Electronic Supplementary Material (ESI) for RSC Advances.

Cu(I)-Catalyzed Multicomponent Cascade Reactions of Terminal Alkynes, Unactivated Primary Alkyl Bromides, CO_2 and NaN_3

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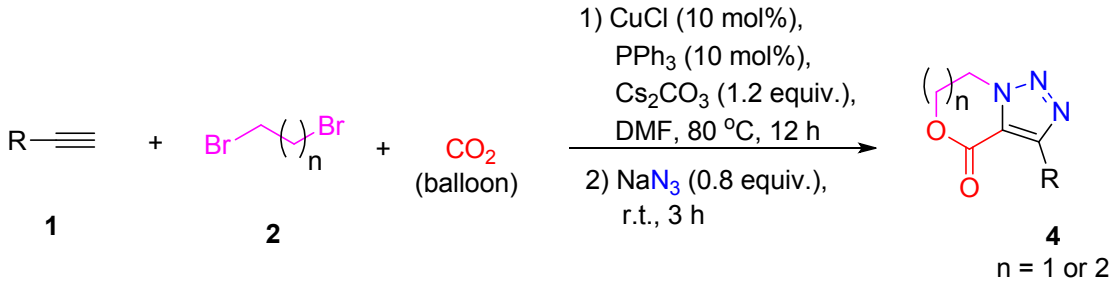
General information.

All the reactions were carried out in dried glasswares with freshly ditilled dry solvents under anhydrous conditions unless otherwise indicated. Column chromatography was performed on silica gel (300-400 mesh). NMR spectra were obtained using a Bruker Avance 500 spectrometer (^{1}H at 500 MHz and ^{13}C at 125MHz) or Bruker Avance 400 spectrometer (^{1}H at 400 MHz and ^{13}C at 100 MHz). High resolution mass spectra (HRMS) were recorded on the Exactive Mass Spectrometer (Thermo Scientific, USA) equipped with ESI ionization source. Gas Chromatography-Mass Spectrometer (GC-MS) were recorded on the Exactive Mass Spectrometer (Shimadzu, Japan) equipped with EI ionization source.

Materials. Unless stated otherwise, commercial reagents were used without further purification. All reagents were weighed and handled in air at room temperature.

Synthesis of 4a-4p.



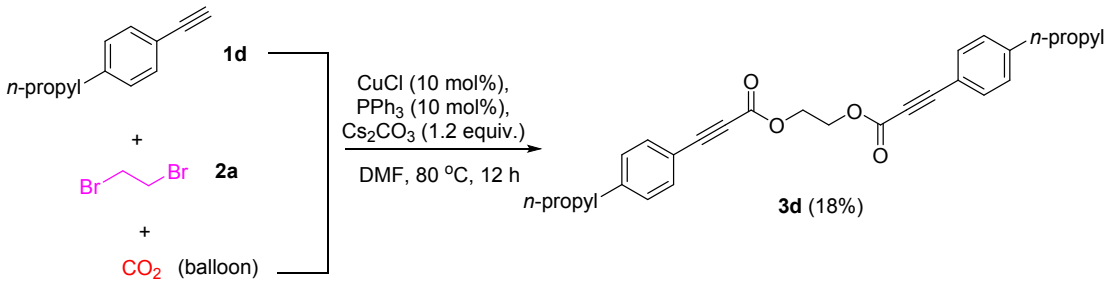
1 **2** **4**

n = 1 or 2

CuCl (0.05 mmol), Cs_2CO_3 (0.6 mmol) and Ph_3P (0.05 mmol) was added in a 10 mL Schlenk flask. The flask was sealed and pumped in CO_2 (99.99%, balloon). Then, the terminal alkyne **1** (0.5 mmol), **2** (0.6 mmol) and DMF (2 mL) was added with syringe. The reaction mixture was stirred at 80 °C for 12 h. After the mixture was cooled to room temperature, CO_2 was degased and NaN_3 (0.4 mmol) was added. The reaction mixture was stirred at room temperature for 3 h under an air atmosphere. The resulting mixture was diluted with ethyl acetate. Then water was added to the mixture, which was extracted with ethyl acetate until no product was detected. The combined organic layer was washed with saturated aqueous NaCl and dried over anhydrous

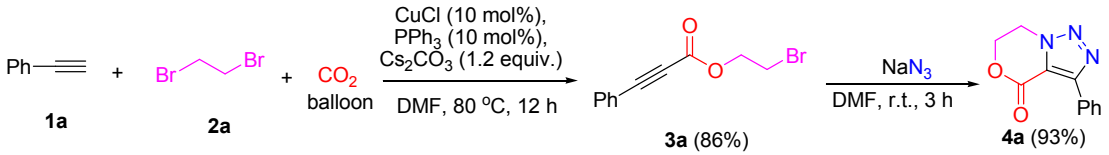
Na_2SO_4. Then the solvent was removed under vacuum. The crud product was purified by colomn chromatography on silica gel (300-400 mesh) to afford the desired product. The products were further identified by NMR and MS.

Synthesis of 3d.



CuCl (0.05 mmol), Cs_2CO_3 (0.6 mmol) and Ph_3P (0.05 mmol) was added in a 10 mL Schlenk flask. The flask was sealed and pumped in CO_2 (99.99%, balloon). Then, the 1-ethynyl-4-propylbenzene **1d** (0.5 mmol), **2a** (0.6 mmol) and DMF (2 mL) was added with syringe. The reaction mixture was stirred at 80 °C for 12 h. After the mixture was cooled to room temperature, CO_2 was degased and NaN_3 (0.4 mmol) was added. The reaction mixture was stirred at room temperature for 3 h under an air atmosphere. The resulting mixture was diluted with ethyl acetate. Then water was added to the mixture, which was extracted with ethyl acetate until no product was detected. The combined organic layer was washed with saturated aqueous NaCl and dried over anhydrous Na_2SO_4. Then the solvent was removed under vacuum. The crud product was purified by colomn chromatography on silica gel (300-400 mesh) to afford the desired product **4d** in 70% yield and side-product **3d** in 18% yield. The products were further identified by NMR and MS.

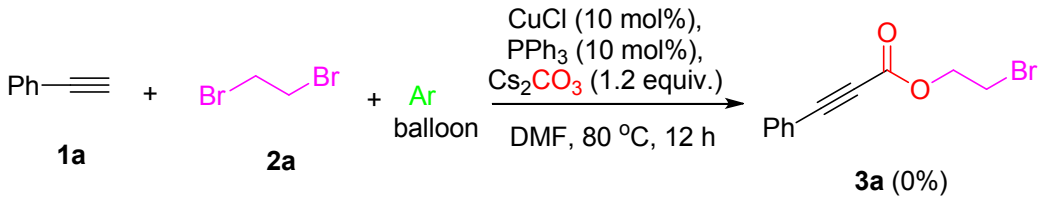
Control experiments.



CuCl (0.05 mmol), Cs_2CO_3 (0.6 mmol) and Ph_3P (0.05 mmol) was added in a 10 mL Schlenk flask. The flask was sealed and pumped in CO_2 (99.99%, balloon). Then, the terminal alkyne **1** (0.5 mmol), **2** (0.6 mmol) and DMF (2 mL) was added with syringe. The reaction mixture was stirred at 80 °C for 12 h. The resulting mixture was diluted with ethyl acetate. Then water was added to the mixture, which was extracted with

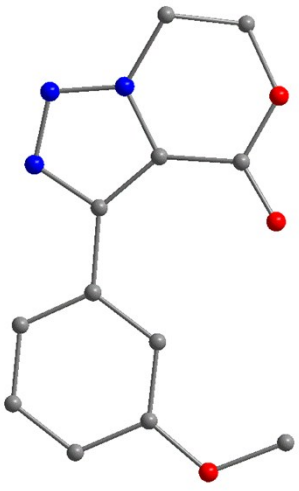
ethyl acetate until no **3a** was detected. The combined organic layer was washed with saturated aqueous NaCl and dried over anhydrous Na_2SO_4. Then the solvent was removed under vacuum. The crud product was purified by colomn chromatography on silica gel (300-400 mesh) to afford **3a** in 86% yield.

3a was dissolved in DMF (2 mL) and NaN_3 (0.275 mmol) was added subsequently. The reaction mixture was stirred at room temperature for 3 h under an air atmosphere. The resulting mixture was diluted with ethyl acetate. Then water was added to the mixture, which was extracted with ethyl acetate until no product was detected. The combined organic layer was washed with saturated aqueous NaCl and dried over anhydrous Na_2SO_4. Then the solvent was removed under vacuum. The crud product was purified by colomn chromatography on silica gel (300-400 mesh) to afford the **4a** in 93% yield.

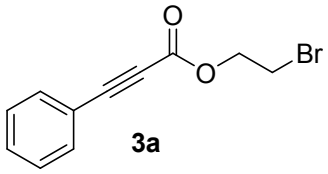


CuCl (0.05 mmol), Cs_2CO_3 (0.6 mmol) and Ph_3P (0.05 mmol) was added in a 10 mL Schlenk flask. The flask was sealed and pumped in Ar (balloon) instead of CO_2. Then, the terminal alkyne **1a** (0.5 mmol), **2a** (0.6 mmol) and DMF (2 mL) was added with syringe. The reaction mixture was stirred at 80 °C for 12 h, which could not afford the desired product **3a**.

X-ray crystal structure of triazolo-fused dihydrooxazinone 4k.



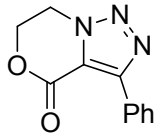
Characterization of the compounds



3a

2-Bromoethyl 3-phenylpropiolate (**3a**).

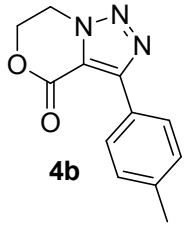
Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 2H), 7.49 – 7.44 (m, 1H), 7.38 (dd, *J* = 10.3, 4.5 Hz, 2H), 4.54 (t, *J* = 6.3 Hz, 2H), 3.57 (t, *J* = 6.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.5, 133.1, 130.9, 128.6, 119.3, 87.5, 80.1, 65.1, 27.8. **MS (EI) m/z** $(M)^+$ 252 and 254. Anal calcd for $C_{11}H_9BrO_2$: C, 52.20; H, 3.58; Found: C, 52.49; H, 3.21.



4a

3-Phenyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4a**).

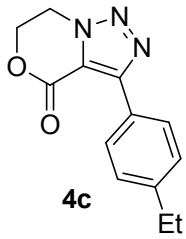
White solid; m.p. 123.5-124.5 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.17 – 8.13 (m, 2H), 7.54 – 7.47 (m, 3H), 4.86 – 4.80 (m, 4H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 157.0, 148.5, 129.5, 129.1, 128.5, 128.1, 121.4,66.1, 44.7. **HRMS (ESI$^+$) m/z** calcd for $C_{11}H_{10}O_2N_3$ $(M+H)^+$ 216.0773 found 216.0767.



4b

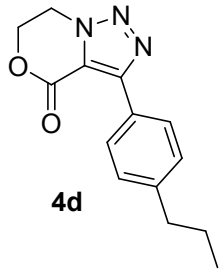
3-(*p*-Tolyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4b**).

White solid; m.p. 100.0-101.0 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.06 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 4.85 – 4.78 (m, 4H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 157.0, 148.6, 139.1, 129.1, 128.0, 126.3, 121.0, 66.0, 44.6, 21.0. **HRMS (ESI$^+$) m/z** calcd for $C_{12}H_{12}O_2N_3$ $(M+H)^+$ 230.0930 found 230.0924.



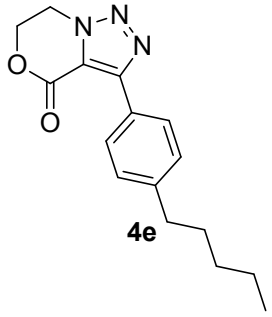
3-(4-Ethylphenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4c).**

White solid; m.p. 91.1-92.1 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.4 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 4.63 (d, *J* = 1.2 Hz, 4H), 2.67 (q, *J* = 7.6 Hz, 2H), 1.24 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.5, 150.7, 146.4, 128.4, 128.1, 125.8, 120.0, 65.5, 44.9, 28.7, 15.4. **HRMS (ESI$^+$) m/z** calcd for $C_{13}H_{14}O_2N_3$ $(M+H)^+$ 244.1086 found 244.1078.



3-(4-Propylphenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4d).**

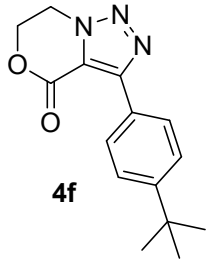
White solid; m.p. 94.0-95.0 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 4.69 (s, 4H), 2.63 – 2.60 (m, 2H), 1.70 – 1.61 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.5, 151.1, 145.1, 128.8, 128.5, 125.8, 120.0, 65.6, 45.0, 38.0, 24.4, 13.9. **HRMS (ESI$^+$) m/z** calcd for $C_{14}H_{16}O_2N_3$ $(M+H)^+$ 258.1243 found 258.1234.



3-(4-Pentylphenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4e**).

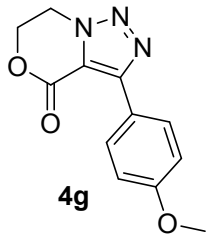
White solid; m. p. 78.5-79.5 °C; **^{1}H NMR** (500 MHz, DMSO-*d6*) δ 8.06 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 8.2 Hz, 2H), 4.81 (m, 4H), 2.65 – 2.59 (m, 2H), 1.64 – 1.56 (m, 2H), 1.30 (m, 4H), 0.87 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, DMSO-*d6*) δ 157.1,

148.6, 144.0, 128.4, 128.0, 126.5, 121.1, 66.1, 44.7, 35.0, 30.9, 30.5, 22.0, 14.0. **HRMS (ESI$^+$) m/z** calcd for $C_{16}H_{20}O_2N_3$ $(M+H)^+$ 286.1556 found 286.1547.



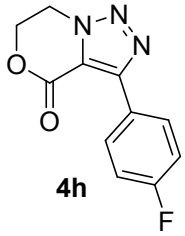
4f

3-(4-(Tert-butyl)phenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4f).** White solid; m.p. 93.6-94.6 ^oC; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.07 (d, J=8.6 Hz, 2H), 7.53 (d, J= 8.7 Hz, 2H), 4.82 (m, 4H), 1.32 (s, 9H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 157.0, 152.1, 148.6, 127.9, 126.2, 125.2, 121.0,66.0, 44.6, 34.5, 31.0. **HRMS (ESI$^+$) m/z** calcd for $C_{15}H_{18}O_2N_3$ $(M+H)^+$ 272.1399 found 272.1391.



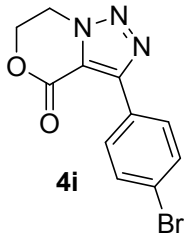
4g

3-(4-Methoxyphenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4g**). White solid; m.p. 103.5-104.5 ^oC; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.14 (d, J = 8.8 Hz, 2H), 7.07 (d, J = 8.9 Hz, 2H), 4.85 – 4.77 (m, 4H), 3.82 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6)) δ 160.2, 157.2, 148.5, 129.6, 121.4, 120.5, 113.9, 66.0, 55.3, 44.6. **HRMS (ESI$^+$) m/z** calcd for $C_{12}H_{12}O_3N_3$ $(M+H)^+$ 246.0879 found 246.0872.



4h

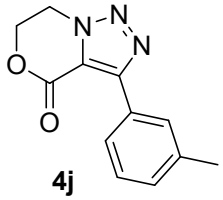
3-(4-Fluorophenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4h**). White solid; m.p. 145.2-146.2 ^oC; ^{1}**H NMR** (500 MHz, DMSO-d_6) δ 8.25 – 8.20 (m, 2H), 7.39 – 7.34 (m , 2H), 4.85 – 4.79 (m,4 H). **^{13}C NMR** (125 MHz, DMSO-*d6*) δ 163.7, 161.7, 157.0, 147.5, 130.3, 130.3, 125.6, 125.5, 121.3 , 115.6 , 115.4, 66.1, 44.6. **HRMS (ESI$^+$) m/z** calcd for $C_{11}H_9O_2N_3F$ $(M+H)^+$ 234.0679 found 234.0910.



4i

3-(4-Bromophenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4i**).

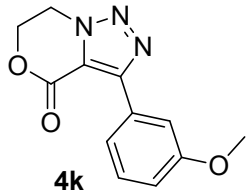
White solid; m.p. 115.0-116.0 °C; **^{1}HNMR** (400 MHz,$CDCl_3$) δ 8.22 (dd, *J*= 8.0, 1.7 Hz, 2H), 7.49–7.44 (m, 2H), 4.75–4.66(m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.4, 150.9, 130.1, 128.7, 128.6, 128.5, 120.4, 65.6, 45.1. **MS (EI) m/z** $(M\text{-}Br+H)^+$ 215. Anal calcd for $C_{11}H_9N_3O_2$: C, 61.39; H, 4.22; Found: C, 61.62; H, 3.08.



4j

3-(*m*-Tolyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4j**).

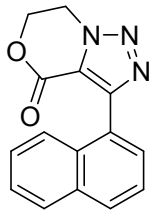
White solid; m.p. 105.4-106.4 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 7.4 Hz, 1H), 4.86–4.78 (m, 4H), 2.38 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 157.0, 148.7, 137.6, 130.2, 129.0, 128.6, 128.4, 125.4, 121.3,66.1, 44.7, 21.1. **HRMS (ESI$^+$) m/z** calcd for $C_{12}H_{12}O_2N_3$ $(M+H)^+$ 230.0930 found 230.0921.



4k

3-(3-Methoxyphenyl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4k**).

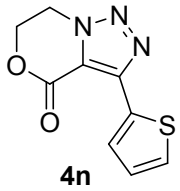
White solid; m.p. 118.0-119.0 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.77 (dd, *J* = 13.2, 4.9 Hz, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.05 (dd, *J* = 8.2, 2.4 Hz, 1H), 4.83 (m, 4H), 3.82 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 159.2, 157.0, 148.3, 130.3, 129.6, 121.5, 120.3, 115.2, 113.5, 66.0, 55.1, 44.7. **HRMS (ESI$^+$) m/z** calcd for $C_{12}H_{12}O_3N_3$ $(M+H)^+$ 246.0879 found 246.0871.



4m

3-(Naphthalen-1-yl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4m**).

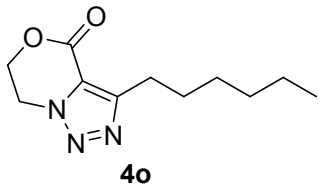
White solid. m.p. 129.0-130.0 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.36 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.96 (dd, *J* = 10.5, 7.6 Hz, 2H), 7.87 (dd, *J* = 5.8, 3.2 Hz, 1H), 7.57 – 7.49 (m, 2H), 4.81 – 4.74 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.5, 151.2, 134.1, 133.3, 129.1, 128.9, 128.4, 127.8, 127.3, 126.6, 126.0, 125.6, 120.6, 65.6, 45.2. **HRMS (ESI$^+$) m/z** calcd for $C_{15}H_{12}O_2N_3$ $(M+H)^+$ 266.0930 found 266.0921.



4n

3-(Thiophen-2-yl)-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4n**).

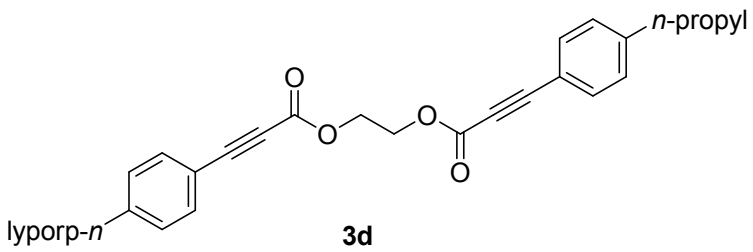
White solid; m.p. 118.0-119.0 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.17 – 8.15 (m, 1H), 7.74 – 7.72 (m, 1H), 7.23 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.81 (s, 4H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 156.9, 143.8, 128.8, 128.6, 128.1, 119.8, 66.1, 44.6. **MS (EI) m/z** $(M)^+$ 221. Anal calcd for $C_9H_7N_3O_2S$: C, 48.86; H, 3.19; Found: C, 48.66; H, 3.48.



4o

3Hexyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazin-4-one (**4o**).

Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.73 – 4.65 (m, 4H), 2.98 – 2.92 (m, 2H), 1.77 – 1.68 (m, 2H), 1.40 – 1.25 (m, 6H), 0.86 (t, *J* = 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 153.9, 121.1,65.8, 44.8, 31.6, 29.0, 28.7, 25.7, 22.6, 14.2. **HRMS (ESI$^+$) m/z** calcd for $C_{11}H_{18}O_2N_3$ $(M+H)^+$ 224.1399 found 224.1392.

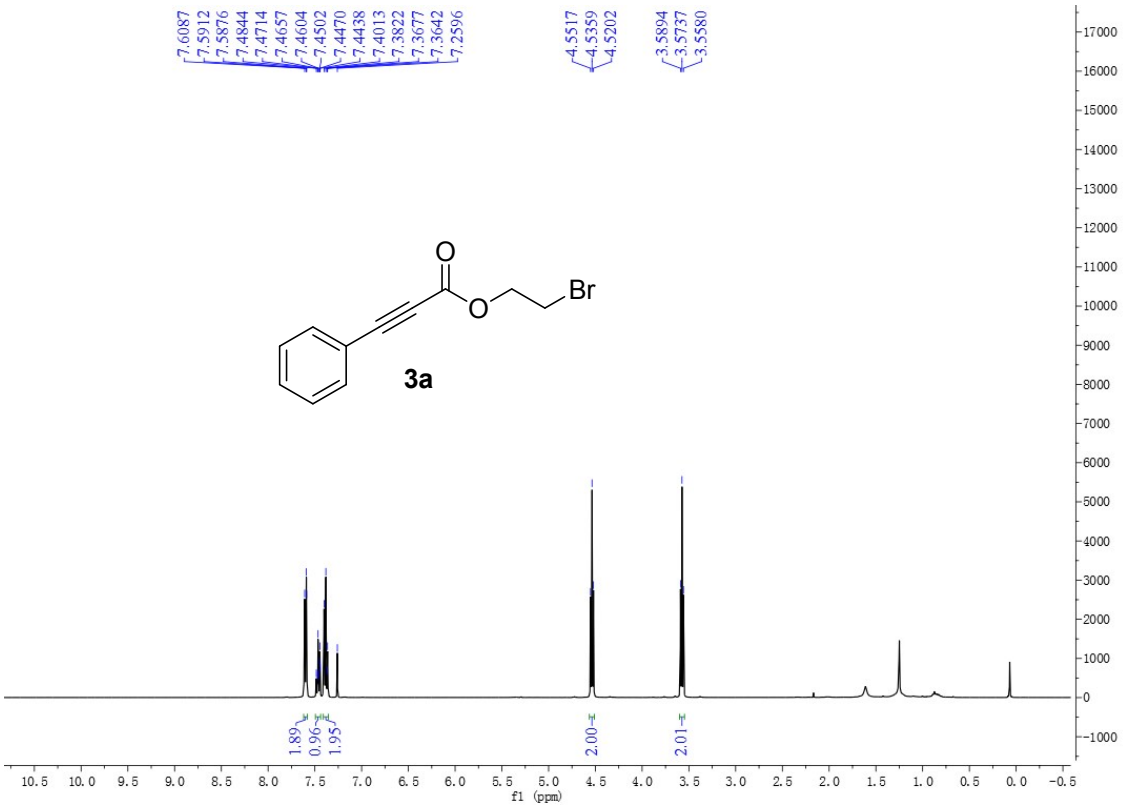


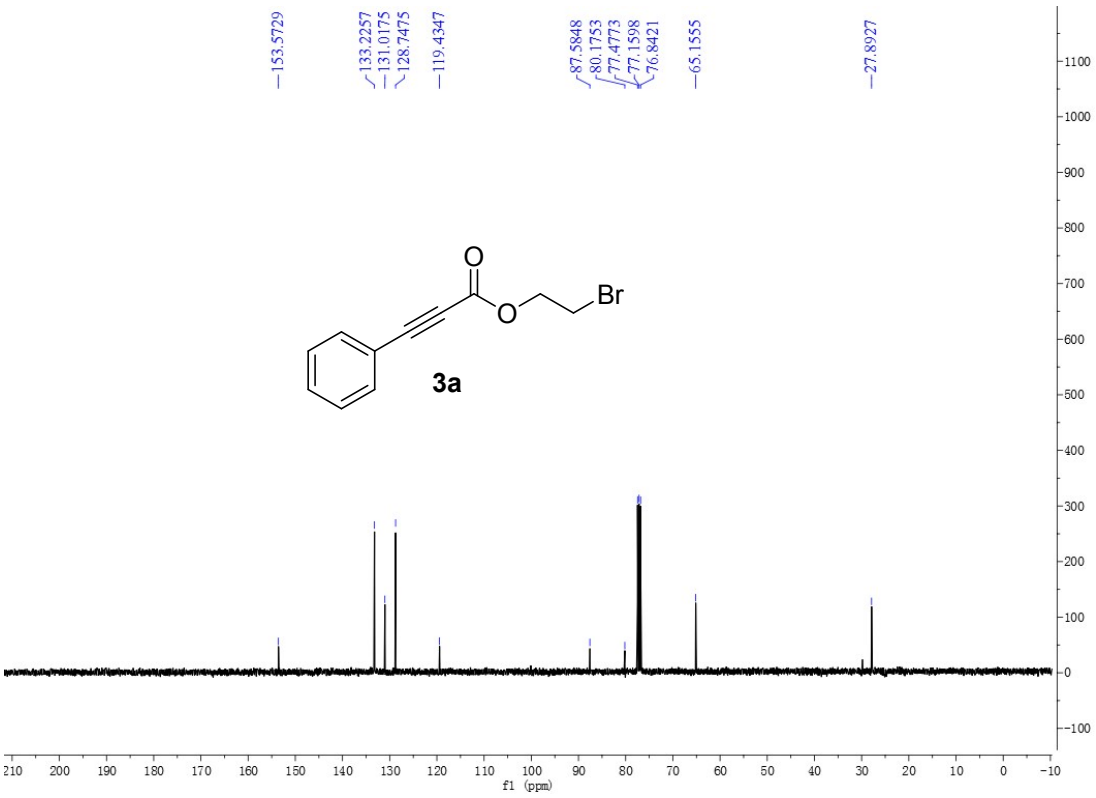
3d

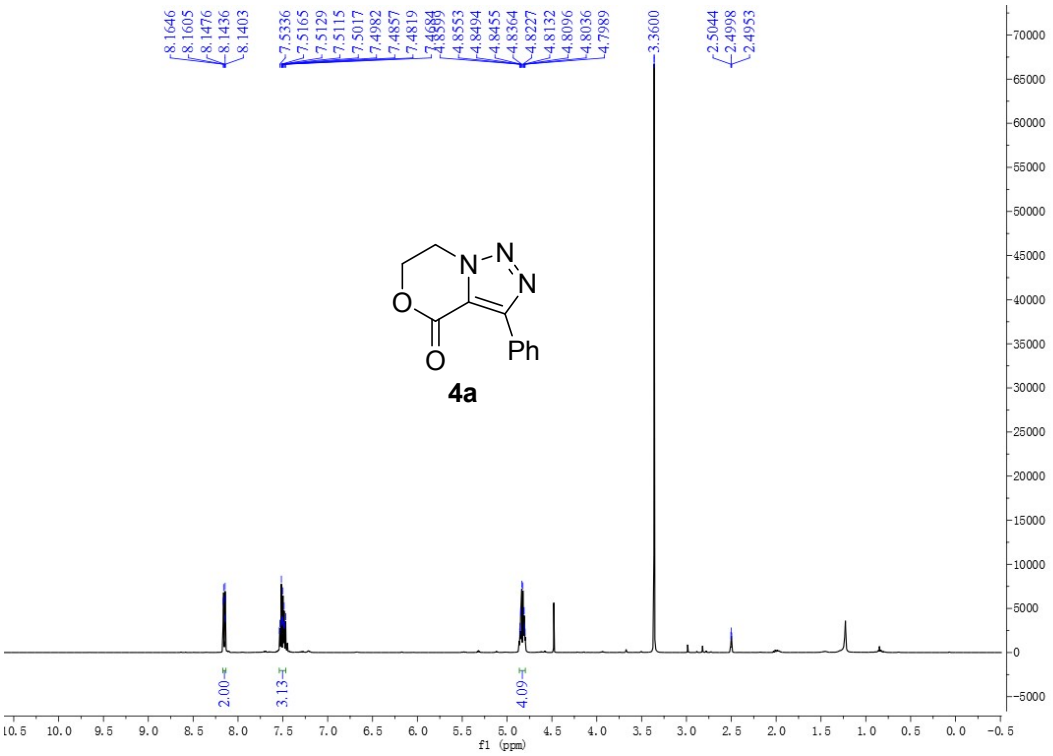
Ethane-1,2-diyl bis(3-(4-propylphenyl)propiolate) (**3d**).

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.2 Hz, 4H), 7.13 (d, *J* = 8.2 Hz, 4H), 4.48 (s, 4H), 2.58 – 2.52 (m, 4H), 1.64 – 1.54 (m, 4H), 0.89 (t, *J* = 7.4 Hz, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 146.1, 133.0, 128.7, 116.4, 87.7, 79.9, 63.1, 38.0, 24.0, 13.6. **MS (EI) m/z** $(M)^+$ 402. Anal calcd for $C_{26}H_{26}O_4$: C, 77.59; H, 6.51; Found: C, 77.40; H, 6.79.

Copies of ^{1}H NMR and ^{13}C NMR spectra of products.



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7.4819
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4.8494
4.8455
4.8364
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4.8132
4.8096
4.8036
4.7989
3.3600
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N
N
O
O
Ph
4a
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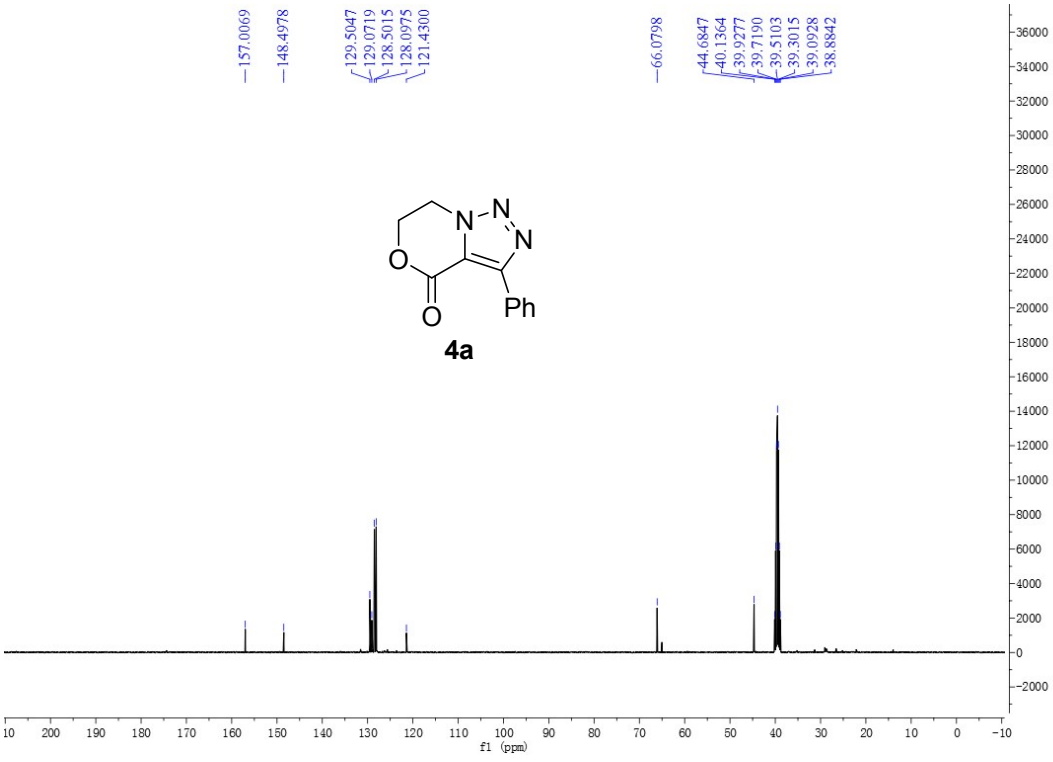
4.09
f1 (ppm)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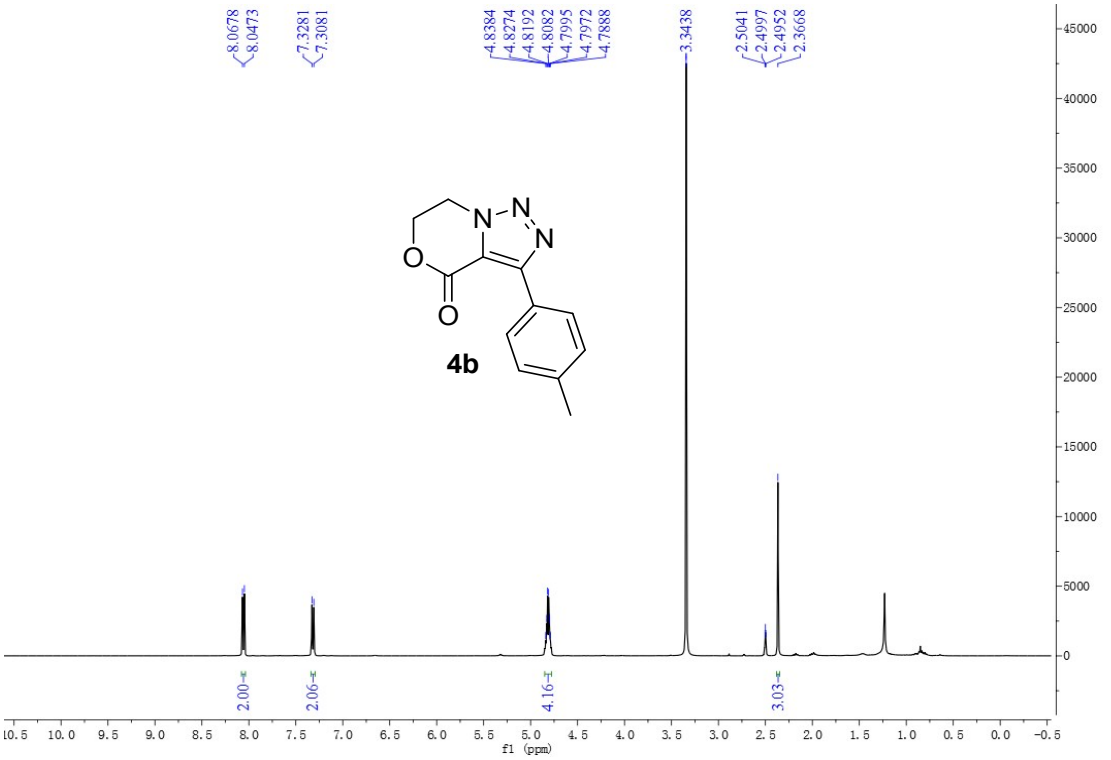
N
N
O
O
Ph
4a
f1 (ppm)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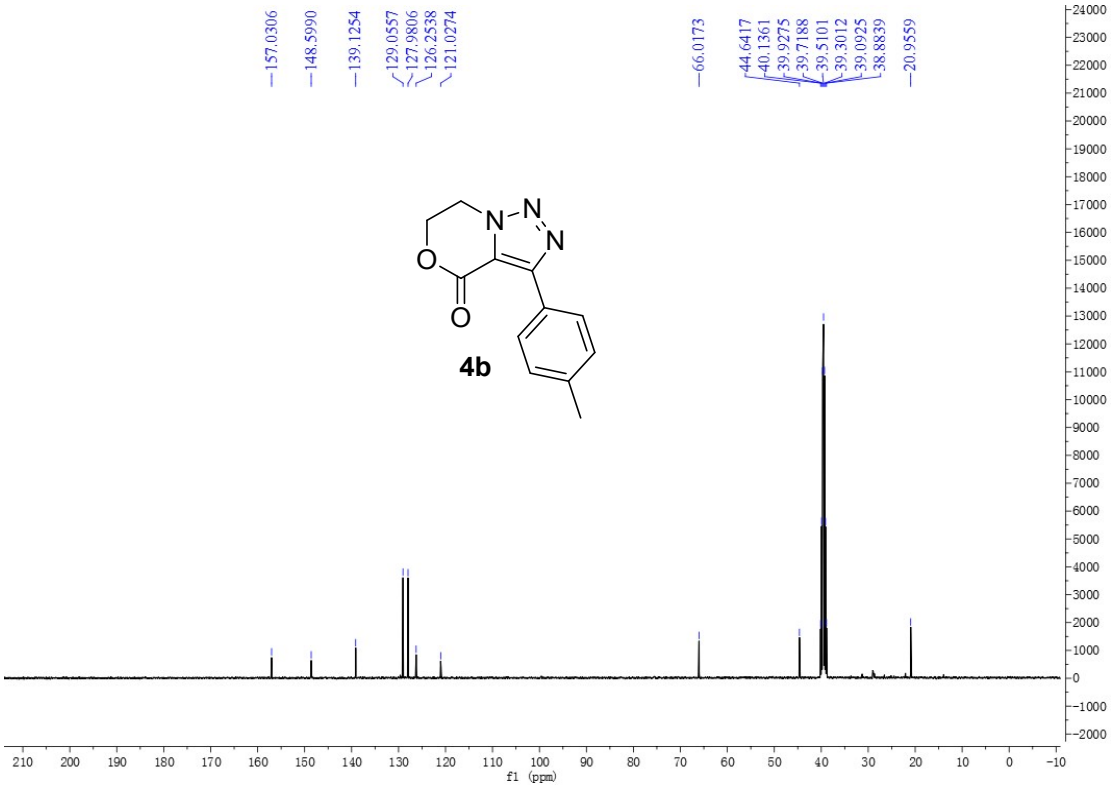
f1 (ppm)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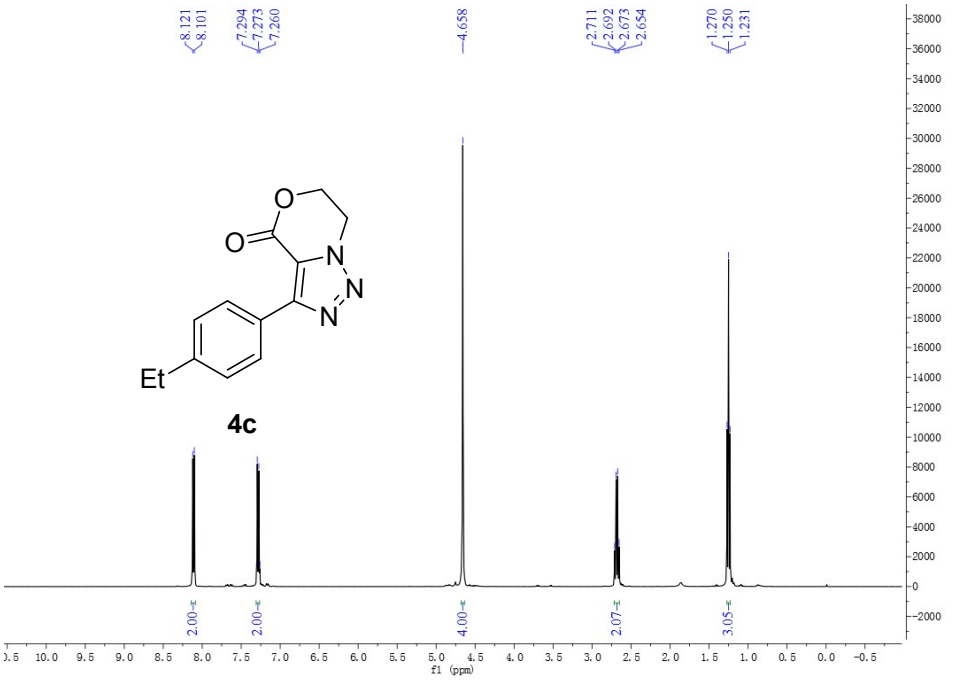
f1 (ppm)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N
N
N
Et
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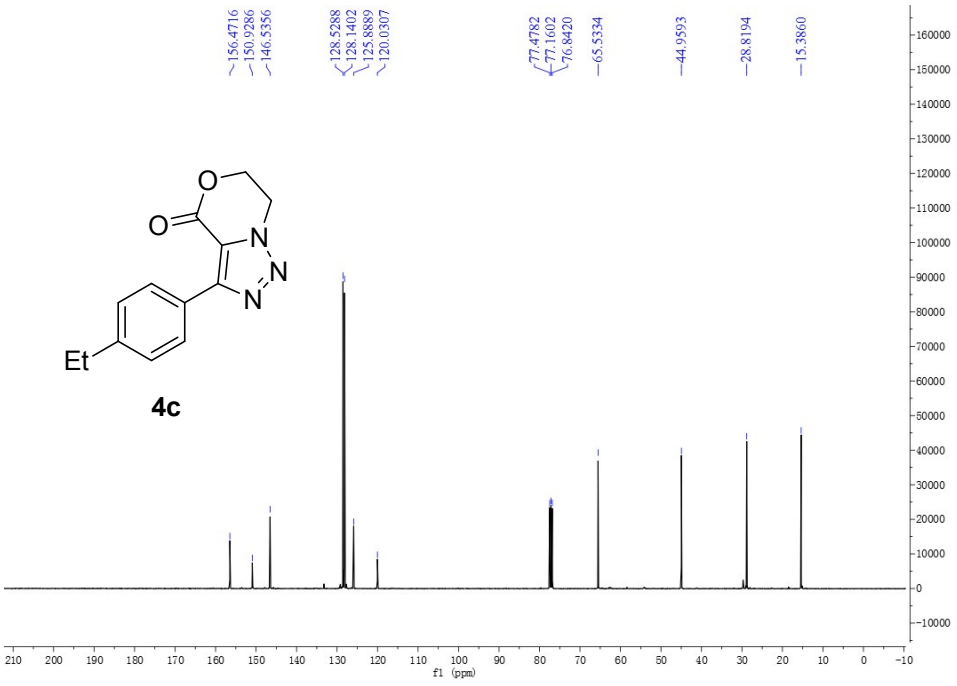
f1 (ppm)

4c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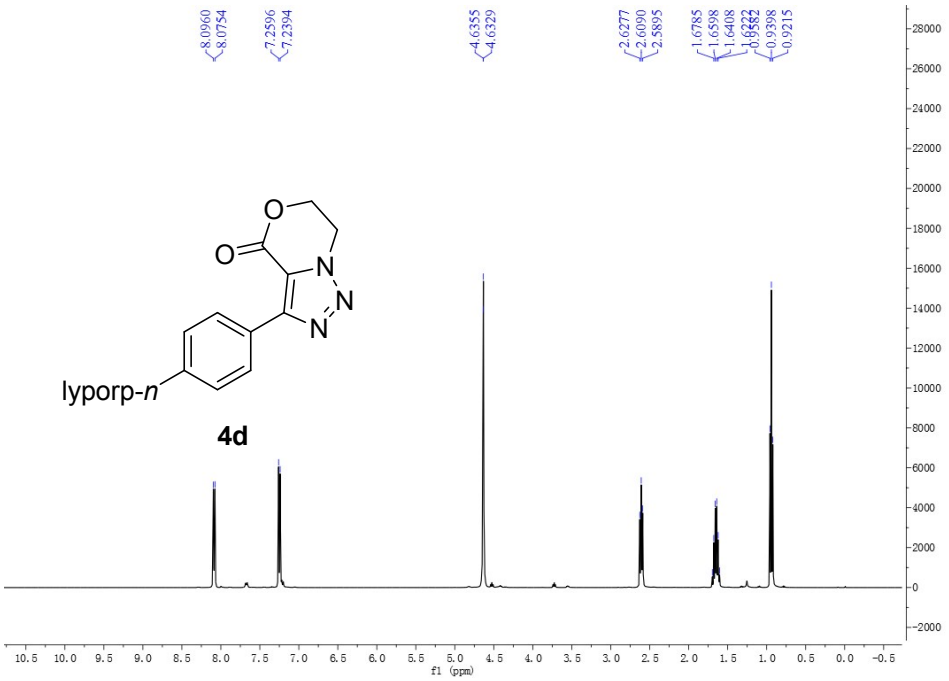
O
N
N
N
Et
f1 (ppm)

4c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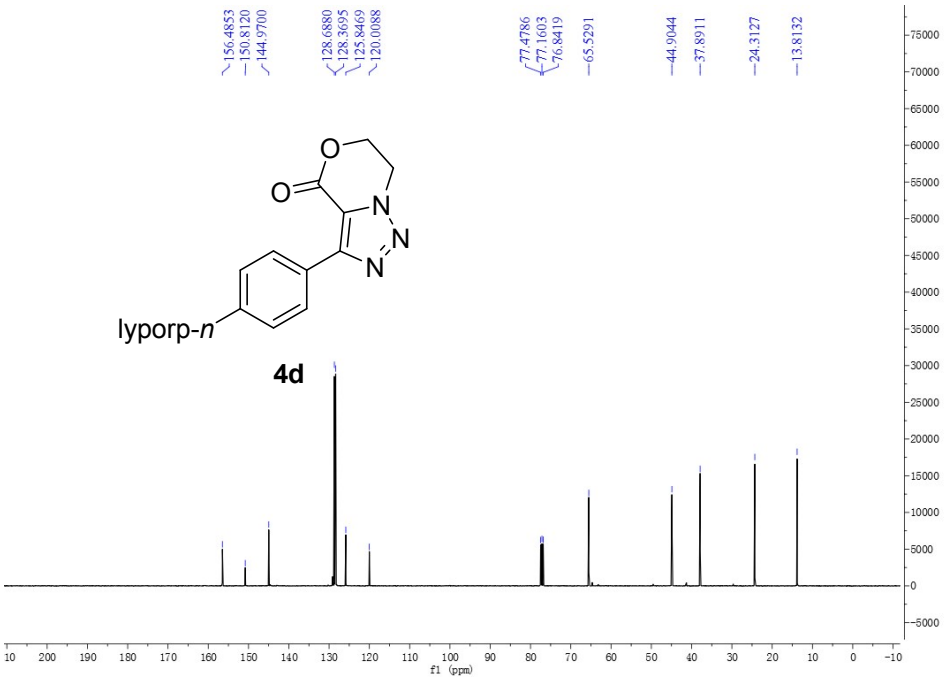
N
N
N
lyporp-n
4d
f1 (ppm)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N
N
lyporp-n
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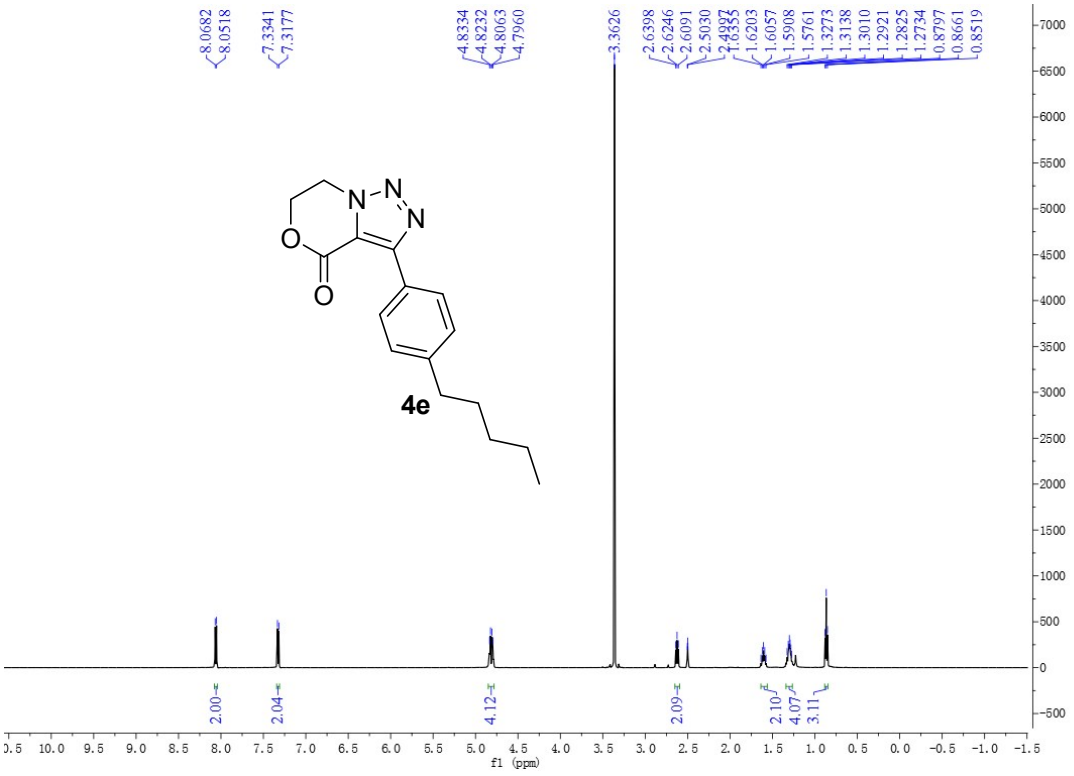
f1 (ppm)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1.3010
1.2921
1.2825
1.2734
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2.10
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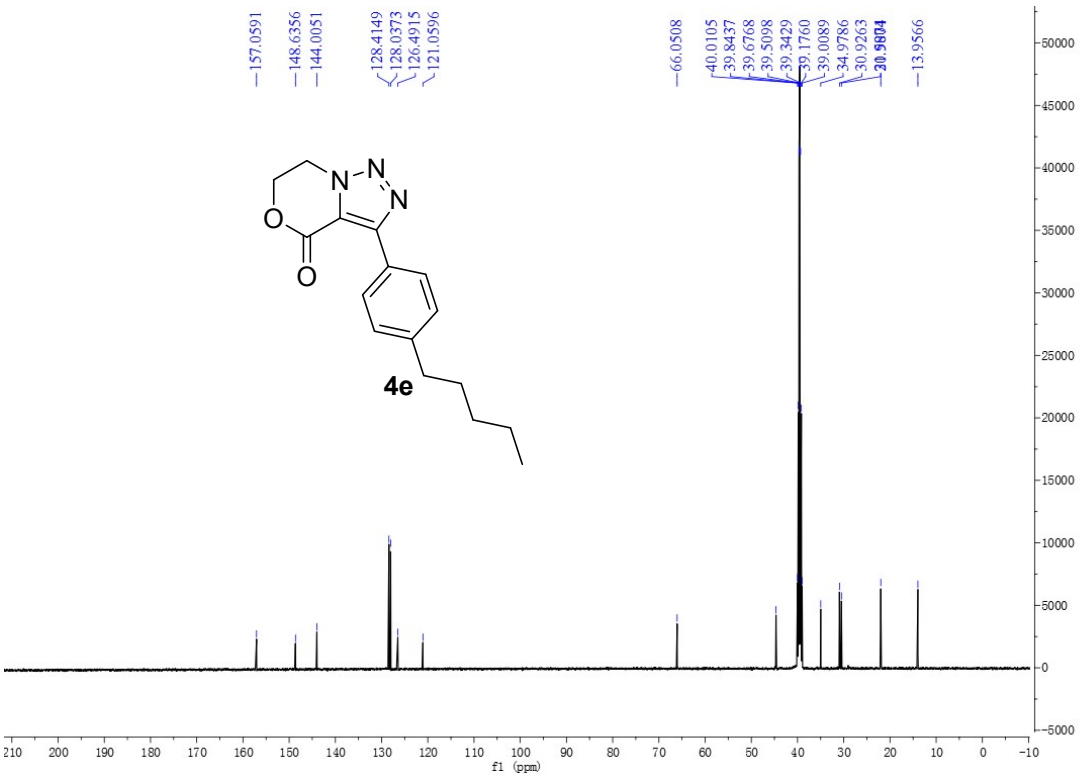
4e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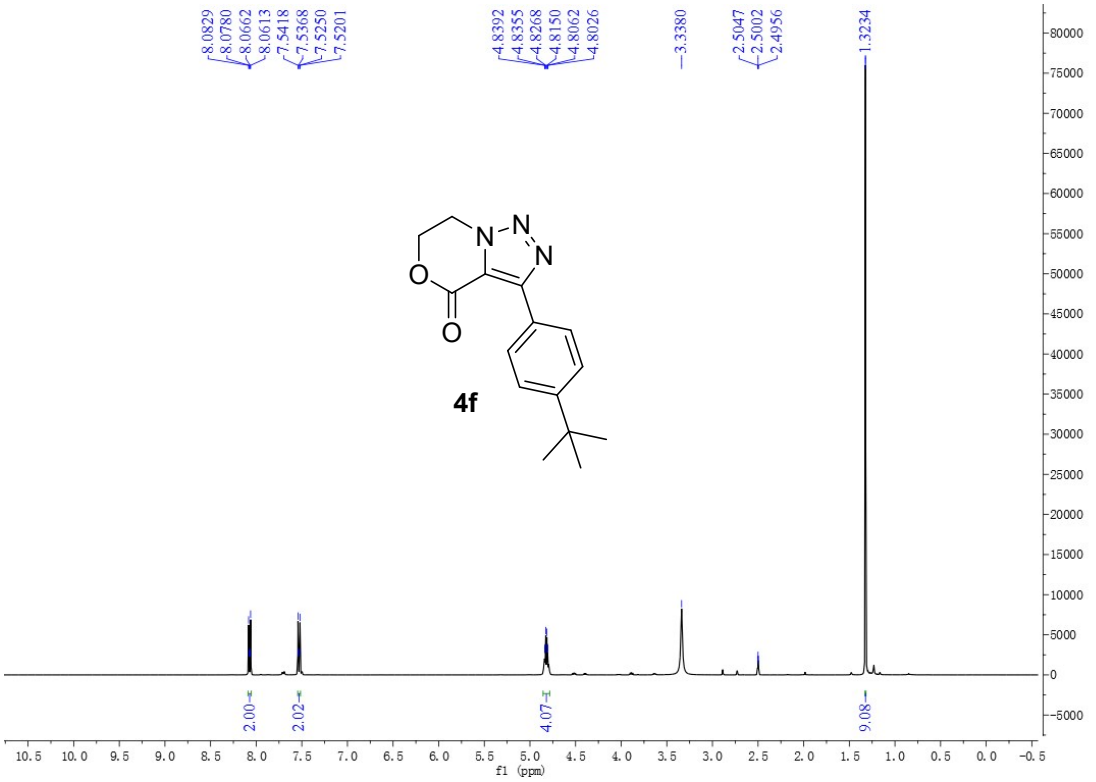
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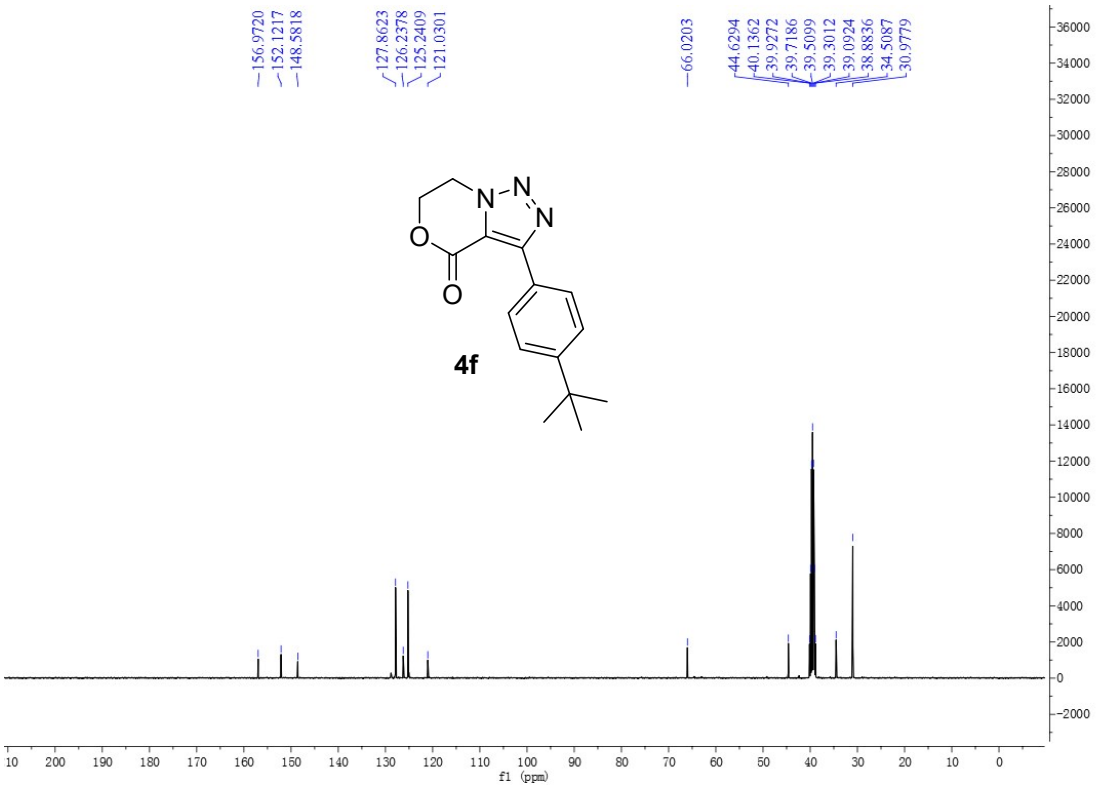
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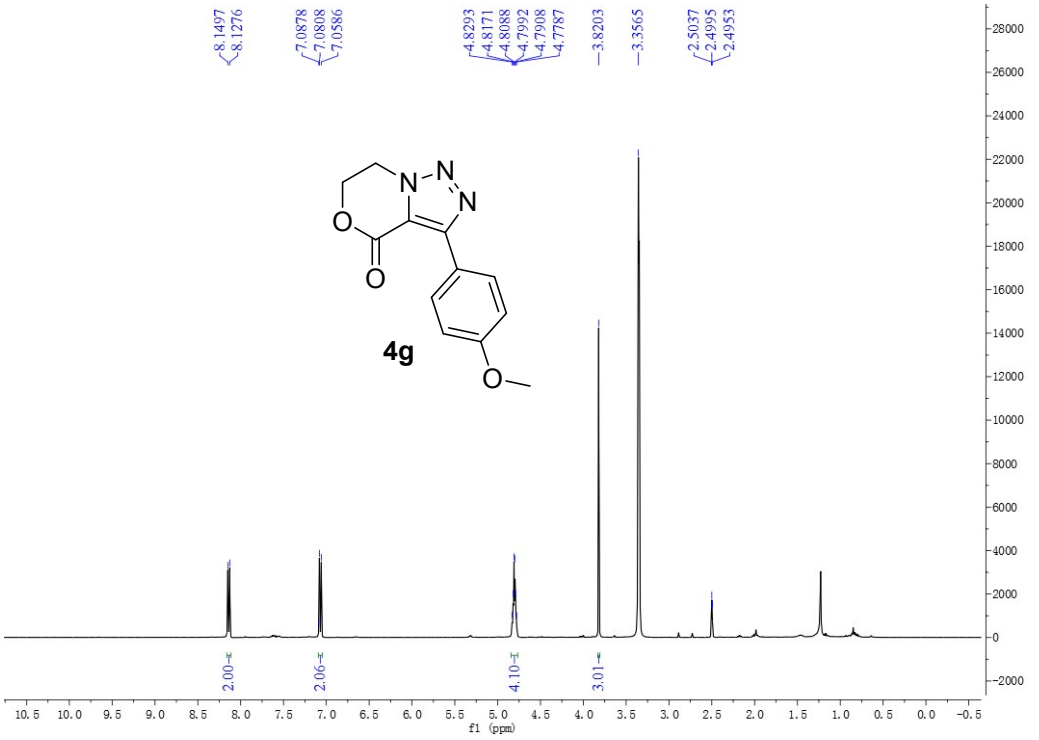
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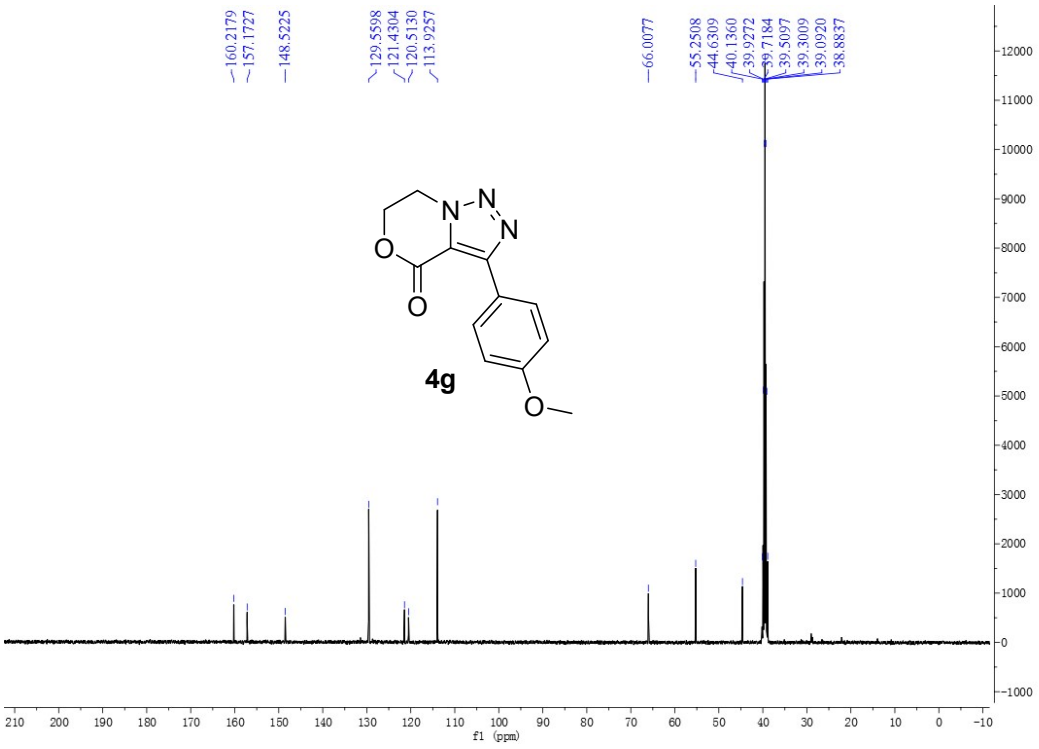
3.01
f1 (ppm)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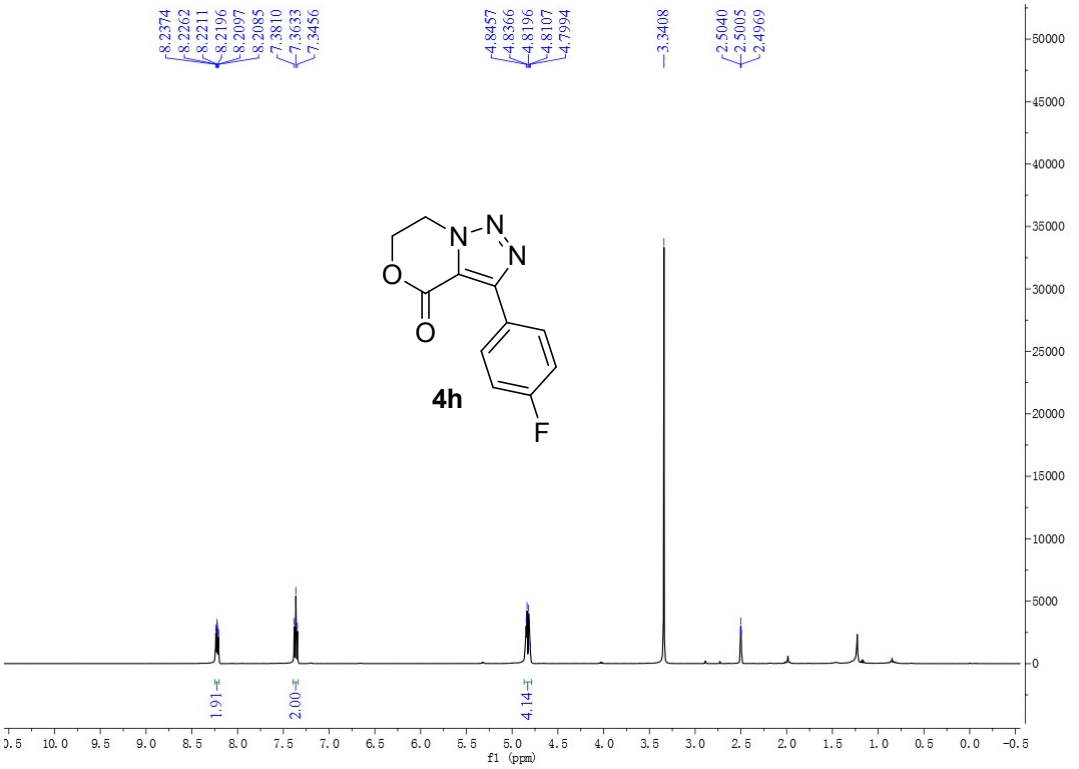
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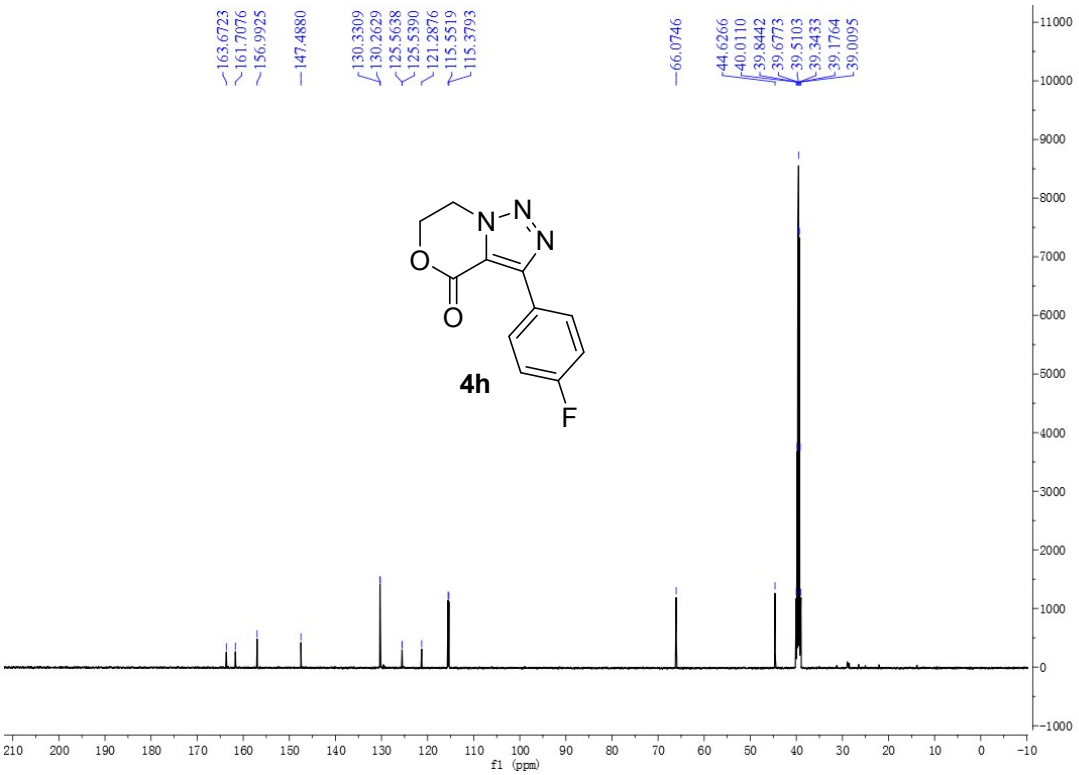
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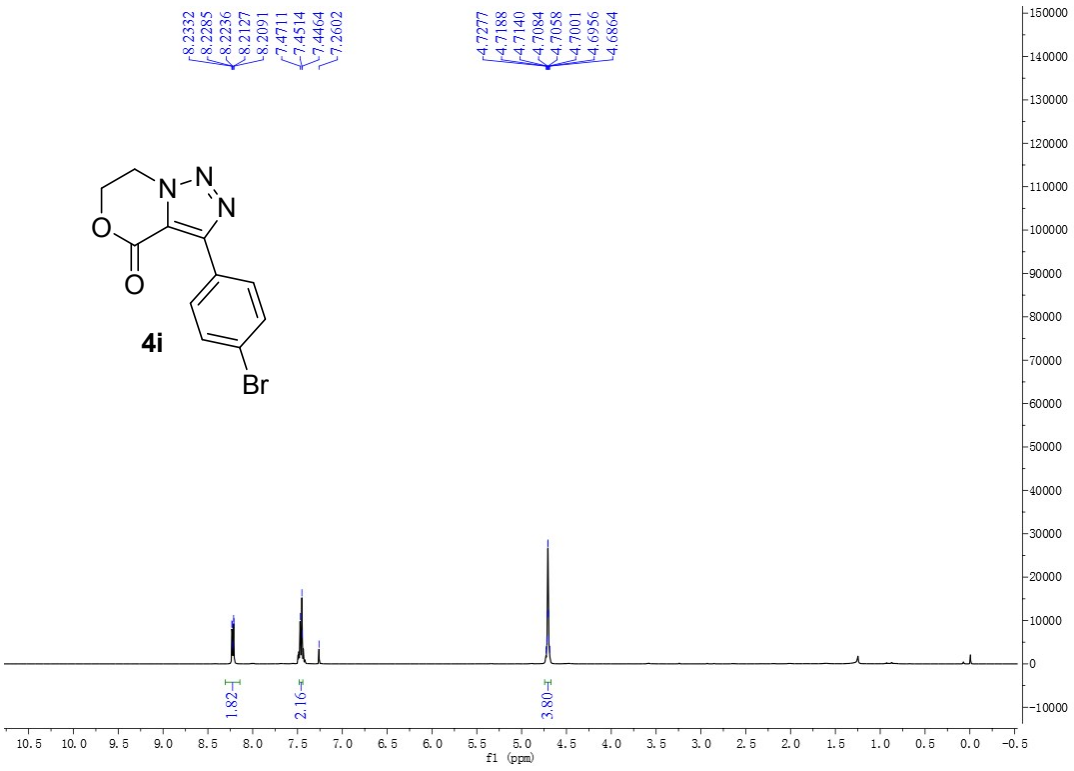
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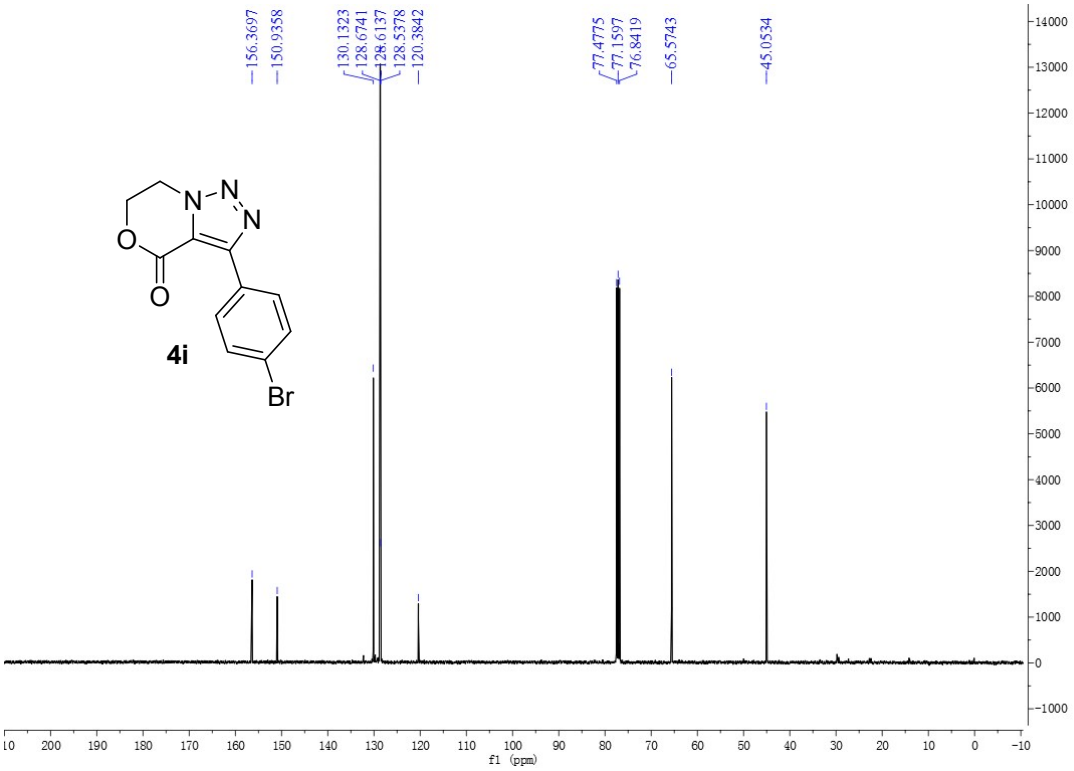
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Br
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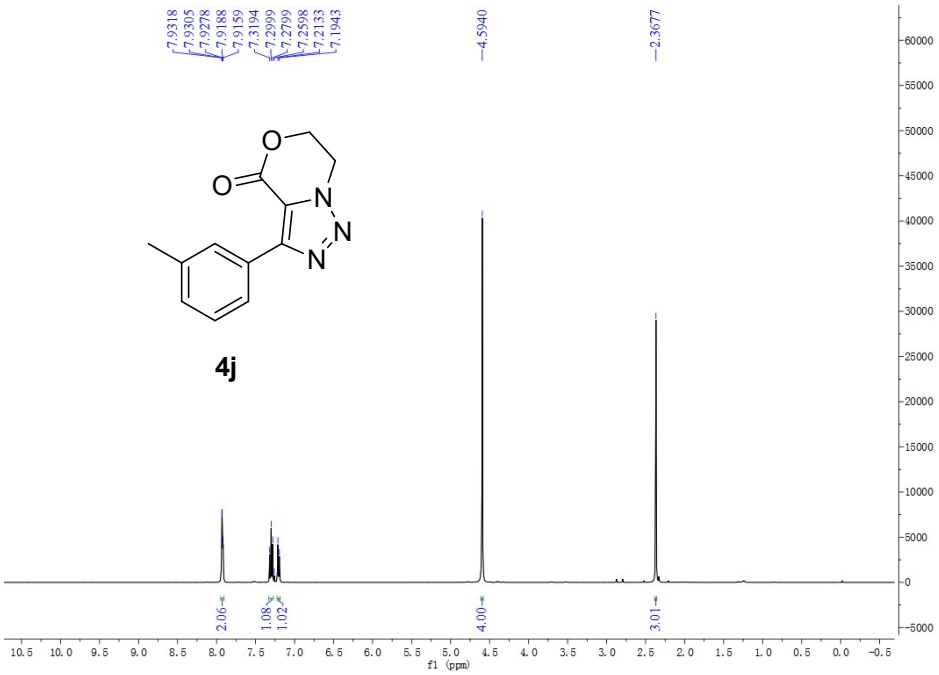
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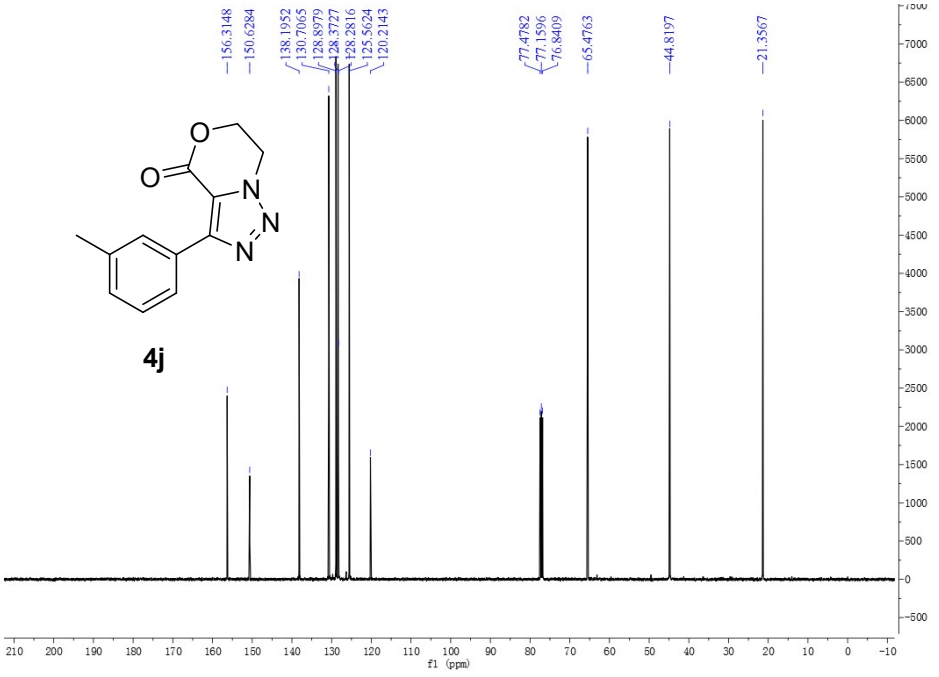
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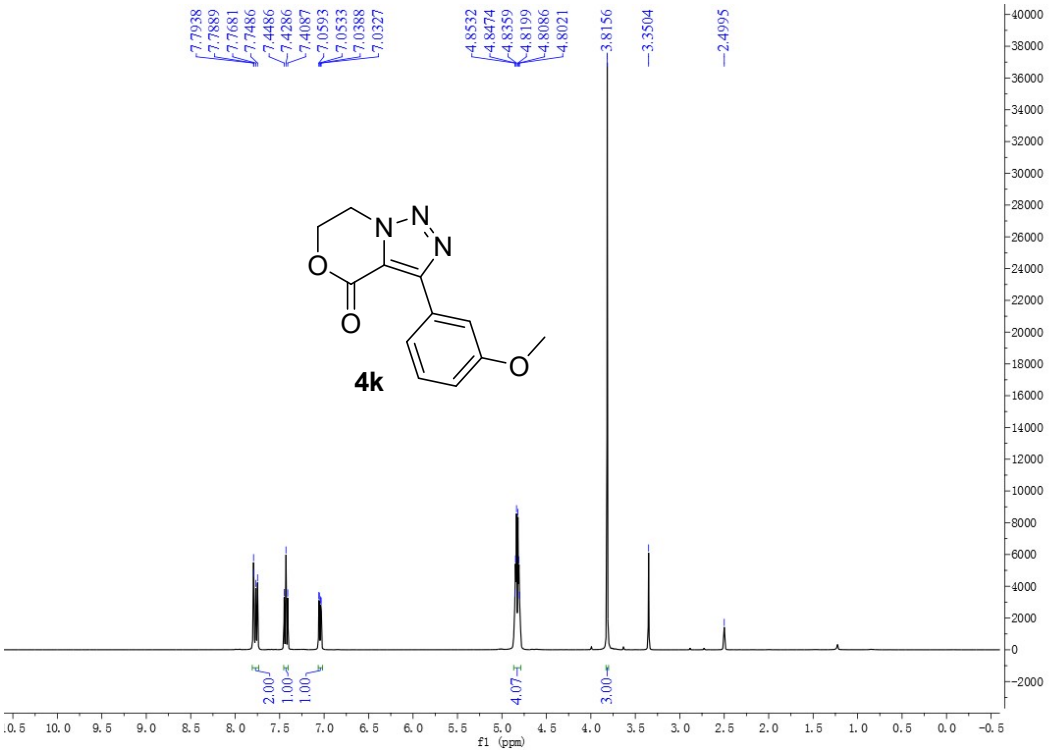
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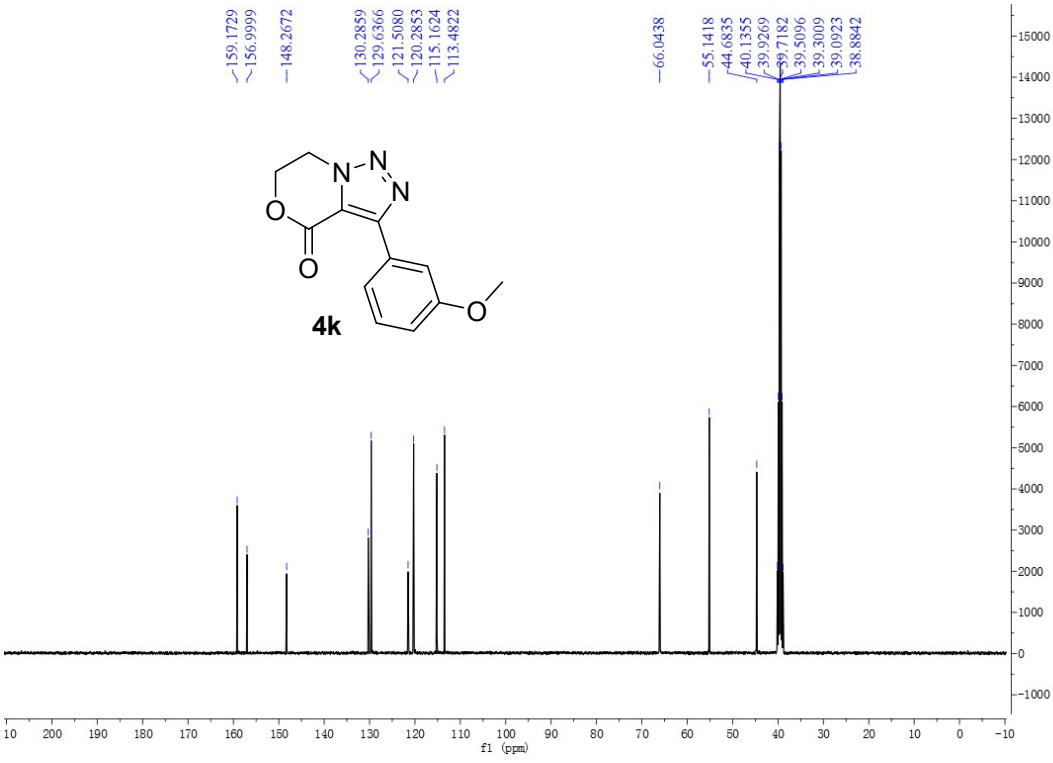
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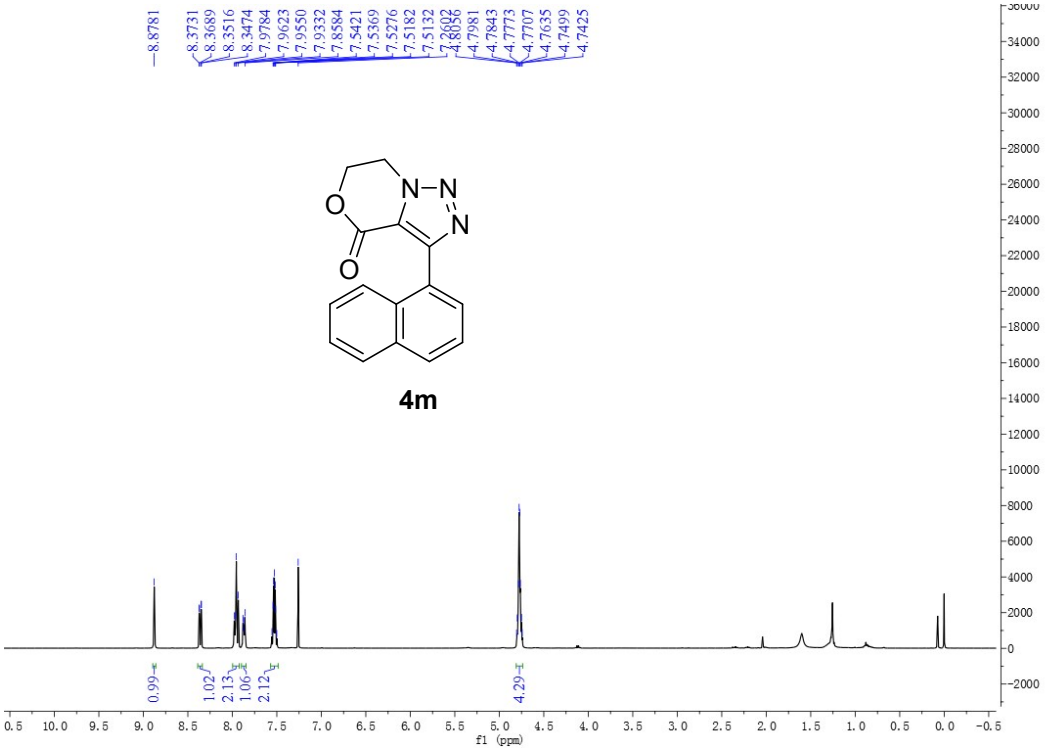
f1 (ppm)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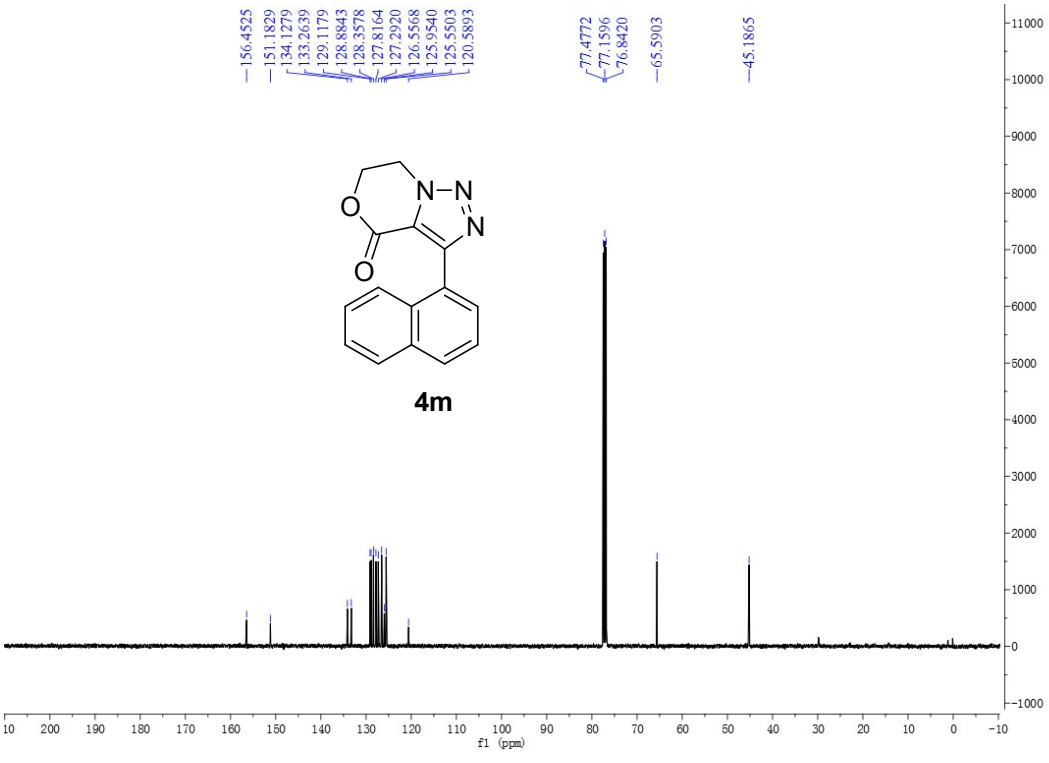
f1 (ppm)

4m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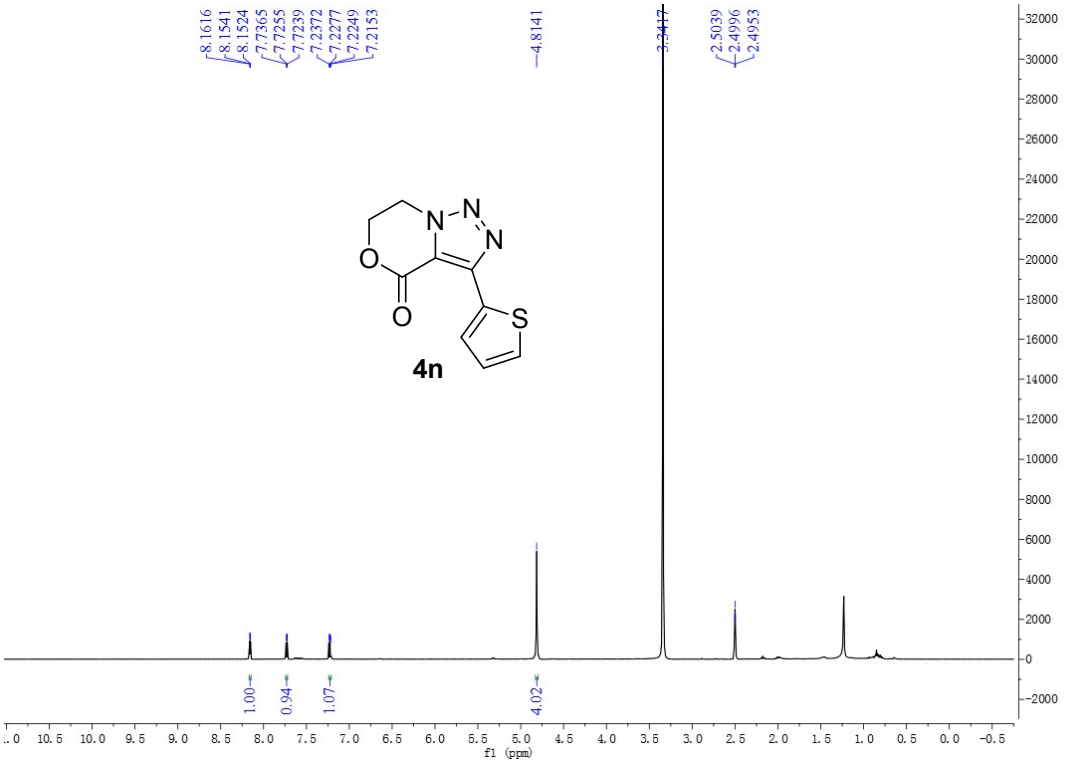
4m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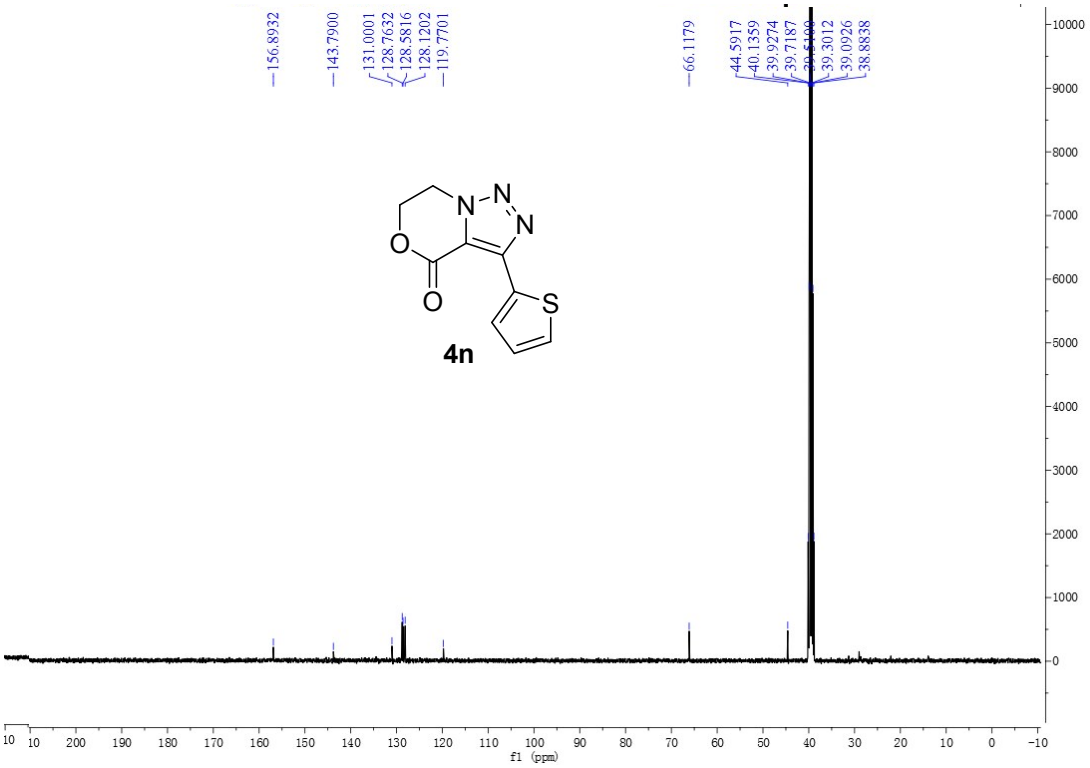
4n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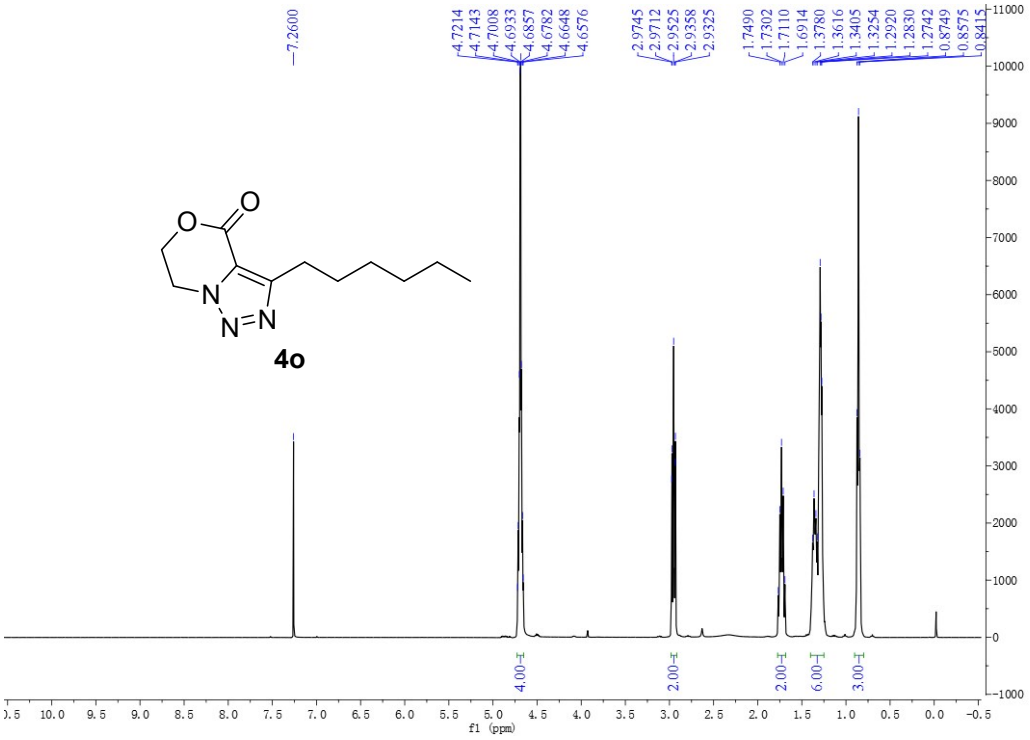
4n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1.3616
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1.3254
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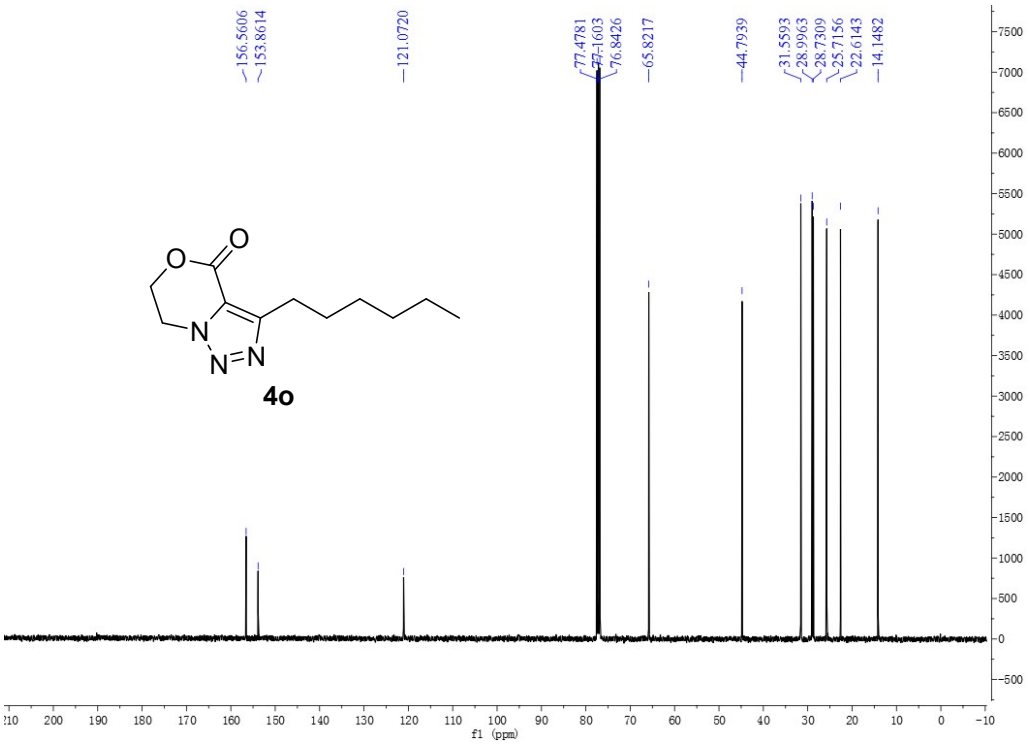
0.8575
0.8415
4.00
2.00
2.00
6.00
3.00
f1 (ppm)

4o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153.8614
121.0720
77.4781
77.1603
76.8426
65.8217
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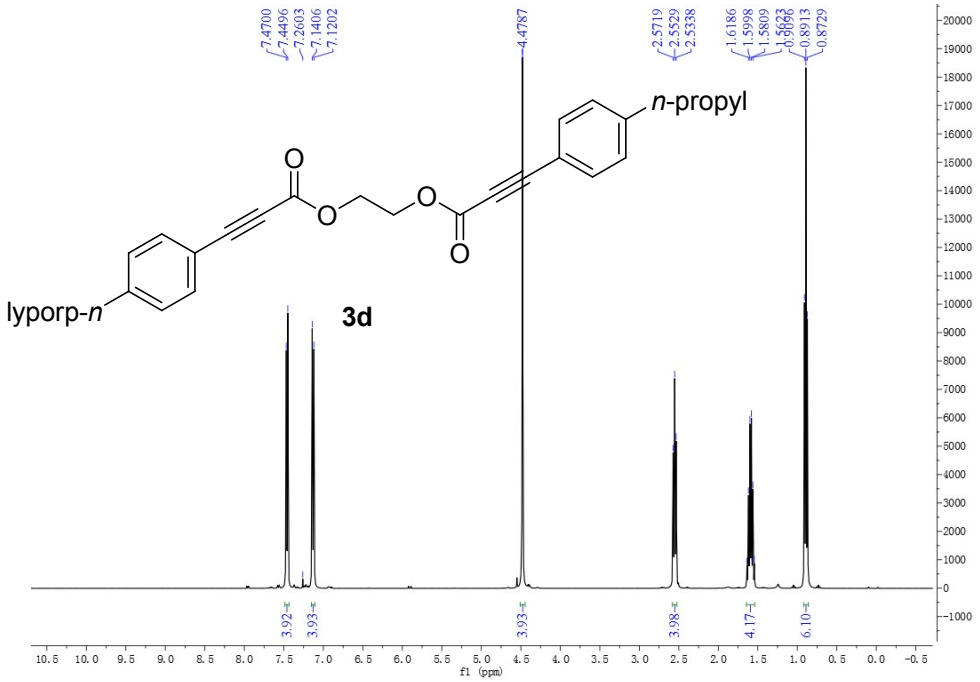
31.5593
28.9963
28.7309
25.7156
22.6143
14.1482
f1 (ppm)

4o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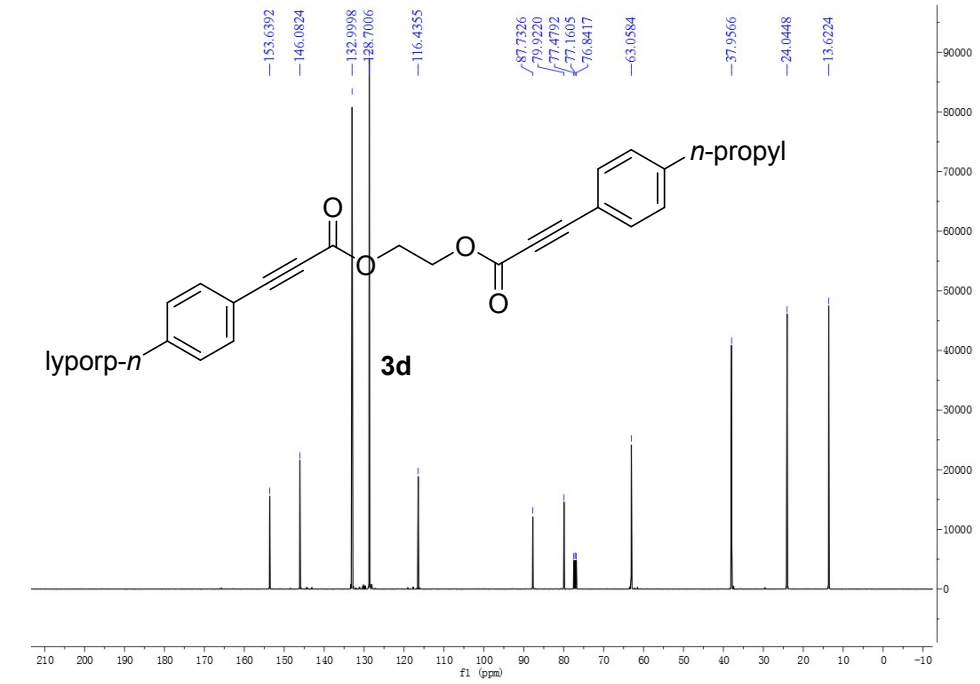
7.4496
7.2603
7.1406
7.1202
4.4787
2.5719
2.5529
2.5338
1.6186
1.5998
1.5809
1.5623
0.9096
0.8913
0.8729
n-propyl
lyporp-n
3d
3.92
3.93
3.93
3.98
4.17
6.10
f1 (ppm)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146.0824
132.9998
128.7006
116.4355
87.7326
79.9220
77.4792
77.1605
76.8417
63.0584
37.9566
24.0448
13.6224
n-propyl
lyporp-n
3d
f1 (ppm)