

Supporting Information for:

Enantioselective Alkynylation of *N*-Sulfonyl α -Ketiminoesters via a Friedel-Crafts Alkylation Strategy

Ren-Rong Liu, Lei Zhu, Jiang-Ping Hu, Chuan-Jun Lu, Jian-Rong Gao, Yu Lan,* and Yi-Xia Jia*

Contents:

1. General information.....	S1
2. Substrate synthesis.....	S2
3. General procedure for catalytic enantioselective alkynylation of <i>N</i> -sulfonyl α -ketiminoesters.....	S6
4. Synthetic transformation of product 3ba.....	S65
5. Computational study of mechanism.....	S68
6. References.....	S90

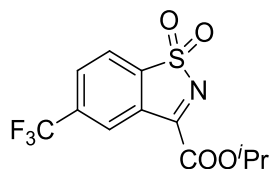
1. General information

Reactions and manipulations involving organometallic or moisture sensitive compounds were carried out under dry nitrogen and glassware heated under oven for two hours prior to use. ^1H and ^{13}C NMR spectra were recorded on Bruker AVANCE III 500MHz with TMS as internal standard. Anhydrous CH_2Cl_2 were freshly distilled over sodium. Melting points were measured on a Buchi Melting Point B-545 apparatus and uncorrected. Optical rotations were determined using a Rudolph Autopol IV polarimeter. HPLC analyses were performed using Waters 1525 chromatography. Chiral columns were purchased from Daicel Chemical Industries, LTD. Commercial reagents were used as received without further purification unless otherwise noticed. HRMS were recorded on Agilent 6210 LCT (EI source) or Waters Xevo Q-ToF Mass Spectrometer (ESI source). Column chromatography was carried out using silica gel (200-300 mesh).

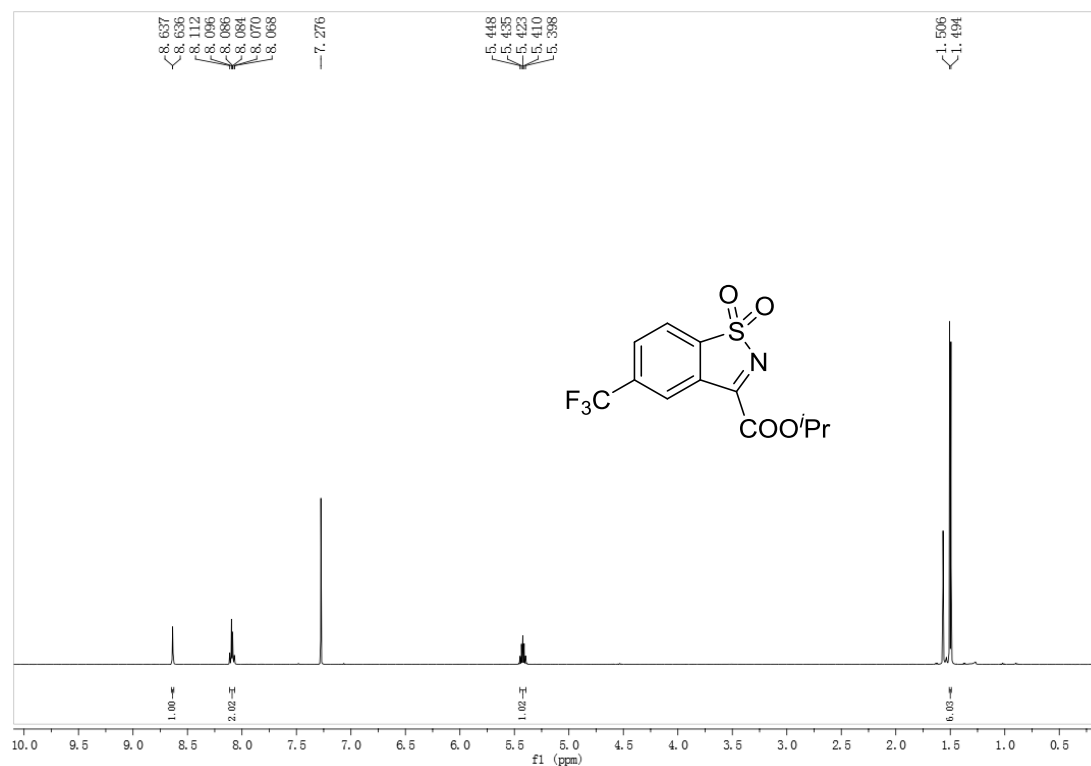
2. Substrate synthesis:

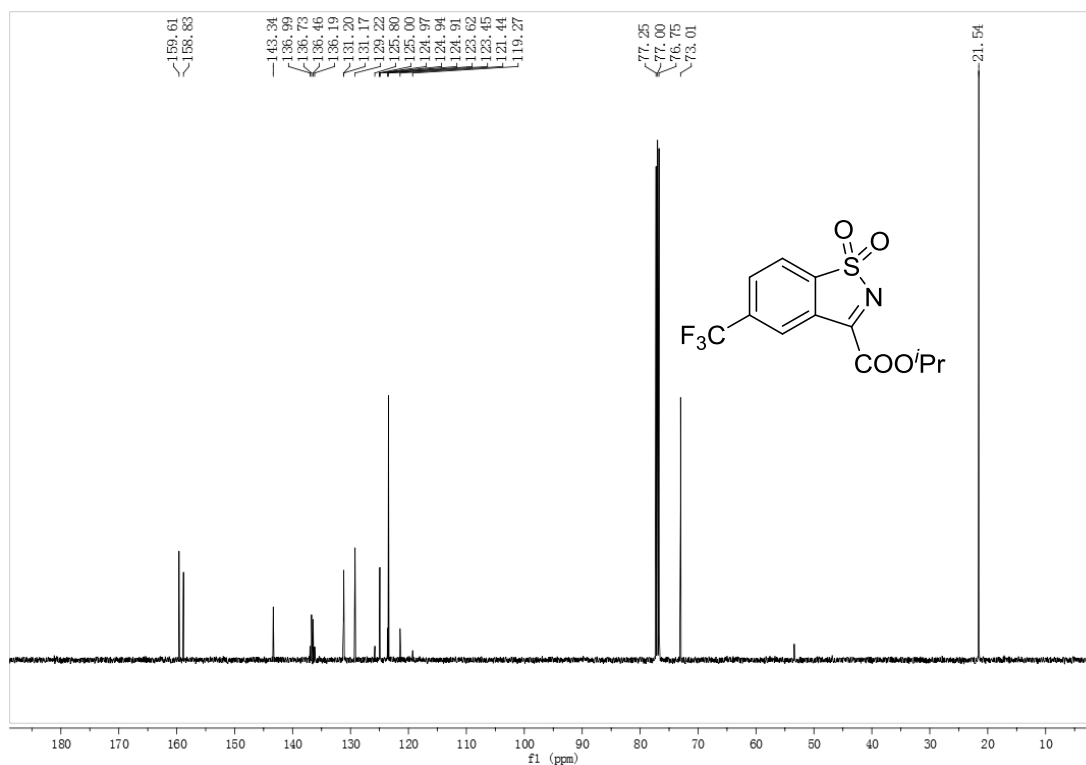
Substrates cyclic *N*-sulfonyl α -ketiminoesters were synthesized according to the known method.¹ **1a-1h** and **1l** are known compounds.¹

Isopropyl 5-(trifluoromethyl)benzo[d]isothiazole-3-carboxylate 1,1-dioxide (**1i**)

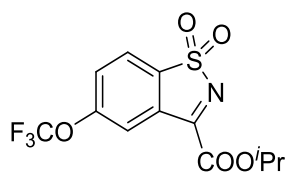


White solid, m.p. 136-137 °C; ¹H NMR (500 MHz, CDCl₃): δ 8.64 (d, *J* = 0.5 Hz, 1H), 8.06-8.12 (m, 2H), 5.42 (dt, *J* = 12.5, 6.5 Hz, 1H), 1.50 (d, *J* = 6.0 Hz, 6H); ¹³C NMR (125 MHz, CDCl₃): δ 159.61, 158.83, 143.34, 136.6 (q, *J* = 32.5 Hz), 131.2 (q, *J* = 3.5 Hz), 129.22, 122.5 (q, *J* = 272.5 Hz), 124.94 (q, *J* = 3.8 Hz), 123.45, 73.01, 21.54; HRMS *m/z* (ESI⁺): calculated for C₁₂H₁₁F₃NO₄S ([M+H]⁺): 322.0355, found 322.0357.

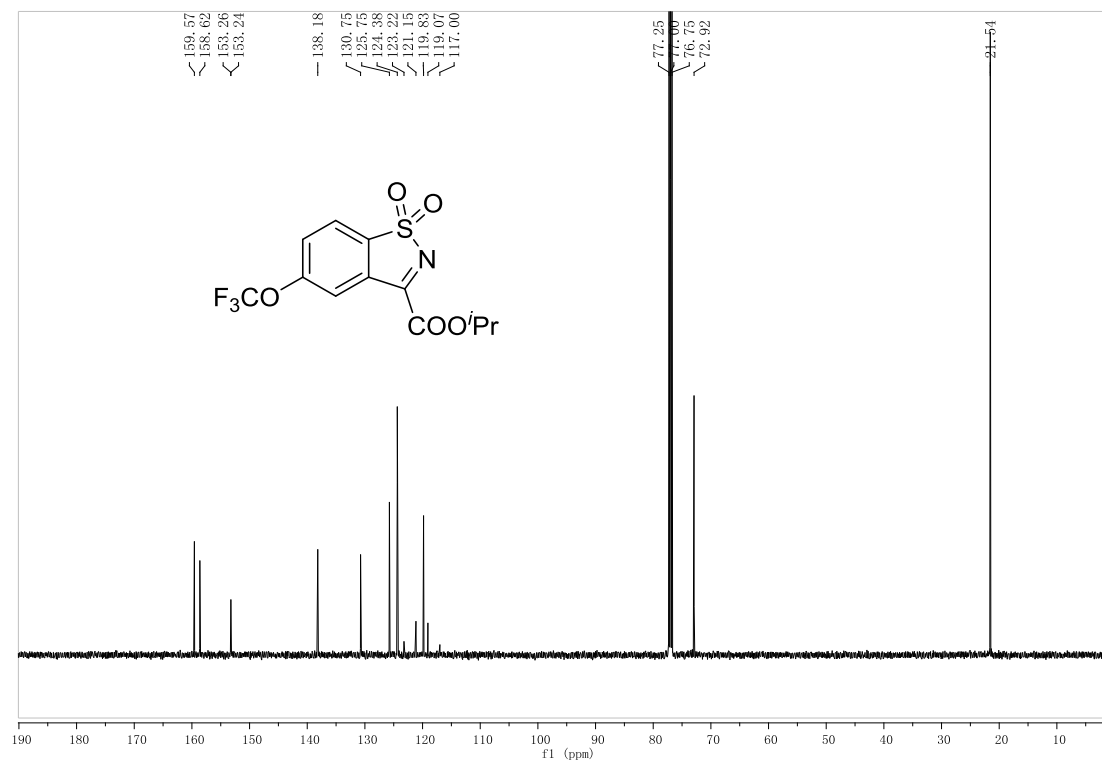
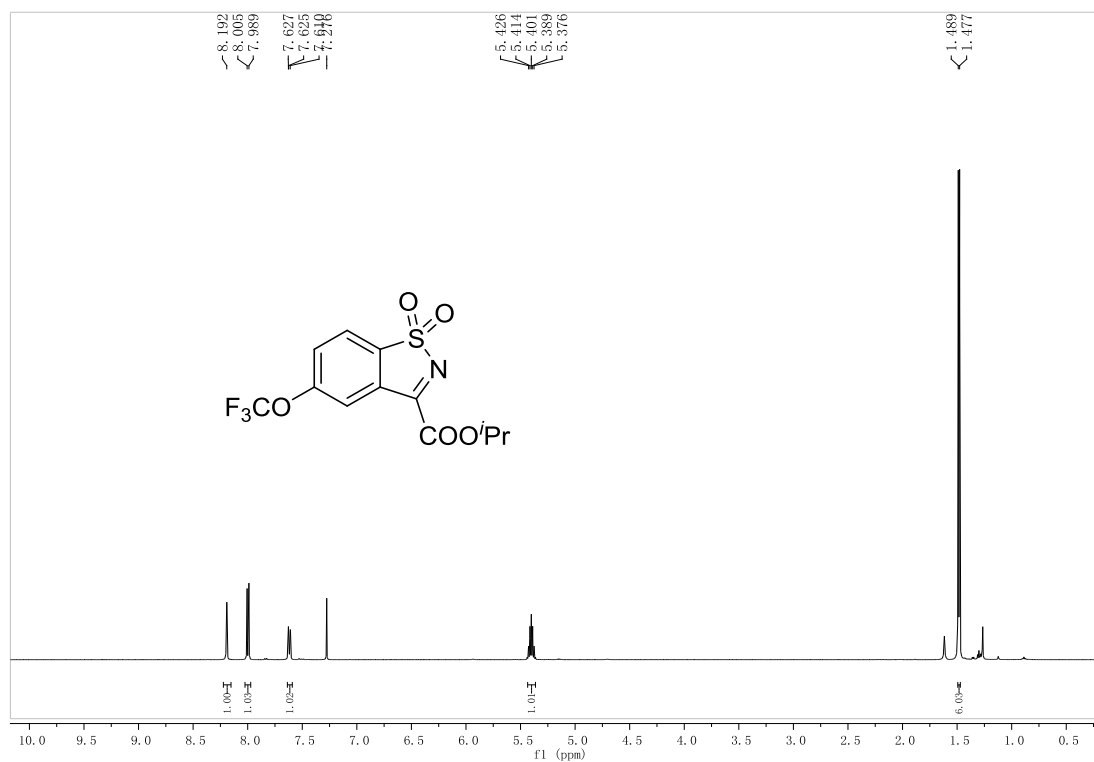




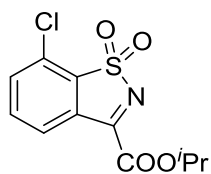
Isopropyl 5-(trifluoromethoxy)benzo[d]isothiazole-3-carboxylate 1,1-dioxide (**1j**)



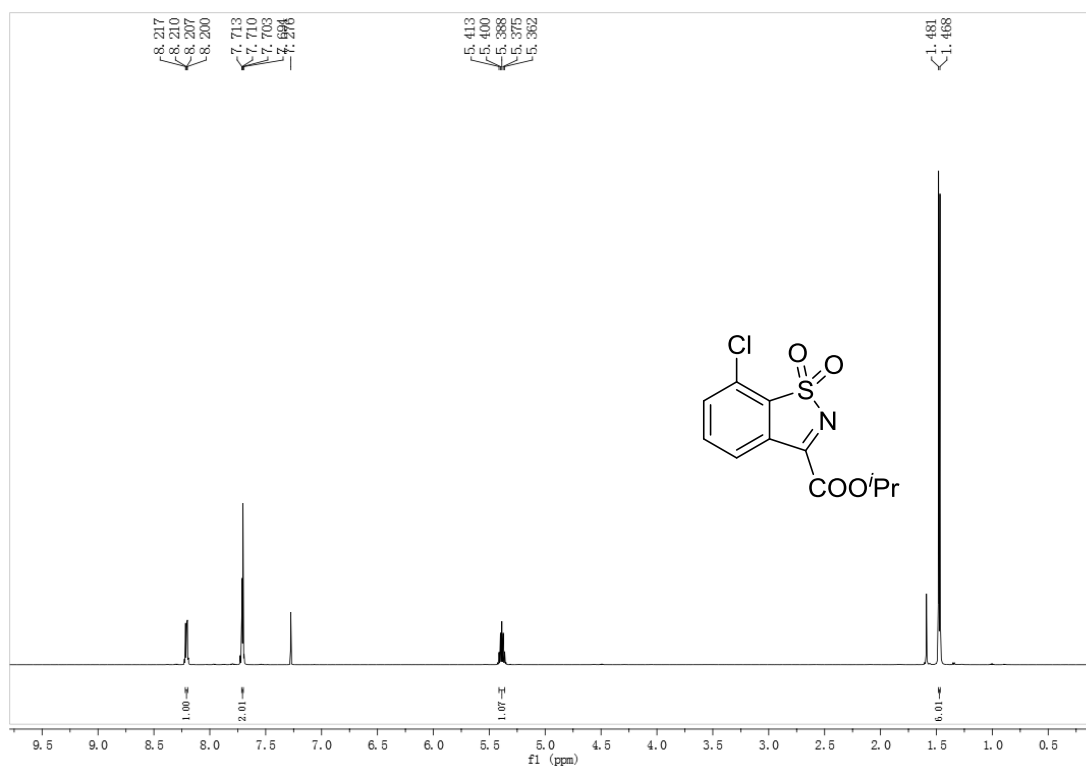
White solid, m.p. 115-117 °C; ^1H NMR (500 MHz, CDCl_3): δ 8.19 (s, 1H), 8.00 (d, $J = 8.0$ Hz, 1H), 7.62 (dd, $J = 8.5, 1.0$ Hz, 1H), 5.40 (dt, $J = 12.5, 6.0$ Hz, 1H), 1.48 (d, $J = 6.0$ Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3): δ 159.6, 158.6, 153.3, 138.2, 130.8, 125.7, 124.4, 120.1 (q, $J = 258.8$ Hz), 119.8, 72.9, 21.5; HRMS m/z (ESI $^+$): calculated for $\text{C}_{12}\text{H}_{11}\text{F}_3\text{NO}_5\text{S}$ ($[\text{M}+\text{H}]^+$): 338.0305, found 338.0309.

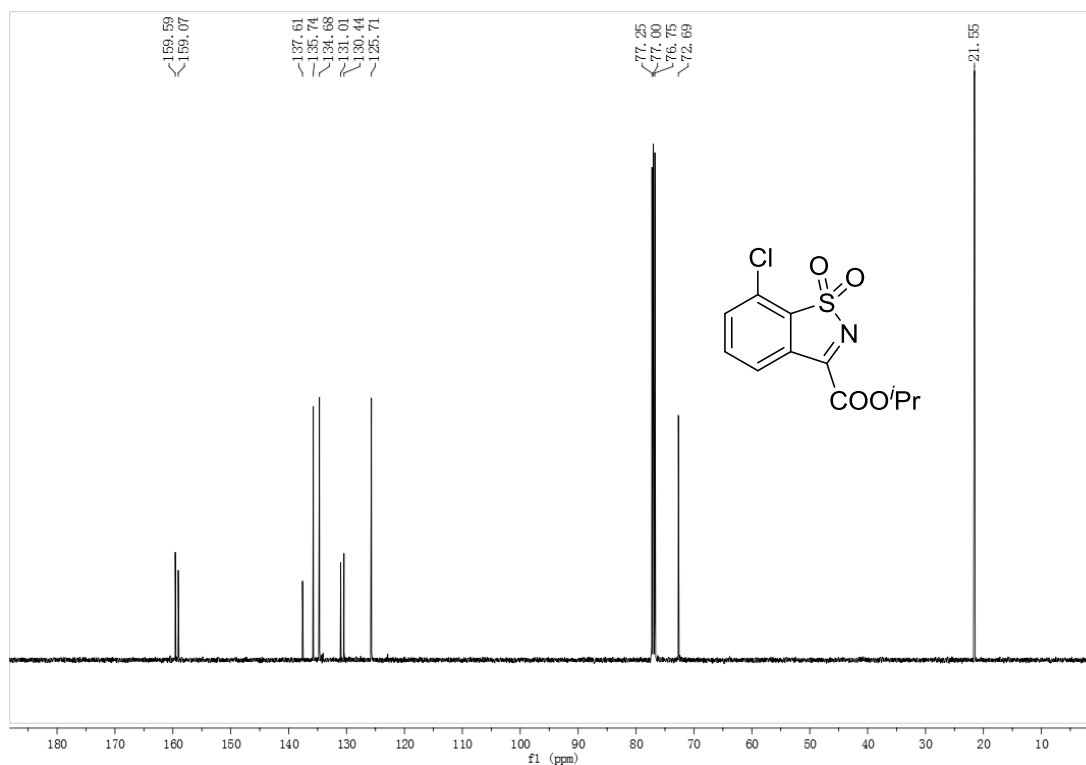


Isopropyl 7-chlorobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**1k**)



White solid, m.p. 137-138 °C; ^1H NMR (500 MHz, CDCl_3): δ 8.21 (dd, $J = 5.0, 3.5$ Hz, 1H), 7.69-7.73 (m, 2H), 5.39 (dt, $J = 12.5, 6.5$ Hz, 1H), 1.47 (d, $J = 6.5$ Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3): δ 159.6, 159.1, 137.6, 135.7, 134.7, 131.0, 130.4, 125.7, 72.7, 21.6; HRMS m/z (ESI $^+$): calculated for $\text{C}_{11}\text{H}_{14}\text{ClN}_2\text{O}_4\text{S}$ ($[\text{M}+\text{NH}_4]^+$): 305.0357, found 305.0350.

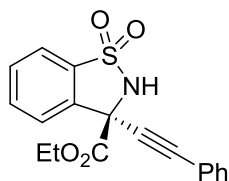




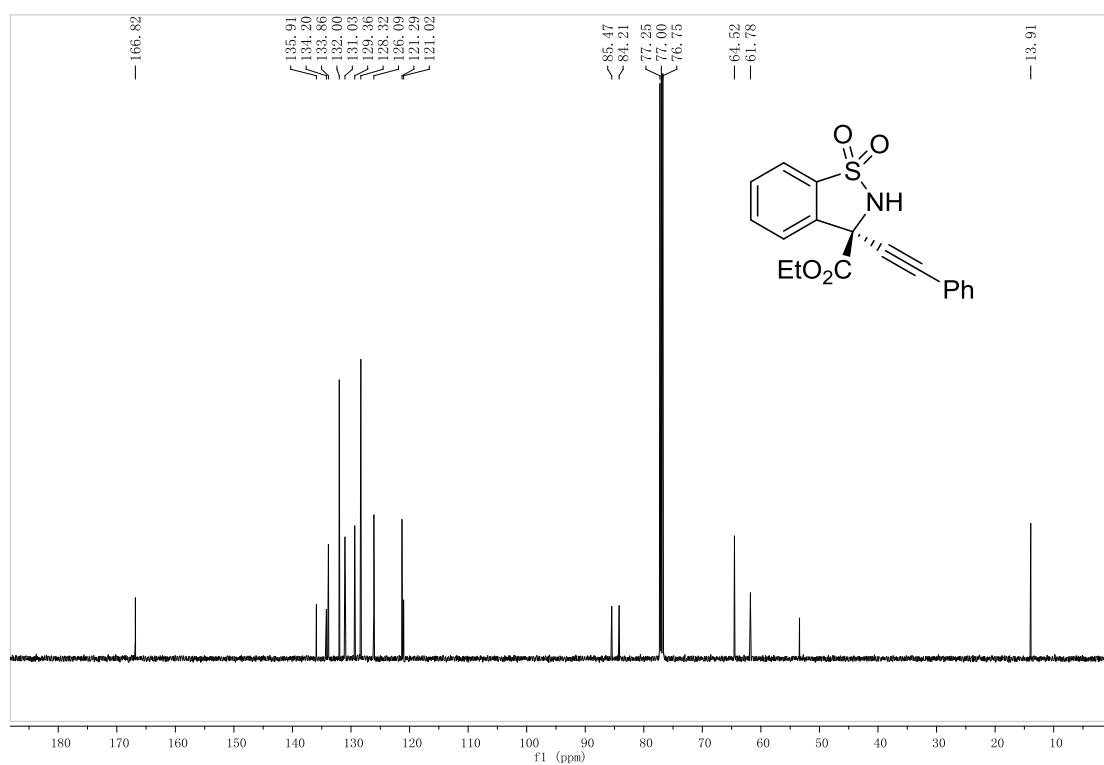
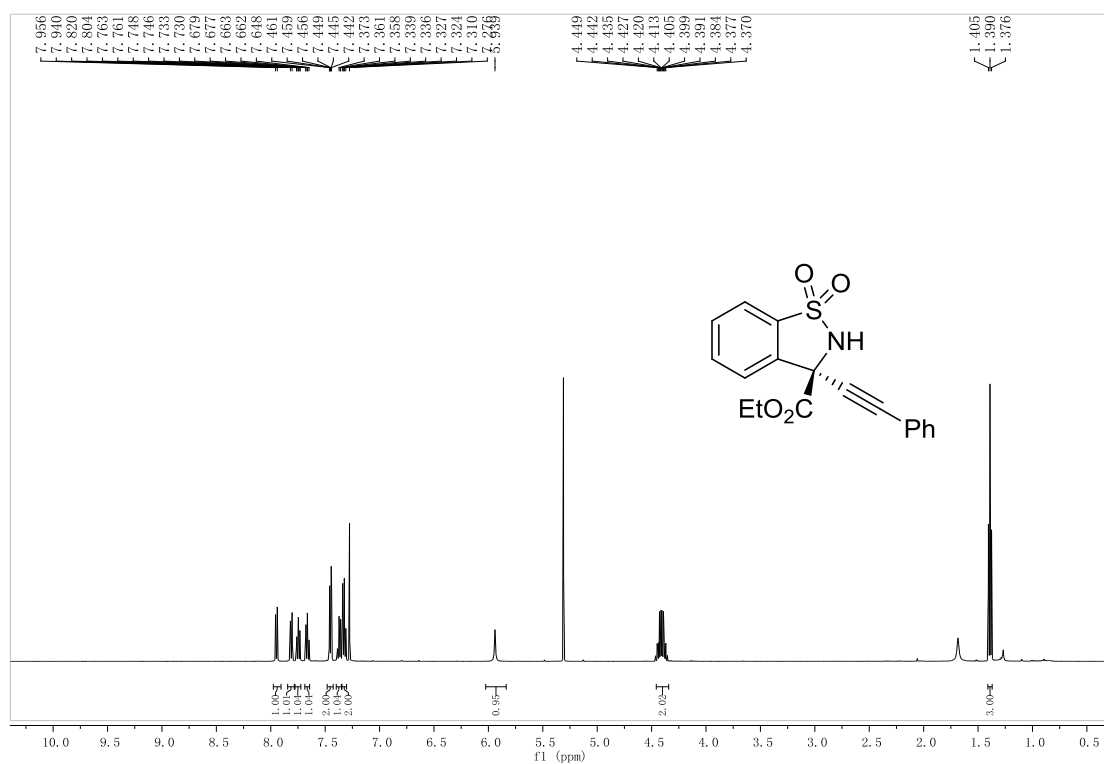
3. General procedure for catalytic enantioselective alkynylation of *N*-sulfonyl α -ketiminoesters:

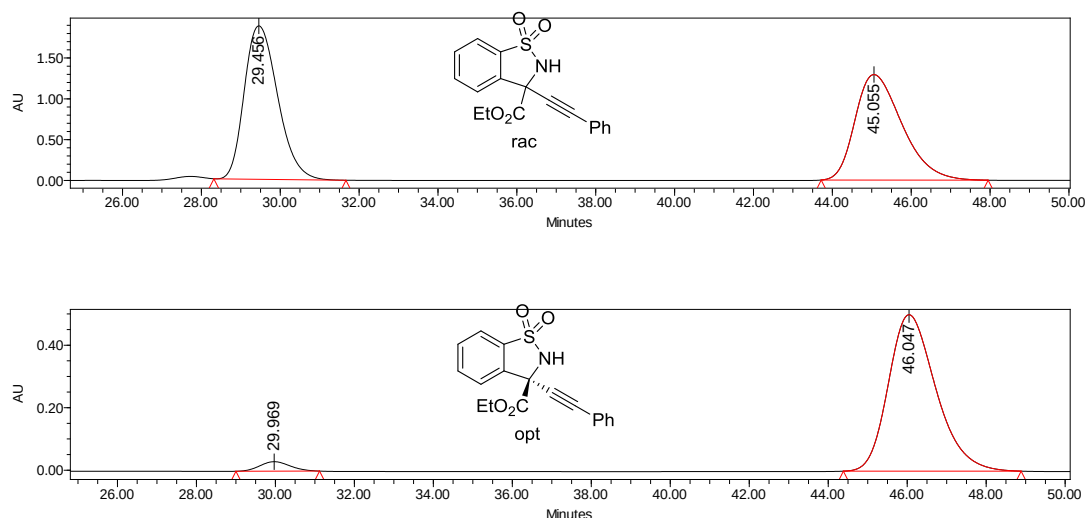
To a dried Schlenk tube was added $\text{Ni}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (7.3 mg, 0.02 mmol) and (*R*)-DTBM-Segphos (28.3 mg, 0.024 mmol) under N_2 , 2.0 mL CH_2Cl_2 was then added via a syringe. The schlenk tube was then sealed with a Teflon cap and the resulting mixture was stirred at 80 °C for 30 min. After cooling to room temperature, *N*-sulfonyl α -ketiminoesters (0.3 mmol) and phenylacetylene (0.2 mmol) were added under N_2 atmosphere. The schlenk tube was sealed again and the mixture was stirred at 50 °C until the reaction was completed. The solvent was then removed under vacuum and the residue was purified by chromatography with ethyl acetate/petroleum ether 1:4 (v/v) on silica gel to give the product.

Ethyl 3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3aa**)



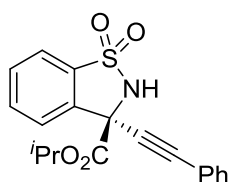
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 72% yield; $[\alpha]_{\text{D}}^{15} = 23.1$ ($c = 1.0$ in CHCl_3), 92% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 46.0$ min, $t_{\text{minor}} = 30.0$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.95 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 8.0$ Hz, 1H), 7.75 (td, $J = 7.5, 1.0$ Hz, 1H), 7.66 (td, $J = 7.5, 1.0$ Hz, 1H), 7.44-7.47 (m, 2H), 7.35-7.39 (m, 1H), 7.30-7.34 (m, 2H), 5.94 (s, 1H), 4.37-4.45 (m, 2H), 1.39 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.8, 135.9, 134.2, 133.9, 132.0, 131.0, 129.4, 128.3, 126.1, 121.3, 121.0, 85.5, 84.2, 64.5, 61.8, 13.9; HRMS m/z (ESI $^+$): calculated for $\text{C}_{18}\text{H}_{16}\text{NO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 342.0795, found 342.0794.



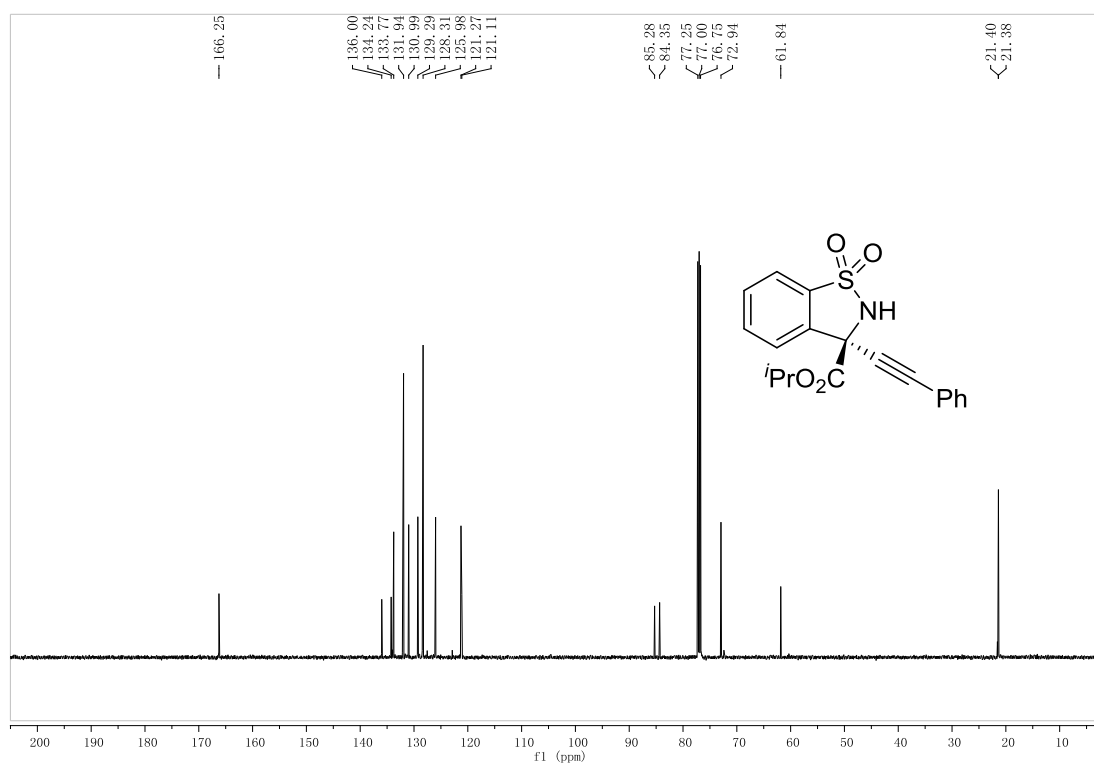
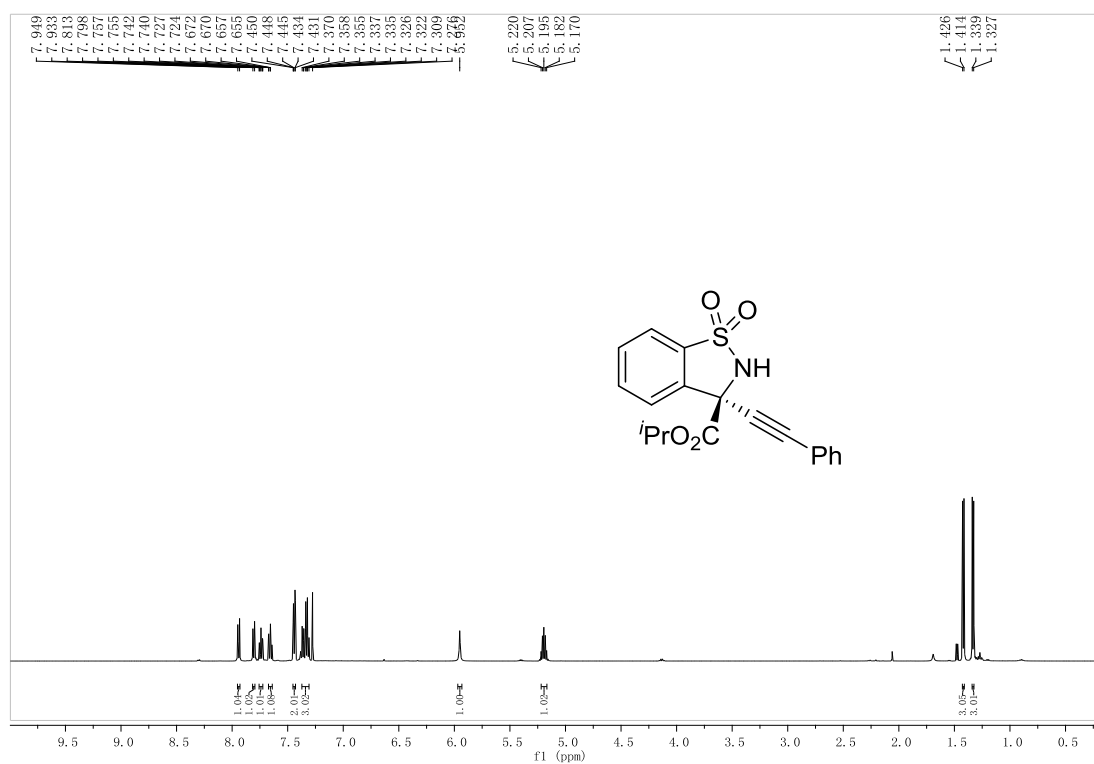


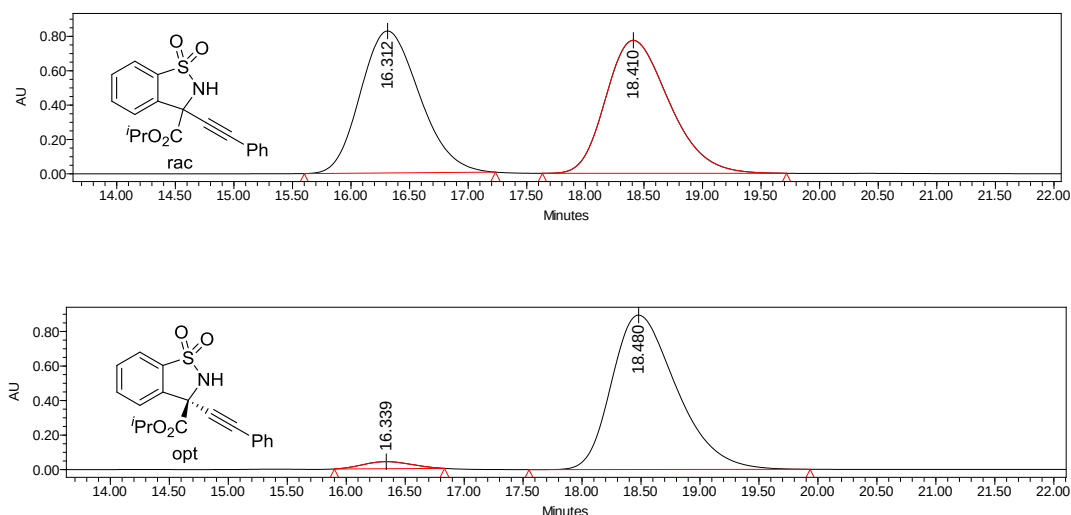
	Retention Time	Area	% Area	Height	% Height
1	29.969	1620948	3.76	30408	5.72
2	46.047	41878803	96.24	500882	94.28

Isopropyl 3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3ba**)



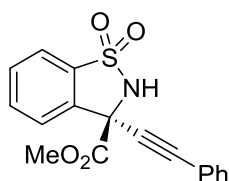
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 84% yield; $[\alpha]_D^{15} = 21.6$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 1.0 mL/min, 254 nm; $t_{\text{major}} = 18.5$ min, $t_{\text{minor}} = 16.3$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.94 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 7.5$ Hz, 1H), 7.74 (td, $J = 7.5, 1.0$ Hz, 1H), 7.66 (td, $J = 7.5, 1.0$ Hz, 1H), 7.43-7.45 (m, 2H), 7.30-7.37 (m, 3H), 5.95 (s, 1H), 5.19 (dd, $J = 12.5, 6.5$ Hz, 1H), 1.42 (d, $J = 6.0$ Hz, 3H), 1.33 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.3, 136.0, 134.2, 133.8, 131.9, 131.0, 129.3, 128.3, 126.0, 121.3, 121.1, 85.3, 84.4, 72.0, 61.8, 21.40, 21.38; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{18}\text{NO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 356.0951, found 356.0951.



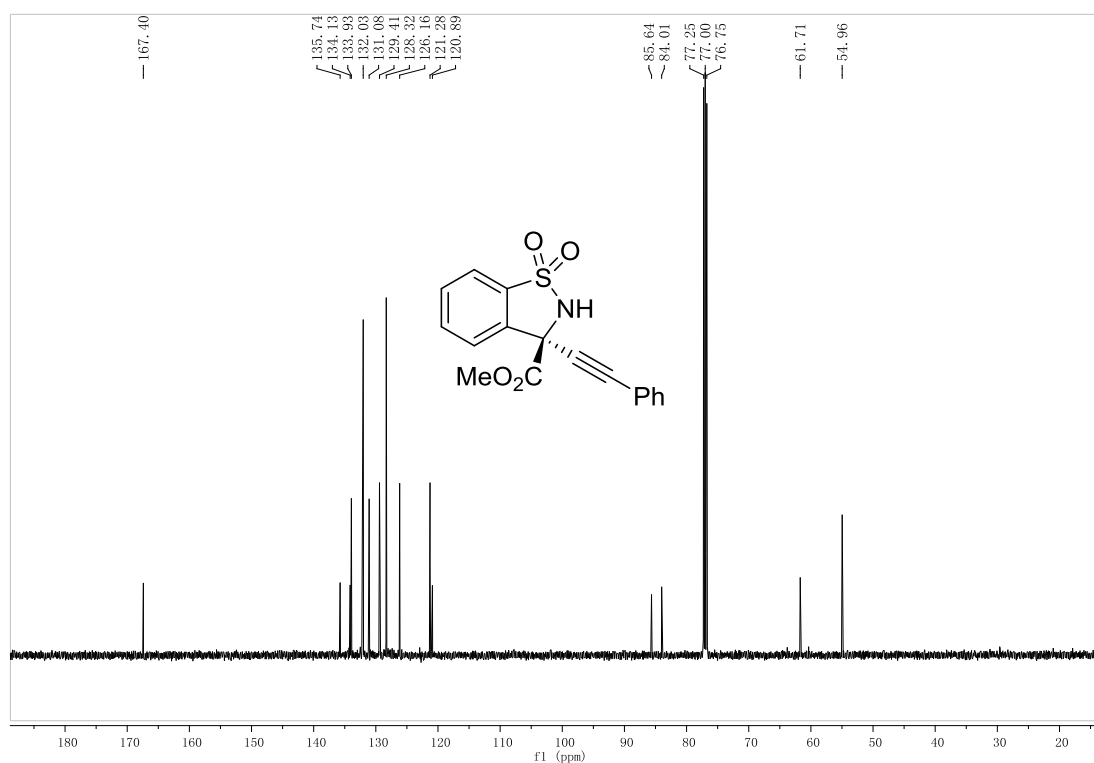
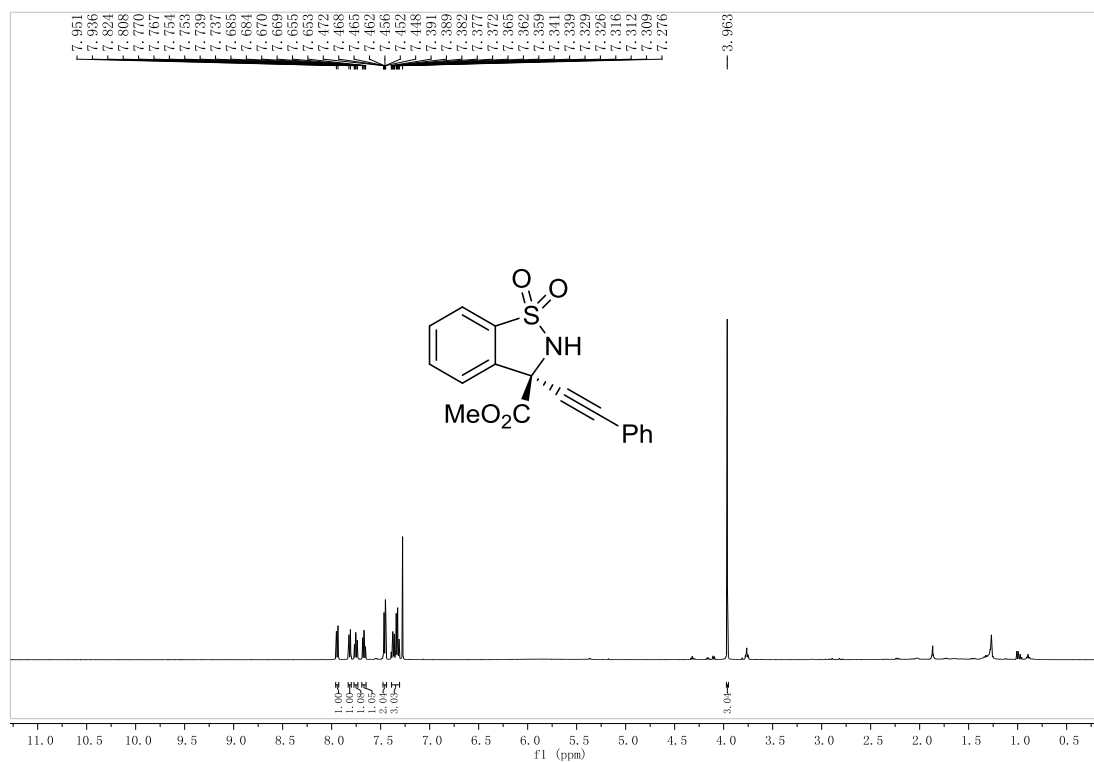


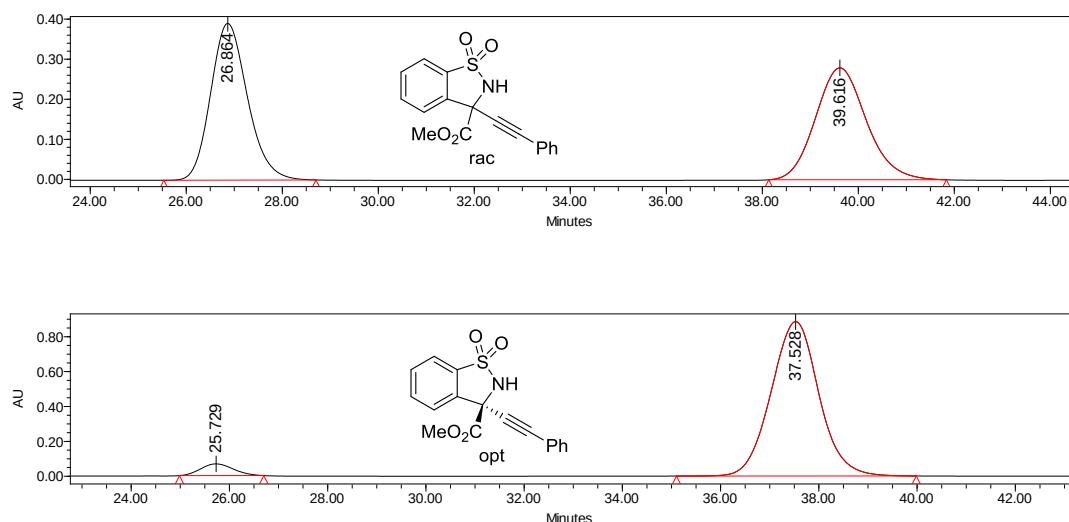
	Retention Time	Area	% Area	Height	% Height
1	16.339	1164923	3.29	40740	4.35
2	18.480	34194355	96.71	894756	95.65

Methyl 3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide
(**3ca**)



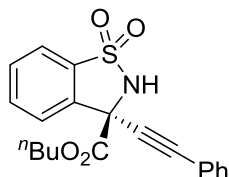
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 76% yield; $[\alpha]_D^{15} = 63.8$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 1.0 mL/min, 254 nm; $t_{\text{major}} = 37.5$ min, $t_{\text{minor}} = 25.7$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.94 (d, $J = 7.5$ Hz, 1H), 7.82 (d, $J = 8.0$ Hz, 1H), 7.75 (td, $J = 8.0, 1.5$ Hz, 1H), 7.67 (td, $J = 7.5, 0.5$ Hz, 1H), 7.44-7.48 (m, 2H), 7.30-7.40 (m, 3H), 3.96 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 167.4, 135.7, 134.1, 133.9, 132.0, 131.1, 129.4, 128.3, 126.2, 121.3, 120.9, 85.6, 84.0, 61.7, 55.0; HRMS m/z (ESI $^+$): calculated for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_4\text{S}$ ($[\text{M}+\text{NH}_4]^+$): 345.0904, found 345.0901.



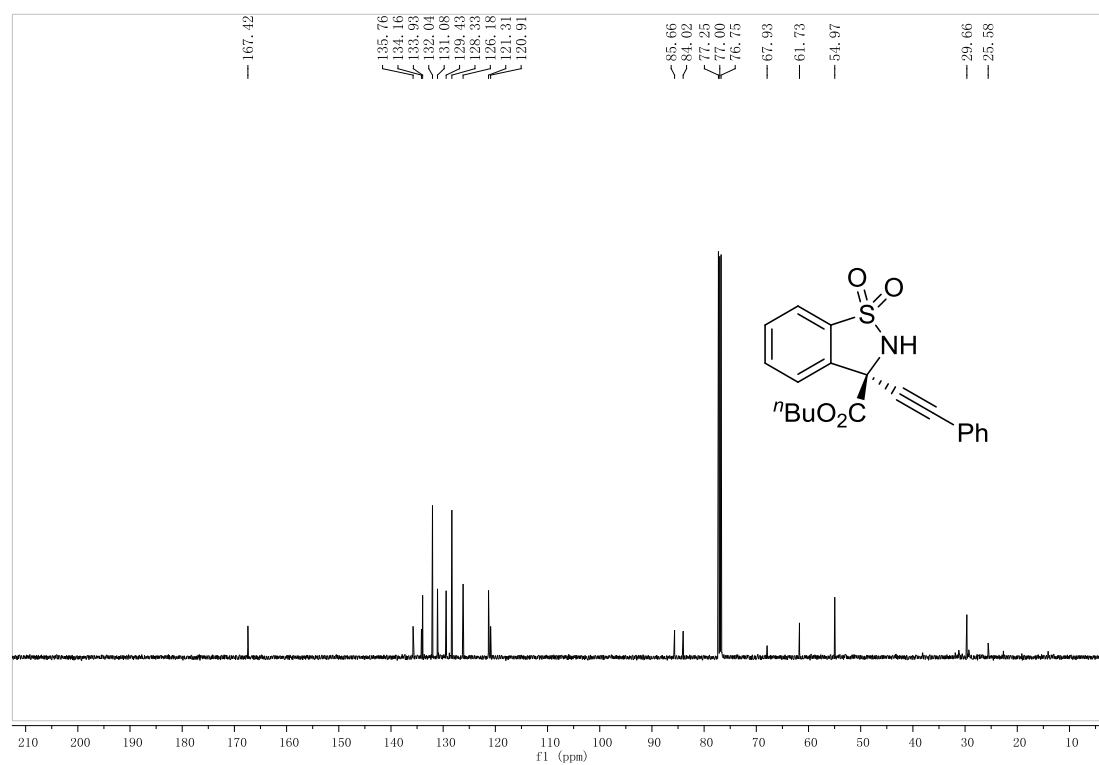
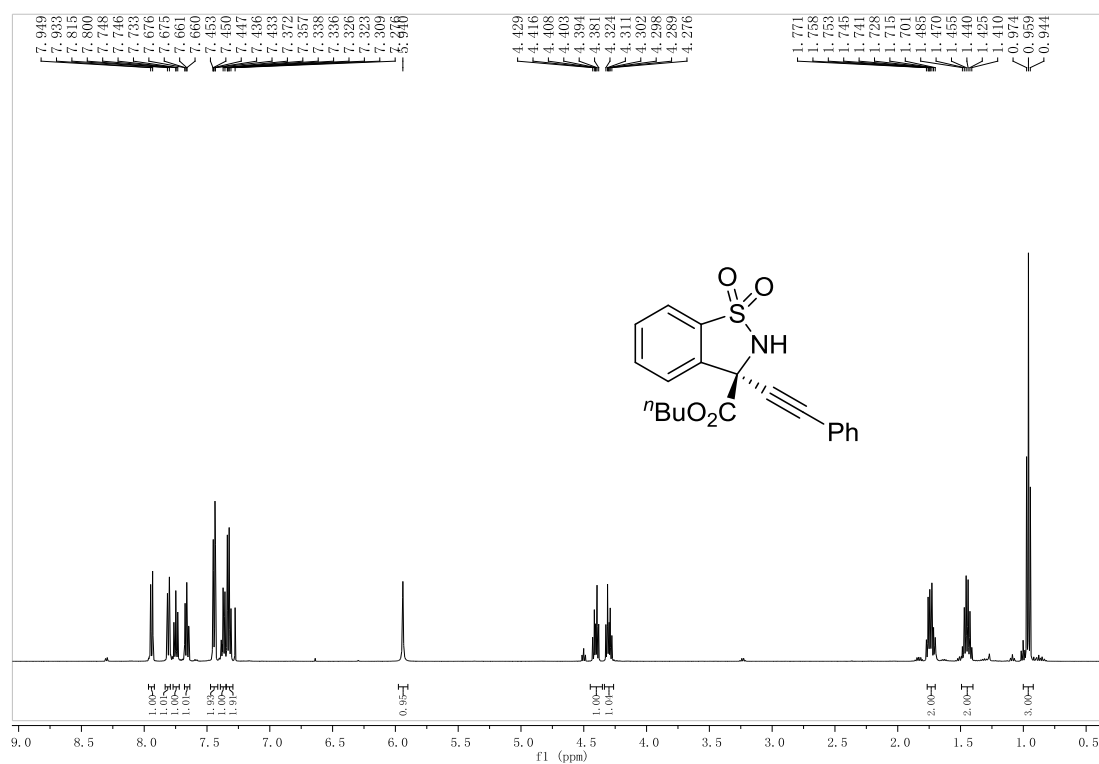


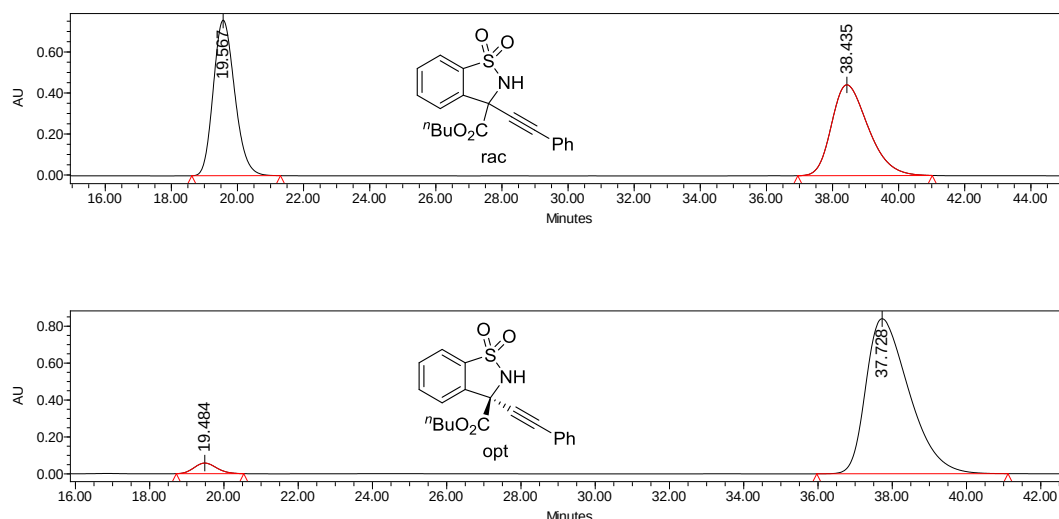
	Retention Time	Area	% Area	Height	% Height
1	25.729	3099516	4.92	67142	7.05
2	37.528	59935065	95.08	885069	92.95

Butyl 3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide
(**3da**)



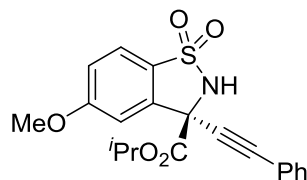
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 75% yield; $[\alpha]_D^{15} = 36.1$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 1.0 mL/min, 254 nm; $t_{\text{major}} = 37.7$ min, $t_{\text{minor}} = 19.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.94 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 7.5$ Hz, 1H), 7.75 (td, $J = 7.5, 1.0$ Hz, 1H), 7.66 (td, $J = 7.5, 0.5$ Hz, 1H), 7.43-7.46 (m, 2H), 7.35-7.39 (m, 1H), 7.30-7.34 (m, 2H), 5.94 (s, 1H), 4.41 (dt, $J = 10.5, 6.5$ Hz, 1H), 4.30 (dt, $J = 11.0, 6.5$ Hz, 1H), 1.70-1.78 (m, 2H), 1.40-1.49 (m, 2H), 0.96 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 167.4, 135.8, 134.2, 133.9, 132.0, 131.1, 129.4, 128.3, 126.2, 121.3, 120.9, 85.7, 84.0, 67.9, 61.7, 55.0, 29.7, 25.6; HRMS m/z (ESI $^+$): calculated for $\text{C}_{20}\text{H}_{19}\text{NNaO}_4\text{S}$ ($[\text{M}+\text{Na}]^+$): 392.0927, found 392.0927.



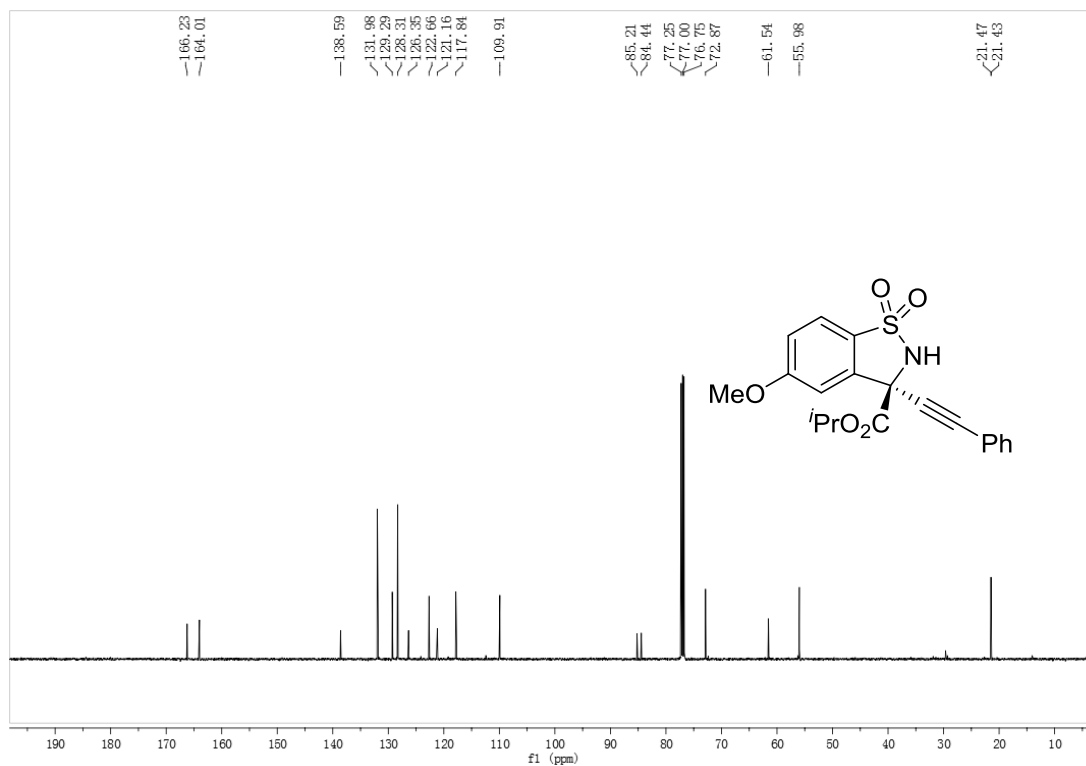
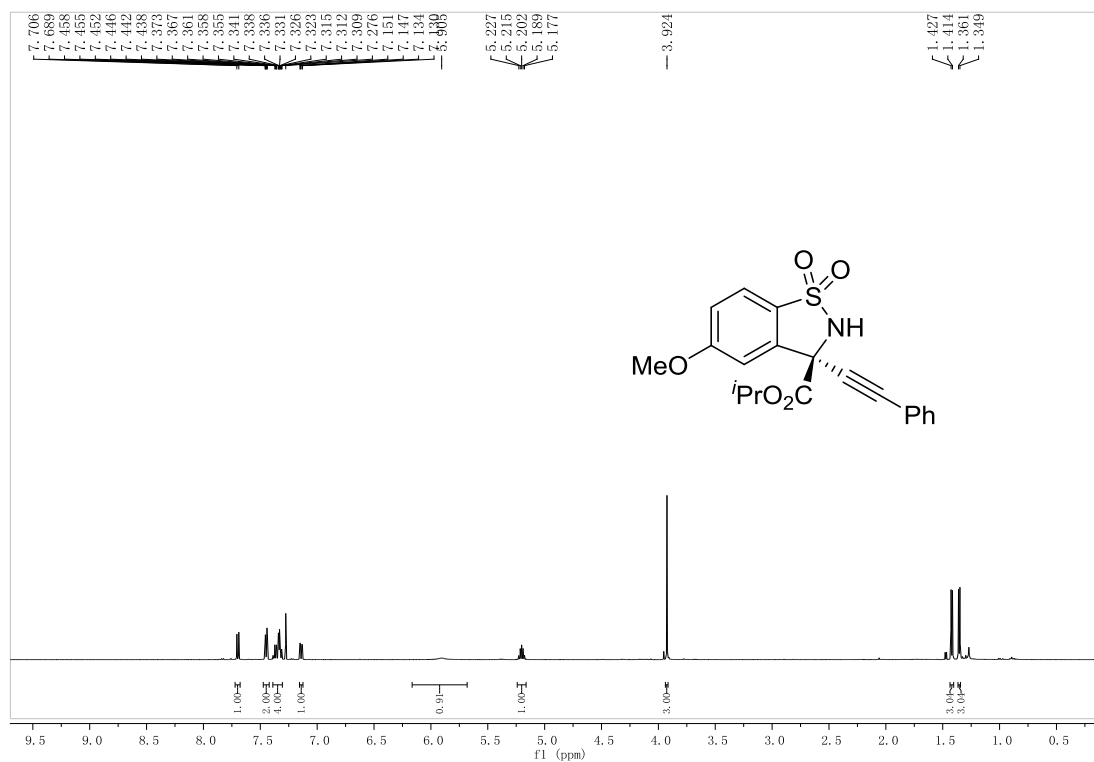


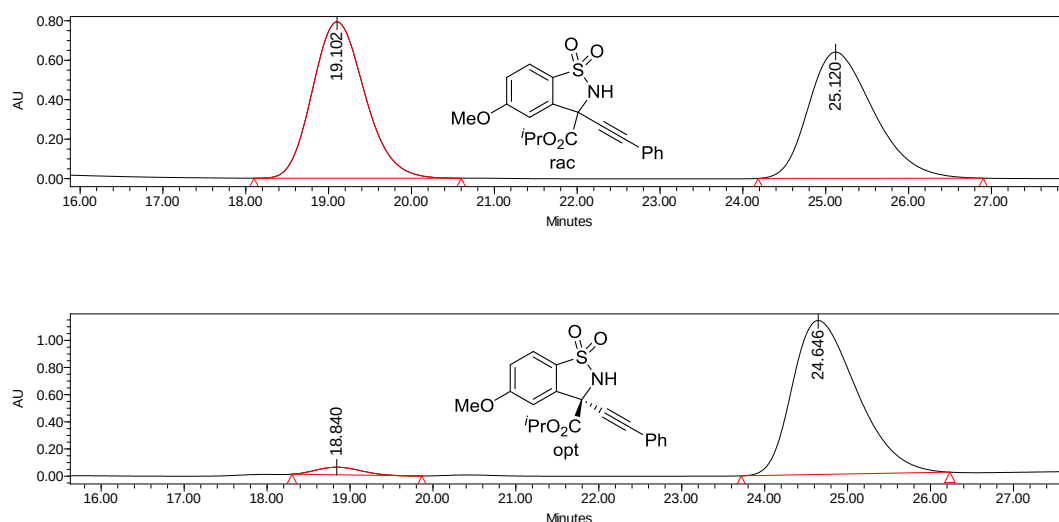
	Retention Time	Area	% Area	Height	% Height
1	19.484	2424614	3.46	57404	6.40
2	37.728	67720899	96.54	839793	93.60

Isopropyl 5-methoxy-3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3ea**)



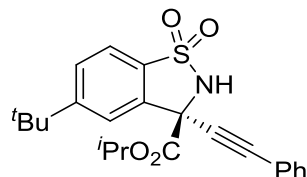
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 74% yield; $[\alpha]_D^{15} = 68.4$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 1.0 mL/min, 254 nm; $t_{\text{major}} = 24.6$ min, $t_{\text{minor}} = 18.8$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.70 (d, $J = 8.5$ Hz, 1H), 7.43-7.46 (m, 2H), 7.30-7.39 (m, 4H), 7.14 (dd, $J = 8.5, 2.0$ Hz, 1H), 5.91 (s, 1H), 5.20 (dt, $J = 12.5, 6.0$ Hz, 1H), 3.92 (s, 3H), 1.42 (d, $J = 6.5$ Hz, 3H), 1.35 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.2, 164.0, 138.6, 132.0, 129.3, 128.3, 126.4, 122.7, 121.2, 117.8, 109.9, 85.2, 84.4, 72.9, 61.5, 56.0, 21.47, 21.43; HRMS m/z (ESI $^+$): calculated for $\text{C}_{20}\text{H}_{20}\text{NO}_5\text{S}$ ($[\text{M}+\text{H}]^+$): 386.1057, found 386.1056.



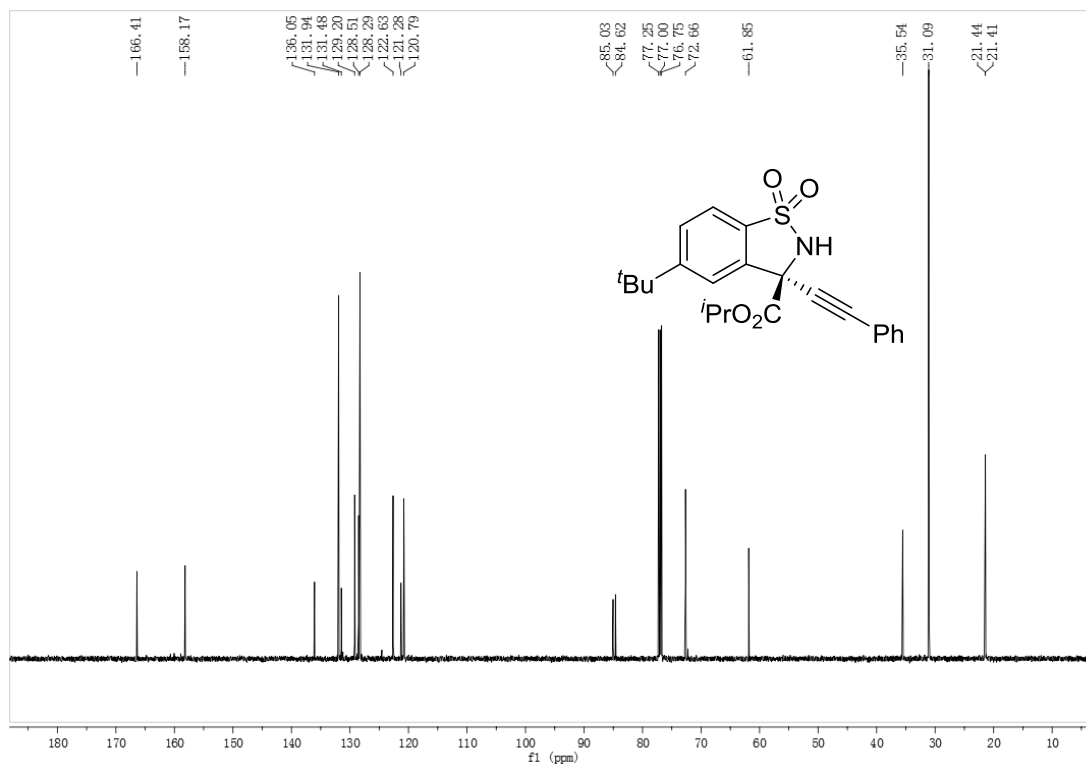
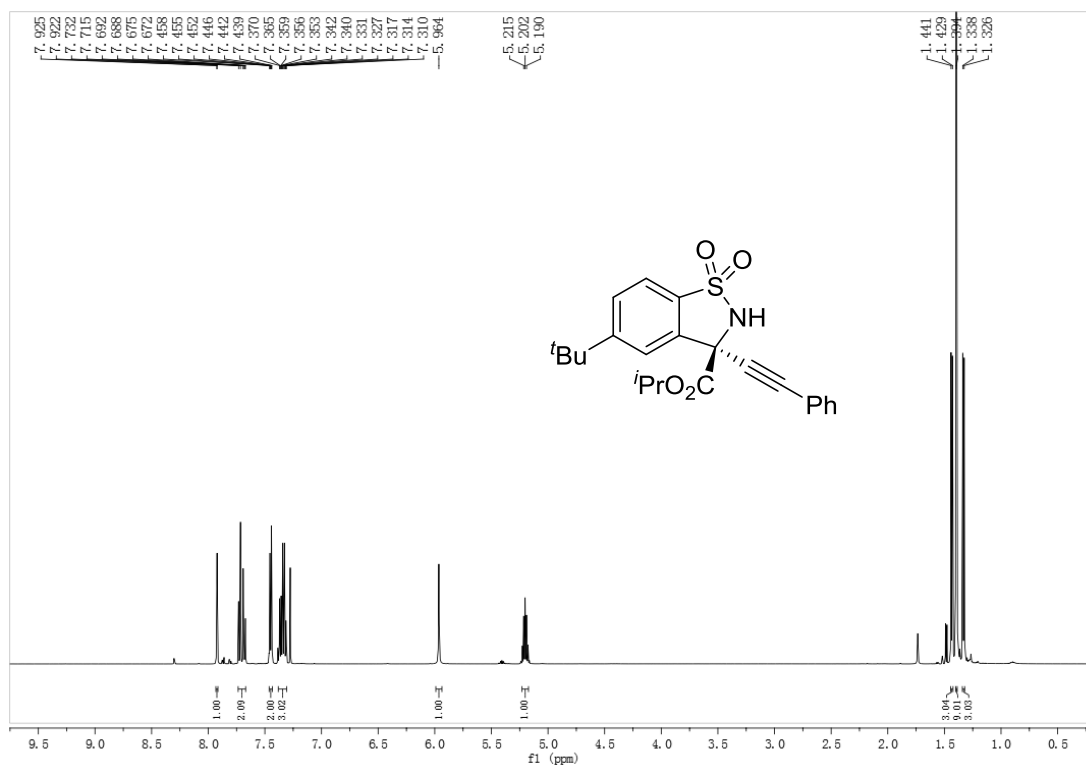


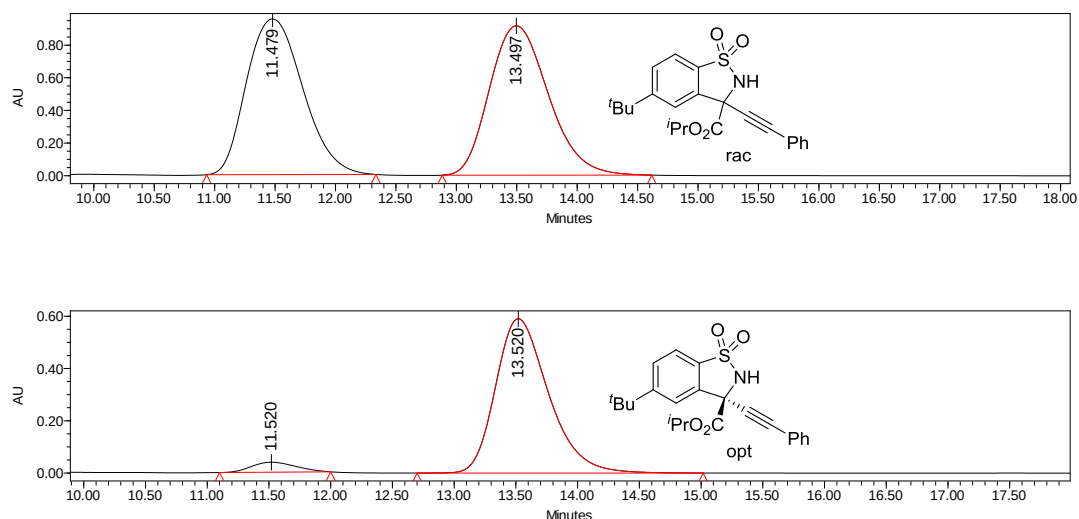
	Retention Time	Area	% Area	Height	% Height
1	18.840	2123618	3.35	56188	4.72
2	24.646	61279293	96.65	1134063	95.28

Isopropyl 5-(tert-butyl)-3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3fa**)



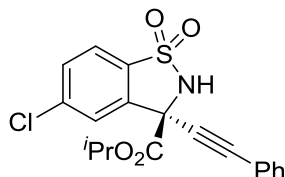
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 80% yield; $[\alpha]_D^{15} = 68.5$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 13.5$ min, $t_{\text{minor}} = 11.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 1.5$ Hz, 1H), 7.67-7.74 (m, 2H), 7.43-7.46 (m, 2H), 7.31-7.37 (m, 3H), 5.96 (s, 1H), 5.19-5.22 (m, 1H), 1.43 (d, $J = 6.0$ Hz, 3H), 1.39 (s, 9H), 1.33 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.4, 158.2, 136.1, 131.9, 131.5, 129.2, 128.5, 128.3, 122.6, 121.3, 120.8, 85.0, 84.6, 72.7, 61.9, 35.5, 31.1, 21.44, 21.41; HRMS m/z (ESI $^+$): calculated for $\text{C}_{23}\text{H}_{26}\text{NO}_4\text{S}$ ($[\text{M}+\text{NH}]^+$): 412.1577, found 412.1575.



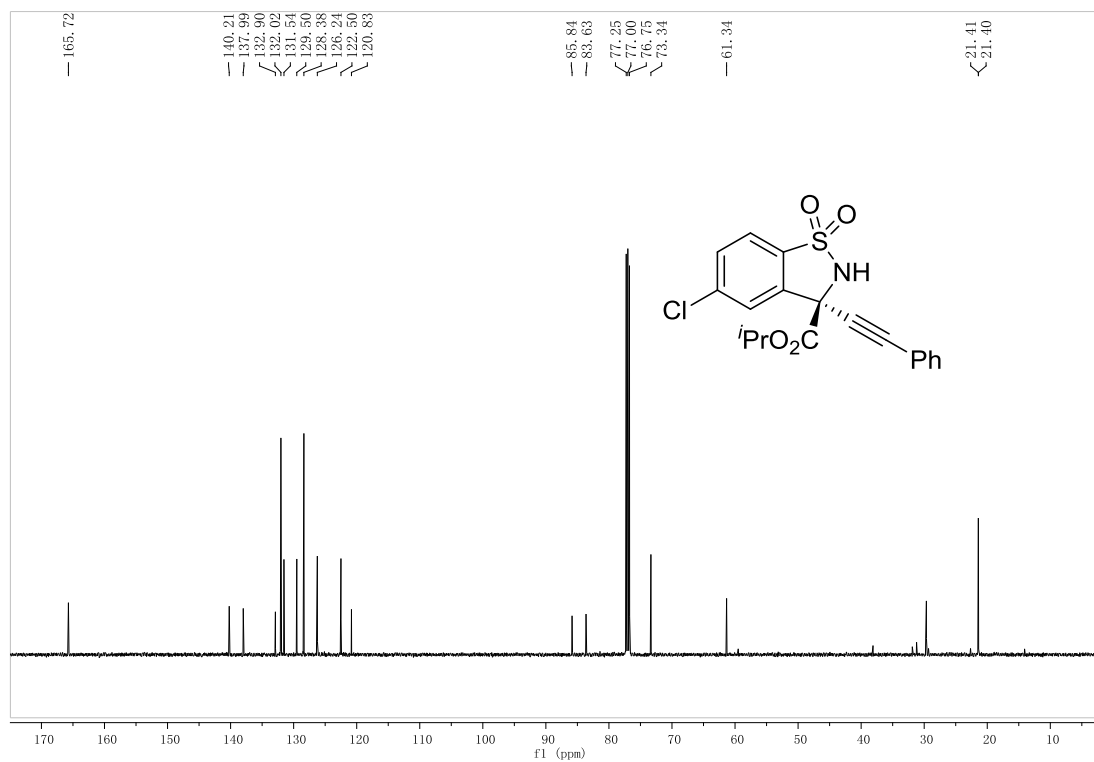
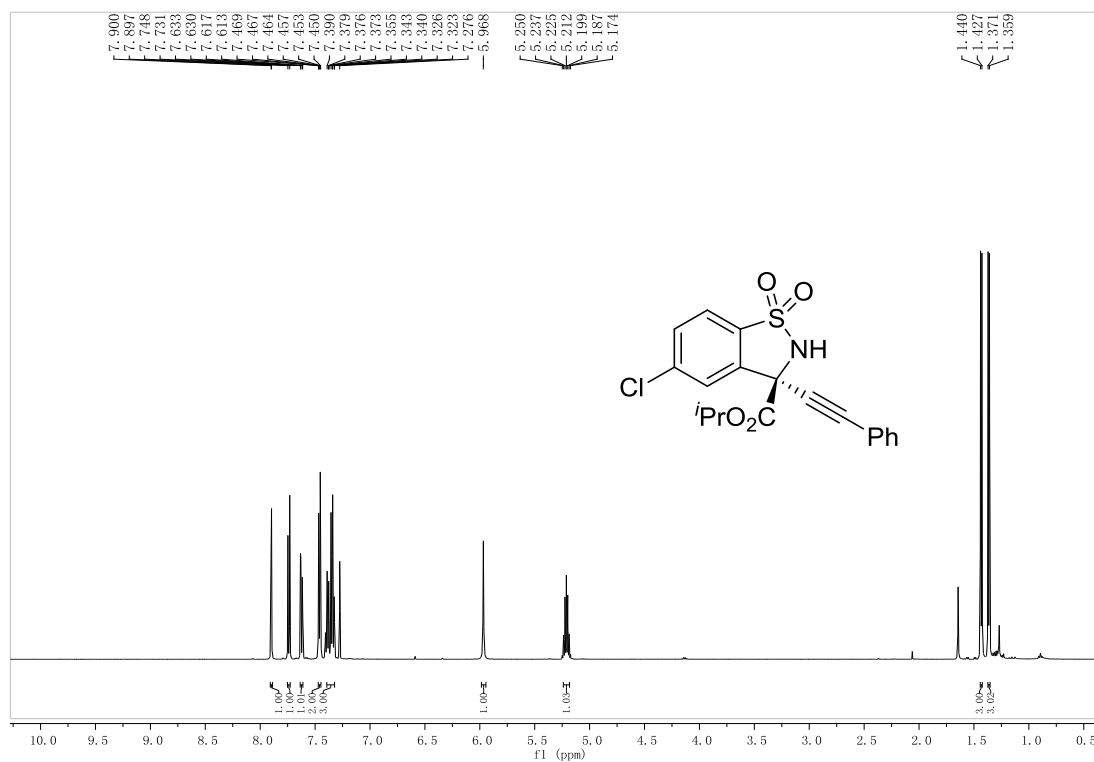


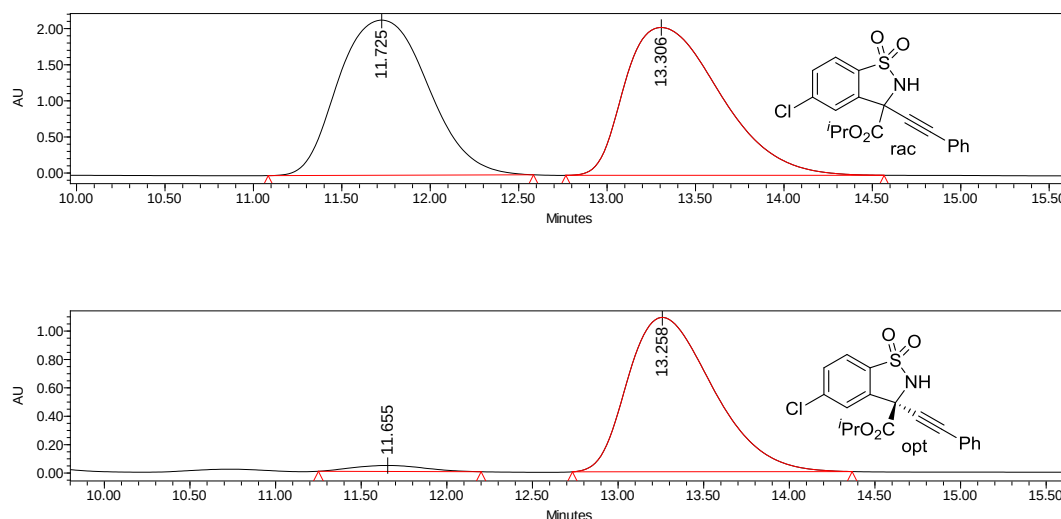
	Retention Time	Area	% Area	Height	% Height
1	11.520	953500	5.14	38192	6.07
2	13.520	17579314	94.86	590728	93.93

Isopropyl 5-chloro-3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3ga**)



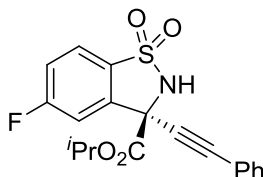
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 65% yield; $[\alpha]_D^{15} = 85.8$ ($c = 1.0$ in CH_2Cl_2), 94% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 1.0 mL/min, 254 nm; $t_{\text{major}} = 13.3$ min, $t_{\text{minor}} = 11.7$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.90 (d, $J = 1.5$ Hz, 1H), 7.74 (d, $J = 8.5$ Hz, 1H), 7.62 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.45-7.47 (m, 2H), 7.32-7.39 (m, 3H), 5.97 (s, 1H), 5.21 (dt, $J = 12.5, 6.5$ Hz, 1H), 1.43 (d, $J = 6.5$ Hz, 3H), 1.36 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 165.7, 140.2, 138.0, 132.9, 132.0, 131.5, 129.5, 128.4, 126.2, 122.5, 120.8, 85.8, 83.6, 73.3, 61.3, 21.41, 21.40; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{16}\text{ClNNaO}_4\text{S}$ ($[\text{M}+\text{Na}]^+$): 412.0381, found 412.0382.



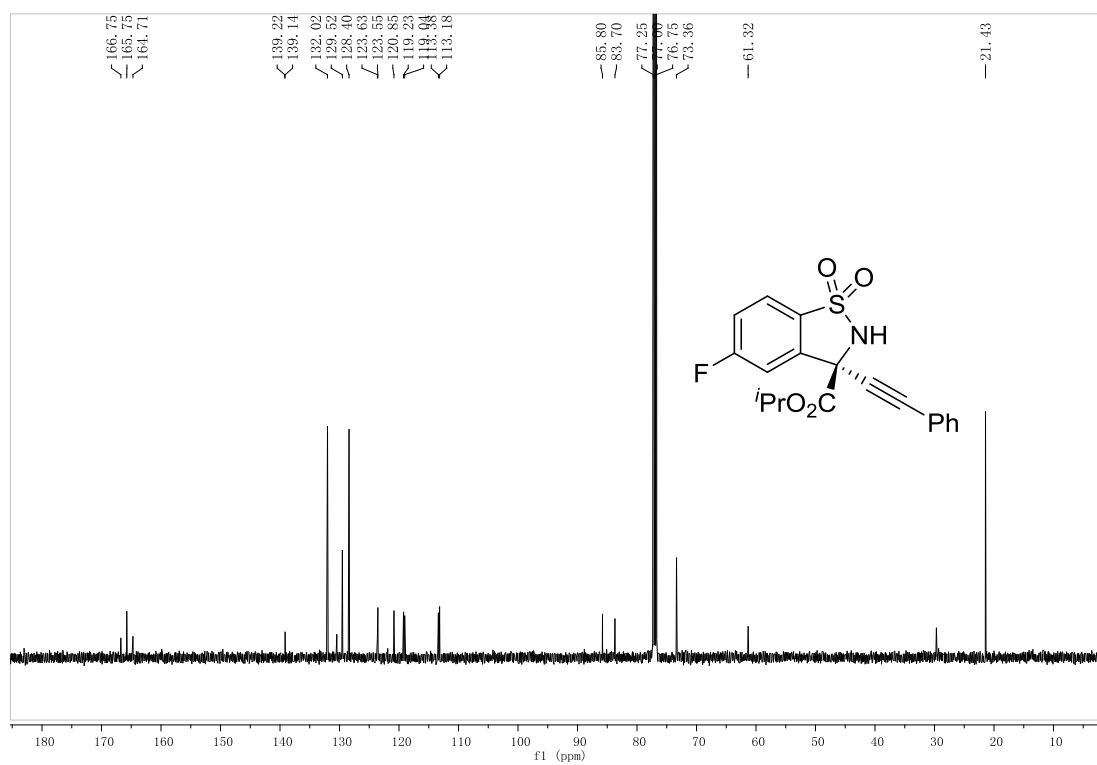
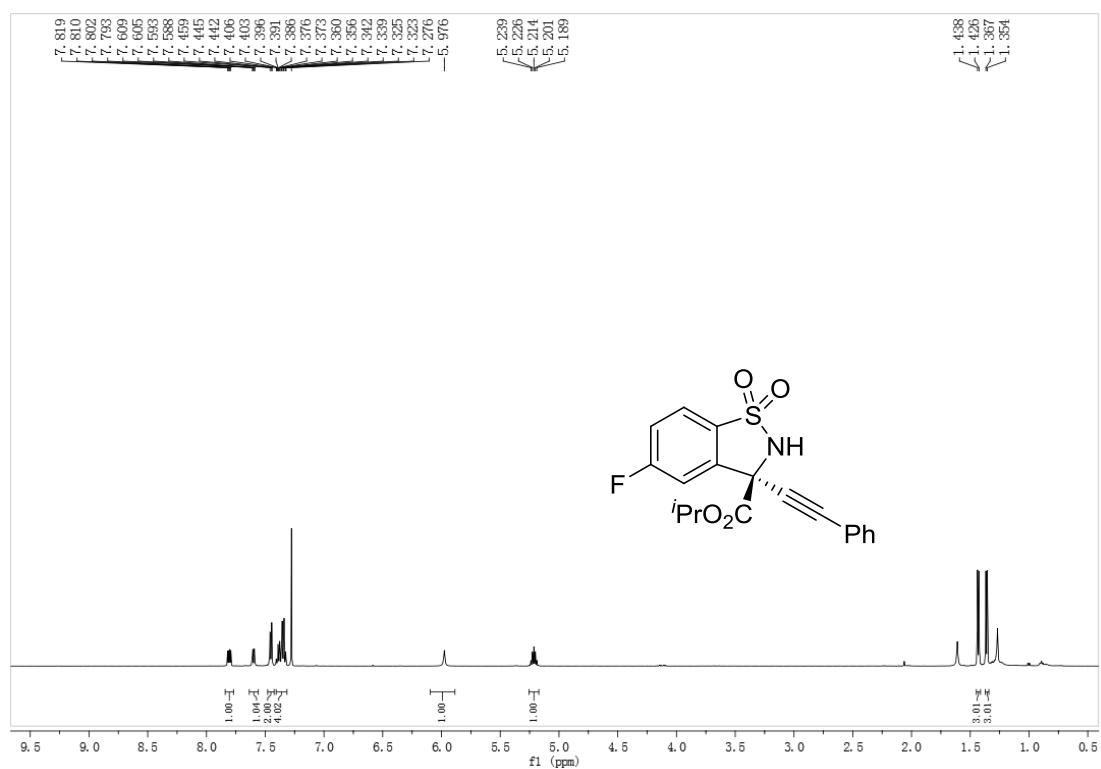


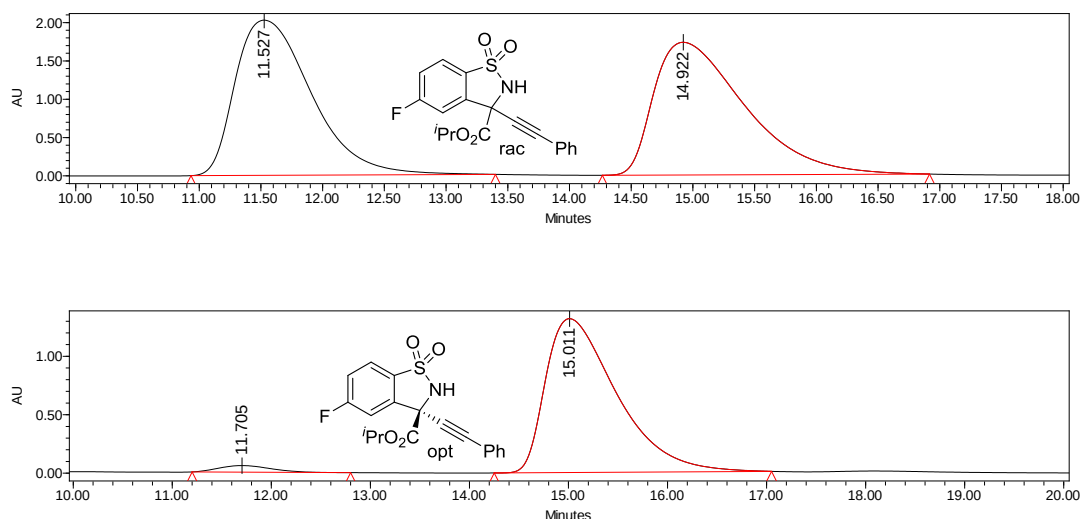
	Retention Time	Area	% Area	Height	% Height
1	11.655	1230568	3.16	42212	3.74
2	13.258	37713696	96.84	1087443	96.26

Isopropyl 5-fluoro-3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3hi**)



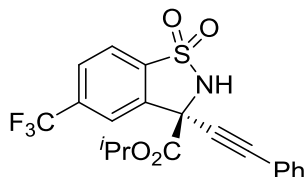
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 65% yield; $[\alpha]_D^{15} = 42.9$ ($c = 1.0$ in CH_2Cl_2), 94% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 15.0$ min, $t_{\text{minor}} = 11.7$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.81 (dd, $J = 8.5, 4.5$ Hz, 1H), 7.60 (dd, $J = 8.0, 2.0$ Hz, 1H), 7.44-7.46 (m, 2H), 7.32-7.41 (m, 4H), 5.98 (s, 1H), 5.21 (dt, $J = 12.5, 6.5$ Hz, 1H), 1.43 (d, $J = 6.0$ Hz, 3H), 1.36 (d, $J = 6.5$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3): δ 165.8, 165.7 (d, $J = 255.0$ Hz), 139.2 (d, $J = 10.0$ Hz), 132.0, 130.5 (d, $J = 3.8$ Hz), 129.5, 128.4, 123.6 (d, $J = 10.0$ Hz), 120.9, 119.1 (d, $J = 23.8$ Hz), 113.3 (d, $J = 25.0$ Hz), 85.8, 83.7, 73.4, 61.3, 21.4; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{16}\text{FNNaO}_4\text{S}$ ($[\text{M}+\text{Na}]^+$): 396.0676, found 396.0669.



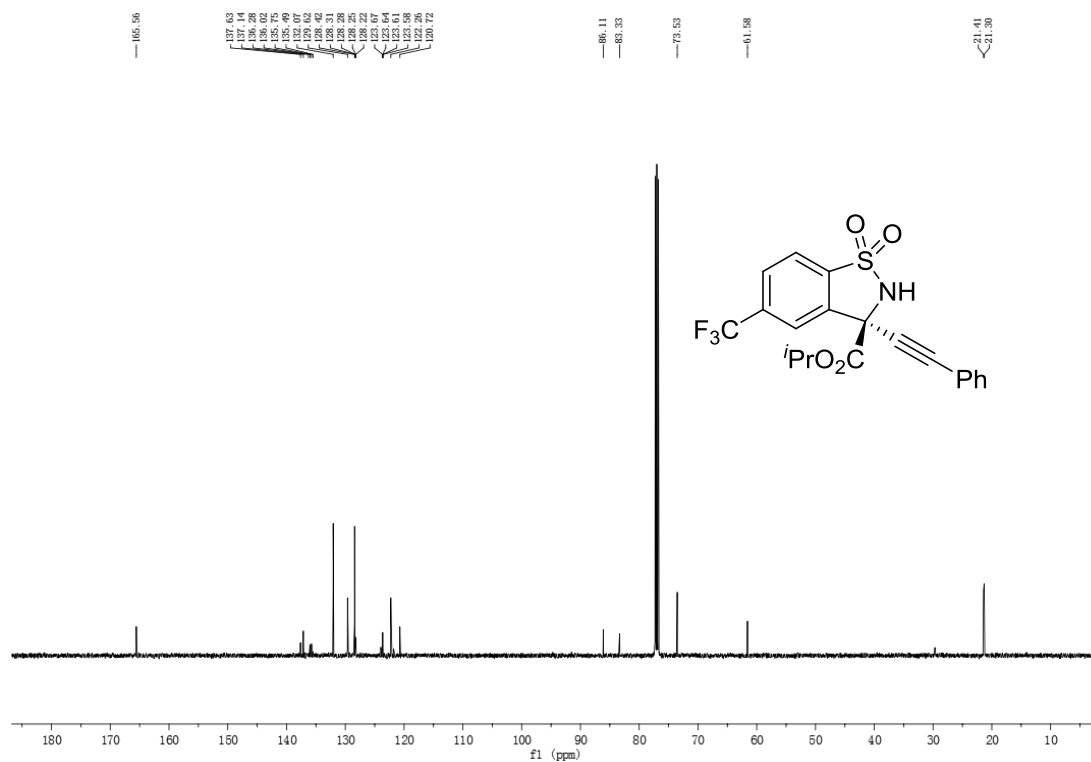
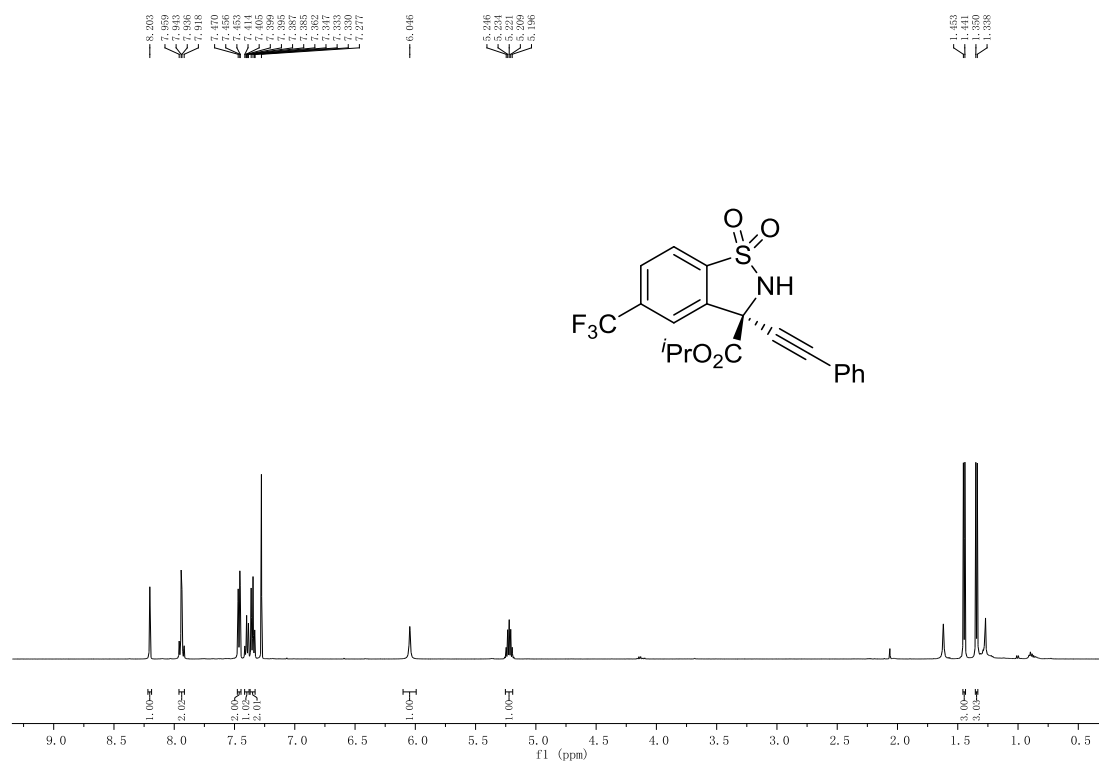


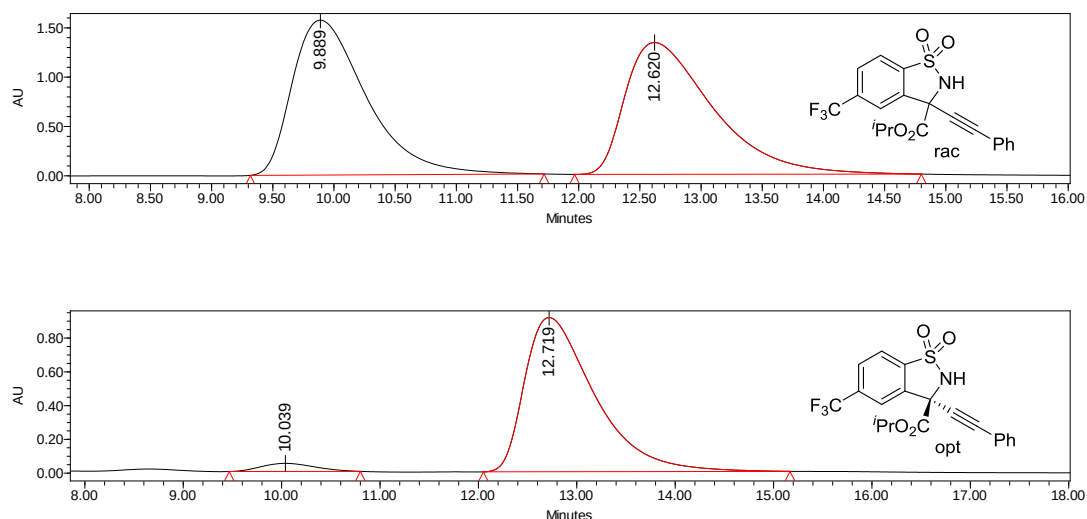
	Retention Time	Area	% Area	Height	% Height
1	11.705	2047139	3.03	56150	4.09
2	15.011	65581269	96.97	1316776	95.91

Isopropyl 3-(phenylethynyl)-5-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3ia**)



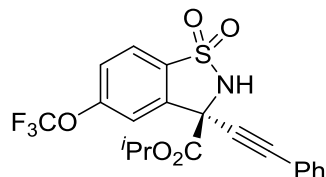
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 62% yield; $[\alpha]_{\text{D}}^{15} = 81.7$ ($c = 1.0$ in CH_2Cl_2), 92% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 12.7$ min, $t_{\text{minor}} = 10.0$ min]; ^1H NMR (500 MHz, CDCl_3): δ 8.20 (s, 1H), 7.91-7.96 (m, 2H), 7.44-7.47 (m, 2H), 7.38-7.42 (m, 1H), 7.32-7.37 (m, 2H), 6.05 (s, 1H), 5.22 (dt, $J = 12.5, 6.0$ Hz, 1H), 1.45 (d, $J = 6.0$ Hz, 3H), 1.34 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 165.6, 137.6, 137.1, 136.2 (q, $J = 32.5$ Hz), 132.1, 129.6, 128.4, 128.2 (q, $J = 3.8$ Hz), 123.6 (q, $J = 261.8$ Hz), 122.3, 120.7, 86.1, 83.3, 73.5, 61.6, 21.41, 21.30; HRMS m/z (ESI $^{+}$): calculated for $\text{C}_{20}\text{H}_{20}\text{F}_3\text{N}_2\text{O}_4\text{S}$ ($[\text{M}+\text{NH}_4]^{+}$): 441.1090, found 441.1095



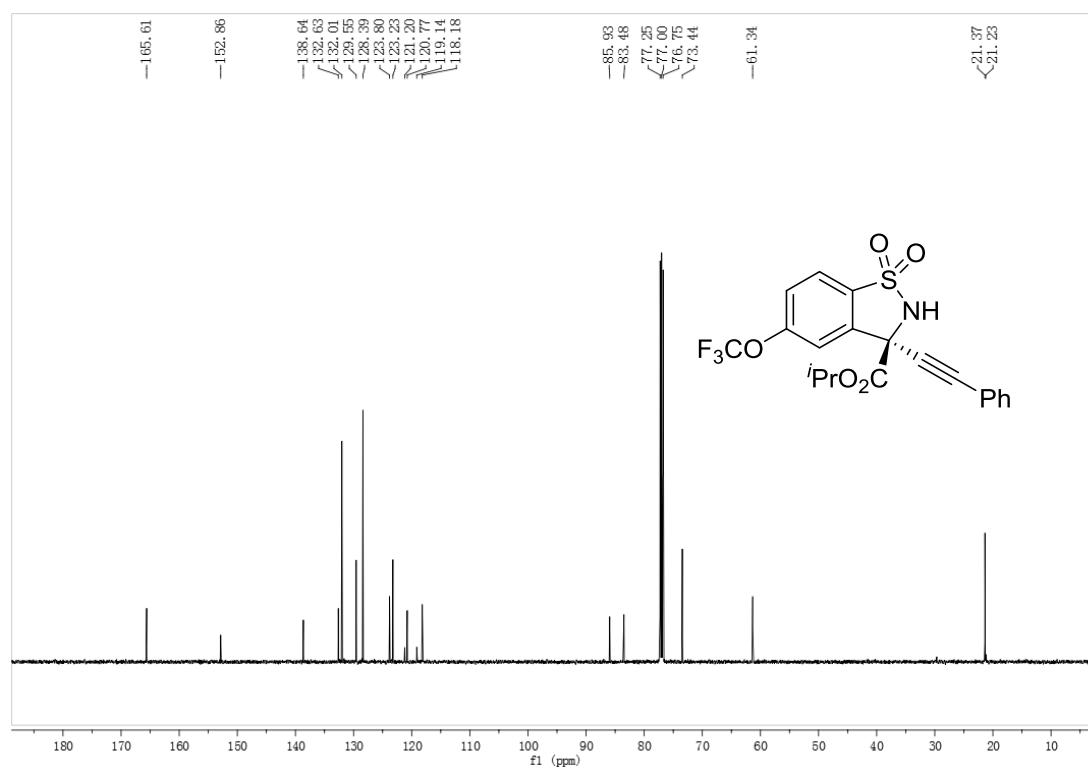
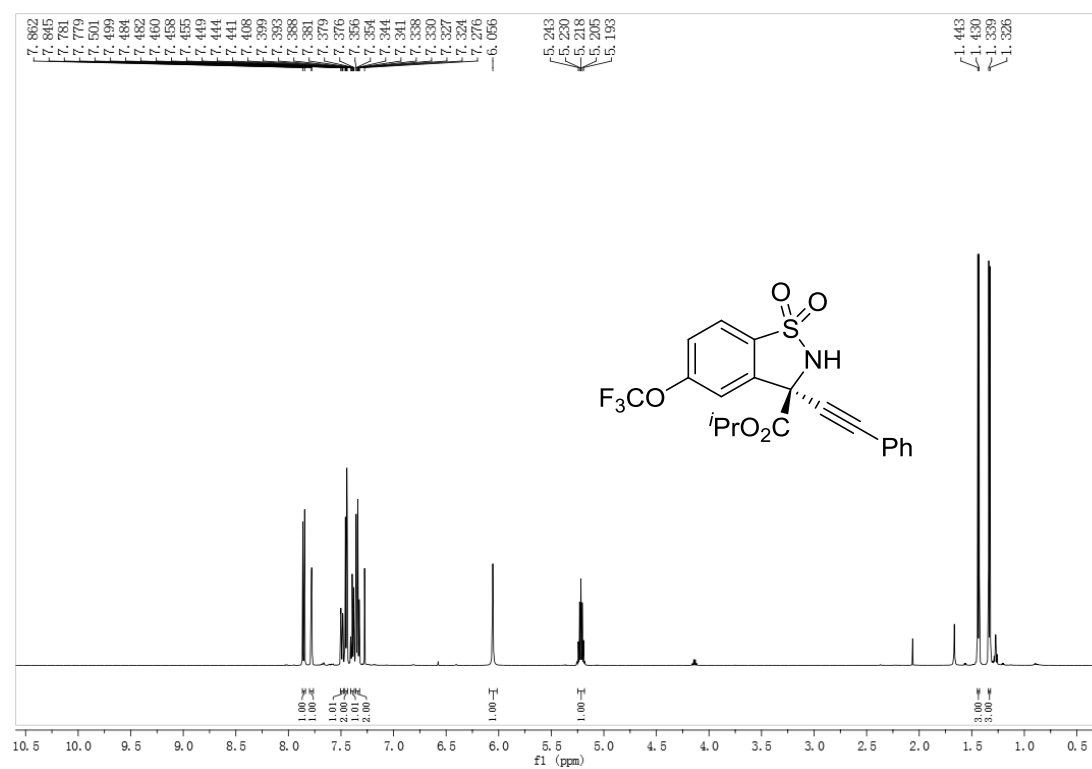


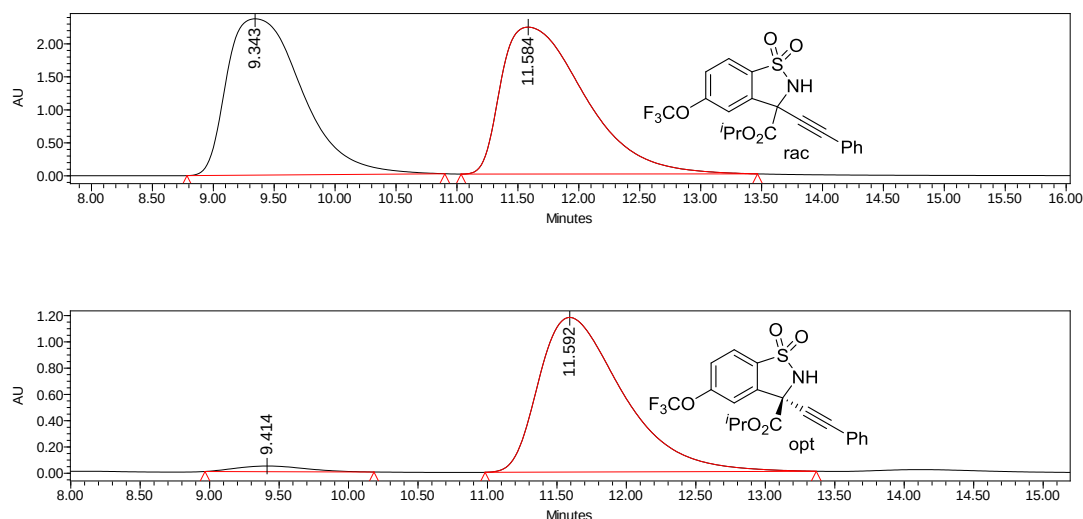
	Retention Time	Area	% Area	Height	% Height
1	10.039	1807811	3.86	47872	4.98
2	12.719	45079548	96.14	913424	95.02

Isopropyl 3-(phenylethynyl)-5-(trifluoromethoxy)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3ja**)



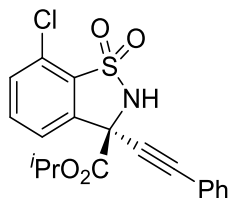
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 64% yield; $[\alpha]_{\text{D}}^{15} = 47.7$ ($c = 1.0$ in CH₂Cl₂), 94% ee [Daicel Chiralcel OD-H column (25 cm × 0.46 cm ID), *n*-hexane/*i*-PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 11.6$ min, $t_{\text{minor}} = 9.4$ min]; ¹H NMR (500 MHz, CDCl₃): δ 7.85 (d, $J = 8.5$ Hz, 1H), 7.78 (d, $J = 1.0$ Hz, 1H), 7.49 (dd, $J = 8.5, 1.0$ Hz, 1H), 7.44-7.46 (m, 2H), 7.37-7.41 (m, 1H), 7.32-7.36 (m, 2H), 6.06 (s, 1H), 5.19-5.25 (m, 1H), 1.44 (d, $J = 6.5$ Hz, 3H), 1.33 (d, $J = 6.5$ Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 165.6, 152.9, 138.6, 132.6, 132.0, 129.6, 128.4, 123.8, 123.2, 120.0 (q, $J = 257.5$ Hz), 120.8, 118.2, 85.9, 83.5, 73.4, 61.3, 21.37, 21.23; HRMS m/z (ESI⁺): calculated for C₂₀H₁₇F₃NO₅S ([M+H]⁺): 440.0774, found 440.0767.



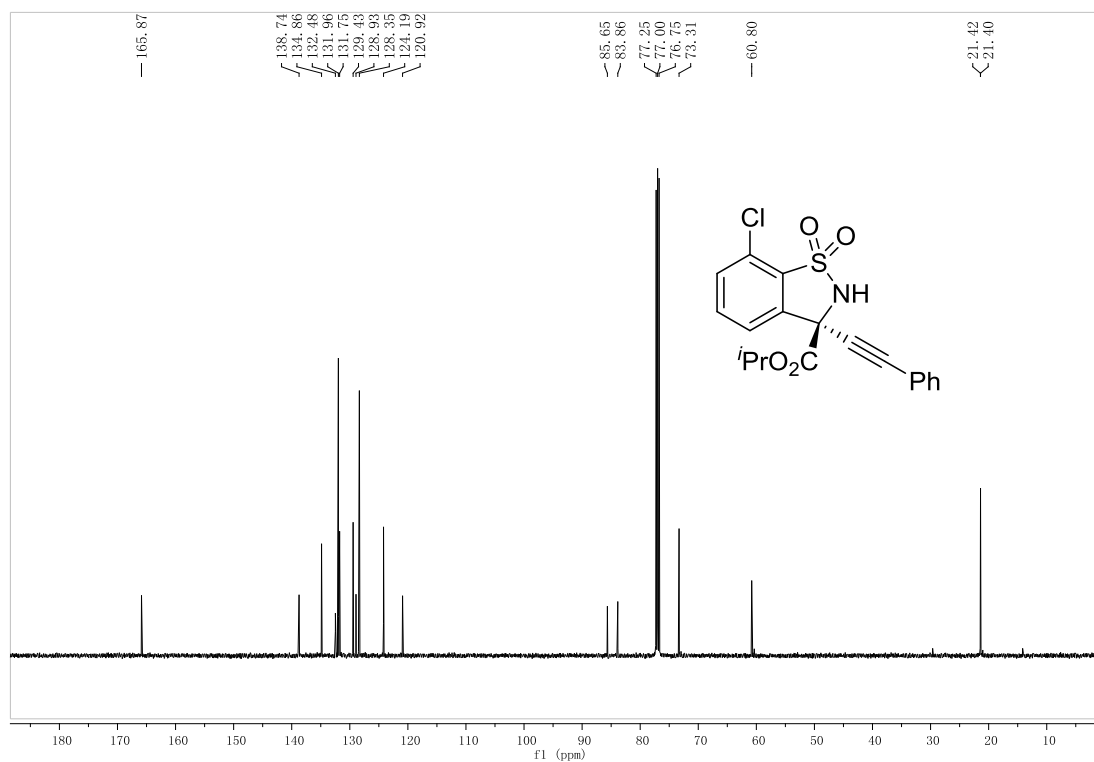
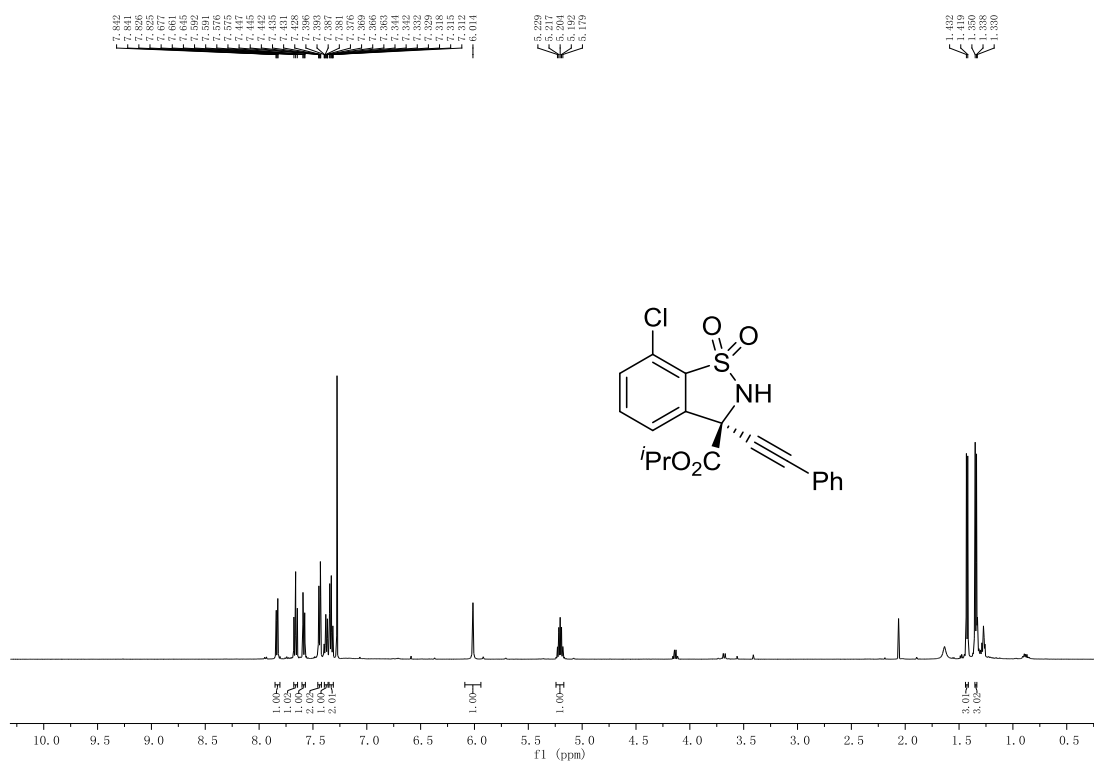


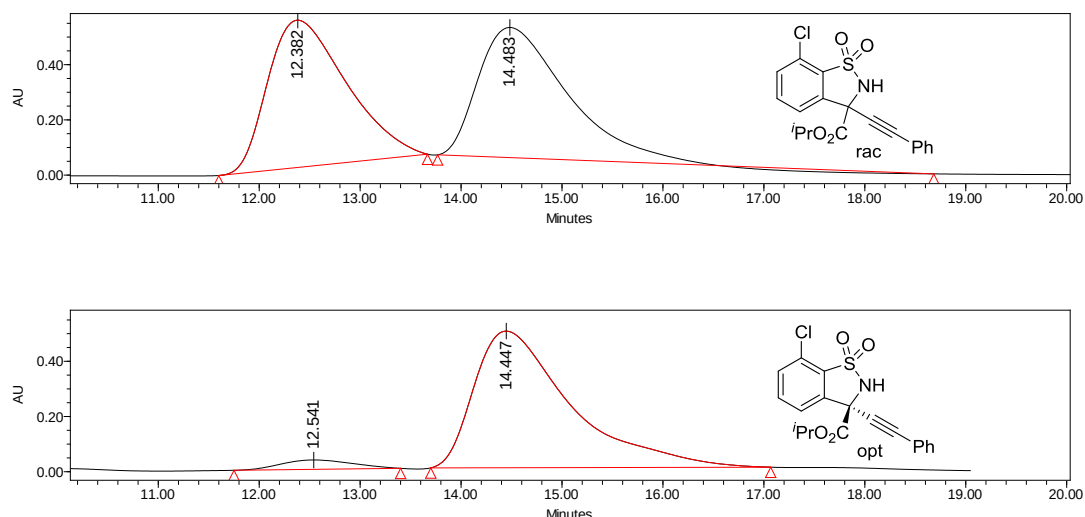
	Retention Time	Area	% Area	Height	% Height
1	9.414	1480901	2.90	43065	3.53
2	11.592	49615404	97.10	1177248	96.47

Isopropyl 7-chloro-3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3ka**)



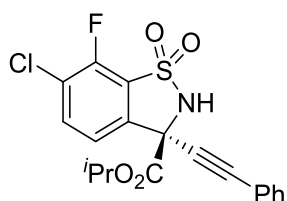
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 55% yield; $[\alpha]_D^{15} = -6.4$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 14.4$ min, $t_{\text{minor}} = 12.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.84 (dd, $J = 8.0, 0.5$ Hz, 1H), 7.66 (t, $J = 8.0$ Hz, 1H), 7.58 (dd, $J = 8.0, 0.5$ Hz, 1H), 7.42-7.45 (m, 2H), 7.36-7.40 (m, 1H), 7.31-7.35 (m, 2H), 6.01 (s, 1H), 5.20 (dt, $J = 12.5, 6.0$ Hz, 1H), 1.42 (d, $J = 6.0$ Hz, 3H), 1.34 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 165.9, 138.7, 134.9, 132.5, 132.0, 131.8, 129.4, 128.9, 128.4, 124.2, 120.9, 85.7, 83.9, 73.3, 60.8, 21.42, 21.40; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{17}\text{ClINO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 390.0561, found 390.0561.



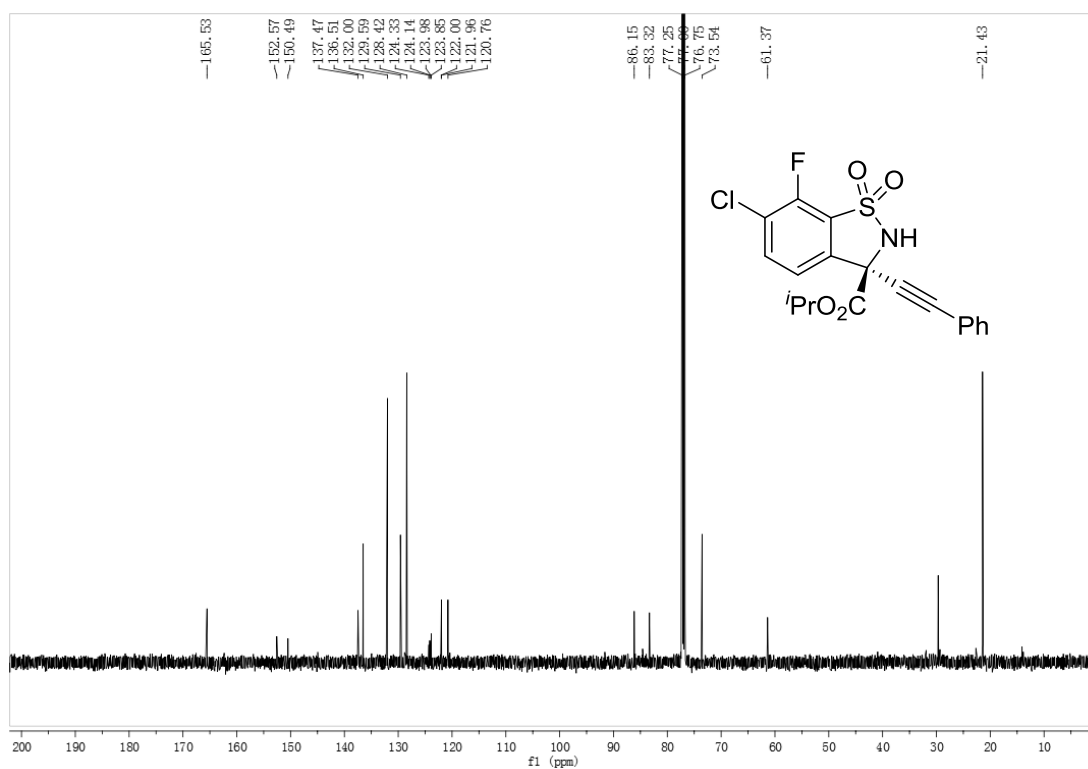
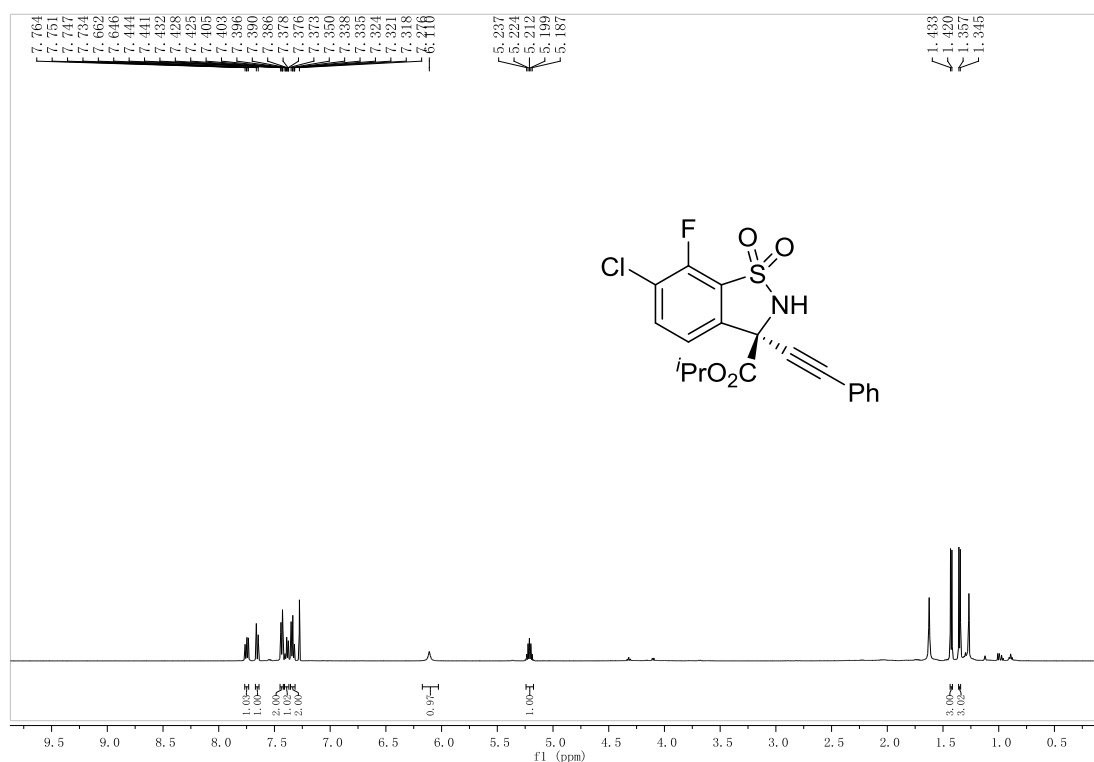


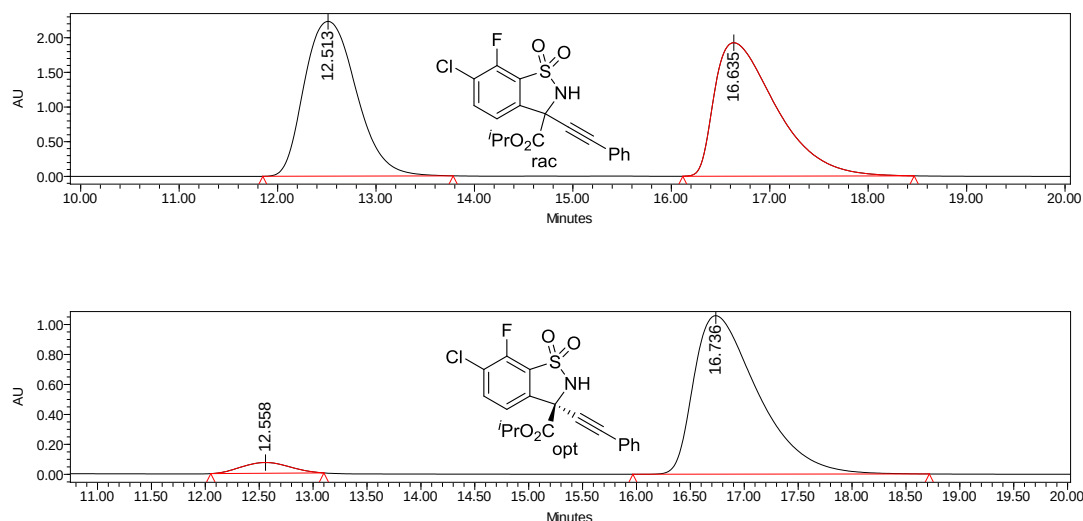
	Retention Time	Area	% Area	Height	% Height
1	12.541	1676384	4.87	34114	6.45
2	14.447	32747337	95.13	495036	93.55

Isopropyl 6-chloro-7-fluoro-3-(phenylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3la**)



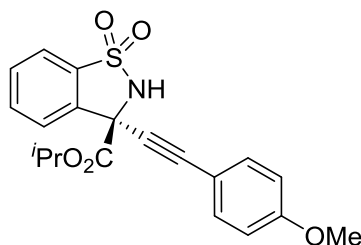
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 62% yield; $[\alpha]_D^{15} = 19.0$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 16.7$ min, $t_{\text{minor}} = 12.6$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.75 (dd, $J = 8.5, 6.5$ Hz, 1H), 7.65 (d, $J = 8.0$ Hz, 1H), 7.42-7.45 (m, 2H), 7.37-7.41 (m, 1H), 7.31-7.35 (m, 2H), 6.11 (s, 1H), 5.21 (dt, $J = 12.5, 6.5$ Hz, 1H), 1.43 (d, $J = 6.5$ Hz, 3H), 1.35 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 165.5, 151.5 (d, $J = 260.0$ Hz), 137.5, 136.5, 132.0, 129.6, 128.4, 124.2 (d, $J = 20.0$ Hz), 123.9 (d, $J = 16.3$ Hz), 122.0 (d, $J = 5.0$ Hz), 120.8, 86.2, 83.3, 73.5, 61.4, 21.4; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{19}\text{ClFN}_2\text{O}_4\text{S}$ ($[\text{M}+\text{NH}_4]^+$): 425.0733, found 425.0744.



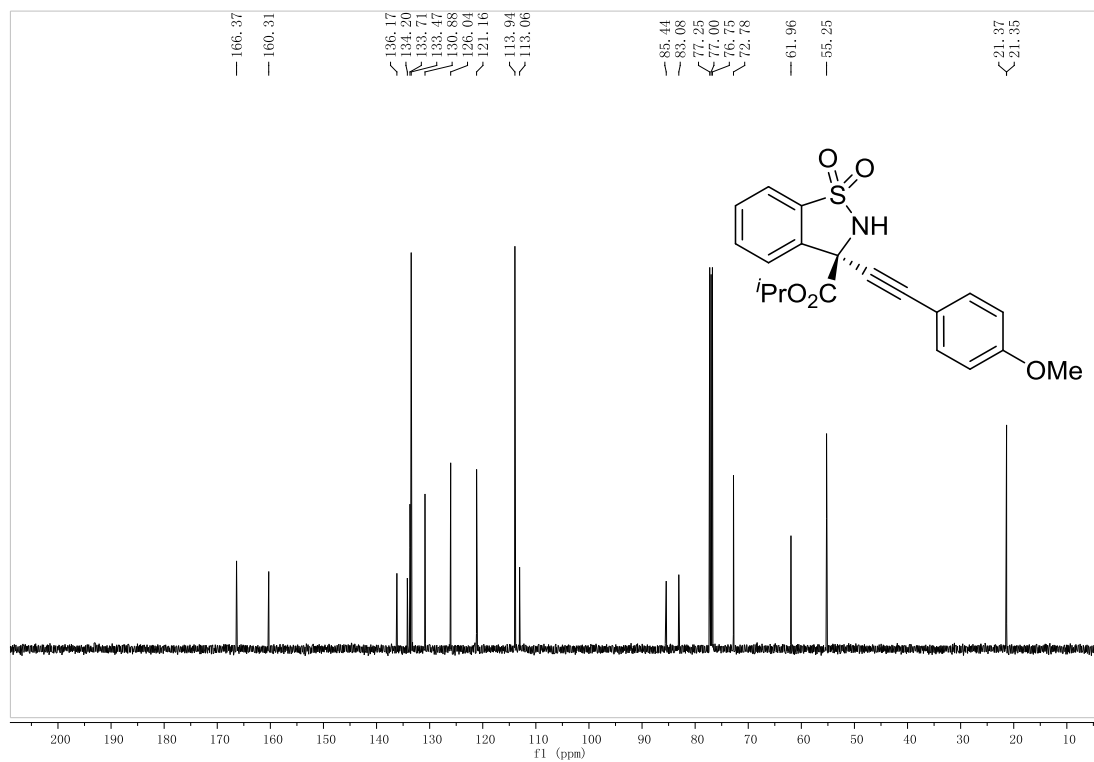
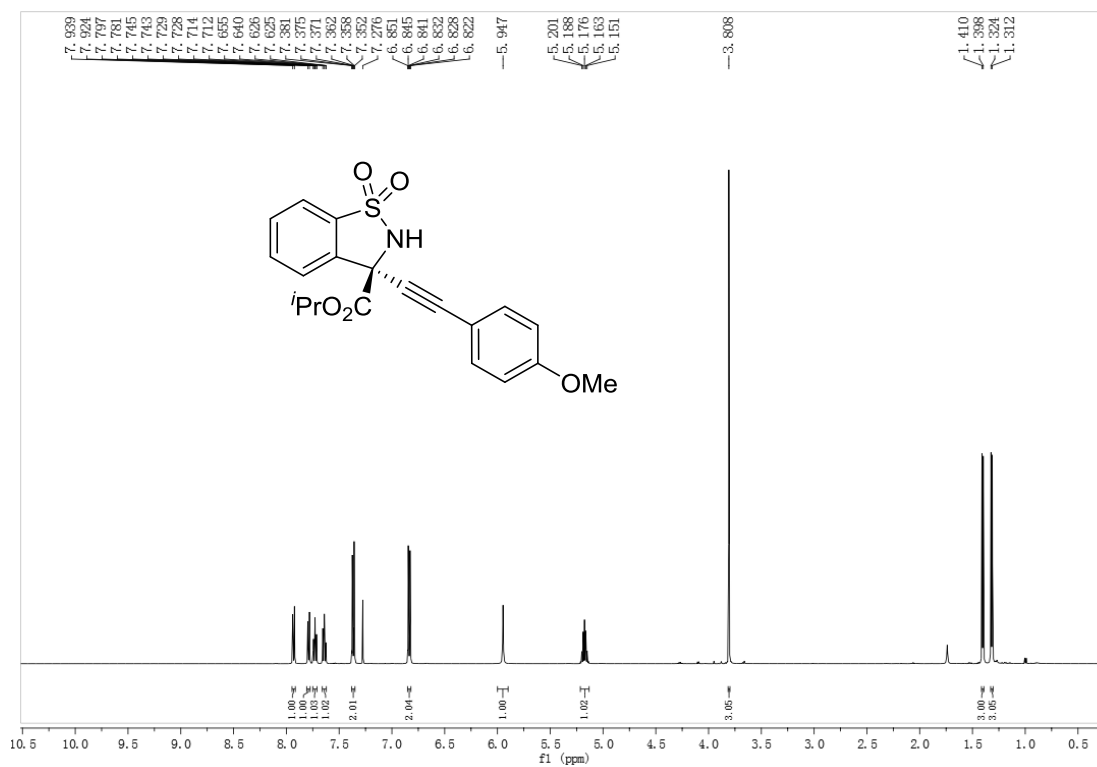


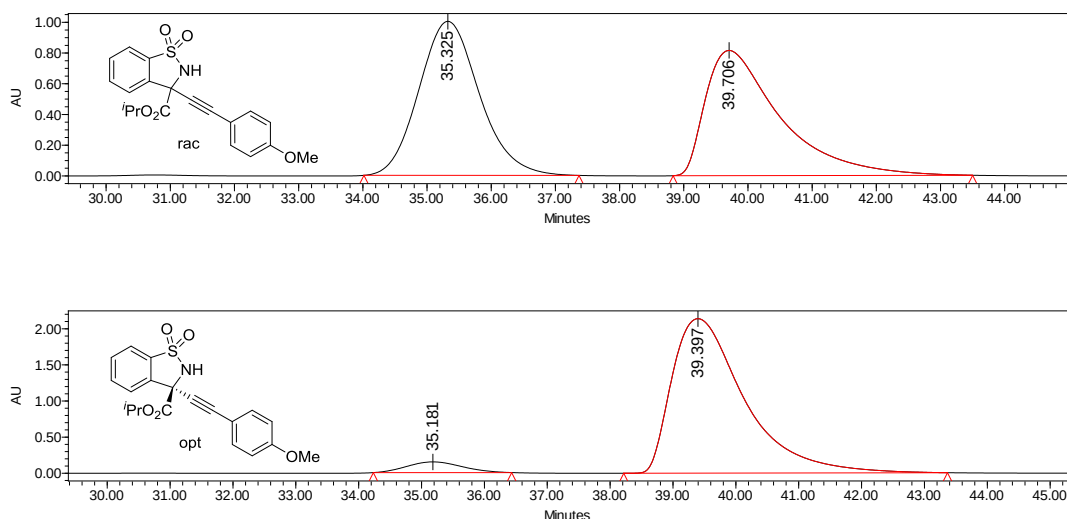
	Retention Time	Area	% Area	Height	% Height
1	12.558	2252335	4.89	72069	6.38
2	16.736	43776900	95.11	1057678	93.62

Isopropyl 3-((4-methoxyphenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bb**)



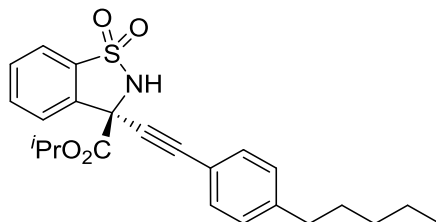
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 80% yield; $[\alpha]_D^{15} = 18.7$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 39.4$ min, $t_{\text{minor}} = 35.2$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.93 (d, $J = 7.5$ Hz, 1H), 7.79 (d, $J = 8.0$ Hz, 1H), 7.73 (td, $J = 8.0, 1.0$ Hz, 1H), 7.62-7.66 (m, 1H), 7.35-7.39 (m, 2H), 6.82-6.86 (m, 2H), 5.95 (s, 1H), 5.15-5.21 (m, 1H), 3.81 (s, 3H), 1.40 (d, $J = 6.0$ Hz, 3H), 1.32 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.4, 160.3, 136.2, 134.2, 133.7, 133.5, 130.9, 126.0, 121.2, 113.9, 113.1, 85.4, 83.1, 72.8, 62.0, 55.3, 21.37, 21.35; HRMS m/z (ESI $^+$): calculated for $\text{C}_{20}\text{H}_{19}\text{NNaO}_5\text{S}$ ($[\text{M}+\text{Na}]^+$): 408.0876, found 408.0875.



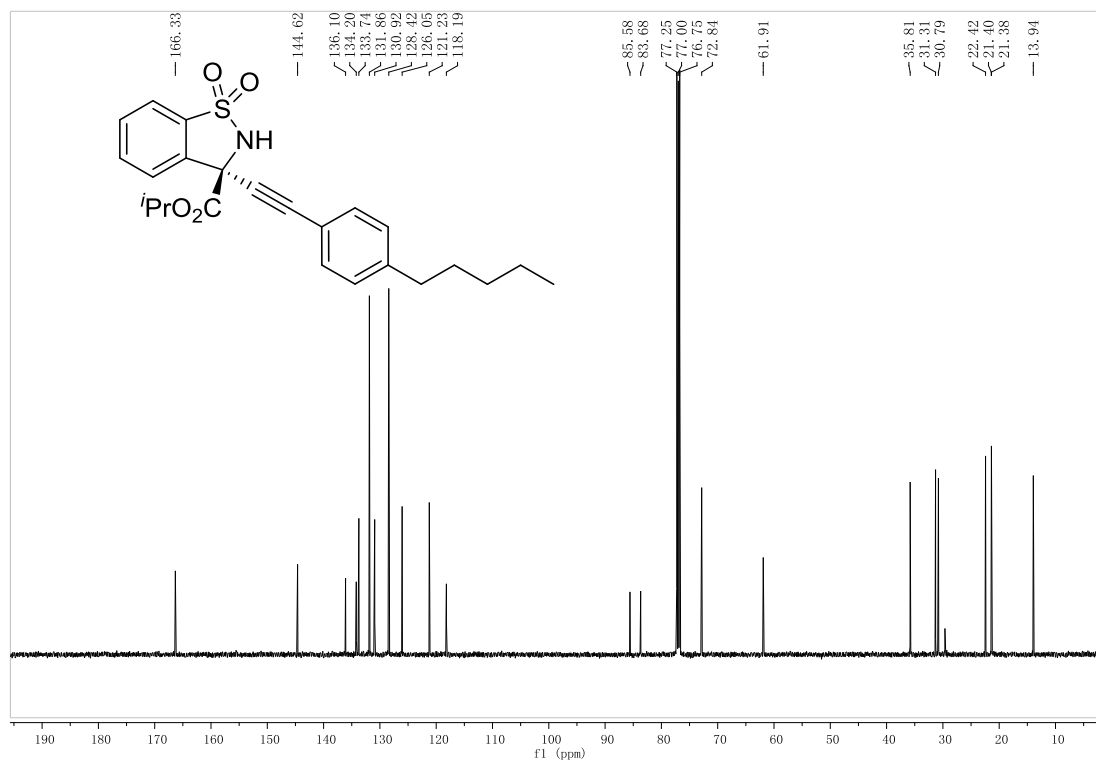
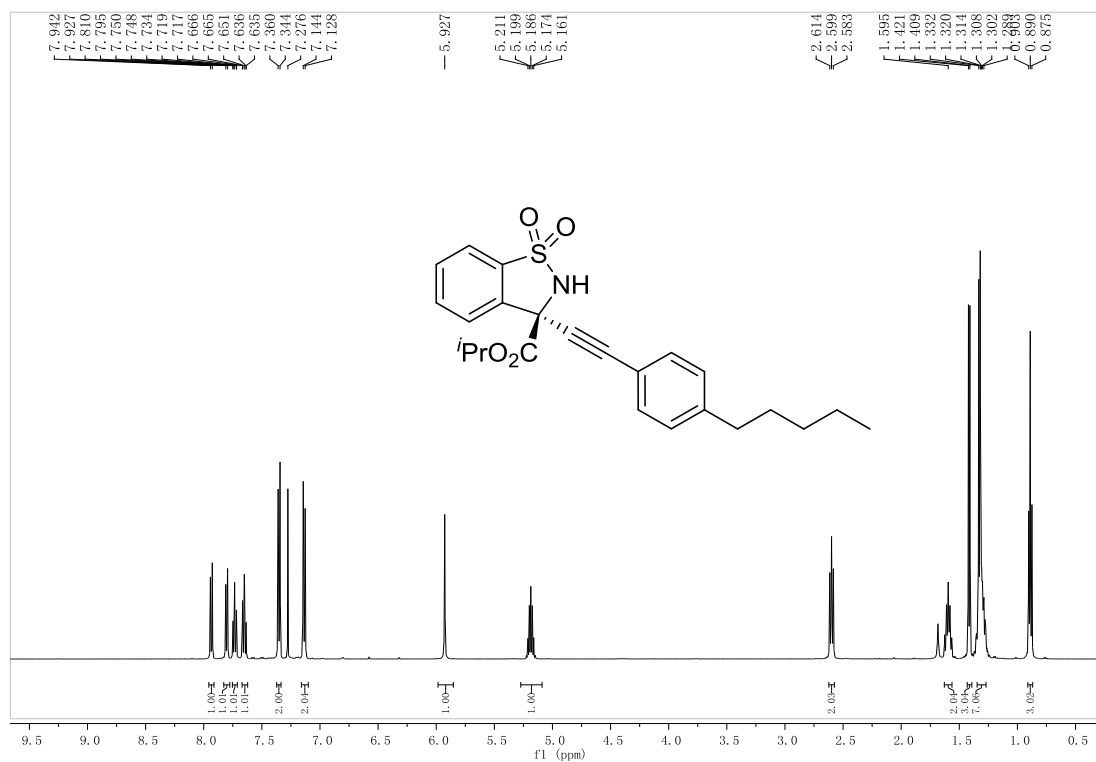


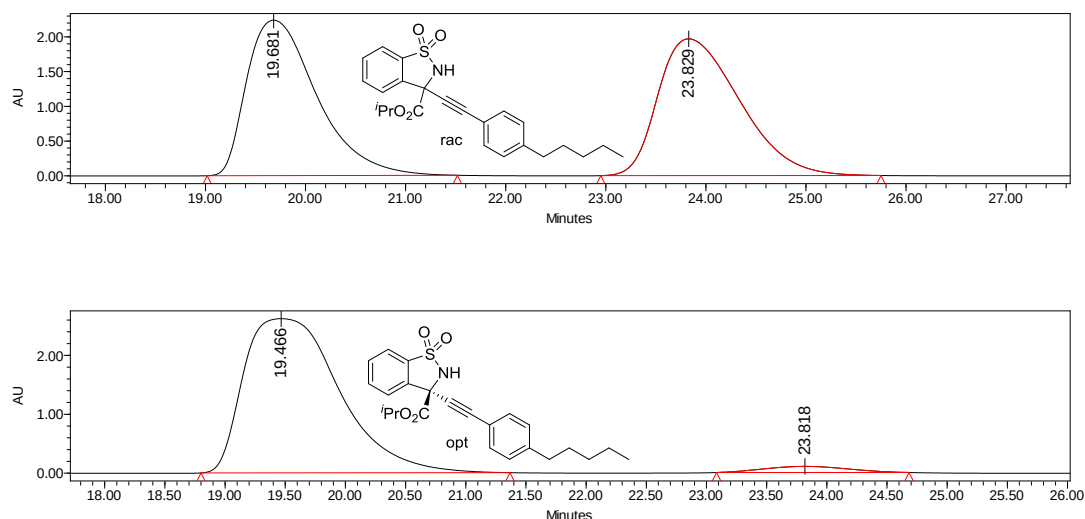
	Retention Time	Area	% Area	Height	% Height
1	35.181	9019755	5.00	148274	6.49
2	39.397	171297596	95.00	2137823	93.51

Isopropyl 3-((4-pentylphenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bc**)



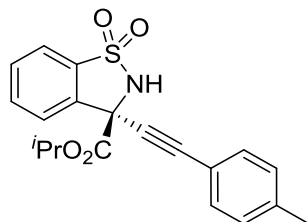
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 73% yield; $[\alpha]_D^{15} = 47.0$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 19.5$ min, $t_{\text{minor}} = 23.8$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.93 (d, $J = 7.5$ Hz, 1H), 7.80 (d, $J = 7.5$ Hz, 1H), 7.71-7.75 (m, 1H), 7.63-7.67 (m, 1H), 7.35 (d, $J = 8.0$ Hz, 2H), 7.14 (d, $J = 8.0$ Hz, 2H), 5.93 (s, 1H), 5.19 (dt, $J = 12.5, 6.0$ Hz, 1H), 2.58-2.62 (m, 2H), 1.60 (dt, $J = 15.5, 8.0$ Hz, 2H), 1.41 (d, $J = 6.0$ Hz, 3H), 1.28-1.34 (m, 7H), 0.89 (t, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.3, 144.6, 136.1, 134.2, 133.7, 131.9, 130.9, 128.4, 126.1, 121.2, 118.2, 85.6, 83.7, 72.8, 61.9, 35.8, 31.3, 30.8, 22.4, 21.40, 21.38, 13.9; HRMS m/z (ESI $^+$): calculated for $\text{C}_{24}\text{H}_{31}\text{N}_2\text{O}_4\text{S}$ ($[\text{M}+\text{NH}_4]^+$): 443.1999, found 443.2001.





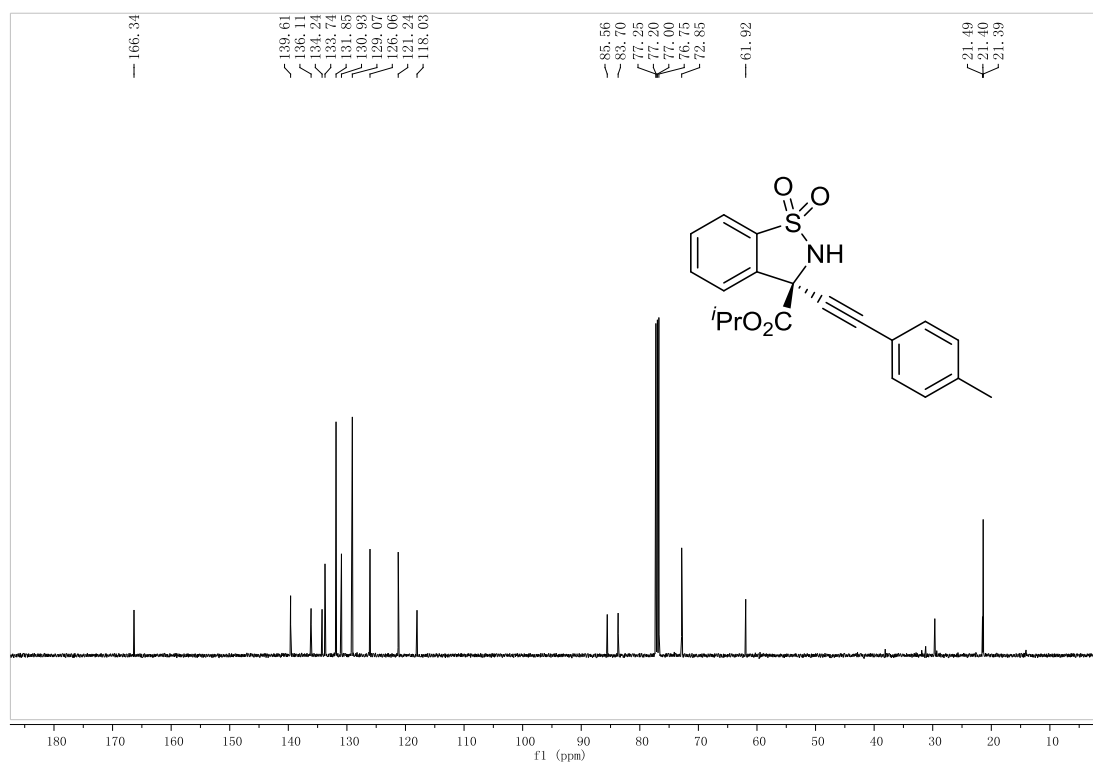
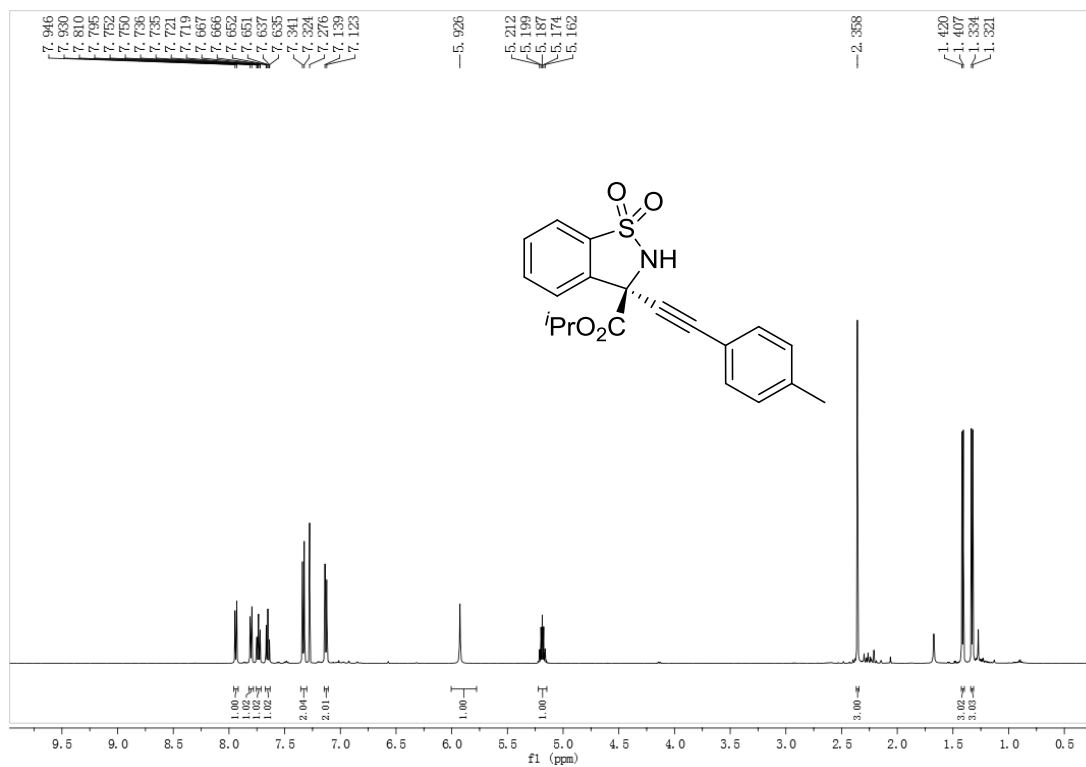
	Retention Time	Area	% Area	Height	% Height
1	19.466	144934408	96.63	2618647	96.18
2	23.818	5052267	3.37	104121	3.82

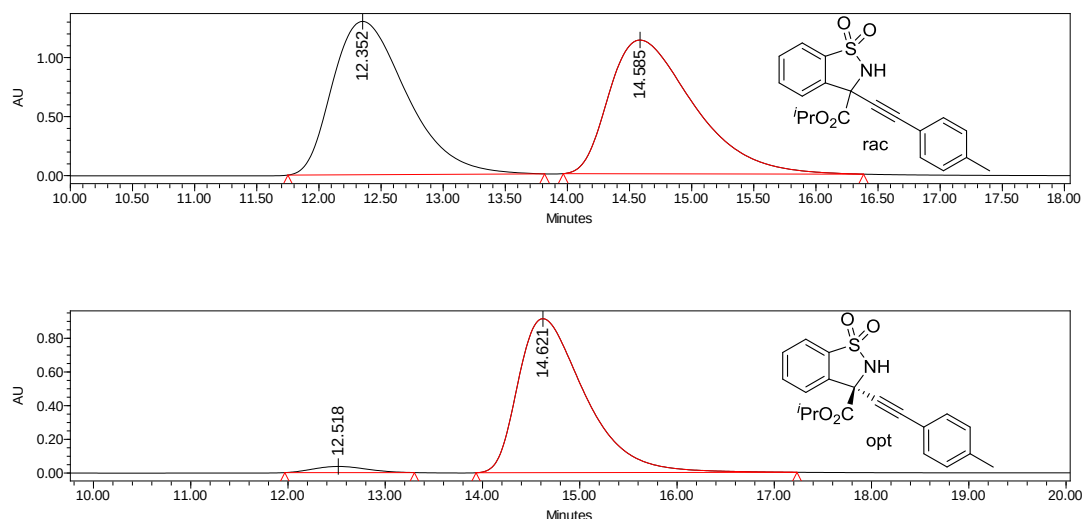
Isopropyl 3-(p-tolyethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bd**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 81% yield; $[\alpha]_{\text{D}}^{15} = 54.0$ ($c = 1.0$ in CH_2Cl_2), 94% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 14.6$ min, $t_{\text{minor}} = 12.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.94 (d, $J = 8.0$ Hz, 1H), 7.80 (d, $J = 7.5$ Hz, 1H), 7.74 (td, $J = 8.0, 1.0$ Hz, 1H), 7.65 (td, $J = 7.5, 0.5$ Hz, 1H), 7.33 (d, $J = 8.5$ Hz, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 5.93 (s, 1H), 5.19 (dt, $J = 12.5, 6.5$ Hz, 1H), 2.36 (s, 3H), 1.41 (d, $J = 6.5$ Hz, 3H), 1.33 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.3, 139.6, 136.1, 134.2, 133.7, 131.9, 130.9, 129.1,

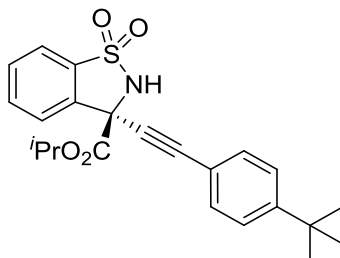
126.1, 121.2, 118.0, 85.6, 83.7, 72.9, 61.9, 21.5, 21.40, 21.39; HRMS m/z (ESI⁺):
calculated for C₂₀H₂₀NO₄S ([M+H]⁺): 370.1108, found 370.1096.





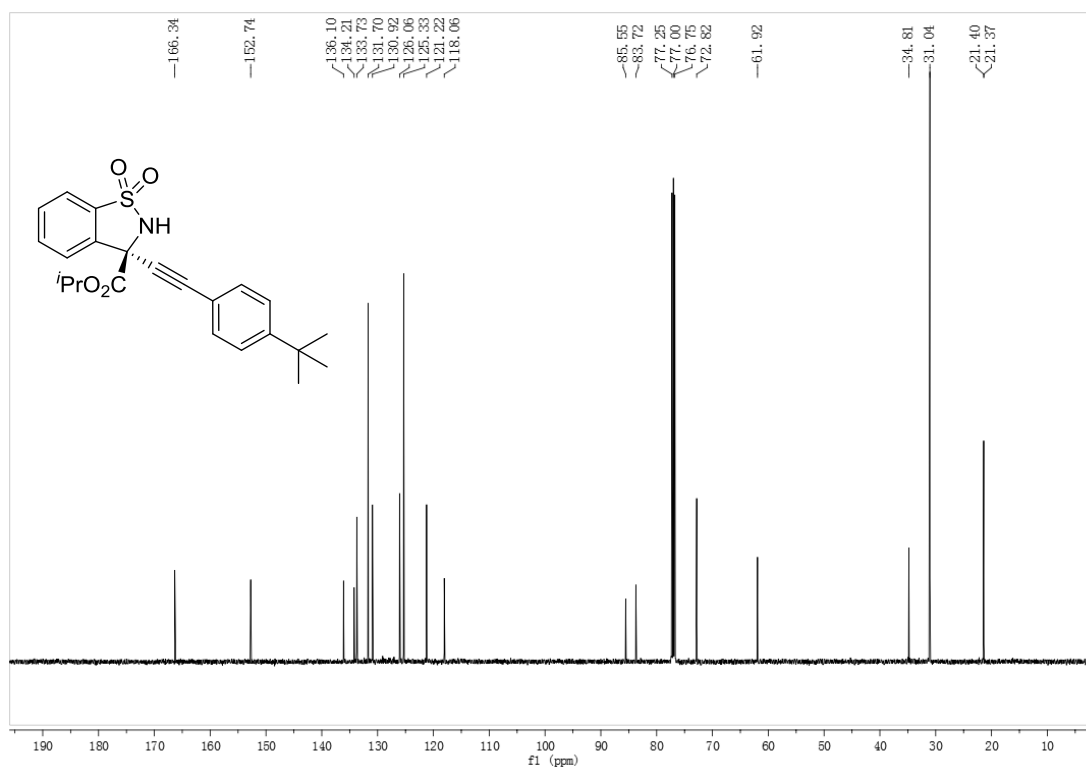
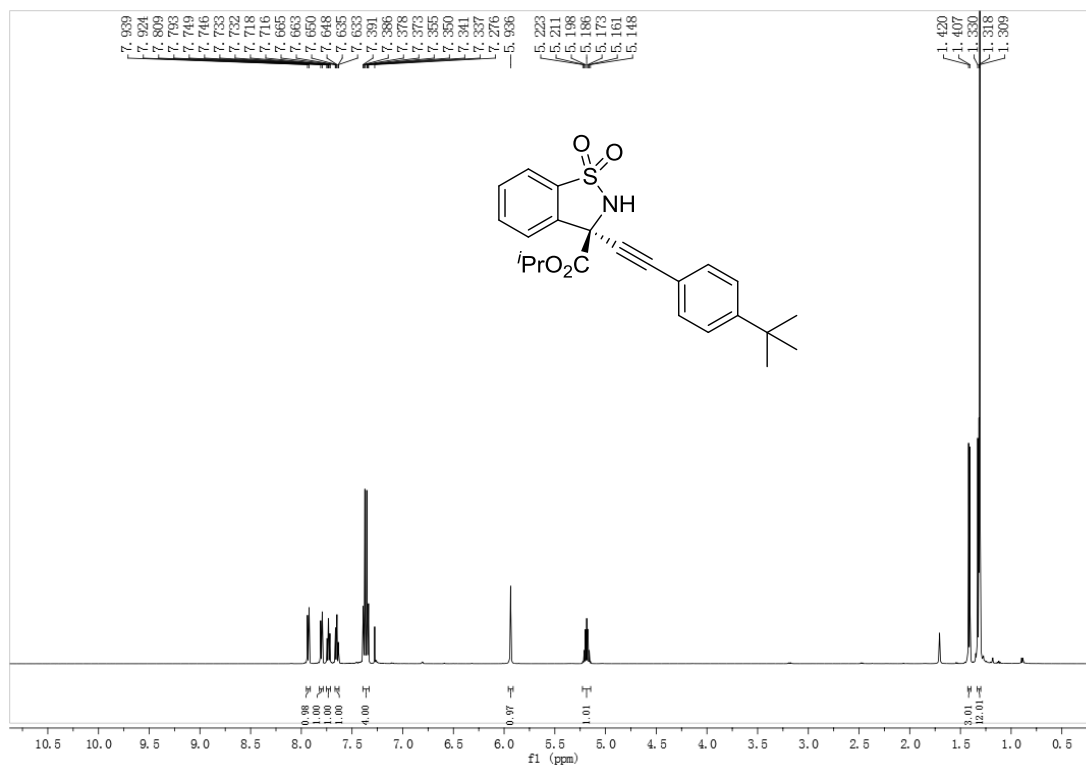
	Retention Time	Area	% Area	Height	% Height
1	12.518	1390595	3.08	36523	3.84
2	14.621	43729777	96.92	913899	96.16

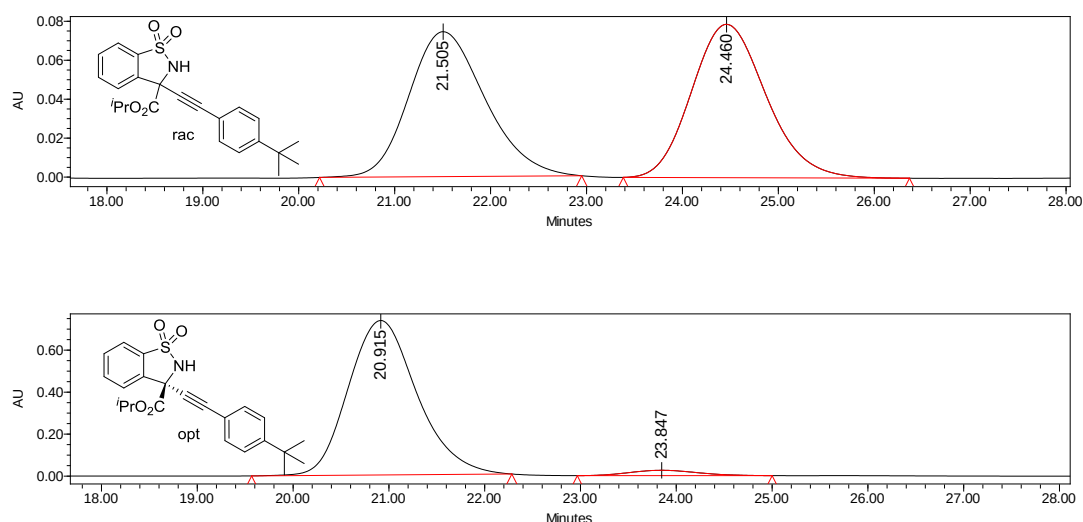
Isopropyl 3-((4-(tert-butyl)phenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3be**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 77% yield; $[\alpha]_D^{15} = 37.8$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 20.9$ min, $t_{\text{minor}} = 23.8$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.93 (d, $J = 7.5$ Hz, 1H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.73 (td, $J = 8.0, 1.5$ Hz, 1H), 7.65 (td, $J = 7.5, 1.0$ Hz, 1H), 7.33-7.40 (m, 4H), 5.94 (s, 1H), 5.19 (td, $J = 12.5, 6.5$ Hz, 1H), 1.41 (d, $J = 6.5$ Hz, 3H), 1.30-1.33 (m, 12H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.3, 152.7, 136.1, 134.2, 133.7, 131.7, 130.9, 126.1, 125.3, 121.2, 118.1, 85.6, 83.7, 72.8, 61.9,

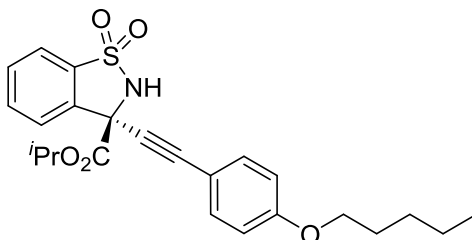
34.8, 31.0, 21.40, 21.37; HRMS m/z (ESI⁺): calculated for C₂₃H₂₆NO₄S ([M+H]⁺): 412.1577, found 412.1564.





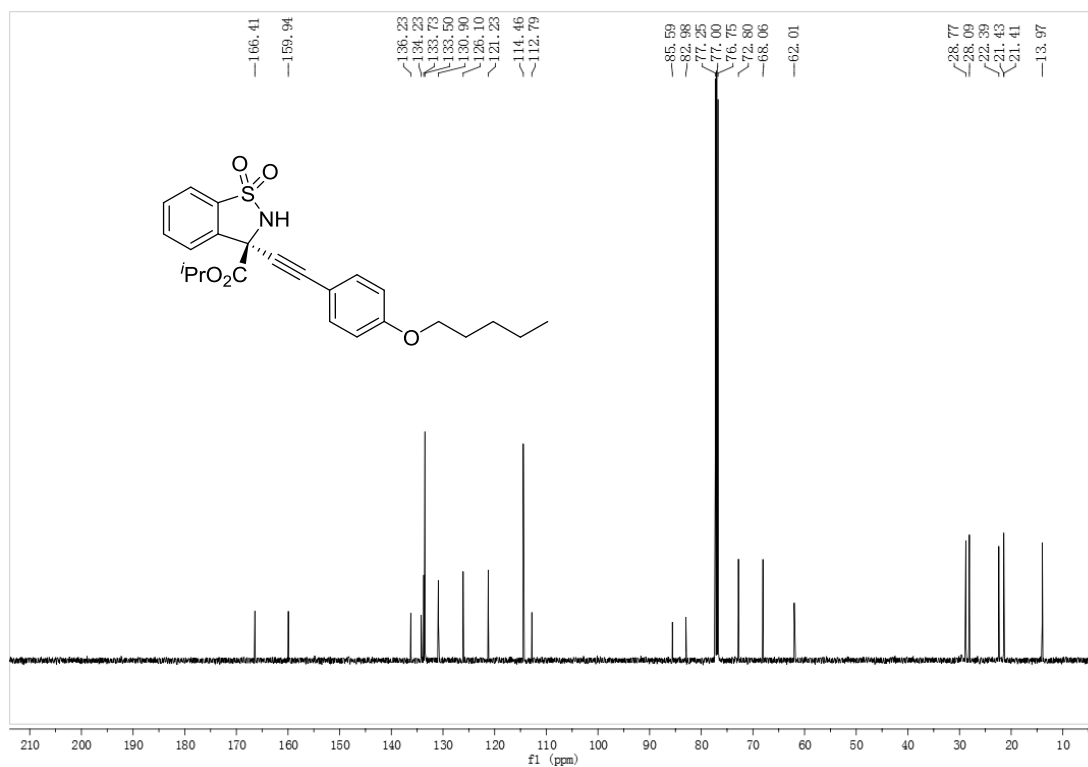
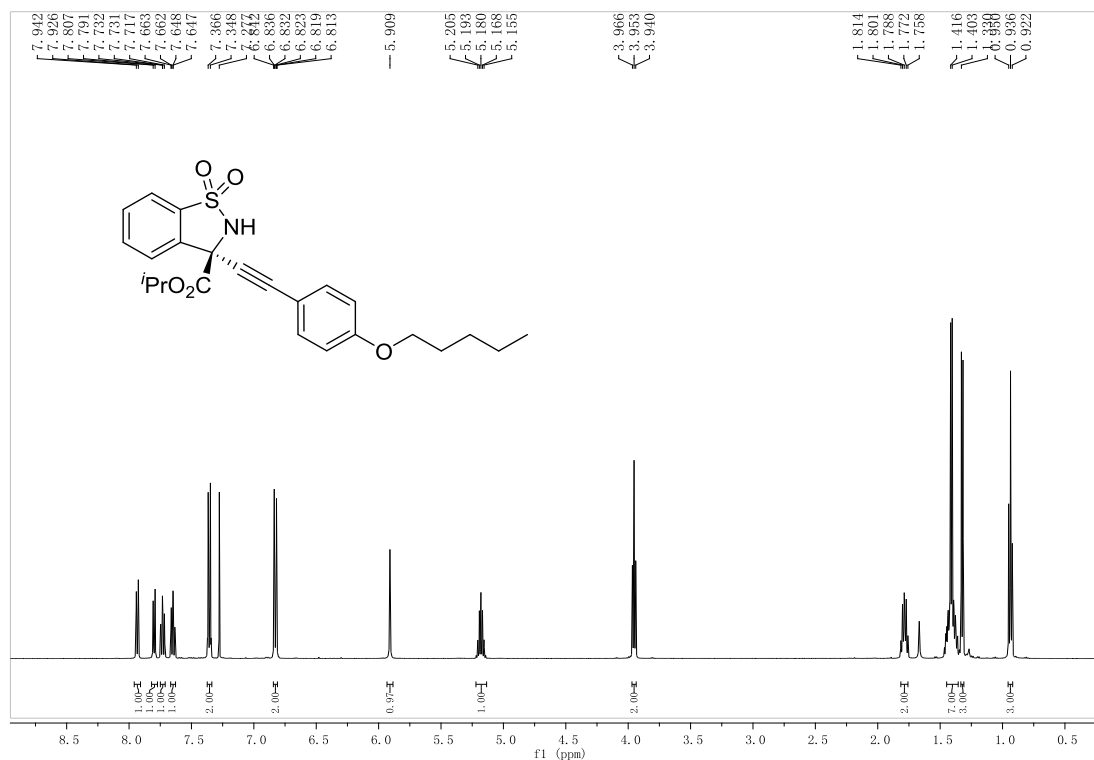
	Retention Time	Area	% Area	Height	% Height
1	20.915	36633649	96.66	735835	96.66
2	23.847	1265160	3.34	25420	3.34

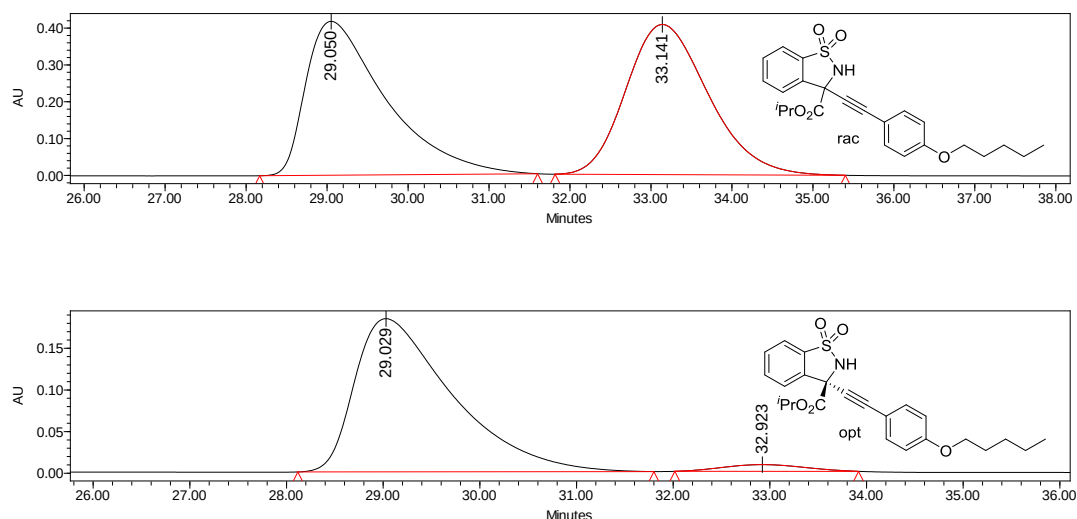
Isopropyl 3-((4-(pentyloxy)phenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bf**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 76% yield; $[\alpha]_D^{15} = 31.1$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 29.0$ min, $t_{\text{minor}} = 32.9$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.93 (d, $J = 8.0$ Hz, 1H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.73 (td, $J = 8.0, 1.5$ Hz, 1H), 7.65 (td, $J = 7.5, 0.5$ Hz, 1H), 7.34-7.38 (m, 2H), 6.81-6.85 (m, 2H), 5.91 (s, 1H), 5.15-5.21 (m, 1H), 3.95 (t, $J = 6.5$ Hz, 2H), 1.75-1.82 (m, 2H), 1.36-1.46 (m, 7H), 1.32 (d, $J = 6.5$ Hz, 3H), 0.94 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.4, 159.9, 136.2, 134.2, 133.7, 133.5, 130.9, 126.1, 121.2, 114.5, 112.8, 85.6, 83.0, 72.8, 68.1, 62.0,

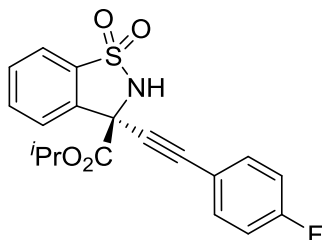
28.8, 28.1, 22.4, 21.43, 21.41, 14.0; HRMS m/z (ESI⁺): calculated for C₂₄H₂₈NO₅S
 ([M+H]⁺): 442.1683, found 442.1684.





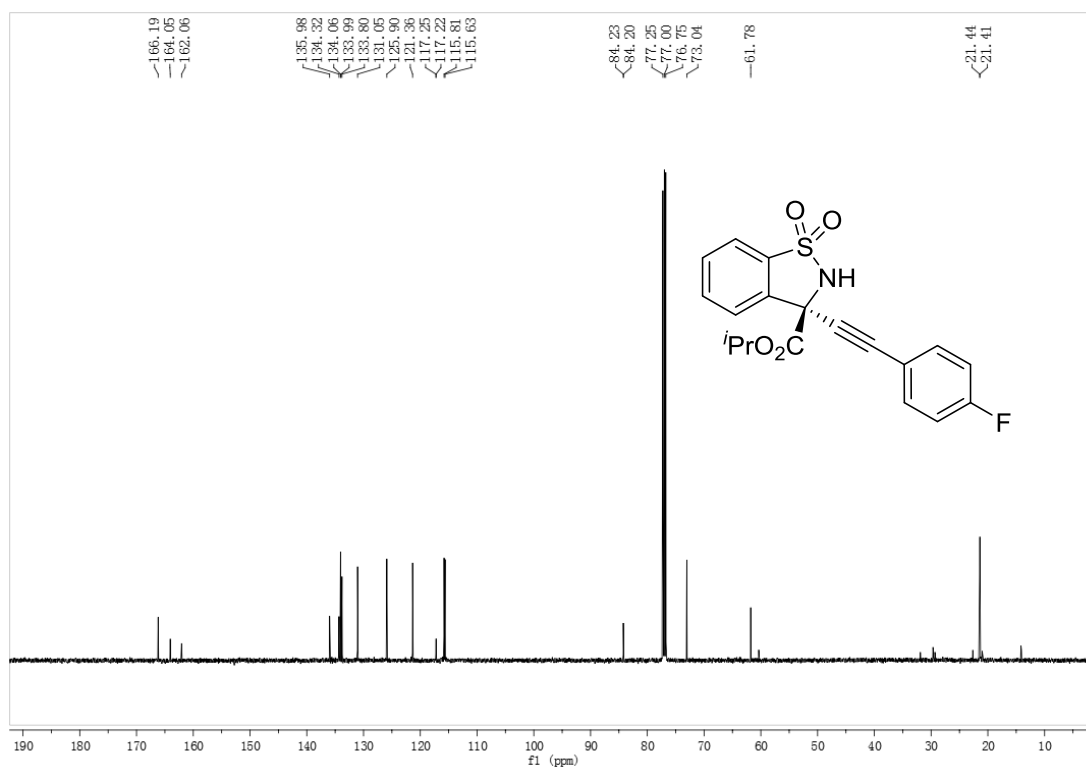
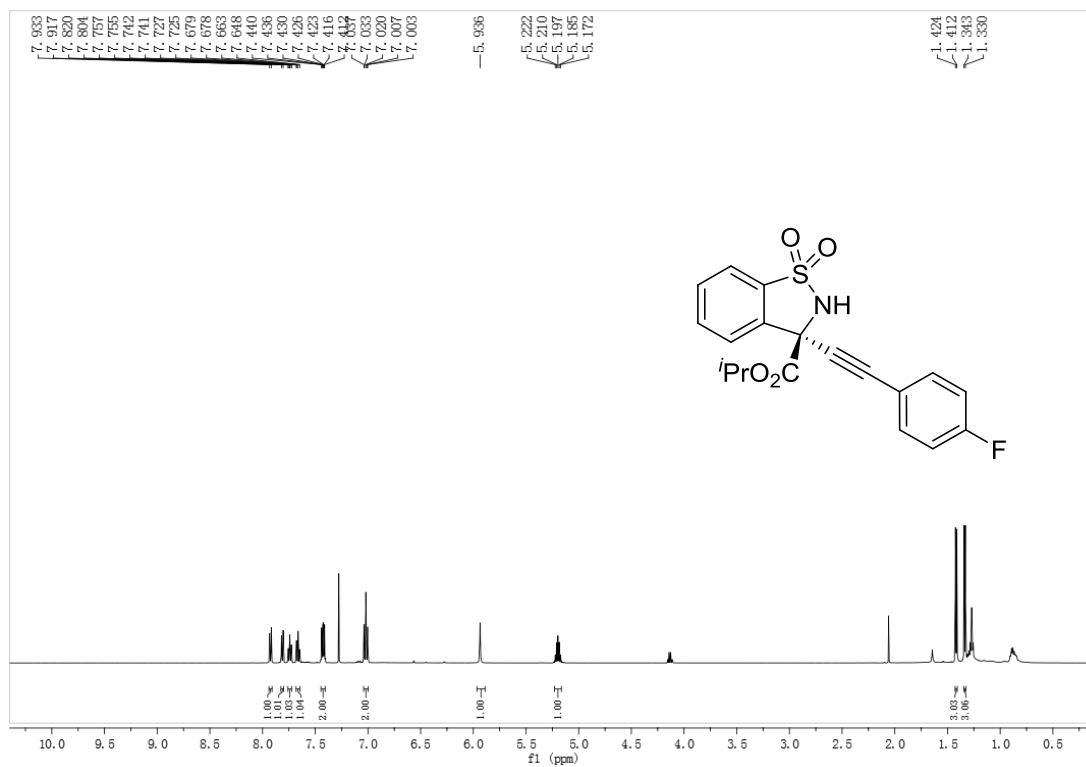
	Retention Time	Area	% Area	Height	% Height
1	29.029	12888034	96.47	183936	95.79
2	32.923	471550	3.53	8079	4.21

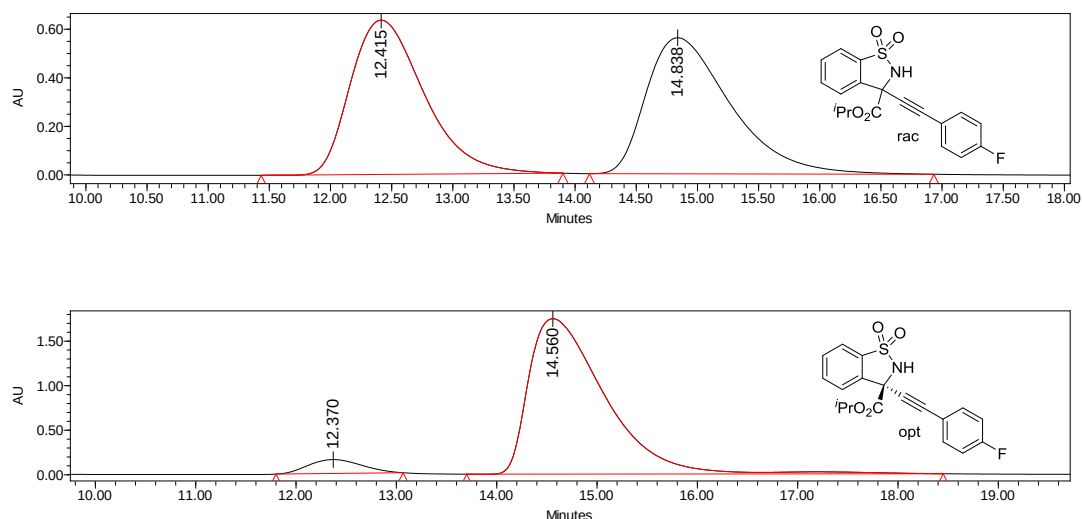
Isopropyl 3-((4-fluorophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bg**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 73% yield; $[\alpha]_D^{15} = 34.7$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 14.6$ min, $t_{\text{minor}} = 12.4$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 8.0$ Hz, 1H), 7.74 (td, $J = 7.5, 1.0$ Hz, 1H), 7.64-7.68 (m, 1H), 7.41-7.44 (m, 2H), 7.00-7.04 (m, 2H), 5.94 (s, 1H), 5.20 (dt, $J = 12.5, 6.0$ Hz, 1H), 1.42 (d, $J = 6.0$ Hz, 3H), 1.34 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.2, 163.1 (d, $J = 248.8$ Hz), 136.0, 134.3, 134.0 (d, $J = 8.8$ Hz), 133.8, 131.1, 125.9, 121.4, 117.2 (d, $J = 3.8$ Hz), 115.7 (d, $J = 22.5$ Hz), 84.23, 84.20, 73.0, 61.8,

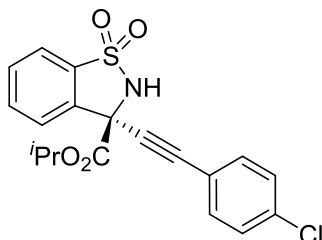
21.44, 21.41; HRMS m/z (ESI⁺): calculated for C₁₉H₁₇FNO₄S ([M+H]⁺): 374.0857, found 374.0858.





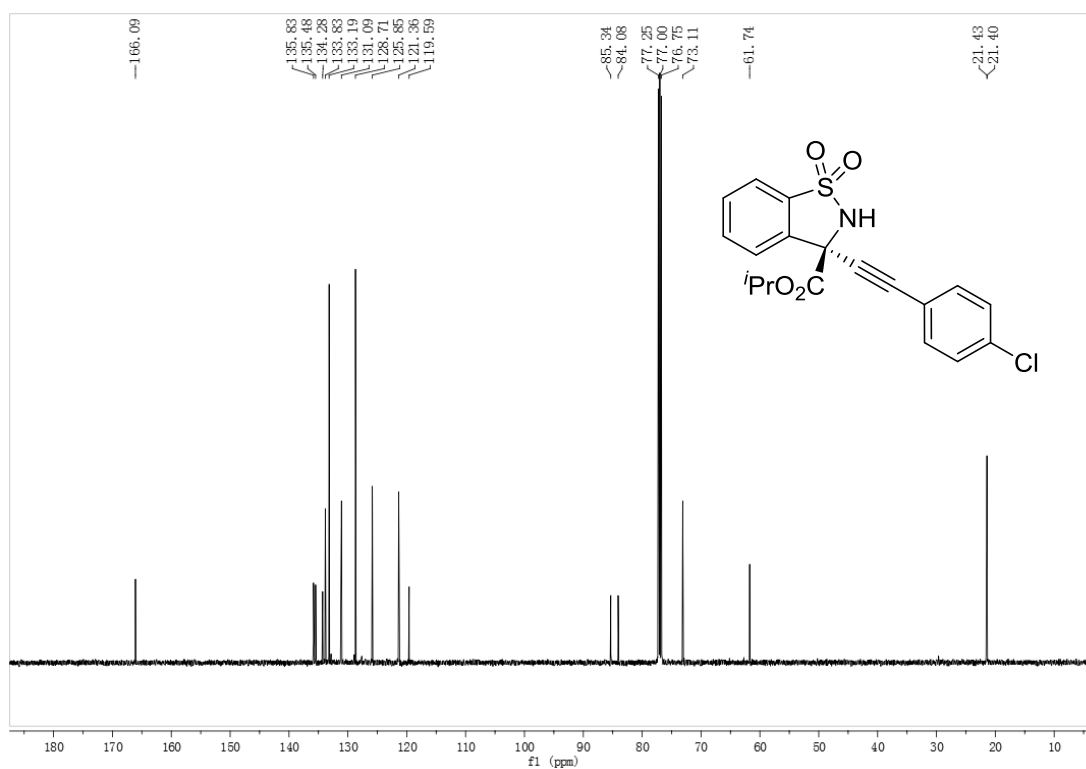
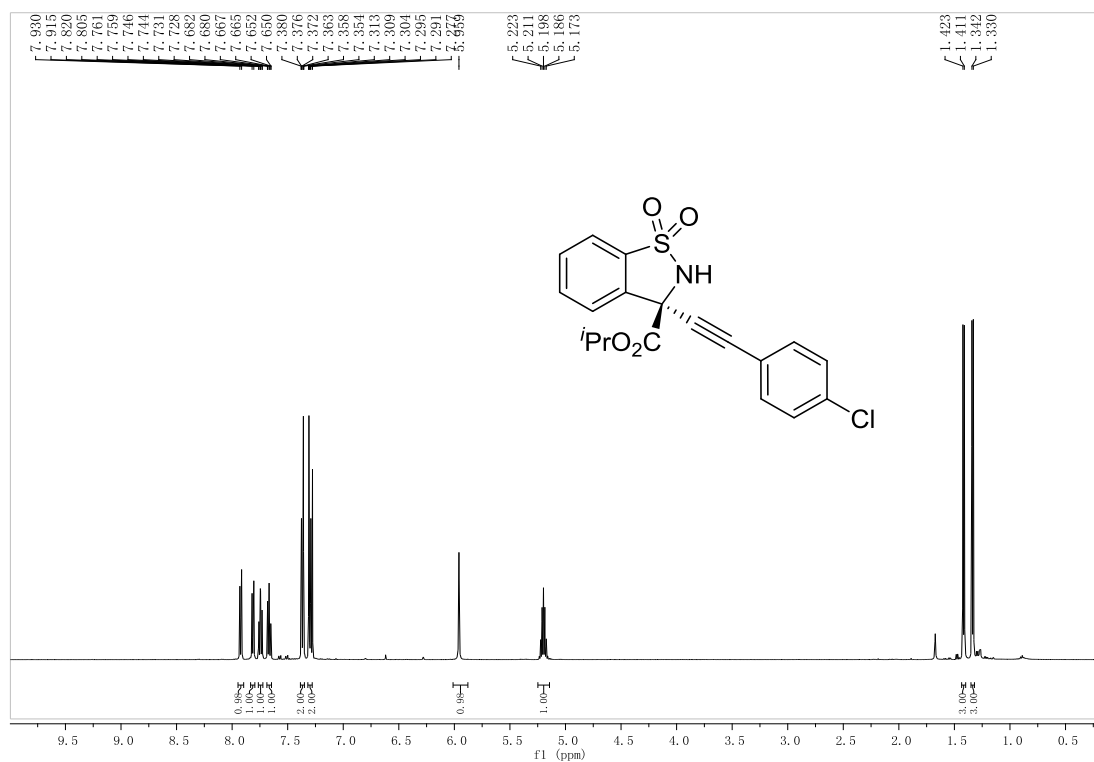
	Retention Time	Area	% Area	Height	% Height
1	12.370	5788562	5.91	156537	8.23
2	14.560	92142147	94.09	1744948	91.77

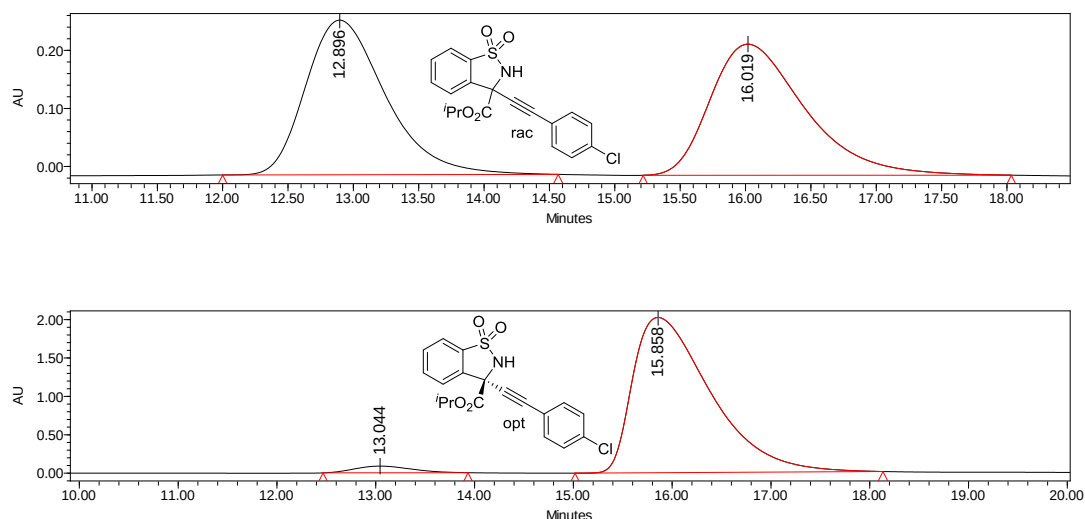
Isopropyl 3-((4-chlorophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bh**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 65% yield; $[\alpha]_D^{15} = 47.7$ ($c = 1.0$ in CH_2Cl_2), 94% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 15.9$ min, $t_{\text{minor}} = 13.0$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 7.5$ Hz, 1H), 7.81 (d, $J = 7.5$ Hz, 1H), 7.74 (td, $J = 7.5, 1.0$ Hz, 1H), 7.67 (td, $J = 7.5, 1.0$ Hz, 1H), 7.35-7.38 (m, 2H), 7.28-7.32 (m, 2H), 5.96 (s, 1H), 5.17-5.23 (m, 1H), 1.42 (d, $J = 6.0$ Hz, 3H), 1.34 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.1, 135.8, 135.5, 134.3, 133.8, 133.2, 131.1, 128.7, 125.9, 121.4, 119.6, 85.3, 84.1,

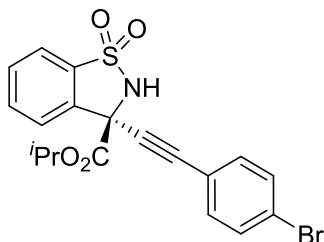
73.1, 61.7, 21.43, 21.40; HRMS m/z (ESI⁺): calculated for C₁₉H₁₇ClNO₄S ([M+H]⁺): 390.0561, found 390.0565.





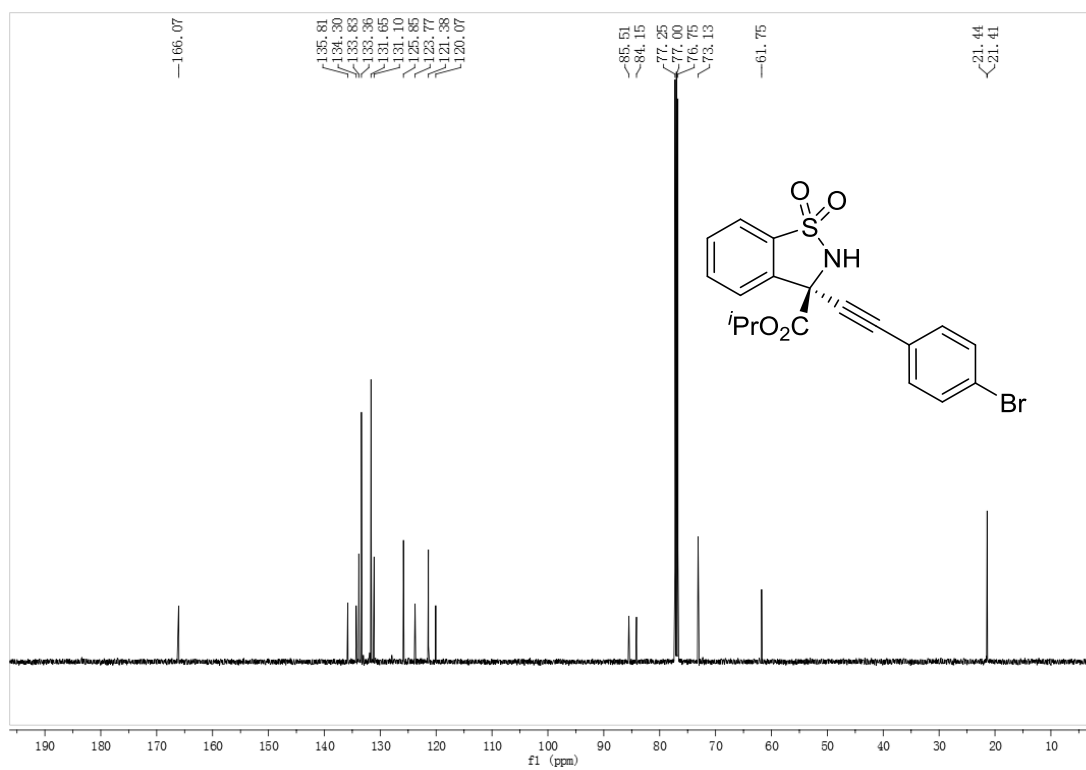
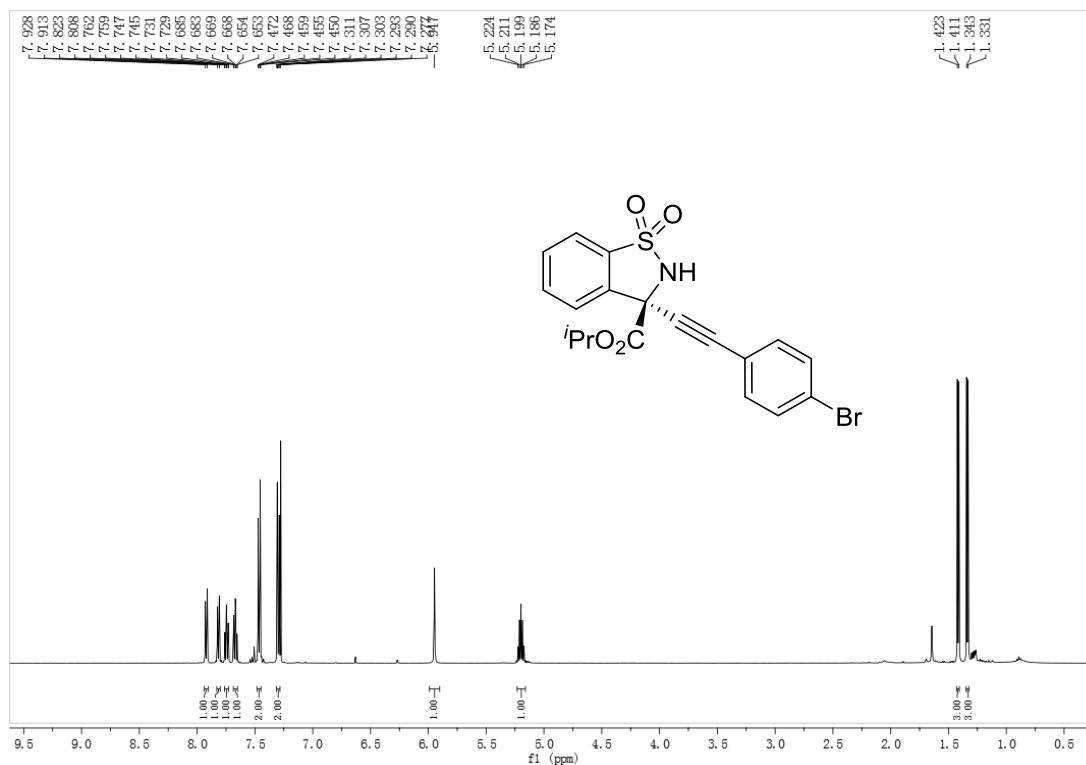
	Retention Time	Area	% Area	Height	% Height
1	13.044	3474655	3.05	87315	4.14
2	15.858	110549882	96.95	2022121	95.86

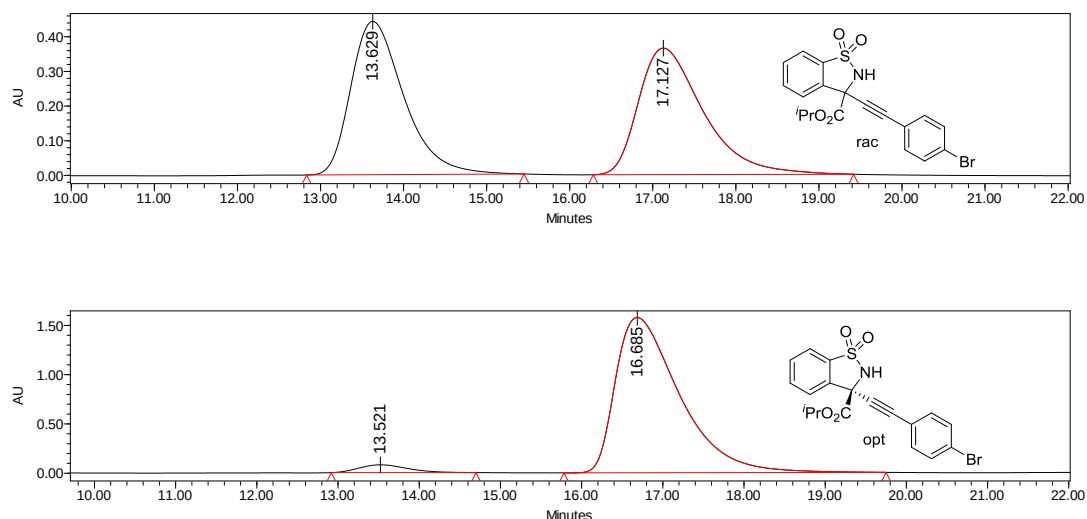
Isopropyl 3-((4-bromophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bi**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 70% yield; $[\alpha]_D^{15} = 31.2$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 16.7$ min, $t_{\text{minor}} = 13.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 7.5$ Hz, 1H), 7.82 (d, $J = 7.5$ Hz, 1H), 7.75 (td, $J = 7.5, 1.5$ Hz, 1H), 7.67 (td, $J = 8.0, 1.0$ Hz, 1H), 7.45-7.48 (m, 2H), 7.27-7.32 (m, 2H), 5.95 (s, 1H), 5.17-5.23 (m, 1H), 1.42 (d, $J = 6.0$ Hz, 3H), 1.34 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.1, 135.8, 134.3, 133.8, 133.4, 131.7, 131.1, 125.9, 123.8, 121.4, 120.1, 85.5, 84.2,

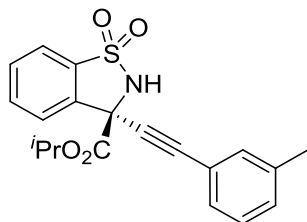
73.1, 61.8, 21.44, 21.41; HRMS m/z (ESI⁺): calculated for C₁₉H₁₇BrNO₄S ([M+H]⁺): 434.0056, found 434.0057.





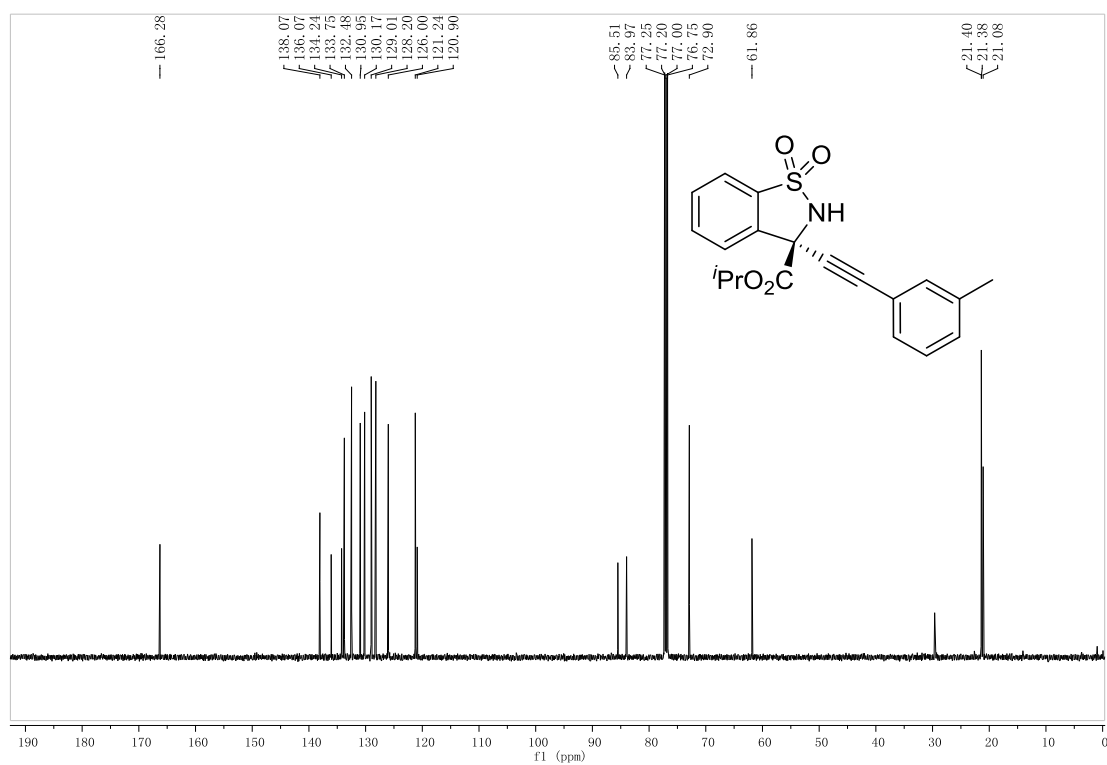
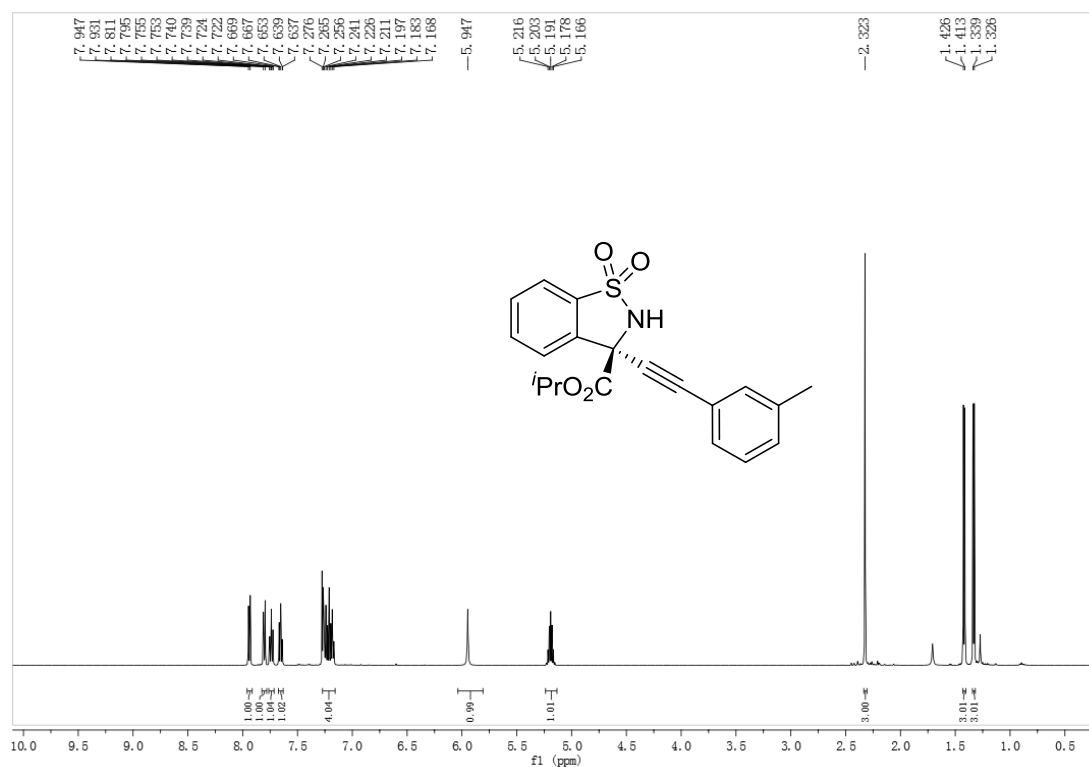
	Retention Time	Area	% Area	Height	% Height
1	13.521	3289383	3.67	79199	4.79
2	16.685	86371600	96.33	1575934	95.21

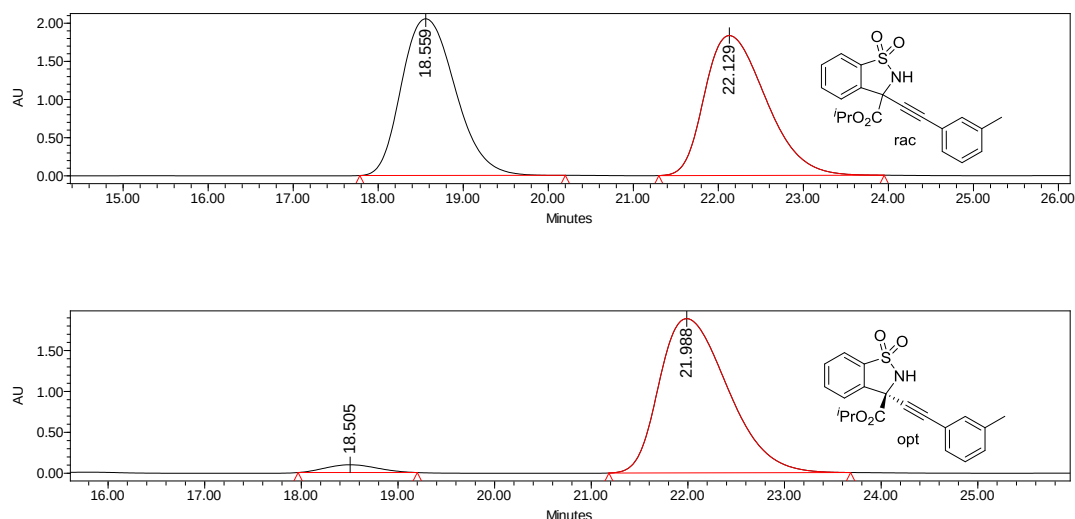
Isopropyl 3-(*m*-tolylethynyl)-2,3-dihydrobenzo[*d*]isothiazole-3-carboxylate 1,1-dioxide (**3bj**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow solid, 72% yield, m.p. 91-94 °C; $[\alpha]_D^{15} = 54.1$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), *n*-hexane/*i*-PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 22.0$ min, $t_{\text{minor}} = 18.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.94 (d, $J = 8.0$ Hz, 1H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.74 (td, $J = 7.5, 1.0$ Hz, 1H), 7.64-7.67 (m, 1H), 7.16-7.28 (m, 4H), 5.95 (s, 1H), 5.19 (dt, $J = 12.5, 6.5$ Hz, 1H), 2.32 (s, 3H), 1.42 (d, $J = 6.5$ Hz, 3H), 1.33 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.3, 138.1, 136.1, 134.2, 133.8, 132.5, 131.0, 130.2, 129.0, 128.2,

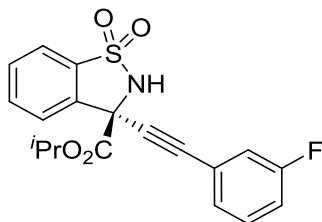
126.0, 121.2, 120.9, 85.5, 84.0, 72.9, 61.9, 21.40, 21.38, 21.1; HRMS m/z (ESI⁺):
calculated for C₂₀H₁₉NNaO₄S ([M+Na]⁺): 392.0927, found 392.0926.





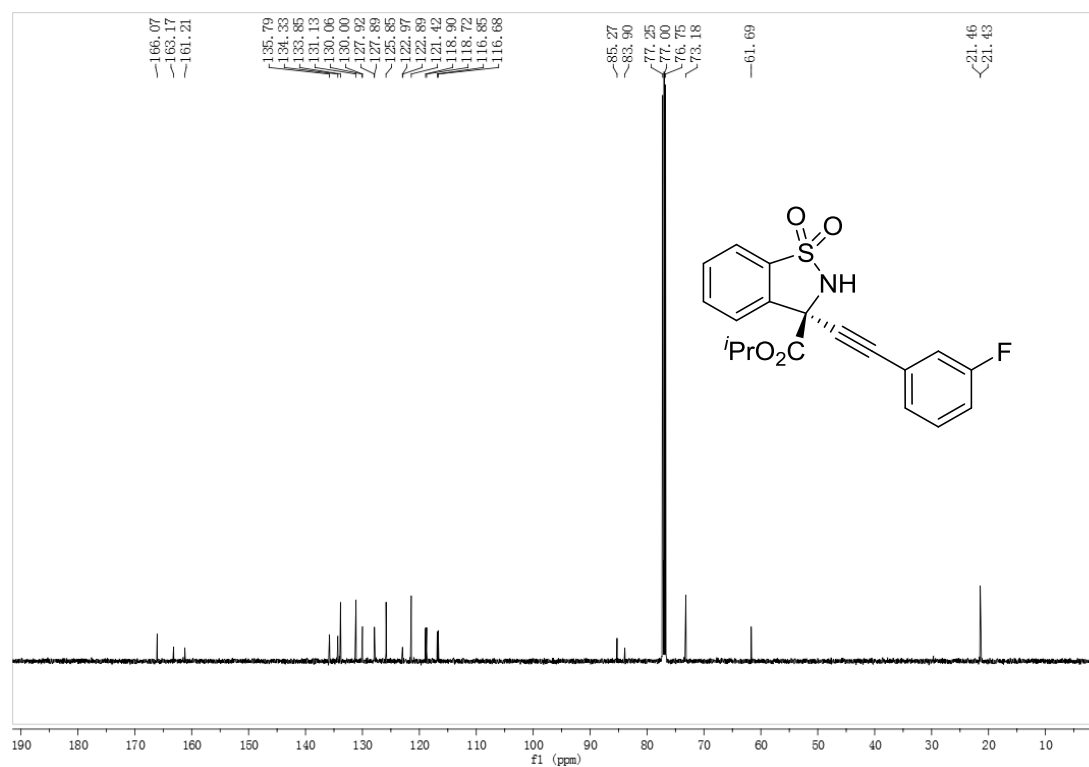
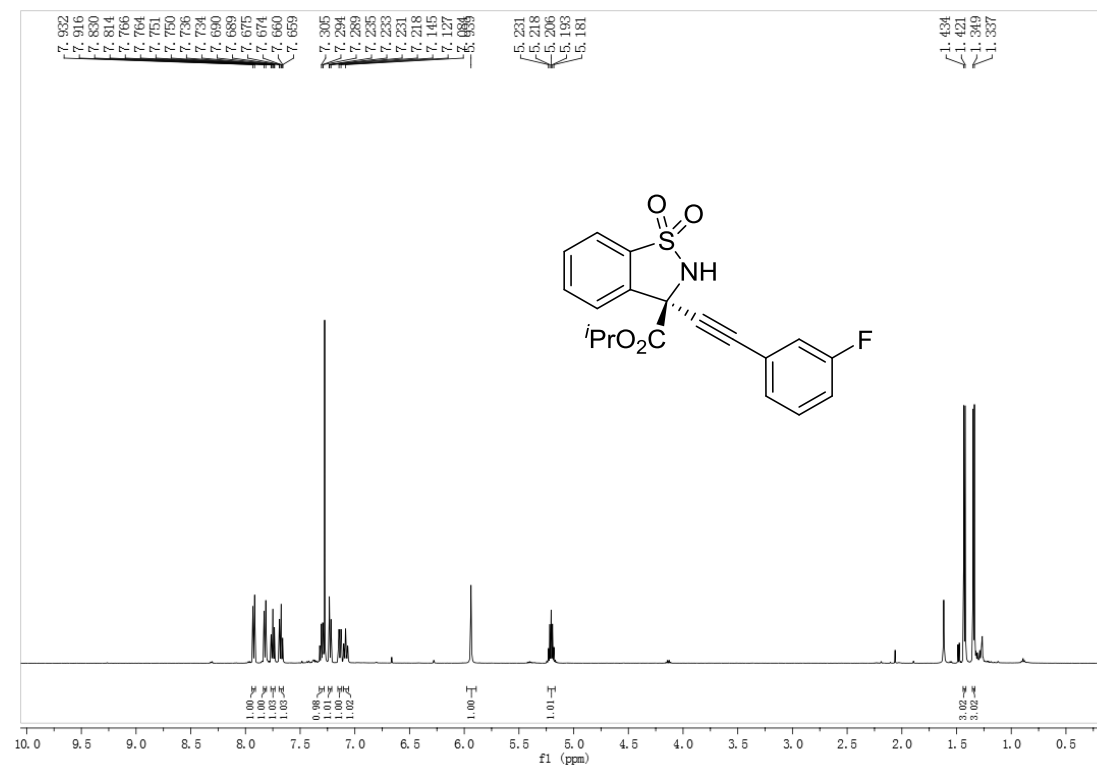
	Retention Time	Area	% Area	Height	% Height
1	18.505	3514079	3.65	95306	4.81
2	21.988	92847879	96.35	1885200	95.19

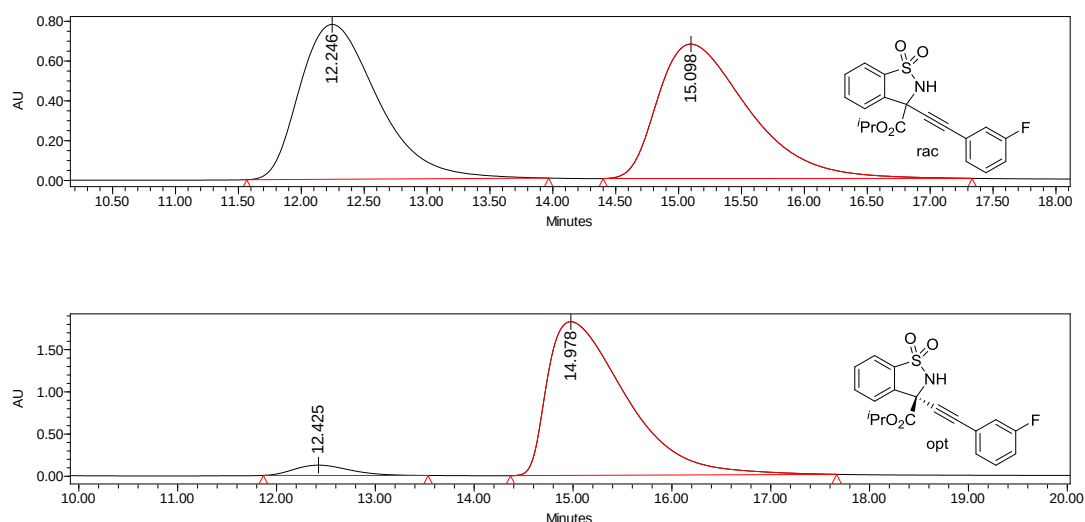
Isopropyl 3-((3-fluorophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bk**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 75% yield; $[\alpha]_D^{15} = 30.8$ ($c = 1.0$ in CH_2Cl_2), 91% ee [Daicel Chiralcel OD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 15.0$ min, $t_{\text{minor}} = 12.4$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 8.0$ Hz, 1H), 7.82 (d, $J = 8.0$ Hz, 1H), 7.75 (td, $J = 7.5, 1.0$ Hz, 1H), 7.67 (td, $J = 7.5, 0.5$ Hz, 1H), 7.28-7.33 (m, 1H), 7.21-7.24 (m, 1H), 7.12-7.15 (m, 1H), 7.06-7.11 (m, 1H), 5.94 (s, 1H), 5.21 (dt, $J = 12.5, 6.5$ Hz, 1H), 1.43 (d, $J = 6.5$ Hz, 3H), 1.34 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.1, 162.2 (d, $J = 245.0$ Hz), 135.8, 134.3, 133.9, 131.1, 130.0 (d, $J = 7.5$ Hz), 127.9 (d, $J = 3.8$ Hz), 125.9, 122.9 (d, $J =$

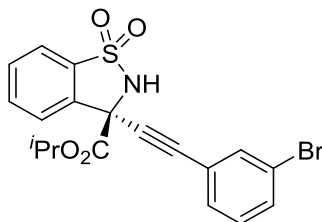
10.0 Hz), 121.4, 118.8 (d, $J = 22.5$ Hz), 116.8 (d, $J = 21.3$ Hz), 85.3, 83.9, 73.2, 61.7, 21.46, 21.43; HRMS m/z (ESI⁺): calculated for C₁₉H₂₀FN₂O₄S ([M+NH₄)⁺): 391.1122, found 391.1125.



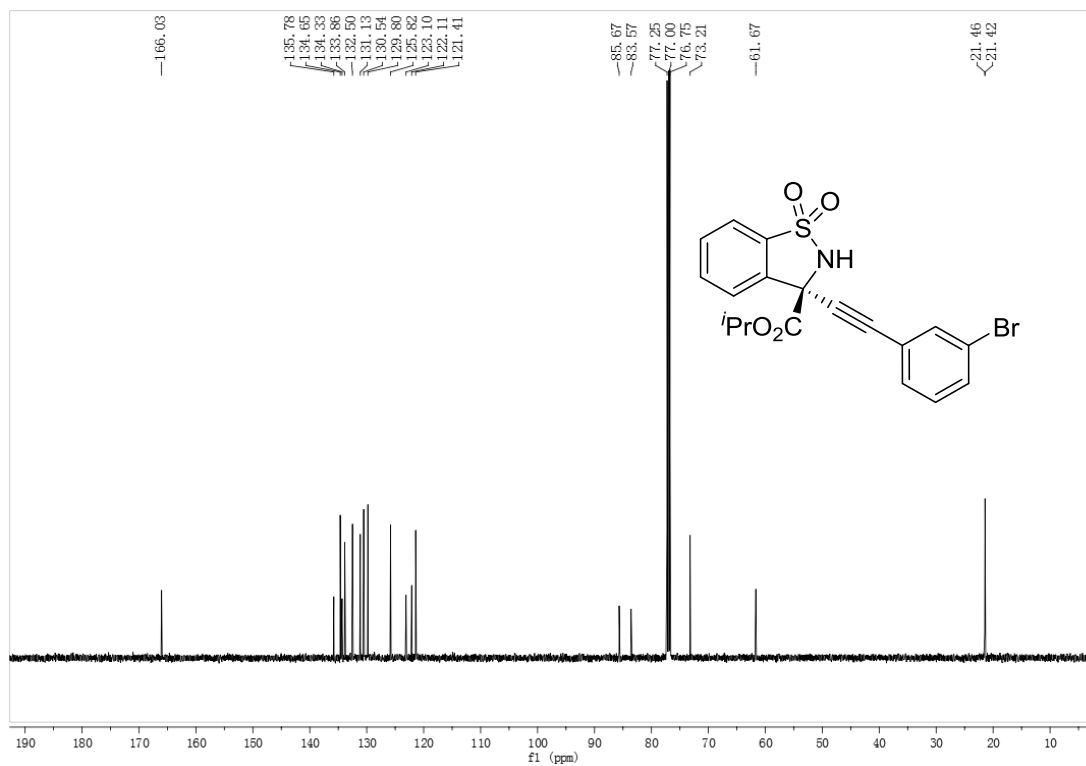
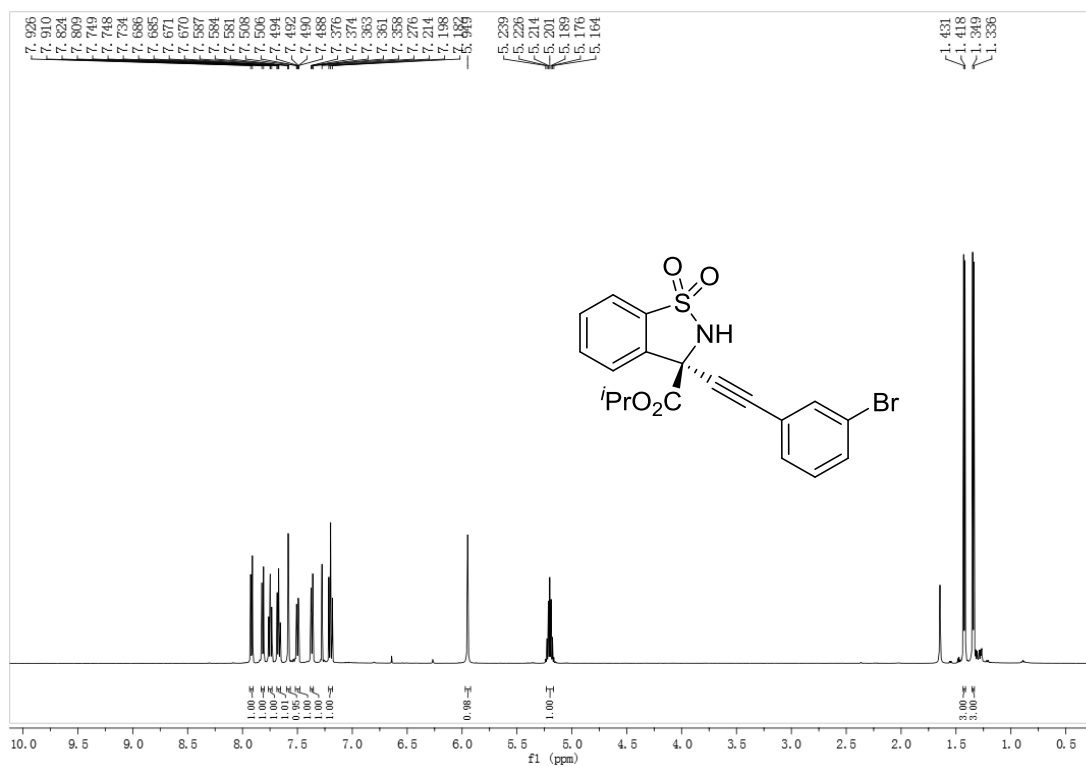


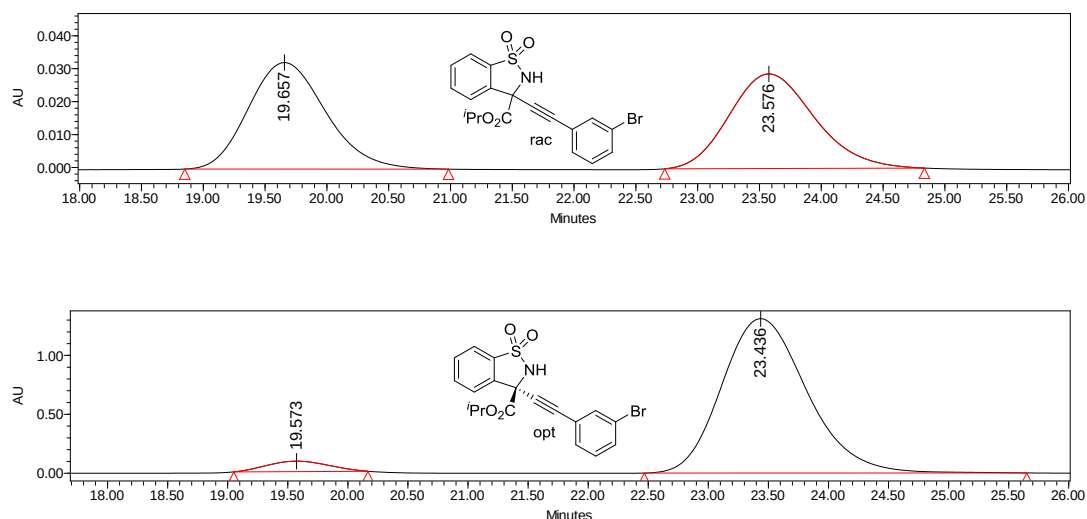
	Retention Time	Area	% Area	Height	% Height
1	12.425	4761823	4.52	122111	6.28
2	14.978	100641214	95.48	1822071	93.72

Isopropyl 3-((3-bromophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bl**)



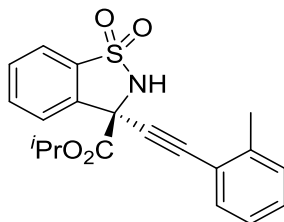
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow solid, 83% yield, m.p. 102-105 °C; $[\alpha]_{\text{D}}^{15} = 31.0$ ($c = 1.0$ in CH_2Cl_2), 91% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 23.4$ min, $t_{\text{minor}} = 19.6$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 8.0$ Hz, 1H), 7.82 (d, $J = 7.5$ Hz, 1H), 7.75 (td, $J = 8.0, 1.0$ Hz, 1H), 7.67 (td, $J = 7.5, 0.5$ Hz, 1H), 7.58 (t, $J = 1.5$ Hz, 1H), 7.48-7.51 (m, 1H), 7.35-7.38 (m, 1H), 7.20 (t, $J = 8.0$ Hz, 1H), 5.95 (s, 1H), 5.16-5.24 (m, 1H), 1.42 (d, $J = 6.5$ Hz, 3H), 1.34 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.0, 135.8, 134.7, 134.3, 133.9, 132.5, 131.1, 130.5, 129.8, 125.8, 123.1, 122.1, 121.4, 85.7, 83.6, 73.2, 61.7, 21.46, 21.42; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{17}\text{BrNO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 434.0056, found 434.0048.



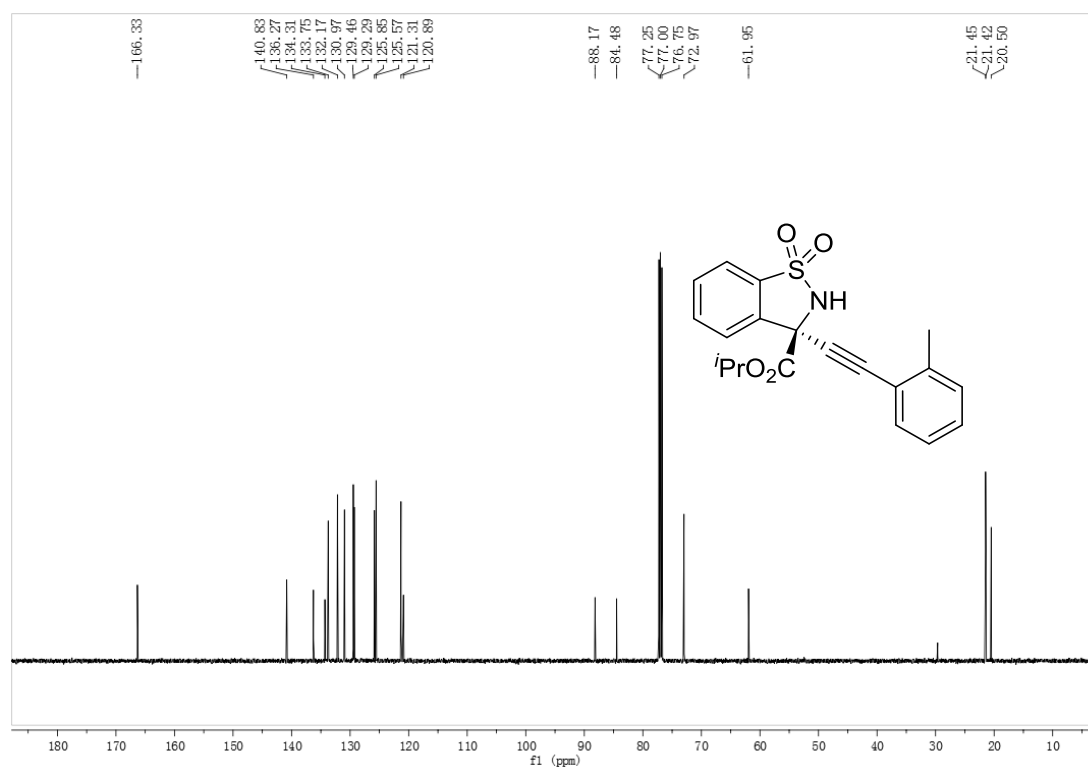


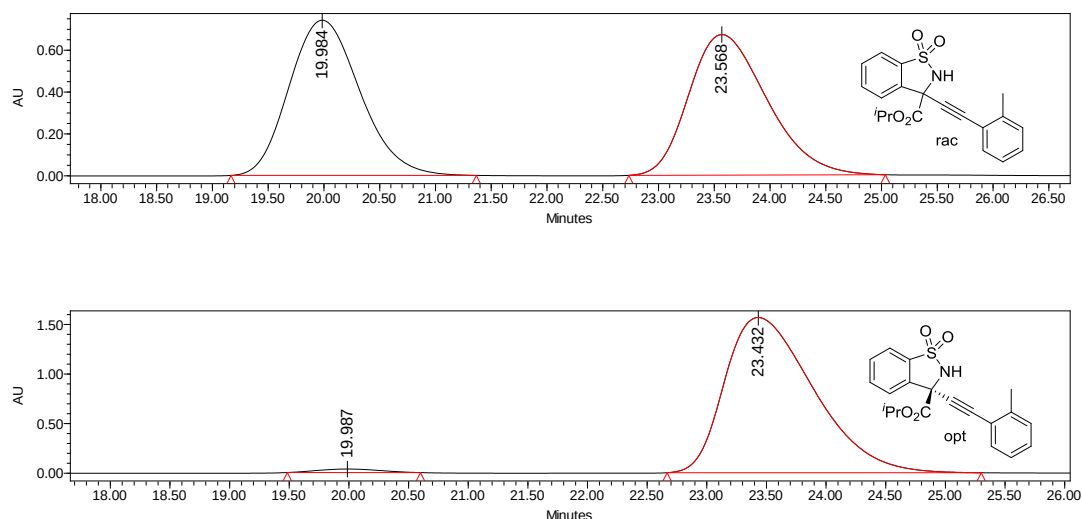
	Retention Time	Area	% Area	Height	% Height
1	19.573	3148230	4.64	88434	6.32
2	23.436	64667680	95.36	1310106	93.68

Isopropyl 3-(o-tolyethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bm**)



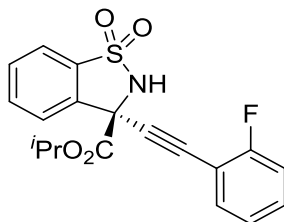
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow solid, 75% yield, m.p. 80-82 °C; $[\alpha]_D^{15} = 30.9$ ($c = 1.0$ in CH_2Cl_2), 97% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 23.4$ min, $t_{\text{minor}} = 20.0$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.93 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 8.0$ Hz, 1H), 7.74 (td, $J = 7.5, 1.0$ Hz, 1H), 7.66 (td, $J = 7.5, 0.5$ Hz, 1H), 7.38-7.41 (m, 1H), 7.26 (dd, $J = 7.0, 6.0$ Hz, 1H), 7.20 (d, $J = 7.5$ Hz, 1H), 7.14 (t, $J = 8.0$ Hz, 1H), 5.95 (s, 1H), 5.20 (dt, $J = 12.5, 6.5$ Hz, 1H), 2.42 (s, 3H), 1.42 (d, $J = 6.5$ Hz, 3H), 1.34 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.3, 140.8, 136.3, 134.3, 133.8, 132.2, 131.0, 129.5, 129.3, 125.9, 125.6, 121.3, 120.9, 88.2, 84.5, 73.0, 62.0, 21.45, 21.42, 20.5; HRMS m/z (ESI $^+$): calculated for $\text{C}_{20}\text{H}_{23}\text{N}_2\text{O}_4\text{S}$ ($[\text{M}+\text{NH}_4]^+$): 387.1373, found 387.1381.





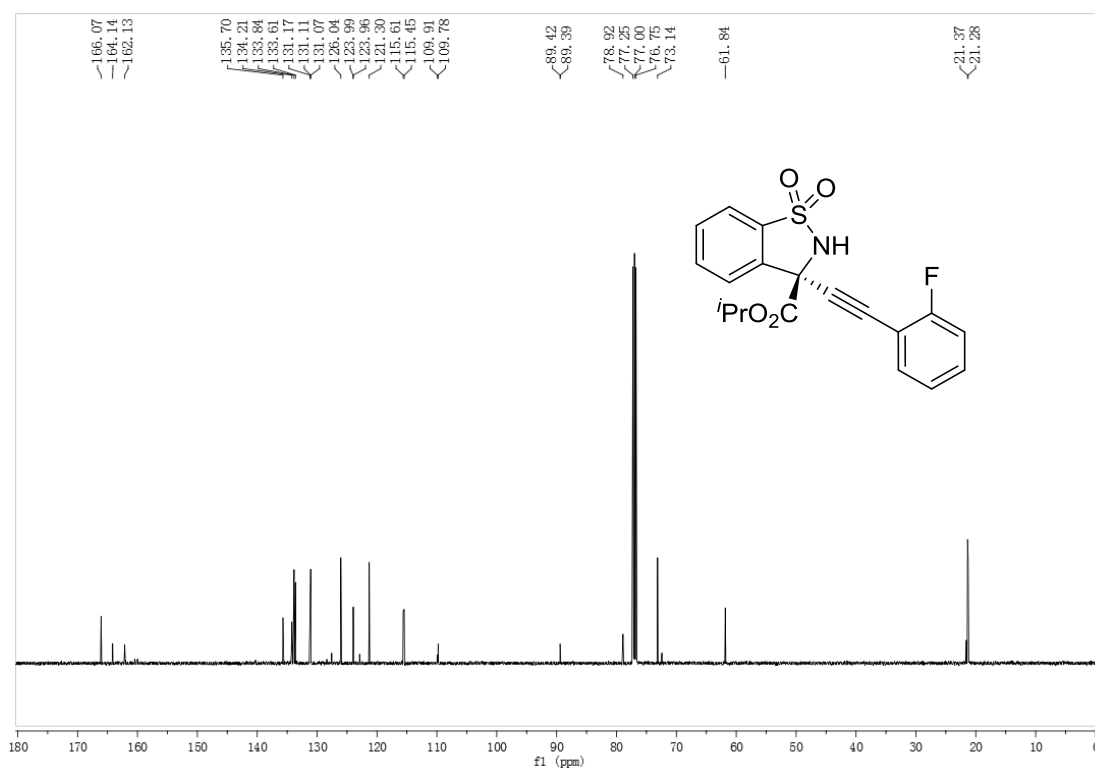
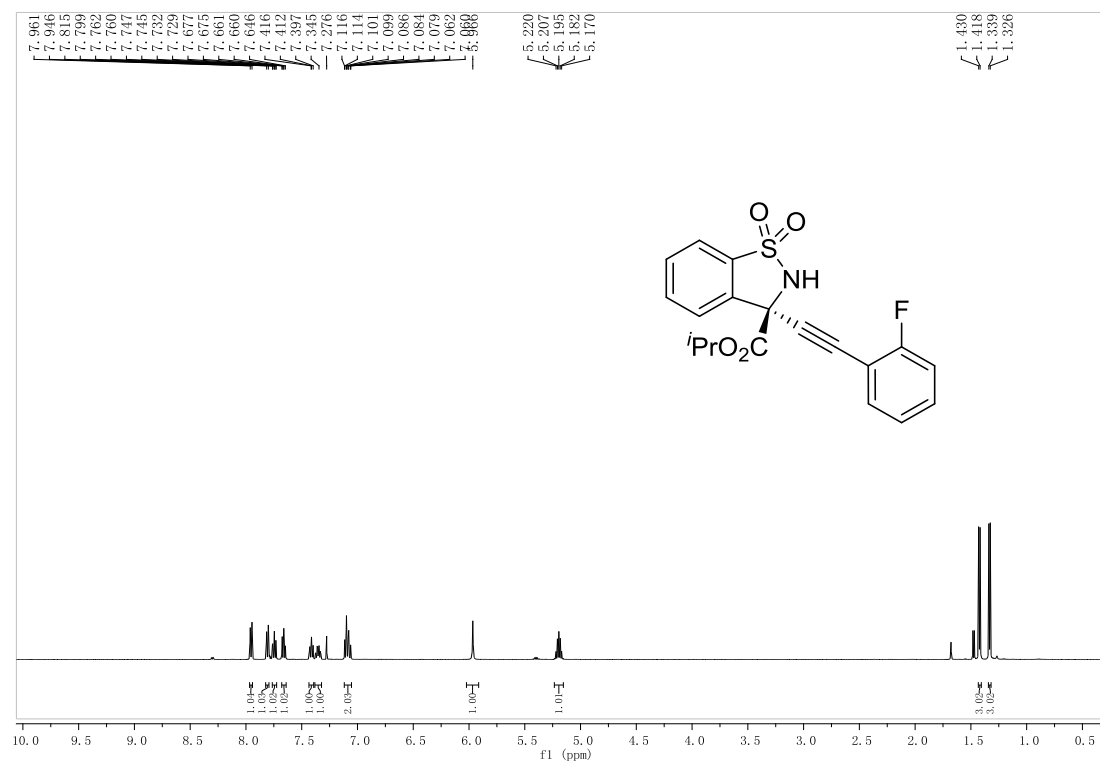
	Retention Time	Area	% Area	Height	% Height
1	19.987	1282137	1.56	35511	2.22
2	23.432	81072457	98.44	1565702	97.78

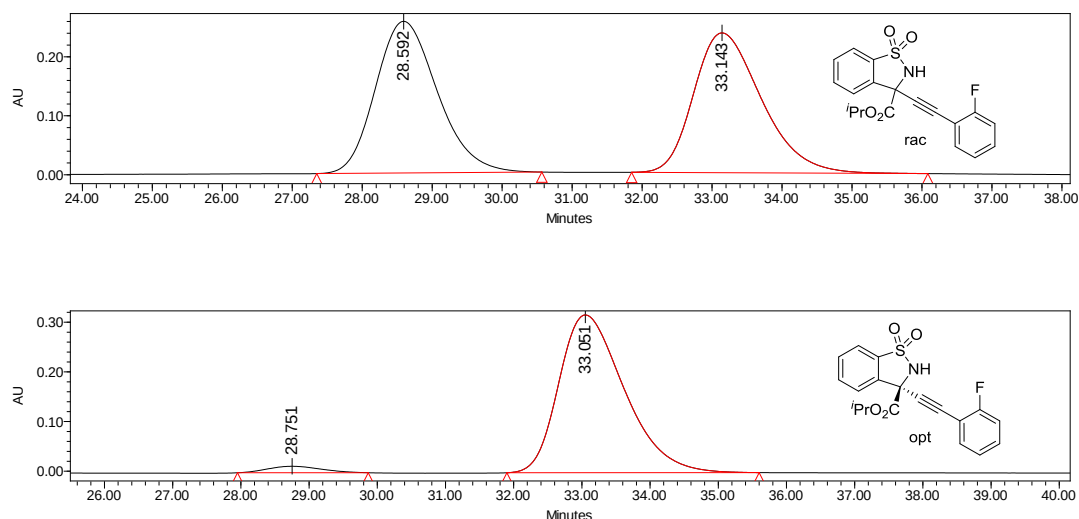
Isopropyl 3-((2-fluorophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bn**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 73% yield; $[\alpha]_D^{15} = 26.7$ ($c = 1.0$ in CH_2Cl_2), 94% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 33.1$ min, $t_{\text{minor}} = 28.8$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.95 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 8.0$, 1H), 7.75 (td, $J = 7.5$, 1.0 Hz, 1H), 7.66 (td, $J = 8.0$, 1.0 Hz, 1H), 7.41 (td, $J = 7.0$, 1.5 Hz, 1H), 7.33-7.38(m, 1H), 7.06-7.12 (m, 2H), 5.97 (s, 1H), 5.19 (dt, $J = 12.5$, 6.0 Hz, 1H), 1.42 (d, $J = 6.0$ Hz, 3H), 1.33 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.1, 163.1 (d, $J = 251.3$ Hz), 135.7, 134.2, 133.8, 133.6, 131.14 (d, $J = 7.5$ Hz), 131.07, 126.0, 124.0 (d, $J = 3.8$ Hz), 121.3,

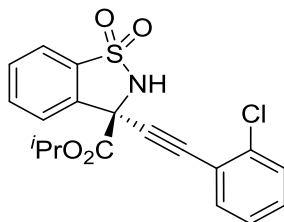
115.5 (d, $J = 20.0$ Hz), 109.8 (d, $J = 16.3$ Hz), 89.4 (d, $J = 3.8$ Hz), 78.9, 73.1, 61.8, 21.37, 21.28; HRMS m/z (ESI⁺): calculated for C₁₉H₁₇FNO₄S ([M+H]⁺): 374.0857, found 374.0855.



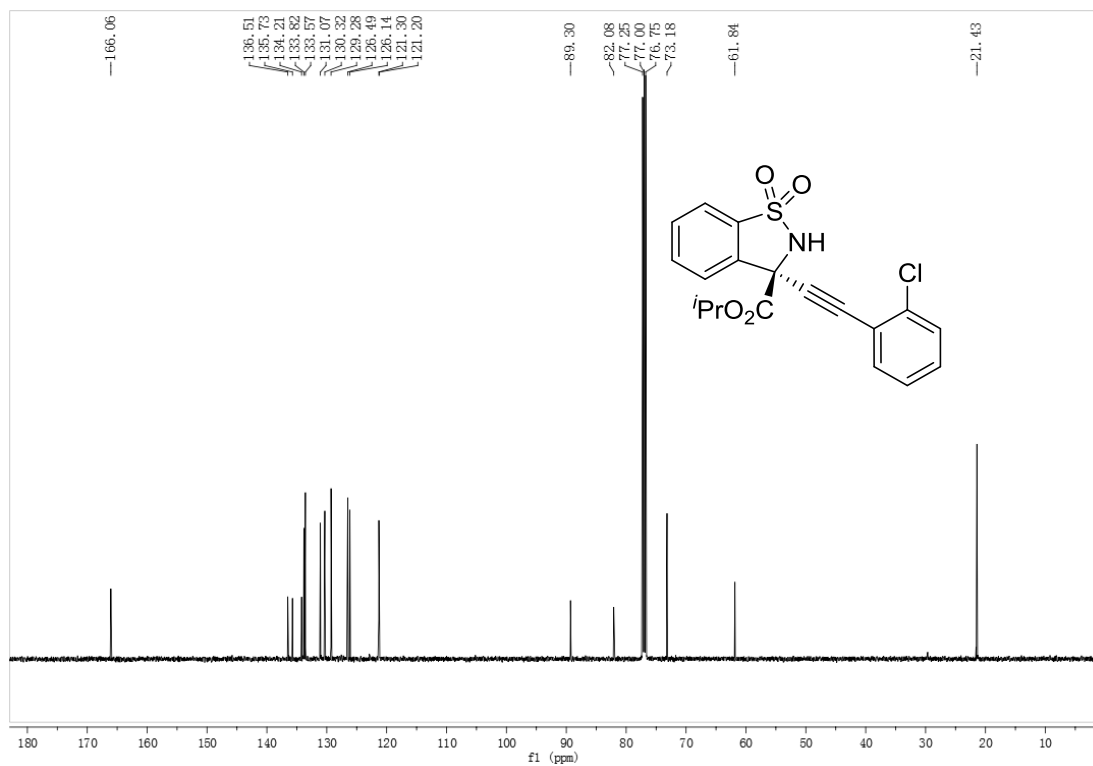
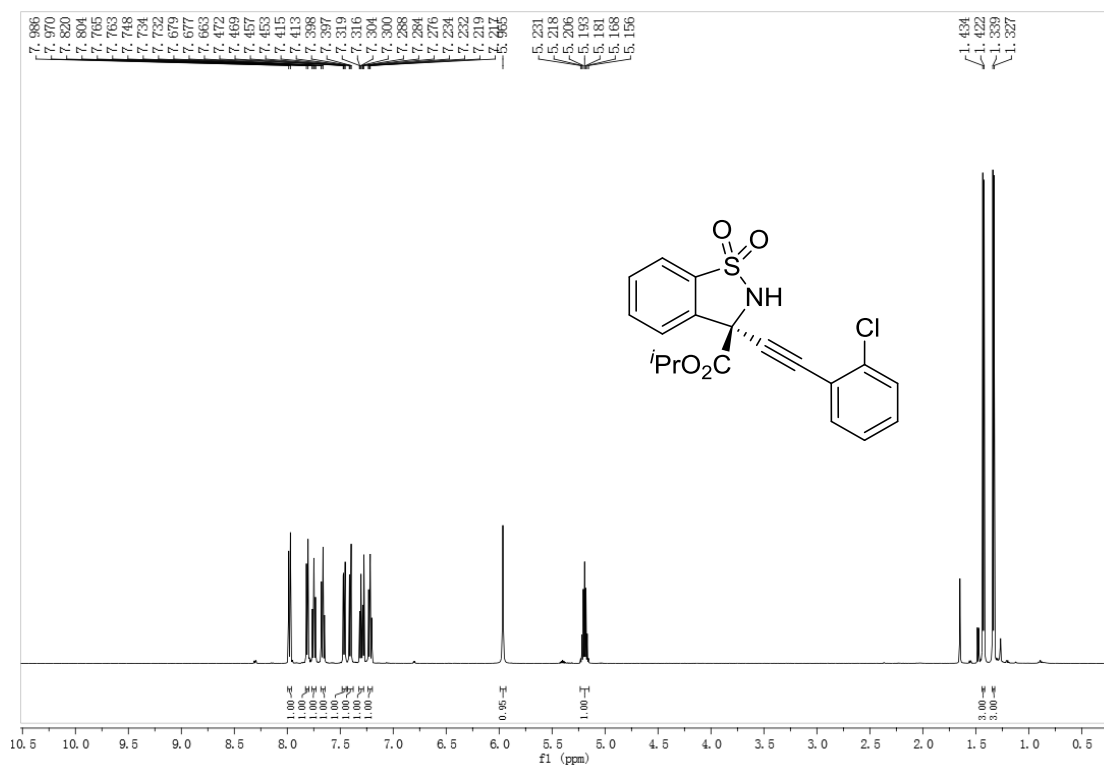


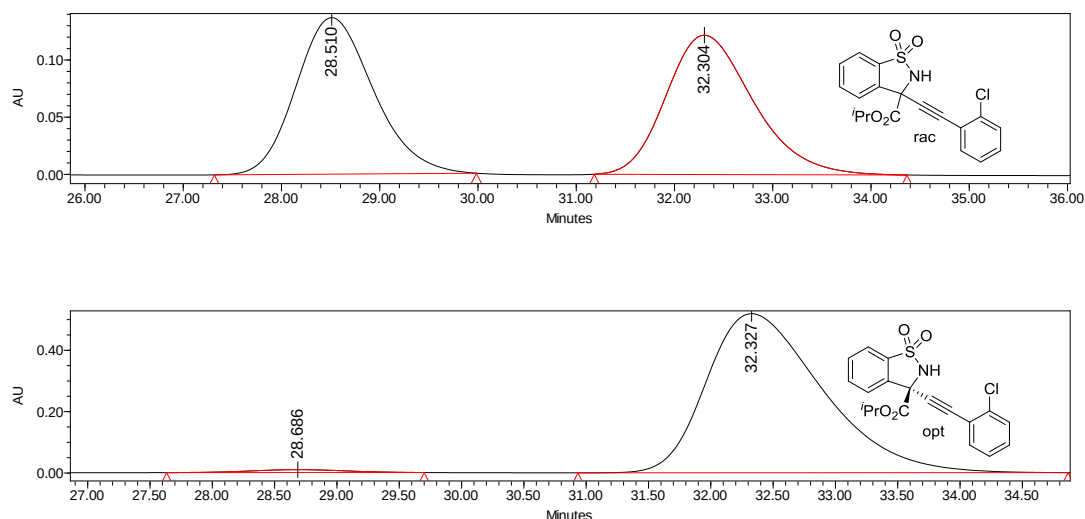
	Retention Time	Area	% Area	Height	% Height
1	28.751	710981	3.25	13065	3.95
2	33.051	21162734	96.75	317672	96.05

Isopropyl 3-((2-chlorophenyl)ethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bo**)



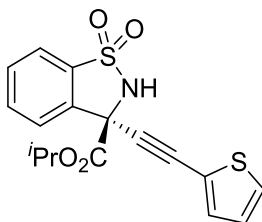
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 73% yield; $[\alpha]_D^{15} = 38.1$ ($c = 1.0$ in CH_2Cl_2), 97% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 32.3$ min, $t_{\text{minor}} = 28.7$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.98 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 8.0$ Hz, 1H), 7.73-7.77 (m, 1H), 7.64-7.68 (m, 1H), 7.46 (dd, $J = 7.5, 1.5$ Hz, 1H), 7.41 (dd, $J = 8.5, 1.0$ Hz, 1H), 7.30 (td, $J = 7.5, 1.5$ Hz, 1H), 7.22 (td, $J = 7.5, 1.0$ Hz, 1H), 5.96 (s, 1H), 5.15-5.24 (m, 1H), 1.43 (d, $J = 6.0$ Hz, 3H), 1.33 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.1, 136.5, 135.7, 134.2, 133.8, 133.6, 131.1, 130.3, 129.3, 126.5, 126.1, 121.3, 89.3, 82.1, 73.2, 61.8, 21.4; HRMS m/z (ESI $^+$): calculated for $\text{C}_{19}\text{H}_{16}\text{ClNNaO}_4\text{S}$ ($[\text{M}+\text{Na}]^+$): 412.0381, found 412.0381.



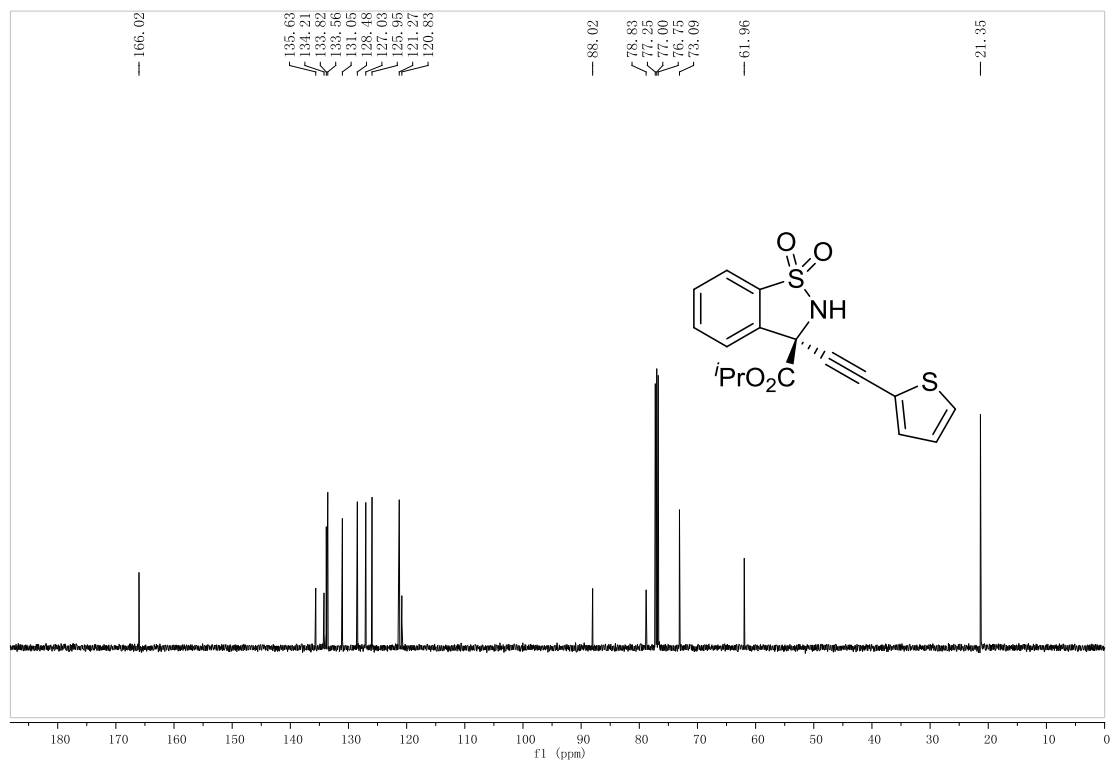
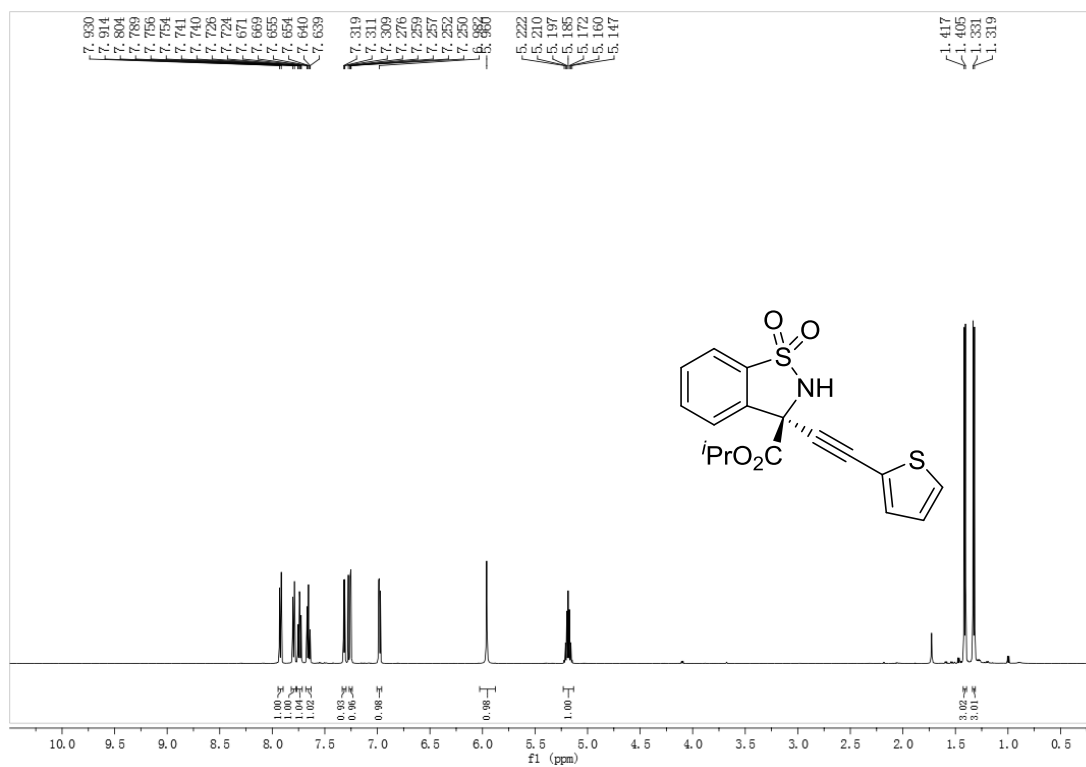


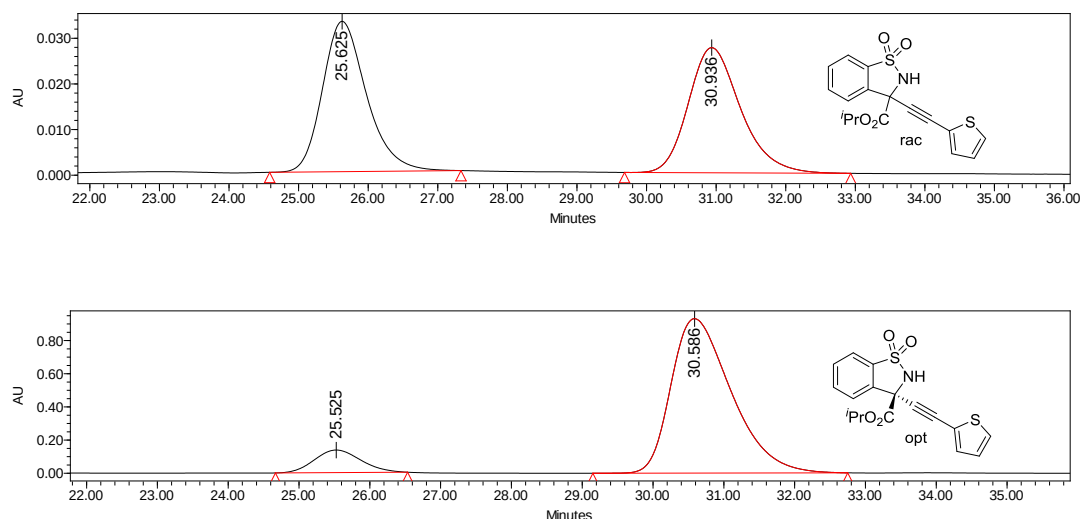
	Retention Time	Area	% Area	Height	% Height
1	28.686	515522	1.52	9601	1.82
2	32.327	33498467	98.48	518489	98.18

Isopropyl 3-(thiophen-2-ylethynyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bp**)



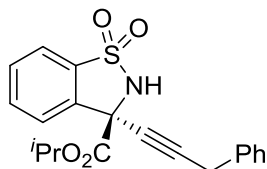
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 50% yield; $[\alpha]_D^{15} = 33.4$ ($c = 1.0$ in CH_2Cl_2), 80% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 30.6$ min, $t_{\text{minor}} = 25.5$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (d, $J = 8.0$ Hz, 1H), 7.80 (d, $J = 7.5$ Hz, 1H), 7.74 (td, $J = 7.5, 1.0$ Hz, 1H), 7.65 (td, $J = 8.0, 1.0$ Hz, 1H), 7.32 (dd, $J = 5.0, 1.0$ Hz, 1H), 7.25 (dd, $J = 3.5, 1.0$ Hz, 1H), 6.98 (dd, $J = 5.0, 3.5$ Hz, 1H), 5.96 (s, 1H), 5.14-5.23 (m, 1H), 1.41 (d, $J = 6.0$ Hz, 3H), 1.33 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.0, 135.6, 134.2, 133.8, 133.6, 131.1, 128.5, 127.0, 126.0, 121.3, 120.8, 88.0, 78.8, 73.1, 62.0, 21.4; HRMS m/z (ESI $^+$): calculated for $\text{C}_{17}\text{H}_{16}\text{NO}_4\text{S}_2$ ($[\text{M}+\text{H}]^+$): 362.0515, found 362.0517.



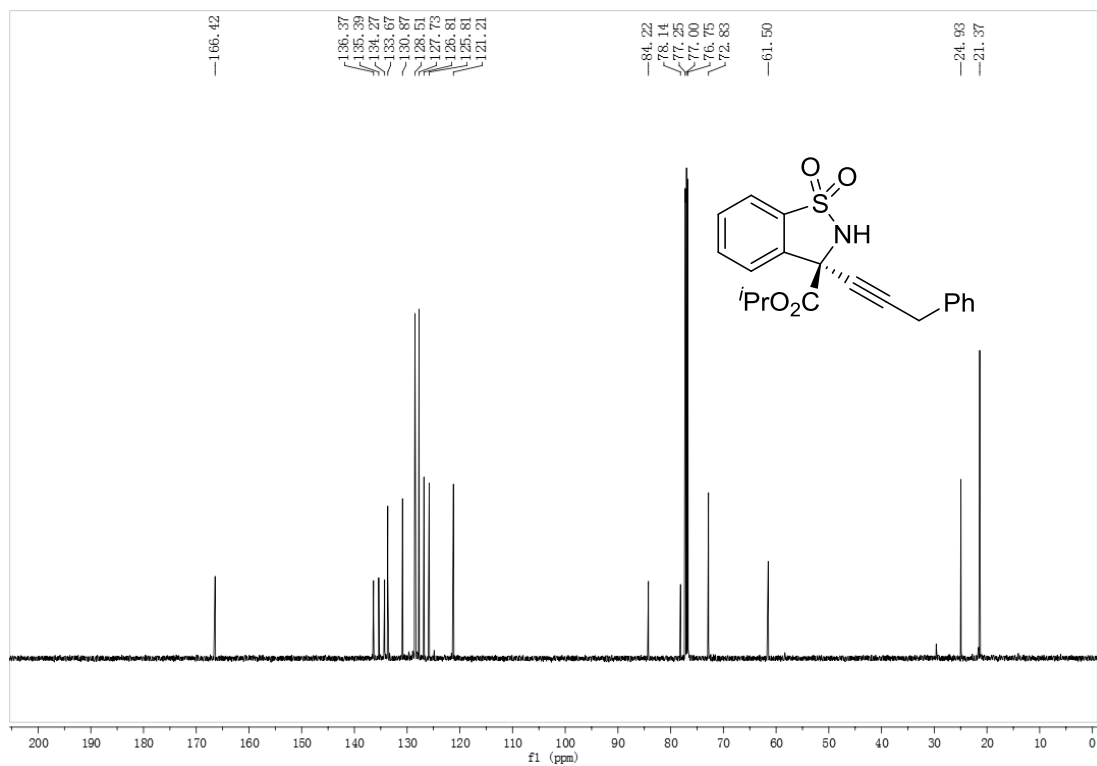
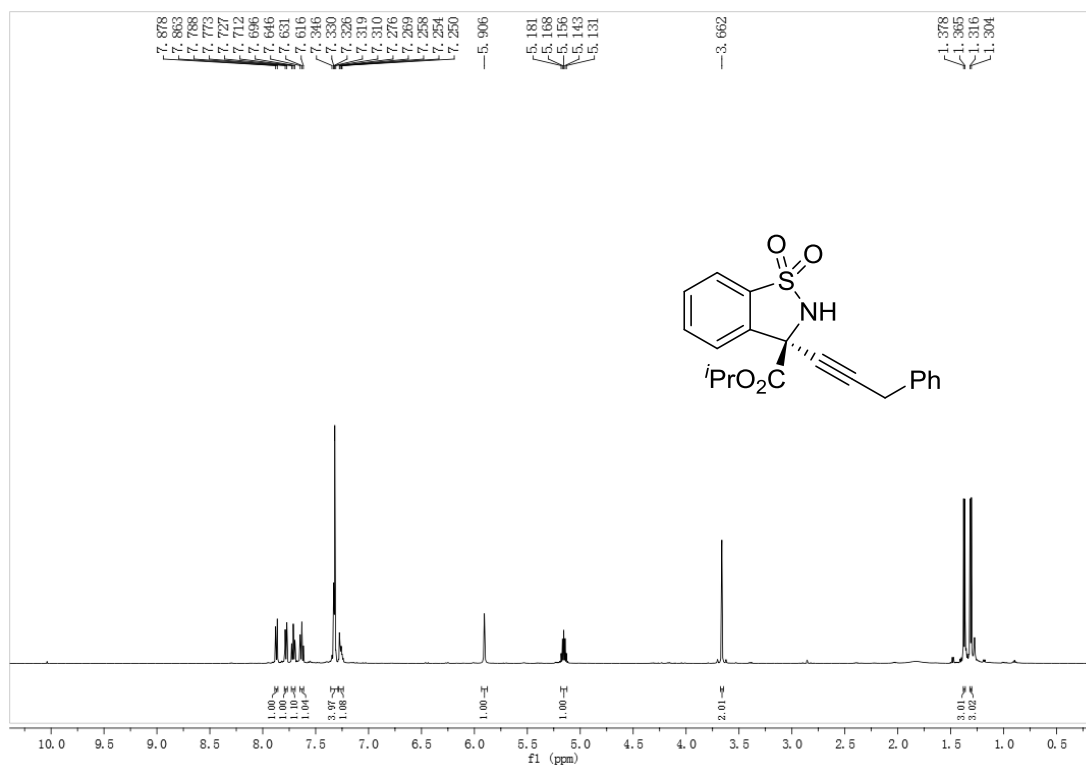


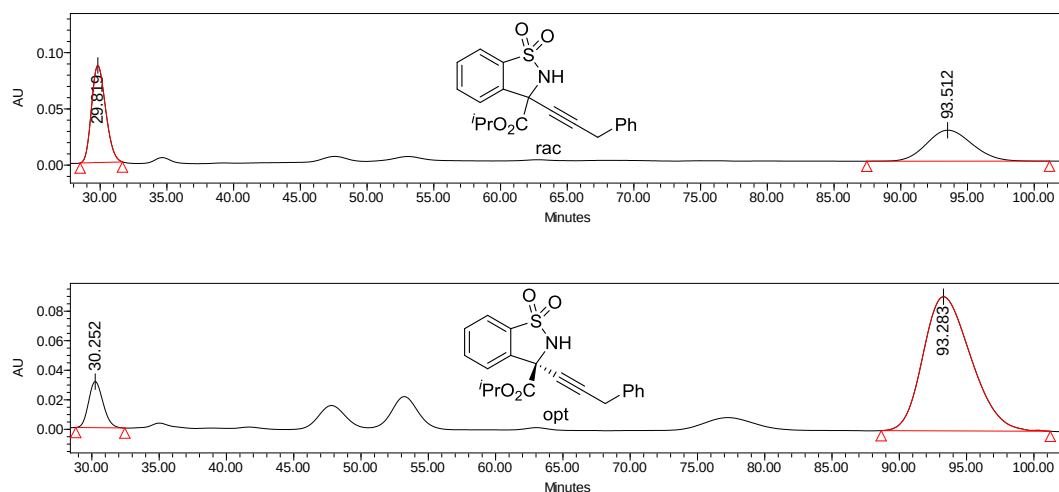
	Retention Time	Area	% Area	Height	% Height
1	25.525	6203933	10.15	136199	12.76
2	30.586	54893788	89.85	930817	87.24

Isopropyl 3-(3-phenylprop-1-yn-1-yl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3bq**)



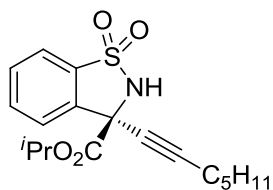
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:4 (v/v); yellow oil, 44% yield; $[\alpha]_D^{25} = 16.4$ ($c = 1.0$ in CHCl_3), 80% ee [Daicel Chiralcel AS-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 220 nm; $t_{\text{major}} = 93.3$ min, $t_{\text{minor}} = 30.3$ min]; ^1H NMR (500 MHz, CDCl_3) δ 7.87 (d, $J = 7.5$ Hz, 1H), 7.78 (d, $J = 8.0$ Hz, 1H), 7.71 (t, $J = 7.5$ Hz, 1H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.31-7.35 (m, 4H), 7.25-7.28 (m, 1H), 5.91 (s, 1H), 5.16 (dt, $J = 12.5, 6.5$ Hz, 1H), 3.66 (s, 2H), 1.37 (d, $J = 6.5$ Hz, 3H), 1.31 (d, $J = 6.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 166.4, 136.4, 135.4, 134.3, 133.7, 130.9, 128.5, 127.7, 126.8, 125.8, 121.2, 84.2, 78.1, 72.8, 61.5, 24.9, 21.4; HRMS m/z (ESI $^+$): calculated for $\text{C}_{20}\text{H}_{20}\text{NO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 370.1108, found 370.1100.



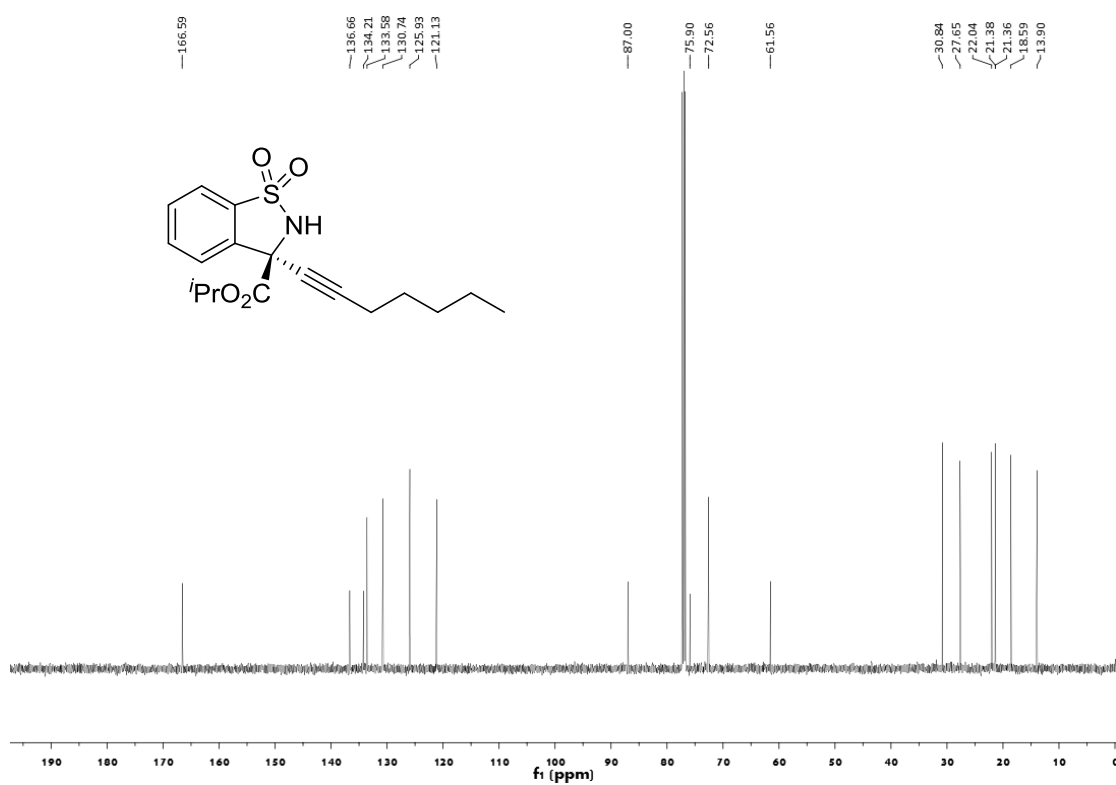
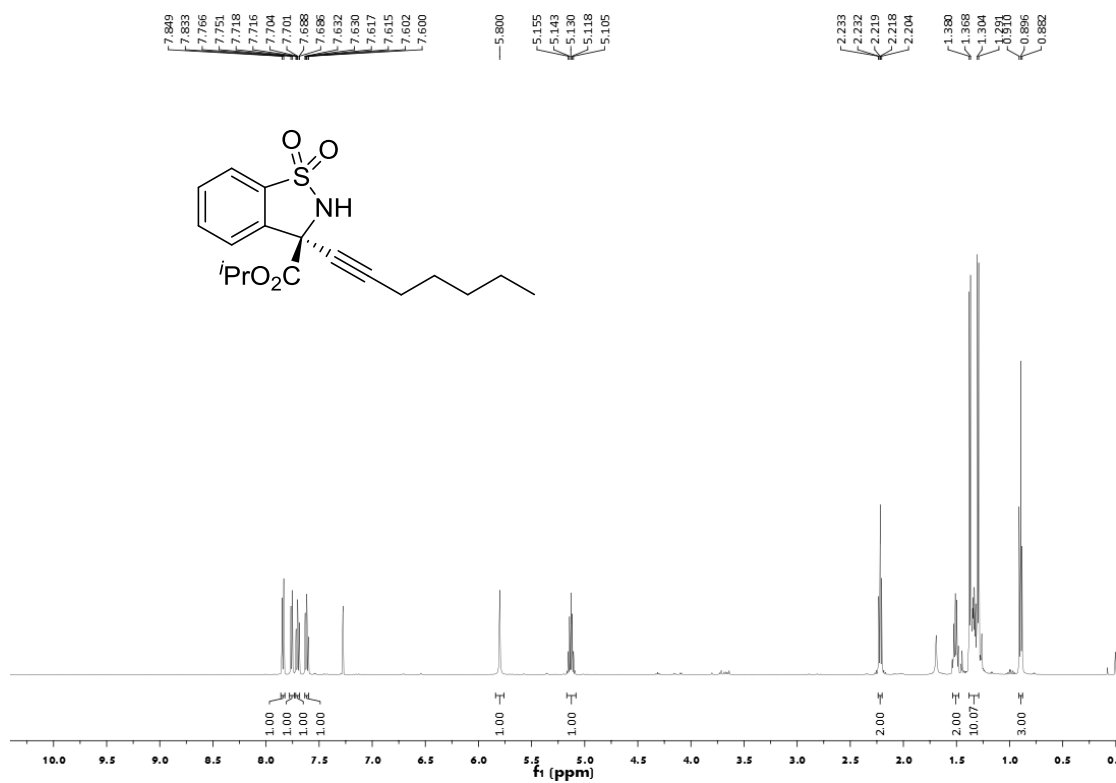


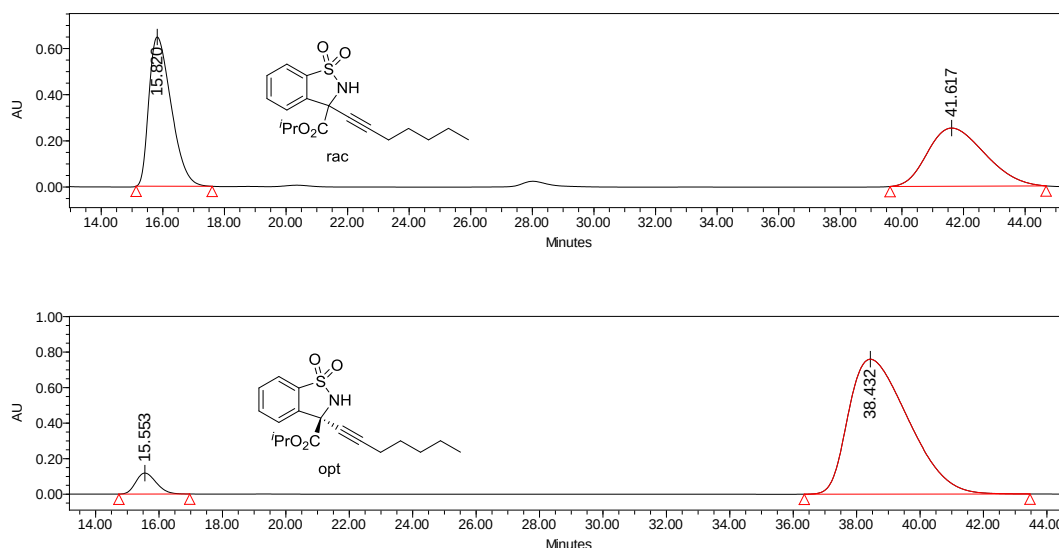
	Retention Time	Area	% Area	Height	% Height
1	30.252	2333883	9.42	31240	25.60
2	93.283	22436245	90.58	90812	74.40

Isopropyl 3-(hept-1-yn-1-yl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**3br**)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:3 (v/v); yellow oil, 37% yield; $[\alpha]_D^{15} = 74.5$ ($c = 1.0$ in CH_2Cl_2), 90% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 38.4$ min, $t_{\text{minor}} = 15.6$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.84 (d, $J = 8.0$ Hz, 1H), 7.76 (d, $J = 7.5$ Hz, 1H), 7.70 (td, $J = 7.0, 1.0$ Hz, 1H), 7.62 (td, $J = 7.5, 1.0$ Hz, 1H), 5.80 (s, 1H), 5.10-5.16 (m, 1H), 2.20-2.24 (m, 2H), 1.50 (dd, $J = 14.5, 7.5$ Hz, 2H), 1.29-1.38 (m, 10H), 0.90 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 166.6, 136.7, 134.2, 133.6, 130.7, 125.9, 121.1, 87.0, 75.9, 72.6, 61.6, 30.8, 27.7, 22.0, 21.38, 21.36, 18.6, 13.9; HRMS m/z (ESI $^+$): calculated for $\text{C}_{18}\text{H}_{24}\text{NO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 350.1421, found 350.1426.

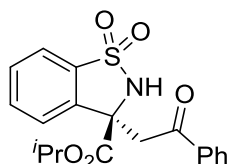




	Retention Time	Area	% Area	Height	% Height
1	15.553	5304102	5.07	118191	13.47
2	38.432	99362429	94.93	759295	86.53

4. Synthetic transformation of product 3ba

Isopropyl 3-(2-oxo-2-phenylethyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide (**4**)



To a dried Schlenk tube was added AuCl_3 (1.8 mg, 0.006 mmol) and compound **3ba** (106.6 mg, 0.3 mmol) under N_2 . Wet acetone (3.0 mL) was then added through a syringe, after which the resulting mixture was stirred at 25 °C for 12 h until the reaction was completed (monitored by TLC). The solvent was removed under vacuum and the residue was purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:2 (v/v), to give compound **4**, yellow oil, 75% yield; $[\alpha]_{\text{D}}^{15} = 186.4$ ($c = 1.0$ in CH_2Cl_2), 93% ee [Daicel Chiralcel AD-H column (25 cm $\times$ 0.46 cm ID), n -hexane/ i -PrOH = 80/20, 0.8 mL/min, 254 nm; $t_{\text{major}} = 55.3$ min, $t_{\text{minor}} = 60.0$ min]; ^1H NMR (500 MHz, CDCl_3): δ 7.92 (dd, $J = 8.5, 1.0$ Hz, 2H), 7.83 (d, $J = 7.5$ Hz, 1H), 7.71 (d, $J = 4.0$ Hz, 2H), 7.59-7.67 (m, 2H), 7.47 (t, $J = 8.0$ Hz, 2H), 6.10 (s,

¹H NMR spectrum (CDCl₃) of the compound, showing peaks in the aromatic region (7.275–7.929 ppm) and aliphatic region (1.227–1.392 ppm). The chemical structure of the compound is shown above the spectrum.

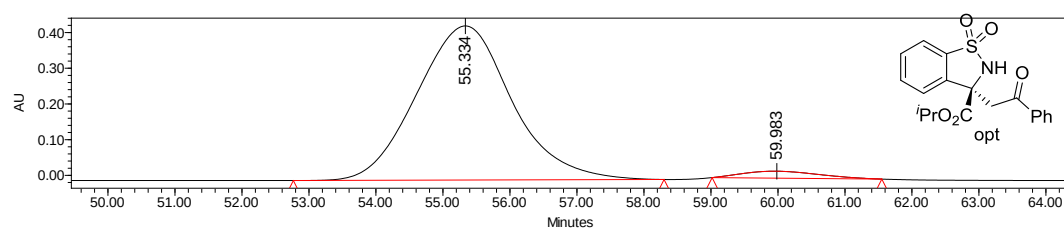
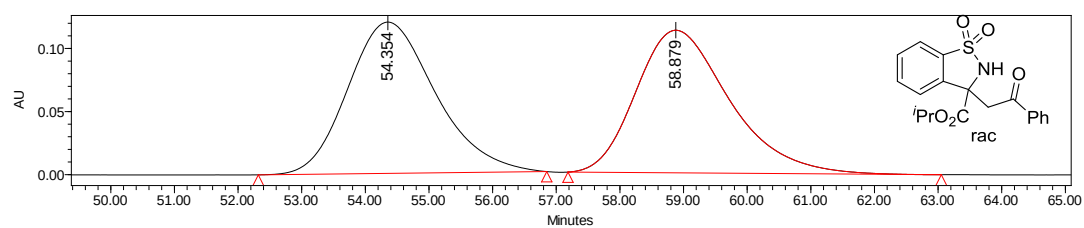
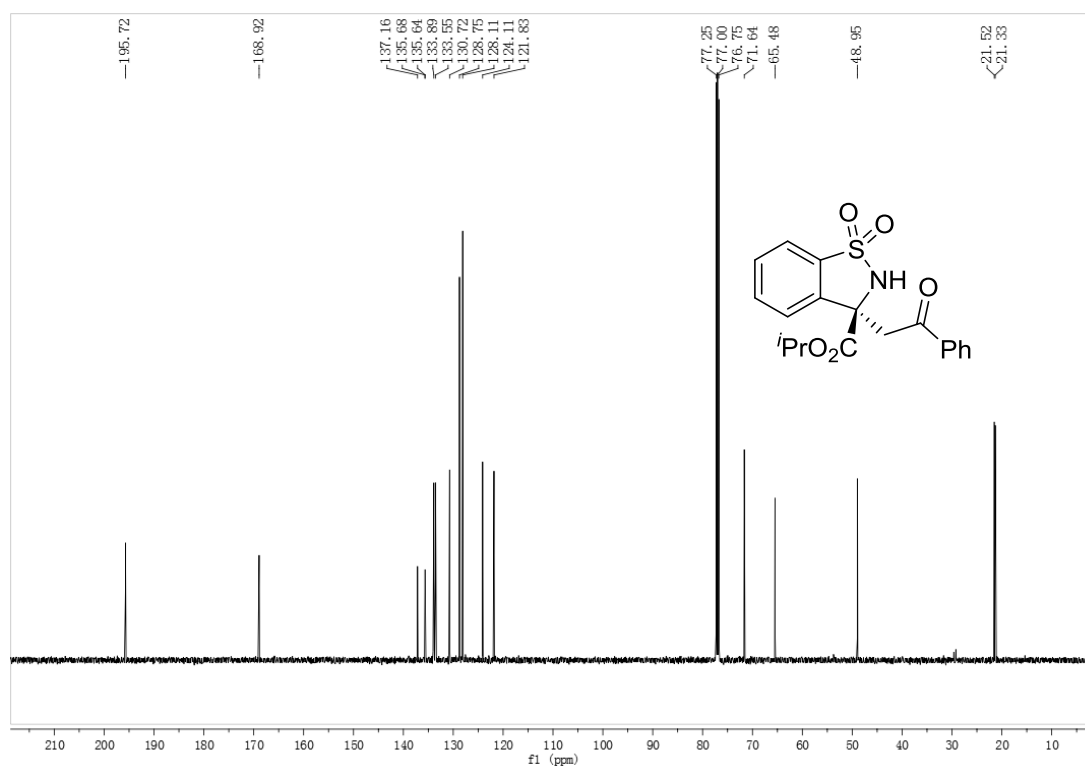
The chemical structure of the compound is shown above the spectrum. It is a benzothiazine derivative with a phenyl group and an isopropoxy group.

The ¹H NMR spectrum (CDCl₃) shows the following peaks (ppm):

- 7.929, 7.927, 7.912, 7.910, 7.841, 7.825, 7.717, 7.709, 7.662, 7.654, 7.641, 7.638, 7.607, 7.592, 7.489, 7.473, 7.468, 7.275
- 6.103
- 5.166, 5.153, 5.141
- 4.076, 4.041
- 3.757, 3.722
- 1.392, 1.329, 1.295, 1.240, 1.227

The integration values for the peaks are:

- 0.94
- 1.03
- 1.03
- 1.06
- 3.02, 3.02



	Retention Time	Area	% Area	Height	% Height
1	55.334	42637666	96.50	431665	95.68
2	59.983	1546008	3.50	19478	4.32

5. Computational study of mechanism

5.1 Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

5.2 Computational Methods

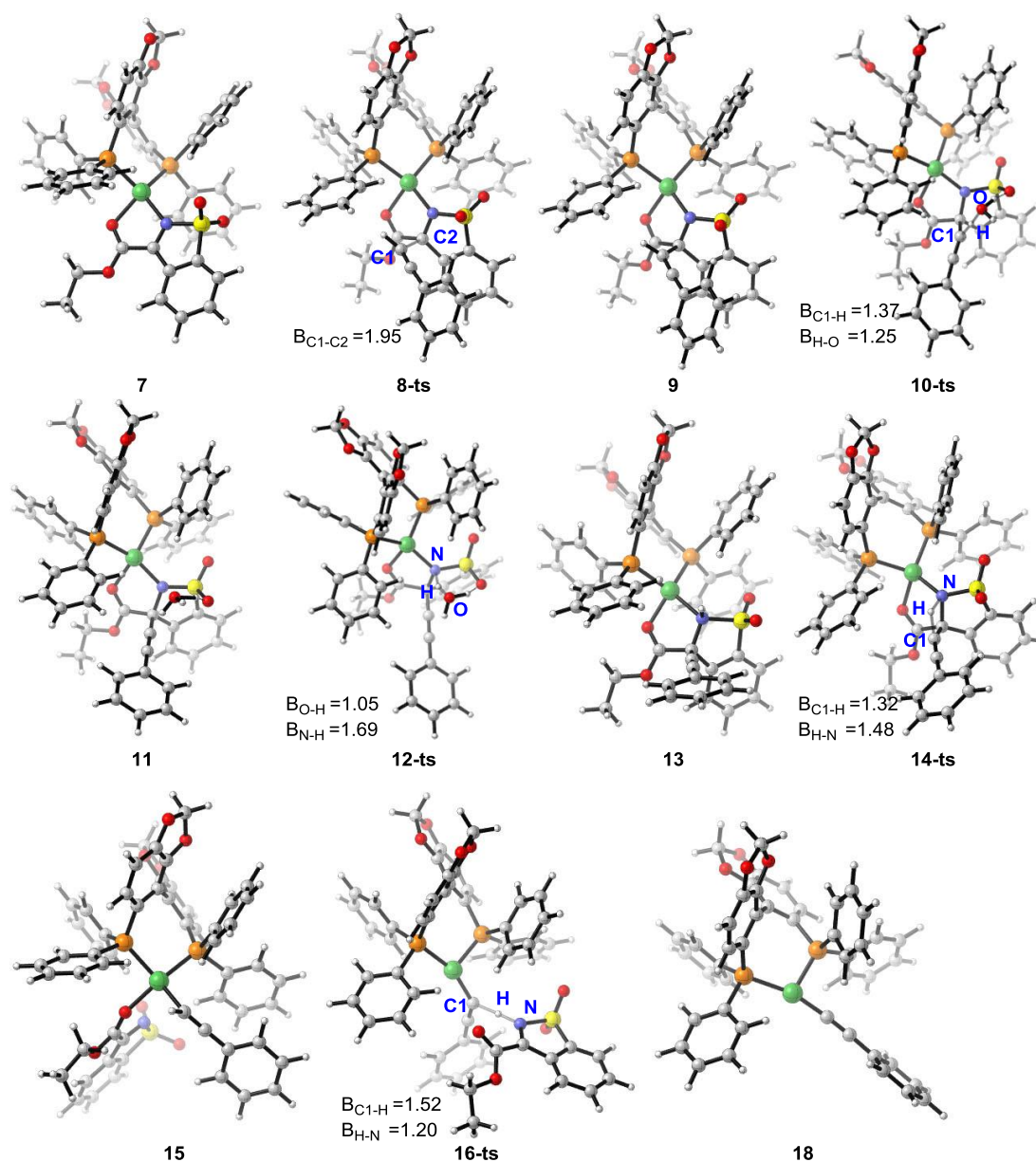
All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. Density functional theory B3LYP² with a standard 6-31G(d) basis set (SDD basis set for Ni) was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. M06-2X³ functional with basis set 6-311+G(d) (SDD basis set for Ni) was employed to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with a SMD continuum solvation model⁴. The energies given in this paper are M06-2X calculated Gibbs free energies

5.3 Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{\text{(elec-B3LYP)}}^1$	$G_{\text{(corr-B3LYP)}}^2$	$H_{\text{(corr-B3LYP)}}^3$	$E_{\text{(solv, M06-2X)}}^4$	IF^5
7	-3759.216652	0.655069	0.803769	-3759.075349	-
8-ts	-4067.594858	0.758394	0.921778	-4067.405666	-302.80
9	-4067.599173	0.759829	0.923323	-4067.415214	-
10-ts	-4144.016932	0.777124	0.945425	-4143.839313	-933.79
11	-4144.038367	0.780669	0.951264	-4143.872402	-
12-ts	-4144.024264	0.77909	0.947681	-4143.856715	-436.72
13	-4067.617339	0.758155	0.925232	-4067.453283	-
14-ts	-4067.549066	0.753366	0.918545	-4067.363308	-
15	-4067.604852	0.75632	0.922823	-4067.416633	-
16-ts	-4067.566444	0.745471	0.91779	-4067.354334	-825.76
17	-1140.577545	0.152091	0.210492	-1140.570766	-
18	-2927.024831	0.577536	0.711401	-2926.794694	-
phenylacetylene	-308.386937	0.079123	0.116977	-308.3412934	-
H₂O	-76.40702351	0.003474	0.024919	-76.42358466	-

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ³The thermal correction to enthalpy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M06-2X in dichloromethan (DCM) solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

5.4 Structures of Key Transition States



5.5 B3LYP Geometries for All the Optimized Compounds and Transition State

7				H	-1.37098400	-1.33919200	3.48287400
C	-4.15283000	0.26098100	1.40235100	H	-3.39319600	-0.50125300	4.64520800
C	-3.04272200	-0.18528000	0.70475100	C	-3.03064000	-0.06489500	-0.77892000
C	-2.00755800	-0.77515600	1.50229900	C	-2.09045800	0.70835800	-1.53350700
C	-2.15054600	-0.87197100	2.89483400	C	-4.01893400	-0.68847200	-1.52108900
C	-3.29126400	-0.40863400	3.57010400	C	-2.19424900	0.80527000	-2.92919600
C	-4.27988200	0.15733800	2.79294800	C	-4.10891300	-0.58707700	-2.91504700

C	-3.21053100	0.15868900	-3.65014400	H	0.02846300	2.48030700	2.02911400
H	-1.48404900	1.40809500	-3.48131100	C	-2.60206100	4.62517400	2.24835900
H	-3.28928400	0.24614900	-4.72757300	H	-3.03536800	5.35616100	2.92455900
O	-5.01866500	-1.48843800	-1.05782500	C	0.22881900	2.49660900	-1.89834400
O	-5.25696900	0.87362800	0.89047400	C	0.23786300	3.90037300	-1.91023600
C	-6.15923800	1.07396800	1.99289800	C	1.02896600	1.79015700	-2.81894300
C	-5.80077800	-1.87180200	-2.20321200	C	1.02158700	4.58485000	-2.84159800
P	-0.48810800	-1.40910800	0.70703900	H	-0.37034600	4.45835600	-1.20628900
P	-0.74090300	1.55625200	-0.66155600	C	1.80884600	2.48162300	-3.74571600
C	-1.01978300	-2.62949300	-0.53834300	H	1.03138200	0.70242600	-2.82718400
C	-2.09537200	-3.48803800	-0.24355000	C	1.80592300	3.87989800	-3.75761900
C	-0.34871100	-2.75035200	-1.76384800	H	2.40797100	4.41754900	-4.48411300
C	-2.47664100	-4.46380800	-1.16347700	O	-5.46244500	0.68667100	3.18802800
H	-2.63323500	-3.39571900	0.69518300	O	-5.16494900	-1.30690900	-3.36130800
C	-0.74158100	-3.72568200	-2.68161900	H	-7.04228800	0.43968500	1.86483000
H	0.48136300	-2.09663600	-2.00719000	H	-6.42896800	2.13087300	2.05527400
C	-1.80165600	-4.58323700	-2.38219200	H	-5.81062200	-2.96154900	-2.28933100
H	-2.10188900	-5.34470500	-3.09595700	H	-6.81254300	-1.46610500	-2.10950200
C	0.46073900	-2.27886500	2.00795600	Ni	0.87899500	0.25319300	0.11514100
C	0.53864500	-3.67853100	2.04984600	C	5.08959900	-0.24239200	-0.06749400
C	1.13551600	-1.51904200	2.98309300	C	6.32574300	0.38912800	0.11527900
C	1.26673300	-4.30581600	3.06214500	C	7.48648800	-0.31804200	-0.21349700
H	0.04144000	-4.27934500	1.29683200	C	7.42300100	-1.62165900	-0.71627300
C	1.85891900	-2.15191700	3.99231100	C	6.18807800	-2.26463000	-0.90800900
H	1.07467400	-0.43239000	2.97002200	C	5.05345700	-1.55059500	-0.57513700
C	1.92527900	-3.54816700	4.03159600	H	6.38494800	1.39594900	0.50902300
H	2.48808700	-4.04240800	4.81778400	H	8.45359900	0.15406200	-0.07429200
C	-1.48494100	2.74252400	0.50581000	H	8.33921700	-2.14838400	-0.96405600
C	-2.66242900	3.42274100	0.14862200	H	6.13616100	-3.27544800	-1.29913600
C	-0.87722000	3.00588900	1.74355100	C	3.73328000	0.23892100	0.19261100
C	-3.21162100	4.36522800	1.01791700	S	3.35277900	-2.08547700	-0.72471600
H	-3.14910800	3.21590200	-0.79971400	O	3.04031000	-3.19747300	0.15617900
C	-1.43802100	3.94331300	2.61124600	O	2.89593300	-2.05101900	-2.11077200

N 2.73449300 -0.57074200 -0.00576400
 C 3.28862000 1.61641200 0.60067700
 O 2.07706500 1.87077200 0.56794900
 O 4.22357600 2.45161800 0.94412300
 C 3.83190000 3.83721100 1.31423400
 C 5.10086700 4.60077600 1.61583100
 H 3.27329400 4.24234600 0.46724900
 H 3.16635900 3.75501500 2.17674500
 H 4.83486700 5.62486800 1.89741700
 H 5.75462400 4.65035100 0.74017300
 H 5.64777900 4.15199000 2.45003000
 H 2.36354100 -1.55981600 4.75030000
 H 1.31848400 -5.38991300 3.08985900
 H 1.00999300 5.67070100 -2.85668400
 H 2.40986800 1.92983000 -4.46252100
 H -3.29873900 -5.13277500 -0.92636400
 H -0.21518100 -3.81597300 -3.62691000
 H -4.11574400 4.89539200 0.73366500
 H -0.96976400 4.13978300 3.57127400

8-ts

C 5.02188400 0.00238100 -0.81297300
 C 3.78431400 -0.33441100 -0.28912600
 C 2.85325100 -0.90994900 -1.21210500
 C 3.21562400 -1.09287200 -2.55566600
 C 4.47856300 -0.73634900 -3.05580900
 C 5.36663300 -0.18914100 -2.15475900
 H 2.51273000 -1.54402400 -3.24327600
 H 4.74328100 -0.89375300 -4.09506400
 C 3.53942900 -0.09256000 1.15766500
 C 2.56089000 0.81228100 1.67945800
 C 4.35311100 -0.70201200 2.09758300
 C 2.47502100 1.05178100 3.05878000

C 4.24758200 -0.46284900 3.47211900
 C 3.31984700 0.41947300 3.98508100
 H 1.75129200 1.76052000 3.43939100
 H 3.25103700 0.62057800 5.04788300
 O 5.34541100 -1.60713100 1.86777000
 O 6.06526900 0.58573300 -0.15520300
 C 7.15040300 0.65032300 -1.09633100
 C 5.90552200 -1.93499500 3.15115700
 P 1.18281900 -1.43113000 -0.65578700
 P 1.40380100 1.62564000 0.52685100
 C 1.44672600 -2.60990400 0.71254600
 C 2.53262100 -3.50233900 0.66381800
 C 0.56089800 -2.65558700 1.79950600
 C 2.71169600 -4.43864600 1.68171500
 H 3.23758700 -3.46472400 -0.16110400
 C 0.75100600 -3.58965300 2.81795300
 H -0.28080500 -1.97325500 1.85698600
 C 1.82198800 -4.48361600 2.75855300
 H 1.96380600 -5.21402700 3.54973600
 C 0.48104600 -2.32255900 -2.09534400
 C 0.51728800 -3.72077600 -2.18135000
 C -0.07053400 -1.57869600 -3.15237900
 C 0.01848600 -4.36249300 -3.31539100
 H 0.91698300 -4.31083800 -1.36430300
 C -0.56668700 -2.22505000 -4.28417600
 H -0.09582200 -0.49205300 -3.10217400
 C -0.52245000 -3.61941500 -4.36612900
 H -0.90775200 -4.12407100 -5.24714700
 C 2.38437900 2.63427400 -0.63577800
 C 3.54839000 3.28628100 -0.19309000
 C 1.95941000 2.79636300 -1.96364400
 C 4.26768200 4.09791900 -1.07025600
 H 3.89420200 3.15776300 0.82829600

C	2.68865100	3.60375900	-2.83734800	O	-3.05393400	-1.98294300	1.51241900
H	1.06308300	2.29355500	-2.31346200	N	-2.02205500	-0.48113000	-0.32545200
C	3.84025300	4.25617800	-2.39147500	C	-2.43130200	1.62514900	-1.29321700
H	4.40540700	4.88537900	-3.07273300	O	-1.24340600	1.88957900	-1.05007300
C	0.38980700	2.78783200	1.52515600	O	-3.22330400	2.37777800	-2.00238000
C	0.47992600	4.17690100	1.35082800	C	-2.68550600	3.64190000	-2.55336900
C	-0.52319500	2.27112900	2.46642900	C	-3.80234000	4.31003400	-3.32359500
C	-0.31524600	5.03397000	2.11587000	H	-2.33406600	4.23670100	-1.70666400
H	1.17570500	4.59362700	0.63082900	H	-1.83169900	3.38158700	-3.18320000
C	-1.30819600	3.13371200	3.23398400	H	-3.43051600	5.25136800	-3.74106100
H	-0.60316300	1.19740900	2.62118900	H	-4.65183400	4.53940900	-2.67360200
C	-1.20590300	4.51737400	3.05836800	H	-4.14443400	3.68314600	-4.15226300
H	-1.81159200	5.18833500	3.66023200	H	-0.98175300	-1.64309300	-5.10212900
O	6.63093100	0.25043800	-2.37405600	H	0.05069000	-5.44626100	-3.37416700
O	5.16765600	-1.19966800	4.14062100	H	-0.22685800	6.10804200	1.98166600
H	7.94234000	-0.04240600	-0.79200800	H	-1.98927200	2.72577100	3.97561300
H	7.51812200	1.67719800	-1.15823600	C	-3.64986100	1.29764000	0.89635900
H	5.79119300	-3.00696200	3.33508100	C	-4.77083000	0.97626000	1.36080200
H	6.95626100	-1.63176600	3.18142000	H	-2.82389900	1.89257400	1.26146400
Ni	-0.18932200	0.29931900	-0.30083400	C	-5.99808600	0.50336500	1.80089800
C	-4.22444100	-0.34590300	-1.24959000	C	-6.05765200	-0.73624400	2.50385300
C	-5.30316900	0.13089100	-1.99456700	C	-7.18605100	1.26110300	1.58879100
C	-6.29044400	-0.77800300	-2.39307000	C	-7.27814400	-1.19186800	2.97586300
C	-6.21883400	-2.13076200	-2.04292100	H	-5.14393600	-1.30453600	2.64408500
C	-5.15069400	-2.61141800	-1.27738700	C	-8.39398500	0.78685400	2.06993500
C	-4.17621800	-1.69703000	-0.90430800	H	-7.12720300	2.20645100	1.05936500
H	-5.37104100	1.17477200	-2.27593200	C	-8.43938300	-0.43447800	2.76217300
H	-7.12464300	-0.42487100	-2.99152400	H	-7.33602600	-2.13310100	3.51299300
H	-6.99419900	-2.81561000	-2.37168600	H	-9.30407700	1.35806200	1.91811900
H	-5.07714100	-3.65913600	-1.00386000	H	-9.39095100	-0.79704500	3.14040900
C	-3.02339600	0.37161200	-0.69715200	H	0.05805700	-3.62151400	3.65321500
S	-2.71623400	-1.99988900	0.08119800	H	3.54452700	-5.13401700	1.63110200
O	-1.89852800	-3.08854700	-0.43872800	H	5.16195900	4.60599100	-0.72157800

H 2.36083900 3.72149700 -3.86607800

9

C 5.00489900 -0.01124600 -0.80247400

C 3.76537900 -0.34588100 -0.28158900

C 2.83356000 -0.91743700 -1.20649600

C 3.19895500 -1.09808300 -2.54918100

C 4.46386800 -0.74334100 -3.04675100

C 5.35198900 -0.20072100 -2.14346800

H 2.49633900 -1.54580000 -3.23925500

H 4.72942900 -0.89891600 -4.08609500

C 3.52054400 -0.10125700 1.16523400

C 2.55127700 0.81568200 1.68200200

C 4.32579700 -0.71574700 2.10902500

C 2.46337900 1.06156700 3.05964700

C 4.21850600 -0.47097200 3.48228000

C 3.29915800 0.42310400 3.99016400

H 1.74483700 1.77868300 3.43502700

H 3.23027200 0.62808600 5.05224000

O 5.31163800 -1.62951200 1.88477300

O 6.04847600 0.56900800 -0.14099300

C 7.13649300 0.62849400 -1.07872800

C 5.85506700 -1.96926000 3.17175900

P 1.15764000 -1.43681600 -0.65251900

P 1.40452800 1.62779400 0.51918500

C 1.43964800 -2.61888100 0.71202200

C 2.51743500 -3.51931600 0.64271200

C 0.58407400 -2.64909300 1.82308900

C 2.71787900 -4.44860500 1.66333000

H 3.20081000 -3.49325800 -0.20065400

C 0.79631800 -3.57398300 2.84524300

H -0.25043600 -1.95967800 1.89340200

C 1.85857100 -4.47683000 2.76485800

H 2.01674700 -5.20110300 3.55865500

C 0.46665900 -2.32661700 -2.09988300

C 0.51779600 -3.72337700 -2.19796100

C -0.08970500 -1.57984800 -3.15152400

C 0.02946800 -4.36067600 -3.33894600

H 0.91968500 -4.31614300 -1.38396200

C -0.57539500 -2.22163700 -4.29080000

H -0.12988900 -0.49437100 -3.09020400

C -0.51573900 -3.61436600 -4.38539200

H -0.89234800 -4.11543000 -5.27227400

C 2.39407800 2.64508800 -0.62857900

C 3.55326000 3.29807500 -0.17503600

C 1.98078800 2.80765700 -1.96008500

C 4.27934700 4.11145100 -1.04502600

H 3.89067900 3.16774100 0.84897000

C 2.71645300 3.61716500 -2.82644300

H 1.08947400 2.30196300 -2.31847200

C 3.86323500 4.27059200 -2.36975600

H 4.43399100 4.90067500 -3.04554200

C 0.37559200 2.78694400 1.51039900

C 0.45819500 4.17647900 1.33955500

C -0.55332600 2.26343300 2.43224300

C -0.36115300 5.02780900 2.08631300

H 1.16708900 4.59877400 0.63557300

C -1.36159100 3.11972900 3.18301200

H -0.62664700 1.18918700 2.58458000

C -1.26819500 4.50456300 3.00895300

H -1.89065700 5.17097200 3.59877600

O 6.61851900 0.23721800 -2.35933800

O 5.13020000 -1.21428200 4.15611700

H 7.92245100 -0.07116600 -0.77408500

H 7.51236700 1.65273500 -1.13565700

H 5.71267500 -3.03799400 3.35649800

H 6.91285200 -1.69275600 3.20809200
 Ni -0.19806400 0.30411700 -0.28976800
 C -4.15635300 -0.26653000 -1.30585900
 C -5.17584800 0.20915000 -2.12989100
 C -6.03669300 -0.71828200 -2.72966500
 C -5.89858700 -2.09160600 -2.49976400
 C -4.89341300 -2.57169800 -1.65472100
 C -4.04070900 -1.63743900 -1.08093400
 H -5.29293500 1.26929400 -2.32246300
 H -6.82081800 -0.36315200 -3.39156600
 H -6.57406300 -2.79047000 -2.98340600
 H -4.77053500 -3.63366900 -1.46688300
 C -3.08773000 0.49895900 -0.51119500
 S -2.70934200 -1.92696700 0.07893500
 O -1.79528800 -2.98562300 -0.33872100
 O -3.28410900 -2.00818800 1.43669400
 N -2.02836700 -0.41164600 -0.16626500
 C -2.43542900 1.71216500 -1.17316500
 O -1.21827200 1.89624400 -1.04634300
 O -3.23827000 2.54094900 -1.78164100
 C -2.66248300 3.76862600 -2.37455000
 C -3.80176400 4.55305100 -2.98624900
 H -2.15579700 4.30703000 -1.56996000
 H -1.92111400 3.45260500 -3.11217800
 H -3.40202600 5.47036900 -3.43052900
 H -4.54063500 4.83586900 -2.23067900
 H -4.29860400 3.98279700 -3.77667100
 H -0.99503200 -1.63664400 -5.10428800
 H 0.07314800 -5.44359600 -3.40672000
 H -0.27713000 6.10262200 1.95484300
 H -2.04813400 2.70693700 3.91749400
 C -3.72643000 1.11738300 0.82966000
 C -4.87663400 0.77535900 1.28274200

H -3.05703000 1.76689500 1.39578400
 C -6.06760200 0.32545300 1.77947800
 C -6.09728100 -0.91133900 2.50913600
 C -7.27139600 1.08490600 1.59932300
 C -7.29537500 -1.35116200 3.04087600
 H -5.17765500 -1.48010700 2.60038900
 C -8.45228100 0.62121300 2.14083400
 H -7.23266500 2.01739900 1.04602300
 C -8.46217500 -0.59003400 2.86016100
 H -7.33714500 -2.28376800 3.59391500
 H -9.37130400 1.18474400 2.01830200
 H -9.39785300 -0.94431000 3.28401300
 H 0.12714300 -3.59317000 3.70016300
 H 3.54390900 -5.15065800 1.59565500
 H 5.17049600 4.61952400 -0.68836500
 H 2.39792100 3.73475500 -3.85811700

10-ts

C 4.88569000 -0.72023800 1.17404500
 C 3.79311700 -0.26603000 0.45401100
 C 3.03633000 0.78522700 1.06387000
 C 3.41372400 1.28412300 2.31983300
 C 4.52588100 0.79728700 3.02697200
 C 5.24828300 -0.20938300 2.42366200
 H 2.84885400 2.09131800 2.76698100
 H 4.80601500 1.20141100 3.99298300
 C 3.50949900 -0.88240300 -0.86955600
 C 2.32856900 -1.62808600 -1.18274900
 C 4.46203400 -0.82007000 -1.87240200
 C 2.18465500 -2.24556800 -2.43349100
 C 4.30039700 -1.43213700 -3.12000200
 C 3.17135500 -2.16140000 -3.42940500
 H 1.29535400 -2.82357000 -2.65028900

H 3.05474900 -2.65085200 -4.38943800
 O 5.66331300 -0.17805100 -1.83228300
 O 5.74039100 -1.72776200 0.82971700
 C 6.75798500 -1.75572700 1.84474600
 C 6.28180500 -0.38648800 -3.11304000
 P 1.58900800 1.51822900 0.19621500
 P 0.98124400 -1.70866300 0.04475400
 C 2.24741400 2.10992100 -1.40273500
 C 3.51271000 2.72030400 -1.45805400
 C 1.50242300 1.95852800 -2.58087200
 C 4.00791100 3.19245400 -2.67366700
 H 4.11267800 2.82323400 -0.55892200
 C 2.00751800 2.42158800 -3.79537200
 H 0.52929400 1.47991700 -2.55158100
 C 3.25672800 3.04407900 -3.84253500
 H 3.64439700 3.41256900 -4.78783000
 C 1.12677700 2.95204800 1.24489000
 C 1.55545800 4.25385400 0.95360800
 C 0.34827400 2.72198900 2.39142300
 C 1.21863400 5.30637100 1.80539600
 H 2.13519200 4.45338900 0.05931500
 C 0.01483300 3.77748600 3.24053700
 H 0.01520400 1.71476100 2.63275600
 C 0.45050400 5.07218400 2.94763900
 H 0.19341400 5.89478200 3.60846500
 C 1.64078800 -2.48436700 1.56073800
 C 2.62885900 -3.48027700 1.47668900
 C 1.12645000 -2.12073700 2.81495800
 C 3.08443100 -4.10887500 2.63575100
 H 3.04506100 -3.75927600 0.51330400
 C 1.59223100 -2.74895300 3.97060900
 H 0.36536500 -1.34999300 2.88731100
 C 2.56841800 -3.74396200 3.88219300

H 2.92904500 -4.23214000 4.78277400
 C -0.27413900 -2.87038600 -0.63371300
 C -0.45958200 -4.15256700 -0.09401600
 C -1.07354800 -2.45818500 -1.71626600
 C -1.41209100 -5.01438000 -0.64212400
 H 0.14478300 -4.48684800 0.74217500
 C -2.01831800 -3.32622000 -2.26444600
 H -0.94957400 -1.46782700 -2.14630400
 C -2.18702900 -4.60739600 -1.73053900
 H -2.90770200 -5.29107700 -2.17072400
 O 6.34367000 -0.86246800 2.88959000
 O 5.38810800 -1.19622400 -3.89413400
 H 7.70739800 -1.40815000 1.42279800
 H 6.84488900 -2.76852300 2.24495600
 H 6.42576200 0.57794800 -3.60931700
 H 7.22983200 -0.91560700 -2.98075400
 Ni -0.20668600 0.17416800 0.19290600
 C -3.83559000 2.07450100 0.53430600
 C -4.95917600 2.21185200 1.34921100
 C -5.48569600 3.49196900 1.55163400
 C -4.92398900 4.61622400 0.93399500
 C -3.81612900 4.48225300 0.09371200
 C -3.29865000 3.20402200 -0.07774800
 H -5.41047200 1.35252700 1.83175900
 H -6.34616400 3.61469500 2.20242300
 H -5.35272000 5.59830900 1.10697600
 H -3.36890000 5.34007400 -0.39807300
 C -3.07802700 0.79802000 0.11309900
 S -1.93174000 2.70811500 -1.10424500
 O -0.73582900 3.52553100 -0.93931700
 O -2.43770800 2.61143900 -2.51737700
 N -1.78178100 1.19882500 -0.44965900
 C -2.76182700 -0.20266200 1.23156400

O -1.63894400 -0.71405000 1.31300500
 O -3.75501500 -0.50918800 2.02268300
 C -3.52746700 -1.51921400 3.07628400
 C -4.84035500 -1.71972400 3.80055100
 H -3.16802500 -2.42645100 2.58466900
 H -2.73971500 -1.13481300 3.72854500
 H -4.70225400 -2.46863000 4.58711500
 H -5.61759000 -2.07981900 3.11984400
 H -5.18057100 -0.79266100 4.27118600
 H -0.57890900 3.58951000 4.13064200
 H 1.55607800 6.31188200 1.57234500
 H -1.53443900 -6.01065500 -0.22727800
 H -2.60897900 -3.00475900 -3.11757900
 C -3.98417300 0.00391600 -0.86261900
 C -5.00176100 -0.72671500 -0.81276400
 H -3.56757600 0.06836500 -2.16137600
 C -6.13940000 -1.53034700 -0.90925100
 C -7.42104400 -0.92921200 -1.03918600
 C -6.02195400 -2.94618700 -0.86635600
 C -8.55021800 -1.72998800 -1.12120600
 H -7.50053400 0.15267400 -1.07189100
 C -7.16170100 -3.73116200 -0.95124400
 H -5.03718200 -3.39474200 -0.77792800
 C -8.42045700 -3.12529100 -1.07758700
 H -9.53185700 -1.27835300 -1.22137500
 H -7.08217000 -4.81314700 -0.92281100
 H -9.30856300 -3.74696000 -1.14491200
 H 4.97948300 3.67698400 -2.70577600
 H 1.42322200 2.30277300 -4.70290500
 H 3.84290100 -4.88297300 2.56466700
 H 1.19690000 -2.45994900 4.94010700
 O -3.02526400 0.26477400 -3.27124400
 H -2.66899700 1.21879700 -3.10221300

H -3.71520100 0.34285100 -3.95821900

11

C 5.02027100 -0.24110800 0.79589400
 C 3.81006900 -0.03241000 0.15465500
 C 3.06743500 1.11346000 0.58387500
 C 3.57117800 1.93868000 1.60095400
 C 4.80129800 1.69641500 2.23397900
 C 5.50856900 0.59334200 1.80617800
 H 3.01286600 2.81235900 1.90992000
 H 5.17786900 2.34961200 3.01270000
 C 3.39904700 -0.98219900 -0.91280600
 C 2.23861100 -1.81946100 -0.86014100
 C 4.21458200 -1.15791700 -2.01809300
 C 1.98641800 -2.75284800 -1.87635200
 C 3.94436300 -2.08659200 -3.02928700
 C 2.83746700 -2.90807100 -2.98233600
 H 1.11919700 -3.39689800 -1.81098000
 H 2.63893600 -3.64163800 -3.75516100
 O 5.36364300 -0.48715000 -2.31202700
 O 5.89444200 -1.26914300 0.59419700
 C 7.03449100 -0.99926600 1.42826300
 C 5.85042900 -1.03121200 -3.55063800
 P 1.46760000 1.53636700 -0.21285300
 P 1.05579700 -1.62922800 0.51640500
 C 1.83827500 1.72165900 -1.99218500
 C 3.02447100 2.35780300 -2.39862400
 C 0.95177200 1.22759000 -2.96064800
 C 3.30122600 2.51795200 -3.75628600
 H 3.73334300 2.72038700 -1.66025700
 C 1.23967300 1.38176000 -4.31670000
 H 0.04381800 0.71356100 -2.65996000
 C 2.40954700 2.03173100 -4.71584300

H 2.62791900 2.15610900 -5.77243400
 C 1.03101700 3.17089700 0.49901600
 C 1.30666900 4.37177200 -0.16924900
 C 0.43631200 3.21076600 1.77204800
 C 1.00106700 5.59256000 0.43368300
 H 1.74313000 4.36006400 -1.16185500
 C 0.13385100 4.43396800 2.37123300
 H 0.22697200 2.28679600 2.30716500
 C 0.41648800 5.62719500 1.70134700
 H 0.18442400 6.58022700 2.16745700
 C 1.94534000 -1.94227800 2.07924200
 C 2.99486900 -2.87629400 2.11987900
 C 1.54634400 -1.29451200 3.25889500
 C 3.62745900 -3.16039300 3.33027600
 H 3.31973300 -3.37645800 1.21244500
 C 2.18961600 -1.57791500 4.46419100
 H 0.73396800 -0.57489500 3.23615100
 C 3.22777500 -2.51154400 4.50164500
 H 3.72563100 -2.73213600 5.44122700
 C -0.18806300 -2.96878200 0.33545000
 C -0.23632800 -4.04687600 1.23284000
 C -1.12133600 -2.90416400 -0.71627500
 C -1.18994700 -5.05366800 1.06868900
 H 0.47340600 -4.11030100 2.05029800
 C -2.06506700 -3.91836400 -0.87878800
 H -1.10209600 -2.07533300 -1.41986000
 C -2.10094000 -4.99462500 0.01249600
 H -2.82998300 -5.78861800 -0.12094300
 O 6.70153900 0.12759200 2.25369600
 O 4.90980400 -2.02977100 -3.97839700
 H 7.89742300 -0.74985900 0.80151700
 H 7.23628700 -1.86678100 2.06091200
 H 5.90402400 -0.23735600 -4.30097900

H 6.82676300 -1.49740900 -3.38839900
 Ni -0.22273300 0.19067700 0.37266000
 C -3.88557600 2.05073500 0.88805100
 C -4.88171400 2.32399400 1.82233700
 C -5.44464000 3.60579300 1.84199500
 C -5.04831400 4.59550600 0.93402400
 C -4.07223400 4.32439300 -0.02778800
 C -3.51789200 3.05053200 -0.01208300
 H -5.21271900 1.56650600 2.52271700
 H -6.20945000 3.83494900 2.57770200
 H -5.50587800 5.57882900 0.97224300
 H -3.75730200 5.07186100 -0.74846000
 C -3.15259400 0.72128700 0.59186500
 S -2.29844300 2.36664700 -1.09152900
 O -1.18514700 3.21071300 -1.48898600
 O -3.17329000 1.95715100 -2.36157300
 N -1.94100800 1.06001000 -0.22974000
 C -2.61119000 -0.03796800 1.81220600
 O -1.45629500 -0.48454000 1.81331100
 O -3.46485100 -0.22473800 2.77626500
 C -3.05672100 -1.04962000 3.93486700
 C -4.24601600 -1.13954900 4.86476300
 H -2.74628600 -2.02081400 3.54207700
 H -2.19478800 -0.55864600 4.39322400
 H -3.97514900 -1.75602600 5.72810400
 H -5.10256200 -1.60504100 4.36872100
 H -4.53961200 -0.15198000 5.23257700
 H -0.31438900 4.45583600 3.36046900
 H 1.22021800 6.51777200 -0.09087600
 H -1.21014500 -5.89056000 1.76048600
 H -2.76952100 -3.87320400 -1.70440800
 C -4.07993100 -0.20486700 -0.08714800
 C -4.92294700 -0.95007700 -0.55061900

H	-3.12558400	-0.78065200	-3.90111800	C	4.09672700	-1.94750700	-3.07343400
C	-5.91525500	-1.79894500	-1.13232200	C	3.00723200	-2.79298700	-3.10759400
C	-6.90256500	-1.25082700	-1.97701400	H	1.25838700	-3.37295200	-2.03027100
C	-5.92118300	-3.18207900	-0.85906300	H	2.85676600	-3.49619300	-3.91854000
C	-7.87286900	-2.07708800	-2.53739400	O	5.45620000	-0.36172000	-2.22259700
H	-6.90442700	-0.18381200	-2.17815200	O	5.86977000	-1.31540400	0.66168500
C	-6.89880800	-3.99694800	-1.42329400	C	6.96478900	-1.09984100	1.56893800
H	-5.16561500	-3.60006000	-0.20086100	C	5.99980300	-0.83313600	-3.46761300
C	-7.87296900	-3.44788300	-2.26259300	P	1.46753300	1.52066200	-0.18102500
H	-8.63392200	-1.65159600	-3.18430100	P	1.06571000	-1.69390400	0.37132600
H	-6.90633000	-5.06074300	-1.20584300	C	1.93572900	1.81895400	-1.92238400
H	-8.63459500	-4.08720300	-2.69869900	C	3.13939800	2.48249700	-2.21870900
H	4.21297200	3.02210300	-4.06298000	C	1.11159700	1.38784100	-2.97177600
H	0.55122200	0.99528700	-5.06238000	C	3.49213900	2.73144700	-3.54521300
H	4.43230900	-3.88904400	3.35765500	H	3.80247600	2.79976900	-1.41960300
H	1.88243800	-1.06978100	5.37363800	C	1.47415000	1.62820900	-4.29654400
O	-2.75046400	-0.51515300	-3.04385000	H	0.18779900	0.86013700	-2.75812800
H	-3.32415500	-0.91028300	-2.35903000	C	2.66080600	2.30605200	-4.58449200
H	-2.93309700	1.02208400	-2.70527600	H	2.93789400	2.50057000	-5.61641000
12-ts				C	0.99642500	3.10632600	0.61519700
C	4.98164600	-0.30428000	0.88492000	C	1.29291100	4.34703700	0.03475600
C	3.80082100	-0.06051400	0.20242400	C	0.35429100	3.06561000	1.86457200
C	3.03215200	1.05490000	0.66427400	C	0.96314600	5.52696500	0.70228300
C	3.48525200	1.81894800	1.75072200	H	1.76504300	4.39836800	-0.93997100
C	4.68563800	1.54166700	2.42530600	C	0.02626900	4.24843600	2.52842400
C	5.41761900	0.46784500	1.96622000	H	0.13159100	2.11006600	2.33521400
H	2.91064100	2.67242000	2.08454800	C	0.33176100	5.48159000	1.94727600
H	5.02246400	2.14829400	3.25806100	H	0.08195300	6.40327400	2.46448400
C	3.44493500	-0.95260300	-0.93268500	C	1.90095400	-2.07122500	1.94994600
C	2.29935800	-1.81136400	-0.96683100	C	2.91335700	-3.04559600	1.99094000
C	4.30748200	-1.06198100	-2.01021100	C	1.50635900	-1.42900600	3.13360500
C	2.10924200	-2.70441400	-2.03194100	C	3.51267300	-3.37552700	3.20644900
				H	3.23530500	-3.54140000	1.07999700

C	2.11603200	-1.75897800	4.34465300	O	-3.15250700	2.13350400	-2.38175700
H	0.72640700	-0.67447900	3.10898500	N	-2.00670100	0.89798100	-0.41723800
C	3.11649900	-2.73284400	4.38266800	C	-2.62488500	-0.21464100	1.66224000
H	3.58856000	-2.98917200	5.32648800	O	-1.46665200	-0.65294200	1.63331200
C	-0.16879700	-3.02812900	0.09647600	O	-3.47419800	-0.48394000	2.61005000
C	-0.33218900	-4.06861200	1.02376600	C	-3.05831400	-1.39416600	3.70009900
C	-1.00326300	-2.98327100	-1.03665300	C	-4.24693100	-1.56721100	4.61895300
C	-1.29890200	-5.05418600	0.81127600	H	-2.74038700	-2.32803300	3.23024000
H	0.30028000	-4.12068700	1.90292500	H	-2.19973600	-0.93474600	4.19597600
C	-1.96086000	-3.97526000	-1.24859700	H	-3.97199900	-2.24967000	5.42975500
H	-0.88110700	-2.19386200	-1.77411400	H	-5.10037600	-1.99590100	4.08599400
C	-2.11110800	-5.01268400	-0.32331200	H	-4.54740600	-0.61468600	5.06524000
H	-2.84853800	-5.79168800	-0.49318600	H	-0.45854000	4.20720700	3.49962400
O	6.59034600	-0.02173100	2.44051600	H	1.20060300	6.48346700	0.24624500
O	5.09901500	-1.83075200	-3.97666300	H	-1.40470000	-5.86363900	1.52756400
H	7.85993700	-0.81832700	1.00428900	H	-2.57771100	-3.94941800	-2.14266900
H	7.13140900	-2.00387200	2.15943200	C	-4.25329300	-0.13890900	-0.11861800
H	6.06014100	-0.00246700	-4.17648200	C	-5.16928200	-0.79747800	-0.57541800
H	6.98049000	-1.28483800	-3.29243500	C	-6.24235900	-1.54859100	-1.14613200
Ni	-0.23413100	0.12335600	0.27092800	C	-7.34556200	-0.88145000	-1.71754000
C	-3.72520300	2.01913100	0.95847800	C	-6.20564900	-2.95836800	-1.13887200
C	-4.60149600	2.30683800	2.00363700	C	-8.38947200	-1.61749500	-2.27053800
C	-5.01943000	3.63031100	2.18075800	H	-7.37491900	0.20369500	-1.71846700
C	-4.59210000	4.65302100	1.32477400	C	-7.25667300	-3.68243500	-1.69376500
C	-3.73254600	4.37131800	0.26136600	H	-5.35803800	-3.46966100	-0.69149700
C	-3.32331600	3.05037900	0.11440800	C	-8.34726800	-3.01487600	-2.25975800
H	-4.95565100	1.52542000	2.66545200	H	-9.23857800	-1.10182900	-2.70823900
H	-5.69385300	3.86647500	2.99814200	H	-7.22994700	-4.76783100	-1.68340300
H	-4.93522100	5.67029500	1.48369100	H	-9.16542200	-3.58406000	-2.69061200
H	-3.39425300	5.14586000	-0.41900300	H	4.41630900	3.25787400	-3.76500000
C	-3.17678500	0.64525100	0.51372600	H	0.82981800	1.29091500	-5.10291700
S	-2.29031500	2.39122300	-1.15715700	H	4.28869500	-4.13477200	3.23423500
O	-1.07214100	3.14340300	-1.42317300	H	1.81336700	-1.25462000	5.25770100

O -2.71974500 -0.23927000 -2.69973400
H -3.00193800 0.82167200 -2.80821700
H -2.29738500 -0.08992900 -1.75353600
H -3.55141100 -0.73307900 -2.52941300

13

C -5.01963700 -0.30965700 -0.65474700
C -3.79266600 -0.07144000 -0.05761900
C -3.08013400 1.07369900 -0.53691600
C -3.62624100 1.87180900 -1.55395900
C -4.87312700 1.60053400 -2.14062300
C -5.55111700 0.49779300 -1.66625300
H -3.08868000 2.74555800 -1.89809600
H -5.28442000 2.23212600 -2.91958000
C -3.33520000 -0.98631000 1.02185400
C -2.16374300 -1.80954400 0.95999200
C -4.11531300 -1.14177400 2.15524900
C -1.86985300 -2.71134600 1.99529200
C -3.80341000 -2.03897800 3.18410500
C -2.68670900 -2.84723900 3.12840500
H -0.99821500 -3.34854500 1.92281400
H -2.45624400 -3.55661400 3.91478200
O -5.26405300 -0.47913500 2.46379400
O -5.87365200 -1.34226600 -0.40239400
C -7.04432500 -1.10410700 -1.20419400
C -5.71264400 -1.00072800 3.72698600
P -1.46738100 1.53267800 0.20073100
P -1.02507500 -1.65028700 -0.45168800
C -1.78298800 1.81278000 1.97552900
C -2.97220100 2.44473900 2.38080200
C -0.84811300 1.41763400 2.94352700
C -3.20306500 2.69443300 3.73352700
H -3.71612900 2.73818100 1.64635700

C -1.08738000 1.66136500 4.29529300
H 0.06706500 0.91507800 2.64744700
C -2.26237800 2.30472800 4.69058600
H -2.44492200 2.50122500 5.74291900
C -1.01773700 3.11399900 -0.60781500
C -1.22929500 4.35223300 0.01468700
C -0.46878900 3.07381400 -1.90219400
C -0.90909300 5.53225900 -0.65648800
H -1.63010700 4.39873900 1.02115700
C -0.14611600 4.25741200 -2.56680100
H -0.31982400 2.12037200 -2.40608000
C -0.36755100 5.48816400 -1.94346900
H -0.12325000 6.41070800 -2.46173700
C -1.94178700 -2.00135300 -1.98772400
C -2.97183300 -2.95802400 -1.98826200
C -1.58272600 -1.36429000 -3.18594100
C -3.62393500 -3.27557800 -3.17977600
H -3.26536500 -3.45028400 -1.06592800
C -2.24546700 -1.68182500 -4.37185800
H -0.78790700 -0.62451800 -3.19318800
C -3.26355400 -2.63829500 -4.37023600
H -3.77675200 -2.88559100 -5.29475000
C 0.25480100 -2.95523000 -0.27573300
C 0.34476500 -4.01205300 -1.19487400
C 1.19553300 -2.87145000 0.76853600
C 1.34817800 -4.97468400 -1.05876900
H -0.37013200 -4.09393600 -2.00611900
C 2.19484400 -3.83478800 0.90044700
H 1.13179900 -2.06836900 1.49955900
C 2.27173900 -4.88889700 -0.01507500
H 3.04416200 -5.64486900 0.09064900
O -6.75165600 0.00899800 -2.06325800
O -4.74135400 -1.96915300 4.15688000

H -7.88903500 -0.85120400 -0.55475400
 H -7.25551700 -1.98715200 -1.81159100
 H -5.76549400 -0.18967100 4.45830800
 H -6.68193100 -1.49127800 3.59853500
 Ni 0.21618800 0.19919200 -0.41162200
 C 3.84584900 1.92322500 -1.00210600
 C 4.70461900 2.14157100 -2.07909600
 C 5.17836000 3.43616600 -2.31275500
 C 4.81339900 4.50523600 -1.48621800
 C 3.96494800 4.29576800 -0.39851600
 C 3.50362300 2.99912800 -0.18782900
 H 5.01149900 1.32278200 -2.71893900
 H 5.84674500 3.61136600 -3.15004800
 H 5.19527200 5.50109100 -1.68648600
 H 3.67300800 5.10901000 0.25794700
 C 3.27412600 0.56897800 -0.53466800
 S 2.49424400 2.50088400 1.17627400
 O 1.27621700 3.28996400 1.28833800
 O 3.26803100 2.16445400 2.36783500
 N 2.10122200 0.91393700 0.38045700
 C 2.68378400 -0.26223400 -1.68994100
 O 1.47819800 -0.54758700 -1.74077100
 O 3.55305000 -0.65964500 -2.56869200
 C 3.10301700 -1.53295200 -3.67809900
 C 4.32468000 -1.88307200 -4.49760100
 H 2.62894300 -2.40466500 -3.22126200
 H 2.35497200 -0.97331900 -4.24501200
 H 4.02250800 -2.54241800 -5.31783100
 H 5.06997700 -2.40804900 -3.89350500
 H 4.78373900 -0.99048400 -4.93253200
 H 0.26628100 4.21959300 -3.57091200
 H -1.08242600 6.48789600 -0.17091400
 H 1.39845100 -5.79847400 -1.76471800

H 2.90826300 -3.76547200 1.71614100
 C 4.27729000 -0.23289800 0.15828700
 C 5.11969900 -0.87034200 0.75866600
 C 6.11179200 -1.59695700 1.47872800
 C 6.76853700 -0.99137200 2.56925000
 C 6.44498900 -2.91463000 1.10510600
 C 7.74135100 -1.69847600 3.26984500
 H 6.50950400 0.02371800 2.85329200
 C 7.42167800 -3.60966800 1.81215600
 H 5.94208200 -3.37566100 0.26025200
 C 8.06953700 -3.00423500 2.89334900
 H 8.24726900 -1.23042500 4.10865300
 H 7.68244300 -4.62234600 1.51976900
 H 8.83210900 -3.54974900 3.44111700
 H -4.11741600 3.19483500 4.03844600
 H -0.35621500 1.35483100 5.03706000
 H -4.41318300 -4.02151500 -3.17762700
 H -1.96953800 -1.18259400 -5.29602400
 H 2.15741400 0.26189600 1.17048300

14-ts

C 5.00951000 0.07974300 -0.57729900
 C 3.75824600 -0.12695500 -0.02033400
 C 2.95668500 -1.13580800 -0.64307900
 C 3.44912800 -1.83736300 -1.75462400
 C 4.72201400 -1.59971500 -2.29898300
 C 5.48516600 -0.63100500 -1.68344700
 H 2.84625800 -2.61114600 -2.21041900
 H 5.08758800 -2.15773600 -3.15331500
 C 3.36474600 0.68883600 1.15892000
 C 2.28301100 1.62658800 1.17611100
 C 4.12677600 0.63147400 2.31317800
 C 2.05167900 2.42741800 2.30443300

C	3.87593300	1.42733600	3.43643500	C	2.48254000	2.10368200	-4.13092000
C	2.84735000	2.34617500	3.45866300	H	0.90730400	1.05412600	-3.10464100
H	1.24706300	3.15130800	2.29660800	C	3.58295000	2.95412900	-4.00130600
H	2.66669400	2.97853200	4.32021200	H	4.14072100	3.25758300	-4.88231900
O	5.19950700	-0.17258500	2.55484300	C	0.00823200	3.11338200	0.05014600
O	5.94319100	0.99771100	-0.19196000	C	0.04774700	4.28334300	-0.72360100
C	7.10503300	0.75361700	-1.00310500	C	-0.96469900	2.99135800	1.06042700
C	5.64368200	0.12743400	3.88910300	C	-0.85853300	5.31795900	-0.47869000
P	1.29799200	-1.55409700	0.02918300	H	0.78936600	4.39599500	-1.50678500
P	1.16367200	1.71846900	-0.26211900	C	-1.86304700	4.03000200	1.30437300
C	1.58973900	-2.03953200	1.76545900	H	-1.00562300	2.09449700	1.67398400
C	2.72346500	-2.80162000	2.09779600	C	-1.81150600	5.19550700	0.53431400
C	0.69383600	-1.65841500	2.77498700	H	-2.50475400	6.00844900	0.72947800
C	2.93792900	-3.19415900	3.41907500	O	6.72832400	-0.19682300	-2.01139500
H	3.43902700	-3.08486000	1.33187100	O	4.77865000	1.15064500	4.40841500
C	0.91953400	-2.04349400	4.09599100	H	7.90335200	0.33057100	-0.38354700
H	-0.18042100	-1.06327800	2.53313900	H	7.41855100	1.68507600	-1.47973800
C	2.03746300	-2.81616300	4.41838900	H	5.56018600	-0.76876000	4.51088300
H	2.20659200	-3.12327000	5.44632900	H	6.67096200	0.50154100	3.85841800
C	0.78382000	-3.01510600	-0.95503700	Ni	-0.26050700	-0.00232500	-0.39916000
C	0.94083900	-4.32421100	-0.48035300	C	-3.89119300	-1.48519700	-1.32590100
C	0.25406900	-2.80492800	-2.23952100	C	-4.75943900	-1.56343300	-2.41510400
C	0.58386600	-5.40551200	-1.28642400	C	-5.28473900	-2.81237000	-2.76244300
H	1.32344000	-4.50332100	0.51816500	C	-4.95820200	-3.96432200	-2.03690200
C	-0.10317400	-3.88971200	-3.04122400	C	-4.09966800	-3.89084700	-0.93660500
H	0.14108600	-1.79408500	-2.62663100	C	-3.58656800	-2.64220300	-0.60784100
C	0.06268500	-5.19241000	-2.56464500	H	-5.02038400	-0.67936900	-2.98559600
H	-0.20987800	-6.03843200	-3.18870700	H	-5.95596900	-2.88779400	-3.61233900
C	2.14707200	2.17158600	-1.73043900	H	-5.37709900	-4.92242000	-2.32809200
C	3.25969100	3.02063400	-1.60313600	H	-3.83730000	-4.77335400	-0.36207500
C	1.76365300	1.71349500	-3.00049500	C	-3.20451300	-0.25814900	-0.74529700
C	3.96931900	3.41180800	-2.73860300	S	-2.57274000	-2.26026800	0.81033500
H	3.57393100	3.36969000	-0.62407100	O	-1.42580800	-3.14927000	0.95230200

O -3.42962000 -2.00951100 1.97461600
 N -2.06537700 -0.71387200 0.16691200
 C -2.61022400 0.71823000 -1.75340500
 O -1.40311400 0.98953400 -1.73047400
 O -3.46664700 1.25268800 -2.57667100
 C -2.97809700 2.26231900 -3.54540800
 C -4.17274500 2.74099500 -4.33929700
 H -2.50206100 3.05650000 -2.96548700
 H -2.22385700 1.77275900 -4.16609100
 H -3.83905100 3.49505300 -5.05959300
 H -4.92421400 3.19943700 -3.69000600
 H -4.63576200 1.92188400 -4.89730000
 H -0.50146700 -3.71848800 -4.03723500
 H 0.71192300 -6.41675900 -0.91192800
 H -0.80818200 6.22560100 -1.07303200
 H -2.59441200 3.93351100 2.10174600
 C -3.94930200 0.52103300 0.31608900
 C -5.00484900 0.88621500 0.88219100
 H -2.84134600 0.25366800 0.98187100
 C -6.08305900 1.24450600 1.68380000
 C -6.64002200 0.26663200 2.55579500
 C -6.63774400 2.55237100 1.63000100
 C -7.72563900 0.60159700 3.34987500
 H -6.19468800 -0.72254800 2.59218600
 C -7.72618800 2.86471400 2.42771700
 H -6.20585500 3.28852700 0.95980200
 C -8.26736400 1.89327800 3.28423900
 H -8.15536000 -0.13449400 4.02148400
 H -8.16099300 3.85831700 2.39182200
 H -9.11989800 2.14740000 3.90740400
 H 0.21919100 -1.74694400 4.87095800
 H 3.80780500 -3.79590600 3.66576300
 H 4.82395500 4.07412800 -2.63658000

H 2.18705100 1.74201800 -5.11147700

15

C 3.47683100 -0.54836500 2.49473200
 C 2.93803100 -0.03546600 1.32564400
 C 1.85695100 0.89009300 1.49436400
 C 1.40258800 1.21545600 2.78252200
 C 1.96787500 0.67179900 3.94644600
 C 3.00955300 -0.21356600 3.76986700
 H 0.59371400 1.92325600 2.90442800
 H 1.60583800 0.94038000 4.93201500
 C 3.53782700 -0.45140900 0.03006900
 C 2.85121200 -1.16668200 -1.00125100
 C 4.88061500 -0.20499100 -0.20168900
 C 3.53393200 -1.57041900 -2.15859800
 C 5.54693700 -0.61230100 -1.36160300
 C 4.89670400 -1.30114600 -2.36363300
 H 3.01498100 -2.13396600 -2.92235200
 H 5.41242600 -1.62843700 -3.25904900
 O 5.74651200 0.47863600 0.60209000
 O 4.49491200 -1.44834500 2.60596300
 C 4.71096300 -1.64919300 4.01320000
 C 7.04167400 0.35649200 -0.01029200
 P 0.99606400 1.62200200 0.05020800
 P 1.08333300 -1.58746400 -0.76549200
 C 2.26813900 2.36404100 -1.03660300
 C 3.44414400 2.89519700 -0.47851600
 C 2.04724700 2.48440000 -2.41720700
 C 4.37436100 3.54214600 -1.29228100
 H 3.63640700 2.80057300 0.58567500
 C 2.98482900 3.12643100 -3.22724400
 H 1.14146000 2.08503700 -2.86086600
 C 4.14778000 3.65774300 -2.66608800

H 4.87535500 4.15967300 -3.29692900
 C 0.03792000 3.03077300 0.73993200
 C 0.56235700 4.33356100 0.74537400
 C -1.19920000 2.78578200 1.35797300
 C -0.13717500 5.36441700 1.37665500
 H 1.51413800 4.54811300 0.27220100
 C -1.88913700 3.81696300 1.99574300
 H -1.62618700 1.78956300 1.35300300
 C -1.35638100 5.10794600 2.00836400
 H -1.88734000 5.91139900 2.51054500
 C 1.01152900 -2.61371700 0.74623900
 C 1.96401800 -3.62786000 0.95585200
 C 0.01731400 -2.38765200 1.70830300
 C 1.89801800 -4.41596500 2.10430200
 H 2.75519600 -3.79801100 0.23140600
 C -0.03748800 -3.17301100 2.86119300
 H -0.69852300 -1.58427000 1.57760200
 C 0.89806200 -4.19069100 3.05627100
 H 0.85502500 -4.80387000 3.95178500
 C 0.65163500 -2.67071900 -2.18946600
 C 0.36543900 -4.03405200 -2.02631800
 C 0.60131300 -2.11141600 -3.48039300
 C 0.06145000 -4.82684300 -3.13753600
 H 0.39322800 -4.48594300 -1.04089300
 C 0.30819400 -2.90706500 -4.58708000
 H 0.81584400 -1.05529400 -3.62572100
 C 0.03998500 -4.26969700 -4.41758300
 H -0.17845100 -4.89289900 -5.27986600
 O 3.72049400 -0.87932300 4.71235700
 O 6.84330800 -0.21578000 -1.31238800
 H 5.70881200 -1.29208000 4.28626300
 H 4.58426100 -2.70841400 4.25309600
 H 7.49177700 1.34615300 -0.11216900

H 7.66994200 -0.31162400 0.58914200
 Ni -0.39120200 0.16434600 -0.92602000
 H -2.83531700 3.59848900 2.48040800
 H 0.28070500 6.36700300 1.38264500
 H -0.14253300 -5.88473200 -2.99977400
 H 0.29666100 -2.46784200 -5.58055700
 H 5.27569400 3.95735900 -0.85100900
 H 2.80667200 3.21249300 -4.29514900
 H 2.62934100 -5.20443200 2.25696100
 H -0.80558800 -2.97480300 3.60232200
 C -3.13367500 6.02665400 -1.44893200
 C -4.47622300 5.84505000 -1.09128000
 C -5.02075500 4.55917600 -0.96064700
 C -4.22744200 3.44751800 -1.19547600
 C -2.86395700 3.61608400 -1.55671900
 C -2.32366700 4.92419800 -1.67679100
 H -2.72923400 7.02868300 -1.54937800
 H -5.10554900 6.71263400 -0.91501100
 H -6.06258100 4.43670800 -0.68271200
 H -4.63356300 2.44546300 -1.10573800
 H -1.28166200 5.04443700 -1.95213000
 C -2.07215300 2.50793300 -1.86244000
 C -1.34012700 1.52387200 -2.12521600
 C -4.74461400 -1.80636300 0.72643100
 C -5.69299300 -2.68462000 0.19120600
 C -6.78533100 -3.05387000 0.98404300
 C -6.93849100 -2.56448800 2.28434700
 C -5.99357700 -1.68517000 2.83463500
 C -4.92272700 -1.33189700 2.03475600
 H -5.59096000 -3.07299100 -0.81305700
 H -7.52717900 -3.73468900 0.57889200
 H -7.79522100 -2.86739800 2.87809600
 H -6.10263600 -1.30241200 3.84419200

C -3.49758400 -1.24035900 0.15612900
 S -3.55279500 -0.25636700 2.44189300
 O -3.96669600 1.14024700 2.55126400
 O -2.65954200 -0.85557600 3.42953600
 N -2.79019100 -0.44292000 0.88266000
 C -2.94200400 -1.50351100 -1.22313800
 O -1.84032300 -1.09317900 -1.59551200
 O -3.74484200 -2.20072000 -1.98681000
 C -3.32034300 -2.51639000 -3.36540900
 C -4.44526100 -3.28829100 -4.01938700
 H -2.39344300 -3.08864800 -3.29521300
 H -3.11406600 -1.56574400 -3.86349600
 H -4.15851200 -3.52806500 -5.04841600
 H -4.63984200 -4.22905000 -3.49559300
 H -5.36704500 -2.70008800 -4.05354600
 H -1.14461400 1.06389400 -3.08978900

16-ts

C -5.06339700 -0.72931500 0.93294600
 C -3.75168900 -0.78579300 0.48965300
 C -2.75279900 -0.73844400 1.52078100
 C -3.13199800 -0.63209500 2.86910000
 C -4.47230600 -0.57798200 3.27973400
 C -5.42223000 -0.62936900 2.28191000
 H -2.37052600 -0.60959000 3.63759400
 H -4.74495200 -0.50589900 4.32621500
 C -3.52461400 -0.90734000 -0.97994000
 C -2.87677200 0.07315300 -1.79802300
 C -4.06391700 -1.98426600 -1.66422300
 C -2.81355500 -0.07335500 -3.18911800
 C -3.99060600 -2.12297300 -3.05494700
 C -3.37534500 -1.17889700 -3.84982100
 H -2.32778000 0.68943600 -3.78641600

H -3.33334500 -1.28156300 -4.92802400
 O -4.71297200 -3.06017100 -1.13349000
 O -6.19132800 -0.72943500 0.16489300
 C -7.30385100 -0.73636300 1.07518500
 C -5.15976300 -3.85302100 -2.24698000
 P -0.96866900 -0.80175300 1.12657300
 P -2.03195900 1.46336100 -0.98737800
 C -0.71085000 -2.29198500 0.09849900
 C -1.44009600 -3.46267900 0.37100600
 C 0.22909300 -2.28848400 -0.94398400
 C -1.21512400 -4.61577000 -0.38074200
 H -2.18418700 -3.47458400 1.16140700
 C 0.43948200 -3.44290600 -1.69885000
 H 0.78772300 -1.38636100 -1.17725000
 C -0.27721400 -4.60736600 -1.41621100
 H -0.10967100 -5.50511000 -2.00398900
 C -0.09368300 -1.04219300 2.71559500
 C 0.35510100 -2.30897100 3.11768800
 C 0.09671400 0.06283300 3.56464000
 C 0.97095300 -2.46696100 4.36153300
 H 0.23447900 -3.16931300 2.46954100
 C 0.70208500 -0.10467900 4.80804700
 H -0.22654500 1.05251700 3.25447500
 C 1.13994300 -1.37157700 5.20817900
 H 1.61417500 -1.50093100 6.17656200
 C -3.26103100 2.47879300 -0.10567700
 C -4.59394500 2.54493000 -0.54304400
 C -2.84804500 3.25470700 0.99016200
 C -5.49791000 3.38408400 0.10940100
 H -4.92475400 1.94372200 -1.38471000
 C -3.75773900 4.08927700 1.63897400
 H -1.81700300 3.21185300 1.33414700
 C -5.08216700 4.15453500 1.19851200

H -5.78929700 4.80624900 1.70305900
 C -1.26899600 2.53173000 -2.26097800
 C -1.76436500 3.81579300 -2.54854700
 C -0.10556800 2.07496600 -2.91367300
 C -1.11905400 4.61655300 -3.48991500
 H -2.65388100 4.18344300 -2.04837900
 C 0.53334300 2.88497400 -3.85254800
 H 0.29740300 1.08691800 -2.70707300
 C 0.02767600 4.15380900 -4.14254700
 H 0.52258100 4.78292500 -4.87661900
 O -6.77084100 -0.58046300 2.39983500
 O -4.59456200 -3.27821000 -3.43456000
 H -7.83029000 -1.69406300 1.00575600
 H -7.96612600 0.10257700 0.84852400
 H -4.79964400 -4.87813400 -2.13133200
 H -6.25270700 -3.81635400 -2.30841000
 Ni -0.16477900 0.93984100 0.08559900
 H 0.83484200 0.75173500 5.46256000
 H 1.31639900 -3.45061600 4.66475500
 H -1.51526000 5.60140400 -3.71834800
 H 1.42216800 2.51694200 -4.35542000
 H -1.77517600 -5.51917000 -0.15792800
 H 1.15940400 -3.43177900 -2.51209500
 H -6.52604600 3.43951300 -0.23612600
 H -3.43423800 4.68771800 2.48539900
 C 3.95740500 5.07757000 2.35938800
 C 4.57810700 4.66177400 3.54278300
 C 4.44070000 3.34290600 3.98926600
 C 3.67766000 2.43502400 3.26287600
 C 3.04927500 2.84551400 2.06425000
 C 3.20178100 4.17771900 1.61644800
 H 4.06832700 6.10241600 2.01855600
 H 5.17086000 5.36736800 4.11749200

H 4.92796700 3.02670700 4.90658700
 H 3.56577100 1.40848000 3.59578500
 H 2.72018900 4.48851400 0.69413400
 C 2.26994100 1.92159300 1.32362900
 C 1.64370800 1.06306300 0.67218700
 H 2.62060900 0.03633200 0.13586300
 C 5.53354300 -1.55346400 -0.93980100
 C 6.58435400 -1.76372200 -1.84122000
 C 7.61659900 -2.63129600 -1.47203400
 C 7.60699000 -3.27983600 -0.23339000
 C 6.55582300 -3.08318400 0.67873200
 C 5.54564300 -2.22243600 0.29593600
 H 6.60077800 -1.25797700 -2.79812900
 H 8.43903700 -2.80220000 -2.15894300
 H 8.42094900 -3.94733300 0.03171400
 H 6.54553100 -3.58851100 1.63891300
 C 4.33956600 -0.71843300 -1.08743700
 S 4.08194000 -1.80309300 1.23514500
 O 3.15389300 -2.91837500 1.32699800
 O 4.37322000 -0.94064700 2.36951300
 N 3.50205900 -0.74638500 -0.09636000
 C 3.96812900 0.13501200 -2.29179100
 O 2.81110700 0.33534700 -2.58813300
 O 5.04750300 0.59497300 -2.90347200
 C 4.83296600 1.47078400 -4.06839700
 C 6.19230900 1.90511700 -4.57189000
 H 4.21911400 2.31064800 -3.73237100
 H 4.26869600 0.89671400 -4.80843900
 H 6.05789200 2.57078100 -5.43061300
 H 6.74543200 2.44981900 -3.80126800
 H 6.78917000 1.04877700 -4.90018700

C -0.25826100 0.68718500 0.00000900
 C 0.38901100 1.93100100 0.00008300
 C -0.39225600 3.08986500 0.00014500
 C -1.78797300 3.01823700 0.00007400
 C -2.45474900 1.77790700 -0.00004700
 C -1.66916400 0.64429000 -0.00004200
 H 1.47008000 1.98450100 0.00015000
 H 0.09438400 4.05955700 0.00024500
 H -2.37465900 3.93160100 0.00011500
 H -3.53874400 1.72648700 -0.00011500
 C 0.33008700 -0.63894900 0.00002800
 S -2.28402200 -1.03919700 -0.00005800
 O -2.84222200 -1.43272300 1.27645800
 O -2.84237800 -1.43277100 -1.27647900
 N -0.54057000 -1.60554900 -0.00015100
 C 1.79144400 -1.08968500 0.00013600
 O 2.03253100 -2.27535900 0.00062400
 O 2.63583900 -0.08090400 -0.00043800
 C 4.07670500 -0.43265000 -0.00039500
 C 4.86145900 0.85939400 0.00013400
 H 4.25477400 -1.04299100 -0.88898200
 H 4.25461000 -1.04367500 0.88775200
 H 5.92997300 0.62097700 -0.00019800
 H 4.64874100 1.45622500 -0.89199300
 H 4.64904500 1.45534400 0.89291700
 H -0.24784000 -2.58755300 0.00002400

18

C 3.37171800 -1.43829900 -0.89863300
 C 2.17826700 -1.10289900 -0.27965300
 C 0.99007400 -1.54028400 -0.95450300
 C 1.08764300 -2.24096400 -2.16735500
 C 2.31637100 -2.55886900 -2.76685900

C 3.44927100 -2.14146400 -2.10290400
 H 0.18477800 -2.56634600 -2.66756000
 H 2.36901700 -3.10617100 -3.70093600
 C 2.26273200 -0.35576200 1.01063500
 C 1.86797700 1.00658200 1.19360800
 C 2.88037700 -0.94810900 2.09941400
 C 2.10005700 1.66315700 2.40691900
 C 3.10051400 -0.28443500 3.30871800
 C 2.72486500 1.02836200 3.49497500
 H 1.79408100 2.69663200 2.52094400
 H 2.90455300 1.54570700 4.43044900
 O 3.34699400 -2.23082400 2.19037900
 O 4.63405200 -1.12727500 -0.47280300
 C 5.53821700 -1.72248800 -1.41484400
 C 3.96201500 -2.34417600 3.48358000
 P -0.69008700 -1.16564400 -0.31473900
 P 0.92958200 1.83396400 -0.14107800
 C -0.81241000 -1.88190300 1.36528700
 C 0.02211900 -2.94408400 1.75254600
 C -1.79776300 -1.41407600 2.25058600
 C -0.13370200 -3.53002500 3.00927900
 H 0.79123400 -3.31323200 1.08224300
 C -1.94250500 -2.00398400 3.50639000
 H -2.45517500 -0.60400000 1.95014800
 C -1.11239400 -3.06027600 3.88789500
 H -1.22898900 -3.51734000 4.86638600
 C -1.84109500 -2.11321400 -1.38066100
 C -2.22109500 -3.41995500 -1.04157900
 C -2.31936400 -1.53834400 -2.56915500
 C -3.06772700 -4.14164200 -1.88528200
 H -1.86825400 -3.87359900 -0.12124000
 C -3.15563100 -2.26816400 -3.41250500
 H -2.05093400 -0.51816800 -2.82710300

C	-3.53240400	-3.57004000	-3.07050200	H	5.31898800	2.35644600	-2.43836600
H	-4.19111200	-4.13430300	-3.72429500	H	1.83019600	2.45952500	-4.95673000
C	2.03836700	2.02531200	-1.58139000	C	-7.58233700	0.97825700	1.36480900
C	3.43264900	2.09480700	-1.43624500	C	-8.37018900	0.62084700	0.26643100
C	1.46676400	2.15510100	-2.85726300	C	-7.76481400	0.28395800	-0.94801200
C	4.24063800	2.29657400	-2.55632900	C	-6.37881700	0.30444900	-1.06912000
H	3.88525700	1.98476900	-0.45524400	C	-5.57276300	0.66155600	0.03322100
C	2.27914000	2.35793100	-3.97304000	C	-6.19553700	0.99966500	1.25379100
H	0.38723900	2.10269200	-2.97833700	H	-8.05201800	1.24210800	2.30805500
C	3.66613100	2.42881600	-3.82307700	H	-9.45259800	0.60643700	0.35622700
H	4.29828200	2.58678300	-4.69212300	H	-8.37649600	0.00725900	-1.80197500
C	0.53868800	3.53251500	0.43436500	H	-5.90211800	0.04406200	-2.00895900
C	1.21902000	4.66537400	-0.03849400	H	-5.57916600	1.28043100	2.10246000
C	-0.53651900	3.69802100	1.32942100	C	-4.15491300	0.67644000	-0.08758600
C	0.83516100	5.93843700	0.38480500	C	-2.93003200	0.73819600	-0.21895600
H	2.04392700	4.55634800	-0.73468700				
C	-0.91555300	4.97346500	1.74784200				
H	-1.07321500	2.83071700	1.70961700				
C	-0.23034800	6.09470500	1.27461300				
H	-0.52744300	7.08844500	1.59669100				
O	4.74973000	-2.30446700	-2.46345600				
O	3.71126000	-1.12350700	4.19177500				
H	6.12122500	-2.50685900	-0.91994100				
H	6.18778900	-0.94954100	-1.83531600				
H	3.51341700	-3.18000400	4.02760200				
H	5.04264800	-2.48198000	3.36357600				
Ni	-1.12819200	0.95485000	-0.32600000				
H	-3.52032600	-1.81724900	-4.33089500				
H	-3.36424300	-5.15001600	-1.61185000				
H	1.36963900	6.80948800	0.01707600				
H	-1.74662900	5.08974000	2.43705100				
H	0.50870800	-4.35709000	3.29815700				
H	-2.70676000	-1.63814300	4.18585600				

6. Reference

1. R.-R. Liu, D.-J. Wang, L. Wu, B. Xiang, G.-Q. Zhang, J.-R. Gao, Y.-X. Jia, *ACS Catal.* **2015**, 5, 6524.
2. a) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785.
3. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, 120, 215
4. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, 113, 6378.