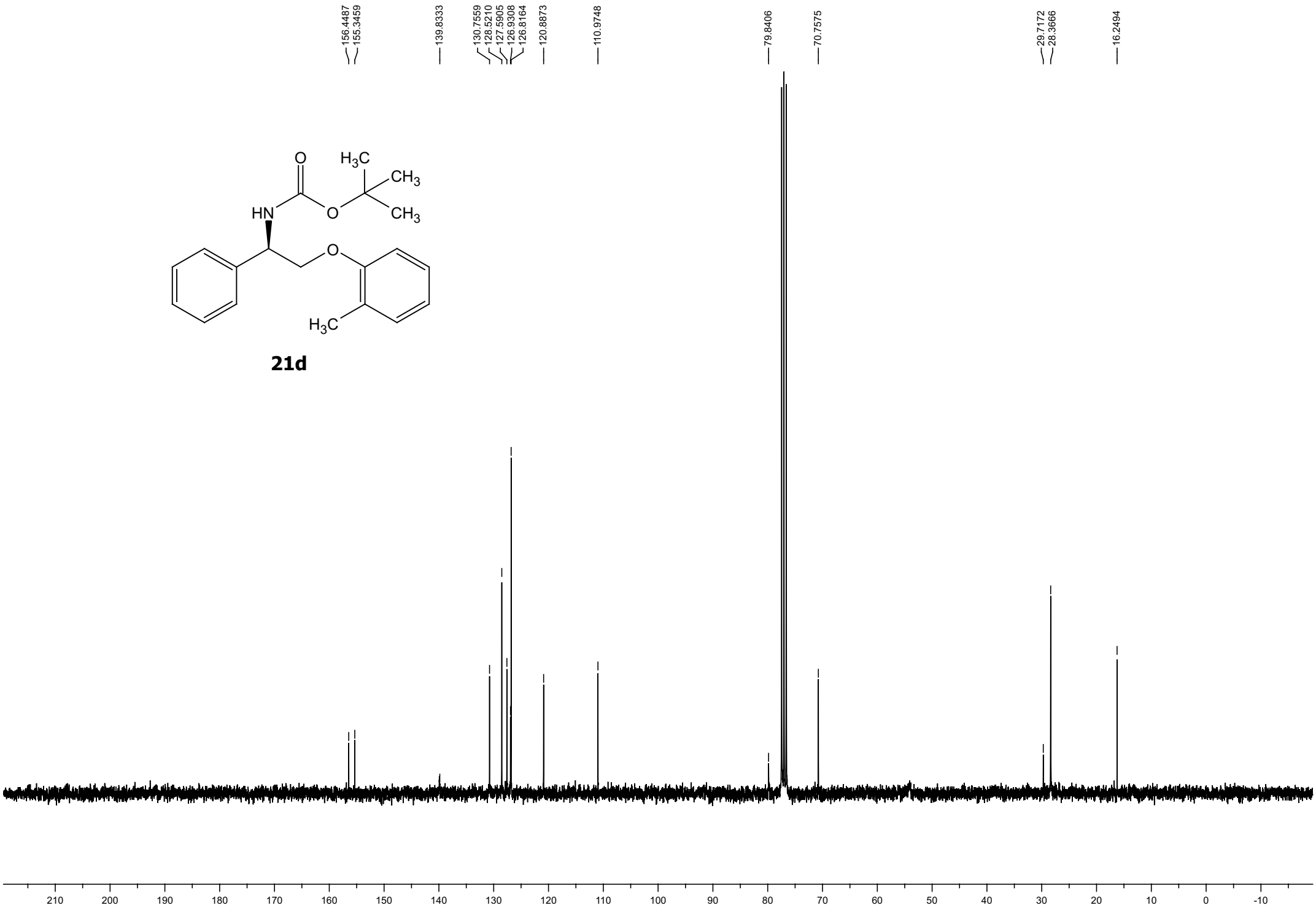
7.3874
7.3525
7.3271
7.3077
7.3022
7.2891
7.2794
7.2605
7.1470
7.1243
7.1001
6.8842
6.8606
6.8357
6.7839
6.7562
5.3116
5.1113
4.2678
4.2527
4.2367
4.2217
4.1527
4.1357
4.1230
4.1050
2.1694
1.4361
O
CH3
CH3
CH3
HN
O
O
H3C
21d
3.76
0.89
1.96
0.99
0.97
0.95
1.00
1.05
1.04
3.00
8.81
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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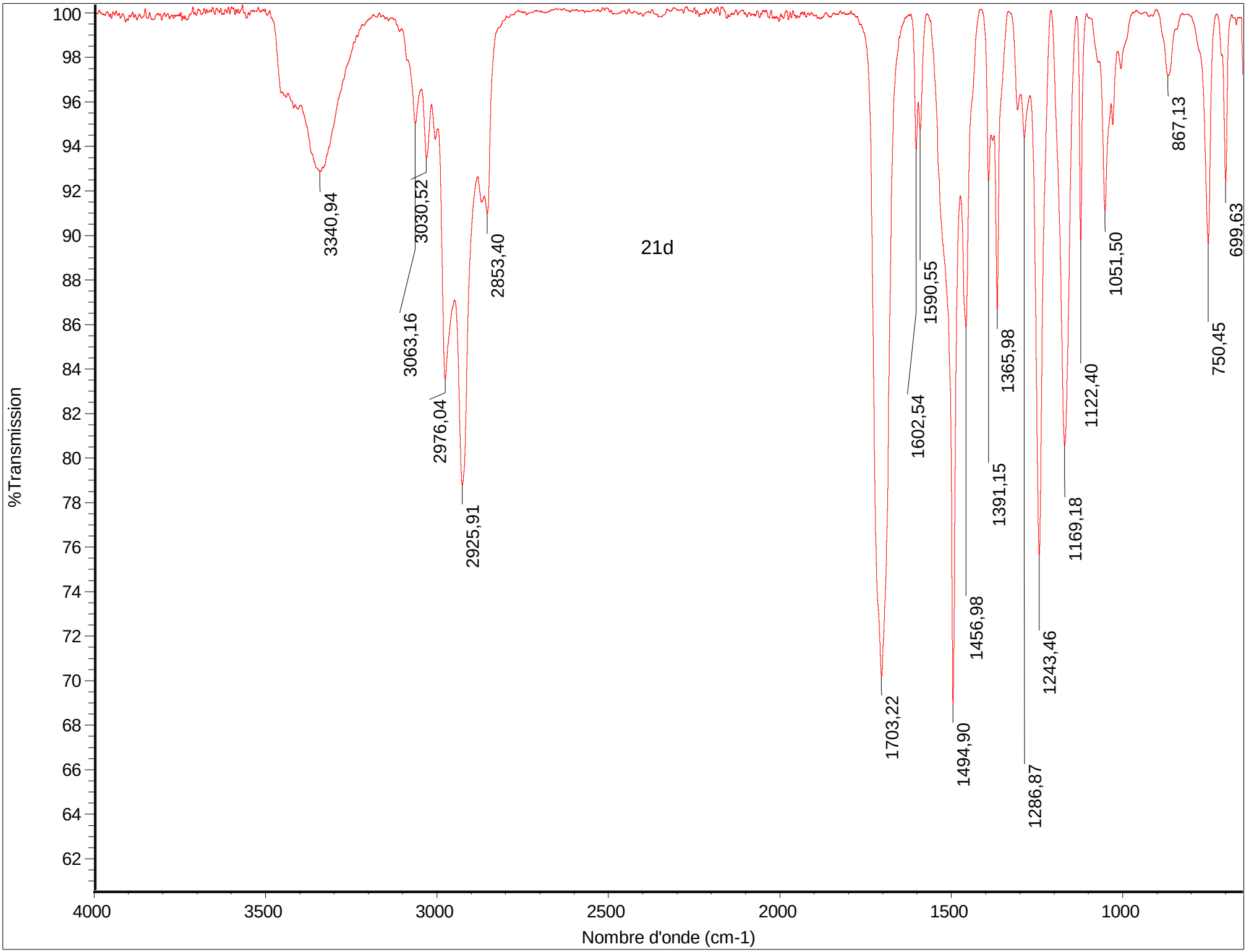
155.3459
139.8333
130.7559
128.5210
127.5905
126.9308
126.8164
120.8873
110.9748
79.8406
70.7575
29.7172
28.3666
16.2494
O
H3C
CH3
HN
O
CH3
O
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

21d


21d
%Transmission
Nombre d'onde (cm-1)
100
98
96
94
92
90
88
86
84
82
80
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76
74
72
70
68
66
64
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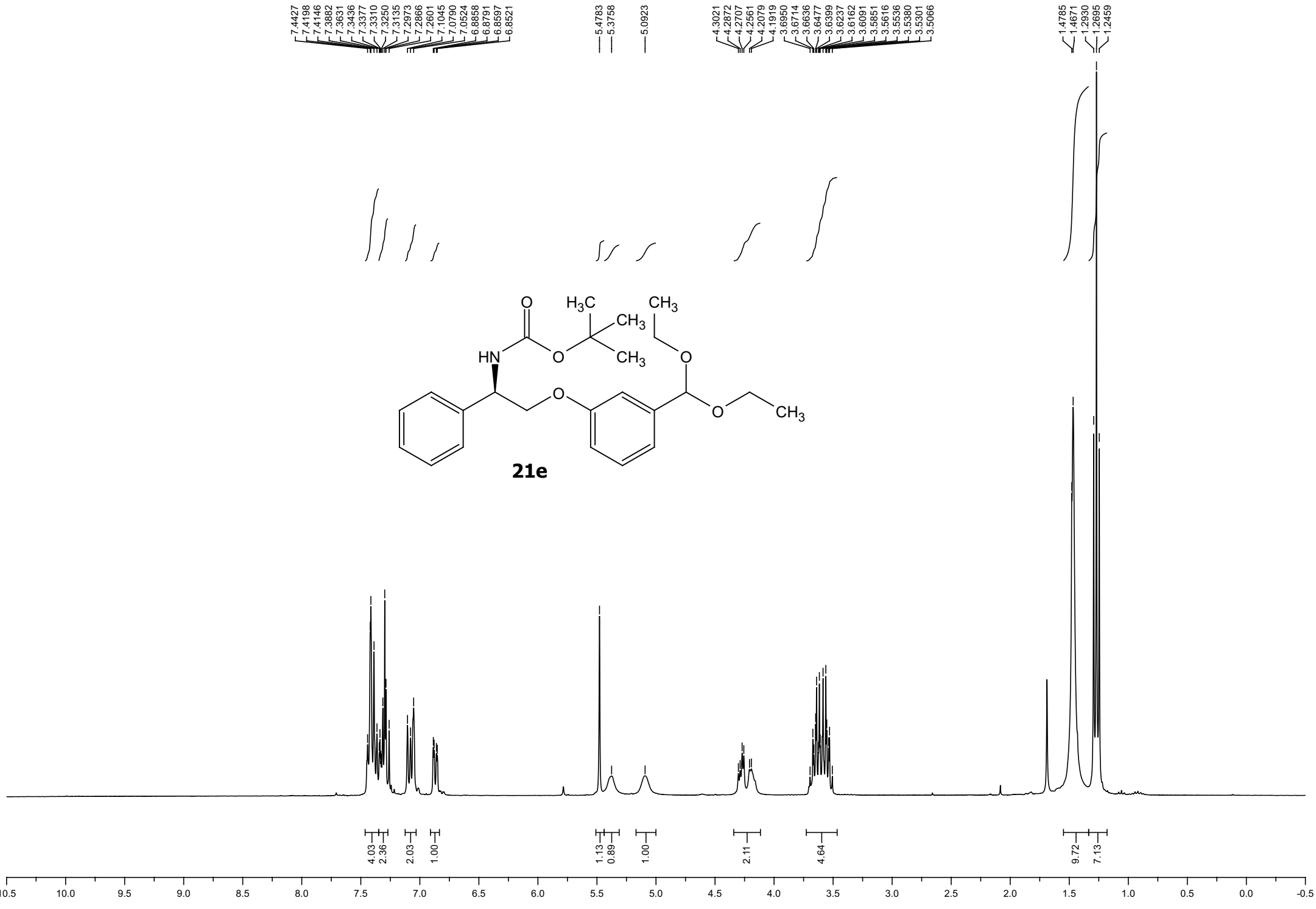
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7.1045
7.0790
7.0524
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6.8791
6.8597
6.8521
5.4783
5.3758
5.0923
4.3021
4.2872
4.2707
4.2561
4.2079
4.1919
3.6950
3.6714
3.6636
3.6477
3.6399
3.6237
3.6162
3.6091
3.5851
3.5616
3.5536
3.5380
3.5301
3.5066
1.4785
1.4671
1.2930
1.2695
1.2459
O
H3C
CH3
CH3
HN
O
O
CH3
O
O
CH3
4.03
2.36
2.03
1.00
1.13
0.89
1.00
2.11
4.64
9.72
7.13
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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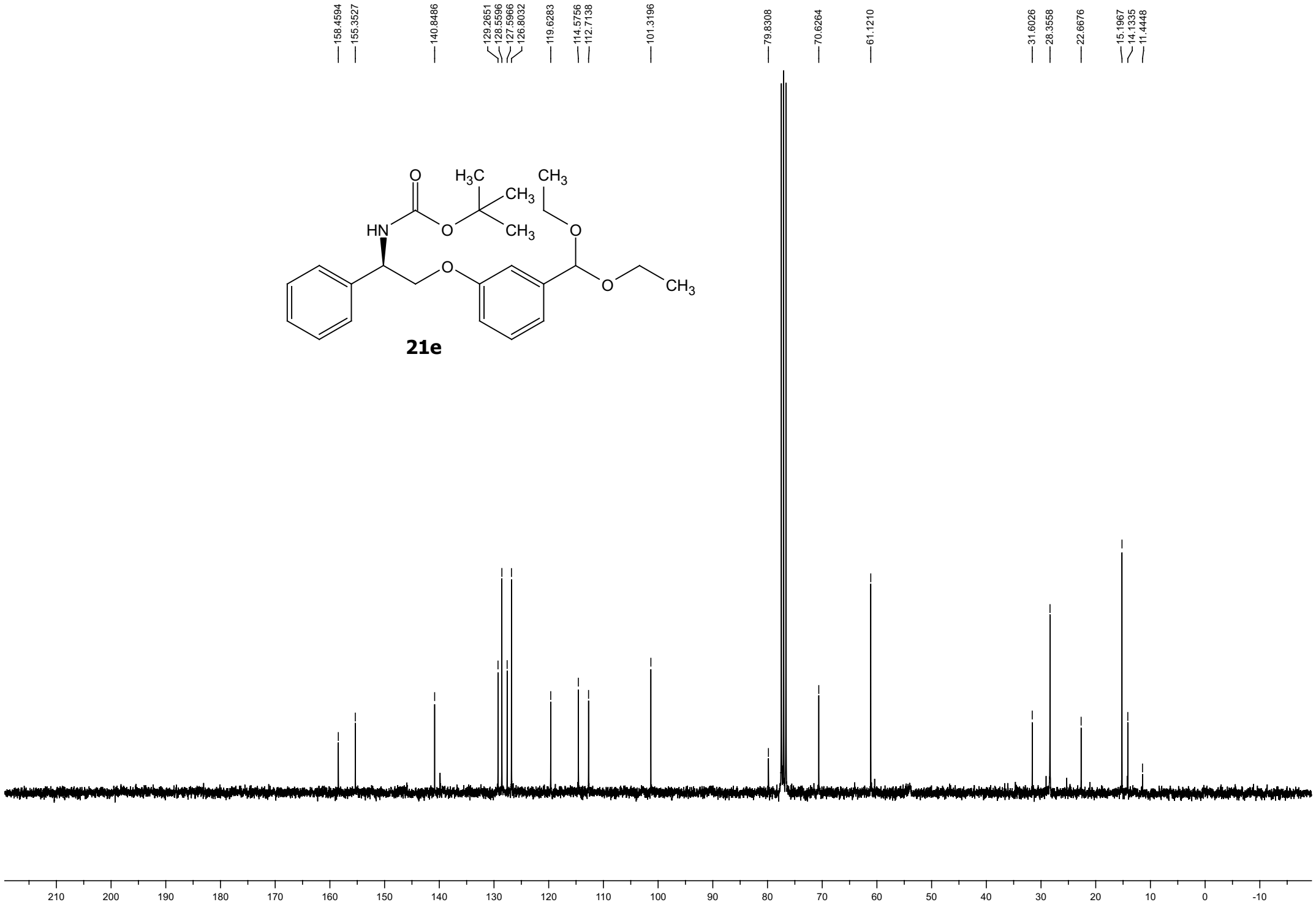
21e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79.8308
70.6264
61.1210
31.6026
28.3558
22.6676
15.1967
14.1335
11.4448
O
H3C
CH3
CH3
CH3
HN
O
O
O
O
O
CH3
21e
210
200
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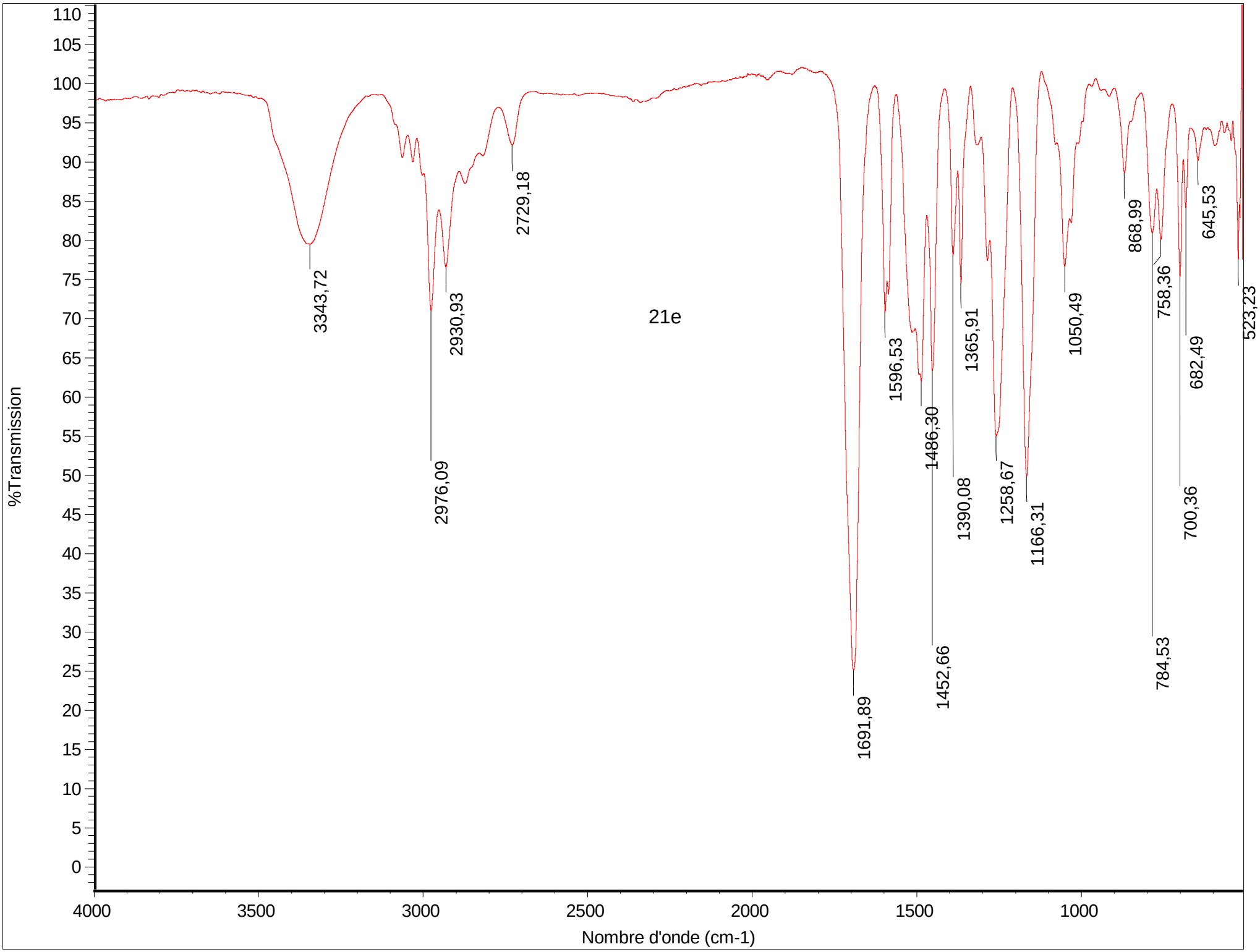
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1390,08
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1166,31
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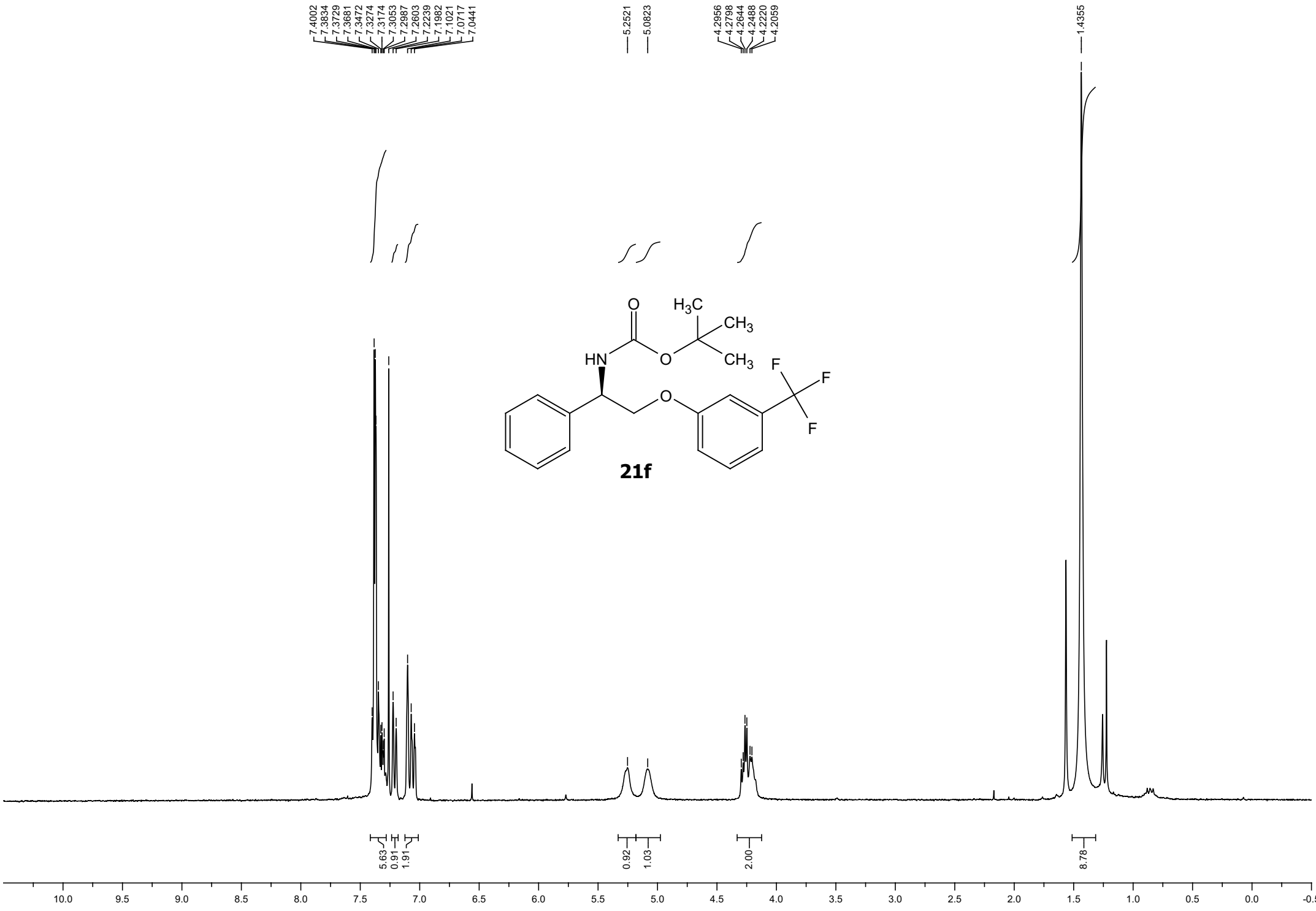
523,23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7.3472
7.3274
7.3174
7.3053
7.2987
7.2603
7.2239
7.1982
7.1021
7.0717
7.0441
5.2521
5.0823
4.2956
4.2798
4.2644
4.2488
4.2220
4.2059
1.4355
O
H3C
CH3
HN
O
CH3
F
F
F
O
21f
5.63
0.91
1.91
0.92
1.03
2.00
8.78
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
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1.0
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0.0
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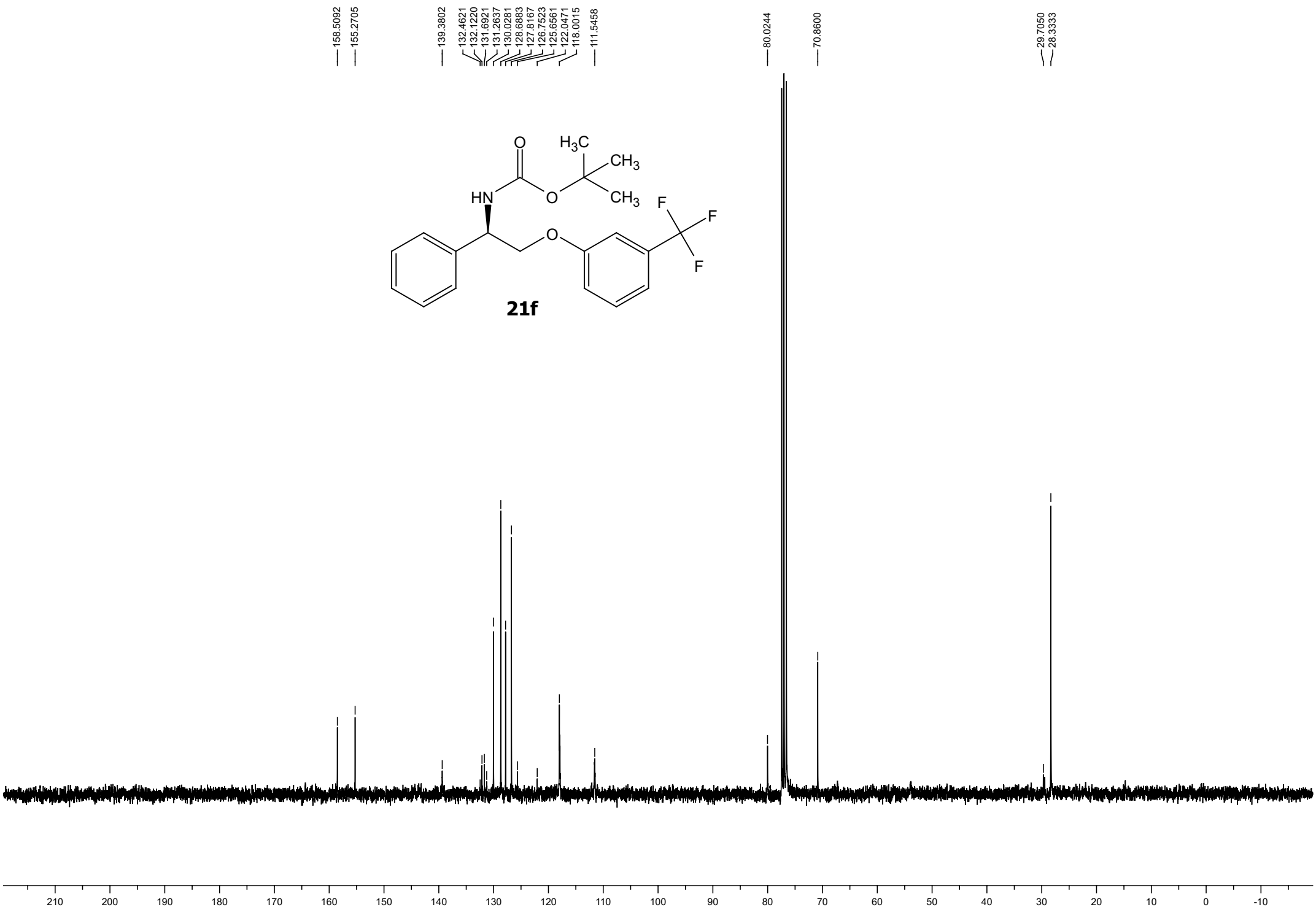
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126.7523
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122.0471
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29.7050
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O
H3C
CH3
HN
O
CH3
F
F
O
F
21f
210
200
190
180
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140
130
120
110
100
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60
50
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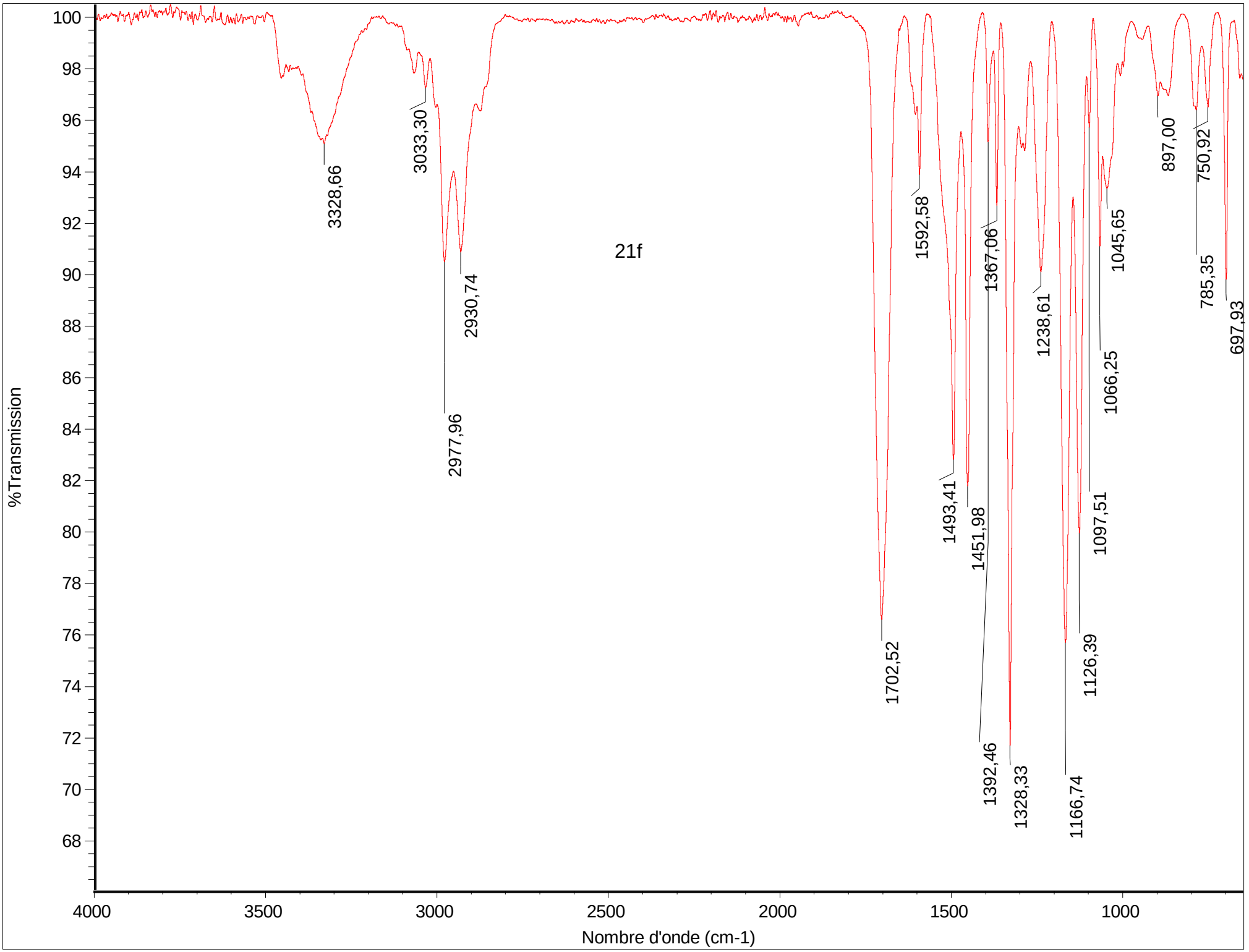
-10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94
92
90
88
86
84
82
80
78
76
74
72
70
68
4000
3500
3000
2500
2000
1500
1000
3328,66
3033,30
2977,96
2930,74
1702,52
1592,58
1493,41
1451,98
1392,46
1367,06
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1126,39
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1045,65
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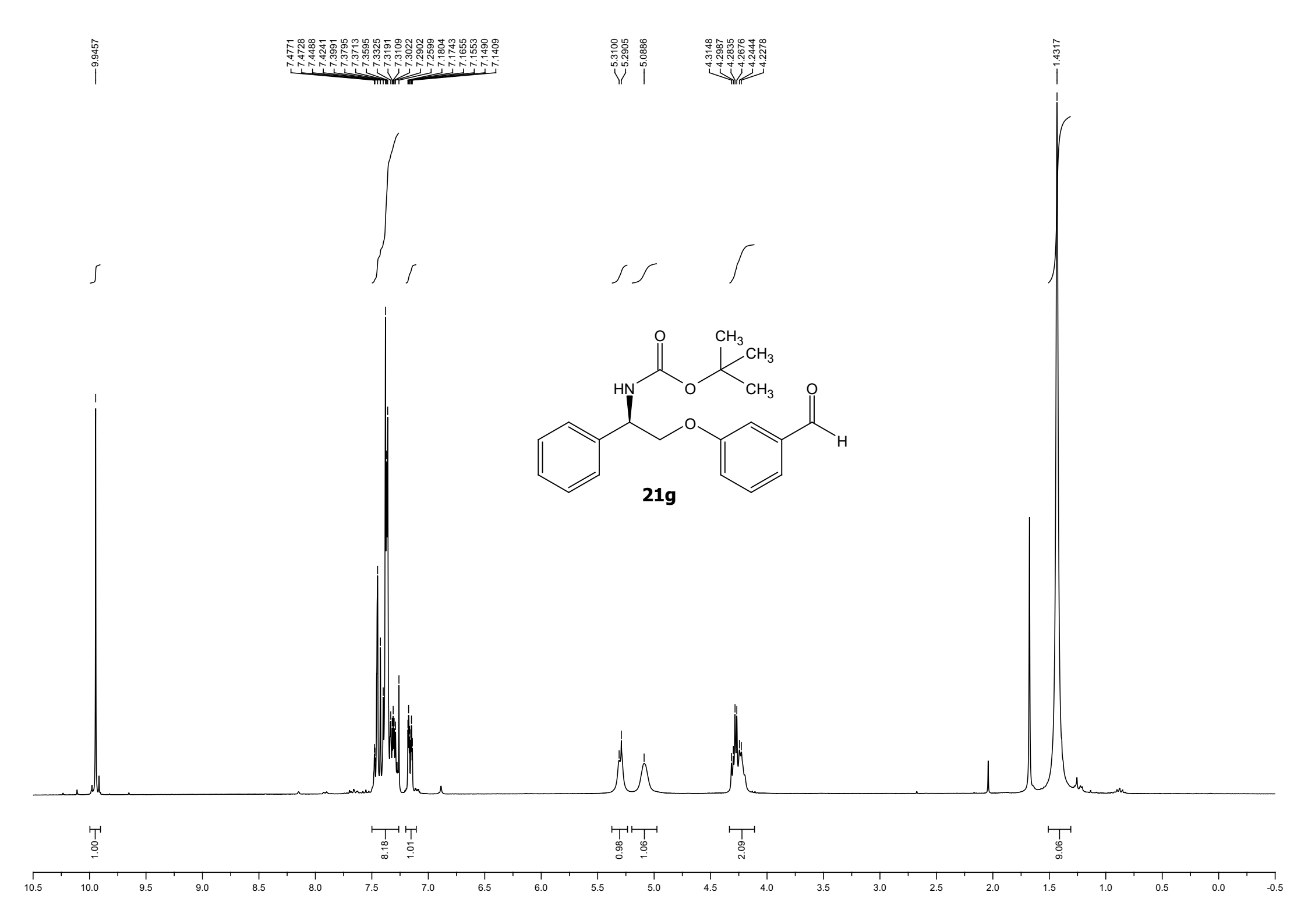
785,35
750,92
697,93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7.3191
7.3109
7.3022
7.2902
7.2599
7.1804
7.1743
7.1655
7.1553
7.1490
7.1409
5.3100
5.2905
5.0886
4.3148
4.2987
4.2835
4.2676
4.2444
4.2278
1.4317
O
CH3
CH3
HN
O
CH3
O
O
H
21g
1.00
8.18
1.01
0.98
1.06
2.09
9.06
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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1.5
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0.0
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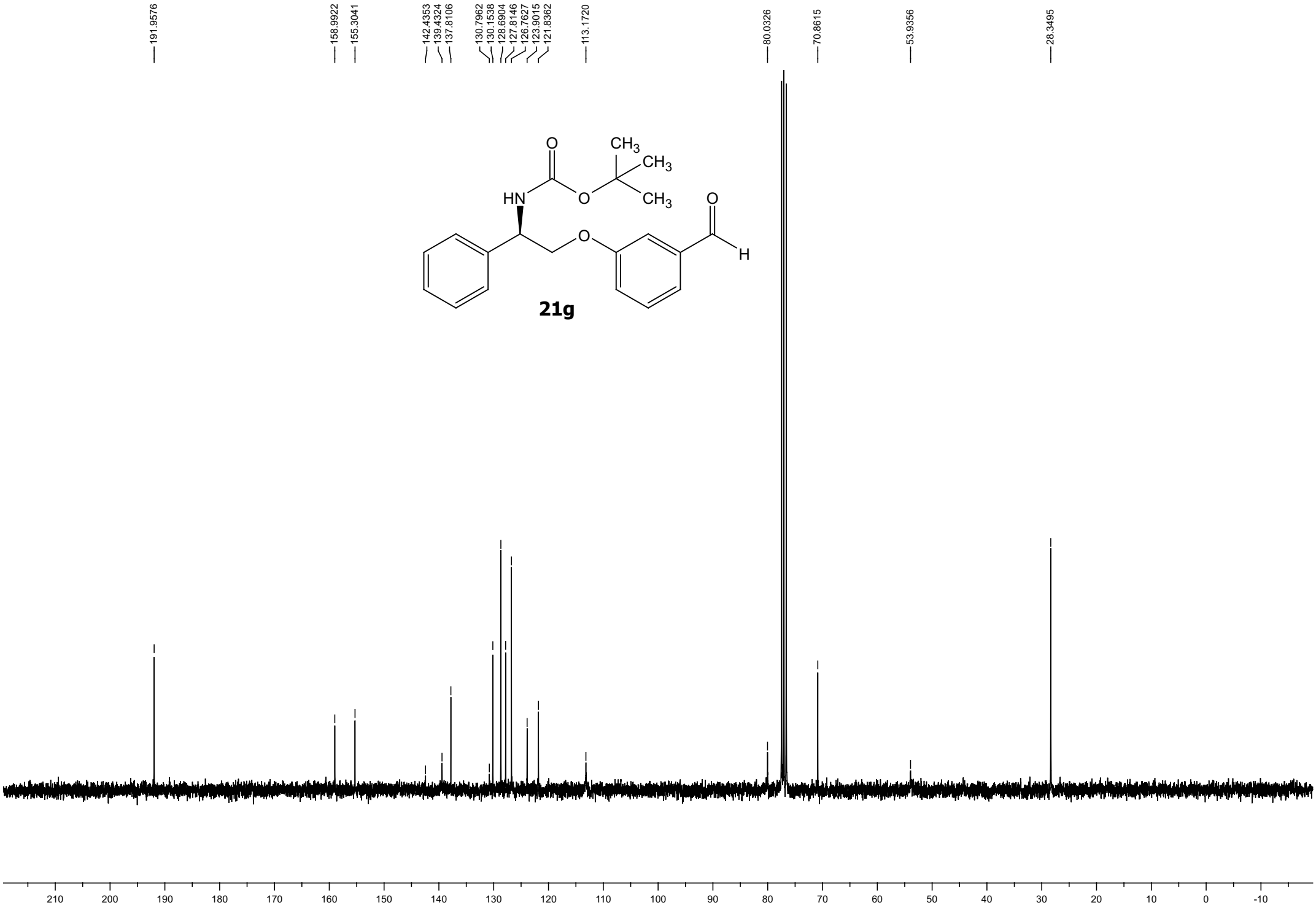
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126.7627
123.9015
121.8362
113.1720
80.0326
70.8615
53.9356
28.3495
O
CH3
CH3
HN
O
CH3
O
O
H
21g
210
200
190
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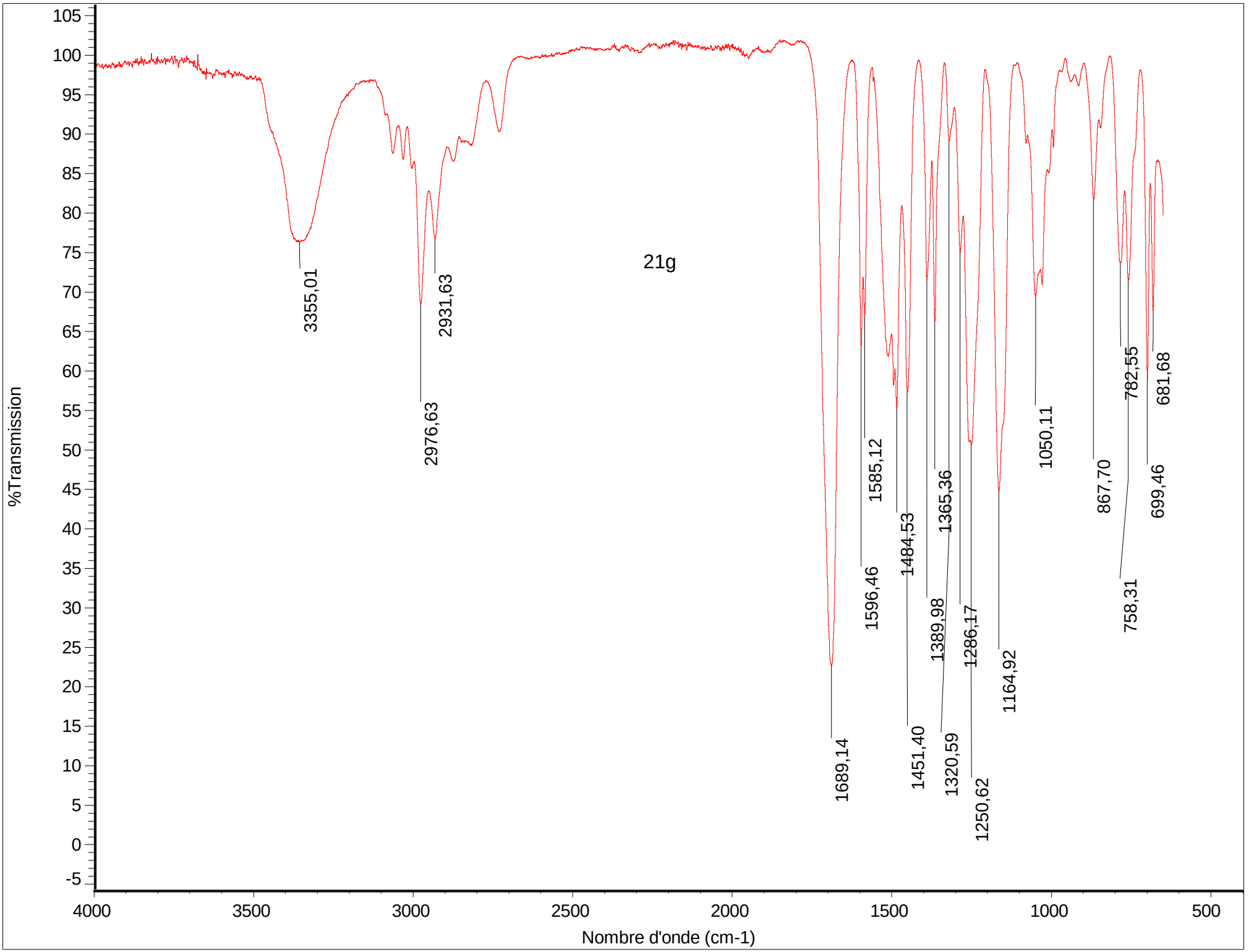
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Nombre d'onde (cm-1)
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70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
4000
3500
3000
2500
2000
1500
1000
500
3355,01
2976,63
2931,63
1689,14
1596,46
1585,12
1484,53
1451,40
1389,98
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1320,59
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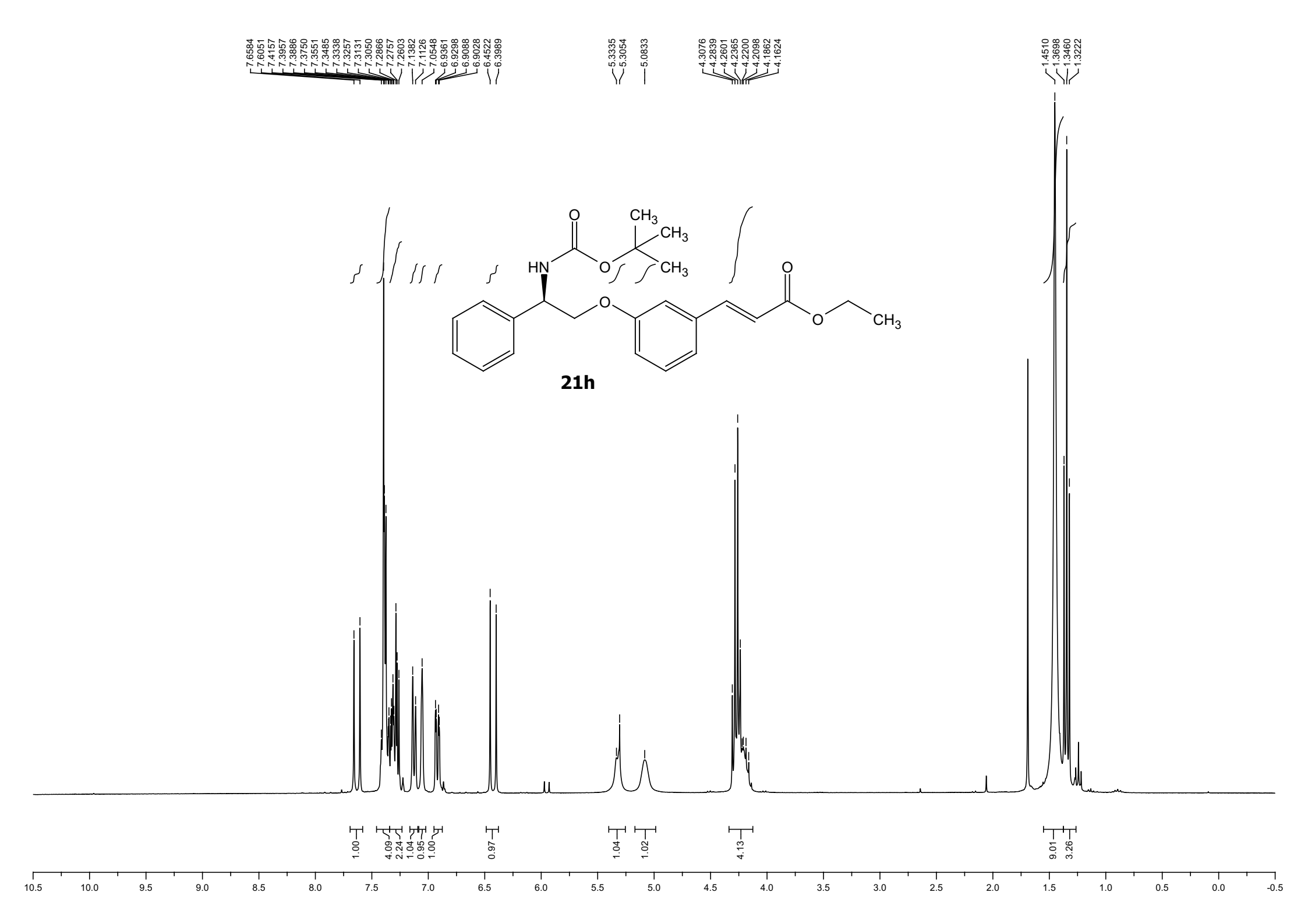
1050,11
867,70
782,55
758,31
699,46
681,68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7.3338
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7.3131
7.3050
7.2866
7.2757
7.2603
7.1382
7.1126
7.0548
6.9361
6.9298
6.9088
6.9028
6.4522
6.3989
5.3335
5.3054
5.0833
4.3076
4.2839
4.2601
4.2365
4.2200
4.2098
4.1862
4.1624
1.4510
1.3698
1.3460
1.3222
HN
O
CH3
CH3
CH3
O
O
O
O
CH3
21h
1.00
4.09
2.24
1.04
0.95
1.00
0.97
1.04
1.02
4.13
9.01
3.26
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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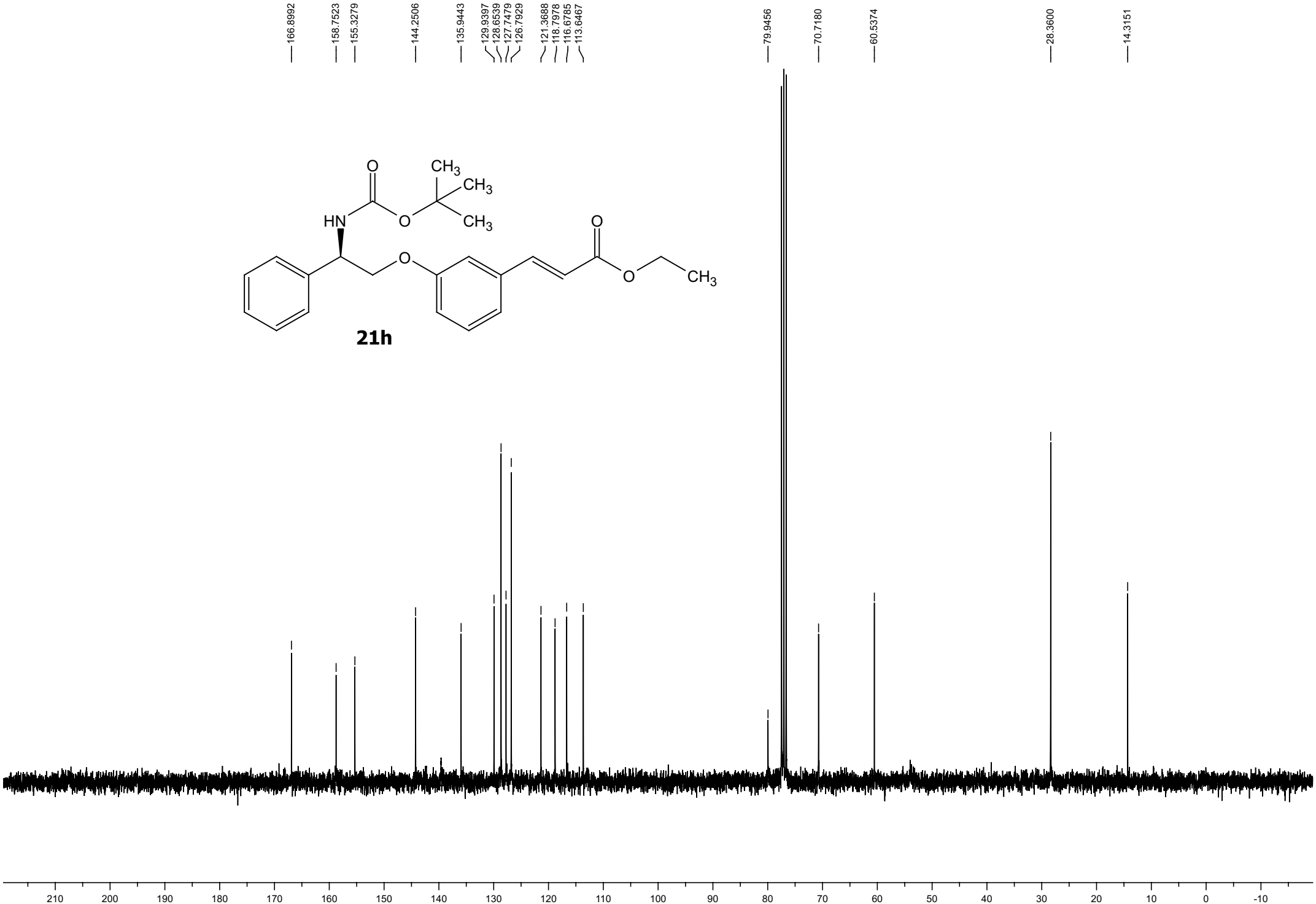
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126.7929
121.3688
118.7978
116.6785
113.6467
79.9456
70.7180
60.5374
28.3600
14.3151
O
CH3
CH3
HN
O
CH3
O
O
O
O
CH3
21h
210
200
190
180
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140
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120
110
100
90
80
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50
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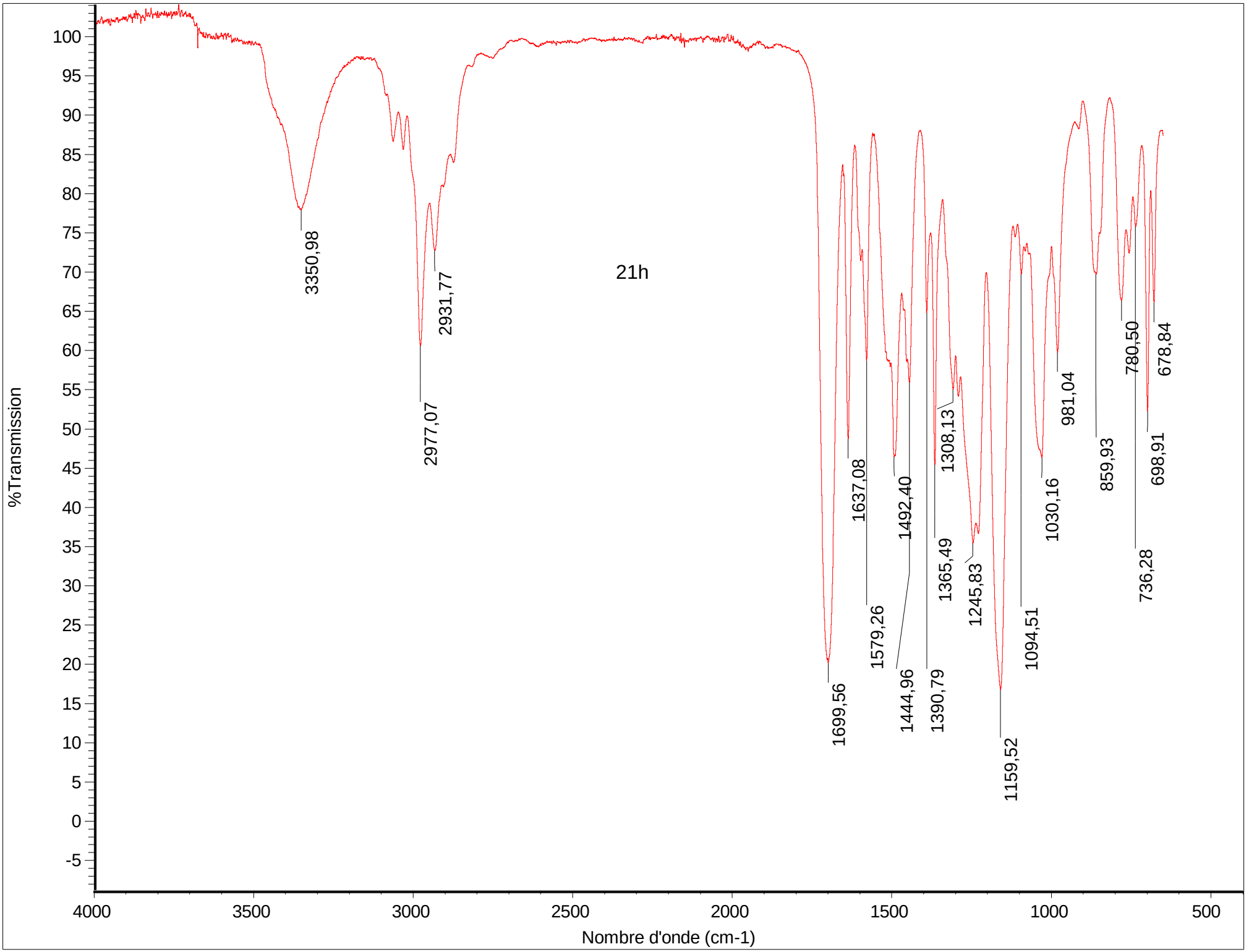
-10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%Transmission
Nombre d'onde (cm-1)
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90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
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3500
3000
2500
2000
1500
1000
500
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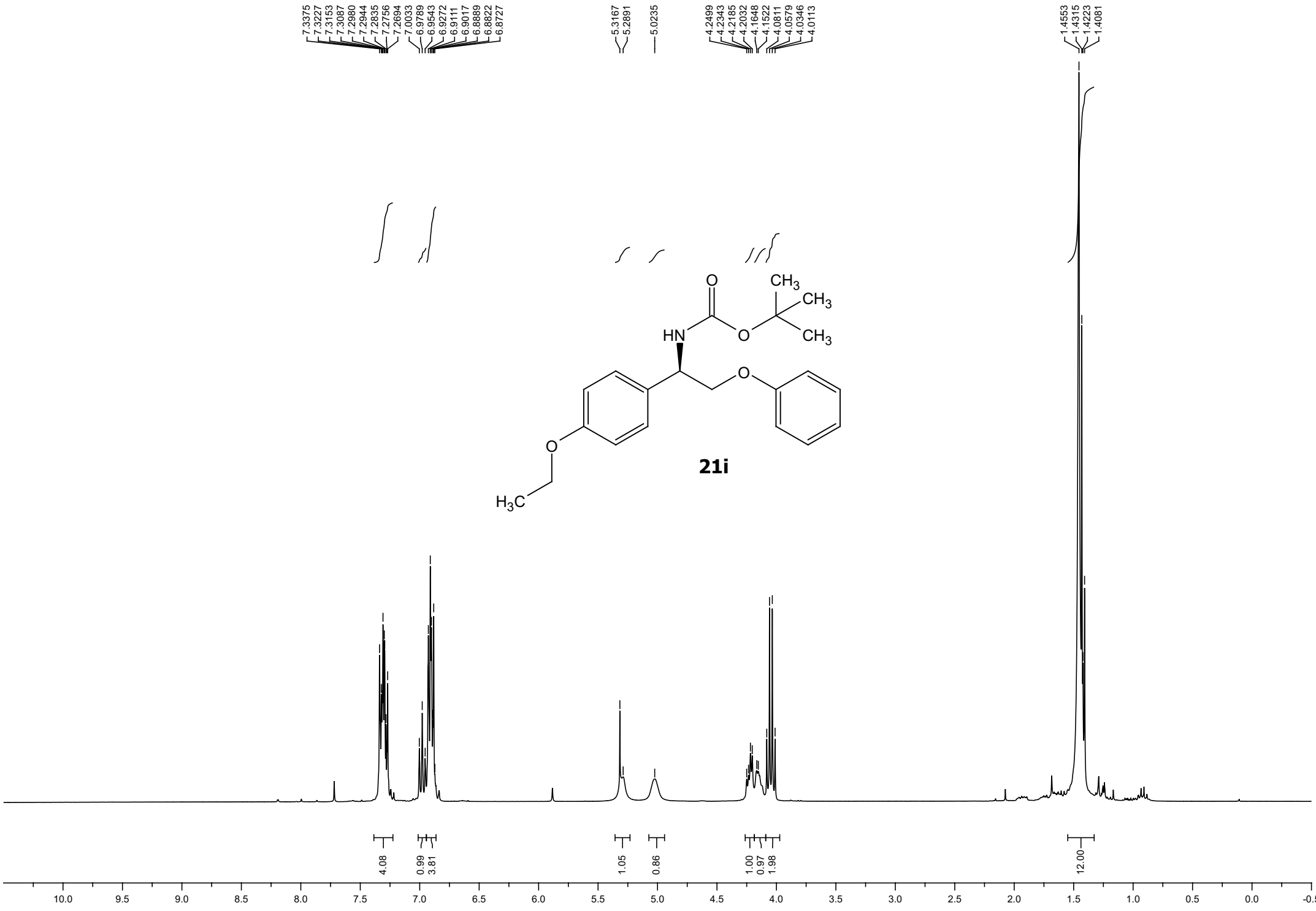
698,91
678,84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6.9111
6.9017
6.8889
6.8822
6.8727
5.3167
5.2891
5.0235
4.2499
4.2343
4.2185
4.2032
4.1648
4.1522
4.0811
4.0579
4.0346
4.0113
1.4553
1.4315
1.4223
1.4081
O
CH3
CH3
HN
O
CH3
O
O
H3C
21i
4.08
0.99
3.81
1.05
0.86
1.00
0.97
1.98
12.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
5.5
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1.5
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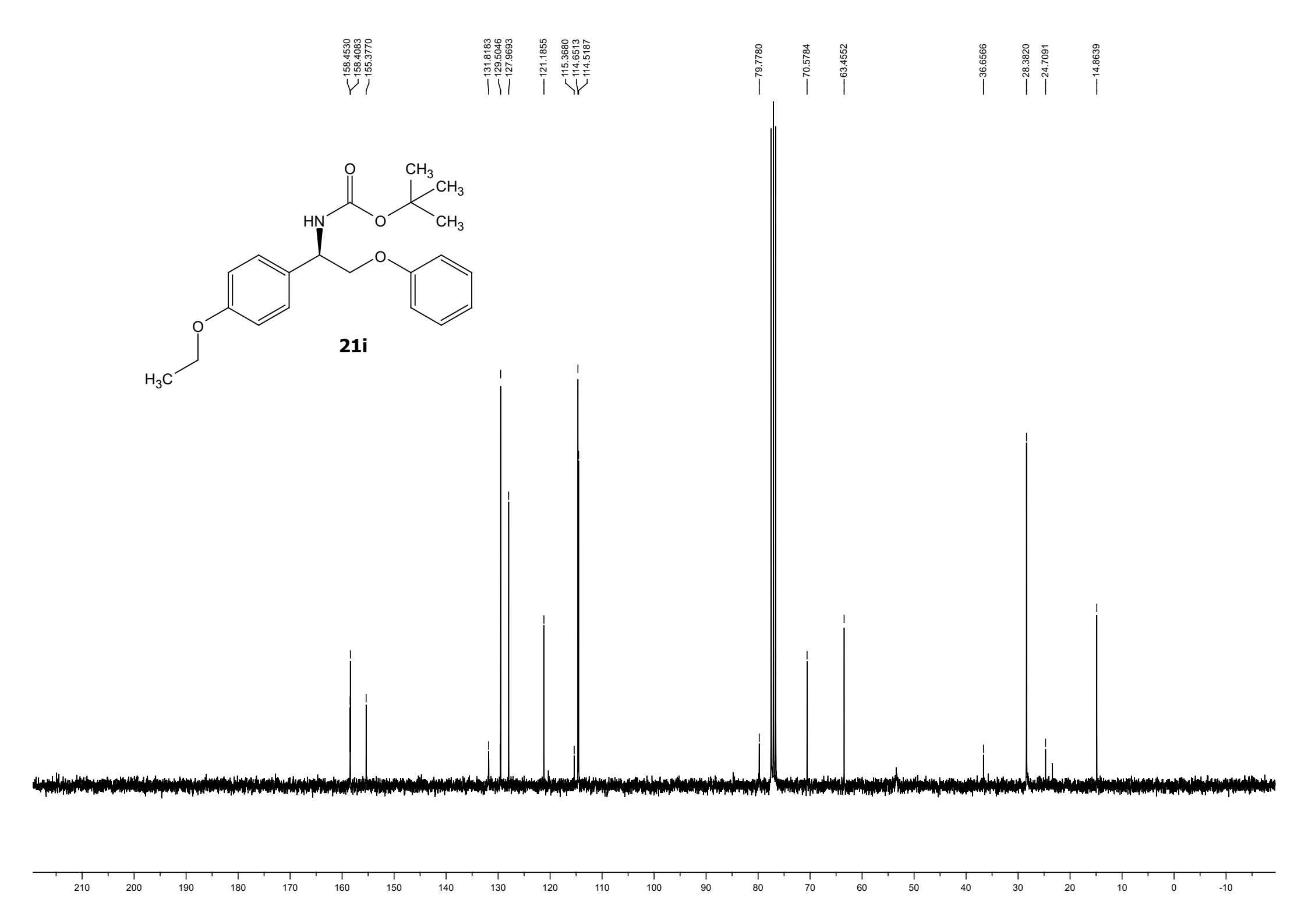
-0.5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24.7091
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CH3
CH3
HN
O
CH3
O
O
H3C
21i
210
200
190
180
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120
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100
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80
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50
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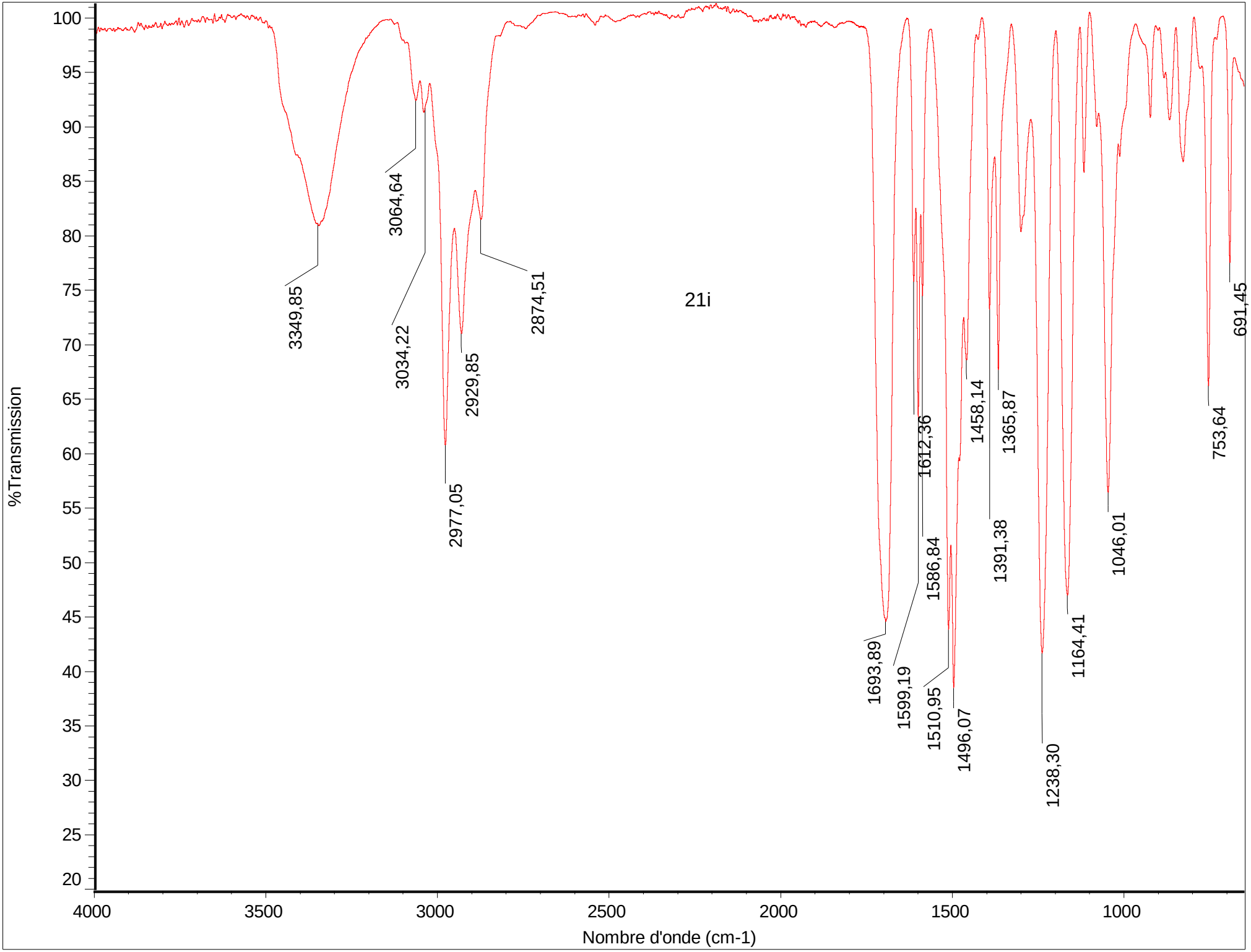
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Nombre d'onde (cm-1)
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75
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65
60
55
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30
25
20
4000
3500
3000
2500
2000
1500
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2874,51
1693,89
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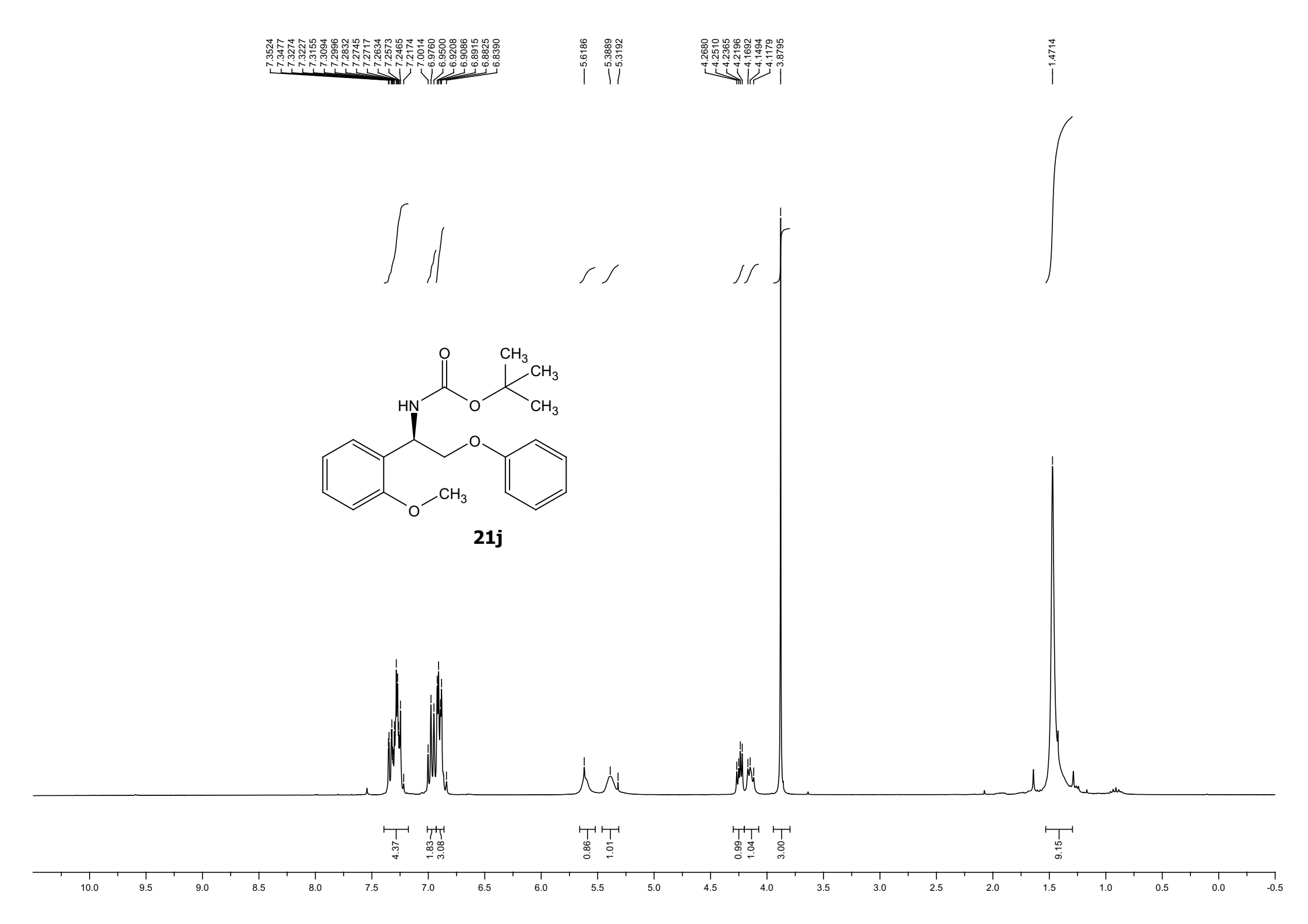
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HN
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CH3
CH3
CH3
O
O
CH3
O
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0.86
1.01
0.99
1.04
3.00
9.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
1.5
1.0
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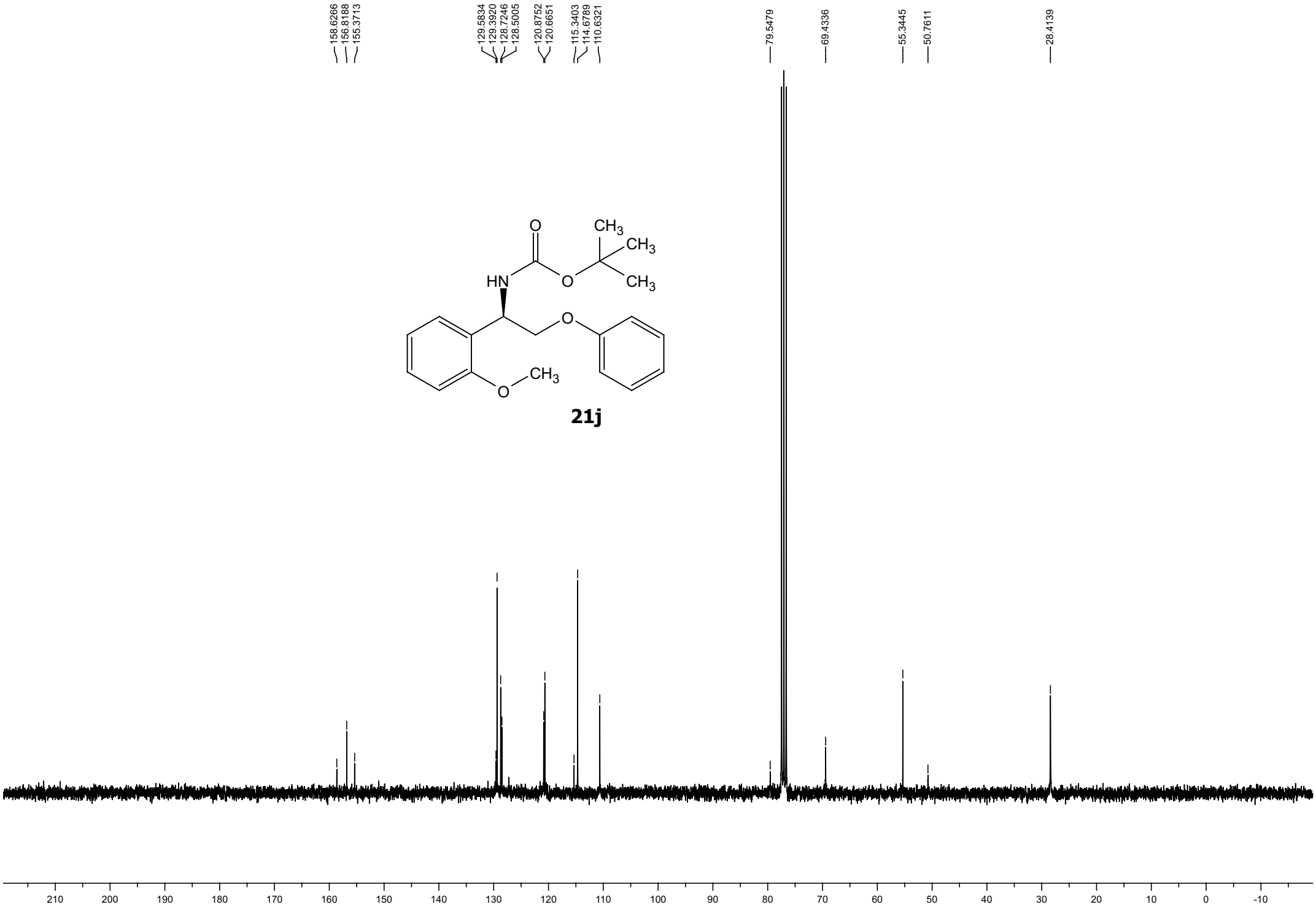
-0.5

21j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CH3
CH3
CH3
HN
O
O
CH3
O
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210
200
190
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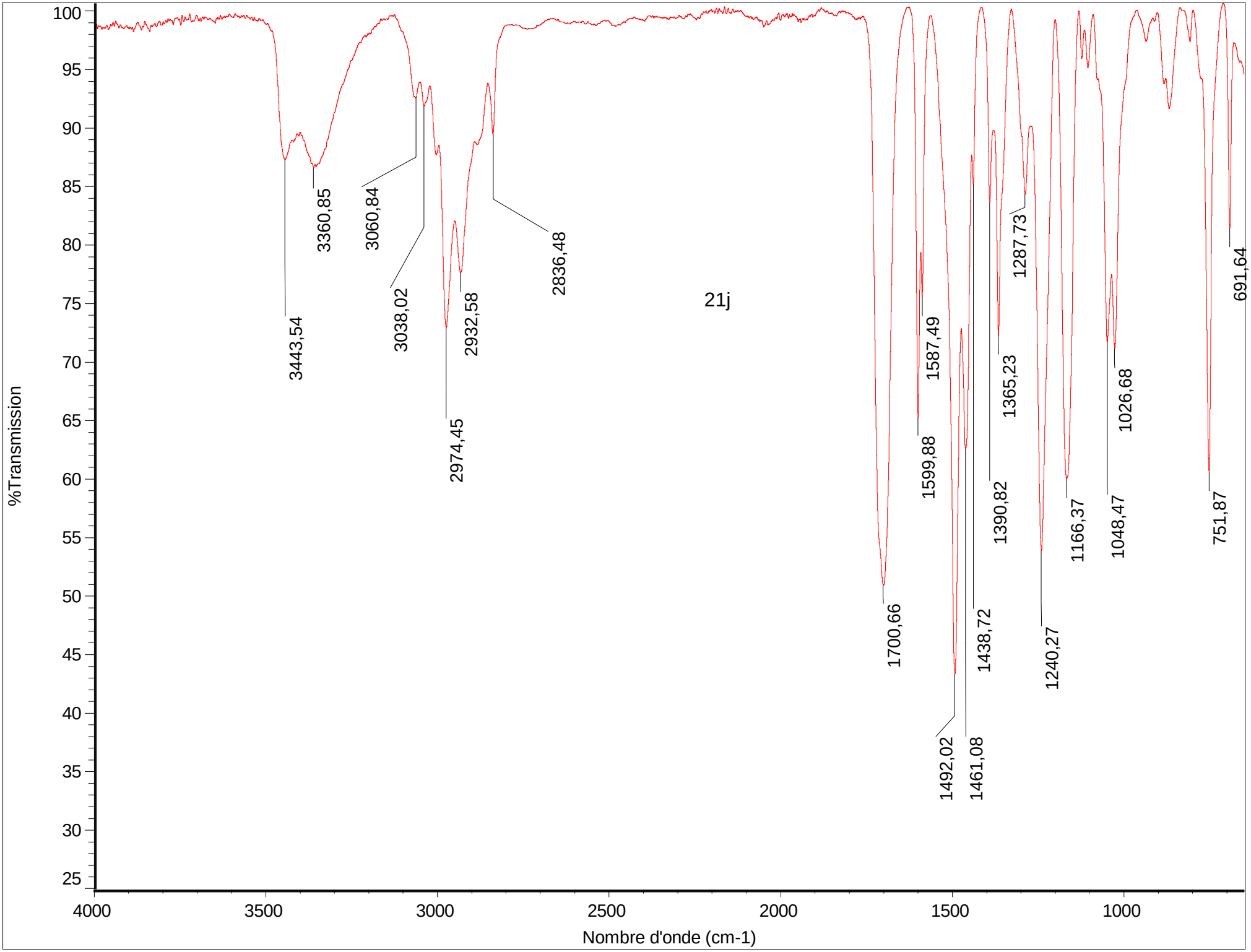
21j
%Transmission
Nombre d'onde (cm-1)
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75
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30
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4000
3500
3000
2500
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2932,58
2836,48
1700,66
1599,88
1587,49
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1461,08
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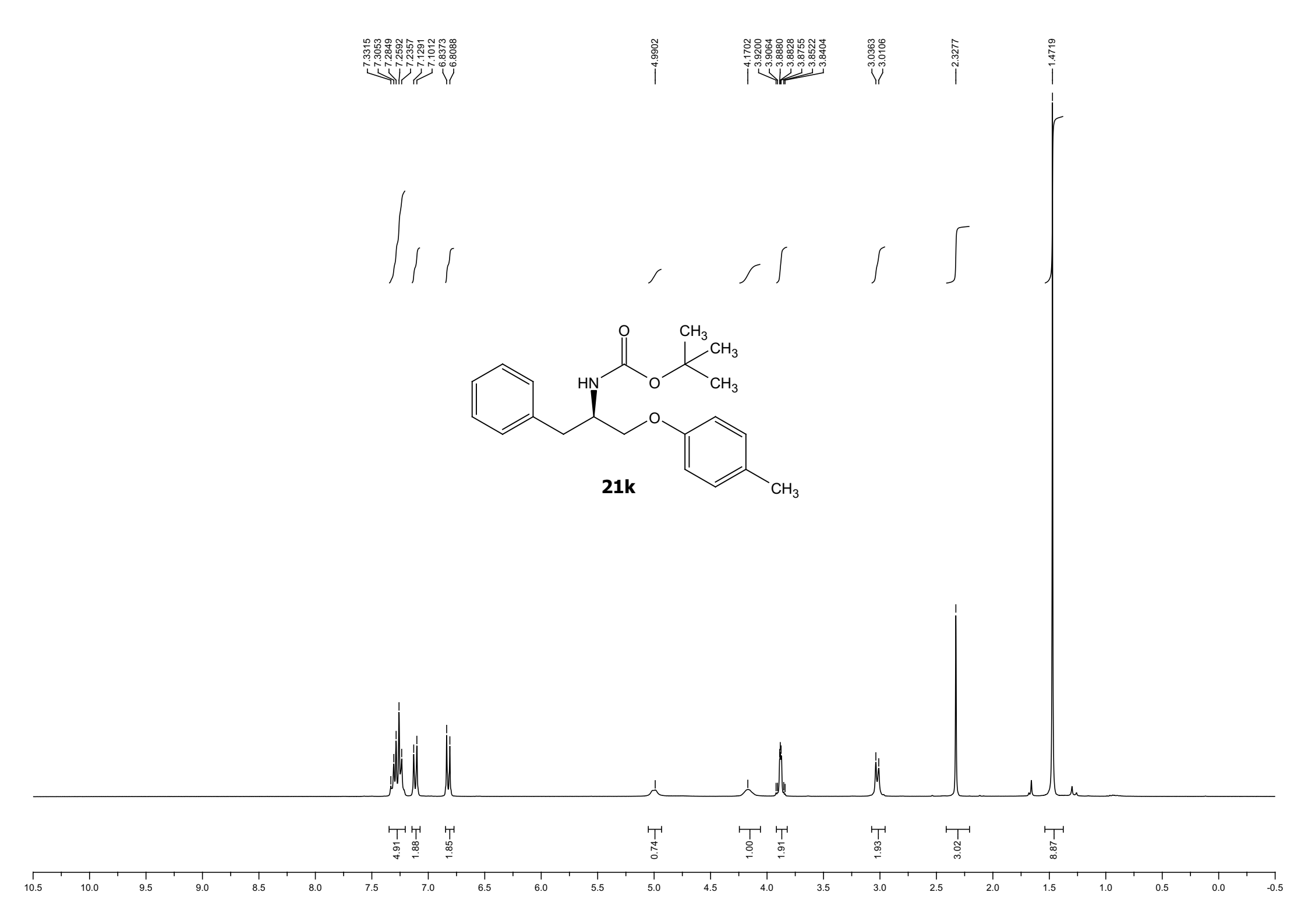
751,87
691,64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4.1702
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3.8828
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3.8404
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2.3277
1.4719
O
CH3
CH3
HN
O
CH3
O
CH3
21k
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1.85
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1.00
1.91
1.93
3.02
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9.0
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8.0
7.5
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5.5
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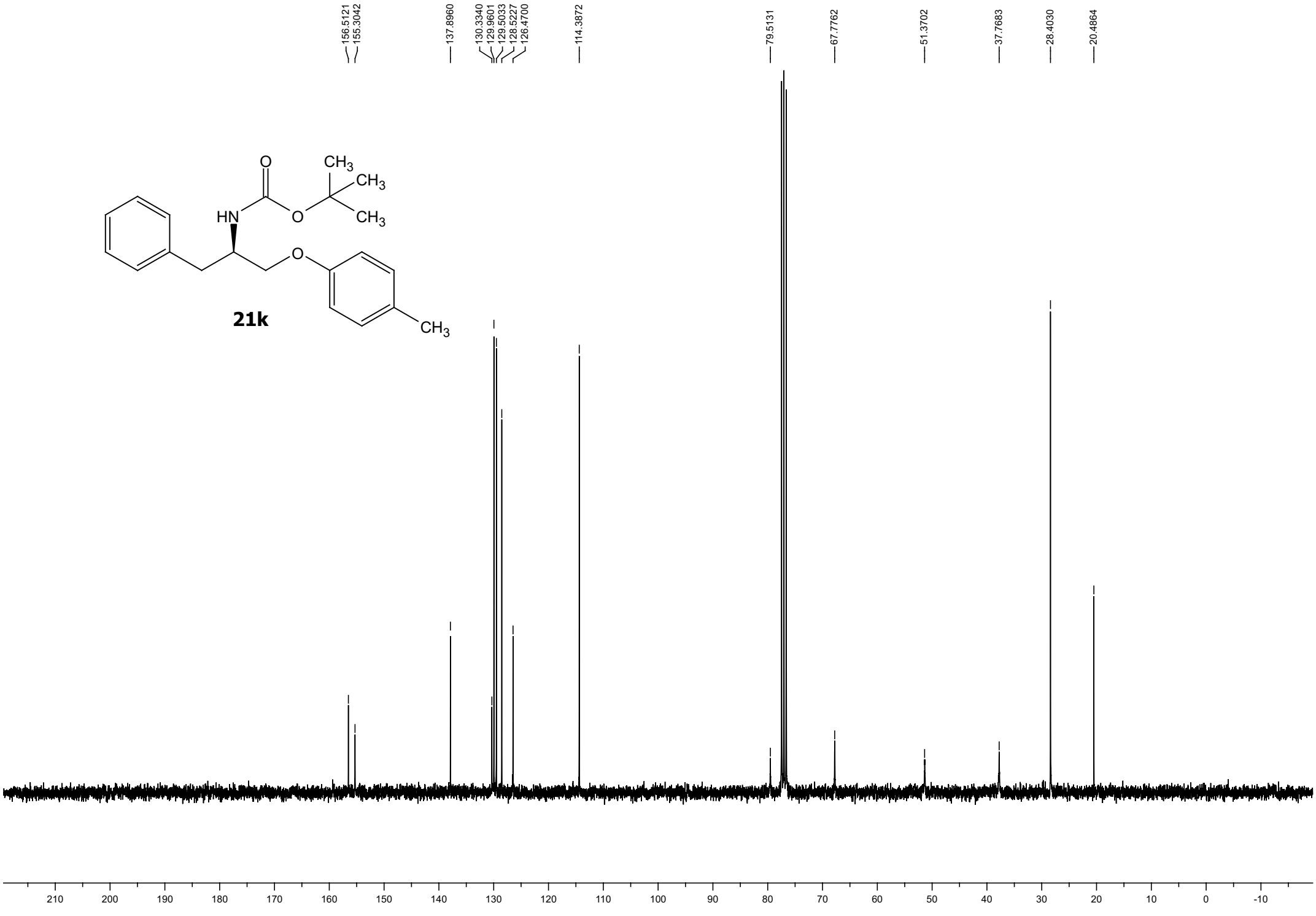
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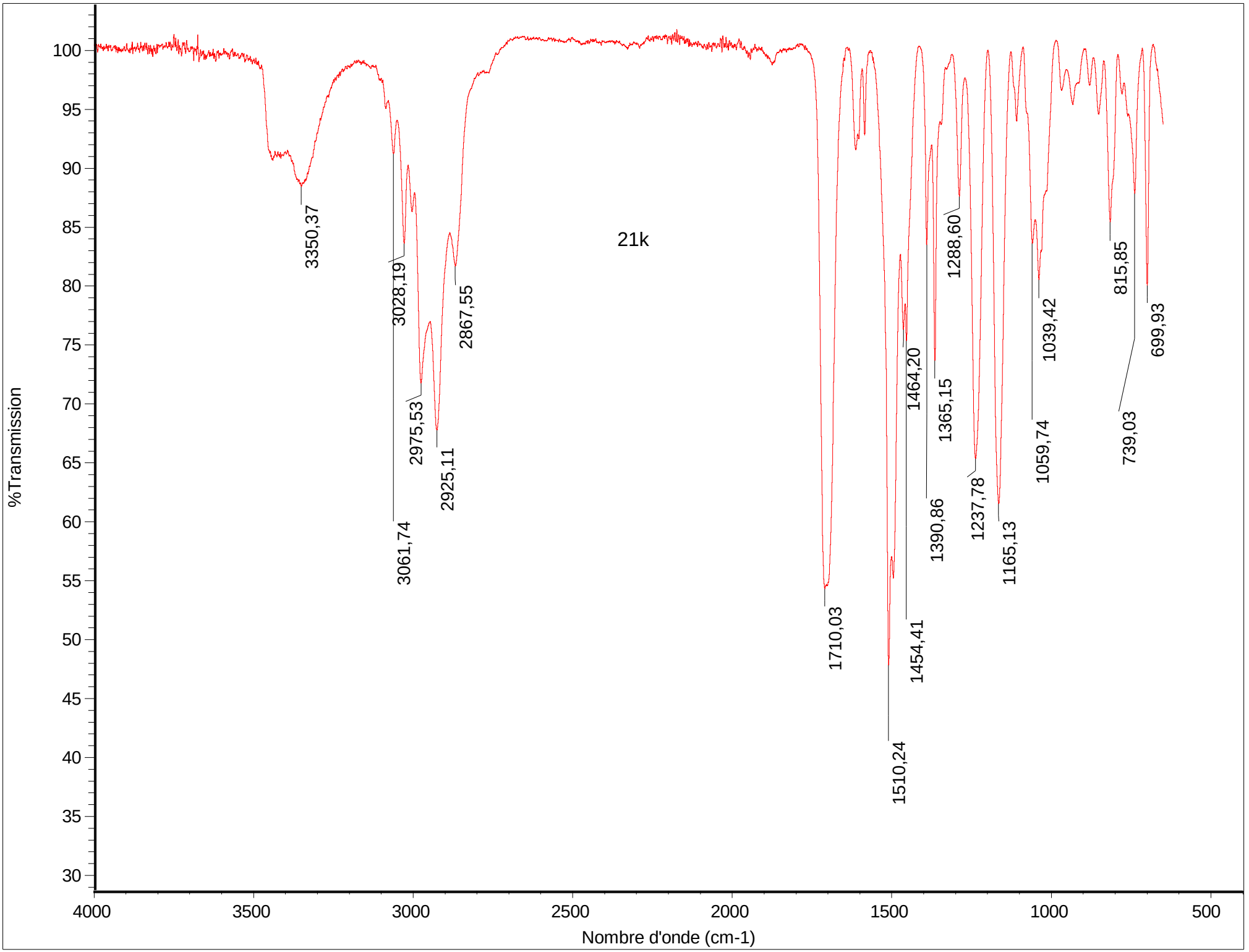
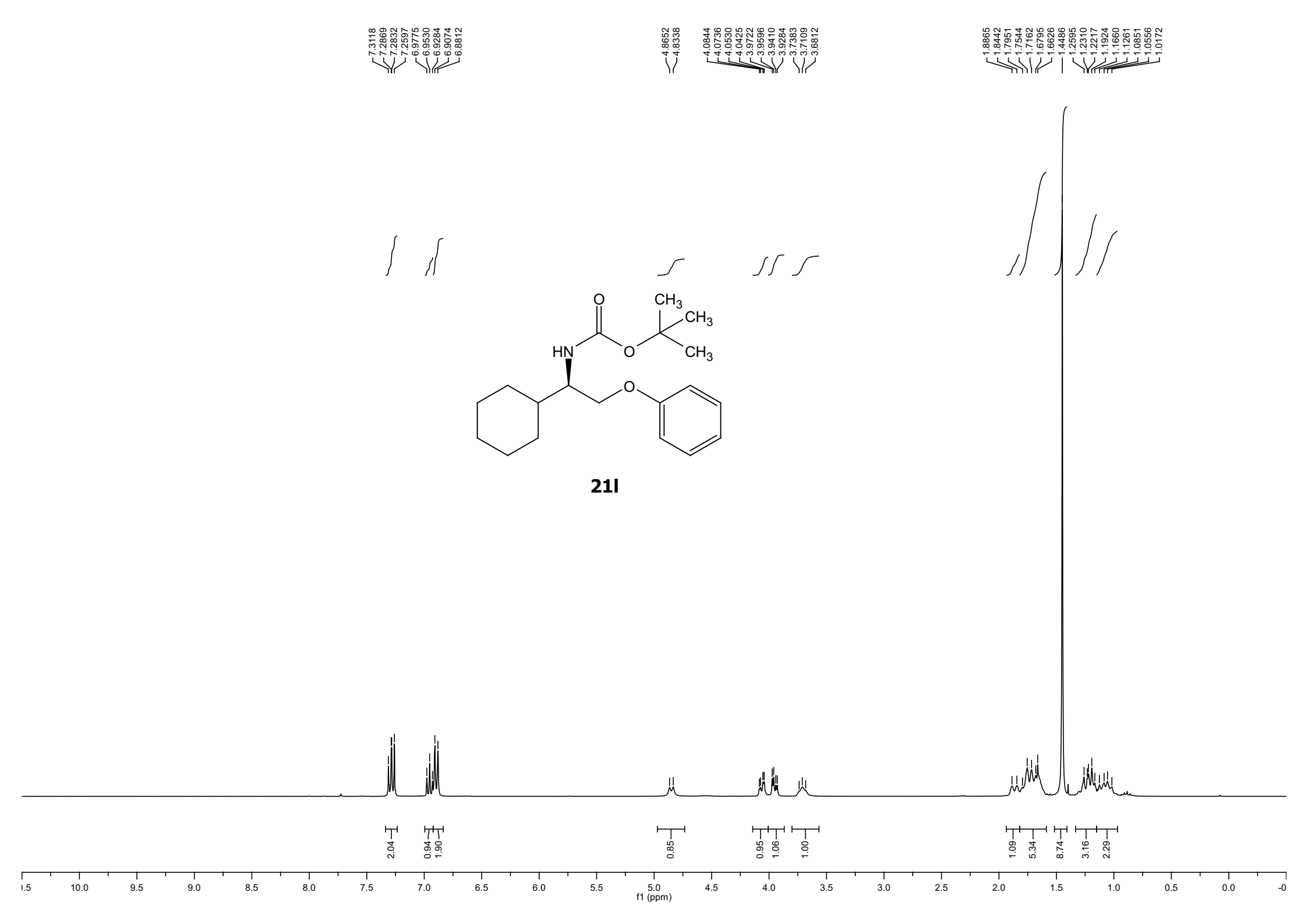
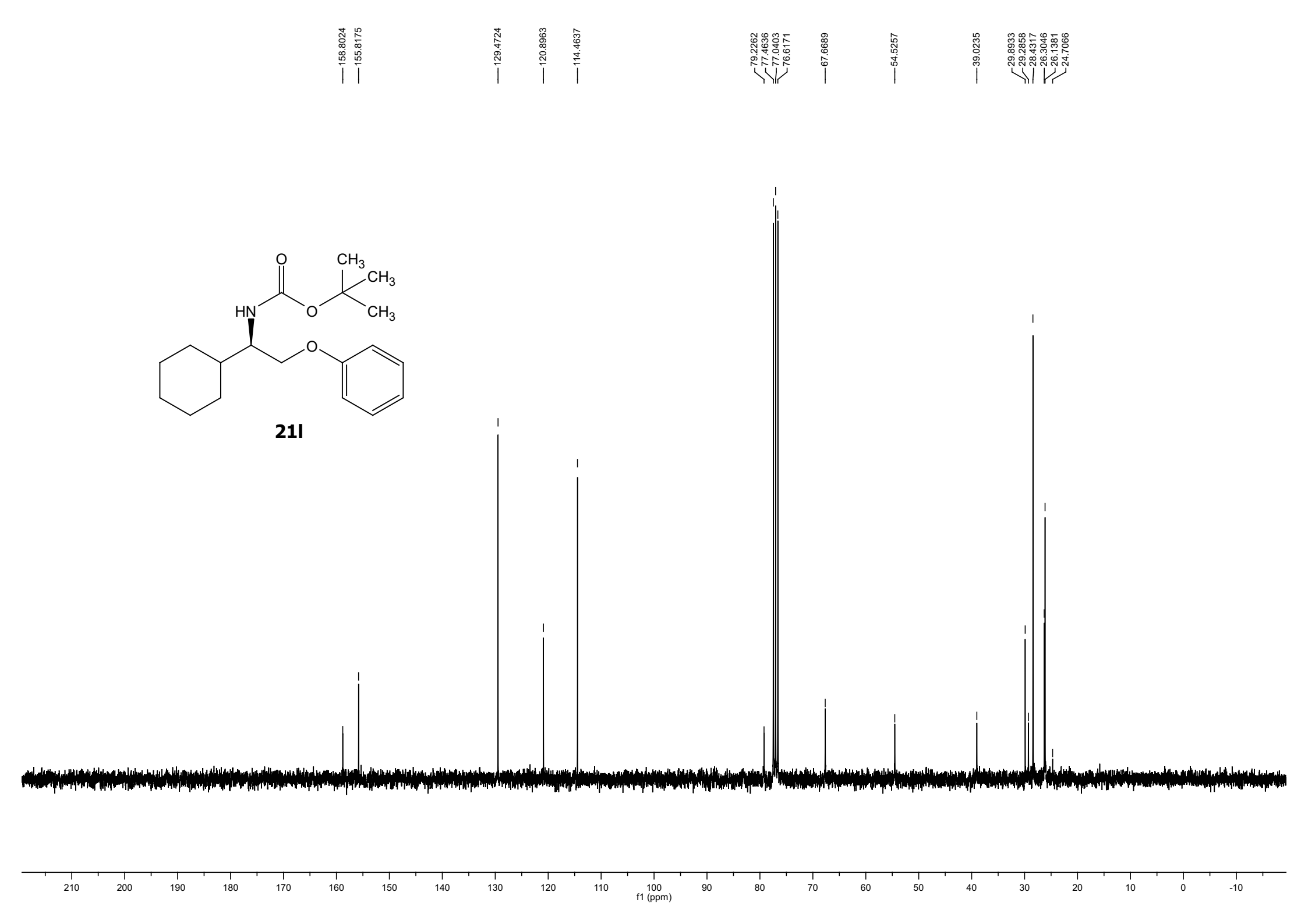
129.5033
128.5227
126.4700
114.3872
79.5131
67.7762
51.3702
37.7683
28.4030
20.4864
O
CH3
CH3
HN
O
CH3
O
CH3
21k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


21k
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
4000
3500
3000
2500
2000
1500
1000
500
3350,37
3028,19
2975,53
2925,11
2867,55
3061,74
1710,03
1510,24
1454,41
1464,20
1390,86
1365,15
1288,60
1237,78
1165,13
1059,74
1039,42
815,85
739,03
699,93


7.3118
7.2869
7.2832
7.2597
6.9775
6.9530
6.9284
6.9074
6.8812
4.8652
4.8338
4.0844
4.0736
4.0530
4.0425
3.9722
3.9596
3.9410
3.9284
3.7383
3.7109
3.6812
1.8865
1.8442
1.7951
1.7544
1.7162
1.6795
1.6626
1.4486
1.2595
1.2310
1.2217
1.1924
1.1660
1.1261
1.0851
1.0556
1.0172
O
CH3
CH3
HN
O
CH3
O
2.04
0.94
1.90
0.85
0.95
1.06
1.00
1.09
5.34
8.74
3.16
2.29
f1 (ppm)

21l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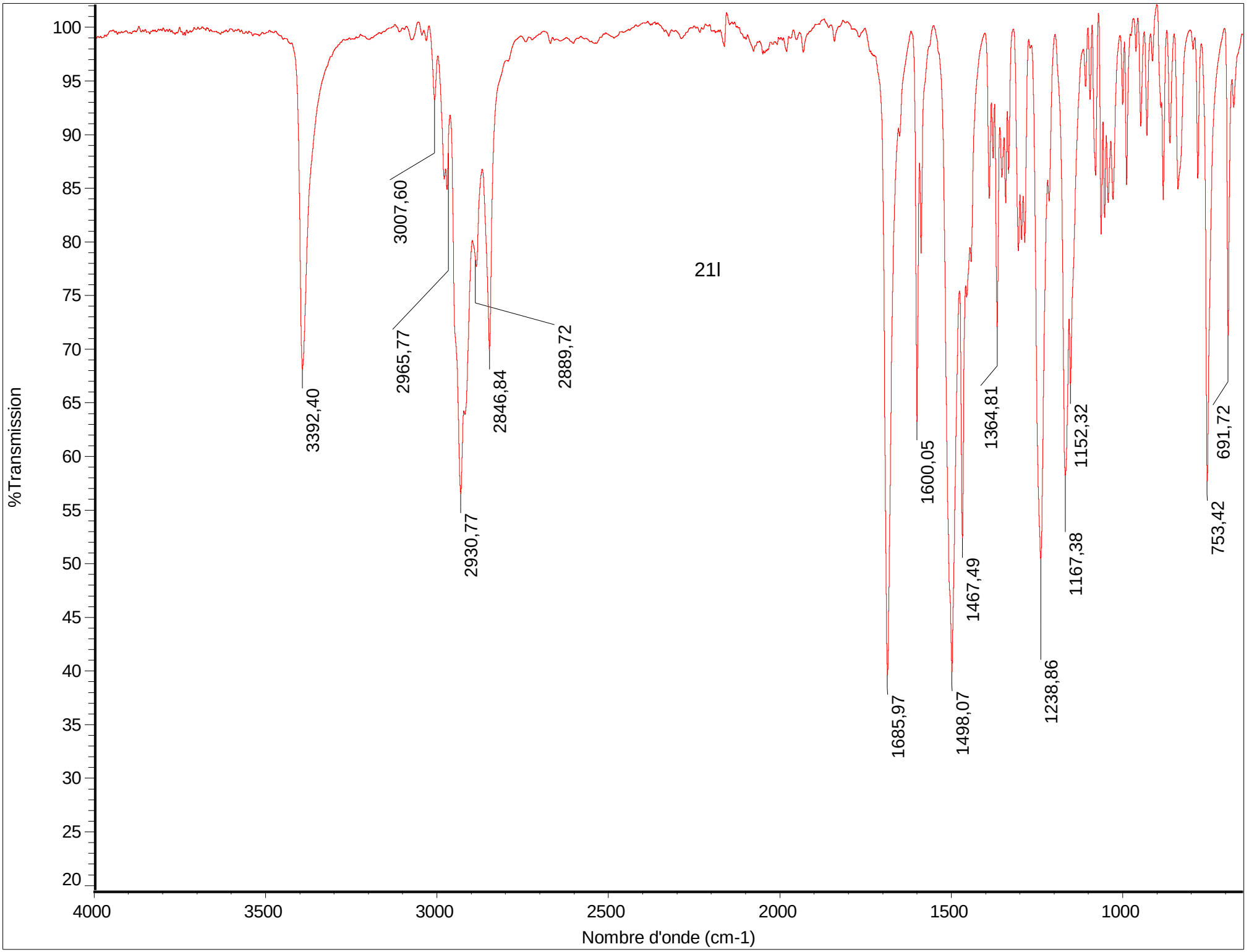
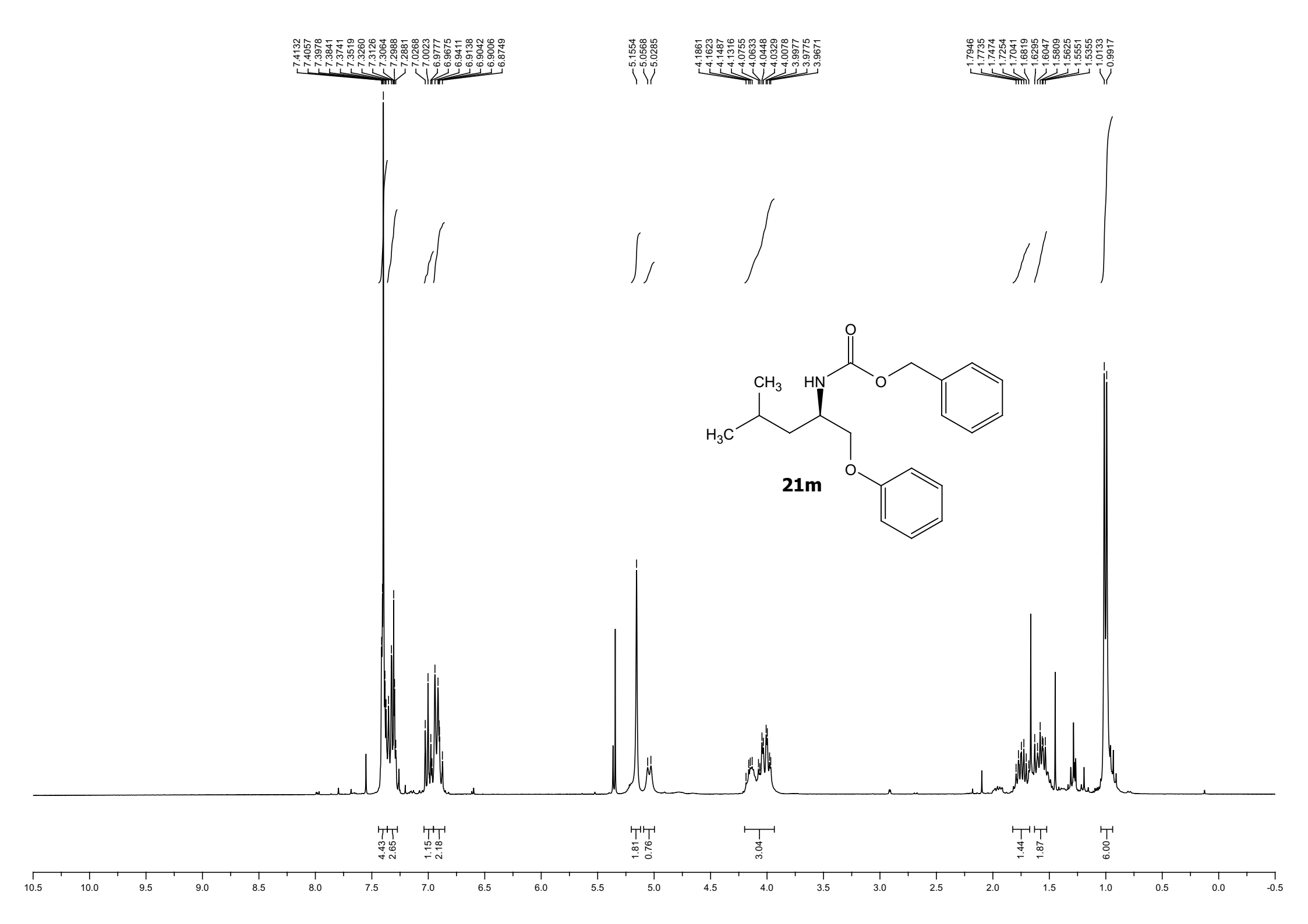
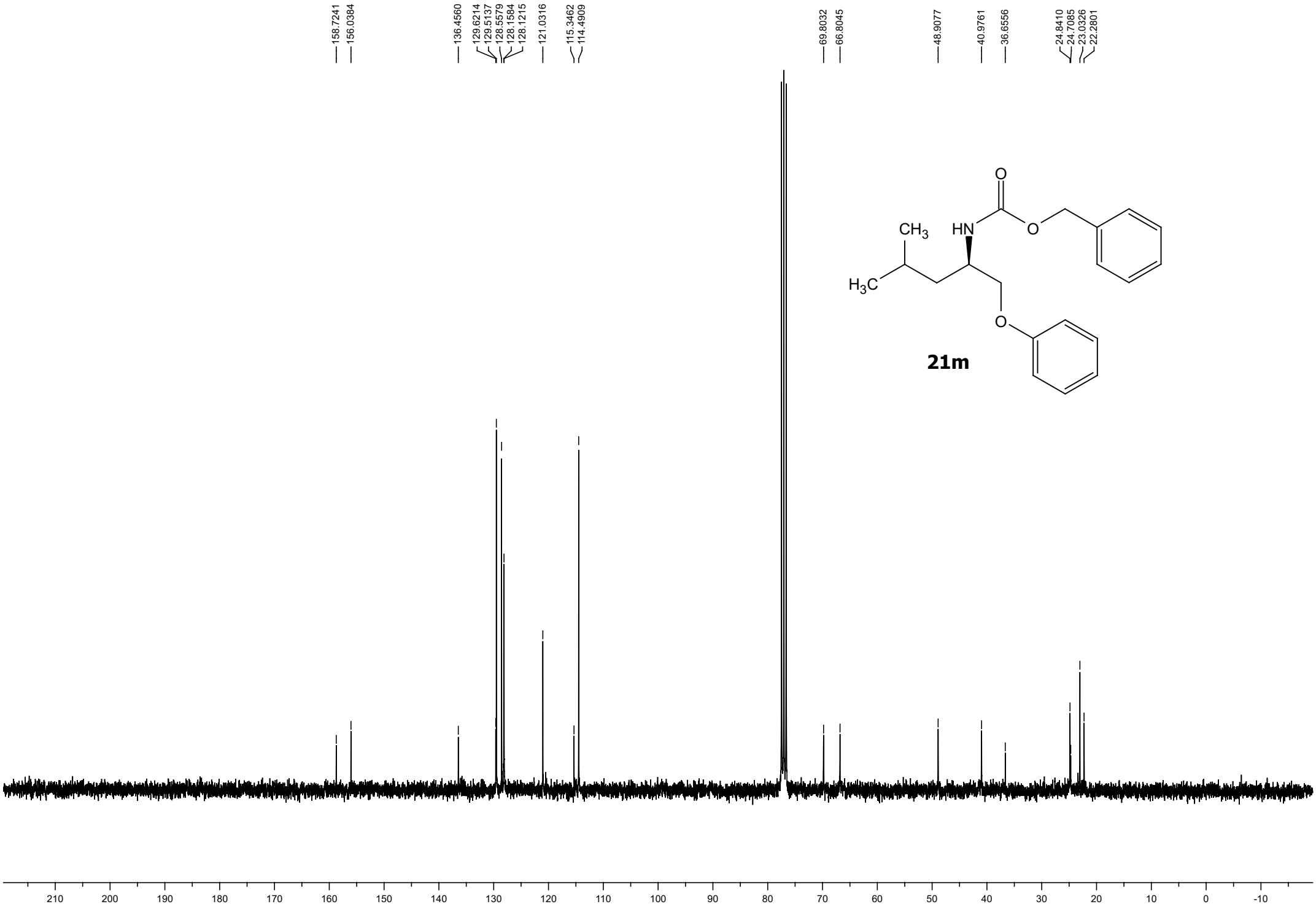
155.8175
129.4724
120.8963
114.4637
79.2262
77.4636
77.0403
76.6171
67.6689
54.5257
39.0235
29.8933
29.2858
28.4317
26.3046
26.1381
24.7066
O
CH3
CH3
HN
O
CH3
O
21l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


21l
%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
3392,40
3007,60
2965,77
2930,77
2846,84
2889,72
1685,97
1600,05
1498,07
1467,49
1364,81
1238,86
1167,38
1152,32
753,42
691,72


7.4132
7.4057
7.3978
7.3841
7.3741
7.3519
7.3260
7.3126
7.3064
7.2988
7.2881
7.0268
7.0023
6.9777
6.9675
6.9411
6.9138
6.9042
6.9006
6.8749
5.1554
5.0568
5.0285
4.1861
4.1623
4.1487
4.1316
4.0755
4.0633
4.0448
4.0329
4.0078
3.9977
3.9775
3.9671
1.7946
1.7735
1.7474
1.7254
1.7041
1.6819
1.6295
1.6047
1.5809
1.5625
1.5551
1.5355
1.0133
0.9917
CH3
HN
O
O
H3C
O
21m
4.43
2.65
1.15
2.18
1.81
0.76
3.04
1.44
1.87
6.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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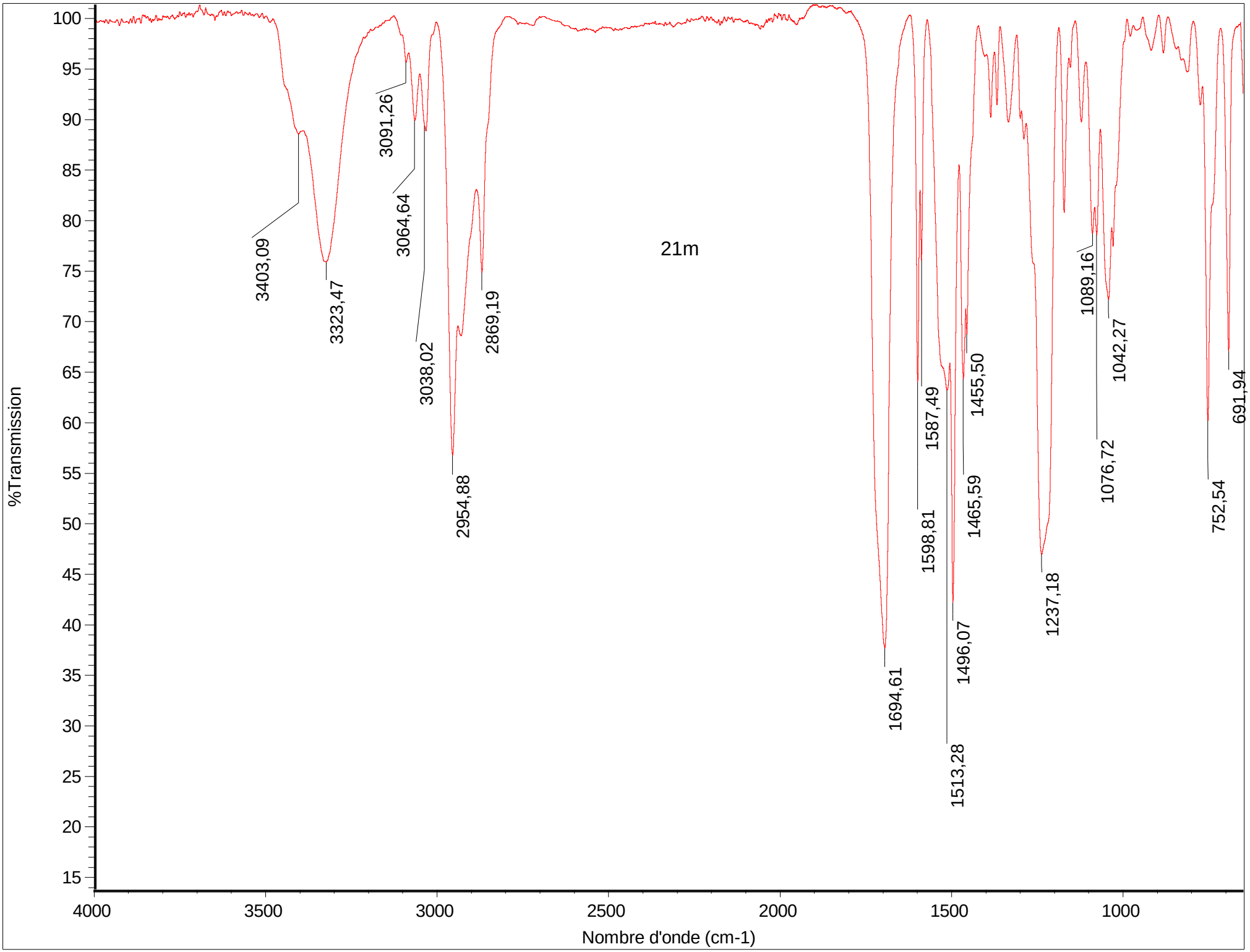
156.0384
136.4560
129.6214
129.5137
128.5579
128.1584
128.1215
121.0316
115.3462
114.4909
69.8032
66.8045
48.9077
40.9761
36.6556
24.8410
24.7085
23.0326
22.2801
O
HN
O
CH3
H3C
O
21m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


21m
%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
3403,09
3323,47
3091,26
3064,64
3038,02
2954,88
2869,19
1694,61
1598,81
1587,49
1513,28
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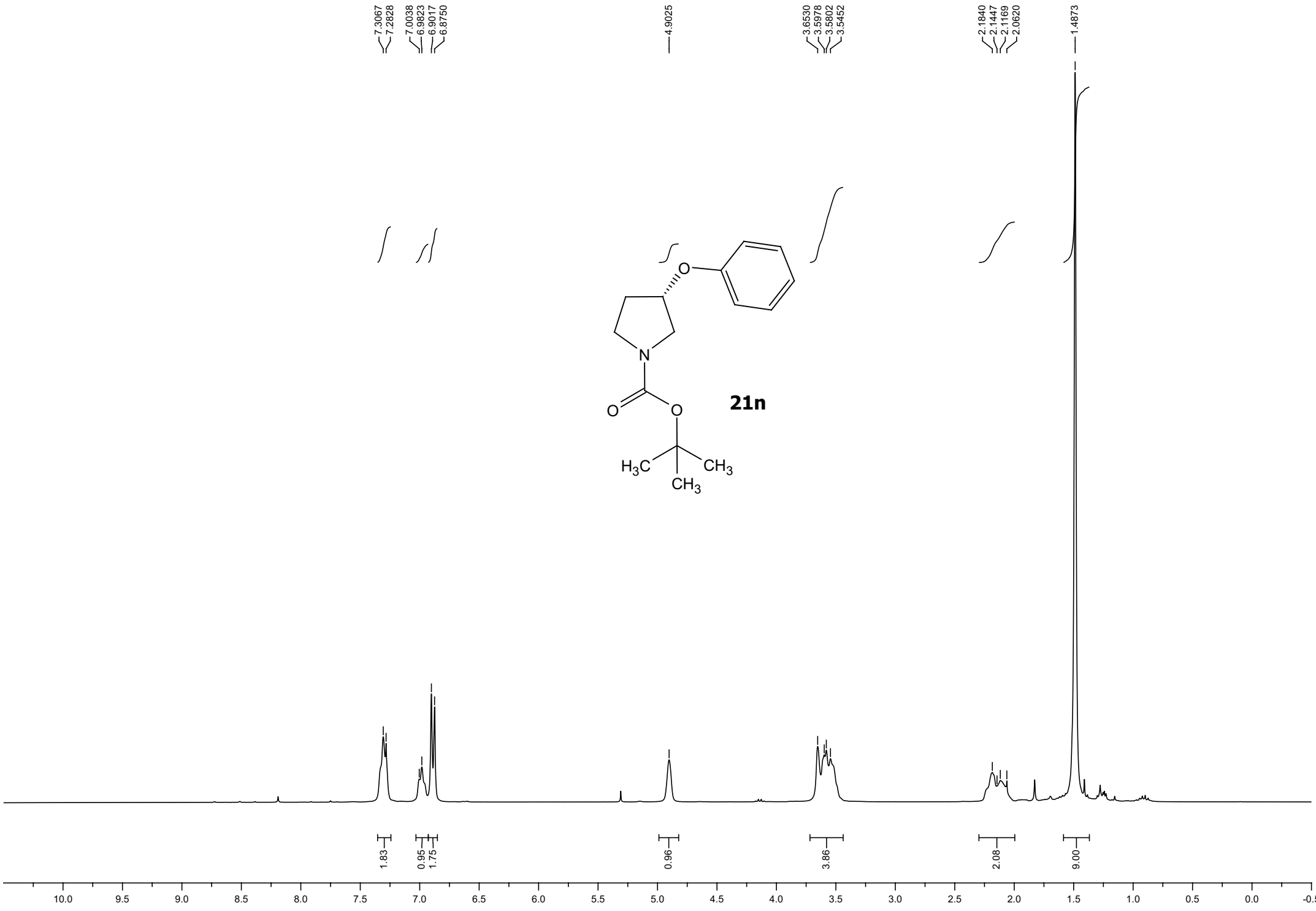
1465,59
1455,50
1237,18
1089,16
1076,72
1042,27
752,54
691,94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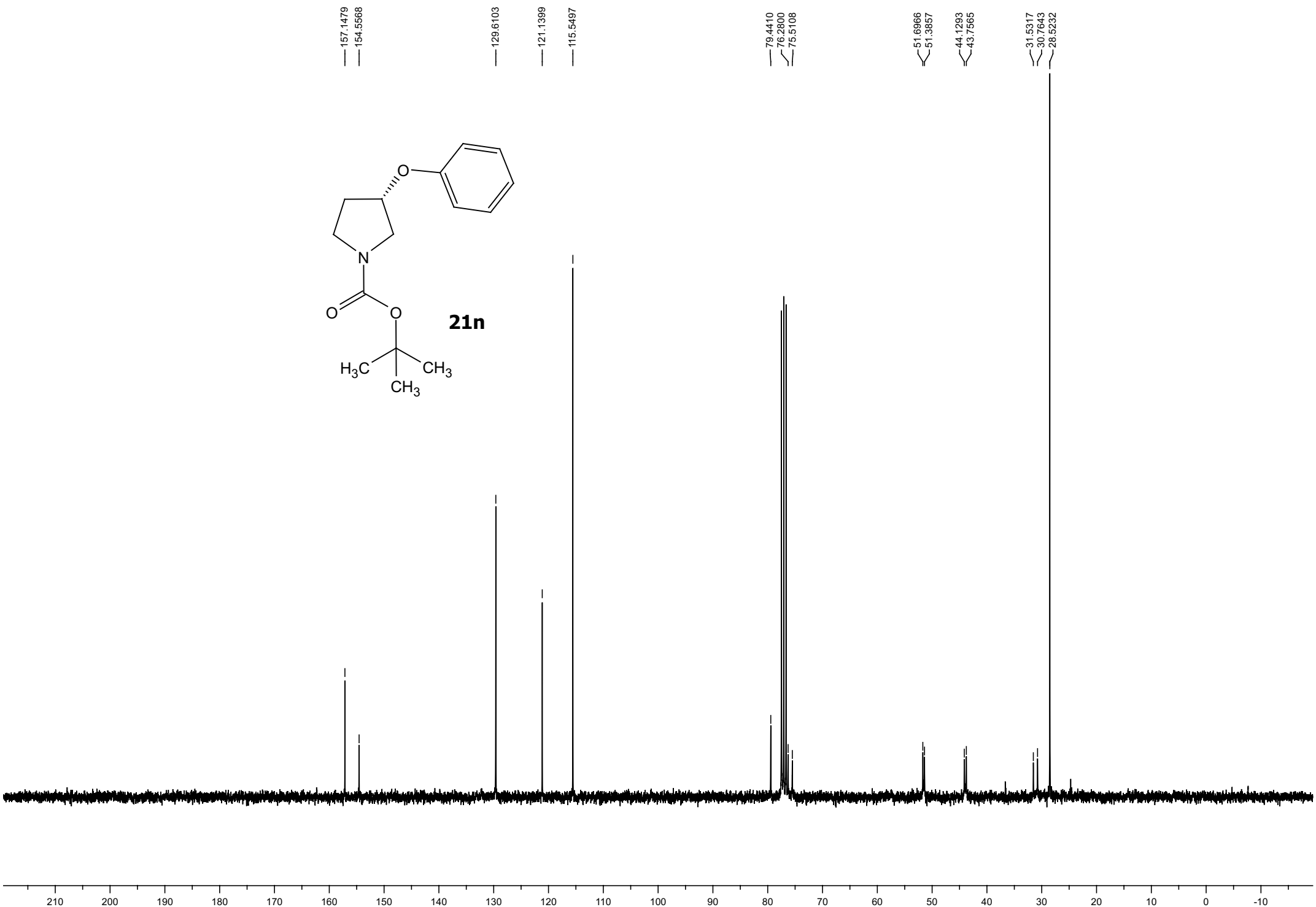
7.2828
7.0038
6.9823
6.9017
6.8750
4.9025
3.6530
3.5978
3.5802
3.5452
2.1840
2.1447
2.1169
2.0620
1.4873
O
N
O
O
H3C
CH3
CH3
21n
1.83
0.95
1.75
0.96
3.86
2.08
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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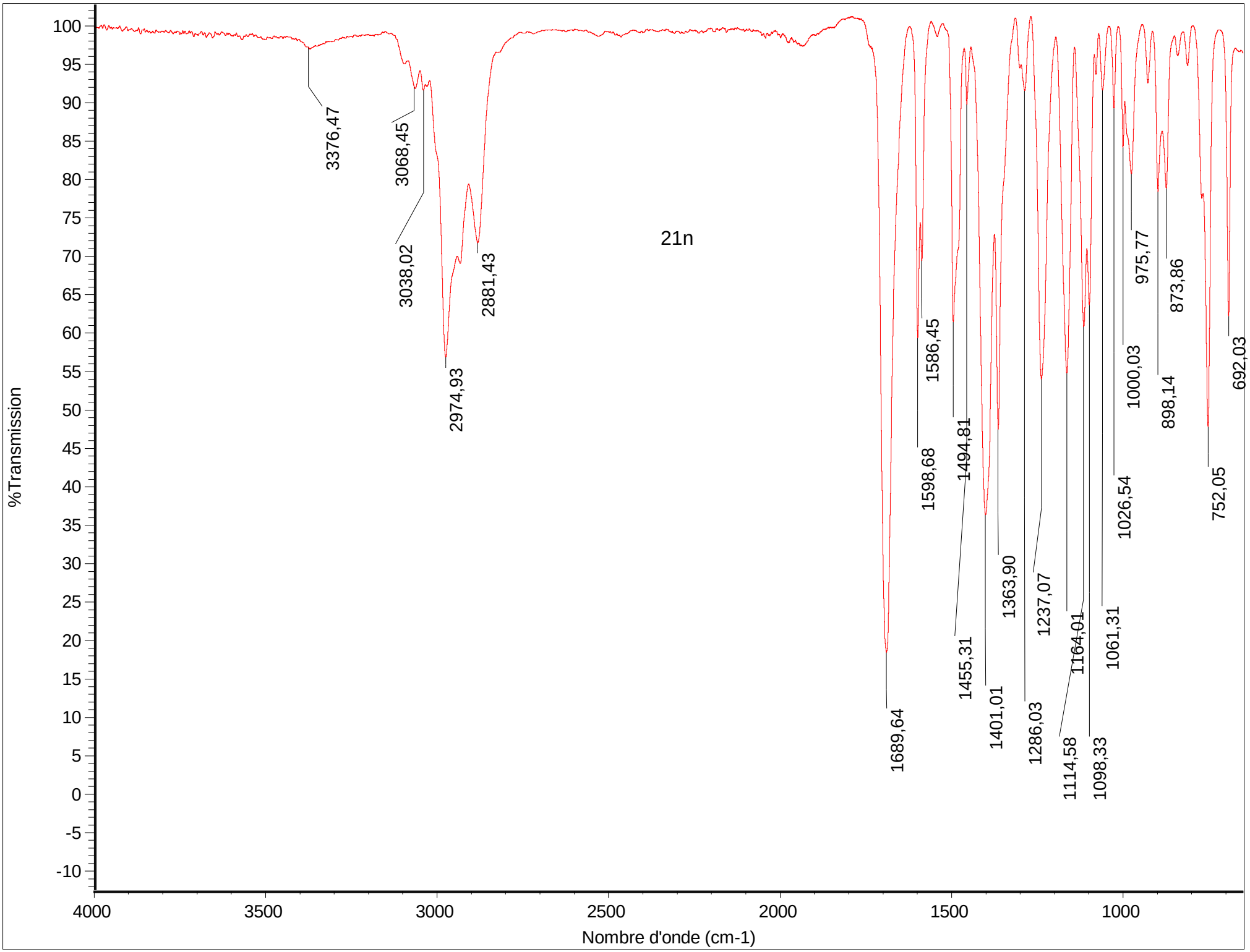
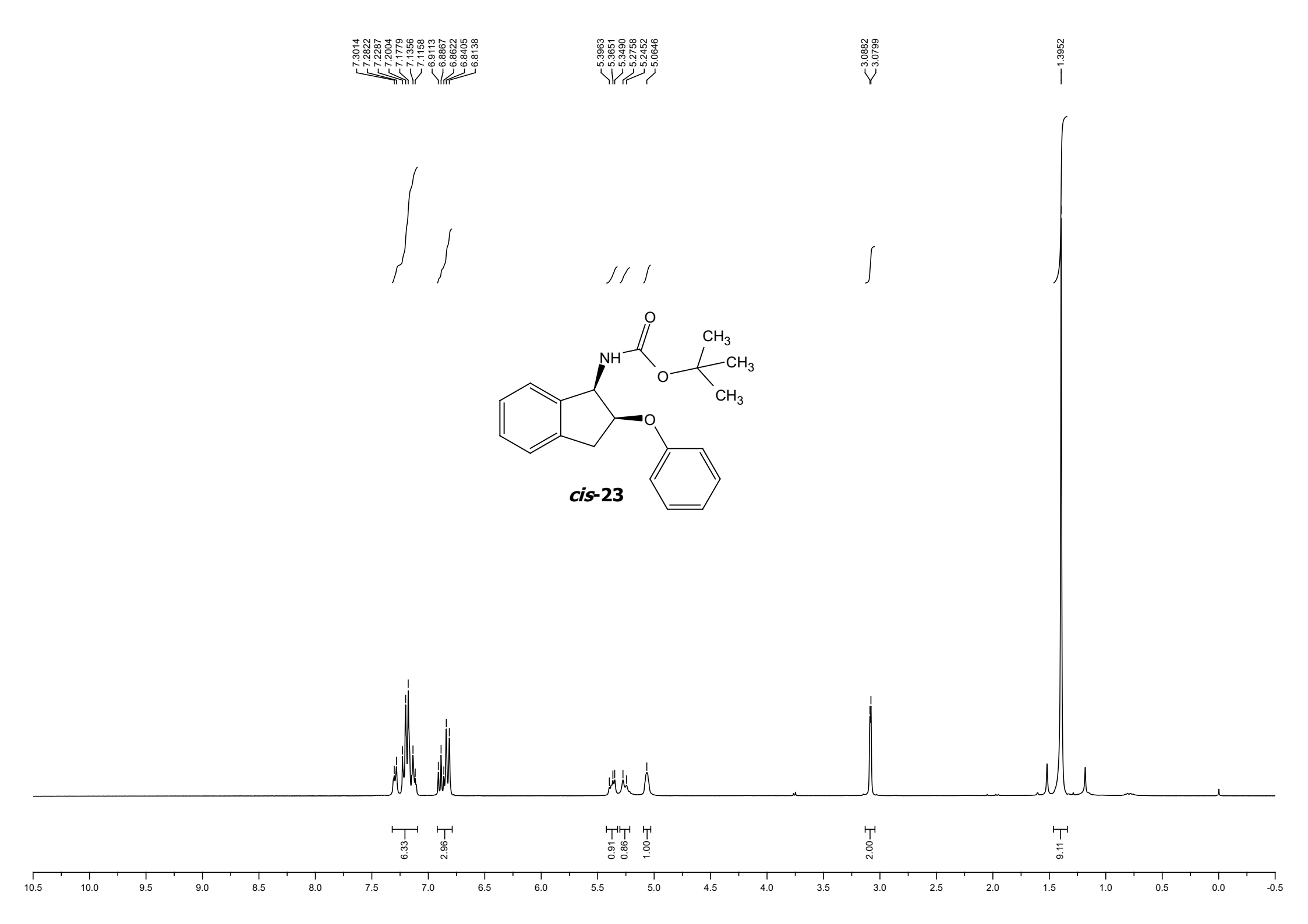
154.5568
129.6103
121.1399
115.5497
79.4410
76.2800
75.5108
51.6966
51.3857
44.1293
43.7565
31.5317
30.7643
28.5232
O
N
O
O
H3C
CH3
CH3
21n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


21n
%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
4000
3500
3000
2500
2000
1500
1000
3376,47
3068,45
3038,02
2974,93
2881,43
1689,64
1598,68
1586,45
1494,81
1455,31
1401,01
1363,90
1286,03
1237,07
1164,01
1114,58
1098,33
1061,31
1026,54
1000,03
975,77
898,14
873,86
752,05
692,03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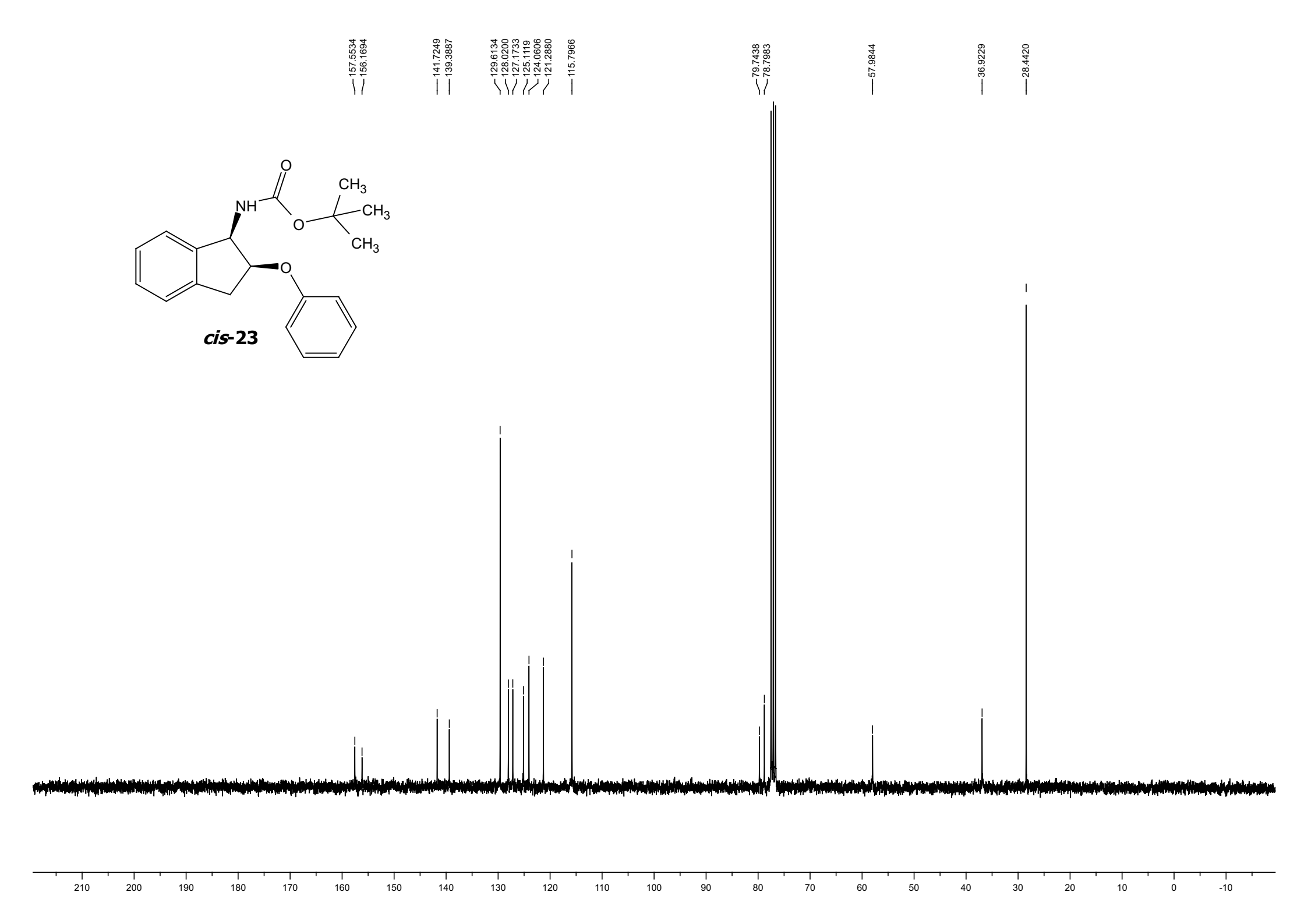
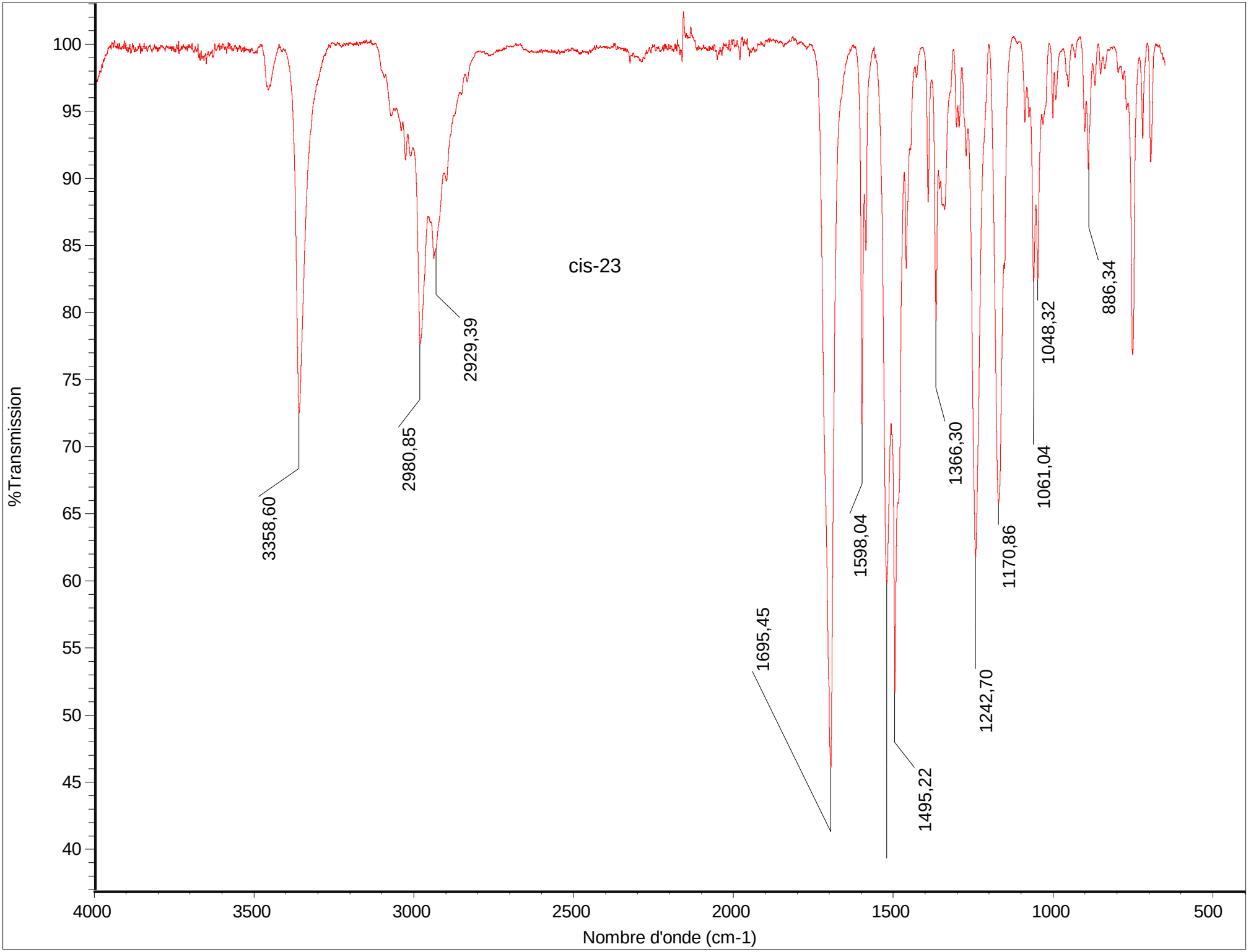
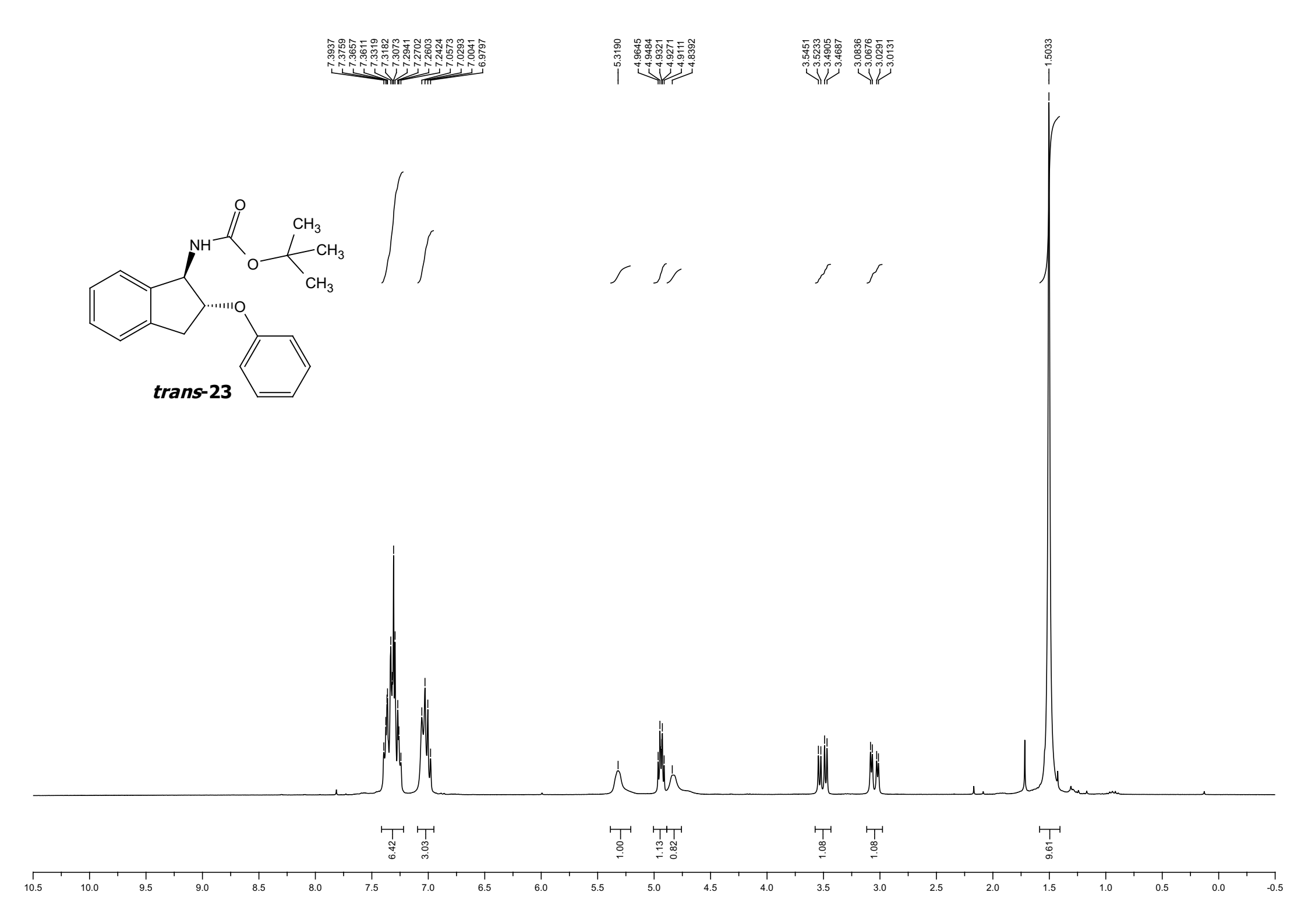
7.2822
7.2287
7.2004
7.1779
7.1356
7.1158
6.9113
6.8867
6.8622
6.8405
6.8138
5.3963
5.3651
5.3490
5.2758
5.2452
5.0646
3.0882
3.0799
1.3952
NH
O
O
O
CH3
CH3
CH3
6.33
2.96
0.91
0.86
1.00
2.00
9.11
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

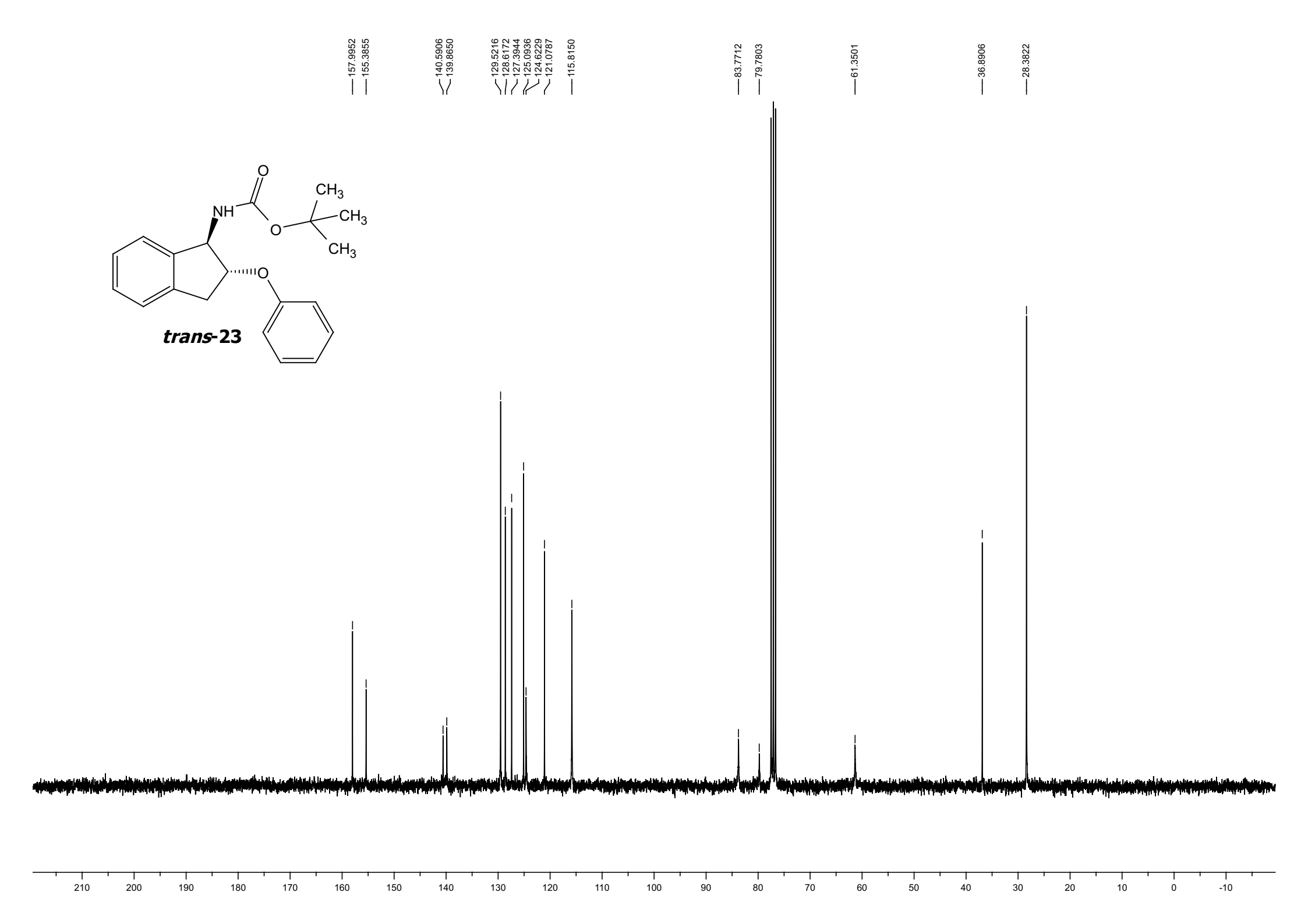
***cis*-23**

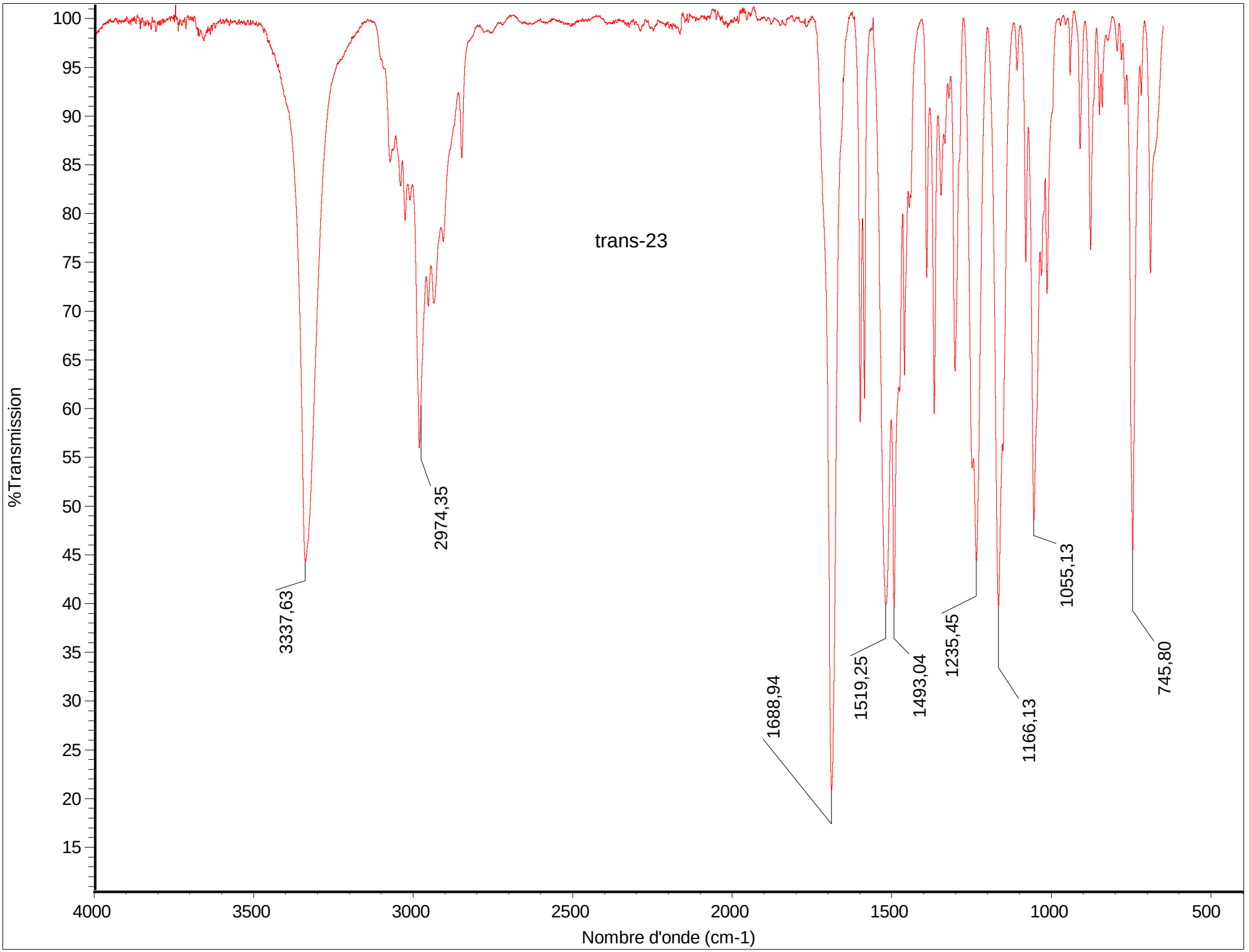

157.5534
156.1694
141.7249
139.3887
129.6134
128.0200
127.1733
125.1119
124.0606
121.2880
115.7966
79.7438
78.7983
57.9844
36.9229
28.4420
O
NH
O
CH3
CH3
CH3
O
cis-23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

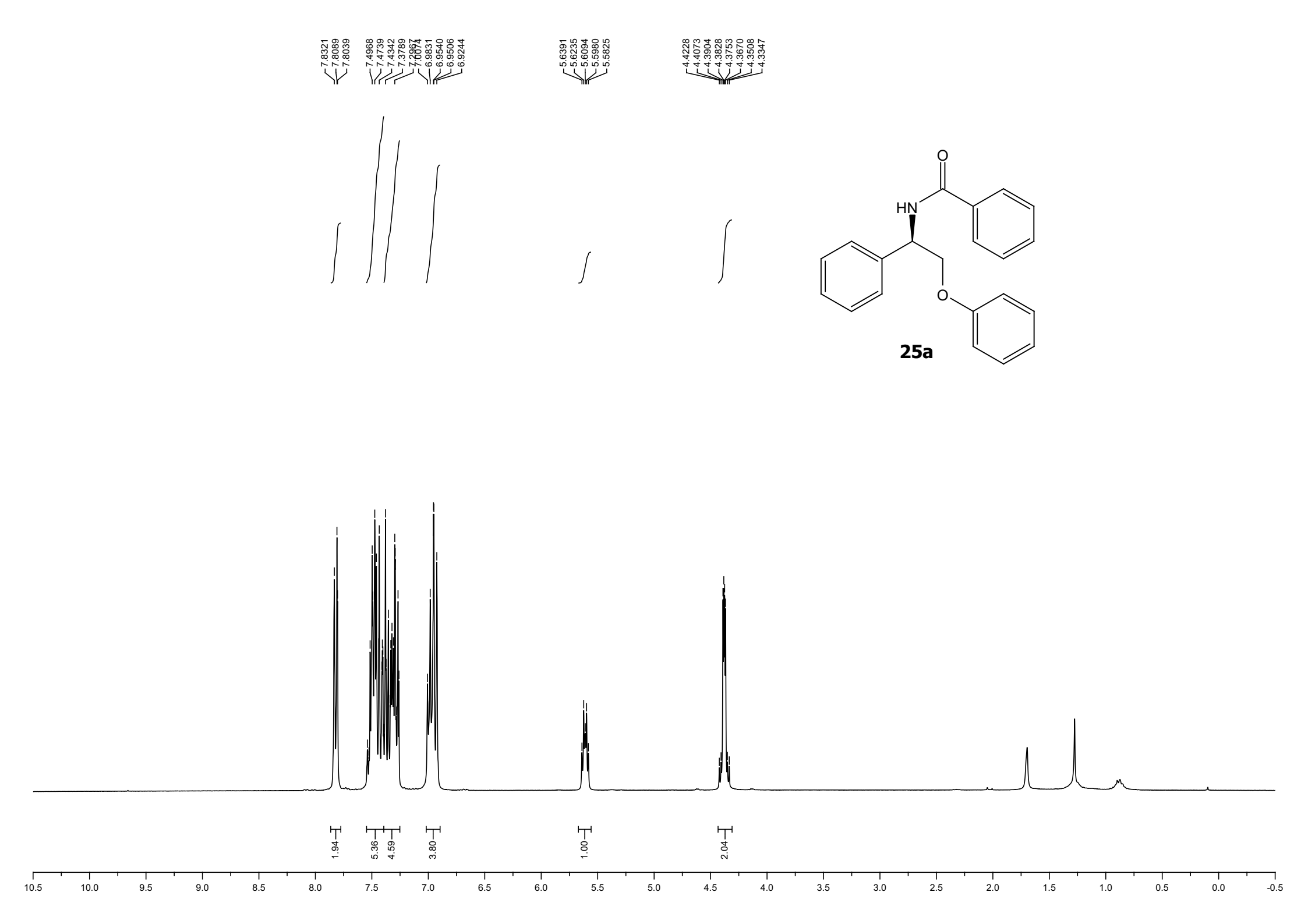

cis-23
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
4000
3500
3000
2500
2000
1500
1000
500
3358,60
2980,85
2929,39
1695,45
1598,04
1495,22
1366,30
1242,70
1170,86
1061,04
1048,32
886,34

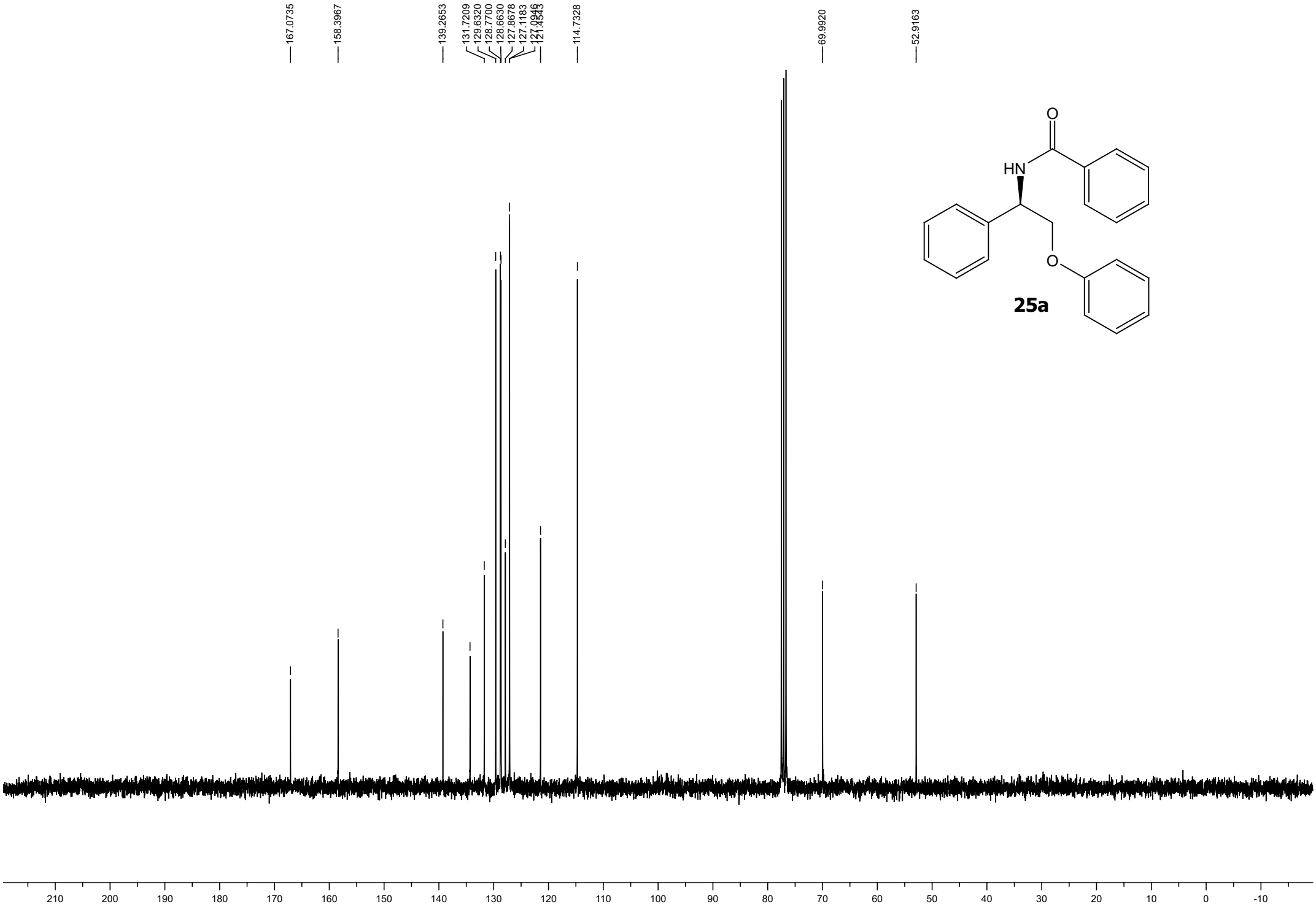

7.3937
7.3759
7.3657
7.3611
7.3319
7.3182
7.3073
7.2941
7.2702
7.2603
7.2424
7.0573
7.0293
7.0041
6.9797
5.3190
4.9645
4.9484
4.9321
4.9271
4.9111
4.8392
3.5451
3.5233
3.4905
3.4687
3.0836
3.0676
3.0291
3.0131
1.5033
NH
O
O
O
CH3
CH3
CH3
6.42
3.03
1.00
1.13
0.82
1.08
1.08
9.61
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

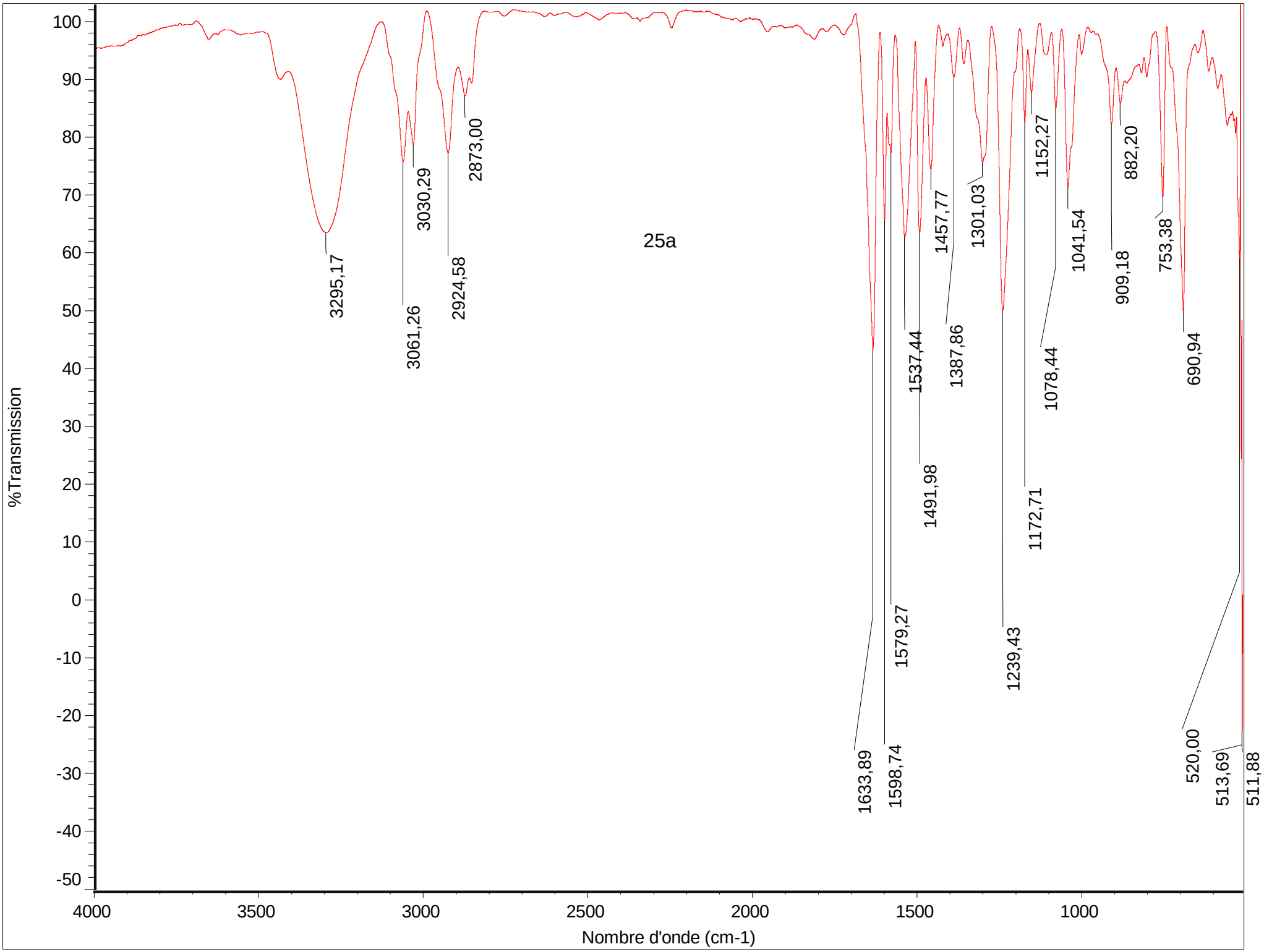
***trans*-23**

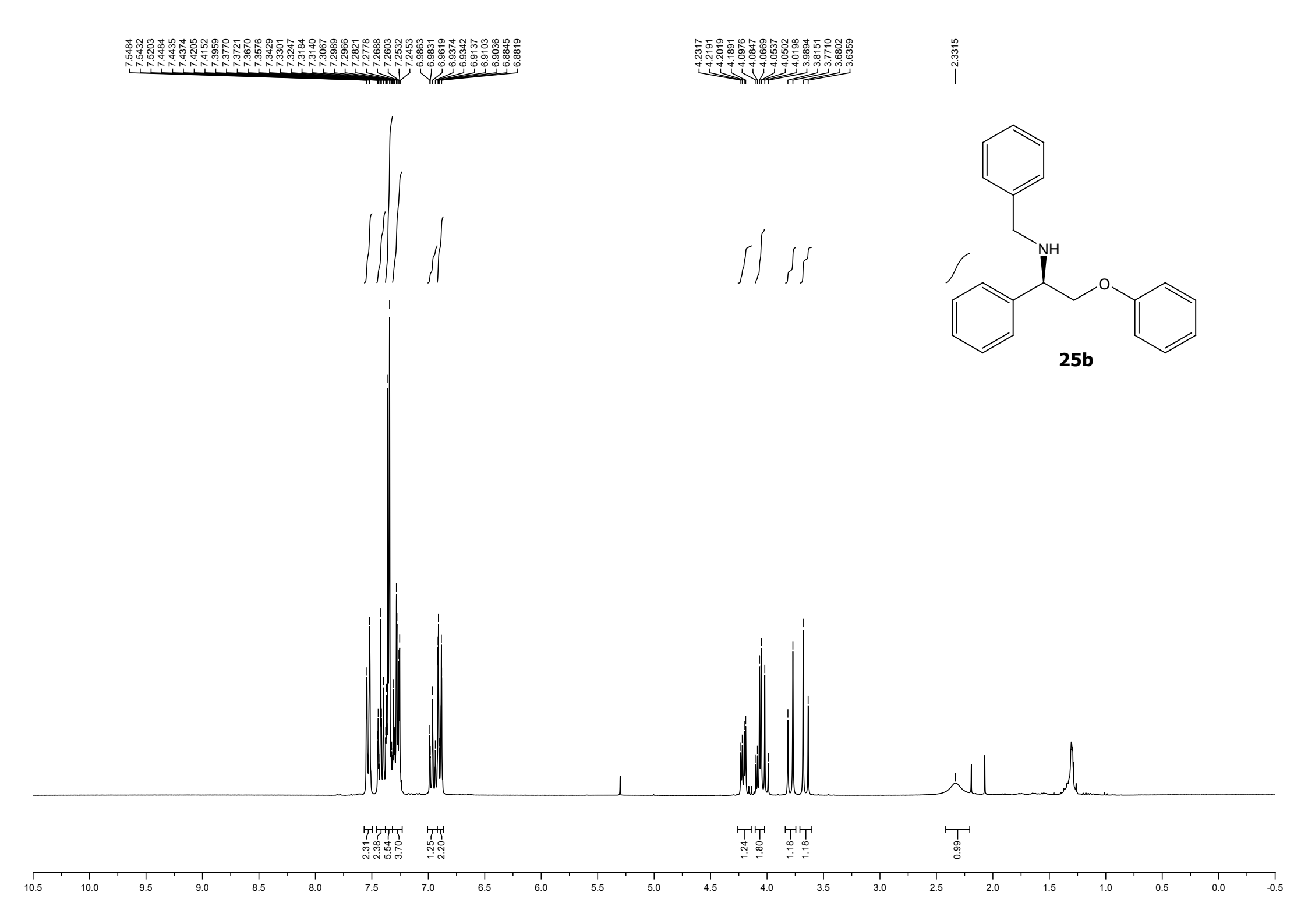

157.9952
155.3855
140.5906
139.8650
129.5216
128.6172
127.3944
125.0936
124.6229
121.0787
115.8150
83.7712
79.7803
61.3501
36.8906
28.3822
NH
O
O
O
CH3
CH3
CH3
trans-23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


trans-23
%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
500
3337,63
2974,35
1688,94
1519,25
1493,04
1235,45
1166,13
1055,13
745,80


7.8321
7.8089
7.8039
7.4968
7.4739
7.4342
7.3789
7.2967
7.0074
6.9831
6.9540
6.9506
6.9244
5.6391
5.6235
5.6094
5.5980
5.5825
4.4228
4.4073
4.3904
4.3828
4.3753
4.3670
4.3508
4.3347
O
HN
O
25a
1.94
5.36
4.59
3.80
1.00
2.04
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


167.0735
158.3967
139.2653
131.7209
129.6320
128.7700
128.6630
127.8678
127.1183
127.0946
121.3543
114.7328
69.9920
52.9163
O
HN
O
25a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


25a
%Transmission
Nombre d'onde (cm-1)
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
4000
3500
3000
2500
2000
1500
1000
3295,17
3061,26
3030,29
2924,58
2873,00
1633,89
1598,74
1579,27
1537,44
1491,98
1457,77
1387,86
1301,03
1239,43
1172,71
1152,27
1078,44
1041,54
909,18
882,20
753,38
690,94
520,00
513,69
511,88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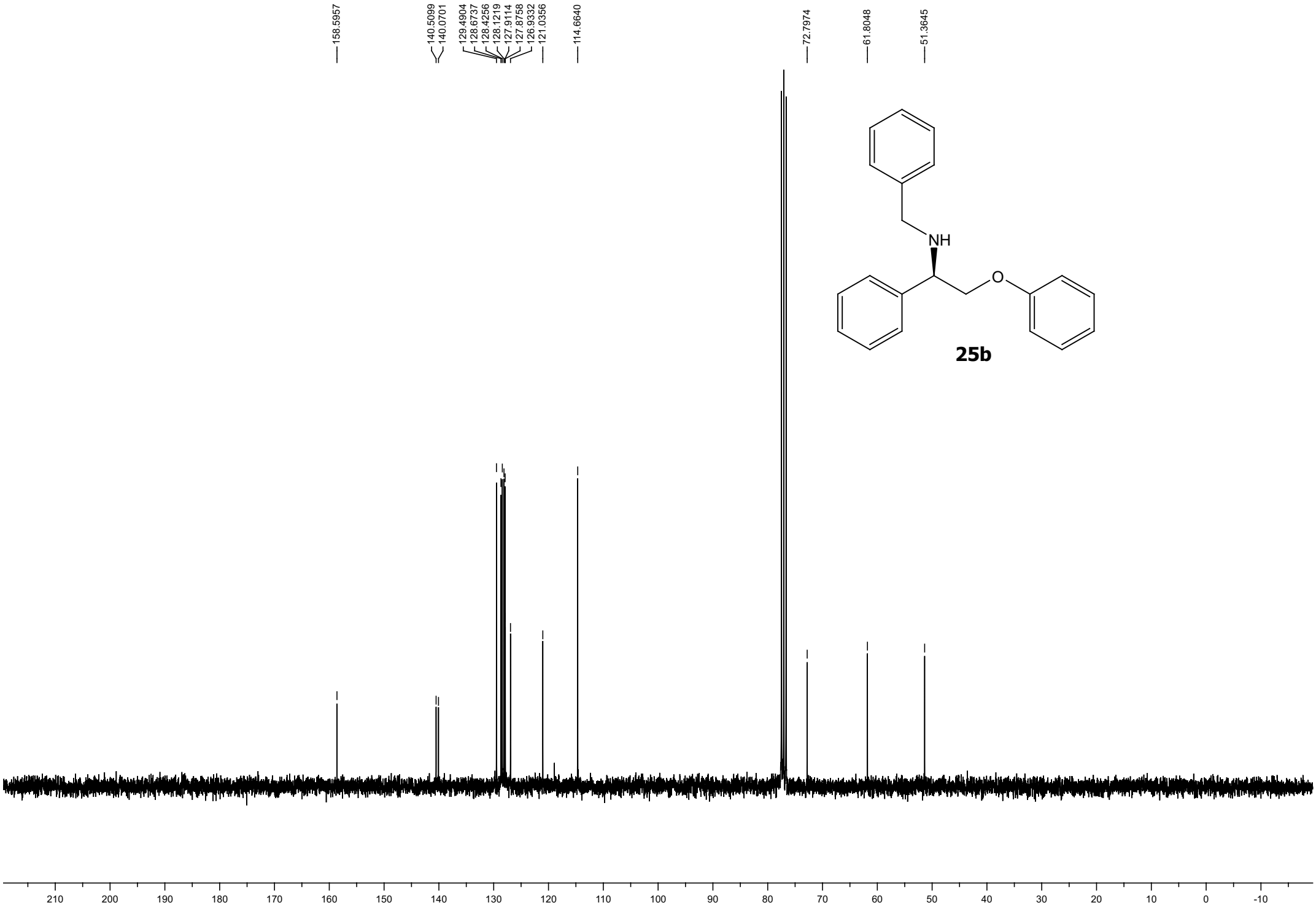
7.5432
7.5203
7.4484
7.4435
7.4374
7.4205
7.4152
7.3959
7.3770
7.3721
7.3670
7.3576
7.3429
7.3301
7.3247
7.3184
7.3140
7.3067
7.2989
7.2966
7.2821
7.2778
7.2688
7.2603
7.2532
7.2453
6.9863
6.9831
6.9619
6.9374
6.9342
6.9137
6.9103
6.9036
6.8845
6.8819
4.2317
4.2191
4.2019
4.1891
4.0976
4.0847
4.0669
4.0537
4.0502
4.0198
3.9894
3.8151
3.7710
3.6802
3.6359
2.3315
NH
O
25b
2.31
2.38
5.54
3.70
1.25
2.20
1.24
1.80
1.18
1.18
0.99
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


158.5957
140.5099
140.0701
129.4904
128.6737
128.4256
128.1219
127.9114
127.8758
126.9332
121.0356
114.6640
72.7974
61.8048
51.3645
NH
O
25b
210
200
190
180
170
160
150
140
130
120
110
100
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80
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60
50
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20
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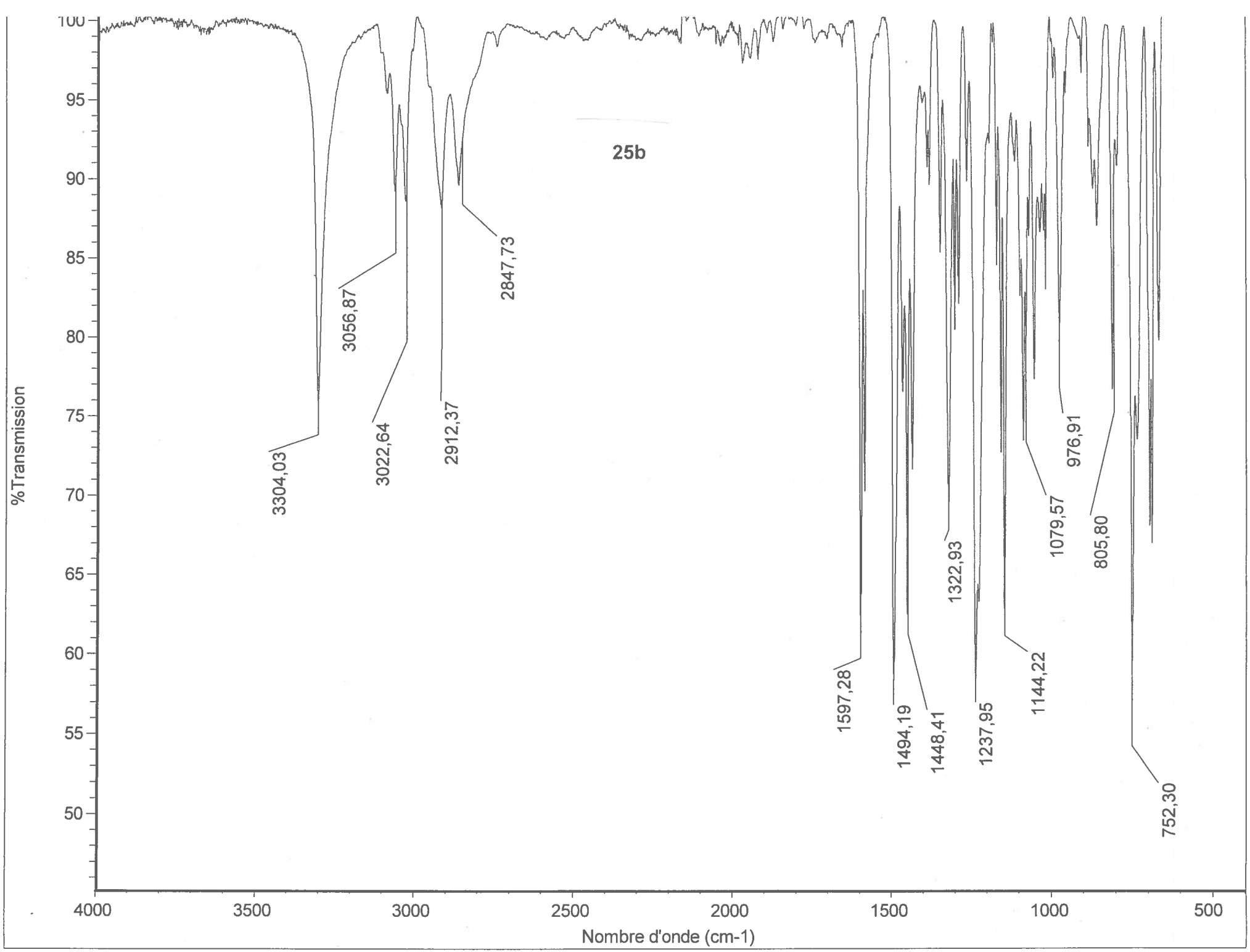
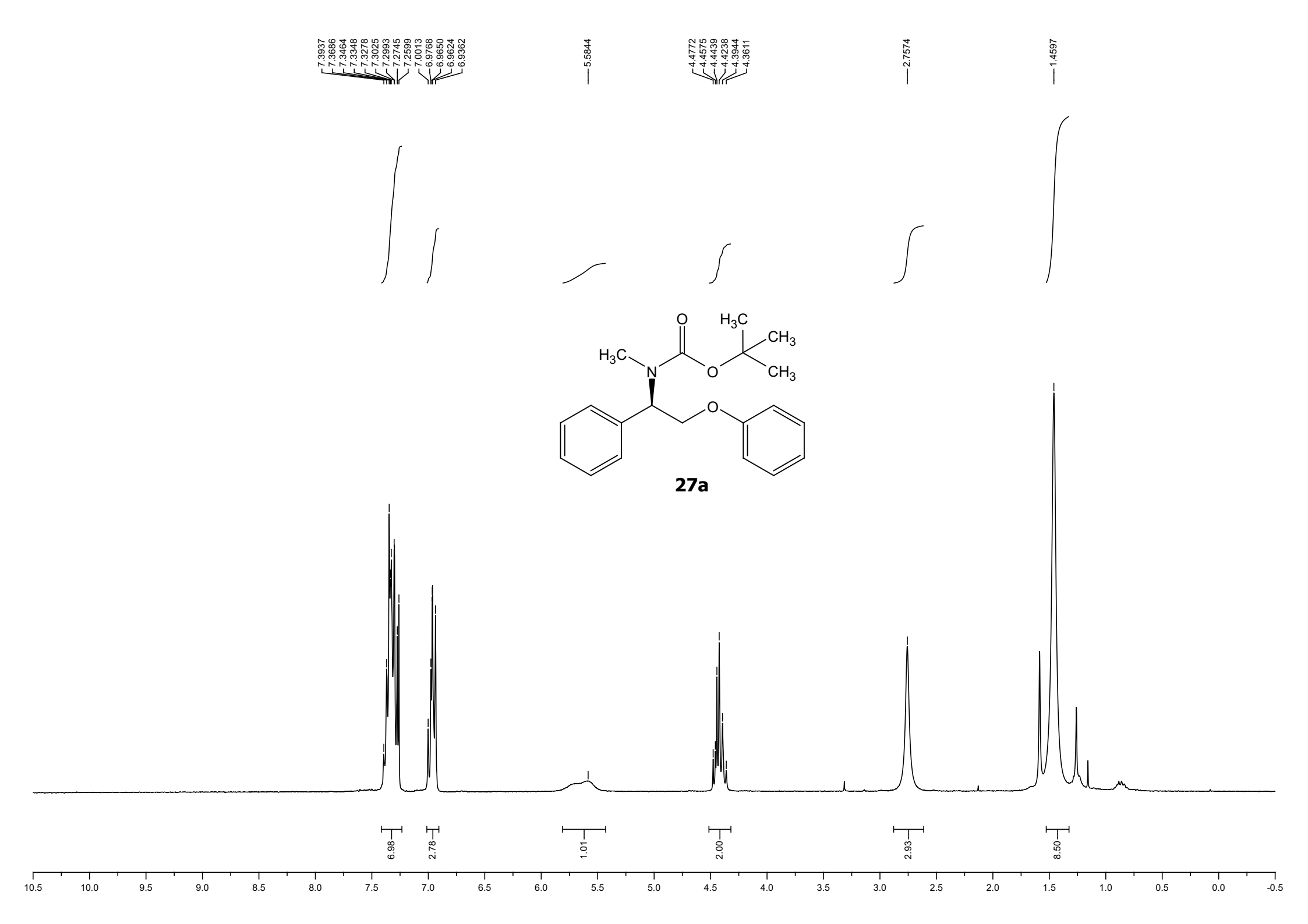
0
-10


25b
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
4000
3500
3000
2500
2000
1500
1000
500
3304,03
3056,87
3022,64
2912,37
2847,73
1597,28
1494,19
1448,41
1322,93
1237,95
1144,22
1079,57
976,91
805,80
752,30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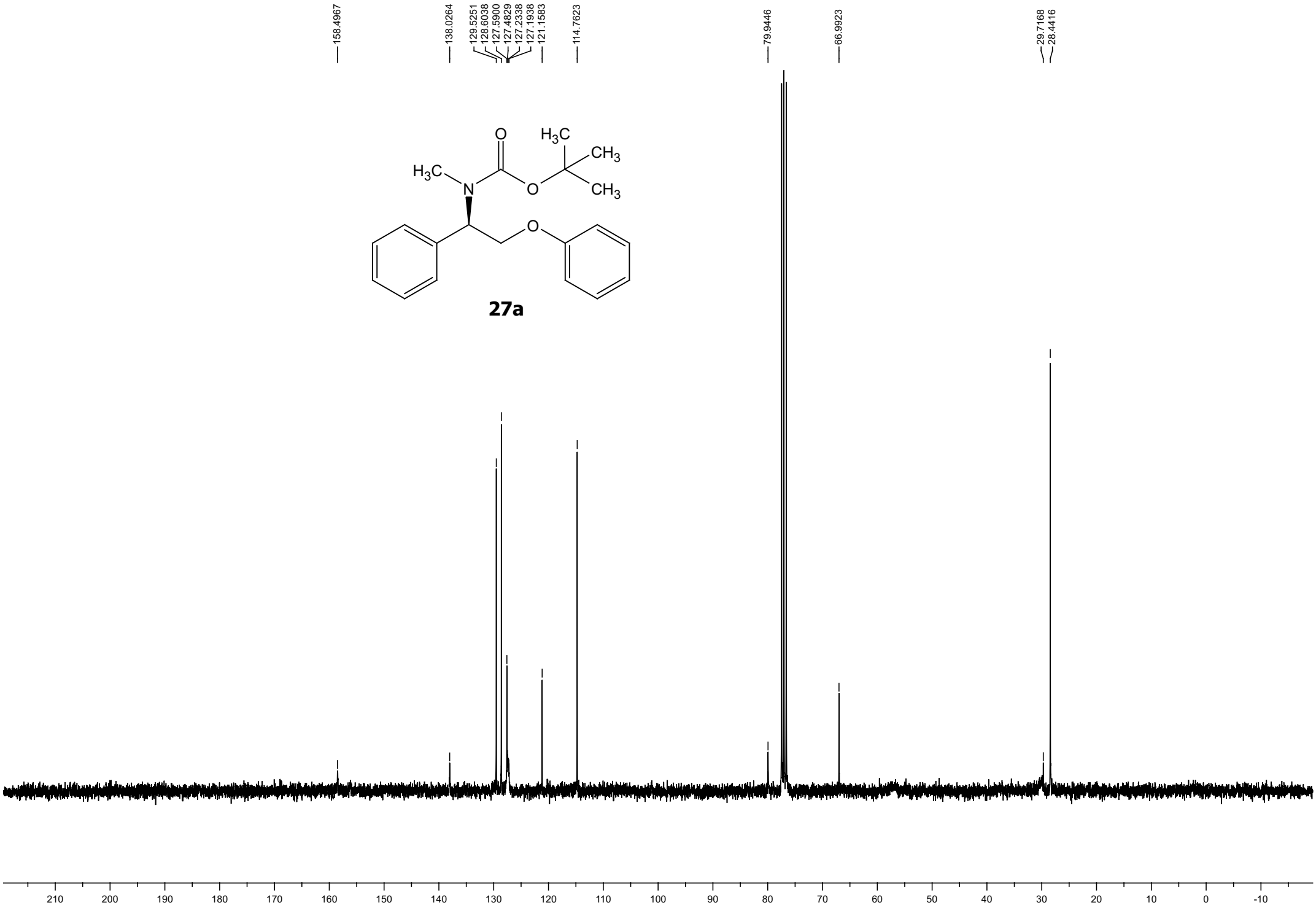
7.3464
7.3348
7.3278
7.3025
7.2993
7.2745
7.2599
7.0013
6.9768
6.9650
6.9624
6.9362
5.5844
4.4772
4.4575
4.4439
4.4238
4.3944
4.3611
2.7574
1.4597
O
H3C
CH3
H3C
N
O
CH3
O
27a
6.98
2.78
1.01
2.00
2.93
8.50
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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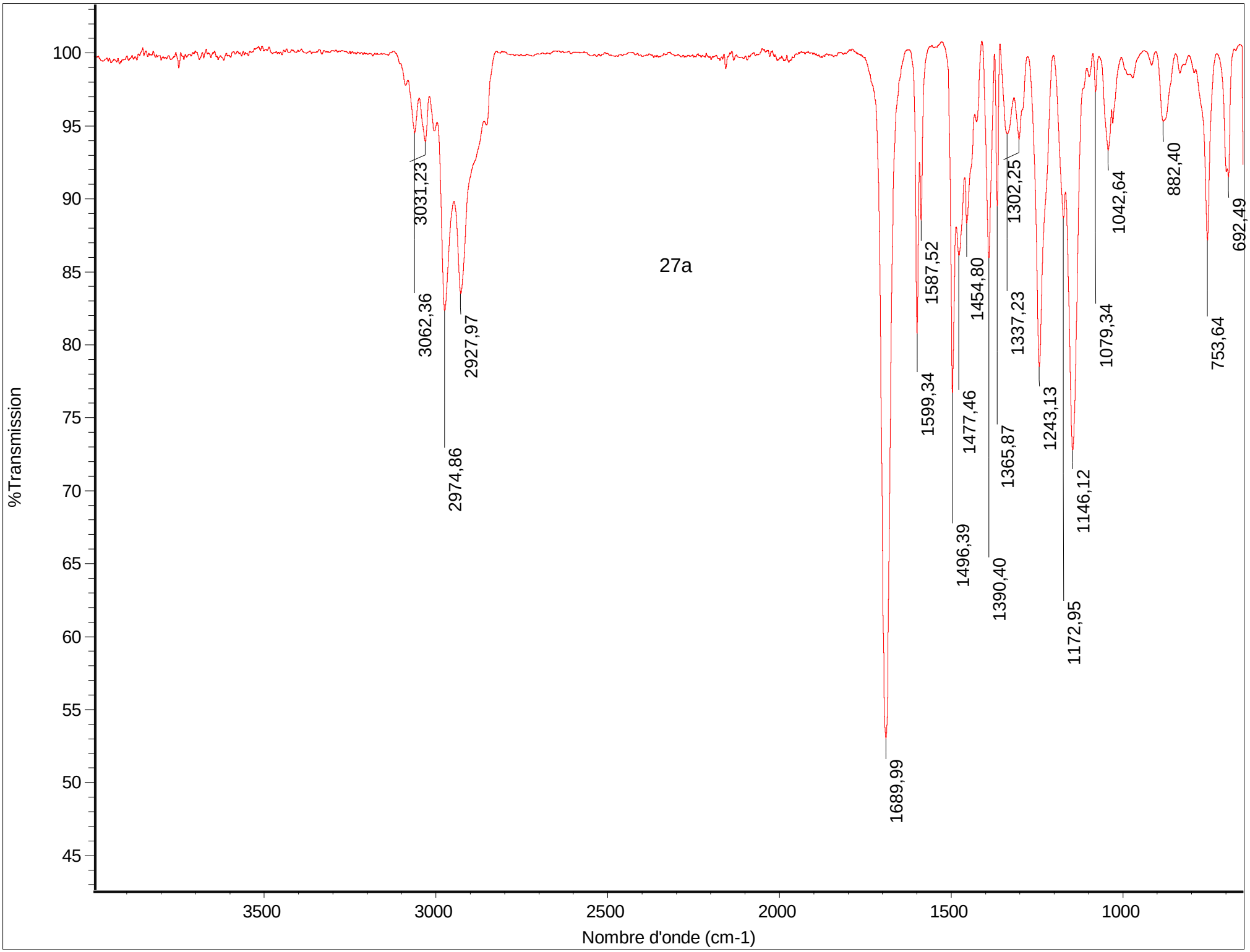
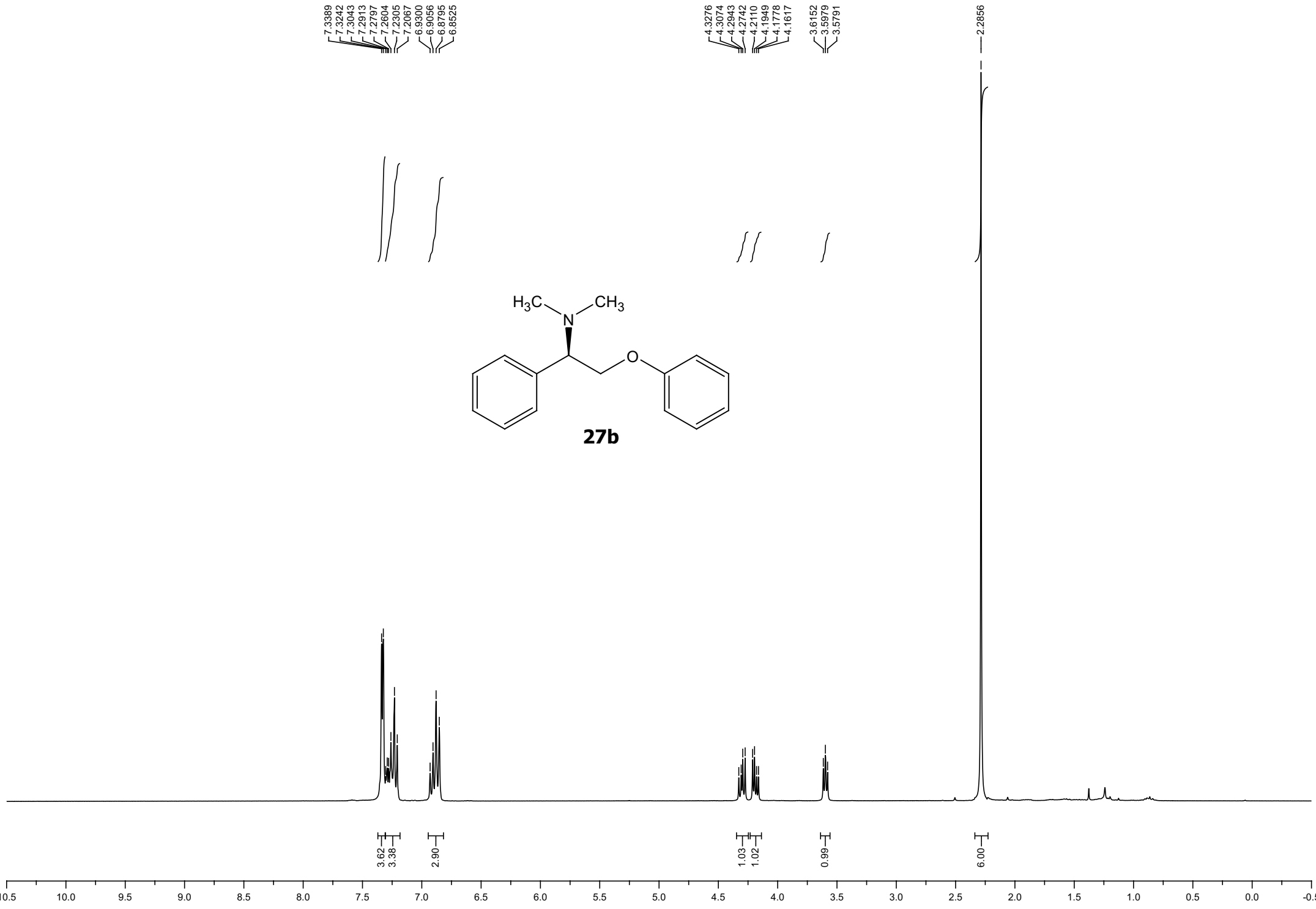
129.5251
128.6038
127.5900
127.4829
127.2338
127.1938
121.1583
114.7623
79.9446
66.9923
29.7168
28.4416
O
H3C
CH3
H3C
N
O
CH3
O
27a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


27a
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
3500
3000
2500
2000
1500
1000
3031,23
3062,36
2974,86
2927,97
1689,99
1599,34
1587,52
1496,39
1477,46
1454,80
1390,40
1365,87
1337,23
1302,25
1243,13
1172,95
1146,12
1079,34
1042,64
882,40
753,64
692,49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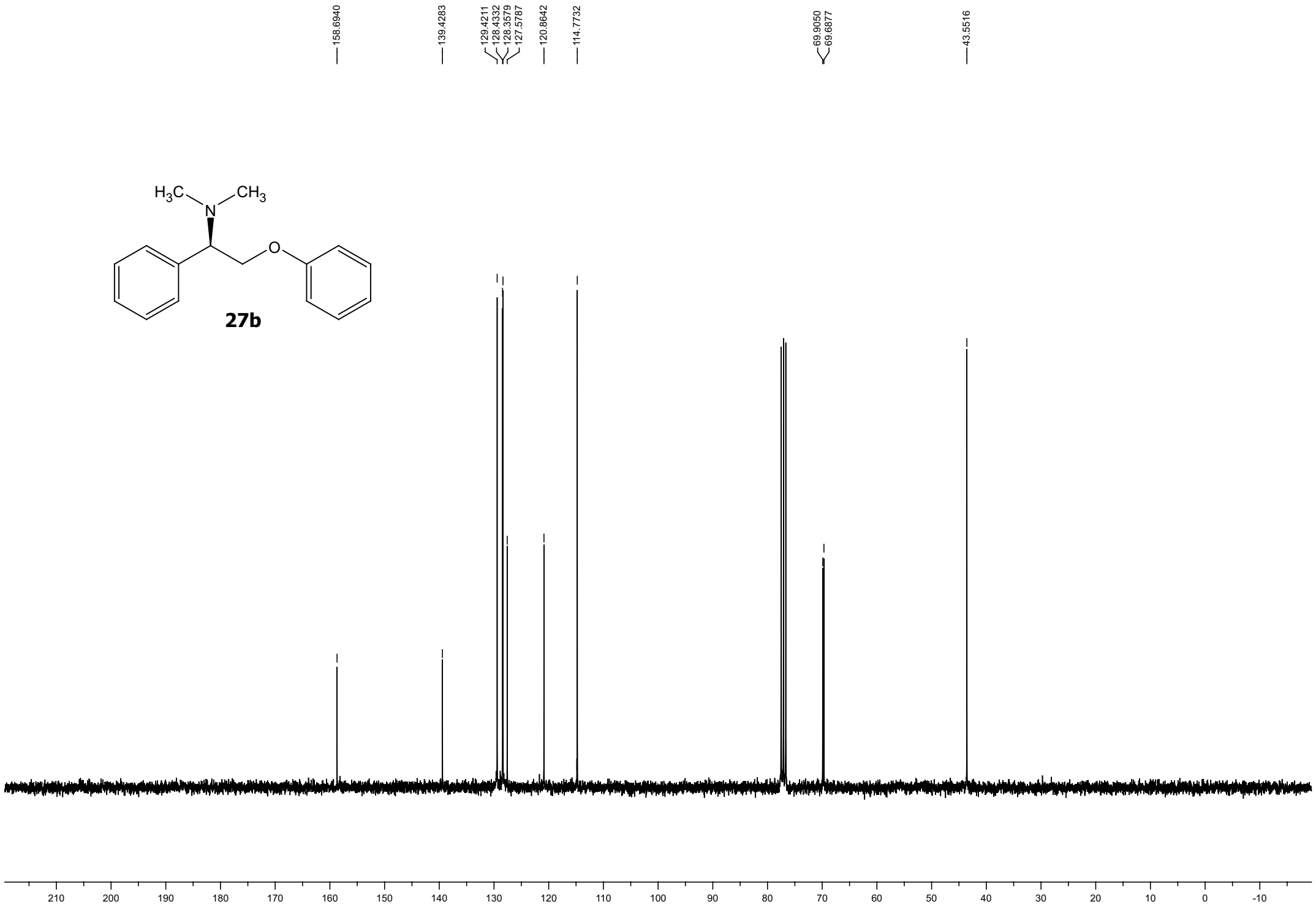
7.3242
7.3043
7.2913
7.2797
7.2604
7.2305
7.2067
6.9300
6.9056
6.8795
6.8525
4.3276
4.3074
4.2943
4.2742
4.2110
4.1949
4.1778
4.1617
3.6152
3.5979
3.5791
2.2856
H3C
N
CH3
O
27b
3.62
3.38
2.90
1.03
1.02
0.99
6.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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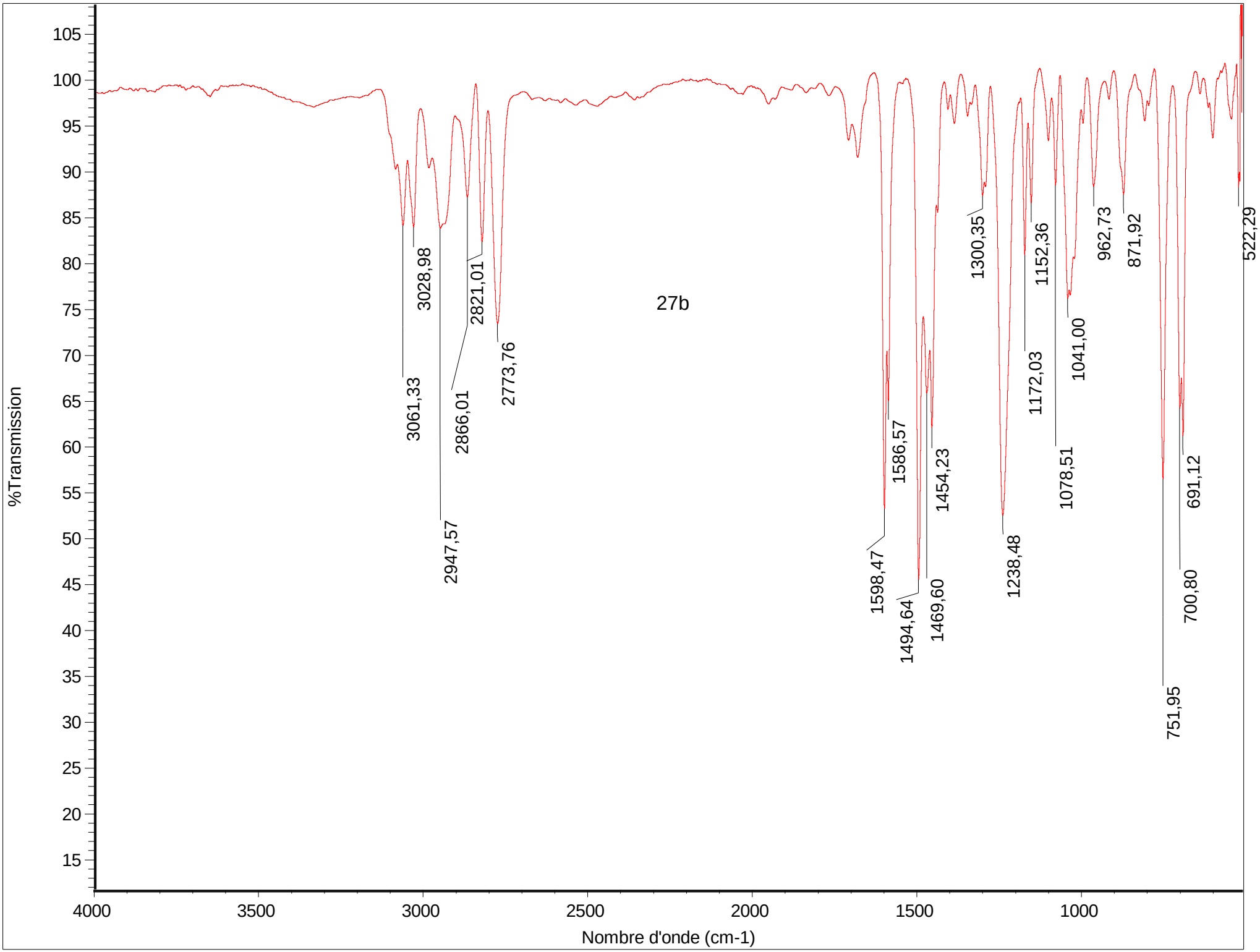
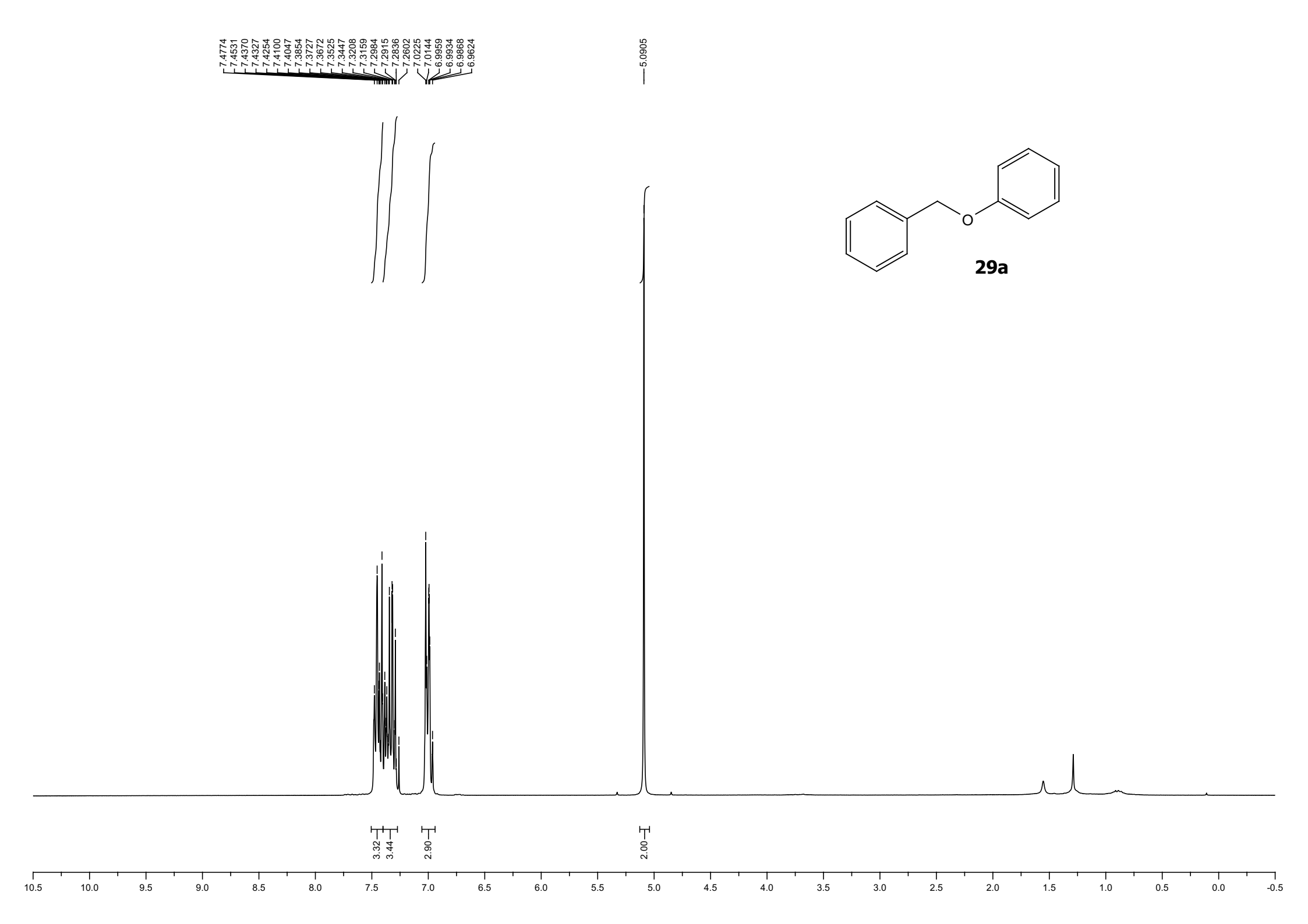
139.4283
129.4211
128.4332
128.3579
127.5787
120.8642
114.7732
69.9050
69.6877
43.5516
H3C
CH3
N
O
27b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


27b
%Transmission
Nombre d'onde (cm-1)
105
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
3061,33
3028,98
2947,57
2866,01
2821,01
2773,76
1598,47
1586,57
1494,64
1469,60
1454,23
1300,35
1238,48
1172,03
1152,36
1078,51
1041,00
962,73
871,92
751,95
700,80
691,12
522,29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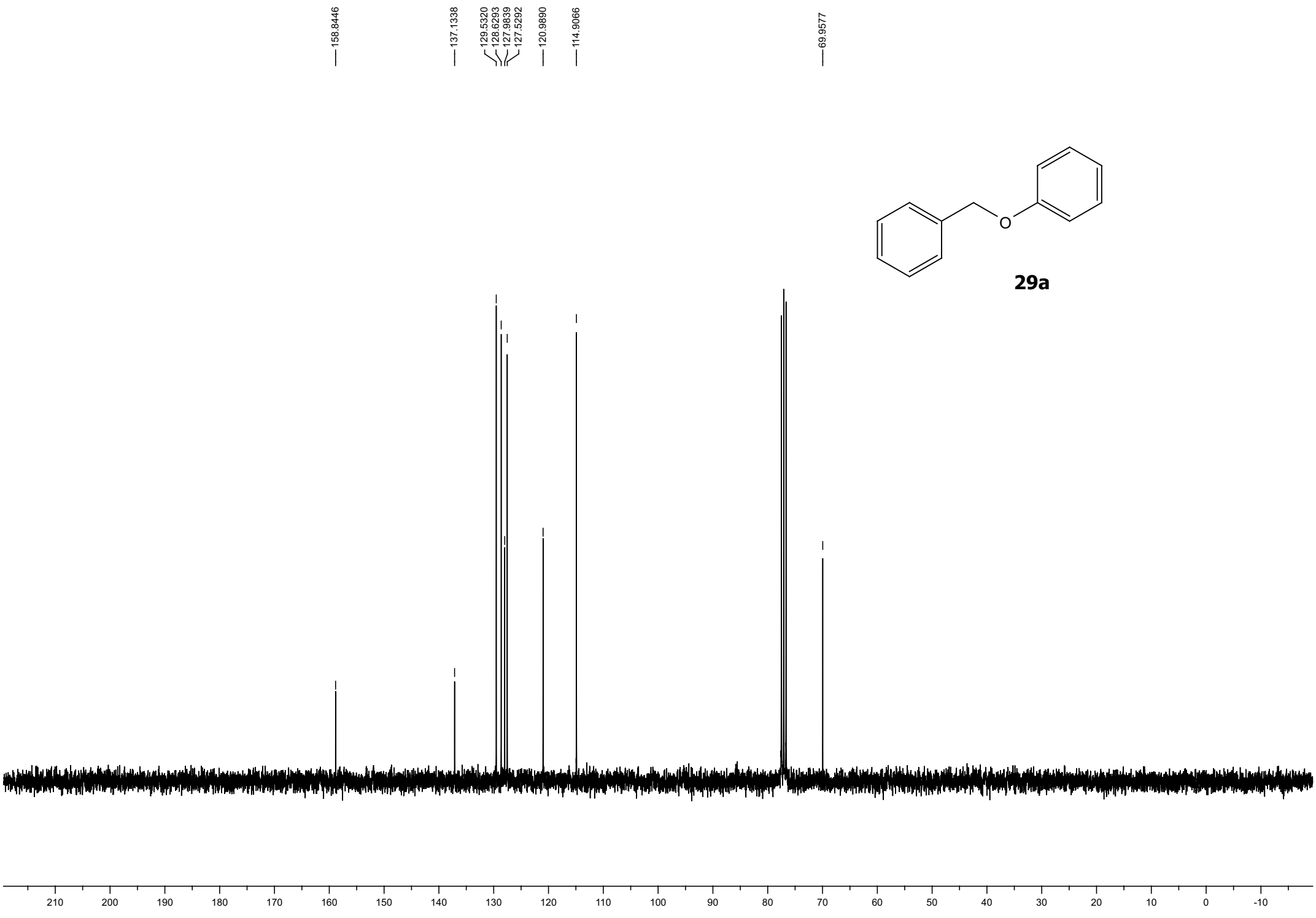
7.4370
7.4327
7.4254
7.4100
7.4047
7.3854
7.3727
7.3672
7.3525
7.3447
7.3208
7.3159
7.2984
7.2915
7.2836
7.2602
7.0225
7.0144
6.9959
6.9934
6.9868
6.9624
5.0905
O
29a
3.32
3.44
2.90
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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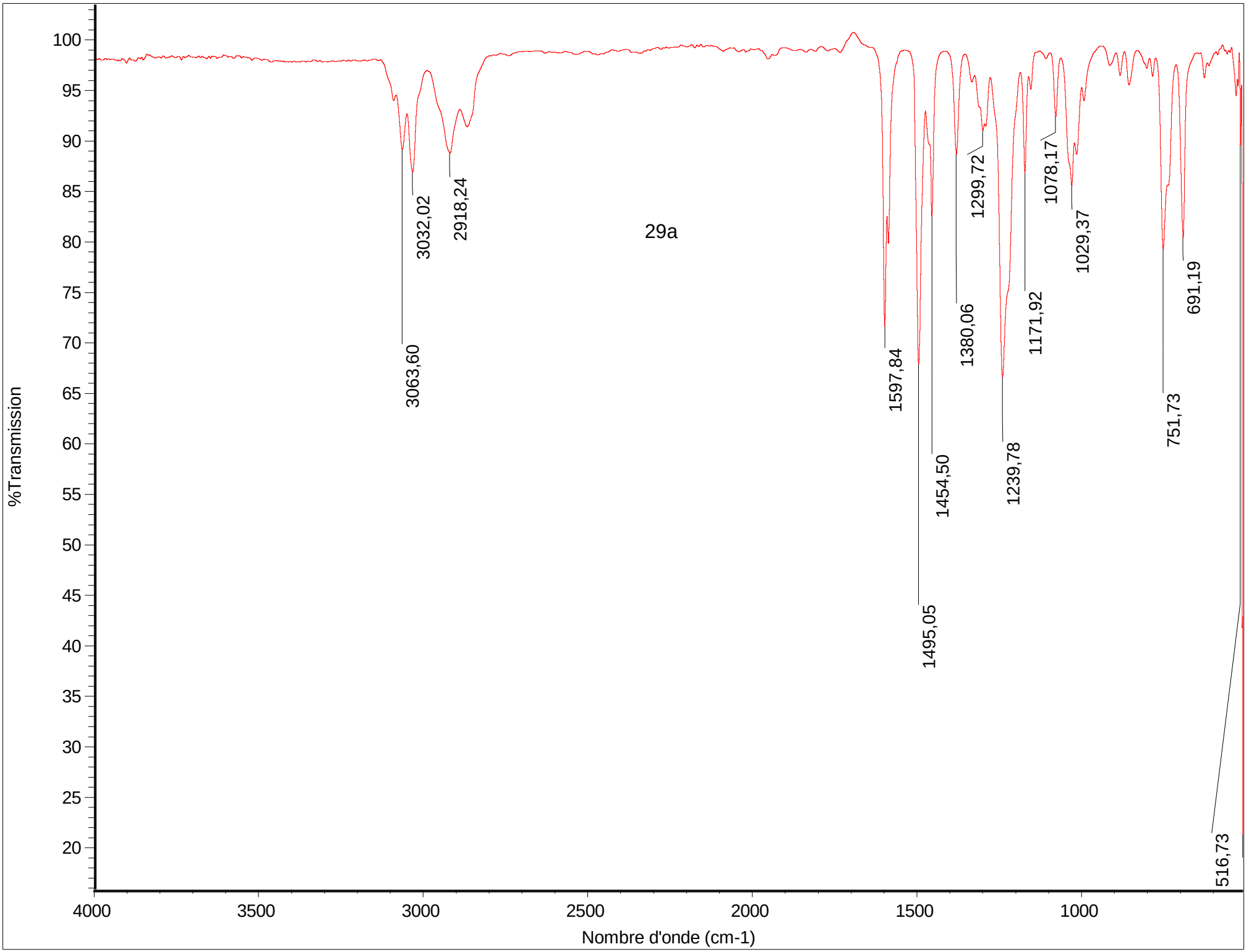
137.1338
129.5320
128.6293
127.9839
127.5292
120.9890
114.9066
69.9577
O
29a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


29a
%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
3063,60
3032,02
2918,24
1597,84
1495,05
1454,50
1380,06
1299,72
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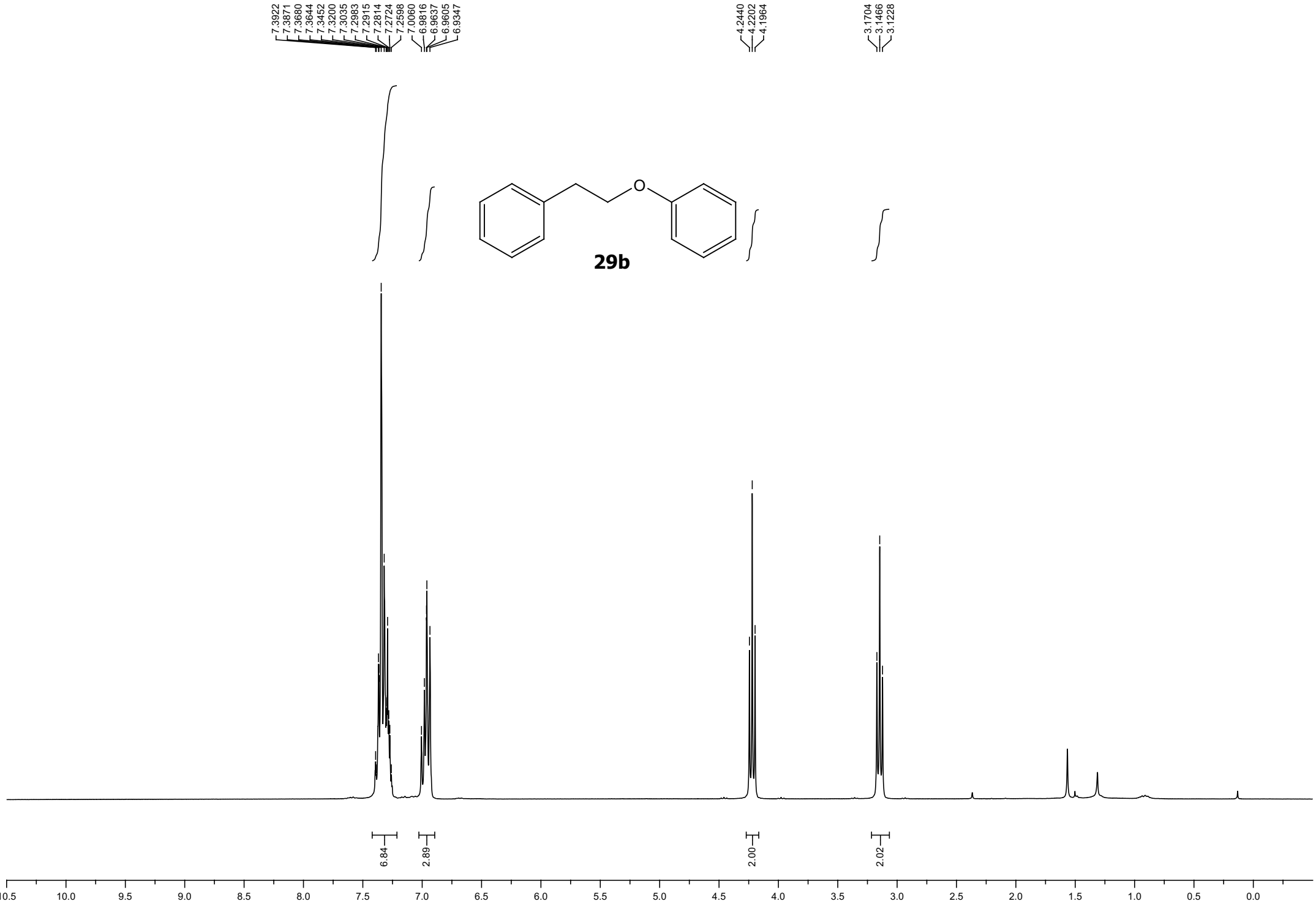
1171,92
1078,17
1029,37
751,73
691,19
516,73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7.3871
7.3680
7.3644
7.3452
7.3200
7.3035
7.2983
7.2915
7.2814
7.2724
7.2598
7.0060
6.9816
6.9637
6.9605
6.9347
4.2440
4.2202
4.1964
3.1704
3.1466
3.1228
O
29b
6.84
2.89
2.00
2.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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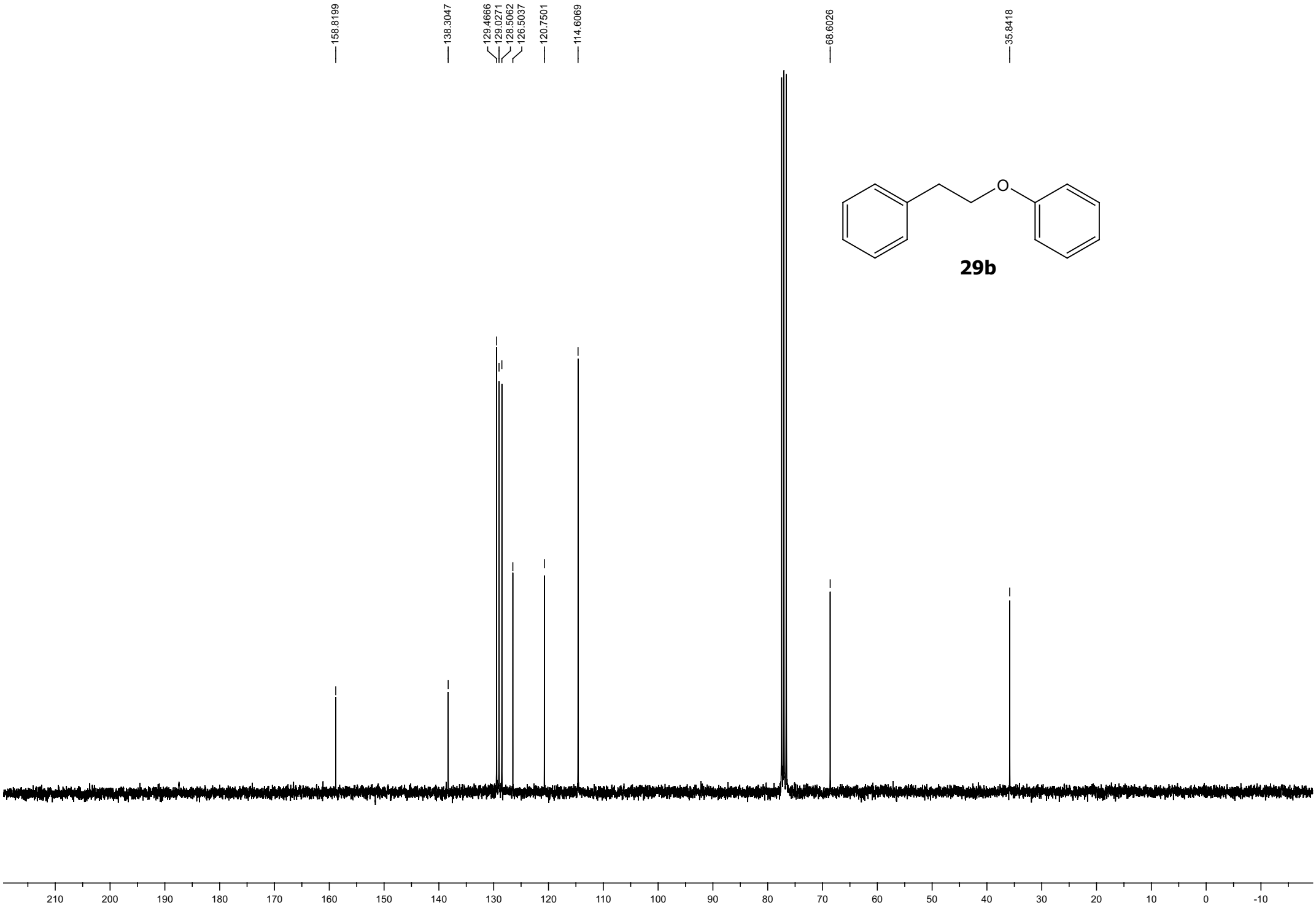
2.0
1.5
1.0
0.5
0.0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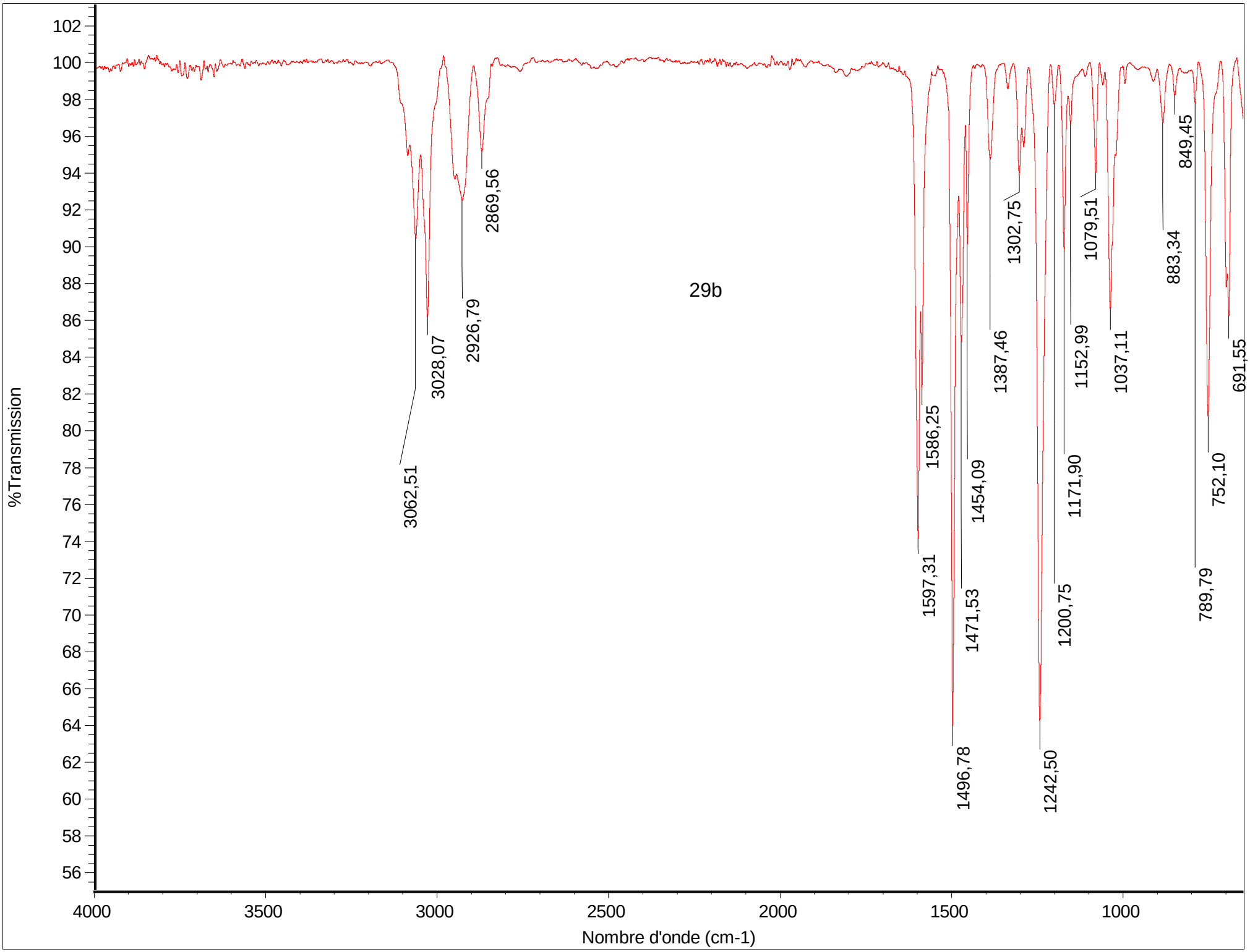
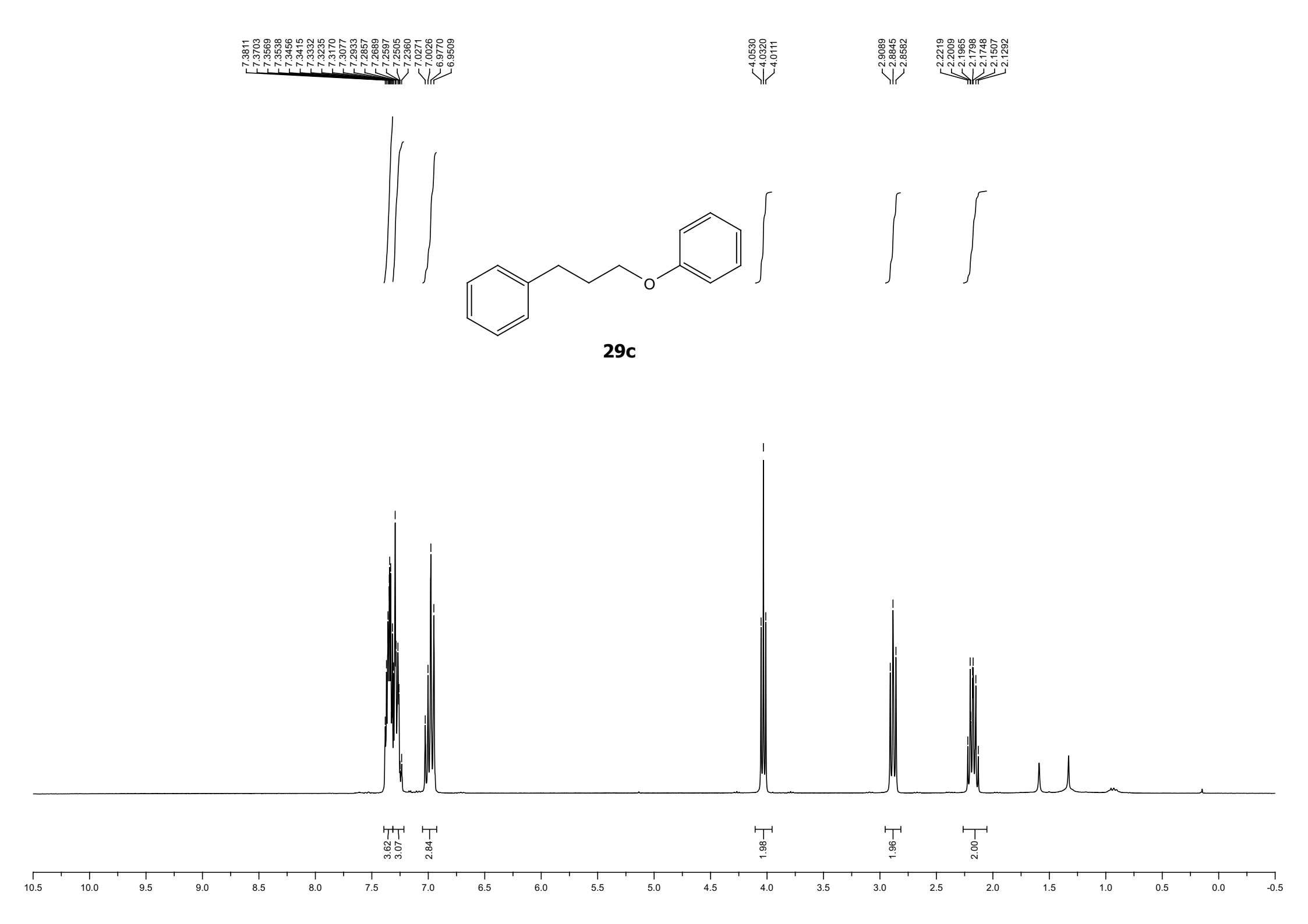
129.0271
128.5062
126.5037
120.7501
114.6069
68.6026
35.8418
O
29b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


29b
%Transmission
Nombre d'onde (cm-1)
4000
3500
3000
2500
2000
1500
1000
102
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56
3062,51
3028,07
2926,79
2869,56
1597,31
1586,25
1496,78
1471,53
1454,09
1387,46
1302,75
1242,50
1200,75
1171,90
1152,99
1079,51
1037,11
883,34
849,45
789,79
752,10
691,55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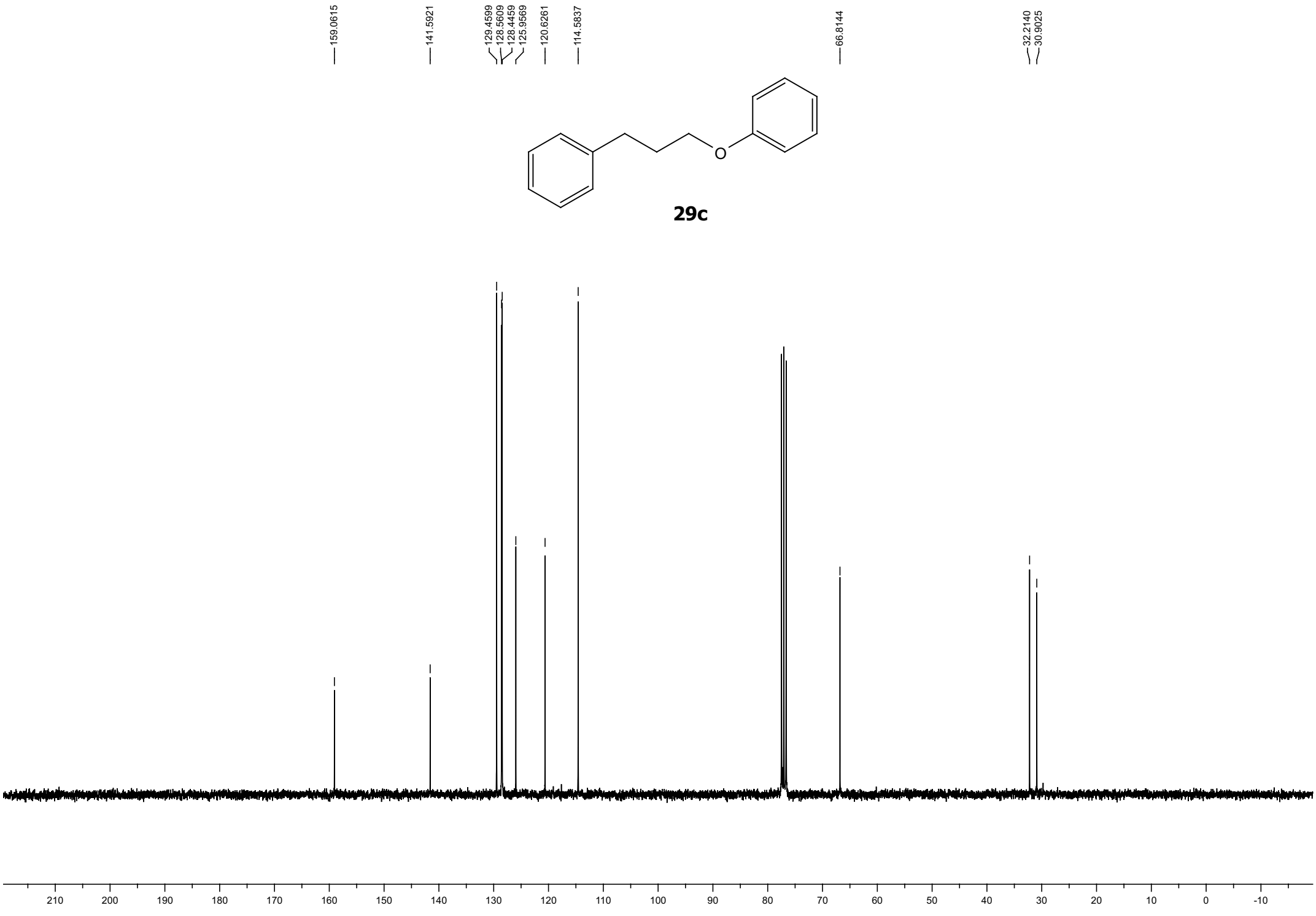
7.3569
7.3538
7.3456
7.3415
7.3332
7.3235
7.3170
7.3077
7.2933
7.2857
7.2689
7.2597
7.2505
7.2360
7.0271
7.0026
6.9770
6.9509
4.0530
4.0320
4.0111
2.9089
2.8845
2.8582
2.2219
2.2009
2.1965
2.1798
2.1748
2.1507
2.1292
O
29c
3.62
3.07
2.84
1.98
1.96
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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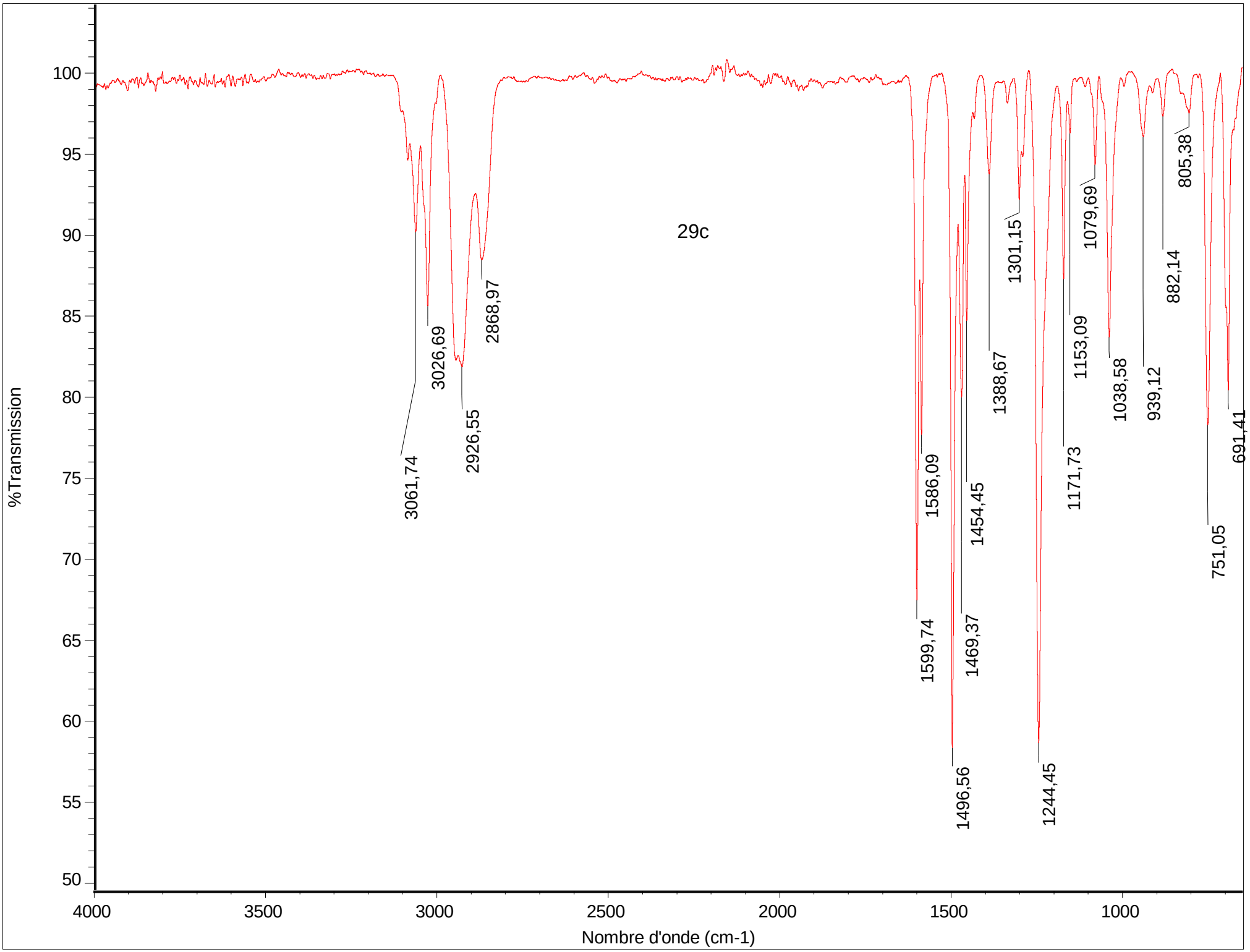
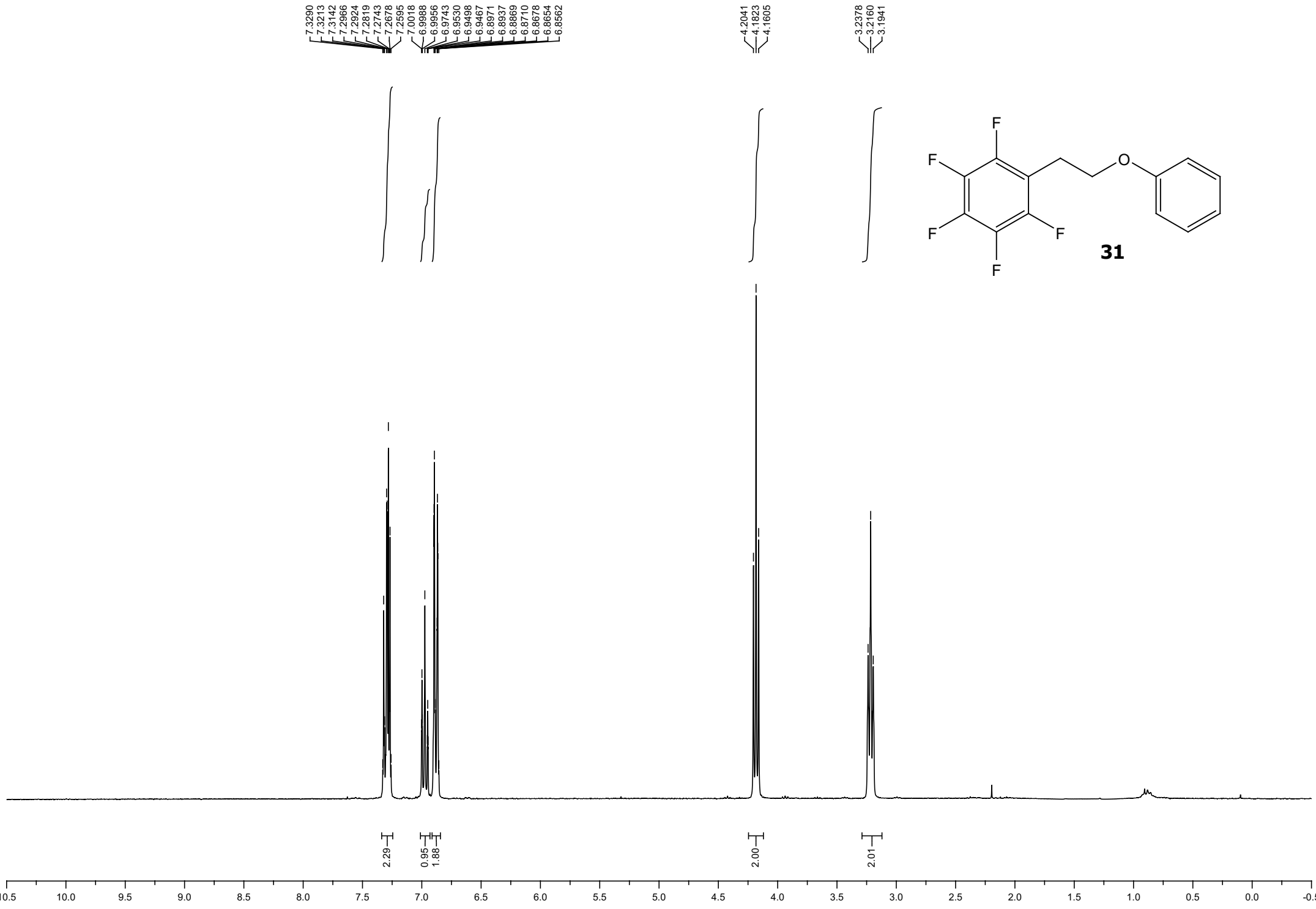
128.5609
128.4459
125.9569
120.6261
114.5837
66.8144
32.2140
30.9025
O
29c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


29c
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
4000
3500
3000
2500
2000
1500
1000
3061,74
3026,69
2926,55
2868,97
1599,74
1586,09
1496,56
1469,37
1454,45
1388,67
1301,15
1244,45
1171,73
1153,09
1079,69
1038,58
939,12
882,14
805,38
751,05
691,41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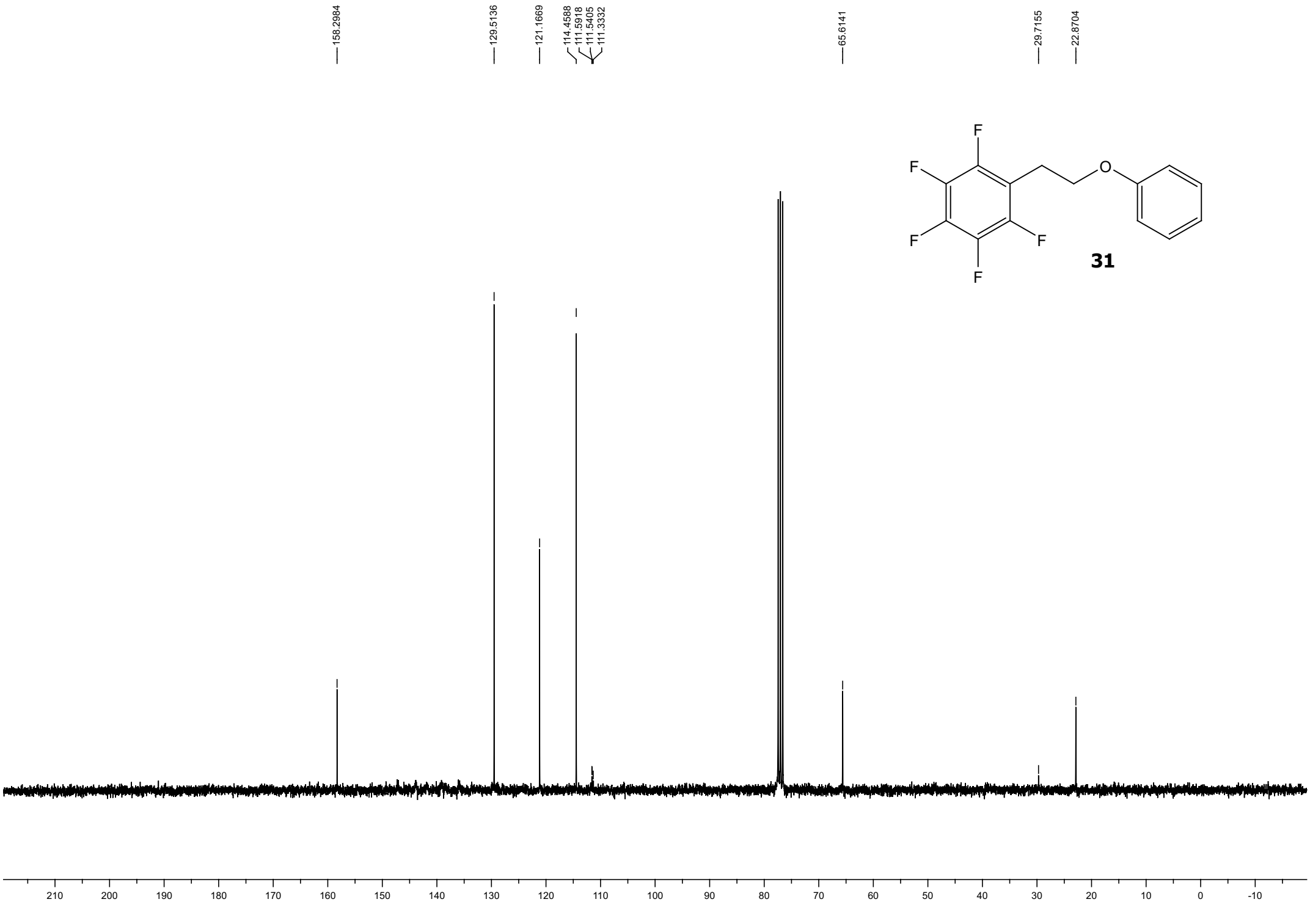
7.2966
7.2924
7.2819
7.2743
7.2678
7.2595
7.0018
6.9988
6.9956
6.9743
6.9530
6.9498
6.9467
6.8971
6.8937
6.8869
6.8710
6.8678
6.8654
6.8562
4.2041
4.1823
4.1605
3.2378
3.2160
3.1941
F
F
F
F
F
O
31
2.29
0.95
1.88
2.00
2.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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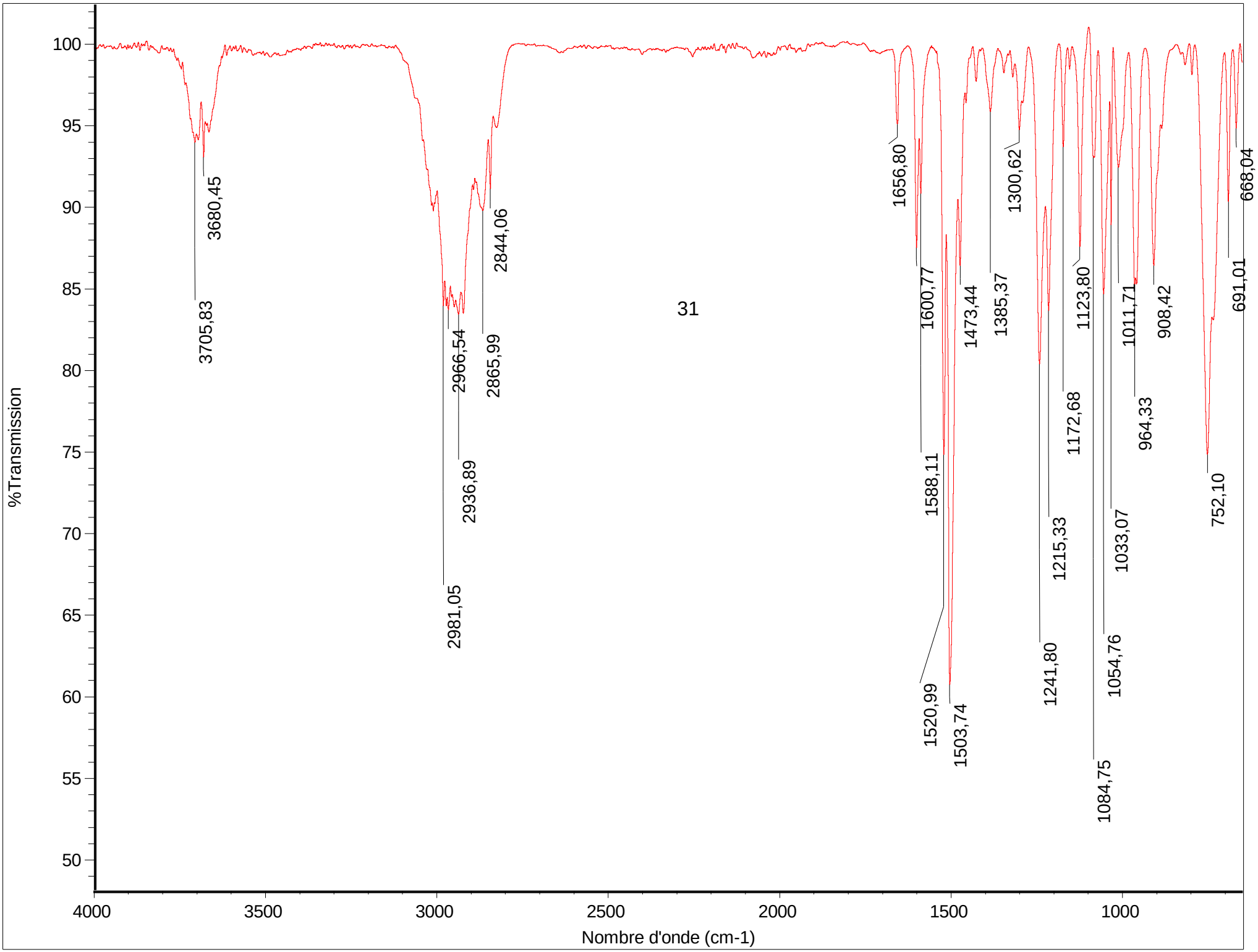
114.4588
111.5918
111.5405
111.3332
65.6141
29.7155
22.8704
F
F
F
F
F
O
31
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


%Transmission
100
95
90
85
80
75
70
65
60
55
50
4000
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)
31
3705,83
3680,45
2981,05
2966,54
2936,89
2865,99
2844,06
1656,80
1600,77
1588,11
1520,99
1503,74
1473,44
1385,37
1300,62
1241,80
1215,33
1172,68
1123,80
1084,75
1054,76
1033,07
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964,33
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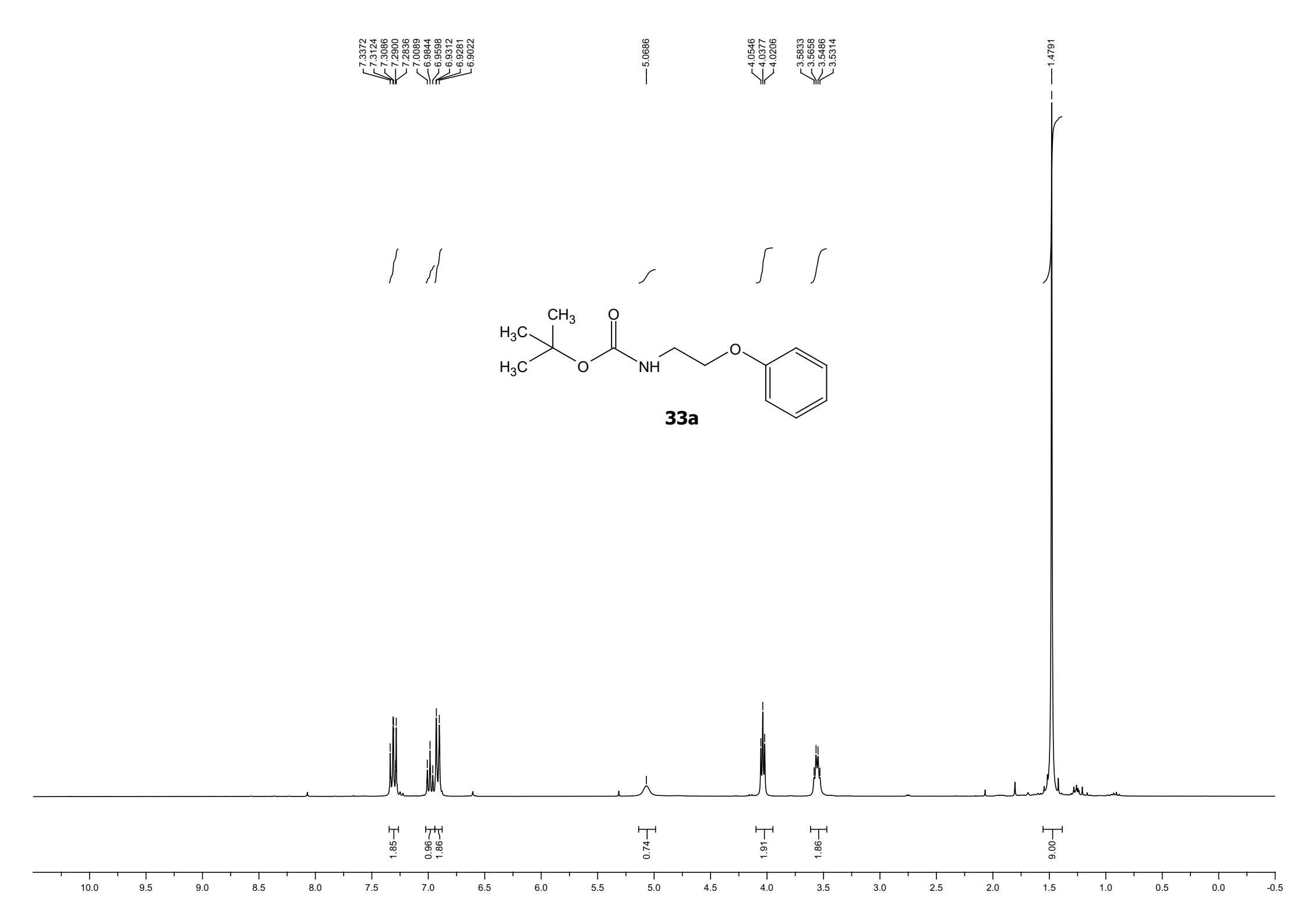
691,01
668,04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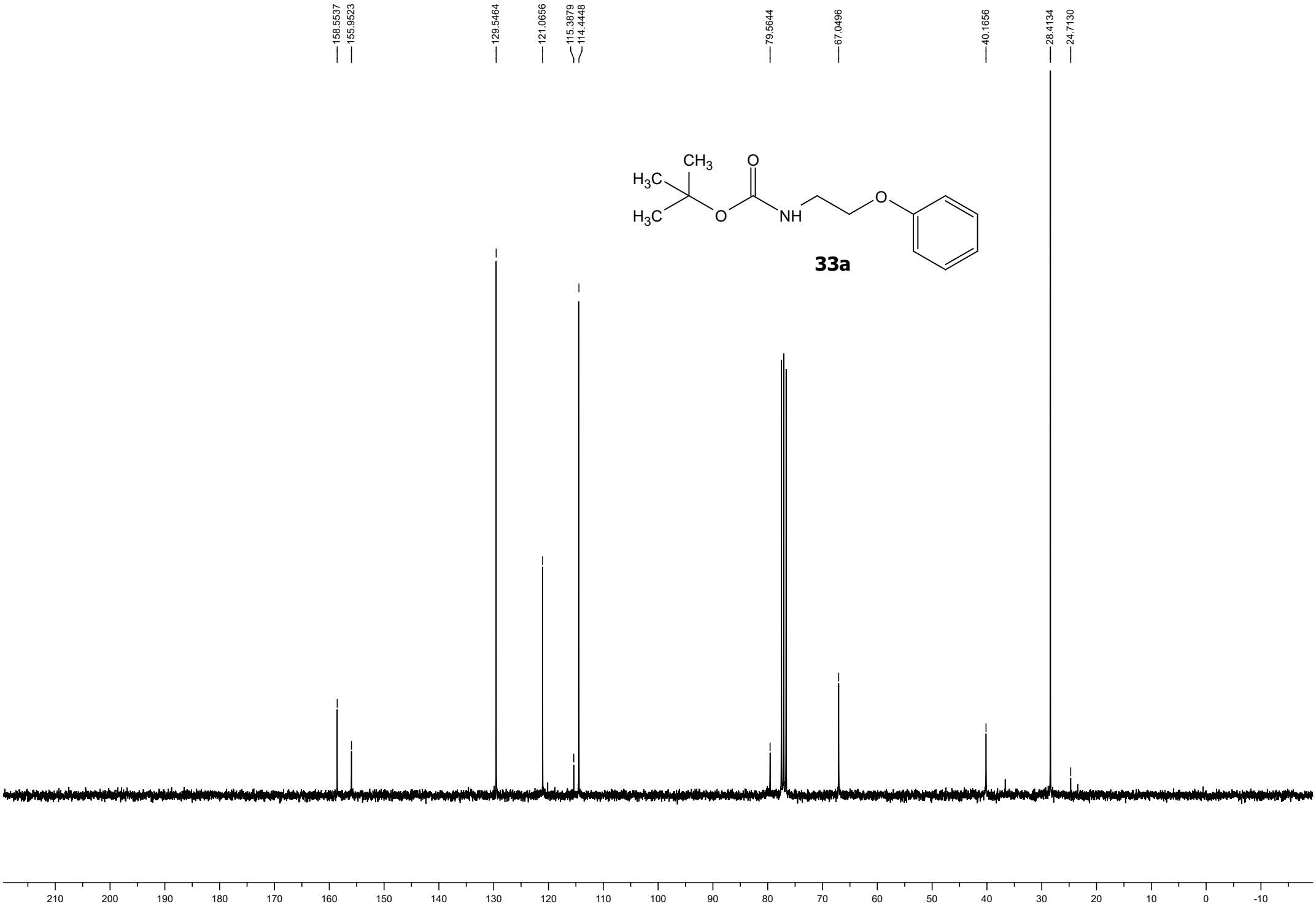
7.2836
7.0089
6.9844
6.9598
6.9312
6.9281
6.9022
5.0686
4.0546
4.0377
4.0206
3.5833
3.5658
3.5486
3.5314
1.4791
CH3
H3C
H3C
O
O
NH
O
33a
1.85
0.96
1.86
0.74
1.91
1.86
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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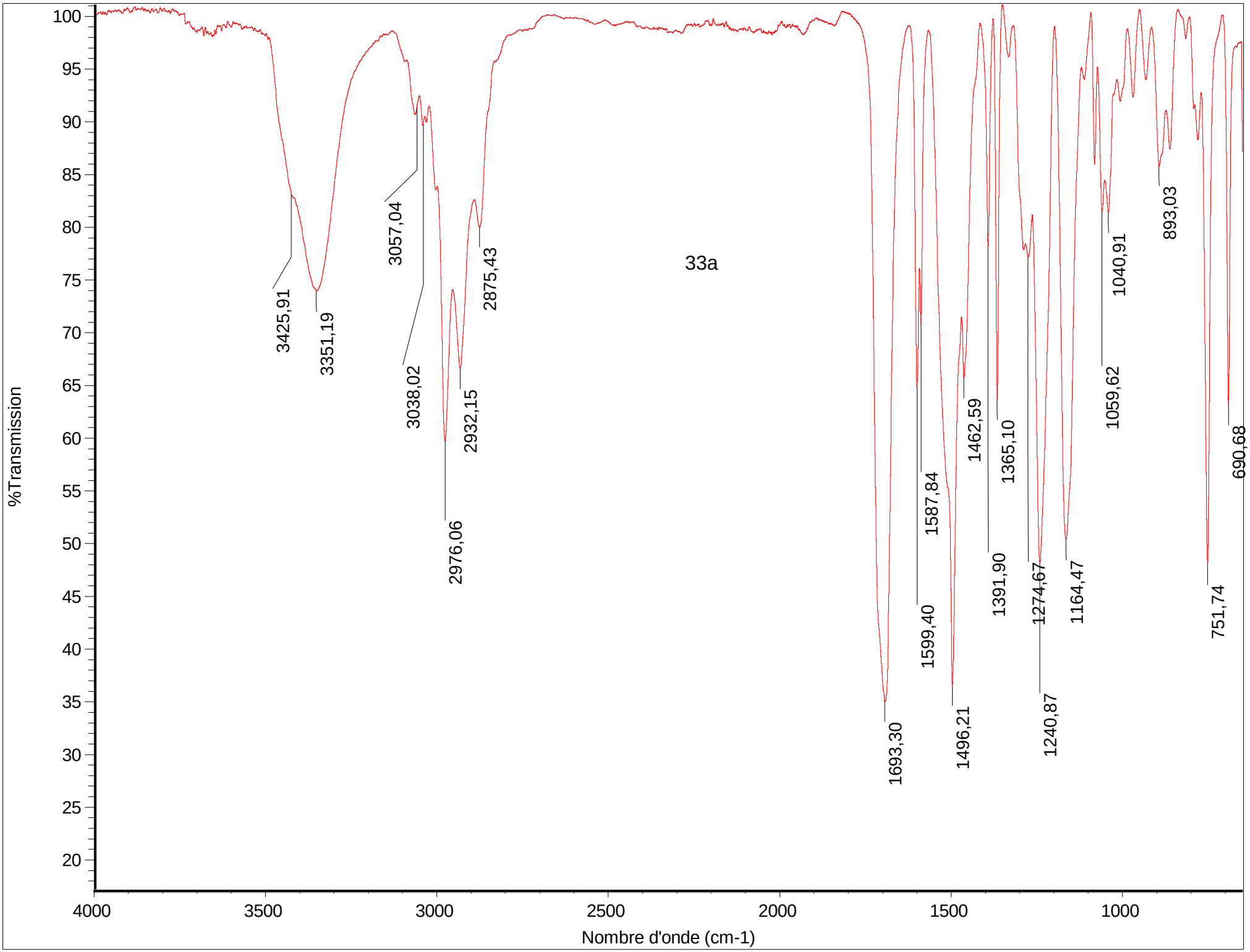
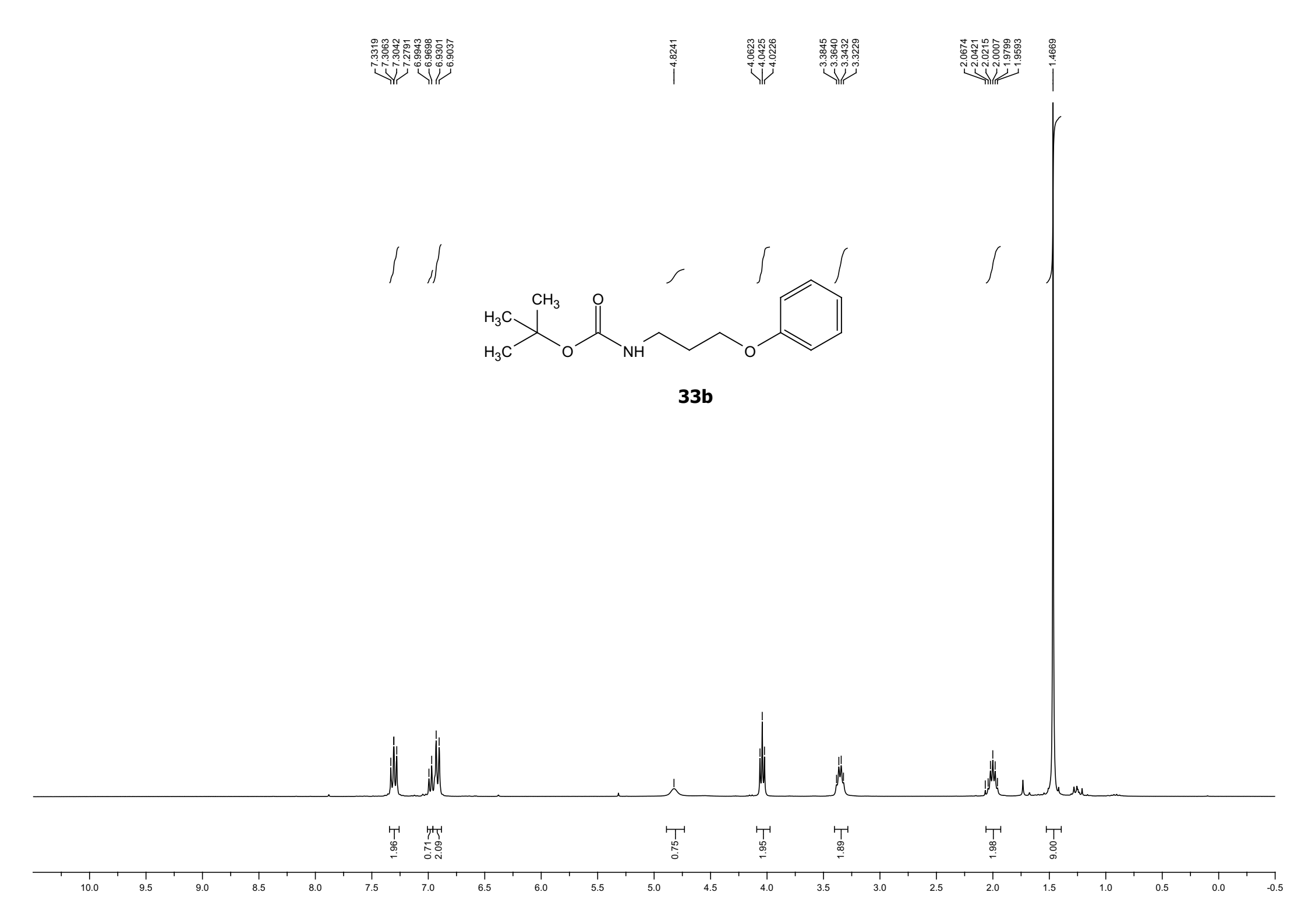
129.5464
121.0656
115.3879
114.4448
79.5644
67.0496
40.1656
28.4134
24.7130
CH3
H3C
H3C
O
O
NH
O
33a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


33a
%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
3425,91
3351,19
3057,04
3038,02
2976,06
2932,15
2875,43
1693,30
1599,40
1587,84
1496,21
1462,59
1391,90
1365,10
1274,67
1240,87
1164,47
1059,62
1040,91
893,03
751,74
690,68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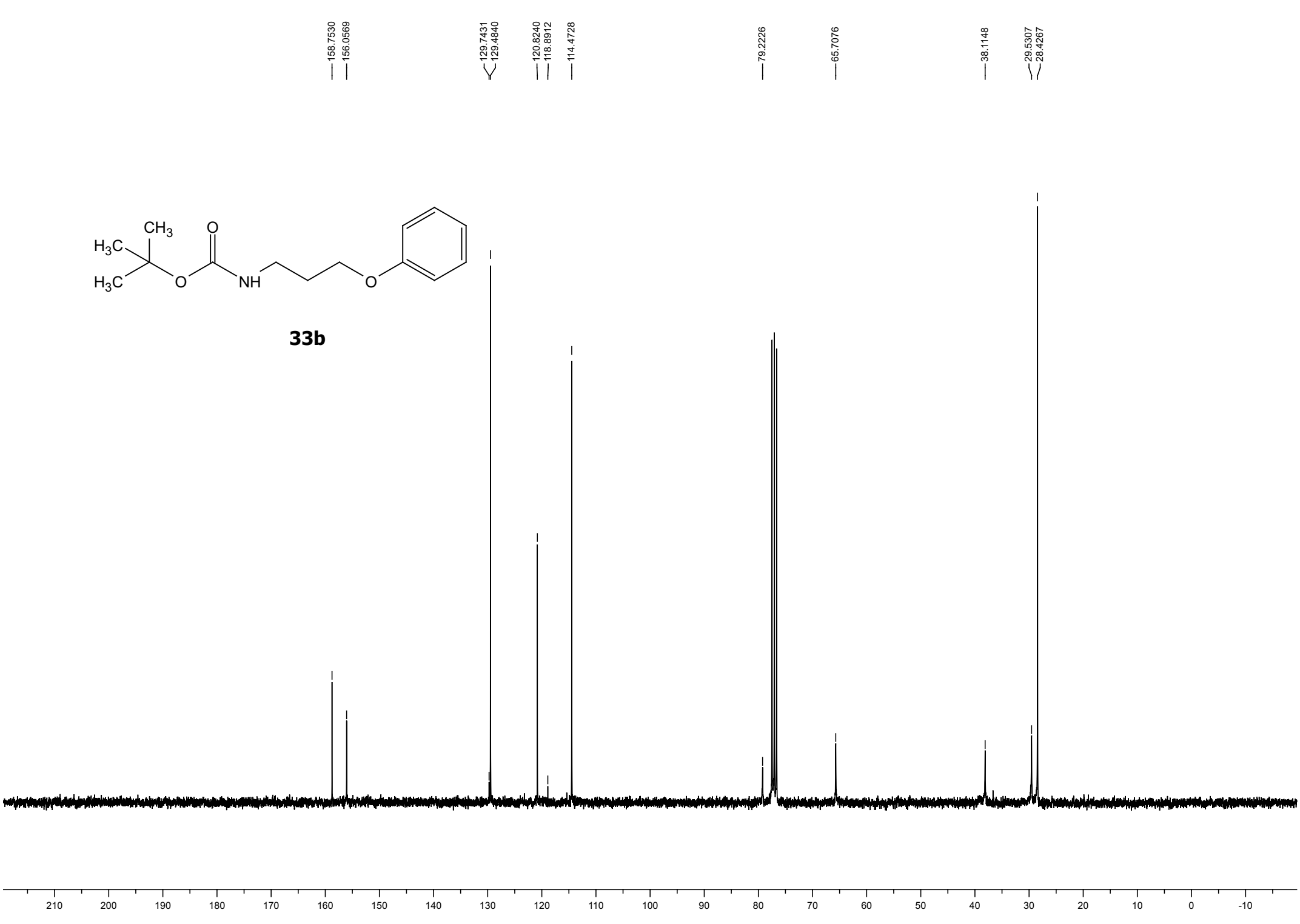
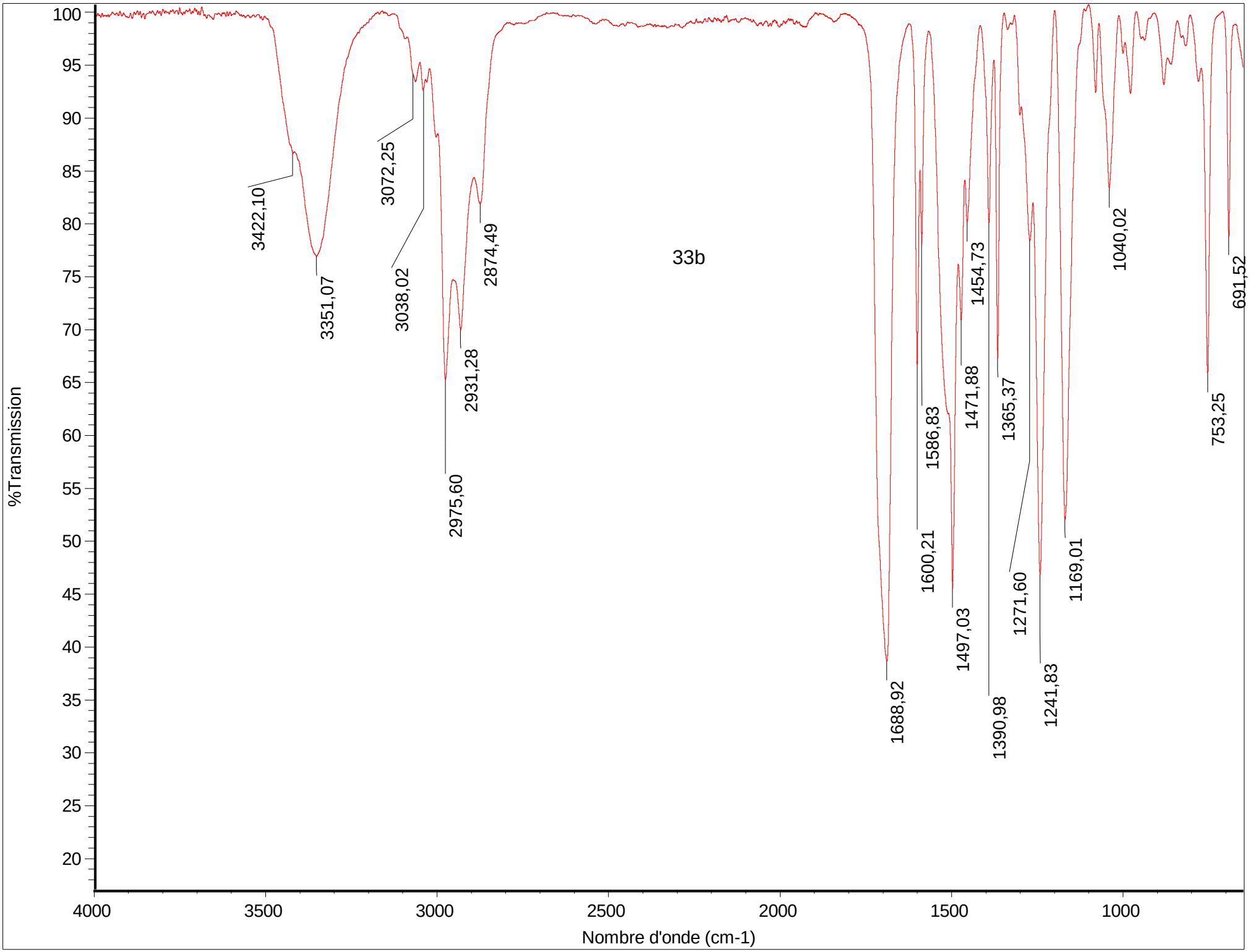
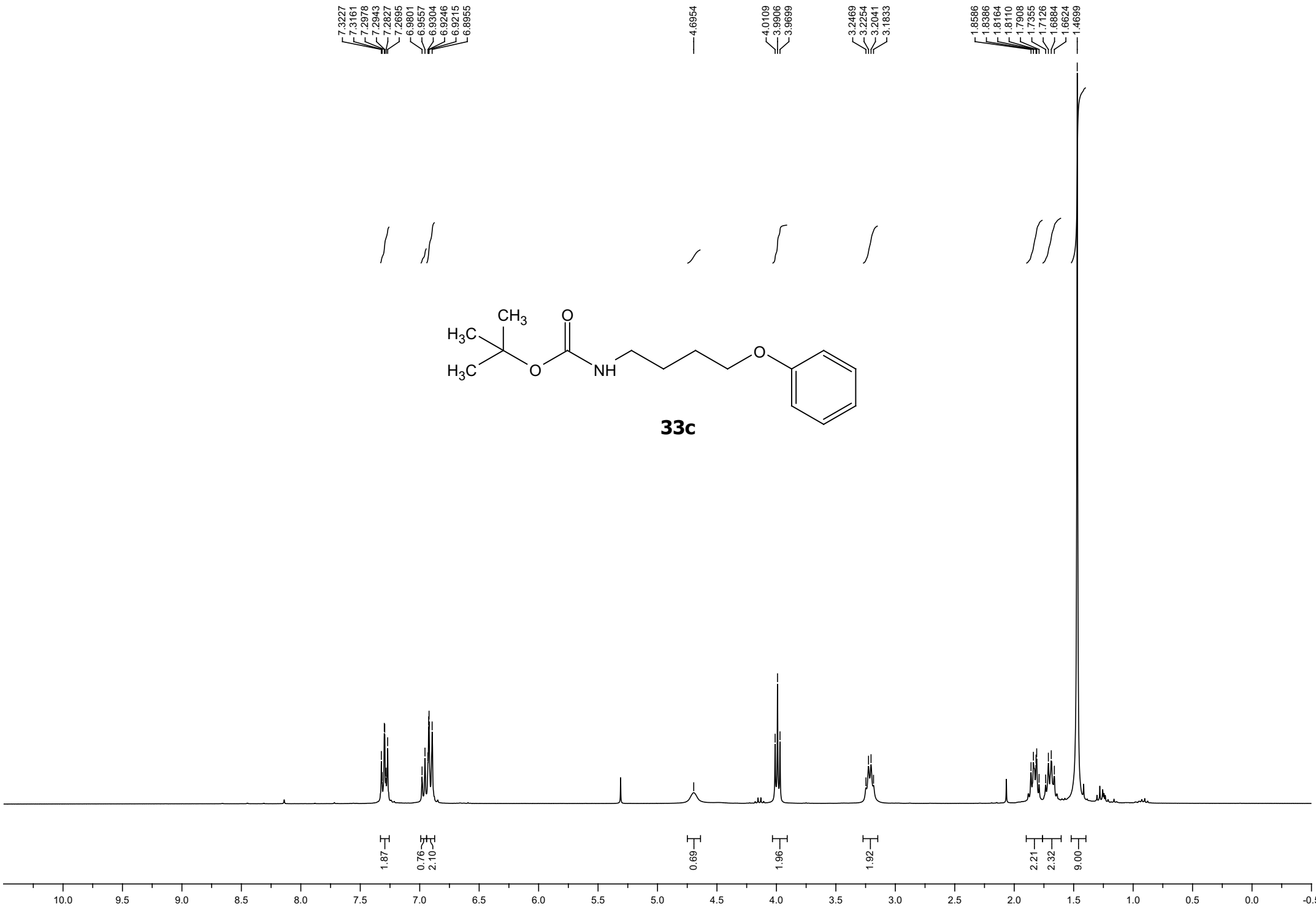
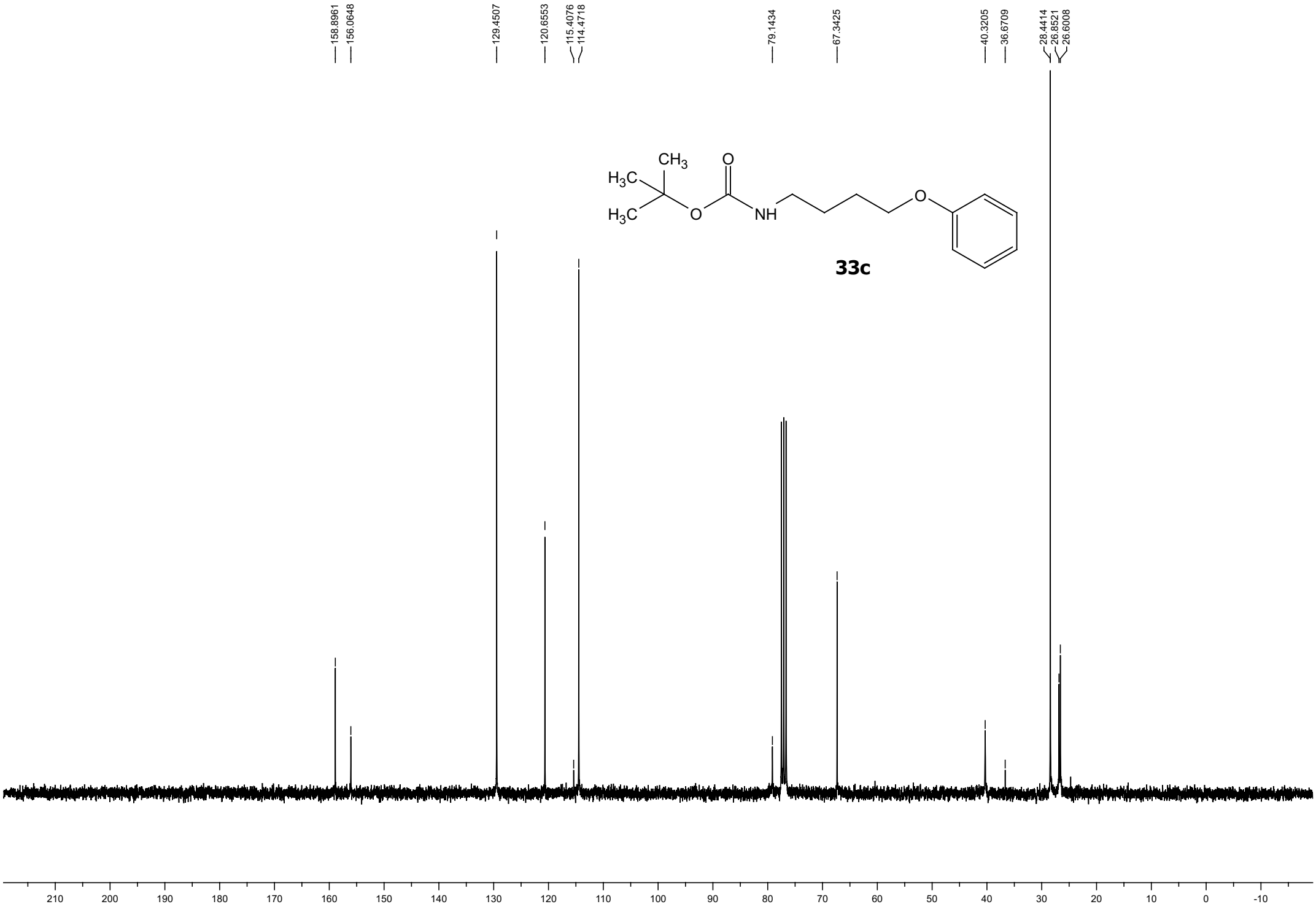
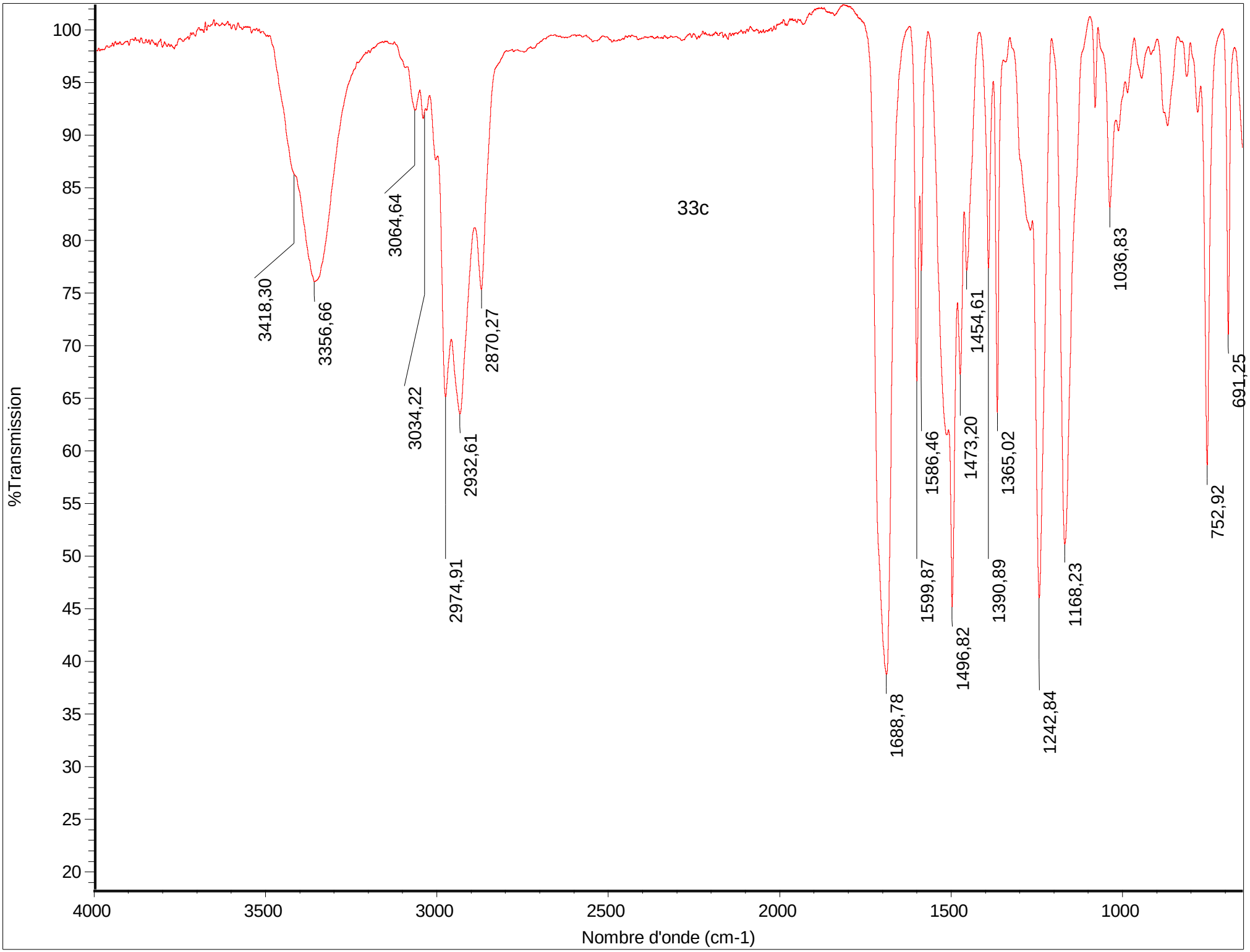
7.3042
7.2791
6.9943
6.9698
6.9301
6.9037
4.8241
4.0623
4.0425
4.0226
3.3845
3.3640
3.3432
3.3229
2.0674
2.0421
2.0215
2.0007
1.9799
1.9593
1.4669
CH3
O
H3C
H3C
O
NH
O
33b
1.96
0.71
2.09
0.75
1.95
1.89
1.98
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

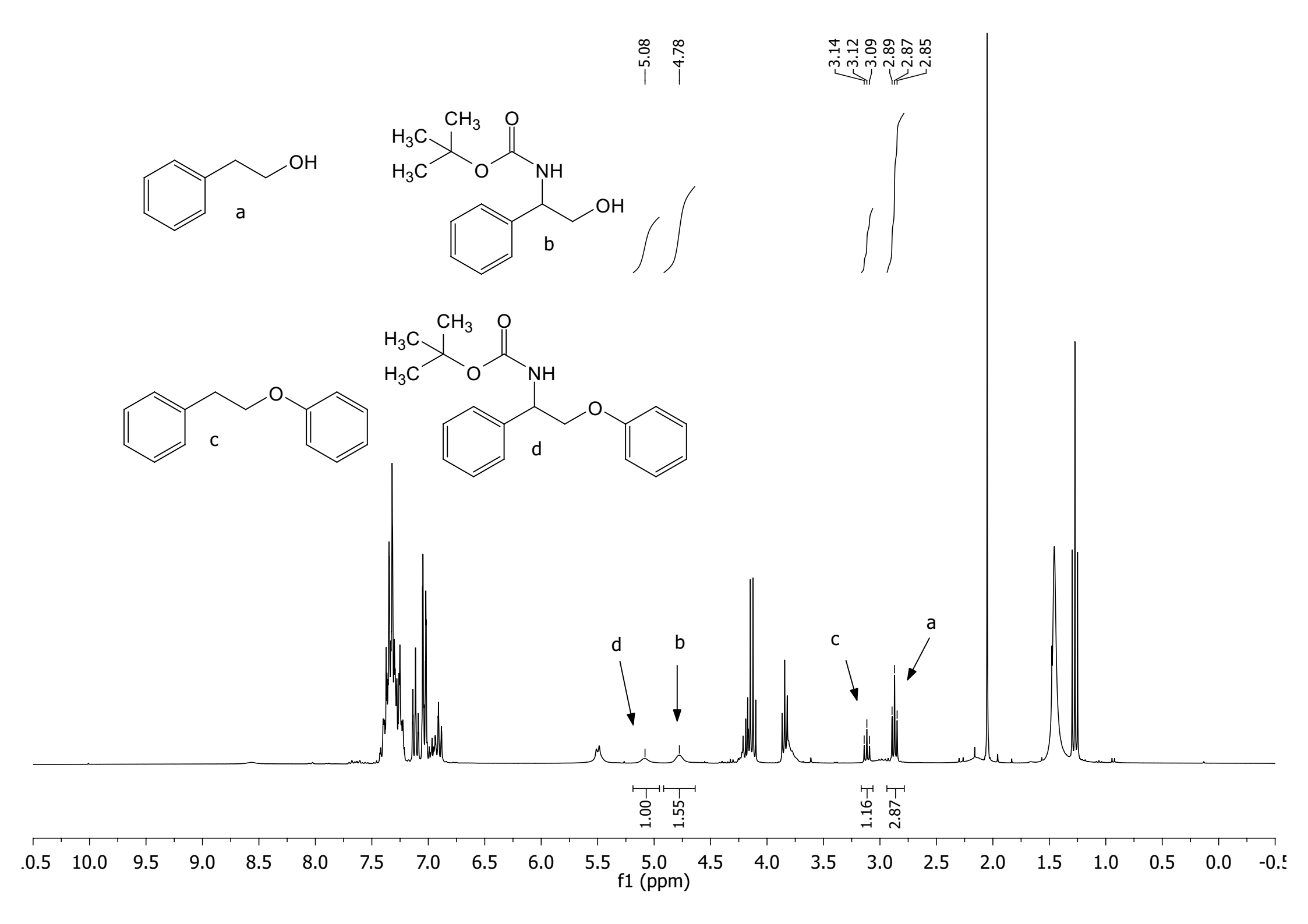

158.7530
156.0569
129.7431
129.4840
120.8240
118.8912
114.4728
79.2226
65.7076
38.1148
29.5307
28.4267
CH3
O
H3C
H3C
O
NH
O
33b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

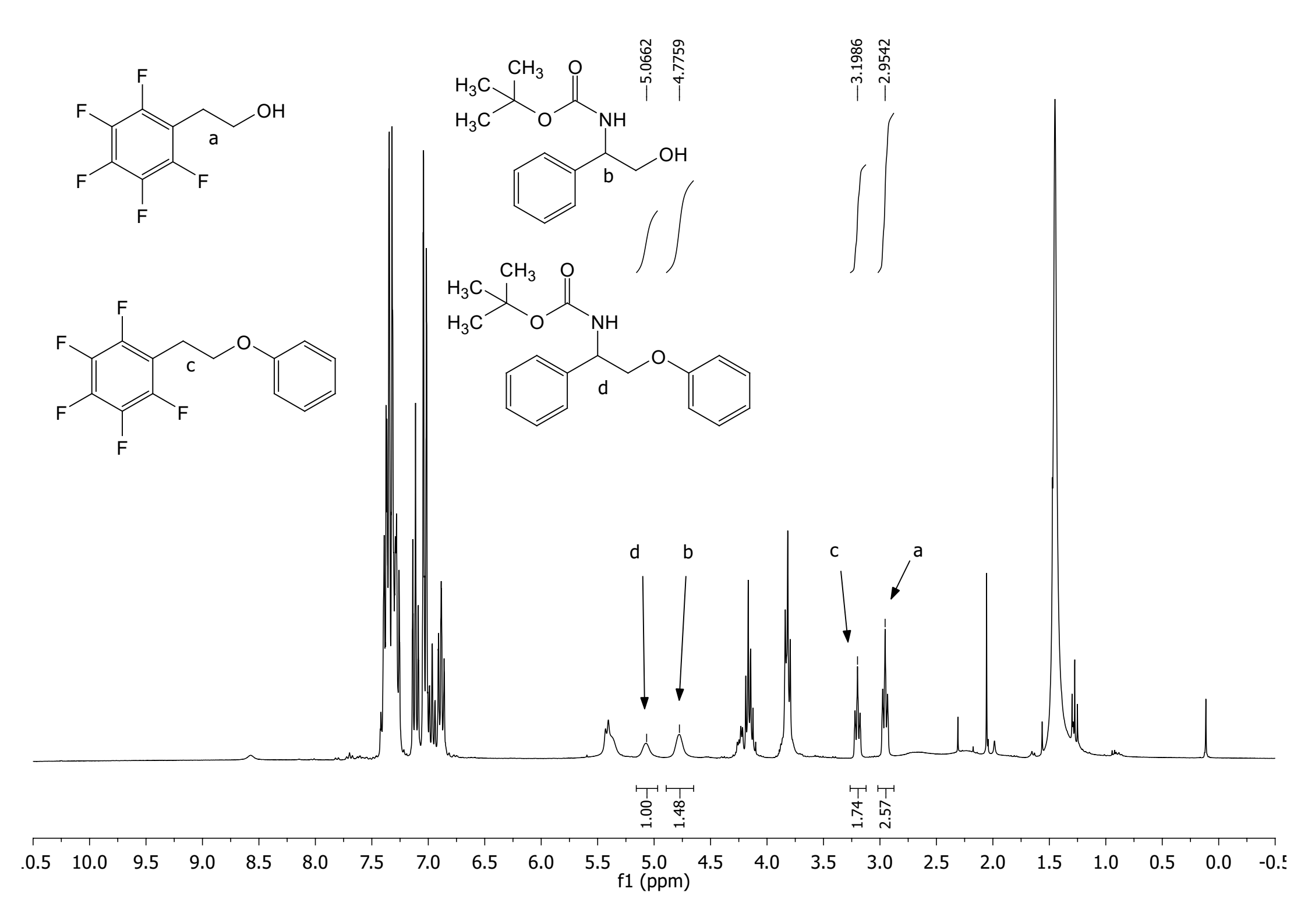

33b
%Transmission
Nombre d'onde (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
4000
3500
3000
2500
2000
1500
1000
3422,10
3351,07
3072,25
3038,02
2975,60
2931,28
2874,49
1688,92
1600,21
1586,83
1497,03
1471,88
1454,73
1390,98
1365,37
1271,60
1241,83
1169,01
1040,02
753,25
691,52


7.3227
7.3161
7.2978
7.2943
7.2827
7.2695
6.9801
6.9557
6.9304
6.9246
6.9215
6.8955
4.6954
4.0109
3.9906
3.9699
3.2469
3.2254
3.2041
3.1833
1.8586
1.8386
1.8164
1.8110
1.7908
1.7355
1.7126
1.6884
1.6624
1.4699
CH3
H3C
H3C
O
O
NH
O
33c
1.87
0.76
2.10
0.69
1.96
1.92
2.21
2.32
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


158.8961
156.0648
129.4507
120.6553
115.4076
114.4718
79.1434
67.3425
40.3205
36.6709
28.4414
26.8521
26.6008
CH3
H3C
H3C
O
O
NH
O
33c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


33c
%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
3418,30
3356,66
3064,64
3034,22
2974,91
2932,61
2870,27
1688,78
1599,87
1586,46
1496,82
1473,20
1454,61
1390,89
1365,02
1242,84
1168,23
1036,83
752,92
691,25


5.08
4.78
3.14
3.12
3.09
2.89
2.87
2.85
OH
a
CH3
O
H3C
H3C
O
NH
OH
b
c
O
CH3
O
H3C
H3C
O
NH
O
d
d
b
c
a
1.00
1.55
1.16
2.87
f1 (ppm)


F
F
F
F
F
OH
a
CH3
O
H3C
H3C
O
NH
OH
b
5.0662
4.7759
3.1986
2.9542
F
F
F
F
F
O
c
CH3
O
H3C
H3C
O
NH
O
d
d
b
c
a
1.00
1.48
1.74
2.57
.0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)