Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Photoinduced synthesis of alkylalkynyl sulfones through a reaction of potassium alkyltrifluoroborates, sulfur dioxide, and alkynyl bromides

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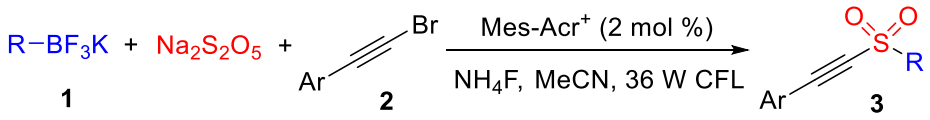
Supporting Information

General experimental methods:

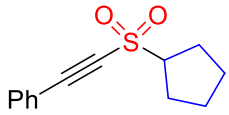
Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

General experimental procedure for the photoredox-catalyzed reaction of potassium alkyltrifluoroborates, sulfur dioxide, and alkynyl bromides.



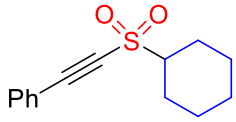
1 **2** **3**

Potassium alkyltrifluoroborate **1** (0.2 mmol), sodium metabisulfite (0.4 mmol), NH_4F (0.4 mmol) and Mes-AcrClO_4 (2 mol %) were combined with in a tube. The tube was evacuated and backfilled with N_2 three times, then alkynyl bromide **2** (0.3 mmol) in MeCN (2.0 mL) was added in the tube under N_2 atmosphere. The mixture was placed around a white CFL (36 W) with a distance of 6 centimeters, and was stirred under light irradiation for 48 hours at room temperature. After completion of reaction as indicated by TLC, the mixture was purified directly by flash column chromatography (EtOAc/n-hexane, 1:8 - 1:2) to provide the desired product **3**.



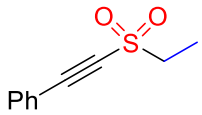
((Cyclopentylsulfonyl)ethynyl)benzene (**3a**), colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.52 (m, 1H), 7.42 (m, 2H), 3.87 – 3.59 (m, 1H), 2.44 – 2.07 (m, 4H), 1.79 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.7, 131.5, 128.7, 117.7, 92.6, 82.5, 66.1, 27.3, 26.0. HRMS (ESI) calcd for $C_{13}H_{14}O_2S^+$: 235.0787 ($M+H^+$), found: 235.0781.



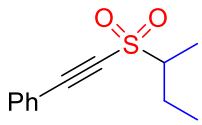
((Cyclohexylsulfonyl)ethynyl)benzene (**3b**), colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.60 (d, *J* = 7.4 Hz, 2H), 7.52 (m, 1H), 7.42 (m, 2H), 3.04 (t, *J* = 11.9 Hz, 1H), 2.36 (d, *J* = 12.5 Hz, 2H), 1.97 (d, *J* = 12.6 Hz, 2H), 1.76 – 1.54 (m, 4H), 1.46 – 1.30 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.8, 131.5, 128.7, 117.7, 93.0, 81.7, 65.1, 25.4, 24.9, 24.8. HRMS (ESI) calcd for $C_{14}H_{16}O_2S^+$: 249.0944 ($M+H^+$), found: 249.0943.



((Ethylsulfonyl)ethynyl)benzene (**3c**), pale yellow oil.

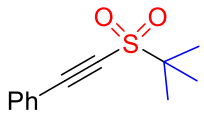
^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.60 (d, *J* = 7.4 Hz, 2H), 7.52 (m, 1H), 7.43 (m, 2H), 3.31 (d, *J* = 7.3 Hz, 2H), 1.54 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.8, 131.6, 128.7, 117.5, 92.4, 82.6, 52.7, 7.6. HRMS (ESI) calcd for $C_{10}H_{10}O_2S^+$: 195.0474 ($M+H^+$), found:195.0475.



((*sec*-Butylsulfonyl)ethynyl)benzene (**3d**), pale yellow oil.

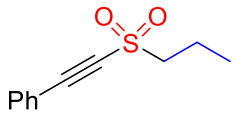
^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.59 (d, *J* = 7.3 Hz, 2H), 7.51 (d, *J* = 7.3 Hz, 1H), 7.42 (m, 2H), 3.07 (m, 1H), 2.37 – 2.19 (m, 1H), 1.79 – 1.62 (m, 1H), 1.52 (m, 3H), 1.11 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.7, 131.5, 128.7, 117.7, 93.0, 81.7, 63.4,

22.6, 12.7, 11.0. HRMS (ESI) calcd for $C_{12}H_{14}O_2S^+$: 223.0787 ($M+H^+$), found: 223.0771.



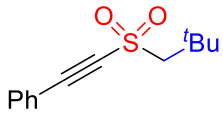
((*tert*-Butylsulfonyl)ethynyl)benzene (**3e**), pale yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.60 (d, *J* = 7.4 Hz, 2H), 7.51 (m, 1H), 7.42 (m, 2H), 1.53 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.7, 131.5, 128.7, 117.8, 93.8, 80.4, 60.9, 22.9. HRMS (ESI) calcd for $C_{12}H_{14}O_2S^+$: 223.0787 ($M+H^+$), found: 223.0780.



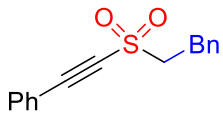
((Propylsulfonyl)ethynyl)benzene (**3f**), pale yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.60 (d, *J* = 7.5 Hz, 2H), 7.53 (m, 1H), 7.43 (m, 2H), 3.27 (dd, *J* = 8.0, 6.7 Hz, 2H), 2.03 (dd, *J* = 14.3, 7.3 Hz, 2H), 1.14 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.7, 131.6, 128.7, 117.6, 92.2, 83.2, 59.9, 16.7, 12.7. HRMS (ESI) calcd for $C_{11}H_{12}O_2S^+$: 209.0631 ($M+H^+$), found: 209.0630.



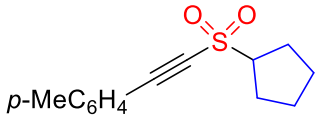
((Neopentylsulfonyl)ethynyl)benzene (**3g**), colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.51 (m, 1H), 7.42 (m, 2H), 3.33 (s, 2H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 132.6, 131.5, 128.7, 117.7, 91.1, 85.4, 70.0, 29.6. HRMS (ESI) calcd for $C_{13}H_{16}O_2S^+$: 237.0944 ($M+H^+$), found: 237.0943.



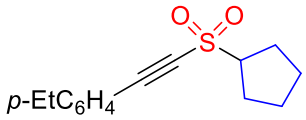
((Phenethylsulfonyl)ethynyl)benzene (**3h**), pale yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.57 (m, 3H), 7.45 (m, 2H), 7.37 (m, 2H), 7.29 (m, 3H), 3.68 – 3.51 (m, 2H), 3.40 – 3.24 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 136.8, 132.8, 131.7, 128.9, 128.7, 128.4, 127.1, 117.4, 92.7, 83.0, 59.4, 29.1. HRMS (ESI) calcd for $C_{16}H_{14}O_2S^+$: 271.0787 ($M+H^+$), found: 271.0779.



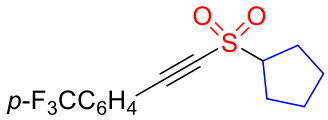
1-((Cyclopentylsulfonyl)ethynyl)-4-methylbenzene (**3i**), white solid.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.47 (d, *J* = 7.4 Hz, 2H), 7.22 (d, *J* = 7.4 Hz, 2H), 3.77 – 3.58 (m, 1H), 2.40 (s, 3H), 2.21 (m, 4H), 1.78 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 142.4, 132.7, 131.5, 129.5, 128.7, 114.6, 93.2, 82.1, 66.2, 27.3, 26.0, 21.7. HRMS (ESI) calcd for $C_{14}H_{16}O_2SNa^+$: 271.0763 ($M+Na^+$), found: 271.0763.



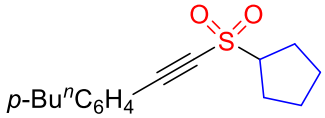
1-((Cyclopentylsulfonyl)ethynyl)-4-ethylbenzene (**3j**), white solid.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 3.67 (s, 1H), 2.69 – 2.59 (m, 2H), 2.32 – 2.05 (m, 4H), 1.91 – 1.79 (m, 2H), 1.73 – 1.59 (m, 4H), 1.35 – 1.28 (m, 4H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 147.3, 132.7, 128.8, 114.8, 93.3, 82.1, 66.2, 36.0, 31.2, 30.6, 27.3, 26.0, 22.3, 139. HRMS (ESI) calcd for $C_{18}H_{24}O_2SNa^+$: 327.1389 ($M+Na^+$), found: 327.1379.



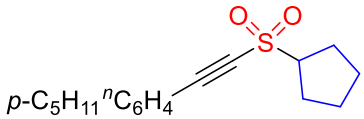
1-((Cyclopentylsulfonyl)ethynyl)-4-(trifluoromethyl)benzene (**3k**), white solid.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.70 (d, *J* = 2.1 Hz, 2H), 7.26 (m, 2H), 3.77 – 3.59 (m, 1H), 2.21 (m, 4H), 1.95 – 1.63 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 133.0, 125.6, 121.6, 90.1, 84.5, 66.1, 27.2, 25.9. HRMS (ESI) calcd for $C_{14}H_{13}F_3O_2SNa^+$: 325.0481 ($M+Na^+$), found: 325.0497.



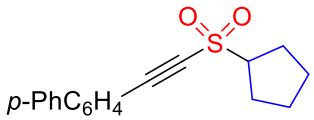
1-Butyl-4-((cyclopentylsulfonyl)ethynyl)benzene (**3l**), colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.56 – 7.41 (m, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 3.67 (m, 1H), 2.69 (q, *J* = 7.6 Hz, 2H), 2.31 – 2.09 (m, 4H), 1.89 – 1.66 (m, 4H), 1.26 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 148.5, 132.8, 129.2, 128.3, 93.3, 82.1, 66.2, 28.9, 27.3, 26.0, 15.0. HRMS (ESI) calcd for $C_{15}H_{18}O_2SNa^+$: 285.0920 ($M+Na^+$), found: 285.0914.



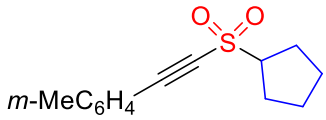
1-((Cyclopentylsulfonyl)ethynyl)-4-pentylbenzene (**3m**), colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 3.73 – 3.61 (m, 1H), 2.74 – 2.60 (m, 2H), 2.37 – 2.02 (m, 4H), 1.91 – 1.66 (m, 4H), 1.62 – 1.56 (m, 2H), 1.35 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 147.3, 132.7, 128.8, 114.8, 93.3, 82.1, 66.2, 35.7, 33.0, 27.3, 26.0, 22.1, 13.8. HRMS (ESI) calcd for $C_{17}H_{22}O_2SNa^+$: 313.1233 (M+Na^+), found: 313.1233.



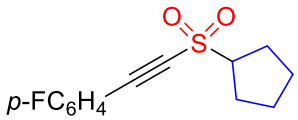
4-((Cyclopentylsulfonyl)ethynyl)-1,1'-biphenyl (**3n**), white solid.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.68 – 7.57 (m, 6H), 7.50 – 7.39 (m, 3H), 3.69 (m, 1H), 2.36 – 2.09 (m, 3H), 1.91 – 1.70 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 144.3, 139.4, 133.2, 128.9, 128.3, 127.3, 127.1, 125.3, 116.4, 92.7, 83.1, 66.2, 27.3, 26.0. HRMS (ESI) calcd for $C_{19}H_{18}O_2SNa^+$: 333.0920 (M+Na^+), found: 333.0924.



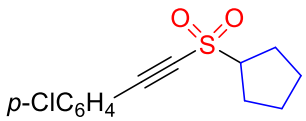
1-((Cyclopentylsulfonyl)ethynyl)-3-methylbenzene (**3o**), colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.39 (m, 2H), 7.30 (d, *J* = 7.5 Hz, 2H), 3.67 (m, 1H), 2.37 (s, 3H), 2.20 (m, 4H), 1.90 – 1.68 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 138.6, 133.1, 132.4, 129.8, 128.6, 117.6, 92.9, 82.2, 66.2, 27.3, 26.0 21.1. HRMS (ESI) calcd for $C_{14}H_{16}O_2S^+$: 249.0944 (M+H^+), found: 249.0945.



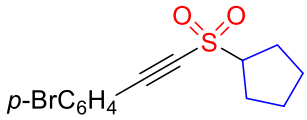
1-((Cyclopentylsulfonyl)ethynyl)-4-fluorobenzene (**3p**), white soild.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.61 (d, *J* = 6.0 Hz, 2H), 7.14 (m, 2H), 3.78 – 3.60 (m, 1H), 2.40 – 2.05 (m, 2H), 1.99 – 1.69 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 165.6, 135.1 (d, *J* = 9.0 Hz), 116.4 (d, *J* = 22.4 Hz), 91.5, 82.6, 66.1, 27.3, 26.0. HRMS (ESI) calcd for $C_{13}H_{13}FO_2S^+$: 253.0693 (M+H^+), found: 253.0695.



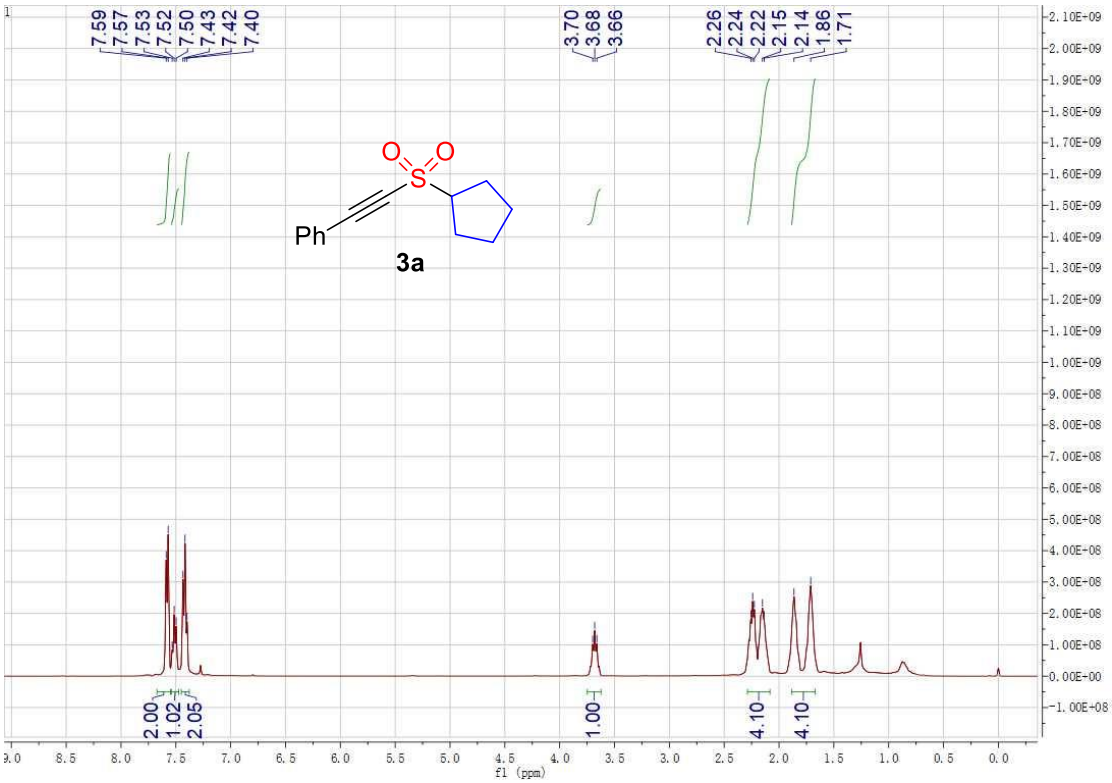
1-Chloro-4-((cyclopentylsulfonyl)ethynyl)benzene (**3q**), white soild.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.52 (d, *J* = 7.9 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 3.75 – 3.60 (m, 1H), 2.26 – 2.08 (m, 4H), 1.86 (m, 2H), 1.72 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 138.0, 133.9, 129.2, 116.2, 91.2, 83.5, 66.1, 27.2, 26.0. HRMS (ESI) calcd for $C_{13}H_{13}ClO_2S^+$: 291.0217 ($M+H^+$), found: 291.0211.



1-Bromo-4-((cyclopentylsulfonyl)ethynyl)benzene (**3r**), white soild.

^{1}H NMR (400 MHz, $CDCl_3$)：δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 3.74 – 3.59 (m, 1H), 2.29 – 2.05 (m, 4H), 1.90 – 1.68 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$)：δ 133.9, 132.1, 126.5, 116.7, 91.2, 83.6, 66.1, 27.2, 26.0. HRMS (ESI) calcd for $C_{13}H_{13}BrO_2S^+$: 312.9892 ($M+H^+$), found: 312.9889.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7.57
7.53
7.52
7.50
7.43
7.42
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3.68
3.66
2.26
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2.22
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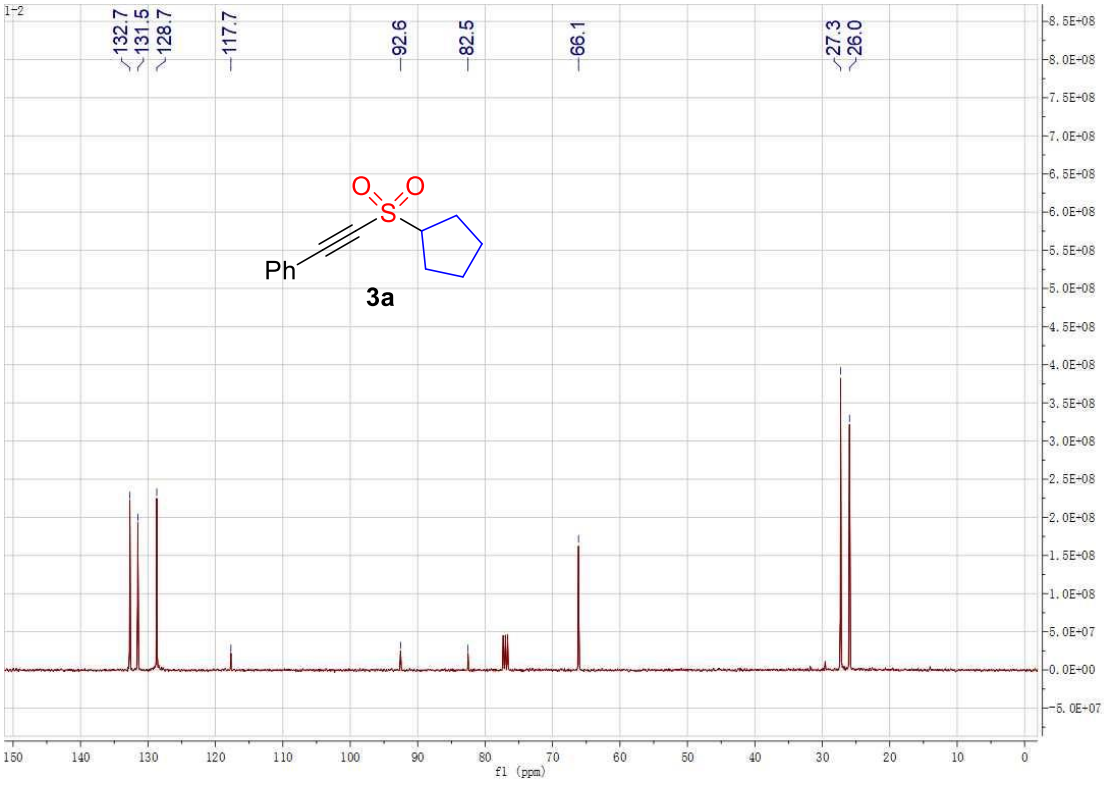
2.05
1.00
4.10
4.10
f1 (ppm)


132.7
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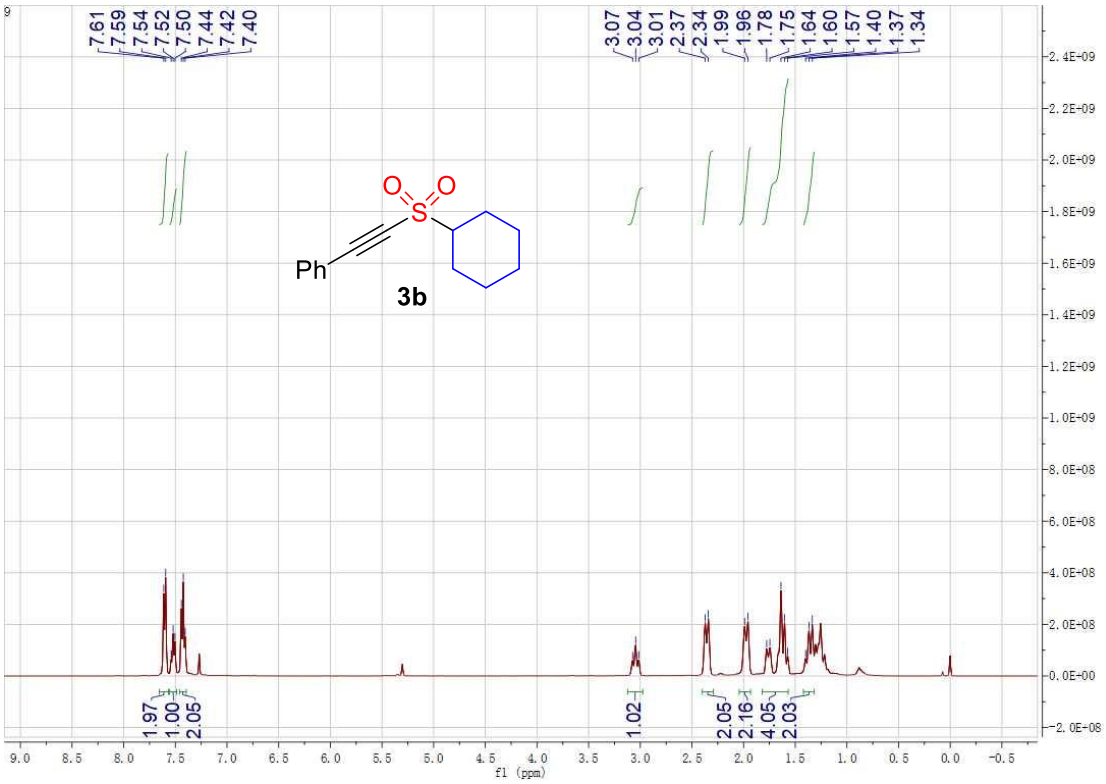
117.7
92.6
82.5
66.1
27.3
26.0
Ph
3a
f1 (ppm)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7.50
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7.42
7.40
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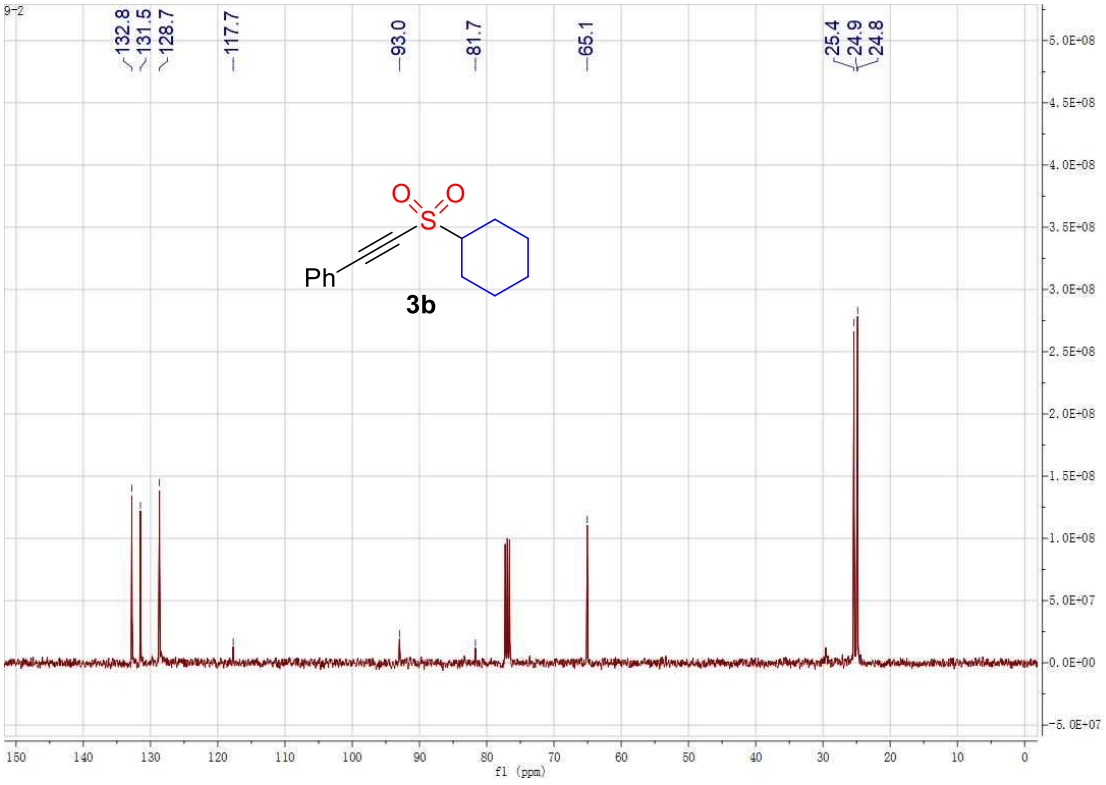
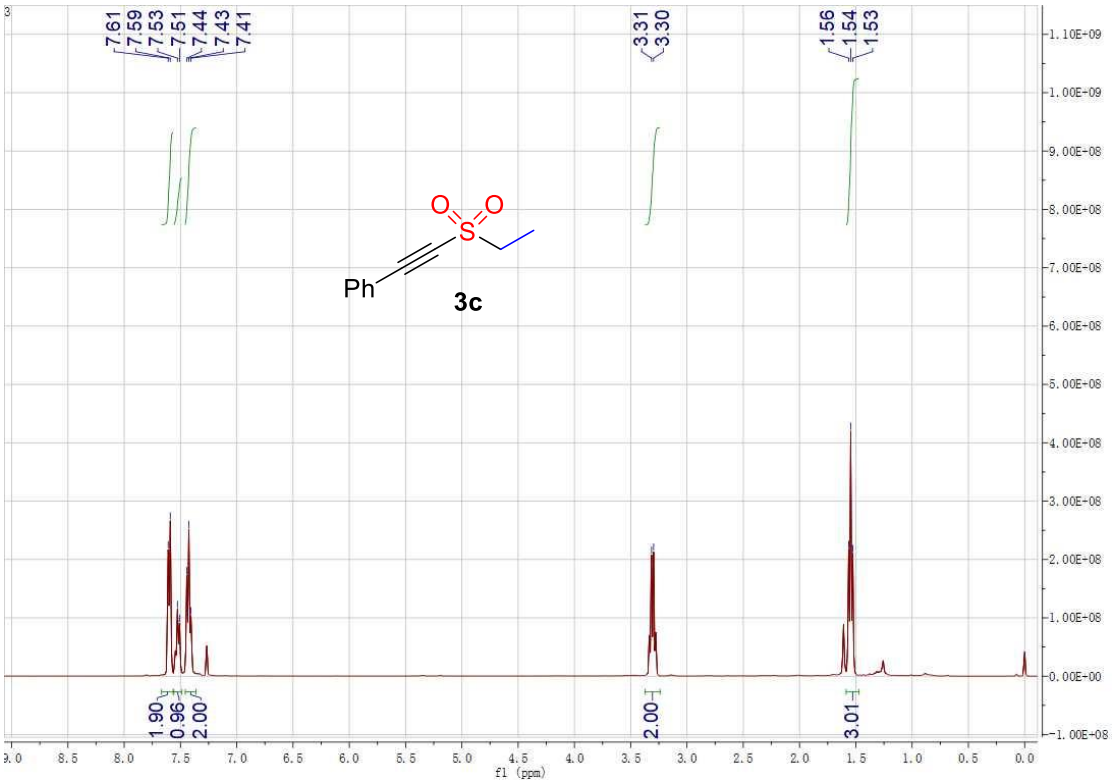
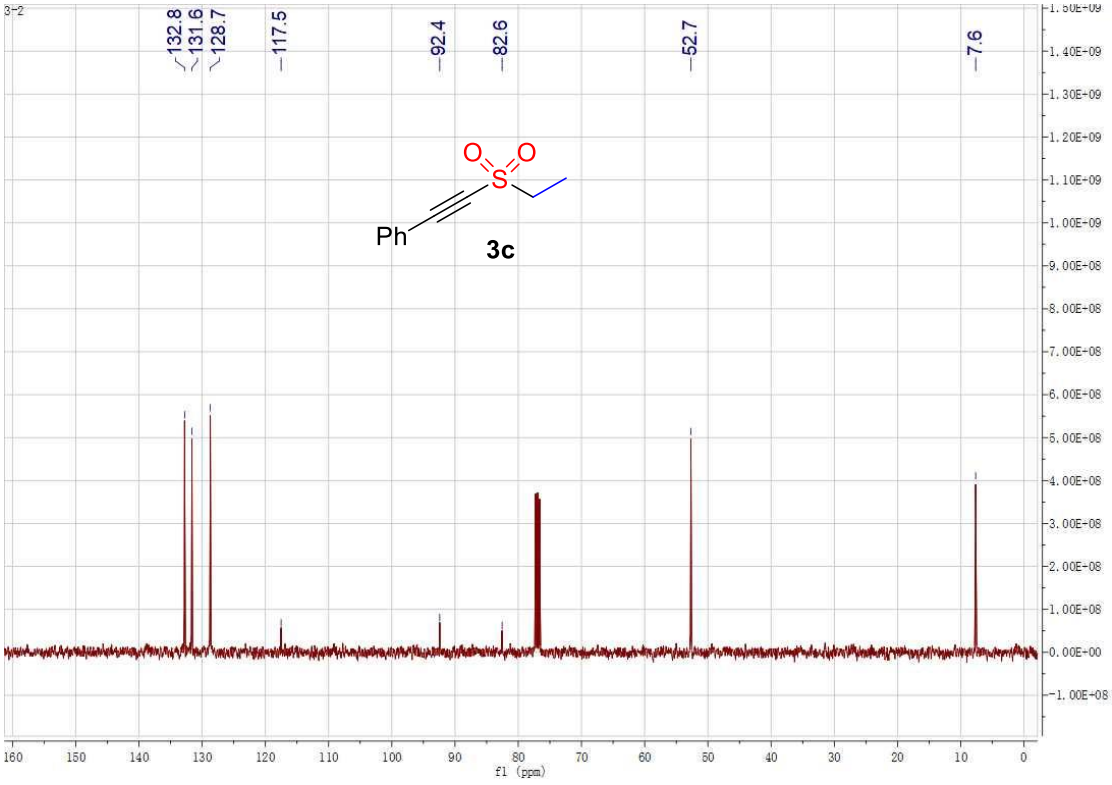
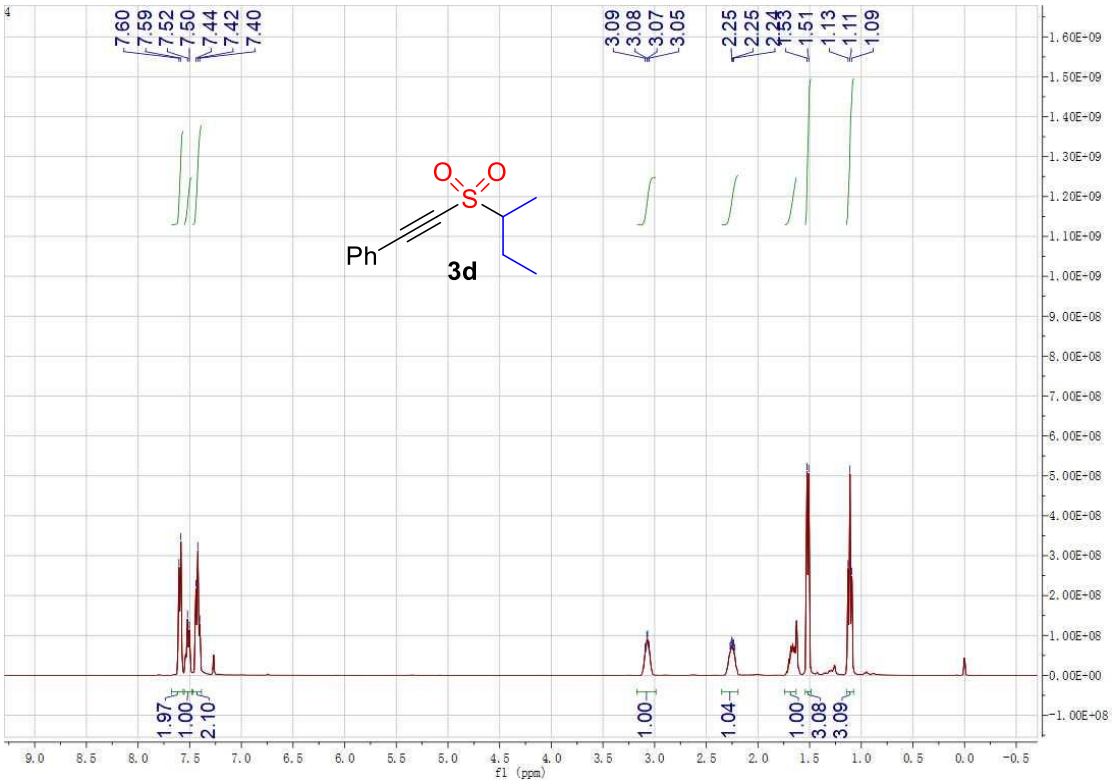
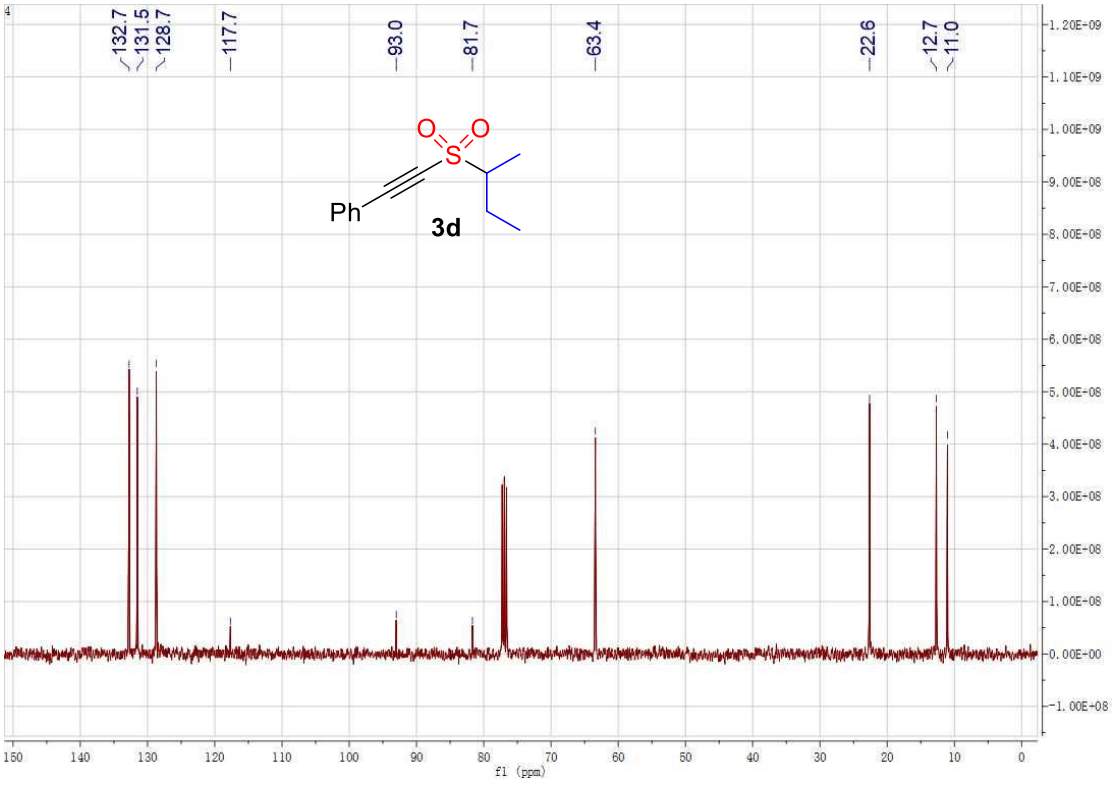
3.04
3.01
2.37
2.34
1.99
1.96
1.78
1.75
1.64
1.60
1.57
1.40
1.37
1.34
Ph
3b
1.97
1.00
2.05
1.02
2.05
2.16
4.05
2.03
f1 (ppm)

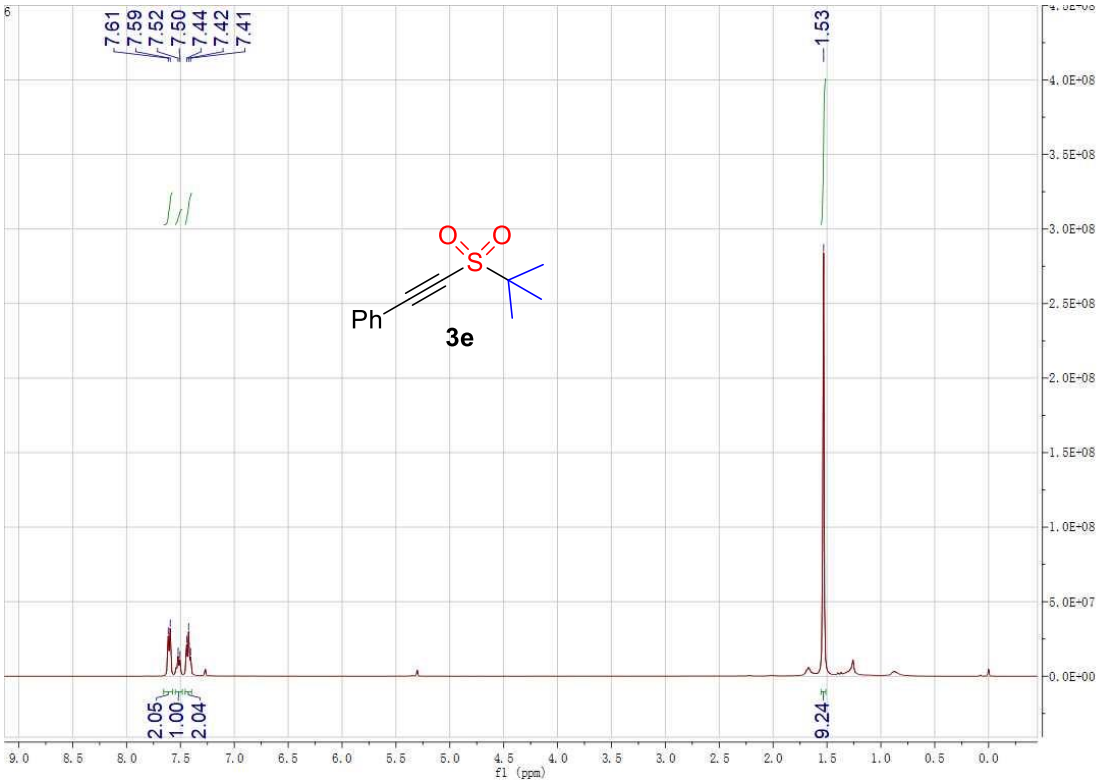

132.8
131.5
128.7
117.7
93.0
81.7
65.1
25.4
24.9
24.8
Ph
3b
f1 (ppm)

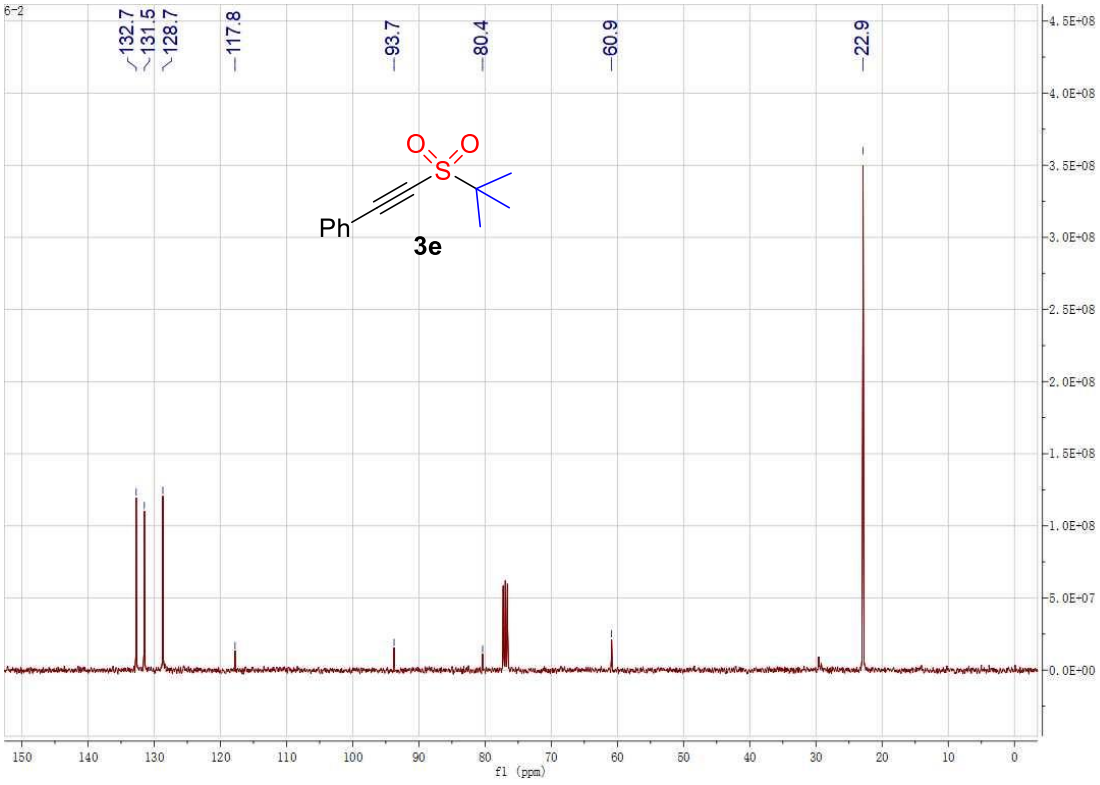

7.61
7.59
7.53
7.51
7.44
7.43
7.41
3.31
3.30
1.56
1.54
1.53
O
O
S
Ph
3c
1.90
0.96
2.00
2.00
3.01
f1 (ppm)

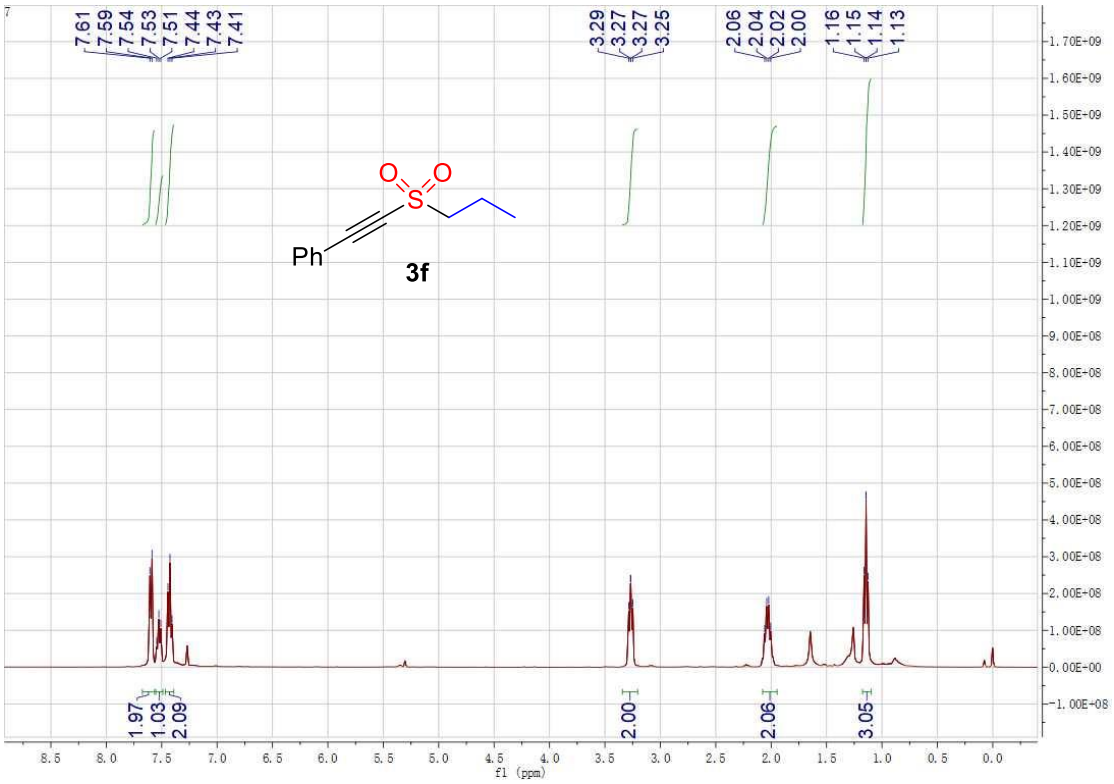

132.8
131.6
128.7
117.5
92.4
82.6
52.7
7.6
O
O
S
Ph
3c
f1 (ppm)

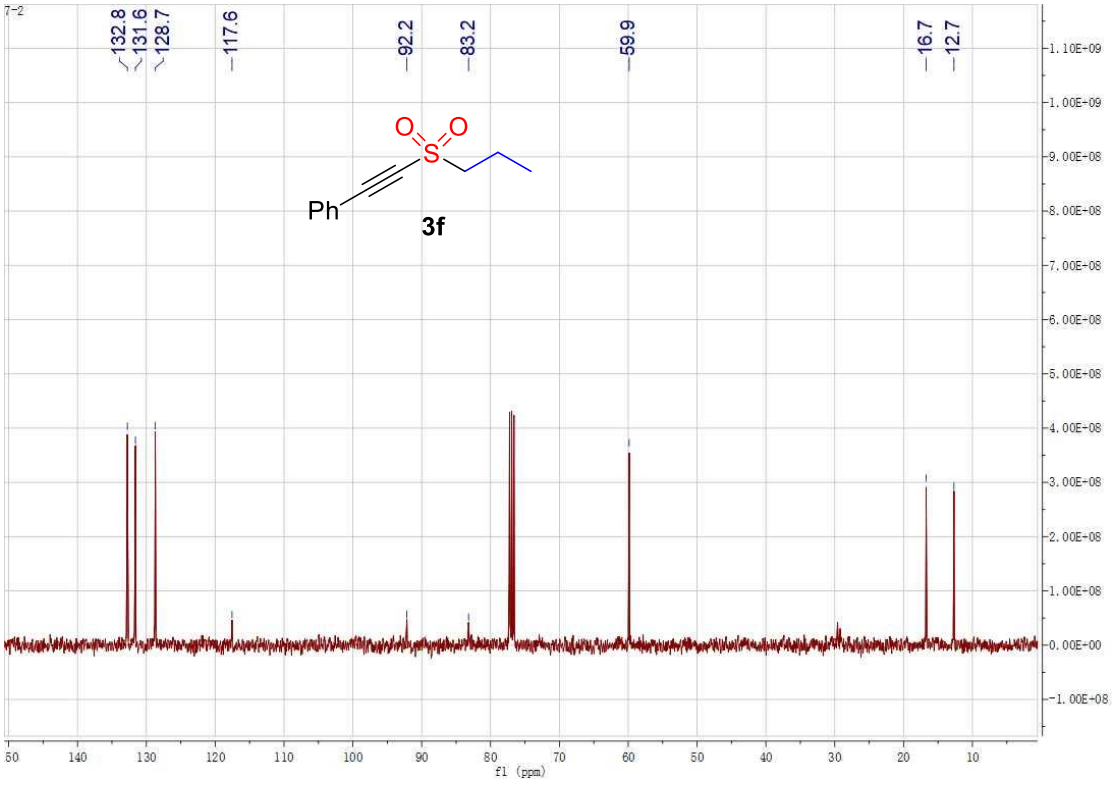

7.60
7.59
7.52
7.50
7.44
7.42
7.40
3.09
3.08
3.07
3.05
2.25
2.25
2.24
1.53
1.51
1.13
1.11
1.09
O
O
S
Ph
3d
1.97
1.00
2.10
1.00
1.04
1.00
3.08
3.09
f1 (ppm)

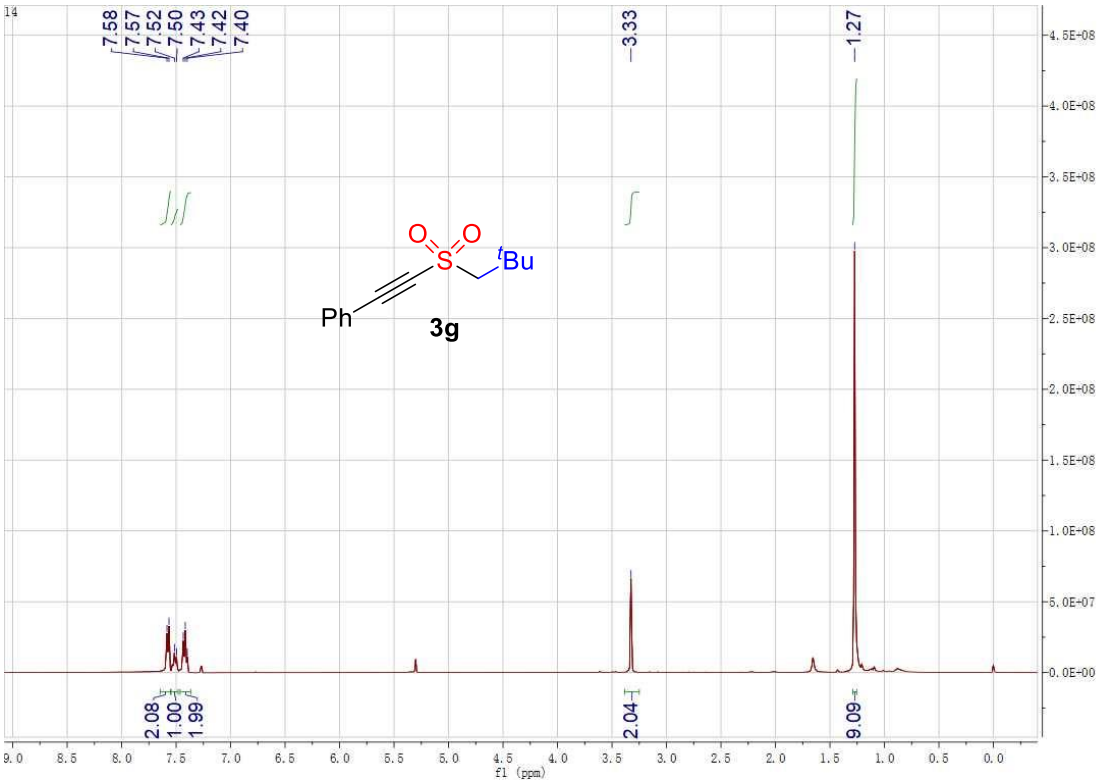

132.7
131.5
128.7
117.7
93.0
81.7
63.4
22.6
12.7
11.0
O
O
S
Ph
3d
f1 (ppm)

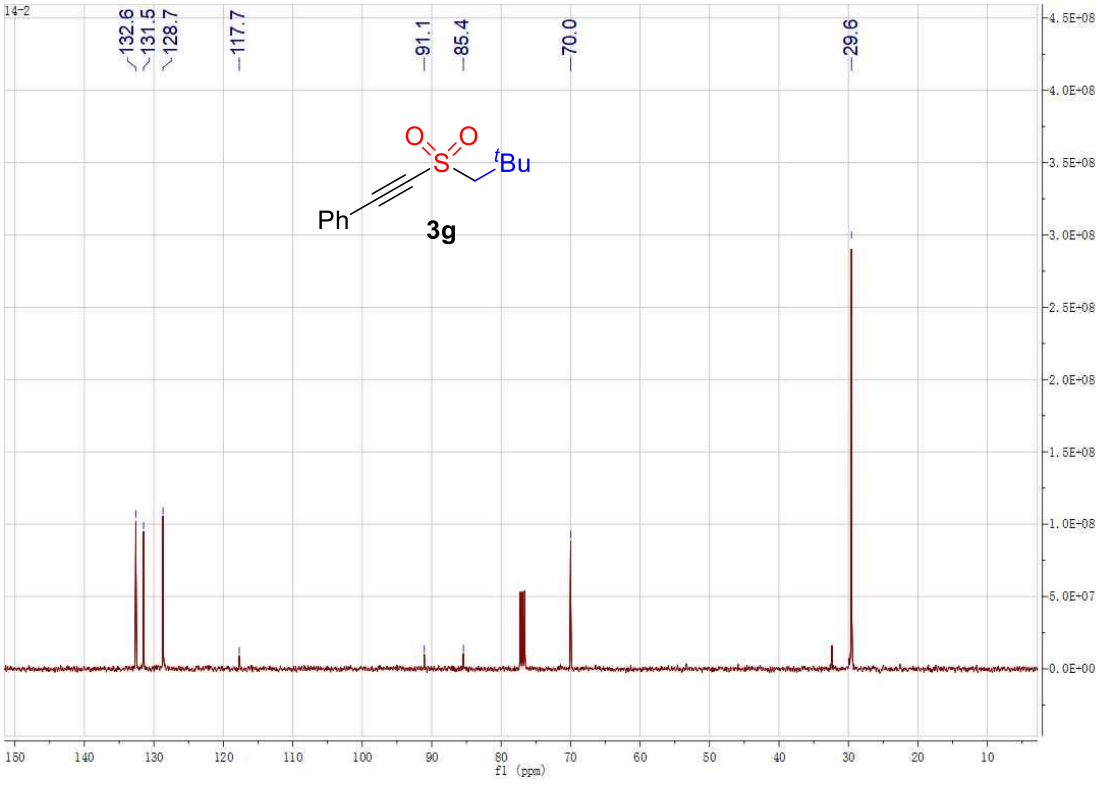

7.61
7.59
7.52
7.50
7.44
7.42
7.41
1.53
2.05
1.00
2.04
9.24
Ph
3e
f1 (ppm)

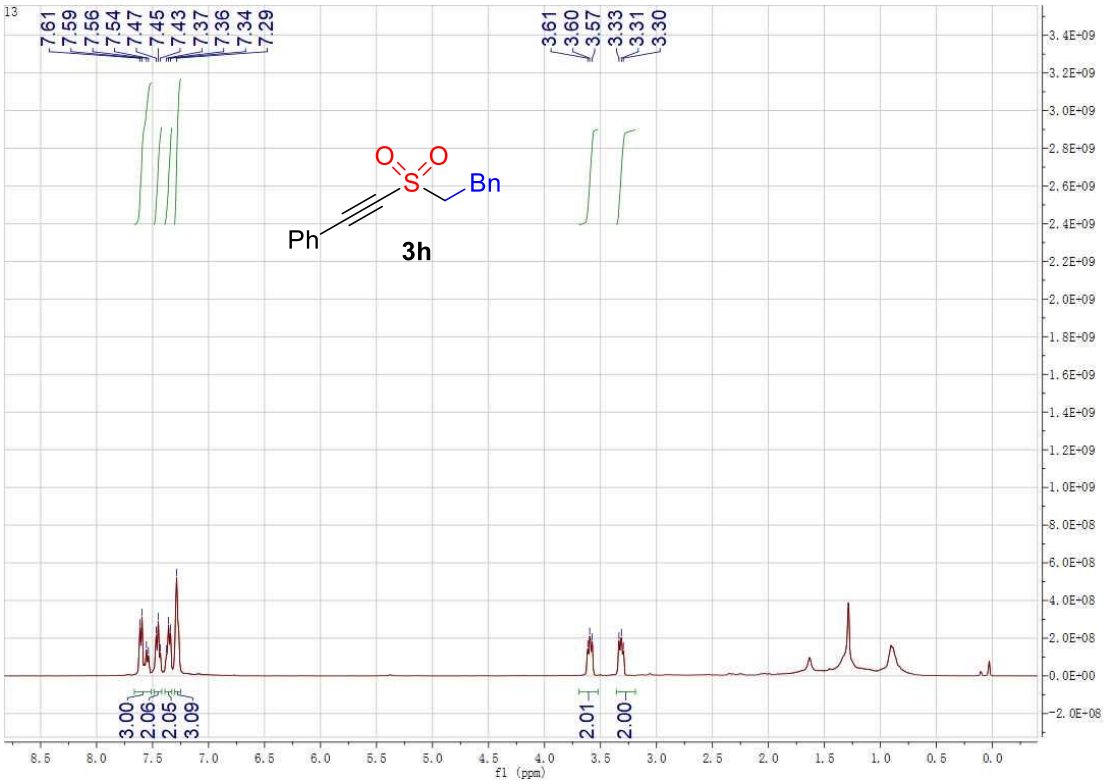

132.7
131.5
128.7
117.8
93.7
80.4
60.9
22.9
Ph
3e
f1 (ppm)

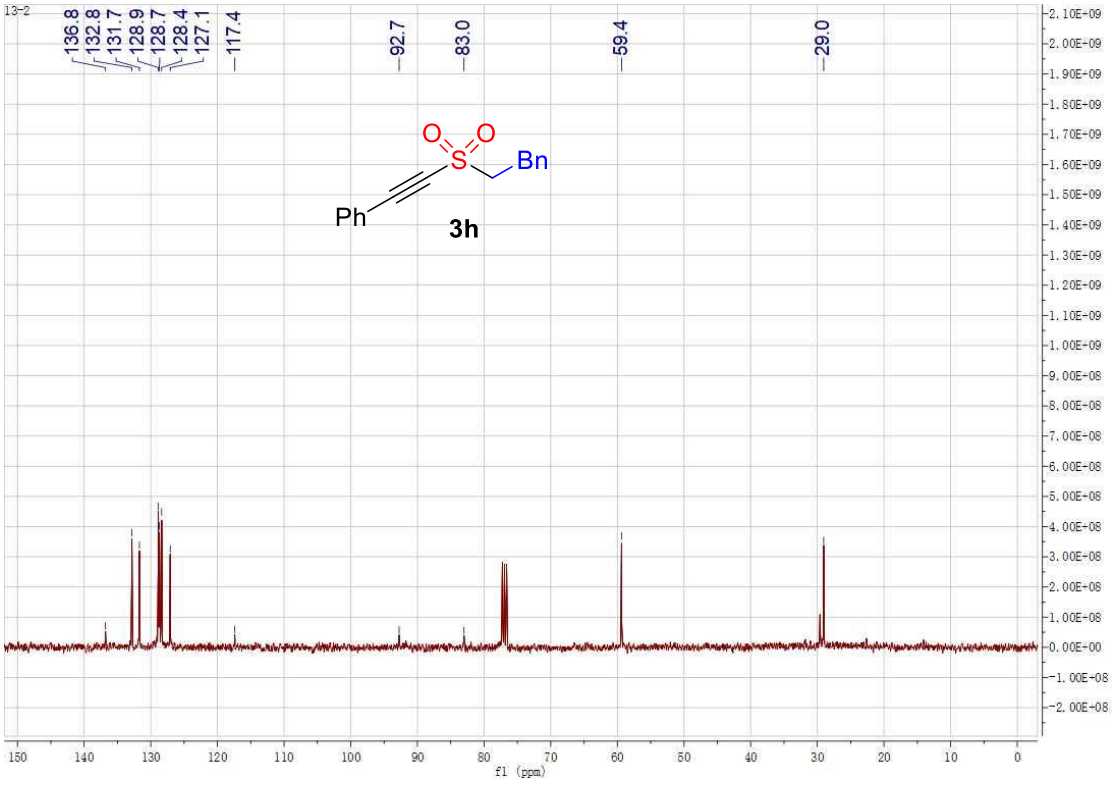

7.61
7.59
7.54
7.53
7.51
7.44
7.43
7.41
3.29
3.27
3.27
3.25
2.06
2.04
2.02
2.00
1.16
1.15
1.14
1.13
Ph
3f
1.97
1.03
2.09
2.00
2.06
3.05
f1 (ppm)

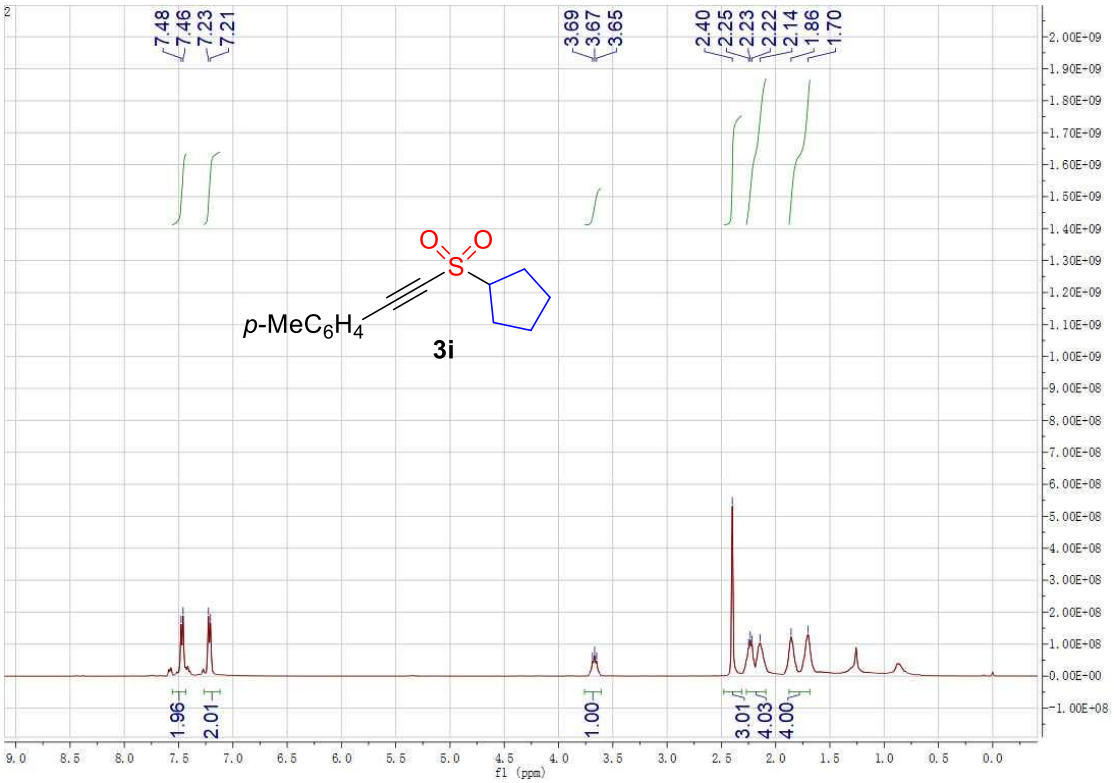

132.8
131.6
128.7
117.6
92.2
83.2
59.9
16.7
12.7
Ph
3f
f1 (ppm)

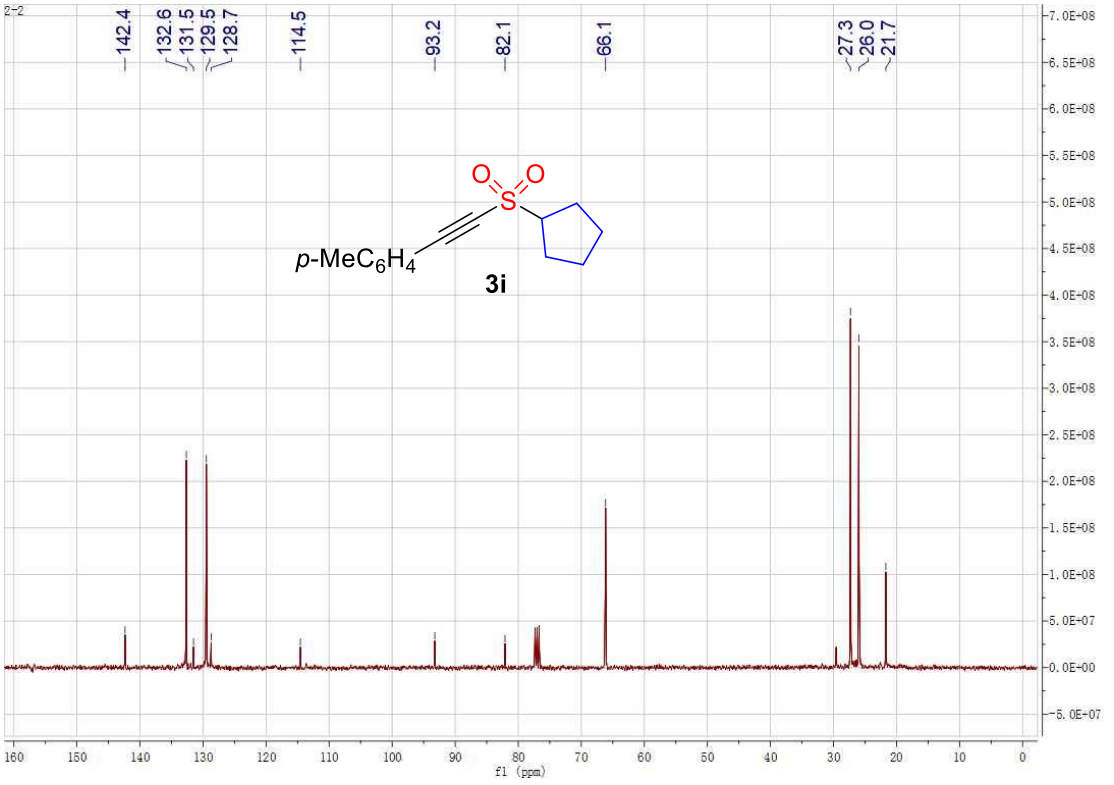

14
7.58
7.57
7.52
7.50
7.43
7.42
7.40
3.33
1.27
O
O
S
tBu
Ph
3g
2.08
1.00
1.99
2.04
9.09
f1 (ppm)

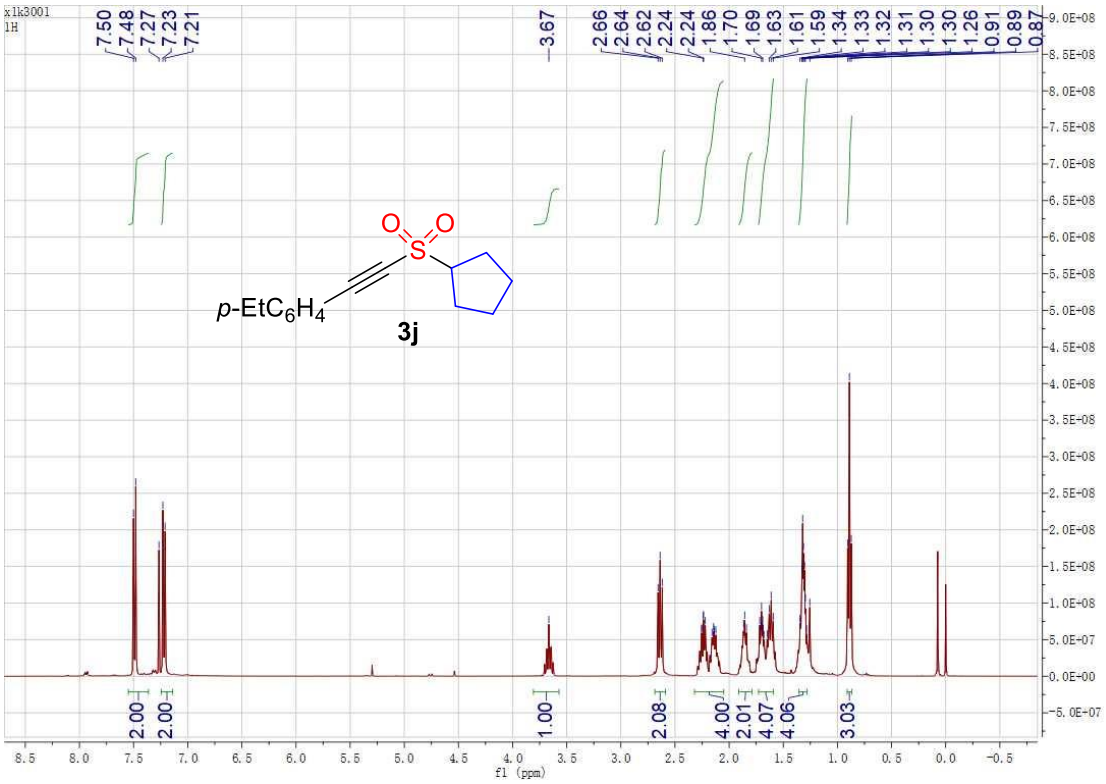

14-2
132.6
131.5
128.7
117.7
91.1
85.4
70.0
29.6
O
O
S
tBu
Ph
3g
f1 (ppm)

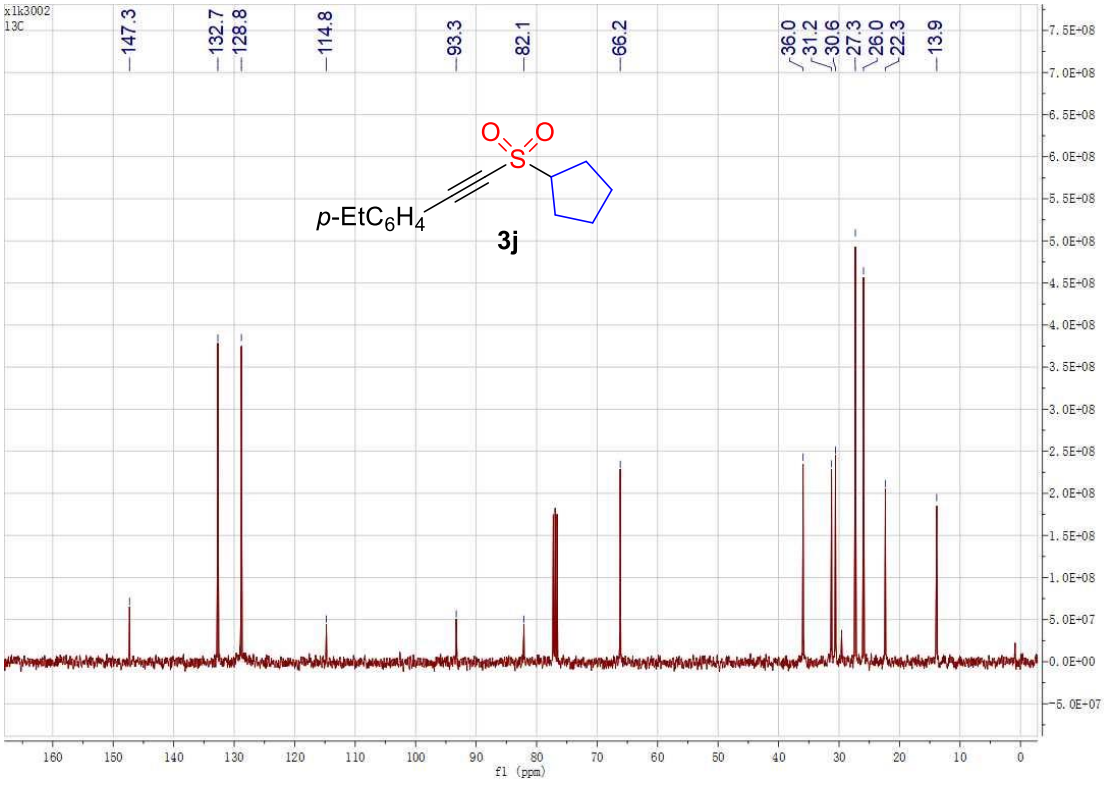

13
7.61
7.59
7.56
7.54
7.47
7.45
7.43
7.37
7.36
7.34
7.29
3.61
3.60
3.57
3.33
3.31
3.30
O
O
S
Bn
Ph
3h
3.00
2.06
2.05
3.09
2.01
2.00
f1 (ppm)

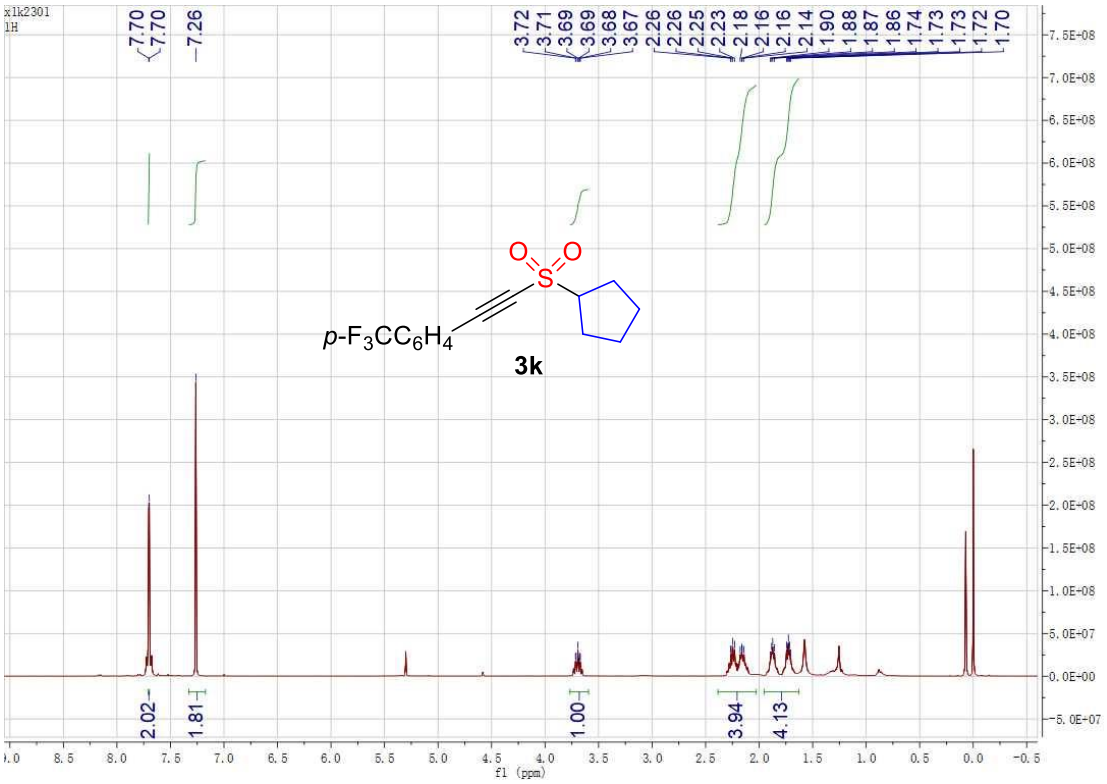

13-2
136.8
132.8
131.7
128.9
128.7
128.4
127.1
117.4
92.7
83.0
59.4
29.0
O
O
S
Bn
Ph
3h
f1 (ppm)

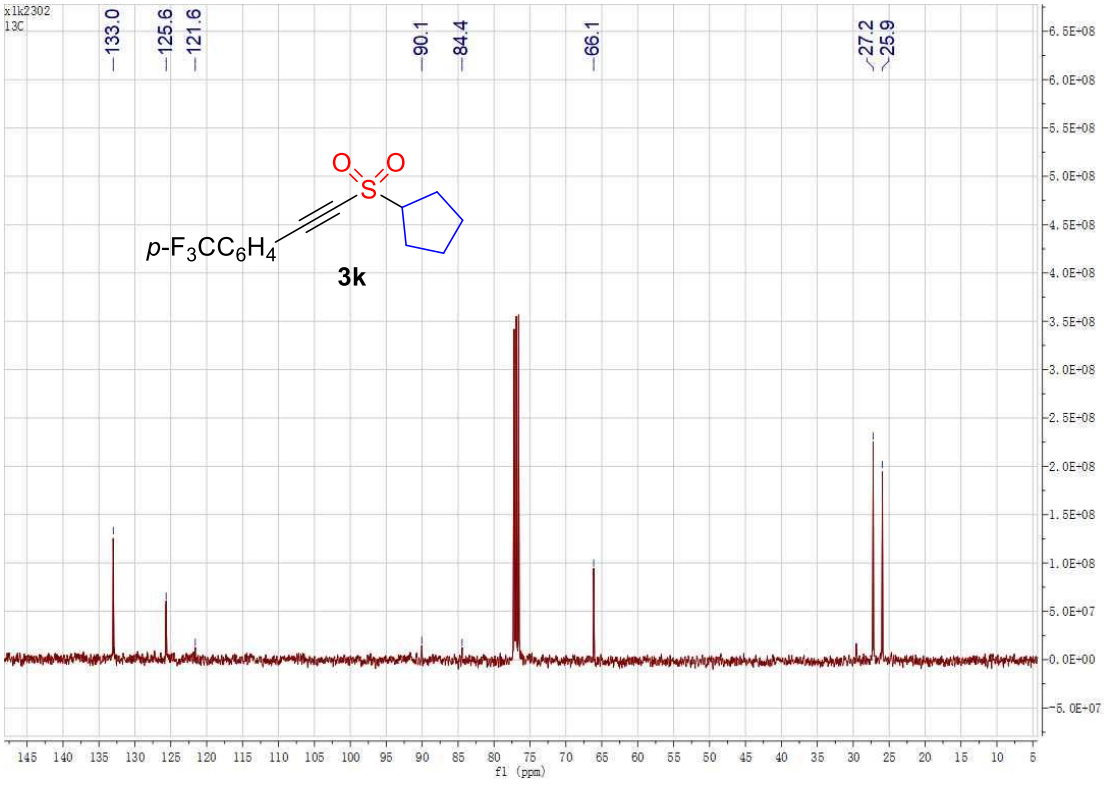

7.48
7.46
7.23
7.21
3.69
3.67
3.65
2.40
2.25
2.23
2.22
2.14
1.86
1.70
O
O
S
p-MeC6H4
3i
1.96
2.01
1.00
3.01
4.03
4.00
f1 (ppm)

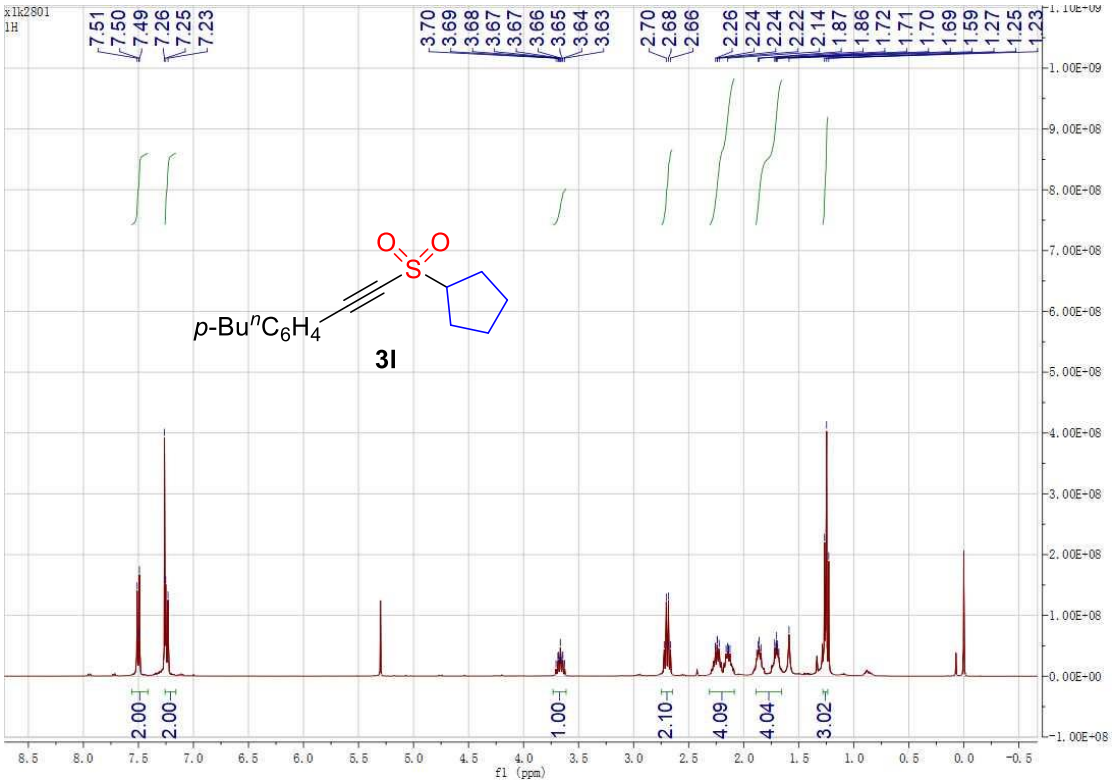

142.4
132.6
131.5
129.5
128.7
114.5
93.2
82.1
66.1
27.3
26.0
21.7
O
O
S
p-MeC6H4
3i
f1 (ppm)

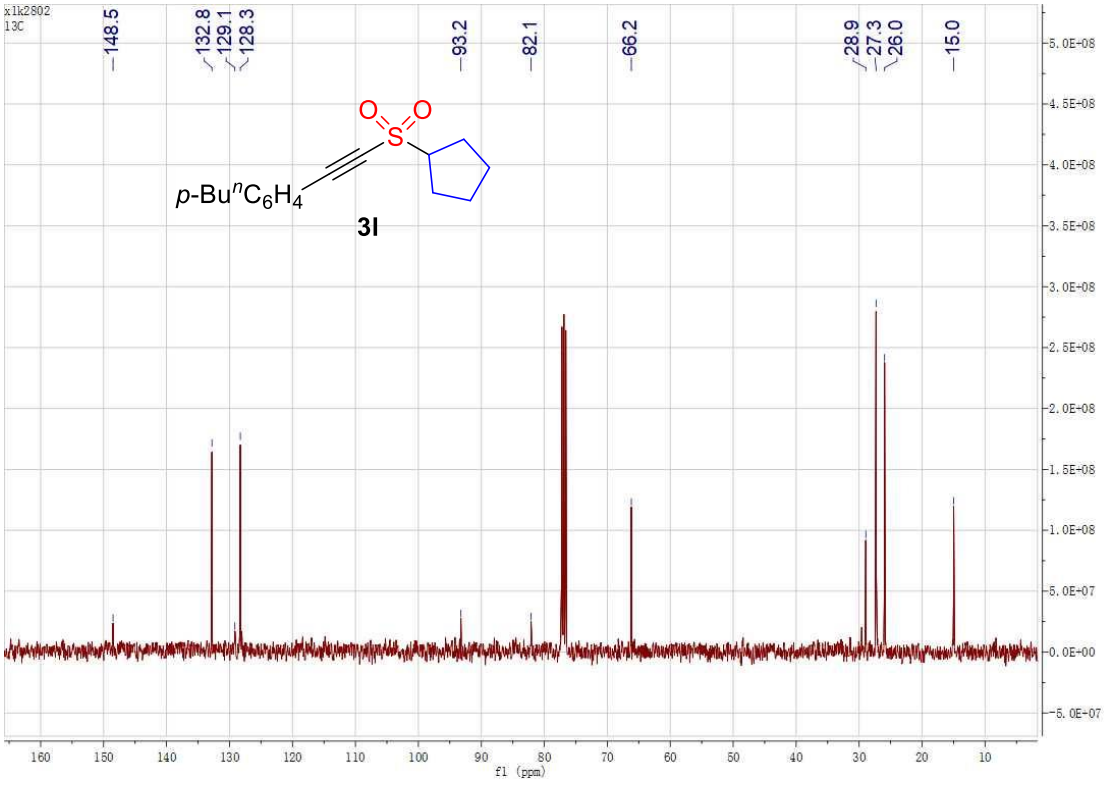

x1k3001
1H
7.50
7.48
7.27
7.23
7.21
3.67
2.66
2.64
2.62
2.24
2.24
1.86
1.70
1.69
1.63
1.61
1.59
1.34
1.33
1.32
1.31
1.30
1.26
0.91
0.89
0.87
2.00
2.00
1.00
2.08
4.00
2.01
4.07
4.06
3.03
f1 (ppm)
p-EtC6H4
3j

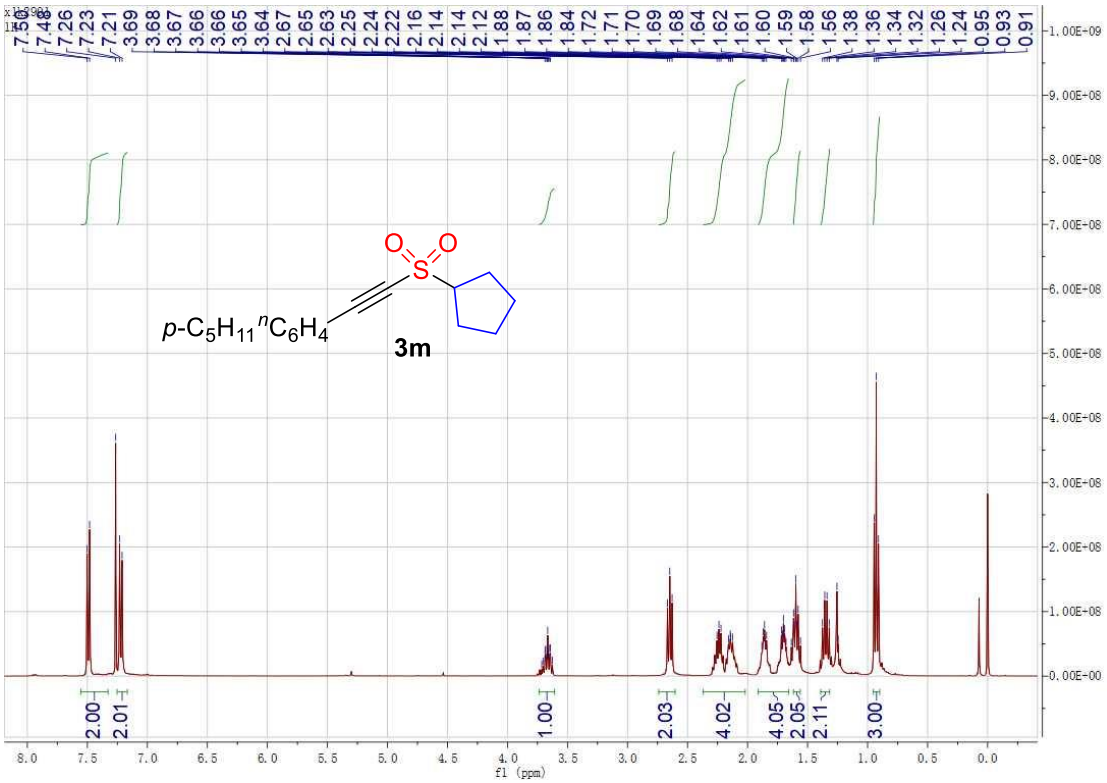

x1k3002
13C
147.3
132.7
128.8
114.8
93.3
82.1
66.2
36.0
31.2
30.6
27.3
26.0
22.3
13.9
f1 (ppm)
p-EtC6H4
3j

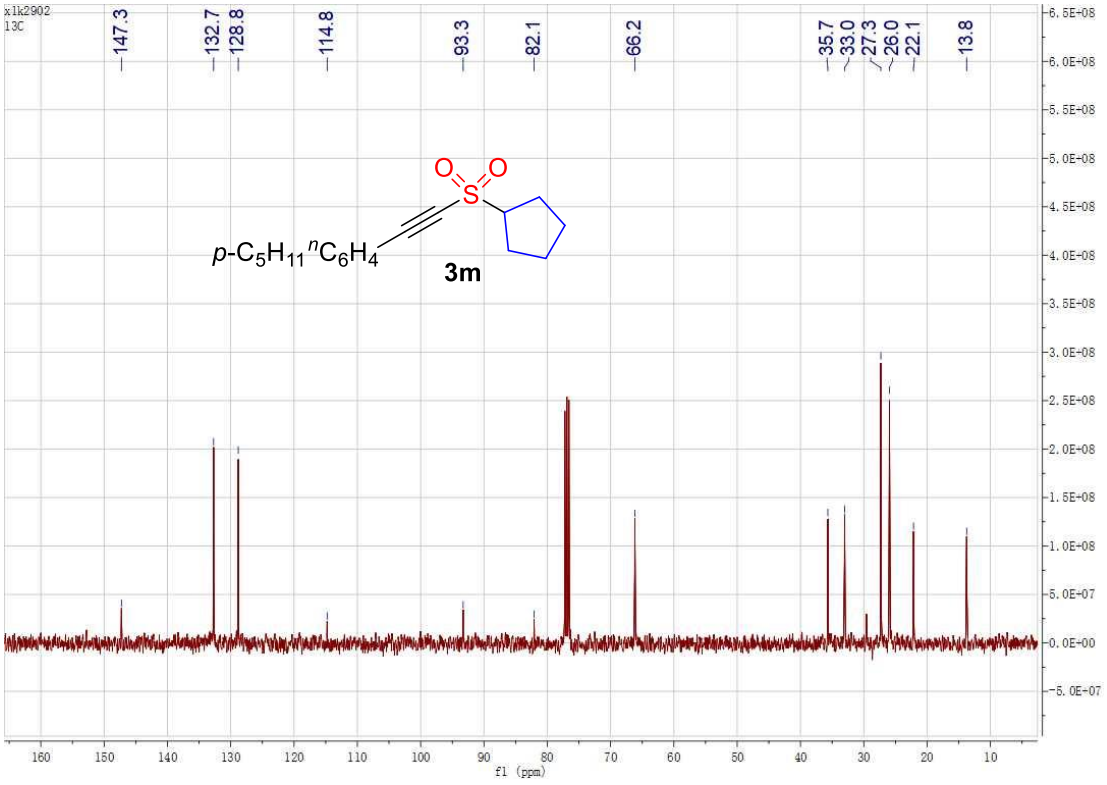

x1k2301
1H
7.70
7.70
7.26
3.72
3.71
3.69
3.69
3.68
3.67
2.26
2.26
2.25
2.23
2.18
2.16
2.16
2.14
1.90
1.88
1.87
1.86
1.74
1.73
1.73
1.72
1.70
O
O
S
p-F3CC6H4
3k
2.02
1.81
1.00
3.94
4.13
f1 (ppm)

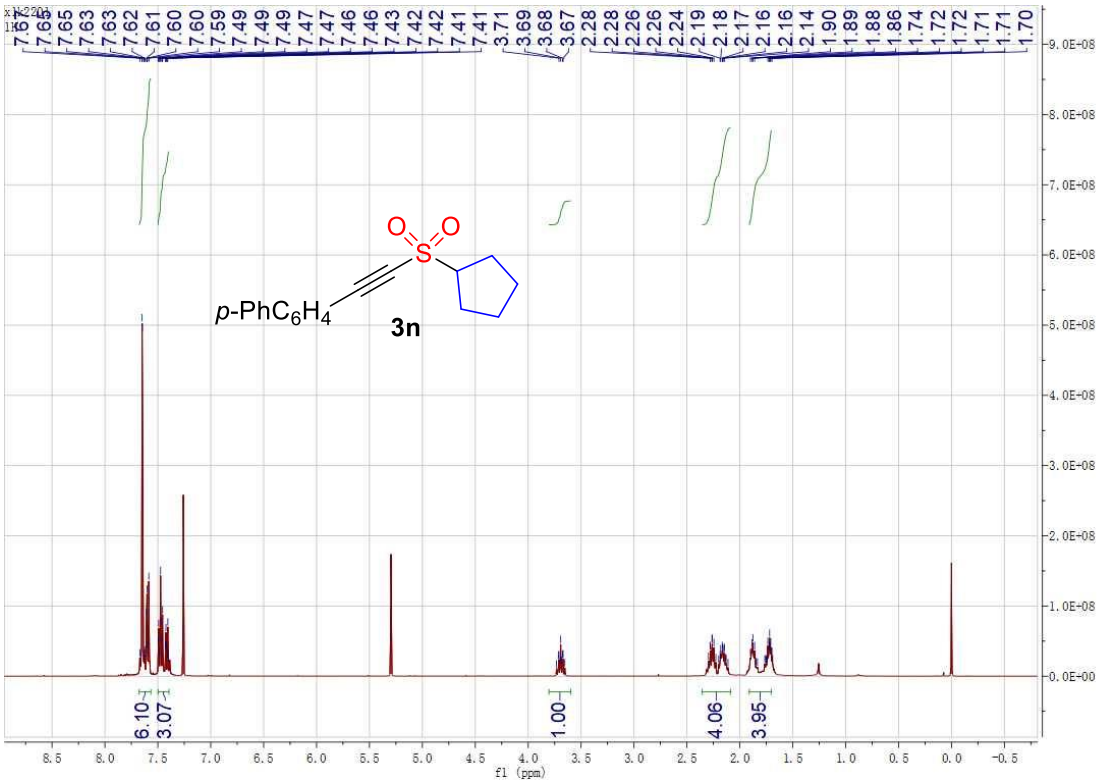

x1k2302
13C
133.0
125.6
121.6
90.1
84.4
66.1
27.2
25.9
O
O
S
p-F3CC6H4
3k
f1 (ppm)

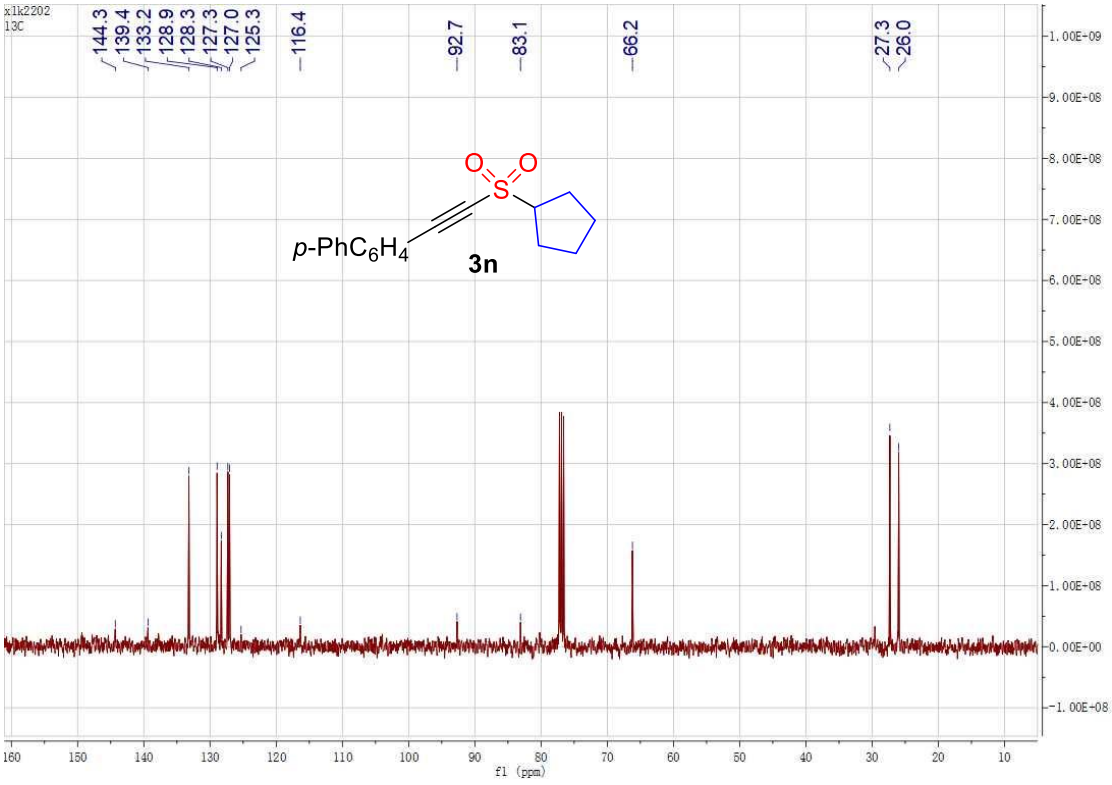

7.51
7.50
7.49
7.26
7.25
7.23
3.70
3.69
3.68
3.67
3.67
3.66
3.65
3.64
3.63
2.70
2.68
2.66
2.26
2.24
2.24
2.22
2.14
1.87
1.86
1.72
1.71
1.70
1.69
1.59
1.27
1.25
1.23
2.00
2.00
1.00
2.10
4.09
4.04
3.02
f1 (ppm)
p-Bu^{n}C$_6$H$_4$
3l

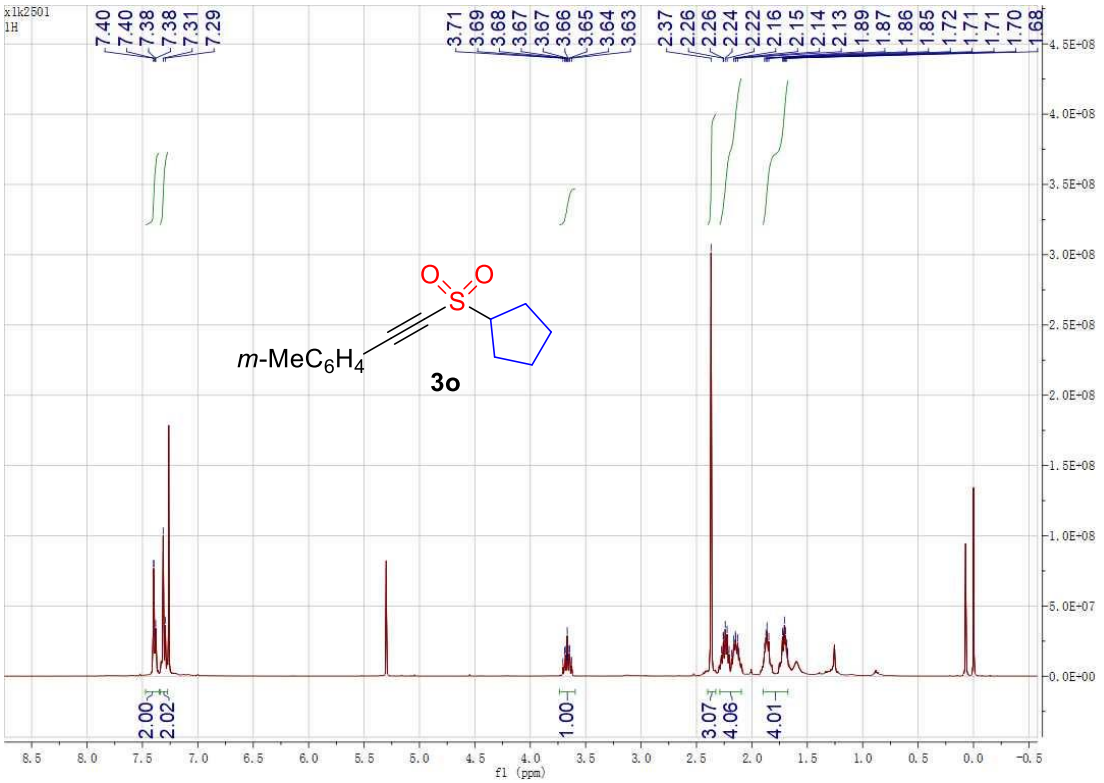

148.5
132.8
129.1
128.3
93.2
82.1
66.2
28.9
27.3
26.0
15.0
f1 (ppm)
p-Bu^{n}C$_6$H$_4$
3l

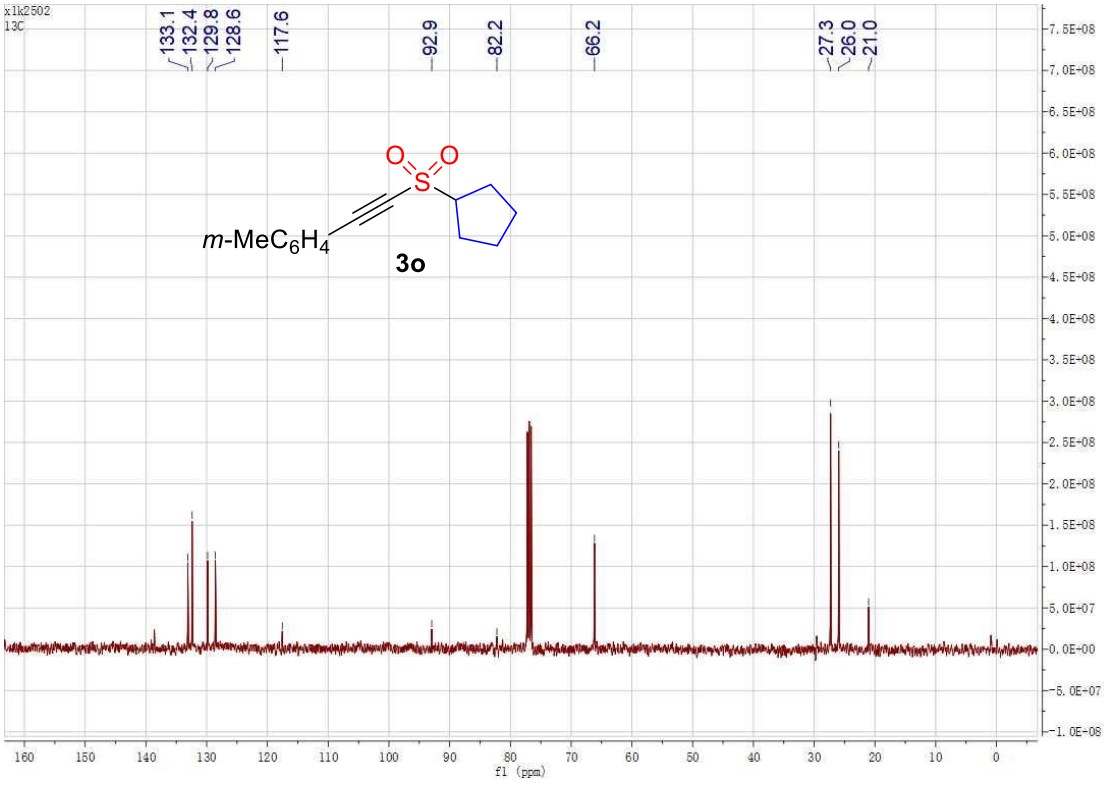

7.50
7.48
7.26
7.23
7.21
3.69
3.68
3.67
3.66
3.66
3.65
3.64
2.67
2.65
2.63
2.25
2.24
2.22
2.16
2.14
2.14
2.12
1.88
1.87
1.86
1.84
1.72
1.71
1.70
1.69
1.68
1.64
1.62
1.61
1.60
1.59
1.58
1.56
1.38
1.36
1.34
1.32
1.26
1.24
0.95
0.93
0.91
O
S
O
p-C5H11nC6H4
3m
2.00
2.01
1.00
2.03
4.02
4.05
2.05
2.11
3.00
f1 (ppm)

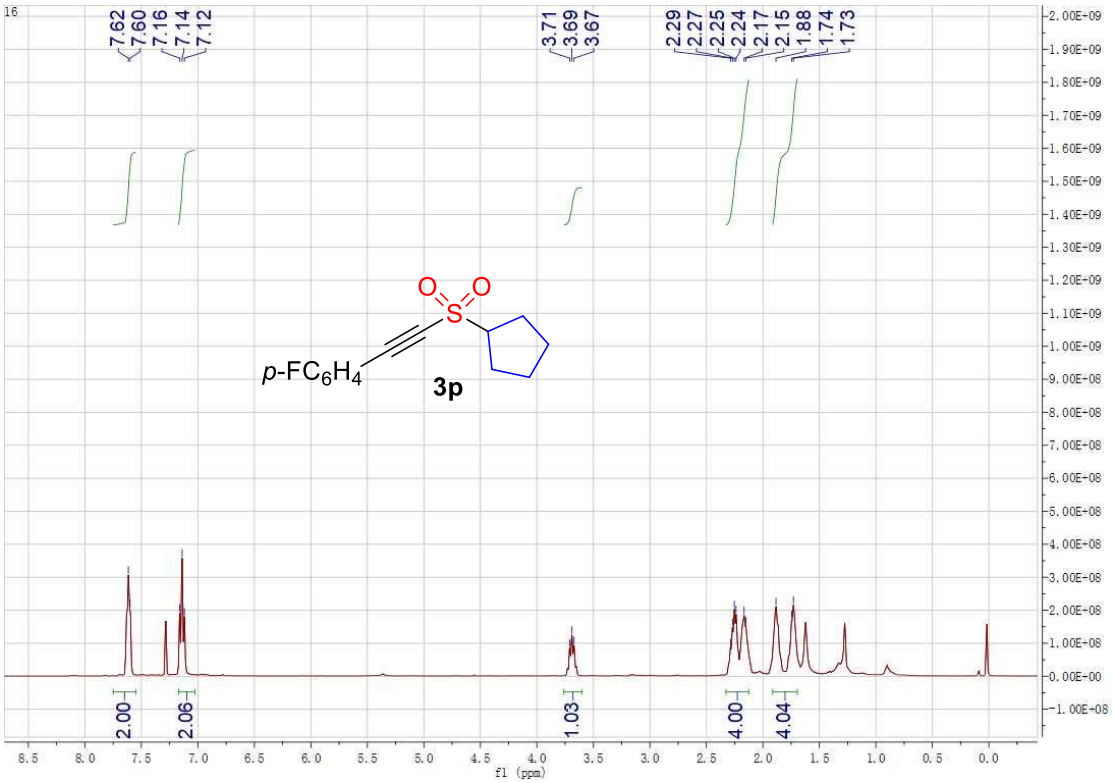

x1k2902
13C
147.3
132.7
128.8
114.8
93.3
82.1
66.2
35.7
33.0
27.3
26.0
22.1
13.8
O
S
O
p-C5H11nC6H4
3m
f1 (ppm)

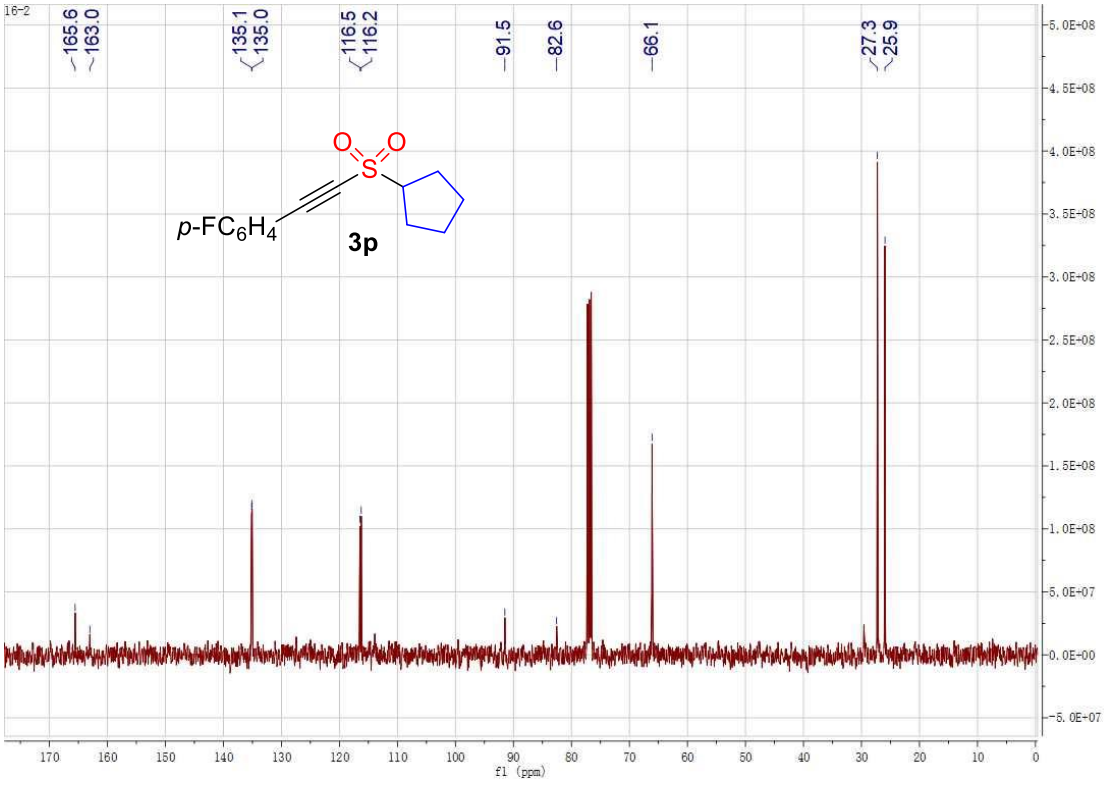

7.67 7.65 7.63 7.63 7.62 7.61 7.60 7.60 7.59 7.49 7.49 7.49 7.47 7.47 7.46 7.46 7.43 7.42 7.42 7.41 7.41 3.71 3.69 3.68 3.67 2.28 2.28 2.26 2.26 2.24 2.19 2.18 2.17 2.16 2.15 2.14 1.90 1.89 1.88 1.86 1.74 1.72 1.72 1.71 1.71 1.70
p-PhC6H4
3n
6.10
3.07
1.00
4.06
3.95
f1 (ppm)

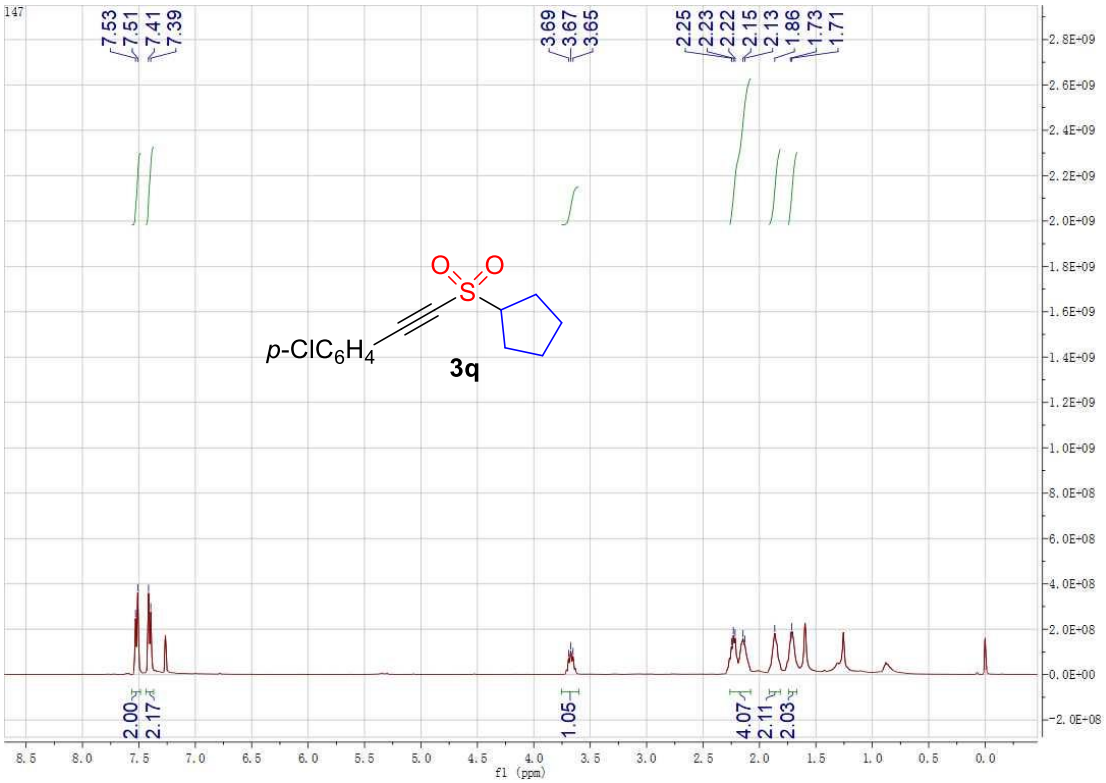

144.3 139.4 133.2 128.9 128.3 127.3 127.0 125.3 116.4 92.7 83.1 66.2 27.3 26.0
p-PhC6H4
3n
f1 (ppm)

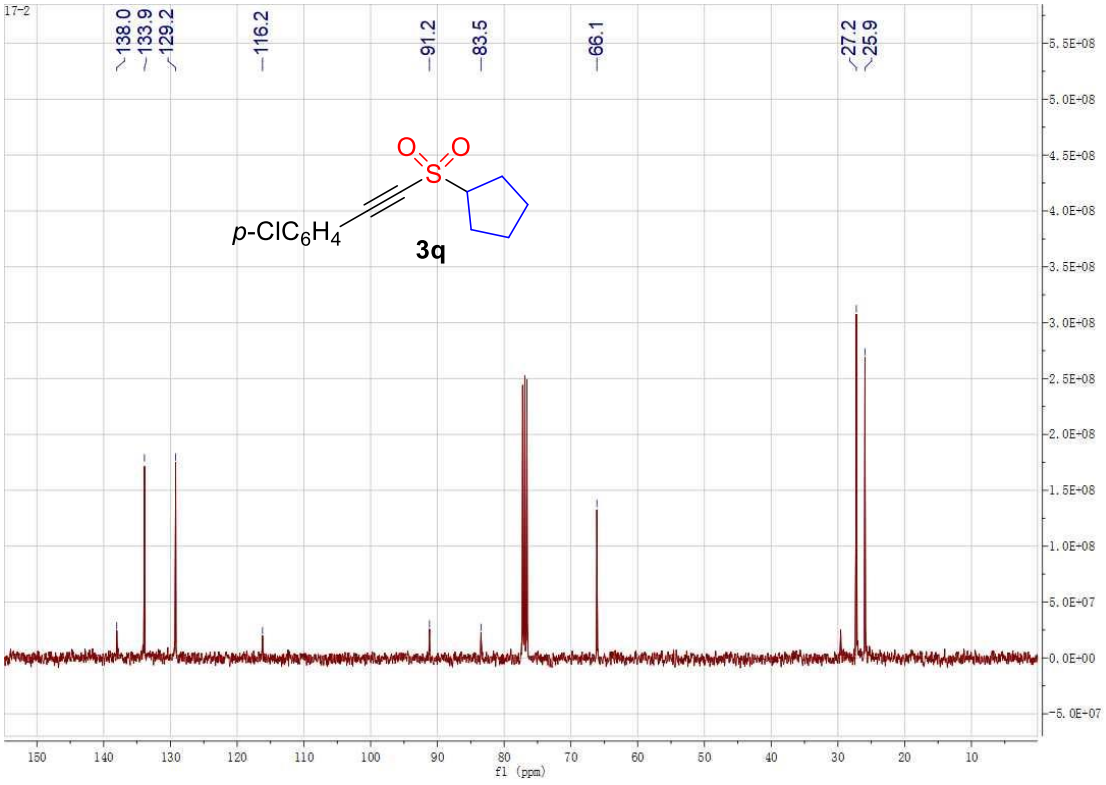

x1k2501
1H
7.40
7.40
7.38
7.38
7.31
7.29
3.71
3.69
3.68
3.67
3.67
3.66
3.65
3.64
3.63
2.37
2.26
2.26
2.24
2.22
2.16
2.15
2.14
2.13
1.89
1.87
1.86
1.85
1.72
1.71
1.71
1.70
1.68
m-MeC6H4
3o
2.00
2.02
1.00
3.07
4.06
4.01
f1 (ppm)

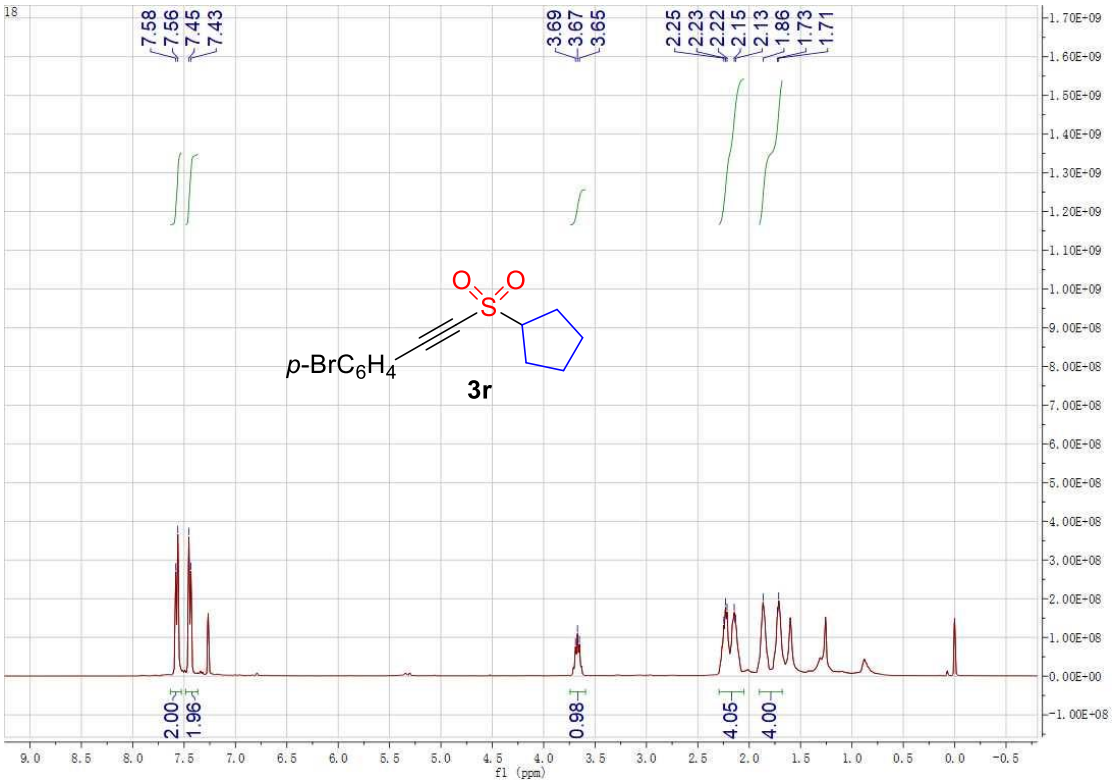

x1k2502
13C
133.1
132.4
129.8
128.6
117.6
92.9
82.2
66.2
27.3
26.0
21.0
m-MeC6H4
3o
f1 (ppm)

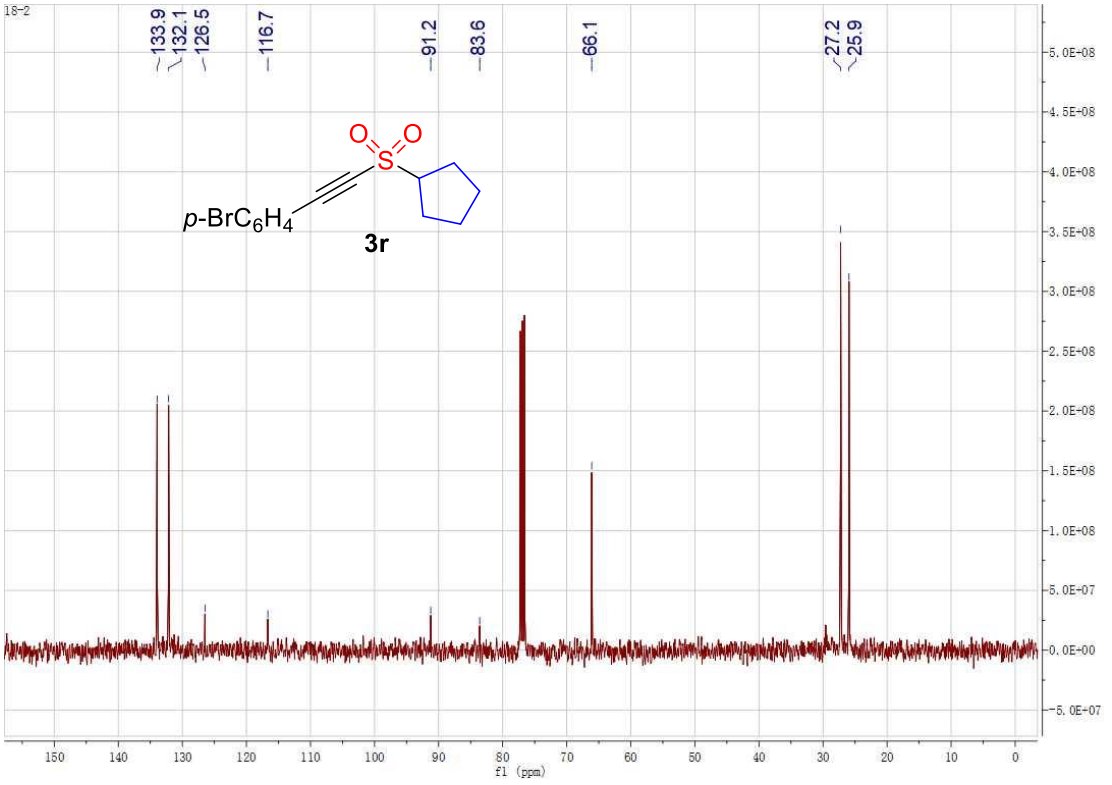

16
7.62
7.60
7.16
7.14
7.12
3.71
3.69
3.67
2.29
2.27
2.25
2.24
2.17
2.15
1.88
1.74
1.73
p-FC6H4
3p
2.00
2.06
1.03
4.00
4.04
f1 (ppm)


16-2
165.6
163.0
135.1
135.0
116.5
116.2
91.5
82.6
66.1
27.3
25.9
p-FC6H4
3p
f1 (ppm)


147
7.53
7.51
7.41
7.39
3.69
3.67
3.65
2.25
2.23
2.22
2.15
2.13
1.86
1.73
1.71
O
O
S
p-ClC6H4
3q
2.00
2.17
1.05
4.07
2.11
2.03
f1 (ppm)


17-2
138.0
133.9
129.2
116.2
91.2
83.5
66.1
27.2
25.9
O
O
S
p-ClC6H4
3q
f1 (ppm)


18
7.58
7.56
7.45
7.43
3.69
3.67
3.65
2.25
2.23
2.22
2.15
2.13
1.86
1.73
1.71
p-BrC6H4
3r
2.00
1.96
0.98
4.05
4.00
f1 (ppm)


18-2
133.9
132.1
126.5
116.7
91.2
83.6
66.1
27.2
25.9
p-BrC6H4
3r
f1 (ppm)