

Supplementary Material

Simultaneous diversity-oriented synthesis of benzothiazoles and related diverse analogues by iodine-catalyzed intramolecular cyclization from identical substrates

Meng Cui^A, Xue-Lin Wang^A, Mengzhou Wang^A and Jian-Wu Xie^{A,}*

^ASchool of Biological and Pharmaceutical Sciences, Shaanxi University of Science and Technology, Xi'an, 710021, PR China

*Correspondence to: Email: xiejw@sust.edu.cn

General methods

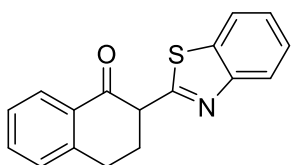
NMR spectra were recorded with tetramethylsilane as the internal standard. TLC was performed on glass-backed silica plates. Column chromatography was performed using silica gel (150–200 mesh) eluting with ethyl acetate and petroleum ether. All NMR spectra were recorded on 600- or 400-MHz instrument. Chemical shifts (δ) are reported in parts per million downfield from CDCl_3 ($\delta = 7.26$ ppm) or DMSO ($\delta = 2.50$ ppm) for ^1H NMR and relative to the central CDCl_3 resonance ($\delta = 77.0$ ppm) or DMSO resonance ($\delta = 39.5$ ppm) for ^{13}C NMR spectroscopy. Coupling constants (J) are given in hertz. ESI-HRMS spectra were measured with an ion trap mass spectrometer.

Experimental

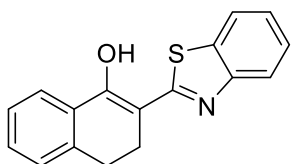
Typical experimental procedure for the Synthesis of benzothiazoles and related diverse analogues (Scheme 3)

A mixture of β -ketothioamides (0.50 mmol), iodine (0.50 mmol) and K_2CO_3 (0.50 mmol) was stirred in DMSO (1.0 mL) at 50°C for 40 min. Then flash chromatography on silica gel (5% ethyl acetate/petroleum ether) gave products **2-5**.

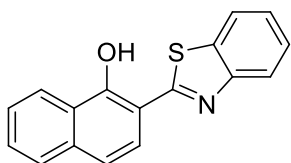
NMR data



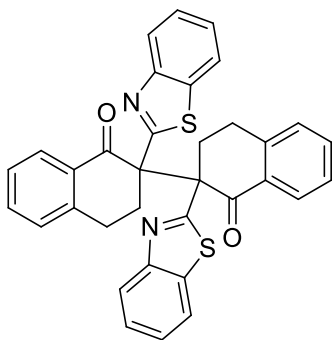
2-(benzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1(2*H*)-one (**2a**). Yellow solid (22% yield). mp $147\text{--}148^\circ\text{C}$. Rf = 0.3(5% EA/PE). ^1H NMR (600 MHz, CDCl_3) δ 8.14 (dd, $J = 7.9, 1.0$ Hz, 1H), 7.90–7.85 (m, 1H), 7.83 (d, $J = 7.7$ Hz, 1H), 7.56 (td, $J = 7.6, 1.3$ Hz, 1H), 7.38 (dd, $J = 11.1, 4.2$ Hz, 2H), 7.34 (td, $J = 7.8, 1.2$ Hz, 1H), 7.27 (d, $J = 7.7$ Hz, 1H), 4.97 (s, 1H), 3.40 (ddd, $J = 17.5, 12.9, 4.7$ Hz, 1H), 3.01 (ddd, $J = 17.3, 4.9, 2.4$ Hz, 1H), 2.80 (ddd, $J = 13.4, 4.8, 2.5$ Hz, 1H), 2.55 (td, $J = 13.1, 5.0$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 196.6, 172.8, 153.3, 145.1, 135.1, 134.6, 130.5, 129.1, 128.6, 127.1, 126.0, 125.4, 123.7, 121.7, 77.5, 36.3, 26.2. HRMS (ESI-TOF) m/z [$\text{M} + \text{H}$] $^+$ Calcd for $\text{C}_{17}\text{H}_{13}\text{NOS}$ 280.0791; found 280.0804.



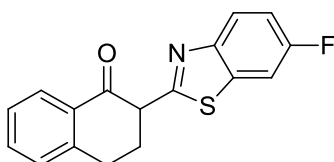
2-(benzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol (**3a**). Yellow solid (20% yield). mp $138\text{--}139^\circ\text{C}$. Rf = 0.4(5% EA/PE). ^1H NMR (400 MHz, CDCl_3) δ 13.89 (s, 1H), 7.93–7.85 (m, 1H), 7.77 (dd, $J = 16.6, 8.0$ Hz, 2H), 7.44–7.36 (m, 1H), 7.33–7.20 (m, 3H), 7.19–7.11 (m, 1H), 2.92 (t, $J = 7.7$ Hz, 2H), 2.71–2.62 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 170.7, 158.2, 151.6, 137.9, 131.9, 131.1, 129.8, 127.4, 126.9, 126.6, 124.4, 124.0, 121.5, 120.4, 100.7, 28.2, 25.1. HRMS (ESI-TOF) m/z [$\text{M} + \text{H}$] $^+$ Calcd for $\text{C}_{17}\text{H}_{13}\text{NOS}$ 280.0791; found 280.0804.



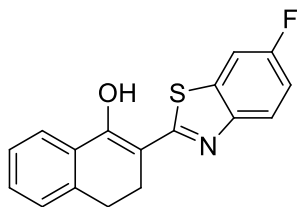
2-(benzo[*d*]thiazol-2-yl)naphthalen-1-ol(**4a**). Yellow solid (38% yield). mp 164–166°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.73 (s, 1H), 8.48 (dd, *J* = 8.5, 0.9 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.79–7.74 (m, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.58–7.51 (m, 2H), 7.51–7.47 (m, 1H), 7.40–7.34 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 167.0, 155.9, 151.9, 135.7, 132.6, 128.6, 127.7, 126.8, 126.0, 125.4, 125.3, 124.4, 124.1, 121.9, 121.6, 119.4, 110.0. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₁NOS 278.0634; found 278.0620.



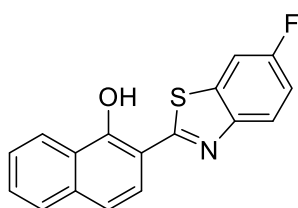
2,2'-bis(benzo[*d*]thiazol-2-yl)-3,3',4,4'-tetrahydro-[2,2'-binaphthalene]-1,1'(2*H*,2'*H*)-dione(**5a**). Yellow solid (13% yield). mp 218–220°C. Rf = 0.7(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.17 (d, *J* = 7.8 Hz, 2H), 8.05 (d, *J* = 8.1 Hz, 2H), 7.88 (d, *J* = 7.9 Hz, 2H), 7.47 (t, *J* = 7.2 Hz, 2H), 7.44–7.36 (m, 4H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 7.5 Hz, 2H), 3.61 (td, *J* = 13.2, 5.1 Hz, 2H), 2.85–2.66 (m, 4H), 2.31 (d, *J* = 12.6 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 197.2, 167.3, 152.7, 142.6, 135.9, 133.7, 132.9, 128.9, 128.4, 126.8, 126.1, 125.6, 123.8, 121.5, 62.2, 35.1, 26.6. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₃₄H₂₄N₂O₂S₂ 557.1352; found 557.1357.



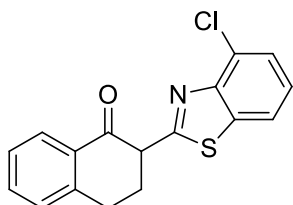
2-(6-fluorobenzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1(2*H*)-one(**2b**). Yellow solid (18% yield). mp 218–220 °C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.14 (dd, *J* = 15.0, 8.0 Hz, 1H), 7.74 (dd, *J* = 9.0, 4.8 Hz, 1H), 7.59–7.49 (m, 2H), 7.38 (dt, *J* = 15.1, 7.6 Hz, 1H), 7.29–7.25 (m, 1H), 7.09 (td, *J* = 8.9, 2.5 Hz, 1H), 5.02 (s, 1H), 3.40 (ddd, *J* = 17.4, 12.9, 4.7 Hz, 1H), 3.00 (ddd, *J* = 17.2, 4.7, 2.3 Hz, 1H), 2.77 (ddd, *J* = 13.4, 4.7, 2.5 Hz, 1H), 2.53 (td, *J* = 13.1, 5.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.4, 172.7, 161.3, 159.7, 150.0, 145.1, 134.7, 130.4, 129.1, 128.5, 127.0, 124.6, 114.6, 107.9, 77.5, 36.2, 26.1. HRMS (ESI-TOF) *m/z* [M + Na]⁺ Calcd for C₁₇H₁₂FNOS 320.0516; found 320.0534.



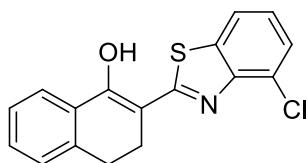
2-(6-fluorobenzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3b**). Yellow solid (27% yield). mp 152–153°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.60 (s, 1H), 7.91–7.83 (m, 1H), 7.76 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.49 (dd, *J* = 8.0, 2.5 Hz, 1H), 7.33–7.28 (m, 2H), 7.20–7.14 (m, 2H), 3.00–2.91 (m, 2H), 2.72–2.65 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 170.8, 160.6, 158.9, 157.3, 148.7, 137.8, 130.8, 129.9, 127.5, 127.0, 124.3, 121.5, 115.1, 108.0, 100.8, 28.2, 25.0. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂FNOS 298.0696; found 298.0698.



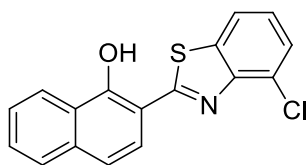
2-(6-fluorobenzo[*d*]thiazol-2-yl)naphthalen-1-ol(**4b**). Yellow solid (23% yield). mp 195–196°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.43 (s, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 7.91 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.66–7.48 (m, 5H), 7.36 (d, *J* = 8.6 Hz, 1H), 7.22 (td, *J* = 8.8, 2.5 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 169.7, 159.7, 155.7, 148.6, 135.7, 128.7, 127.7, 126.1, 124.2, 124.1, 122.8, 119.5, 115.5, 115.3, 109.9, 108.1, 108.0. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₀FNOS 296.0467; found 296.0471.



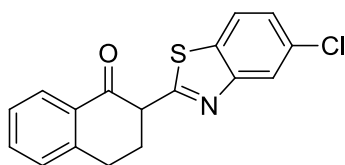
2-(4-chlorobenzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1(2*H*)-one(**2c**). Yellow oil (45% yield). mp 120–121°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.09 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.26 (t, *J* = 7.9 Hz, 1H), 5.06 (s, 1H), 3.68 (ddd, *J* = 17.5, 12.7, 5.0 Hz, 1H), 3.06 (dd, *J* = 17.4, 3.4 Hz, 1H), 2.87–2.80 (m, 1H), 2.55 (td, *J* = 13.0, 5.3 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.3, 173.6, 150.5, 145.4, 136.6, 134.8, 130.1, 129.1, 128.6, 128.4, 127.0, 126.3, 125.9, 120.3, 77.6, 35.9, 26.2. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂ClNOS 314.0401; found 314.0454.



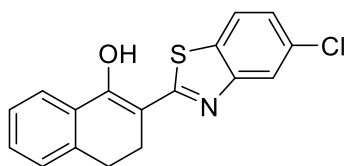
2-(4-chlorobenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3c**). Yellow solid (10% yield). mp 163-164°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.91 (s, 1H), 7.93 (dd, *J* = 5.7, 3.2 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.36–7.32 (m, 2H), 7.23 (t, *J* = 7.8 Hz, 2H), 3.00 (t, *J* = 7.7 Hz, 2H), 2.77–2.72 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 171.4, 159.0, 149.1, 138.1, 133.3, 130.9, 130.1, 127.5, 127.1, 126.8, 125.4, 124.7, 124.5, 120.0, 100.8, 28.3, 25.1. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂ClNOS 314.0401; found 314.0403.



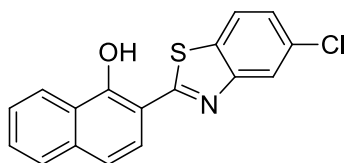
2-(4-chlorobenzo[d]thiazol-2-yl)naphthalen-1-ol(**4c**). Yellow solid (13% yield). mp 208-210°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.63 (s, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 7.78 (dd, *J* = 7.6, 4.4 Hz, 2H), 7.61–7.48 (m, 4H), 7.37 (d, *J* = 8.6 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 170.6, 156.4, 149.2, 135.9, 133.9, 128.9, 127.7, 127.0, 126.8, 126.2, 125.8, 125.5, 124.2, 124.2, 120.1, 119.6, 109.7. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₀ClNOS 312.0244; found 312.0245.



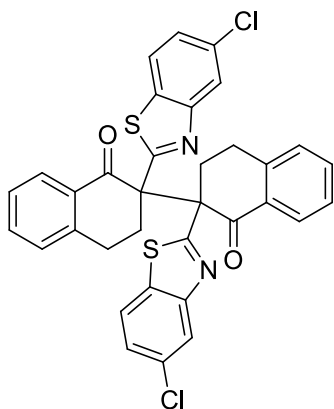
2-(5-chlorobenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1(2H)-one(**2d**). Yellow oil (25% yield). mp 127-128°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.16–8.10 (m, 1H), 7.75 (ddd, *J* = 15.2, 9.1, 2.2 Hz, 1H), 7.57 (td, *J* = 7.6, 1.2 Hz, 1H), 7.39 (dd, *J* = 11.6, 4.3 Hz, 1H), 7.36–7.26 (m, 3H), 5.00 (d, *J* = 6.8 Hz, 1H), 3.43 (ddd, *J* = 17.5, 13.0, 4.7 Hz, 1H), 3.05–2.98 (m, 1H), 2.78 (tdd, *J* = 14.3, 4.8, 2.4 Hz, 1H), 2.55 (tdd, *J* = 12.9, 7.7, 5.1 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.3, 174.0, 154.0, 145.1, 134.7, 129.2, 128.6, 127.1, 127.0, 125.9, 125.1, 123.5, 122.5, 122.0, 77.6, 36.3, 26.1. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂ClNOS 314.0401; found 314.0398.



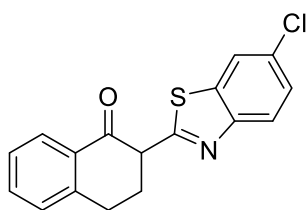
2-(5-chlorobenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3d**). Yellow solid (23% yield). mp 139-140°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.70 (d, *J* = 17.6 Hz, 1H), 7.88 (dd, *J* = 5.4, 3.6 Hz, 1H), 7.70 (ddd, *J* = 8.4, 2.2, 0.7 Hz, 1H), 7.42–7.34 (m, 1H), 7.34–7.29 (m, 2H), 7.28–7.24 (m, 1H), 7.22–7.17 (m, 1H), 2.98 (dd, *J* = 16.8, 15.5, 8.6 Hz, 2H), 2.76–2.66 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 171.4, 158.8, 152.6, 138.1, 130.8, 130.1, 127.6, 127.5, 127.0, 124.5, 123.6, 122.2, 120.4, 118.7, 100.7, 28.2, 25.1. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂ClNOS 314.0401; found 314.0407.



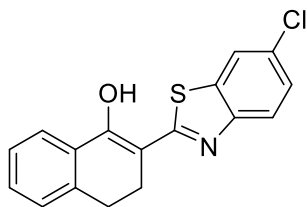
2-(5-chlorobenzo[d]thiazol-2-yl)naphthalen-1-ol(**4d**). Yellow solid (18% yield). mp 220-221°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.45 (d, *J* = 17.2 Hz, 1H), 8.49–8.44 (m, 1H), 7.96–7.84 (m, 1H), 7.77 (t, *J* = 8.1 Hz, 1H), 7.64–7.51 (m, 3H), 7.43 (t, *J* = 7.9 Hz, 1H), 7.39–7.32 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 170.6, 156.2, 135.9, 128.9, 127.8, 127.7, 126.2, 125.7, 125.4, 124.9, 124.2, 124.1, 122.3, 121.7, 120.1, 119.6, 109.7. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₀ClNOS 311.0172; found 311.0175.



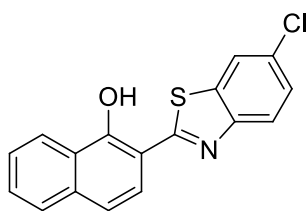
2,2'-bis(5-chlorobenzo[d]thiazol-2-yl)-3,3',4,4'-tetrahydro-[2,2'-binaphthalene]-1,1'(2*H*,2'*H*)-dione(**5d**). White solid (14% yield). mp 164-165°C. Rf = 0.7(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.16 (t, *J* = 8.2 Hz, 2H), 8.04 (d, *J* = 1.7 Hz, 1H), 7.98–7.92 (m, 1H), 7.79 (dd, *J* = 8.5, 5.3 Hz, 1H), 7.49–7.36 (m, 5H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.06 (d, *J* = 7.5 Hz, 2H), 3.67–3.54 (m, 2H), 2.80 (ddd, *J* = 8.7, 5.3, 2.4 Hz, 2H), 2.75–2.63 (m, 2H), 2.34–2.23 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 196.9, 168.1, 153.3, 142.5, 133.9, 132.8, 132.3, 128.9, 128.5, 126.9, 126.2, 125.3, 123.6, 122.1, 62.3, 35.2, 26.6. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₃₄H₂₂Cl₂N₂O₂S₂ 625.0573; found 625.0571.



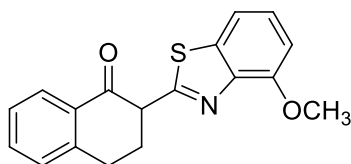
2-(6-chlorobenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1(2*H*)-one(**2e**). Yellow solid (38% yield). mp >259°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.14 (d, *J* = 7.8 Hz, 1H), 7.77 (dd, *J* = 9.0, 4.8 Hz, 1H), 7.60–7.53 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.12 (td, *J* = 8.9, 2.5 Hz, 1H), 4.95 (s, 1H), 3.42 (ddd, *J* = 17.4, 13.0, 4.7 Hz, 1H), 3.06–2.99 (m, 1H), 2.78 (ddd, *J* = 13.3, 4.6, 2.4 Hz, 1H), 2.55 (td, *J* = 13.1, 11.9, 5.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.4, 145.1, 134.7, 130.4, 129.2, 128.6, 127.1, 124.8, 124.7, 114.9, 114.7, 108.0, 107.8, 100.1, 77.5, 36.3, 26.2. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂ClNOS 314.0401; found 314.0407.



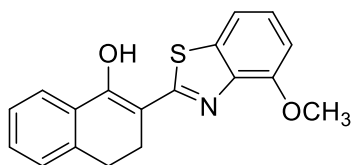
2-(6-chlorobenzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3e**). Yellow solid (22% yield). mp>259°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.67 (s, 1H), 7.91–7.87 (m, 1H), 7.83–7.70 (m, 2H), 7.40 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.34–7.29 (m, 2H), 7.22–7.18 (m, 1H), 3.01–2.94 (m, 2H), 2.75–2.68 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 171.4, 158.1, 150.6, 137.9, 133.3, 130.0, 127.5, 127.4, 127.0, 124.5, 121.3, 121.2, 115.2, 108.0, 100.7, 28.3, 25.1. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₂ClNOS 314.0401; found 314.0401.



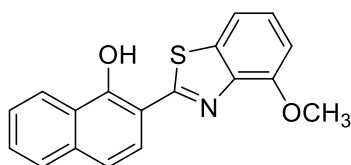
2-(6-chlorobenzo[*d*]thiazol-2-yl)naphthalen-1-ol(**4e**). Yellow solid (16% yield). mp>259°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.45 (s, 1H), 8.47 (d, *J* = 8.1 Hz, 1H), 7.90 (ddd, *J* = 14.1, 7.2, 3.3 Hz, 2H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.61–7.53 (m, 3H), 7.45 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.37 (dd, *J* = 8.6, 4.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 170.4, 160.8, 156.0, 135.8, 133.9, 131.2, 128.8, 127.7, 127.6, 126.2, 124.2, 124.1, 122.6, 121.3, 119.6, 119.6, 109.8. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₇H₁₀ClNOS 312.0172; found 312.0177.



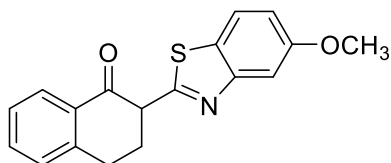
2-(4-methoxybenzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1(2*H*)-one(**2f**). White solid (23% yield). mp 174-175°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.11 (d, *J* = 7.8 Hz, 1H), 7.53 (td, *J* = 7.6, 1.1 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.27 (dd, *J* = 13.2, 5.1 Hz, 2H), 6.84 (d, *J* = 7.9 Hz, 1H), 4.91 (s, 1H), 3.86 (s, 3H), 3.47 (ddd, *J* = 17.2, 12.3, 4.8 Hz, 1H), 3.05 (ddd, *J* = 17.4, 4.8, 2.9 Hz, 1H), 2.91 (ddd, *J* = 13.4, 4.8, 2.9 Hz, 1H), 2.54 (td, *J* = 12.9, 12.6, 5.1 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.6, 170.4, 153.7, 145.0, 143.4, 137.2, 134.5, 130.5, 129.1, 128.6, 127.0, 126.5, 113.9, 108.4, 77.5, 56.8, 36.0, 26.3. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₆NO₂S 310.0896; found 310.0882.



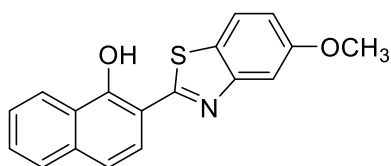
2-(4-methoxybenzo[*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3f**). Yellow solid (25% yield). mp 174-175°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.98 (s, 1H), 7.98–7.83 (m, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.31 (dd, *J* = 9.1, 3.8 Hz, 2H), 7.27–7.23 (m, 1H), 7.22–7.17 (m, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 4.02 (s, 3H), 2.98 (t, *J* = 7.7 Hz, 2H), 2.79–2.68 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 169.2, 158.8, 151.6, 141.6, 138.0, 133.2, 131.5, 129.7, 127.4, 127.0, 124.9, 124.4, 113.6, 107.6, 100.7, 56.2, 28.4, 25.2. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₆NO₂S 310.0896; found 310.0882.



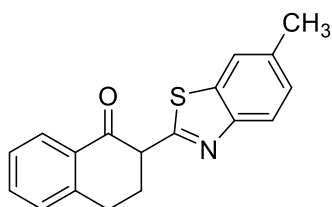
2-(4-methoxybenzo[d]thiazol-2-yl)naphthalen-1-ol (**4f**). Yellow solid (20% yield). mp 201-202°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.85 (s, 1H), 8.56–8.44 (m, 1H), 7.83–7.72 (m, 1H), 7.61 (d, *J* = 8.6 Hz, 1H), 7.58–7.51 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.38–7.29 (m, 2H), 6.92 (d, *J* = 7.9 Hz, 1H), 4.05 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 168.4, 155.9, 152.8, 142.2, 135.6, 134.3, 128.4, 127.6, 126.3, 126.0, 125.5, 124.4, 124.1, 119.2, 113.5, 110.1, 107.7, 56.2. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₄NO₂S 308.0740; found 308.0745.



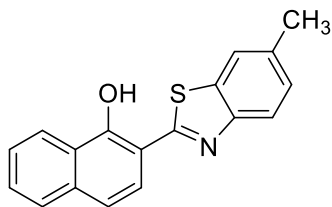
2-(5-methoxybenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1(2H)-one (**2g**). Yellow solid (25% yield). mp 97-98°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.15 (t, *J* = 6.9 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.58–7.55 (m, 1H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.32 (d, *J* = 2.4 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.00 (dd, *J* = 8.8, 2.5 Hz, 1H), 4.91 (s, 1H), 3.80 (s, 3H), 3.42–3.37 (m, 1H), 3.01 (ddd, *J* = 12.3, 4.8, 2.4 Hz, 1H), 2.82–2.78 (m, 1H), 2.55 (td, *J* = 13.1, 5.0 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 196.6, 173.9, 154.6, 145.1, 134.5, 130.5, 129.1, 128.5, 127.0, 126.9, 121.9, 115.9, 105.8, 77.5, 77.37 (s), 77.2, 76.9, 55.6, 36.3, 26.2. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₆NO₂S 310.0896; found 310.0887.



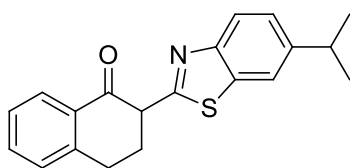
2-(5-methoxybenzo[d]thiazol-2-yl)naphthalen-1-ol (**4g**). Yellow solid (41% yield). mp 152-154°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.73 (s, 1H), 8.49 (d, *J* = 7.9 Hz, 1H), 7.77 (dd, *J* = 19.7, 19.2, 8.2 Hz, 2H), 7.63 (d, *J* = 8.6 Hz, 1H), 7.60–7.52 (m, 2H), 7.48 (d, *J* = 1.7 Hz, 1H), 7.37 (d, *J* = 8.6 Hz, 1H), 7.04 (dd, *J* = 8.7, 1.9 Hz, 1H), 3.93 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 171.1, 159.6, 155.8, 153.3, 135.7, 128.5, 127.7, 126.0, 125.5, 124.5, 124.3, 124.1, 121.9, 119.4, 115.3, 110.2, 104.5, 55.8. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₃NO₂S 308.0740; found 308.0743.



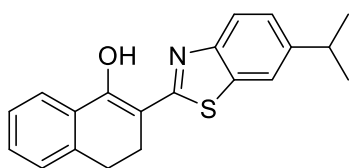
2-(6-methylbenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1(2H)-one (**2h**). Yellow oil (28% yield). mp 107-108°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.14 (d, *J* = 7.9 Hz, 1H), 7.71 (d, *J* = 9.0 Hz, 1H), 7.56 (td, *J* = 7.6, 1.3 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 2.5 Hz, 1H), 7.28 (d, *J* = 7.7 Hz, 1H), 6.98 (dd, *J* = 9.0, 2.5 Hz, 1H), 4.90 (d, *J* = 6.5 Hz, 1H), 3.85 (s, 3H), 3.39 (ddd, *J* = 17.2, 13.1, 4.3 Hz, 1H), 3.04–2.97 (m, 1H), 2.80 (ddd, *J* = 13.3, 4.7, 2.4 Hz, 1H), 2.53 (td, *J* = 13.1, 5.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.8, 169.8, 157.9, 145.1, 136.5, 134.6, 130.6, 129.1, 128.6, 127.1, 124.3, 115.5, 104.0, 77.5, 55.9, 36.3, 26.2, 18.6. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₆NOS 294.0947; found 294.0951.



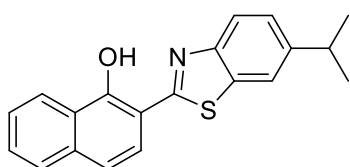
2-(6-methylbenzo[d]thiazol-2-yl)naphthalen-1-ol(**4h**). Yellow solid (41% yield). mp 218-220°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.53 (s, 1H), 8.51–8.45 (m, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.81–7.77 (m, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.55 (pd, *J* = 6.8, 1.5 Hz, 2H), 7.38 (t, *J* = 5.7 Hz, 2H), 7.11 (dd, *J* = 8.9, 2.5 Hz, 1H), 3.91 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 167.6, 158.0, 146.5, 135.5, 134.1, 128.4, 127.7, 126.0, 125.4, 124.3, 124.0, 122.5, 119.4, 116.0, 110.3, 104.4, 100.1, 56.0. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₄NOS 292.0791; found 292.0787.



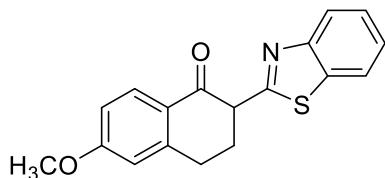
2-(6-isopropylbenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1(2H)-one(**2i**). Yellow solid (20% yield). mp 104-105°C. Rf = 0.3(5% EA/PE) ¹H NMR (600 MHz, CDCl₃) δ 8.17–8.11 (m, 1H), 7.72 (dd, *J* = 26.0, 5.0 Hz, 2H), 7.53 (tt, *J* = 7.2, 3.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.27–7.24 (m, 2H), 4.93 (s, 1H), 3.38 (ddd, *J* = 17.4, 12.9, 4.7 Hz, 1H), 3.02–2.96 (m, 2H), 2.80 (ddd, *J* = 13.4, 4.7, 2.5 Hz, 1H), 2.53 (td, *J* = 13.1, 5.0 Hz, 1H), 1.27 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 196.7, 171.6, 151.7, 146.7, 145.0, 135.3, 134.5, 130.6, 129.1, 128.5, 127.0, 125.2, 123.4, 118.8, 77.5, 36.2, 34.4, 26.2, 24.3, 24.3. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₂₀H₁₉NOS 322.1260; found 322.1246.



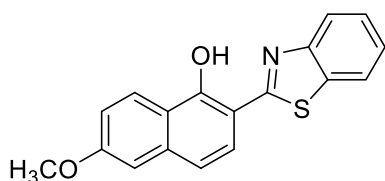
2-(6-isopropylbenzo[d]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3i**). Yellow solid (26% yield). mp 208-110°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.90 (s, 1H), 7.89 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 1.5 Hz, 1H), 7.35–7.27 (m, 3H), 7.20 (d, *J* = 6.7 Hz, 1H), 3.02 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.97 (t, *J* = 7.7 Hz, 2H), 2.80–2.66 (m, 2H), 1.31 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 170.1, 157.7, 150.0, 145.3, 137.8, 132.2, 131.2, 129.7, 127.4, 126.9, 125.8, 124.3, 120.2, 118.8, 100.9, 34.3, 28.3, 25.1, 24.4. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₂₀H₁₉NOS 322.1260; found 322.1246.



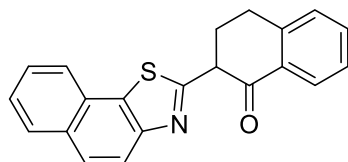
2-(6-isopropylbenzo[d]thiazol-2-yl)naphthalen-1-ol(**4i**). Yellow solid (27% yield). mp 173-175°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.80 (s, 1H), 8.55–8.50 (m, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.84–7.77 (m, 2H), 7.67 (d, *J* = 8.6 Hz, 1H), 7.63–7.55 (m, 2H), 7.45–7.39 (m, 2H), 3.16–3.04 (m, 1H), 1.37 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 169.1, 155.7, 150.3, 146.7, 135.6, 132.9, 128.5, 127.7, 126.0, 126.0, 125.5, 124.4, 124.0, 121.6, 119.3, 118.8, 110.2, 34.4, 24.3. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₂₀H₁₈NOS 320.1104; found 320.1109.



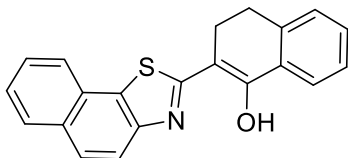
2-(benzo[*d*]thiazol-2-yl)-6-methoxy-3,4-dihydronaphthalen-1(2*H*)-one (**2j**). Yellow oil (31% yield). mp 120-122°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.11 (d, *J* = 8.8 Hz, 1H), 7.94–7.79 (m, 2H), 7.43–7.32 (m, 2H), 6.90 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.73 (d, *J* = 2.3 Hz, 1H), 5.01 (s, 1H), 3.88 (s, 3H), 3.45 (ddd, *J* = 17.5, 13.0, 4.8 Hz, 1H), 2.96 (ddd, *J* = 17.3, 4.9, 2.4 Hz, 1H), 2.78 (ddd, *J* = 13.3, 4.8, 2.5 Hz, 1H), 2.52 (td, *J* = 13.2, 5.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 195.0, 173.3, 164.7, 153.5, 147.9, 135.2, 131.1, 126.0, 125.3, 123.9, 123.7, 121.7, 114.0, 112.9, 77.3, 55.7, 36.2, 26.5. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₆NO₂S 310.0896; found 310.0882.



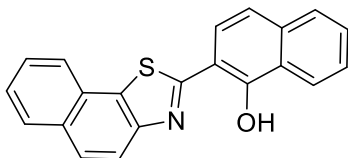
2-(benzo[*d*]thiazol-2-yl)-6-methoxynaphthalen-1-ol (**4j**). Yellow solid (36% yield). mp 202-203°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.69 (s, 1H), 8.38 (d, *J* = 9.1 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 8.6 Hz, 1H), 7.53–7.46 (m, 1H), 7.41–7.34 (m, 1H), 7.26 (d, *J* = 3.3 Hz, 1H), 7.17 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.07 (d, *J* = 2.4 Hz, 1H), 3.94 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 170.1, 160.0, 156.2, 152.0, 137.5, 132.5, 126.8, 125.9, 125.3, 125.1, 121.7, 121.6, 120.3, 118.4, 118.1, 108.7, 106.3, 55.5. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₁₈H₁₃NO₂S 308.0740; found 308.0743.



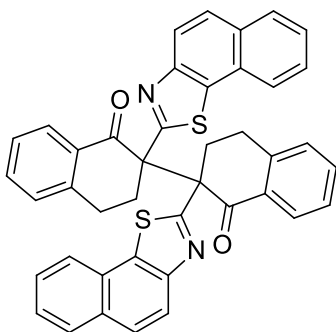
2-(naphtho[2,1-*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1(2*H*)-one (**2k**). White solid (20% yield). mp 140-141°C. Rf = 0.3(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 8.39–8.27 (m, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 7.86 (dd, *J* = 10.8, 7.9 Hz, 2H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.59 (td, *J* = 7.6, 1.2 Hz, 1H), 7.55–7.46 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 5.07 (s, 1H), 3.59 (ddd, *J* = 17.5, 12.8, 4.9 Hz, 1H), 3.05 (ddd, *J* = 17.4, 5.0, 2.0 Hz, 1H), 2.85 (ddd, *J* = 13.4, 4.9, 2.2 Hz, 1H), 2.59 (td, *J* = 13.1, 5.2 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 196.7, 171.6, 149.6, 145.2, 134.6, 131.8, 130.6, 129.0, 128.7, 128.5, 128.0, 127.0, 126.9, 126.1, 126.1, 123.8, 119.0, 77.7, 36.3, 26.3. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₂₁H₁₆NOS 330.0947; found 330.0951.



2-(naphtho[2,1-*d*]thiazol-2-yl)-3,4-dihydronaphthalen-1-ol(**3k**). Yellow solid (19% yield). mp 137-138°C. Rf = 0.4(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.94 (s, 1H), 8.65–8.60 (m, 1H), 7.91 (t, *J* = 7.7 Hz, 2H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.69 (d, *J* = 8.6 Hz, 1H), 7.66–7.62 (m, 1H), 7.55 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.36–7.27 (m, 2H), 7.19 (dd, *J* = 7.2, 0.7 Hz, 1H), 2.98 (t, *J* = 7.8 Hz, 2H), 2.76–2.71 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 170.4, 156.4, 148.3, 137.7, 132.3, 131.1, 129.6, 128.5, 128.3, 127.5, 127.0, 126.9, 126.8, 126.3, 124.8, 124.1, 123.7, 118.9, 101.3, 28.3, 25.2. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₂₁H₁₆NOS 330.0947; found 330.0951.



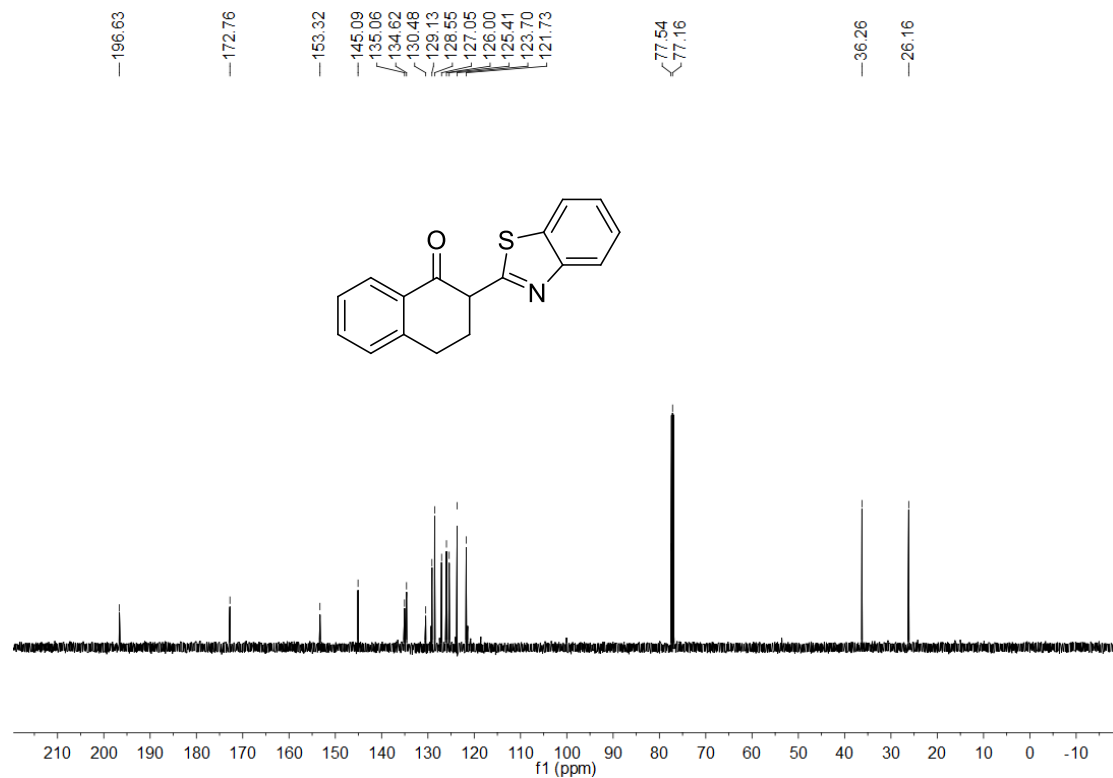
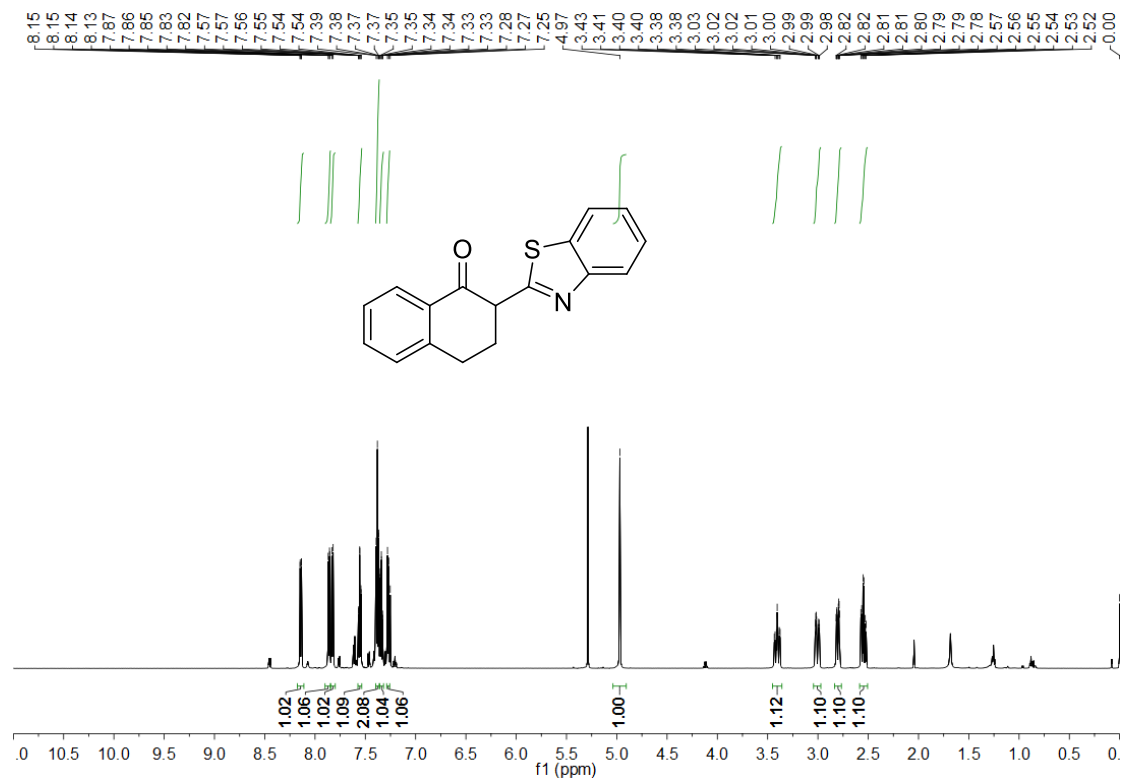
2-(naphtho[2,1-*d*]thiazol-2-yl)naphthalen-1-ol(**4k**). Yellow solid (13% yield). mp 171-173°C. Rf = 0.5(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 13.87 (s, 1H), 8.72 (d, *J* = 8.2 Hz, 1H), 8.56–8.49 (m, 1H), 7.96 (t, *J* = 6.5 Hz, 1H), 7.90 (d, *J* = 8.7 Hz, 1H), 7.83–7.77 (m, 2H), 7.73–7.67 (m, 2H), 7.63–7.59 (m, 1H), 7.59–7.54 (m, 2H), 7.39 (d, *J* = 8.6 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 169.11 (s), 155.4, 148.2, 135.6, 132.3, 129.3, 128.5, 128.4, 127.7, 127.4, 126.6, 126.2, 126.1, 125.5, 124.9, 124.2, 124.0, 123.7, 119.5, 118.8, 110.4. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₂₁H₁₄NOS 328.0791; found 328.0791.



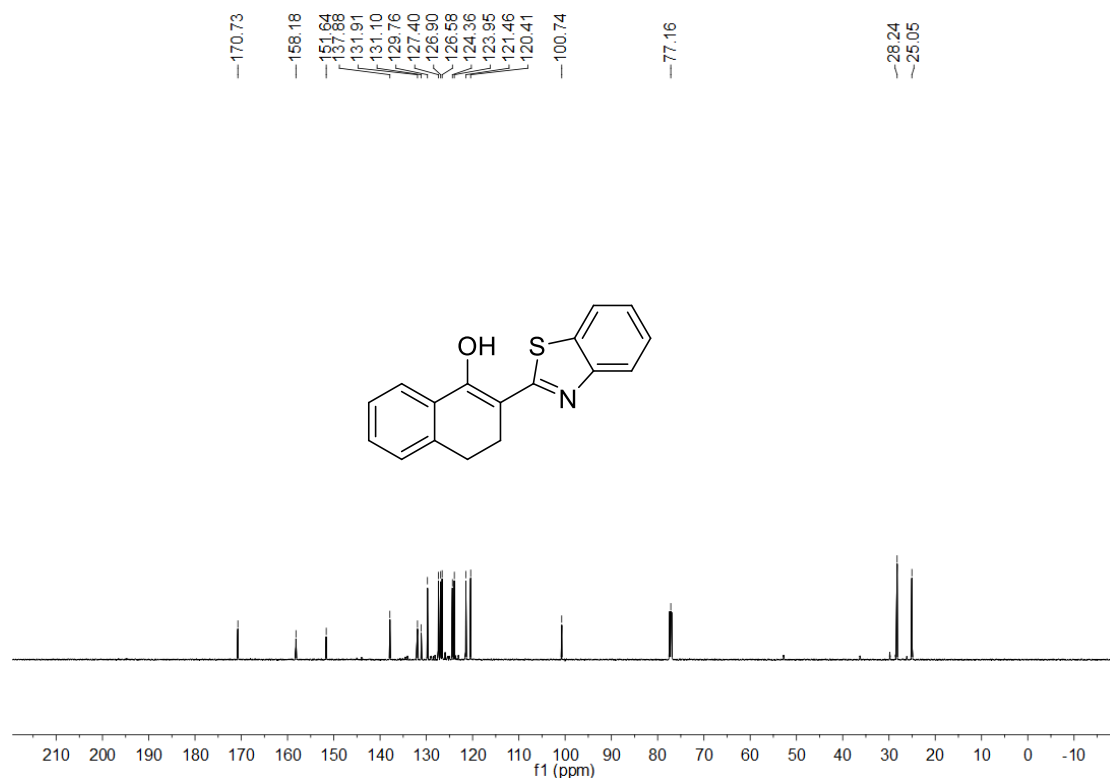
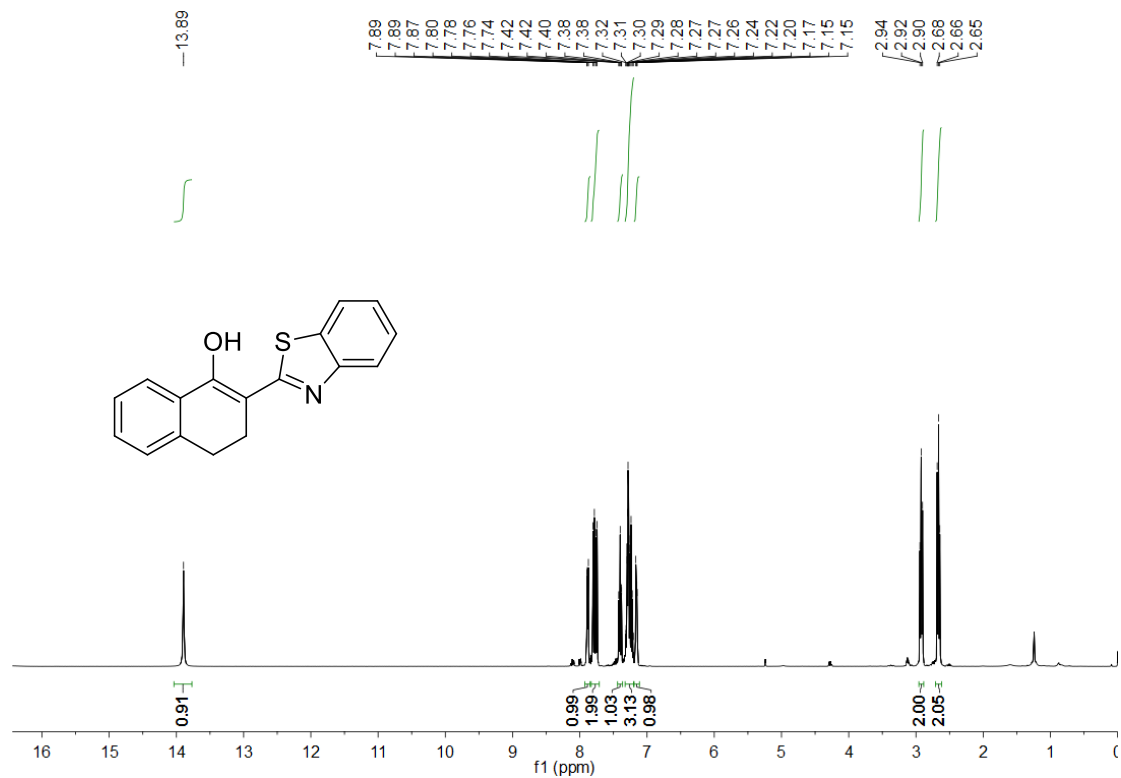
2,2'-bis(naphtho[2,1-*d*]thiazol-2-yl)-3,3',4,4'-tetrahydro-[2,2'-binaphthalene]-1,1'(2*H*,2'*H*)-dione(**5k**). White solid (25% yield). mp 130-131°C. Rf = 0.7(5% EA/PE). ¹H NMR (600 MHz, CDCl₃) δ 9.07 (s, 1H), 8.23 (d, *J* = 25.2 Hz, 2H), 8.04 (s, 1H), 7.80 (d, *J* = 22.7 Hz, 3H), 7.65 (s, 4H), 7.59–7.30 (m, 6H), 7.09 (d, *J* = 46.6 Hz, 3H), 3.73 (d, *J* = 26.7 Hz, 2H), 3.08 (s, 1H), 2.85 (d, *J* = 15.1 Hz, 2H), 2.67 (d, *J* = 66.1 Hz, 2H), 2.42 (s, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 133.9, 133.3, 131.7, 128.7, 128.5, 127.7, 127.2, 127.0, 126.1, 125.5, 124.2, 120.5, 119.2, 119.0, 32.8, 26.6, 15.7. HRMS (ESI-TOF) *m/z* [M + H]⁺ Calcd for C₄₂H₂₉N₂O₂S₂ 657.1665; found 657.1664.

^1H NMR and ^{13}C NMR spectra

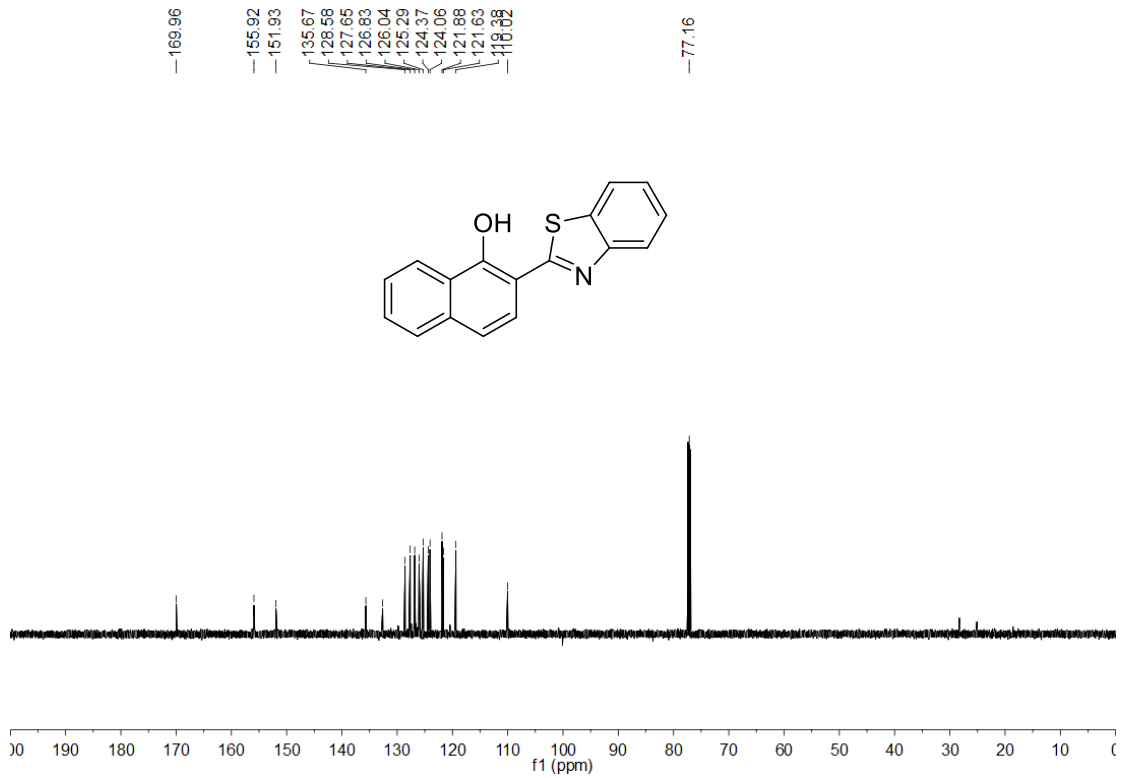
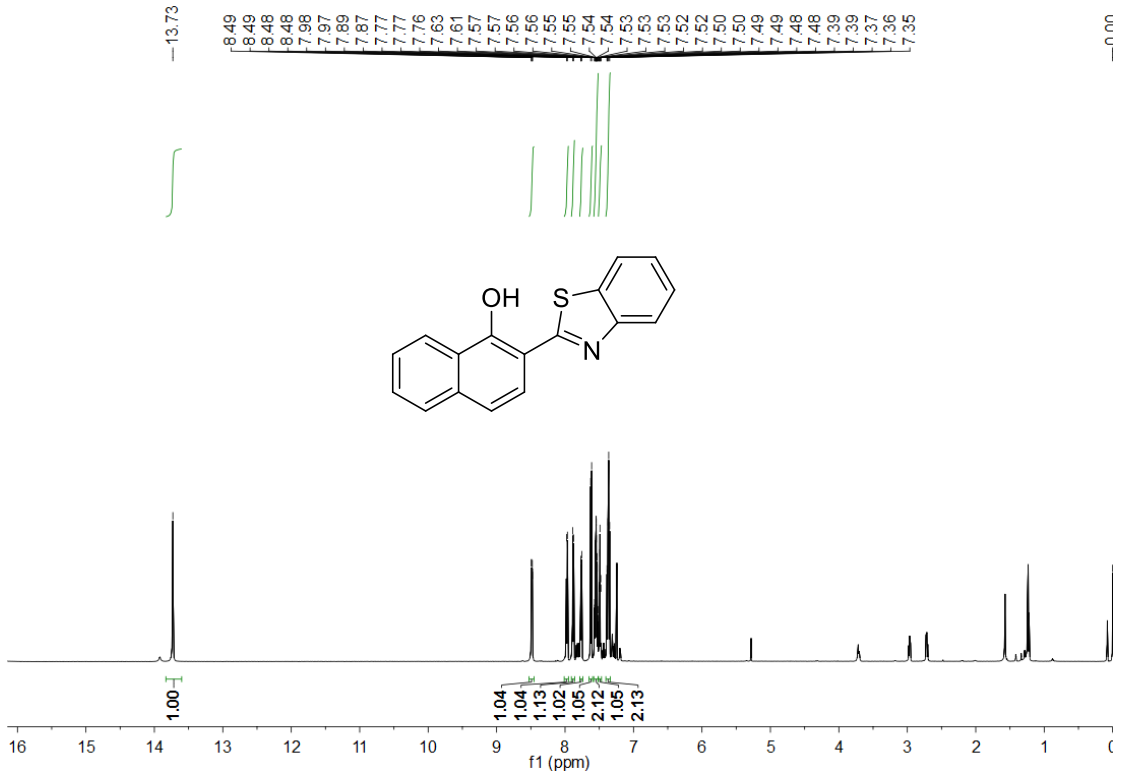
2a



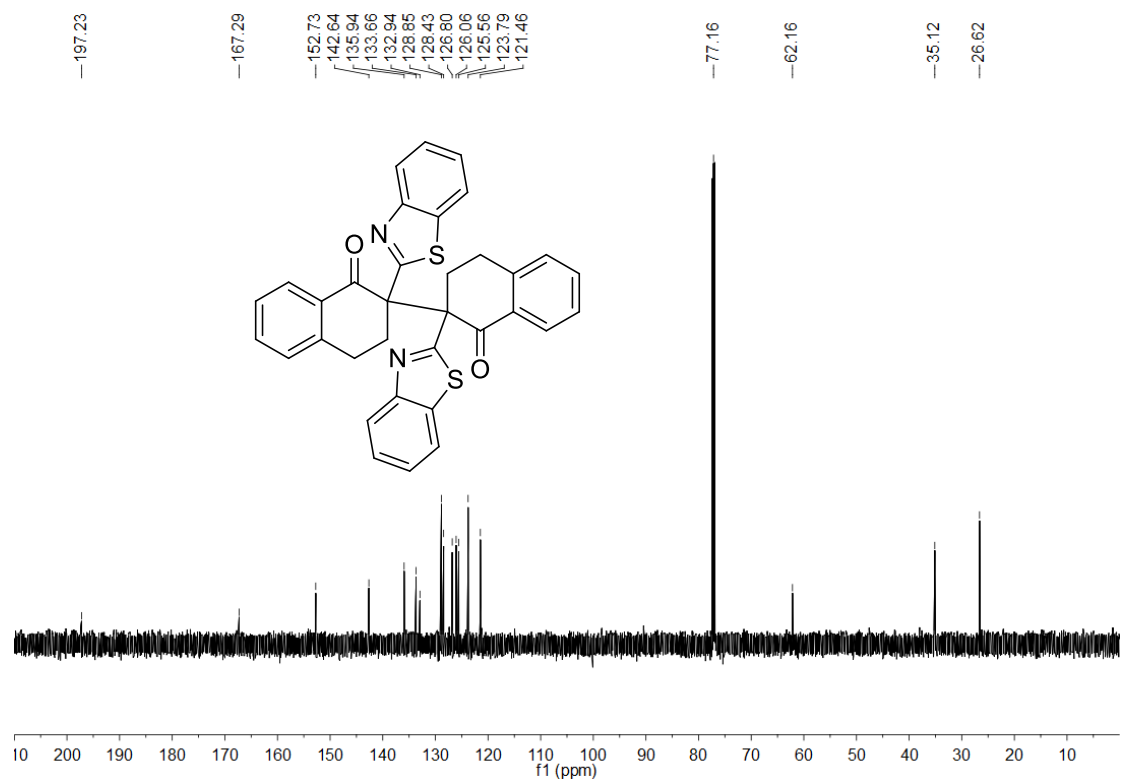
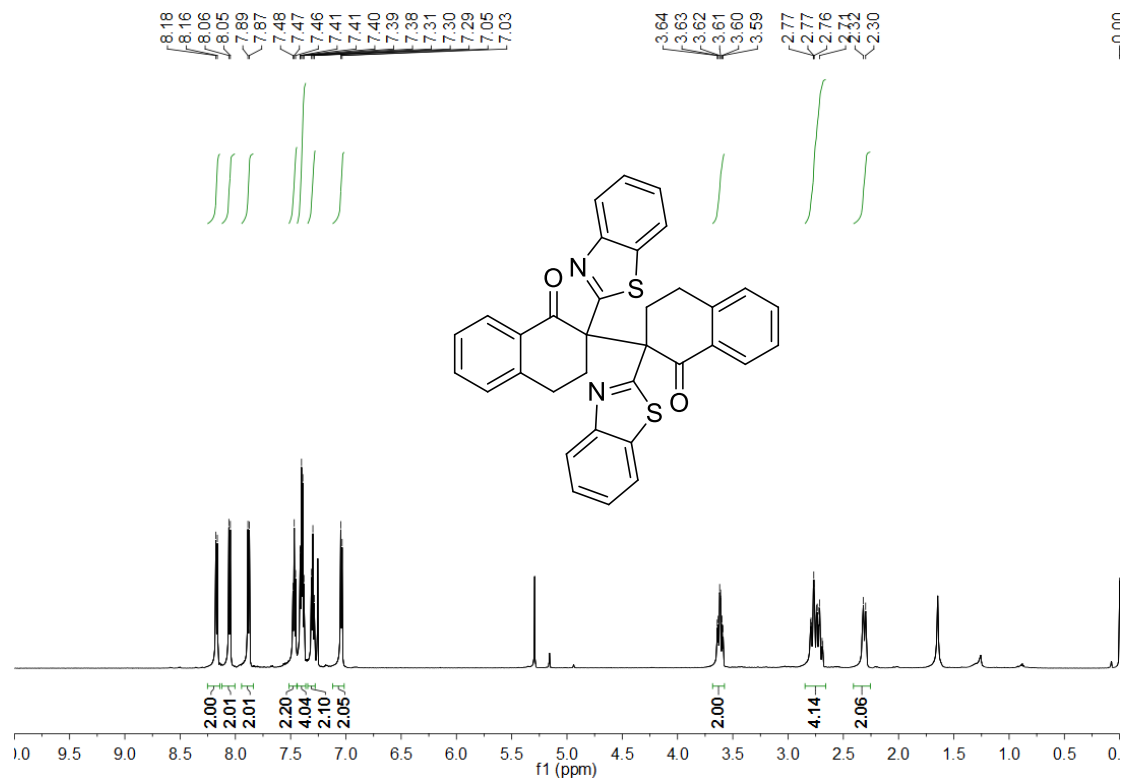
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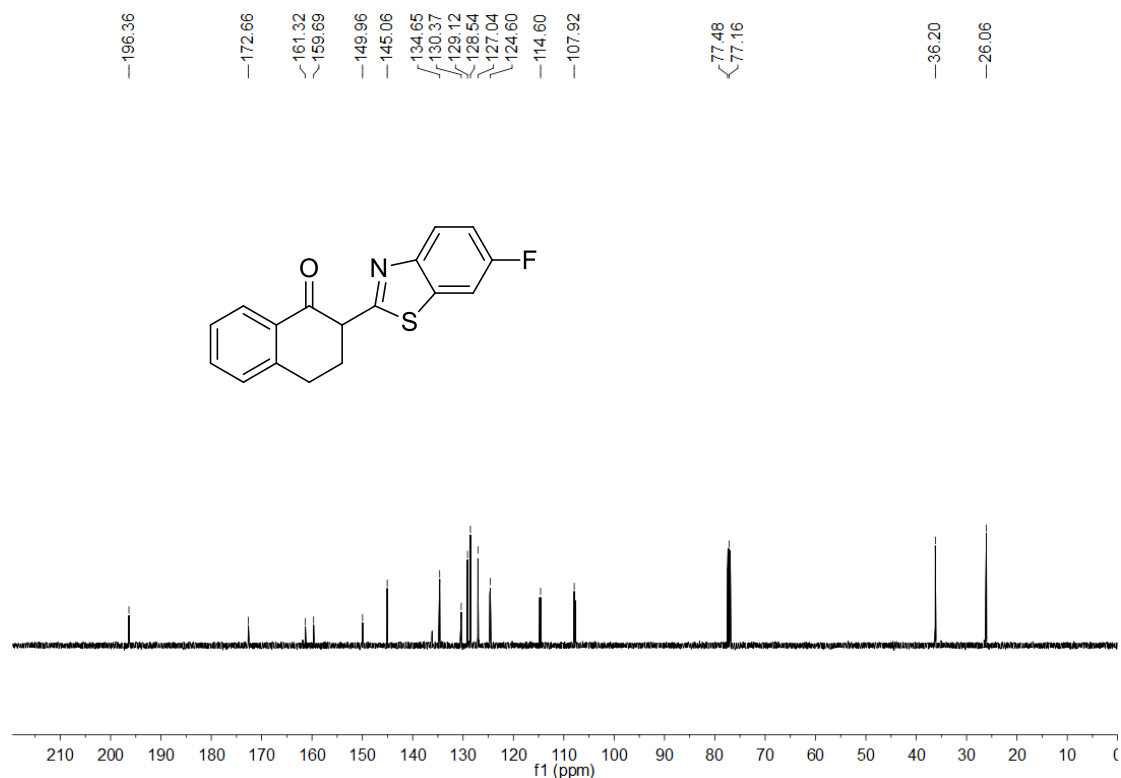
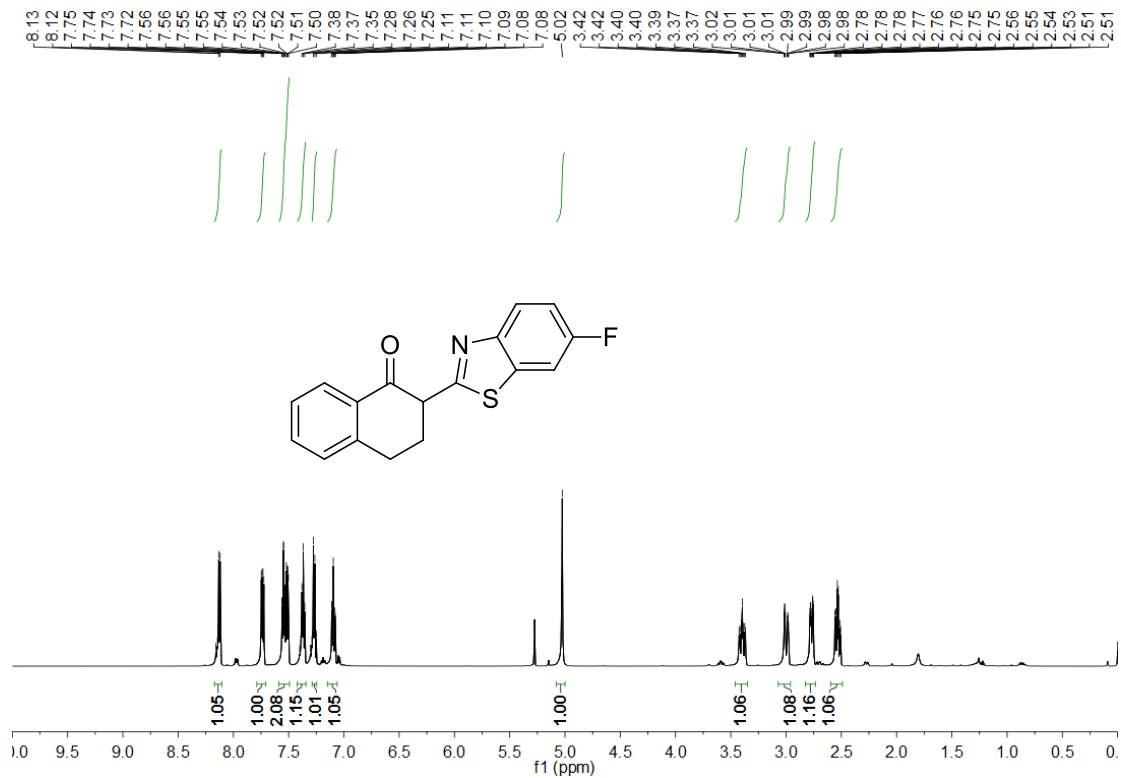
4a



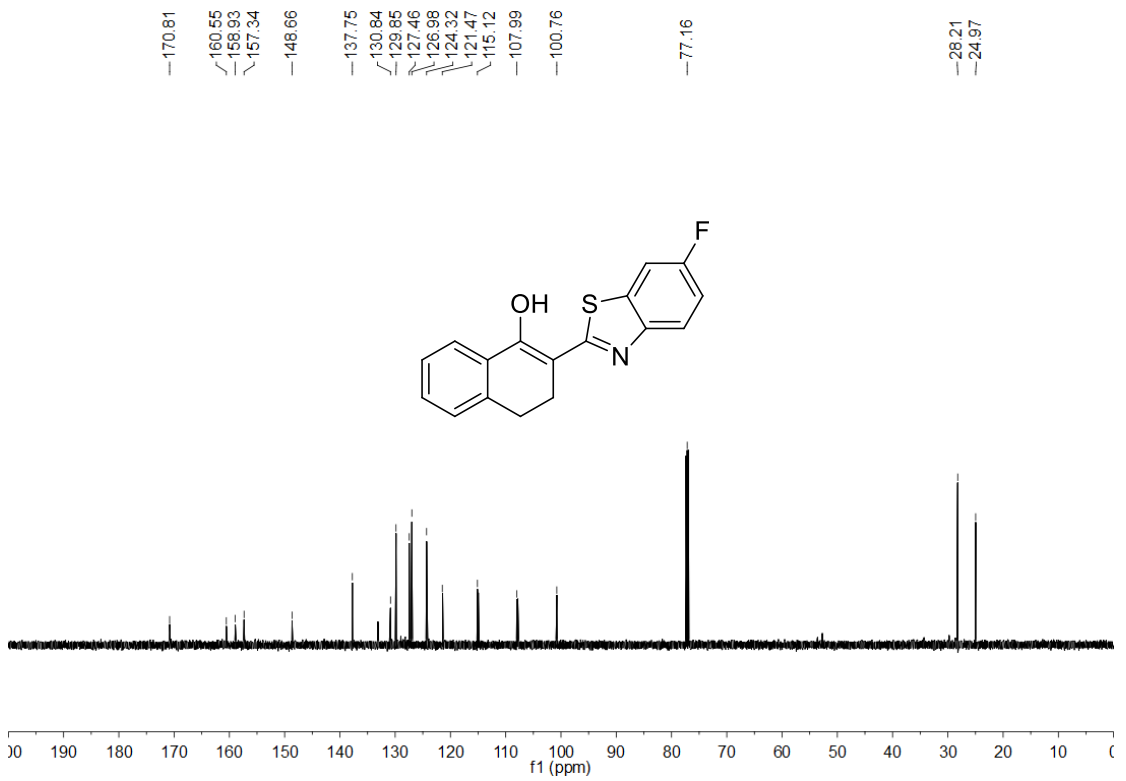
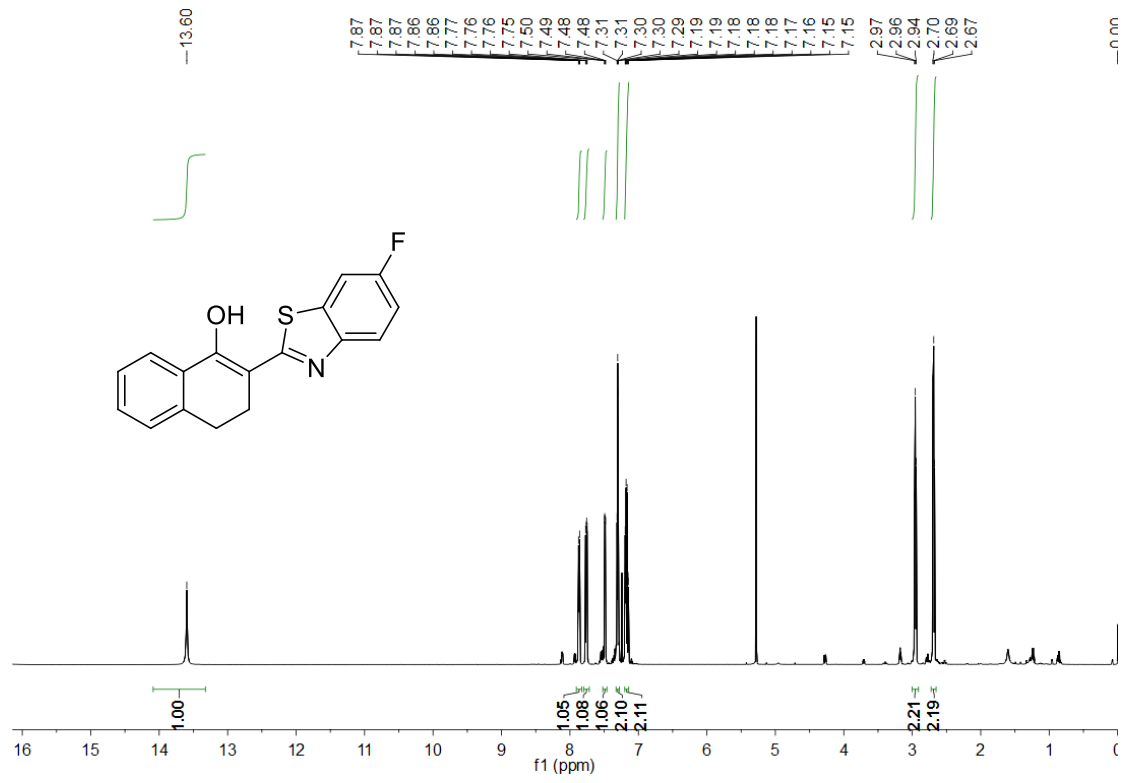
5a



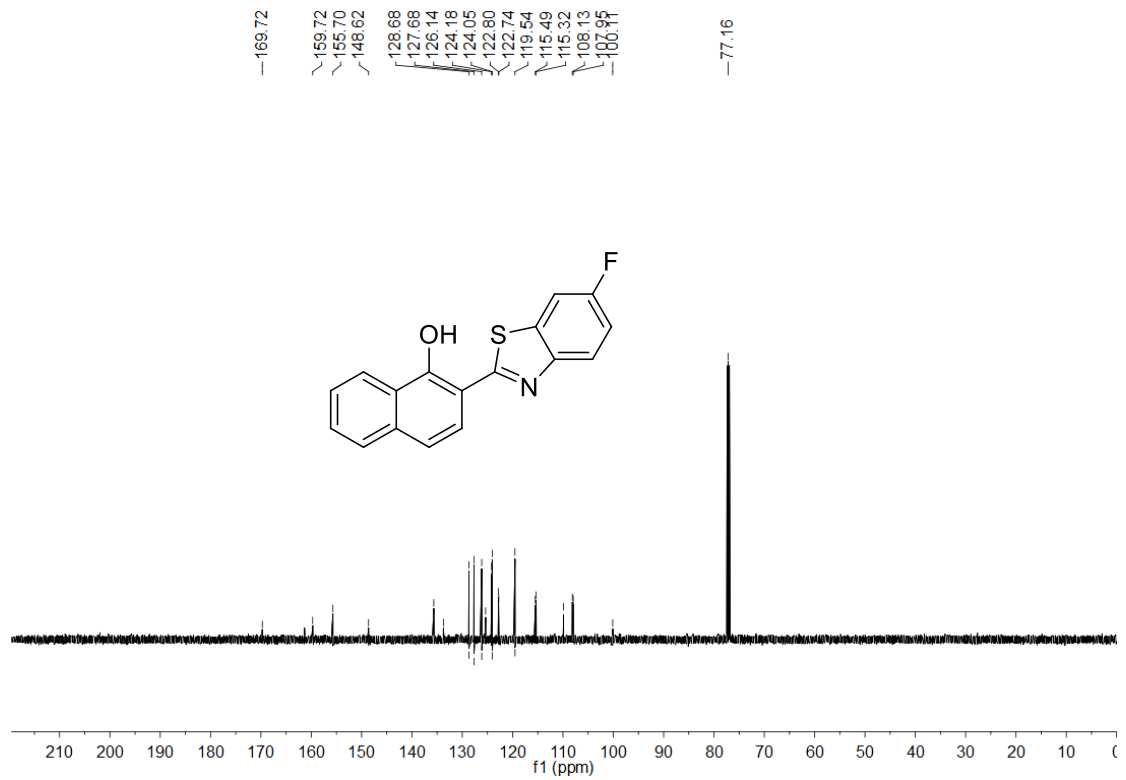
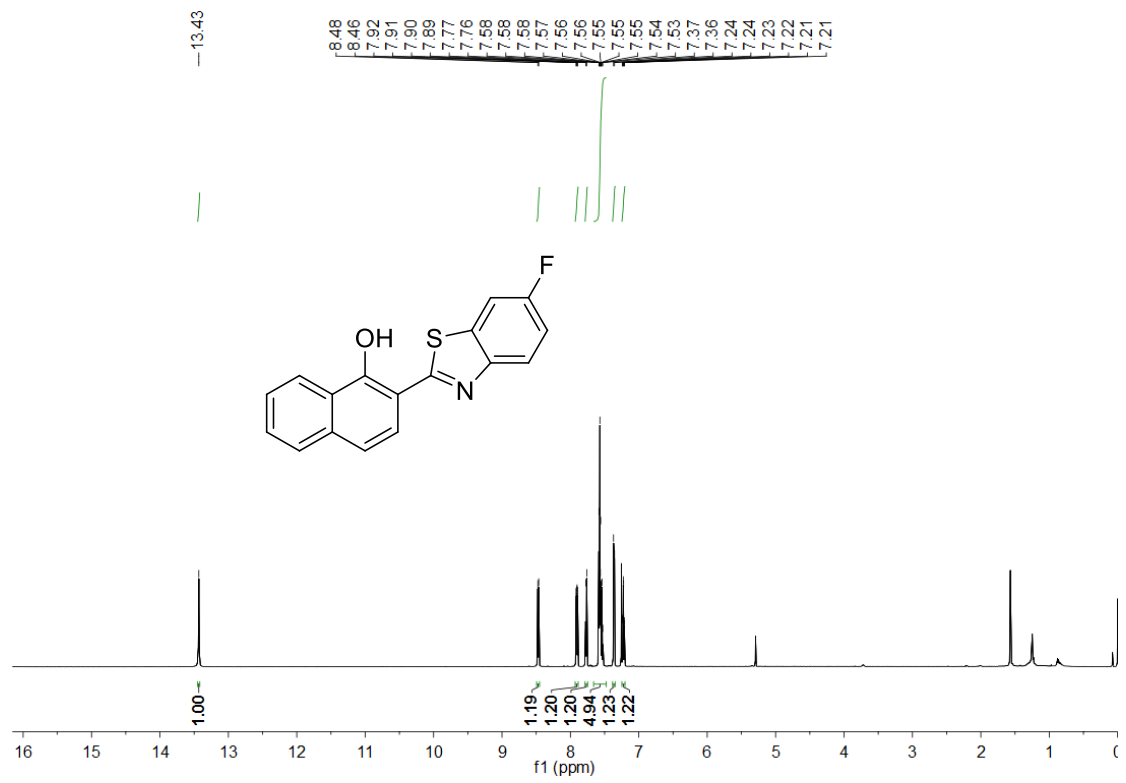
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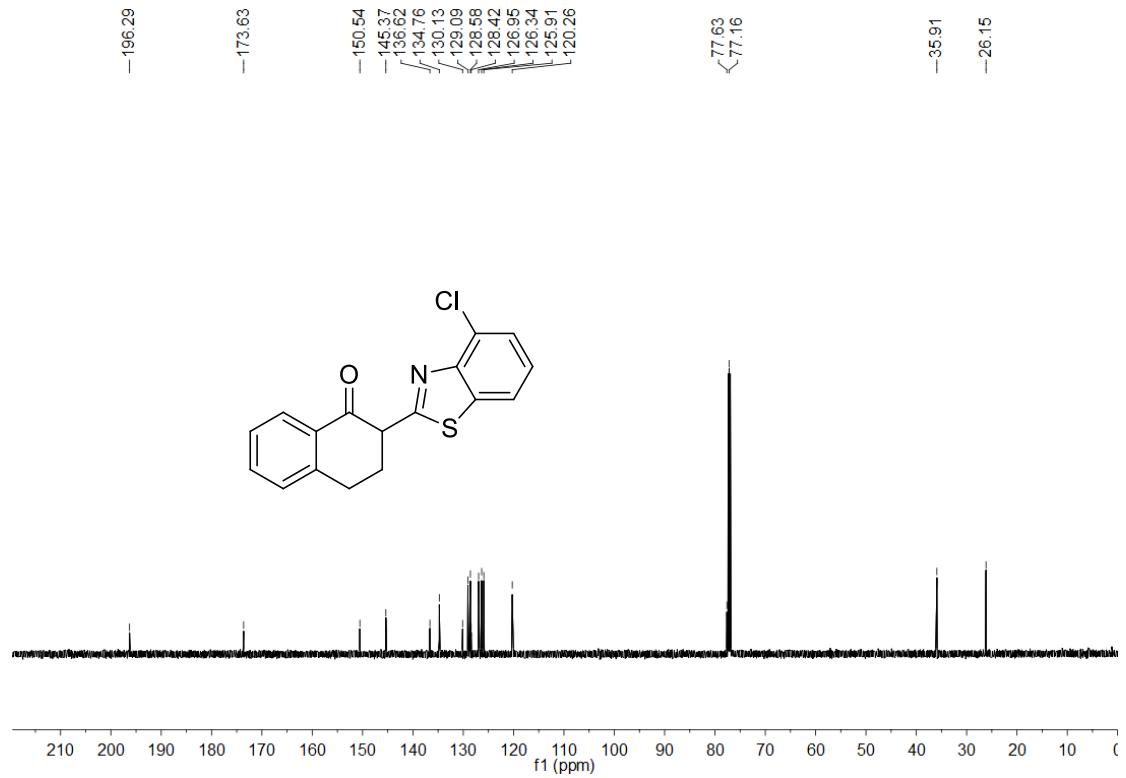
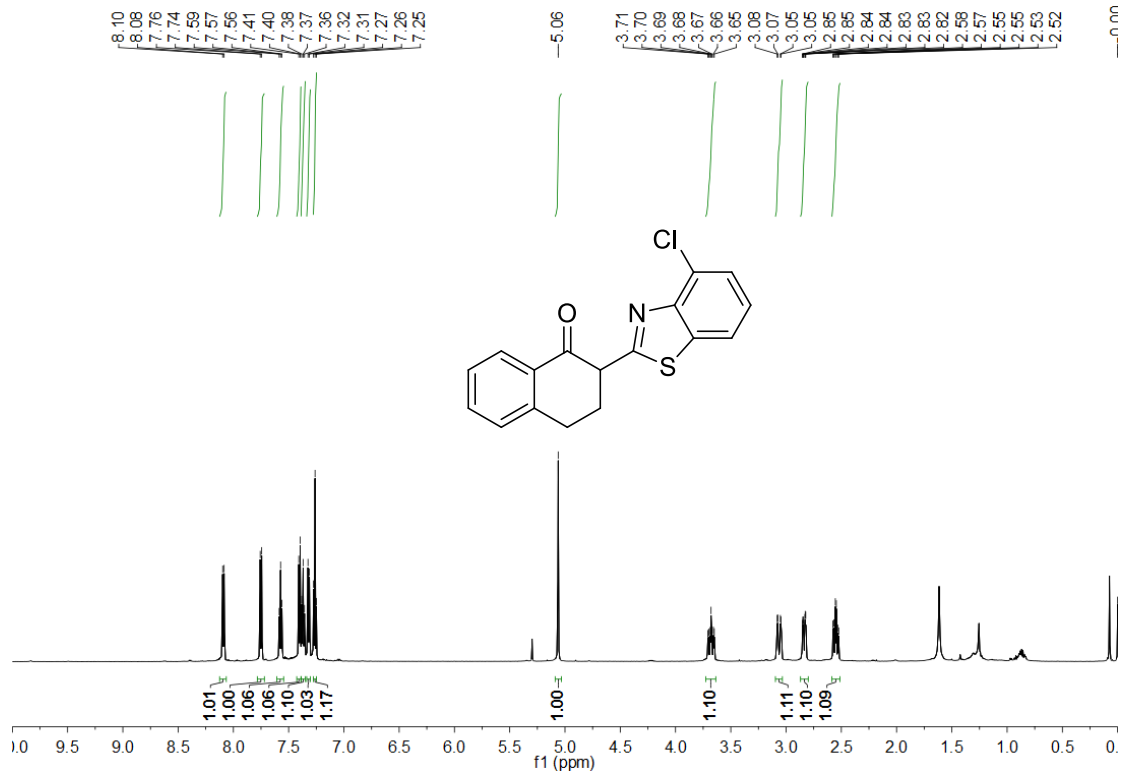
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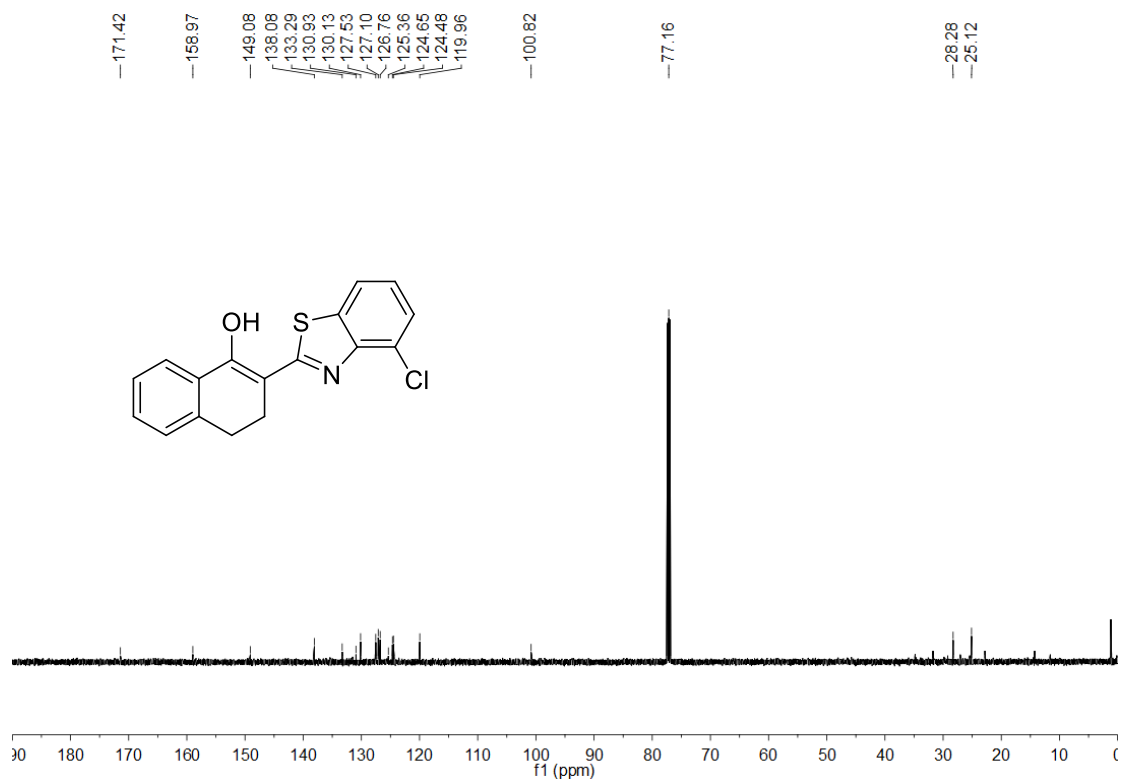
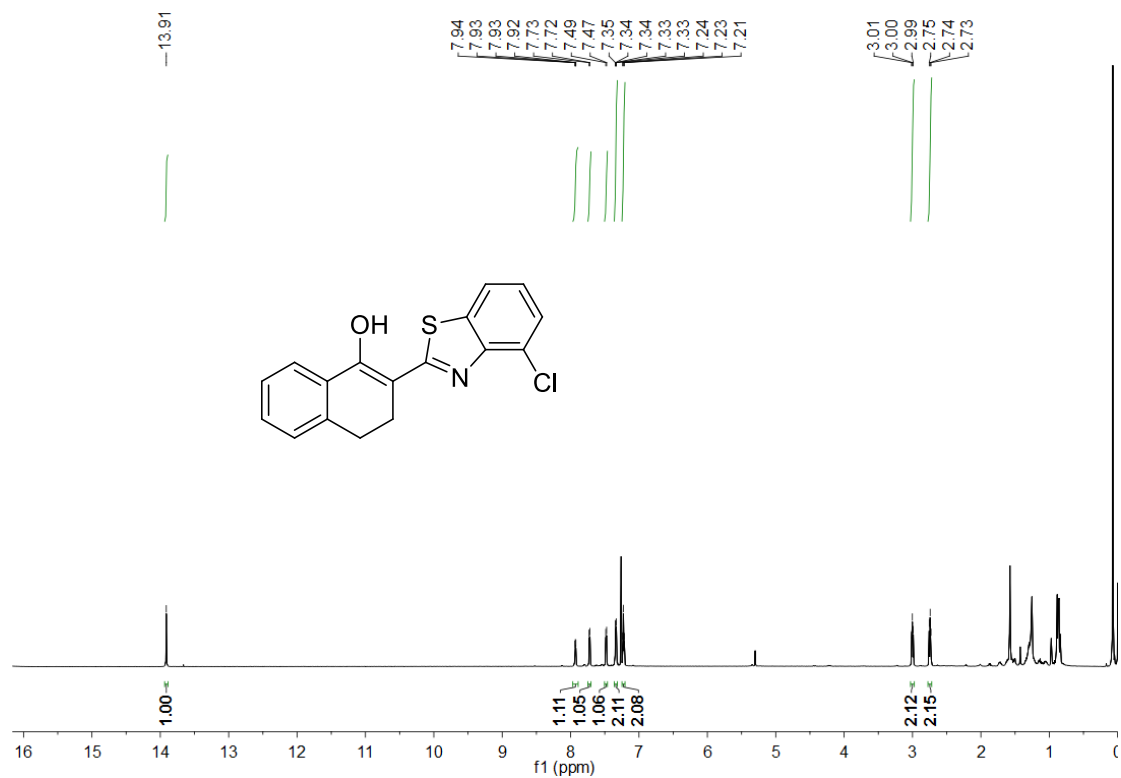
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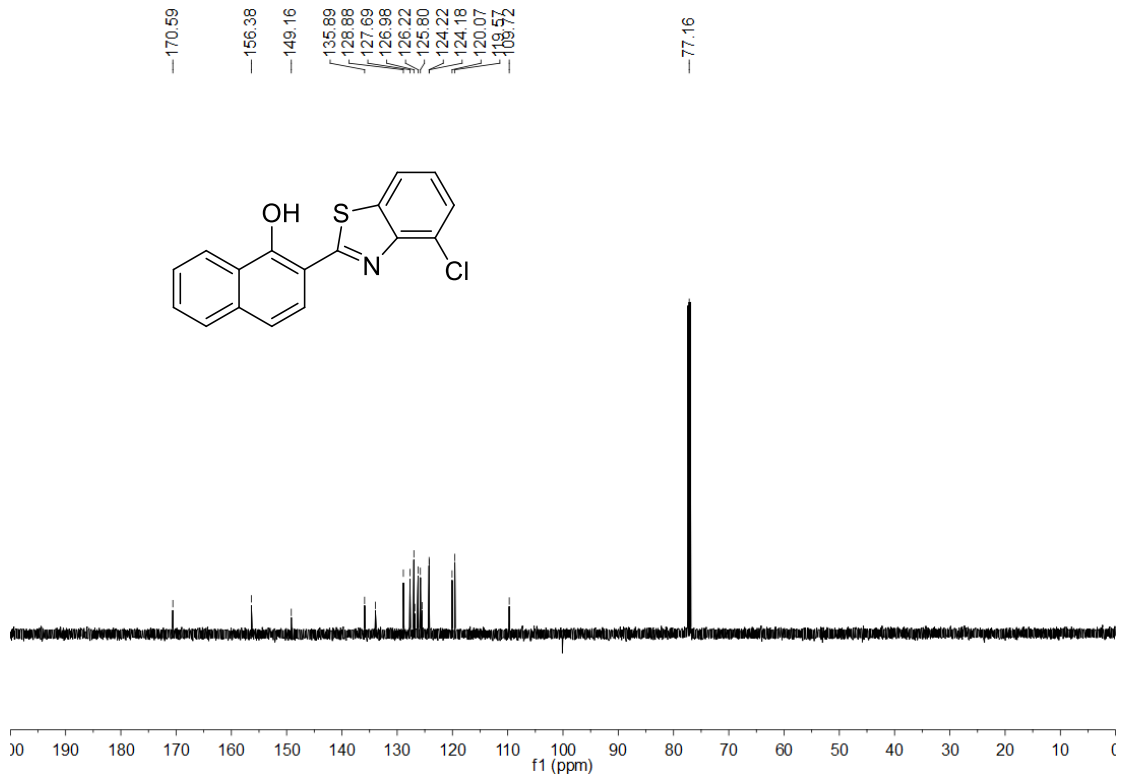
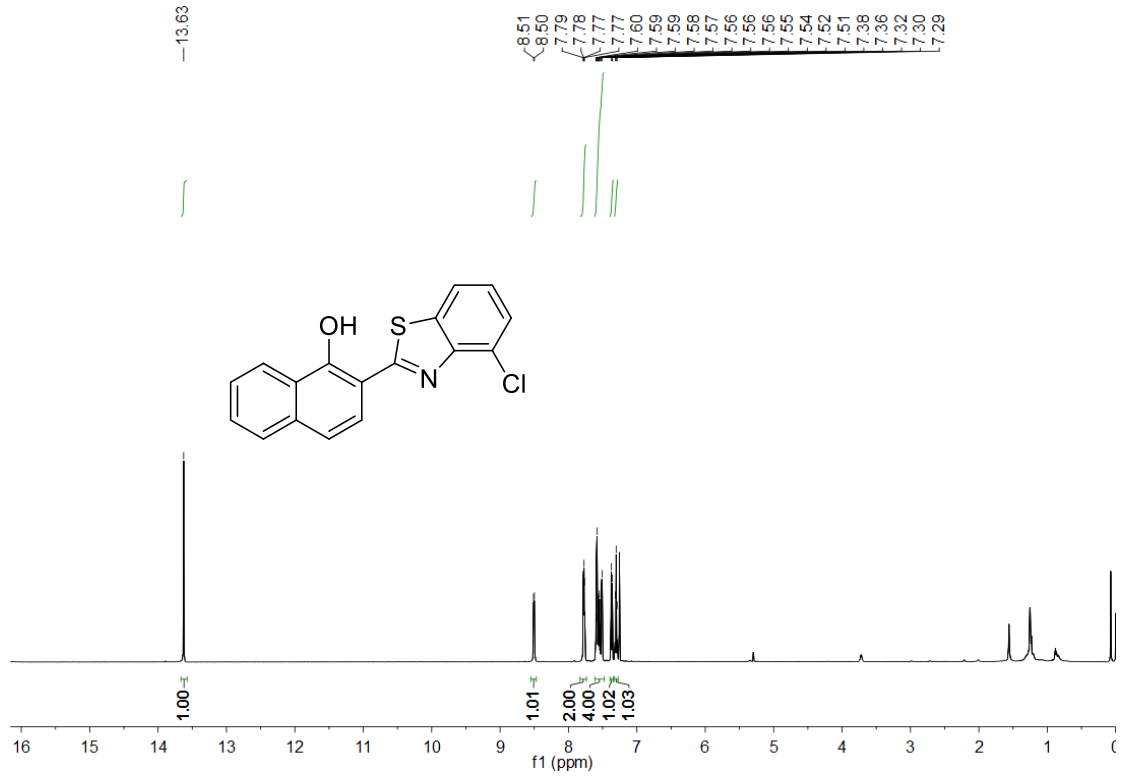
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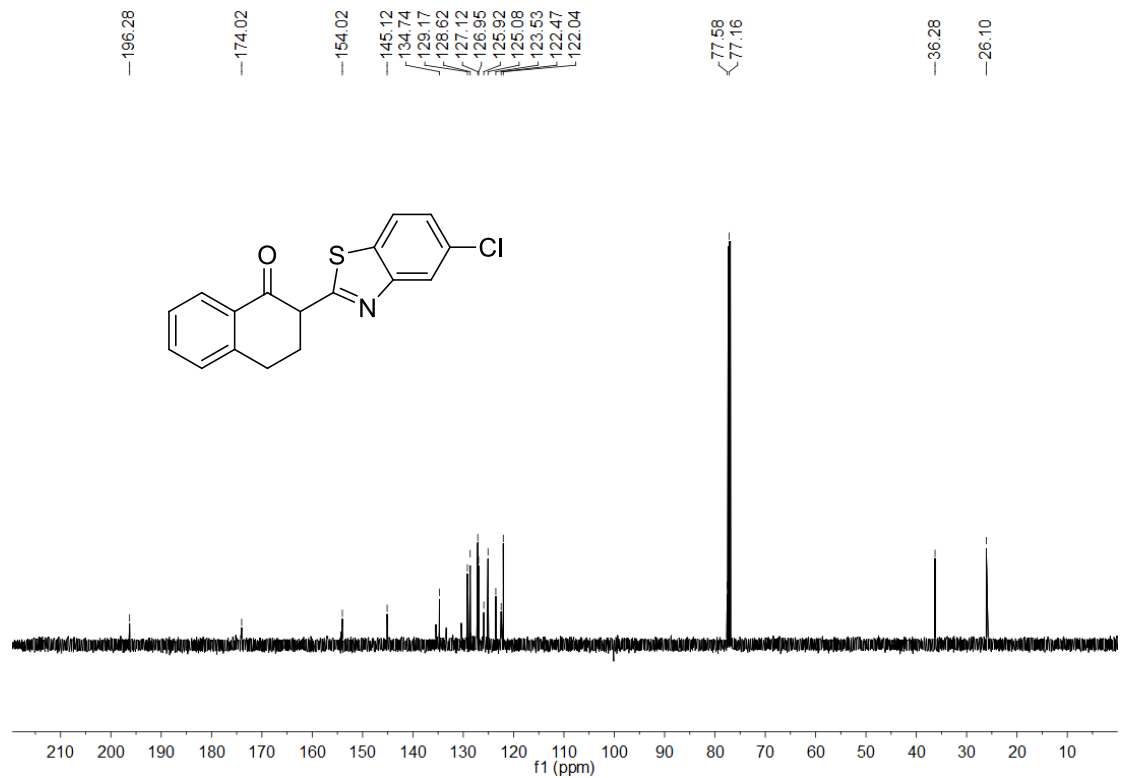
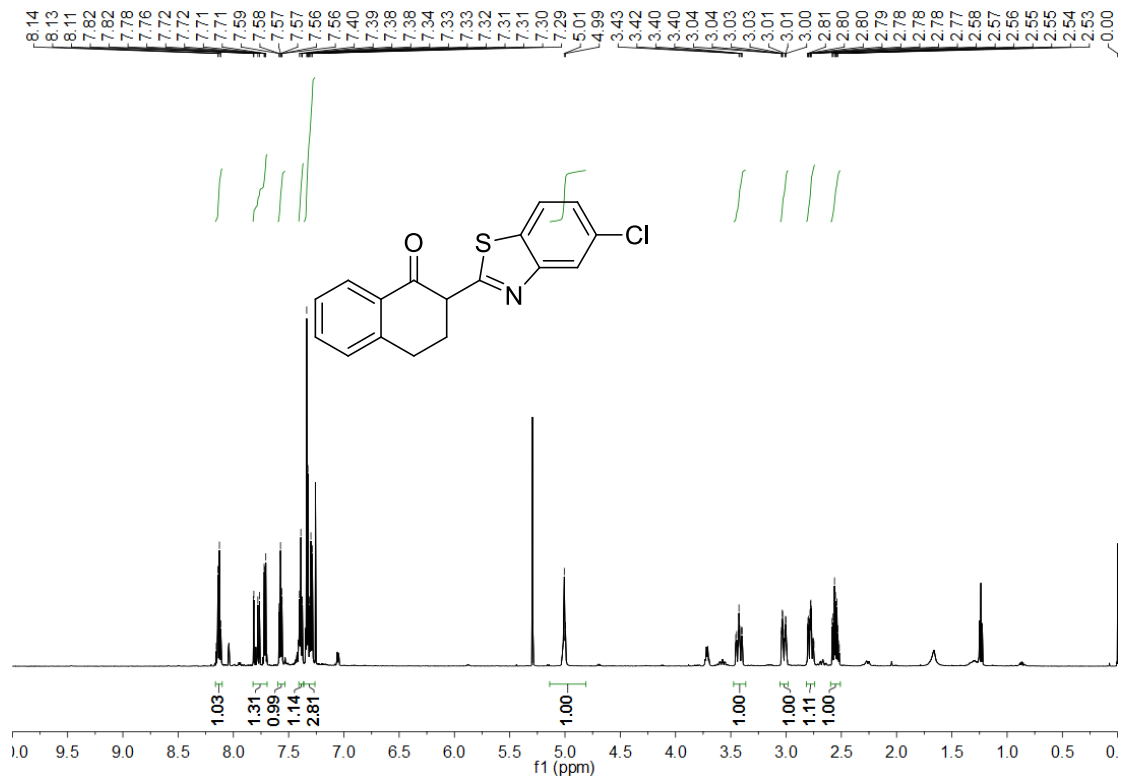
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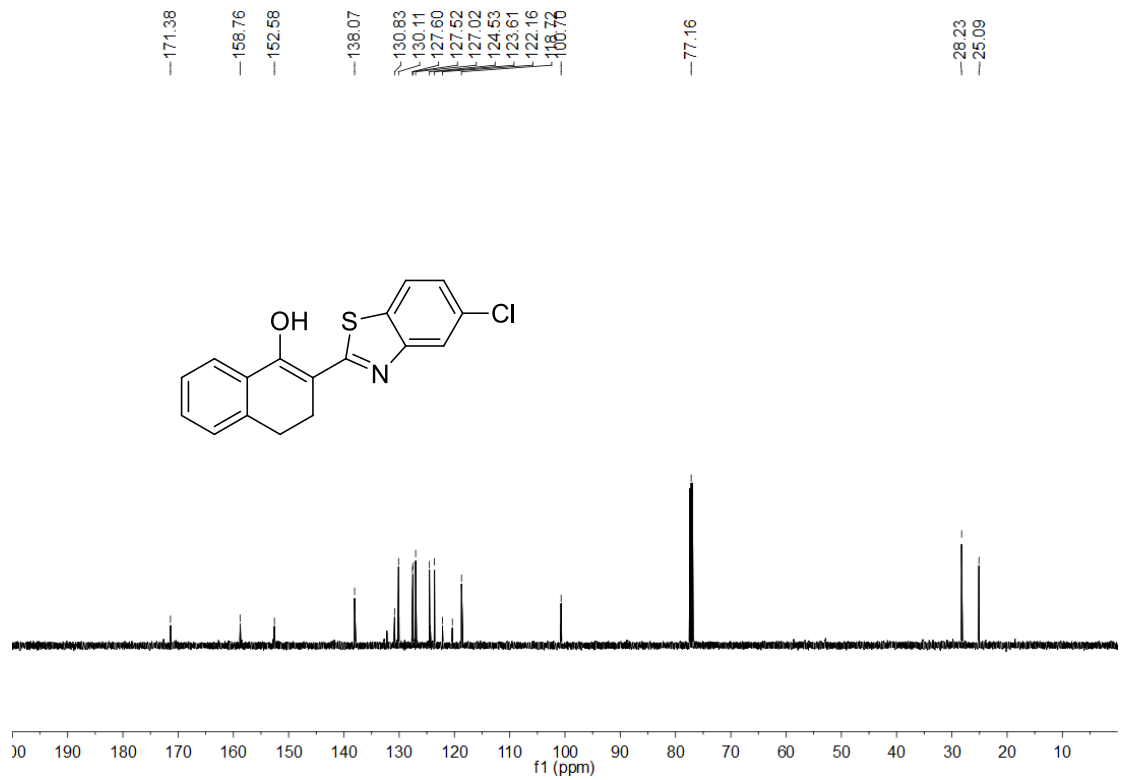
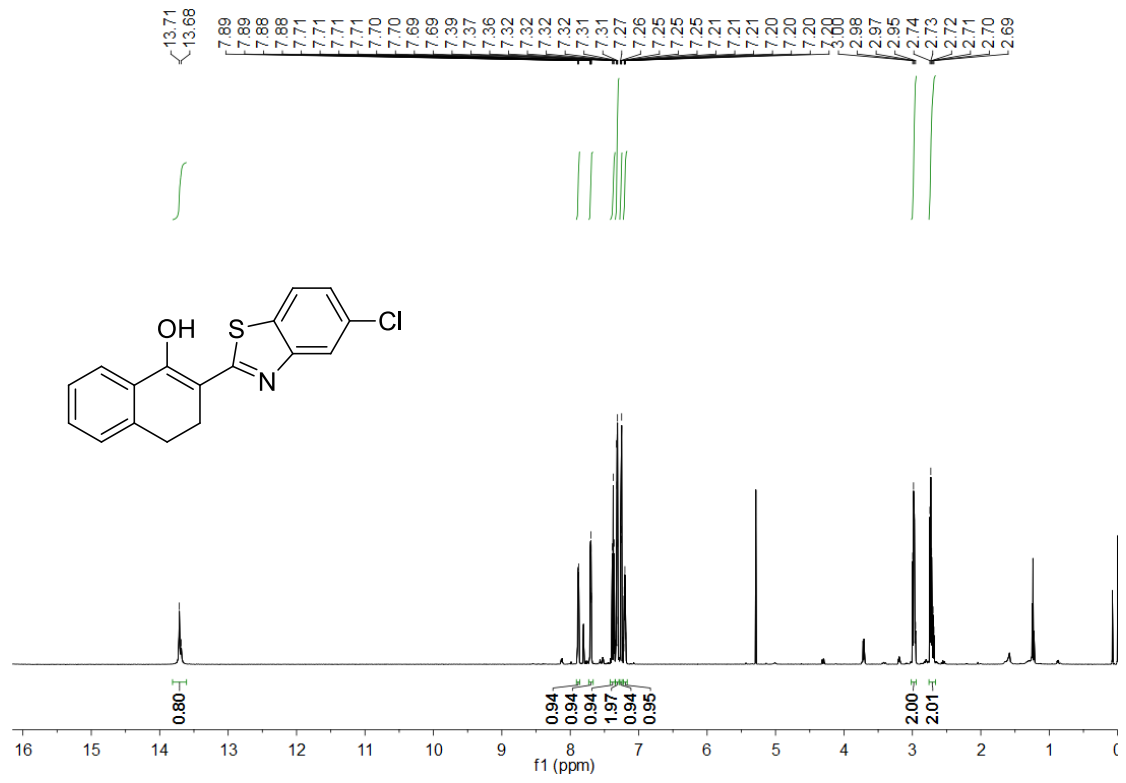
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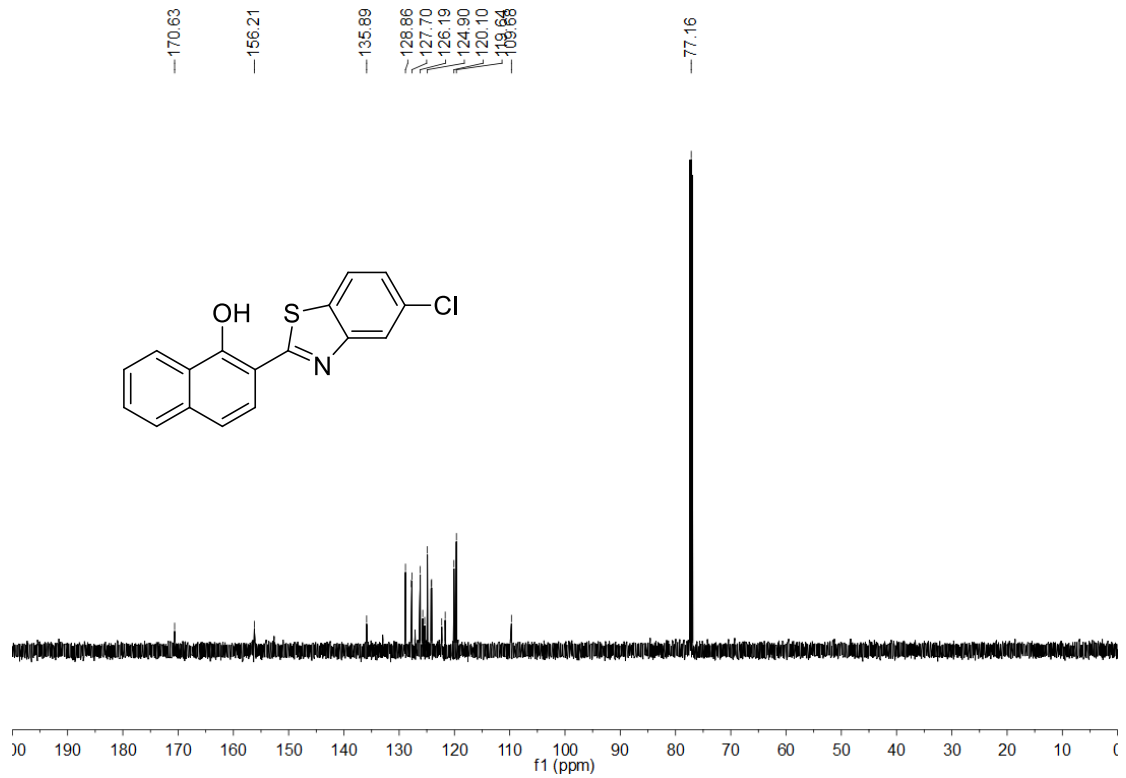
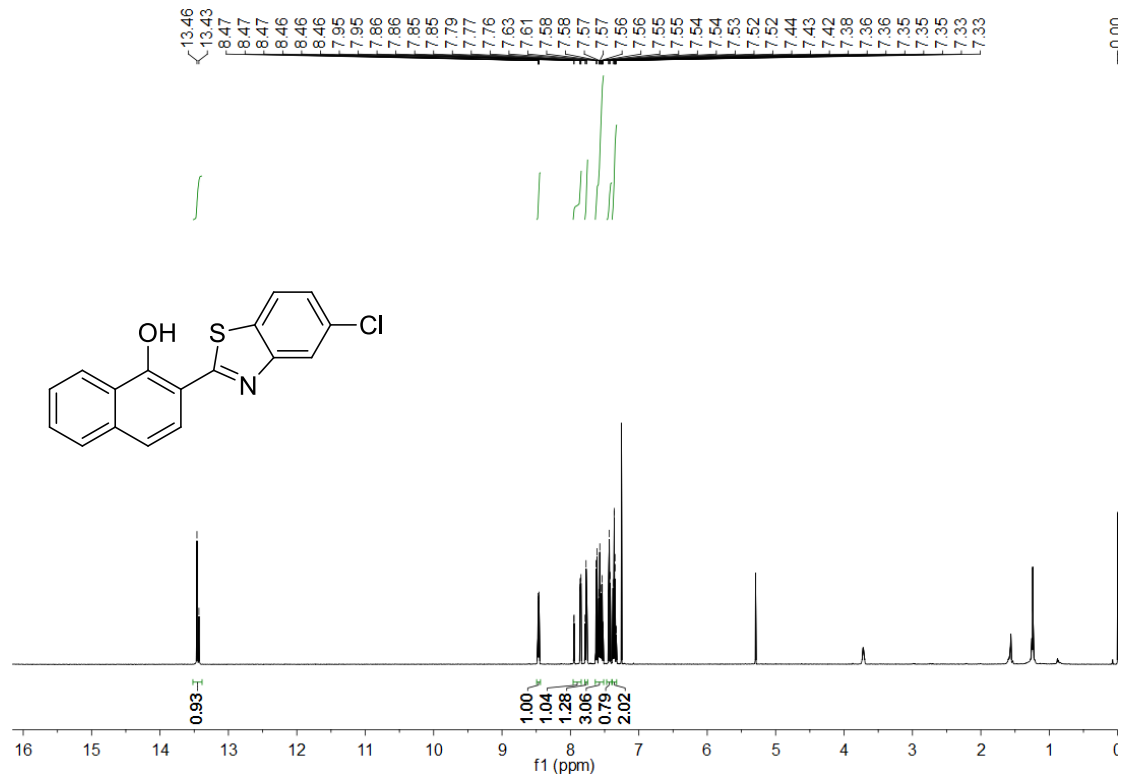
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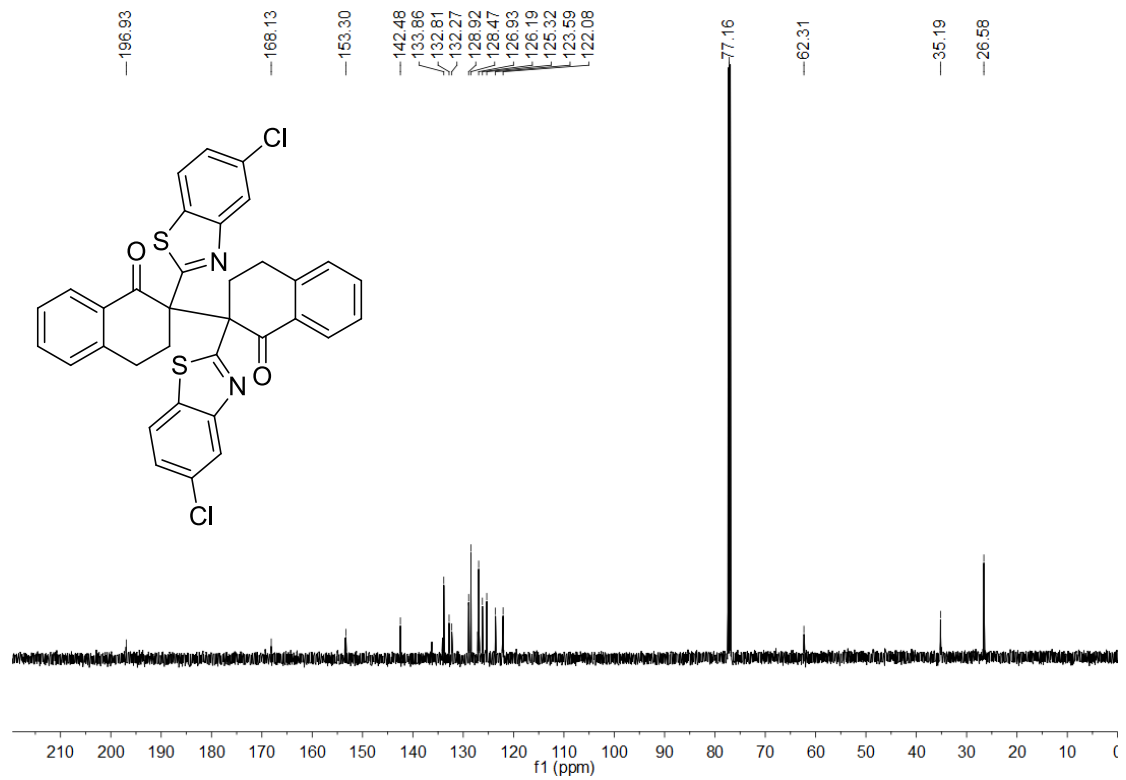
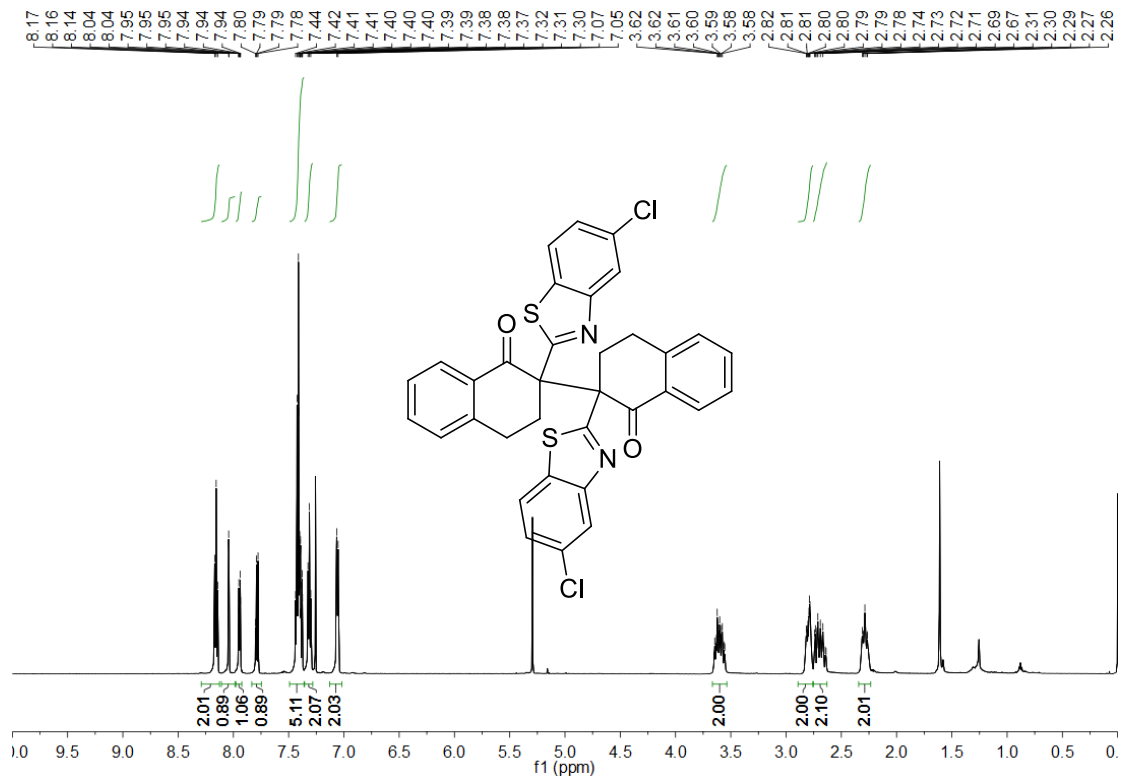
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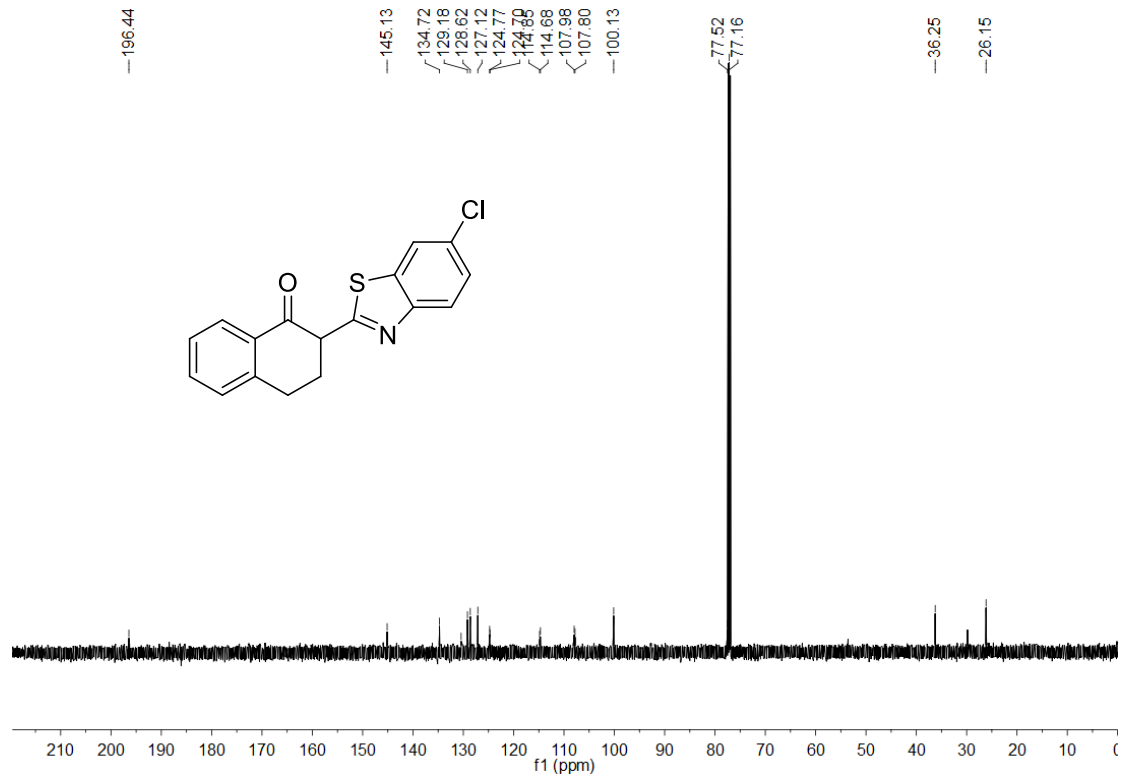
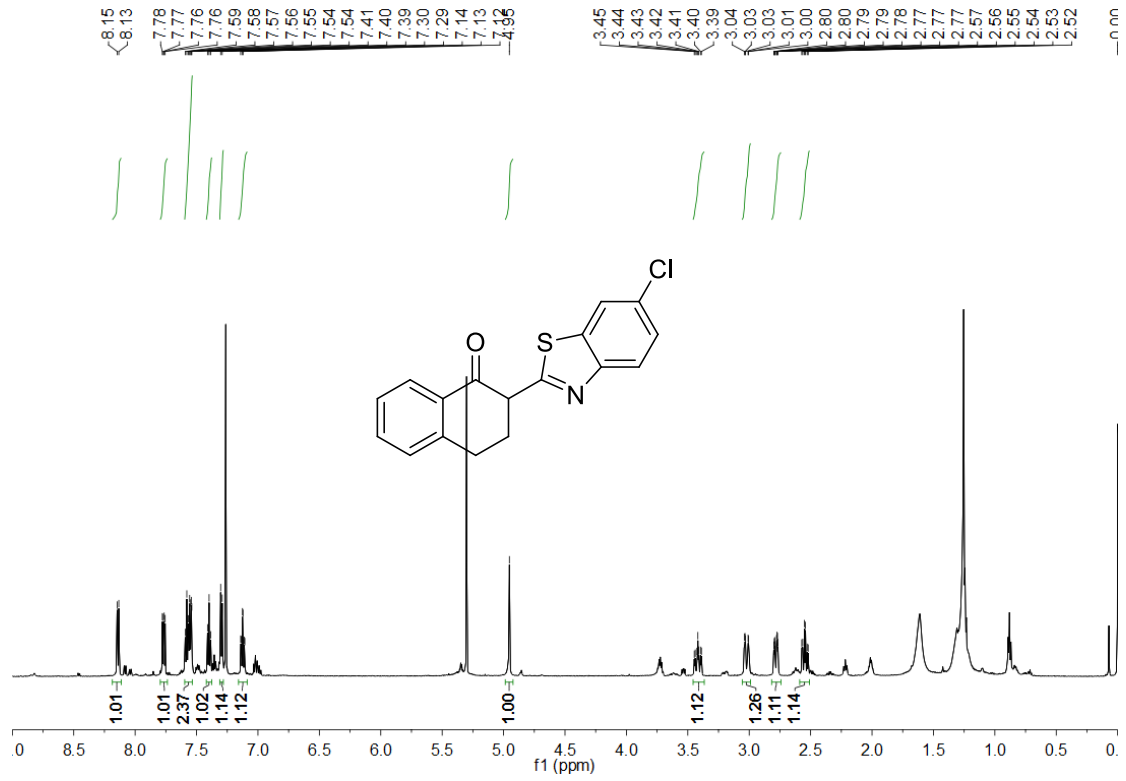
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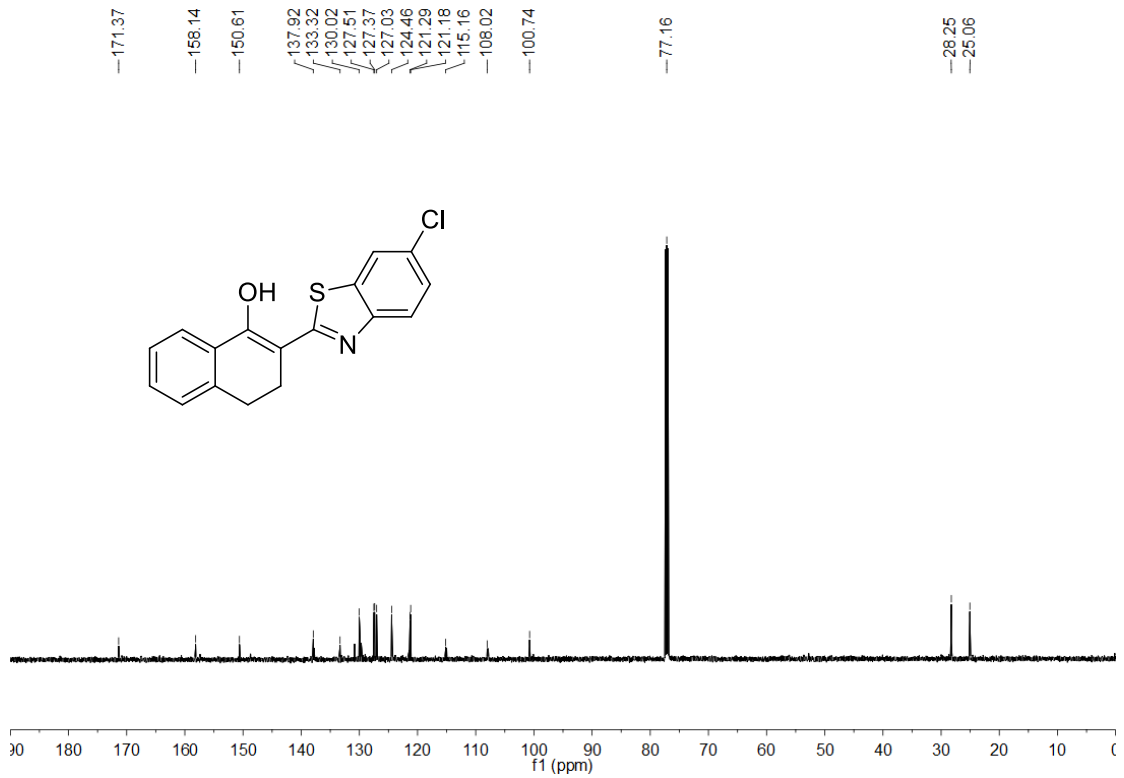
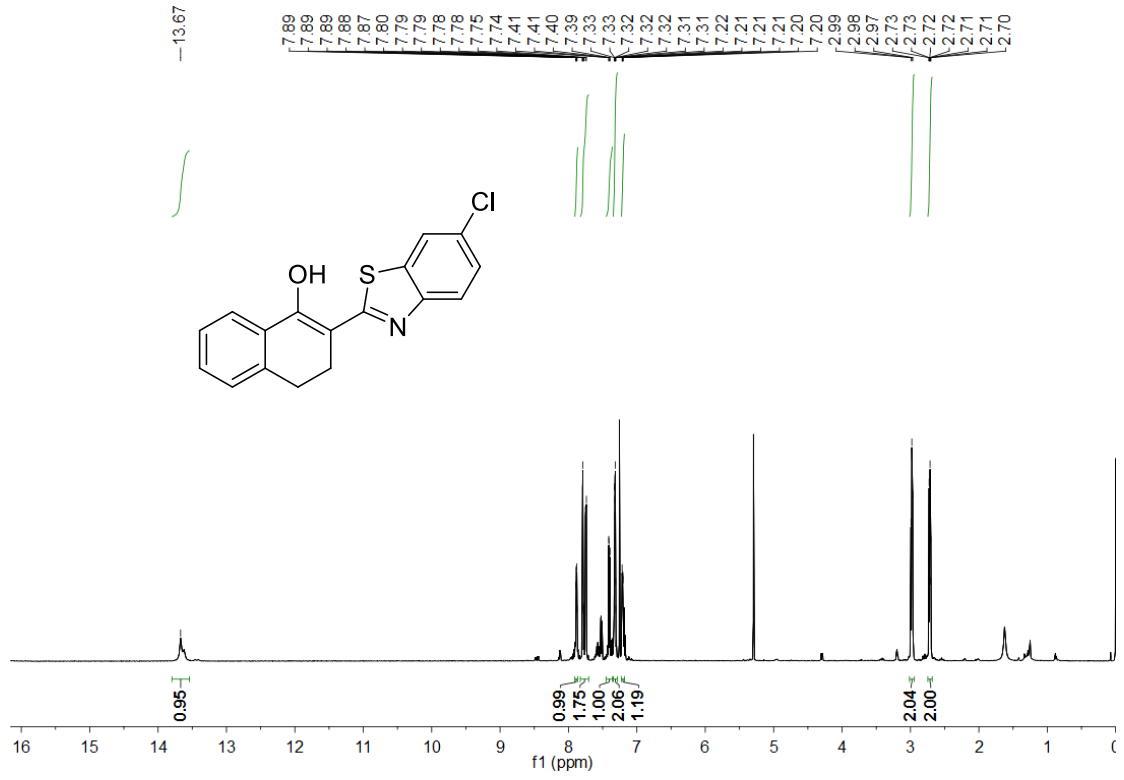
5d



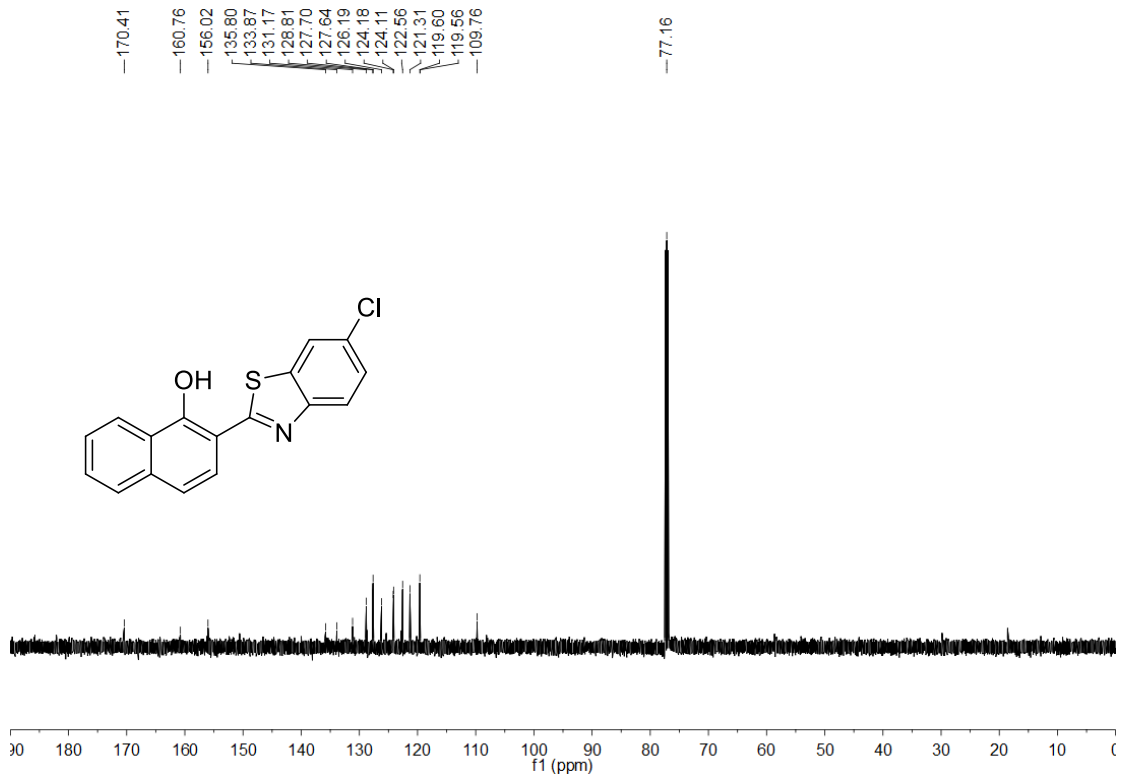
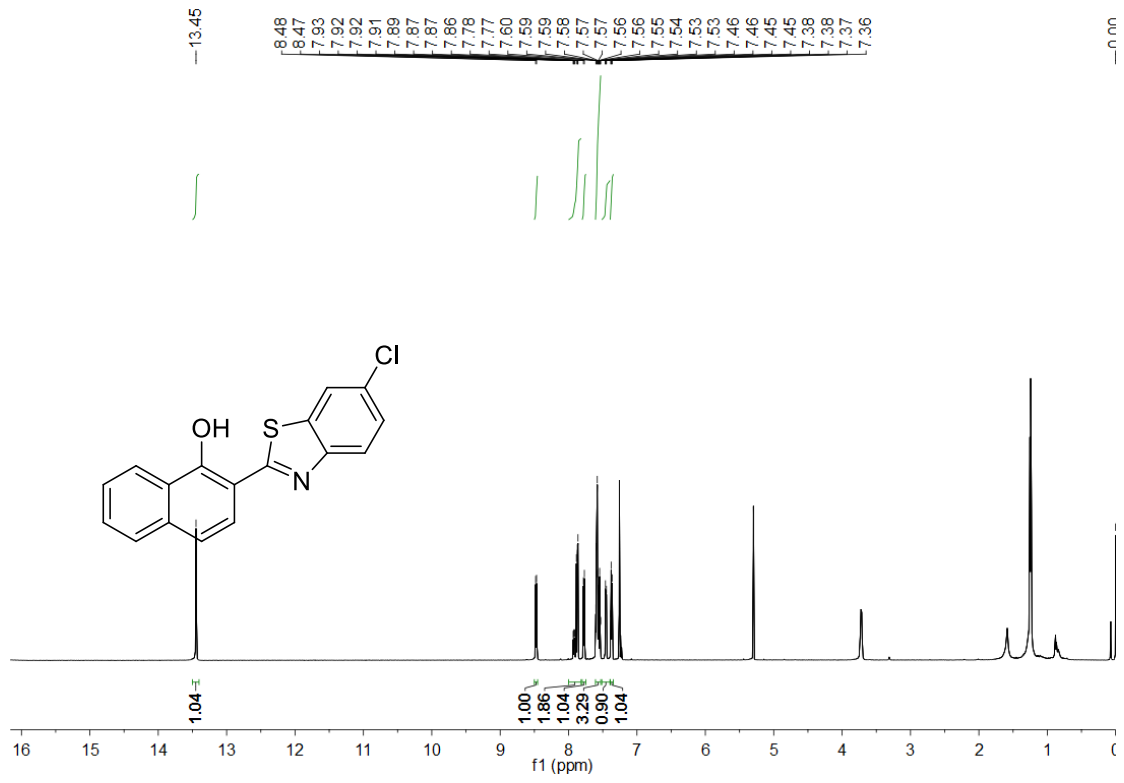
2e



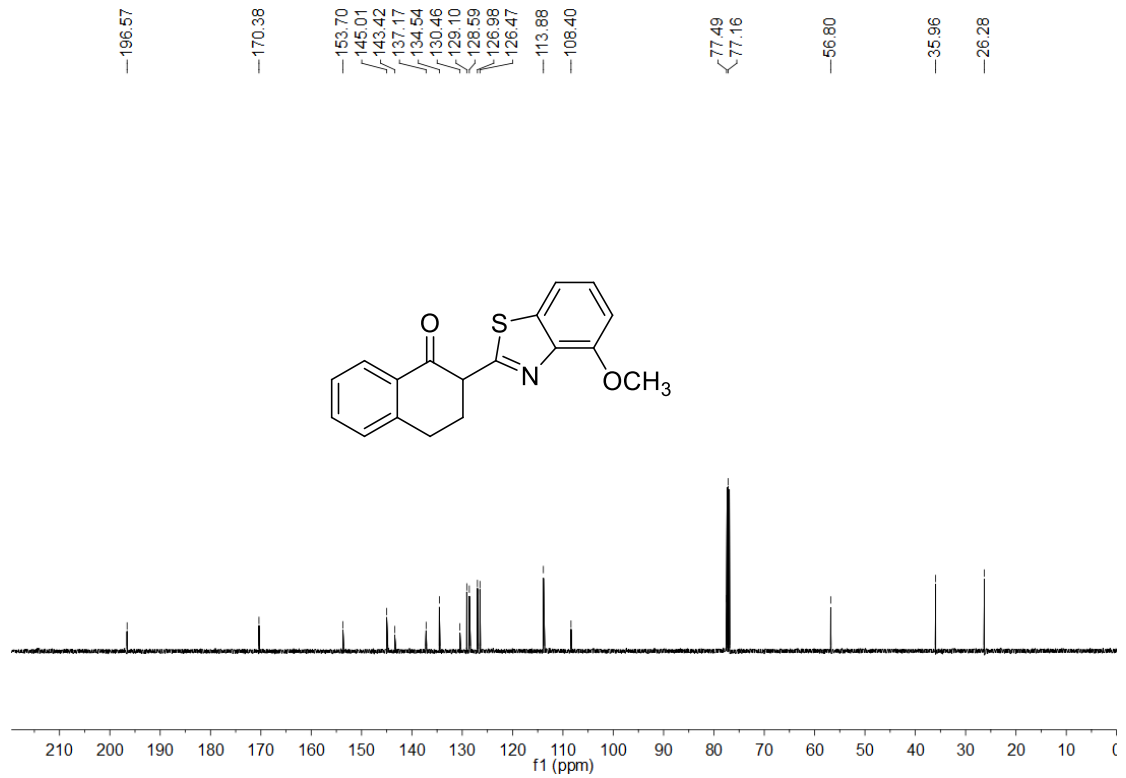
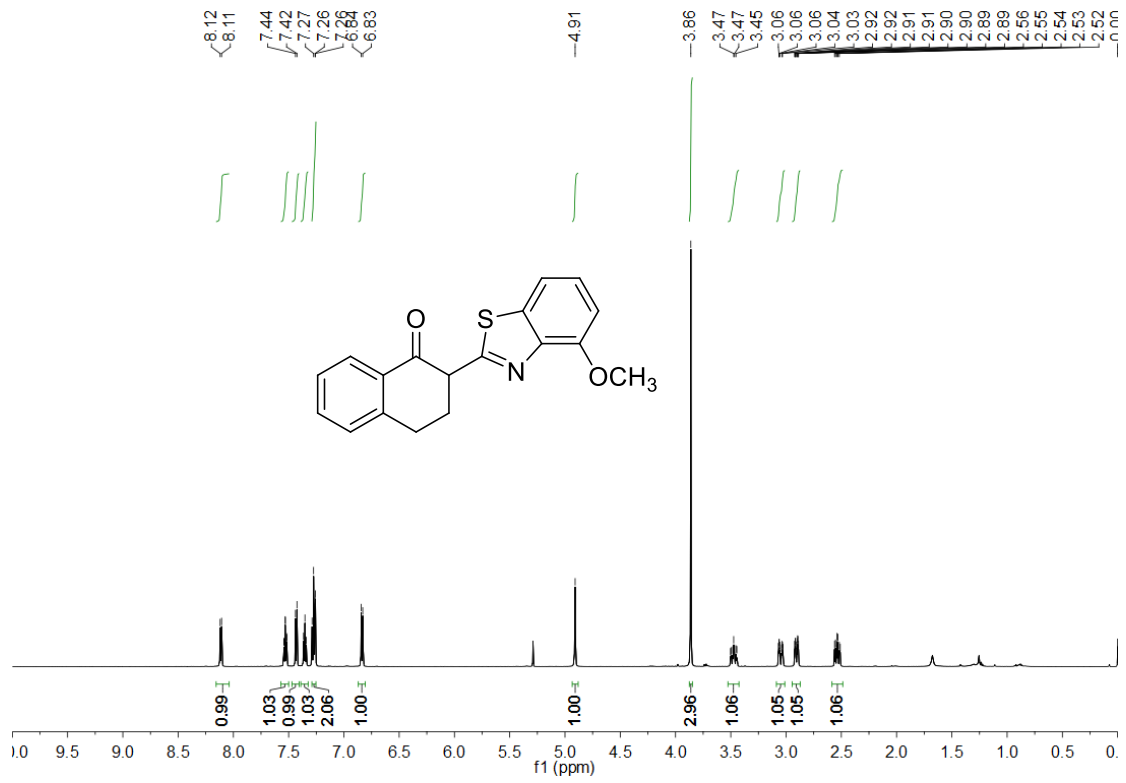
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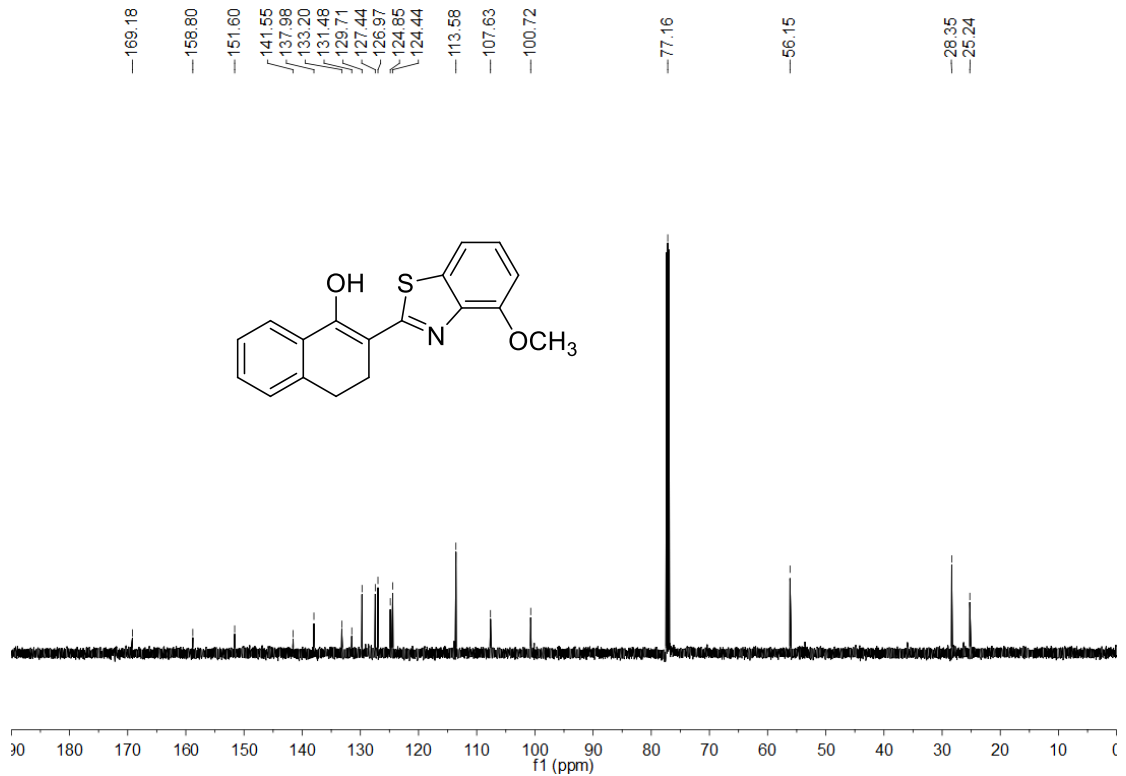
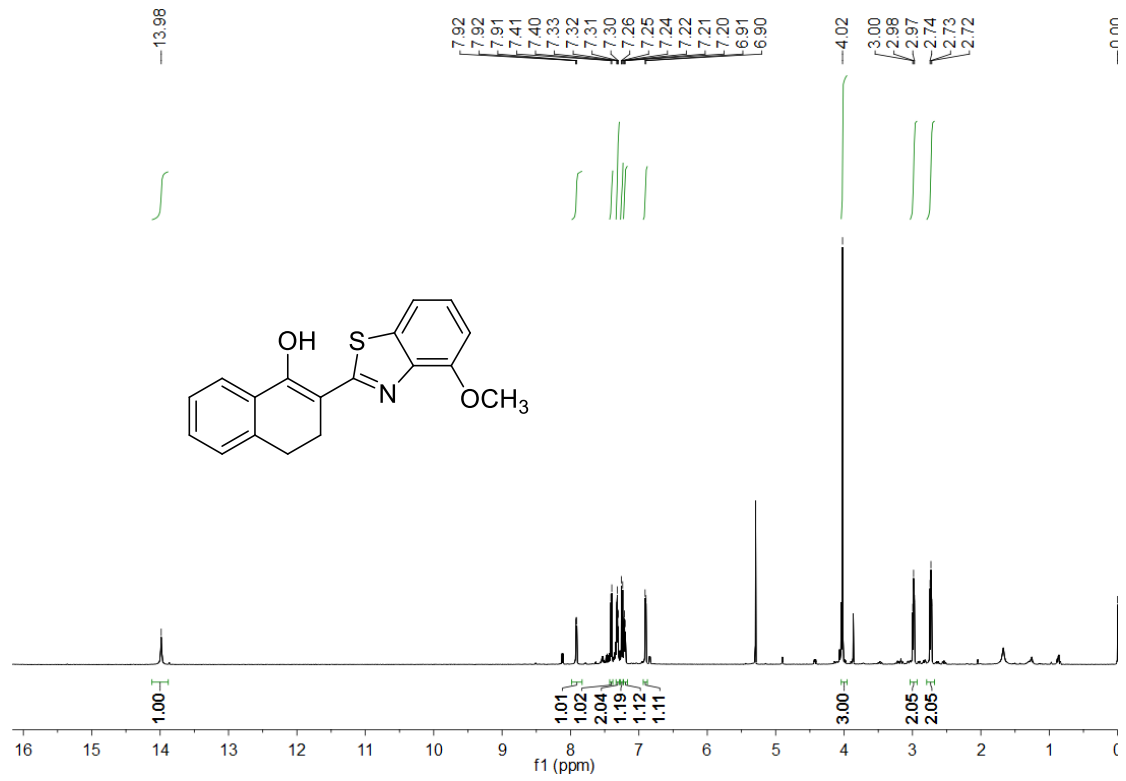
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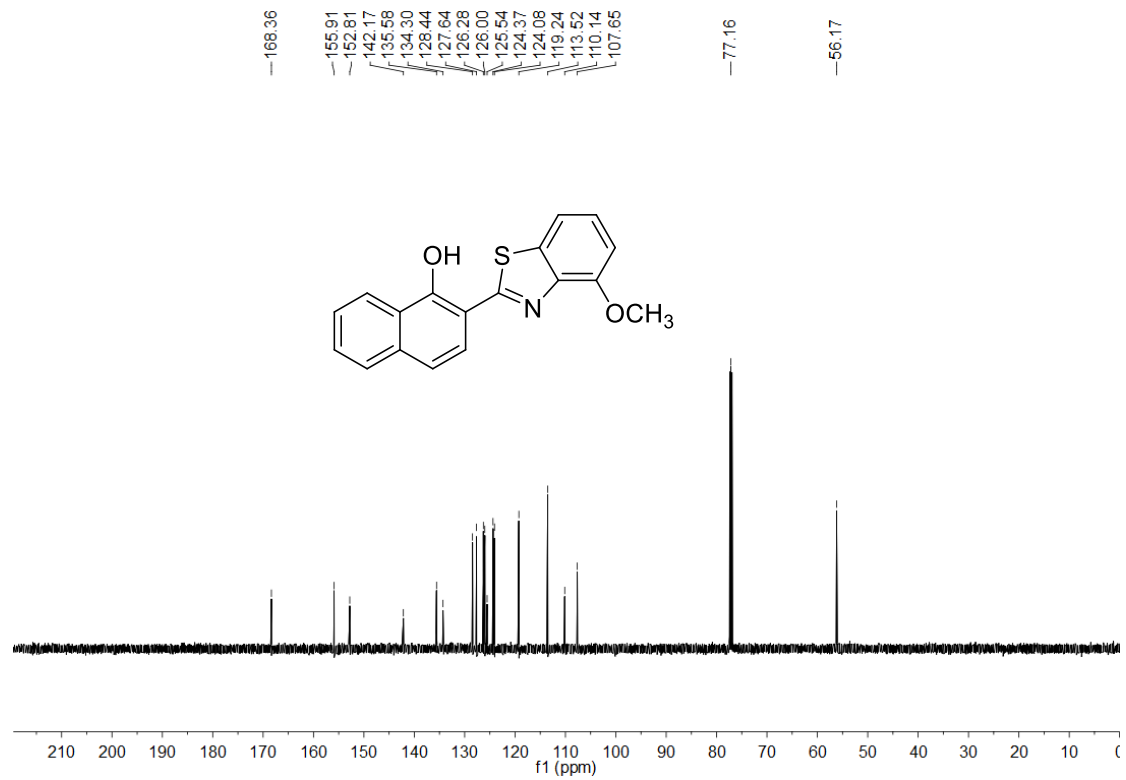
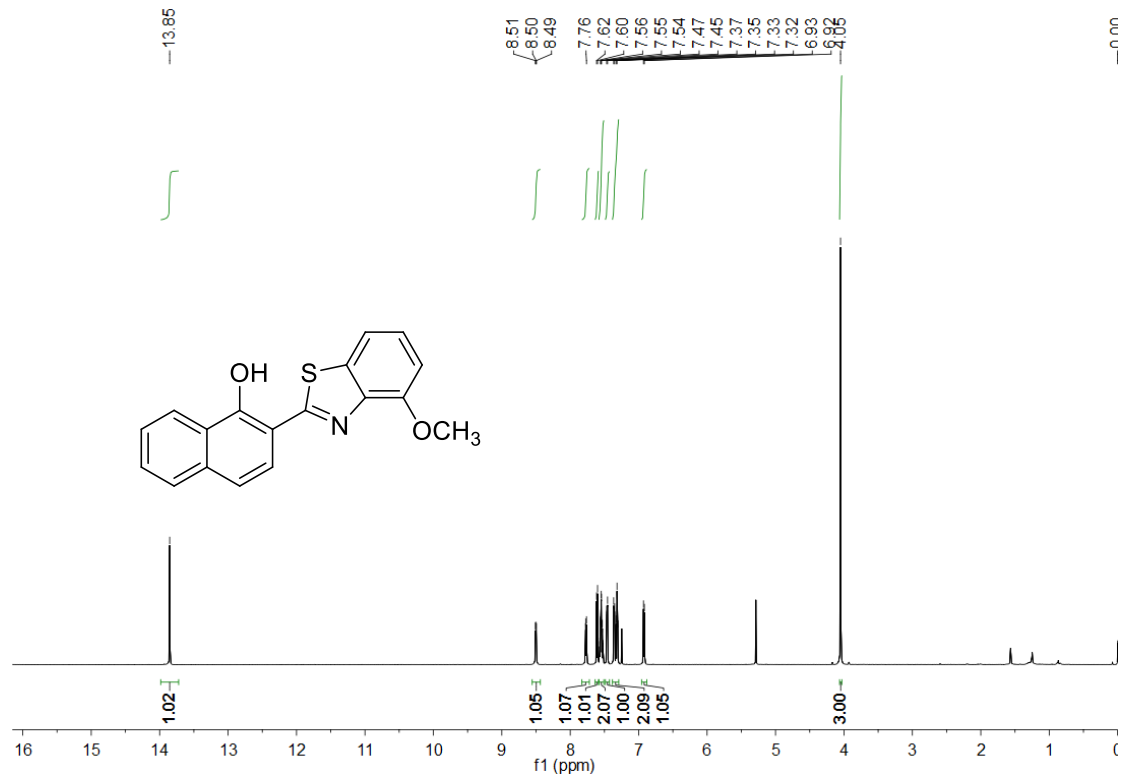
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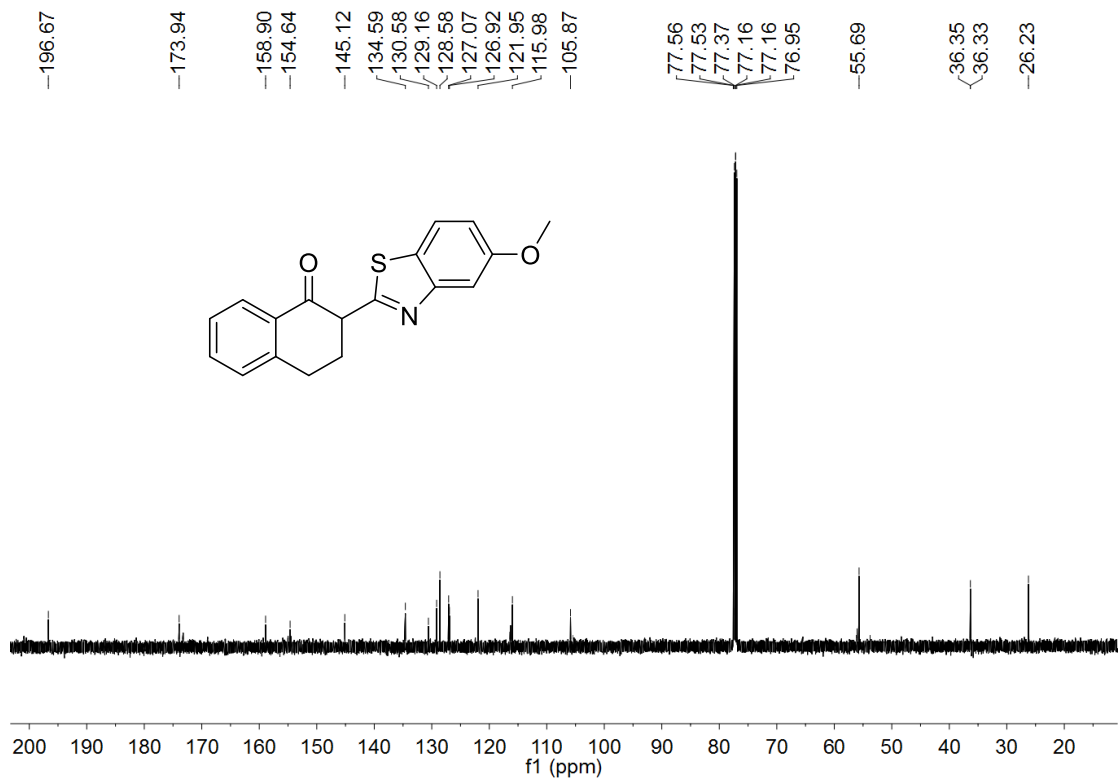
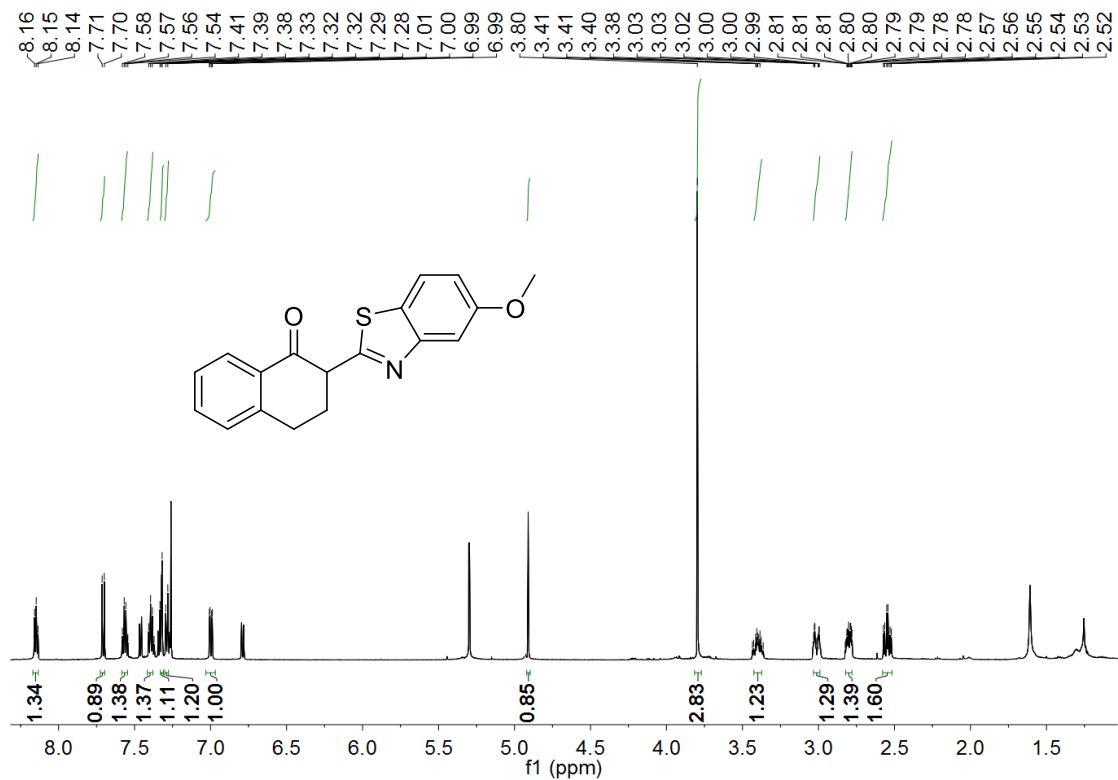
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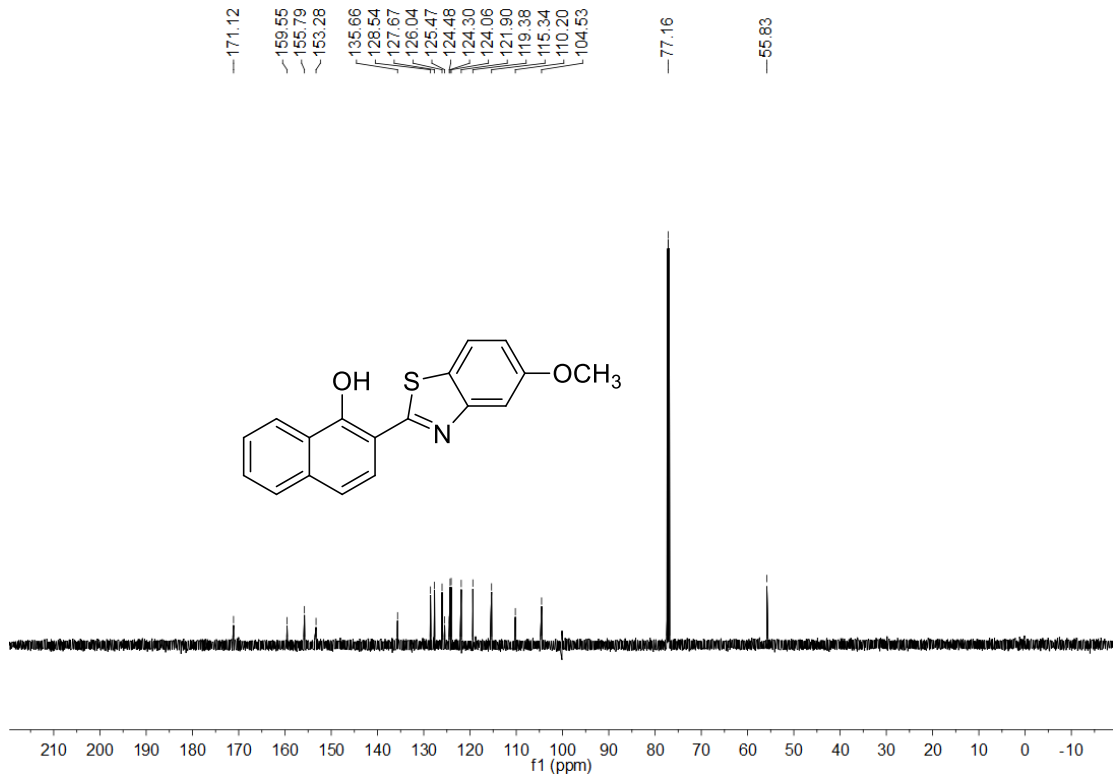
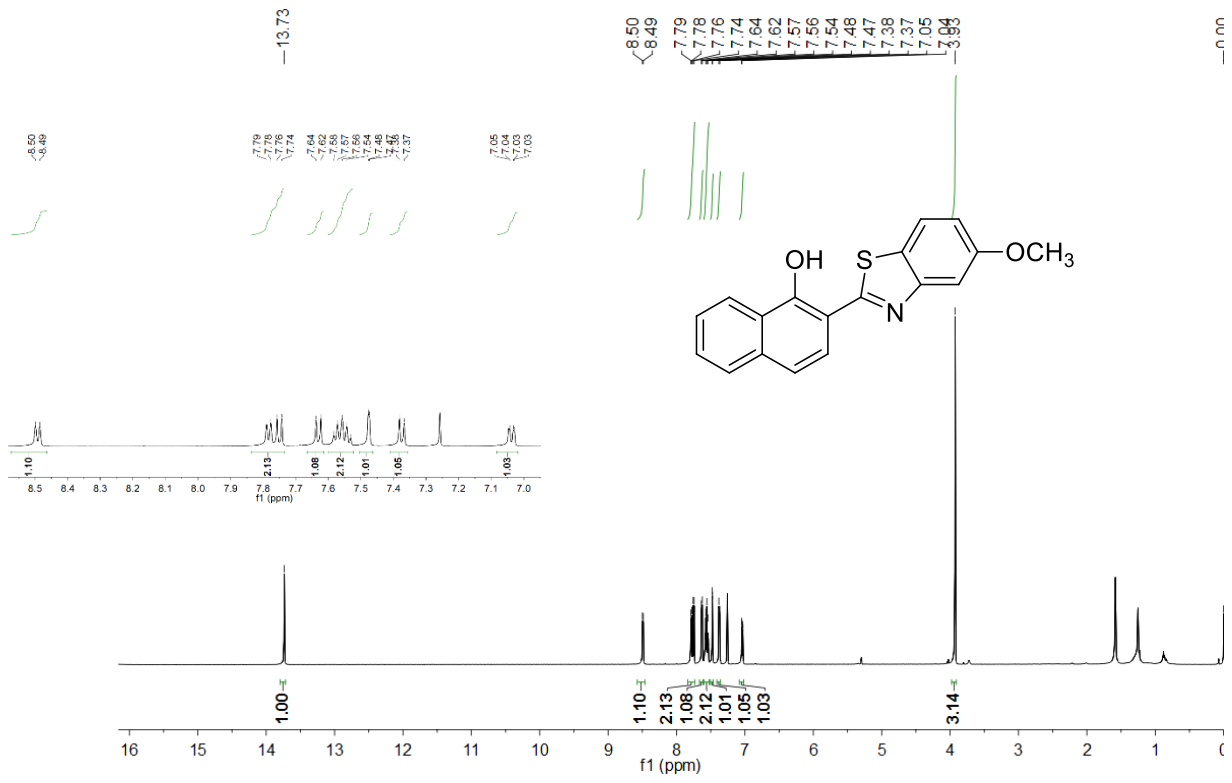
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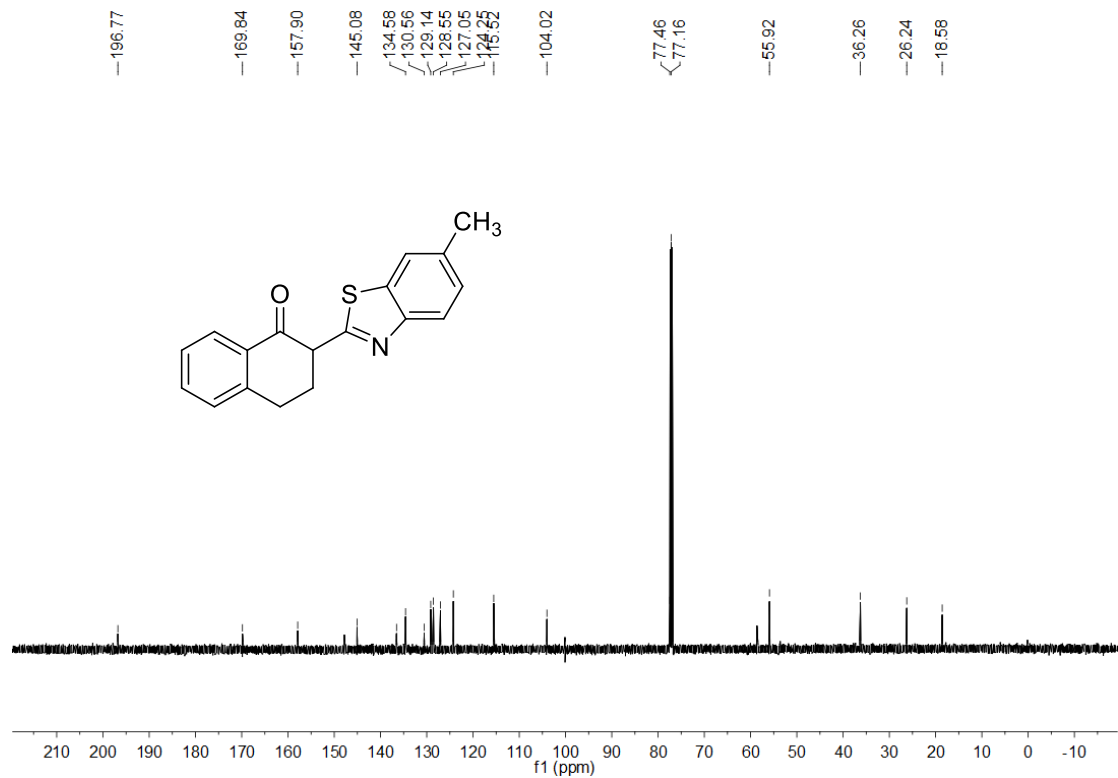
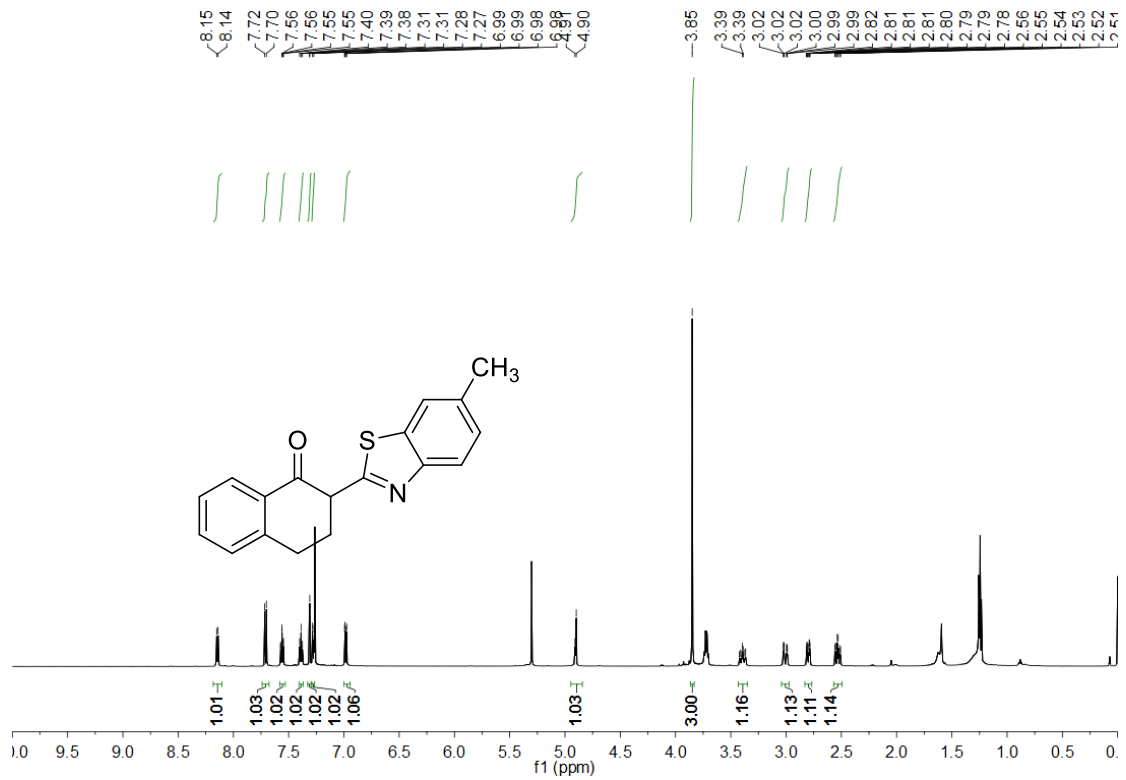
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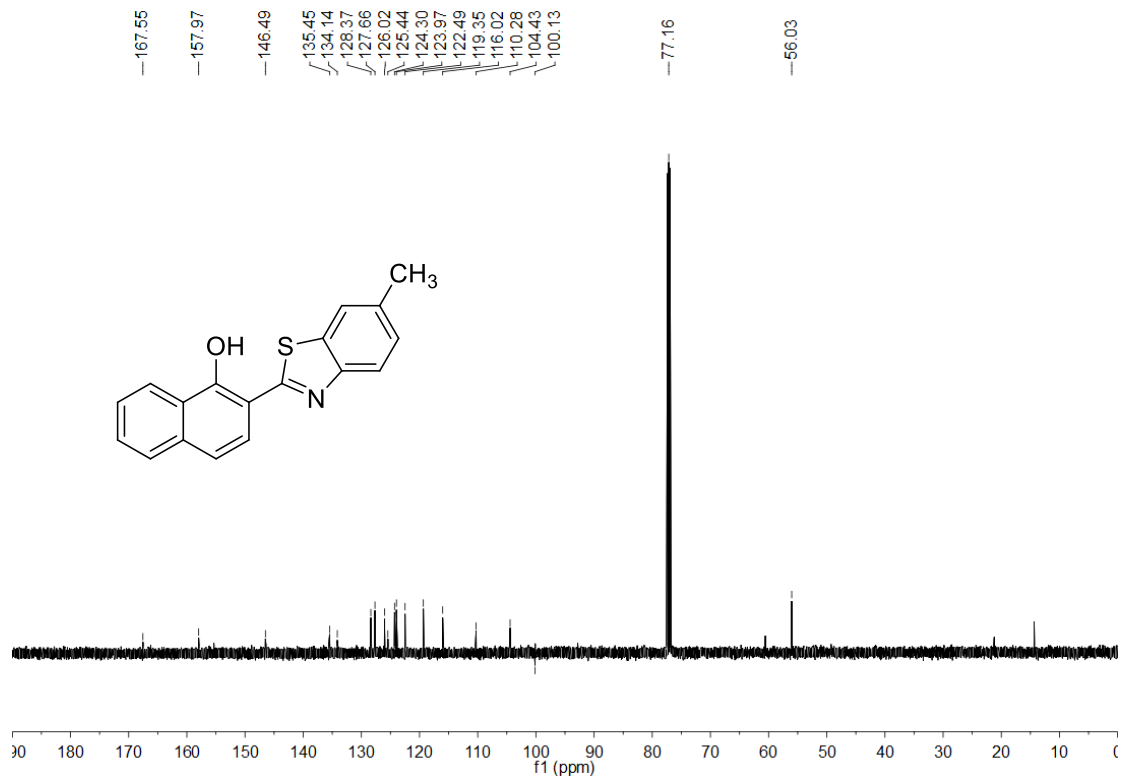
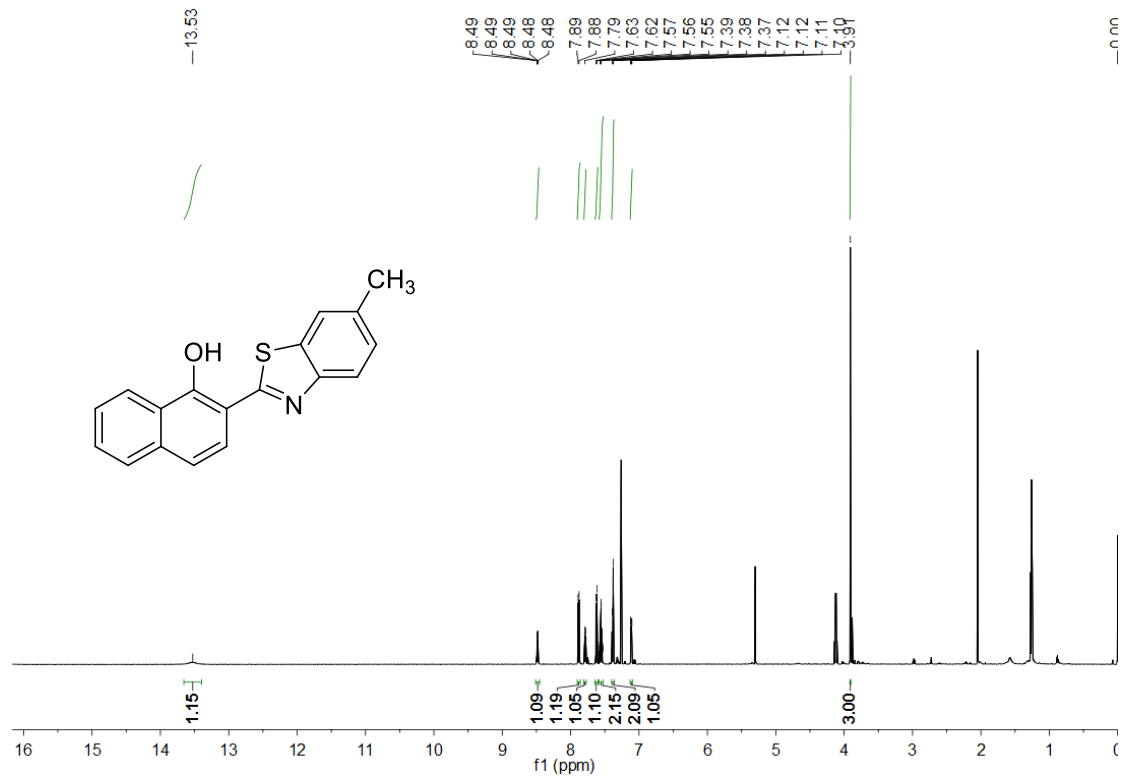
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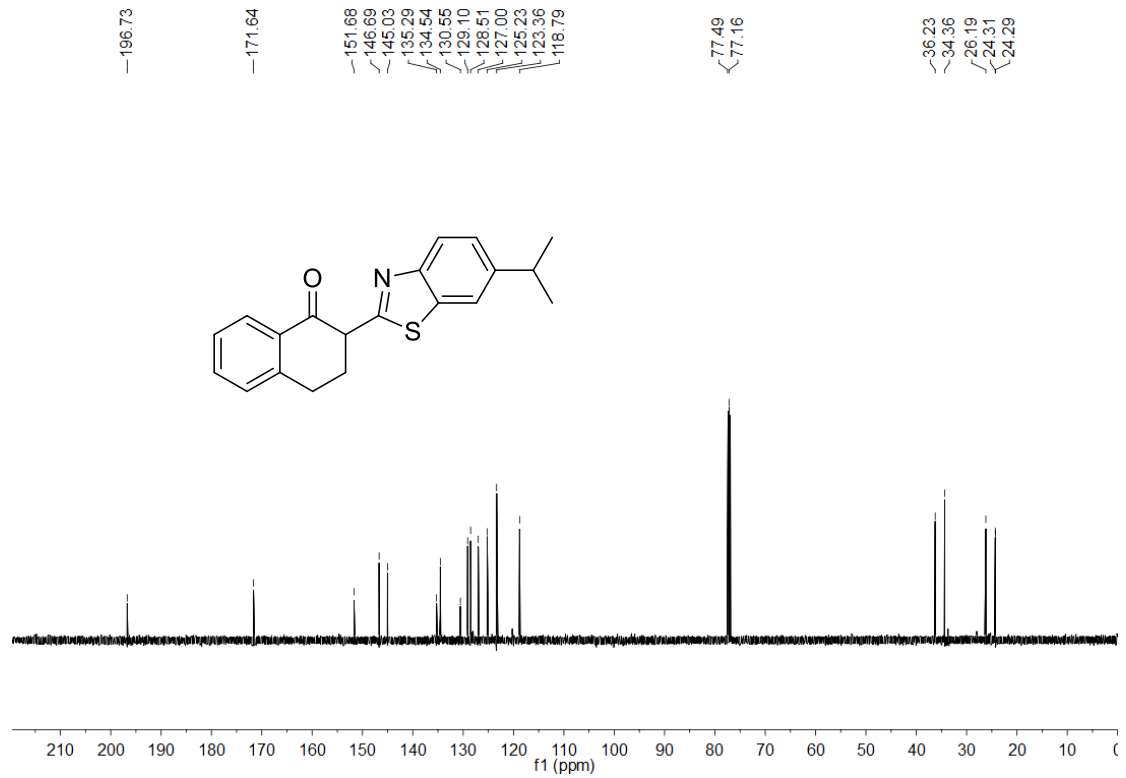
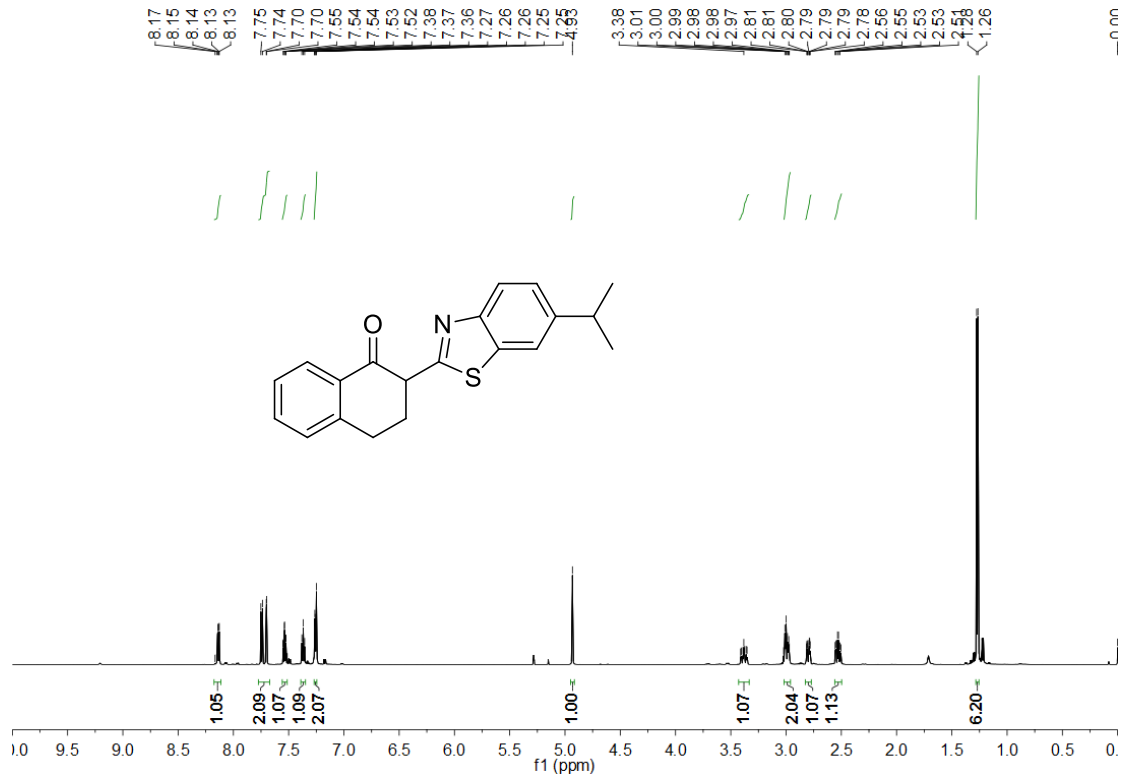


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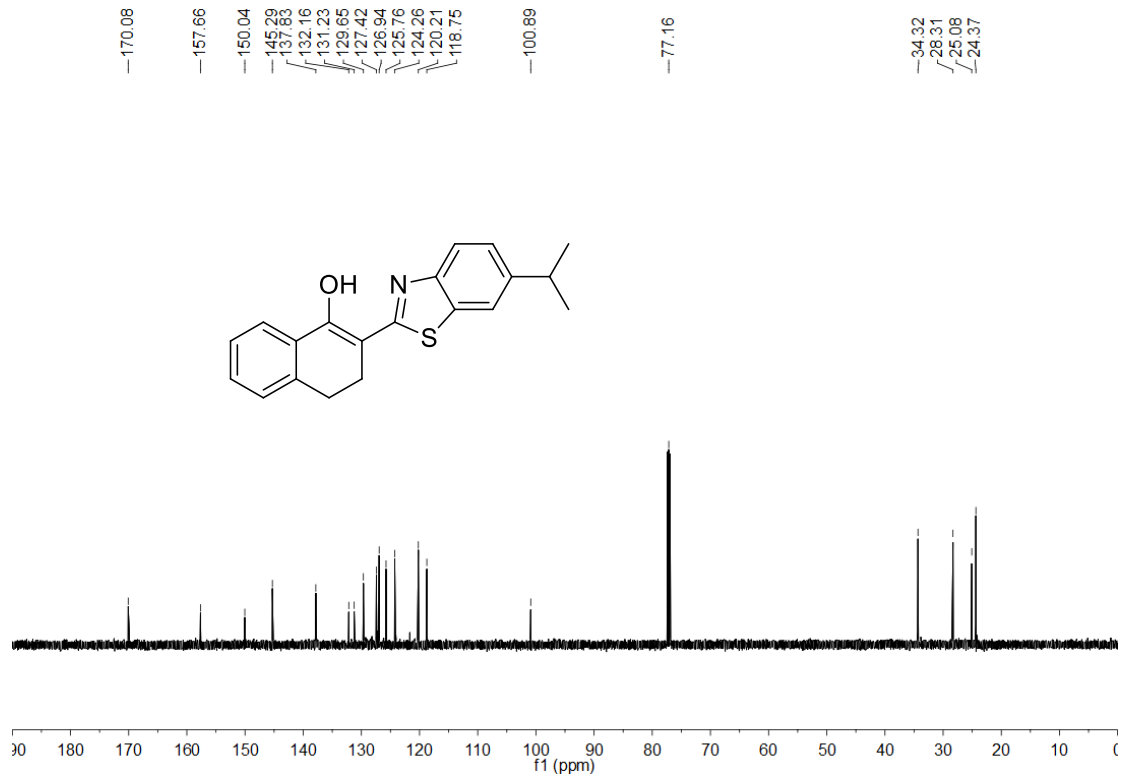
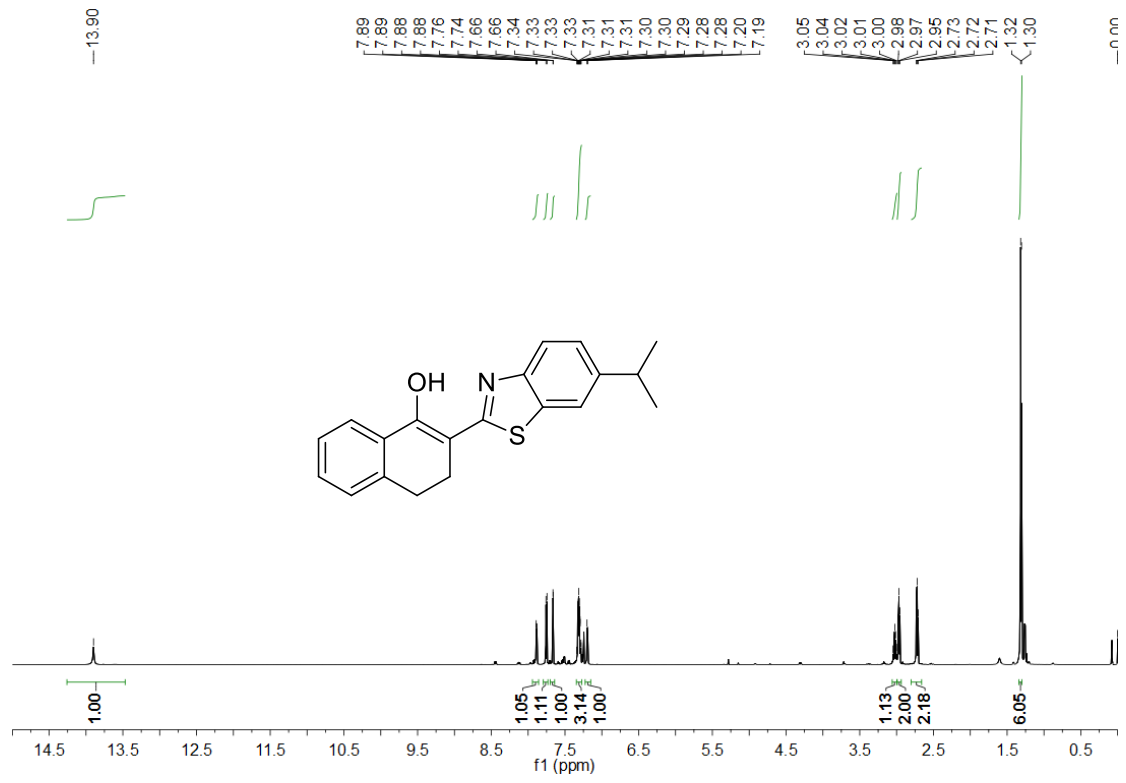


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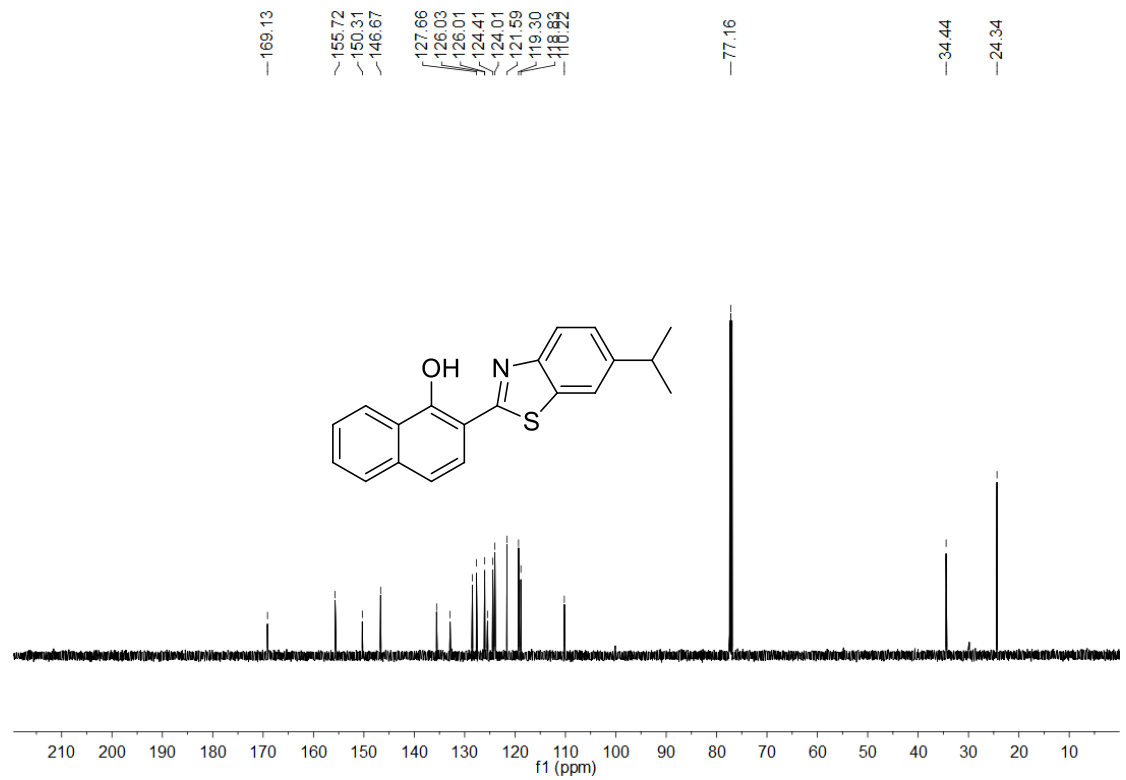
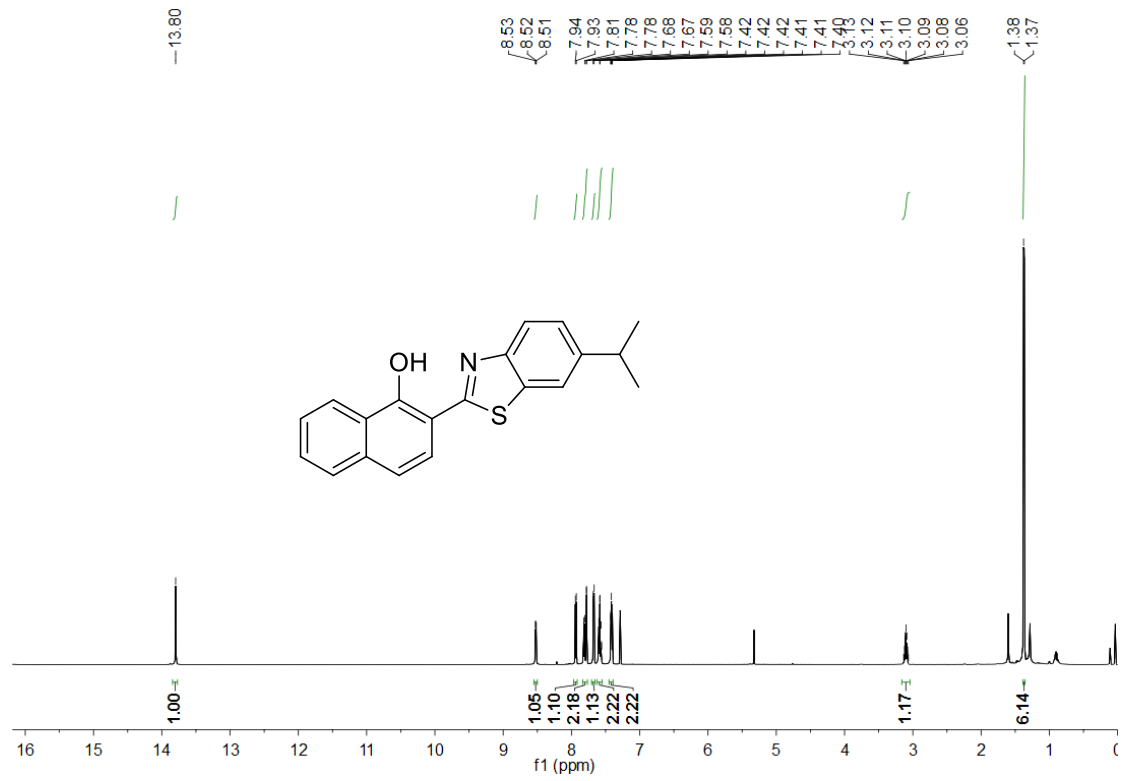




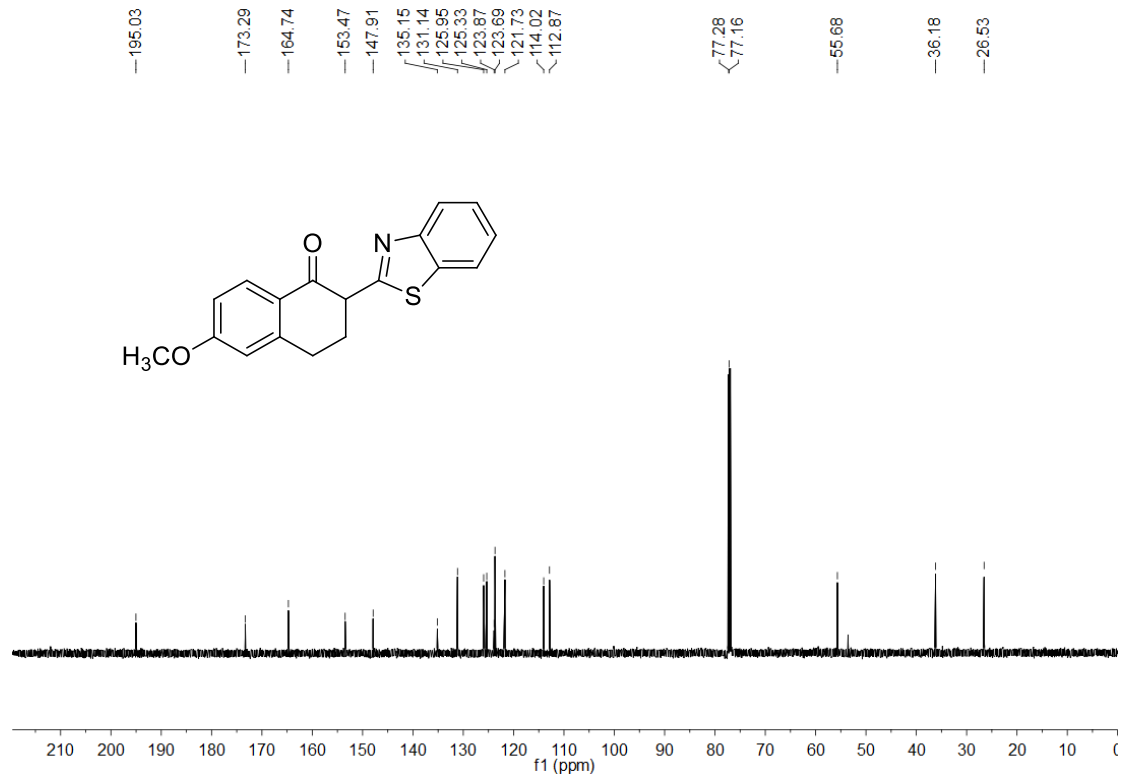
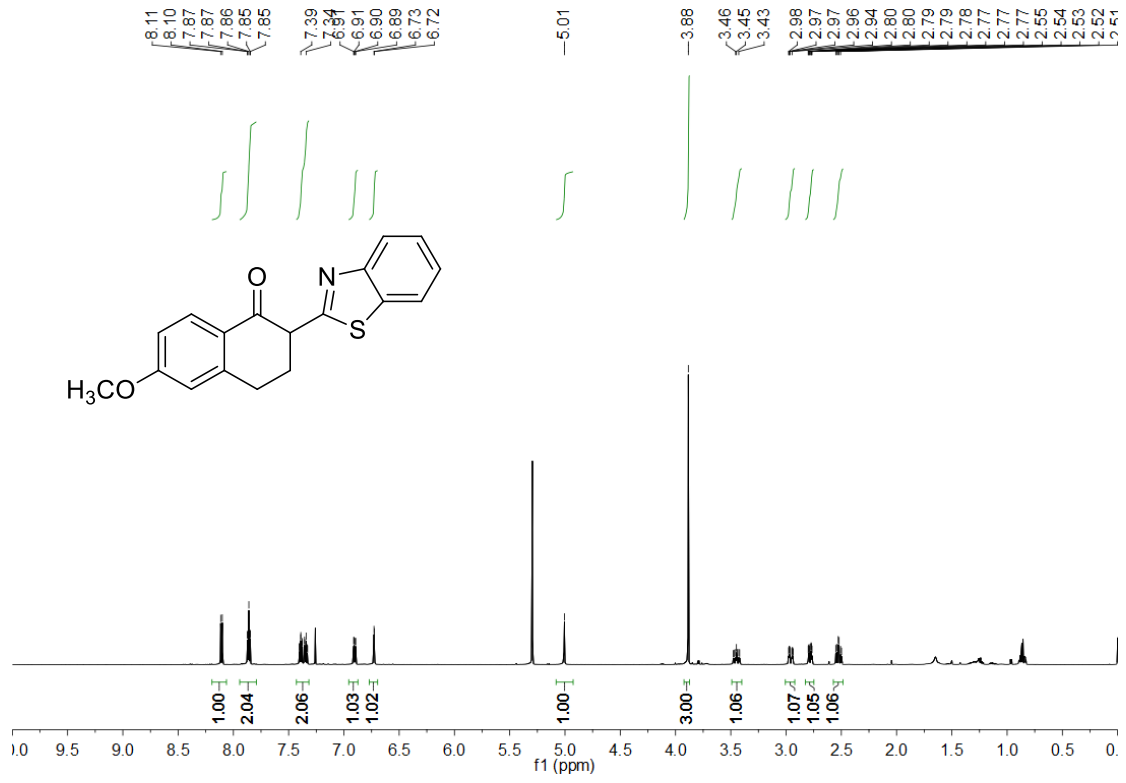
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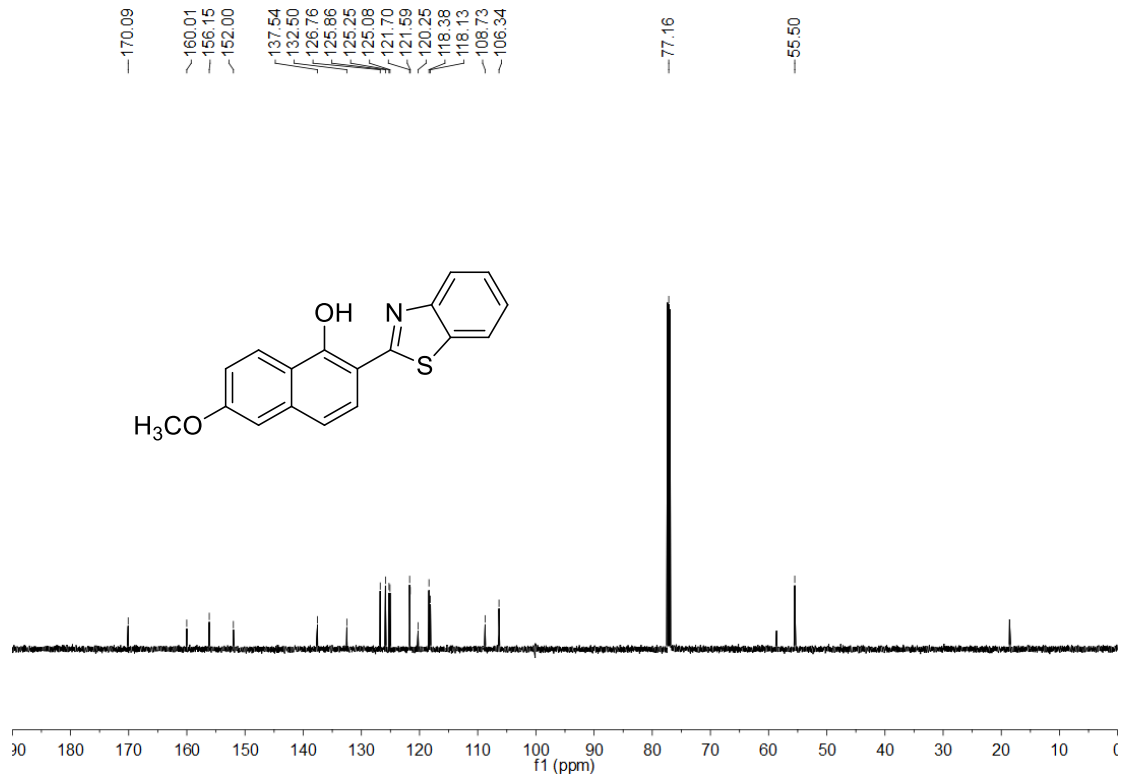
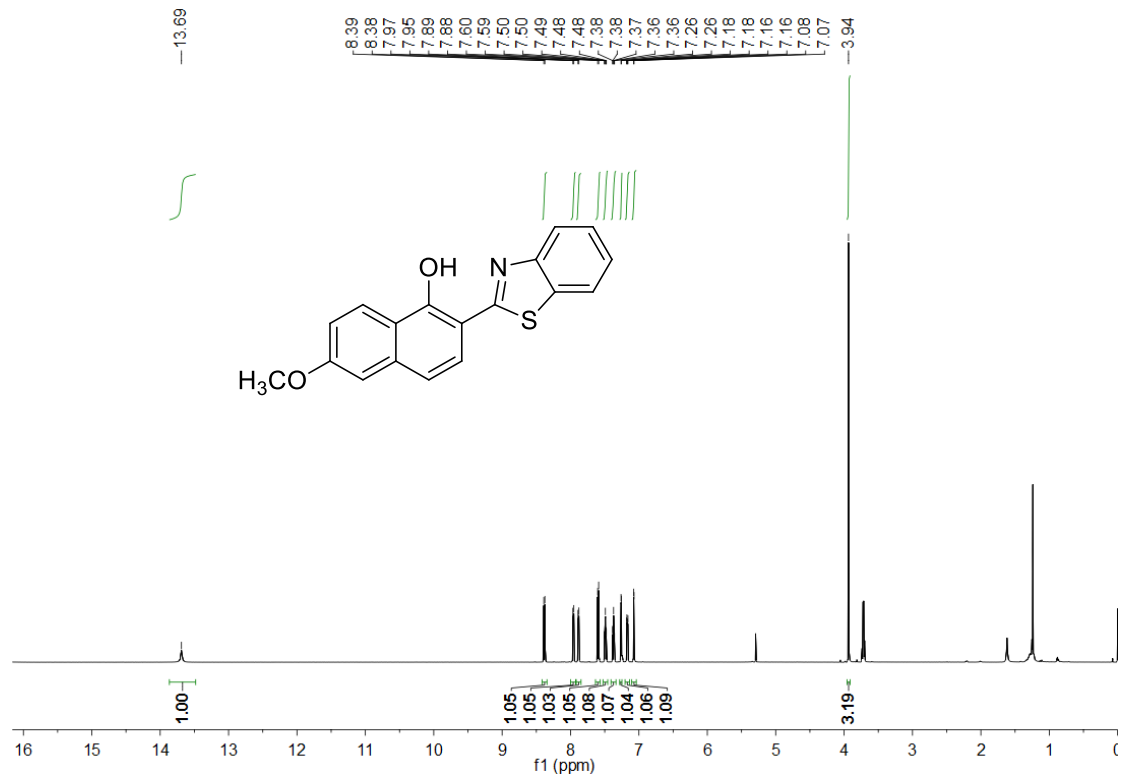
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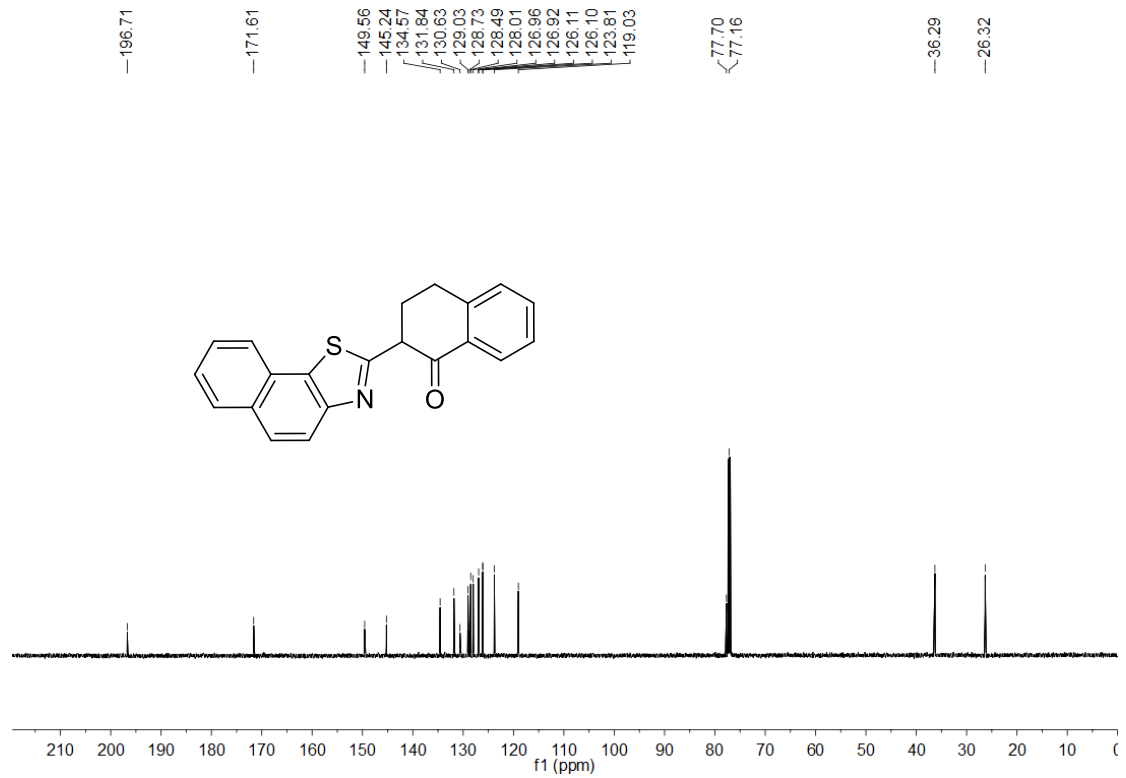
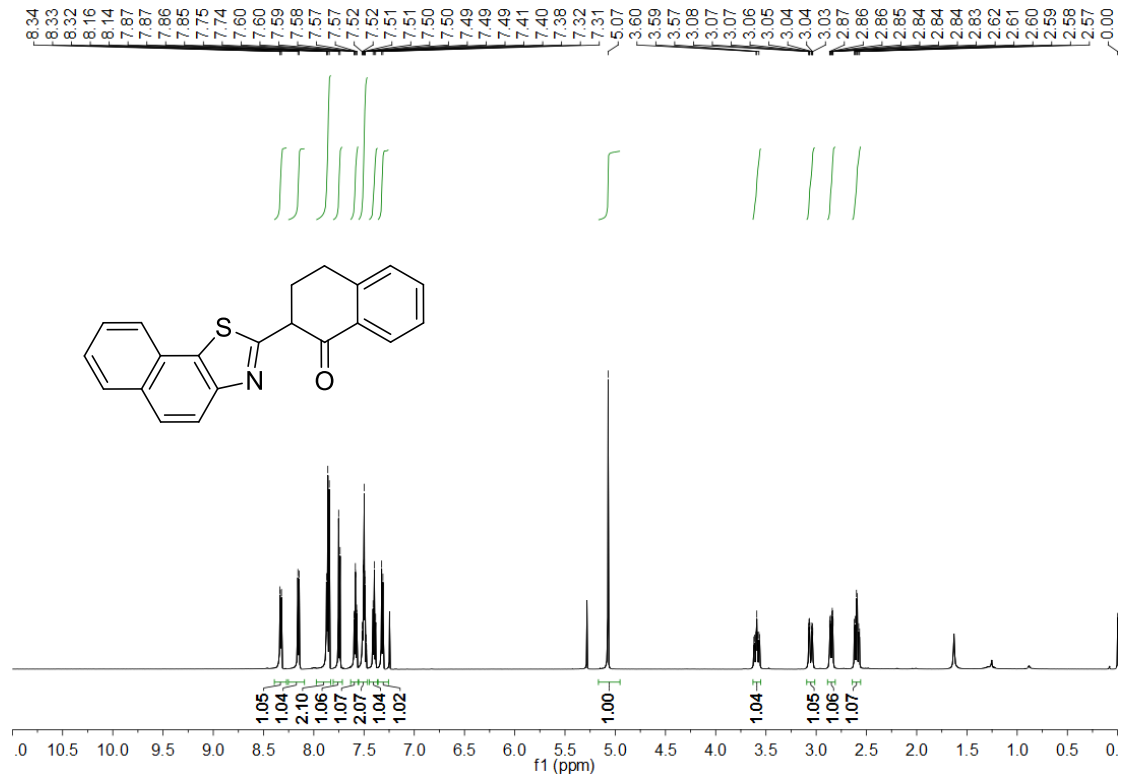
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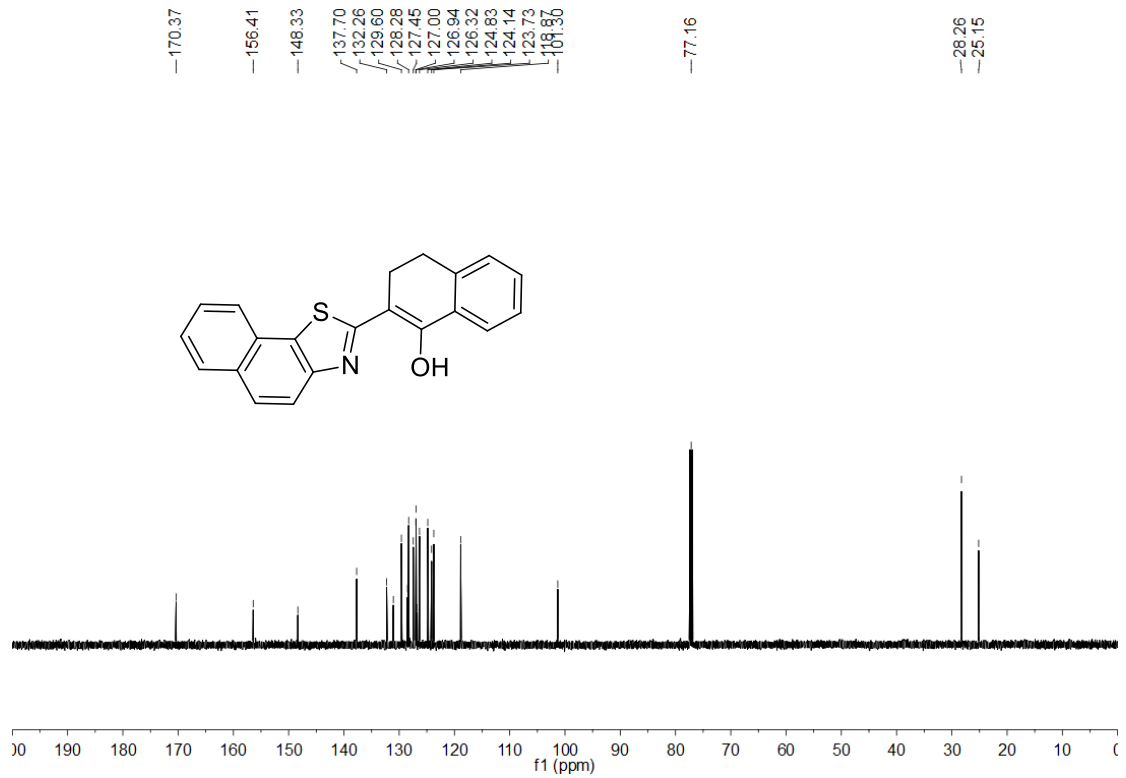
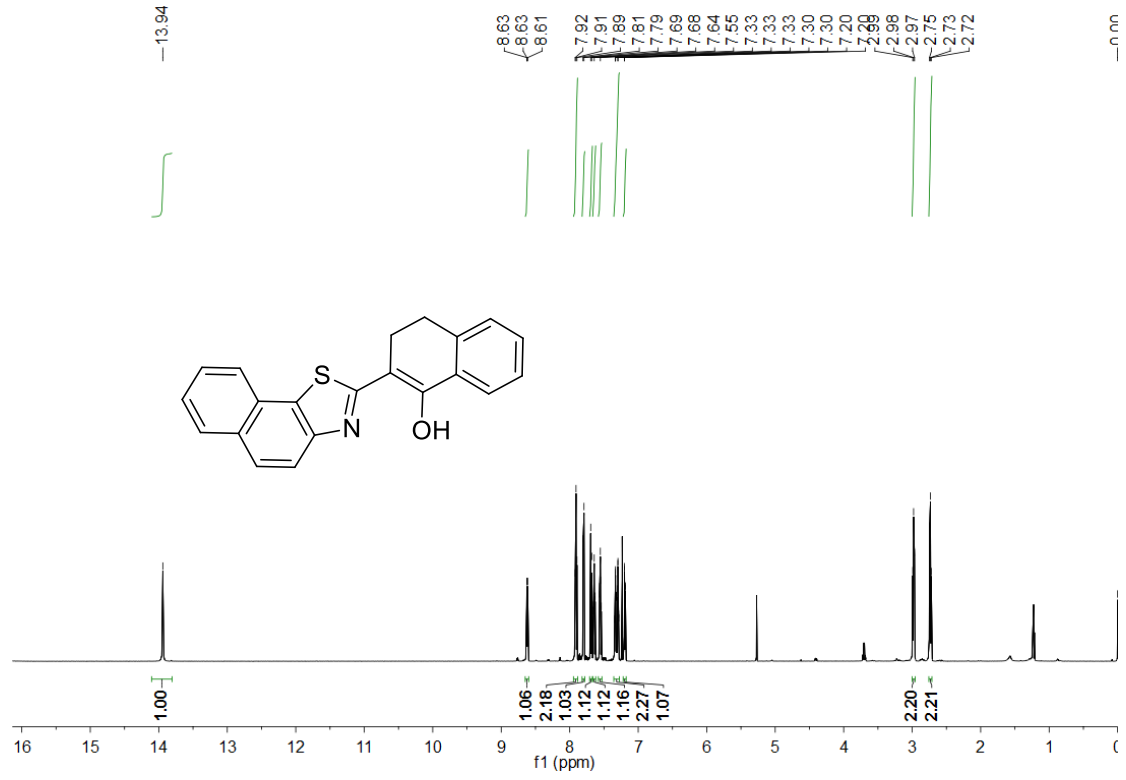
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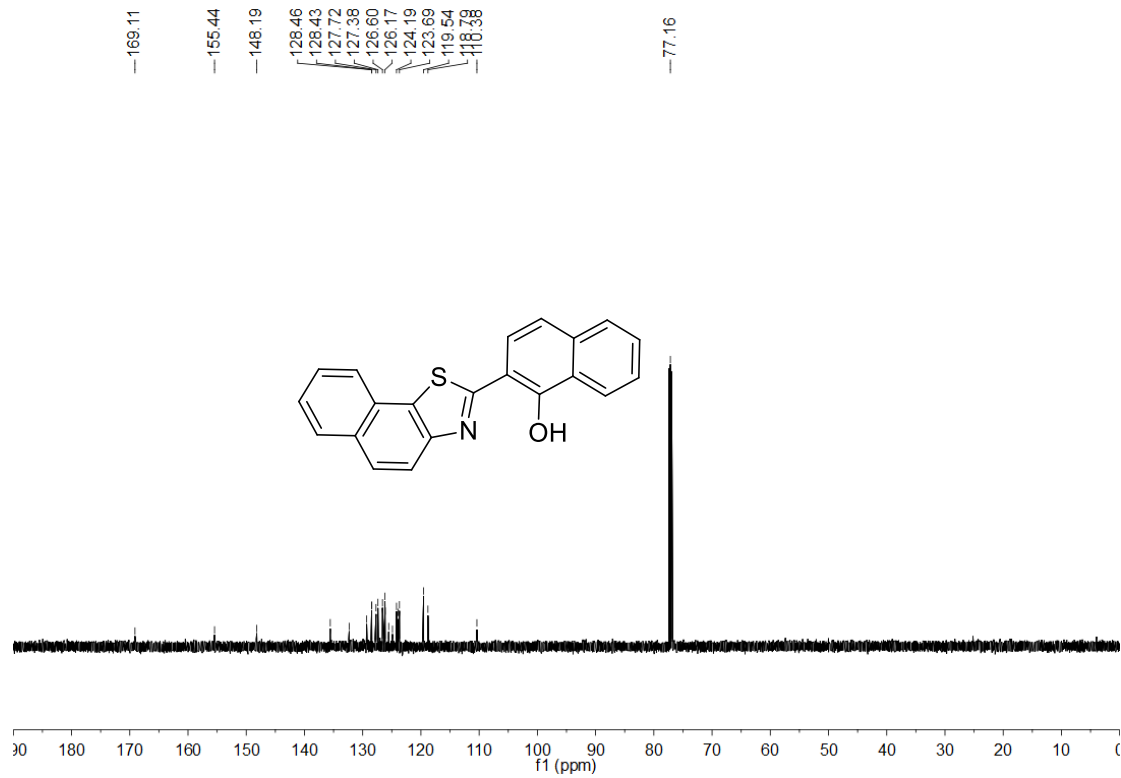
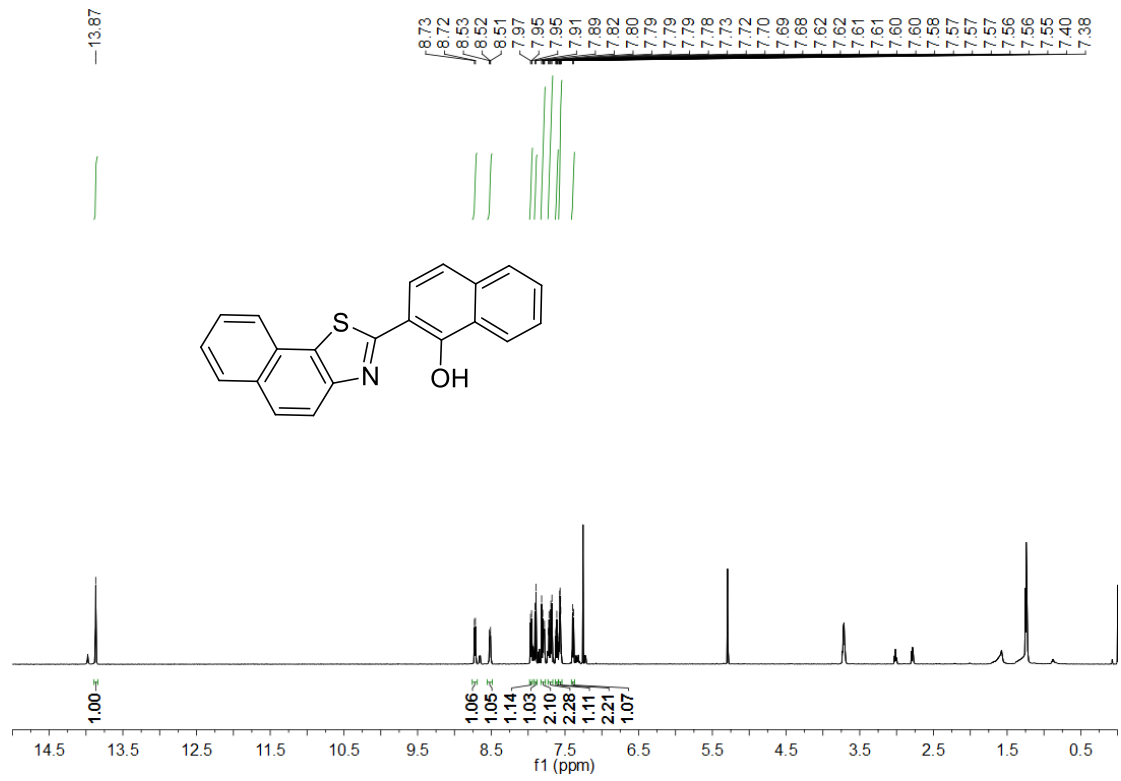
2k



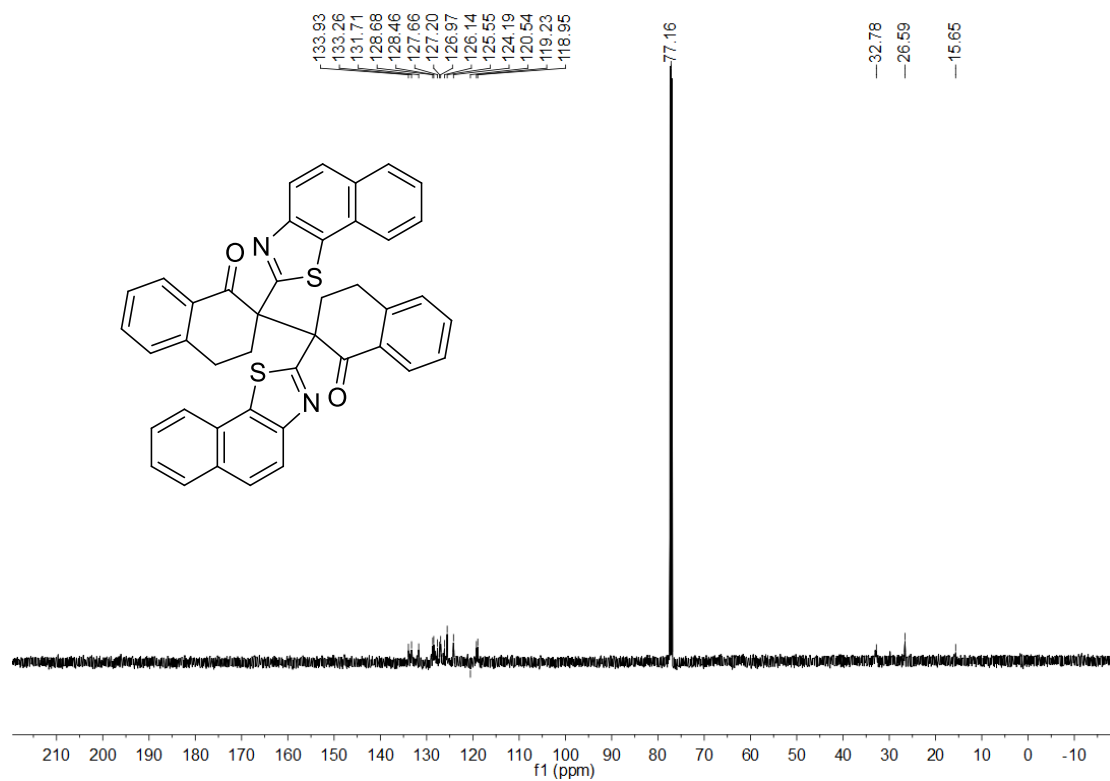
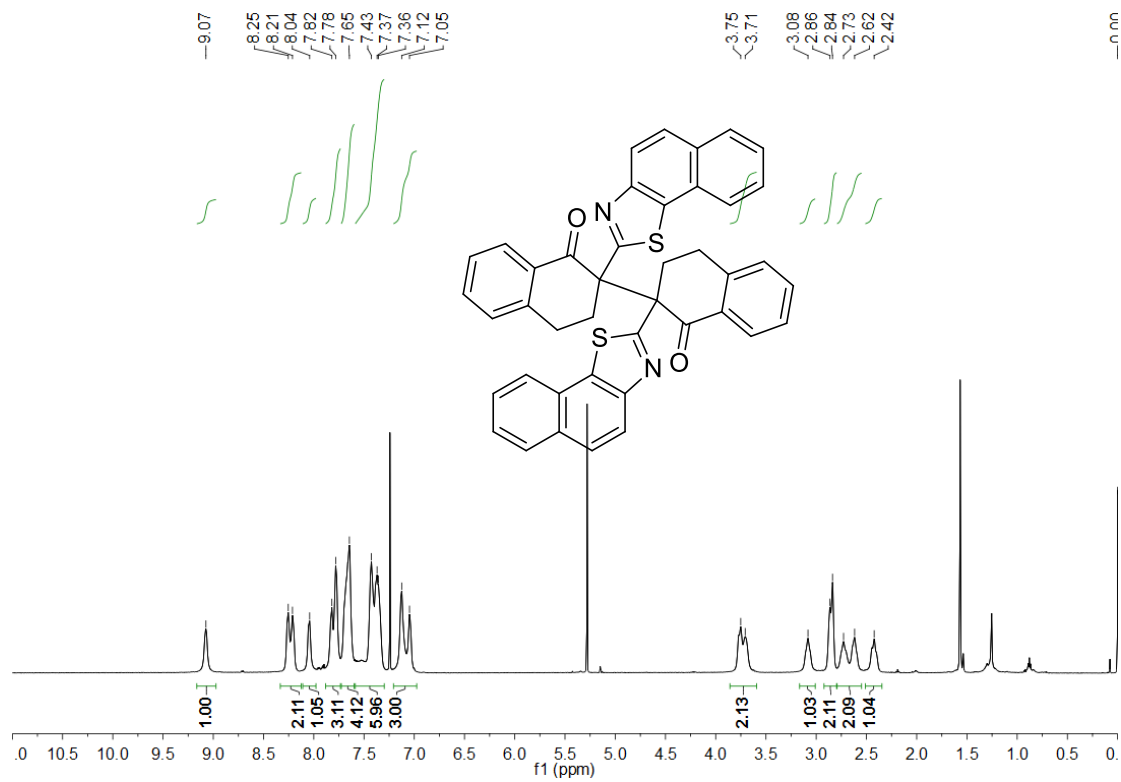
3k



4k

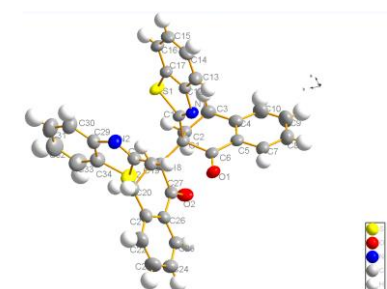
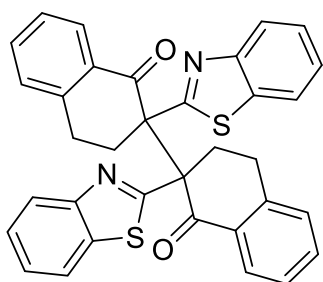


5k



Crystal data and structure refinement for 5a and 4e

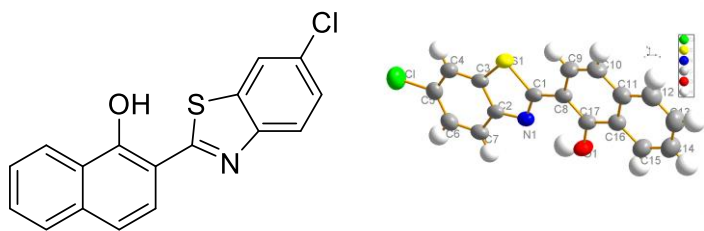
Crystal data and structure refinement for 5a



5a

Identification code	5a
Empirical formula	C ₃₄ H ₂₄ N ₂ O ₂ S ₂
Formula weight	556.12
Temperature	294(2) K
Wavelength	1.54178 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.8581(3) Å alpha = 79.6440(10) deg. b = 12.2068(4) Å beta = 74.2510(10) deg. c = 15.0389(5) Å gamma = 74.0600(10) deg.
Volume	1663.95(9) Å ³
Z, Calculated density	22, 1.111 Mg m ⁻³
Absorption coefficient	1.679 mm ⁻¹
F(000)	580
Crystal size	0.23 x 0.18 x 0.11 mm
Theta range for data collection	3.07 to 68.26 deg.
Limiting indices	-8<=h<=11, -14<=k<=14, -18<=l<=18
Reflections collected / unique	20663 / 6025 [R(int) = 0.0583]
Completeness to theta = 68.26	98.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6025 / 0 / 362
Goodness-of-fit on F ²	1.109
Final R indices [I>2sigma(I)]	R1 = 0.0864, wR2 = 0.2554
R indices (all data)	R1 = 0.0902, wR2 = 0.2640
Extinction coefficient	0.021(3)
Largest diff. peak and hole	1.211 and -0.395 e.Å ⁻³

Crystal data and structure refinement for 4e



4e

Identification code	4e
Empirical formula	C ₁₇ H ₁₀ ClNOS
Formula weight	95.62
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 15.3266(10) Å alpha = 90 deg. b = 5.7203(4) Å beta = 105.487(3) deg. c = 16.2604(12) Å gamma = 90 deg.
Volume	1373.83(17) Å ³
Z, Calculated density	13, 1.502 Mg m ⁻³
Absorption coefficient	0.426 mm ⁻¹
F(000)	636
Theta range for data collection	2.60 to 27.47 deg.
Limiting indices	-17<=h<=19, -7<=k<=7, -21<=l<=21
Reflections collected / unique	12139 / 3136 [R(int) = 0.0661]
Completeness to theta = 27.47	99.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3136 / 0 / 190
Goodness-of-fit on F ²	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0621, wR2 = 0.1737
R indices (all data)	R1 = 0.0753, wR2 = 0.1882
Largest diff. peak and hole	0.662 and -0.483 e.Å ⁻³