Supporting Information

A Route to Convert CO_2: Synthesis of 3,4,5-Trisubstituted Oxazolones

Jiayin Hu, Jun Ma*, Zhaofu Zhang, Qinggong Zhu, Huacong Zhou, Wenjing Lu, Buxing Han*

Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, PR China; Tel: (+) 86-10-62562821; E-mail: Majun@iccas.ac.cn; Hanbx@iccas.ac.cn

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1. Experimental Results

1.1 Table S1

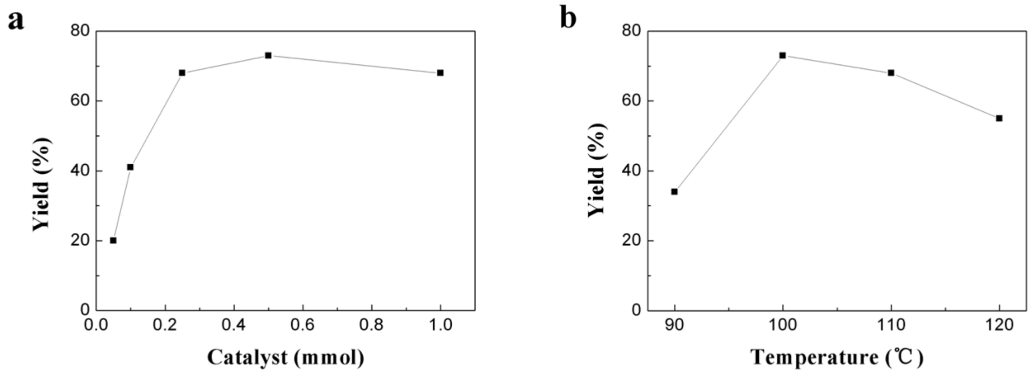
Table S1 Reaction of CO_2 with propargylic amine **1a** in various cataylsts.[a]

Entry	Catalyst	Conversion[b]/%	Yield[b]/%	Selectivity/%
1	--	0	0	--
2	Cs_2CO_3	40	4	10
3	TBD[c]	>99	22	22
4	DBU[d]	>99	32	32
5	[Bmim][OAc]	>99	45	45

[a] Typical reaction conditions were as follows until otherwise stated: 0.5 mmol of **1a**, 0.05 mmol of catalyst, 0.5 mL solvent of N,N-dimethylformamide, 0.1 MPa CO_2, 100 ℃, 2 h. [b] Conversion and yield were determined by ^{1}H NMR spectroscopy using 1,3,5-trioxane as an internal standard. [c] TBD =1,5,7-triazabicyclo[4.4.0]dec-5-ene. [d] DBU = 1,8-diazabicyclo[5.4.0]undec-7-ene.

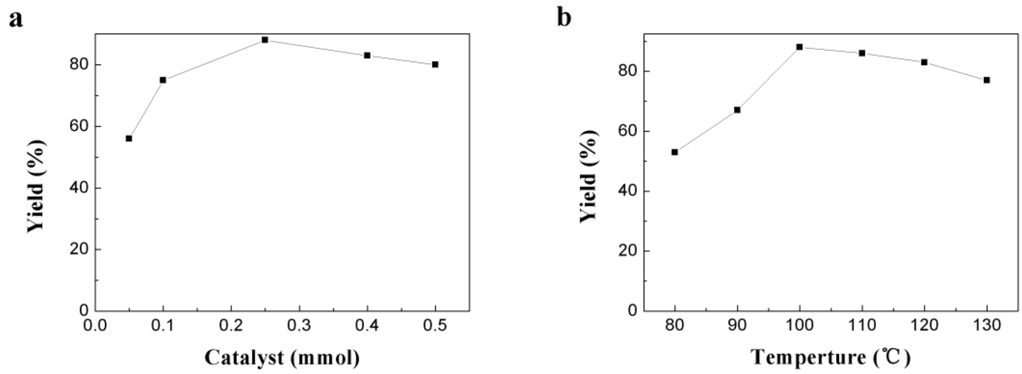
1.2. Figures S1-S4

Figure S1 Optimization of catalyst amount and temperature



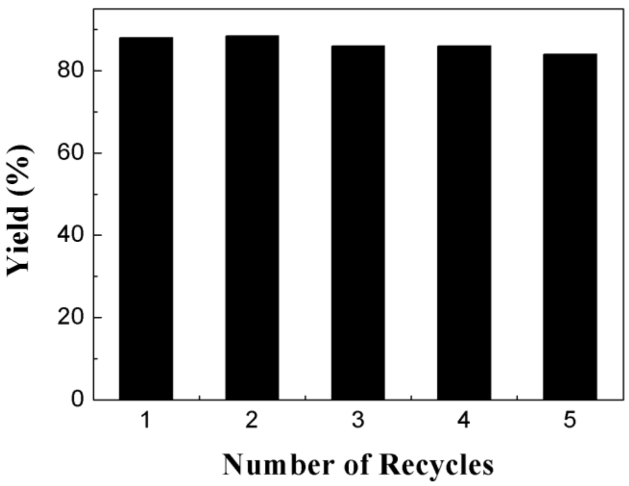
Typical reaction conditions were as follows until otherwise stated: **a**) 0.5 mmol of **1a**, 0.1 MPa CO_2 and different dosage of [Bmim][OAc], 100 ^oC, 2h. **b**) 0.5 mmol of **1a**, 0.5 mmol of [Bmim][OAc], 0.1 MPa CO_2, different temperatures, 2 h. Yields were determined by ^1H NMR spectroscopy using 1,3,5-trioxane as an internal standard.

Figure S2 Optimization of IL system amount and temperature



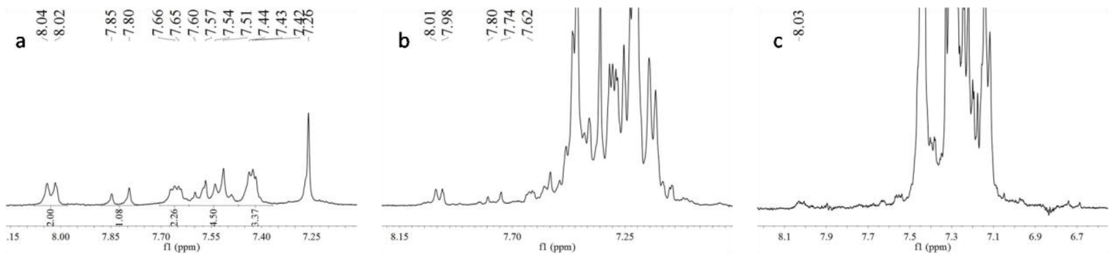
Typical reaction conditions were as follows until otherwise stated: **a**) 0.5 mmol of **1a**, 0.5 mmol of [Bmim][Tf_2N] and different dosage of [Bmim][OAc], 0.1 MPa CO_2, 100 ^oC, 12 h. **b**) 0.5 mmol of **1a**, , 0.25 mmol of [Bmim][OAc] and 0.5 mmol of [Bmim][Tf_2N], 0.1 MPa CO_2, different temperatures, 12 h. Yields were determined by ^1H NMR spectroscopy using 1,3,5-trioxane as an internal standard.

Figure S3 Recyclability of the IL system



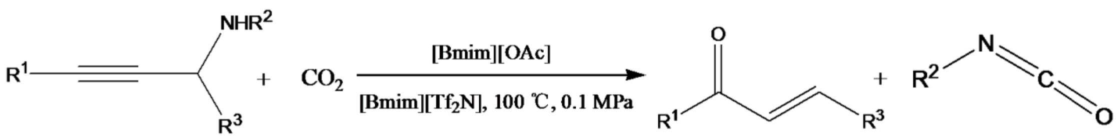
Typical reaction conditions were as follows until otherwise stated: 0.5 mmol of **1a**, 0.25 mmol of [Bmim][OAc] and 0.5 mmol of [Bmim][Tf_2N], 0.1 MPa CO_2, 100 ^oC, 12 h. After the reaction, the product was extracted by diethyl ether and yields were determined by ^1H NMR spectroscopy using 1,3,5-trioxane as an internal standard. The IL mixture was used directly for the next run after drying.

Figure S4 The characteristic peak of chalcone in different reaction



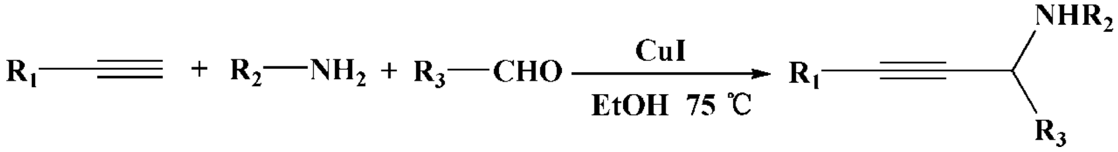
a: the pure chalcone isolated by silica gel column chromatography. b: reaction condition was 0.5 mmol of **1a**, 0.5 mmol of [Bmim][OAc], 0.1 MPa CO_2, 100 ^oC, 2 h. c: reaction condition was 0.5 mmol of **1a**, 0.25 mmol of [Bmim][OAc] and 0.5 mmol of [Bmim][Tf_2N], 0.1 MPa CO_2, 100 ^oC, 12 h.

Scheme S1 Possible side reaction.[S2]

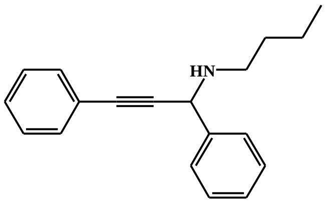


1.3. Substrates

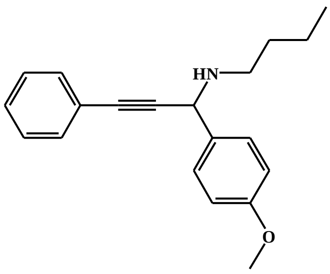
Preparation propargylic amines[s3]



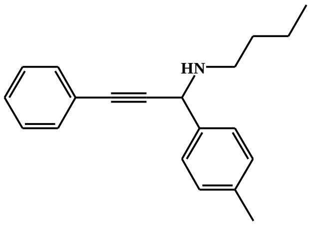
Data:



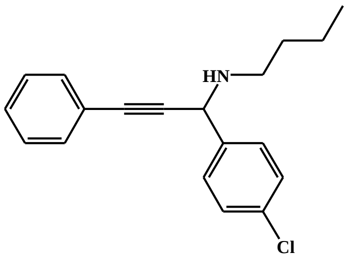
Butyl-(1,3-diphenyl-prop-2-ynyl)-amine (1a). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.3 Hz, 2H), 7.48 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.35 to 7.27 (m, 4H), 4.82 (s, 1H), 2.87 (dt, *J* = 11.2, 7.3 Hz, 1H), 2.74 (dt, *J* = 11.2, 7.1 Hz, 1H), 1.65 to 1.45 (m, 3H), 1.45 to 1.33 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.70, 131.74, 128.53, 128.27, 128.11, 127.70, 127.61, 123.27, 89.67, 85.27, 54.77, 47.11, 32.17, 20.53, 14.03.



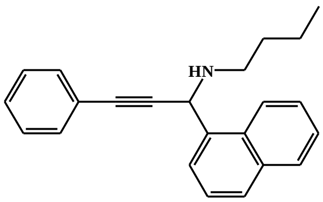
Butyl-[1-(4-methoxy-phenyl)-3-phenyl-prop-2-ynyl]-amine (1b). yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 to 7.42 (m, 4H), 7.40 to 7.27 (m, 3H), 6.91 (d, *J* = 8.6 Hz, 2H), 4.77 (s, 1H), 3.82 (s, 3H), 2.85 (dt, *J* = 11.2, 7.3 Hz, 1H), 2.72 (dt, *J* = 11.2, 7.1 Hz, 1H), 1.65 to 1.45 (m, 3H), 1.39 (dq, *J* = 14.6, 7.3 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.16, 132.92, 131.72, 128.74, 128.26, 128.06, 123.31, 113.86, 89.91, 85.09, 55.32, 54.15, 47.02, 32.15, 20.55, 14.03.



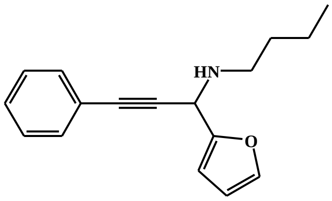
Butyl-(3-phenyl-1-p-tolyl-prop-2-ynyl)-amine (1c). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 8.6, 3.7 Hz, 4H), 7.39 to 7.29 (m, 3H), 7.21 (d, *J* = 7.8 Hz, 2H), 4.81 (s, 1H), 2.89 (dt, *J* = 11.3, 7.3 Hz, 1H), 2.75 (dt, *J* = 11.2, 7.1 Hz, 1H), 2.39 (s, 3H), 1.56 (dt, *J* = 13.8, 7.1 Hz, 3H), 1.47 to 1.35 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.79, 137.37, 131.75, 129.22, 128.27, 128.07, 127.53, 123.37, 89.91, 85.10, 54.52, 47.10, 32.19, 21.17, 20.57, 14.07.



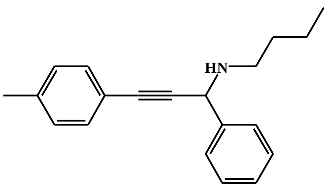
Butyl-[1-(4-chloro-phenyl)-3-phenyl-prop-2-ynyl]-amine (1d). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.3 Hz, 2H), 7.51 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.42 to 7.28 (m, 5H), 4.81 (s, 1H), 2.86 (dt, *J* = 11.2, 7.2 Hz, 1H), 2.74 (dt, *J* = 11.2, 7.0 Hz, 1H), 1.56 (ddd, *J* = 15.3, 10.1, 4.6 Hz, 2H), 1.49 to 1.36 (m, 3H), 0.96 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.26, 133.45, 131.77, 129.06, 128.62, 128.36, 128.30 , 123.07, 89.18, 85.67, 54.08, 46.99, 32.19, 20.55, 14.07.



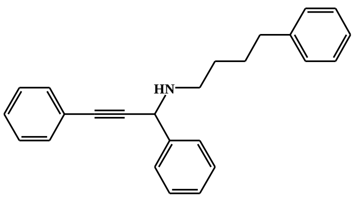
Butyl-(1-naphthalen-1-yl-3-phenyl-prop-2-ynyl)-amine (1e). yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 6.9 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.72 to 7.49 (m, 5H), 7.39 (d, *J* = 5.0 Hz, 3H), 5.60 (s, 1H), 3.20 to 3.04 (m, 1H), 3.04 to 2.87 (m, 1H), 1.89 to 1.57 (m, 3H), 1.57 to 1.43 (m, 2H), 1.04 (td, *J* = 7.3, 1.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.04, 134.26, 131.86, 131.23, 128.92, 128.73, 128.40, 128.22, 126.31, 125.78, 125.45, 125.41, 123.97, 123.44, 89.86, 85.87, 52.47, 47.86, 32.28, 20.70, 14.16.



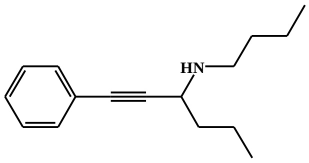
Butyl-(1-furan-2-yl-3-phenyl-prop-2-ynyl)-amine (1f). brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.41 (s, 1H), 7.37 to 7.27 (m, 3H), 6.44 (d, *J* = 3.1 Hz, 1H), 6.35 (dd, *J* = 2.9, 1.9 Hz, 1H), 4.91 (s, 1H), 2.91 to 2.67 (m, 2H), 1.65 (s, 1H), 1.59 to 1.44 (m, 2H), 1.44 to 1.31 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.00, 142.42, 131.81, 128.32, 128.28, 122.86, 110.18, 107.36, 87.00, 84.29, 48.62, 46.59, 32.04, 20.49, 14.00.



Butyl-(1-phenyl-3-p-tolyl-prop-2-ynyl)-amine (1g). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 6.8 Hz, 4H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 2H), 4.84 (s, 1H), 2.90 (dt, *J* = 11.4, 7.3 Hz, 1H), 2.77 (dt, *J* = 11.3, 7.0 Hz, 1H), 2.38 (s, 3H), 1.70 to 1.50 (m, 3H), 1.43 (dq, *J* = 14.6, 7.3 Hz, 2H), 0.98 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.85, 138.18, 131.67, 129.07, 128.54, 127.69, 127.67, 120.25, 88.95, 85.43, 54.82, 47.12, 32.21, 21.51, 20.59, 14.09.

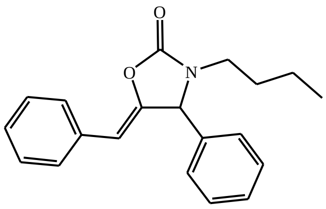


(1,3-Diphenyl-prop-2-ynyl)-(4-phenyl-butyl)-amine (1h). yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.6 Hz, 2H), 7.49 to 7.39 (m, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.30 to 7.18 (m, 6H), 7.13 (d, *J* = 7.6 Hz, 3H), 4.76 (s, 1H), 2.85 (dt, *J* = 11.3, 7.1 Hz, 1H), 2.77 to 2.65 (m, 1H), 2.59 (t, *J* = 7.5 Hz, 2H), 1.75 to 1.61 (m, 2H), 1.55 (dq, *J* = 14.3, 7.0 Hz, 2H), 1.40 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.57, 140.72, 131.85, 128.64, 128.57, 128.40, 128.25, 127. 83, 127.73, 125.83, 123.33, 89.73, 85.48, 54.85, 47.28, 35.92, 29.77, 29.34.

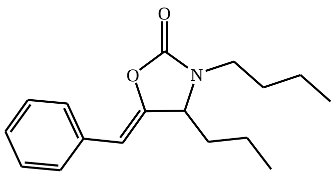


Butyl-(1-phenylethynyl-butyl)-amine (1i). yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.36 to 7.26 (m, 3H), 3.59 (dd, *J* = 7.7, 5.9 Hz, 1H), 2.93 (ddd, *J* = 11.1, 8.1, 6.6 Hz, 1H), 2.66 (ddd, *J* = 11.2, 8.2, 6.0 Hz, 1H), 1.68 (ddd, *J* = 13.5, 8.4, 6.3 Hz, 2H), 1.63 to 1.46 (m, 4H), 1.38 (dd, *J* = 15.3, 7.5 Hz, 3H), 0.95 (dt, *J* = 14.3, 7.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.66, 128.21, 127.82, 123.52, 91.34, 83.55, 50.64, 47.33, 38.32, 32.25, 20.56, 19.44, 14.03, 13.94.

1.4. Intermediate data:

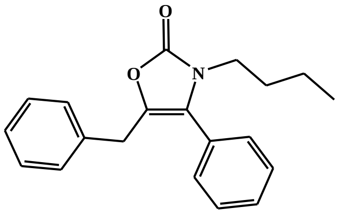


5-benzylidene-3-butyl-4-phenyloxazolidin-2-one (intermediate of 1a). white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.5 Hz, 2H), 7.48 to 7.40 (m, 3H), 7.38 to 7.31 (m, 2H), 7.31 to 7.24 (m, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 5.39 (d, *J* = 1.4 Hz, 1H), 5.25 (d, *J* = 1.7 Hz, 1H), 1.58 (s, 1H), 1.53 to 1.38 (m, 2H), 1.38 to 1.18 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.05, 147.70, 137.33, 133.46, 129.37, 129.33, 128.45, 128.33, 127.81, 126.94, 104.55, 63.85, 41.61, 28.96, 19.81, 13.64.

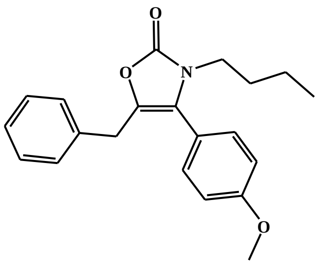


5-Benzylidene-3-butyl-4-propyl-oxazolidin-2-one (intermediate of 1i). colourless liquid; ^{1}H NMR (400 MHz, CDCl3) δ 7.58 (d, J = 7.5 Hz, 2H), 7.32 (t, J = 7.7 Hz, 2H), 7.20 (t, J = 7.4 Hz, 1H), 5.47 (d, J = 1.4 Hz, 1H), 4.51 (s, 1H), 3.59 (dt, J = 14.4, 8.0 Hz, 1H), 3.02 (ddd, J = 13.9, 8.3, 5.3 Hz, 1H), 1.92 – 1.78 (m, 1H), 1.74 – 1.62 (m, 1H), 1.57 (ddd, J = 21.5, 14.1, 7.9 Hz, 2H), 1.44 – 1.25 (m, 4H), 0.95 (dd, J = 7.8, 6.8 Hz, 6H). ^{13}C NMR (100 MHz, CDCl3) δ 155.17, 147.04, 133.67, 128.46, 128.28, 126.72, 102.31, 58.43, 41.14, 34.41, 29.25, 19.91, 15.83, 13.90, 13.67.

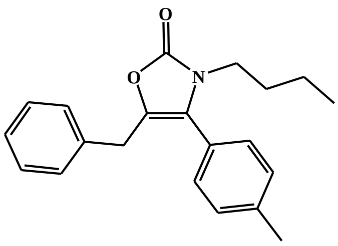
1.5. Products data:



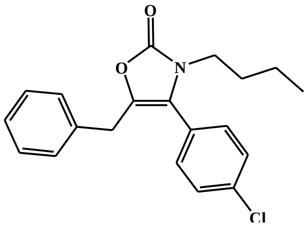
5-Benzyl-3-butyl-4-phenyl-3H-oxazol-2-one (2a). colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 to 7.43 (m, 3H), 7.38 to 7.21 (m, 5H), 7.21 to 7.14 (m, 2H), 3.70 (s, 2H), 3.58 to 3.43 (m, 2H), 1.51 to 1.36 (m, 2H), 1.23 to 1.08 (m, 2H), 0.77 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.51, 136.93, 135.17, 129.68, 129.41, 129.04, 128.64, 128.42, 126.82, 126.79, 124.08, 42.01, 30.98, 30.67, 19.59, 13.45.



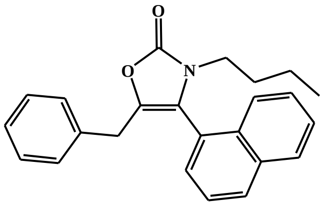
5-Benzyl-3-butyl-4-(4-methoxy-phenyl)-3H-oxazol-2-one (2b). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 to 7.11 (m, 7H), 6.99 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 3.67 (s, 2H), 3.47 (t, *J* = 7.4 Hz, 2H), 1.54 to 1.37 (m, 2H), 1.24 to 1.08 (m, 2H), 0.78 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.39, 155.50, 137.11, 134.94, 131.16, 128.62, 128.42, 126.74, 123.80, 118.77, 114.49, 55.38, 41.91, 30.97, 30.72, 19.63, 13.52.



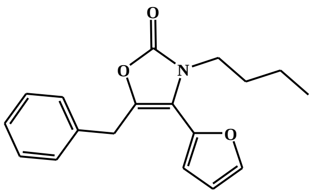
5-Benzyl-3-butyl-4-p-tolyl-3H-oxazol-2-one (2c). colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 to 7.25 (m, 4H), 7.25 to 7.15 (m, 5H), 3.68 (s, 2H), 3.53 to 3.43 (m, 2H), 2.42 (s, 3H), 1.52 to 1.36 (m, 2H), 1.23 to 1.09 (m, 2H), 0.78 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.55, 139.49, 137.07, 134.99, 129.73，129.59, 128.62，128.43, 126.75, 124.06, 123.77, 41.97, 30.96, 30.70, 21.39, 19.62, 13.50.



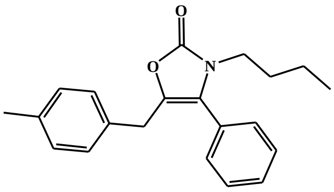
5-Benzyl-3-butyl-4-(4-chloro-phenyl)-3H-oxazol-2-one (2d). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.3 Hz, 2H), 7.33 to 7.19 (m, 5H), 7.16 (d, *J* = 7.2 Hz, 2H), 3.68 (s, 2H), 3.53 to 3.43 (m, 2H), 1.41 (dd, *J* = 15.0, 7.7 Hz, 2H), 1.24 to 1.08 (m, 2H), 0.79 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.34, 136.62, 135.66， 135.57, 130.94, 129.42, 128.71, 128.38, 126.91, 125.27, 122.94, 42.06, 30.99, 30.72, 19.60, 13.48.



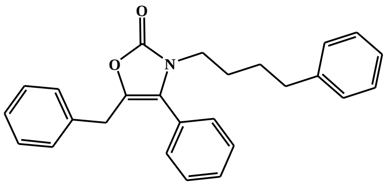
5-Benzyl-3-butyl-4-naphthalen-1-yl-3H-oxazol-2-one (2e). colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.97 to 7.90 (m, 1H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.64 to 7.50 (m, 3H), 7.48 (d, *J* = 6.8 Hz, 1H), 7.25 to 7.13 (m, 3H), 7.09 (d, *J* = 6.8 Hz, 2H), 3.60 (q, *J* = 15.8 Hz, 2H), 3.47 (dt, *J* = 14.3, 7.3 Hz, 1H), 3.22 to 3.05 (m, 1H), 1.37 to 1.19 (m, 2H), 1.14 to 0.98 (m, 2H), 0.62 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.63, 136.61, 136.32, 133.66, 132.61, 130.54, 129.86, 128.67， 128.61， 128.51, 127.35, 126.74， 126.68, 125.28, 124.87, 123.80, 121.84, 42.31, 31.26, 30.80, 19.45, 13.33.



5-Benzyl-3-butyl-4-furan-2-yl-3H-oxazol-2-one (2f). croci oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 to 7.51 (m, 1H), 7.37 to 7.27 (m, 2H), 7.24 (dd, *J* = 8.1, 4.7 Hz, 3H), 6.50 (dt, *J* = 11.8, 2.7 Hz, 2H), 3.85 (s, 2H), 3.72 to 3.59 (m, 2H), 1.64 to 1.49 (m, 2H), 1.37 to 1.21 (m, 2H), 0.87 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.01, 143.75, 140.90, 137.16, 136.41, 128.73, 128.46, 126.95, 115.56, 111.31, 111.11, 42.75, 31.47, 30.83, 19.71, 13.60.



3-Butyl-5-(4-methyl-benzyl)-4-phenyl-3H-oxazol-2-one (2g). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 to 7.40 (m, 3H), 7.32 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.16 to 7.02 (m, 4H), 3.66 (s, 2H), 3.58 to 3.43 (m, 2H), 2.31 (s, 3H), 1.50 to 1.37 (m, 2H), 1.24 to 1.10 (m, 2H), 0.77 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.53, 136.38, 135.44, 133.88, 129.69, 129.36, 129.32, 129.02, 128.31, 126.89, 123.86, 41.99, 30.61, 21.03, 19.59, 13.46.

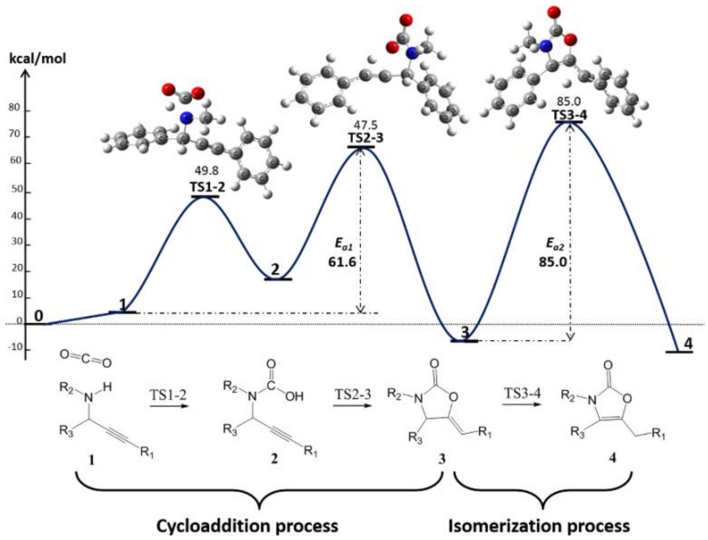


5-Benzyl-4-phenyl-3-(4-phenyl-butyl)-3H-oxazol-2-one (2h). pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 to 7.38 (m, 3H), 7.33 to 7.19 (m, 7H), 7.15 (dd, *J* = 12.0, 7.0 Hz, 3H), 7.03 (d, *J* = 7.2 Hz, 2H), 3.68 (s, 2H), 3.52 (t, *J* = 6.7 Hz, 2H), 2.47 (t, *J* = 6.8 Hz, 2H), 1.59 to 1.37 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.56, 141.77, 136.91, 135.27, 129.66, 129.45, 129.09, 128.68, 128.44, 128.35, 128.32, 126.84, 126.72, 125.82, 123.98, 42.04, 35.05, 30.97, 28.07, 27.97.

2. Theoretical Section

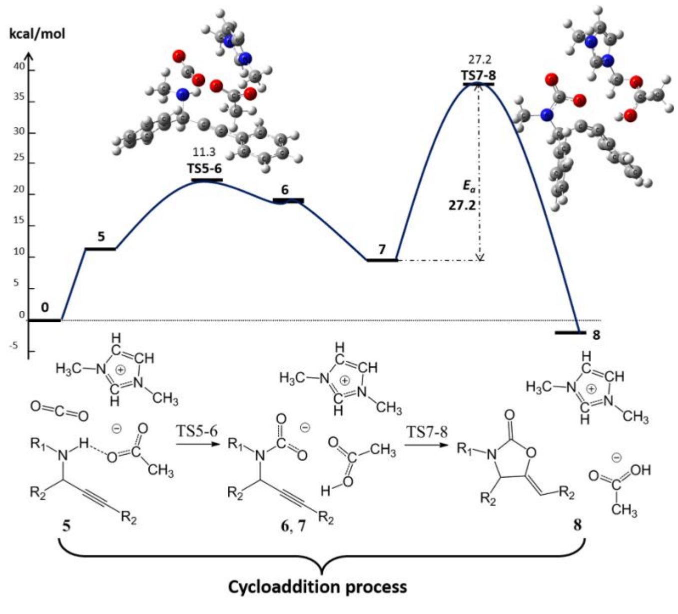
2.1. Figures S5-S7

Figure S5 Non-catalytic potential energy curve



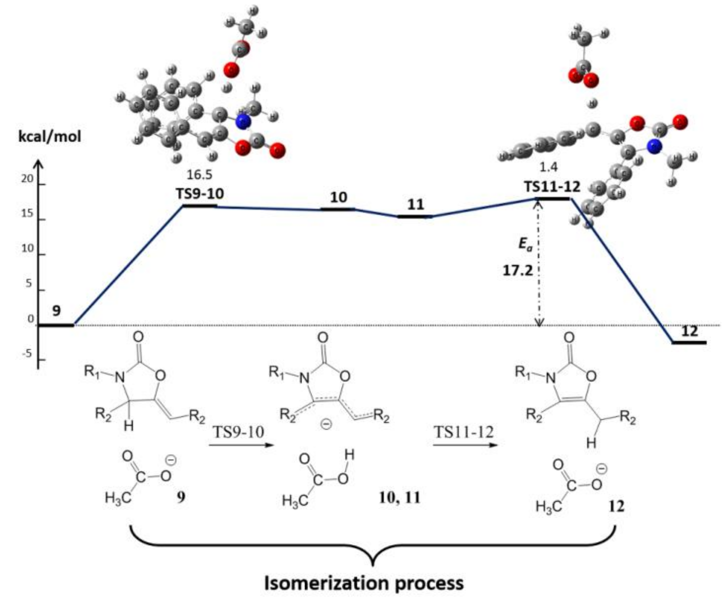
E_{a1}: the overall energy barrier (kcal/mol) of the cycloaddition process; E_{a2}: the overall energy barrier (kcal/mol) of the synthesis of 3.4.5-trisubstituted oxazolone from propargylic amines and CO_2.

Figure S6 [Bmim][OAc] promoted potential energy curve



E_a: the overall energy barrier (kcal/mol).

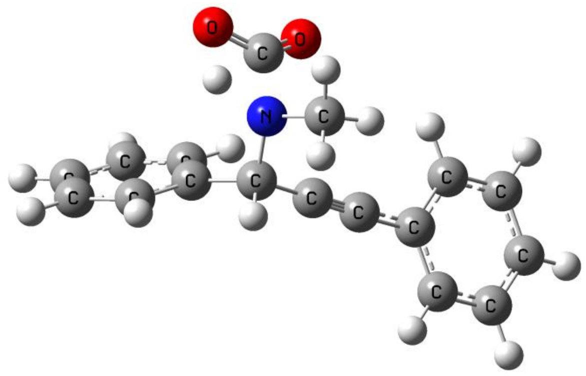
Figure S7 The potential energy curve of the double-bond isomerization promoted by $[OAc]^-$



E_a: the overall energy barrier (kcal/mol)

2.2. Optimized geometries of the transition states

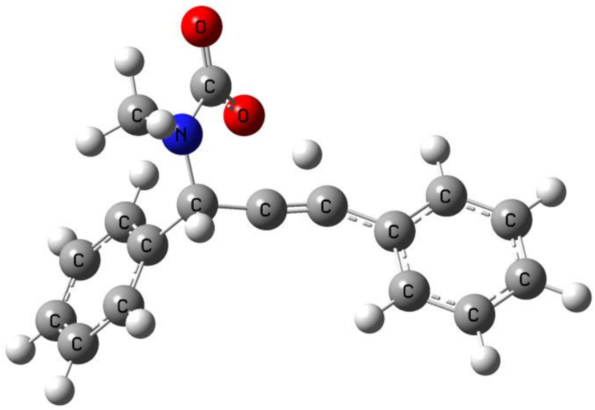
TS1-2			
N	-0.61085976	0.79185519	0.00000000
H	0.62260424	1.03458119	0.34099900
C	-0.49071176	1.09231619	1.53987500
O	-1.39441676	1.09968519	2.32104500
O	0.77411724	1.31974819	1.56956400
C	-1.03764576	-0.60206781	-0.37632300
H	-0.90346376	-0.64409581	-1.46361500
C	-1.36192676	1.84439219	-0.71011700
H	-0.92923776	2.81416019	-0.46039700
H	-2.41452876	1.83129119	-0.41882800
C	-2.45253176	-0.83876581	-0.08735600
C	-3.62383976	-1.01626581	0.14020800
C	-0.09839376	-1.63406481	0.24061100
C	1.07334424	-1.97499081	-0.44137800
C	-0.36803576	-2.22750281	1.47539500
C	1.96786324	-2.89185181	0.10438300
H	1.28695824	-1.52446981	-1.40595000
C	0.52833324	-3.14308581	2.02264400
H	-1.27860276	-1.97437781	2.00505600
C	1.69625724	-3.47704581	1.33998800
H	2.87192624	-3.15084181	-0.43485800
H	0.31188724	-3.59597281	2.98338200
H	2.39053224	-4.19188081	1.76691700
C	-5.00492276	-1.20460881	0.44705900
C	-5.83555276	-1.95807381	-0.39964800
C	-5.55099276	-0.63063381	1.60868200
C	-7.18009376	-2.13152281	-0.08920400
H	-5.41748676	-2.40277381	-1.29480300
C	-6.89708276	-0.80797681	1.90959600
H	-4.91041076	-0.05060281	2.26214100
C	-7.71503276	-1.55739281	1.06393200
H	-7.81191976	-2.71567381	-0.74867900
H	-7.30836876	-0.36078181	2.80743400
H	-8.76362076	-1.69402181	1.30258400
H	-1.28028876	1.68463819	-1.78742700



1724.1 *i*

Optimized geometries of transition states TS1-2. The imaginary vibrational frequency (cm^{-1}) is shown.

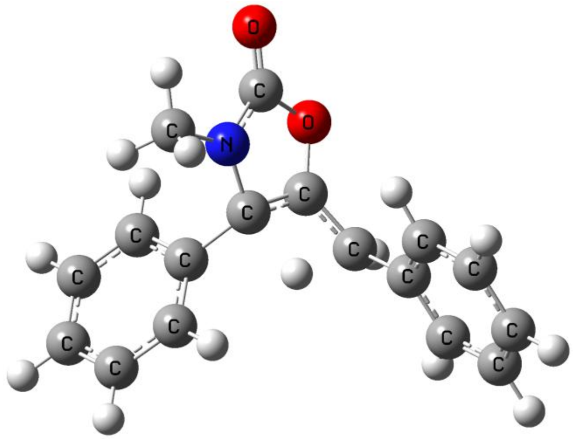
TS2-3			
N	0.18099548	-0.04524887	0.00000000
H	2.62030348	-0.61176987	-1.59879700
C	0.64726748	0.76112413	-1.08638900
O	0.40111348	1.95444013	-1.10805000
O	1.29752648	0.03621813	-1.94817600
C	0.56552848	-1.44313887	0.05473300
H	0.69548948	-1.70682187	1.11843100
C	-0.65694152	0.49849713	1.05386900
H	-0.90791852	1.51804913	0.76734900
H	-0.13409452	0.52617813	2.01824700
C	1.92381048	-1.56231587	-0.48136400
C	3.11276948	-1.49163787	-0.88005700
C	-0.42391152	-2.44967287	-0.53823800
C	-0.79588752	-3.56815587	0.20985200
C	-0.96481652	-2.26176887	-1.81389600
C	-1.69942652	-4.49681787	-0.30682400
H	-0.38684452	-3.71467187	1.20544500
C	-1.86656252	-3.18951187	-2.32742800
H	-0.66942952	-1.39801387	-2.39643000
C	-2.23547052	-4.30775187	-1.57779200
H	-1.98707752	-5.35836587	0.28510900
H	-2.28277652	-3.03940187	-3.31718900
H	-2.94052052	-5.02514687	-1.98239500
C	4.49792248	-1.90663987	-0.81748000
C	4.90109748	-2.92999087	0.05627000
C	5.45074348	-1.28215087	-1.63461300
C	6.23475348	-3.31564287	0.10780500
H	4.16687448	-3.41908587	0.68559200
C	6.78503548	-1.67121887	-1.57407900
H	5.13993448	-0.49407487	-2.31023000
C	7.17944448	-2.68708287	-0.70517400
H	6.53921448	-4.10720587	0.78271400
H	7.51589148	-1.18171187	-2.20691700
H	8.21914648	-2.99017987	-0.66102500
H	-1.57856652	-0.08306787	1.16597200



1354.5 *i*

Optimized geometries of transition states TS2-3. The imaginary vibrational frequency (cm^{-1}) is shown.

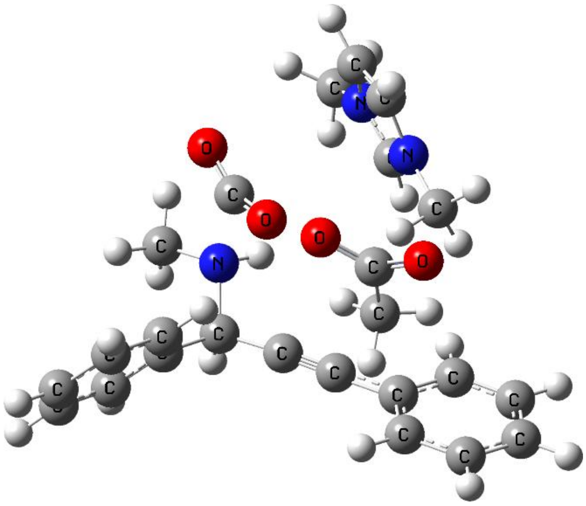
TS3-4			
C	-0.13574661	0.38461538	0.00000000
C	0.66511739	0.78999638	-1.07397400
N	-0.62519461	1.64696138	0.51130900
C	-0.34535661	2.65027938	-0.38403300
O	-0.65228661	3.80903638	-0.36667000
O	0.44745639	2.09180838	-1.41557500
C	-1.44814561	1.86413438	1.69102200
H	-1.74490761	2.91176338	1.70589400
H	-0.88198061	1.63804138	2.59757100
C	1.68025539	-0.11617962	-1.46117000
H	0.93867739	-0.60615062	-0.10789000
H	1.82100739	-0.28342562	-2.53146800
C	-1.18072261	-0.71366562	-0.04249700
C	-1.04006061	-1.89147962	0.69368800
C	-2.34174761	-0.52037062	-0.80413200
C	-2.03168061	-2.87188862	0.65775800
H	-0.14913561	-2.04125062	1.29302800
C	-3.32794361	-1.50105362	-0.84457500
H	-2.46717961	0.39446338	-1.37314100
C	-3.17516261	-2.67970662	-0.11260100
H	-1.90815461	-3.78269162	1.23239600
H	-4.21369761	-1.34810262	-1.45076500
H	-3.94524361	-3.44202562	-0.14385800
C	2.93943239	-0.33630362	-0.69171000
C	3.78706739	-1.39176562	-1.06691900
C	3.34618039	0.49171738	0.36796300
C	4.98198939	-1.62541962	-0.39393600
H	3.49894739	-2.03652762	-1.89075600
C	4.53650139	0.24631038	1.04728900
H	2.73827839	1.34313938	0.65239400
C	5.36192439	-0.81347062	0.67453400
H	5.61780939	-2.44749562	-0.70441200
H	4.83037339	0.90325338	1.85886500
H	6.29336539	-0.99427562	1.19822900
H	-2.34007761	1.23464938	1.65891000



1671.9 *i*

Optimized geometries of transition states TS3-4. The imaginary vibrational frequency (cm^{-1}) is shown.

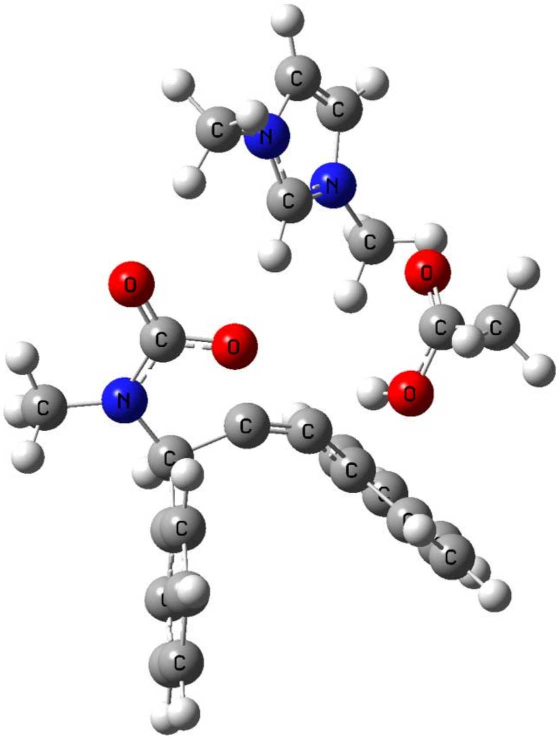
TS5-6			
O	-1.04865774	1.05704696	0.00000000
C	-1.38382474	0.10488196	0.64304500
O	-1.51468174	-1.07871404	0.75722400
C	2.05151926	0.35349296	1.07693200
N	2.17308826	0.81232096	-0.17692200
C	2.04702926	-0.24464304	-1.06121100
C	1.85590526	-1.36647104	-0.31155300
N	1.86029526	-0.97188804	1.01449600
C	2.26124926	2.22823596	-0.53890000
C	1.65784326	-1.84115504	2.18061000
H	2.51910226	2.80256296	0.35102900
H	3.03409526	2.36048596	-1.29992200
H	1.34217826	-1.21086204	3.01787700
H	2.58637926	-2.37022804	2.41400100
H	0.86544526	-2.55407804	1.94401800
H	1.69510726	-2.39294804	-0.60196500
H	2.08085726	-0.10477804	-2.13055000
H	2.08811426	0.96093896	2.00584700
H	1.29202326	2.56469996	-0.91494300
N	-1.93066974	0.81442096	2.47246100
C	-2.45160074	2.21519296	2.60599500
C	-2.78633874	-0.16898504	3.15694800
C	-1.43754874	3.19749196	2.20490300
H	-3.76760074	-0.21526804	2.67799400
H	-2.31154474	-1.14730604	3.08119800
H	-2.91038274	0.08632996	4.21846900
C	-0.60811274	4.05054196	1.96759900
H	-1.00630774	0.79200596	2.94434600
O	0.46907826	0.53053296	3.98503100
C	1.33026826	1.40800396	4.31537900
O	2.20533226	1.88925196	3.53694200
C	1.29536026	1.93638896	5.75093200
H	0.74523126	2.88678996	5.76540300
H	2.30810126	2.13842896	6.11372200
H	0.78537526	1.23497696	6.41739600
C	0.38314826	5.04314996	1.68392900
C	0.07128326	6.15731196	0.87847400
C	1.68430326	4.92004896	2.21657000
C	1.03833126	7.12668996	0.61229800
H	-0.93154974	6.25433896	0.47189400
C	2.64273726	5.89719796	1.94230200
H	1.92920326	4.05669196	2.83239500
C	2.32678026	7.00110096	1.14283000
H	0.78471126	7.98319896	-0.00764300
H	3.64103026	5.79613596	2.36157800
H	3.07749626	7.76025796	0.93719800
C	-3.79585474	2.42450096	1.90569900
C	-3.89191674	2.54379896	0.51162100
C	-4.96348074	2.51559696	2.67398800
C	-5.13431574	2.73432296	-0.09625100
H	-2.99157474	2.48998696	-0.09146600
C	-6.20817574	2.70946596	2.06726900
H	-4.90072674	2.43921996	3.75775200
C	-6.29645874	2.81701196	0.67787900
H	-5.19402774	2.82369696	-1.17826600
H	-7.10322974	2.77926796	2.68041900
H	-7.26160074	2.96951496	0.20120500
H	-2.62888074	2.37445896	3.68300000



84.0*i*

Optimized geometries of transition states TS5-6. The imaginary vibrational frequency (cm^{-1}) is shown.

TS7-8			
C	-3.25179500	-0.52165000	-0.42004900
N	-4.26686300	-1.38920100	-0.35036400
C	-5.42818200	-0.74748500	-0.74227200
C	-5.08710000	0.52965100	-1.06217600
N	-3.72485700	0.64671900	-0.86014200
C	-4.14737900	-2.78164200	0.10528500
C	-2.92496600	1.86580200	-1.02312000
H	-4.75495200	-3.41453300	-0.54151600
H	-3.09844300	-3.08284300	0.03118600
H	-3.09450200	2.27449900	-2.01966100
H	-1.87375900	1.61188500	-0.89393900
H	-3.20714400	2.58493900	-0.25584000
H	-5.68677100	1.35137800	-1.41319600
H	-6.37975700	-1.24933000	-0.76548200
H	-2.21379000	-0.73897600	-0.16098200
H	-4.49936700	-2.85907900	1.13514100
C	0.66722200	1.03517600	-0.34716500
C	0.85081900	-0.19018000	-0.53432500
O	-0.44849100	-1.31229000	0.09697700
C	1.74308800	-1.27603000	-1.06582300
H	2.06293200	-0.96635400	-2.07061000
C	-0.26848700	-2.45108900	-0.52212900
O	-1.08368800	-3.38022600	-0.55045600
N	0.94629100	-2.48668600	-1.17293000
C	1.40725500	-3.62971400	-1.93070000
H	2.35490900	-4.01014000	-1.53490400
H	0.65068900	-4.40882700	-1.85594700
H	1.55152900	-3.37112800	-2.98720700
C	-1.63824700	1.14784500	2.73386900
C	-1.83501300	1.26853300	4.22622600
H	-2.89183300	1.39281100	4.45366300
H	-1.45113600	0.37170800	4.71872700
H	-1.26511400	2.11791300	4.60925700
O	-0.35427900	1.05555900	2.41034900
O	-2.55210800	1.13604600	1.92901200
H	-0.21702000	0.95744800	1.42420100
C	3.00612400	-1.44908300	-0.21853700
C	4.21579200	-0.90556600	-0.65289800
C	2.96696000	-2.12939900	1.00213700
C	5.37131400	-1.03361100	0.11798300
H	4.25492600	-0.37287500	-1.59802300
C	4.11941200	-2.26106300	1.77193500
H	2.03160400	-2.55392900	1.34887300
C	5.32555700	-1.71310200	1.33278900
H	6.30408700	-0.60551600	-0.23236900
H	4.07719300	-2.79078300	2.71743900
H	6.22208300	-1.81708800	1.93384900
C	1.13898800	2.36104500	-0.62174800
C	0.93039500	2.96101800	-1.88416500
C	1.78790100	3.13432000	0.36580700
C	1.36171800	4.25806100	-2.14460100
H	0.43501700	2.38982200	-2.66223700
C	2.22378900	4.42571100	0.09154600
H	1.95048900	2.70449700	1.34731500
C	2.01349600	5.00345700	-1.16189800
H	1.19217200	4.68731100	-3.12710500
H	2.73028900	4.98967200	0.86822800
H	2.35023400	6.01294800	-1.36768000



277.0 *i*

Optimized geometries of transition states TS7-8. The imaginary vibrational frequency (cm^{-1}) is shown.

TS9-10			
C	-0.84470988	0.20477815	0.00000000
C	-2.17459688	-0.01148885	-0.24382600
O	-2.97510388	1.12958815	-0.13986200
C	-3.02710488	-1.14450285	-0.55096700
H	-3.11434988	-1.94555785	0.84651800
C	-4.29013688	0.81841215	-0.42489200
O	-4.90658988	-3.63814385	1.33491000
O	-5.17518888	1.65435815	-0.38722400
C	-4.03625688	-3.27082585	2.11373300
C	-3.94234488	-3.81851285	3.53027000
H	-4.03614888	-2.99886285	4.24729200
H	-4.72731188	-4.55447085	3.70165000
H	-2.96087988	-4.27368485	3.68505400
O	-3.09896988	-2.39202485	1.85730500
N	-4.34724888	-0.49823085	-0.69957500
C	-5.60713588	-1.17477685	-0.93308100
H	-5.74468088	-1.98579685	-0.21432300
H	-6.40031488	-0.43546685	-0.81954200
H	-5.64874388	-1.58809285	-1.94588000
H	-0.59951988	1.25135115	0.15259900
C	0.26114712	-0.71429685	0.14785600
C	1.56759912	-0.17859885	0.27714000
C	0.15183812	-2.12309785	0.21670900
C	2.68285612	-0.98625885	0.45263100
H	1.69079712	0.89991715	0.23860300
C	1.27200812	-2.92758785	0.39725300
H	-0.82026188	-2.58914685	0.14941800
C	2.54944512	-2.37653185	0.51215600
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H	-3.58668788	-5.18391485	-2.81411000
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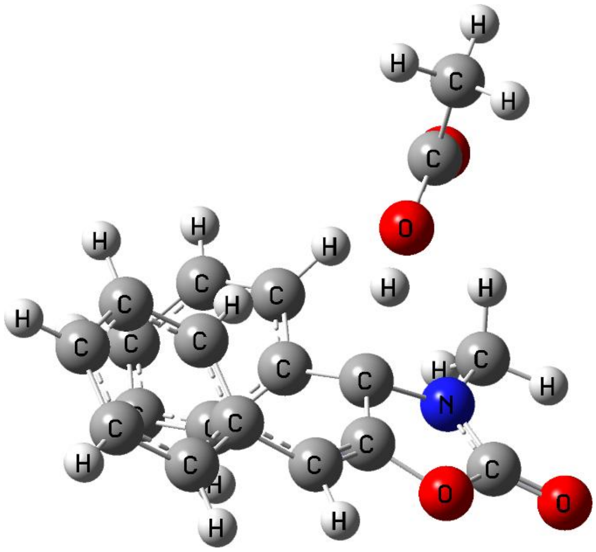

367.6 *i*

Optimized geometries of transition states TS9-10. The imaginary vibrational frequency (cm^{-1}) is shown.

Charge = -1 Multiplicity = 1

TS11-12			
C	0.38395903	0.97269623	0.00000000
C	-0.68446697	0.02210523	0.21703900
O	-0.25832097	-1.31435677	0.10027300
C	-2.00124797	-0.00212477	0.59465300
C	-1.27921997	-2.16060177	0.40988200
O	-1.21452797	-3.37239877	0.32674200
N	-2.34133797	-1.38401577	0.78552400
C	-3.67010797	-1.95396177	0.87944400
H	-4.35266797	-1.45990377	0.18209500
H	-3.58481997	-3.01020477	0.62358400
H	-4.08460697	-1.87036077	1.88807500
H	0.93149303	0.73044623	-0.91347300
C	0.25648103	2.41946323	0.22818000
C	-0.33259897	2.97042623	1.38602800
C	0.85837503	3.32947323	-0.66693800
C	-0.33374797	4.34079223	1.62171200
H	-0.77697397	2.30715923	2.11877900
C	0.86100003	4.70057723	-0.42892200
H	1.34584503	2.93909023	-1.55455000
C	0.25818503	5.22386723	0.71619900
H	-0.79781897	4.72329923	2.52600400
H	1.33929303	5.36502423	-1.14287400
H	0.25641103	6.29270723	0.90298300
C	-2.97883197	1.06430923	0.78118800
C	-3.88785197	1.05678423	1.85882900
C	-3.05119297	2.14384023	-0.12032600
C	-4.83374697	2.06555223	2.01358800
H	-3.83297497	0.26557923	2.59699900
C	-3.98947097	3.15657623	0.04385500
H	-2.36190297	2.17725223	-0.95425100
C	-4.89462597	3.12295623	1.10531600
H	-5.51554097	2.03381023	2.85774700
H	-4.01352697	3.97781623	-0.66467900
H	-5.62740697	3.91310223	1.22899700
C	3.46197803	0.18928723	1.24271900
O	2.25754703	0.27368923	1.72547900
O	3.80573203	0.45143823	0.09313100
C	4.48203603	-0.29790877	2.27437600
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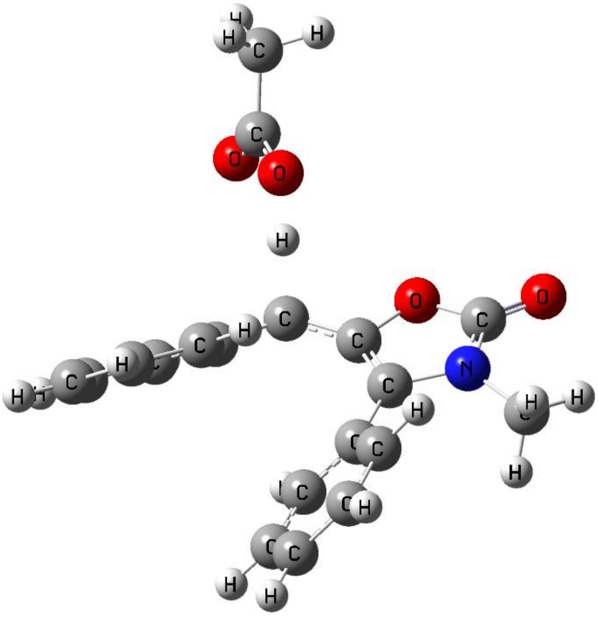
H	5.48727803	-0.28150477	1.85177900
H	4.44022503	0.33136423	3.16742200
H	1.41055103	0.59020123	0.90979000



1135.9 *i*

Optimized geometries of transition states TS9-10. The imaginary vibrational frequency (cm^{-1}) is shown.

Charge = -1 Multiplicity = 1

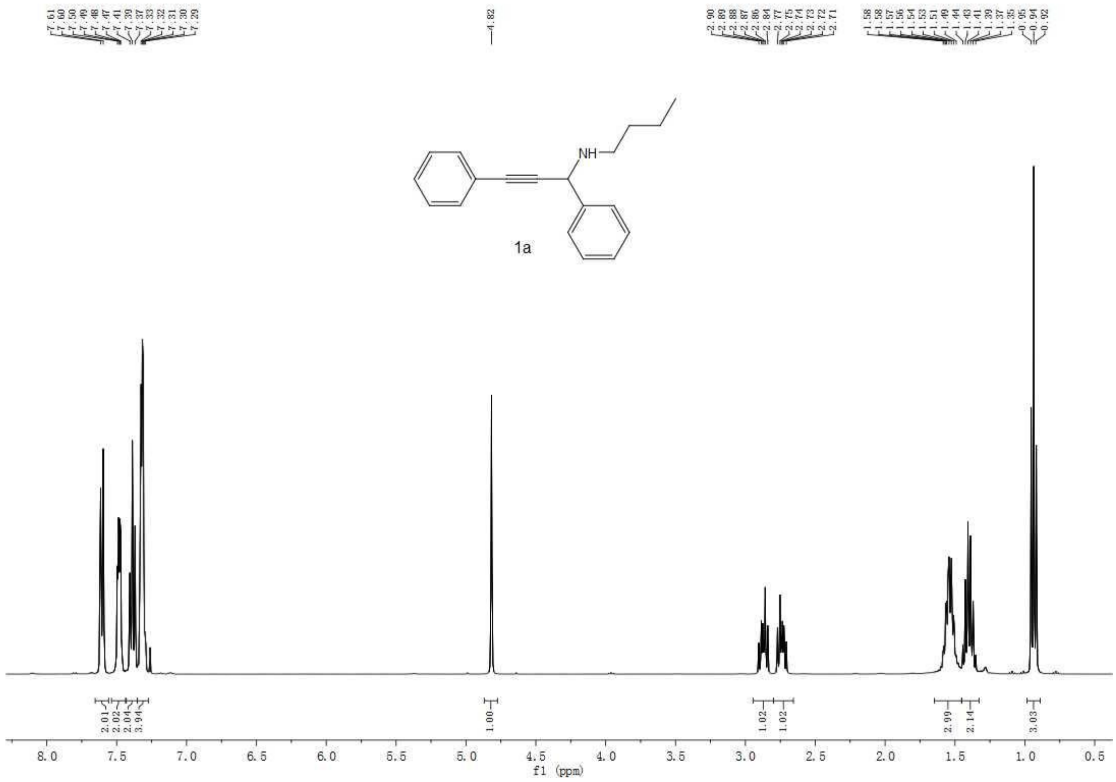
3. References

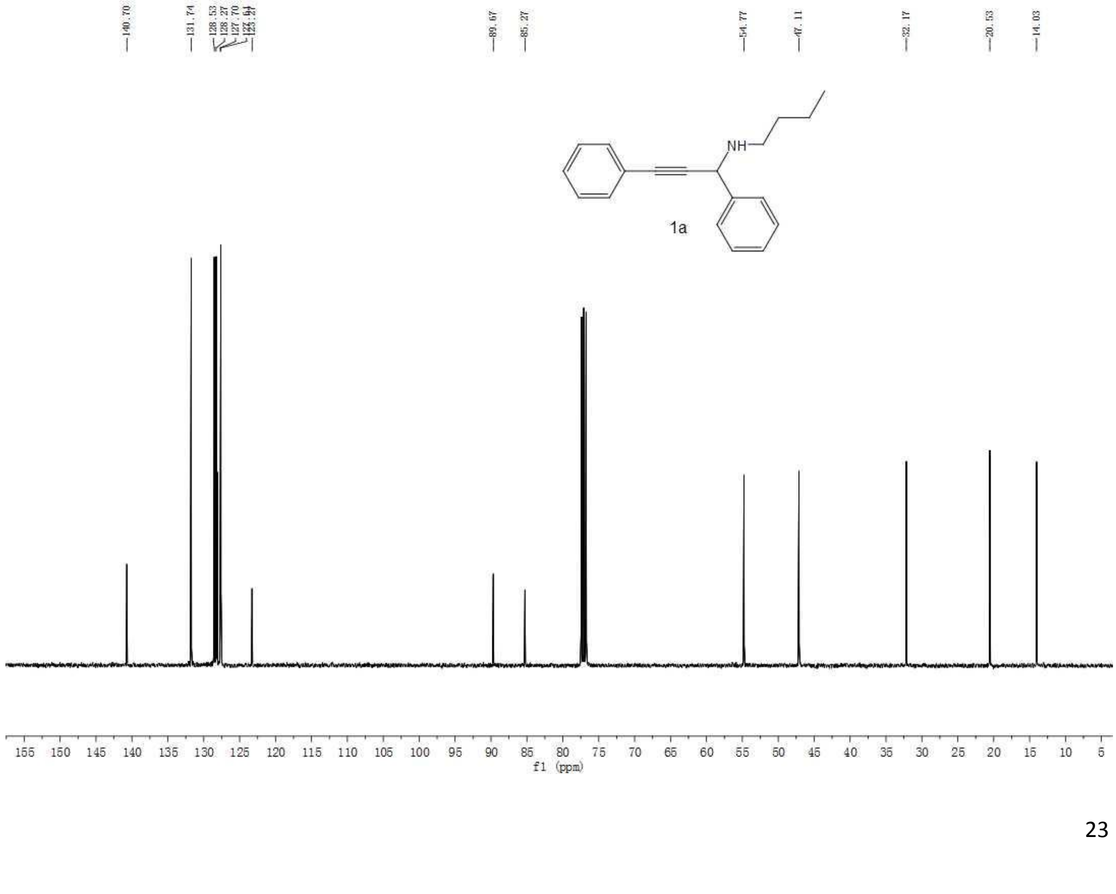
S1. Gaussian 09, Revision A.01, Frisch,M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr.,J. A.; Peralta,J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev,O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

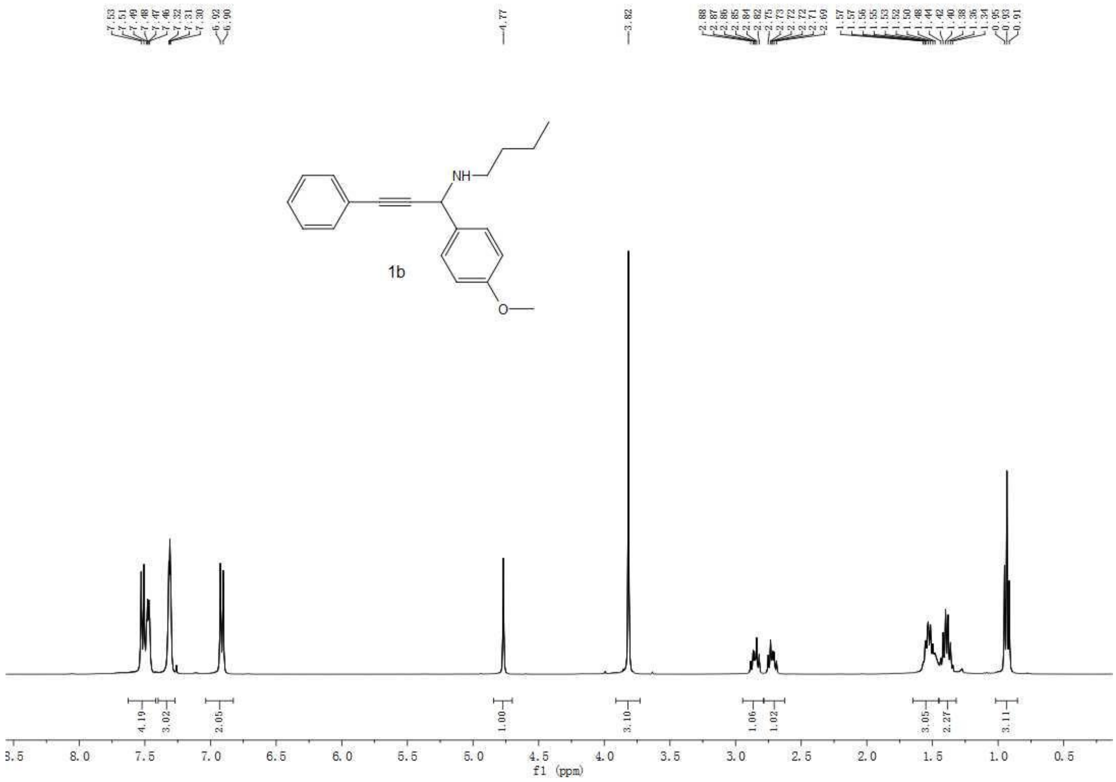
S2. Y. Sugawara, W. Yamada, S.Yoshida, T. Ikeno, T. Yamada, *J. Am. Chem. Soc.* 2007, **129**, 12902.

S3. W. J. Yoo and C. J. Li, *Adv. Synth. Catal.* 2008, **350**, 1503.

4. NMR Spectra



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1.00
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3.05
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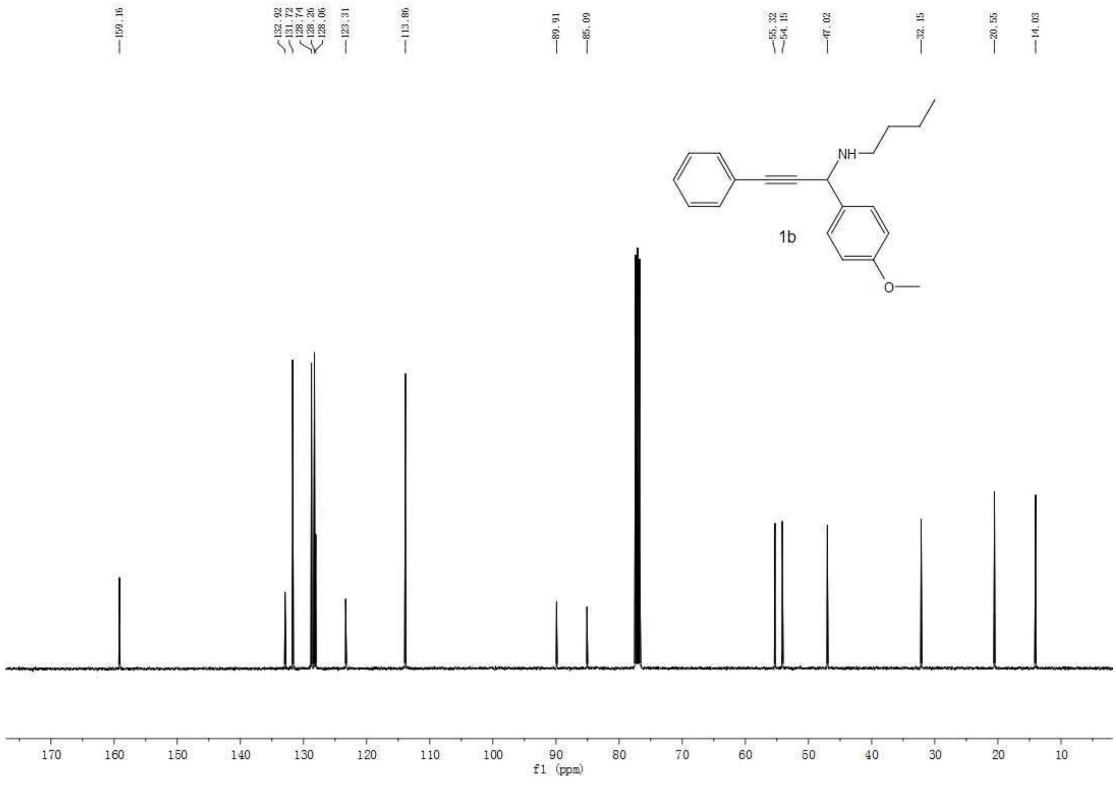
f1 (ppm)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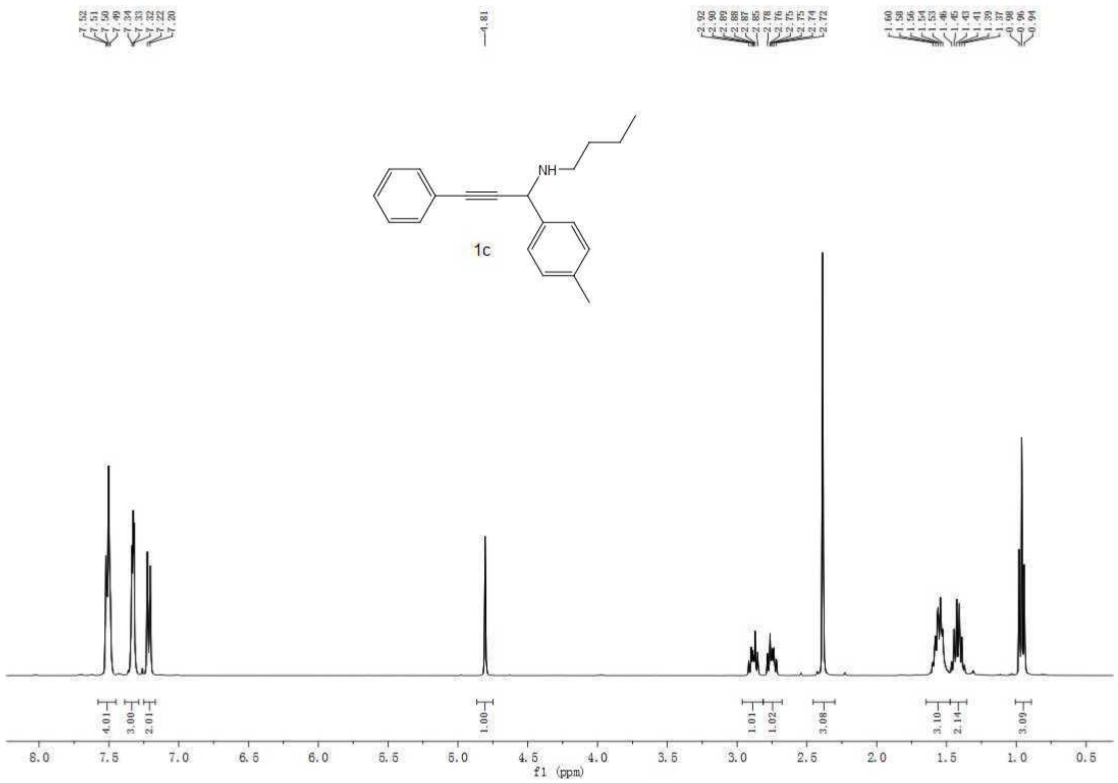
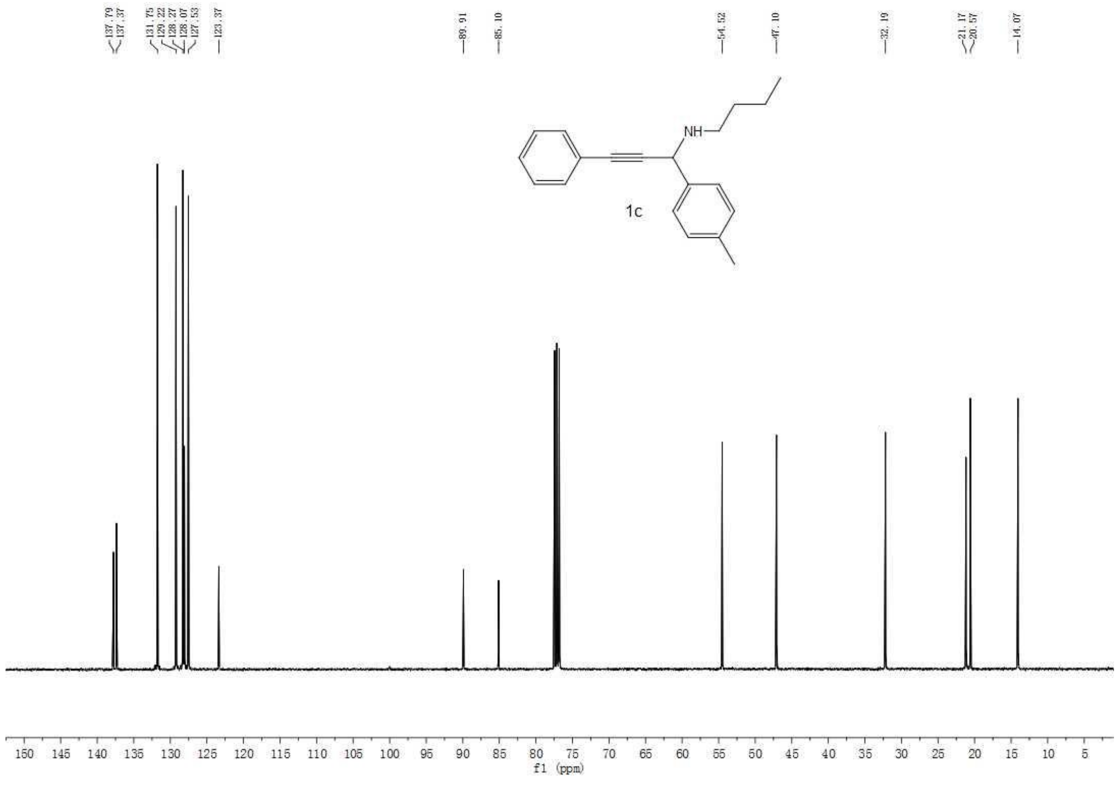
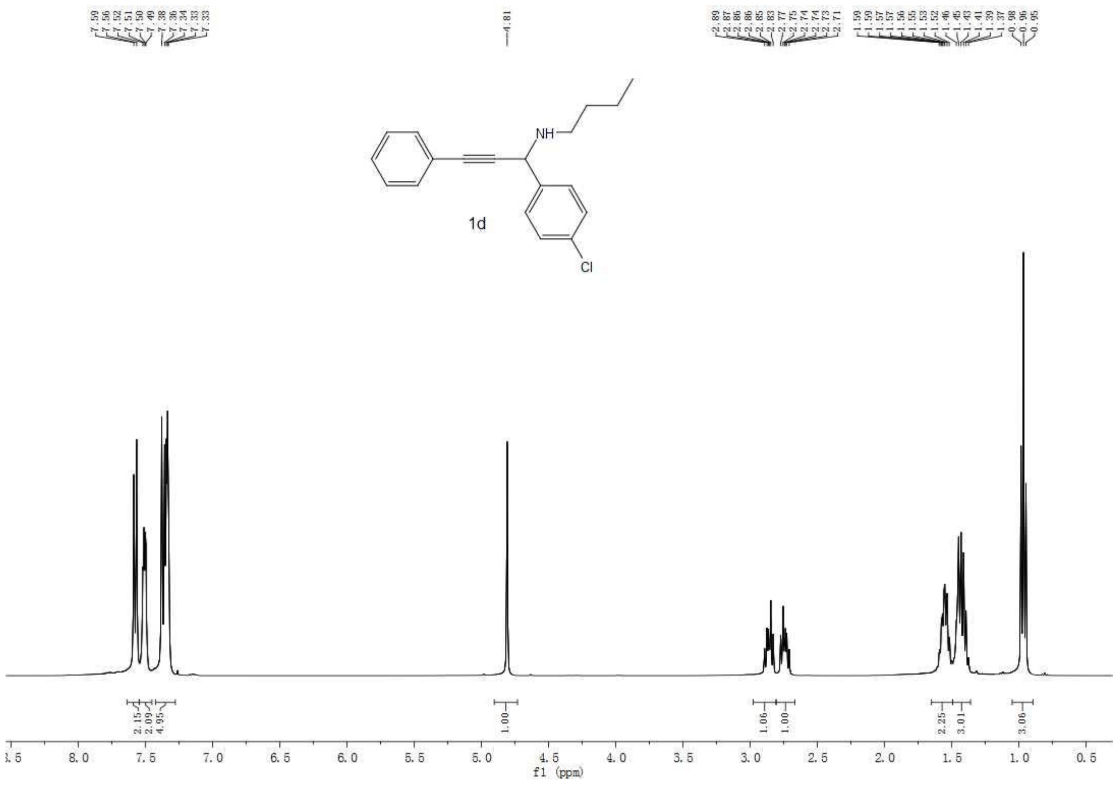
NH
1b
O
f1 (ppm)



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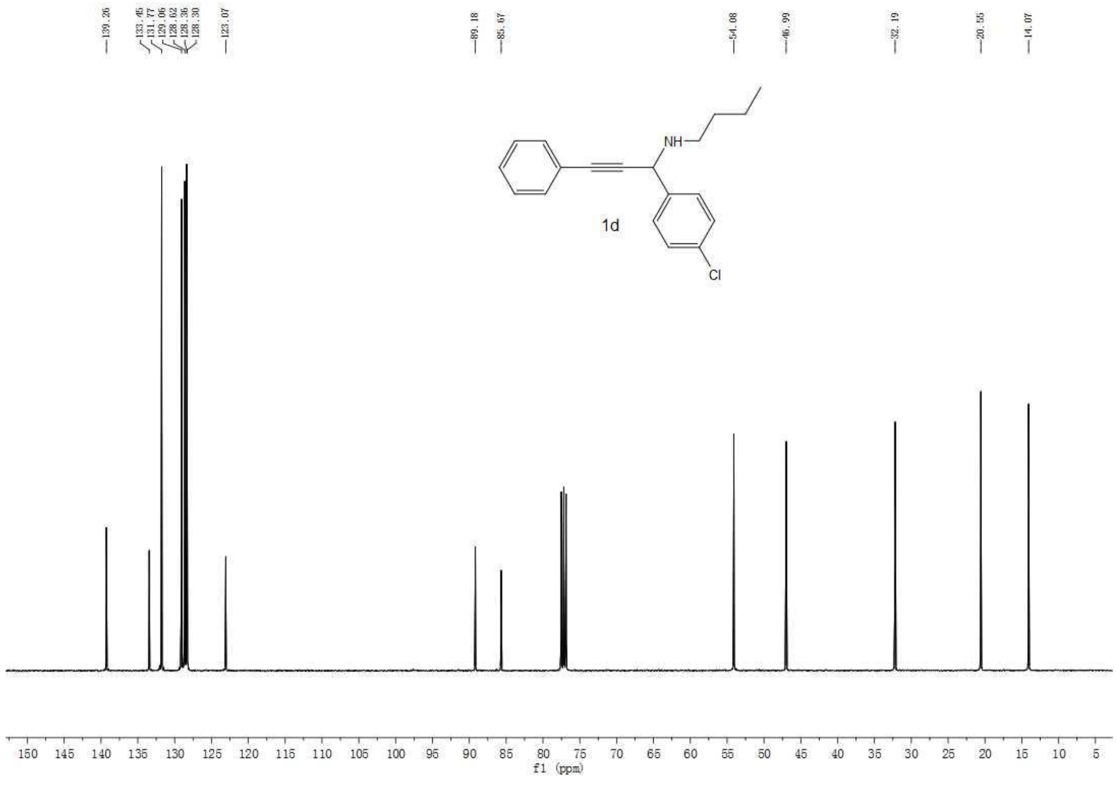
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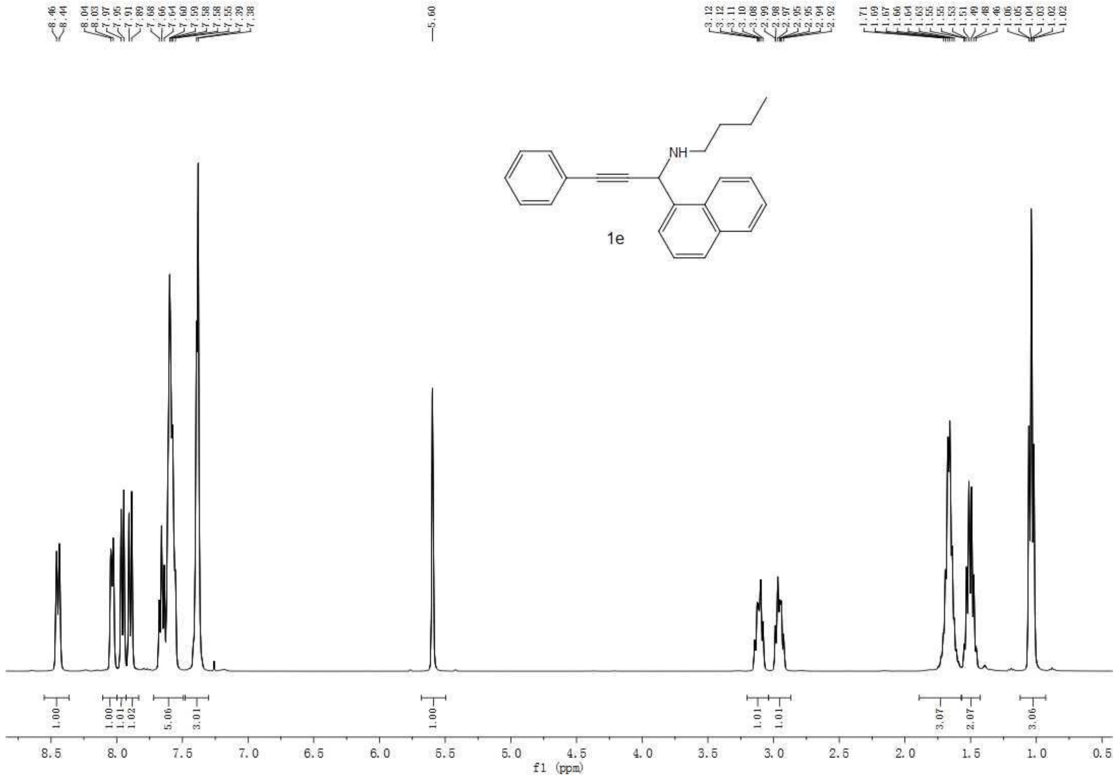
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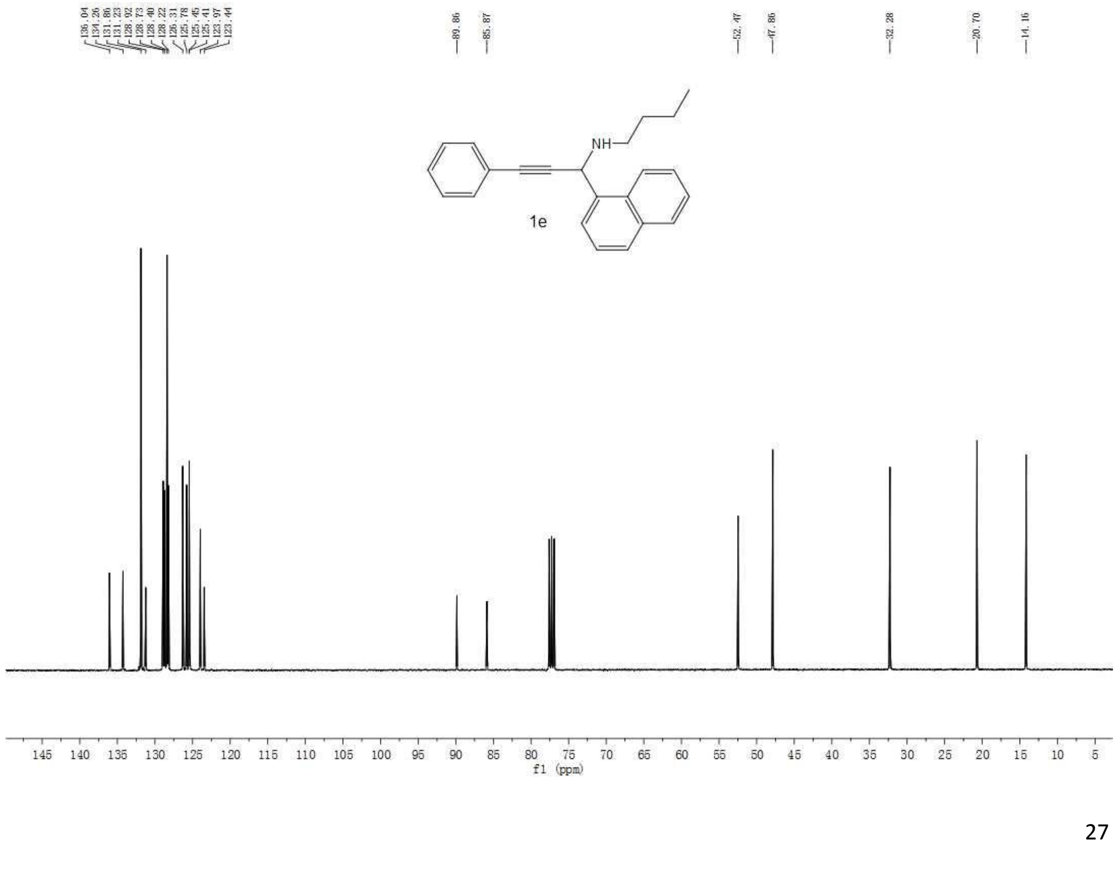
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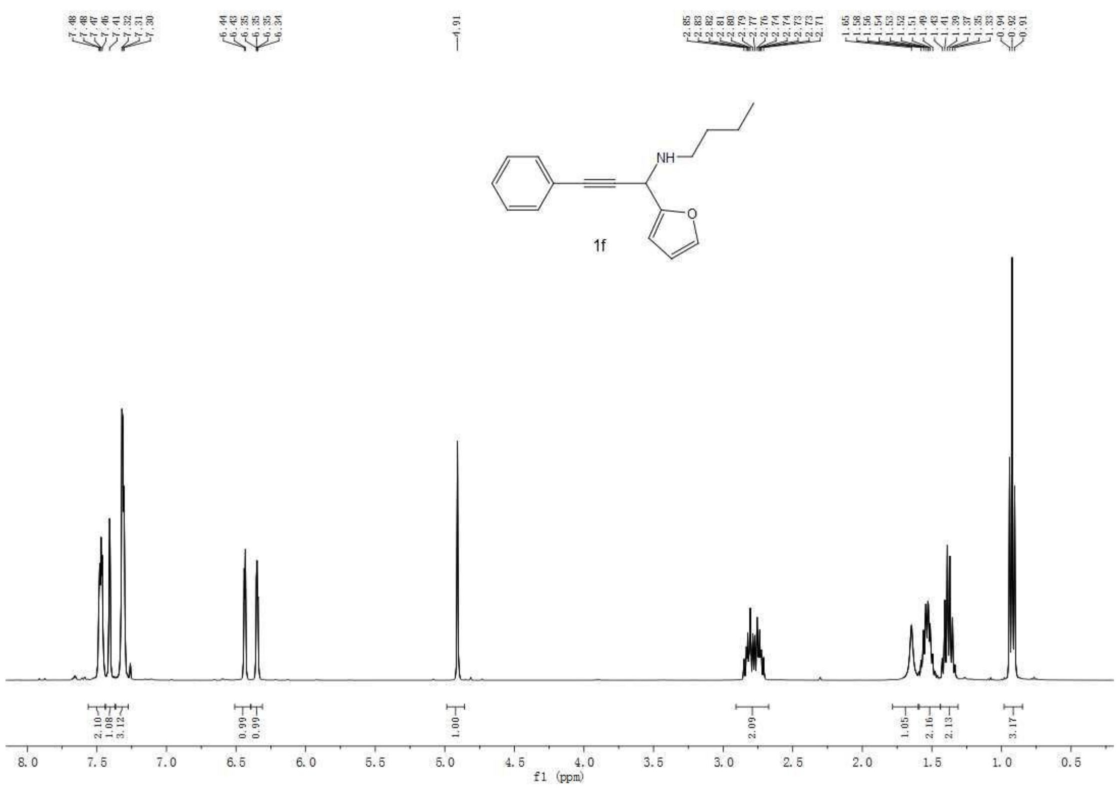
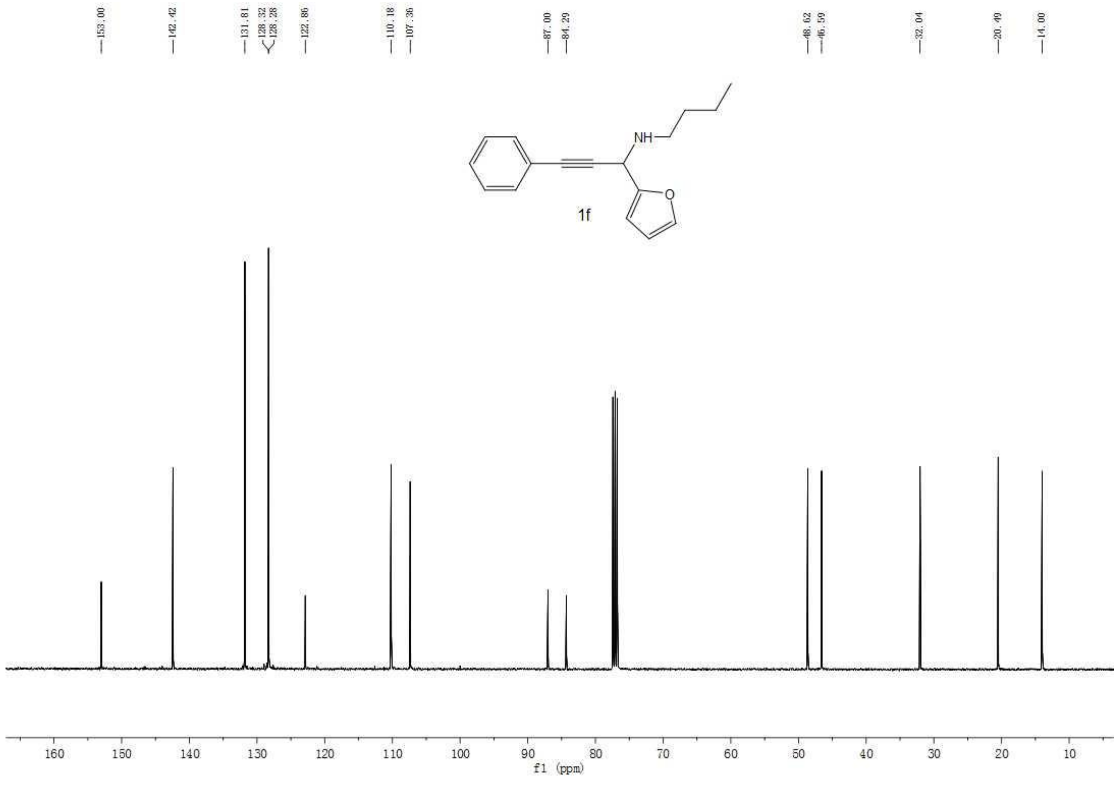
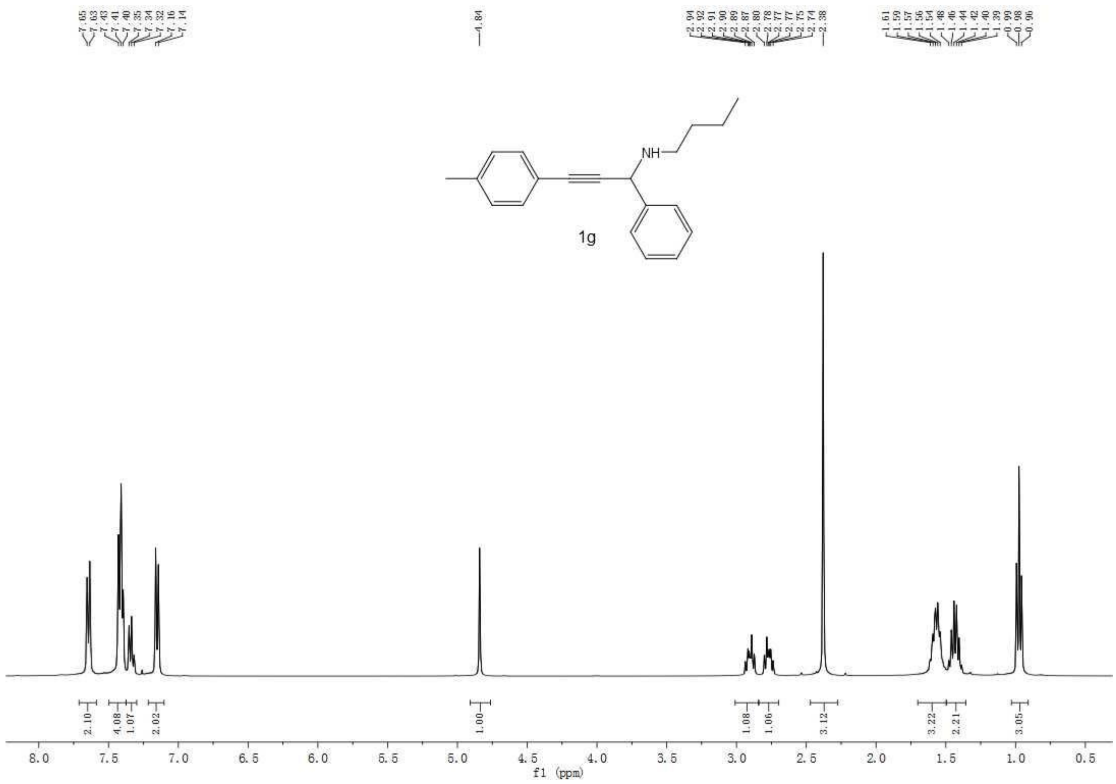
f1 (ppm)



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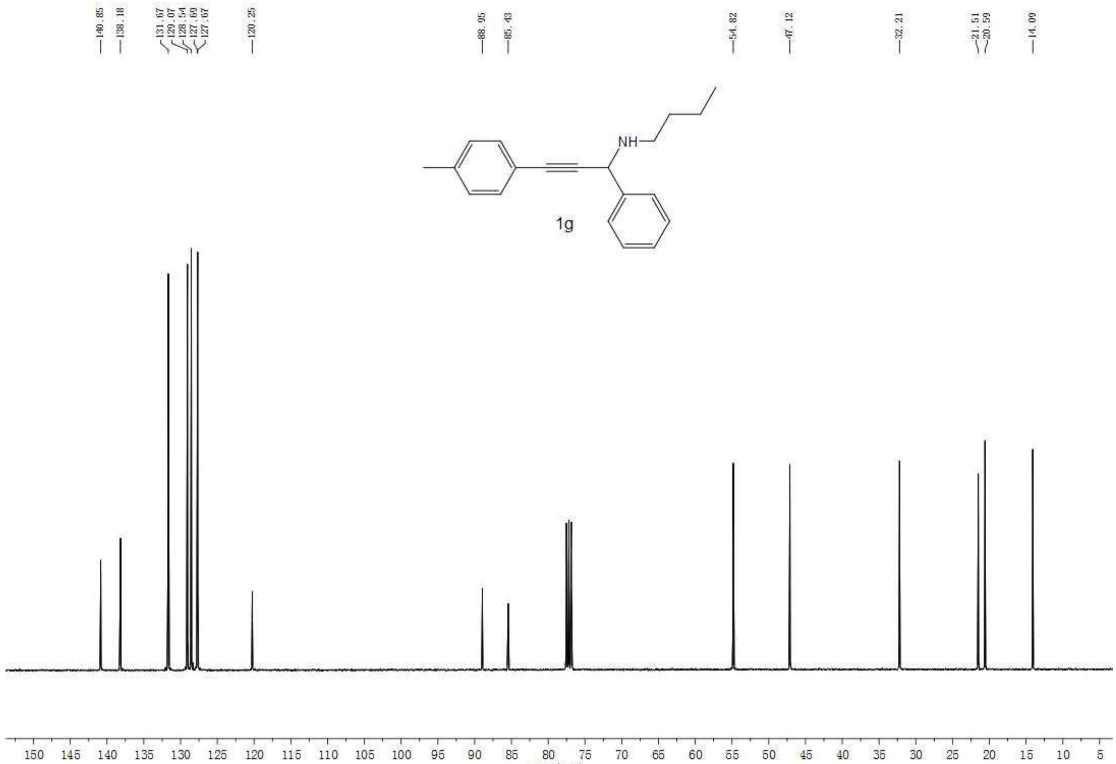
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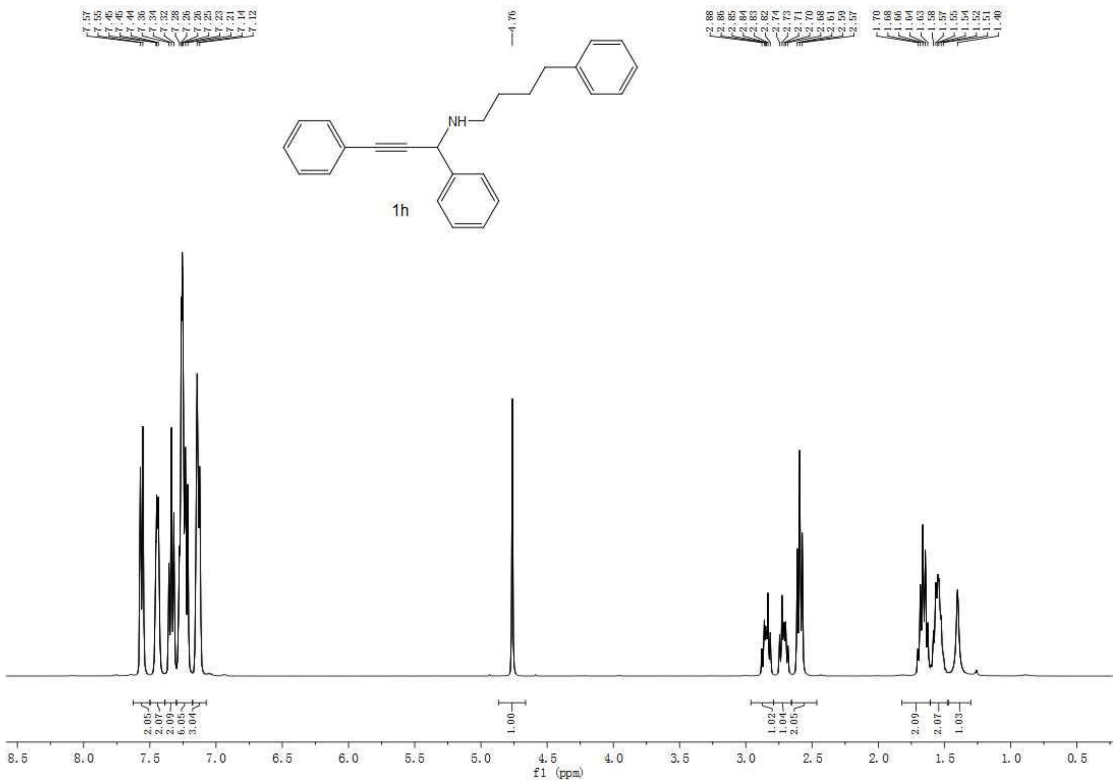

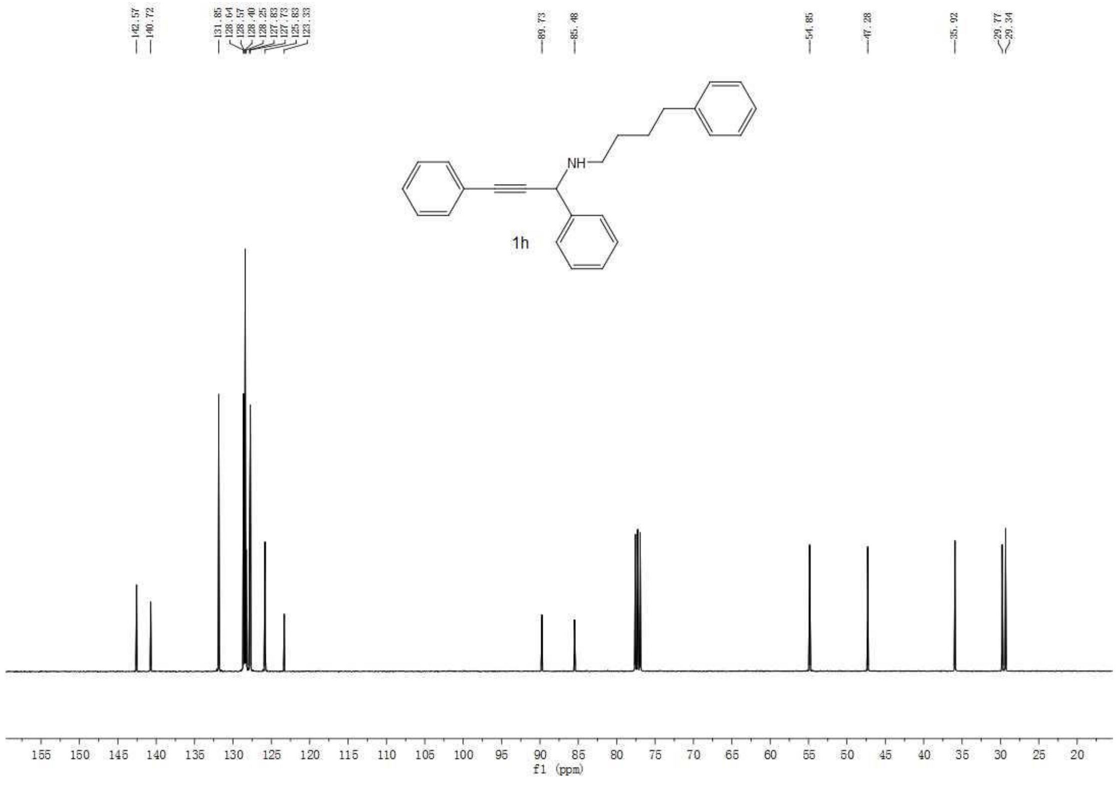

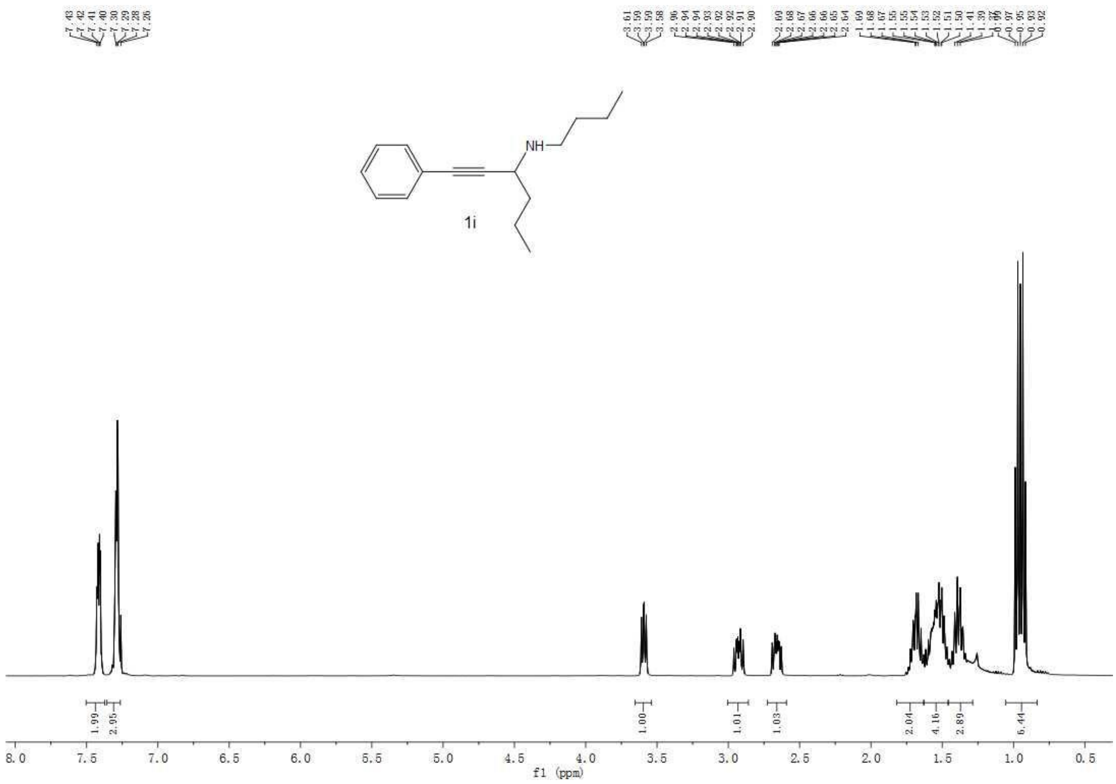
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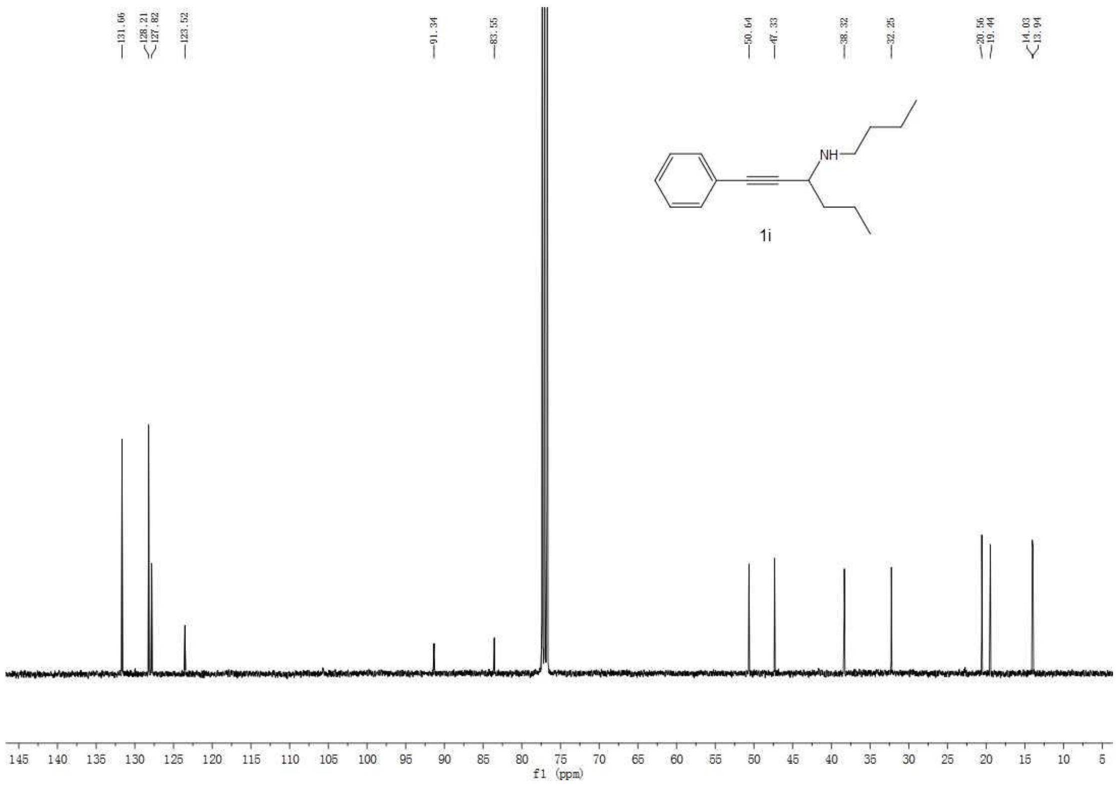
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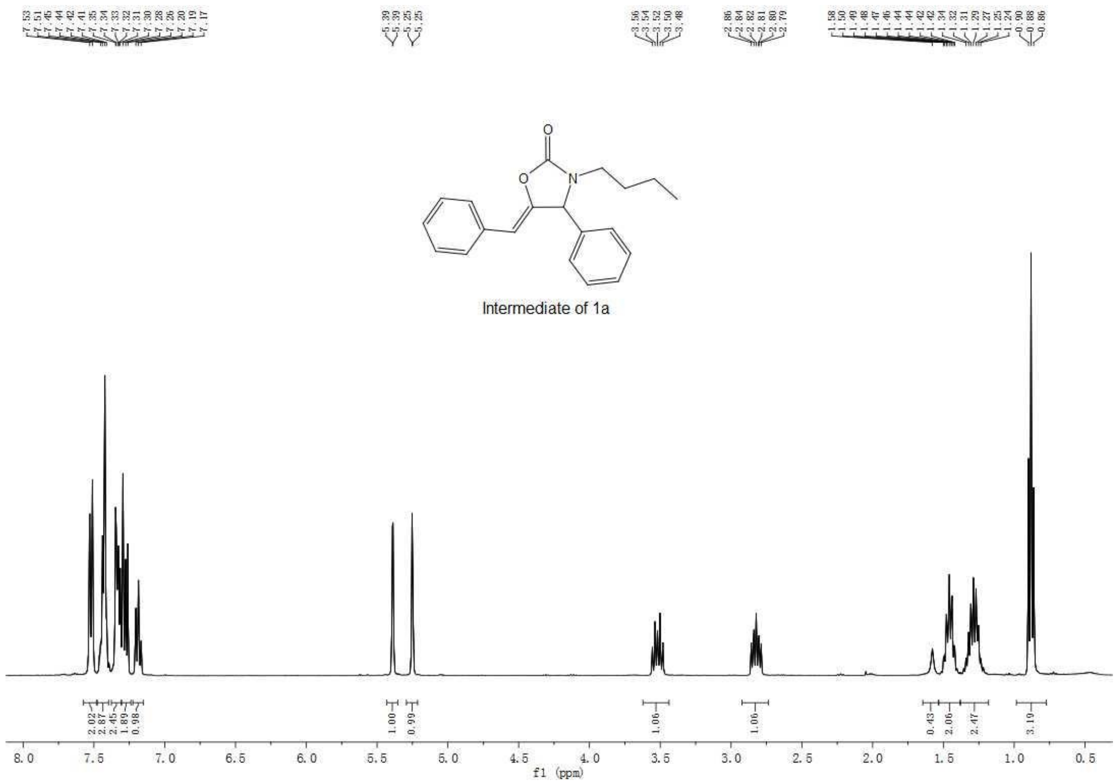
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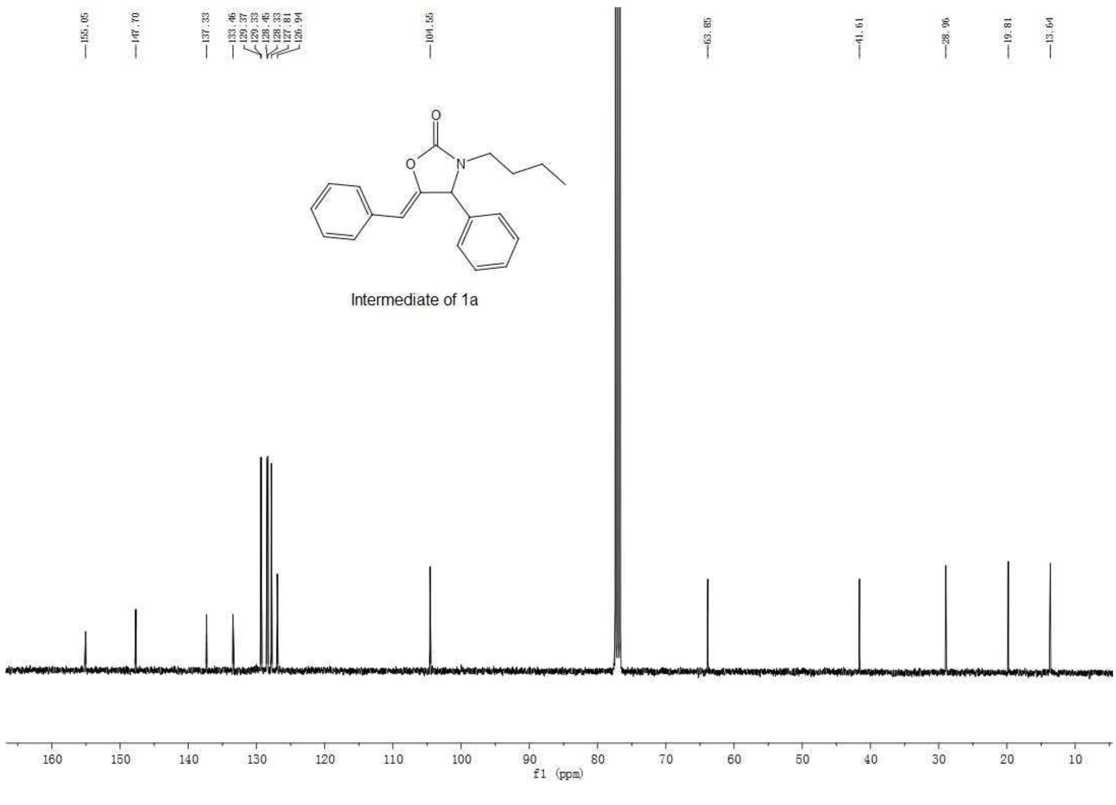
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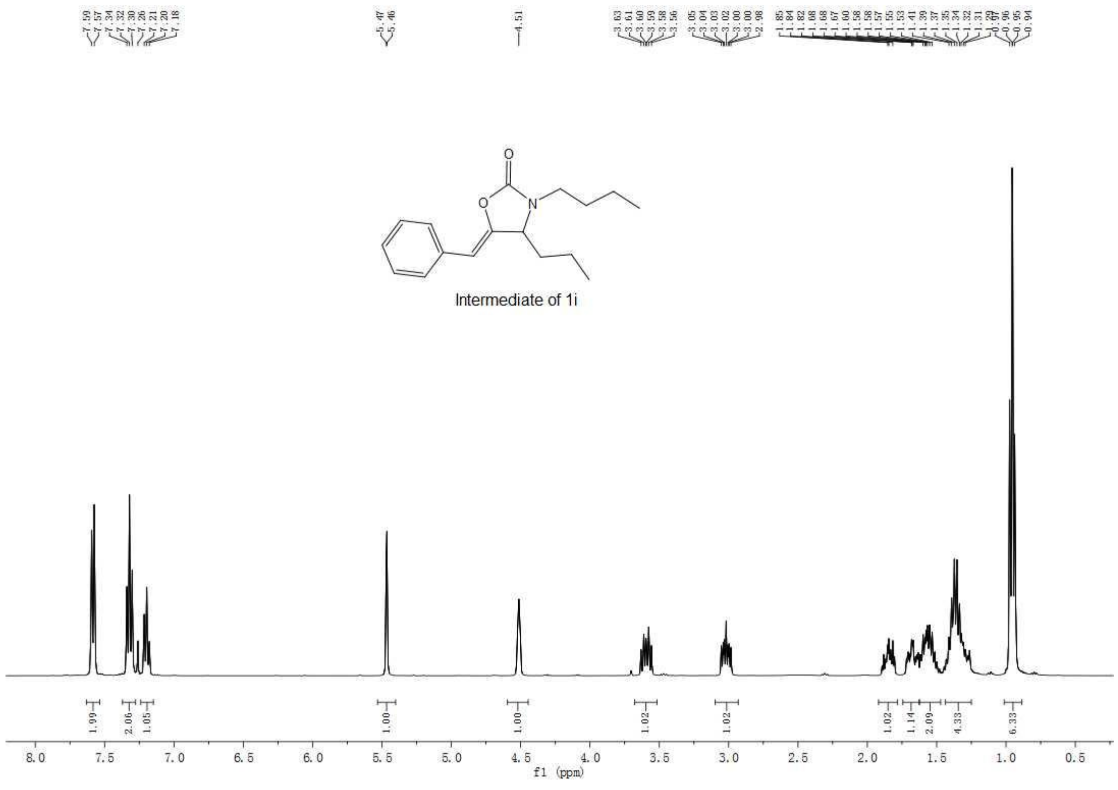
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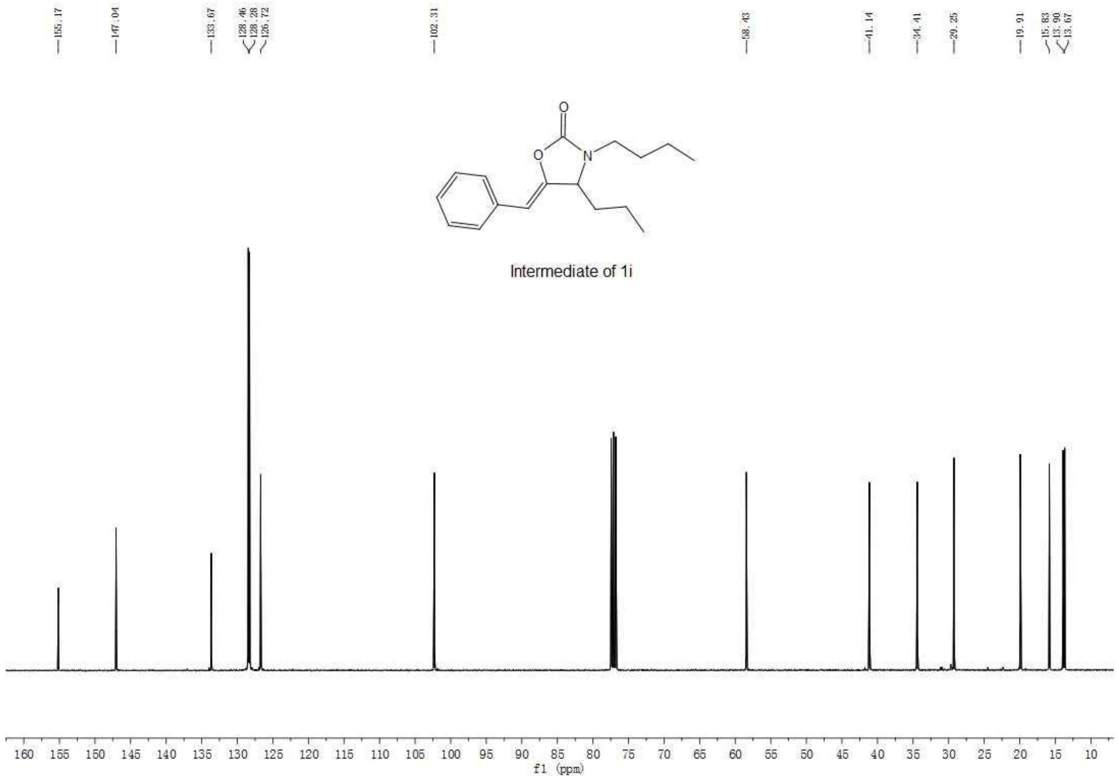
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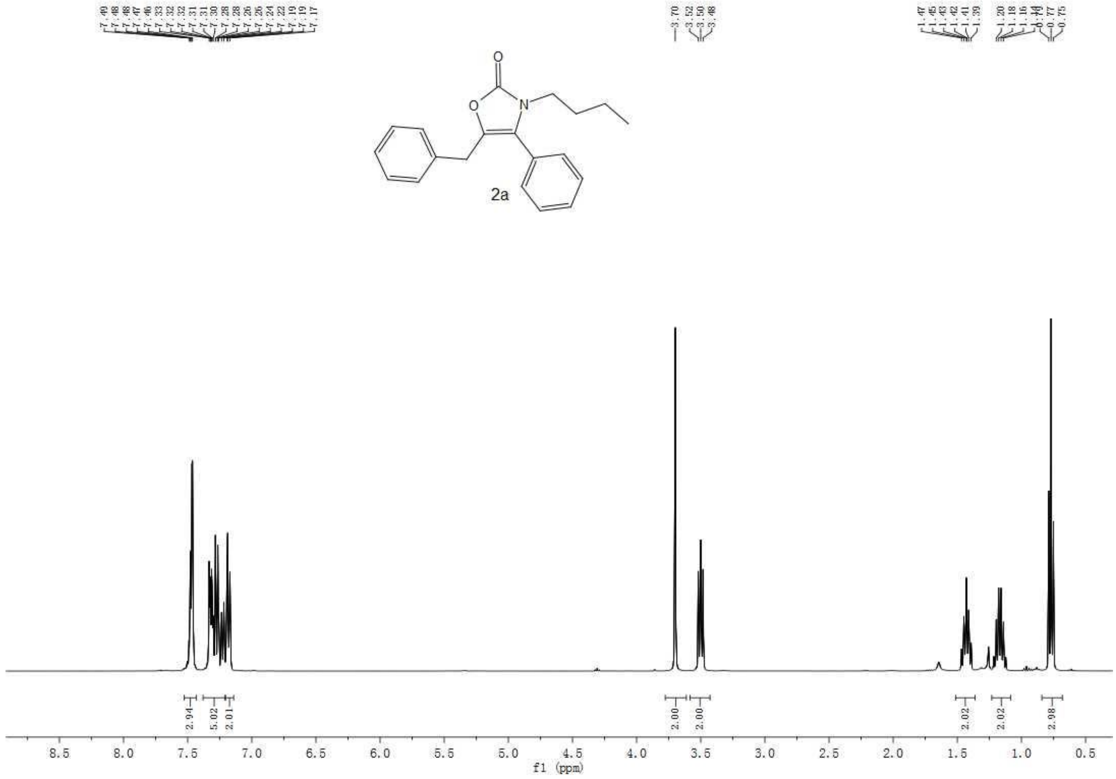
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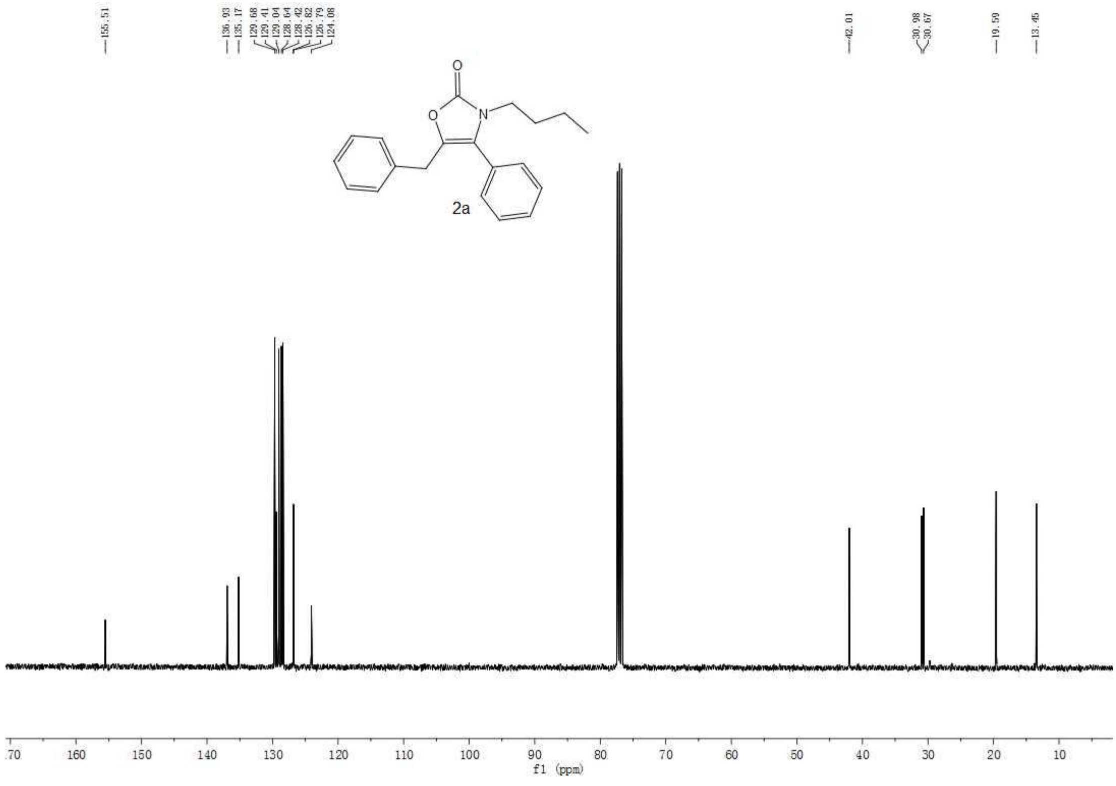
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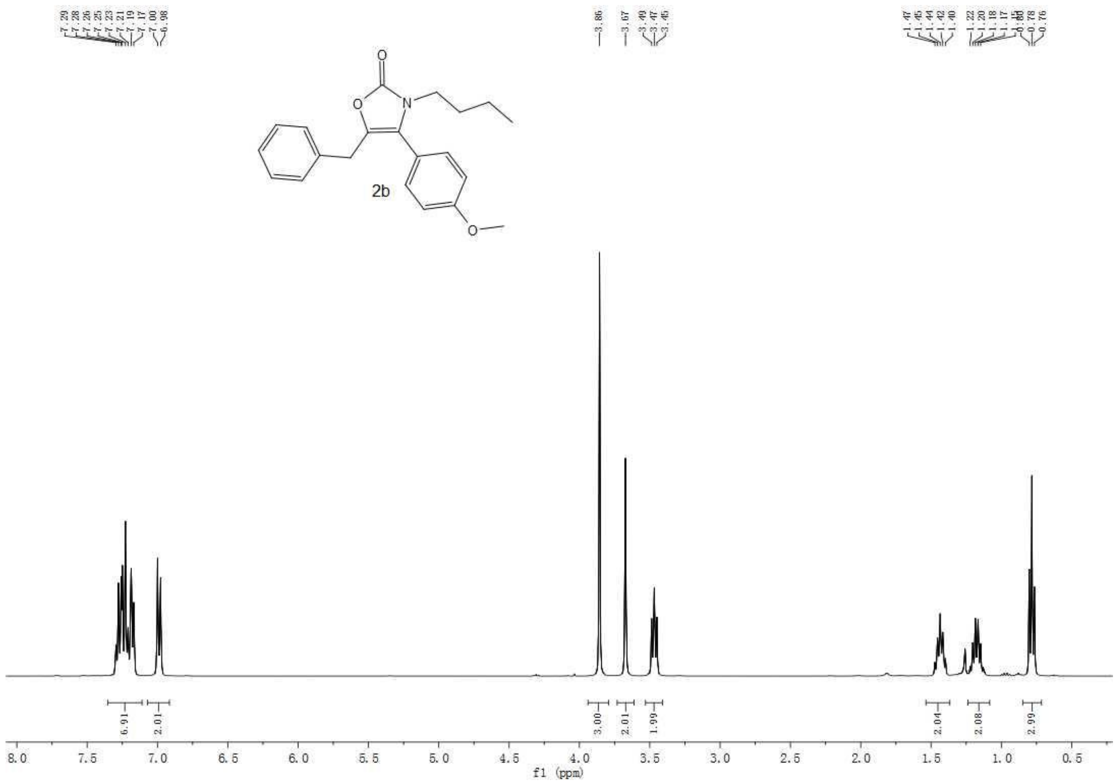

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O
N
O
O
2b
6.91 2.01 3.00 2.01 1.99 2.04 2.08 2.99
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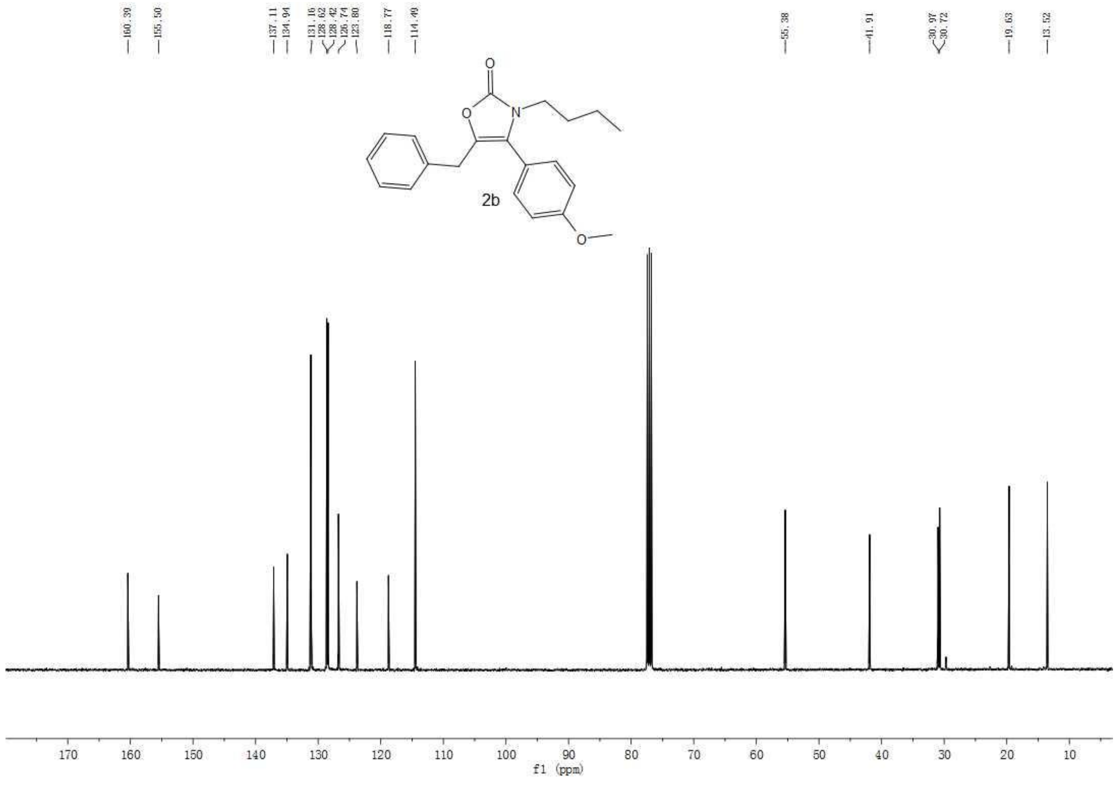

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O
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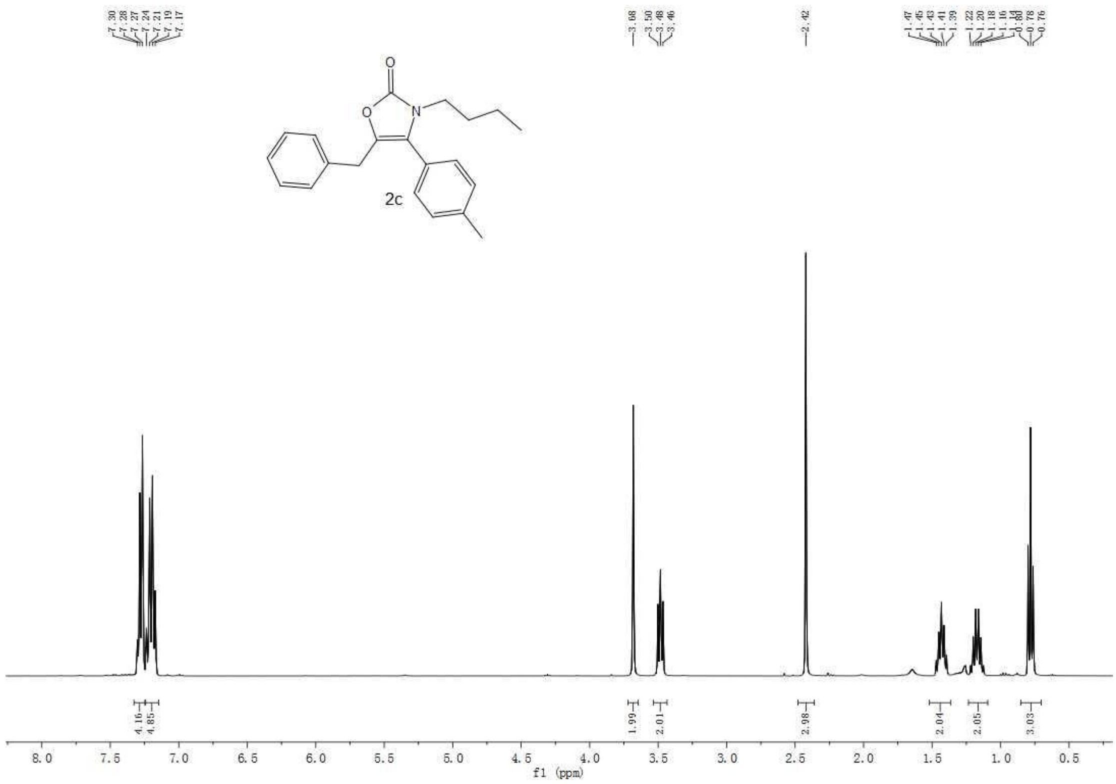

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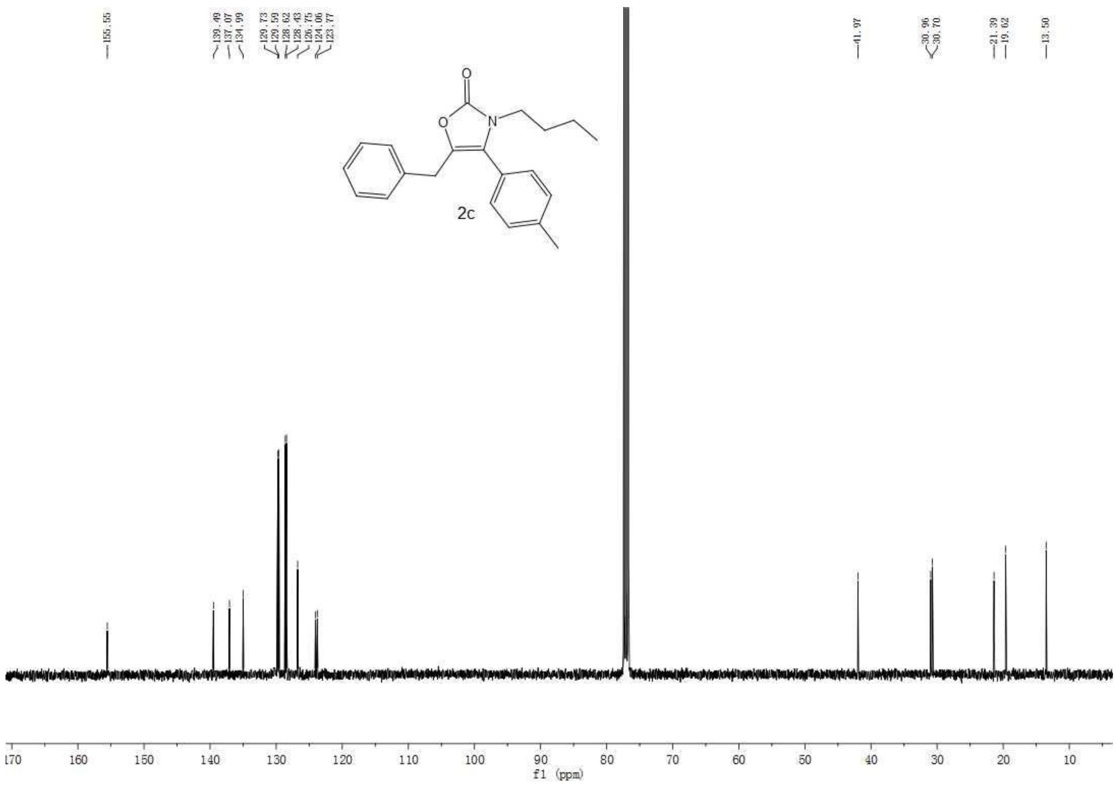

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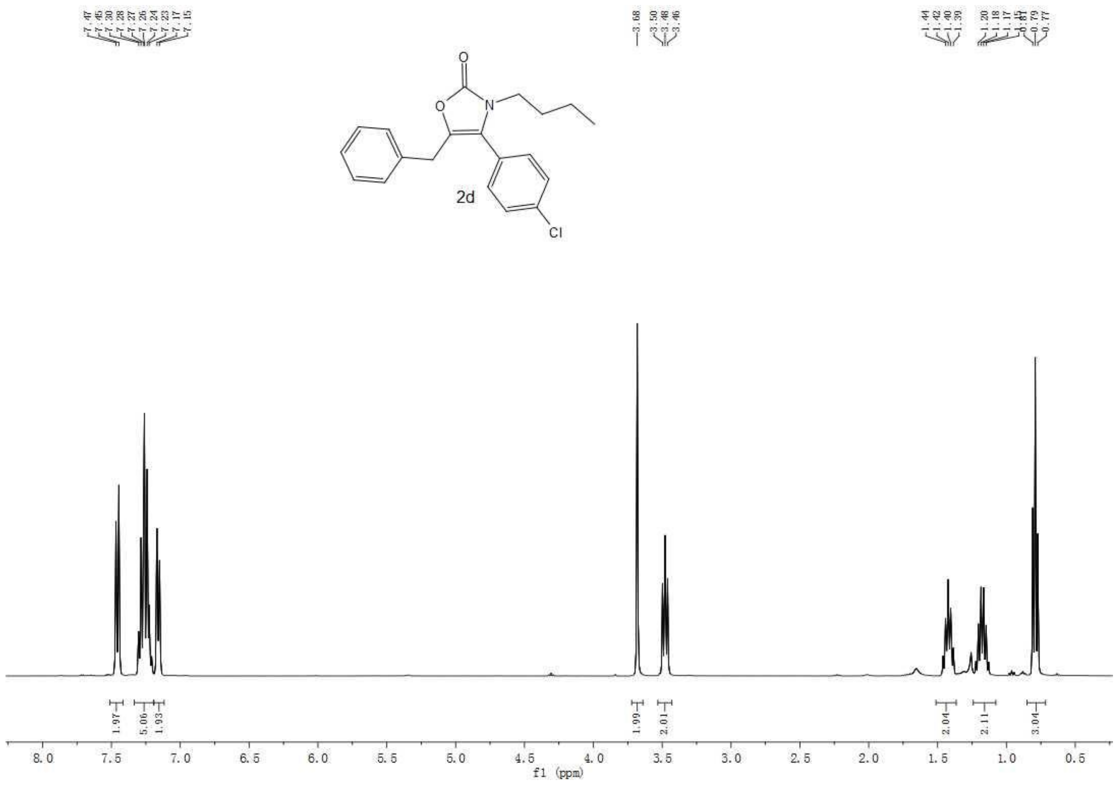

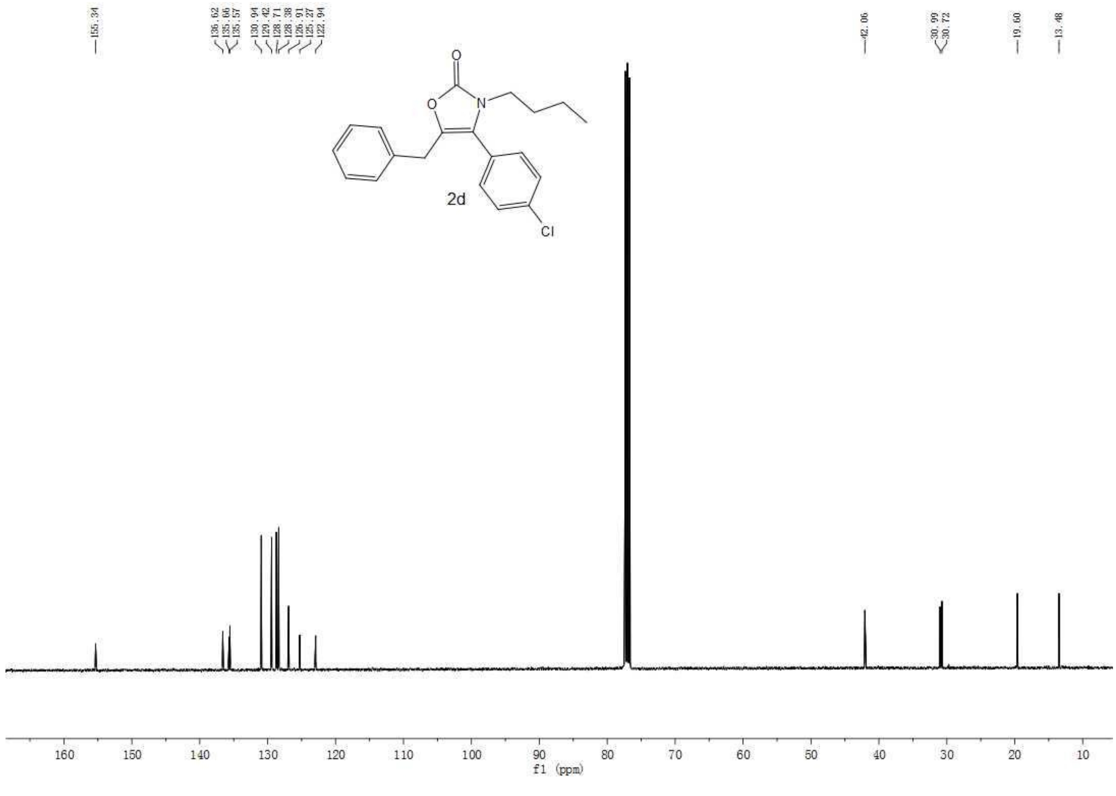

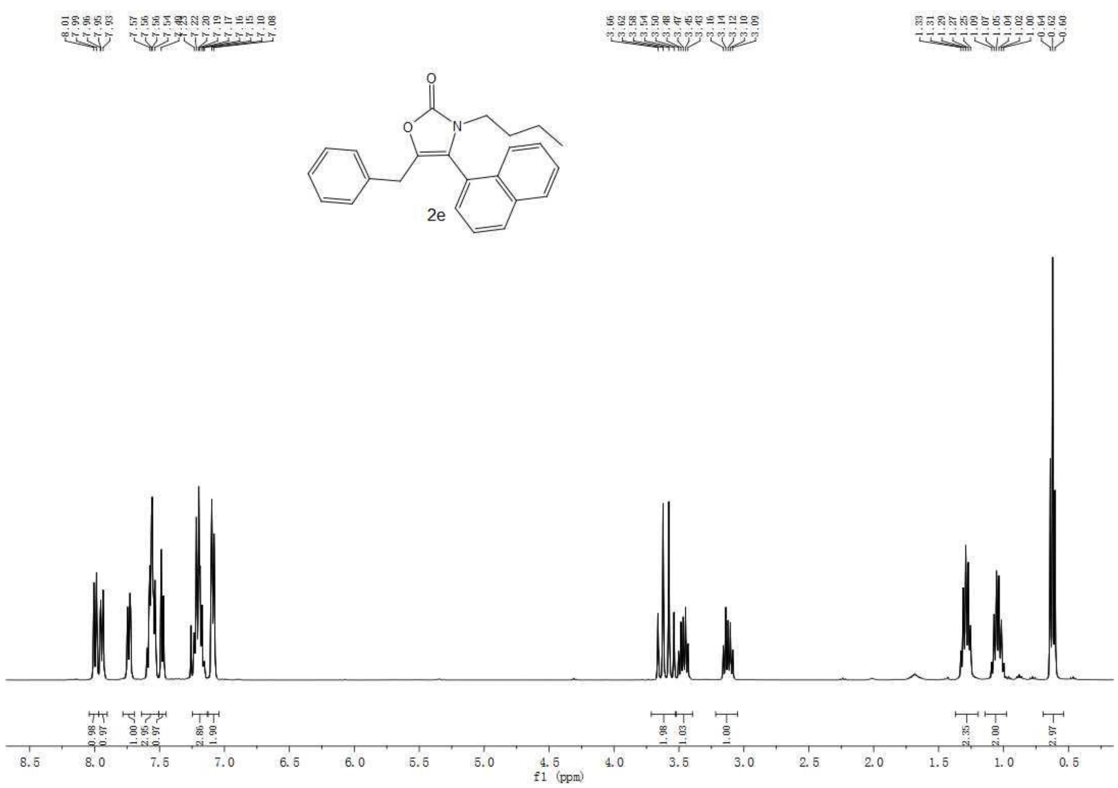

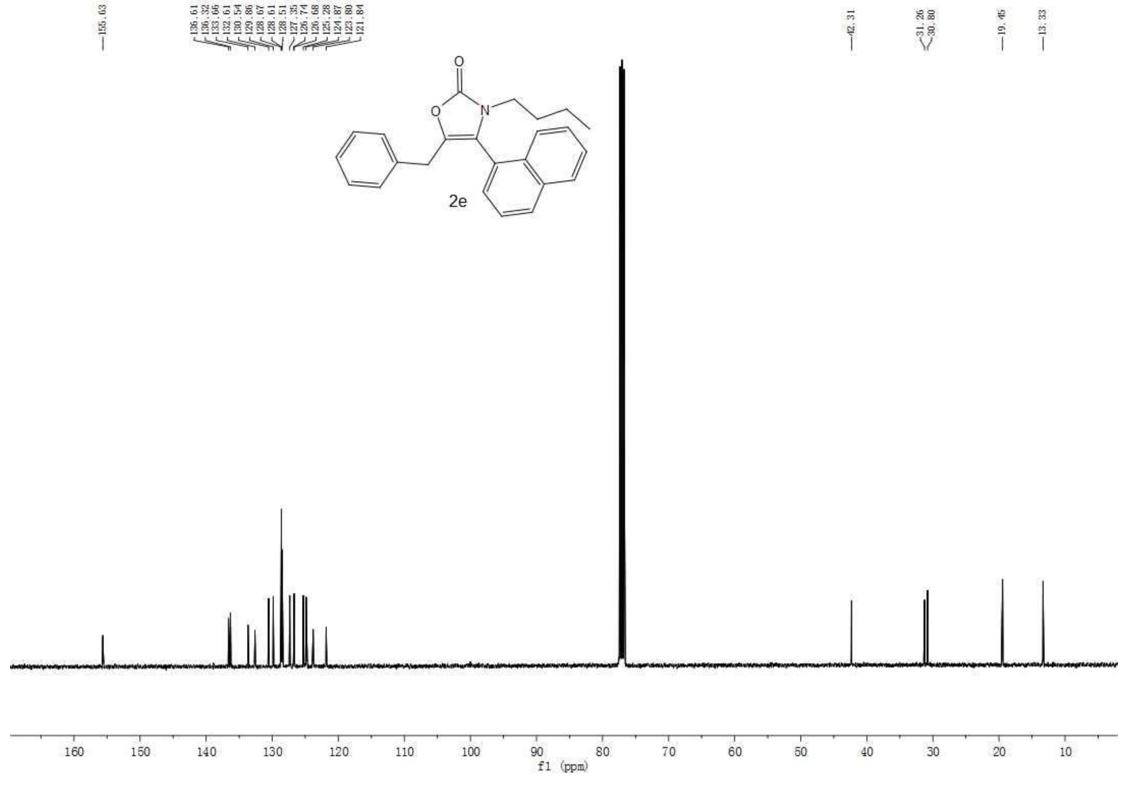

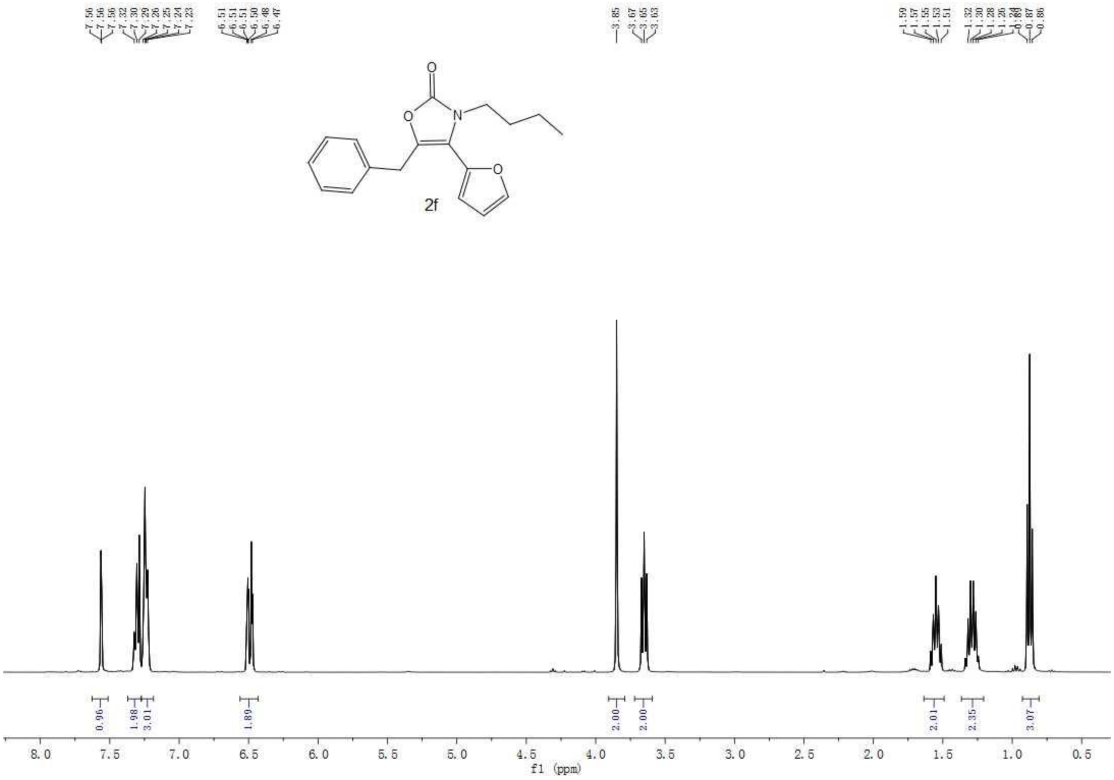
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2.01
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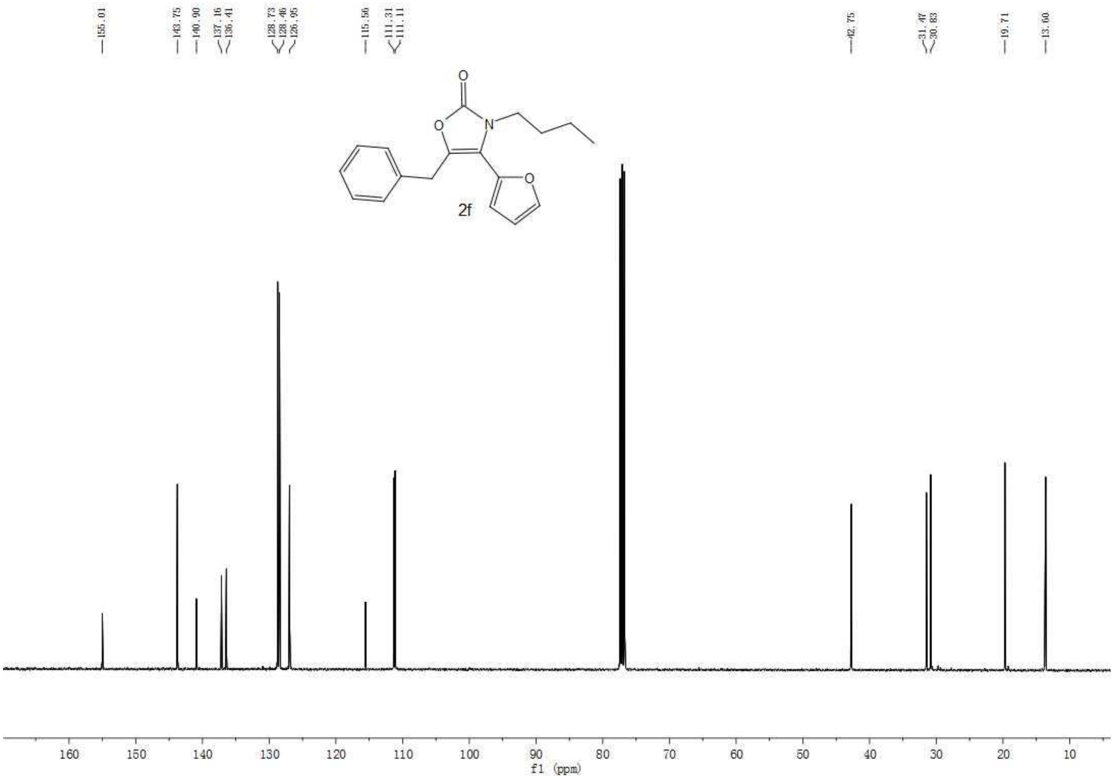
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O
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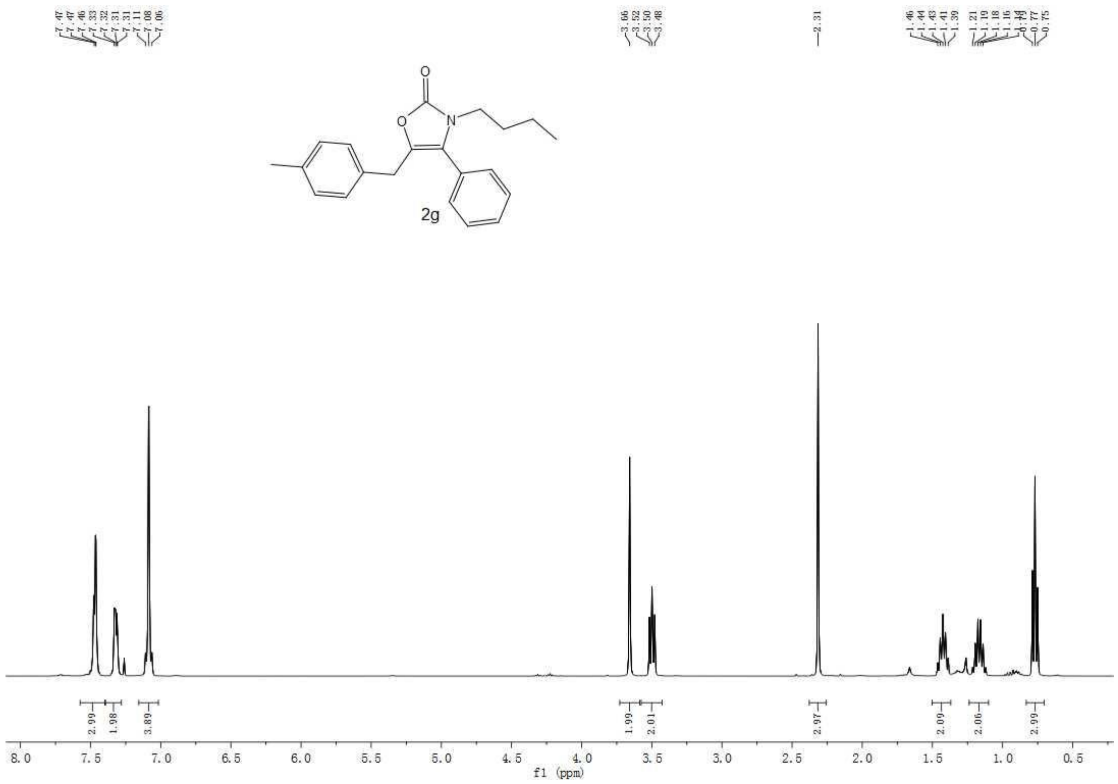
f1 (ppm)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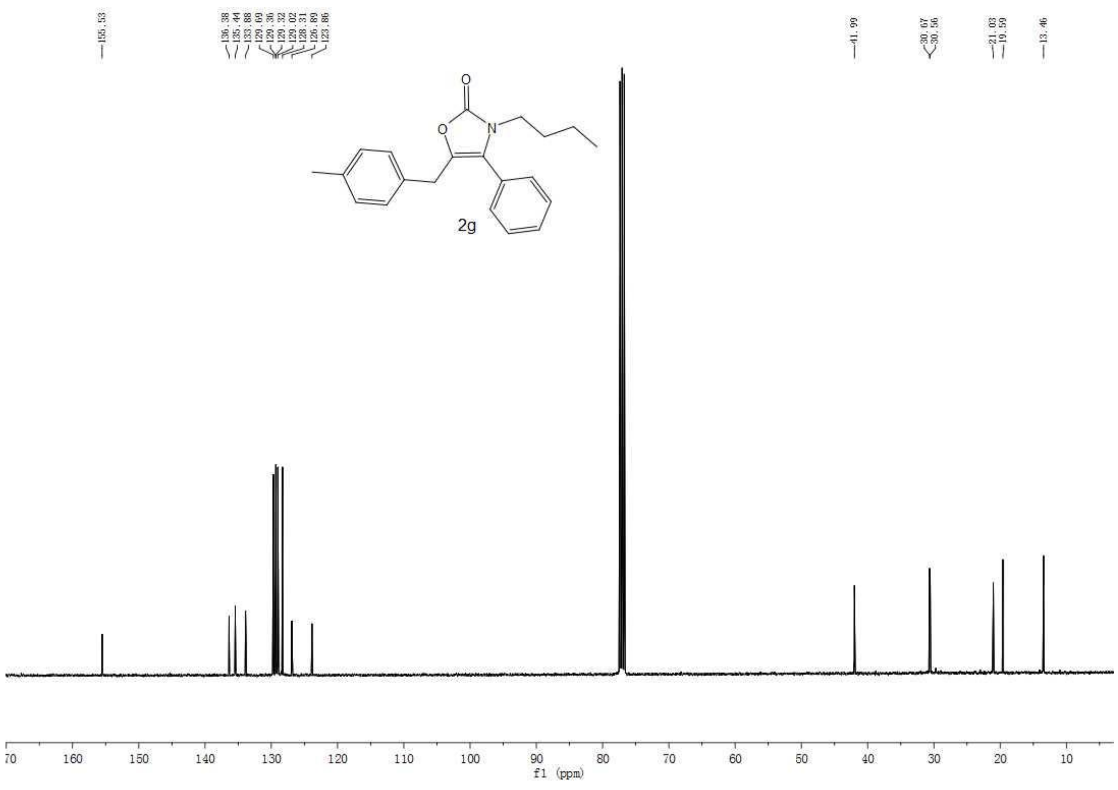
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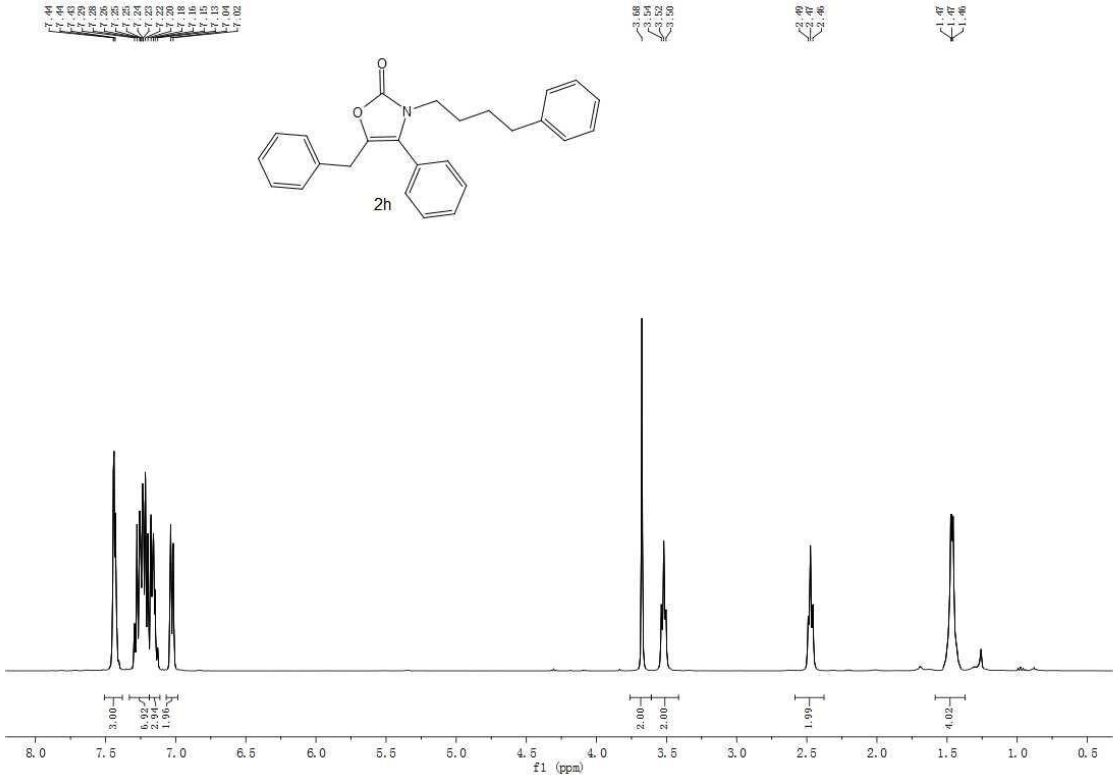
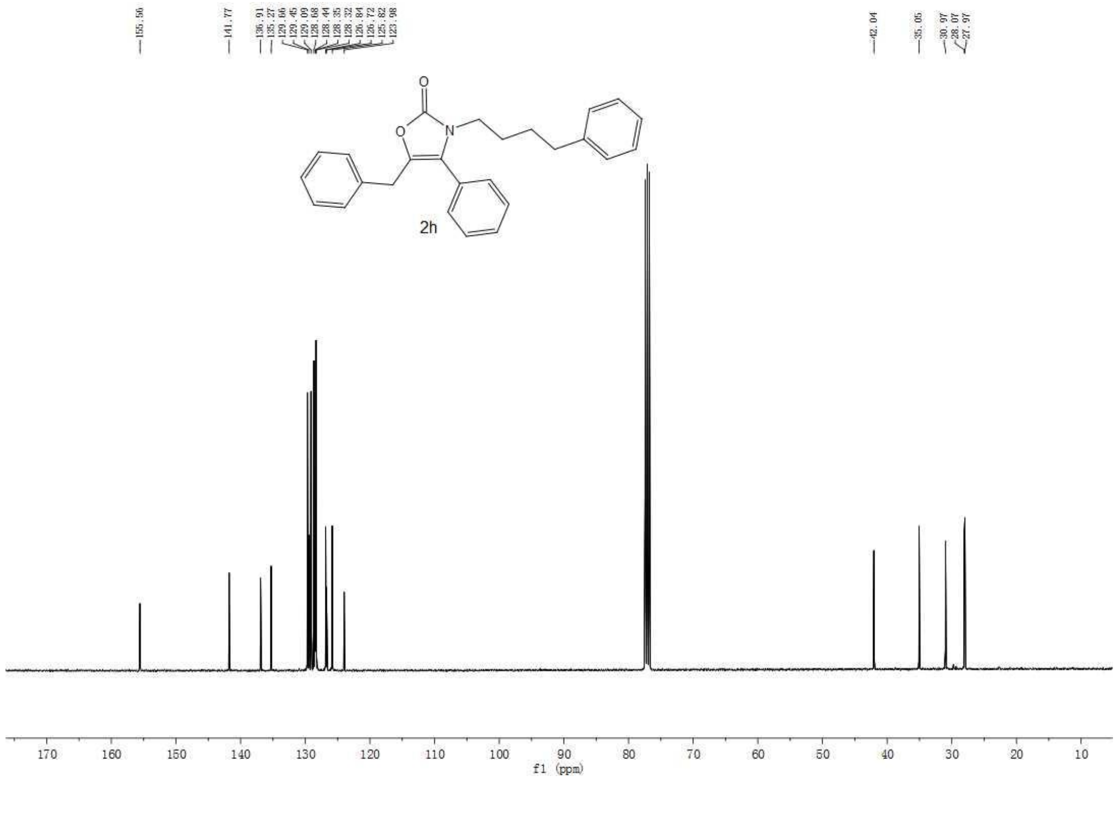
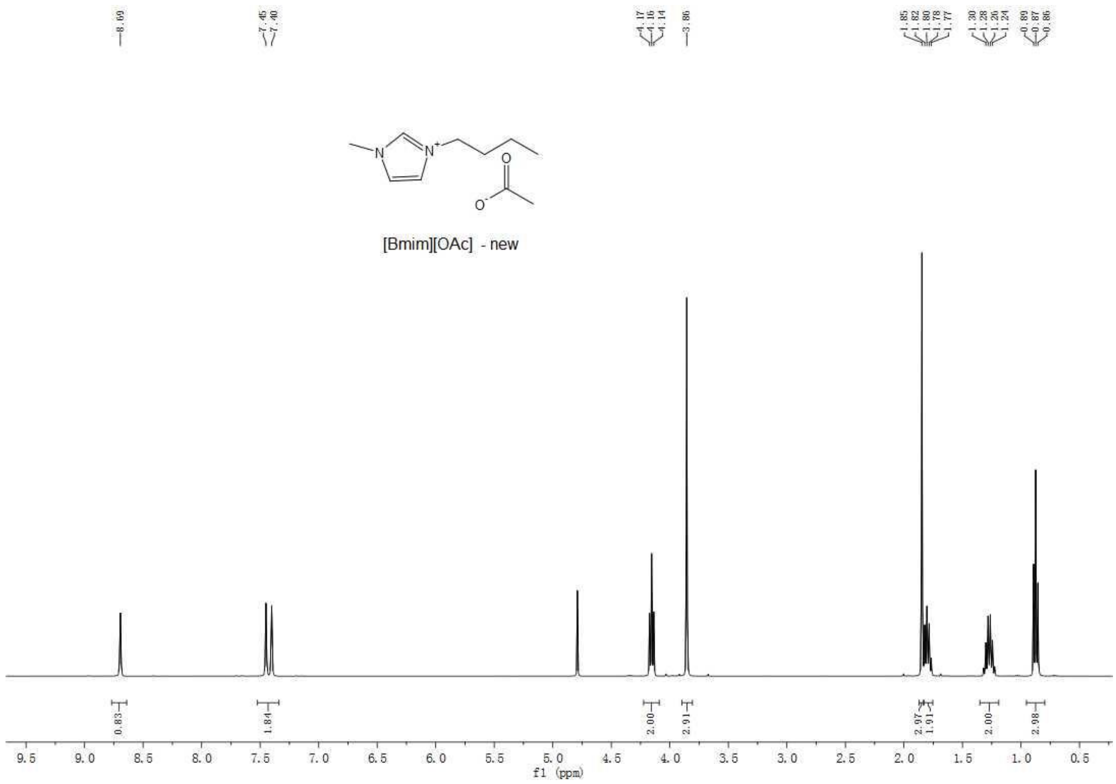
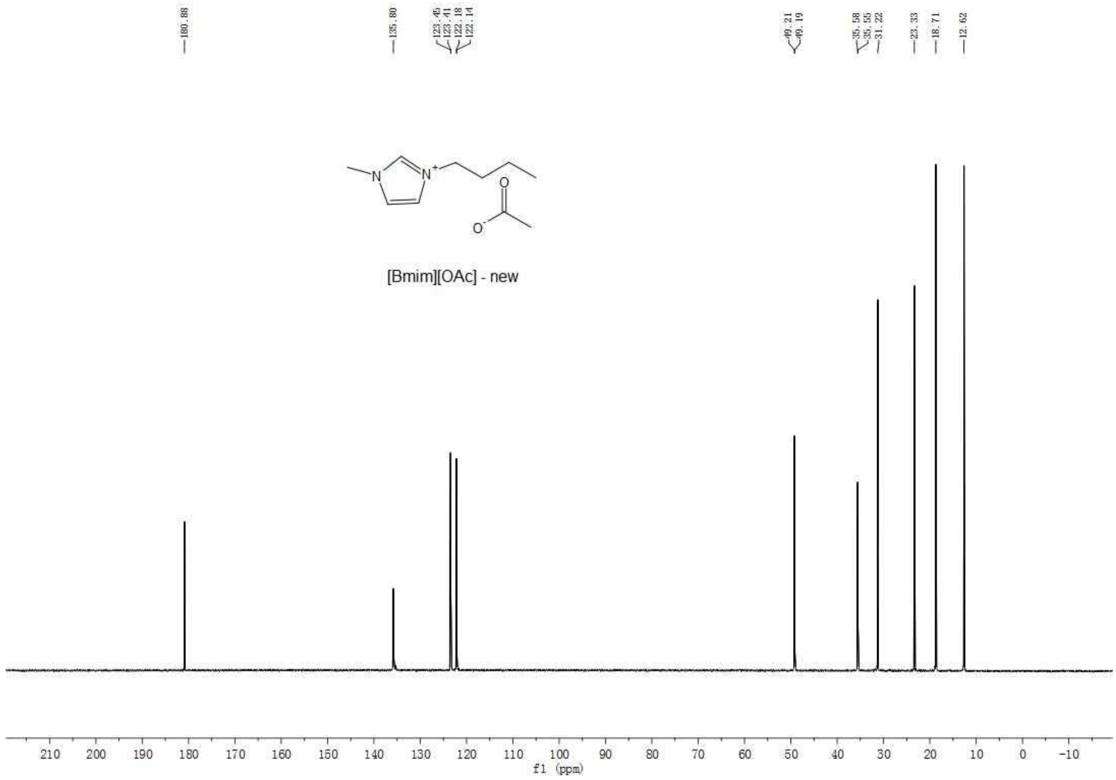
O
N
O
2g
f1 (ppm)

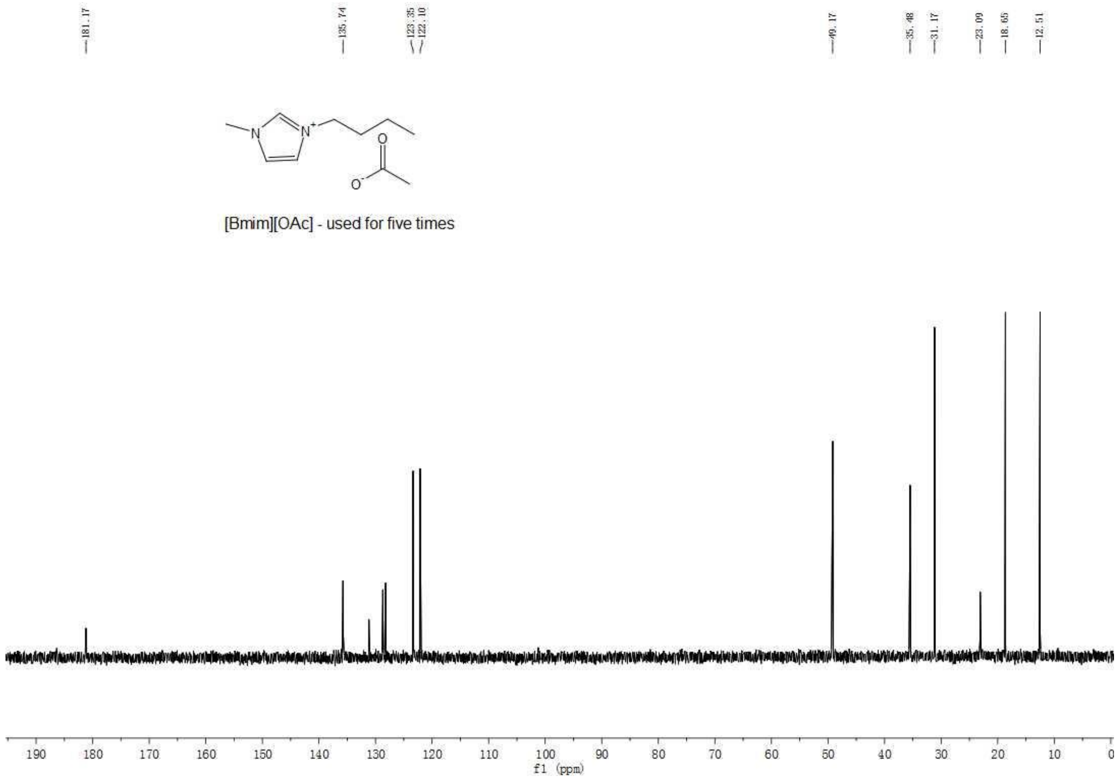

7.44
7.44
7.43
7.29
7.28
7.26
7.25
7.25
7.24
7.23
7.22
7.20
7.18
7.16
7.15
7.13
7.04
7.02
3.68
3.54
3.52
3.50
2.49
2.47
2.46
1.47
1.47
1.46
O
N
2h
3.00
6.92
2.94
1.96
2.00
2.00
1.99
4.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

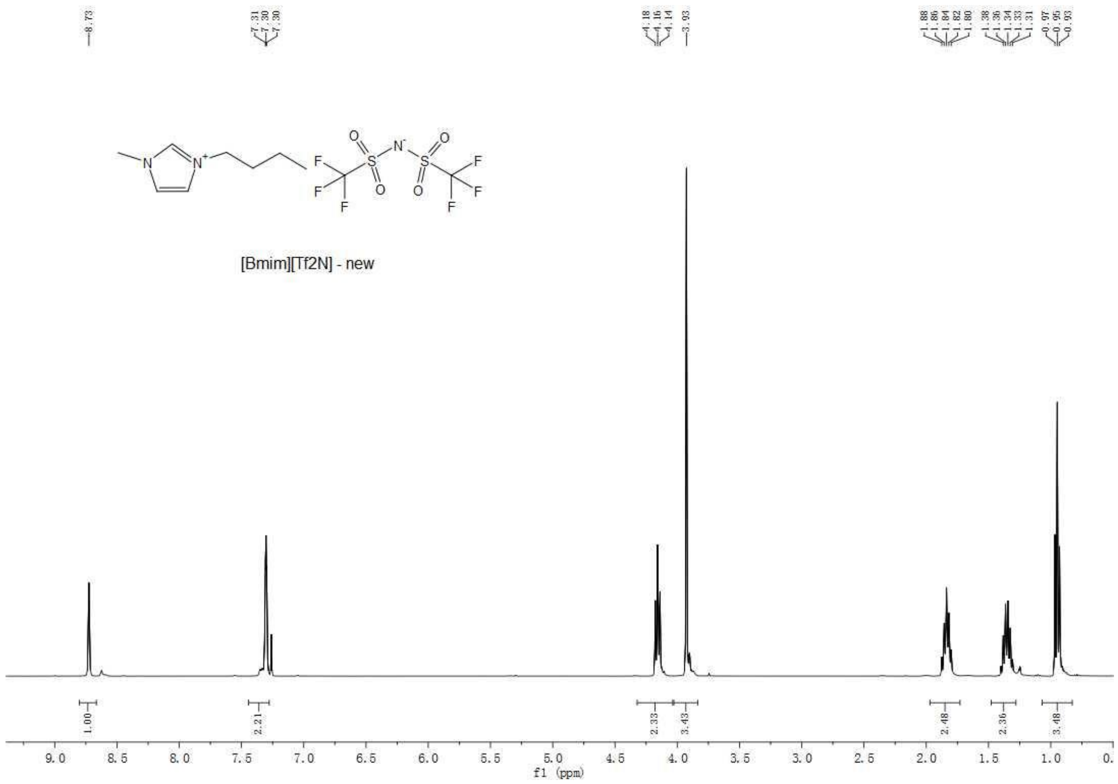

155.56
141.77
136.91
135.27
129.66
129.45
129.09
128.68
128.44
128.35
128.32
126.84
126.72
125.82
123.98
42.04
35.05
30.97
28.07
27.97
O
N
2h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

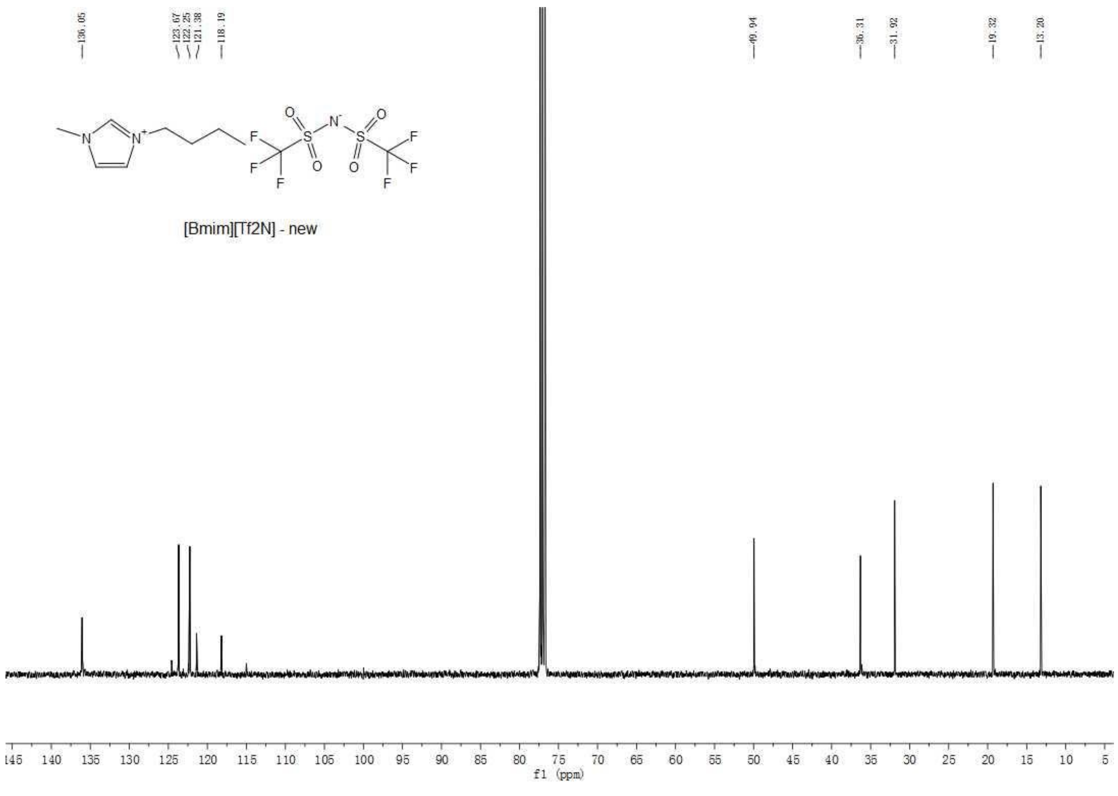

[Bmim][OAc] - new
f1 (ppm)

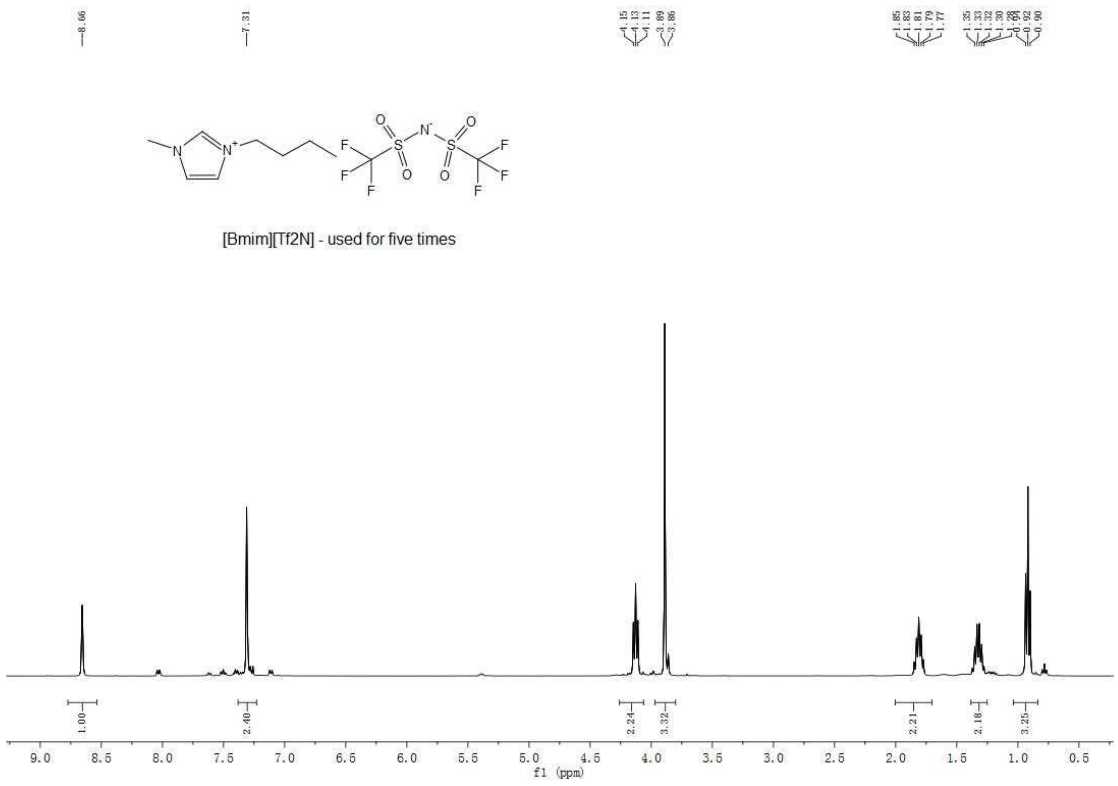

[Bmim][OAc] - new
f1 (ppm)

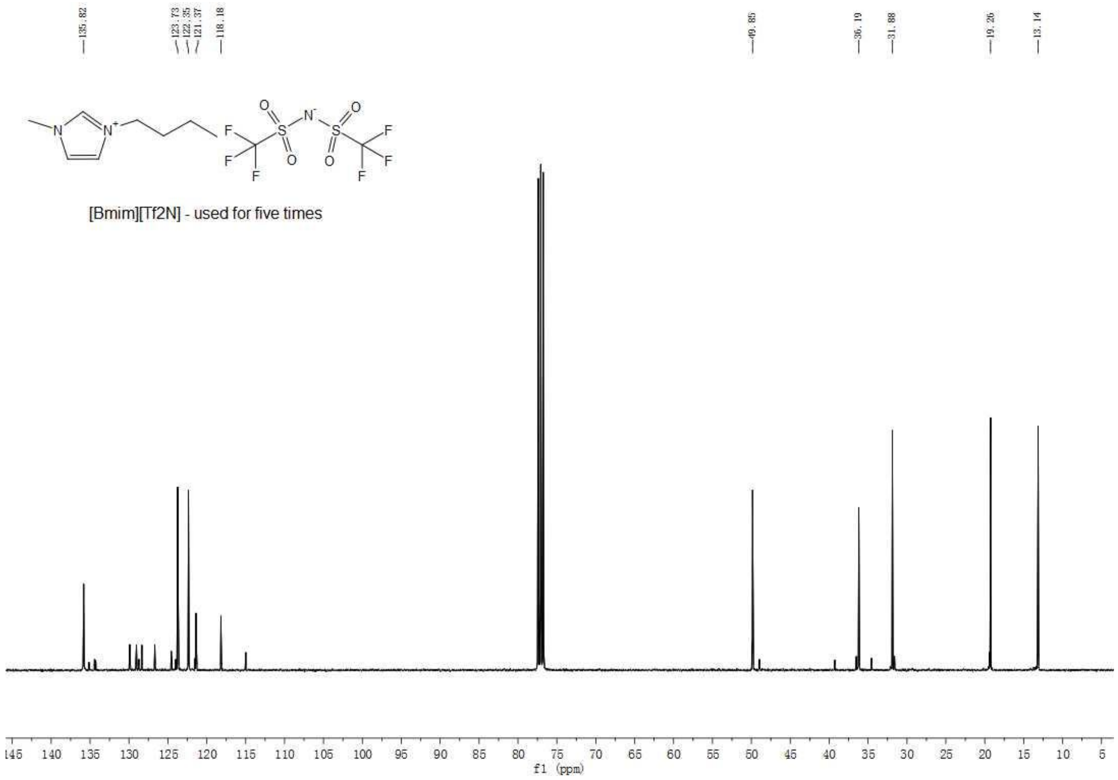

[Bmim][OAc] - used for five times
8.65
7.41
7.37
4.79
4.15
4.13
4.12
3.83
1.87
1.83
1.81
1.79
1.77
1.75
1.29
1.27
1.25
1.23
0.87
0.85
0.94
2.13
2.00
2.91
2.34
2.10
2.05
3.05
f1 (ppm)


[Bmim][OAc] - used for five times
181.17
135.74
123.35
122.10
49.17
35.48
31.17
23.09
18.65
12.51
f1 (ppm)


8.73
7.31
7.30
7.30
4.18
4.16
4.14
3.93
1.88
1.86
1.84
1.82
1.80
1.38
1.36
1.34
1.33
1.31
0.97
0.95
0.93
[Bmim][Tf2N] - new
1.00
2.21
2.33
3.43
2.48
2.36
3.48
f1 (ppm)


136.05
123.67
122.25
121.38
118.19
49.94
36.31
31.92
19.32
13.20
[Bmim][Tf2N] - new
f1 (ppm)


[Bmim][Tf2N] - used for five times
f1 (ppm)


[Bmim][Tf2N] - used for five times
f1 (ppm)