Experimental Section

All reagents were purchased from Sigma-Aldrich Chemical Company or Strem Chemicals and used without further purification. Toluene and diethyl ether were distilled over K, DMF over CaH_2 under atmosphere of argon. For testing the activity of precatalysts HPLC grade (Aldrich) solvents CH_2Cl_2, MeOH and toluene were used as recieved. Analytical thin-layer chromatography (TLC) was performed using silica gel 60 F_{254} precoated plates (0.25 mm thickness) with a fluorescent indicator. Visualization of TLC plates was performed by UV light either $KMnO_4$ or I_2 stains. Flash chromatography was performed using silica gel 60 (230-400 mesh). NMR spectra were recorded in $CDCl_3$ or CD_2Cl_2 on a Varian VNMRS 500 MHz spectrometer. The ^1H and ^{13}C chemical shifts are referenced to $SiMe_4$ (δ=0 ppm) or CD_2Cl_2 (δ=5.32 and 54 ppm respectively). The following abbreviations are used in reporting NMR data: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad), appt (apparent triplet). Coupling constants (*J*) are in Hz. Spectra are reported as follows: chemical shift (δ, ppm), multiplicity, integration, coupling constants (Hz). IR spectra were recorded on a Perkin-Elmer Spectrum One FTIR spectrometer with diamond ATR accessory. Wave numbers are in cm^{-1}. GC analyses were performed using Clarus 580 chromatograph. Micro-analyses were made using Vario EL III apparatus. Melting points were recorded on OptiMelt SRS with heating rate 4 °C/min. MS spectra were recorded by Quattro LC (triple quadrupole mass spectrometer).

N-(2,4,6-Trimethylphenyl)-1,2-diaminoethane was prepared according to Marshall's procedure.[1]

2-(Methylthio)benzoic acid (1c) was prepared according to the method reported in the literature.[2]

***N*-(2-(2,4,6-Trimethylphenylamino)ethyl)-2-(methylthio)benzamide**

2-(methylthio)benzoic acid (4.72 g, 28 mmol) was dissolved in MeCN (60 ml) and 1,1'-carbonyldiimidazole (CDI; 4.78 g, 29.4 mmol) was added portionwise. Resulting mixture was stirred for 30 min at 60 °C. Then the resulting mixture was placed in the ice cooled bath and stirred for 5 minutes. Next the *N*-(2,4,6-Trimethylphenyl)-1,2-diaminoethane (5 g, 28 mmol) was dissolved in MeCN (30 ml)

and added to the stirring mixture. The ice cooled bath was removed and the reaction mixture was left stirring at RT. After 10 min reaction mixture was placed in an oil bath and stirred for 2 h at 60 °C. Progress of the reaction was monitored by TLC (*c*-Hex:EtOc, 3:7). After full consumption of the substrates the reaction mixture was cooled down to RT and the solvent was evaporated delivering orange colored oil. The oil was washed with 5% $NaHCO_3$ (2x50ml) and brine (2x50 ml). The mixture was extracted with DCM (2x100 ml) and combined organic layers were dried over magnesium sulfate, filtered and concentrated. Purification of the crude mixture by silica-gel chromatography (*c*-Hex:EtOAc, 3:7) yielded the product as a white crystals (7.74 g, 84%), mp: 96-98 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.52 (dd, 1H, *J*=7.7, 1.4, Ar-H), 7.37 (dt, 1H, *J*=7.6, 1.5, Ar-H), 7.30 (dd, 1H, *J*=7.8, 0.9, Ar-H), 7.18 (dt, 1H, *J*=7.4, 1.1, Ar-H), 6.82 (s, 2H, Mes-H), 6.78 (bs, 1H, NH), 3.66 (q, 2H, CH_2), 3.19 (appt, 2H, CH_2), 2.46 (s, 3H, SCH_3), 2.27 (s, 6H, Mes-CH_3), 2.22 (s, 3H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=168.5, 142.5, 137.1, 135.0, 132.2, 130.8, 130.2, 129.7, 128.5, 127.1, 125.3, 48.0, 41.0, 20.7, 18.5, 16.7; IR (KBr): ν=3353, 3248, 3073, 2917, 2860, 1629, 1585, 1547, 1482, 1426, 1350,1312, 1219, 1161, 1108, 851, 796, 741, 731, 696 cm^{-1}; Anal. Calcd. for $C_{19}H_{24}N_2OS$: C, 69.47; H, 7.36; N, 8.53; S, 9.76; Found: C, 69.37; H, 7.36; N, 8.66; S, 9.74; MS (ESI): m/z 351 $[M+Na]^+$; HR-MS: calcd 351.1507, found 351.1518.

_N_-(2,4,6-Trimethylphenyl)-_N_^{2}-(2-(methylthio)benzyl)-1,2-diaminoethane (2c)

A solution of *N*-(2-(2,4,6-trimethylphenylamino)ethyl)-2-(methylthio)benzamide (4.63 g, 14.1 mmol) in THF (20 ml) was added dropwise to a vigorously stirred suspension of $LiAlH_4$ (2.25 g, 56.4 mmol) in THF (30 ml) at 0 ºC. Next the cooling bath was removed and the resulting mixture was left stirring at RT for 10 min and then placed in an oil bath and refluxed for 4 h. The progress of the reaction was monitored by TLC (*c*-Hex:EtOAc 4:1). After consumption of starting material the reaction mixture was cooled down in an ice cooling bath and the excess of $LiAlH_4$ was quenched with water (8 ml, dropwise addition), followed by NaOH (10% aq., 2.5 ml). Precipitate was filtered through Celite pad and washed with EtOAc. The mixture was extracted with EtOAc (2x30 ml) and combined organic layers were dried

over sodium sulfate, filtered and concentrated. Purification of the crude mixture by silica-gel chromatography (*c*-Hex:EtOAc, 7:3) yielded the product as a white crystals (3.3 g, 74%), mp: 85-87 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.31 (d, 1H, *J*=7.9, Ar-H), 7.27-7.22 (m, 2H, Ar-H), 7.12 (m, 1H, Ar-H), 6.80 (s, 2H, Mes-H), 3.91 (s, 2H, CH_2), 3.06 (t, 2H, *J*=5.8, ImdCH_2), 2.83 (t, 2H, *J*=5.8, ImdCH_2), 2.47 (s, 3H, SCH_3), 2.26 (s, 6H, Mes-CH_3), 2.21 (s, 3H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=143.9, 137.8, 137.6, 131.1, 129.8, 129.5, 129.1, 128.0, 125.9, 125.0, 51.6, 49.4, 48.3, 20.7, 18.6, 15.9; IR (KBr): ν=3350, 3291, 2842, 1586, 1484, 1463, 1439, 1334, 1243, 1143, 1112, 1045, 845, 793, 740, 687 cm^{-1}; Anal. Calcd. for $C_{19}H_{26}N_2S$: C, 72.56; H, 8.33; N, 8.91; S, 10.20; Found: C, 73.54; H, 8.36; N, 8.86; S, 10.42; MS (ESI): m/z 337.2 $[M+Na]^+$; HR-MS calcd 337.1714, found 337.1723.

2-(Dimethylamino)benzaldehyde (1b)

To the stirred solution of *N*,*N*-dimethylaniline (3 g, 24.6 mmol) in dry diethyl ether (37 ml), *n*-BuLi (2.5 M in hexane, 10.8 ml, 27.1 mmol) was added dropwise at RT. The resulting mixture was stirred for 30 h at 40 °C. After that an oil bath was replaced by the ice bath and DMF (dry, 2.5 ml) was added dropwise at 0 °C. The mixture was stirred for 15 min and then the bath was removed and the mixture was stirred for additional 30 min. Water (40 ml) was added and the organic phase was separated and washed with brine (2x20ml). Water phase was extracted with EtOAc and resulting organic phase was washed also with brine. Combined organic phases were dried over sodium sulfate, filtered and concentrated. Purification of the crude mixture by silica-gel chromatography (*c*-Hex:EtOAc, 9:1) yielded the product as yellow colored oil (2.21 g, 60%). Spectral data are in agreement with those reported in the literature.[3]

General procedure for the preparation of diamines via aldehyde-amine condensation and *in situ* reduction.

To the solution of an appropriate aldehyde (1 mmol) in methanol, a catalytic amount of formic acid and *N*-(2,4,6-Trimethylphenyl)-1,2-diaminoethane (1 mmol) were added. The resulting mixture was left

stirring for 48 h at RT. After that, $NaBH_4$ (5 mmol) was added in 5 portions (with 10 min intervals) and the mixture was left stirring for overnight. The solvent was evaporated *in vacuo*, the crude mixture was washed with saturated $NaHCO_3$ aq. solution until pH became slightly basic. The product was extracted with EtOAc (3x40 ml). Purification of the crude mixture was accomplished by silica-gel chromatography (*c*-Hex/EtOAc).

***N*^{1}-2,4,6-Trimethylphenyl-*N*^{2}-(2-methoxybenzyl)-1,2-diaminoethane (2a)**

To the solution of 2-methoxybenzaldehyde (2 g, 14.4 mmol) in MeOH (10 ml), formic acid (2 drops) and *N*-(2,4,6-trimethylphenyl)-1,2-diaminoethane (2.57 g, 14.4 mmol) were added. Reduction with $NaBH_4$ (2.87 g, 72 mmol). Purification by silica-gel chromatography (*c*-Hex:EtOAc 3:1, following by *c*-Hex/EtOAc 1:1) yielded a yellow oil (2.65g, 60%). ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.26-7.22 (m, 2H, Ar-H), 6.91(dt, 1H, *J*=7.4, 0.97, Ar-H), 6.87-6.85 (m, 1H, Ar-H), 6.8 (s, 2H, Mes-H), 3.83 (s, 2H, CH_2), 3.82 (s, 3H, OCH_3), 3.05-3.03 (m, 2H, ImdCH_2), 2.8 (m, 2H, ImdCH_2), 2.26 (s, 6H, Mes-CH_3), 2.22 (s, 3H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=157.8, 143.9, 131.1, 129.9, 129.7, 129.5, 128.4,120.5, 110.4, 55.4, 49.2, 48.9, 48.3, 20.7, 18.6; IR (KBr): ν=3359, 3276, 2905, 2833, 1599, 1586, 1488, 1442, 1302, 1241, 1158, 1101, 1050, 1027, 945, 928, 900, 861, 796, 755, 716 cm^{-1}; Anal. Calcd. for $C_{19}H_{26}N_2O$: C, 76.47; H, 8.78; N, 9.39; Found: C, 76.41; H, 9.02; N, 9.43; MS (ESI): m/z 321.2 $[M+Na]^+$; HR-MS calcd 321.1943, found 321.1946.

***N*^{1}-(2-(dimethylamino)benzyl)-*N*^{2}-mesityl-1,2-diaminoethane (2b)**

To the solution of 2-(dimethylamino)benzaldehyde (1 g, 6.7 mmol) in MeOH (10ml), formic acid (2 drops) and *N*-(2,4,6-Trimethylphenyl)-1,2-diaminoethane (1.19 g, 6.7 mmol) were added. Reduction with $NaBH_4$ (1.43 g, 36 mmol). Purification by silica-gel chromatography (*c*-Hex/EtOAc 3:1, following by *c*-Hex/EtOAc 1:1) yielded a yellow oil (1.31 g, 63%). ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.28 (dd, 1H, *J*=7.4, 1.7, Ar-H), 7.15 (dt, 1H, *J*=7.6, 1.7, Ar-H), 7.06-6.93 (m, 2H, Ar-H), 6.74 (s, 2H, Mes-H), 3.83 (s, 2H, CH_2), 2.98-2.95 (m, 2H, Imd-CH_2), 2.77-2.72 (m, 2H, Imd-CH_2), 2.62 (s, 6H, CH_3), 2.19 (s, 6H,

Mes-CH_3), 2.15 (s, 3H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=152.8, 144.0, 134.7, 131.1, 129.7, 129.5, 127.8, 123.4, 119.4, 50.1, 49.7, 48.4, 45.1, 20.7, 18.6; IR (KBr): ν=3026, 3276, 2912, 1603, 1485, 1453, 1372, 1304, 1234, 1114, 1028, 854, 734, 697 cm^{-1}; Anal. Calcd. for $C_{20}H_{29}N_3$: C, 77.12; H, 9.38; N, 13.49; Found: C, 76.86; H, 9.47; N, 13.62; MS (ESI): m/z 312.2 $[M+H]^+$; HR-MS calcd 312.2440, found 312.2430.

General procedure for the preparation of dihydroimidazolium salts by the ring closure of diamines

A mixture of diamine (1 mmol), triethyl orthoformate (10 mmol) and HCl in dioxane (4 M, 2.1 mmol) was heated at 100 °C for 4 h. Next the reaction mixture was cooled down to RT and the solvent was evaporated to 1/3 of its volume. Filtration and washing with cold triethyl orthoformate followed by washing with cold diethyl ether yielded pure imidazolium salt as white crystals which were dried *in vacuo* ($5x10^{-2}$ mbar).

3-(2,4,6-Trimethylphenyl)-1-(2-methoxybenzyl)-4,5-dihydro-1H-imidazol-3-ium chloride (3a)

Starting from *N*-(2,4,6-trimethylphenyl)-N^2-(2-methoxybenzyl)-1,2-diaminoethane (1.5 g, 5.03 mmol), triethylorthoformate (8.5 ml) and HCl (4 M solution, 2.64 ml) **3a** was obtained as a white crystals (1.31 g, 76%), mp: decomposes without melting in the range of 223-241 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ=9.62 (s, 1H, CH-Imd), 7.52 (dd, 1H, *J*=7.4, 1.78, Ar-H), 7.39-7.35 (m, 1H, Ar-H), 6.97 (dt, 1H, *J*=7.5, 1.1, Ar-H), 6.93 (d, 1H, *J*=8.4, Ar-H), 6.9 (s, 2H, Mes-H), 5.1 (s, 2H, CH_2), 4.1 (s, 4H, Imd-CH_2), 3.86 (s, 3H, OCH_3), 2.27 (s, 9H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=159.5, 158.0, 140.1, 135.3, 131.8, 131.0, 130.8, 129.9, 121.3, 120.9, 110.8, 55.6, 51.1, 48.3, 48.0, 21.0, 17.9; IR (KBr): ν=3365, 2970, 2917, 1643, 1601, 1512, 1496, 1447, 1367, 1287, 1267, 1248, 1216, 1164, 1141, 1050, 1020, 761 cm^{-1}; Anal. Calcd. for $C_{20}H_{25}ClN_2O$: C, 69.65; H, 7.31; Cl, 10.28; N, 8.12; Found: C, 68.45; H, 7.25; Cl, 10.63; N, 8.12; MS (ESI): m/z 309.2 $[M-Cl]^+$; HR-MS calcd 309.1967, found 309.1966.

1-(2-(dimethylamino)benzyl)-3-(2,4,6-trimethylphenyl)-4,5-dihydro-1H-imidazol-3-ium chloride (3b)

Starting from N^1-(2-(dimethylamino)benzyl)-N^2-(2,4,6-trimethylphenyl)-1,2-diaminoethane (1.2 g, 3.85 mmol), triethylorthoformate (6.8 ml), HCl (4 M solution, 2 ml) **3b** was obtained as white crystals (1.1 g, 80%), mp: 174-177 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ=9.96 (s, 1H, Imd-H), 7.40-7.35 (bs, 1H, Ar-H), 7.28 (t, 1H, *J*=7.3, Ar-H), 7.14-6.99 (bs, 2H, Ar-H), 6.83 (s, 2H, Mes-H), 5.3 (s, 2H, CH_2), 4.08-3.81 (m, 4H, Imd-CH_2), 2.61 (s, 6H, CH_3), 2.22 (s, 6H, Mes-CH_3), 2.20 (s, 3H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=159.7, 153.6, 140.2, 135.2, 130.9, 130.8, 130.1, 130.0, 127.3, 124.5, 120.2, 50.9, 48.6, 48.0, 45.5, 21.0, 18.0; IR (Kbr): ν=3395, 2937, 2762, 1644, 1492, 1448, 1361, 1306, 1264, 1226, 1097, 1044, 1010, 946, 849, 777, 758 cm^{-1}; Anal. Calcd. for $C_{21}H_{28}ClN_3$: C, 70.47; H, 7.89; Cl, 9.91; N, 11.74; Found: C, 70.49; H, 7.78; Cl, 10.18; N, 11.68; MS (ESI): m/z 322.2 $[M\text{-}Cl]^+$; HR-MS calcd 322.2283, found 322.2277.

3-(2,4,6-Trimethylphenyl)-1-(2-(methylthio)benzyl)-4,5-dihydro-1H-imidazol-3-ium chloride (3c)

Starting from N^1-(2,4,6-trimethylphenyl)-N^2-(2-(methylthio)benzyl)-1,2-diaminoethane (0.3 g, 0.954 mmol), triethylorthoformate (1.6 ml) and HCl (4 M solution, 0.5 ml), **3c** was obtained as white crystals (0.275 g, 80%), mp: decomposes without melting in the range of 192-246 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ=9.46 (s, 1H, CH-Imd), 7.6 (d, 1H, *J*=8.6, Ar-H), 7.38 (dt, 1H, *J*=7.6, 1.4, Ar-H), 7.28 (d, 1H, *J*=8.6, Ar-H), 7.22 (dt, 1H, *J*=7.5, 1.1, Ar-H), 6.90 (s, 2H, Mes-H), 5.24 (bs, 2H, CH_2), 4.12 (m, 4H, Imd-CH_2), 2.50 (s, 3H, SCH_3), 2.31 (s, 6H, Mes-CH_3), 2.27 (s, 3H, Mes-CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): δ=159.5, 140.3, 138.7, 135.4, 131.7, 130.7, 130.6, 130.1, 130.0, 126.8, 126.2, 51.0, 50.7, 48.3, 21.1, 18.1, 16.2; IR (KBr): ν=3447, 2994, 2899, 1640, 1508, 1470, 1447, 1267, 1214, 1179, 1142, 853, 768, 742 cm^{-1}; Anal. Calcd. for $C_{20}H_{25}ClN_2S$: C, 66.55; H, 6.98; Cl, 9.82; N, 7.76; S, 8.88; Found: C, 65.5; H, 7.02; Cl, 9.7; N, 7.64; S, 8.68; MS (ESI): m/z 325.2 $[M\text{-}Cl]^+$; HR-MS calcd 325.1739, found 325.1745.

General procedure for the preparation of precatalysts 4a, 4b and 4c

In a flame dried Schlenk vessel with the vigorously stirred suspension of imidazolium salt (1.1 mmol) in toluene (to obtain concentration of carbene c=0.02 mmol/ml), potassium *t*-amylate (1.7 M in toluene, 1.1 mmol) was added under Ar atmosphere at RT. After the solution became clear the indenylidene catalyst **M1** (1 mmol) was added at once and the reaction vessel was submerged into a preheated (65 °C) oil bath. The progress of the reaction was monitored by TLC (*c*-Hex:EtOAc 4:1). After 40 min the reaction mixture was cooled down to RT and the solvent was evaporated. Purification by silica-gel chromatography (*c*-Hex:EtOAc, 95:5, followed by *c*-Hex/EtOAc 9:1) yielded a carmine-colored film. Pentane was added to the resulting film and the flask was submerged in ultrasound bath for 15 min. Further decantation provided a carmine colored powder which was dried *in vacuo*.

{[1-(2,4,6-Trimethylphenyl)-3(2-methoxybenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene)(tricyclohexylphosphine)}ruthenium(II) (4a)

Prepared from imidazolium salt **3a** (200 mg, 0.580 mmol), potassium *t*-amylate (1.7 M in toluene, 350 µl, 598.4 mmol), **M1** (487 mg, 0.527 mmol) in toluene (29 ml). Purification by silica-gel chromatography (*c*-Hex:EtOAc 95:5). Carmine, microcrystalline solid (280 mg, 56%). ^{1}H NMR (500 MHz, $CDCl_3$): δ=8.42 (s, 1H , *J*=10, Ar-H), δ=8.42 (s, 1H , *J*=10, Ar-H), 7.6 (d, 1H, *J*=10, Ar-H), 7.38 (dt, 1H, *J*=7.6, 1.4, Ar-H), 7.28 (d, 1H, *J*=8.6, Ar-H), 7.22 (dt, 1H, *J*=7.5, 1.1, Ar-H), 6.38 (s, 1H, Mes-H), 5.99 (s, 1H, Mes-H), 5.78-5.72 (m, 2H, CH_2), 3.75-3.60 (m, 4H, Imd-CH_2), 3.91 (s, 3H, OMe), 2.39-2.32 (m, 3H, Cy), 2.11 (s, 3H, Mes-CH_3), 2.00 (s, 3H, Mes-CH_3), 1.87 (s, 3H, Mes-CH_3), 1.85-1.75 (m, 3H, Cy), 1.60-1.45 (m, 9H, Cy), 1.40-1.25 (m, 7H, Cy), 1.15-0.90 (m, 9H, Cy); ^{13}C NMR (125 MHz, $CDCl_3$): δ=159.5, 140.3, 138.7, 135.4, 131.7, 130.7, 130.6, 130.1, 130.0, 126.8, 126.2, 51.0, 50.7, 48.3, 21.1, 18.1, 16.2; IR (KBr): ν=3051, 2924, 2848, 1601,1588, 1537, 1489, 1448, 1354, 1266, 1247, 1173,1111, 1027, 885, 846,774, 753, 698 cm^{-1}; Anal. Calcd. for $C_{53}H_{67}Cl_2N_2OPRu$: C, 66.93; H, 7.10; Cl, 7.46; N, 2.95; Found: C, 67.02; H, 7.18; Cl, 7.52; N, 2.7; MS (ESI): m/z 951.1 $[M\text{-}Cl]^+$; HR-MS calcd 915.3735, found 915.3760.

{[1-(2,4,6-Trimethylphenyl)-3(2-*N*,*N*-dimethylaminobenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene)(tricyclohexylphosphine)}ruthenium(II) (4b)

Prepared from imidazolium salt **3b** (200mg, 0.559 mmol), potassium *t*-amylate (1.7 M in toluene, 330 µl, 561 mmol), **M1** (469 mg, 0.508 mmol) toluene (28 ml). Purification by silica-gel chromatography (*c*-Hex:EtOAc 95:5). Deep carmine microcrystalline solid (212 mg, 43%). ^{1}H NMR (500 MHz, $CDCl_3$): δ=8.44 (d, 1H , *J*=7.5, Ar-H), δ=8.18 (d, 1H , *J*=7.5, Ar-H), 7.74-7.72 (m, 2H, Ar-H), 7.53-7.45 (m, 1H, Ar-H), 7.45-7.41 (m, 2H, Ar-H), 7.37-7.33 (m, 1H, Ar-H), 7.25-7.22 (m, 3H, Ar-H), 7.19-7.15 (m, 2H, Ar-H), 7.05-7.03 (m, 1H, Ar-H), 6.38(s, 1H, Mes-H), 5.99 (s, 1H, Mes-H), 5.77-5.74 (m, 2H, CH_2), 3.70-3.58 (m, 4H, Imd-CH_2), 2.78(s, 6H, $N(CH_3)_2$), 2.39-2.32 (m, 3H, Cy) 2.12 (s, 3H, Mes-CH_3), 2.00 (s, 3H, Mes-CH_3), 1.86 (s, 3H, Mes-CH_3), 1.57-1.55 (m, 3H, Cy), 1.53-1.51 (m, 3H, Cy), 1.49-1.46 (m, 10H, Cy), 1.41-1.24 (m, 7H, Cy), 1.13-1.02 (m, 6H, Cy), 0.94-0.86 (m, 4H, Cy); ^{13}C NMR (125 MHz, $CDCl_3$): δ=291.3, 215.9, 214.4, 154.5, 144.6, 141.2, 137.3, 137.2, 136.7, 131.7, 131.2, 129.4, 129.2, 129.1, 128.9, 128.4, 128.1, 127.6, 126.9, 124.7, 120.4, 116.6, 52.4, 50.6, 48.9, 46.1, 33.2, 33.0, 30.1, 30.0, 28.4, 28.3, 28.2, 27.5, 27.0, 18.7; IR (KBr): ν=3052, 2922, 2849, 1731, 1598, 1537, 1488, 1447, 1354, 1319, 1265, 1027, 100, 845, 775, 753, 698 cm^{-1}; Anal. Calcd. for $C_{54}H_{70}Cl_2N_3PRu$: C, 67.27; H, 7.32; Cl, 7.35; N, 4.36; Found: C, 67.32; H, 7.43; Cl, 7.19; N, 4.30; MS (ESI): m/z 928.4 $[M-Cl]^+$; HR-MS calcd 928.4052, found 928.4058.

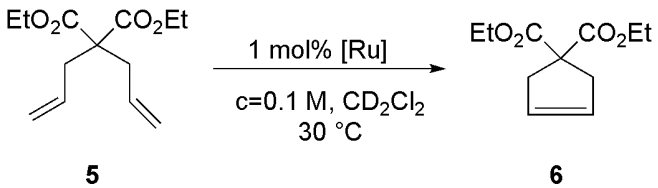
{[1-(2,4,6-Trimethylphenyl)-3(2-thiomethylbenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene)(tricyclohexylphosphine)}ruthenium(II) (4c)

Prepared from imidazolium salt **3c** (150 mg, 0.416 mmol), potassium *t*-amylate (1.7 M in toluene, 250 µl, 425 mmol), **M1** (349 mg, 0.378 mmol) in toluene (21 ml). Purification by silica-gel chromatography (*c*-Hex:EtOAc 95:5). Carmine microcrystalline solid (245 mg, 67%). ^{1}H NMR (500 MHz, $CDCl_3$): δ=8.41 (d, 1H, *J*=8, Ar-H), δ=8.15 (d, 1H, *J*=8, Ar-H), 7.72-7.70 (m, 2H, Ar-H), 7.52 (m, 1H, Ar-H), 7.42 (t, 2H, *J*=15.1, 7.7, Ar-H), 7.39-7.35 (m, 2H, Ar-H), 7.33-7.30 (m, 1H, Ar-H), 7.23 (m, 1H, Ar-H), 7.16 (s, 2H, Mes-H), 7.03 (d, 1H, Ar-H, *J*= 8.5), 6.39 (s, 1H, CH_2), 6.00 (bs, 1H, CH_2), 3.73-3.63 (m,

4H, Imd-CH_2), 2.54 (s, 3H, SCH_3), 2.38-2.31 (m, 3H, Cy), 2.12 (s, 3H, Mes-CH_3), 2.01 (s, 3H, Mes-CH_3), 1.87 (s, 3H, Mes-CH_3), 1.80-1.65 (m, 10H, Cy), 1.60-1.45 (m, 10H, Cy), 1.42-1.17 (m, 10H, Cy), 1.12-0.87 (m, 10H, Cy); ^{13}C NMR (125 MHz, $CDCl_3$): δ=291.4, 217.7, 216.3, 144.4, 141.1, 138.7, 137.7, 137.4, 137.1, 136.5, 134.4, 130.8, 129.4, 129.2, 129.1, 128.9, 128.4, 128.2, 127.7, 126.9, 126.5, 116.6, 48.9, 33.1, 32.8, 31.6, 30.0, 28.5, 28.3, 28.1, 27.5, 27.0, 21.3, 18.7, 18.6, 17.1; IR (KBr): ν=3052, 2920, 2848, 1608,1588, 1536, 1488, 1444, 1353, 1267, 1218, 1027, 846, 774, 752, 697 cm^{-1}; Anal. Calcd. for $C_{53}H_{67}Cl_2N_2SPRu$: C, 65.82; H, 6.98; Cl, 7.33; N, 2.90; S, 3.32; Found: C, 65.72; H, 6.84; Cl, 7.13; N, 2.78; S, 3.55; MS (ESI): m/z 931.4 $[M-Cl]^+$; HR-MS calcd 931.3506, found 931.3504.

General procedure for kinetic studies:

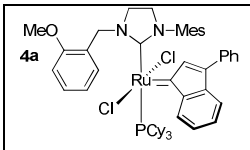
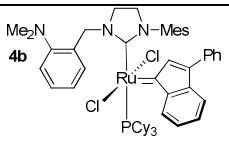
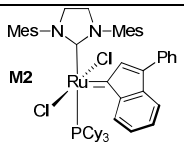
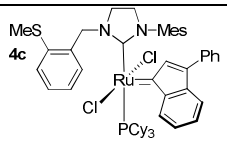
On the benchtop under air, a NMR tube equipped with a septum was filled with the diethyl diallylmalonate **5** (16.8 mg, 0.07 mmol) and non-distilled, non-degassed CD_2Cl_2 (600 µL) was added. The sample was equilibrated at 30 °C in the NMR probe. Then it was locked and shimmed. Stock solution of precatalyst was prepared in the following manner: precatalyst (3.5 µmol) was weighed in the 2 ml vial, then it was closed with the rubber septum and CD_2Cl_2 (500 µL) was injected. An aliquot of the precatalyst (100 µL, 0.7 µmol) was taken from the stock solution and injected through the septum into a solution of substrate. The reaction progress was monitored by the periodical acquisition of data over 1.5 h. The conversion of **5** to **6** was determined by comparing the ratio of the integrals of the methylene protons in the starting material, δ 2.67-2.64 , with those in the product, δ 2.93-2.88. Conversion was calculated according to the equation: Conv. (%) = [P] x 100%/[P]+[S]



5 **6**

Scheme S1. RCM of diethyl diallylmalonate

Table S1. Conversion to disubstituted olefin product **6** using **4a**, **4b**, **M2** and **4c**

							
Time (min)	Conversion (%)	Time (min)	Conversion (%)	Time (min)	Conversion (%)	Time (min)	Conversion (%)
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2.77	3.0	3.17	9.8	7.22	4.7	5.67	1.9
2.82	5.0	3.92	13.3	7.97	5.2	6.42	2.1
3.67	7.6	4.77	17.4	8.82	5.6	7.27	2.2
4.64	12.0	5.74	21.0	9.79	6.6	8.24	2.2
5.76	15.3	6.86	25.5	10.91	6.9	9.36	2.3
7.04	18.9	8.14	30.2	12.19	7.5	10.64	2.7
8.52	22.8	9.62	35.3	13.67	8.6	12.12	2.8
10.26	27.4	11.36	40.5	15.41	10.1	13.86	3.0
12.29	32.4	13.39	46.5	17.44	10.6	15.89	3.2
14.67	37.9	15.77	52.1	19.82	12.4	18.27	3.5
17.49	43.8	18.59	58.1	22.64	13.4	21.09	3.6
20.82	50.3	21.92	63.7	25.97	14.9	24.42	3.7
24.77	57.7	25.87	69.6	29.92	17.0	28.37	3.9
29.45	64.3	30.55	74.9	34.60	19.6	33.05	4.2
35.02	71.9	36.12	79.5	40.17	21.4	38.62	4.6
41.65	77.6	42.75	83.2	46.80	23.7	45.25	4.9
49.57	83.7	50.67	86.0	54.72	26.5	53.17	5.5
59.02	88.6	60.12	88.5	64.17	29.8	62.62	5.6
70.43	91.9	71.53	90.1	75.58	33.3	74.03	6.1
84.16	94.3	85.26	91.6	89.31	37.3	87.76	6.6
100.54	95.6	101.64	92.6	105.69	42.0	104.14	6.9

Preparative RCM, CM and Ene-Yne Reactions

Ene-Yne metathesis of [1-(Alliloksy)-1-fenylo-2-propynylo]benzene (7)

A round bottom flask (25 ml) was equipped with a stirring bar and charged with the substrate **7** (200 mg, 0.805 mmol), followed by the addition of DCM (HPLC grade, 7 ml). In a 2 ml vial the precatalyst **4b** (2 mol%, 15.5 mg, 0.0161 mmol) was weighed and 1 ml of DCM (HPLC grade) was added and the resulting solution of precatalyst was transfered to the vigorously stirred substrate solution. The resulting mixtrure was left stirring at 30 °C. Progress of the reaction was monitored by GC. Aliquots were taken every 30 min. After completion of the reaction the solvent was evaporated and the crude product was purified via column (*c*-Hex:EtOAc 39:1) providing a colourless oil (192 mg, 96%). ^{1}H and ^{13}C NMR spectra are in agreement with those previously reported.[4]

Ring Closing Metathesis of (S)-tert-butyl 2-(diallylcarbamoyl)pyrrolidine-1-carboxylate (9)

A round bottom flask (25 ml) was equipped with a stirring bar and charged with the substrate **9** (196 mg, 0.666 mmol), followed by the addition of toluene (HPLC grade, 5.6 ml). In a 2 ml vial the precatalyst **4b**, (1 mol%, 6.4 mg, 6.66 μmol) was weighed and toluene (HPLC grade, 1 ml) was added and the resulting solution of precatalyst was transfered to the vigorously stirred substrate solution. The resulting mixture was left stirring at 50 °C. Progress of the reaction was monitored by GC. Aliquots were taken every 30 min. After completion of the reaction the solvent was evaporated and the crude product was purified via column chromatography (*c*-Hex:EtOAc 1:1) providing a brownish-coloured oil (162 mg, 91%). ^{1}H and ^{13}C NMR spectra are in agreement with those previously reported.[5]

Cross metathesis of allylbenzene (11) with *cis*-1,4-diacetoxy-2-butene (12)

A round bottom flask (25 ml) was equipped with a stirring bar and charged with the substrates allylbenzene **11** (100 mg, 0.829 mmol) and *cis*-1,4-diacetoxy-2-butene **12** (286 mg, 1.66 mmol) followed by the addition of DCM (HPLC grade, 7 ml). In a 2 ml vial the precatalyst **4b** (20mg, 0.0207 mmol, 2.5 mol%) was weighed and DCM (HPLC grade, 1 ml) was added. The resulting solution of precatalyst was transfered to the vigorously stirred substrate solution and left stirring at 30 °C. After 20 h the reaction mixture was cooled down and the solvent was evaporated. The crude product was purified via column chromatography (*c*-Hex:EtOAc 9:1) providing a colourless oil (114 mg, 74%, *E*/*Z* 9:1). ^{1}H and ^{13}C NMR spectra are in agreement with those previously reported.[6]

Ring Closing Metathesis of *N*,*N*-di(but-3-enyl)-4-methylbenzenesulfonamide (14)

A round bottom flask (25 ml) was equipped with a stirring bar and charged with the substrate **14** (200 mg, 0.716 mmol), followed by the addition of DCM (HPLC grade, 6 ml). In a 2 ml vial the precatalyst **4b** (6.9 mg, 7.16 μmol, 1 mol%) was weighed and DCM (HPLC grade, 1 ml) was added. The resulting solution of precatalyst was transfered to the vigorously stirred substrate solution and left stirring at 30 °C. Progress of the reaction was monitored by GC. Aliquots were taken every 30 min. After completion

of the reaction the solvent was evaporated and the crude product was purified via column chromatography (*c*-Hex:EtOAc 9:1) providing a colourless oil (185 mg, 97%). ^{1}H and ^{13}C NMR spectra are in agreement with those previously reported.[7]

X-ray measurement details

The collection of the X-ray diffraction data for **4a** was performed on a Kuma KM4CCD - axis diffractometer with the graphite-monochromated MoK radiation and equipped with an Oxford Cryosystems nitrogen gas-flow apparatus. The crystal was positioned at 50 mm from the KM4CCD camera. 540 frames were measured at 1 ° intervals with a counting time of 10 sec. The data were corrected for Lorentz and polarization effects. The multi-scan absorption correction was applied. Data reduction and analysis were carried out with the Oxford Diffraction Ltd. programs.[7]

The structure was solved by direct methods[8] and refined using SHELXL.[9] The refinement was based on F^2 for all reflections except those with negative F^2. Weighted R factors (wR) and all goodness-of-fit S values are based on F^2. Conventional R factors are based on F with F set to zero for negative F^2. The $Fo^2>2(Fo^2)$ criterion was used only for calculating R factors and is not relevant to the choice of reflections for the refinement. The R factors based on F^2 are about twice as large as those based on F. Scattering factors were taken from Tables 6.1.1.4 and 4.2.4.2 in Ref. 9.

Table S5. X-ray measurement details of precatalyst **4a**

Chemical formula	$C_{53}H_{67}Cl_2N_2OPRu$
M_r	951.03
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, *b*, *c* (Å)	12.7022 (3), 15.6607 (3), 23.8898 (5)
V (Å^3)	4752.3 (2)
Z	4
Radiation type	Sealed tube Mo, λ = 0.71073 Å
μ (mm^{-1})	0.52
Crystal size (mm)	0.40 × 0.30 × 0.30
Data collection	
Diffractometer	KUMA4 CCD diffractometer
Absorption correction	Multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.15 (release 03-08-2011 CrysAlis171

	.NET) (compiled Aug 3 2011,13:03:54) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.820, 0.861
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	116009, 11014, 9508
R_{int}	0.063
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.140, 1.22
No. of reflections	11014
No. of parameters	545
No. of restraints	0
H-atom treatment	H-atom parameters constrained
$\rangle\Delta_{max}$, $\rangle\Delta_{min}$ (e Å^{-3})	0.73, -1.29
Absolute structure	Flack H D (1983), Acta Cryst. A39, 876-881
Flack parameter	-0.01 (3)

Computer programs: *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.7 (release 14-02-2011 CrysAlis171 .NET) (compiled Feb 15 2011,09:34:54), *SHELXS97* (Sheldrick, 1990), *SHELXL97* (Sheldrick, 1997), *WinGX*, *SHELXTL*, Bruker.

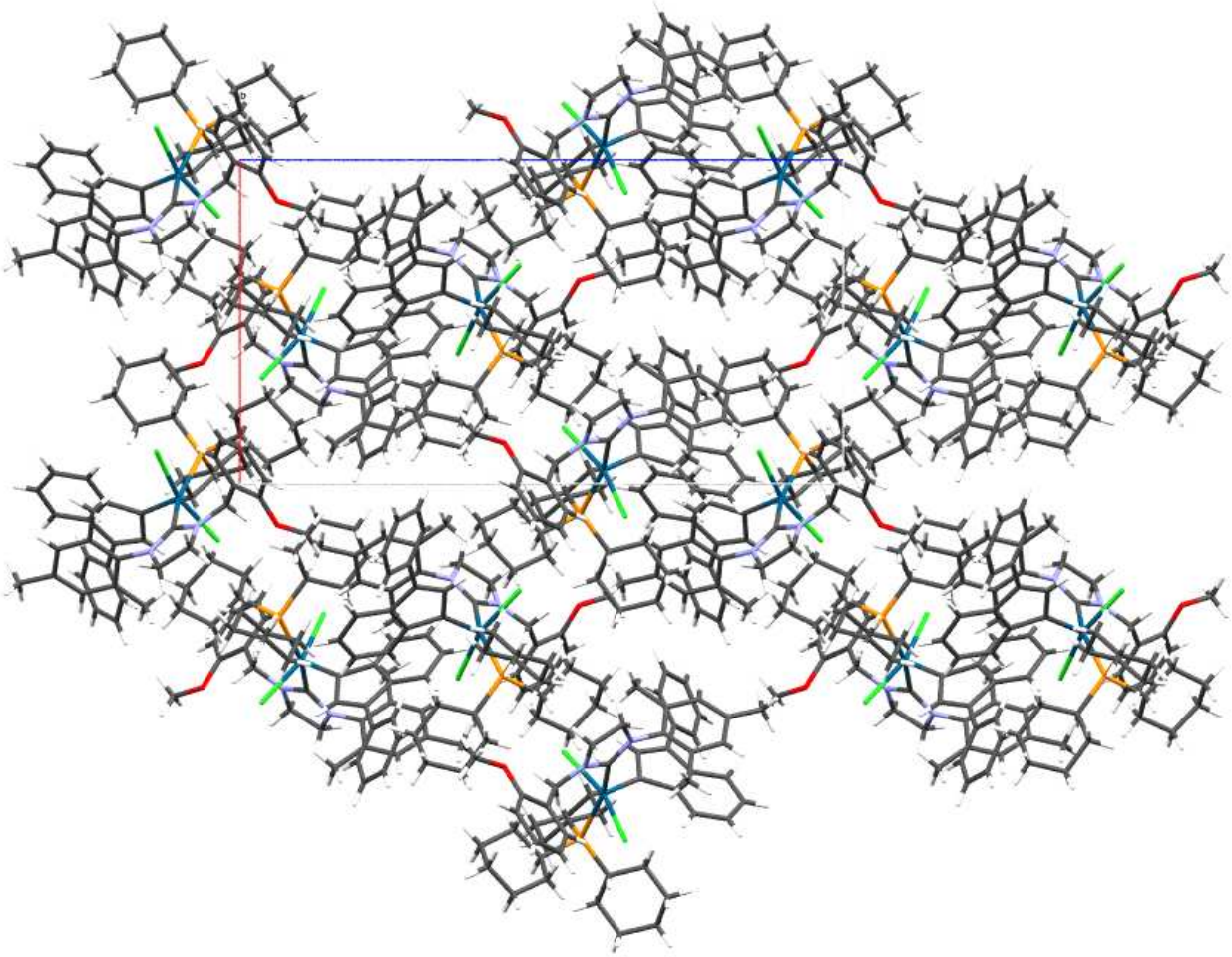

Figure S2. Packing of **4a** molecules in the crystal lattice – projection along the Y axis

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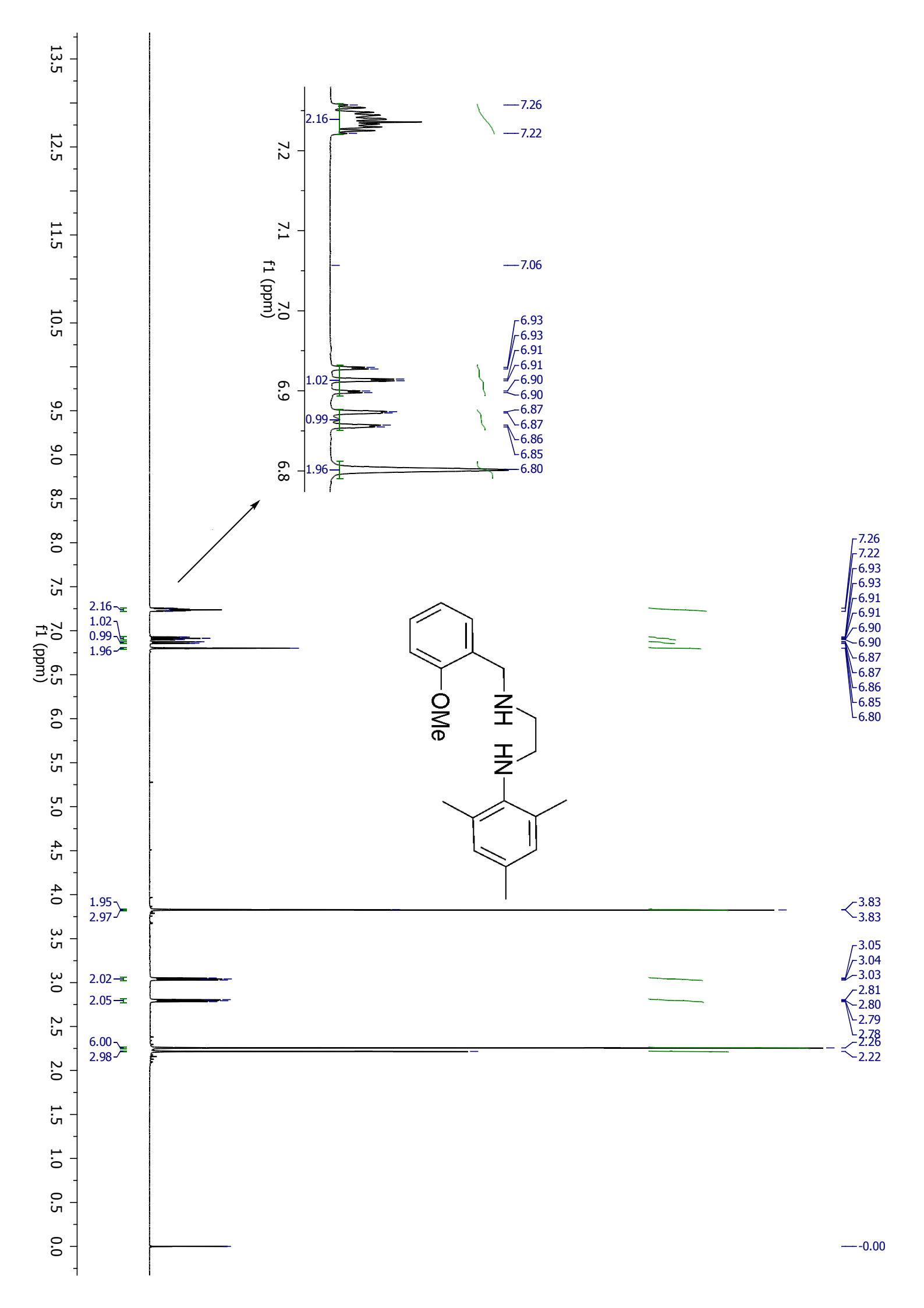
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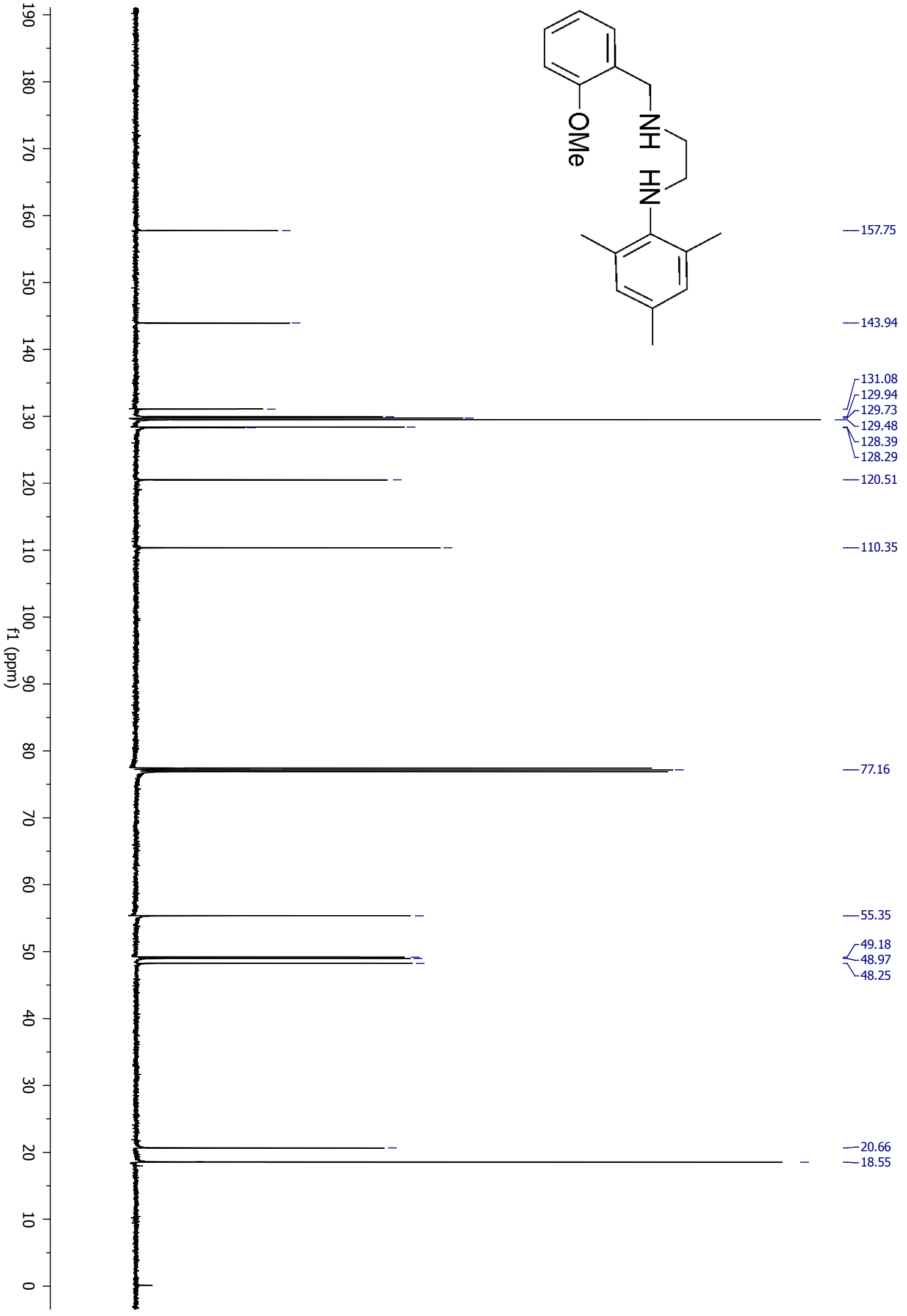
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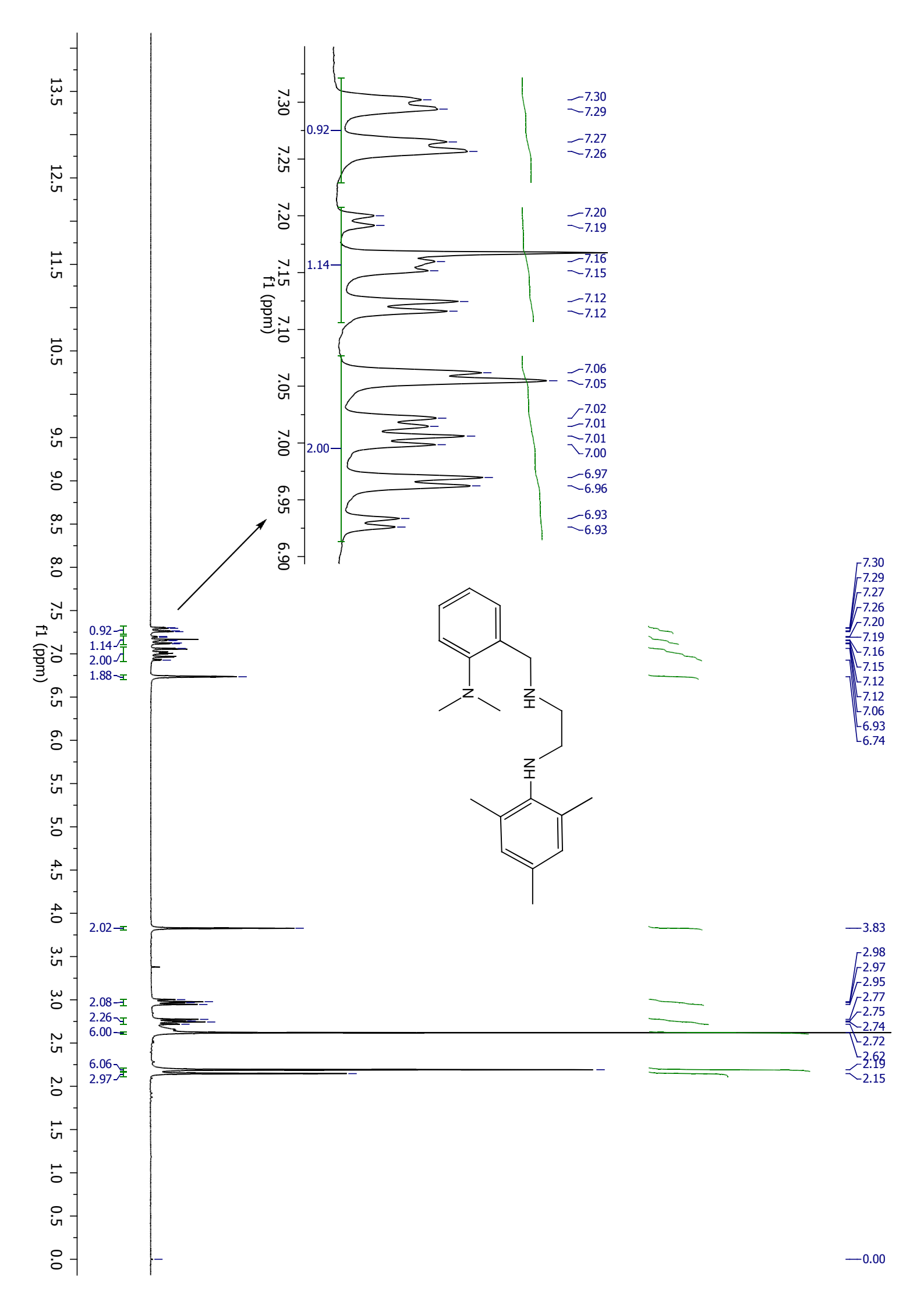
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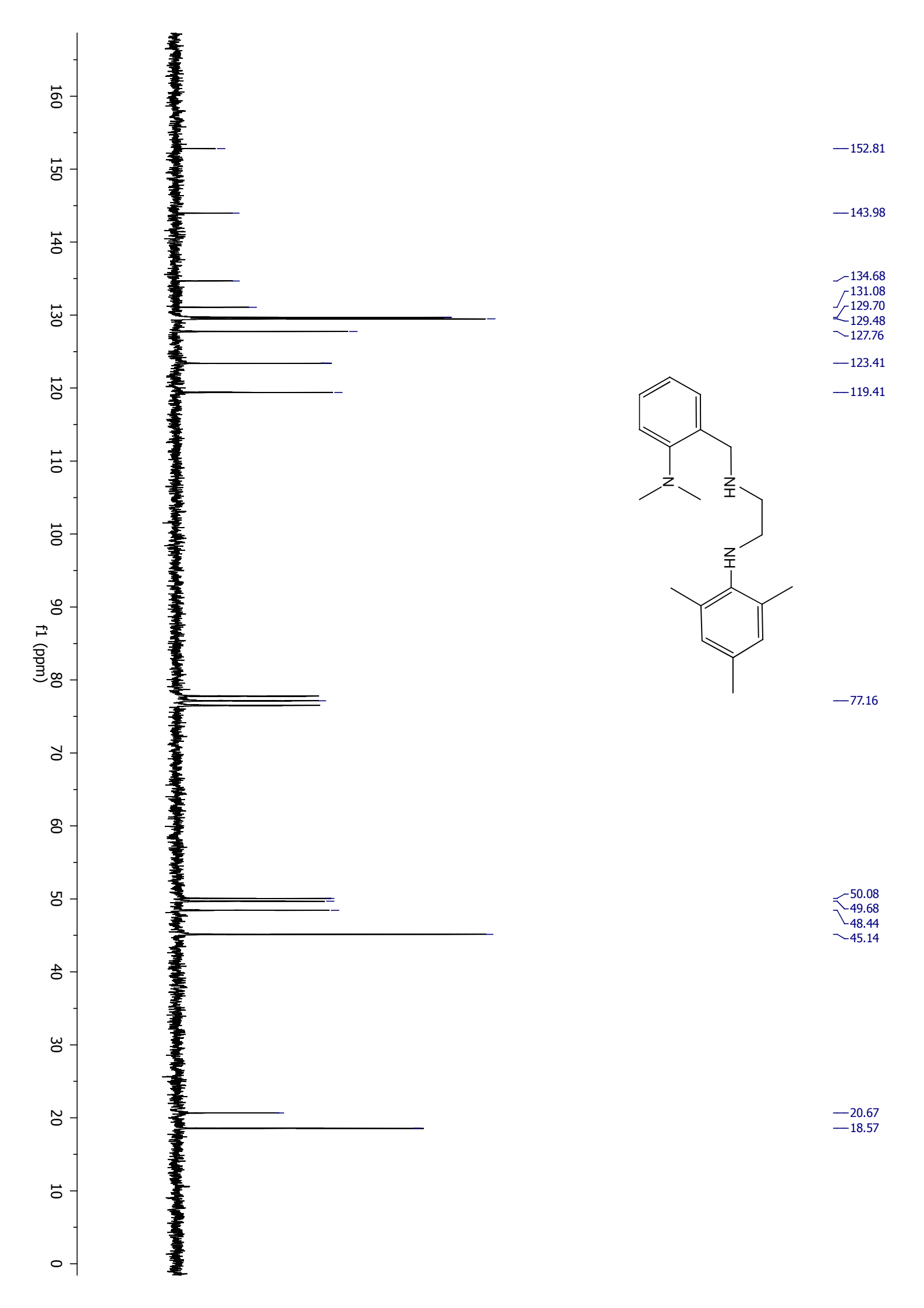
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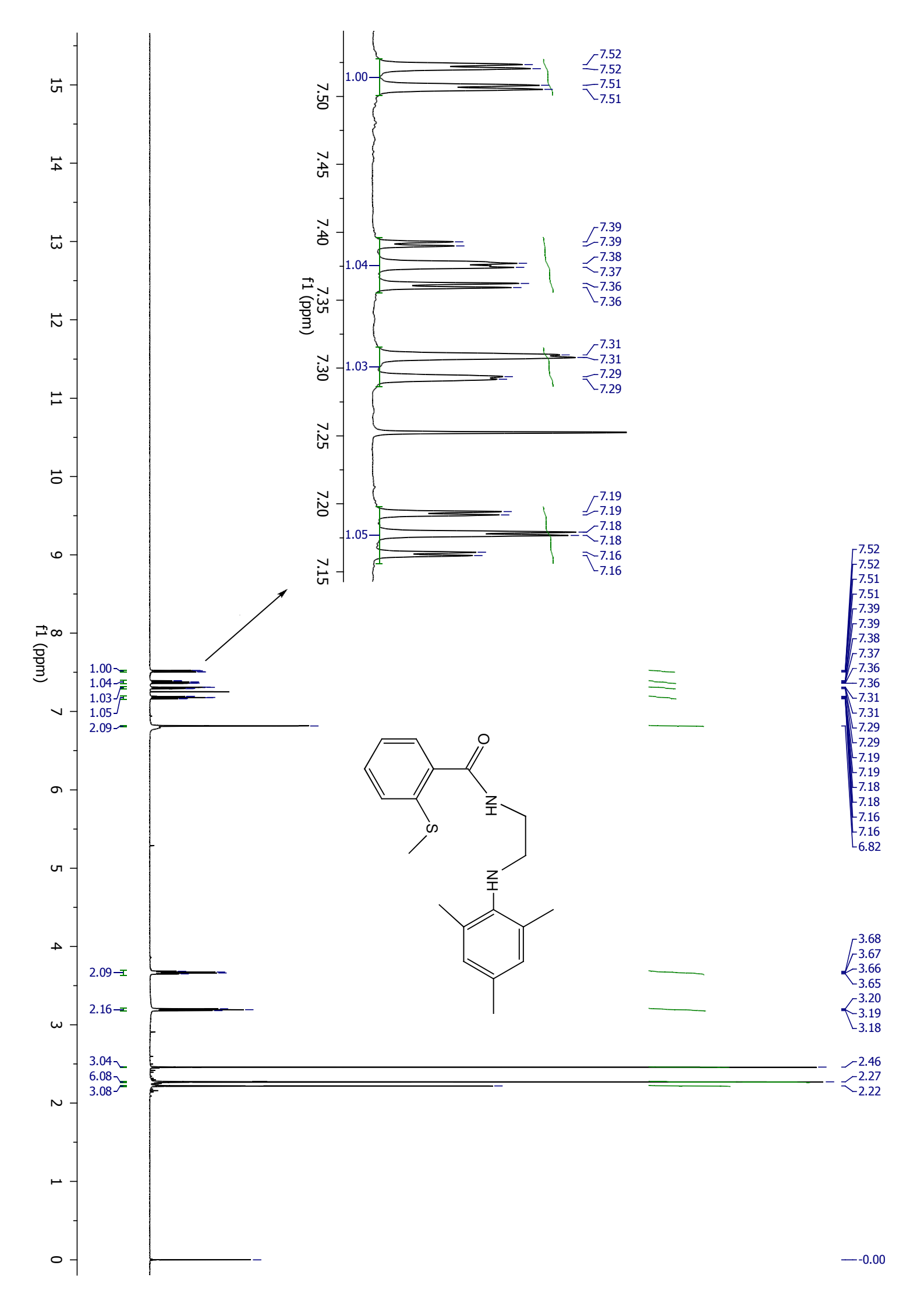
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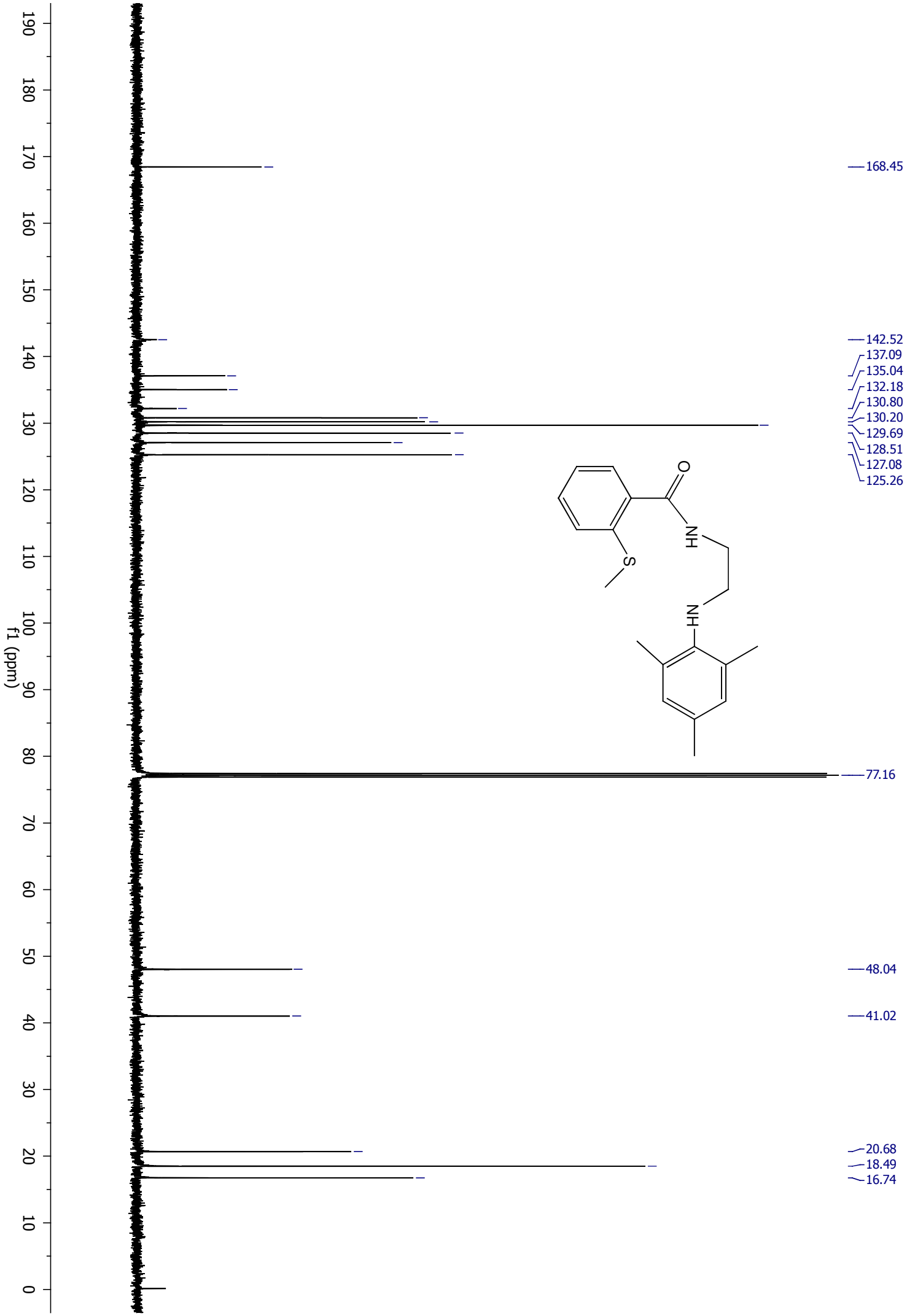
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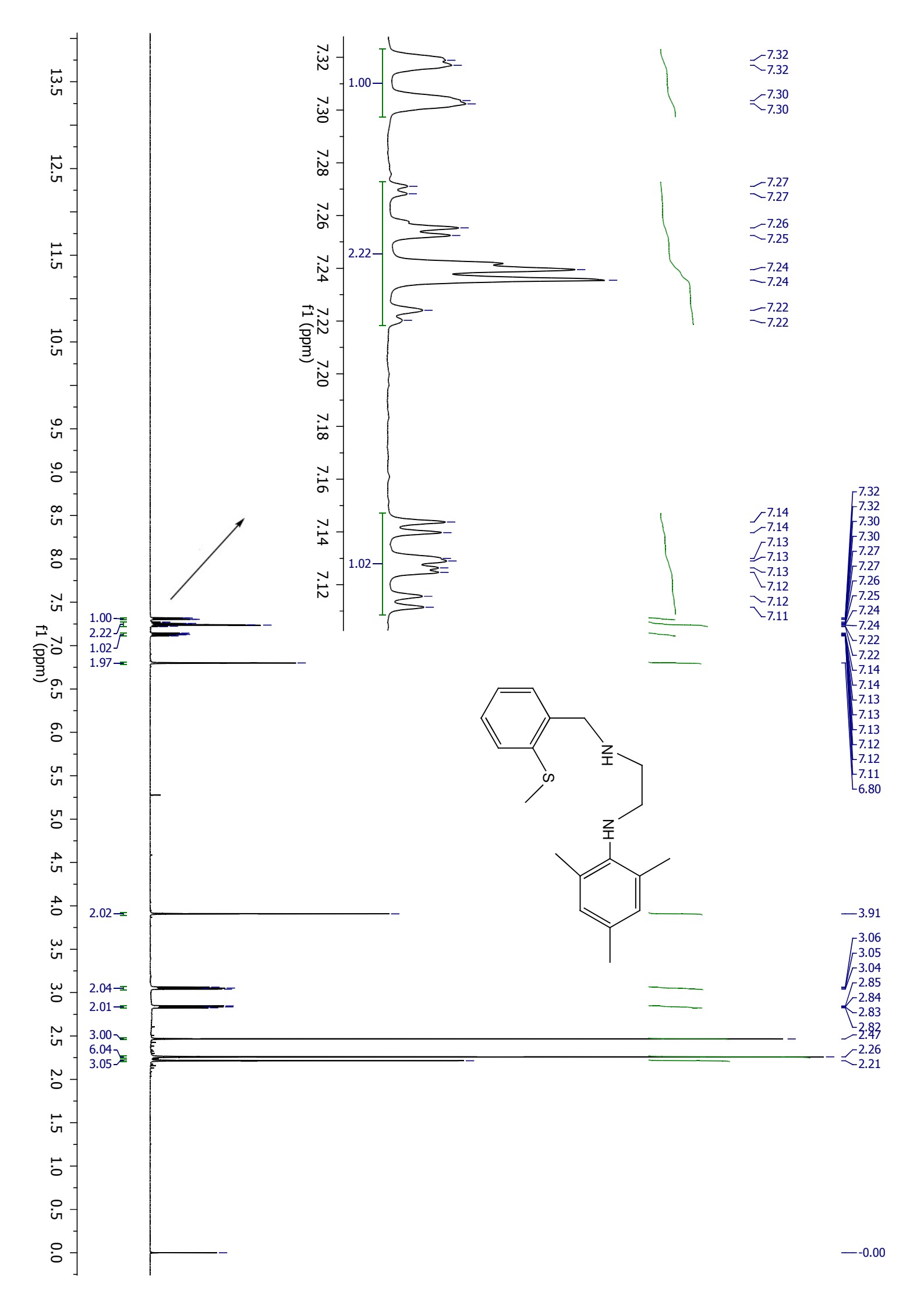
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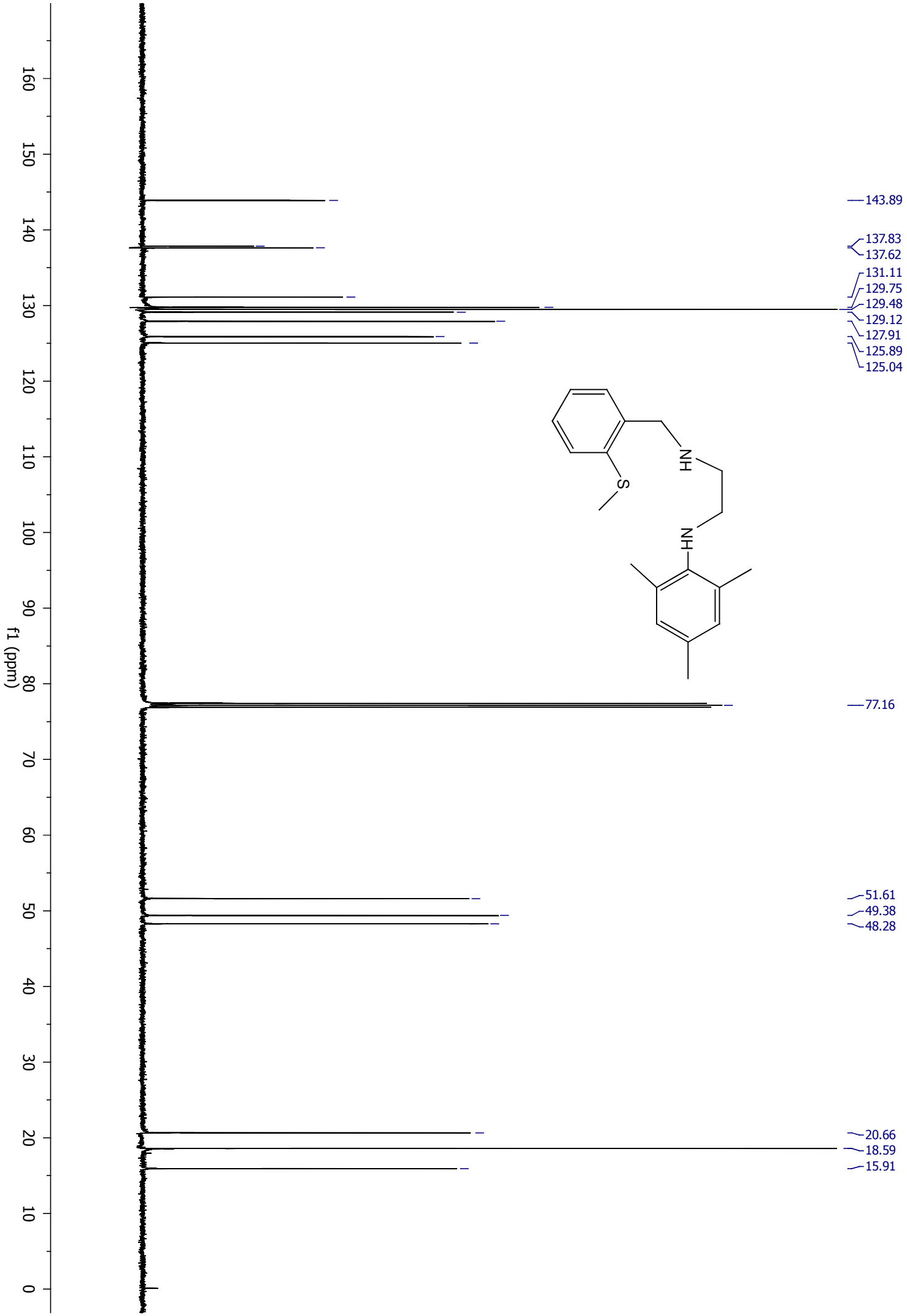
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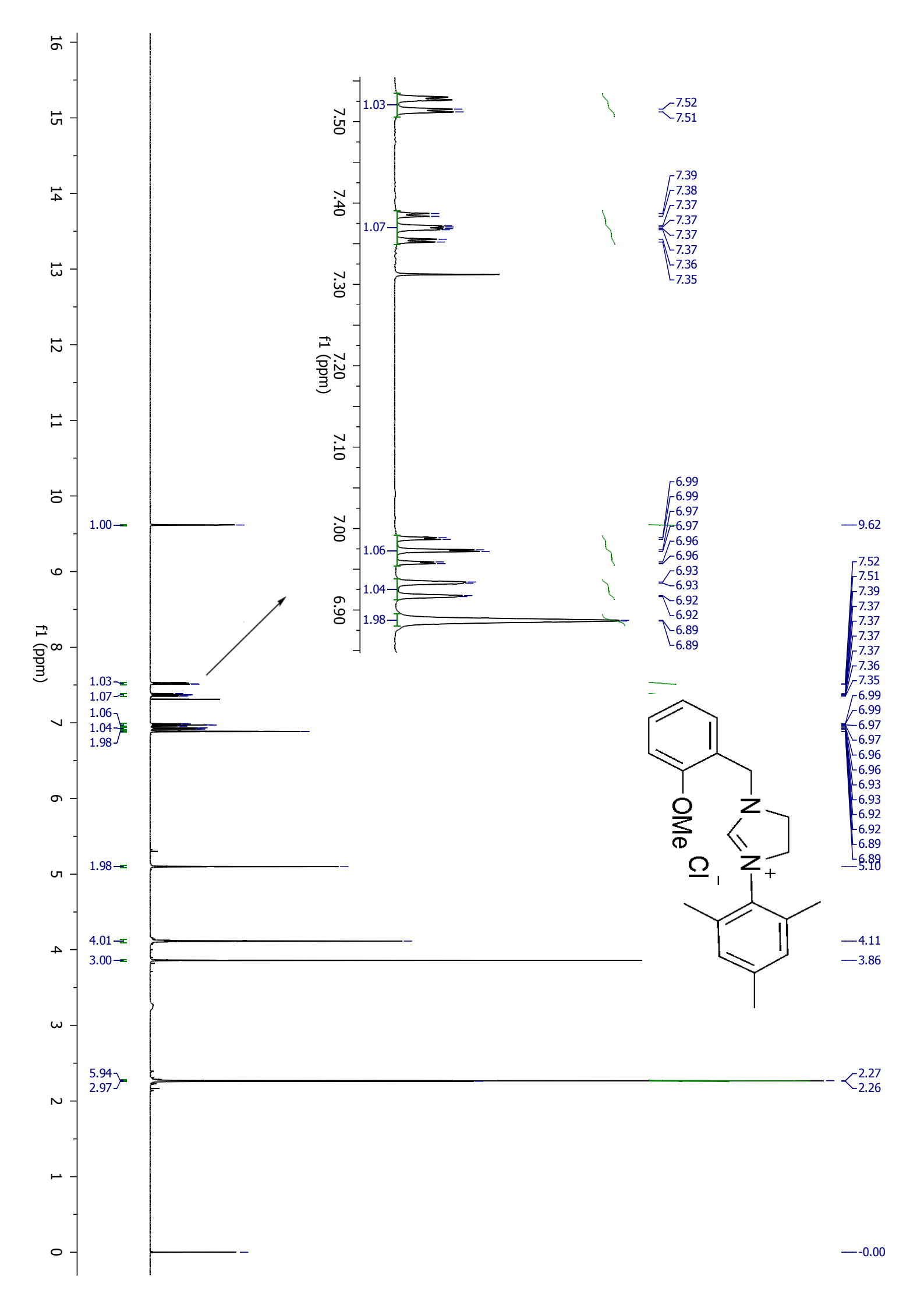
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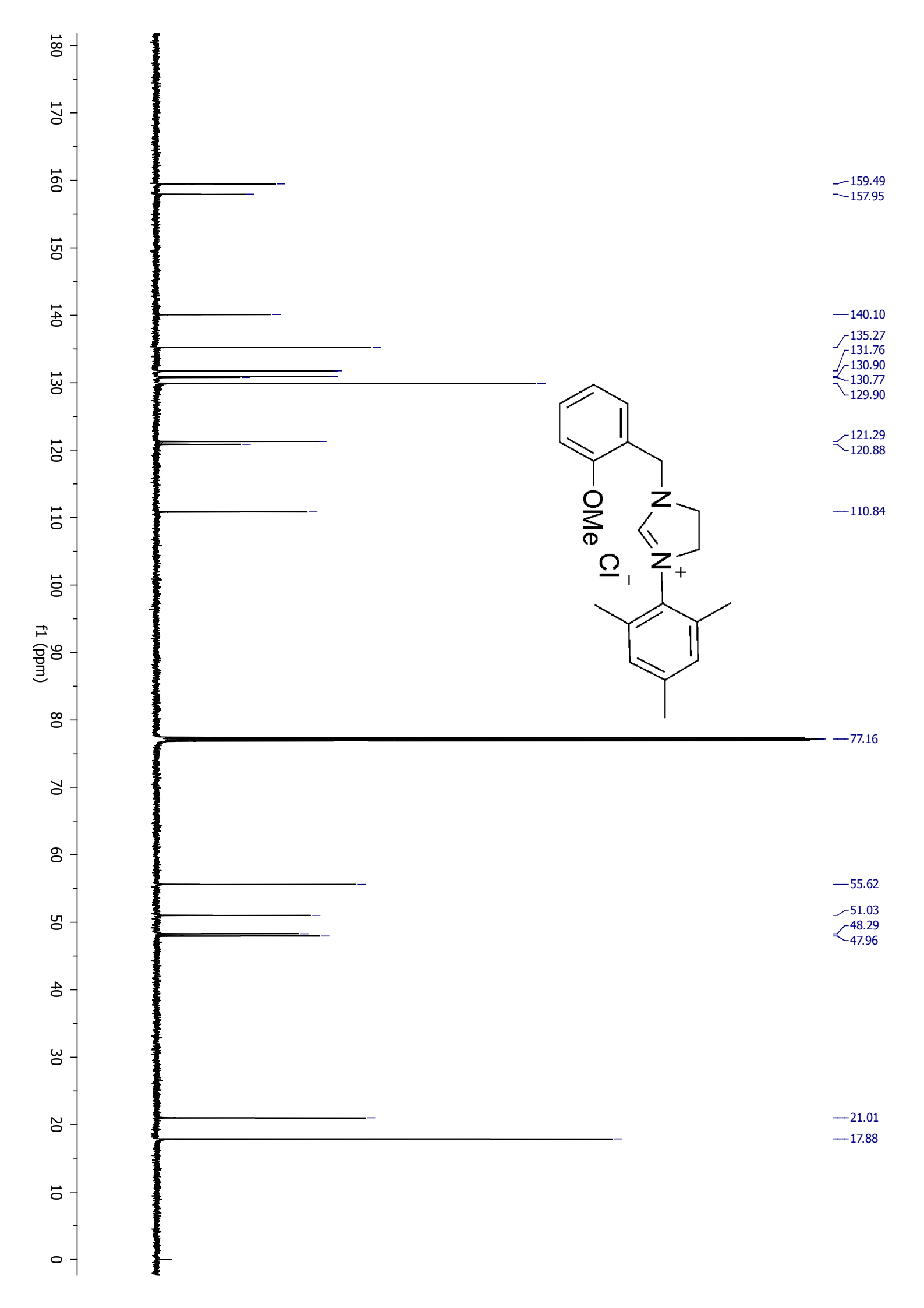
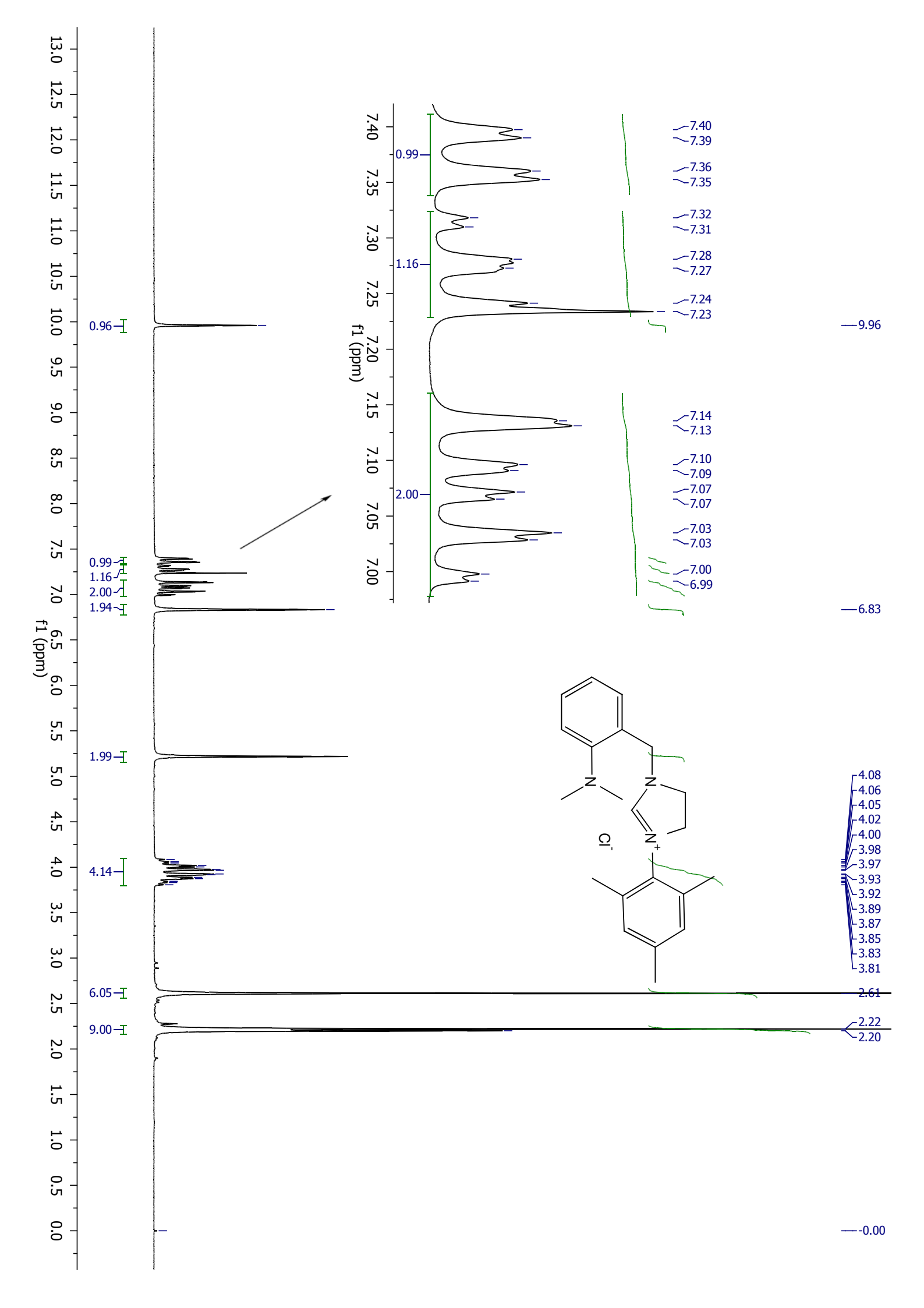
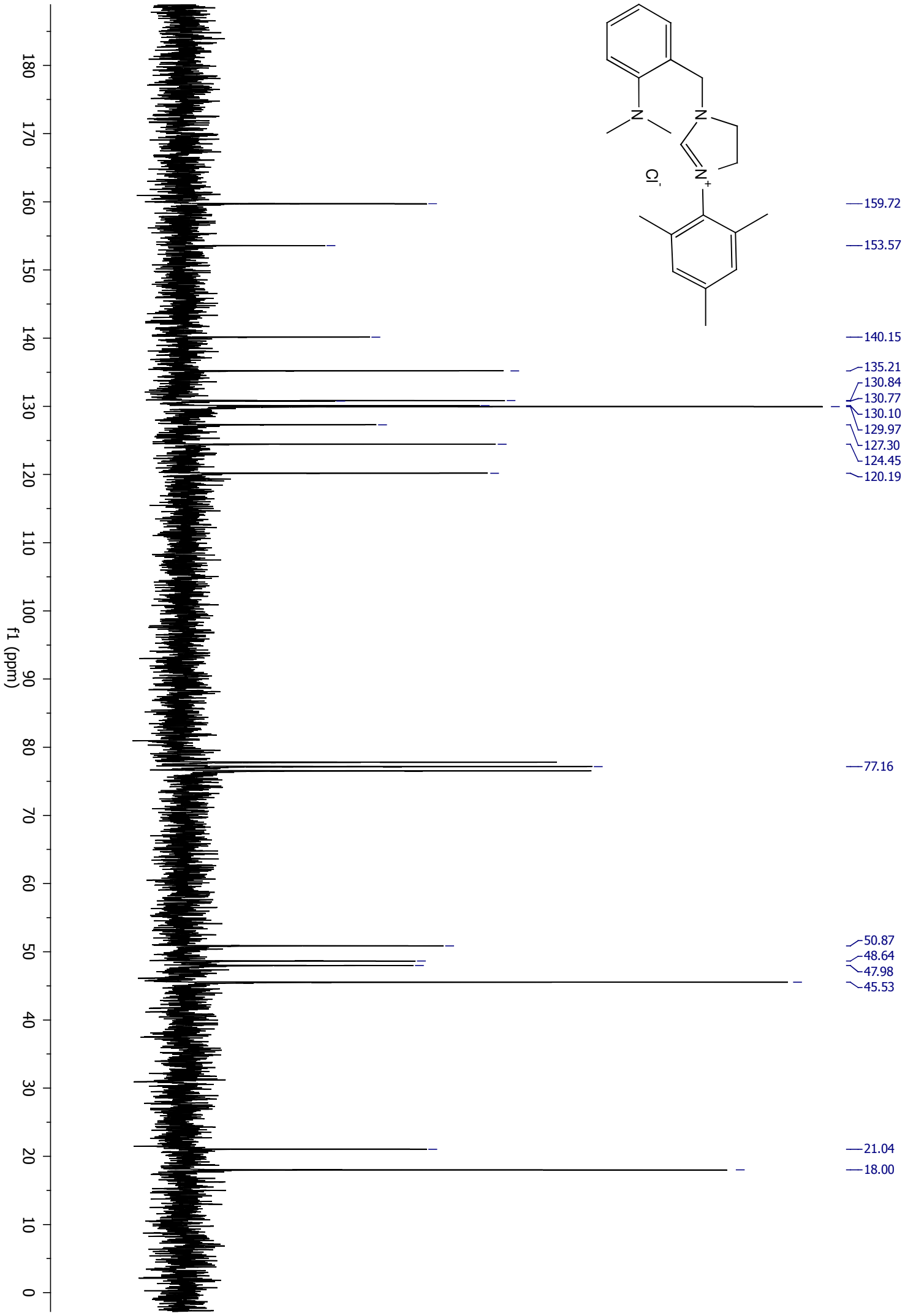
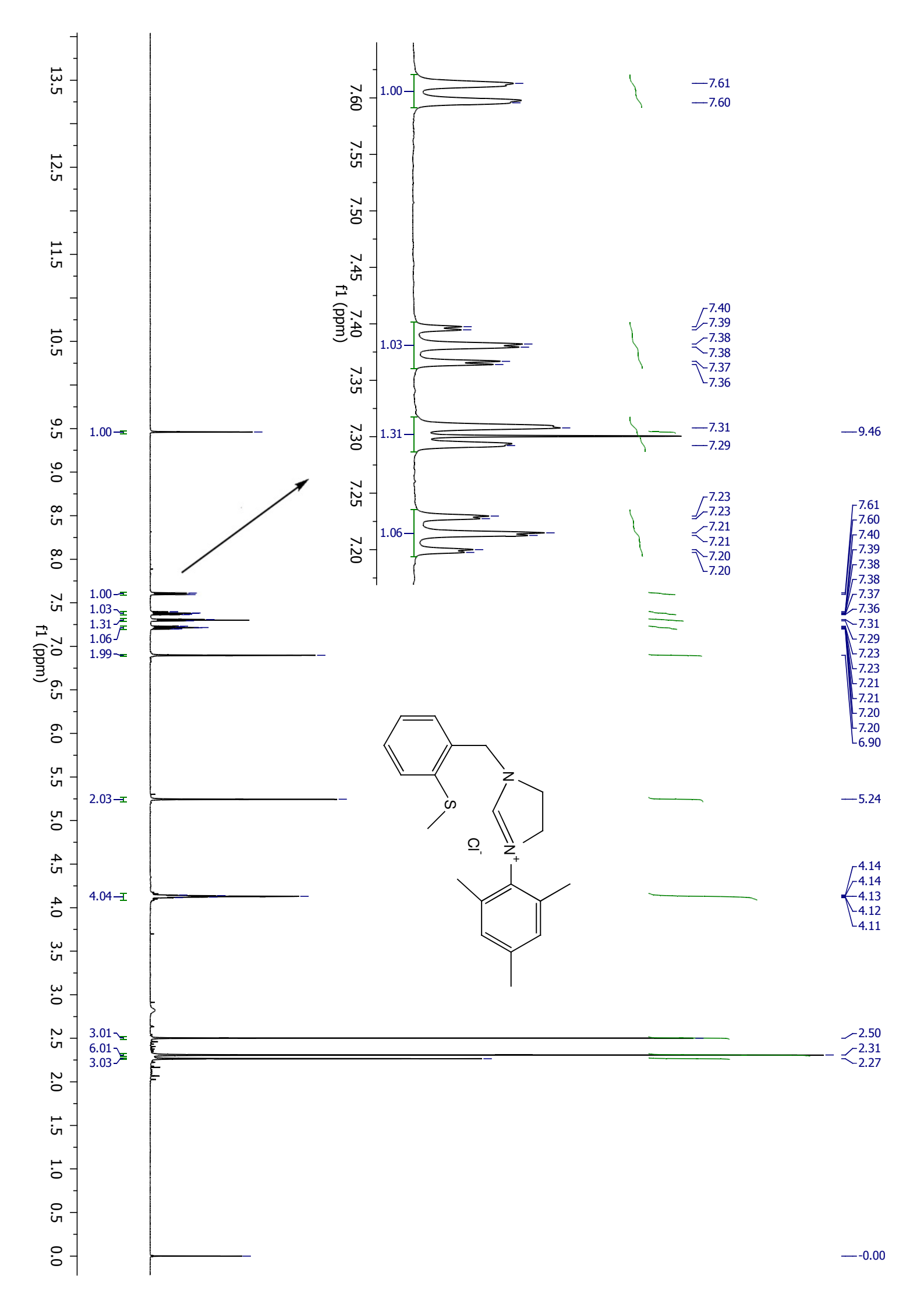
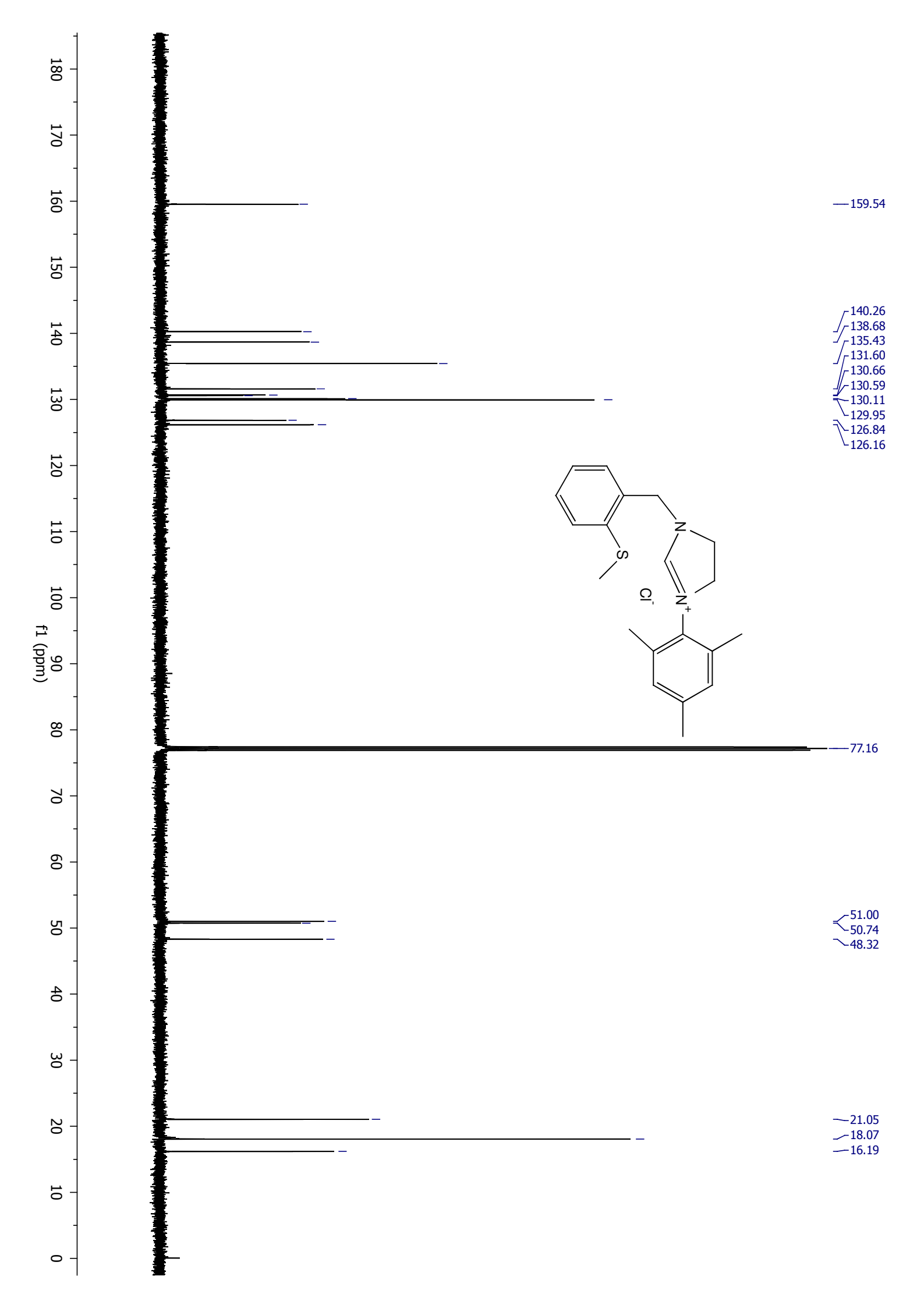
4.11
3.86
2.27
2.26
-0.00
OMe
Cl
N
N
+
−

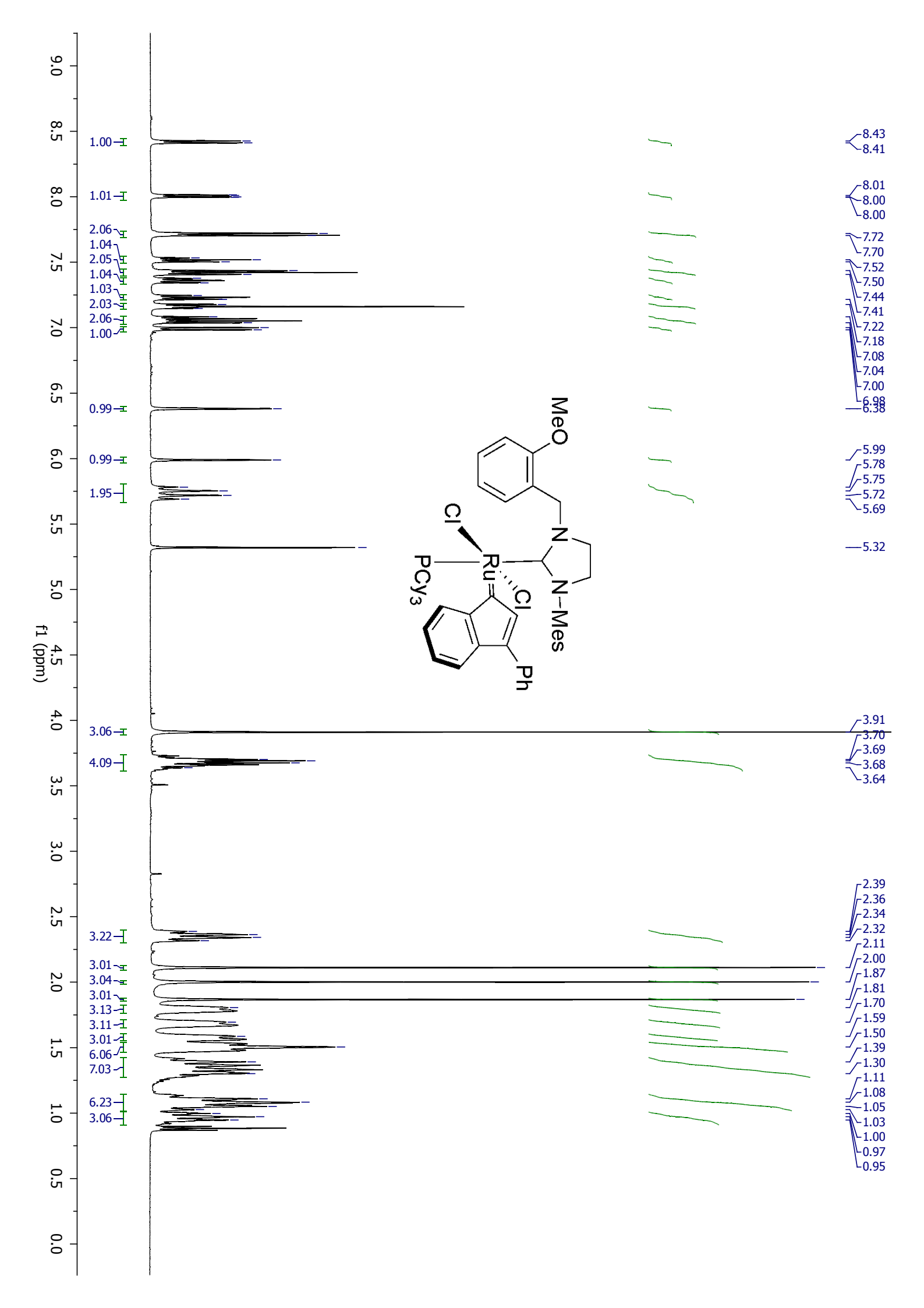

159.49
157.95
140.10
135.27
131.76
130.90
130.77
129.90
121.29
120.88
110.84
77.16
55.62
51.03
48.29
47.96
21.01
17.88
OMe
Cl
N
N+
f1 (ppm)

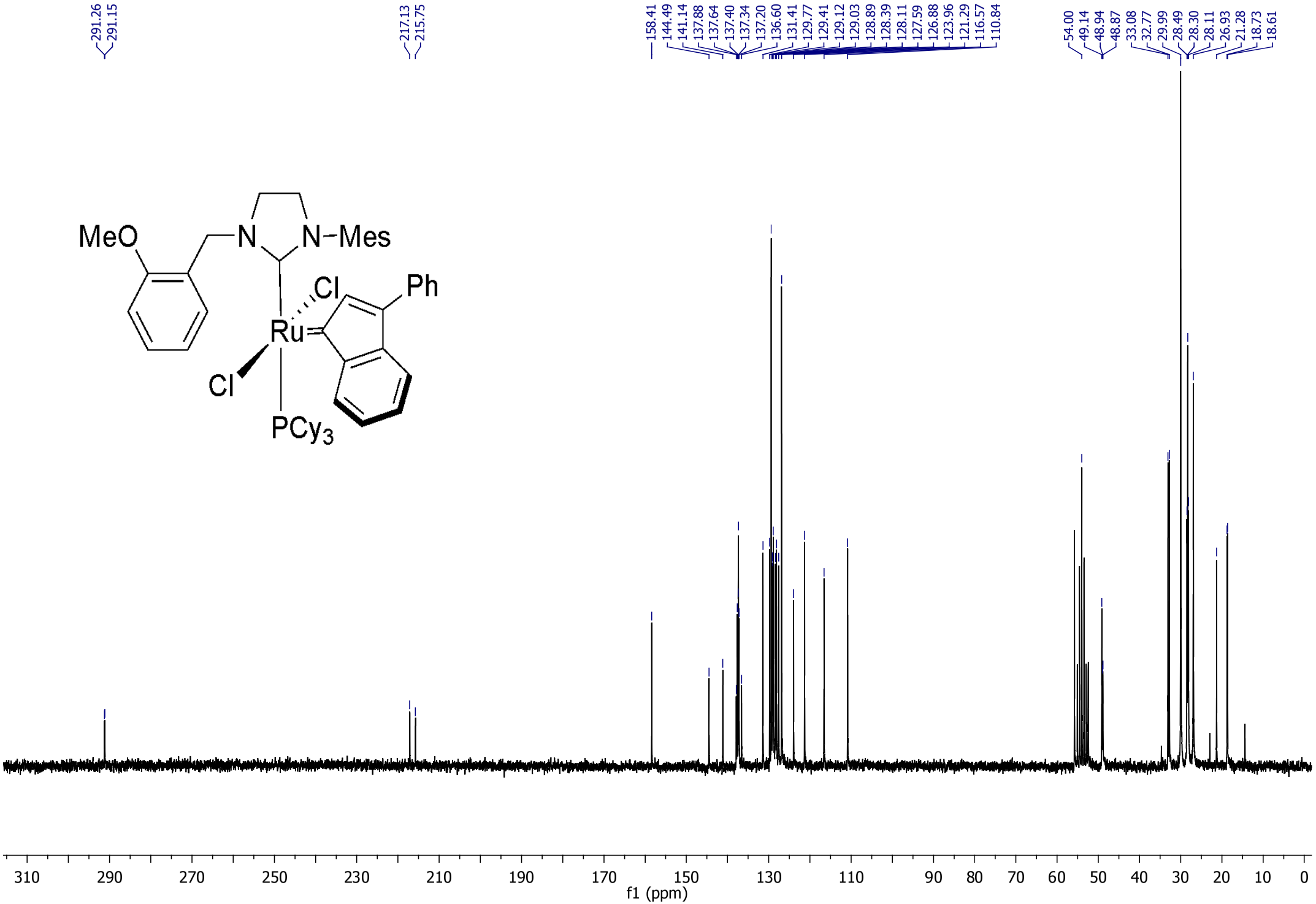

f1 (ppm)
0.96
0.99
1.16
2.00
1.94
1.99
4.14
6.05
9.00
9.96
6.83
-0.00
7.40
7.39
7.36
7.35
7.32
7.31
7.28
7.27
7.24
7.23
7.14
7.13
7.10
7.09
7.07
7.07
7.03
7.03
7.00
6.99
4.08
4.06
4.05
4.02
4.00
3.98
3.97
3.93
3.92
3.89
3.87
3.85
3.83
3.81
2.61
2.22
2.20
N
N
N+
Cl-

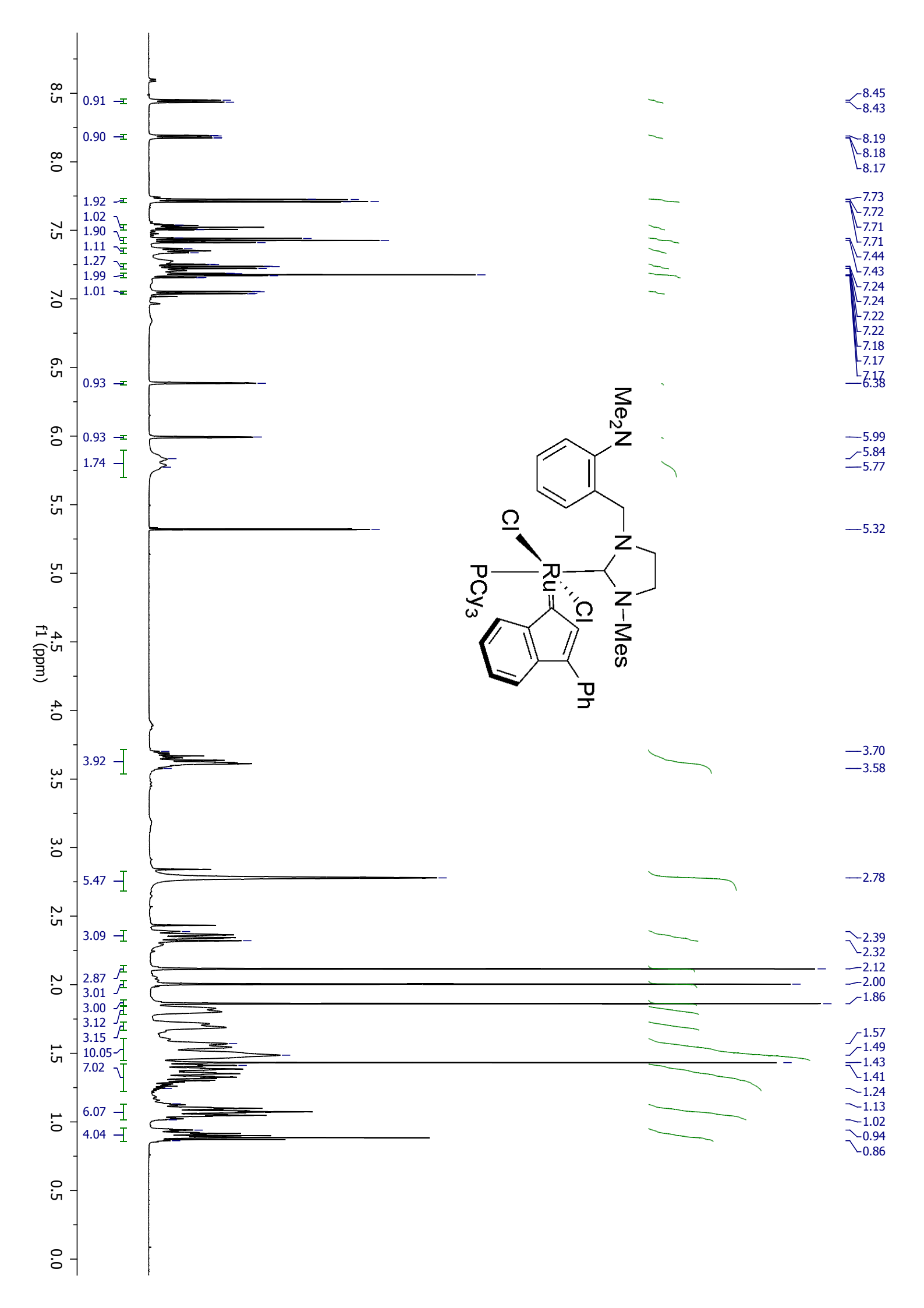

159.72
153.57
140.15
135.21
130.84
130.77
130.10
129.97
127.30
124.45
120.19
77.16
50.87
48.64
47.98
45.53
21.04
18.00
f1 (ppm)

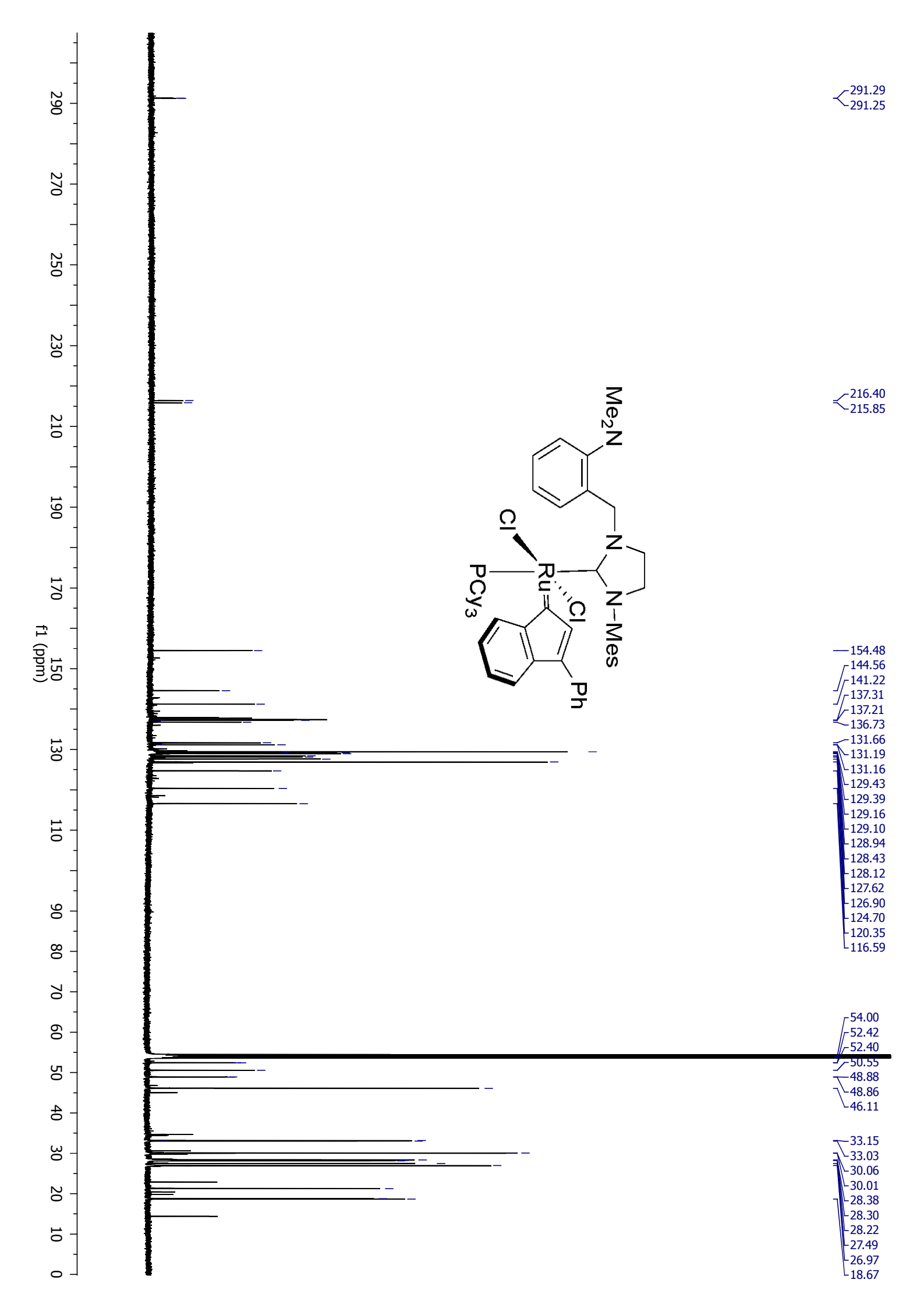

f1 (ppm)
1.00
1.03
1.31
1.06
1.99
2.03
4.04
3.01
6.01
3.03
7.61
7.60
7.40
7.39
7.38
7.38
7.37
7.36
7.31
7.29
7.23
7.23
7.21
7.21
7.20
7.20
9.46
7.61
7.60
7.40
7.39
7.38
7.38
7.37
7.36
7.31
7.29
7.23
7.23
7.21
7.21
7.20
7.20
6.90
5.24
4.14
4.14
4.13
4.12
4.11
2.50
2.31
2.27
-0.00
S
N
N+
Cl-

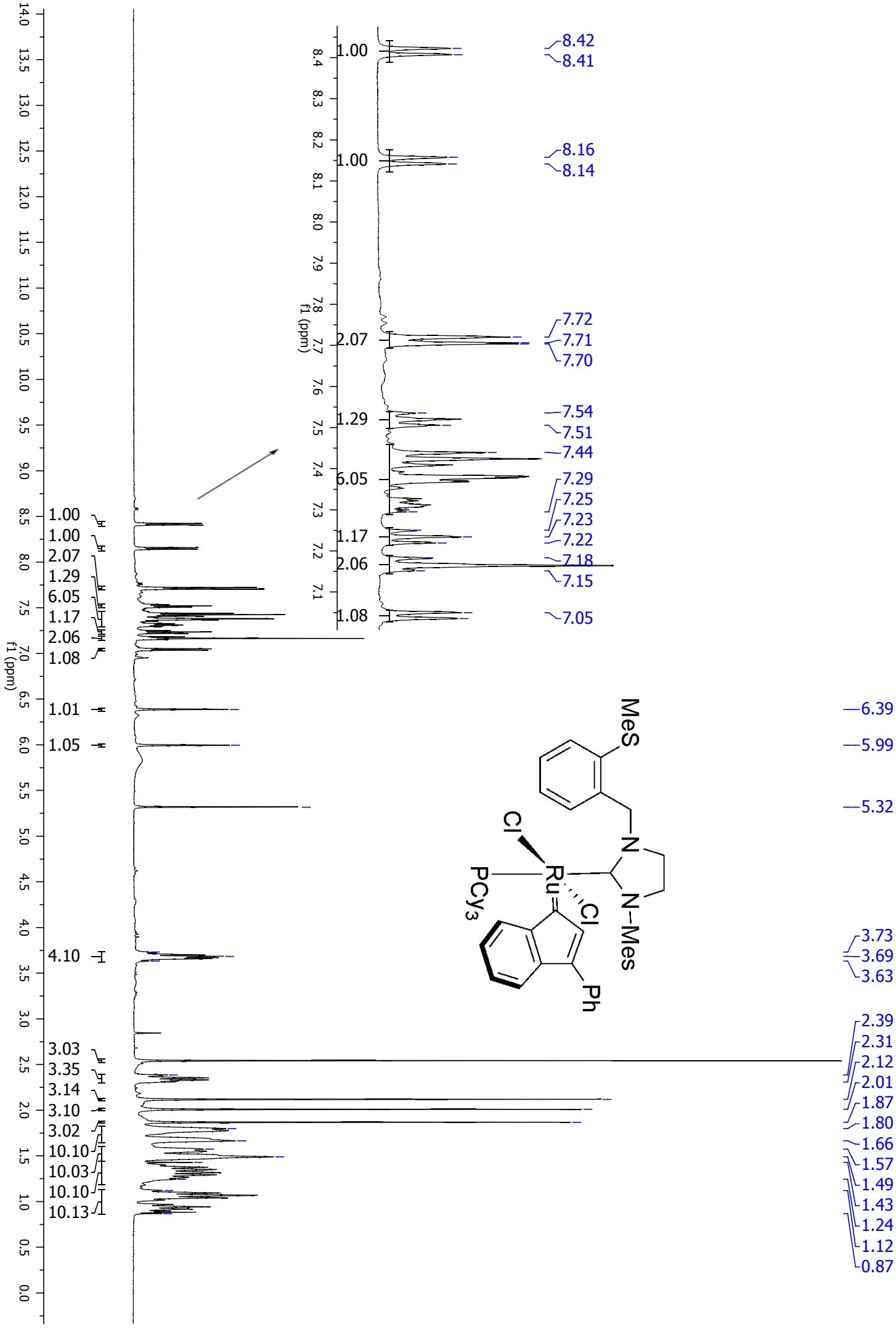

f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
159.54
140.26
138.68
135.43
131.60
130.66
130.59
130.11
129.95
126.84
126.16
77.16
51.00
50.74
48.32
21.05
18.07
16.19
N
S
Cl-
N+

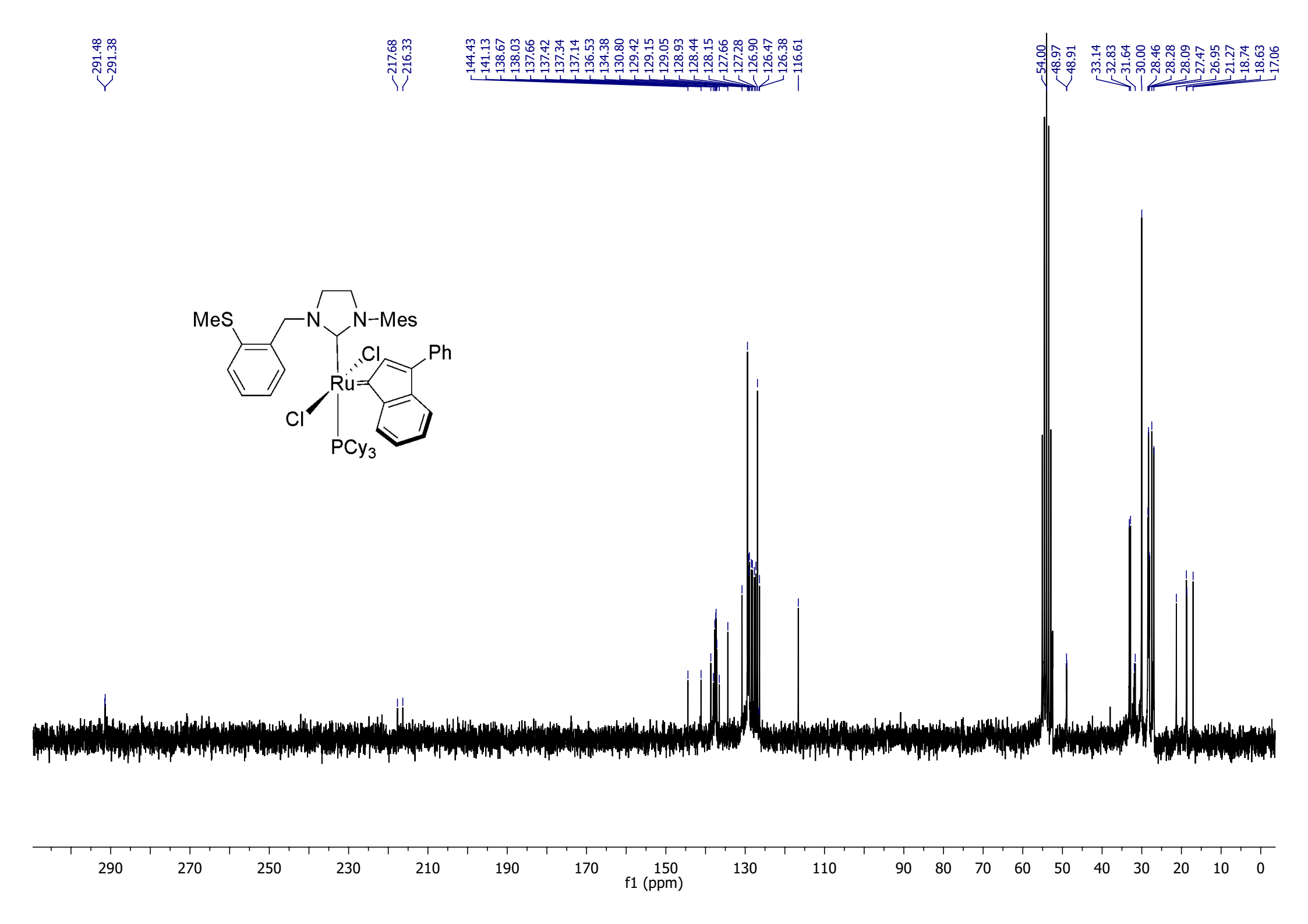

f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.00
1.01
2.06
1.04
2.05
1.04
1.03
2.03
2.06
1.00
0.99
0.99
1.95
3.06
4.09
3.22
3.01
3.04
3.01
3.13
3.11
3.01
6.06
7.03
6.23
3.06
8.43
8.41
8.01
8.00
8.00
7.72
7.70
7.52
7.50
7.44
7.41
7.22
7.18
7.08
7.04
7.00
6.98
6.38
5.99
5.78
5.75
5.72
5.69
5.32
3.91
3.70
3.69
3.68
3.64
2.39
2.36
2.34
2.32
2.11
2.00
1.87
1.81
1.70
1.59
1.50
1.39
1.30
1.11
1.08
1.05
1.03
1.00
0.97
0.95
MeO
N
N–Mes
Cl
Ru
Cl
PCy3
Ph


291.26
291.15
217.13
215.75
158.41
144.49
141.14
137.88
137.64
137.40
137.34
137.20
136.60
131.41
129.77
129.41
129.12
129.03
128.89
128.39
128.11
127.59
126.88
123.96
121.29
116.57
110.84
54.00
49.14
48.94
48.87
33.08
32.77
29.99
28.49
28.30
28.11
26.93
21.28
18.73
18.61
MeO
N
N–Mes
Cl
Ph
Ru
Cl
PCy3
310
290
270
250
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


f1 (ppm)
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
0.91
0.90
1.92
1.02
1.90
1.11
1.27
1.99
1.01
0.93
0.93
1.74
3.92
5.47
3.09
2.87
3.01
3.00
3.12
3.15
10.05
7.02
6.07
4.04
8.45
8.43
8.19
8.18
8.17
7.73
7.72
7.71
7.71
7.44
7.43
7.24
7.24
7.22
7.22
7.18
7.17
7.17
6.38
5.99
5.84
5.77
5.32
3.70
3.58
2.78
2.39
2.32
2.12
2.00
1.86
1.57
1.49
1.43
1.41
1.24
1.13
1.02
0.94
0.86
Me2N
N
N–Mes
Cl
Ru
Cl
PCy3
Ph


291.29
291.25
216.40
215.85
154.48
144.56
141.22
137.31
137.21
136.73
131.66
131.19
131.16
129.43
129.39
129.16
129.10
128.94
128.43
128.12
127.62
126.90
124.70
120.35
116.59
54.00
52.42
52.40
50.55
48.88
48.86
46.11
33.15
33.03
30.06
30.01
28.38
28.30
28.22
27.49
26.97
18.67
f1 (ppm)
Me2N
N
N–Mes
Cl
Ru
Cl
PCy3
Ph


f1 (ppm)
1.00
1.00
2.07
1.29
6.05
1.17
2.06
1.08
1.01
1.05
4.10
3.03
3.35
3.14
3.10
3.02
10.10
10.03
10.10
10.13
8.42
8.41
8.16
8.14
7.72
7.71
7.70
7.54
7.51
7.44
7.29
7.25
7.23
7.22
7.18
7.15
7.05
6.39
5.99
5.32
3.73
3.69
3.63
2.39
2.31
2.12
2.01
1.87
1.80
1.66
1.57
1.49
1.43
1.24
1.12
0.87
MeS
N
N-Mes
Cl
Ru
Cl
PCy3
Ph


291.48
291.38
217.68
216.33
144.43
141.13
138.67
138.03
137.66
137.42
137.34
137.14
136.53
134.38
130.80
129.42
129.15
129.05
128.93
128.44
128.15
127.66
127.28
126.90
126.47
126.38
116.61
54.00
48.97
48.91
33.14
32.83
31.64
30.00
28.46
28.28
28.09
27.47
26.95
21.27
18.74
18.63
17.06
MeS
N
N–Mes
Cl
Ph
Ru
Cl
PCy3
290
270
250
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)