Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Rhodium-catalyzed benzoisothiazoles synthesis by tandem annulation reactions of sulfoximines and activated olefins

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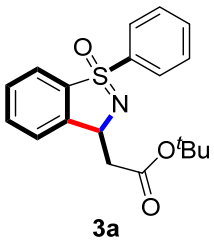
1. General Methods

NMR data were obtained for ^{1}H at 400 MHz or 600 MHz, and for ^{13}C at 100 MHz or 151 MHz. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in CDCl3 solution. ESI HRMS was recorded on a Waters SYNAPT G2 and Water XEVO G2 Q-ToF. UV detection was monitored at 220 nm. TLC was performed on glass-backed silica plates. Column chromatography was performed on silica gel (200-300 mesh), eluting with ethyl acetate and petroleum ether. These substrates **1b-o** were prepared according to the literatures.[1,2] Acrylates were commercially available.

2. General Procedure for Synthesis of Benzothiazines Compounds and Characterization Data

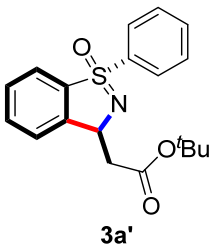
iminodiphenyl-λ^6-sulfanone **1a** (10.9 mg, 0.05 mmol), *tert*-butyl acrylate **2a** (32 mg, 0.25 mmol) , $Cu(OAc)_2 \cdot H_2O$ (21 mg, 2.1 equiv.), Na_2CO_3 (1.1 mg, 0.2 equiv.) and $[Cp^*RhCl_2]_2$ (1.6 mg, 5 mol %) were stirred in DCE (0.5 mL) at 110 °C for 20 h. After completion, the reaction mixture was purified by flash chromatography eluting to give the product **3a+3a'** as yellow oil (15.5 mg, 90%). Noteworthy, these series of benzothiazines were not very stable for svereral days.[3] Almost all of those products were yellow oil, except **3j** (**3j'**) and **3o** were light yellow solid.

tert-butyl 2-((1S*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3a**). 20 h, 7.6 mg, 44% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 7.6 Hz, 2H), 7.61 (t, J = 7.2 Hz, 1H), 7.56-7.52 (m, 5H), 7.45-7.41 (m, 1H), 5.60 (t, J = 6.4Hz, 1H), 2.90-2.79 (m, 2H), 1.50 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.5, 147.9, 140.0, 139.0, 133.4, 132.3, 129.8, 129.1, 129.0, 123.8, 122.4, 81.1, 65.7, 43.4, 28.2 ppm. ESI HRMS: calcd. for $C_{19}H_{21}NO_3S$+H 344.1320, found 344.1315.



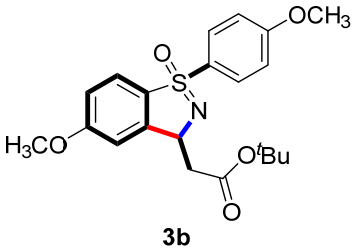
3a

tert-butyl 2-((1R*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3a'**). 20 h, 7.9 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 7.2 Hz, 2H), 7.60-7.55 (m, 3H), 7.53-7.48 (m, 3H), 7.45-7.41 (m, 1H), 5.50 (t, J = 6.4 Hz, 1H), 3.02 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.80 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.6, 148.1, 140.8, 138.8, 133.3, 132.3, 129.3, 129.1, 129.1 124.1, 122.5, 81.0, 66.4, 44.8, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{21}NO_3S$+H 344.1320, found 344.1320.



3a'

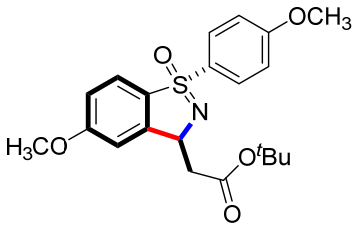
tert-butyl 2-((1S*,3S*)-5-methoxy-1-(4-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3b**). 20 h, 9.3 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, J = 9.2 Hz, 2H), 7.38 (d, J = 8.4 Hz, 1H), 6.98 (d, J = 8.4 Hz, 3H), 6.94-6.91 (m, 1H), 5.50 (t, J = 6.4 Hz, 1H), 3.86 (s, 3H), 3.84 (s, 3H), 2.89 (dd, J_1 = 6.4 Hz, J_2 = 15.2 Hz, 1H), 2.74 (dd, J_1 = 7.2 Hz, J_2 = 15.2 Hz, 1H), 1.51 (s, 9H) ppm. ^{13}C



3b

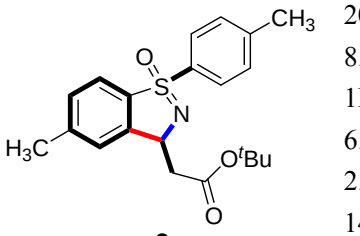
NMR (100 MHz, $CDCl_3$): δ 170.6, 163.6, 163.1, 150.7, 131.8, 131.7, 131.7, 123.3, 116.5 114.3, 107.4, 81.1, 64.8, 55.8, 55.7, 43.6, 28.2 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_5S$+H 404.1532, found 404.1530.

tert-butyl 2-((1R*,3S*)-5-methoxy-1-(4-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3b'**). 20 h, 9.5 mg, 47% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 9.2 Hz, 2H), 7.37(d, J = 8.4 Hz, 1H), 7.01 (d, J = 2.0 Hz, 1H), 6.96-6.91 (m, 3H), 5.41 (t, J = 6.0 Hz, 1H), 3.85 (s, 3H), 3.84 (s, 3H), 3.04 (dd, J_1 = 5.6 Hz, J_2 = 16.0 Hz, 1H), 2.73 (dd, J_1 = 7.6 Hz, J_2 = 16.0 Hz, 1H), 1.49 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.9, 163.5, 163.1, 150.9, 132.4, 131.4, 123.4, 116.6, 114.3 107.8, 81.0, 65.5, 55.8, 55.6, 45.0, 28.2 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_5S$+H 404.1532, found 404.1537.



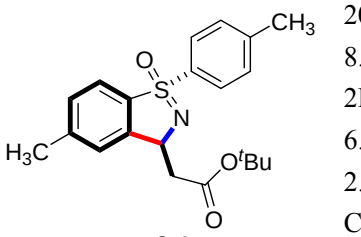
3b'

tert-butyl 2-((1S*,3S*)-5-methyl-1-oxido-1-(p-tolyl)-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3c**). 20 h, 6.6 mg, 34% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, J = 8.4 Hz, 2H), 7.38 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 4.4 Hz, 2H), 7.30 (s, 1H), 7.21 (d, J = 8.0 Hz, 1H), 5.54 (t, J = 6.4 Hz, 1H), 2.85 (dd, J_1 = 6.8 Hz, J_2 = 15.2 Hz, 1H), 2.74 (dd, J_1 = 6.8 Hz, J_2 = 14.8 Hz, 1H), 2.42 (s, 6H), 1.51 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.6, 148.3, 144.2, 143.1, 137.3, 136.7, 130.1, 129.8, 129.7, 124.1, 122.0, 81.0, 65.2, 43.6, 28.2, 21.7, 21.5 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_3S$+H 372.1633, found 372.1630.



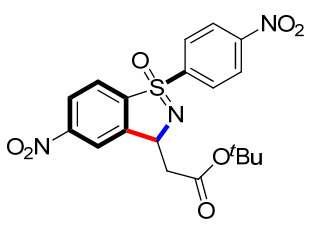
3c

tert-butyl 2-((1R*,3S*)-5-methyl-1-oxido-1-(p-tolyl)-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3c'**). 20 h, 6.7 mg, 36% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.0 Hz, 1H), 7.34 (s, 1H), 7.30 (d, J = 9.6 Hz, 2H), 7.21 (d, J = 8.0 Hz, 1H), 5.43 (t, J = 6.4 Hz, 1H), 3.01 (dd, J_1 = 6.4 Hz, J_2 = 16.0 Hz, 1H), 2.76 (dd, J_1 = 7.2 Hz, J_2 = 15.6 Hz, 1H), 2.43 (s, 3H), 2.40 (s, 3H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.8, 148.5, 144.0, 143.1, 138.0, 136.5, 130.1, 129.7, 129.3, 124.4, 122.1, 80.9, 66.0, 44.9, 28.5, 28.2, 21.7 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_3S$+H 372.1633, found 372.1634.



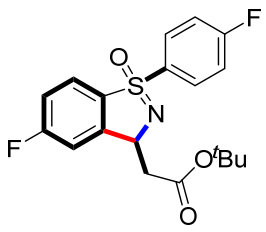
3c'

tert-butyl 2-((5-nitro-1-(4-nitrophenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3d**). 20 h, 2.8 mg, 13% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (s, 1H), 8.39 (d, J = 6.0 Hz, 2H), 8.34 (dd, J_1 = 1.2 Hz, J_2 = 5.6 Hz, 1H), 8.27 (d, J = 6.0 Hz, 2H), 7.67 (d, J = 6.0 Hz, 1H), 5.62 (t, J = 4.0 Hz, 1H), 3.07-2.99 (m, 2H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.5, 151.1, 150.6, 150.3, 144.5, 142.7, 131.6, 125.0, 124.4, 123.4, 119.4, 81.9, 65.7, 41.4, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Cl_2NO_3S$+Na 456.0841, found 456.0850.



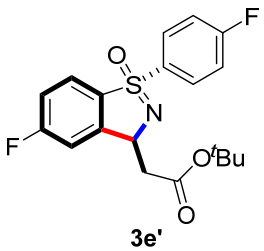
3d

tert-butyl 2-((1S*,3S*)-5-fluoro-1-(4-fluorophenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3e**). 20 h, 7.4 mg, 39% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06-8.02 (m, 2H), 7.49-7.46 (m, 1H), 7.26-7.19 (m, 3H), 7.14 (td, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 5.51 (t, J = 6.4 Hz, 1H), 2.90 (dd, J_1 = 6.4 Hz, J_2 = 15.6 Hz, 1H), 2.81 (dd, J_1 = 6.8 Hz, J_2 = 15.6 Hz, 1H), 1.49 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.1, 166.0 (d, J = 170.1 Hz), 165.3 (d, J = 169.0 Hz), 151.4 (d, J = 6.1 Hz), 135.5, 134.8, 132.7 (d, J = 6.5 Hz), 124.2 (d, J = 6.8 Hz), 117.1 (d, J = 16.4 Hz), 116.5 (d, J = 15.0 Hz), 111.0 (d, J = 16.0 Hz), 81.4, 64.9, 42.7, 28.1 ppm. ESI HRMS: calcd. for $C_{19}F_{19}Cl_2NO_3S$+H 380.1132, found 380.1134.



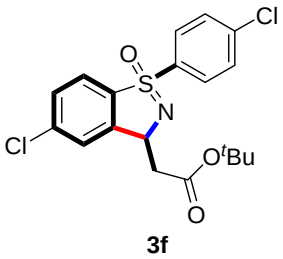
3e

tert-butyl 2-((1R*,3S*)-5-fluoro-1-(4-fluorophenyl)-1-oxido-3H-1λ^4-benzo [d]isothiazol-3-yl) acetate (**3e'**). 20 h, 7.6 mg, 40% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93-7.90 (m, 2H), 7.48 (d, J = 4.8 Hz, 1H), 7.22-7.12 (m, 4H), 5.44 (t, J = 6.4 Hz, 1H), 3.03 (dd, J_1 = 5.6 Hz, J_2 = 16.4 Hz, 1H), 2.76 (dd, J_1 = 7.6 Hz, J_2 = 16.0 Hz, 1H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.3, 165.9 (d, J = 254.8 Hz), 165.4 (d, J = 253.6 Hz), 151.7 (d, J = 9.1 Hz), 136.4, 134.6, 132.2 (d, J = 9.6 Hz), 124.3 (d, J = 10.4 Hz), 117.3 (d, J = 24.7 Hz), 116.5 (d, J = 22.5 Hz), 111.5 (d, J = 23.8 Hz), 81.3, 65.7, 44.5, 28.1 ppm. ESI HRMS: calcd. for $C_{19}F_{19}Cl_2NO_3S$+H 380.1132, found 380.1132.



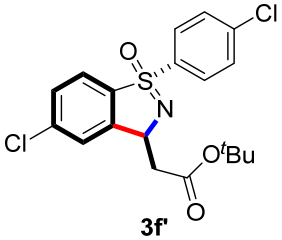
3e'

tert-butyl 2-((1S*,3S*)-5-chloro-1-(4-chlorophenyl)-1-oxido-3H-1λ^4-benzo[d] isothiazol-3-yl) acetate (**3f**). 20 h, 7.6 mg, 37% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 8.4 Hz, 2H), 7.56 (s, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 7.2 Hz, 2H), 5.52 (t, J = 6.8 Hz, 1H), 2.91-2.79 (m, 2H), 1.49 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 150.0, 140.6, 139.3, 138.1, 137.4, 131.3, 129.7, 129.5, 124.3, 123.3, 81.4, 65.2, 42.7, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Cl_2NO_3S$+H 412.0541, found 412.0537.

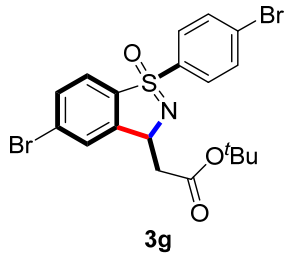


3f

tert-butyl 2-((1R*,3S*)-5-chloro-1-(4-chlorophenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3f'**). 20 h, 7.9 mg, 38% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 8.8 Hz, 2H), 7.58 (s, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.42 (s, 2H), 5.44 (t, J = 6.8 Hz, 1H), 3.01 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.77 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.2, 150.3, 140.4, 139.4, 138.8, 137.0, 130.8, 129.7, 129.6, 124.7, 123.4, 81.4, 66.0, 44.4, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Cl_2NO_3S$+H 412.0541, found 412.0537.



3f'

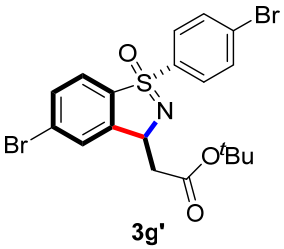


3g

tert-butyl 2-((1S*,3S*)-5-bromo-1-(4-bromophenyl)-1-oxido-3H-1λ^4-benzo [d]isothiazol-3-yl) acetate (**3g**). 20 h, 8.8 mg, 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, J = 8.4 Hz, 2H), 7.74 (s, 1H), 7.67 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.4 Hz, 1H), 7.35 (d, J = 8.4 Hz, 1H), 5.51 (t, J = 6.4 Hz, 1H), 2.91-2.78 (m, 2H), 1.49 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 150.0, 138.5, 137.8, 132.5, 132.5, 131.4,

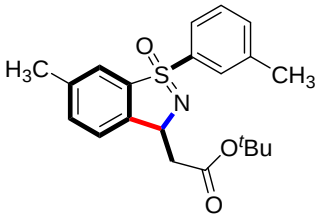
129.3, 127.7, 127.3, 123.4, 81.4, 65.2, 42.6, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Br_2NO_3S$+H 499.9531, found 499.9533.

tert-butyl 2-((1R*,3S*)-5-bromo-1-(4-bromophenyl)-1-oxido-3H-1λ^4-benzo[d] isothiazol-3-yl) acetate (**3g'**). 20 h, 9.2 mg, 37% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.8 Hz, 3H), 7.65 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.35 (d, J = 8.4 Hz, 1H), 5.44 (t, J = 6.4 Hz, 1H), 3.01 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.77 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.2, 150.4, 139.4, 137.5, 132.6, 132.6, 130.9, 129.1, 127.8, 127.8, 123.6, 81.4, 66.1, 44.4, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Br_2NO_3S$+H 499.9531, found 499.9537.



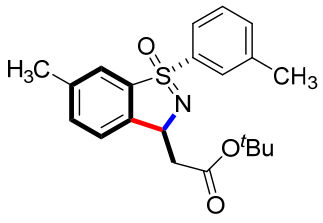
3g'

tert-butyl 2-((1S*,3S*)-6-methyl-1-oxido-1-(m-tolyl)-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3h**). 20 h, 8.1 mg, 44% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (s, 1H), 7.82-7.79 (m, 1H), 7.44-7.40 (m, 3H), 7.34 (d, J = 8.0 Hz, 1H), 7.30 (s, 1H), 5.55 (t, J = 6.8 Hz, 1H), 2.87 (dd, J_1 = 6.4 Hz, J_2 = 15.2 Hz, 1H), 2.76 (dd, J_1 = 6.8 Hz, J_2 = 15.2 Hz, 1H), 2.43 (s, 3H), 2.37 (s, 3H), 1.51 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.6, 145.1, 139.9, 139.5, 139.3, 134.2, 133.4, 130.1, 129.4, 129.0, 127.0, 123.3, 122.3, 81.0, 65.3, 43.5, 28.2, 21.4, 21.1 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_3S$+H 372.1633, found 372.1629.



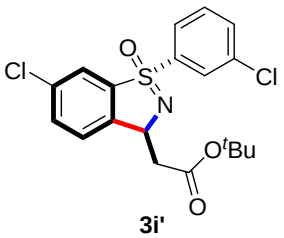
3h

tert-butyl 2-((1R*,3S*)-6-methyl-1-oxido-1-(m-tolyl)-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3h'**). 20 h, 8.5 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, J = 6.4 Hz, 1H), 7.69 (s, 1H), 7.45 (d, J = 7.6 Hz, 1H), 7.41-7.34 (m, 3H), 7.30 (s, 1H), 5.46 (t, J = 6.4 Hz, 1H), 3.00 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.75 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 2.40 (s, 3H), 2.37 (s, 3H), 1.49 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.8, 145.4, 140.7, 139.5, 139.3, 139.0, 134.0, 133.5, 129.6, 129.0, 126.5, 123.7, 122.3, 80.9, 66.0, 44.9, 28.2, 21.3, 21.1 ppm.



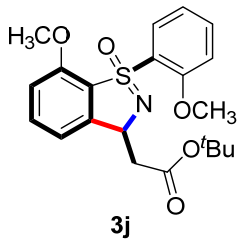
3h'

tert-butyl 2-((1R*,3S*)6-chloro-1-(3-chlorophenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3i'**). 20 h, 8.4 mg, 41% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (s, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.4 Hz, 2H), 7.54 (s, 1H), 7.48 (t, J = 8.4 Hz, 2H), 5.47 (t, J = 6.8 Hz, 1H), 2.99 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.78 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.3, 146.7, 142.0, 139.9, 135.5, 135.3, 133.8, 132.9, 130.5, 129.4, 127.6, 125.3, 122.4, 81.4, 66.2, 44.4, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Cl_2NO_3S$+H 412.0541, found 412.0539.



3i'

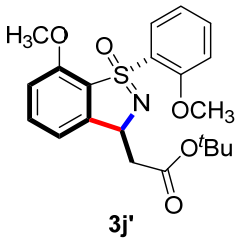
tert-butyl 2-((1S*,3S*)-7-methoxy-1-(2-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)



3j

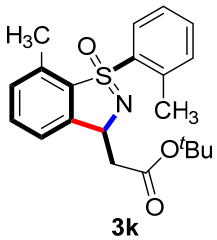
acetate (**3j**). 20 h, 7.9 mg, 39% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H), 7.56-7.49 (m, 2H), 7.13-7.10 (m, 2H), 6.88 (d, J = 8.0 Hz, 1H), 6.82 (d, J = 8.0Hz, 1H), 5.55 (t, J = 6.8 Hz, 1H), 3.73 (s, 3H), 3.54 (s, 3H), 2.86 (dd, J_1 = 6.4 Hz, J_2 = 15.2 Hz, 1H), 2.62 (dd, J_1 = 6.8 Hz, J_2 = 15.6 Hz, 1H), 1.52 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.2, 157.5, 154.9, 152.0, 135.0, 134.7, 132.3, 127.5, 126.1, 120.5, 115.4, 112.2, 110.0, 80.9, 65.7, 56.0, 55.2, 43.0, 28.2 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_5S$+H 404.1532, found 404.1529.

tert-butyl 2-((1R*,3S*)-7-methoxy-1-(2-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3j'**). 20 h, 8.5 mg, 42% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H), 7.53-7.47 (m, 2H), 7.08 (t, J = 7.6 Hz, 2H), 6.84-6.79 (m, 2H), 5.26 (t, J = 6.8 Hz, 1H), 3.74 (s, 3H), 3.55 (s, 3H), 2.95 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.80 (dd, J_1 = 6.8 Hz, J_2 = 16.0 Hz, 1H), 1.47 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.0, 157.9, 155.1, 153.0, 134.8, 134.7, 132.0, 128.7, 125.3, 120.2, 115.2, 112.1, 109.9, 80.8, 65.3, 56.0, 55.9, 43.9, 28.1 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_5S$+H 404.1532, found 404.1534.



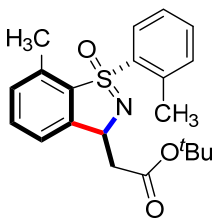
3j'

tert-butyl 2-((1S*,3S*)-7-methyl-1-oxido-1-(o-tolyl)-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3k**). 20 h, 7.6 mg, 40% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, J = 8.0 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 7.6 Hz, 1H), 7.20 (d, J = 7.2 Hz, 1H), 5.45 (t, J = 7.2 Hz, 1H), 2.89 (dd, J_1 = 6.4 Hz, J_2 = 15.6 Hz, 1H), 2.75 (dd, J_1 = 7.6 Hz, J_2 = 15.6 Hz, 1H), 2.20 (s, 3H), 2.15 (s, 3H), 1.51 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.8, 148.7, 138.9, 137.3, 137.2, 134.0, 133.4, 132.9, 132.9, 131.3, 130.4, 126.8, 121.4, 81.1, 65.1, 42.1, 28.2, 20.5, 17.3 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_3S$+H 372.1633, found 372.1632.

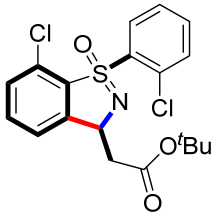


3k

tert-butyl 2-((1R*,3S*)-7-methyl-1-oxido-1-(o-tolyl)-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3k'**). 20 h, 8 mg, 43% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, J = 8.0 Hz, 1H), 7.48-7.45 (m, 2H), 7.41 (t, J = 6.8 Hz, 2H), 7.18 (d, J = 7.2 Hz, 2H), 5.35 (t, J = 6.8 Hz, 1H), 2.97 (dd, J_1 = 6.4 Hz, J_2 = 16.0 Hz, 1H), 2.78 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 2.16 (s, 3H), 1.93 (s, 3H), 1.48 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.7, 149.2, 139.2, 137.6, 135.8, 134.3, 133.4, 133.0, 132.8, 131.9, 130.5, 126.6, 121.5, 80.9, 65.4, 44.6, 28.1, 18.9, 16.8 ppm. ESI HRMS: calcd. for $C_{21}H_{25}NO_3S$+H 372.1633, found 372.1630.



3k'

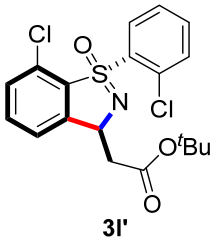


3l

tert-butyl 2-((1S*,3S*)-7-chloro-1-(2-chlorophenyl)-1-oxido-3H-1λ^4-benzo [d]isothiazol-3-yl) acetate (**3l**). 20 h, 7.9 mg, 38% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (d, J = 7.8 Hz, 1H), 7.57-7.52 (m, 4H), 7.44-7.38 (m, 2H), 5.62 (t, J = 6.8 Hz, 1H), 3.00 (dd, J_1 = 6.4 Hz, J_2 = 16.0 Hz, 1H), 2.81 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 1.53 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.9, 151.4, 135.9, 135.5, 134.9, 134.4, 133.6, 133.2, 132.1, 129.4, 128.6,

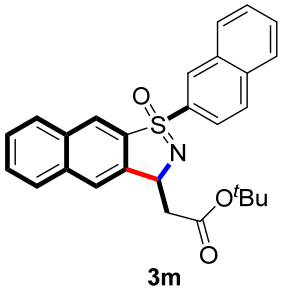
127.6, 122.6, 81.3, 65.6, 41.2, 28.2 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Cl_2NO_3S$+H 412.0541, found 412.0543.

tert-butyl 2-((1R*,3S*)-7-chloro-1-(2-chlorophenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl) acetate (**3l'**). 20 h, 8.2 mg, 40% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, J = 7.8 Hz, 1H), 7.60 (t, J = 7.2 Hz, 1H), 7.51 (t, J = 6.4 Hz, 4H), 7.34 (dd, J_1 = 2.4 Hz, J_2 = 5.2 Hz, 1H), 5.50 (t, J = 6.4 Hz, 1H), 3.01 (dd, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 2.79 (dd, J_1 = 6.8 Hz, J_2 = 16.0 Hz, 1H), 1.47 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.4, 151.0, 139.7, 136.3, 134.1, 133.6, 130.6, 129.8, 129.3, 129.1, 128.8, 122.6, 81.2, 66.1, 44.7, 28.1 ppm. ESI HRMS: calcd. for $C_{19}H_{19}Cl_2NO_3S$+H 412.0541, found 412.0543.

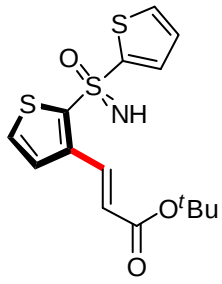


3l'

tert-butyl 2-((1S*,3S*)-1-(naphthalen-2-yl)-1-oxido-3H-1λ^4-naphtho[2,3-d]isothiazol-3-yl)acetate (**3m**). 20 h, 9.1 mg, 41% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81 (s, 1H), 8.04 (s, 1H), 8.02 (s, 1H), 7.94 (t, J = 8.4 Hz, 4H), 7.86 (d, J = 8.0 Hz, 1H), 7.70-7.60 (m, 4H), 7.53 (t, J = 7.8 Hz, 1H), 5.82 (t, J = 6.4 Hz, 1H), 3.08 (dd, J_1 = 6.4 Hz, J_2 = 15.2 Hz, 1H), 2.98 (dd, J_1 = 6.8 Hz, J_2 = 15.2 Hz, 1H), 1.57 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.7, 135.3, 135.0, 132.4, 131.9, 129.6, 129.4, 129.2, 129.2, 128.7, 128.5, 127.9, 127.5, 127.1, 124.5, 122.9, 122.7, 100.0, 81.1, 65.1, 44.1, 28.3 ppm. ESI HRMS: calcd. for $C_{27}H_{25}NO_3S$+H 444.1633, found 444.1633.



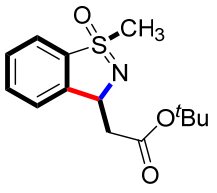
3m



3o"

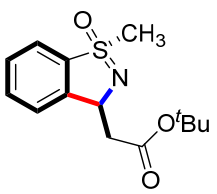
tert-butyl (E)-3-(2-(thiophene-2-sulfonimidoyl)thiophen-3-yl)acrylate (**3o"**). 20 h, 10.8 mg, 61% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, J = 16.0 Hz, 1H), 7.74 (dd, J_1 = 1.2 Hz, J_2 = 4.0 Hz, 1H), 7.62 (dd, J_1 = 1.4 Hz, J_2 = 4.4 Hz, 1H), 7.50 (d, J = 5.2 Hz, 1H), 7.25 (d, J = 5.2 Hz, 1H), 7.08-7.05 (m, 1H), 6.21 (d, J = 16.0 Hz, 1H), 3.68 (s, 1H), 1.55 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.5, 145.4, 139.4, 134.0, 133.4, 133.2, 131.2, 128.0, 127.4, 124.6, 81.0, 28.2 ppm. ESI HRMS: calcd. for $C_{15}H_{17}NO_3S_3$+H 356.0449, found 356.0448.

tert-butyl 2-((1S*,3S*)-1-methyl-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3p**). 12 h, 4.4 mg, 31% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 7.8 Hz, 1H), 7.62 (t, J = 7.2Hz, 1H), 7.57-7.52 (m, 2H), 5.37 (t, J = 5.6 Hz, 1H), 3.40 (s, 3H), 2.84-2.73 (m, 2H), 1.39 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.1, 148.9, 137.3, 132.6, 128.9, 123.8, 123.5, 121.9, 80.7, 66.0, 45.1, 42.0, 28.1 ppm. ESI HRMS: calcd. for $C_{14}H_{19}NO_3S$+H 282.1164, found.282.1169.



3p

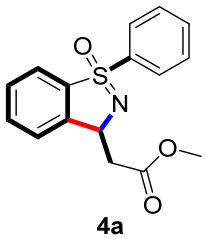
tert-butyl 2-((1R*,3S*)-1-methyl-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3p'**). 12 h, 4.5 mg, 32% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 5.2 Hz, 1H), 7.63 (t, J = 4.8Hz, 1H), 7.56 (t, J = 4.8 Hz, 2H), 5.23 (t, J = 4.4 Hz, 1H), 3.33 (s, 3H), 2.81 (dd, J_1 = 4.4 Hz, J_2 = 10.8 Hz, 1H), 2.72 (dd, J_1 = 4.4 Hz, J_2 = 10.8 Hz, 1H), 1.45 (s, 9H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 170.5, 149.1, 137.2, 132.8, 129.1, 124.4, 122.0, 123.8, 121.9, 80.7, 66.0, 45.1, 42.0, 28.1 ppm. ESI



3p'

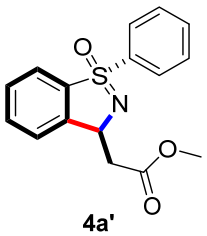
HRMS: calcd. for $C_{14}H_{19}NO_3S$+H 282.1164, found.282.1165.

methyl 2-((1S*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4a**). 20 h, 6.7 mg, 45% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 5.2 Hz, 2H), 7.62 (t, J = 4.8 Hz, 1H), 7.59-7.53 (m, 5H), 7.45 (t, J = 4.8 Hz, 1H), 5.65 (t, J = 4.4 Hz, 1H), 3.79 (s, 3H), 3.01 (dd, J_1 = 3.6 Hz, J_2 = 10.0 Hz, 1H), 2.85 (dd, J_1 = 5.2 Hz, J_2 = 10.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 147.3, 139.7, 139.0, 133.5, 132.4, 129.7, 129.3, 129.2, 123.6, 122.5, 65.4, 52.0, 42.1 ppm. ESI HRMS: calcd. for $C_{16}H_{15}NO_3S$+H 302.0851, found 302.0960.



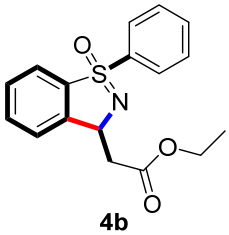
4a

methyl 2-((1R*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4a'**). 20 h, 7 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 7.6 Hz, 2H), 7.61-7.49 (m, 6H), 7.45 (t, J = 7.2 Hz, 1H), 5.56 (t, J = 6.8 Hz, 1H), 3.77 (s, 3H), 3.02-2.92 (m, 2H), ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ 171.8, 147.5, 140.4, 138.7, 133.3, 132.4, 129.3, 129.2, 129.1, 123.9, 122.6, 66.3, 51.9, 43.7 ppm. ESI HRMS: calcd. for $C_{16}H_{15}NO_3S$+H 302.0851, found 302.0965.



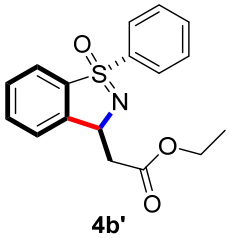
4a'

ethyl 2-((1S*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4b**). 20 h, 6.9 mg, 44% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 7.6 Hz, 2H), 7.62 (t, J = 7.2 Hz, 1H), 7.59-7.53 (m, 5H), 7.45 (t, J = 6.8 Hz, 1H), 5.65 (t, J = 6.4 Hz, 1H), 4.25 (q, J = 6.8 Hz, 2H), 2.98 (dd, J_1 = 5.6 Hz, J_2 = 15.2 Hz, 1H), 2.86 (dd, J_1 = 7.6 Hz, J_2 = 15.2 Hz, 1H), 1.29 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.1, 147.5, 139.8, 139.0, 133.5, 132.4, 129.7, 129.2, 129.2, 123.6, 122.5, 65.5, 60.9, 42.3, 14.2 ppm. ESI HRMS: calcd. for $C_{17}H_{17}NO_3S$+H 316.1007, found 316.1002.



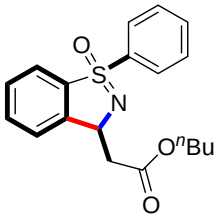
4b

ethyl 2-((1R*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4b'**). 20 h, 7.4 mg, 47% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 7.6 Hz, 2H), 7.59-7.49 (m, 6H), 7.46-7.44 (m, 1H), 5.55 (t, J = 6.8 Hz, 1H), 4.23 (q, J = 7.2 Hz, 2H), 3.03-2.90 (m, 2H), 1.28 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.3, 147.7, 140.5, 138.7, 133.3, 132.4, 129.3, 129.2, 129.1, 124.0, 122.5, 66.3, 60.7, 43.8, 14.2 ppm. ESI HRMS: calcd. for $C_{17}H_{17}NO_3S$+H 316.1007, found 316.1010.



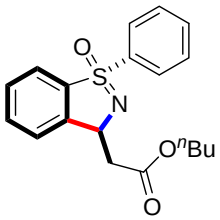
4b'

butyl 2-((1S*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4c**). 20 h, 7.7 mg, 45% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02-8.00 (m, 2H), 7.64-7.58 (m, 1H), 7.57-7.52 (m, 5H), 7.46-7.42 (m, 1H), 5.64 (t, J = 6.8 Hz, 1H), 4.19 (t, J = 6.8 Hz, 2H), 3.00-2.85 (m, 2H), 1.67-1.60 (m, 2H), 1.41-1.35 (m, 2H), 0.92 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.2, 147.5, 139.8, 139.0, 133.5, 132.4, 129.7, 129.2, 129.2, 123.6, 122.5, 65.5, 64.8, 42.3, 30.6, 19.1, 13.7 ppm. ESI HRMS: calcd. for $C_{19}H_{21}NO_3S$+H 344.1320, found 344.1316.



4c

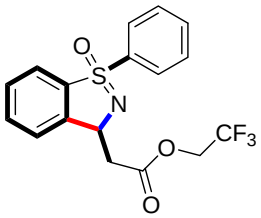
butyl 2-((1R*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4c'**). 20 h, 8.1 mg,



4c'

47% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92-7.90 (m, 2H), 7.60-7.42 (m, 7H), 5.55 (t, J = 6.8 Hz, 1H), 4.20-4.16 (m, 2H), 3.02 (dd, J_1 = 6.8 Hz, J_2 = 16.0 Hz, 1H), 2.91 (dd, J_1 = 6.4 Hz, J_2 = 15.6 Hz, 1H), 1.66-1.59 (m, 2H), 1.41-1.34 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.4, 147.8, 140.6, 138.8, 133.3, 132.4, 129.4, 129.2, 129.1, 124.0, 122.6, 66.3, 64.7, 43.8, 30.6, 19.1, 13.7 ppm. ESI HRMS: calcd. for $C_{19}H_{21}NO_3S$+H 344.1320, found 344.1321.

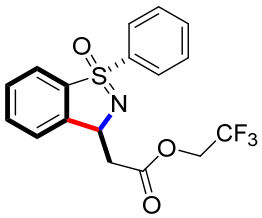
2,2,2-trifluoroethyl 2-((1S*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4d**).



4d

20 h, 8.1 mg, 44% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 7.6 Hz, 2H), 7.66-7.53 (m, 6H), 7.47 (t, J = 8.0Hz, 1H), 5.66 (t, J = 6.0 Hz, 1H), 4.60-4.55 (m, 2H), 3.15 (dd, J_1 = 5.2 Hz, J_2 = 15,2 Hz, 1H), 2.89 (dd, J_1 = 8.4 Hz, J_2 = 15.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.5, 146.8, 139.5, 139.1, 133.6, 132.5, 129.7, 129.5, 129.3, 123.0 (t, J = 90 Hz), 65.1, 60.6 (t, J = 40 Hz), 41.6 ppm. ESI HRMS: calcd. for $C_{17}H_{14}F_3NO_3S$+H 370.0725, found 370.0795.

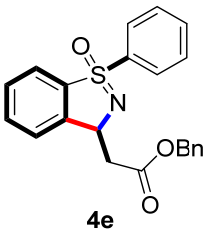
2,2,2-trifluoroethyl 2-((1R*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4d'**).



4d'

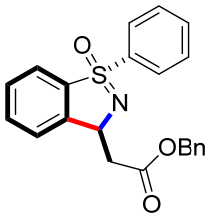
20 h, 8.5 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 7.6 Hz, 2H), 7.60 (t, J = 7.2 Hz, 2H), 7.53 (t, J = 7.2Hz, 3H), 7.50-7.45 (m, 2H), 5.55 (t, J = 6.4 Hz, 1H), 4.70-4.61 (m, 1H), 4.52-4.42 (m, 1H), 3.15-3.02 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.6, 147.0, 140.3, 138.9, 133.5, 132.6, 129.5, 129.4, 129.2, 123.3 (t, J = 100 Hz), 65.9, 60.5 (t, J = 40 Hz), 43.1 ppm. ESI HRMS: calcd. for $C_{17}H_{14}F_3NO_3S$+H 370.0725, found 370.0791.

benzyl 2-((1S*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4e**). 20 h, 7.8 mg, 41% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 8.0 Hz, 2H), 7.62-7.58 (m, 1H), 7.53-7.49 (m, 4H), 7.47-7.40 (m, 2H), 7.37-7.31 (m, 5H), 5.67 (t, J = 7.2 Hz, 1H), 5.23 (s, 2H), 3.02 (dd, J_1 = 6.0 Hz, J_2 = 15.2 Hz, 1H), 2.92 (dd, J_1 = 7.6 Hz, J_2 = 15.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.9, 147.3, 139.7, 139.0, 135.7, 133.5, 132.4, 129.7, 129.3, 129.2, 128.6, 128.4, 128.3, 123.6, 122.5, 66.7, 65.5, 42.3 ppm. ESI HRMS: calcd. for $C_{22}H_{19}NO_3S$+H 378.1164, found 378.1163.

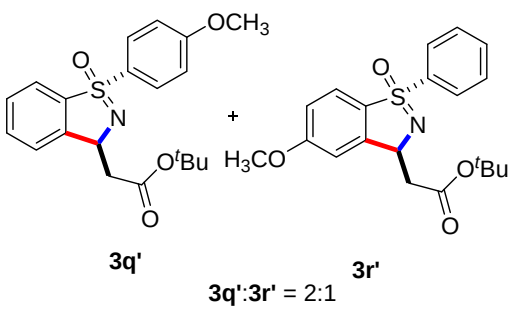


4e

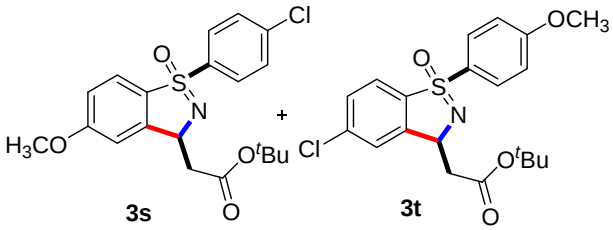
benzyl 2-((1R*,3S*)-1-oxido-1-phenyl-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**4e'**). 20 h, 8.1 mg, 43% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 8.0 Hz, 2H), 7.59 (t, J = 6.8 Hz, 1H), 7.50 (t, J = 7.8 Hz, 4H), 7.47-7.42 (m, 2H), 7.39-7.32 (m, 5H), 5.56 (t, J = 6.8 Hz, 1H), 5.29-5.17 (m, 2H), 3.08 (dd, J_1 = 7.2 Hz, J_2 = 16.0 Hz, 1H), 2.96 (dd, J_1 = 6.4 Hz, J_2 = 15.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.1, 147.6, 140.6, 138.8, 135.8, 133.4, 132.4, 129.4, 129.2, 129.2, 128.5, 128.4, 128.2, 124.0, 122.6, 66.6, 66.3, 43.9 ppm. ESI HRMS: calcd. for $C_{22}H_{19}NO_3S$+H 378.1164, found 378.1168.



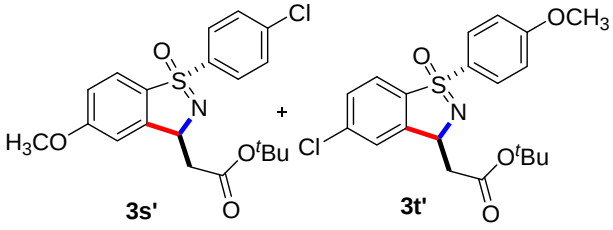
4e'



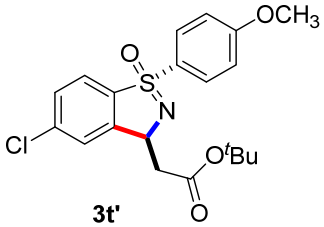
tert-butyl 2-((1R*,3S*)-1-(4-methoxyphenyl)-1-oxido-3H-1λ^4-benzo [d]isothiazol-3-yl)acetate (**3q'**). tert-butyl 2-((1R*,3S*)-5-methoxy-1-oxido -1-phenyl-3H-1l4-benzo [d]isothiazol-3-yl)acetate (**3r'**). 20 h, 8.6 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89-7.83 (m, 3H), 7.57-7.43 (m, 5H), 7.41-7.39 (m, 2H), 7.02 (s, 1H), 6.98-6.93 (m, 3H), 5.48 (t, *J* = 6.8 Hz, 1H), 5.43 (t, J = 6.4 Hz, 1H), 3.85 (s, 3H), 3.85 (s, 3H), 3.04-3.00 (m, 2H), 2.80-2.75 (m, 2H), 1.50 (s, 9H), 1.48 (s, 9H) ppm.



tert-butyl 2-((1S*,3S*)-1-(4-chlorophenyl)-5-methoxy-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3s**). tert-butyl 2-((1S*,3S*)-5-chloro-1-(4-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3t**). 20 h, 8.3 mg, 41% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.8 Hz, 2H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.53 (s, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.41-7.37 (m, 2H), 7.00-6.94 (m, 3H), 5.50 (t, *J* = 6.4 Hz, 1H), 5.40 (t, *J* = 6.4 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 3.02-2.98 (m, 1H), 2.93-2.89 (m, 1H), 2.87-2.73 (m, 2H), 1.49 (s, 14H) ppm.



tert-butyl 2-((1R*,3S*)-1-(4-chlorophenyl)-5-methoxy-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3s'**). tert-butyl 2-((1R*,3S*)-5-chloro-1-(4-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3t'**). 20 h, 8.5 mg, 42% yield. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.83-7.80 (m, 3H), 7.56 (s, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.40 (d, J = 8.4 Hz, 2H), 7.01 (s, 1H), 6.98-6.94 (m, 3H), 5.44 (t, *J* = 6.6 Hz, 1H), 5.40 (t, *J* = 6.6 Hz, 1H), 3.86 (s, 3H), 3.85 (s, 3H), 3.06-3.00 (m, 2H), 2.76-2.72 (m, 2H), 1.49 (s, 13H) ppm.



tert-butyl 2-((1R*,3S*)-5-chloro-1-(4-methoxyphenyl)-1-oxido-3H-1λ^4-benzo[d]isothiazol-3-yl)acetate (**3t'**). 20 h, 5.6 mg, 29% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 8.8 Hz, 2H), 7.56 (s, 1H), 7.39 (t, *J* = 8.8 Hz, 2 H), 6.97 (d, J = 8.8 Hz, 2H), 5.44 (t, *J* = 6.8 Hz, 1H), 3.86 (s, 3H), 3.04 (dd, J_1 = 5.6 Hz, J_2 = 16 Hz, 1H), 2.74 (dd, J_1 = 7.6 Hz, J_2 = 16 Hz, 1H), 1.49 (s, 9H) ppm.

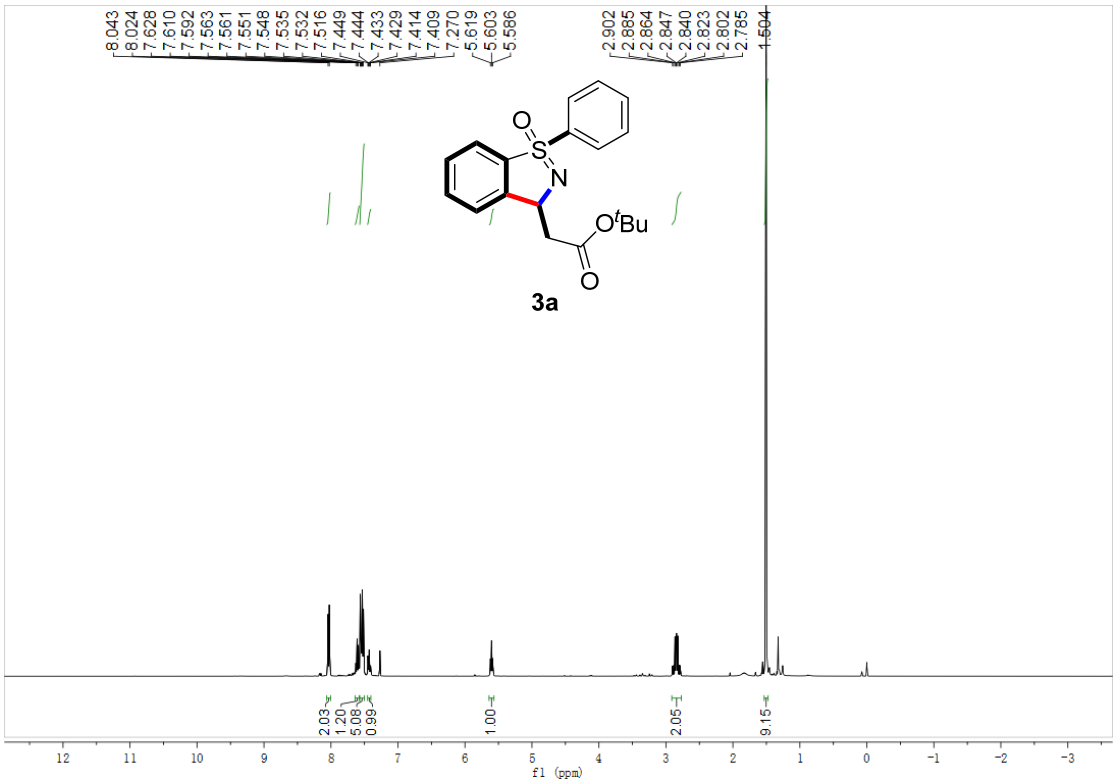
Reference

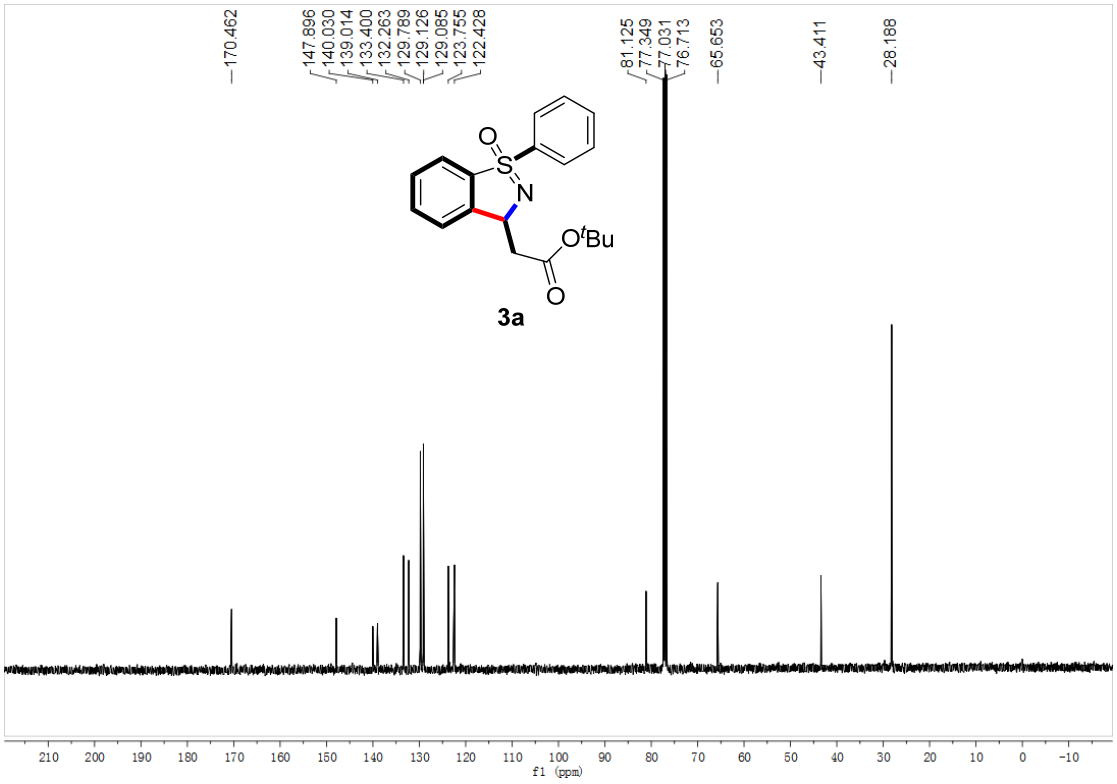
[1] Y.-M. Li, C.-P. Nie, H.-F. Wang, X.-Y. Li, F. Verpoort and C.-Y. Duan, *Eur. J. Org. Chem.*, **2011**, 7331.

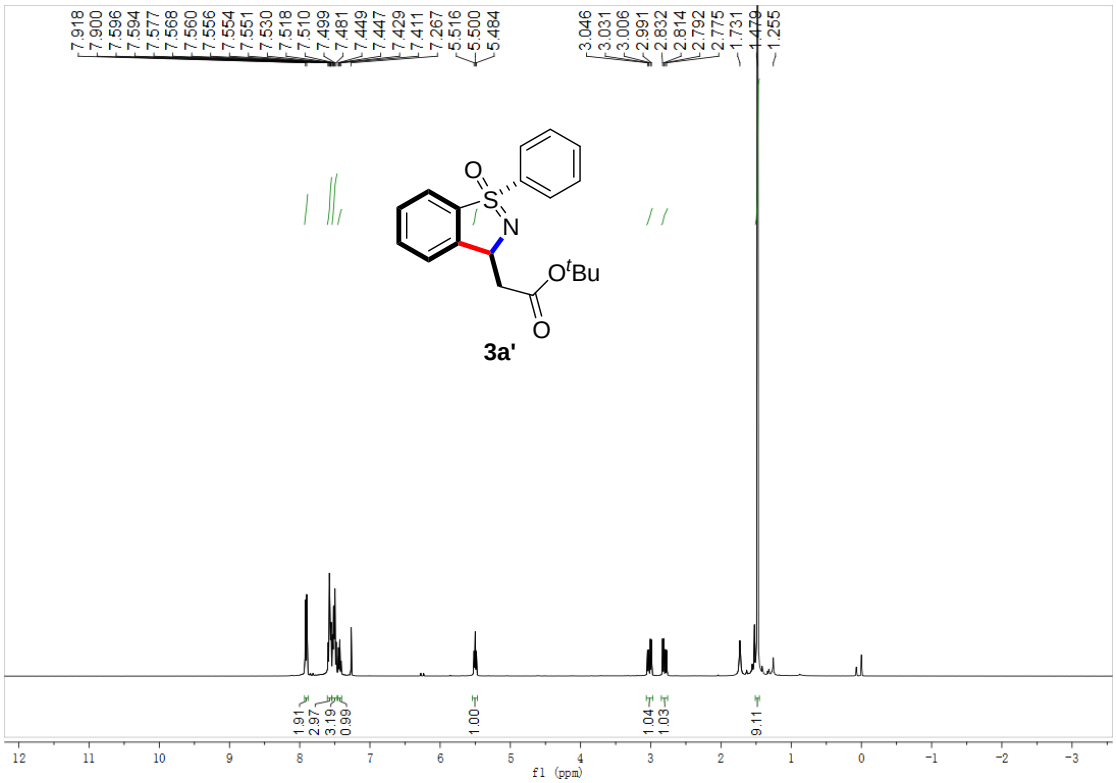
[2] M. Zenzola, R. Doran, L. Degennaro, R. Luisi and J.-A. Bull, *Angew. Chem. Int. Ed.*, **2016**, 55, 7203.

[3] M. Harmata, N. K.-O. Rayanil, M. G. Gomes, P. Zheng, N. L. Calkins, S.-Y. Kim, Y. Fan, V. Bumbu, D. Y. Lee, S. Wacharasindhu, X. Hong, *Org. Lett.*, **2005**, 7, 143.

3. NMR Spectra of benzothiazines Compounds and Structure Determination



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7.594
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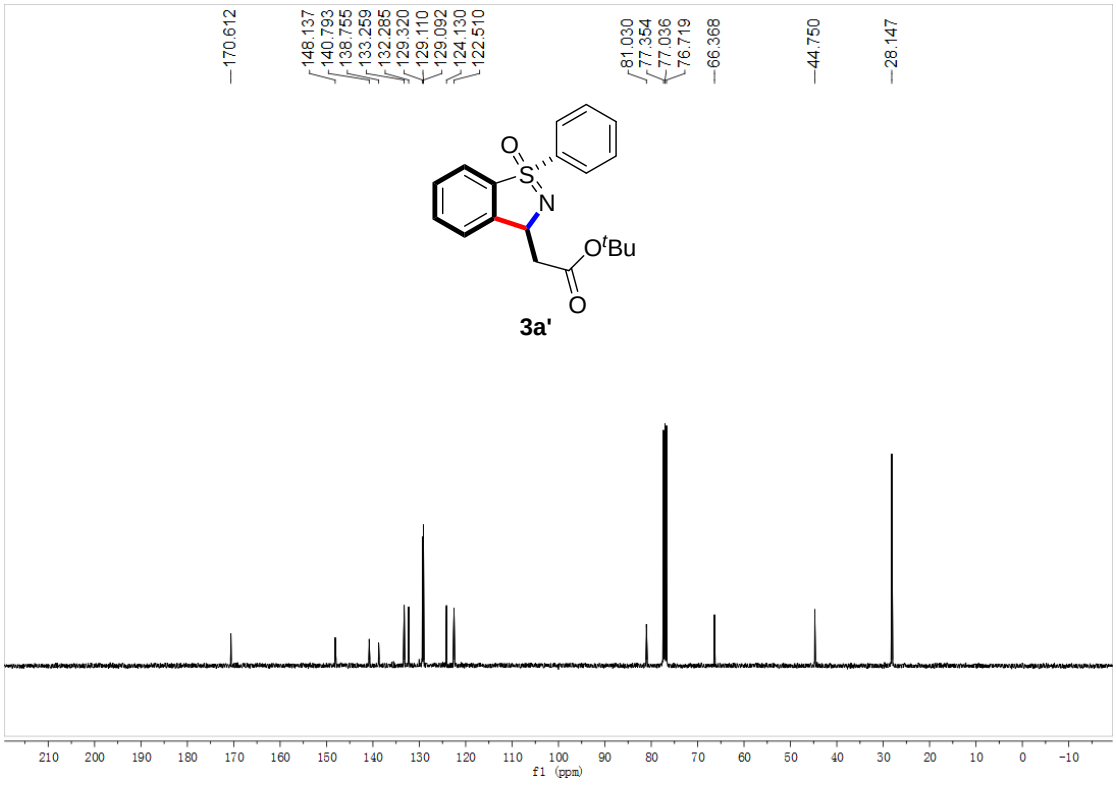
7.568
7.560
7.556
7.554
7.551
7.530
7.518
7.510
7.499
7.481
7.449
7.447
7.429
7.411
7.267
5.516
5.500
5.484
3.046
3.031
3.006
2.991
2.832
2.814
2.792
2.775
1.731
1.479
1.255
O
S
N
O^{t}Bu
O
1.91
2.97
3.19
0.99
1.00
1.04
1.03
9.11
f1 (ppm)

3a'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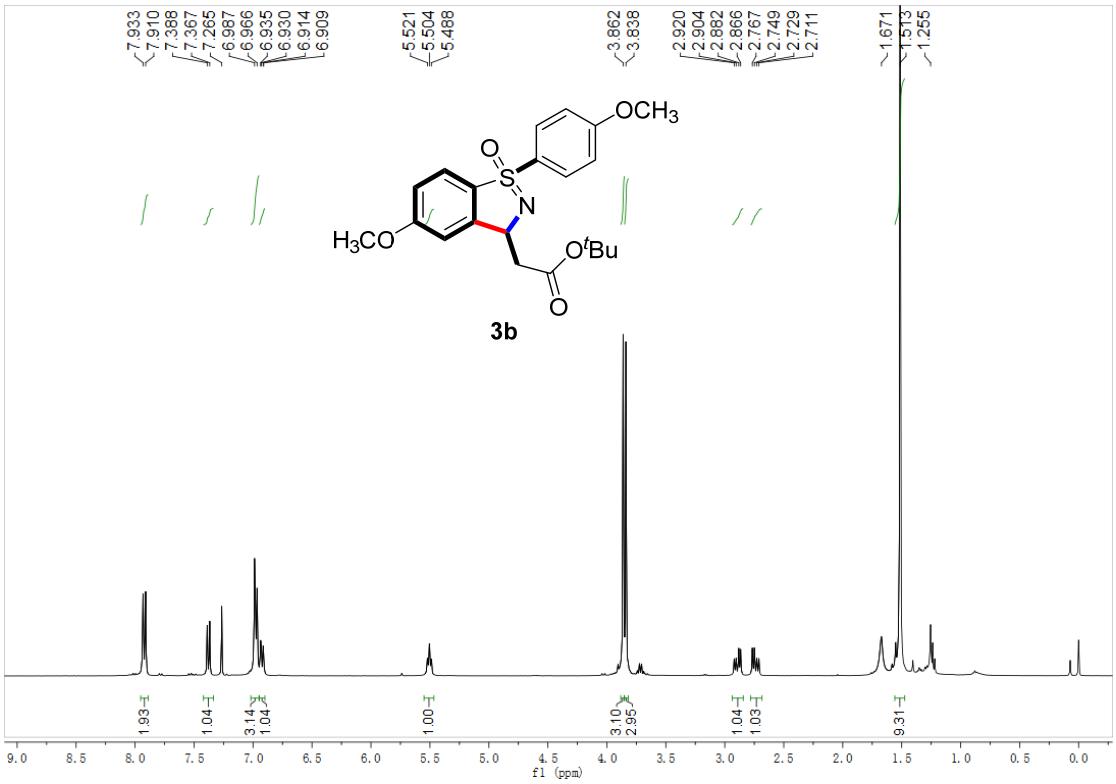
140.793
138.755
133.259
132.285
129.320
129.110
129.092
124.130
122.510
81.030
77.354
77.036
76.719
66.368
44.750
28.147
O
S
N
O^{t}Bu
O
f1 (ppm)

3a'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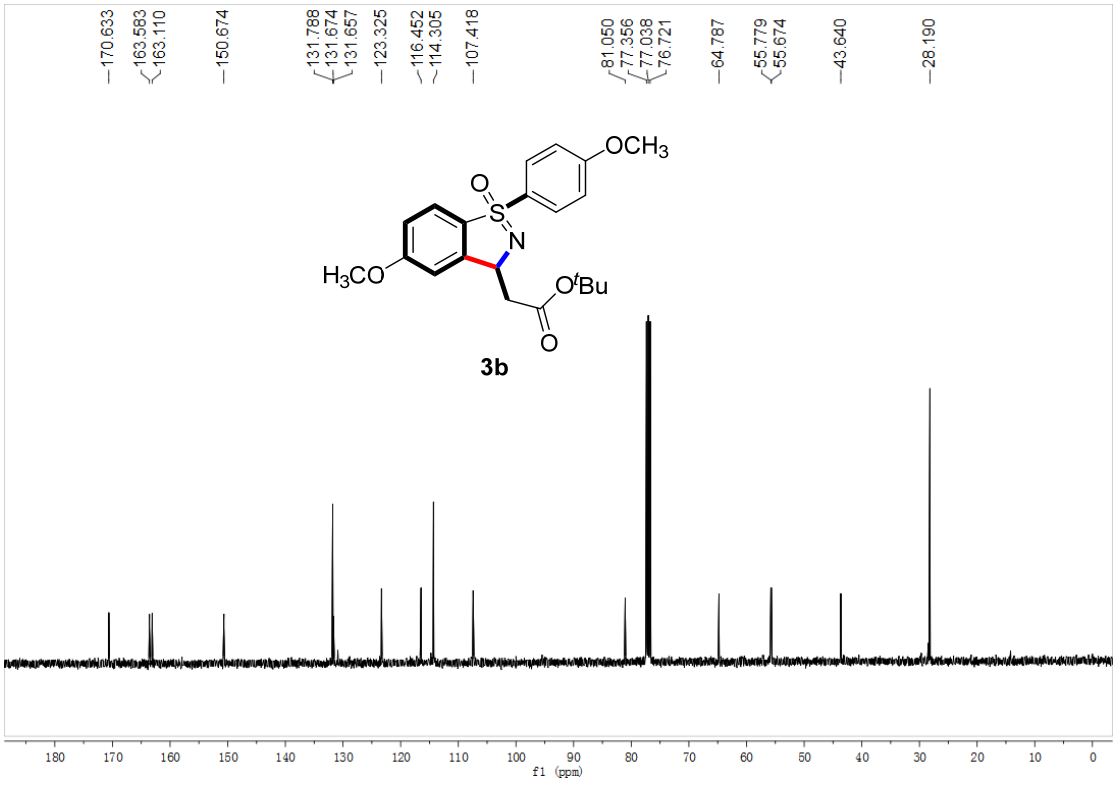
7.910
7.388
7.367
7.265
6.987
6.966
6.935
6.930
6.914
6.909
5.521
5.504
5.488
3.862
3.838
2.920
2.904
2.882
2.866
2.767
2.749
2.729
2.711
1.671
1.513
1.255
OCH3
O
S
N
H3CO
OtBu
O
3b
1.93
1.04
3.14
1.04
1.00
3.10
2.95
1.04
1.03
9.31
f1 (ppm)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150.674
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131.674
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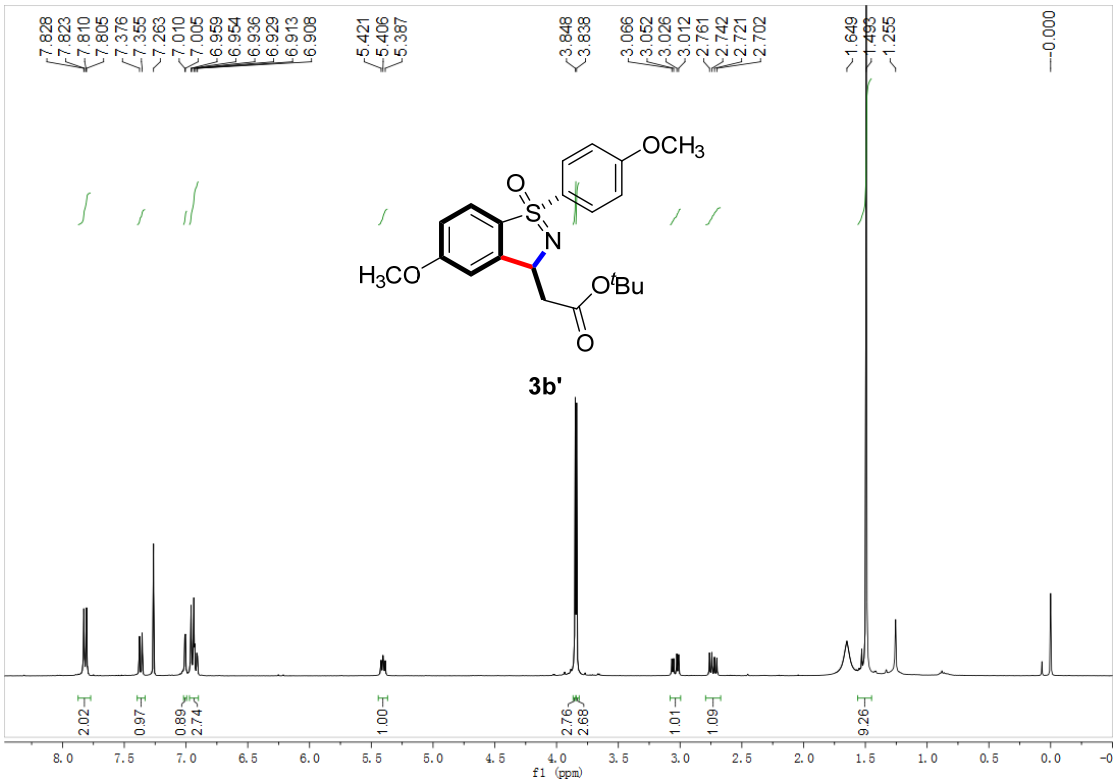
77.038
76.721
64.787
55.779
55.674
43.640
28.190
OCH3
O
S
N
H3CO
OtBu
O
3b
f1 (ppm)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7.823
7.810
7.805
7.376
7.355
7.263
7.010
7.005
6.959
6.954
6.936
6.929
6.913
6.908
5.421
5.406
5.387
3.848
3.838
3.066
3.052
3.026
3.012
2.761
2.742
2.721
2.702
1.649
1.493
1.255
0.000
OCH3
O
S
N
H3CO
OtBu
O
2.02
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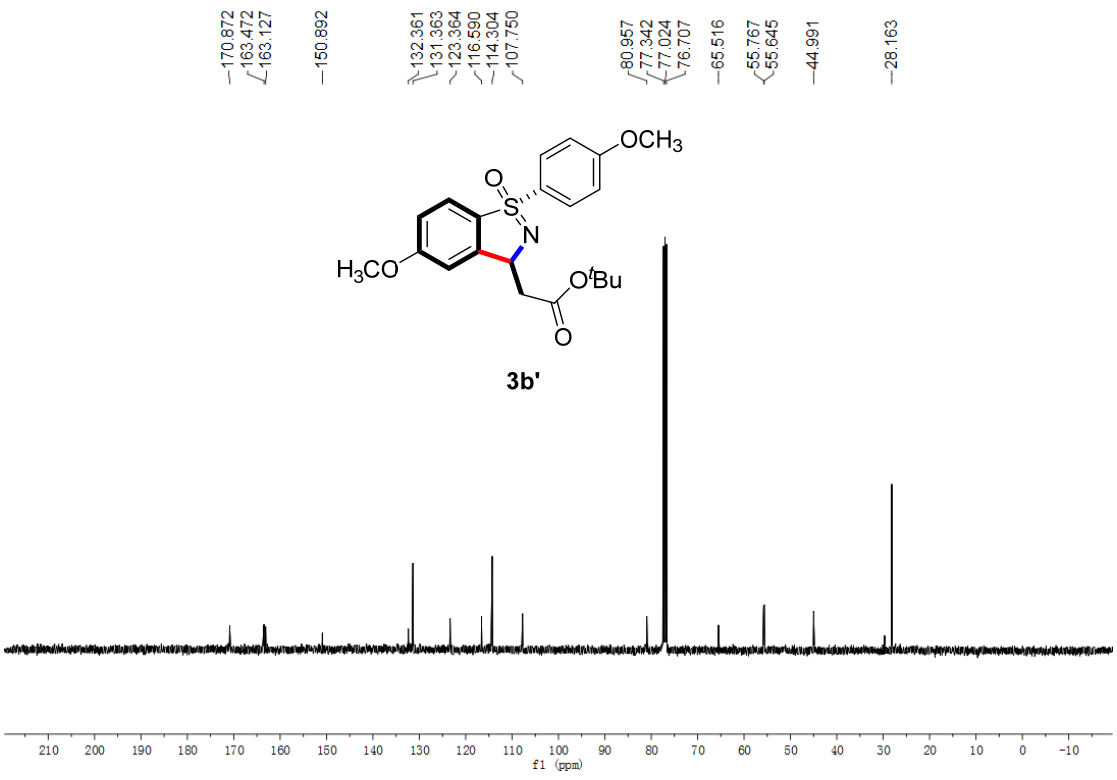
2.74
1.00
2.76
2.68
1.01
1.09
9.26
f1 (ppm)

3b'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163.472
163.127
150.892
132.361
131.363
123.364
116.590
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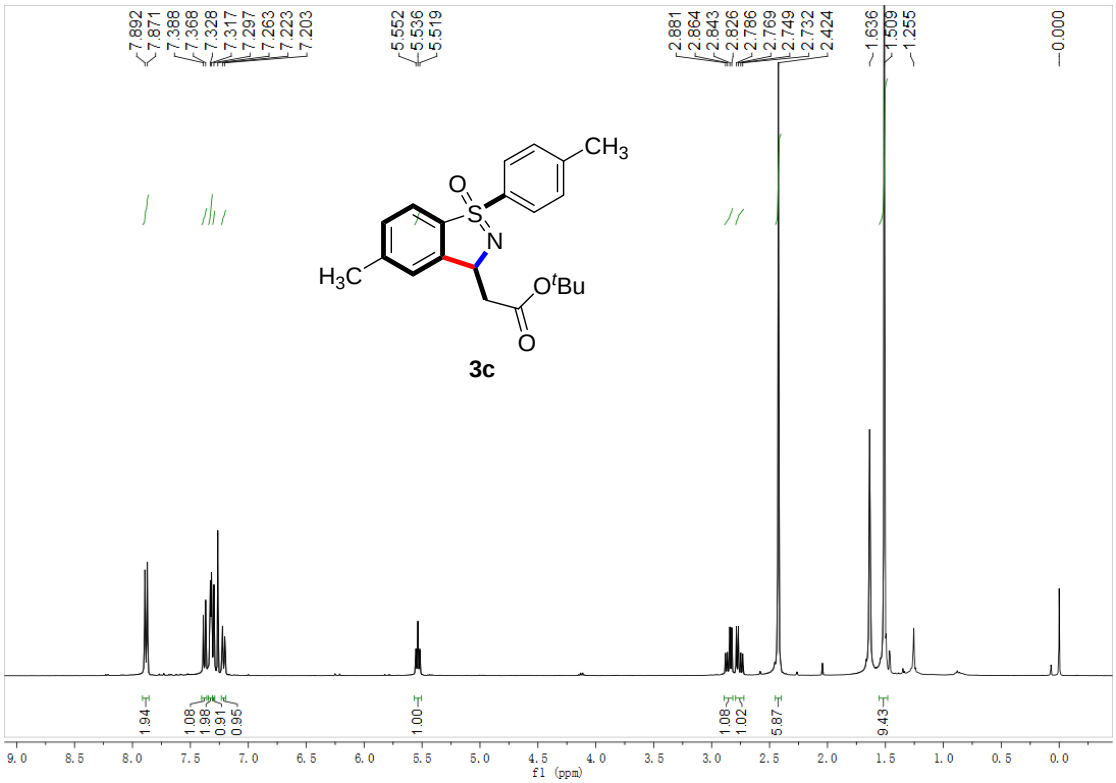
107.750
80.957
77.342
77.024
76.707
65.516
55.767
55.645
44.991
28.163
OCH3
O
S
N
H3CO
OtBu
O
f1 (ppm)

3b'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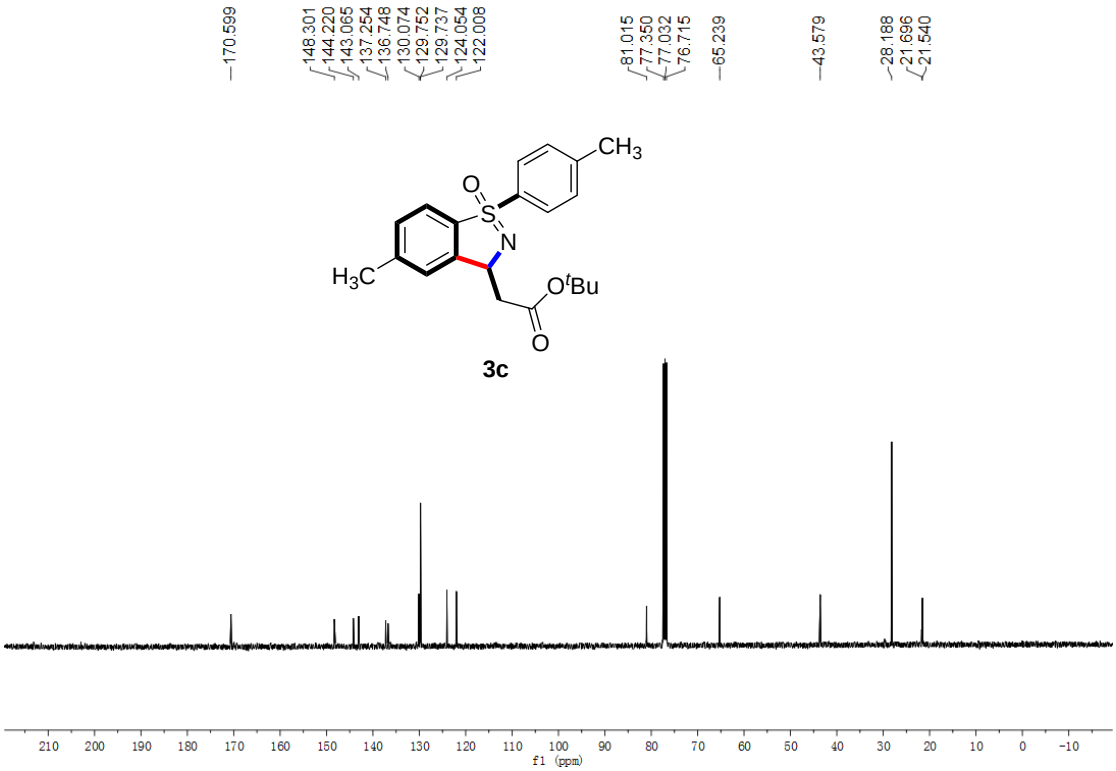
7.328
7.317
7.297
7.263
7.223
7.203
5.552
5.536
5.519
2.881
2.864
2.843
2.826
2.786
2.769
2.749
2.732
2.424
1.636
1.509
1.255
0.000
CH3
O
S
N
H3C
OtBu
O
1.94
1.08
1.98
0.91
0.95
1.00
1.08
1.02
5.87
9.43
f1 (ppm)

3c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129.752
129.737
124.054
122.008
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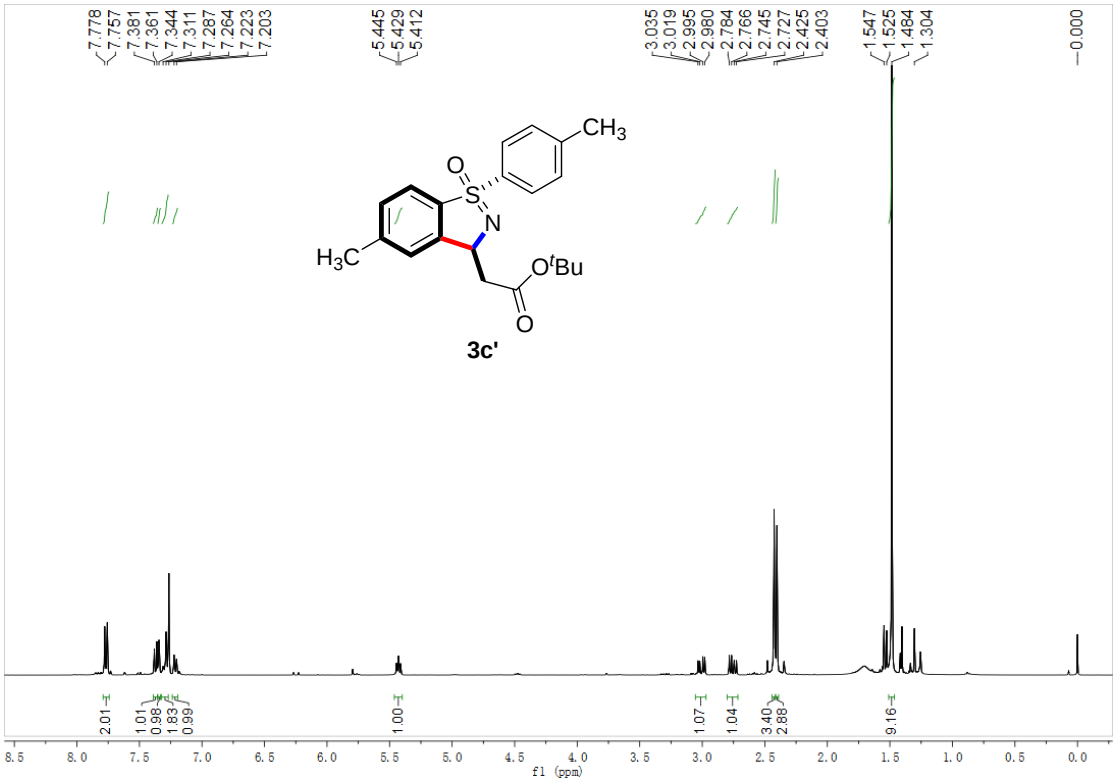
77.350
77.032
76.715
65.239
43.579
28.188
21.696
21.540
CH3
O
S
N
H3C
OtBu
O
f1 (ppm)

3c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7.381
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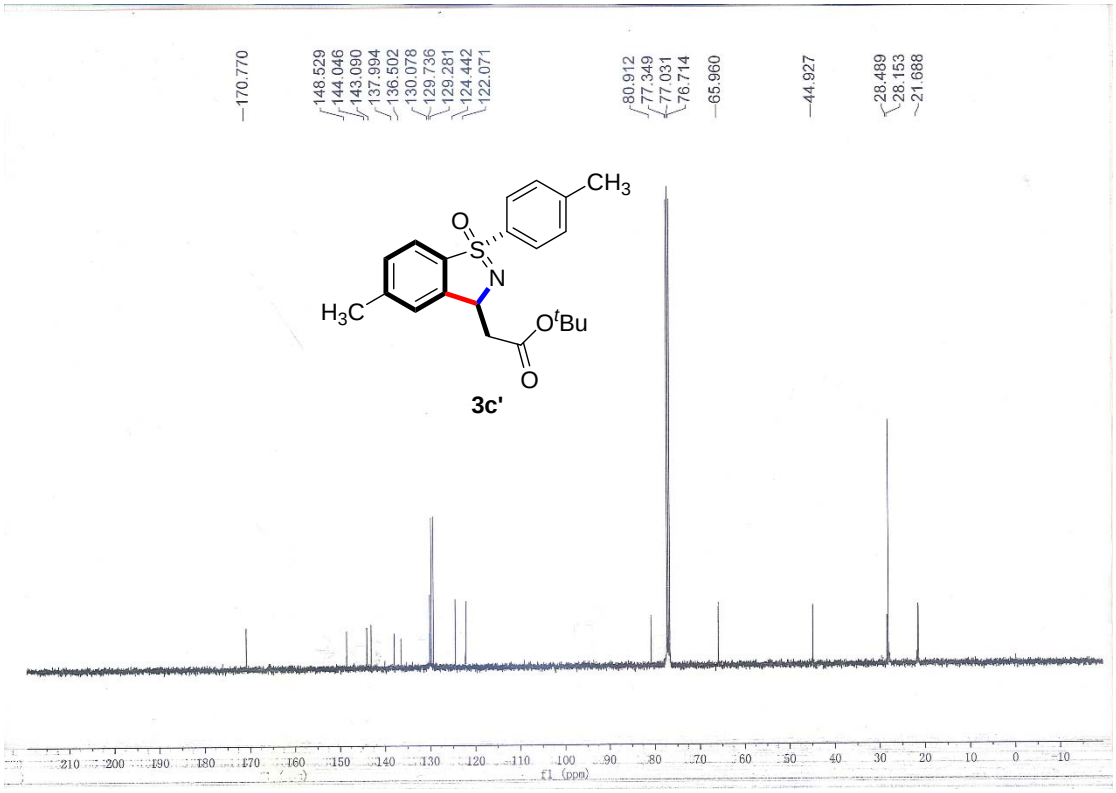
7.311
7.287
7.264
7.223
7.203
5.445
5.429
5.412
3.035
3.019
2.995
2.980
2.784
2.766
2.745
2.727
2.425
2.403
1.547
1.525
1.484
1.304
0.000
CH3
O
S
N
H3C
OtBu
O
3c'
2.01
1.01
0.98
1.83
0.99
1.00
1.07
1.04
3.40
2.88
9.16
f1 (ppm)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77.349
77.031
76.714
65.960
44.927
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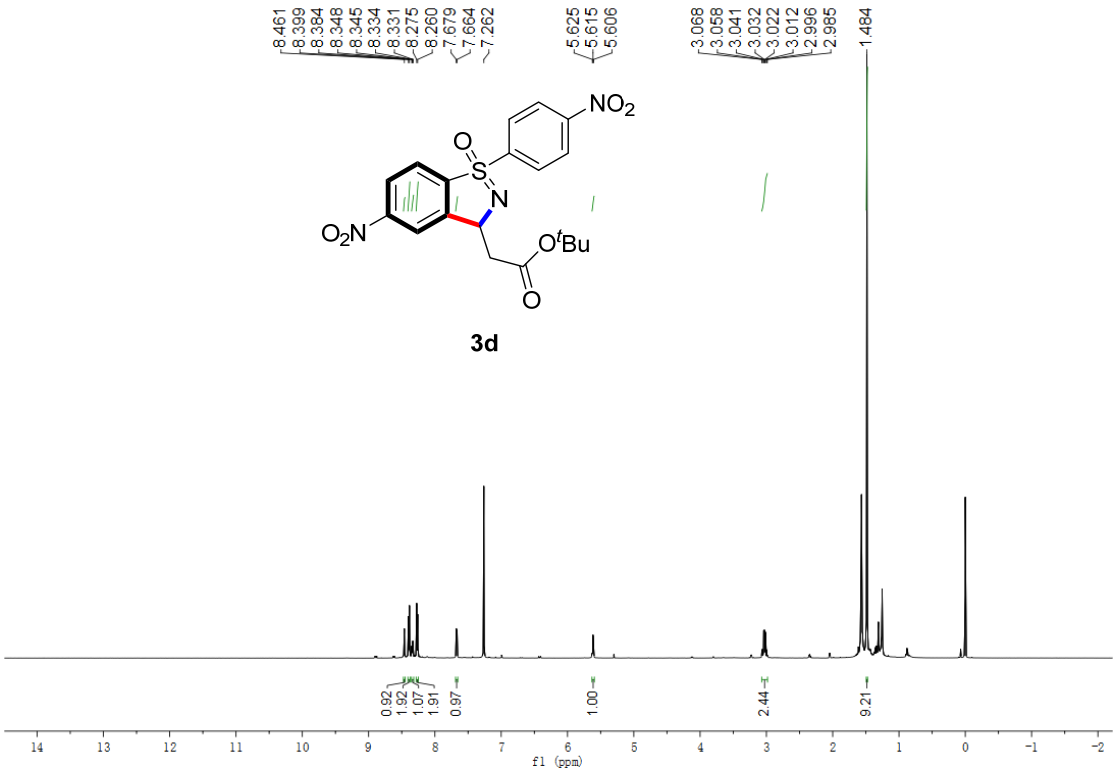
28.153
21.688
CH3
O
S
N
H3C
OtBu
O
3c'
f1 (ppm)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5.615
5.606
3.068
3.058
3.041
3.032
3.022
3.012
2.996
2.985
1.484
NO2
O
S
N
O2N
OtBu
O
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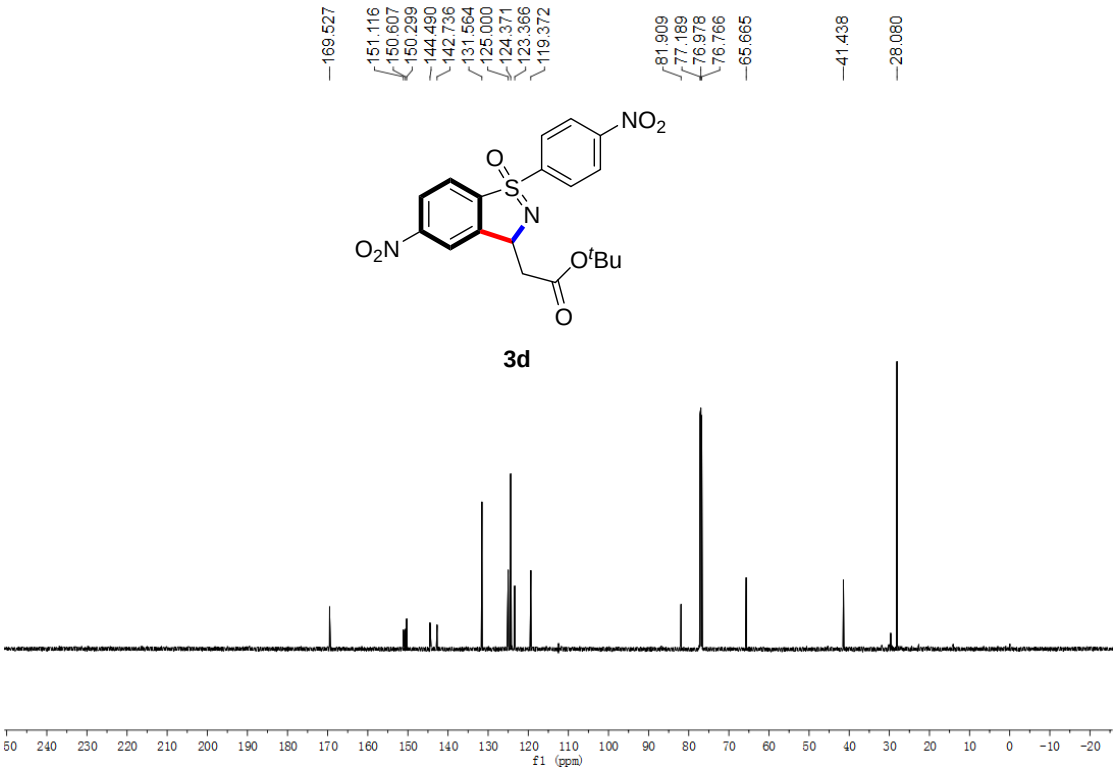
1.92
1.07
1.91
0.97
1.00
2.44
9.21
f1 (ppm)

3d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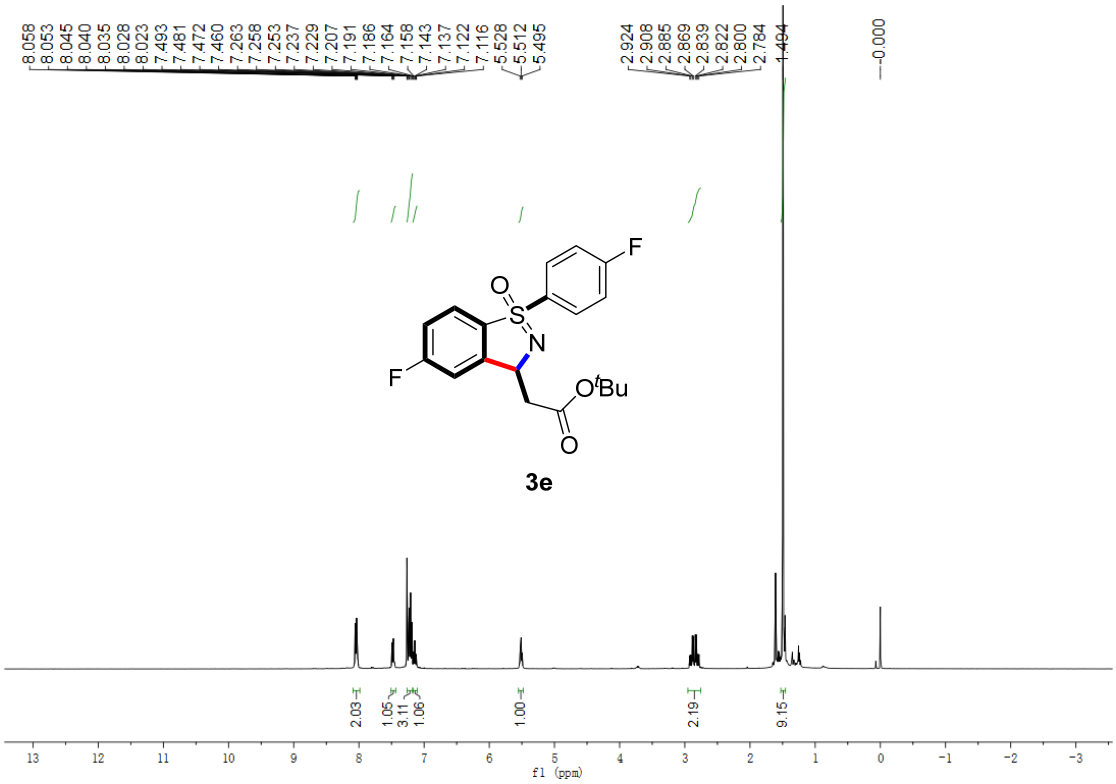
125.000
124.371
123.366
119.372
81.909
77.189
76.978
76.766
65.665
41.438
28.080
NO2
O
S
N
O2N
OtBu
O
f1 (ppm)

3d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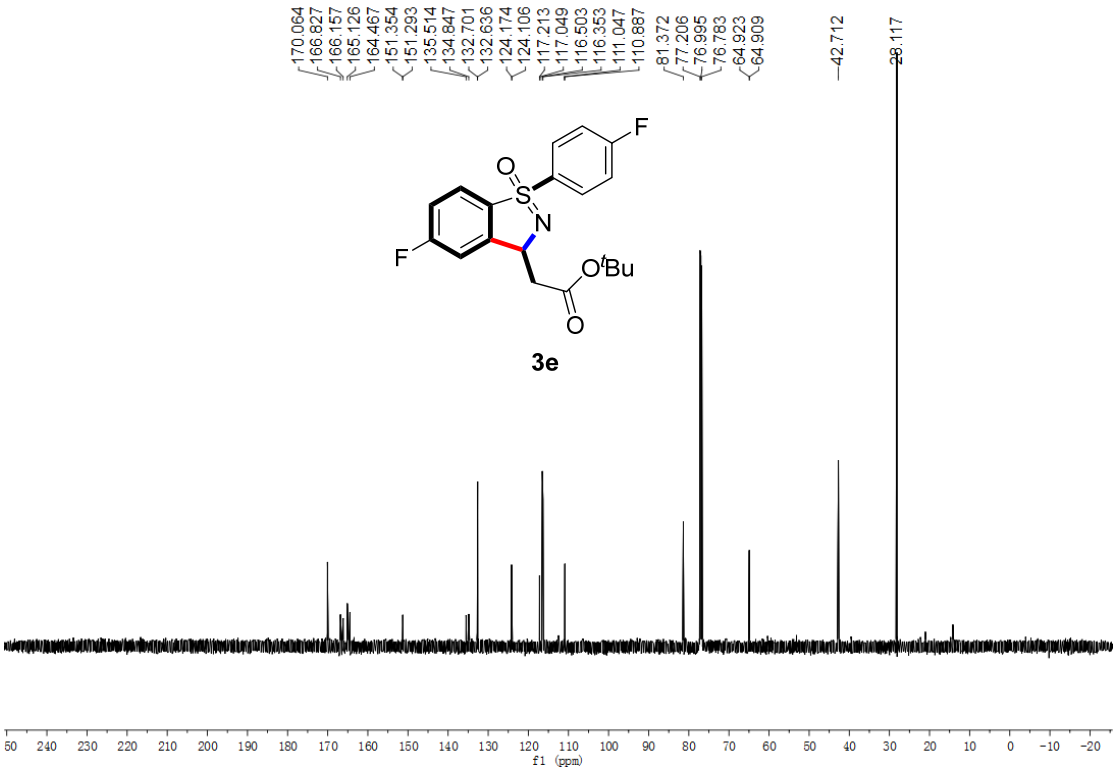
8.053
8.045
8.040
8.035
8.028
8.023
7.493
7.481
7.472
7.460
7.263
7.258
7.253
7.237
7.229
7.207
7.191
7.186
7.164
7.158
7.143
7.137
7.122
7.116
5.528
5.512
5.495
2.924
2.908
2.885
2.869
2.839
2.822
2.800
2.784
1.494
0.000
F
O
S
N
F
O
tBu
O
3e
2.03
1.05
3.11
1.06
1.00
2.19
9.15
f1 (ppm)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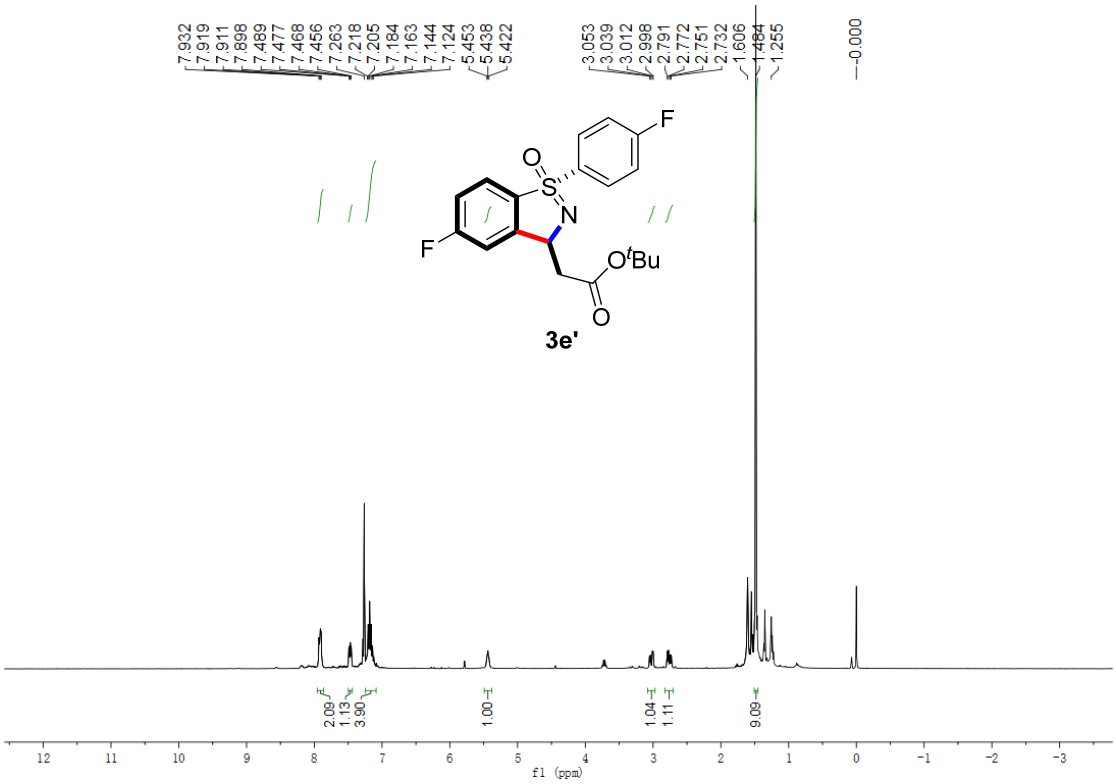
166.827
166.157
165.126
164.467
151.354
151.293
135.514
134.847
132.701
132.636
124.174
124.106
117.213
117.049
116.503
116.353
111.047
110.887
81.372
77.206
76.995
76.783
64.923
64.909
42.712
28.117
F
O
S
N
F
O
tBu
O
3e
f1 (ppm)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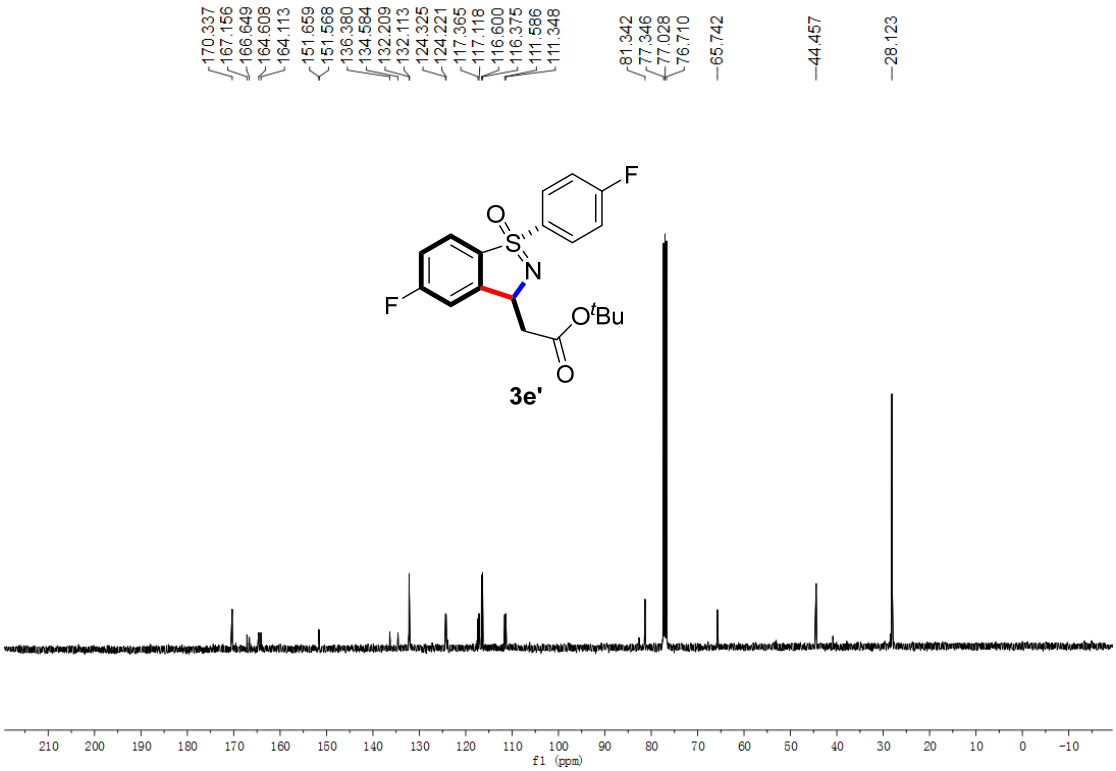
7.919
7.911
7.898
7.489
7.477
7.468
7.456
7.263
7.218
7.205
7.184
7.163
7.144
7.124
5.453
5.438
5.422
3.053
3.039
3.012
2.998
2.791
2.772
2.751
2.732
1.606
1.484
1.255
0.000
F
O
S
N
F
O^{t}Bu
O
3e'
2.09
1.13
3.90
1.00
1.04
1.11
9.09
f1 (ppm)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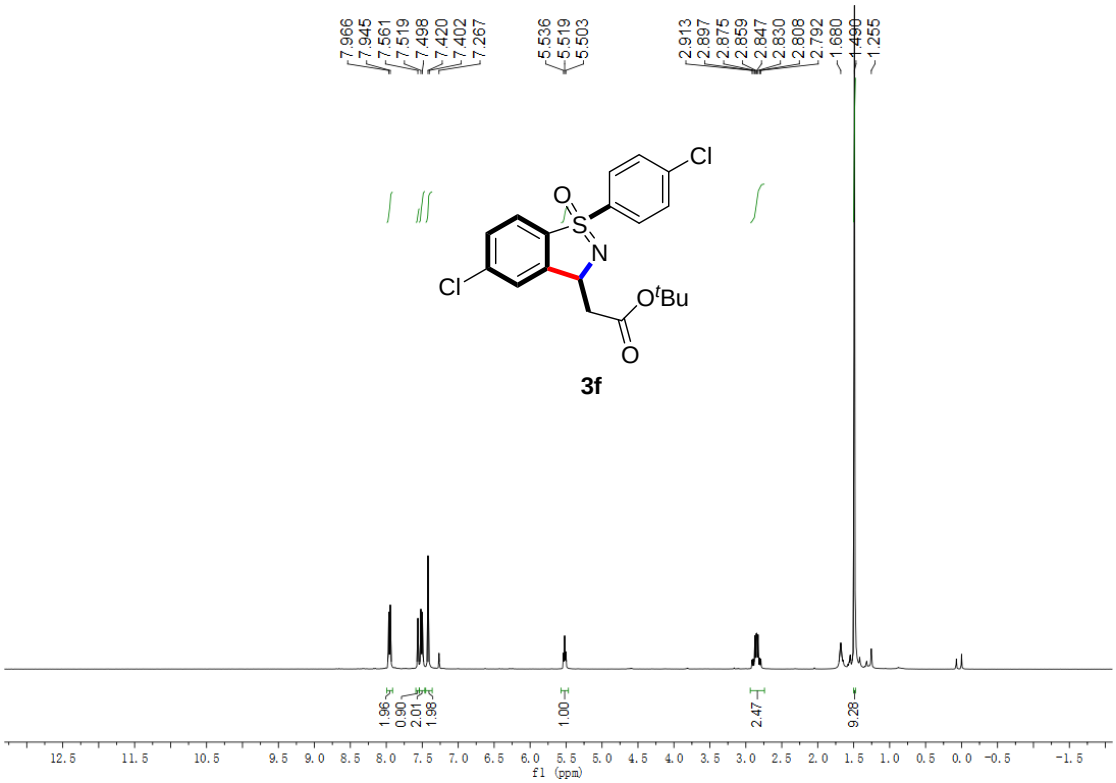
166.649
164.608
164.113
151.659
151.568
136.380
134.584
132.209
132.113
124.325
124.221
117.365
117.118
116.600
116.375
111.586
111.348
81.342
77.346
77.028
76.710
65.742
44.457
28.123
F
O
S
N
F
O^{t}Bu
O
3e'
f1 (ppm)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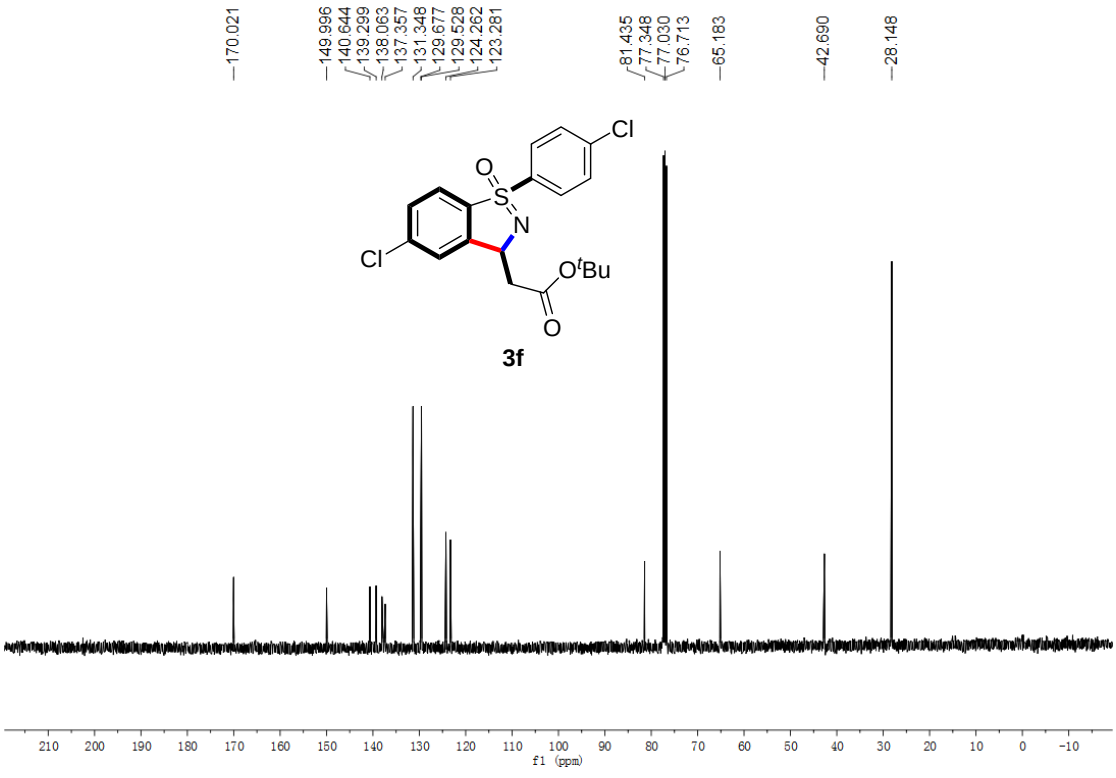
7.945
7.561
7.519
7.498
7.420
7.402
7.267
5.536
5.519
5.503
2.913
2.897
2.875
2.859
2.847
2.830
2.808
2.792
1.680
1.490
1.255
Cl
O
S
N
Cl
O^{t}Bu
O
1.96
0.90
2.01
1.98
1.00
2.47
9.28
f1 (ppm)

3f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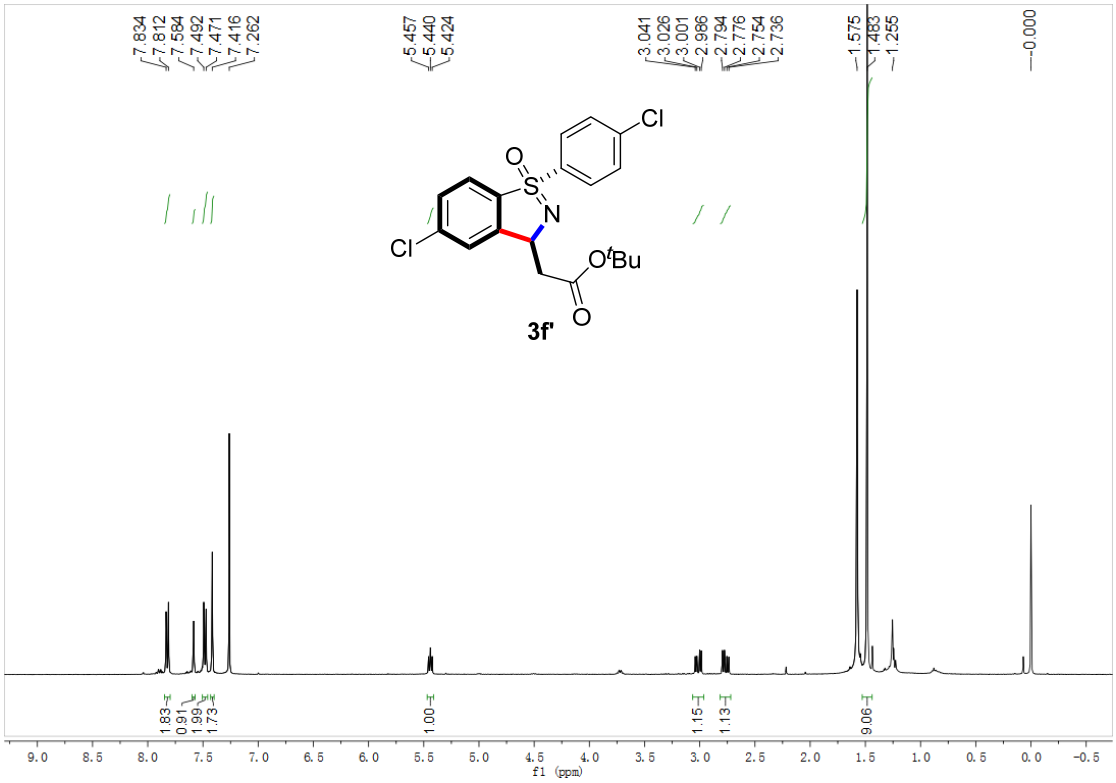
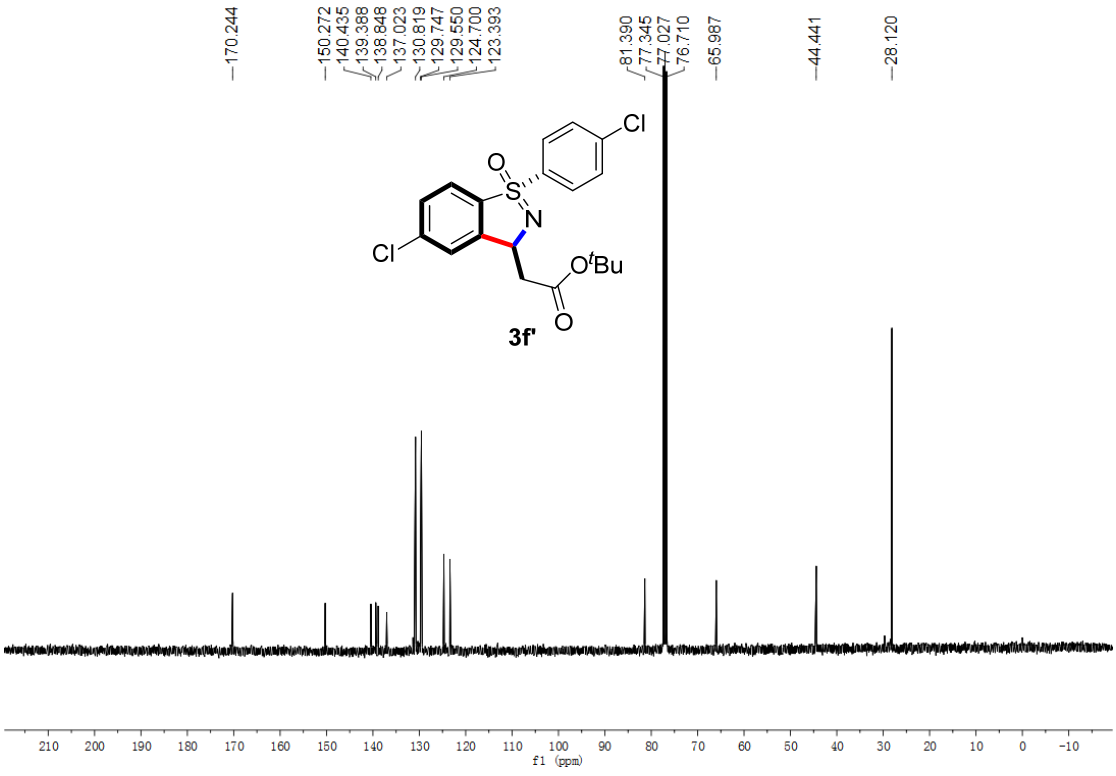
149.996
140.644
139.299
138.063
137.357
131.348
129.677
129.528
124.262
123.281
81.435
77.348
77.030
76.713
65.183
42.690
28.148
Cl
O
S
N
Cl
O^{t}Bu
O
f1 (ppm)

3f


7.834
7.812
7.584
7.492
7.471
7.416
7.262
5.457
5.440
5.424
3.041
3.026
3.001
2.986
2.794
2.776
2.754
2.736
1.575
1.483
1.255
0.000
Cl
O
S
N
Cl
O^{t}Bu
O
3f'
1.83
0.91
1.99
1.73
1.00
1.15
1.13
9.06
f1 (ppm)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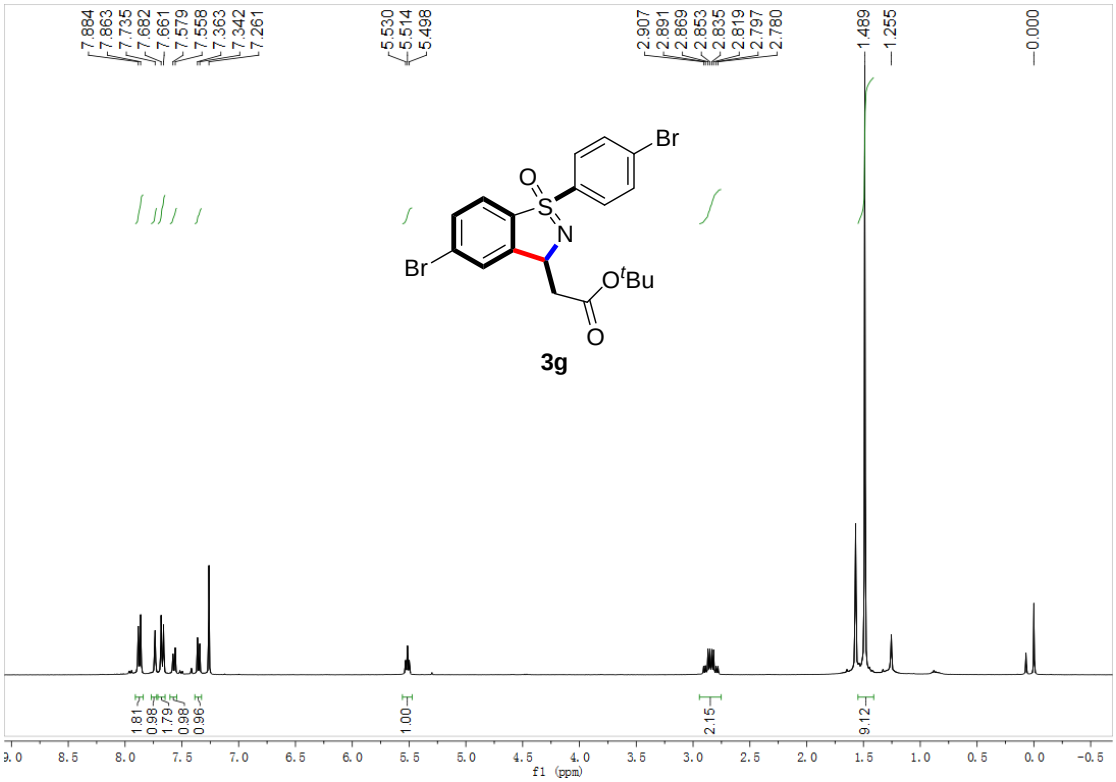
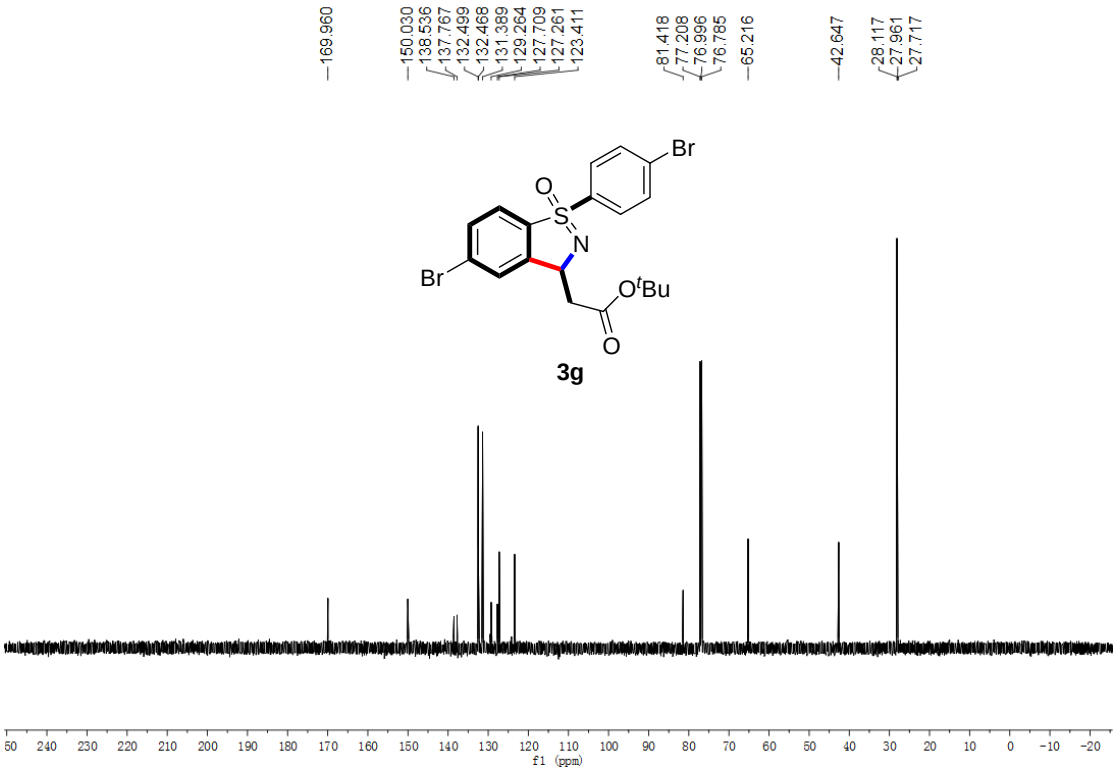
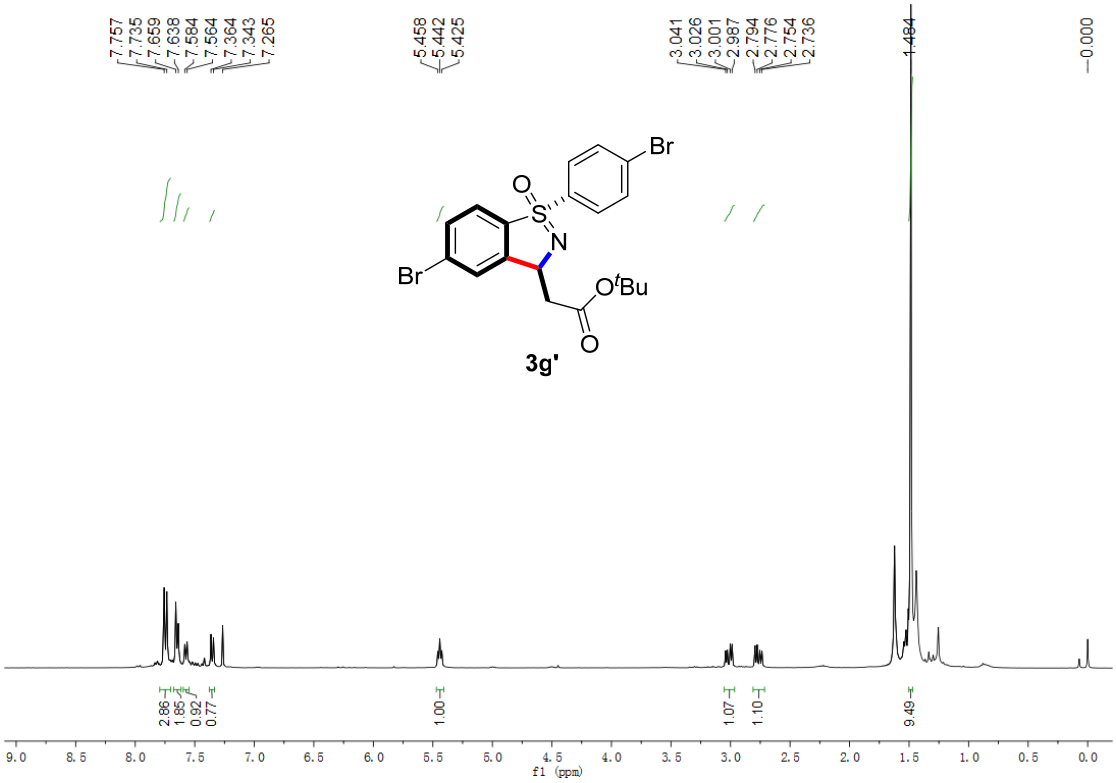
150.272
140.435
139.388
138.848
137.023
130.819
129.747
129.550
124.700
123.393
81.390
77.345
77.027
76.710
65.987
44.441
28.120
Cl
O
S
N
Cl
O^{t}Bu
O
3f'
f1 (ppm)

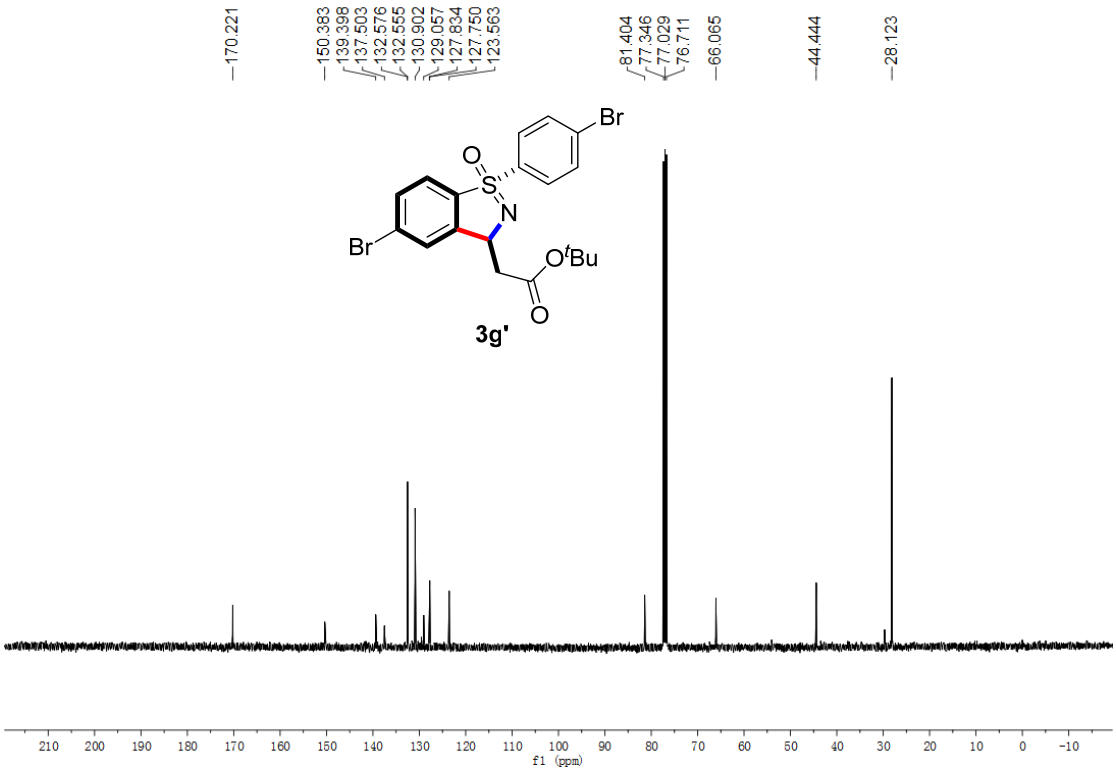

7.884
7.863
7.735
7.682
7.661
7.579
7.558
7.363
7.342
7.261
5.530
5.514
5.498
2.907
2.891
2.869
2.853
2.835
2.819
2.797
2.780
1.489
1.255
0.000
Br
O
S
N
Br
O^{t}Bu
O
1.81
0.98
1.79
0.98
0.96
1.00
2.15
9.12
f1 (ppm)

3g


169.960
150.030
138.536
137.767
132.499
132.468
131.389
129.264
127.709
127.261
123.411
81.418
77.208
76.996
76.785
65.216
42.647
28.117
27.961
27.717
Br
O
S
N
Br
O^{t}Bu
O
f1 (ppm)

3g


7.757
7.735
7.659
7.638
7.584
7.564
7.364
7.343
7.265
5.458
5.442
5.425
3.041
3.026
3.001
2.987
2.794
2.776
2.754
2.736
1.484
0.000
Br
O
S
N
Br
O^{t}Bu
O
3g'
2.86
1.85
0.92
0.77
1.00
1.07
1.10
9.49
f1 (ppm)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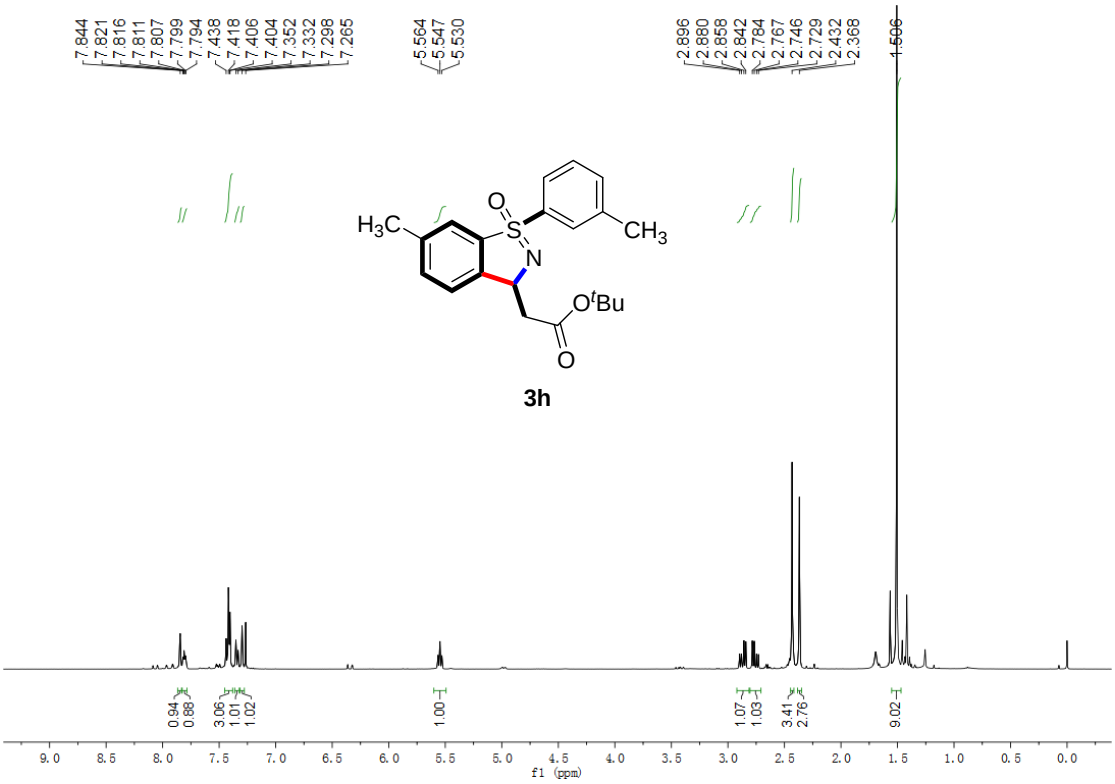
150.383
139.398
137.503
132.576
132.555
130.902
129.057
127.834
127.750
123.563
81.404
77.346
77.029
76.711
66.065
44.444
28.123
Br
O
S
N
Br
O^{t}Bu
O
3g'
f1 (ppm)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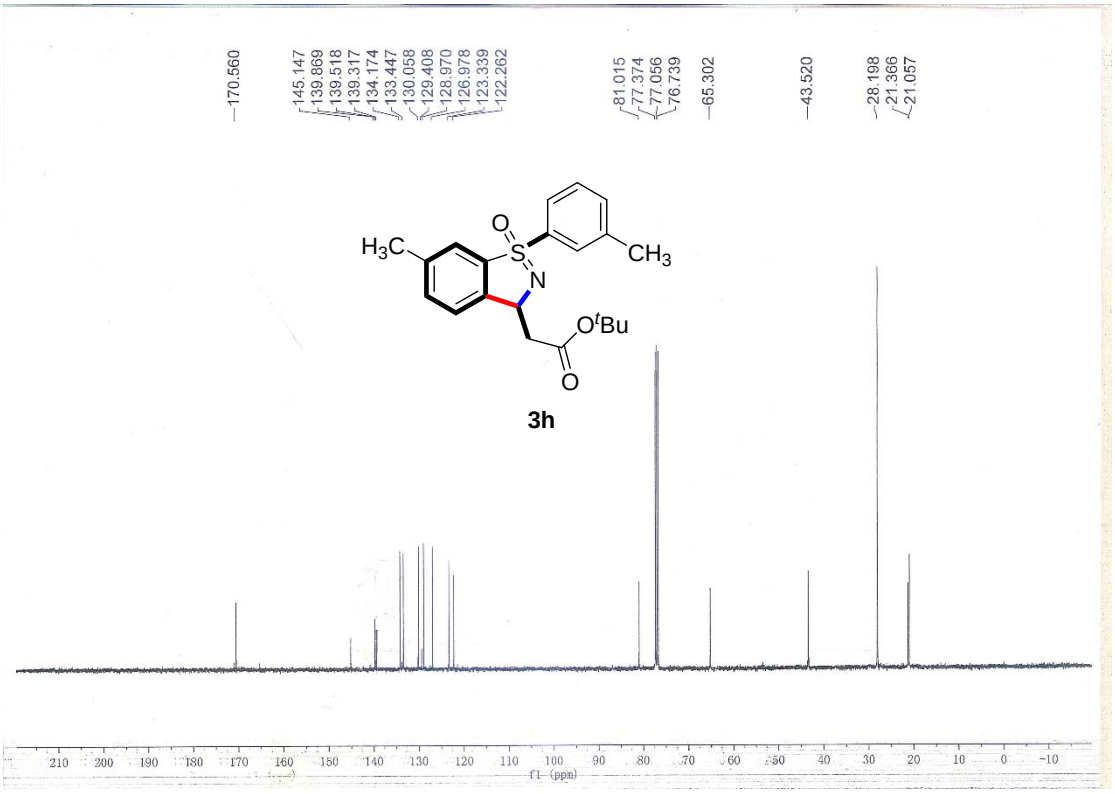
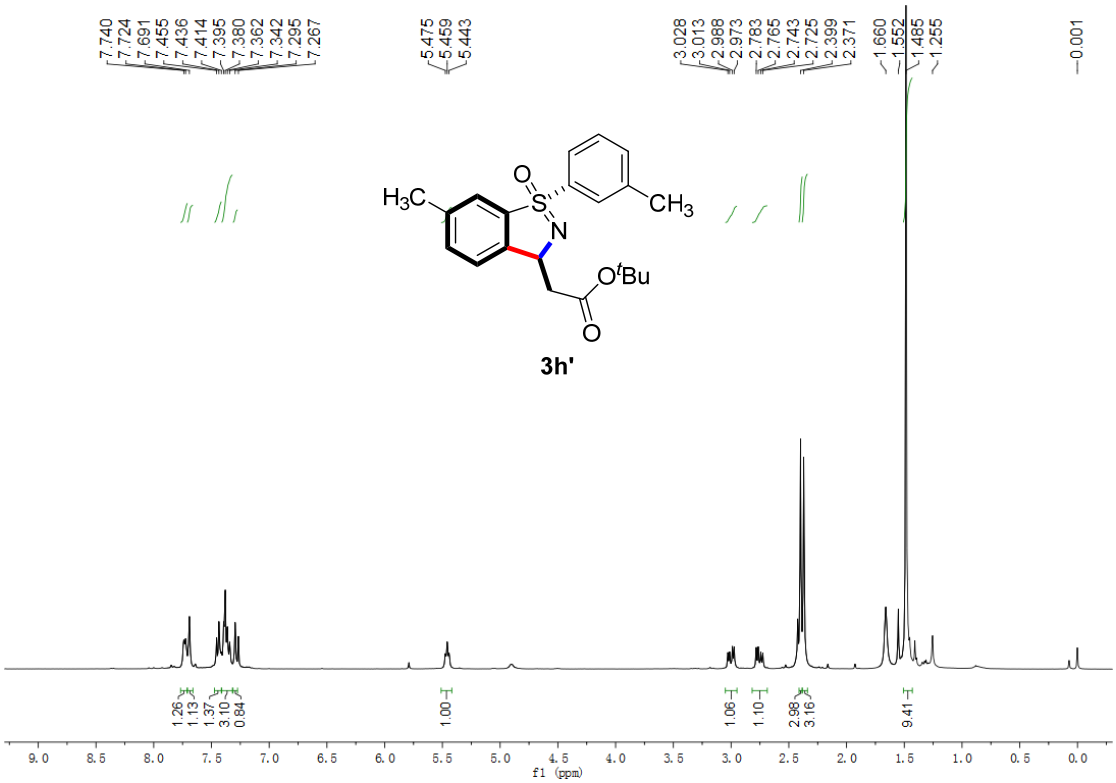
7.821
7.816
7.811
7.807
7.799
7.794
7.438
7.418
7.406
7.404
7.352
7.332
7.298
7.265
5.564
5.547
5.530
2.896
2.880
2.858
2.842
2.784
2.767
2.746
2.729
2.432
2.368
1.596
H3C
CH3
O
S
N
OtBu
O
0.94
0.88
3.06
1.01
1.02
1.00
1.07
1.03
3.41
2.76
9.02
f1 (ppm)

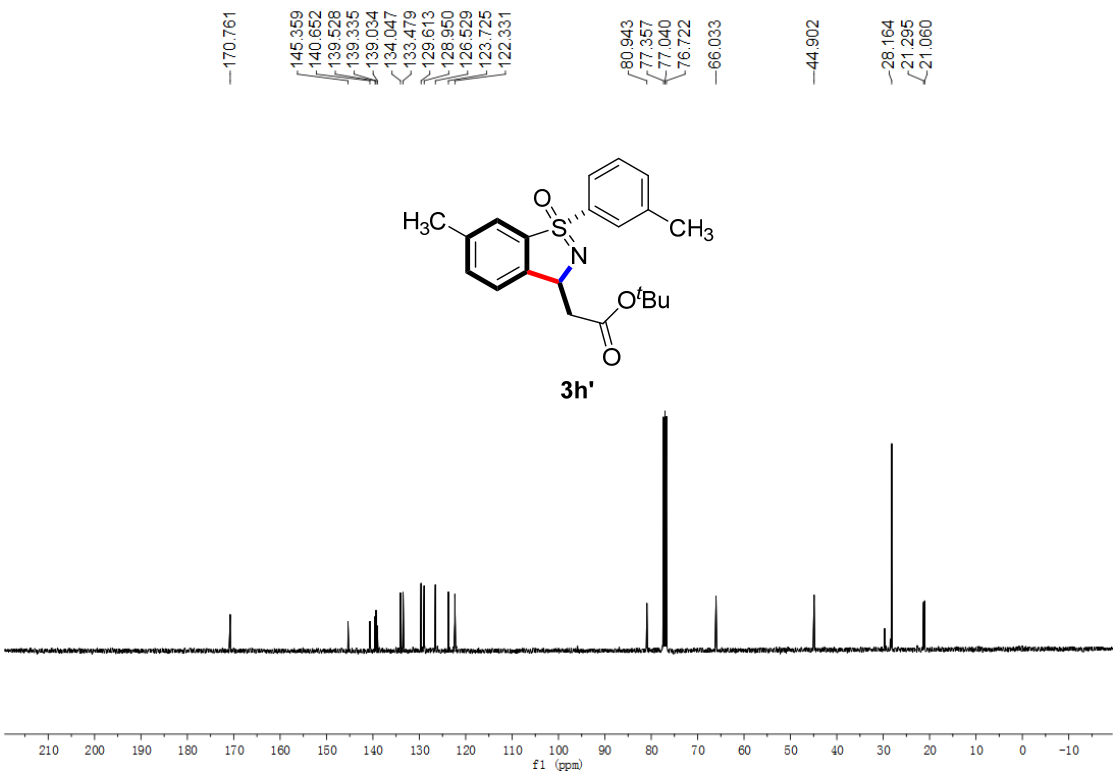
3h


170.560
145.147
139.869
139.518
139.317
134.174
133.447
130.058
129.408
128.970
126.978
123.339
122.262
81.015
77.374
77.056
76.739
65.302
43.520
28.198
21.366
21.057
H3C
CH3
O
S
N
OtBu
O
f1 (ppm)

3h


7.740
7.724
7.691
7.455
7.436
7.414
7.395
7.380
7.362
7.342
7.295
7.267
5.475
5.459
5.443
3.028
3.013
2.988
2.973
2.783
2.765
2.743
2.725
2.399
2.371
1.660
1.552
1.485
1.255
0.001
H3C
CH3
O
S
N
OtBu
O
1.26
1.13
1.37
3.10
0.84
1.00
1.06
1.10
2.98
3.16
9.41
f1 (ppm)

3h'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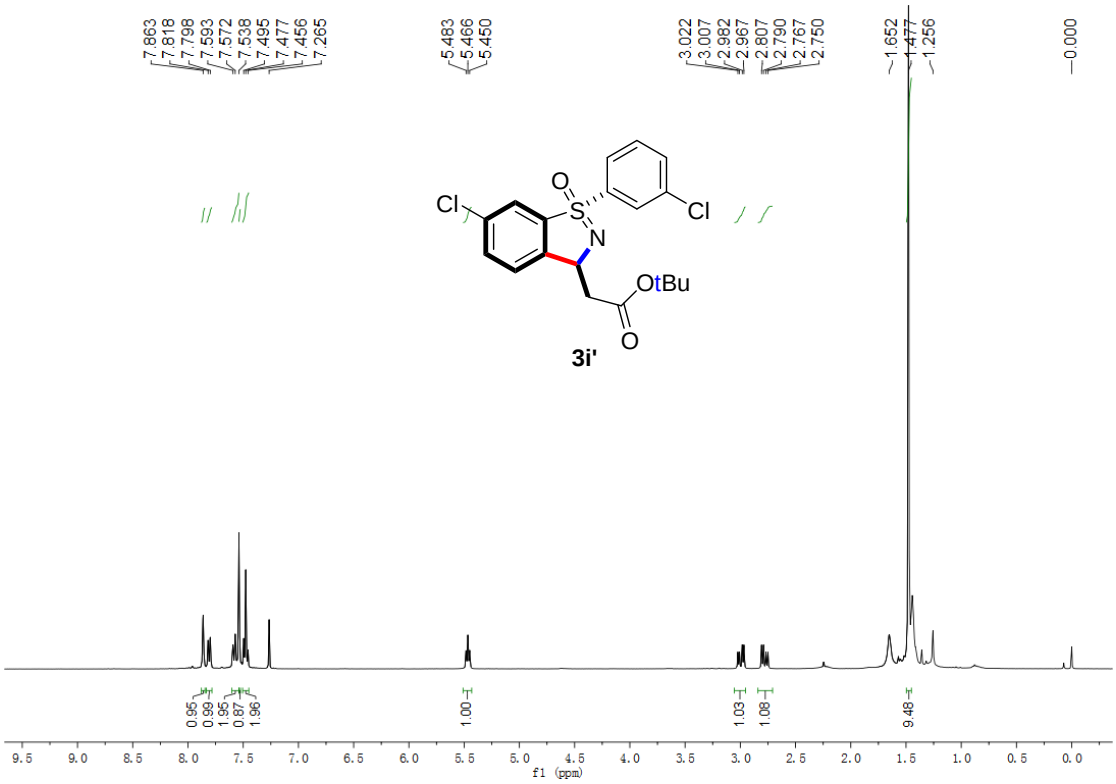
140.652
139.528
139.335
139.034
134.047
133.479
129.613
128.950
126.529
123.725
122.331
80.943
77.357
77.040
76.722
66.033
44.902
28.164
21.295
21.060
H3C
CH3
O
S
N
OtBu
O
f1 (ppm)

3h'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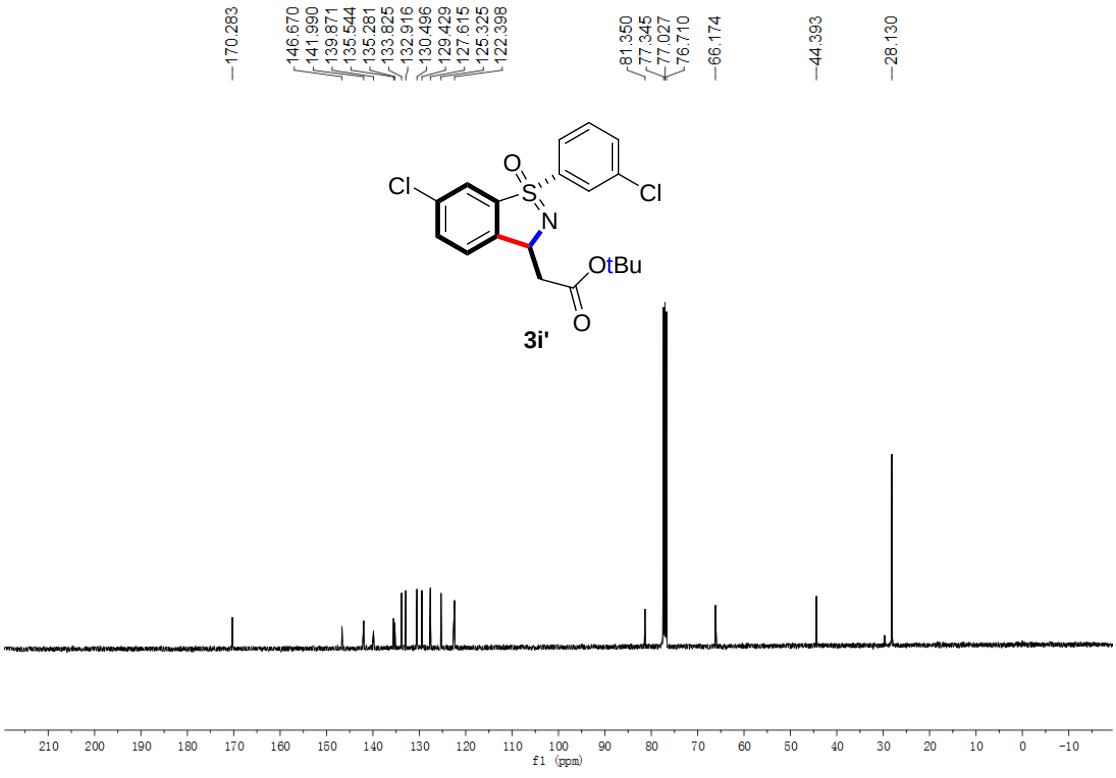
7.818
7.798
7.593
7.572
7.538
7.495
7.477
7.456
7.265
5.483
5.466
5.450
3.022
3.007
2.982
2.967
2.807
2.790
2.767
2.750
1.652
1.477
1.256
0.000
Cl
O
S
N
Cl
OtBu
O
3i'
0.95
0.99
1.95
0.87
1.96
1.00
1.03
1.08
9.48
f1 (ppm)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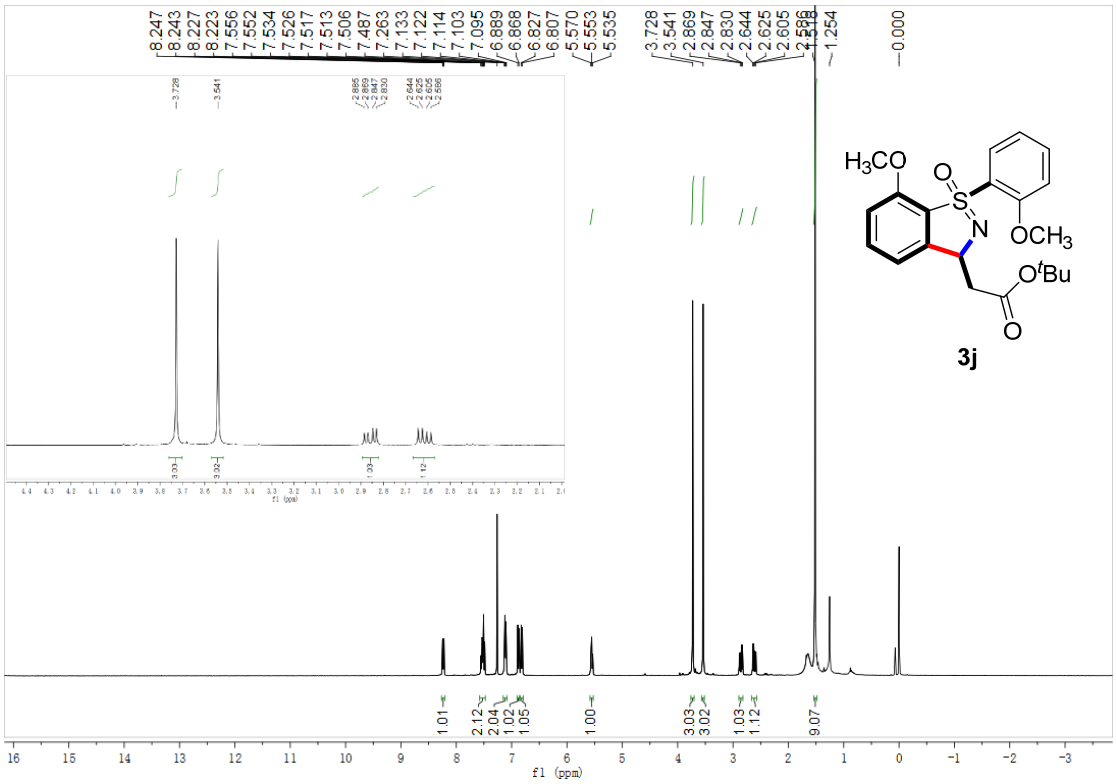
135.281
133.825
132.916
130.496
129.429
127.615
125.325
122.398
81.350
77.345
77.027
76.710
66.174
44.393
28.130
Cl
O
S
N
Cl
OtBu
O
3i'
f1 (ppm)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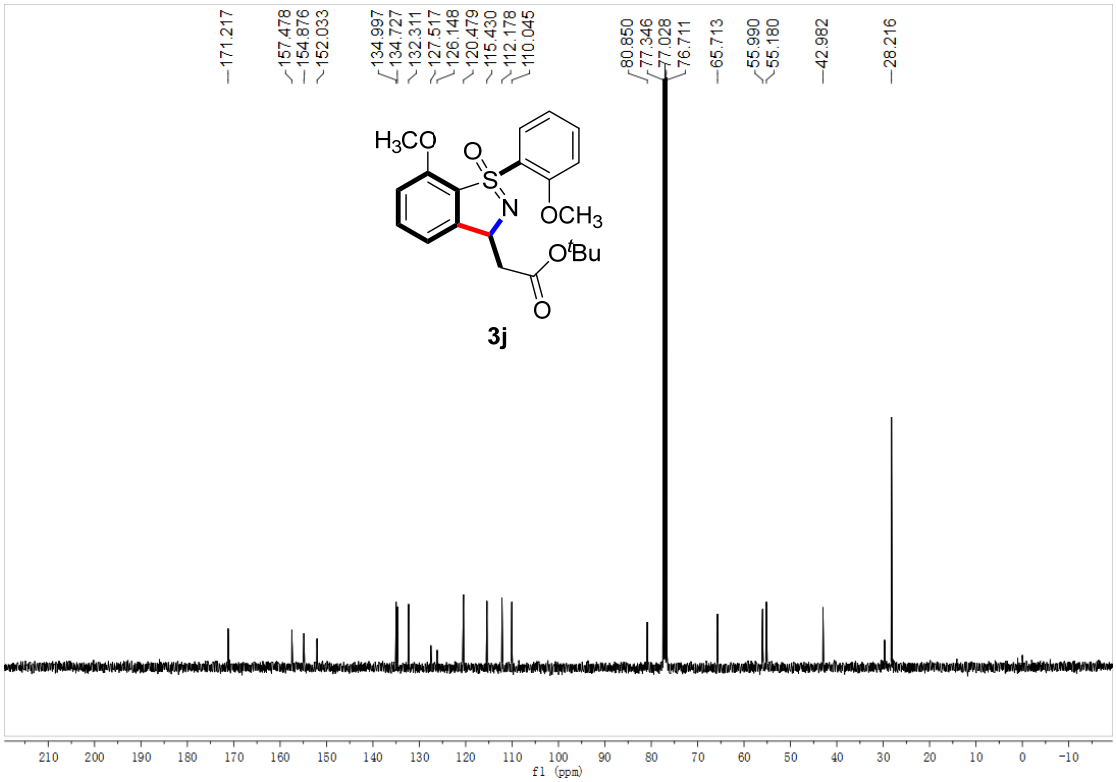
8.227
8.223
7.556
7.552
7.534
7.526
7.517
7.513
7.506
7.487
7.263
7.133
7.122
7.114
7.103
7.095
6.889
6.868
6.827
6.807
5.570
5.553
5.535
3.728
3.541
2.869
2.847
2.830
2.644
2.625
2.605
1.254
0.000
1.01
2.12
2.04
1.02
1.05
1.00
3.03
3.02
1.03
1.12
9.07
f1 (ppm)
H3CO
OCH3
OtBu
3j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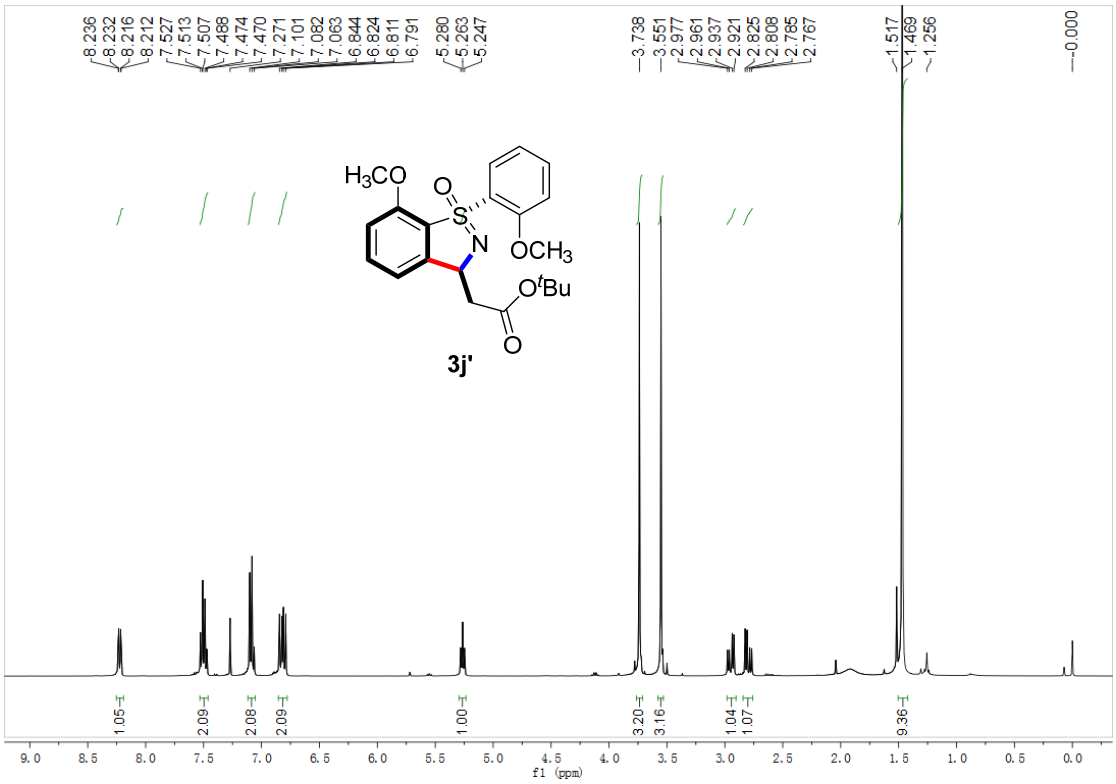
157.478
154.876
152.033
134.997
134.727
132.311
127.517
126.148
120.479
115.430
112.178
110.045
80.850
77.346
77.028
76.711
65.713
55.990
55.180
42.982
28.216
f1 (ppm)
H3CO
OCH3
OtBu
3j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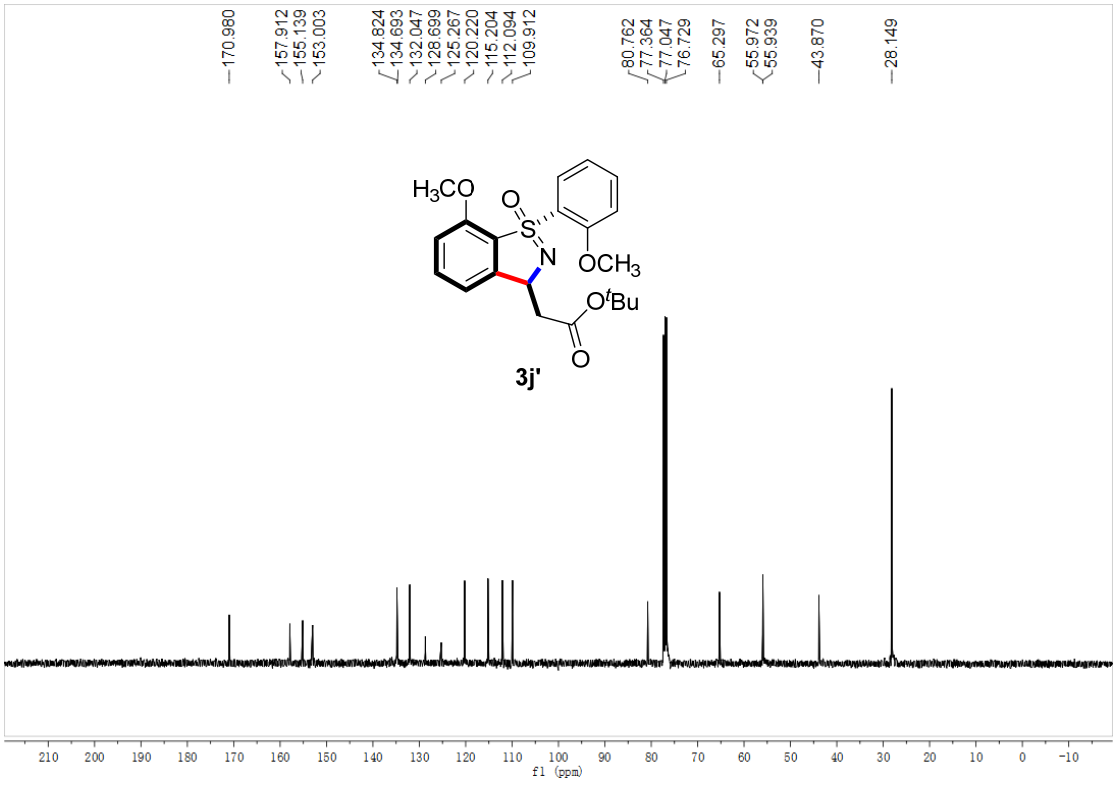
8.232
8.216
8.212
7.527
7.513
7.507
7.488
7.474
7.470
7.271
7.101
7.082
7.063
6.844
6.824
6.811
6.791
5.260
5.263
5.247
3.738
3.551
2.977
2.961
2.937
2.921
2.825
2.808
2.785
2.767
1.517
1.469
1.256
0.000
H3CO
O
S
N
OCH3
OtBu
O
3j'
1.05
2.09
2.08
2.09
1.00
3.20
3.16
1.04
1.07
9.36
f1 (ppm)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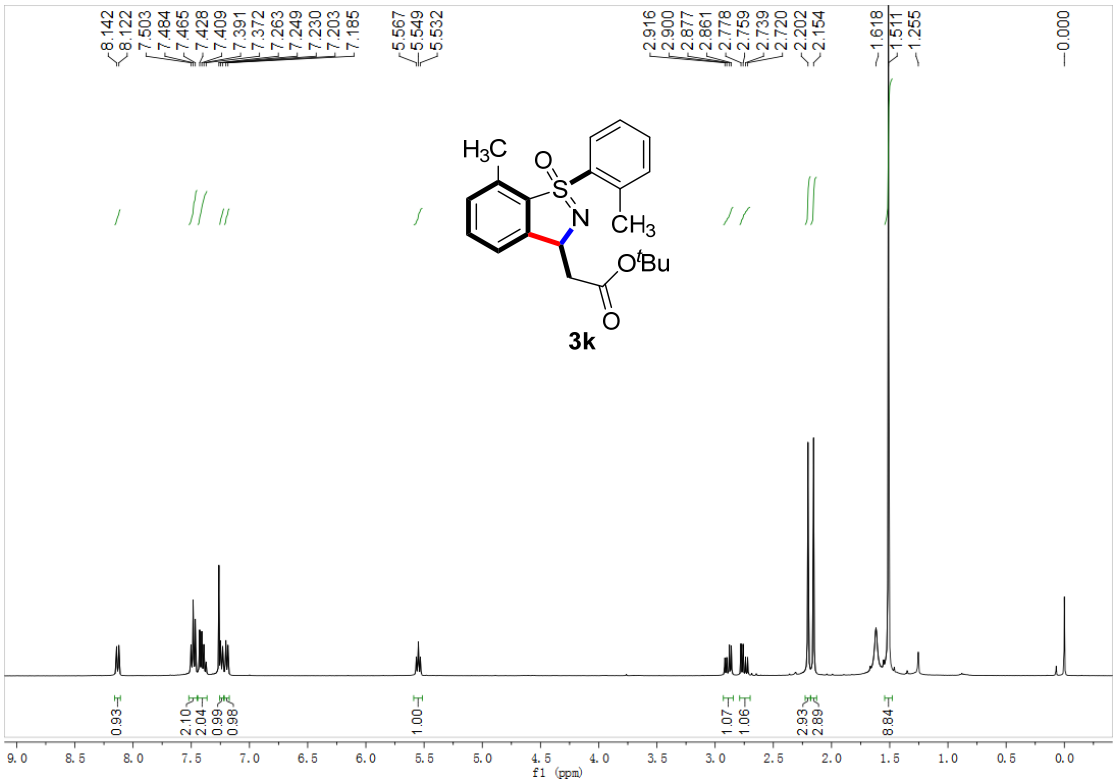
157.912
155.139
153.003
134.824
134.693
132.047
128.699
125.267
120.220
115.204
112.094
109.912
80.762
77.364
77.047
76.729
65.297
55.972
55.939
43.870
28.149
H3CO
O
S
N
OCH3
OtBu
O
3j'
f1 (ppm)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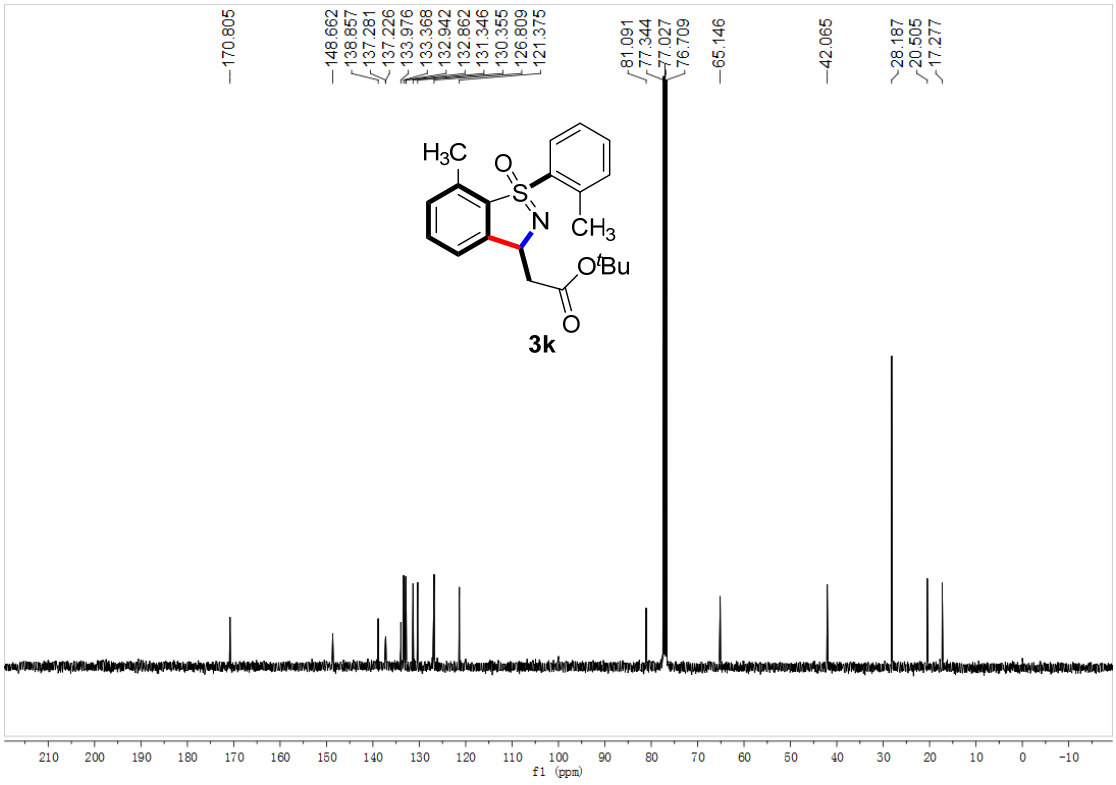
7.465
7.428
7.409
7.391
7.372
7.263
7.249
7.230
7.203
7.185
5.567
5.549
5.532
2.916
2.900
2.877
2.861
2.778
2.759
2.739
2.720
2.202
2.154
1.618
1.511
1.255
0.000
H3C
O
S
N
CH3
OtBu
O
3k
0.93
2.10
2.04
0.99
0.98
1.00
1.07
1.06
2.93
2.89
8.84
f1 (ppm)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137.226
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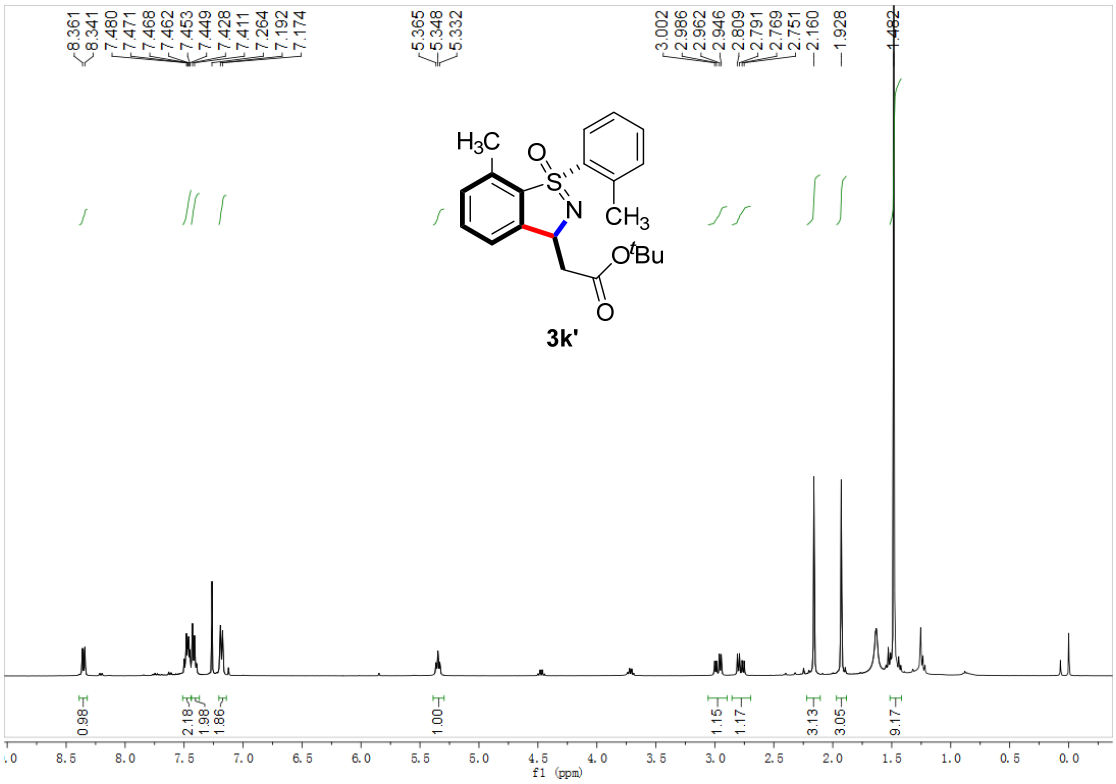
133.368
132.942
132.862
131.346
130.355
126.809
121.375
81.091
77.344
77.027
76.709
65.146
42.065
28.187
20.505
17.277
H3C
O
S
N
CH3
OtBu
O
3k
f1 (ppm)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7.471
7.468
7.462
7.453
7.449
7.428
7.411
7.264
7.192
7.174
5.365
5.348
5.332
3.002
2.986
2.962
2.946
2.809
2.791
2.769
2.751
2.160
1.928
1.482
H3C
O
S
N
CH3
OtBu
O
3k'
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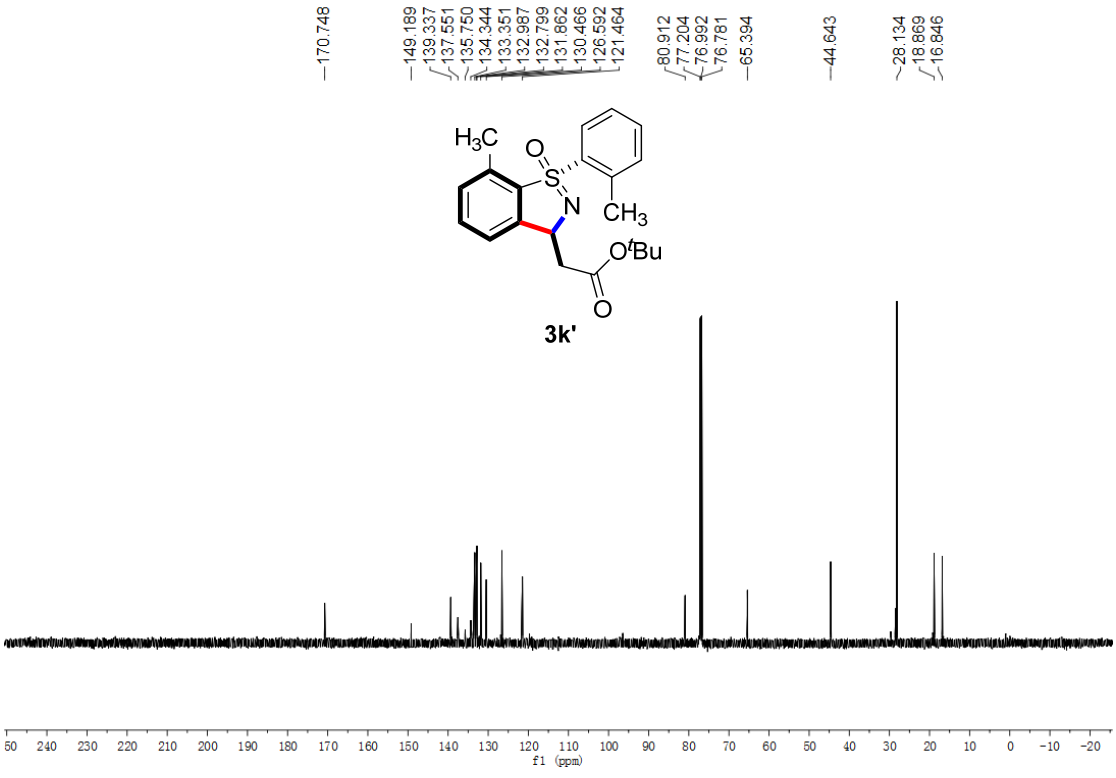
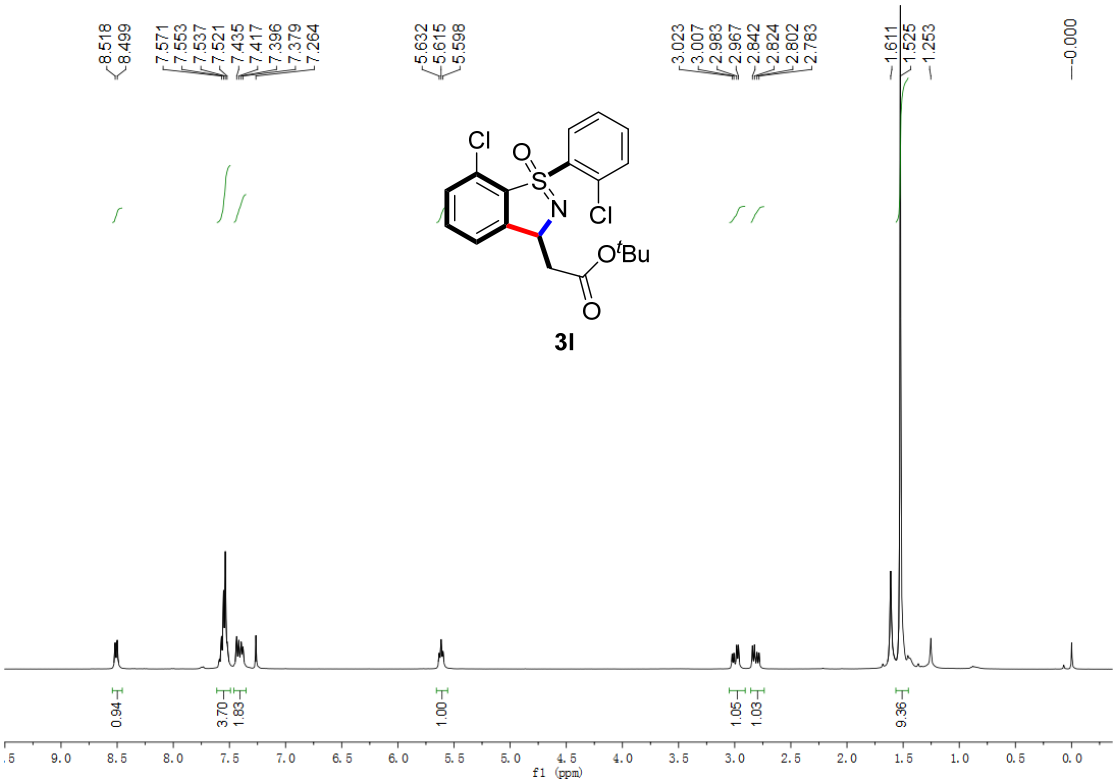
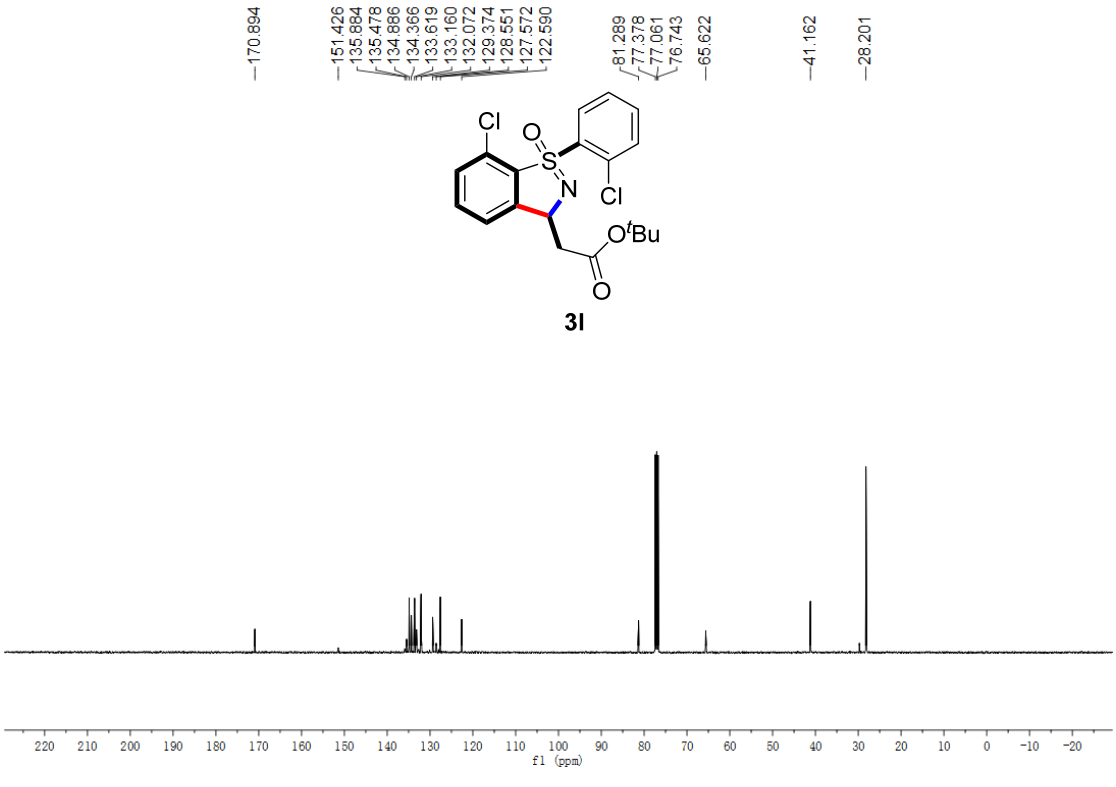
1.98
1.86
1.00
1.15
1.17
3.13
3.05
9.17
f1 (ppm)

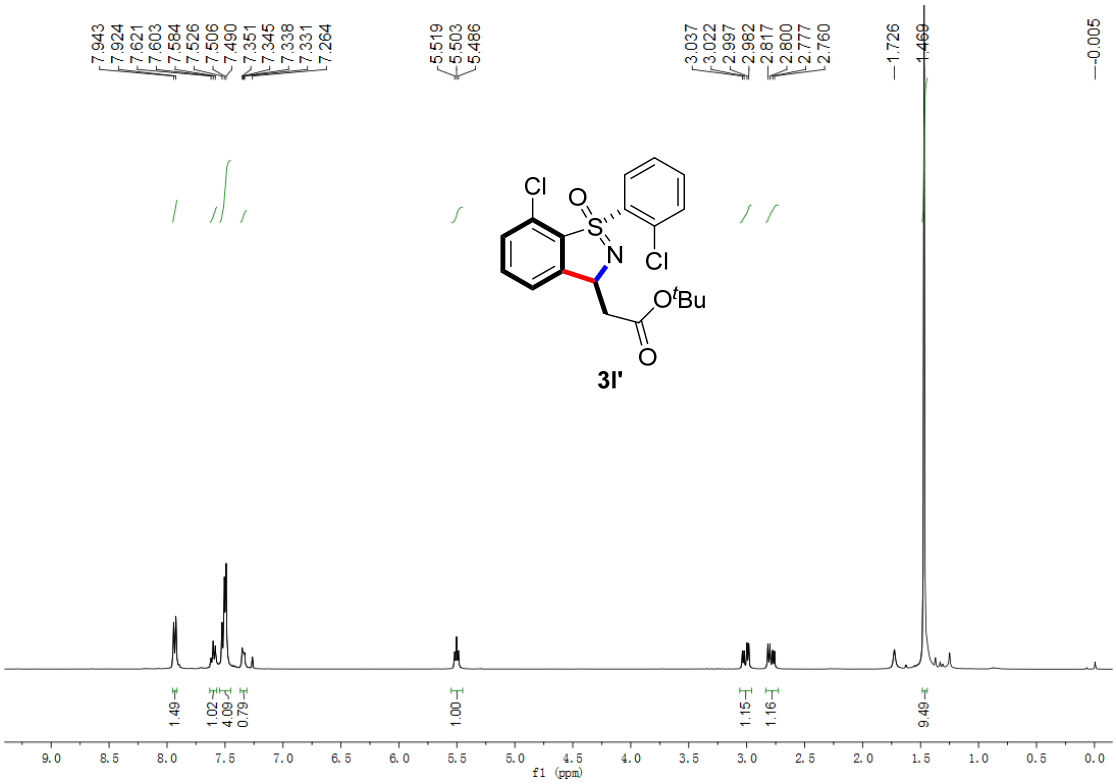

170.748
149.189
139.337
137.551
135.750
134.344
133.351
132.987
132.799
131.862
130.466
126.592
121.464
80.912
77.204
76.992
76.781
65.394
44.643
28.134
18.869
16.846
H3C
O
S
N
CH3
OtBu
O
3k'
f1 (ppm)

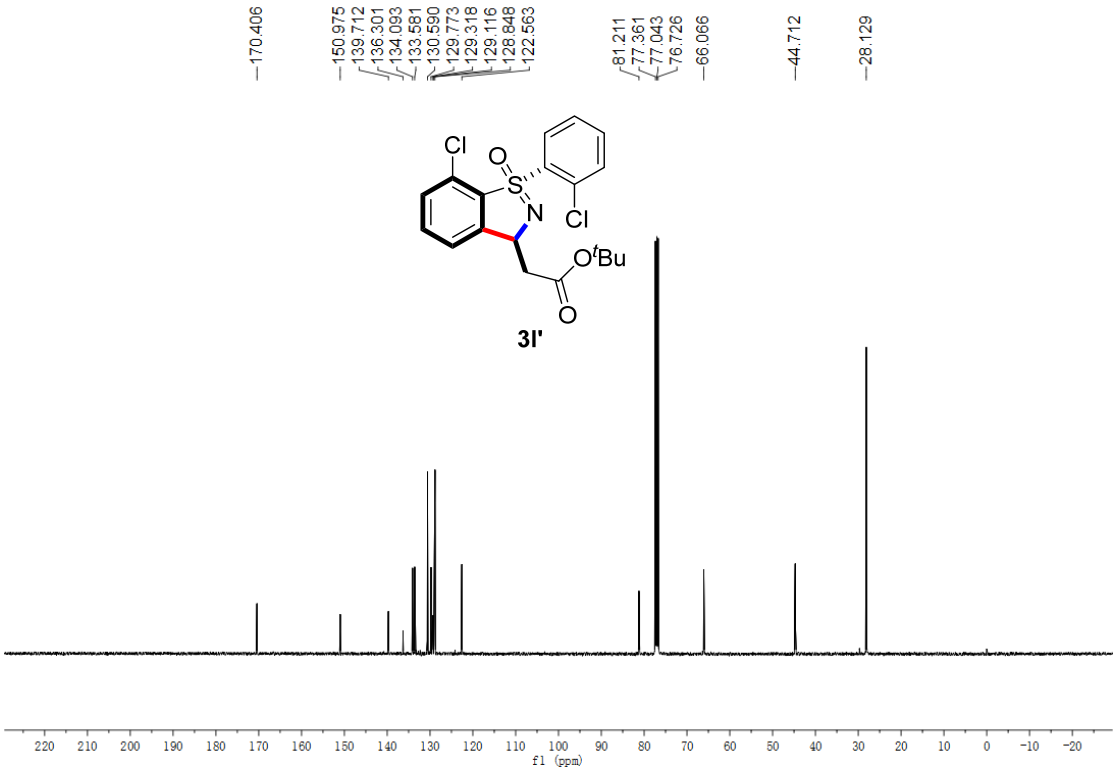

8.518
8.499
7.571
7.553
7.537
7.521
7.435
7.417
7.396
7.379
7.264
5.632
5.615
5.598
3.023
3.007
2.983
2.967
2.842
2.824
2.802
2.783
1.611
1.525
1.253
0.000
Cl
O
S
N
Cl
O^{t}Bu
O
0.94
3.70
1.83
1.00
1.05
1.03
9.36
f1 (ppm)

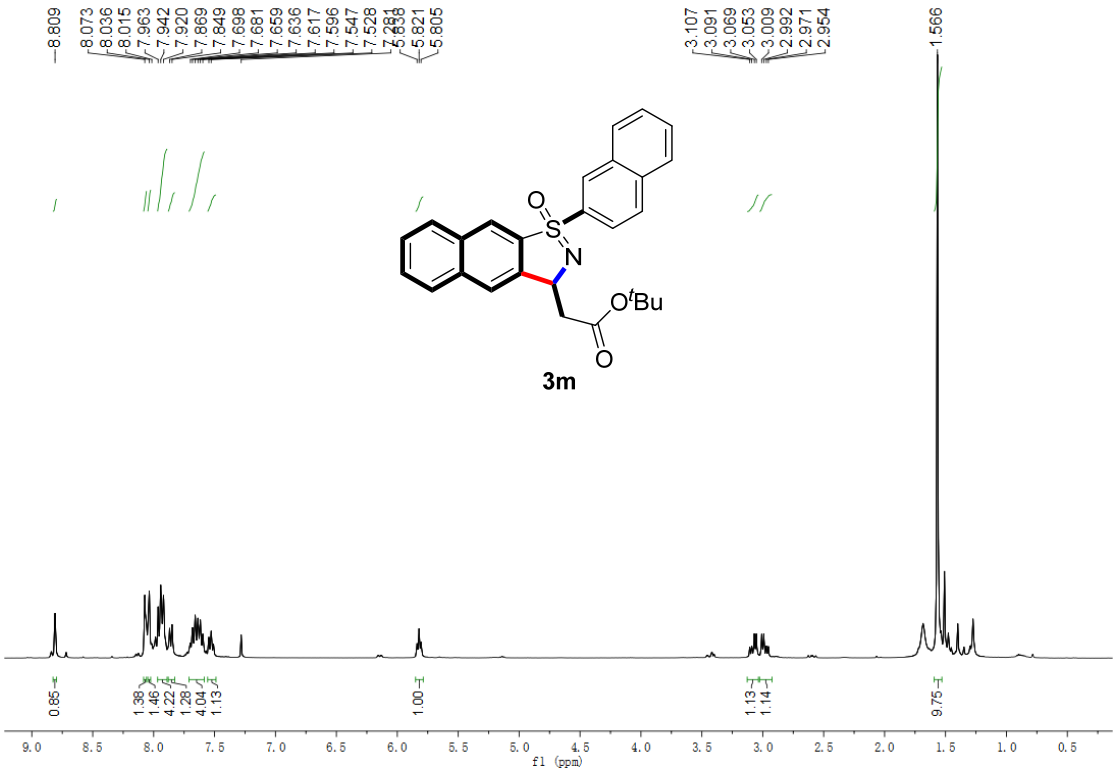
3l

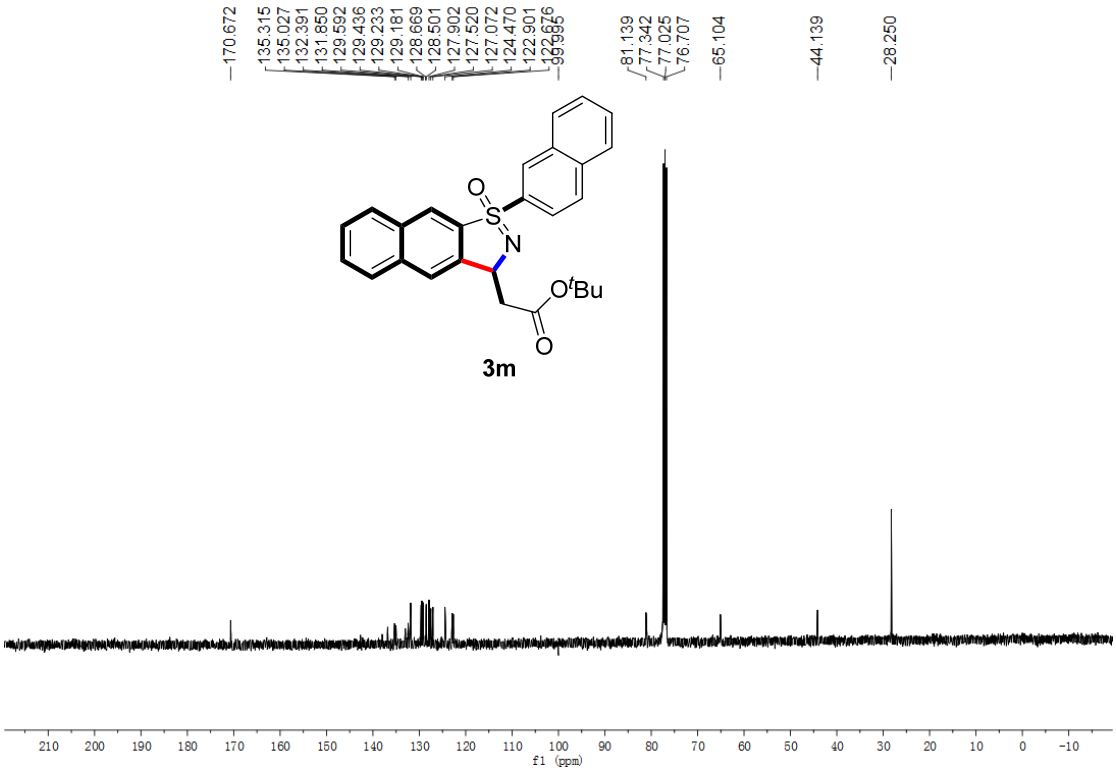

170.894
151.426
135.884
135.478
134.886
134.366
133.619
133.160
132.072
129.374
128.551
127.572
122.590
81.289
77.378
77.061
76.743
65.622
41.162
28.201
Cl
O
S
N
Cl
O^{t}Bu
O
f1 (ppm)

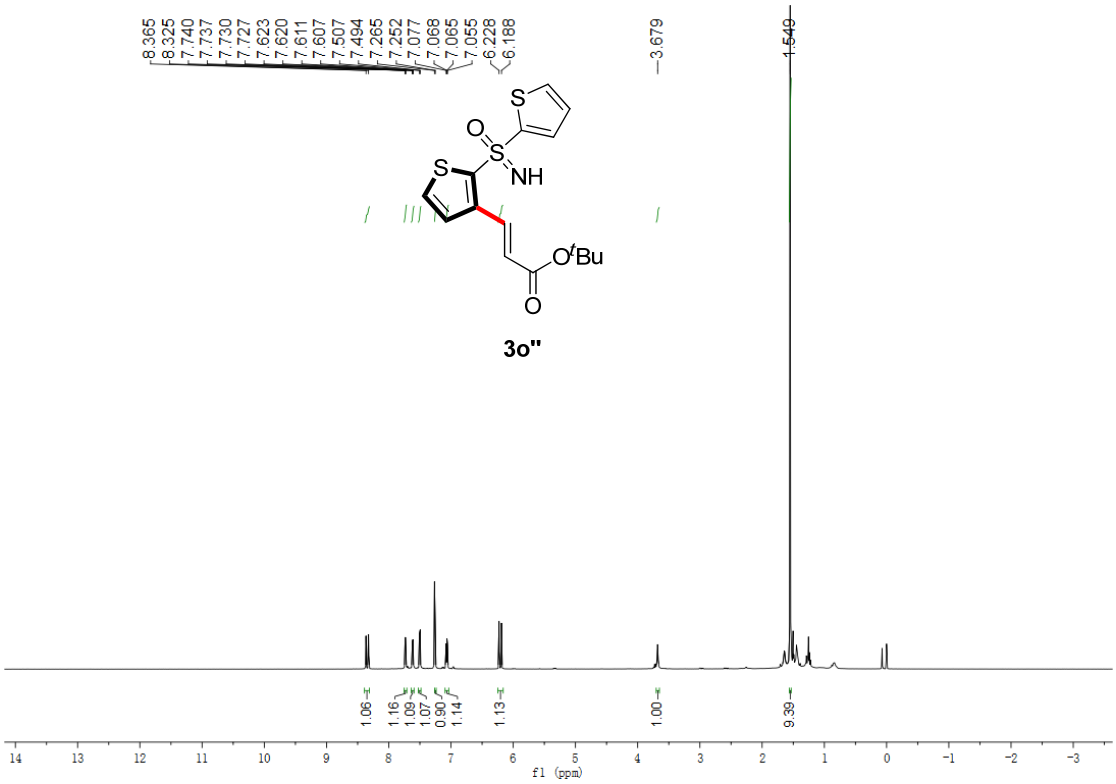
3l


7.943
7.924
7.621
7.603
7.584
7.526
7.506
7.490
7.351
7.345
7.338
7.331
7.264
5.519
5.503
5.486
3.037
3.022
2.997
2.982
2.817
2.800
2.777
2.760
1.726
1.469
0.005
Cl
O
S
N
Cl
O^{t}Bu
O
3l'
1.49
1.02
4.09
0.79
1.00
1.15
1.16
9.49
f1 (ppm)

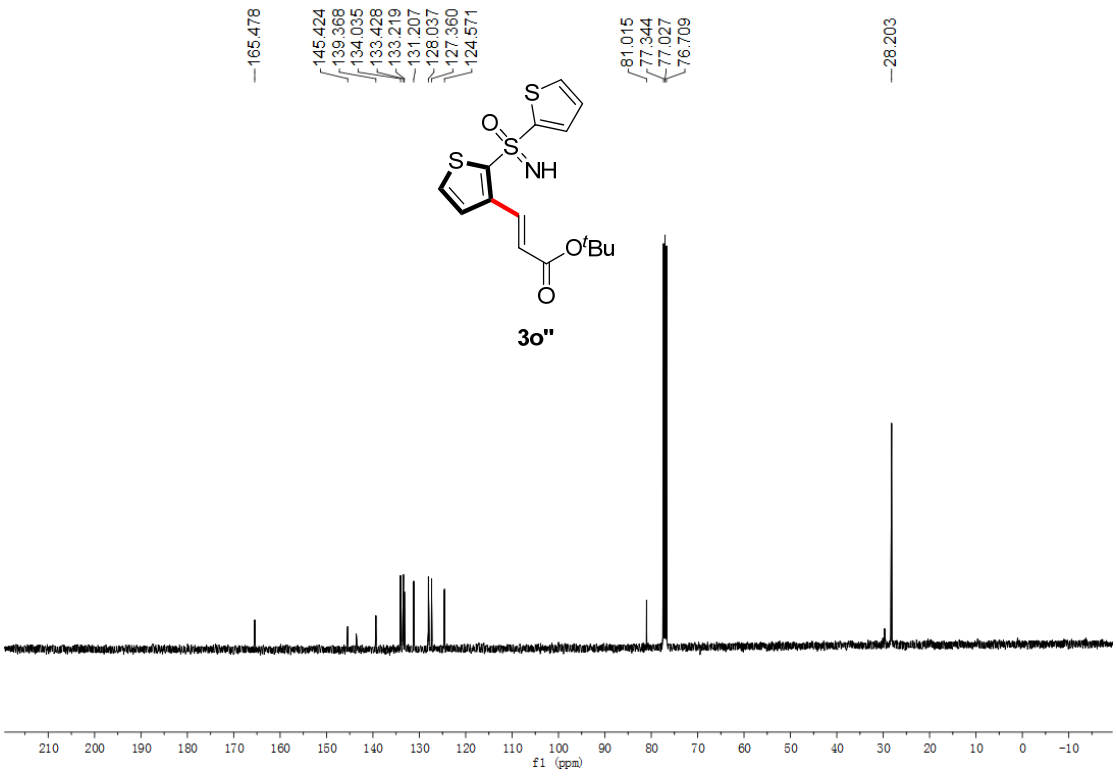

170.406
150.975
139.712
136.301
134.093
133.581
130.590
129.773
129.318
129.116
128.848
122.563
81.211
77.361
77.043
76.726
66.066
44.712
28.129
Cl
O
S
N
Cl
O^{t}Bu
O
3l'
f1 (ppm)


8.809
8.073
8.036
8.015
7.963
7.942
7.920
7.869
7.849
7.698
7.681
7.659
7.636
7.617
7.596
7.547
7.528
7.281
7.838
5.821
5.805
3.107
3.091
3.069
3.053
3.009
2.992
2.971
2.954
1.566
O
S
N
O
tBu
O
3m
0.85
1.38
1.46
4.22
1.28
4.04
1.13
1.00
1.13
1.14
9.75
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)

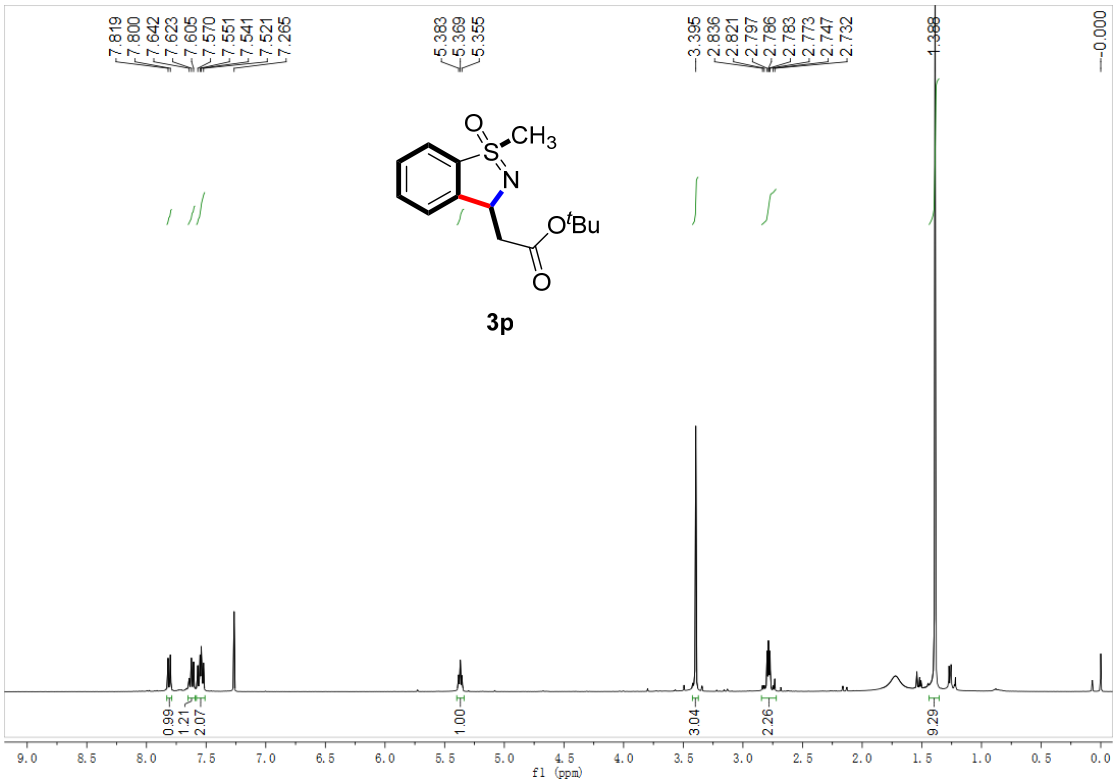

170.672
135.315
135.027
132.391
131.850
129.592
129.436
129.233
129.181
128.669
128.501
127.902
127.520
127.072
124.470
122.901
122.676
81.139
77.342
77.025
76.707
65.104
44.139
28.250
O
S
N
O
tBu
O
3m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.365
8.325
7.740
7.737
7.730
7.727
7.623
7.620
7.611
7.607
7.507
7.494
7.265
7.252
7.077
7.068
7.065
7.055
6.228
6.188
3.679
1.549
S
O
S
NH
S
O
tBu
O
1.06
1.16
1.09
1.07
0.90
1.14
1.13
1.00
9.39
f1 (ppm)

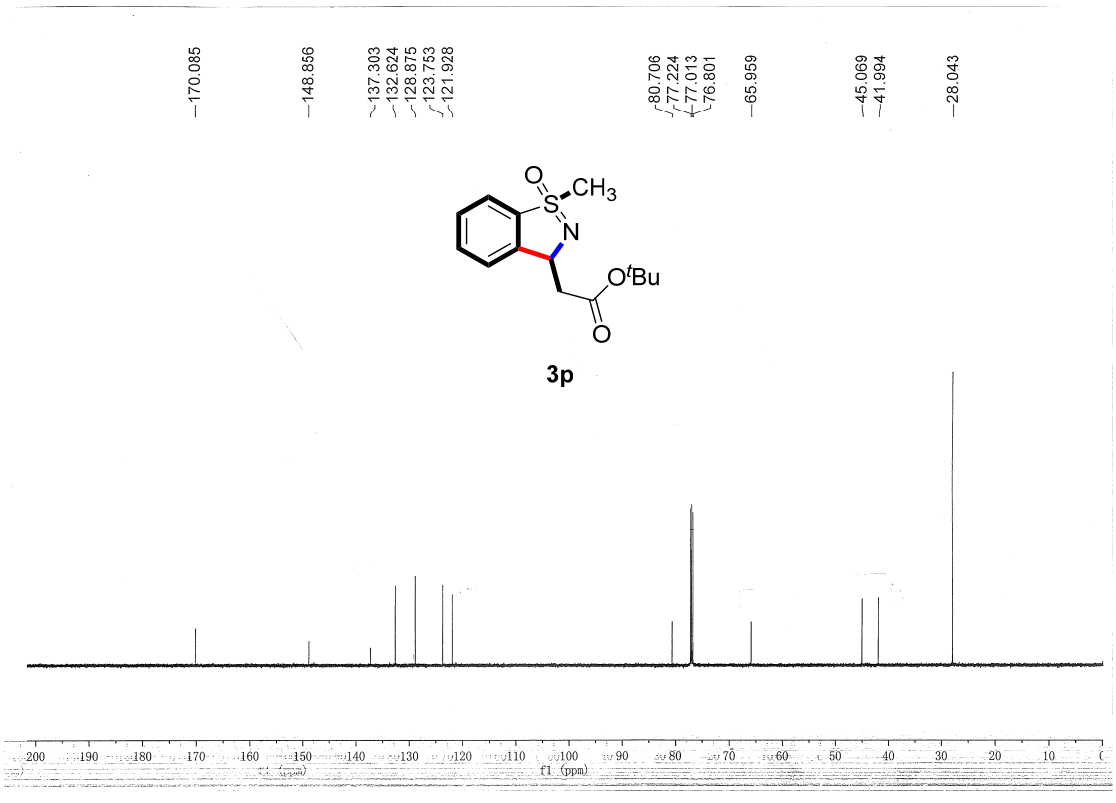
3o''


165.478
145.424
139.368
134.035
133.428
133.219
131.207
128.037
127.360
124.571
81.015
77.344
77.027
76.709
28.203
S
O
S
NH
O
tBu
O
f1 (ppm)

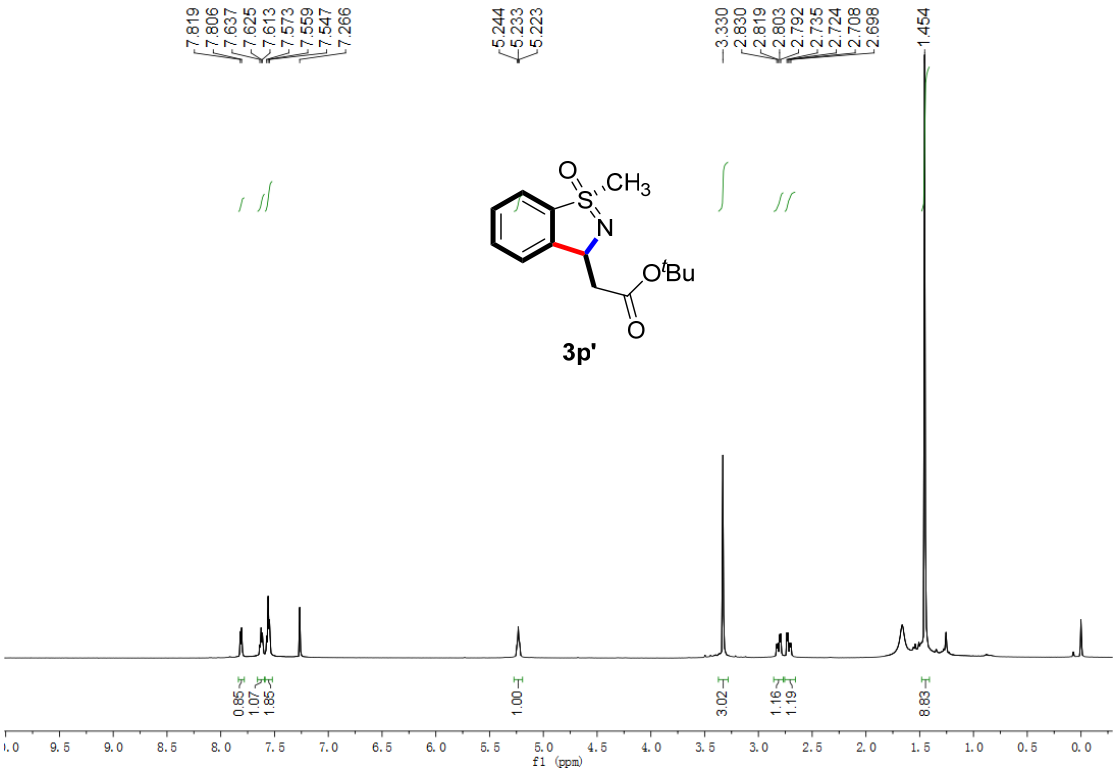
3o''

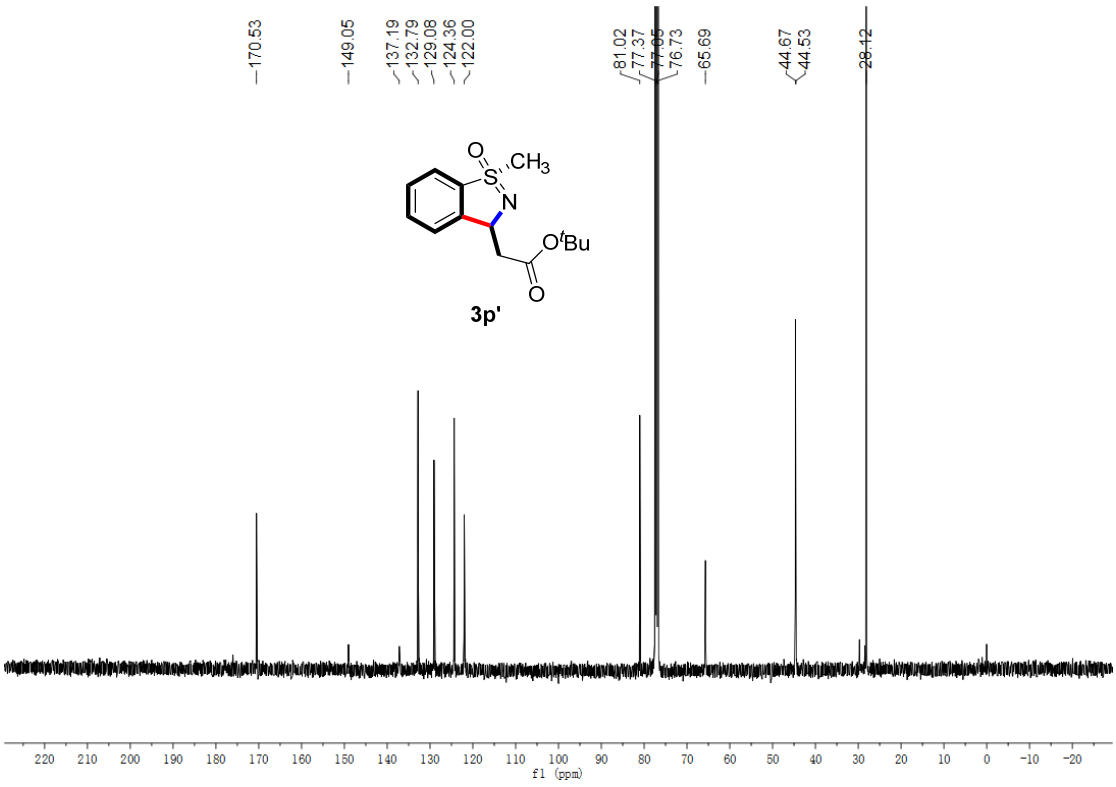

7.819
7.800
7.642
7.623
7.605
7.570
7.551
7.541
7.521
7.265
5.383
5.369
5.355
3.395
2.836
2.821
2.797
2.786
2.783
2.773
2.747
2.732
1.388
0.000
O
S
CH3
N
O
tBu
O
0.99
1.21
2.07
1.00
3.04
2.26
9.29
f1 (ppm)

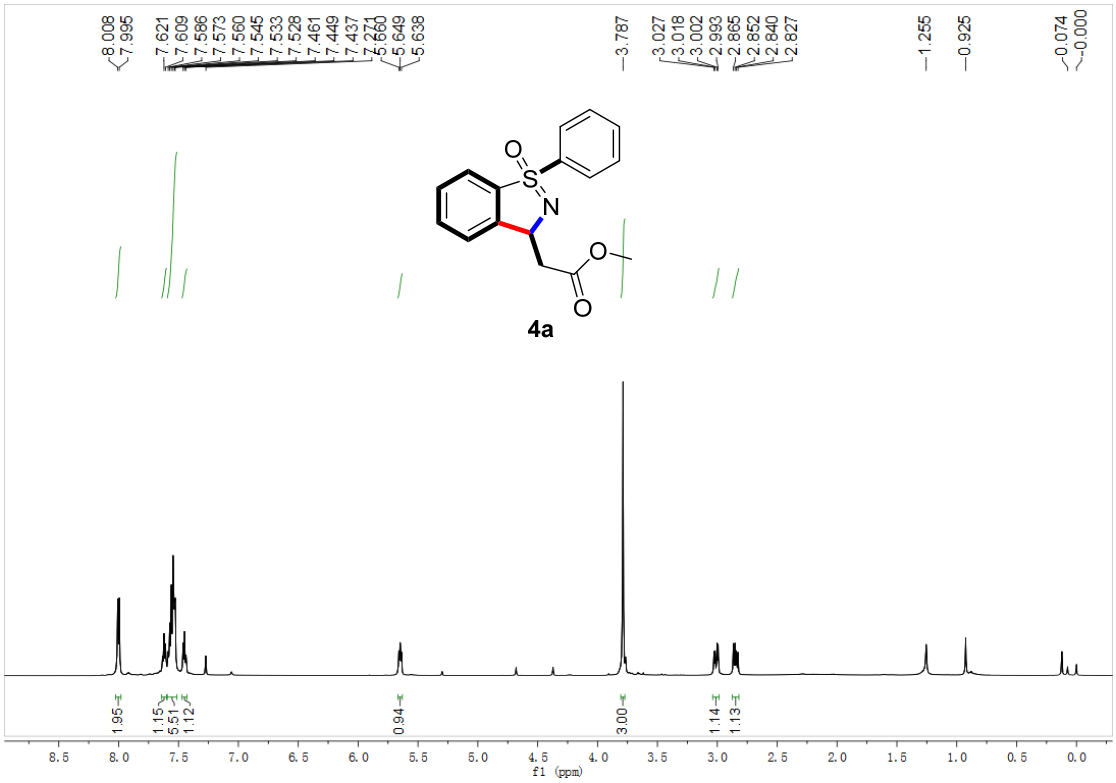
3p


170.085
148.856
137.303
132.624
128.875
123.753
121.928
80.706
77.224
77.013
76.801
65.959
45.069
41.994
28.043
O
S
CH3
N
O
tBu
O
f1 (ppm)

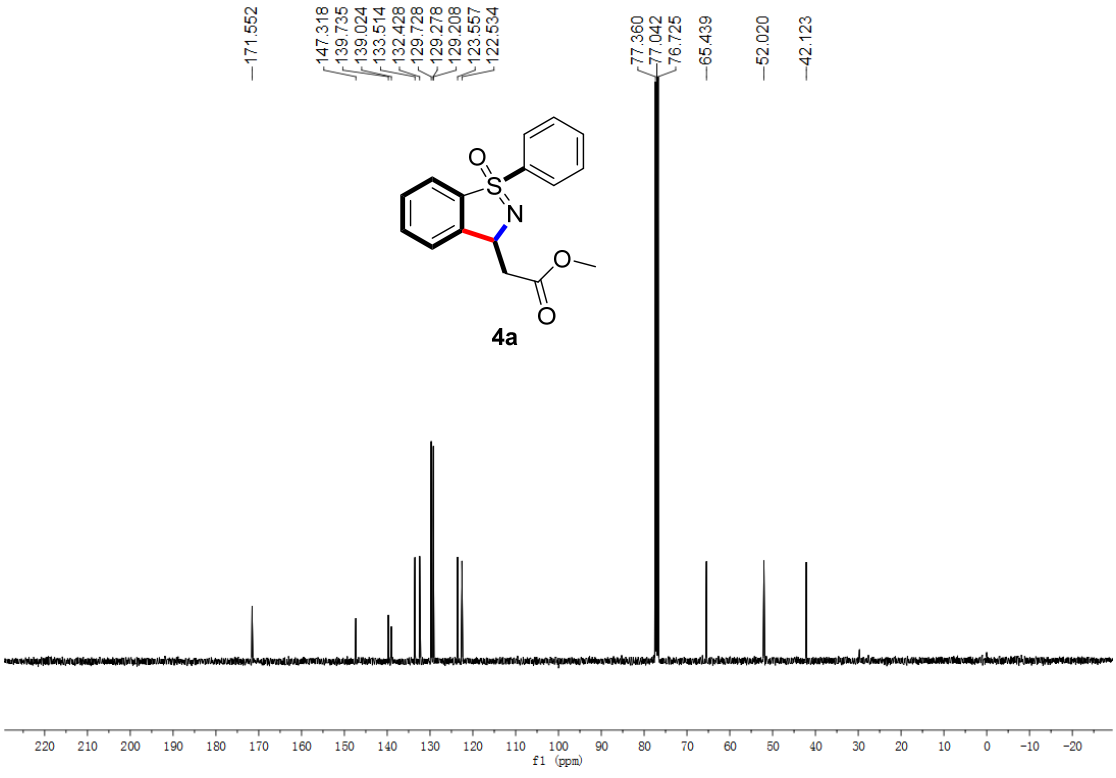
3p


7.819
7.806
7.637
7.625
7.613
7.573
7.559
7.547
7.266
5.244
5.233
5.223
3.330
2.830
2.819
2.803
2.792
2.735
2.724
2.708
2.698
1.454
O
S
CH3
N
O
tBu
O
3p'
0.85
1.07
1.85
1.00
3.02
1.16
1.19
8.83
f1 (ppm)

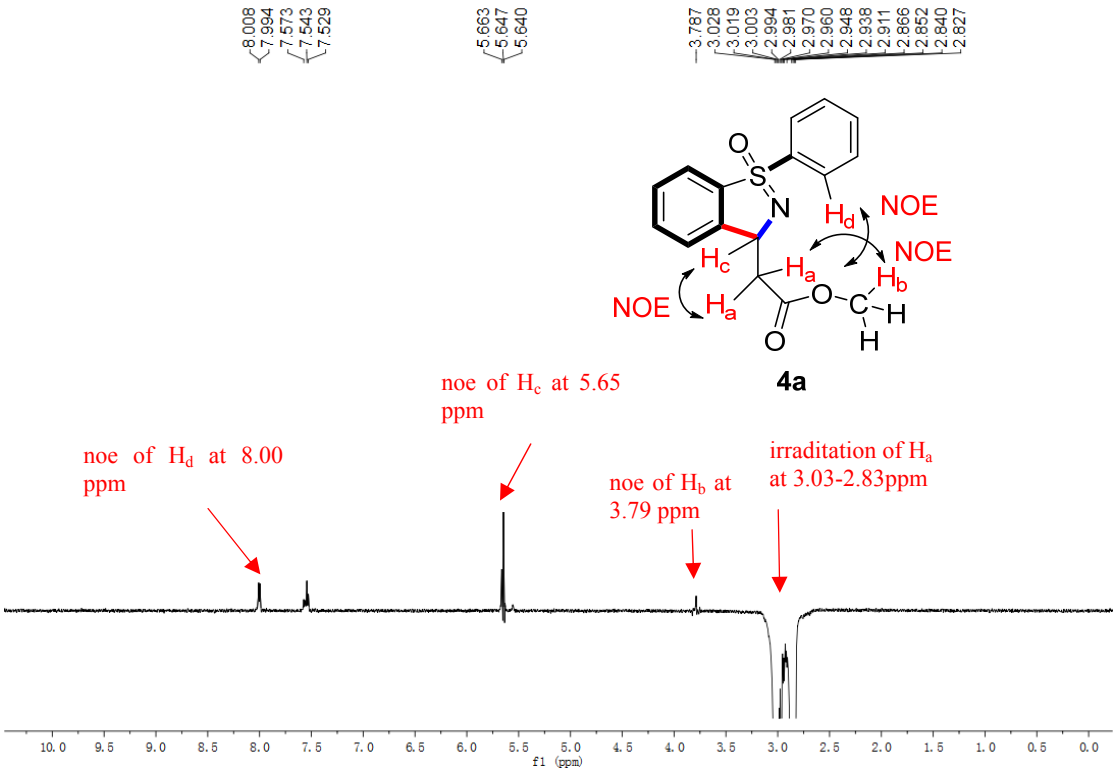

170.53
149.05
137.19
132.79
129.08
124.36
122.00
81.02
77.37
77.05
76.73
65.69
44.67
44.53
28.12
O
S
CH3
N
O
tBu
O
3p'
f1 (ppm)


8.008
7.995
7.621
7.609
7.586
7.573
7.560
7.545
7.533
7.528
7.461
7.449
7.437
7.421
5.660
5.649
5.638
3.787
3.027
3.018
3.002
2.993
2.865
2.852
2.840
2.827
1.255
0.925
0.074
0.000
O
S
N
O
O
1.95
1.15
5.51
1.12
0.94
3.00
1.14
1.13
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)

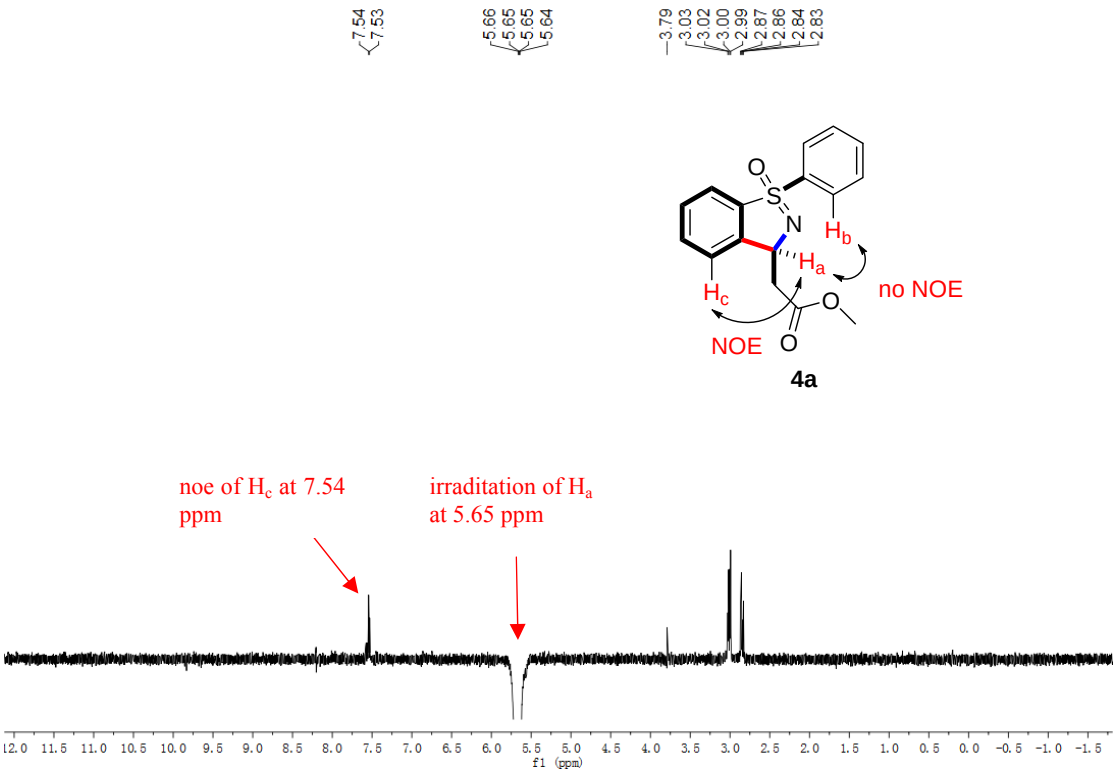
4a


171.552
147.318
139.735
139.024
133.514
132.428
129.728
129.278
129.208
123.557
122.534
77.360
77.042
76.725
65.439
52.020
42.123
O
S
N
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

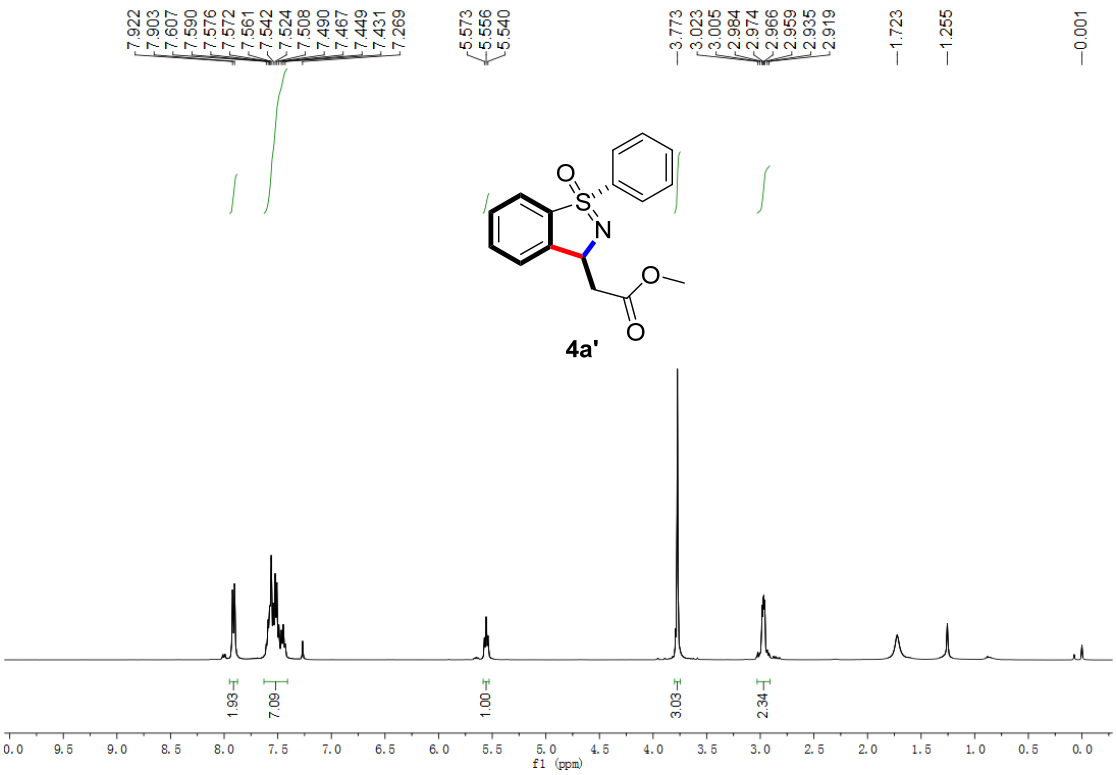
4a


8.008
7.994
7.573
7.543
7.529
5.663
5.647
5.640
3.787
3.028
3.019
3.003
2.994
2.981
2.970
2.960
2.948
2.938
2.911
2.866
2.852
2.840
2.827
O
S
N
Hd
NOE
NOE
Hc
Ha
Hb
NOE
Ha
O
C
H
O
H
noe of Hc at 5.65 ppm
noe of Hd at 8.00 ppm
noe of Hb at 3.79 ppm
irraditation of Ha at 3.03-2.83ppm
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)

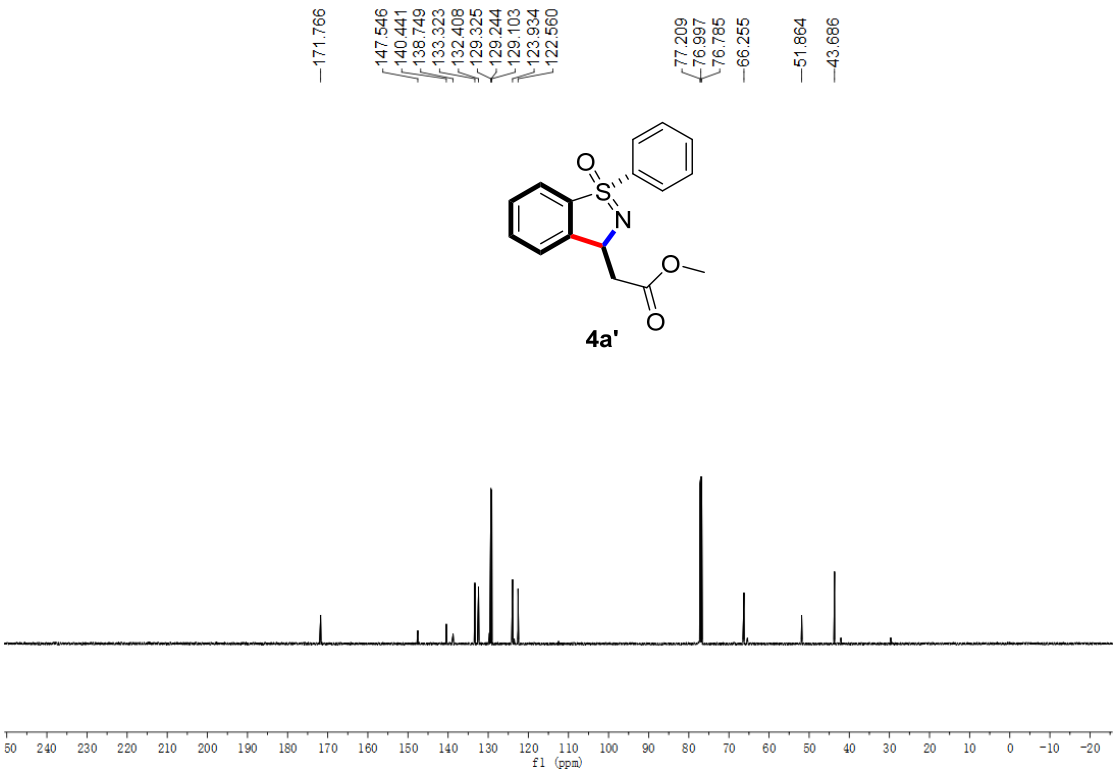
4a


7.54
7.53
5.66
5.65
5.65
5.64
3.79
3.03
3.02
3.00
2.99
2.87
2.86
2.84
2.83
O
S
N
Hb
Ha
Hc
no NOE
O
NOE
O
noe of Hc at 7.54 ppm
irraditation of Ha at 5.65 ppm
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
f1 (ppm)

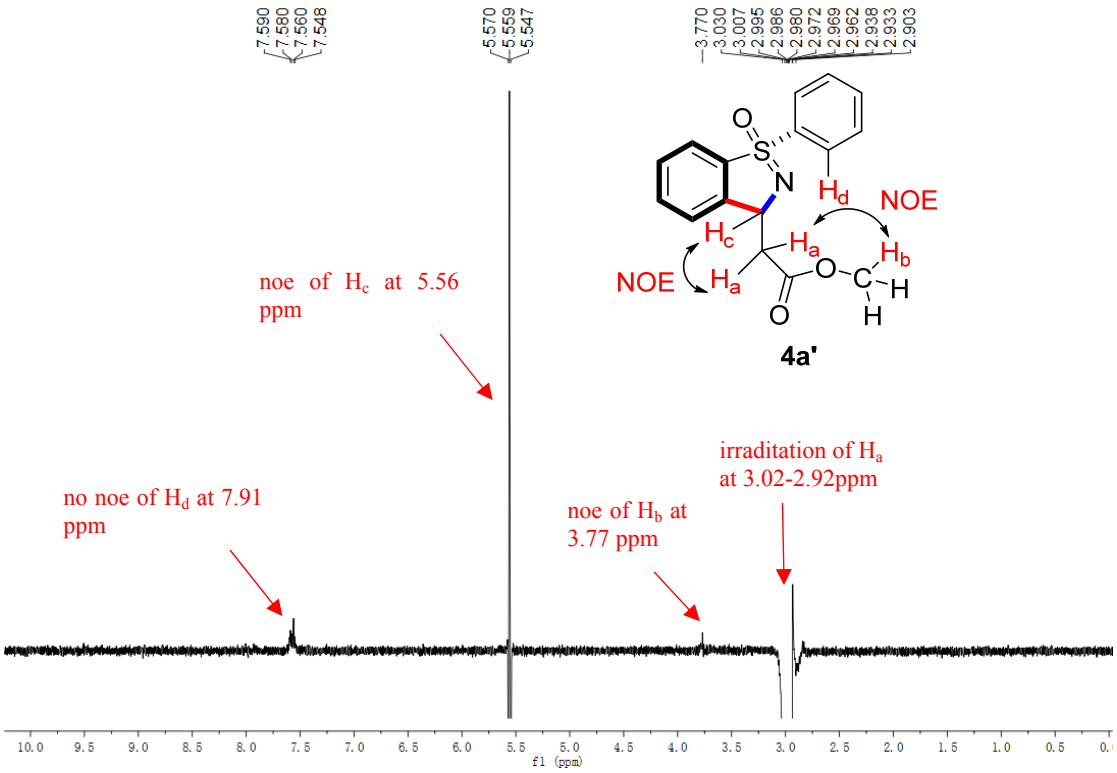
4a


7.922
7.903
7.607
7.590
7.576
7.572
7.561
7.542
7.524
7.508
7.490
7.467
7.449
7.431
7.269
5.573
5.556
5.540
3.773
3.023
3.005
2.984
2.974
2.966
2.959
2.935
2.919
1.723
1.255
0.001
1.93
7.09
1.00
3.03
2.34
f1 (ppm)

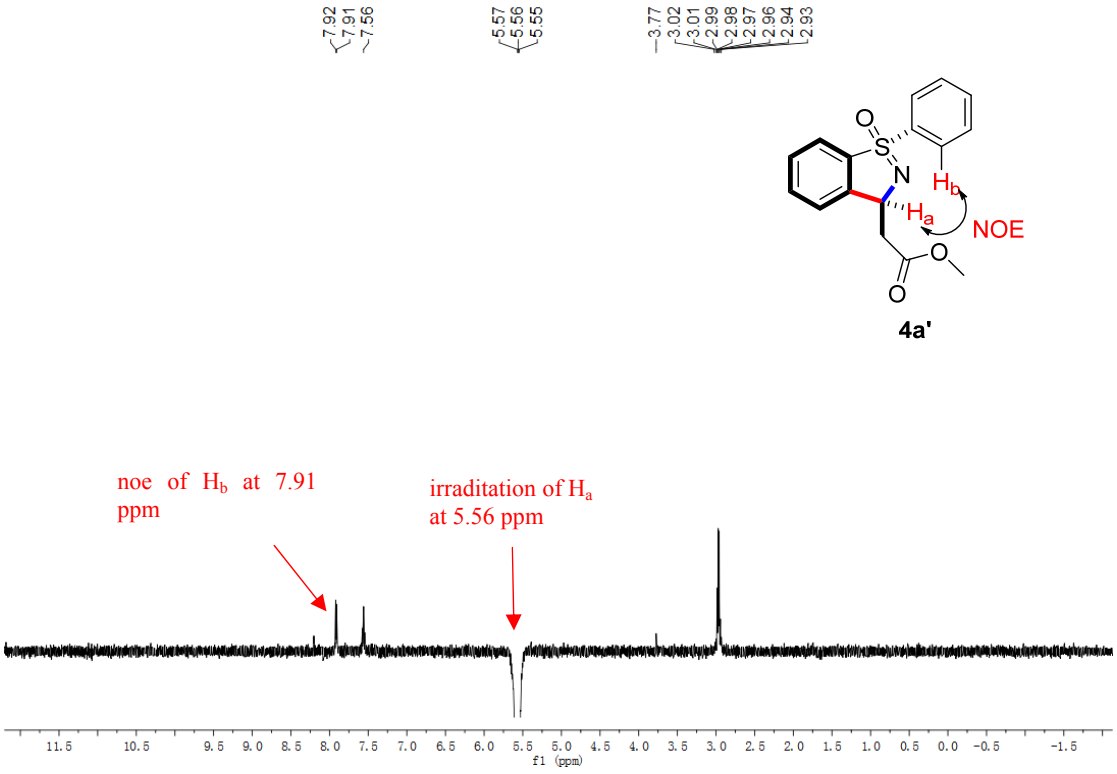
4a'


171.766
147.546
140.441
138.749
133.323
132.408
129.325
129.244
129.103
123.934
122.560
77.209
76.997
76.785
66.255
51.864
43.686
f1 (ppm)

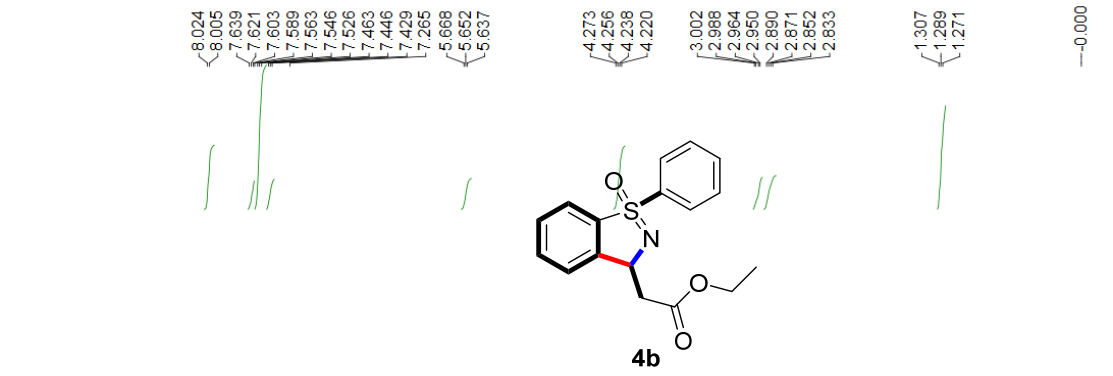
4a'


7.590
7.580
7.560
7.548
5.570
5.559
5.547
3.770
3.030
3.007
2.995
2.986
2.980
2.972
2.969
2.962
2.938
2.933
2.903
noe of Hc at 5.56 ppm
no noe of Hd at 7.91 ppm
noe of Hb at 3.77 ppm
irraditation of Ha at 3.02-2.92ppm
NOE
NOE
f1 (ppm)

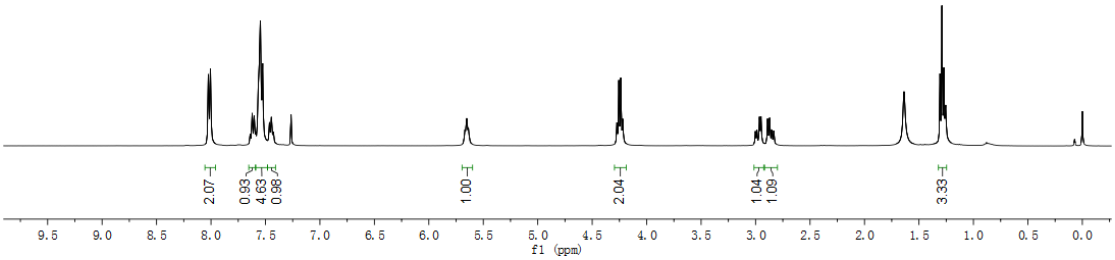
4a'

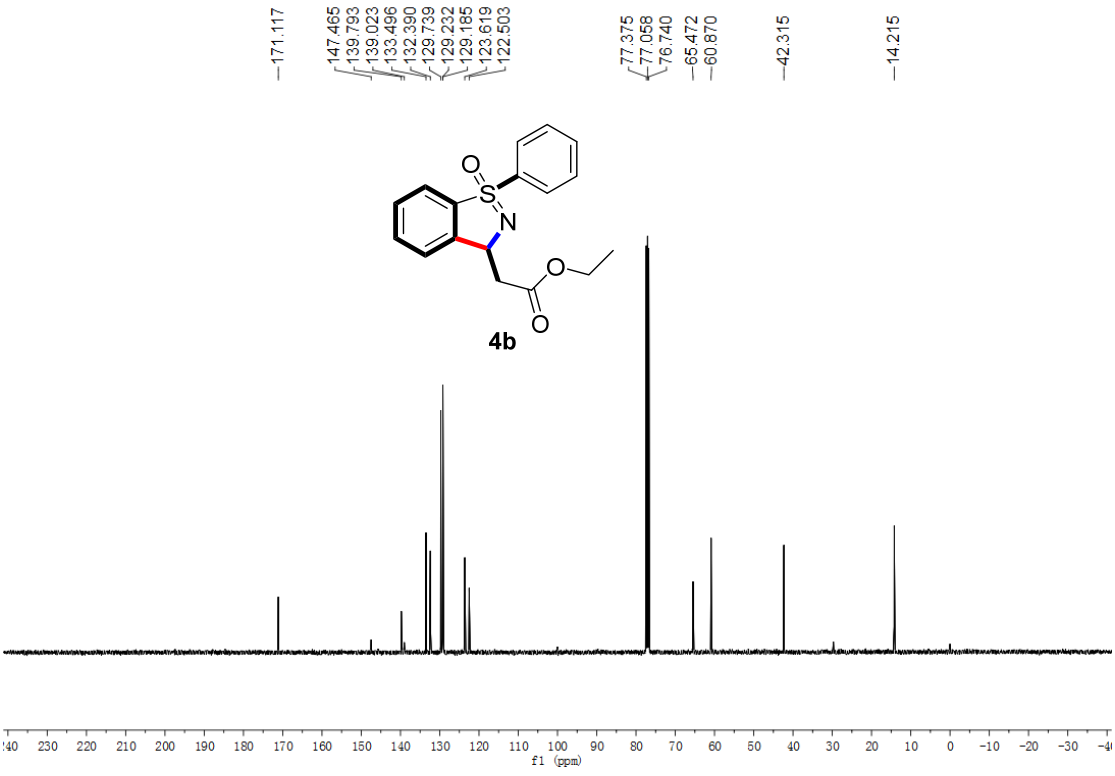

7.92
7.91
7.56
5.57
5.56
5.55
3.77
3.02
3.01
2.99
2.98
2.97
2.96
2.94
2.93
noe of Hb at 7.91 ppm
irraditation of Ha at 5.56 ppm
NOE
f1 (ppm)

4a'

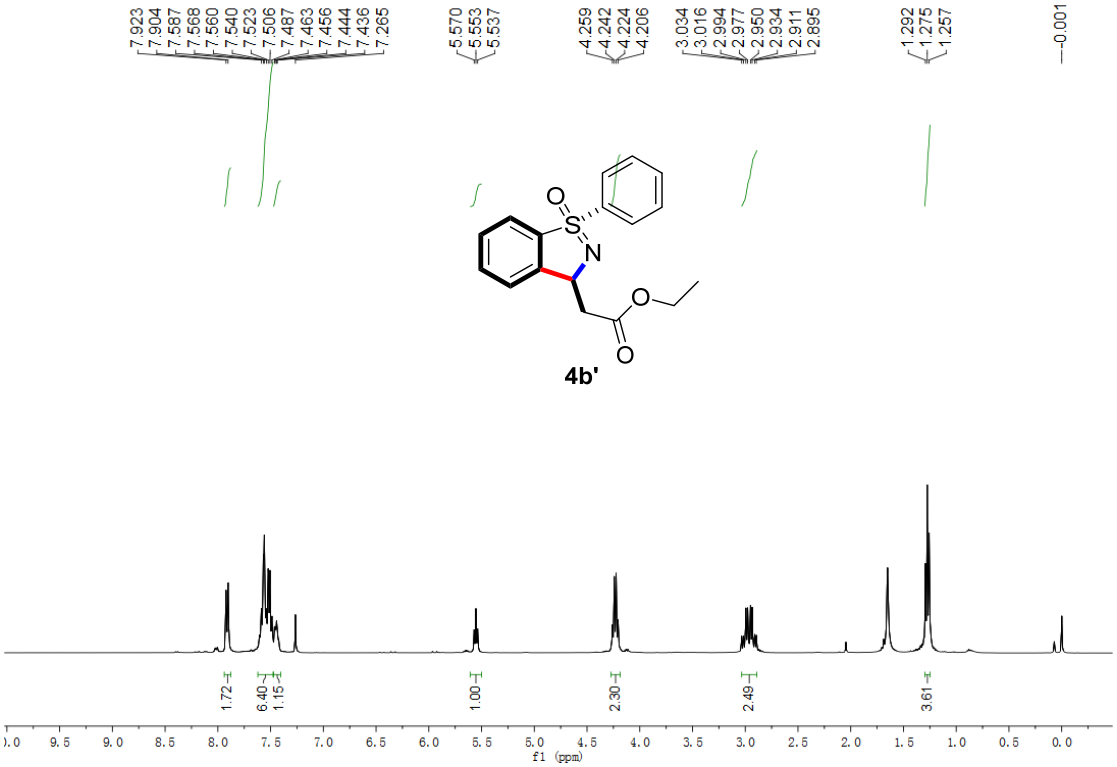

8.024
8.005
7.639
7.621
7.603
7.589
7.563
7.546
7.526
7.463
7.446
7.429
7.265
5.668
5.652
5.637
4.273
4.256
4.238
4.220
3.002
2.988
2.964
2.950
2.890
2.871
2.852
2.833
1.307
1.289
1.271
0.000
O
S
N
O
O

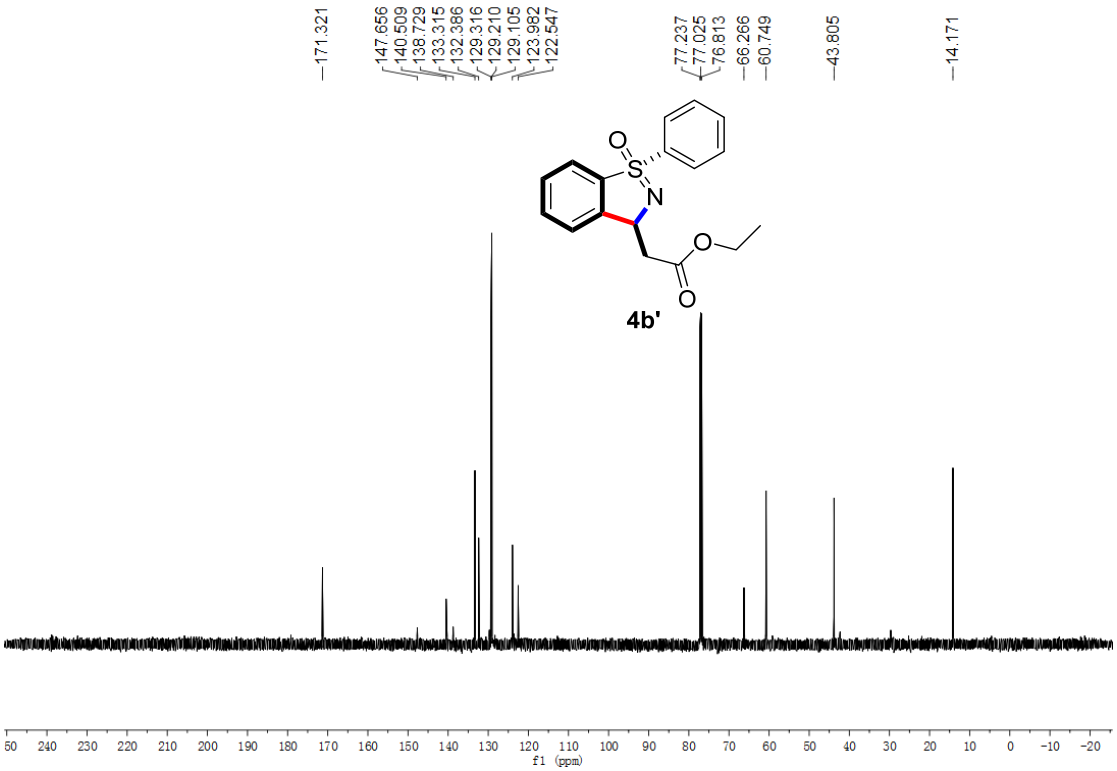
4b

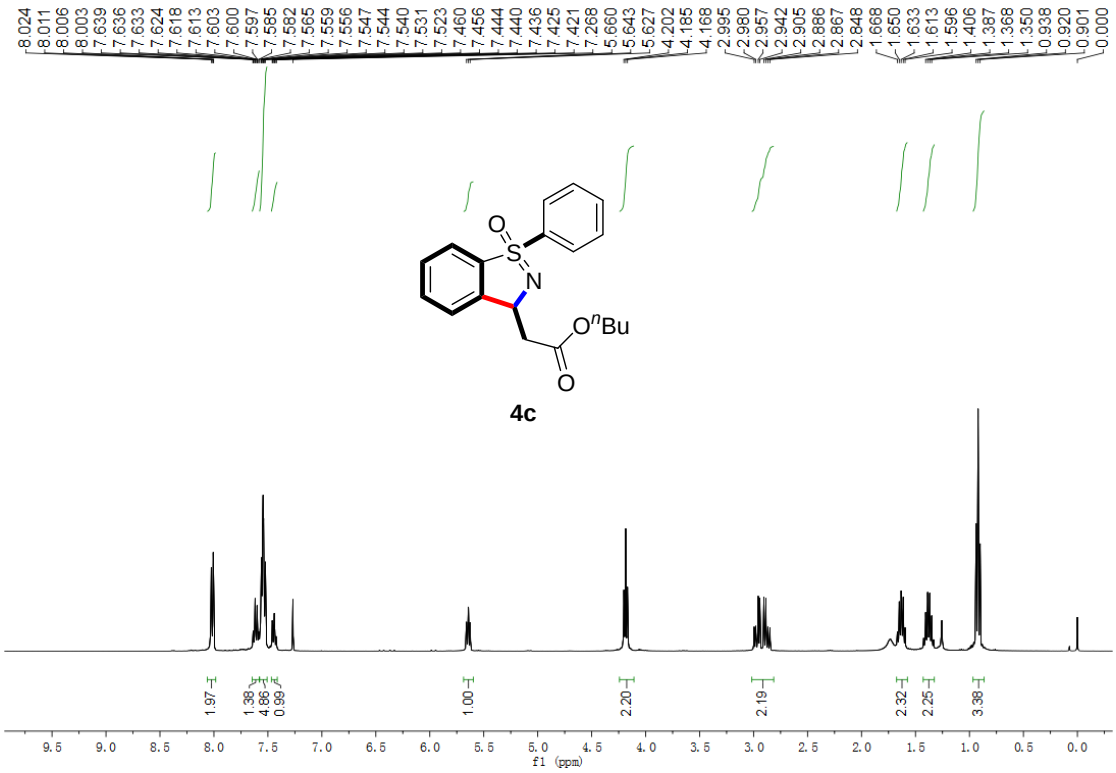

2.07
0.93
4.63
0.98
1.00
2.04
1.04
1.09
3.33
f1 (ppm)


171.117
147.465
139.793
139.023
133.496
132.390
129.739
129.232
129.185
123.619
122.503
77.375
77.058
76.740
65.472
60.870
42.315
14.215
O
S
N
O
O
f1 (ppm)

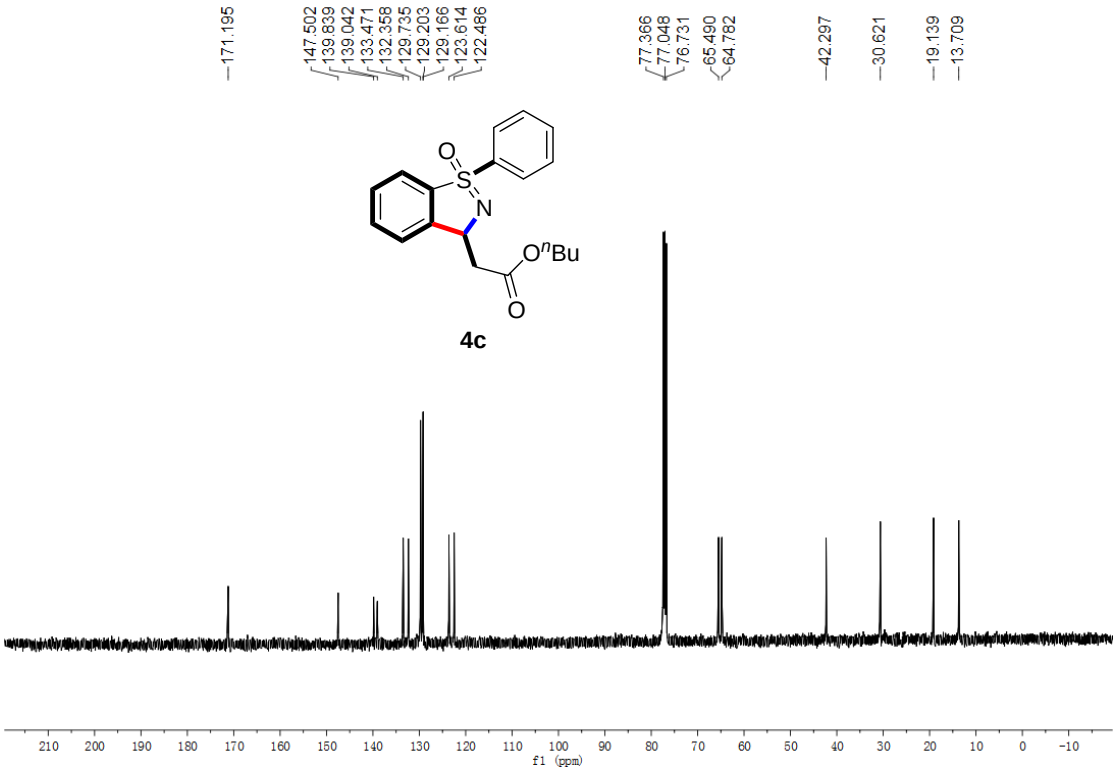
4b


7.923
7.904
7.587
7.568
7.560
7.540
7.523
7.506
7.487
7.463
7.456
7.444
7.436
7.265
5.570
5.553
5.537
4.259
4.242
4.224
4.206
3.034
3.016
2.994
2.977
2.950
2.934
2.911
2.895
1.292
1.275
1.257
0.001
O
S
N
O
O
4b'
1.72
6.40
1.15
1.00
2.30
2.49
3.61
f1 (ppm)

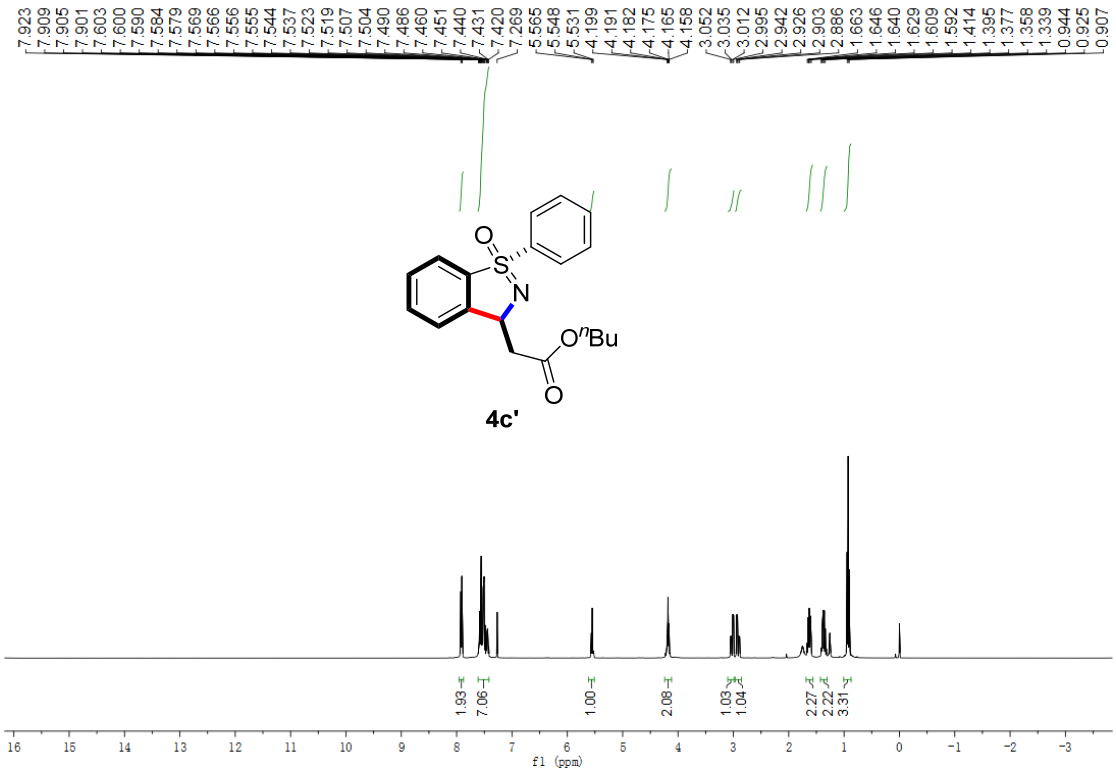

171.321
147.656
140.509
138.729
133.315
132.386
129.316
129.210
129.105
123.982
122.547
77.237
77.025
76.813
66.266
60.749
43.805
14.171
O
S
N
O
O
4b'
f1 (ppm)

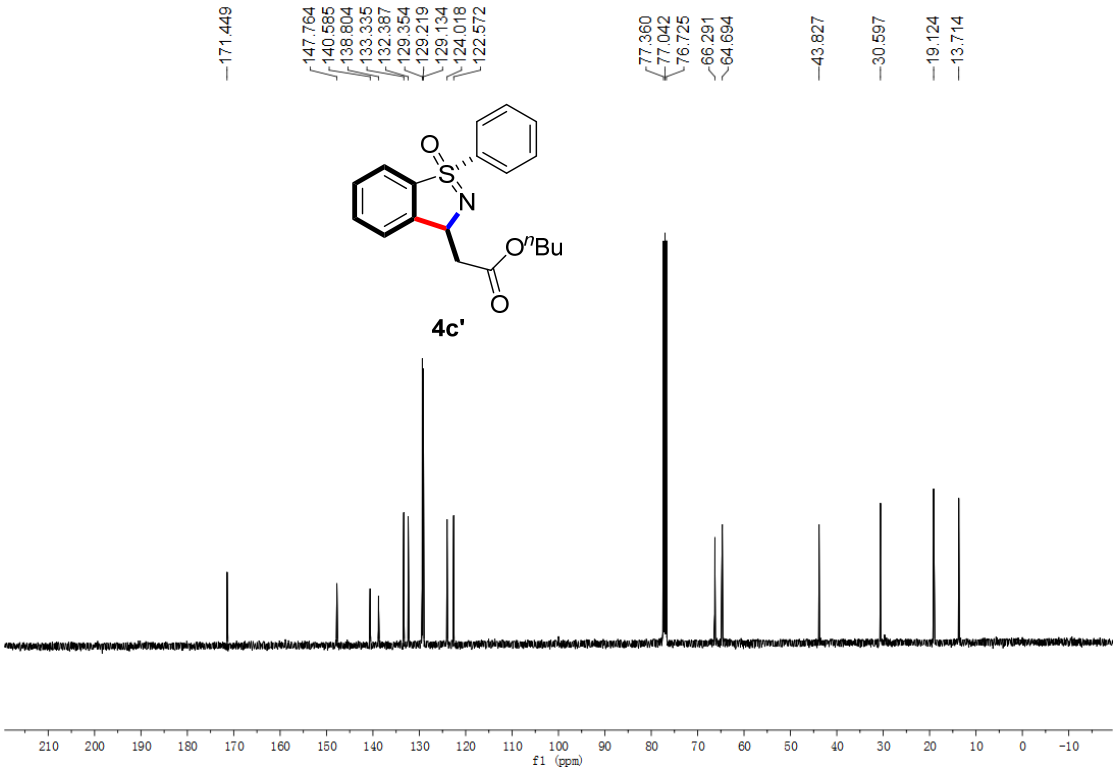

8.024
8.011
8.006
8.003
7.639
7.636
7.633
7.624
7.618
7.613
7.603
7.600
7.597
7.585
7.582
7.565
7.559
7.556
7.547
7.544
7.540
7.531
7.523
7.460
7.456
7.444
7.440
7.436
7.425
7.421
7.268
5.660
5.643
5.627
4.202
4.185
4.168
2.995
2.980
2.957
2.942
2.905
2.886
2.867
2.848
1.668
1.650
1.633
1.613
1.596
1.406
1.387
1.368
1.350
0.938
0.920
0.901
0.000
O
S
N
O
O^{n}Bu
1.97
1.38
4.86
0.99
1.00
2.20
2.19
2.32
2.25
3.38
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)

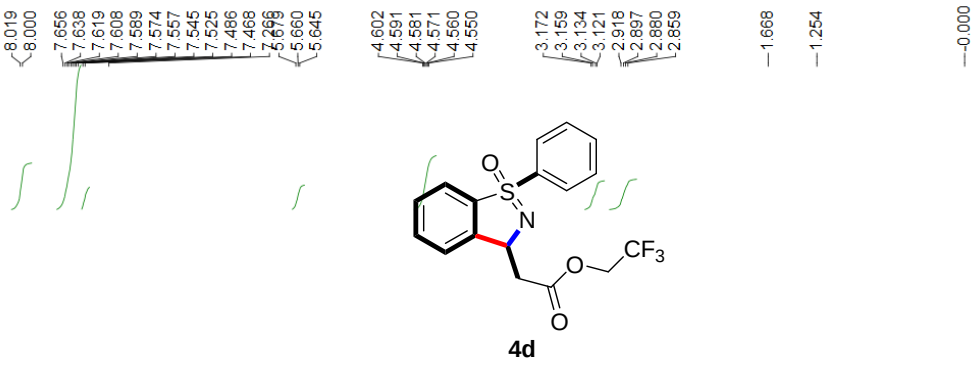
4c


171.195
147.502
139.839
139.042
133.471
132.358
129.735
129.203
129.166
123.614
122.486
77.366
77.048
76.731
65.490
64.782
42.297
30.621
19.139
13.709
O
S
N
O
O^{n}Bu
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

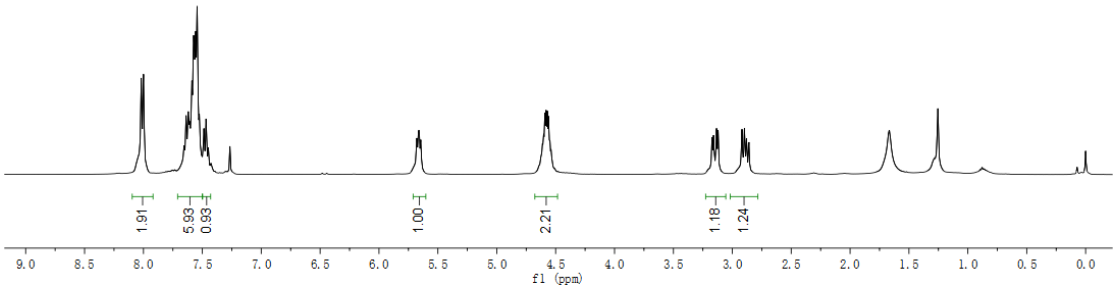
4c

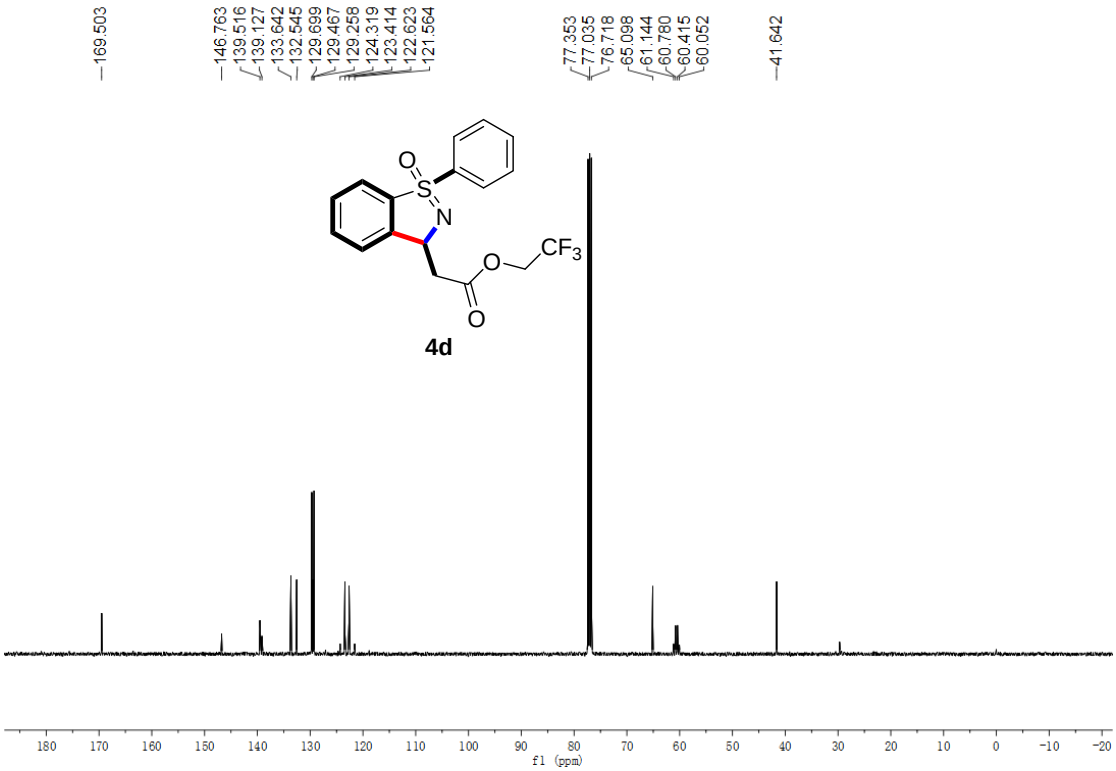

7.923
7.909
7.905
7.901
7.603
7.600
7.590
7.584
7.579
7.569
7.566
7.556
7.555
7.544
7.537
7.523
7.519
7.507
7.504
7.490
7.486
7.460
7.451
7.440
7.431
7.420
7.269
5.565
5.548
5.531
4.199
4.191
4.182
4.175
4.165
4.158
3.052
3.035
3.012
2.995
2.942
2.926
2.903
2.886
1.663
1.646
1.640
1.629
1.609
1.592
1.414
1.395
1.377
1.358
1.339
0.944
0.925
0.907
O
S
N
O
O
nBu
4c'
1.93
7.06
1.00
2.08
1.03
1.04
2.27
2.22
3.31
f1 (ppm)


171.449
147.764
140.585
138.804
133.335
132.387
129.354
129.219
129.134
124.018
122.572
77.360
77.042
76.725
66.291
64.694
43.827
30.597
19.124
13.714
O
S
N
O
O
nBu
4c'
f1 (ppm)

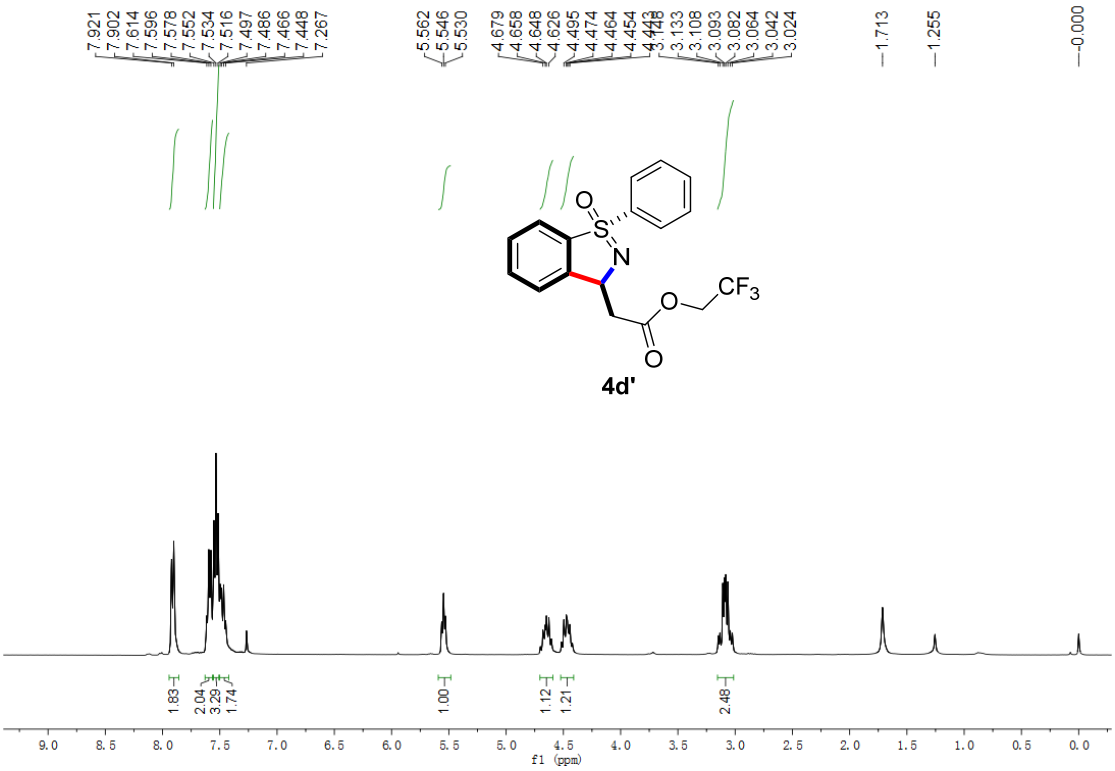

8.019
8.000
7.656
7.638
7.619
7.608
7.589
7.574
7.557
7.545
7.525
7.486
7.468
7.266
5.679
5.660
5.645
4.602
4.591
4.581
4.571
4.560
4.550
3.172
3.159
3.134
3.121
2.918
2.897
2.880
2.859
1.668
1.254
0.000
O
S
N
O
O
CF3

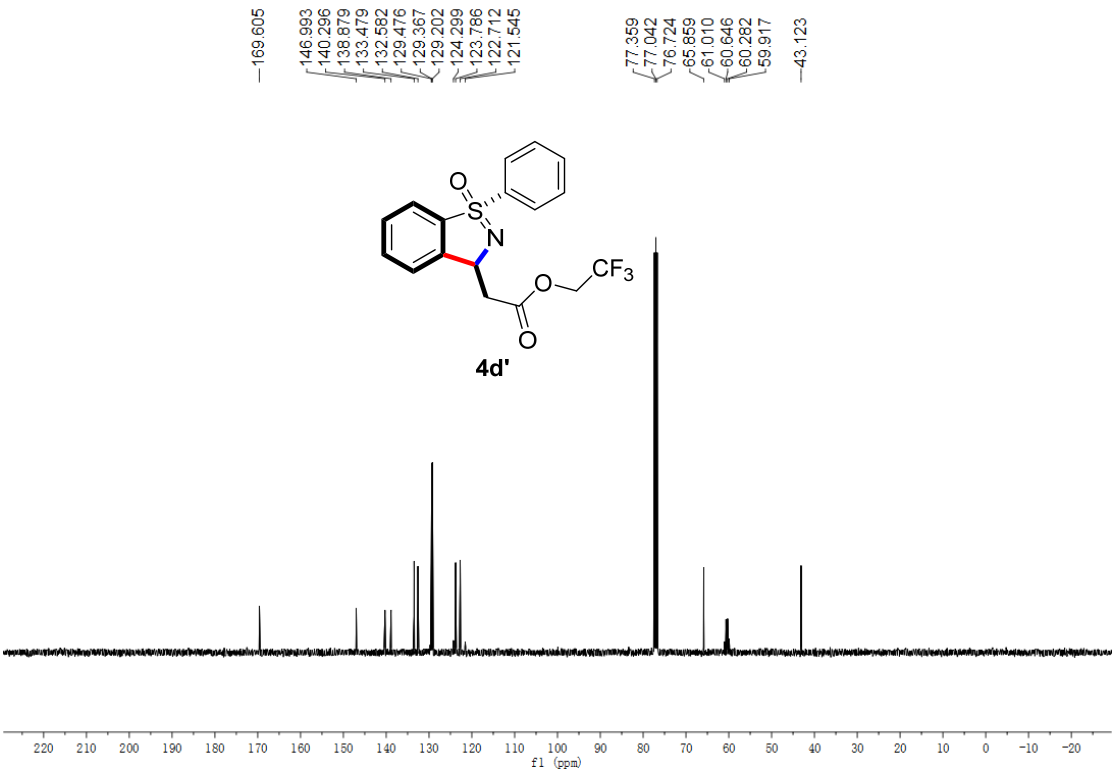
4d

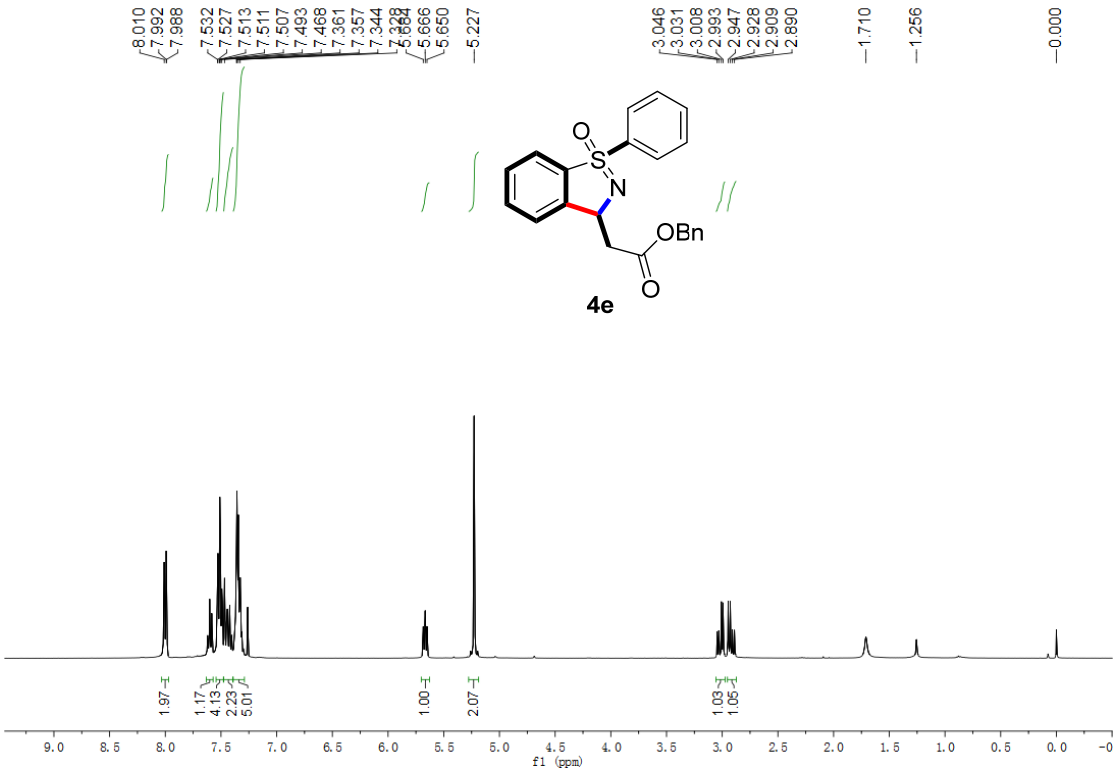

1.91
5.93
0.93
1.00
2.21
1.18
1.24
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

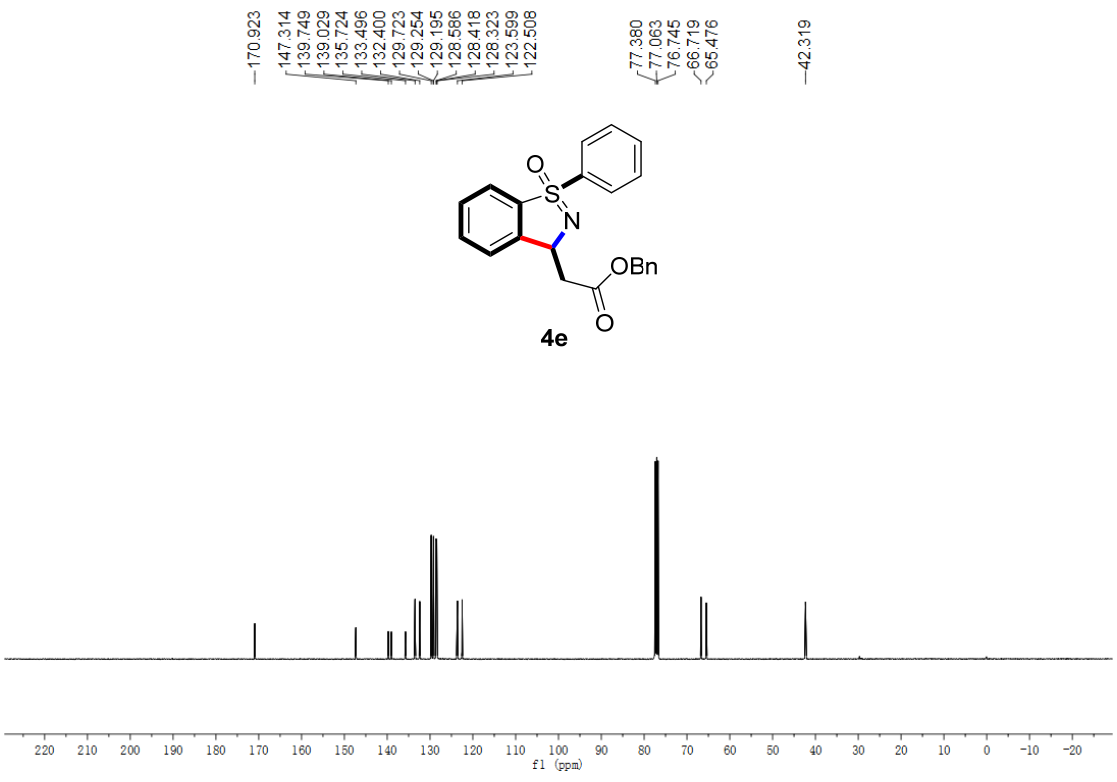

169.503
146.763
139.516
139.127
133.642
132.545
129.699
129.467
129.258
124.319
123.414
122.623
121.564
77.353
77.035
76.718
65.098
61.144
60.780
60.415
60.052
41.642
O
S
N
O
O
CF3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

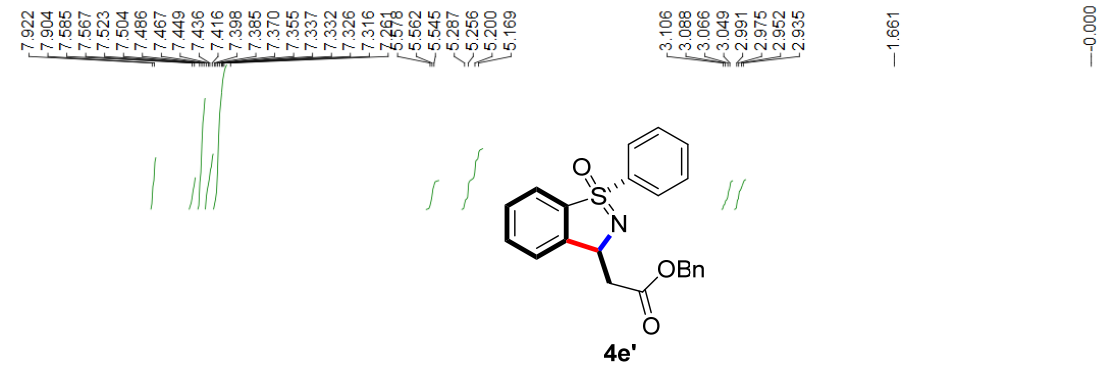
4d


7.921
7.902
7.614
7.596
7.578
7.552
7.534
7.516
7.497
7.486
7.466
7.448
7.267
5.562
5.546
5.530
4.679
4.658
4.648
4.626
4.495
4.474
4.464
4.454
3.133
3.108
3.093
3.082
3.064
3.042
3.024
1.713
1.255
0.000
O
S
N
O
O
CF3
4d'
1.83
2.04
3.29
1.74
1.00
1.12
1.21
2.48
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)

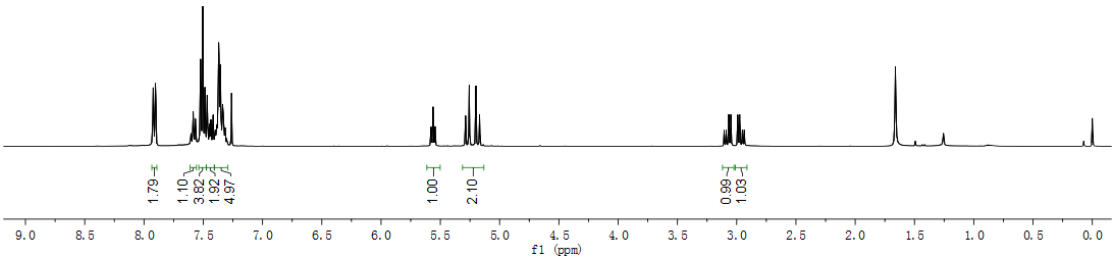

169.605
146.993
140.296
138.879
133.479
132.582
129.476
129.367
129.202
124.299
123.786
122.712
121.545
77.359
77.042
76.724
65.859
61.010
60.646
60.282
59.917
43.123
O
S
N
O
O
CF3
4d'
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

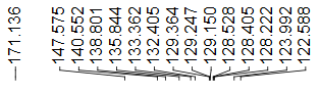

8.010
7.992
7.988
7.532
7.527
7.513
7.511
7.507
7.493
7.468
7.361
7.357
7.344
5.666
5.650
5.227
3.046
3.031
3.008
2.993
2.947
2.928
2.909
2.890
1.710
1.256
0.000
O
S
N
OBn
O
4e
1.97
1.17
4.13
2.23
5.01
1.00
2.07
1.03
1.05
f1 (ppm)

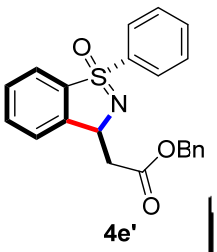

170.923
147.314
139.749
139.029
135.724
133.496
132.400
129.723
129.254
129.195
128.586
128.418
128.323
123.599
122.508
77.380
77.063
76.745
66.719
65.476
42.319
O
S
N
OBn
O
4e
f1 (ppm)


7.922
7.904
7.585
7.567
7.523
7.504
7.486
7.467
7.449
7.436
7.416
7.398
7.385
7.370
7.355
7.337
7.332
7.326
7.316
7.261
5.578
5.562
5.545
5.287
5.256
5.200
5.169
3.106
3.088
3.066
3.049
2.991
2.975
2.952
2.935
1.661
0.000
O
S
N
OBn
O

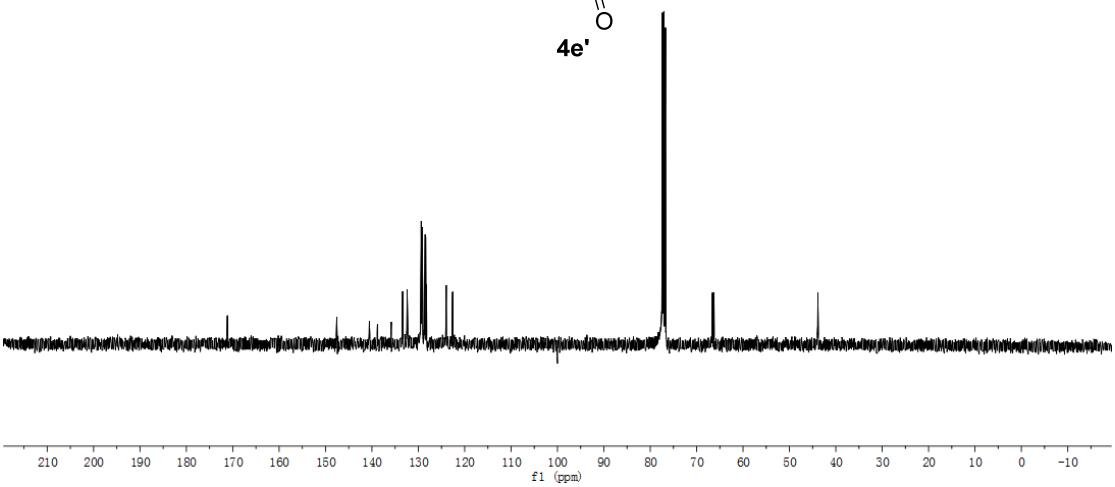
4e'

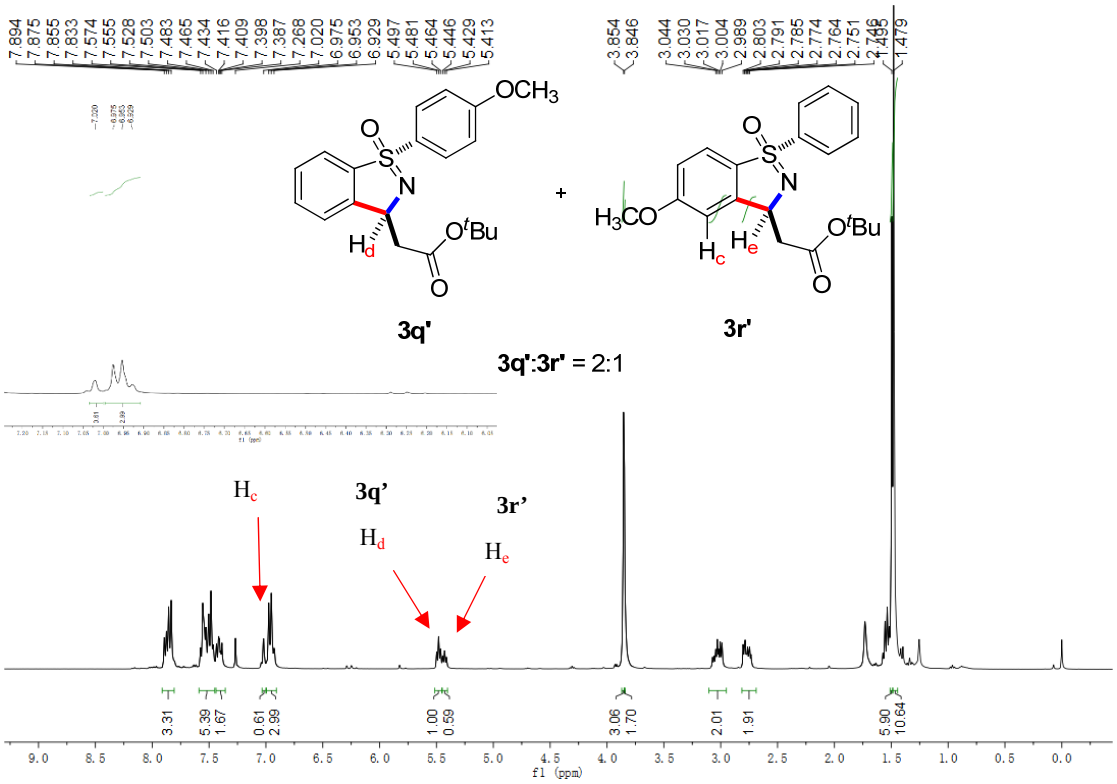

1.79
1.10
3.82
1.92
4.97
1.00
2.10
0.99
1.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

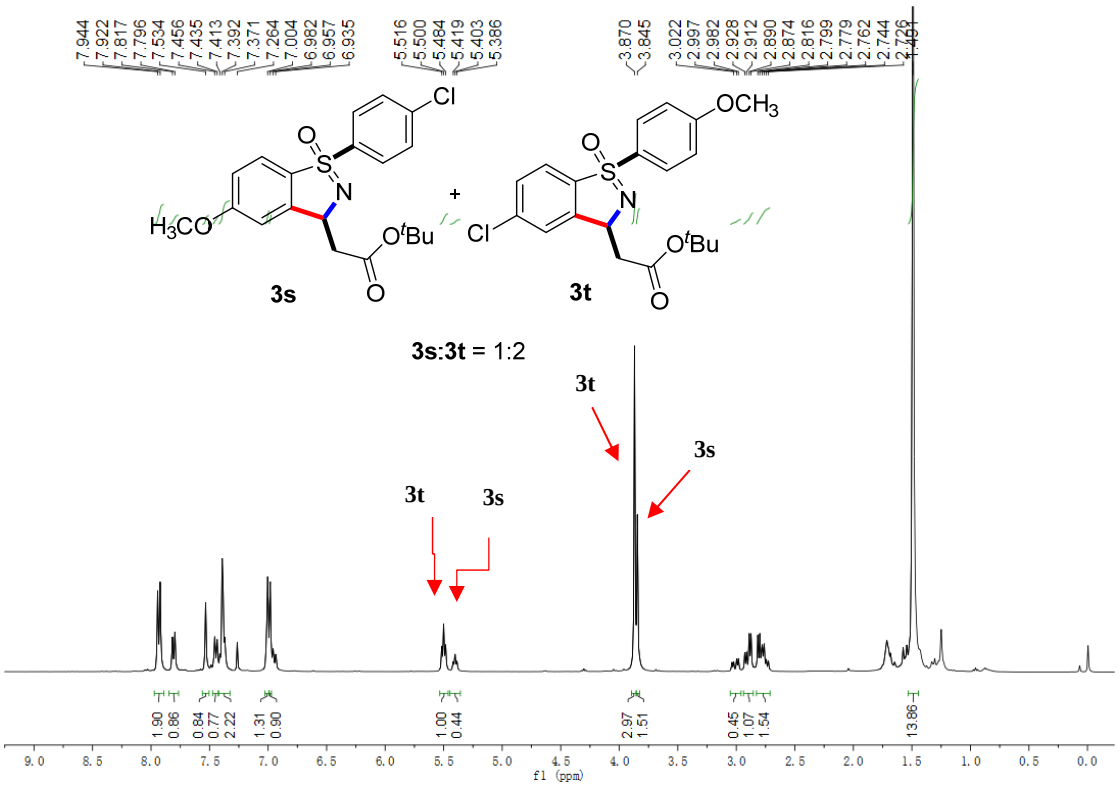

171.136
147.575
140.552
138.801
135.844
133.362
132.405
129.364
129.247
129.150
128.528
128.405
128.222
123.992
122.588
77.359
77.041
76.724
66.577
66.256
43.865

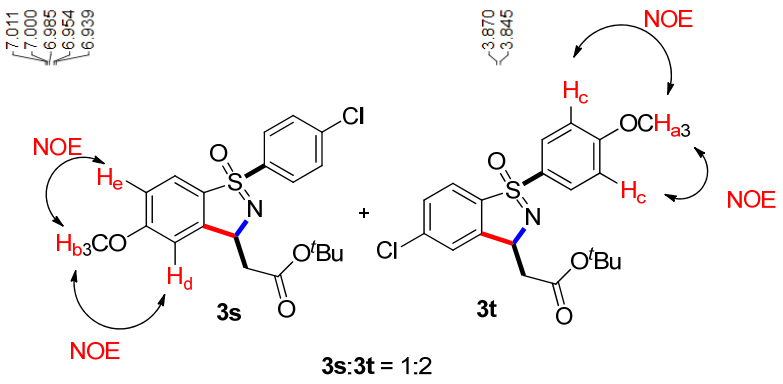

O
S
N
OBn
O

4e'

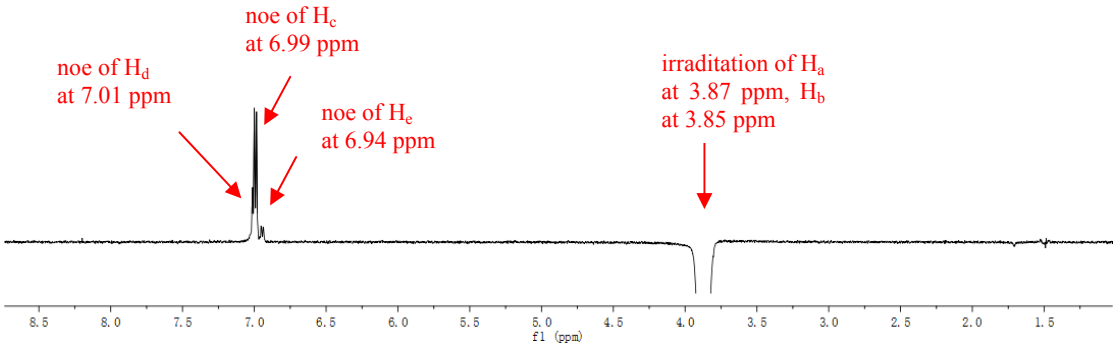

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

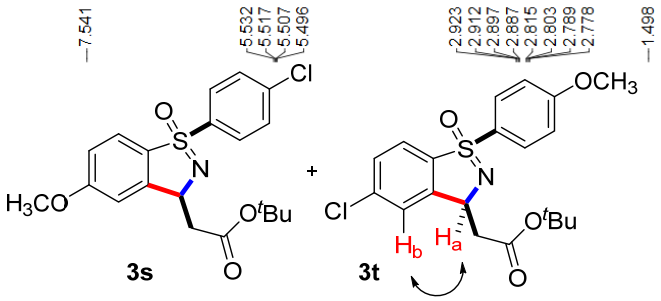

OCH3
O
S
N
Hd
OtBu
O
H3CO
Hc
He
3q'
3r'
3q':3r' = 2:1
Hc
3q'
Hd
3r'
He
f1 (ppm)


Cl
OCH3
O
S
N
H3CO
OtBu
3s
3t
3s:3t = 1:2
3t
3s
3t
3s
f1 (ppm)

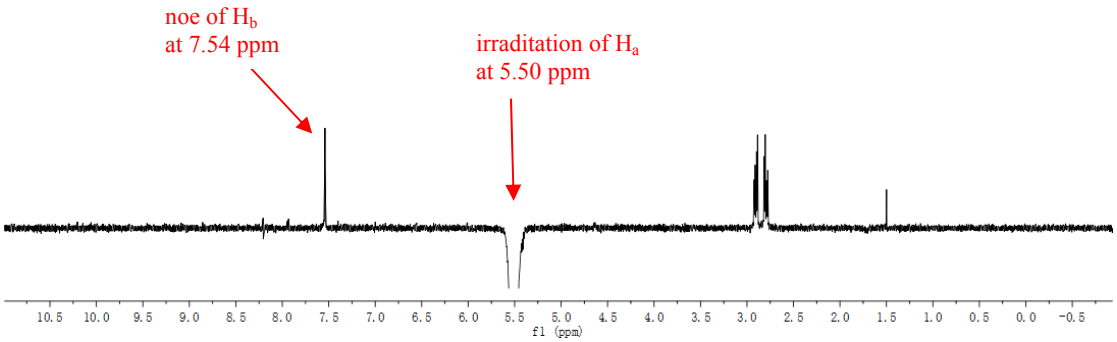


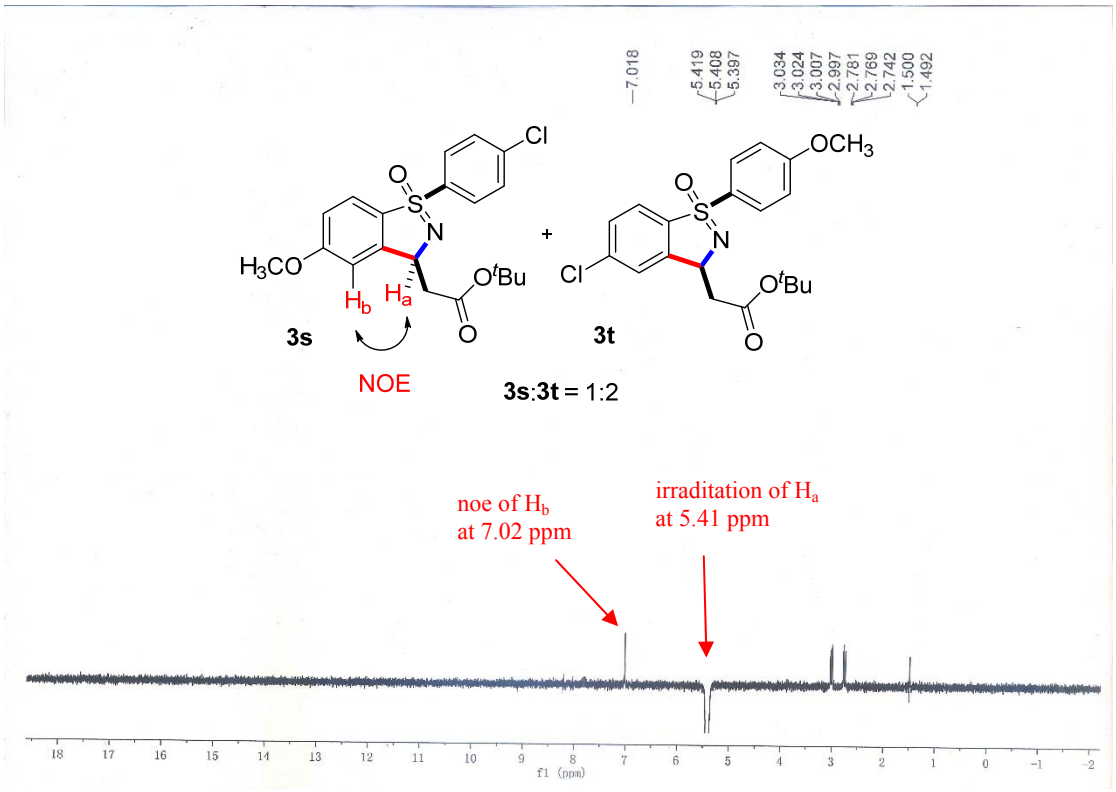
3s:**3t** = 1:2

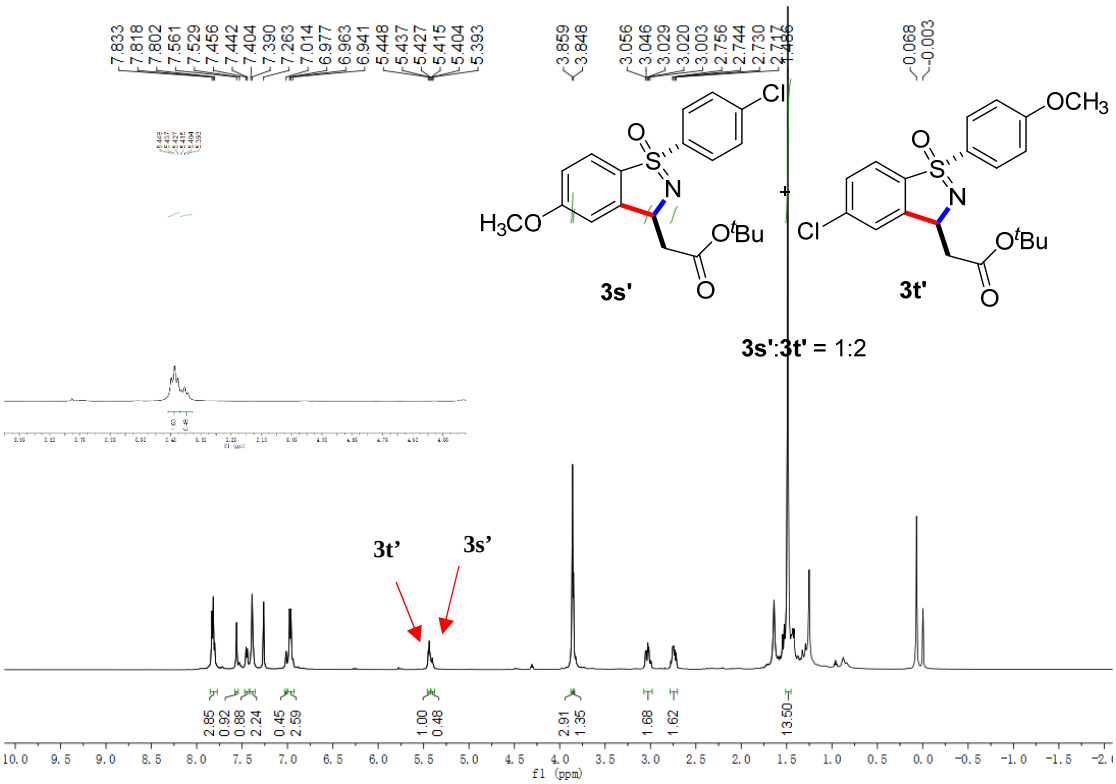


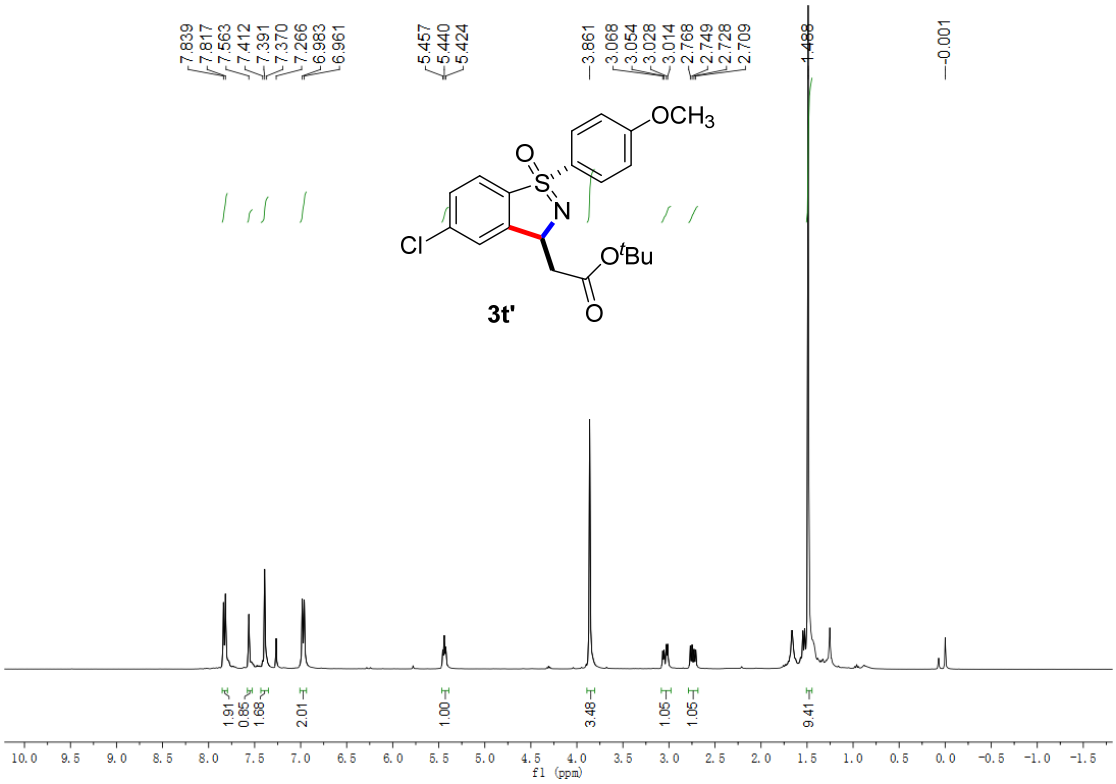


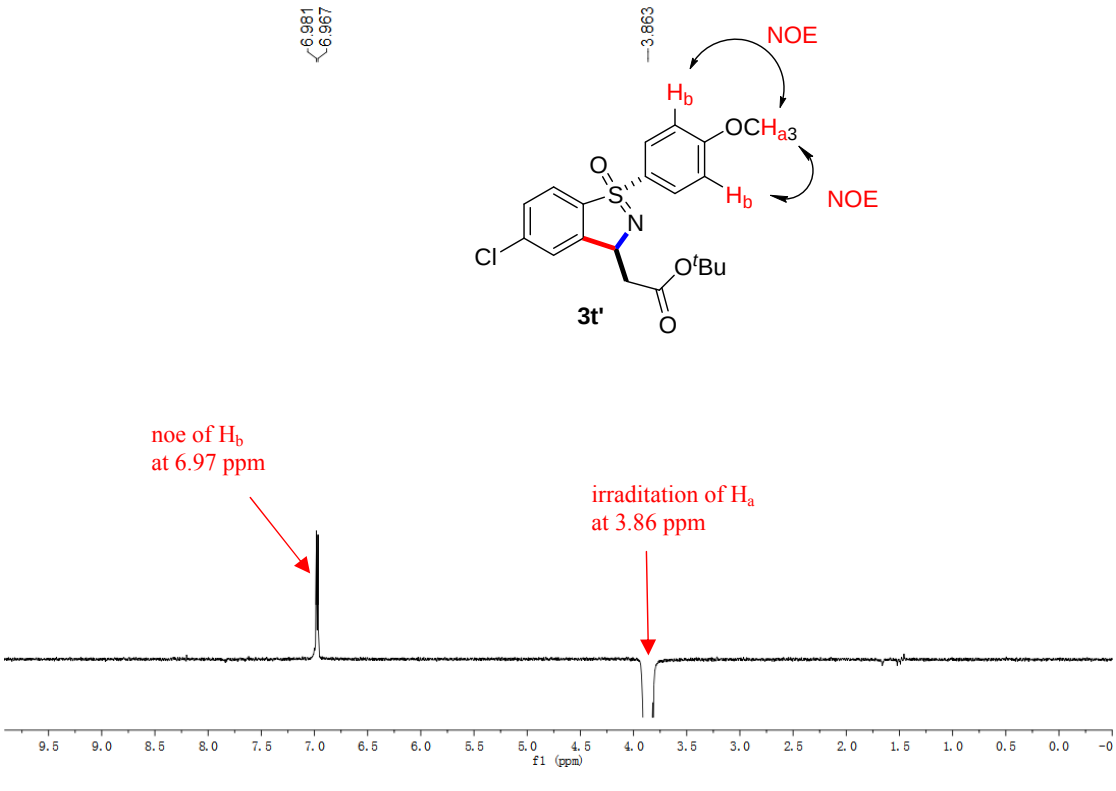
3s:**3t** = 1:2




7.018
5.419
5.408
5.397
3.034
3.024
3.007
2.997
2.781
2.769
2.742
1.500
1.492
Cl
O
S
N
H3CO
Hb
Ha
OtBu
O
3s
+
OCH3
Cl
3t
NOE
3s:3t = 1:2
noe of Hb
at 7.02 ppm
irraditation of Ha
at 5.41 ppm
f1 (ppm)


7.833
7.818
7.802
7.561
7.529
7.456
7.442
7.404
7.390
7.263
7.014
6.977
6.963
6.941
5.448
5.437
5.427
5.415
5.404
5.393
3.859
3.848
3.056
3.046
3.029
3.020
3.003
2.756
2.744
2.730
1.486
0.068
-0.003
Cl
OCH3
H3CO
OtBu
3s'
3t'
3s':3t' = 1:2
3t'
3s'
2.85
0.92
0.88
2.24
0.45
2.59
1.00
0.48
2.91
1.35
1.68
1.62
13.50
f1 (ppm)


7.839
7.817
7.563
7.412
7.391
7.370
7.266
6.983
6.961
5.457
5.440
5.424
3.861
3.068
3.054
3.028
3.014
2.768
2.749
2.728
2.709
1.488
-0.001
OCH3
O
S
N
Cl
OtBu
O
3t'
1.91
0.85
1.88
2.01
1.00
3.48
1.05
1.05
9.41
f1 (ppm)


6.981
6.967
3.863
NOE
Hb
OCHa3
Hb
NOE
O
S
N
Cl
OtBu
O
3t'
noe of Hb
at 6.97 ppm
irraditation of Ha
at 3.86 ppm
f1 (ppm)