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Base-promoted direct amidation of esters: beyond the current scope and practical applications

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1. General and chemistry

For thin layer chromatography (TLC) aluminum sheets pre-coated with silica gel 60 F_{254} (Merck) were used. Flash column chromatography was carried out using silica gel 60 (0.040–0.063 mm, 230-400 mesh ASTM, Merck). Commercially available solvents for reactions, TLC and column chromatography were used after distillation (and were dried if needed) – water, acetic acid (AcOH), methanol (MeOH), petroleum ether (PE), diethyl ether (Et_2O), ethylacetate (EA), dichloromethane (DCM), chloroform, methyl *tert*-butyl ether (MTBE), diisopropyl ether (DIPE), tetrahydrofurane (THF), dimethylformamide (DMF), *iso*-propanol (*i*-PrOH), dimethylsulfoxyde (DMSO). Any fine chemical, whose synthesis is not described or mentioned in the references in this study, is commercially available from Sigma-Aldrich, Fluorochem, Fluka, Acros or Alfa Aesar. Melting temperatures were determined in capillary tubes on an Electrothermal MEL-TEMP 1102D-230 VAC apparatus without corrections. The NMR spectra were recorded on a Bruker Avance II+ 600 spectrometer (600.13 MHz for ^{1}H and 150.92 MHz for ^{13}C). In case of $CDCl_3$, TMS was used as internal standard (δ=0.00). For other deuterated solvents ^{1}H spectra were calibrated to the residual solvent peaks (DMSO-d_6 δ=2.50). ^{13}C spectra were calibrated in all cases to the residual solvent peaks ($CDCl_3$ δ=77.00, DMSO-d_6 δ=39.52). The following additional NMR techniques were used for all compounds: DEPT 135, COSY, HSQC and HMBC. Mass spectra (MS) were recorded in direct regime on Thermo Scientific High Resolution Magnetic Sector MS DFS by chemical ionization (CI), or on a Waters ZQ 2000 by electrospray ionization (ESI). Direct MS-regime for ESI: each compound was dissolved in MeOH with concentration 1 mg/ml; injection volume 3-5 µl; mobile phase – formic acid in MeOH. MS spectra are reported as fragmentation in m/z with relative intensities (%). Optical angle of rotation was measured with JASCO P-2000 apparatus. The compound names are in agreement with the IUPAC nomenclature.

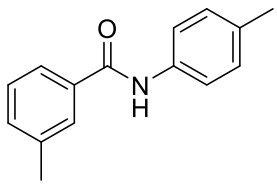
General procedure

Method A (DMSO/*t*-BuOK system). 2 mmol of the respective amine were dissolved in 4 ml dry DMSO, together with 4 mmol of the respective ester at r.t, and were stirred vigorously. 5 mmol of *t*-BuOK were added slowly, portion wise to the mixture. After stirring for 5 min. 50 ml of DCM were added to the mixture and the organic layer was washed with brine 3x100 ml and with water 1x100 ml. After that the organic layer was dried over K_2CO_3 or Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was later purified by column chromatography.

Method B (THF/*n*-BuLi system). 2 mmol of the respective amine were dissolved in 10 ml dry THF under argon at r.t. The solution was cooled on an ice bath, and 4 mmol of *n*-BuLi were added to it. The cooling was removed and the mixture was stirred at r.t. for 5 min. Then 4 mmol of the respective ester were added and the mixture was stirred for 5 more minutes. The mixture was concentrated under reduced pressure and 50 ml of DCM were added to it. It was washed with water 1x100 ml. the organic layer was dried over K_2CO_3 or Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was later purified by column chromatography.

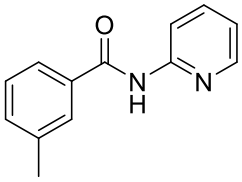
ANALYTICAL AND SPECTRAL DATA

3-methyl-*N*-(*p*-tolyl)benzamide (**3**) [1]:



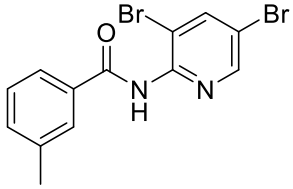
Pale yellow solid, 94% yield (Method A). TLC: DCM/PE 2:1 2x. Column chromatography: DCM/PE 2:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.06 (*s*, 1H), 7.65 – 7.62 (*m*, 1H), 7.60 (*dt*, *J* = 6.6, 2.1 Hz, 1H), 7.53 – 7.49 (*m*, 2H), 7.31 – 7.25 (*m*, 2H), 7.11 (*dd*, *J* = 7.4, 1.5 Hz, 2H), 2.35 (*s*, 3H), 2.31 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 166.0, 138.4, 135.4, 134.9, 134.0, 132.3, 129.4, 129.4, 129.4, 128.4, 127.8, 123.9, 120.3, 21.3, 20.8.

- 3-methyl-*N*-(pyridin-2-yl)benzamide (**24**) [2]:



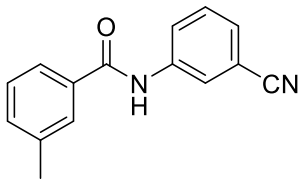
White solid, 89% yield. (Method A). TLC: DCM/MTBE 20:1, 2x. Column chromatography: DCM-DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 9.12 (*s*, 1H), 8.41 (*dt*, *J* = 8.4, 1.0 Hz, 1H), 8.15 (*ddd*, *J* = 4.9, 1.9, 0.9 Hz, 1H), 7.77 – 7.68 (*m*, 3H), 7.38 – 7.32 (*m*, 2H), 7.03 (*ddd*, *J* = 7.3, 4.9, 1.0 Hz, 1H), 2.39 (*s*, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) = 166.1, 151.7, 147.8, 138.6, 138.4, 134.2, 132.9, 128.6, 127.9, 124.3, 119.7, 114.2, 21.3.

N-(3,5-dibromopyridin-2-yl)-3-methylbenzamide (**25**):



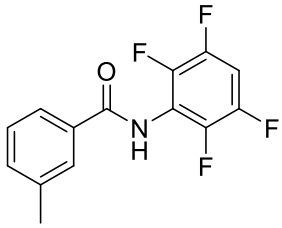
White solid, 72% yield. (Method A). M.p. 148-149ºC. TLC: DCM/MTBE 20:1, 1x. Column chromatography: DCM/MTBE 50:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.49 (*d*, *J* = 2.2 Hz, 1H), 8.46 (*s*, 1H), 8.06 (*d*, *J* = 2.2 Hz, 1H), 7.75 (*d*, *J* = 2.1 Hz, 1H), 7.71 (*dt*, *J* = 6.6, 2.1 Hz, 1H), 7.43 – 7.36 (*m*, 2H), 2.44 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 165.1, 148.5, 147.7, 143.3, 139.0, 133.9, 133.5, 128.9, 128.4, 124.5, 115.7, 112.8, 21.5. MS (CI+) m/z (rel. int.): 289 (M-Br, 33), 291 (M-Br, 34), 369 (M+1, 52), 371 (M+1, 100).

N-(3-cyanophenyl)-3-methylbenzamide (**26**):



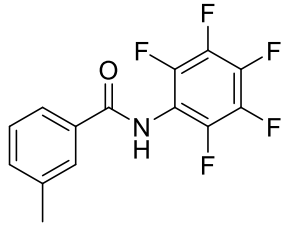
Pale yellow solid, 94% yield. (Method A). M.p. 119-120ºC. TLC: DCM, 1x. Column chromatography: DCM. ^{1}H NMR (600 MHz, DMSO-d^6) δ (ppm) = 10.52 (*s*, 1H), 8.28 – 8.24 (*m*, 1H), 8.05 (*dt*, *J* = 7.4, 2.2 Hz, 1H), 7.79 – 7.72 (*m*, 2H), 7.60 – 7.53 (*m*, 2H), 7.46 – 7.40 (*m*, 2H), 2.40 (*s*, 3H). ^{13}C NMR (151 MHz, DMSO-d^6) δ (ppm) = 166.1, 140.1, 137.9, 134.4, 132.6, 130.1, 128.4, 128.2, 127.1, 125.0, 124.8, 122.9, 118.8, 111.5, 40.1, 21.0. MS (ESI+) m/z (rel. int.): 237 (M+1, 100), 259 (M+Na, 34), 282 (M+2Na, 43).

3-methyl-*N*-(2,3,5,6-tetrafluorophenyl)benzamide (**27**):



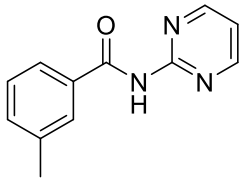
White solid, 75% yield. (Method A). M.p. 146-147ºC. TLC: DCM/PE 1:1, 1x. Column chromatography: DCM/PE 5:1 - 1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 7.76 – 7.64 (*m*, 2H), 7.62 (*s*, 1H), 7.45 – 7.33 (*m*, 2H), 7.01 (*tt*, *J* = 9.8, 7.2 Hz, 1H), 2.42 (*s*, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, C-F-decoupling) δ (ppm) = 165.7, 146.2, 142.3, 139.1, 133.7, 132.7, 128.9, 128.5, 124.8, 117.4, 103.9, 21.5. MS (CI+) m/z (rel. int.): 284 (M+1, 100).

3-methyl-*N*-(perfluorophenyl)benzamide (**28**):



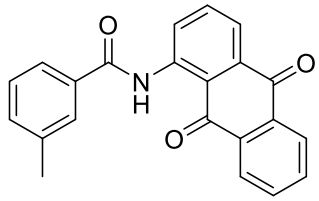
White solid, 78% yield. (Method A). M.p. 144-145ºC. TLC: DCM/PE 1:1, 1x. Column chromatography: DCM/PE 5:1 - 1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) =7.76 – 7.66 (*m*, 2H), 7.66 (*s*, 1H), 7.45 – 7.35 (*m*, 2H), 2.44 (*s*, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, C-F Decoupling) δ (ppm) = 166.1, 139.1, 133.7, 132.5, 128.9, 128.5, 124.8, 21.4. MS (CI+) m/z (rel. int.): 302 (M+1, 100).

3-methyl-*N*-(pyrimidin-2-yl)benzamide (**29**):



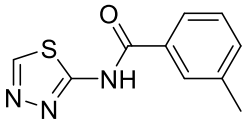
White solid, 94% yield. (Method A). M.p. 154-155ºC. TLC: DCM/MTBE 20:1, 2x. Column chromatography: DCM - DCM/MTBE 10:1. ^{1}H NMR (600 MHz, DMSO-d^6) δ (ppm) = 10.95 (*s*, 1H), 8.73 (*d*, *J* = 4.8 Hz, 2H), 7.80 (*d*, *J* = 2.2 Hz, 1H), 7.76 (*dt*, *J* = 7.1, 2.0 Hz, 1H), 7.43 – 7.36 (*m*, 2H), 7.25 (*t*, *J* = 4.8 Hz, 1H), 2.37 (*s*, 3H). ^{13}C NMR (151 MHz, DMSO-d^6) δ (ppm) = 165.61, 158.40, 158.25, 137.70, 134.23, 132.68, 128.79, 128.28, 125.38, 117.32, 40.06, 20.93. MS (ESI+) m/z (rel. int.): 214 (M+1, 100), 236 (M+Na, 57), 449 (2M+Na, 26).

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3-methylbenzamide (**30**):



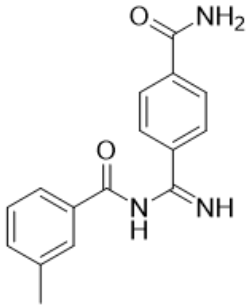
Yellow-orange solid, 55% yield. (Method A). M.p. 198-199ºC. TLC: PE/MTBE 10:1, 3x. Column chromatography: PE/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 13.22 (*s*, 1H), 9.33 (*dd*, *J* = 8.5, 1.2 Hz, 1H), 8.36 – 8.30 (*m*, 1H), 8.30 – 8.24 (*m*, 1H), 8.07 (*dd*, *J* = 7.6, 1.2 Hz, 1H), 7.95 (*d*, *J* = 7.1 Hz, 2H), 7.80 (*qd*, *J* = 7.5, 3.8 Hz, 3H), 7.47 (*td*, *J* = 7.2, 1.5 Hz, 1H), 7.42 (*d*, *J* = 7.5 Hz, 1H), 2.50 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 187.6, 182.8, 166.9, 142.6, 138.9, 136.0, 134.6, 134.5, 134.4, 134.1, 133.3, 132.9, 128.9, 128.7, 127.6, 127.2, 126.4, 124.7, 122.7, 118.0, 29.8, 21.7. MS (CI+) m/z (rel. int.): 342 (M+1, 100).

3-methyl-*N*-(1,3,4-thiadiazol-2-yl)benzamide (**31**) [3]:



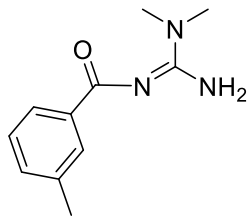
White solid (Method A - 30% yield; Method B – 72% yield). TLC: DCM/MTBE 10:1, 1x. Column chromatography: DCM/MTBE 20:1. ^{1}H NMR (400 MHz, DMSO-d^6) δ (ppm) = 13.01 (s, 1H), 9.23 (s, 1H), 7.98 – 7.88 (m, 2H), 7.50 – 7.39 (m, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d^6) δ (ppm) = 165.3, 159.5, 149.0, 138.0, 133.5, 131.5, 128.9, 128.5, 125.5, 20.9.

N-((4-carbamoylphenyl)(imino)methyl)-3-methylbenzamide (**32**):



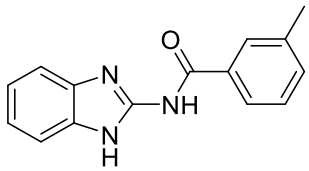
White solid, 69% yield. (Method A). M.p. 191-192ºC. TLC: DCM/MTBE 10:1, 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, DMSO-d^6) δ (ppm) = 10.40 (*s*, 1H), 9.40 (*s*, 1H), 8.25 – 8.21 (m, 2H), 8.15 (*s*, 1H), 8.06 (*dd*, *J* = 8.8, 3.2 Hz, 2H), 8.04 – 7.99 (*m*, 2H), 7.57 (*s*, 1H), 7.41 – 7.36 (*m*, 2H), 2.39 (*s*, 3H). ^{13}C NMR (151 MHz, DMSO-d^6) δ (ppm) = 178.6, 167.2, 165.3, 137.7, 137.4, 137.0, 132.6, 129.6, 128.1, 127.94, 127.6, 126.5, 40.1, 21.1. MS (ESI+) m/z (rel. int.): 119 (3-methylbenzoyl, 55), 282 (M+1, 100).

N-(*N*,*N*-dimethylcarbamimidoyl)-3-methylbenzamide (**33**):



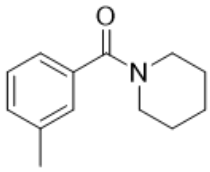
White solid, 60% yield. (Method A) M.p. 180-181ºC. TLC: DCM/MTBE 1:1, 1x. Column chromatography: DCM/MTBE 2:1. ^{1}H NMR (600 MHz, DMSO-d^{6}) δ (ppm) = 8.39 (s, 2H), 7.96 – 7.85 (m, 2H), 7.28 – 7.20 (m, 2H), 2.35 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d^{6}) δ (ppm) = 174.5, 160.8, 139.2, 136.1, 130.5, 128.6, 127.0, 125.3, 36.0, 20.5. MS (ESI+) m/z (rel. int.): 119 (3-methylbenzoyl, 55), 206 (M+1, 100).

N-(1*H*-benzo[*d*]imidazol-2-yl)-3-methylbenzamide (**34**) [4]:



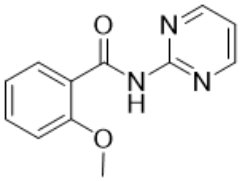
White solid, 62% yield. (Method A) TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM/MTBE10:1. ^{1}H NMR (400 MHz, DMSO-d^{6}) δ (ppm) = 11.98 (s, 2H), 7.98 (tt, *J* = 1.6, 0.9 Hz, 1H), 7.94 (tdd, *J* = 4.4, 1.8, 0.7 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.42 – 7.38 (m, 2H), 7.17 – 7.09 (m, 2H), 2.40 (d, *J* = 0.7 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d^{6}) δ (ppm) = 168.2, 148.6, 137.2, 134.3, 134.1, 132.1, 128.4, 127.7, 125.0, 121.0, 113.0, 20.5.

Piperidin-1-yl(*m*-tolyl)methanone (**35**) [5]:



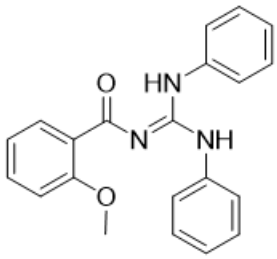
Pale yellow oil. (Method A - 71% yield; Method B – 85% yield). TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM/MTBE 15:1 - 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.31 – 7.24 (*m*, 1H), 7.22 – 7.18 (*m*, 2H), 7.18 – 7.14 (*m*, 1H), 3.71 (*s*, 2H), 3.34 (*s*, 2H), 2.37 (*d*, *J* = 0.8 Hz, 2H), 1.68 (*dd*, *J* = 7.5, 3.8 Hz, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 170.5, 138.2, 136.4, 130.0, 128.2, 127.4, 123.6, 48.7, 43.0, 26.5, 25.6, 24.6, 21.4.

2-methoxy-*N*-(pyrimidin-2-yl)benzamide (**36**):



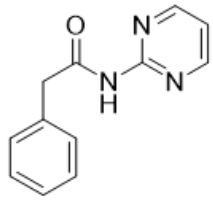
White solid, 63% yield. (Method A). M.p. 102-103ºC. TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 10.54 (*s*, 1H), 8.68 (*d*, *J* = 4.8 Hz, 2H), 8.33 (*dd*, *J* = 7.8, 1.9 Hz, 1H), 7.52 (*ddd*, *J* = 8.8, 7.3, 1.9 Hz, 1H), 7.17 – 7.11 (*m*, 1H), 7.07 – 7.01 (*m*, 2H), 4.09 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 162.8, 158.5, 158.1, 157.4, 1334.0, 133.2, 121.8, 121.6, 116.7, 111.6, 56.4. MS (CI+) m/z (rel. int.): 135 (2-methoxybenzoyl, 100), 198 (M-OMe, 52), 230 (M+1, 92).

N-(bis(phenylamino)methylene)-2-methoxybenzamide (**37**):



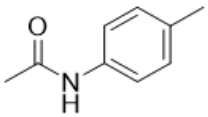
Pale pink solid, 85% yield. (Method A). M.p. 137-138ºC. TLC: DCM/MTBE 5:1, 2x. Column chromatography: DCM/MTBE 5:1. ^{1}HNMR (600 MHz, $CDCl_3$) δ (ppm) = 10.69 (*s*, 1H), 10.14 (*s*, 1H), 8.21 (*dd*, *J* = 7.9, 1.8 Hz, 1H), 7.78 (*d*, *J* = 8.0 Hz, 2H), 7.48 (*ddd*, *J* = 8.7, 7.3, 1.9 Hz, 1H), 7.37 (*t*, *J* = 7.7 Hz, 2H), 7.32 (*t*, *J* = 7.7 Hz, 2H), 7.13 – 7.06 (*m*, 2H), 7.04 (*d*, *J* = 7.4 Hz, 1H), 7.00 (*d*, J=7.5 Hz, 2H), 6.83 (*d*, *J* = 8.4 Hz, 1H), 3.26 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 165.7, 157.8, 147.9, 141.6, 139.5, 134.8, 132.6, 129.7, 128.9, 123.1, 122.8, 122.7, 121.6, 120.1, 119.5, 111.52, 55.6. MS (CI+) m/z (rel. int.): 135 (2-methoxybenzoyl, 72), 314 (M-OMe, 66), 346 (M+1, 100).

2-phenyl-*N*-(pyrimidin-2-yl)acetamide (**38**) [6]:



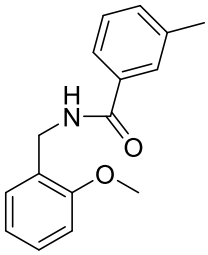
White solid, 58% yield. (Method A). TLC: DCM/MTBE 10:1, 2x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.74 (s, 1H), 8.53 (d, *J* = 4.8 Hz, 2H), 7.38 – 7.33 (m, 4H), 7.30 (m, 1H), 6.91 (t, *J* = 4.9 Hz, 1H), 3.97 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 158.48, 157.53, 134.29, 129.72, 129.06, 127.53, 116.62, 44.67.

N-(*p*-tolyl)acetamide (**39**) [7]:



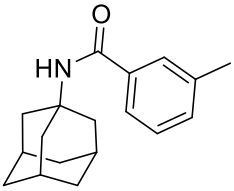
White solid. (Method A - 65% yield; Method B - 83% yield). TLC: DCM:MTBE 5:1, 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.42 (*s*, 1H), 7.40 – 7.34 (*m*, 2H), 7.13 – 7.08 (*m*, 2H), 2.30 (*s*, 3H), 2.15 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 168.3, 135.3, 133.9, 129.4, 120.0, 24.5, 20.8.

N-(2-methoxybenzyl)-3-methylbenzamide (**48**) [6]:



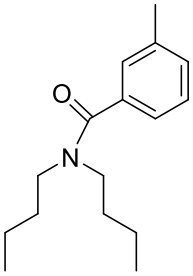
White solid, 78% yield. (Method B). TLC: DCM, 1x. Column chromatography: DCM. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (tt, *J* = 1.9, 0.9 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.34 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.30 – 7.24 (m, 3H), 6.93 (td, *J* = 7.4, 1.1 Hz, 1H), 6.89 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.67 (s, 1H), 4.63 (d, *J* = 5.8 Hz, 2H), 3.87 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.5, 157.7, 138.4, 134.9, 132.1, 130.0, 129.0, 128.5, 128.5, 127.9, 126.3, 123.9, 120.9, 110.5, 55.5, 40.0, 21.5.

N-(adamantan-1-yl)-3-methylbenzamide (**49**):



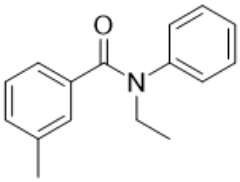
White solid, 70% yield. (Method B). M.p. 139-140ºC. TLC: PE/DCM 1:2, 2x. Column chromatography: PE/DCM 1:2. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 2.2 Hz, 1H), 7.48 (dt, *J* = 7.1, 2.0 Hz, 1H), 7.32 – 7.22 (m, 2H), 5.80 (s, 1H), 2.38 (s, 3H), 2.12 (s, 9H), 1.78 – 1.65 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.9, 138.4, 136.1, 131.8, 128.4, 127.6, 123.8, 52.3, 41.8, 36.5, 29.6, 21.5. MS (CI+) m/z (rel. int.): 135 (59, 2-methoxybenzoyl), 270 (M+1, 100).

N,*N*-dibutyl-3-methylbenzamide (**50**) [8]:



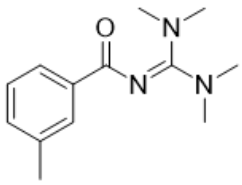
Colorless oil, 89% yield. (Method B). TLC: DCM/MTBE 10:1 1x. Column chromatography: DCM-DCM/MTBE 50:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.39 – 7.33 (*m*, 1H), 7.30 – 7.27 (*m*, 1H), 7.26 (*d*, *J* = 2.0 Hz, 1H), 7.25 – 7.21 (*m*, 1H), 3.58 (*t*, *J* = 7.7 Hz, 2H), 3.28 (*t*, *J* = 7.6 Hz, 2H), 2.47 (*s*, 3H), 1.81 – 1.67 (*m*, 2H), 1.59 (*p*, *J* = 7.6 Hz, 2H), 1.50 (*q*, *J* = 7.6 Hz, 2H), 1.24 (*q*, *J* = 7.3 Hz, 2H), 1.08 (*t*, *J* = 7.3 Hz, 3H), 0.89 (*t*, *J* = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 171.9, 138.2, 137.5, 129.8, 128.3, 127.2, 123.5, 48.8, 44.5, 30.9, 29.8, 21.5, 20.4, 19.9, 14.1, 13.8.

N-ethyl-3-methyl-*N*-phenylbenzamide (**51**):



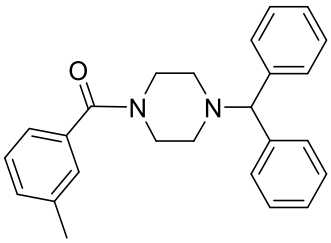
Colorless oil, 80% yield. (Method B). TLC: DCM, 1x. Column chromatography: DCM/PE 1:1 – DCM. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.25 – 7.18 (*m*, 3H), 7.17 – 7.11 (*m*, 1H), 7.05 – 6.97 (*m*, 5H), 3.98 (*q*, *J* = 7.1 Hz, 2H), 2.22 (*s*, 3H), 1.22 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 170.5, 143.4, 137.6, 136.3, 130.3, 129.5, 129.1, 128.0, 127.5, 126.7, 125.8, 45.5, 21.3, 13.1. MS (CI+) m/z (rel. int.): 240 (M+1, 100).

N-(bis(dimethylamino)methylene)-3-methylbenzamide (**52**):



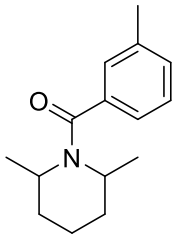
Colorless oil, 98% yield. (Method B). TLC: DCM/MTBE 1:1, 1x. Column chromatography: DCM/MTBE 1:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.97 – 7.91 (*m*, 2H), 7.33 – 7.22 (*m*, 2H), 2.94 (*s*, 12H), 2.39 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 173.4, 168.5, 138.0, 137.4, 131.5, 129.7, 127.8, 126.3, 40.2, 21.4. MS (CI+) m/z (rel. int.): 119 (3-methylbenzoyl, 100) 234 (M+1, 64).

(4-benzhydrylpiperazin-1-yl)(m-tolyl)methanone (**53**):



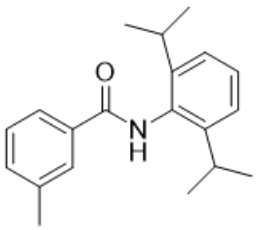
White solid, 70% yield. (Method B). M.p. 123-124ºC. TLC: DCM/MTBE 10:1 1x. Column chromatography: DCM - DCM/MTBE 20:1. ^{1}H NMR (400 MHz, DMSO-d^{6}) δ (ppm) = 7.45 – 7.40 (m, 4H), 7.33 – 7.25 (m, 5H), 7.24 – 7.11 (m, 5H), 4.40 (s, 1H), 3.52 (s, 4H), 2.39 – 2.33 (m, 4H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d^{6}) δ (ppm) = 168.6, 141.9, 137.3, 135.6, 129.5, 128.0, 127.7, 127.3, 126.9, 126.5, 123.5, 74.3, 51.0, 38.9, 20.4. MS (CI+) m/z (rel. int.): 167 ($CH(Ph)_2$, 100), 208 (93), 369 (M+1, 16).

(2,6-dimethylpiperidin-1-yl)(m-tolyl)methanone (**54**):



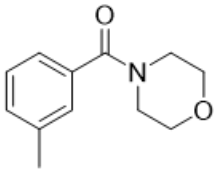
Colorless solid, 63% yield. (Method B). M.p. 78-79ºC. TLC: DCM 1x. Column chromatography: DCM. ^{1}H NMR (600 MHz, DMSO-d^{6}) δ (ppm) = 7.29 (t, *J* = 7.5 Hz, 1H), 7.23 – 7.19 (m, 1H), 7.17 – 7.06 (m, 2H), 4.31 (t, *J* = 7.2 Hz, 2H), 2.34 (s, 3H), 1.84 (qt, *J* = 12.9, 3.6 Hz, 1H), 1.63 (tdd, *J* = 12.9, 6.1, 4.0 Hz, 2H), 1.57 – 1.44 (m, 3H), 1.22 (d, *J* = 7.1 Hz, 6H). ^{13}C NMR (151 MHz, DMSO-d^{6}) δ (ppm) = 169.8, 137.6, 137.3, 128.7, 127.7, 125.8, 122.3, 45.7, 29.3, 20.5, 20.4, 13.5. MS (CI+) m/z (rel. int.): 232 (M+1, 100).

N-(2,6-diisopropylphenyl)-3-methylbenzamide (**55**):



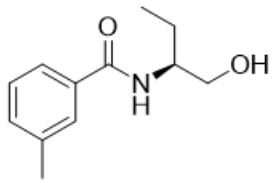
White solid, 70% yield. (Method B). M.p.= 207-208ºC. TLC: DCM/PE 1:1, 1x. Column chromatography: DCM/PE 1:1 – DCM. ^{1}H NMR (600 MHz, DMSO-d^{6}) δ (ppm) = 9.81 (s, 1H), 7.93 – 7.89 (m, 2H), 7.55 – 7.48 (m, 2H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 2H), 3.18 (*hept*, *J* = 6.9 Hz, 2H), 2.50 (*s*, 3H), 1.27 (*d*, *J* = 6.9 Hz, 6H), 1.20 (*d*, *J* = 6.9 Hz, 6H). ^{13}C NMR (151 MHz, DMSO-d^{6}) δ (ppm) = 166.3, 146.2, 137.8, 134.4, 132.9, 132.1, 128.4, 128.1, 127.6, 124.6, 122.9, 40.1, 39.9, 28.2, 23.6, 23.3, 21.0. MS (ESI+) m/z (rel. int.): 206 (88), 296 (M+1, 100), 318 (M+Na, 79).

Morpholino(*m*-tolyl)methanone (**56**) [9]:



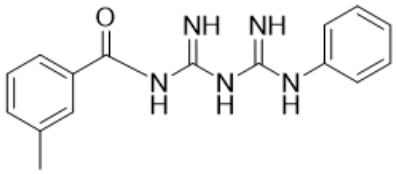
Colorless oil, 75% yield. (Method B). TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM - DCM/MTBE 5:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.32 – 7.26 (*m*, 1H), 7.28 – 7.21 (*m*, 2H), 7.20 – 7.15 (*m*, 1H), 3.78 (*s*, 4H), 3.65 – 3.60 (*m*, 2H), 3.45 (s, 2H), 2.37 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 170.6, 138.4, 135.1, 130.5, 128.3, 127.6, 123.9, 66.8, 48.1, 42.4, 21.3.

(*S*)-*N*-(1-hydroxybutan-2-yl)-3-methylbenzamide (**57**):



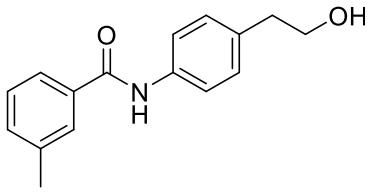
Pale yellow solid, 64% yield. (Method B). M.p. 93-94ºC. $[\alpha]_D^{20}$ = +33.1 (*c*=1.0, $CHCl_3$) TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.57 (*tt*, *J* = 1.6, 0.8 Hz, 1H), 7.57 – 7.50 (*m*, 1H), 7.31 – 7.23 (*m*, 2H), 6.54 (*d*, *J* = 8.0 Hz, 1H), 4.04 (*tddd*, *J* = 8.2, 6.3, 5.2, 3.5 Hz, 1H), 3.75 (*dd*, *J* = 11.2, 3.6 Hz, 1H), 3.68 (*dd*, *J* = 11.1, 5.2 Hz, 1H), 3.42 (*s*, 1H), 2.35 (*s*, 3H), 1.75 – 1.56 (*m*, 2H), 0.99 (*t*, *J* = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.6, 138.5, 134.5, 132.4, 128.5, 127.8, 124.1, 65.1, 53.7, 53.7, 24.4, 21.4, 10.8. MS (CI+) m/z (rel. int.): 119 (3-methylbenzoyl, 100), 208 (M+1, 45).

3-methyl-*N*-(*N*-(*N*-phenylcarbamimidoyl)carbamimidoyl)benzamide (**58**):



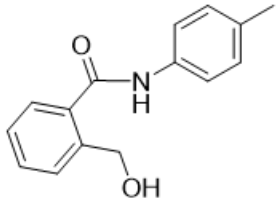
White solid, 76% yield. (Method B). M.p. 79-80ºC. TLC: DCM/MTBE 10:1, 1x. Column chromatography: DCM - DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.16 – 8.11 (m, 2H), 7.65 (s, 1H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.36 – 7.29 (m, 2H), 7.32 – 7.27 (m, 2H), 7.09 – 7.03 (m, 1H), 5.67 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 172.4, 167.5, 165.0, 138.5, 138.1, 136.5, 132.6, 129.0, 128.9, 128.4, 125.7, 123.6, 120.8, 53.6, 21.6. MS (CI+) m/z (rel. int.): 278 (M-OH, 100).

N-(4-(3-hydroxypropyl)phenyl)-3-methylbenzamide (**59**):



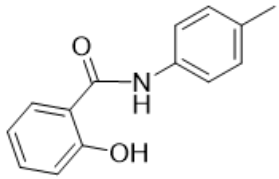
Pale brown solid, 42% yield. (Method B). M.p. 110-111ºC. TLC: DCM/MTBE 10:1, 1x. Column chromatography: DCM - DCM/MTBE 20:1. ^{1}H NMR (600 MHz, DMSO-d^6) δ (ppm) = 10.25 (*s*, 1H), 7.89 – 7.82 (*m*, 2H), 7.80 – 7.75 (*m*, 2H), 7.54 – 7.47 (*m*, 2H), 7.31 – 7.27 (*m*, 2H), 4.76 (*t*, *J* = 5.2 Hz, 1H), 3.70 (*td*, *J* = 7.2, 5.2 Hz, 2H), 2.80 (*t*, *J* = 7.1 Hz, 2H), 2.50 (*s*, 3H). ^{13}C NMR (151 MHz, DMSO-d^6) δ (ppm) = 165.5, 137.7, 137.2, 135.1, 134.8, 132.1, 129.0, 128.3, 128.1, 124.8, 120.3, 62.3, 40.1, 38.6, 21.0. MS (ESI+) m/z (rel. int.): 256 (M+1, 45), 278 (M+Na, 100).

2-(hydroxymethyl)-*N*-(*p*-tolyl)benzamide (**60**):



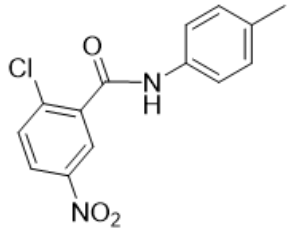
White solid, 81% yield. (Method B). M.p. 169-170ºC. TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, DMSO-d^6) δ (ppm) = 10.29 (*s*, 1H), 7.64 – 7.57 (*m*, 3H), 7.54 – 7.46 (*m*, 2H), 7.37 (*td*, *J* = 7.5, 1.3 Hz, 1H), 7.14 (*d*, *J* = 8.2 Hz, 2H), 5.32 (*t*, *J* = 5.5 Hz, 1H), 4.66 (*d*, *J* = 5.4 Hz, 2H), 2.27 (*s*, 3H). ^{13}C NMR (151 MHz, DMSO-d^6) δ (ppm) = 167.2, 140.3, 136.8, 135.3, 132.5, 129.9, 129.1, 127.5, 127.5, 126.7, 119.8, 60.8, 40.1, 20.5. MS (ESI+) m/z (rel. int.): 224 (M-OH, 55), 242 (M+1, 25), 264 (M+23, 100).

2-hydroxy-*N*-(*p*-tolyl)benzamide (**61**) [10]:



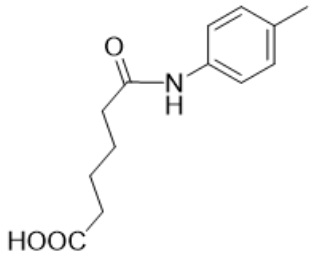
White solid, 81% yield. (Method B). M.p. 169-170ºC. TLC: DCM/MTBE 5:1, 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 12.06 (*s*, 1H), 7.89 (*s*, 1H), 7.50 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.47 – 7.41 (m, 3H), 7.22 – 7.17 (*m*, 2H), 7.03 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.91 (*ddd*, *J* = 8.2, 7.2, 1.2 Hz, 1H), 2.35 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 168.3, 161.8, 135.2, 134.6, 133.9, 129.7, 125.3, 121.3, 118.9, 118.9, 114.5, 20.9.

2-chloro-5-nitro-*N*-(*p*-tolyl)benzamide (**62**) [11]:



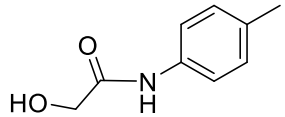
Pale yellow solid, 25% yield. (Method B). TLC: DCM/PE 1:1, 1x. Column chromatography: DCM/PE 1:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.57 (*d*, *J* = 2.7 Hz, 1H), 8.23 (*dd*, *J* = 8.8, 2.7 Hz, 1H), 7.86 (*s*, 1H), 7.63 (*d*, *J* = 8.8 Hz, 1H), 7.52 – 7.47 (*m*, 2H), 7.22 – 7.17 (*m*, 2H), 2.36 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 162.0, 146.6, 137.5, 136.6, 135.3, 134.3, 131.5, 129.7, 125.9, 125.3, 120.4, 21.0.

6-oxo-6-(*p*-tolylamino)hexanoic acid (**63**):



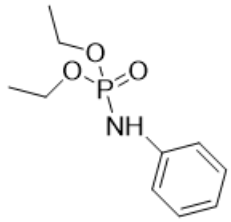
White solid, 63% yield. (Method B). M.p. 164-165ºC. TLC: DCM/*i*PrOH 20:1. Column chromatography: DCM/*i*PrOH 40:1. ^{1}H NMR (600 MHz, DMSO-d^{6}) δ (ppm) = 12.03 (*s*, 1H), 9.78 (*s*, 1H), 7.48 – 7.44 (*m*, 2H), 7.07 (*d*, *J* = 8.2 Hz, 2H), 2.33 – 2.16 (*m*, 9H), 1.63 – 1.48 (*m*, 2H). ^{13}C NMR (151 MHz, DMSO-d^{6}) δ (ppm) = 174.4, 170.8, 136.9, 131.8, 129.1, 119.1, 72.2, 40.1, 38.6, 36.1, 33.5, 25.3, 25.0, 24.7, 24.2, 23.0, 20.5, 14.2. MS (CI+) m/z (rel. int.): 107 (4-methylaniline, 32), 218 (M-OH, 100), 235 (M+1, 19).

2-hydroxy-N-(p-tolyl)acetamide (**64**) [12]:



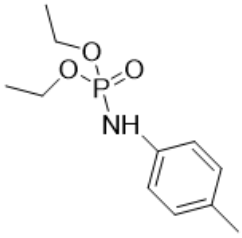
White solid, 53% yield. (Method B). TLC: DCM/MTBE 5:1 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, CD_3OD) δ (ppm) = 7.45 – 7.48 (m, 2H), 7.12 – 7.15 (m, 2H), 4.09 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, CD_3OD) δ (ppm) = 173.2, 136.3, 135.3, 130.3, 121.6, 62.9, 20.9.

Diethyl phenylphosphoramidate (**70**) [13]:



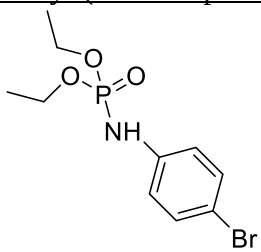
White solid, 81% yield. (Method B). TLC: DCM/MTBE 5:1 1x. Column chromatography: DCM/MTBE 20:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.27 – 7.21 (*m*, 2H), 7.06 – 7.01 (*m*, 2H), 6.94 (*tt*, *J* = 7.4, 1.1 Hz, 1H), 6.89 (*d*, *J* = 9.6 Hz, 1H), 4.18 (*dp*, *J* = 10.1, 7.2 Hz, 2H), 4.09 (*ddq*, *J* = 10.1, 7.9, 7.1 Hz, 2H), 1.31 (*td*, *J* = 7.1, 0.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 139.9, 129.2, 121.3, 117.2 (J_{CP} = 7.4 Hz), 62.6, 62.6, 16.1, 16.0.

Diethyl *p*-tolylphosphoramidate (**71**) [14]:



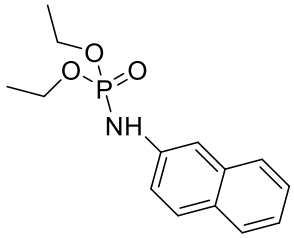
White solid, 87% yield. (Method B). TLC: DCM/MTBE 10:1. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.06 – 7.01 (*m*, 2H), 6.96 – 6.90 (*m*, 2H), 6.61 (d, *J* = 9.6 Hz, 1H), 4.17 (*dp*, *J* = 10.1, 7.2 Hz, 2H), 4.07 (*ddq*, *J* = 10.1, 7.9, 7.1 Hz, 2H), 2.27 (*s*, 3H), 1.30 (*td*, *J* = 7.0, 0.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 137.2, 130.7, 129.7, 117.2 (J_{CP} = 7.1 Hz), 62.5, 62.5, 20.5, 16.1, 16.0.

Diethyl (4-bromophenyl)phosphoramidate (**72**) [15]:



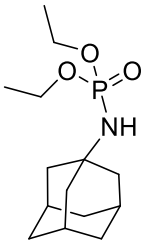
White solid, 84% yield. (Method B). TLC: DCM/MTBE 10:1 2x. Column chromatography: DCM, DCM/MTBE 20:1-10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.35 – 7.29 (m, 2H), 7.26 (d, *J* = 9.6 Hz, 1H), 6.95 – 6.89 (m, 2H), 4.20 – 4.01 (m, 4H), 1.30 (td, *J* = 7.1, 0.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 139.4, 132.2, 118.8 (J_{CP} = 7.6 Hz), 113.9, 62.77, 62.74, 16.07, 16.02.

Diethyl naphthalen-2-ylphosphoramidate (**73**):



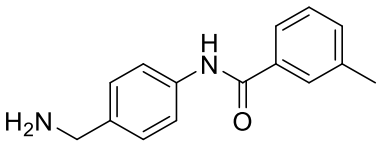
Colorless oil, 78% yield. (Method B). TLC: DCM/MTBE 10:1 2x. Column chromatography: DCM, DCM/MTBE 20:1-10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.80 – 7.73 (*m*, 3H), 7.49 – 7.43 (*m*, 2H), 7.39 – 7.25 (*m*, 2H), 4.27 (*dp*, *J* = 10.2, 7.2 Hz, 2H), 4.16 (*ddt*, *J* = 15.1, 10.1, 7.1 Hz, 2H), 1.36 (*td*, *J* = 7.1, 0.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 137.8, 134.4, 129.3, 127.7, 126.9, 126.6, 124.0, 119.2, 119.1, 112.4, 112.3, 62.9, 62.9, 16.3, 16.2. MS (ESI+) m/z (rel. int.): 280 (M+1, 100), 302 (M+Na, 46), 581 (2M+Na, 30).

Diethyl-(adamantan-1-yl)phosphoramidate (**74**) [16]:



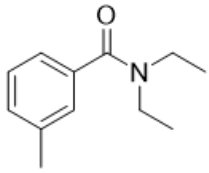
White solid, 81% yield. (Method B). M.p 96-97ºC. TLC: DCM/MTBE 5:1 1x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 4.13 – 4.00 (m, 4H), 2.50 (d, *J* = 7.8 Hz, 1H), 2.06 (q, *J* = 3.3 Hz, 3H), 1.81 (d, *J* = 2.9 Hz, 6H), 1.68 – 1.58 (m, 6H), 1.33 (td, *J* = 7.1, 0.8 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) =62.2, 62.1, 50.9, 44.33 (J_{CP} = 4.5 Hz), 36.2, 29.8, 16.4, 16.3. MS (CI+) m/z (rel. int.): 135 (adamantane-1, 23), 230 (M-H-2Et, 28), 288 (M+1, 100).

N-(4-(aminomethyl)phenyl)-3-methylbenzamide (**77**):



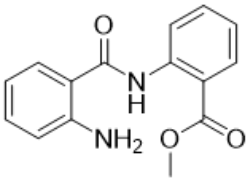
White solid, 70% yield. (Method B). TLC: MTBE/i-PrOH 10:1 1x. Column chromatography: MTBE/i-PrOH 10:1. ^{1}H NMR (600 MHz, DMSO-d^6) δ (ppm) = 10.16 (s, 1H), 7.78 – 7.72 (m, 2H), 7.72 – 7.66 (m, 2H), 7.44 – 7.36 (m, 2H), 7.35 – 7.28 (m, 2H), 3.70 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d^6) δ (ppm) = 165.5, 139.0, 137.7, 137.5, 135.0, 132.2, 128.3, 128.1, 127.3, 124.8, 120.2, 5.1, 40.1, 21.0. MS (CI+) m/z (rel. int.): 224 (M-NH_3, 100), 241 (M+1, 49).

N,*N*-diethyl-3-methylbenzamide (**78**) [17]:



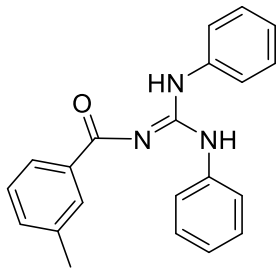
Colorless oil, 94% yield. (Method B). TLC: DCM/MTBE 10:1, 1x. Column chromatography: DCM-DCM/MTBE 20:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 7.28-7.24 (*m*, 1H), 7.22 – 7.12 (*m*, 3H), 3.54 (br. *s*, 2H), 3.25 (br. *s*, 2H), 2.37 (*s*, 3H), 1.24 (br. *s*, 3H), 1.10 (br. *s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 171.5, 138.2, 137.2, 129.7, 128.2, 126.9, 123.1, 43.2, 39.1, 21.4, 14.2, 12.9.

Methyl 2-(2-aminobenzamido)benzoate (**79**) [18]:



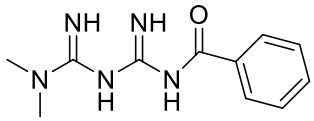
White solid, 80% yield. (Method A). TLC: DCM/MTBE 5:1, 2x. Column chromatography: DCM/MTBE 10:1. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 11.80 (*s*, 1H), 8.80 (*dd*, *J* = 8.6, 1.1 Hz, 1H), 8.08 – 8.02 (*m*, 1H), 7.72 (*dd*, *J* = 8.0, 1.4 Hz, 1H), 7.57 (*ddd*, *J* = 8.8, 7.2, 1.7 Hz, 1H), 7.27 – 7.22 (*m*, 1H), 7.11 – 7.05 (*m*, 1H), 6.76 (*ddd*, *J* = 8.1, 7.1, 1.2 Hz, 1H), 6.69 (*dd*, *J* = 8.2, 1.1 Hz, 1H), 5.75 (*s*, 2H), 3.93 (*s*, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm) = 168.9, 168.1, 149.8, 141.9, 134.6, 132.8, 130.9, 127.6, 122.3, 120.4, 117.5, 116.9, 115.7, 115.3, 52.4.

N-(bis(phenylamino)methylene)-3-methylbenzamide (**81**):



White solid, 88% yield. (Method A). M.p. 96-97ºC. TLC: DCM/MTBE 20:1, 1x. Column chromatography: DCM - DCM/MTBE 20:1. ^{1}H NMR (600 MHz, DMSO-d^{6}) δ (ppm) = 10.29 (br s, 2H, NH), 7.81 (br s, 2H), 7.00-7.67 (m, 12H), 2.35 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d^{6}) δ (ppm) = 136.66, 131.46, 128.81, 128.29, 127.40, 125.27, 122.84, 20.45. MS (ESI+) m/z (rel. int.): 330 (M+1, 100).

N-(*N*-(*N*,*N*-dimethylcarbamimidoyl)carbamimidoyl)benzamide (**83**) [19]:



White solid, 76% yield. (Method A). TLC: DCM/MTBE 10:1 1x. Column chromatography: DCM/i-PrOH. ^{1}H NMR (600 MHz, DMSO-d^{6}): δ (ppm) = 8.30 (*m*, 2H), 7.54 – 7.49 (*m*, 1H), 7.49 – 7.44 (*m*, 2H), 6.87 (*s*, 2H), 3.20 (*s*, 3H), 3.09 (*s*, 3H). ^{13}C NMR (151 MHz, DMSO-d^{6}) δ (ppm) = 169.3, 167.1, 165.5, 137.2, 131.1, 128.2, 127.8, 40.1, 35.8.

References:

1. *Org. Lett.*, **2019**, *21*, pp 4878–4881. https://doi.org/10.1021/acs.orglett.9b01772
2. *J. Org. Chem.*, **2018**, *83*, pp 14307–14313. https://doi.org/10.1021/acs.joc.8b01956
3. *Tetrahedron*, **2018**, *74*, pp 2030-2040. https://doi.org/10.1016/j.tet.2018.03.007
4. *Tetrahedron*, **2020**, *76*, 131079. https://doi.org/10.1016/j.tet.2020.131079
5. *J. Org. Chem.*, **2016**, *81*, pp 10688–10697. https://doi.org/10.1021/acs.joc.6b01686
6. *Org. Biomol. Chem.*, **2015**, *13*, pp 10888-10894. https://doi.org/10.1039/C5OB01801C
7. *J. Org. Chem.*, **2012**, *77*, pp 9553–9561. https://doi.org/10.1021/jo301466w
8. *Chem. Commun.*, **2014**, *50*, pp 14775-14777. https://doi.org/10.1039/C4CC07378A
9. *Green Chem.*, **2015**, *17*, pp 2741-2744. https://doi.org/10.1039/C5GC00299K
10. *Synth. Comm.*, **2011**, *41*, pp 1275-1266. https://doi.org/10.1080/00397911.2010.481745
11. *Bioorg. Med. Chem. Lett.*, **2010**, *20*, pp 149-152. https://doi.org/10.1016/j.bmcl.2009.11.022
12. *J. Am. Chem. Soc.*, **2016**, *138*, pp 14218–14221. https://doi.org/10.1021/jacs.6b09482
13. *J. Org. Chem.*, **2020**, *85*, pp 14545–14558. https://doi.org/10.1021/acs.joc.0c01151
14. *Org. Lett.*, **2020**, *22*, pp 6143–6149. https://doi.org/10.1021/acs.orglett.0c02207
15. *Org. Biomol. Chem.*, **2021**, *24*, pp 5342-5347. https://doi.org/10.1039/D1OB00779C
16. *Tetrahedron Lett.*, **2006**, *47*, pp 6281-6284. https://doi.org/10.1016/j.tetlet.2006.06.126
17. *Synthesis*, **2016**, *48*, pp 2069-2078. http://dx.doi.org/10.1055/s-0035-1561427
18. *RSC Adv.*, **2016,** *6*, pp 27378-27387. https://doi.org/10.1039/C6RA00855K
19. *Eur. J. Med. Chem.*, **2020**, *200*, 112462. https://doi.org/10.1016/j.ejmech.2020.112462

2. X-ray

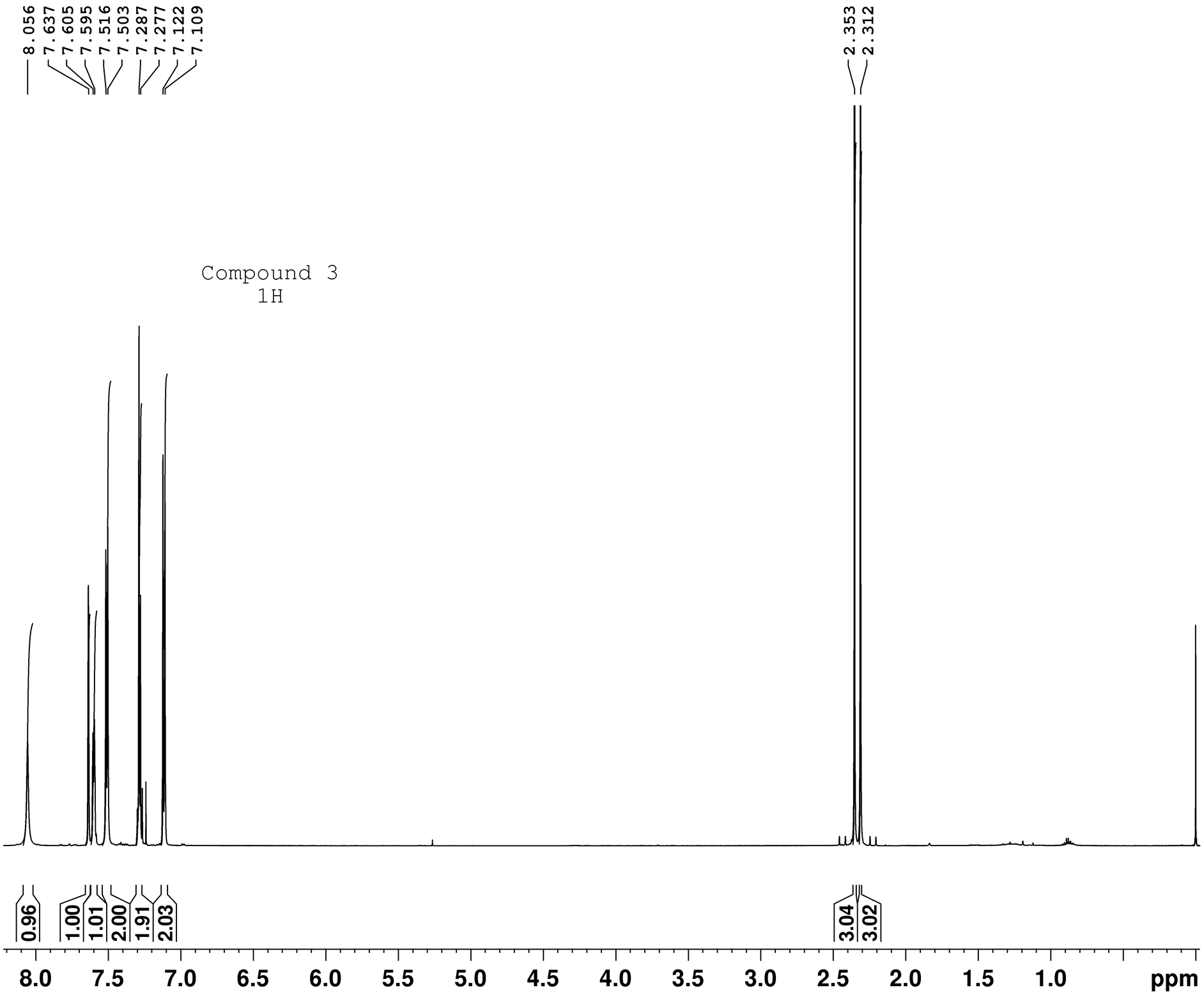
X-ray data for **77·HCl** was measured using a Bruker-Nonius KappaCCD diffractometer with an APEX-II detector with graphite-monochromatized Mo-*K*α (λ = 0.71073 Å) radiation. Data collection and reduction were performed using the program *COLLECT*[1] and *HKL DENZO AND SCALEPACK*,[2] respectively, and the intensities were corrected for absorption using *SADABS*.[3] Single-crystal X-ray data for **81** was measured using an Agilent SuperNova dual-source Oxford diffractometer equipped with an Eos detector using mirror-monochromated Cu-*K*α (λ = 1.54184 Å) radiation. The data collection and reduction were performed using the program *CrysAlisPro* and Gaussian face index absorption correction method was applied.[4] The structures were solved with intrinsic phasing (ShelXT)[5] and refined by full-matrix least squares on F^2 using the *Olex2* software,[6] which utilises the ShelXL-2015 module.[7] Anisotropic displacement parameters were assigned to non-H atoms and isotropic displacement parameters for all H atoms were constrained to multiples of the equivalent displacement parameters of their parent atoms with $U_{iso}(H) = 1.2\ U_{eq}$ (aromatic) or $U_{iso}(H) = 1.5\ U_{eq}$ (alkyl) of their respective parent atoms. The X-ray single crystal data and CCDC numbers of all new structures are included below.

Crystals suitable for single crystal X-ray diffraction were obtained by slow evaporation of a 4:1 dichloromethane:acetonitrile solution of **77**. Crystal data for **77·HCl**: CCDC-2127766, $[C_{15}H_{17}N_2O]Cl$, M = 276.75, colourless needle, 0.04 × 0.06 × 0.28=2 mm^3, monoclinic, space group $P2_1/n$, a = 4.8798(3) Å, b = 17.8602(9) Å, c = 15.7045(8) Å, β = 90.206(3)°, V = 1368.70(13) $Å^3$, Z = 4, D_{calc} = 1.343 gcm^{-3}, F(000) = 584, μ = 0.27 mm^{-1}, T = 170.0(1) K, θ_{max} = 27.9°, 2490 total reflections, 1526 with $I_o > 2\sigma(I_o)$, R_{int} = 0.088, 2490 data, 177 parameters, no restraints, GooF = 1.03, 0.30 < dΔρ < –0.30 $eÅ^{-3}$, $R[F^2 > 2\sigma(F^2)] = 0.071$, $wR(F^2) = 0.151$.

Crystals suitable for single crystal X-ray diffraction were obtained by slow evaporation of a diisopropyl ether solution of **81**. Crystal data for **81**: CCDC-2127765, $C_{21}H_{19}N_3O$, M = 329.39, colourless plate, 0.03 × 0.19 × 0.28 mm^3, monoclinic, space group $P2_1/c$, a = 8.7084(3) Å, b = 10.2040(5) Å, c = 19.0448(7) Å, β = 92.691(4)°, V = 1690.46(12) $Å^3$, Z = 4, D_{calc} = 1.294 gcm^{-3}, F(000) = 696, μ = 0.64 mm^{-1}, T = 120.0(1) K, θ_{max} = 76.0°, 3428 total reflections, 2754 with $I_o > 2\sigma(I_o)$, R_{int} = 0.029, 3428 data, 233 parameters, no restraints, GooF = 1.03, 0.26 < dΔρ < –0.23 $eÅ^{-3}$, $R[F^2 > 2\sigma(F^2)] = 0.043$, $wR(F^2) = 0.118$.

[1] R.W.W. Hooft, *COLLECT* **1998**, Nonius BV, Delft, The Netherlands.
(computer program - no DOI: https://iucrdata.iucr.org/x/services/stdswrefs.html)
[2] Otwinowski, Z.; Minor, W. *Methods in Enzymology, Macromolecular Crystallography, Part A* **1997**, 276, 307-326. Edited by C. W. Carter Jr & R. M. Sweet, New York: Academic Press.
(https://doi.org/10.1016/S0076-6879(97)76066-X)
[3] Sheldrick, G. M. *SADABS* Version 2008/2 **1996**, University of Göttingen, Germany.
(computer program - no DOI: https://iucrdata.iucr.org/x/services/stdswrefs.html)
[4] Rigaku Oxford Diffraction, 2018, *CrysAlisPro* Software system, Rigaku Corporation, Oxford, UK.
(computer program - no DOI: https://iucrdata.iucr.org/x/services/stdswrefs.html)
[5] G. M. Sheldrick, *Acta Crystallogr. Sect. A*, 2015, **71**, 3–8.
(https://doi.org/10.1107/S2053273314026370)
[6] O. V Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339–341.
(https://doi.org/10.1107/S0021889808042726)
[7] G. M. Sheldrick, *Acta Crystallogr. Sect. C*, 2015, **71**, 3–8.
(https://doi.org/10.1107/S2053229614024218)

^{1}H and ^{13}C NMR images

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TE                 293.0 K
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P0                  3.60 usec
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PLW1         20.00000000 W

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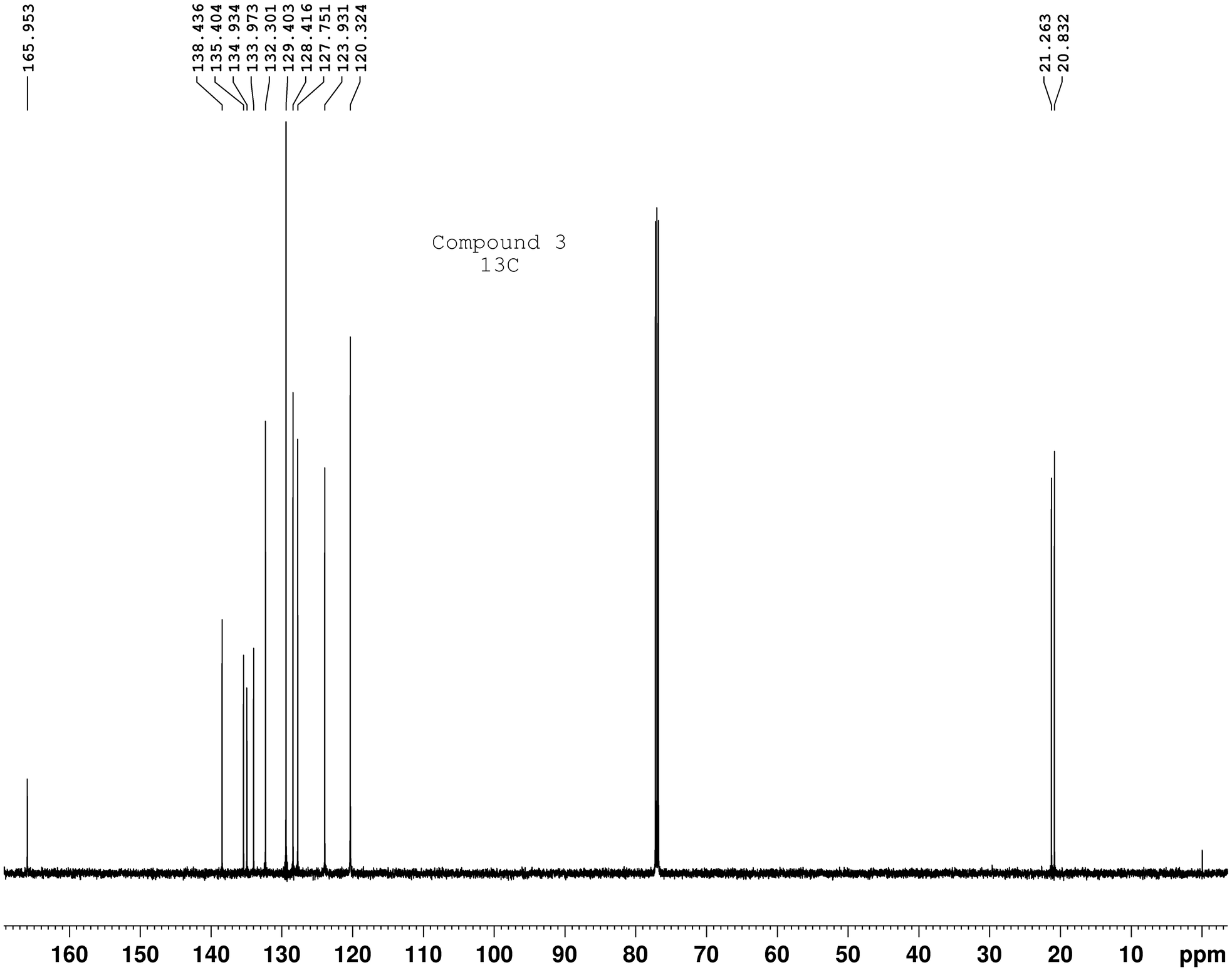


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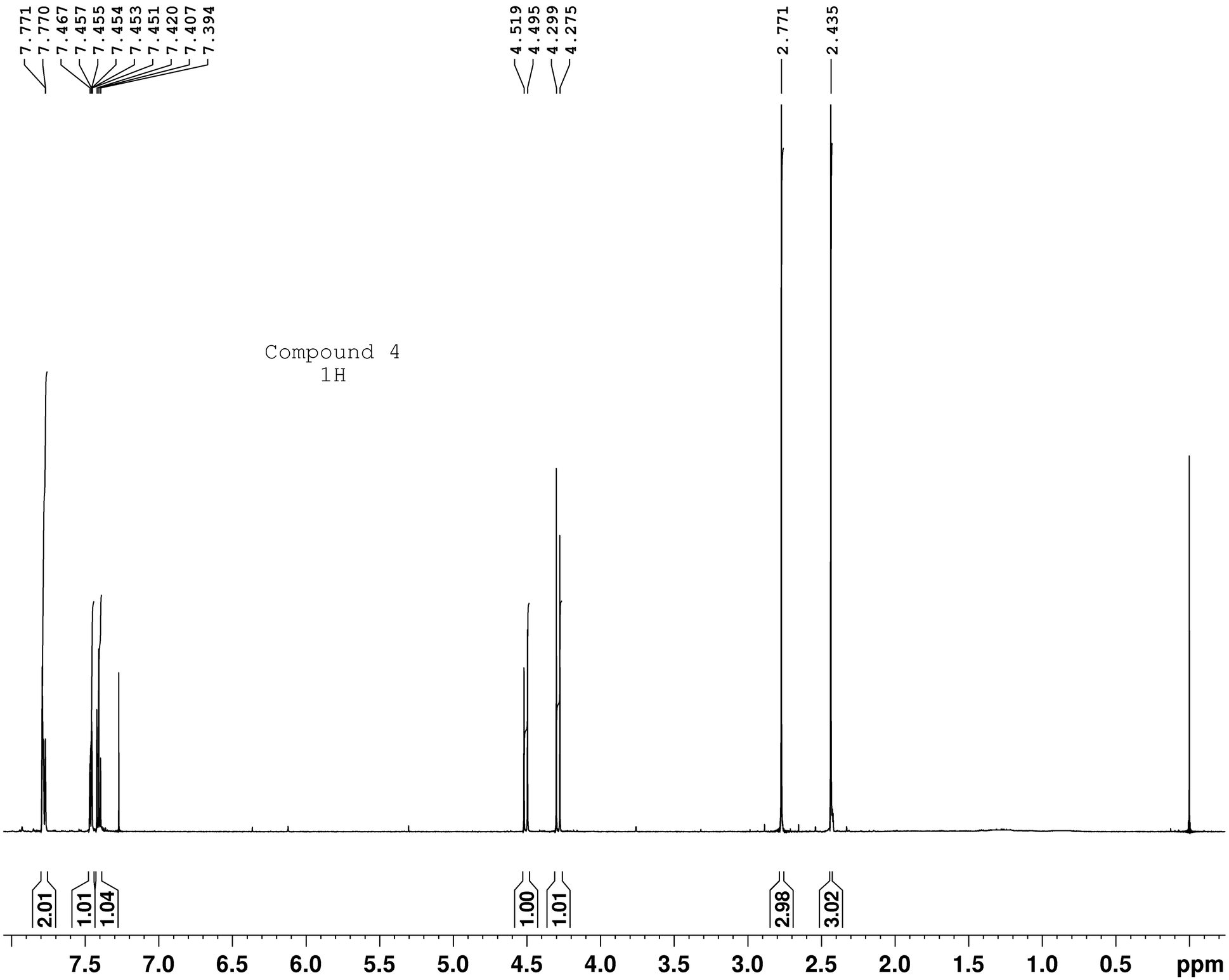


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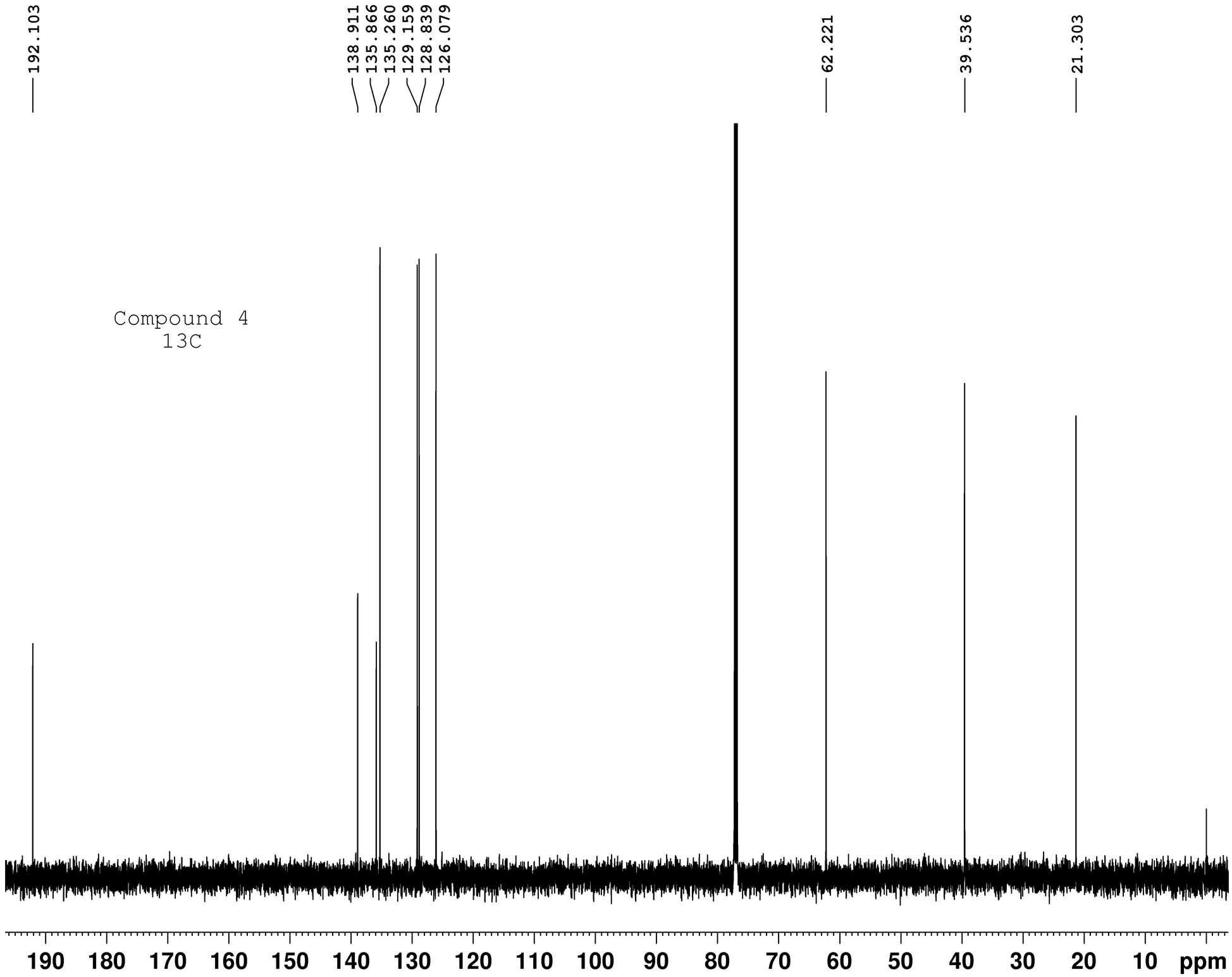


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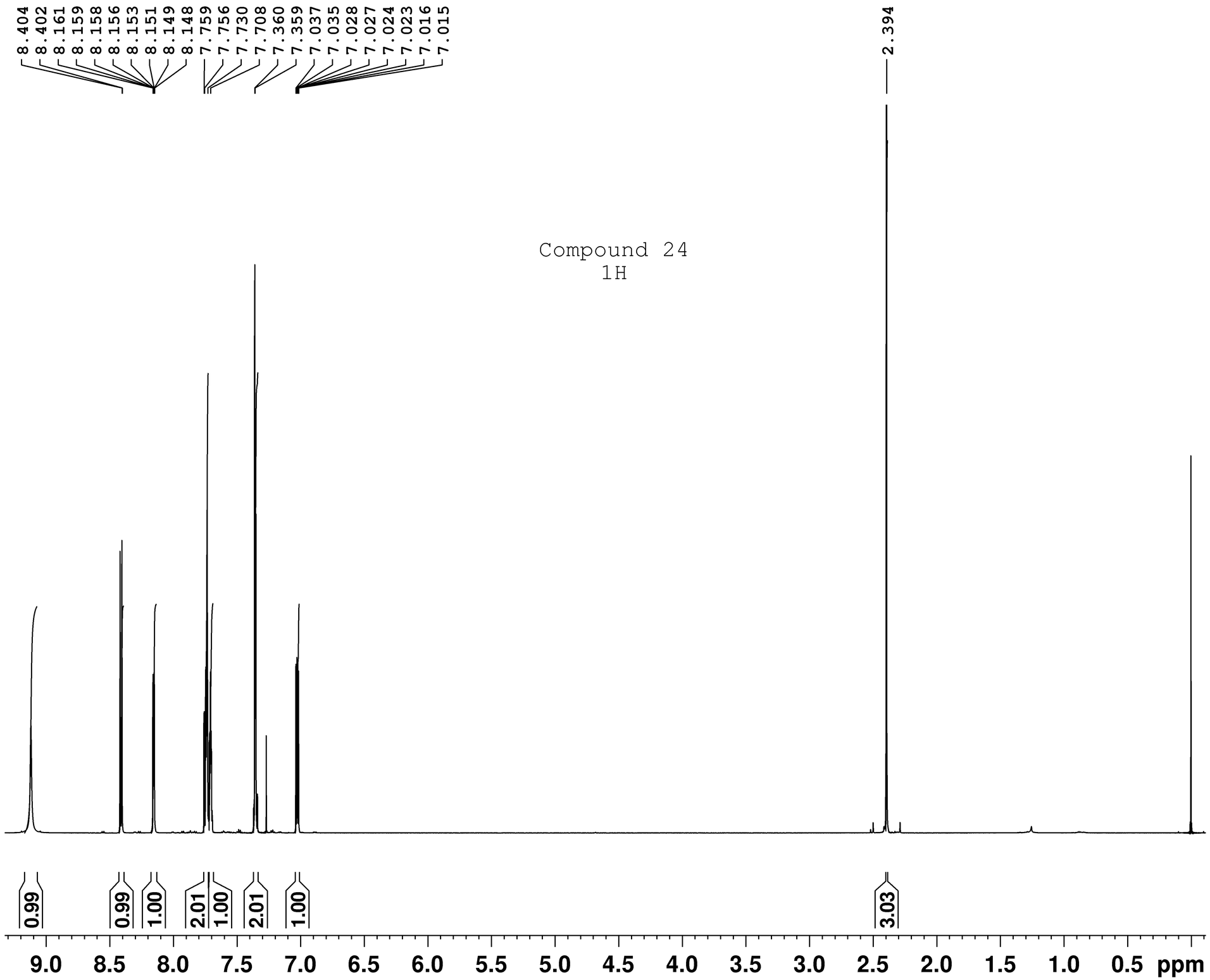
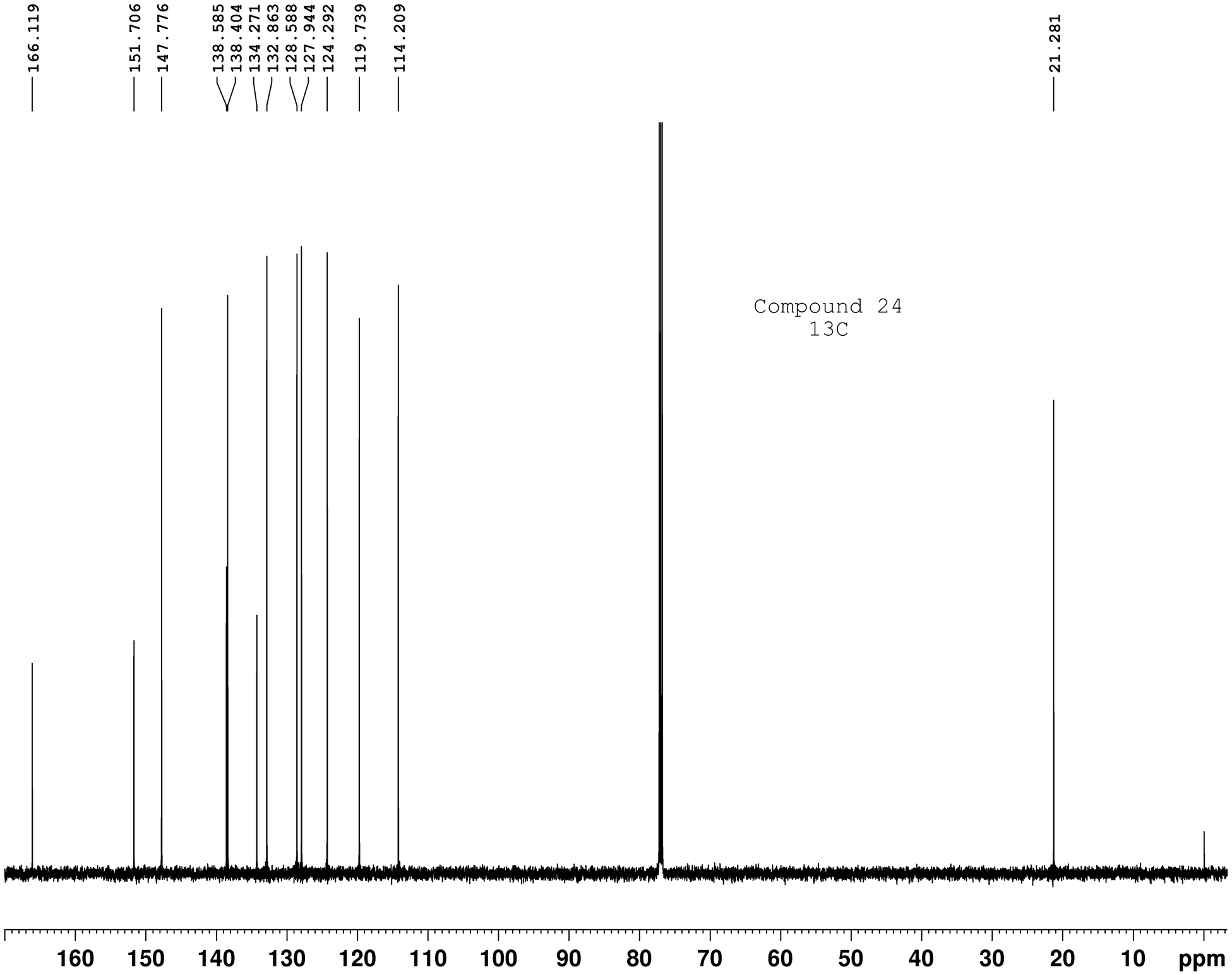
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          24-CD-109
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20220111
Time              16.43 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ            1.7039360 sec
RG                 90.5
DW               52.000 usec
DE                14.38 usec
TE                293.0 K
D1           1.00000000 sec
TD0                   1
SFO1        599.9845606 MHz
NUC1                 1H
P0                 3.60 usec
P1                10.80 usec
PLW1        20.00000000 W

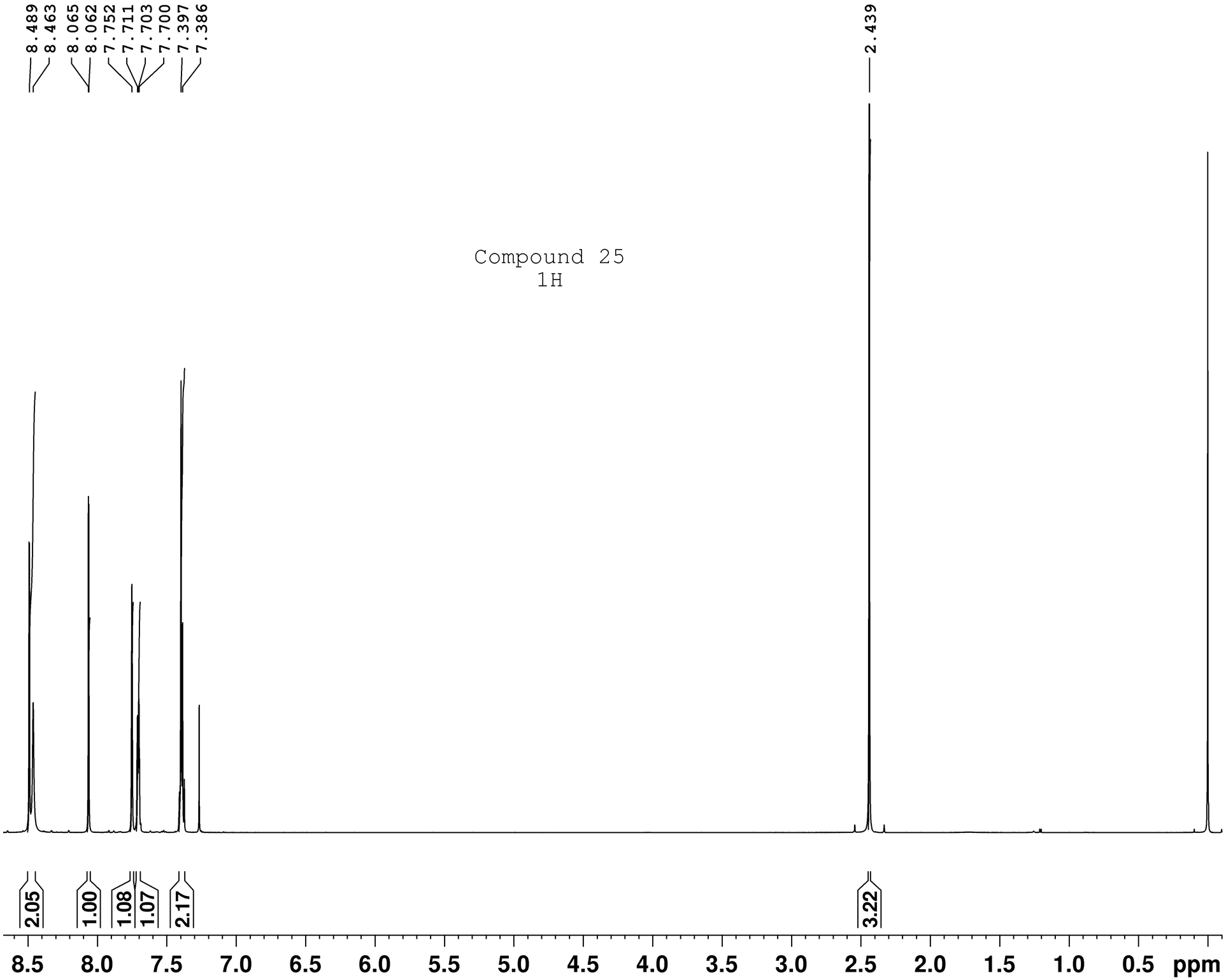
F2 - Processing parameters
SI                65536
SF          599.9800087 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME              CD-109
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220111
Time               16.49 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                 2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                 3.27 usec
P1                 9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

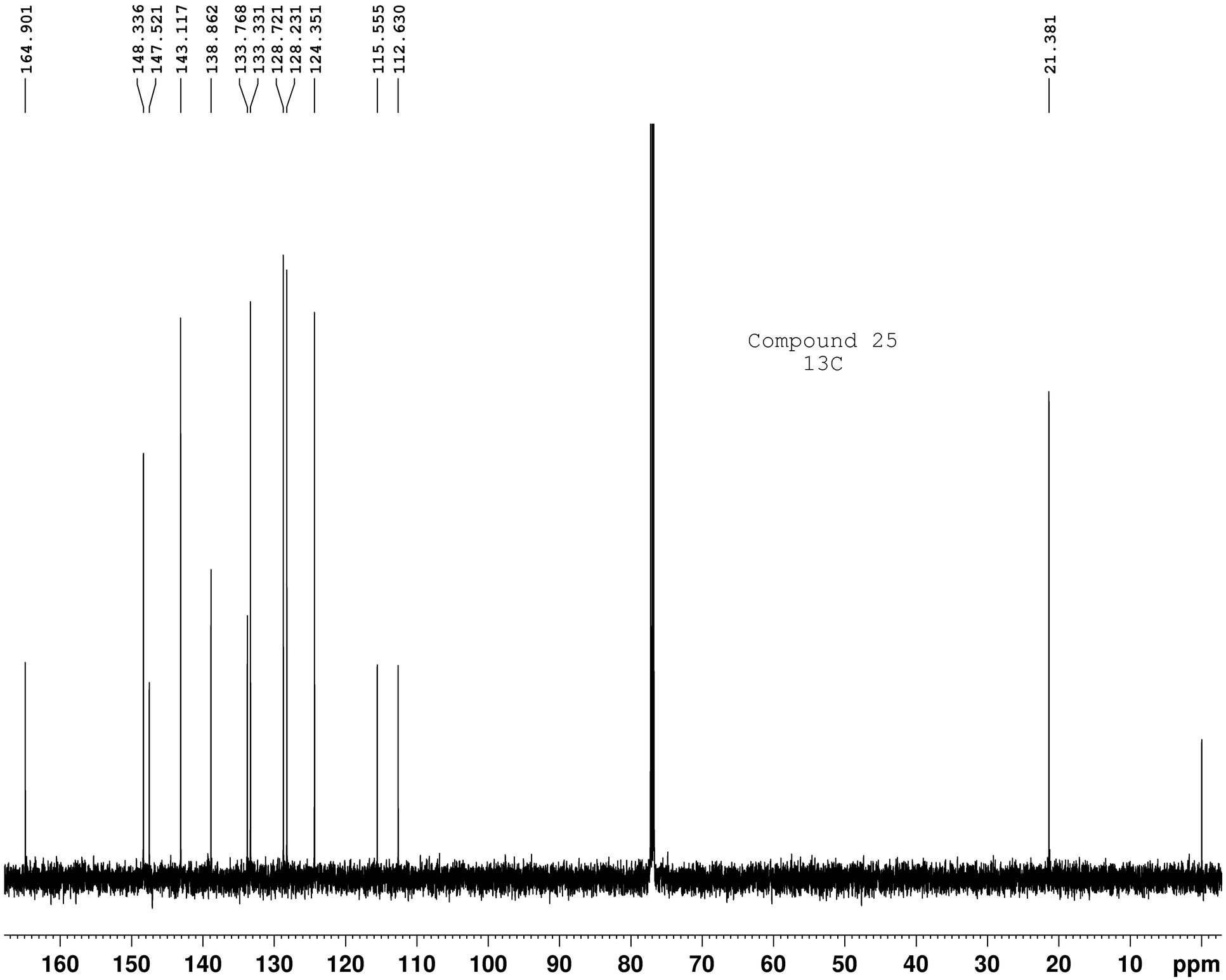
F2 - Processing parameters
SI                65536
SF           150.8651044 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME              CD-99A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210217
Time               18.33 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   161
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

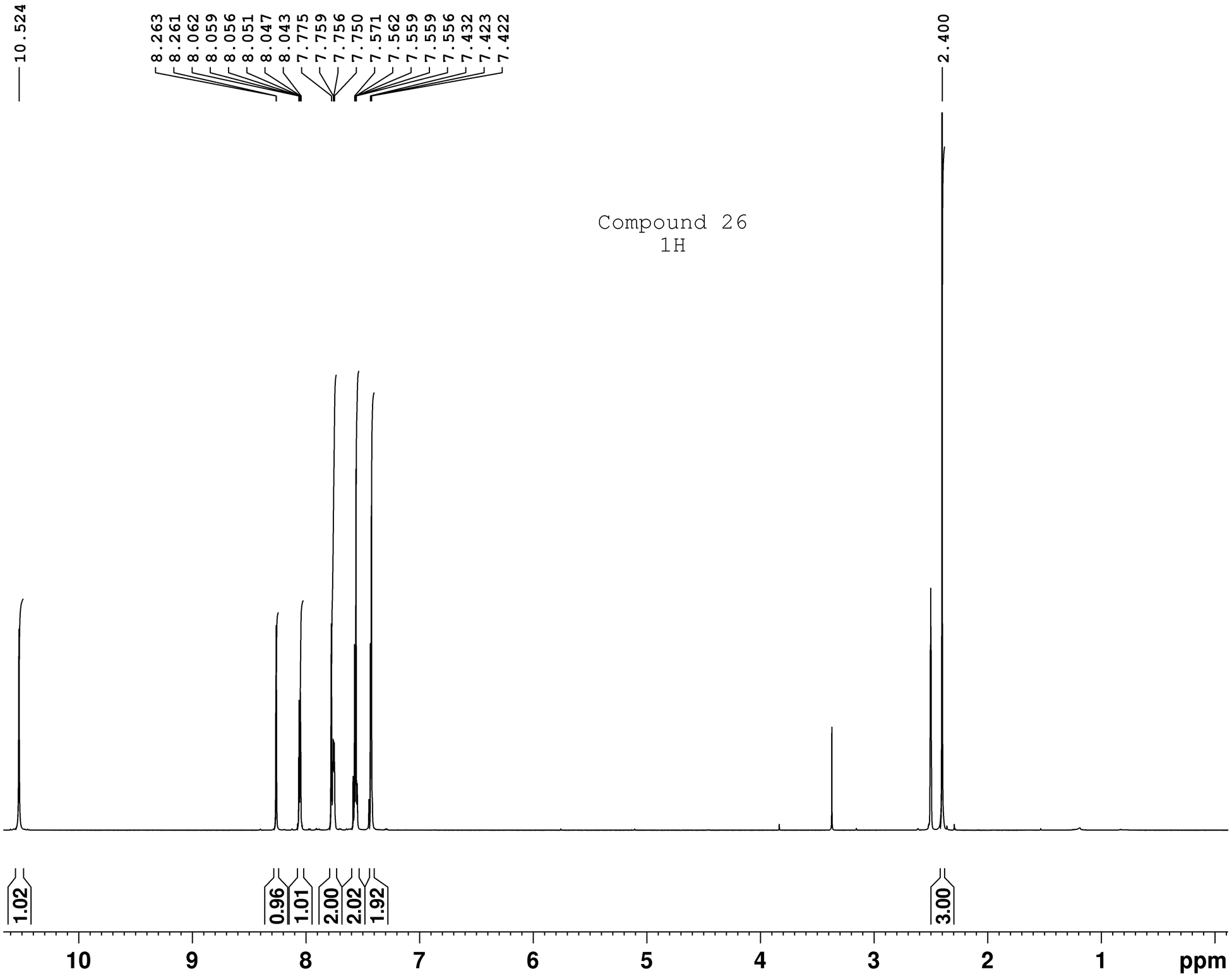
F2 - Processing parameters
SI                 65536
SF           600.0100104 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CD-99A
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210217
Time              19.08 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8892338 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        600.0124004 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        20.00000000 W
PLW12        0.33800000 W

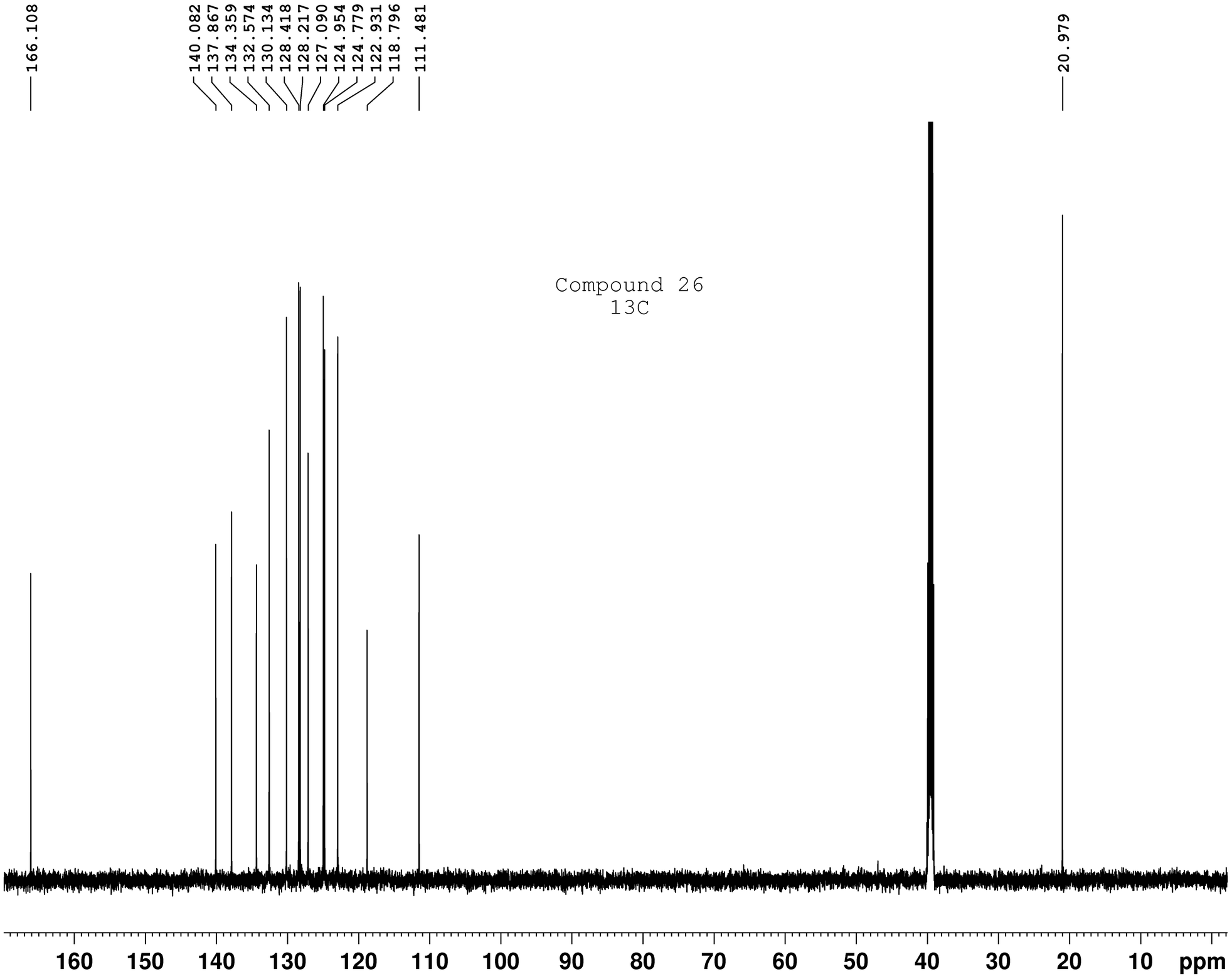
F2 - Processing parameters
SI                65536
SF          150.8726459 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME              CD-130A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210426
Time               18.08 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                     32
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  90.5
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                     1
SFO1         600.0145608 MHz
NUC1                   1H
P0                   3.62 usec
P1                  10.85 usec
PLW1         20.00000000 W

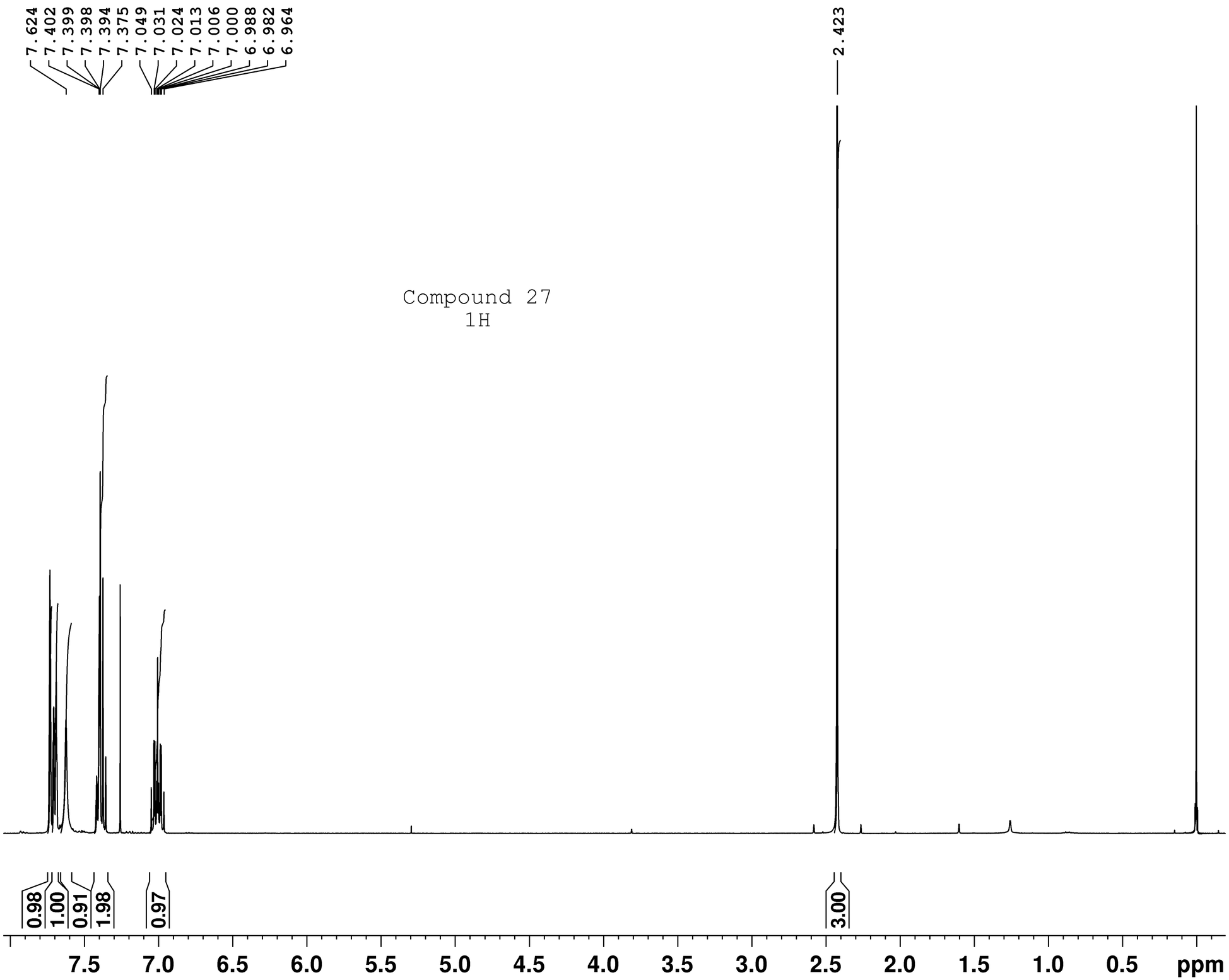
F2 - Processing parameters
SI                  65536
SF           600.0100047 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME                CD-130A
EXPNO                    16
PROCNO                    1

F2 - Acquisition Parameters
Date_             20210426
Time                 18.43 h
INSTRUM              spect
PROBHD    Z847801_0047 (
PULPROG             zgdc30
TD                   32768
SOLVENT               DMSO
NS                     128
DS                       0
SWH              36057.691 Hz
FIDRES            2.200787 Hz
AQ               0.4543829 sec
RG                    2050
DW                  13.867 usec
DE                    6.50 usec
TE                   293.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           150.8892338 MHz
NUC1                   13C
P0                    3.27 usec
P1                    9.80 usec
PLW1           40.00000000 W
SFO2           600.0124004 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           20.00000000 W
PLW12           0.33800000 W

F2 - Processing parameters
SI                    65536
SF             150.8727014 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

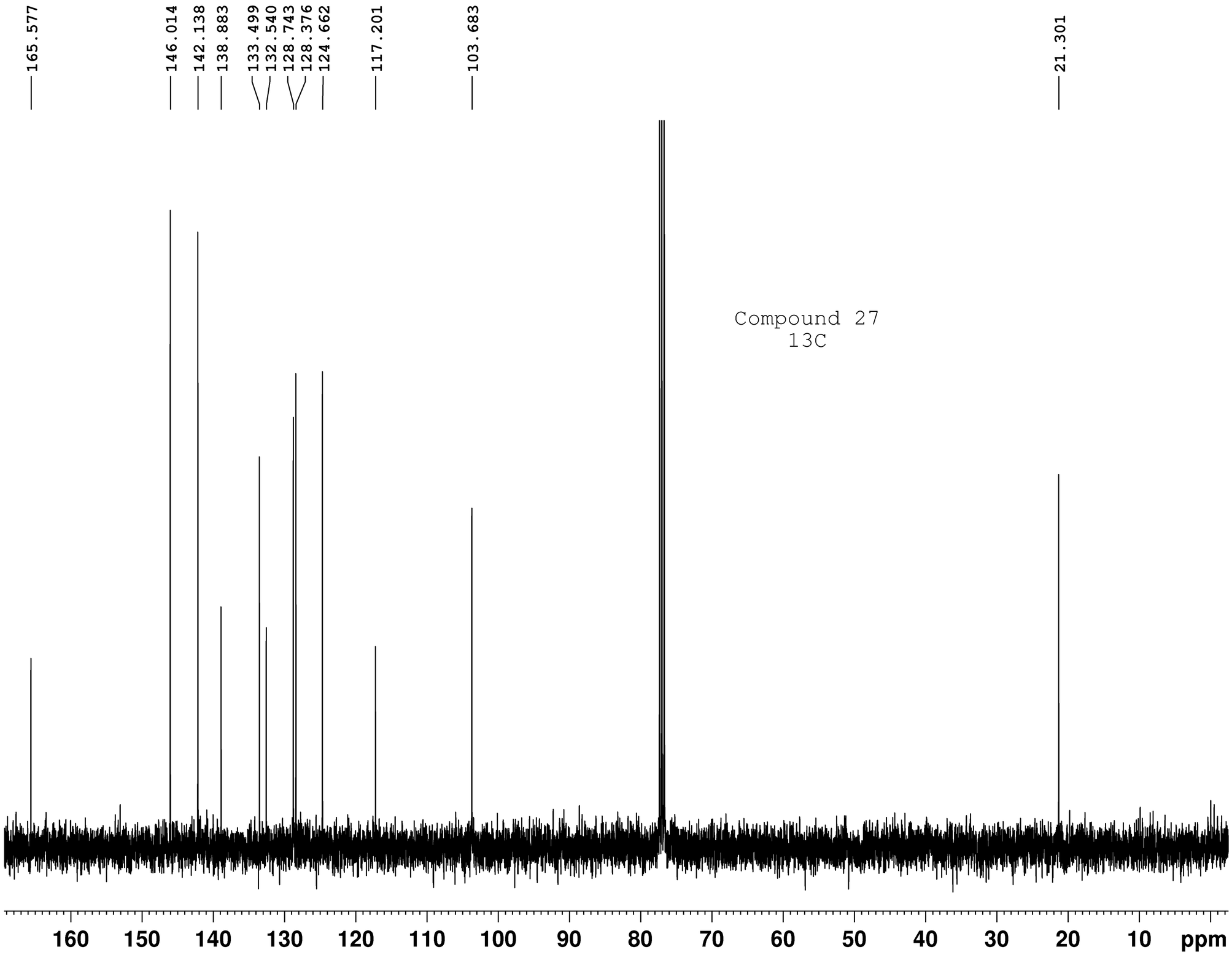


Compound 27
1H

```
Current Data Parameters
NAME            CD-129F
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20211215
Time              14.53 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             6578.947 Hz
FIDRES          0.401547 Hz
AQ             2.4903679 sec
RG                   101
DW                76.000 usec
DE                  7.79 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         400.1330415 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1         20.07200050 W

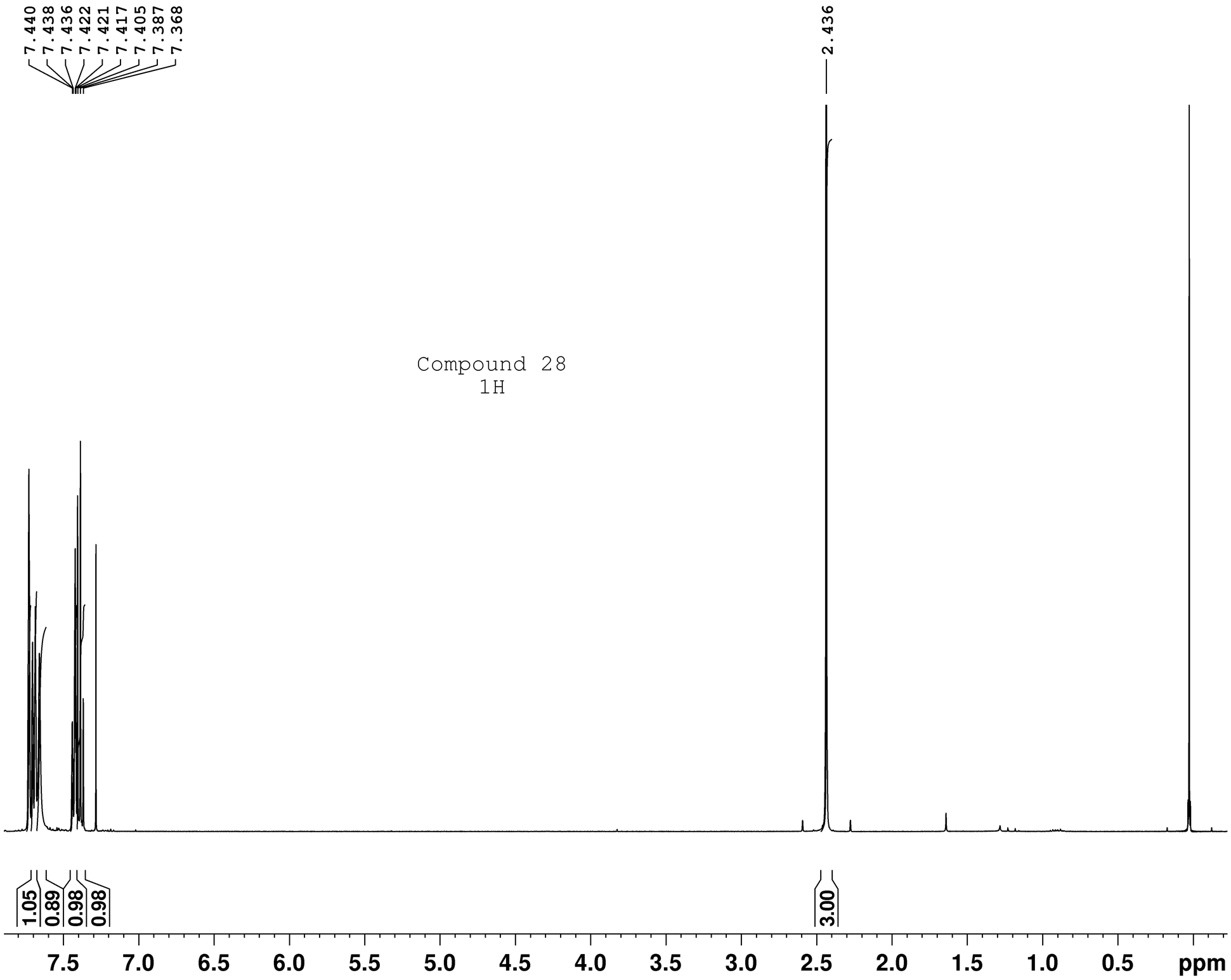
F2 - Processing parameters
SI                 65536
SF           400.1300103 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME                  CD-129F
EXPNO                      16
PROCNO                      1

F2 - Acquisition Parameters
Date_              20211215
Time                  15.37 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG  zg30igf2igf3.yavor
TD                      32768
SOLVENT                 CDCl3
NS                        128
DS                          0
SWH                23809.523 Hz
FIDRES              1.453218 Hz
AQ                 0.6881280 sec
RG                   25.7622
DW                    21.000 usec
DE                      6.50 usec
TE                    298.4 K
D1                1.50000000 sec
D11               0.03000000 sec
P1                     10.00 usec
TD0                         1
SFO1             100.6238383 MHz
NUC1                      13C
P0                      3.30 usec
PLW1             58.46900177 W
SFO2             376.4607162 MHz
NUC2                      19F
CPDPRG[2 bi_p5m4sp_4sp.2
P63                  1500.00 usec
PLW2             65.31900024 W
PLW12                       0 W
SPNAM[14 Crp120,0.75,30.4
SPOAL14                 0.500
SPOFFS14                    0 Hz
SPW14            23.06747055 W
SPNAM[31 Crp120,1.5,30.4
SPOAL31                 0.500
SPOFFS31                    0 Hz
SPW31            11.53349972 W
SFO3             400.1328009 MHz
NUC3                       1H
CPDPRG[3             waltz16
PCPD3                  90.00 usec
PLW3             20.00000000 W
PLW16             0.24717240 W

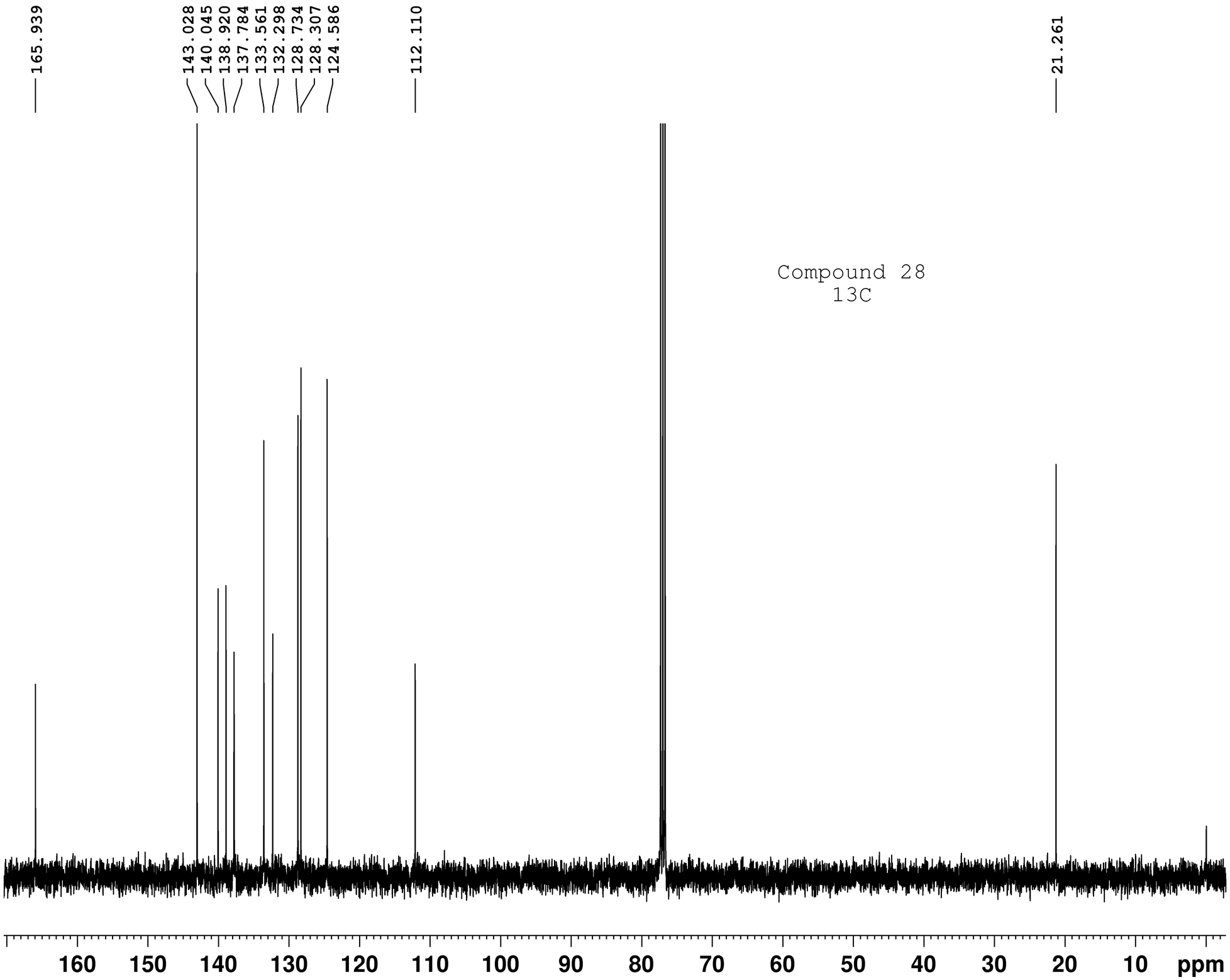
F2 - Processing parameters
SI                      65536
SF               100.6127716 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```




```
Current Data Parameters
NAME            CD-114A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20211208
Time              15.06 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             6578.947 Hz
FIDRES          0.401547 Hz
AQ             2.4903679 sec
RG                   101
DW                76.000 usec
DE                  7.79 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         400.1330415 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1         20.07200050 W

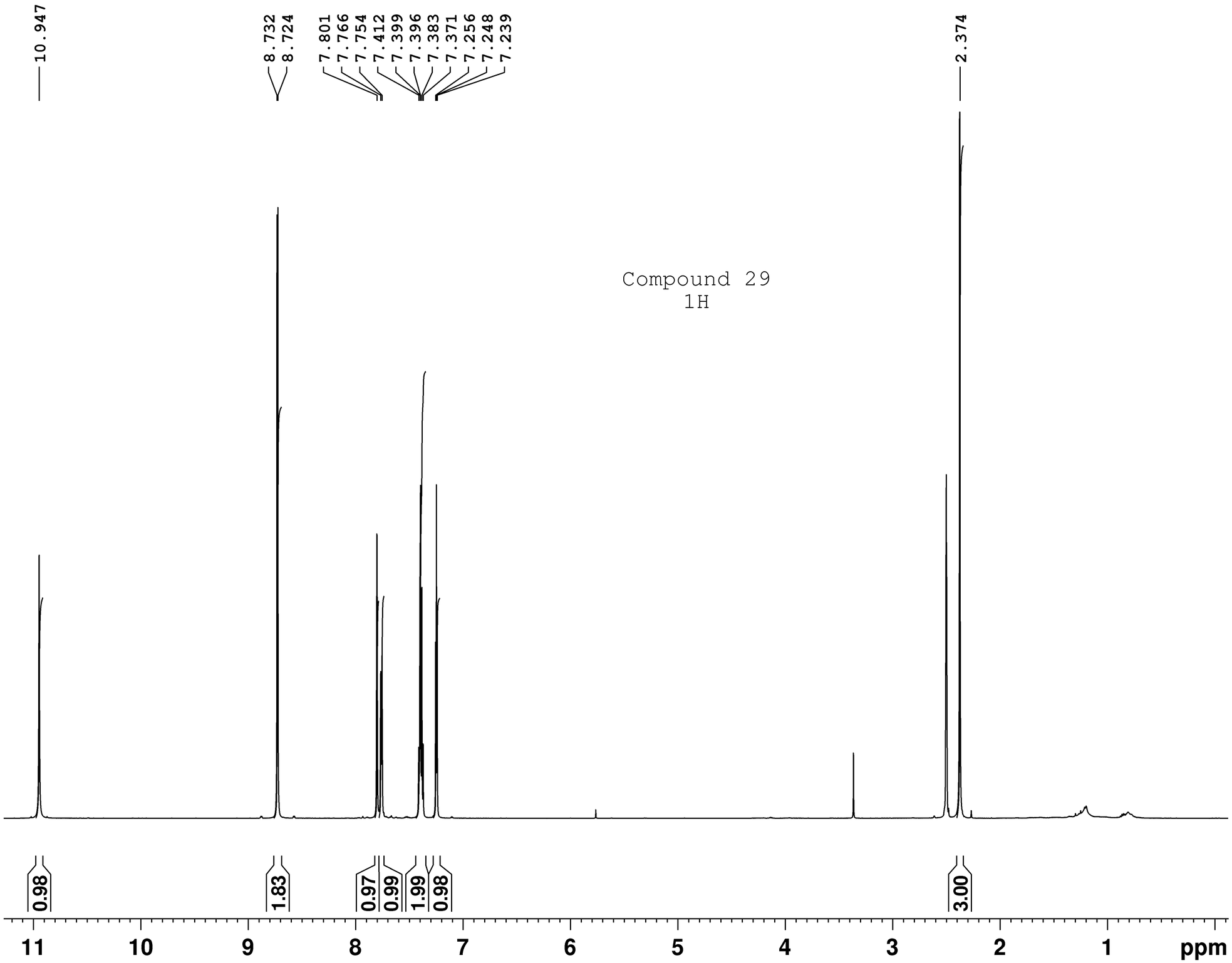
F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-114A
EXPNO               100
PROCNO                1

F2 - Acquisition Parameters
Date_           20211208
Time              15.17 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG  zg30igf2igf3.yavor
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           23809.523 Hz
FIDRES         1.453218 Hz
AQ            0.6881280 sec
RG               16.25
DW               21.000 usec
DE                 6.50 usec
TE                298.2 K
D1           1.50000000 sec
D11          0.03000000 sec
P1                10.00 usec
TD0                   1
SFO1        100.6238383 MHz
NUC1                13C
P0                 3.30 usec
PLW1        58.46900177 W
SFO2        376.4494212 MHz
NUC2                19F
CPDPRG[2 bi_p5m4sp_4sp.2
P63             1500.00 usec
PLW2        65.31900024 W
PLW12                 0 W
SPNAM[14 Crp32,0.75,20.2
SPOAL14           0.500
SPOFFS14              0 Hz
SPW14        6.00000000 W
SPNAM[31 Crp32,1.5,20.2
SPOAL31           0.500
SPOFFS31              0 Hz
SPW31        3.00000000 W
SFO3        400.1328009 MHz
NUC3                 1H
CPDPRG[3         waltz16
PCPD3             90.00 usec
PLW3        20.00000000 W
PLW16        0.24717240 W

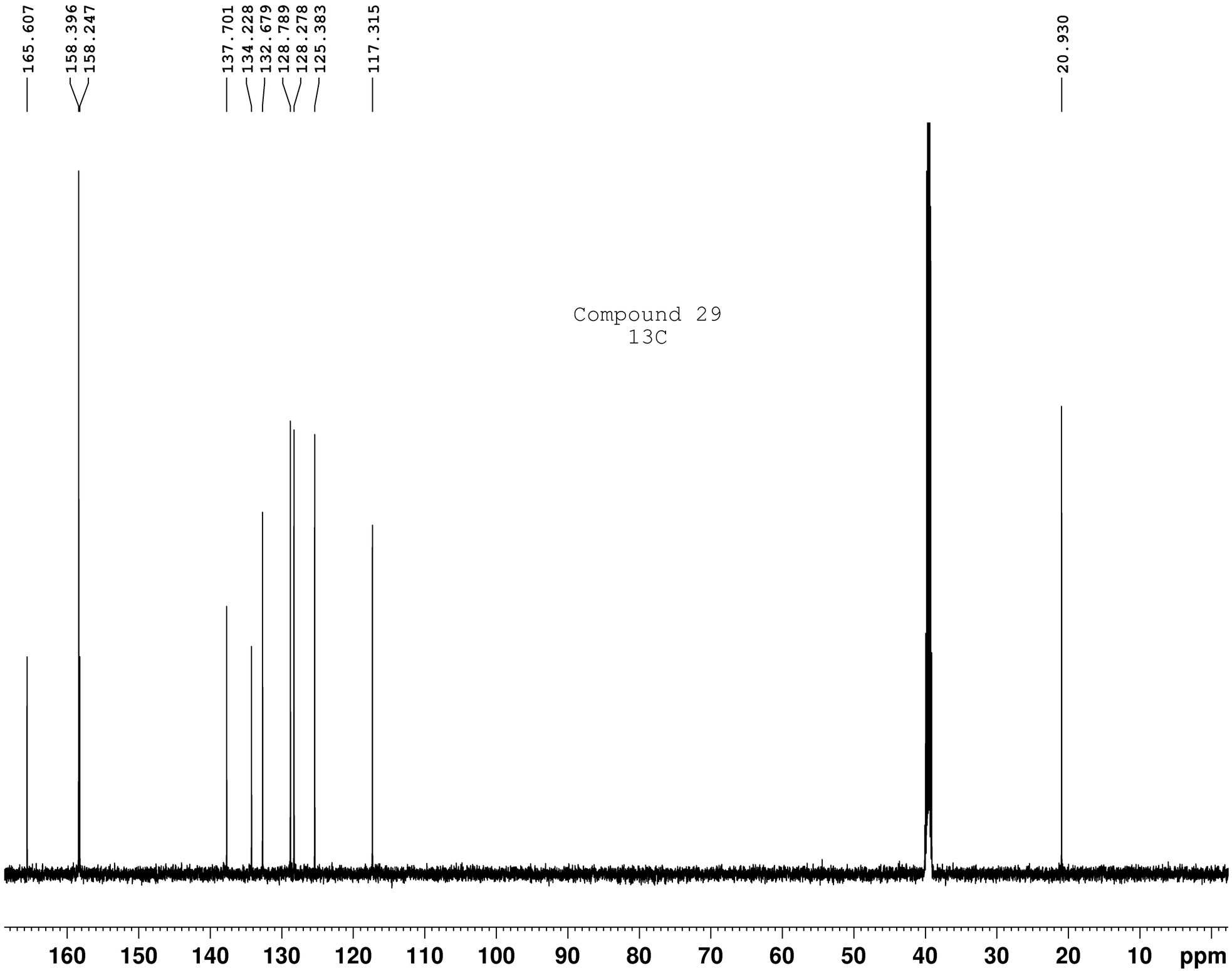
F2 - Processing parameters
SI                65536
SF          100.6127715 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME              CD-69A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210426
Time              17.23 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                    16
DS                     0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ            1.7039360 sec
RG                   101
DW               52.000 usec
DE               14.37 usec
TE               293.1 K
D1           1.00000000 sec
TD0                    1
SFO1        600.0145608 MHz
NUC1                  1H
P0                 3.62 usec
P1                10.85 usec
PLW1        20.00000000 W

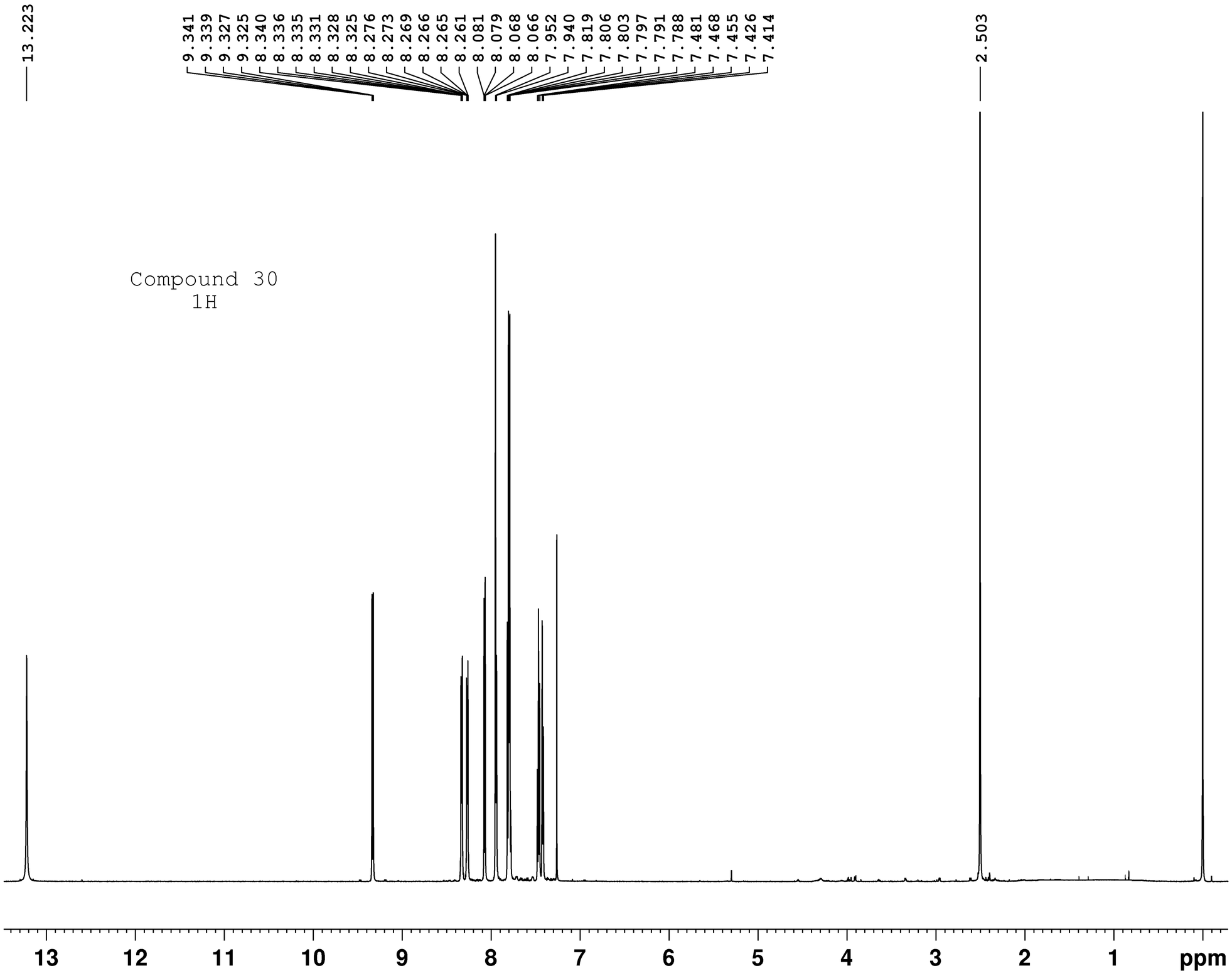
F2 - Processing parameters
SI                65536
SF          600.0100049 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CD-69A
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210426
Time               17.57 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT             DMSO
NS                    128
DS                      0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                   2050
DW                 13.867 usec
DE                  6.50 usec
TE                 293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8892338 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

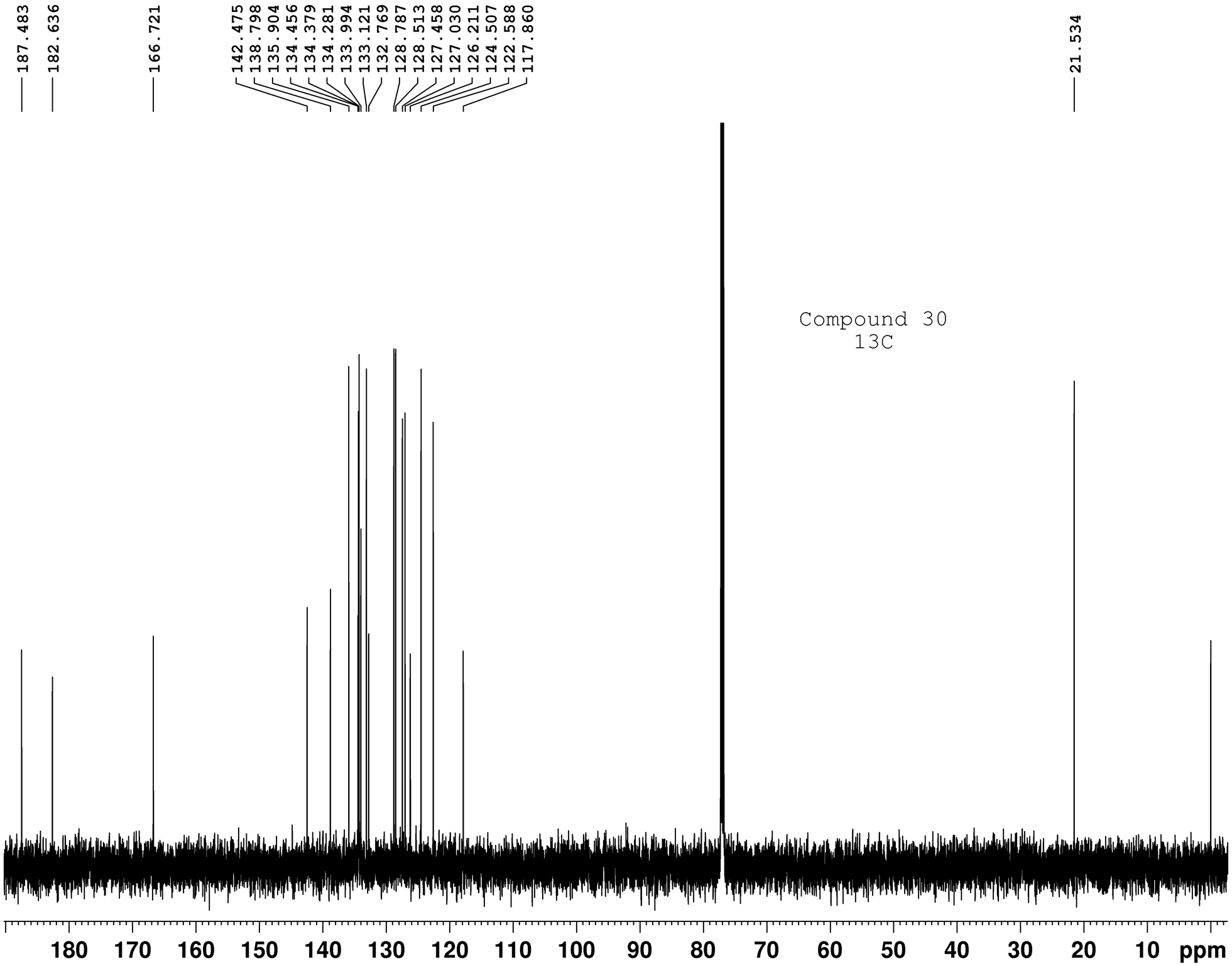
F2 - Processing parameters
SI                  65536
SF          150.8727007 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
Current Data Parameters
NAME            CD-118A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20210219
Time               17.14 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   161
DW                52.000 usec
DE                14.37 usec
TE                293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

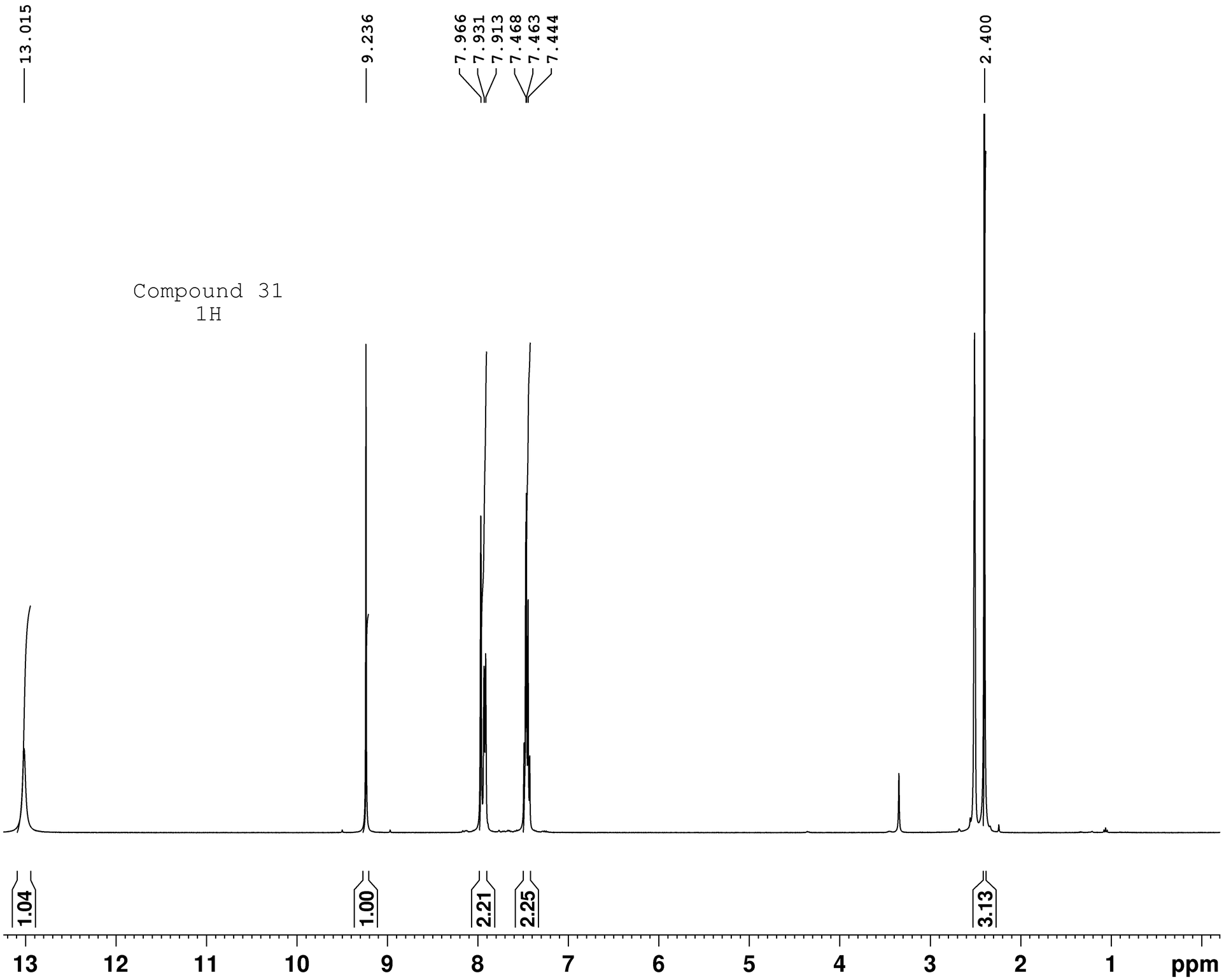
F2 - Processing parameters
SI                 65536
SF           600.0100136 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-118A
EXPNO                16
PROCNO                1

F2 - Acquisition Parameters
Date_           20210219
Time              17.50 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8892338 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        600.0124004 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        20.00000000 W
PLW12        0.33800000 W

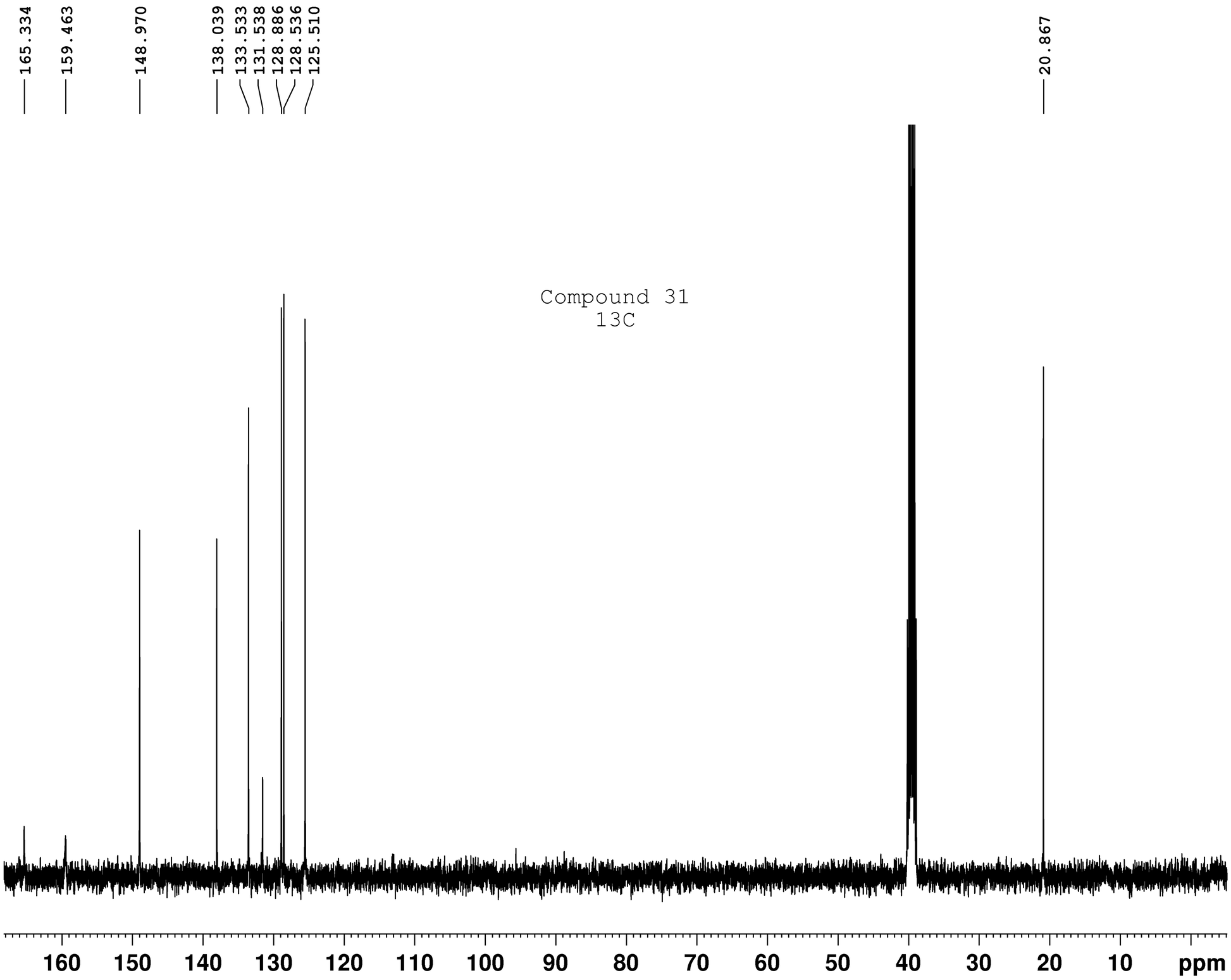
F2 - Processing parameters
SI                65536
SF          150.8726390 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME            CD-185B
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20220414
Time             18.13 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                    32
DS                     0
SWH            6578.947 Hz
FIDRES         0.401547 Hz
AQ            2.4903679 sec
RG                   101
DW               76.000 usec
DE                 7.79 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1
SFO1        400.1330415 MHz
NUC1                  1H
P0                 3.33 usec
P1                10.00 usec
PLW1        20.07200050 W

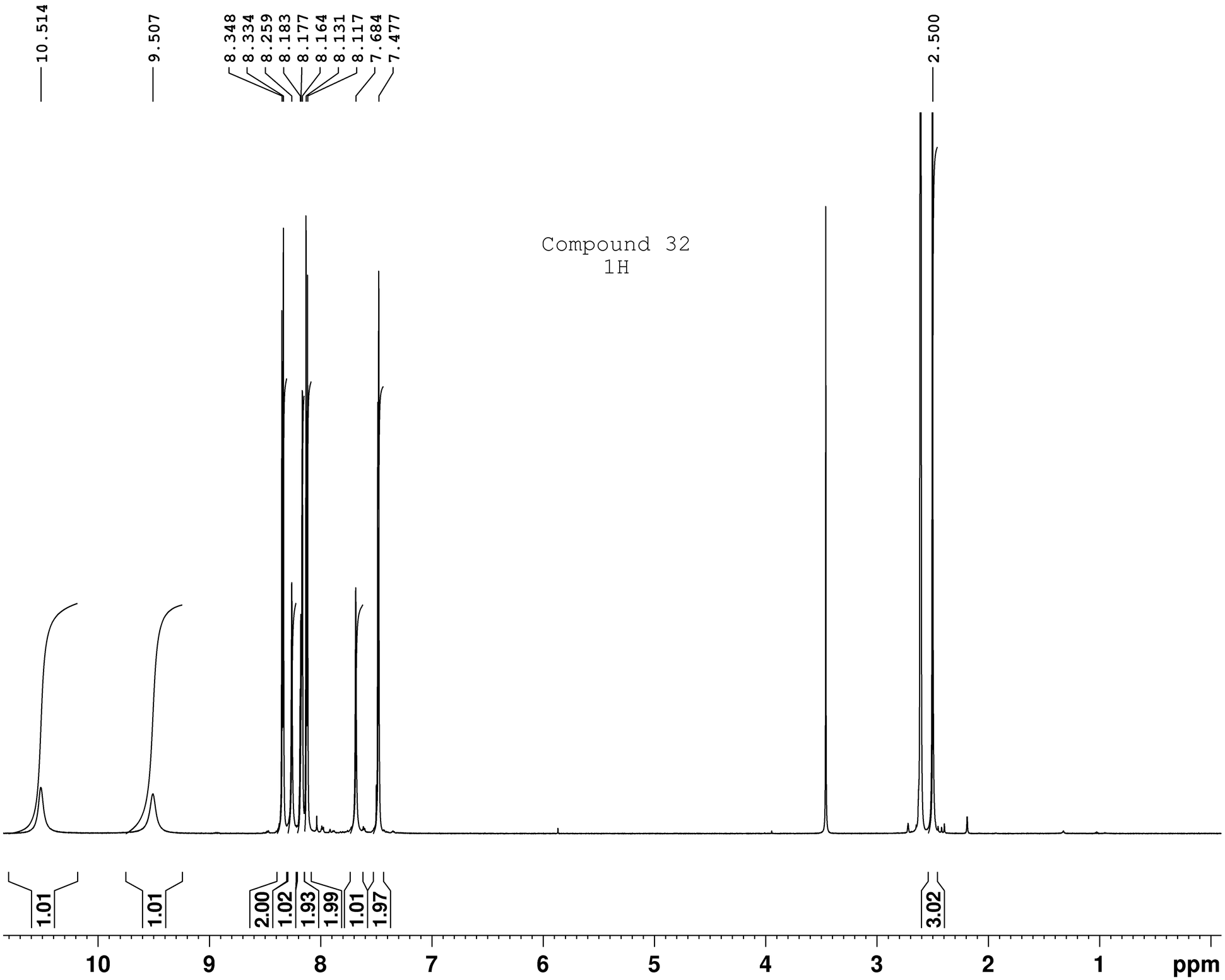
F2 - Processing parameters
SI                65536
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME            CD-185B
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220414
Time              18.18 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG          zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH           23809.523 Hz
FIDRES         1.453218 Hz
AQ            0.6881280 sec
RG                 11.3
DW               21.000 usec
DE                6.50 usec
TE               298.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6238383 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        58.46900177 W
SFO2        400.1316008 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        20.07200050 W
PLW12        0.24781001 W

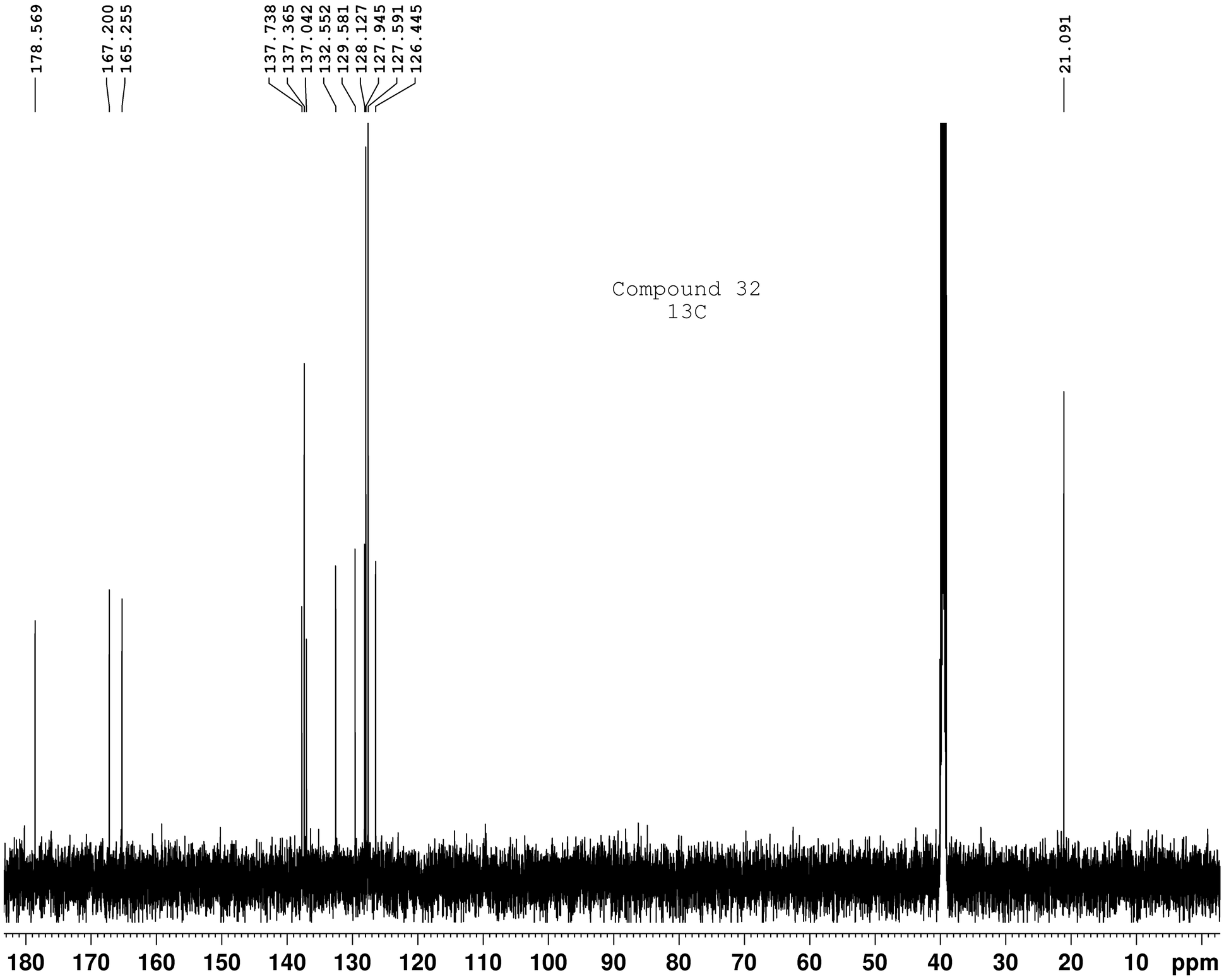
F2 - Processing parameters
SI                65536
SF          100.6128162 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME            CD-112-A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210316
Time               19.23 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                     32
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    161
DW                 52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                     1
SFO1         600.0145608 MHz
NUC1                   1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

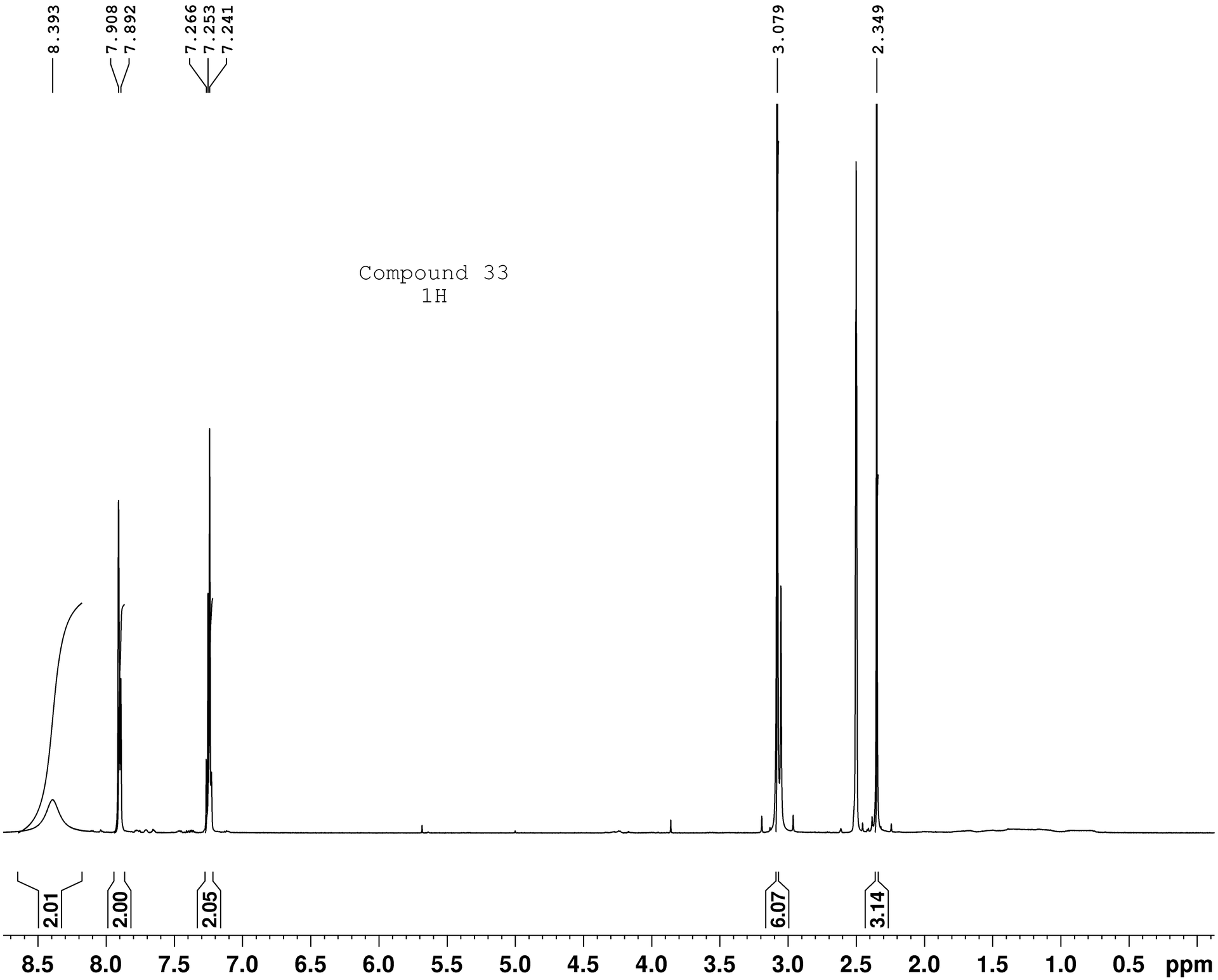
F2 - Processing parameters
SI                  65536
SF           600.0099403 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CD-112-A
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210316
Time               19.58 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT             DMSO
NS                    128
DS                      0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                   2050
DW                13.867 usec
DE                  6.50 usec
TE                 293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         150.8892338 MHz
NUC1                 13C
P0                   3.27 usec
P1                   9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2               90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

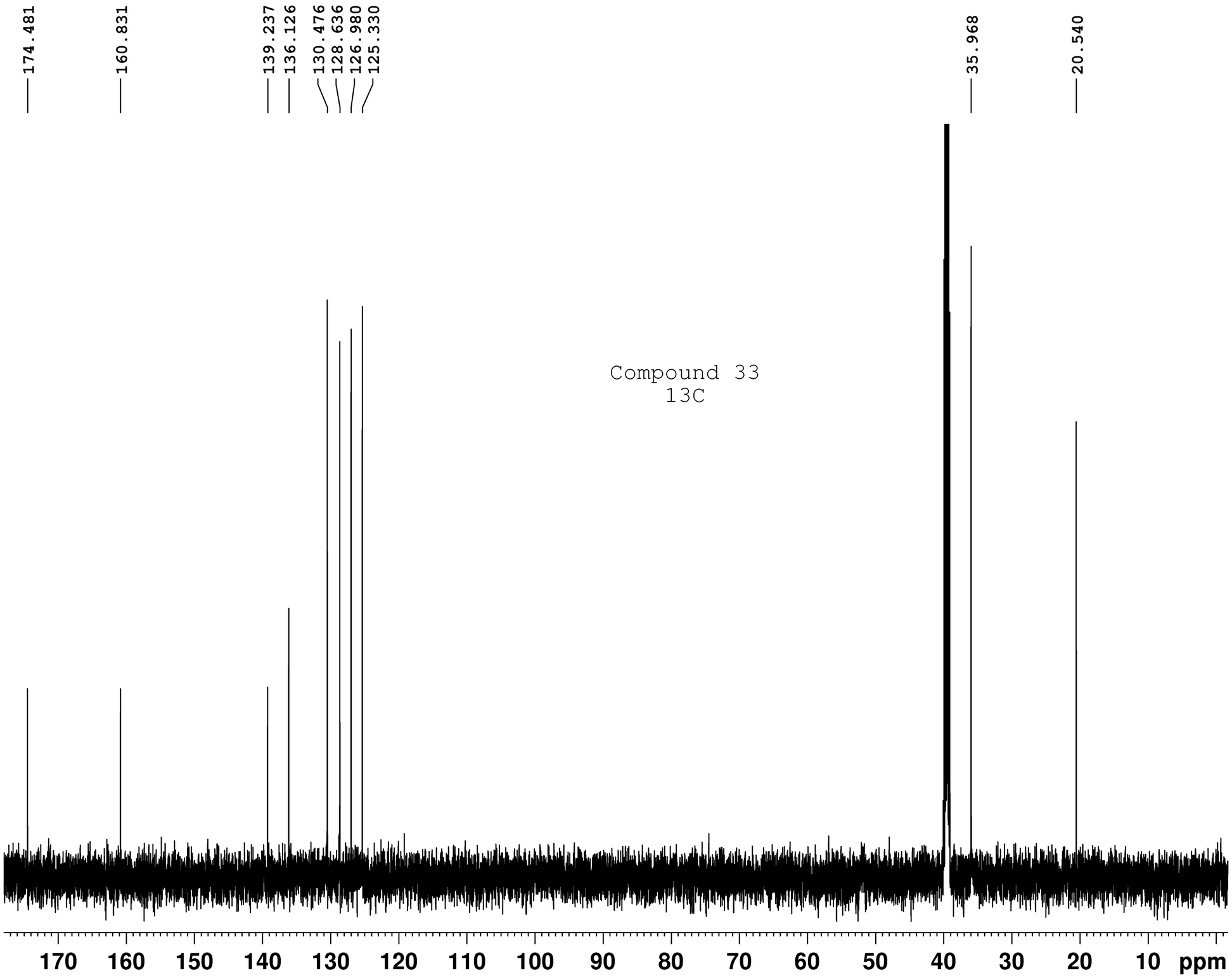
F2 - Processing parameters
SI                  65536
SF           150.8727009 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
Current Data Parameters
NAME            CD-163A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20220225
Time               21.00 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                     32
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    181
DW                52.000 usec
DE                 14.38 usec
TE                 353.1 K
D1            1.00000000 sec
TD0                     1
SFO1         599.9845606 MHz
NUC1                   1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

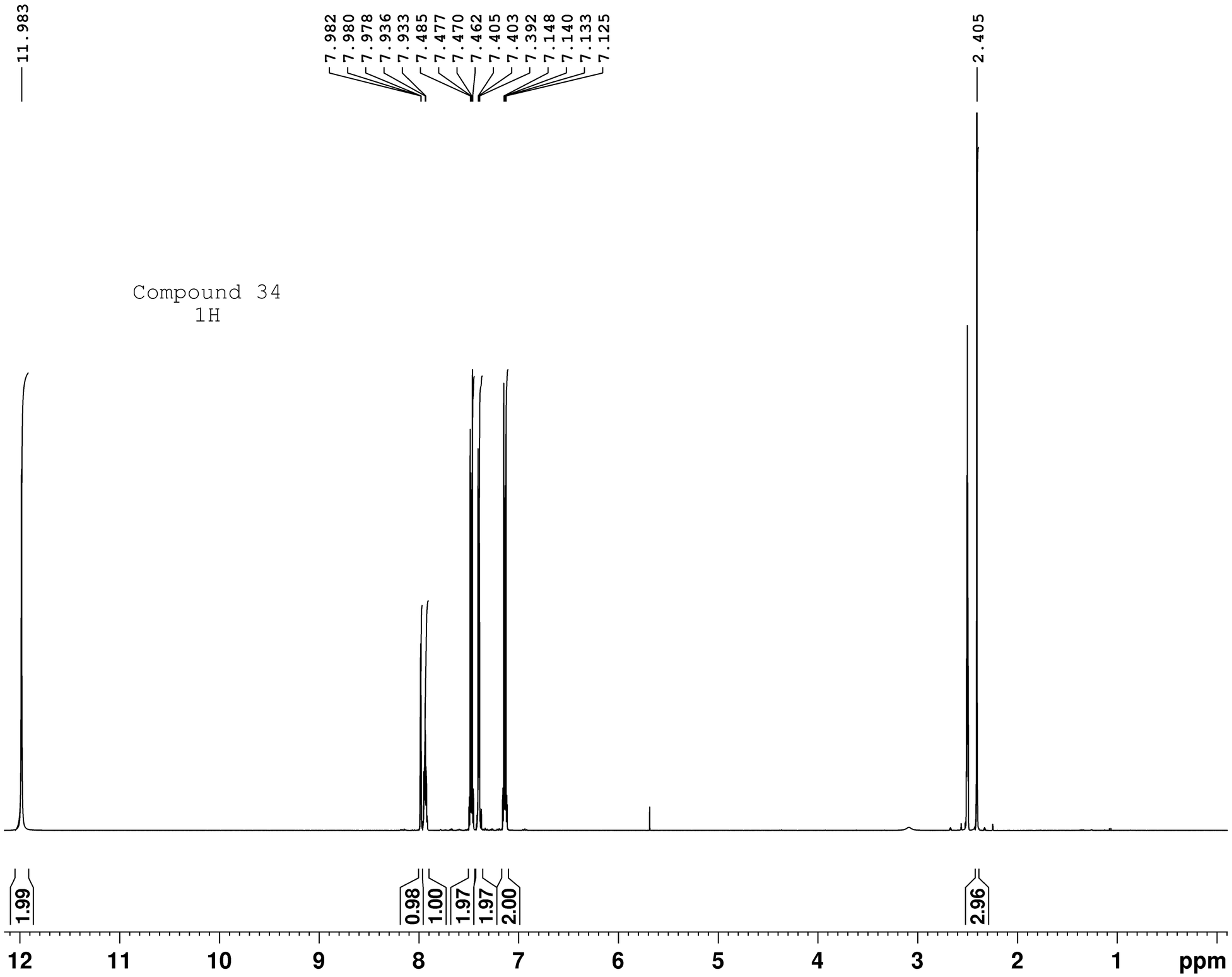
F2 - Processing parameters
SI                  65536
SF           599.9800045 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CD-163A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220225
Time              21.06 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                  2050
DW               13.867 usec
DE                6.50 usec
TE               353.1 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

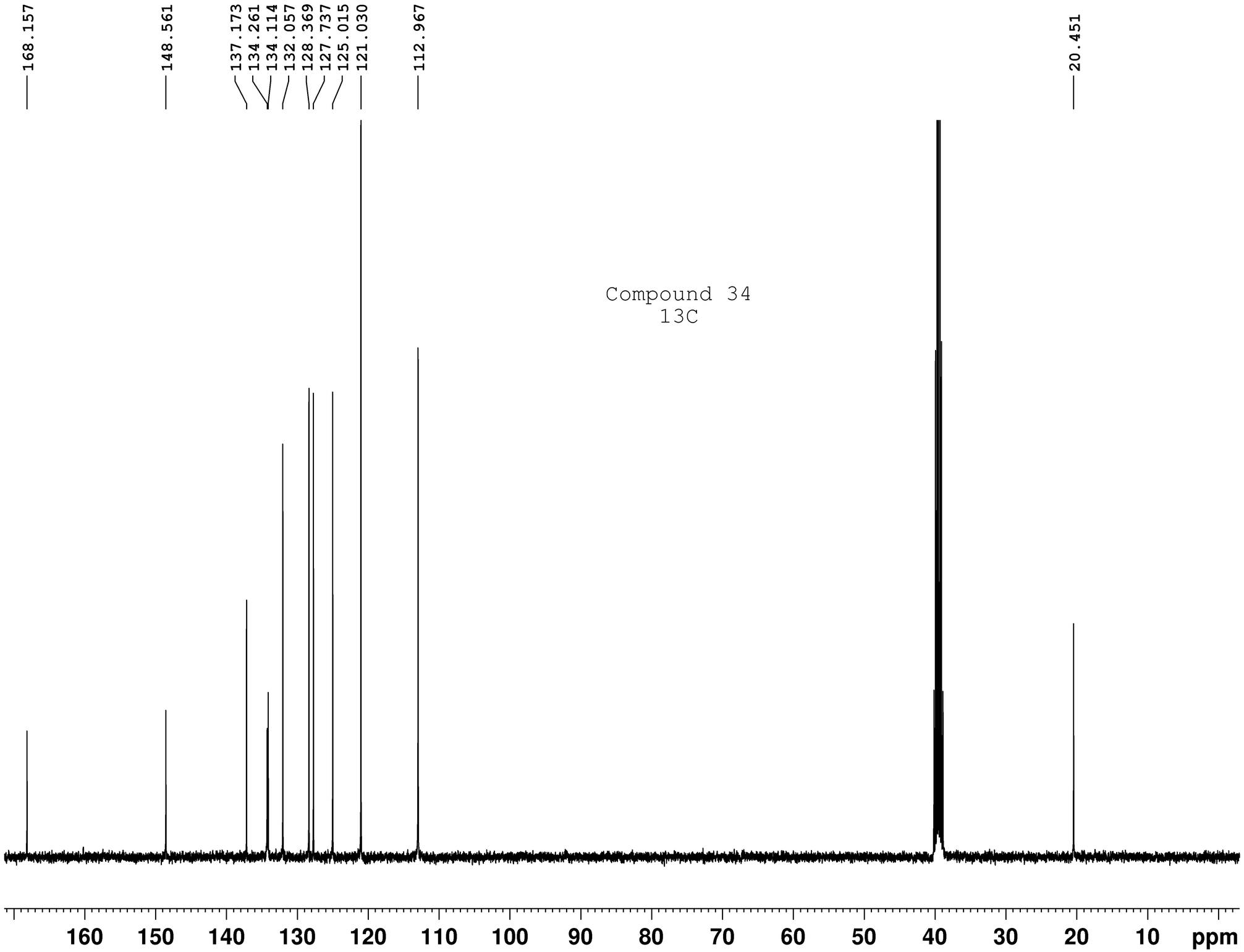
F2 - Processing parameters
SI                65536
SF          150.8652273 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME            CD-102B
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20220416
Time              10.51 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                     32
DS                      0
SWH            6578.947 Hz
FIDRES         0.401547 Hz
AQ            2.4903679 sec
RG                    101
DW               76.000 usec
DE                 7.79 usec
TE                353.0 K
D1           2.00000000 sec
TD0                     1
SFO1        400.1330415 MHz
NUC1                   1H
P0                 3.33 usec
P1                10.00 usec
PLW1        20.07200050 W

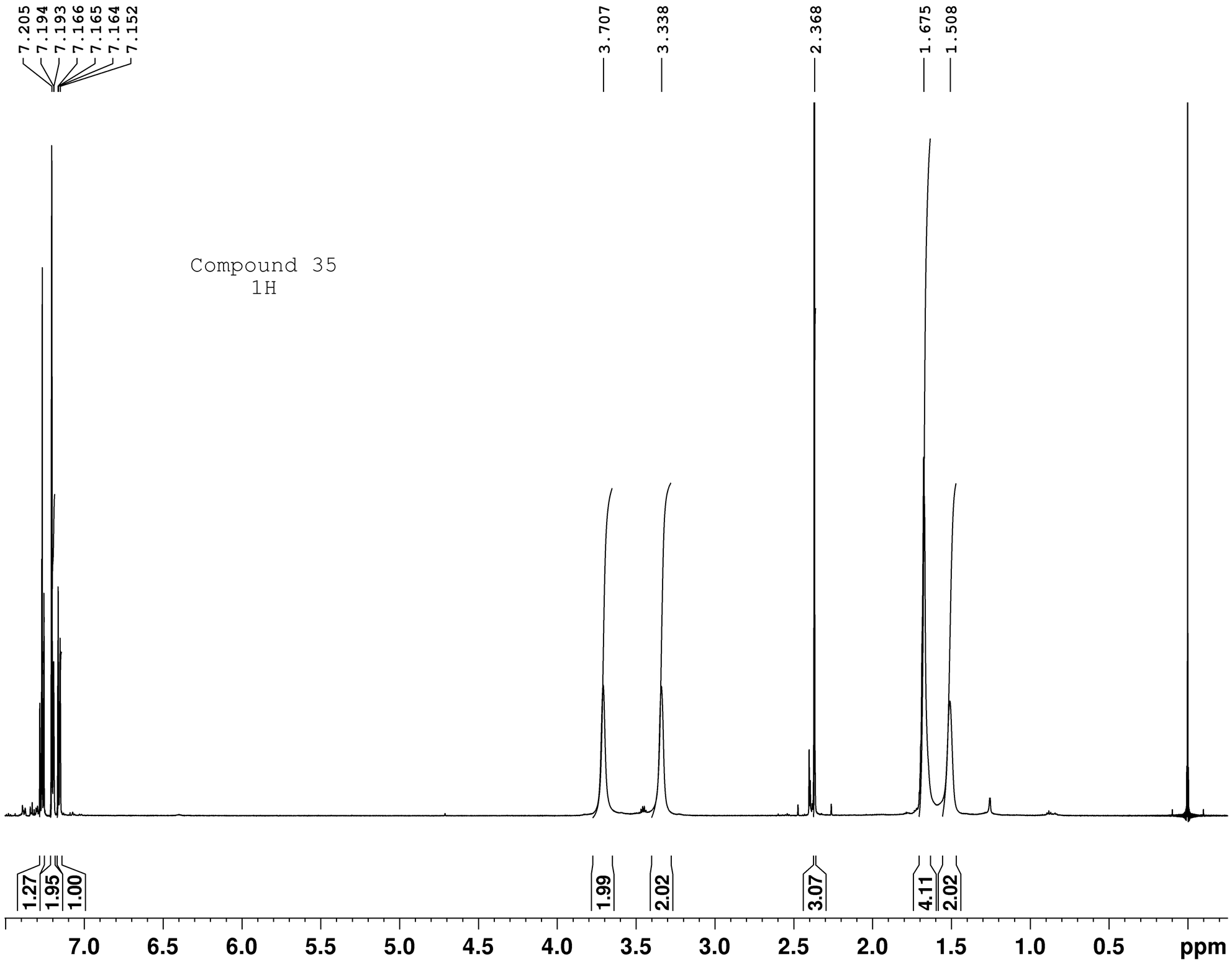
F2 - Processing parameters
SI                  65536
SF          400.1300037 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME              CD-102B
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220416
Time               11.30 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG           zgdc30
TD                 32768
SOLVENT             DMSO
NS                  1024
DS                     0
SWH            23809.523 Hz
FIDRES          1.453218 Hz
AQ             0.6881280 sec
RG                  45.2
DW                21.000 usec
DE                 6.50 usec
TE                353.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6238383 MHz
NUC1                 13C
P0                 3.33 usec
P1                10.00 usec
PLW1         58.46900177 W
SFO2         400.1316008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         20.07200050 W
PLW12         0.24781001 W

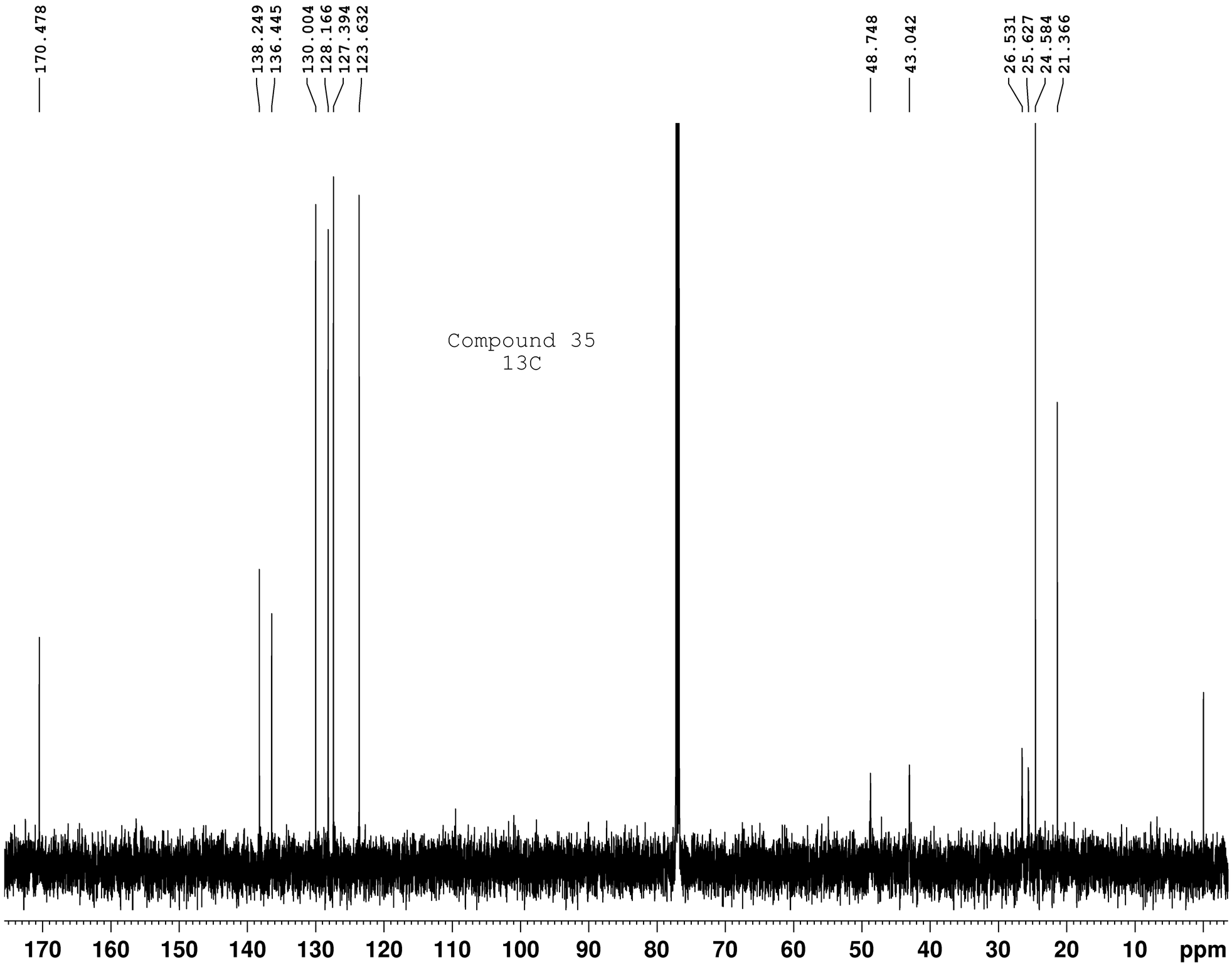
F2 - Processing parameters
SI                 65536
SF           100.6128564 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          35-CD-111A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220111
Time              16.59 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ            1.7039360 sec
RG                  203
DW               52.000 usec
DE               14.38 usec
TE               293.0 K
D1           1.00000000 sec
TD0                   1
SFO1        599.9845606 MHz
NUC1                 1H
P0                 3.60 usec
P1                10.80 usec
PLW1        20.00000000 W

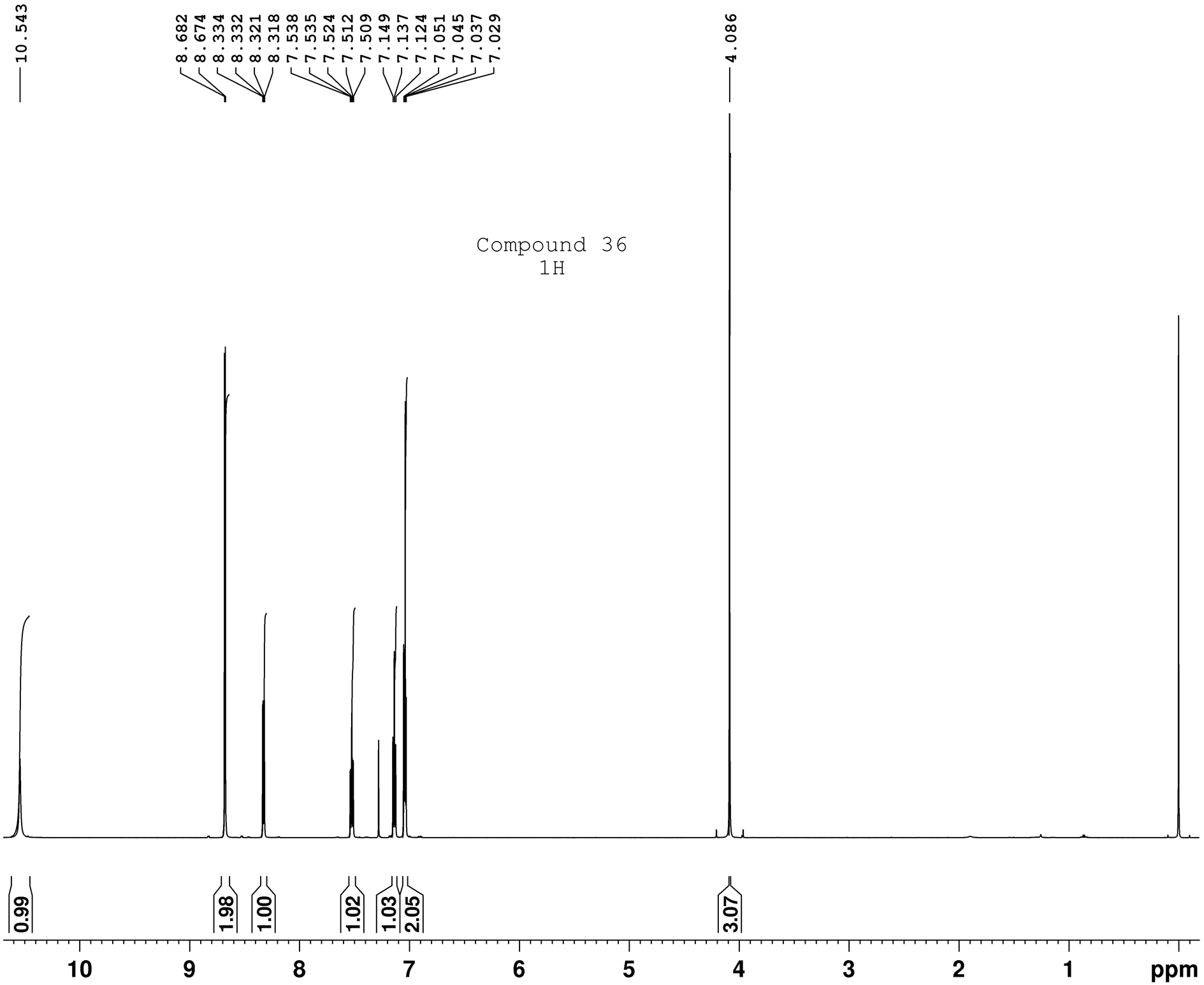
F2 - Processing parameters
SI                65536
SF          599.9800107 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME            CD-111A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20220111
Time              17.04 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2            70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

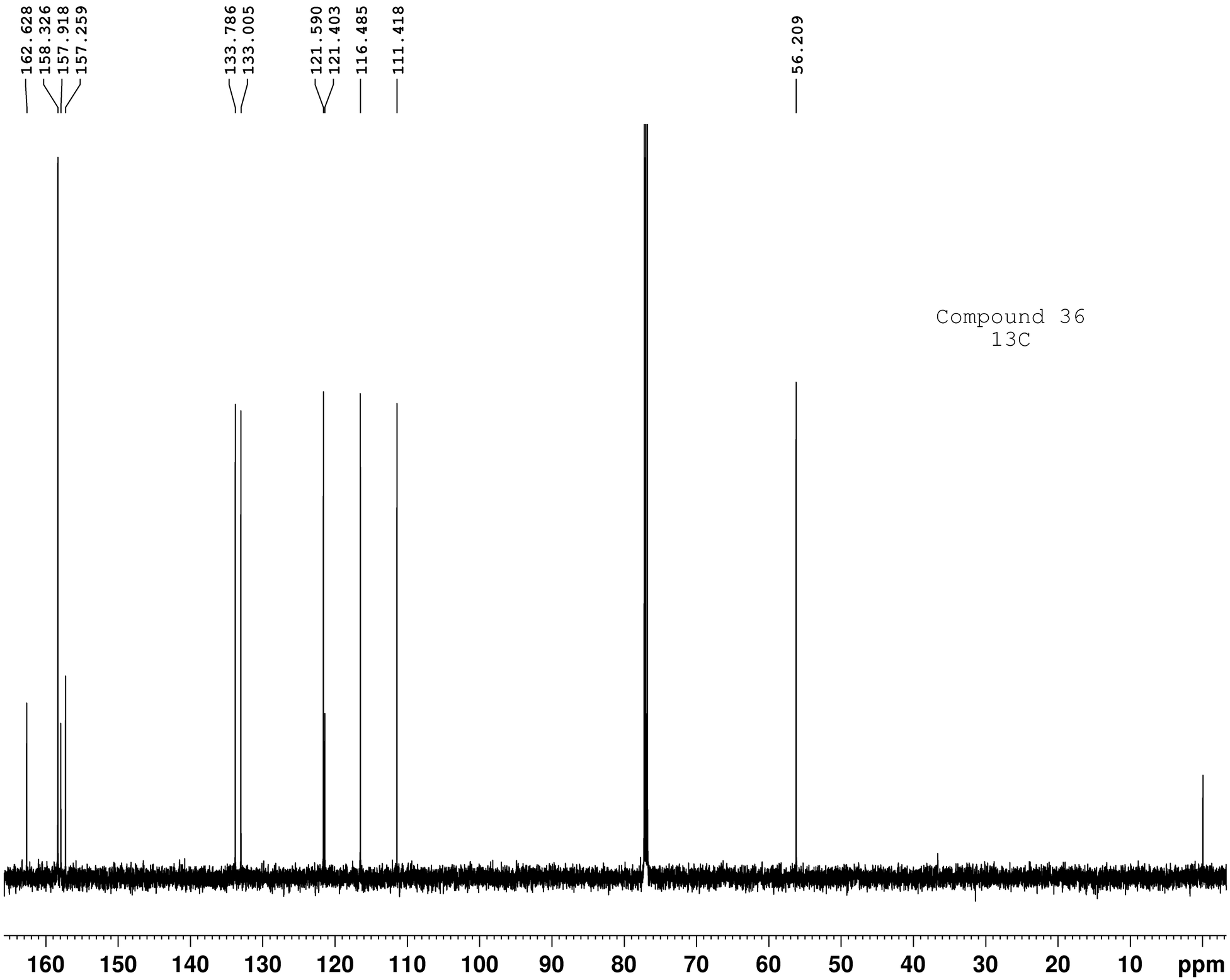
F2 - Processing parameters
SI                65536
SF          150.8650981 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME              CD-62A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210217
Time               17.48 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   161
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1        600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1        20.00000000 W

F2 - Processing parameters
SI                 65536
SF          600.0100031 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

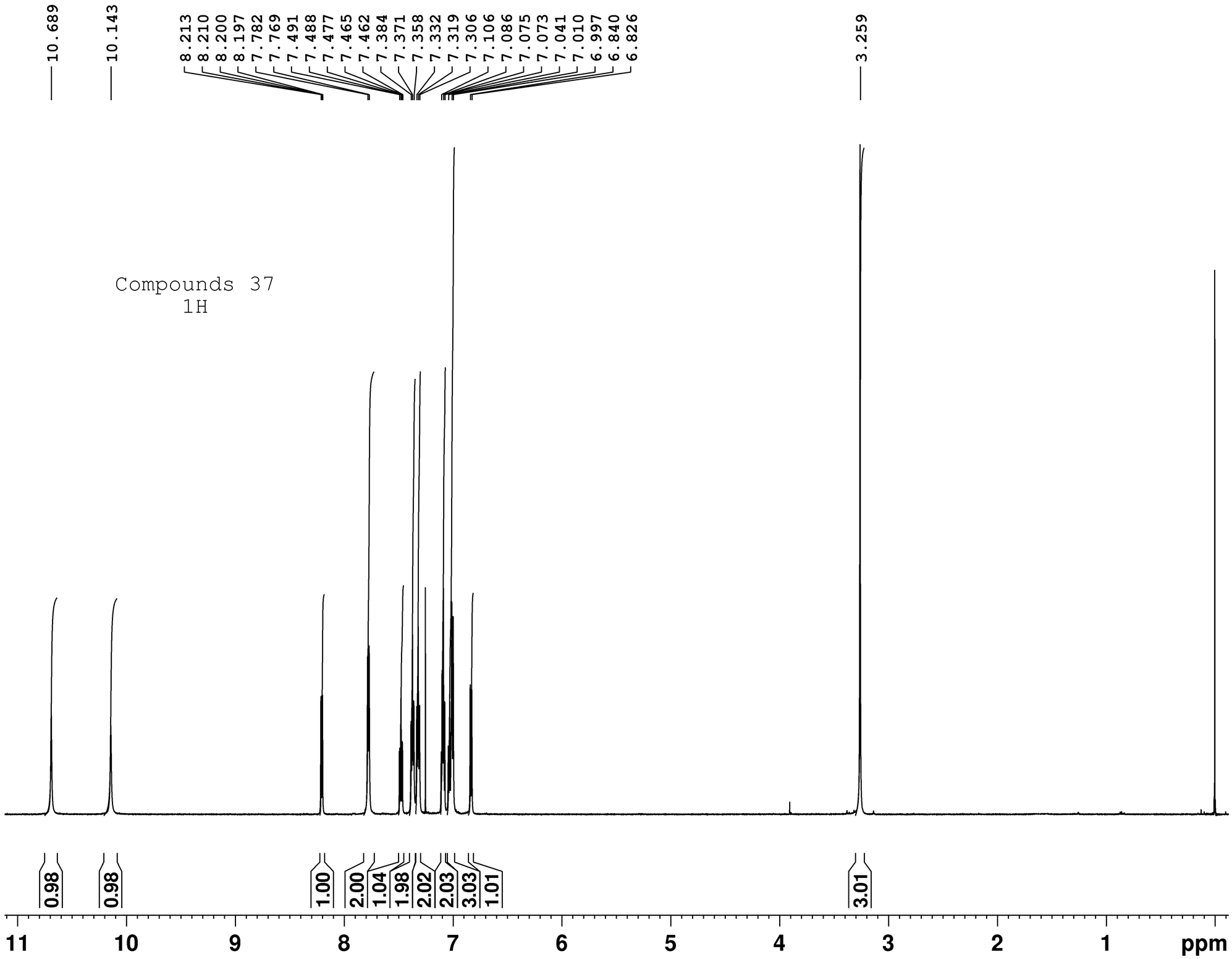


Compound 36
13C

```
Current Data Parameters
NAME                CD-62A
EXPNO                   16
PROCNO                   1

F2 - Acquisition Parameters
Date_             20210217
Time                 18.22 h
INSTRUM               spect
PROBHD    Z847801_0047 (
PULPROG             zgdc30
TD                   32768
SOLVENT              CDCl3
NS                     128
DS                       0
SWH              36057.691 Hz
FIDRES            2.200787 Hz
AQ               0.4543829 sec
RG                    2050
DW                  13.867 usec
DE                    6.50 usec
TE                   293.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           150.8892338 MHz
NUC1                   13C
P0                    3.27 usec
P1                    9.80 usec
PLW1           40.00000000 W
SFO2           600.0124004 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           20.00000000 W
PLW12           0.33800000 W

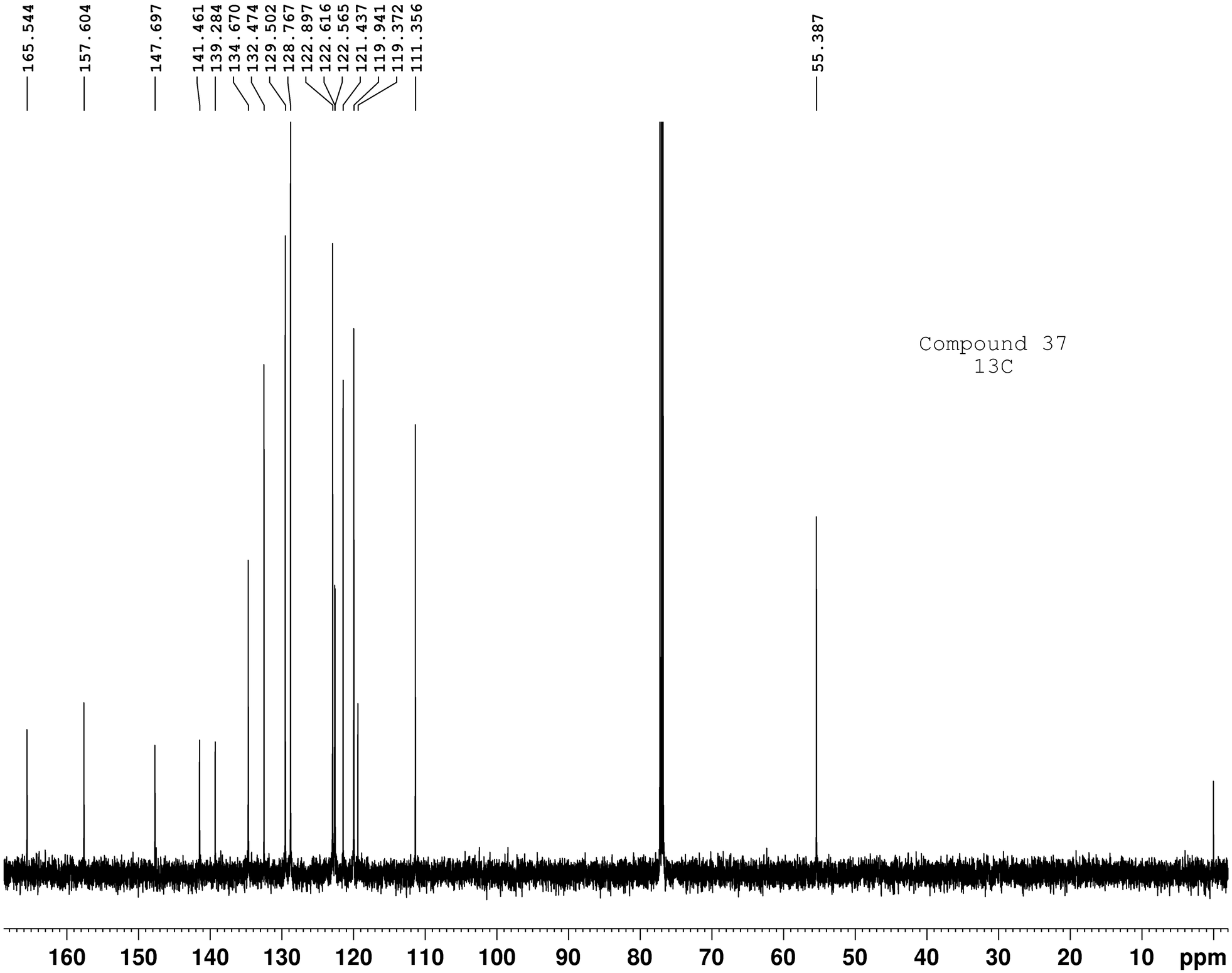
F2 - Processing parameters
SI                   65536
SF             150.8726472 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```




```
Current Data Parameters
NAME              CD-63A
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191111
Time                8.55 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   161
DW                52.000 usec
DE                 13.95 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P1                 10.85 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                 65536
SF          600.0100204 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

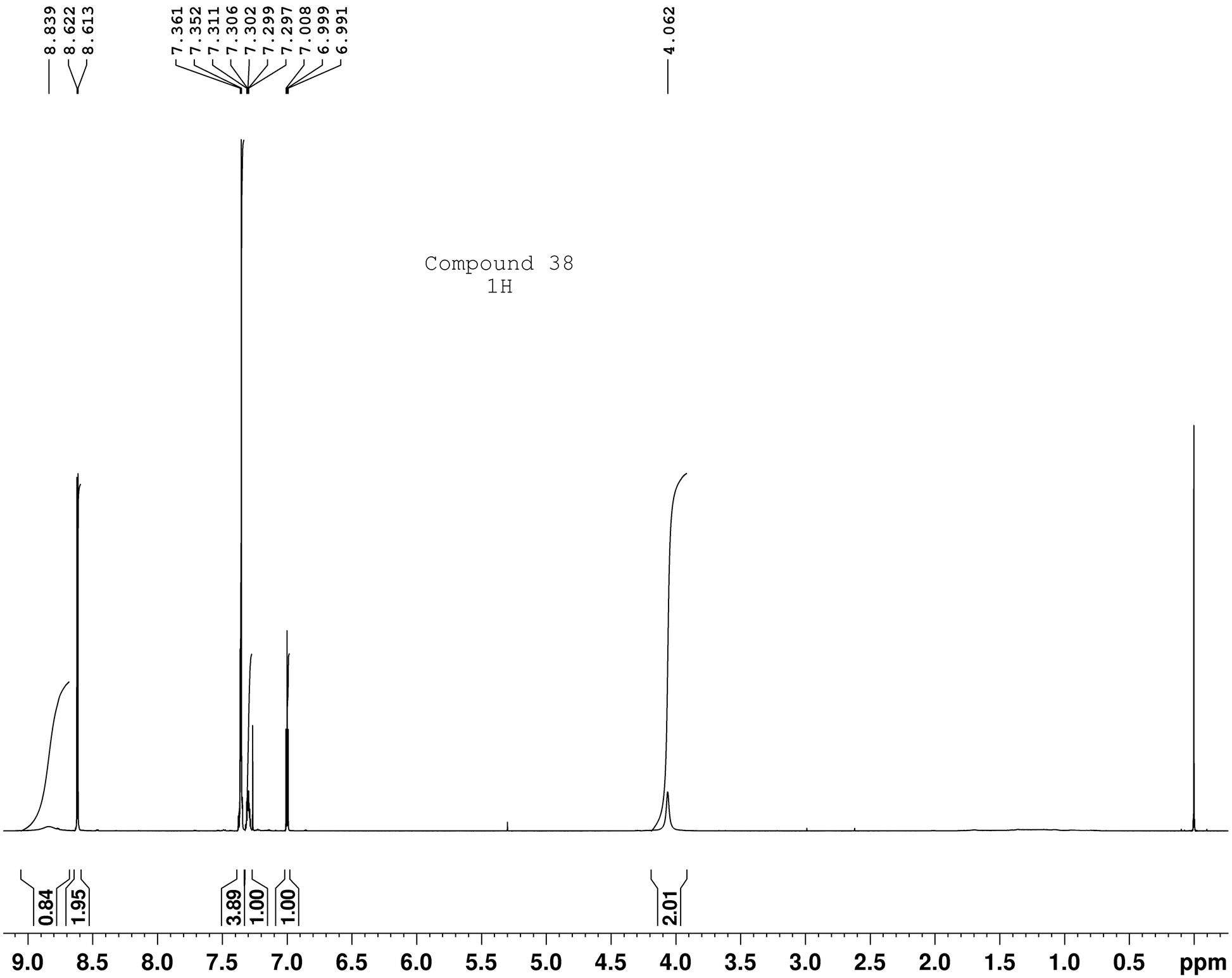


Compound 37
13C

```
Current Data Parameters
NAME              CD-63A
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191111
Time               9.38 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE                293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8892338 MHz
NUC1                13C
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        600.0124004 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        20.00000000 W
PLW12        0.33800000 W

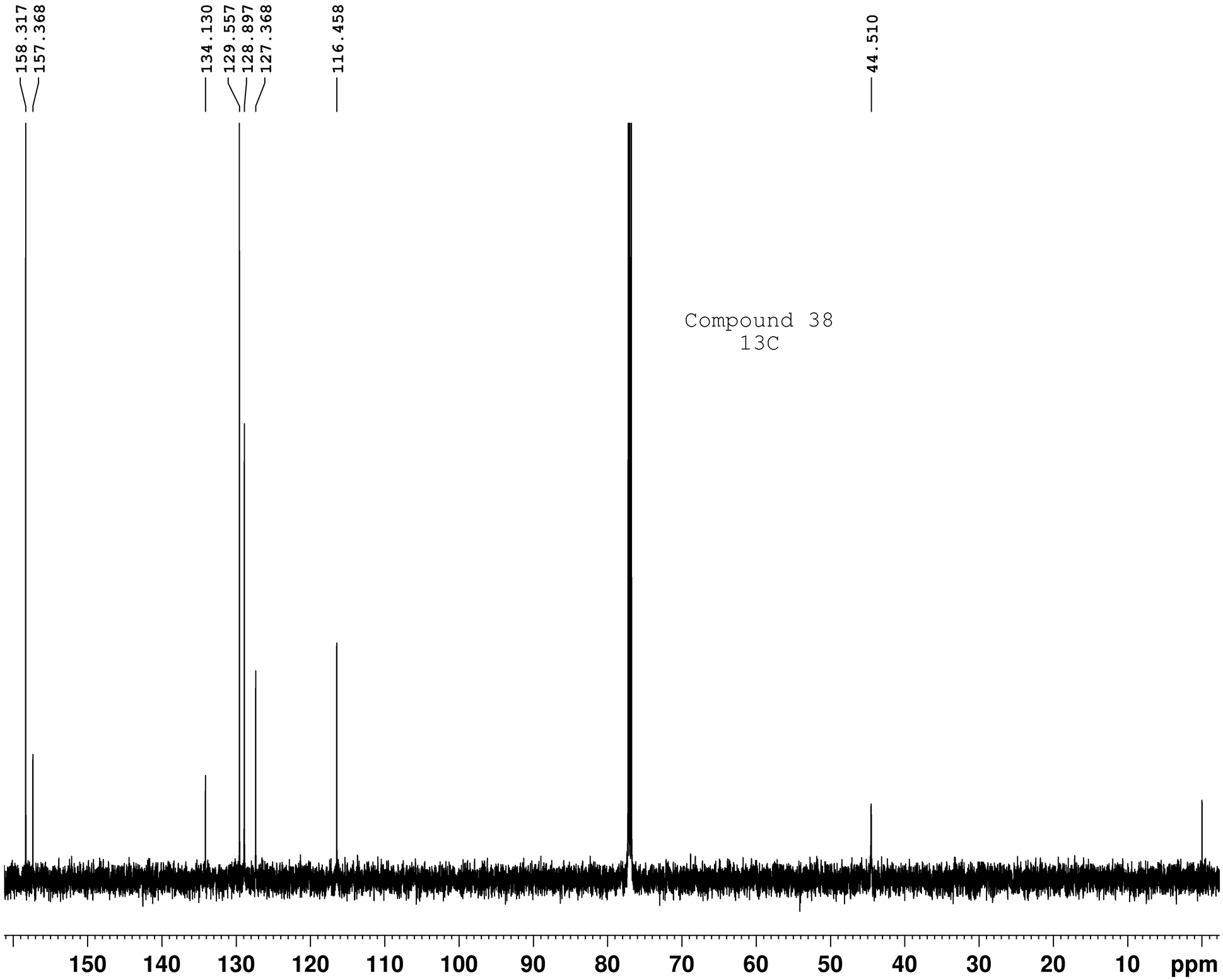
F2 - Processing parameters
SI                65536
SF          150.8726444 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME          38-CD-80A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20220112
Time              16.51 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   228
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

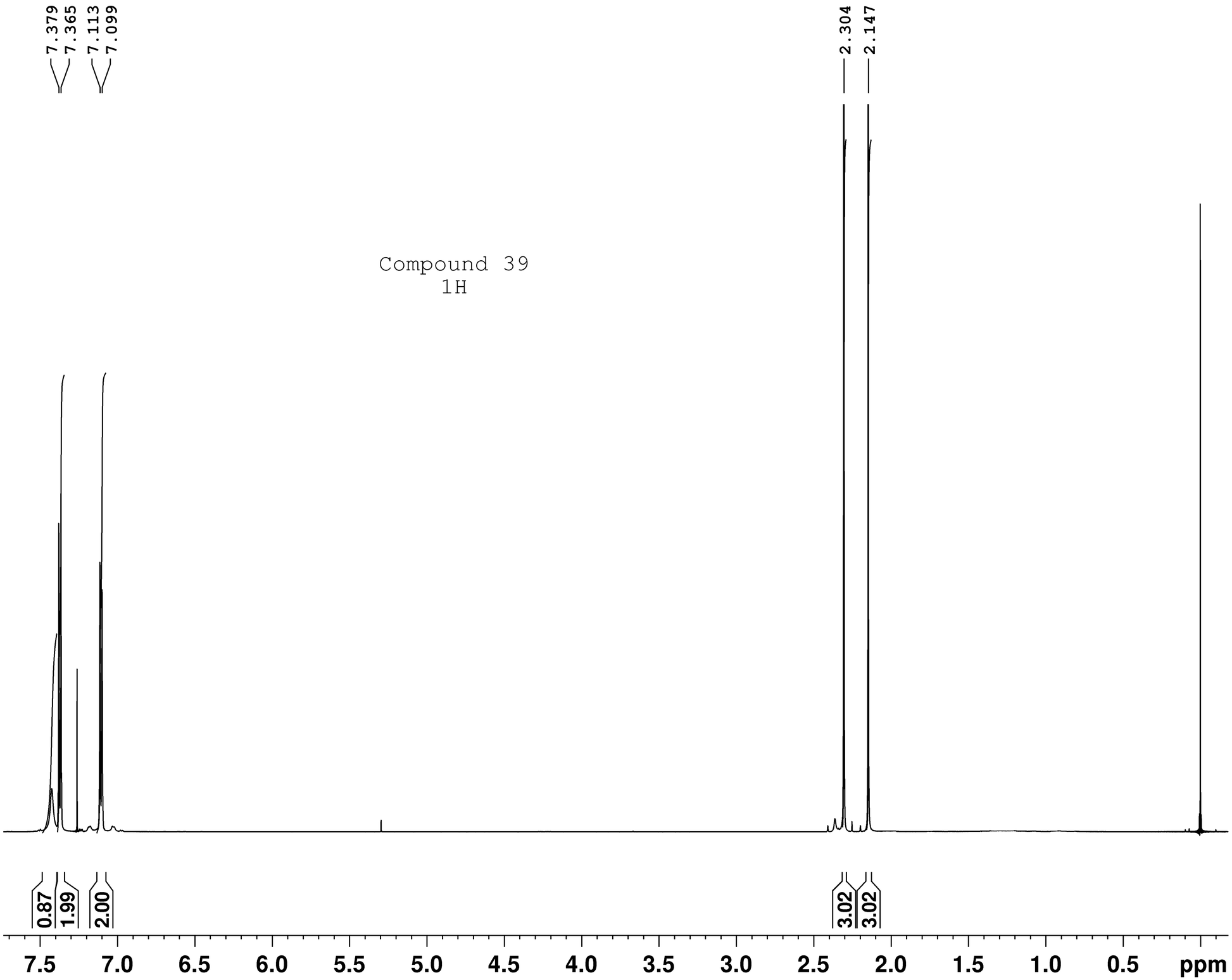
F2 - Processing parameters
SI                 65536
SF           599.9800112 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CD-80A
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_            20220112
Time               16.56 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                  6.50 usec
TE                 293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

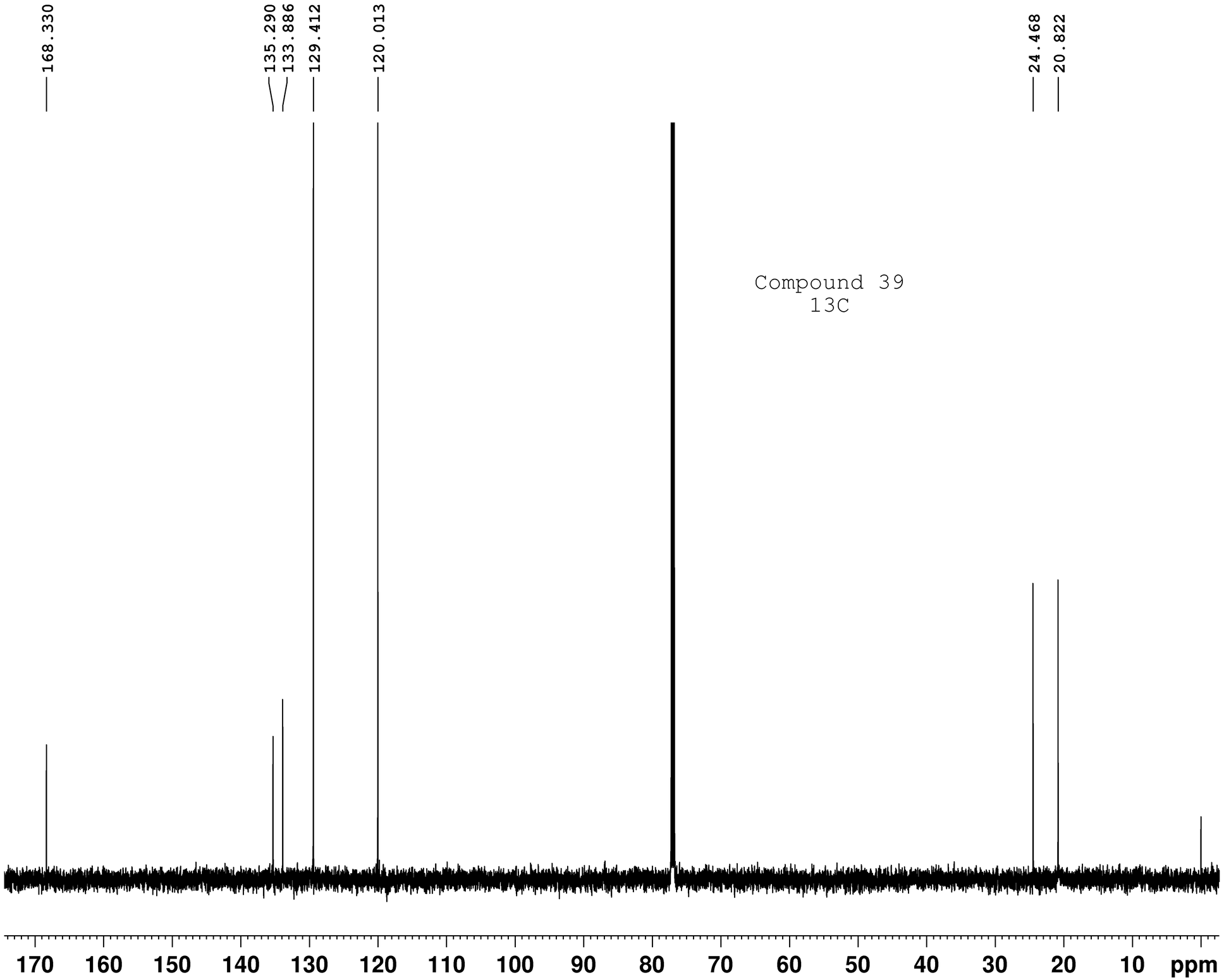
F2 - Processing parameters
SI                 65536
SF          150.8650999 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          39-CD-125A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_            20220112
Time                17.07 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    161
DW                 52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1             1.00000000 sec
TD0                     1
SFO1         599.9845606 MHz
NUC1                   1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

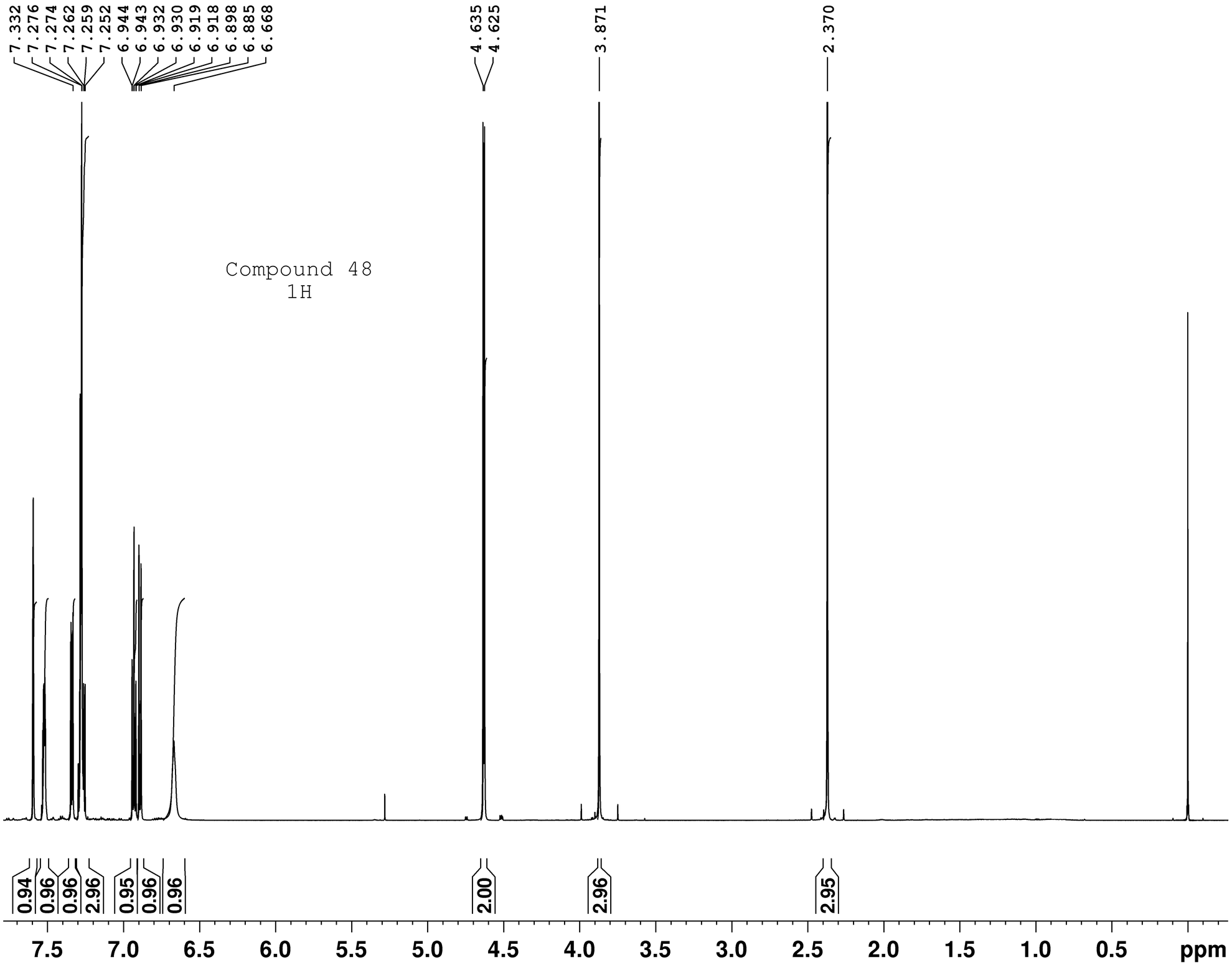
F2 - Processing parameters
SI                  65536
SF           599.9800136 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME              CD-125A
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220112
Time                17.13 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

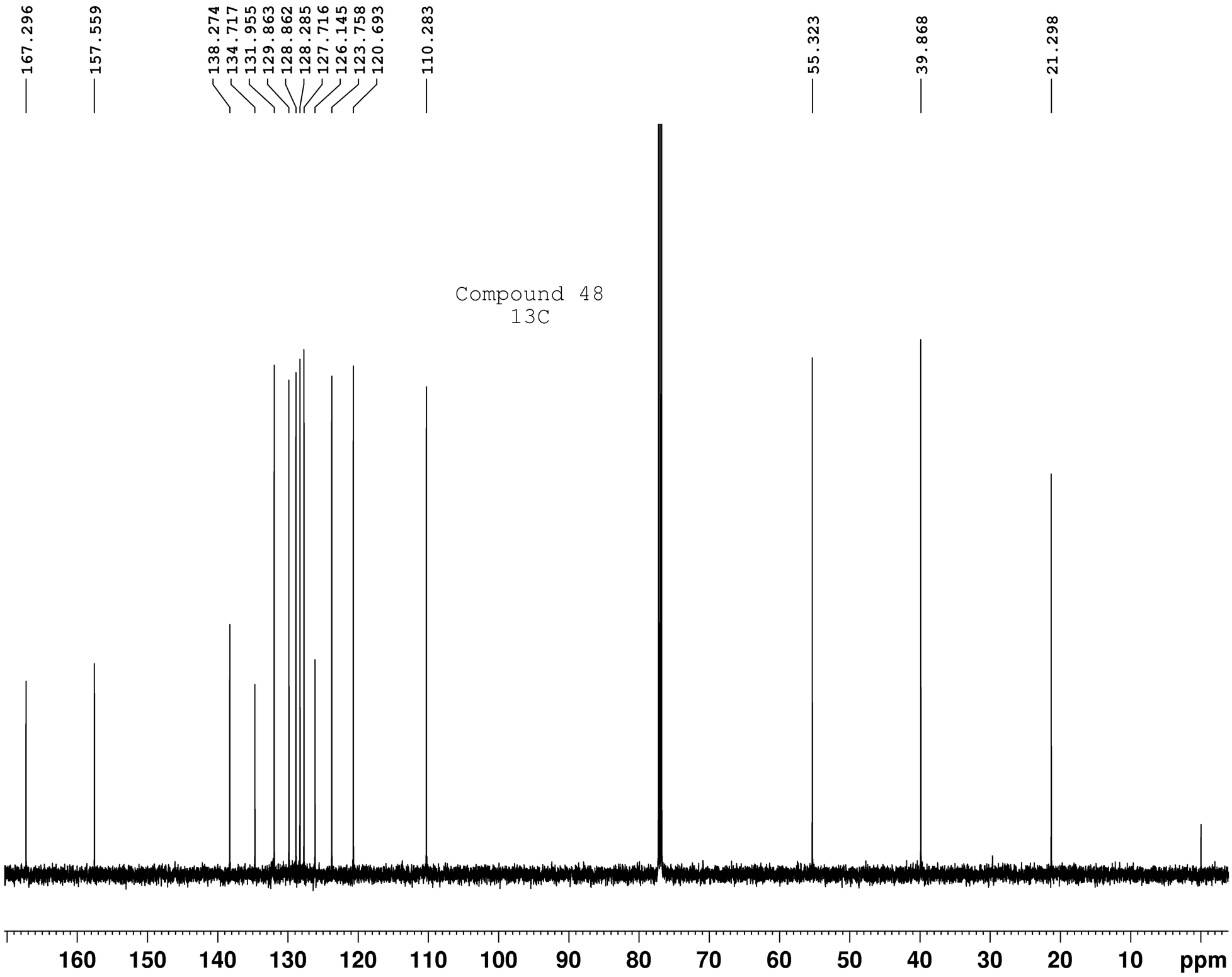
F2 - Processing parameters
SI                 65536
SF           150.8651004 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-103A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220224
Time                20.53 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    101
DW                 52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1             1.00000000 sec
TD0                     1
SFO1         599.9845606 MHz
NUC1                   1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

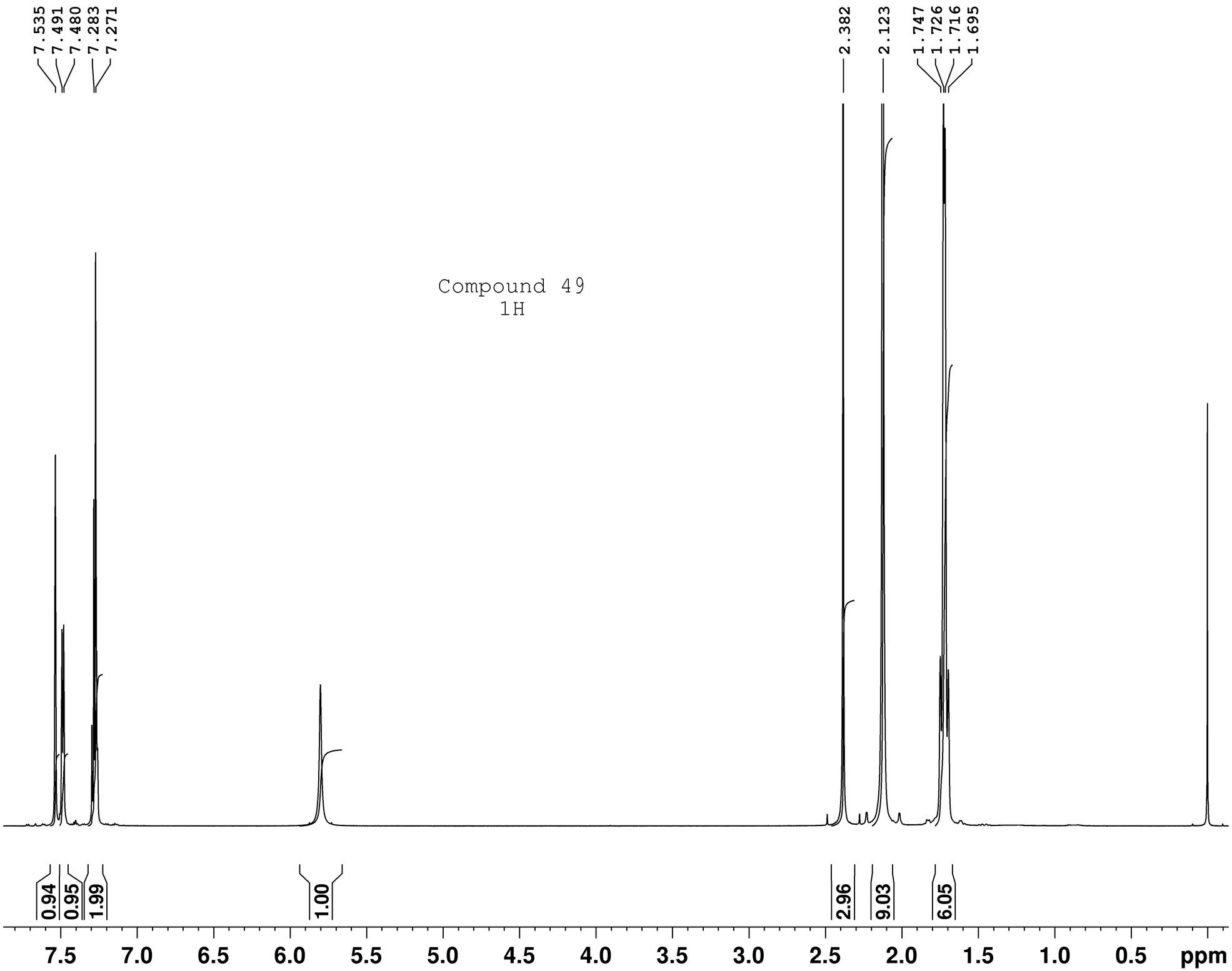
F2 - Processing parameters
SI                  65536
SF           599.9800185 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CE-103A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20220224
Time              20.58 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD               32768
SOLVENT          CDCl3
NS                 128
DS                   0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                2050
DW               13.867 usec
DE                6.50 usec
TE               293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

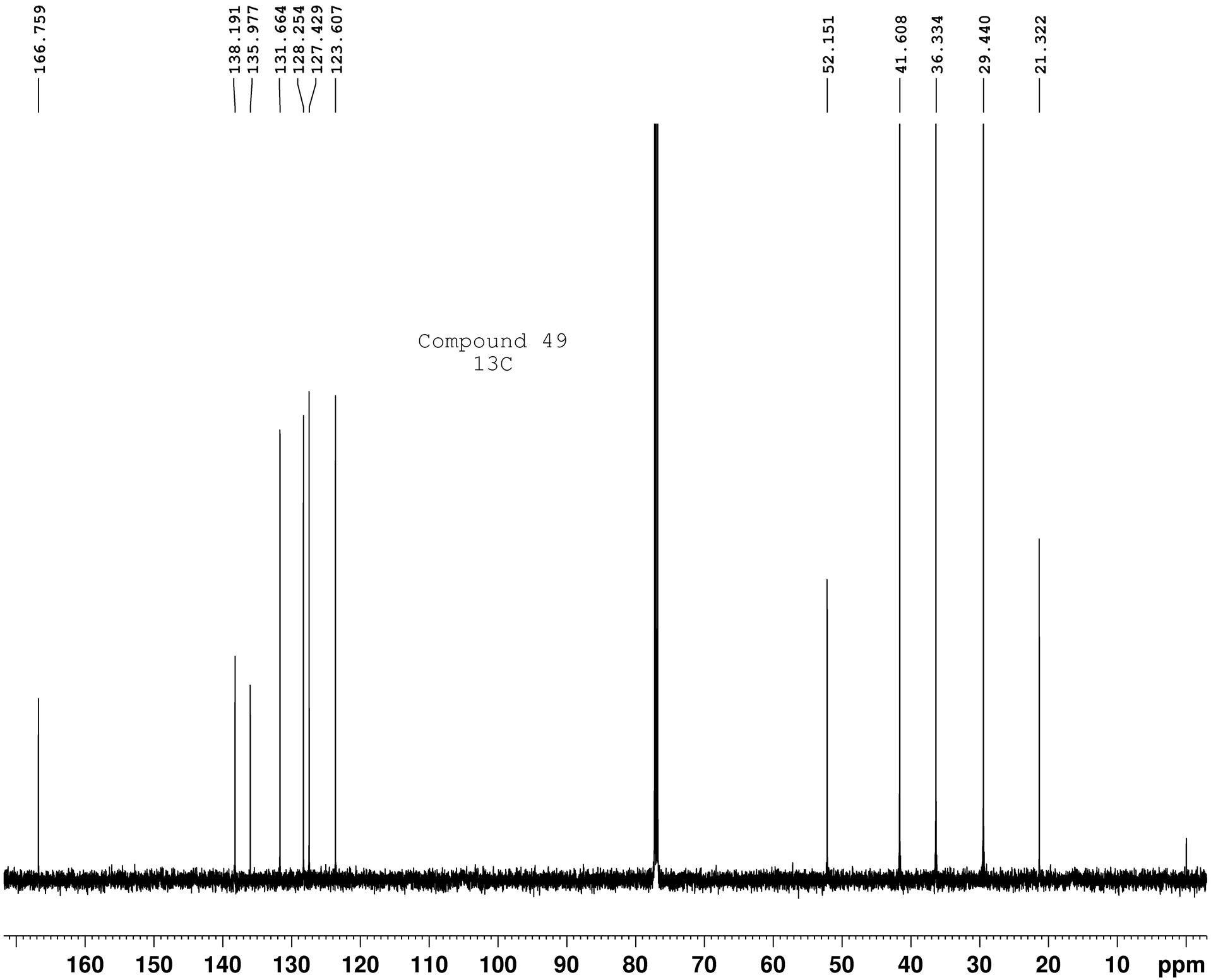
F2 - Processing parameters
SI                65536
SF          150.8651046 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME            CD-170A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20220224
Time               20.21 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  80.6
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

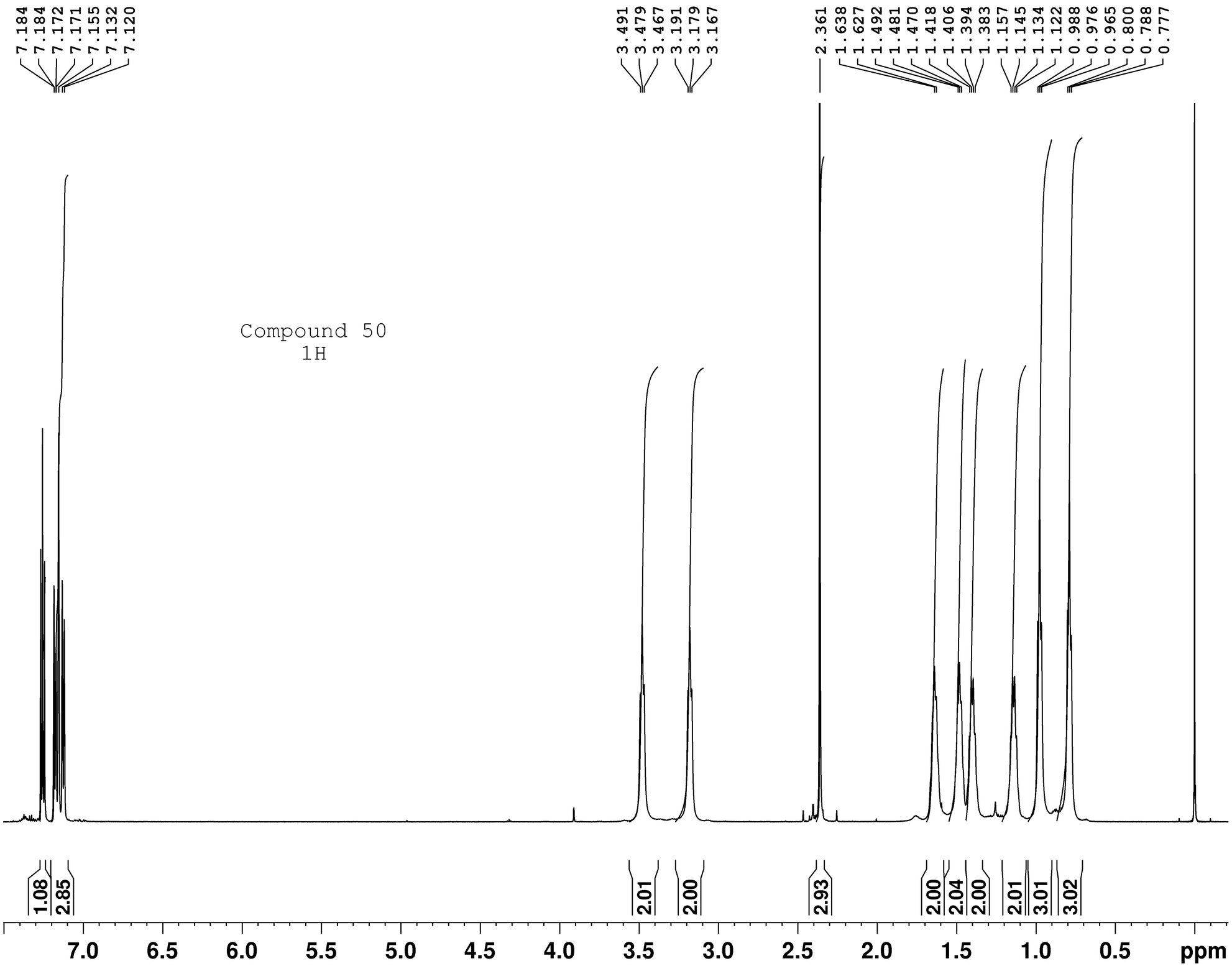
F2 - Processing parameters
SI                 65536
SF           599.9800112 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-170A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20220224
Time              20.26 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2            70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

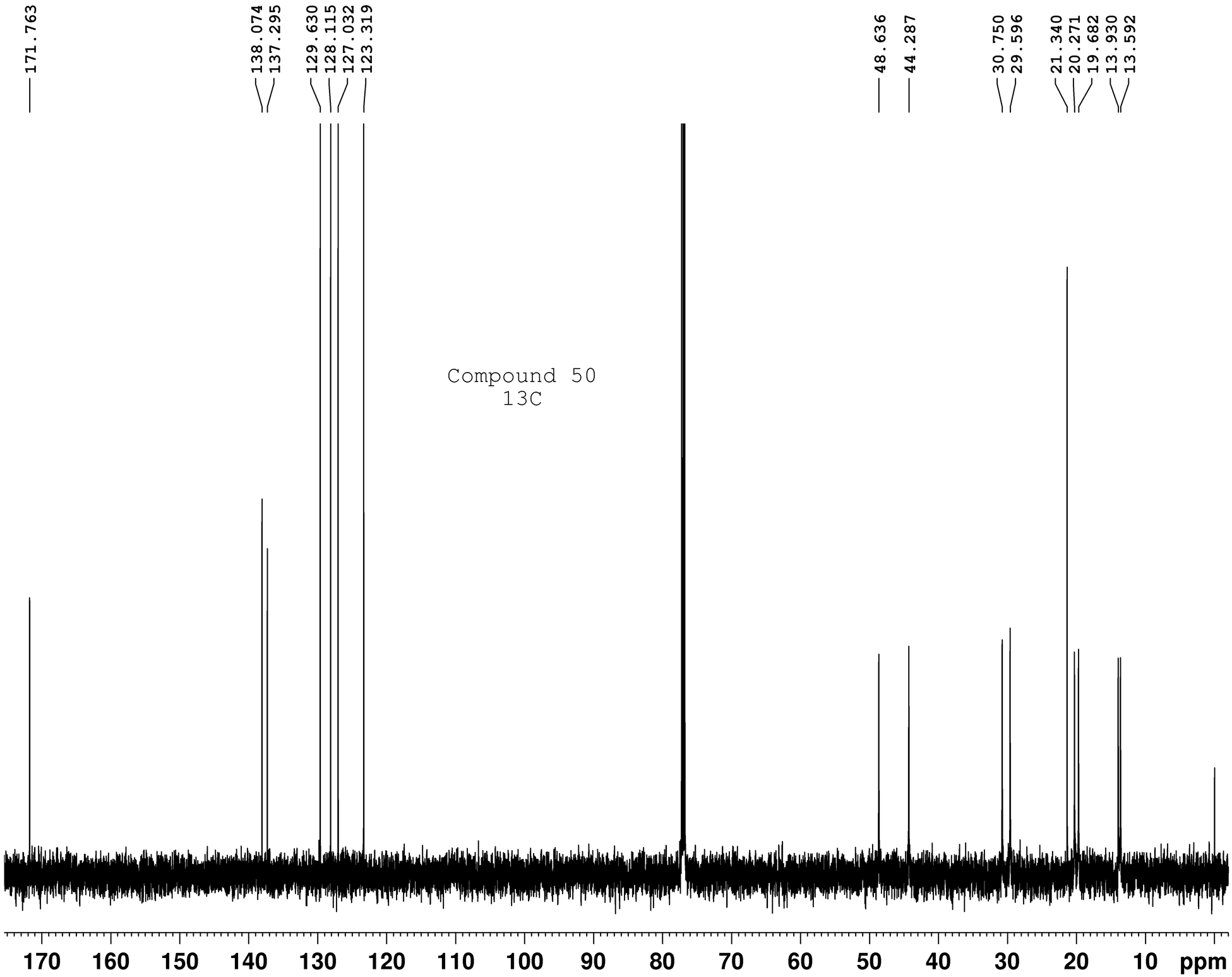
F2 - Processing parameters
SI                65536
SF          150.8651018 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME              CD-194A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220224
Time               20.37 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   101
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

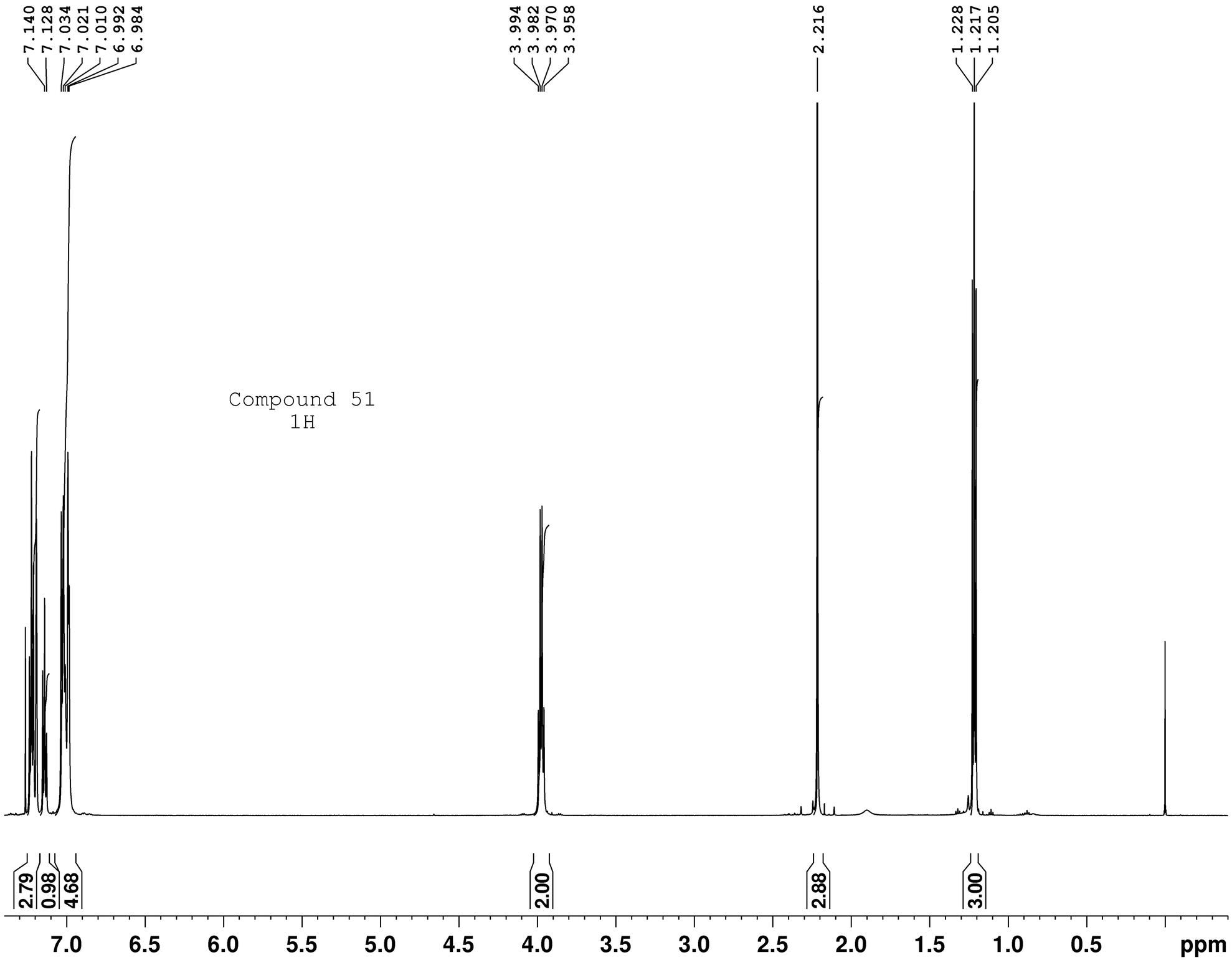
F2 - Processing parameters
SI                 65536
SF           599.9800097 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CD-194A
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220224
Time               20.43 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG            zgdc30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

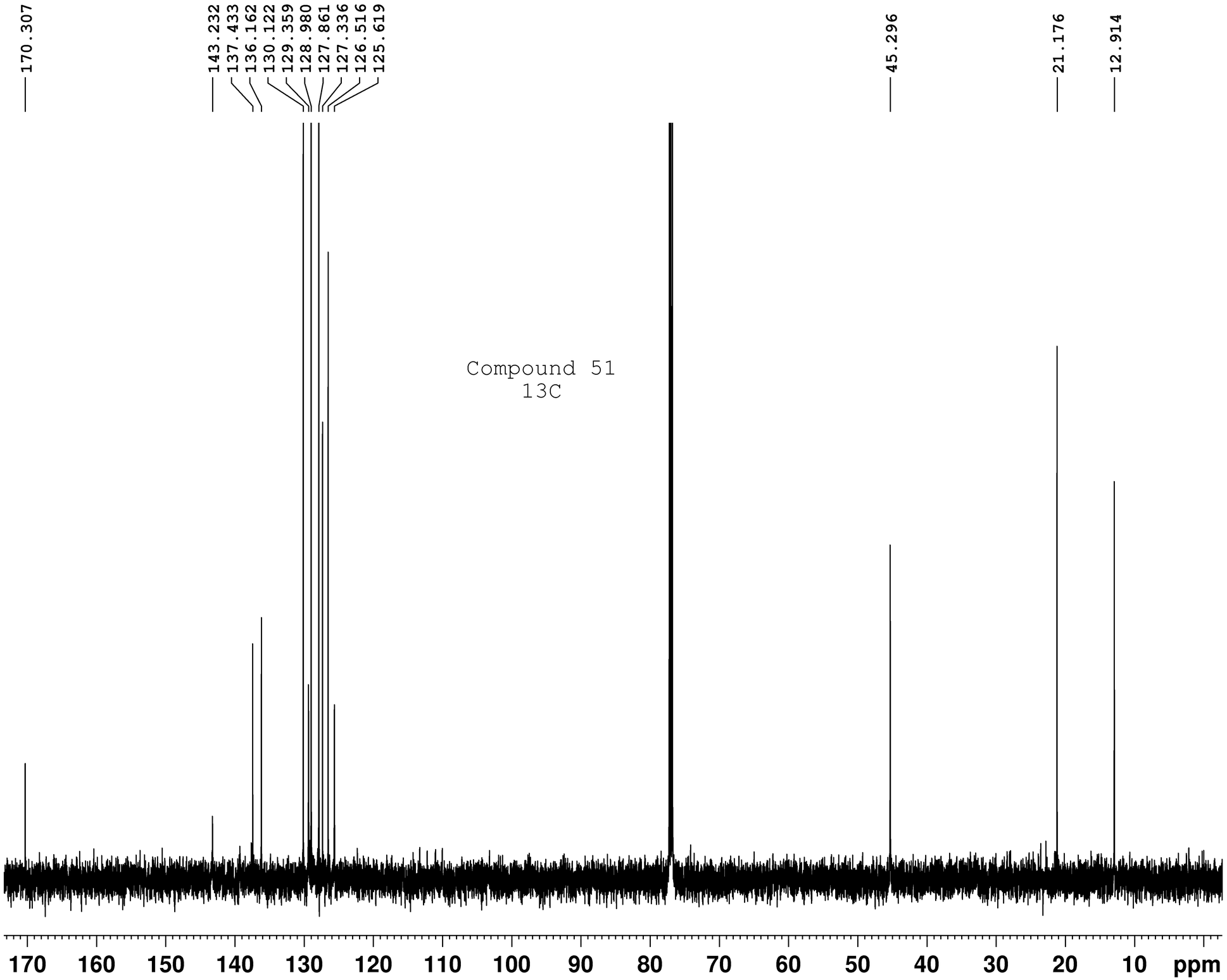
F2 - Processing parameters
SI                 65536
SF           150.8650996 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME            CD-175A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20210316
Time              20.10 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ            1.7039360 sec
RG                 80.6
DW               52.000 usec
DE                14.37 usec
TE                293.0 K
D1           1.00000000 sec
TD0                   1
SFO1        600.0145608 MHz
NUC1                 1H
P0                 3.62 usec
P1                10.85 usec
PLW1        20.00000000 W

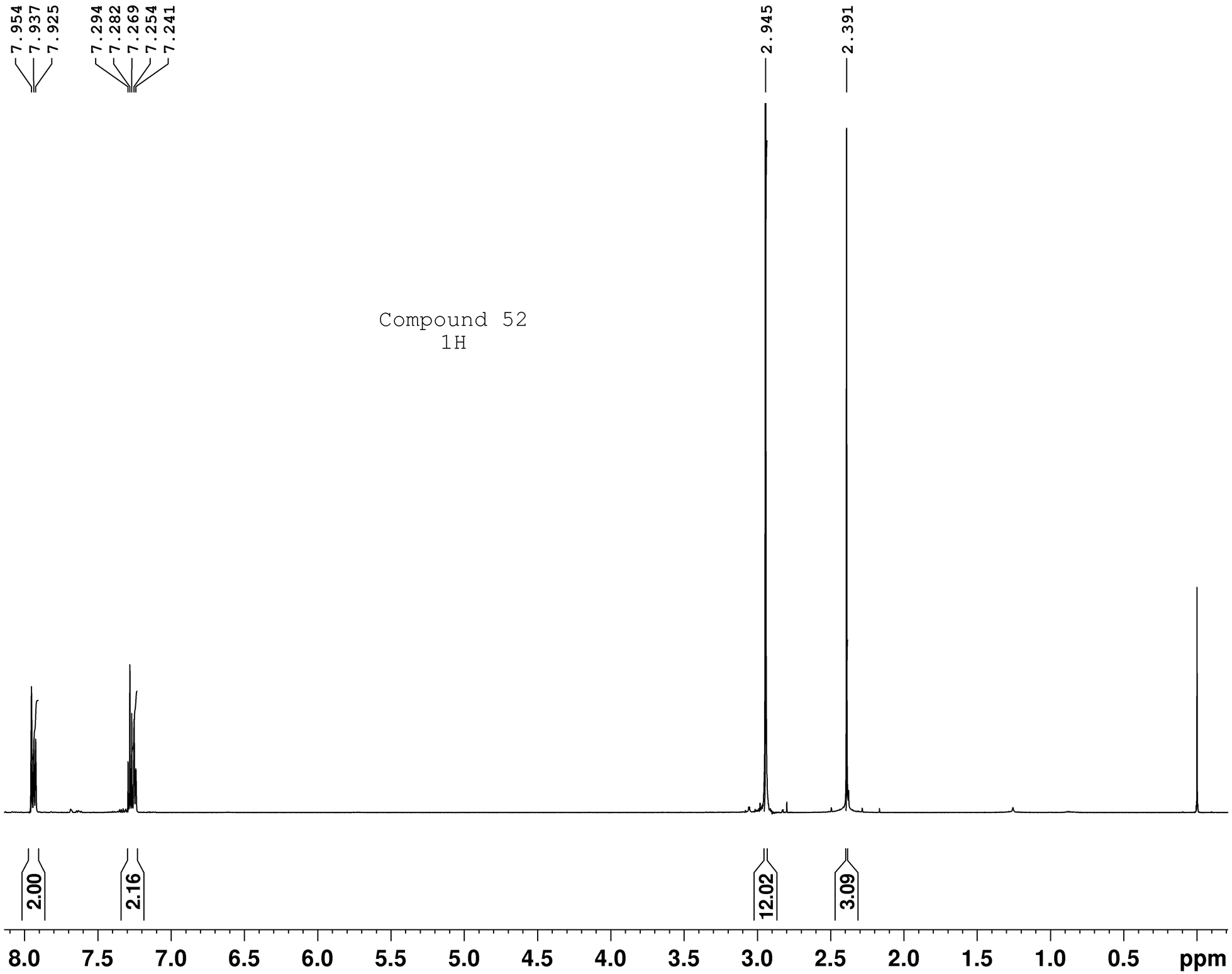
F2 - Processing parameters
SI                65536
SF          600.0100129 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME              CD-175A
EXPNO                  16
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210316
Time                20.46 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8892338 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

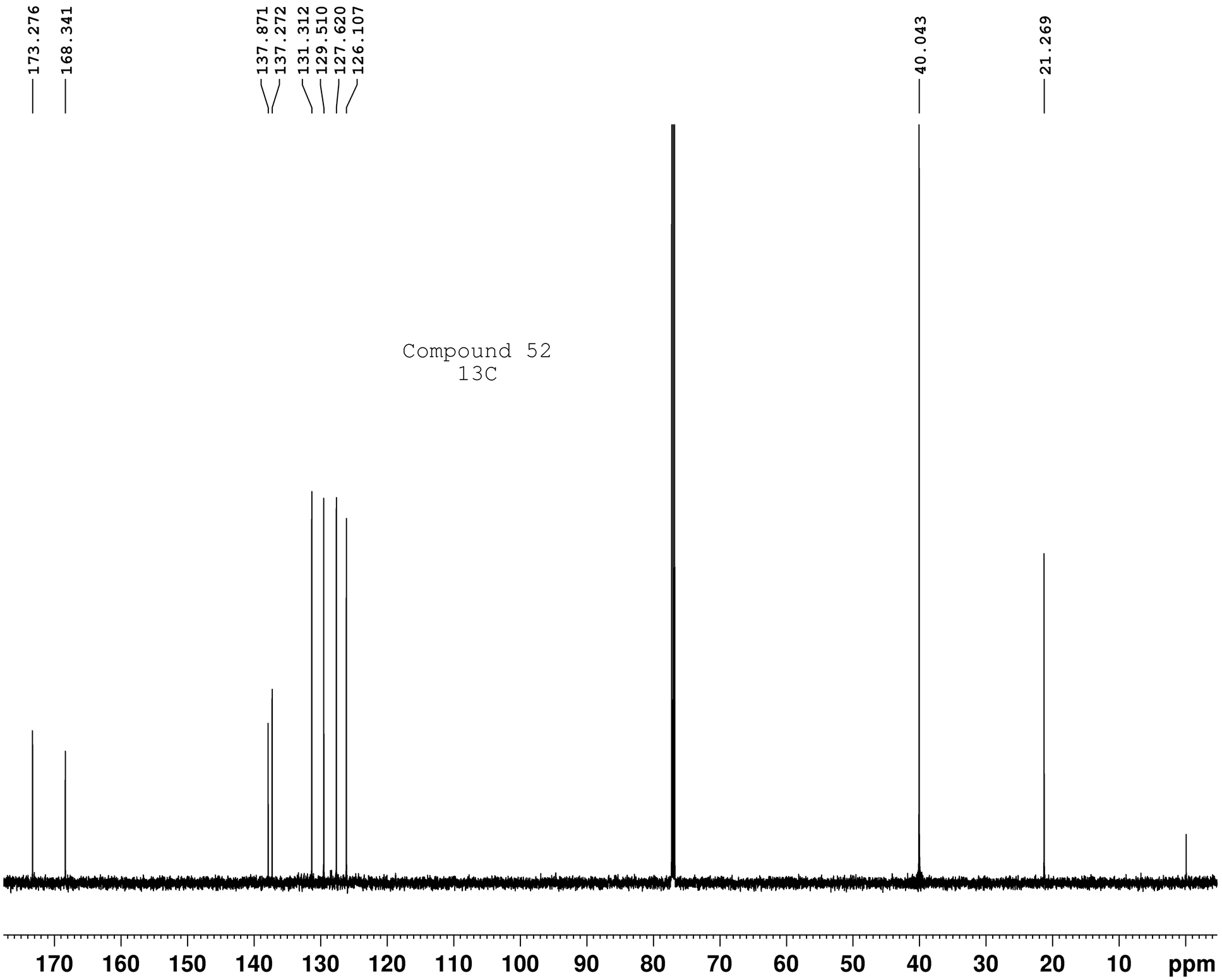
F2 - Processing parameters
SI                 65536
SF           150.8726437 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-23A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210222
Time               18.40 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  50.8
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

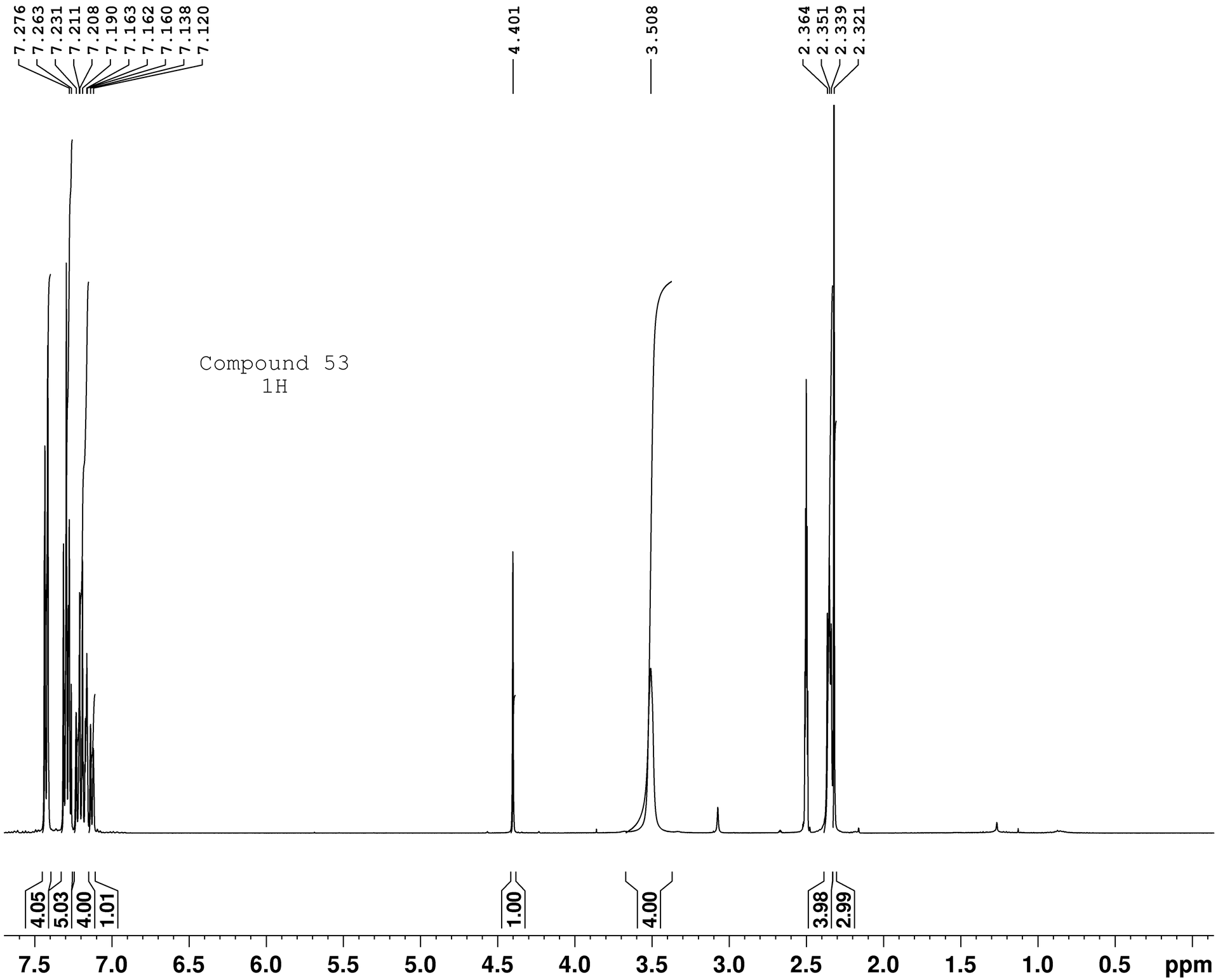
F2 - Processing parameters
SI                 65536
SF           600.0100013 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME                CE-23A
EXPNO                   16
PROCNO                   1

F2 - Acquisition Parameters
Date_             20210222
Time                 19.15 h
INSTRUM              spect
PROBHD   Z847801_0047 (
PULPROG             zgdc30
TD                   32768
SOLVENT              CDCl3
NS                     128
DS                       0
SWH              36057.691 Hz
FIDRES            2.200787 Hz
AQ               0.4543829 sec
RG                    2050
DW                  13.867 usec
DE                    6.50 usec
TE                   293.1 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           150.8892338 MHz
NUC1                   13C
P0                    3.27 usec
P1                    9.80 usec
PLW1           40.00000000 W
SFO2           600.0124004 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           20.00000000 W
PLW12           0.33800000 W

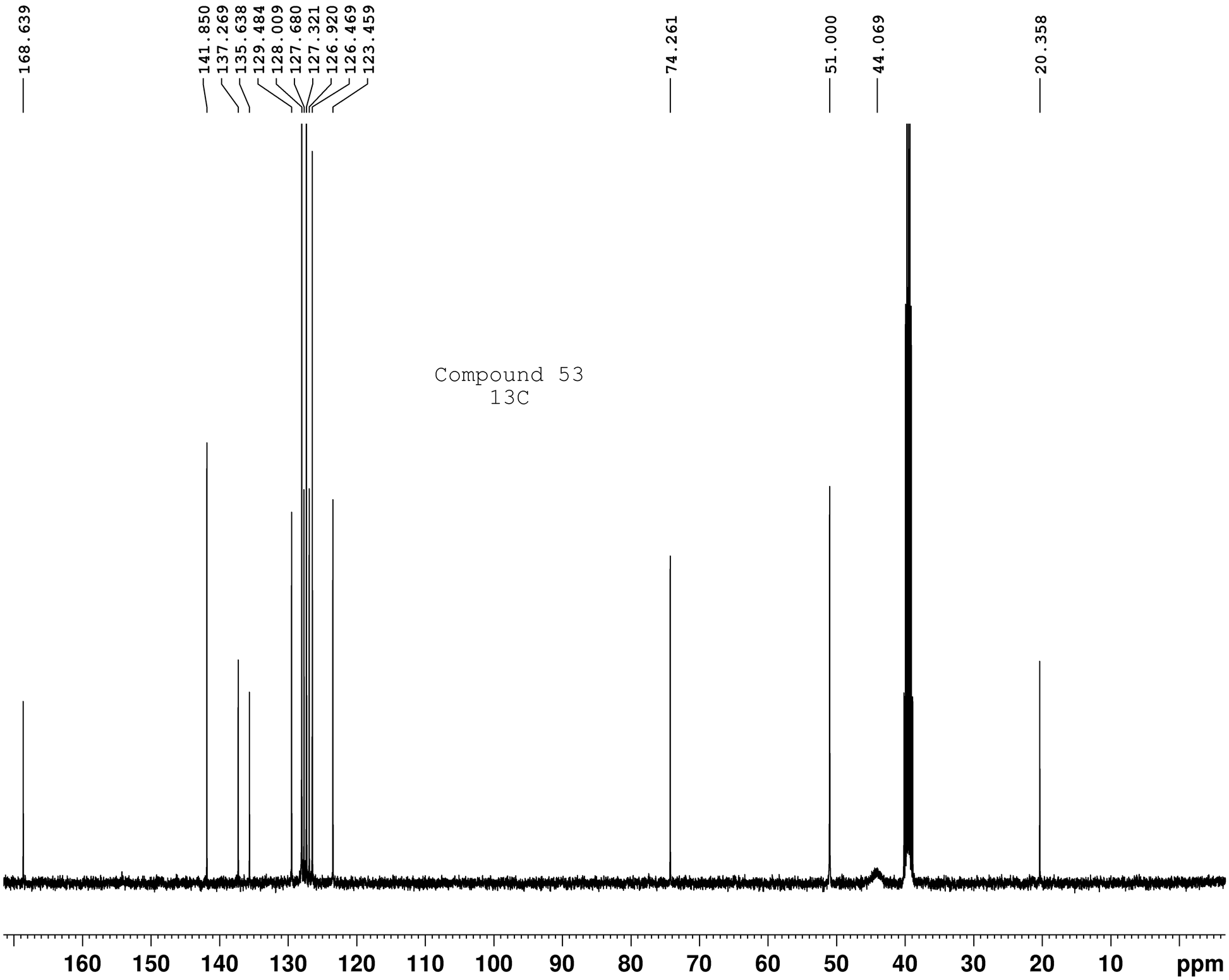
F2 - Processing parameters
SI                    65536
SF             150.8726510 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```




```
Current Data Parameters
NAME            CD-197B
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_            20220416
Time                12.56 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH            6578.947 Hz
FIDRES         0.401547 Hz
AQ            2.4903679 sec
RG                   101
DW                76.000 usec
DE                 7.79 usec
TE                353.0 K
D1            2.00000000 sec
TD0                    1
SFO1        400.1330415 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1        20.07200050 W

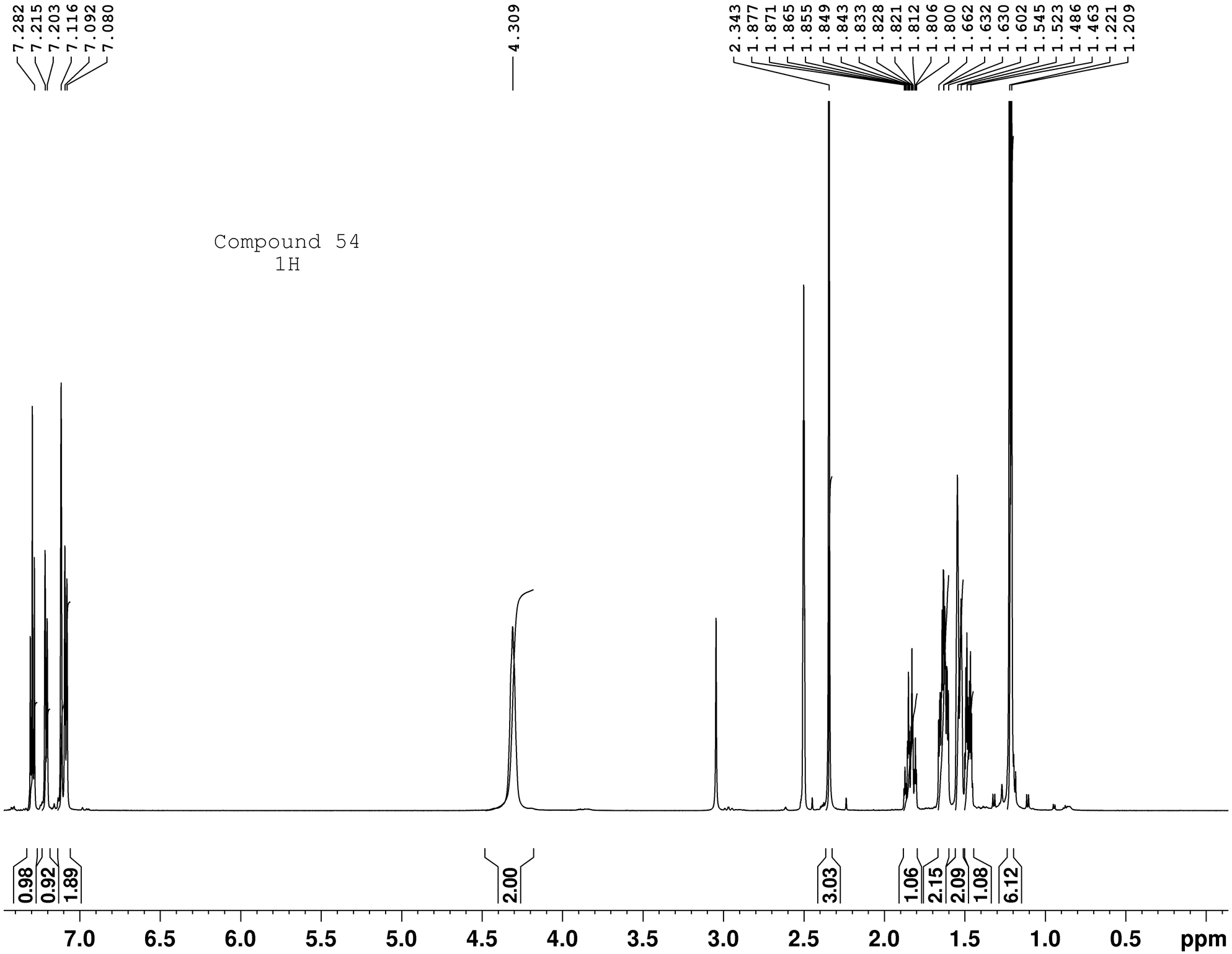
F2 - Processing parameters
SI                 65536
SF          400.1300034 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-197B
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220416
Time              13.35 h
INSTRUM  Avance Neo 400
PROBHD   Z175272_0007 (
PULPROG           zgdc30
TD                32768
SOLVENT            DMSO
NS                  1024
DS                     0
SWH           23809.523 Hz
FIDRES         1.453218 Hz
AQ            0.6881280 sec
RG                 45.2
DW                21.000 usec
DE                 6.50 usec
TE                353.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6238383 MHz
NUC1                13C
P0                  3.33 usec
P1                 10.00 usec
PLW1        58.46900177 W
SFO2        400.1316008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        20.07200050 W
PLW12        0.24781001 W

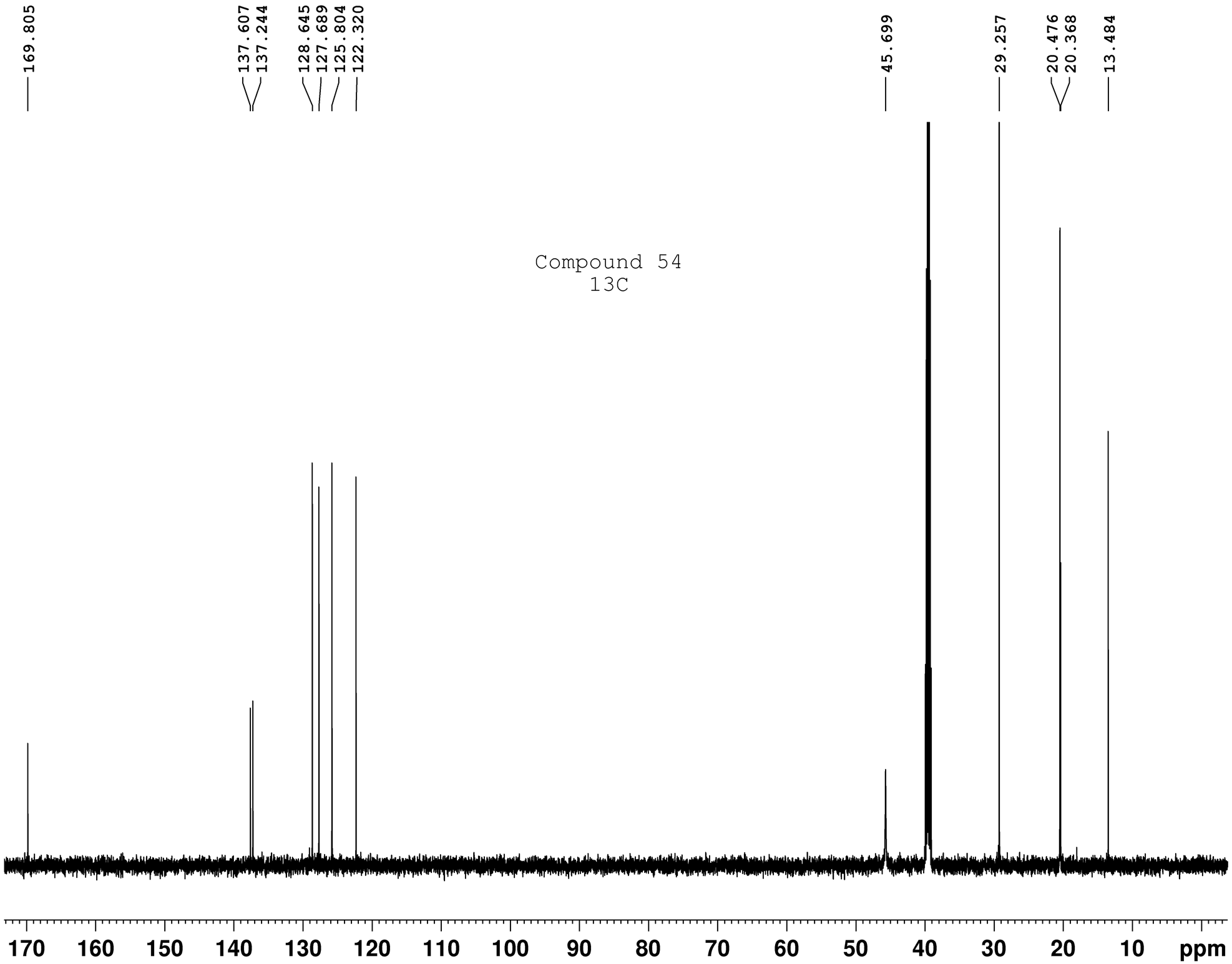
F2 - Processing parameters
SI                 65536
SF          100.6128587 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME            CD-192A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20220225
Time              21.18 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ            1.7039360 sec
RG                 90.5
DW                52.000 usec
DE                14.38 usec
TE                353.1 K
D1            1.00000000 sec
TD0                    1
SFO1        599.9845606 MHz
NUC1                  1H
P0                 3.60 usec
P1                10.80 usec
PLW1        20.00000000 W

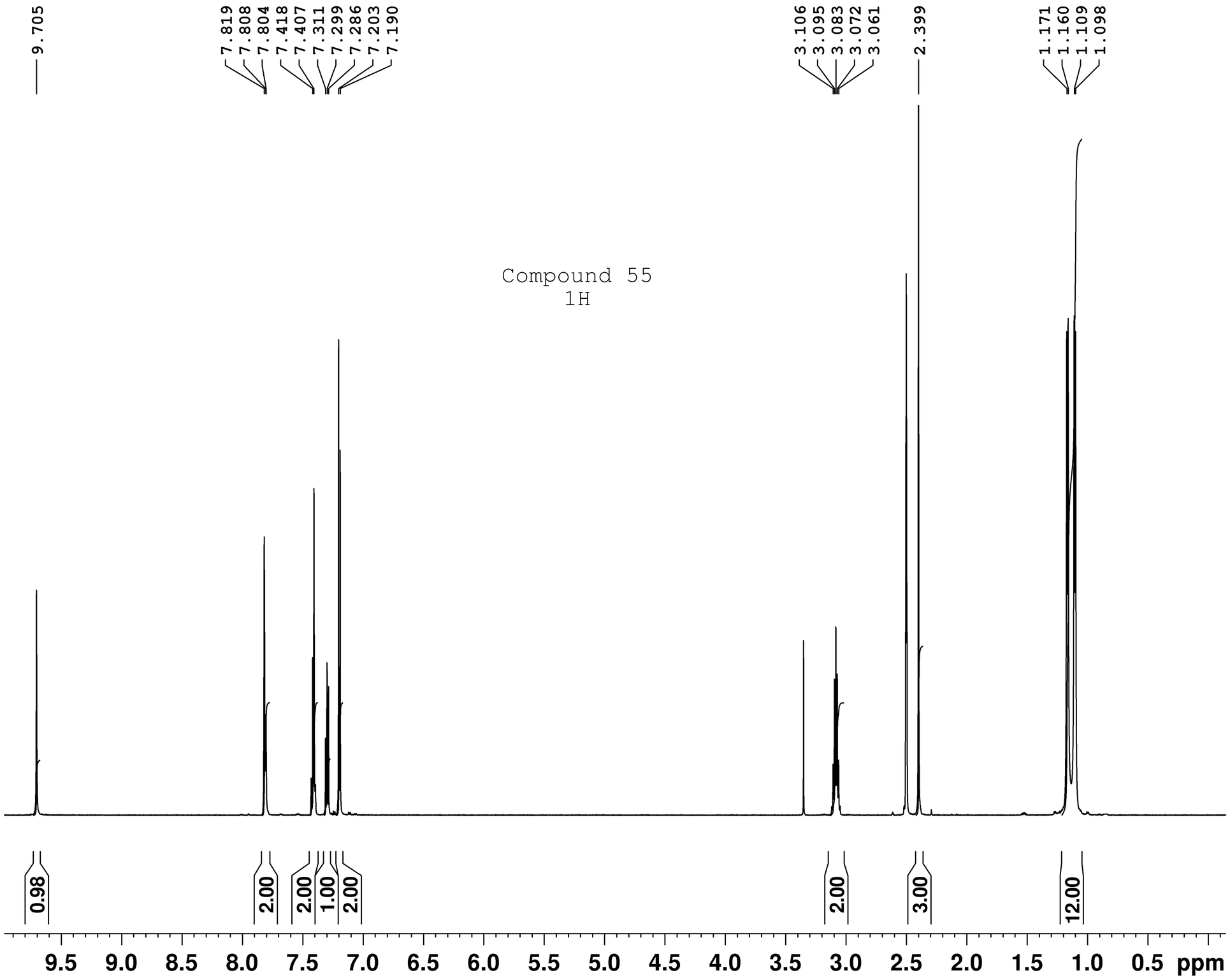
F2 - Processing parameters
SI                65536
SF          599.9800046 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CD-192A
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220225
Time               21.23 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT             DMSO
NS                    128
DS                      0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                   2050
DW                13.867 usec
DE                  6.50 usec
TE                 353.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         150.8816889 MHz
NUC1                  13C
P0                   3.27 usec
P1                   9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

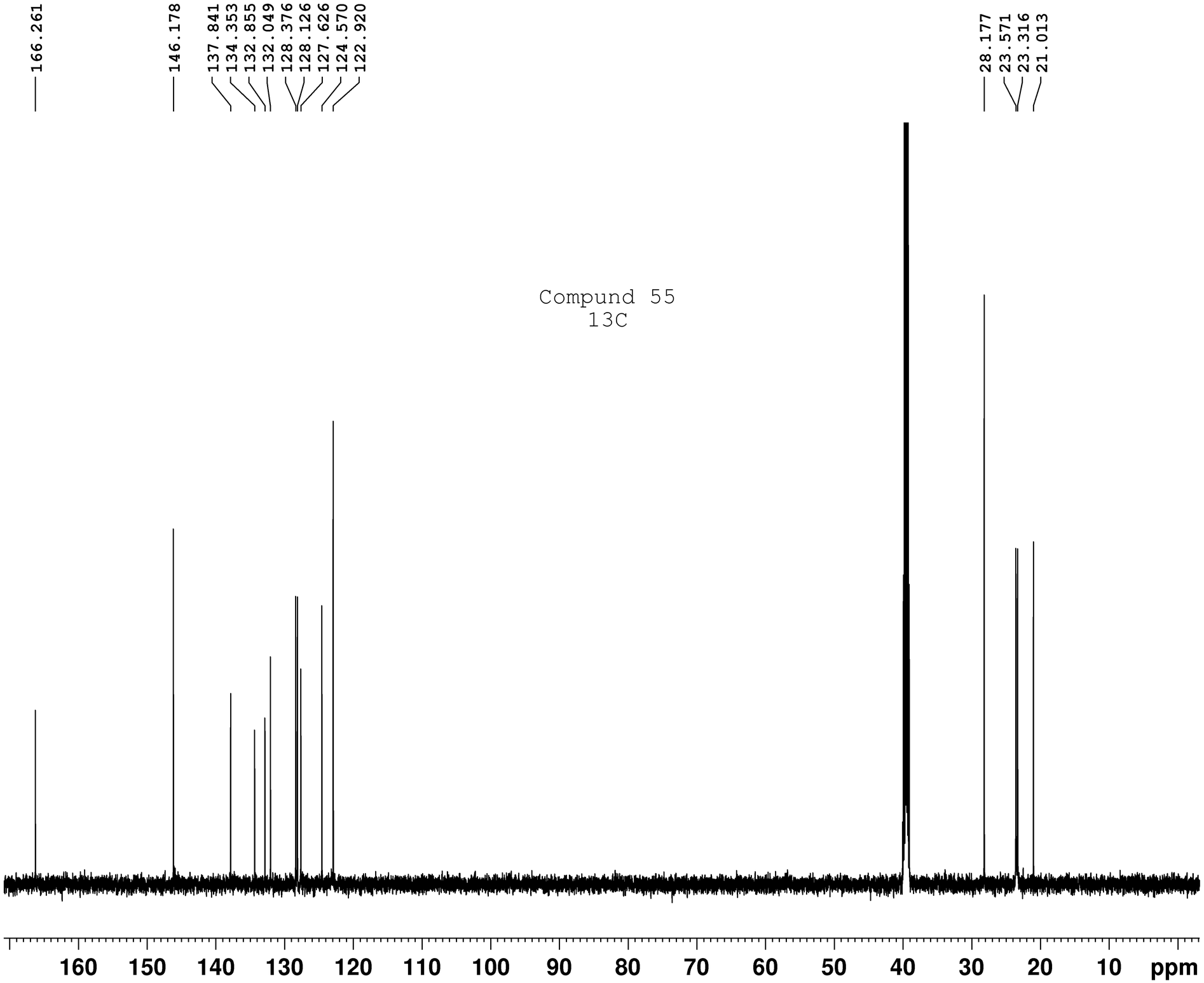
F2 - Processing parameters
SI                  65536
SF           150.8652284 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
Current Data Parameters
NAME              CD-181A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210428
Time                 0.15 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                      1
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   90.5
DW                 52.000 usec
DE                  14.37 usec
TE                  293.0 K
D1             1.00000000 sec
TD0                     1
SFO1         600.0145608 MHz
NUC1                   1H
P0                   3.62 usec
P1                  10.85 usec
PLW1         20.00000000 W

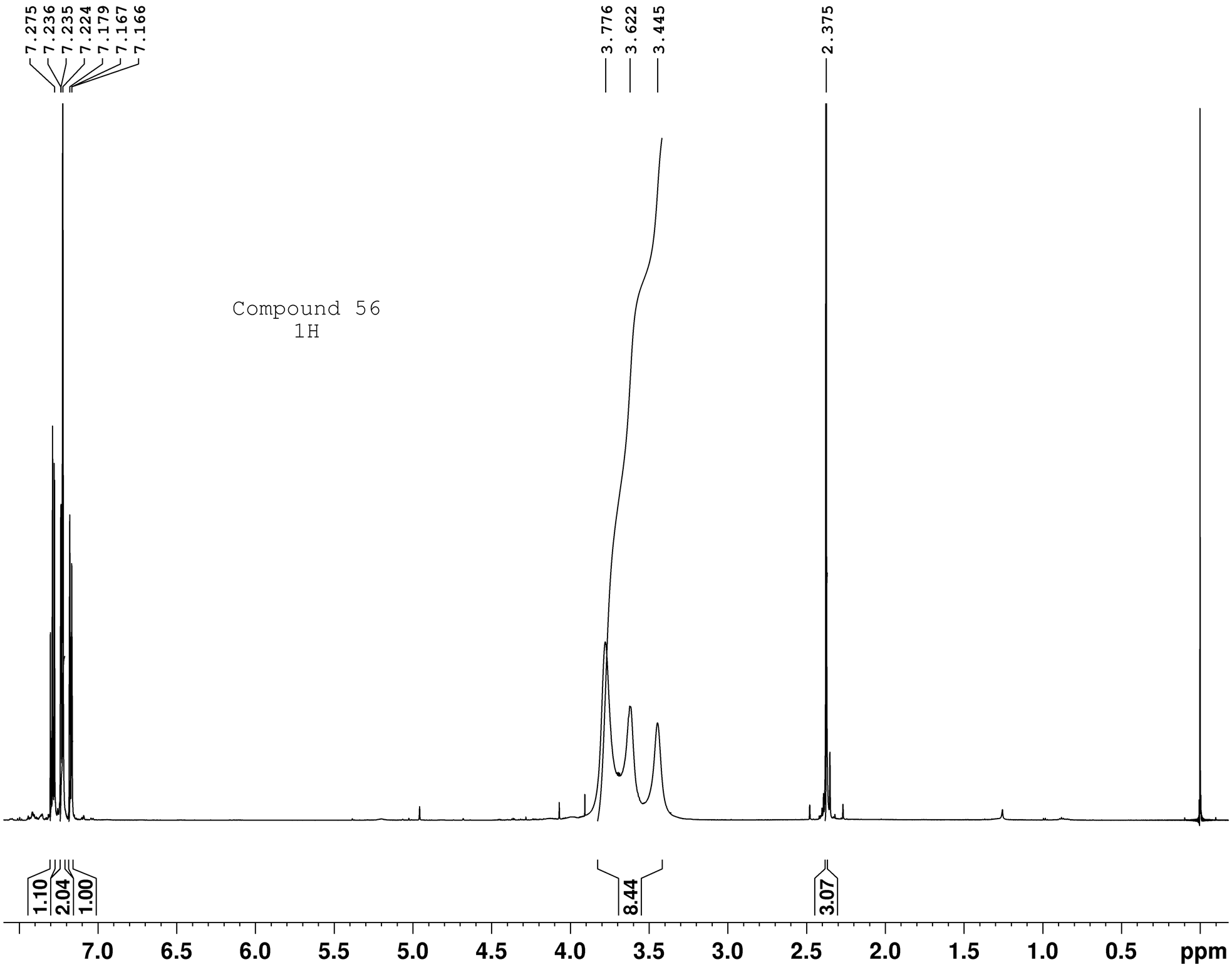
F2 - Processing parameters
SI                  65536
SF           600.0100047 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CD-181A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20210428
Time               0.20 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8892338 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

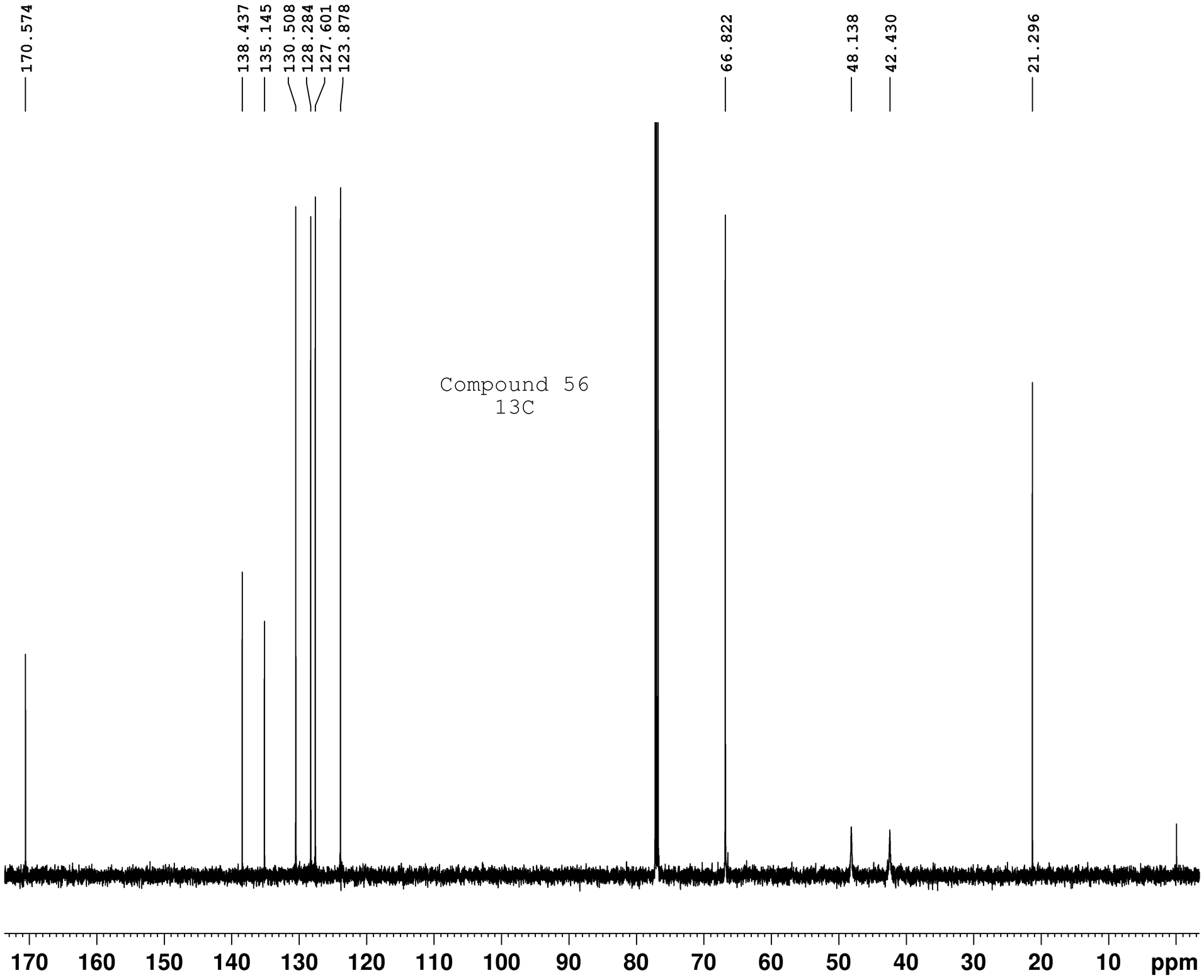
F2 - Processing parameters
SI                 65536
SF           150.8727027 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          56-CD-186A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220112
Time               17.23 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  80.6
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

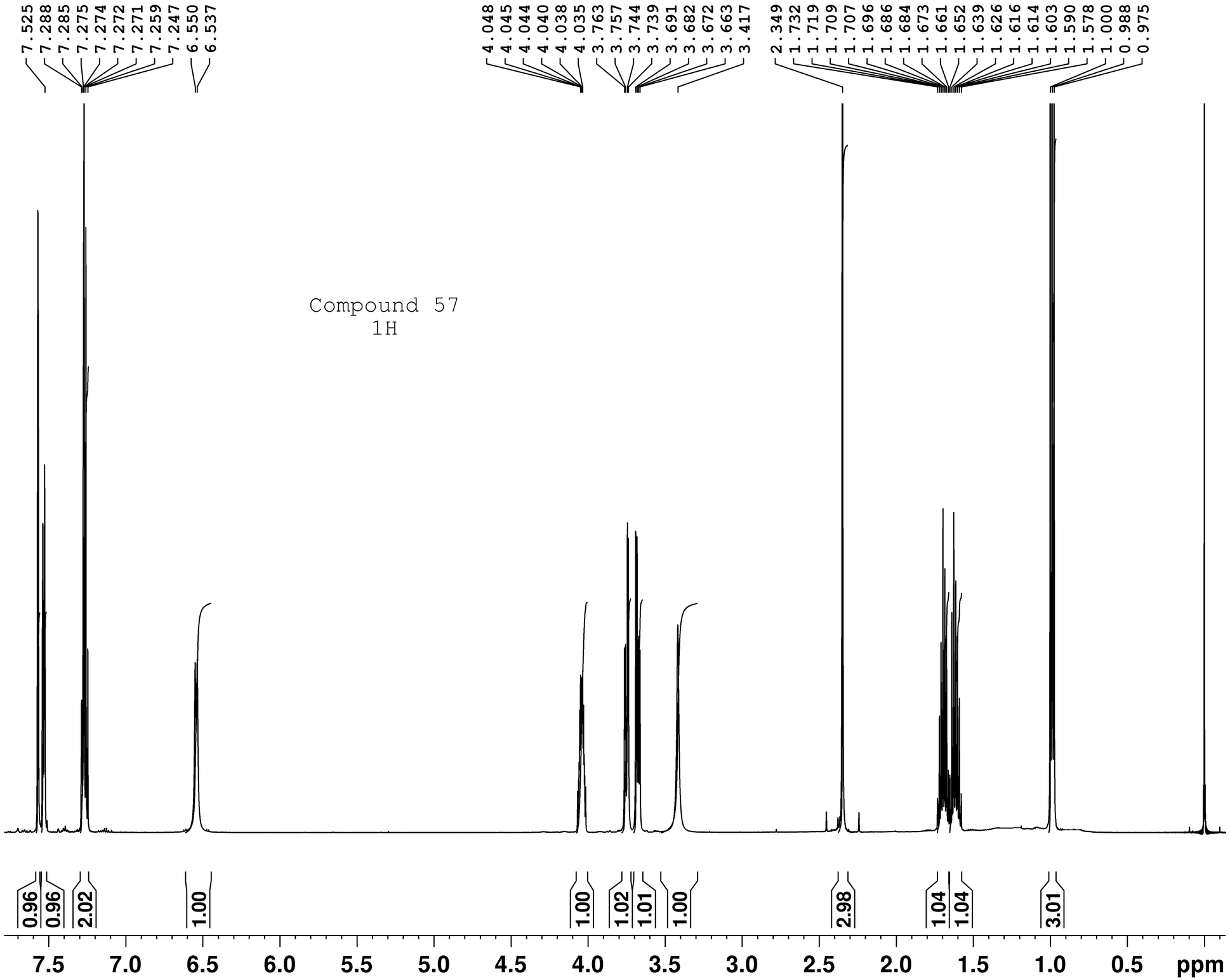
F2 - Processing parameters
SI                 65536
SF          599.9800034 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CD-186A
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220112
Time                17.29 h
INSTRUM             spect
PROBHD    Z847801_0047 (
PULPROG            zgdc30
TD                  32768
SOLVENT             CDCl3
NS                    128
DS                      0
SWH             36057.691 Hz
FIDRES           2.200787 Hz
AQ              0.4543829 sec
RG                   2050
DW                 13.867 usec
DE                   6.50 usec
TE                  293.1 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          150.8816889 MHz
NUC1                  13C
P0                   3.27 usec
P1                   9.80 usec
PLW1          40.00000000 W
SFO2          599.9824003 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               70.00 usec
PLW2          20.00000000 W
PLW12          0.53044999 W

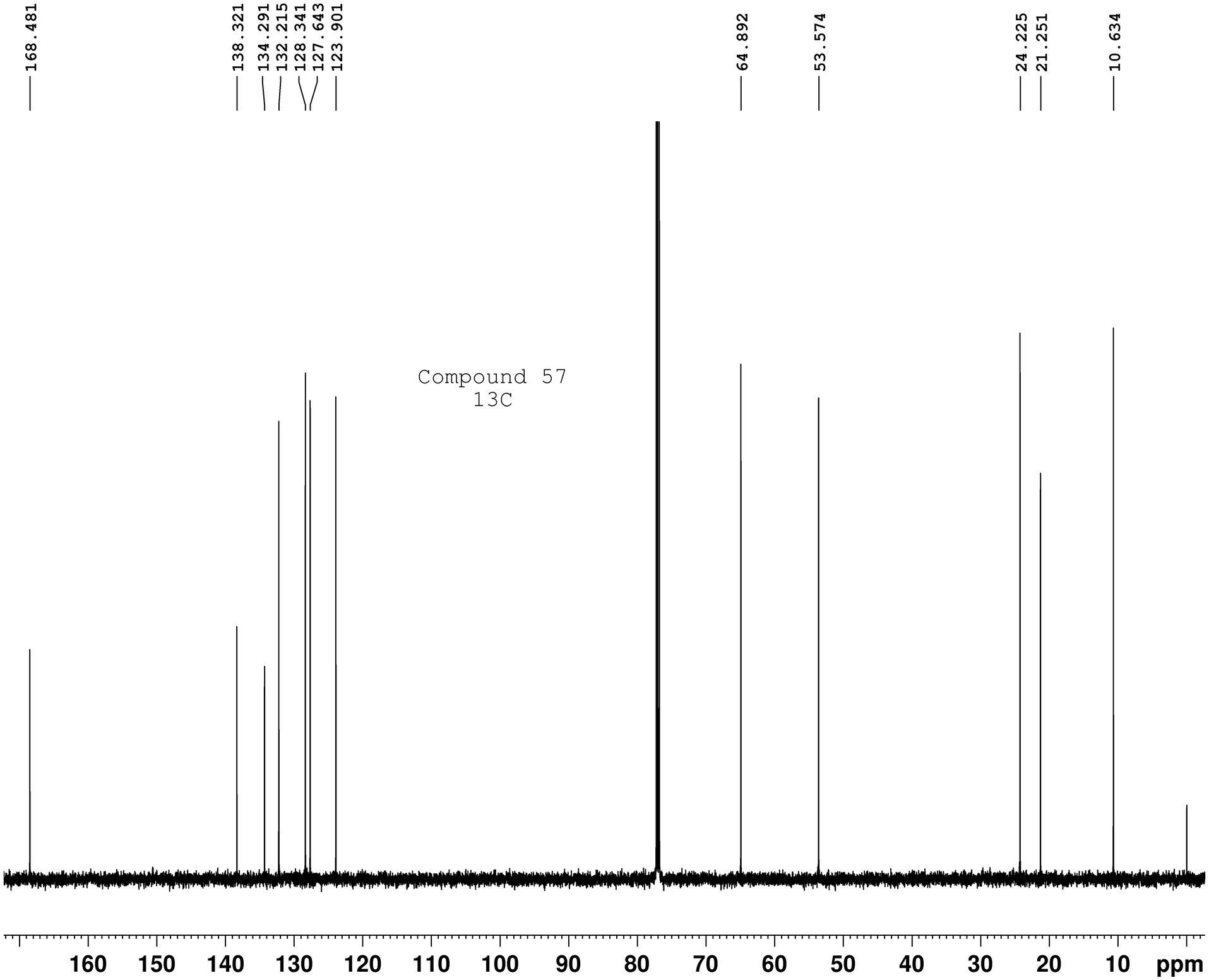
F2 - Processing parameters
SI                  65536
SF            150.8651060 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
Current Data Parameters
NAME              CE-15A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210219
Time               18.49 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  50.8
DW                52.000 usec
DE                14.37 usec
TE                293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

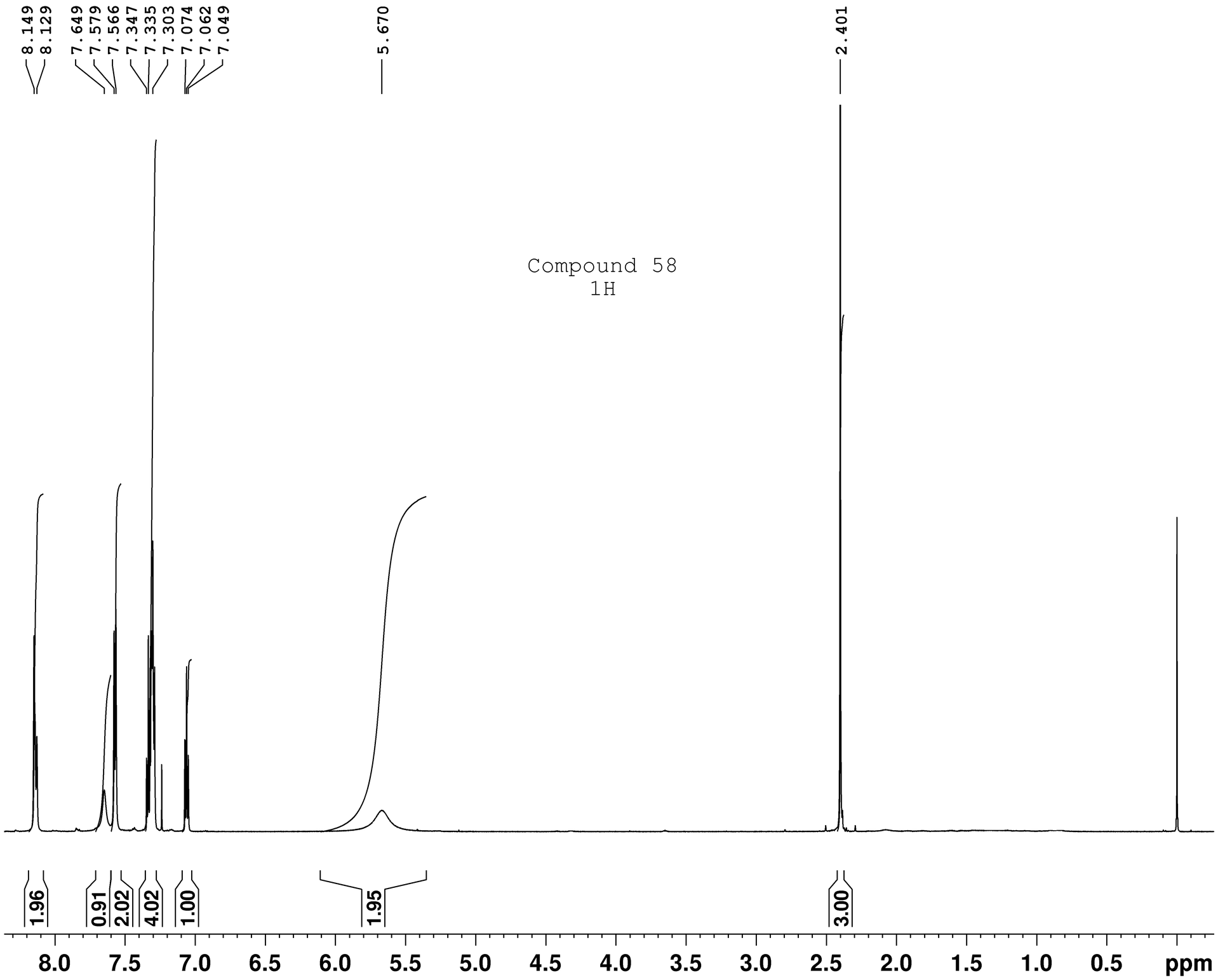
F2 - Processing parameters
SI                 65536
SF          600.0100095 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CE-15A
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210219
Time               19.24 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8892338 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

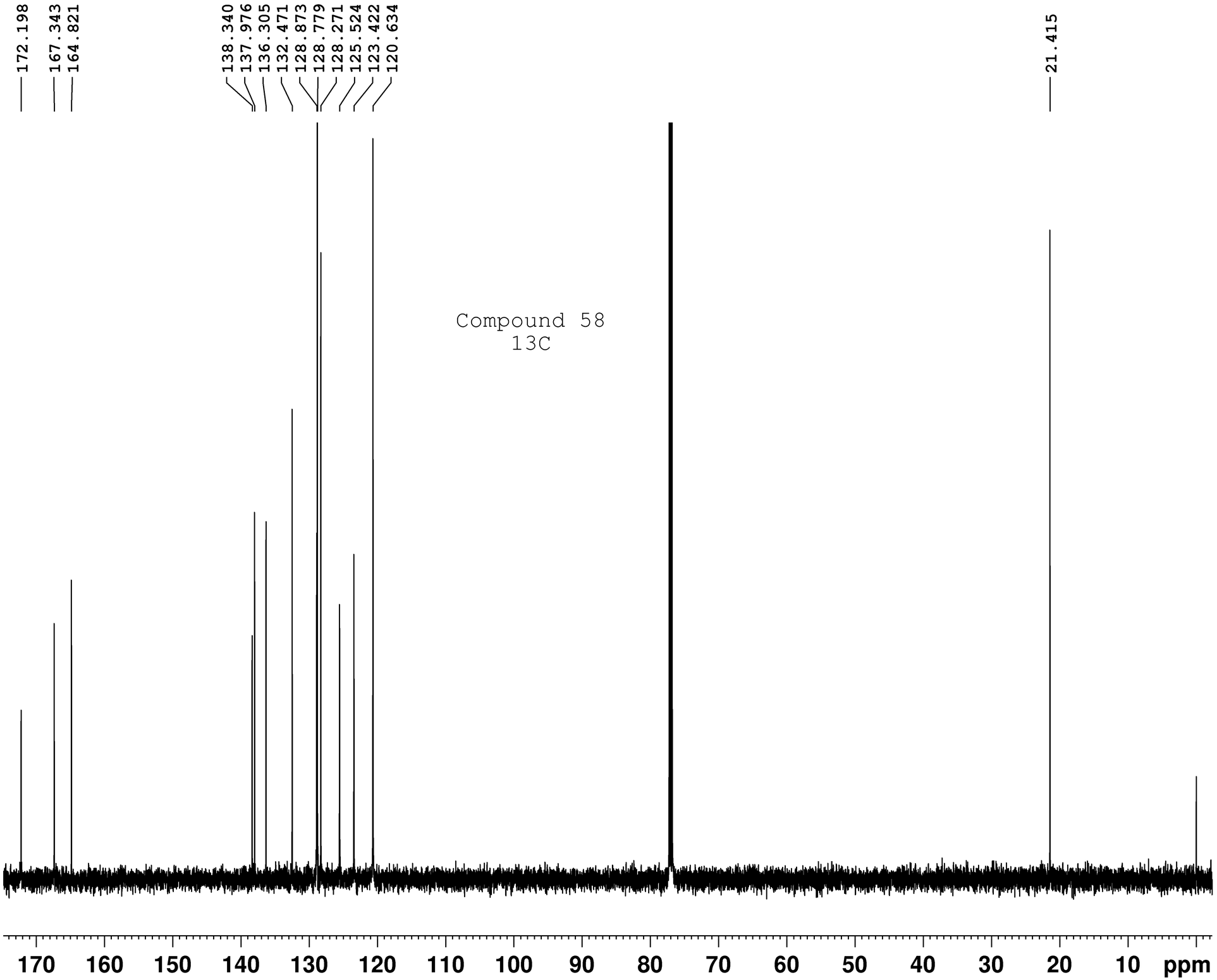
F2 - Processing parameters
SI                 65536
SF           150.8726471 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-14A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210222
Time               17.54 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  50.8
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

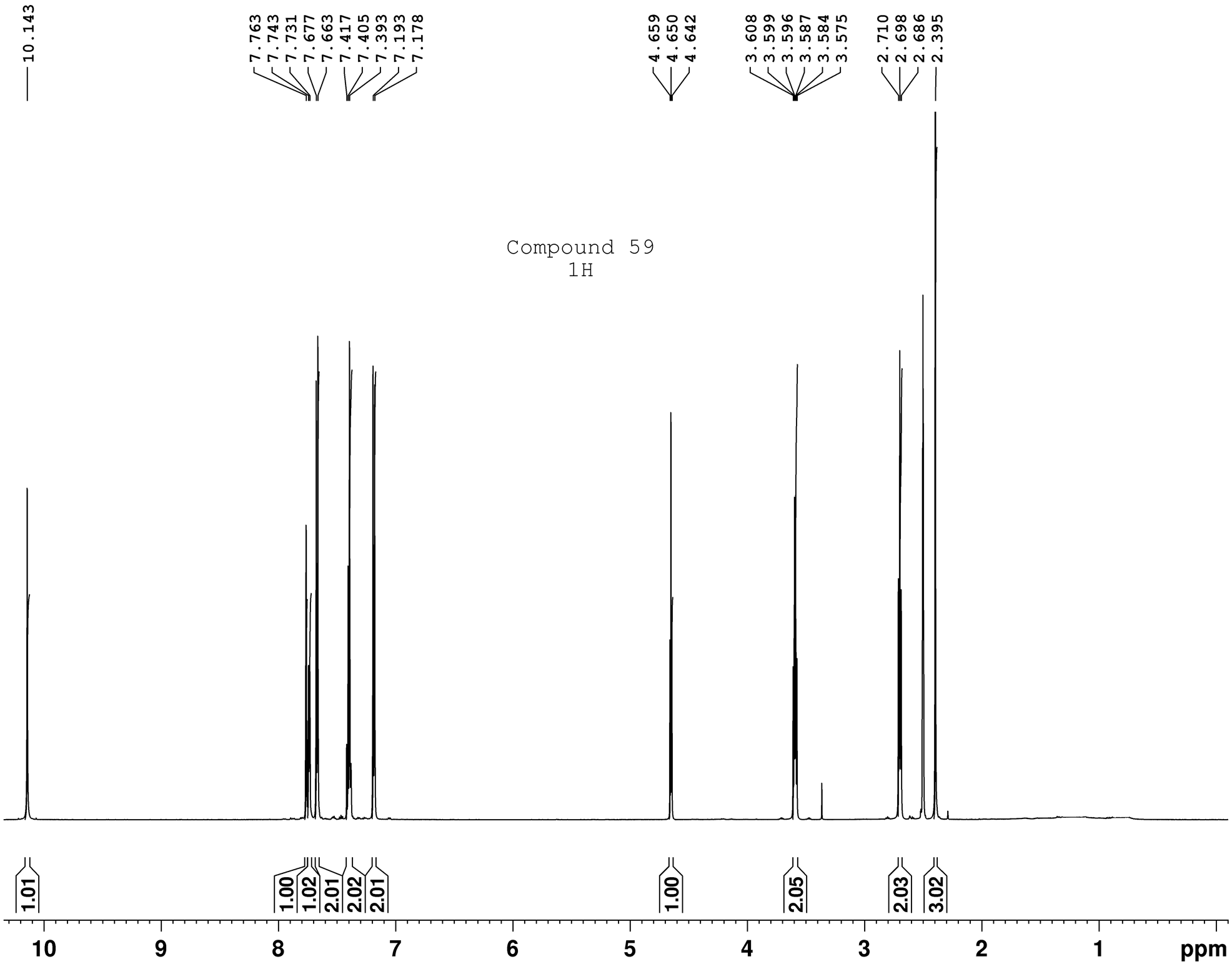
F2 - Processing parameters
SI                 65536
SF           600.0100278 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CE-14A
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210222
Time               18.29 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                 2050
DW                13.867 usec
DE                 6.50 usec
TE                293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8892338 MHz
NUC1                 13C
P0                 3.27 usec
P1                 9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

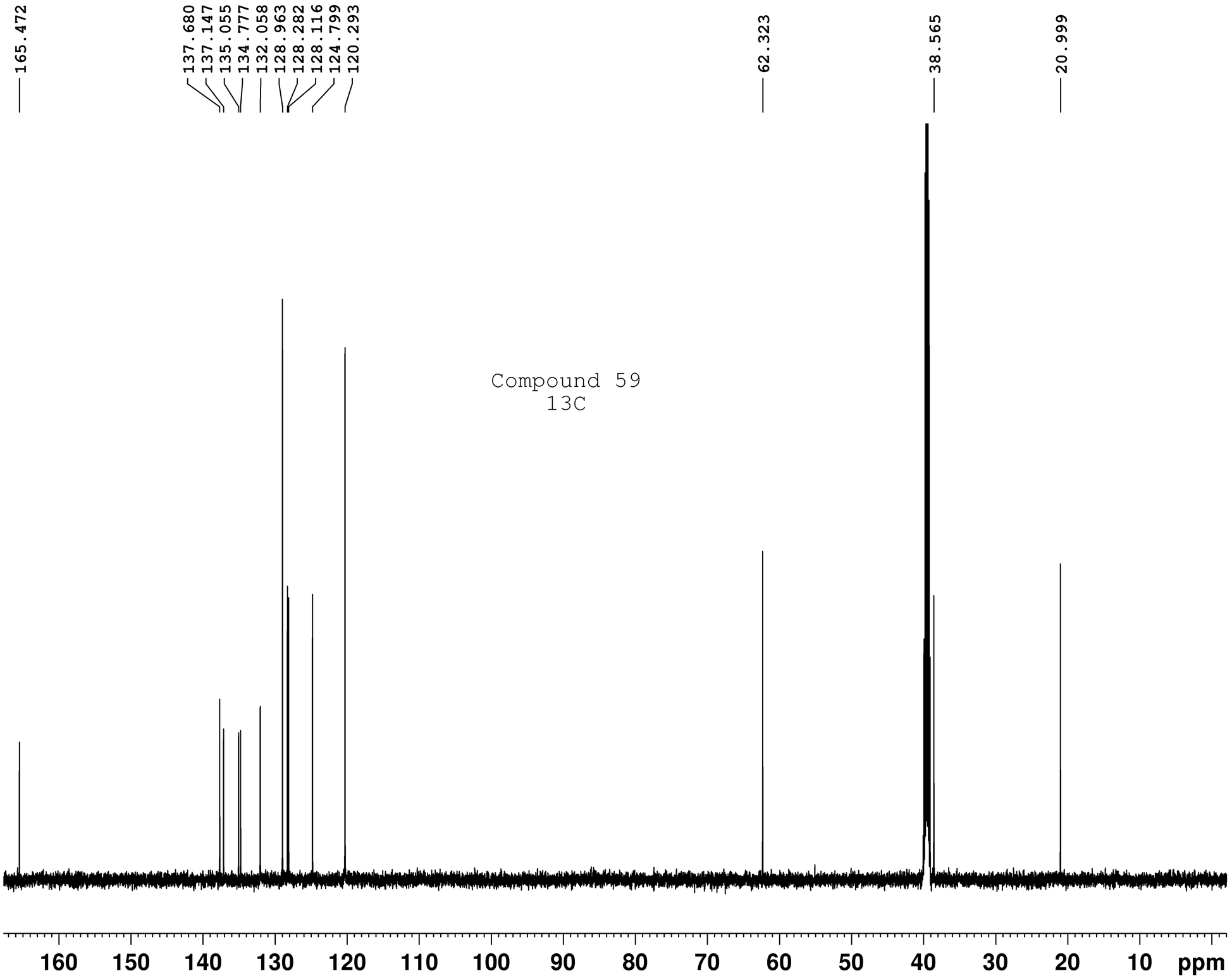
F2 - Processing parameters
SI                 65536
SF           150.8726505 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-03A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210217
Time               19.20 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    64
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.0145608 MHz
NUC1                  1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

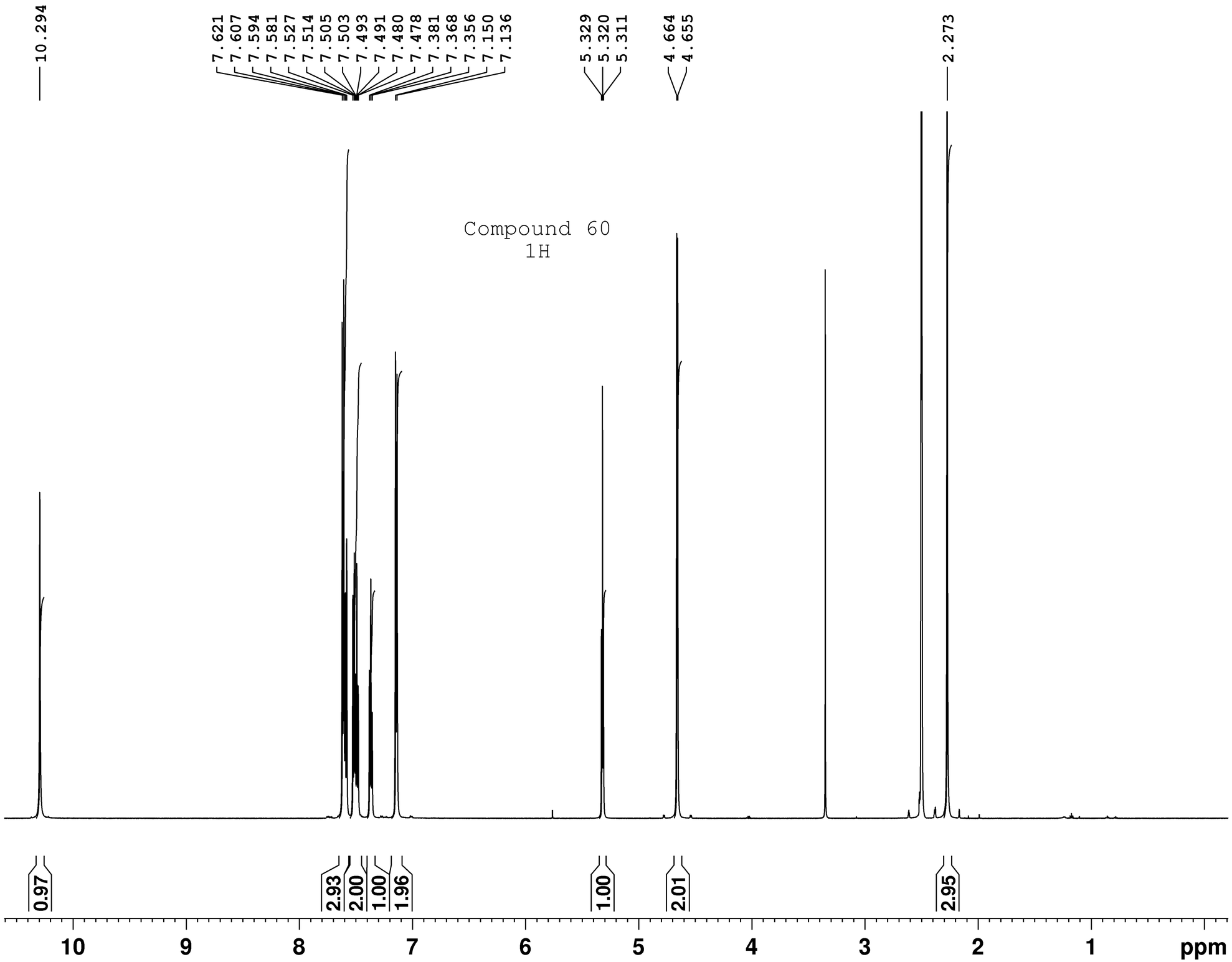
F2 - Processing parameters
SI                 65536
SF           600.0100050 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME                CE-03A
EXPNO                   16
PROCNO                   1

F2 - Acquisition Parameters
Date_             20210217
Time                 19.55 h
INSTRUM              spect
PROBHD   Z847801_0047 (
PULPROG             zgdc30
TD                   32768
SOLVENT               DMSO
NS                     128
DS                       0
SWH              36057.691 Hz
FIDRES            2.200787 Hz
AQ               0.4543829 sec
RG                    2050
DW                  13.867 usec
DE                    6.50 usec
TE                   293.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           150.8892338 MHz
NUC1                    13C
P0                    3.27 usec
P1                    9.80 usec
PLW1           40.00000000 W
SFO2           600.0124004 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                90.00 usec
PLW2           20.00000000 W
PLW12           0.33800000 W

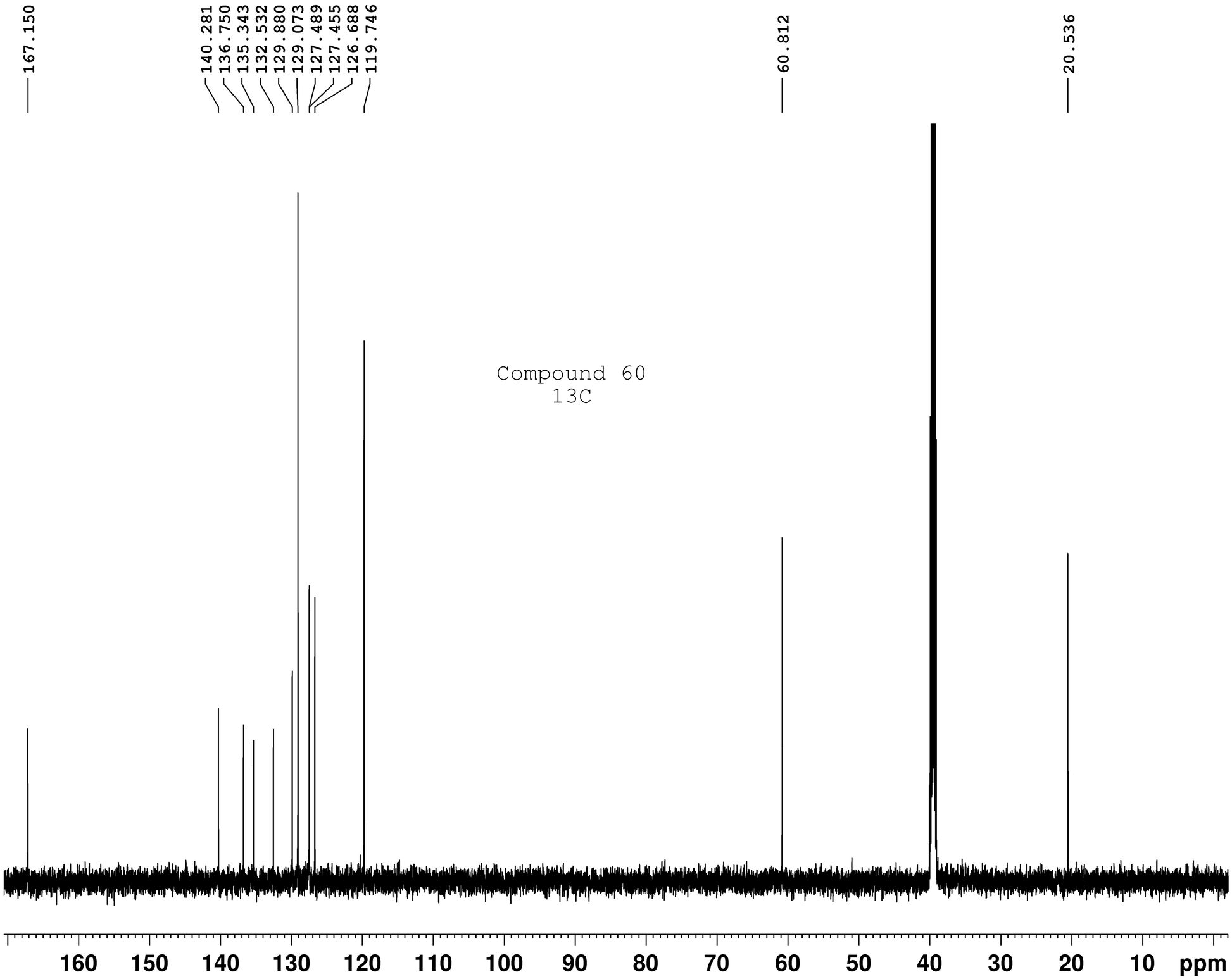
F2 - Processing parameters
SI                    65536
SF             150.8727017 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```




```
Current Data Parameters
NAME                CE-08A
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20210428
Time                  1.01 h
INSTRUM              spect
PROBHD    Z847801_0047 (
PULPROG               zg30
TD                   32768
SOLVENT               DMSO
NS                      32
DS                       0
SWH               9615.385 Hz
FIDRES            0.586877 Hz
AQ               1.7039360 sec
RG                     144
DW                  52.000 usec
DE                   14.37 usec
TE                   293.0 K
D1              1.00000000 sec
TD0                      1
SFO1           600.0145608 MHz
NUC1                    1H
P0                    3.62 usec
P1                   10.85 usec
PLW1           20.00000000 W

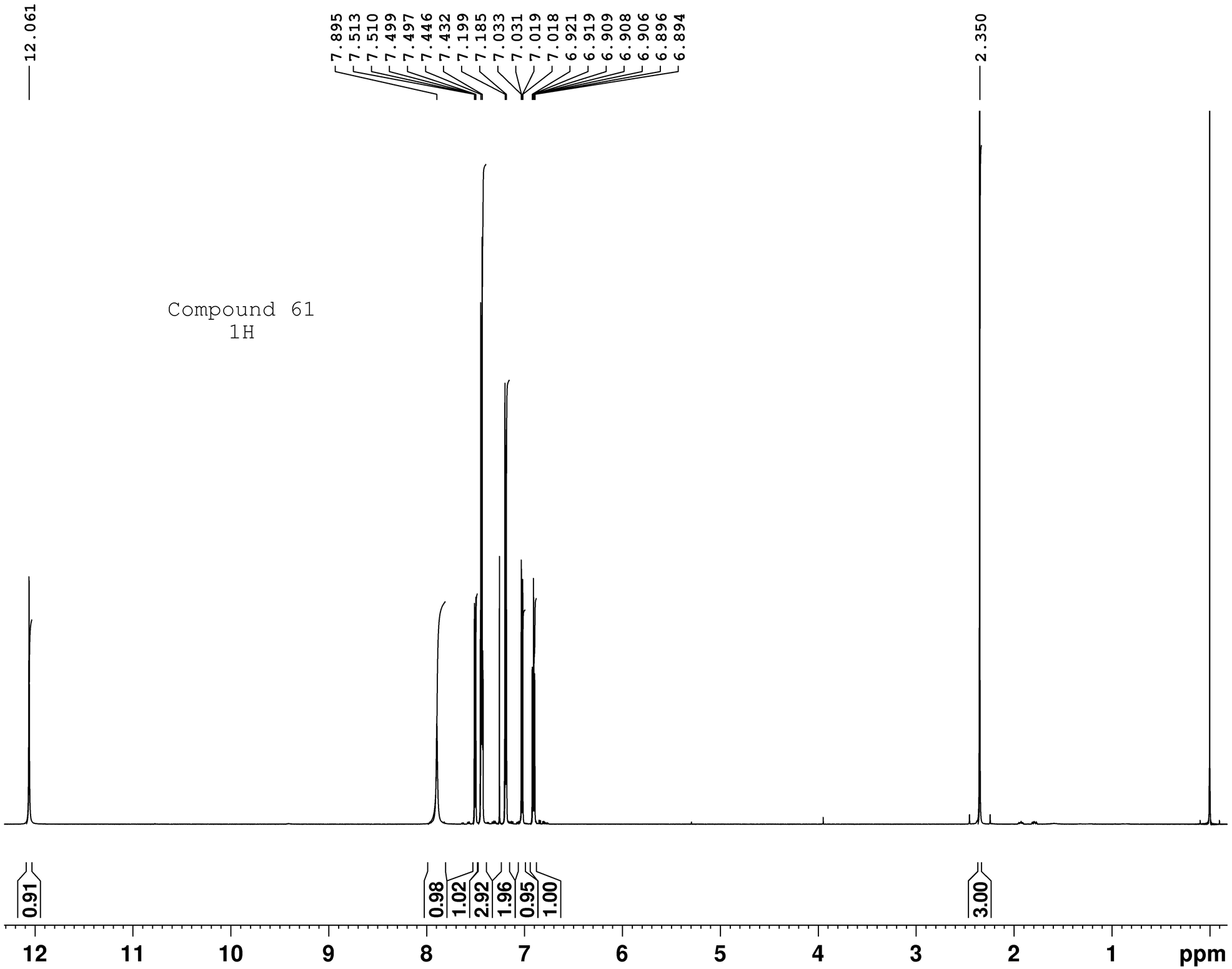
F2 - Processing parameters
SI                   65536
SF             600.0100048 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```




```
Current Data Parameters
NAME              CE-08A
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_            20210428
Time                1.06 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT             DMSO
NS                    128
DS                      0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                   2050
DW                 13.867 usec
DE                  6.50 usec
TE                 293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         150.8892338 MHz
NUC1                  13C
P0                   3.27 usec
P1                   9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2               90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

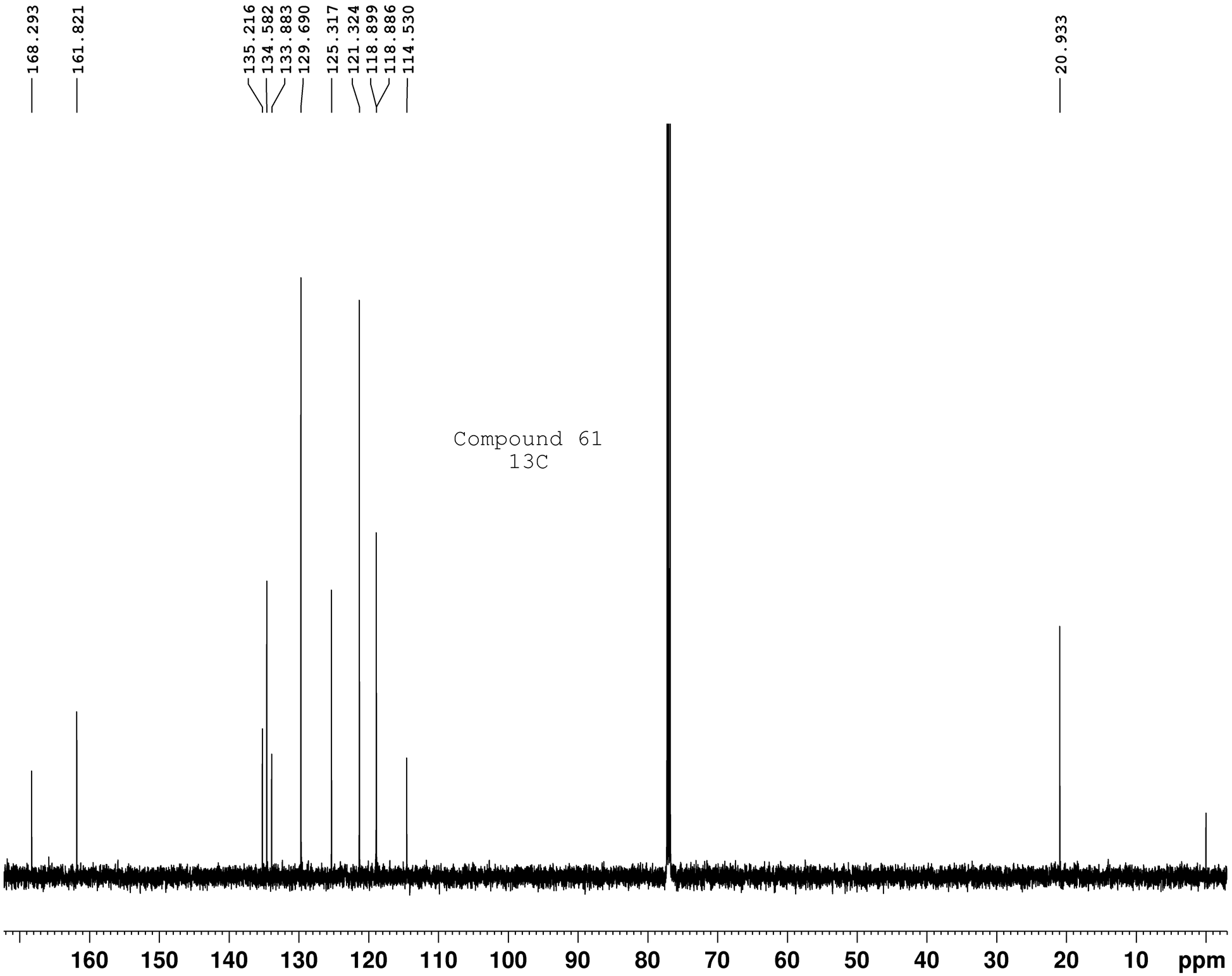
F2 - Processing parameters
SI                  65536
SF           150.8727011 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
Current Data Parameters
NAME          61-CD-203A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220118
Time              18.02 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ           1.7039360 sec
RG                   203
DW               52.000 usec
DE                14.38 usec
TE                293.0 K
D1           1.00000000 sec
TD0                    1
SFO1        599.9845606 MHz
NUC1                  1H
P0                 3.60 usec
P1                10.80 usec
PLW1        20.00000000 W

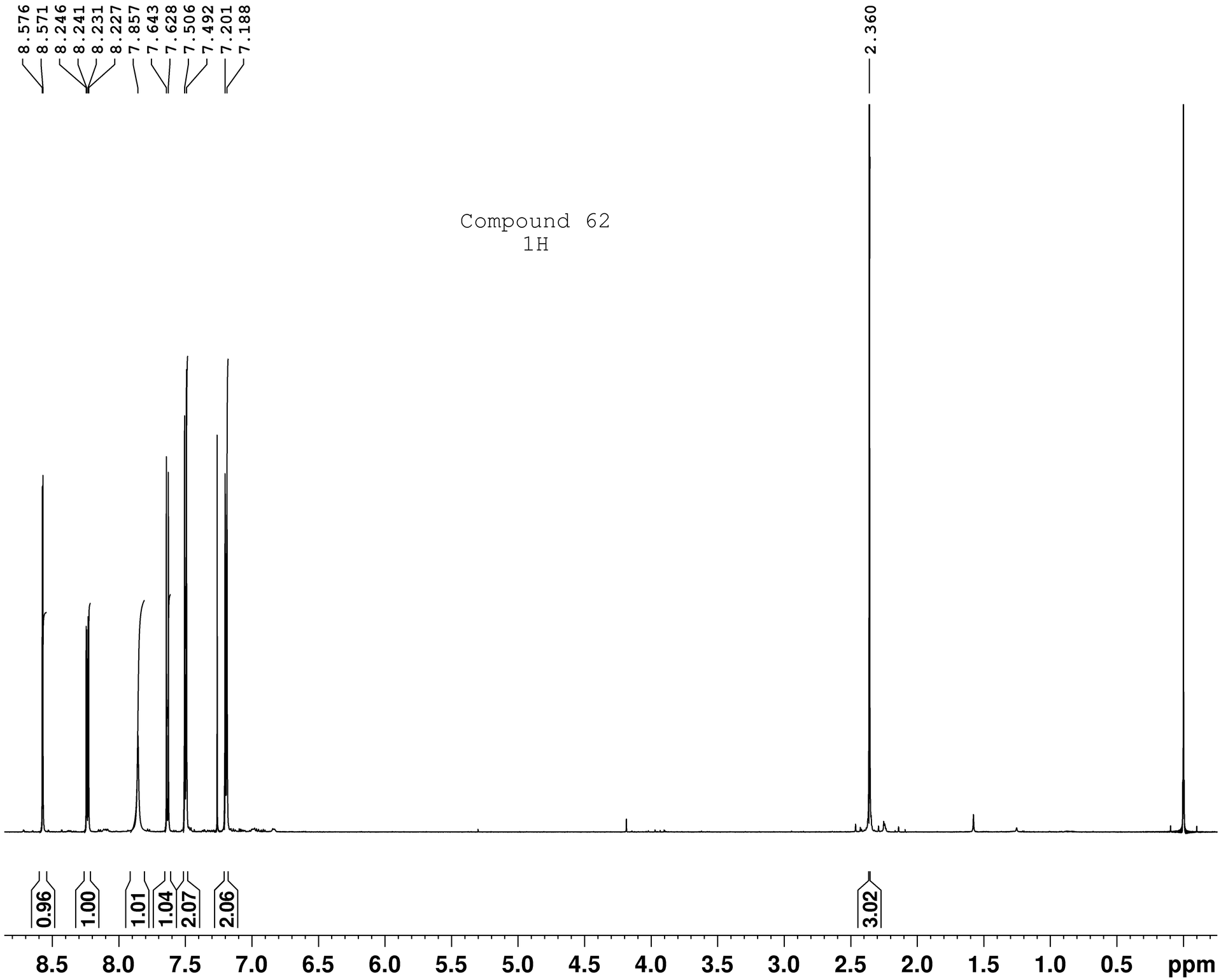
F2 - Processing parameters
SI                65536
SF          599.9800167 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME              CD-203A
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220118
Time               18.07 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                  6.50 usec
TE                 293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

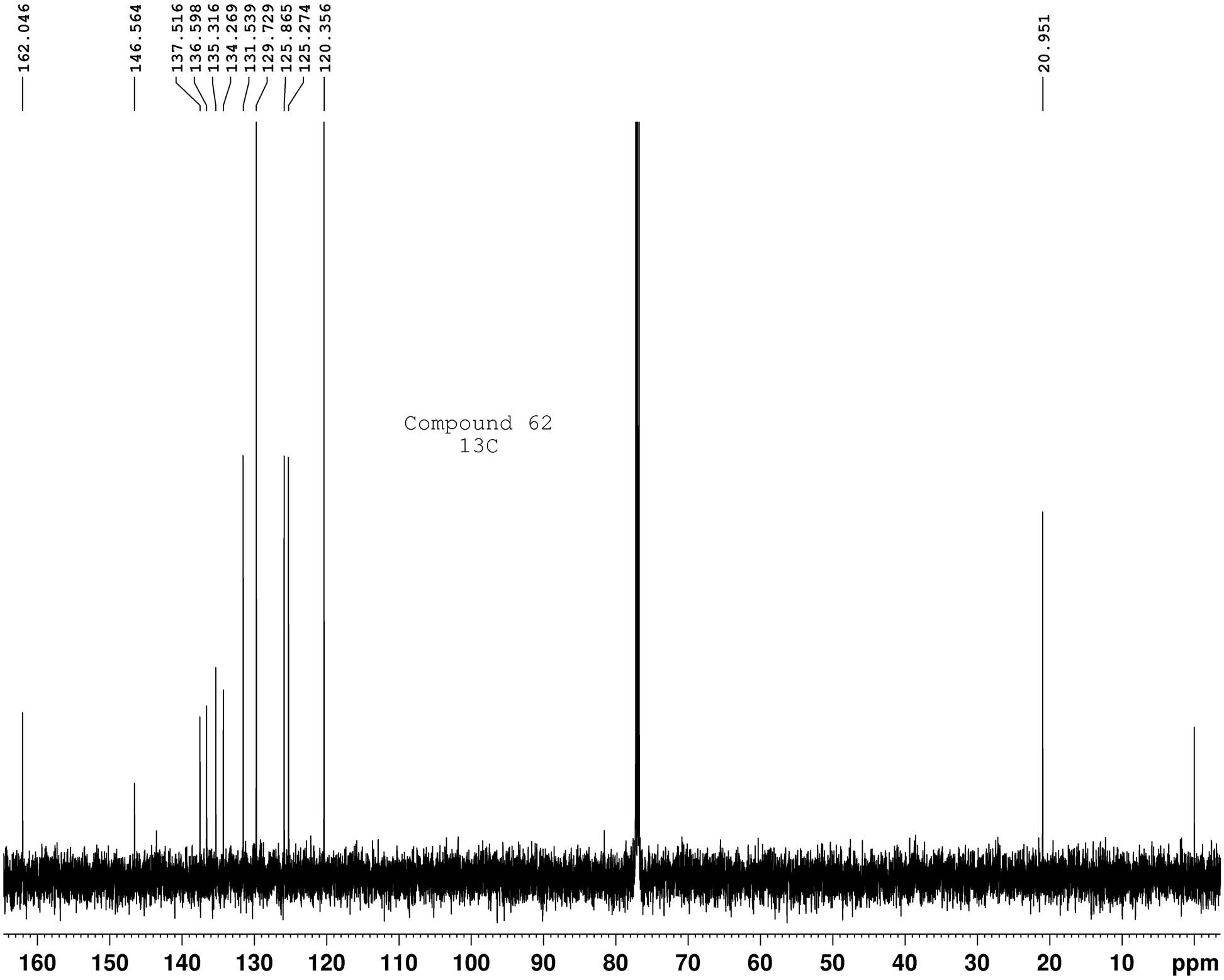
F2 - Processing parameters
SI                 65536
SF           150.8650988 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          62-CD-198A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220118
Time               17.45 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   287
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

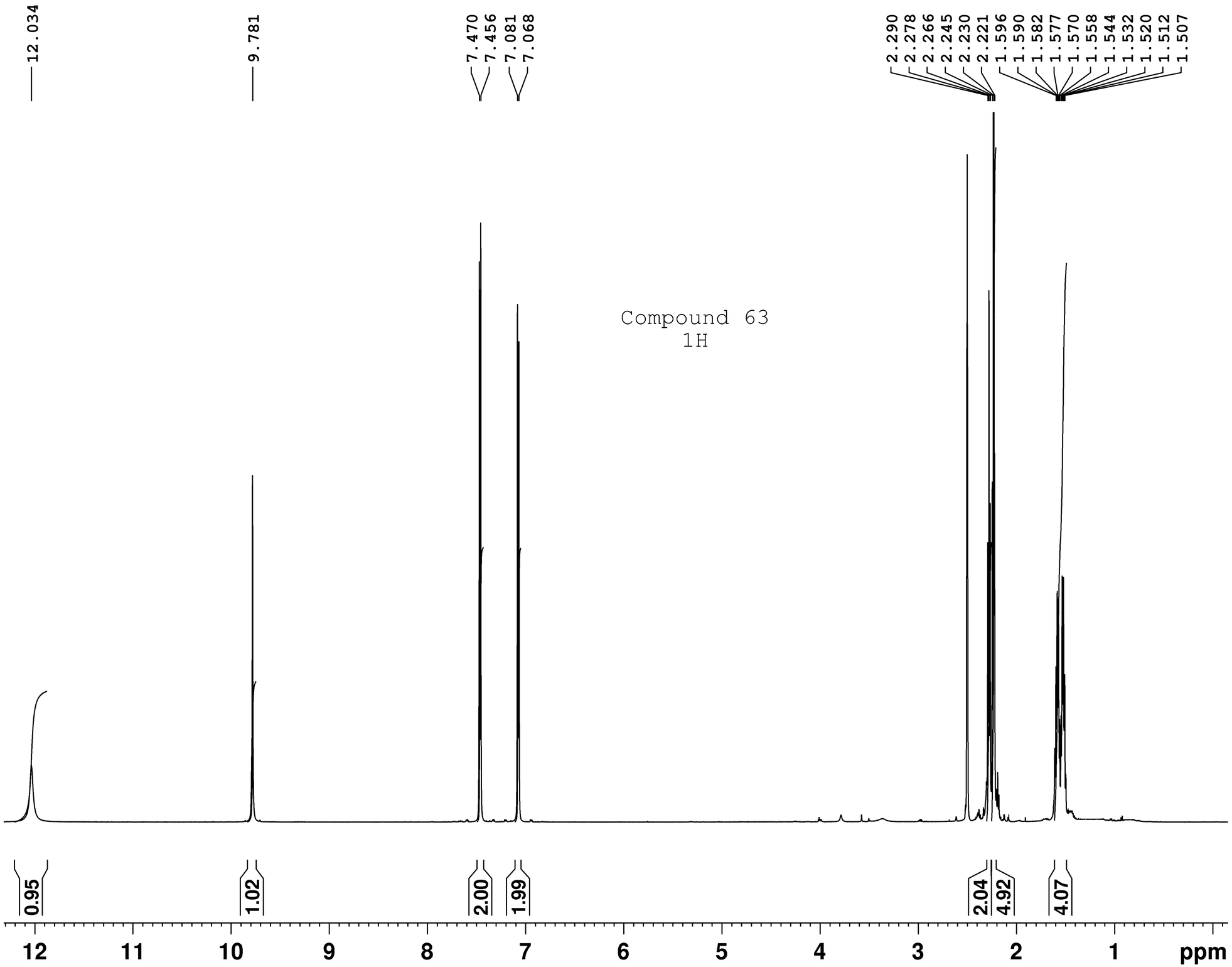
F2 - Processing parameters
SI                 65536
SF           599.9800131 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-198A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220118
Time              17.50 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE                293.1 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

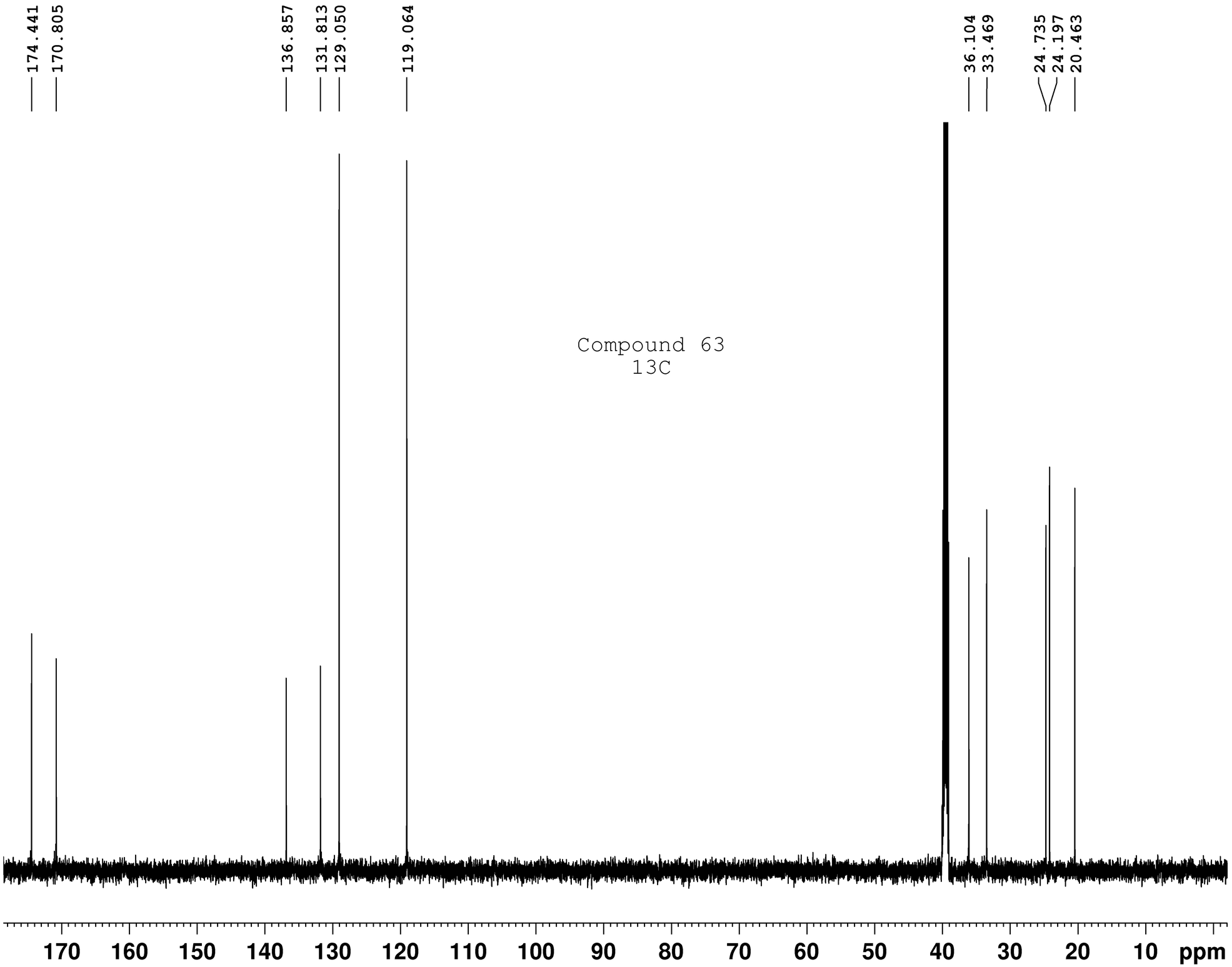
F2 - Processing parameters
SI                65536
SF          150.8650977 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME          63. CD-199A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210219
Time                18.02 h
INSTRUM             spect
PROBHD    Z847801_0047 (
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                     32
DS                      0
SWH              9615.385 Hz
FIDRES           0.586877 Hz
AQ             1.7039360 sec
RG                     57
DW                52.000 usec
DE                 14.37 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                     1
SFO1         600.0145608 MHz
NUC1                   1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

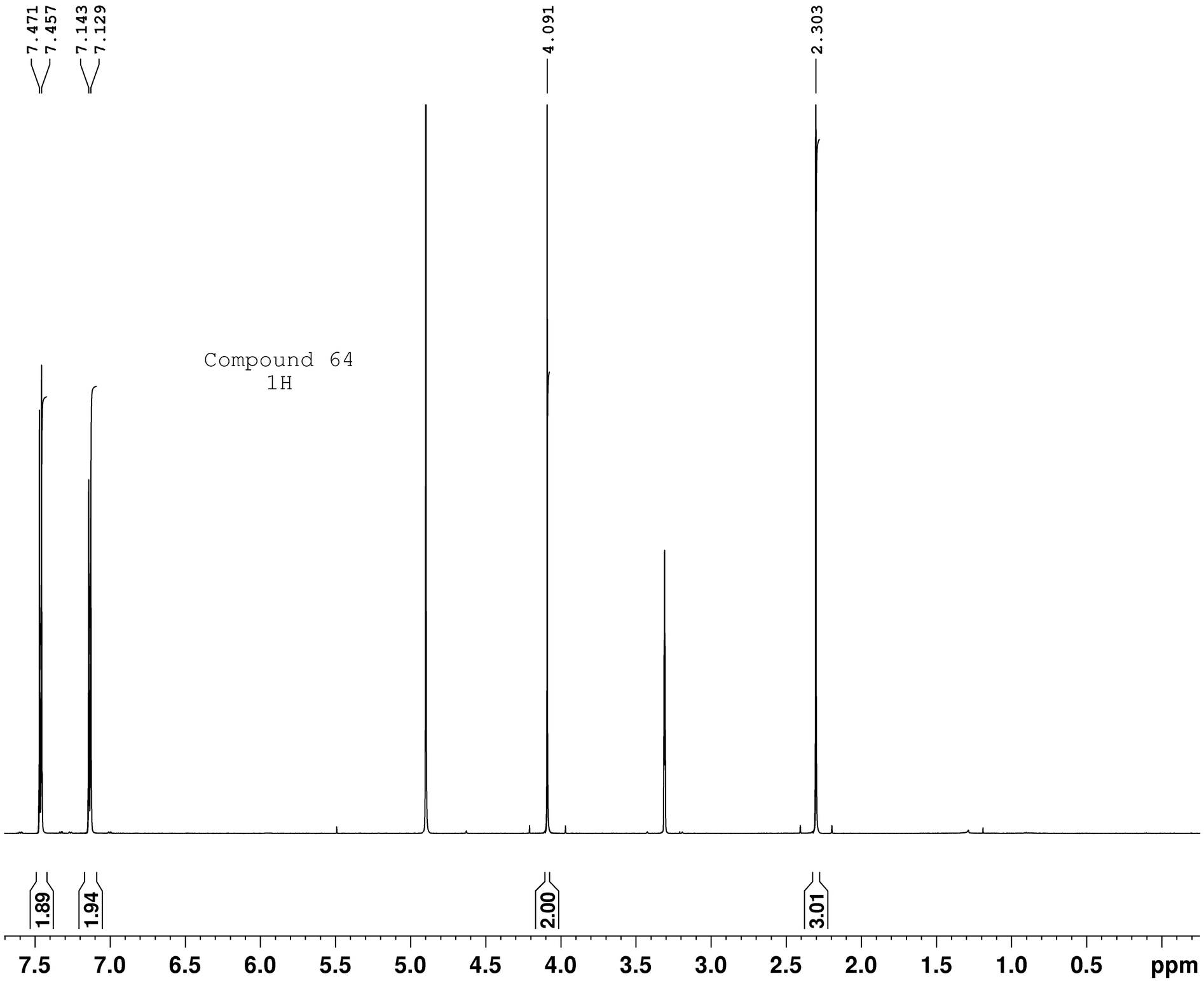
F2 - Processing parameters
SI                  65536
SF           600.0100049 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CD-199A
EXPNO                16
PROCNO                1

F2 - Acquisition Parameters
Date_           20210219
Time              18.36 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8892338 MHz
NUC1                13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         600.0124004 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         20.00000000 W
PLW12         0.33800000 W

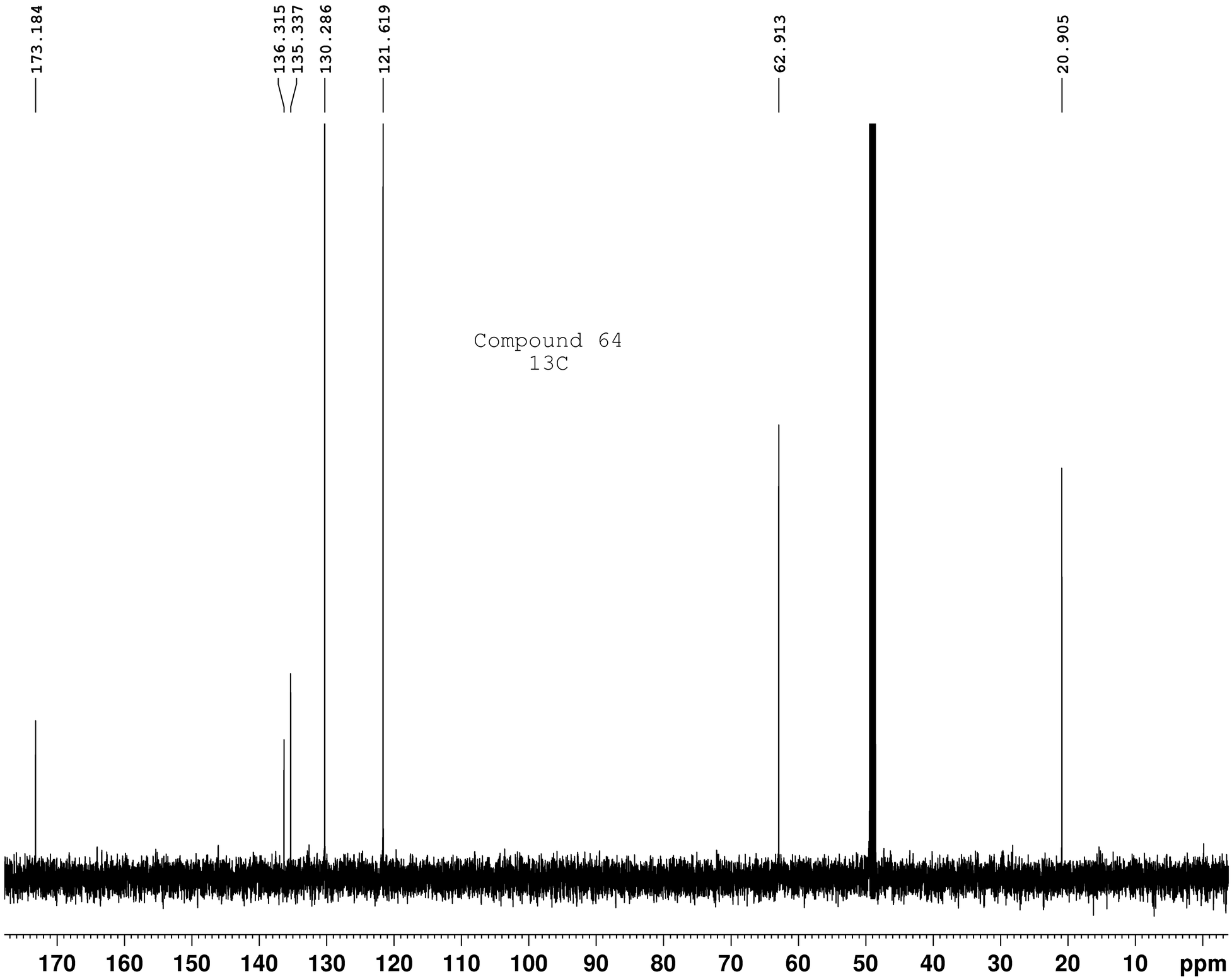
F2 - Processing parameters
SI                  65536
SF           150.8726989 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CD-200A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220224
Time               19.39 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             MeOD
NS                     16
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    256
DW                 52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                     1
SFO1         599.9845606 MHz
NUC1                   1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

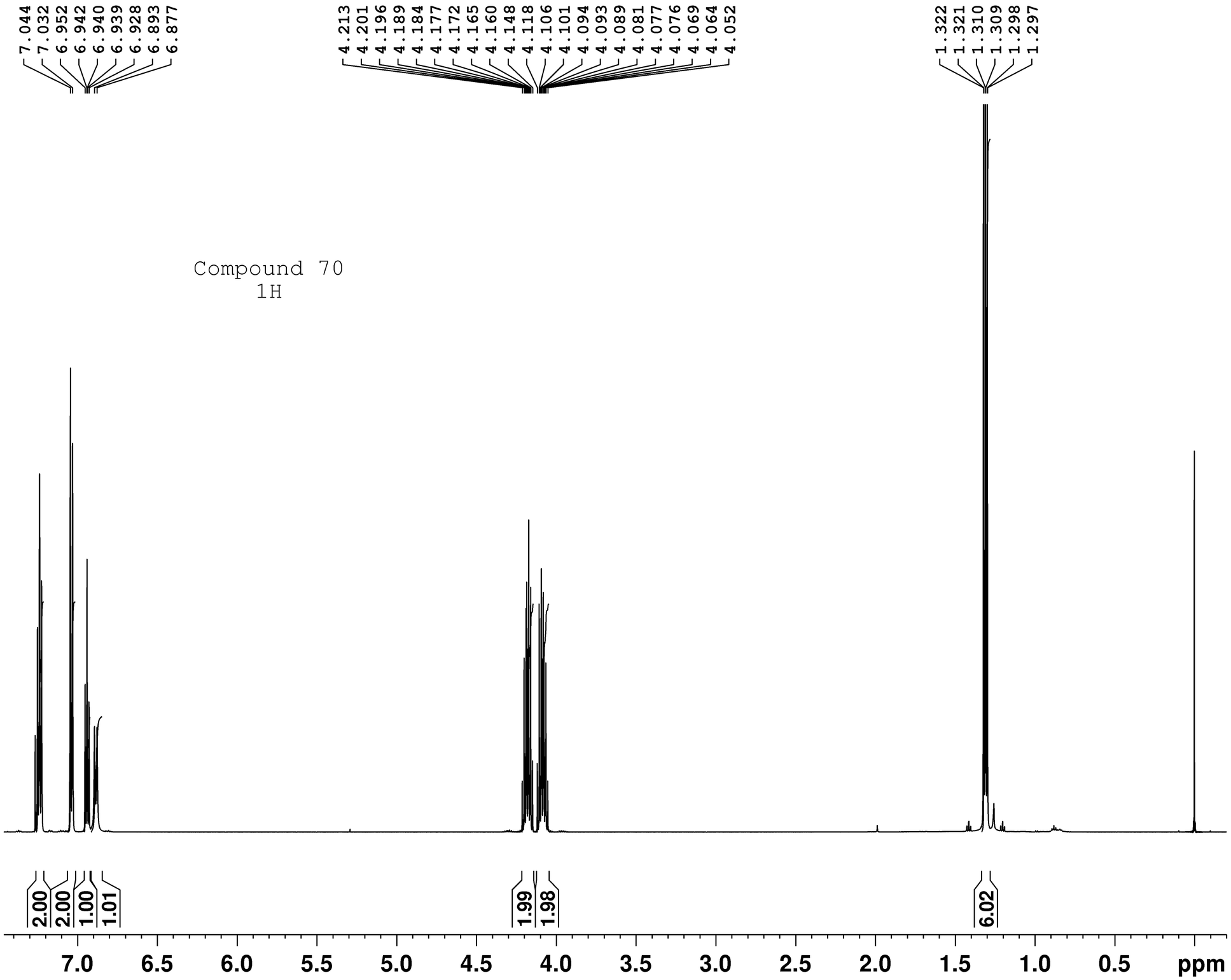
F2 - Processing parameters
SI                  65536
SF           599.9800114 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME              CD-200A
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220224
Time               19.44 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                 32768
SOLVENT             MeOD
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

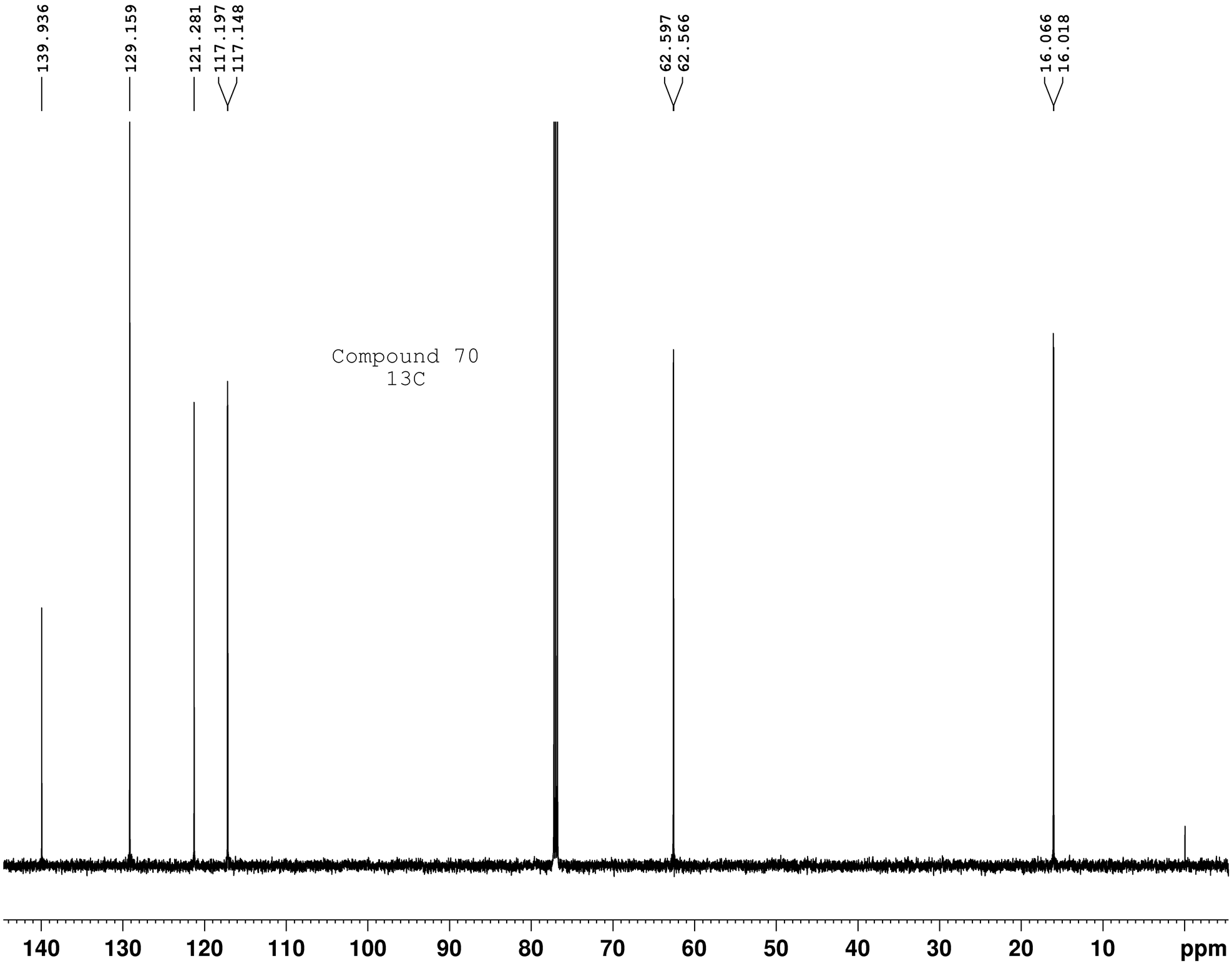
F2 - Processing parameters
SI                 65536
SF           150.8648802 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          70-CE-110A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220118
Time               18.36 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  80.6
DW                52.000 usec
DE                14.38 usec
TE                293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

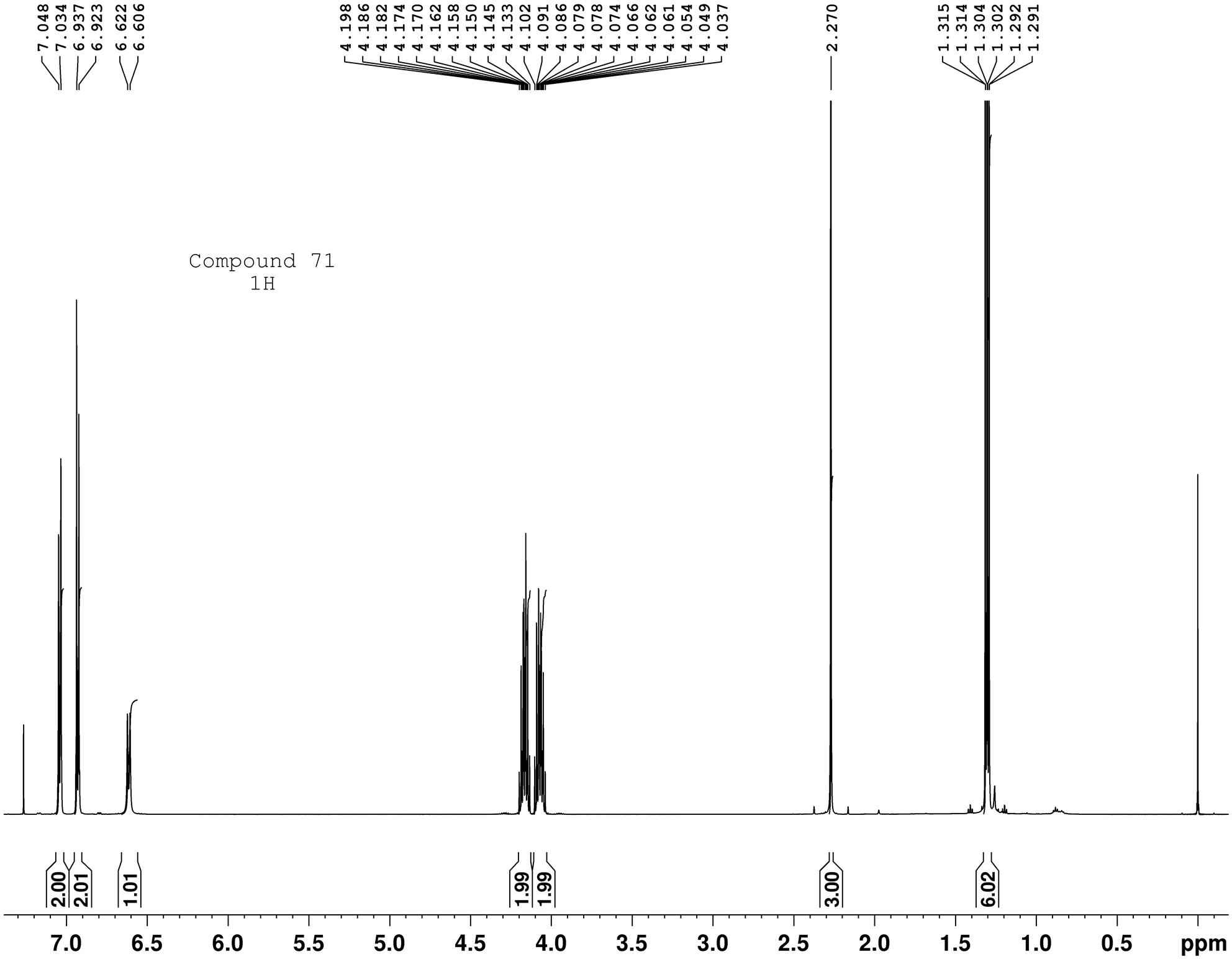
F2 - Processing parameters
SI                 65536
SF           599.9800107 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CE-110A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220118
Time              18.41 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.1 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

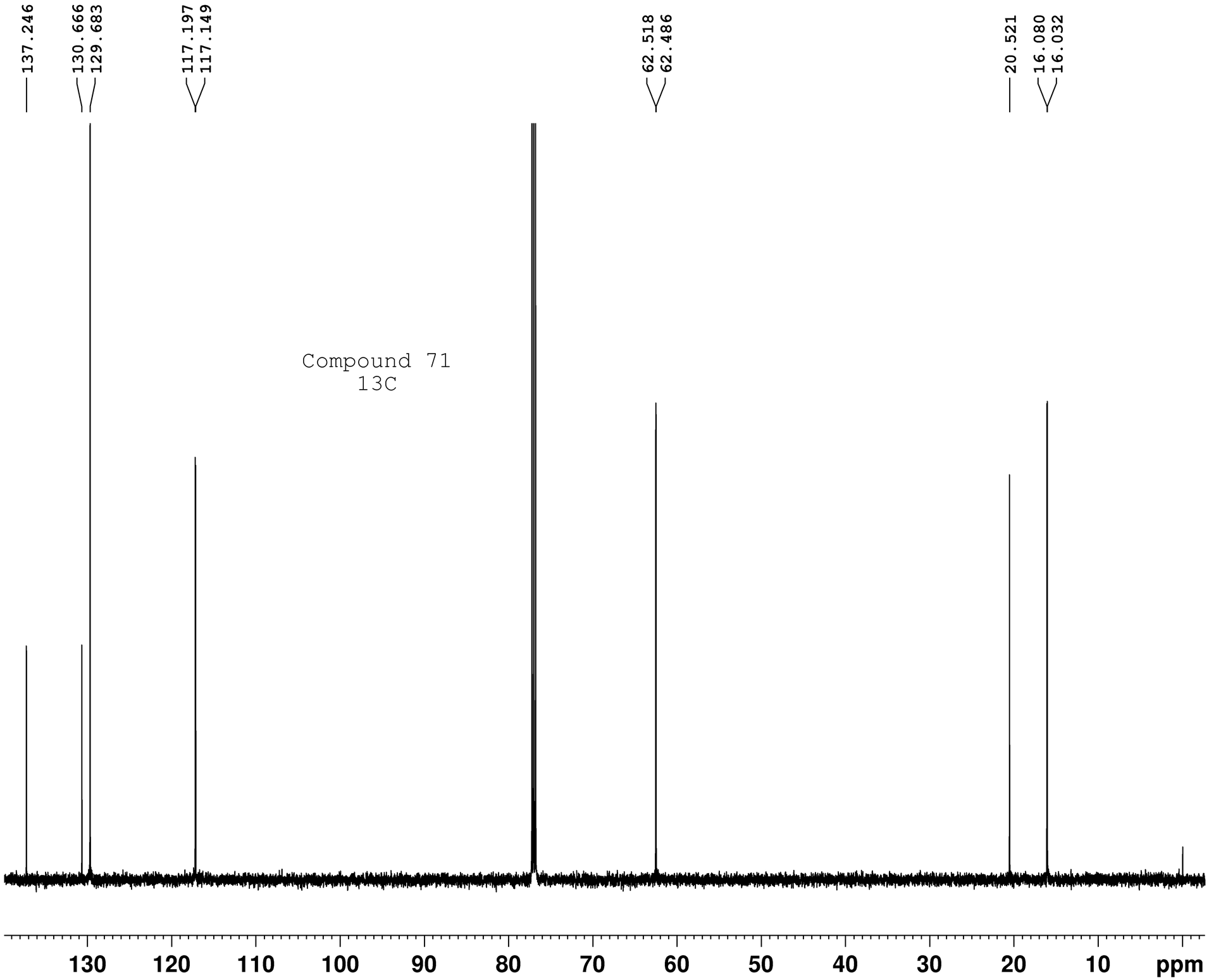
F2 - Processing parameters
SI                65536
SF          150.8651021 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME          71-CE-66A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20220118
Time              18.19 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ            1.7039360 sec
RG                 80.6
DW               52.000 usec
DE                14.38 usec
TE                293.0 K
D1           1.00000000 sec
TD0                    1
SFO1        599.9845606 MHz
NUC1                  1H
P0                 3.60 usec
P1                10.80 usec
PLW1        20.00000000 W

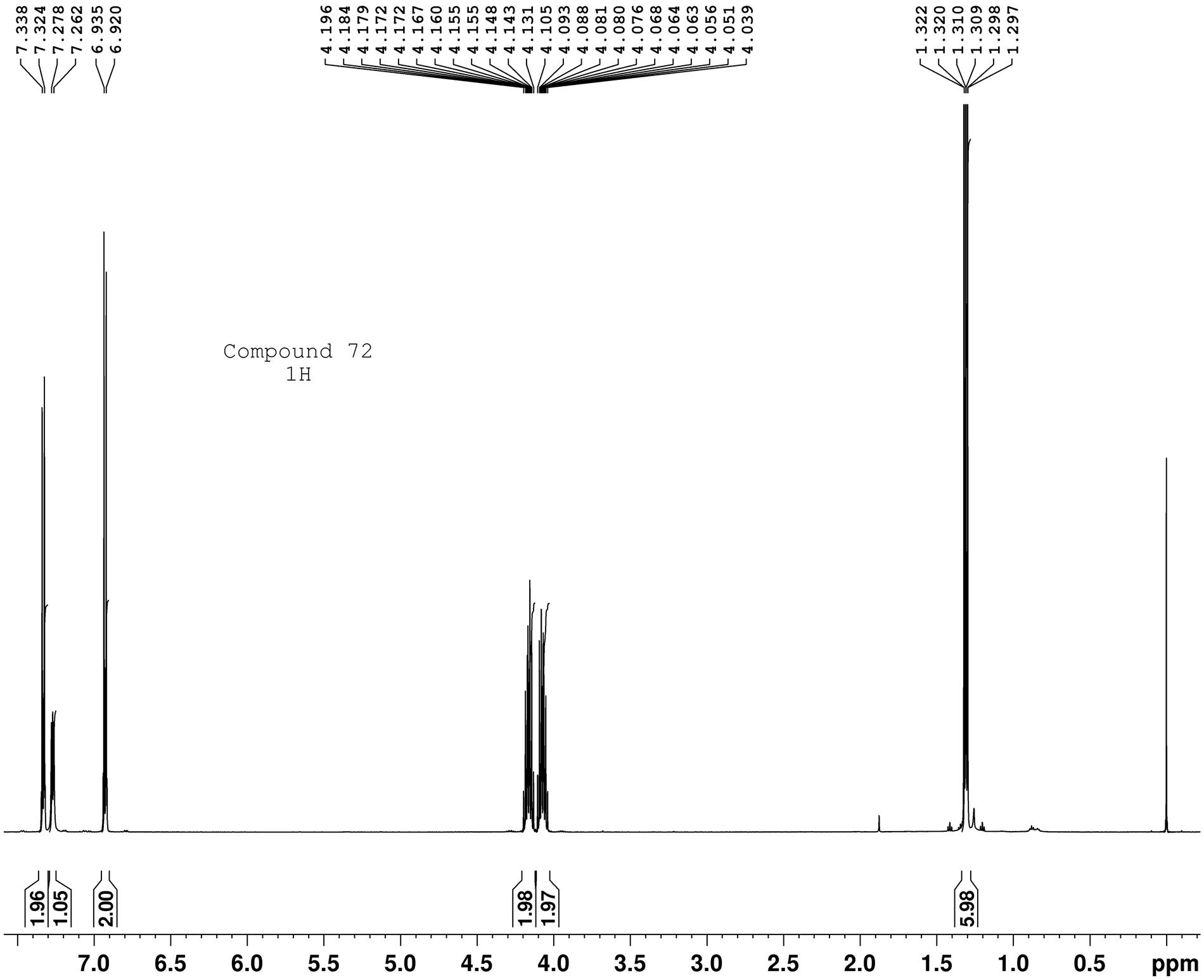
F2 - Processing parameters
SI                65536
SF          599.9800111 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME              CE-66A
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_            20220118
Time               18.25 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                 2050
DW                13.867 usec
DE                 6.50 usec
TE                293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

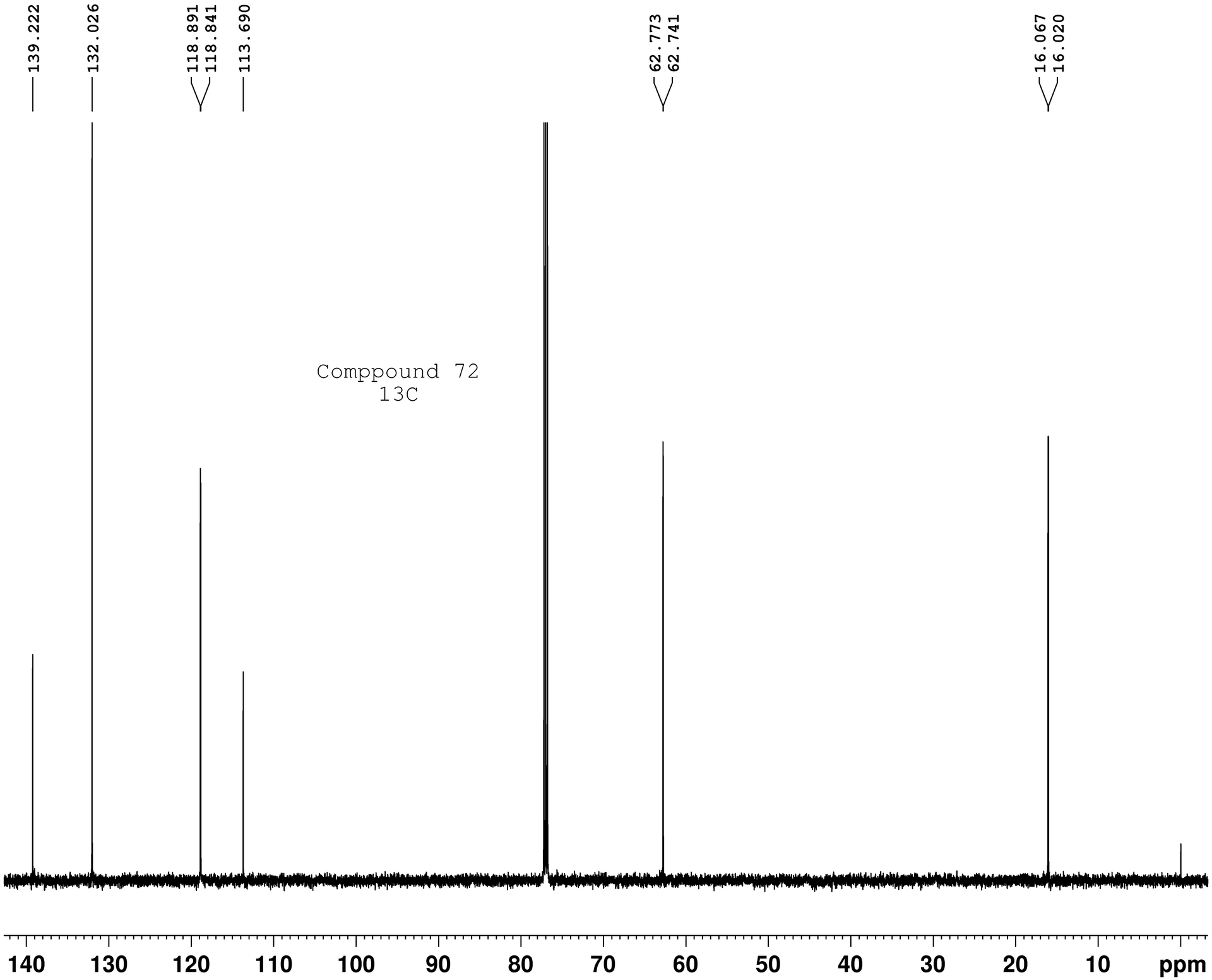
F2 - Processing parameters
SI                 65536
SF          150.8651015 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-108A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220221
Time                17.52 h
INSTRUM             spect
PROBHD   Z847801_0047 (
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    101
DW                 52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1             1.00000000 sec
TD0                     1
SFO1         599.9845606 MHz
NUC1                   1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

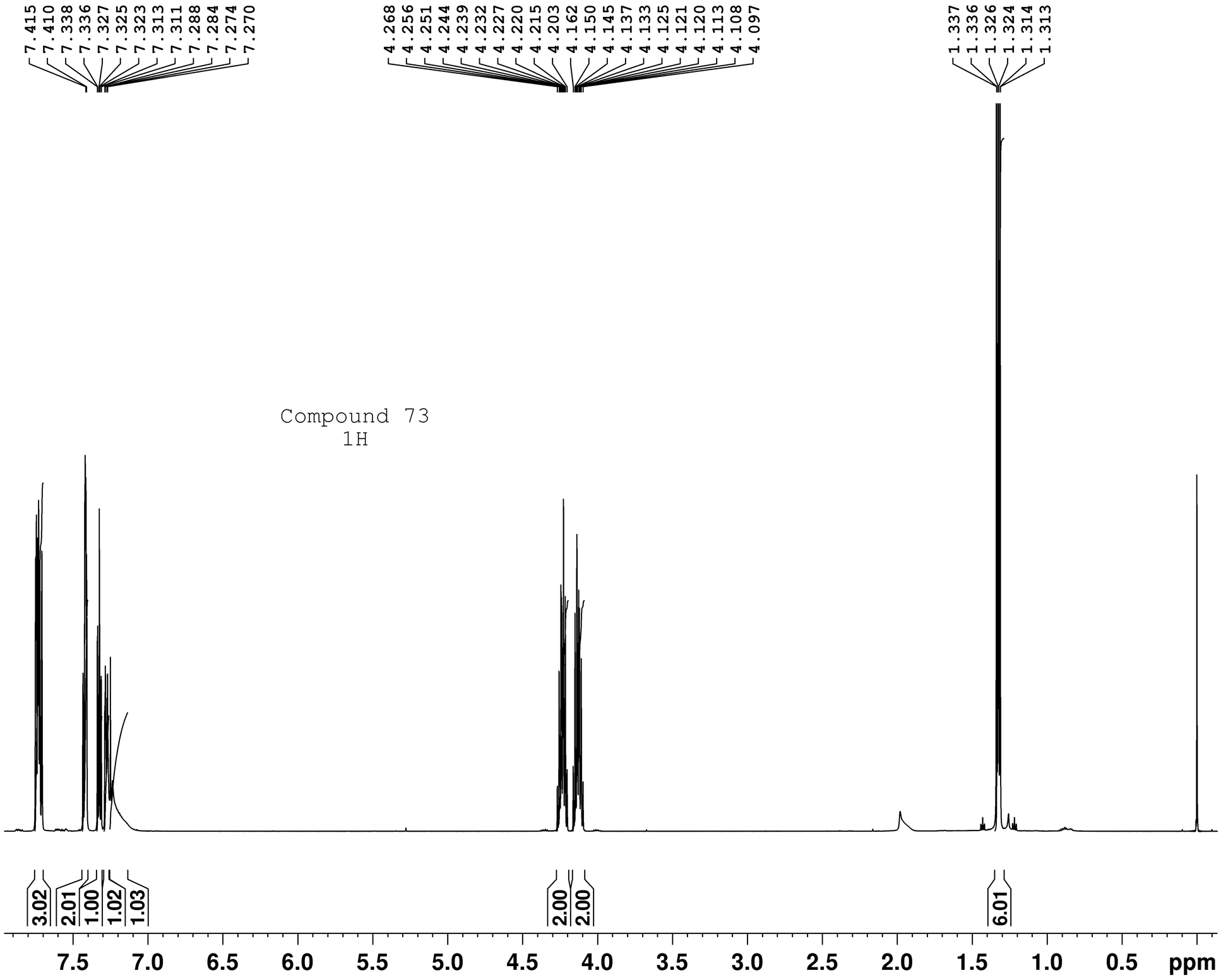
F2 - Processing parameters
SI                  65536
SF           599.9800078 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CE-108A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220221
Time              17.57 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE                293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

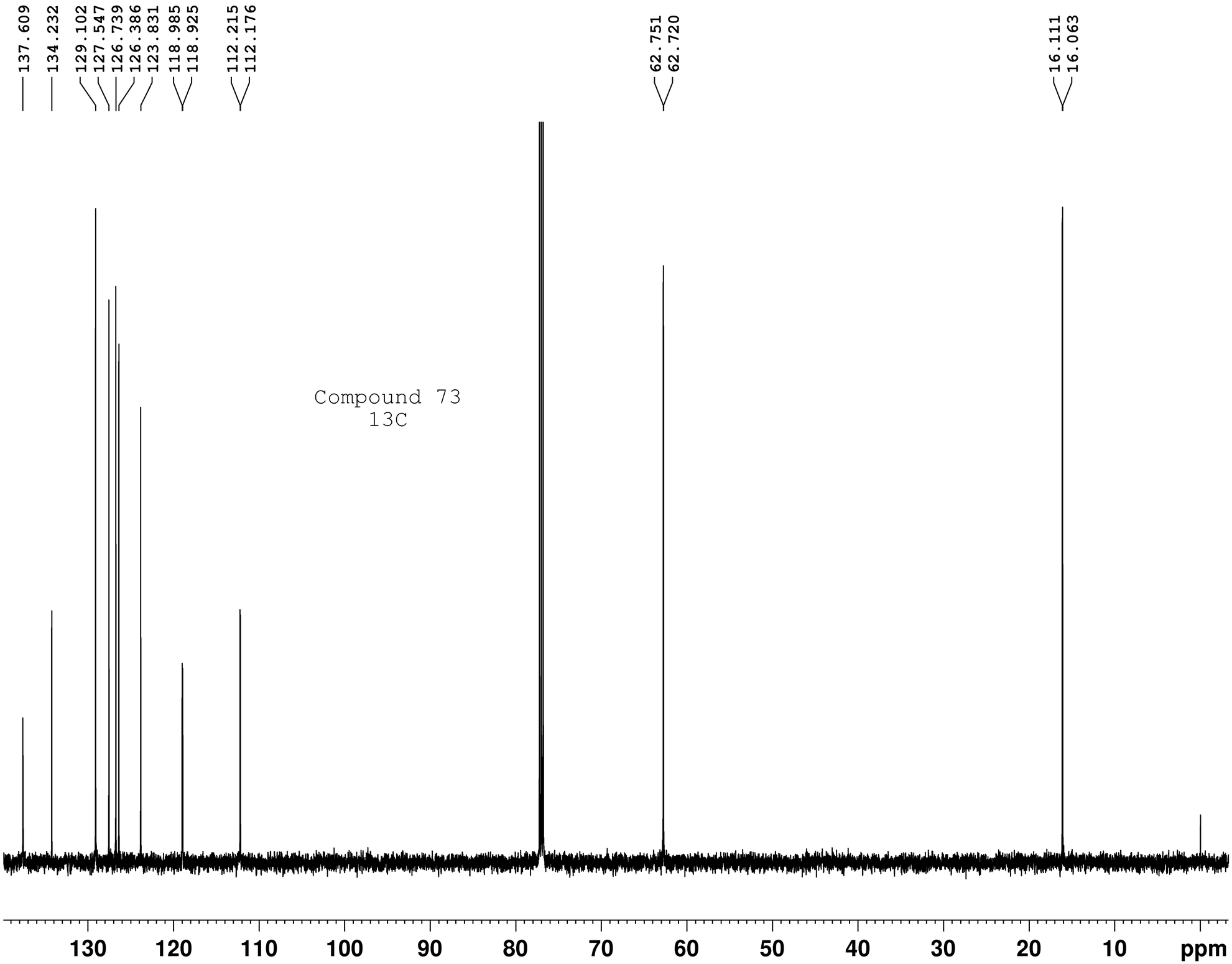
F2 - Processing parameters
SI                 65536
SF          150.8651001 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-107A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220221
Time               17.36 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                  90.5
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

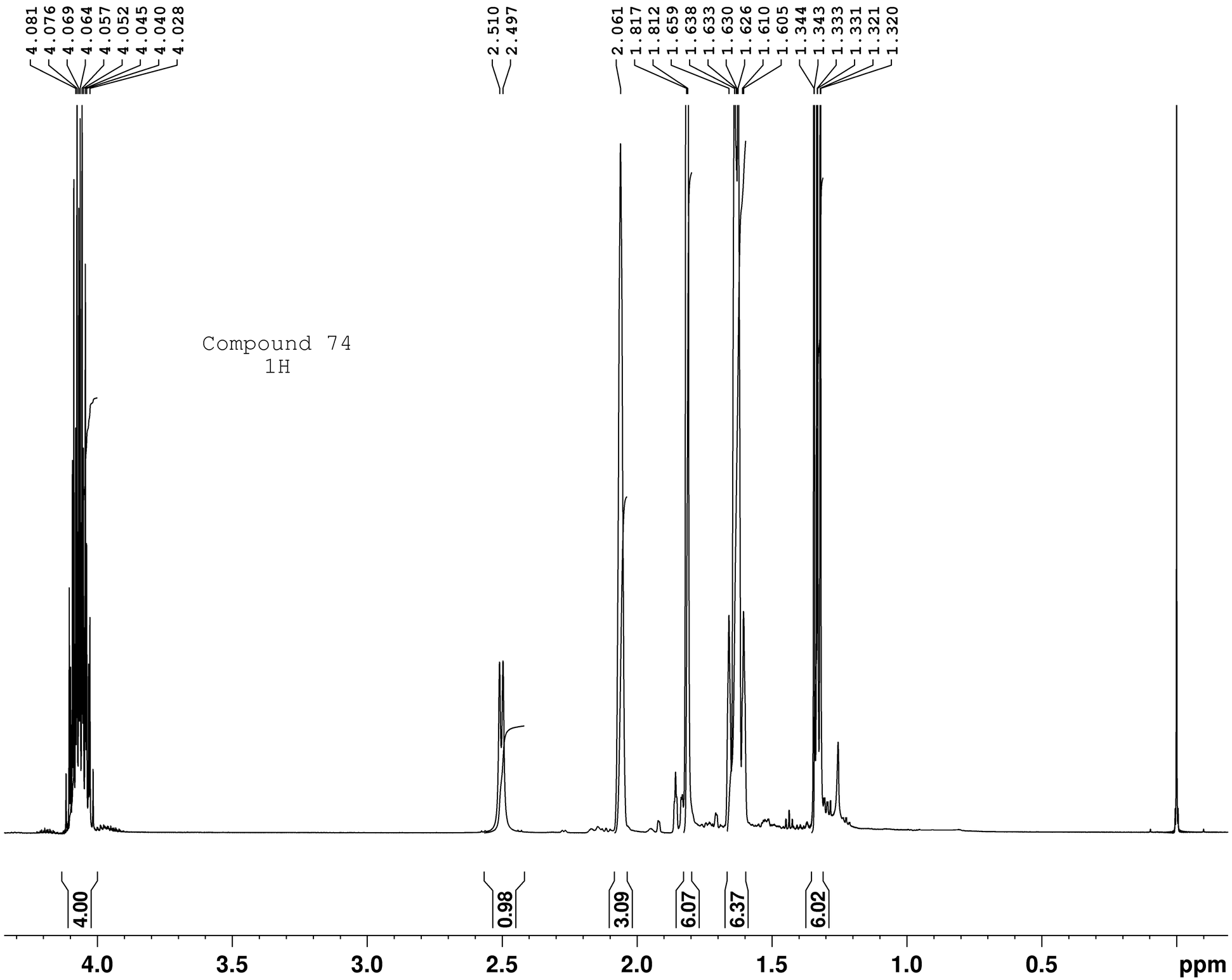
F2 - Processing parameters
SI                 65536
SF           599.9800195 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CE-107A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20220221
Time             17.42 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE                293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                 13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

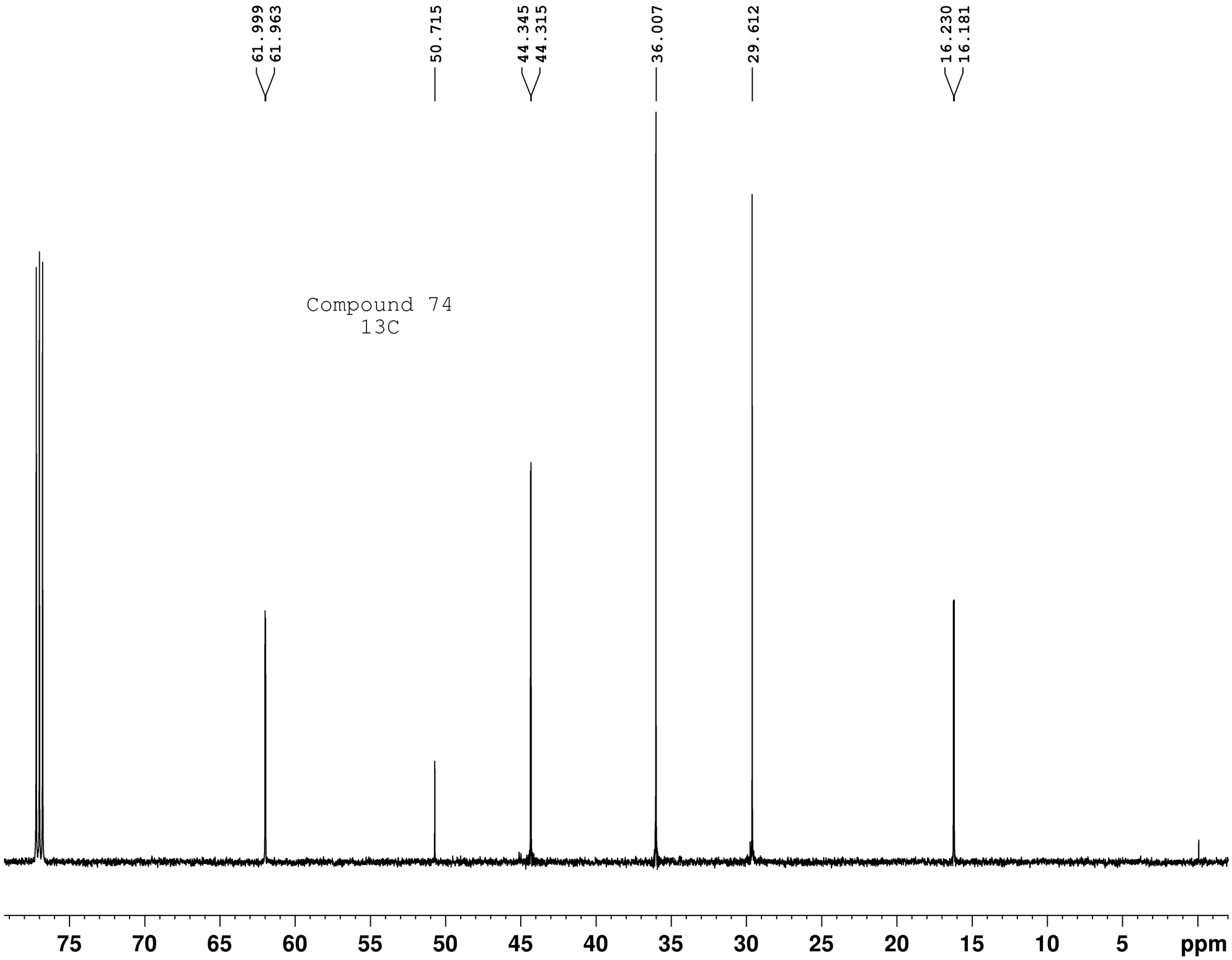
F2 - Processing parameters
SI                65536
SF          150.8651040 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME            CE-115A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20220221
Time              18.27 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH            9615.385 Hz
FIDRES         0.586877 Hz
AQ           1.7039360 sec
RG                   64
DW               52.000 usec
DE               14.38 usec
TE               293.0 K
D1          1.00000000 sec
TD0                   1
SFO1        599.9845606 MHz
NUC1                 1H
P0                3.60 usec
P1               10.80 usec
PLW1        20.00000000 W

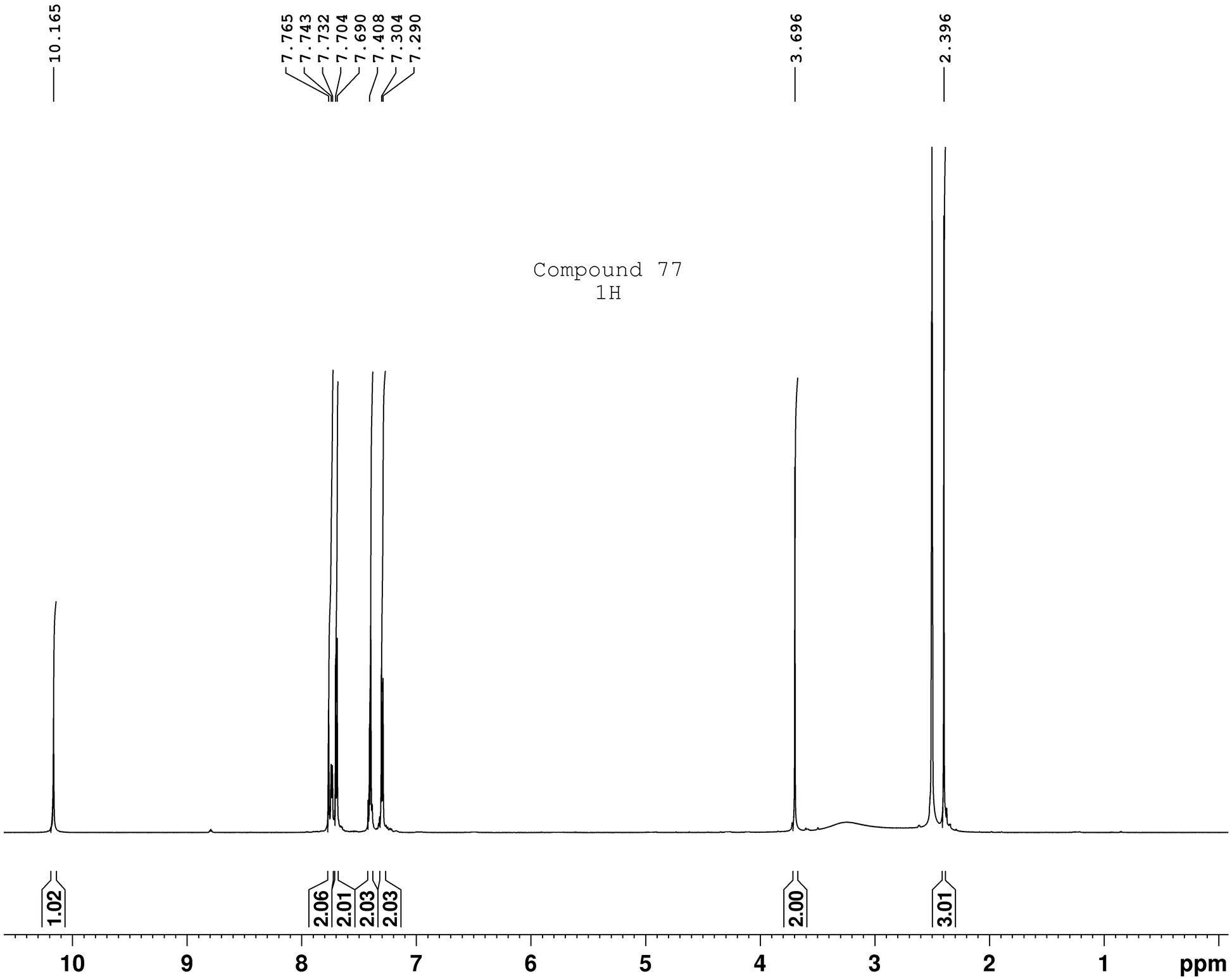
F2 - Processing parameters
SI                65536
SF          599.9799954 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME            CE-115A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220221
Time               18.32 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW                13.867 usec
DE                 6.50 usec
TE                293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

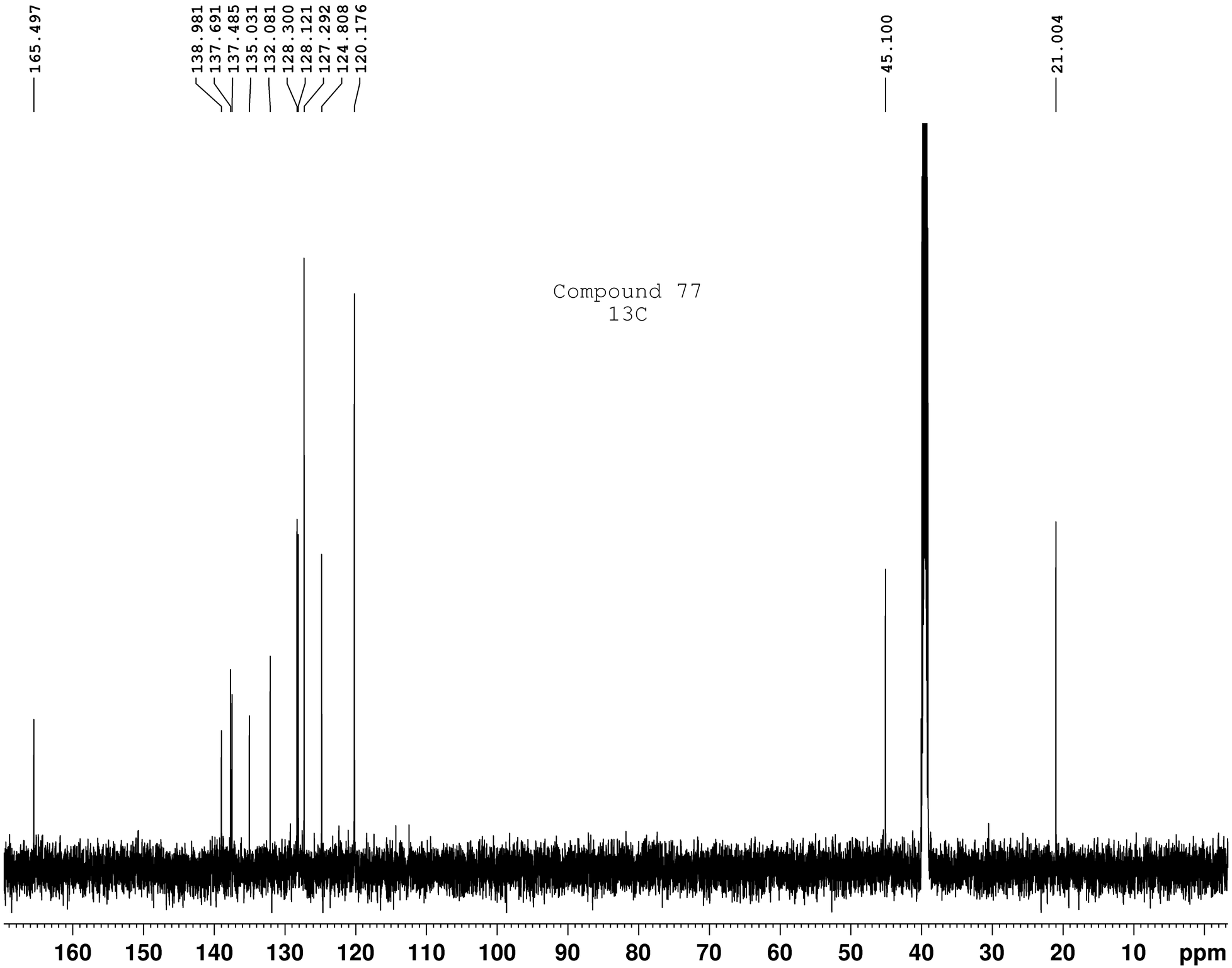
F2 - Processing parameters
SI                65536
SF          150.8651013 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME            CD-195A
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20200723
Time               19.17 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                     32
DS                      0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                    181
DW                52.000 usec
DE                14.37 usec
TE                293.0 K
D1            1.00000000 sec
TD0                     1
SFO1         600.0145608 MHz
NUC1                   1H
P0                  3.62 usec
P1                 10.85 usec
PLW1         20.00000000 W

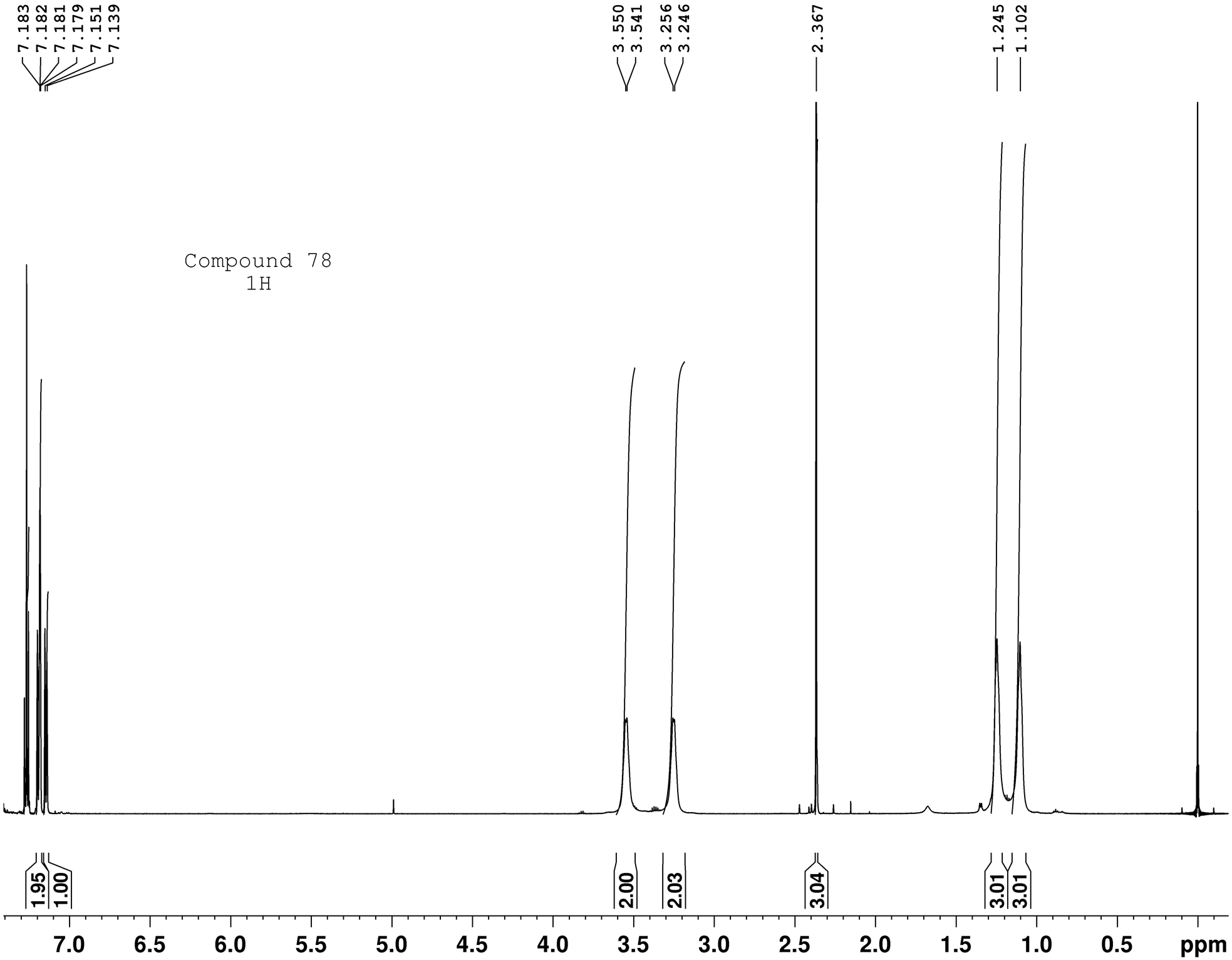
F2 - Processing parameters
SI                  65536
SF           600.0100048 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME            CD-195A
EXPNO                16
PROCNO                1

F2 - Acquisition Parameters
Date_           20200723
Time               20.38 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                  6.50 usec
TE                 293.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1        150.8892338 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1        40.00000000 W
SFO2        600.0124004 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        20.00000000 W
PLW12        0.33800000 W

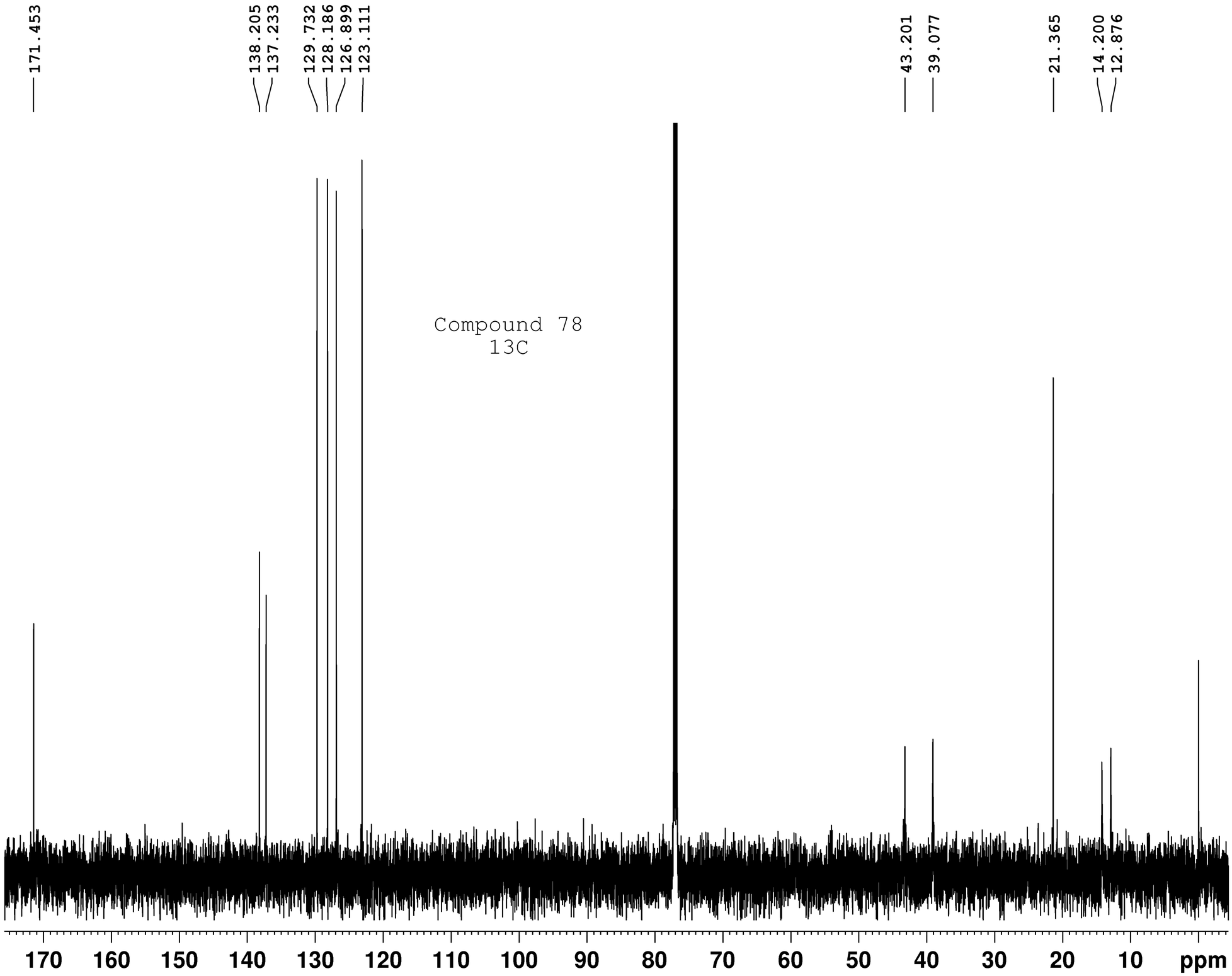
F2 - Processing parameters
SI                 65536
SF          150.8727013 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          80-CD-202A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220112
Time               17.40 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   203
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1           1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1        20.00000000 W

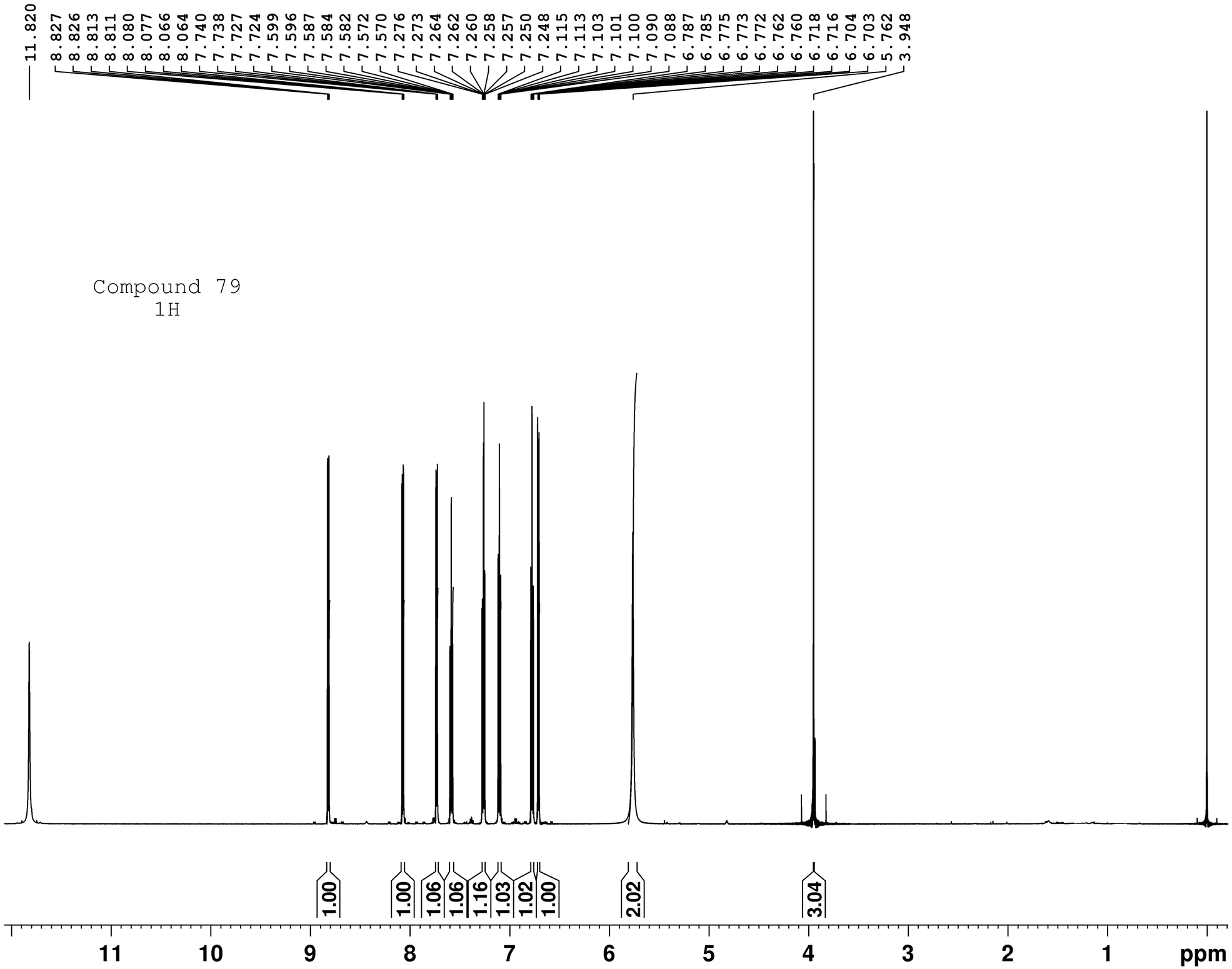
F2 - Processing parameters
SI                 65536
SF          599.9800111 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-202A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20220112
Time              17.45 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.1 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                 13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

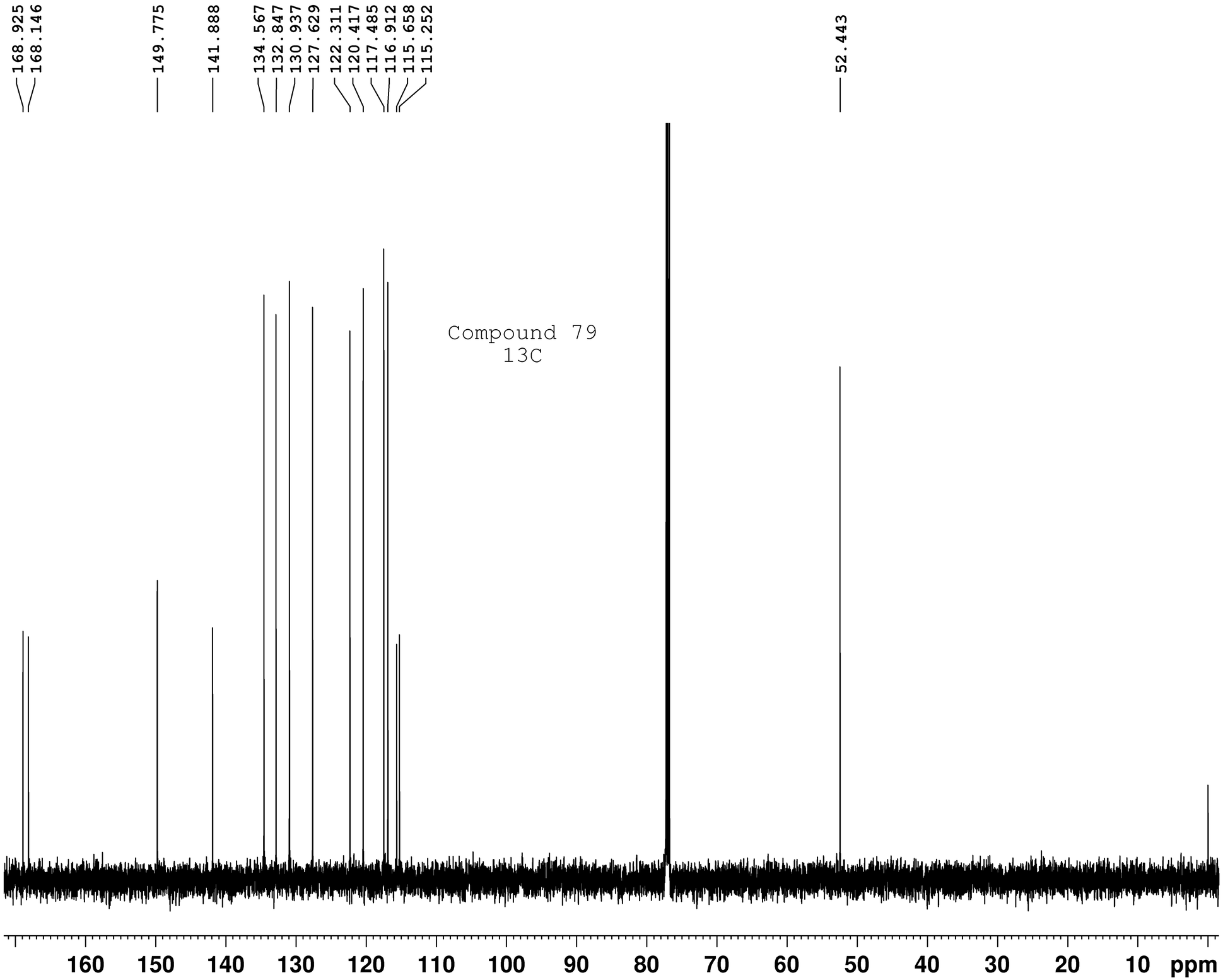
F2 - Processing parameters
SI                 65536
SF          150.8650977 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME          81-CD-152A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220118
Time               17.28 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   161
DW                52.000 usec
DE                14.38 usec
TE                293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

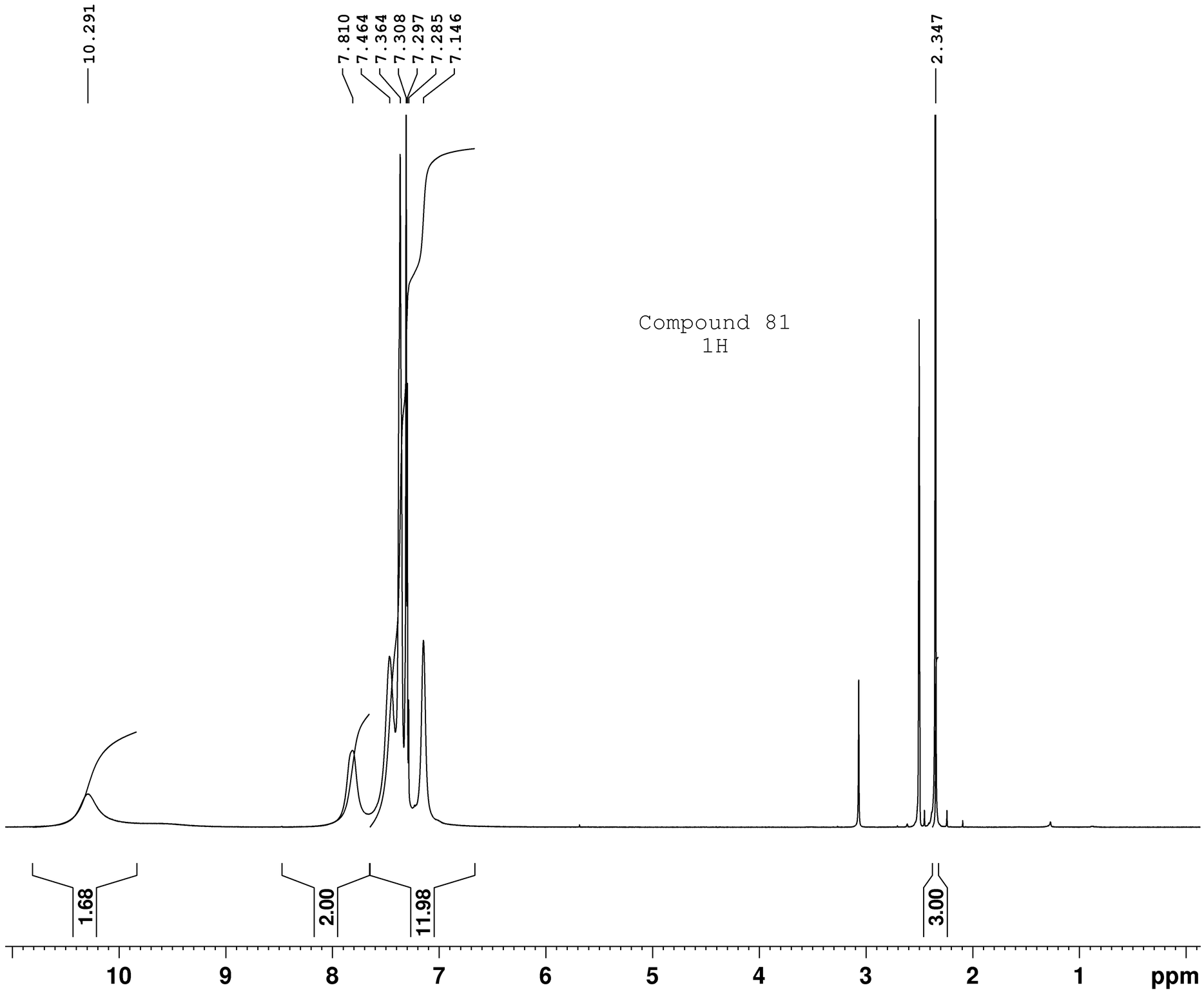
F2 - Processing parameters
SI                 65536
SF           599.9800158 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME            CD-152A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20220118
Time              17.33 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                 2050
DW               13.867 usec
DE                6.50 usec
TE               293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        150.8816889 MHz
NUC1                 13C
P0                 3.27 usec
P1                 9.80 usec
PLW1         40.00000000 W
SFO2        599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

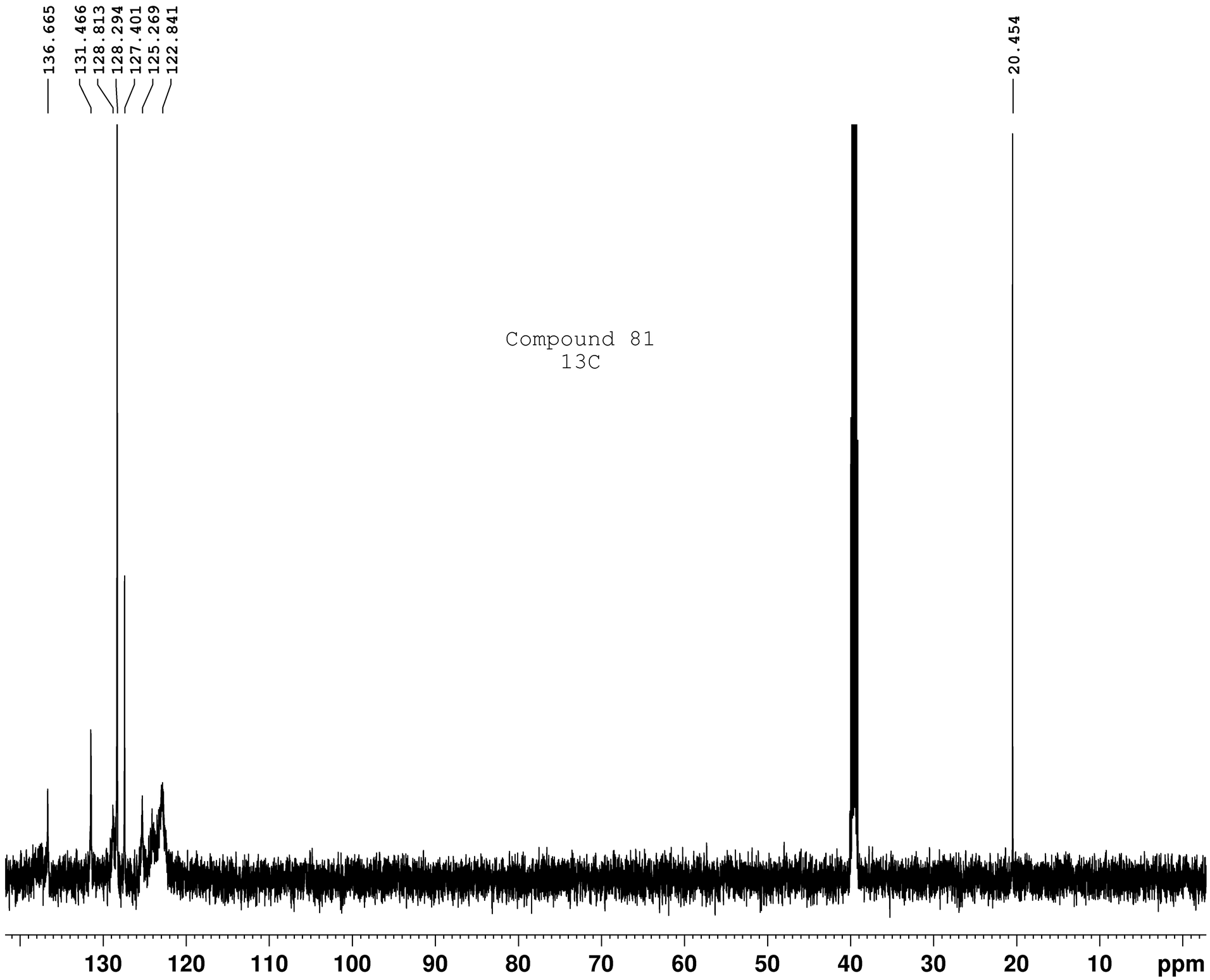
F2 - Processing parameters
SI                  65536
SF          150.8650994 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME                CD-68A
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220225
Time                 20.12 h
INSTRUM              spect
PROBHD   Z847801_0047 (
PULPROG               zg30
TD                   32768
SOLVENT               DMSO
NS                       32
DS                        0
SWH               9615.385 Hz
FIDRES            0.586877 Hz
AQ               1.7039360 sec
RG                    90.5
DW                  52.000 usec
DE                   14.38 usec
TE                   353.2 K
D1              1.00000000 sec
TD0                       1
SFO1           599.9845606 MHz
NUC1                     1H
P0                    3.60 usec
P1                   10.80 usec
PLW1           20.00000000 W

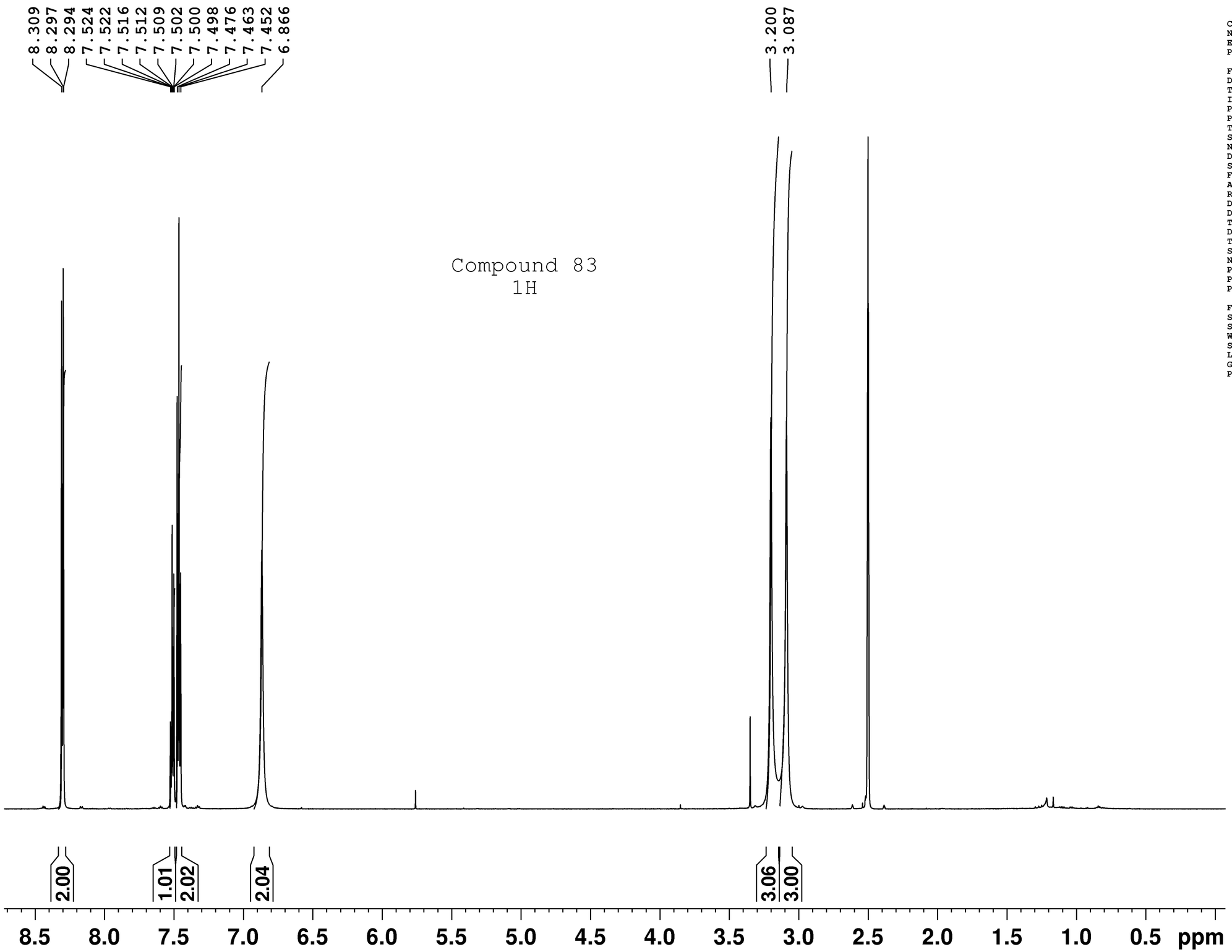
F2 - Processing parameters
SI                   65536
SF             599.9800043 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```




```
Current Data Parameters
NAME              CD-68A
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220225
Time              20.18 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG          zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          2.200787 Hz
AQ             0.4543829 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                353.2 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.8816889 MHz
NUC1                 13C
P0                  3.27 usec
P1                  9.80 usec
PLW1         40.00000000 W
SFO2         599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2         20.00000000 W
PLW12         0.53044999 W

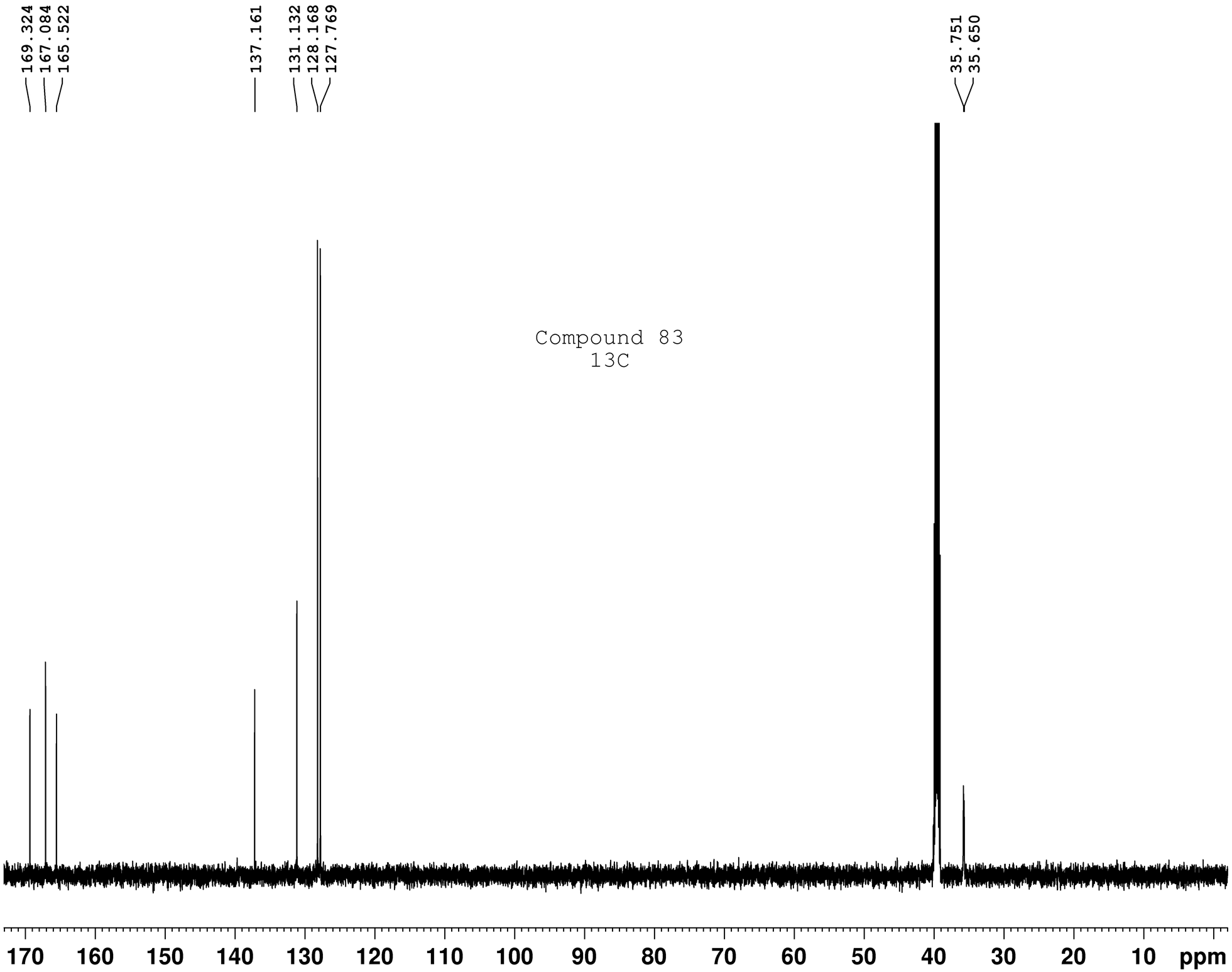
F2 - Processing parameters
SI                 65536
SF          150.8652289 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME              CE-60A
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220224
Time              22.27 h
INSTRUM           spect
PROBHD   Z847801_0047 (
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                    16
DS                     0
SWH             9615.385 Hz
FIDRES          0.586877 Hz
AQ             1.7039360 sec
RG                   144
DW                52.000 usec
DE                 14.38 usec
TE                 293.0 K
D1            1.00000000 sec
TD0                    1
SFO1         599.9845606 MHz
NUC1                  1H
P0                  3.60 usec
P1                 10.80 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                 65536
SF           599.9800038 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME              CE-60A
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220224
Time              22.32 h
INSTRUM            spect
PROBHD   Z847801_0047 (
PULPROG           zgdc30
TD                32768
SOLVENT            DMSO
NS                   128
DS                     0
SWH           36057.691 Hz
FIDRES         2.200787 Hz
AQ            0.4543829 sec
RG                  2050
DW               13.867 usec
DE                6.50 usec
TE               293.1 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        150.8816889 MHz
NUC1                 13C
P0                 3.27 usec
P1                 9.80 usec
PLW1        40.00000000 W
SFO2        599.9824003 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        20.00000000 W
PLW12        0.53044999 W

F2 - Processing parameters
SI                65536
SF          150.8651586 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```