Supporting Information

NBS-activated cross-dehydrogenative esterification of carboxylic acids with DMSO

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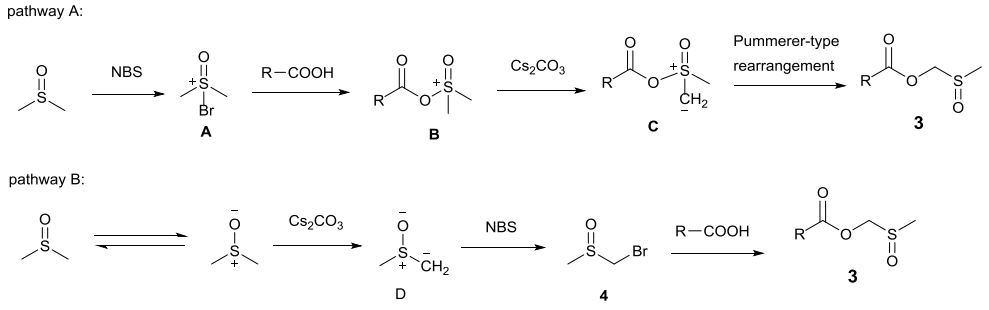
General remarks

Proton nuclear magnetic resonance (^{1}H NMR) spectra, carbon nuclear magnetic resonance (^{13}C NMR) spectra and ^{19}F fluorine spectra (^{19}F NMR) were recorded on a JNM-ECZ600R/S3 (^{1}H NMR 600 MHz, ^{13}C NMR 150 MHz, ^{19}F NMR 564 MHz). HRMS were recorded on a MicroMass Waters Xevo G2-XS QTof. GC and MS samples were recorded on an Agilent 7890A-5975C GC-MS system. Unless otherwise indicated, all reagents were purchased commercially without further purification.

Typical reaction procedure for the synthesis of compounds 3

To a 10 mL schlenk tube was added carboxylic acids **1** (0.25 mmol), CS_2CO_3 (0.25 mmol), DMSO (1.0 mL) and NBS (0.375 mmol), and the resulting mixture was stirred at 50 ^{o}C for 20 hours. When the reaction was finished, appropriate ethyl acetate was added to the mixture and DMSO was extracted by saturated NaCl solution. The obtained organic phase was evaporated to remove the solvent and the resulting residue was further purified by flash column chromatography using petroleum ether/ethyl acetate to afford the products **3**.

Possible reaction pathway



Scheme S1 Possible reaction pathway for synthesis of **3a**.

^{81}Br NMR monitoring the reaction residue

To a 10 mL schlenk tube was added NBS (3.0 mmol) and DMSO (1.0 mL), and the resulting mixture was stirred at room temperature for 10 minutes. When the reaction was finished, the reaction mixture was filtrated, and the obtained residue was detected by ^{81}Br NMR with D_2O as solvent. ^{81}Br NMR signal (δ = -8.05 ppm) of the reaction mixture was determined, which indicates that bromine-containing sulfur cation A

should be generated.

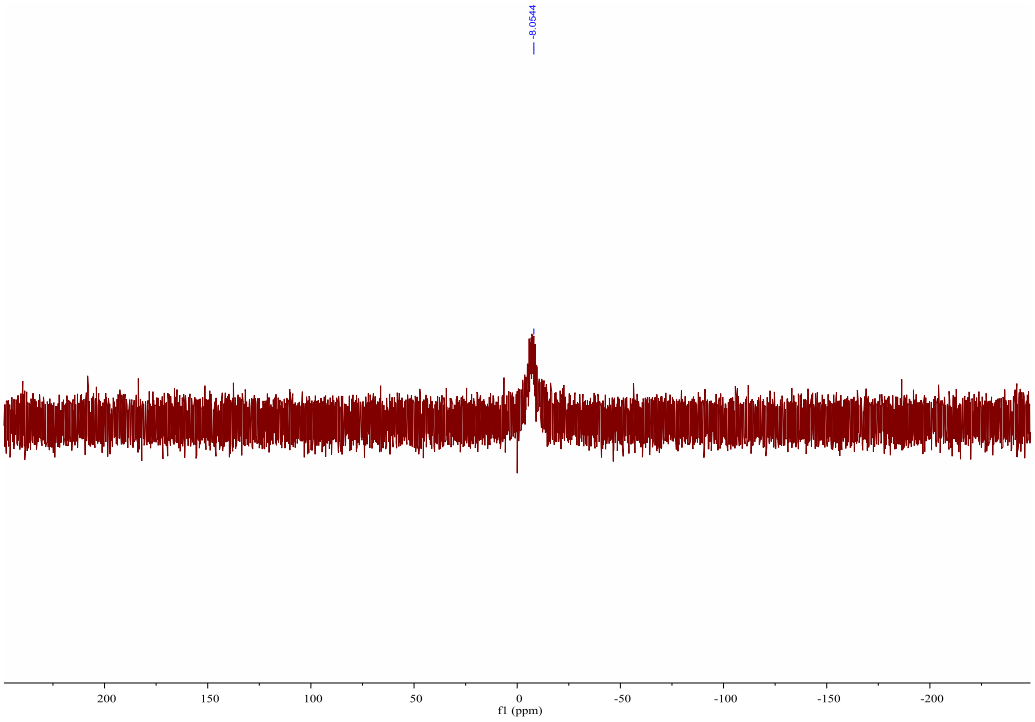


Figure S1 ^{81}Br NMR spectrum of residue

Kinetic hydrogen isotope experiment

To a 10 mL schlenk tube was added **1a** (0.25 mmol), CS_2CO_3 (0.25 mmol), DMSO (0.5 mL), deuterium-labelled DMSO (0.5 mL) and NBS (0.375 mmol), and the resulting mixture was stirred at 50 ^{o}C for 2 hours. When the reaction was finished, appropriate ethyl acetate was added to the mixture and DMSO was extracted by saturated NaCl solution. The obtained organic phase was evaporated to remove the solvent and the resulting residue was further purified by flash column chromatography using petroleum ether/ethyl acetate to afford the products **3aa** and **3aa-d$_5$**. The ^{1}H NMR spectrum of the products **3aa** and **3aa-d$_5$** shows that the ratio of **3aa**/**3aa-d$_5$** is about 9:1.

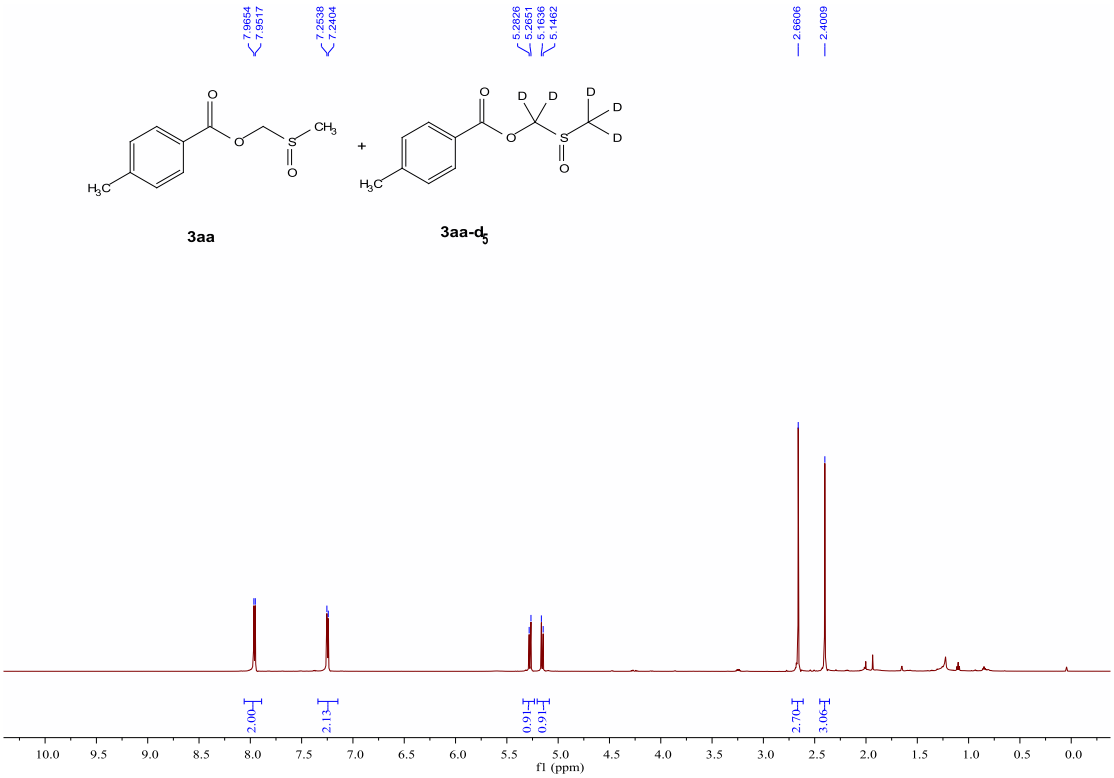
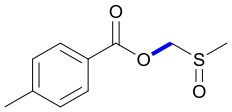


Figure S2 ^{1}H NMR spectrum of the products **3aa** and **3aa-d$_5$**

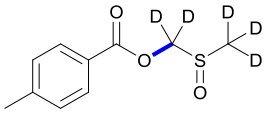
Characterization data of products

(methylsulfinyl)methyl 4-methylbenzoate **(3aa)**



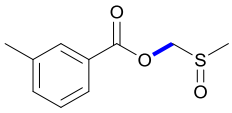
Colorless oil; 37.7 mg, 71%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.95-7.93 (d, J = 8.0 Hz, 2H), 7.24-7.22 (d, J = 7.9 Hz, 2H), 5.27-5.25 (d, J = 10.5 Hz, 1H), 5.14-5.12 (d, J = 10.4 Hz, 1H), 2.64 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.4, 145.2, 130.3, 129.5, 125.4, 79.0, 36.0, 21.9; HRMS (ESI-TOF): calcd. for $C_{10}H_{13}O_3S$ $[M+H]^+$ 213.0585, found 213.0578.

((methyl-d_3)sulfinyl)methyl-d_2 4-methylbenzoate (**3aa-d_5**)



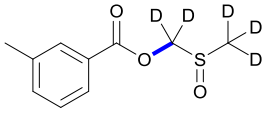
Colorless oil; 37.1 mg, 69%; ^{1}H NMR (600 MHz, d^6-DMSO): δ [ppm] = 7.94-7.93 (d, J = 8.3 Hz, 2H), 7.39-7.38 (d, J = 8.3 Hz, 2H), 2.40 (s, 3H).

(methylsulfinyl)methyl 3-methylbenzoate **(3ba)**



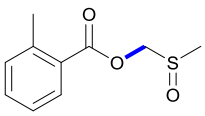
Colorless oil; 37.0 mg, 70%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.89-7.86 (m, 2H), 7.41-7.40 (d, J = 7.6 Hz, 1H), 7.35-7.32 (t, J = 7.7 Hz, 1H), 5.29-5.28 (d, J = 10.4 Hz, 1H), 5.16-5.14 (d, J = 10.5 Hz, 1H), 2.66 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.5, 138.7, 135.0, 130.7, 128.6, 128.1, 127.4, 79.0, 35.9, 21.3; HRMS (ESI-TOF): calcd. for $C_{10}H_{13}O_3S$ $[M+H]^+$ 213.0585, found 213.0589.

((methyl-d_3)sulfinyl)methyl-d_2 3-methylbenzoate (**3ba-d_5**)



Colorless oil; 38.0 mg, 70%; ^{1}H NMR (600 MHz, d^6-DMSO): δ [ppm] = 7.85-7.83 (m, 2H), 7.54-7.53 (d, J = 7.6 Hz, 1H), 7.48-7.45 (t, J = 7.6 Hz, 1H), 2.40 (s, 3H).

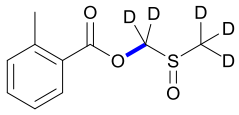
(methylsulfinyl)methyl 2-methylbenzoate (**3ca**)



Colorless oil; 38.6 mg, 73%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.01-8.00 (m, 1H), 7.45-7.42 (m, 1H), 7.26-7.24 (m, 2H), 5.29-5.27 (d, J = 10.5 Hz, 1H), 5.14-5.12

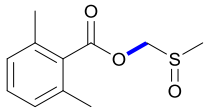
(d, *J* = 10.5 Hz, 1H), 2.66 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.7, 141.5, 133.3, 132.1, 131.2, 127.3, 126.1, 78.9, 36.0, 22.0; HRMS (ESI-TOF): calcd. for $C_{10}H_{13}O_3S$ $[M+H]^+$ 213.0585, found 213.0578.

((methyl-d_3)sulfinyl)methyl-d_2 2-methylbenzoate (**3ca-d$_5$**)



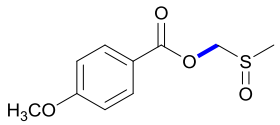
Colorless oil; 39.1 mg, 72%; ^{1}H NMR (600 MHz, d^6-DMSO): δ [ppm] = 7.94-7.92 (m, 1H), 7.56-7.52 (m, 1H), 7.39-7.53 (m, 2H), 2.55 (s, 3H).

(methylsulfinyl)methyl 2,6-dimethylbenzoate **(3da)**



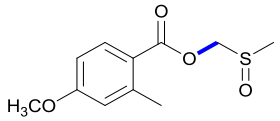
Colorless oil; 37.9 mg, 67%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.23-7.21 (t, *J* = 7.7 Hz, 1H), 7.05-7.03 (d, *J* = 7.7 Hz, 2H), 5.35-5.33 (d, *J* = 10.5 Hz, 1H), 5.11-5.09 (d, *J* = 10.4 Hz, 1H), 2.68 (s, 3H), 2.34 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 168.5, 135.7, 131.8, 130.3, 127.9, 79.0, 36.2, 20.2; HRMS (ESI-TOF): calcd. for $C_{11}H_{15}O_3S$ $[M+H]^+$ 227.0742, found 227.0751.

(methylsulfinyl)methyl 4-methoxybenzoate (**3ea**)



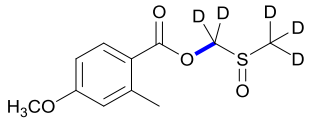
Colorless oil; 37.0 mg, 65%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.02-8.01 (d, *J* = 8.0 Hz, 2H), 6.92-6.90 (d, *J* = 7.9 Hz, 2H), 5.26-5.25 (d, *J* = 10.5 Hz, 1H), 5.14-5.12 (d, *J* = 10.4 Hz, 1H), 3.84 (s, 3H), 2.65 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.0, 164.3, 132.4, 120.4, 114.0, 78.9, 55.6, 35.9; HRMS (ESI-TOF): calcd. for $C_{10}H_{13}O_4S$ $[M+H]^+$ 229.0535, found 229.0536.

(methylsulfinyl)methyl 4-methoxy-2-methylbenzoate (**3fa**)



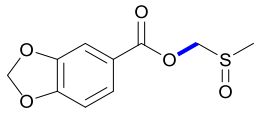
Colorless oil; 39.9 mg, 66%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.03-8.01 (m, 1H), 6.75-6.73 (m, 2H), 5.24-5.23 (d, *J* = 10.5 Hz, 1H), 5.12-5.10 (d, *J* = 10.5 Hz, 1H), 3.83 (s, 3H), 2.65 (s, 3H), 2.59 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.1, 163.3, 144.6, 133.7, 119.3, 117.3, 111.3, 78.8, 55.5, 36.0, 22.6; HRMS (ESI-TOF): calcd. for $C_{11}H_{15}O_4S$ $[M+H]^+$ 243.0691, found 243.0699.

((methyl-d_3)sulfinyl)methyl-d_2 4-methoxy-2-methylbenzoate (**3fa-d$_5$**)



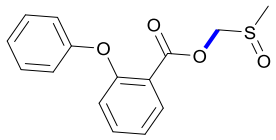
Colorless oil; 40.8 mg, 66%; ^{1}H NMR (600 MHz, d^{6}-DMSO): δ [ppm] = 7.96-7.94 (d, J = 8.5 Hz, 1H), 6.92-6.89 (m, 2H), 3.82 (s, 3H), 2.54 (s, 3H).

(methylsulfinyl)methyl 6-methylbenzo[d][1,3]dioxole-5-carboxylate (**3ga**)



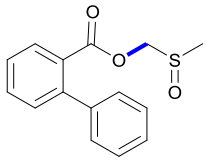
Colorless oil; 36.9 mg, 61%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.70-7.68 (dd, J = 8.1, 1.7 Hz, 1H), 7.46 (d, J = 1.7 Hz, 1H), 6.84-6.83 (d, J = 8.1 Hz, 1H), 6.04 (s, 2H), 5.26-5.25 (d, J = 10.5 Hz, 1H), 5.12-5.10 (d, J = 10.5 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 164.6, 152.7, 148.1, 126.4, 122.0, 109.8, 108.3, 102.2, 79.1, 35.9; HRMS (ESI-TOF): calcd. for $C_{10}H_{11}O_5S$ $[M+H]^+$ 243.0327, found 243.0332.

(methylsulfinyl)methyl 2-phenoxybenzoate (**3ha**)



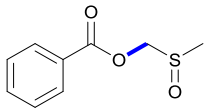
Colorless oil; 46.4 mg, 64%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.99-7.98 (dd, J = 8.2, 1.7 Hz, 1H), 7.50-7.49 (m, 1H), 7.33-7.30 (m, 2H), 7.19-7.16 (m, 1H), 7.11-7.08 (m, 1H), 6.96-6.94 (m, 3H), 5.15-5.13 (d, J = 10.6 Hz, 1H), 5.12-5.11 (d, J = 10.5 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 164.2, 157.1, 157.0, 134.9, 132.5, 130.0, 123.8, 123.6, 120.7, 120.5, 118.6, 78.4, 36.0; HRMS (ESI-TOF): calcd. for $C_{15}H_{15}O_4S$ $[M+H]^+$ 291.0691, found 291.0680.

(methylsulfinyl)methyl [1,1'-biphenyl]-2-carboxylate **(3ia)**



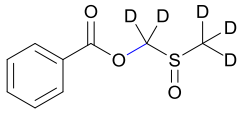
Colorless oil; 47.2 mg, 69%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.91-7.90 (dd, J = 8.2, 1.8 Hz, 1H), 7.58-7.55 (td, J = 8.2, 1.7 Hz, 1H), 7.44-7.42 (td, J = 8.2, 1.8 Hz, 1H), 7.41-7.34 (m, 4H), 7.30-7.29 (m, 2H), 5.00-4.99 (d, J = 10.5 Hz, 1H), 4.86-4.84 (d, J = 10.5 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 167.1, 143.1, 141.2, 132.4, 131.2, 130.6, 128.7, 128.5, 127.7, 127.5, 78.2, 36.1; HRMS (ESI-TOF): calcd. for $C_{15}H_{15}O_3S$ $[M+H]^+$ 275.0742, found 275.0740.

(methylsulfinyl)methyl benzoate (**3ja**)



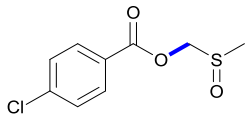
Colorless oil; 36.1 mg, 73%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.09-8.07 (m, 2H), 7.62-7.59 (m, 1H), 7.47-7.44 (m, 2H), 5.31-5.30 (d, J = 10.5 Hz, 1H), 5.17-5.16 (d, J = 10.5 Hz, 1H), 2.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 1653, 134.2, 130.2, 128.8, 128.2, 79.1, 36.0; HRMS (ESI-TOF): calcd. for $C_9H_{11}O_3S$ $[M+H]^+$ 199.0429, found 199.0430.

((methyl-d_3)sulfinyl)methyl-d_2 benzoate (**3ja-d$_5$**)



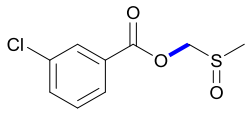
Colorless oil; 35.5 mg, 70%; ^{1}H NMR (600 MHz, d^6-DMSO): δ [ppm] = 8.05-8.03 (m, 2H), 7.73-7.70 (m, 1H), 7.59-7.56 (m, 2H).

(methylsulfinyl)methyl 4-chlorobenzoate (**3ka**)



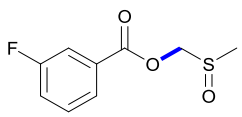
Colorless oil; 31.8 mg, 55%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.02-8.01 (d, J = 8.6 Hz, 2H), 7.44-7.43 (d, J = 8.6 Hz, 2H), 5.33-5.32 (d, J = 10.5 Hz, 1H), 5.14-5.12 (d, J = 10.5 Hz, 1H), 2.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 164.6, 140.8, 131.6, 129.2, 126.6, 79.2, 35.9; HRMS (ESI-TOF): calcd. for $C_9H_{10}ClO_3S$ $[M+H]^+$ 233.0039, found 233.0034.

(methylsulfinyl)methyl 3-chlorobenzoate (**3la**)



Colorless oil; 26.1 mg, 45%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.02-8.01 (t, J = 1.9 Hz, 1H), 7.95-7.94 (dt, J = 8.5, 1.9 Hz, 1H), 7.57-7.55 (m, 1H), 7.41-7.38 (t, J = 8.6 Hz, 1H), 5.35-5.33 (d, J = 10.5 Hz, 1H), 5.17-5.15 (d, J = 10.5 Hz, 1H), 2.70 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 178.4, 164.2, 134.9, 134.2, 130.1, 129.9, 128.3, 79.1, 35.7; HRMS (ESI-TOF): calcd. for $C_9H_{10}ClO_3S$ $[M+H]^+$ 233.0039, found 233.0032.

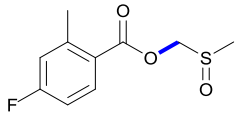
(methylsulfinyl)methyl 3-fluorobenzoate (**3ma**)



Colorless oil; 22.7 mg, 42%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.80-7.79 (dt, J = 8.5, 1.9 Hz, 1H), 7.67-7.65 (m, 1H), 7.40-7.36 (m, 1H), 7.25-7.22 (m, 1H), 5.31-5.30 (d, J = 10.6 Hz, 1H), 5.12-5.10 (d, J = 10.5 Hz, 1H), 2.64 (s, 3H); ^{13}C NMR

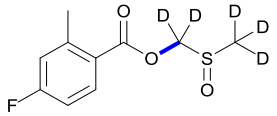
(150 MHz, $CDCl_3$): δ [ppm] = 178.9, 164.2 (d, J_{CF} = 2.5 Hz), 162.5 (d, J_{CF} = 246.5 Hz), 130.5 (d, J_{CF} = 8.1 Hz), 125.9 (d, J_{CF} = 2.4 Hz), 121.2 (d, J_{CF} = 21.0 Hz), 116.9 (d, J_{CF} = 23.5 Hz), 78.9, 35.5; ^{19}F NMR (564 MHz, $CDCl_3$): δ [ppm] = -111.5; HRMS (ESI-TOF): calcd. for $C_9H_{10}FO_3S$ $[M+H]^+$ 217.0335, found 217.0325.

(methylsulfinyl)methyl 4-fluoro-2-methylbenzoate (**3na**)



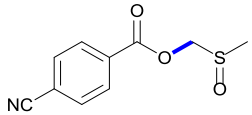
Colorless oil; 32.2 mg, 56%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.08-8.05 (dd, J = 8.7, 5.9 Hz, 1H), 6.98-6.93 (m, 2H), 5.30-5.29 (d, J = 10.5 Hz, 1H), 5.11-5.09 (d, J = 10.5 Hz, 1H), 2.65 (s, 3H), 2.62 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.4 (d, J_{CF} = 253.7 Hz), 164.8, 145.3 (d, J_{CF} = 9.2 Hz), 134.0 (d, J_{CF} = 9.7 Hz), 123.4 (d, J_{CF} = 2.9 Hz), 118.9 (d, J_{CF} = 21.4 Hz), 113.2 (d, J_{CF} = 21.3 Hz), 79.0, 36.0, 22.3 (d, J_{CF} = 1.2 Hz); ^{19}F NMR (564 MHz, $CDCl_3$): δ [ppm] = -105.1; HRMS (ESI-TOF): calcd. for $C_{10}H_{12}FO_3S$ $[M+H]^+$ 231.0491, found 231.0490.

((methyl-d_3)sulfinyl)methyl-d_2 4-fluoro-2-methylbenzoate (**3na-d_5**)



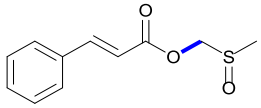
Colorless oil; 30.0 mg, 51%; ^{1}H NMR (600 MHz, d^6-DMSO): δ [ppm] = 8.03-8.00 (m, 1H), 7.26-7.18 (m, 2H), 2.55 (s, 3H).

(methylsulfinyl)methyl 4-cyanobenzoate (**3oa**)



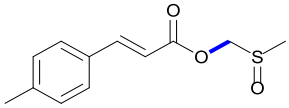
Colorless oil; 19.5 mg, 35%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.19-8.18 (d, J = 8.5 Hz, 2H), 7.77-7.76 (d, J = 8.5 Hz, 2H), 5.41-5.39 (d, J = 10.5 Hz, 1H), 5.15-5.13 (d, J = 10.5 Hz, 1H), 2.69 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 163.7, 132.6, 132.1, 130.7, 117.7, 117.5, 79.4, 35.8; HRMS (ESI-TOF): calcd. for $C_{10}H_{10}NO_3S$ $[M+H]^+$ 224.0381, found 224.0395.

(methylsulfinyl)methyl cinnamate (**3pa**)



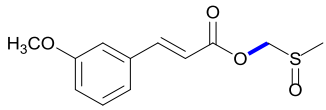
Colorless oil; 38.0 mg, 68%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.82-7.80 (d, J = 16.1 Hz, 1H), 7.54-7.53 (m, 2H), 7.42-7.39 (m, 3H), 6.52-6.49 (d, J = 16.0 Hz, 1H), 5.22-5.20 (d, J = 10.4 Hz, 1H), 5.07-5.05 (d, J = 10.5 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.6, 147.8, 133.9, 131.1, 129.1, 128.5, 115.7, 78.7, 35.8; HRMS (ESI-TOF): calcd. for $C_{11}H_{13}O_3S$ $[M+H]^+$ 225.0585, found 225.0581.

(methylsulfinyl)methyl (E)-3-(p-tolyl)acrylate (**3qa**)



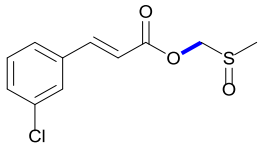
Colorless oil; 41.7 mg, 70%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.79-7.76 (d, J = 16.1 Hz, 1H), 7.43-7.42 (d, J = 8.1 Hz, 2H), 7.20-7.19 (d, J = 8.2 Hz, 2H), 6.46-6.44 (d, J = 16.1 Hz, 1H), 5.20-5.18 (d, J = 10.4 Hz, 1H), 5.06-5.04 (d, J = 10.4 Hz, 1H), 2.64 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.8, 147.8, 141.8, 131.2, 129.9, 128.5, 114.6, 78.6, 35.8, 21.6; HRMS (ESI-TOF): calcd. for $C_{12}H_{15}O_3S$ $[M+H]^+$ 239.0742, found 239.0735.

(methylsulfinyl)methyl (E)-3-(3-methoxyphenyl)acrylate (**3ra**)



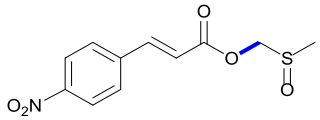
Colorless oil; 47.0 mg, 74%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.79-7.76 (d, J = 16.1 Hz, 1H), 7.33-7.30 (t, J = 7.9 Hz, 1H), 7.13-7.12, (dt, J = 8.0, 2.3 Hz, 1H), 7.05-7.04 (t, J = 2.3 Hz, 1H), 6.97-6.95 (m, 1H), 6.51-6.48 (d, J = 16.1 Hz, 1H), 5.22-5.20 (d, J = 10.5 Hz, 1H), 5.06-5.05 (d, J = 10.4 Hz, 1H), 3.83 (s, 3H), 2.65 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.5, 160.0, 147.7, 135.2, 130.1, 121.2, 117.1, 116.0, 113.2, 78.6, 55.4, 35.8; HRMS (ESI-TOF): calcd. for $C_{12}H_{15}O_4S$ $[M+H]^+$ 255.0691, found 255.0689.

(methylsulfinyl)methyl (E)-3-(3-chlorophenyl)acrylate (**3sa**)



Colorless oil; 38.7 mg, 60%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.74-7.71 (d, J = 16.0 Hz, 1H), 7.51-7.50 (m, 1H), 7.40-7.25 (m, 3H), 6.51-6.48 (d, J = 16.1 Hz, 1H), 5.22-5.20 (d, J = 10.5 Hz, 1H), 5.04-5.03 (d, J = 10.4 Hz, 1H), 2.64 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 165.2, 146.0, 135.6, 135.2, 131.0, 130.4, 128.2, 126.6, 117.2, 78.7, 35.8; HRMS (ESI-TOF): calcd. for $C_{11}H_{12}ClO_3S$ $[M+H]^+$ 259.0196, found 259.0187.

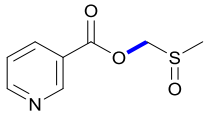
(methylsulfinyl)methyl (E)-3-(4-nitrophenyl)acrylate (**3ta**)



Colorless oil; 27.6 mg, 41%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 8.26-8.24 (d, J = 8.6 Hz, 2H), 7.84-7.81 (d, J = 16.0 Hz, 1H), 7.69-7.68 (d, J = 8.4 Hz, 2H), 6.64-6.62 (d, J = 16.0 Hz, 1H), 5.28-5.26 (d, J = 10.5 Hz, 1H), 5.04-5.02 (d, J = 10.5 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 164.7, 148.9, 144.5, 139.8, 129.1, 124.4, 120.1, 78.8, 35.8; HRMS (ESI-TOF): calcd. for $C_{11}H_{12}NO_5S$

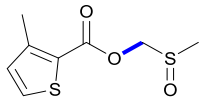
$[M+H]^+$ 270.0436, found 270.0429.

(methylsulfinyl)methyl nicotinate (**3ua**)



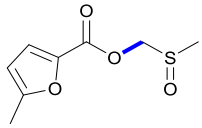
Colorless oil; 22.4 mg, 45%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 9.28-9.27 (dd, J = 2.1, 0.7 Hz, 1H), 8.84-8.82 (dd, J = 4.9, 1.9 Hz, 1H), 8.37-8.35 (dt, J = 8.0, 2.1 Hz, 1H), 7.45-7.43 (m, 1H), 5.40-5.38 (d, J = 10.4 Hz, 1H), 5.17-5.15 (d, J = 10.5 Hz, 1H), 2.70 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 164.1, 154.5, 151.3, 137.7, 124.4, 123.7, 79.1, 36.0; HRMS (ESI-TOF): calcd. for $C_8H_{10}NO_3S$ $[M+H]^+$ 200.0381, found 200.0389.

(methylsulfinyl)methyl 3-methylthiophene-2-carboxylate (**3va**)



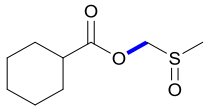
Colorless oil; 38.7 mg, 71%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.46-7.45 (d, J = 8.1 Hz, 2H), 6.93-6.92 (d, J = 8.1 Hz, 2H), 5.24-5.22 (d, J = 10.5 Hz, 1H), 5.14-5.12 (d, J = 10.4 Hz, 1H), 2.70 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 161.1, 148.8, 132.1, 132.0, 124.3, 78.2, 35.8, 16.3; HRMS (ESI-TOF): calcd. for $C_8H_{11}O_3S_2$ $[M+H]^+$ 219.0150, found 219.0164.

(methylsulfinyl)methyl 5-methylfuran-2-carboxylate (**3wa**)



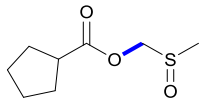
Colorless oil; 32.3 mg, 64%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.25-7.24 (d, J = 8.1 Hz, 1H), 6.17-6.16 (d, J = 8.0 Hz, 1H), 5.26-5.24 (d, J = 10.4 Hz, 1H), 5.12-5.11 (d, J = 10.4 Hz, 1H), 2.66 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 159.1, 157.1, 141.1, 122.0, 109.1, 78.4, 35.9, 14.2; HRMS (ESI-TOF): calcd. for $C_8H_{11}O_4S$ $[M+H]^+$ 203.0378, found 203.0384.

(methylsulfinyl)methyl cyclohexanecarboxylate (**3xa**)



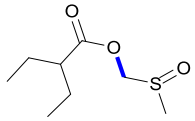
Colorless oil; 38.3 mg, 75%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 5.06-5.04 (d, J = 10.5 Hz, 1H), 4.92-4.90 (d, J = 10.4 Hz, 1H), 2.58 (s, 3H), 2.43-2.38 (m, 1H), 1.92-1.88 (m, 2H), 1.72-1.70 (m, 2H), 1.62-1.58 (m, 1H), 1.46-1.39 (m, 2H), 1.28-1.16 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 178.5, 174.8, 78.0, 42.8, 35.5, 28.9, 28.9, 25.6, 25.3, 25.3; HRMS (ESI-TOF): calcd. for $C_9H_{17}O_3S$ $[M+H]^+$ 205.0898, found 205.0899.

(methylsulfinyl)methyl cyclopentanecarboxylate (**3ya**)



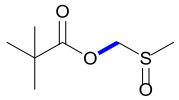
Colorless oil; 34.2 mg, 72%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 5.08-5.06 (d, *J* = 10.5 Hz, 1H), 4.92-4.90 (d, *J* = 10.5 Hz, 1H), 2.85-2.79 (m, 1H), 2.59 (s, 3H), 1.92-1.87 (m, 2H), 1.80-1.75 (m, 2H), 1.70-1.64 (m, 2H), 1.59-1.53 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 178.4, 175.6, 78.2, 43.3, 35.5, 30.1, 25.9, 25.8; HRMS (ESI-TOF): calcd. for $C_8H_{15}O_3S$ $[M+H]^+$ 191.0742, found 191.0736.

(methylsulfinyl)methyl 2-ethylbutanoate (**3za**)



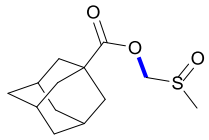
Colorless oil; 33.1 mg, 69%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 5.11-5.09 (d, *J* = 10.5 Hz, 1H), 4.94-4.93 (d, *J* = 10.5 Hz, 1H), 2.61 (s, 3H), 2.37-2.32 (m, 1H), 1.68-1.61 (m, 2H), 1.60-1.52 (m, 2H), 0.91-0.87 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 177.9, 175.1, 78.4, 48.6, 35.8, 29.7, 24.9, 24.9, 11.8, 11.8; HRMS (ESI-TOF): calcd. for $C_8H_{17}O_3S$ $[M+H]^+$ 193.0898, found 193.0905.

(methylsulfinyl)methyl pivalate (**3ab**)



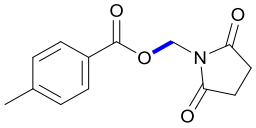
Colorless oil; 19.1 mg, 43%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 5.03-5.02 (d, *J* = 10.5 Hz, 1H), 4.90-4.88 (d, *J* = 10.5 Hz, 1H), 2.56 (s, 3H), 1.18 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 178.7, 177.3, 78.2, 39.1, 35.5, 27.1; HRMS (ESI-TOF): calcd. for $C_7H_{15}O_3S$ $[M+H]^+$ 179.0742, found 179.0742.

(methylsulfinyl)methyl (3r,5r,7r)-adamantane-1-carboxylate (**3ac**)



Colorless oil; 34.6 mg, 54%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 5.04-5.02 (d, *J* = 10.5 Hz, 1H), 4.91-4.90 (d, *J* = 10.4 Hz, 1H), 2.58 (s, 3H), 2.01 (s, 3H), 194-1.91 (m, 6H), 1.73-1.66 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 176.3, 78.1, 41.1, 38.8, 36.3, 35.8, 27.8; HRMS (ESI-TOF): calcd. for $C_{13}H_{21}O_3S$ $[M+H]^+$ 257.1211, found 257.1225.

(2,5-dioxopyrrolidin-1-yl)methyl 4-methylbenzoate (**x**)

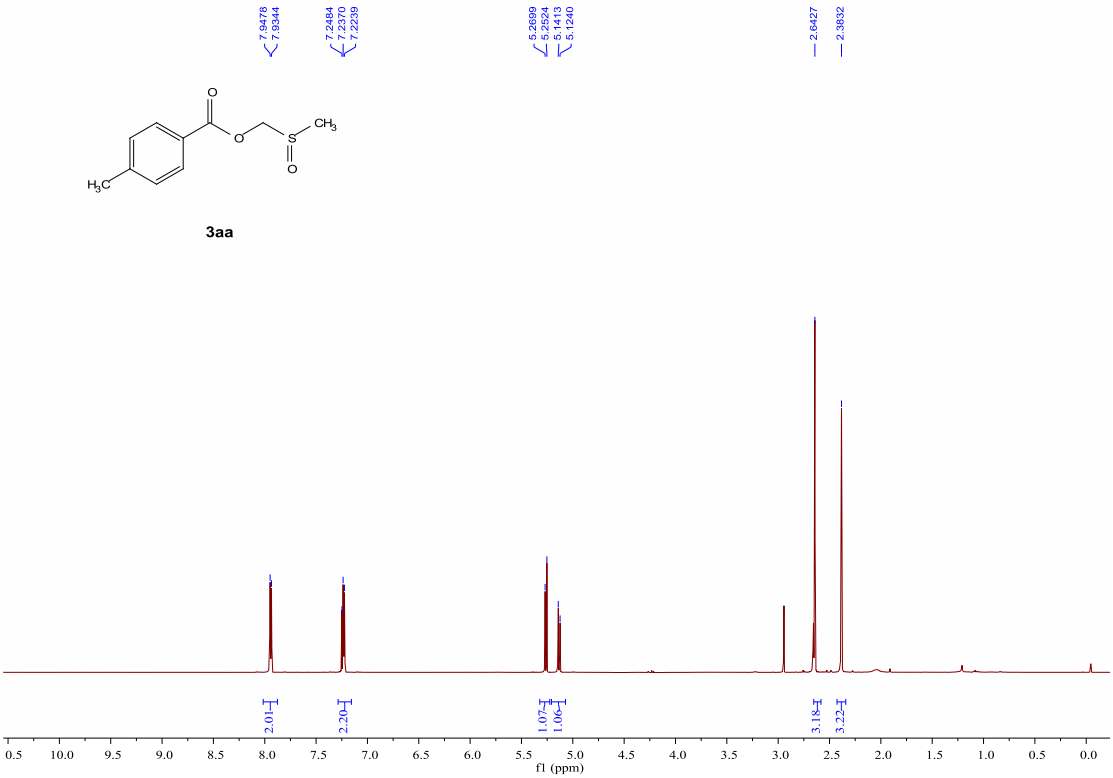


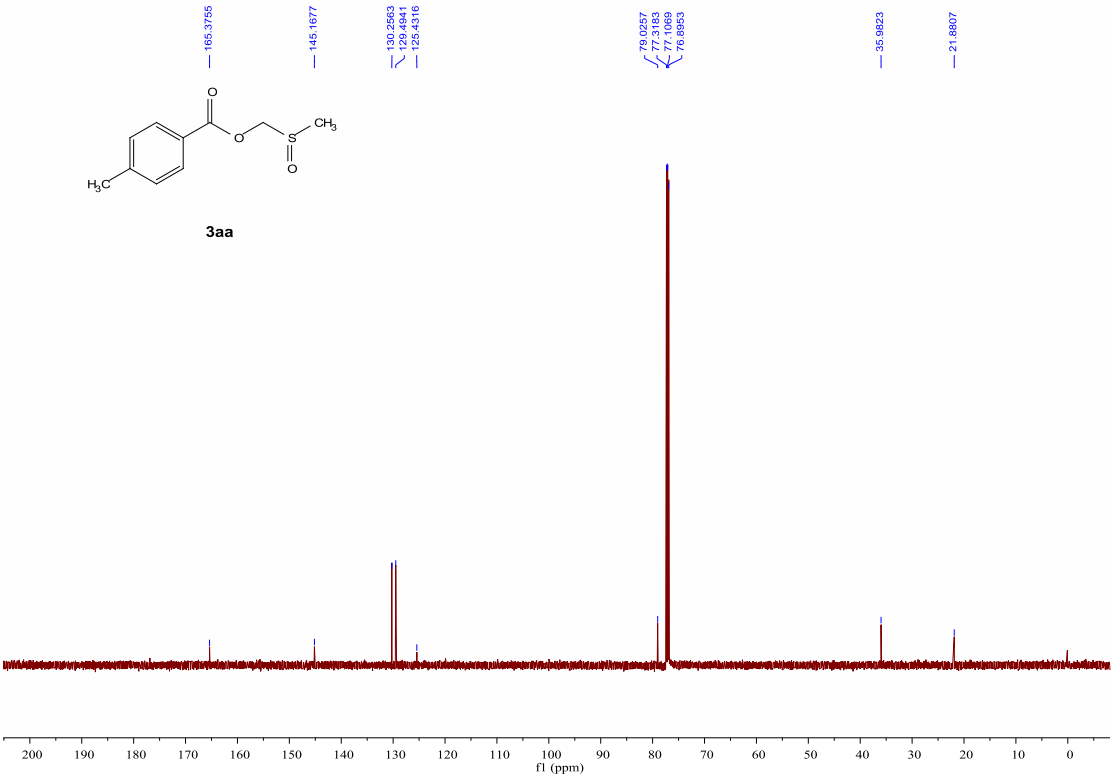
White solid, 125-127 ^{o}C; 25.9 mg, 35%; ^{1}H NMR (600 MHz, $CDCl_3$): δ [ppm] = 7.88-7.87 (d, J = 8.2 Hz, 2H), 7.21-7.20 (d, J = 8.1 Hz, 2H), 5.74 (s, 2H), 2.81 (s, 4H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ [ppm] = 175.7, 165.4, 144.4, 130.0, 129.2, 126.3, 61.5, 28.3, 21.8.[1]

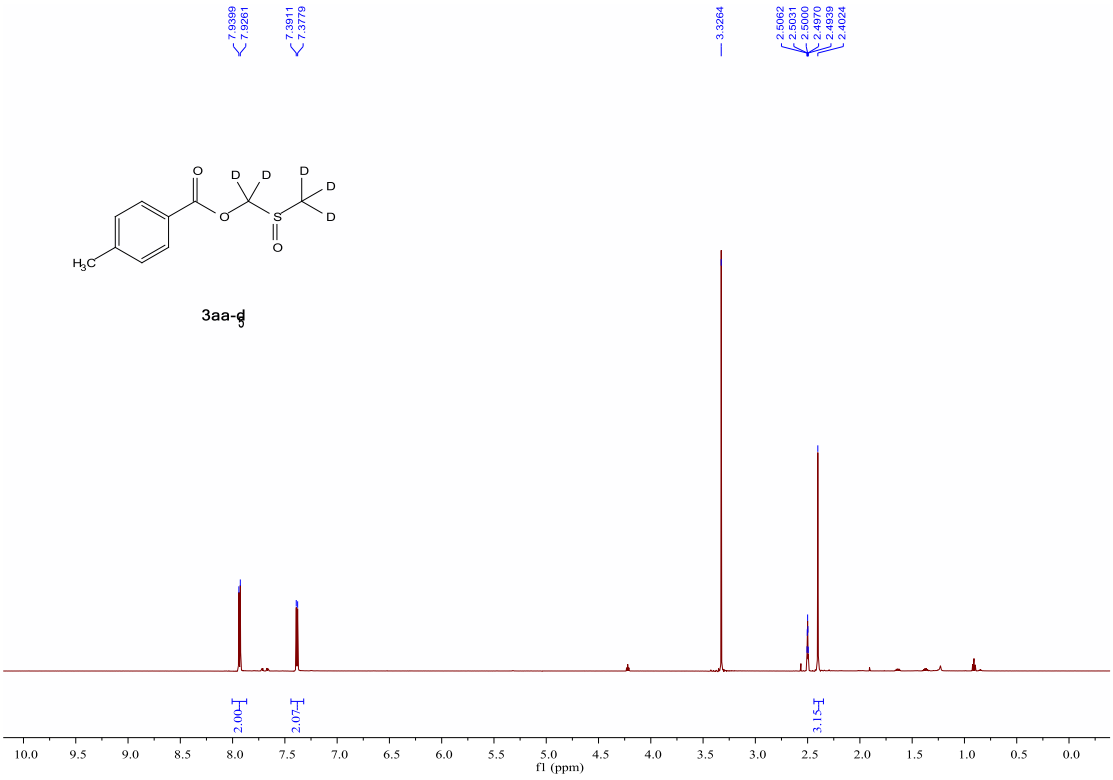
References:

[1] C. S. C. Kumar, W.-S. Loh, Si. Chandraju, Y.-F. Win, W. K. Tan, C. K. Quah, H.-K. Fun, Plos One, 2015, **10**, e0119440.

NMR Spectra of products



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7.3911
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3.3264
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2.5031
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2.4970
2.4939
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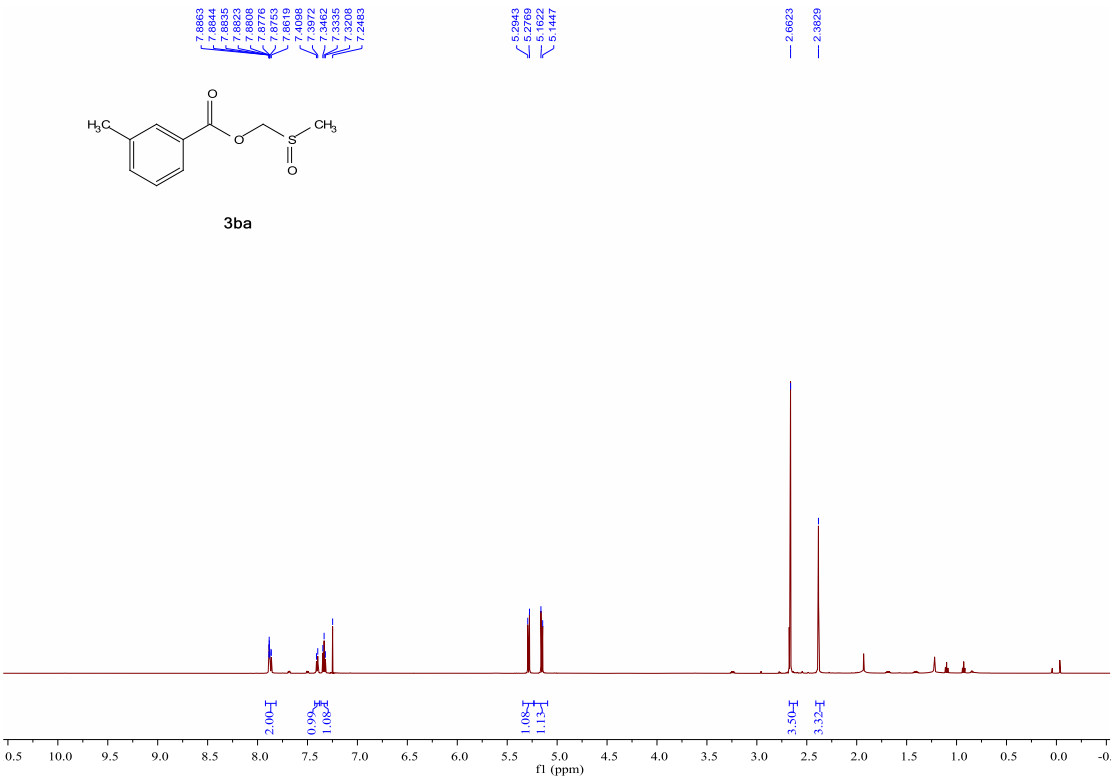
O
D
D
D
D
D
O
S
O
H3C
2.00
2.07
3.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3aa-d6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7.8835
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2.3829
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H3C
O
S
CH3
O
2.00
0.96
1.08
1.08
1.13
3.50
3.32
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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1.5
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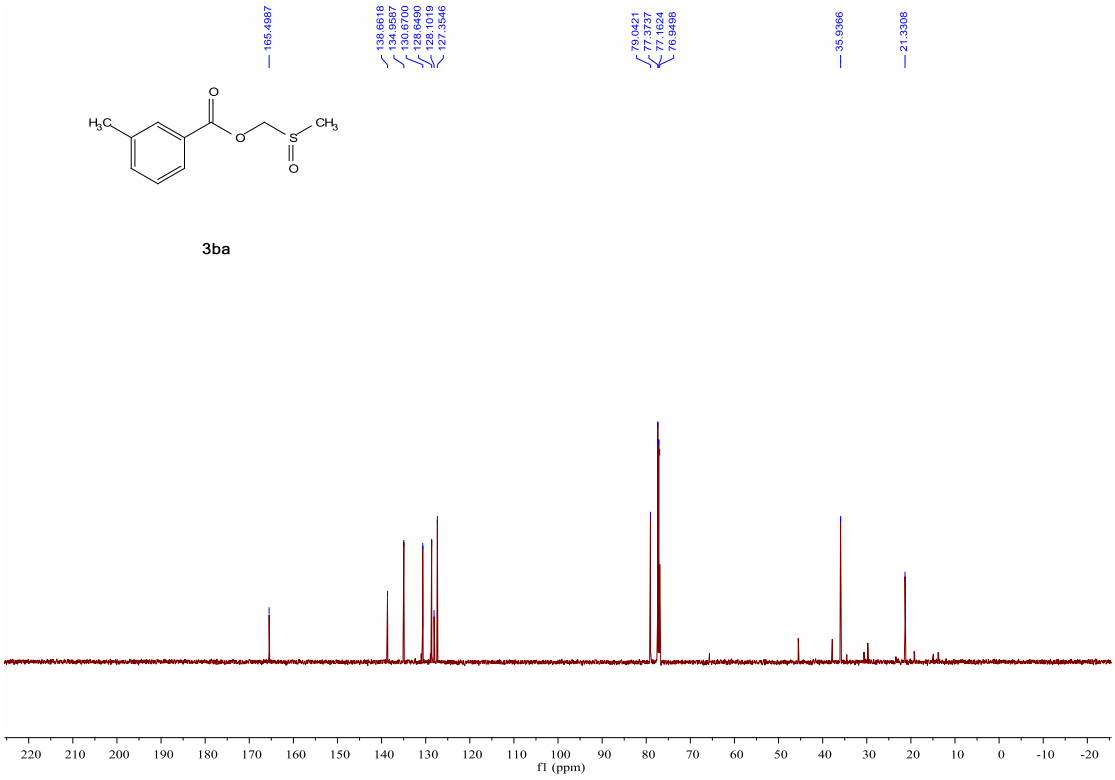
-0.
f1 (ppm)

3ba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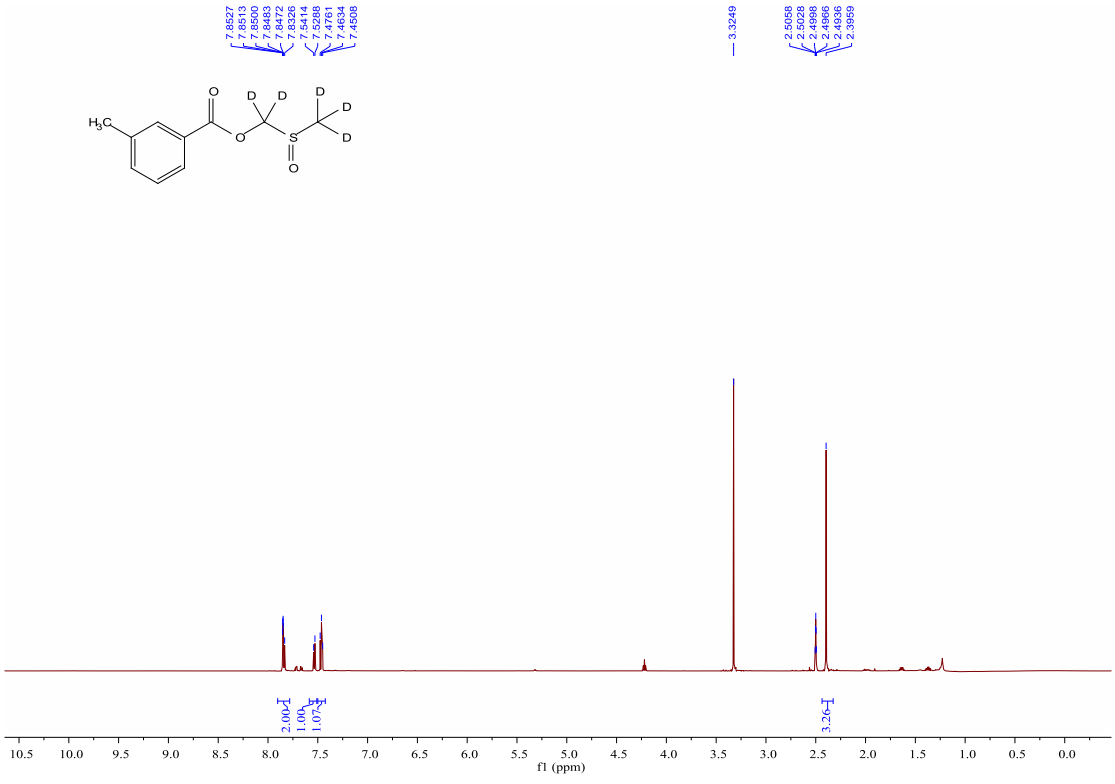
3ba
f1 (ppm)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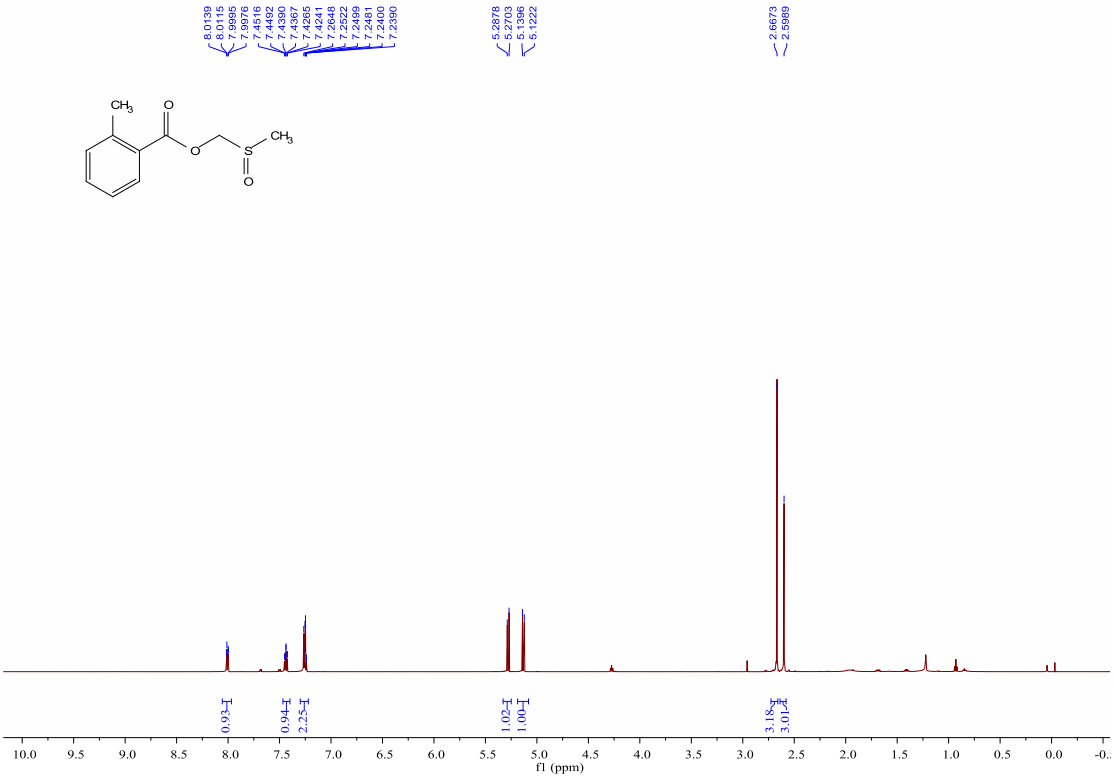
2.00
1.00
1.07
3.26
f1 (ppm)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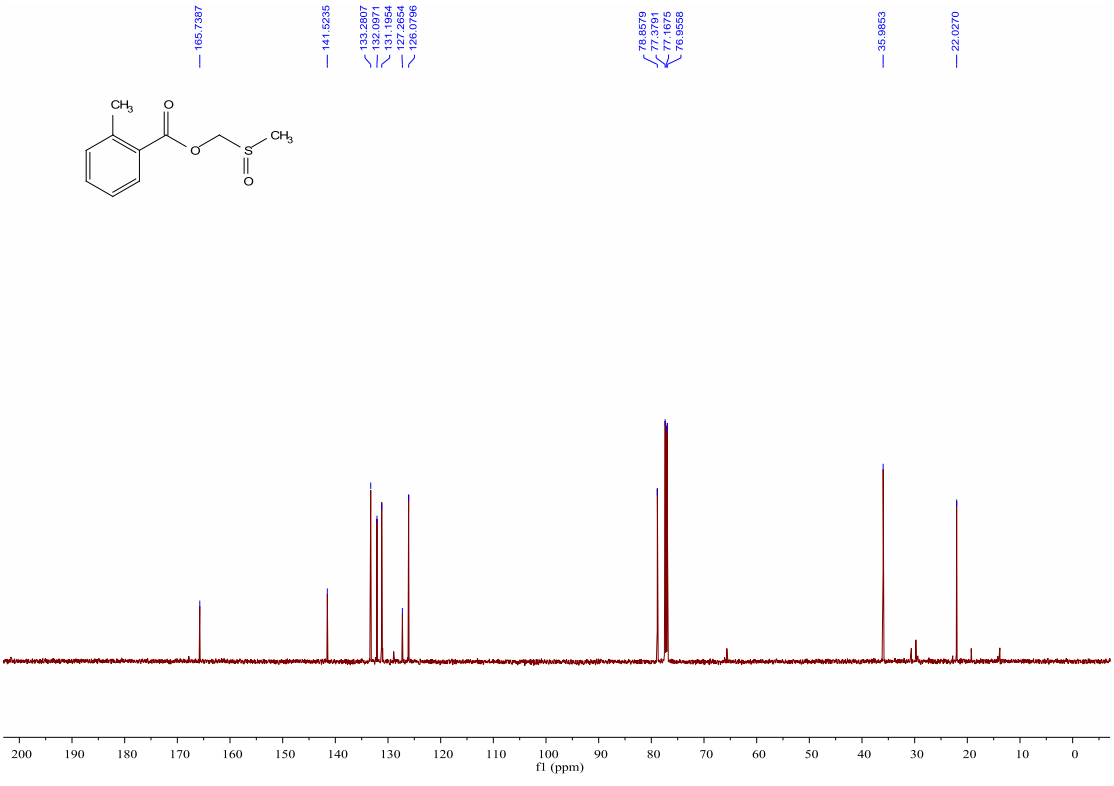
7.2400
7.2390
5.2878
5.2703
5.1396
5.1222
2.6673
2.5989
CH3
O
O
S
CH3
O
0.93
0.94
2.25
1.02
1.00
3.18
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.0796
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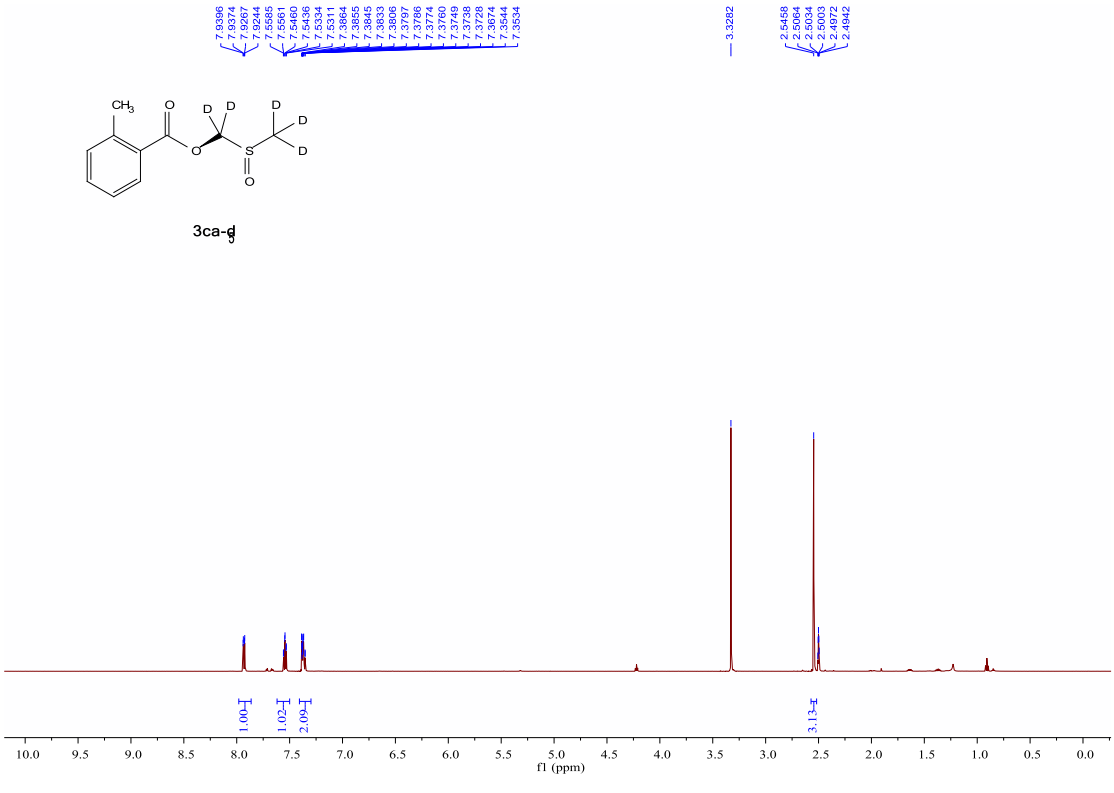
77.1675
76.9558
35.9853
22.0270
CH3
O
O
S
CH3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.9267
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7.5460
7.5436
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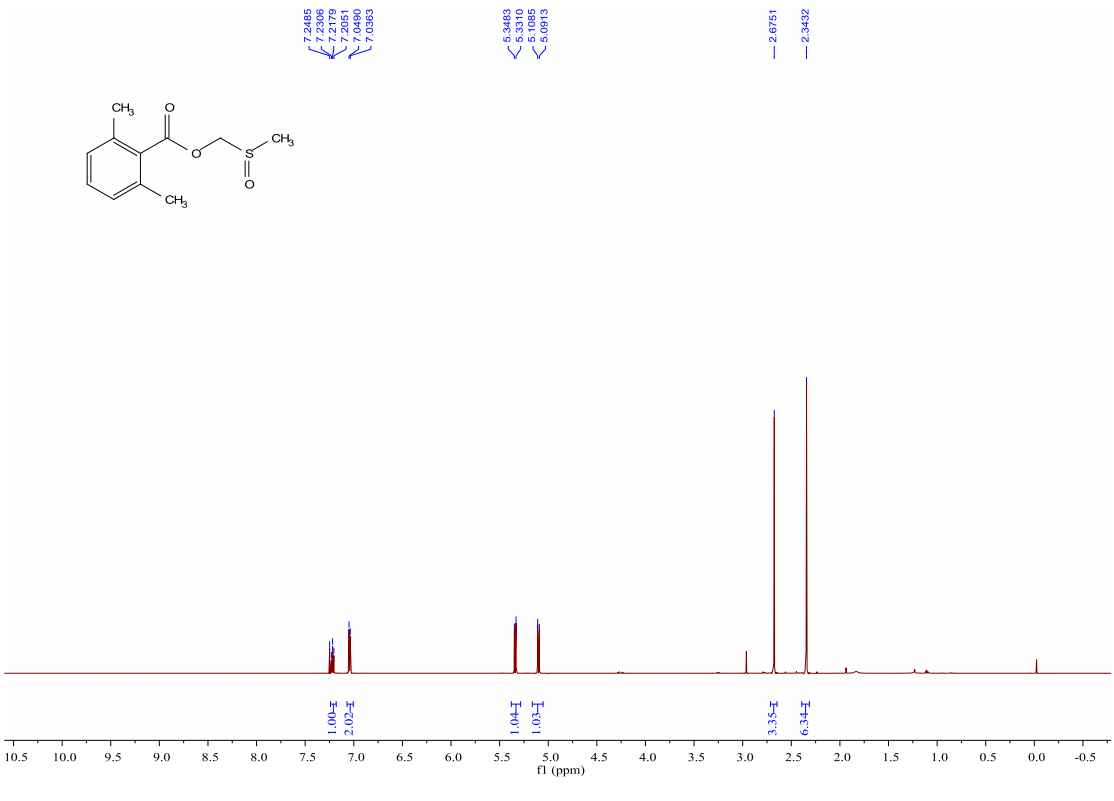
7.3864
7.3855
7.3845
7.3833
7.3806
7.3797
7.3786
7.3774
7.3760
7.3749
7.3738
7.3728
7.3674
7.3544
7.3534
3.3282
2.5458
2.5064
2.5034
2.5003
2.4972
2.4942
CH3
O
D
D
D
D
D
O
S
O
3ca-d3
1.00
1.02
2.09
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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7.2179
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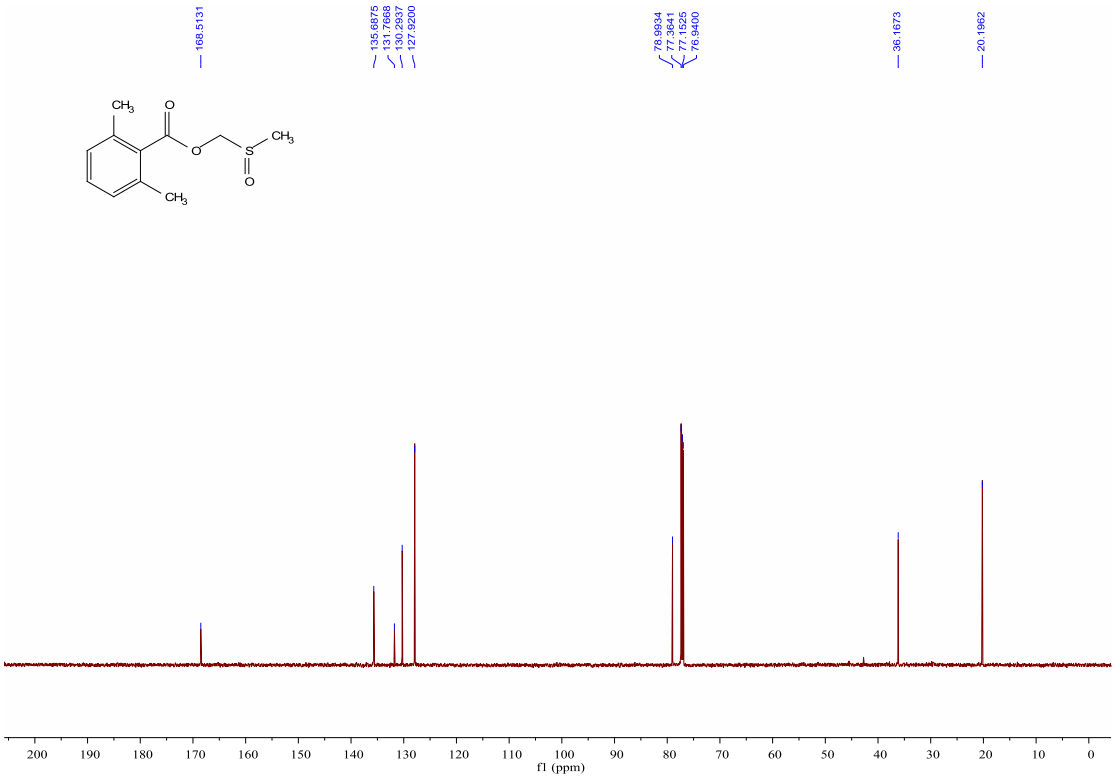
7.0490
7.0363
5.3493
5.3310
5.1085
5.0913
2.6751
2.3432
CH3
O
O
S
CH3
O
CH3
1.00
2.02
1.04
1.03
3.35
6.34
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


168.5131
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127.9200
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77.3641
77.1525
76.9400
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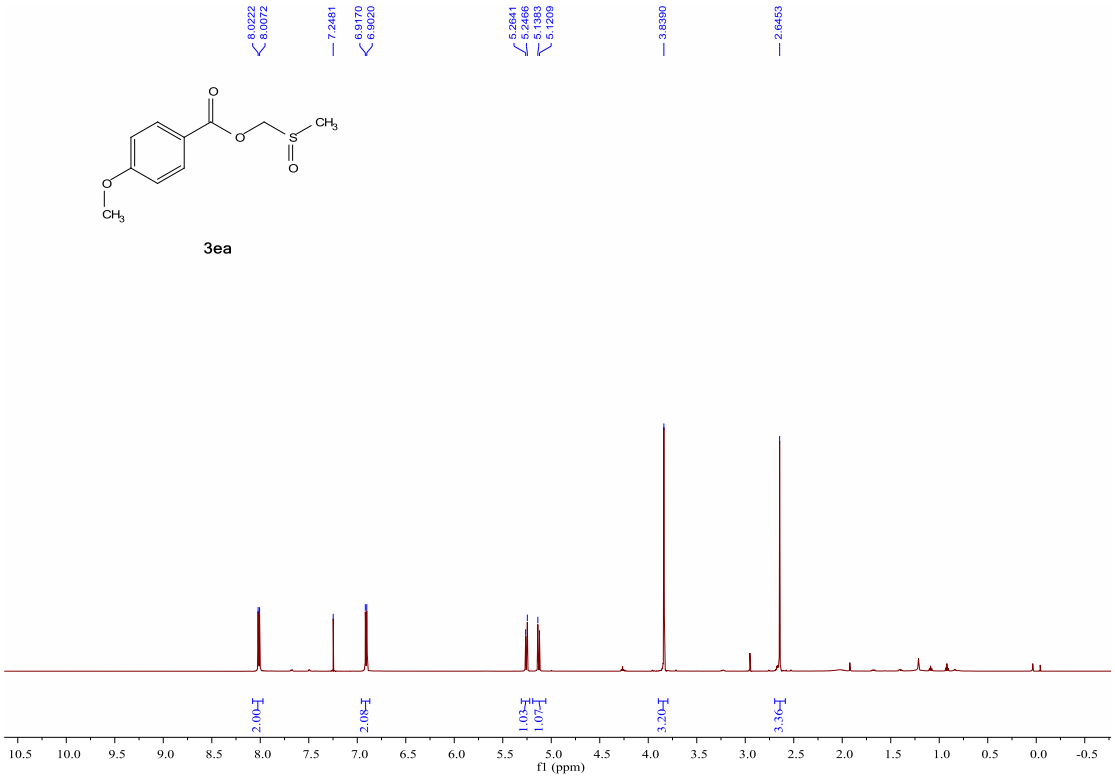
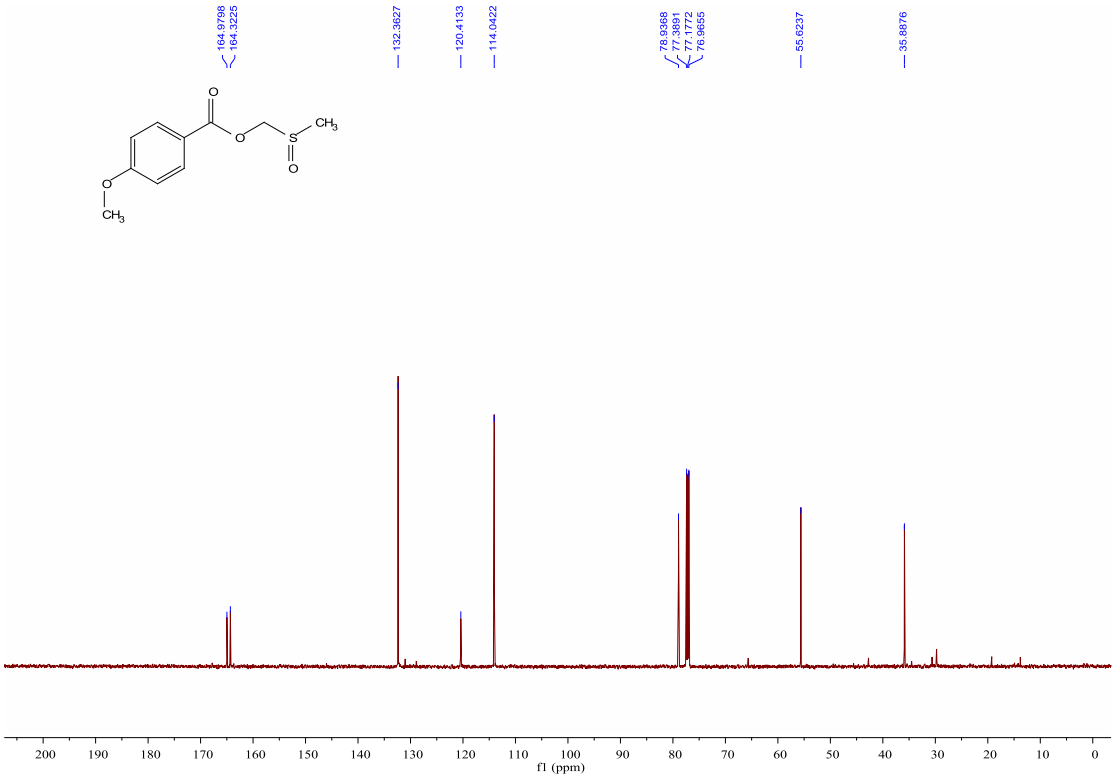
20.1962
f1 (ppm)


8.0222
8.0072
7.2481
6.9170
6.9020
5.2641
5.2466
5.1383
5.1209
3.8390
2.6453
2.00
2.08
1.03
1.07
3.20
3.36
f1 (ppm)

3ea


164.9798
164.3225
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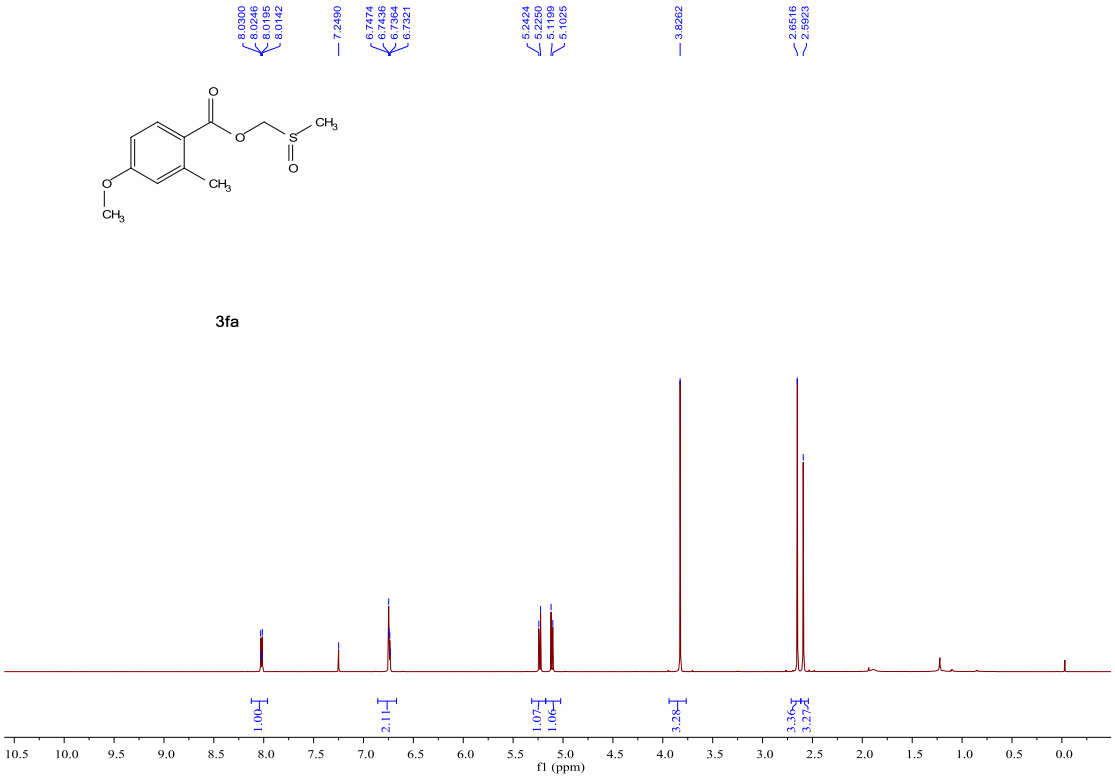
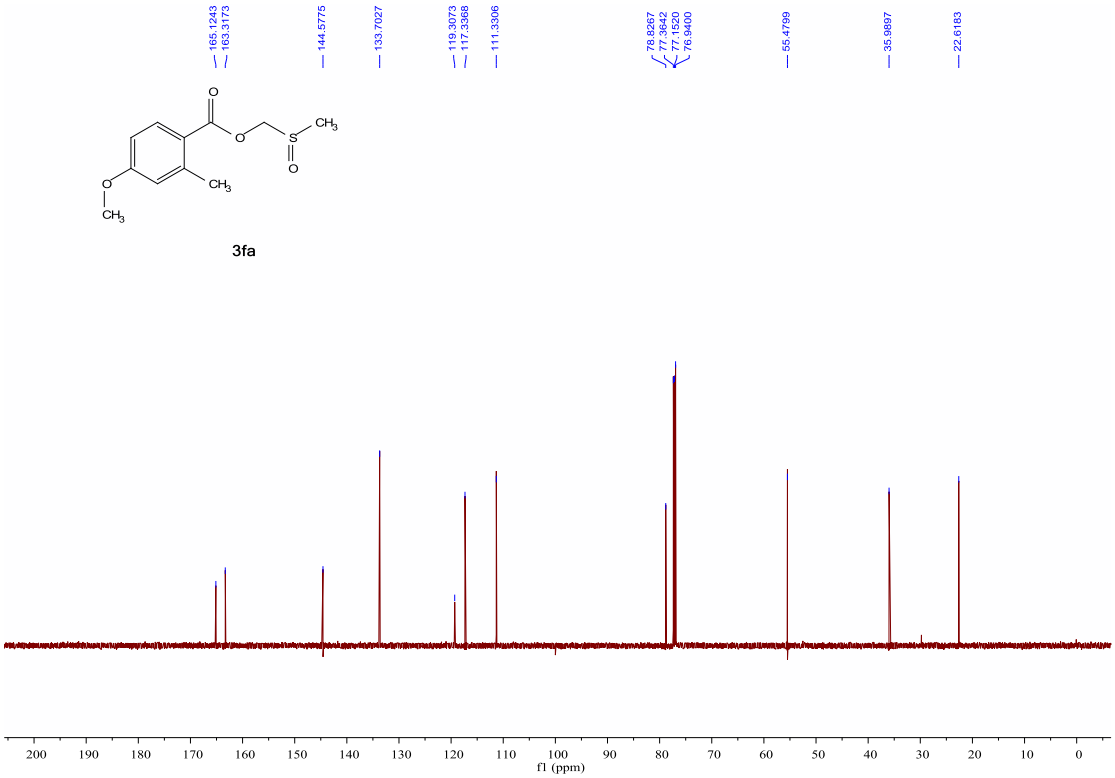
120.4133
114.0422
78.9368
77.3891
77.1772
76.9655
55.6237
35.8876
f1 (ppm)


8.0300
8.0046
8.0195
8.0142
7.2490
6.7474
6.7438
6.7364
6.7321
5.2424
5.2250
5.1199
5.1025
3.8262
2.6516
2.5923
1.00
2.11
1.07
1.06
3.28
3.36
3.27
f1 (ppm)

3fa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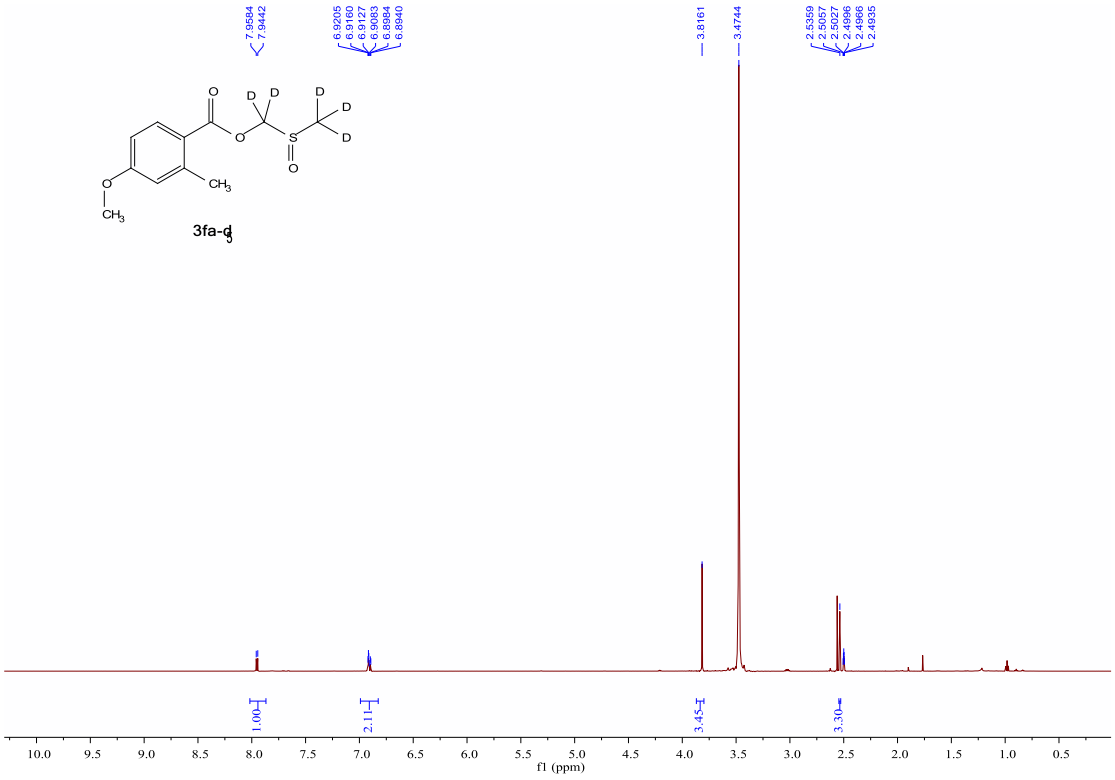
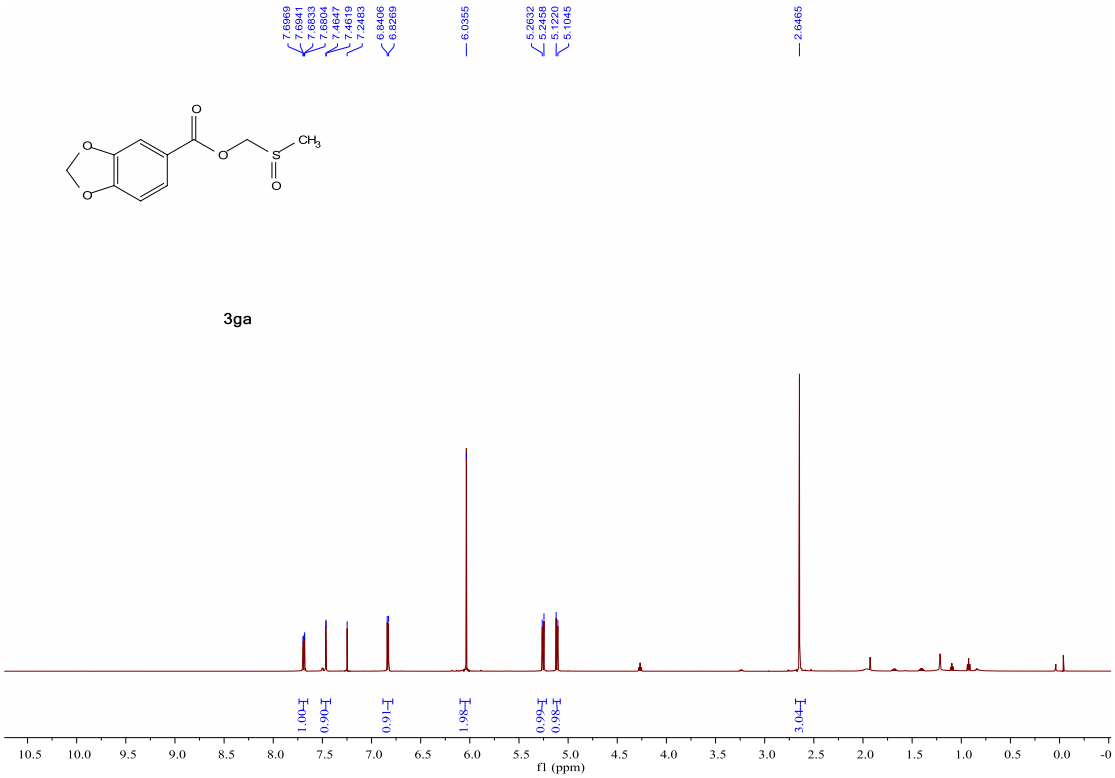
163.3173
144.5775
133.7027
119.3073
117.3368
111.3306
78.8267
77.3642
77.1520
76.9400
55.4799
35.9897
22.6183
O
O
S
CH3
O
CH3
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3fa


7.9584
7.9442
6.9205
6.9160
6.9127
6.9083
6.8984
6.8940
3.8161
3.4744
2.5359
2.5057
2.5027
2.4966
2.4935
O
D
D
D
D
D
O
S
O
O
CH3
CH3
1.00
2.11
3.45
3.30
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
f1 (ppm)

3fa-d$_5$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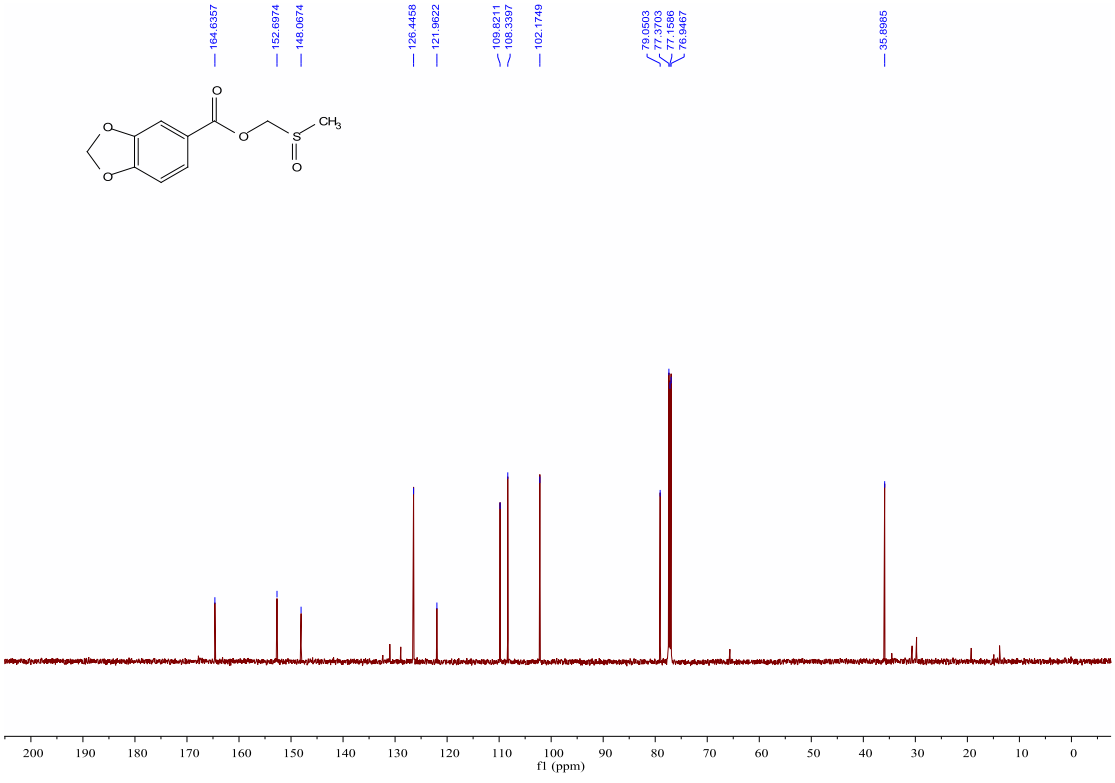
7.6941
7.6833
7.6804
7.4647
7.4619
7.2483
6.8406
6.8299
6.0355
5.2632
5.2458
5.1220
5.1045
2.6465
O
O
O
O
S
CH3
1.00
0.90
0.91
1.98
0.99
0.98
3.04
f1 (ppm)

3ga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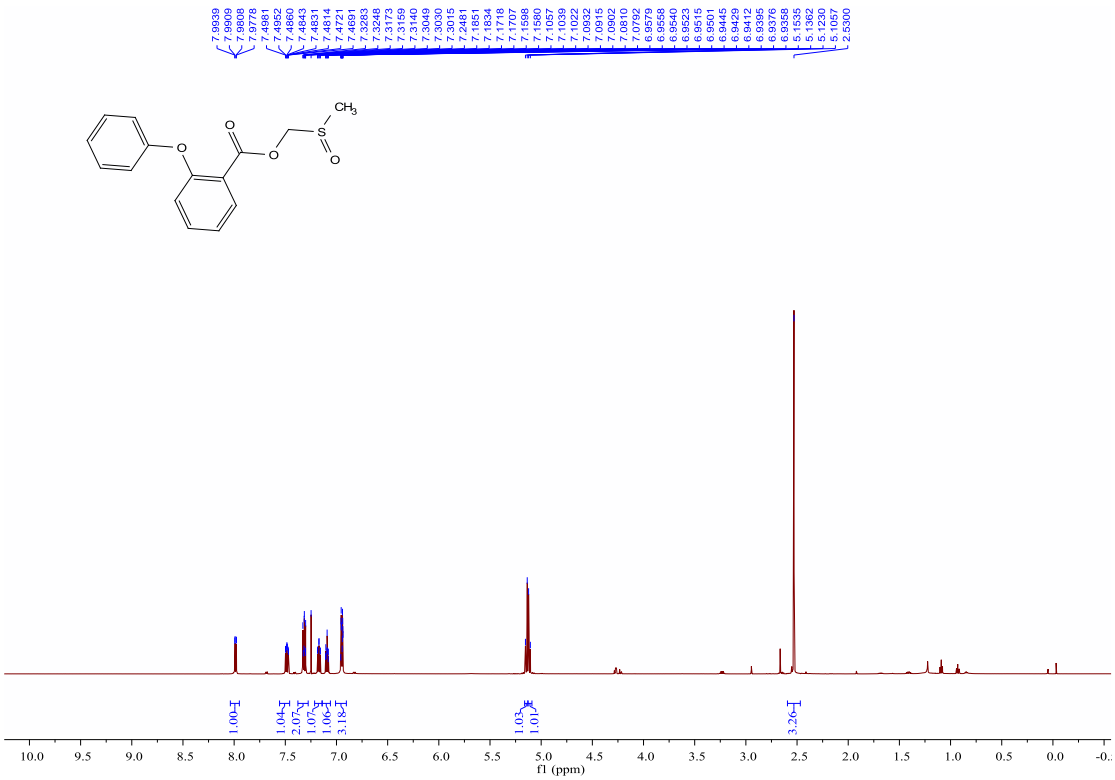
152.6974
148.0674
126.4458
121.9622
109.8211
108.3397
102.1749
79.0503
77.3703
77.1586
76.9467
35.8985
O
O
O
O
S
CH3
f1 (ppm)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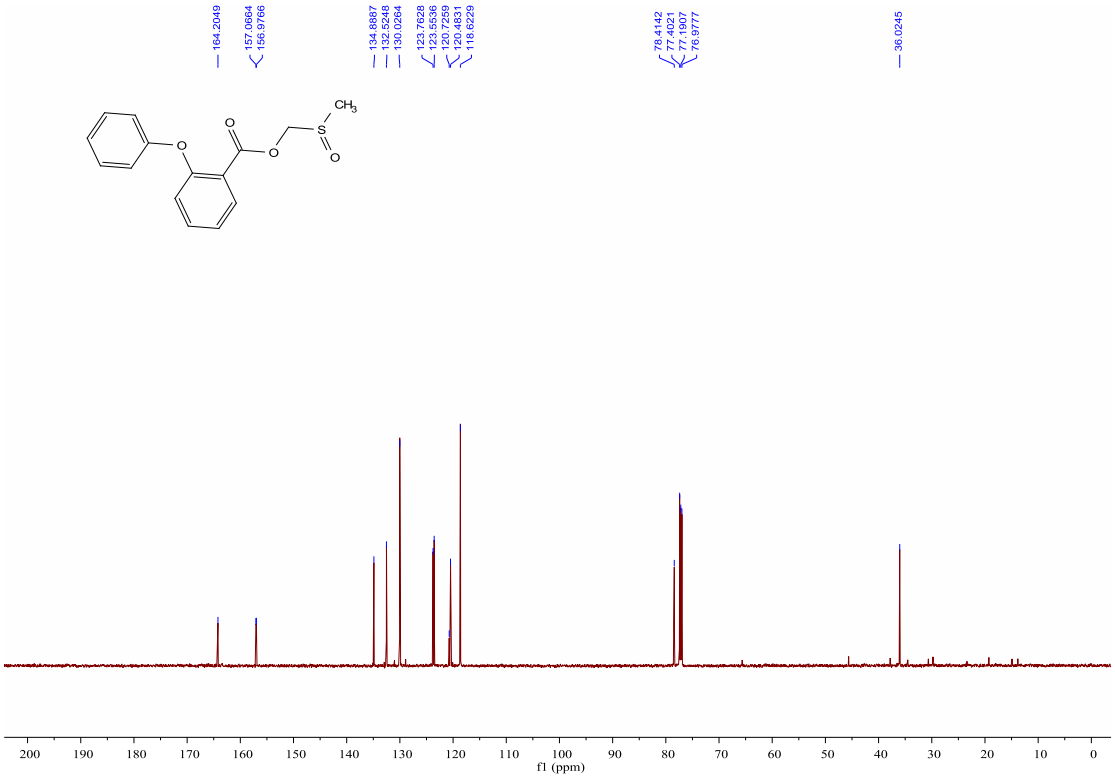
7.9909
7.9898
7.9778
7.4981
7.4952
7.4860
7.4843
7.4831
7.4814
7.4721
7.4691
7.3283
7.3248
7.3173
7.3159
7.3140
7.3049
7.3030
7.2915
7.2491
7.1851
7.1834
7.1718
7.1707
7.1598
7.1580
7.1057
7.1039
7.1022
7.0932
7.0915
7.0902
7.0810
7.0792
6.9579
6.9558
6.9540
6.9523
6.9515
6.9501
6.9445
6.9429
6.9412
6.9395
6.9378
6.9358
5.1535
5.1362
5.1230
5.1057
2.5300
CH3
S
O
O
O
O
1.00
1.04
2.07
1.07
1.06
3.18
1.03
1.01
3.26
f1 (ppm)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132.5248
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123.5536
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120.4831
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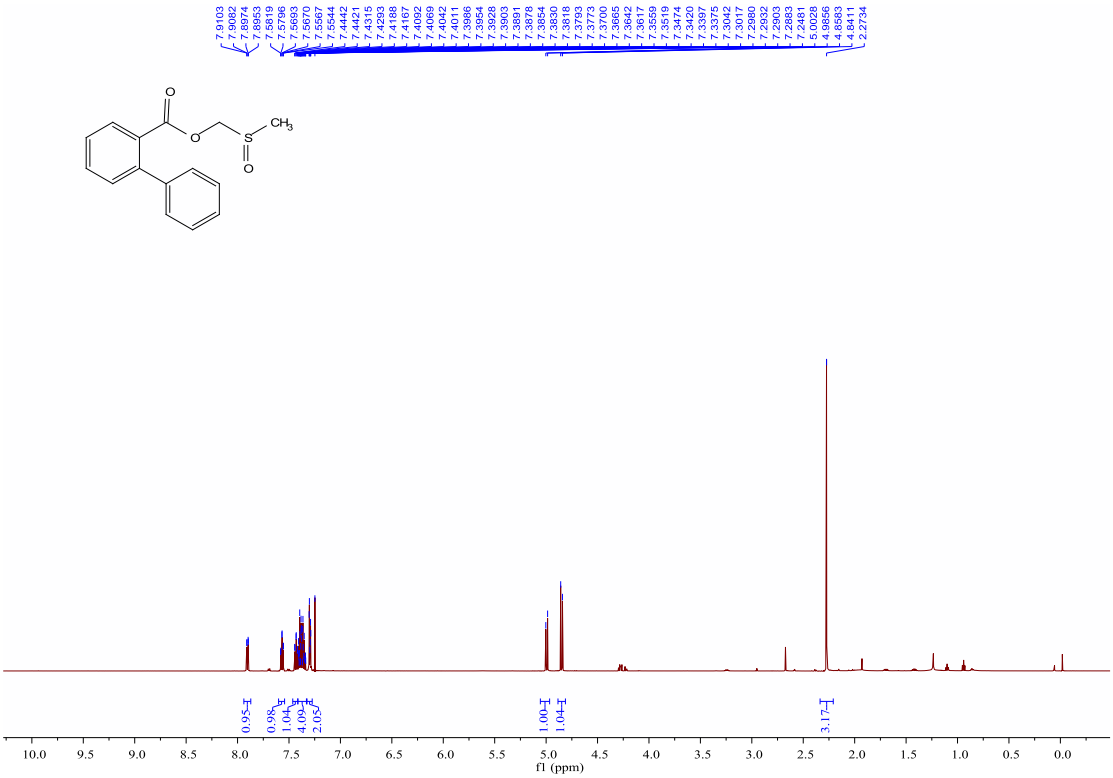
78.4142
77.4021
77.1907
76.9777
36.0245
CH3
S
O
O
O
O
f1 (ppm)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7.5796
7.5693
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7.5567
7.5544
7.4442
7.4421
7.4315
7.4293
7.4168
7.4167
7.4092
7.4069
7.4042
7.4011
7.3986
7.3954
7.3928
7.3903
7.3891
7.3878
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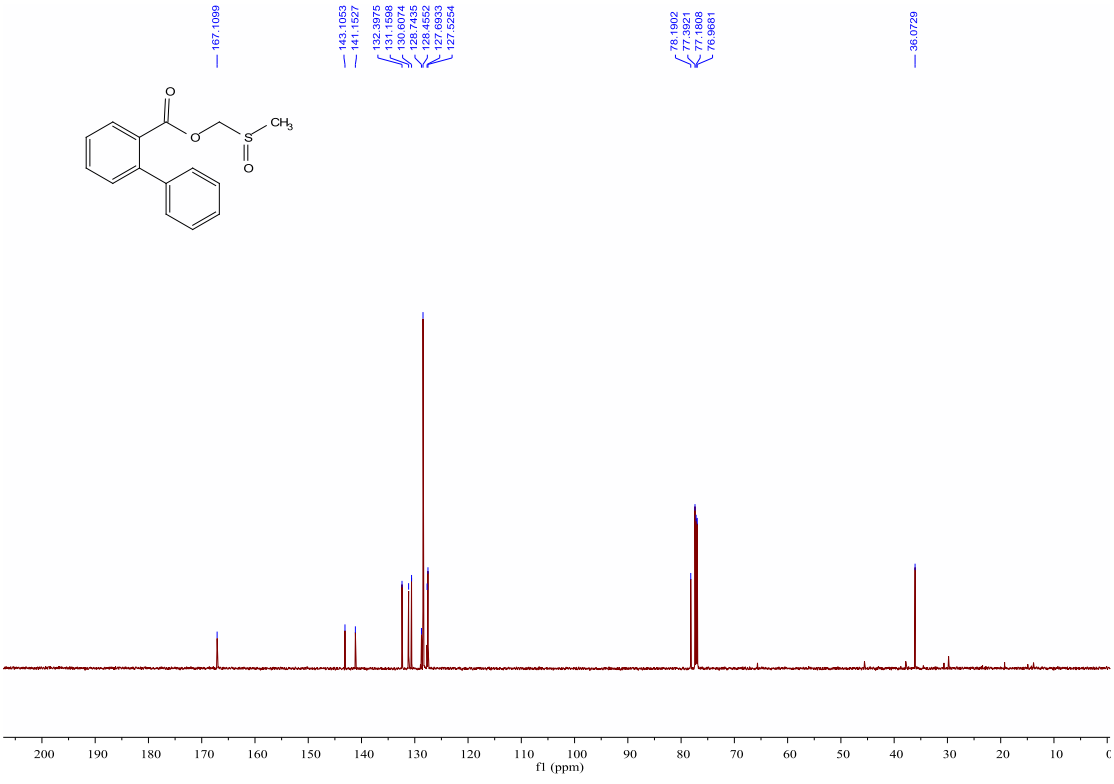
7.3793
7.3773
7.3700
7.3665
7.3642
7.3617
7.3559
7.3519
7.3474
7.3420
7.3397
7.3375
7.3042
7.3017
7.2980
7.2932
7.2903
7.2883
7.2481
4.6078
4.6056
4.8583
4.8411
2.2734
O
O
S
CH3
O
0.95
0.98
1.04
4.09
2.05
1.00
1.04
3.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.1598
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128.7435
128.4552
127.6933
127.5254
78.1902
77.3831
77.1808
76.9681
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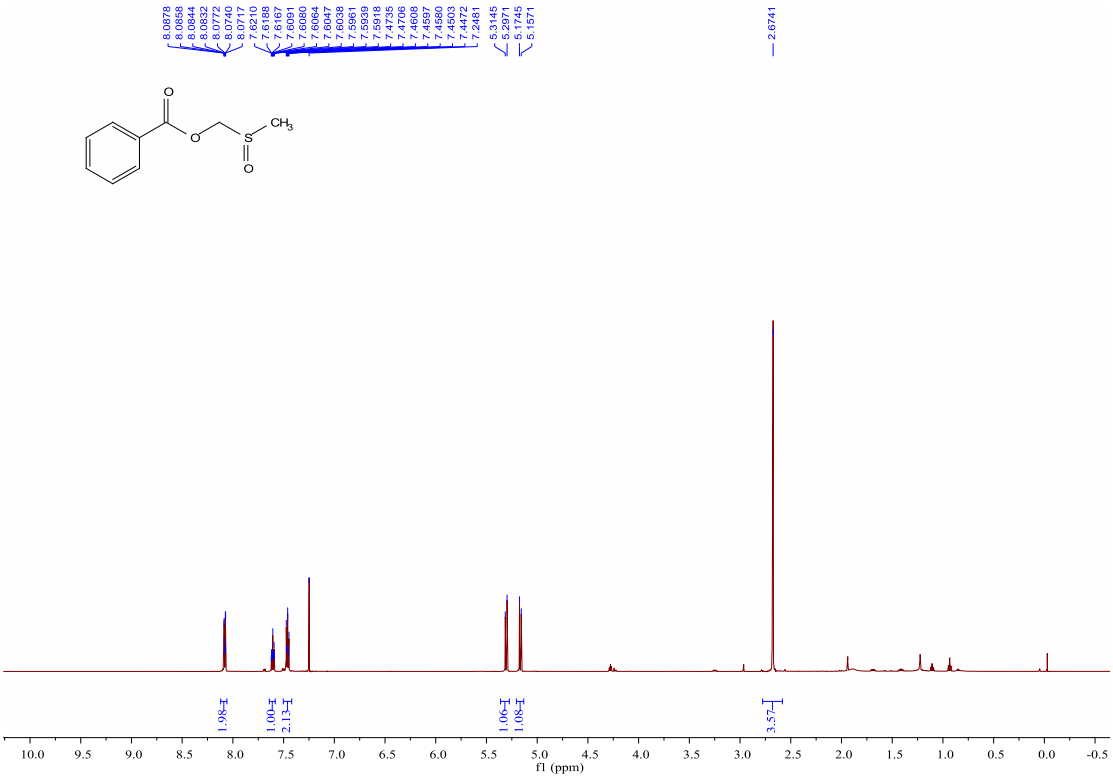
O
O
S
CH3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.6080
7.6064
7.6047
7.6038
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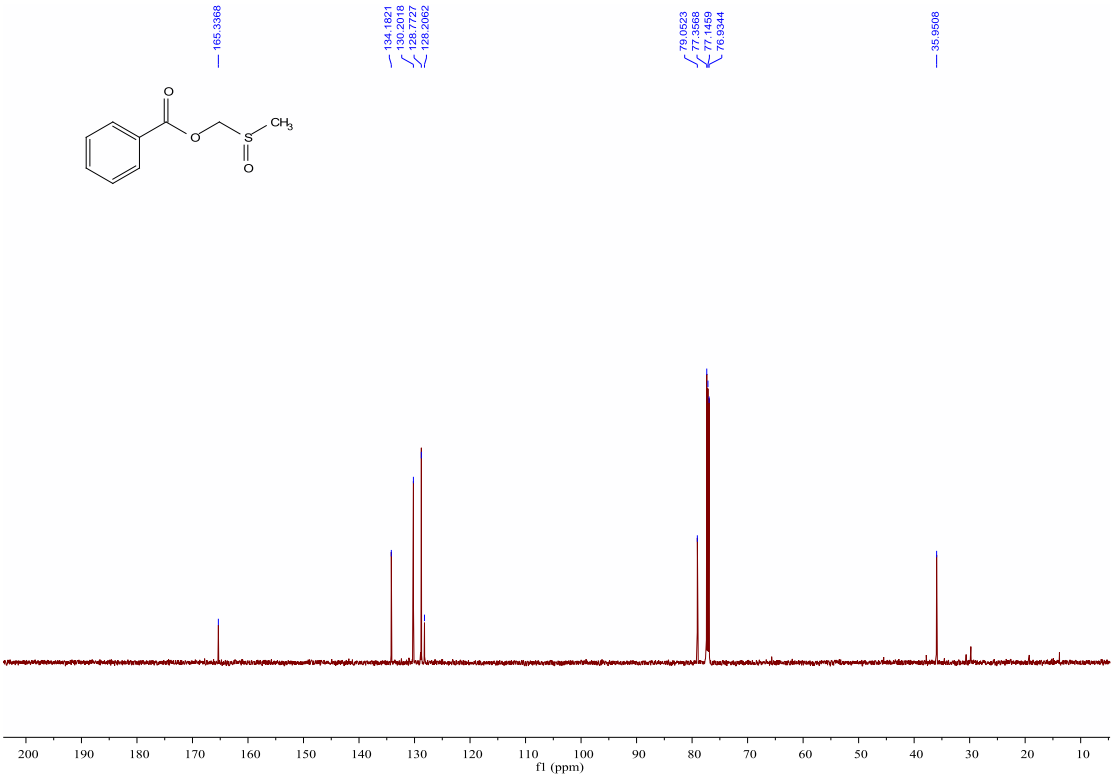
7.4580
7.4503
7.4472
7.4452
7.2461
5.3145
5.2971
5.1745
5.1571
2.6741
O
O
S
CH3
O
1.98
1.00
2.13
1.06
1.08
3.57
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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130.2018
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128.2062
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77.3568
77.1459
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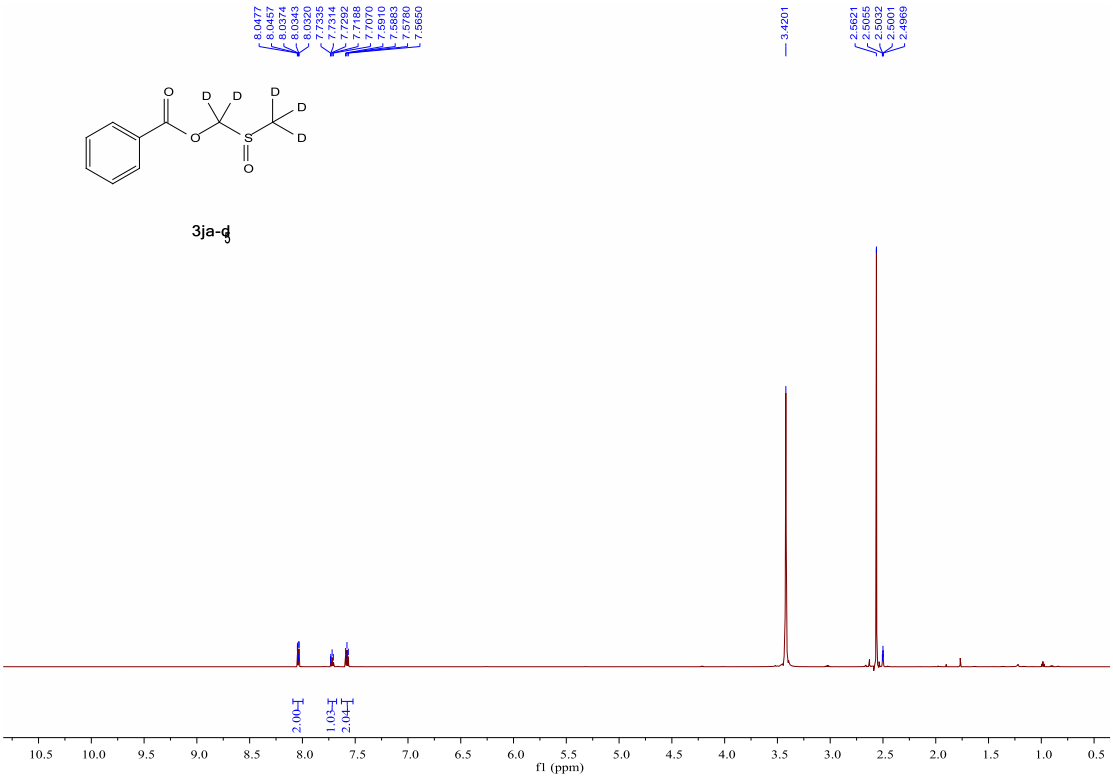
35.9508
O
O
S
CH3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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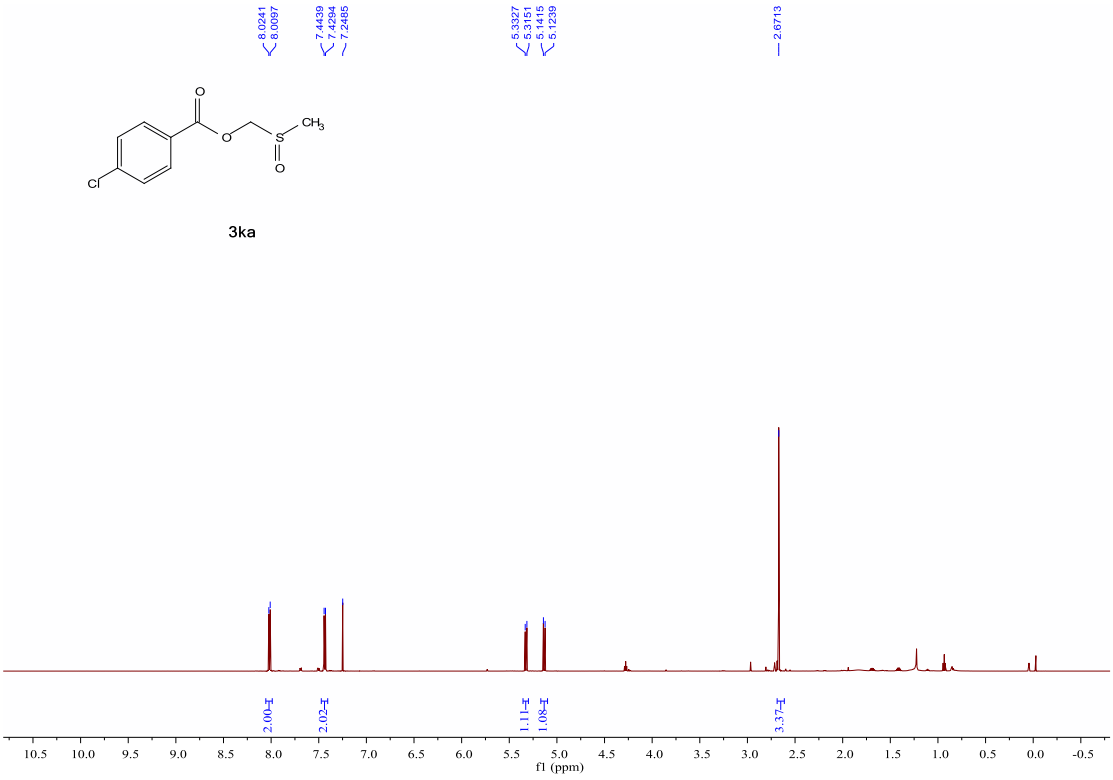
8.0374
8.0343
8.0320
7.7335
7.7314
7.7292
7.7188
7.7070
7.5910
7.5883
7.5790
7.5650
3.4201
2.5621
2.5055
2.5032
2.5001
2.4969
O
D
D
D
D
D
O
S
O
2.00
1.03
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

3ja-d$_5$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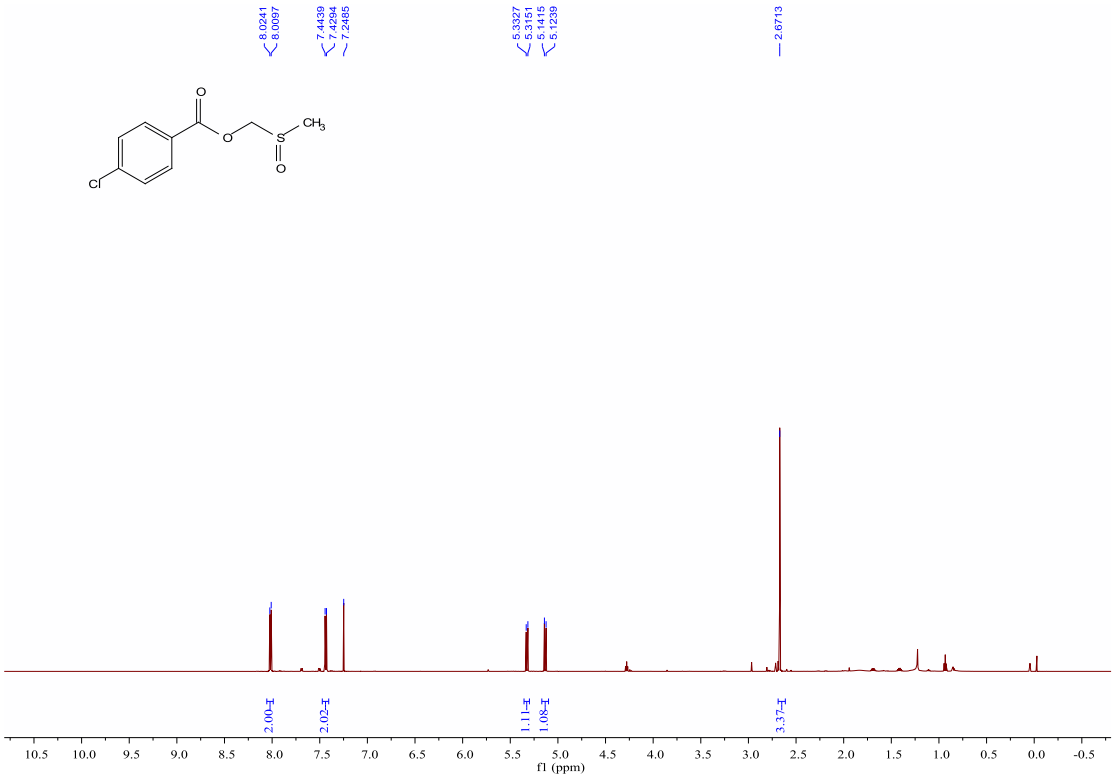
5.3327
5.3151
5.1415
5.1239
2.6713
O
O
S
CH3
O
Cl
2.00
2.02
1.11
1.08
3.37
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3ka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7.4439
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5.3327
5.3151
5.1415
5.1239
2.6713
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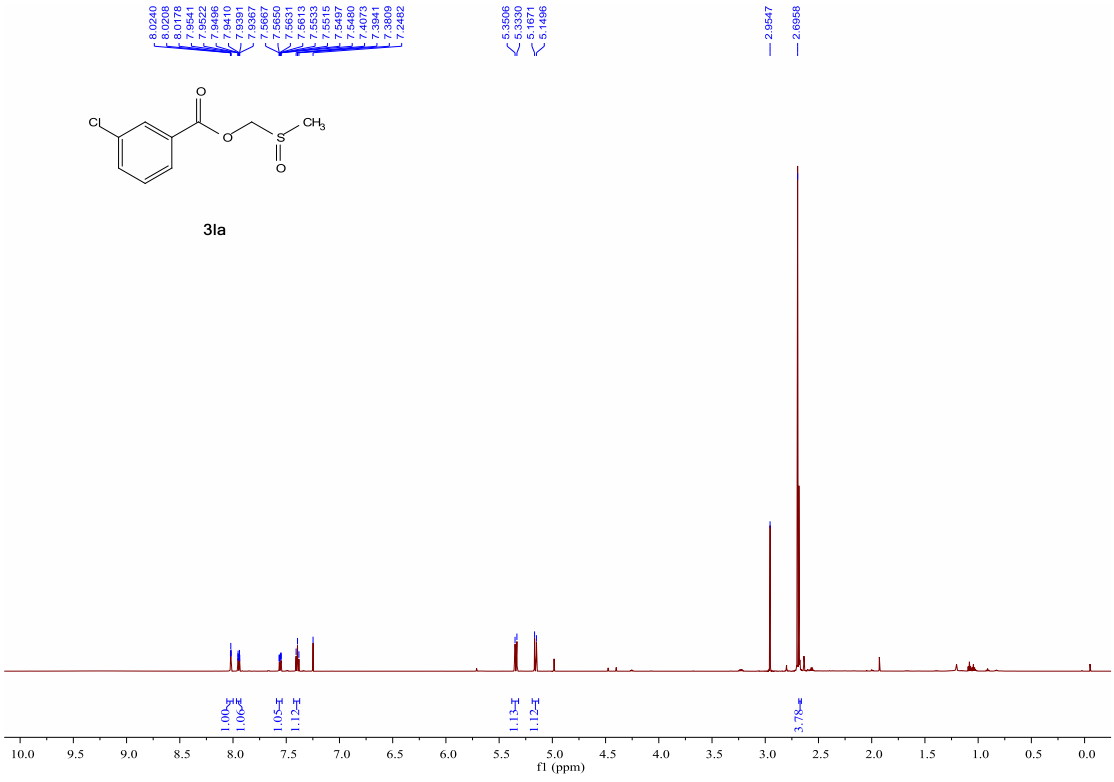
2.02
1.11
1.08
3.37
f1 (ppm)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8.0178
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7.9522
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7.9410
7.9381
7.9367
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7.5650
7.5631
7.5613
7.5533
7.5515
7.5487
7.5469
7.4073
7.3941
7.3869
7.2482
5.3506
5.3330
5.1671
5.1496
2.9547
2.6958
O
O
S
CH3
O
Cl
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1.05
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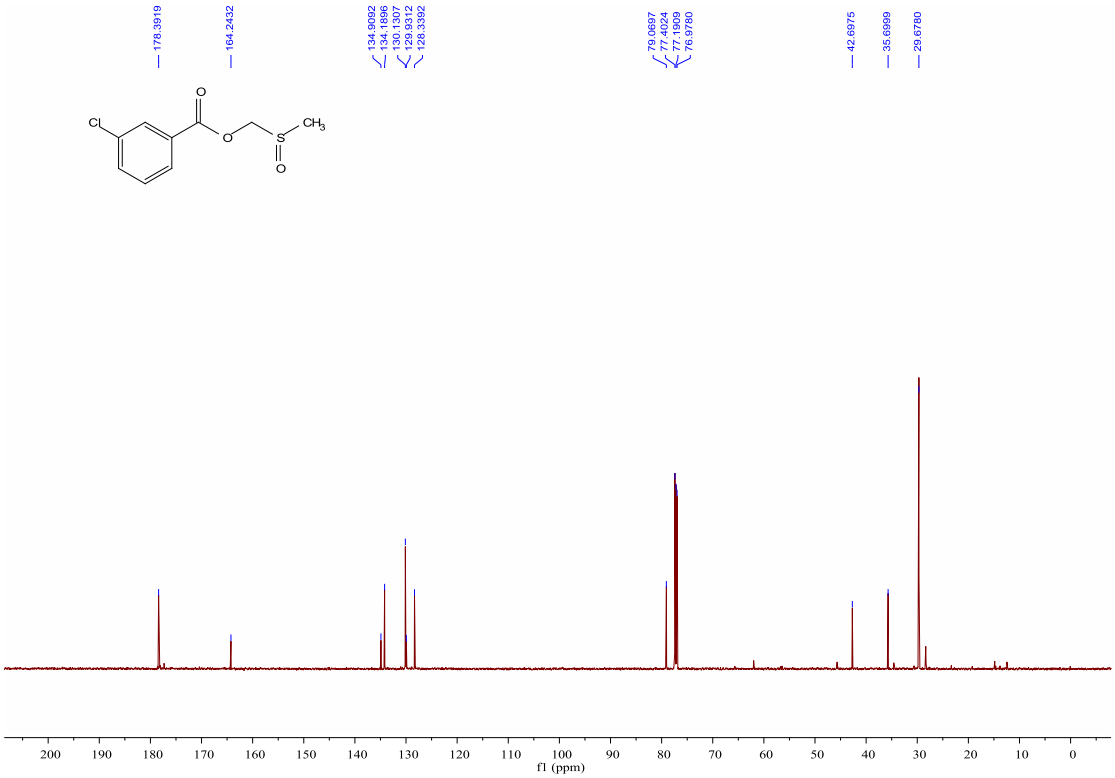
1.13
1.12
3.78
f1 (ppm)

3la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128.3392
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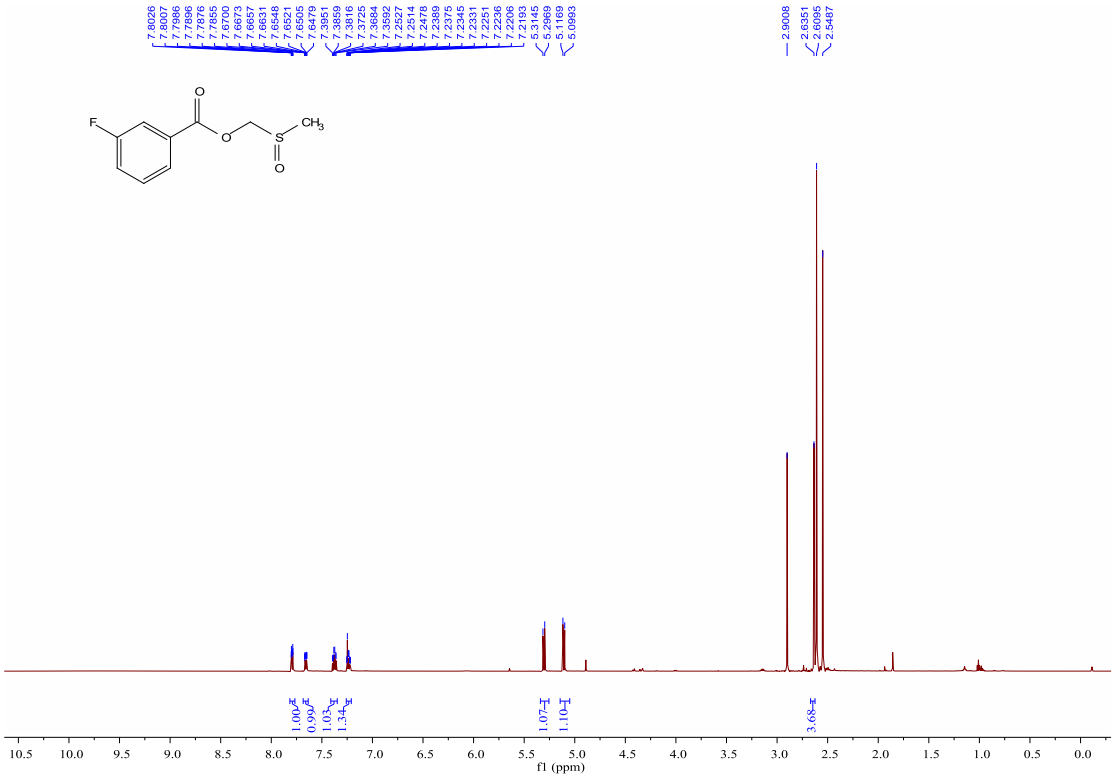
77.4024
77.1909
76.9780
42.6975
35.6999
29.6780
Cl
O
O
S
CH3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.6521
7.6505
7.6479
7.3851
7.3816
7.3725
7.3684
7.3592
7.2527
7.2514
7.2478
7.2369
7.2375
7.2345
7.2331
7.2251
7.2236
7.2206
7.2193
5.3145
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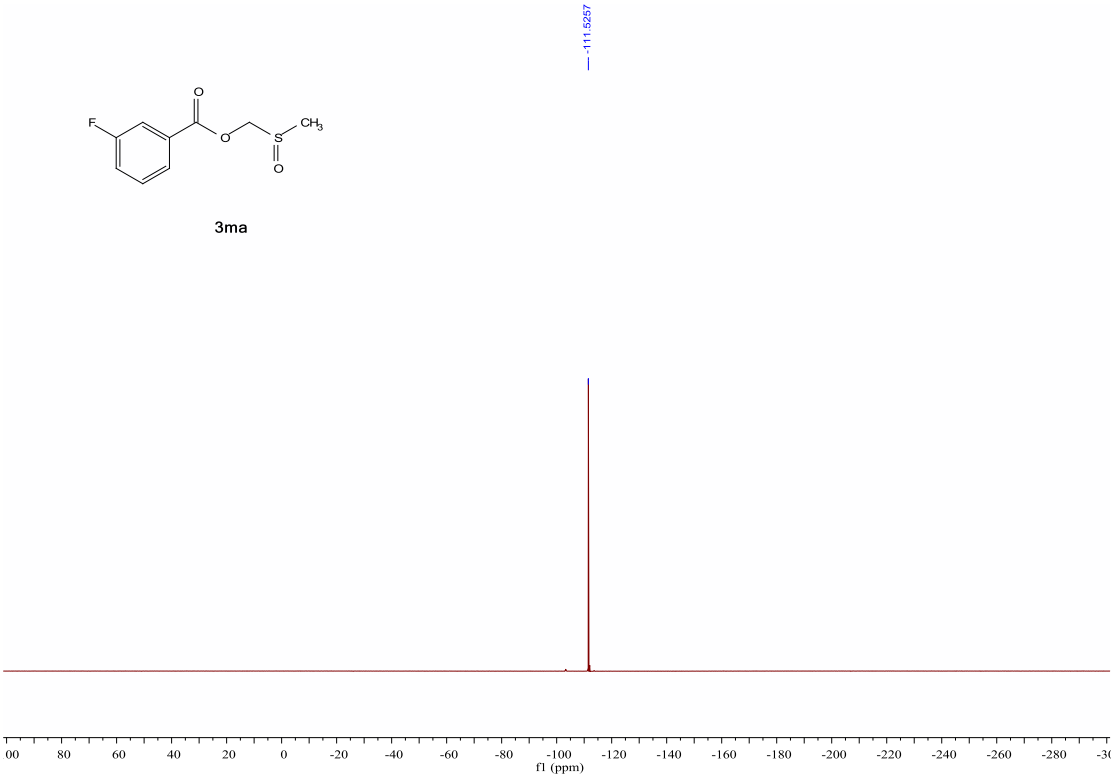
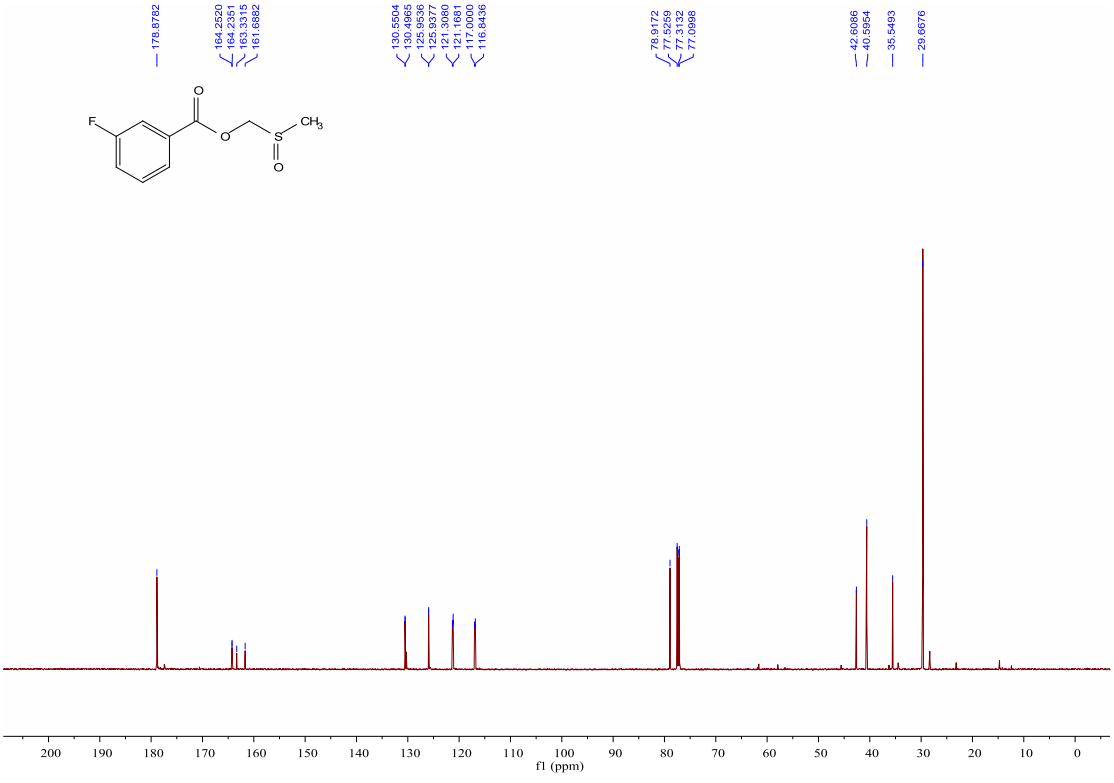
5.1169
5.0993
2.9008
2.6351
2.6095
2.5487
F
O
O
S
CH3
O
1.00
0.99
1.03
1.34
1.07
1.10
3.68
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-111.5257
F
O
O
S
O
CH3
f1 (ppm)

3ma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130.4965
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125.9377
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117.0000
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78.9172
77.5259
77.3132
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40.5954
35.5493
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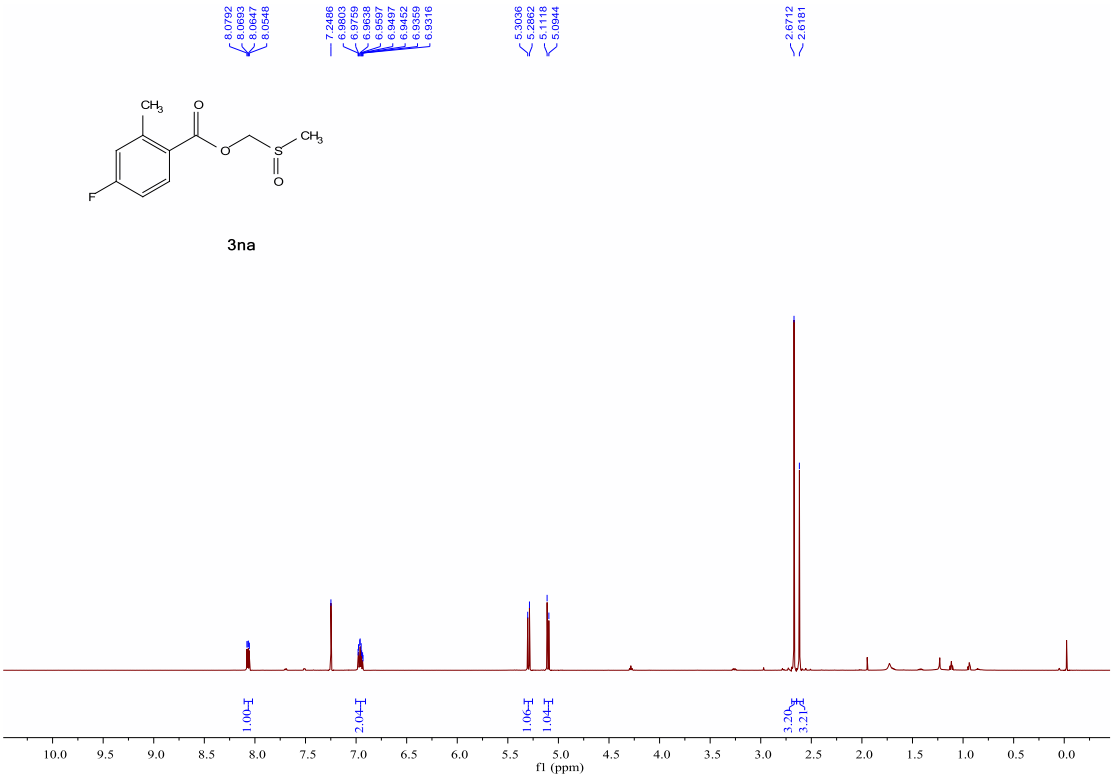
F
O
O
S
O
CH3
f1 (ppm)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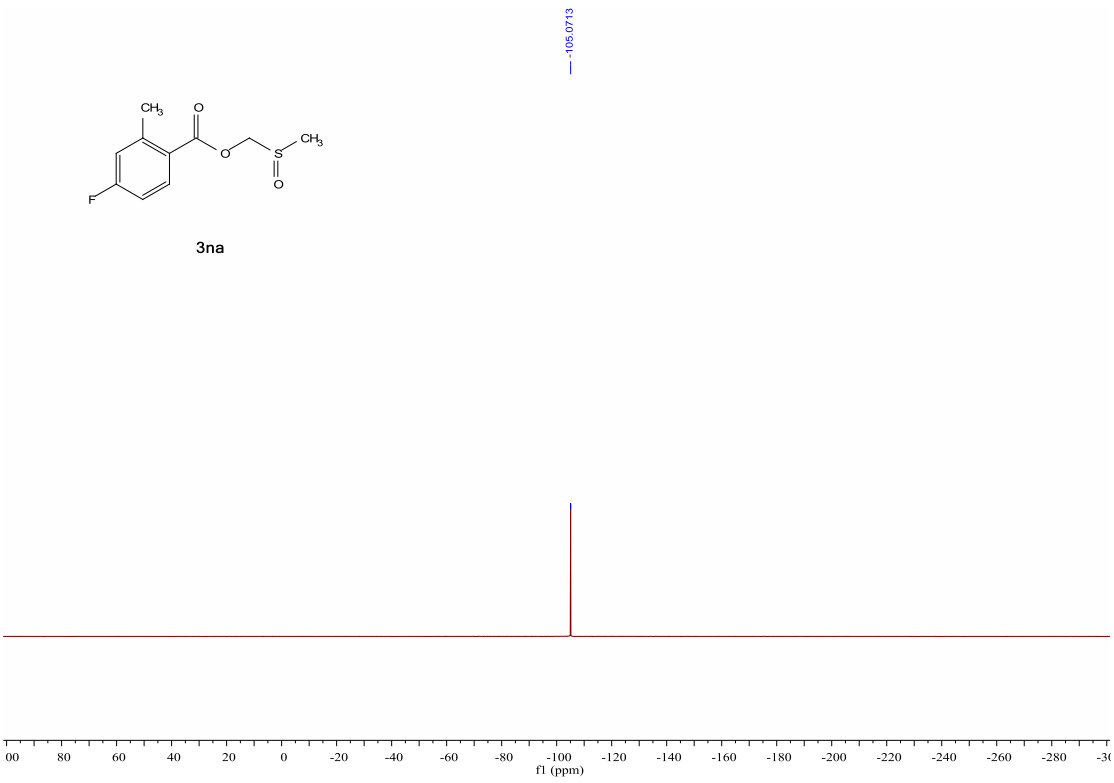
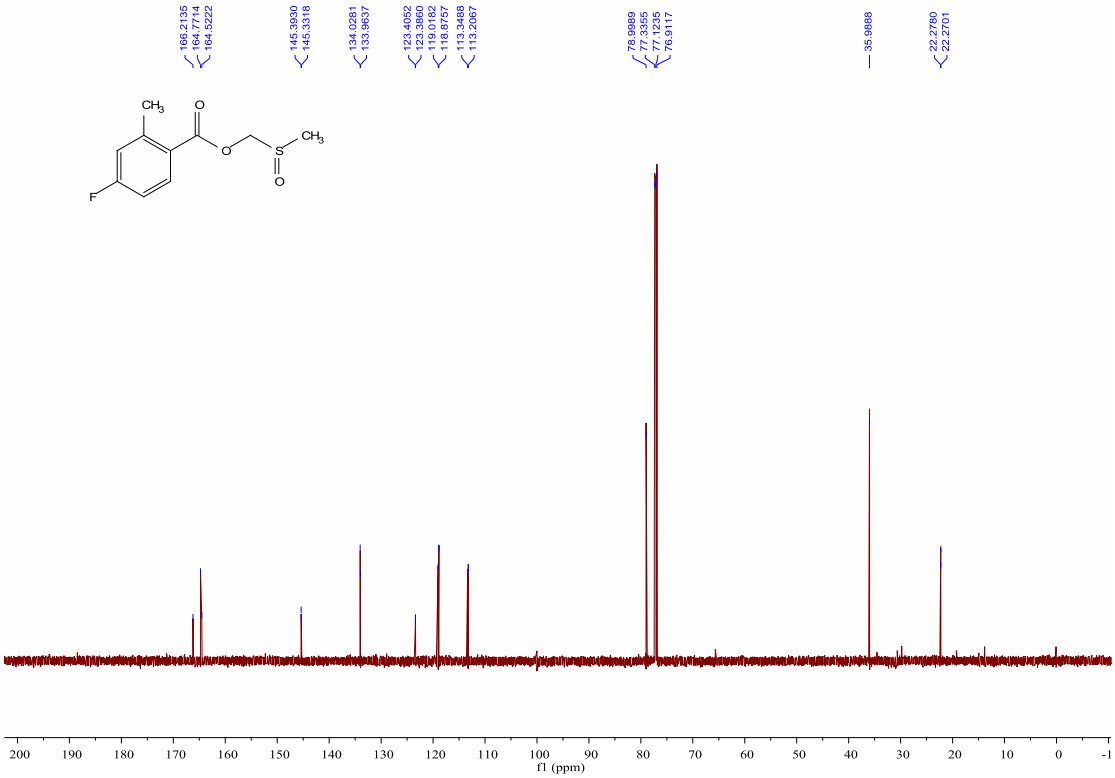
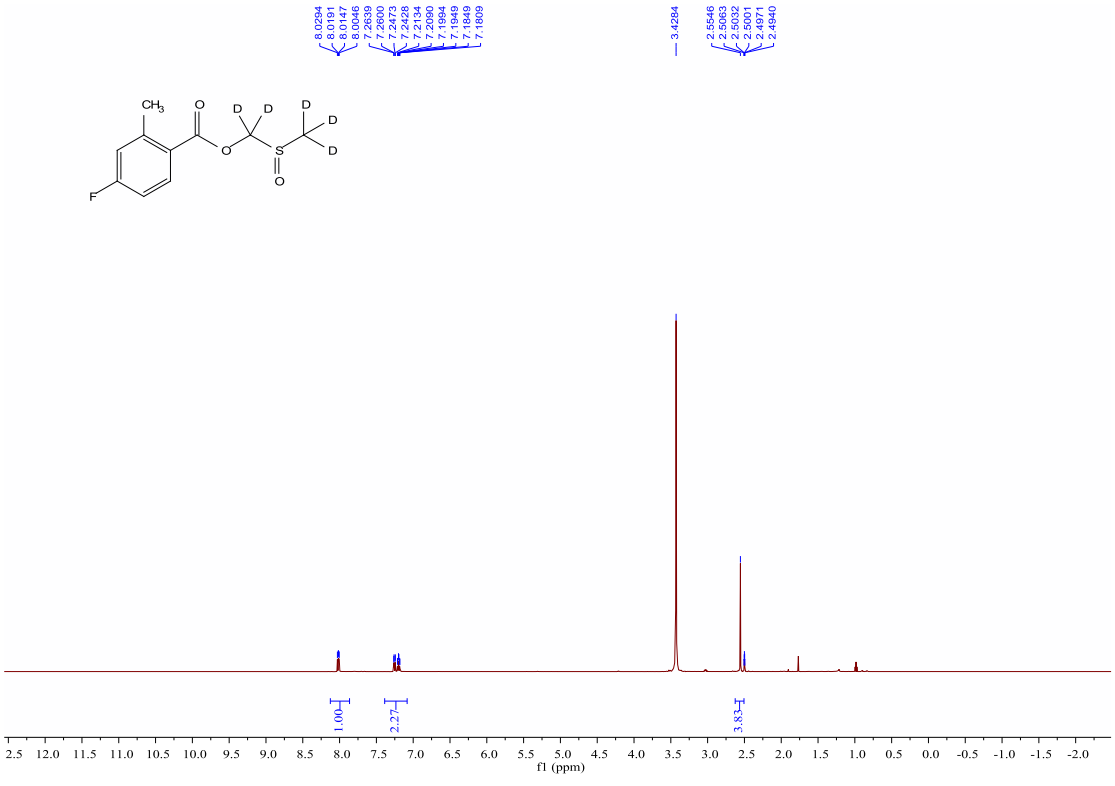
6.9759
6.9638
6.9597
6.9497
6.9452
6.9359
6.9316
5.3036
5.2862
5.1118
5.0944
2.6712
2.6181
CH3
O
O
S
CH3
O
F
1.00
2.04
1.06
1.04
3.20
3.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

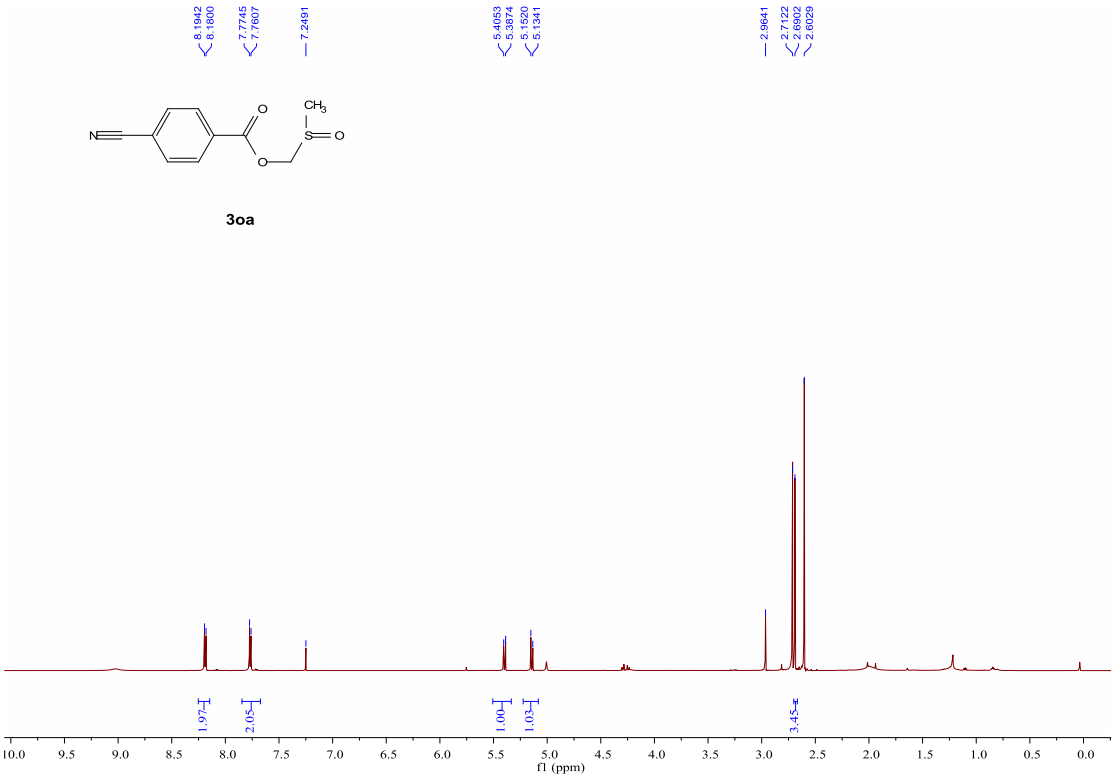
3na


-105.0713
CH3
O
O
S
CH3
O
F
00 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280
f1 (ppm)

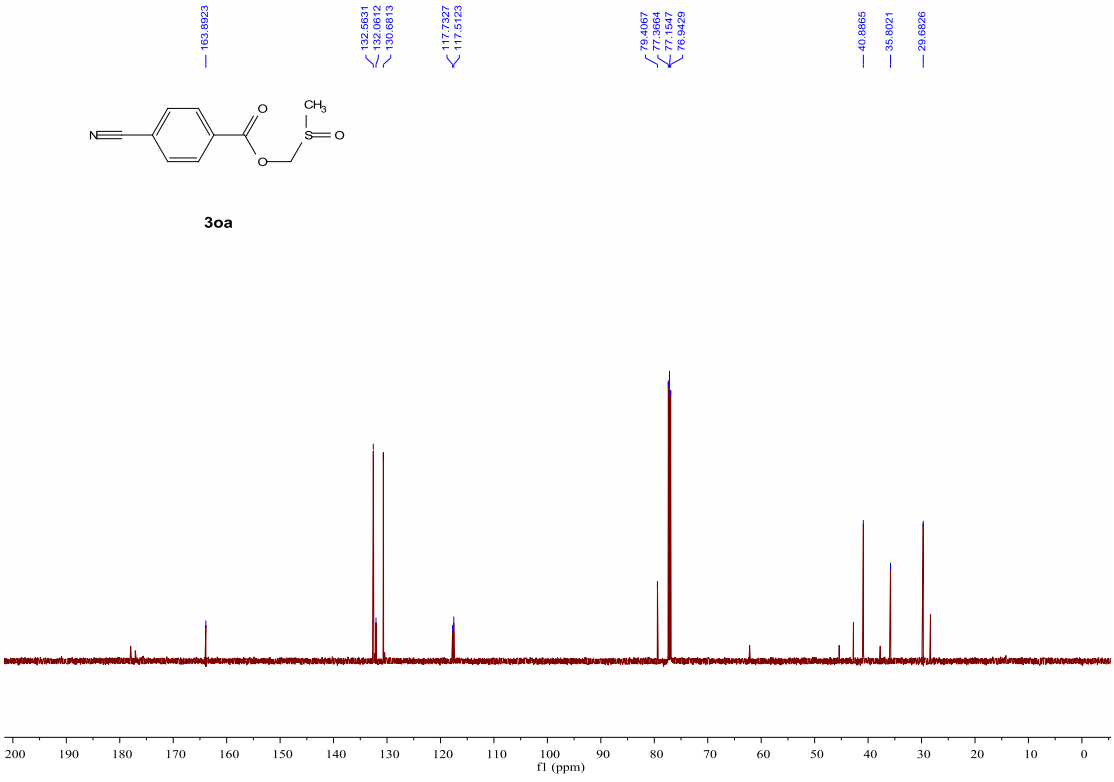
3na


166.2135
164.7714
164.5222
145.3930
145.3318
134.0261
133.9637
123.4052
123.3860
119.0182
118.8757
113.3488
113.2067
78.9889
77.3355
77.1235
76.9117
35.9888
22.2780
22.2701
CH3
O
O
S
CH3
O
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

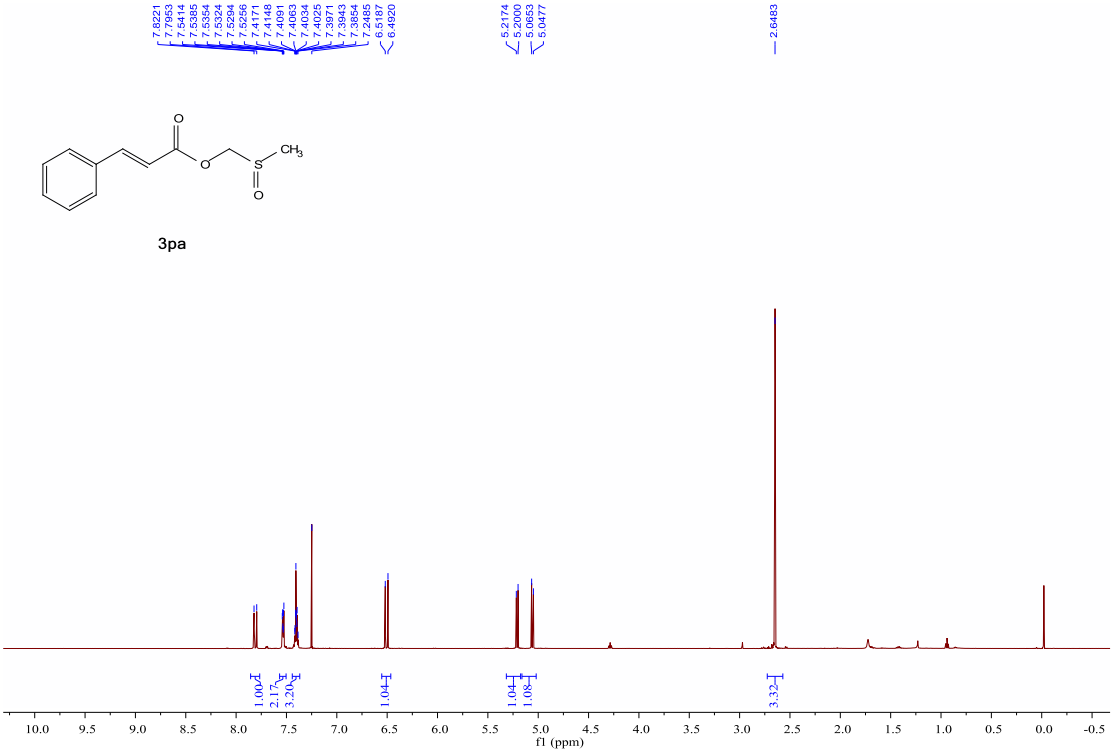

8.0294
8.0191
8.0147
8.0046
7.2639
7.2600
7.2473
7.2428
7.2134
7.2090
7.1994
7.1949
7.1849
7.1609
3.4284
2.5546
2.5063
2.5032
2.5001
2.4971
2.4940
CH3
O
D
D
D
O
S
D
D
O
F
1.00
2.27
3.83
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


8.1942
8.1800
7.7745
7.7607
7.2491
5.4053
5.3874
5.1520
5.1341
2.9641
2.7122
2.6902
2.6029
1.97
2.05
1.00
1.03
3.45
f1 (ppm)

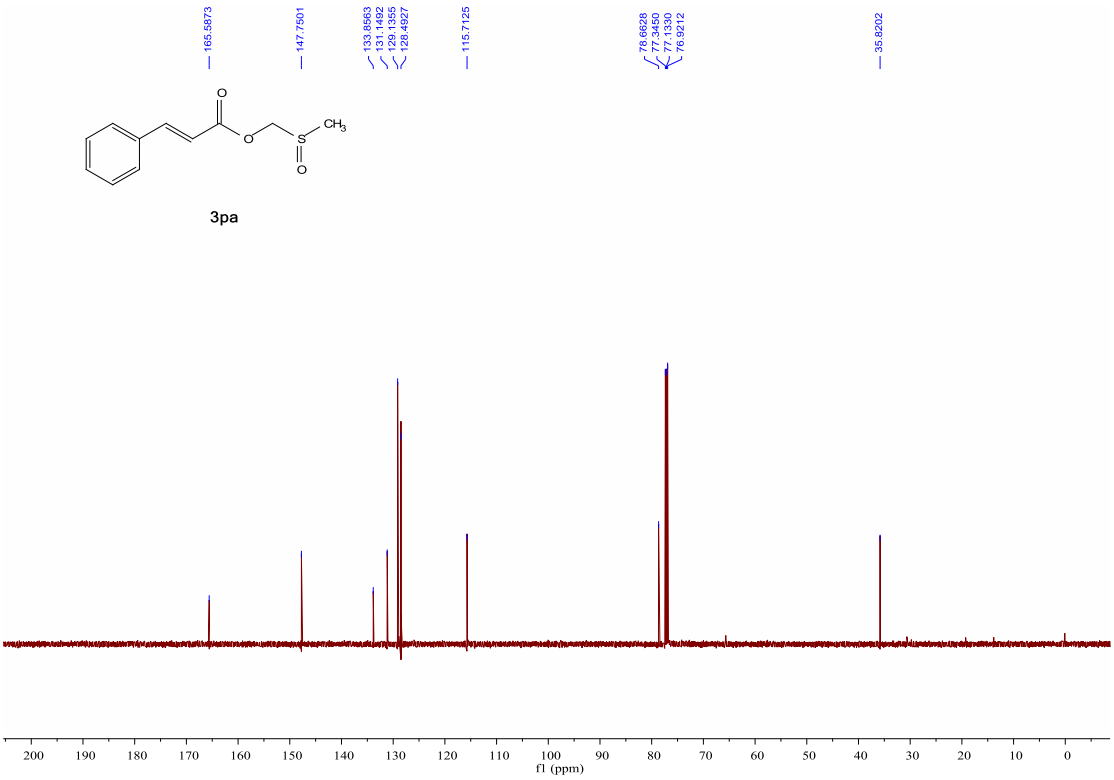
3oa


163.8923
132.5631
132.0612
130.6813
117.7327
117.5123
79.4067
77.3664
77.1547
76.9429
40.8865
35.8021
29.6826
f1 (ppm)

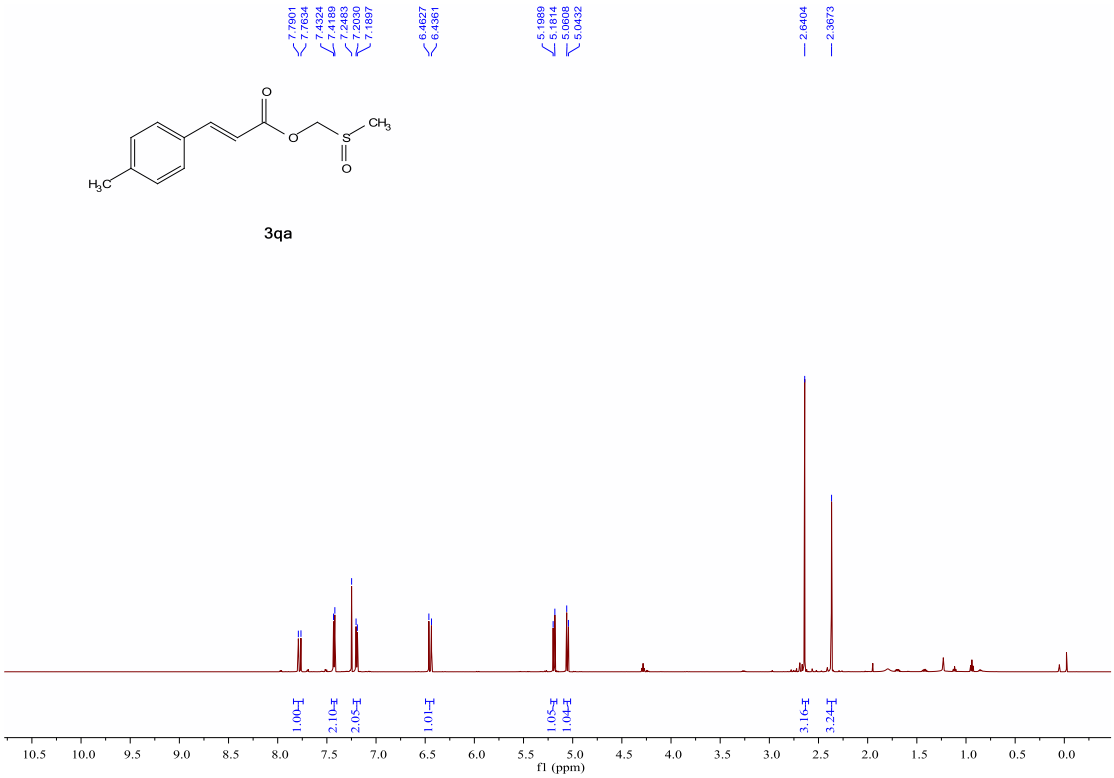
3oa


7.8221
7.7955
7.5414
7.5385
7.5364
7.5324
7.5294
7.5256
7.4171
7.4146
7.4091
7.4063
7.4034
7.4025
7.3971
7.3943
7.3854
7.2485
6.5597
6.4920
5.2174
5.2000
5.0653
5.0477
2.6483
O
O
S
CH3
O
1.00
2.17
3.20
1.04
1.04
1.08
3.32
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)

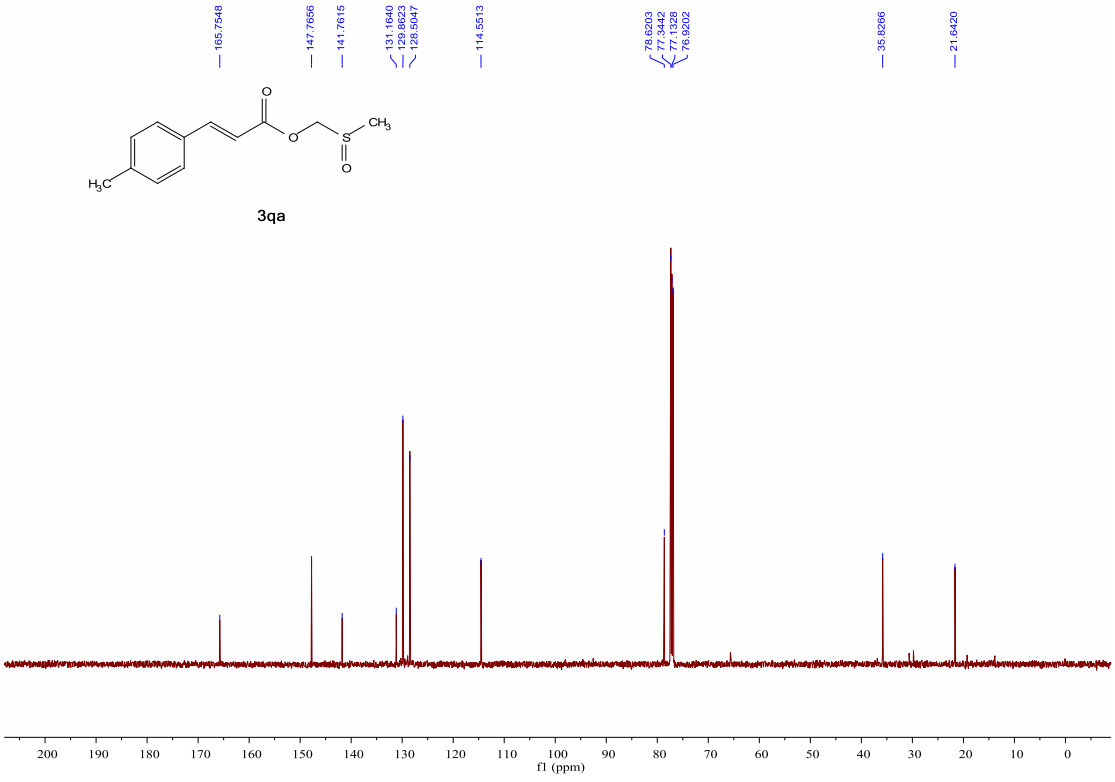
3pa


165.5873
147.7501
133.8563
131.1492
130.1355
128.4927
115.7125
78.6628
77.3450
77.1330
76.9212
35.8202
O
O
S
CH3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

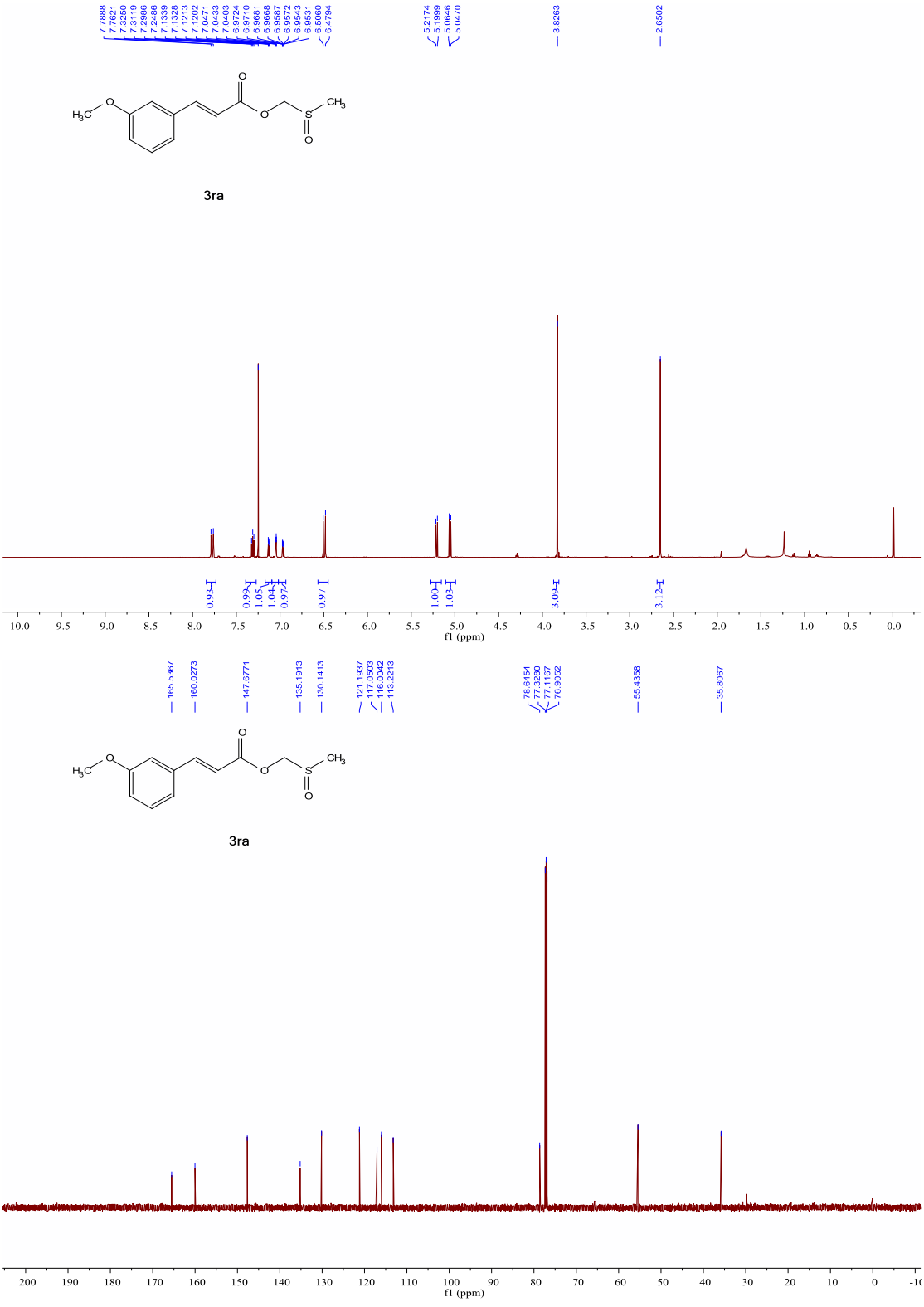
3pa

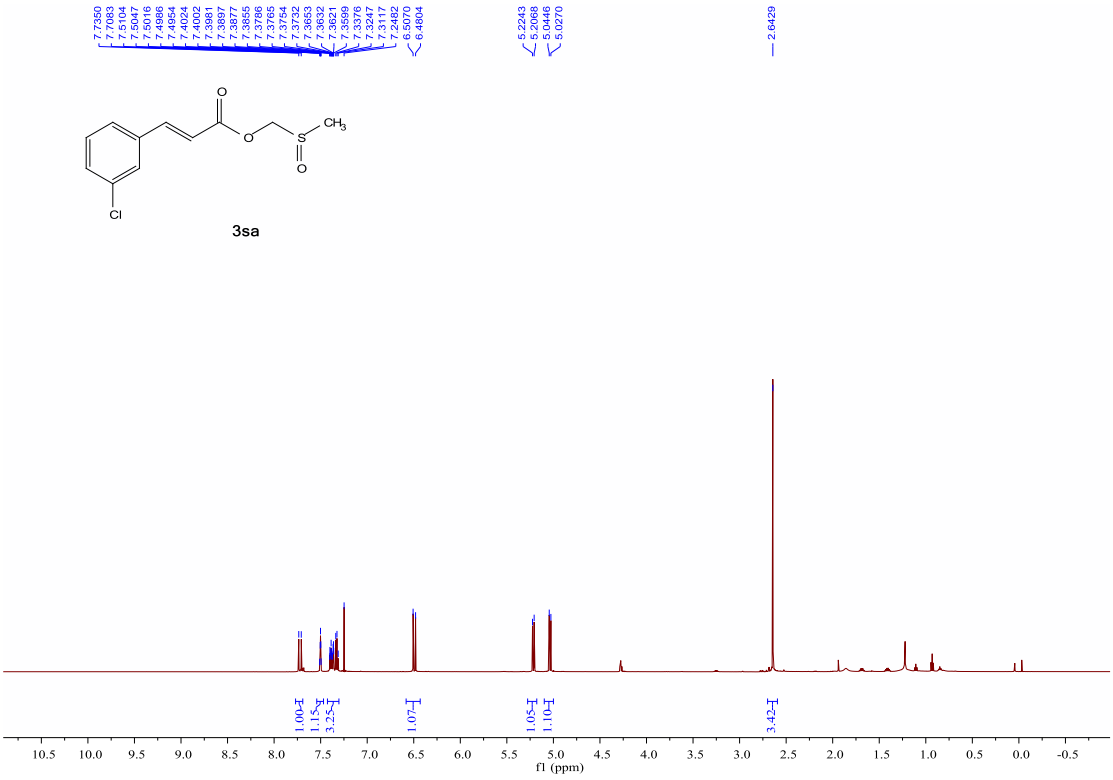

7.7901
7.7634
7.4324
7.4189
7.2483
7.2030
7.1897
6.4627
6.4351
5.1989
5.1814
5.0608
5.0432
2.6404
2.3673
O
O
S
CH3
O
H3C
1.00
2.10
2.05
1.01
1.05
1.04
3.16
3.24
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

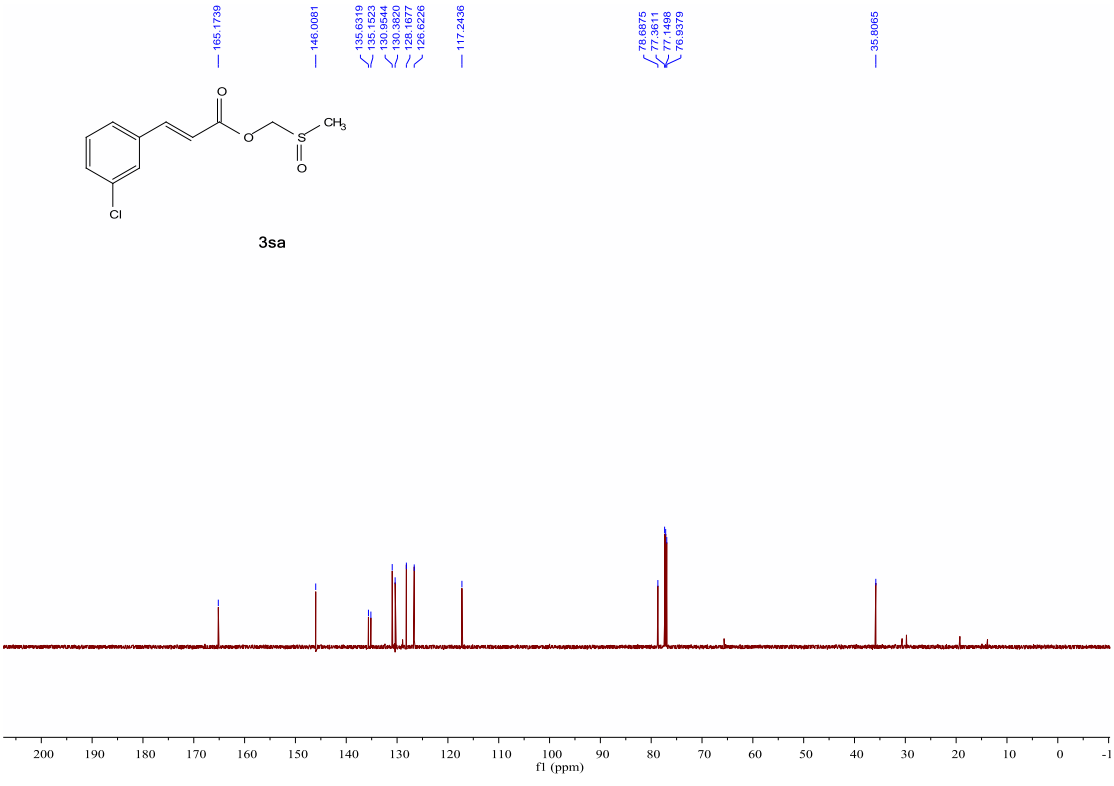
3qa

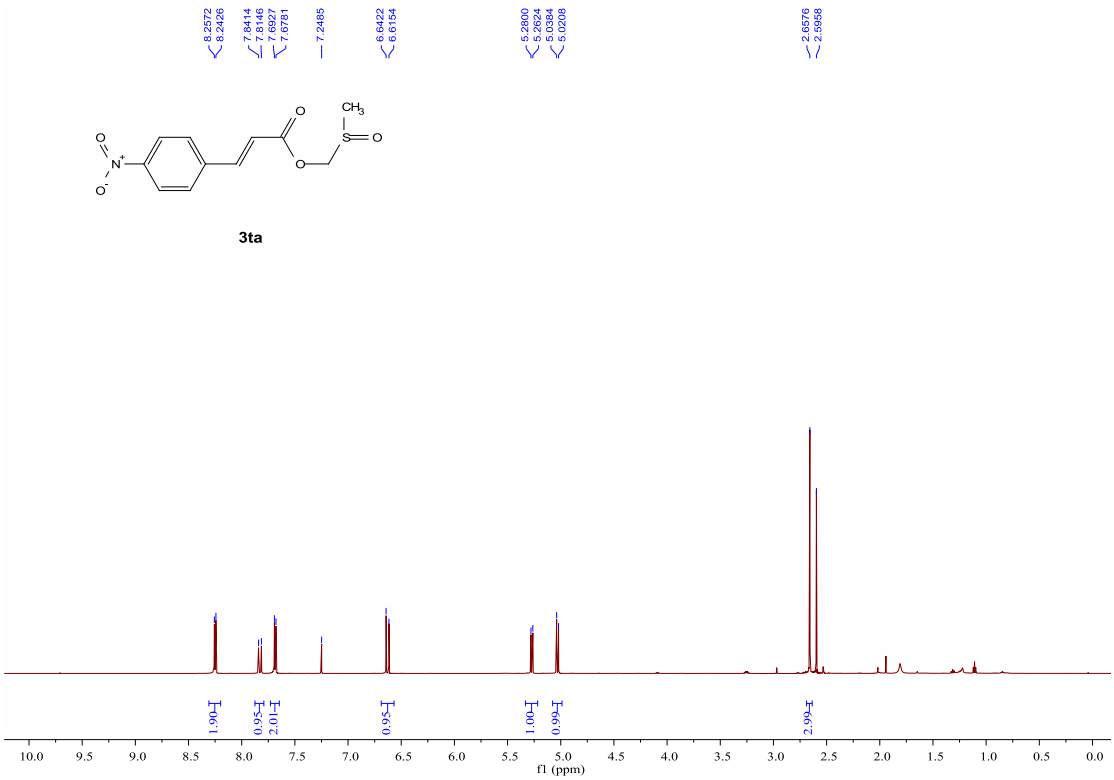

165.7548
147.7656
141.7615
131.1640
129.8623
128.5047
114.5513
78.6203
77.3442
77.1328
76.9202
35.8266
21.6420
O
O
S
CH3
O
H3C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3qa

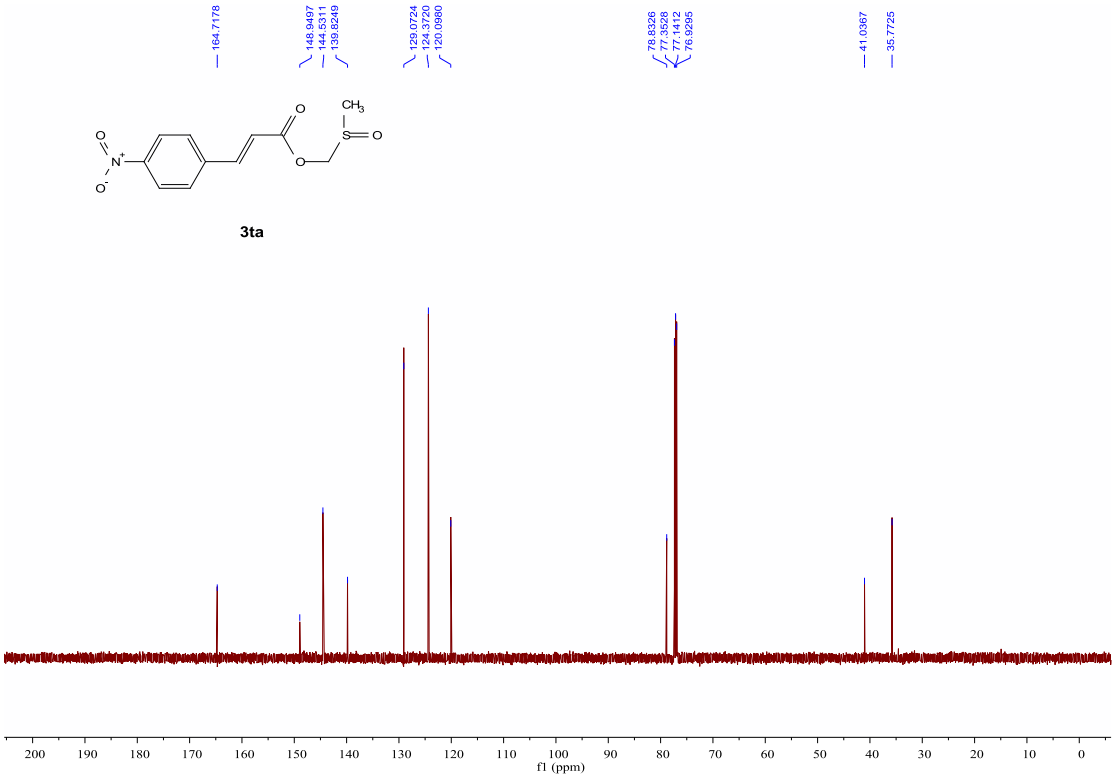

7.7888
7.7621
7.3250
7.3119
7.2986
7.2486
7.1339
7.1238
7.1213
7.1202
7.0471
7.0433
7.0403
6.9724
6.9710
6.9681
6.9668
6.9587
6.9572
6.9543
6.9531
6.5060
6.4794
5.2174
5.1999
5.0646
5.0470
3.8263
2.6502
O
H3C
O
O
S
CH3
O
3ra
0.93
0.99
1.05
1.04
0.97
0.97
1.00
1.03
3.09
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 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)
165.5367
160.0273
147.6771
135.1913
130.1413
121.1937
117.0503
116.0042
113.2213
78.6454
77.3280
77.1167
76.9052
55.4358
35.8067
O
H3C
O
O
S
CH3
O
3ra
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.7350
7.7083
7.5104
7.5047
7.5016
7.4986
7.4954
7.4024
7.4002
7.3981
7.3897
7.3877
7.3855
7.3786
7.3765
7.3754
7.3732
7.3653
7.3632
7.3621
7.3599
7.3376
7.3247
7.3117
7.2482
6.6770
6.4804
5.2243
5.2068
5.0446
5.0270
2.6429
O
O
S
CH3
O
Cl
3sa
1.00
1.15
3.25
1.07
1.05
1.10
3.43
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)

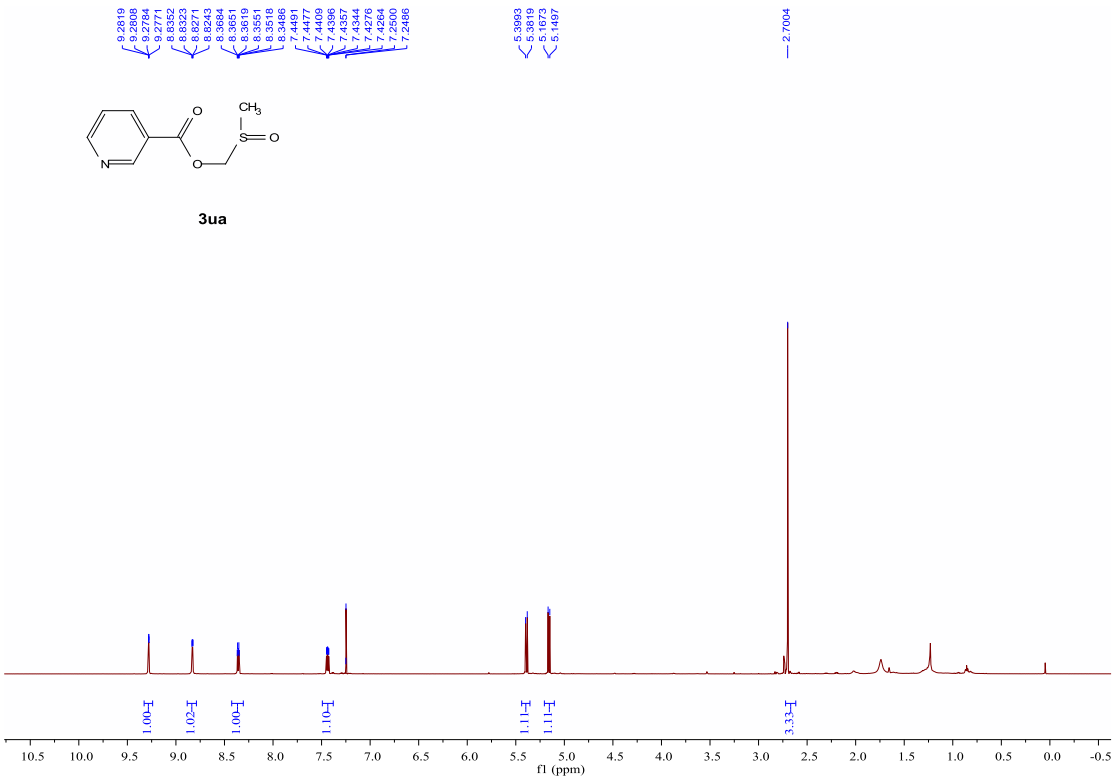

165.1739
146.0081
135.6319
135.1523
130.9544
130.3820
128.1677
126.6226
117.2436
78.6875
77.3611
77.1498
76.9379
35.8065
O
O
S
CH3
O
Cl
3sa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

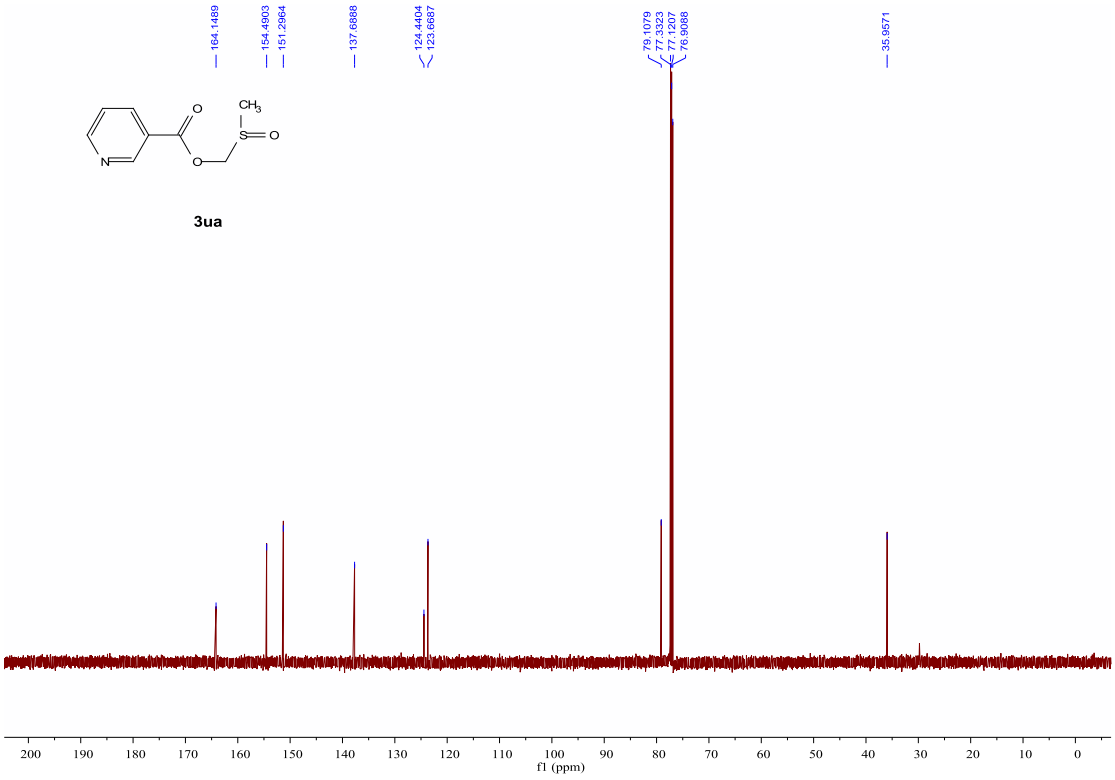

8.2572
8.2426
7.8414
7.8146
7.6927
7.6781
7.2485
6.6422
6.6154
5.2800
5.2624
5.0384
5.0208
2.6576
2.5998
CH3
S
O
O
O
N+
O-
1.90
0.95
2.01
0.95
1.00
0.99
2.99
f1 (ppm)

3ta


164.7178
148.9497
144.5311
139.8249
129.0724
124.3720
120.0980
78.8326
77.3528
77.1412
76.9295
41.0367
35.7725
CH3
S
O
O
O
N+
O-
f1 (ppm)

3ta


9.2819
9.2808
9.2784
9.2771
8.8552
8.8523
8.8271
8.8243
8.3684
8.3651
8.3619
8.3551
8.3518
8.3486
7.4491
7.4477
7.4409
7.4396
7.4357
7.4344
7.4276
7.4264
7.2600
7.2486
5.3993
5.3819
5.1673
5.1497
2.7004
CH3
S
O
N
3ua
1.00
1.02
1.00
1.10
1.11
1.11
3.33
f1 (ppm)


164.1489
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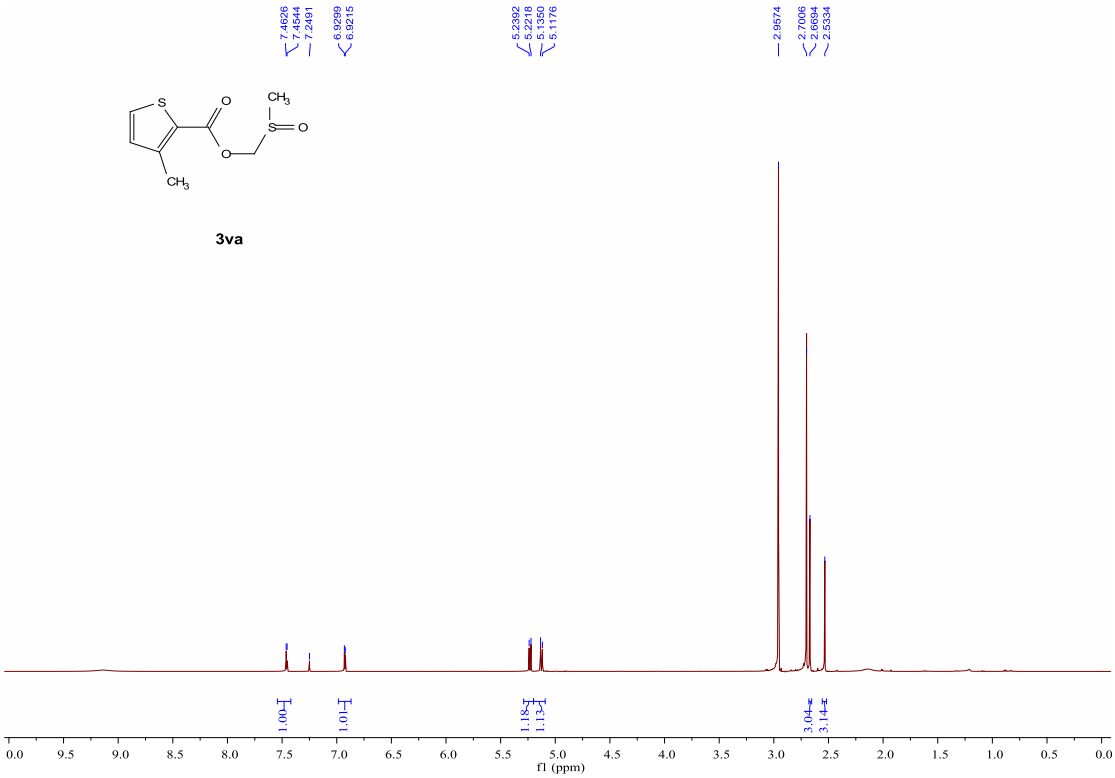
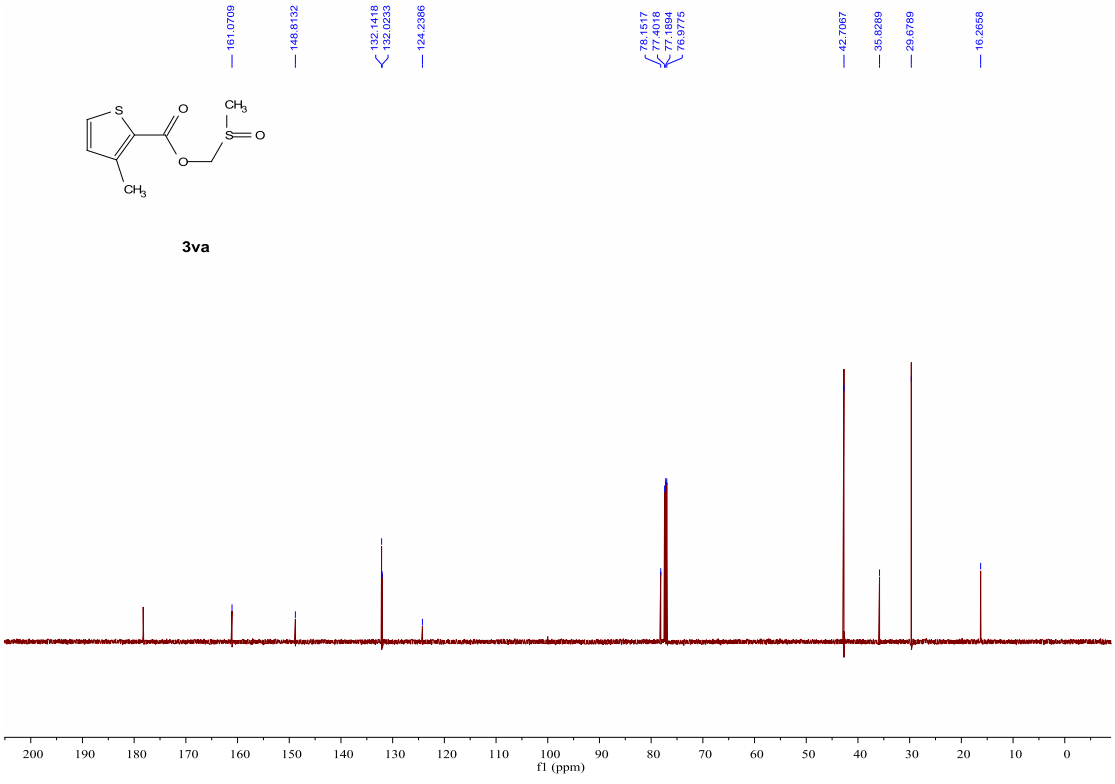
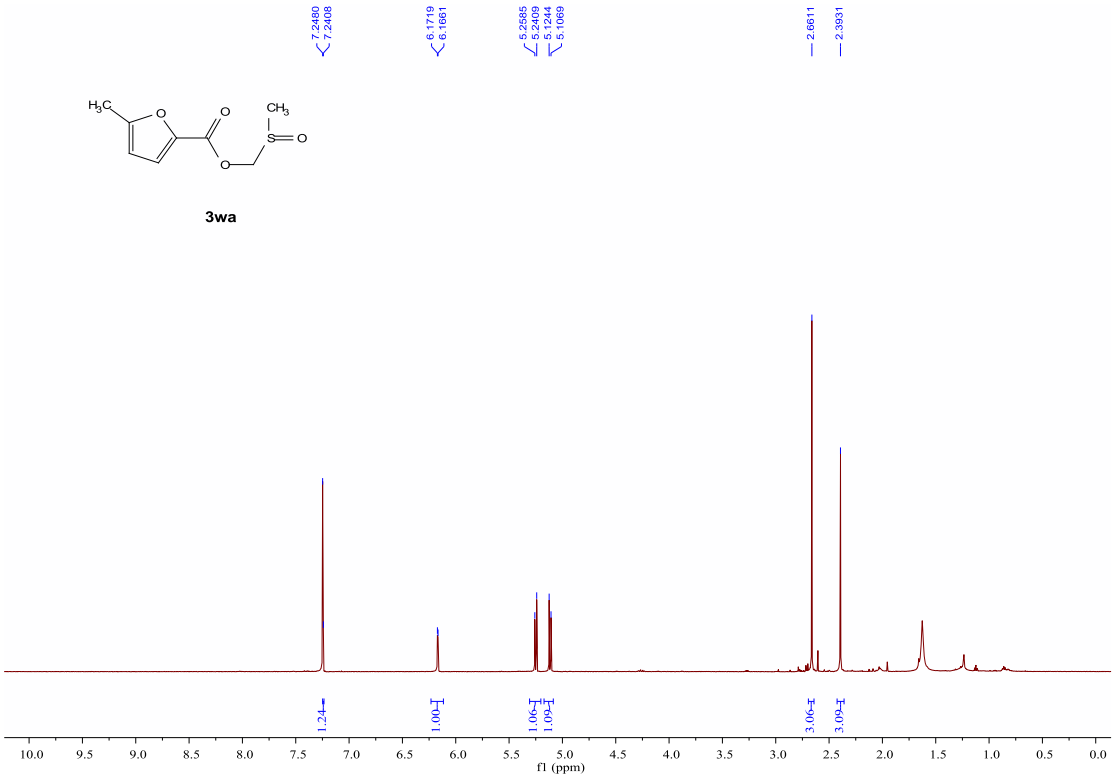
151.2964
137.6888
124.4404
123.6687
79.1079
77.3323
77.1207
76.9088
35.9571
CH3
S
O
N
3ua
f1 (ppm)


7.4626
7.4544
7.2491
6.9299
6.9215
5.2392
5.2218
5.1350
5.1176
2.9574
2.7006
2.6694
2.5334
1.00
1.01
1.18
1.13
3.04
3.14
f1 (ppm)

3va


161.0709
148.8132
132.1418
132.0233
124.2386
78.1517
77.4018
77.1894
76.9775
42.7067
35.8289
29.6789
16.2658
f1 (ppm)

3va


7.2480
7.2408
6.1719
6.1661
5.2585
5.2469
5.2354
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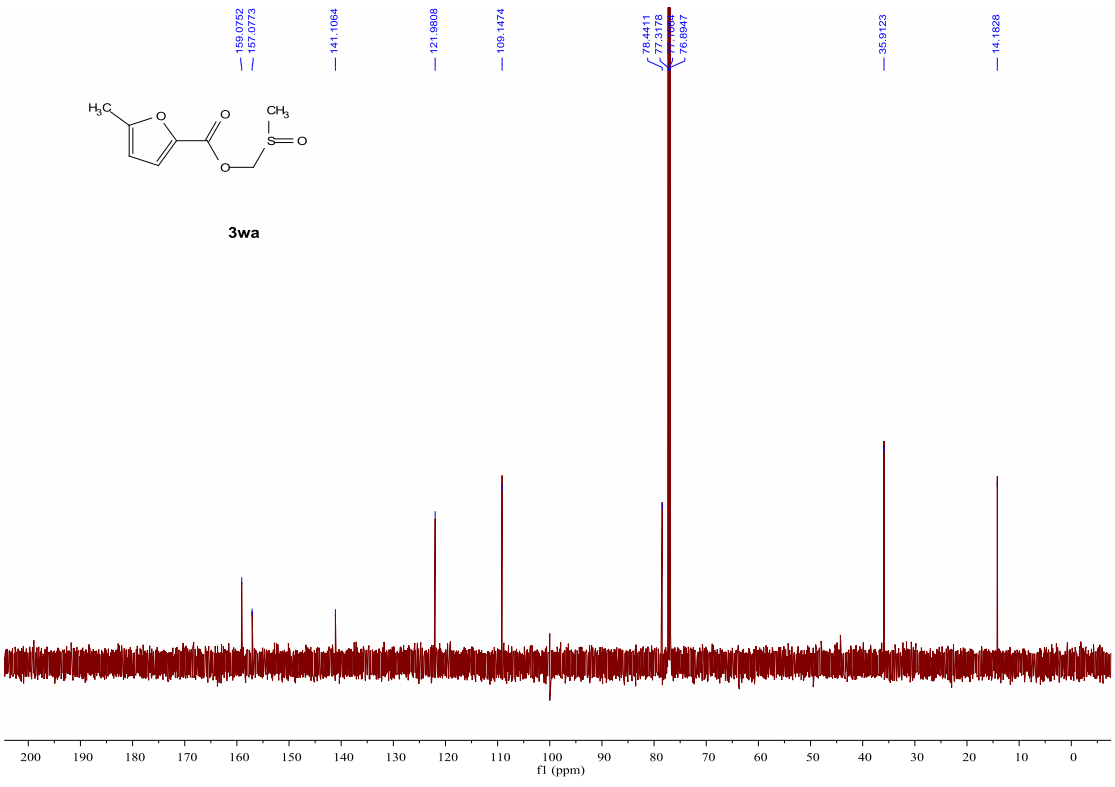
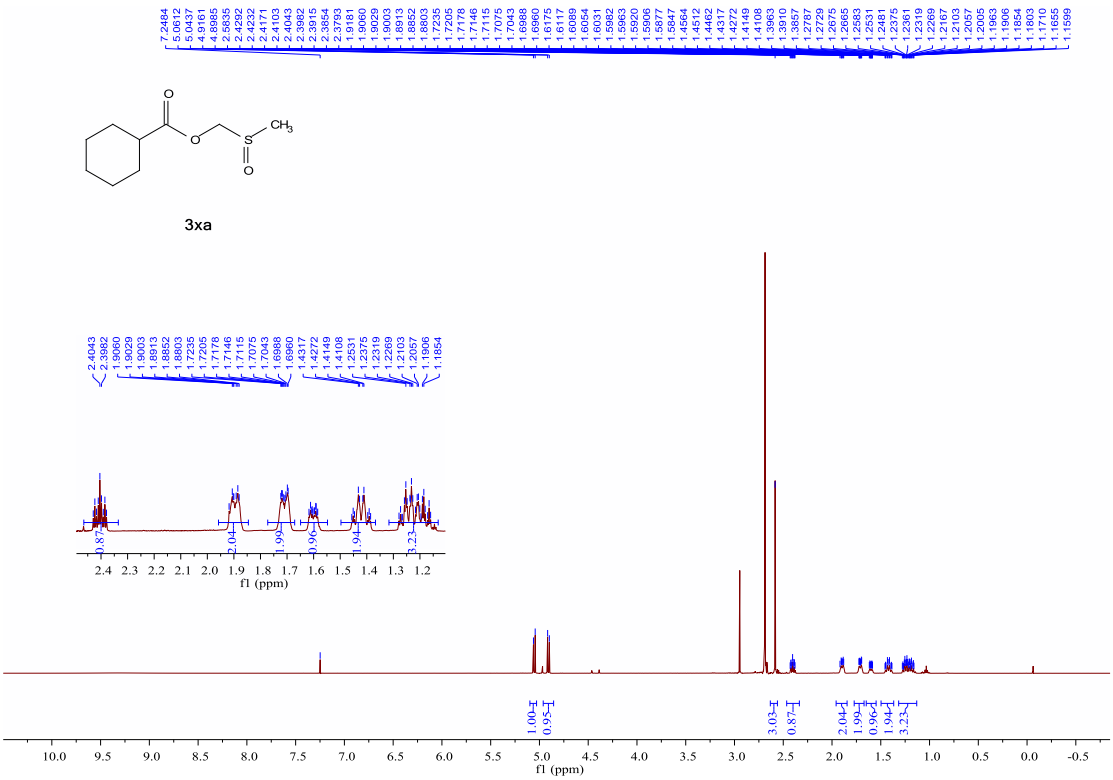
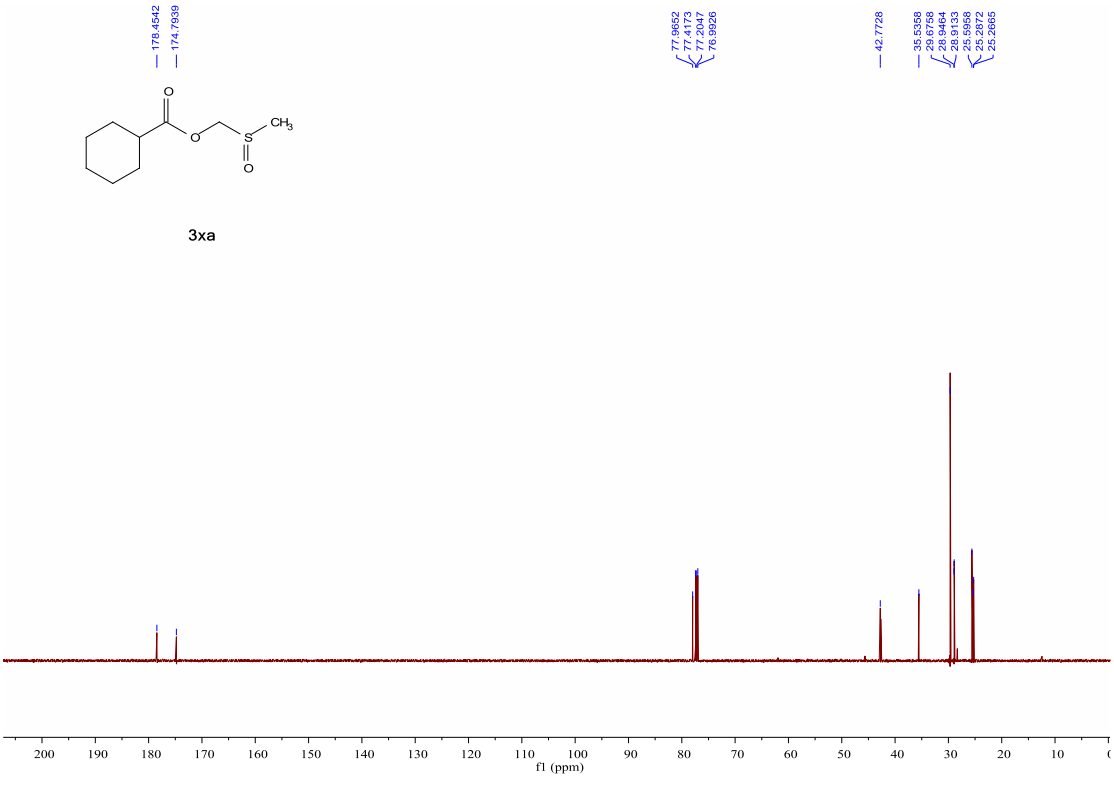
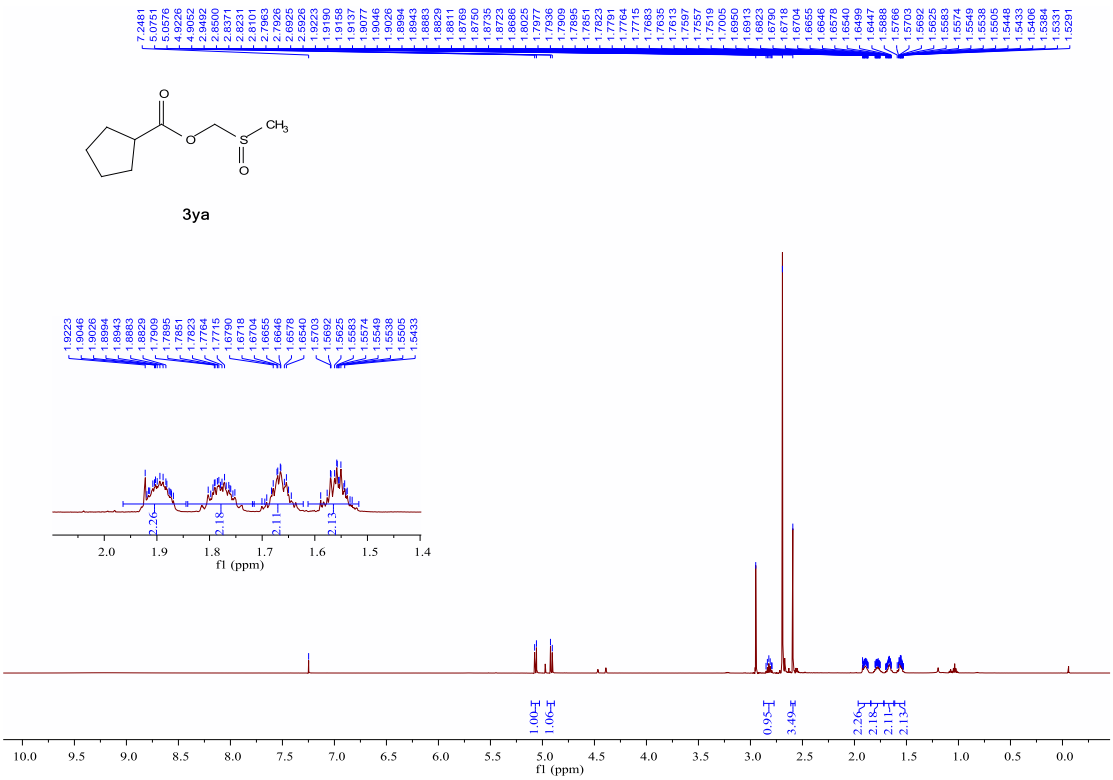
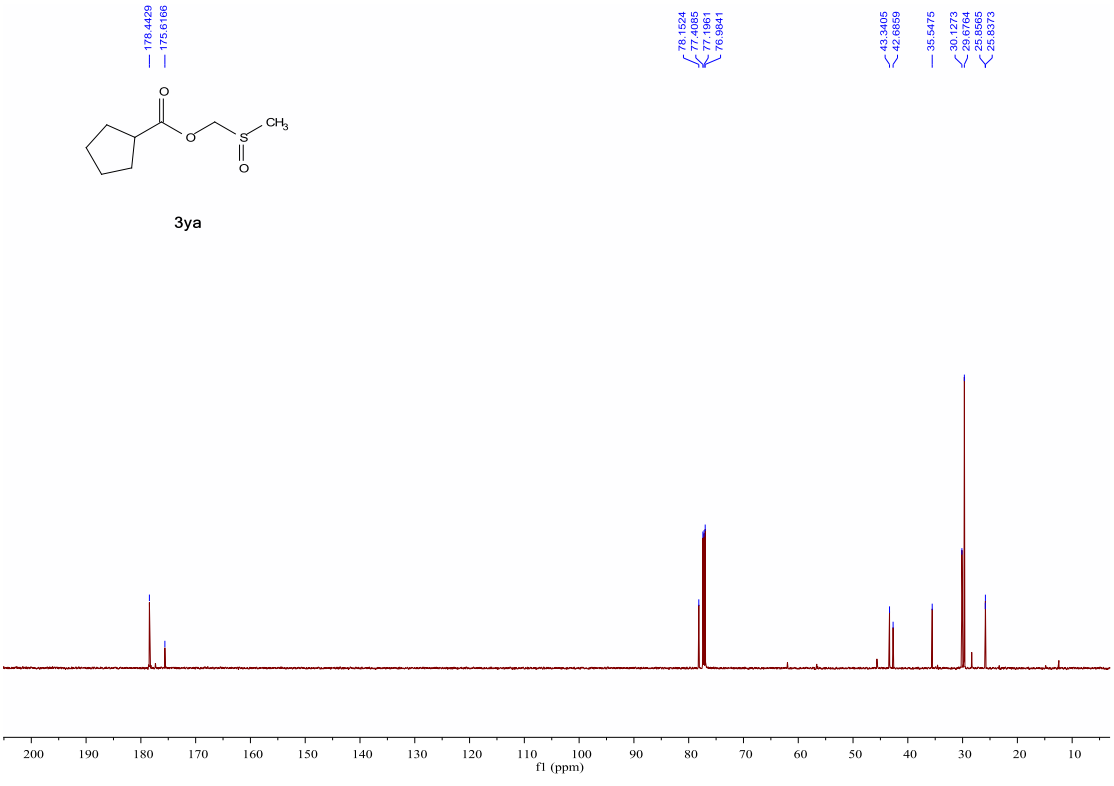
2.6611
2.3931
3wa
1.24
1.00
1.06
1.09
3.06
3.09
f1 (ppm)

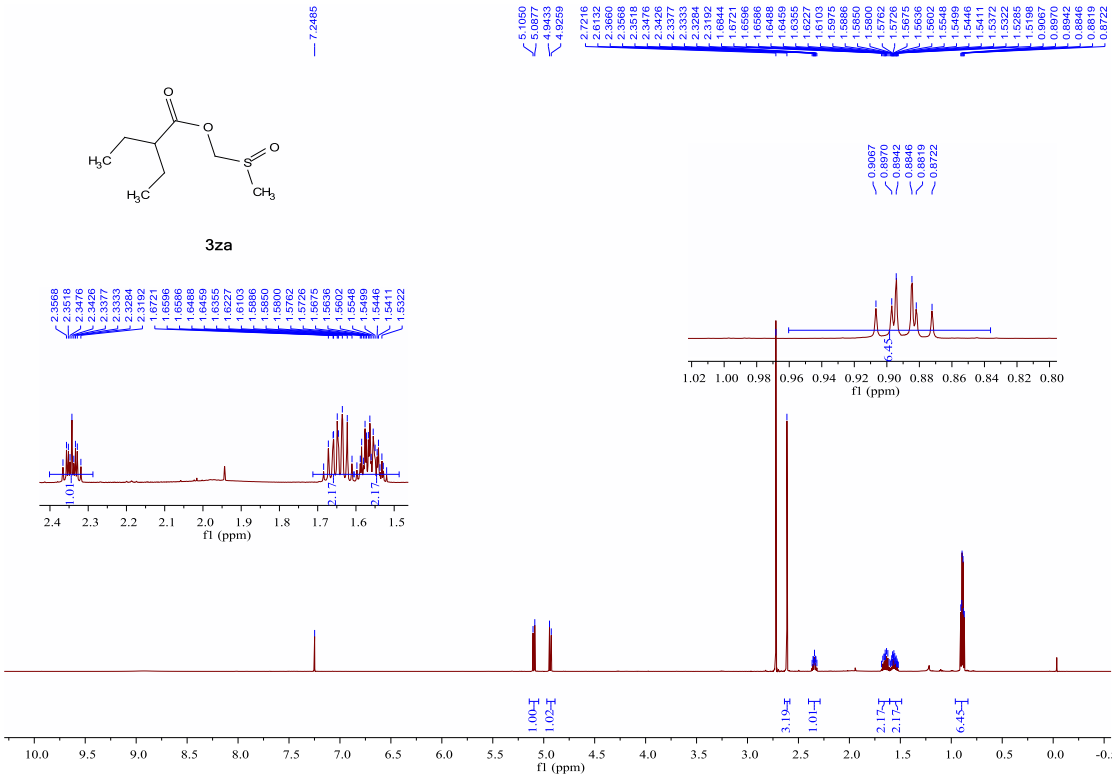

159.0752
157.0773
141.1064
121.9808
109.1474
78.4411
77.3178
76.8947
35.9123
14.1828
3wa
f1 (ppm)

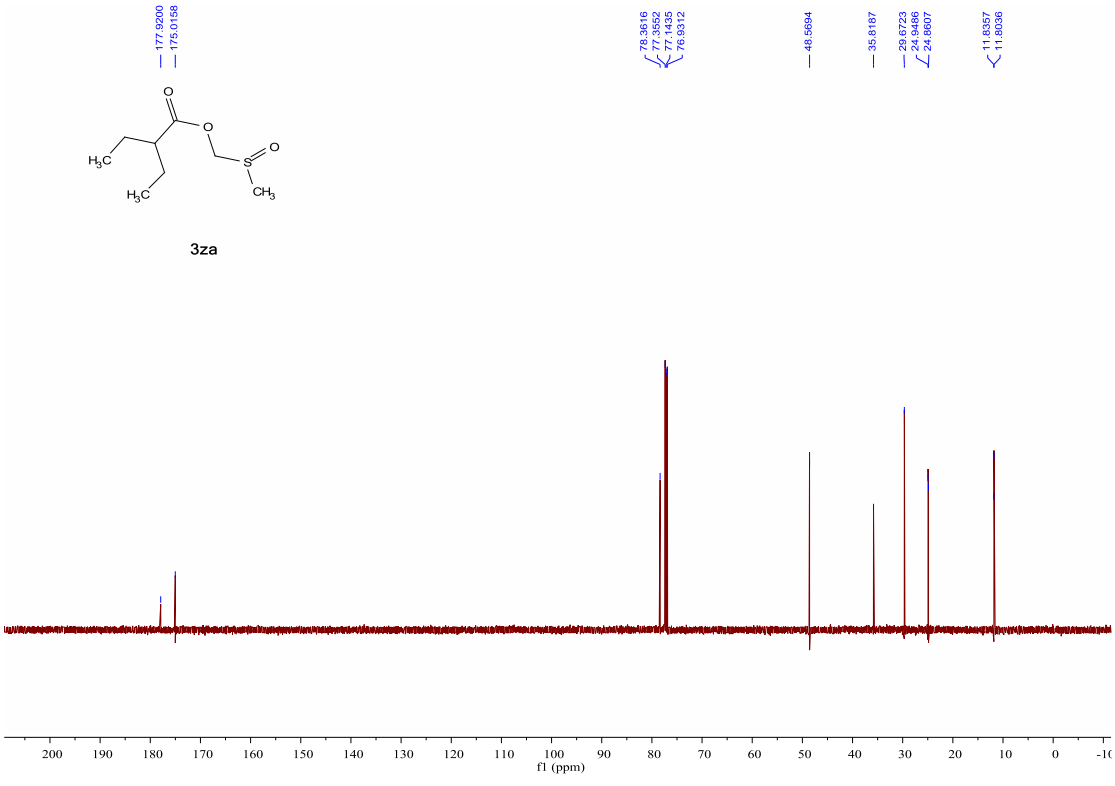

3xa
f1 (ppm)

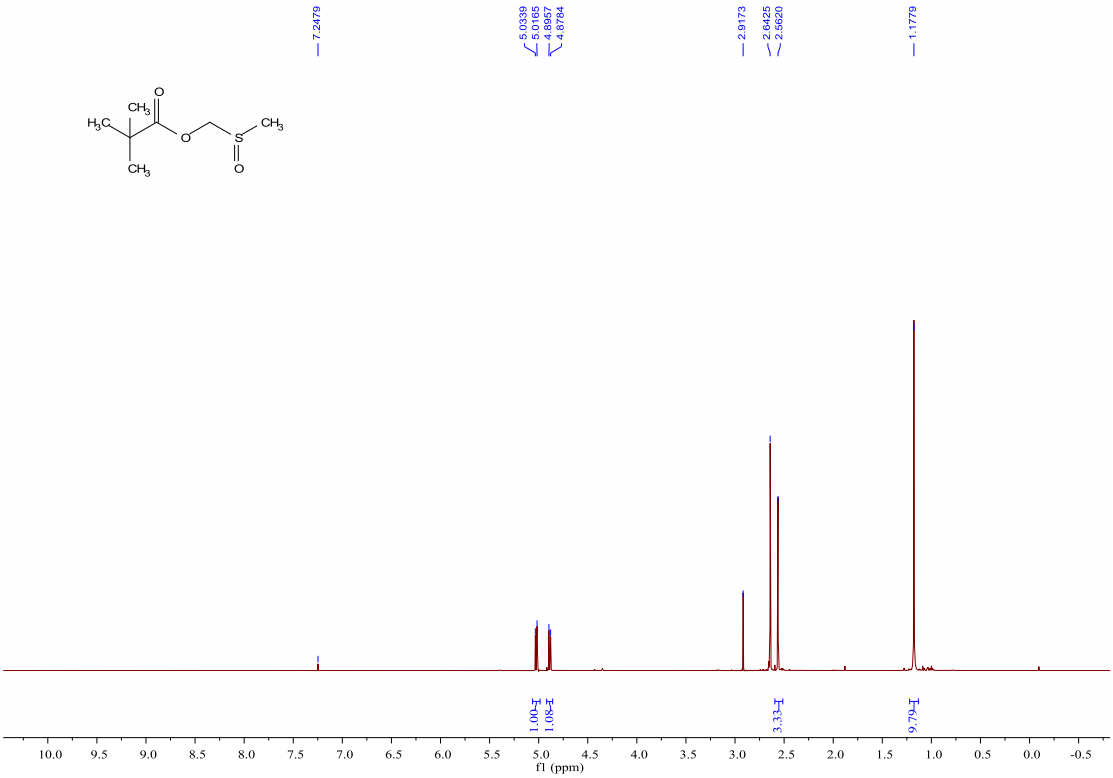

3xa
f1 (ppm)

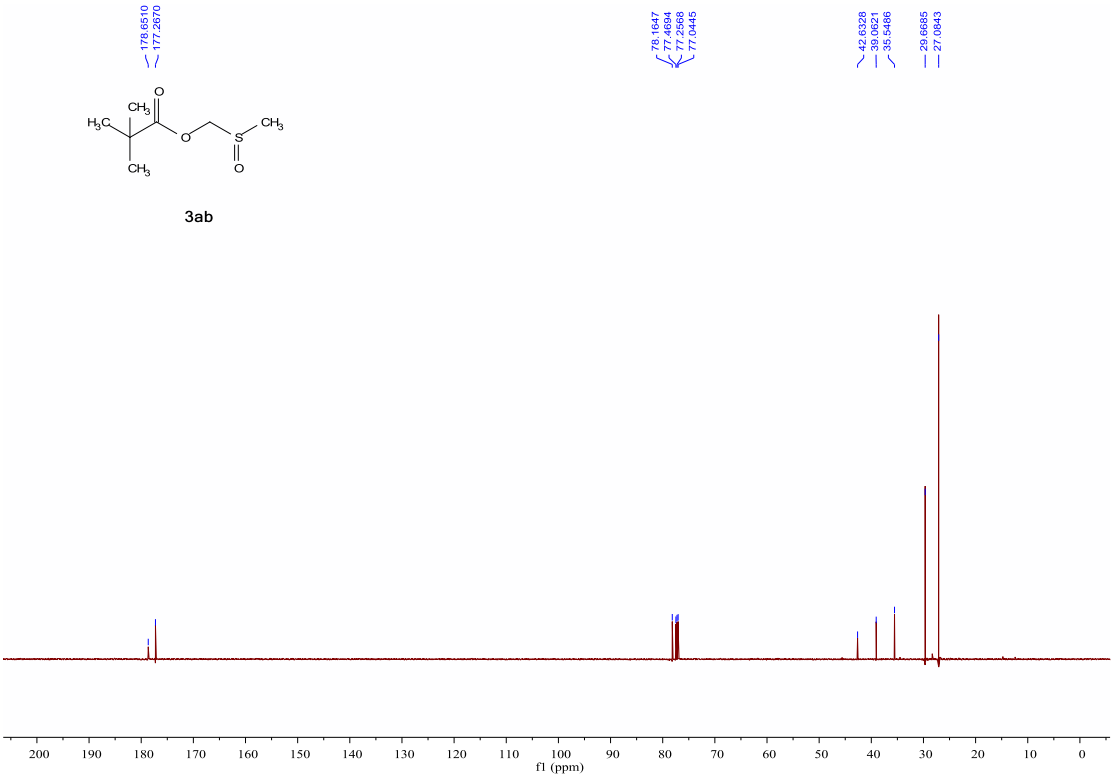

3ya
f1 (ppm)


3ya
f1 (ppm)

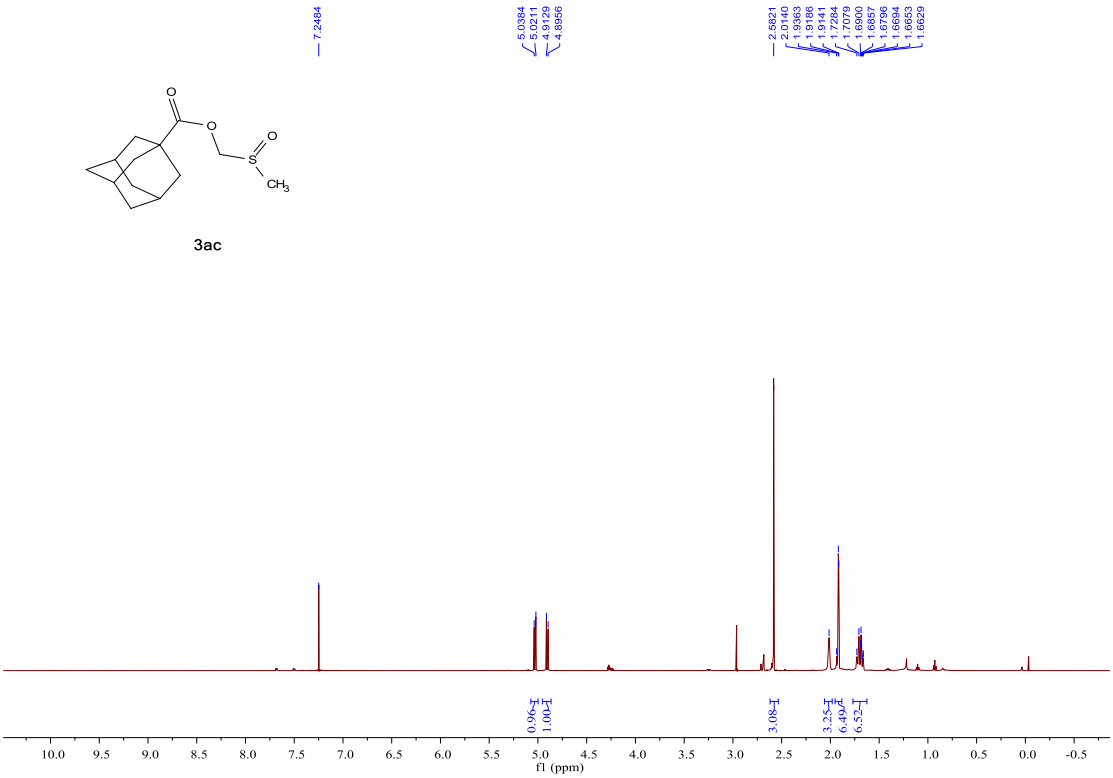

3za
f1 (ppm)


3za
f1 (ppm)

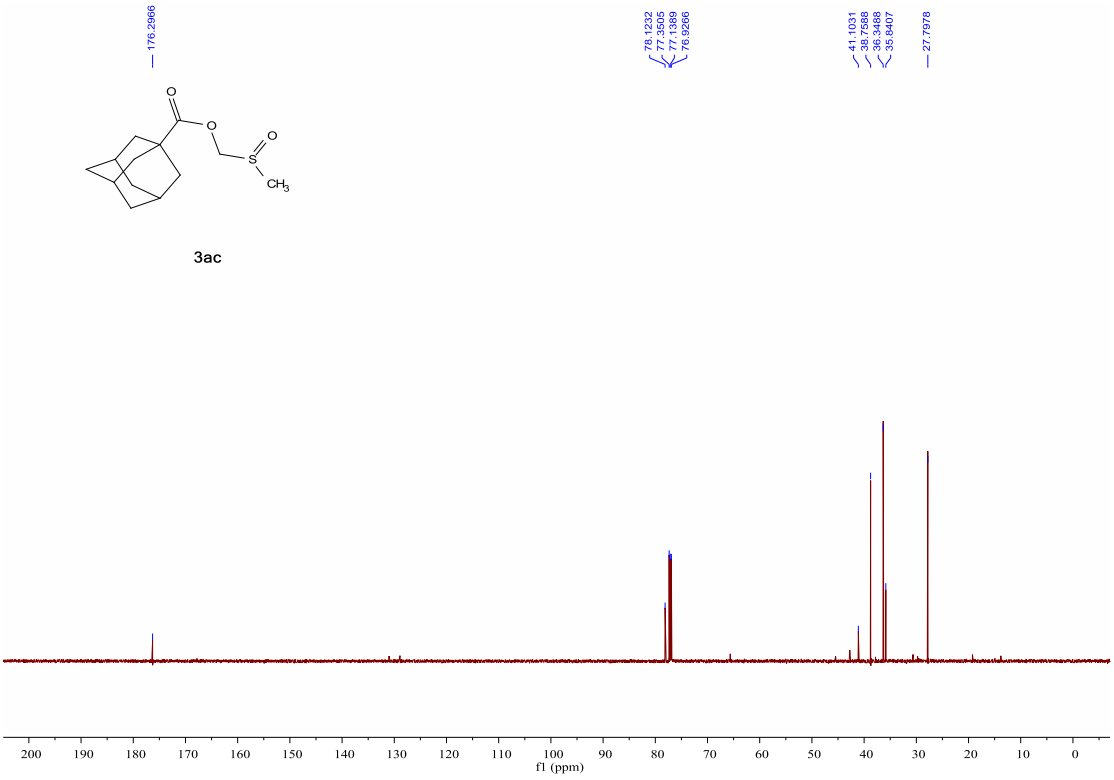

7.2479
5.0339
5.0165
4.8957
4.6784
2.9173
2.6425
2.5620
1.1779
1.00
1.00
3.33
9.79
f1 (ppm)


178.6510
177.2670
78.1647
77.4694
77.2568
77.0445
42.6328
39.0621
35.5486
29.6685
27.0843
f1 (ppm)

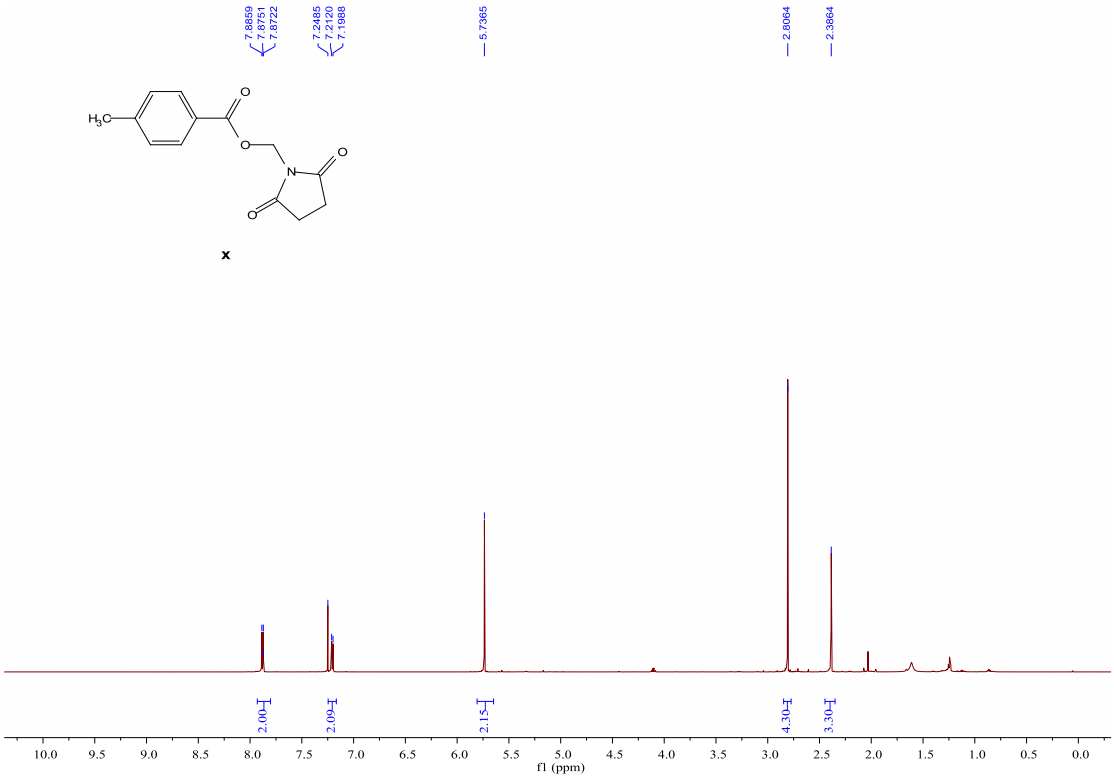
3ab


7.2484
5.0384
5.0231
4.9229
4.8956
2.5621
2.0446
1.9363
1.9186
1.9141
1.7284
1.7079
1.6900
1.6857
1.6796
1.6694
1.6653
1.6629
0.96
1.00
3.08
3.25
6.49
6.52
f1 (ppm)

3ac


176.2966
78.1232
77.3505
77.1398
76.9286
41.1031
38.7588
36.3488
35.8407
27.7978
f1 (ppm)

3ac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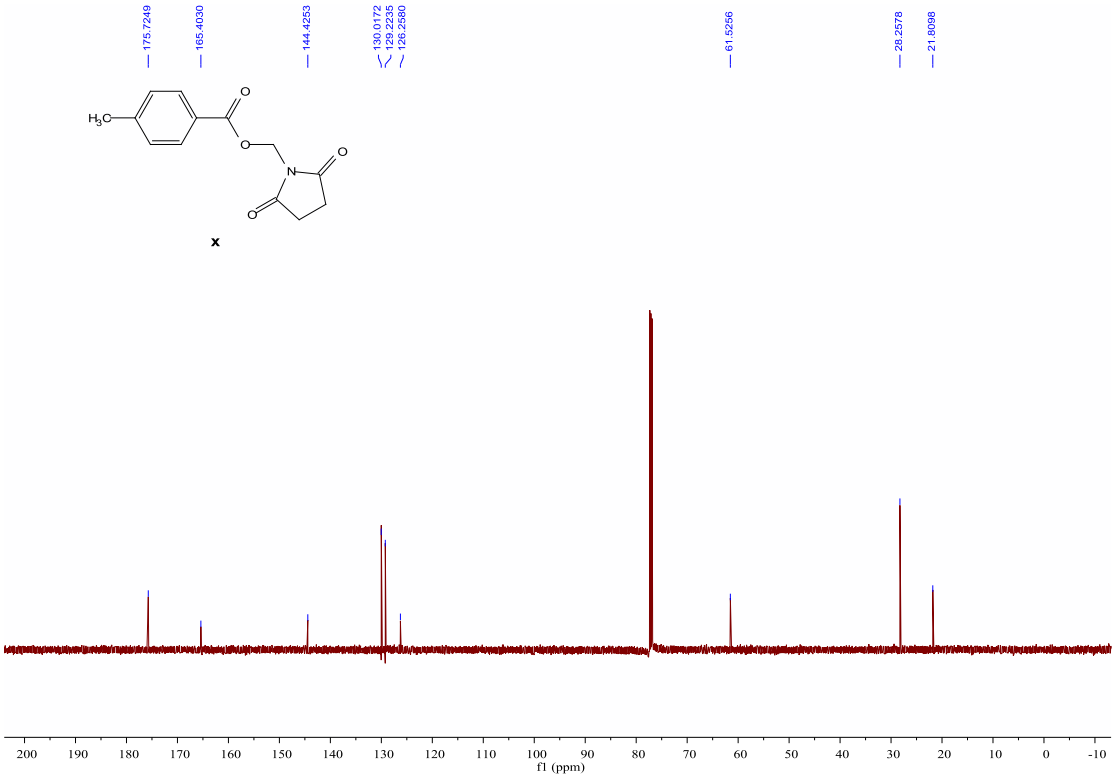
7.8751
7.8722
7.2485
7.2120
7.1988
5.7365
2.8064
2.3864
H3C
O
O
N
O
O
x
2.00
2.09
2.15
4.30
3.30
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


175.7249
165.4030
144.4253
130.0172
129.2235
126.2580
61.5256
28.2578
21.8098
H3C
O
O
N
O
O
x
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)