Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Efficient imidation of C(sp^3)−H bonds adjacent to oxygen atoms of aryl ether under metal-free condition

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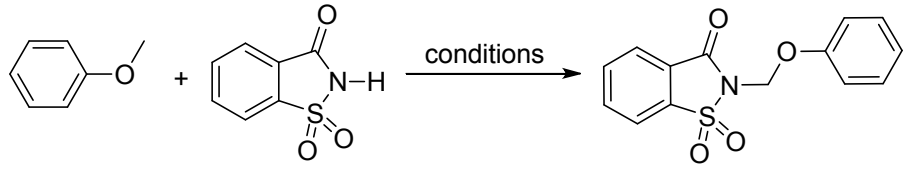
I. General Remarks:

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. All the reactions were carried out under air atmosphere. ^{1}H NMR spectra were recorded at 25ºC on a Bruker Ascend^{TM} 400 spectrometer, ^{13}C NMR spectra were recorded at 25ºC on a Bruker 100 MHz, and TMS as internal standard. Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. HRMS data were obtained on a Waters LCT Premierxe^{TM} (USA). All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

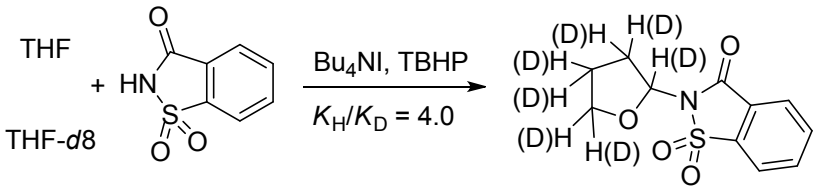
II. General procedure for the synthesis of 3 and 5 (**1a** as an example).



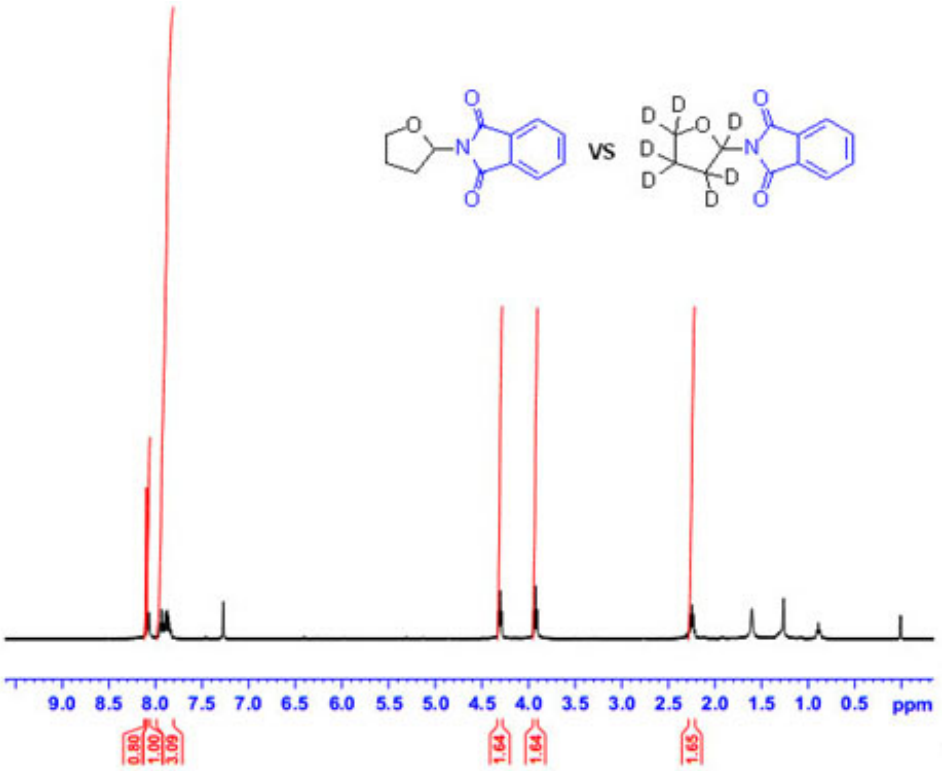
1a **2** **3a**

Anisole **1a** (54.0 mg, 0.5 mmol), saccharin **2** (183.0 mg, 1.0 mmol) were added to Bu_4NI (18.5 mg, 0.05 mmol) and TBHP (180.2 mg, 2.0 mmol) solution. The mixture was stirred at 120 ^{o}C for 8.0-12.0 h (monitored by TLC), quenched with water, extracted with dichloromethane (5×3 mL), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (EtOAc/petro ether=1:6) to give compound **3a** as a white solid (127.2 mg, 88%).

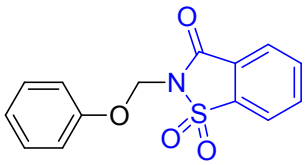
III. The Kinetic Isotope Effect Experiment



Reaction conditions: The mixture of THF (0.25 mmol), THF-*d*8 (0.25 mmol), saccharin (1.0 mmol), Bu_4NI (0.05 mmol) and TBHP (2.0 mmol) was stirred at 120 ^{o}C under air atmosphere for 6 h. There is a high kinetic isotope effect (K_H/K_D = 4.0) in the deuterated experiment between THF and THF-*d*8.

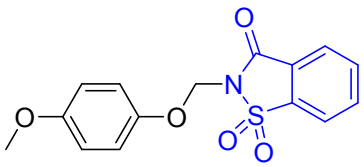


IV. Analytical data of products obtained in this study



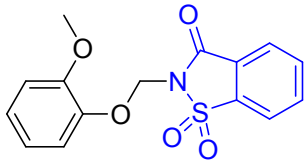
2-(3-oxo-3-phenylpropyl)benzo[d]isothiazol-3(2*H*)-one 1,1-dioxide 3a

White solid. Mp: 113-115 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.84 (s, 2H), 7.07 (t, J= 7.6 Hz, 1H), 7.14-7.16 (m, 2H), 7.31-7.35 (m, 2H), 7.85-7.94 (m, 3H), 7.95-8.11 (m, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.2, 116.7, 121.0, 121.2, 123.1, 125.7, 126.7, 129.6, 134.5, 137.8, 155.9, 158.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{11}NO_4S$, $[M+H]^+$ 290.0487; Found 290.0485.



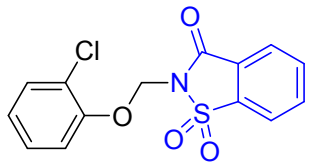
2-((4-methoxyphenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3b

White solid. Mp: 130-132 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.77 (s, 3H), 5.76 (s, 2H), 6.85 (dd, J_1= 1.2 Hz, J_2= 8.0 Hz, 2H), 6.87-7.11 (m, 2H), 7.83-7.85 (m, 3H), 7.89 (dd, J_1= 2.0 Hz, J_2= 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 55.6, 68.2, 114.7, 118.7, 121.1, 125.7, 126.7, 134.5, 135.4, 137.9, 149.9, 155.7, 158.6. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}NO_5S$, $[M+H]^+$ 320.0593; Found 320.0597.



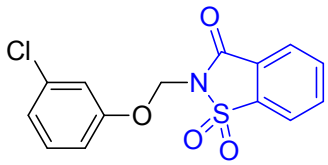
2-((2-methoxyphenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3c

White solid. Mp: 137-139 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.91 (s, 3H), 5.83 (s, 2H), 6.86 (d, *J*= 7.6 Hz, 1H), 6.97 (J_1= 1.6 Hz, J_2= 8.0 Hz, 1H), 7.09-7.16 (m, 2H), 7.84-7.94 (m, 3H), 8.05 (d, *J*= 7.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 55.9, 68.8, 112.6, 120.9, 121.1, 125.0, 125.6, 126.7, 134.4, 135.3, 137.9, 144.9, 151.6, 158.6. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}NO_5S$, $[M+H]^+$ 320.0593; Found 320.0591.



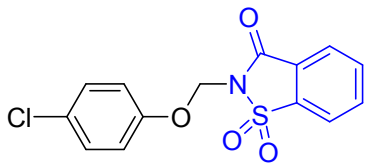
2-((2-chlorophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3d

White solid. Mp: 193-195 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.84 (s, 2H), 7.06 (d, *J*= 6.4 Hz, 1H), 7.23-7.26 (m, 2H), 7.41 (dd, J_1= 1.2 Hz, J_2= 8.0 Hz, 1H), 7.87-7.91 (m, 3H), 7.93 (d, *J*= 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 68.2, 119.0, 121.2, 124.7, 125.6, 125.8, 126.5, 127.8, 130.7, 134.5, 135.5, 137.8, 152.0, 158.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}ClNO_4S$, $[M+H]^+$ 324.0097; Found 324.0095.



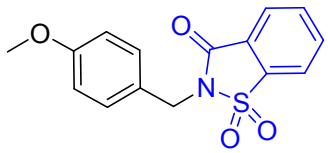
2-((3-chlorophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3e

White solid. Mp: 196-199 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.81 (s, 2H), 7.05 (dd, J_1= 2.4 Hz, J_2= 8.0 Hz, 2H), 7.17 (d, *J*= 6.0 Hz, 1H), 7.25 (d, *J*= 8.0 Hz, 1H), 7.88-7.93 (m, 3H), 7.94 (d, *J*= 6.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.0, 114.7, 117.4, 121.2, 123.3, 125.8, 126.6, 130.4, 134.6, 135.0, 135.5, 137.8, 156.6, 158.5. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}ClNO_4S$, $[M+H]^+$ 324.0097; Found 324.0092.



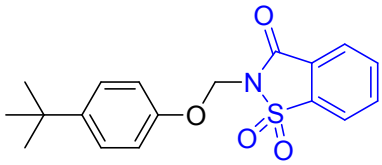
2-((4-chlorophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3f

White solid. Mp:192-194 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.81 (s, 2H), 7.08 (dd, J_1= 2.0 Hz, J_2= 6.8 Hz, 2H), 7.28 (dd, J_1 = 2.4 Hz, J_2 = 6.8 Hz, 2H), 7.87-7.91 (m, 3H), 7.93 (d, *J*= 6.4 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.4, 118.3, 121.2, 125.8, 126.5, 128.3, 129.6, 134.6, 135.5, 137.8, 154.5, 158.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}ClNO_4S$, $[M+H]^+$ 324.0097; Found 324.0091.



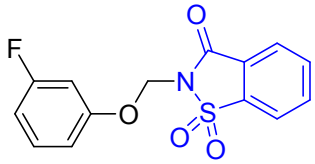
2-(4-methoxybenzyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3g

White solid. Mp: 150-152 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.80 (s, 3H), 4.87 (s, 2H), 6.88 (d, *J*= 8.8 Hz, 2H), 7.46 (d, *J*= 8.8 Hz, 2H), 7.82-7.86 (m, 3H), 7.93 (d, *J*= 6.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 42.3, 55.2, 114.1, 121.0, 125.2, 126.6, 127.4, 130.4, 134.3, 134.7, 137.8, 158.8, 159.6. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}NO_4S$, $[M+H]^+$ 304.0644; Found 304.0639.



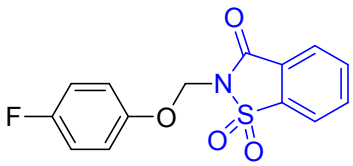
2-((4-(*tert*-butyl)phenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3h

White solid. Mp: 164-166 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.30 (s, 9H), 5.82 (s, 2H), 7.07 (dd, J_1= 2.0 Hz, J_2= 6.4 Hz, 2H), 7.34 (dd, J_1= 2.0 Hz, J_2= 6.4 Hz, 2H), 7.84-7.88 (m, 3H), 7.90 (dd, J_1= 1.2 Hz, J_2= 7.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.4, 34.2, 67.3, 115.9, 121.2, 125.7, 126.4, 126.7, 134.5, 135.4, 137.9, 145.7, 153.7, 158.6. HRMS (ESI-TOF) Calcd for $C_{18}H_{19}NO_4S$, $[M+H]^+$ 346.1113; Found 346.1117.



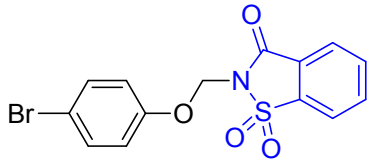
2-((3-fluorophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3i

White solid. Mp: 148-150 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.82 (s, 2H), 6.68-6.88 (m, 1H), 6.89-6.96 (m, 2H), 7.25-7.31 (m, 1H), 7.86-7.93 (m, 3H), 7.95-8.01 (m, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.0, 104.5, 104.8, 109.8,110.0, 112.0, 121.2, 125.8, 126.6, 130.4, 130.5, 134.6, 135.0, 135.5, 137.8, 157.1, 157.2, 158.5, 162.2, 164.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}FNO_4S$, $[M+H]^+$ 308.0393; Found 308.0391.



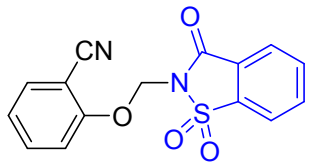
2-((4-fluorophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3j

White solid. Mp: 108-110 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.78 (s, 2H), 6.97-7.02 (m, 2H), 7.09-7.13 (m, 2H), 7.86-7.92 (m, 3H), 7.93 (d, *J*= 6.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 68.1, 116.0, 116.2, 118.6, 118.7, 121.2, 125.7, 126.5, 134.6, 135.5, 137.8, 151.9, 157.6, 158.6, 159.9. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}FNO_4S$, $[M+H]^+$ 308.0393; Found 308.0389.



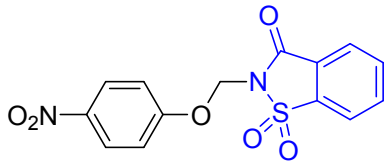
2-((4-bromophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3k

White solid. Mp: 167-170 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.81 (s, 2H), 7.05 (dd, J_1= 2.0 Hz, J_2= 6.8 Hz, 2H), 7.34 (dd, J_1 = 2.4 Hz, J_2 = 6.8 Hz, 2H), 7.85-7.91 (m, 3H), 7.92 (d, J= 6.4 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.2, 115.7, 118.7, 121.2, 125.8, 126.5, 132.6, 134.6, 135.5, 137.8, 155.0, 158.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}BrNO_4S$, $[M+H]^+$ 367.9592; Found 367.9596.



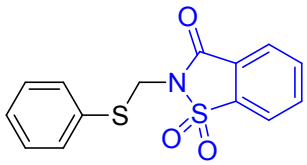
2-((1,1-dioxido-3-oxobenzo[*d*]isothiazol-2(3*H*)-yl)methoxy)benzonitrile 3l

White solid. Mp: 116-118 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.93 (s, 2H), 7.13-7.17 (m, 1H), 7.35 (d, J= 8.4 Hz, 1H), 7.56-7.60 (m, 2H), 7.61-7.63 (m, 3H), 7.87 (t, J= 6.4 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.3, 104.4, 115.4, 115.6, 121.3, 123.3, 125.9, 126.4, 134.1, 134.2, 134.6, 135.7, 137.8, 157.6, 158.6. HRMS (ESI-TOF) Calcd for $C_{15}H_{10}N_2O_4S$, $[M+H]^+$ 315.0440; Found 315.0445.



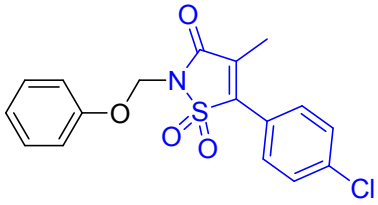
2-((4-nitrophenoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3m

White solid. Mp: 207-209 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.92 (s, 2H), 7.25 (d, J = 9.2 Hz, 2H), 7.90-7.95 (m, 3H), 7.96 (d, J = 6.8 Hz, 1H), 8.12-8.26 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 67.0, 114.8, 117.4, 121.2, 123.3, 125.8, 126.6, 133.4, 134.6, 135.0, 135.5, 156.6, 158.5. HRMS (ESI-TOF) Calcd for $C_{14}H_{11}N_2O_6S$, $[M+H]^+$ 335.0338; Found 335.0386.



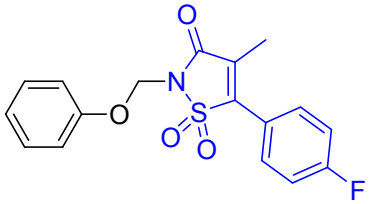
2-((phenylthio)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3o

White solid. Mp: 110-112 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.17 (s, 2H), 7.33-7.60 (m, 3H), 7.62 (dd, J_1= 1.2 Hz, J_2= 6.8 Hz, 2H),), 7.83-7.91 (m, 3H), 8.03 (d, J= 7.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 44.4, 121.0, 125.4, 126.9, 127.4, 128.4, 129.4, 132.8, 134.4, 135.0, 137.9, 158.3. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}NO_3S_2$, $[M+H]^+$ 306.0259; Found 306.0255.



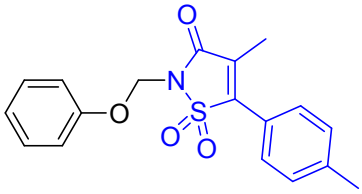
5-(4-chlorophenyl)-4-methyl-2-(phenoxymethyl)isothiazol-3(2*H*)-one 1,1-dioxide 3p

White solid. Mp: 76-79 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.19 (s, 3H), 5.75 (s, 2H), 7.08 (t, *J*=7.6 Hz, 1H), 7.14 (d, *J*= 8.0 Hz, 2H), 7.32-7.36 (m, 2H), 7.51-7.54 (m, 2H), 7.61-7.64 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 10.2, 67.6, 116.6, 122.9, 123.1, 129.7, 129.8, 129.9, 130.3, 130.4, 132.3, 138.2, 144.4, 155.9, 160.6. HRMS (ESI-TOF) Calcd for $C_{17}H_{15}NClO_4S$, $[M+H]^+$ 364.0410; Found 364.0419.



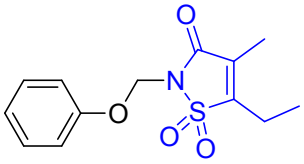
5-(4-fluorophenyl)-4-methyl-2-(phenoxymethyl)isothiazol-3(2*H*)-one 1,1-dioxide 3q

White solid. Mp: 81-84 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.19 (s, 3H), 5.75 (s, 2H), 7.08 (t, *J*=7.2 Hz, 1H), 7.14 (d, *J*= 7.6 Hz, 2H), 7.15-7.26 (m, 2H), 7.32-7.36 (m, 2H), 7.67-7.70 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 10.2, 67.6, 116.6, 116.8, 117.0, 120.6, 123.1, 129.7, 131.4, 131.5, 131.9, 144.5, 155.9, 160.7, 163.2, 165.7. HRMS (ESI-TOF) Calcd for $C_{17}H_{15}NFO_4S$, $[M+H]^+$ 348.0706; Found 348.0701.



4-methyl-2-(phenoxymethyl)-5-(p-tolyl)isothiazol-3(2*H*)-one 1,1-dioxide 3r

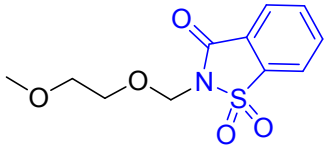
White solid. Mp: 73-76 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.20 (s, 3H), 2.44 (s, 3H), 5.75 (s, 2H), 7.08 (t, *J*=7.6 Hz, 1H), 7.14 (d, *J*= 7.2 Hz, 2H), 7.32 (d, *J*= 6.0 Hz, 3H), 7.58 (d, *J*= 8.0 Hz, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 10.3, 21.6, 67.5, 116.6, 121.6, 122.9, 128.9, 129.0, 129.6, 130.1, 130.9, 142.3, 145.5, 156.0, 161.1. HRMS (ESI-TOF) Calcd for $C_{18}H_{18}NO_4S$, $[M+H]^+$ 344.0957; Found 344.0952.



5-ethyl-4-methyl-2-(phenoxymethyl)isothiazol-3(2*H*)-one 1,1-dioxide 3s

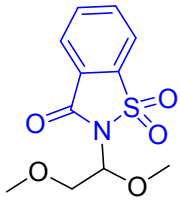
White solid. Mp: 55-57 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.36 (t, *J*= 6.0 Hz, 3H), 2.04 (s, 3H), 2.70 (q, *J*= 7.6 Hz, 2H), 5.66 (s, 2H), 7.08 (d, *J*= 7.2 Hz, 1H), 7.09 (d, *J*= 8.0 Hz, 2H), 7.30-7.34 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 8.8, 12.1, 17.6, 67.3, 116.5, 122.9, 129.6, 132.1，

148.6, 155.9, 160.9. HRMS (ESI-TOF) Calcd for $C_{13}H_{16}NO_4S$, $[M+H]^+$ 282.0800; Found 282.0801.



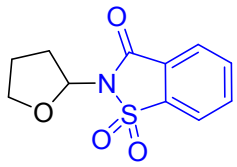
2-((2-methoxyethoxy)methyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 5a

White solid. Mp: 105-107 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.38 (s, 3H), 3.58-3.60 (m, 2H), 3.83-3.85 (m, 2H), 5.36 (s, 2H), 7.87-7.90 (m, 3H), 7.93 (dd, J_1= 1.2 Hz, J_2= 7.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 59.0, 69.4, 70.0, 71.4, 121.1, 125.5, 126.9, 134.5, 135.3, 137.9, 159.2. HRMS (ESI-TOF) Calcd for $C_{11}H_{13}NO_5S$, $[M+H]^+$ 272.0593; Found 272.0599.



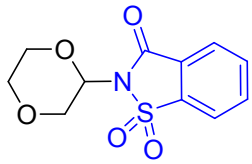
2-(1,2-dimethoxyethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 5a'

White solid. Mp: 90-92 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.45 (s, 3H), 3.57 (s, 3H), 3.97 (d, J= 6.0 Hz, 2H), 5.62 (t, J= 6.0 Hz, 1H), 7.85-7.94 (m, 3H), 8.08 (t, J= 7.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 57.7, 59.4, 71.6, 85.6, 120.8, 125.5, 126.6, 134.3, 135.1, 138.1, 159.2. HRMS (ESI-TOF) Calcd for $C_{11}H_{13}NO_5S$, $[M+H]^+$ 272.0593; Found 272.0596.



2-(tetrahydrofuran-2-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 5b

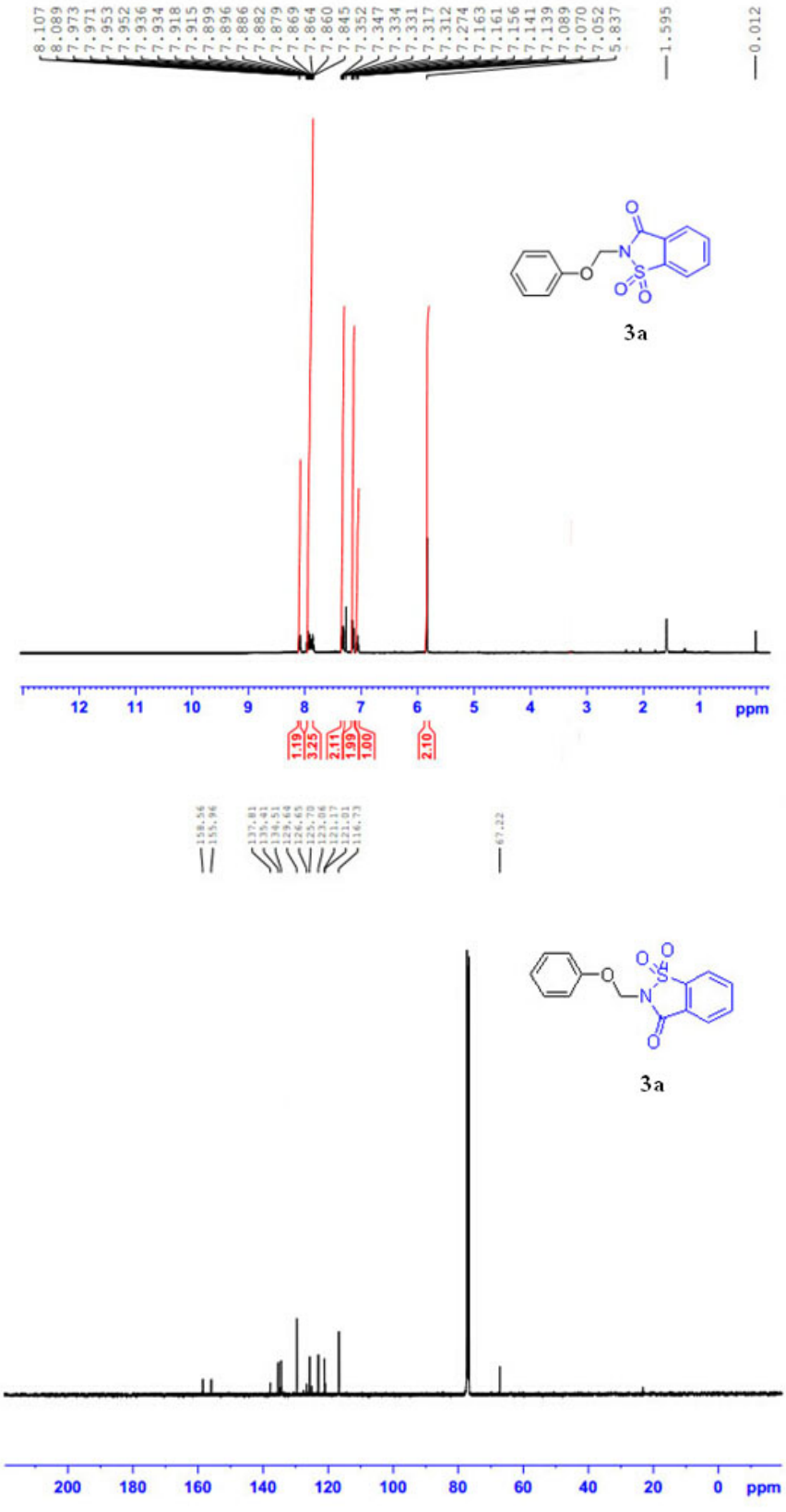
White solid. Mp: 107-110 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.25 (t, J= 6.8 Hz, 2H), 3.93 (t, J= 7.2 Hz, 2H), 4.31 (t, J= 6.4 Hz, 2H), 7.86-7.95 (m, 3H), 8.10 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 27.4, 36.0, 60.8, 121.0, 125.2, 127.3, 134.4, 134.9, 137.7, 158.9, 160.8. HRMS (ESI-TOF) Calcd for $C_{11}H_{11}NO_4S$, $[M+H]^+$ 254.0487; Found 254.0481.

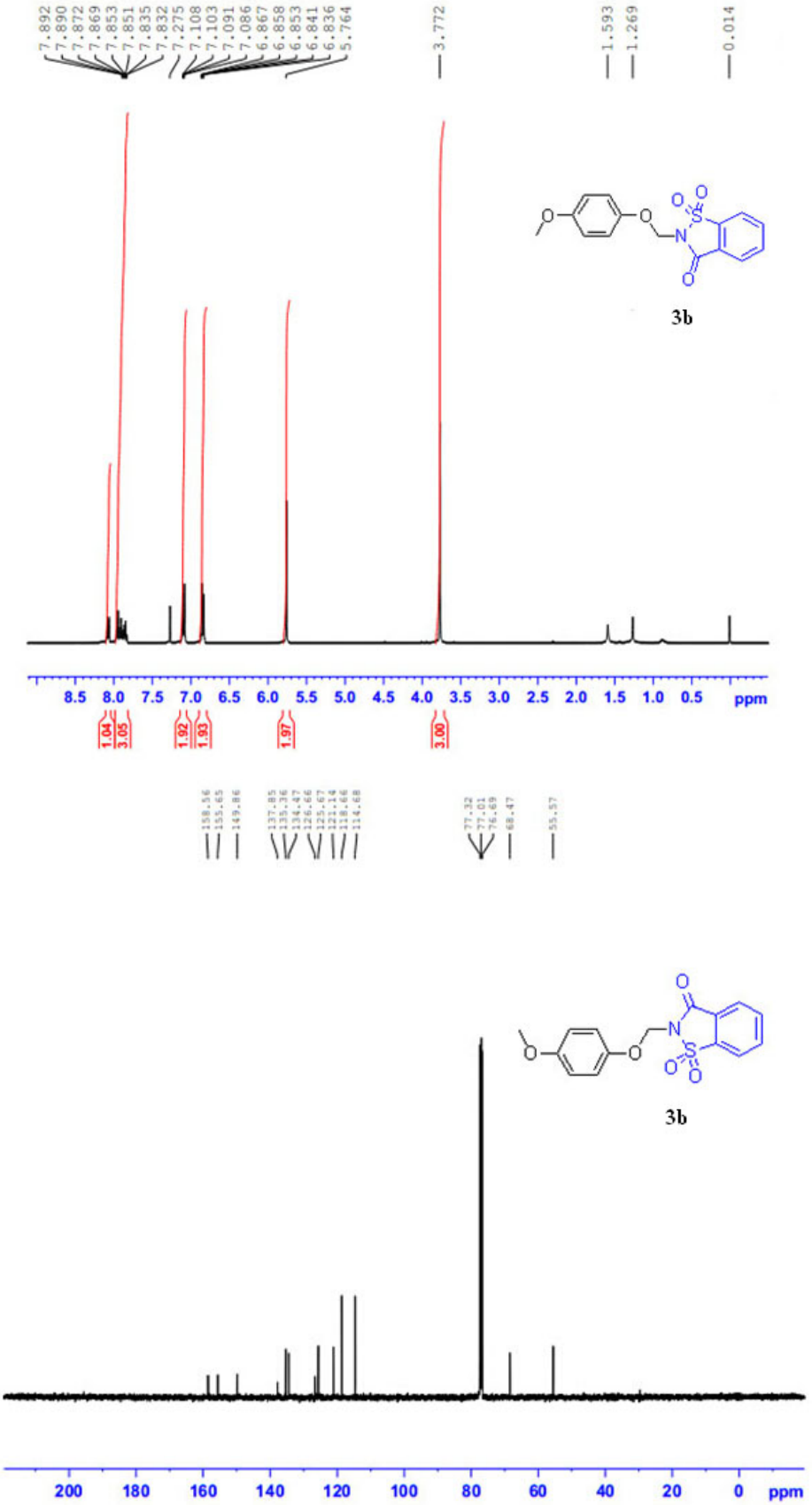


2-(1,4-dioxan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 5c

White solid. Mp: 161-163 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.79-3.93 (m, 2H), 4.02 (dd, J_1= 2.8 Hz, J_2= 7.6 Hz, 1H), 4.11 (d, J= 7.6 Hz, 2H), 4.36 (m, 1H), 5.70 (dd, J_1= 2.8 Hz, J_2= 8.8 Hz, 1H), 7.85-7.93 (m, 3H), 8.07 (t, J= 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 65.9, 66.5, 66.7, 78.9, 120.9, 125.5, 126.4, 134.4, 135.3, 137.9, 158.5. HRMS (ESI-TOF) Calcd for $C_{11}H_{11}NO_5S$, $[M+H]^+$ 270.0436; Found 270.0433.

V. ^{1}H NMR and ^{13}C NMR spectra copies of compounds 3, 5 and H.

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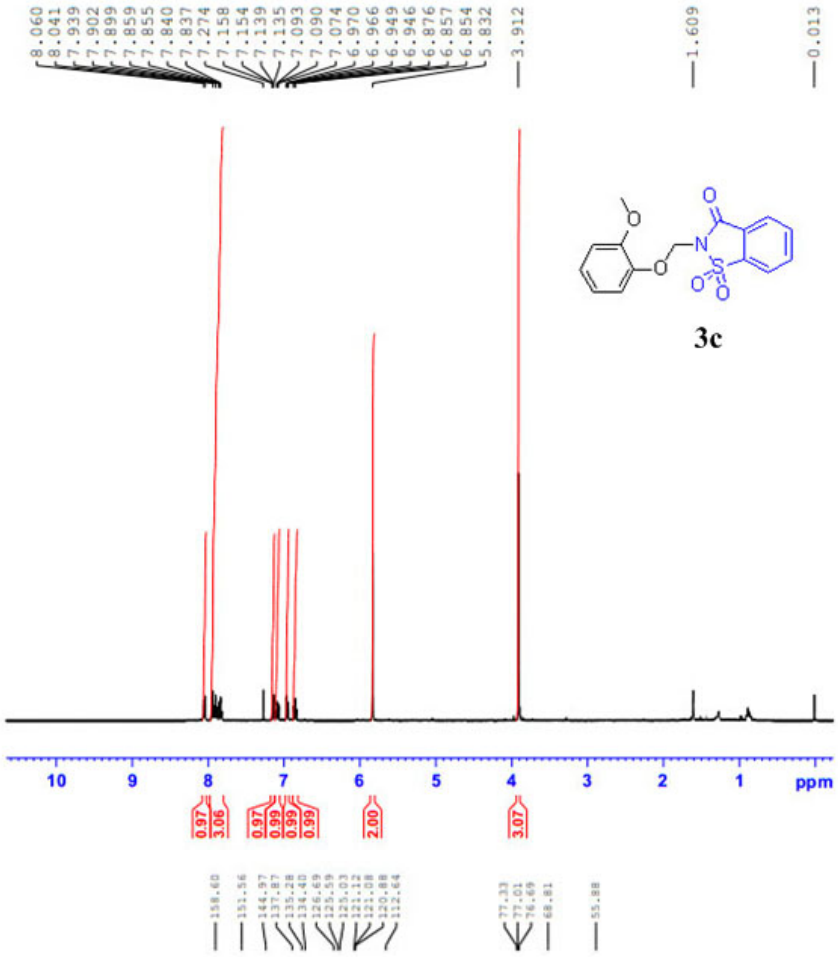
7.275
7.108
7.103
7.091
7.086
6.867
6.858
6.853
6.841
6.836
5.764
3.772
1.593
1.269
0.014
3b
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.04
3.05
1.92
1.93
1.97
3.00
158.56
155.65
149.86
137.85
135.36
134.47
126.46
125.67
121.14
118.66
114.68
77.32
77.01
76.69
68.47
55.57
3b
200 180 160 140 120 100 80 60 40 20 0 ppm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7.840
7.837
7.274
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7.154
7.139
7.135
7.093
7.090
7.074
6.970
6.966
6.949
6.946
6.876
6.857
6.854
5.832
3.912
1.609
0.013
10
9
8
7
6
5
4
3
2
1
ppm
0.97
3.06
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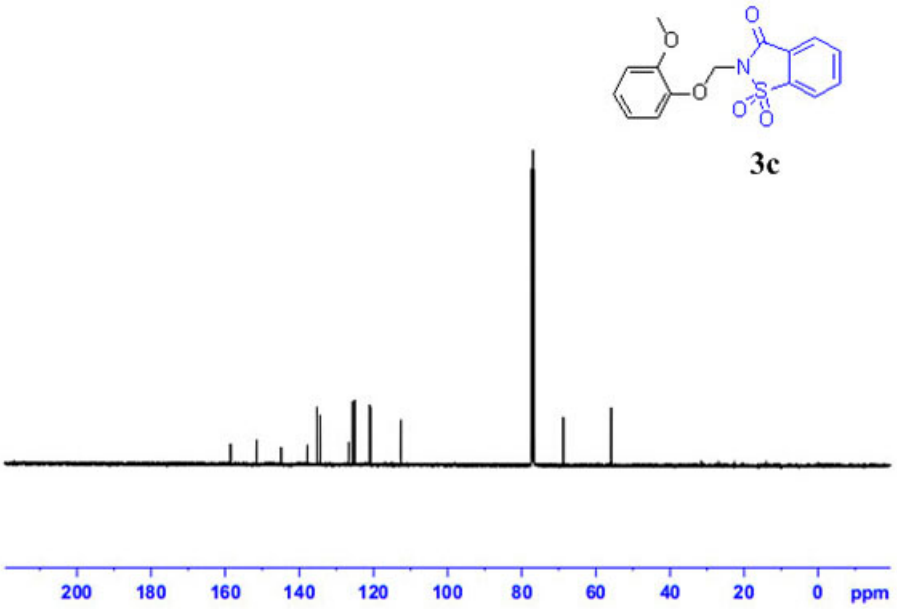
0.99
0.99
0.99
2.00
3.07

3c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125.59
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121.12
120.08
113.08
112.64
77.33
77.01
76.69
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55.88
200
180
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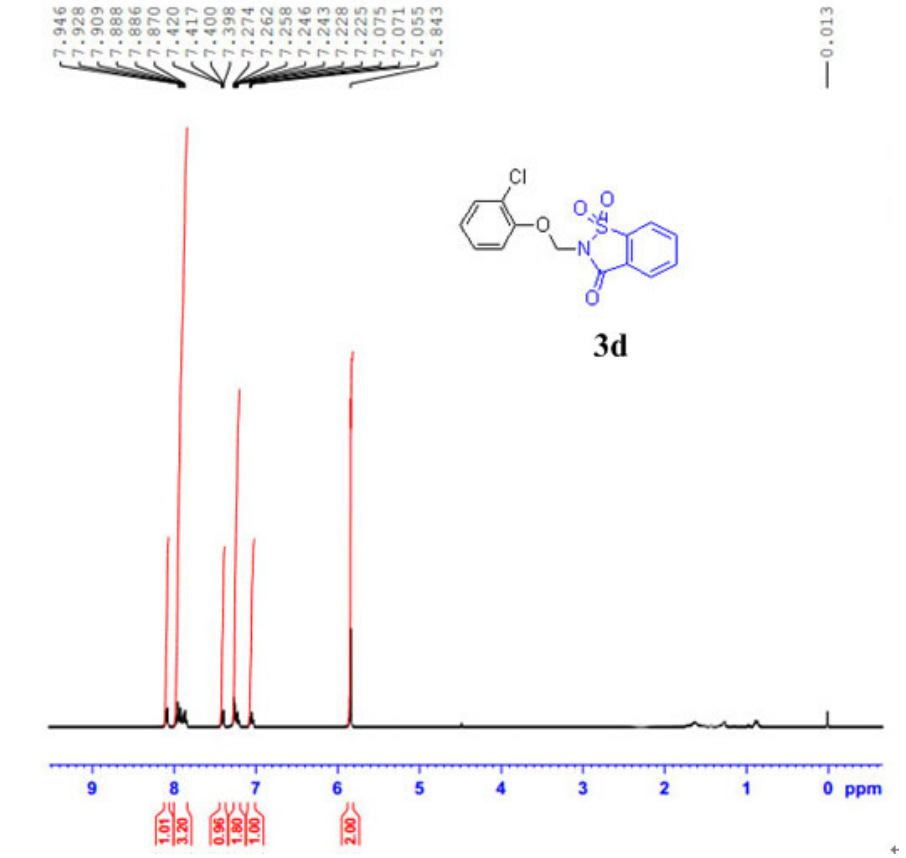
140
120
100
80
60
40
20
0
ppm

3c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7.417
7.400
7.398
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7.258
7.246
7.243
7.228
7.225
7.075
7.071
7.055
5.843
0.013
Cl
O
O
S
N
O
O
3d
9
8
7
6
5
4
3
2
1
0 ppm
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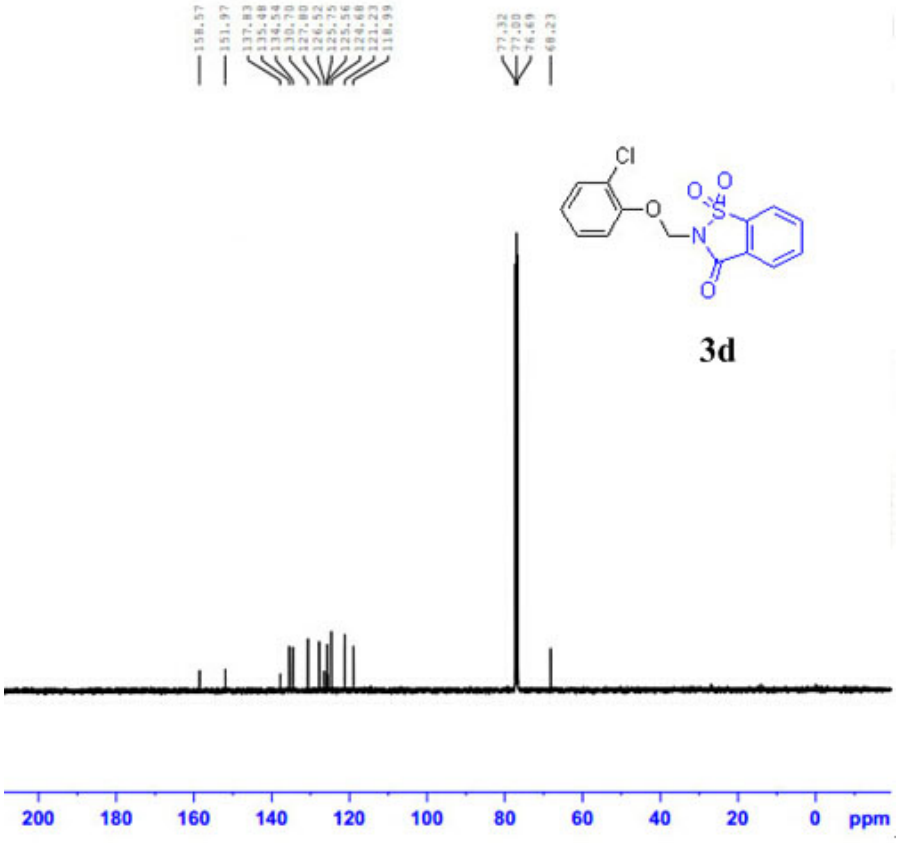
3.20
0.96
1.80
1.00
2.00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124.68
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77.32
77.00
76.69
60.23
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S
N
O
O
3d
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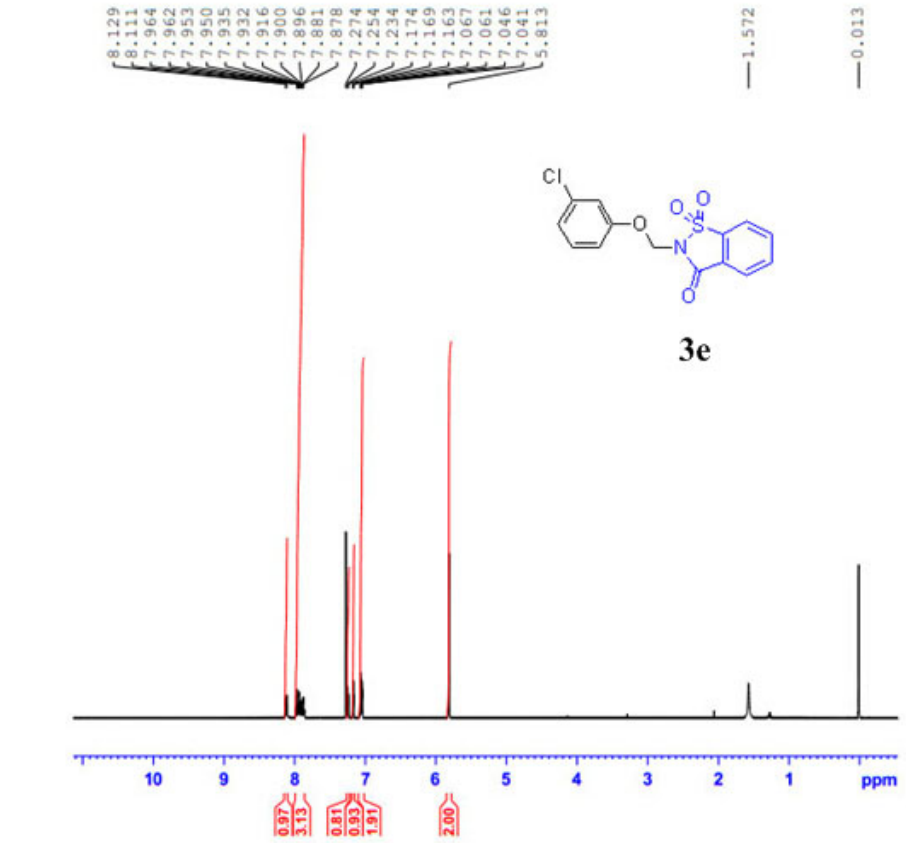
140
120
100
80
60
40
20
0 ppm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7.916
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7.881
7.878
7.274
7.254
7.234
7.174
7.169
7.163
7.067
7.061
7.046
7.041
5.813
1.572
0.013
Cl
O
O
O
S
N
O
3e
10
9
8
7
6
5
4
3
2
1
ppm
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0.93
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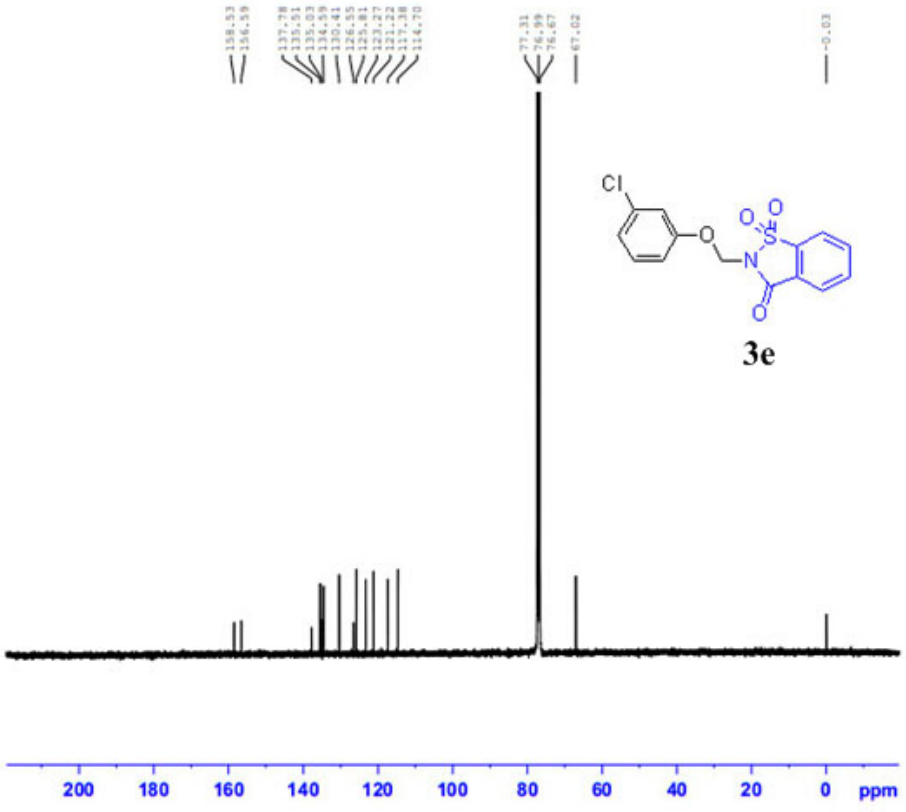
2.00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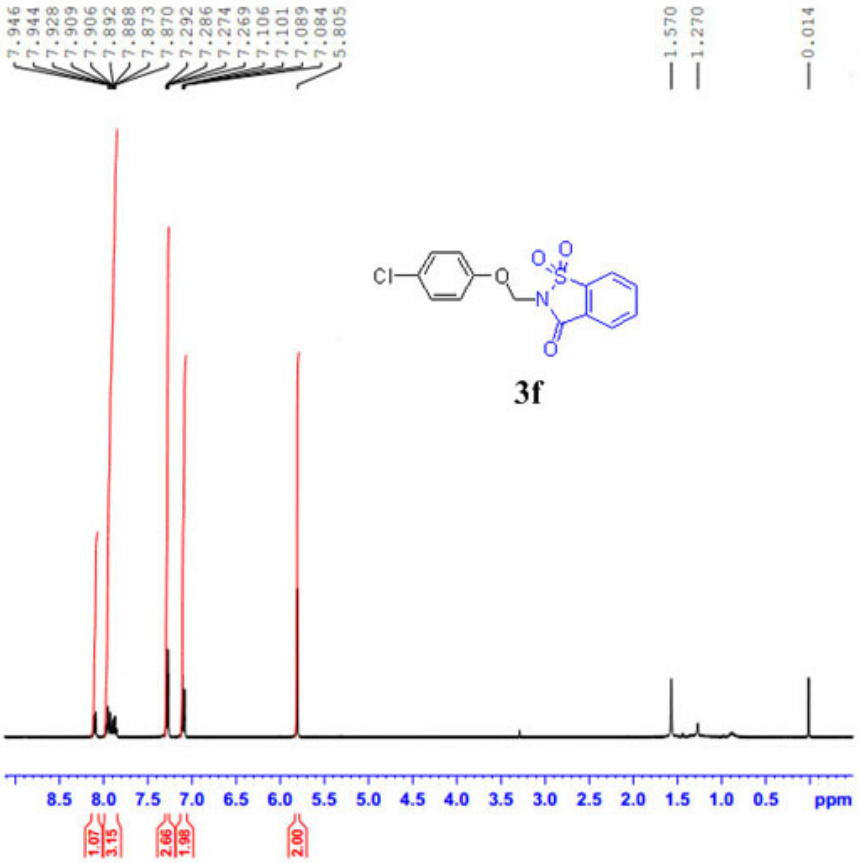
126.55
125.81
123.27
121.22
117.38
114.70
77.31
76.99
76.67
67.02
-0.03
Cl
O
O
O
S
N
O
3e
200
180
160
140
120
100
80
60
40
20
0
ppm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7.269
7.106
7.101
7.089
7.084
5.805
1.570
1.270
0.014
Cl
O
O
O
S
N
O
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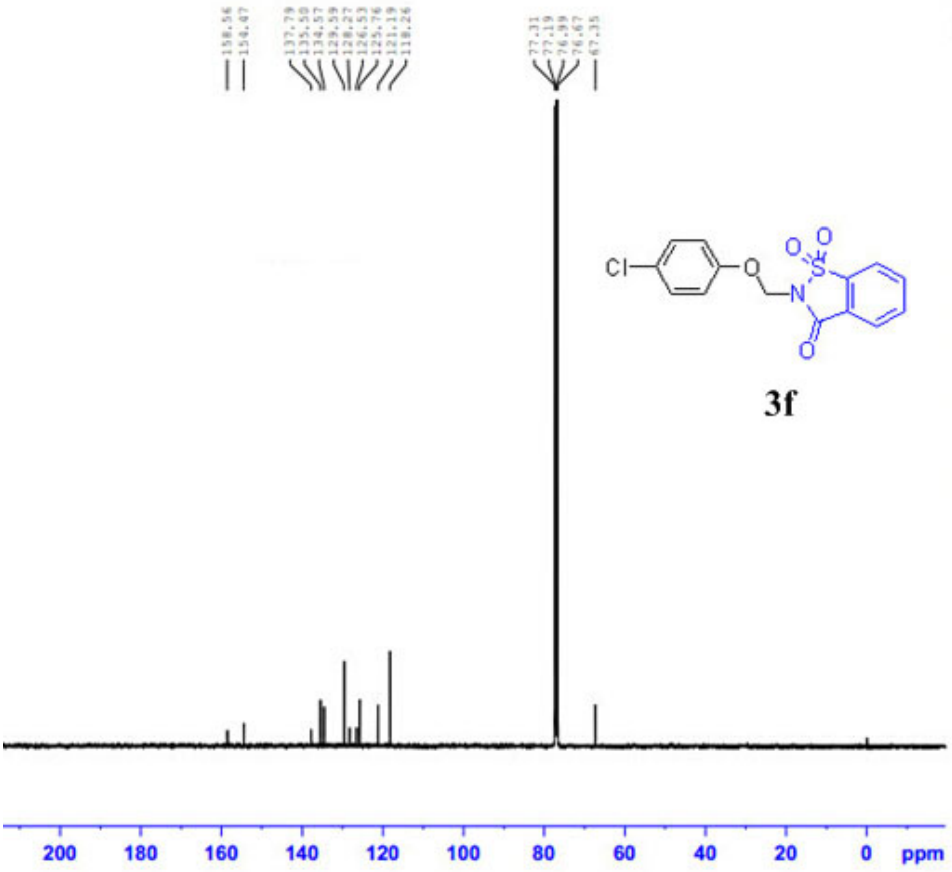
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129.59
128.27
126.53
125.76
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118.26
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77.19
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76.67
67.35
Cl
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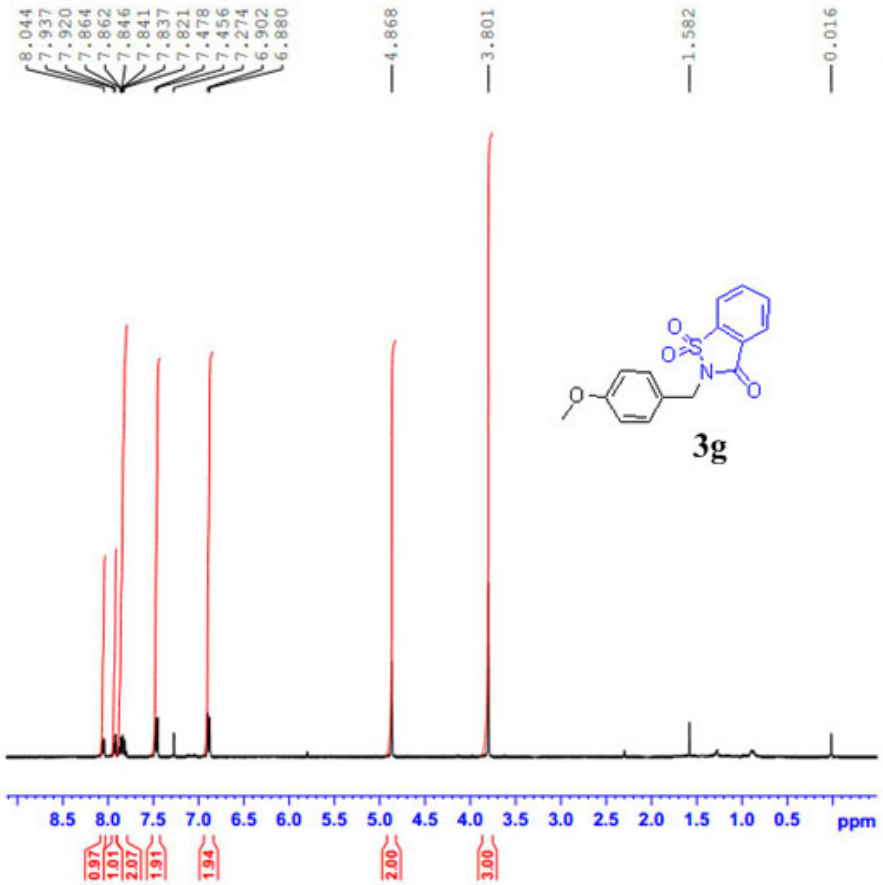
O
O
S
N
O
200 180 160 140 120 100 80 60 40 20 0 ppm

3f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7.846
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7.837
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7.478
7.456
7.274
6.902
6.880
4.868
3.801
1.582
0.016
3g
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1.01
2.07
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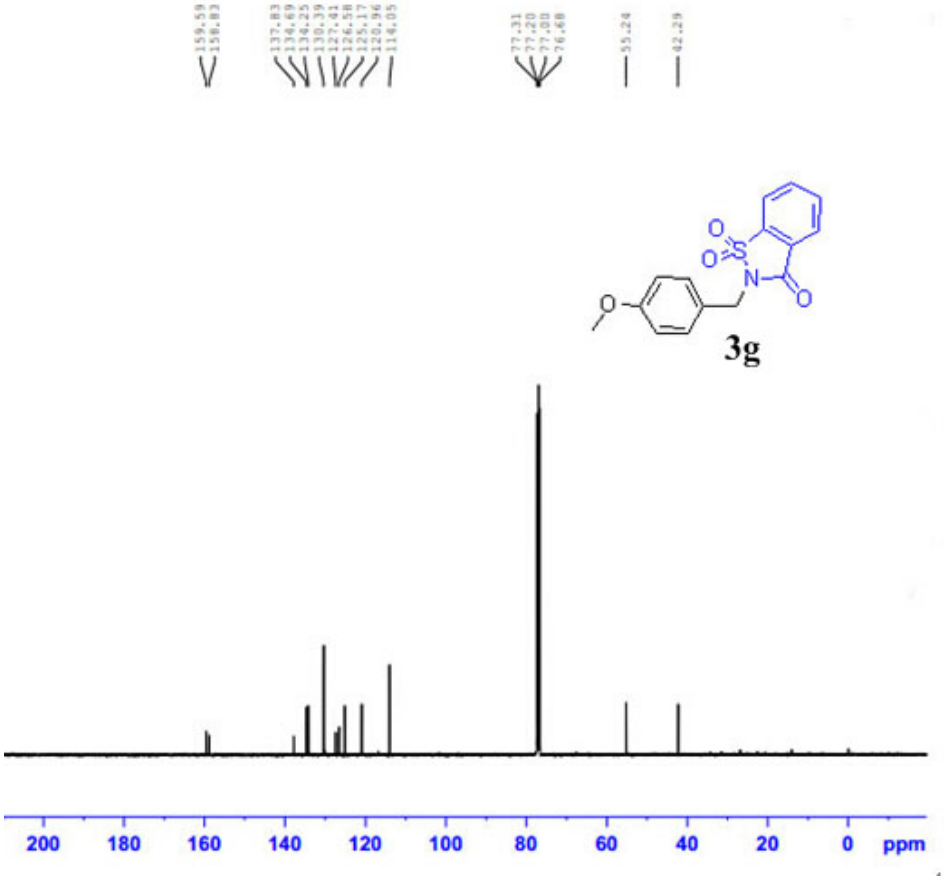
2.00
3.00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42.29
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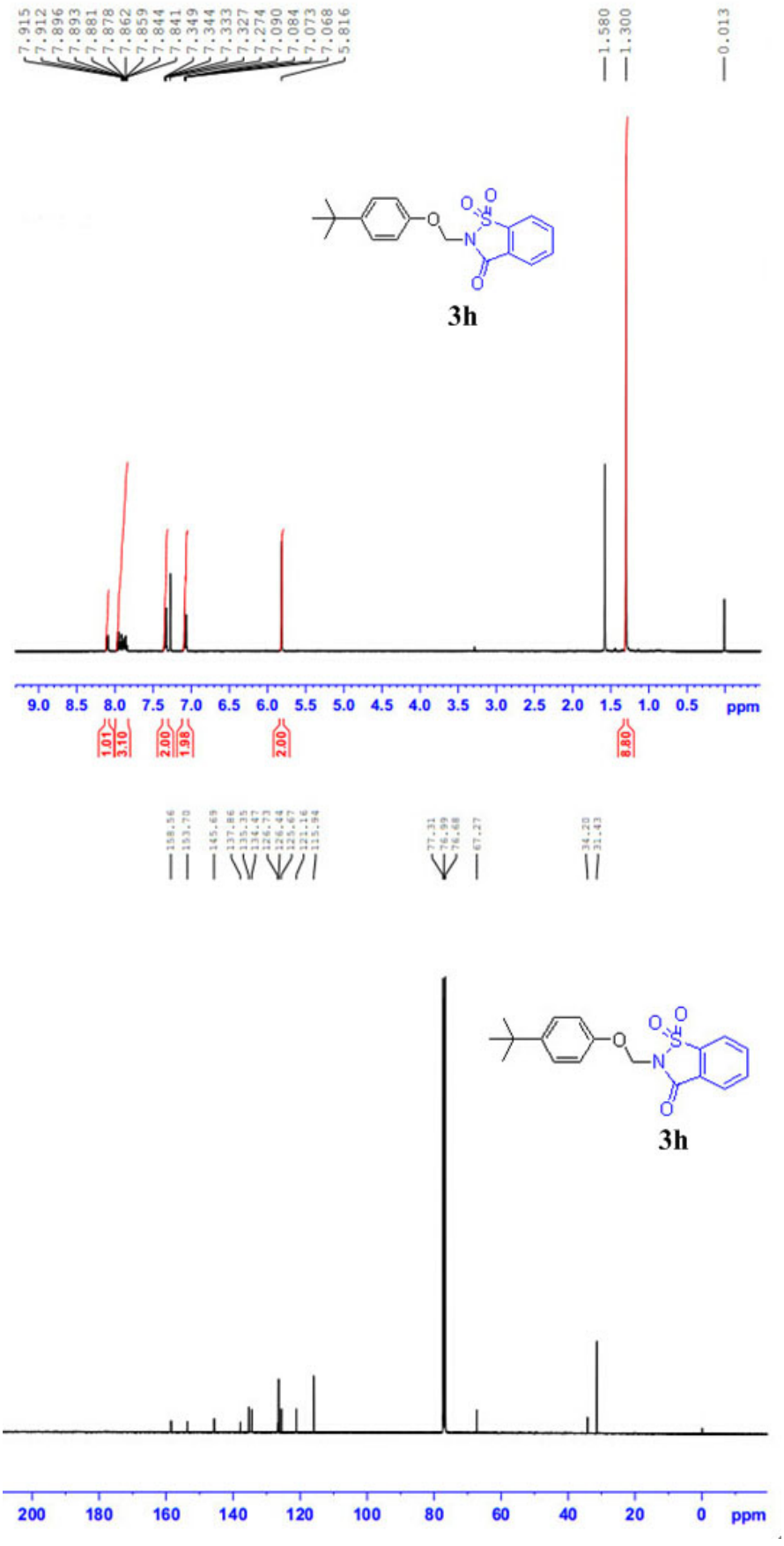
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7.333
7.327
7.274
7.090
7.084
7.073
7.068
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1.580
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0.013
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3.10
2.00
1.98
2.00
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145.69
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135.35
134.47
126.73
126.44
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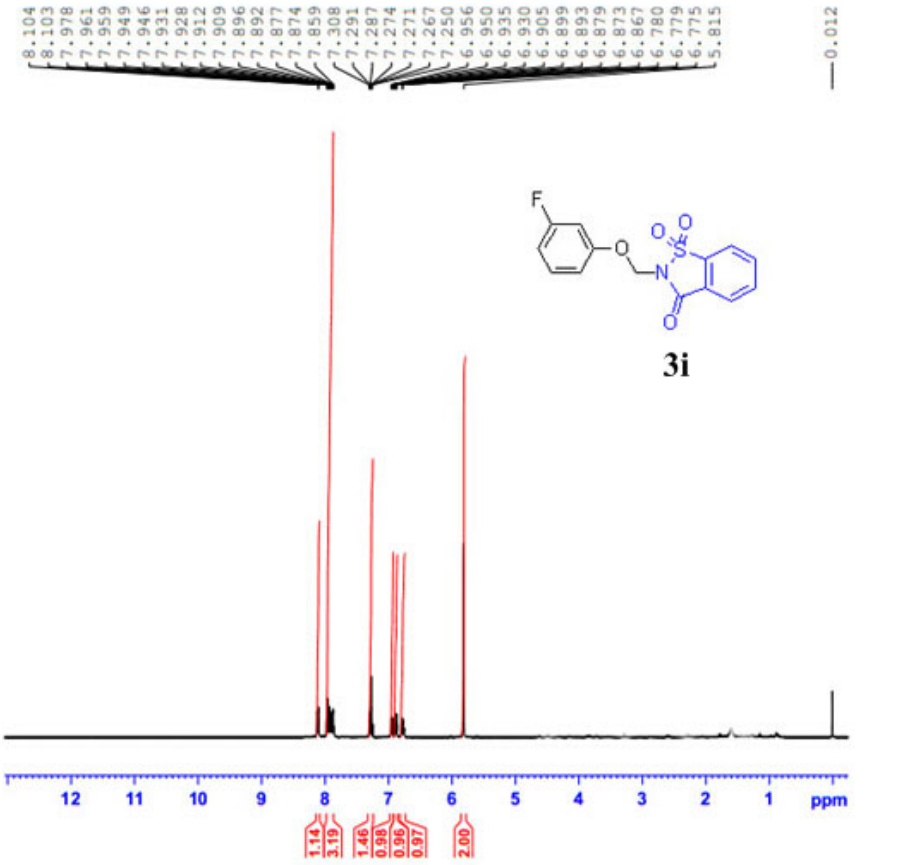
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6.930
6.905
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6.873
6.867
6.780
6.779
6.775
5.815
0.012
F
O
O
O
S
N
O
12
11
10
9
8
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2
1
ppm
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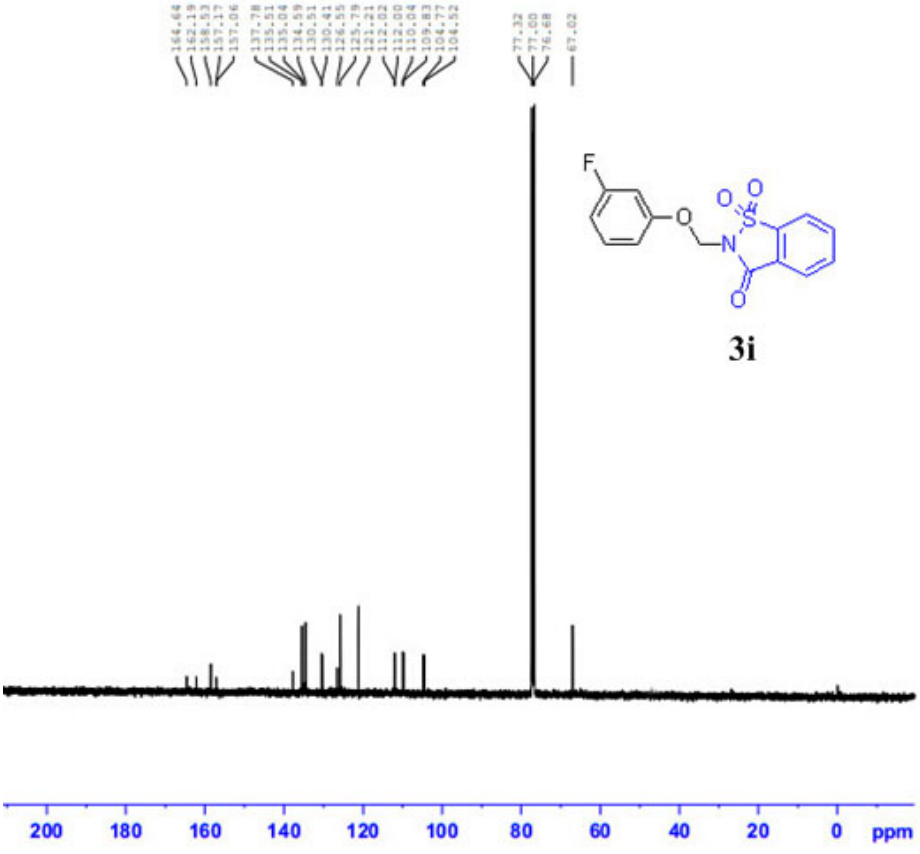
3i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130.41
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125.79
121.21
112.02
112.00
110.04
109.83
104.77
104.52
77.32
77.00
76.68
67.02
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S
N
O
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140
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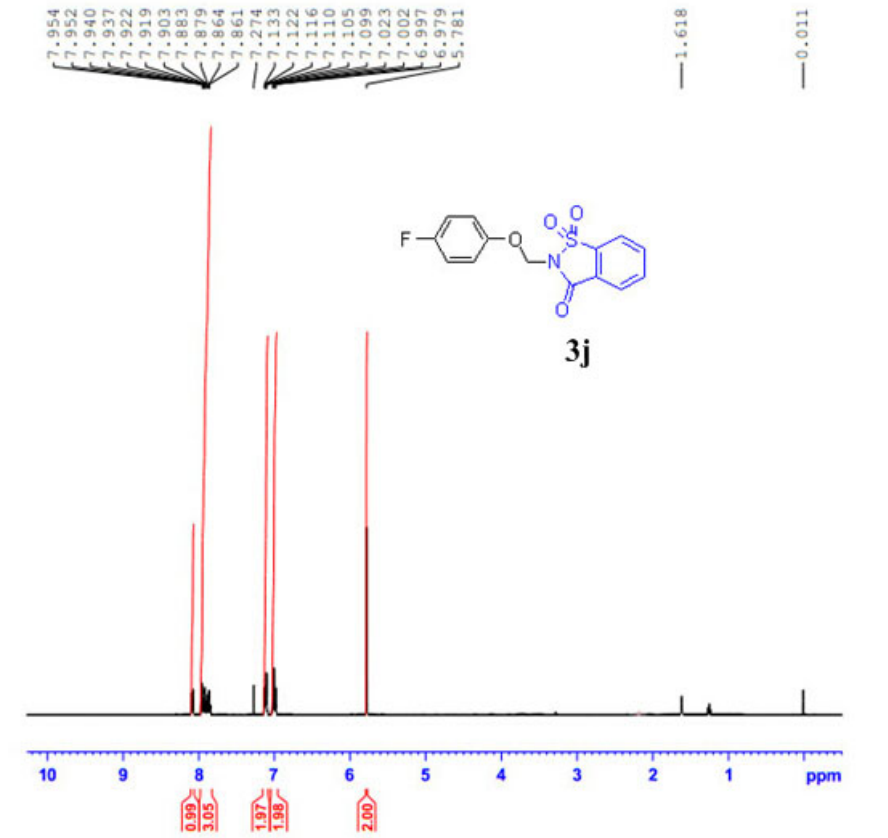
100
80
60
40
20
0
ppm

3i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7.122
7.116
7.110
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7.023
7.002
6.997
6.979
5.781
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0.011
F
O
S
N
O
O
O
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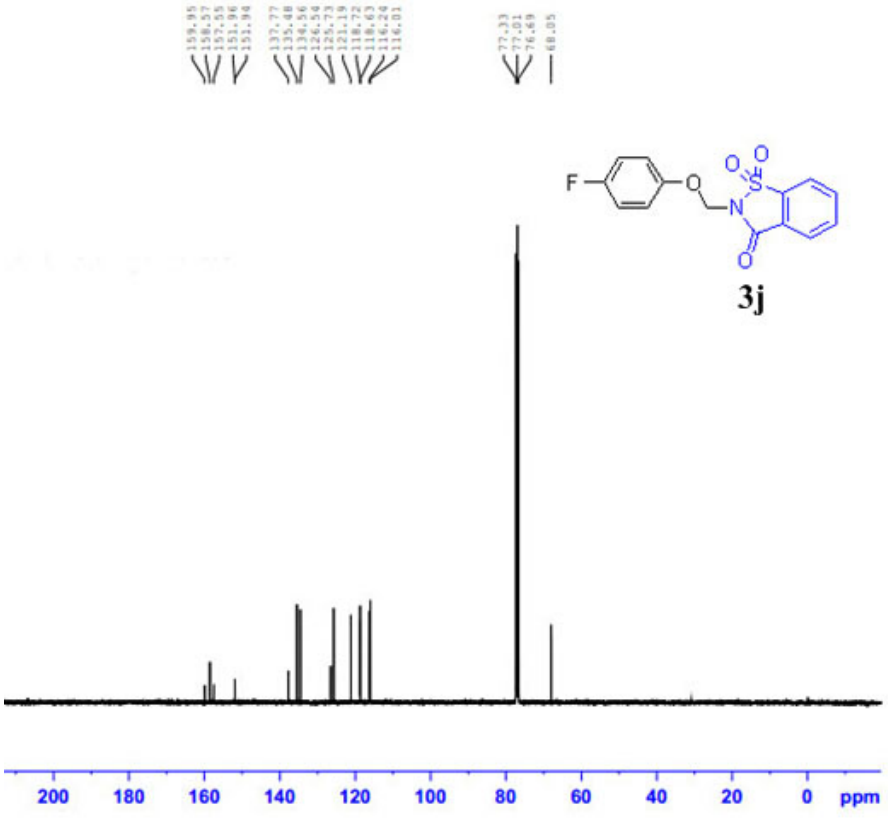
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134.56
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77.01
76.69
68.05
F
O
S
N
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O
O
3j
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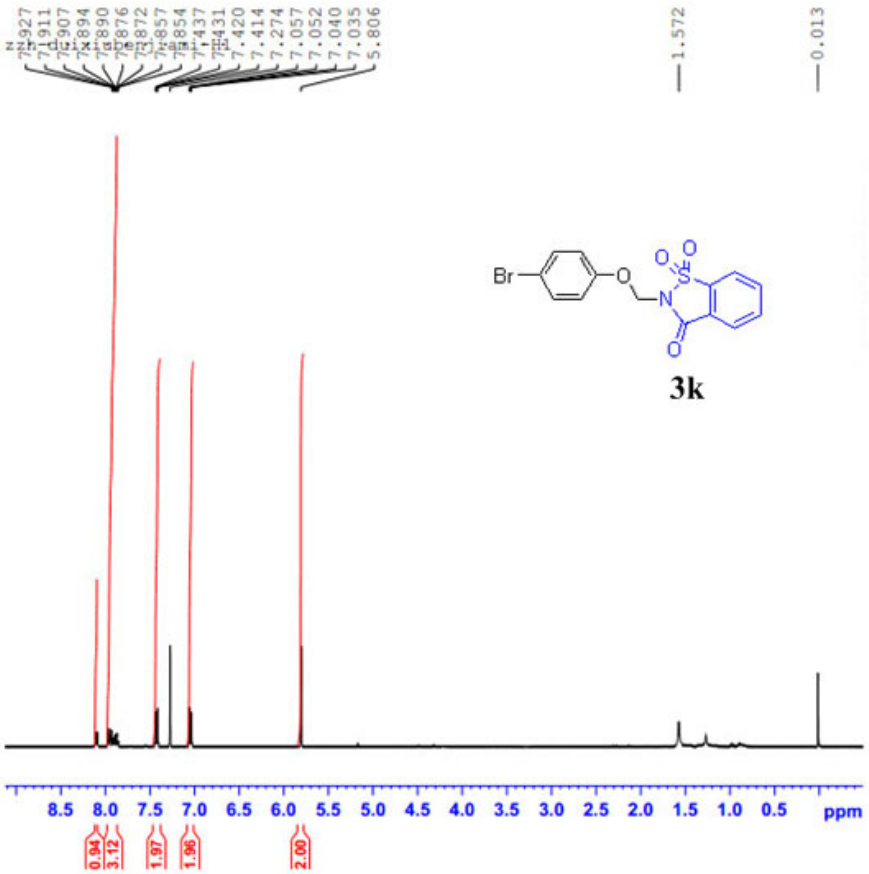
140
120
100
80
60
40
20
0
ppm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7.057
7.052
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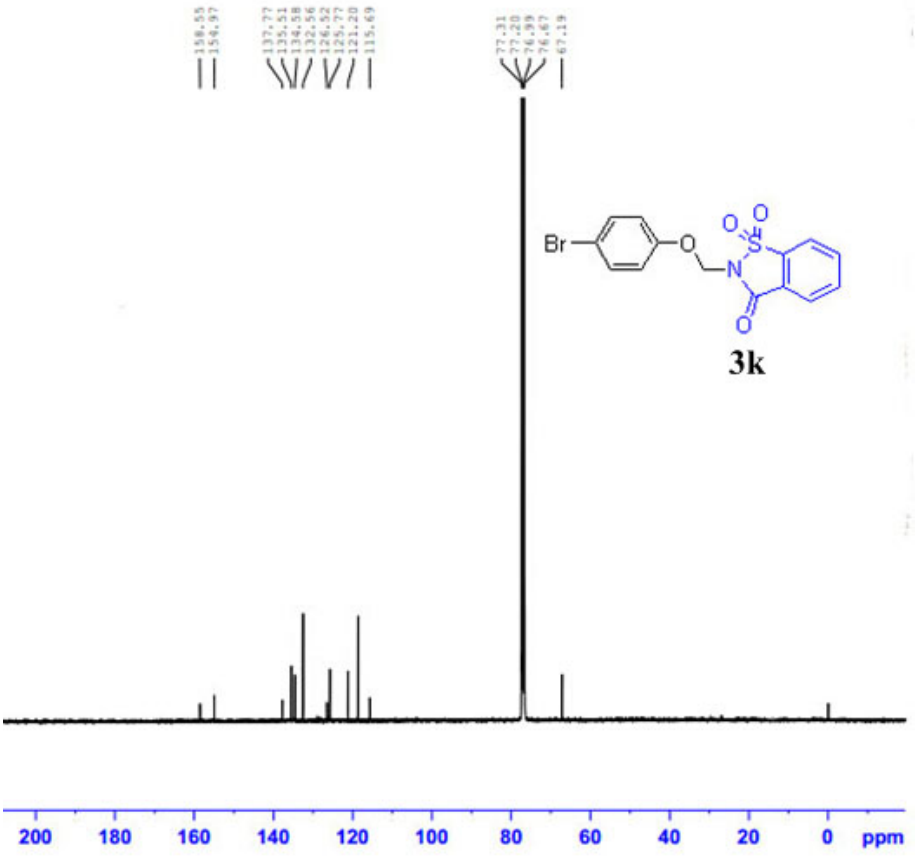
5.806
1.572
0.013
Br
O
O
O
Se
N
O
3k
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.94
3.12
1.97
1.96
2.00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121.20
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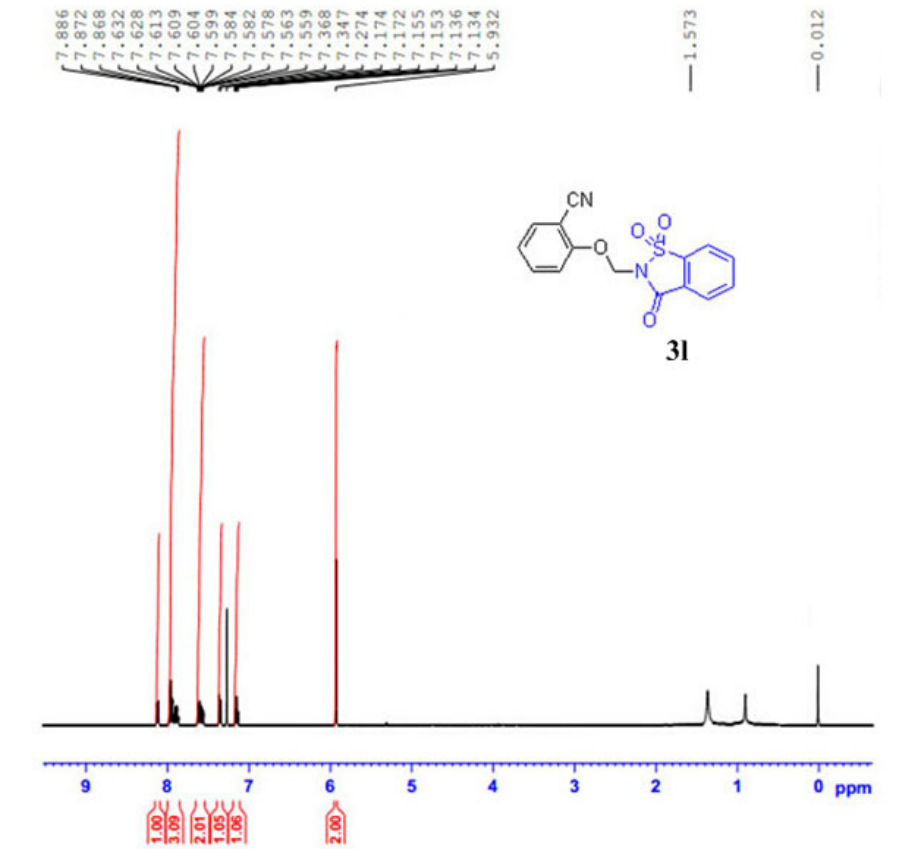
76.67
67.19
Br
O
O
O
Se
N
O
3k
200 180 160 140 120 100 80 60 40 20 0 ppm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7.559
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7.274
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7.172
7.155
7.153
7.136
7.134
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1.573
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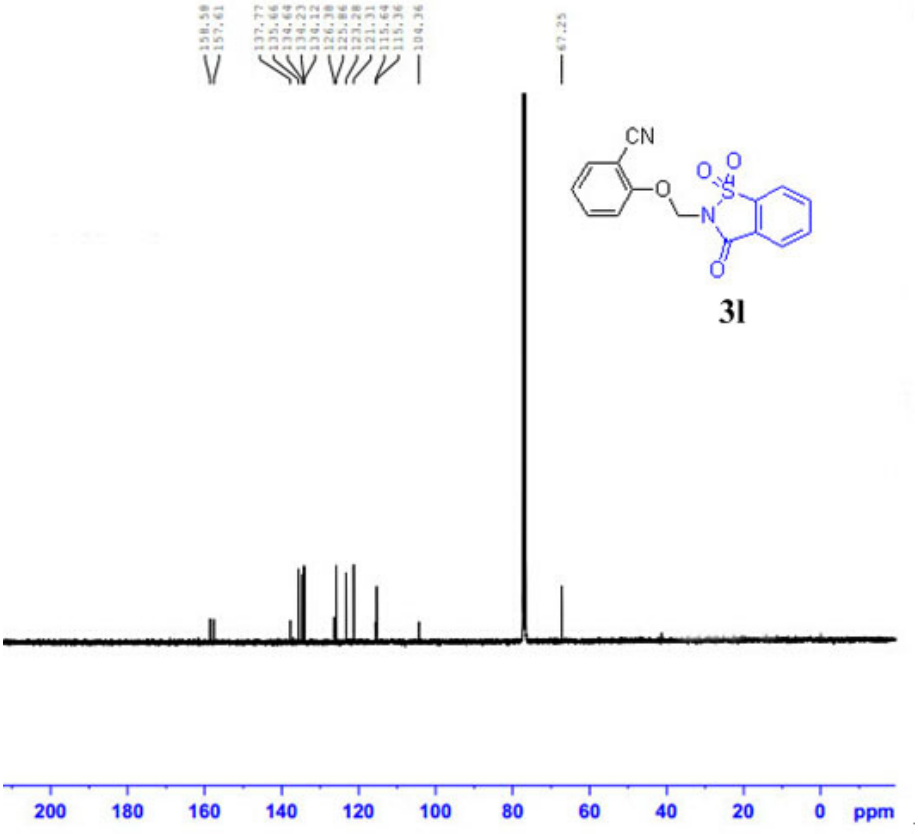
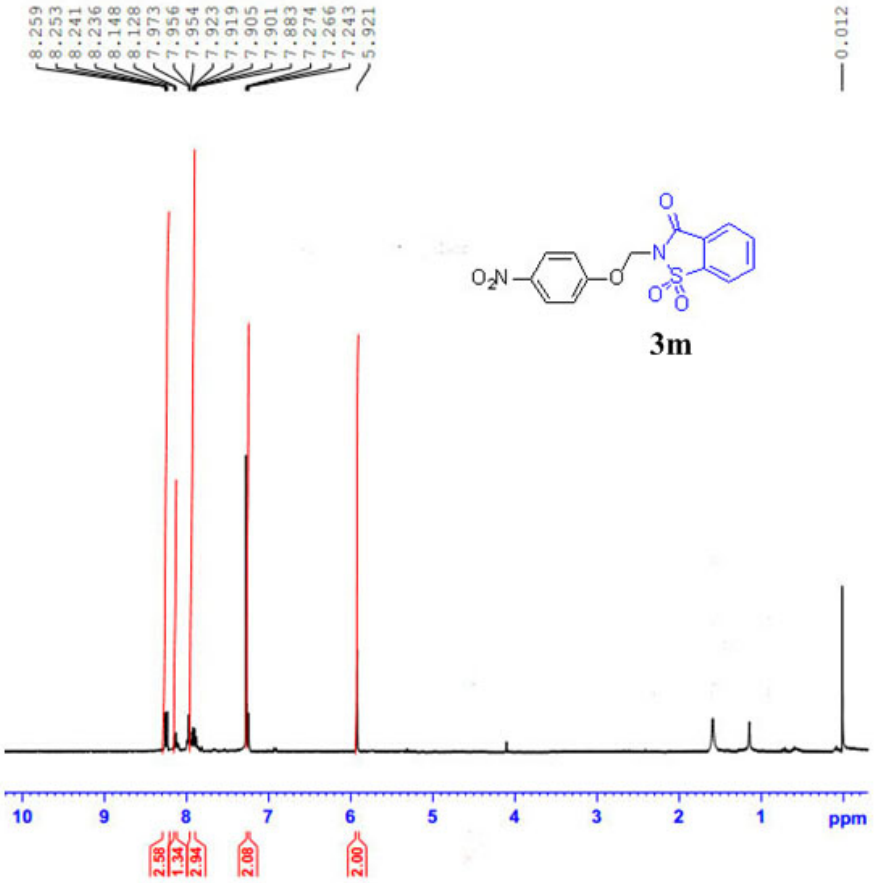
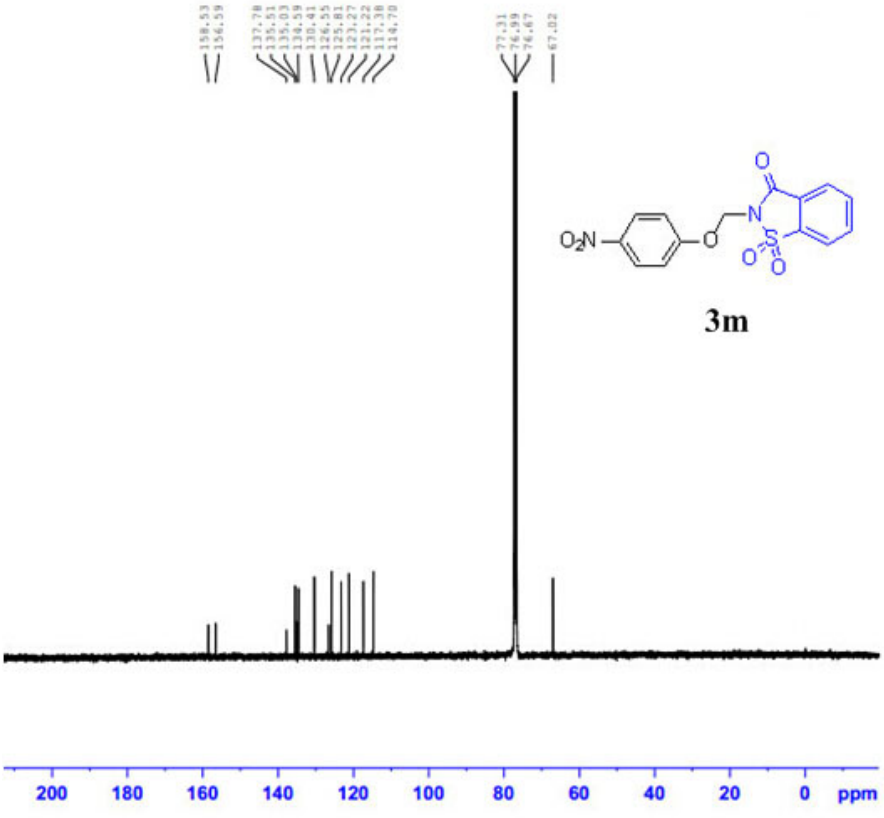
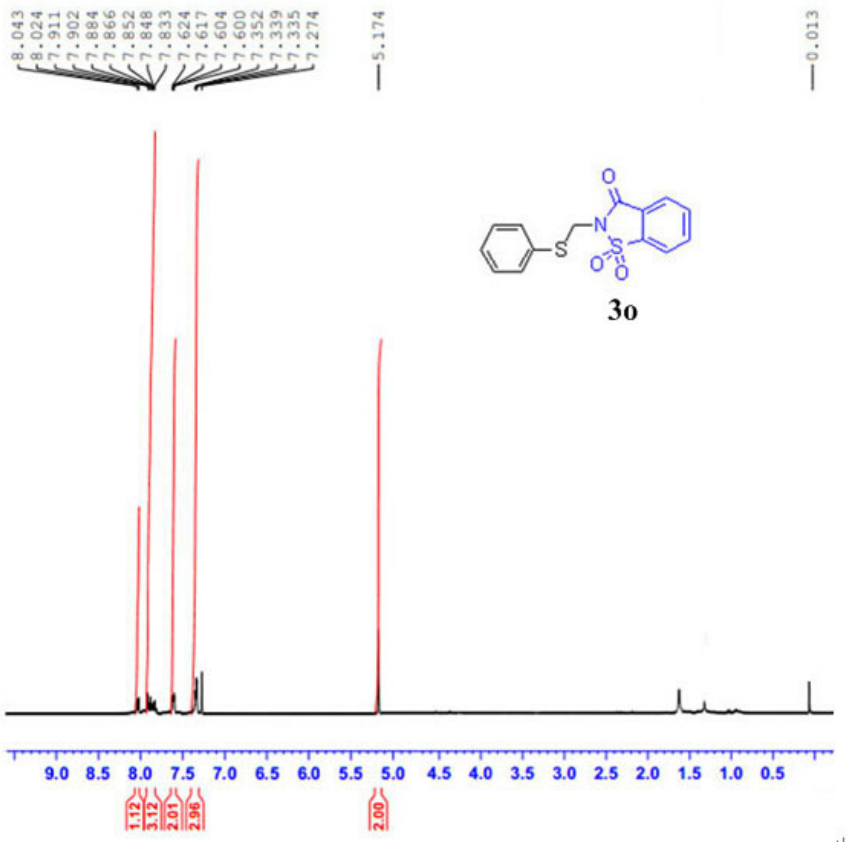
CN
O
S
N
O
O
O
3l
9
8
7
6
5
4
3
2
1
0 ppm
1.00
3.09
2.01
1.05
1.06
2.00

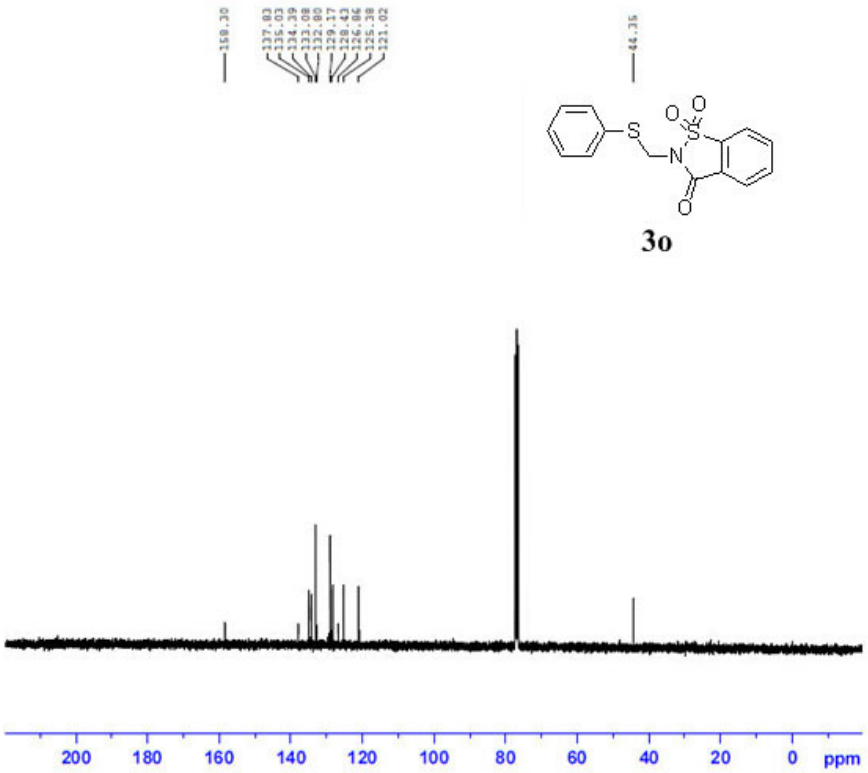

168.58
157.61
137.77
135.66
134.64
134.23
134.12
126.30
125.86
123.28
121.31
115.64
115.36
104.36
67.25
CN
O
S
N
O
O
O
3l
200
180
160
140
120
100
80
60
40
20
0 ppm


8.259
8.253
8.241
8.236
8.148
8.128
7.973
7.956
7.954
7.923
7.919
7.905
7.901
7.883
7.274
7.266
7.243
5.921
0.012
3m
10
9
8
7
6
5
4
3
2
1
ppm
2.58
1.34
2.94
2.08
2.00

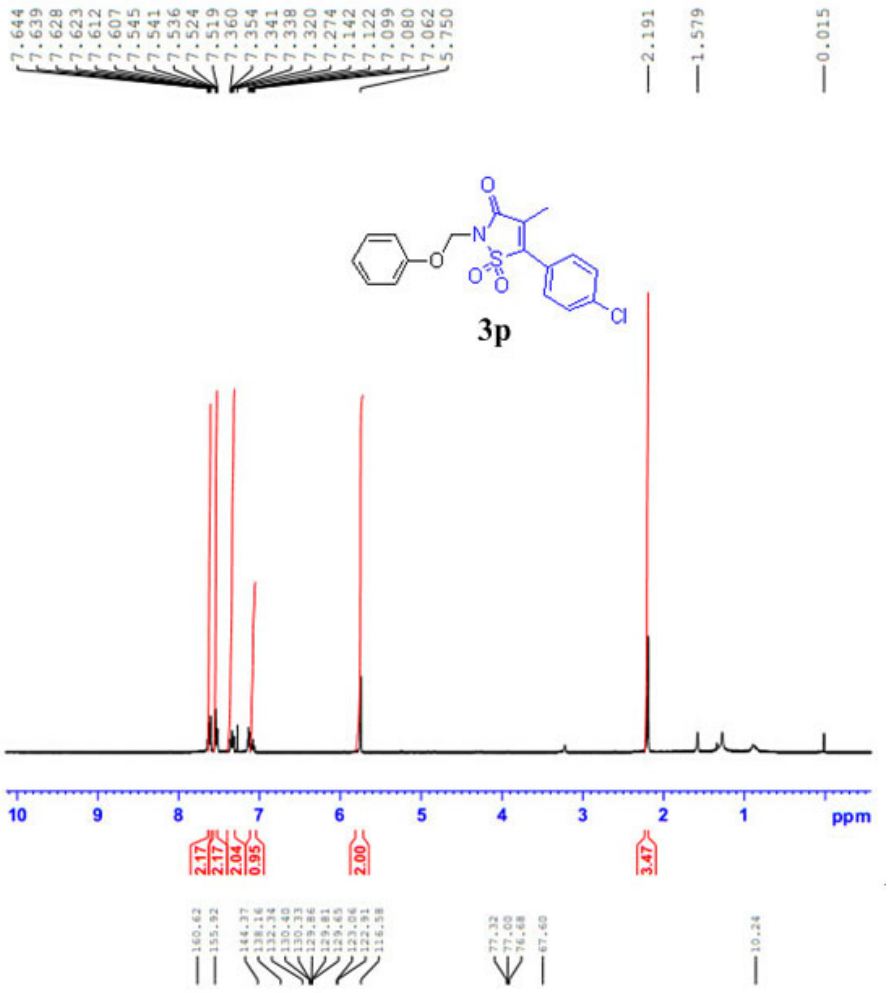

158.53
156.59
137.78
135.51
135.03
134.59
130.41
126.55
125.81
123.27
121.22
117.38
114.70
77.31
76.99
76.67
67.02
3m
200
180
160
140
120
100
80
60
40
20
0
ppm

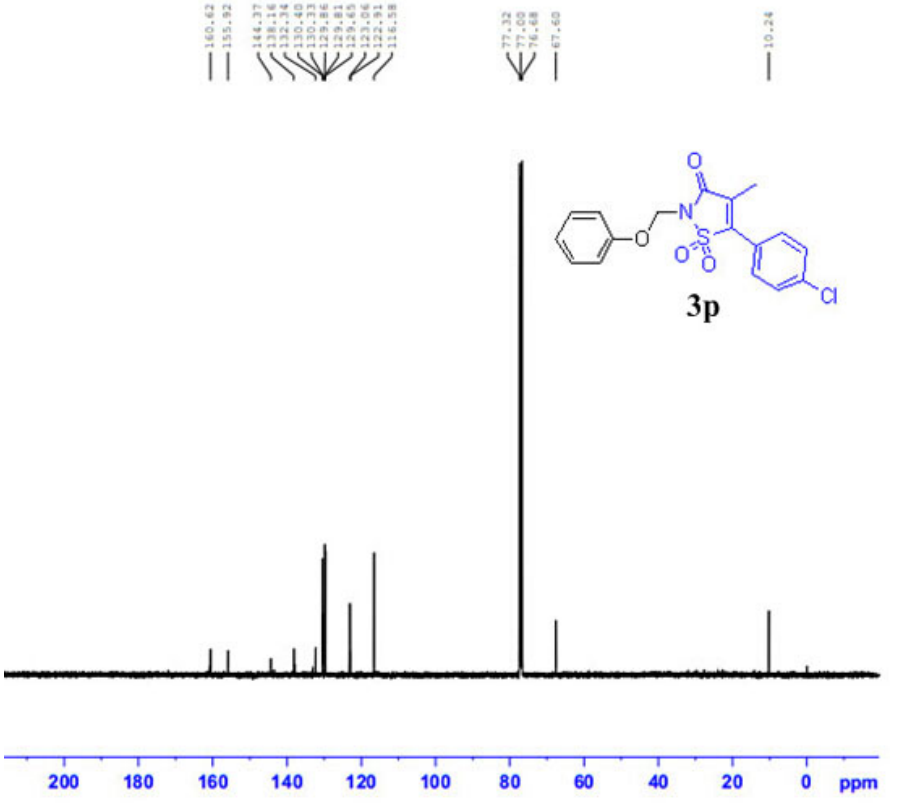

8.043
8.024
7.911
7.902
7.884
7.866
7.852
7.848
7.833
7.624
7.617
7.604
7.600
7.352
7.339
7.335
7.274
5.174
0.013
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
1.12
3.12
2.01
2.96
2.00

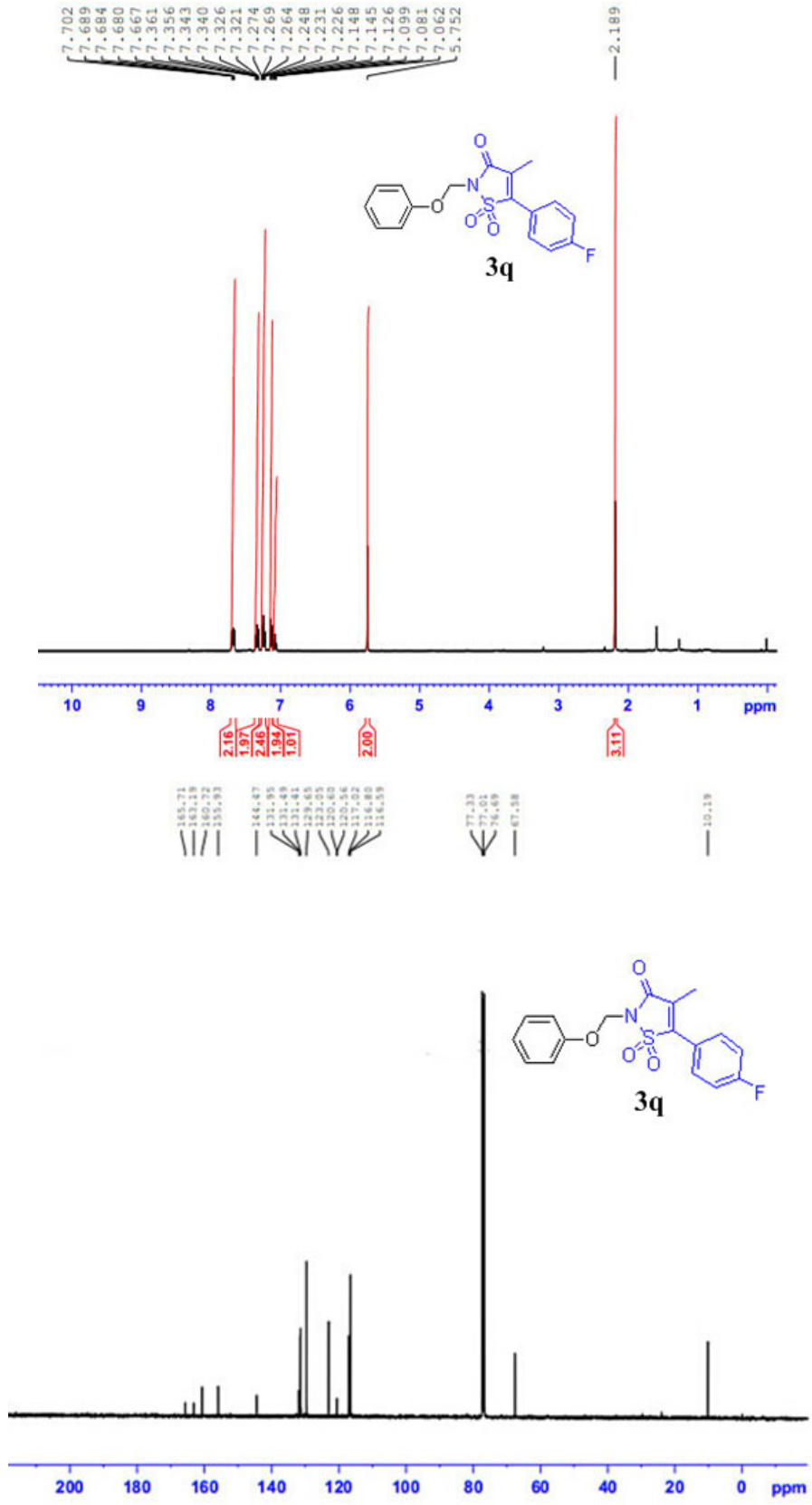
3o

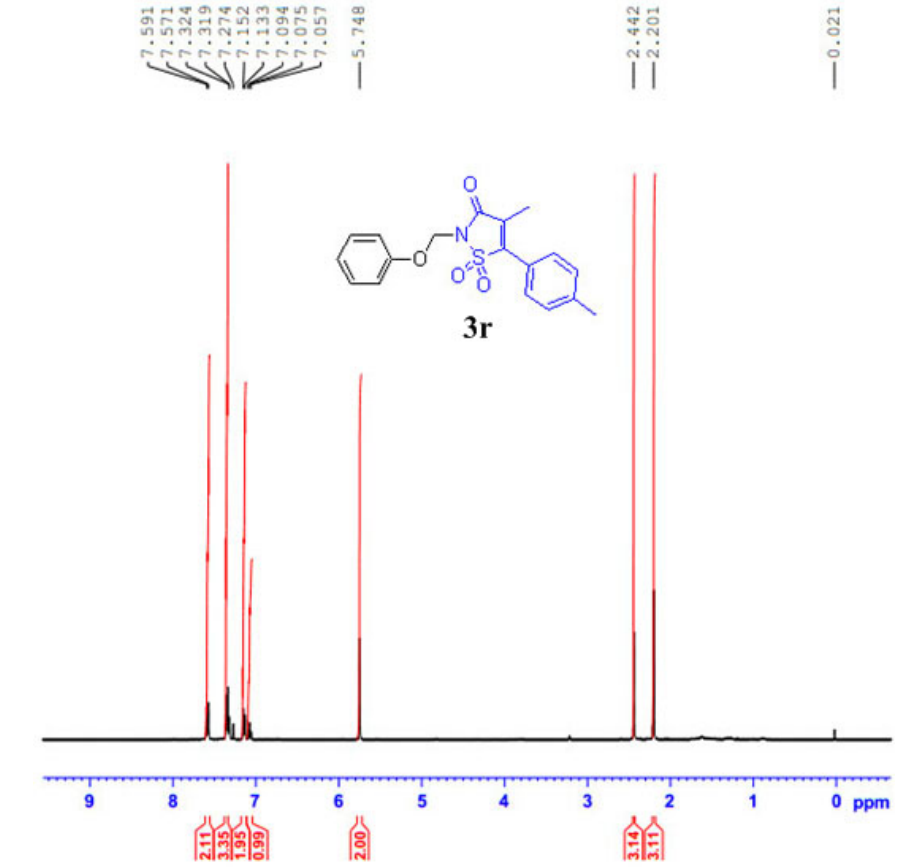

160.30
137.03
135.03
134.39
133.08
132.80
129.17
128.43
126.86
125.38
121.02
44.35
200 180 160 140 120 100 80 60 40 20 0 ppm

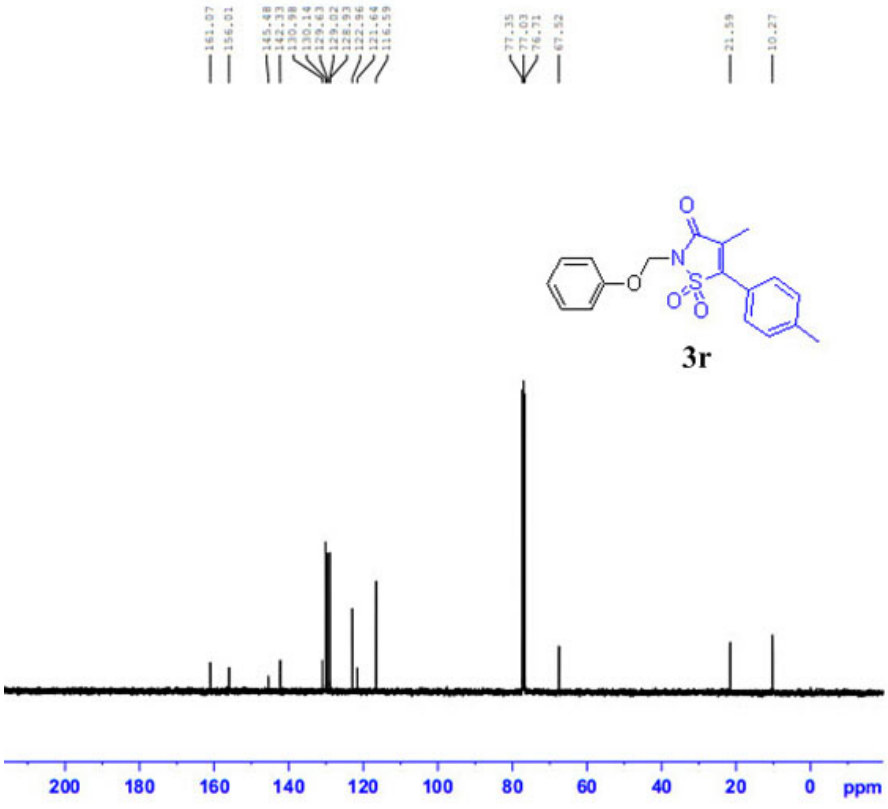
3o

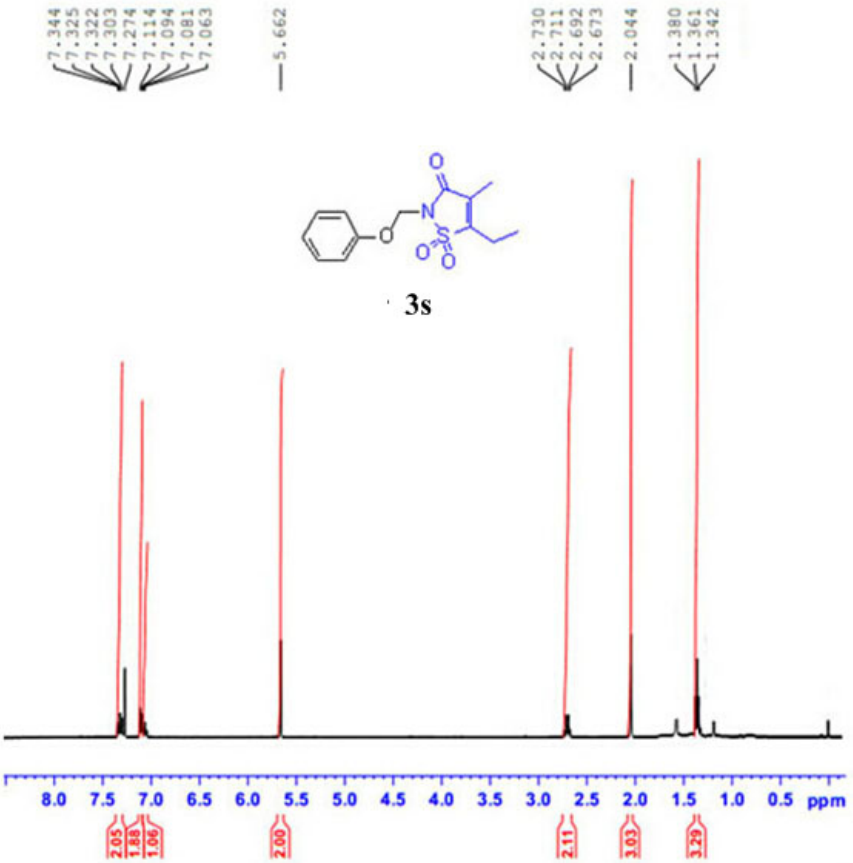

7.644
7.639
7.628
7.623
7.612
7.607
7.545
7.541
7.536
7.524
7.519
7.360
7.354
7.341
7.338
7.320
7.274
7.142
7.122
7.099
7.080
7.062
5.750
2.191
1.579
0.015
3p
10
9
8
7
6
5
4
3
2
1
ppm
2.17
2.17
2.04
0.95
2.00
3.47

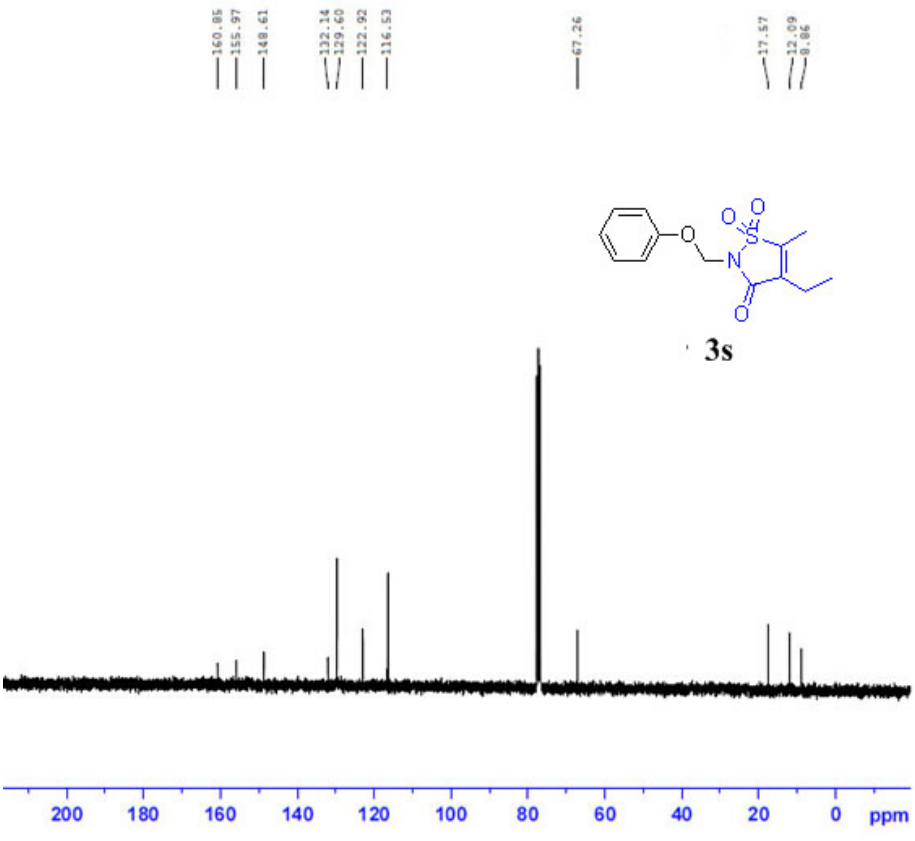

160.62
155.92
144.37
138.16
132.34
130.40
130.23
129.86
129.81
129.45
123.06
122.91
116.58
77.32
77.00
76.68
67.60
10.24
3p
200
180
160
140
120
100
80
60
40
20
0
ppm

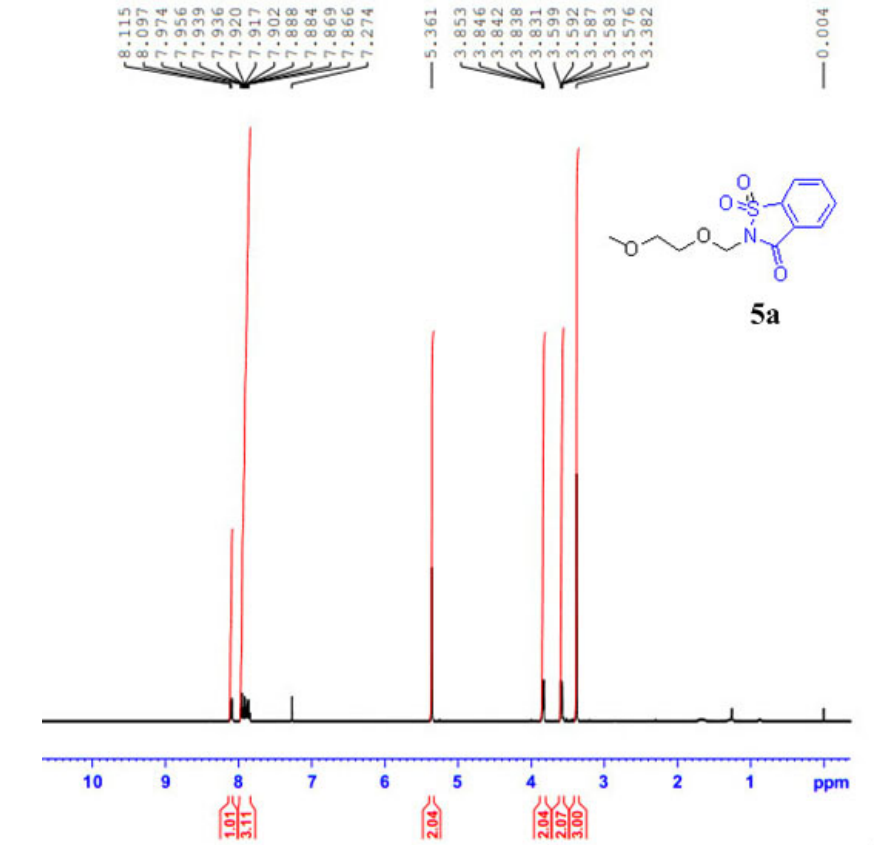

7.702
7.689
7.684
7.680
7.667
7.361
7.356
7.343
7.340
7.326
7.321
7.274
7.269
7.264
7.248
7.231
7.226
7.148
7.145
7.126
7.099
7.081
7.062
5.752
2.189
3q
10 9 8 7 6 5 4 3 2 1 ppm
2.16 1.97 2.46 1.94 1.01 2.00 3.11
165.71
163.19
160.72
155.93
146.47
131.95
131.89
131.41
129.65
123.05
120.60
120.56
117.72
116.80
116.59
77.33
77.01
76.69
67.38
10.19
3q
200 180 160 140 120 100 80 60 40 20 0 ppm


7.591
7.571
7.324
7.319
7.274
7.152
7.133
7.094
7.075
7.057
5.748
2.442
2.201
0.021
3r
9
8
7
6
5
4
3
2
1
0 ppm
2.11
3.35
1.95
0.99
2.00
3.14
3.11

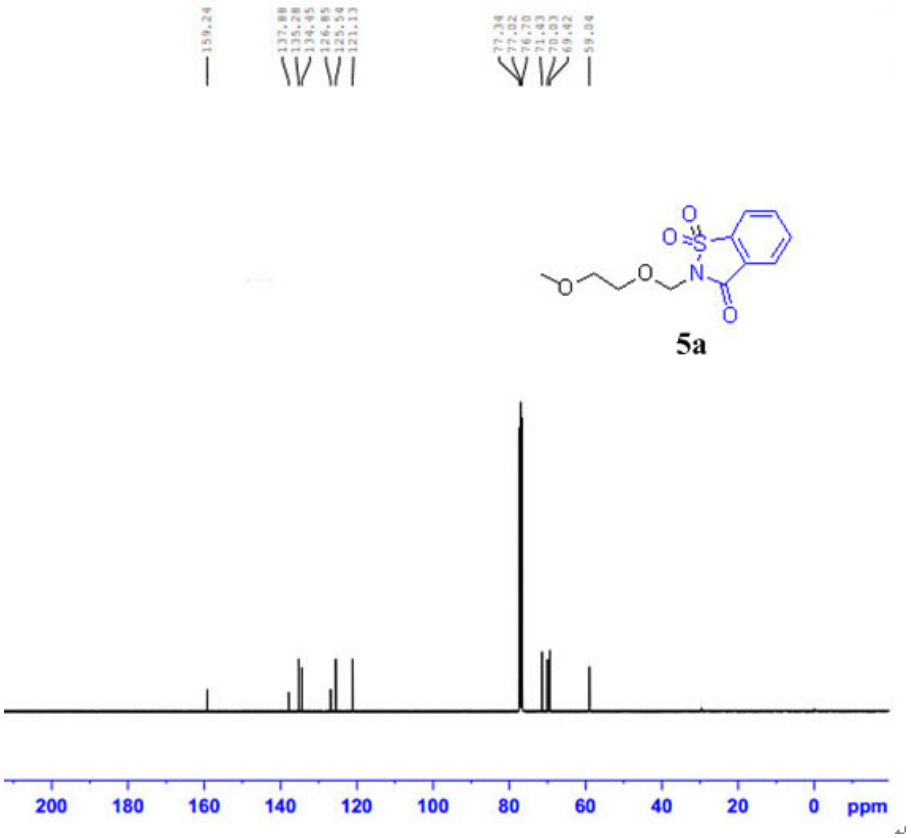

161.07
156.01
145.48
142.33
130.98
130.14
129.63
129.02
128.93
122.26
121.64
116.59
77.35
77.03
76.71
67.52
21.59
10.27
3r
200
180
160
140
120
100
80
60
40
20
0 ppm


7.344
7.325
7.322
7.303
7.274
7.114
7.094
7.081
7.063
5.662
2.730
2.711
2.692
2.673
2.044
1.380
1.361
1.342
3s
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 ppm
2.05
1.88
1.06
2.00
2.11
3.03
3.29

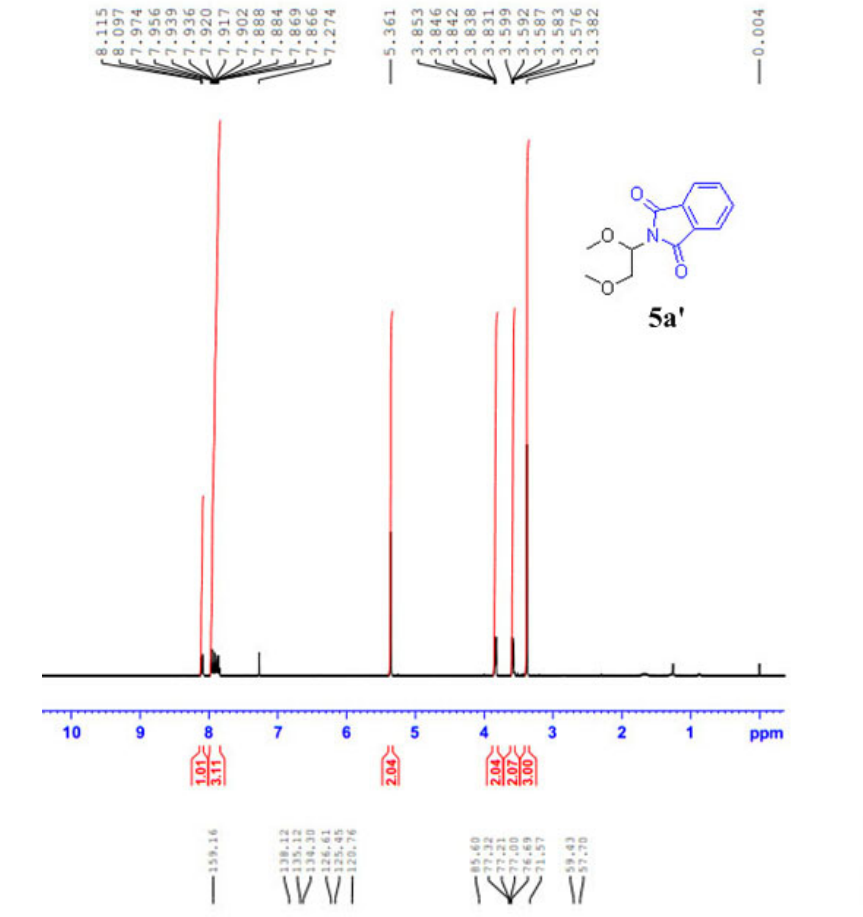

160.85
155.97
148.61
132.14
129.60
122.92
116.53
67.26
17.57
12.09
8.86
3s
200 180 160 140 120 100 80 60 40 20 0 ppm

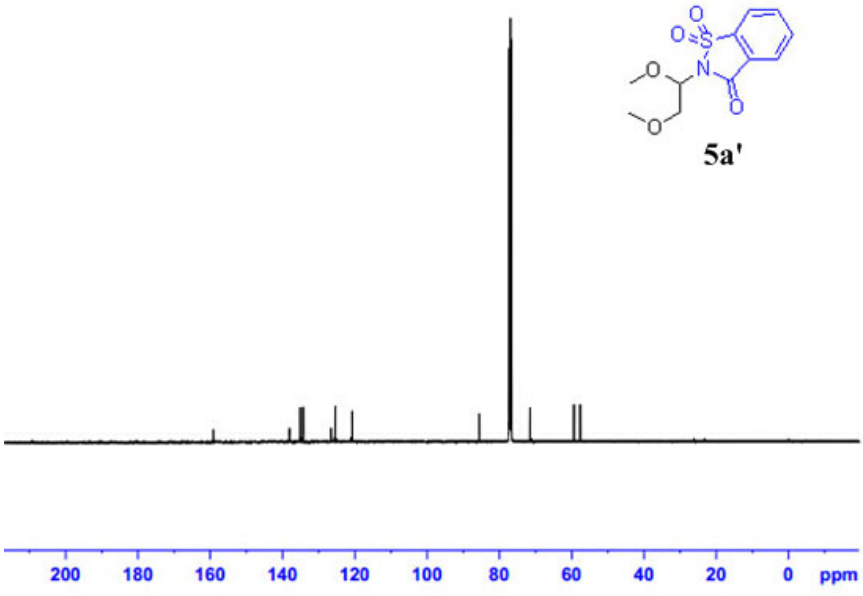

8.115
8.097
7.974
7.956
7.939
7.936
7.920
7.917
7.902
7.888
7.884
7.869
7.866
7.274
5.361
3.853
3.846
3.842
3.838
3.831
3.599
3.592
3.587
3.583
3.576
3.382
0.004
10
9
8
7
6
5
4
3
2
1
ppm
1.01
3.11
2.04
2.04
2.07
3.00

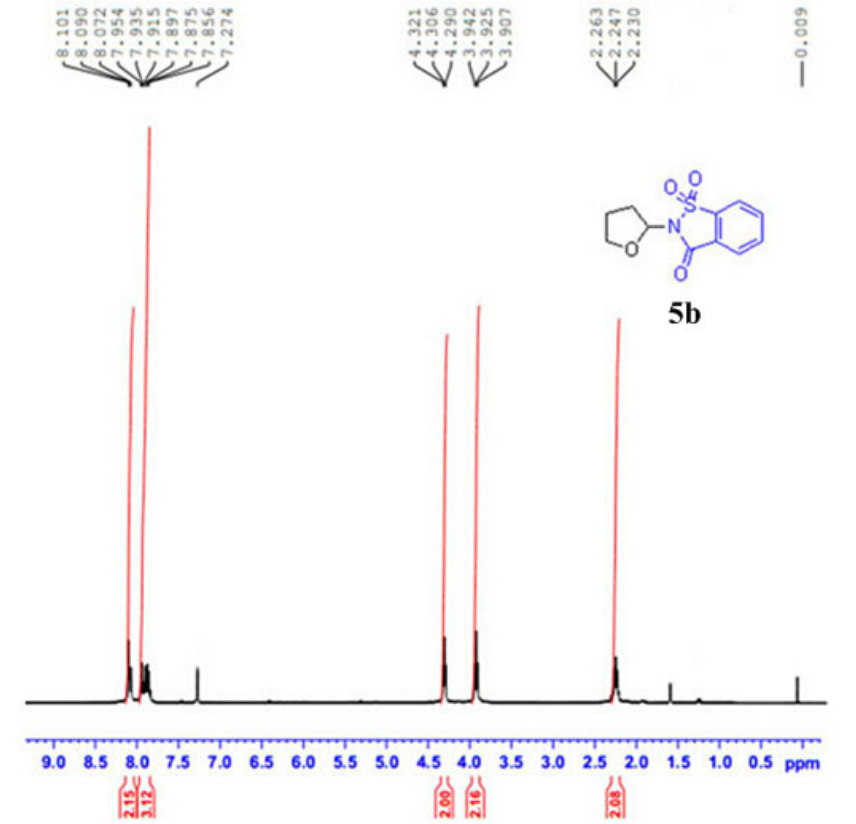
5a

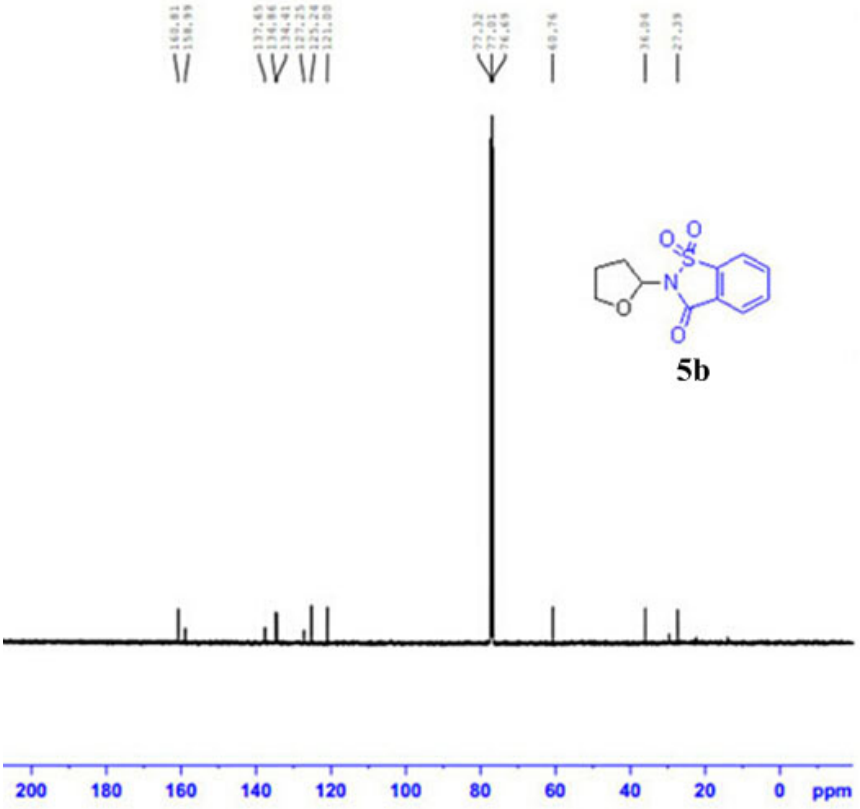

159.24
137.88
135.28
134.45
126.85
125.54
121.13
77.34
77.02
76.70
71.43
70.03
69.42
59.04
200
180
160
140
120
100
80
60
40
20
0
ppm

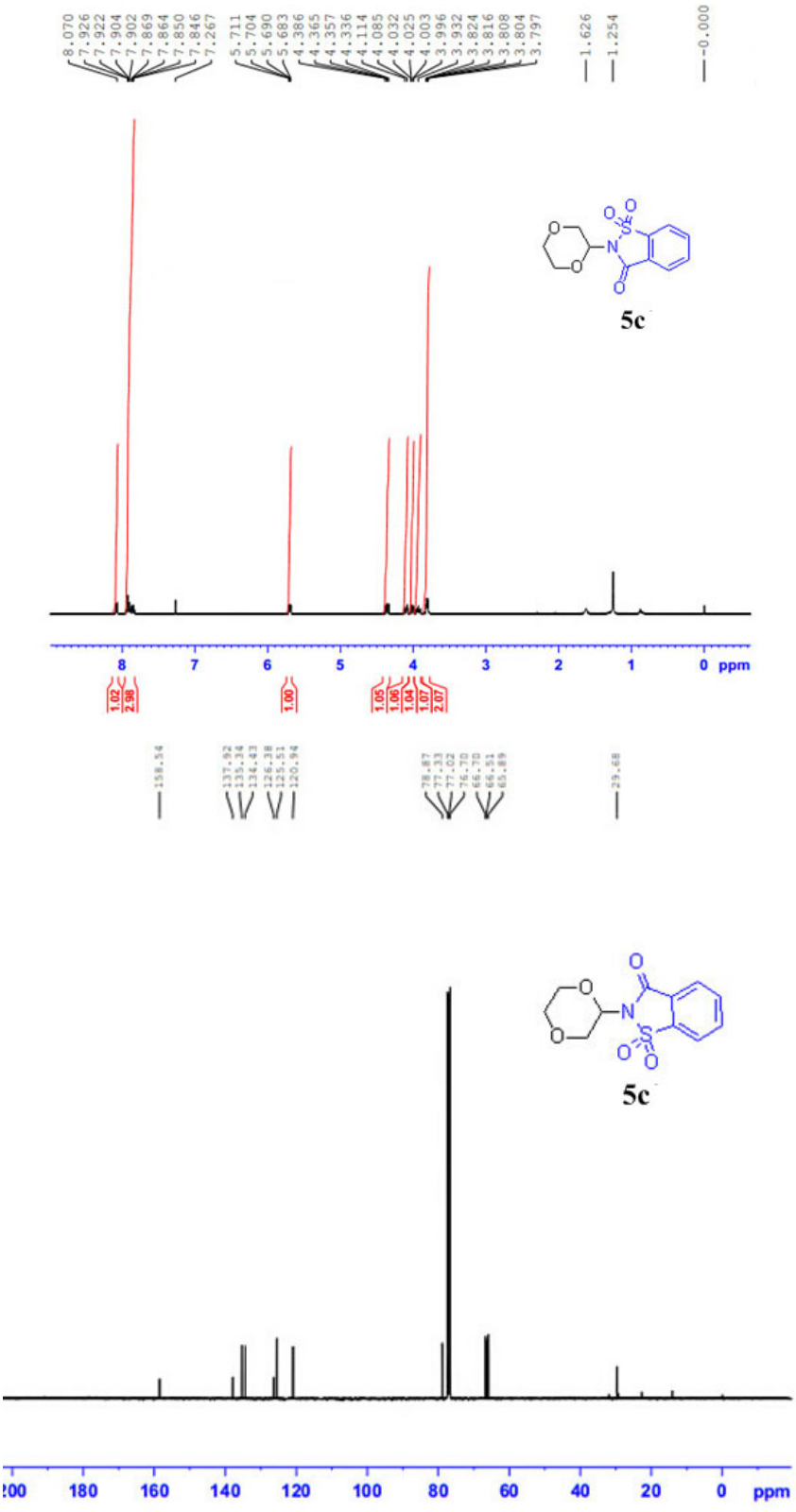
5a


8.115
8.097
7.974
7.956
7.939
7.936
7.920
7.917
7.902
7.888
7.884
7.869
7.866
7.274
5.361
3.853
3.846
3.842
3.838
3.831
3.599
3.592
3.587
3.583
3.576
3.382
0.004
5a'
10
9
8
7
6
5
4
3
2
1
ppm
1.01
3.11
2.04
2.04
2.02
3.00


159.16
138.12
135.12
134.30
126.61
125.45
120.76
85.60
77.32
77.21
77.00
76.69
71.57
59.43
57.70
5a'
200
180
160
140
120
100
80
60
40
20
0
ppm


8.101
8.090
8.072
7.954
7.935
7.915
7.897
7.875
7.856
7.274
4.321
4.306
4.290
3.942
3.925
3.907
2.263
2.247
2.230
0.009
5b
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 ppm
2.15
3.12
2.00
2.16
2.08


160.81
158.99
137.45
134.86
134.41
127.25
125.24
121.00
77.32
77.01
76.69
68.76
36.04
27.39
5b
200 180 160 140 120 100 80 60 40 20 0 ppm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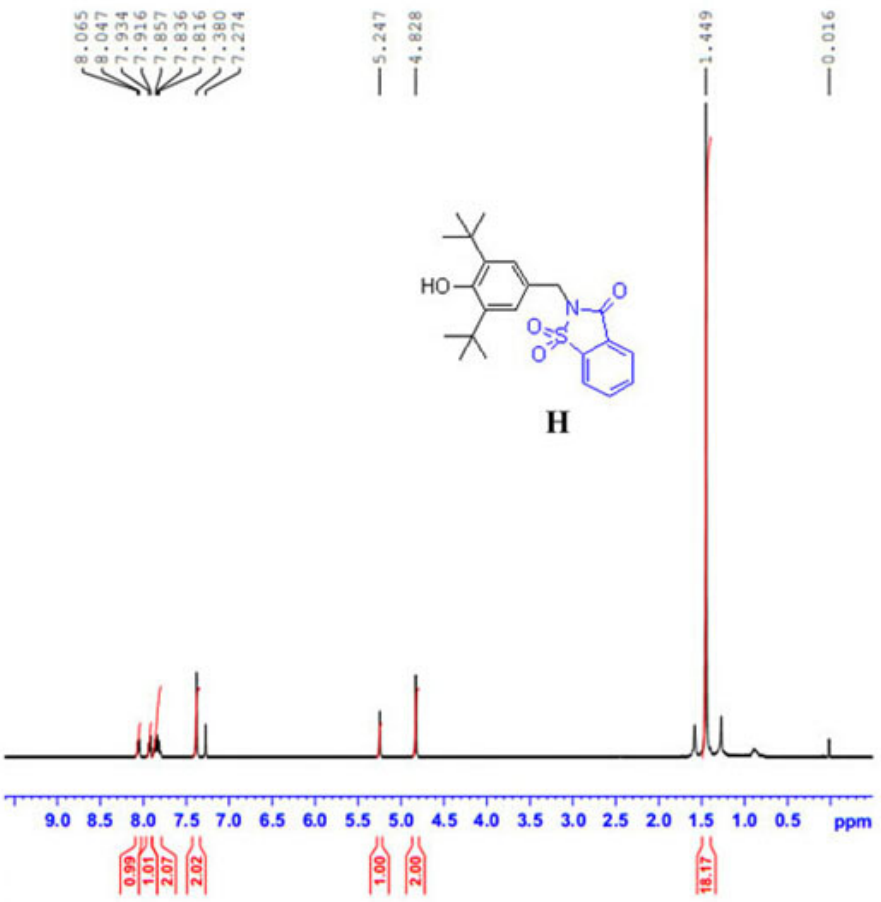
7.926
7.922
7.904
7.902
7.869
7.864
7.850
7.846
7.267
5.711
5.704
5.690
5.683
4.386
4.365
4.357
4.336
4.114
4.085
4.032
4.025
4.003
3.996
3.932
3.824
3.816
3.808
3.804
3.797
1.626
1.254
0.000
5c
8
7
6
5
4
3
2
1
0 ppm
1.02
2.98
1.00
1.05
1.06
1.04
1.07
2.07
158.54
137.92
135.34
134.43
126.38
125.51
120.94
78.87
77.33
77.02
76.70
66.51
65.89
29.68
5c
200
180
160
140
120
100
80
60
40
20
0 ppm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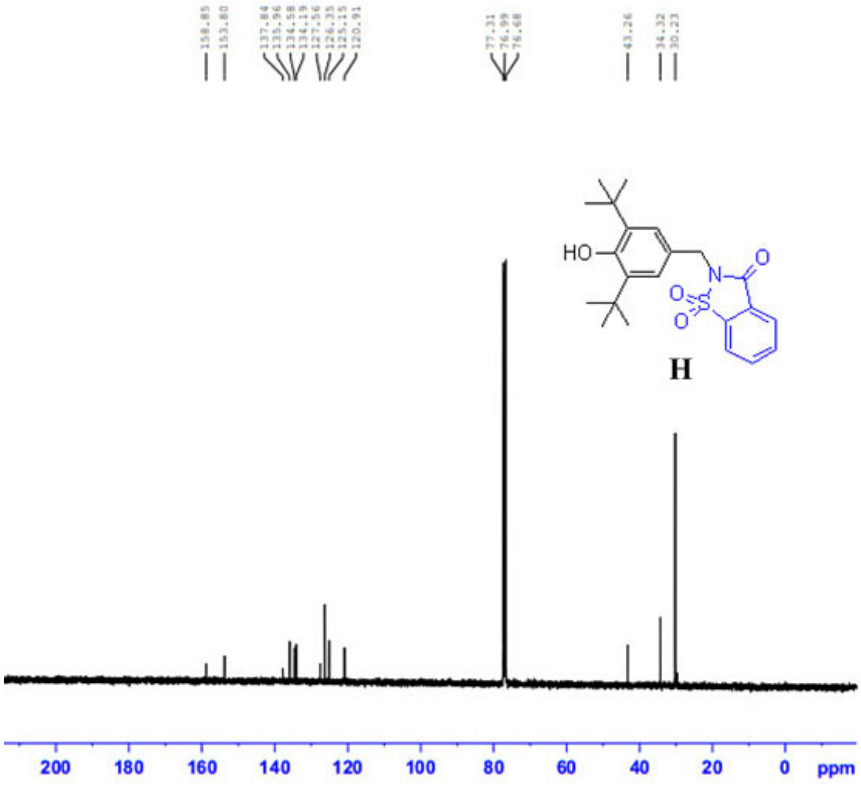
8.047
7.934
7.916
7.857
7.836
7.816
7.380
7.274
5.247
4.828
1.449
0.016
HO
N
O
O
S
O
H
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.99
1.01
2.07
2.02
1.00
2.00
18.17


156.85
153.80
137.84
135.96
134.58
134.19
127.56
126.35
125.15
120.91
77.31
76.99
76.68
43.26
34.32
30.23

HO
N
O
O
S
O
H
200 180 160 140 120 100 80 60 40 20 0 ppm