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Supporting Information

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N-Heterocyclic Carbene Catalyzed C–C Bond Cleavage in Redox Esterifications of Chiral Formylcyclopropanes

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General Methods. All reactions utilizing air- or moisture-sensitive reagents were performed in dried glassware under an atmosphere of dry Ar. CH_2Cl_2 was distilled over CaH_2. Toluene and THF were dried by passage over activated alumina under Ar atmosphere. Triazolium salts were prepared according to a reported protocol.[1] All aldehydes, thiols, and alcohols were purified by distillation or column chromatography prior to use. Enantiomerically enriched cyclopropanes were prepared by the method of MacMillan and the enantiopurities of the products were determined by analyses in our laboratory using the reported conditions.[2] *N*,*N*-Diisopropylethylamine (DIPEA) and 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) were distilled from KOH. Other reagents were used without further purification. Thin layer chromatography (TLC) was performed on Merck precoated plates (silica gel 60 F_{254}, Art 5715, 0.25 mm) and was visualized by fluorescence quenching under UV light or by staining with phosphomolybdic acid or permanganate. Silica-gel preparative thin-layer chromatography (PTLC) was performed using plates prepared from Merck Kieselgel 60 PF_{254} (Art 7747). Column chromatography was performed on E. Merck Silica Gel 60 (230–400 Mesh) using a forced flow of 0.5–1.0 bar. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) were measured on a Varian Unity 400 spectrometer. Chemical shifts are expressed in parts per million (PPM) downfield from residual solvent peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Infrared (IR) spectra were recorded on a JASCO FT/IR-430 spectrophotometer and are reported as wavenumbers (cm^{-1}). Optical rotations were measured on a JASCO DIP-1000 polarimeter operating at the sodium D

(1) (a) R. L. Knight, F. J. Leeper, *J. Chem. Soc. Perkins Trans. 1* **1998**, 1891–1893. (b) M. S. Kerr, J. Read de Alaniz, T. Rovis, *J. Org. Chem.* **2005**, *70*, 5725–5728.

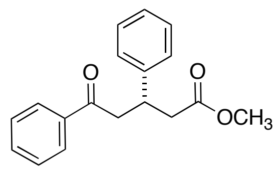
(2) R. K. Kunz, D. W. C. MacMillan, *J. Am. Chem. Soc.* **2005**, *127*, 3240–3241.

line with a 100 mm path length cell, and are reported as follows: $[\alpha]^T$ (concentration (g/100 ml), solvent).

Gas chromatography (GC) was performed on a Hewlett-Packard 6890 Series gas chromatograph equipped with a split-mode capillary injection system and flame ionization detectors using Chiraldex Γ-TA and β-DM (30 m x 0.25 mm) columns at a flow rate of 1 mL/min.

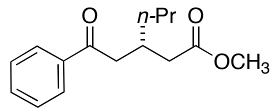
HPLC Conditions. Column, Diacel Chiralpak AD-H, (4.6 x 250mm) Eluent: hexanes/ EtOH. Flow Rate 1.0 mL/min. Detection: 254 nm.

General Procedure for Catalytic Redox Esterifications of Cyclopropanes and Alcohols:

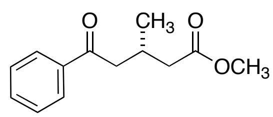


(S)-Methyl 5-oxo-3,5-diphenylpentanoate *(Table 1, entry 1). The reaction of (1R, 2S, 3R)-2-benzoyl-3-phenyl-cyclopropanecarbaldehyde and MeOH is representative.* Into an oven dried vial was weighed triazolium salt **7** (9.0 mg, 0.034 mmol, 5.0 mol %) and the cyclopropanecarbaldehyde **1** (0.168 mg, 0.671 mmol, 1.00 equiv). The vial was closed with a septum and filled with argon. To this was added sequentially THF (1.4 mL), MeOH (0.136 mL, 3.36 mmol, 5.00 equiv) and DBU (0.020 mL, 0.134 mmol, 0.20 equiv). The septum was removed and replaced with a crimp seal, and the resulting solution stirred 15 h at room temperature (20–25 °C). The mixture was concentrated under reduced pressure and purified by flash chromatography (3:1 hexanes/EtOAc) to afford ester **2** as a white solid (170 mg, 90 % yield, 89% ee). $[\alpha]_D^{20}$ (c 0.1, $CHCl_3$) = –2.0; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, 2H, *J* = 7.5), 7.54 (t, 1H, *J* = 7.2), 7.44 (t, 2H, *J* = 7.5), 7.29 (s, 4H), 7.22–7.21 (m, 1H), 3.92 (quintet, 1H, *J* = 7.1), 3.59 (s, 3H), 3.42 (dd, 1H, *J* = 17.2, 7.2), 3.35 (dd, 1H, *J* = 17.1, 7.1), 2.84 (dd, 1H, *J* = 14.6, 7.0), 2.71 (dd, 1H, *J* = 15.5, 7.8); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 172.4, 143.4, 139.6, 133.2, 128.7, 128.7, 128.1, 127.4, 126.9, 51.6, 44.6, 40.6, 37.5. Other spectral data were consistent with a previous report.[3] The enantiomeric ratio was determined by HPLC, using a AD-H column (8% EtOH/hexanes); major enantiomer t_r = 17.0 min and minor enantiomer t_r = 15.8 min.

(3) A. Diaz-Ortiz, E. Diez-Barra, A. de la Hoz, P. Prieto, A. Moreno, *J. Chem. Soc., Perkin Trans. 1,* **1996**, *3*, 259-263.

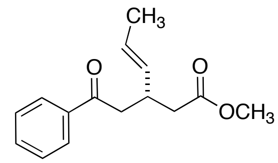


(S)-Methyl 5-oxo-5-phenyl-3-propylpentanoate *(Table 1, entry 2)*. Prepared according to the general procedure with (1*R*, 2*S*, 3*R*)-2-Benzoyl-3-propyl-cyclopropanecarbaldehyde at 40 ºC in 87% yield and 90% ee. $[\alpha]_D^{20}$ (c 0.96, $CHCl_3$) = – 0.2 ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, 2H, *J* = 7.1), 7.57 (t, 1H, *J* = 7.3), 7.45 (t, 2H, *J* = 7.3), 3.66 (s, 3H), 3.09 (dd, 1H, *J* = 16.7, 6.8), 2.96 (dd, 1H, *J* = 16.6, 6.4), 2.62–2.55 (m, 1H), 2.44 (dd, 1H, *J* = 15.3, 6.0), 2.39 (dd, 1H, *J* = 15.3, 7.2), 1.41–1.32 (m, 4H), 0.90 (t, 3H, *J* = 7.0); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 173.3, 137.2, 133.1, 128.6, 128.1, 51.5, 42.7, 38.4, 36.5, 31.3, 20.0, 14.2; IR (thin film) *v* 3061, 2956, 2932, 2872, 1736, 1685, 1448, 1201, 1161, 691cm^{-1}; HREI-MS: calc'd for $C_{15}H_{20}O_3$ (M^+), 248.1412; found, 248.1414. The enantiomeric ratio was determined by HPLC, using a AD-H column (1% EtOH/hexanes); major enantiomer t_r = 14.5 min and minor enantiomer t_r = 16.3 min.

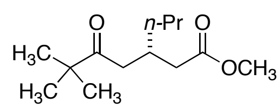


(S)-Methyl 3-methyl-5-oxo-5-phenylpentanoate *(Table 1, entry 3)*. Prepared according to the general procedure with (1*R*, 2*S*, 3*R*)-2-benzoyl-3-methyl-cyclopropanecarbaldehyde at 40 ºC in 84% yield and 77% ee. $[\alpha]_D^{20}$ (c 1.28, C_6H_6) = – 2.9; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, 2H, *J* = 7.2), 7.55 (t, 1H, *J* = 7.4), 7.45 (t, 2H, *J* = 7.4), 3.66 (s, 3H), 3.10 (dd, 1H, *J* = 16.2, 5.9), 2.84 (dd, 1H, *J* = 16.2, 7.4), 2.67 (sextet, 1H, *J* = 6.8), 2.43 (dd, 1H, *J* = 15.3, 6.5), 2.31 (dd, 1H, *J* = 15.3, 7.0), 1.04 (d, 3H, *J* = 6.7); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 173.2, 137.1, 133.2, 128.8, 128.3, 51.6, 45.0, 41.0, 27.0, 20.3; Other spectral data were consistent with a previous report.[4] The enantiomeric ratio was determined by HPLC, using an AD-H column (1% ethanol/hexanes); major enantiomer t_r = 20.4 min and minor enantiomer t_r = 22.8 min.

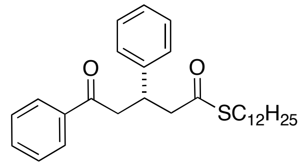
(4) Y. Shi, W. D. Wulff, G. P. A. Yap, A. L. Rheingold, *Chem. Commun.* **1996**, 2601–2602.



(S)-Methyl 5-oxo-5-phenyl-3-(prop-1-enyl)pentanoate *(Table 1, entry 4)*. Prepared according to the general procedure with (*1R, 2S, 3R, E)*-2-benzoyl-3-(prop-1-enyl)cyclopropanecarbaldehyde (83% ee of *trans* isomer, 75% ee of *cis* isomer, 8:1 *trans*: *cis*) at 40 ºC in 96% yield and 81% ee (of combined *cis* and *trans* isomers). $[\alpha]_D^{20}$ (c 0.88, $CHCl_3$) = – 0.9; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, 2H, *J* = 7.1), 7.54 (t, 1H, *J* = 7.3), 7.45 (t, 2H, *J* = 7.3), 5.51–5.46 (m, 1H), 5.42–5.36 (m, 1H), 3.64 (s, 3H), 3.22–3.17 (m, 1H), 3.10 (dd, 1H, *J* = 16.2, 6.3), 3.00 (dd, 1H, *J* = 16.2, 7.2), 2.50 (dd, 1H, *J* = 15.4, 6.5), 2.41 (dd, 1H, *J* = 15.4, 7.4), 1.59 (d, 3H, *J* = 6.0); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 172.8, 137.1, 133.2, 132.4, 128.7, 128.2, 126.3, 51.6, 43.4, 39.5, 35.1, 18.0; IR (thin film) *v* 2951, 2855, 1737, 1685, 1597, 1580, 1448, 1363, 1212, 969 cm^{-1} ; HREI-MS: calc'd for $C_{15}H_{18}O_3$ (M^+), 246.1256, found, 246.1249. The enantiomeric ratio was determined by HPLC, using an OB column (1% isopropanol/hexanes); major enantiomers (of both *cis* and *trans* isomers) t_r = 32.2 min and minor enantiomers (of both *cis* and *trans* isomers) t_r = 26.3 min.

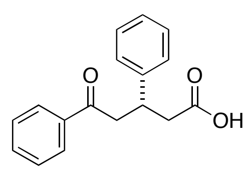


(S)-Methyl 6,6-dimethyl-5-oxo-3-propylheptanoate *(Table 1, entry 5)*. Prepared according to the general procedure with (1*R*, 2*S*, 3*R*)-2-(2,2-Dimethyl-propionyl)-3-propyl-cyclopropanecarbaldehyde (93% ee, 6:1 dr) at 40 ºC in 95% yield. $[\alpha]_D^{20}$ (c 1.09, $CHCl_3$) = + 0.23; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.65 (s, 3H), 2.57 (dd, 1H, *J* = 17.9, 7.0), 2.51 (dd, 1H, *J* = 17.9, 5.8), 2.43–2.37 (m, 1H), 2.35–2.25 (m, 2H), 1.34–1.16 (m, 4H), 1.13 (s, 9H), 0.89 (t, 3H, *J* = 6.4); ^{13}C NMR (100 MHz, $CDCl_3$) δ 214.9, 173.3, 51.3, 44.2, 40.6, 38.1, 36.4, 30.4, 26.4, 20.0, 14.1; IR (thin film) *v* 2958, 2873, 1738, 1706, 1366, 1164, 735 cm^{-1}; HRCI-MS: calc'd for $C_{13}H_{25}O_3$ $(M+H)^+$, 229.1804, found, 229.1811.



(S)-S-dodecyl 5-oxo-3,5-diphenylpentanethioate *(Table 1, entry 6)*. Prepared according to the general procedure with 1.2 equiv of 1-dodecanethiol in 99% yield. and 87% ee (as determined by HPLC analysis of the methyl ester). $[\alpha]_d^{20}$ (c 1.05, $CHCl_3$) = + 1.85. ^1H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, 2H, *J* = 7.1), 7.55 (t, 1H, *J* = 7.3), 7.44 (t, 2H, *J* = 7.3), 7.31–7.25 (m, 4H), 7.22–7.18 (m, 1H), 3.95 (quintet, 1H, *J* = 7.2), 3.44–3.32 (m, 2H), 3.01 (dd, 1H, *J* = 15.1, 7.1), 2.93 (dd, 1H, *J* = 15.0, 7.5), 2.81 (t, 2H, *J* = 7.4), 1.50–1.44 (m, 2H), 1.31–1.21 (m, 18H), 0.89 (t, 3H, *J* = 6.8); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 198.1, 143.0, 137.0, 133.7, 128.8, 128.7, 128.7, 127.6, 127.0, 50.1, 44.5, 38.3, 32.1, 29.8, 29.8, 29.7, 29.7, 29.6, 29.6, 29.3, 29.2, 28.9, 22.9, 14.3; IR (thin film) *v* 3062, 3029, 2925, 2853, 1687, 1449, 984 cm^{-1}; HREI-MS: calc'd for $C_{29}H_{40}O_2S$ (M^+), 452.2749, found, 452.2738. The thioester was converted into the methyl ester by means of Na metal in MeOH. The enantiomeric ratio of the methyl ester was determined by HPLC, using an AD-H column (8% ethanol/ hexanes); major enantiomer t_r = 17.1 min and minor enantiomer t_r = 15.8 min.

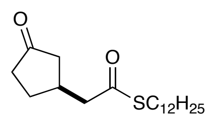
Conversion of the thioester into the methyl ester: To the thioester (63 mg, 0.139 mmol) was added 7 ml MeOH and 2 pieces (~ 3 mm^3) of Na metal. The mixture was stirred for 15 min. EtOAc and NH_4Cl (aq) were added. The layers were separated and the organic layer was washed with brine, dried with Na_2SO_4, filtered and concentrated under vacuum. The crude product was purified by PTLC to provide 20 mg (50% yield) of the methyl ester.



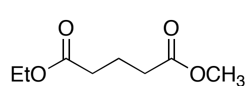
(S)-5-Oxo-3,5-diphenylpentanoic acid *(Table 1, entry 7)*. Prepared according to the general procedure with 1.2 equiv of DBU and 5 equiv of H_2O. Upon termination of the reaction, 1 N HCl and EtOAc were added, and the layers were separated. The organic layer was washed with brine, dried with Na_2SO_4, filtered and concentrated under reduced pressure. The residue was recrystallized from EtOAc to provide the product in 92% yield and 88% ee (as determined by HPLC analysis of the methyl ester). $[\alpha]_d^{20}$ (c 0.92, CH_2Cl_2) = + 1.02. ^1H NMR (400 MHz, CD_6OS) δ 7.92 (d, 2H, *J* = 7.2), 7.61 (t, 1H, *J* =

7.1), 7.49 (t, 2H, *J* = 7.5), 7.30–7.22 (m, 4H), 7.14 (t, 1H, *J* = 7.0), 5.75 (s, 1H), 3.70-3.62 (m, 1H), 3.46 (dd, 1H, J = 17.7, 7.8), 3.37 (dd, 1H, J = 17.7, 6.6), 2.69 (dd, 1H, *J* = 15.8, 6.3), 2.56 (dd, 1H, *J* = 15.8, 8.7); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 173.0, 143.9, 136.7, 128.7, 128.7, 128.2, 127.9, 127.6, 126.3, 44.0, 40.4, 37.3. Other spectral data were consistent with a previous report.[5] The acid was converted into the methyl ester by means of $TMSCHN_2$ in MeOH. The enantiomeric ratio of the ester was determined by HPLC, using an AD-H column (8% EtOH/ hexanes); major enantiomer t_r = 17.1 min and minor enantiomer t_r = 15.8 min.

Conversion of acid into methyl ester: To the acid (80 mg, 0.298 mmol) was added 5 ml MeOH and 0.5 ml $TMSCHN_2$ (2 M soln in Et_2O, 0.954 mmol). The solution was stirred under Ar for 10 min and then concentrated under vacuum. The crude product was purified by PTLC to yield 67 mg (80% yield) of the methyl ester.

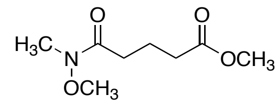


S-Dodecyl 2-(3-oxocyclopentyl)ethanethioate *(Table 2, entry 1)*. Prepared according to the general procedure with 2-oxobicyclo[3.1.0]hexane-6-carbaldehyde and 1.5 equiv of 1-dodecanethiol at 40 °C in 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.89 (t, 2H, *J* = 7.4), 2.72–2.65 (m, 3H), 2.50–2.44 (m, 1H), 2.36–2.30 (m, 1H), 2.24–2.16 (m, 2H), 1.94–1.87 (m, 1H), 1.66–1.53 (m, 3H), 1.37–1.26 (m, 18H), 0.89 (t, 3H, *J* = 6.8); ^{13}C NMR (100 MHz, $CDCl_3$) δ 218.0, 197.9, 49.2, 44.4, 38.2, 34.1, 32.0, 29.7, 29.7, 29.6, 29.6, 29.4, 29.2, 29.2, 29.1, 28.9, 22.8, 14.2; IR (thin film) ν 2925, 2853, 1744, 1687, 1465, 1157, 991 cm^{-1}; HREI-MS: cal'd for $C_{19}H_{34}O_2S$ (M^+), 326.2280; found, 326.2287.

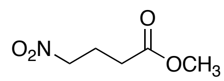


Ethyl methyl glutarate *(Table 2, entry 2)*. Prepared according to the general procedure with ethyl 2-formyl-1-cyclopropanecarboxylate in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.11 (q, 2H, *J* = 7.2), 3.66 (s, 3H), 2.36 (q, 4H, *J* = 7.4), 1.94 (quintet, 2H, *J* = 7.4), 1.24 (t, 3H, *J* = 7.2). Other spectral data were consistent with a previous report.[6]

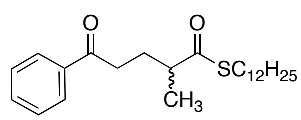
(5) A. Diaz-Ortiz, E. Diez-Barra, A. de la Hoz, P. Prieto, A. Moreno, *J. Chem. Soc., Perkin Trans. 1*, **1996**, *3*, 259–263.
(6) G. Kaupp, H. Frey, G. Behmann, *Synthesis*, **1985**, 555–556.



Methyl 5-(methoxy(methyl)amino)-5-oxopentanoate. *(Table 2, entry 3).* Prepared according to the general procedure with Weinreb amide cyclopropanecarbaldehyde in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.62 (s, 3 H), 3.61 (s, 3H). 3.11 (s, 3H), 2.43 (t, 2H, *J* = 7.0), 2.35 (t, 2H, *J* = 7.1), 1.92–1.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 61.3, 51.6, 33.3, 32.1, 30.9, 19.8; IR (thin film) ν 3504, 2952, 1736, 1663, 1439, 1175, 996 cm^{-1}; HRESI-MS: calc'd for $C_8H_{15}NO_4Na$ $(M+Na)^+$, 212.0893, found, 212.0885.

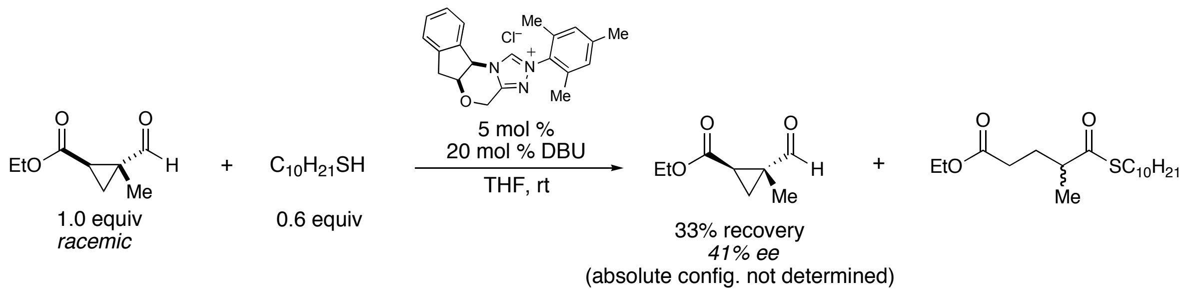


Methyl 4-nitrobutyrate *(Tabel 2, entry 4)*. Prepared according to the general procedure with 2-nitrocyclopropanecarbaldehyde in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.49 (t, 2H, *J* = 6.8), 3.71 (s, 3H), 2.48 (t, 2H, *J* = 7.1), 2.32 (quintet, 2H, *J* = 6.8); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 74.4, 52.0, 30.3, 22.4. Other spectral data were consistent with commercially available material (Aldrich Cat. No. 227846).



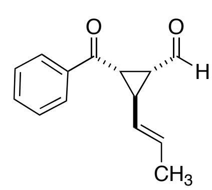
S-dodecyl 2-methyl-5-oxo-phenylpentanethioate *(Table 2, entry 5)*. Prepared according to the general procedure with 2-benzoyl-1-methylcyclopropanecarbaldehyde and 1.5 equiv of 1-dodecanethiol in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, 2H, *J* = 7.1), 7.57 (t, 1H, *J* = 7.3), 7.46 (t, 2H, *J* = 7.3), 3.08–2.94 (m, 2H), 2.87 (t, 2H, *J* = 7.4), 2.83–2.76 (m, 1H), 2.15–2.06 (m, 1H), 1.98–1.90 (m, 1H), 1.60–1.52 (m, 2H), 1.36-1.19 (m, 21H), 0.88 (t, 3H, *J* = 6.8); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 199.5, 137.0, 133.3, 128.8, 128.2, 48.0, 36.0, 32.1, 29.8, 29.8, 29.7, 29.5, 29.3, 29.0, 28.9, 28.4, 22.9, 18.3, 14.3; IR (thin film) *v* 3062, 3028, 2925, 2854, 1686, 1449, 1209, 973 cm^{-1}; HRCI-MS: cal'd for $C_{24}H_{39}O_2S$ $(M+H)^+$, 391.2671; found, 391.2664.

Enantioselective Kinetic Resolution:

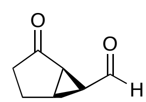


Ethyl 5-(dodecylthio)-4-methyl-5-oxopentanoate. Prepared according to the general procedure in 24 h with ethyl 2-formyl-2-methylcyclopropanecarboxylate and 0.6 equiv of 1-dodecanethiol. Ethyl 2-formyl-2-methylcyclopropanecarboxylate was recovered by column chromatography in 32% yield and 41% ee. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.13 (q, 2H, *J* = 7.2), 2.86 (t, 2H, *J* = 7.4), 2.73–2.65 (m, 1H), 2.37–2.29 (m, 2H), 2.05–1.96 (m, 1H), 1.82–1.73 (m, 1H), 1.59–1.52 (m, 1H), 1.34–1.26 (m, 2H), 1.34–1.26 (m, 18H), 1.19 (d, 3H, *J* = 7.0), 0.88 (t, 3H, *J* = 6.9); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.5, 173.2, 60.6, 47.9, 32.1, 32.0, 29.8, 29.8, 29.8, 29.7, 29.6, 29.3, 29.1, 29.1, 29.0, 28.9, 22.9, 18.0, 14.4, 14.3; IR (thin film) *v* 2925, 2854, 1737, 1686, 1459, 1179, 964, 735 cm^{-1}; HREI-MS: cal'd for $C_{20}H_{39}O_3S$ $(M+H)^+$, 359.2620; found, 359.2605. The the enantiomeric ratio of the recovered aldehyde was determined by GC using a β-DM Chiraldex column (85°C isotherm, 1 mL/min); major enantiomer t_r= 42.8 min, minor enantiomer t_r= 44.1 min.

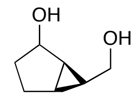
Preparation of Cyclopropane Aldehydes:



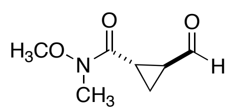
(*1R, 2S, 3R, E*)-2-Benzoyl-3-(prop-1-enyl)cyclopropanecarbaldehyde. Prepared in analogy to the method of MacMillan:[2] To 2-(dimethyl-l-sulfanylidene)-λ-phenyl-ethanone (0.770 g, 4.27 mmol, 1.00 equiv) was added 60 mL $CHCl_3$, (S)-(–)-indoline-2-carboxylic acid (0.139 g, 0.854 mmol, 0.20 equiv) and *trans*-2-hexenal (0.70 mL, 6.34 mmol, 1.48 equiv). The reaction was stirred for 24 h at rt, followed by filtration through a plug of silica, elution with EtOAc and concentration *in vacuo*. The crude product was purified by column (10:1 Hexanes/EtOAc) to yield 0.164 g (18% yield, 8:1 *trans*/*cis*, 83% ee of *trans* isomer) of product. $[\alpha]_D^{20}$ (c 1.32, $CHCl_3$) = –142.0; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (d, 1H, *J* = 5.5), 7.96 (d, 2H, *J* = 7.0), 7.58 (t, 1H, *J* = 7.3), 7.47 (t, 2H, *J* = 7.5), 5.82–5.76 (m, 1H), 5.24–5.18 (m, 1H), 3.19–3.16 (m, 1H), 3.03–2.98 (m, 1H), 2.31–2.26 (m, 1H), 1.72-1.70 (d, 3H, *J* = 6.5); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 195.6, 136.9, 133.7, 129.2, 128.9, 128.5, 127.7, 40.0, 35.3, 31.7, 18.0; IR (thin film) *v* 3061, 3028, 2965, 2938, 2918, 2855, 2764, 1703, 1597, 1580, 1450, 1225, 962 cm^{-1}; HREI-MS: cal'd for $C_{14}H_{14}O_2$ $(M)^+$, 214.0994; found, 214.0999. The *trans* to *cis* isomeric ratio and the enantiomeric ratios were determined by GC using a Γ-TA Chiraldex column (145°C isotherm, 1 mL/min); *cis* major enantiomer t_r= 156.8 min, *cis* minor enantiomer t_r= 160.2 min, *trans* major enatiomer t_r = 194.7 min, *trans* minor enantiomer t_r = 199.6 min.



2-oxobicyclo[3.1.0]hexane-6-carbaldehyde. To a solution of 6-(hydroxymethyl)bicyclo[3.1.0]hexane-2-ol (0.277 g, 2.16 mmol, 1.00 equiv) and *N*-methyl-morpholine-*N*-oxide (0.380 g, 3.24 mmol, 1.50 equiv) in CH_2Cl_2 (11 mL) was added activated, powdered 4A molecular sieves (2.20 g, 1 g /1 mmol of the diol). The reaction mixture was stirred at rt for 20 minutes before tetrapropyl ammonium perruthanate (TPAP) (0.076 g, 0.216 mmol, 0.10 equiv) was added in portions. After 1 h, the reaction was diluted with pentane, filtered over a plug of silica gel, and eluted with 1:1 pentane/Et_2O. The filtrate was concentrated under reduced pressure, and the residue was purified by flash chromatography (1:1 hexanes/EtOAc) on silica gel to yield 60% (0.162 g) of the aldehyde product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (d, 1H, *J* = 4.1), 2.61–2.58 (m, 1H), 2.42–2.40 (m, 1H), 2.34–2.15 (m, 2H), 2.14–1.99 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.1, 196.3, 35.5, 34.8, 32.0, 29.5, 22.5; IR (thin film) *v* 3063, 2951, 2885, 2743, 1731, 1185 cm^{-1}; HREI-MS: calc'd for $C_7H_8O_2$ (M^+), 124.0524; found, 124.0528.

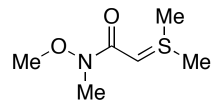


6-(Hydroxymethyl)bicyclo[3.1.0]hexan-2-ol. Ethyl 2-oxobicyclo[3.1.0]hexane-6-carboxylate[7] (0.770 g, 4.58 mmol, 1.00 equiv) was dissolved in 70 ml THF. The solution was cooled in an ice bath and $LiAlH_4$ (0.500 g, 13.2 mmol, 2.87 equiv) was added in portions. After 1 h of stirring, the reaction was quenched with 1.0 mL MeOH. The flask was removed from the bath and stirred at rt. To the mixture was added Na_2SO_4•$10H_2O$ and water and the mixture was stirred 1 h. The mixture was filtered and extracted with EtOAc. The organic layer was washed water and brine, dried with Na_2SO_4 and concentrated under reduced pressure. Purification by flash chromatography (6:1 CH_2Cl_2/MeOH) afforded the aldehyde (0.277 g, 2.16 mmol, 47% yield) or the product was continued to the next reaction without prior purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.57–4.51 (m, 1H), 3.79 (dd, 1H, *J* = 11.1, 5.4), 3.45–3.30 (m, 2H), 3.10–3.05 (m, 1H), 1.92–1.85 (m, 1H), 1.82–1.71 (m, 2H), 1.45–1.42 (m, 1H), 1.37–1.32 (m, 1H), 1.26–1.22 (m, 1H), 1.17–1.07 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 73.7, 64.6, 29.4, 28.4, 25.2, 21.8, 19.4; IR (thin film) v 3324, 3025, 2870, 1657, 1452, 1340, 1266, 1025, 909 cm^{-1}; HRESI-MS: calc'd for $C_7H_{12}O_2Na$ $(M+Na)^+$, 151.0729, found, 151.0730.

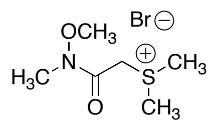


To Weinreb sulfur ylide (2.15g, 13.2 mmol, 1.00 equiv) was added 26 mL PhMe and acrolein (1.76 mL, 26.3 mmol, 2.00 equiv). The solution was heated at 60 °C for 90 min under Ar, concentrated in vacuo and purified by column chromatography (1:1 Hexanes/EtOAc) to yield the aldehyde (0.707 g, 34% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (d, 1H, *J* = 3.8), 3.75 (s, 3H), 3.22 (s, 3H), 2.85–2.79 (m, 1H), 2.47–2.42 (m, 1H), 1.65–1.60 (m, 1H), 1.52–1.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 169.9, 61.3, 32.0, 30.0, 18.9, 14.0; IR (thin film) *v* 3404, 2939, 2850, 2736, 1711, 1656, 1443, 1177, 1002 cm^{-1}; HRESI-MS: calc'd for $C_7H_{11}NO_3Na$ $(M+Na)^+$, 180.0631, found, 180.0635.

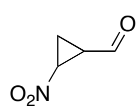
(7) I. Collado, C. Dominguez, J. Ezquerra, Concepcion, P. *Tetrahedron Lett.* **1997**, *38*, 2133–2136



Weinreb Sulfur Ylide. To the Weinreb amide sulfur ylide bromide salt (2.64g, 13.3 mmol, 1.00 equiv) was added 13 mL $CHCl_3$. After the starting materials had dissolved, the solution was cooled in ice-bath. To this was added 7.5 mL of K_2CO_3 (sat. aq.) and 1.38 mL of 12.5 M aq. NaOH. The ice-bath was removed, and the reaction stirred 20 min. The solution was filtered through celite and eluted with CH_2Cl_2. The filtrate was dried with K_2CO_3, filtered and concentrated under vacuum to yield 2.15 g ylide (99% yield).



Weinreb Amide Sulfur Ylide Bromide Salt. To 2-chloro-N-methoxy-N-methylethanamide[8] (6.30 g, 45.6 mmol, 1.00 equiv) was added of dimethyl sulfide (DMS) (10.5 mL, 143 mmol, 3.14 equiv). The mixture was heated at 65 °C for 20 h. The excess DMS was decanted and the remaining clear gel was rinsed with EtOAc to afford 3.25g (36% yield) of the product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.56 (s, 2H), 3.91 (s, 3H), 3.41 (s, 6H), 3.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 62.0, 47.1, 31.9, 24.7; IR (thin film) ν 2994, 2190, 1645, 1435, 1182, 929 cm^{-1}; HRESI-MS: calc'd for $C_6H_{14}NO_2S^+$ (M^+), 164.0740, found, 164.0737.

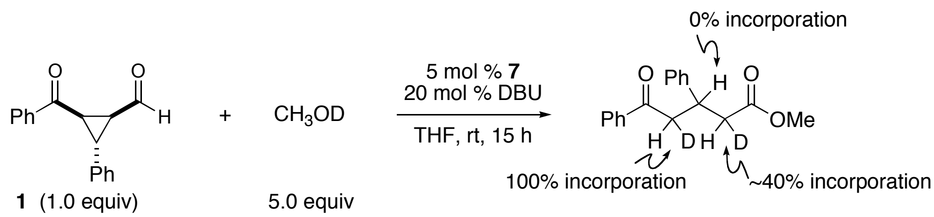


2-nitrocyclopropanecarbaldehyde. Into a 50 mL flask with a rubber septa was weighed *trans*-2-nitrocyclopropyl)methanol[9] (0.291 g, 2.48 mmol, 1.00 equiv). The flask was filled with argon and cooled in an ice-bath. To this was added 21 mL CH_2Cl_2, 5.2 mL DMSO, NEt_3 (1.7 mL, 12.2 mmol, 4.90 equiv), and SO_3•pyr complex (1.40 g, 8.68 mmol, 3.50 equiv). The reaction was stirred for 1 h, followed by the addition of Na_2CO_3 (sat. aq.) and EtOAc. The layers were separated, and the organic layer was washed with NaCl (aq.), dried with Na_2SO_4 and concentrated under reduced pressure. The

(8) D. Netz, J. Seidel, *Tetrahedron Lett*. **1992**, *33*, 1957–1958.
(9) O. V. Larinov, T. F. Savel'eva, K. A. Kochetkov, N. S. Ikonnokov, S. I. Kozhushkov, D. S. Yufit, J. A. K. Howard, V. N. Khrustalev, Y. N. Belokon, A. de Meijere, *Eur. J. Org. Chem.* **2003**, 869–877.

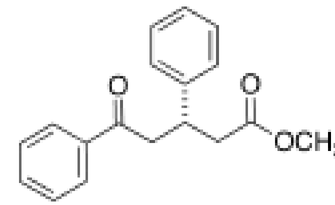
crude product was purified by column chromatography (3:1 hexanes/EtOAc) to yield 0.223 g (78% yield) of aldehyde. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 4.68–4.65 (m, 1H), 3.13–3.07 (m, 1H), 2.19–2.14 (m, 1H), 1.83–1.79 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 59.9, 31.7, 17.9; IR (thin film) v 3110, 2862, 2744, 1717, 1550, 1364, 981 cm^{-1}; HREI-MS: calc'd for $C_4H_5NO_3$ (M^+), 115.0269; found, 115.0270.

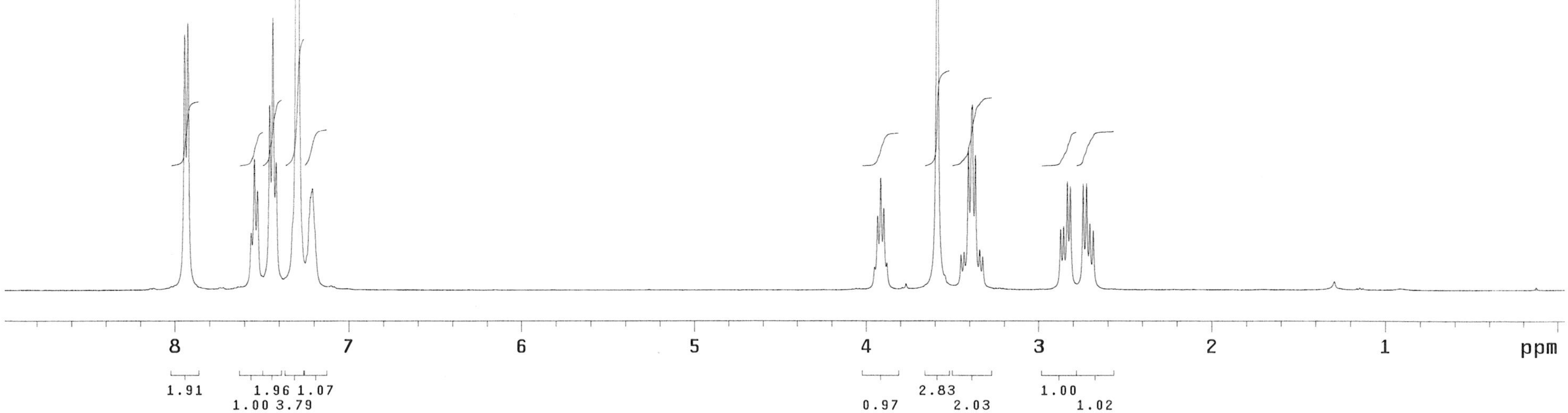
Deuterium Labeling Studies:



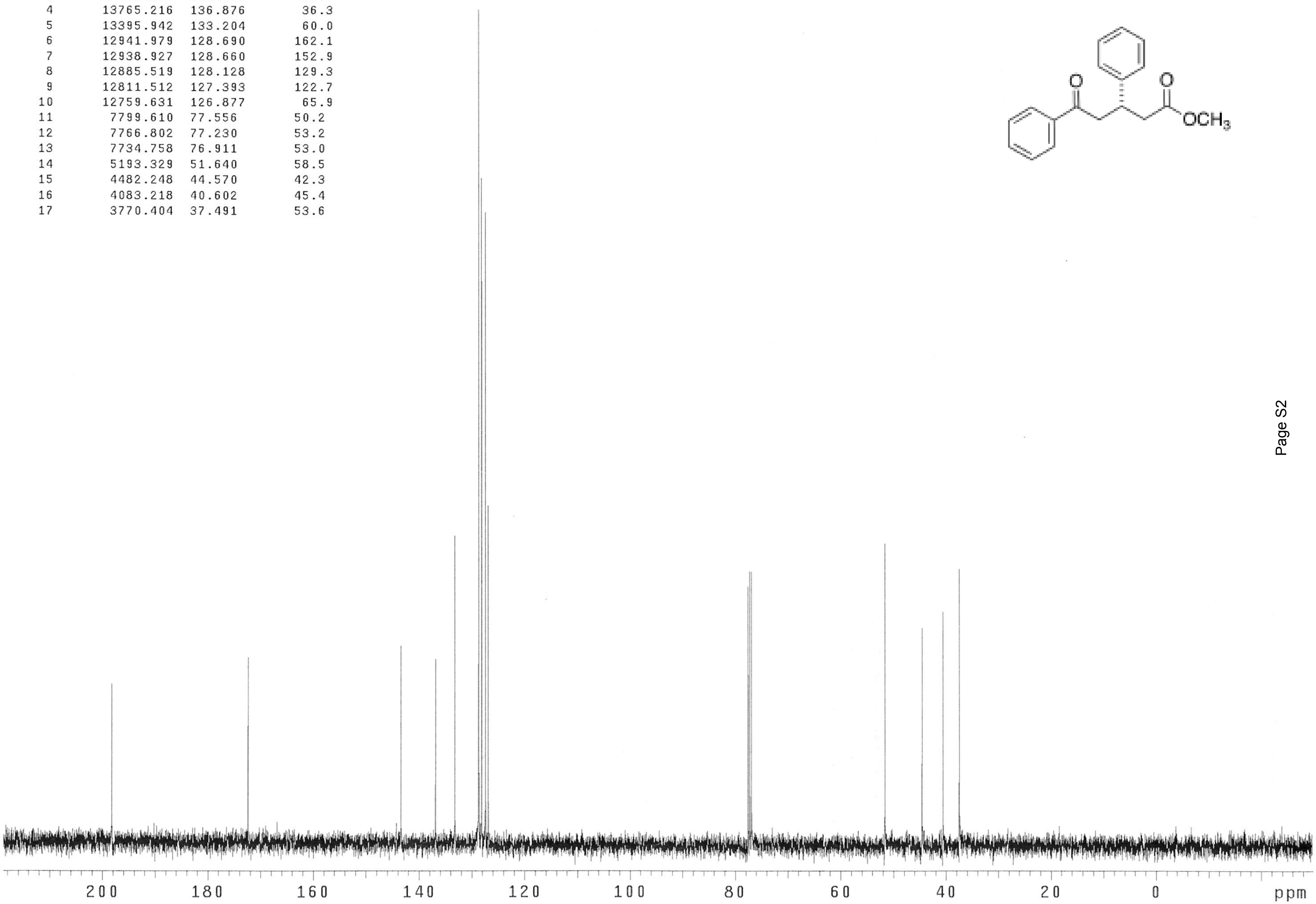
The reaction of aldehyde and alcohol was conducted according the general procedure. Following purification, the product was analyzed by ^{1}H and ^{2}D NMR, revealing the deuteration pattern shown in the above scheme.

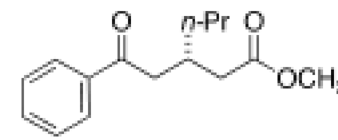
INDEX	FREQUENCY	PPM	HEIGHT
1	3176.921	7.943	41.3
2	3169.441	7.925	43.2
3	3024.130	7.561	9.1
4	3016.968	7.543	21.1
5	3009.646	7.525	16.1
6	2981.794	7.455	29.8
7	2974.154	7.436	44.1
8	2966.833	7.418	20.6
9	2916.380	7.292	125.5
10	2888.209	7.221	15.0
11	2883.434	7.210	16.3
12	1579.932	3.950	3.6
13	1572.929	3.933	11.9
14	1565.767	3.915	18.0
15	1558.605	3.897	13.1
16	1551.602	3.880	4.4
17	1434.780	3.587	151.2
18	1379.393	3.449	5.7
19	1372.390	3.431	6.0
20	1362.522	3.407	23.0
21	1355.042	3.388	29.4
22	1353.450	3.384	29.9
23	1346.129	3.366	21.7
24	1336.102	3.341	6.5
25	1329.258	3.324	5.3
26	1148.614	2.872	9.7
27	1141.611	2.854	10.2
28	1133.017	2.833	17.5
29	1126.173	2.816	16.6
30	1096.729	2.742	17.1
31	1088.930	2.723	17.1
32	1081.291	2.704	10.6
33	1073.492	2.684	9.5



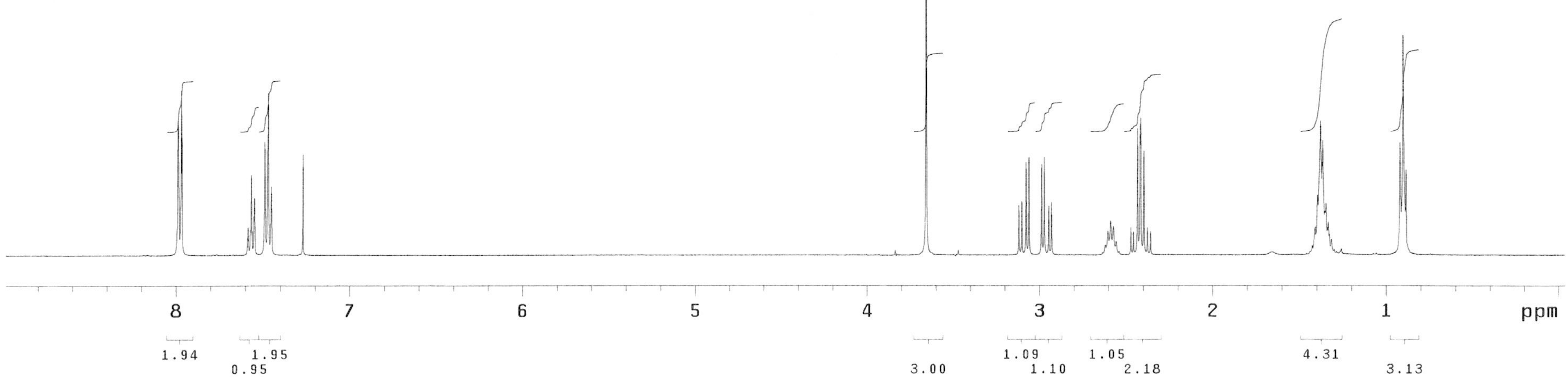


INDEX	FREQUENCY	PPM	HEIGHT
1	19930.717	198.183	31.5
2	17335.118	172.374	36.6
3	14422.126	143.408	38.7
4	13765.216	136.876	36.3
5	13395.942	133.204	60.0
6	12941.979	128.690	162.1
7	12938.927	128.660	152.9
8	12885.519	128.128	129.3
9	12811.512	127.393	122.7
10	12759.631	126.877	65.9
11	7799.610	77.556	50.2
12	7766.802	77.230	53.2
13	7734.758	76.911	53.0
14	5193.329	51.640	58.5
15	4482.248	44.570	42.3
16	4083.218	40.602	45.4
17	3770.404	37.491	53.6

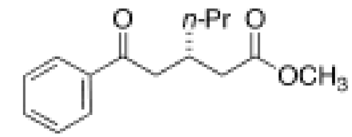


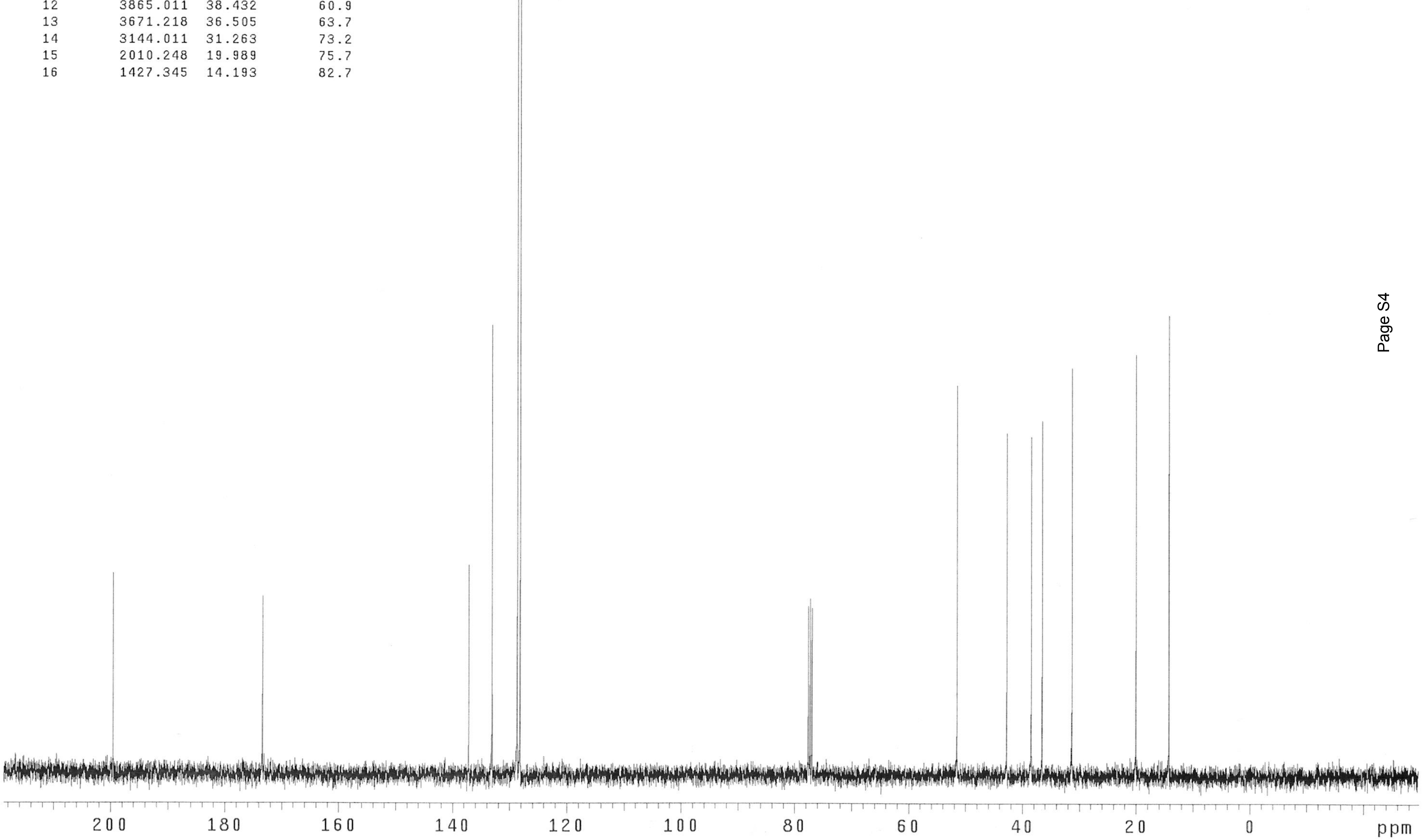


INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3195.384	7.989	20.5	40	558.458	1.396	9.8
2	3194.588	7.987	22.1	41	551.295	1.378	21.7
3	3189.177	7.974	7.9	42	547.953	1.370	15.1
4	3187.426	7.970	26.7	43	546.521	1.366	18.5
5	3185.994	7.966	19.0	44	542.064	1.355	7.2
6	3033.680	7.585	4.5	45	540.473	1.351	7.1
7	3028.109	7.571	4.0	46	538.881	1.347	8.5
8	3026.359	7.567	13.0	47	535.539	1.339	4.6
9	3024.449	7.562	4.0	48	533.629	1.334	5.4
10	3020.151	7.551	6.4	49	531.082	1.328	3.4
11	3019.037	7.549	9.3	50	368.264	0.921	18.1
12	3017.764	7.545	4.9	51	361.420	0.904	35.5
13	2995.164	7.489	18.4	52	354.258	0.886	13.8
14	2993.731	7.485	7.5				
15	2987.365	7.469	26.2				
16	2981.476	7.455	5.2				
17	2980.044	7.451	11.1				
18	2907.627	7.270	16.3				
19	1462.156	3.656	149.8				
20	1246.974	3.118	8.1				
21	1240.130	3.101	8.7				
22	1230.263	3.076	15.0				
23	1223.419	3.059	15.9				
24	1194.134	2.986	14.7				
25	1187.768	2.970	15.8				
26	1177.581	2.944	8.0				
27	1171.215	2.928	8.6				
28	1041.183	2.603	4.0				
29	1034.817	2.587	5.6				
30	1028.451	2.571	4.7				
31	988.184	2.471	4.5				
32	982.295	2.456	3.8				
33	972.905	2.433	20.4				
34	966.857	2.417	21.2				
35	965.742	2.415	22.2				
36	958.421	2.396	16.8				
37	950.304	2.376	4.5				
38	943.142	2.358	3.9				
39	563.232	1.408	4.6				

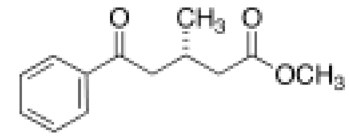


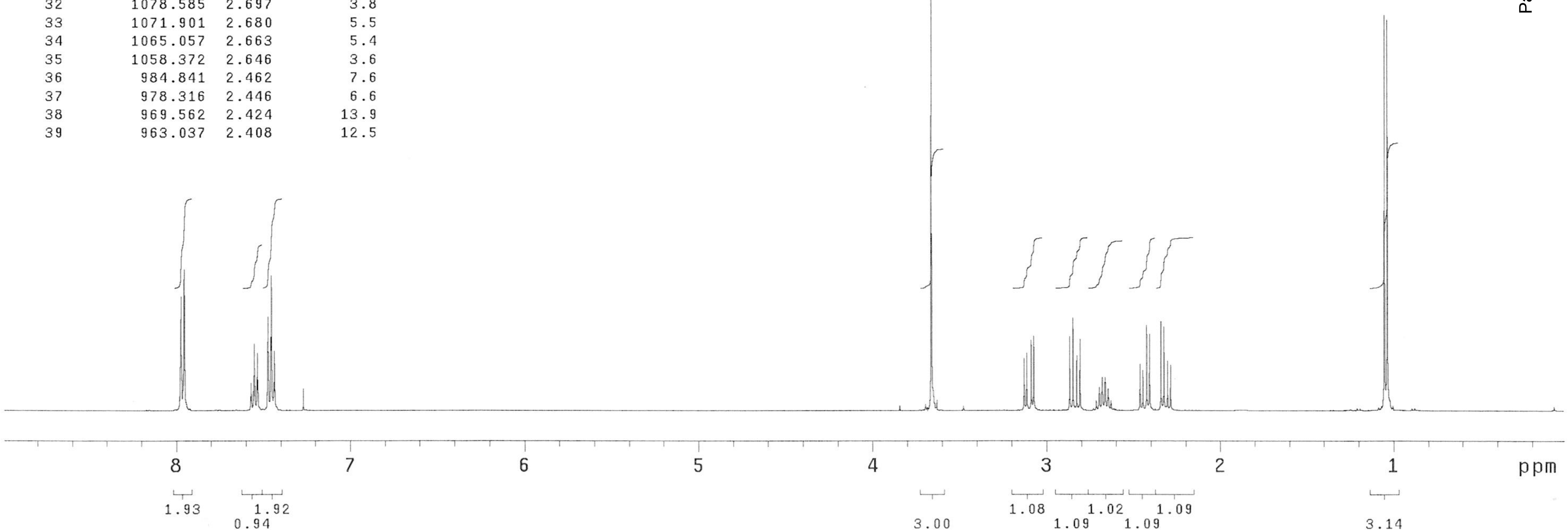
INDEX	FREQUENCY	PPM	HEIGHT
1	20064.236	199.511	36.4
2	17432.014	173.337	32.3
3	13793.445	137.157	38.0
4	13382.208	133.067	80.9
5	12935.875	128.629	164.4
6	12886.282	128.136	152.7
7	7798.847	77.549	30.5
8	7766.802	77.230	31.9
9	7734.758	76.911	30.2
10	5177.307	51.481	70.1
11	4299.136	42.749	61.5
12	3865.011	38.432	60.9
13	3671.218	36.505	63.7
14	3144.011	31.263	73.2
15	2010.248	19.989	75.7
16	1427.345	14.193	82.7





INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3190.291	7.977	14.9	40	936.776	2.342	14.5
2	3189.177	7.974	18.6	41	929.614	2.324	13.7
3	3187.745	7.970	8.7	42	921.337	2.304	8.1
4	3184.084	7.961	6.0	43	914.334	2.286	7.4
5	3182.015	7.956	23.0	44	421.104	1.053	64.3
6	3180.582	7.952	18.8	45	414.420	1.036	63.6
7	3028.109	7.571	4.5				
8	3022.857	7.558	3.2				
9	3020.788	7.553	11.0				
10	3018.719	7.548	4.0				
11	3014.740	7.538	5.4				
12	3013.308	7.534	9.4				
13	3012.034	7.531	5.0				
14	2989.116	7.474	15.3				
15	2987.683	7.470	6.9				
16	2982.590	7.457	12.0				
17	2981.317	7.454	22.0				
18	2975.746	7.440	4.6				
19	2973.996	7.436	9.7				
20	2973.200	7.434	6.7				
21	2907.627	7.270	3.5				
22	1464.702	3.662	150.9				
23	1460.405	3.651	3.3				
24	1251.272	3.129	8.5				
25	1245.383	3.114	9.4				
26	1235.037	3.088	11.5				
27	1229.149	3.073	12.2				
28	1146.387	2.866	12.1				
29	1138.906	2.848	15.1				
30	1130.152	2.826	9.0				
31	1122.672	2.807	11.7				
32	1078.585	2.697	3.8				
33	1071.901	2.680	5.5				
34	1065.057	2.663	5.4				
35	1058.372	2.646	3.6				
36	984.841	2.462	7.6				
37	978.316	2.446	6.6				
38	969.562	2.424	13.9				
39	963.037	2.408	12.5				





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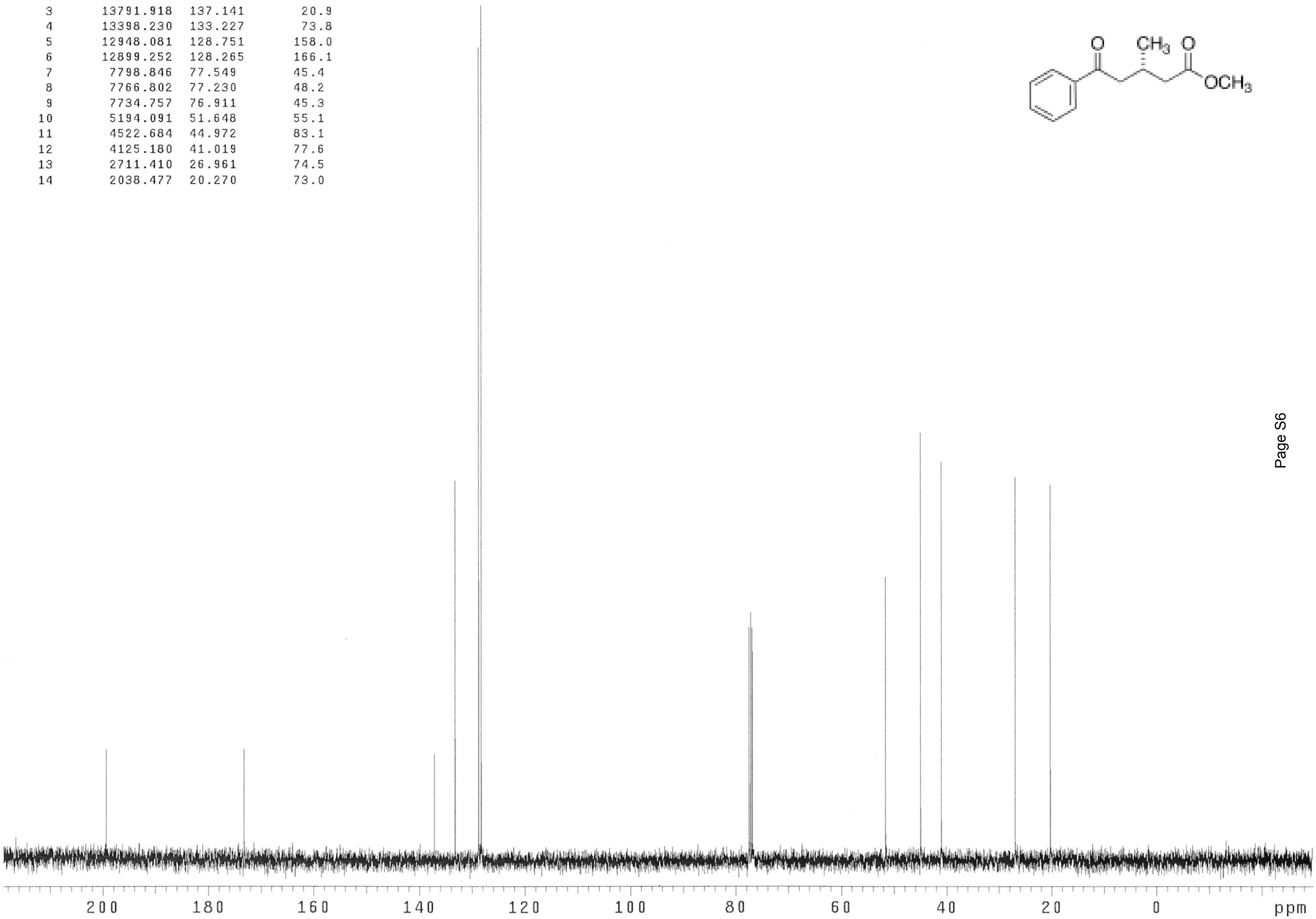
3	13791.918	137.141	20.9
4	13398.230	133.227	73.8
5	12948.081	128.751	158.0
6	12899.252	128.265	166.1
7	7798.846	77.549	45.4
8	7766.802	77.230	48.2
9	7734.757	76.911	45.3
10	5194.091	51.648	55.1
11	4522.684	44.972	83.1
12	4125.180	41.019	77.6
13	2711.410	26.961	74.5
14	2038.477	20.270	73.0



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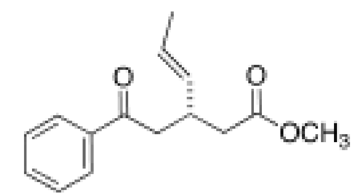
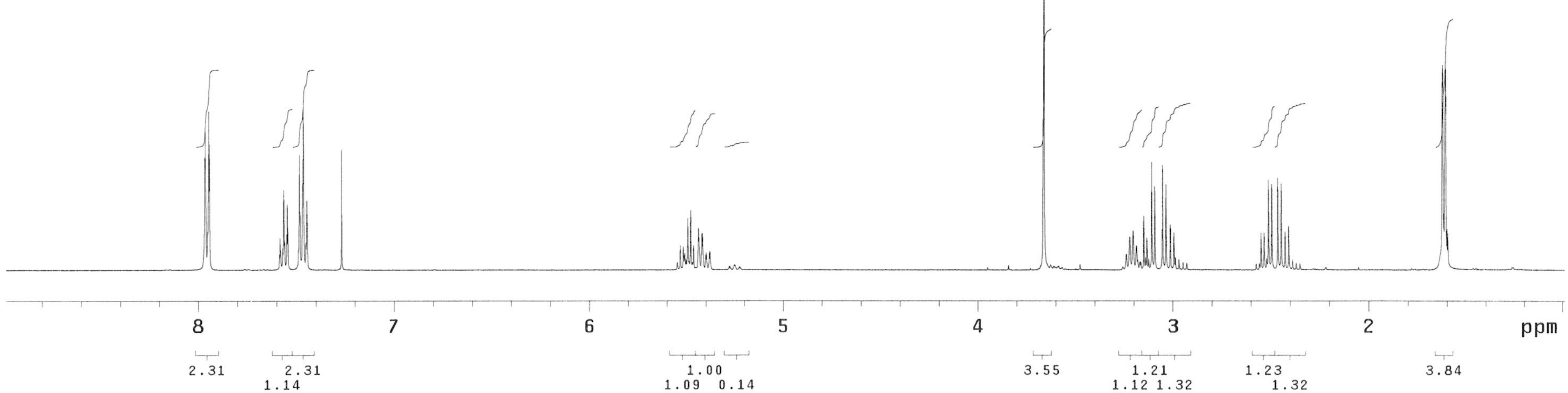
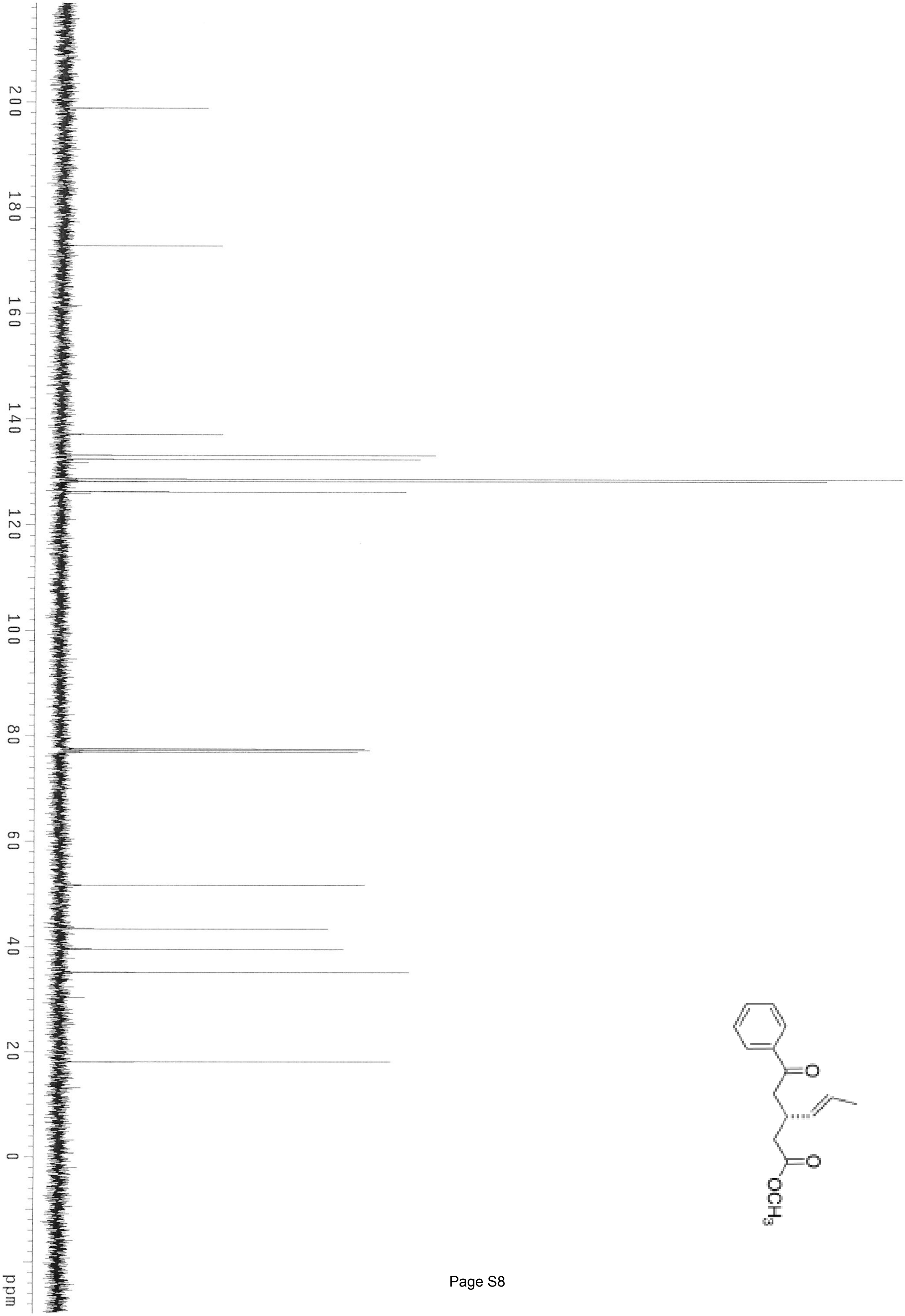
1	3187.092	7.969	18.3	40	1288.265	3.221	5.4
2	3186.324	7.967	22.4	41	1281.355	3.204	6.4
3	3181.257	7.954	6.2	42	1274.292	3.186	4.0
4	3179.261	7.949	25.8	43	1259.397	3.149	8.8
5	3177.879	7.946	20.4	44	1253.101	3.133	5.2
6	3033.233	7.584	5.2	45	1243.120	3.108	17.6
7	3031.851	7.581	3.3	46	1236.825	3.092	13.6
8	3027.858	7.571	3.5	47	1221.162	3.053	17.1
9	3025.708	7.565	13.0	48	1213.946	3.035	13.9
10	3023.866	7.561	4.8	49	1204.886	3.013	7.4
11	3019.720	7.550	5.8	50	1197.669	2.995	6.1
12	3018.492	7.547	10.7	51	1019.548	2.549	6.0
13	3017.110	7.544	6.1	52	1013.099	2.533	6.1
14	2995.612	7.490	3.4	53	1004.347	2.511	14.7
15	2993.923	7.486	18.6	54	997.744	2.495	14.0
16	2992.388	7.482	8.8	55	985.613	2.464	15.0
17	2987.320	7.469	13.9	56	978.243	2.446	14.1
18	2986.092	7.466	26.5	57	970.412	2.426	6.2
19	2980.411	7.452	4.5	58	963.041	2.408	7.1
20	2978.722	7.448	11.3	59	650.562	1.627	32.7
21	2977.954	7.446	9.1	60	649.795	1.625	33.4
22	2907.627	7.270	19.6	61	649.180	1.623	32.0
23	2213.110	5.533	3.3	62	647.184	1.618	9.2
24	2212.496	5.532	4.0	63	644.267	1.611	33.3
25	2206.507	5.517	3.8	64	643.806	1.610	32.6
26	2203.436	5.509	2.7	65	643.038	1.608	28.3
27	2197.908	5.495	7.0	66	640.274	1.601	6.7
28	2197.294	5.494	8.4	67	638.432	1.596	5.9
29	2191.152	5.479	9.7				
30	2185.471	5.464	4.0				
31	2175.643	5.440	6.8				
32	2174.415	5.437	6.6				
33	2168.119	5.421	6.0				
34	2166.737	5.418	5.9				
35	2159.213	5.399	2.8				
36	2152.918	5.383	2.7				
37	2151.536	5.380	3.0				
38	1465.925	3.665	24.4				
39	1464.389	3.661	151.2				







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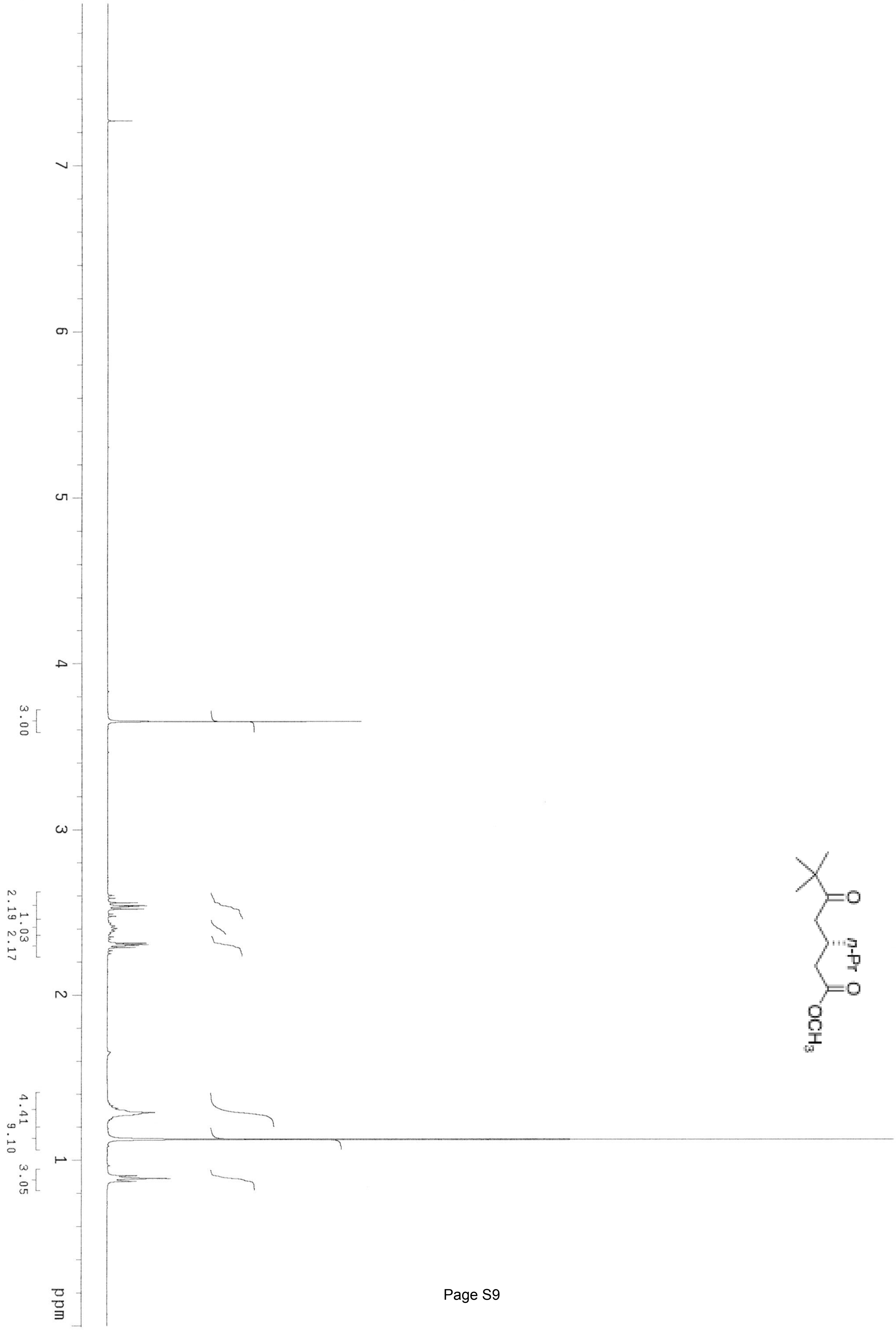
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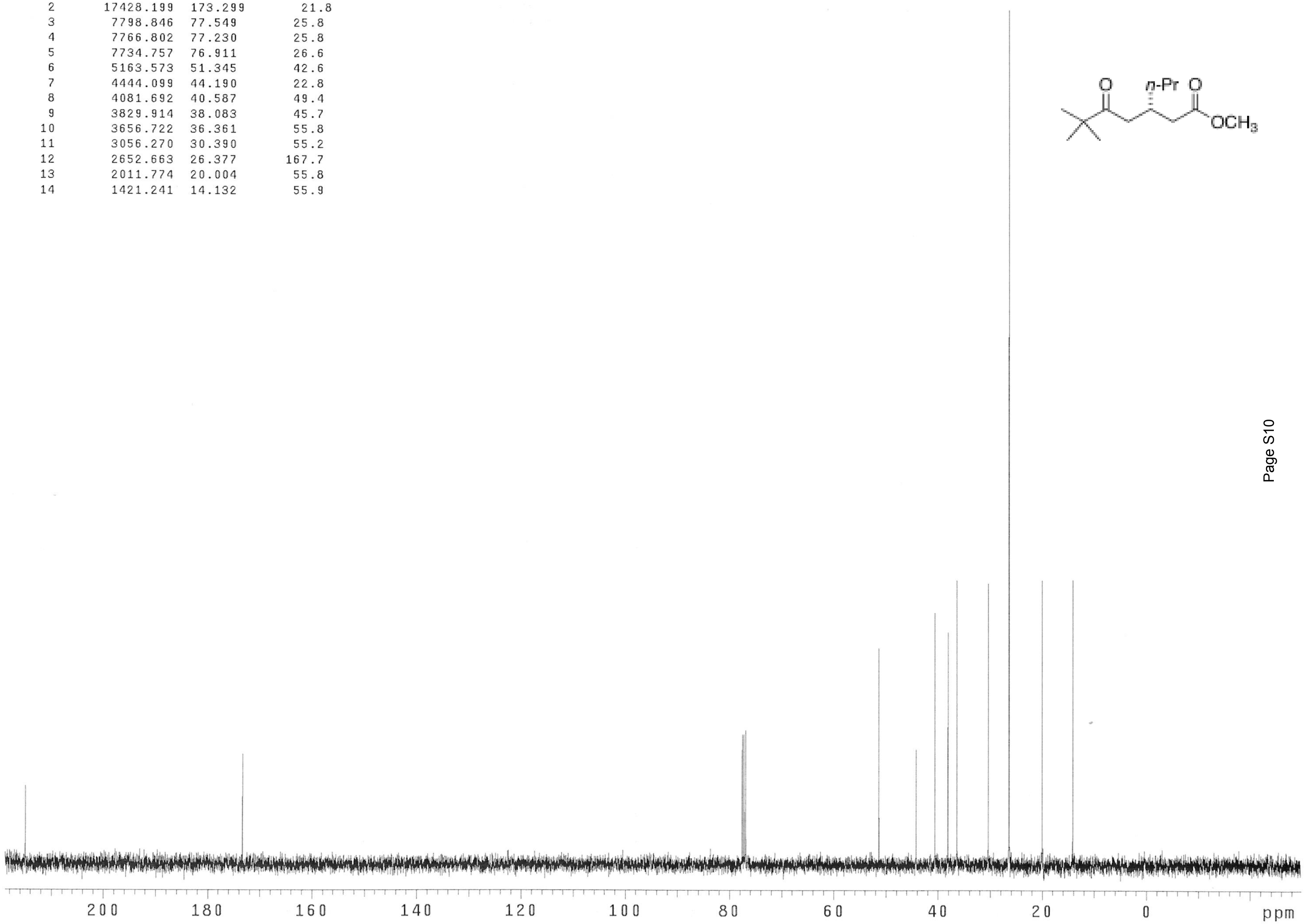
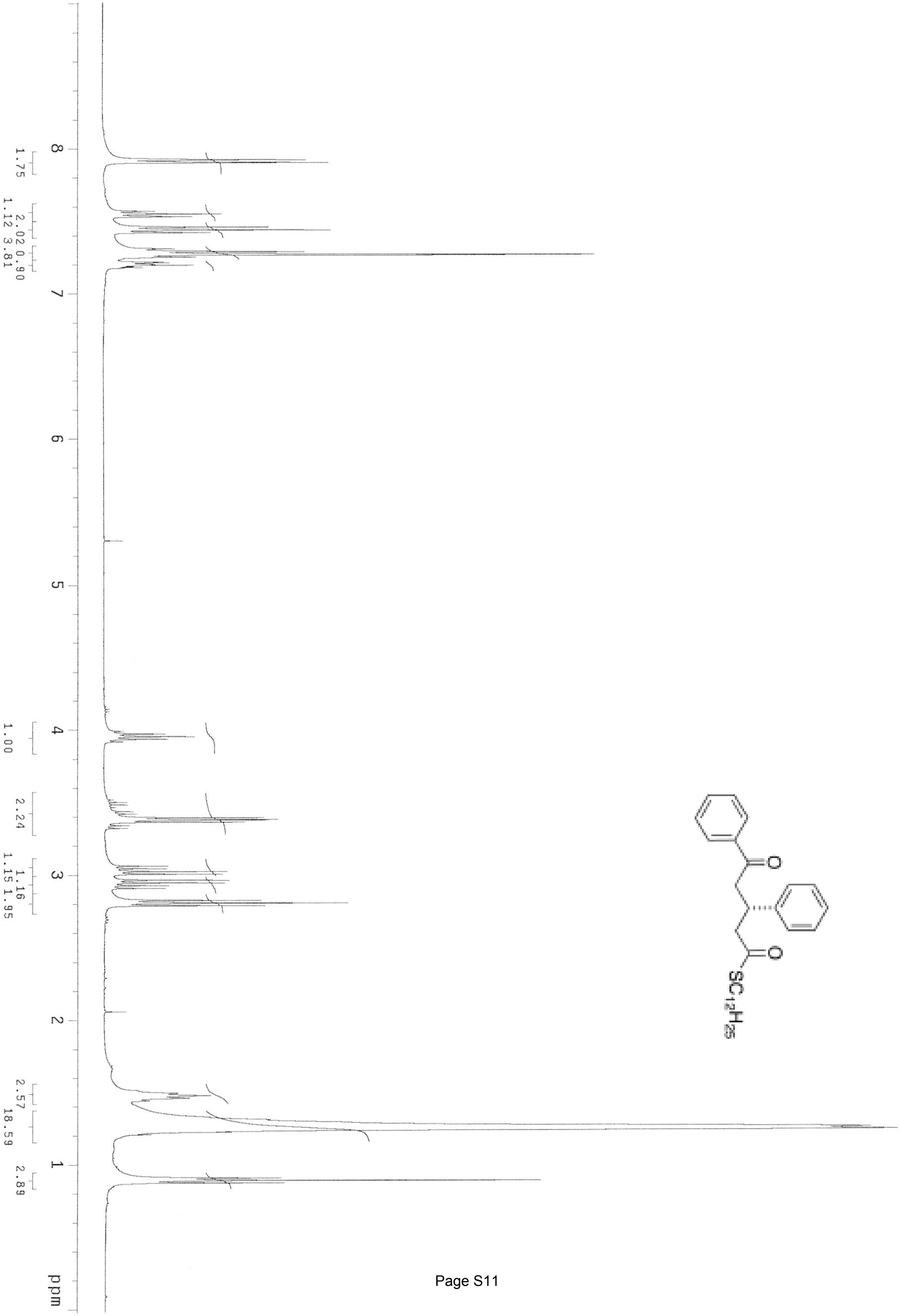
n-Pr O
OCH3

INDEX	FREQUENCY	PPM	HEIGHT
1	21612.287	214.904	15.5
2	17428.199	173.299	21.8
3	7798.846	77.549	25.8
4	7766.802	77.230	25.8
5	7734.757	76.911	26.6
6	5163.573	51.345	42.6
7	4444.099	44.190	22.8
8	4081.692	40.587	49.4
9	3829.914	38.083	45.7
10	3656.722	36.361	55.8
11	3056.270	30.390	55.2
12	2652.663	26.377	167.7
13	2011.774	20.004	55.8
14	1421.241	14.132	55.9

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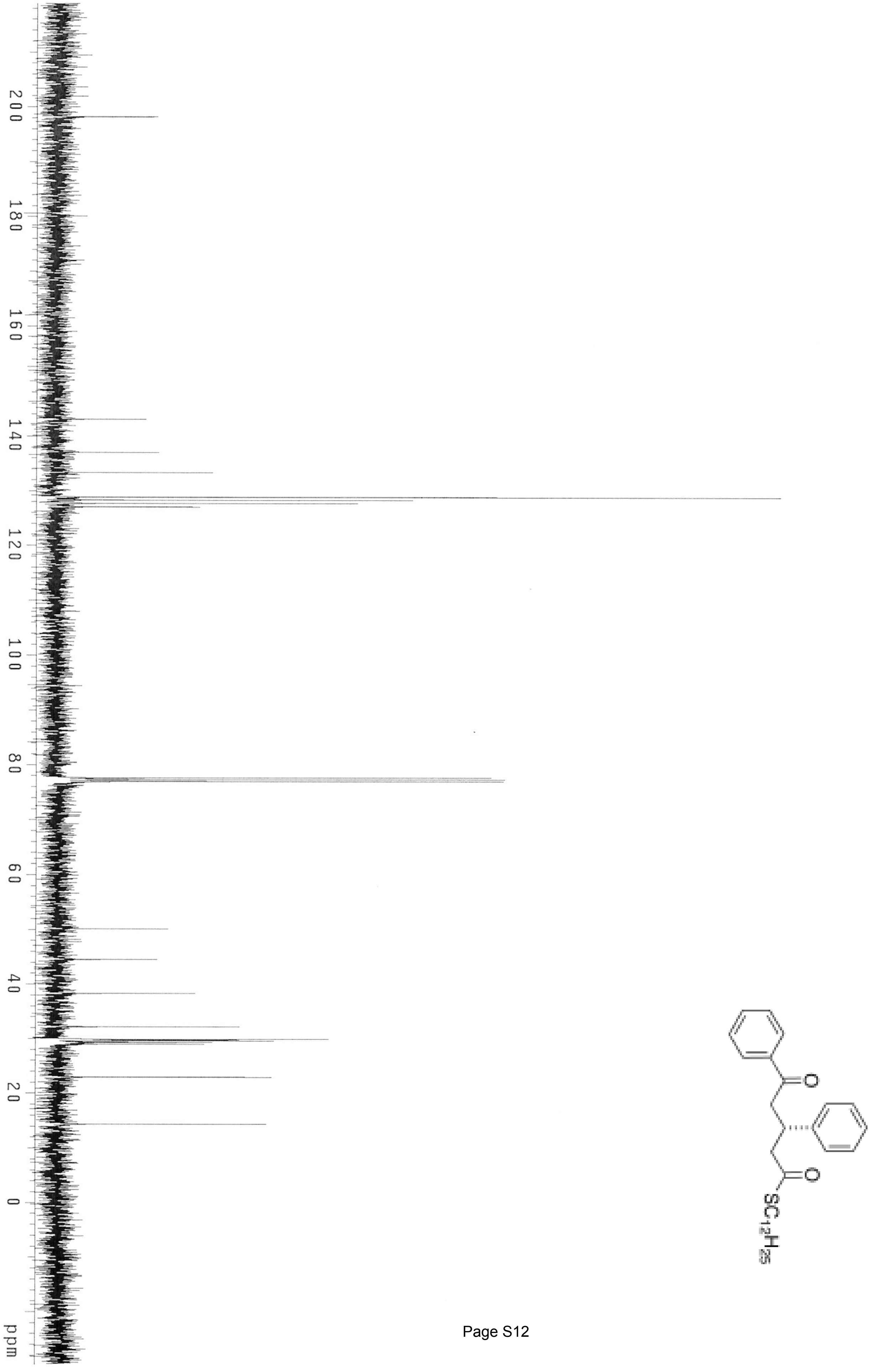
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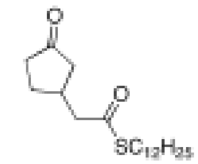
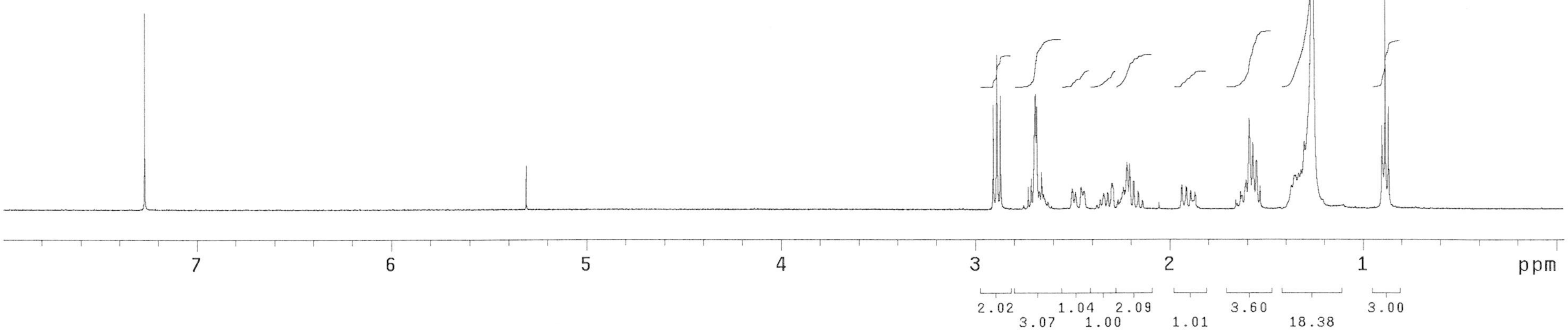
1	2907.627	7.270	32.0	40	650.928	1.628	2.3
2	2123.456	5.309	7.2	41	649.496	1.624	2.3
3	1162.780	2.907	17.1	42	641.856	1.605	4.9
4	1155.459	2.889	25.2	43	635.172	1.588	14.9
5	1147.978	2.870	18.5	44	627.691	1.569	10.9
6	1091.000	2.728	3.6	45	620.688	1.552	8.0
7	1084.633	2.712	5.0	46	612.571	1.532	3.8
8	1078.744	2.697	12.1	47	548.271	1.371	3.9
9	1076.198	2.691	18.8	48	542.223	1.356	5.6
10	1073.015	2.683	16.8	49	539.040	1.348	5.6
11	1068.240	2.671	3.0	50	532.833	1.332	5.9
12	1063.465	2.659	6.1	51	527.899	1.320	6.4
13	1061.715	2.655	3.7	52	521.533	1.304	11.1
14	1059.009	2.648	2.4	53	504.185	1.261	151.9
15	1000.598	2.502	3.3	54	360.784	0.902	13.7
16	993.754	2.485	2.8	55	354.099	0.885	42.6
17	981.977	2.455	3.6	56	347.096	0.868	16.8
18	976.724	2.442	3.0				
19	975.610	2.439	3.0				
20	943.142	2.358	1.6				
21	935.980	2.340	2.6				
22	928.181	2.321	2.7				
23	920.064	2.300	4.2				
24	918.313	2.296	4.2				
25	895.713	2.240	3.6				
26	892.371	2.231	3.2				
27	888.551	2.222	7.7				
28	887.118	2.218	7.2				
29	882.662	2.207	7.4				
30	874.386	2.186	4.6				
31	864.996	2.163	3.0				
32	863.722	2.160	2.5				
33	774.435	1.936	3.9				
34	765.840	1.915	3.7				
35	764.726	1.912	3.5				
36	755.972	1.890	3.0				
37	747.537	1.869	2.8				
38	663.024	1.658	1.5				
39	653.316	1.633	2.9				





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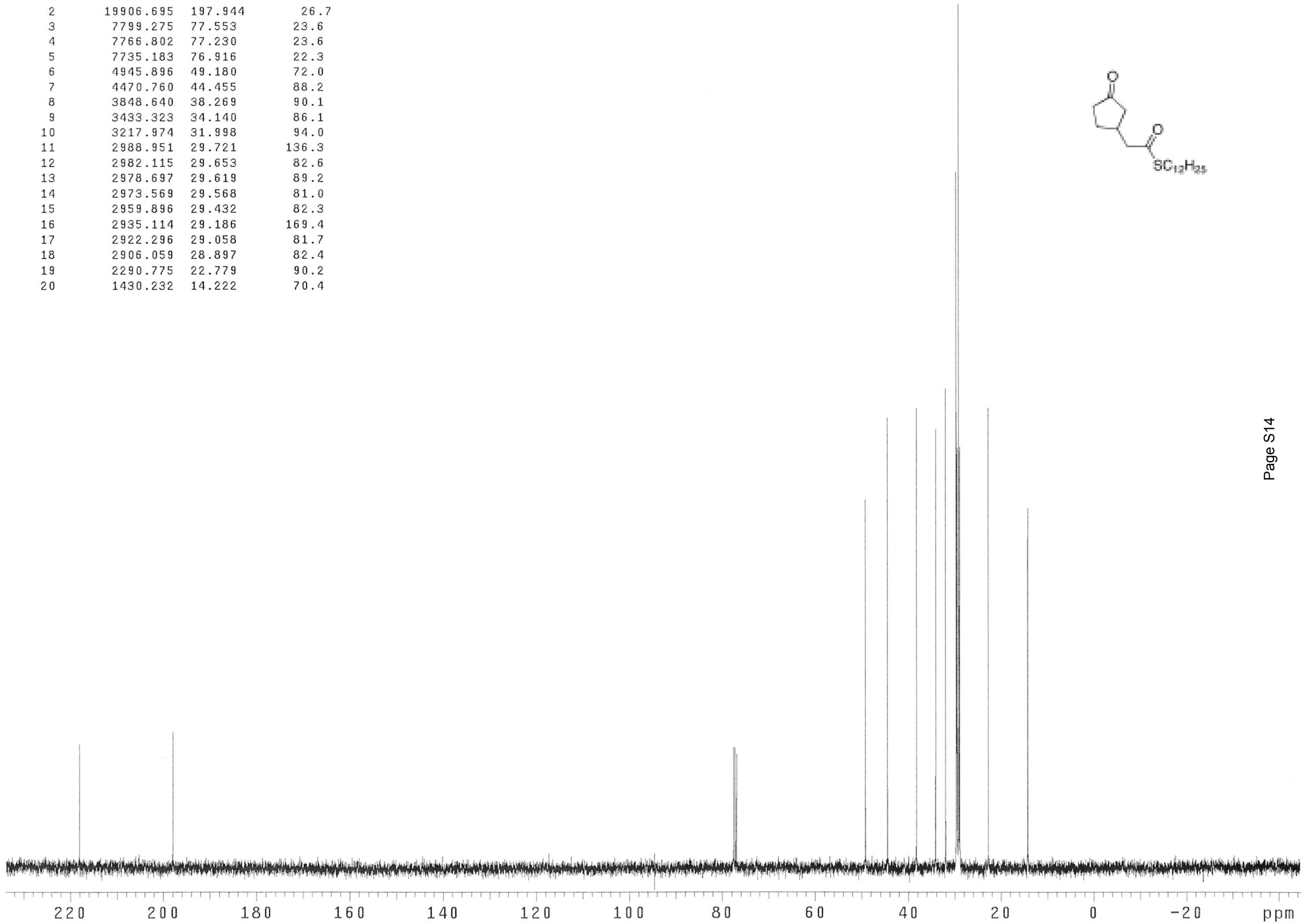
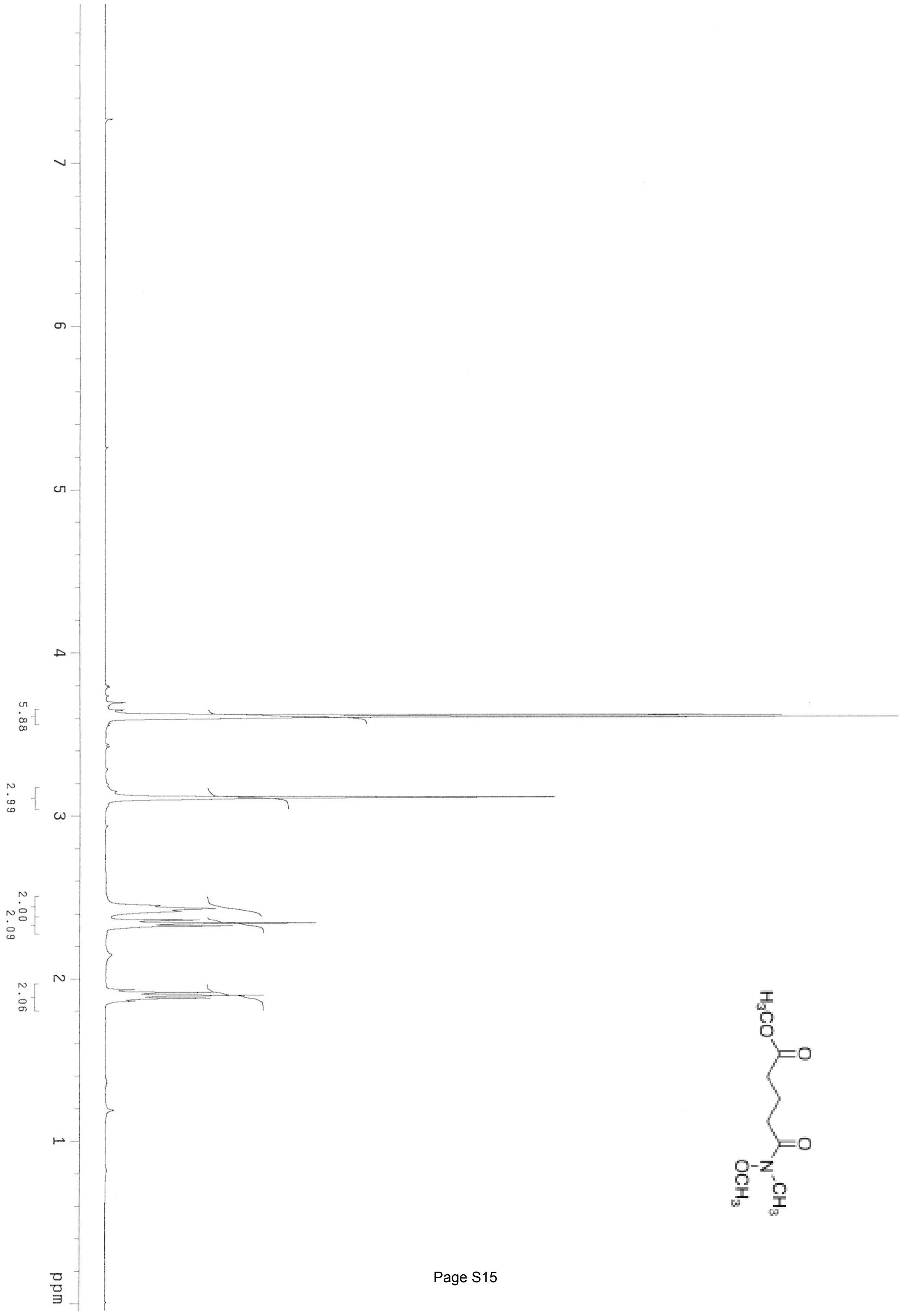
1	21927.732	218.041	24.2
2	19906.695	197.944	26.7
3	7799.275	77.553	23.6
4	7766.802	77.230	23.6
5	7735.183	76.916	22.3
6	4945.896	49.180	72.0
7	4470.760	44.455	88.2
8	3848.640	38.269	90.1
9	3433.323	34.140	86.1
10	3217.974	31.998	94.0
11	2988.951	29.721	136.3
12	2982.115	29.653	82.6
13	2978.697	29.619	89.2
14	2973.569	29.568	81.0
15	2959.896	29.432	82.3
16	2935.114	29.186	169.4
17	2922.296	29.058	81.7
18	2906.059	28.897	82.4
19	2290.775	22.779	90.2
20	1430.232	14.222	70.4

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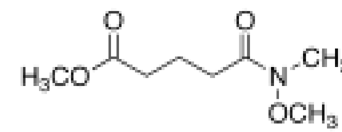
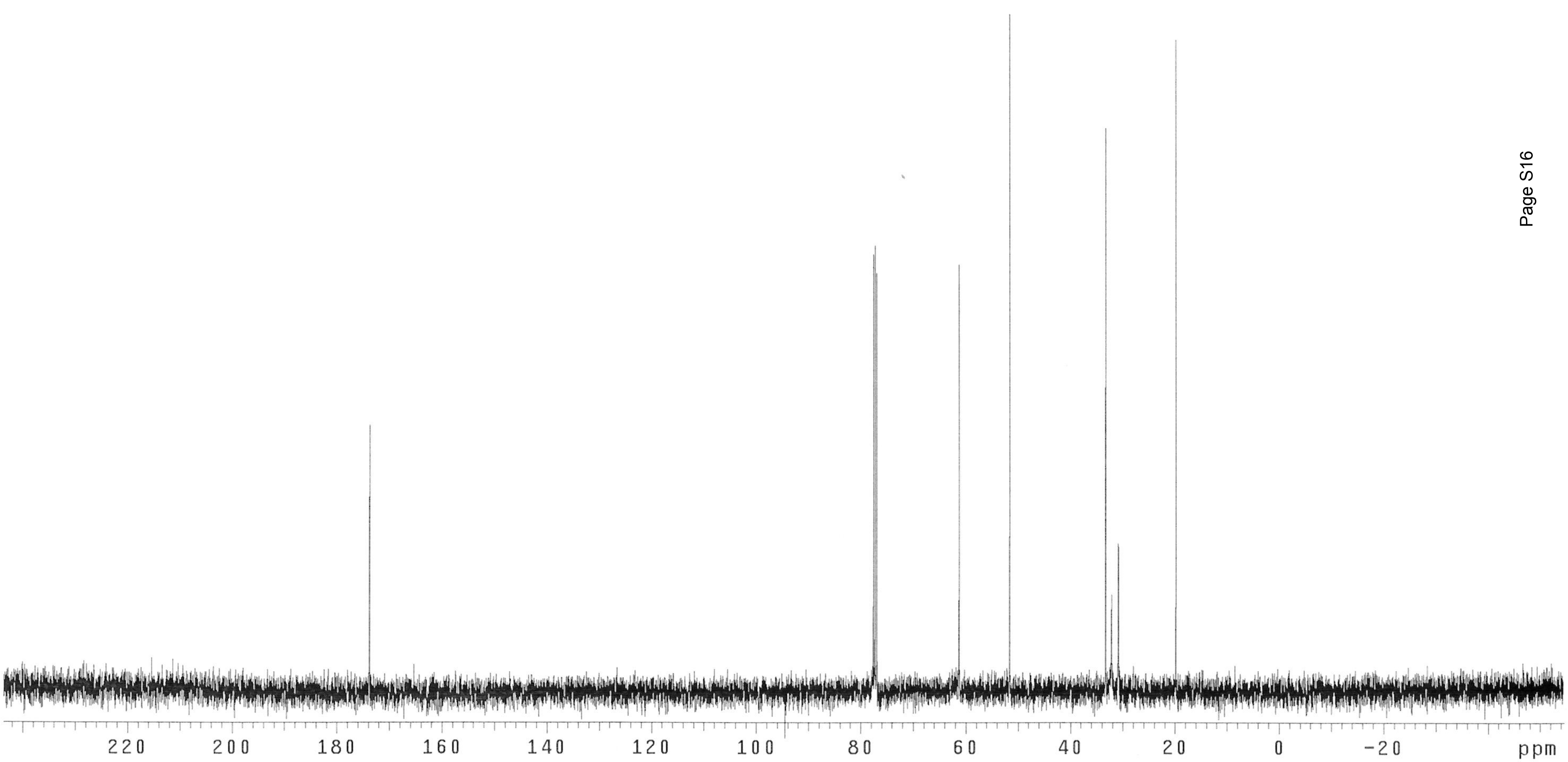
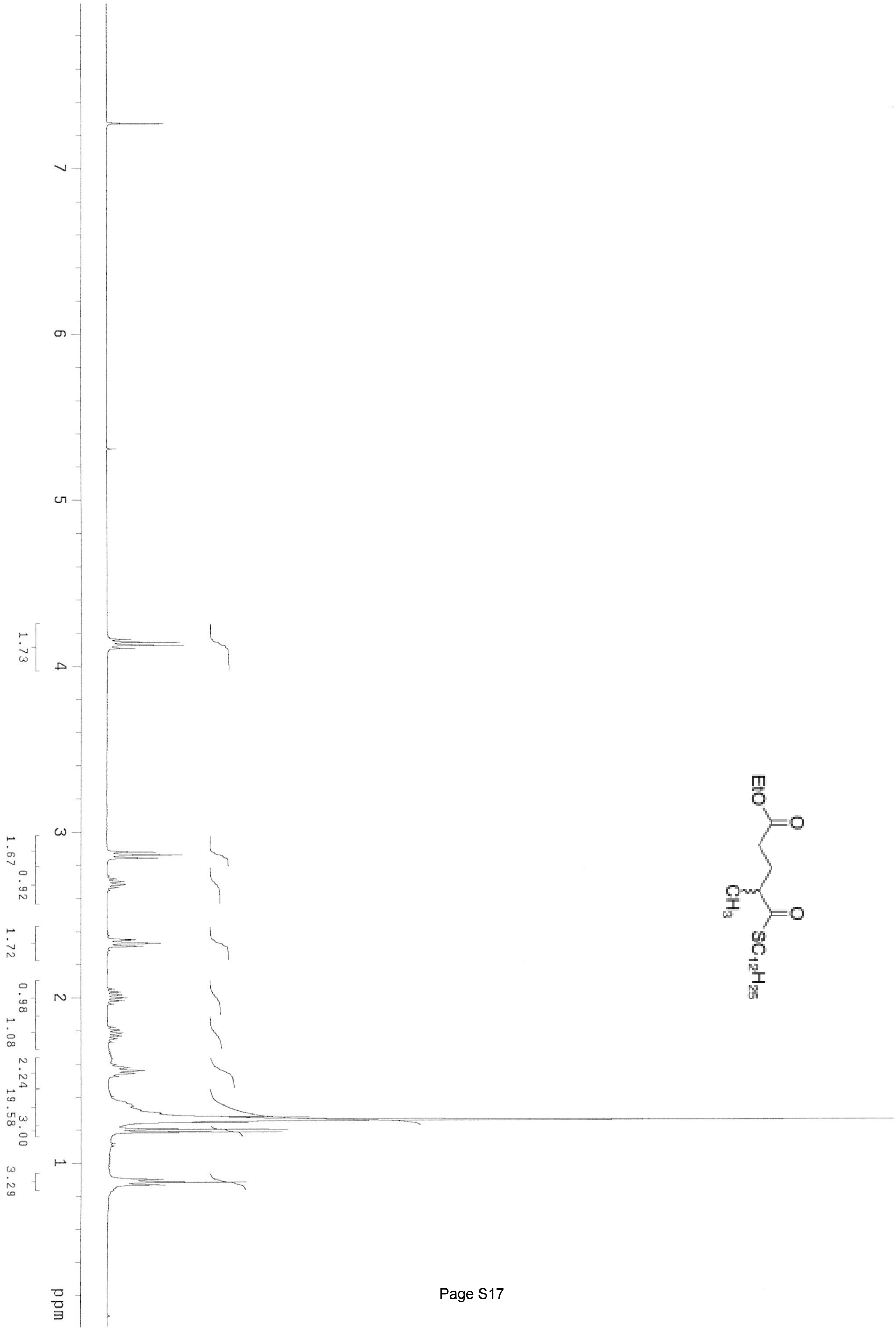
1	17474.137	173.756	43.6
2	7798.842	77.549	71.4
3	7766.802	77.230	72.8
4	7734.761	76.911	68.3
5	6161.119	61.264	69.6
6	5186.174	51.569	110.6
7	3345.223	33.264	92.0
8	3233.539	32.153	16.0
9	3102.631	30.851	24.4
10	1991.286	19.801	106.4



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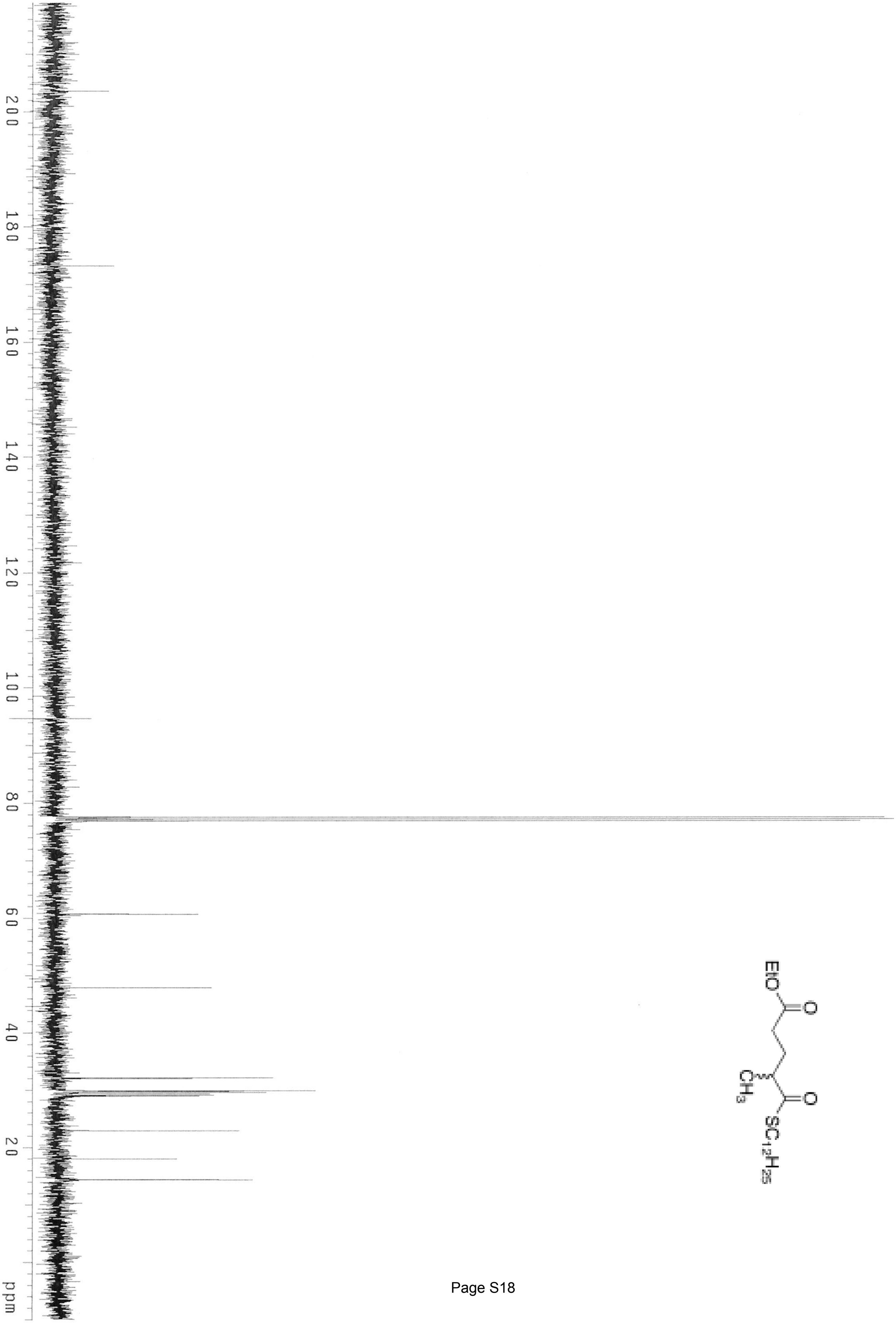
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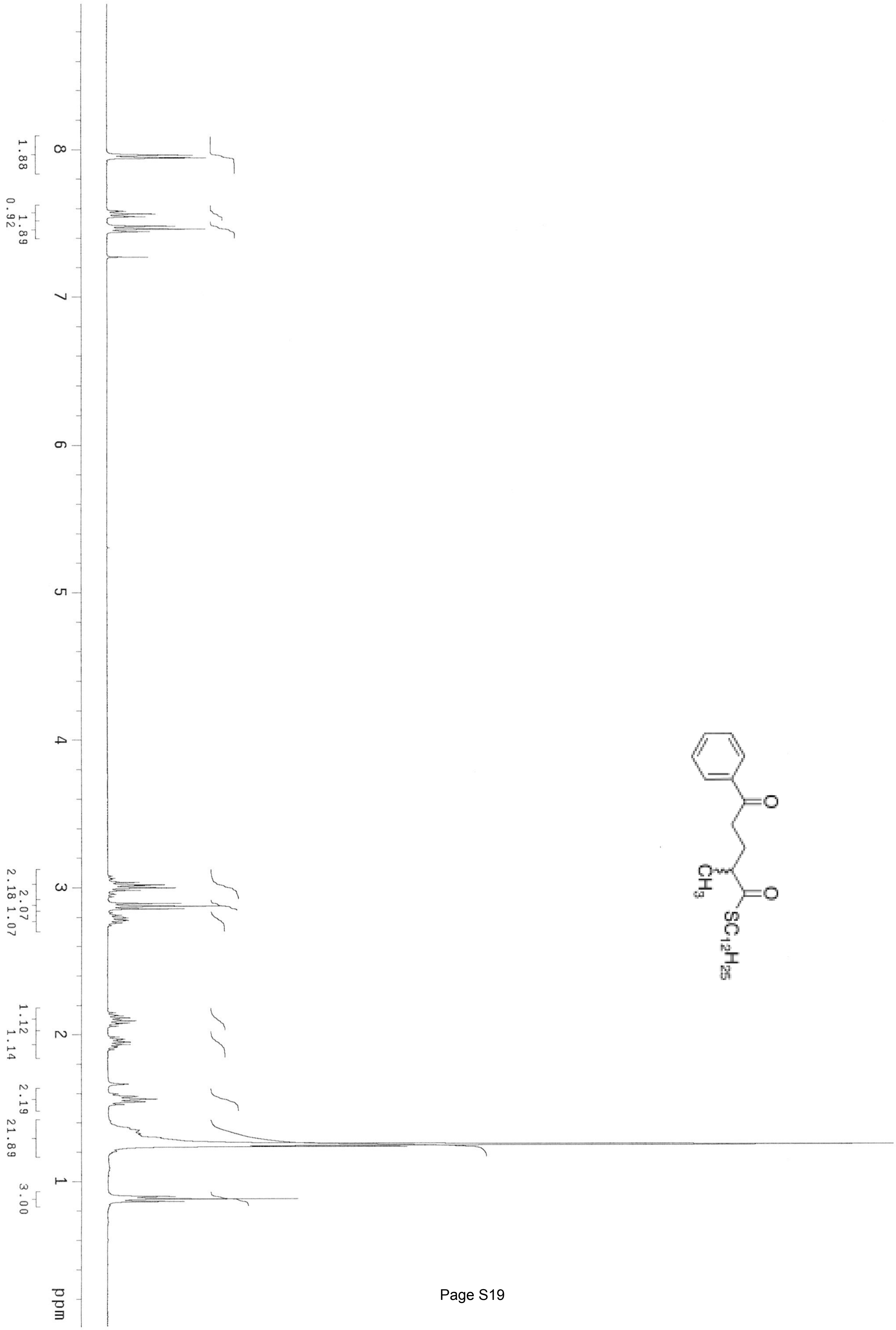

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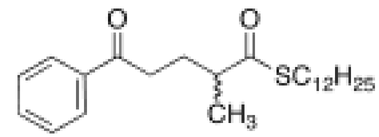
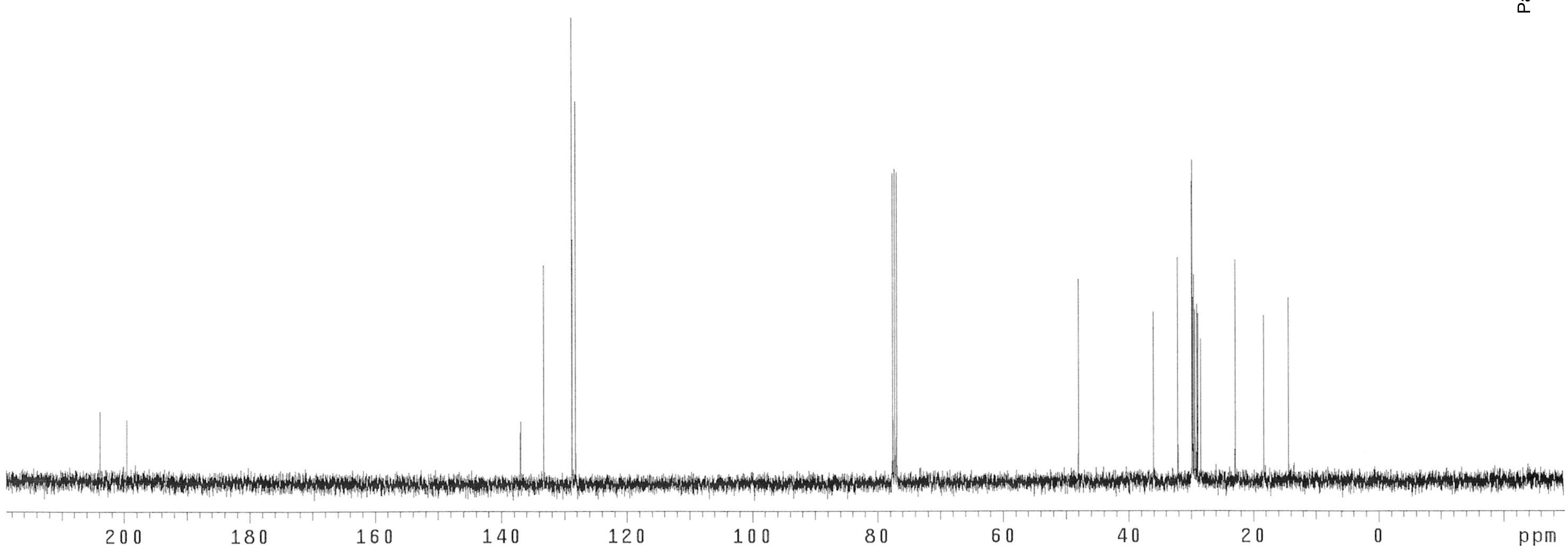
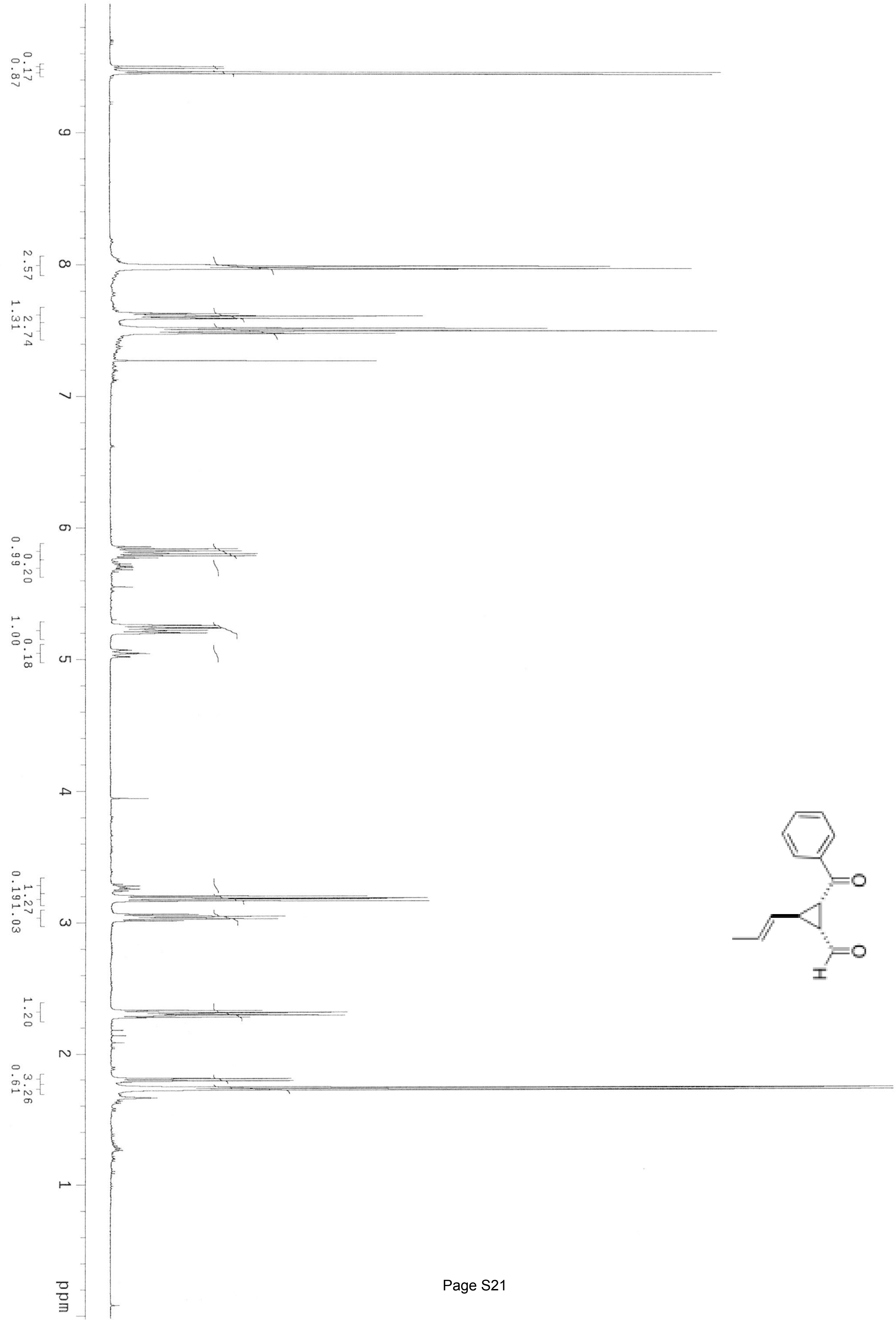
INDEX	FREQUENCY	PPM	HEIGHT
1	20502.938	203.873	11.4
2	20068.049	199.549	10.1
3	13773.607	136.959	9.7
4	13403.570	133.280	35.3
5	12951.896	128.789	75.6
6	12894.674	128.220	61.9
7	7798.846	77.549	50.2
8	7766.801	77.230	50.9
9	7734.757	76.911	50.4
10	4827.869	48.006	33.0
11	3622.388	36.020	27.7
12	3229.462	32.112	36.5
13	2999.810	29.829	48.9
14	2994.469	29.776	52.3
15	2986.840	29.700	30.0
16	2971.580	29.548	33.8
17	2950.217	29.336	28.1
18	2920.462	29.040	29.0
19	2905.203	28.888	27.4
20	2857.899	28.418	23.3
21	2302.462	22.895	36.2
22	1840.107	18.297	27.1
23	1441.840	14.337	30.0







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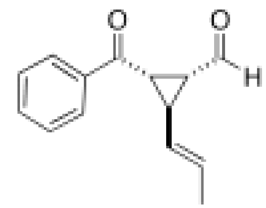
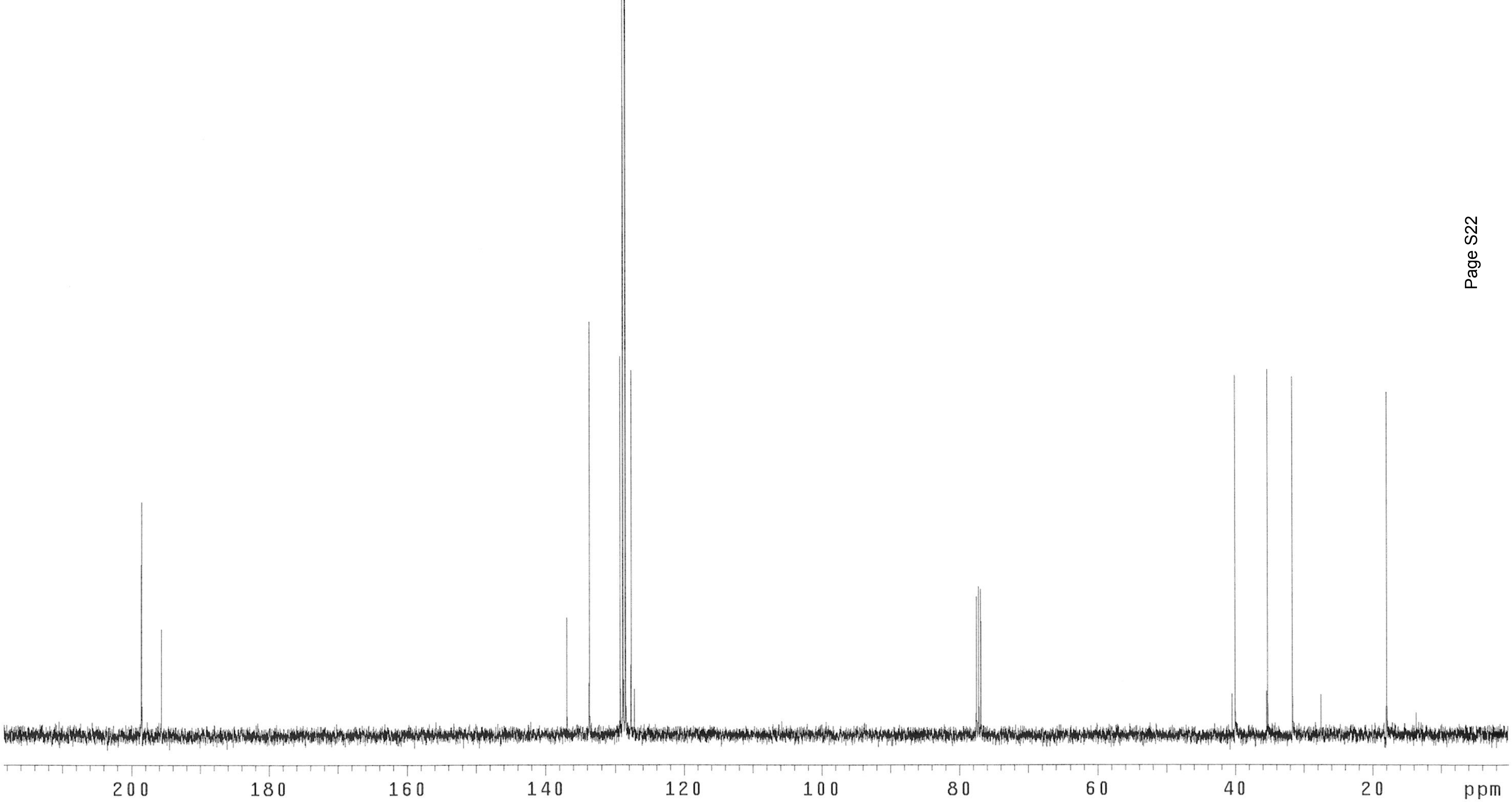
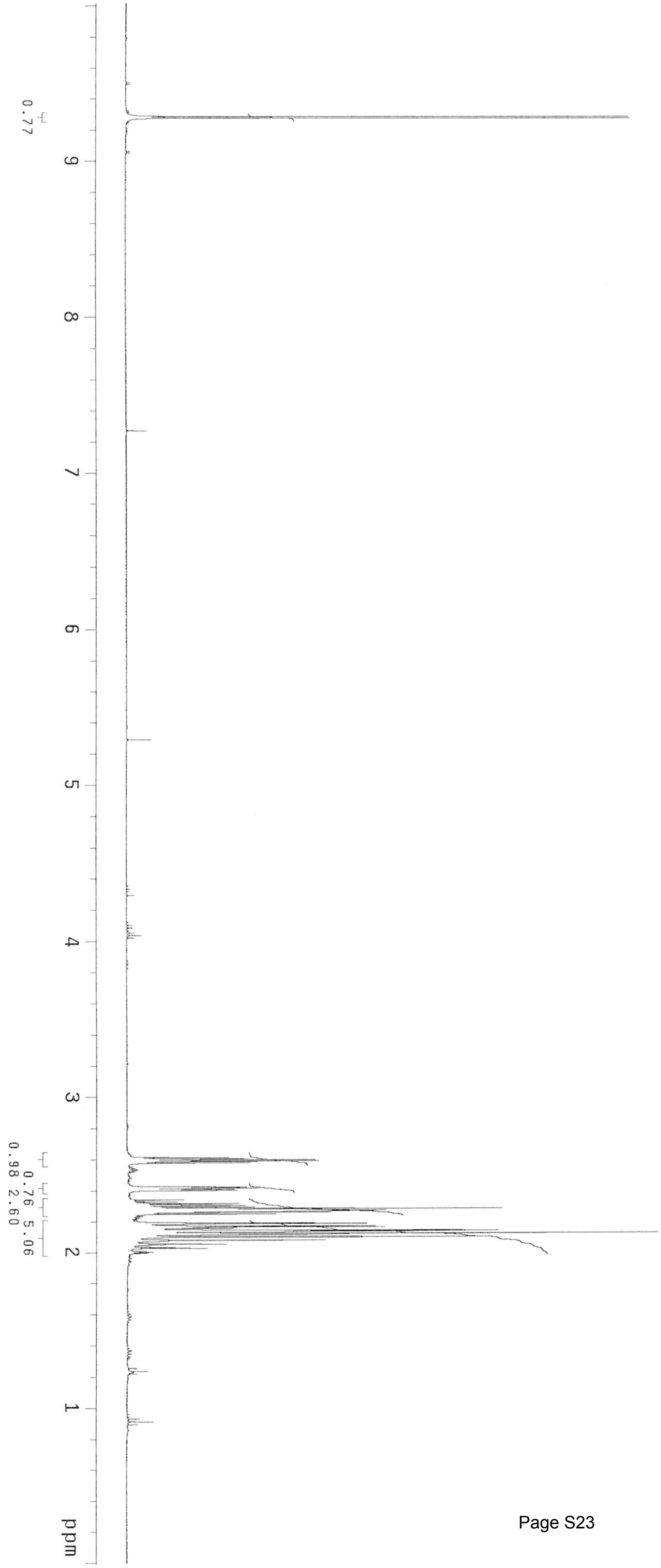
2	19674.362	195.634	18.1
3	13772.845	136.952	20.1
4	13446.297	133.705	69.9
5	12997.675	129.244	64.0
6	12958.764	128.857	139.9
7	12921.378	128.485	136.3
8	12838.215	127.658	61.7
9	7798.847	77.549	23.6
10	7766.802	77.230	25.3
11	7734.758	76.911	24.9
12	4025.996	40.033	60.8
13	3549.144	35.291	61.8
14	3182.922	31.650	60.6
15	1809.589	17.994	58.0



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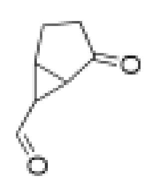

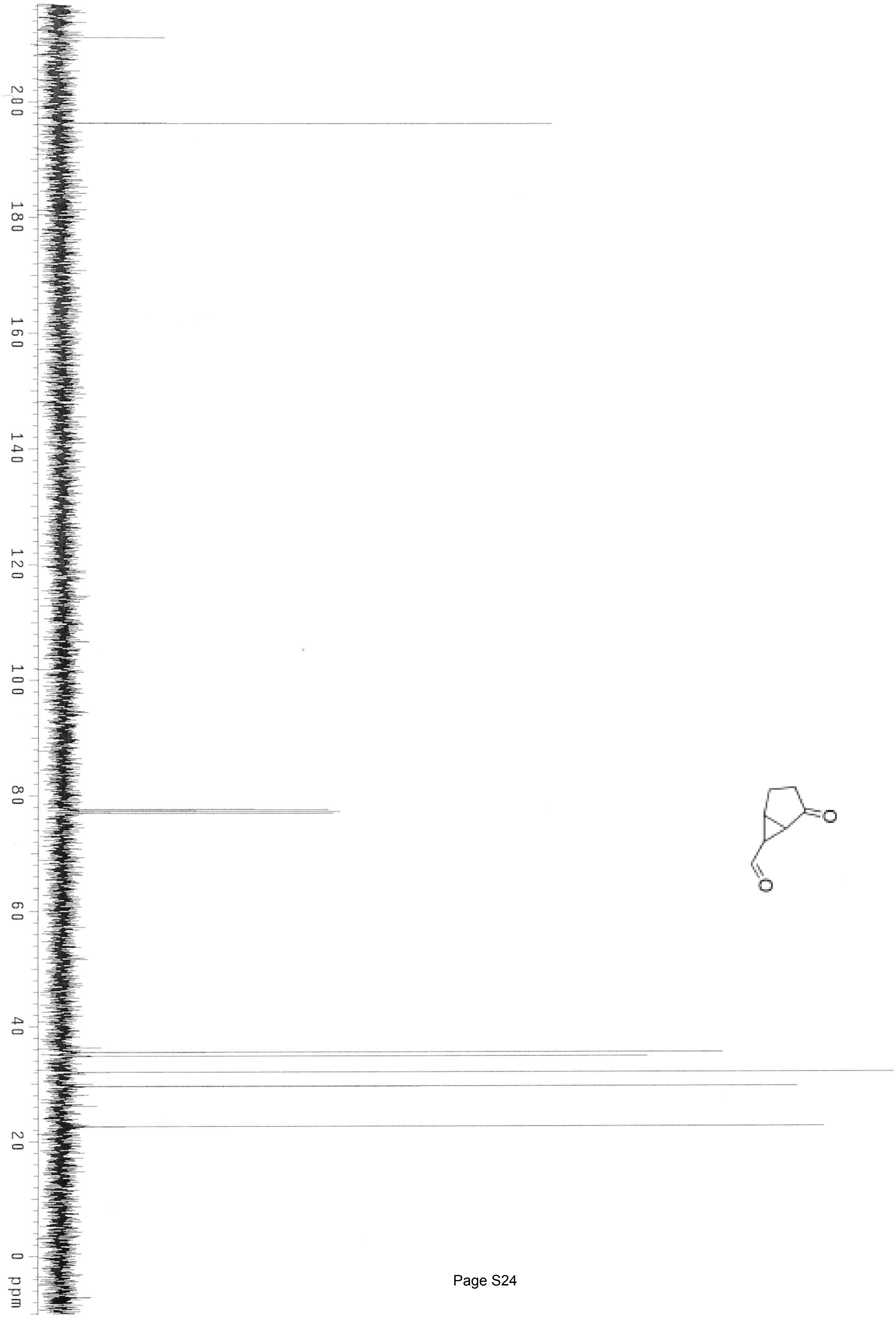
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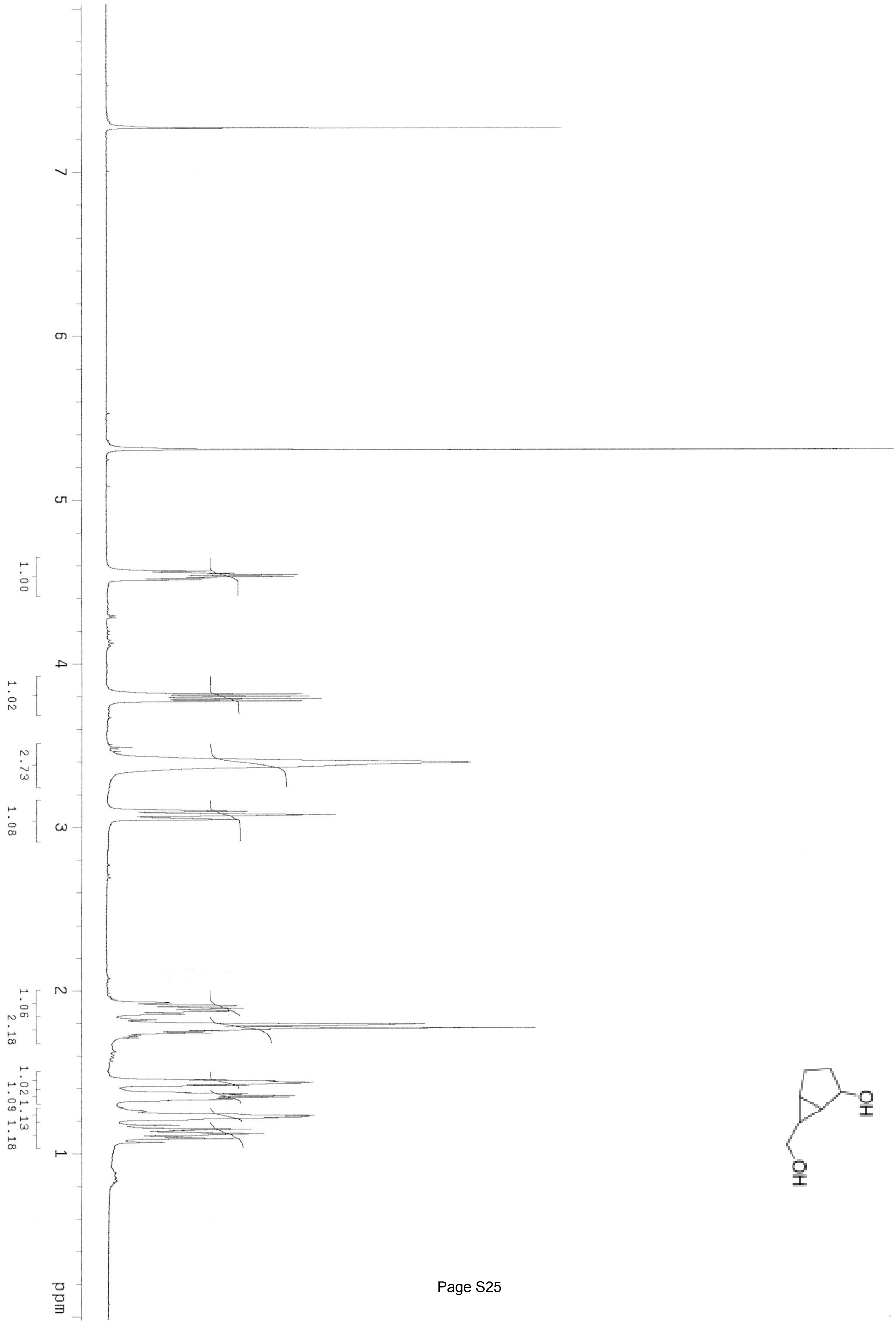
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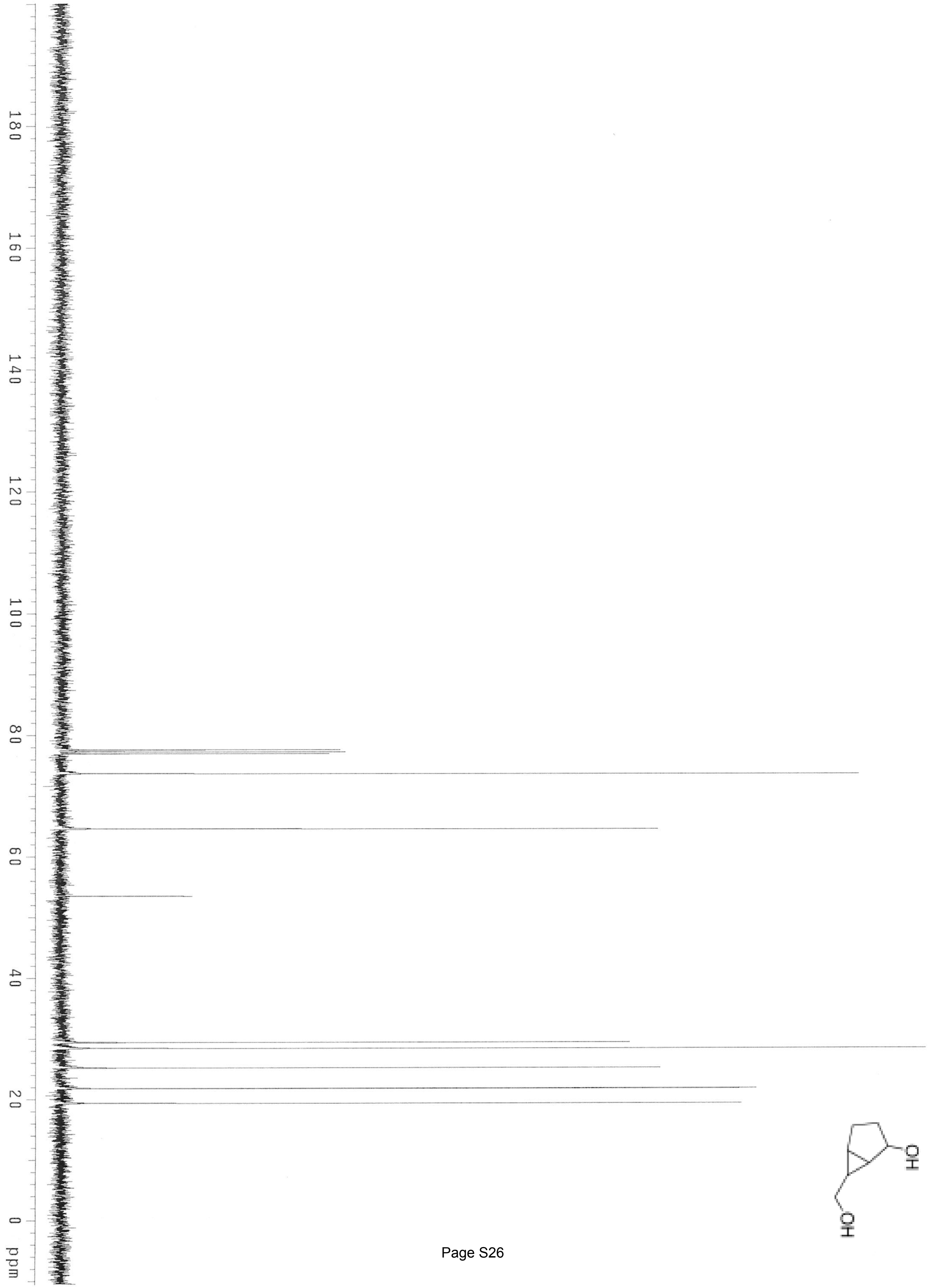
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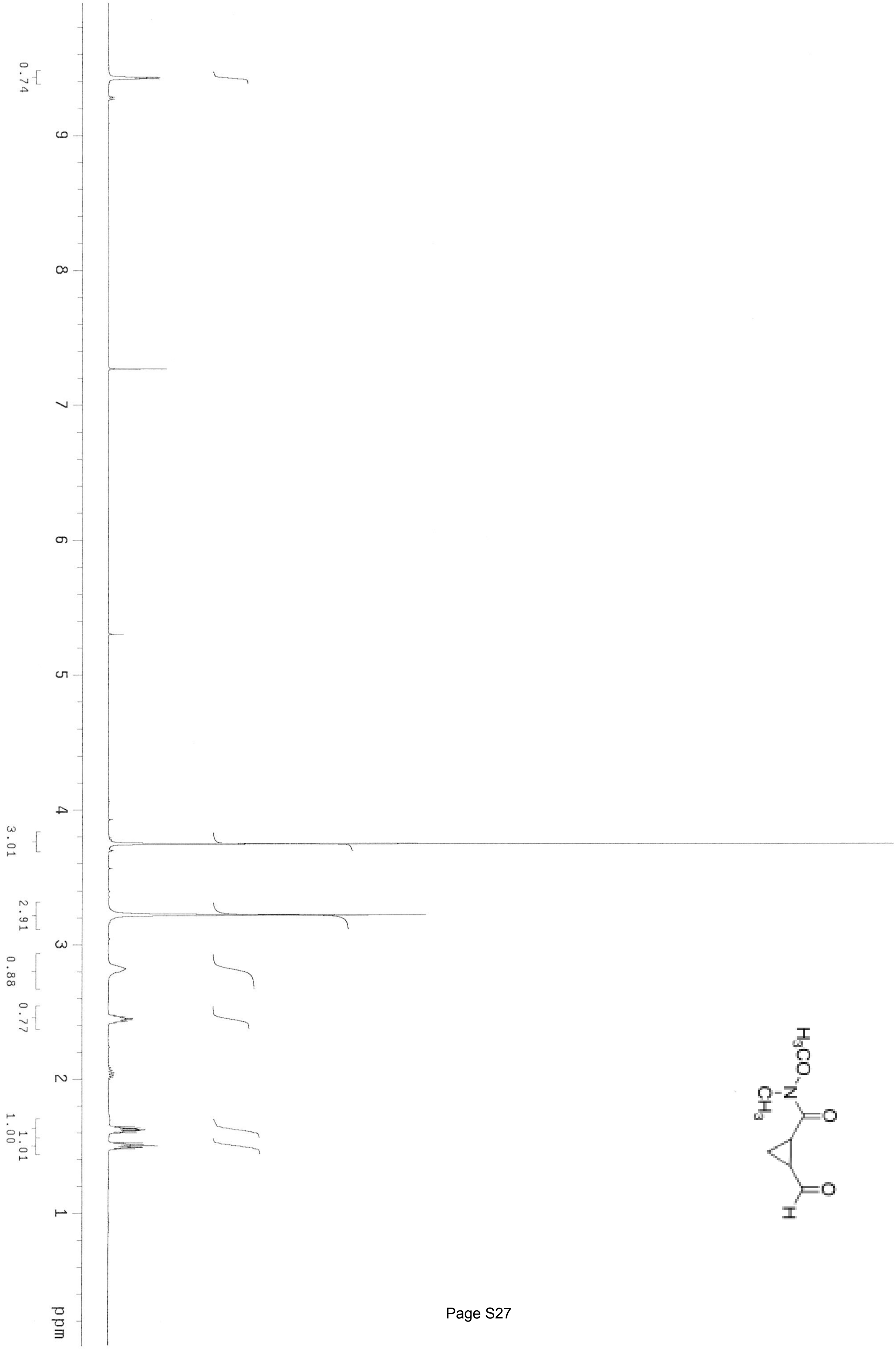

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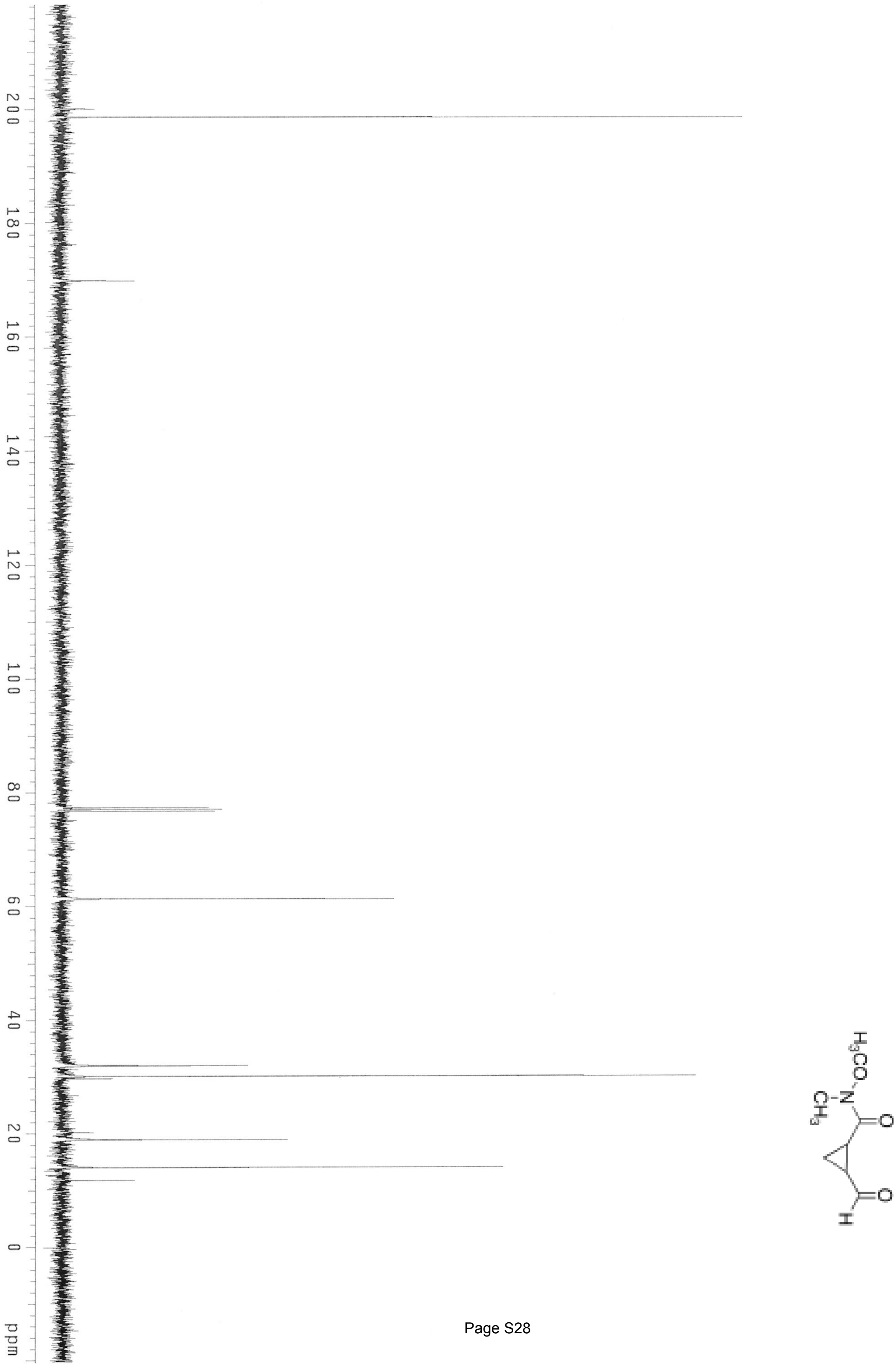

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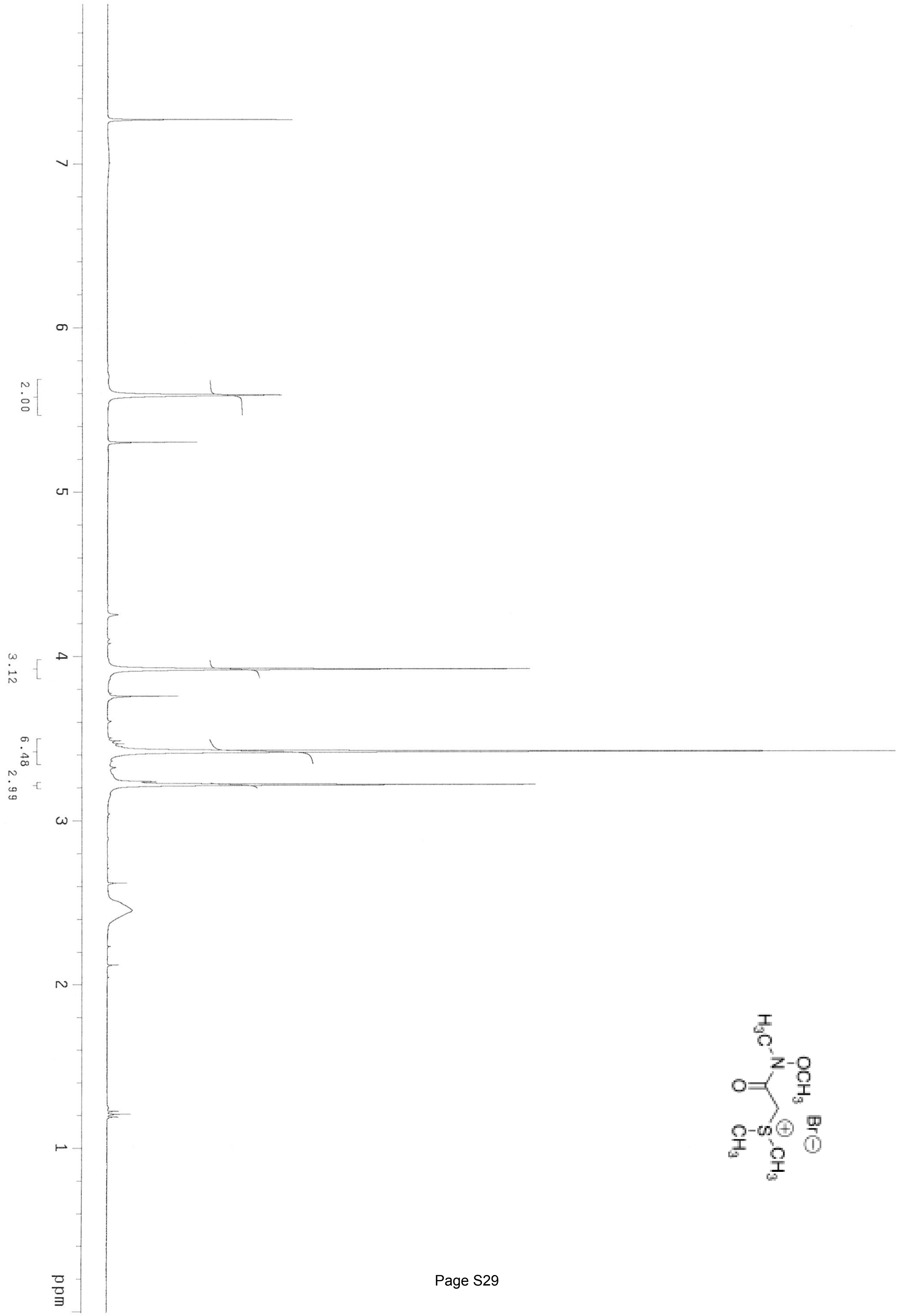

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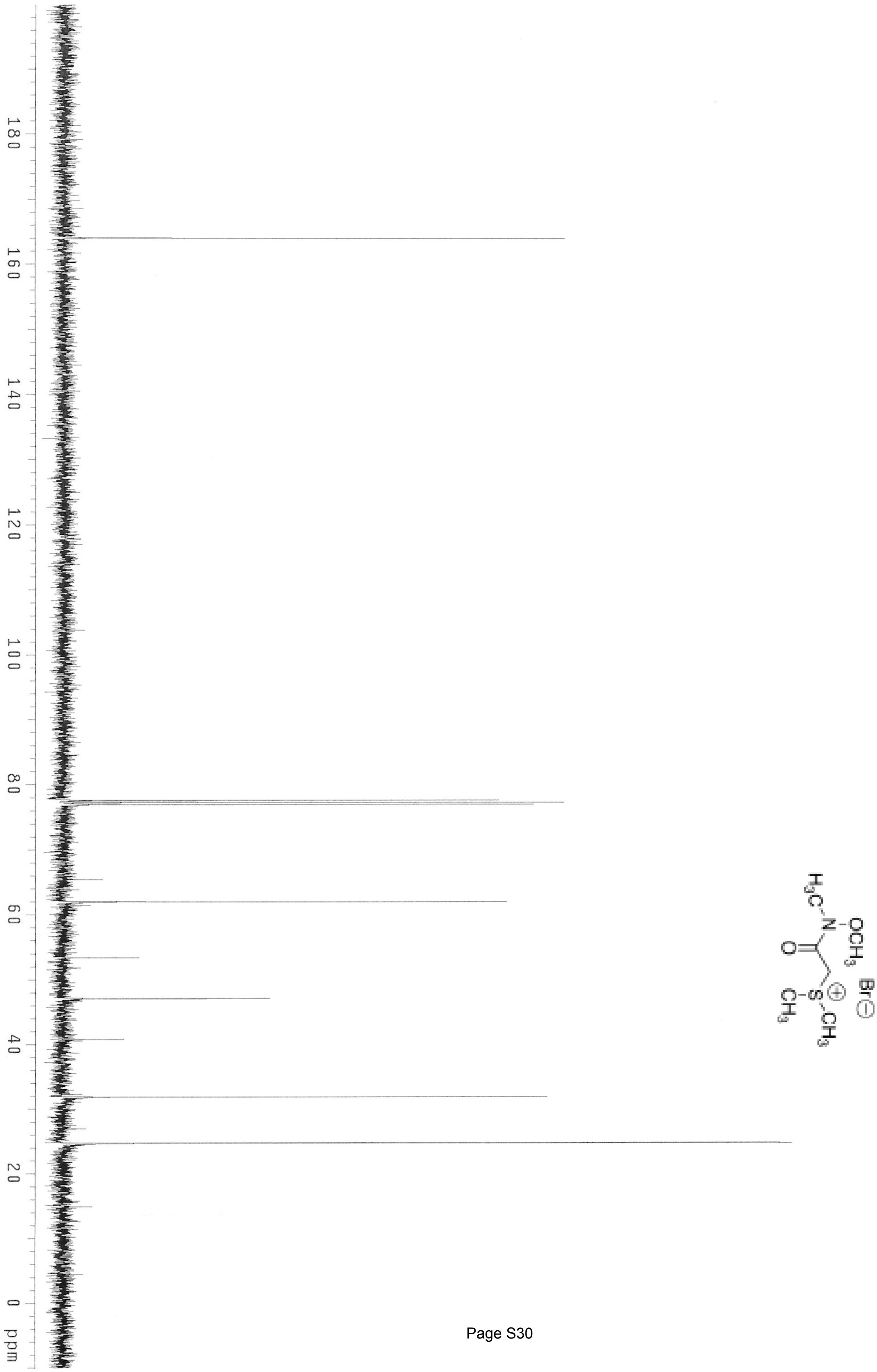
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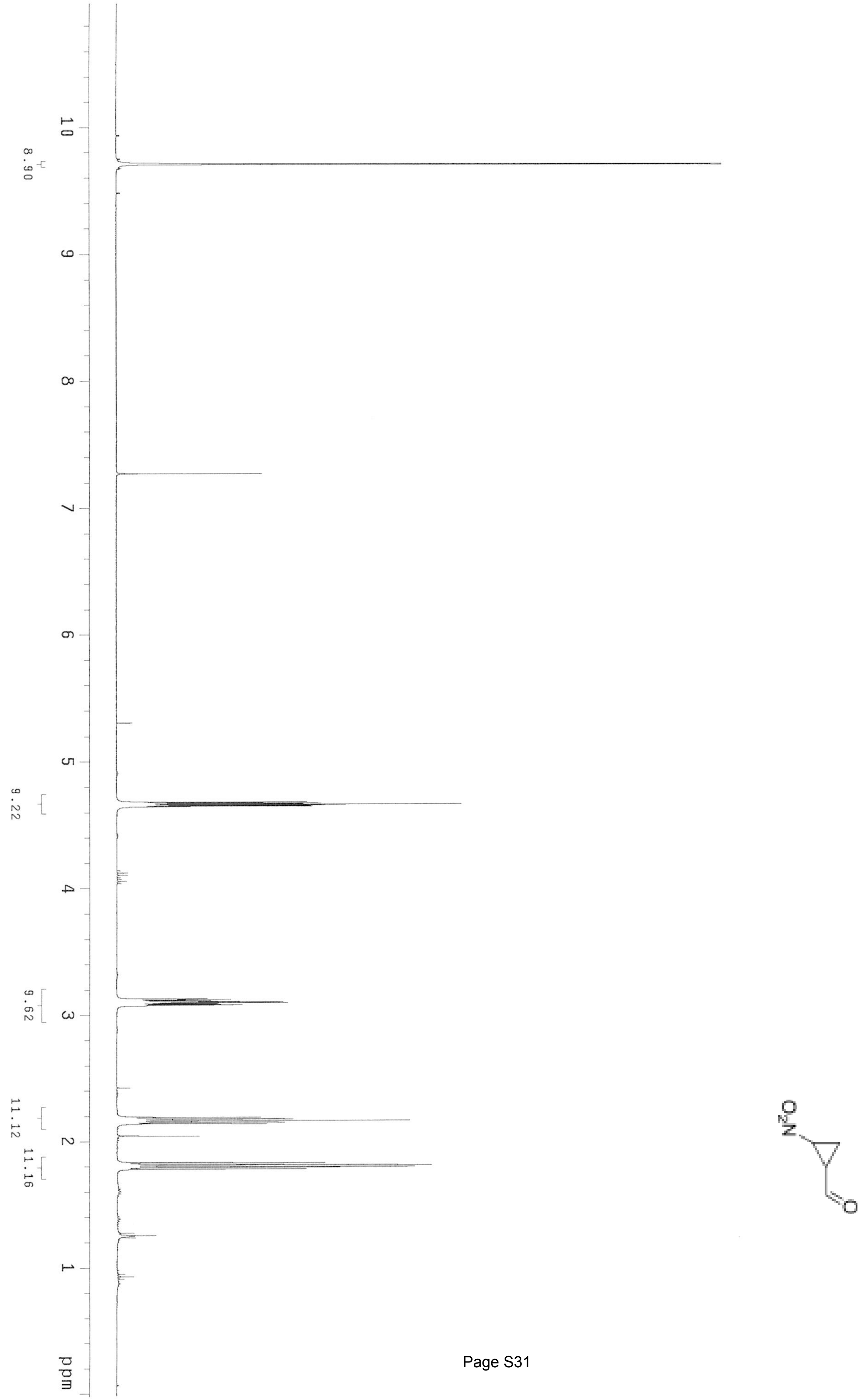
O
S
CH3
Br


10
9
8
7
6
5
4
3
2
1
ppm
8.90
9.22
9.62
11.12
11.16
O2N
O

INDEX	FREQUENCY	PPM	HEIGHT
1	19670.546	195.596	46.3
2	7798.846	77.549	65.1
3	7766.801	77.230	67.6
4	7734.757	76.911	66.5
5	6026.483	59.925	16.7
6	3182.921	31.650	68.2
7	1798.144	17.880	87.2