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Supporting Information

Nitroepoxide ring opening with thionucleophiles in water: Synthesis of *α*-xanthyl ketones, *β*-ketosulfones and *β*-ketosulfonic acids

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Experimental

General. All chemicals and solvents were obtained from commercial sources and used as received. Nitroepoxides were prepared according to the literature.[1] ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AMX 300 MHz spectrometers referenced to internal Me_4Si at 0.00 ppm. Reaction monitoring was carried out by thin-layer chromatography using TLC silica gel 60 F254 plates. Elemental analyses were conducted with a Perkin Elmer 2004 Series II CHN analyzer. High-resolution mass spectra (HRMS) were recorded on a THERMO SCIENTIFIC Advantage and a THERMO SCIENTIFIC Exactive instrument with ESI-/APCI-Source.

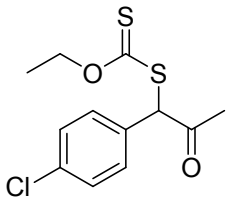
General procedure for the synthesis of α-xantyl ketones ***3a-o***

To a solution of xanthate (0.6 mmol) in H_2O (3 mL), nitroepoxide (0.5 mmol) was added and the mixture was stirred at 70 °C for 5 h. In the end, the product was extracted with EtOAc (3 × 10 mL). The organic extracts were combined, washed with water (2×10 mL), dried with anhydrous Na_2SO_4, and evaporated under reduced pressure to give the crude product. Purification was carried out by column chromatography (SiO_2; EtOAc/petrolium ether, 1/8).

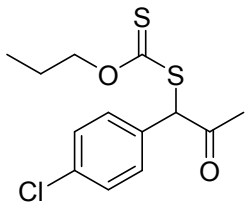
General procedure for the synthesis of β-keto sulfones ***4a-g*** *and β-keto sulfonic acids* ***5a-g***

Sodium aryl sulfinate/Sodium bisulfite (1.0 mmol) was added to a suspension of nitroepoxide (1.0 mmol) in H_2O (5 mL) and the mixture was stirred at 60 °C for 6h. The solvent was evaporated under reduced pressure to give a precipitate. The precipitate was dissolved in EtOAc and again filtered to remove the inorganic salts. The filtrate was evaporated under reduced pressure and the residue was washed with petroleum ether to remove unreacted nitroepoxide to afford the pure product.

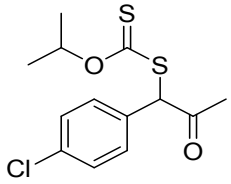
Characterization data for all products



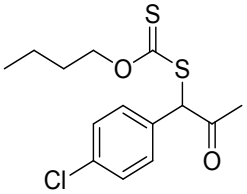
S-(1-(4-chlorophenyl)-2-oxopropyl) O-ethyl carbonodithioate (**3a**)[2]: Yellow viscous oil; (137 mg, yield 95%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.27 (m, 4H), 5.61 (s, 1H), 4.64 (q, J = 7.7 Hz, 2H), 2.28 (s, 3H), 1.42 (t, J = 7.1 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.1, 200.9, 134.9, 131.4, 130.3, 129.4, 70.6, 63.7, 28.7, 13.6 ppm.



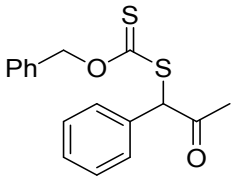
S-(1-(4-chlorophenyl)-2-oxopropyl) O-propyl carbonodithioate **(3b):** Pale yellow viscous oil; (136 mg, yield 90%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.28 (m, 4H), 5.61(s, 1H), 4.50 (t, J = 6.7 Hz, 2H), 2.28 (s, 3H), 1.84-1.76 (m, 2H), 1.01-0.96 (t, J= 7.4 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.4, 200.9, 134.9, 131.4, 130.4, 129.4, 76.2, 63.8, 28.8, 21.6, 10.3 ppm; HRMS (ESI^-) calculated for $C_{13}H_{14}ClO_2S_2$ $[M–H]^-$ 301.0124; found: 301.0129.



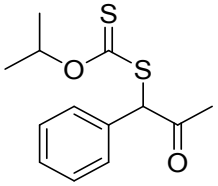
S-(1-(4-chlorophenyl)-2-oxopropyl) O-isopropyl carbonodithioate **(3c)** : Yellow oil; (136 mg, yield 90%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36- 7.28 (m, 4H), 5.69 (m, 1H), 5.59 (s, 1H), 2.28 (s, 3H), 1.36-1.38 (d, J = 6.2 Hz, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.3, 201.0, 134.8, 131.4, 130.3, 129.3, 78.8, 63.4, 28.7, 21.2, 21.1 ppm; HRMS (ESI^-) calculated for $C_{13}H_{14}ClO_2S_2$ $[M–H]^-$ 301.0124; found: 301.0128.



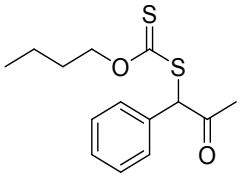
O-butyl S-(1-(4-chlorophenyl)-2-oxopropyl) carbonodithioate (**3d**) : yellow viscous oil; (147 mg, yield 93%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.27 (m, 4H), 5.60 (s, 1H), 4.57 (t, J = 6.6 Hz, 2H), 2.28 (s, 3H), 1.80-1.70 (m, 2H), 1.45-1.37 (m, 2H), 0.97- 0.92 (t, J = 7.3 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.4, 200.9, 134.9, 131.4, 130.3, 129.4, 74.6, 63.8, 30.1, 28.8, 19.0, 13.6 ppm; HRMS (ESI^-) calculated for $C_{14}H_{16}ClO_2S_2$ $[M–H]^-$ 315.0280; found: 315.0287.



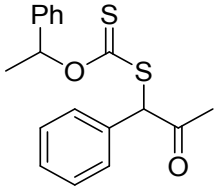
O-benzyl S-(2-oxo-1-phenylpropyl) carbonodithioate (**3e**): Yellow viscous oil, (145 mg, yield 92%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41-7.23 (m, 10H), 5.57 (s, 1H), 5.55 (s, 2H), 2.18 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.7, 200.8, 134.9, 133.9, 131.2, 130.4, 129.4, 128.9, 128.9, 128.7, 75.9, 63.7, 28.7 ppm; Anal calcd for $C_{17}H_{16}O_2S_2$: C, 64.53; H, 5.10; Found: C, 64.12; H, 5.19.



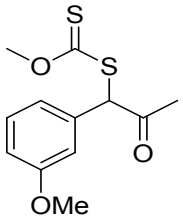
O-isopropyl S-(2-oxo-1-phenylpropyl) carbonodithioate (**3f**) : Yellow viscous oil, (123 mg, yield 92%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.27 (m, 5H), 5. 69 (m, 1H), 5.60 (s, 1H) 2.28 (s, 3H), 1.38-1.35 (d, J = 6.3 Hz, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.8, 201.3, 132.6, 129.2, 128.9, 128.7, 78.6, 64.2, 28.6, 21.2, 21.1 ppm; HRMS (ESI$^+$) calculated for $C_{13}H_{17}O_2S_2$ $[M+H]^+$ 269.0670; found: 269.0660.



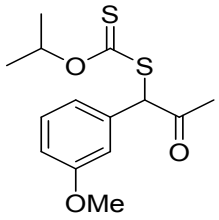
O-butyl S-(2-oxo-1-phenylpropyl) carbonodithioate (**3g**): Yellow viscous oil; (125 mg, yield 89%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39-7.33 (m, 5H), 5.62 (S, 1H), 4.57(t, J = 6.5 Hz, 2H), 2.28 (s, 3H), 1.78-1.73 (m, 2H), 1.45-1.38 (m, 2H), 0.98 (t, J = 7.3 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.8, 201.3, 132.5, 129.2, 129.0, 128.8, 74.4, 64.5, 30.1, 28.7, 19.0, 13.6 ppm; HRMS (ESI$^+$) calculated for $C_{14}H_{19}O_2S_2$ $[M+H]^+$ 283.0826; found: 283.0820.



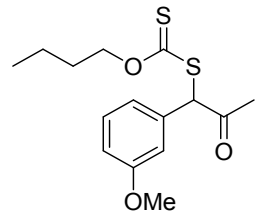
S-(2-oxo-1-phenylpropyl) O-(1-phenylethyl) carbonodithioate (**3h**): Yellow viscous oil, (143 mg, yield 87%); ^{1}H NMR for a diasteromer (300 MHz, $CDCl_3$) δ 7.39-7.30 (m, 10H), 6.57 (m, 1H), 5.61(s, 1H), 2.25 (ds, 3H), 1.69(d, J = 6.7 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.7, 201.3, 139.9, 132.8, 129.2, 129.0, 128.8, 128.5, 128.3, 126.5, 82.2, 64.5, 28.7, 21.5 ppm; HRMS (ESI$^+$) calculated for $C_{18}H_{19}O_2S_2$ $[M+H]^+$ 331.0826; found: 331.0816.



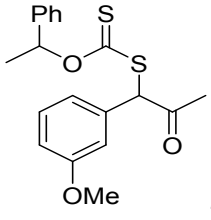
S-(1-(3-methoxyphenyl)-2-oxopropyl) O-methyl carbonodithioate (**3i**): Yellow viscous oil, (120 mg, yield 89%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31-7.25 (m, 1H), 6.94- 6.86 (m, 3H), 5.59 (s, 1H), 4.15 (s, 3H), 3.80 (s, 3H), 2.28 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 213.7, 201.1, 160.1, 133.7, 130.2, 121.3, 114.6, 114.4, 64.8, 60.4, 55.2, 28.8 ppm; Anal. calcd for $C_{12}H_{14}O_3S_2$: C, 53.31; H, 5.22; Found: C, 53.27; H, 5.14.



O-isopropyl S-(1-(3-methoxyphenyl)-2-oxopropyl) carbonodithioate (**3j**): yellow viscous oil, (124 mg, yield: 83%); ^{1}H NMR (300 MHz, Chloroform-*d) δ* 7.27 (m, 1H), 6.94-6.86 (m, 3H), 5.70 (m, 1H), 5.57 (s, 1H), 3.80 (s, 3H), 2.28 (s, 3H), 1.38 (d, J = 6.2 Hz, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.9, 201.2, 160.0, 133.8, 130.2, 121.3, 114.6, 114.3, 78.6, 64.2, 55.3, 28.7, 21.2 ppm; HRMS (ESI$^+$) calculated for $C_{14}H_{18}NaO_3S_2$ $[M+Na]^+$ 321.0595; found: 321.0598.

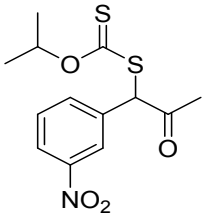


O-butyl S-(1-(3-methoxyphenyl)-2-oxopropyl) carbonodithioate (**3k**): Yellow viscous oil, (133 mg, yield 85%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (m, 1H), 6.94-6.86 (m, 3H), 5.59 (s, 1H), 4.56 (t, J = 6.6 Hz, 2H), 3.80 (s, 3H), 2.28 (s, 3H), 1.79-1.73 (m, 2H), 1.46-1.39 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.9, 201.2, 160.0, 133.8, 130.2, 121.3, 114.6, 114.3, 74.4, 64.5, 55.3, 30.1, 28.7, 19.0, 13.6 ppm; HRMS (ESI$^+$) calculated for $C_{15}H_{20}NaO_3S_2$ $[M+Na]^+$ 335.0752; found: 335.0745.

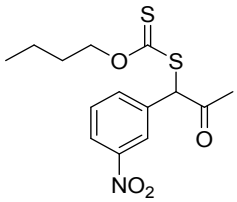


S-(1-(3-methoxyphenyl)-2-oxopropyl) O-(1-phenylethyl) carbonodithioate (**3l**): Yellow viscous oil, (144 mg, yield 80%); The product was obtained as a 1:1 mixture of diastereomers; spectroscopic for one of the diastereomers: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.22 (m, 6H), 6.92-6.85(m, 4H), 6.57 (q, J = 6.6 Hz 1H), 5.55 (s, 1H), 3.79 (s, 3H), 2.5 (s, 3H), 1.66 (d, J = 6.6 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.7, 201.1, 160.1, 139.9, 134.1,

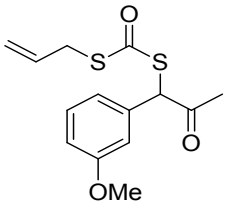
130.2, 128.5, 128.3, 126.5, 121.3, 114.6, 114.3, 82.2, 64.4, 55.3, 28.7, 21.5 ppm; Anal. calcd for $C_{19}H_{20}NaO_3S_2$ 383.0752; 383.0755



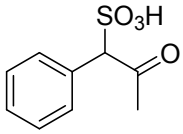
O-isopropyl S-(1-(3-nitrophenyl)-2-oxopropyl) carbonodithioate (**3m**) : Yellow viscous oil; (141 mg, yield 90%);^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27- 8.19 (m, 2H), 7.72-7.69 (m, 1H), 7.57 (t, J = 7.9 Hz, 1H), 5.76 (s,1H), 5.70 (m, 1H), 2.35 (s, 3H), 1.40-1.36 (d, J = 6.3 Hz, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.3, 200.4, 148.4, 136.0, 135.0, 129.9, 124.2, 123.6, 79.5, 63.2, 28.9, 21.2 ppm; HRMS (ESI$^+$) calculated for $C_{13}H_{16}O_4NS_2$ $[M+H]^+$ 314.0521; found: 314.0513.



O-butyl S-(1-(3-nitrophenyl)-2-oxopropyl) carbonodithioate (**3n**): Yellow viscous oil, (140 mg, yield 86%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (t, J = 1.9 Hz, 1H), 8.23-8.19 (m, 1H), 7.72-7.69 (m, 1H), 7.56 (t, J = 7.9 Hz, 1H), 5.77 (s, 1H), 4.56 (t, J = 6.7 Hz, 2H), 2.34 (s, 3H), 1.81-1.71(m, 2H), 1.44-1.37 (m, 2H), 0.94 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 211.3, 200.4, 148.4, 135.9, 135.0, 129.9, 124.2, 123.6, 75.0, 63.5, 30.1, 28.9, 19.0, 13.6 ppm; HRMS (ESI$^-$) calculated for $C_{14}H_{16}O_4NS_2$ $[M–H]^–$ 326.0521; found: 326.0526.

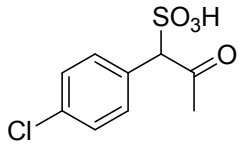


S-allyl S-(1-(3-methoxyphenyl)-2-oxopropyl) carbonodithioate (**3o**): Pale yellow viscous oil, (112 mg, yield 76%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30-7.24 (m, 1H), 6.91-6.81(m, 3H), 5.85-5.76 (m, 1H), 5.47 (s, 1H), 5.30-5.12 (m, 2H), 3.80 (s, 3H), 3.62 (dd, J = 6.7, 2.2 Hz, 2H), 2.24 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.1, 188.0, 160.1, 134.6, 132.2, 130.3, 121.1, 118.8, 114.5, 114.1, 59.6, 55.3, 33.4, 28.1 ppm; HRMS (ESI$^+$) calculated for $C_{14}H_{17}O_3S_2$ $[M+H]^+$ 297.0619; found: 297.0613.

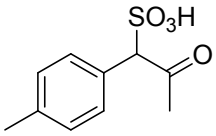


2-Oxo-1-phenylpropane-1-sulfonic acid (**4a**); Cream powder (197 mg, 92%); mp 128-130 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ (ppm) 7.51-7.20 (m, 5H), 4.93 (s, 1H), 2.32 (s, 3H,

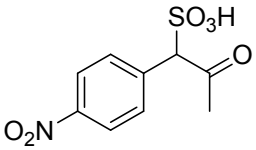
CH_3) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 202.1, 134.7, 129.9, 127.4, 126.8, 77.3, 30.2 ppm; HRMS (ESI^-) calculated for $C_9H_9O_4S$ $[M–H]^-$ 213.0222; found: 213.0227.



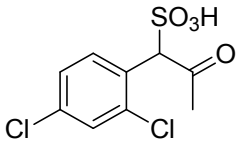
1-(4-Chlorophenyl)-2-oxopropane-1-sulfonic acid (**4b**): White powder (153 mg, 62%); mp 235 °C (decomposed); ^1H NMR (300 MHz, D_2O) δ 7.49-7.41, 5.41 (brs, 1H), 2.36 (s, 3H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 204.6, 134.3, 131.2, 129.6, 128.7, 74.5, 30.2 ppm; HRMS (ESI^-) calculated for $C_9H_8ClO_4S$ $[M–H]^-$ 246.9832; found: 246.9837.



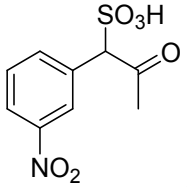
2-Oxo-1-(p-tolyl)propane-1-sulfonic acid (**4c**): White powder (166 mg, 73%); mp 229 °C (decomposed); ^1H NMR (300 MHz, DMSO-d_6) δ 7.37 (d, J = 7.8 Hz, 2H), 7.05 (d, J = 7.6 Hz, 2H), 4.81 (s, 1H), 2.29 (s, 3H), 2.25 (s, 3H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 202.2, 135.7, 131.9, 129.7, 127.9, 77.3, 29.9, 20.7 ppm; HRMS (ESI^-) calculated for $C_{10}H_{11}O_4S$ $[M–H]^-$ 227.0378; found: 227.0385.



1-(4-Nitrophenyl)-2-oxopropane-1-sulfonic acid (**4d**): Pale yellow powder (225 mg, 87%); mp 190 °C (decomposed); ^1H NMR (300 MHz, D_2O) δ 8.13 (d, J = 8.5 Hz, 2H), 7.77 (d, J = 8.8 Hz, 2H), 5.31 (s, 1H), 2.40 (s, 3H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 200.8, 146.3, 142.8, 131.3, 122.2, 76.4, 30.9 ppm; HRMS (ESI^-) calculated for $C_9H_8NO_6S$ $[M–H]^-$ 258.0072; found: 258.0078.

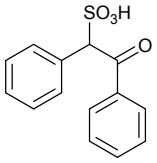


1-(2,4-Dichlorophenyl)-2-oxopropane-1-sulfonic acid (**4e**): White powder (256 mg, 91%); mp 210-212 °C; ^1H NMR (300 MHz, D_2O) δ 7.69 (d, J = 8.2 Hz, 1H), 7.60 (s, 1H), 7.40 (d, J = 8.2 Hz, 1H), 5.89 (s, 1H), 2.37 (s, 3H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 203.4, 134.9, 134.5, 130.9, 129.0, 127.4, 127.0, 70.4, 29.8 ppm; HRMS (ESI^-) calcd for $C_9H_7Cl_2O_4S$ $[M–H]^-$ 280.9442; found: 280.9448.

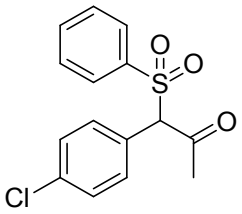


1-(3-Nitrophenyl)-2-oxopropane-1-sulfonic acid (**4f**): Yellow powder (194 mg, 75%); mp 134-136 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.10 (dd, J = 8.2, 2.4 Hz, 1H),

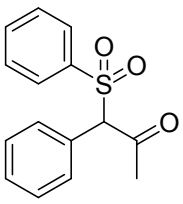
7.88 (d, J = 7.5 Hz, 1H), 7.54 (t, J = 8.0 Hz, 1H), 5.35 (s, 1H), 2.40 (s, 3H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 201.2, 147.1, 137.2, 135.4, 128.6, 124.8, 121.6, 75.7, 31.0 ppm; HRMS (ESI$^-$) calculated for $C_9H_8NO_6S$ [M–H]$^-$ 258.0072; found: 258.0076.



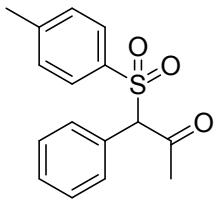
2-oxo-1,2-diphenylethane-1-sulfonic acid (**4g**): White solid (198 mg, 72%); mp 124-127 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.0 (2H, dd, J = 8.5, 1.6 Hz, 2H), 7.57-7.53 (m, 1H), 7.46-7.40 (m, 4H), 7.32-7.29 (m, 2H), 7.24-7.21 (m, 1H), 6.07 (s, 1H), 6.03 (s, 1H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 199.1, 139.7, 134.7, 133.2, 128.8, 128.6, 128.4, 127.7, 127.2, 75.6 ppm; HRMS (ESI$^-$) calculated for $C_{14}H_{11}O_4S$ [M–H]$^-$ 275.0387; found: 275.0378.



1-(4-Chlorophenyl)-1-(phenylsulfonyl)propan-2-one (**5a**): White powder (175 mg, 57%); mp 114-115 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, J = 7.6 Hz, 2H), 7.43-7.26 (m, 7H), 5.24 (s, 1H), 2.38 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 136.7, 134.0, 130.3, 129.7, 129.6, 128.7, 128.5, 127.9, 80.2, 31.6 ppm; Anal. calcd for $C_{15}H_{13}ClO_3S$: C, 58.35; H, 4.24; Found: C, 58.06; H, 4.18.

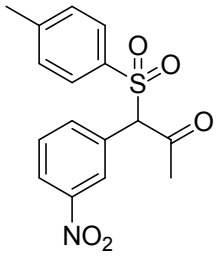


1-Phenyl-1-(phenylsulfonyl)propan-2-one (5b): White powder (214 mg, 78%); mp 111-112 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61-7.56 (m, 3H), 7.43-7.23 (m, 7 H), 5.25 (s, 1H), 2.49 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 136.6, 134.0, 130.3, 129.7, 129.6, 128.7, 128.5, 127.8, 80.1, 31.6 ppm; HRMS (ESI$^+$) calculated for $C_{15}H_{18}NO_3S$ [M+NH_4]$^+$ 292.1007; found: 292.1001.

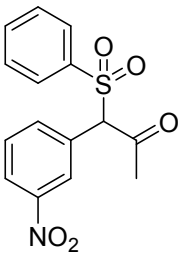


1-Phenyl-1-tosylpropan-2-one (**5c**): White powder (219 mg, 76%); mp 148-150°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (d, J = 8.2 Hz, 2H), 7.37-7.25 (m, 5H), 7.21 (d, J = 9.3

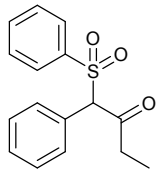
Hz, 2H), 5.22 (s, 1H), 2.46 (s, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.0, 145.1, 133.7, 130.3, 129.7, 129.5, 129.2, 128.7, 128.0, 80.2, 31.6, 21.6 ppm; HRMS (ESI^+) calculated for $C_{16}H_{20}NO_3S$ $[M+NH_4]^+$ 306.1164; found: 306.1157.



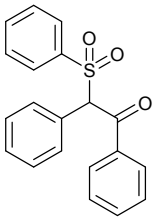
1-(3-Nitrophenyl)-1-tosylpropan-2-one (**5d**): White powder (240 mg, 72%); mp 148-150°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.24-8.21 (m, 2H), 7.75 (d, J = 7.4 Hz, 1H), 7.63 (t, J = 7.6 Hz, 1H), 7.51 (d, J = 8.0 Hz, 2H), 7.37 (d, J = 7.8 Hz, 2H), 6.50 (s, 1H), 2.36 (s, 3H), 2.27 (s, 3H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 197.9, 147.5, 145.4, 137.1, 133.9, 130.6, 129.9, 129.7, 128.9, 125.2, 124.0, 76.1, 32.2, 21.1 ppm; HRMS (ESI^-) calculated for $C_{16}H_{14}NO_5S$ $[M-H]^-$ 332.0593; found: 332.0598.



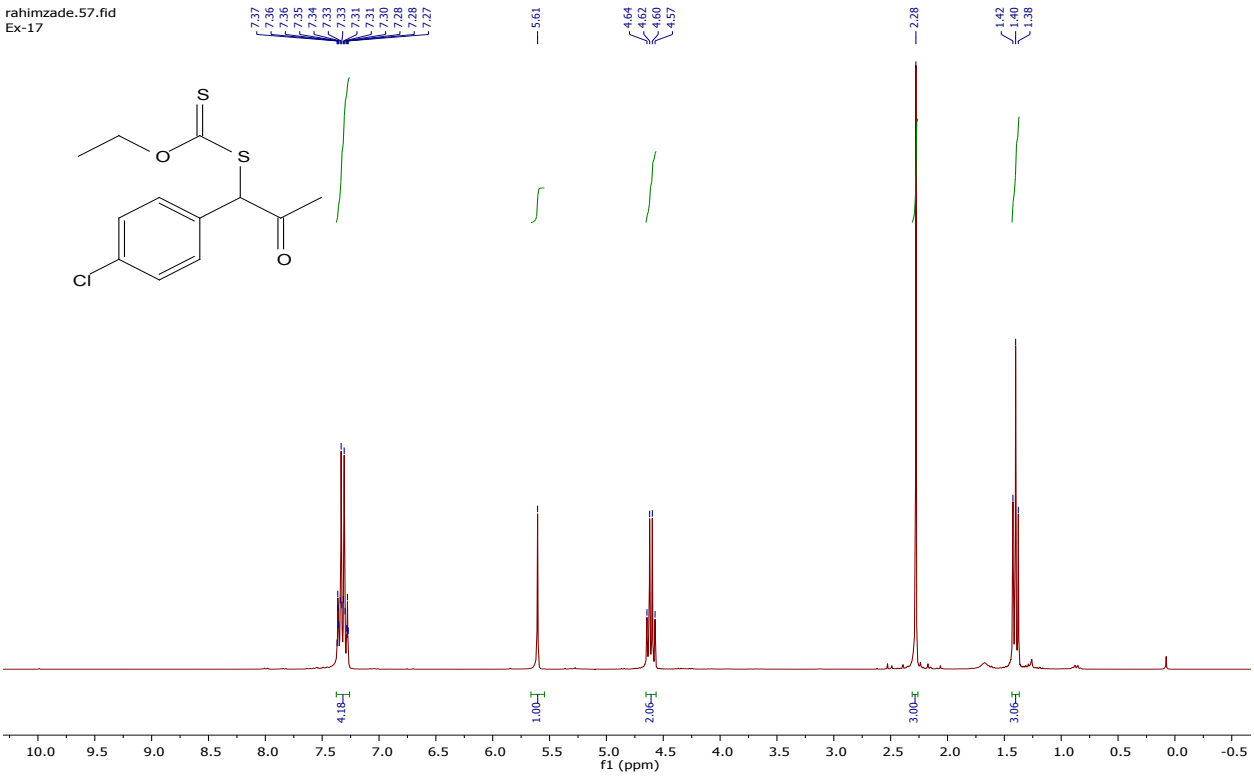
1-(3-Nitrophenyl)-1-(phenylsulfonyl)propan-2-one (**5e**): Grey powder (239 mg, 75%); mp 139-140 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (d, J = 7.9 Hz, 1H), 8.03 (s, 1H), 7.79 (d, J = 7.5 Hz, 1H), 7.67-7.46 (m, 6H), 5.34 (s, 1H), 2.41 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.0, 148.1, 136.3, 135.8, 135.6, 134.8, 130.0, 129.6, 129.0, 125.4, 124.3, 78.9, 32.6; HRMS (ESI^-) calculated for $C_{15}H_{12}NO_5S$ $[M-H]^-$ 318.0436; found: 318.0442.



1-phenyl-1-(phenylsulfonyl)butan-2-one (**5f**): White solid (173 mg, 60%); mp 97-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.26 (m, 5H), 5.09 (s, 1H), 3.93 (brs, 1H), 2.43-2.27 (m, 2H), 1.00 (t, J = 7.3 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 136.7, 134.0, 130.3, 130.0, 129.6, 128.7, 128.5, 128.2, 79.6, 38.2, 7.6 ppm; HRMS (ESI) calculated for $C_{16}H_{16}NaO_3S$ $[M+Na]^+$ 311.0718; found: 311.0712.



1,2-diphenyl-2-(phenylsulfonyl)ethan-1-one (**5g**): White solid (233 mg, 70%); mp 117-120 °C (lit.[3]118-120 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.85 (m, 2H), 7.66-7.52 (m, 4H), 7.44-7.26 (m, 9H), 6.13 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.7, 136.9, 136.2, 134.0, 133.9, 130.5, 130.4, 129.7, 129.0, 128.9, 128.8, 128.6, 128.4, 76.3 ppm.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Ex-17
7.37
7.36
7.36
7.35
7.34
7.33
7.33
7.31
7.31
7.30
7.28
7.28
7.27
5.61
4.64
4.62
4.60
4.57
2.28
1.42
1.40
1.38
S
O
S
O
Cl
4.18
1.00
2.06
3.00
3.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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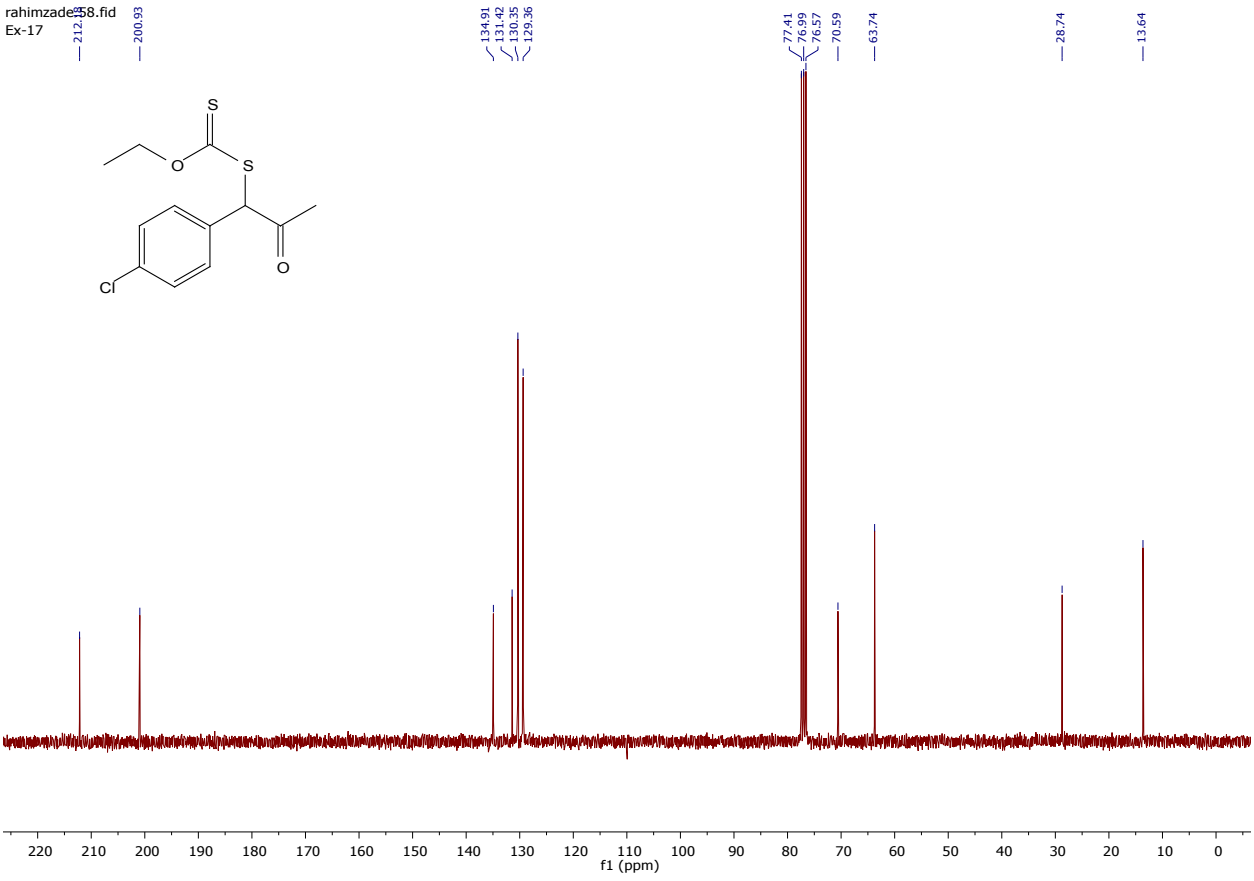
0.5
0.0
-0.5
f1 (ppm)


rahimzade.58.fid
Ex-17
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131.42
130.35
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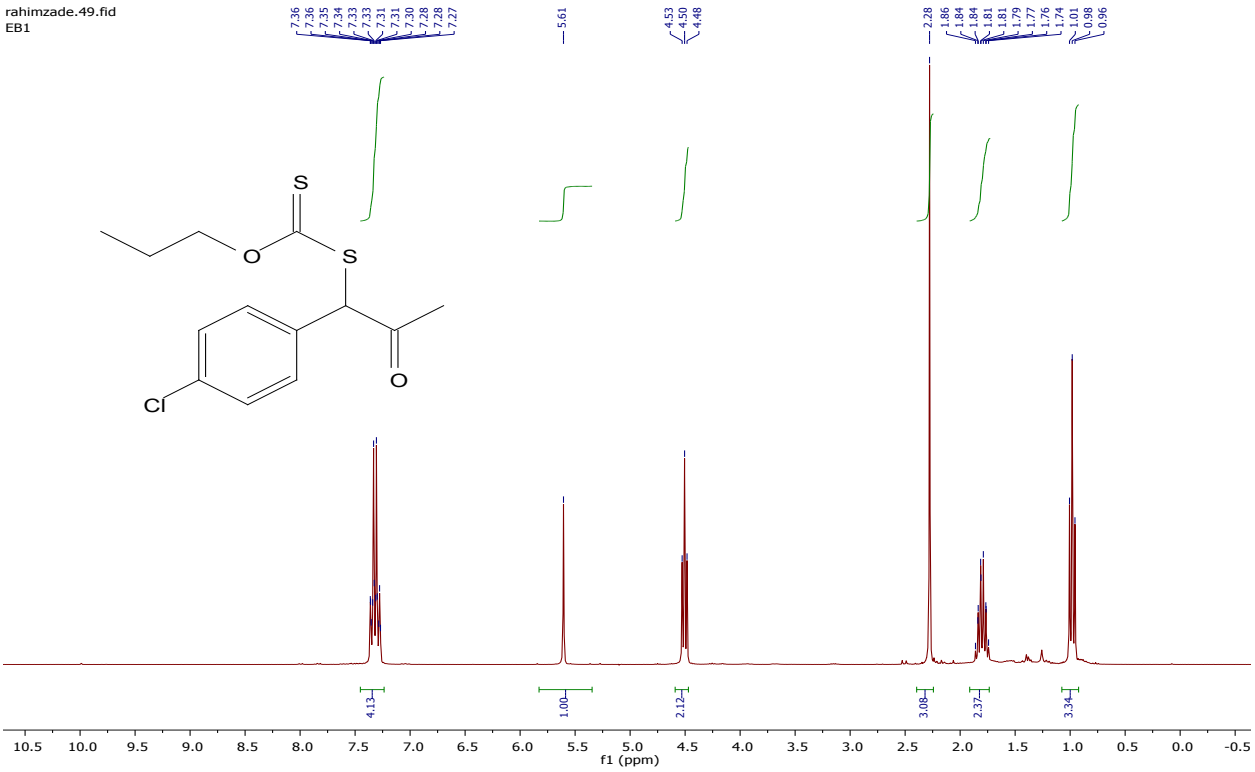
77.41
76.99
76.57
70.59
63.74
28.74
13.64
S
O
S
O
Cl
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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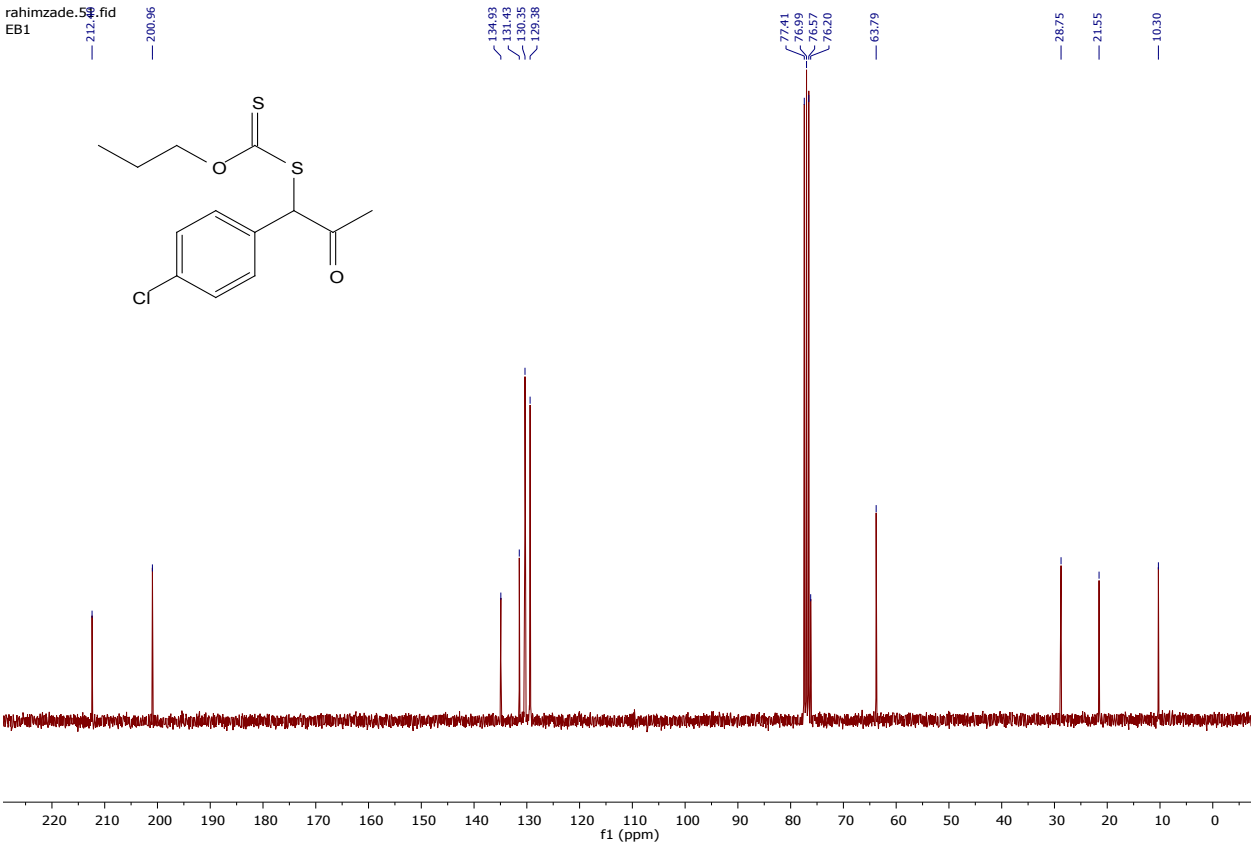
7.36
7.35
7.34
7.33
7.33
7.31
7.31
7.30
7.28
7.28
7.27
5.61
4.53
4.50
4.48
2.28
1.86
1.84
1.84
1.81
1.81
1.79
1.77
1.76
1.74
1.01
0.98
0.96
S
O
S
Cl
O
4.13
1.00
2.12
3.08
2.37
3.34
f1 (ppm)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EB1
212.24
200.96
134.93
131.43
130.35
129.38
77.41
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76.20
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28.75
21.55
10.30
S
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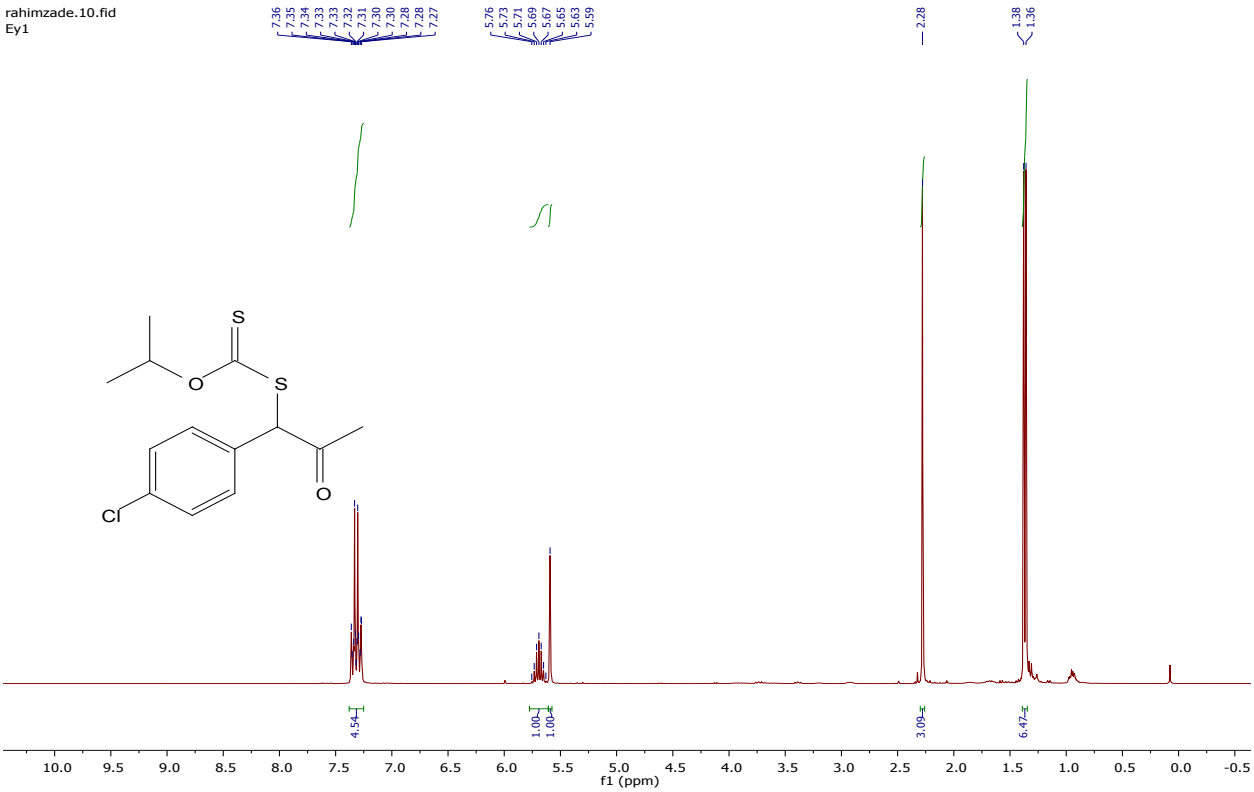
S
Cl
O
f1 (ppm)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Ey1
7.36
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.28
7.28
7.27
5.76
5.73
5.71
5.69
5.67
5.65
5.63
5.59
2.28
1.38
1.36
S
O
S
O
Cl
4.54
1.00
1.00
3.09
6.47
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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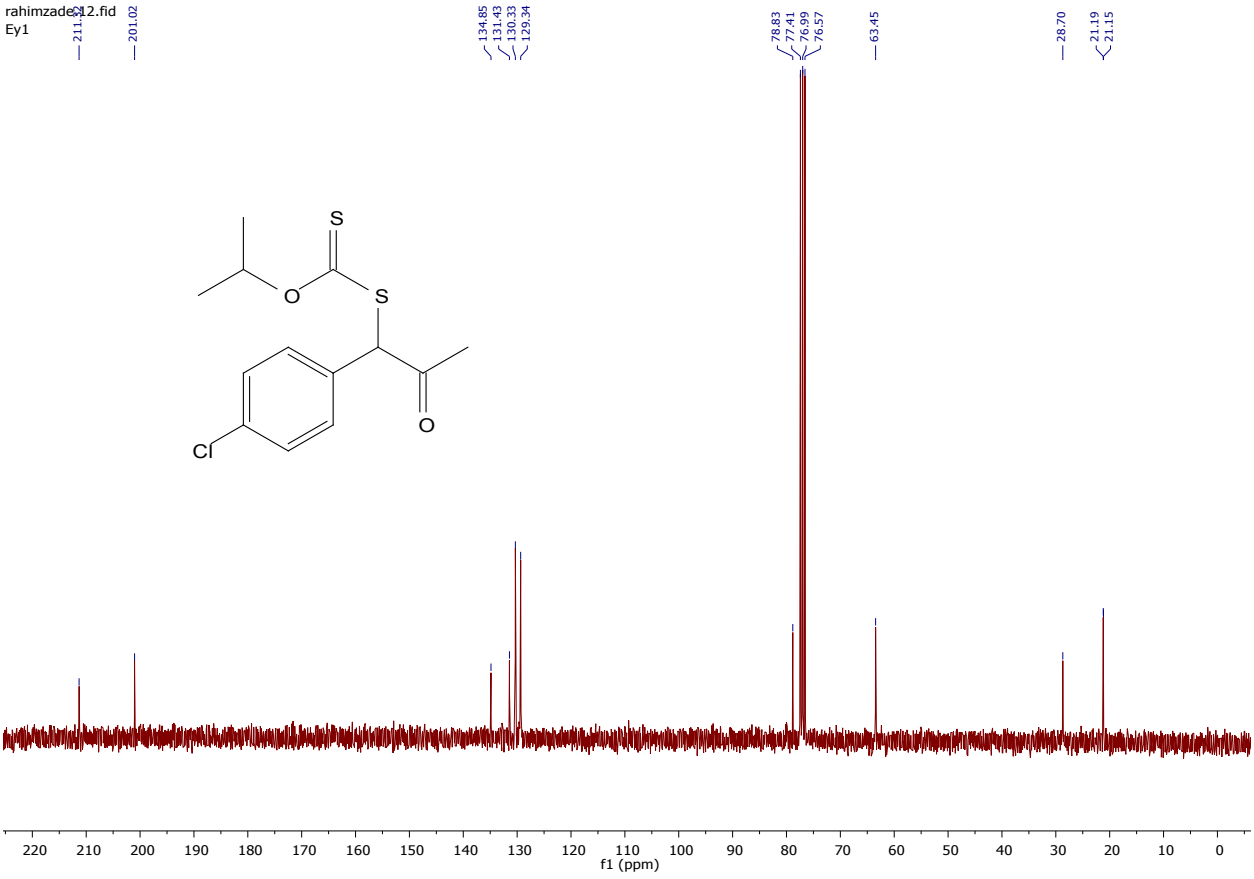
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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130.33
129.34
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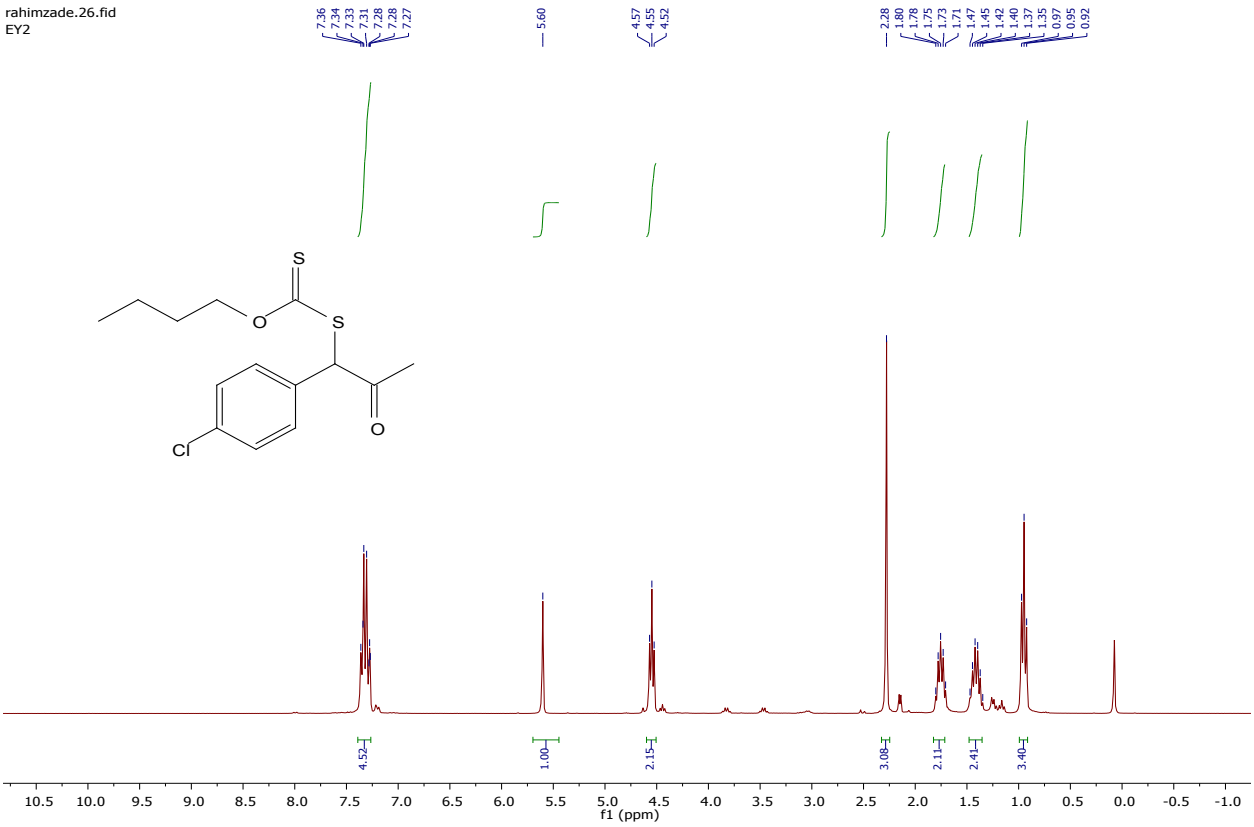
76.57
63.45
28.70
21.19
21.15
S
O
S
O
Cl
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


rahimzade.26.fid
EY2
7.36
7.34
7.33
7.31
7.28
7.28
7.27
5.60
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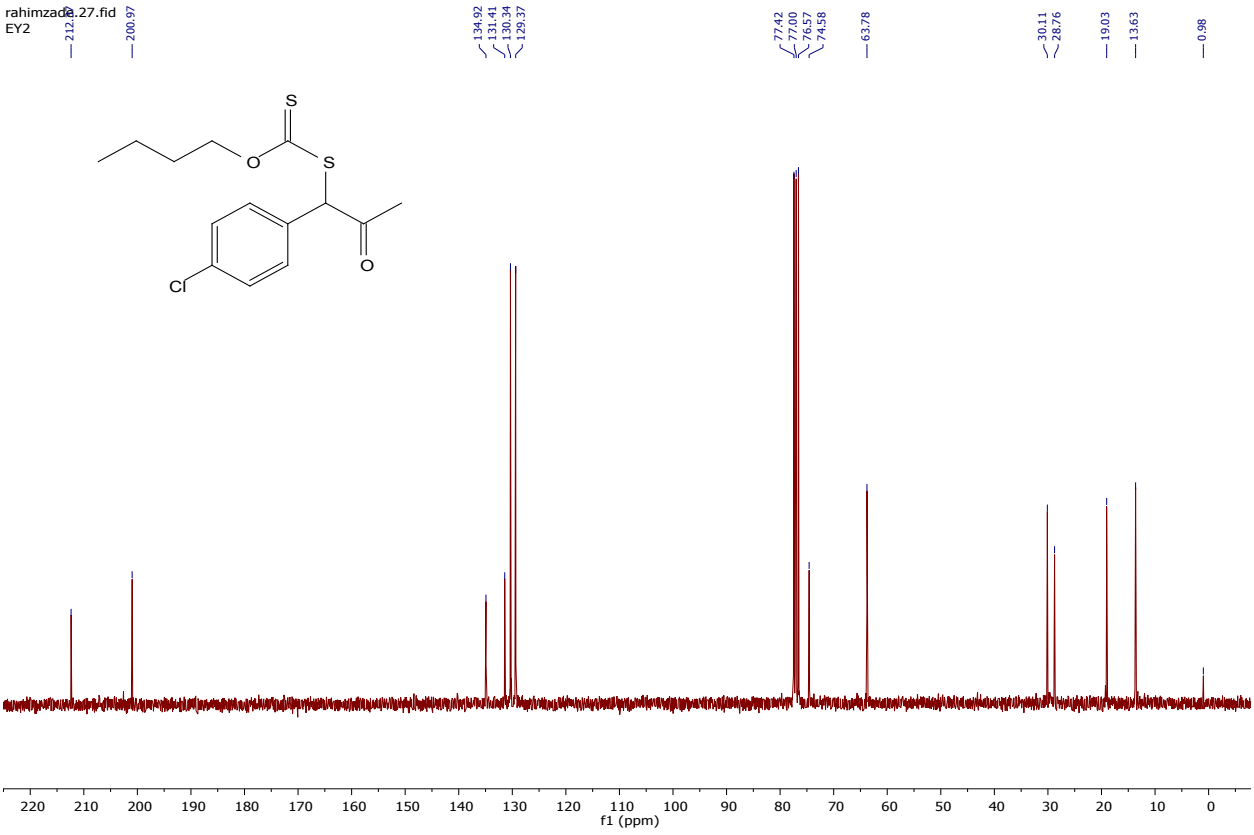
4.55
4.52
2.28
1.80
1.78
1.75
1.73
1.71
1.47
1.45
1.42
1.40
1.37
1.35
0.97
0.95
0.92
S
O
S
Cl
O
4.52
1.00
2.15
3.08
2.11
2.41
3.40
f1 (ppm)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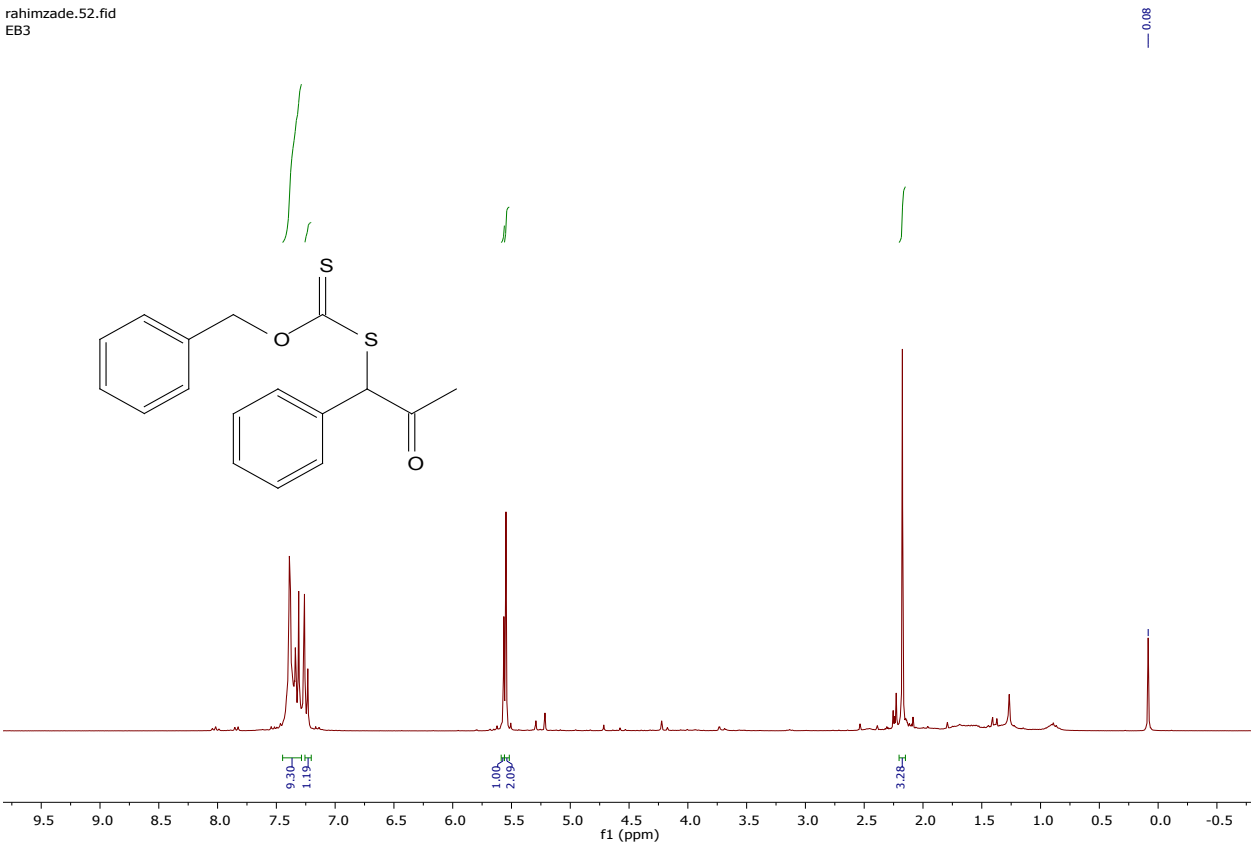
EY2
212.
200.97
134.92
131.41
130.34
129.37
77.42
77.00
76.57
74.58
63.78
30.11
28.76
19.03
13.63
0.98
S
O
S
Cl
O
f1 (ppm)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S
O
S
O
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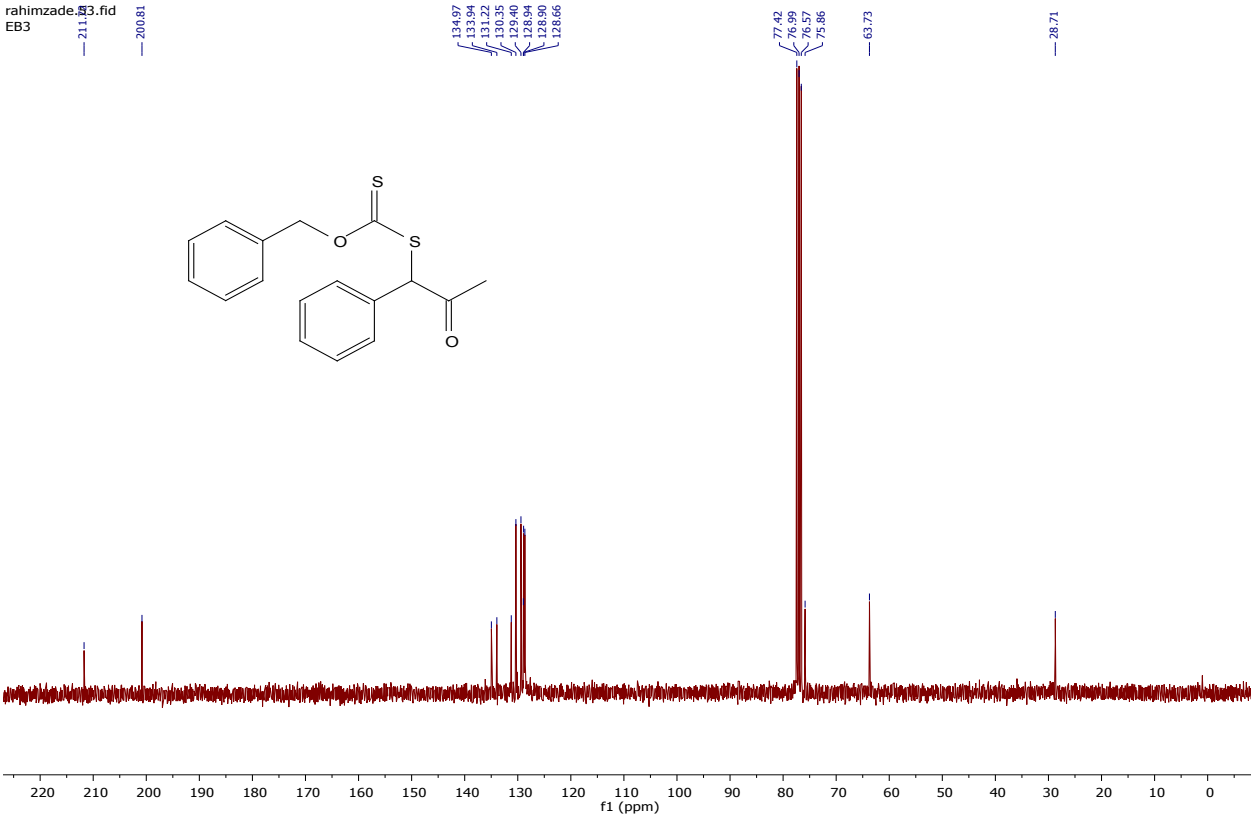
1.19
1.00
2.09
3.28
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.97
133.94
131.22
130.35
129.40
128.94
128.90
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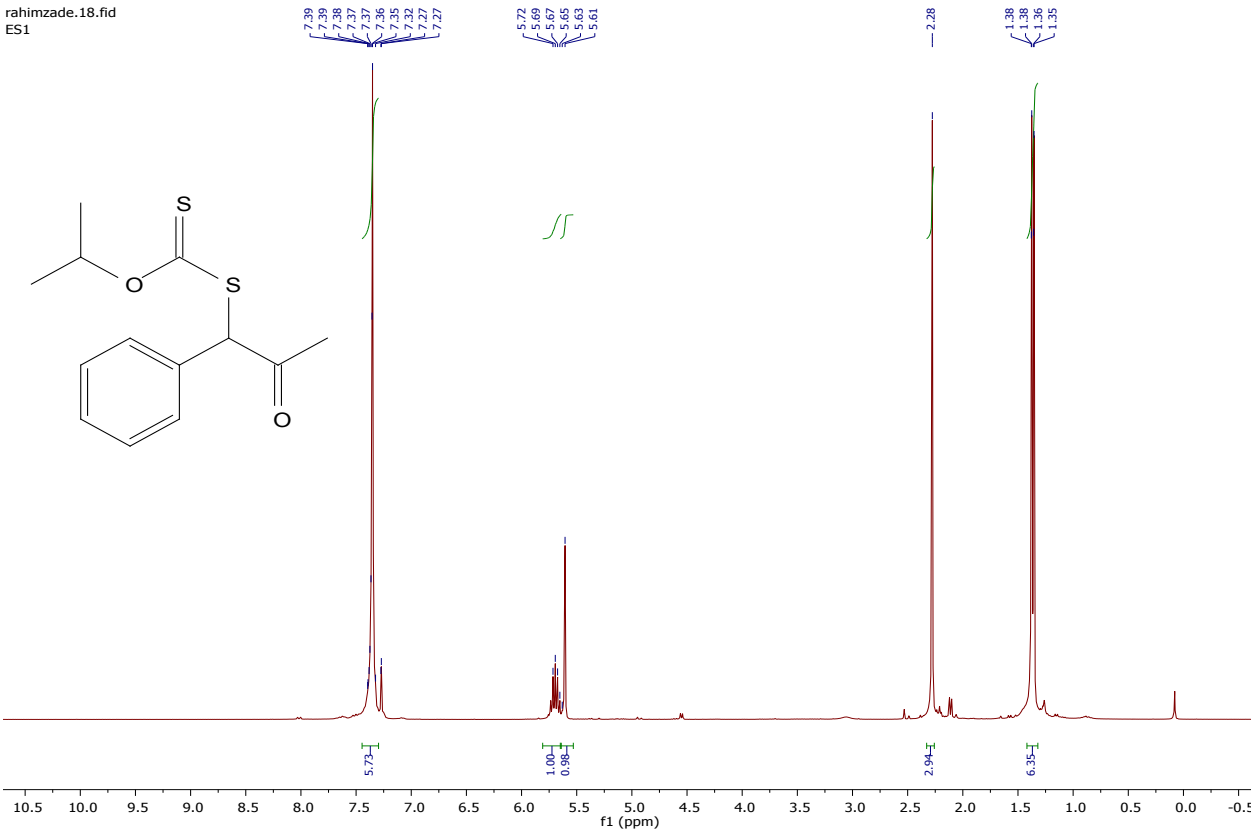
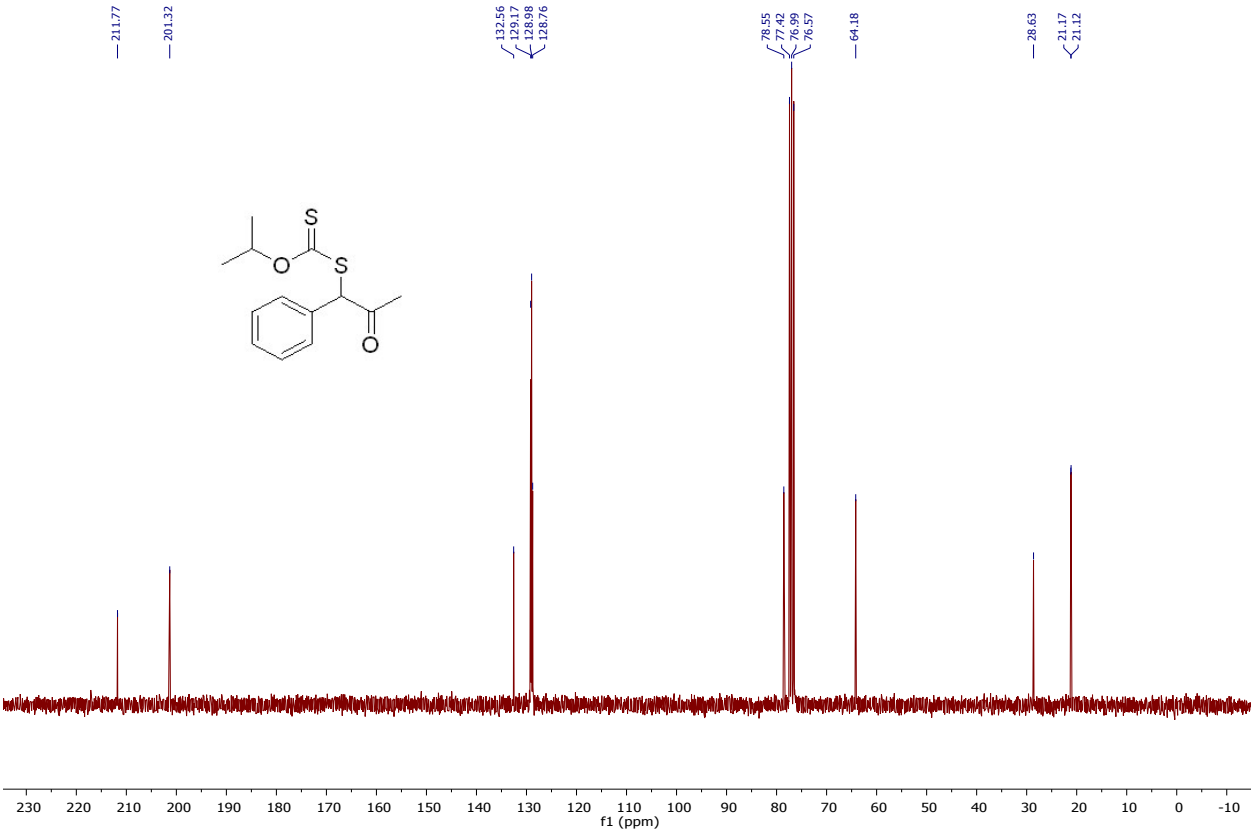
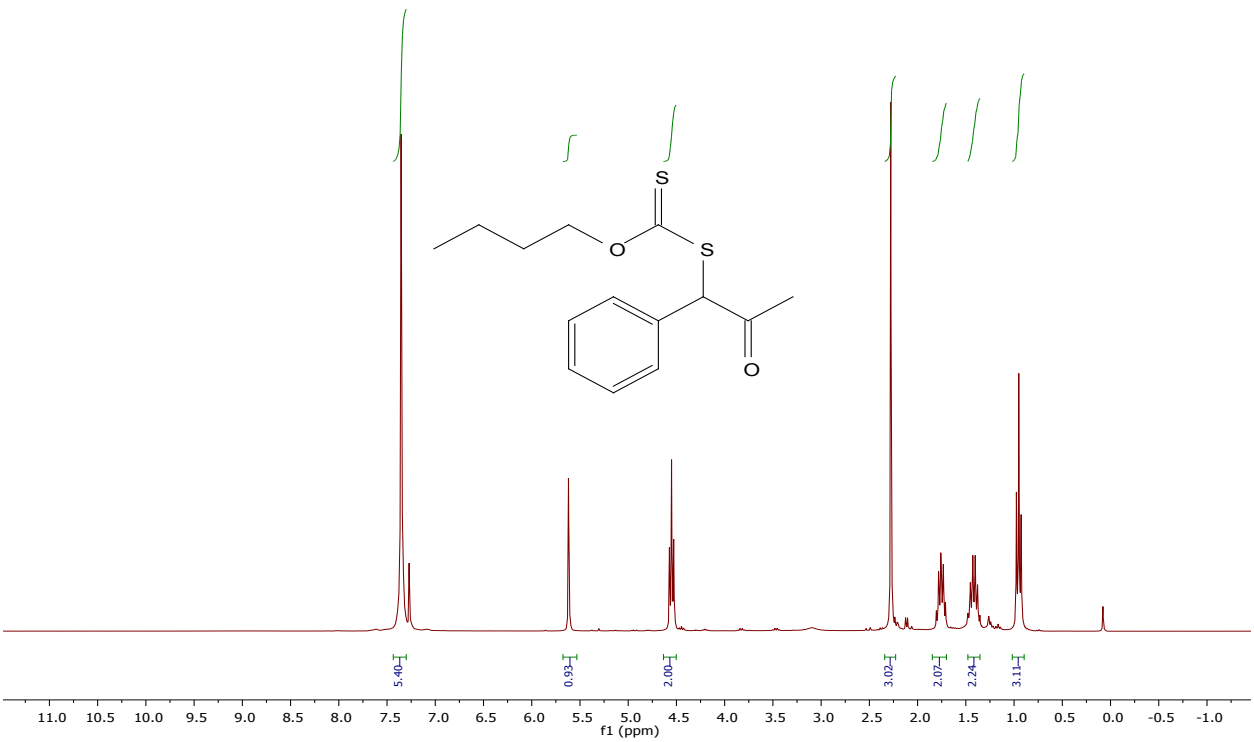
76.99
76.57
75.86
63.73
28.71
S
O
S
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

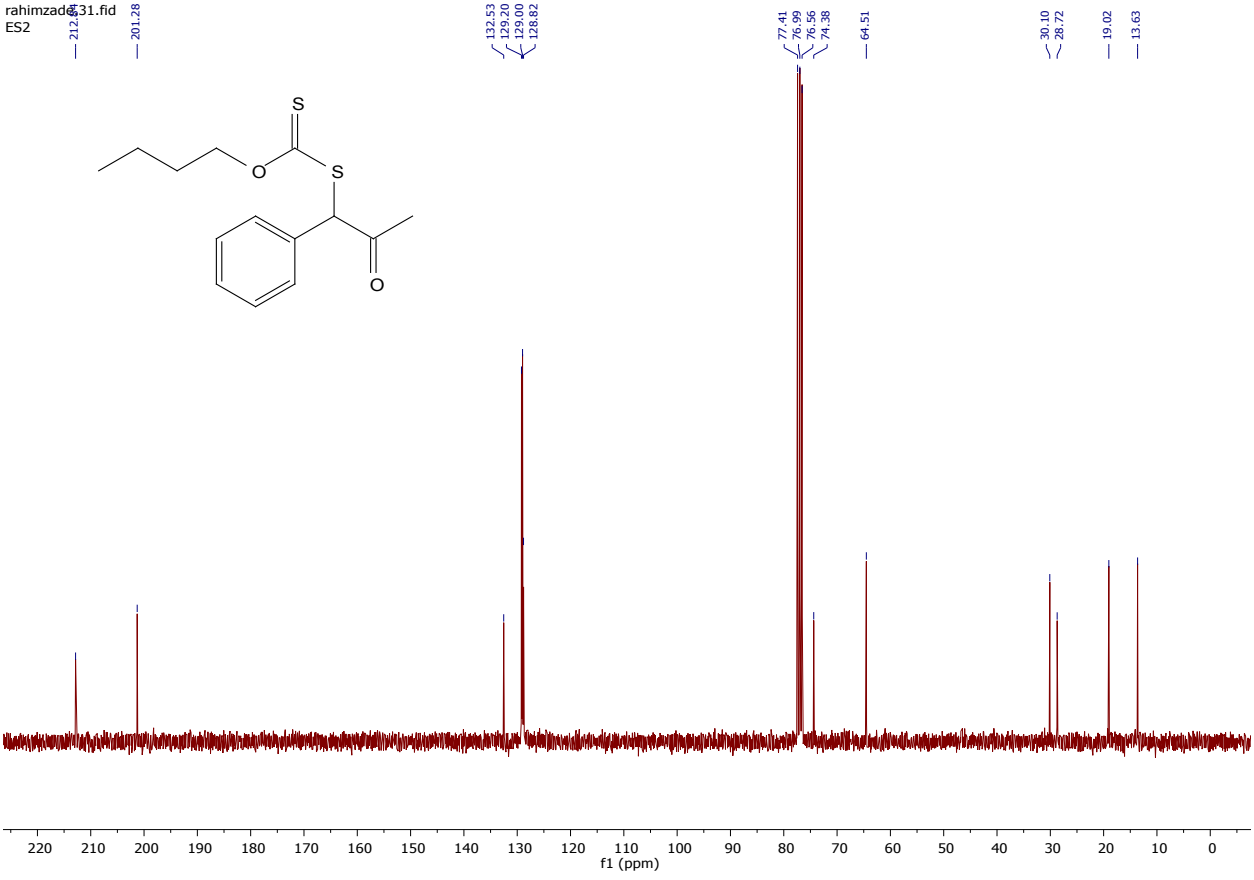

rahimzade.18.fid
ES1
7.39
7.39
7.38
7.37
7.37
7.36
7.35
7.32
7.27
7.27
5.72
5.69
5.67
5.65
5.63
5.61
2.28
1.38
1.38
1.36
1.35
S
O
S
O
5.73
1.00
0.98
2.94
6.35
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

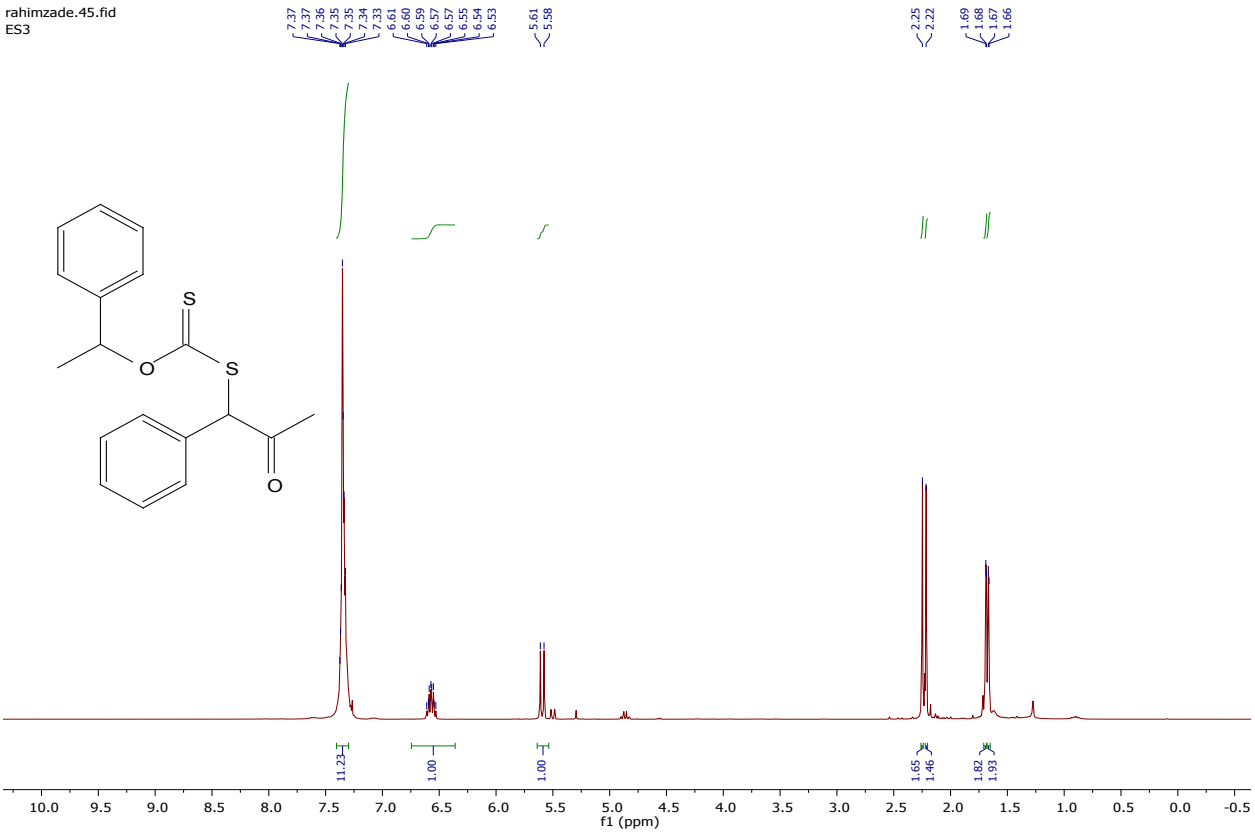

211.77
201.32
132.56
129.17
128.98
128.76
78.55
77.42
76.99
76.57
64.18
28.63
21.17
21.12
S
O
S
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

rahimzade.30.fid
ES2



rahimzade.31.fid
ES2




rahimzade.45.fid
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7.37
7.36
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7.35
7.34
7.33
6.61
6.60
6.59
6.57
6.57
6.55
6.54
6.53
5.61
5.58
2.25
2.22
1.69
1.68
1.67
1.66
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S
O
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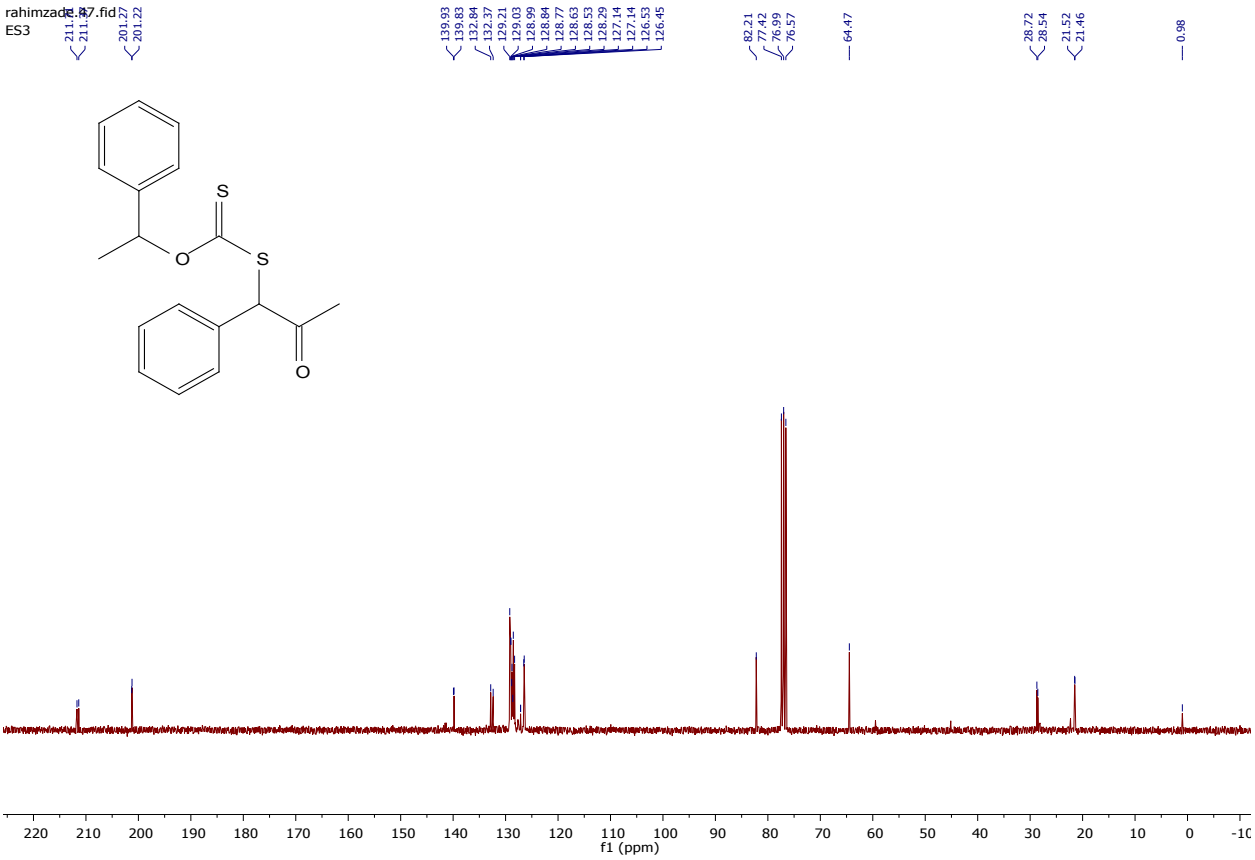
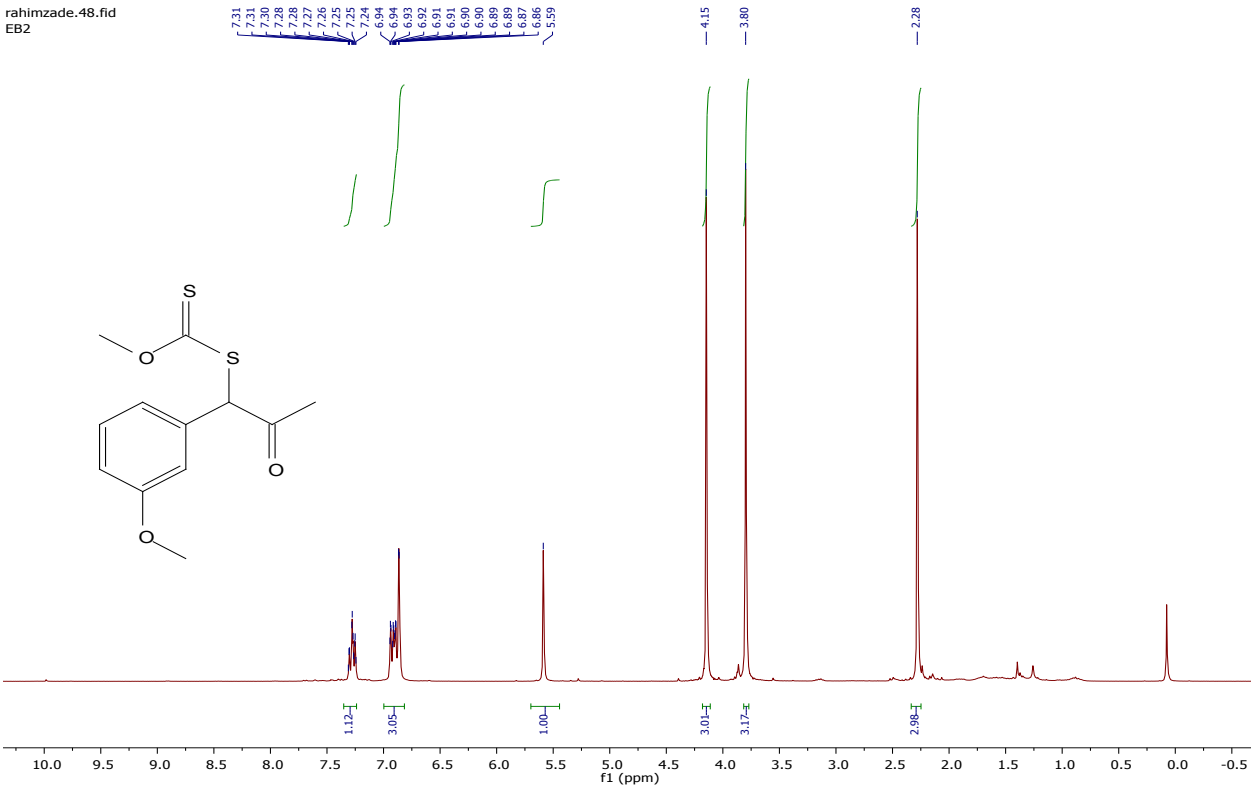
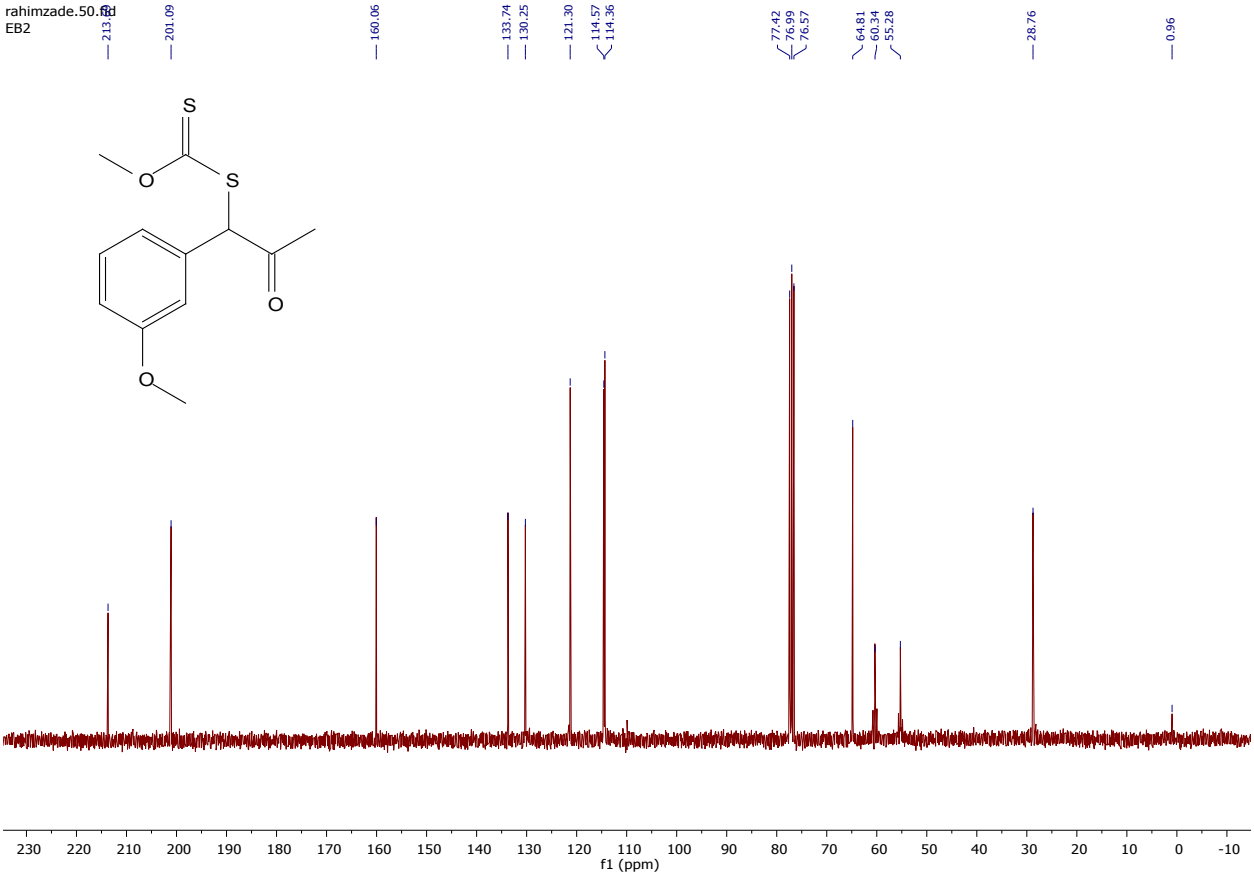
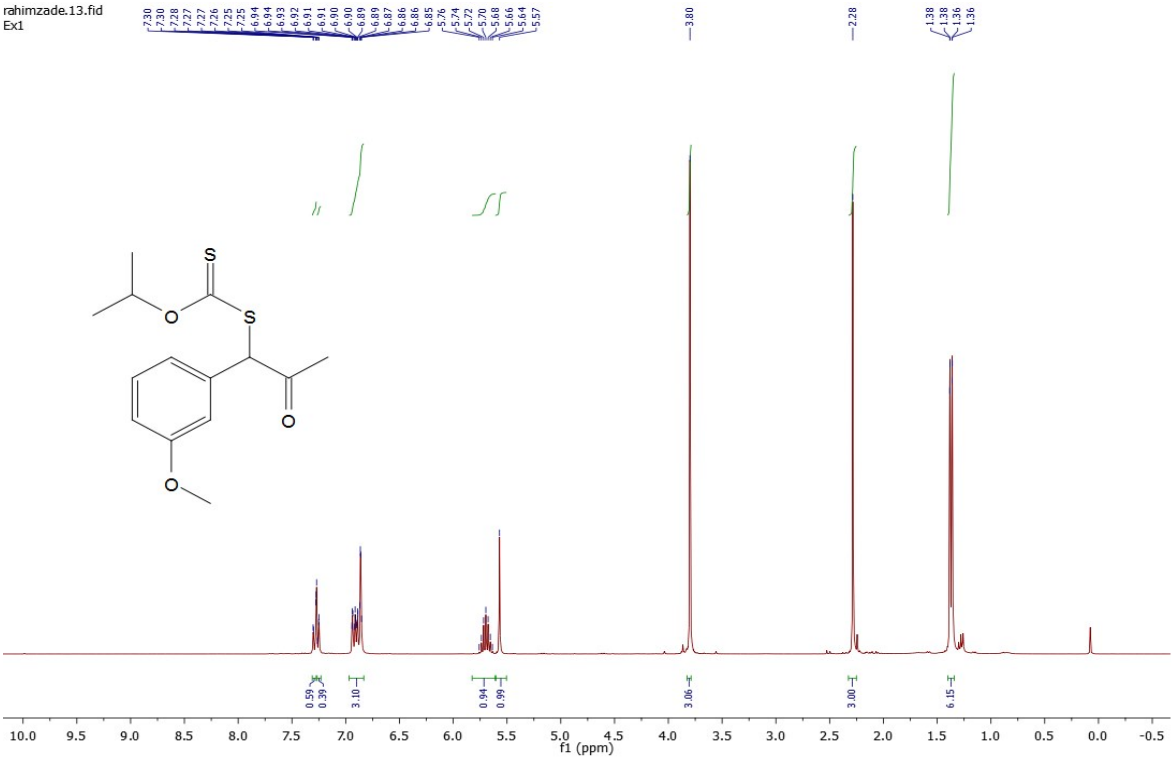
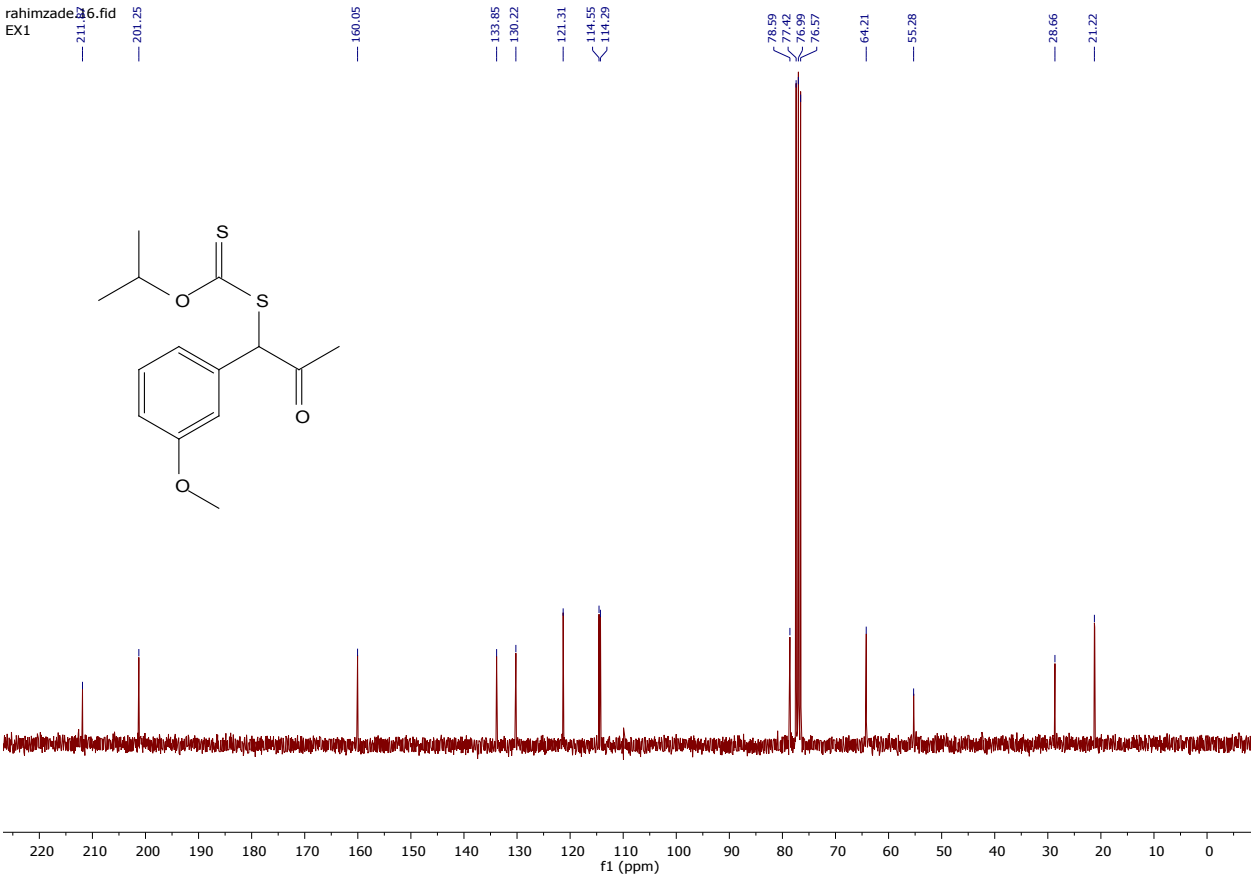
1.65
1.46
1.82
1.93
f1 (ppm)

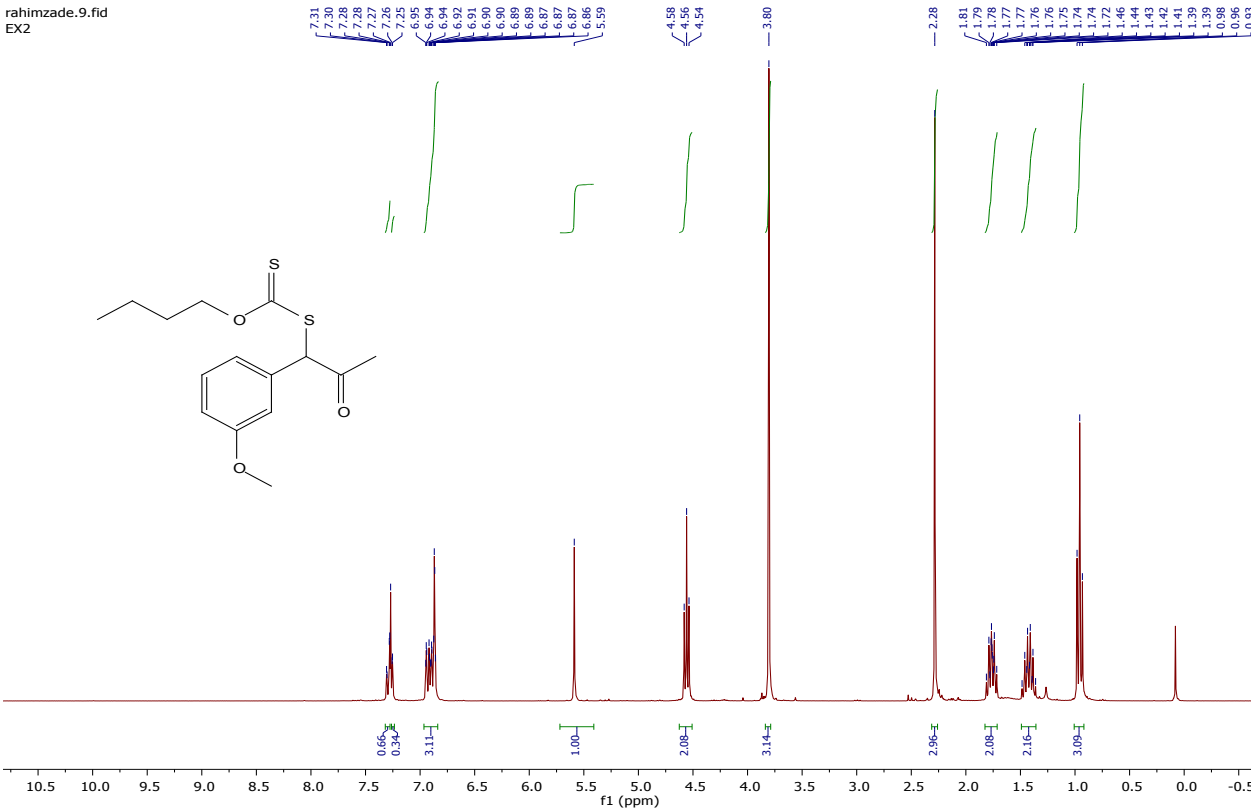

rahimzade.47.fid
ES3
211.77
211.47
201.27
201.22
139.93
139.83
132.84
132.37
129.21
129.03
128.99
128.84
128.77
128.63
128.53
128.29
127.14
127.14
126.53
126.45
82.21
77.42
76.99
76.57
64.47
28.72
28.54
21.52
21.46
0.98
S
O
S
O
f1 (ppm)

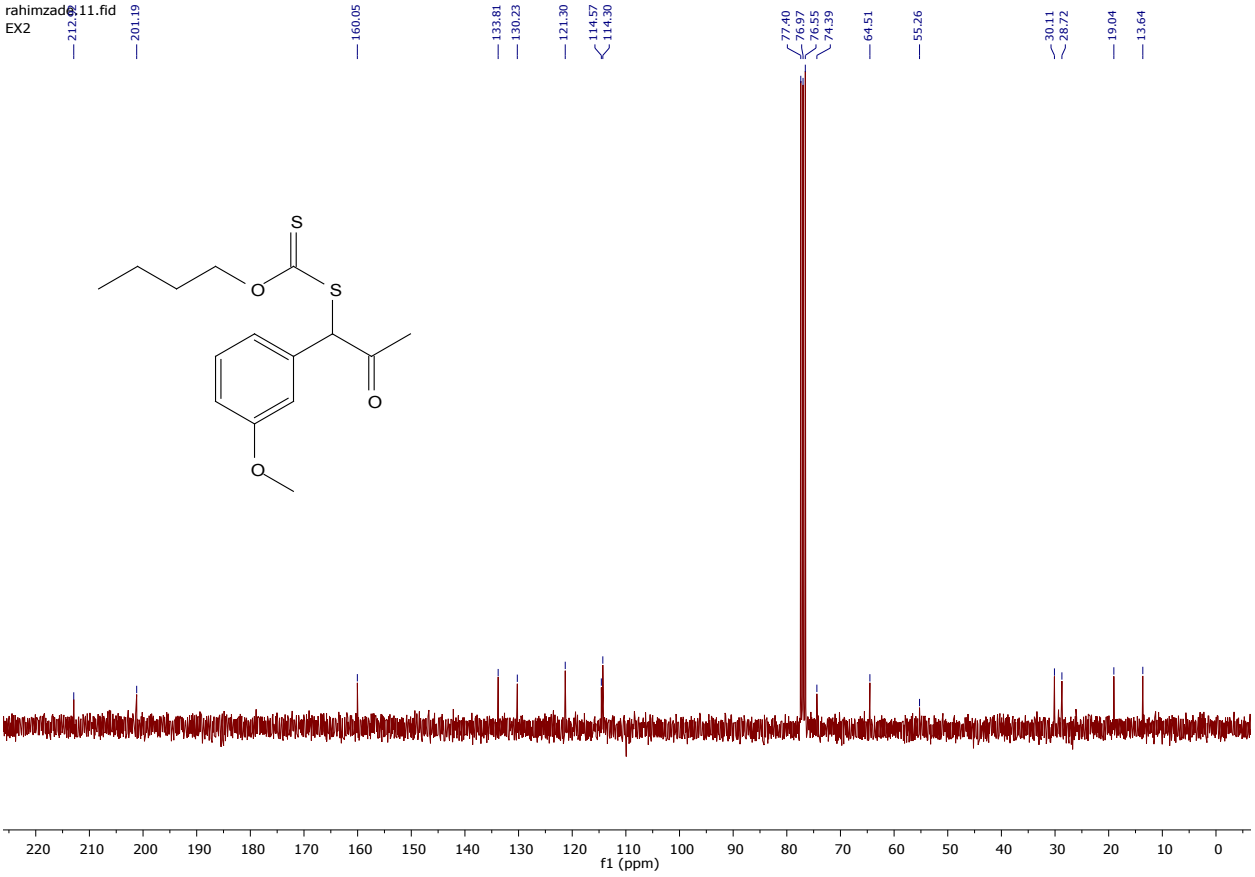

rahimzade.48.fid
EB2
7.31
7.31
7.30
7.28
7.28
7.27
7.26
7.25
7.25
7.24
6.94
6.94
6.93
6.92
6.91
6.91
6.90
6.90
6.89
6.89
6.87
6.86
5.59
4.15
3.80
2.28
S
O
S
O
O
1.12
3.05
1.00
3.01
3.17
2.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

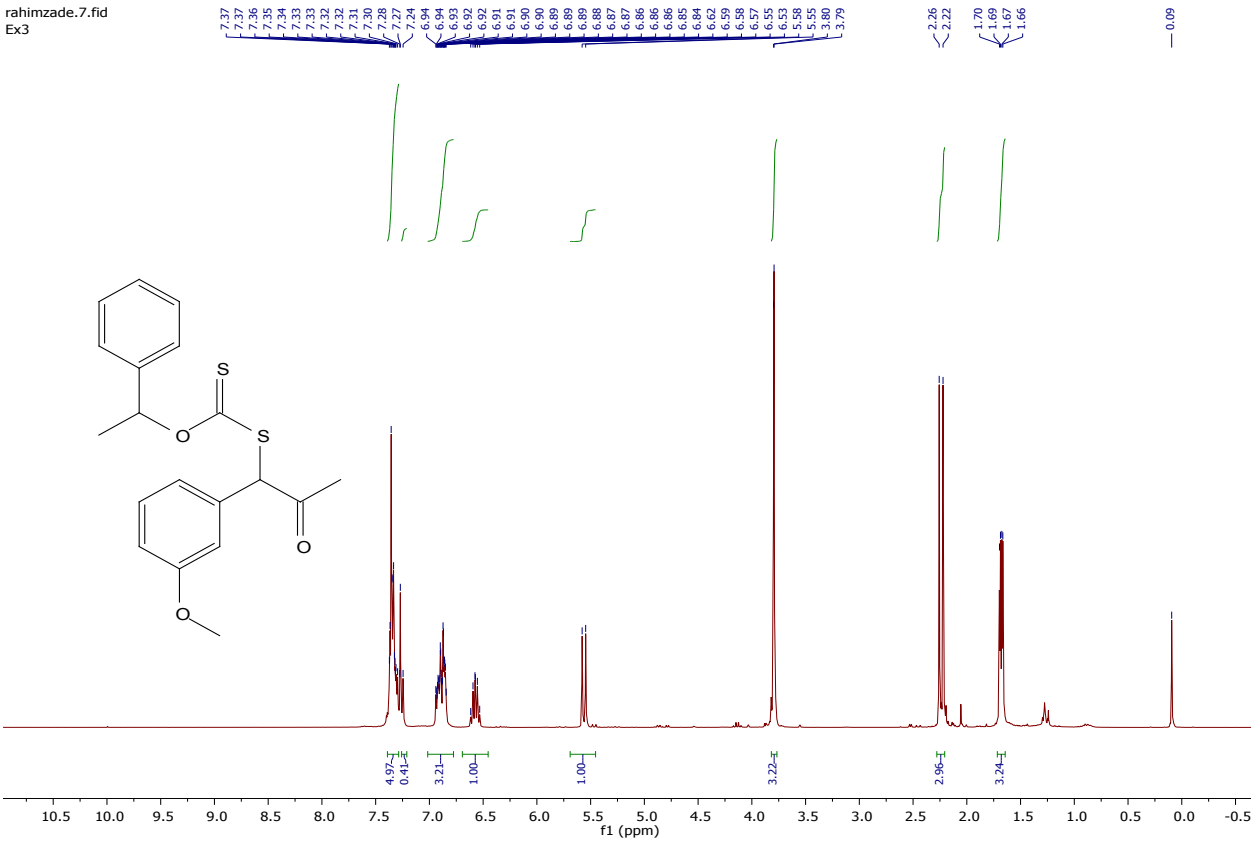

rahimzade.50.fid
EB2
213.81
201.09
160.06
133.74
130.25
121.30
114.57
114.36
77.42
76.99
76.57
64.81
60.34
55.28
28.76
0.96
S
O
S
O
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

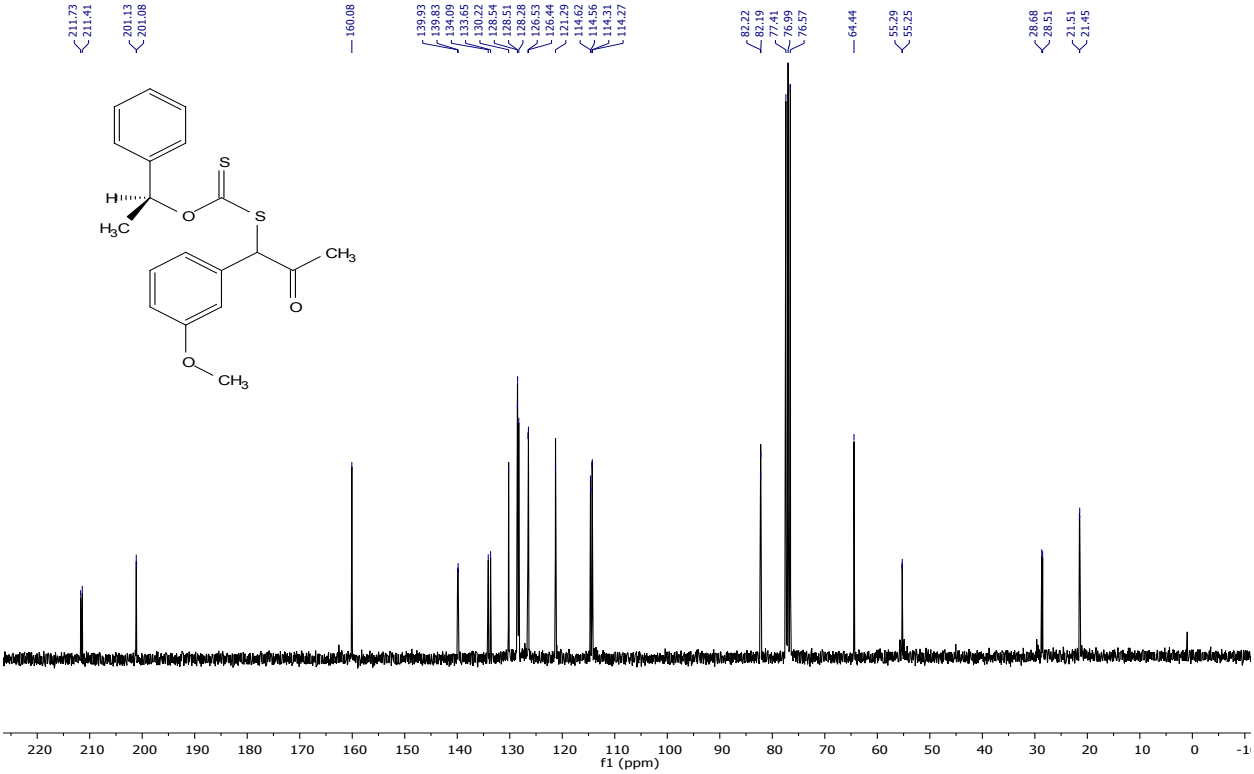

rahimzade.13.fid
Ex1
7.30
7.30
7.28
7.27
7.27
7.26
7.25
7.25
6.94
6.93
6.92
6.91
6.91
6.90
6.90
6.89
6.89
6.87
6.86
6.86
6.85
5.76
5.74
5.72
5.70
5.68
5.66
5.64
5.57
3.80
2.28
1.38
1.38
1.36
1.36
S
O
S
O
O
0.59
0.39
3.10
0.94
0.99
3.06
3.00
6.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

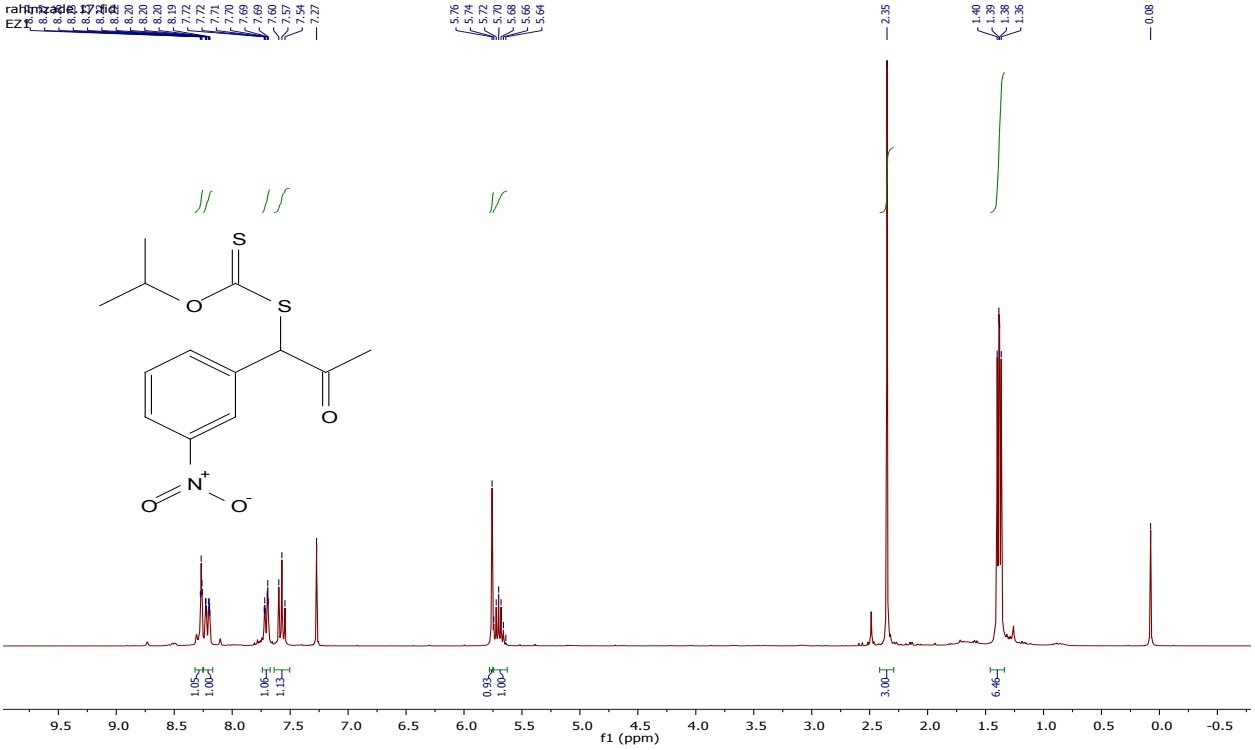

rahimzade.16.fid
EX1
211.84
201.25
160.05
133.85
130.22
121.31
114.55
114.29
78.59
77.42
76.99
76.57
64.21
55.28
28.66
21.22
S
O
S
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

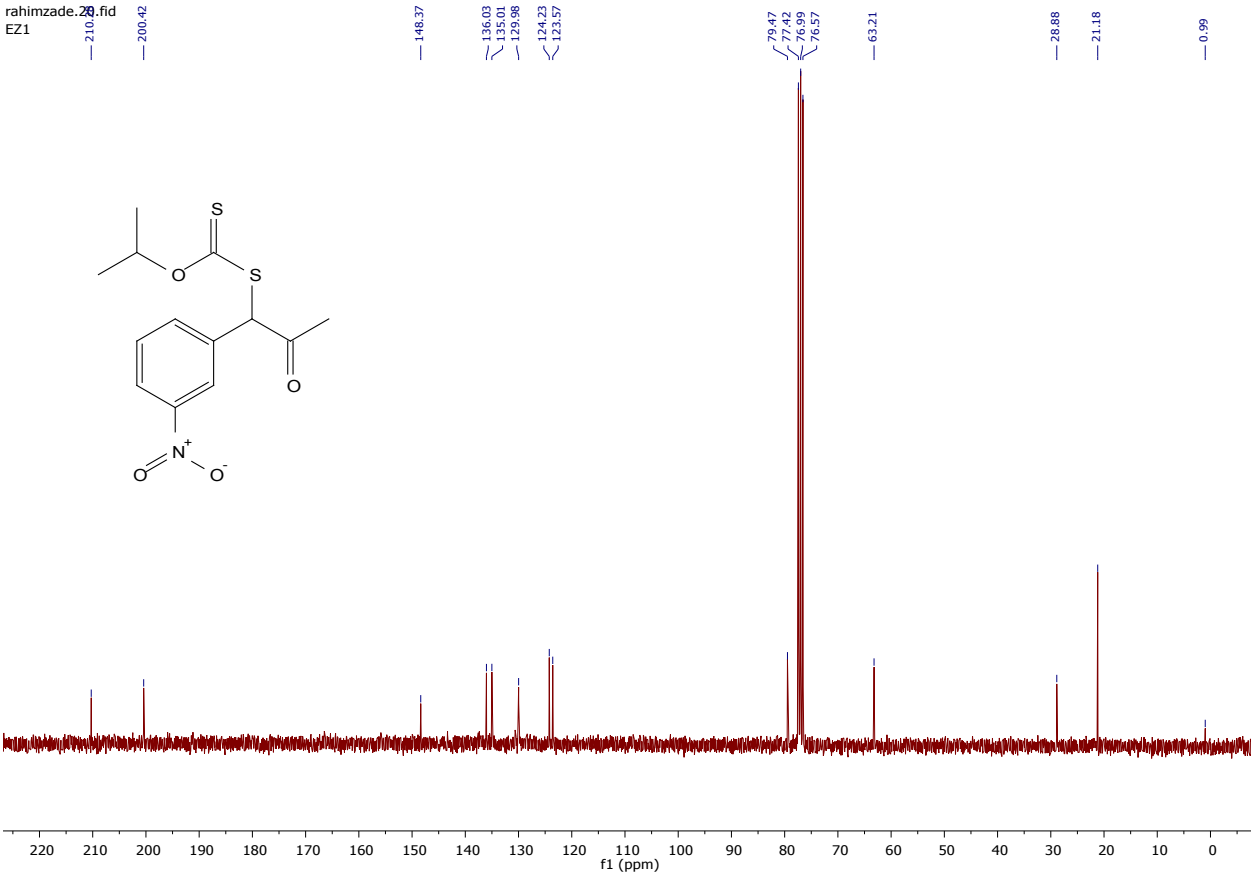

rahimzade.9.fid
EX2
7.31
7.30
7.28
7.28
7.27
7.26
7.25
6.95
6.94
6.94
6.92
6.91
6.90
6.90
6.89
6.89
6.87
6.87
6.87
6.86
5.59
4.58
4.56
4.54
3.80
2.28
1.81
1.79
1.78
1.77
1.77
1.76
1.76
1.75
1.74
1.74
1.72
1.46
1.44
1.43
1.42
1.41
1.39
1.39
0.98
0.96
S
O
S
O
O
0.66
0.34
3.11
1.00
2.08
3.14
2.96
2.08
2.16
3.09
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

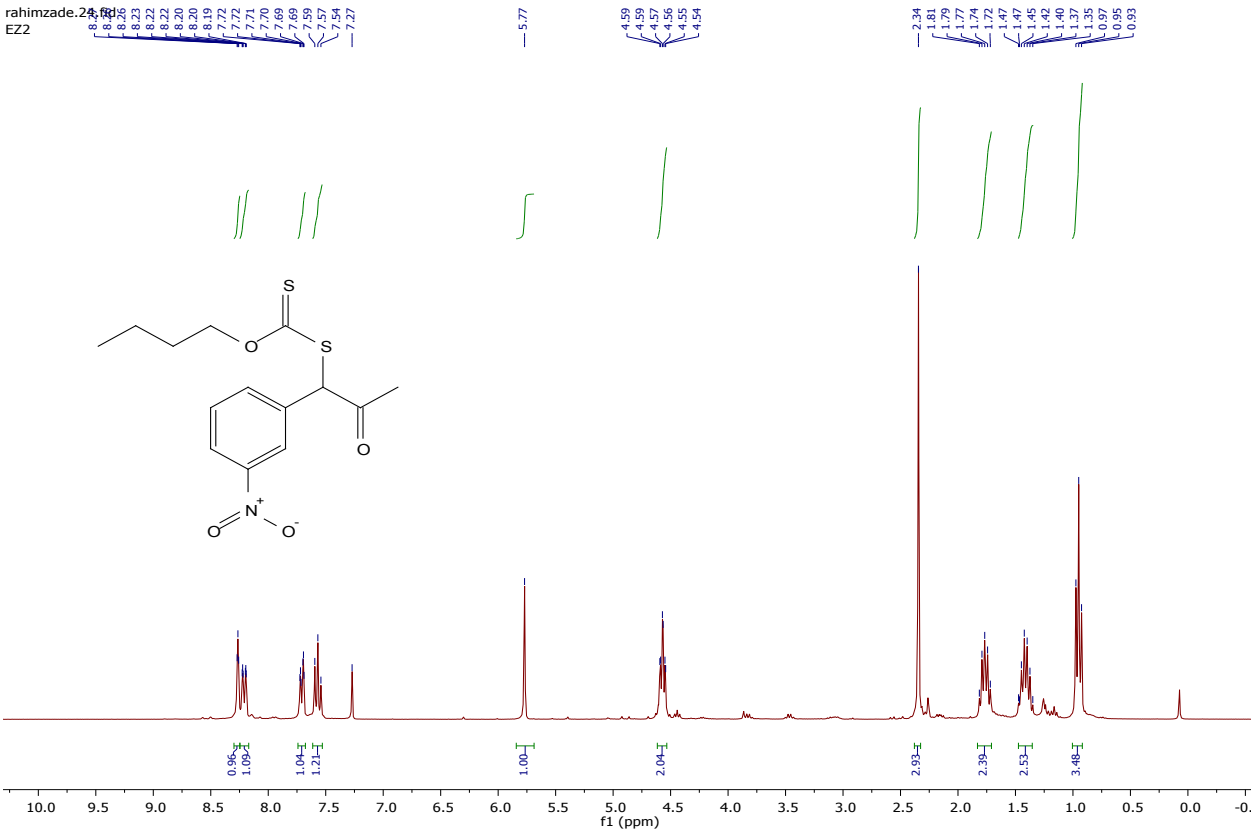

rahimzade.11.fid
EX2
212.6
201.19
160.05
133.81
130.23
121.30
114.57
114.30
77.40
76.97
76.55
74.39
64.51
55.26
30.11
28.72
19.04
13.64
S
O
S
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

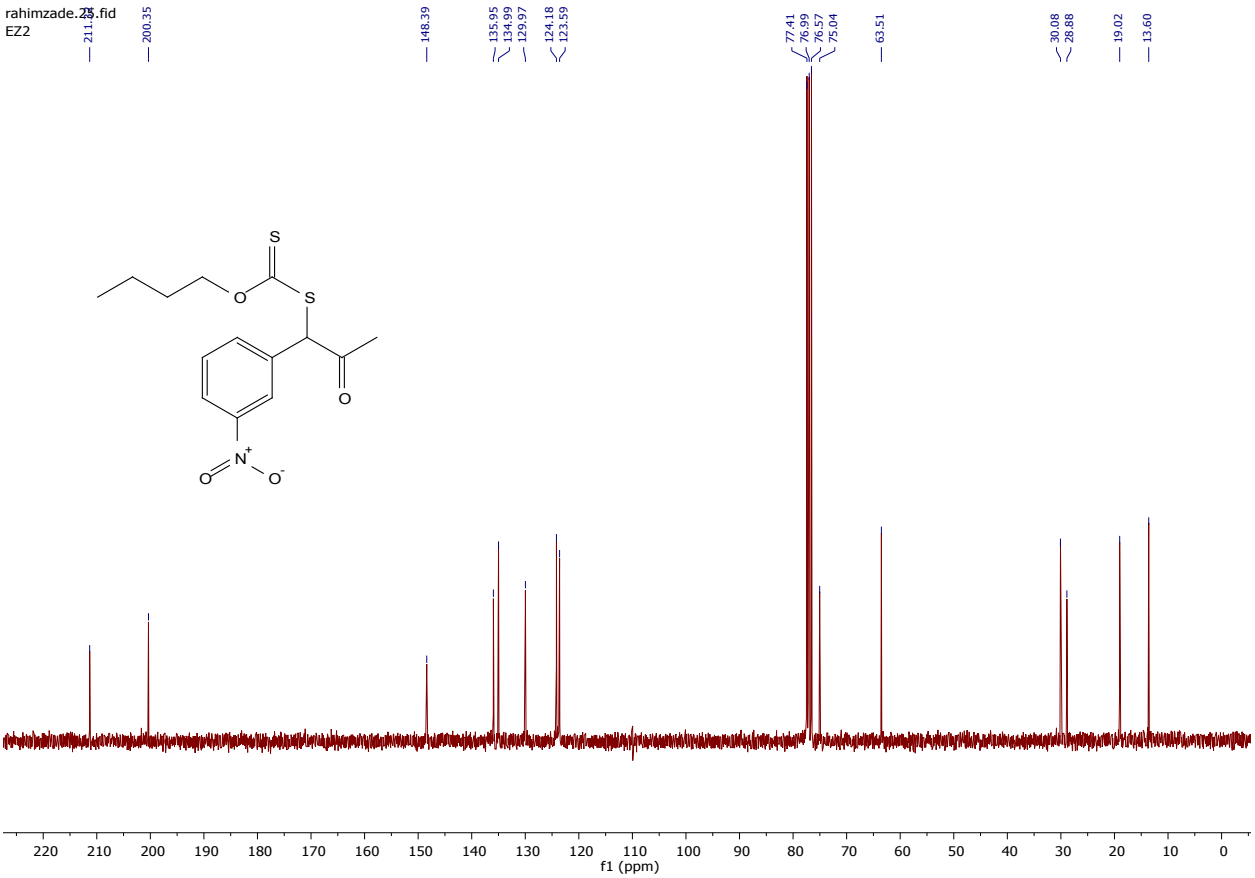

rahimzade.7.fid
Ex3
f1 (ppm)

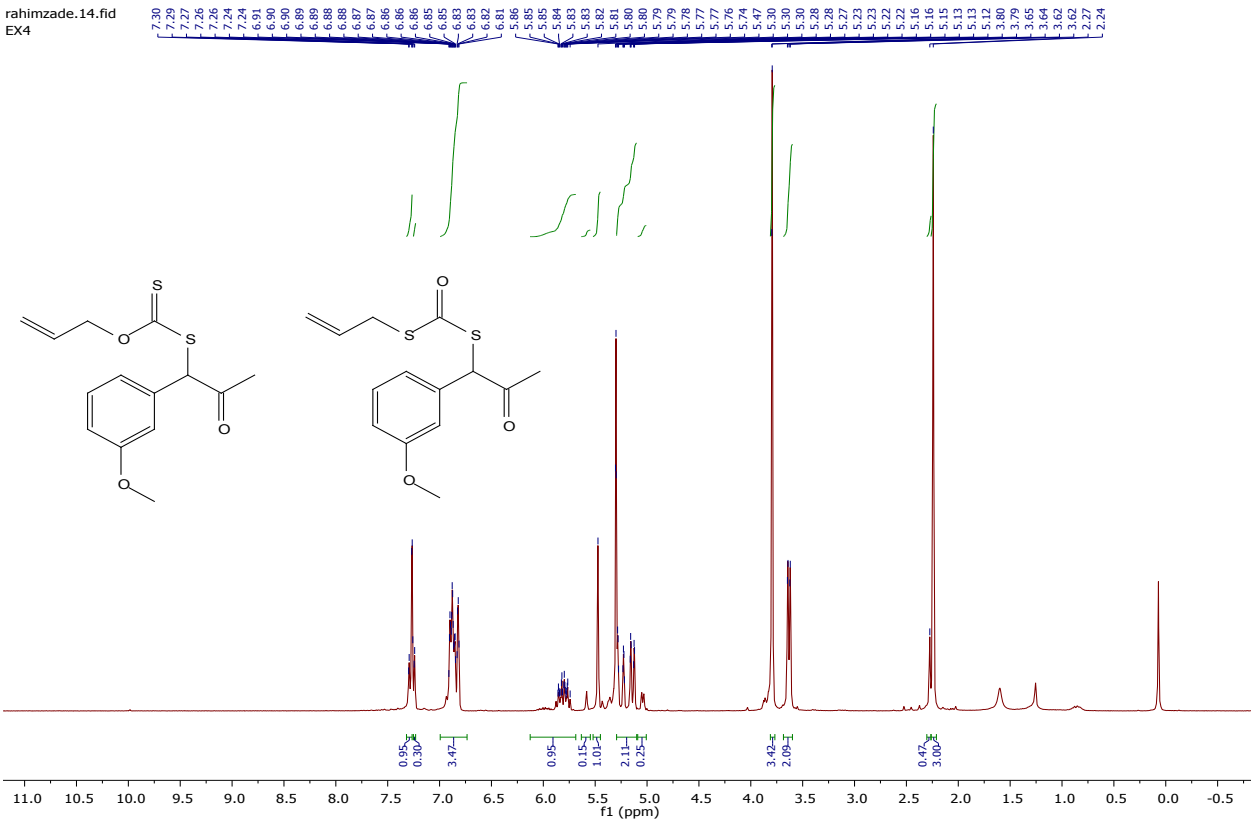

f1 (ppm)

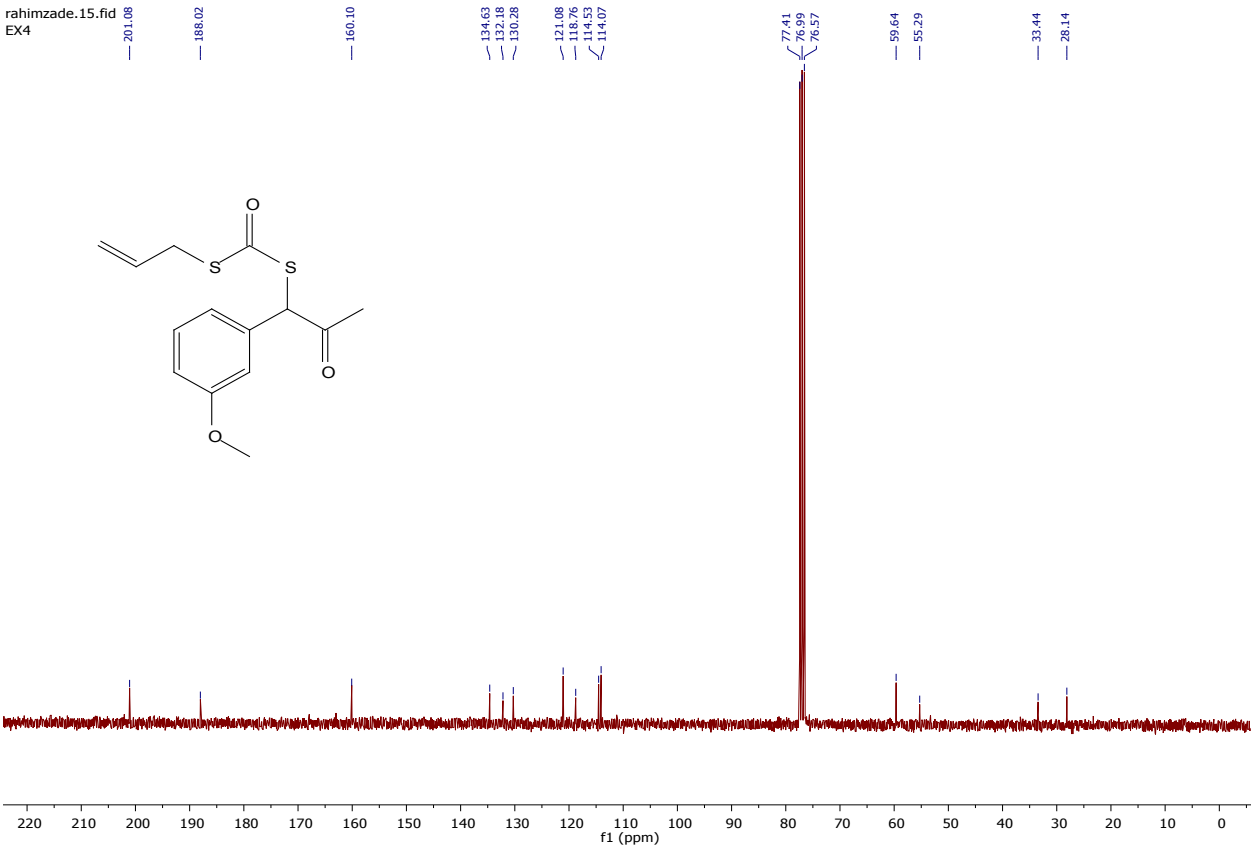

rahimzade.17.fid
EZ1
f1 (ppm)

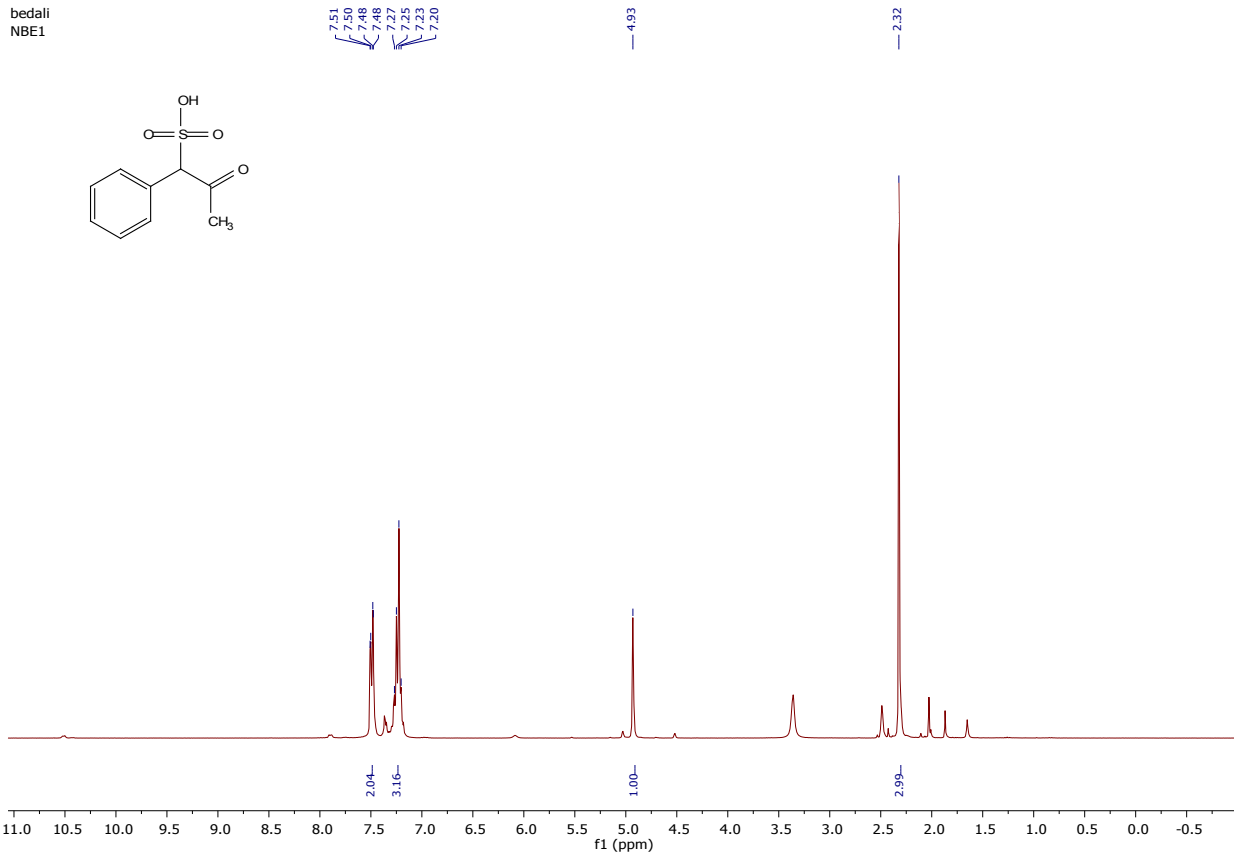

rahimzade.28.fid
EZ1
f1 (ppm)

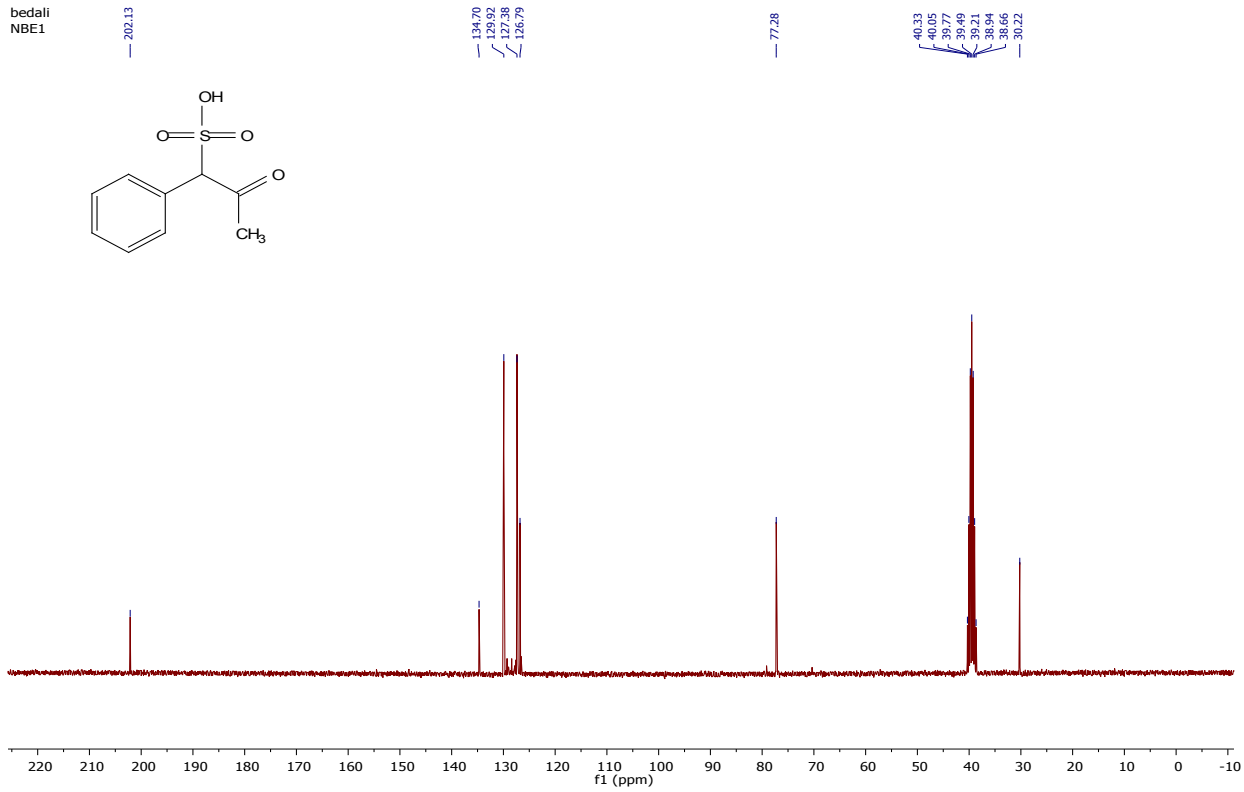

rahimzade.24.fid
EZ2
8.27
8.26
8.26
8.23
8.22
8.22
8.20
8.20
8.19
7.72
7.72
7.71
7.70
7.69
7.69
7.59
7.57
7.54
7.27
5.77
4.59
4.59
4.57
4.56
4.55
4.54
2.34
1.81
1.79
1.77
1.74
1.72
1.47
1.47
1.45
1.42
1.40
1.37
1.35
0.97
0.95
0.93
S
O
S
O
N+
O
O-
0.96
1.09
1.04
1.21
1.00
2.04
2.93
2.39
2.53
3.48
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

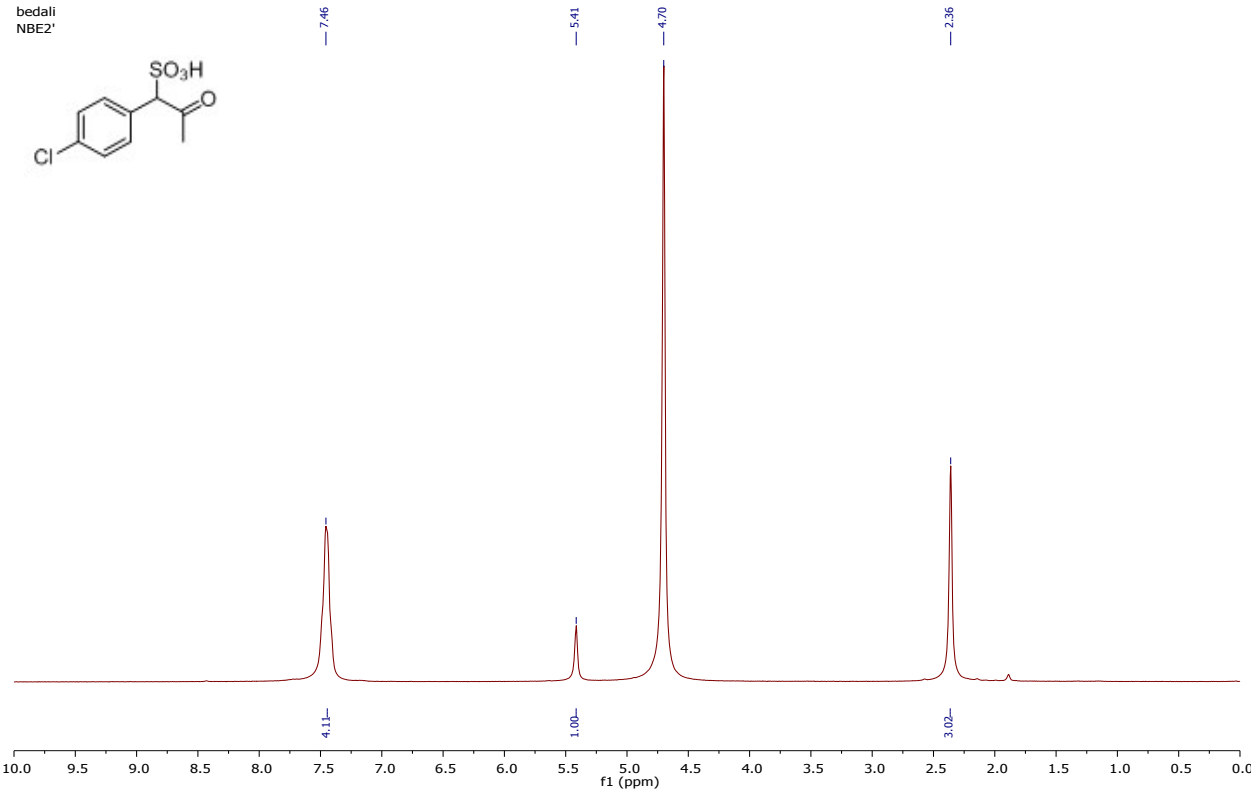

rahimzade.25.fid
EZ2
211.45
200.35
148.39
135.95
134.99
129.97
124.18
123.59
77.41
76.99
76.57
75.04
63.51
30.08
28.88
19.02
13.60
f1 (ppm)

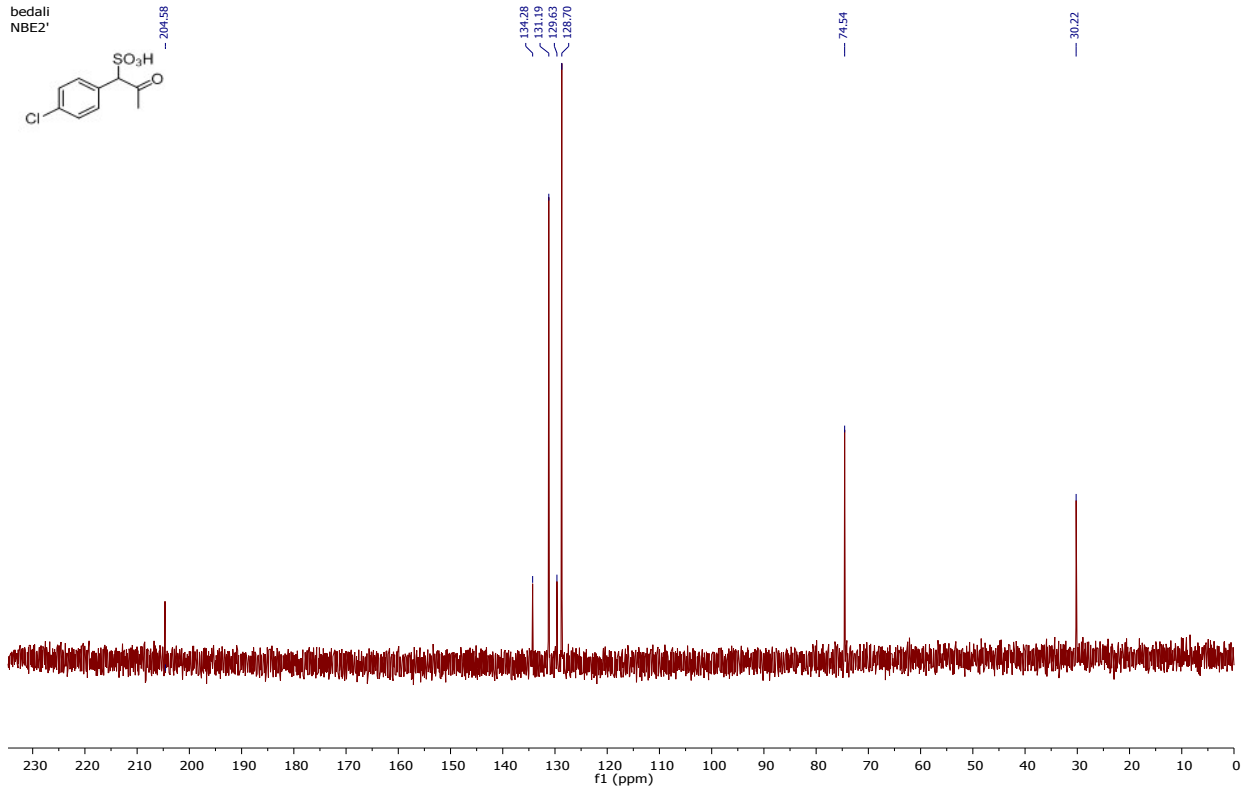

rahimzade.14.fid
EX4
0.95
0.30
3.47
0.95
0.15
1.01
2.11
0.25
3.42
2.09
0.47
3.00
f1 (ppm)

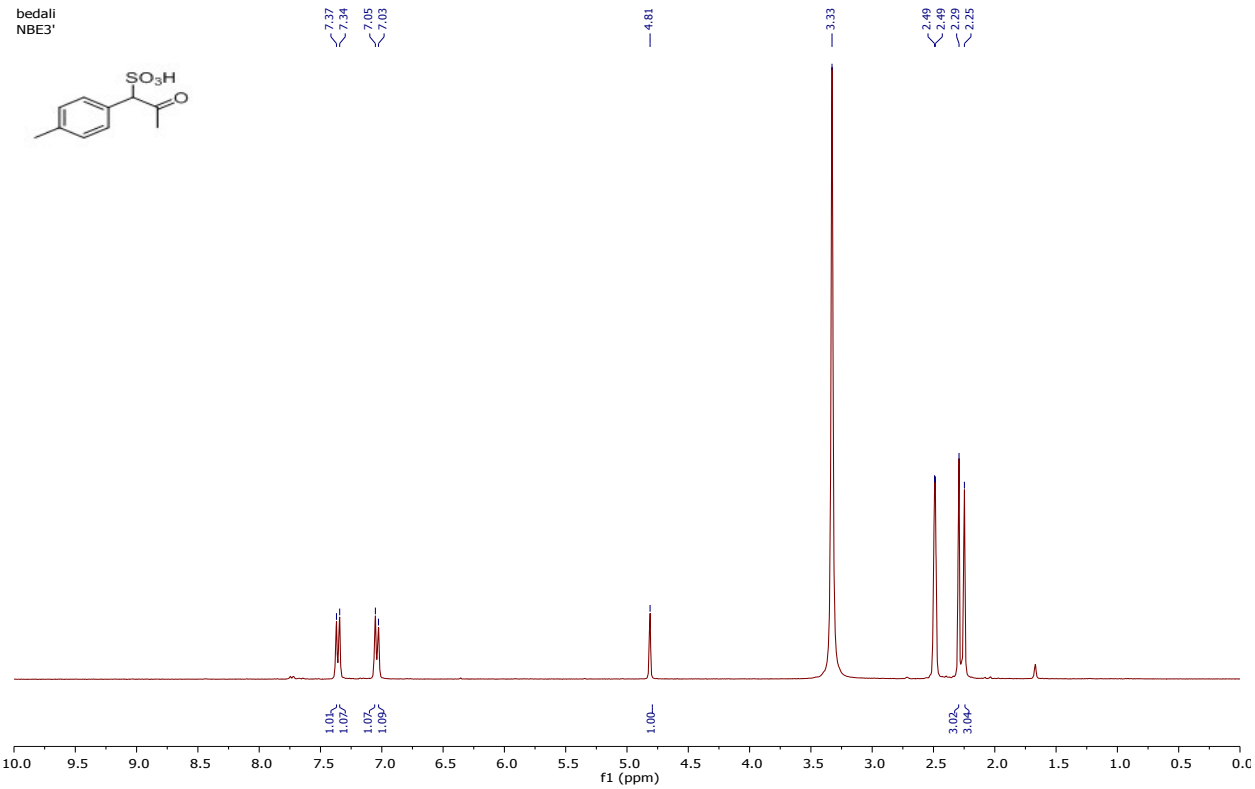

rahimzade.15.fid
EX4
201.08
188.02
160.10
134.63
132.18
130.28
121.08
118.76
114.53
114.07
77.41
76.99
76.57
59.64
55.29
33.44
28.14
O
S
S
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

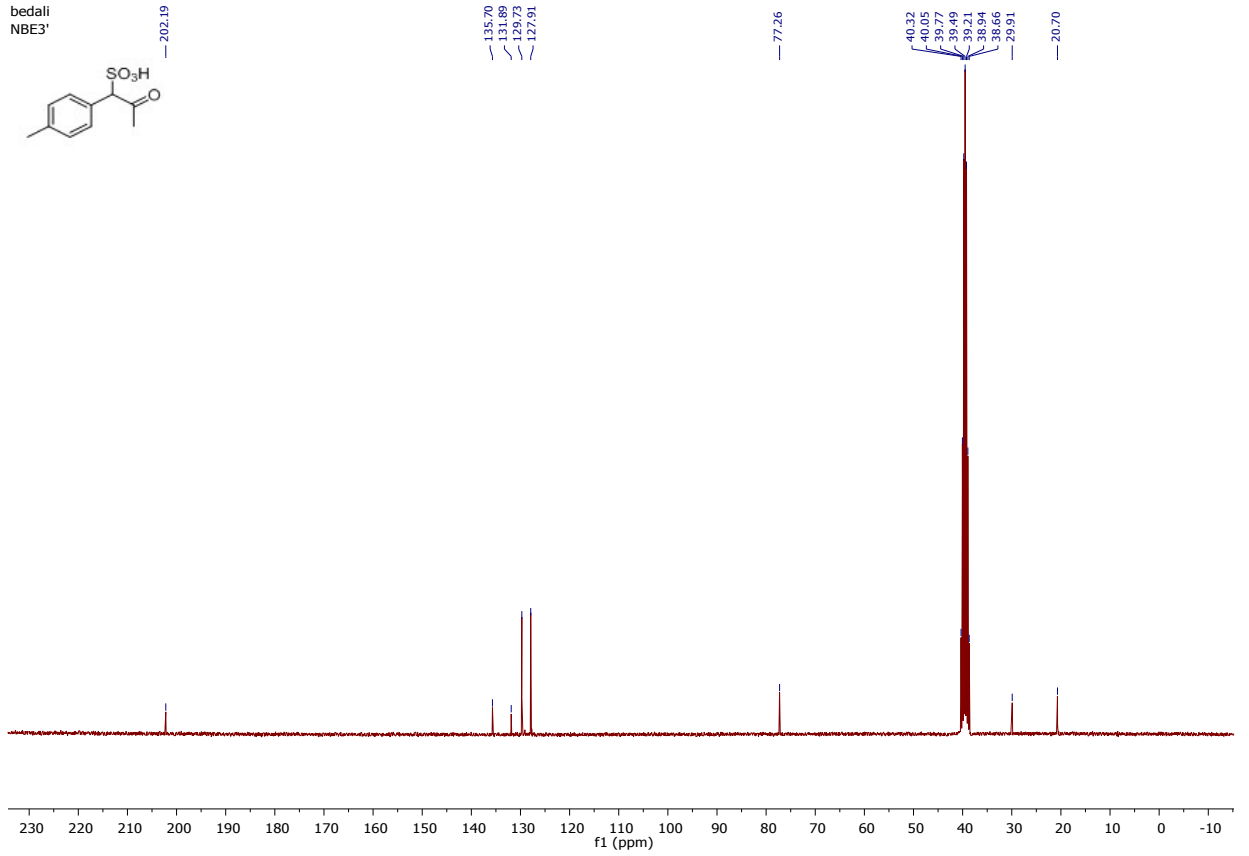

bedali
NBE1
7.51
7.50
7.48
7.48
7.27
7.25
7.23
7.20
4.93
2.32
OH
O
S
O
O
CH3
2.04
3.16
1.00
2.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

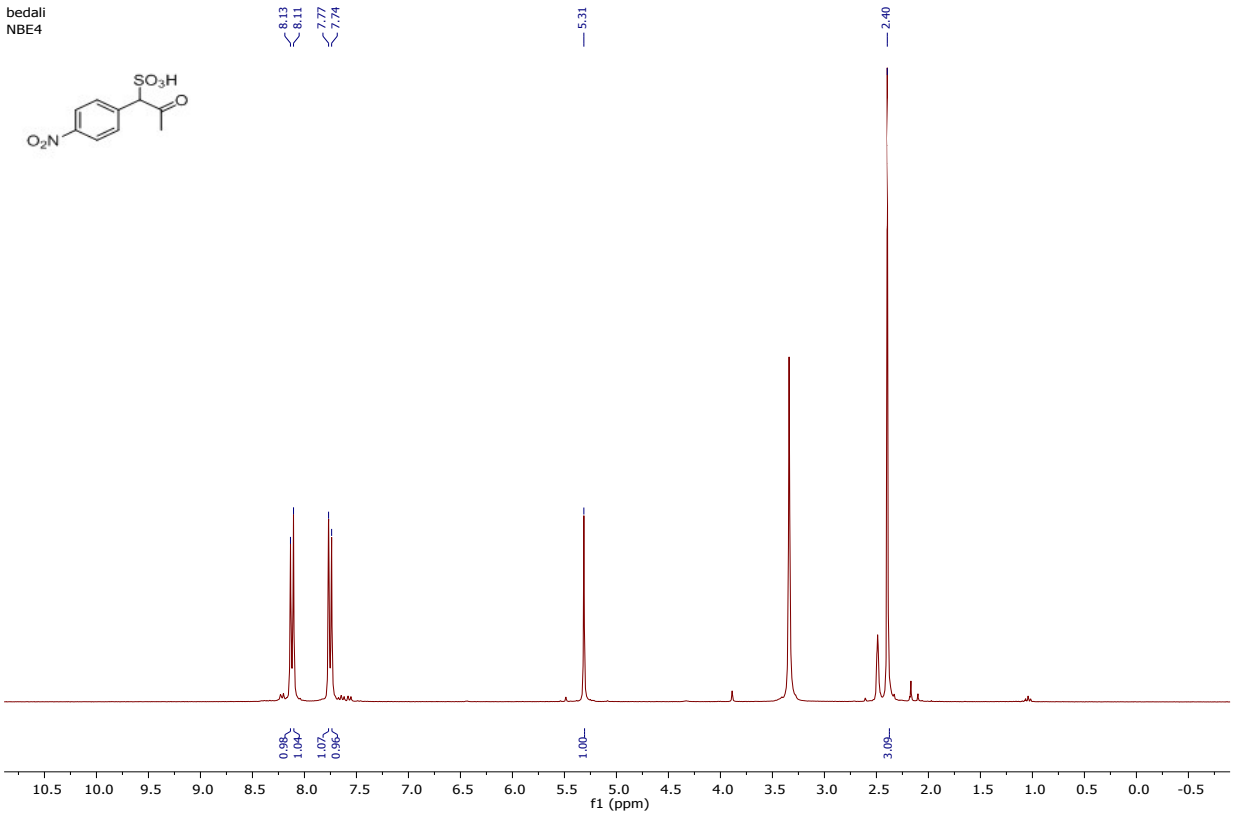

bedali
NBE1
202.13
134.70
129.92
127.38
126.79
77.28
40.33
40.05
39.77
39.49
39.21
38.94
38.66
30.22
OH
O
S
O
O
CH3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

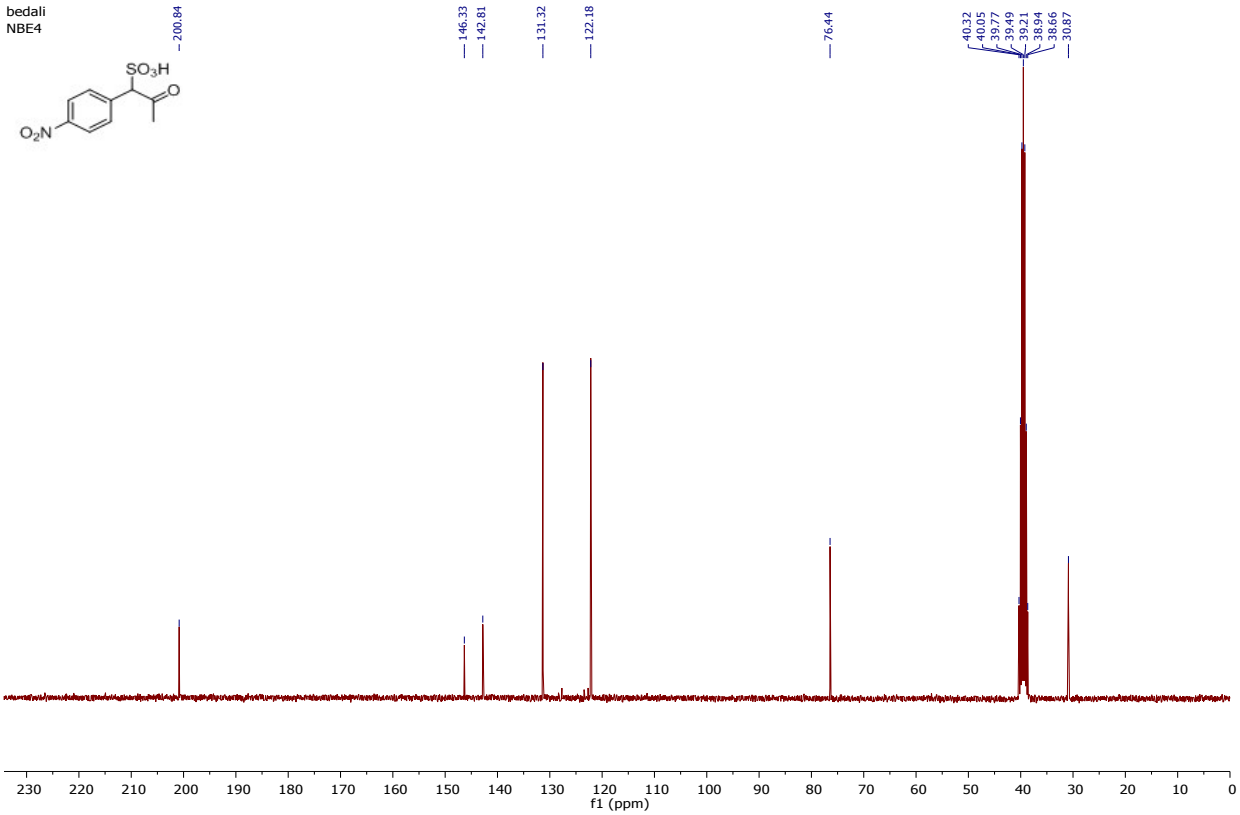

bedali
NBE2'
SO3H
O
Cl
7.46
5.41
4.70
2.36
4.11
1.00
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

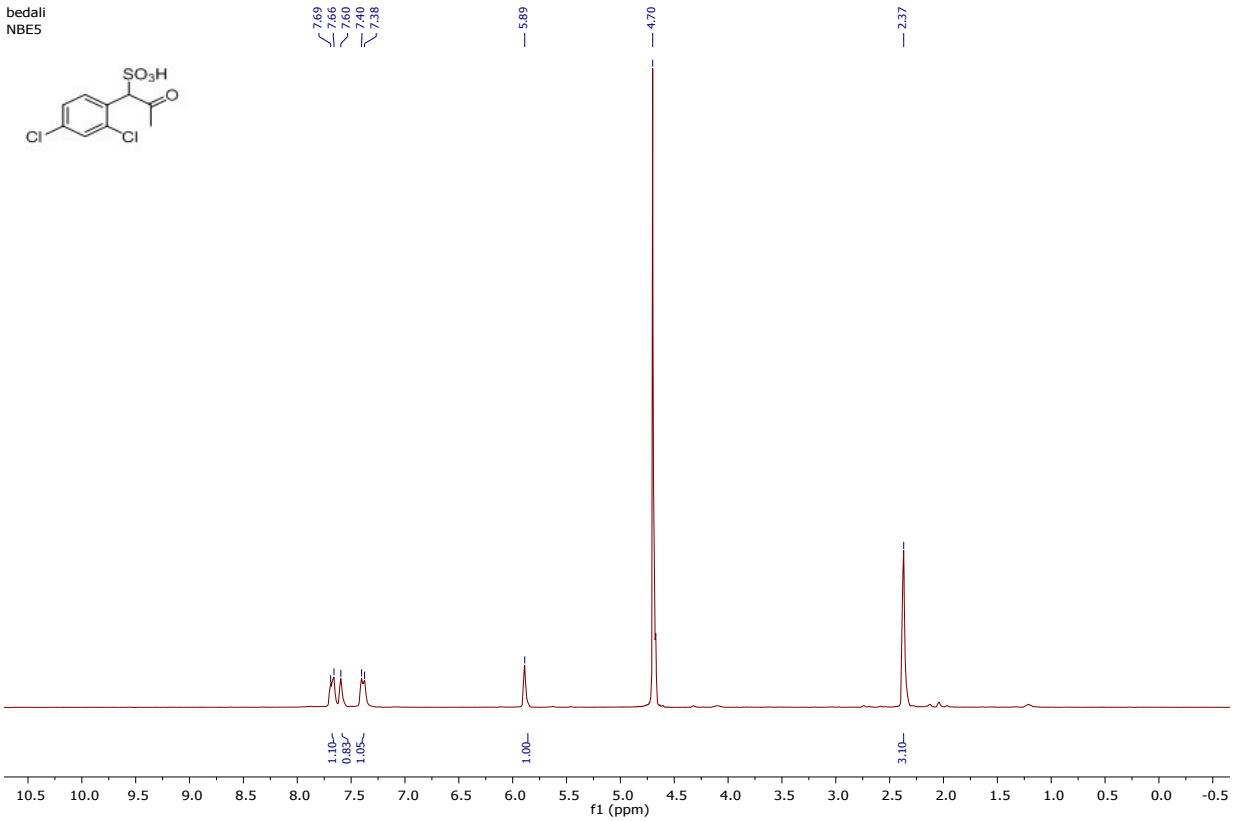

bedali
NBE2'
SO3H
O
Cl
204.58
134.28
131.19
129.63
128.70
74.54
30.22
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

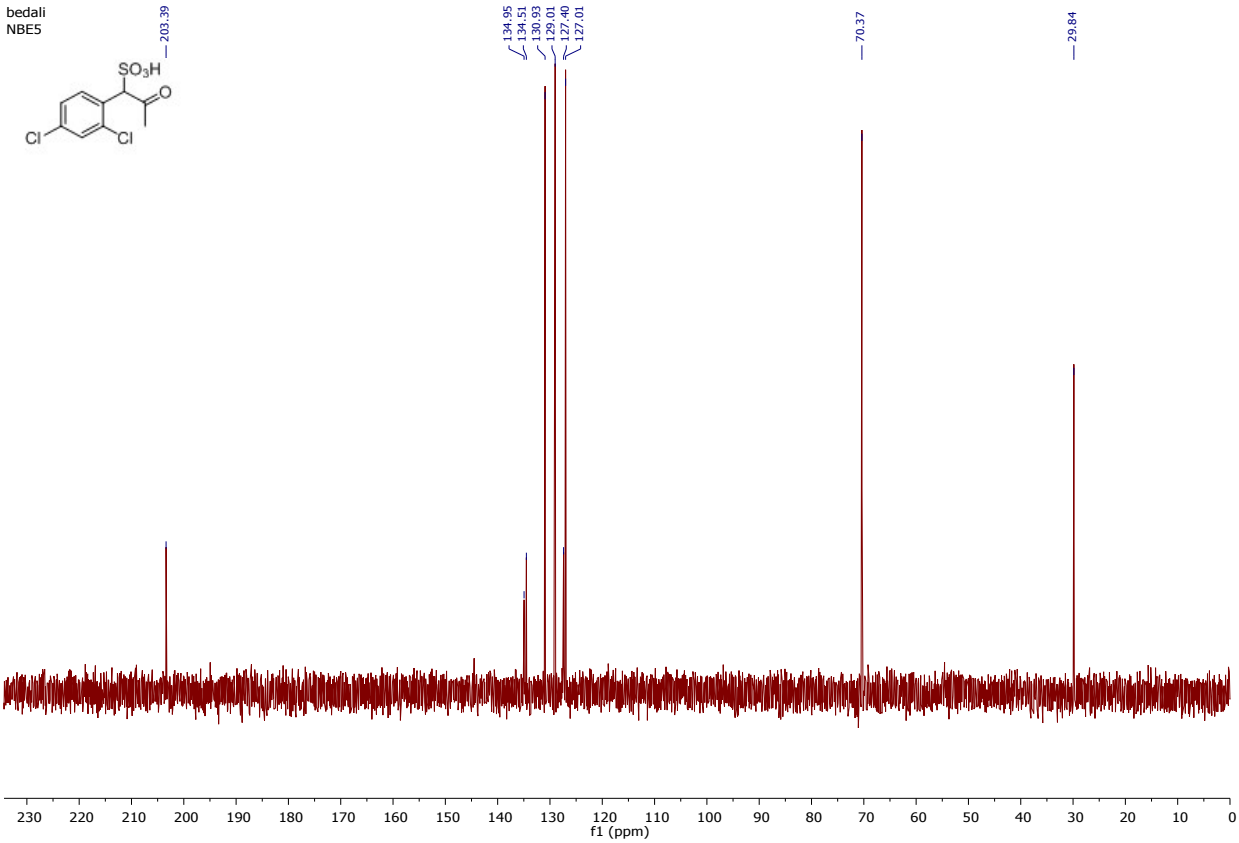

bedali
NBE3'
SO3H
O
7.37
7.34
7.05
7.03
4.81
3.33
2.49
2.49
2.29
2.25
1.01
1.07
1.07
1.09
1.00
3.02
3.04
f1 (ppm)

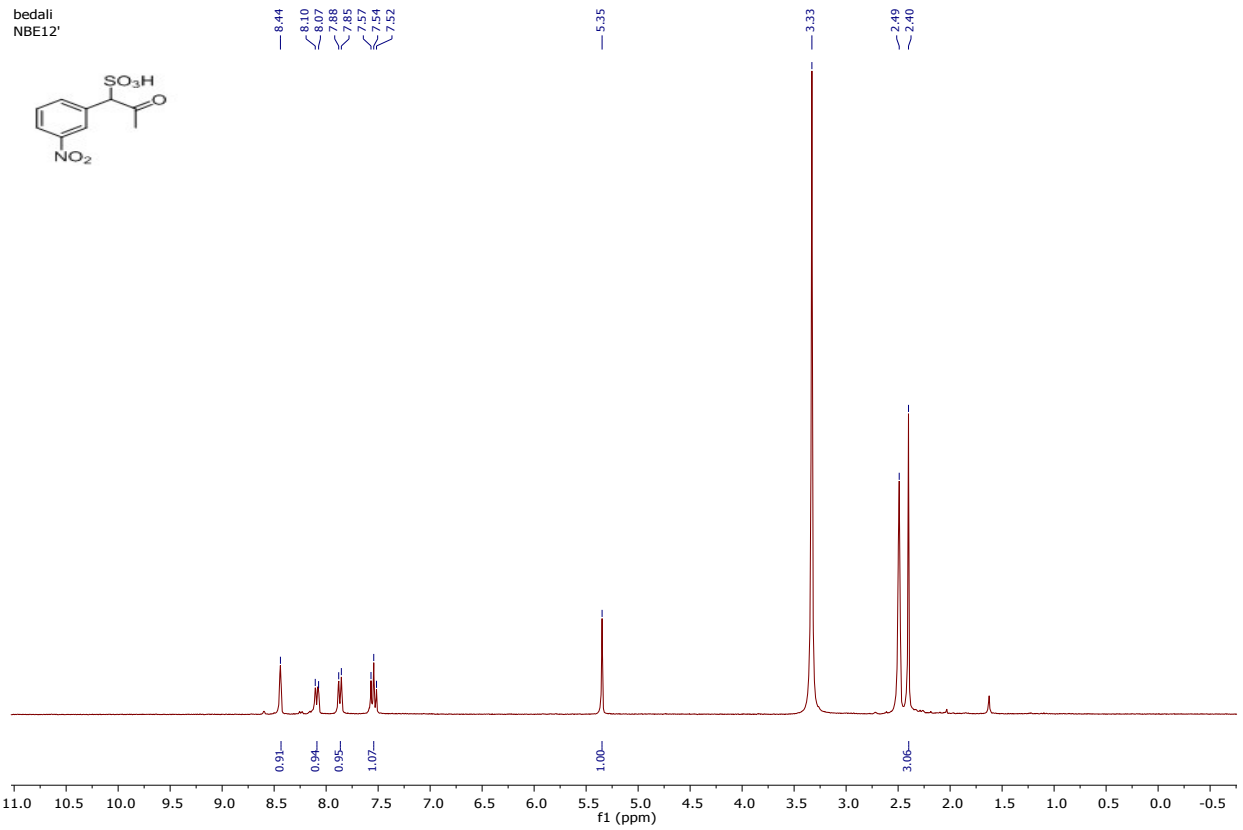

bedali
NBE3'
SO3H
O
202.19
135.70
131.89
129.73
127.91
77.26
40.32
40.05
39.77
39.49
39.21
38.94
38.66
29.91
20.70
f1 (ppm)

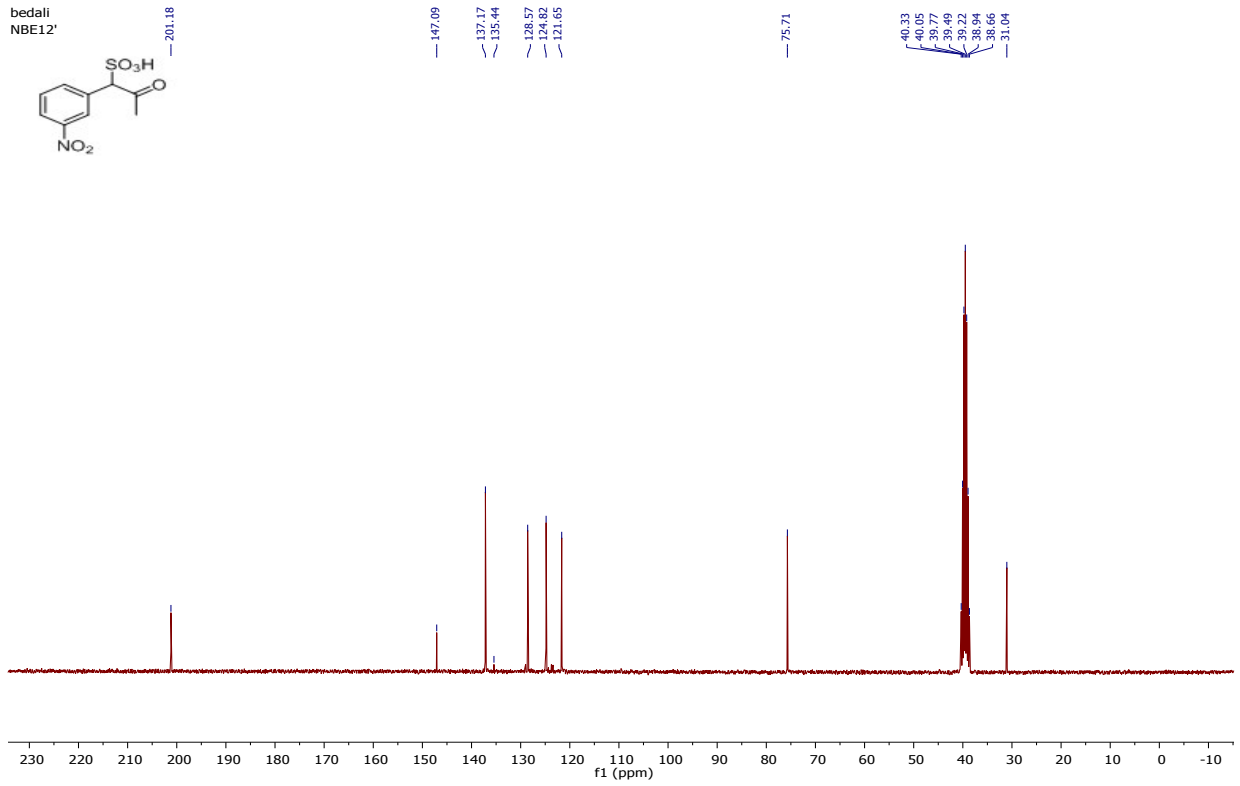

bedali
NBE4
8.13
8.11
7.77
7.74
5.31
2.40
SO3H
O
O2N
0.98
1.04
1.07
0.96
1.00
3.09
f1 (ppm)

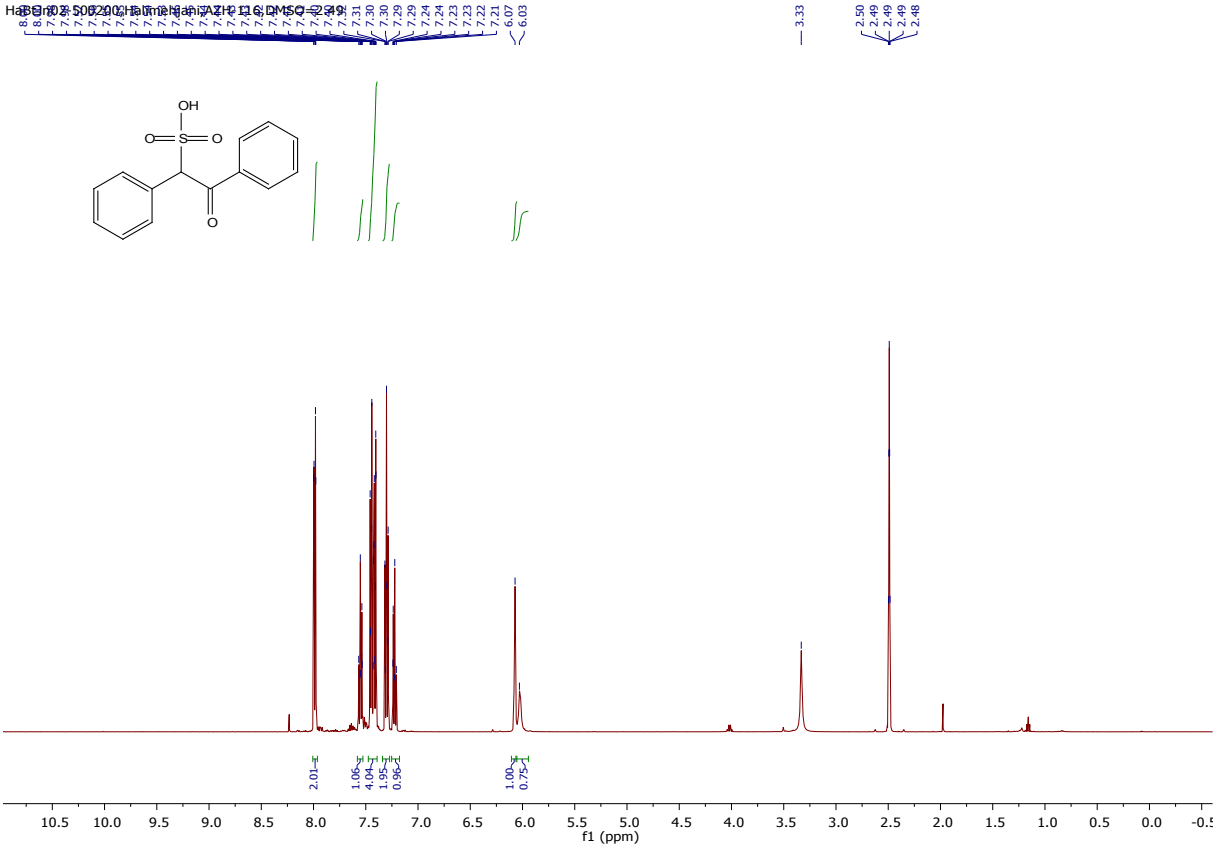

bedali
NBE4
200.84
146.33
142.81
131.32
122.18
76.44
40.32
40.05
39.77
39.49
39.21
38.94
38.66
30.87
SO3H
O
O2N
f1 (ppm)

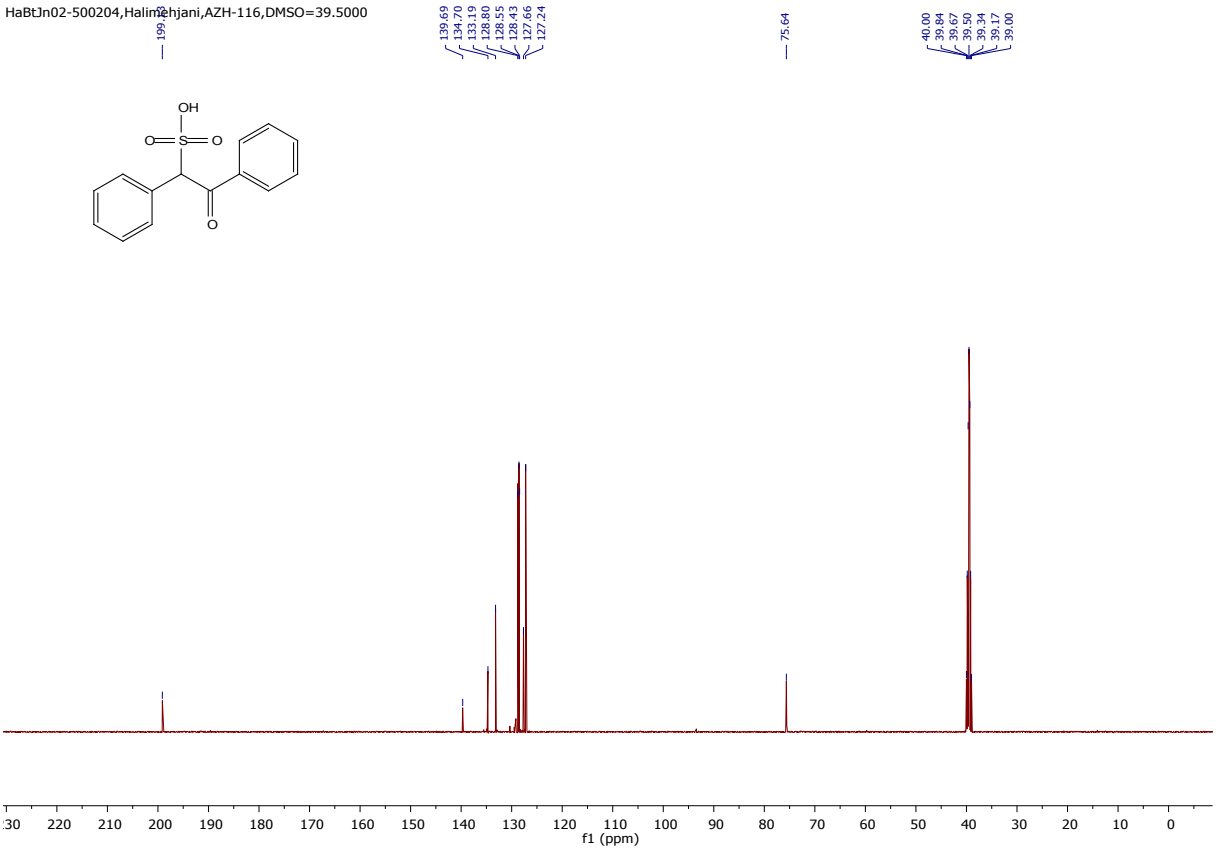

bedali
NBE5
SO3H
O
Cl
Cl
7.69
7.66
7.60
7.40
7.38
5.89
4.70
2.37
1.10
0.83
1.05
1.00
3.10
f1 (ppm)

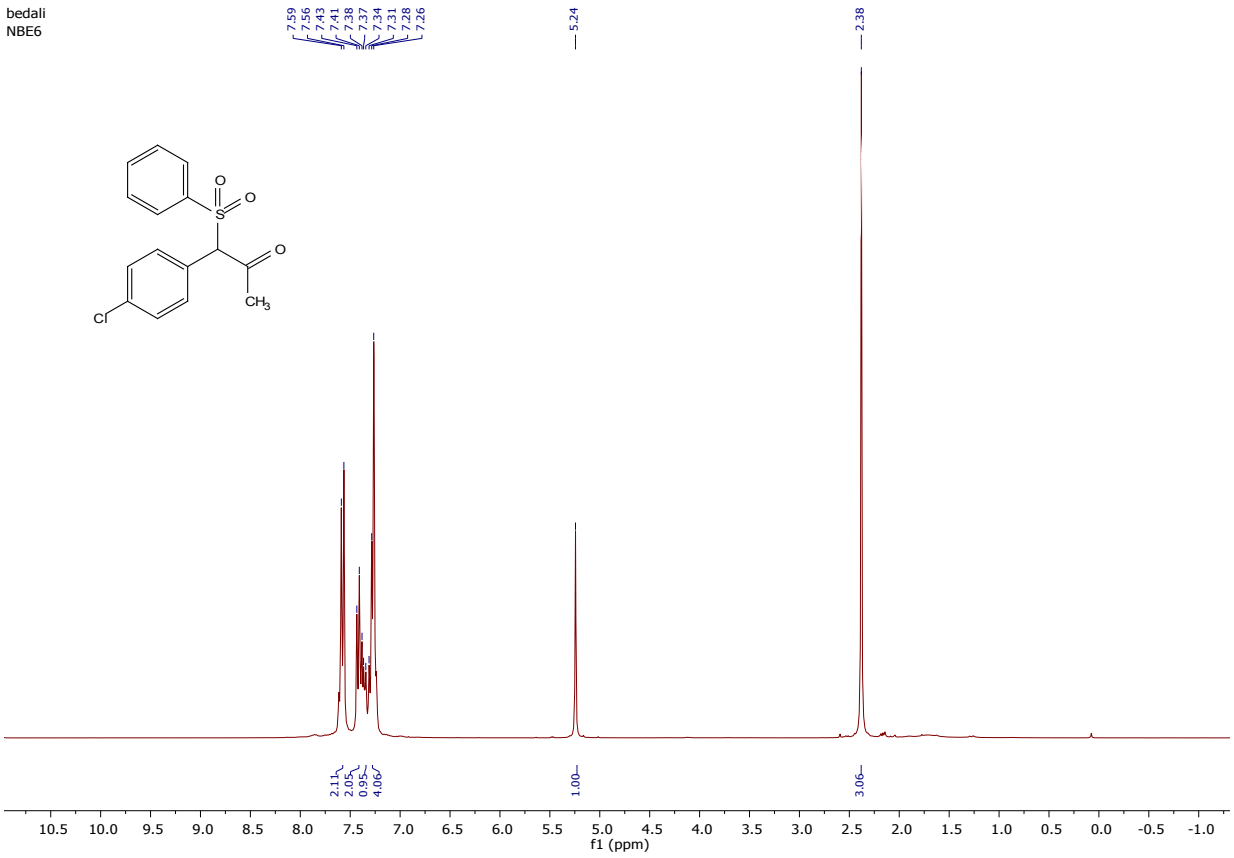

bedali
NBE5
SO3H
O
Cl
Cl
203.39
134.95
134.51
130.93
129.01
127.40
127.01
70.37
29.84
f1 (ppm)

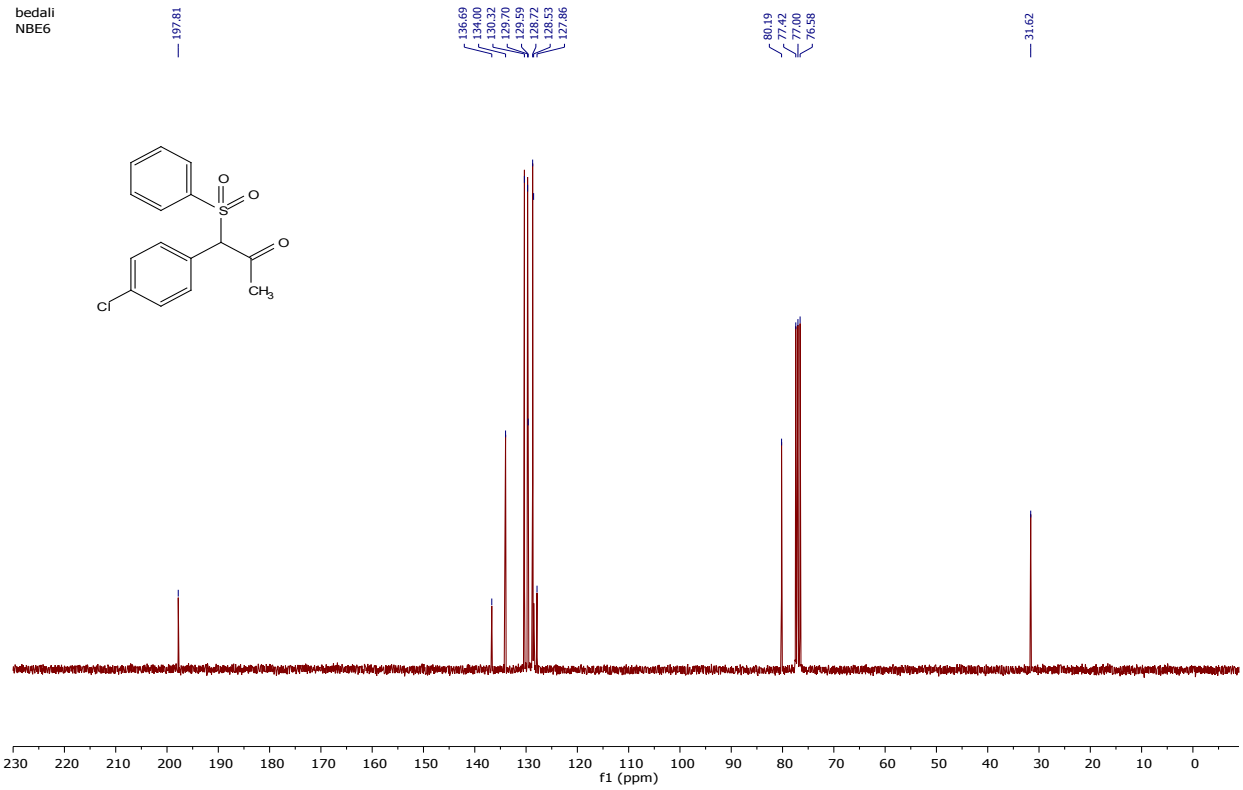

bedali
NBE12'
8.44
8.10
8.07
7.88
7.85
7.57
7.54
7.52
5.35
3.33
2.49
2.40
0.91
0.94
0.95
1.07
1.00
3.06
f1 (ppm)

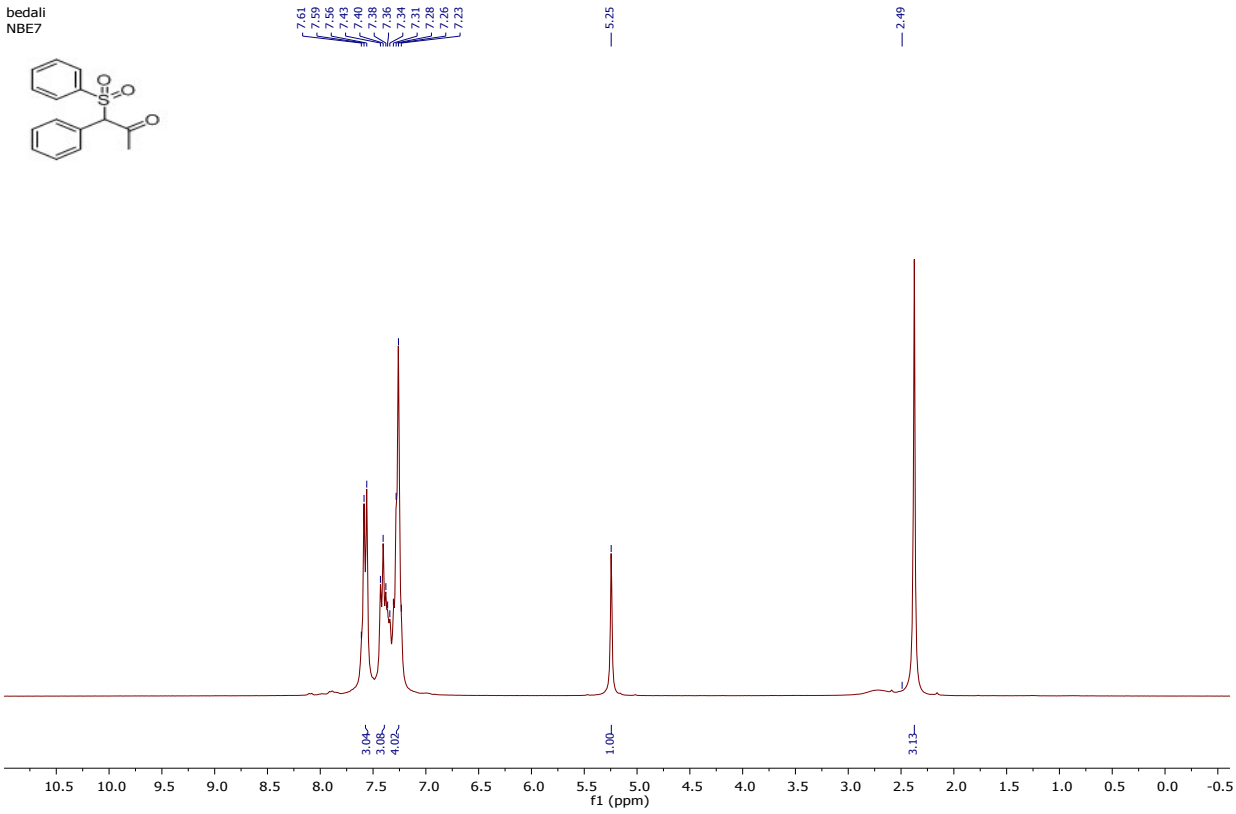

bedali
NBE12'
201.18
147.09
137.17
135.44
128.57
124.82
121.65
75.71
40.33
40.05
39.77
39.49
39.22
38.94
38.66
31.04
f1 (ppm)

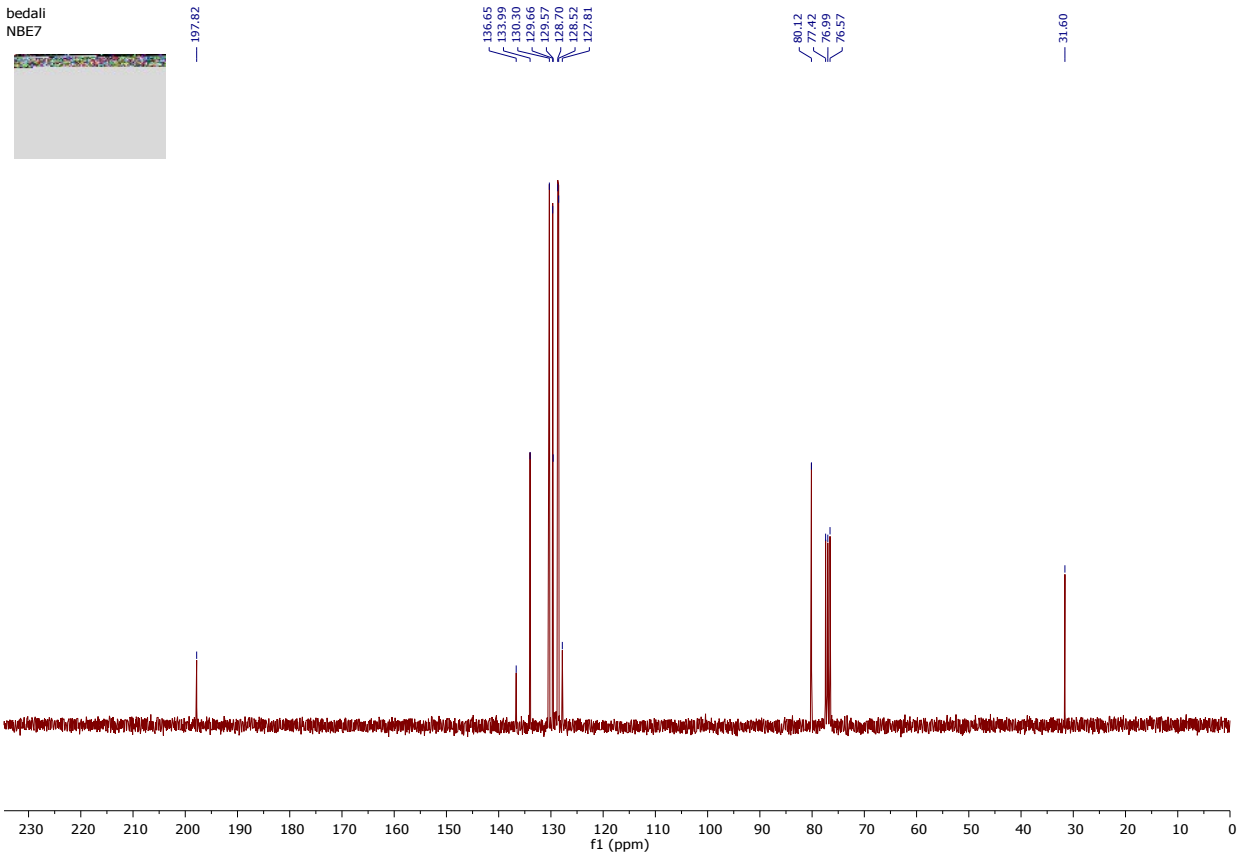

OH
O
S
O
O
3.33
2.50
2.49
2.49
2.49
2.48
7.31
7.30
7.30
7.29
7.29
7.24
7.24
7.23
7.23
7.22
7.21
6.07
6.03
2.01
1.06
4.04
1.95
0.96
1.00
0.75
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

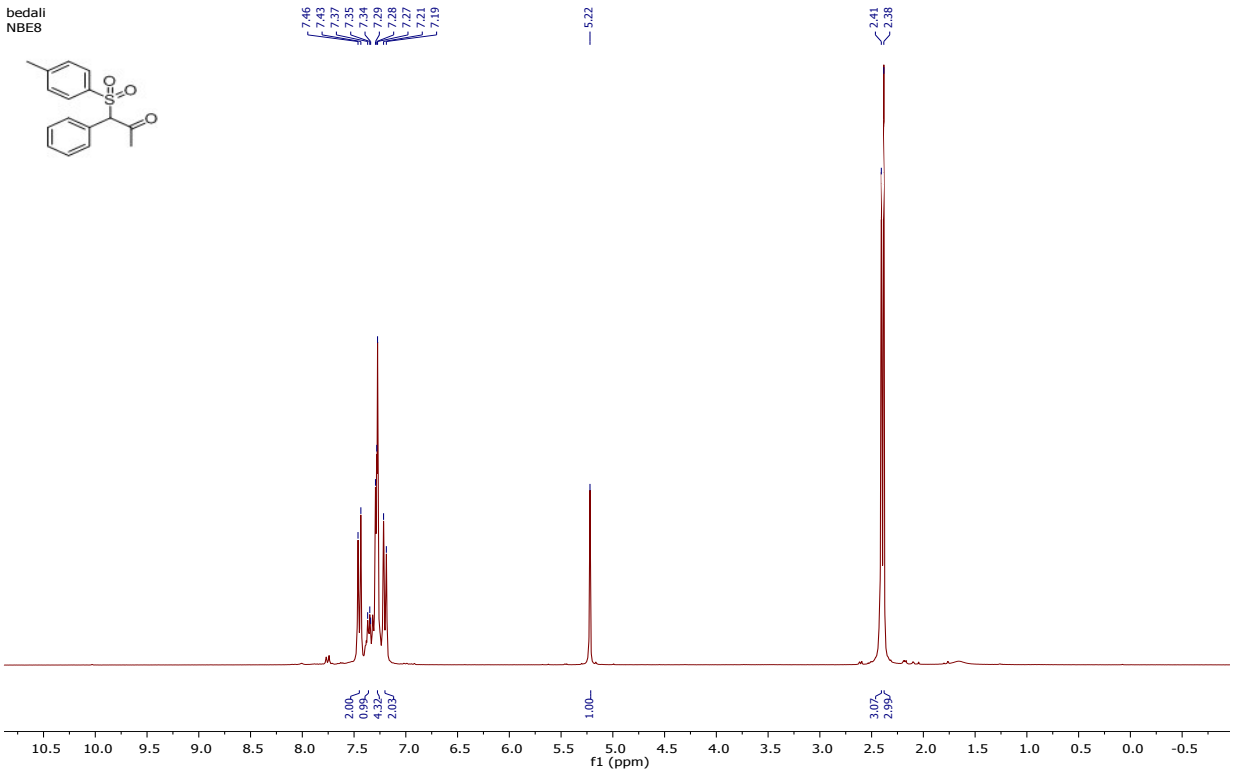

HaBtJn02-500204,Halimehjani,AZH-116,DMSO=39.5000
199.22
139.69
134.70
133.19
128.80
128.55
128.43
127.66
127.24
75.64
40.00
39.84
39.67
39.50
39.34
39.17
39.00
OH
O
S
O
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

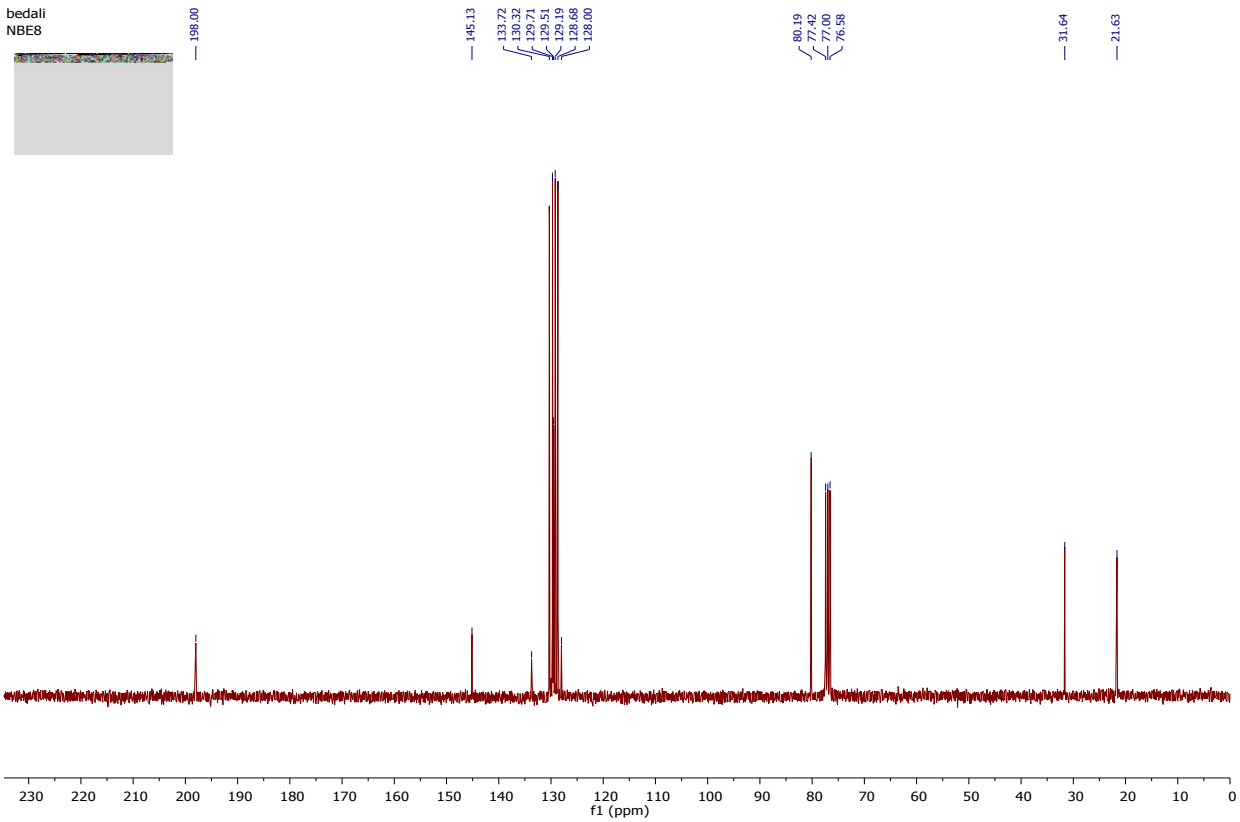

bedali
NBE6
7.59
7.56
7.43
7.41
7.38
7.37
7.34
7.31
7.28
7.26
5.24
2.38
O
S
O
O
CH3
Cl
2.11
2.05
0.95
4.06
1.00
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

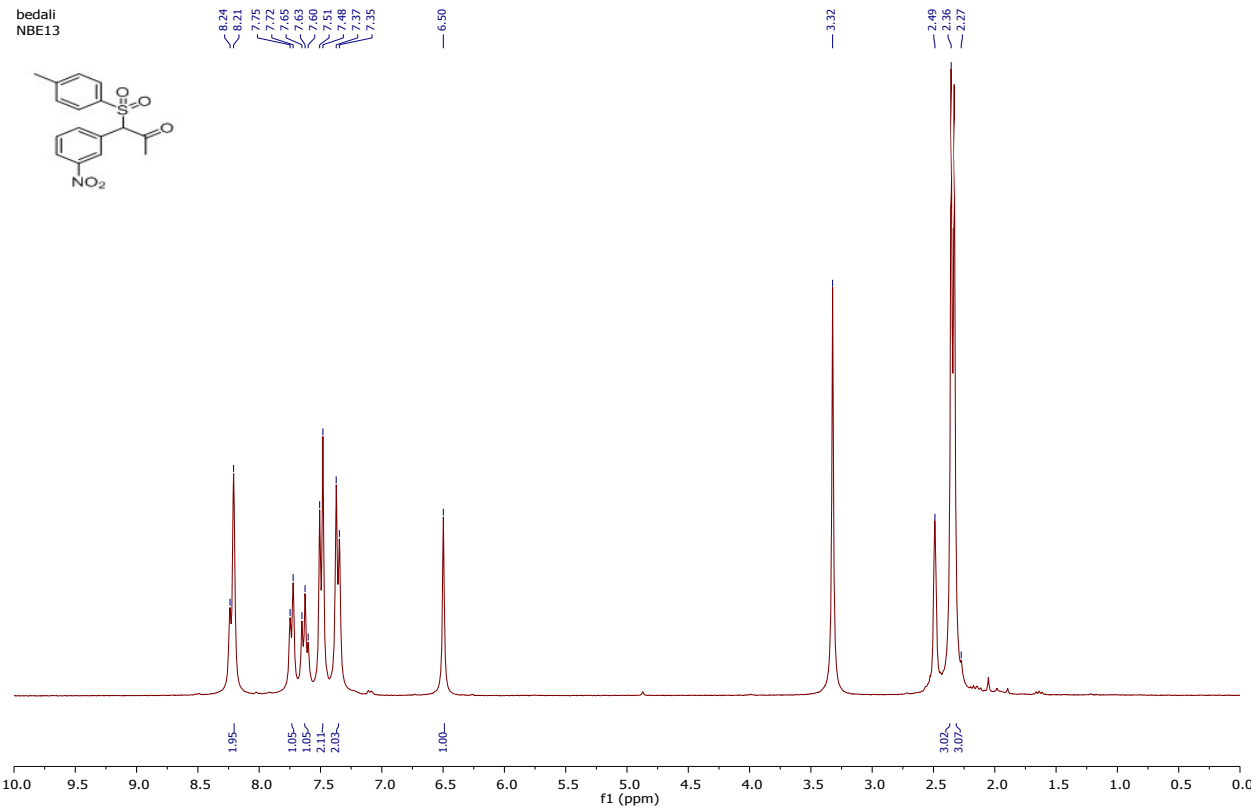

bedali
NBE6
197.81
136.69
134.00
130.32
129.70
129.59
128.72
128.53
127.86
80.19
77.42
77.00
76.58
31.62
O
S
O
O
CH3
Cl
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

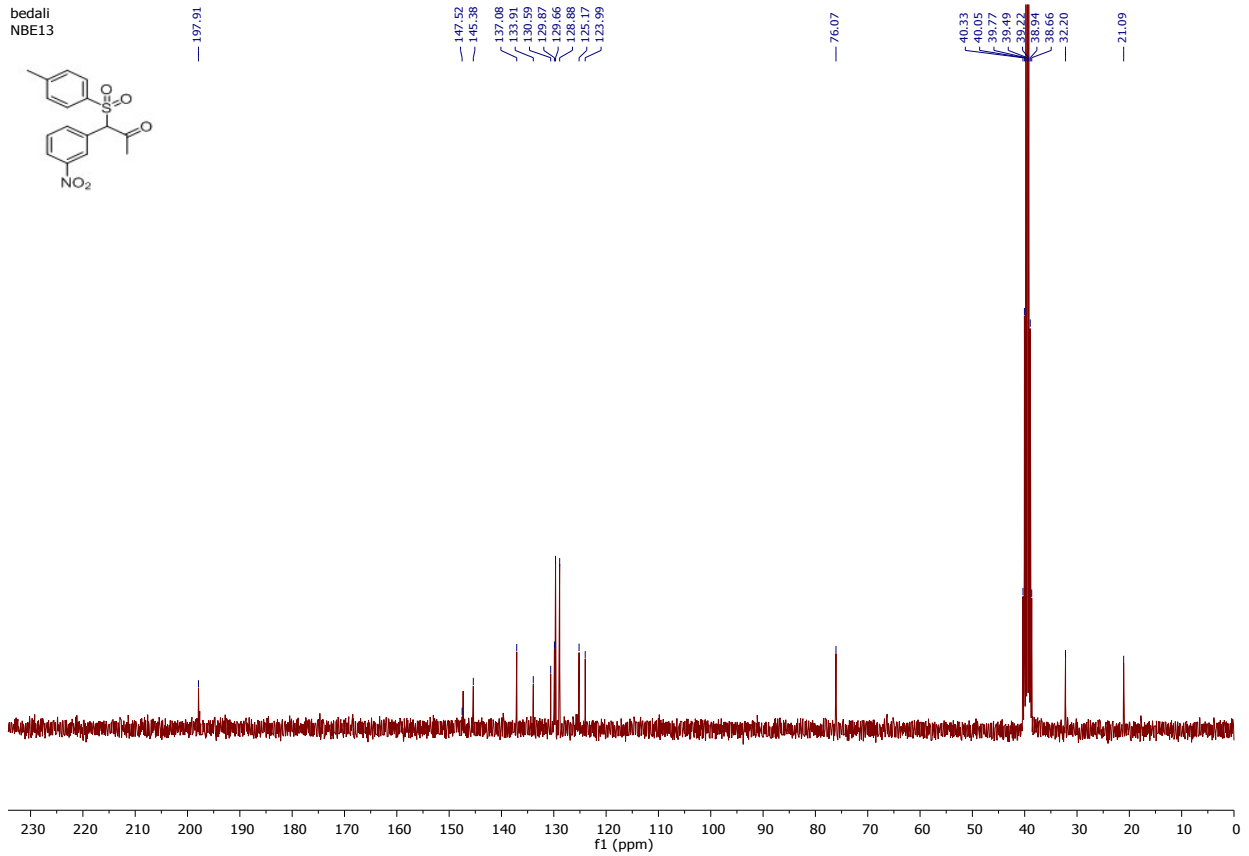

bedali
NBE7
7.61
7.59
7.56
7.43
7.40
7.38
7.36
7.34
7.31
7.28
7.26
7.23
5.25
2.49
3.04
3.08
4.02
1.00
3.13
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


bedali
NBE7
197.82
136.65
133.99
130.30
129.66
129.57
128.70
128.52
127.81
80.12
77.42
76.99
76.57
31.60
f1 (ppm)


bedali
NBE8
7.46
7.43
7.37
7.35
7.34
7.29
7.28
7.27
7.21
7.19
5.22
2.41
2.38
2.00
0.99
4.32
2.03
1.00
3.07
2.99
f1 (ppm)


bedali
NBE8
198.00
145.13
133.72
130.32
129.71
129.51
129.19
128.68
128.00
80.19
77.42
77.00
76.58
31.64
21.63
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


bedali
NBE13
8.24
8.21
7.75
7.72
7.65
7.63
7.60
7.51
7.48
7.37
7.35
6.50
3.32
2.49
2.36
2.27
1.95
1.05
1.05
2.11
2.03
1.00
3.02
3.07
f1 (ppm)


bedali
NBE13
197.91
147.52
145.38
137.08
133.91
130.59
129.87
129.66
128.88
125.17
123.99
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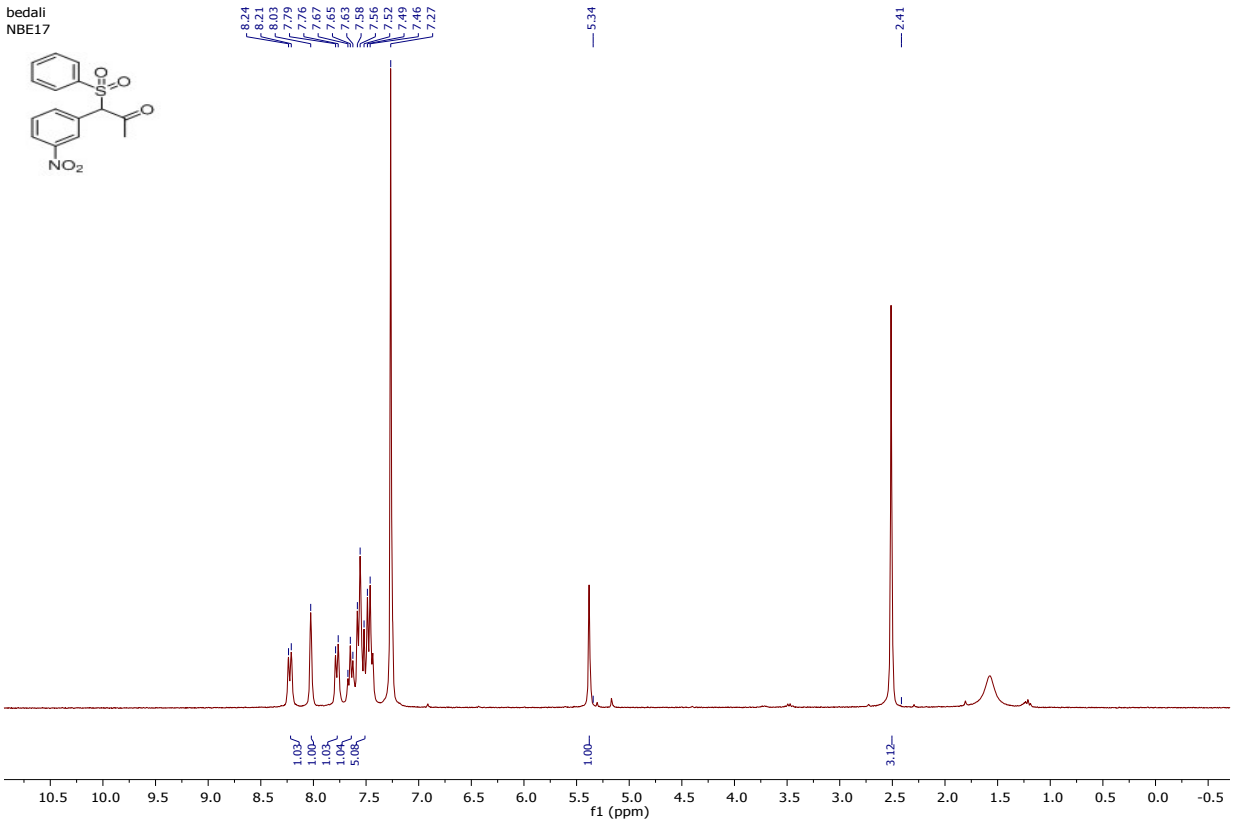
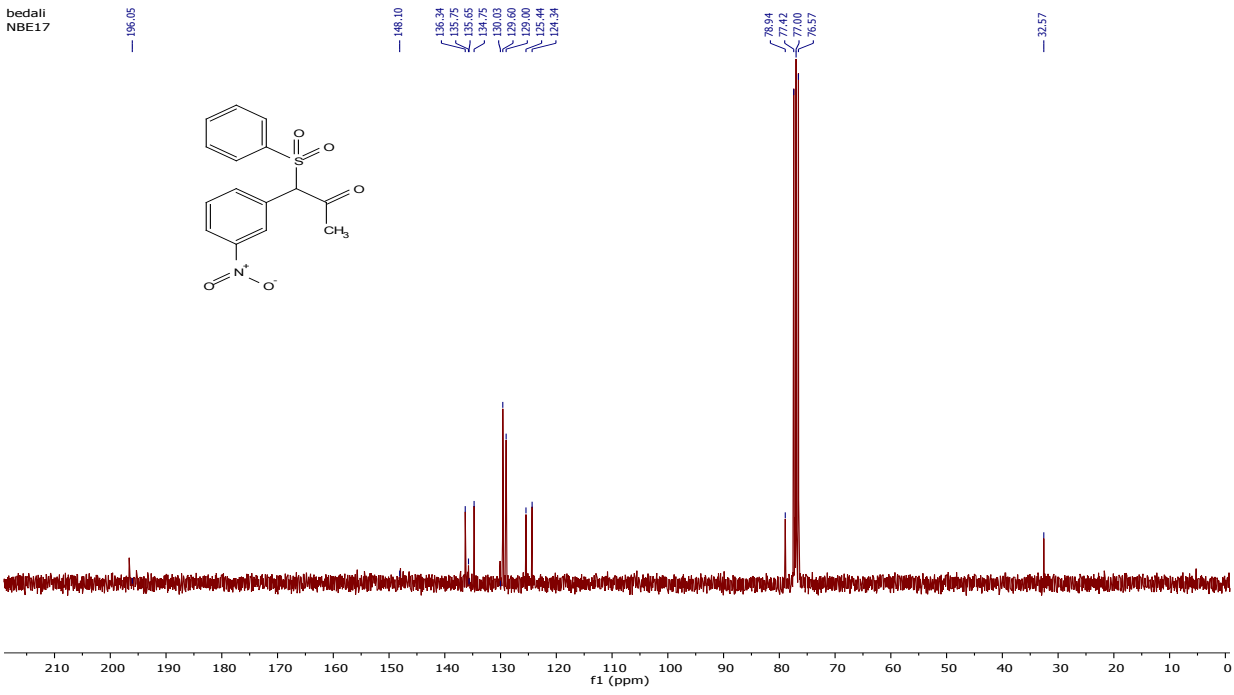
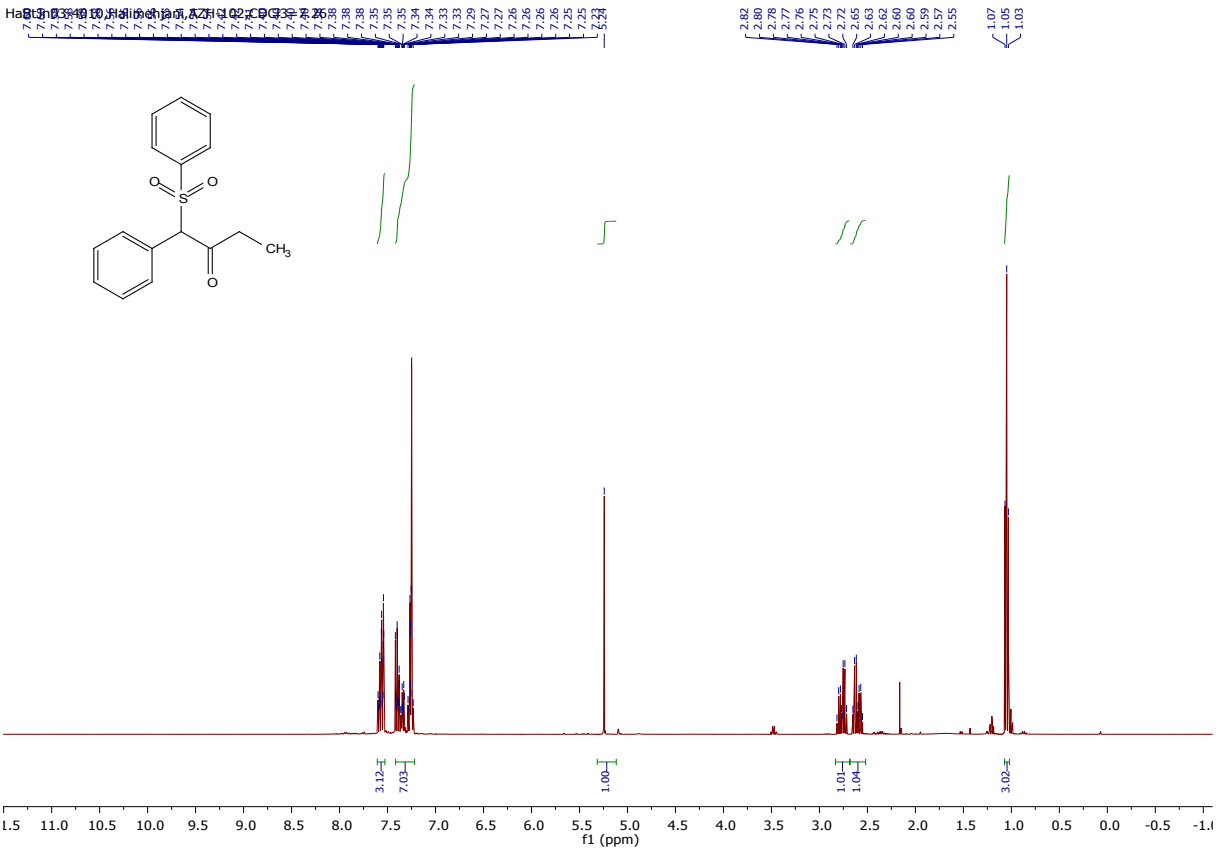
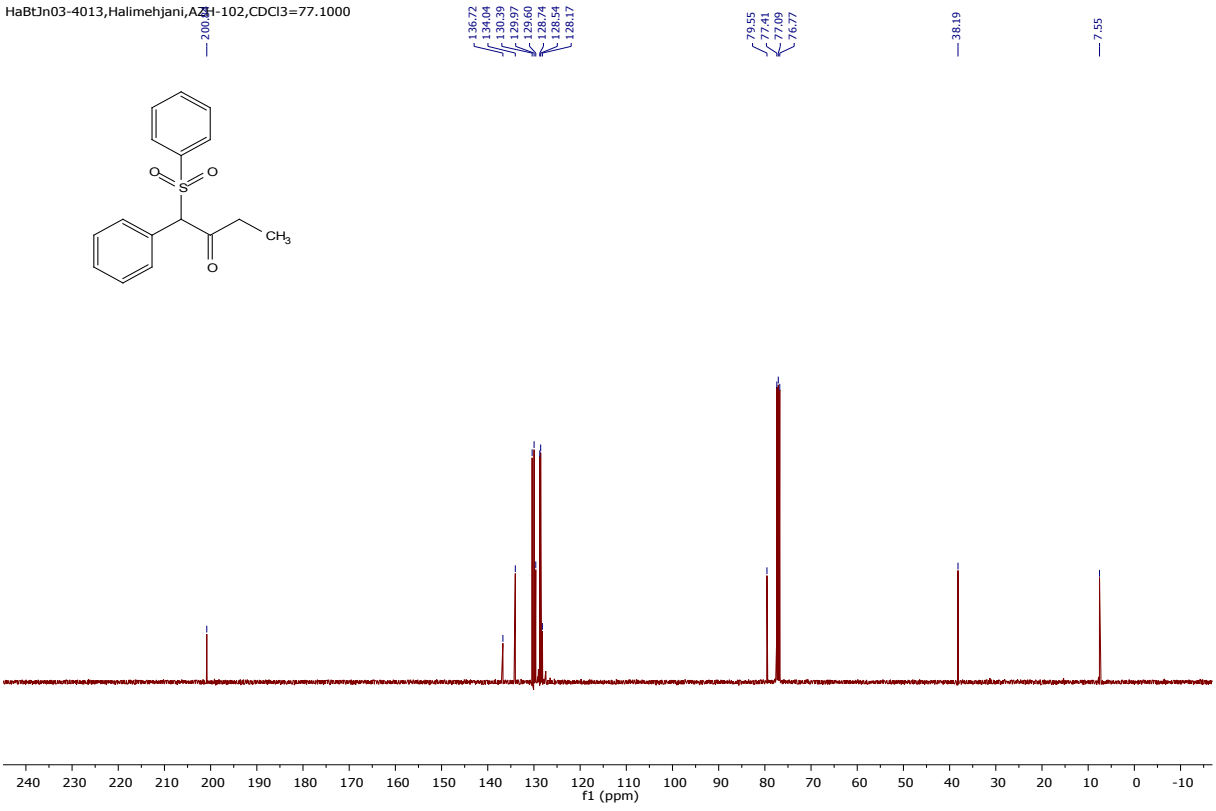
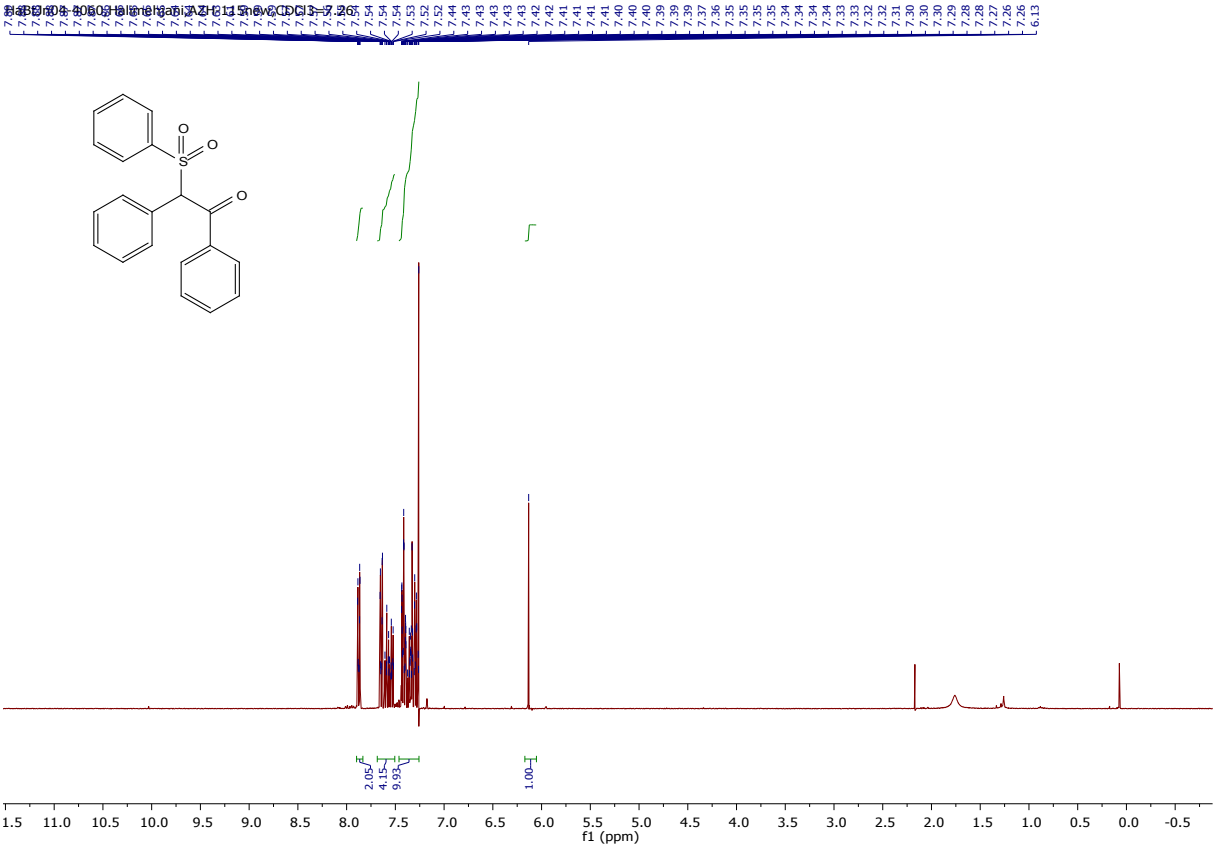
38.94
38.66
32.20
21.09
f1 (ppm)

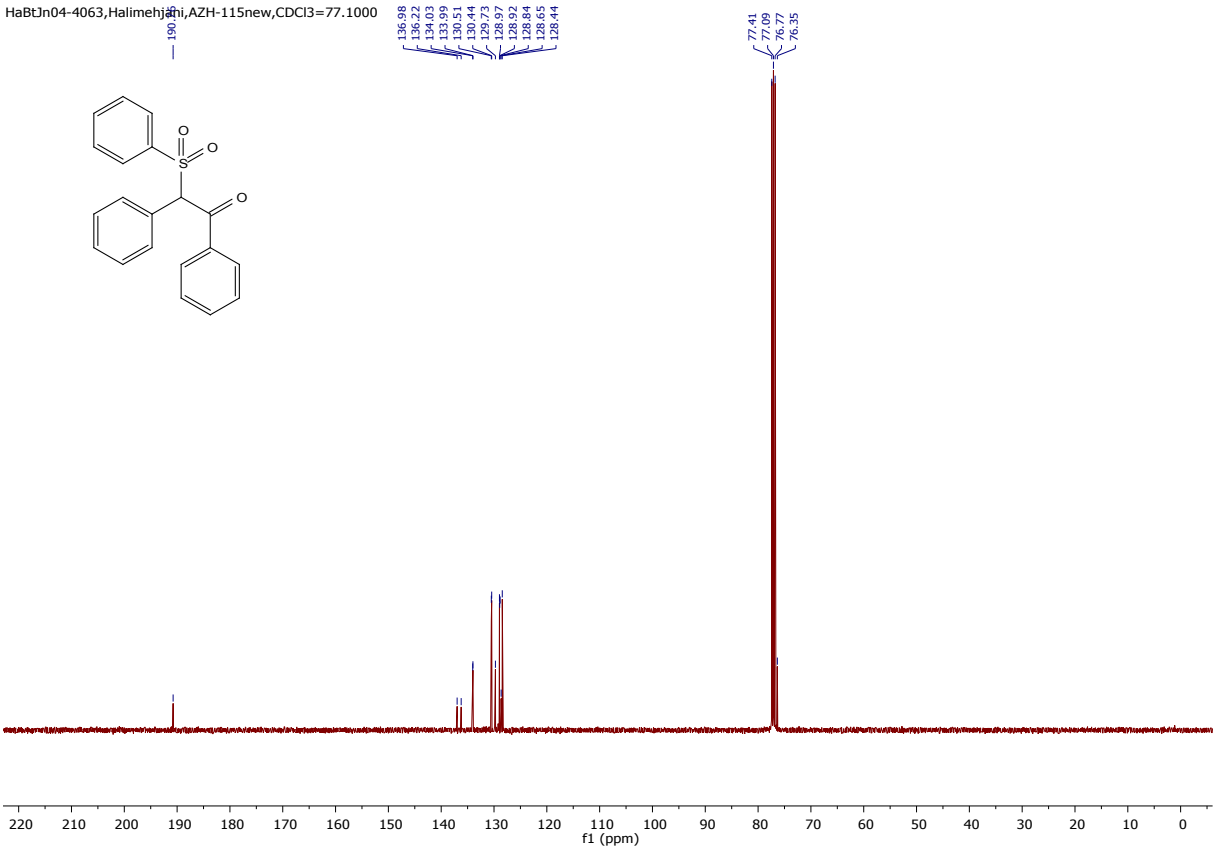

bedali
NBE17
8.24
8.21
8.03
7.79
7.76
7.67
7.65
7.63
7.58
7.56
7.52
7.49
7.46
7.27
5.34
2.41
1.03
1.00
1.03
1.04
5.08
1.00
3.12
f1 (ppm)


bedali
NBE17
196.05
148.10
136.34
135.75
135.65
134.75
130.03
129.60
129.00
125.44
124.34
78.94
77.42
77.00
76.57
32.57
f1 (ppm)


O
O
S
CH3
O
f1 (ppm)


HaBtJn03-4013,Halimehjani,AZH-102,CDCl3=77.1000
O
O
S
CH3
O
f1 (ppm)


HaBtJn04-4063,Halimehjani,AZH-115new,CDCl3=7.26
2.05
4.15
9.93
1.00
f1 (ppm)


HaBtJn04-4063,Halimehjani,AZH-115new,CDCl3=77.1000
190.41
136.98
136.22
134.03
133.99
130.51
130.44
129.73
128.97
128.92
128.84
128.65
128.44
77.41
77.09
76.77
76.35
f1 (ppm)

References

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