Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

CuI Assited Desulfurative Sonogashira Reaction of Mercapto N-heterocyclic derivatives with Alkynes

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Experimental:

^{1}H and ^{13}CNMR spectra were recorded in $CDCl_3$ on a Bruker AV-400 spectrometer. Chemical shifts for ^{1}H NMR spectra are reported in ppm relative to residual $CDCl_3$ as internal reference (δ 7.26 ppm for ^{1}H) downfield from TMS, chemical shifts for ^{13}C NMR spectra are reported in ppm relative to internal $CDCl_3$ (δ 77.16 ppm for ^{13}C). Coupling constants (J) are given in Hertz (Hz). The terms m, s, d, t, q refer to multiplet, singlet, doublet, triplet, quartlet respectively; br refers to a broad signal.Reagents and solvents used were mostly AR grade. Silica gel coated plates were used for TLC.

Experimental procedure:

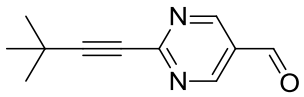
Thioamides (1 mmol), alkynes (2 mmol), $Pd(OAc)_2$ (2%), PPh_3 (10%),CuI (3mmol) and Na_2CO_3 (5mmol) was added in DMF (4 ml) under N_2 atmosphere, the resulting mixture was stirred at 110 ℃ for 1h. After cooling to r.t., the reaction was quenched with saturated aq NH_4Cl (5 mL). The suspension was diluted with EtOAc(25 mL) and filtered through celite with EtOAc (50 mL). The filtrate was washed with 2MNaOH (1 mL) andbrine(2 × 20ml). After drying over $MgSO_4$,the mixture was concentrated in vacuo and the residue was purified by column chromatography on silica gel to afford pure product.

Computational method:

All the DFT calculations were carried out with the Gaussian 09 series of programs.[1] Geometry optimizations and frequency calculations were performed with the B3LYP method with BSI (the LANL2DZ basis set and corresponding effective core potentials (ECPs)for elements with atomic number higher than 36,and the 6-31G(d) basis set for other atoms). All the TS stationary points were correctly connected to the corresponding species. Vibrational frequency calculations also provide thermal corrections for enthalpies and Gibbs free energies (at 298.15 K and 1 atm).

Characterization data:

2-(3,3-Dimethylbut-1-yn-1-yl)pyrimidne-5-carbaldehyde(3a)[2]:

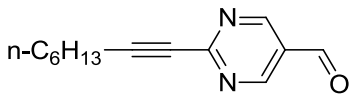


Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave 160 mg (85%) of colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (s, 9H), 9.12 (s, 2H), 10.13 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 28.30, 30.34, 79.12, 103.22, 126.38, 156.51, 158.36, 188.39.

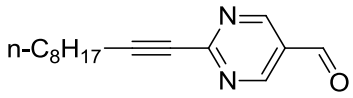
2-(Oct-1-yn-1-yl)pyrimidne-5-carbaldehyde(3b):



Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave 158 mg (73%) of pale yellow solid.

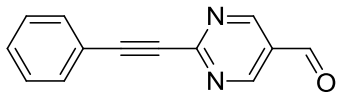
^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, *J* = 7.2 Hz; 3 H), 1.25 – 1.32 (m, 4 H), 1.41 – 1.49 (m, 2 H), 1.67 (p, J = 7.6 Hz; 2 H), 2.50 (t, J = 7.6 Hz; 2 H), 9.08 (s, 2H), 10.09 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 14.15, 19.65, 22.59, 27.96, 28.79, 31.39, 80.40, 96.26, 126.44, 156.41, 158.39 , 188.38.

2-(Oct-1-yn-1-yl)pyrimidine-5-carbaldehyde(3c):



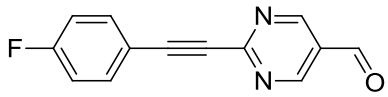
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave 159 mg (65%) of pale yellow solid.
^{1}H NMR (400 MHz, CDCl3): δ 0.83 (t, J = 7.0 Hz; 3 H), 1.20 – 1.31 (m, 4 H), 1.40 – 1.51 (m, 2 H), 1.62 (p, J = 7.1 Hz; 2 H), 2.49 (t, J = 7.2 Hz; 2 H), 9.04 (s, 2 H), 10.05 (s, 1 H).
13C NMR (100 MHz, CDCl3): δ 1.0, 14.13, 19.64, 22.63, 27.94, 29.02, 29.05, 29.1, 31.85, 80.38, 96.24, 126.41, 156.38, 158.36, 188.35.

2-(Phenylethynyl)pyrimidne-5-carbaldehyde(3d):



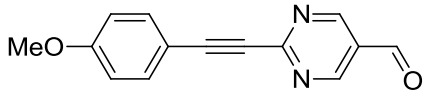
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave146 mg (70%) of yellow solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 – 7.45 (m, 3 H), 7.71 (d, *J* = 8.0 Hz, 2H), 9.18 (s, 2 H), 10.15 (s, 1 H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 88.26, 92.66, 120.72, 126.4, 128.74, 130.62, 133.08, 156.45, 158.46, 188.31

2-((4-Fluorophenyl)ethynyl)pyrimidne-5-carbaldehyde(3e)



Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave113 mg (50%) of yellow solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.08 – 7.16 (m, 2 H), 7.65–7.71 (m, 2 H), 9.16 (s, 2 H), 10.14 (s, 1 H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 88.05, 91.41, 116.10, 116.35, 116.81, 116.85, 126.37, 135.18, 135.28, 156.26, 158.36, 162.05, 165.24, 188.12.

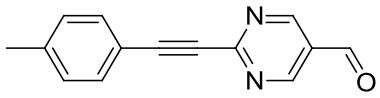
2-((4-Methoxyphenyl)ethynyl)pyrimidne-5-carbaldehyde(3f)



Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave 136 mg (57%) of yellow solid.

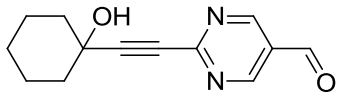
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.85 (s, 3 H), 6.93 (d, *J* = 10.8 Hz; 2 H), 7.64 (d, *J* = 10.8 Hz; 2 H), 9.14 (s, 2 H), 10.12 (s, 1 H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 55.44, 87.96, 93.80, 112.59, 114.48, 126.11, 135.0, 156.64, 158.44, 161.58, 188.33.

2-((4-Tolyl)ethynyl)pyrimidine-5-carbaldehyde(3g):



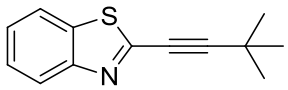
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h.Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave171 mg (77%) of yellow solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 2.40 (s, 3 H), 7.19 (d, *J* = 8.0 Hz; 2 H), 7.58 (d, J = 8.0 Hz; 2 H), 9.13 (s, 2 H), 10.14(s, 1 H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 21.79, 88.10, 93.36, 117.75, 126.32, 129.62, 133.07, 141.20, 156.51, 158.46, 188.33.

2-((1-Hydroxy-1-cyclohexyl)ethynyl)pyrimidine-5-carbaldehyde(3i):



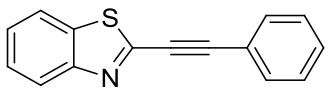
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (CH_2Cl_2/MeOH=100:1-20:1) gave74 mg (32%) of orange solid.
^{1}H NMR (400MHz, CDCl3): δ 1.28 – 1.38 (m, 1 H), 1.58 – 1.81 (m, 7 H), 2.05–2.11 (m, 2 H), 3.09 (s, 1 H), 9.15 (s, 2 H), 10.13 (s, 1 H).
^{13}C NMR (100 MHz, CDCl3): δ 22.95, 24.95, 39.27, 68.70, 82.82, 96.88, 126.55, 155.72, 158.20, 188.14.

2-(3,3-Dimethylbut-1-yn-1-yl)benzo[*d*]thiazole(3j):



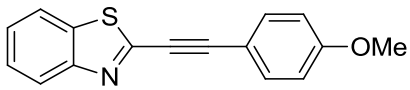
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/EA=20:1) gave166 mg (77%) of colorless solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (s, 9 H), 7.42 – 7.53 (m, 2 H), 7.5 (d, *J* = 8.0 Hz; 1 H), 8.04 (d, *J* = 8.0 Hz; 1 H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 28.48, 30.44, 73.41, 106.13, 121.35, 123.49, 126.0, 126.61, 135.21, 149.52, 152.9.

2-(phenylethynyl)benzo[*d*]thiazole(3k):



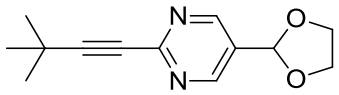
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h.Purification by column chromatography (hexane/EA=20:1) gave188 mg (80%) of yellow solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.47 (m, 4H), 7.51 – 7.55 (m, 1H), 7.63-7.66 (dd, *J*= 7.7, 1.6 Hz, 2H), 7.87 (d, *J*= 8.0 Hz; 1 H), 8.08 (d, *J* = 8.0 Hz; 1H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 82.85, 96.01, 121.14, 121.45, 123.74, 126.32, 126.83, 128.70, 130.06, 132.33, 135.48, 148.76, 153.09.

2-((4-methoxyphenyl)ethynyl)benzo[*d*]thiazole(3l):



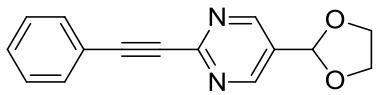
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/EA=20:1) gave233 mg (88%) of yellow solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (s, 3H), 6.95 (d, *J* = 8.0 Hz; 2 H), 7.45 – 7.50 (m, 1 H), 7.55 (t, *J* = 12.0 Hz; 1 H), 7.62 (d, *J* = 12.0 Hz; 2 H), 7.89 (d, *J* = 8.0 Hz; 2 H), 8.09 (d, *J* = 8.0 Hz; 1 H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 55.54, 82.08, 96.66, 114.27, 114.44, 121.43, 123.63, 126.15, 126.78, 134.07, 134.19, 135.44, 149.18, 153.17.

2-(3,3-Dimethylbut-1-yn-1-yl)-5-(1,3-dioxolan-2-yl)pyrimidine(3o)[3]:



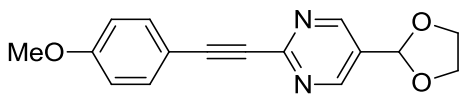
Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave144 mg (62% over 2 steps) of yellow oil.
^{1}H NMR (400 MHz, $CDCl_3$): δ 1.41 (s, 9 H), 4.05 – 4.14 (m, 4 H), 5.89 (s, 1 H), 8.77 (s, 2 H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 27.96, 30.45, 65.49, 78.69, 98.57, 100.26, 129.58, 153.82, 155.95.

5-(1,3-dioxolan-2-yl)-2-(phenylethynyl)pyrimidine(3p):



Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave161 mg (64% over 2 steps) of yellow solid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.97 - 4.09 (m, 4 H), 5.82 (s, 1 H), 7.26 - 7.34 (m, 3 H), 7.59 - 7.61 (d, *J* = 8.0 Hz; 2 H), 8.75 (s, 2 H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 155.96, 153.67, 132.79, 129.90, 128.57, 127.07, 121.32, 100.24, 88.60, 87.98, 65.64.

5-(1,3-dioxolan-2-yl)-2-((4-methoxyphenyl)ethynyl)pyrimidine(3q):

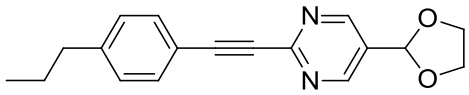


Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h.Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave200 mg (71% over 2 steps) of yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.84 (s, 3H), 4.05 – 4.17 (m, 4 H), 5.90 (s, 1 H), 6.89 – 6.92 (m, 2 H), 7.61 – 7.65 (m, 2 H), 8.81 (s, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 55.49, 65.65, 87.29, 89.28, 100.32, 113.26, 114.29, 114.49, 129.42, 134.55, 135.04, 153.93, 155.96, 158.49, 160.95.

5-(1,3-dioxolan-2-yl)-2-((4-propylphenyl)ethynyl)pyrimidine(3r):

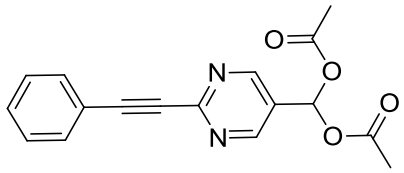


Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave223 mg (76% over 2 steps) of yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.96 (t, *J* = 16.0 Hz; 3 H), 1.64 – 1.69 (dt, *J* = 15.0, 7.5 Hz; 2 H), 2.63 (t, *J* = 12.0 Hz; 2 H), 4.08 – 4.17 (m, 4 H), 5.91 (s, 1 H), 7.21 (d, *J* = 8.0 Hz; 2 H),7.61 (d, *J* = 8.0 Hz; 2 H), 8.83 (s, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 13.90, 24.36, 38.18, 65.64, 87.60, 89.16, 100.28, 118.44, 128.78, 129.60, 132.77, 145.11, 153.82, 155.96.

(2-(phenylethynyl)pyrimidn-5-yl)methylene dicetate(3s)[4]:

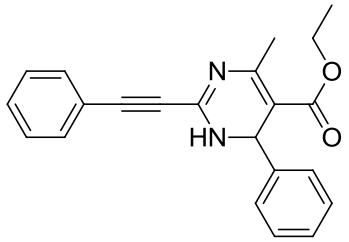


Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave96 mg (31% over 2 steps) of orange solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.18 (s, 6 H), 7.27 (s, 1 H), 7.34 – 7.45 (m, 3 H), 7.68 (d, *J* = 8.0 Hz; 2 H), 8.89 (s, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 20.84, 86.65, 87.80, 89.44, 121.11, 127.62, 128.63, 130.11, 132.86, 154.07, 156.15, 168.60.

Ethyl-4-methyl-6-phenyl-2-(phenylethynyl)-6*H*-1,3-thiazine-5-carboxylate(3t)[5]:

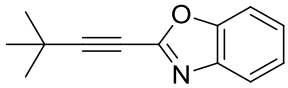


Prepared according to the general procedure with 2.0equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (hexane/CH_2Cl_2=1:3) gave72 mg (21%) of yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.17 (t, *J* = 16.0 Hz; 3H), 1.59 (s, 1 H), 2.41 (s, 3 H), 2.91 (d, *J* = 56.0 Hz; 1 H), 4.05 – 4.11 (m, 2 H), 5.72 (s, 1 H), 7.26 – 7.52 (m, 10 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 14.25, 22.76, 48.3, 59.97, 87.63, 88.26, 120.65, 127.53, 127.53, 128.59, 129.28, 129.96, 132.37, 132.7, 144.69, 151.94, 163.06, 166.71.

2-(3,3-dimethylbut-1-yn-1-yl)benzo[d]oxazole(3u):

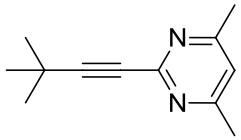


Prepared according to the general procedure with 2.0 equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (CH_2Cl_2) gave 131 mg (82%) of yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.38 (s, 9 H), 7.32 – 7.39 (m, 2 H), 7.47 – 7.50 (dd, *J* = 2.2 Hz; 1 H), 7.69 – 7.71 (m, 1 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 28.27, 30.21, 68.28, 103.69, 110.53, 120.27, 124.9, 126.03, 141.01, 147.99, 150.2.

2-(3,3-dimethylbut-1-yn-1-yl)-4,6-dimethylpyrimidine(3v):

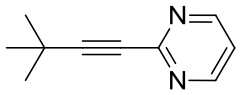


Prepared according to the general procedure with 2.0 equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (CH_2Cl_2) gave 164 mg (87%) of colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.36 (s, 9 H), 2.46 (s, 6 H), 6.92 (s, 1 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 24.05, 27.9, 30.6, 78.9, 96.74, 118.78, 152.83, 167.04.

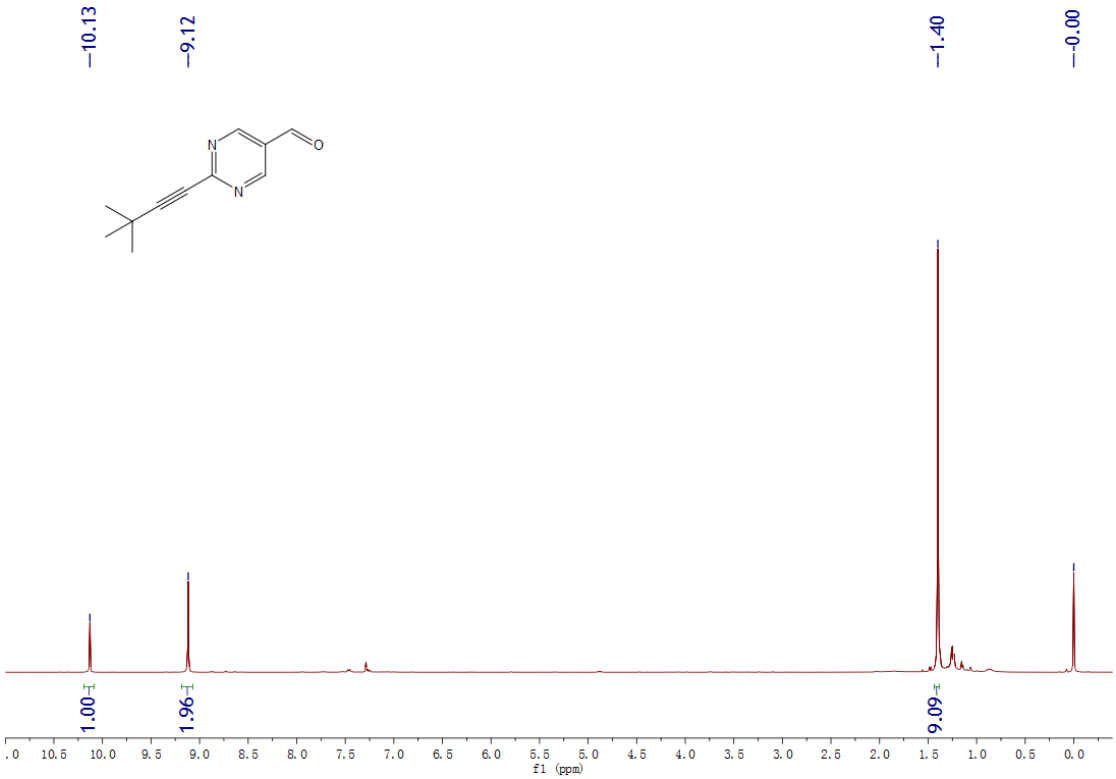
2-(3,3-dimethylbut-1-yn-1-yl)pyrimidine(3w):



Prepared according to the general procedure with 2.0 equiv of the alkyne at 110 °C for 1h. Purification by column chromatography (CH_2Cl_2) gave88 mg (55%) of colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.35 (s, 9 H), 7.17 (t, *J* = 5.8 Hz; 1 H), 8.67 (d, *J* = 5.0 Hz; 2 H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 28.1, 30.69, 78.82, 98.23, 119.52, 153.48, 157.28.


10.13
9.12
1.40
0.00
N
N
O
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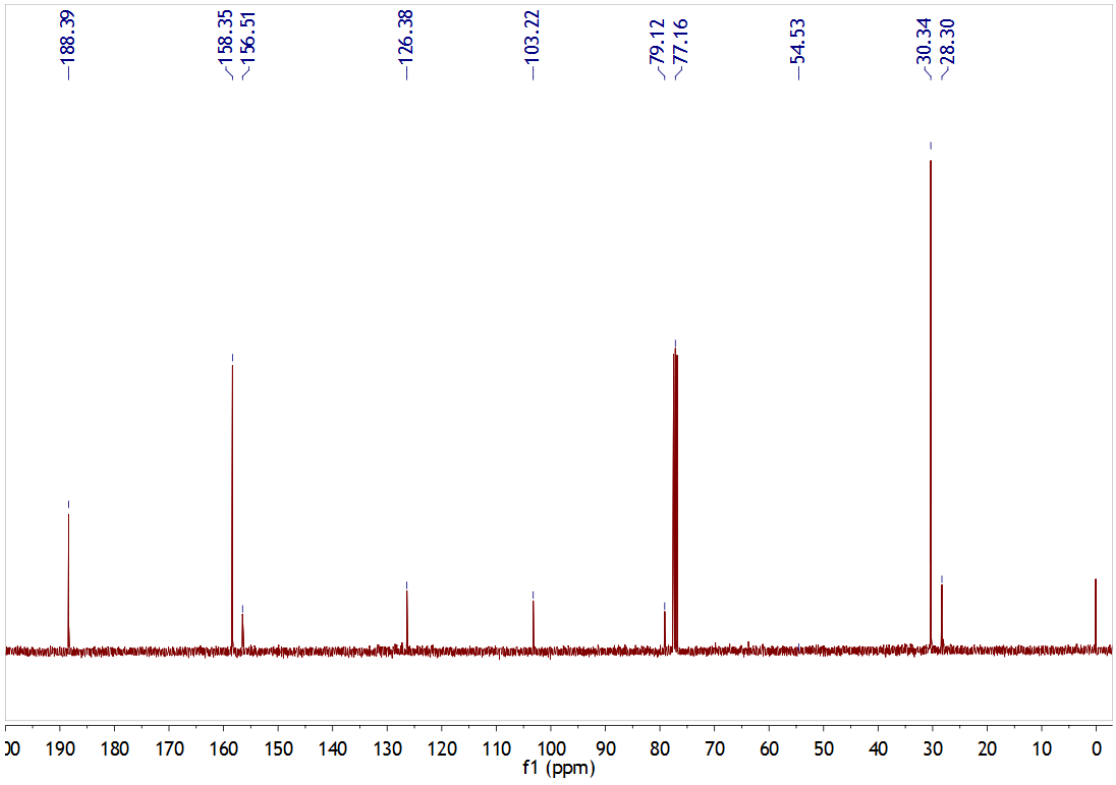
1.96
9.09
f1 (ppm)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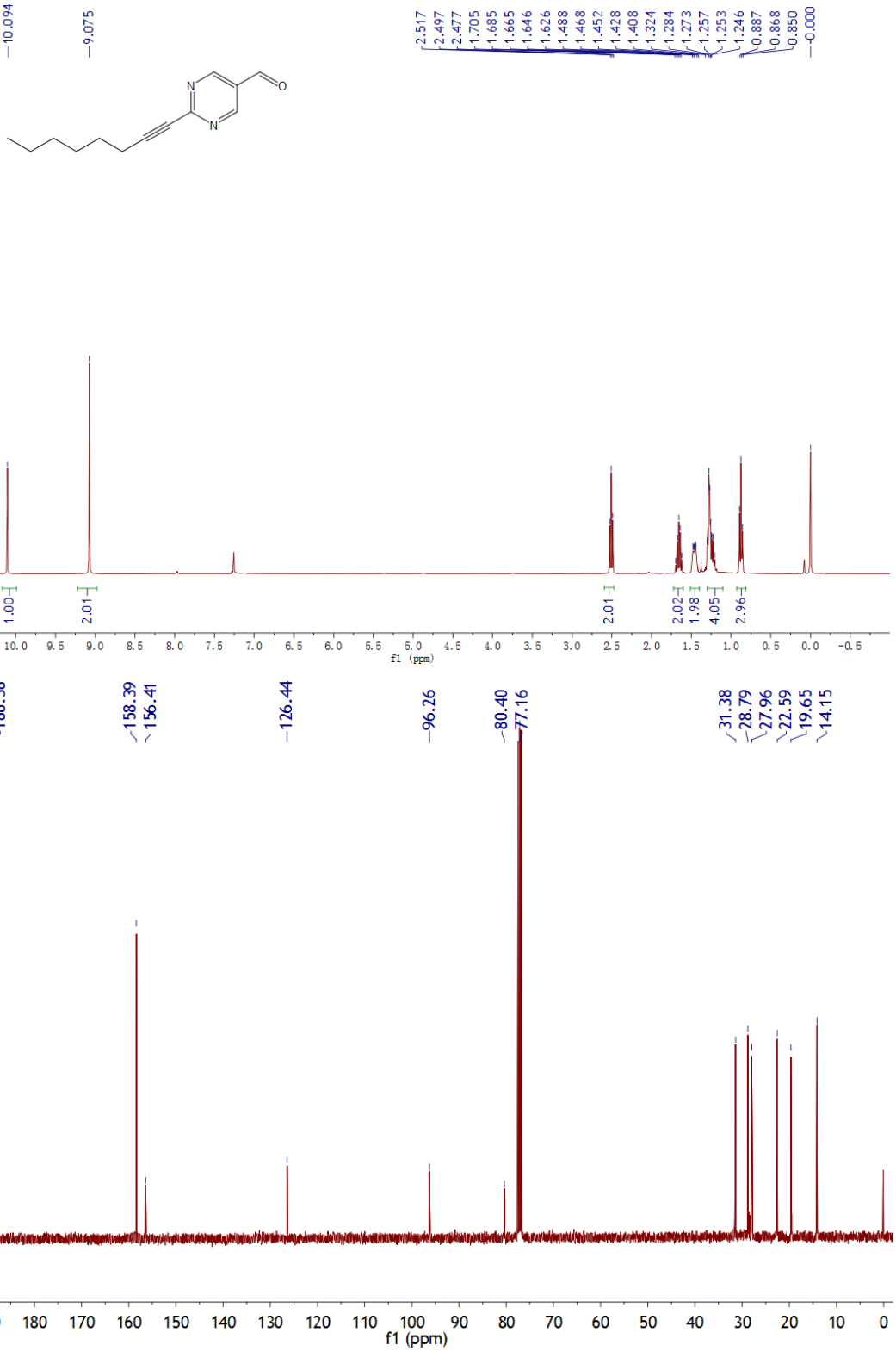
126.38
103.22
79.12
77.16
54.53
30.34
28.30
f1 (ppm)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1.705
1.685
1.665
1.646
1.626
1.488
1.468
1.452
1.428
1.408
1.324
1.284
1.273
1.257
1.253
1.246
0.887
0.868
0.850
0.000
N
N
O
1.00
2.01
2.01
2.02
1.98
4.05
2.96
f1 (ppm)
190.35
188.38
158.39
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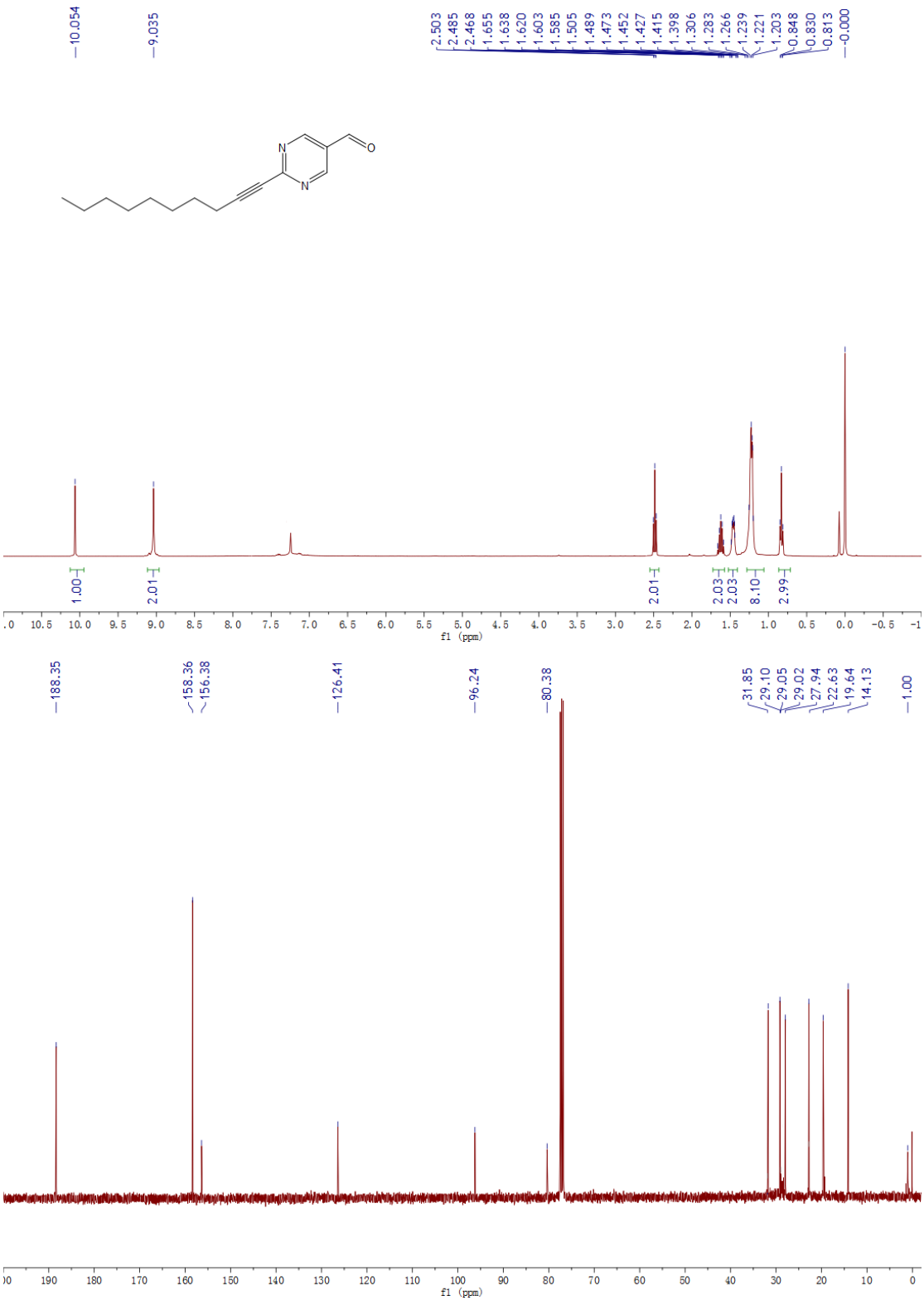
80.40
77.16
31.38
28.79
27.96
22.59
19.65
14.15
f1 (ppm)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1.505
1.489
1.473
1.452
1.427
1.415
1.398
1.306
1.283
1.266
1.239
1.221
1.203
0.848
0.830
0.813
0.000
N
N
O
1.00
2.01
2.01
2.03
2.03
8.10
2.99
f1 (ppm)
188.35
158.36
156.38
126.41
96.24
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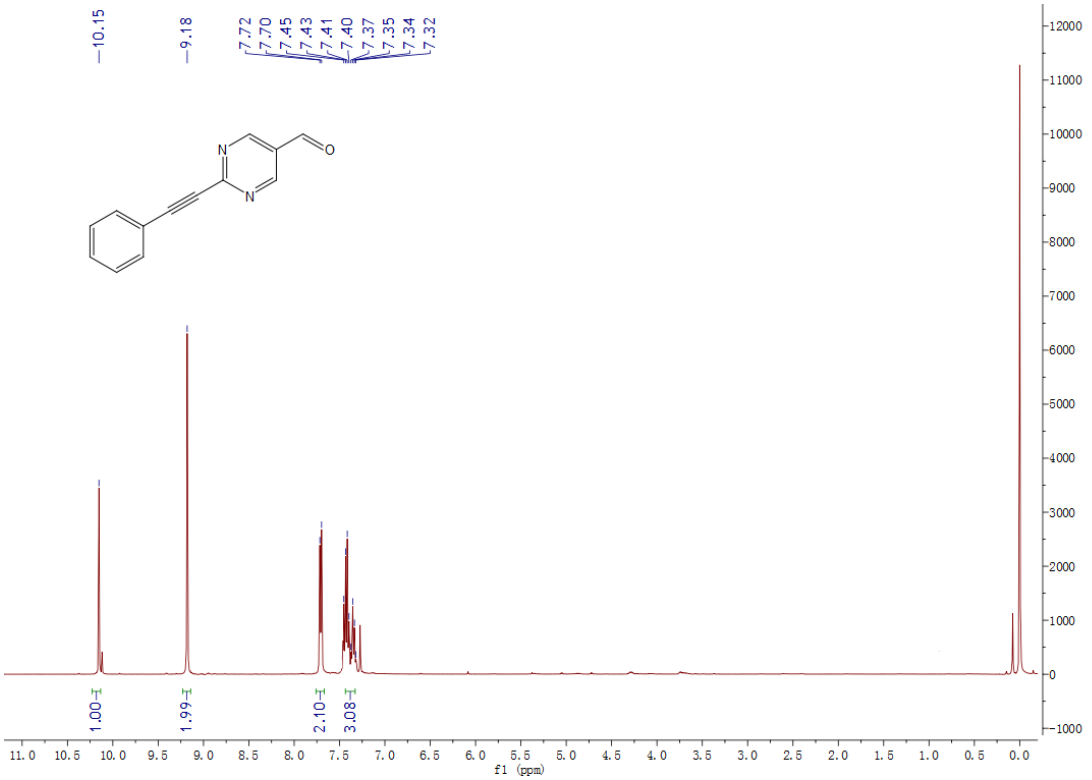
29.05
29.02
27.94
22.63
19.64
14.13
1.00
f1 (ppm)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7.72
7.70
7.45
7.43
7.41
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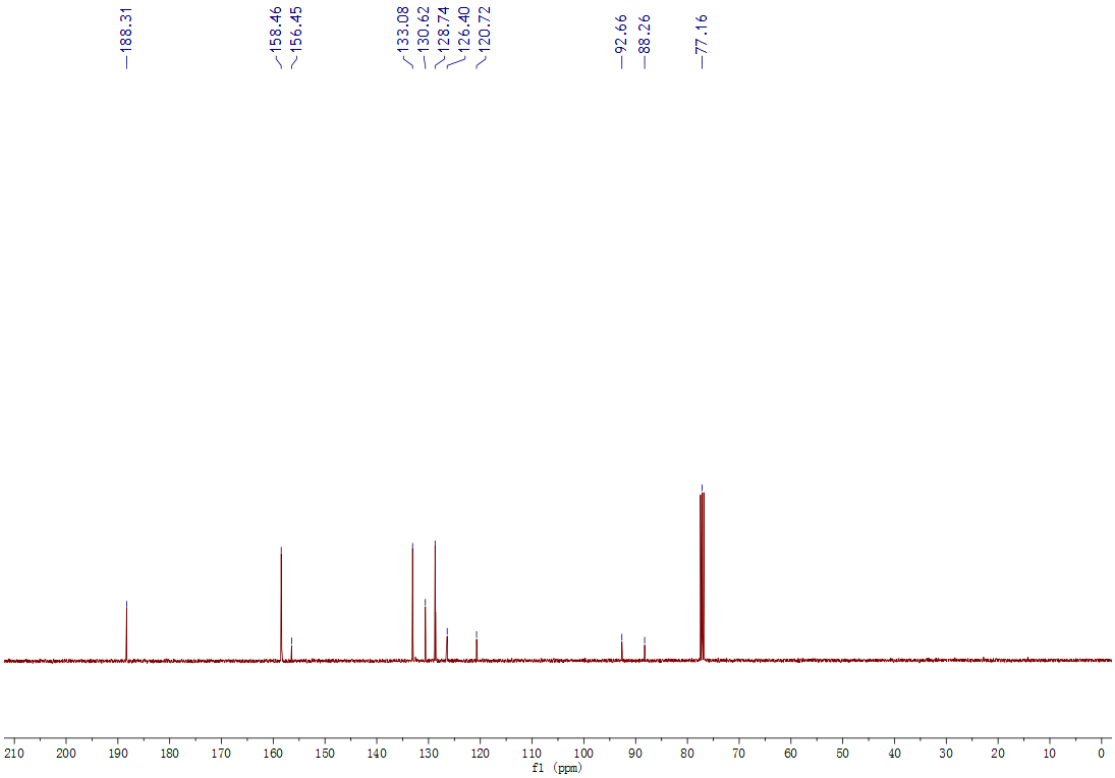
1.99
2.10
3.08
f1 (ppm)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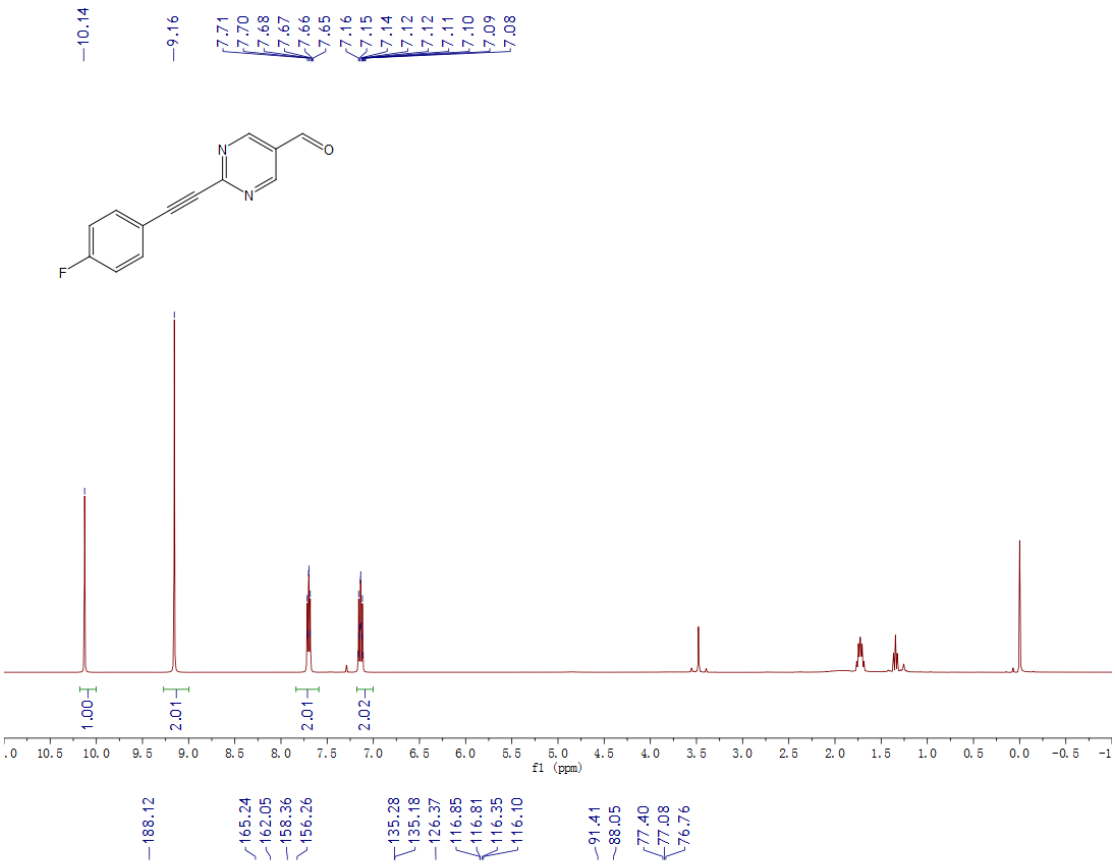
128.74
126.40
120.72
92.66
88.26
77.16
f1 (ppm)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9.16
7.71
7.70
7.68
7.67
7.66
7.65
7.16
7.15
7.14
7.12
7.12
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7.09
7.08
N
N
O
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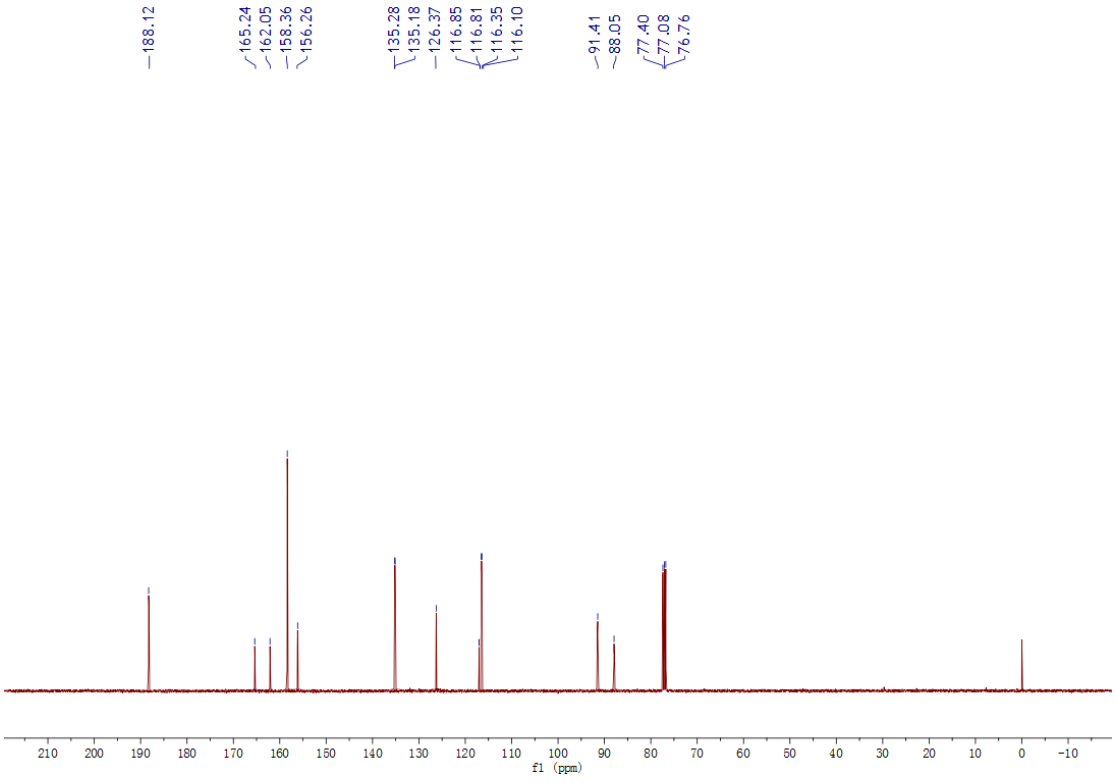
1.00
2.01
2.01
2.02
f1 (ppm)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156.26
135.28
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126.37
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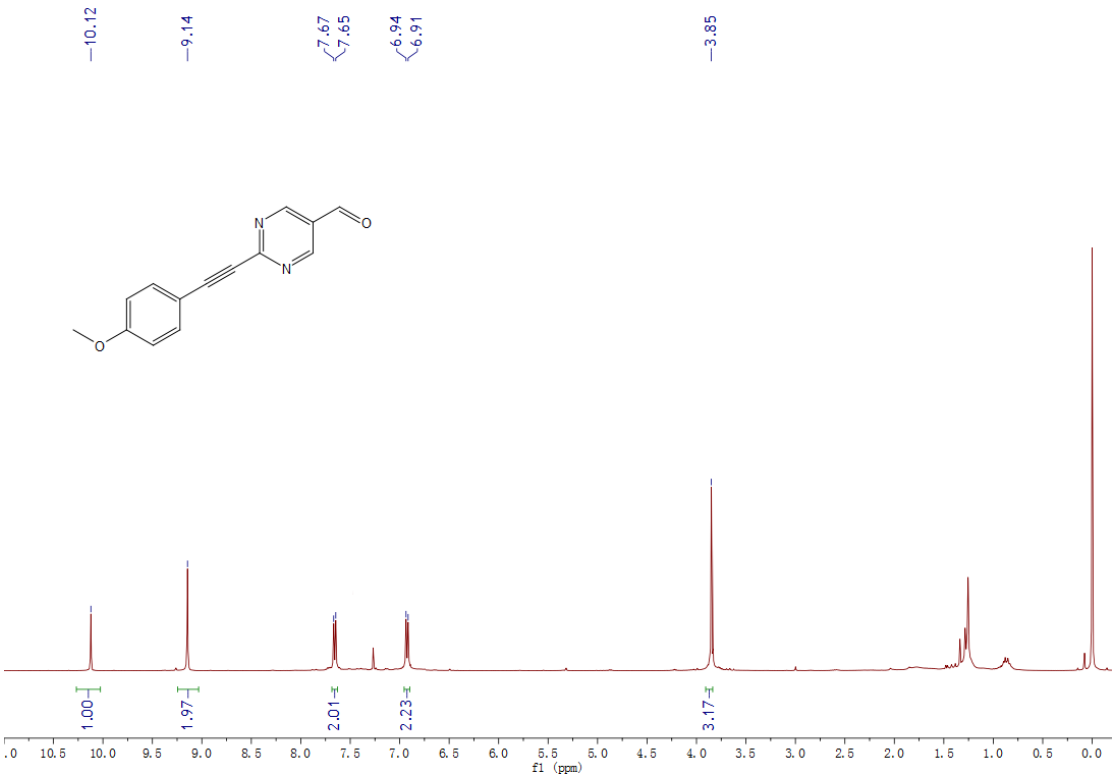
116.10
91.41
88.05
77.40
77.08
76.76
f1 (ppm)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9.14
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7.65
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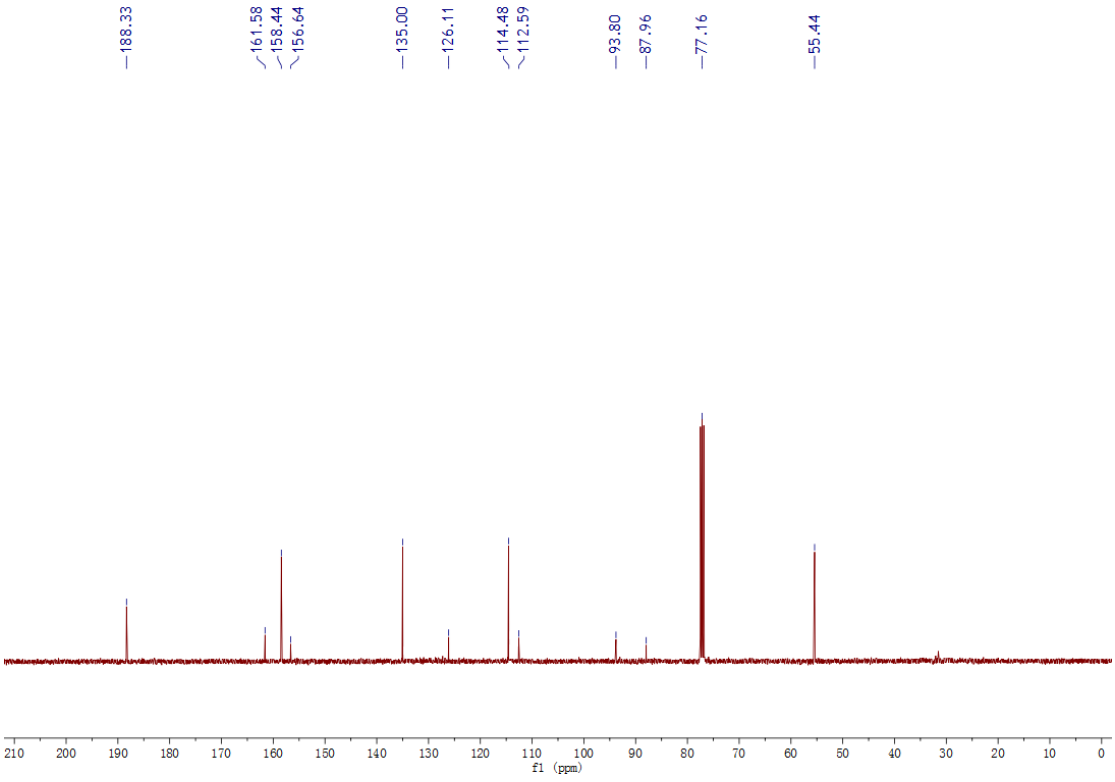
3.85
N
N
O
O
1.00
1.97
2.01
2.23
3.17
f1 (ppm)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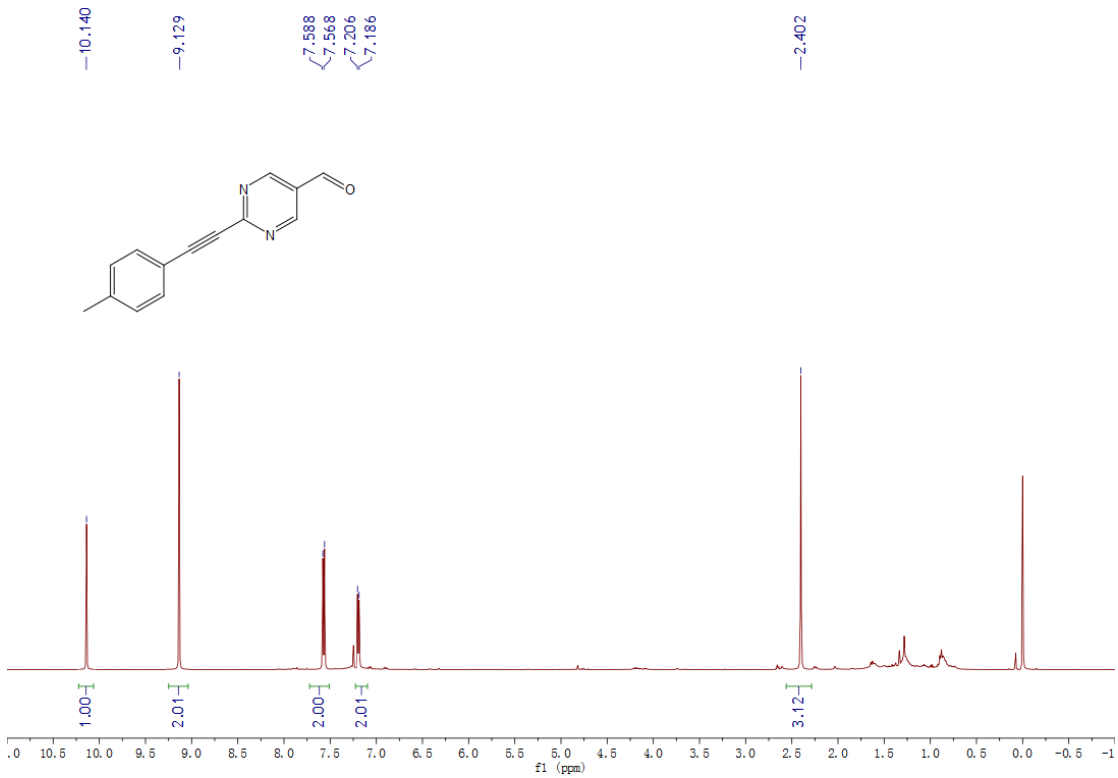
114.48
112.59
93.80
87.96
77.16
55.44
f1 (ppm)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9.129
7.588
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7.206
7.186
2.402
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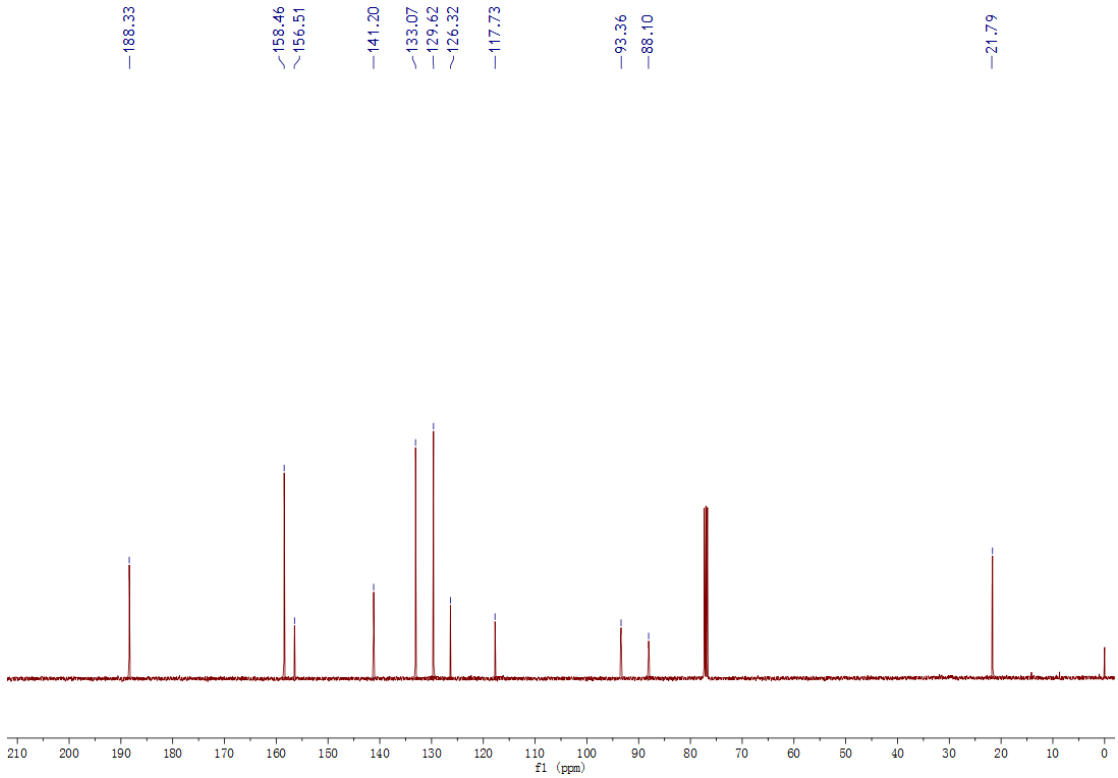
2.01
2.00
2.01
3.12
f1 (ppm)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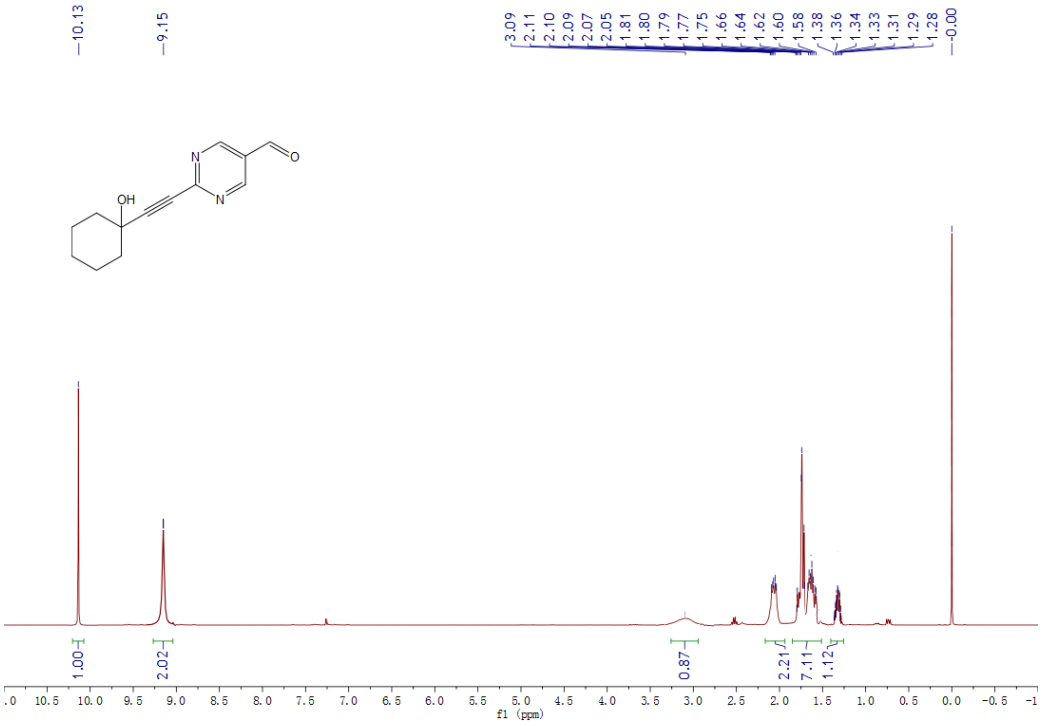
129.62
126.32
117.73
93.36
88.10
21.79
f1 (ppm)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2.10
2.09
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2.05
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1.79
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1.38
1.36
1.34
1.33
1.31
1.29
1.28
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2.21
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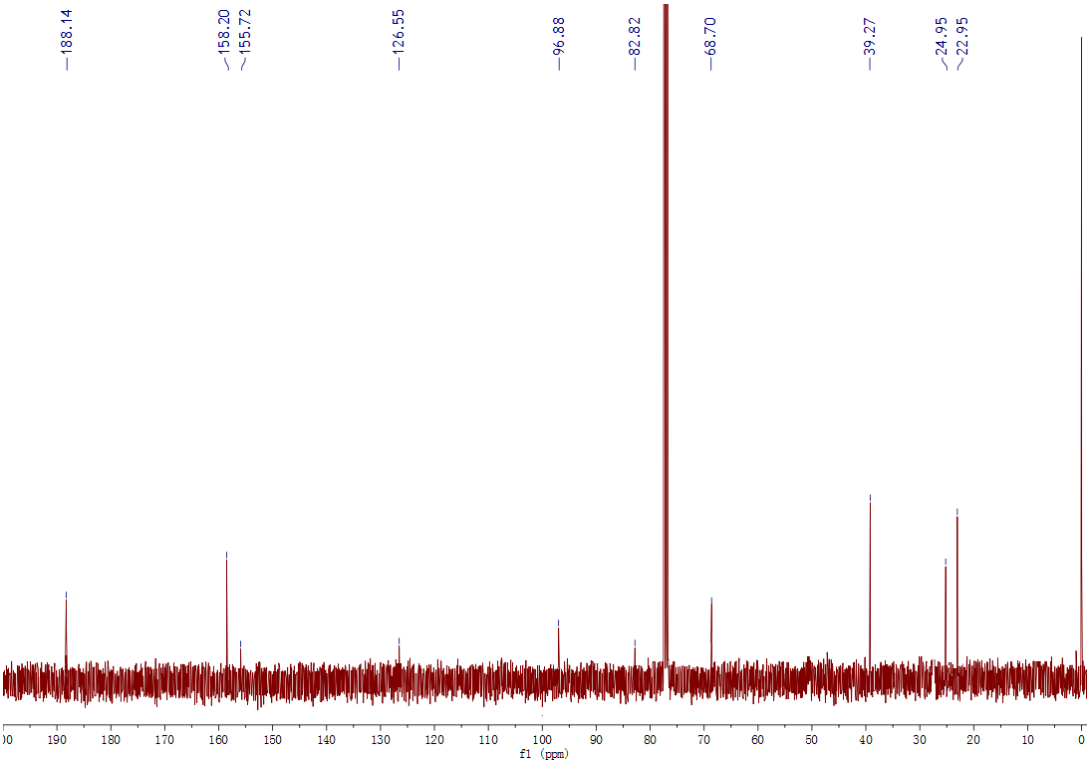
1.12
f1 (ppm)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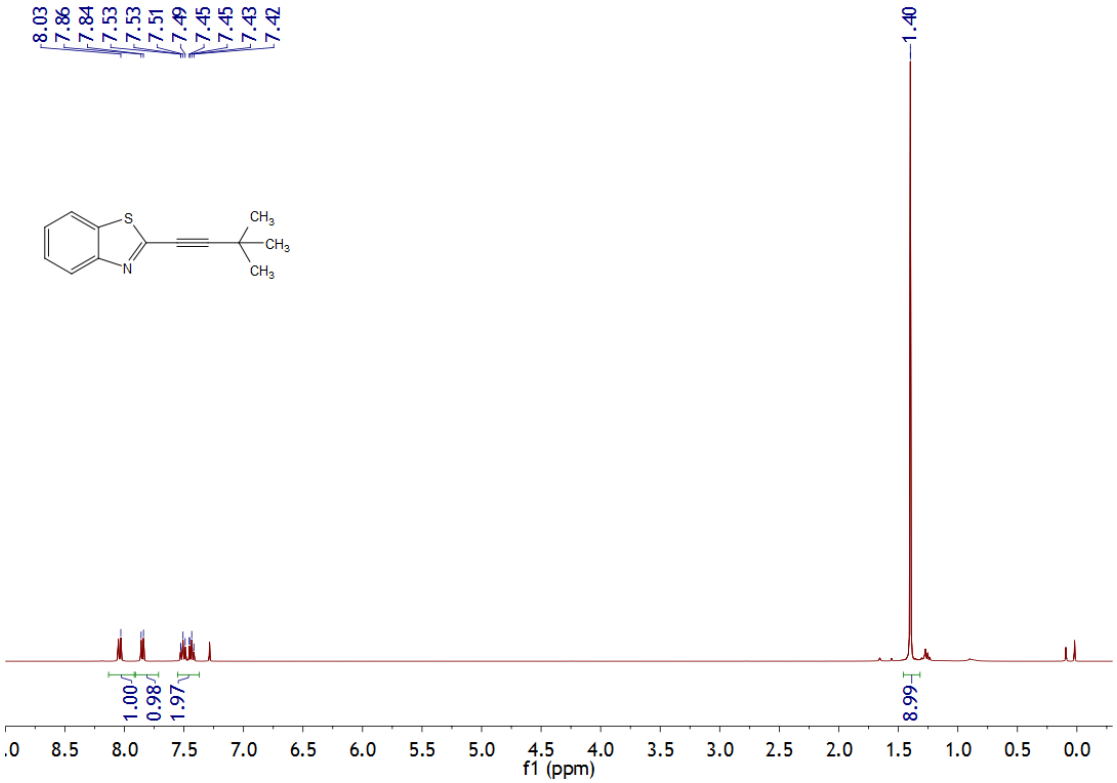
82.82
68.70
39.27
24.95
22.95
f1 (ppm)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7.86
7.84
7.53
7.53
7.51
7.49
7.45
7.45
7.43
7.42
1.40
S
N
CH3
CH3
CH3
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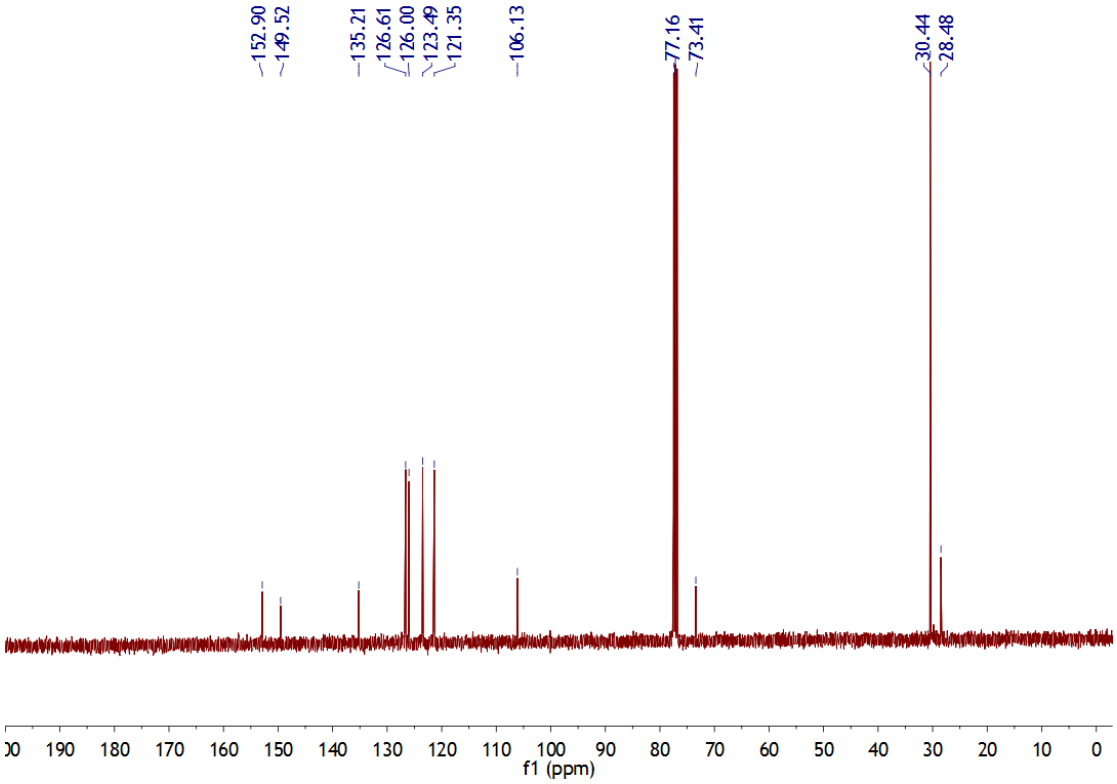
0.98
1.97
8.99
f1 (ppm)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126.00
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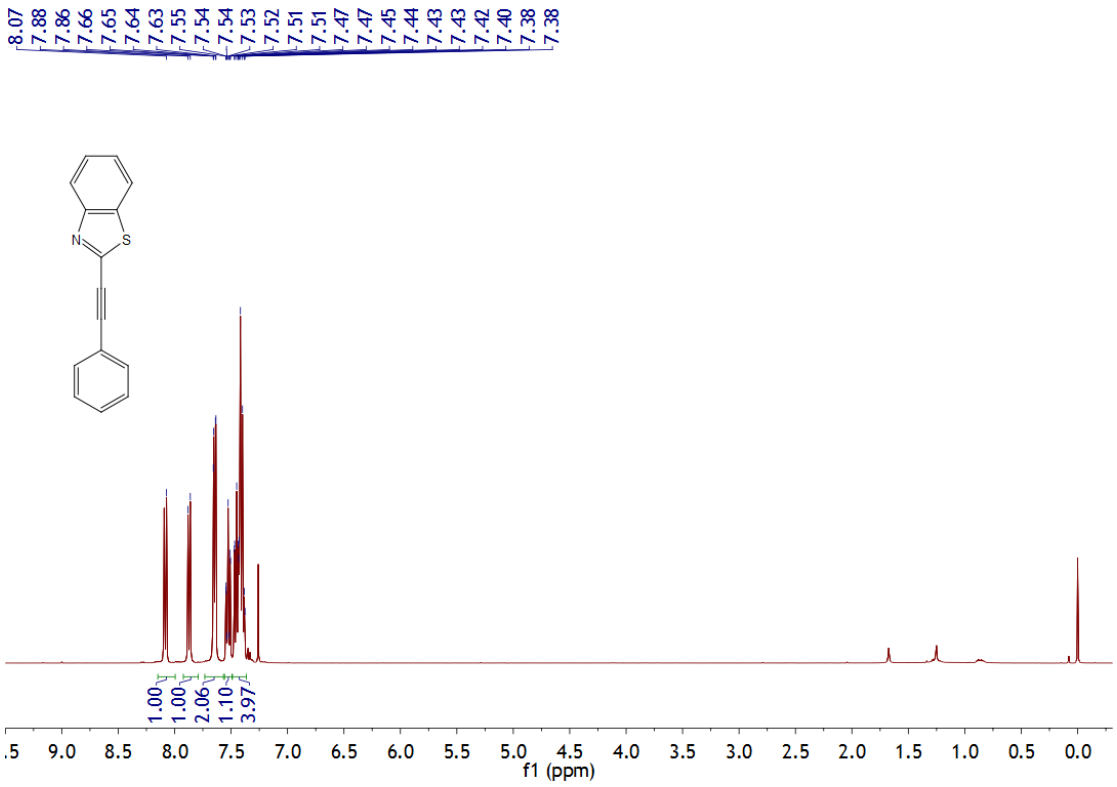
121.35
106.13
77.16
73.41
30.44
28.48
f1 (ppm)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7.86
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7.64
7.63
7.55
7.54
7.54
7.53
7.52
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7.51
7.47
7.47
7.45
7.44
7.43
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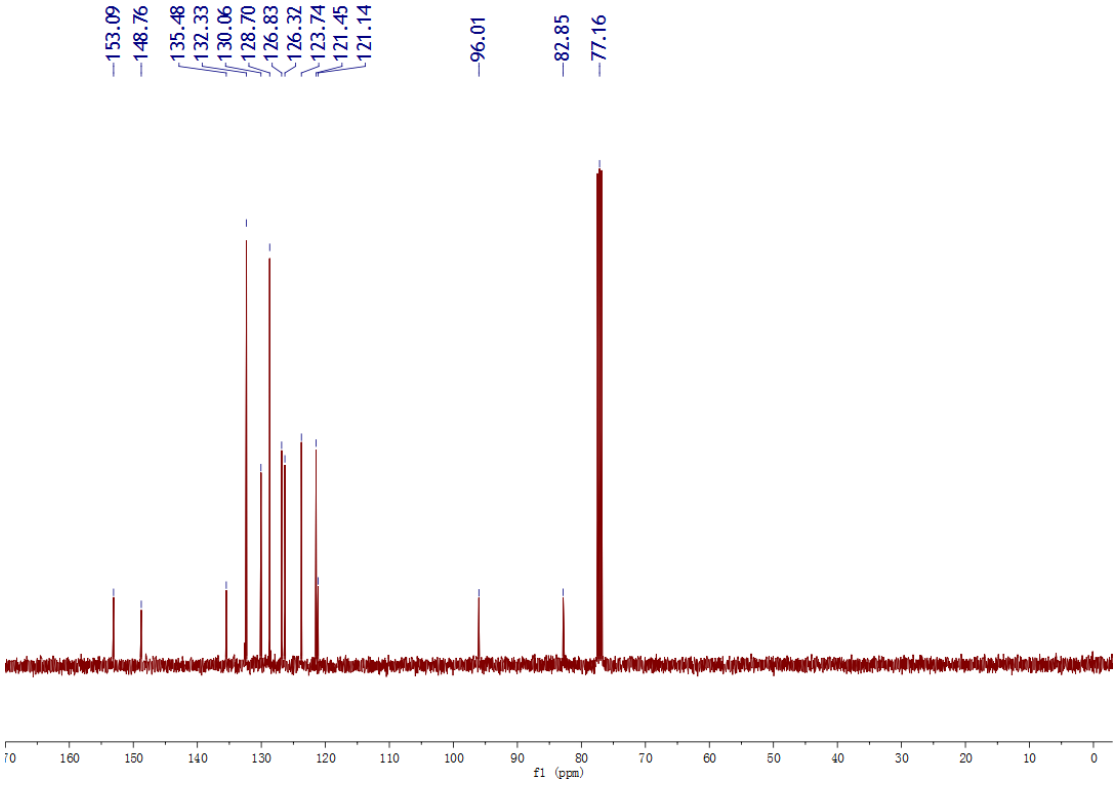
1.00
2.06
1.10
3.97
f1 (ppm)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130.06
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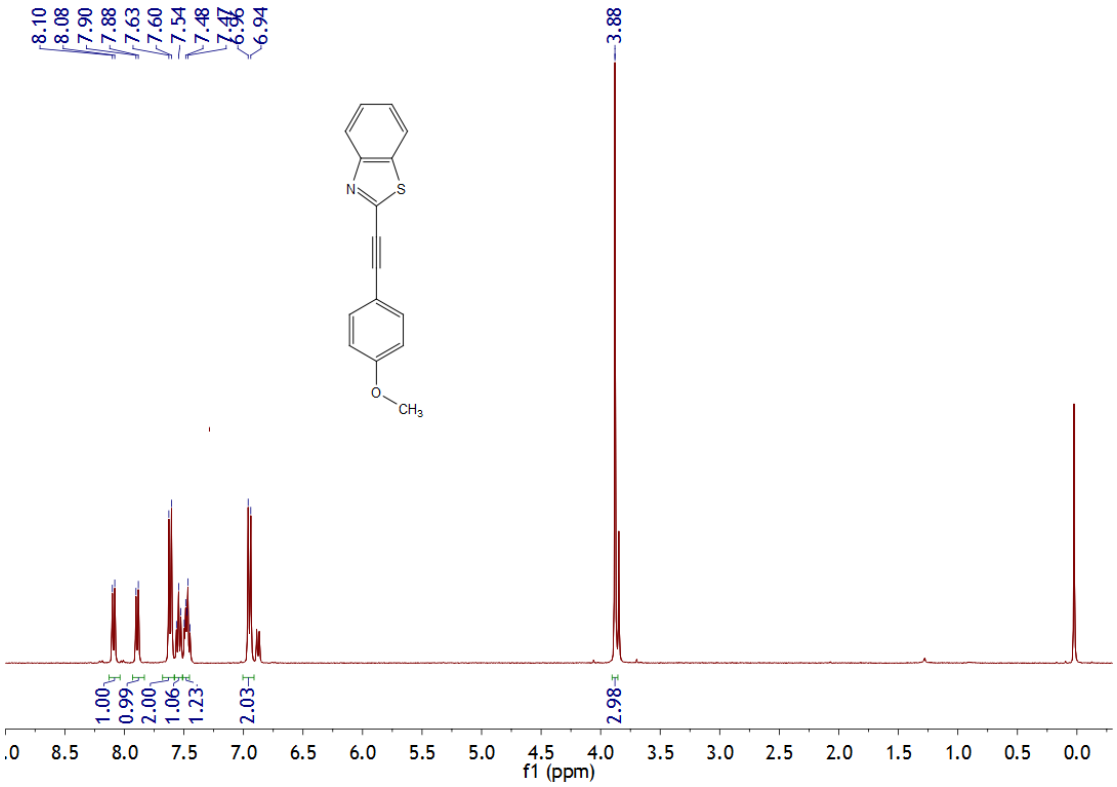
126.32
123.74
121.45
121.14
96.01
82.85
77.16
f1 (ppm)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8.08
7.90
7.88
7.63
7.60
7.54
7.48
7.47
6.96
6.94
3.88
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S
O
CH3
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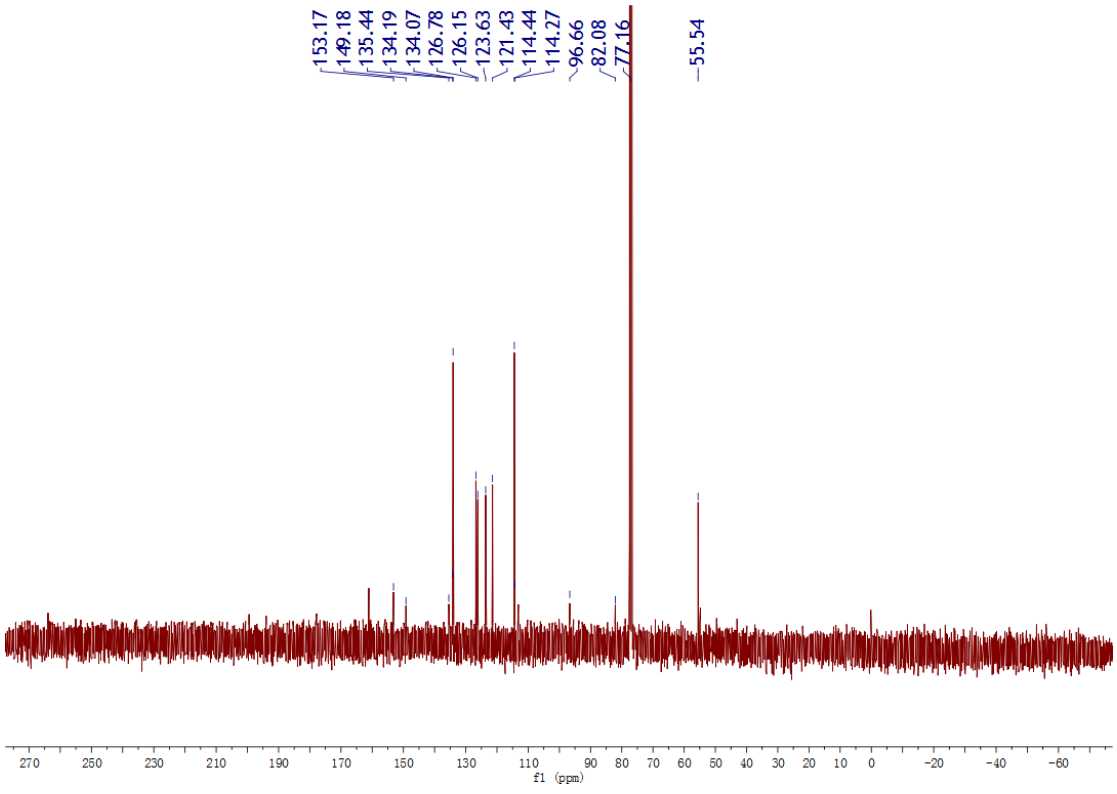
0.99
2.00
1.06
1.23
2.03
2.98
f1 (ppm)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134.19
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114.44
114.27
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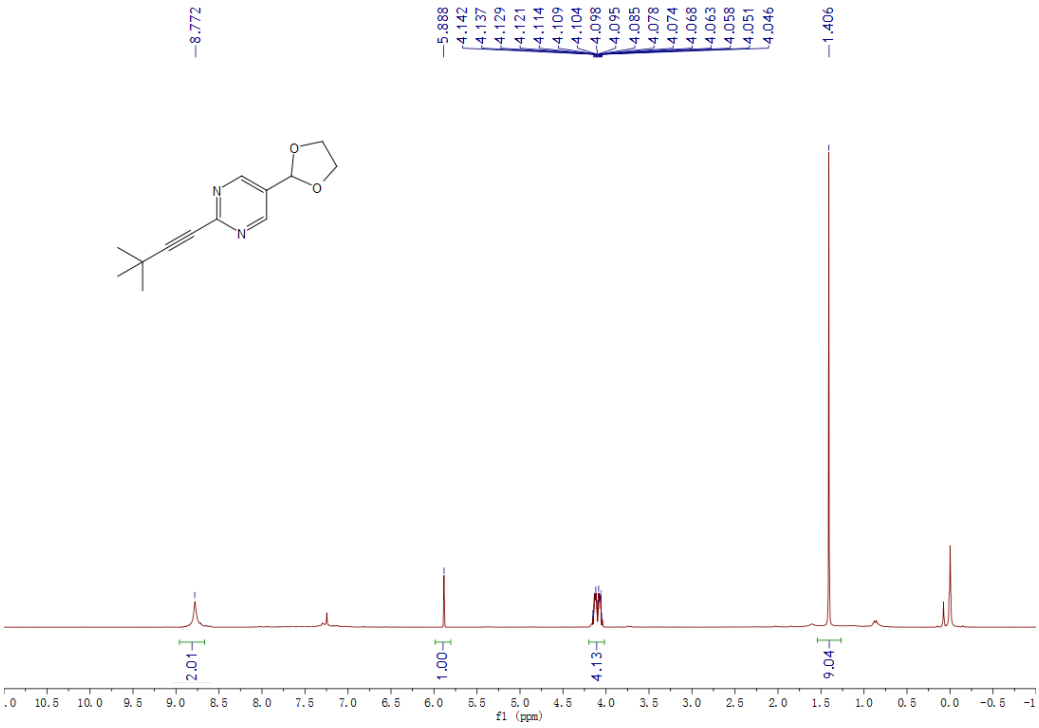
77.16
55.54
f1 (ppm)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4.095
4.085
4.078
4.074
4.068
4.063
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4.046
1.406
O
O
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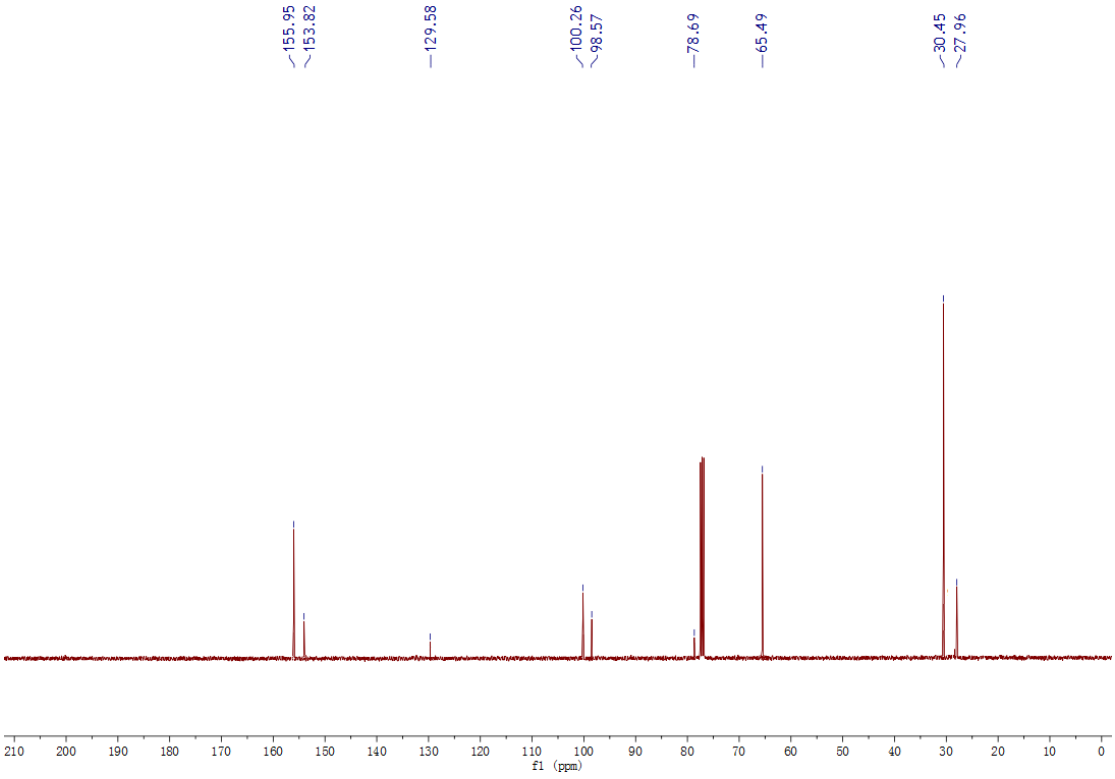
1.00
4.13
9.04
f1 (ppm)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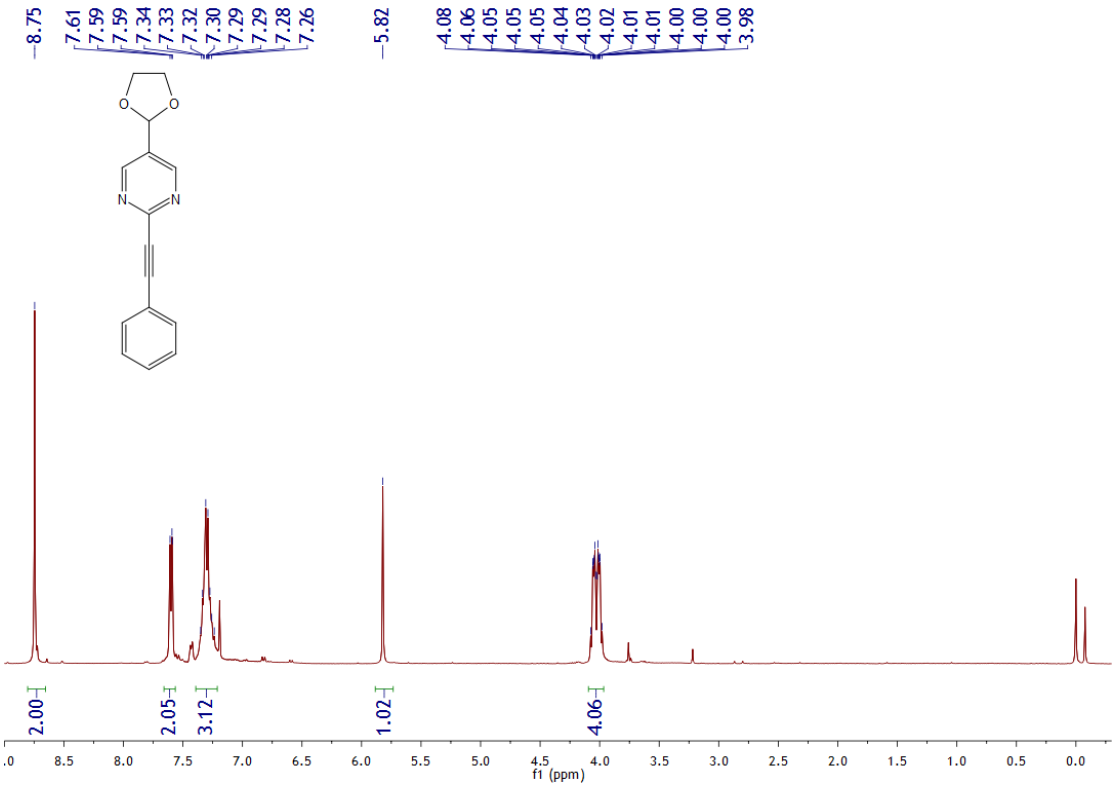
30.45
27.96
f1 (ppm)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7.28
7.26
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4.08
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4.05
4.05
4.05
4.04
4.03
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4.01
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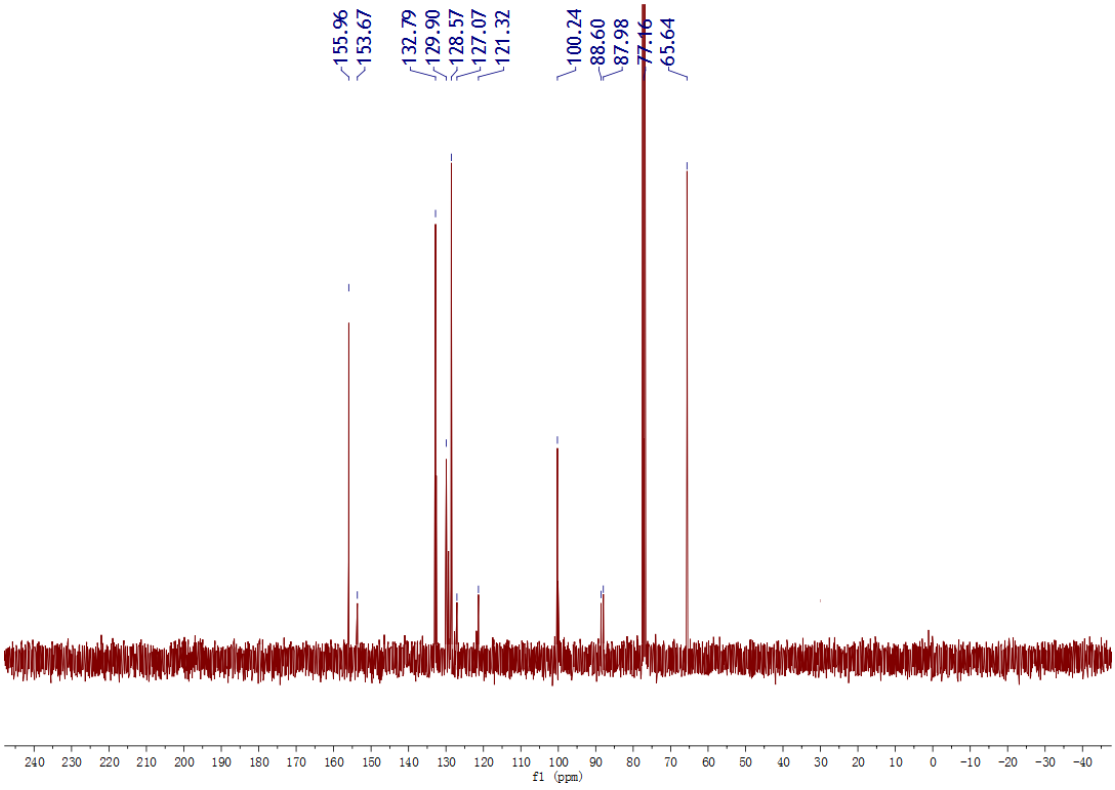
1.02
4.06
f1 (ppm)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128.57
127.07
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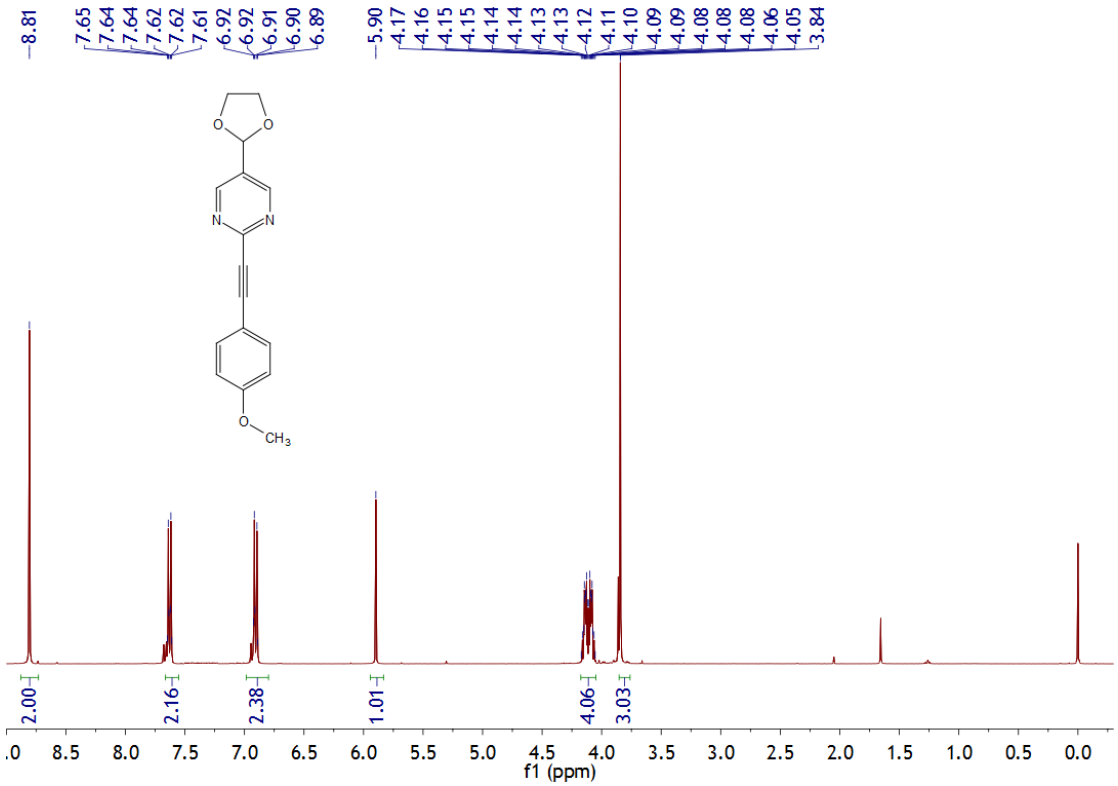
100.24
88.60
87.98
77.16
65.64
f1 (ppm)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6.91
6.90
6.89
5.90
4.17
4.16
4.15
4.15
4.14
4.14
4.13
4.13
4.12
4.11
4.10
4.09
4.09
4.08
4.08
4.08
4.06
4.05
3.84
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O
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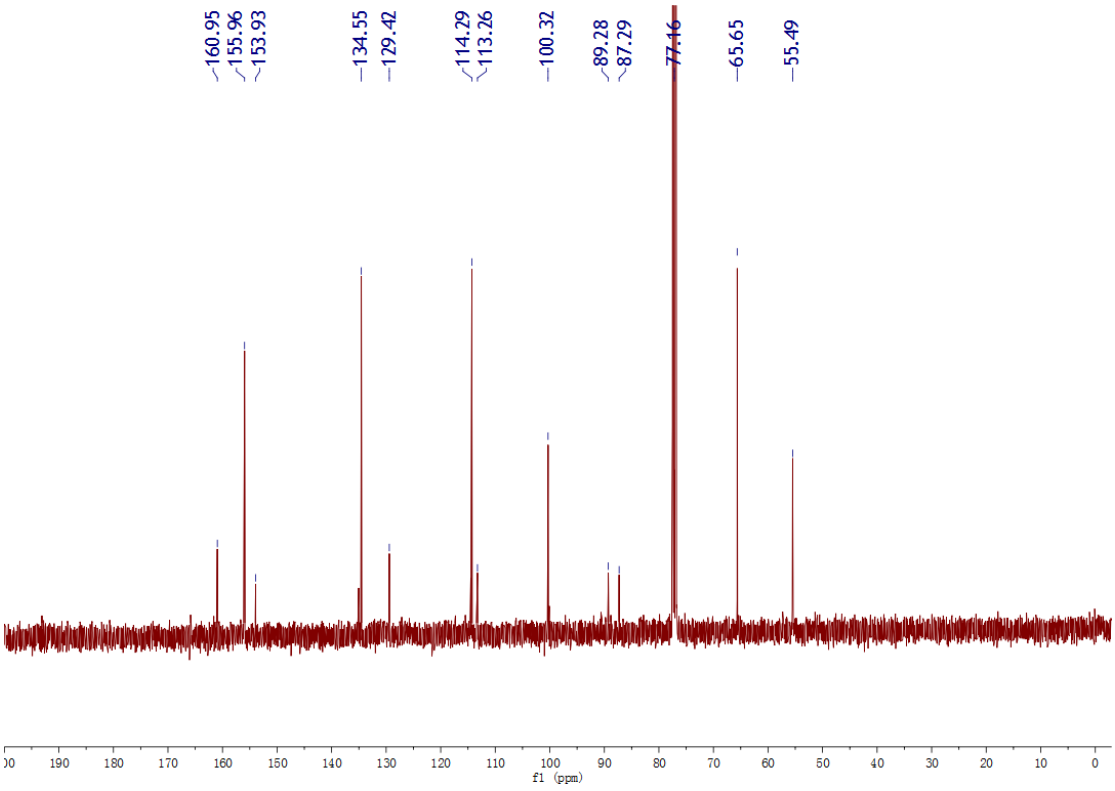
2.38
1.01
4.06
3.03
f1 (ppm)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114.29
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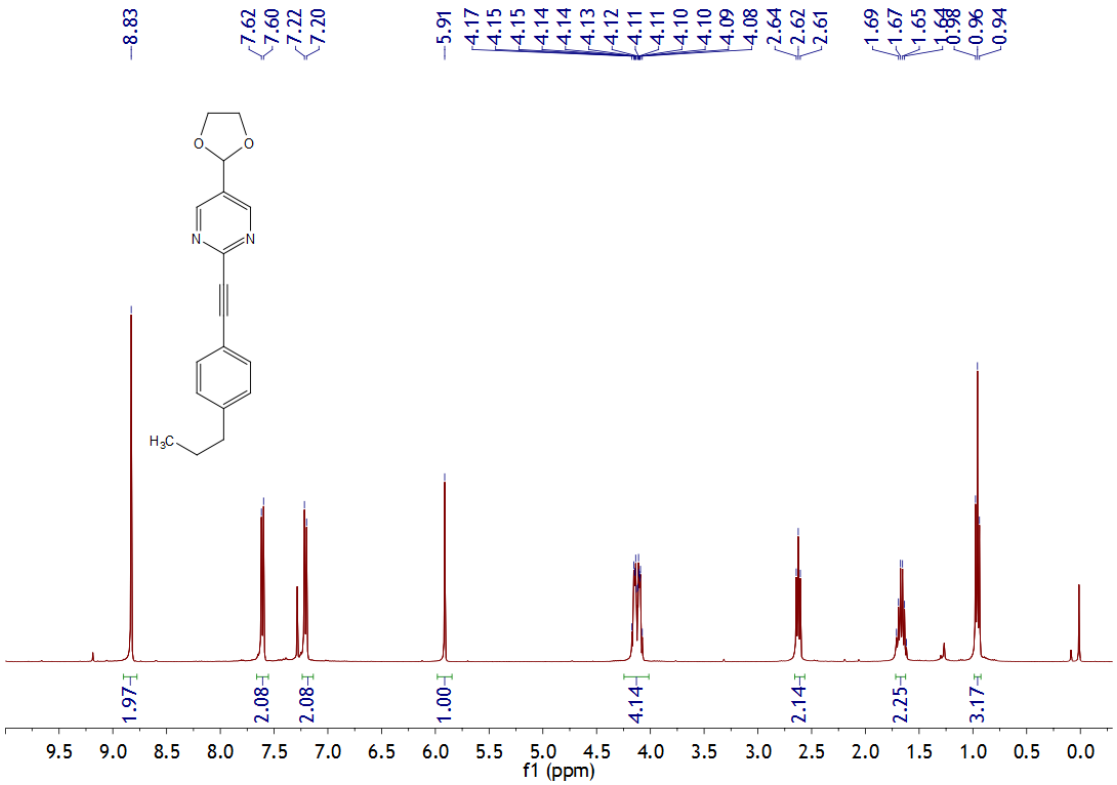
100.32
89.28
87.29
77.46
65.65
55.49
f1 (ppm)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4.15
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4.14
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4.13
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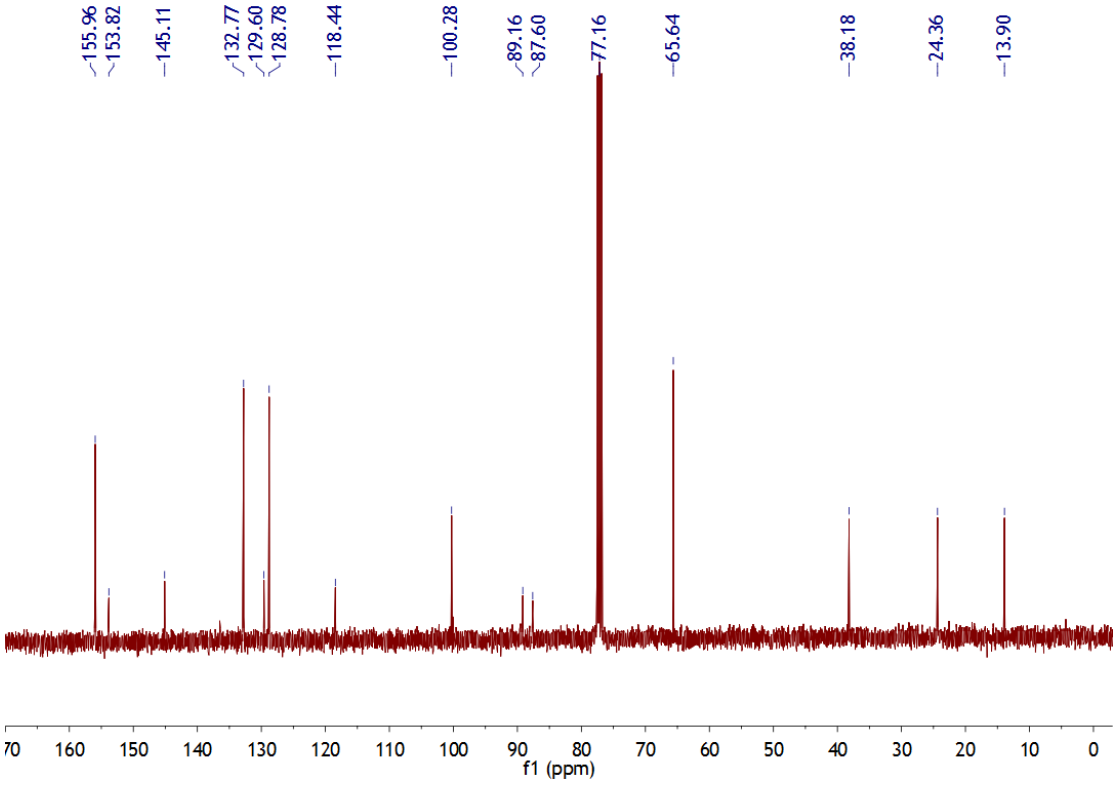
4.11
4.11
4.10
4.10
4.09
4.08
2.64
2.62
2.61
1.69
1.67
1.65
0.98
0.96
0.94
O
O
N
N
H3C
1.97
2.08
2.08
1.00
4.14
2.14
2.25
3.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.78
118.44
100.28
89.16
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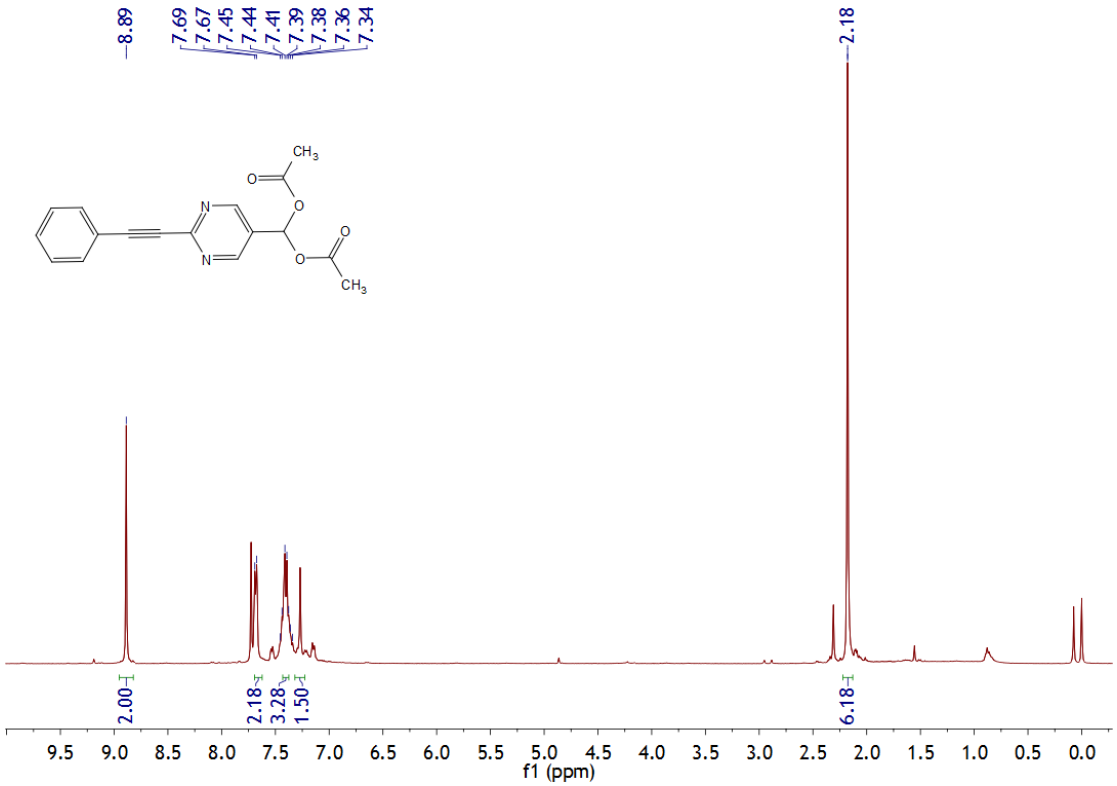
77.16
65.64
38.18
24.36
13.90
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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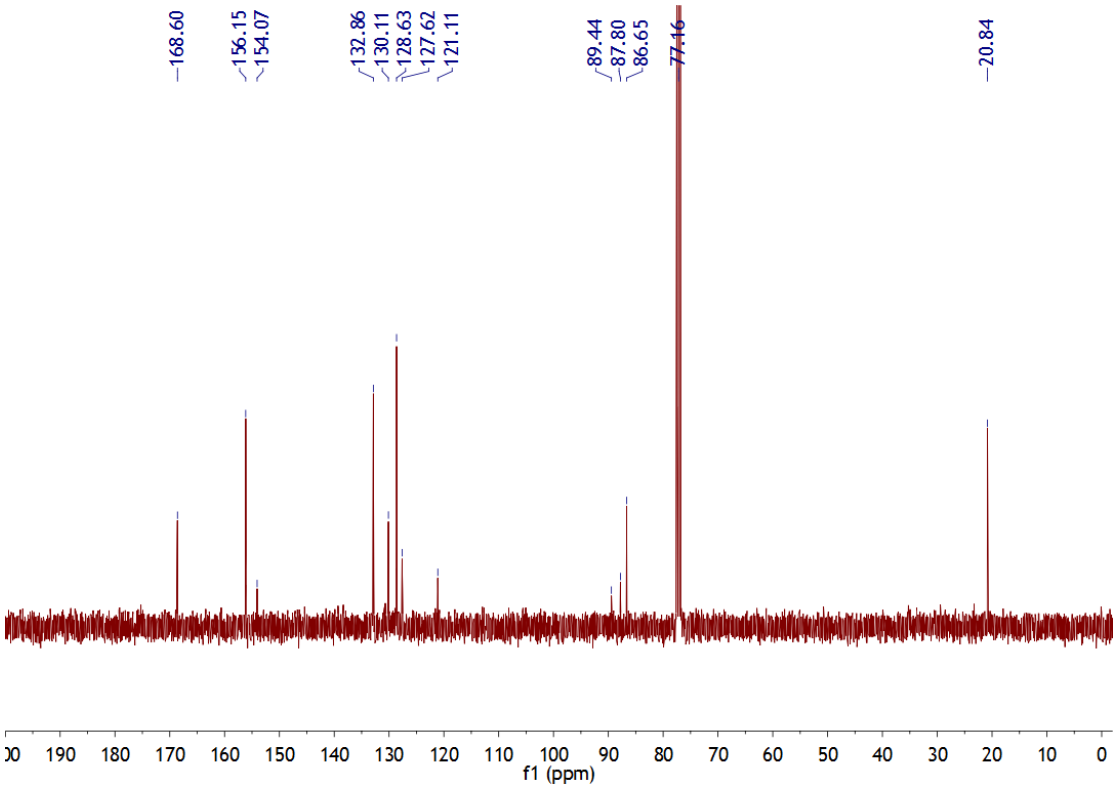
7.34
2.18
2.00
2.18
3.28
1.50
6.18
f1 (ppm)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121.11
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86.65
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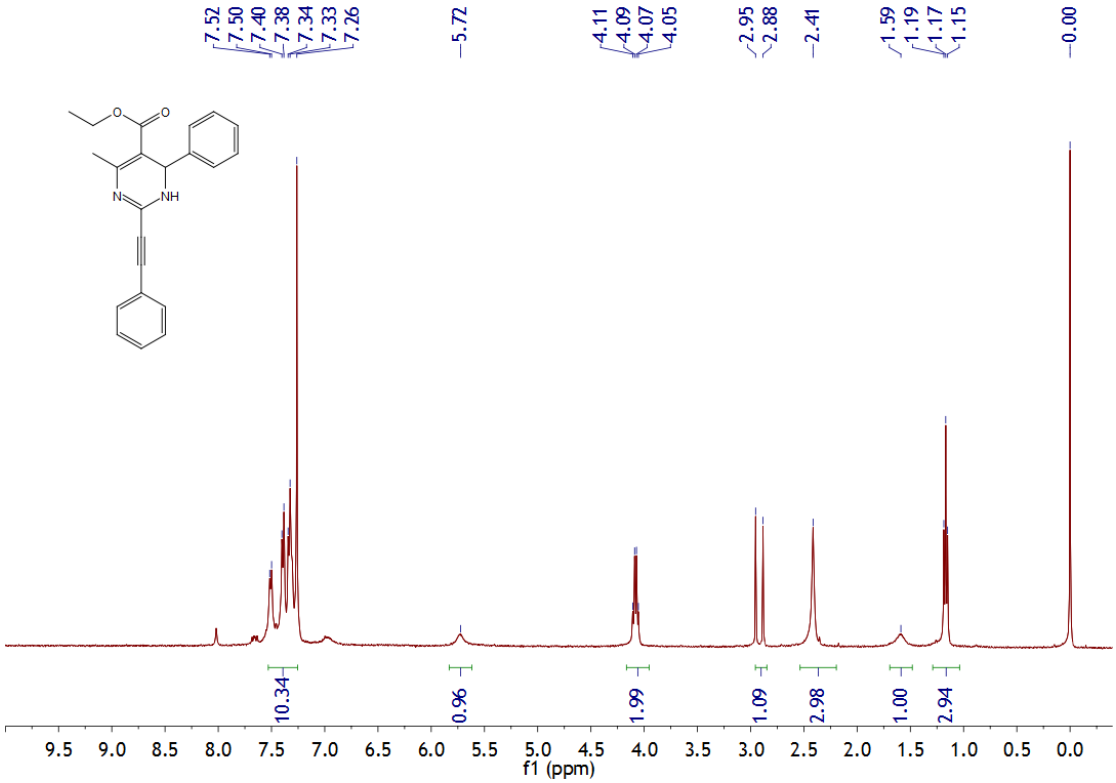
20.84
f1 (ppm)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7.34
7.33
7.26
5.72
4.11
4.09
4.07
4.05
2.95
2.88
2.41
1.59
1.19
1.17
1.15
0.00
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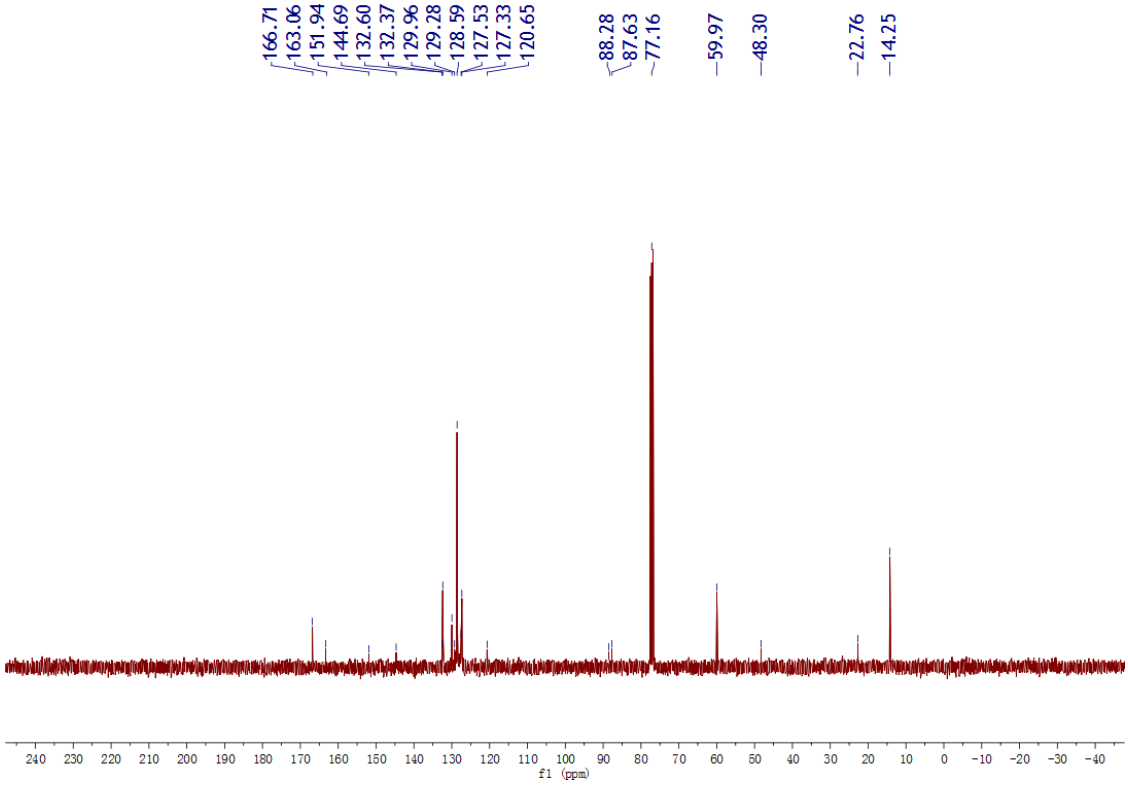
O
N
NH
10.34
0.96
1.99
1.09
2.98
1.00
2.94
f1 (ppm)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163.06
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144.69
132.60
132.37
129.96
129.28
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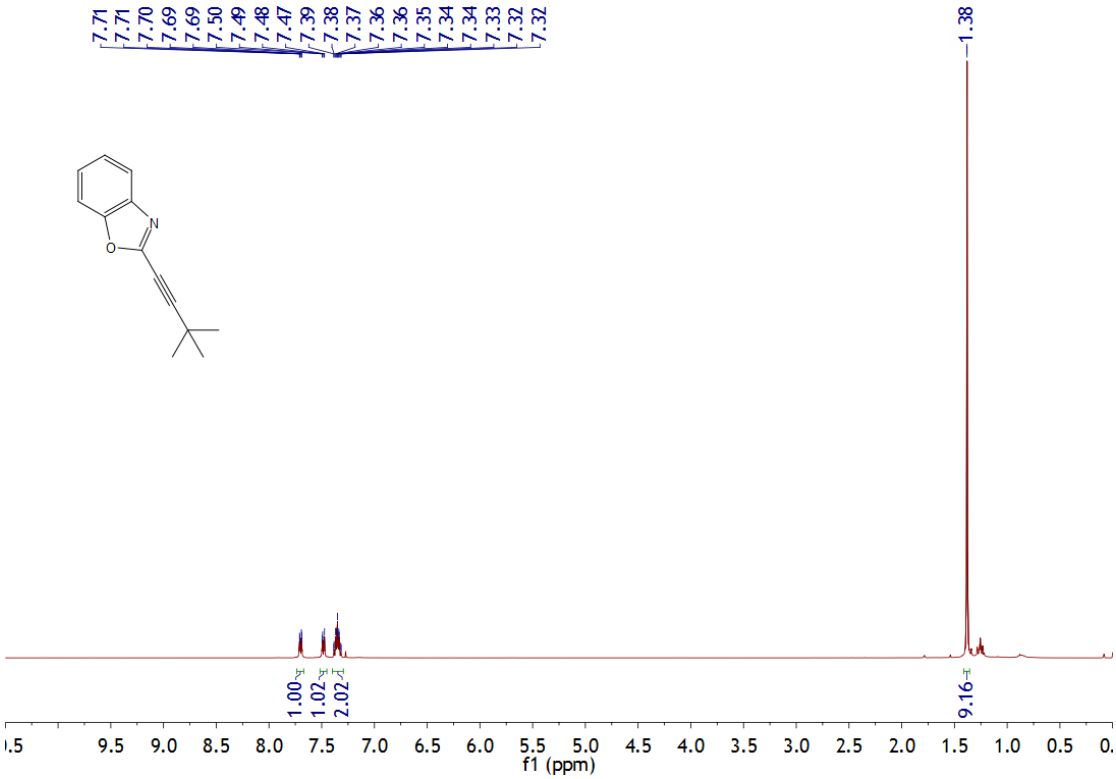
127.53
127.33
120.65
88.28
87.63
77.16
59.97
48.30
22.76
14.25
f1 (ppm)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7.50
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7.38
7.37
7.36
7.36
7.35
7.34
7.34
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7.32
7.32
1.38
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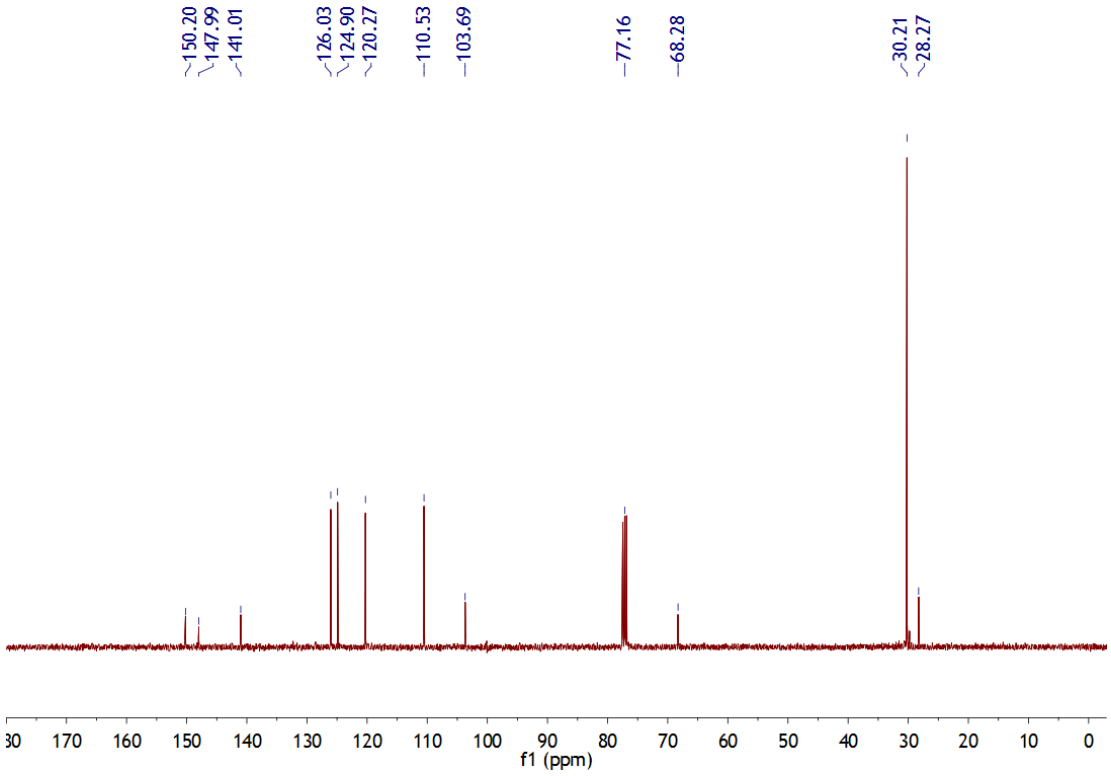
2.02
9.16
f1 (ppm)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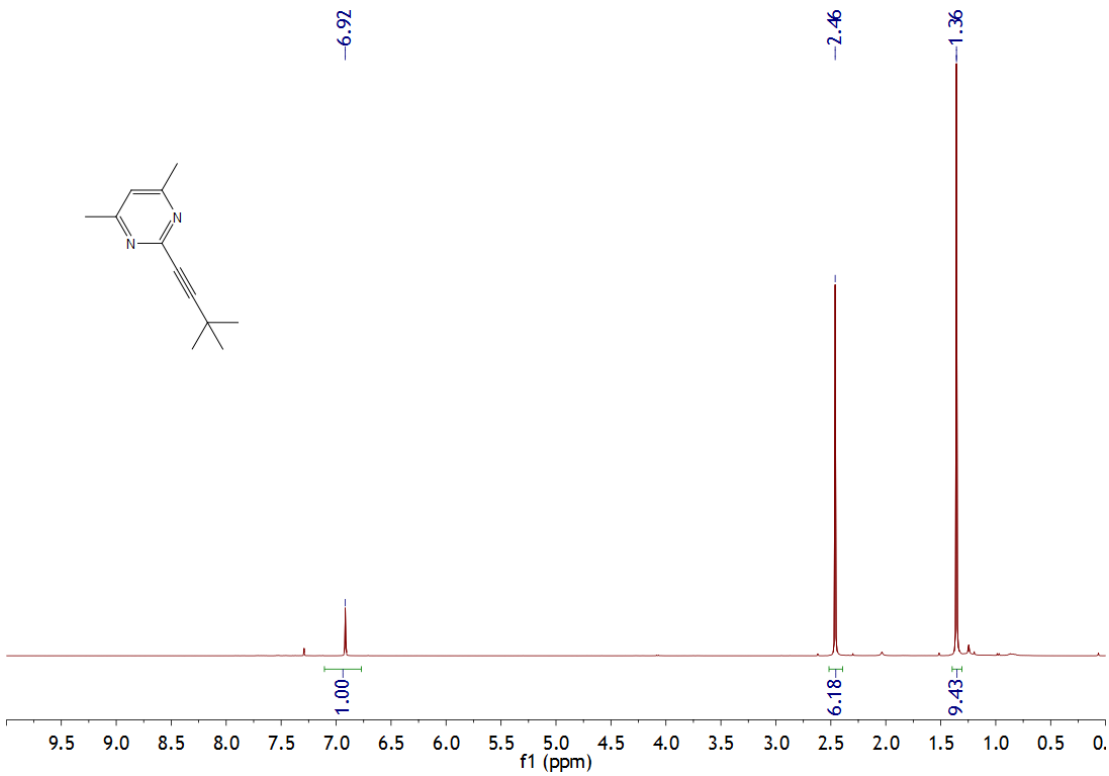
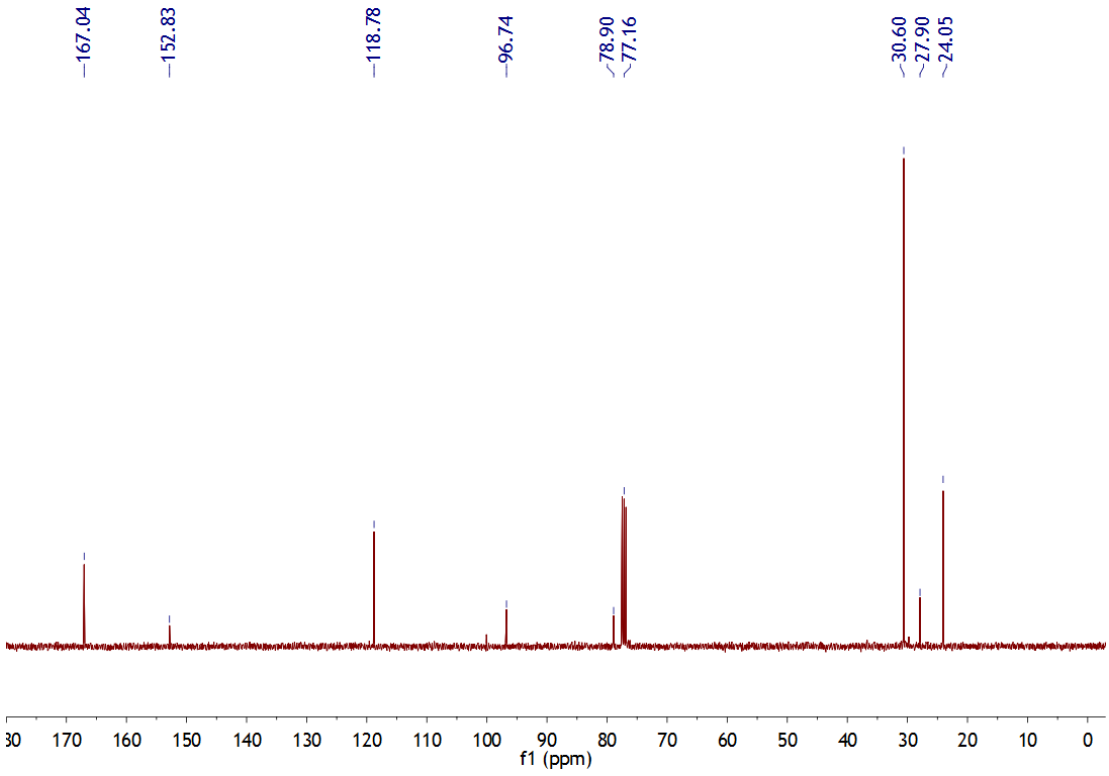
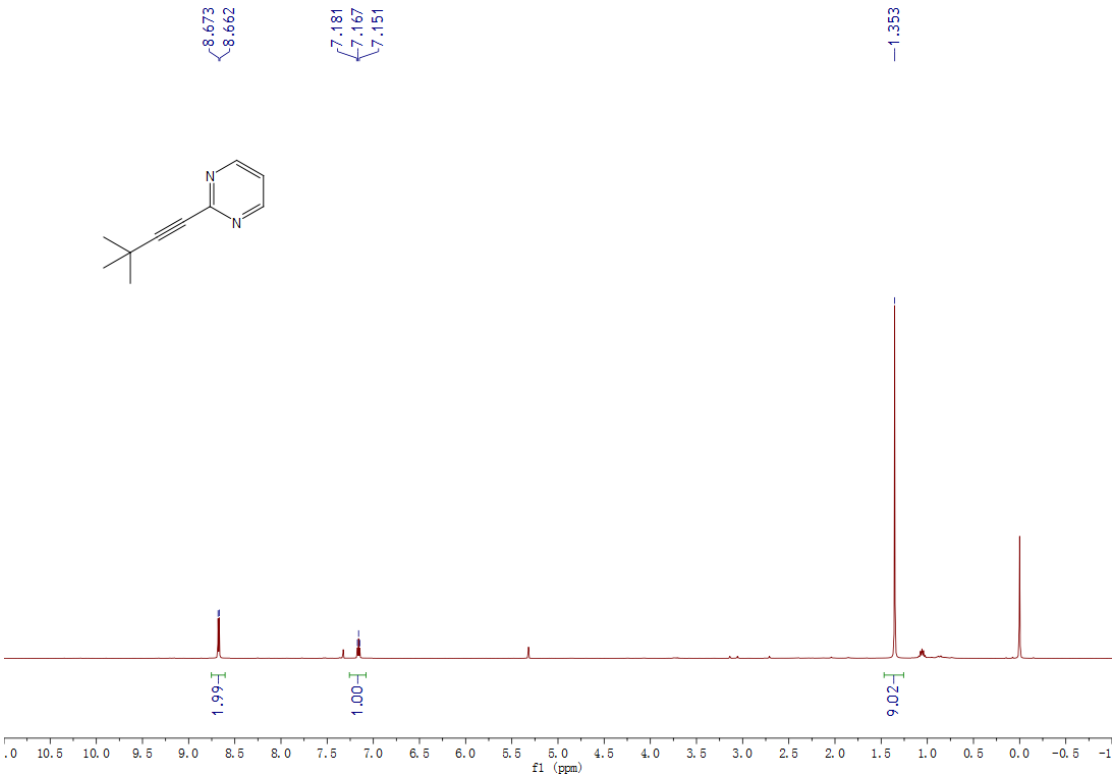
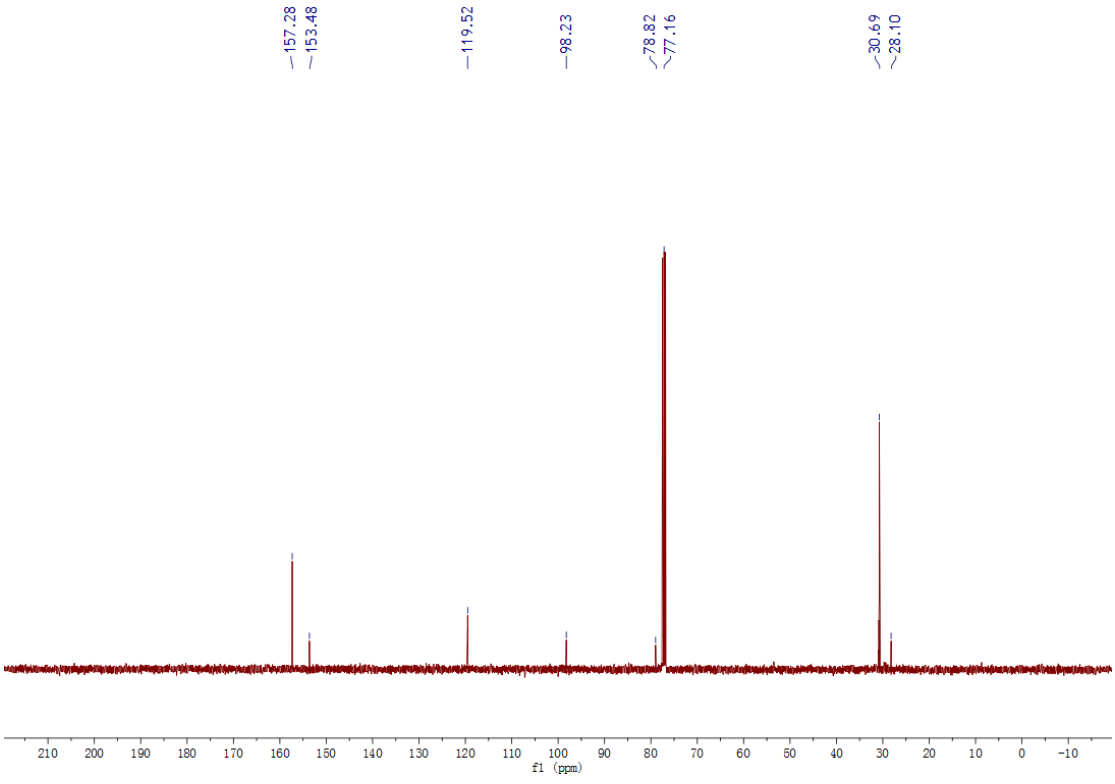
110.53
103.69
77.16
68.28
30.21
28.27
f1 (ppm)


6.92
2.46
1.36
1.00
6.18
9.43
f1 (ppm)


167.04
152.83
118.78
96.74
78.90
77.16
30.60
27.90
24.05
f1 (ppm)


8.673
8.662
7.181
7.167
7.151
1.353
N
N
1.99
1.00
9.02
f1 (ppm)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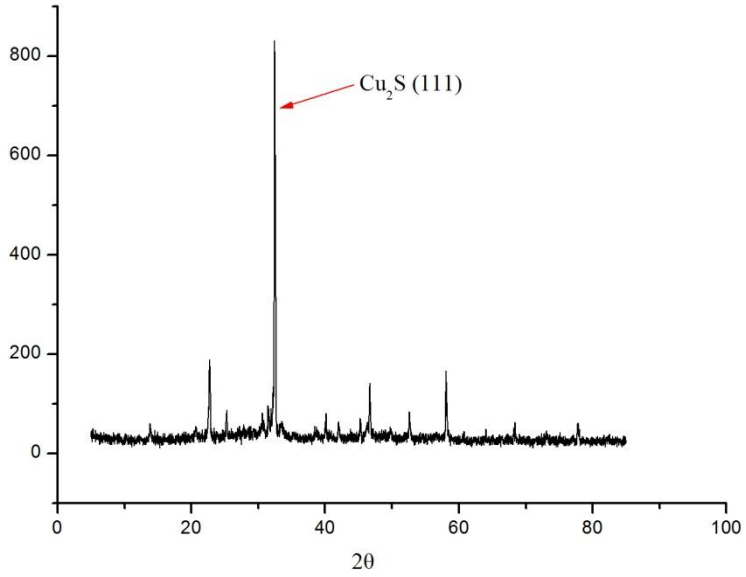
119.52
98.23
78.82
77.16
30.69
28.10
f1 (ppm)



XRD analysis of the reaction solid mixture

Substrate **a**

Sum of electronic and thermal Free Energies= -2487.416978

Cu	1.52814300	0.18450300	-0.05118800
Cu	-1.52820300	0.18465900	0.04886700
I	0.00006900	2.39090700	-0.00286400
I	0.00011900	-2.04906200	-0.00289500
P	3.83170900	0.01879400	-0.01976300
P	-3.83171100	0.01870600	0.02113500
C	4.76796100	1.52217800	-0.52530000
C	5.99875600	1.47054900	-1.19809200
C	4.21016000	2.77332000	-0.21490500
C	6.66336000	2.64945200	-1.54184800
H	6.43580000	0.51187500	-1.46025400
C	4.88135100	3.94861100	-0.55331800
H	3.24345600	2.82667300	0.27805600
C	6.10848200	3.88899900	-1.21725800
H	7.61394300	2.59757400	-2.06619300
H	4.43728200	4.90968600	-0.30910400
H	6.62644300	4.80503700	-1.48862500
C	4.49033500	-1.32824900	-1.08715200
C	5.64129400	-2.06449800	-0.76648300
C	3.79937200	-1.62287400	-2.27292500
C	6.09954500	-3.06491800	-1.62576000
H	6.17479300	-1.86285100	0.15783800
C	4.26356300	-2.61808700	-3.13324900
H	2.88803100	-1.08223900	-2.51476500
C	5.41448200	-3.34025500	-2.81108800
H	6.98981700	-3.63158900	-1.36607500
H	3.71757400	-2.83811200	-4.04643200
H	5.77075500	-4.12212700	-3.47641900
C	4.45112700	-0.37714900	1.66990500
C	5.63970600	0.15137900	2.19517100
C	3.67941100	-1.24604200	2.46019500
C	6.05337400	-0.19175900	3.48439900
H	6.23941300	0.83508400	1.60201600
C	4.10052400	-1.59153500	3.74426600
H	2.74771700	-1.64899000	2.07039300
C	5.28737400	-1.06448200	4.25912100
H	6.97410000	0.22639100	3.88267800
H	3.49526000	-2.26493500	4.34494800
H	5.61025200	-1.32773600	5.26283000
C	-4.48892600	-1.33038100	1.08678800
C	-5.64025900	-2.06606600	0.76617800
C	-3.79641900	-1.62725600	2.27110000

C	-6.09735900	-3.06816100	1.62411900
H	-6.17496200	-1.86266200	-0.15706000
C	-4.25945800	-2.62414400	3.13010100
H	-2.88478100	-1.08705700	2.51278600
C	-5.41075700	-3.34575000	2.80802900
H	-6.98793800	-3.63437200	1.36448700
H	-3.71228400	-2.84590800	4.04215400
H	-5.76613300	-4.12892300	3.47230900
C	-4.45341000	-0.37391800	-1.66846400
C	-5.64264600	0.15570900	-2.19112400
C	-3.68278800	-1.24130500	-2.46147500
C	-6.05802800	-0.18486800	-3.48048100
H	-6.24153000	0.83828600	-1.59584200
C	-4.10560500	-1.58424400	-3.74566900
H	-2.75059800	-1.64506800	-2.07370200
C	-5.29309900	-1.05610800	-4.25792400
H	-6.97924900	0.23412200	-3.87672600
H	-3.50116800	-2.25648600	-4.34847500
H	-5.61730800	-1.31736700	-5.26172500
C	-4.76720400	1.52113800	0.53091900
C	-5.99715600	1.46816900	1.20516000
C	-4.20974800	2.77289000	0.22239600
C	-6.66127900	2.64638200	1.55218500
H	-6.43390800	0.50897500	1.46589700
C	-4.88046300	3.94750700	0.56409300
H	-3.24368500	2.82722400	-0.27171200
C	-6.10675200	3.88657700	1.22946000
H	-7.61120500	2.59346100	2.07761500
H	-4.43666300	4.90906300	0.32128800
H	-6.62433400	4.80207300	1.50337000

Substrate **b**

Sum of electronic and thermal Free Energies=-3251.171414

C	0.79876200	2.96944200	1.14326700
N	1.75252300	2.56818500	0.24092500
C	2.67231300	3.44899000	-0.13861800
C	2.70046900	4.75562300	0.36322000
C	1.69456700	5.06845000	1.28931300
N	0.76107900	4.20915200	1.67818500
H	4.42866500	0.53927800	-1.46791500
H	1.64782000	6.06424400	1.73367500
S	-0.38382700	1.79787200	1.64820200

C	3.72836600	5.71996700	-0.05011600
H	3.63323900	6.72764400	0.41158600
O	4.63133600	5.47446800	-0.83097400
Cu	1.47356500	0.60089100	-0.37031900
Cu	-1.29139500	0.76056800	-0.25979400
I	-0.05856300	0.81468000	-2.62958600
P	2.80291300	-1.20863500	0.14232000
C	2.90410300	-2.56252800	-1.10106100
C	1.75663400	-2.85683400	-1.85389900
C	4.07360600	-3.31023900	-1.31395000
C	1.77341200	-3.89411400	-2.78742200
H	0.85872400	-2.25918200	-1.72711000
C	4.08758300	-4.34333400	-2.25241900
H	4.97497100	-3.08058600	-0.75312000
C	2.93713100	-4.63898700	-2.98738000
H	0.87997500	-4.10824300	-3.36727500
H	4.99881800	-4.91371700	-2.41203900
H	2.95161600	-5.44083500	-3.72077400
C	4.55048700	-0.64917100	0.33543800
C	5.05933700	0.22927000	-0.63725200
C	5.37392500	-1.03034700	1.40384000
C	6.36652700	0.70573200	-0.54913000
H	3.41935000	3.11932500	-0.85496300
C	6.68122300	-0.54411600	1.49463500
H	4.99674900	-1.70269100	2.16810400
C	7.17984000	0.32149100	0.52063800
H	6.74554700	1.38451300	-1.30811500
H	7.30818600	-0.84363700	2.33031800
H	8.19532000	0.70058600	0.59581500
C	2.39984200	-2.05785500	1.72874800
C	1.78850600	-1.30310800	2.74336700
C	2.68307300	-3.41329300	1.96179500
C	1.48706600	-1.88908300	3.97465900
H	1.53051400	-0.26206900	2.56734100
C	2.37280400	-3.99736000	3.19108200
H	3.13944000	-4.01520600	1.18198000
C	1.77917300	-3.23614600	4.20091600
H	1.01696800	-1.29123400	4.75060400
H	2.59486800	-5.04794100	3.35873300
H	1.54198200	-3.69272000	5.15834700
P	-3.42127800	-0.12398400	0.11740600
C	-3.57626600	-0.93836200	1.76238000
C	-4.68442400	1.21701600	0.14145000
C	-4.07030100	-1.36406200	-1.08072600

C	-2.45546500	-1.61728800	2.26587700
C	-4.75323800	-0.90603000	2.52628100
C	-5.98254900	1.05877900	-0.36646000
C	-4.30860000	2.45457900	0.69198300
C	-3.70397600	-1.22277100	-2.42948500
C	-4.90563400	-2.42857600	-0.70753400
C	-2.51618100	-2.27064600	3.49714900
H	-1.52737200	-1.62325300	1.69994700
C	-4.80968200	-1.55430700	3.76152000
H	-5.62247800	-0.36716600	2.16059000
C	-6.89186200	2.11773800	-0.31551800
H	-6.28271100	0.11271200	-0.80671700
C	-5.22338900	3.50620900	0.74741500
H	-3.30015000	2.59478600	1.07446500
C	-4.18119900	-2.11800900	-3.38746300
H	-3.03272000	-0.42180800	-2.72622200
C	-5.37443500	-3.32672000	-1.66847800
H	-5.18637200	-2.56129800	0.33283500
C	-3.69401600	-2.24033400	4.24655600
H	-1.63761100	-2.78800800	3.87226500
H	-5.72507800	-1.51943000	4.34634400
C	-6.51542700	3.34057100	0.24284200
H	-7.89385500	1.98574400	-0.71532700
H	-4.92112300	4.45777000	1.17611800
C	-5.01674300	-3.17121400	-3.00922000
H	-3.88924800	-1.99698200	-4.42707000
H	-6.01828700	-4.14893000	-1.36723600
H	-3.74025100	-2.74120600	5.20994000
H	-7.22405900	4.16373400	0.27862700
H	-5.38189400	-3.87249000	-3.75490700

Substrate **c**

Sum of electronic and thermal Free Energies=-5450.058463

C	-0.25015900	-0.95252600	-2.11975000
N	-1.52579300	-1.12671300	-2.59070100
C	-1.68107900	-1.67292100	-3.79286900
C	-0.59293400	-2.08779100	-4.57092300
C	0.67180000	-1.87707300	-4.00367200
N	0.84820700	-1.32158200	-2.81033900
H	-4.43004700	-3.22012200	-2.58805700
H	1.58005000	-2.16522600	-4.53457400
S	-0.04227200	-0.26666300	-0.53088600
C	-0.77982200	-2.71341900	-5.88711300

H	0.16258100	-2.97749800	-6.41500900
O	-1.86479100	-2.94524600	-6.39206300
Cu	-3.01411500	-0.48882300	-1.29533900
Cu	-1.30286800	1.70347400	-0.40839100
I	-3.47453500	2.08018400	-2.00887200
P	-4.38286400	-1.85173600	-0.04309000
C	-6.19290200	-1.58714200	-0.25708700
C	-6.64561200	-0.28817100	-0.53770100
C	-7.12828300	-2.62842400	-0.14073700
C	-8.01055600	-0.03418400	-0.68310100
H	-5.92929800	0.51990200	-0.65903000
C	-8.49167900	-2.37046700	-0.29125200
H	-6.79124800	-3.64129600	0.05967000
C	-8.93484500	-1.07324700	-0.55998200
H	-8.34759200	0.97470500	-0.90480300
H	-9.20678300	-3.18405100	-0.20245500
H	-9.99656800	-0.87558800	-0.68136700
C	-4.14663200	-3.62918100	-0.48259800
C	-4.21701900	-3.98192200	-1.84160600
C	-3.86459600	-4.62482500	0.46242000
C	-4.02208800	-5.30175200	-2.24472500
H	-2.69576400	-1.79343500	-4.16214400
C	-3.65937100	-5.94671500	0.05519600
H	-3.80138500	-4.37197800	1.51593100
C	-3.73869200	-6.28817300	-1.29533700
H	-4.08358200	-5.55812900	-3.29886200
H	-3.43951800	-6.70822700	0.79876900
H	-3.57884200	-7.31614800	-1.60910100
C	-4.09360100	-1.77548600	1.77262800
C	-2.78684500	-1.51421300	2.21707100
C	-5.11194900	-1.97633800	2.71738000
C	-2.49998100	-1.47232900	3.58233200
H	-1.99240200	-1.33825500	1.49595700
C	-4.82336800	-1.92379200	4.08235100
H	-6.12895300	-2.16935600	2.38997100
C	-3.51901700	-1.67533700	4.51541700
H	-1.48558700	-1.27286900	3.91368000
H	-5.61954200	-2.07817100	4.80617900
H	-3.29660100	-1.63524200	5.57845700
Pd	2.67369100	-0.61869800	0.06096000
P	3.93825300	0.61493700	-1.50827600
C	3.24271800	2.20980700	-2.15762100
C	5.65181400	1.11527200	-0.97945500
C	4.28700500	-0.31793200	-3.07824900

C	2.04706300	2.15368600	-2.89778500
C	3.78500000	3.46944300	-1.86264600
C	6.62580200	1.60553300	-1.86566400
C	5.98737200	0.97845800	0.37488500
C	4.35869300	-1.71795900	-2.99781500
C	4.48522600	0.29226800	-4.32669700
C	1.43109700	3.31877700	-3.35352300
H	1.60323600	1.18839200	-3.12136800
C	3.16010100	4.63829100	-2.30801500
H	4.70164200	3.54477400	-1.28685700
C	7.89436500	1.95862000	-1.40493400
H	6.39732000	1.70708000	-2.92239000
C	7.25639000	1.33547200	0.83948700
H	5.24674100	0.56399400	1.05458700
C	4.64369600	-2.48584400	-4.12860400
H	4.16618700	-2.20000200	-2.04269600
C	4.76226800	-0.47538400	-5.46066100
H	4.40700900	1.37129400	-4.42103700
C	1.98695400	4.56844100	-3.05939500
H	0.51592700	3.25019400	-3.93662700
H	3.59895600	5.60414500	-2.07029900
C	8.21195600	1.82742000	-0.04976600
H	8.63720500	2.33356100	-2.10470100
H	7.49836600	1.21523100	1.89234900
C	4.84716500	-1.86587900	-5.36464700
H	4.69925700	-3.56850200	-4.04475700
H	4.91124700	0.01511200	-6.41950200
H	1.50953700	5.47793000	-3.41524100
H	9.20214600	2.10028800	0.30650600
H	5.06553800	-2.46229900	-6.24696800
P	2.91130600	-2.13889800	1.81187500
C	2.30112600	-3.85013800	1.41870200
C	4.64438300	-2.47606400	2.40185600
C	2.03463100	-1.78324500	3.41338300
C	1.06920000	-3.95951900	0.74970900
C	2.99776100	-5.02530100	1.73915100
C	4.98311900	-2.74394100	3.73767600
C	5.67034400	-2.45762900	1.44276800
C	1.89519000	-0.43899600	3.79538200
C	1.51467600	-2.77711900	4.25780900
C	0.53988600	-5.20947500	0.42838900
H	0.53054100	-3.05630500	0.47506300
C	2.47372000	-6.27704700	1.40329500
H	3.95303800	-4.96699700	2.25131100

C	6.30982400	-2.99127200	4.10073400
H	4.21212600	-2.75841300	4.50151500
C	6.99270100	-2.71939800	1.80192100
H	5.42365000	-2.21571300	0.41244000
C	1.27510400	-0.09657000	4.99821600
H	2.26996500	0.34116600	3.13826700
C	0.88818600	-2.43559900	5.45940400
H	1.59902700	-3.82283400	3.97724800
C	1.24364400	-6.37297100	0.75179700
H	-0.41909200	-5.27467300	-0.07971300
H	3.02992900	-7.17693100	1.65454500
C	7.31719000	-2.98450100	3.13465700
H	6.55359400	-3.19060300	5.14146800
H	7.77059300	-2.69954900	1.04303500
C	0.77113700	-1.09550500	5.83563600
H	1.17848300	0.94987900	5.27548000
H	0.49318500	-3.21891900	6.10175900
H	0.83765100	-7.34755100	0.49241600
H	8.34861700	-3.17701900	3.41889600
H	0.28644700	-0.83093100	6.77210200
P	-1.04606200	3.46514300	1.11324800
C	-2.02998400	3.12217300	2.63548600
C	0.64845500	3.87319200	1.70630000
C	-1.69702100	5.08032400	0.51091900
C	-3.33004800	2.61446400	2.46370000
C	-1.54356300	3.32104500	3.93534100
C	0.95260900	5.10628200	2.30857600
C	1.66782300	2.92339900	1.54255900
C	-1.42200500	5.44009700	-0.81780900
C	-2.43685400	5.95740600	1.31745400
C	-4.12902100	2.32801300	3.56978200
H	-3.71530800	2.44476600	1.46112900
C	-2.34526800	3.02599200	5.04133400
H	-0.54064000	3.70704700	4.08741100
C	2.24589100	5.37247900	2.75827500
H	0.18039400	5.86239300	2.41706000
C	2.96229700	3.19426300	1.99363600
H	1.46697800	1.97669100	1.04601300
C	-1.86254100	6.66308000	-1.32272500
H	-0.86964800	4.75865100	-1.45896700
C	-2.88313400	7.17815000	0.80598600
H	-2.67110600	5.68653000	2.34264000
C	-3.63754900	2.53184700	4.86179100
H	-5.13038400	1.93354900	3.42180800

H	-1.95626800	3.18538700	6.04379400
C	3.25197500	4.41493200	2.60447300
H	2.46890500	6.33005100	3.22171000
H	3.74204700	2.45306900	1.84620600
C	-2.59469800	7.53403100	-0.51244000
H	-1.64658500	6.92889900	-2.35399200
H	-3.45862500	7.84861100	1.43895200
H	-4.25849600	2.30198600	5.72354500
H	4.26121100	4.62579200	2.94837600
H	-2.94597300	8.48249000	-0.91004500

Substrate **TS1**

Sum of electronic and thermal Free Energies=-5450.016563

C	0.68892900	-0.64240700	-2.03987600
N	-0.53322200	-1.23777500	-1.76021300
C	-1.18993700	-1.80030400	-2.77011900
C	-0.69105000	-1.87014300	-4.07590700
C	0.62131700	-1.38299600	-4.23156000
N	1.29476300	-0.80671100	-3.25501000
H	-3.74806500	-3.55329000	-2.27548600
H	1.13822900	-1.48997400	-5.18761800
S	0.52105500	1.71286400	-1.61032200
C	-1.45089900	-2.50940800	-5.14204100
H	-0.93438000	-2.54090100	-6.12754000
O	-2.57063400	-2.99311400	-5.01763500
Cu	-1.51064100	-1.33243400	0.03582800
Cu	-1.17342500	1.96002100	-0.13064700
I	-1.49923900	0.35043900	2.10417900
P	-3.11095900	-3.06603400	0.54718300
C	-4.86585000	-2.49765000	0.48728400
C	-5.13388400	-1.14067900	0.72890000
C	-5.93651700	-3.36647900	0.21775600
C	-6.44593900	-0.66481000	0.70889300
H	-4.31571200	-0.45776200	0.93750000
C	-7.24710300	-2.88667700	0.19837800
H	-5.74700400	-4.41575200	0.01317000
C	-7.50392300	-1.53607100	0.44399300
H	-6.63498300	0.39013800	0.88519600
H	-8.06641000	-3.56904100	-0.01265100
H	-8.52488000	-1.16388400	0.42260400
C	-3.13874500	-4.60801700	-0.47800300
C	-3.45503600	-4.50596100	-1.84472200
C	-2.78839200	-5.86541700	0.03706700

C	-3.41001700	-5.62369700	-2.67628500
H	-2.15225100	-2.24655300	-2.55056800
C	-2.75188000	-6.98797200	-0.79596400
H	-2.54622900	-5.97413600	1.08914700
C	-3.05725800	-6.87063400	-2.15266100
H	-3.63655500	-5.50632000	-3.73177000
H	-2.48224600	-7.95466600	-0.37836100
H	-3.02011800	-7.74371000	-2.79871700
C	-2.87175400	-3.69362400	2.26439600
C	-1.57610400	-3.66615900	2.80280800
C	-3.92038900	-4.20947200	3.04132700
C	-1.32823900	-4.16413400	4.08286700
H	-0.75843300	-3.23952300	2.22867700
C	-3.67309400	-4.69667100	4.32544600
H	-4.93195900	-4.22466200	2.64704600
C	-2.37698500	-4.67907200	4.84649300
H	-0.31810800	-4.13343500	4.48143900
H	-4.49443200	-5.08853700	4.91966600
H	-2.18795600	-5.05810600	5.84742000
Pd	1.99254500	0.05789800	-0.64877100
P	3.59254800	1.72377000	0.43669500
C	2.97540700	2.76825800	1.83756600
C	5.24751600	1.20281800	1.09922000
C	4.05360600	2.95612100	-0.86658600
C	1.59144400	2.93240100	1.98561500
C	3.83322300	3.41504600	2.74503800
C	6.45313400	1.48982800	0.44356100
C	5.29663100	0.48193100	2.30591200
C	3.94926600	2.58036300	-2.21429100
C	4.51817100	4.24384100	-0.55646300
C	1.07233400	3.73129900	3.00671300
H	0.92090800	2.42672000	1.29945700
C	3.31363700	4.21488400	3.76389700
H	4.90814900	3.28698100	2.66594200
C	7.67422300	1.07977100	0.98586600
H	6.44452800	2.04465600	-0.48840500
C	6.51577800	0.07949700	2.84941000
H	4.37855300	0.24641800	2.83565600
C	4.32262900	3.46509000	-3.22809500
H	3.54558800	1.60610900	-2.47038400
C	4.88249200	5.13011900	-1.57108600
H	4.58749700	4.56339200	0.47850000
C	1.93237900	4.37673000	3.89605700
H	-0.00467600	3.83388600	3.10868900

H	3.99034400	4.70819200	4.45719000
C	7.71143900	0.38014900	2.19159700
H	8.59746400	1.31709500	0.46355100
H	6.53031700	-0.46606700	3.78952800
C	4.78965400	4.74090600	-2.90951700
H	4.22758500	3.16031500	-4.26685000
H	5.23593900	6.12564000	-1.31452100
H	1.52980500	4.99612700	4.69348100
H	8.66282200	0.07092700	2.61685500
H	5.07158400	5.43269300	-3.69934300
P	3.12485800	-2.01383900	-0.25006200
C	2.53632000	-3.54176500	-1.12170100
C	4.87952200	-1.90947000	-0.80805900
C	3.11895200	-2.59169800	1.50390200
C	1.21789400	-3.96969900	-0.89389100
C	3.34658600	-4.29347000	-1.98514200
C	5.98529800	-2.33311200	-0.06089500
C	5.08693200	-1.37775500	-2.09454200
C	2.47418000	-1.79644100	2.46324100
C	3.66057700	-3.82778800	1.89789200
C	0.72310900	-5.11891100	-1.50869100
H	0.56876200	-3.39540000	-0.23926700
C	2.84866700	-5.44300300	-2.60474000
H	4.36867300	-3.98787000	-2.17875300
C	7.27359000	-2.24162000	-0.59440500
H	5.85081900	-2.72265200	0.94221400
C	6.37329500	-1.29965300	-2.62733600
H	4.23492600	-1.03645200	-2.67847300
C	2.39758500	-2.21263600	3.79593600
H	2.01312800	-0.85952300	2.16110300
C	3.59264500	-4.23750900	3.22930800
H	4.12198200	-4.47777200	1.15980400
C	1.53910800	-5.85871200	-2.36850000
H	-0.29889400	-5.43343100	-1.32187700
H	3.49180000	-6.01222100	-3.27118600
C	7.47049700	-1.73344900	-1.87830200
H	8.12323200	-2.56650700	0.00008700
H	6.51819000	-0.89472100	-3.62549300
C	2.96486300	-3.42834800	4.18178000
H	1.88870300	-1.58648000	4.52357400
H	4.02076400	-5.19260500	3.52232000
H	1.15154300	-6.75172400	-2.85165800
H	8.47361000	-1.66783700	-2.29157900
H	2.91156900	-3.75093600	5.21854300

P	-2.74848600	3.69244700	-0.32825000
C	-3.27221000	4.63804500	1.16925800
C	-2.20370100	4.98628800	-1.52353600
C	-4.32639300	3.06989700	-1.05451600
C	-3.47245600	3.91683900	2.35952000
C	-3.45364900	6.02961600	1.18087100
C	-3.10528600	5.74661600	-2.28642300
C	-0.82591700	5.20854400	-1.67269100
C	-4.22814300	2.10093400	-2.06872600
C	-5.59659200	3.50351900	-0.64820900
C	-3.86405200	4.57242900	3.52727600
H	-3.30914900	2.84291300	2.37452700
C	-3.83704100	6.68328200	2.35444100
H	-3.29168100	6.60606500	0.27575000
C	-2.63612800	6.72147700	-3.16795300
H	-4.17383800	5.57104900	-2.19848900
C	-0.36018300	6.18772300	-2.55229000
H	-0.11673200	4.59474800	-1.12433900
C	-5.37666000	1.59006100	-2.67304300
H	-3.24815800	1.74933000	-2.38421600
C	-6.74603300	2.98280000	-1.24982900
H	-5.68997500	4.24868900	0.13615400
C	-4.04662500	5.95741000	3.52802200
H	-4.01478300	3.99999900	4.43875600
H	-3.97049700	7.76204100	2.34874200
C	-1.26319400	6.94595200	-3.29902000
H	-3.34269300	7.30164800	-3.75597900
H	0.70968300	6.34066500	-2.66367200
C	-6.63887100	2.02878100	-2.26309300
H	-5.28569600	0.84494100	-3.45878300
H	-7.72498300	3.32926300	-0.92796700
H	-4.34361200	6.46867100	4.44004700
H	-0.89980600	7.70192200	-3.99038000
H	-7.53350200	1.62532600	-2.72977400

Substrate **d**

Sum of electronic and thermal Free Energies=-5450.018562

C	-2.13969700	2.05130500	-0.39248300
C	-4.08329300	0.99443700	-1.16197700
C	-4.73380900	2.21394400	-1.32015600
C	-3.98541000	3.34632800	-0.96331200
H	-4.59365300	0.06098300	-1.39325900
H	-4.43023600	4.33648400	-1.05227200

C	-6.11926800	2.29566900	-1.81018100
H	-6.58598200	1.31358500	-2.04988000
O	-6.74088600	3.33264600	-1.95197700
N	-2.74188700	3.26785900	-0.50838300
N	-2.82191000	0.90110700	-0.71665900
Pd	-0.19441900	1.94969700	0.27121100
S	2.05589800	1.72153300	1.12253700
Cu	2.45667900	-0.27508600	0.18362300
I	0.48491100	-1.65866800	-1.42999100
Cu	-1.95603100	-0.96360700	-0.64735000
P	-3.31570200	-2.89905000	-0.41701000
C	-5.08027500	-2.56666300	0.01438100
C	-3.40354500	-3.83611900	-2.00134800
C	-2.77660600	-4.16660100	0.81001900
C	-5.33752500	-1.58768500	0.98995000
C	-6.16469400	-3.21432200	-0.59805400
C	-3.63123600	-5.22024100	-2.05418100
C	-3.23753900	-3.12837600	-3.20183500
C	-1.41606100	-4.52076800	0.82832500
C	-3.65808500	-4.79050200	1.70521800
C	-6.64751600	-1.27516300	1.35384100
H	-4.51318700	-1.06178600	1.46531600
C	-7.47561000	-2.89133900	-0.23930300
H	-5.98799400	-3.96902700	-1.35793000
C	-3.70621100	-5.87683700	-3.28371000
H	-3.74272200	-5.78635300	-1.13408800
C	-3.31822400	-3.78509000	-4.43033400
H	-3.02601900	-2.06247900	-3.17384400
C	-0.95443000	-5.49451700	1.71477600
H	-0.71787700	-4.03440000	0.15215800
C	-3.18785900	-5.75568800	2.59963100
H	-4.71122000	-4.52719200	1.70567700
C	-7.72006200	-1.92395000	0.73715600
H	-6.82307400	-0.51364300	2.10808700
H	-8.30549300	-3.39779200	-0.72511400
C	-3.55317200	-5.16064200	-4.47289200
H	-3.87989000	-6.94925300	-3.31164800
H	-3.18163600	-3.22530900	-5.35151400
C	-1.83860100	-6.11205500	2.60403100
H	0.09919600	-5.76105400	1.71027300
H	-3.88034900	-6.23048500	3.28980800
H	-8.74093900	-1.67253600	1.01192800
H	-3.60672900	-5.67463700	-5.42877600
H	-1.47705400	-6.86612000	3.29824700

P	4.34780500	-1.65396400	0.18694500
C	4.11324200	-3.40472900	0.72973000
C	5.23150500	-1.81245400	-1.42757100
C	5.62948700	-1.03207600	1.36191400
C	3.27674900	-3.63001800	1.83528800
C	4.72360600	-4.50248400	0.10607000
C	6.61480700	-1.63212900	-1.57479000
C	4.46116600	-2.11261100	-2.56443000
C	5.58149200	0.31816600	1.74297700
C	6.63786300	-1.85608000	1.88969600
C	3.07758500	-4.92262100	2.32008900
H	2.77993600	-2.79205500	2.31723700
C	4.50924600	-5.79817200	0.58388900
H	5.36689300	-4.34808000	-0.75466600
C	7.21600100	-1.76007700	-2.82968100
H	7.22641900	-1.39147900	-0.71129600
C	5.06643900	-2.25267900	-3.81292100
H	3.38475200	-2.22960900	-2.47415700
C	6.53769500	0.83626100	2.61967500
H	4.78189400	0.95570800	1.37377200
C	7.58901400	-1.33495900	2.76752300
H	6.67534900	-2.90794200	1.62032500
C	3.69136700	-6.01151800	1.69408600
H	2.43955200	-5.07939300	3.18641700
H	4.98728400	-6.63952000	0.08870700
C	6.44567300	-2.07585200	-3.94977700
H	8.28903200	-1.61576000	-2.92784400
H	4.45624600	-2.48871700	-4.68066200
C	7.54226600	0.01354300	3.13113300
H	6.48438300	1.88158200	2.91187500
H	8.36330700	-1.98276300	3.17074600
H	3.53178200	-7.01928200	2.06892500
H	6.91594000	-2.17937800	-4.92436300
H	8.28114600	0.41717700	3.81878100
P	0.64094500	2.92595900	-1.80486500
C	2.22730400	2.40565300	-2.59510900
C	-0.55262900	2.89057200	-3.22155600
C	0.87784800	4.73412300	-1.49626500
C	3.43075900	2.57397600	-1.88437000
C	2.27508000	1.85366800	-3.88436600
C	-0.93142900	4.04101700	-3.92787500
C	-1.09645900	1.65180200	-3.60248100
C	0.00198100	5.38051700	-0.60818000
C	1.87288500	5.48745500	-2.13818700

C	4.64709000	2.20782800	-2.46255300
H	3.40583000	2.97117100	-0.87673100
C	3.49482000	1.47884600	-4.45162700
H	1.36466600	1.71641200	-4.45606900
C	-1.83376500	3.95583700	-4.99122100
H	-0.52506500	5.00754700	-3.64925600
C	-1.98506400	1.56817000	-4.67544900
H	-0.81611800	0.75125000	-3.06257800
C	0.12518800	6.74958900	-0.36650000
H	-0.78725500	4.81216900	-0.12565700
C	1.99652200	6.85607700	-1.88793200
H	2.55789700	5.00723700	-2.82873700
C	4.68422500	1.65612300	-3.74458100
H	5.56783100	2.34832100	-1.90226900
H	3.51043600	1.05189800	-5.45108600
C	-2.36029100	2.72067100	-5.37055700
H	-2.12115300	4.85830700	-5.52450900
H	-2.38388400	0.59989200	-4.96860100
C	1.12535000	7.48995300	-1.00067200
H	-0.55927900	7.23534000	0.32418600
H	2.77635200	7.42453800	-2.38822100
H	5.63232800	1.36039200	-4.18537600
H	-3.05867600	2.65596300	-6.20090300
H	1.22487300	8.55464800	-0.80518700
P	-0.71022000	1.73645700	2.58748200
C	0.00651800	0.29922600	3.48857900
C	-0.25141400	3.24792400	3.55517100
C	-2.51721600	1.62013200	3.04439900
C	-0.14779700	-0.97830900	2.92842900
C	0.64721900	0.42352800	4.72784100
C	-0.82640300	3.48682600	4.81652200
C	0.65080400	4.18599200	3.03375600
C	-3.35767500	2.68955700	2.68533000
C	-3.07394200	0.53923700	3.74346700
C	0.29443800	-2.11106500	3.61180300
H	-0.60089300	-1.09084600	1.94700200
C	1.11067200	-0.70940600	5.40052700
H	0.79811800	1.40375000	5.16621400
C	-0.49615800	4.63129100	5.54276300
H	-1.53916300	2.78182500	5.23335200
C	0.97098500	5.33550600	3.75997100
H	1.11369800	4.00260100	2.07087800
C	-4.71044600	2.68044800	3.02056200
H	-2.94854400	3.53764700	2.14532900

C	-4.43236200	0.53132800	4.08110800
H	-2.44893800	-0.29394300	4.04546500
C	0.92619000	-1.97894900	4.85197000
H	0.14667800	-3.09224900	3.16954500
H	1.61468200	-0.59564700	6.35676000
C	0.40251300	5.56065800	5.01401200
H	-0.94649900	4.79804400	6.51790700
H	1.66964200	6.05330900	3.33856200
C	-5.25360200	1.60089800	3.72422600
H	-5.33989700	3.52096800	2.73991200
H	-4.83984300	-0.30972900	4.63663600
H	1.27523200	-2.85992100	5.38474400
H	0.65481500	6.45584400	5.57687600
H	-6.30511000	1.60171600	4.00049700

Substrate **e**

Sum of electronic and thermal Free Energies=-2809.726998

P	1.69305800	-1.27346100	-0.10326600
Pd	0.16209700	0.61267300	-0.20514800
N	2.28168600	2.13450200	1.00364800
C	1.74065700	1.87335200	-0.20903000
C	3.28634900	3.00561500	1.04925700
N	2.17192600	2.39750500	-1.37134700
C	3.78568500	3.63846700	-0.09868300
H	3.72654900	3.22001300	2.02161900
C	3.17924500	3.26772600	-1.30316000
C	4.89302300	4.60497200	-0.04736000
H	3.52488700	3.69013200	-2.24883400
H	5.18700000	5.02399300	-1.03660100
O	5.47177100	4.94698100	0.96840800
P	-2.10498000	-0.42751100	0.02247100
C	-0.81796300	2.36868700	-0.21863700
C	-1.39785600	3.44533600	-0.24286900
C	-2.12726100	4.72660600	-0.29053500
C	-3.53742700	4.54876900	0.32131200
H	-4.11095700	3.80013300	-0.23540000
H	-3.47205000	4.21665900	1.36323500
H	-4.08869800	5.49784100	0.29606300
C	-2.26389000	5.18432200	-1.76247000
H	-2.80940300	4.43833900	-2.35010000
H	-2.80741600	6.13659000	-1.81868900
H	-1.27808300	5.32130100	-2.21974300
C	-1.35182600	5.79941300	0.51030300

H	-1.23849300	5.49799100	1.55737100
H	-0.35059000	5.94883400	0.09224900
H	-1.88484400	6.75873000	0.48294000
C	-2.85774700	-0.08541200	1.67895400
C	-3.87116600	-0.89885000	2.21520400
C	-2.41183400	1.01992500	2.42192900
C	-4.42879600	-0.61003000	3.46173100
H	-4.22099600	-1.76726700	1.66616800
C	-2.97205200	1.30303600	3.66929800
H	-1.64431000	1.66700400	2.01078100
C	-3.97945900	0.49120600	4.19278500
H	-5.21173400	-1.24951100	3.86116200
H	-2.61498900	2.16148900	4.23210700
H	-4.41100500	0.71303800	5.16542800
C	-2.40534000	-2.24798900	-0.16282000
C	-1.84613100	-3.12434600	0.78358200
C	-3.12287700	-2.79111400	-1.23894400
C	-2.00722300	-4.50344400	0.65939700
H	-1.28971000	-2.72926600	1.62795400
C	-3.27745500	-4.17457800	-1.36468300
H	-3.56978600	-2.13626000	-1.97954900
C	-2.72222900	-5.03440000	-0.41729900
H	-1.57111500	-5.16253700	1.40533900
H	-3.84069700	-4.57647700	-2.20305900
H	-2.84601900	-6.10965500	-0.51466700
C	-3.27424000	0.29668200	-1.20821000
C	-4.64995800	0.42027400	-0.96556600
C	-2.76162100	0.70827700	-2.44763200
C	-5.49676400	0.93873500	-1.94720800
H	-5.06227900	0.12386600	-0.00605100
C	-3.61126100	1.21353300	-3.43308700
H	-1.69165100	0.66119500	-2.62806400
C	-4.98024100	1.33154400	-3.18396100
H	-6.55978400	1.03735100	-1.74340600
H	-3.19960500	1.53023800	-4.38759300
H	-5.64070500	1.73549500	-3.94675200
C	1.58801300	-2.01485400	1.58329400
C	1.51959600	-1.11432900	2.66268200
C	1.55060200	-3.39275300	1.83948000
C	1.42657600	-1.59097800	3.97092900
H	1.54791800	-0.04313100	2.47459400
C	1.44806900	-3.86347400	3.15123400
H	1.58664600	-4.10172000	1.01915800
C	1.38688400	-2.96558400	4.21821100

H	1.37702700	-0.88570200	4.79597000
H	1.41647000	-4.93410900	3.33664100
H	1.30604000	-3.33444700	5.23724000
C	3.49547300	-0.89802000	-0.29937000
C	4.43492900	-1.09526100	0.72110100
C	3.93214300	-0.40590200	-1.54114500
C	5.78619100	-0.81182800	0.50257900
H	4.11881700	-1.46933300	1.68900000
C	5.28112100	-0.12984400	-1.75711300
H	3.21541100	-0.22938900	-2.33787700
C	6.21289600	-0.33213900	-0.73521800
H	6.50289700	-0.96850300	1.30437700
H	5.60402900	0.24788900	-2.72364300
H	7.26388200	-0.11293600	-0.90341400
C	1.51051200	-2.65181000	-1.31595700
C	2.46374700	-3.68198500	-1.41033600
C	0.43253100	-2.64445300	-2.21011500
C	2.31943700	-4.69441200	-2.35766100
H	3.32886000	-3.68249000	-0.75352900
C	0.29148600	-3.65633600	-3.16274300
H	-0.29290500	-1.83955400	-2.16459800
C	1.23090800	-4.68431300	-3.23476500
H	3.06246500	-5.48513200	-2.41897000
H	-0.55220500	-3.63633700	-3.84664700
H	1.12331100	-5.47087000	-3.97695800

Substrate **TS2**

Sum of electronic and thermal Free Energies=-2809.715902

Pd	-0.10401000	0.45768600	0.03037600
N	-2.27166700	2.04698900	-1.07445800
C	-1.62984000	1.83632100	0.10873800
C	-3.44025800	2.66961000	-1.02095600
N	-2.13501200	2.14598700	1.32812100
C	-4.01952100	3.10306900	0.18549500
H	-3.96541300	2.83617100	-1.96026200
C	-3.30436000	2.77260700	1.34581200
C	-5.30703300	3.79781700	0.23380100
H	-3.70917400	3.02060500	2.32927600
H	-5.65335100	4.05541300	1.26130400
O	-5.98290700	4.09205600	-0.73913200
C	0.22753300	2.44524500	0.00927400
C	0.60337500	3.61410900	0.00590200

C	1.00807100	5.02965700	0.01205500
C	-0.12981400	5.87680400	0.63396700
H	-1.05189200	5.78143600	0.05089300
H	-0.34082100	5.55443200	1.65906800
H	0.15682400	6.93586100	0.65542000
C	1.27277300	5.50397200	-1.43642300
H	1.56541900	6.56158800	-1.44106600
H	2.07726100	4.91953800	-1.89420000
H	0.37491400	5.39153600	-2.05331300
C	2.29475400	5.20071100	0.85546300
H	2.12810100	4.87829000	1.88903400
H	3.11653900	4.60828500	0.44062400
H	2.59873500	6.25512300	0.86861700
P	2.28426600	-0.24362200	0.00444000
C	2.81449800	-0.42770000	1.76681700
C	2.96589200	-1.73255200	-0.86080700
C	3.40490500	1.07057400	-0.65537900
C	2.37573300	0.55616700	2.67325300
C	3.56678600	-1.50774600	2.25219500
C	4.34810300	-1.94236100	-1.01646700
C	2.07844400	-2.66218700	-1.41778700
C	3.10633800	1.60643200	-1.91798200
C	4.54807900	1.51980100	0.01980200
C	2.70028700	0.46611400	4.02628300
H	1.77477500	1.38800000	2.31489400
C	3.88032100	-1.59905000	3.61182000
H	3.90963000	-2.28179100	1.57337100
C	4.82324500	-3.06695600	-1.68992200
H	5.05462200	-1.21827700	-0.62152100
C	2.55408900	-3.78576200	-2.09845900
H	1.01009300	-2.49920300	-1.33960500
C	3.94900900	2.55011900	-2.50426100
H	2.20583100	1.29201300	-2.43814200
C	5.38428200	2.47667600	-0.56302900
H	4.78803600	1.12842700	1.00362800
C	3.45154200	-0.61291800	4.50040500
H	2.35649900	1.23561200	4.71224400
H	4.46395800	-2.44244900	3.97209700
C	3.92644400	-3.99305400	-2.23121000
H	5.89416900	-3.21572800	-1.80107500
H	1.84666700	-4.48848100	-2.52997100
C	5.09070000	2.98878300	-1.82744800
H	3.70862400	2.95041100	-3.48562600
H	6.26648400	2.81731800	-0.02712000

H	3.69658500	-0.68551700	5.55669700
H	4.29901400	-4.86493800	-2.76248900
H	5.74355800	3.72942900	-2.28167800
P	-1.53890900	-1.51620200	-0.02134600
C	-1.63718100	-2.11431100	-1.76844800
C	-1.17754600	-3.01025100	1.00590200
C	-3.30559500	-1.21284600	0.43717900
C	-1.72832800	-1.13064300	-2.77155700
C	-1.59162500	-3.46549100	-2.14248900
C	-2.10746800	-4.05600600	1.14970800
C	0.03697800	-3.08830000	1.69984400
C	-3.57713500	-0.81736700	1.75820700
C	-4.37227700	-1.35791100	-0.46033400
C	-1.78831400	-1.49997700	-4.11568700
H	-1.75680900	-0.07795200	-2.49711300
C	-1.63866900	-3.82802300	-3.49161700
H	-1.51238100	-4.23913200	-1.38568000
C	-1.81140900	-5.16245200	1.94488200
H	-3.07014900	-3.99731200	0.64999200
C	0.33055000	-4.19386600	2.50199600
H	0.74781200	-2.27240200	1.63237600
C	-4.88853200	-0.59295500	2.17389700
H	-2.76088000	-0.67890800	2.46154200
C	-5.68511600	-1.12147000	-0.04287900
H	-4.18434900	-1.65660700	-1.48633800
C	-1.73980000	-2.84813500	-4.47984100
H	-1.86445500	-0.73051600	-4.87929000
H	-1.59946400	-4.87898900	-3.76666500
C	-0.58968200	-5.23481200	2.62101400
H	-2.53864700	-5.96387600	2.04536900
H	1.27543200	-4.22994800	3.03712100
C	-5.94697900	-0.74321200	1.27372700
H	-5.08306700	-0.29343900	3.20043100
H	-6.50165800	-1.23599400	-0.75086200
H	-1.77753000	-3.13227400	-5.52814500
H	-0.36427000	-6.09469600	3.24630700
H	-6.96865100	-0.56219100	1.59683900

Substrate **3a**

Sum of electronic and thermal Free Energies=-610.873803

C	-2.43500100	1.34566900	-0.00060500
C	-0.53379100	0.09614900	-0.00348800

C	-2.51617900	-1.02778600	-0.00134600
C	-3.21905600	0.18743200	-0.00018600
H	-2.90138000	2.33199400	0.00029500
H	-3.06216200	-1.96924400	-0.00100000
C	-4.69389700	0.23909000	0.00153300
H	-5.12480600	1.26446800	0.00201500
C	0.89362300	0.04498600	-0.00434400
C	2.10564600	-0.00044300	-0.00558400
C	3.57509700	-0.05915000	-0.00193300
C	4.04082800	-1.19748500	-0.94114800
H	5.13573700	-1.25361600	-0.94046500
H	3.64419900	-2.16384100	-0.61372300
H	3.70585900	-1.02100200	-1.96850900
C	4.05835100	-0.34266200	1.44192000
H	5.15343500	-0.39175300	1.46033200
H	3.73692200	0.44875600	2.12674300
H	3.66328800	-1.29539400	1.80889300
C	4.14533300	1.29371500	-0.48911300
H	3.81185300	1.51642100	-1.50793800
H	3.82318400	2.11289800	0.16182100
H	5.24110800	1.25840700	-0.48486100
O	-5.41244900	-0.74218800	0.00214500
N	-1.18928000	-1.08906600	-0.00290300
N	-1.10405800	1.32082800	-0.00209700

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