Supporting Information

Oxidative C–S Bond Cleavage Reaction of DMSO for C–N and C–C Bond Formation: New Mannich-type Reaction for β-amino Ketones

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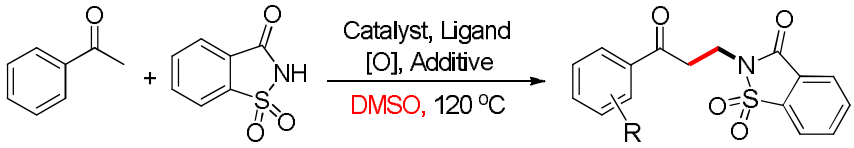
I. General Remarks:

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 25 ºC on a Bruker Ascend^{TM} 400 spectrometer (Germany), ^{13}C NMR spectra were recorded at 25 ºC 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. Optimization Study for Ruthenium catalyzed mannich reaction

Table 1: Screening of Reaction Conditions [a, b]

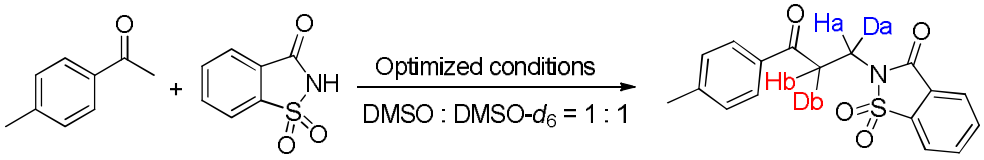


1a **2a**

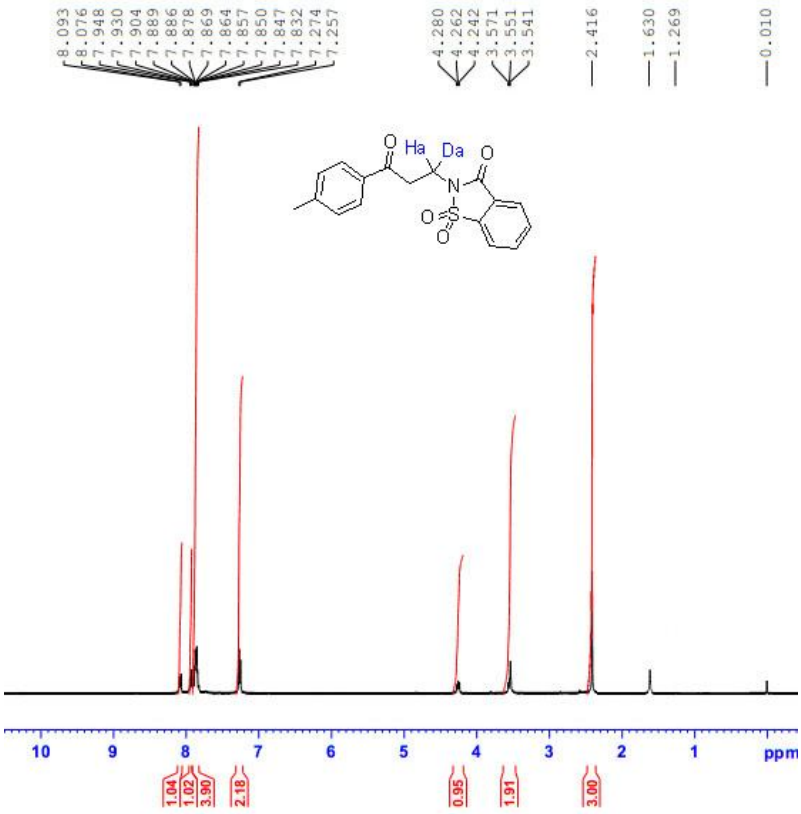
Entry	Catalyst	Ligand	Oxidant	Additive	Yield
1	$Cu(OTf)_2$	1,10-phen [c]	selectflour	Na_2CO_3	41
2	$Cu(OTf)_2$	2,2-bipyl [d]	selectflour	Na_2CO_3	38
3	$Cu(OTf)_2$	No	selectflour	Na_2CO_3	30
4	$Cu(OAc)_2$	1,10-phen	selectflour	Na_2CO_3	46
5	$CuSO_4$	1,10-phen	selectflour	Na_2CO_3	27
6	CuCl	1,10-phen	selectflour	Na_2CO_3	24
7	$Pd(OAc)_2$	1,10-phen	selectflour	Na_2CO_3	33
8	$FeCl_3$	1,10-phen	selectflour	Na_2CO_3	57
9	$FeCl_2$	1,10-phen	selectflour	Na_2CO_3	39
10	$AgNO_3$	1,10-phen	selectflour	Na_2CO_3	46
11	$RuCl_3$	1,10-phen	selectflour	Na_2CO_3	91
12	$RuCl_3$	1,10-phen	NFSI	Na_2CO_3	0
13	$RuCl_3$	1,10-phen	TBHP	Na_2CO_3	0
14	$RuCl_3$	1,10-phen	$K_2S_2O_8$	Na_2CO_3	0
15	$RuCl_3$	1,10-phen	O_2	Na_2CO_3	0
16	$RuCl_3$	1,10-phen	selectflour	CH_3COOH	86

[a] Raction conditions: **1a** (0.5 mmol), saccharin (1.0 mmol), $RuCl_3$ (5 mol%), 1,10-phen (0.025 mmol), selectflour (1.0 mmol), Na_2CO_3 (1.0 mmol) and DMSO (2 mL) at 120 °C for 3 h. [b] Yield of the isolated products. [c] 1,10-phen = 1,10-phenanthroline. [d] 2,2-bipyl = 2,2-bipyridine.

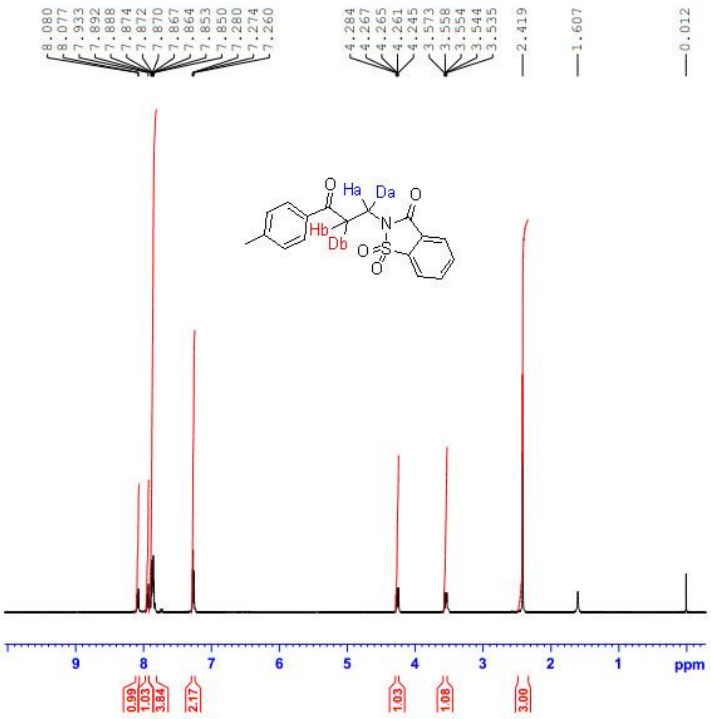
III. The KIE for reactions between 1d and saccharin.



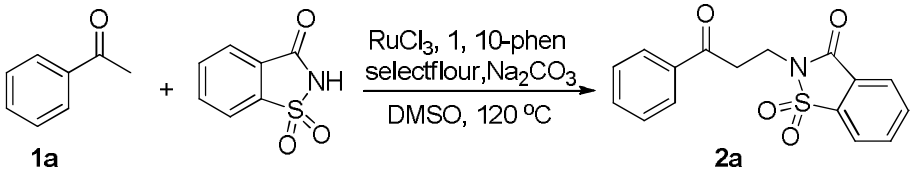
To a solution of 1-(*p*-tolyl)ethanone (**1d**) (67.0 mg, 0.5 mmol) in DMSO (1.0 mL) and DMSO-d_6 (1.0 mL) was added $RuCl_3$ (4.3 mg, 0.025 mmol), 1,10-phen (4.95 mg, 0.025 mmol), selectflour (354 mg, 1.0 mmol), Na_2CO_3 (108 mg, 1.0 mmol) and saccharin (183.2 mg, 1.0 mmol). The mixture was stirred at 120 ^oC for 0.5 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 flash column chromatography. The KIE value was determined by average of two runs and representative ^{1}HNMR spectrum was provided as follows:



To a solution of 1-(*p*-tolyl)ethanone (**1d**) (67.0 mg, 0.5 mmol) in DMSO (1.0 mL) and DMSO-d_6 (1.0 mL) was added $RuCl_3$ (4.3 mg, 0.025 mmol), 1,10-phen (4.95 mg, 0.025 mmol), selectflour (354 mg, 1.0 mmol), Na_2CO_3 (108 mg, 1.0 mmol) and saccharin (183.2 mg, 1.0 mmol). The mixture was stirred at 120 ^oC for 3.0 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 flash column chromatography. The KIE value was determined by average of two runs and representative ^{1}HNMR spectrum was provided as follows:

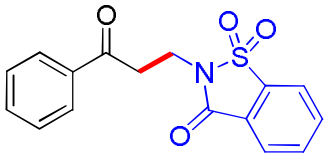


IV. General procedure for the preparation of 2 and 4 (**2a** as an example).



To a solution of acetophenone (**1a**) (60.1 mg, 0.5 mmol) in DMSO (2.0 mL) was added $RuCl_3$ (4.3 mg, 0.025 mmol), 1,10-phen (4.95 mg, 0.025 mmol), selectflour (354 mg, 1.0 mmol) and Na_2CO_3 (108 mg, 1.0 mmol). The mixture was stirred at 120 ^oC for 3.0 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 **2a** as a white solid (143.3 mg, 91%).

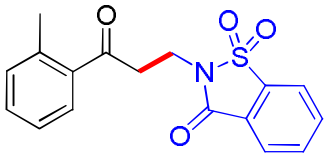
V. Analytical data of products obtained in this study



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

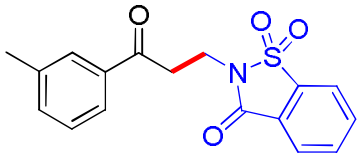
White solid. Mp: 138-140 ^oC; ^1H NMR (400 MHz; $CDCl_3$): δ = 3.59 (t, J = 7.6 Hz, 2H), 4.28 (t, J = 7.6 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.58 (d, J = 7.2 Hz, 1H), 7.86 (d, J = 8.6 Hz, 2H), 7.89-7.95 (m, 3H), 7.98 (dd, J_1 = 2.8 Hz, J_2 = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.5, 36.8, 121.0, 125.2, 127.4, 128.1, 128.7, 133.5, 134.4, 134.8, 136.2, 137.8, 158.8, 196.8. HRMS

(ESI-TOF) Calcd for $C_{16}H_{14}NO_4S$, $[M+H]^+$ 316.0644; Found 316.0641.



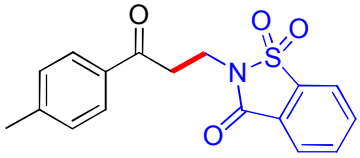
2-(3-oxo-3-(*o*-tolyl)propyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2b

White solid. Mp: 134-135 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.56 (s, 3H), 3.52 (t, J = 7.6 Hz, 2H), 4.25 (t, J = 7.6 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 8.6 Hz, 1H), 7.88 (dd, J_1 = 2.4 Hz, J_2 = 7.6 Hz, 2H), 7.94 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.5, 34.6, 39.2, 121.0, 125.2, 125.8, 127.4, 128.9, 131.9, 132.2, 134.4, 134.8, 137.8, 138.9, 158.8, 200.0. HRMS (ESI-TOF) Calcd for $C_{17}H_{16}NO_4S$, $[M+H]^+$ 330.0794; Found 330.0797.



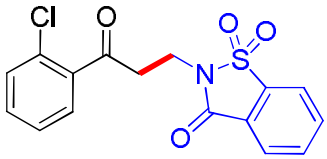
2-(3-oxo-3-(*m*-tolyl)propyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2c

White solid. Mp: 106-107 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.41 (s, 3H), 3.56 (t, J = 7.6 Hz, 2H), 4.26 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 8.0 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.76 (d, J = 9.2 Hz, 2H), 7.85-7.90 (m, 2H), 7.91-8.09 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.3, 34.5, 36.9, 121.0, 125.2, 125.3, 127.4, 128.6, 134.3, 134.4, 134.8, 136.2, 137.7, 138.5, 158.8, 197.0. HRMS (ESI-TOF) Calcd for $C_{17}H_{16}NO_4S$, $[M+H]^+$ 330.0794; Found 330.0784.



2-(3-oxo-3-(*p*-tolyl)propyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2d

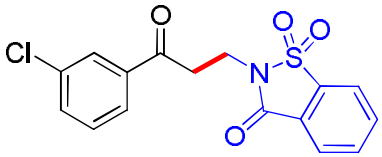
White solid. Mp: 132-133 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.42(s, 3H), 3.55 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 2H), 4.25 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 2H), 7.26 (d, J = 6.8 Hz, 2H), 7.85-7.91 (m, 4H), 8.08 (d, J=8.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.7, 34.6, 36.7, 121.0, 125.2, 127.4, 128.2, 129.4, 133.8, 134.4, 134.8, 137.8, 144.4, 158.8, 196.4. HRMS (ESI-TOF) Calcd for $C_{17}H_{16}NO_4S$, $[M+H]^+$ 330.0794; Found 330.0793.



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

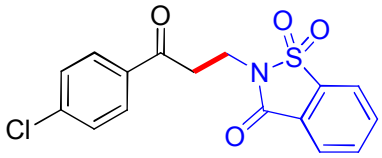
White solid. Mp: 132-134 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.58 (t, J = 7.5 Hz, 2H), 4.25 (t, J = 7.5 Hz, 2H), 7.33 (dd, J_1 = 2.4 Hz, J_2 = 6.4 Hz, 1H), 7.35-7.59 (m, 2H), 7.60 (d, J = 6.8 Hz, 1H), 7.85-8.08 (m, 3H), 8.09(d, J = 6.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.2, 41.0, 121.0,

125.2, 127.0, 127.3, 129.6, 130.8, 131.4, 132.3, 134.4, 134.8, 137.7, 138.0, 158.7, 199.2. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}ClNO_4S$, $[M+H]^+$ 350.0251; Found 350.0253.



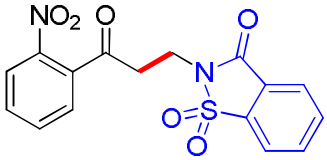
2-(3-(3-chlorophenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2f

White solid. Mp: 105-106 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.56 (t, J = 8.0 Hz, 2H), 4.27 (t, J = 8.0 Hz, 2H), 7.29 (t, J = 8.0 Hz, 1H), 7.55-7.58 (m, 1H), 7.84-7.88 (m, 3H), 7.90-7.95 (m, 2H), 8.08 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.3, 36.9, 121.0, 125.2, 126.1, 127.3, 128.2, 130.1, 133.5, 134.4, 134.9, 135.1, 137.7, 158.8, 195.5. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}ClNO_4S$, $[M+H]^+$ 350.0251; Found 350.0247.



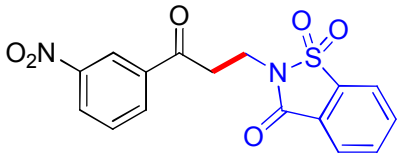
2-(3-(4-chlorophenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2g

White solid. Mp: 153-154 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.54 (t, J = 8.0 Hz, 2H), 4.26 (t, J = 8.0 Hz, 2H), 7.46 (dd, J_1 = 2.0 Hz, J_2 = 6.8 Hz, 2H), 7.86-8.08 (m, 5H), 8.09 (d, J = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.3, 36.8, 120.9, 125.2, 127.3, 129.1, 129.5, 134.4, 134.5, 134.9, 137.7, 140.1, 195.6. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}ClNO_4S$, $[M+H]^+$ 350.0251; Found 350.0254.



2-(3-(2-nitrophenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2h

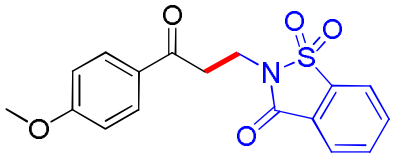
White solid. Mp: 131-132 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.39 (t, J = 7.6 Hz, 2H), 4.32 (t, J = 7.6 Hz, 2H), 7.48 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1H), 7.61-7.65 (m, 1H), 7.75 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1H), 7.83-8.07 (m, 3H), 8.08 (d, J = 7.5 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.0, 40.9, 121.0, 124.5, 125.3, 125.4, 127.3, 127.5, 130.9, 134.4, 134.5, 134.9, 137.0, 137.7, 158.7, 198.8. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}N_2O_6S$, $[M+H]^+$ 361.0486; Found 361.0483.



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

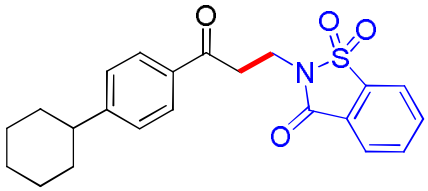
White solid. Mp: 89-91 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.64 (t, J = 6.8 Hz, 2H), 4.31 (t, J = 6.8 Hz, 2H), 7.10 (d, J = 8.0 Hz, 1H), 7.81-7.96 (m, 3H), 8.10 (d, J = 8.0 Hz, 1H), 8.30 (d, J = 7.6

Hz, 1H), 8.46 (dd, J_1 = 2.0 Hz, J_1 = 8.0 Hz, 1H), 8.79 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.0, 37.1, 121.0, 122.9, 125.3, 127.2, 127.8, 130.0, 133.5, 134.5, 134.9, 137.4, 148.5, 158.8, 194.7. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}N_2O_6S$, $[M+H]^+$ 361.0486; Found 361.0481.



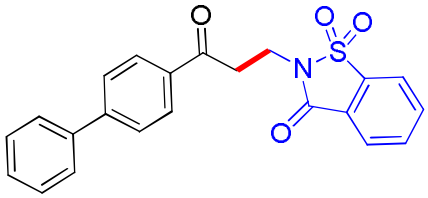
2-(3-(4-methoxyphenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2j

White solid. Mp: 127-128 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.52 (t, J = 7.6 Hz, 2H), 3.88 (s, 3H), 4.26 (t, J = 7.6 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H), 7.85-7.96 (m, 5H), 8.08 (d, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.6, 36.4, 55.5, 113.8, 121.0, 125.2, 127.3, 129.3, 130.3, 134.4, 134.8, 137.7, 158.8, 163.8, 196.3. HRMS (ESI-TOF) Calcd for $C_{17}H_{16}NO_5S$, $[M+H]^+$ 346.0741; Found 346.0748.



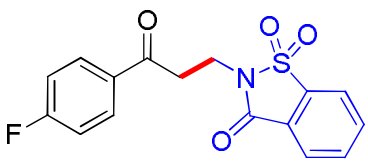
2-(3-(4-cyclohexylphenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2k

White solid. Mp: 153-154 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.28-1.45 (m, 5H), 1.59-1.88 (m, 5H), 2.56 (q, J = 4.4 Hz, 1H), 3.55 (t, J = 7.6 Hz, 2H), 4.26 (t, J = 7.6 Hz, 2H), 7.30 (d, J = 8.4 Hz, 2H), 7.85-7.95(m, 5H), 8.09 (d, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 26.0, 26.7, 34.1, 34.6, 36.7, 44.7, 121.0, 125.2, 127.2, 127.4, 128.3, 134.1, 134.4, 134.8, 137.8, 154.2, 158.8, 196.4. HRMS (ESI-TOF) Calcd for $C_{22}H_{24}NO_4S$, $[M+H]^+$ 398.1418; Found 398.1413.



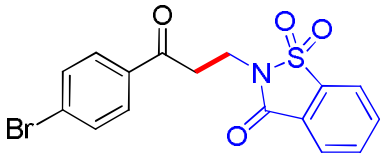
2-(3-([1,1'-biphenyl]-4-yl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2l

White solid. Mp: 151-152 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.62 (t, J = 7.6 Hz, 2H), 4.30 (t, J = 7.6 Hz, 2H), 7.41-7.63 (m, 3H), 7.65 (d, J = 6.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.86-7.89 (m, 3H), 7.90-8.11 (m, 3H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.5, 36.9, 121.0, 125.2, 127.3, 127.4, 128.3, 128.7, 129.0, 134.4, 134.8, 134.9, 137.7, 139.8, 146.2, 158.8, 196.4. HRMS (ESI-TOF) Calcd for $C_{22}H_{18}NO_4S$, $[M+H]^+$ 392.0968; Found 392.0966.



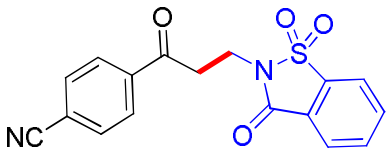
2-(3-(4-fluorophenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2m

White solid. Mp: 150-151 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.55 (t, J = 7.6 Hz, 2H), 4.28 (t, J = 7.6 Hz, 2H), 7.15 (dd, J_1 = 2.4 Hz, J_2 = 8.4 Hz, 2H), 7.86-7.93 (m, 3H), 7.94-8.02 (m, 2H), 8.07 (dd, J_1 = 1.6 Hz, J_2 = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.4, 36.7, 115.7, 116.0, 121.0, 125.2, 127.3, 130.7, 130.8, 132.7, 134.4, 134.9, 137.7, 158.8, 164.7, 167.3, 195.2. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}FNO_4S$, $[M+H]^+$ 334.0549; Found 334.0546.



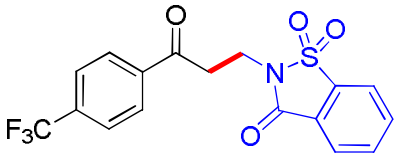
2-(3-(4-bromophenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2n

White solid. Mp: 179-180 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.59 (t, J = 8.0 Hz, 2H), 4.29 (t, J = 7.6 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 7.83-7.87 (m, 2H), 7.88-7.91 (m, 1H), 7.93-8.08 (m, 3H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.2, 37.1, 121.0, 121.1, 125.3, 125.4, 125.7, 125.8, 127.2, 128.4, 134.3, 134.5, 134.9, 135.2, 137.6, 138.8, 158.8, 195.9. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}BrNO_4S$, $[M+H]^+$ 393.9749; Found 393.9747.



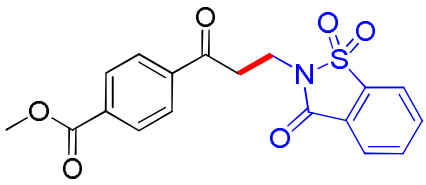
4-(3-(1,1-dioxido-3-oxobenzo[*d*]isothiazol-2(3*H*)-yl)propanoyl)benzonitrile 2o

White solid. Mp: 177-178 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.59 (t, J = 7.2 Hz, 2H), 4.28 (s, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.89-7.94 (m, 3H), 8.05-8.11 (m, 3H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.1, 37.1, 116.9, 117.8, 121.0, 125.3, 127.2, 128.5, 129.9, 132.2, 134.5, 134.9, 137.7, 139.1, 158.8, 195.5. HRMS (ESI-TOF) Calcd for $C_{17}H_{13}N_2O_4S$, $[M+H]^+$ 341.0591; Found 341.0596.



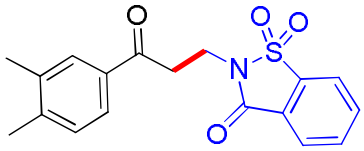
2-(3-oxo-3-(4-(trifluoromethyl)phenyl)propyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2p

White solid. Mp: 123-124 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.59 (t, J = 7.6 Hz, 2H), 4.28 (t, J = 7.6 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 7.85 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 2H), 7.87-7.91 (m, 1H), 7.93-8.08 (m, 3H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.2, 37.1, 121.0, 121.1, 125.3, 125.4, 125.7, 125.8, 127.2, 128.4, 134.3, 134.5, 134.9, 135.2, 137.6, 138.8, 158.8, 159.9. HRMS (ESI-TOF) Calcd for $C_{17}H_{13}F_3NO_4S$, $[M+H]^+$ 384.0517; Found 384.0516.



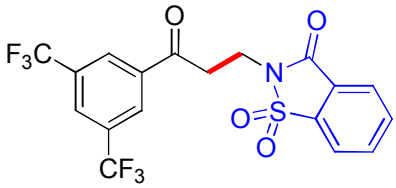
methyl 4-(3-(1,1-dioxido-3-oxobenzo[*d*]isothiazol-2(3*H*)-yl)propanoyl)benzoate 2q

White solid. Mp: 132-133 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.60 (t, J = 8.0 Hz, 2H), 3.95 (s, 3H), 4.27 (t, J = 8.0 Hz, 2H), 7.85-8.91 (m, 3H), 7.94 (d, J = 7.2 Hz, 2H)，8.01(d, J = 8.4 Hz, 1H), 8.07-8.13 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.3, 37.2, 52.5, 121.1, 125.2, 127.3, 127.9, 129.9, 134.2, 134.3, 134.5, 137.7, 139.3, 158.8, 166.1, 196.4. HRMS (ESI-TOF) Calcd for $C_{18}H_{16}NO_6S$, $[M+H]^+$ 374.0696; Found 374.0693.



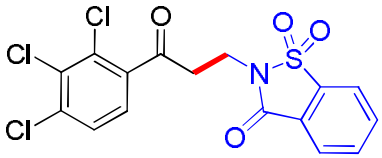
2-(3-(3,4-dimethylphenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2r

White solid. Mp: 126-128 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ =2.31 (s, 3H), 2.32 (s, 3H)，3.55 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 2H), 4.25 (q, J = 6.4 Hz, 2H), 7.22 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 6.4 Hz, 1H), 7.74 (s, 1H), 7.83-7.89 (m, 3H), 7.91 (d, J = 6.4 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 19.7, 20.2, 34.6, 36.7, 120.9, 125.2, 125.8, 127.4, 129.2, 134.2, 134.3, 137.0, 137.8, 143.1, 158.8, 196.7. HRMS (ESI-TOF) Calcd for $C_{18}H_{18}NO_4S$, $[M+H]^+$ 344.0951; Found 344.0953.



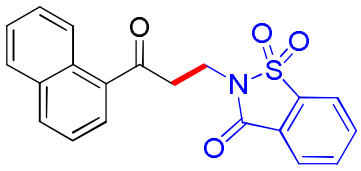
2-(3-(3,5-bis(trifluoromethyl)phenyl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2s

White solid. Mp: 129-130 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.63 (t, J = 7.6 Hz, 2H), 4.31 (t, J = 7.6 Hz, 2H), 7.87-7.97 (m, 3H), 8.10 (t, J = 6.8 Hz, 2H), 8.37 (s, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 33.9, 37.1, 121.0, 121.4, 124.1, 125.3, 126.7, 127.2, 128.1, 132.1, 132.4, 132.7, 133.1, 134.5, 134.9, 137.6, 137.7, 158.8, 194.1. HRMS (ESI-TOF) Calcd for $C_{18}H_{12}F_6NO_4S$, $[M+H]^+$ 452.0383; Found 452.0382.



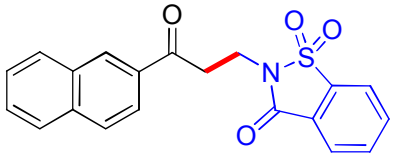
2-(3-oxo-3-(2,3,4-trichlorophenyl)propyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2t

White solid. Mp: 142-143 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.52 (t, J = 6.8 Hz, 2H), 4.25 (t, J = 6.8 Hz, 2H), 7.39 (d, J = 8.4 Hz, 1H), 7.47 (d, J = 8.4 Hz, 1H), 7.86-8.08 (m, 3H), 8.09 (d, J = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.0, 41.0, 121.0, 125.3, 127.1, 127.2, 128.7, 131.3, 133.2, 134.5, 134.9, 137.1, 137.7, 138.6, 158.7, 198.0. HRMS (ESI-TOF) Calcd for $C_{16}H_{11}Cl_3NO_4S$, $[M+H]^+$ 417.9486; Found 417.9491.



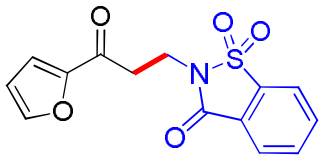
2-(3-(naphthalen-1-yl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2u

White solid. Mp: 146-148 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.68 (t, J = 7.6 Hz, 2H), 4.35 (t, J = 7.6 Hz, 2H), 7.48-7.63 (m, 6H), 7.83-8.03 (m, 4H), 8.07 (dd, J_1 = 1.6 Hz, J_2 = 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.7, 39.7, 121.0, 124.3, 125.2, 125.9, 126.6, 127.3, 128.3, 128.4, 128.5, 130.2, 133.5, 134.0, 134.8, 137.7, 158.8, 200.2. HRMS (ESI-TOF) Calcd for $C_{20}H_{16}NO_4S$, $[M+H]^+$ 366.0876; Found 366.0873.



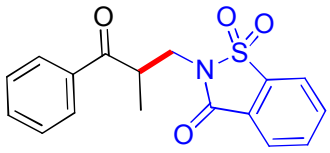
2-(3-(naphthalen-2-yl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2v

White solid. Mp: 138-138 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.73 (t, J = 7.6 Hz, 2H), 4.34 (t, J = 7.6 Hz, 2H), 7.57-7.60 (m, 2H), 7.62-8.06 (m, 8H), 8.10 (dd, J_1 = 1.2 Hz, J_2 = 7.2 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.6, 36.9, 121.0, 123.6, 125.2, 126.9, 127.4, 127.8, 128.6, 128.7, 129.6, 130.0, 132.5, 133.6, 134.4, 134.8, 135.8, 137.8, 158.8, 196.7. HRMS (ESI-TOF) Calcd for $C_{20}H_{16}NO_4S$, $[M+H]^+$ 366.0876; Found 366.0874.



2-(3-(furan-2-yl)-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 2w

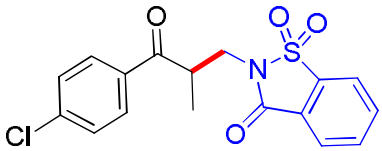
White solid. Mp: 103-105 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.44 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 2H), 4.24 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 2H), 6.55 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1H), 7.25 (dd, J_1 = 0.8 Hz, J_2 = 6.4 Hz, 1H), 7.60 (t, J = 1.6 Hz, 1H), 7.85-7.95 (m, 3H), 8.07-8.09 (m, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 34.0, 36.7, 112.4, 117.5, 121.0, 125.2, 127.3, 134.4, 134.8, 137.7, 146.7, 152.2, 158.7, 185.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}NO_5S$, $[M+H]^+$ 306.0438; Found 306.0436.



(*R*)-2-(2-methyl-3-oxo-3-phenylpropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 4a

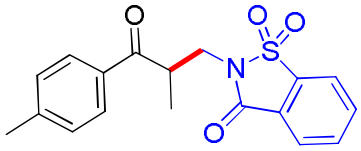
White solid. Mp: 113-114 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.35 (d, J = 7.2 Hz, 3H), 3.99 (t, J = 6.4 Hz, 1H), 4.24 (dd, J_1 = 3.2 Hz, J_2 = 7.2 Hz, 2H), 7.26 (d, J = 8.8 Hz, 2H), 7.57 (d, J = 7.2 Hz, 1H), 7.84-7.88 (m, 2H), 7.88-7.94 (m, 1H), 8.01-8.08 (m, 3H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 16.3, 39.5, 41.6, 121.0, 125.3, 127.2, 128.5, 128.8, 133.4, 134.4, 134.8, 135.7, 137.6, 159.1, 201.0.

HRMS (ESI-TOF) Calcd for $C_{17}H_{16}NO_4S$, $[M+H]^+$ 330.0800; Found 330.0803.



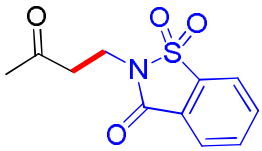
(*R*)-2-(3-(4-chlorophenyl)-2-methyl-3-oxopropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 4b

White solid. Mp: 160-161 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.33 (d, J = 7.2 Hz, 3H), 3.96 (m, 1H), 4.16-4.26 (m, 2H), 7.44-7.47 (m, 2H), 8.46 (dd, J_1 = 1.6 Hz, J_2 = 7.2 Hz, 3H), 7.88-7.93 (m, 2H), 7.94-8.06 (m, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 16.2, 39.5, 41.5, 121.0, 125.3, 127.2, 134.0, 134.4, 134.9, 159.1, 199.8. HRMS (ESI-TOF) Calcd for $C_{17}H_{15}ClNO_4S$, $[M+H]^+$ 364.0409; Found 364.0405.



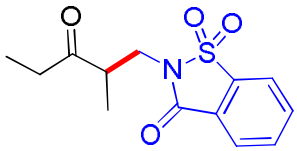
(*R*)-2-(2-methyl-3-oxo-3-(p-tolyl)propyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 4c

White solid. Mp: 131-133 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.33 (d, J = 7.2 Hz, 3H), 2.41 (s, 3H), 3.98 (t, J = 6.4 Hz, 1H), 4.19-4.24 (m, 2H), 7.28 (d, J = 6.4 Hz, 2H), 7.84 (dd, J_1 = 1.6 Hz, J_2 = 7.2 Hz, 2H), 7.87-7.83 (m, 3H), 8.06 (dd, J_1 = 1.2 Hz, J_2 = 6.4 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 16.3, 21.6, 39.3, 41.6, 120.9, 125.3, 127.2, 128.7, 129.5, 133.1, 134.4, 134.8, 137.6, 144.3, 159.1, 200.7. HRMS (ESI-TOF) Calcd for $C_{18}H_{18}NO_4S$, $[M+H]^+$ 344.0951; Found 344.0954.



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

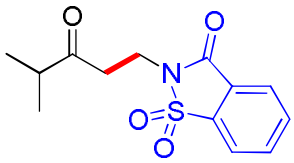
White solid. Mp: 113-115 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.21 (s, 3H), 3.03 (t, J = 7.6 Hz, 2H), 4.05 (t, J = 7.6 Hz, 2H), 7.83-7.89 (m, 3H), 7.91-8.07 (m, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 30.1, 33.8, 41.2, 121.0, 125.2, 127.2, 134.4, 134.9, 137.6, 158.7, 205.4. HRMS (ESI-TOF) Calcd for $C_{11}H_{12}NO_4S$, $[M+H]^+$ 254.0479; Found 254.0472.



(*R*)-2-(2-methyl-3-oxopentyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 4e

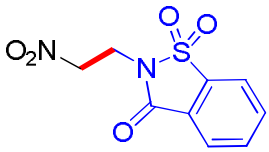
White solid. Mp: 90-91 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.08 (t, J = 7.2 Hz, 3H), 1.24 (d, J = 7.2 Hz, 3H), 2.50 (q, J = 7.2 Hz, 1H), 2.63 (q, J = 7.2 Hz, 1H), 3.27 (q, J = 7.6 Hz, 1H), 3.80 (q, J = 7.2 Hz, 1H), 4.10 (q, J = 7.6 Hz, 1H), 7.84-7.94 (m, 3H), 8.08 (dd, J_1 = 1.6 Hz, J_2 = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 7.5, 15.3, 34.7, 41.0, 44.2, 120.9, 125.3, 127.2, 134.4, 134.8,

137.6, 159.0, 211.8. HRMS (ESI-TOF) Calcd for $C_{13}H_{16}NO_4S$, $[M+H]^+$ 282.0792; Found 282.0794.



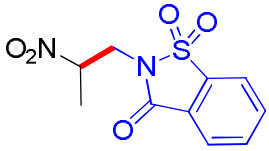
2-(4-methyl-3-oxopentyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 4f

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.14 (d, J = 7.2 Hz, 6H), 2.59-2.66 (m, 1H), 3.05 (t, J = 7.6 Hz, 2H), 4.08 (t, J = 7.6 Hz, 2H), 7.84-7.94 (m, 3H), 8.08 (dd, J_1 = 1.2 Hz, J_2 = 6.4 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 18.0, 34.1, 38.2, 41.0, 120.9, 125.2, 127.4, 134.3, 134.8, 137.8, 158.7, 211.1. HRMS (ESI-TOF) Calcd for $C_{13}H_{16}NO_4S$, $[M+H]^+$ 281.0722; Found 282.0795.



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

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.43 (t, J = 6.4 Hz, 2H), 4.80 (t, J = 6.4 Hz, 2H), 7.88-7.96 (m, 3H), 8.09 (d, J = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 35.4, 71.7, 121.2, 125.6, 126.8, 134.7, 135.3, 137.5, 158.7. HRMS (ESI-TOF) Calcd for $C_9H_9N_2O_5S$, $[M+H]^+$ 257.0232; Found 257.0235.

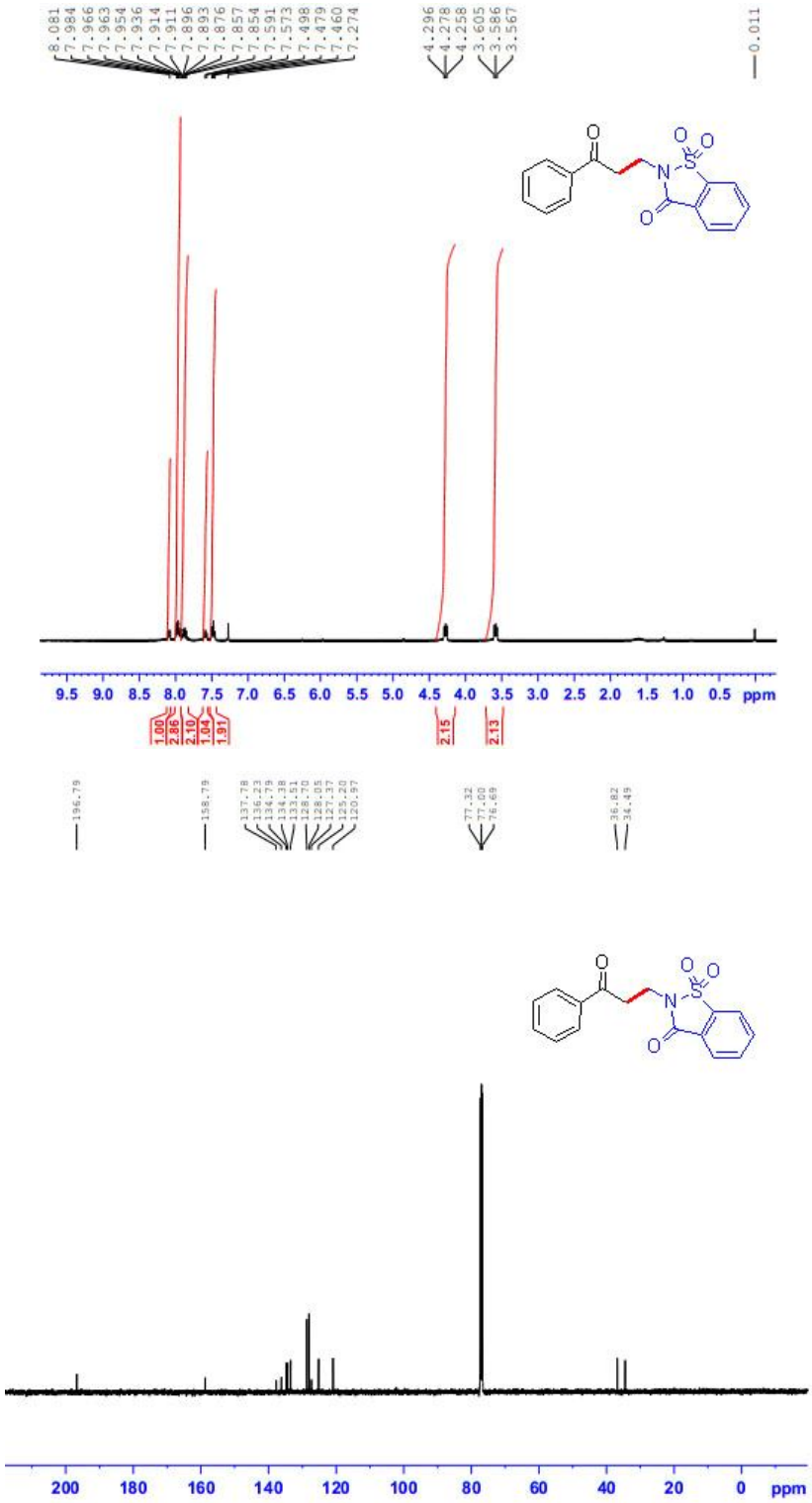


(*R*)-2-(2-nitropropyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 4h

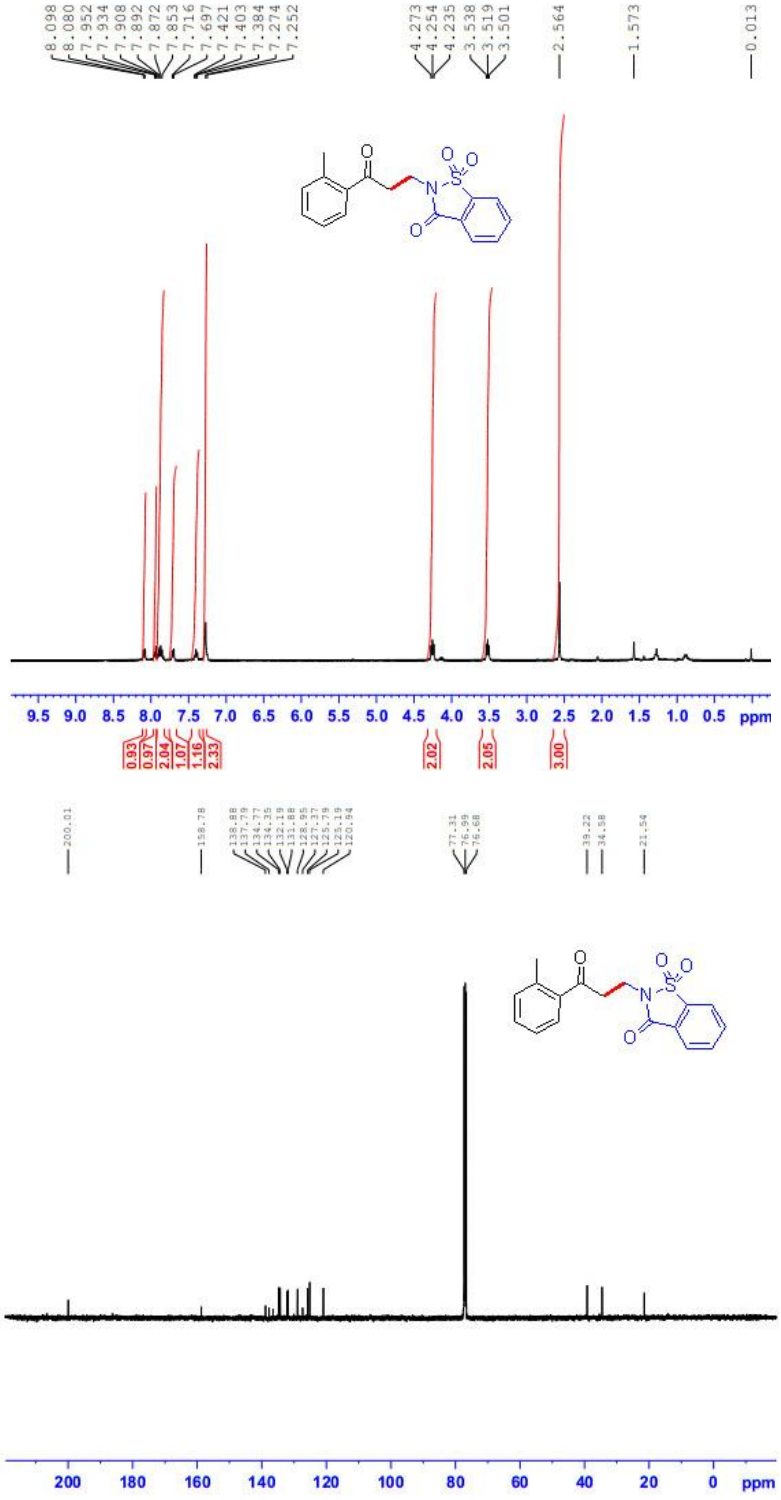
Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.69 (d, J = 6.8 Hz, 3H), 4.03-4.17 (m, 1H), 4.41-4.49 (m, 1H), 5.07-5.12 (m, 1H), 7.88-8.04 (m, 3H), 8.09 (d, J = 6.8 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 17.3, 41.6, 80.0, 121.2, 125.6, 126.1, 134.7, 135.3, 137.4, 158.9. HRMS (ESI-TOF) Calcd for $C_{10}H_{11}N_2O_5S$, $[M+H]^+$ 271.0381; Found 271.0385.

VI. ^{1}H NMR and ^{13}C NMR spectra copies of compounds 2, 4, C and H.

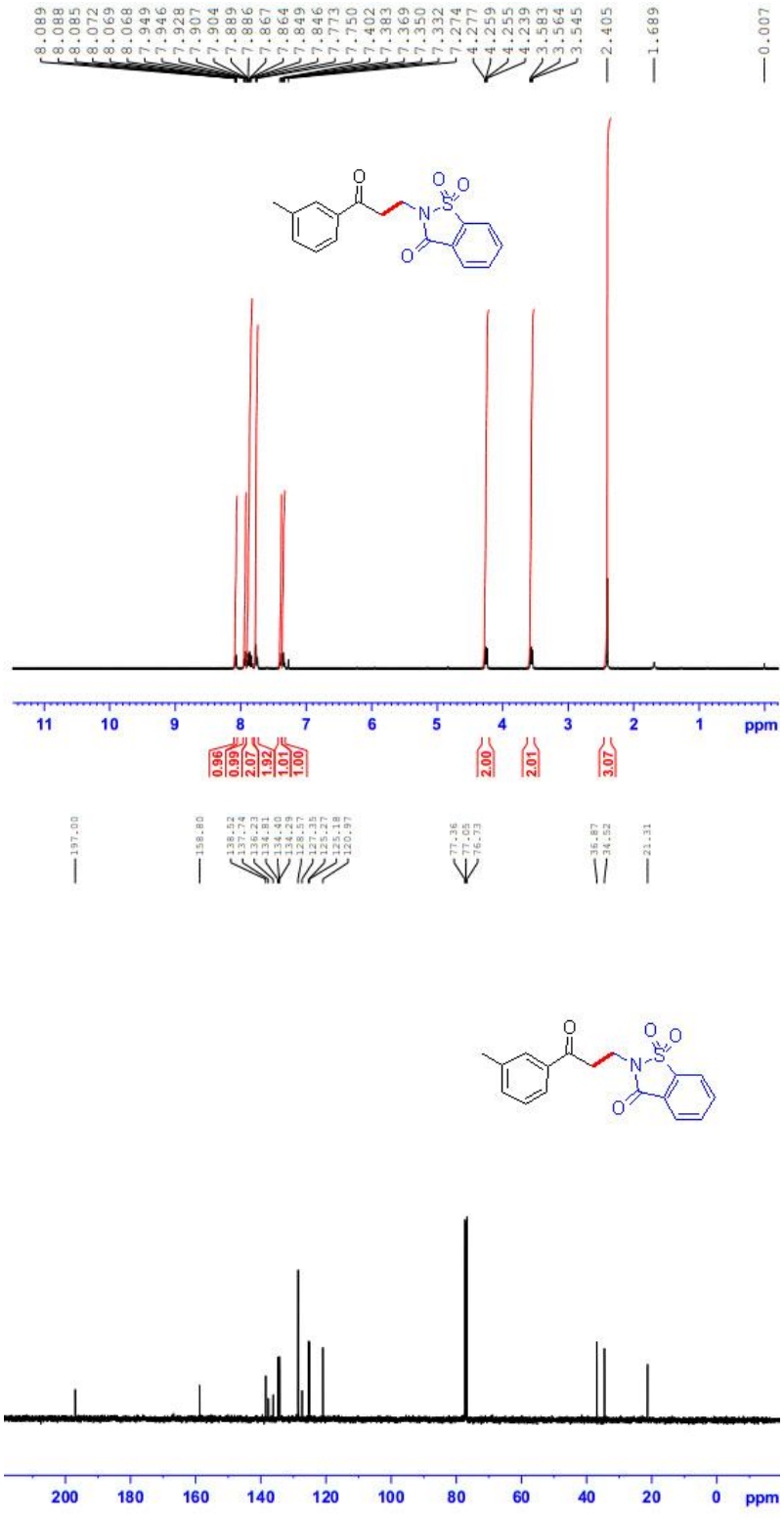
Compound 2a



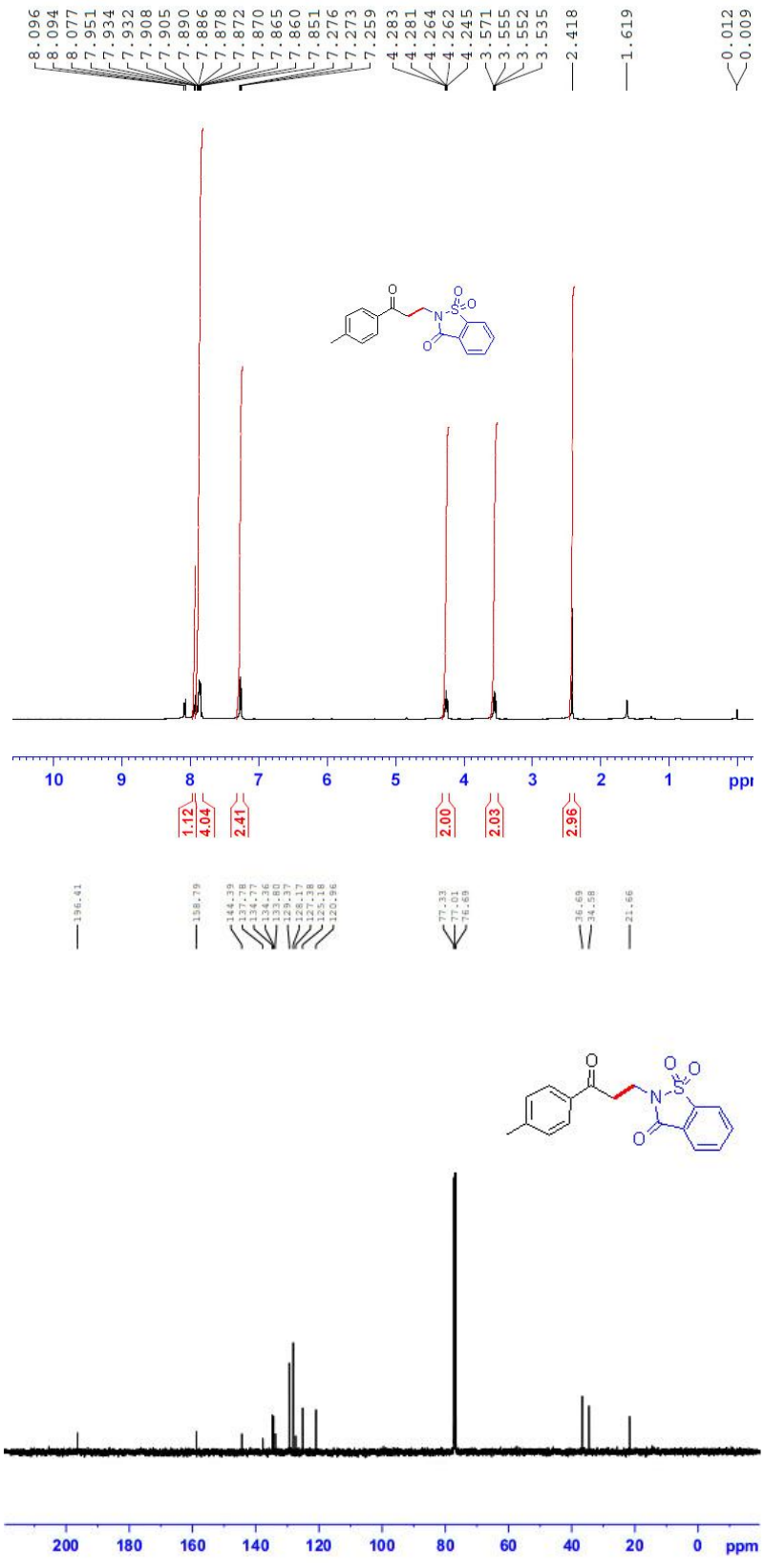
Compound 2b


8.098
8.080
7.952
7.934
7.908
7.892
7.872
7.853
7.716
7.697
7.421
7.403
7.384
7.274
7.252
4.273
4.254
4.235
3.538
3.519
3.501
2.564
1.573
0.013
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 ppm
0.93
0.97
2.04
1.07
1.16
2.33
2.02
2.05
3.00
200.01
158.78
138.88
137.79
134.77
133.15
132.19
131.88
128.95
127.37
125.79
123.58
120.54
77.31
76.99
76.68
39.22
34.58
21.54
200 180 160 140 120 100 80 60 40 20 0 ppm

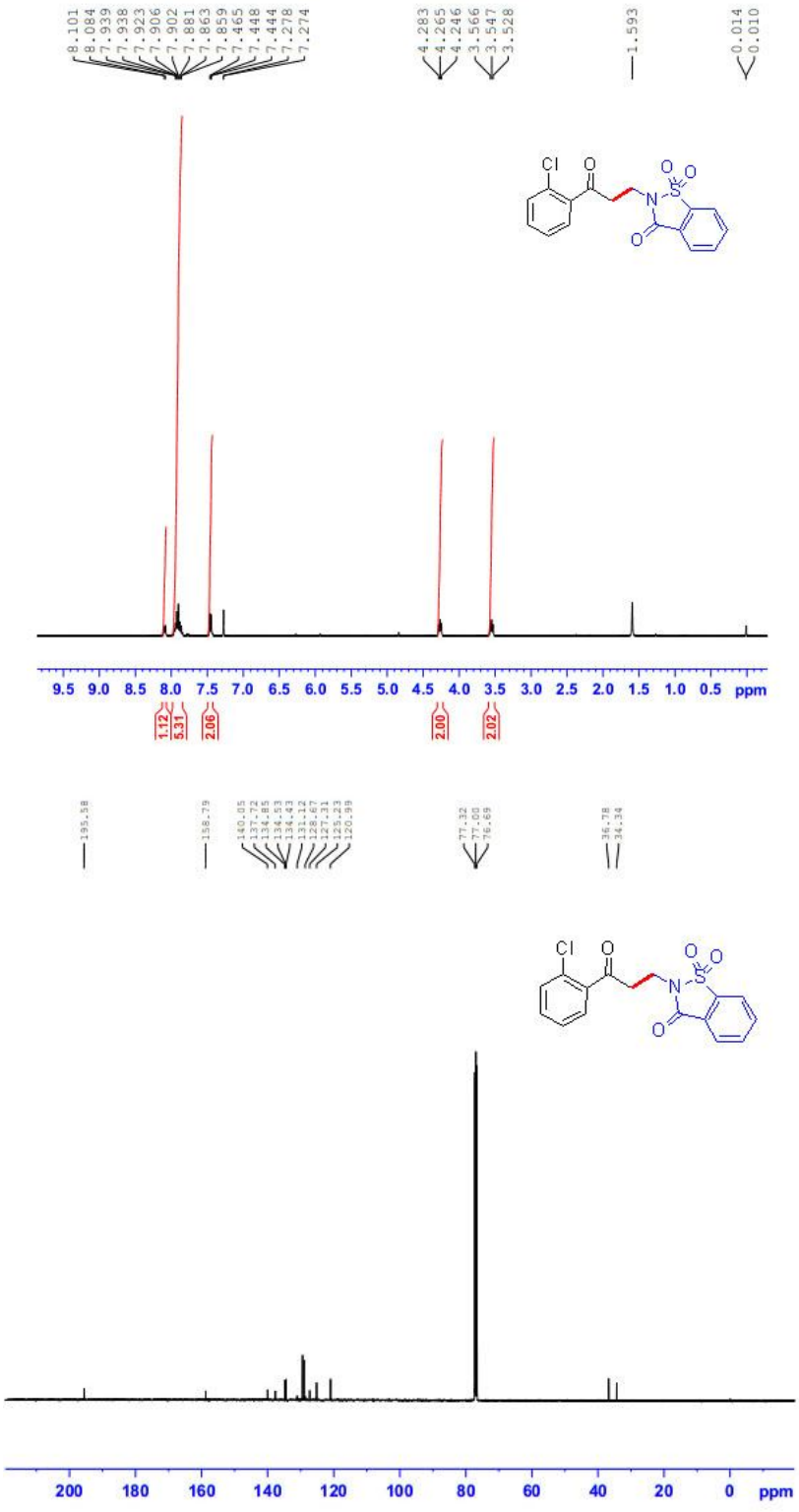
Compound 2c


8.089
8.088
8.085
8.072
8.069
8.068
7.949
7.946
7.928
7.907
7.904
7.889
7.886
7.867
7.864
7.849
7.846
7.773
7.750
7.402
7.383
7.369
7.350
7.332
7.274
4.277
4.259
4.255
4.239
3.583
3.564
3.545
2.405
1.689
0.007
11 10 9 8 7 6 5 4 3 2 1 ppm
0.96 0.99 2.07 1.92 1.01 1.00
2.00 2.01 3.07
197.00
158.80
136.52
137.74
136.23
134.81
134.40
134.29
129.57
128.35
125.27
125.18
120.97
77.36
77.05
76.73
36.87
34.52
21.31
200 180 160 140 120 100 80 60 40 20 0 ppm

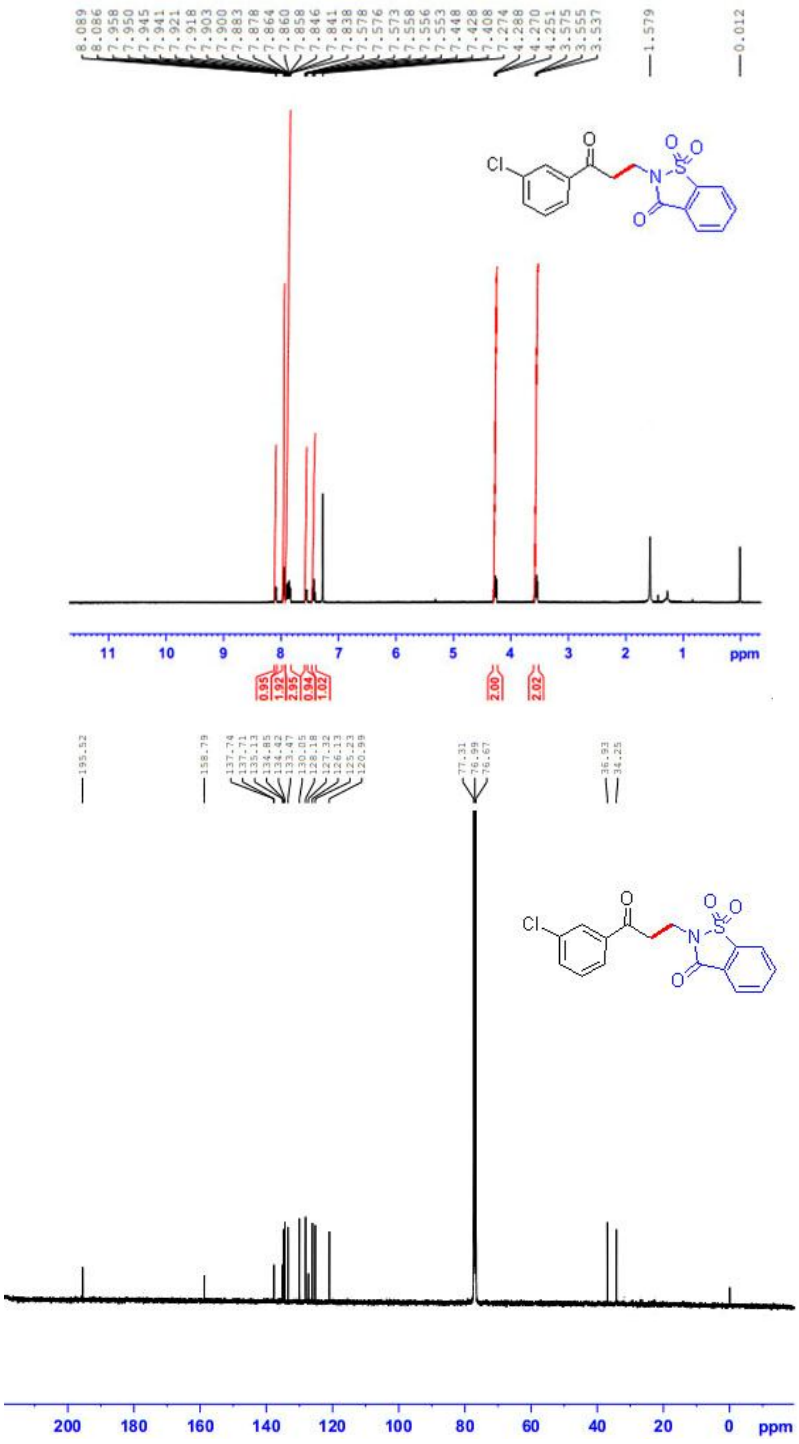
Compound 2d


8.096
8.094
8.077
7.951
7.934
7.932
7.908
7.905
7.890
7.886
7.878
7.872
7.870
7.865
7.860
7.851
7.276
7.273
7.259
4.283
4.281
4.264
4.262
4.245
3.571
3.555
3.552
3.535
2.418
1.619
0.012
0.009
10
9
8
7
6
5
4
3
2
1
ppm
1.12
4.04
2.41
2.00
2.03
2.96
196.41
158.79
144.39
137.58
134.77
134.66
133.80
129.37
128.17
127.38
125.18
120.96
77.33
77.01
76.69
36.69
34.58
21.66
200
180
160
140
120
100
80
60
40
20
0
ppm

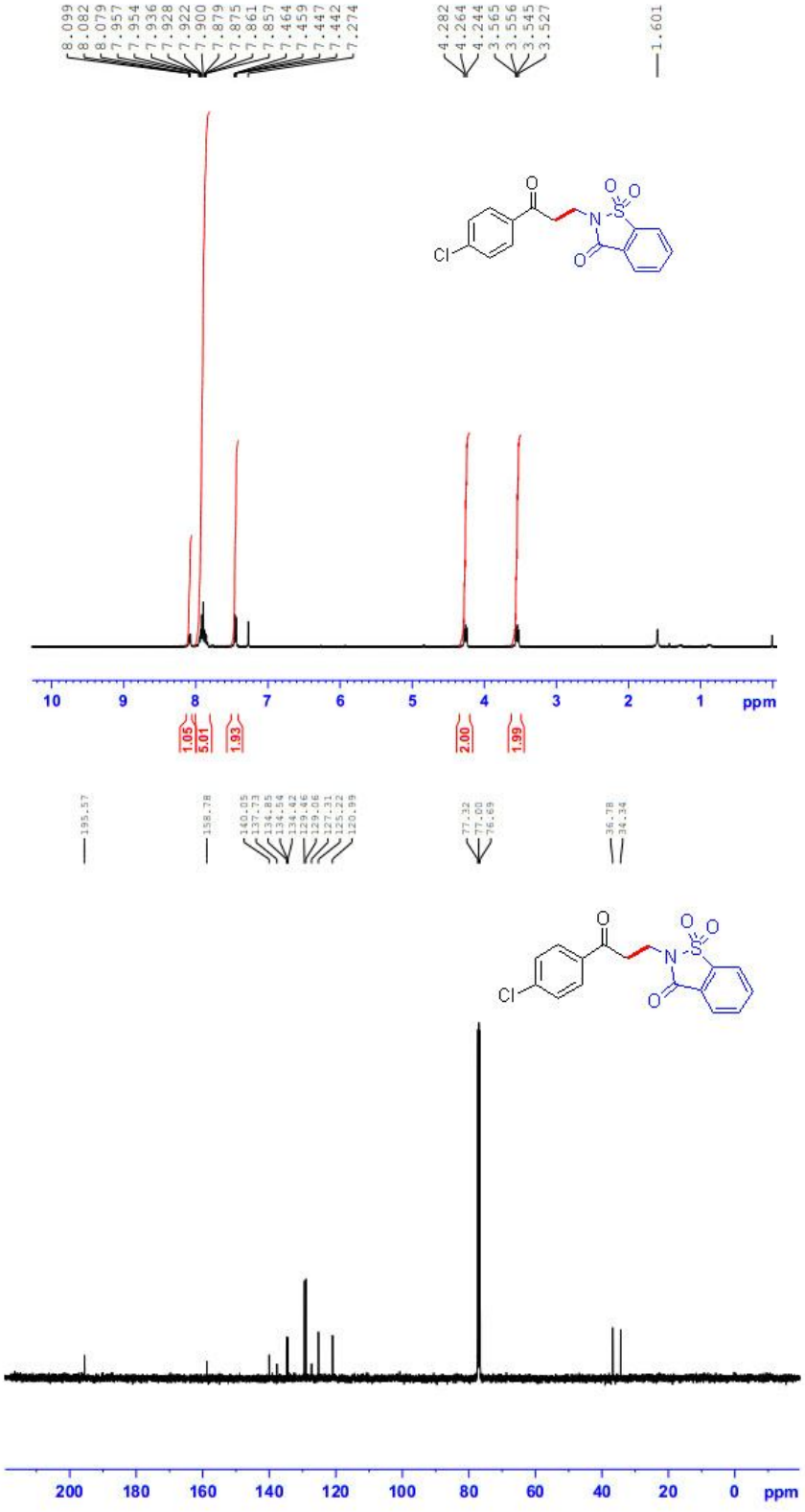
Compound 2e


8.101
8.084
7.939
7.938
7.923
7.906
7.902
7.881
7.863
7.859
7.465
7.448
7.444
7.278
7.274
4.283
4.265
4.246
3.566
3.547
3.528
1.593
0.014
0.010
Cl
O
O
O
S
N
O
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 ppm
1.12
5.31
2.06
2.00
2.02
195.58
158.79
140.05
137.72
134.85
134.53
134.43
131.12
130.87
129.31
126.23
120.99
77.32
77.00
76.69
36.78
34.34
200 180 160 140 120 100 80 60 40 20 0 ppm

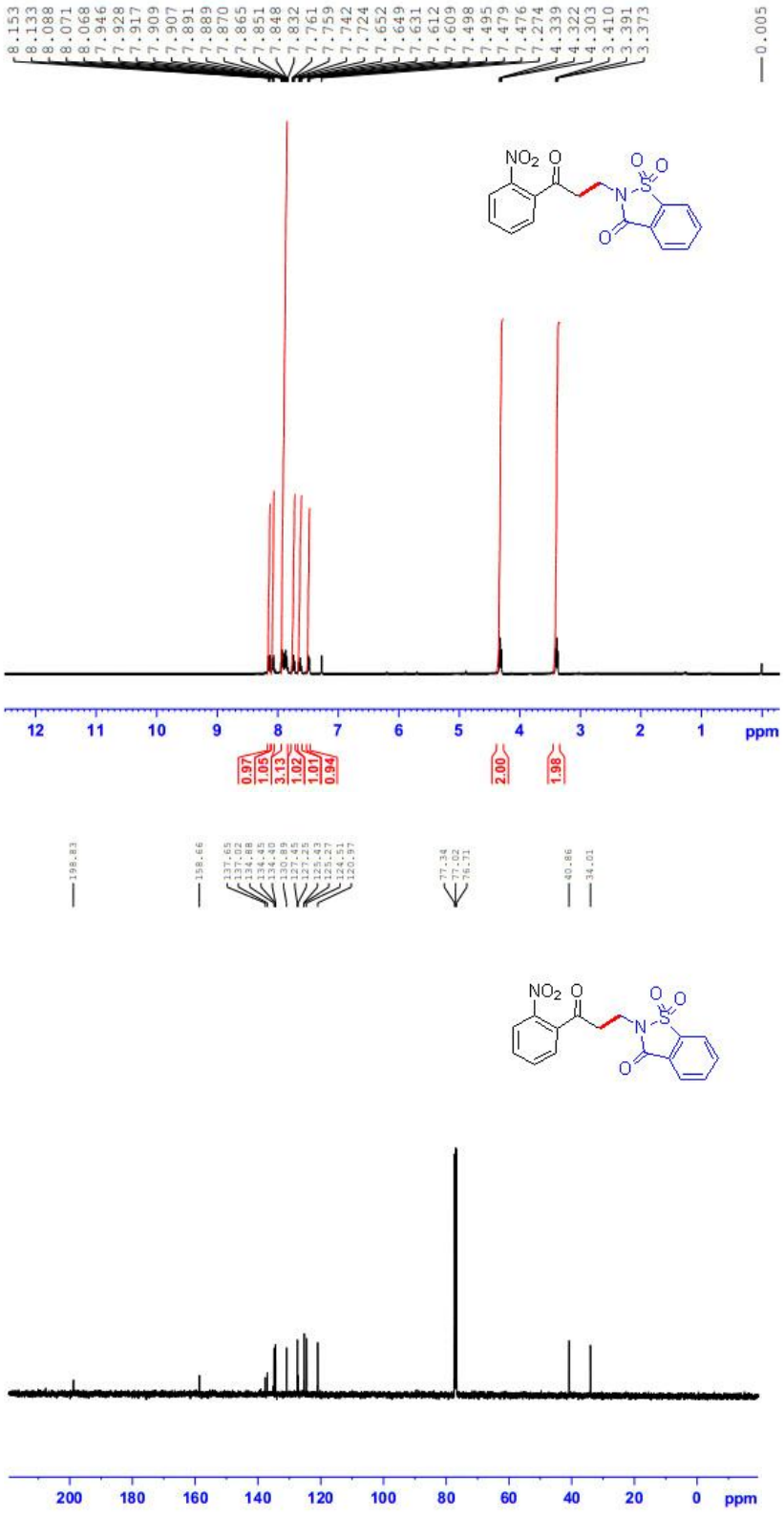
Compound 2f


8.089
8.086
7.958
7.950
7.945
7.941
7.921
7.918
7.903
7.900
7.883
7.878
7.864
7.860
7.858
7.846
7.841
7.838
7.578
7.576
7.573
7.558
7.556
7.553
7.448
7.428
7.408
7.274
4.288
4.270
4.251
3.575
3.555
3.537
1.579
0.012
Cl
O
O
O
S
N
O
11 10 9 8 7 6 5 4 3 2 1 ppm
0.85
1.92
1.92
2.85
0.94
1.02
2.00
2.02
195.52
158.79
137.74
137.71
135.13
134.85
134.42
133.47
130.65
128.18
127.32
126.13
125.23
120.98
77.31
77.00
76.67
36.93
34.25
200 180 160 140 120 100 80 60 40 20 0 ppm

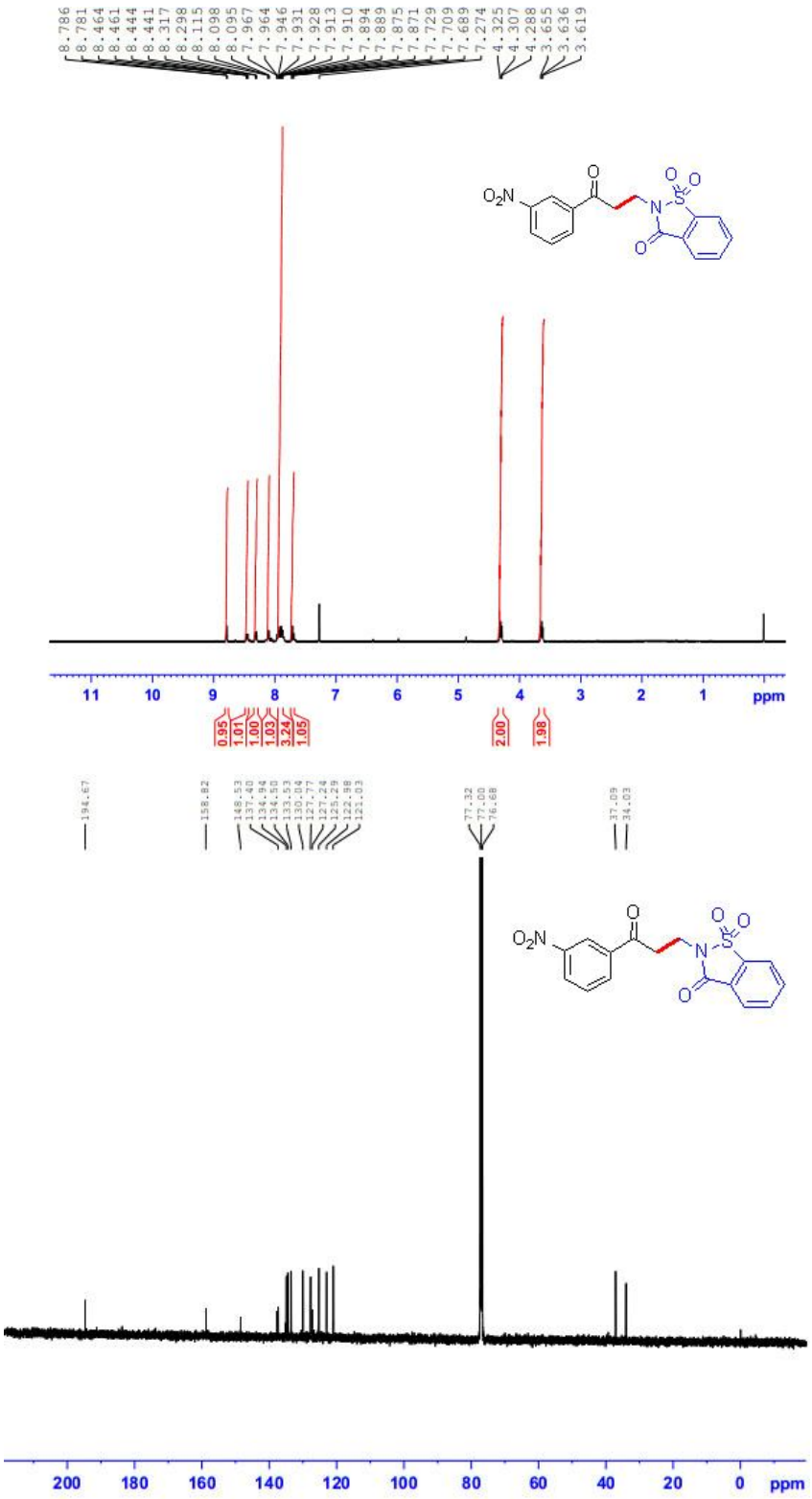
Compound 2g


8.099
8.082
8.079
7.957
7.954
7.936
7.928
7.922
7.900
7.879
7.875
7.861
7.857
7.464
7.459
7.447
7.442
7.274
4.282
4.264
4.244
3.565
3.556
3.545
3.527
1.601
Cl
O
O
O
N
S
10
9
8
7
6
5
4
3
2
1
ppm
1.05
5.01
1.93
2.00
1.99
195.57
158.78
140.05
137.73
134.85
134.54
134.42
129.46
129.06
127.31
125.22
120.99
77.32
77.00
76.69
36.78
34.34
200
180
160
140
120
100
80
60
40
20
0
ppm

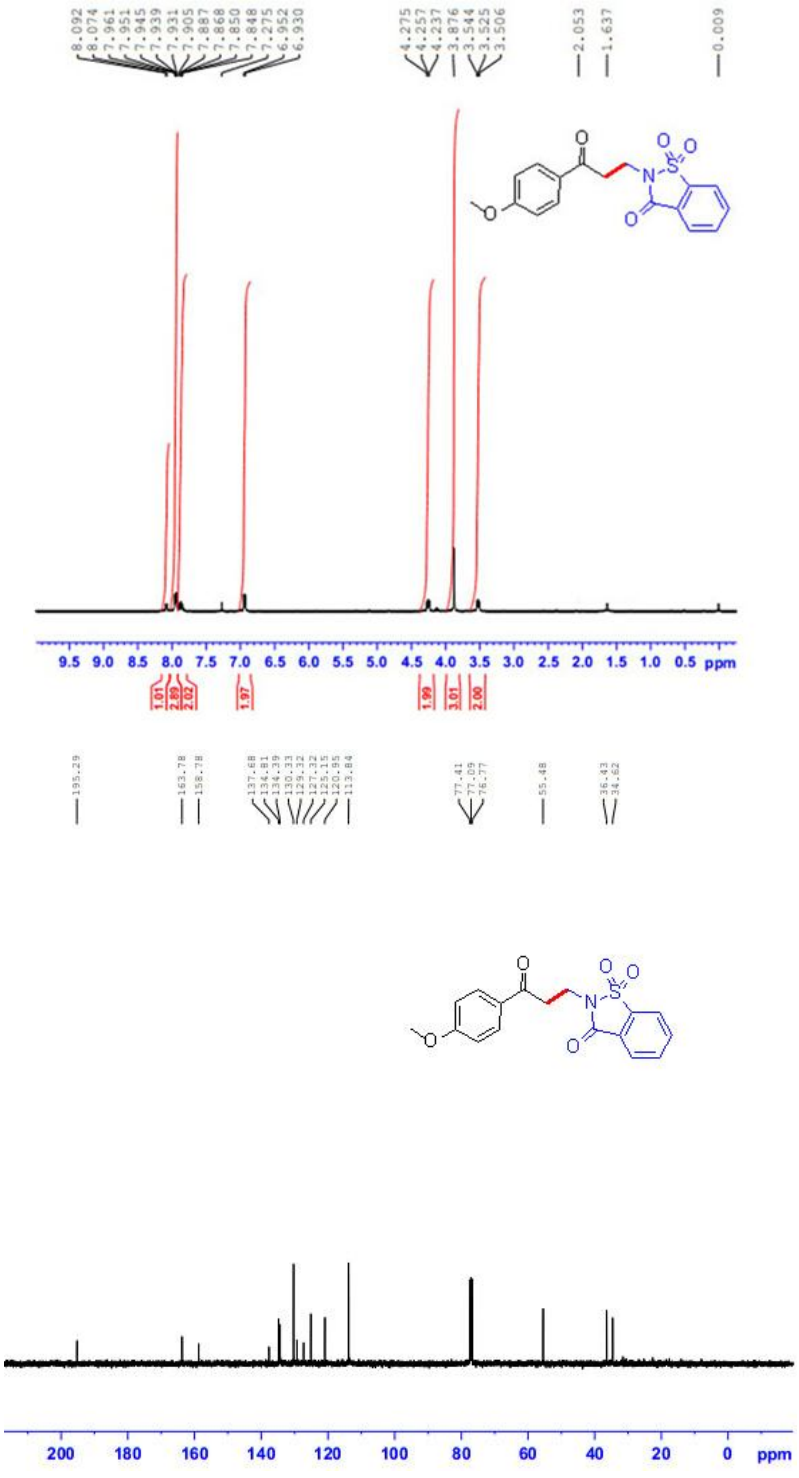
Compound 2h


8.153
8.133
8.088
8.071
8.068
7.946
7.928
7.917
7.909
7.907
7.891
7.889
7.870
7.865
7.851
7.848
7.832
7.761
7.759
7.742
7.724
7.652
7.649
7.631
7.612
7.609
7.498
7.495
7.479
7.476
7.274
4.339
4.322
4.303
3.410
3.391
3.373
0.005
NO2
O
O
O
N
S
O
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.97
1.05
3.13
1.02
1.01
0.94
2.00
1.98
198.83
158.66
137.65
137.02
134.88
134.45
134.40
130.89
127.45
127.25
125.43
125.27
124.51
120.97
77.34
77.02
76.71
40.86
34.01
NO2
O
O
O
N
S
O
200
180
160
140
120
100
80
60
40
20
0
ppm

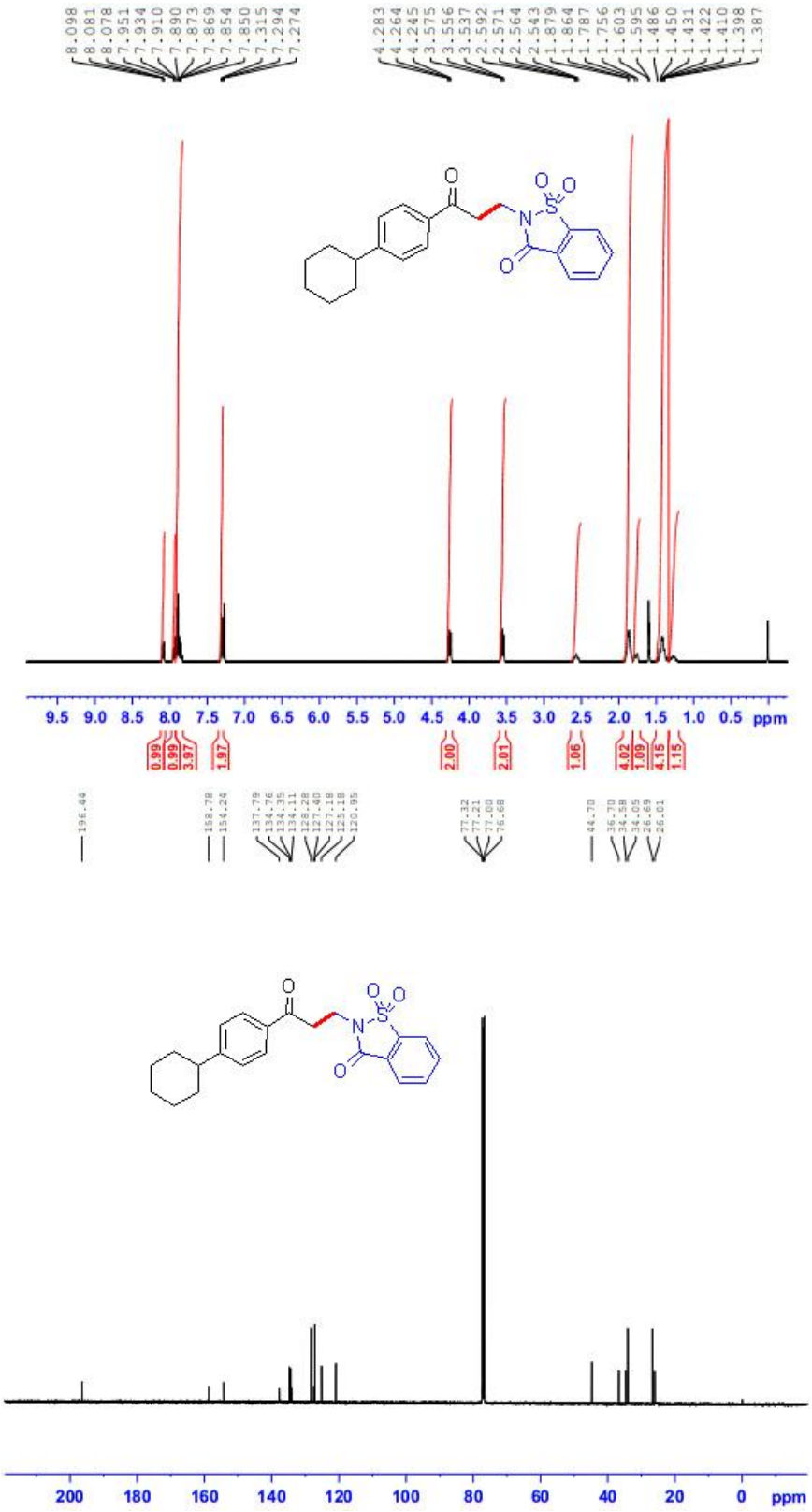
Compound 2i


8.786
8.781
8.464
8.461
8.444
8.441
8.317
8.298
8.115
8.098
8.095
7.967
7.964
7.946
7.931
7.928
7.913
7.910
7.894
7.889
7.875
7.871
7.729
7.709
7.689
7.274
4.325
4.307
4.288
3.655
3.636
3.619
O2N
O
O
O
S
N
O
11 10 9 8 7 6 5 4 3 2 1 ppm
0.95
1.01
1.00
1.03
3.24
1.05
2.00
1.98
194.67
158.82
148.53
137.60
134.98
134.50
133.53
130.04
127.77
127.24
125.29
122.98
121.03
77.32
77.00
76.68
37.09
34.03
O2N
O
O
O
S
N
O
200 180 160 140 120 100 80 60 40 20 0 ppm

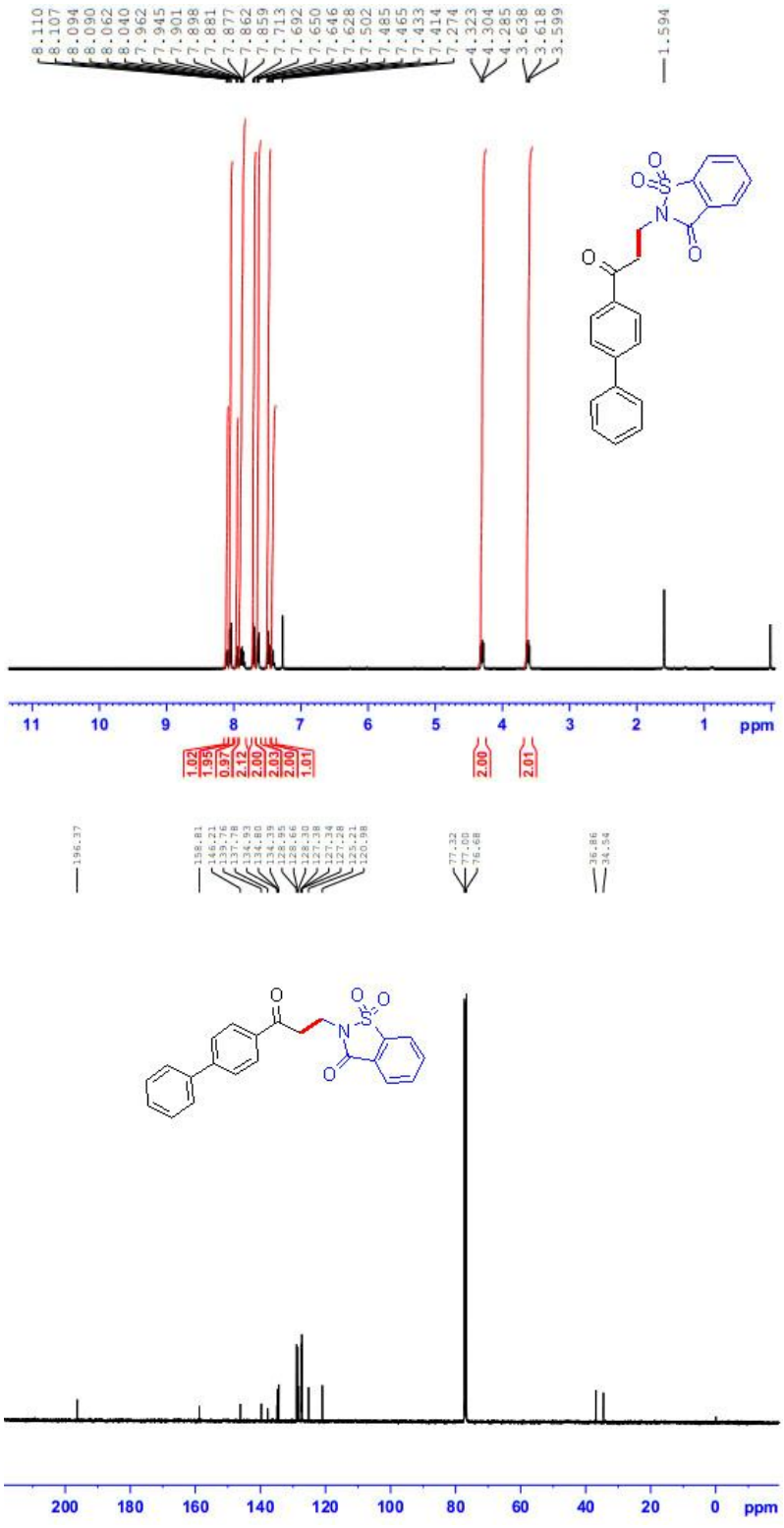
Compound 2j


8.092
8.074
7.961
7.952
7.945
7.939
7.931
7.905
7.887
7.868
7.850
7.848
7.275
6.952
6.930
4.275
4.257
4.237
3.876
3.544
3.525
3.506
2.053
1.637
0.009
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 ppm
1.01
2.89
2.02
1.97
1.99
3.01
2.00
195.29
163.78
158.78
137.68
134.81
134.39
130.33
129.32
127.32
125.15
120.95
113.84
77.41
77.09
76.77
55.48
36.43
34.82
200 180 160 140 120 100 80 60 40 20 0 ppm

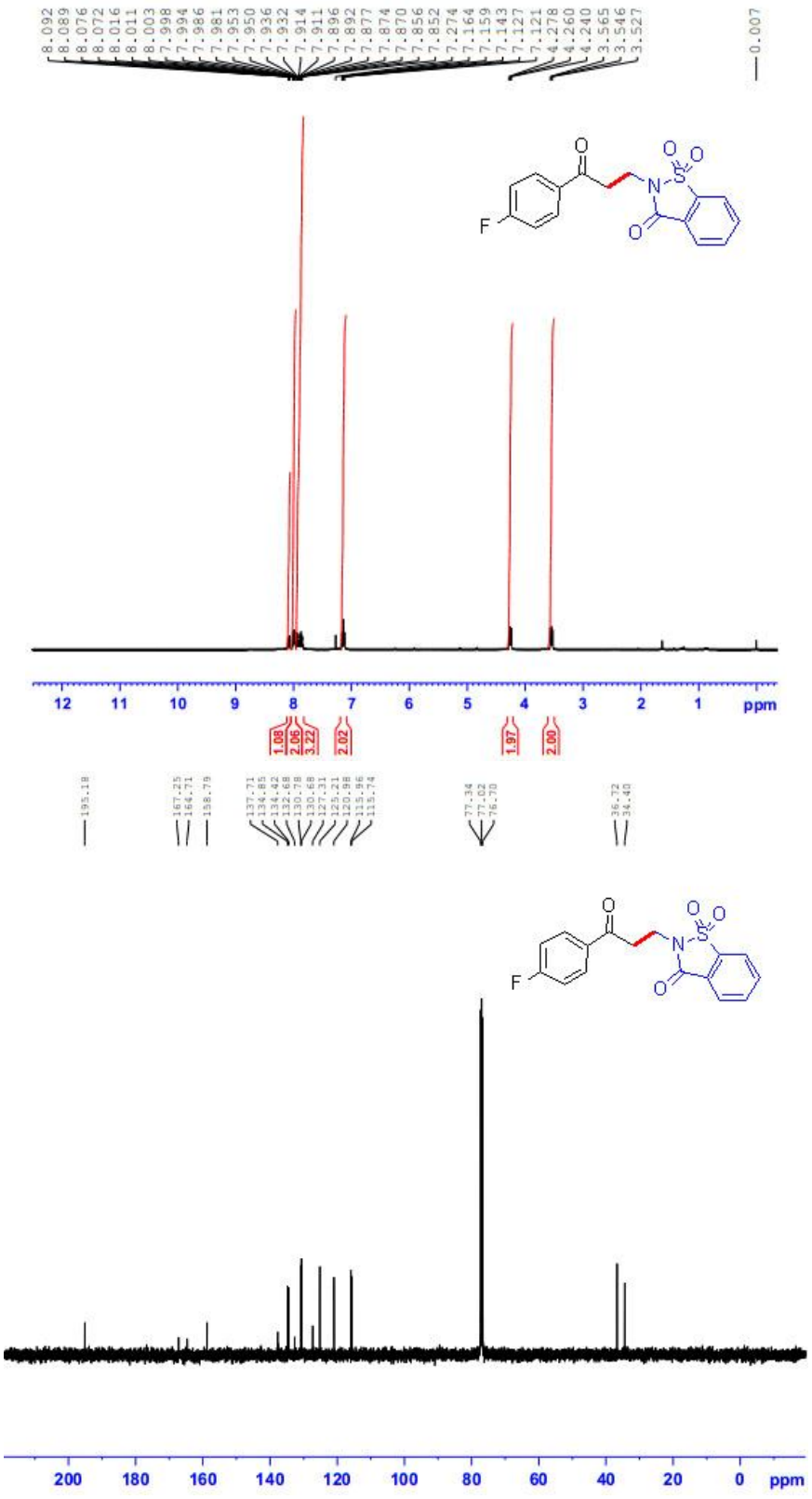
Compound 2k


8.098
8.081
8.078
7.951
7.934
7.910
7.890
7.873
7.869
7.854
7.850
7.315
7.294
7.274
4.283
4.264
4.245
3.575
3.556
3.537
2.592
2.571
2.564
2.543
1.879
1.864
1.787
1.756
1.603
1.595
1.486
1.450
1.431
1.422
1.410
1.398
1.387
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 ppm
0.99
0.99
3.97
1.97
2.00
2.01
1.06
4.02
1.09
4.15
1.15
196.44
158.78
154.24
137.79
134.76
134.35
134.11
128.48
127.80
127.18
126.18
120.55
77.32
77.21
77.00
76.68
44.70
36.70
34.58
34.05
26.69
26.01
200 180 160 140 120 100 80 60 40 20 0 ppm

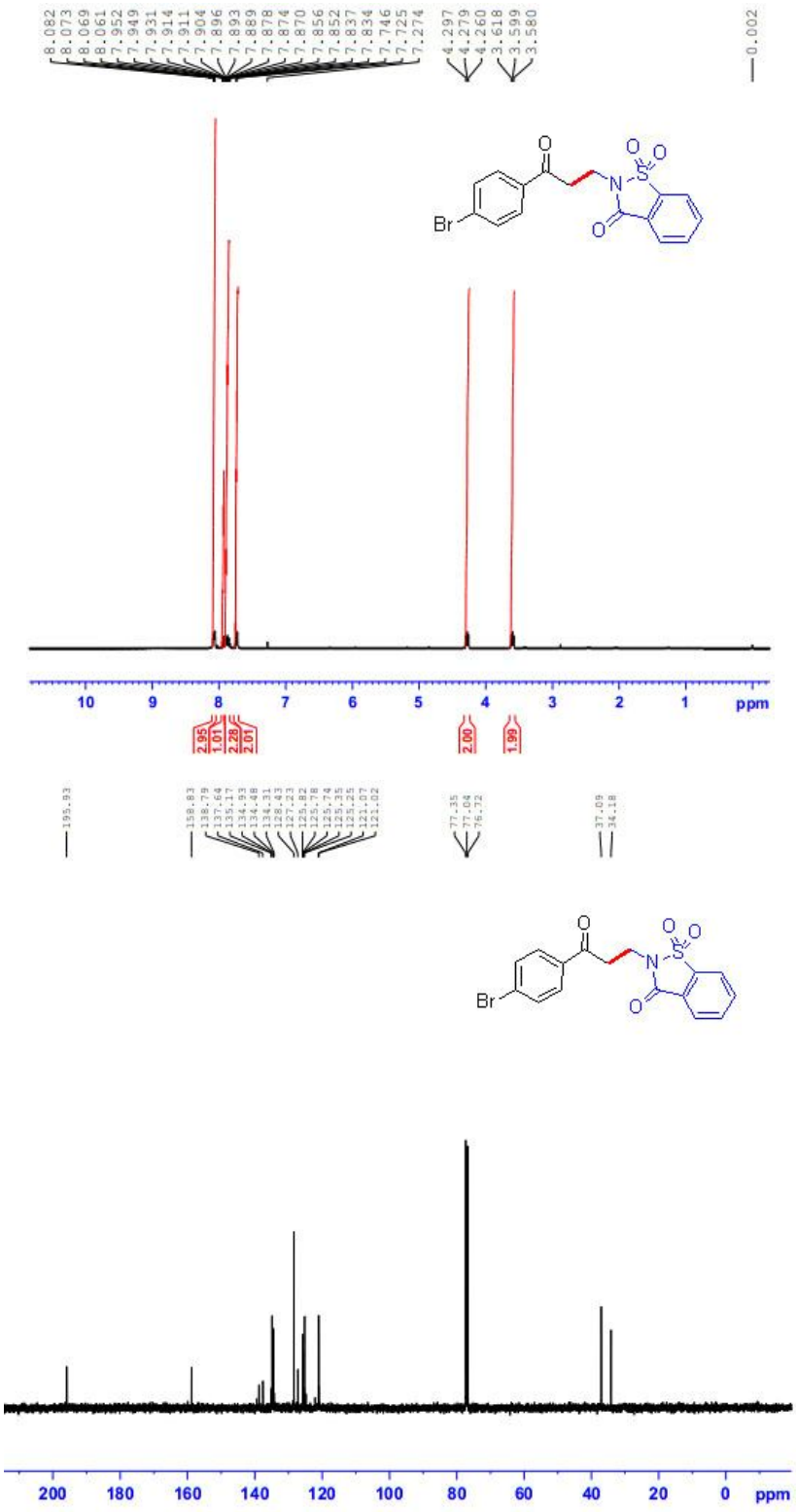
Compound 2l


8.110
8.107
8.094
8.090
8.062
8.040
7.962
7.945
7.901
7.898
7.881
7.877
7.862
7.859
7.713
7.692
7.650
7.646
7.628
7.502
7.485
7.465
7.433
7.414
7.274
4.323
4.304
4.285
3.638
3.618
3.599
1.594
11 10 9 8 7 6 5 4 3 2 1 ppm
1.02 1.95 0.97 2.12 2.00 2.03 2.00 1.01
2.00 2.01
196.37
158.81
146.21
139.76
137.78
134.83
134.80
134.39
128.95
128.66
128.30
127.38
127.34
127.24
125.21
120.98
77.32
77.00
76.68
36.86
34.54
200 180 160 140 120 100 80 60 40 20 0 ppm

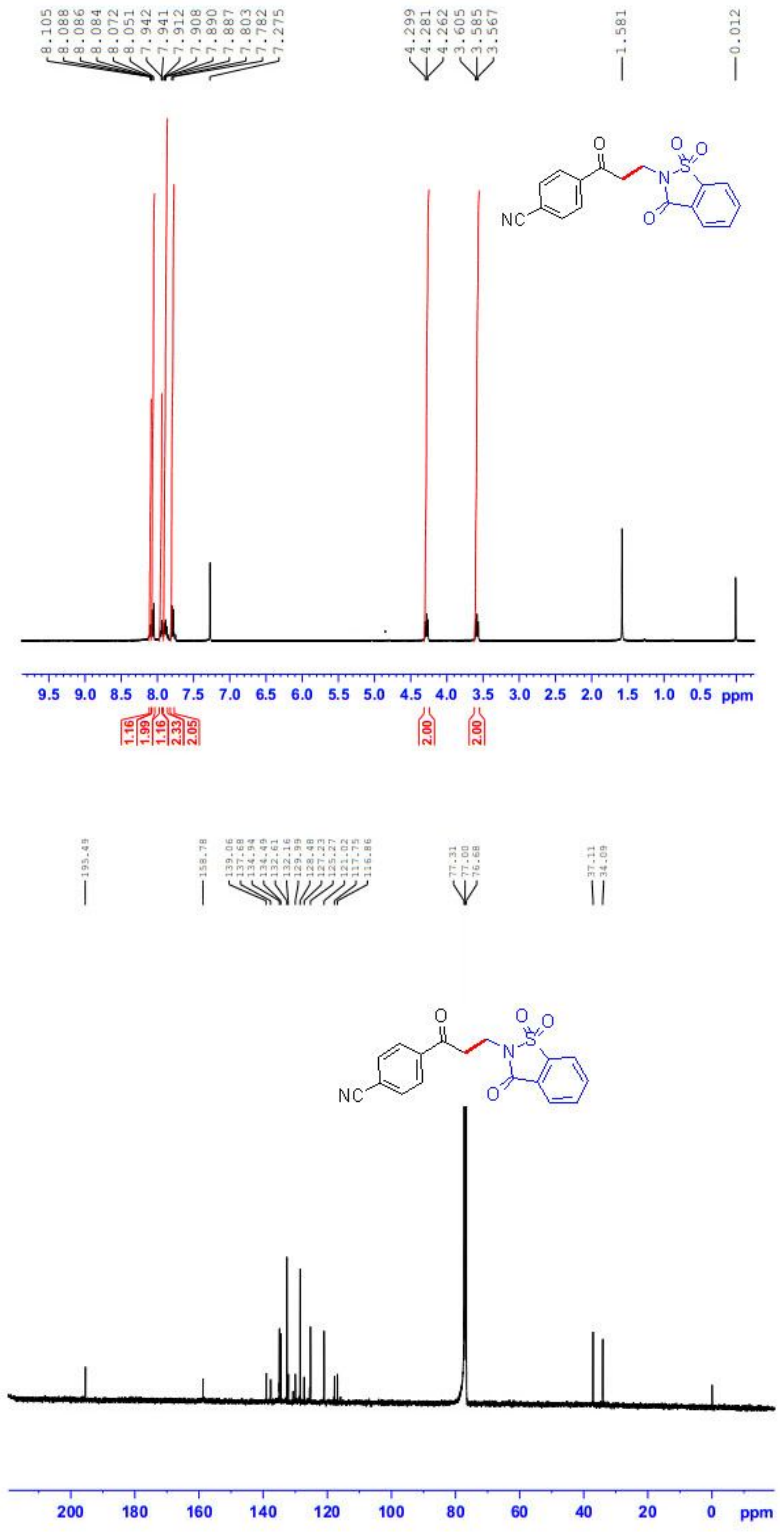
Compound 2m


8.092
8.089
8.076
8.072
8.016
8.011
8.003
7.998
7.994
7.986
7.981
7.953
7.950
7.936
7.932
7.914
7.911
7.896
7.892
7.877
7.874
7.870
7.856
7.852
7.274
7.164
7.159
7.143
7.127
7.121
4.278
4.260
4.240
3.565
3.546
3.527
0.007
F
O
O
O
N
S
O
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.08
1.06
3.22
2.02
1.97
2.00
195.18
167.25
164.71
158.79
137.71
134.85
134.42
132.68
130.78
130.68
127.31
125.21
120.98
115.96
115.74
77.34
77.02
76.70
36.72
34.40
200
180
160
140
120
100
80
60
40
20
0
ppm

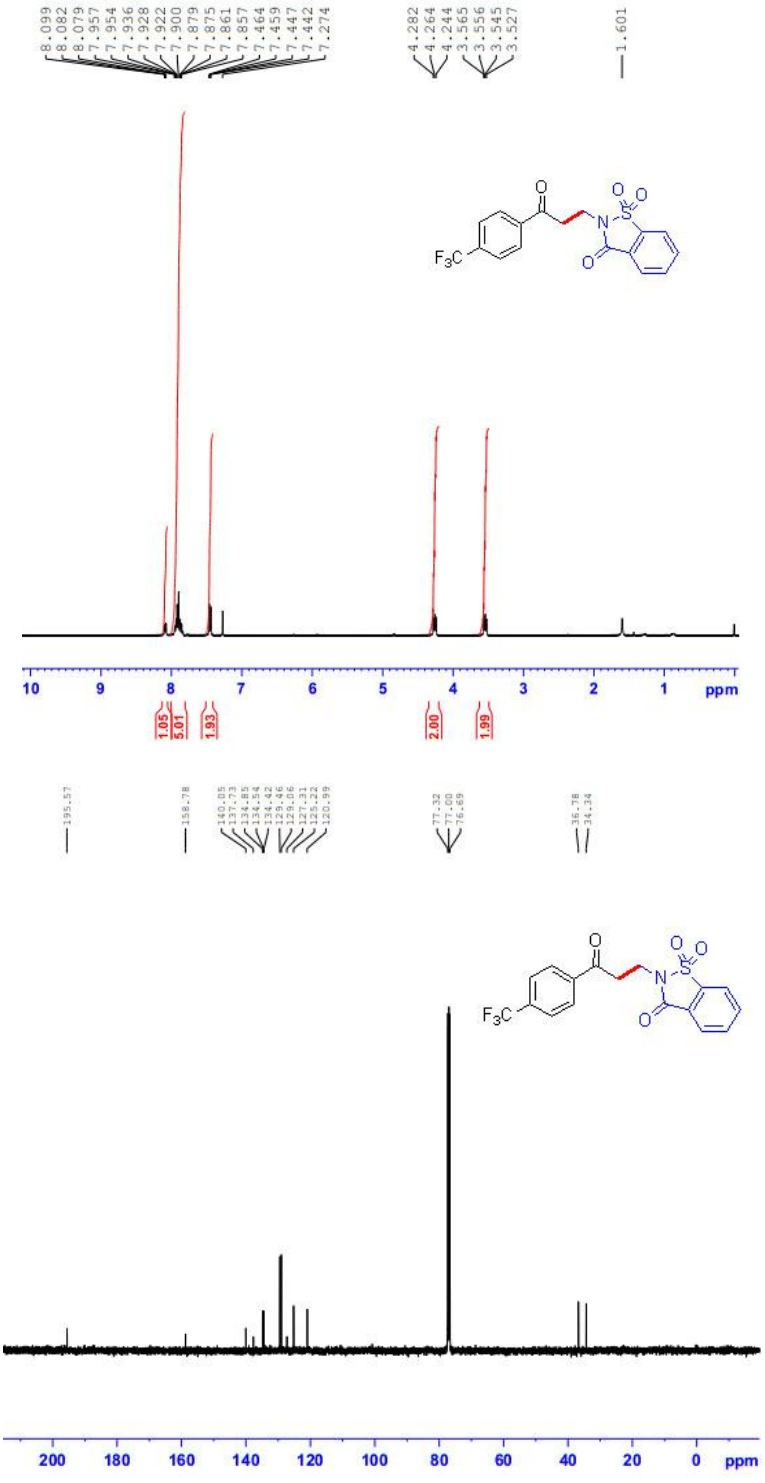
Compound 2n


8.082
8.073
8.069
8.061
7.952
7.949
7.931
7.914
7.911
7.904
7.896
7.893
7.889
7.878
7.874
7.870
7.856
7.852
7.837
7.834
7.746
7.725
7.274
4.297
4.279
4.260
3.618
3.599
3.580
0.002
Br
10
9
8
7
6
5
4
3
2
1
ppm
2.95
1.01
2.28
2.01
2.00
1.99
195.93
159.83
138.79
137.64
135.17
134.93
134.68
134.31
128.43
127.23
125.82
125.78
125.74
125.35
125.25
121.77
121.02
77.35
77.04
76.72
37.09
34.18
Br
200
180
160
140
120
100
80
60
40
20
0
ppm

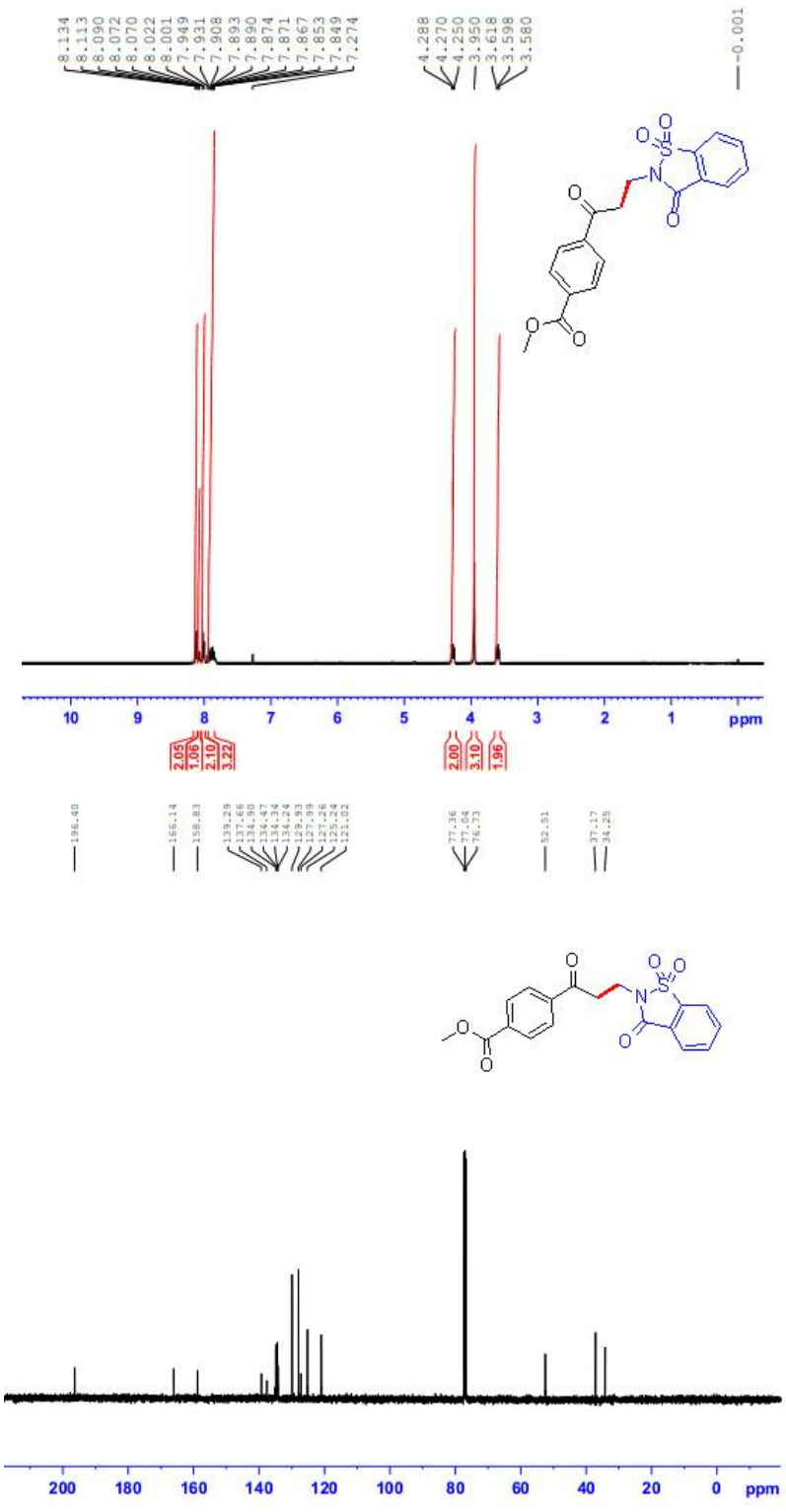
Compound 2o


8.105
8.088
8.086
8.084
8.072
8.051
7.942
7.941
7.912
7.908
7.890
7.887
7.803
7.782
7.275
4.299
4.281
4.262
3.605
3.585
3.567
1.581
0.012
NC
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 ppm
1.16
1.99
1.16
2.33
2.05
2.00
2.00
195.49
158.78
139.06
137.88
134.84
134.49
132.61
132.16
129.99
129.88
129.33
125.27
121.02
117.75
116.86
77.31
77.00
76.68
37.11
34.09
NC
200 180 160 140 120 100 80 60 40 20 0 ppm

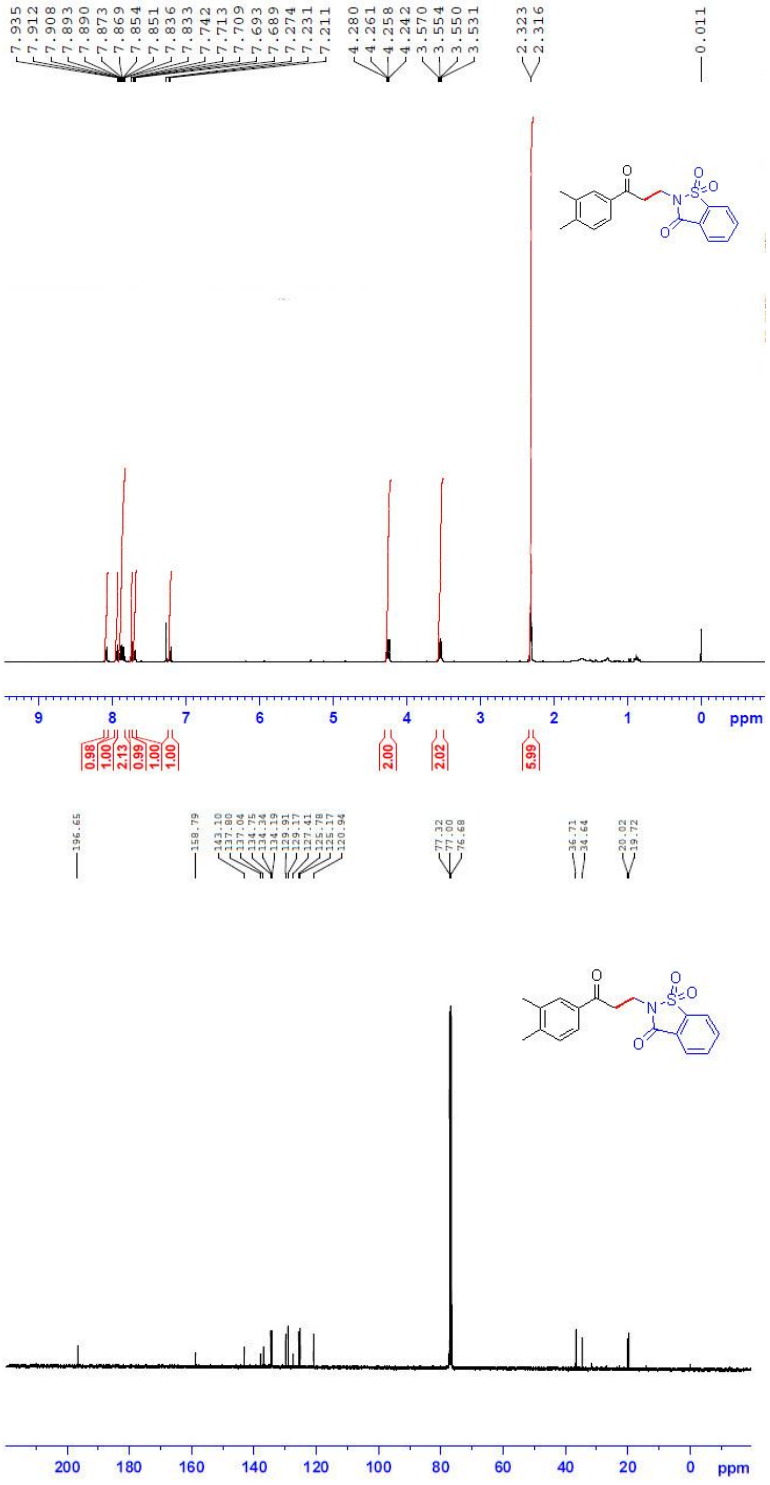
Compound 2p


8.099
8.082
8.079
7.957
7.954
7.936
7.928
7.922
7.900
7.879
7.875
7.861
7.857
7.464
7.459
7.447
7.442
7.274
4.282
4.264
4.244
3.565
3.556
3.545
3.527
1.601
F3C
10 9 8 7 6 5 4 3 2 1 ppm
1.05
5.01
1.93
2.00
1.99
195.57
158.78
140.05
137.73
134.85
134.54
134.42
129.46
129.06
128.31
127.22
120.99
77.32
77.00
76.69
36.78
34.34
F3C
200 180 160 140 120 100 80 60 40 20 0 ppm

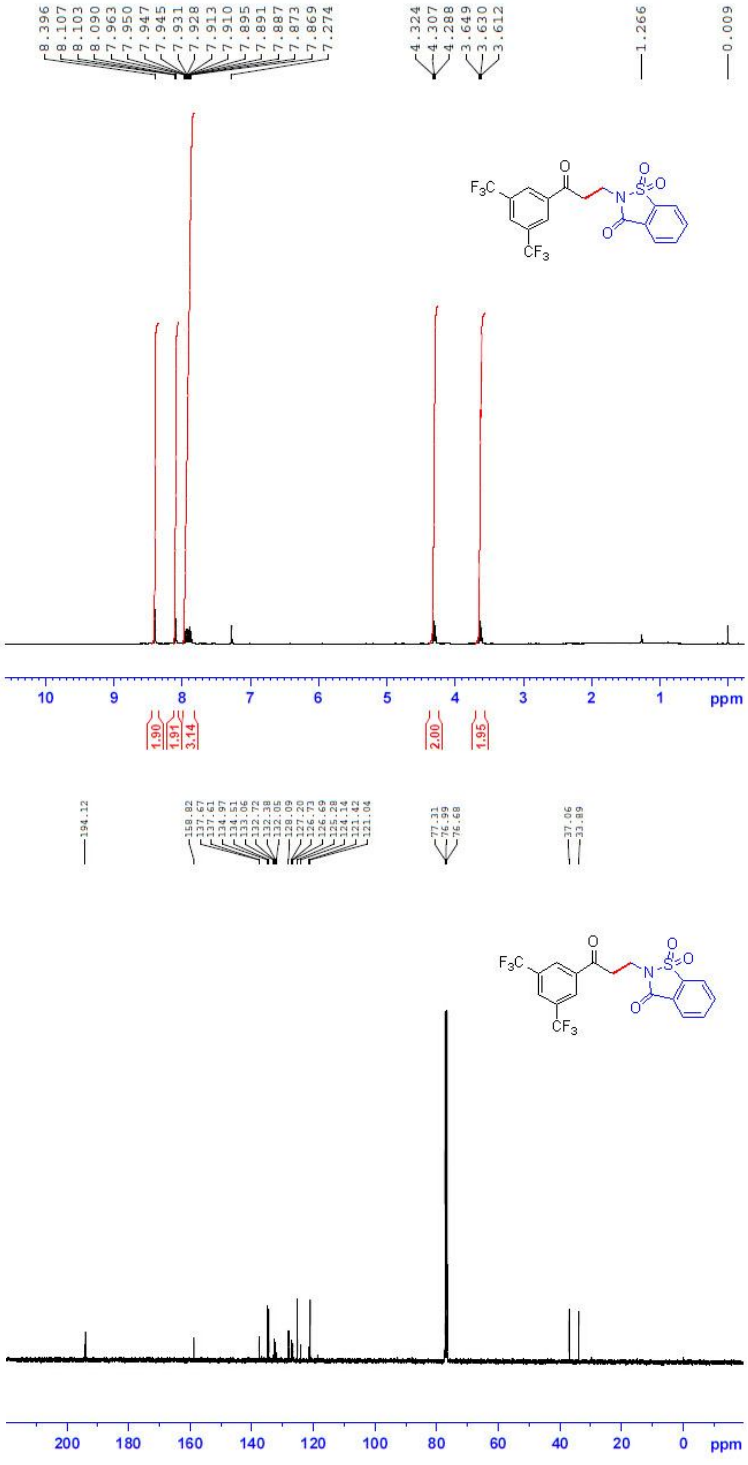
Compound 2q


8.134
8.113
8.090
8.072
8.070
8.022
8.001
7.949
7.931
7.908
7.893
7.890
7.874
7.871
7.867
7.853
7.849
7.274
4.288
4.270
4.250
3.950
3.618
3.598
3.580
-0.001
10
9
8
7
6
5
4
3
2
1
ppm
2.05
1.06
2.10
3.22
2.00
3.10
1.96
196.40
166.14
158.83
139.29
137.66
134.90
134.47
134.34
134.24
129.93
127.99
127.26
125.24
121.02
77.36
77.04
76.73
52.51
37.17
34.25
200
180
160
140
120
100
80
60
40
20
0
ppm

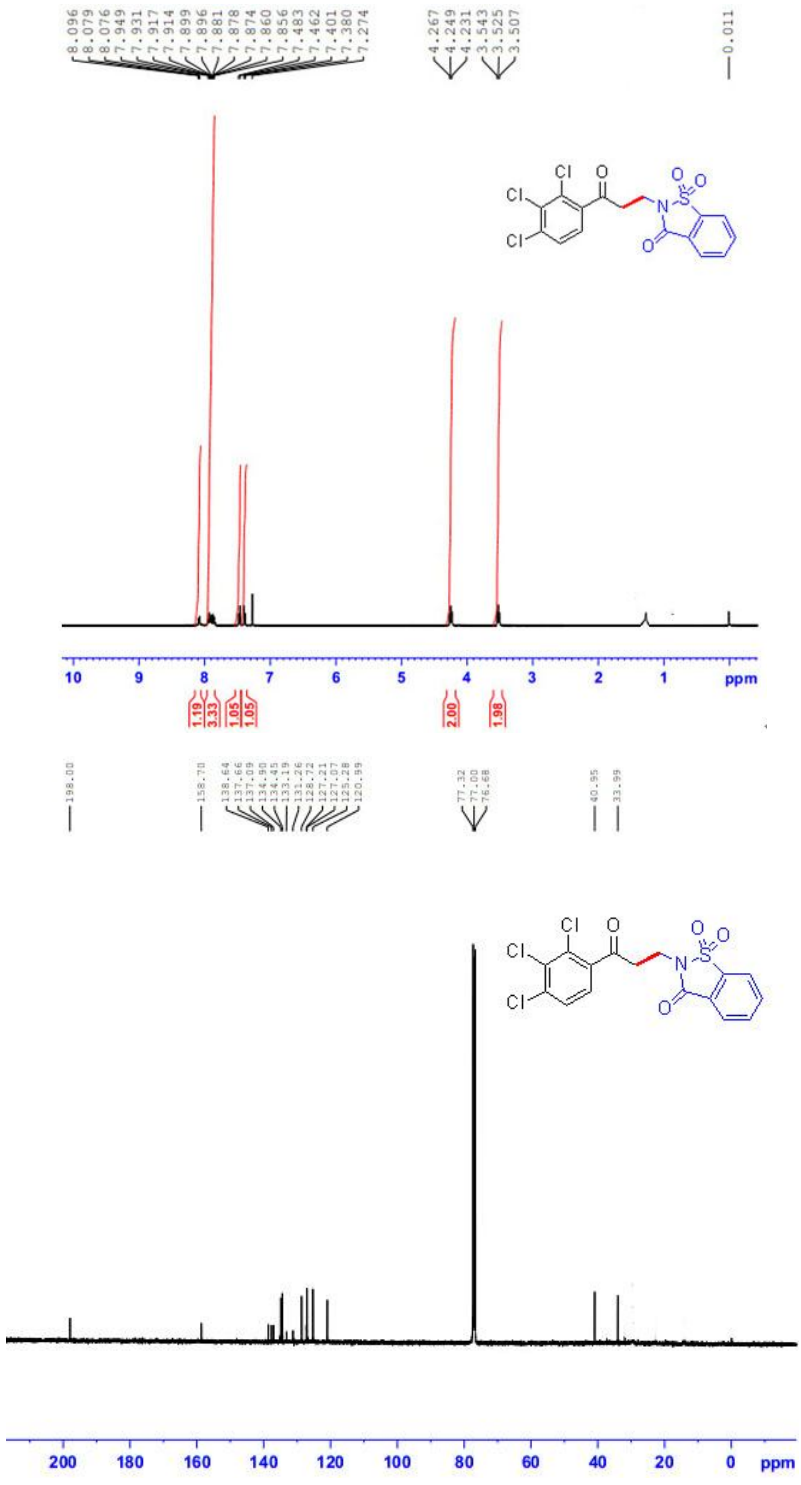
Compound 2r


7.935
7.912
7.908
7.893
7.890
7.873
7.869
7.854
7.851
7.836
7.833
7.742
7.713
7.709
7.693
7.689
7.274
7.231
7.211
4.280
4.261
4.258
4.242
3.570
3.554
3.550
3.531
2.323
2.316
0.011
ppm
0.98
1.00
2.13
0.99
1.00
1.00
2.00
2.02
5.99
196.65
158.79
143.10
137.80
137.04
134.75
134.34
134.19
132.31
129.17
127.41
125.78
125.37
120.84
77.32
77.00
76.68
36.71
34.64
20.02
19.72
ppm

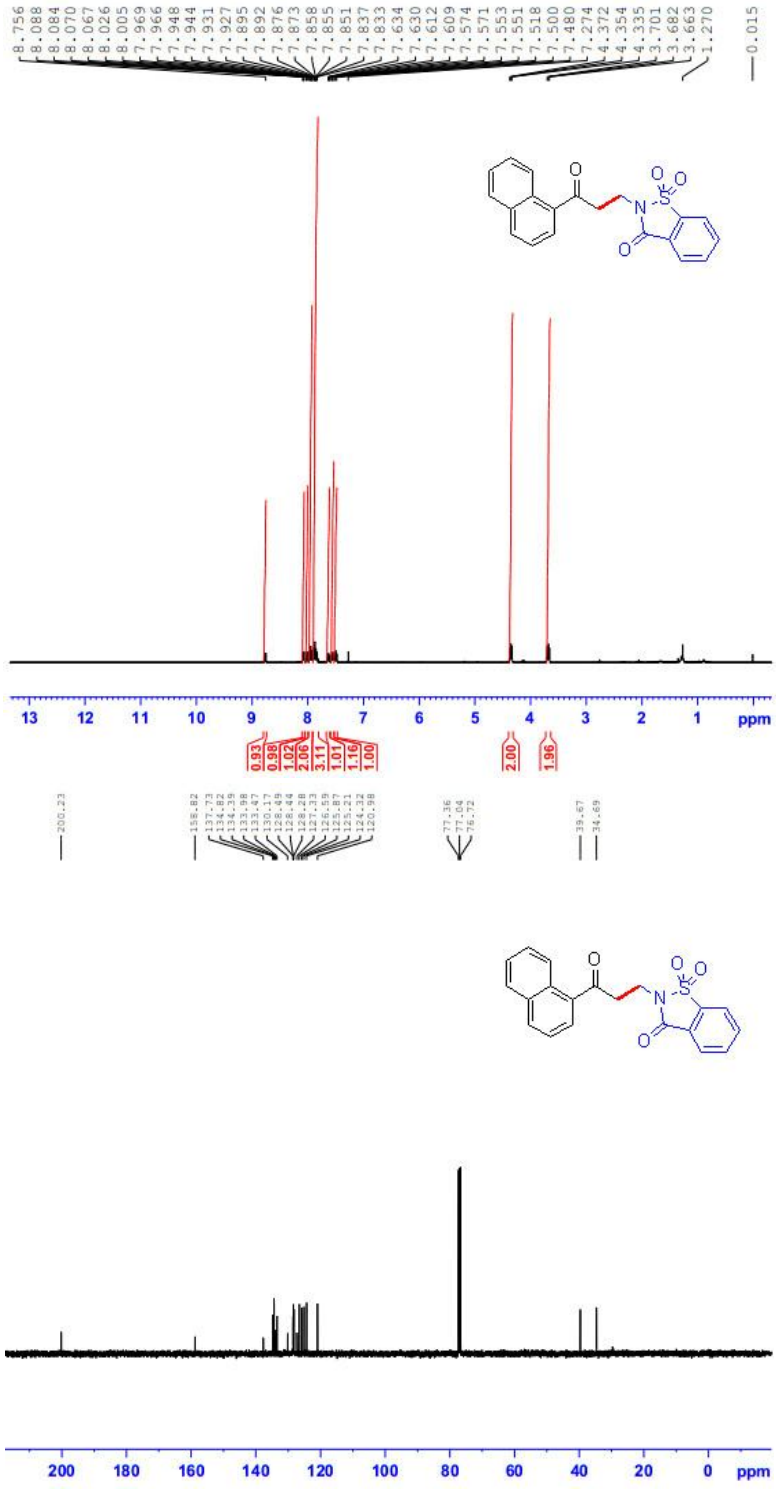
Compound 2s


8.396
8.107
8.103
8.090
7.963
7.950
7.947
7.945
7.931
7.928
7.913
7.910
7.895
7.891
7.887
7.873
7.869
7.274
4.324
4.307
4.288
3.649
3.630
3.612
1.266
0.009
F3C
CF3
O
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
1.90
1.91
3.14
2.00
1.96
194.12
158.82
137.67
137.61
134.97
134.51
133.06
132.78
132.38
132.05
128.09
127.20
126.73
126.69
125.28
124.14
121.42
121.04
77.31
76.99
76.68
37.06
33.89
200
180
160
140
120
100
80
60
40
20
0
ppm

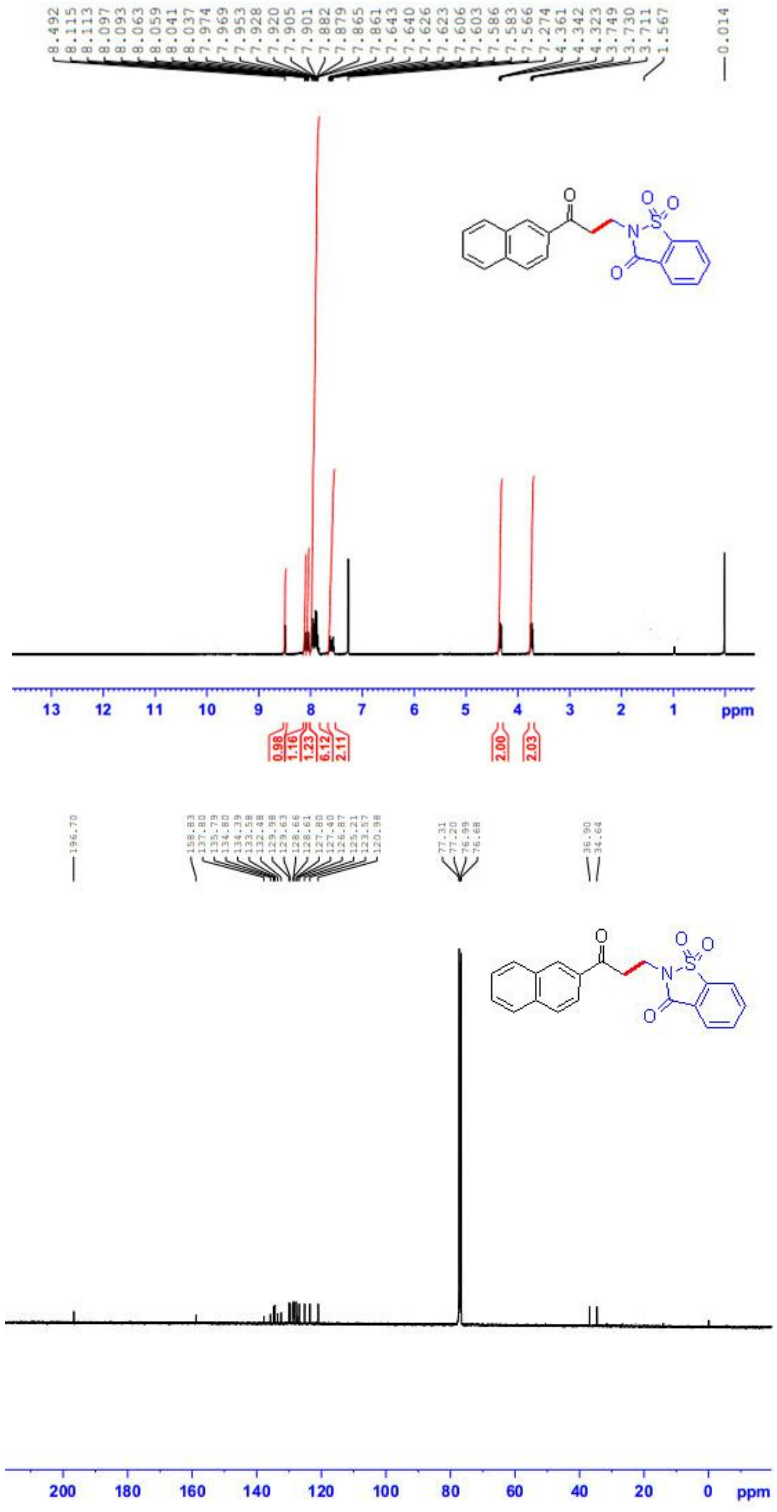
Compound 2t


8.096
8.079
8.076
7.949
7.931
7.917
7.914
7.899
7.896
7.881
7.878
7.874
7.860
7.856
7.483
7.462
7.401
7.380
7.274
4.267
4.249
4.231
3.543
3.525
3.507
0.011
Cl
Cl
Cl
O
O
O
O
N
S
10
9
8
7
6
5
4
3
2
1
ppm
1.19
3.33
1.05
1.05
2.00
1.98
198.00
158.70
138.64
137.66
137.09
134.90
134.45
133.19
131.26
128.72
128.21
127.07
125.28
120.99
77.32
77.00
76.68
40.95
33.99
200
180
160
140
120
100
80
60
40
20
0
ppm

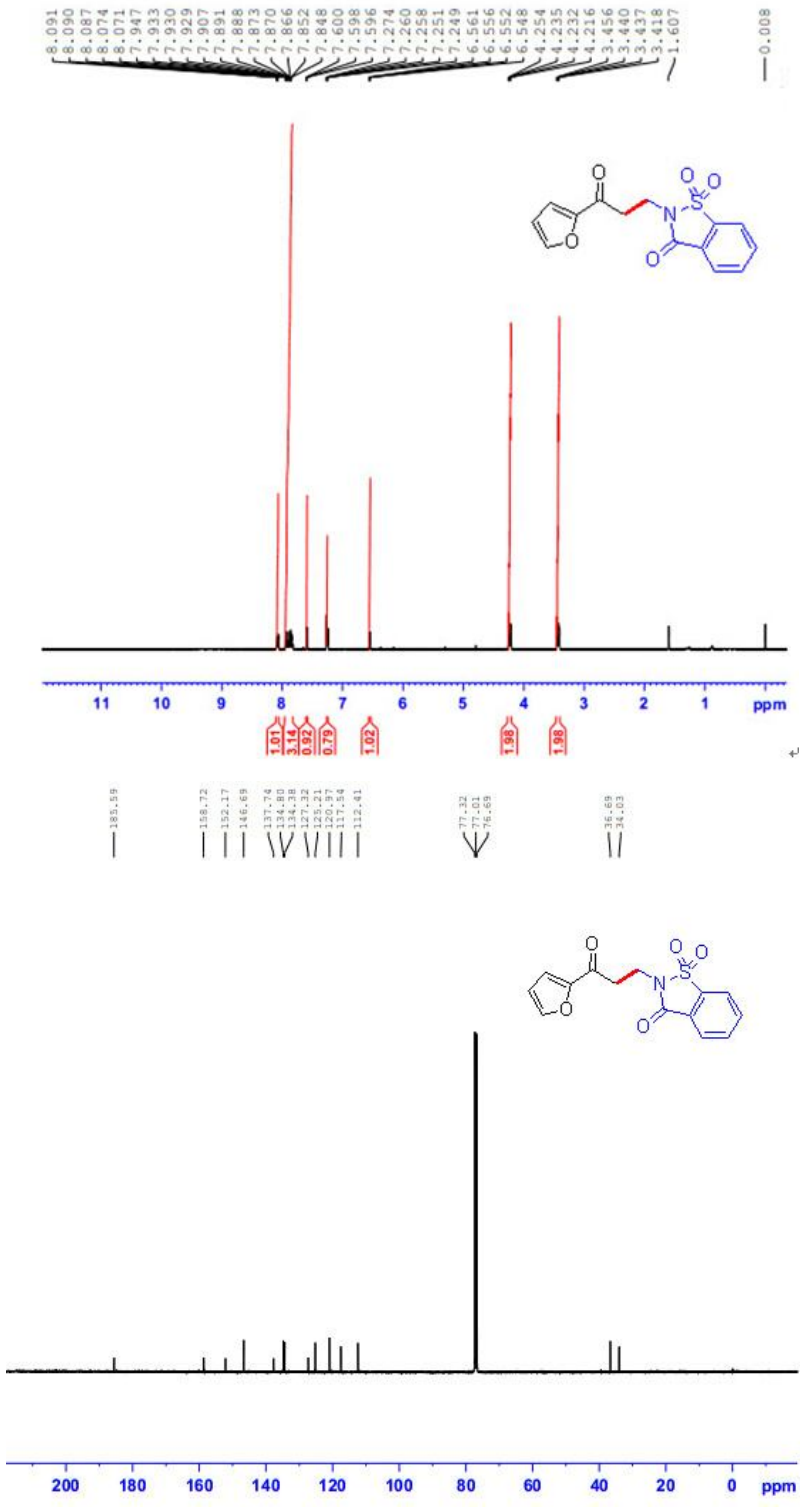
Compound 2u



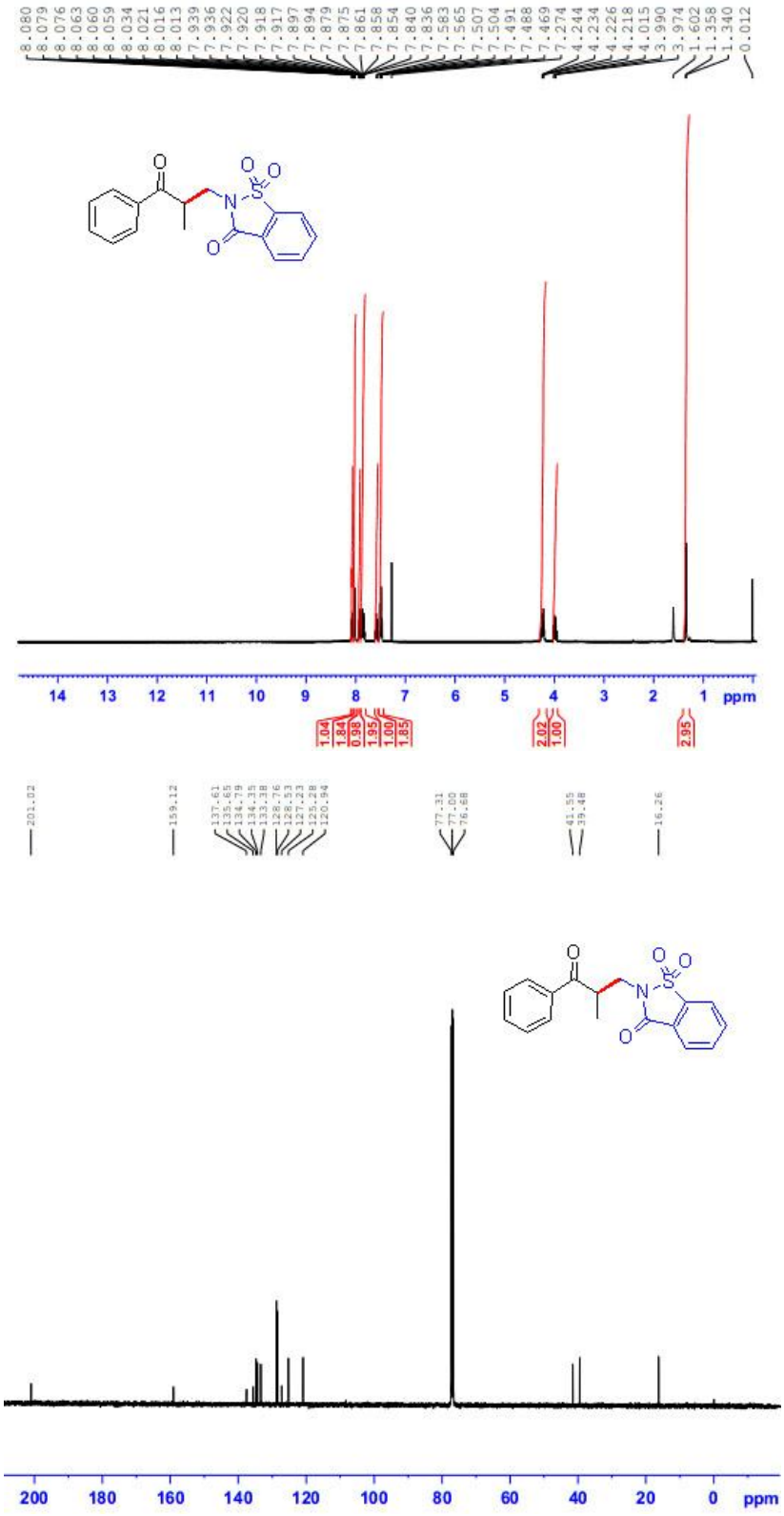
Compound 2v


8.492
8.115
8.113
8.097
8.093
8.063
8.059
8.041
8.037
7.974
7.969
7.953
7.928
7.920
7.905
7.901
7.882
7.879
7.865
7.861
7.643
7.640
7.626
7.623
7.606
7.603
7.586
7.583
7.566
7.274
4.361
4.342
4.323
3.749
3.730
3.711
1.567
0.014
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.98 1.16 1.23 6.12 2.11 2.00 2.03
196.70
158.83
137.80
135.79
134.20
134.39
133.58
132.48
129.88
129.63
128.66
128.61
127.80
127.40
126.87
125.21
124.27
120.98
77.31
77.20
76.99
76.68
36.90
34.64
200 180 160 140 120 100 80 60 40 20 0 ppm

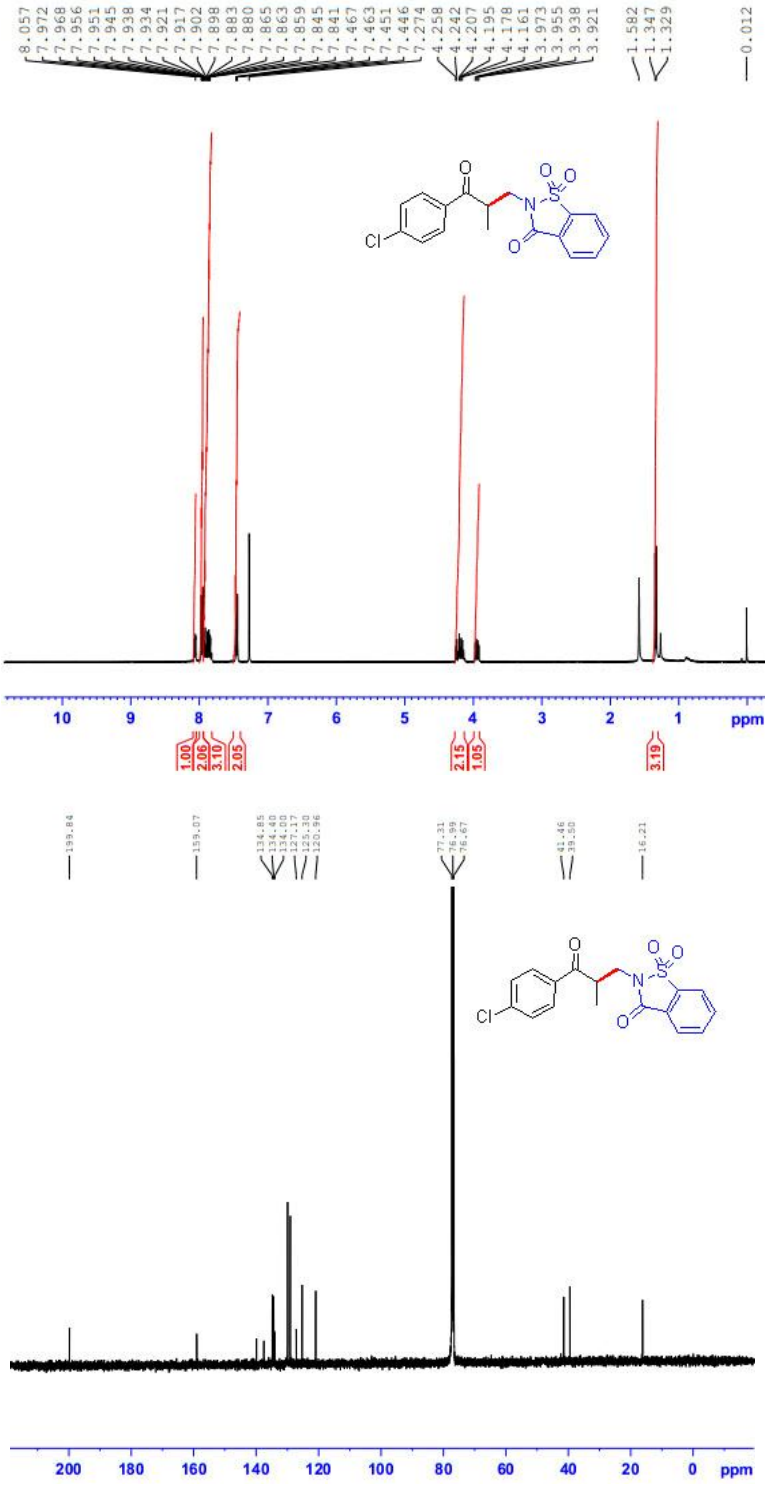
Compound 2w


8.091
8.090
8.087
8.074
8.071
7.947
7.933
7.930
7.929
7.907
7.891
7.888
7.873
7.870
7.866
7.852
7.848
7.600
7.598
7.596
7.274
7.260
7.258
7.251
7.249
6.561
6.556
6.552
6.548
4.254
4.235
4.232
4.216
3.456
3.440
3.437
3.418
11.607
0.008
11 10 9 8 7 6 5 4 3 2 1 ppm
1.01
3.14
0.92
0.79
1.02
1.98
1.98
185.59
158.72
152.17
146.69
137.74
134.80
134.38
127.32
125.21
120.97
117.54
112.41
77.32
77.01
76.69
36.69
34.03
200 180 160 140 120 100 80 60 40 20 0 ppm

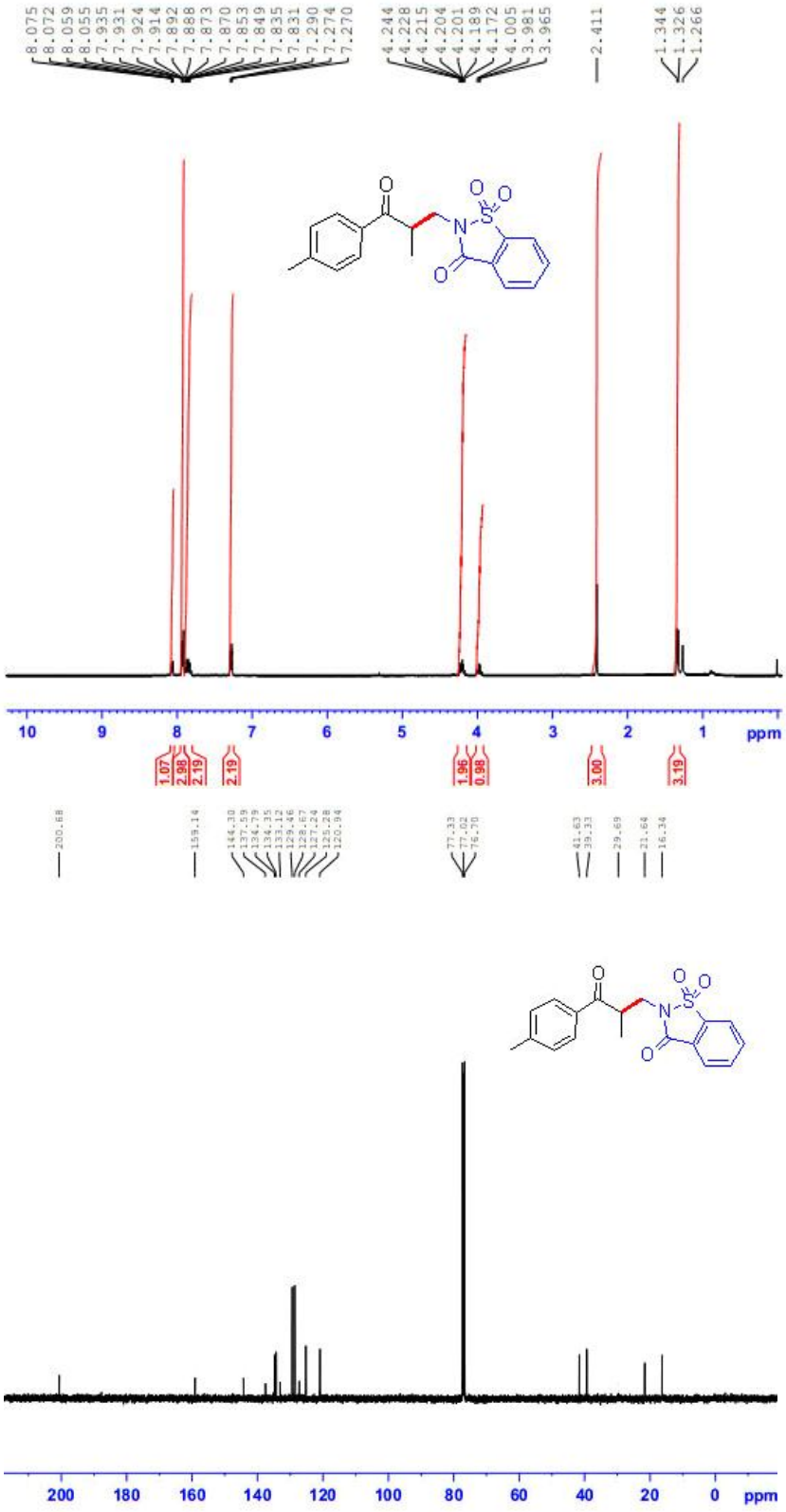
Compound 4a



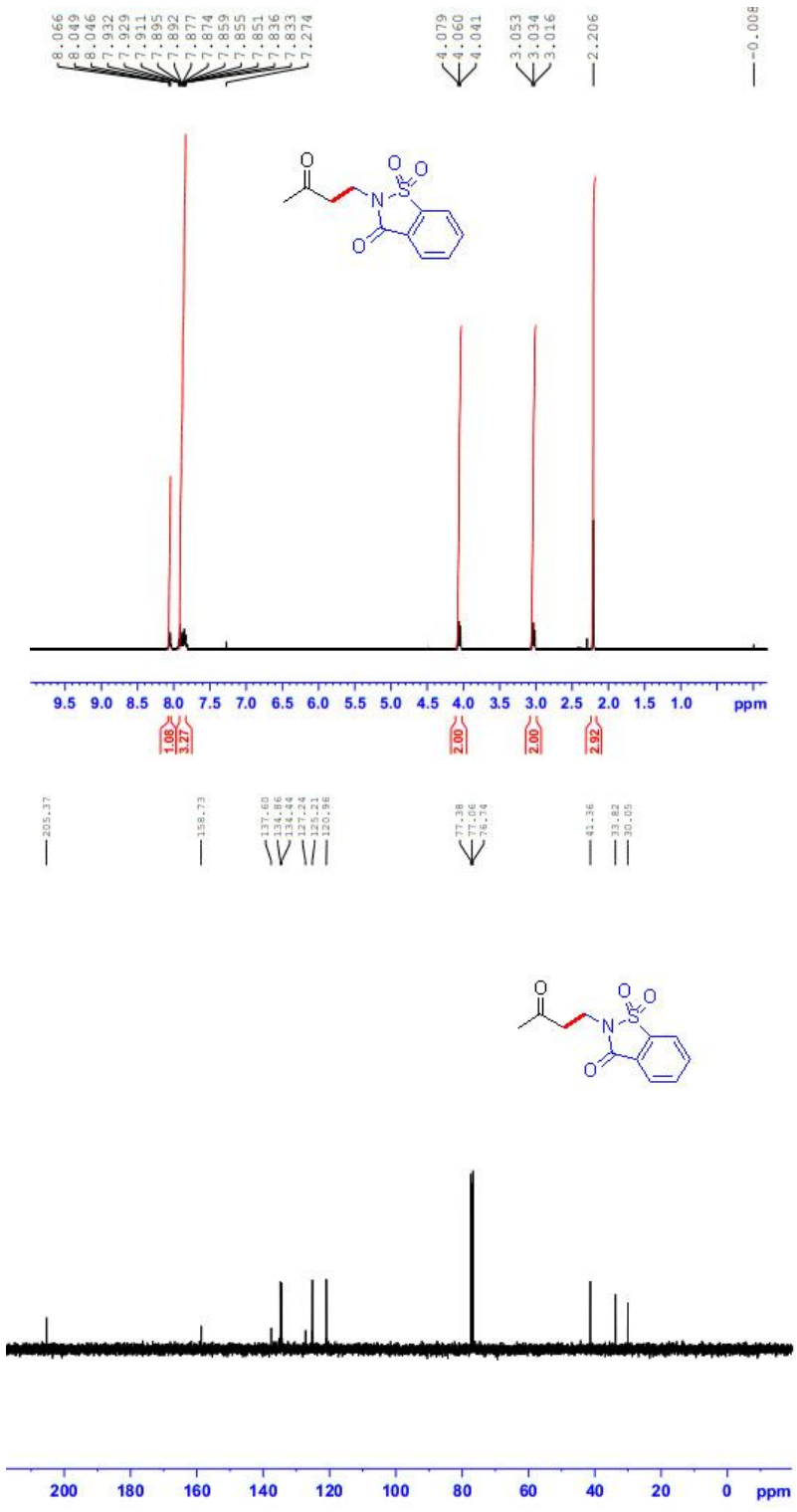
Compound 4b


8.057
7.972
7.968
7.956
7.951
7.945
7.938
7.934
7.921
7.917
7.902
7.898
7.883
7.880
7.865
7.863
7.859
7.845
7.841
7.467
7.463
7.451
7.446
7.274
4.258
4.242
4.207
4.195
4.178
4.161
3.973
3.955
3.938
3.921
1.582
1.347
1.329
0.012
Cl
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.06
3.10
2.05
2.15
1.05
3.19
199.84
159.07
134.85
134.40
134.00
127.17
125.30
120.96
77.31
76.99
76.67
41.46
39.50
16.21
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

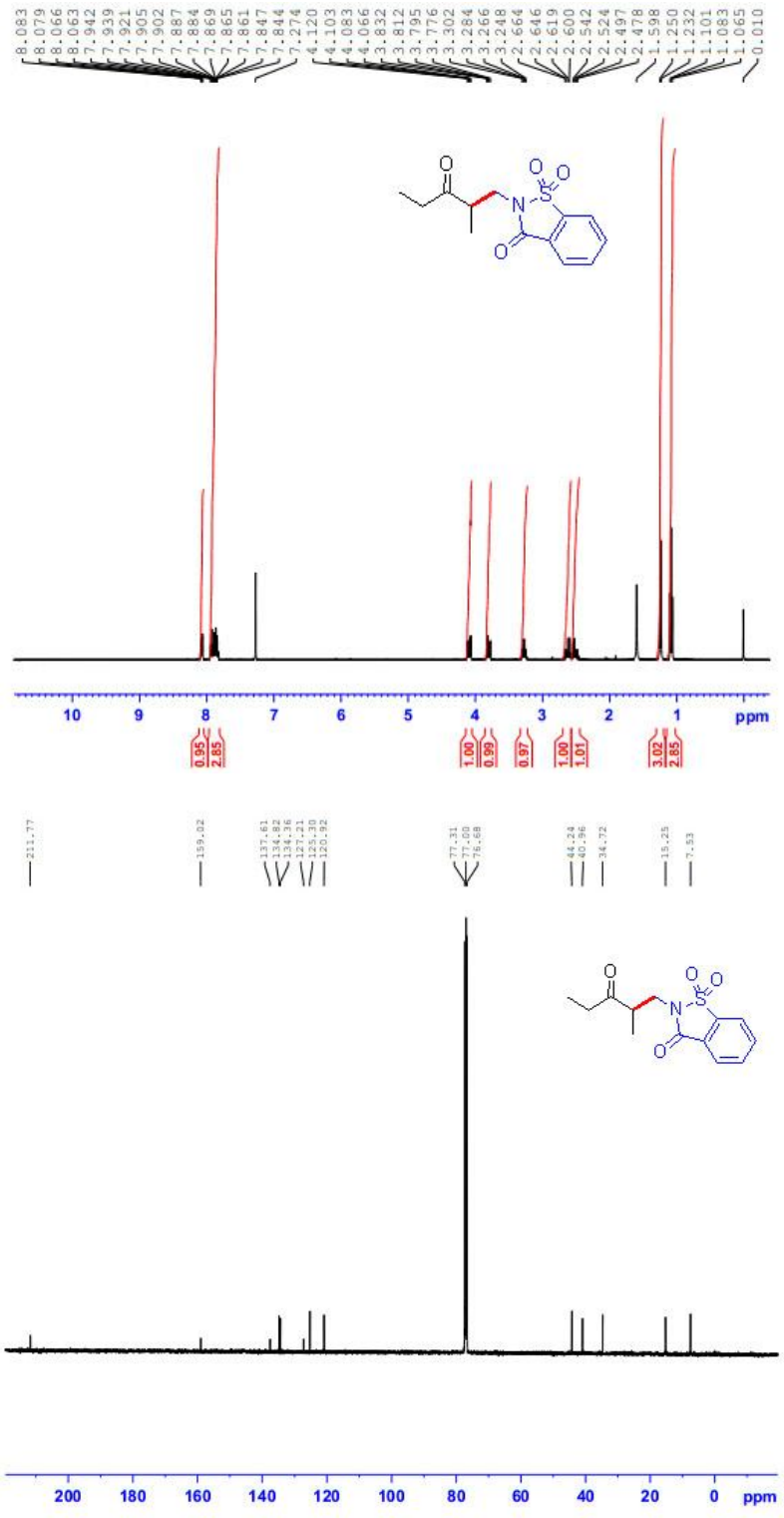
Compound 4c


8.075
8.072
8.059
8.055
7.935
7.931
7.924
7.914
7.892
7.888
7.873
7.870
7.853
7.849
7.835
7.831
7.290
7.274
7.270
4.244
4.228
4.215
4.204
4.201
4.189
4.172
4.005
3.981
3.965
2.411
1.344
1.326
1.266
10 9 8 7 6 5 4 3 2 1 ppm
1.07
2.08
2.19
2.19
1.96
0.98
3.00
3.19
200.68
159.14
144.30
137.59
134.79
134.35
133.12
129.46
128.67
127.74
125.28
120.94
77.33
77.02
76.70
41.63
39.33
29.69
21.64
16.34
200 180 160 140 120 100 80 60 40 20 0 ppm

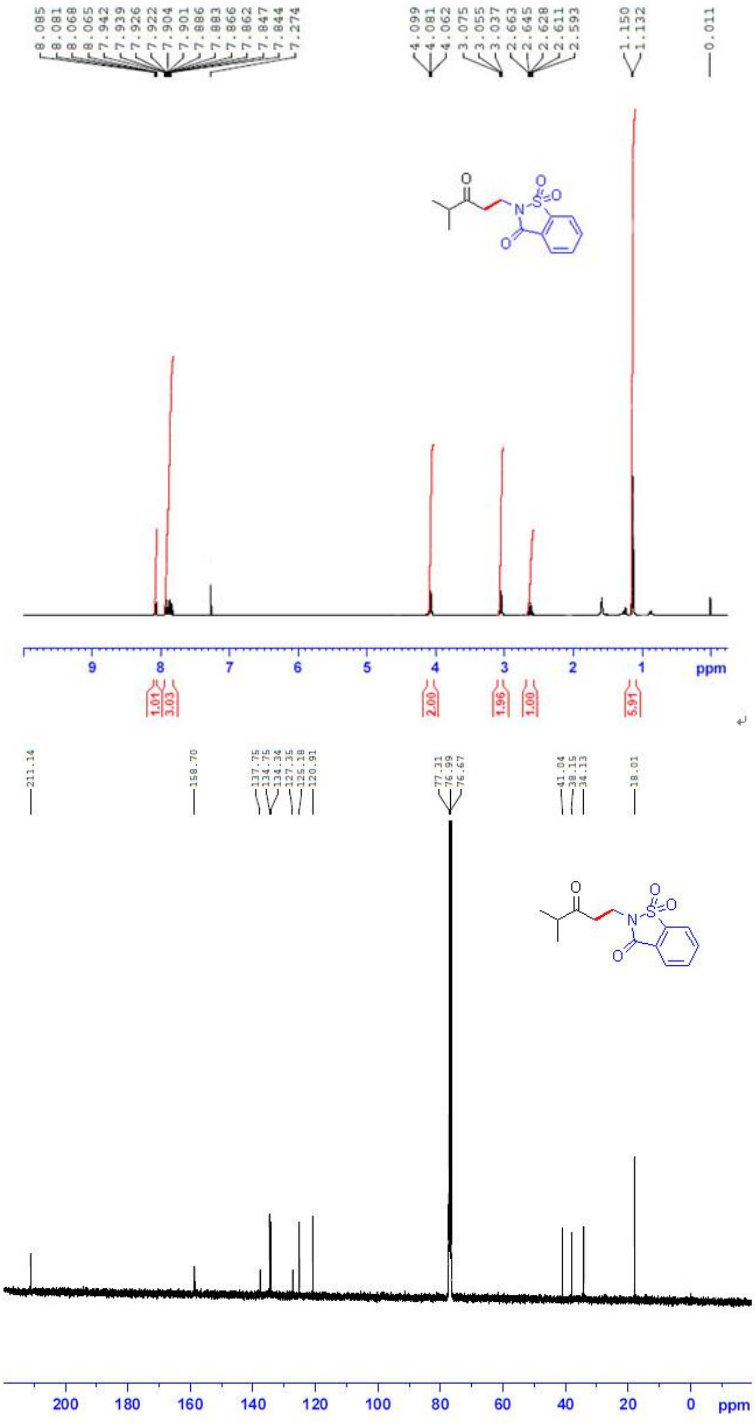
Compound 4d


8.066
8.049
8.046
7.932
7.929
7.911
7.895
7.892
7.877
7.874
7.859
7.855
7.851
7.836
7.833
7.274
4.079
4.060
4.041
3.053
3.034
3.016
2.206
-0.008
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 ppm
1.00
3.27
2.00
2.00
2.92
205.37
158.73
137.60
134.86
134.44
127.24
125.21
120.96
77.38
77.06
76.74
41.36
33.82
30.05
200 180 160 140 120 100 80 60 40 20 0 ppm

Compound 4e

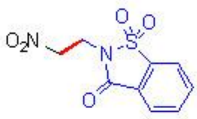

8.083
8.079
8.066
8.063
7.942
7.939
7.921
7.905
7.902
7.887
7.884
7.869
7.865
7.861
7.847
7.844
7.274
4.120
4.103
4.083
4.066
3.832
3.812
3.795
3.776
3.302
3.284
3.266
3.248
2.664
2.646
2.619
2.600
2.542
2.524
2.497
2.478
1.598
1.250
1.232
1.101
1.083
1.065
0.010
10
9
8
7
6
5
4
3
2
1
ppm
0.95
2.85
1.00
0.99
0.97
1.00
1.01
3.02
2.85
211.77
159.02
137.61
134.82
134.36
127.21
125.30
120.92
77.31
77.00
76.68
44.24
40.96
34.72
15.25
7.53
200
180
160
140
120
100
80
60
40
20
0
ppm

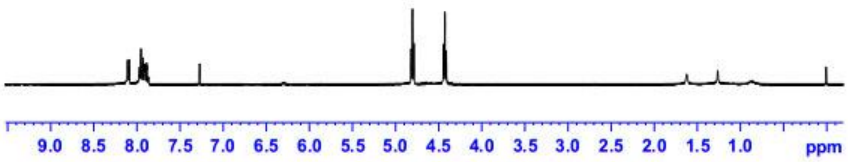
Compound 4f


8.085
8.081
8.068
8.065
7.942
7.939
7.926
7.922
7.904
7.901
7.886
7.883
7.866
7.862
7.847
7.844
7.274
4.099
4.081
4.062
3.075
3.055
3.037
2.663
2.645
2.628
2.611
2.593
1.150
1.132
0.011
ppm
1.01
3.03
2.00
1.96
1.00
5.91
211.14
168.70
137.75
134.75
134.34
127.35
125.18
120.91
77.31
77.00
76.67
41.04
38.16
34.13
18.01
ppm

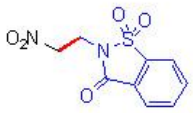
Compound 4g

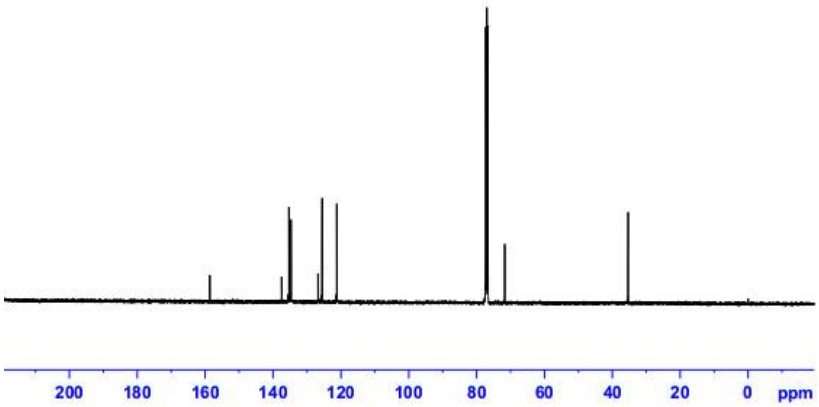

8.108
8.091
7.956
7.952
7.947
7.931
7.929
7.905
7.901
7.887
7.883
4.821
4.805
4.790
4.445
4.430
4.414


O2N
N
S
O
O
O

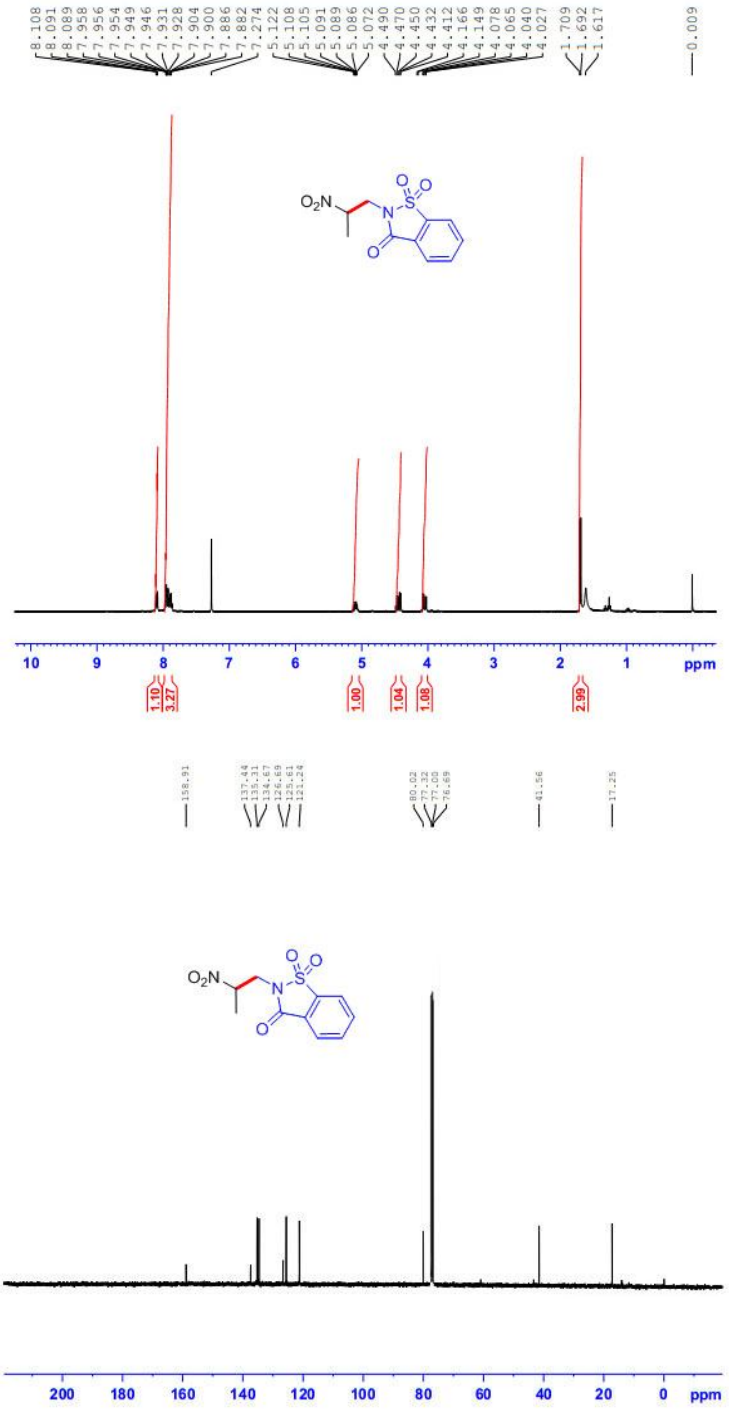

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


158.67
137.49
135.32
134.70
126.75
126.57
121.23
77.33
77.01
76.69
71.74
35.38

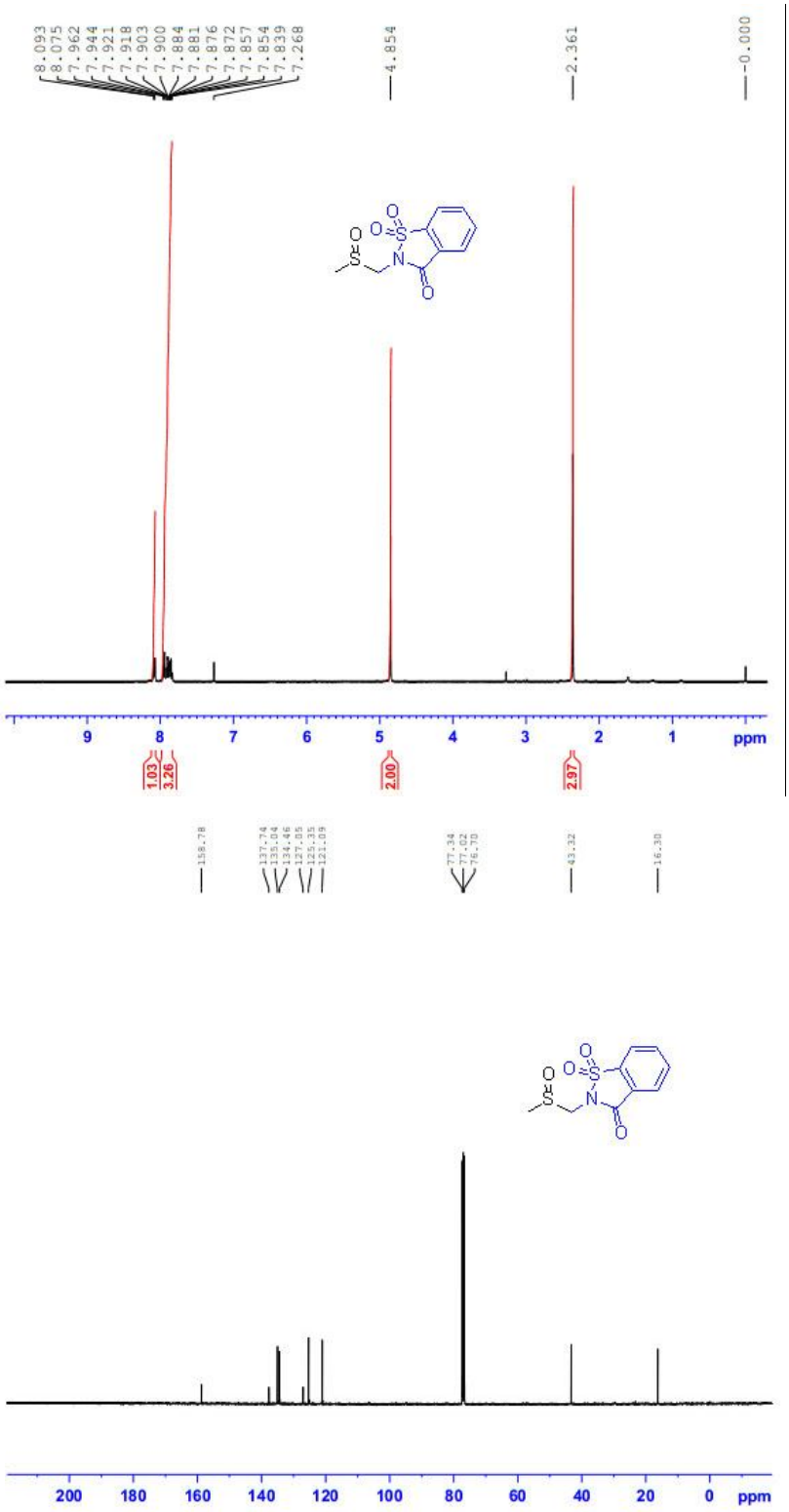

O2N
N
S
O
O
O


200 180 160 140 120 100 80 60 40 20 0 ppm

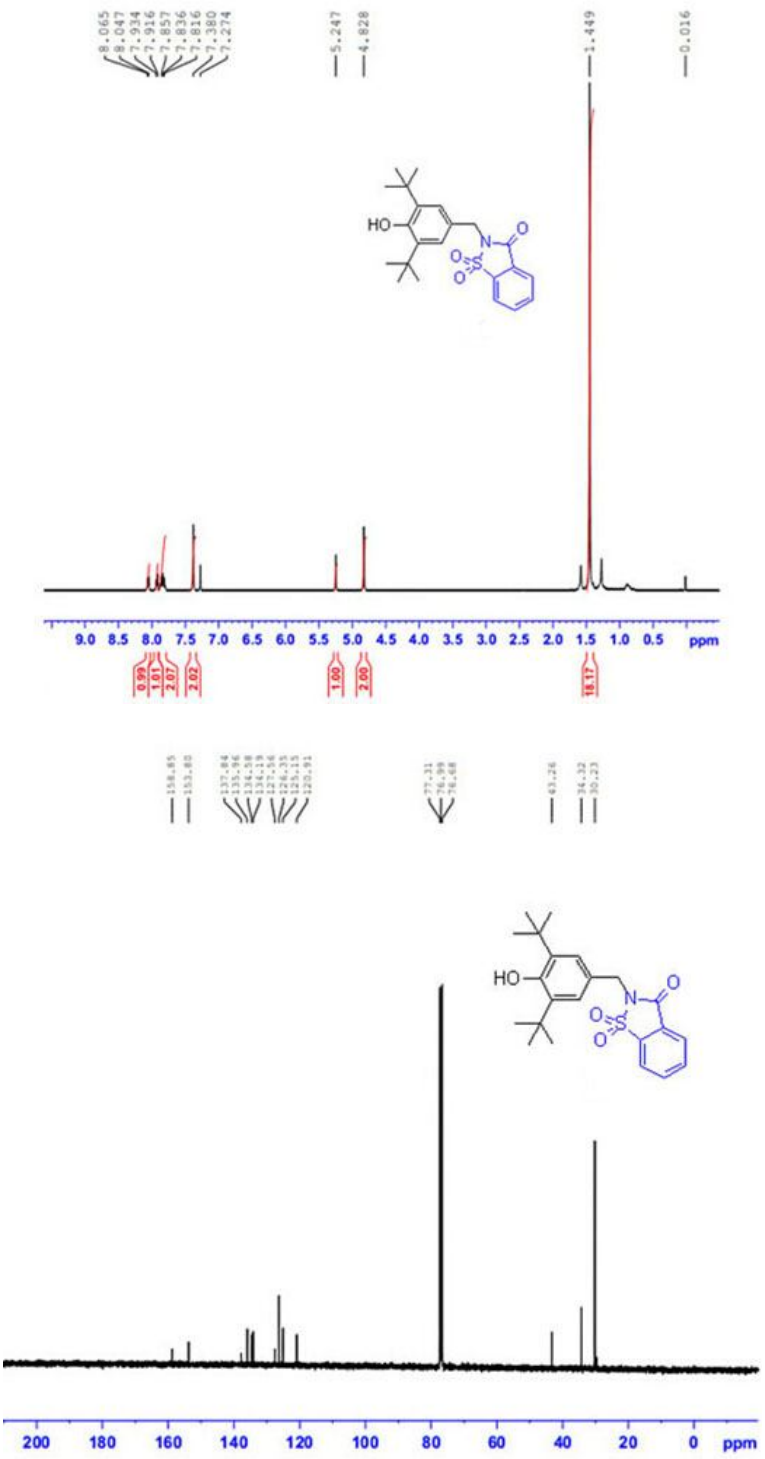
Compound 4h


8.108
8.091
8.089
7.958
7.956
7.954
7.949
7.946
7.931
7.928
7.904
7.900
7.886
7.882
7.274
5.122
5.108
5.105
5.091
5.089
5.086
5.072
4.490
4.470
4.450
4.432
4.412
4.166
4.149
4.078
4.065
4.040
4.027
1.709
1.692
1.617
0.009
O2N
10 9 8 7 6 5 4 3 2 1 ppm
1.10
3.27
1.00
1.04
1.08
2.99
158.91
137.44
135.31
134.67
126.69
125.61
121.24
80.02
77.32
77.00
76.69
41.56
17.25
O2N
200 180 160 140 120 100 80 60 40 20 0 ppm

Compound C


8.093
8.075
7.962
7.944
7.921
7.918
7.903
7.900
7.884
7.881
7.876
7.872
7.857
7.854
7.839
7.268
4.854
2.361
0.000
9
8
7
6
5
4
3
2
1
ppm
1.03
3.26
2.00
2.97
158.78
137.74
135.04
134.46
127.05
125.35
121.09
77.34
77.02
76.70
43.32
16.30
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound H


8.065
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
O
N
O
O
S
O
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
158.85
153.80
137.84
135.96
134.58
134.18
127.54
126.35
125.15
120.91
77.31
76.99
76.68
63.26
34.32
30.23
HO
O
N
O
O
S
O
200 180 160 140 120 100 80 60 40 20 0 ppm