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***N*-bromosuccinimide/carboxylic acid combination: mild and efficient
access to dibromination of unsaturated carbonyl compounds**

Hongxun Xue, Hui Tan, Donglei Wei, Ying Wei, Shaoxia Lin, Fushun Liang,* and
Baozhong Zhao*

Department of Chemistry, Northeast Normal University, Changchun 130024, China

liangfs112@nenu.edu.cn

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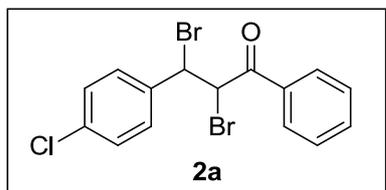
I. General

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. ^1H NMR and ^{13}C NMR spectra were recorded at 25 °C on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. Elemental analyses were measured on an E-2400 analyzer (Perkin-Elmer). Mass spectra were recorded on Agilent 1100 LCMsD mass spectrometer. All the reactions were performed under normal conditions, without the necessity for inert gas protection.

II. Synthesis and analytical data of 2a-p, 3a-c and 4a-c.

General procedure for the Synthesis of **2** (**2a** as an example): 1.0 mmol chalcone **1a** was dispensed in 2 mL THF. 2.2 mmol NBS and 0.2 mmol benzoic acid was added and stirring for 6.0 h at ambient temperature. After the starting material **1a** was consumed as indicated by TLC, the reaction mixture was poured into water (10 mL) and extracted with CH_2Cl_2 (3 \times 10 mL). The combined organic phase was washed with water (3 \times 10 mL), and dried over anhydrous MgSO_4 . The solvent was removed under reduced pressure, and the residue was purified by recrystallization in dichloromethane and petroleum ether to give compound **2a** (366 mg, 91%) as a white solid.

2,3-dibromo-3-(4-chlorophenyl)-1-phenylpropan-1-one (**2a**)

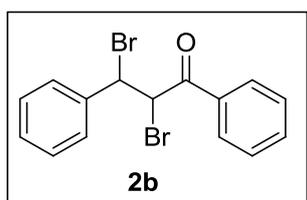


White solid. m.p. 184-186 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.60-5.63 (d, J = 11.0 Hz, 1H), 5.76-5.78 (d, J = 11.5 Hz, 1H), 7.40-7.42 (m, 2H), 7.46-7.48 (m, 2H), 7.54-7.57 (t, J = 8.0 Hz, 2H), 7.66-7.68 (d, J = 8.0 Hz, 1H), 8.08-8.10 (t, J = 8.0 Hz, 2H). ^{13}C NMR

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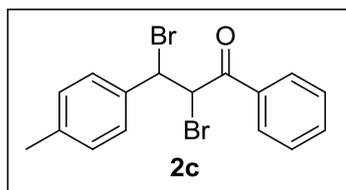
(DMSO-*d*₆, 125 MHz) δ = 48.8, 73.3, 121.5, 129.3, 129.4, 130.7, 131.2, 134.5, 135.2, 141.5, 193.8. MS calcd *m/z* 399.8, Found 401.2 [(M + 1)]⁺. Anal. Calcd for C₁₅H₁₁Br₂ClO: C, 44.76; H, 2.75; Found: C, 44.88; H, 2.72.

2,3-dibromo-1,3-diphenylpropan-1-one (2b)



White solid. m.p. 166-168 °C. ¹H NMR (CDCl₃, 500 MHz) δ = 5.64-5.66 (d, *J* = 11.5 Hz, 1H), 5.82-5.84 (d, *J* = 11.5 Hz, 1H), 7.39-7.45 (m, 3H), 7.52-7.57 (m, 4H), 7.66-7.68 (t, 1H). 8.10-8.12 (d, *J* = 8.0 Hz, 2H). ¹³C NMR (CDCl₃, 125 MHz) δ = 46.7, 49.7, 128.3, 128.8, 128.8, 128.9, 129.2, 134.1, 134.3, 138.1, 191.1. MS calcd *m/z* 365.9, Found 3676.1 [(M + 1)]⁺. Anal. Calcd for C₁₅H₁₂Br₂O: C, 48.95; H, 3.29; Found: C, 49.16; H, 3.34.

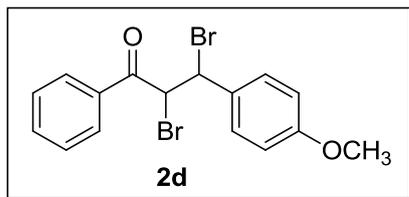
2,3-dibromo-1-phenyl-3-p-tolylpropan-1-one (2c)



White solid. 187-189 °C. ¹H NMR (CDCl₃, 500 MHz) δ = 2.39 (s, 3H), 5.63-5.65 (d, *J* = 11.0 Hz, 1H), 5.82-5.84 (d, *J* = 11.5 Hz, 1H), 7.22-7.25 (t, *J* = 5.5 Hz, 2H), 7.41-7.42 (d, *J* = 8.0 Hz, 2H), 7.53-7.56 (t, *J* = 7.5 Hz, 2H), 7.64-7.67 (t, *J* = 7.0 Hz, 1H), 8.09-8.11 (d, *J* = 7.5 Hz, 2H). ¹³C NMR (CDCl₃, 125 MHz) δ = 46.8, 49.9, 128.1, 128.8, 128.9, 129.5, 134.1, 134.4, 135.2, 135, 139.3, 191.2. MS calcd *m/z* 379.9, Found 381.0 [(M + 1)]⁺. Anal. Calcd for C₁₆H₁₄Br₂O: C, 50.29; H, 3.69; Found: C, 50.52; H, 3.62.

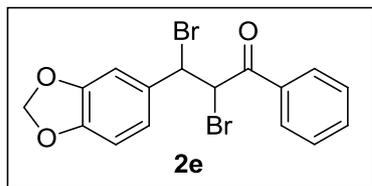
2,3-dibromo-3-(4-methoxyphenyl)-1-phenylpropan-1-one (2d)

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White solid. 149-151 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 3.98 (s, 3H), 6.02-6.04 (d, J = 10.5 Hz, 1H), 6.20-6.22 (d, J = 9.5 Hz, 1H), 6.96-6.97 (d, J = 8.5 Hz, 1H), 7.00-7.03 (t, J = 7.5 Hz, 1H), 7.35-7.39 (m, 1H), 7.45-7.46 (d, J = 7.5 Hz, 1H), 7.53-7.56 (m, 2H), 7.63-7.67 (m, 1H), 8.09-8.11 (t, J = 7.0 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 45.5, 55.9, 111.7, 120.9, 126.3, 128.9, 128.9, 134.0, 134.7, 191.5 (one carbon peak was missed due to overlap). MS calcd m/z 395.9, Found 397.2 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{16}\text{H}_{14}\text{Br}_2\text{O}_2$: C, 48.27; H, 3.54; Found: C, 48.51; H, 3.59.

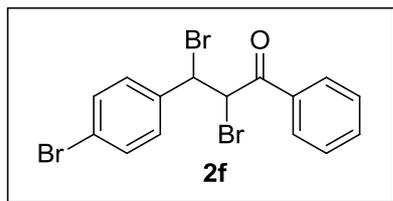
3-(benzo[d][1,3]dioxol-5-yl)-2,3-dibromo-1-phenylpropan-1-one (2e)



White solid. m.p. 194-196 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.59-5.62 (d, J = 11.0 Hz, 1H), 5.75-5.77 (d, J = 11.5 Hz, 1H), 6.03 (s, 2H), 6.81-6.83 (d, J = 7.0 Hz, 1H), 6.99-7.01 (t, J = 5.5 Hz, 2H), 7.54-7.57 (t, J = 8.0 Hz, 2H), 7.65-7.66 (d, J = 7.0 Hz, 1H), 8.08-8.10 (d, J = 7.5 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 47.0, 50.3, 101.5, 108.0, 108.2, 122.6, 128.8, 128.9, 131.8, 134.1, 134.5, 148.1, 148.4, 191.2. MS calcd m/z 409.9, Found 411.1 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{16}\text{H}_{12}\text{Br}_2\text{O}_3$: C, 46.64; H, 2.94; Found: C, 46.75; H, 2.90.

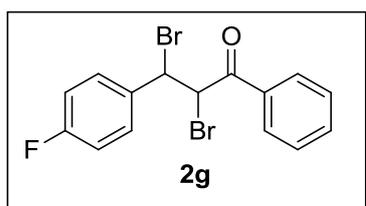
2,3-dibromo-3-(4-bromophenyl)-1-phenylpropan-1-one (2f)

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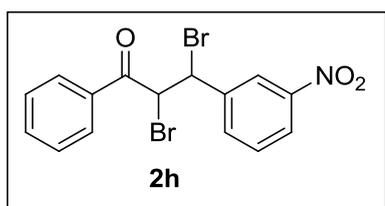
White solid. m.p. 186-188 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.59-5.61 (d, J = 11.0 Hz, 1H), 5.75-5.77 (d, J = 11.5 Hz, 1H), 7.39-7.41 (d, J = 8.5 Hz, 2H), 7.54-7.58 (m, 4H), 7.61-7.68 (m, 1H), 8.08-8.09 (d, J = 7.0 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 46.5, 48.6, 123.3, 128.8, 129.0, 129.9, 132.0, 134.2, 137.3, 190.8 (one carbon peak was missed due to overlap).. MS calcd m/z 443.8, Found 445.0 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{15}\text{H}_{11}\text{Br}_3\text{O}$: C, 40.31; H, 2.48; Found: C, 40.59; H, 2.42.

2,3-dibromo-3-(4-fluorophenyl)-1-phenylpropan-1-one (2g)



White solid. m.p. 156-158 °C . ^1H NMR (CDCl_3 , 500 MHz) δ = 5.63–5.65 (d, J = 11.0 Hz, 1H), 5.76-5.78 (d, J = 11.5 Hz, 1H), 7.10-7.14 (t, J = 8.5 Hz, 2H), 7.50-7.52 (m, 2H) , 7.53- 7.57 (m, 2H), 7.66-7.67 (d, J = 7.5 Hz, 1H), 8.09-8.10 (d, J = 7.5 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 48.8, 48.9, 115.8, 116.0, 128.9, 129.0, 130.2, 130.2, 134.2, 161.9, 163.9,191.0. MS calcd m/z 383.9, Found 385.0 (M + 1)] $^+$. Anal. Calcd for $\text{C}_{15}\text{H}_{11}\text{Br}_2\text{FO}$: C, 46.67; H, 2.87; Found: C, 46.80; H, 2.90.

2,3-dibromo-3-(3-nitrophenyl)-1-phenylpropan-1-one (2h)

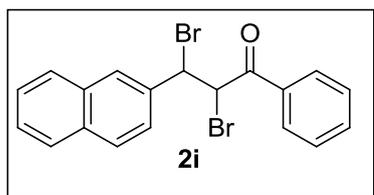


White solid. m.p. 188-190 °C . ^1H NMR (CDCl_3 , 500 MHz) δ = 5.70–5.72 (d, J = 11.0 Hz,

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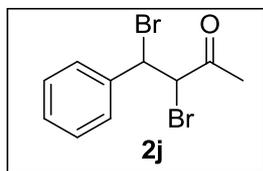
1H), 5.79-5.82 (d, $J = 11.0$ Hz, 1H), 7.57-7.65 (m, 3H), 7.68-7.71 (t, $J = 7.5$ Hz, 1H), 7.83-7.85 (d, $J = 7.5$ Hz, 1H), 8.11-8.12 (m, 2H), 8.25-8.27 (m, 1H). 8.43 (t, $J = 2.0$ Hz, 1H). ^{13}C NMR (CDCl_3 , 125 MHz) $\delta = 46.1, 47.3, 123.3, 124.1, 128.9, 129.1, 129.9, 133.9, 134.5, 134.5, 140.4, 148.4, 190.4$. MS calcd m/z 410.9, Found 412.2 $[(M + 1)]^+$.
Anal. Calcd for $\text{C}_{15}\text{H}_{11}\text{Br}_2\text{NO}_3$: C, 43.62; H, 2.68; Found: C, 43.85; H, 2.73.

2,3-dibromo-3-(naphthalen-2-yl)-1-phenylpropan-1-one (2i)



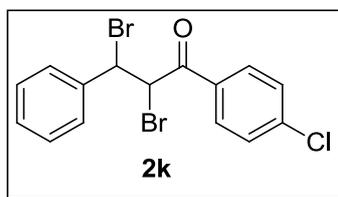
White solid. m.p. 216-218 °C. ^1H NMR (CDCl_3 , 500 MHz) $\delta = 6.11-6.13$ (d, $J = 11.0$ Hz, 1H), 6.63-6.65 (d, $J = 11.5$ Hz, 1H), 6.74 (d, $J = 9.0$ Hz, 1H), 7.54-7.60 (m, 4H), 7.65-7.70 (m, 2H), 7.90-7.93 (m, 3H), 8.16-8.18 (d, $J = 7.5$ Hz, 2H), 8.26-8.28 (d, $J = 8.5$ Hz, 1H). ^{13}C NMR (CDCl_3 , 125 MHz) $\delta = 44.1, 45.9, 122.5, 125.3, 125.7, 126.2, 127.0, 128.9, 128.9, 129.0, 129.8, 130.9, 133.7, 133.7, 134.1, 134.4, 191.2$. MS calcd m/z 415.9, Found 417.1 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{19}\text{H}_{14}\text{Br}_2\text{O}$: C, 54.58; H, 3.37; Found: C, 54.73; H, 3.45.

3,4-dibromo-4-phenylbutan-2-one (2j)



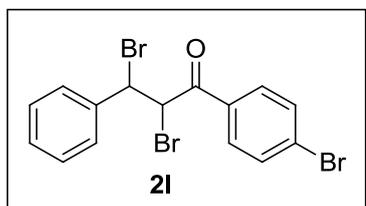
White solid. m.p. 200-202 °C. ^1H NMR (CDCl_3 , 500 MHz) $\delta = 2.49$ (s, 6H), 3.44 (s, 3H), 4.92-4.94 (d, $J = 11.5$ Hz, 1H), 5.30-5.33 (d, $J = 11.5$ Hz, 1H), 7.38-7.41 (m, 5H). ^{13}C NMR (CDCl_3 , 125 MHz) $\delta = 26.6, 49.4, 52.7, 128.0, 128.8, 129.3, 137.7, 198.4$. MS calcd m/z 303.9, Found 305.0 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{10}\text{H}_{10}\text{Br}_2\text{O}$: C, 39.25; H, 3.29; Found: C, 39.46; H, 3.35.

2,3-dibromo-1-(4-chlorophenyl)-3-phenylpropan-1-one (2k)



White solid. m.p. 203-205 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.61-5.63 (d, J = 11.5 Hz, 1H), 5.75-5.77 (d, J = 11.5 Hz, 1H), 7.39-7.45 (m, 3H), 7.51-7.54 (m, 4H), 8.03-8.05 (t, J = 2.0 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 46.6, 49.6, 128.3, 128.8, 129.3, 130.2, 132.6, 137.9, 140.8, 190.0 (one carbon peak was missed due to overlap). MS calcd m/z 399.8, Found 401.1 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{15}\text{H}_{11}\text{Br}_2\text{ClO}$: C, 44.76; H, 2.75; Found: C, 44.55; H, 2.70.

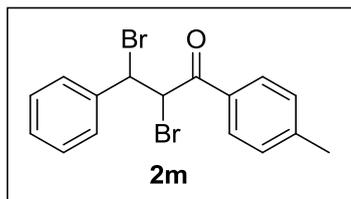
2,3-dibromo-1-(4-bromophenyl)-3-phenylpropan-1-one (2l)



White solid. m.p. 199-201 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.61-5.63 (d, J = 11.5 Hz, 1H), 5.74-5.76 (d, J = 11.5 Hz, 1H), 7.37-7.44 (m, 3H), 7.50-7.52 (d, J = 7.5 Hz, 2H), 7.68-7.01 (d, J = 8.5 Hz, 2H), 7.95-7.96 (d, J = 9.0 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 46.7, 49.6, 128.3, 128.8, 129.3, 129.5, 130.3, 132.3, 133.1, 138.0, 190.2. MS calcd m/z 443.8, Found 445.1 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{15}\text{H}_{11}\text{Br}_3\text{O}$: C, 40.31; H, 2.48; Found: C, 40.16; H, 2.42.

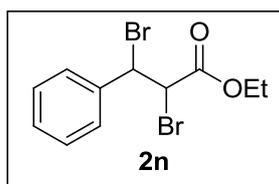
2,3-dibromo-3-phenyl-1-(p-tolyl)propan-1-one (2m)

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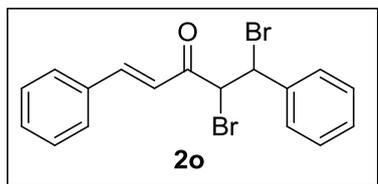
White solid. m.p. 188-190 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 3.46 (s, 3H), 5.63-5.65 (d, J = 11.0 Hz, 1H), 5.80-5.83 (d, J = 11.0 Hz, 1H), 7.34-7.44 (m, 5H), 7.52-7.53 (d, J = 7.0 Hz, 2H), 8.00-8.01 (d, J = 8.5 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 21.8, 46.7, 49.8, 128.3, 128.8, 129.0, 129.2, 129.7, 131.8, 138.3, 145.3, 190.7. MS calcd m/z 379.9, Found 381.0 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{16}\text{H}_{14}\text{Br}_2\text{O}$: C, 50.29; H, 3.69; Found: C, 50.42; H, 3.75.

ethyl 2,3-dibromo-3-phenylpropanoate (2n)



White solid. m.p. 89-91 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 1.36-1.39 (t, J = 7.0 Hz, 3H), 4.34-4.38 (m, 2H), 4.84-4.87 (d, J = 12.0 Hz, 1H), 5.36-5.38 (d, J = 12.0 Hz, 1H), 7.35-7.42 (m, 5H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 13.9, 47.0, 50.7, 62.6, 128.0, 128.9, 129.3, 137.6, 167.7. MS calcd m/z 333.9, Found 335.2 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{11}\text{H}_{12}\text{Br}_2\text{O}_2$: C, 39.32; H, 3.60; Found: C, 39.54; H, 3.65.

(E)-4,5-dibromo-1,5-diphenylpent-1-en-3-one (2o)

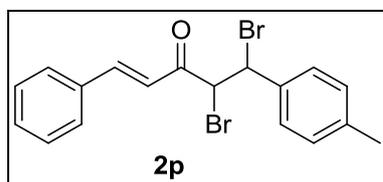


White solid. m.p. 150-152 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.21-5.24 (d, J = 11.5 Hz, 1H), 5.48-5.50 (d, J = 11.5 Hz, 1H), 6.96-6.99 (d, J = 16 Hz, 1H), 7.38-7.49 (m, 8H), 7.64-7.66 (m, 2H), 7.86-7.89 (d, J = 16 Hz, 1H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 49.4, 51.5, 122.1, 128.1, 128.1, 128.7, 128.8, 128.8, 129.0, 129.2, 131.2, 133.9, 138.1,

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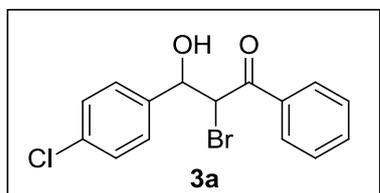
146.0, 189.8. MS calcd m/z 391.9, Found 393.0 $[(M + 1)]^+$. Anal. Calcd for $C_{17}H_{14}Br_2O$:
C, 51.81; H, 3.58; Found: C, 51.92; H, 3.66.

(E)-4,5-dibromo-1-phenyl-5-(p-tolyl)pent-1-en-3-one (2p)



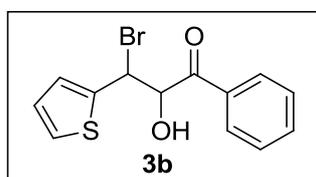
White solid. m.p. 178-180 °C. 1H NMR ($CDCl_3$, 500 MHz) δ = 2.38 (s, 3H), 5.21-5.23 (d, J = 11.5 Hz, 1H), 5.47-5.49 (d, J = 11.5 Hz, 1H), 6.90-6.99 (m, 1H), 7.22-7.26 (m, 2H), 7.36-7.38 (d, J = 8.0 Hz, 2H), 7.44-7.45 (m, 3H), 7.64-7.66 (m, 2H), 7.85-7.88 (d, J = 16 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ = 21.3, 49.6, 51.6, 122.0, 128.0, 128.7, 129.0, 129.6, 131.2, 133.9, 135.1, 139.3, 146.0, 189.9. MS calcd m/z 405.9, Found 407.0 $[(M + 1)]^+$. Anal. Calcd for $C_{18}H_{16}Br_2O$: C, 52.97; H, 3.95; Found: C, 52.72; H, 3.89.

2-bromo-3-(4-chlorophenyl)-3-hydroxy-1-phenylpropan-1-one (3a)



White solid. 1H NMR ($CDCl_3$, 500 MHz) δ = 3.45-3.46 (d, J = 5.0 Hz, 1H), 5.12-5.14 (d, J = 11.5 Hz, 1H), 5.29-5.32 (m, 1H), 7.36-7.38 (d, J = 8.5 Hz, 2H), 7.49-7.54 (m, 4H), 7.62-7.65 (t, J = 7.5 Hz, 1H), 8.00-8.02 (t, J = 7.0 Hz, 2H). MS calcd m/z 337.9, Found 339.2 $[(M + 1)]^+$. Anal. Calcd for $C_{15}H_{12}BrClO_2$: C, 53.05; H, 3.56; Found: C, 53.30; H, 3.64.

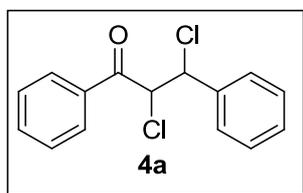
3-bromo-2-hydroxy-1-phenyl-3-(thiophen-2-yl)propan-1-one (3b)



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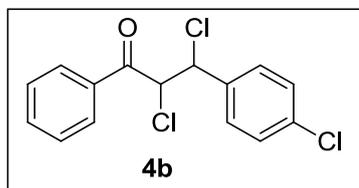
White solid. m.p. 101-103 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 3.08-3.81 (d, J = 5.5 Hz, 1H), 5.25-5.27 (d, J = 8.0 Hz, 1H), 5.25-5.61 (m, 1H), 6.98-7.00 (m, 1H), 7.14-7.15 (d, J = 3.0 Hz, 1H), 7.30-7.31 (m, 1H), 7.47-7.50 (t, J = 7.5 Hz, 2H), 7.59-7.62 (t, J = 7.5 Hz, 1H), 8.00-8.02 (t, J = 8.0 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 47.9, 71.2, 125.6, 126.3, 126.6, 128.8, 128.9, 134.2, 134.3, 142.8, 194.4. MS calcd m/z 309.9, Found 311.4 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{13}\text{H}_{11}\text{BrO}_2\text{S}$: C, 50.17; H, 3.56; Found: C, 50.30; H, 3.62.

2,3-dichloro-1,3-diphenylpropan-1-one (4a)



White solid. m.p. 117-119 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.46-5.48 (d, J = 10.5 Hz, 1H), 5.49-5.51 (d, J = 10.5 Hz, 1H), 7.41-7.46 (m, 3H), 7.45-7.47 (m, 2H), 7.52-7.57 (m, 4H), 7.65-7.68 (t, J = 7.5 Hz, 1H), 8.08-8.10 (t, J = 7.5 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 56.9, 60.0, 60.6, 63.5, 127.8, 128.1, 128.3, 128.4, 128.6, 128.7, 128.8, 128.9, 129.1, 129.3, 129.9, 134.1, 134.2, 134.6, 137.0, 191.3. MS calcd m/z 278.0, Found 279.3 $[(M + 1)]^+$. Anal. Calcd for $\text{C}_{15}\text{H}_{12}\text{Cl}_2\text{O}$: C, 64.54; H, 4.33; Found: C, 64.76; H, 4.41.

2,3-dichloro-3-(4-chlorophenyl)-1-phenylpropan-1-one (4b)

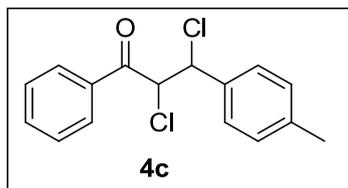


White solid. m.p. 180-183 °C. ^1H NMR (CDCl_3 , 500 MHz) δ = 5.42-5.44 (d, J = 10.5 Hz, 1H), 5.45-5.47 (d, J = 10.5 Hz, 1H), 7.40-7.42 (m, 2H), 7.45-7.47 (m, 2H), 7.54-7.57 (m, 2H), 7.66-7.69 (m, 1H), 8.07-8.08 (t, J = 7.5 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz) δ = 56.7, 59.1, 128.9, 128.9, 129.0, 129.6, 134.3, 135.2, 135.5, 190.9 (one carbon peak

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was missed due to overlap). MS calcd m/z 311.9, Found 313.2 $[(M + 1)]^+$. Anal. Calcd for $C_{15}H_{11}Cl_3O$: C, 57.45; H, 3.54; Found: C, 57.65; H, 3.61.

2,3-dichloro-1-phenyl-3-(p-tolyl)propan-1-one (4c)

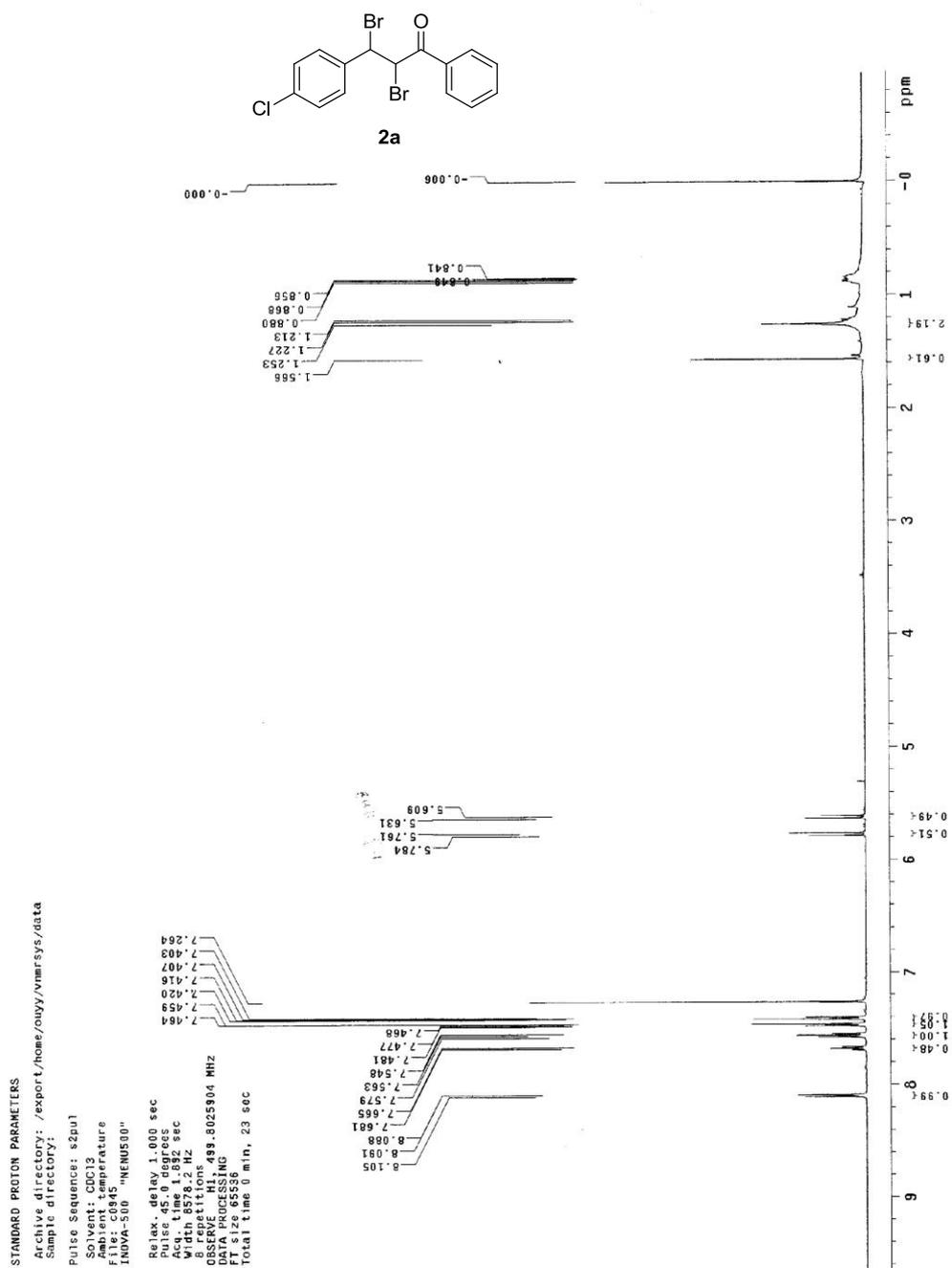


White solid. m.p. 172-174 °C. 1H NMR ($CDCl_3$, 500 MHz) 2.39 (s, 3H), 5.44-5.46 (d, $J = 10.5$ Hz, 1H), 5.48-5.51 (d, $J = 10.5$ Hz, 1H), 7.24-7.25 (d, $J = 9.5$ Hz, 2H), 7.40-7.42 (d, $J = 8.0$ Hz, 2H), 7.53-7.56 (t, $J = 8.0$ Hz, 2H), 7.64-7.67 (m, 1H), 8.07-8.09 (m, 2H). MS calcd m/z 292.0, Found 293.3 $[(M + 1)]^+$. Anal. Calcd for $C_{16}H_{14}Cl_2O$; C, 65.55; H, 4.81; Found: C, 65.32; H, 4.73.

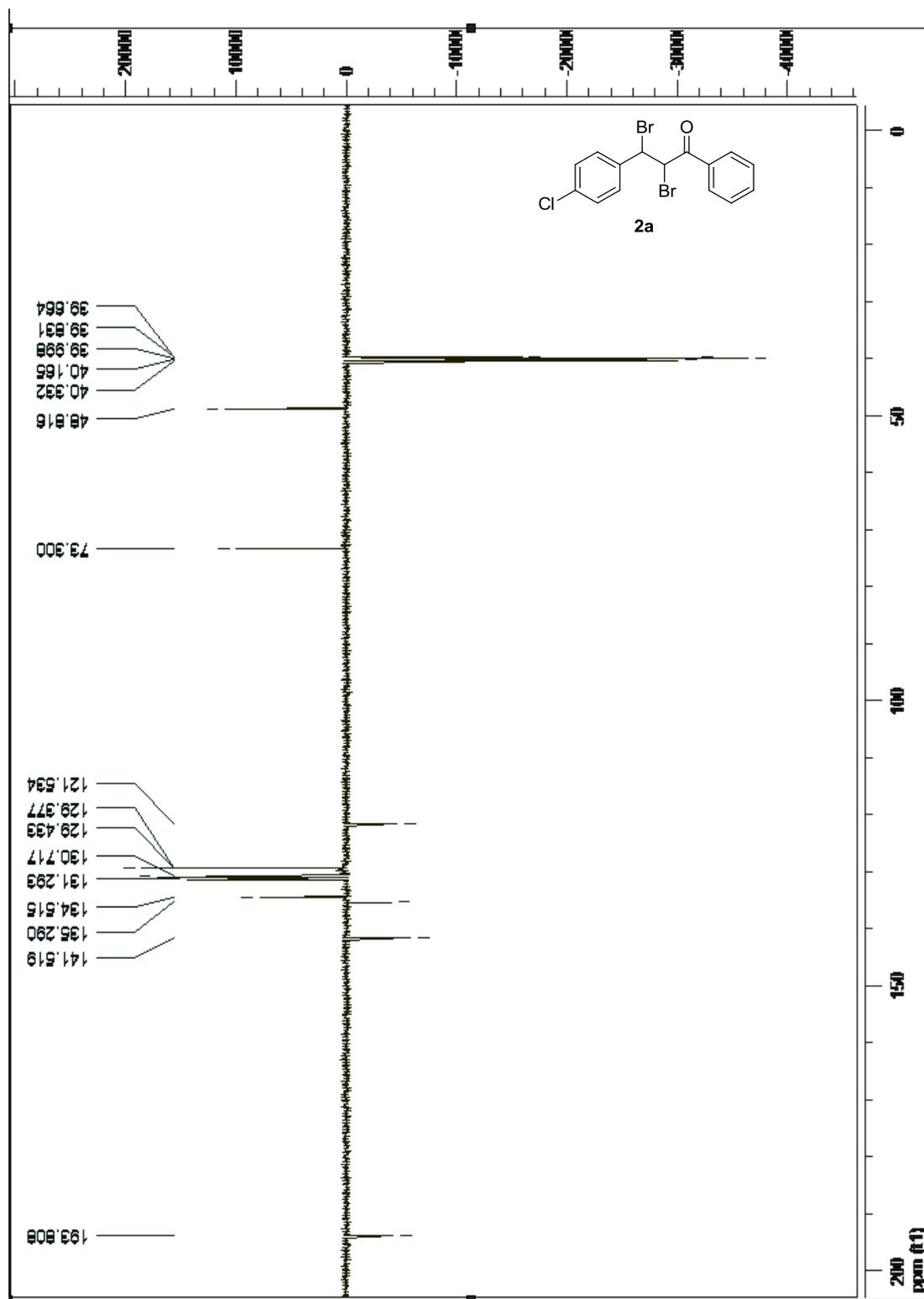
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III. Copies of ^1H and ^{13}C NMR spectra for compounds 2a-p, 3a-c and 4a-c.

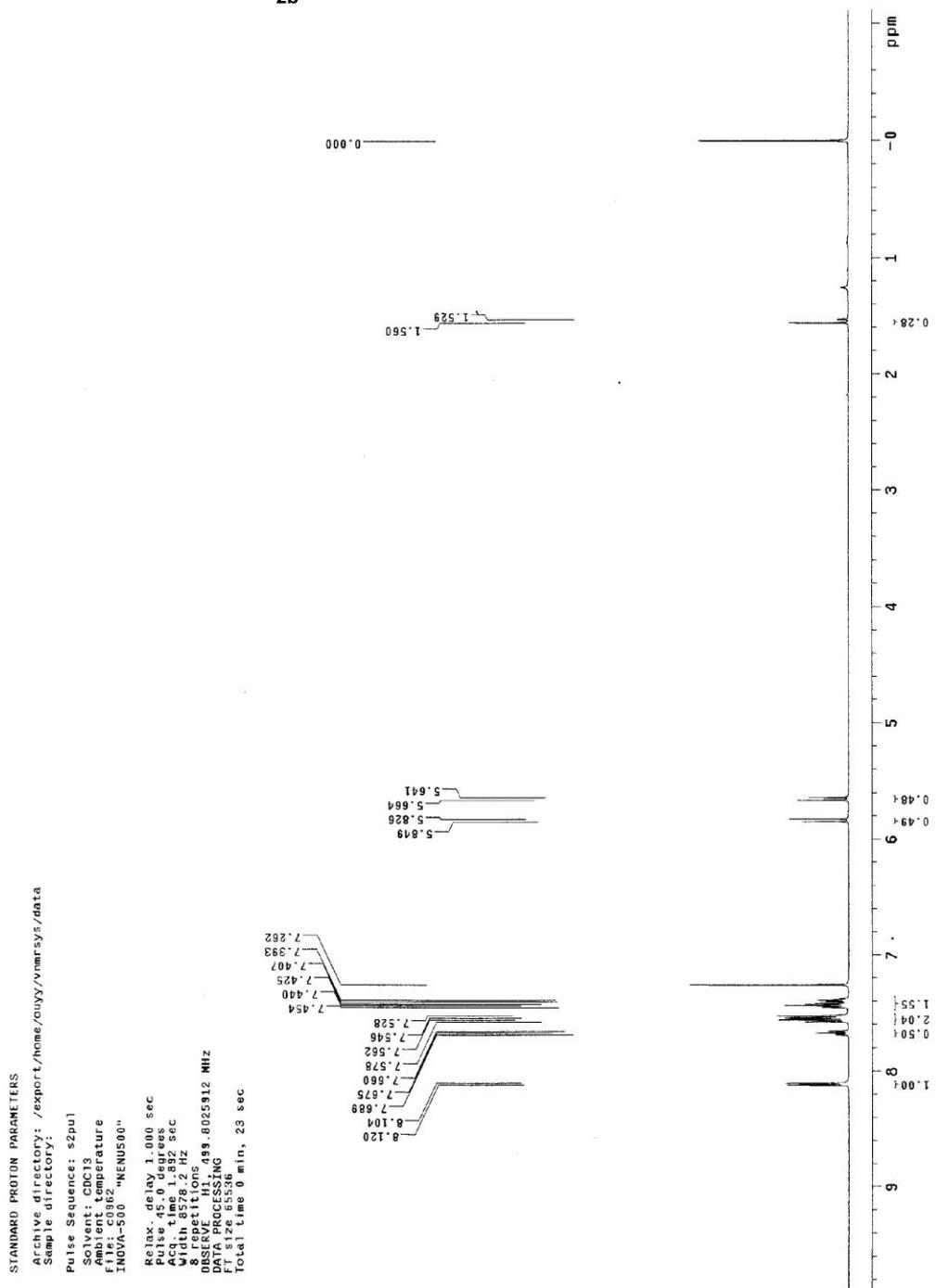
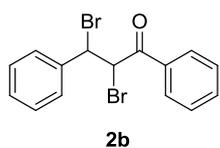
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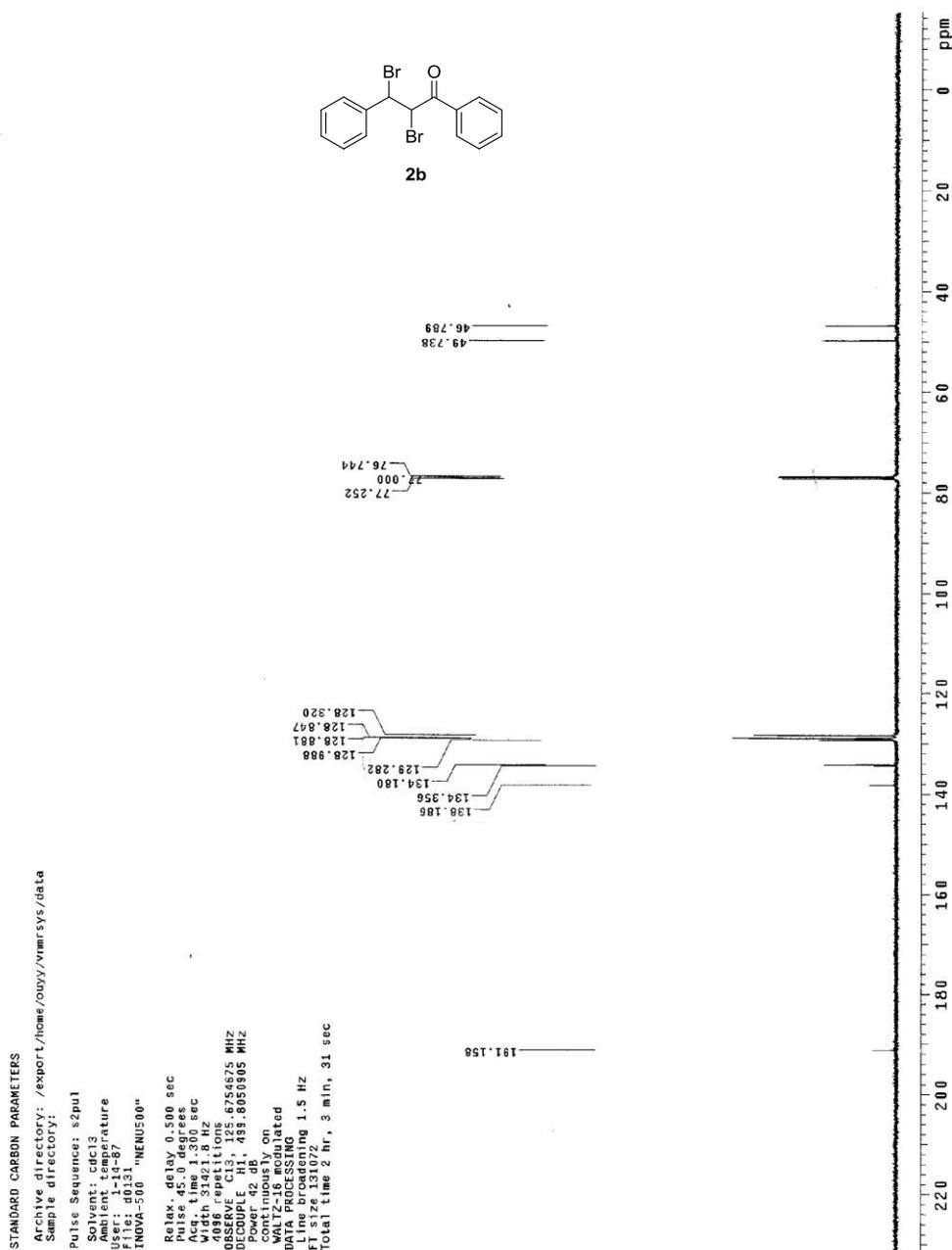
Electronic Supplementary Material (ESI) for RSC Advances
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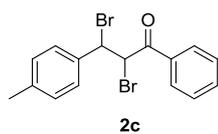
Electronic Supplementary Material (ESI) for RSC Advances
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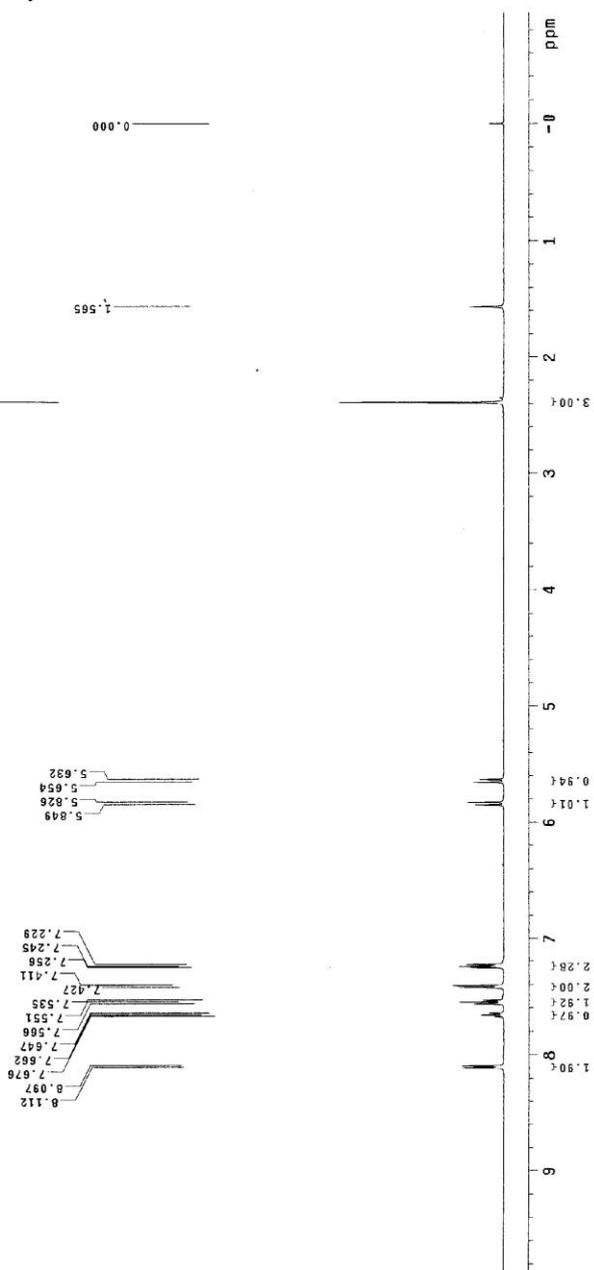
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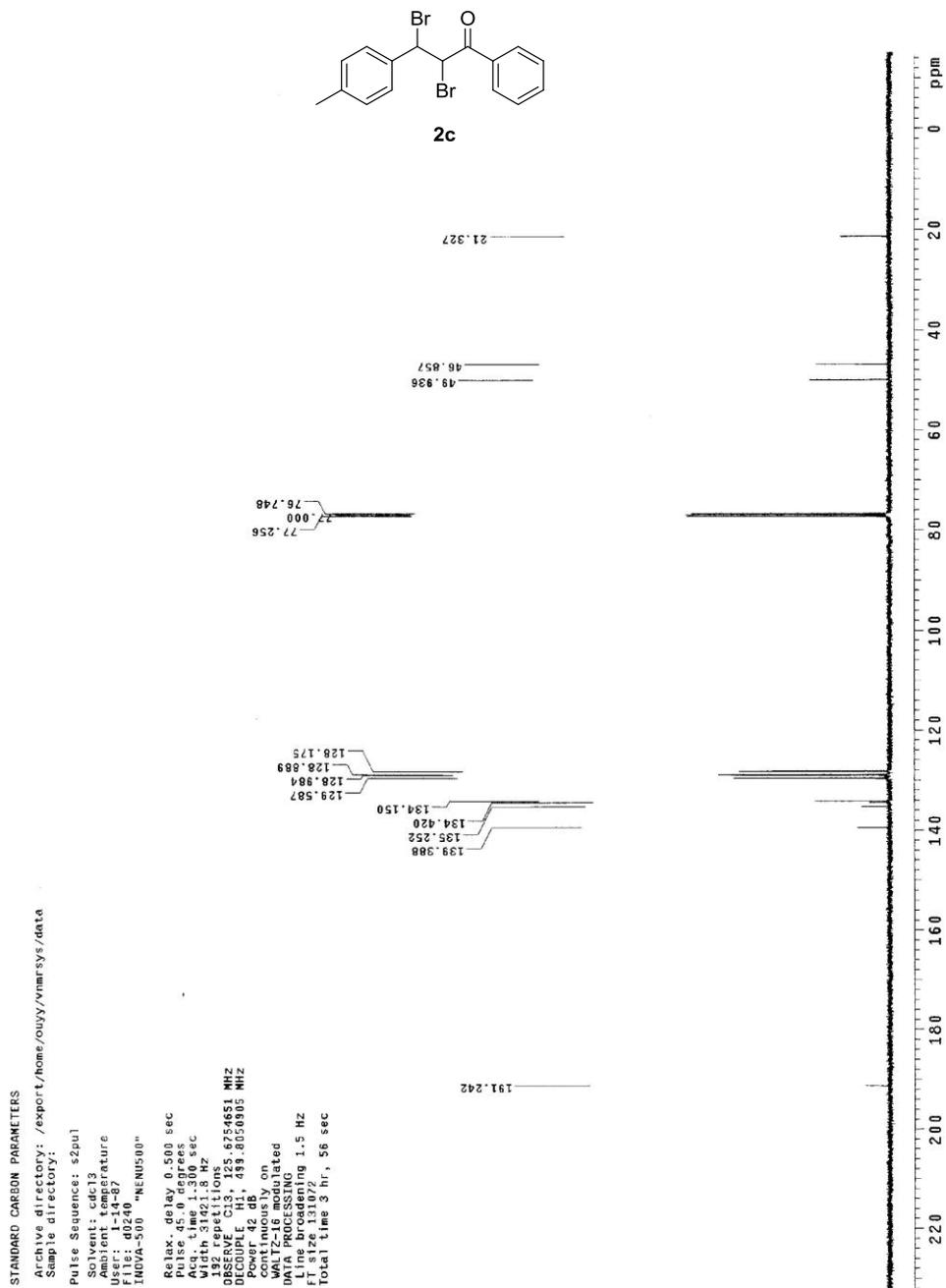
Electronic Supplementary Material (ESI) for RSC Advances
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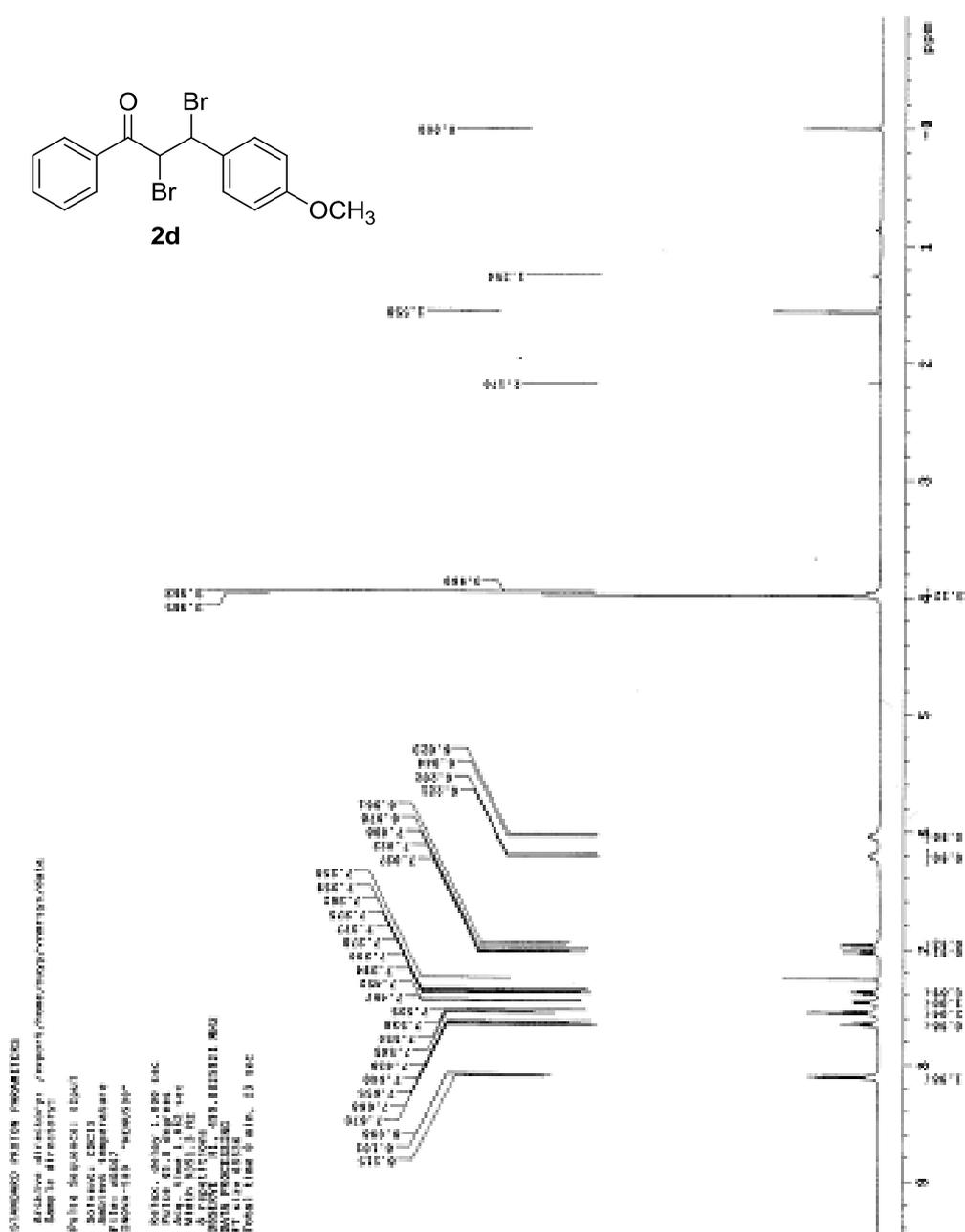
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Ambient temperature
File: c0456
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DATA PROCESSING
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Total time: 0 min, 23 sec



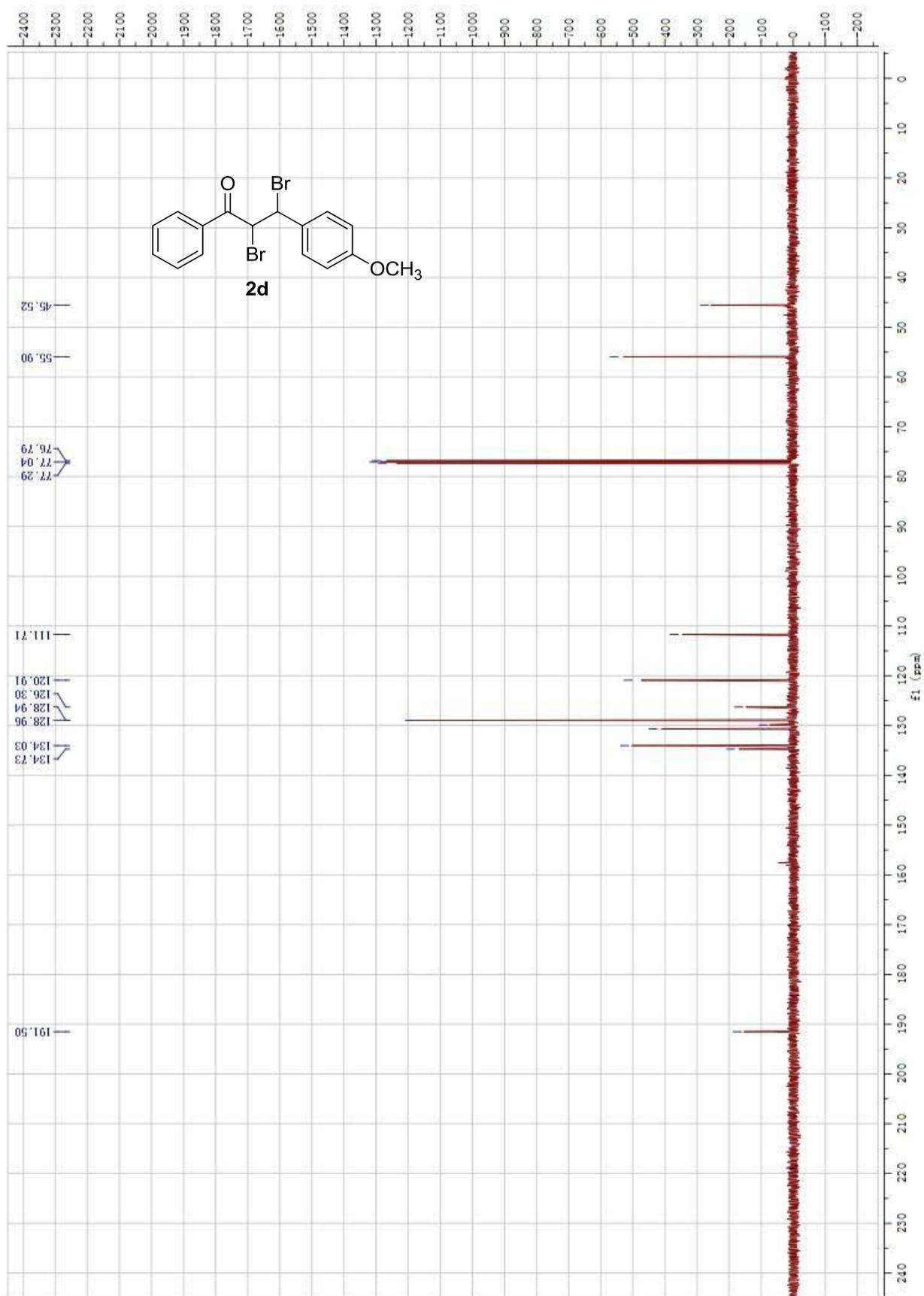
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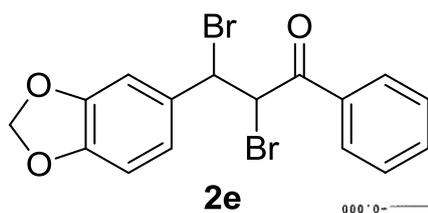
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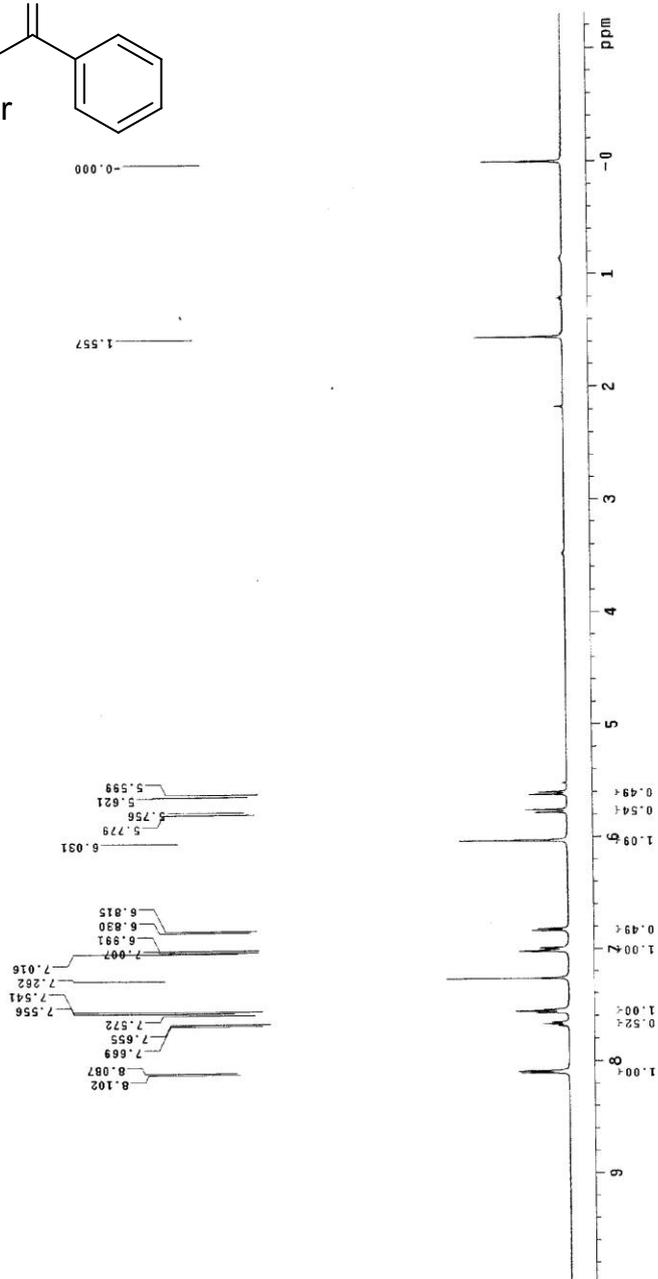
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2e



STANDARD PROTON PARAMETERS

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Sample directory:

Pulse Sequence: s2pu1

Solvent: CDCl₃

Shift reference: TMS

File: 00241

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8 repetitions

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FT size 655396

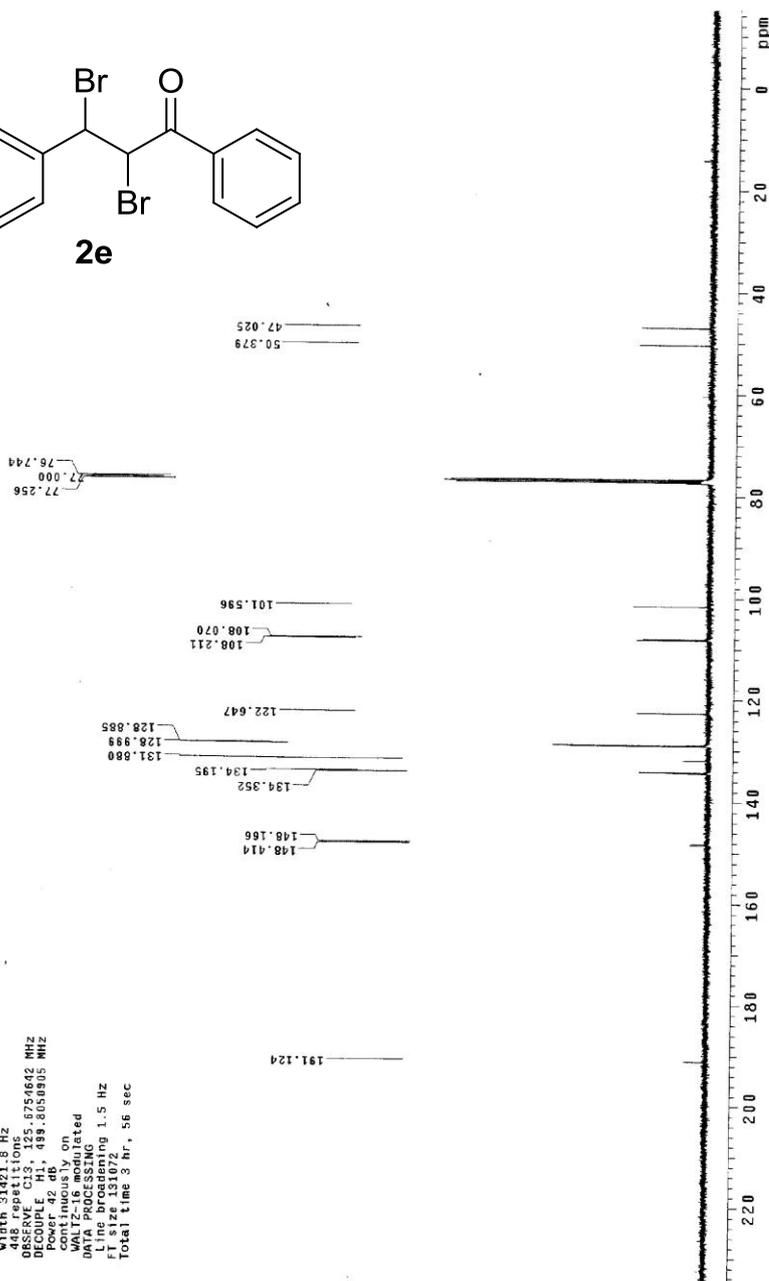
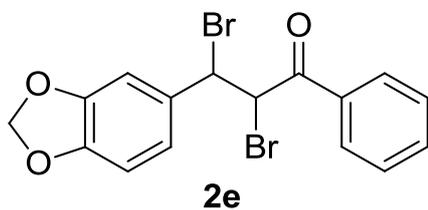
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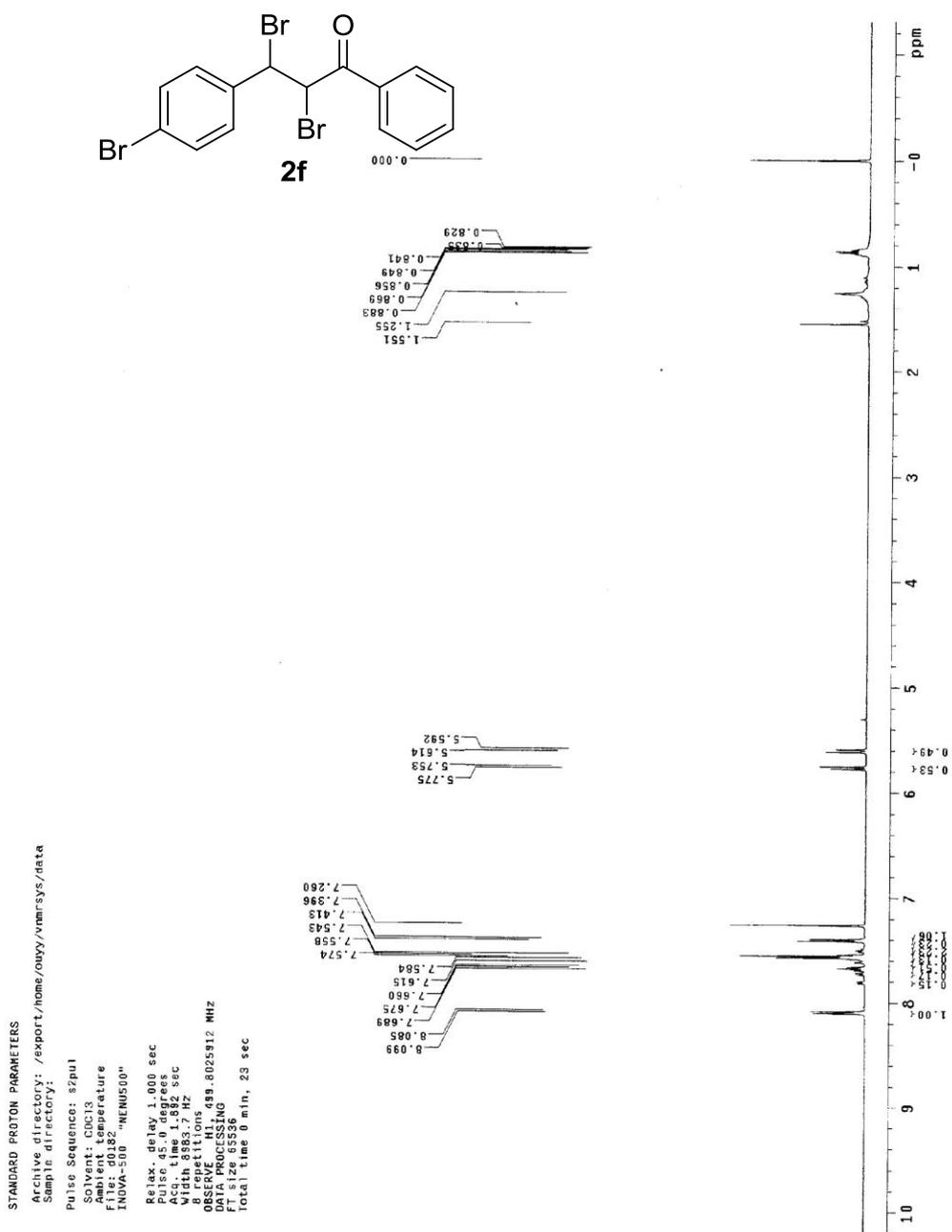
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Date: 11-14-07
User: 1-14-07
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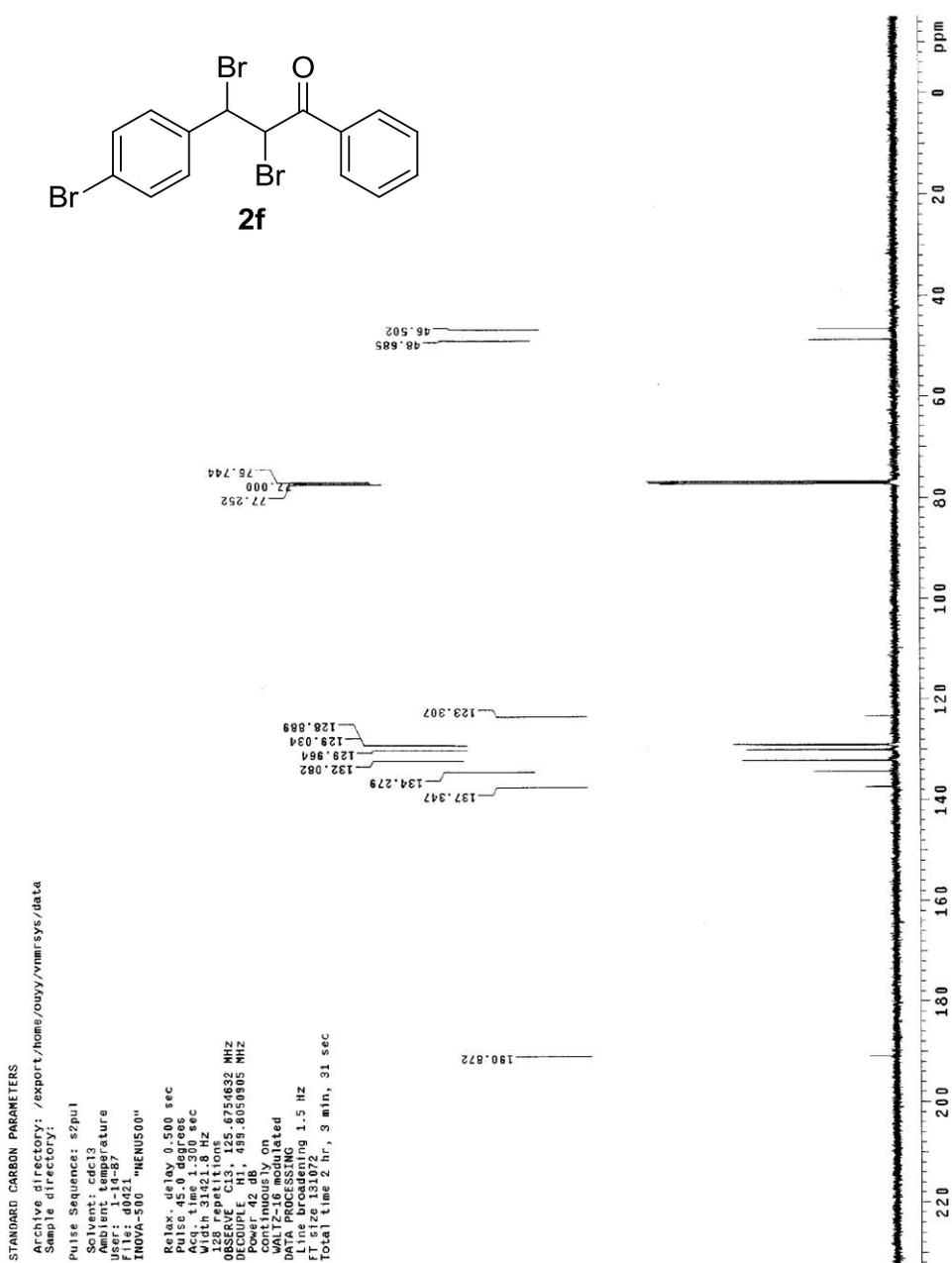
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Pulse 45.0 degrees
Acq. time 1.300 sec
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OBSERVED 131.005 MHz
DECOUPLE H1, 499.3058905 MHz
Power 42 dB
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DATA PROCESSING
Line broadening 1.5 Hz
FI size 131072
Total time 3 hr, 56 sec



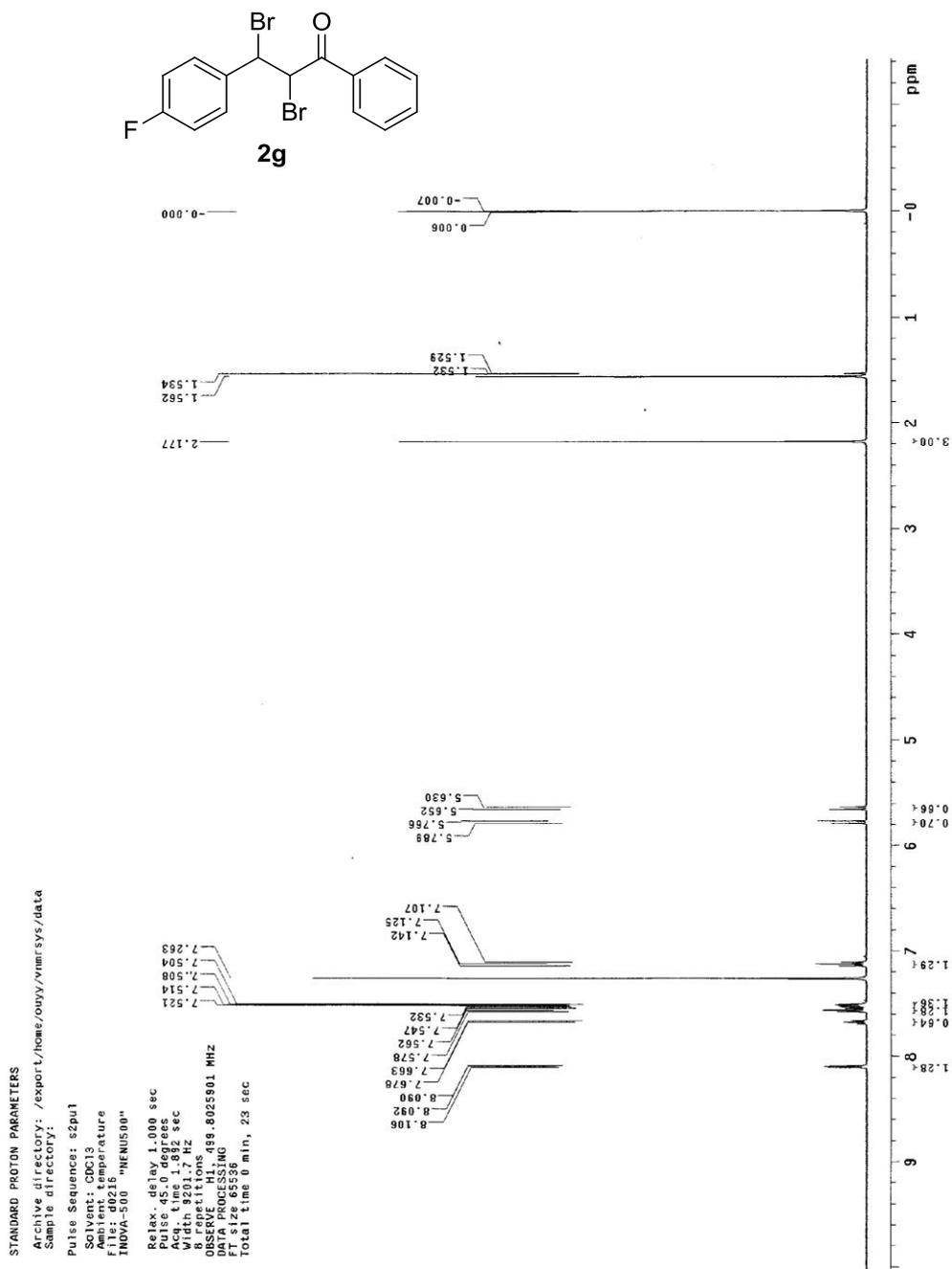
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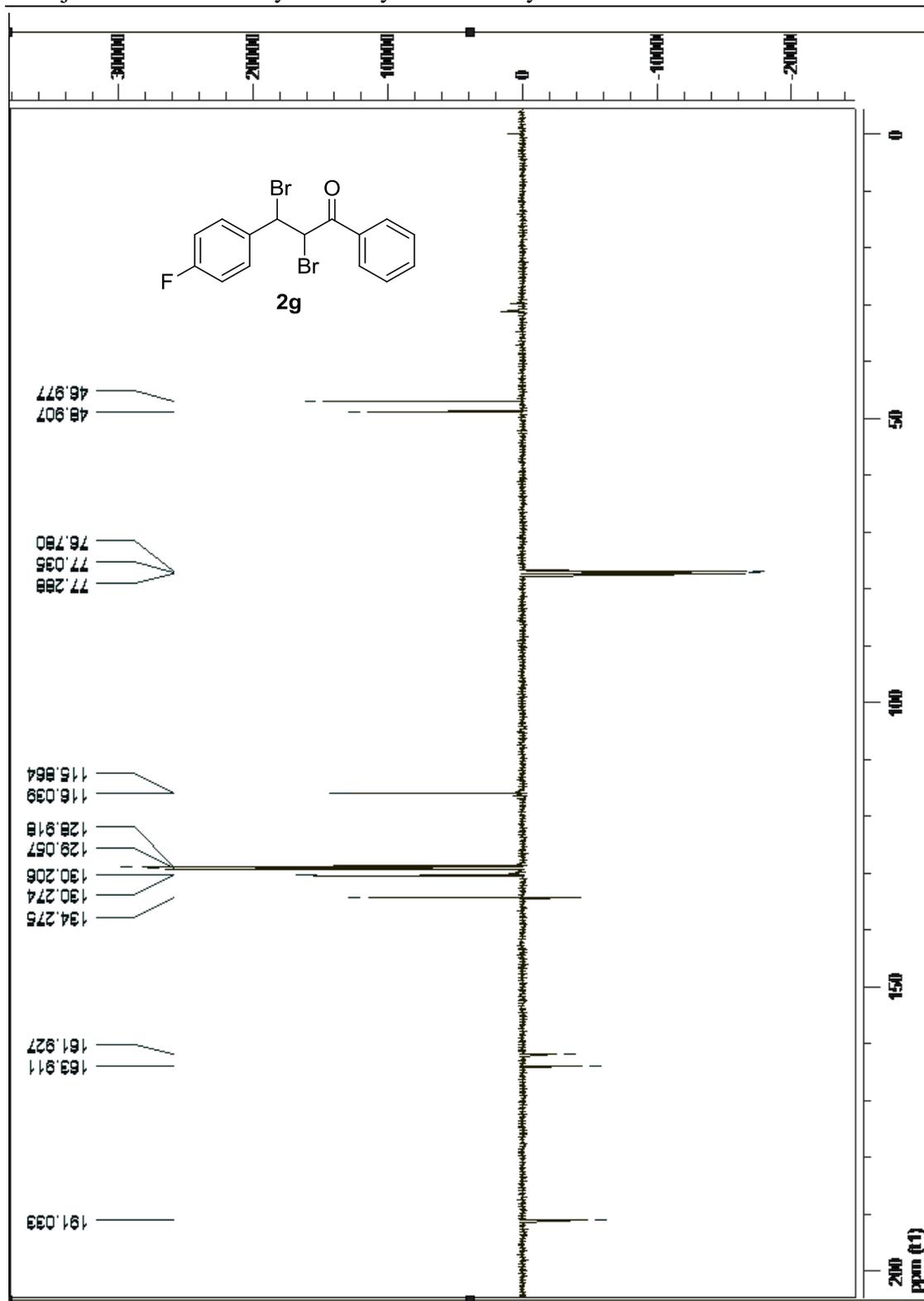
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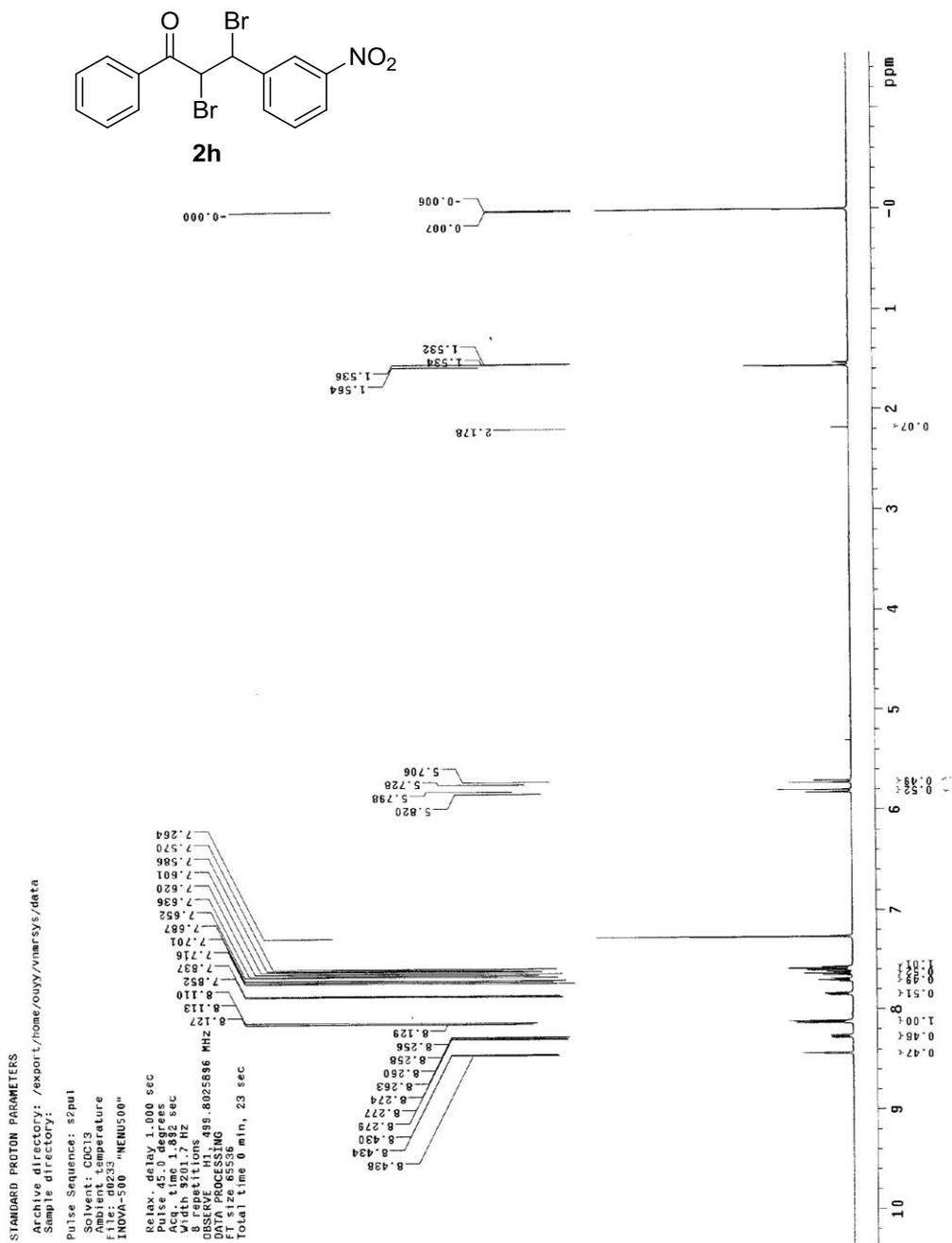
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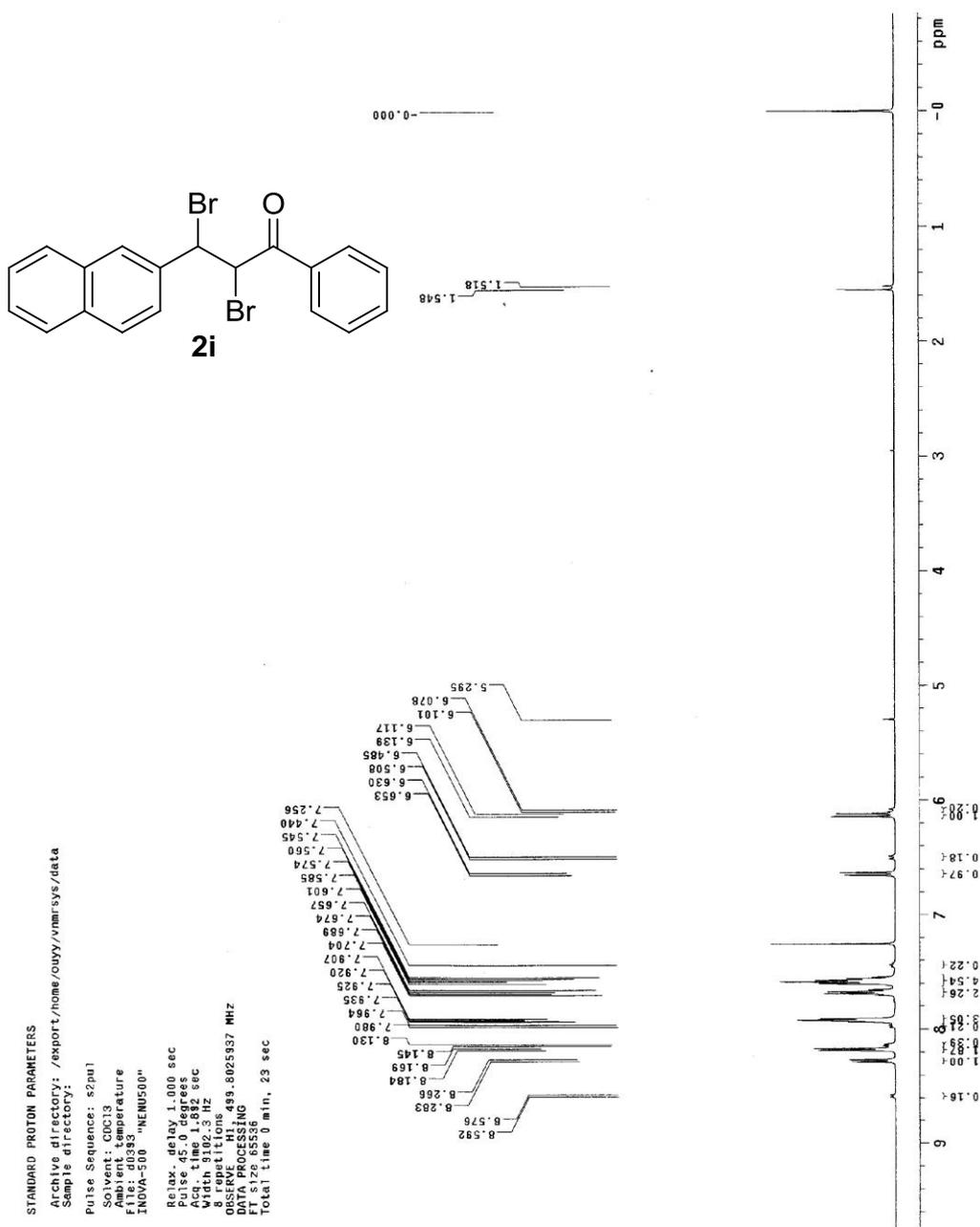
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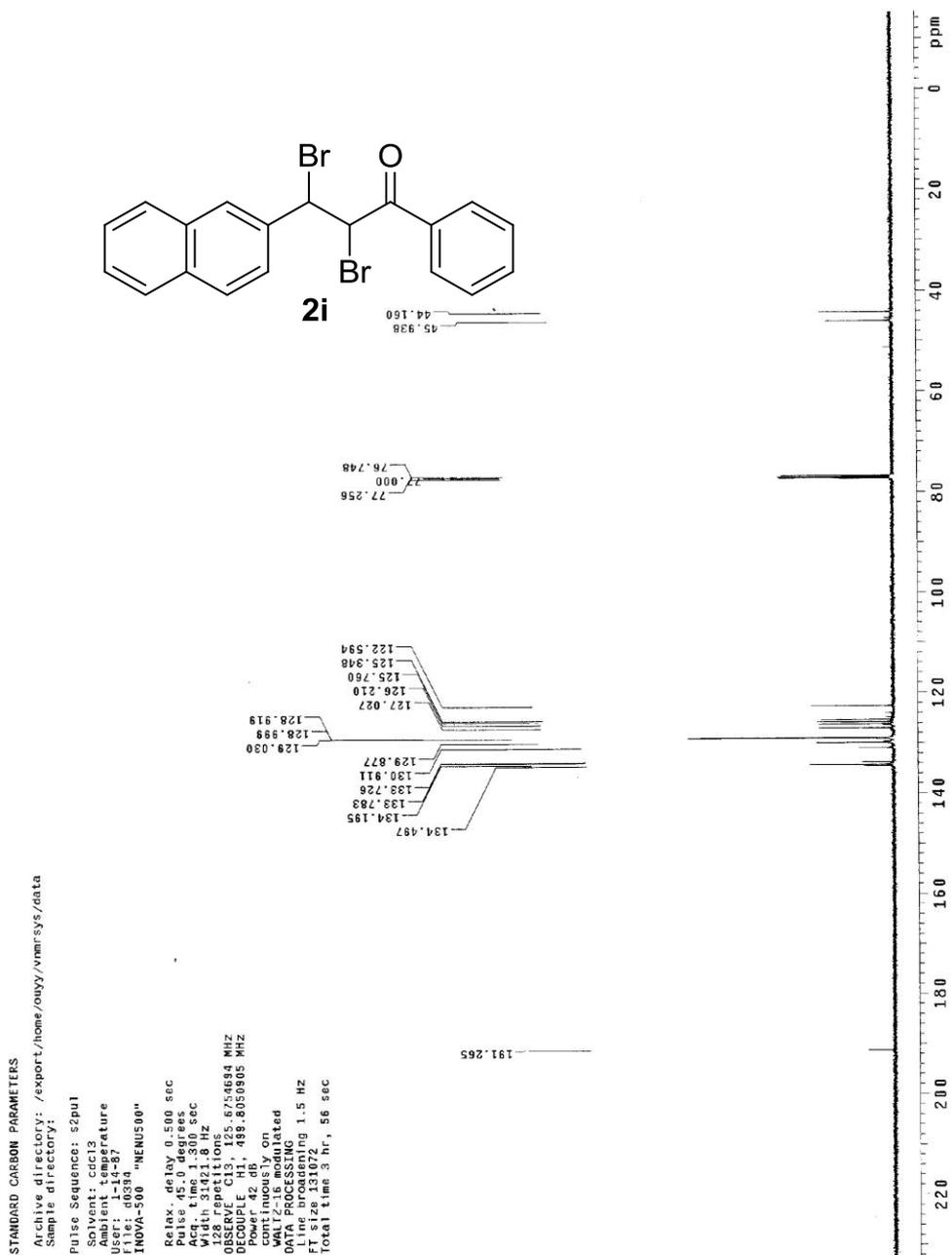
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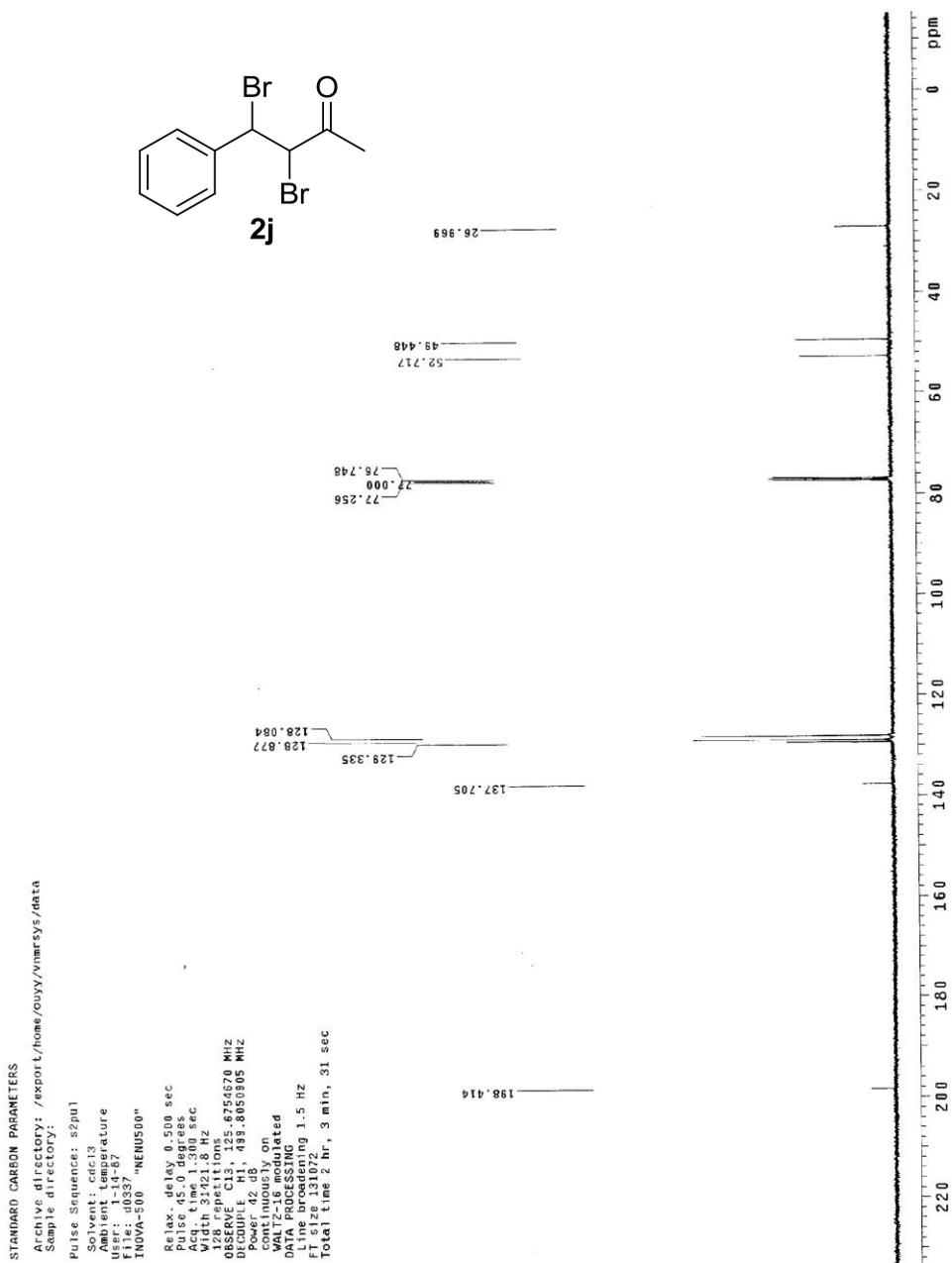
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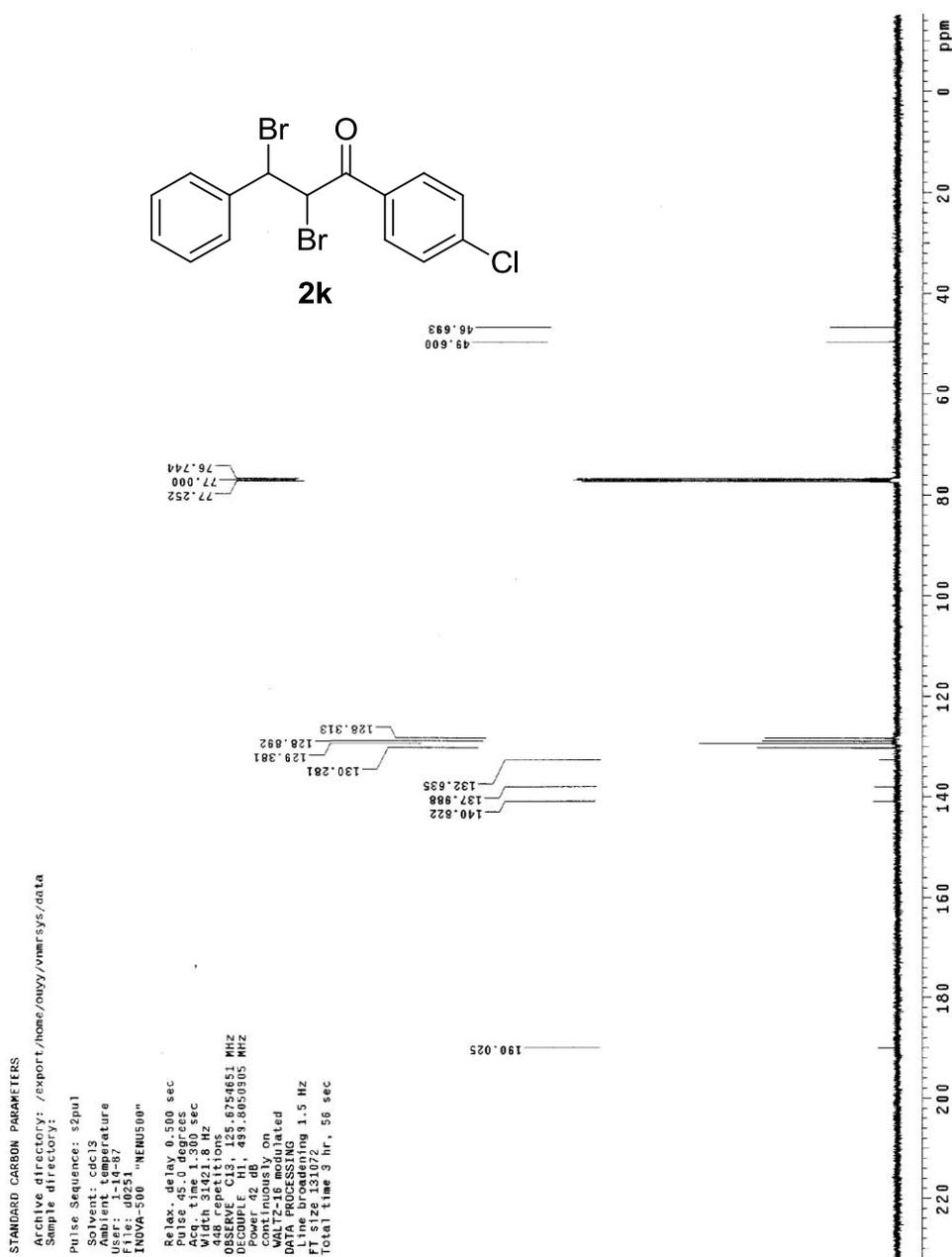
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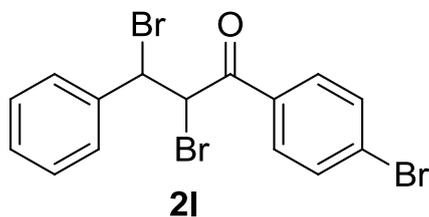
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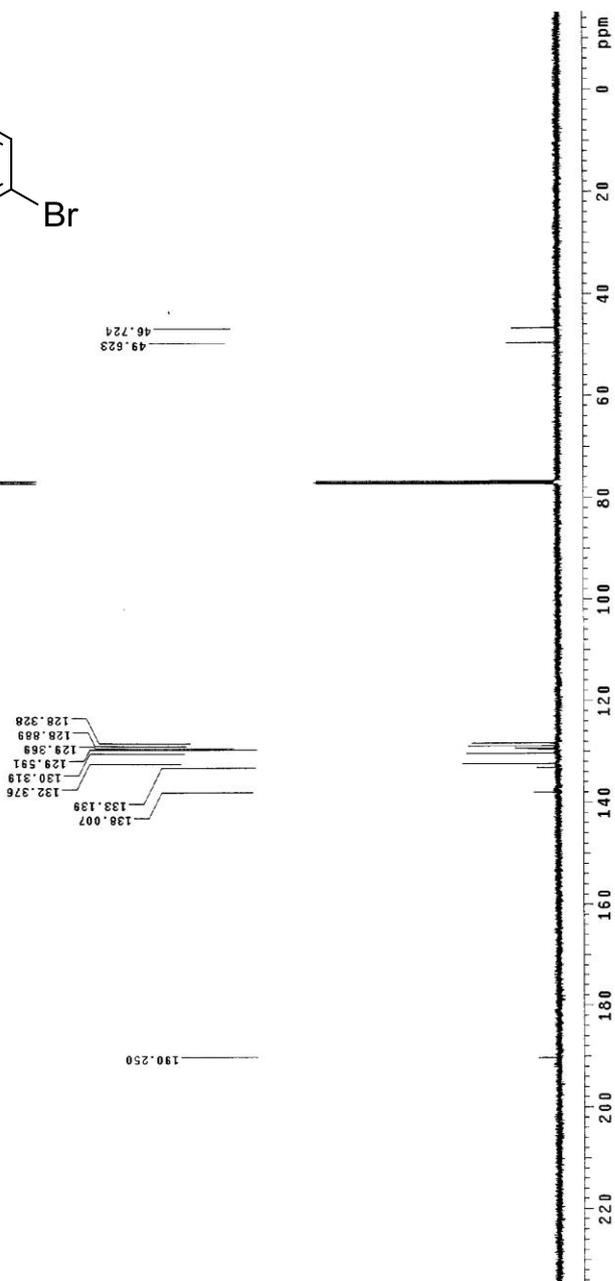
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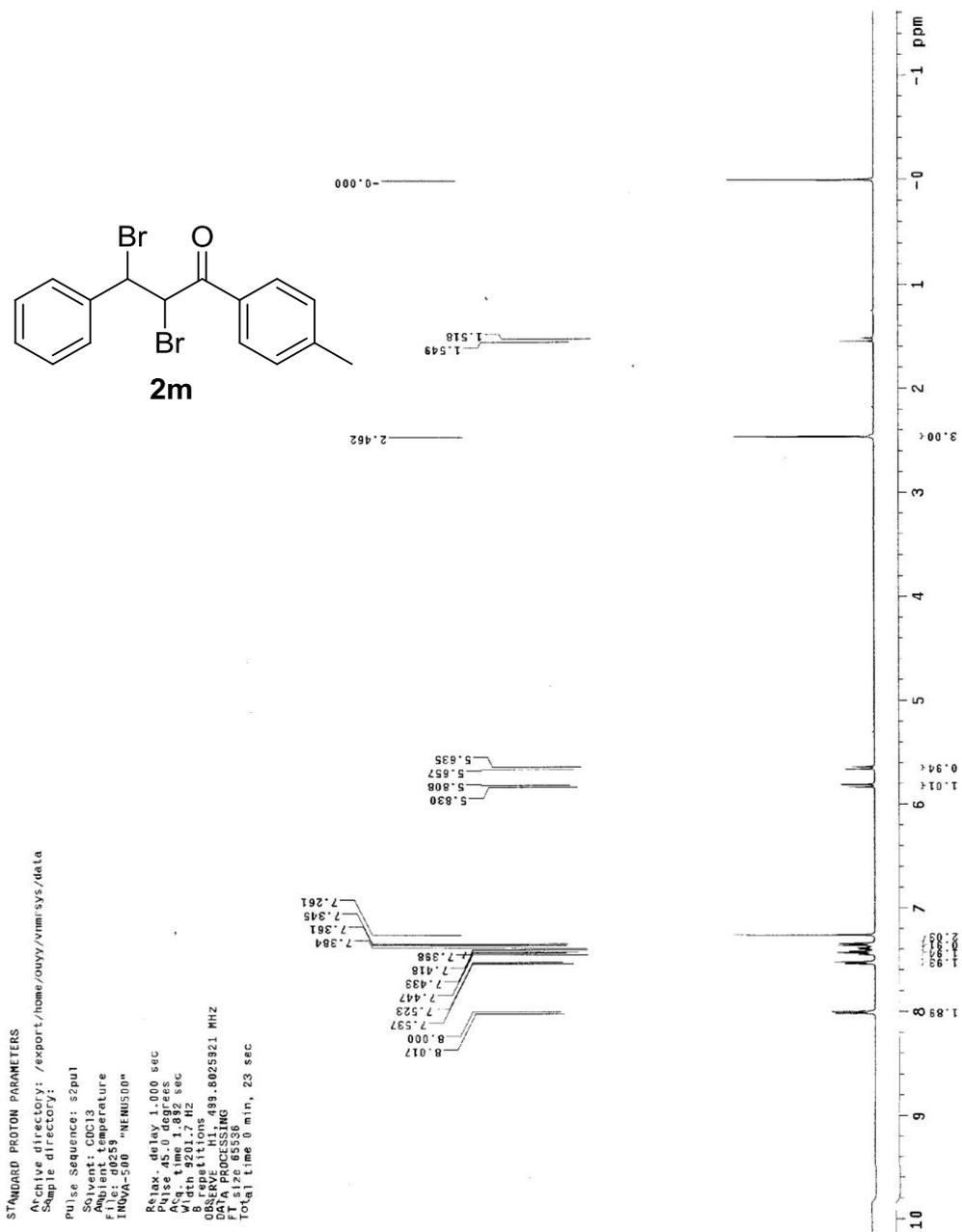
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Date: 11-14-07
User: L-14-07
File: d0552
INOVA-500 "NMRUS00"

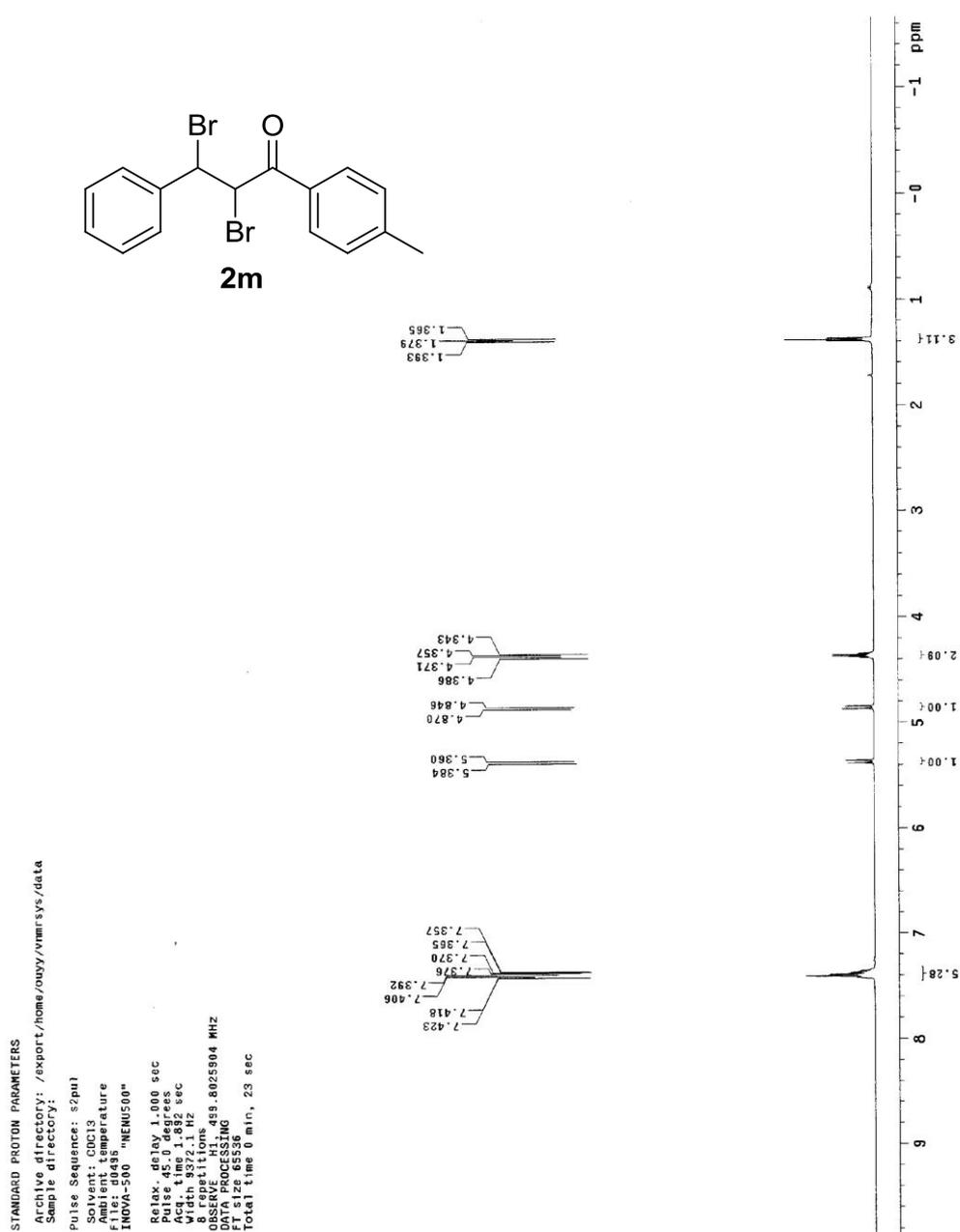
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DECOUPLE: H1, 499.8050305 MHz
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continuously on
cont. 1.5 Hz
DATA PROCESSING
Line broadening 1.5 Hz
F1 size 131072
Total time 3 hr, 56 sec



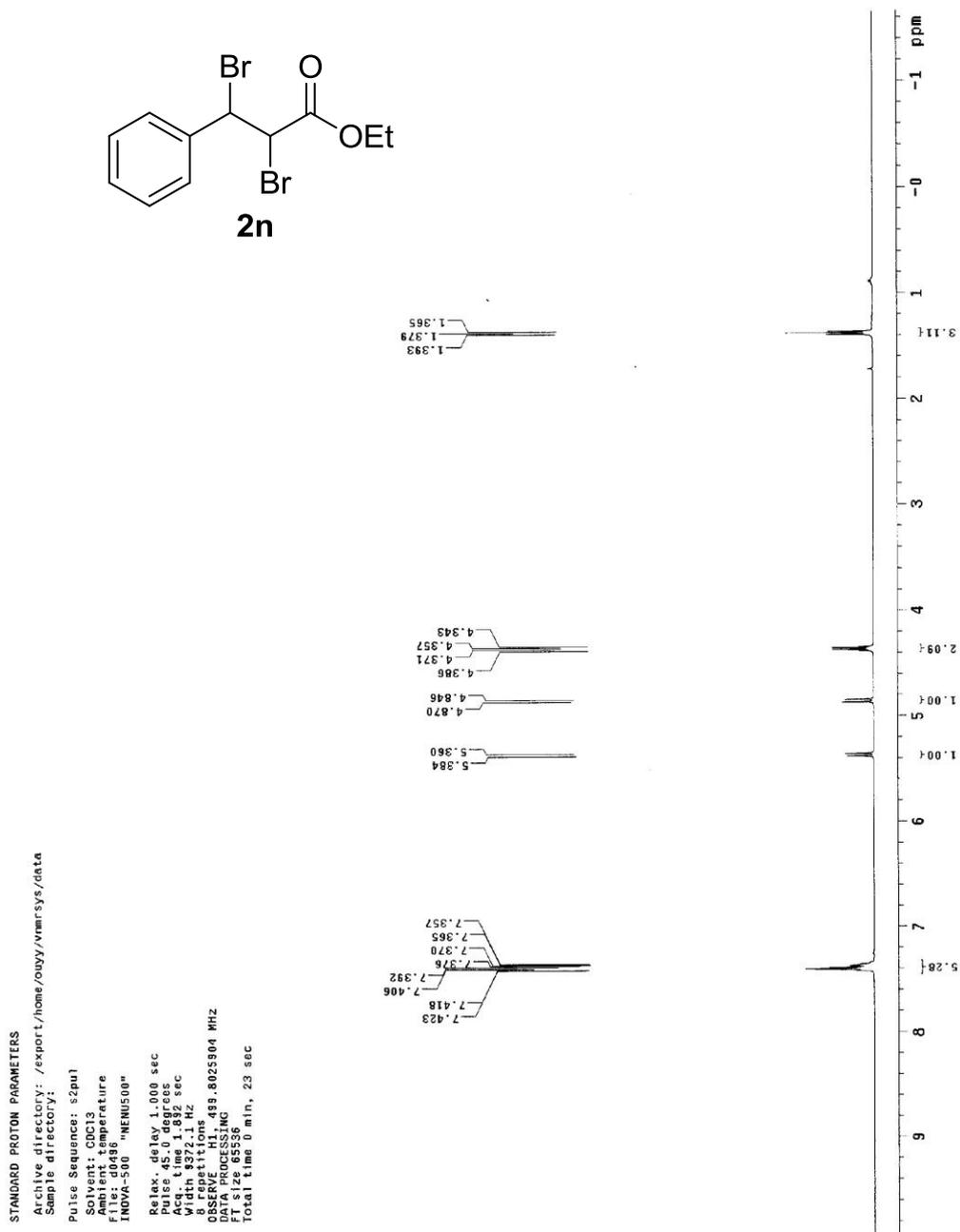
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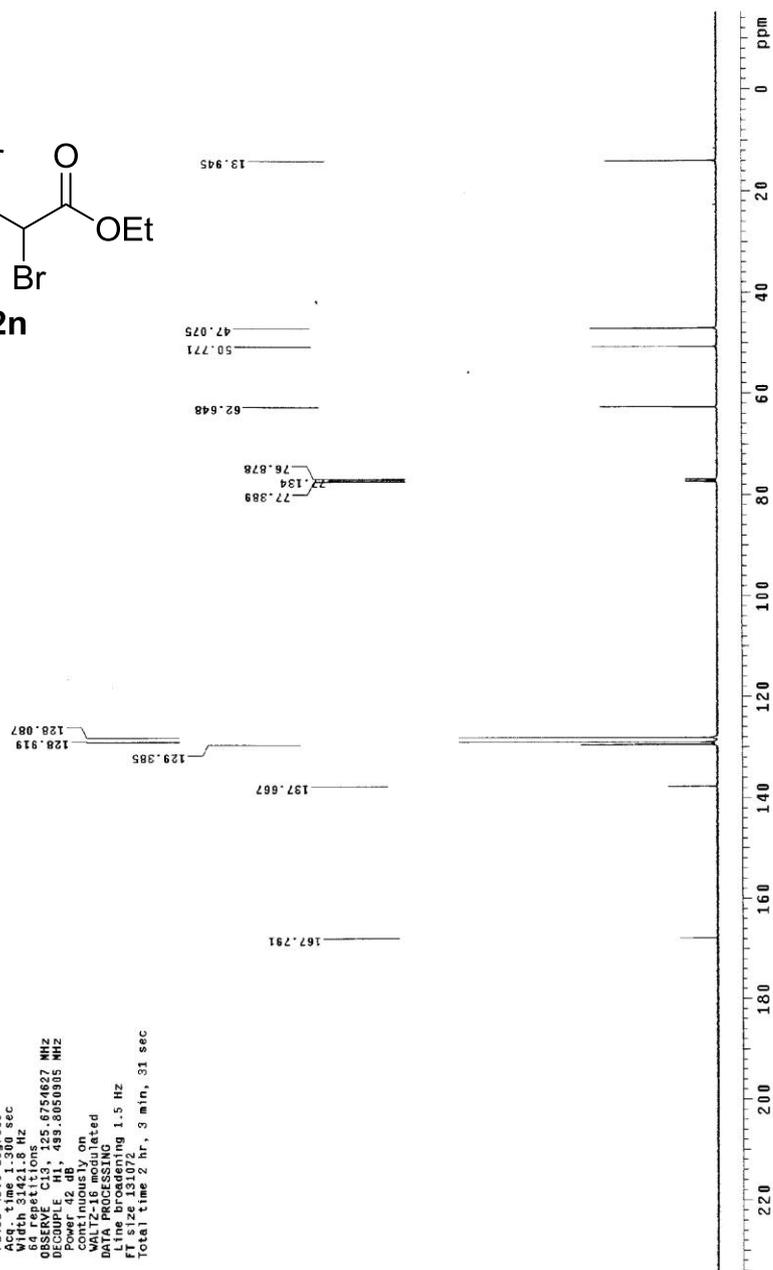
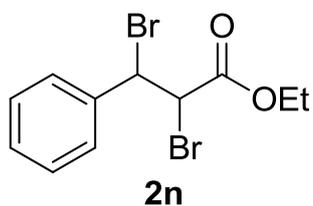


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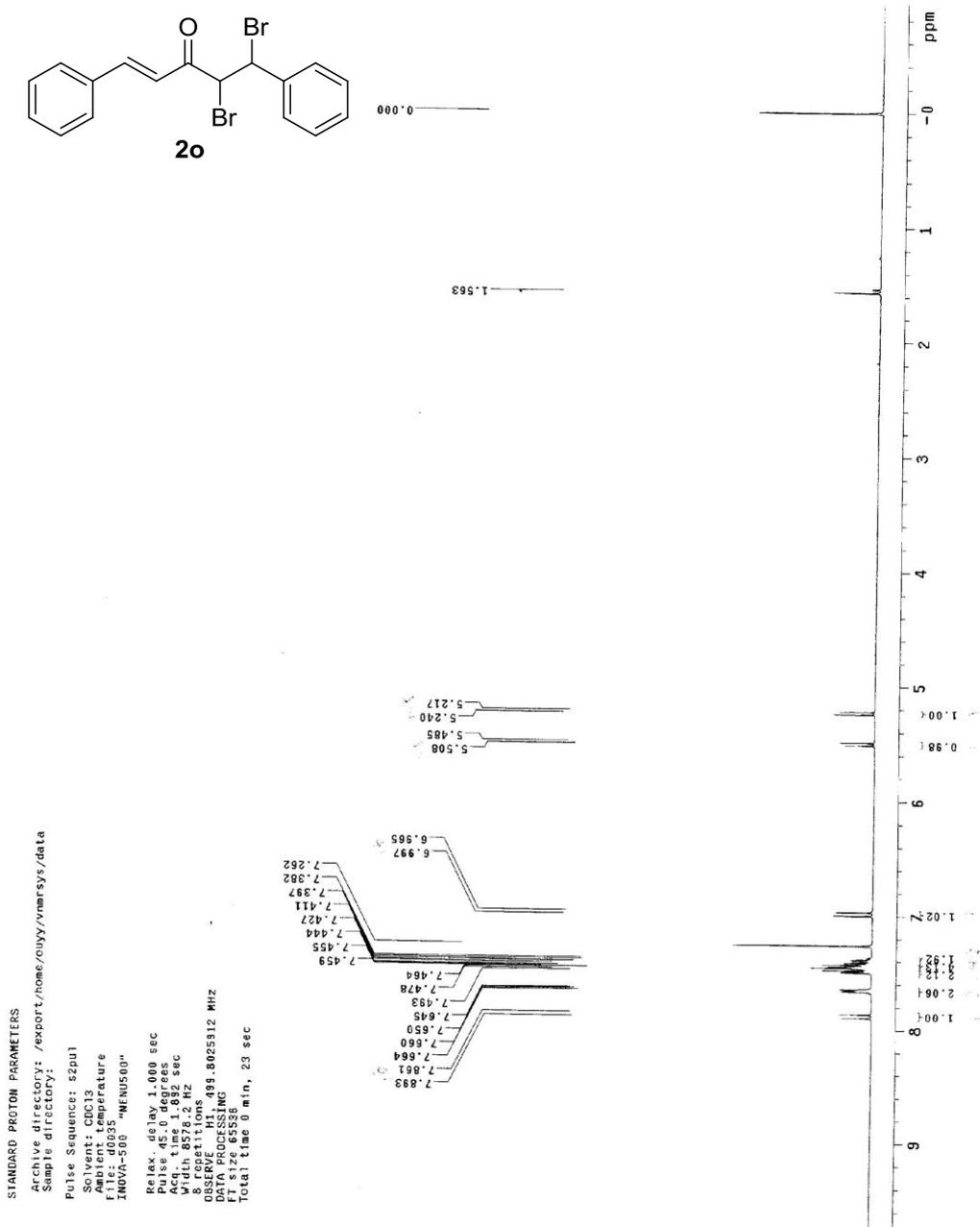


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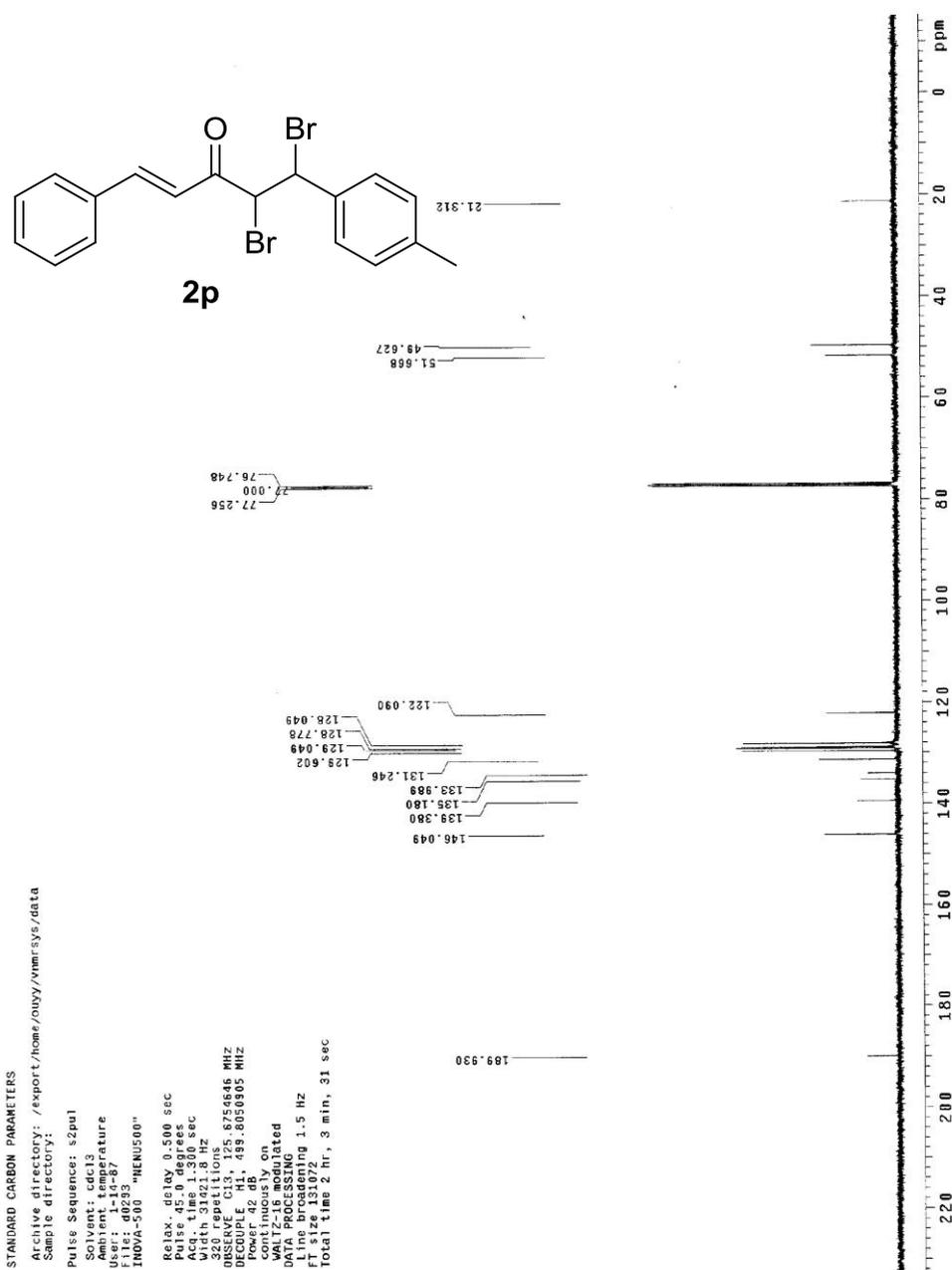
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Acquisition Temperature
User: 1-14-87
File: d0497
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Pulse 45.0 degrees
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DECOUPLE H1 495.8050905 MHZ
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WALTZ16
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Total time 2 hr, 3 min, 31 sec



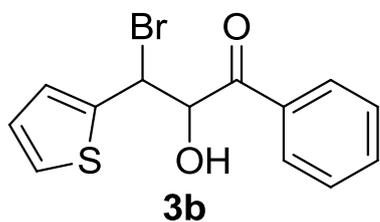
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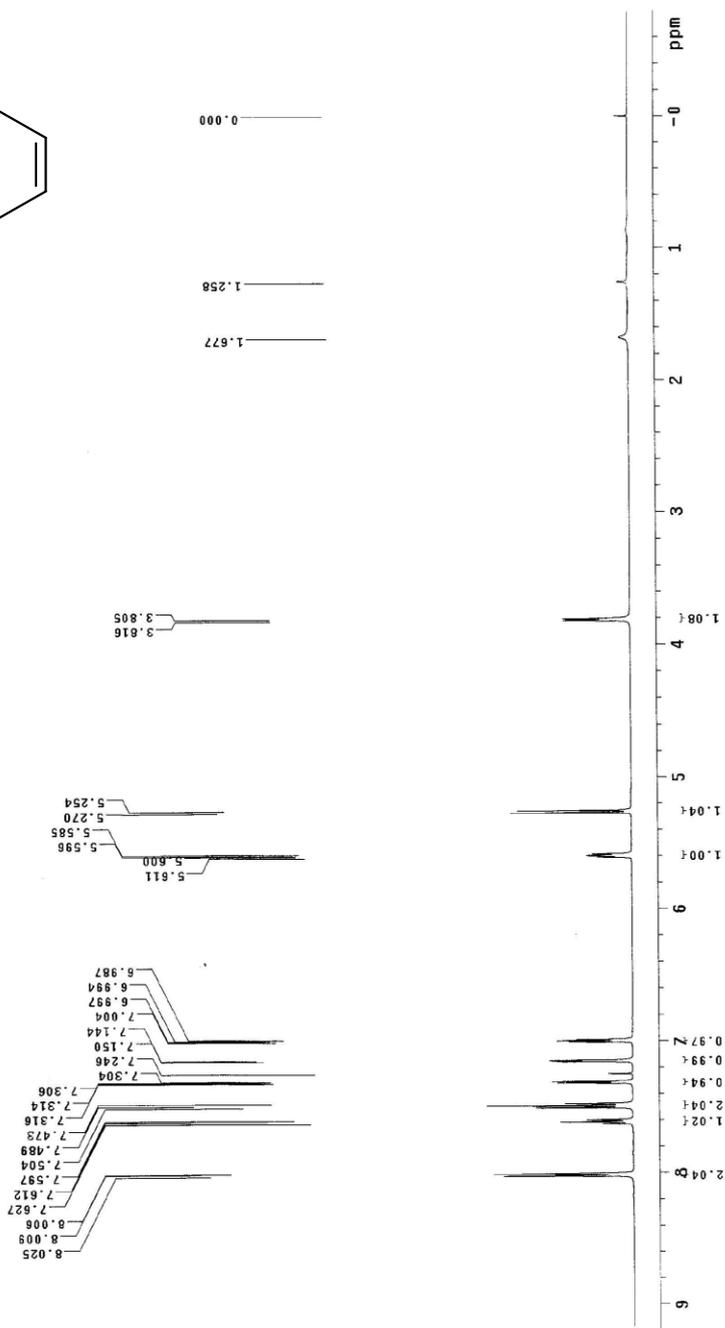
Electronic Supplementary Material (ESI) for RSC Advances
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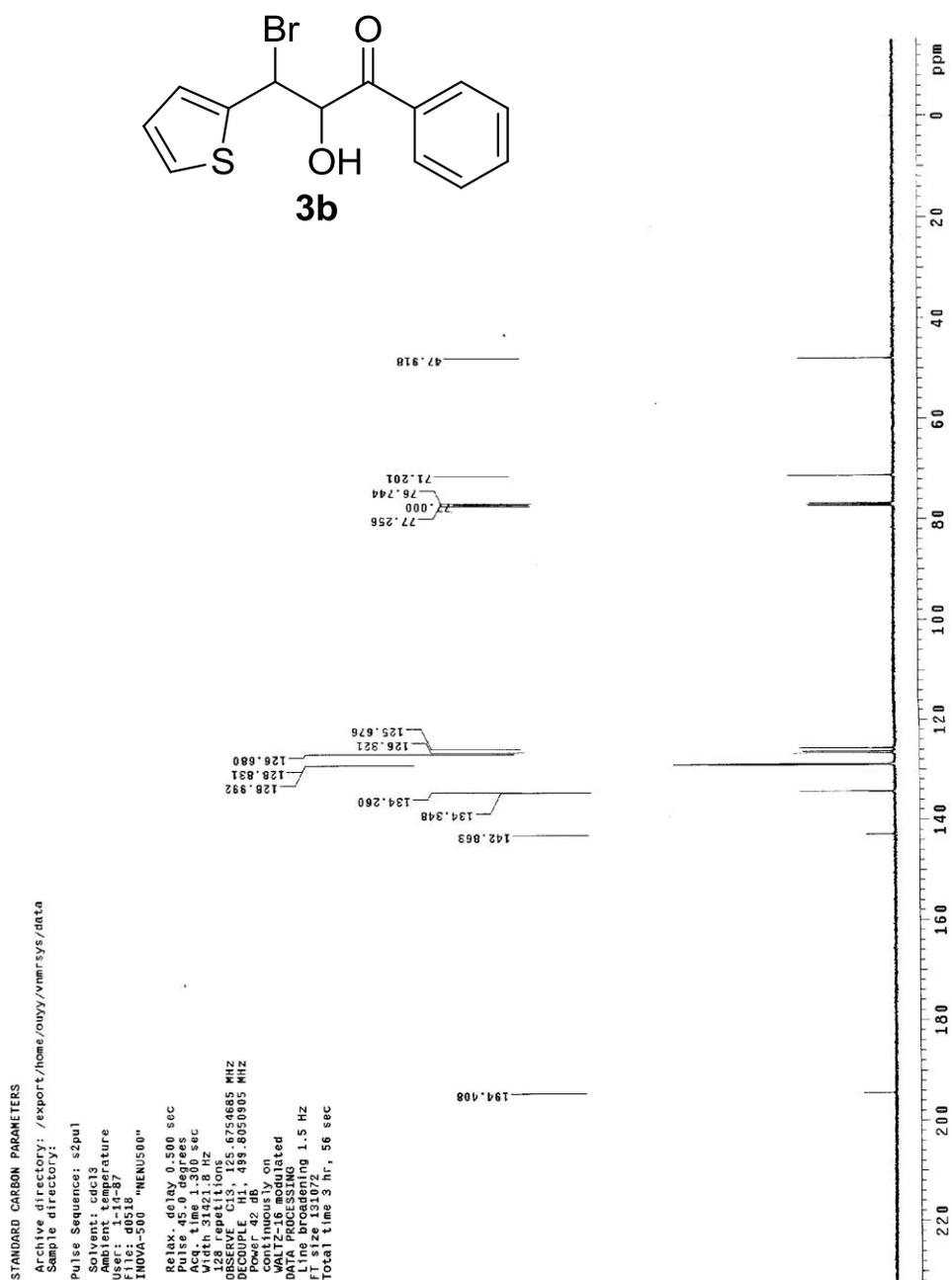
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Temperature: 300 K
File: d0516
INVA-500 "MENU500"

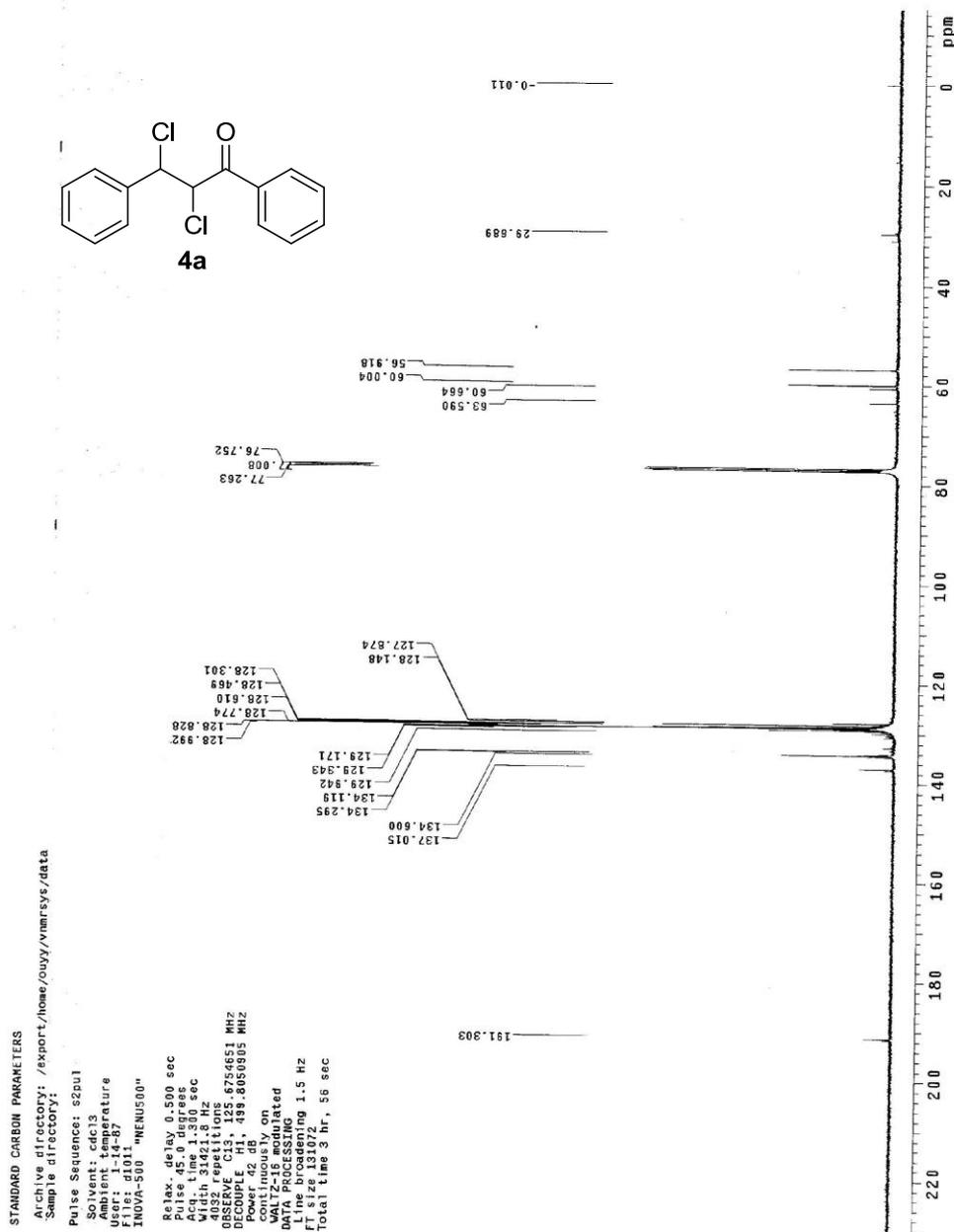
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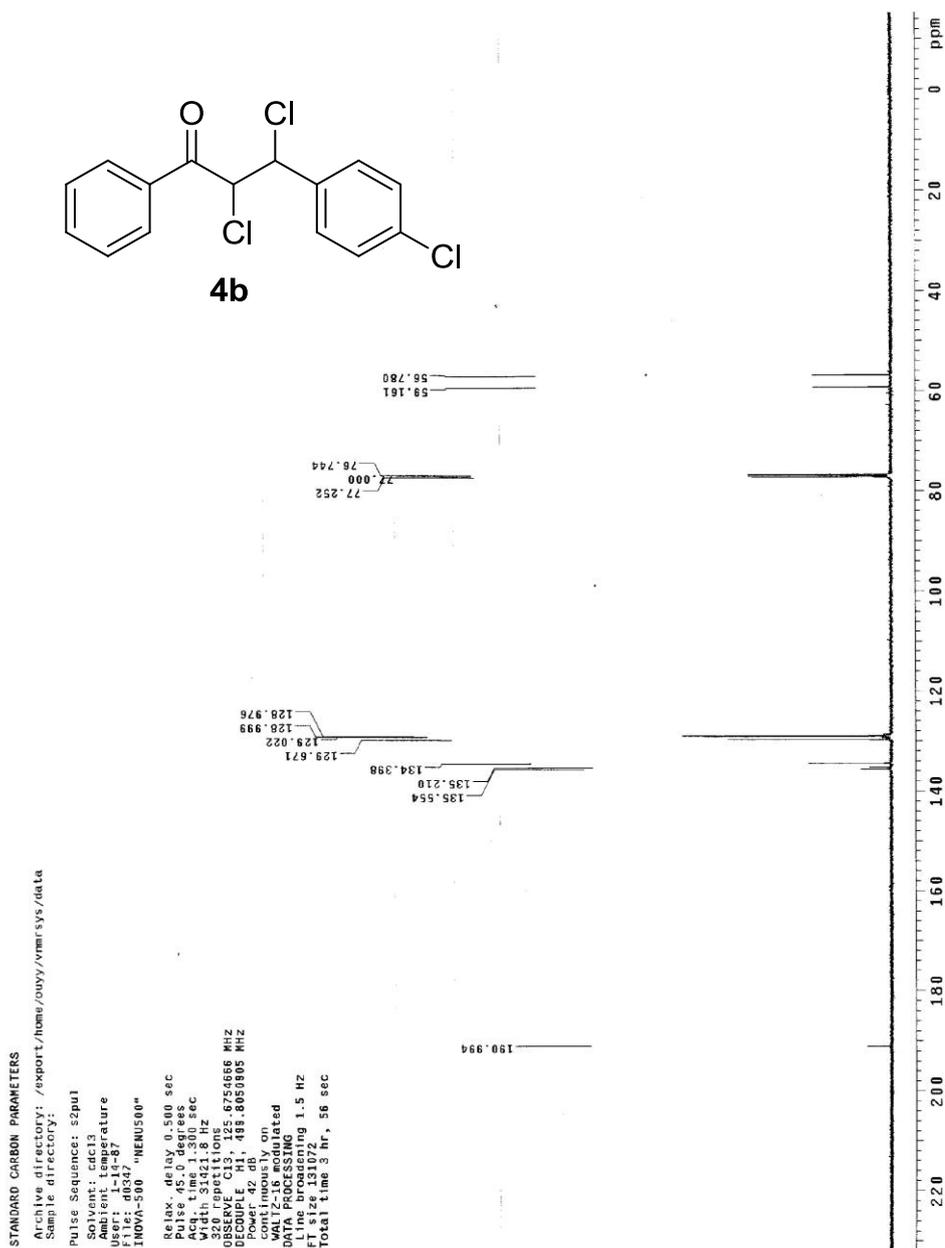
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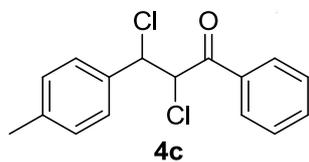
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STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouxy/vnmrsys/data

Sample directory:

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Solvent: CDCl3

Amplitude: 10.000

Temperature: 300

INVA-500 "HENU500"

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Pulse: 45.0 degree

Acq. time: 1.500 sec

Width: 9951.3 Hz

8 repetitions

OBSERVE: h1, 499.8025816 MHz

FT size: 65536

Total time: 0 min, 23 sec

