Electronic Supporting Information

Silica-supported metal acetylacetonate catalysts with a robust and flexible linker constructed by using 2-butoxy-3,4-dihydropyrans as dual anchoring reagents and ligand donors

Bingbing Lai,[a] Zhipeng Huang,[a] Zhifang, Jia,[a] Rongxian Bai[a,] * and Yanlong Gu[a, b] *

[a]Hubei Key Laboratory of Material Chemistry and Service Failure, Key Laboratory for Large-Format Battery, Materials and System, Ministry of Education, Huazhong University of Science and Technology, 1037 Luoyu road, Hongshan District, Wuhan 430074, China. Fax: (0)86-(0)27-87 54 45 32; E-mail: klgyl@hust.edu.cn

[b]State Key Laboratory for Oxo Synthesis and Selective Oxidation, Lanzhou Institute of Chemical Physics, Lanzhou, 730000 (P.R. China)

Table of Contents

1. General remarks:

Zinc(II) acetylacetonate, cupric(II) acetylacetonate, ruthenium (III) 2,4-pentanedionate, 4-fluorophenylacetylene and *p*-methoxybenzaldehyde were purchased from Heowns Biochem Technologies Co. Ltd. Benzyl mercaptan, 4-*tert*-butylphenylacetylene, (2-bromoethyl)benzene, p-anisidine, benzylamine, furfurylamine, allylamine, 2-(1-cyclohexenyl)ethylamine, 2-carboxy-3,4-dimethoxybenzaldehyde, *p*-tolualdehyde and 4-chlorobenzaldehyde were purchased from Alfa Aesar Chemical Company. 1-Hexadecylamine, iodoethane and 4-aminoacetophenone were purchased from Aladdin Industrial Corporation. Sodium azide was purchased from Tianjing Damaotie Chemical Company. 4-Ethylphenylacetylene, 1-eth-1-ynyl-4-propylbenzene, 1-*n*-butyl-4-eth-1-ynylbenzene, 3-aminophenylacetylene, benzhydrol, 2-carboxybenzaldehyde, 1-ethynyl-4-pentylbenzene, 4-aminophenyl boronic acid pinacol ester were purchased from Energy Chemical. *p*-Toluidine was purchased from Shanghai Jinshantingxin Industry Co. Ltd. 4-Bromoaniline, 4-fluoroaniline, 4-amino benzoic acid ethyl ester and tryptamine were purchased from Shanghai Shaoyuan Co., Ltd. 3,4-Dimethoxyaniline and 1-Boc-6-aminoindole were purchased from Adamas Reagent. Co., Ltd. 4-Morpholinoaniline and 2-methylallylamine were purchased from Accella Chemical Company. 2-Propynylamine was purchased from ChangCheng Chemical Company. 4-(1-Propenyl)-1,2-dimethoxybenzene was purchased from TCI Chemical Company. TEOS, MTPMS, $Zn(Cl)_2$, nitromethane, EtOH, phenylacetylene, benzyl bromide, 4-nitrobenzyl bromide, benzyl chloride, 4-nitroaniline, 1-bromooctane, 1-bromohexane, *n*-butylamine, cyclohexane and cyclohexane were purchased from *Sinopharm* Chemical Reagent Co. Ltd.

2. Elemental and XRD analysis of the catalysts

Table S1. Elemental analysis of the catalysts.

Name	Weight[mg]	Method	N[%]	C[%]	H[%]	S[%]
HMS	2.3360	2mg80s	0.00	14.22	2.955	7.086
HMS-acac	2.2470	2mg80s	0.40	20.93	3.636	5.110

Sufur loading =2.21 mmol/g. acac loading = 0.67mmol/g.

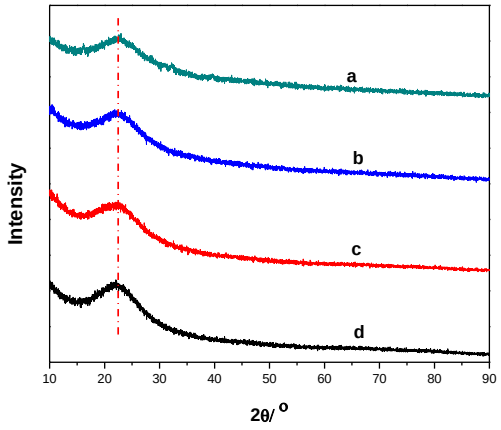


Figure S1. XRD pattern of a) HMS-SH, b) HMS-acac, c) Fresh HMS-DP-Cu **II**, d) Resycled HMS-DP-Cu **II.**

3. IR spectra of acetylacetone complexs

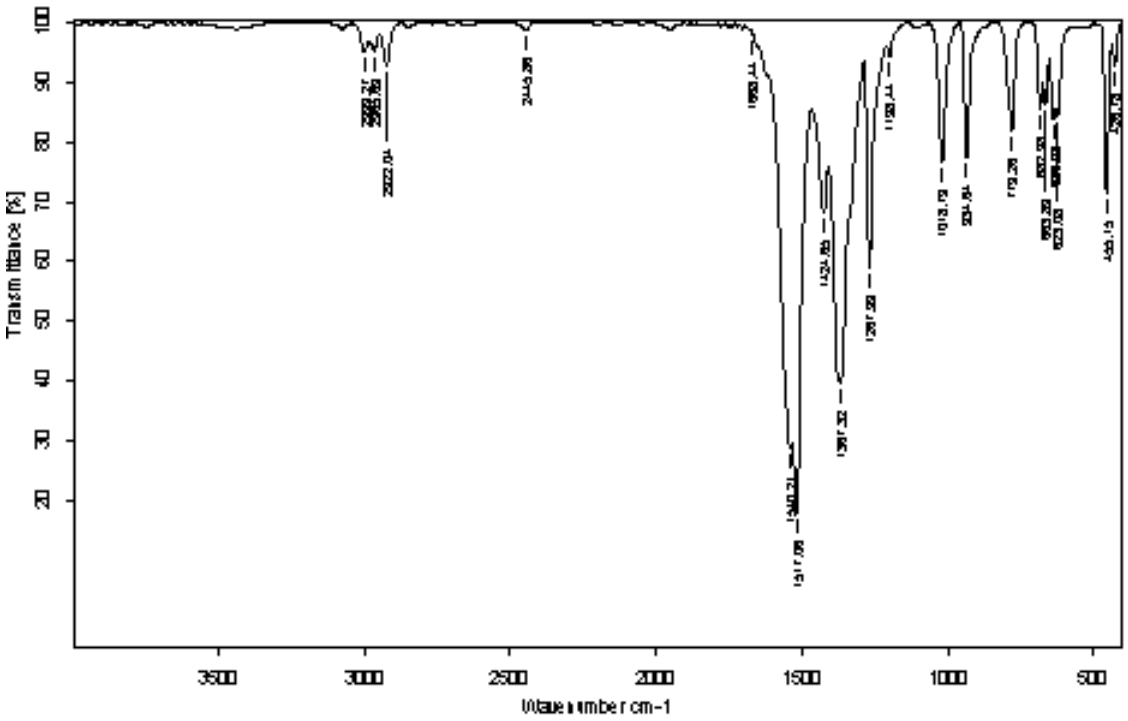


Figure S2. IR spectrogram of $Ru(acac)_3$.

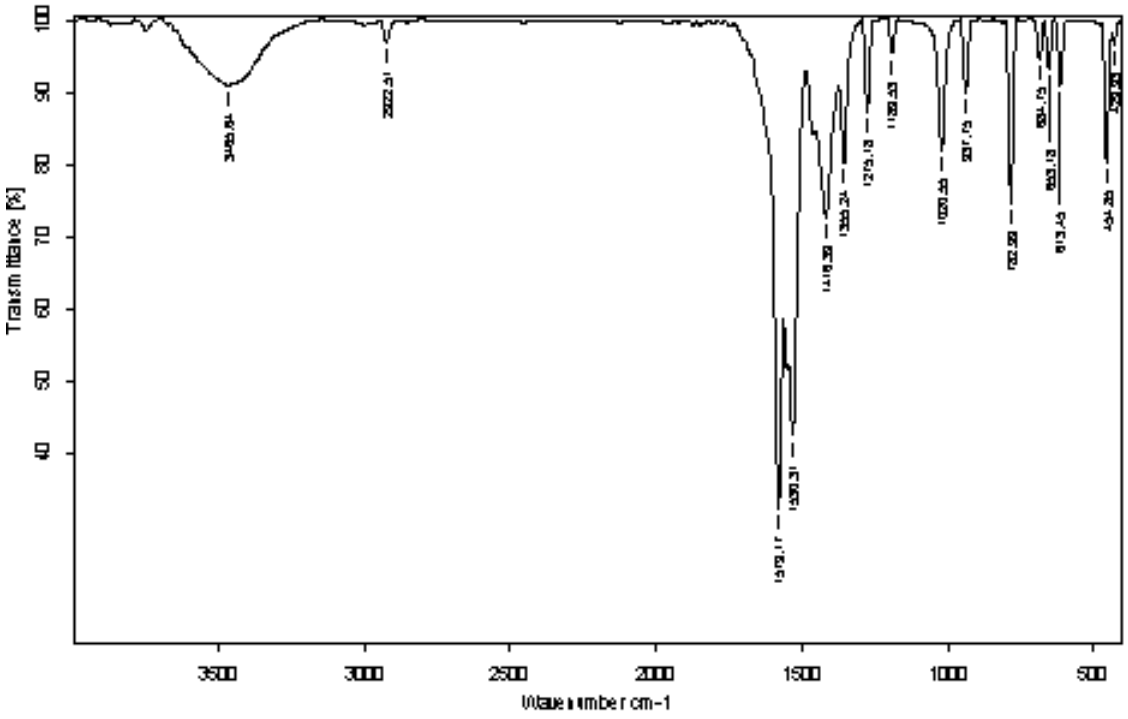


Figure S3. IR spectrogram of $Cu(acac)_2$.

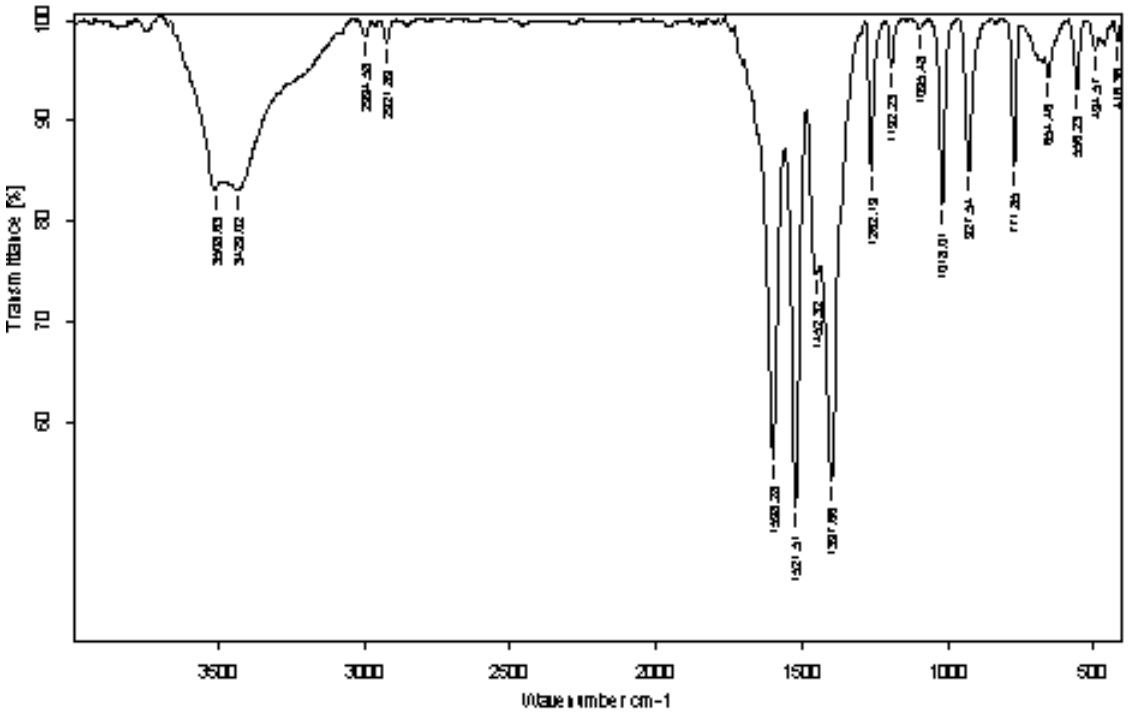


Figure S4. IR spectrogram of $Zn(acac)_2$.

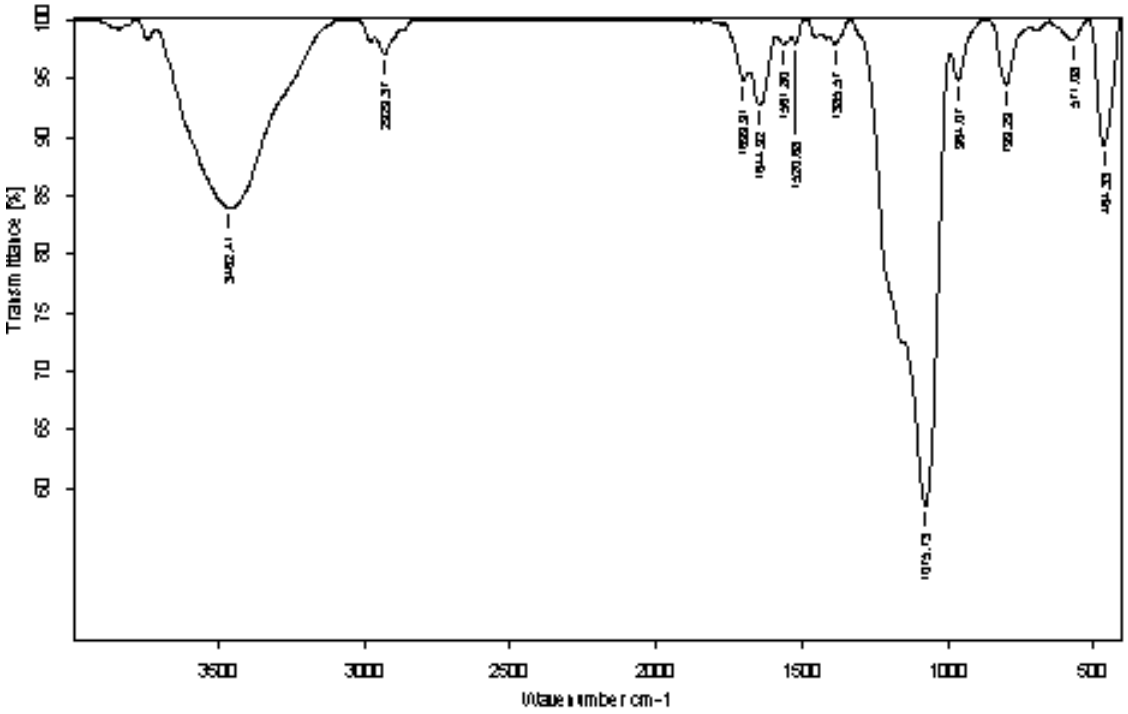


Figure S5. IR spectrogram of HMS-DP-Ru after six run.

4. Experimental Section

4.1 General procedure of the catalysts

Preparation of the HMS-DP-Cu I:

HMS-DP-Cu **I** was synthesized as same as HMS-DP-Cu **II** that we have mentioned before except the mass ratio of the HMS-acac and $Cu(acac)_2$ was 1:1 and the reaction time was 12 h.

Preparation of the HMS-DP-Zn:

The method of prepare HMS-DP-Zn was as same as HMS-DP-Cu **II**.

Preparation of the HMS-DP-Ru:

HMS-DP-Ru was synthesized as same as HMS-DP-Cu **I** that we have mentioned before except the mass ratio of the HMS-acac and $Cu(acac)_2$ was 3:1.

Preparation of the HMS-DP-Cu II@IL

To a 100 mL round flask, 0.6 g of ionic liquid $[OMIm]NTf_2$ was dissolved in 20 mL EA, then 2 g of the HNM-DP-Cu was added and the mixture was stirred for 10 min at room temperature. Removal the EA by rotary evaporator at 40 ^oC, then the flowable solid HMS-DP-Cu **II**@IL was obtained.

Procedure for the synthesis of 1a[1]

In a V-type reaction flask equipped with magnetic stirring, vinyl n-butyl ether (100.0 mg, 1.0 mmol), was mixed with acetylacetone (200.1 mg, 2.0 mmol) and formaldehyde aqueous solution (37 wt%, 202.8 mg, 2.5 mmol) under air. The mixture was stirred at 80 ^oC for 7 h. After reaction, the reaction mixture was cooled to room temperature. After addition of brine (5.0 mL), the aqueous phase was extracted with a mixture of ethyl acetate and heptane (v/v=1/1, 5.0 mL*3). The obtained organic phases were then combined together and dried with anhydrous Na_2SO_4. After evaporation under reduced pressure, the desired product 1c was obtained by silica gel column chromatography using a mixed solution of ethyl acetate and petroleum ether as eluting solvent (the ratio of ethyl acetate/petroleum ether is 1/20); yield: 184.6 mg (87%).

5. Spectroscopic Data for the New Compounds

3-(Nitromethyl)-2-phenylisoindolin-1-one (10a): Light yellow solid, mp: 139-141 ^oC, ^1H NMR (400 MHz, $CDCl_3$, 25 ^oC, TMS): δ = 7.95 (d, J = 4.0 Hz, 1H), 7.65 (t, J = 8.0 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 8.0 Hz, 2H), 7.51-7.45 (m, 3H), 7.29 (q, J = 8.0 Hz, 1H), 5.81 (dd, J_a = 4.0 Hz, J_b=8.0 Hz, 1H), 4.82 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.49 ppm (dd, J_a = 8.0 Hz, J_b = 12.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^oC) δ = 166.6, 140.5, 132.9, 131.8, 130.6, 130.0, 129.7, 126.8, 126.5, 124.7, 123.9, 122.6, 122.2, 75.8, 75.4, 58.0 ppm. IR: v = 3053, 3026, 2957, 2901, 2851, 1758, 1686, 1597, 1548, 1496, 1461, 1384, 1296, 1215, 1159, 1105, 766, 746, 694, 616, 499 cm^{-1}. HRMS (ESI): m/z: calcd for $C_{15}H_{12}N_2NaO_3$: 291.0746 $[M+Na]^+$; found: 291.0731.

3-(Nitromethyl)-2-(*p*-tolyl)isoindolin-1-one (10b): Light yellow solid, mp: 144-146 ^oC, ^1H NMR (400 MHz, $CDCl_3$, 25 ^oC, TMS): δ = 7.92 (d, J = 8.0 Hz, 1H), 7.59 (sext, J = 8.0 Hz, 2H), 7.47 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 5.73 (t, J = 4.0 Hz, 1H), 4.79 (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H), 4.46 (q, J = 8.0 Hz, 1H), 2.36 ppm (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^oC) δ = 166.6, 140.5, 136.8, 133.0, 132.7, 132.0, 130.2, 129.9, 124.6, 124.0, 122.6, 75.4, 58.2, 21.1 ppm; IR: v = 3370, 3062, 3026, 2956, 2915, 2854, 1706, 1689, 1616, 1547, 1514, 1467, 1419, 1387, 1297,

1210, 1152, 819, 747, 686, 611, 507 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{16}H_{14}N_2NaO_3$: 305.0902 $[M+Na]^+$; found: 305.0900.

2-(4-Bromophenyl)-3-(nitromethyl)isoindolin-1-one (10c): Light yellow solid, mp: 114-116 °C, ^1H NMR (400 MHz, DMSO, 25 °C): δ = 7.84 (t, *J* = 8.0 Hz, 2H), 7.75 (t, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.63-7.60 (m, 3H), 6.12 (t, *J* = 3.6 Hz, 1H), 5.31 (dd, J_a = 4.0 Hz, J_b=16.0 Hz, 1H), 5.05 ppm (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H). ^{13}C NMR (100 MHz, DMSO, 25 °C) *δ* = 166.6, 141.3, 136.0, 133.2, 132.4, 131.9, 129.9, 126.5, 124.0, 123.8, 118.9, 74.9, 58.5 ppm. IR: *v* = 3055, 2921, 1706, 1553, 1493, 1470, 1411, 1375, 1300, 1217, 1153, 1105, 1071, 1011, 833, 747, 690, 600, 504 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{15}H_{11}BrN_2NaO_3$: 368.9851 $[M+Na]^+$; found: 368.9848.

2-(4-Fluorophenyl)-3-(nitromethyl)isoindolin-1-one (10d): Light yellow solid, mp: 137-139 °C, ^1H NMR (400 MHz, DMSO, 25 °C): *δ* = 7.86-7.81 (m, 2H), 7.75 (t, *J* = 8.0 Hz, 1H), 7.67-7.60 (m, 3H), 7.37-7.32 (m, 2H), 6.09 (t, *J* = 4.0 Hz, 1H), 5.28 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 5.04 ppm (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H). ^{13}C NMR (100 MHz, DMSO, 25 °C) *δ* = 166.7, 161.74, 159.3, 141.3, 133.0, 132.8, 132.8, 132.0, 129.8, 127.3, 127.2, 123.9, 123.8, 116.4, 116.2, 75.1, 59.0 ppm. ^{19}F NMR (377 MHz, DMSO, 25°C): *δ*= -115.8 ppm (sex, *J* = 3.8 Hz, 1F). IR: *v* = 3117, 3077, 3021, 2962, 2925, 1772, 1685, 1598, 1551, 1509, 1470, 1380, 1337, 1224, 1161, 1102, 1018, 848, 813, 754, 694, 659, 605, 527, 503 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{15}H_{11}FN_2NaO_3$: 309.0651 $[M+Na]^+$; found: 309.0645.

2-(4-Methoxyphenyl)-3-(nitromethyl)isoindolin-1-one (10e): Light yellow solid, mp: 138-140 °C, ^1H NMR (400 MHz, DMSO, 25 °C): *δ* = 7.83-7.80 (m, 2H), 7.73 (t, *J* = 4.0 Hz, 1H), 7.60 (t, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 12.0 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 5.99 (t, *J* = 4.0 Hz, 1H), 5.24 (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H), 4.97 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 3.79 ppm (s, 3H). ^{13}C NMR (100 MHz, DMSO, 25 °C) *δ* = 166.6, 158.0, 145.7, 141.4, 135.1, 132.8, 132.3, 130.5, 129.7, 129.2, 126.9, 125.7, 123.8, 123.6, 114.7, 77.1, 77.0, 75.2, 59.1, 55.8 ppm. IR: *v* = 2919, 2843, 1774, 1678, 1552, 1514, 1466, 1423, 1380, 1297, 1249, 1159, 1109, 1026, 826, 744, 689, 611, 520 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{16}H_{14}N_2NaO_4$: 321.0851 $[M+Na]^+$; found: 321.0842.

3-(Nitromethyl)-2-(4-nitrophenyl)isoindolin-1-one (10f): Light yellow solid, mp: 140-143 °C, 1H NMR (400 MHz, DMSO, 25 °C): *δ* = 8.38 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 12.0 Hz, 2H), 7.90-7.85 (m, 2H), 7.83-7.78 (m, 1H), 7.65 (q, *J* = 8.0 Hz, 1H), 6.31-6.29 (m, 1H), 5.54-5.38 (m, 1H), 5.15-5.06 ppm (m, 1H). ^{13}C NMR (100 MHz, DMSO, 25 °C) *δ* = 169.6, 167.0, 145.7, 144.3, 142.8, 141.3, 135.1, 133.8, 131.4, 130.5, 130.1, 126.1, 125.7, 125.2, 124.3, 123.9, 123.6, 123.4, 77.1, 77.0, 74.6, 58.1 ppm. IR: v = 3118, 3084, 2926, 2854, 1775, 1714, 1597, 1556, 1517, 1375, 1341, 1300, 1219, 1108, 1026, 851, 751, 691, 602 cm-1. HRMS (ESI): m/z: calcd for $C_{15}H_{11}N_3NaO_5$: 336.0596 $[M+Na]^+$; found: 336.0585.

Methyl 4-(1-(nitromethyl)-3-oxoisoindolin-2-yl)benzoate (10g): Brown oil, ^1H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): *δ* = 8.08 (dd, J_a = 4.0 Hz, J_b =8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 6.63 (d, *J* = 8.0 Hz, 1H), 5.54 (d, *J* = 8.0 Hz, 1H), 4.95 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.83 (dd, J_a = 8.0 Hz, J_b = 12.0 Hz, 1H), 3.99 ppm (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) *δ* = 167.5, 166.8, 166.6, 149.5, 139.1, 133.4, 132.0, 131.6, 131.4, 128.7, 127.8, 113.8, 112.6, 79.4, 60.3, 53.2, 52.7 ppm; IR: *v* = 3480, 3372, 3228, 2982, 2957, 1710, 1606, 1555, 1523, 1437, 1371, 1278, 1176, 1108, 1021, 843, 770, 703, 617, 511 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{17}H_{14}N_2NaO_5$: 349.0800 $[M+Na]^+$; found: 349.0795.

2-(4-Acetylphenyl)-3-(nitromethyl)isoindolin-1-one (10h): Light yellow solid, mp: 120-122 °C, ^1H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): *δ* = 8.09 (d, *J* = 12.0 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.77-7.75 (m, 2H), 7.70 (t, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 5.92 (dd,

J_a = 4.0 Hz, J_b =8.0 Hz, 1 H), 4.89 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1 H), 4.55 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1 H), 2.63 ppm (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 196.9, 166.6, 140.3, 140.1, 134.9, 134.4, 133.5, 131.4, 130.8, 130.7, 130.2, 129.9, 125.0, 122.6, 122.2, 113.7, 75.3, 57.4, 26.6 ppm. IR: ν = 3476, 3364, 3237, 3059, 3012, 2924, 2853, 1772, 1701, 1671, 1598, 1553, 1514, 1422, 1374, 1272, 1218, 1177, 1106, 1025, 958, 837, 752, 692, 591, 496 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{17}H_{14}N_2NaO_4$: 333.0851 $[M+Na]^+$; found: 333.0842.

2-(3,4-Dimethoxyphenyl)-3-(nitromethyl)isoindolin-1-one (10i): Light yellow solid, mp: 133-135 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.92 (d, J = 8.0 Hz, 1H), 7.66-7.56 (m, 2H), 7.49 (d, J = 4.0 Hz, 1H), 7.19 (s, 1H), 6.92 (s, 2H), 5.71 (q, J = 4.0 Hz, 1H), 4.82 (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H), 4.52 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 3.90 ppm (d, J = 4.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 166.8, 149.6, 148.0, 140.4, 132.7, 131.9, 129.9, 128.6, 124.5, 122.5, 116.3, 111.5, 108.9, 75.5, 58.8, 56.1 ppm. IR: ν = 3032, 2968, 2940, 2913, 2849, 1700, 1595, 1551, 1515, 1456, 1391, 1325, 1271, 1239, 1217, 1146, 1102, 1022, 847, 793, 749, 688, 617, 578 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{17}H_{16}N_2NaO_5$: 351.0957 $[M+Na]^+$; found: 351.0951.

2-(4-Morpholinophenyl)-3-(nitromethyl)isoindolin-1-one (10j): Brown oil, ^{1}H NMR (400 MHz, DMSO, 25 ^{o}C): δ = 7.79 (t, J = 8.0 Hz, 2H), 7.72 (t, J = 8.0 Hz, 1H), 7.60 (t, J = 8.0 Hz, 1H), 7.42 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 12.0 Hz, 2H), 5.97 (t, J = 4.0 Hz, 1H), 5.23 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.95 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 3.75 (t, J = 8.0 Hz, 4H), 3.15 ppm (t, J = 4.0 Hz, 4H). ^{13}C NMR (100 MHz, DMSO, 25 ^{o}C) δ = 166.6, 149.8, 141.4, 132.7, 132.4, 129.7, 127.8, 126.2, 123.7, 115.6, 75.2, 66.6, 59.0, 48.8 ppm. IR: ν = 2962, 2922, 2854, 1694, 1613, 1552, 1517, 1452, 1378, 1301, 1262, 1235, 1116, 1051, 1023, 929, 821, 799, 746, 691, 643, 524 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{19}H_{19}N_3NaO_4$: 376.1273 $[M+Na]^+$; found: 376.1269.

***tert*-Butyl 6-(1-(nitromethyl)-3-oxoisoindolin-2-yl)-1H-indole-1-carboxylate (10k):** Light yellow solid, mp: 164-166 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 8.36 (s, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.65-7.60 (m, 4H), 7.51 (d, J = 8.0 Hz, 1H), 7.40 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 6.59 (d, J = 8.0 Hz, 1H), 5.83 (dd, J_a = 4.0 Hz, J_b = 8.0 Hz, 1H), 4.86 (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H), 4.52 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 1.67 ppm (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 166.8, 149.5, 140.5, 132.7, 132.0, 131.9, 129.9, 129.4, 128.3, 127.9, 127.1, 124.7, 122.6, 121.8, 112.0, 107.1, 75.4, 58.9, 28.2 ppm. IR: ν = 2978, 2928, 1776, 1733, 1703, 1616, 1555, 1483, 1444, 1379, 1342, 1257, 1210, 1157, 1128, 1025, 851, 817, 768, 745, 690, 612 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{22}H_{21}N_3NaO_5$: 430.1379 $[M+Na]^+$; found: 430.1370.

3-(Nitromethyl)-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)isoindolin-1-one (10l): Light yellow solid, mp: 144-146 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.94 (t, J = 8.0 Hz, 3H), 7.75 (t, J = 8.0 Hz, 1H), 7.62-7.60 (m, 3H), 7.51 (t, J = 8.0 Hz, 1H), 5.86 (dd, J_a = 4.0 Hz, J_b = 8.0 Hz, 1H), 4.86-4.83 (m, 1H), 4.48 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 1.36 ppm (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 166.6, 144.4, 140.5, 138.2, 136.2, 134.9, 133.1, 131.7, 130.6, 130.0, 129.7, 126.5, 124.8, 122.6, 122.3, 122.2, 84.0, 75.8, 75.3, 75.0, 63.7, 57.6, 24.9, 24.8 ppm. IR: ν = 2980, 2928, 1776, 1706, 1606, 1557, 1469, 1363, 1273, 1216, 1145, 1093, 1025, 961, 858, 746, 689, 660 cm^{-1}; HRMS (ESI): *m/z*: calcd for $C_{21}H_{23}BN_2NaO_5$: 417.1598 $[M+Na]^+$; found: 417.1592.

2-*n*-Butyl-3-(nitromethyl)isoindolin-1-one (10m): Brown oil, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.85 (d, J = 4.0 Hz, 1H), 7.56 (sex, J = 8.0 Hz, 2H), 7.47 (d, J =4.0 HZ, 1H), 5.25 (t, J = 80 Hz, 1H), 4.80 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.71 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.02 (quintet, J = 8.0 Hz, 1H), 3.19-3.12(m, 1H), 1.70-1.54 (m, 2H), 1.36 (q, J = 8.0 Hz, 2H), 0.94 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 168.0, 140.7, 132.1, 132.1, 129.5, 124.1, 122.4,

76.4, 56.8, 40.4, 30.3, 20.0, 13.7 ppm. IR: *v* = 3025, 2961, 2932, 2971, 1692, 1553, 1468, 1411, 1377, 1302, 1204, 1095, 798, 747, 693, 616, 534 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{13}H_{16}N_2NaO_3$: 271.1059 $[M+Na]^+$; found: 271.1061.

2-Benzyl-3-(nitromethyl)isoindolin-1-one (10n): Light yellow solid, mp: 73-75 °C, ^1H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.93 (d, *J* = 4.0 Hz, 1H), 7.51 (q. *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.35-7.26 (m, 5H), 5.27 (d, *J* = 16.0 Hz, 1H), 5.05 (t, *J* = 4.0 Hz, 1H), 4.70 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 4.60(dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 4.39 ppm (d, *J* = 16.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 168.3, 140.9, 136.3, 132.5, 131.7, 129.7, 129.1, 128.1, 128.0, 124.5, 122.5, 76.0, 56.8, 44.7 ppm. IR: *v* = 3061, 3031, 2924, 2956, 1696, 1616, 1553, 1469, 1405, 1377, 1295, 1199, 1147, 1098, 1078, 979, 747, 699, 617, 553, 512 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{16}H_{14}N_2NaO_3$: 305.0902 $[M+Na]^+$; found: 305.0900.

2-Cyclohexyl-3-(nitromethyl)isoindolin-1-one (10o): Brown oil, ^1H NMR (400 MHz, DMSO, 25 °C): δ = 7.65-7.59 (m, 3H), 7.53-7.49 (m, 1H), 5.39 (dd, J_a = 4.0 Hz, J_b = 12. 0 Hz, 1H), 5.26-5.19 (m, 2H), 3.72-3.66 (m, 1H), 2.12-2.02 (m, 1H), 1.84-1.77 (m, 4H), 1.63 (d, *J* = 12.0 Hz, 1H), 1.37-1.27 (m, 2H), 1.23-1.14 ppm (m, 2H). ^{13}C NMR (100 MHz, DMSO, 25 °C) δ = 168.0, 142.5, 133.0, 132.1, 129.2, 123.4, 123.1, 75.9, 57.8, 53.8, 30.4, 30.2, 26.2, 26.1, 25.4 ppm. IR: *v* = 2934, 2858, 1681, 1552, 1470, 1402, 1375, 1328, 1220, 1128, 1024, 893, 800, 753, 695, 616, 541 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{15}H_{18}N_2NaO_3$: 297.1215 $[M+Na]^+$; found: 297.1200.

2-(2-(1H-Indol-3-yl)ethyl)-3-(nitromethyl)isoindolin-1-one (10p): Brown oil, ^1H NMR (400 MHz, DMSO, 25 °C): δ = 10.85 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.66-7.62 (m, 2H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.21 (s, 1H), 7.10 (t, *J* = 8.0 Hz, 1H), 7.01 (t, *J* = 8.0 Hz, 1H), 5.36 (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H), 5.30 (q, *J* = 4.0 Hz, 2H), 4.23-4.16 (m, 1H), 3.61-3.54 (m, 1H), 3.19-3.12 (m, 1H), 3.03-2.95 ppm (m, 1H). ^{13}C NMR (100 MHz, DMSO, 25 °C) δ = 167.8, 142.0, 136.7, 132.5, 132.2, 129.4, 127.6, 123.7, 123.3, 123.2, 121.5, 118.9, 118.8, 111.9, 111.6, 75.1, 57.5, 41.1, 24.3 ppm. IR: *v* = 3412, 3306, 3054, 2923, 2855, 1773, 1688, 1618, 1553, 1457, 1412, 1375, 1227, 1097, 1022, 746, 692, 613, 426 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{19}H_{17}N_3NaO_3$: 358.1168 $[M+Na]^+$; found: 358.1153.

2-(Furan-2-ylmethyl)-3-(nitromethyl)isoindolin-1-one (10q): Light yellow solid, mp: 89-91 °C, ^1H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.86 (d, *J* = 8.0 Hz, 1H), 7.55 (dt, J_a = 8.0 Hz, J_b = 24.0 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.35 (s, 1H), 6.35-6.33 (m, 2H), 5.17 (d, *J* = 16.0 Hz, 1H), 5.11 (t, J_a = 8.0 Hz, J_b = 12.0 Hz, 1H), 4.87 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.74 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 4.48 ppm (d, *J* = 16.0 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ= 167.9, 149.5, 142.9, 140.9, 132.5, 131.5, 129.6, 124.4, 122.5, 110.7, 109.2, 75.7, 57.2, 37.4 ppm. IR: *v* = 3156, 3103, 3045, 2988, 2919, 2854, 1692, 1617, 1552, 1469, 1407, 1384, 1355, 1278, 1232, 1191, 1143, 1073, 1011, 915, 797, 749, 689, 616, 564, 533 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{14}H_{12}N_2NaO_4$: 295.0695 $[M+Na]^+$; found: 295.0694.

2-(3-Ethynylphenyl)-3-(nitromethyl)isoindolin-1-one (10r): Light yellow solid, mp: 121-123 °C, ^1H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.94 (d, *J* = 8.0 Hz, 1H), 7.67-7.64 (m, 2H), 7.61-7.58 (m, 2H), 7.52-7.49 (m, 1H), 7.45-7.40 (m, 2H), 5.79 (dd, J_a = 4.0 Hz, J_b = 8.0 Hz, 1H), 4.84 (dd, J_a = 4.0 Hz, J_b = 16.0 Hz, 1H), 4.51 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 3.14 ppm (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 166.6, 140.3, 135.8, 133.1, 131.6, 130.3, 130.0, 129.7, 127.0, 124.8, 124.4, 123.6, 122.6, 82.6, 78.6, 75.2, 57.9 ppm. IR: *v* = 3291, 3071, 2958, 2924, 2855, 1774, 1706, 1600, 1554, 1484, 1431, 1376, 1216, 1154, 1104, 792, 747, 690, 618, 530 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{17}H_{12}N_2NaO_3$: 315.0746 $[M+Na]^+$; found: 315.0739.

3-(Nitromethyl)-2-(prop-2-yn-1-yl)isoindolin-1-one (10s): Brown oil, ^1H NMR (400 MHz, DMSO,

25 °C): δ = 7.76 (t, J = 8.0 Hz, 2H), 7.69 (t, J = 8.0 Hz, 1H), 7.57 (t, J = 8.0 Hz, 1H), 5.38-5.37 (m, 2H), 5.33-5.51 (m, 1H), 4.63 (dd , J_a = 2.4 Hz, J_b = 18 Hz, 1H), 4.26 (dd, J_a = 2.4 Hz, J_b = 18.0 Hz, 1H), 3.30 ppm (t, J = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO, 25 °C) δ = 167.4, 142.0, 132.8, 131.6, 129.6, 123.8, 123.6, 79.2, 75.3, 74.7, 57.4, 30.2 ppm. IR: v = 3293, 2922, 1775, 1701, 1617, 1555, 1470, 1402, 1378, 1295, 1151, 748, 693 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{12}H_{10}N_2NaO_3$: 253.0589 [M+Na]$^+$; found: 253.0593.

2-Allyl-3-(nitromethyl)isoindolin-1-one (10t): Colorless oil, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.68 (d, J = 8.0 Hz, 1H), 7.57 (sextet, J = 8.0 Hz, 2H), 7.46 (d, J = 8.0 Hz, 1H), 5.88-5.78 (m, 1H), 5.28 (d, J = 8.0 Hz, 1H), 5.24-5.21 (m, 2H), 4.82 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 4.69 (dd, J_a = 4.0 Hz, J_b = 8.0 Hz, 1H), 4.61 (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H), 3.89 ppm (dd, J_a = 8.0 Hz, J_b = 16.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 167.9, 140.9, 132.5, 132.4, 131.7, 129.6, 124.3, 122.5, 118.8, 76.1, 57.0, 43.6 ppm. IR: v = 3083, 3021, 2982, 2921, 1774, 1695, 1617, 1553, 1470, 1403, 1378, 1294, 1203, 1099, 996, 931, 798, 748, 694, 613, 534 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{12}H_{12}N_2NaO_3$: 255.0746 [M+Na]$^+$; found: 255.0740.

2-(2-Methylallyl)-3-(nitromethyl)isoindolin-1-one (10u): Light yellow solid, mp: 98-100 °C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.88 (d, J = 8.0 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 7.55 (t, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 5.14 (t, J = 8.0 Hz, 1H), 4.96 (s, 1H), 4.87-4.82 (m, 2H), 4.68(dd, J_a = 5.6 Hz. J_b = 13.2 Hz, 1H), 4.57 (d, J = 16.0 Hz, 1H), 3.83 (d, J = 16.0 Hz, 1H), 1.70 ppm (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 168.2, 140.9, 140.4, 132.4, 131.6, 129.6, 124.4, 122.5, 113.8, 75.9, 57.0, 46.8, 19.9 ppm. IR: v = 3079, 3048, 2976, 2921, 2857, 1761,1694, 1618, 1552, 1467, 1410, 1382, 1274, 1224, 1190, 1030, 906, 745, 689, 621, 585, 537 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{13}H_{14}N_2NaO_3$: 269.0902 [M+Na]$^+$; found: 269.0897.

2-(2-(Cyclohex-1-en-1-yl)ethyl)-3-(nitromethyl)isoindolin-1-one (10v): Brown oil, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.85 (d, J = 8.0 Hz, 1H), 7.56 (dt, J_a = 7.2 Hz, J_b = 23.2 Hz, 2H), 7.45 (d, J = 4.0 Hz, 1H), 5.42 (s, 1H), 5.28 (t, J = 5.6 Hz, 1H), 4.78 (dd, J_a = 5.6 Hz, J_b = 13.2 Hz, 1H), 4.66 (dd, J_a = 5.6 Hz, J_b = 13.2 Hz, 1H), 4.14 (quintet, J = 8.0 Hz, 1H), 3.22-3.15 (m, 1H), 2.35-2.29 (m, 1H), 2.25-2.18 (m, 1H), 2.06-1.99 (m, 2H), 1.94-1.89 (m, 2H), 1.64-1.58 (m, 2H), 1.52-1.47 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 167.9, 140.8, 134.2, 132.1, 132.1, 129.5, 124.1, 124.0, 122.3, 56.9, 39.3, 36.6, 28.1, 25.2, 22.8, 22.2 ppm. IR: v = 2928, 2857, 2836, 1693, 1618, 1553, 1468, 1409, 1376, 1300, 1201, 1129, 1098, 1019, 921, 799, 747, 693, 614, 537 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{17}H_{20}N_2NaO_3$: 323.1372 [M+Na]$^+$; found: 323.1767.

6,7-Dimethoxy-3-(nitromethyl)-2-(*p*-tolyl)isoindolin-1-one (10w): Light yellow solid, mp: 149-151 °C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.41 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.13 (dd, J_a = 8.0 Hz, J_b = 12.0 Hz, 2H), 5.67 (q, J = 4.0 Hz, 1H), 4.75 (dd, J_a = 4.0 Hz, J_b = 12.0 Hz, 1H), 4.42 (dd, J_a = 8.0 Hz. J_b = 12.0 Hz, 1H), 4.09 (s, 3H), 3.92 (s, 3H), 2.37 ppm (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 164.7, 153.8, 147.9, 136.7, 133.4, 133.0, 130.1, 124.0, 117.7, 117.1, 76.0, 62.6, 57.2, 56.7, 21.1 ppm. IR: v = 3074, 3009, 2940, 2839, 1690, 1557, 1515, 1493, 1426, 1371, 1264, 1218, 1179, 1059, 1033, 968, 835, 742, 686, 517 cm^{-1}. HRMS (ESI): *m/z*: calcd for $C_{18}H_{18}N_2NaO_5$: 365.1113 [M+Na]$^+$; found: 365.1107.

6. Spectroscopic Data for the Old Compounds

1-(4-butoxy-2-methylcyclohex-1-en-1-yl)ethan-1-one (1a)[1] Brown liquid, ^{1}H NMR (400 MHz, $CDCl_3$, 25℃, TMS): δ = 5.04 (s, 1H), 3.81-3.77 (m, 1H), 3.57-3.52 (m, 1H), 2.46-2.44 (m, 1H), 2.31-2.28 (m, 1H), 2.21-2.20 (m, 6H), 1.92-1.90 (m, 1H), 1.80-1.78 (m, 1H), 1.56-1.55 (m, 2H),

1.39-1.35 (m, 2H), 0.93-0.90 ppm (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 198.88, 161.06, 110.31, 97.43, 68.27, 31.52, 29.26, 26.08, 20.52, 19.07, 18.81, 13.64 ppm.

3-(3-(benzylthio)-4-(phenylthio)butyl)pentane-2,4-dione (2a)[2] Colorless liquid, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.30-7.22 (m, 10H), 3.84-3.70 (m, 4H), 3.48 (t, J = 6.4 Hz, 0.4H), 3.40 (t, J = 6.8 Hz, 0.6H), 3.30 (t, J = 7.2 Hz, 0.6H), 2.29-2.24 (m. 1H), 2.05-2.00 (m, 6H), 1.90-1.84 (m, 1H), 1.80-1.75 (m, 1H), 1.67-1.62 ppm (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 204.0, 191.2, 138.1, 129.1, 129.0, 128.7, 128.6, 127.2, 127.1, 109.3, 67.3, 49.7, 49.4, 36.5, 35.3, 34.8, 32.8, 29.1, 25.4, 24.9, 22.9 ppm.

1-benzyl-4-phenyl-1H-1,2,3-triazole (5a)[3] White solid, mp: 127-128 ℃, ^{1}H NMR (400 MHz, $CDCl_3$, 25^{o}C, TMS): δ = 7.78 (d, J = 8.0 Hz, 2H), 7.68 (s, 1H), 7.39-7.34 (m, 5H), 7.30-7.27 (m, 3H), 5.52 ppm (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25^{o}C) δ = 148.2, 134.8, 130.6, 129.1, 128.8, 128.7, 128.2, 128.0, 125.7, 119.7, 54.2 ppm.

1-Benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole (5b)[3] White solid, mp: 109-110 ℃, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.77 (m, 2H), 7.64 (s, 1H), 7.38-7.36 (m, 3H), 7.31-7.29 (m, 2H), 7.07 (t, J = 8.0 Hz, 2H), 5.55 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 163.9, 161.4, 147.4, 134.6, 129.2, 128.9, 128.1, 127.5, 127.4, 119.4, 115.9, 115.7, 54.3.

1-Benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (5c)[4] White solid, mp: 135–136 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.71 (d, J = 8.0 Hz, 2H), 7.58 (s, 1H), 7.37-7.34 (m, 3H), 7.30-7.28 (m, 2H), 6.92 (d, J = 8.0 Hz, 2H), 5.54 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 159.6, 148.1, 134.8, 129.1, 128.7, 128.1, 127.0, 123.3, 118.8, 114.2, 55.3, 54.2.

1-Benzyl-4-(4-(*tert*-butyl)phenyl)-1H-1,2,3-triazole (5d)[5] White solid, mp: 113-114 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.73 (d, J = 8.0 Hz, 2H), 7.64(s, 1H), 7.42 (d, J = 8.0 Hz, 2H), 7.37-7.34 (m, 3H), 7.29-7.27 (m, 2H), 5.55 (s, 2H), 1.32 ppm (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 151.3, 148.2, 134.8, 129.1, 128.7, 128.0, 127.7, 125.8, 125.5, 119.3, 54.2, 34.7, 31.3 ppm.

1-Benzyl-4-(4-ethylphenyl)-1H-1,2,3-triazole (5e)[5] White solid, mp: 148-149 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.71 (d, J=12.0 Hz, 2H), 7.63 (s, 1H), 7.31-7.36 (m, 3H), 7.30-7.28 (m, 2H), 7.22 (d, J = 8.0 Hz, 2H), 5.54 (s, 2H), 2.65 (q, J = 8.0 Hz, 2H), 1.23 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 148.3, 144.4, 134.8, 129.1, 128.8, 128.3, 128.1, 125.7, 119.3, 54.2, 28.7, 15.5 ppm.

1-Benzyl-4-(4-propylphenyl)-1H-1,2,3-triazole (5f)[5] White solid, mp: 113-115 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.70 (d, J = 8.0 Hz, 2H), 7.63 (s, 1H), 7.37-7.34 (m, 3H), 7.29-7.27 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 5.54 (s, 2H), 2.58 (t, J = 8.0 Hz, 2H), 1.64 (sextet, J = 8.0 Hz, 2H), 0.93 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 148.3, 142.9, 134.8, 129.1, 128.9, 128.7, 128.0, 128.0, 125.6, 119.3, 54.2, 37.8, 24.5, 13.8 ppm

1-Benzyl-4-(4-butylphenyl)-1H-1,2,3-triazole (5g)[5] White solid, mp: 110-112 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.70 (d, J=8.0 Hz, 2H), 7.62 (s, 1H), 7.38-7.36 (m, 3H), 7.30-7.28 (m, 2H), 7.21 (d, J = 8.0 Hz, 2H), 5.56 (s, 2H), 2.61 (t, J = 8.0 Hz, 2H), 1.60 (quintet, J = 8.0 Hz, 2H), 1.35 (q, J = 8.0 Hz, 2H), 0.92 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ =148.4, 143.1, 134.8, 129.1, 128.9, 128.8, 128.0, 127.9, 125.6, 119.2, 54.2, 35.4, 33.6, 22.3, 14.0 ppm.

1-Benzyl-4-(4-pentylphenyl)-1H-1,2,3-triazole (5h)[5] White solid, mp: 102–103 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.70 (d, J = 8.0 Hz, 2H), 7.62 (s, 1H), 7.37-7.34 (m, 3H), 7.29-7.27 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 5.54 (s, 2H), 2.60 (t, J = 8.0 Hz, 2H), 1.61 (quintet, J = 8.0 Hz, 2H), 1.32-1.30 (m, 4H), 0.88 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 148.3, 143.1, 134.8, 129.1, 128.9, 128.7, 128.0, 127.9, 125.6, 119.3, 54.2, 35.7, 31.5, 31.1, 22.6, 14.1 ppm.

1-(4-Nitrobenzyl)-4-phenyl-1H-1,2,3-triazole (5i)[3] White solid, mp: 156-157 ℃, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 8.20 (d, J = 8.0 Hz, 2H), 7.81-7.79 (m, 3H), 7.44-7.39 (m, 4H), 7.35-7.32 (m, 1H), 5.68 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ =148.6, 148.0, 141.8, 130.1, 128.9, 128.6, 128.5, 125.7, 124.3, 119.9, 53.2 ppm.

1-Octyl-4-phenyl-1H-1,2,3-triazole (5j)[3] White solid, mp: 78-79 ℃, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.83 (d, J=8.0 Hz, 2H), 7.75 (s, 1H), 7.42 (t, J = 8.0 Hz, 2H), 7.32 (t, J = 8.0 Hz, 1H), 4.37 (t, J = 8.0 Hz, 2H), 4.93 (t, J = 8.0 Hz, 2H), 1.33-1.26 (m, 10H), 0.89-0.86 ppm (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 147.7, 130.7, 128.8, 128.1, 125.7, 119.5, 50.5, 31.7, 30.4, 29.1, 29.0, 26.5, 22.6, 14.1 ppm.

1-Hexyl-4-phenyl-1H-1,2,3-triazole (5k)[3] White solid, mp: 62-63 ℃, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.83 (d, J = 8.0 Hz, 2H), 7.75 (s, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.32 (t, J = 8.0 Hz, 1H), 4.37 (t, J = 8.0 Hz, 2H), 1.94-1.91 (m, 2H), 1.32 (s, 6H), 0.88 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 147.7, 130.7, 128.8, 128.1, 125.7, 119.5, 50.4, 31.2, 30.3, 26.2, 22.4, 14.0 ppm.

1-Phenethyl-4-phenyl-1H-1,2,3-triazole (5l)[3] White Solid, mp: 124-126 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.76 (d, J = 4.0 Hz, 2H), 7.47 (s, 1H), 7.39 (t, J = 8.0 Hz, 2H), 7.32-7 24 (m, 4H), 7.11 (d, J = 8.0 Hz, 2H), 4.60 (t, J = 8.0 Hz, 2H), 3.22 ppm (t, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 147.5, 137.1, 130.7, 128.9, 128.9, 128.8, 128.1, 127.2, 125.7, 120.0, 51.7, 36.8 ppm.

1-Ethyl-4-phenyl-1H-1,2,3-triazole (5m)[6] White solid, mp: 53–55 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.83 (d, J = 8.0 Hz, 2H), 7.77 (s, 1H), 7.43 (t, J = 8.0 Hz, 2H), 7.33 (t, J = 8.0 Hz, 1H), 4.46 (q, J = 8.0 Hz, 2H), 1.60 ppm (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 147.8, 130.7, 128.9, 128.1, 125.7, 119.0, 45.4, 15.6 ppm.

1,4-Diphenylbuta-1,3-diyne (7a)[5] White solid, mp 82-84 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.53 (dd, J_a = 4. 0 Hz, J_b = 8.0 Hz, 5H), 7.37-7.31 ppm (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ= 132.5, 129.2, 128.5, 121.8, 81.6, 74.0 ppm.

1,4-Bis(4-ethylphenyl)buta-1,3-diyne (7b)[7] White solid, mp: 96-97 ^{o}C , ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.43 (d, J = 8.0 Hz, 4H), 7.15 (d, J = 4.0 Hz, 4H), 2.64 ppm (q, J = 8.0 Hz, 4H), 1.22 (t, J = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 145.8, 132.5, 128.1, 119.1, 81.6, 73.6, 29.0, 15.3 ppm.

1,4-bis(4-fluorophenyl)buta-1,3-diyne (7c)[8] White solid, mp 192-193 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.53-7.49 (m, 4H), 7.04 (t, J = 8.0 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 164.3, 161.8, 134.6, 134.5, 117.9, 116.0, 115.8, 80.4, 73.6 ppm.

1,4-Bis(4-methoxyphenyl)buta-1,3-diyne (7d)[8] White solid, mp: 143-144 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.46 (d, J = 8.0 Hz, 4H), 6.85 (d, J = 8.0 Hz, 4H), 3.82 ppm (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 160.3, 134.1, 114.2, 114.0, 81.3, 73.0, 55.4 ppm.

1,4-Bis(4-propylphenyl)buta-1,3-diyne (7e)[7] White solid, mp: 107-108 ^{o}C , ^{1}H NMR (400 MHz, $CDCl_3$, 25℃, TMS): δ = 7.42 (d, J = 8.0 Hz, 4H), 7.13 (d, J = 8.0 Hz, 4H), 2.51 (t, J = 8.0 Hz, 4H), 1.62 (q, J = 8.0 Hz, 4H), 0.92 ppm (t, J = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, 25℃) δ = 144.3, 132.4, 128.7, 119.1, 81.6, 73.6, 38.1, 24.3, 13.8 ppm.

1,4-Bis(4-butylphenyl)buta-1,3-diyne (7f)[5] White solid, mp: 66-67 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, TMS): δ = 7.42 (d, J = 8.0 Hz, 4H), 7.12 (d, J = 8.0 Hz, 4H), 2.59 (t, J = 8.0 Hz, 4H), 1.57 (quint, J = 8.0 Hz, 4H), 1.33 (q, J = 8.0 Hz, 4H), 0.91 ppm (t, J = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ= 144.5, 132.5, 128.6, 119.1, 81.7, 73.6, 35.8, 33.4, 22.4, 14.0 ppm.

1,4-Bis(4-pentylphenyl)buta-1,3-diyne (7g)[7] White solid, mp 86-87 °C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.41 (d, J = 8.0 Hz, 4H), 7.12 (d, J = 8.0 Hz, 4H), 2.58 (t, J = 8.0 Hz, 4H), 1.58 (quintet, J = 8.0 Hz, 4H), 1.33-1.28 (m, 8H), 0.88 ppm (t, J = 4.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 144.5, 132.5, 128.6, 119.1, 81.7, 73.6, 36.0, 31.5, 30.9, 22.6, 14.1 ppm.

1,4-Bis(4-(tert-butyl)phenyl)buta-1,3-diyne (7h)[9] White solid, mp: 209-210 °C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.37 (d, J = 8.0 Hz, 4H), 7.26 (d, J = 8.0 Hz, 4H), 1.22 ppm (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ= 152.6, 132.3, 125.5, 118.9, 81.6, 73.6, 34.9, 31.2 ppm.

3,3'-(buta-1,3-diyne-1,4-diyl)dianiline (7i)[10] Black Solid, mp: 94-96 °C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.10 (t, J = 8.0 Hz, 2H), 6.93 (d, J = 4.0 Hz, 2H), 6.81 (t, J = 4.0 Hz, 2H), 6.68 (dd, J_a = 4.0 Hz, J_b = 8.0 Hz, 2H), 3.12-3.10 ppm (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 146.3, 129.4, 123.0, 122.5, 118.4, 116.3, 81.7, 73.4 ppm.

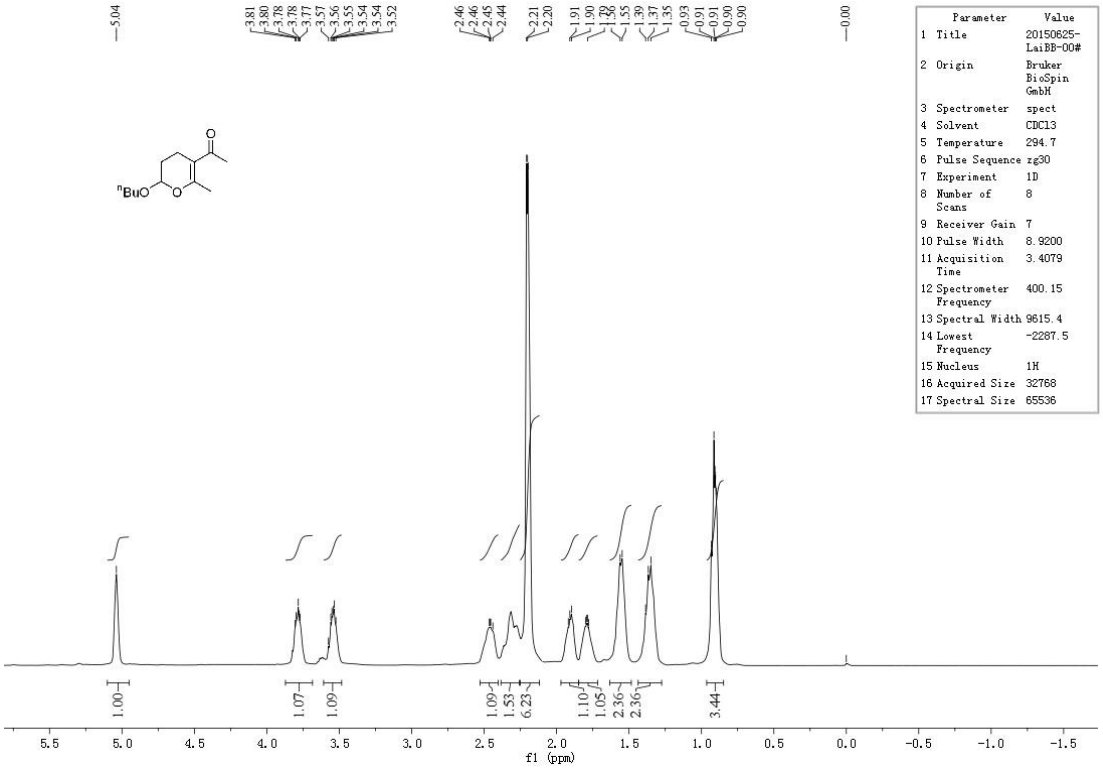
Benzophenone (9a)[11] White oli, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.72-7.70 (m, 4H), 7.51-7.48 (m, 2H), 7.39 ppm (t, J = 8.0 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 196.77, 137.62, 132.43, 130.07, 128.30 ppm.

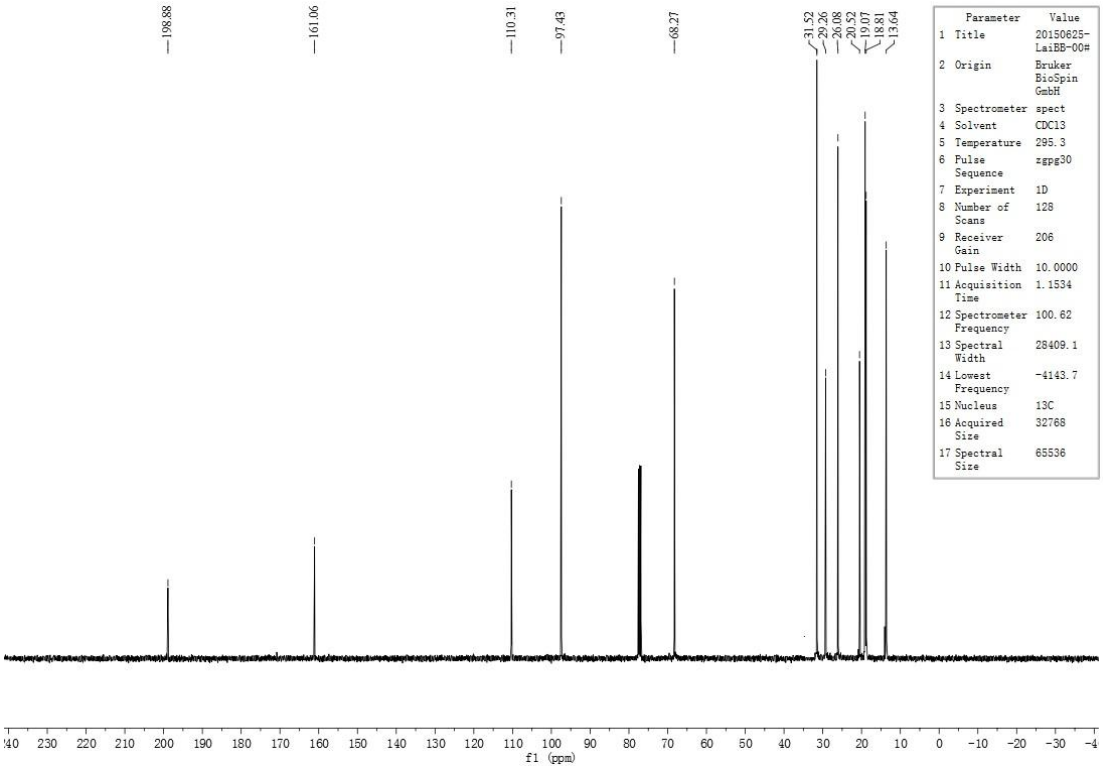
1-(1,3-Diphenylprop-2-yn-1-yl)piperidine (14a)[12] Pale yellow oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.55 (d, J = 8.0 Hz, 2H), 7.44-7.42 (m, 2H), 7.28-7.17 (m, 6H), 4.71 (s, 1H), 2.48 (s, 4H), 1.53-1.48 (m, 4H), 1.36-1.34 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 137.6, 130.8, 127.5, 127.2, 127.0, 126.4, 122.3, 86.8, 85.0, 61.3, 49.7, 25.1, 23.4 ppm.

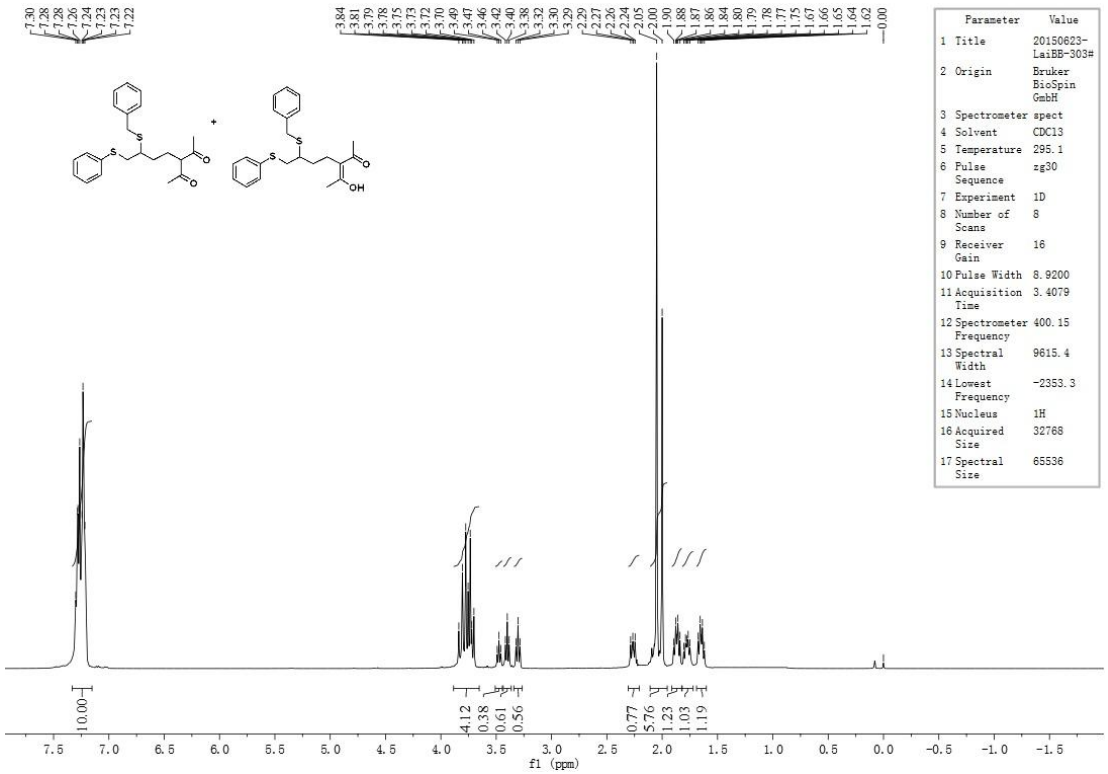
1-(1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-yl)piperidine (14b)[12] Yellow oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.57 (d, J = 8.0 Hz, 2H), 7.52-7.49 (m, 2H), 7.32-7.30 (m, 5H), 4.75 (s, 1H), 2.53 (s, 4H), 1.62-1.52 (m, 4H), 1.45-1.42 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 137.4, 133.2, 131.9, 129.9, 128.4, 128.2, 123.1, 88.3, 85.4, 61.8, 50.7, 26.2, 24.4 ppm.

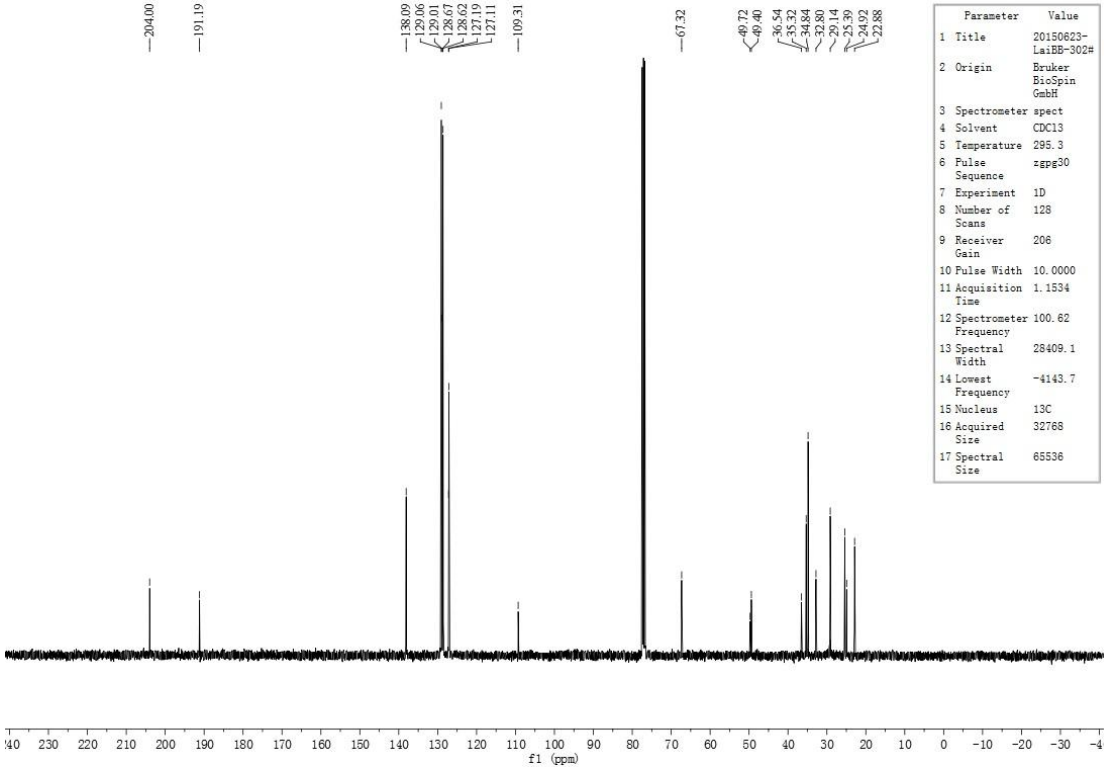
1-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-yl)piperidine (14c)[12] Dark yellowish oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 7.54-7.49 (m, 4H), 7.31-7.29 (m, 3H), 6.88 (d, J = 8.0 Hz, 2H), 4.73 (s, 1H), 3.78 (s, 3H), 2.55 (s, 4H), 1.62-1.54 (m, 4H), 1.44-1.43 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 159.0, 131.8, 130.7, 129.7, 128.3, 128.1, 123.4, 113.4, 87.7, 86.5, 61.8, 55.3, 26.2, 24.5 ppm.

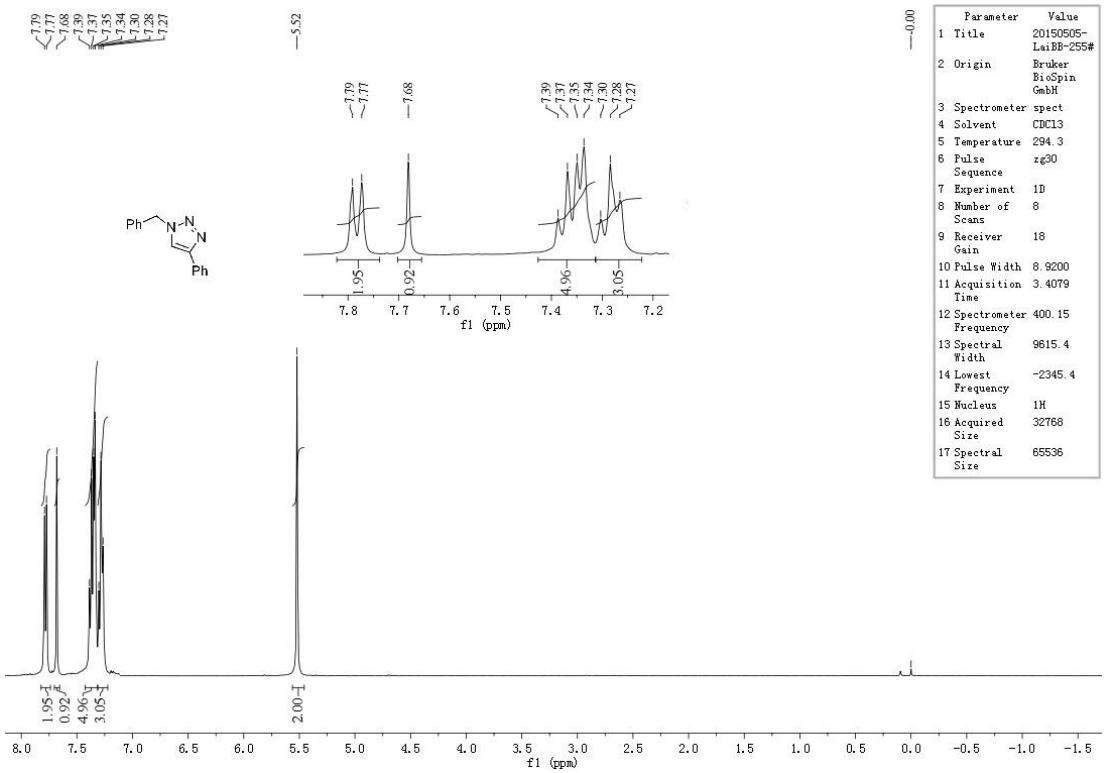
3,4-Dimethoxybenzaldehyde (16a)[13] White solid, mp: 40-41 °C, ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C, TMS): δ = 9.86 (s, 1H), 7.47 (dd, J_a = 4.0 Hz, J_b=8.0 Hz, 1H), 7.41 (d, J = 2.0 Hz, 1H), 6.99 (d, J = 8.0 Hz, 1H), 3.96 ppm (d, J = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 190.8, 154.4, 149.5, 130.0, 126.7, 110.4, 108.8, 56.1, 55.9, 55.9 ppm.

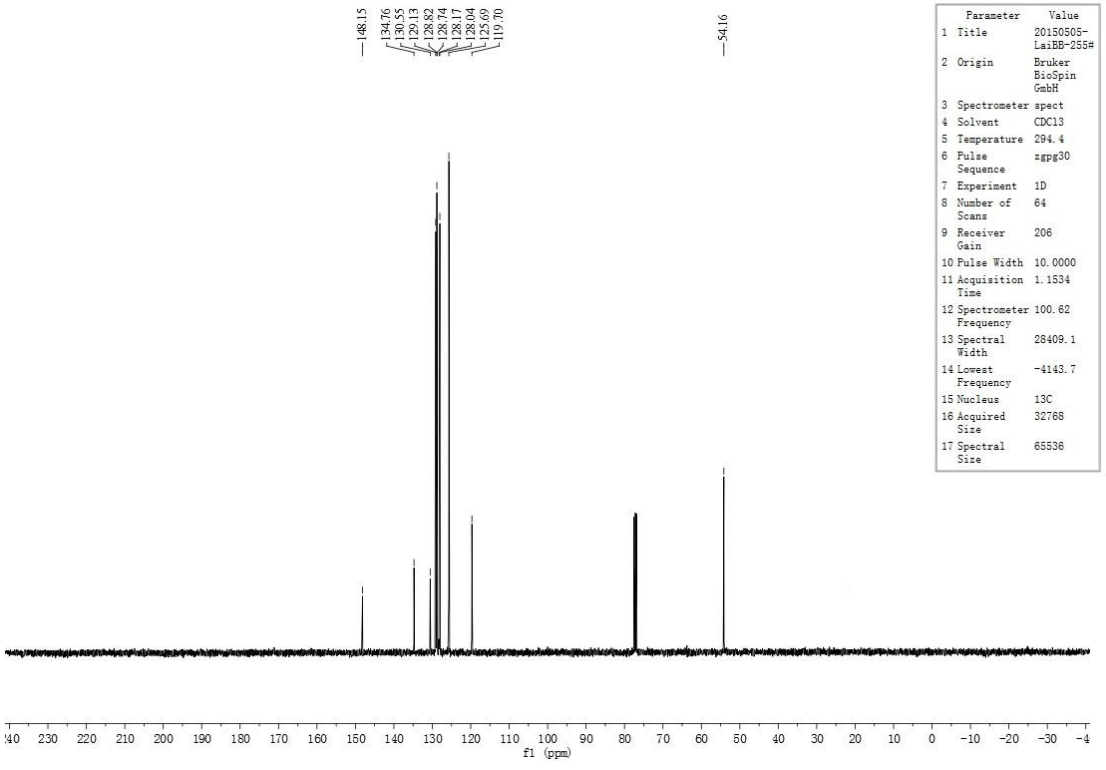

5.04
3.81
3.80
3.78
3.78
3.77
3.57
3.56
3.55
3.54
3.54
3.52
2.46
2.46
2.45
2.44
2.21
2.20
1.91
1.90
1.55
1.39
1.37
1.35
0.93
0.91
0.91
0.90
0.90
0.00
nBuO
O
O
Parameter Value
1 Title 20150625-LaiBB-00#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 7
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2287.5
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
1.00
1.07
1.09
1.09
1.53
6.23
1.10
1.05
2.36
2.36
3.44
f1 (ppm)

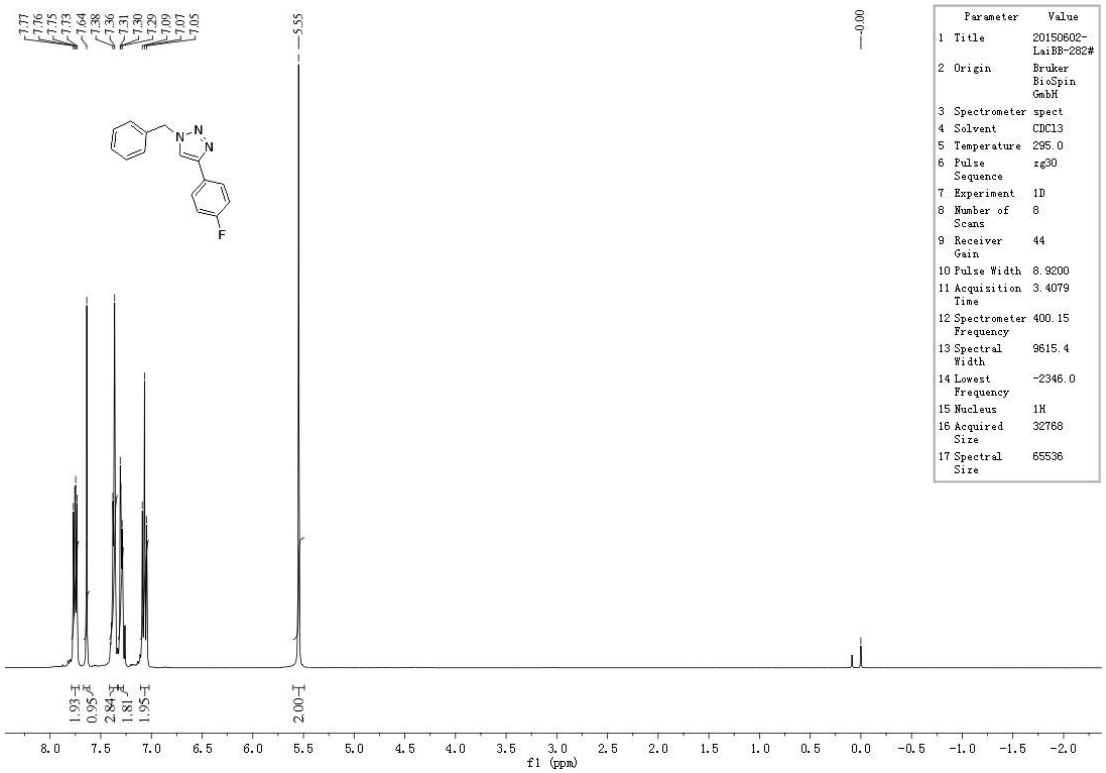

198.88
161.06
110.31
97.43
68.27
31.52
29.26
26.08
20.52
19.07
18.81
13.64
Parameter Value
1 Title 20150625-LaiBB-00#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

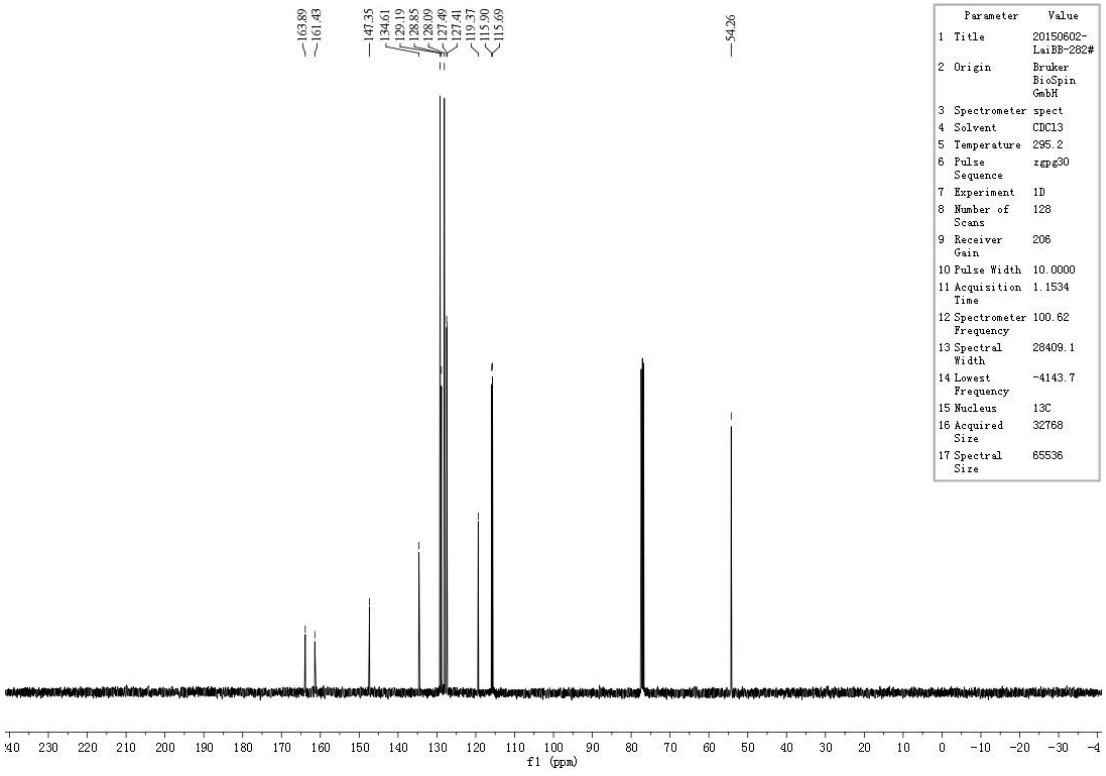

7.30 7.28 7.28 7.26 7.24 7.23 7.23 7.22
3.84 3.81 3.79 3.78 3.75 3.73 3.72 3.70 3.49 3.47 3.46 3.42 3.40 3.38 3.32 3.30 3.29 2.29 2.27 2.26 2.24 2.05 2.00 1.90 1.88 1.87 1.86 1.84 1.80 1.79 1.78 1.77 1.75 1.67 1.66 1.65 1.64 1.62 0.00
OH
10.00 4.12 0.38 0.61 0.56 0.77 5.76 1.23 1.03 1.19
7.5 7.0 6.5 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 -0.5 -1.0 -1.5
f1 (ppm)
Parameter Value
1 Title 20150623-LaiBB-303#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 16
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2353.3
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

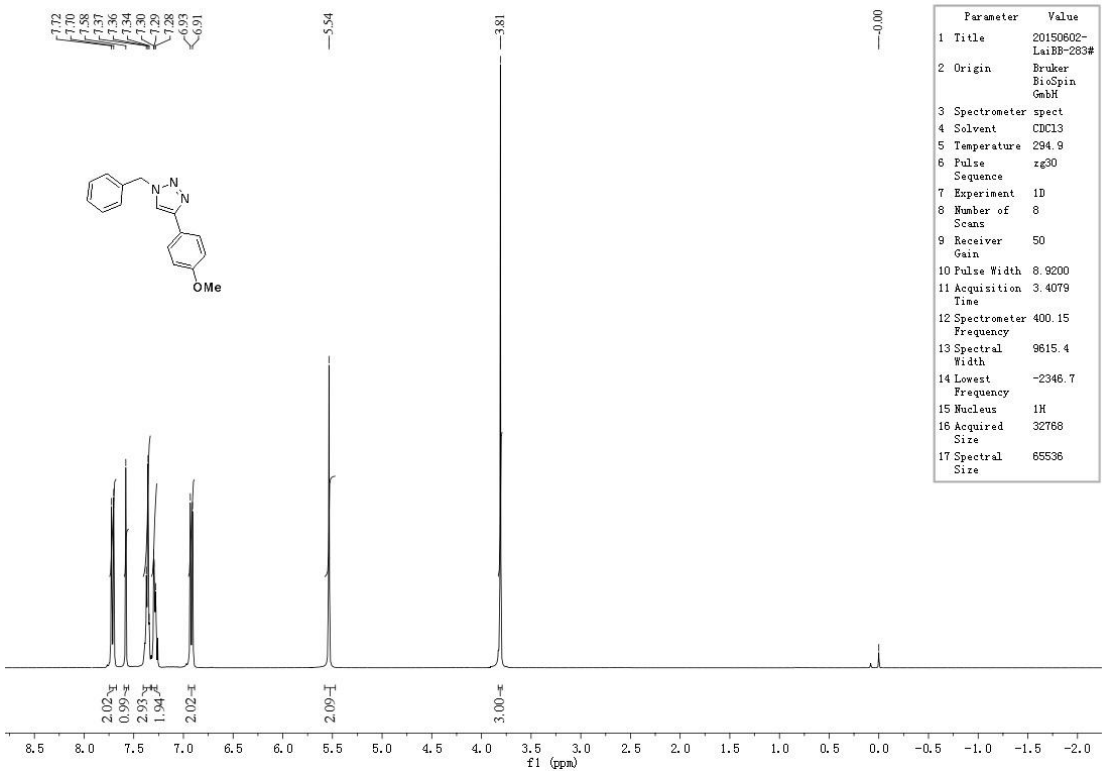

204.00 191.19 138.09 129.06 129.01 128.67 128.62 127.19 127.11 109.31 67.32 49.72 49.40 36.54 35.32 34.84 32.80 29.14 25.39 24.92 22.88
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)
Parameter Value
1 Title 20150623-LaiBB-302#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.79
7.77
7.68
7.39
7.37
7.35
7.34
7.30
7.28
7.27
5.52
-0.00
Ph
N
N
N
Ph
1.95
0.92
4.96
3.05
2.00
f1 (ppm)
Parameter Value
1 Title 20150505-LaiBB-255#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 18
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2345.4
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

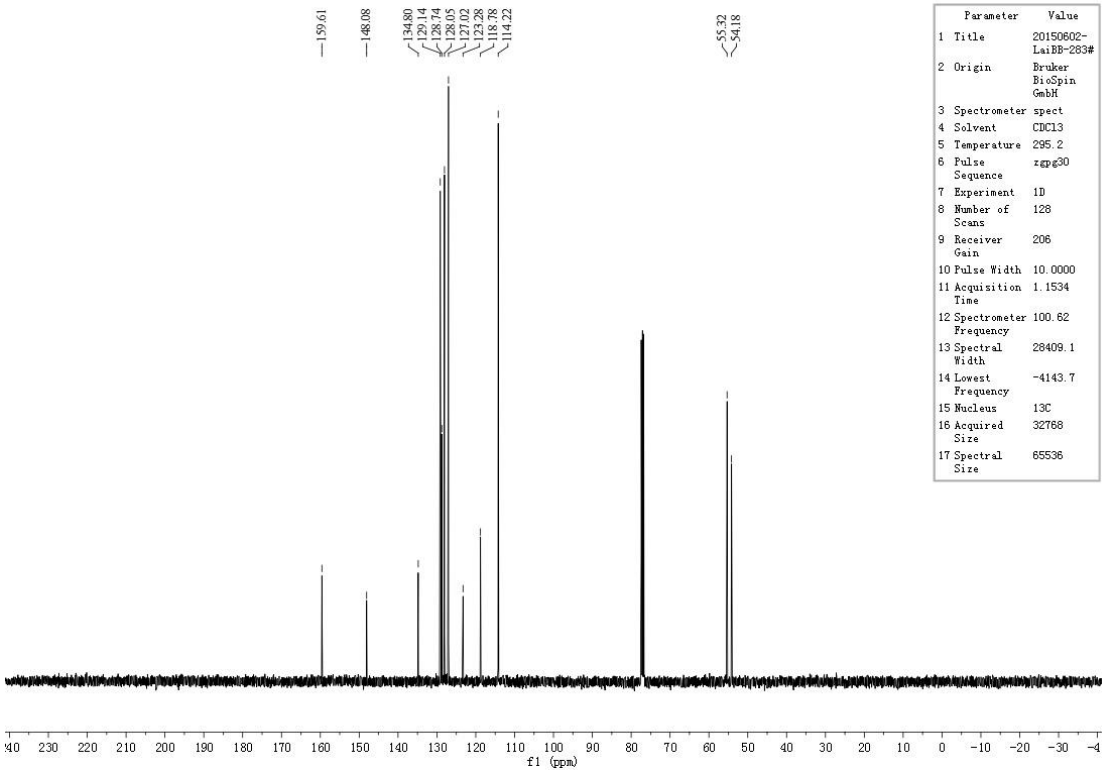

148.15
134.76
130.55
129.13
128.82
128.74
128.17
128.04
125.69
119.70
54.16
f1 (ppm)
Parameter Value
1 Title 20150505-LaiBB-255#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.4
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.77
7.76
7.75
7.73
7.64
7.38
7.36
7.31
7.30
7.20
7.09
7.07
7.05
5.55
0.00
N
N
N
F
1.93
0.95
2.84
1.81
1.95
2.00
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 -0.5 -1.0 -1.5 -2.0
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-282#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 44
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2346.0
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

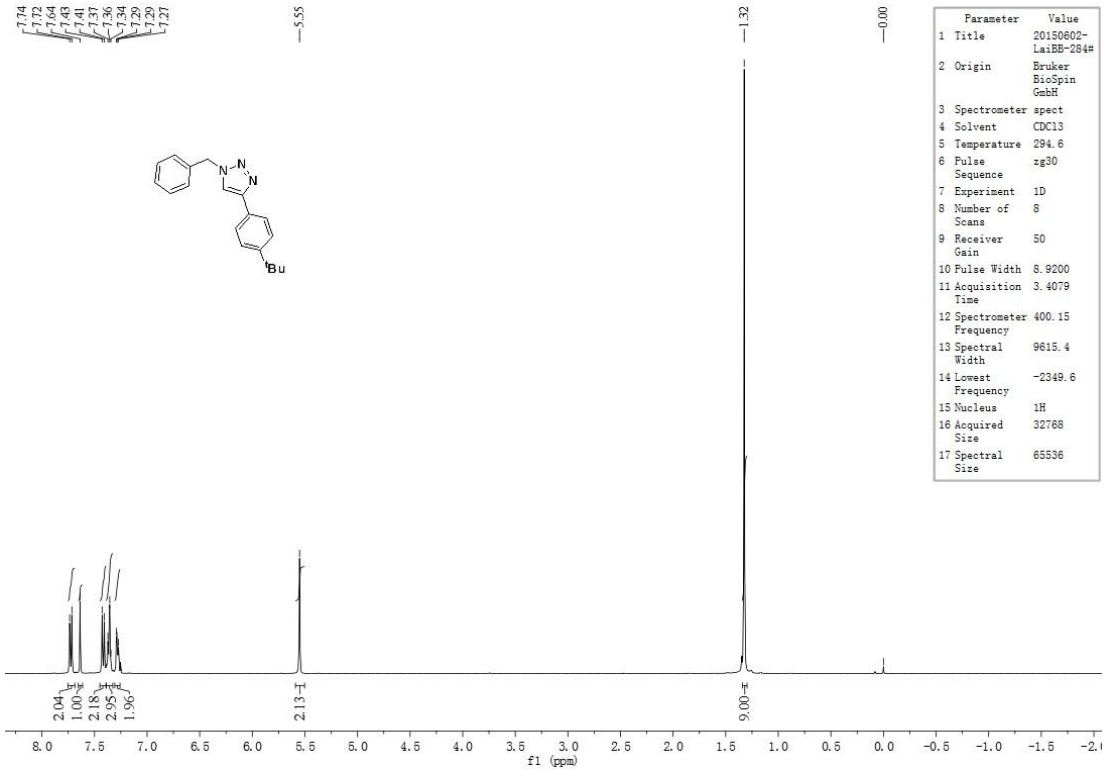

163.89
161.43
147.35
134.61
129.19
128.85
128.09
127.49
127.41
119.37
115.90
115.69
54.26
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-282#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

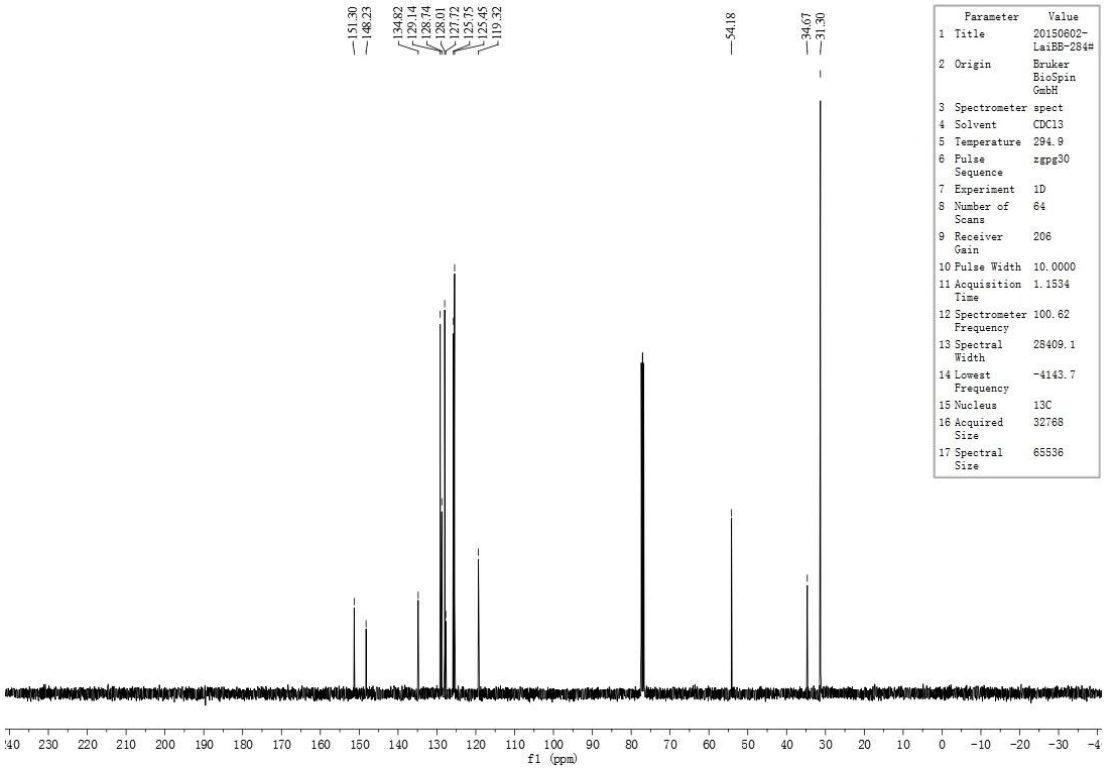


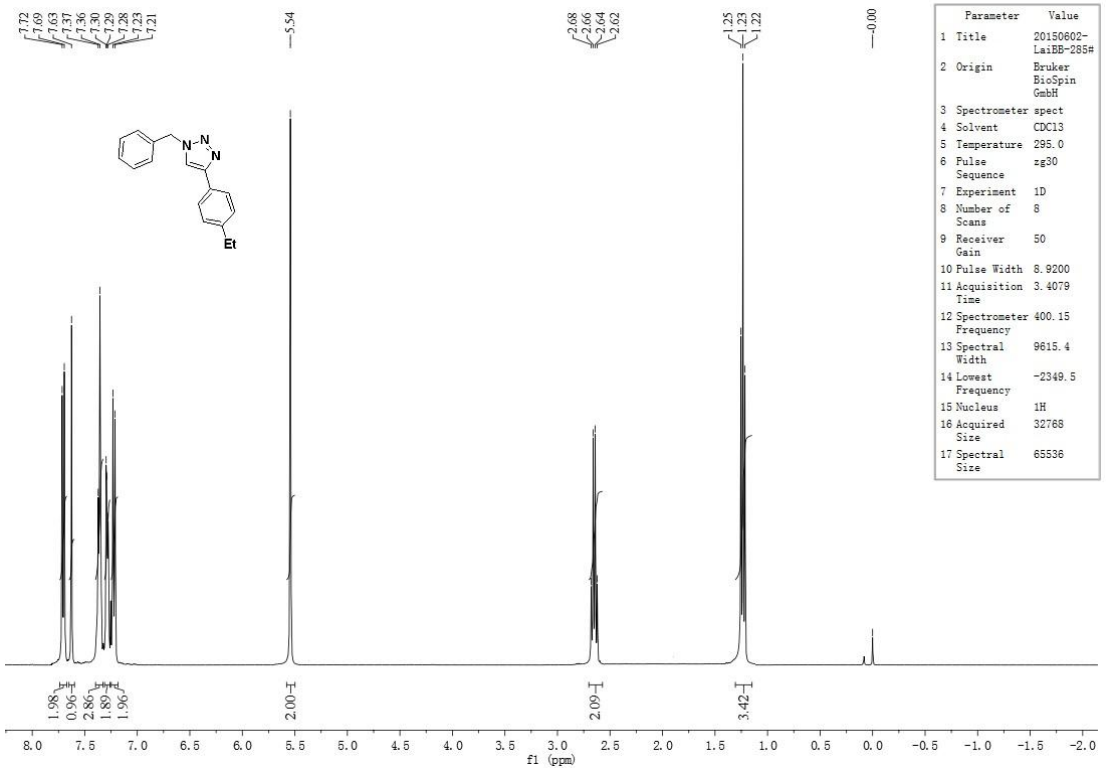
	Parameter	Value
1	Title	20150602-LaiBB-283#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	294.9
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	50
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2346.7
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

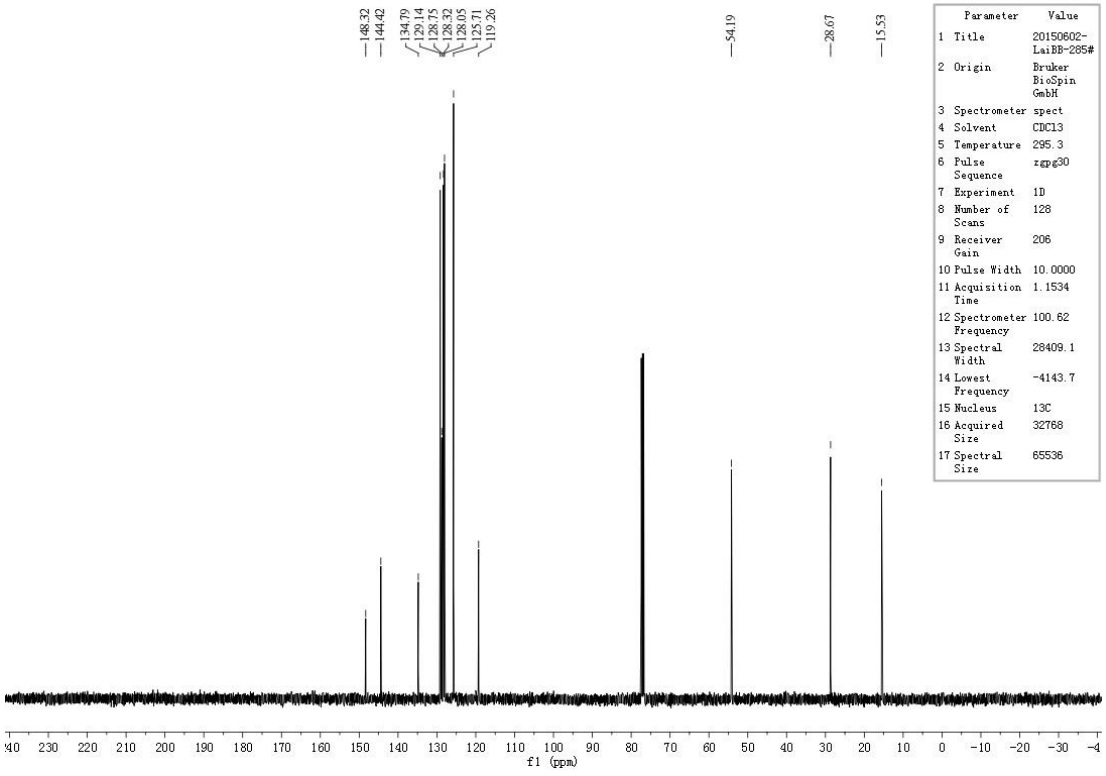


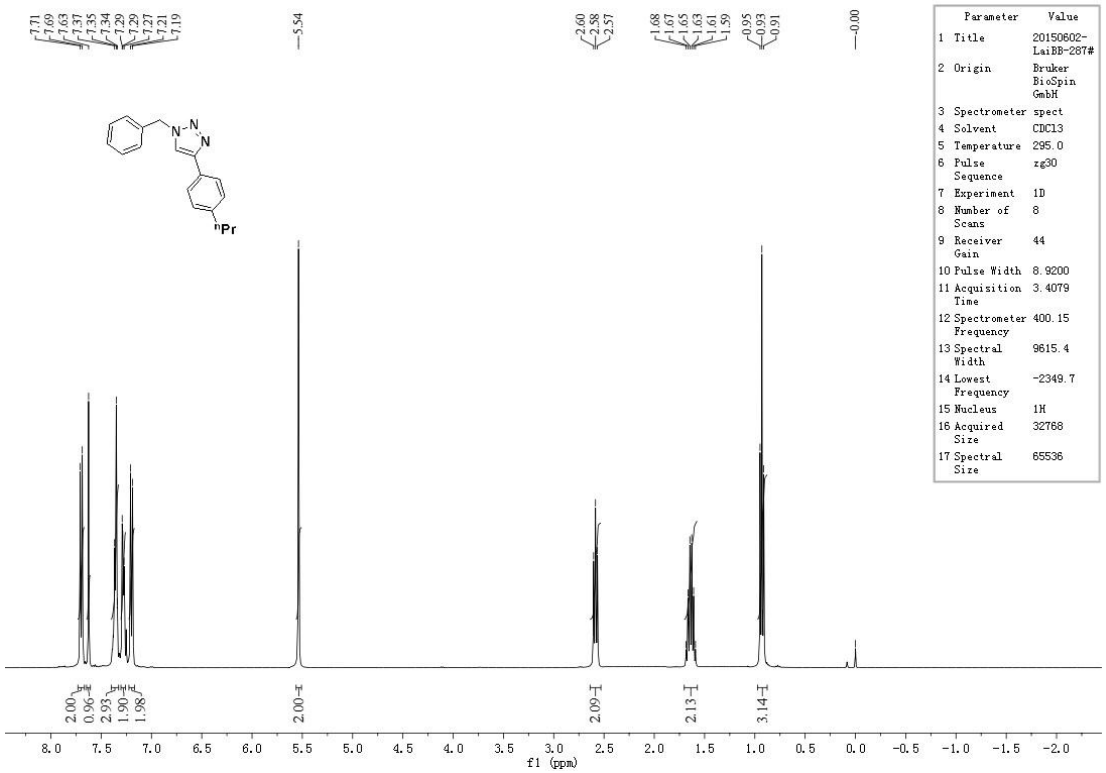
	Parameter	Value
1	Title	20150602-LaiBB-283#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

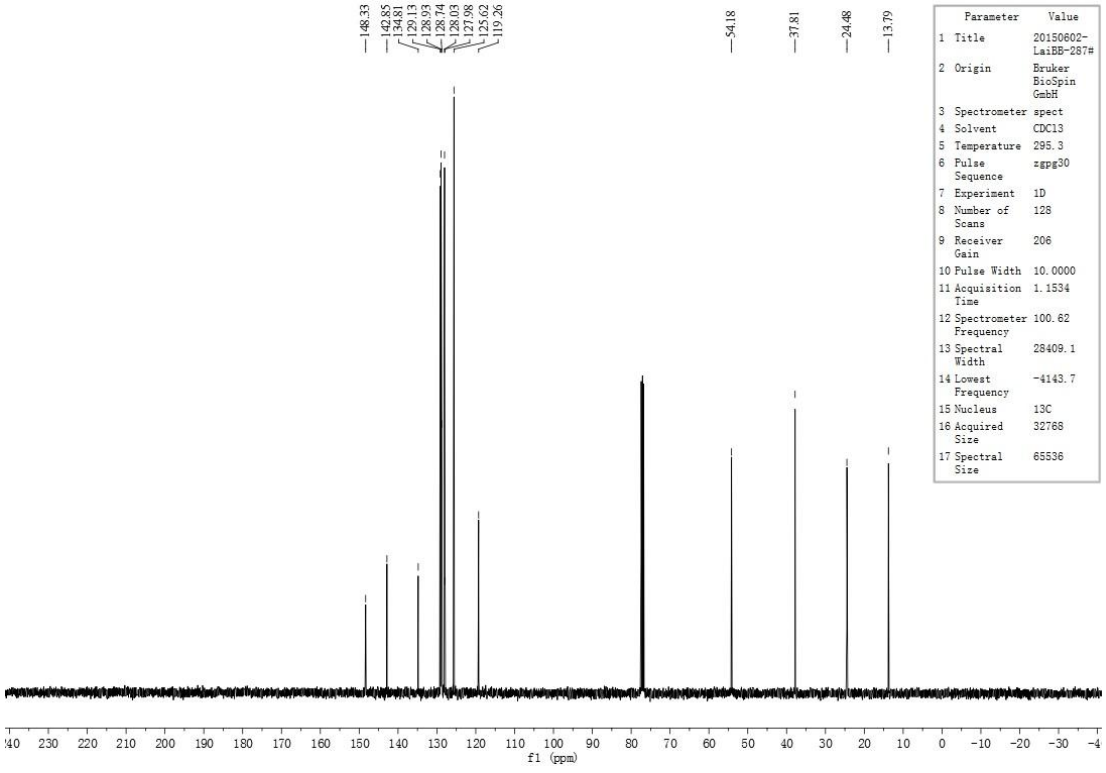

7.74
7.72
7.64
7.43
7.41
7.37
7.36
7.34
7.29
7.29
7.27
5.55
1.32
0.00
tBu
2.04
1.00
2.18
2.95
1.96
2.13
9.00
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-284#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.6
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 50
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2349.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

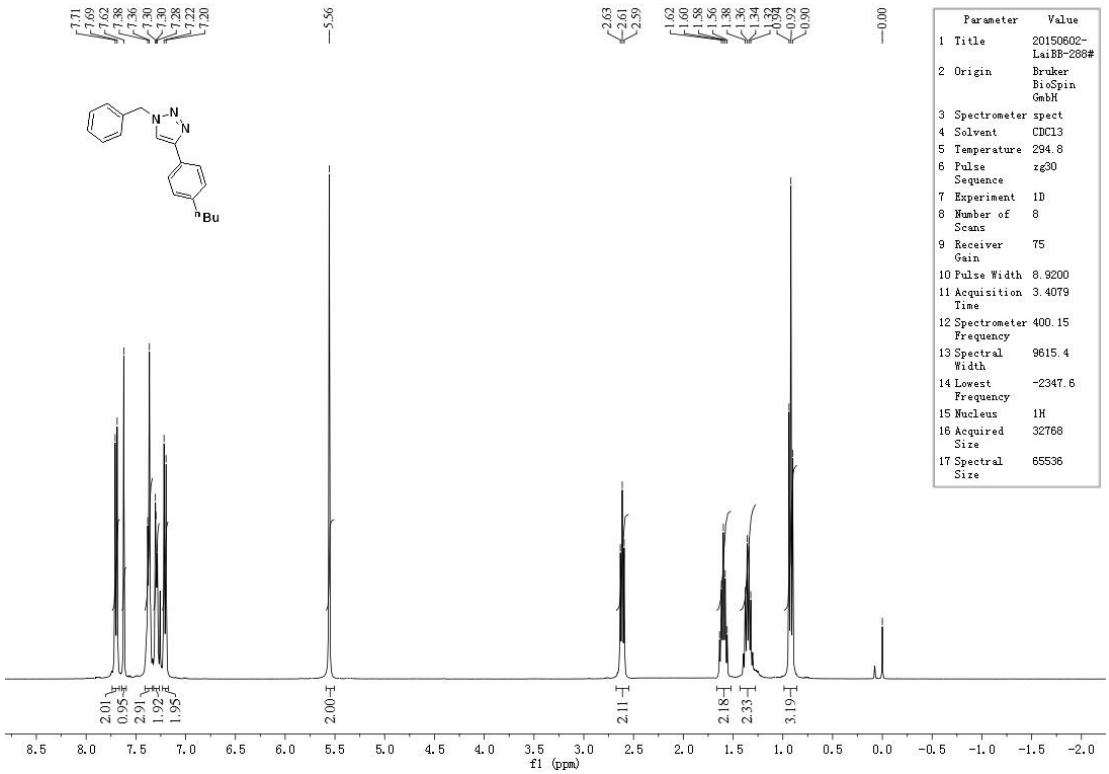

151.30
148.23
134.82
129.14
128.74
128.01
127.72
125.75
125.45
119.32
54.18
34.67
31.30
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-284#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

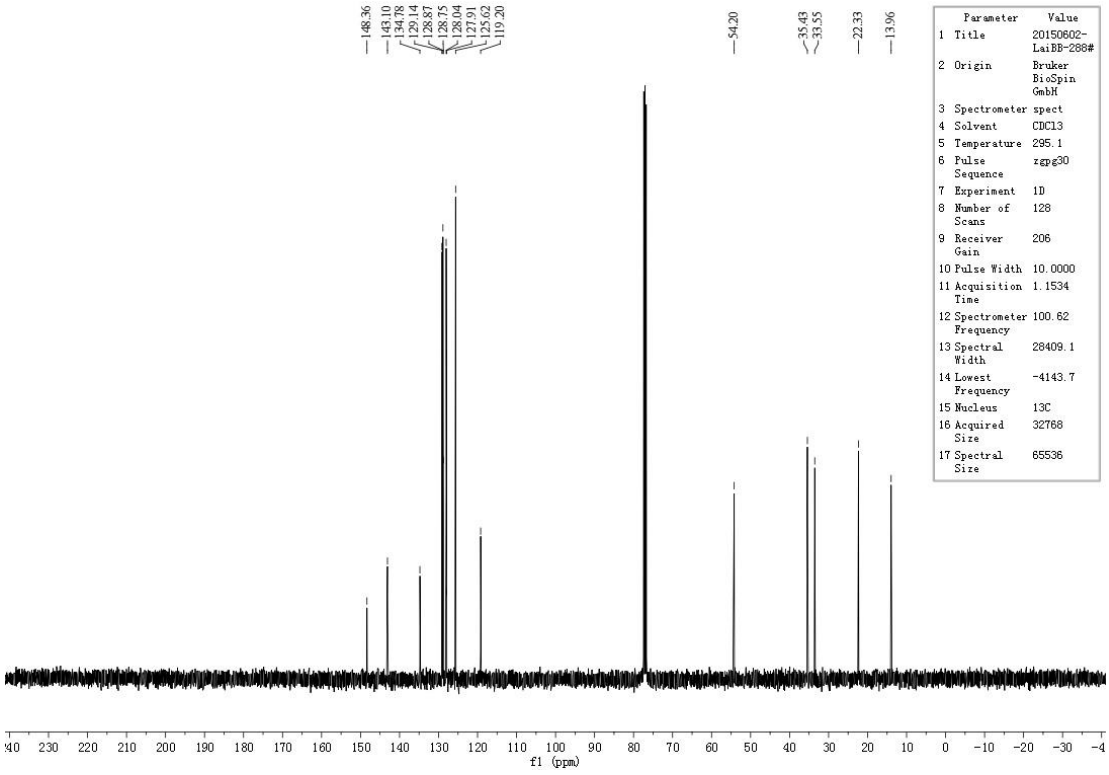

7.72
7.69
7.63
7.37
7.36
7.30
7.29
7.28
7.23
7.21
5.54
2.68
2.66
2.64
2.62
1.25
1.23
1.22
0.00
Et
1.98
0.96
2.86
1.89
1.96
2.00
2.09
3.42
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-285#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 50
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2349.5
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

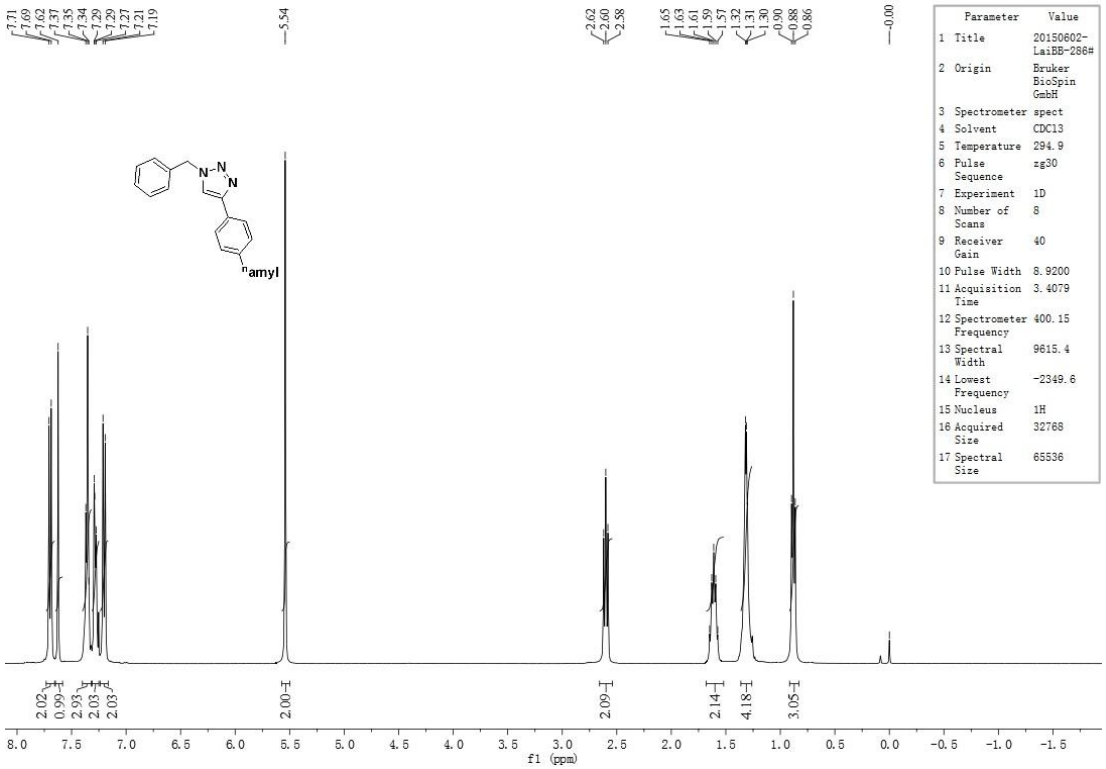

148.32
144.42
134.79
129.14
128.75
128.32
128.05
125.71
119.26
54.19
28.67
15.53
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-285#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

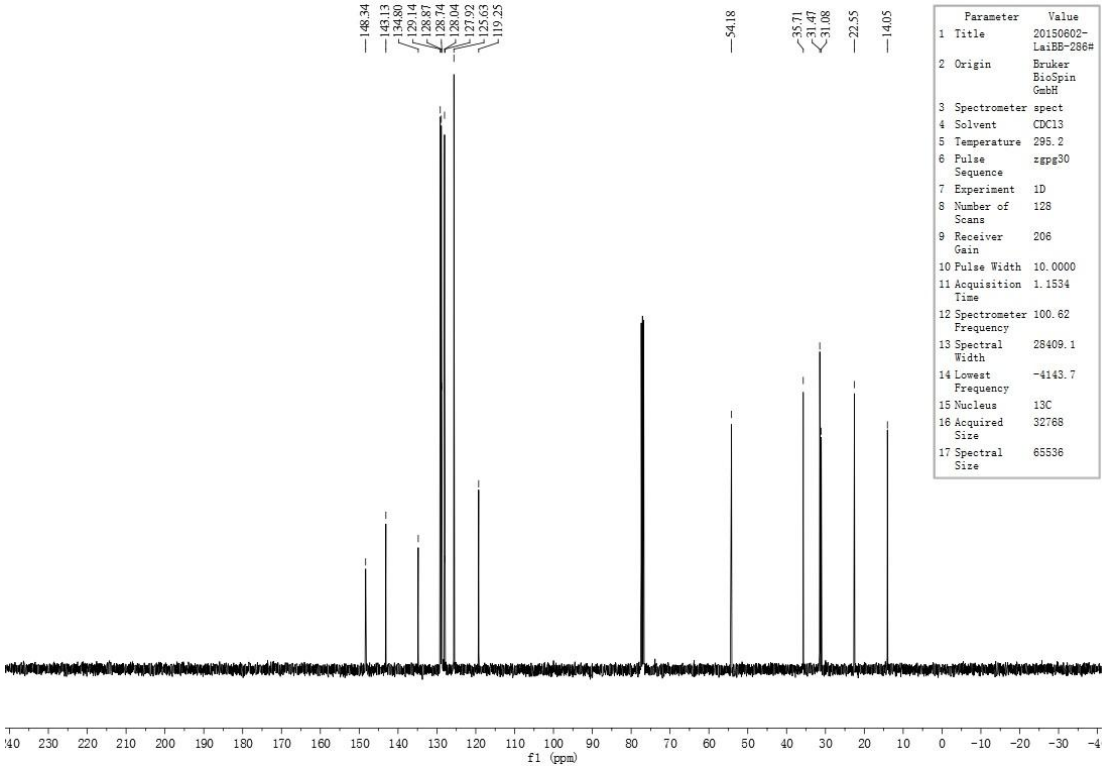

7.71
7.69
7.63
7.37
7.35
7.34
7.29
7.29
7.27
7.21
7.19
5.54
2.60
2.58
2.57
1.68
1.67
1.65
1.63
1.61
1.59
0.95
0.93
0.91
0.00
nPr
2.00
0.96
2.93
1.90
1.98
2.00
2.09
2.13
3.14
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-287#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 44
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2349.7
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

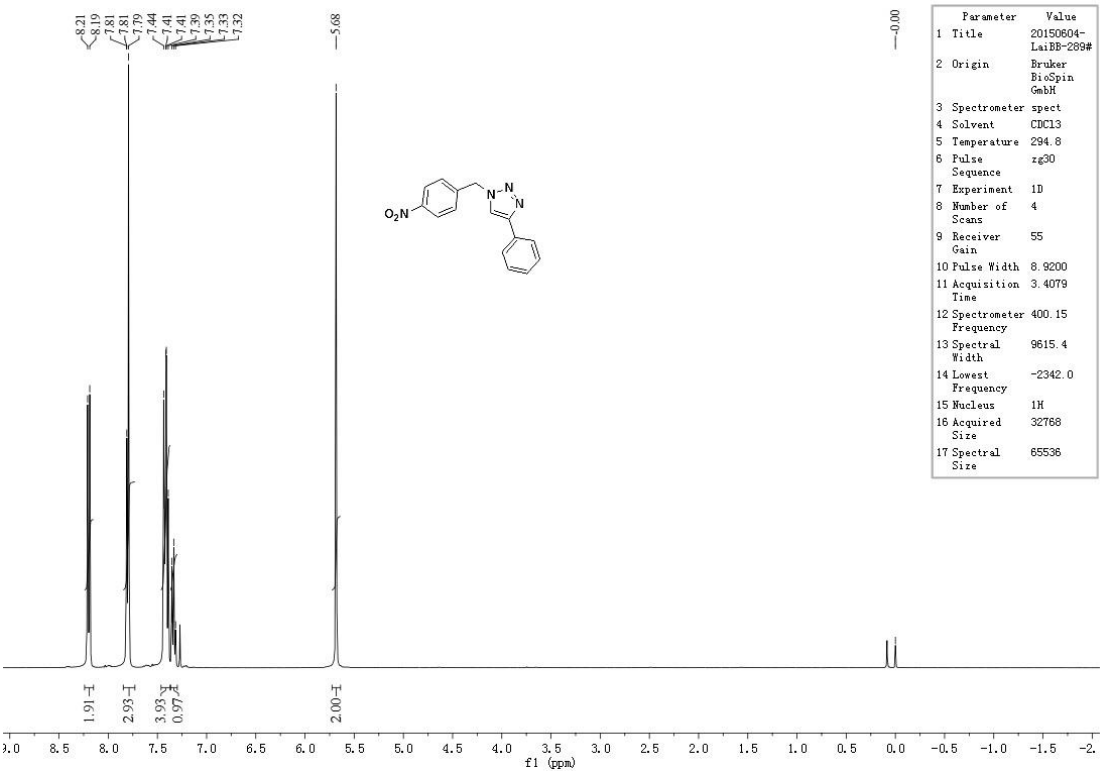

148.33
142.85
134.81
129.13
128.93
128.74
128.03
127.98
125.62
119.26
54.18
37.81
24.48
13.79
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-287#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.71
7.69
7.62
7.38
7.36
7.30
7.30
7.28
7.22
7.20
5.56
2.63
2.61
2.59
1.62
1.60
1.58
1.56
1.38
1.36
1.34
1.32
0.94
0.92
0.90
0.00
nBu
2.01
0.95
2.91
1.92
1.95
2.00
2.11
2.18
2.33
3.19
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-288#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.8
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2347.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

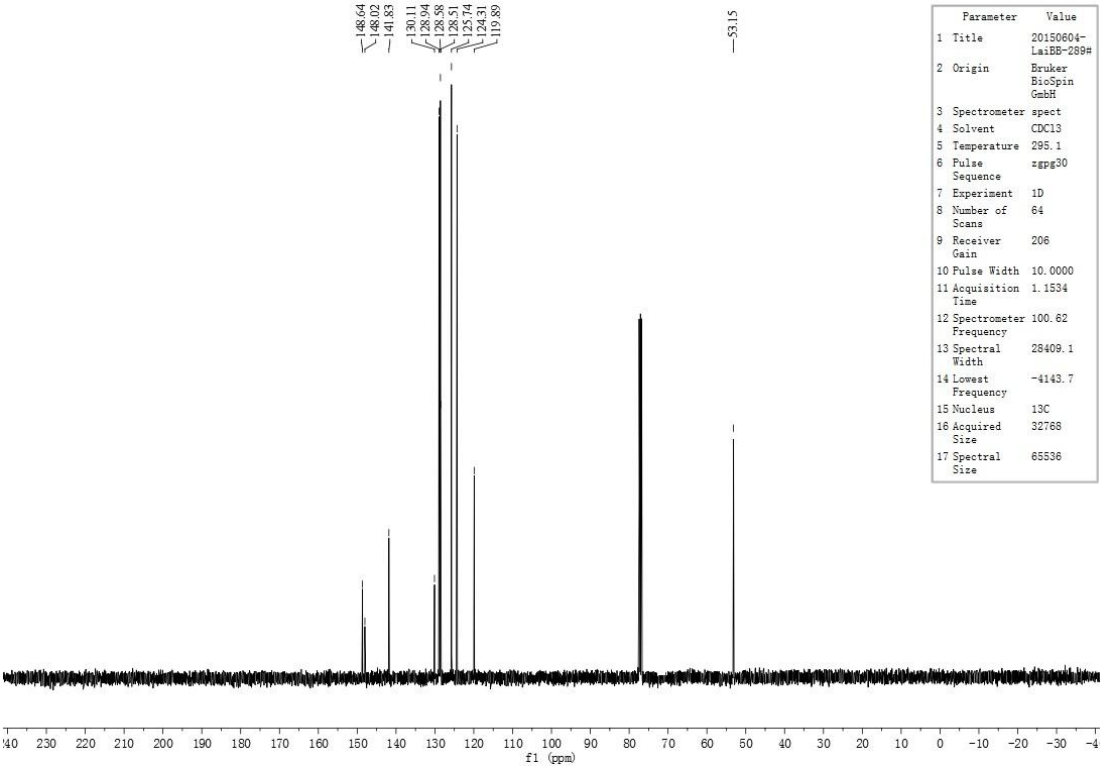

148.36
143.10
134.78
129.14
128.87
128.75
128.04
127.91
125.62
119.20
54.20
35.43
33.55
22.33
13.96
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-288#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.71
7.69
7.62
7.37
7.35
7.34
7.29
7.27
7.21
7.19
5.54
2.62
2.60
2.58
1.65
1.63
1.61
1.59
1.57
1.32
1.31
1.30
0.90
0.88
0.86
0.00
nAmyl
2.02
0.99
2.93
2.03
2.03
2.00
2.09
2.14
4.18
3.05
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-286#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 40
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2349.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

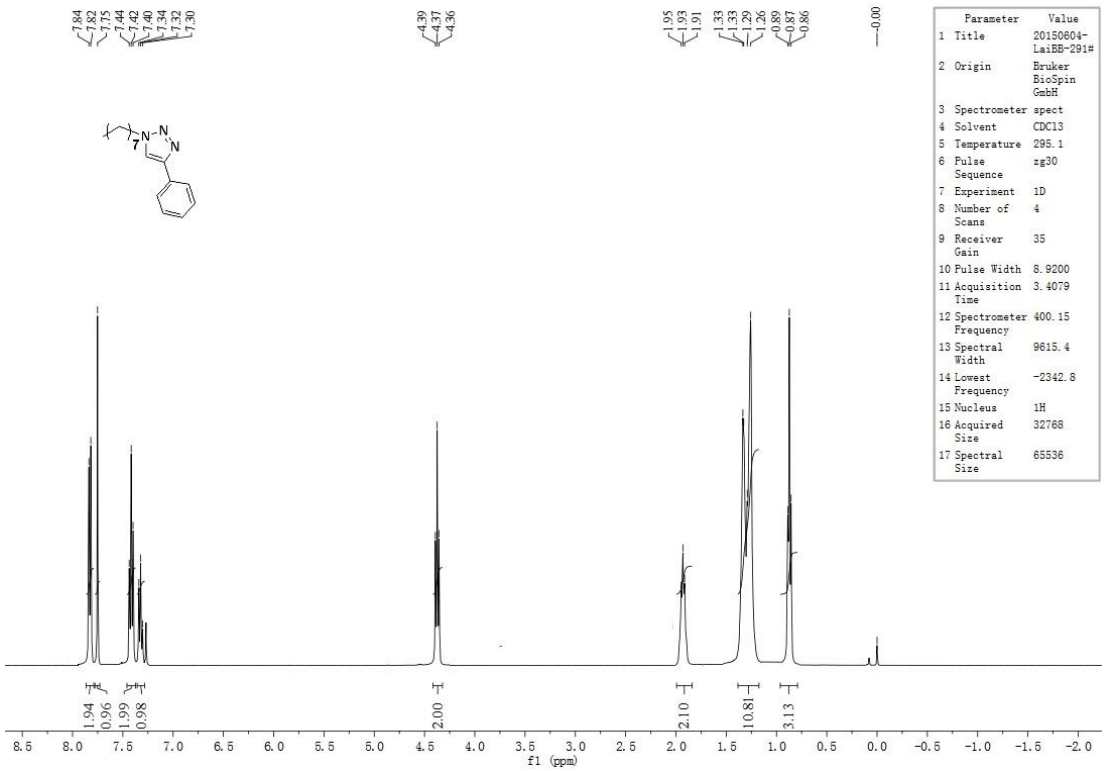

148.34
143.13
134.80
129.14
128.87
128.74
128.04
127.92
125.63
119.25
54.18
35.71
31.47
31.08
22.55
14.05
f1 (ppm)
Parameter Value
1 Title 20150602-LaiBB-286#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

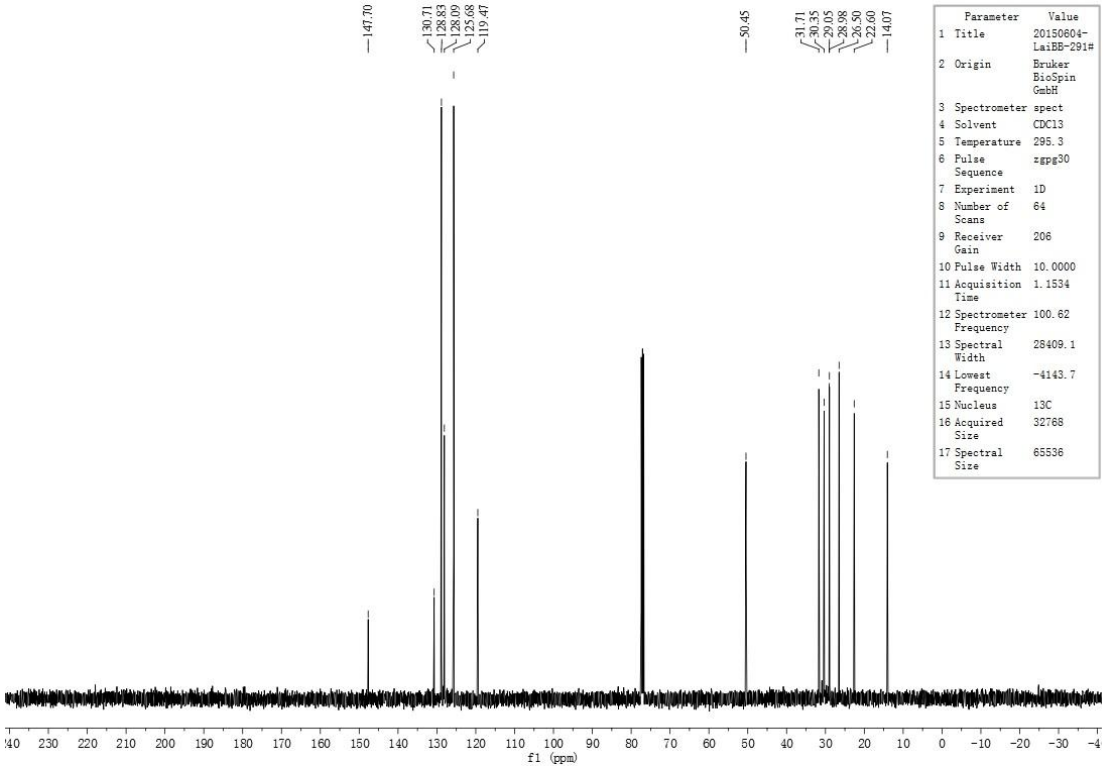


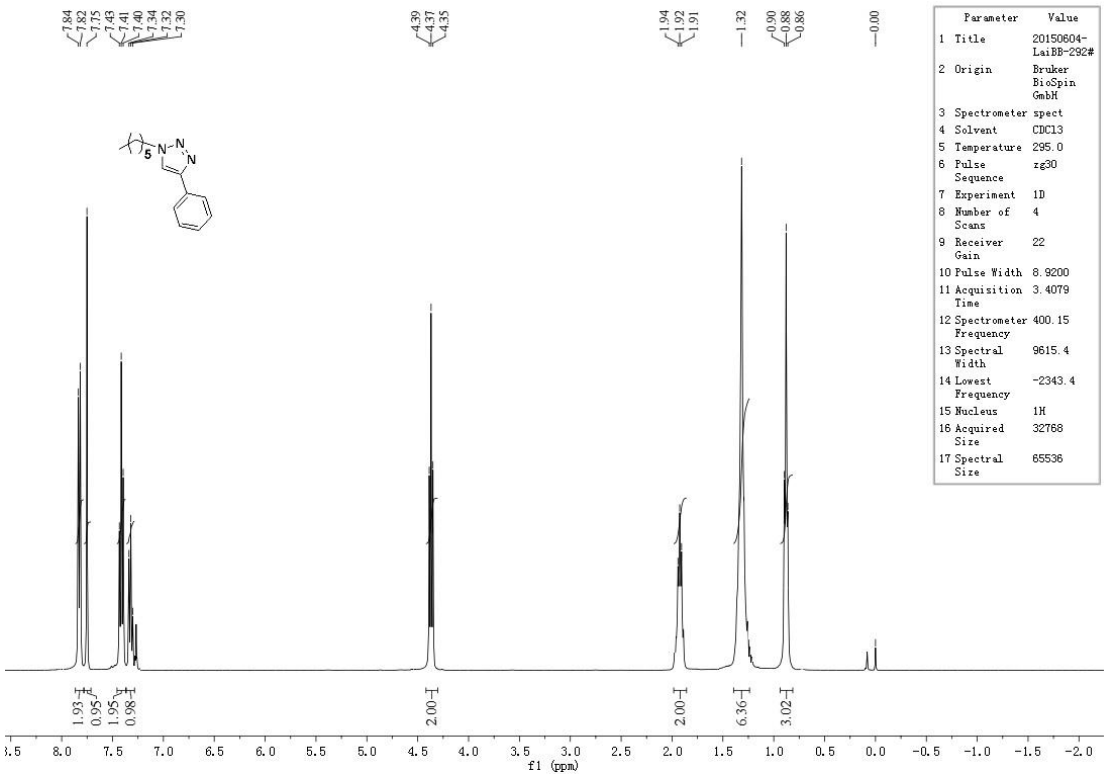
	Parameter	Value
1	Title	20150604-LaiBB-289#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	294.8
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	4
9	Receiver Gain	55
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2342.0
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

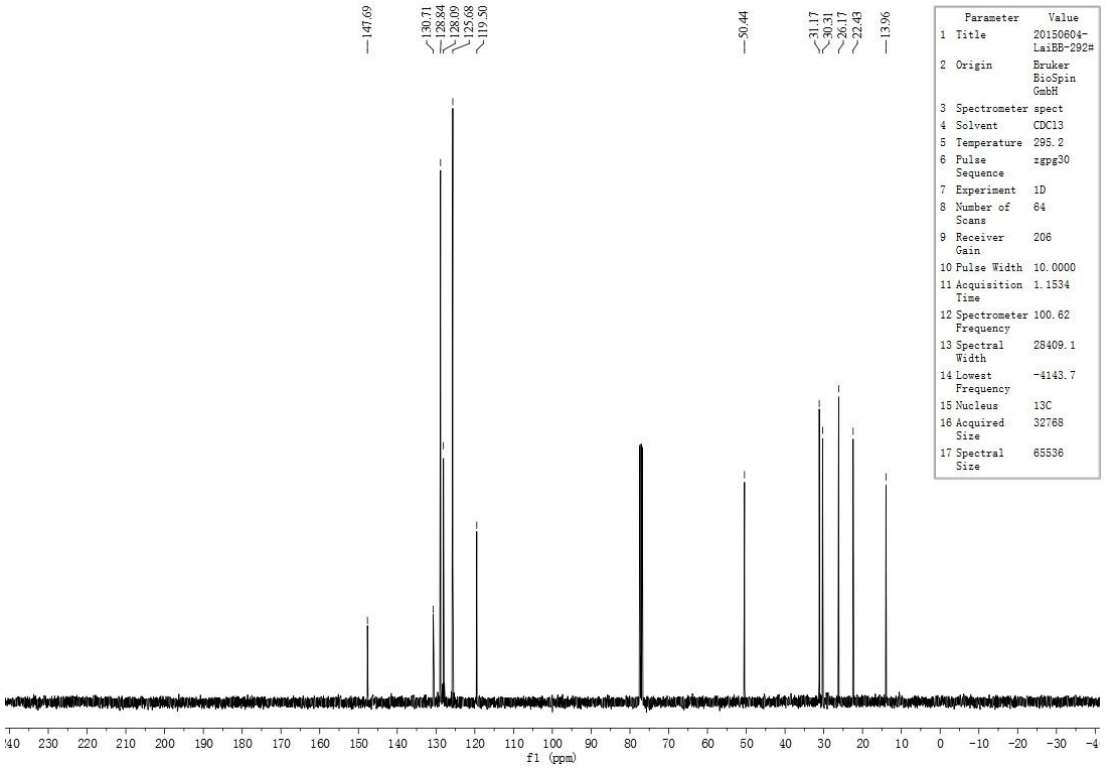


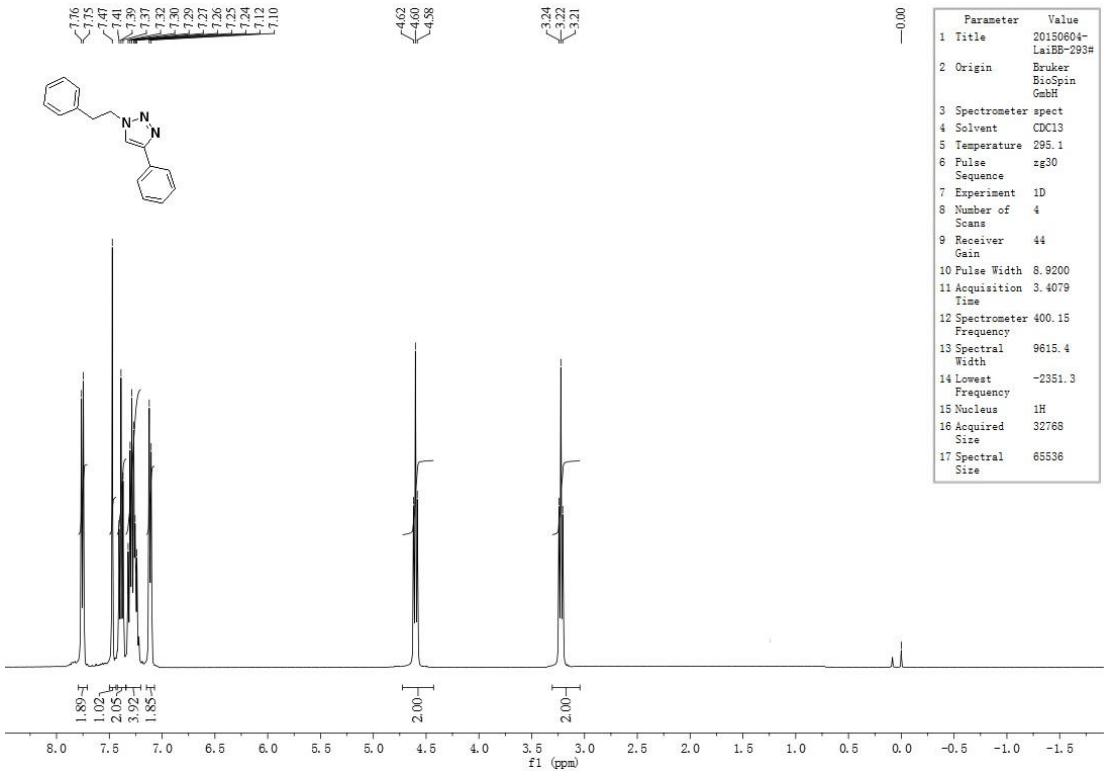
	Parameter	Value
1	Title	20150604-LaiBB-289#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	64
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

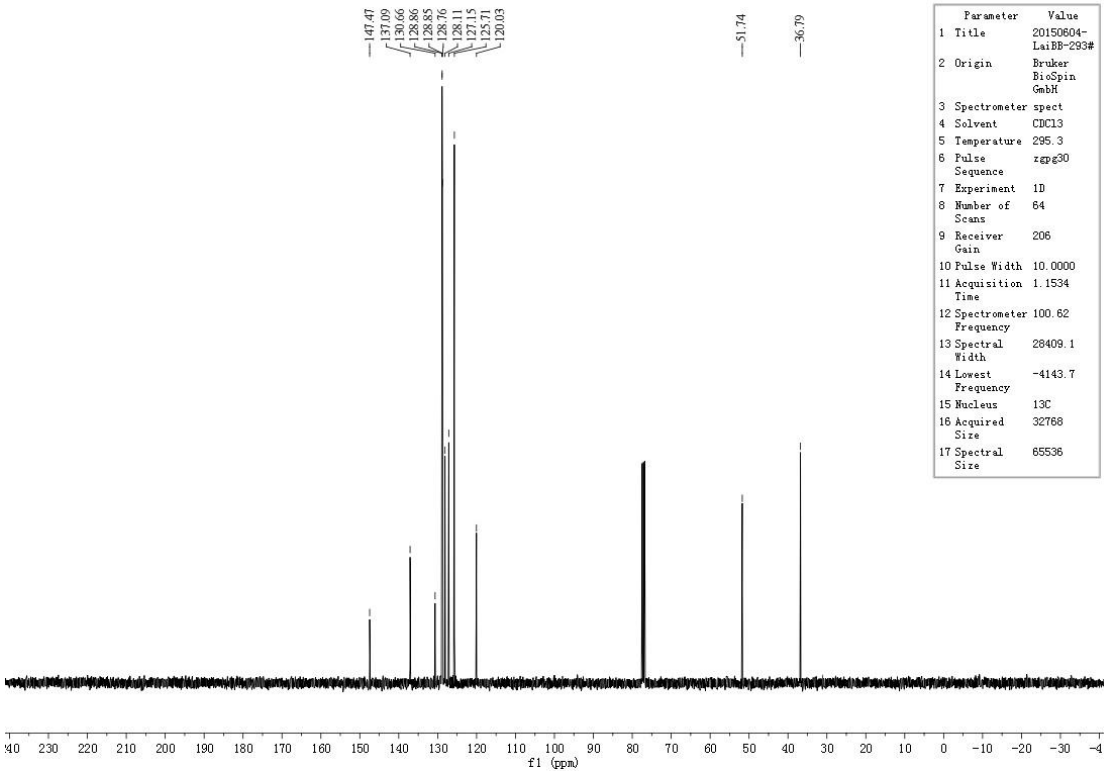

7.84
7.82
7.75
7.44
7.42
7.40
7.34
7.32
7.30
4.39
4.37
4.36
1.95
1.93
1.91
1.33
1.33
1.29
1.26
0.89
0.87
0.86
0.00
1.94
0.96
1.99
0.98
2.00
2.10
10.81
3.13
f1 (ppm)
Parameter Value
1 Title 20150604-LaiBB-291#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 35
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2342.8
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

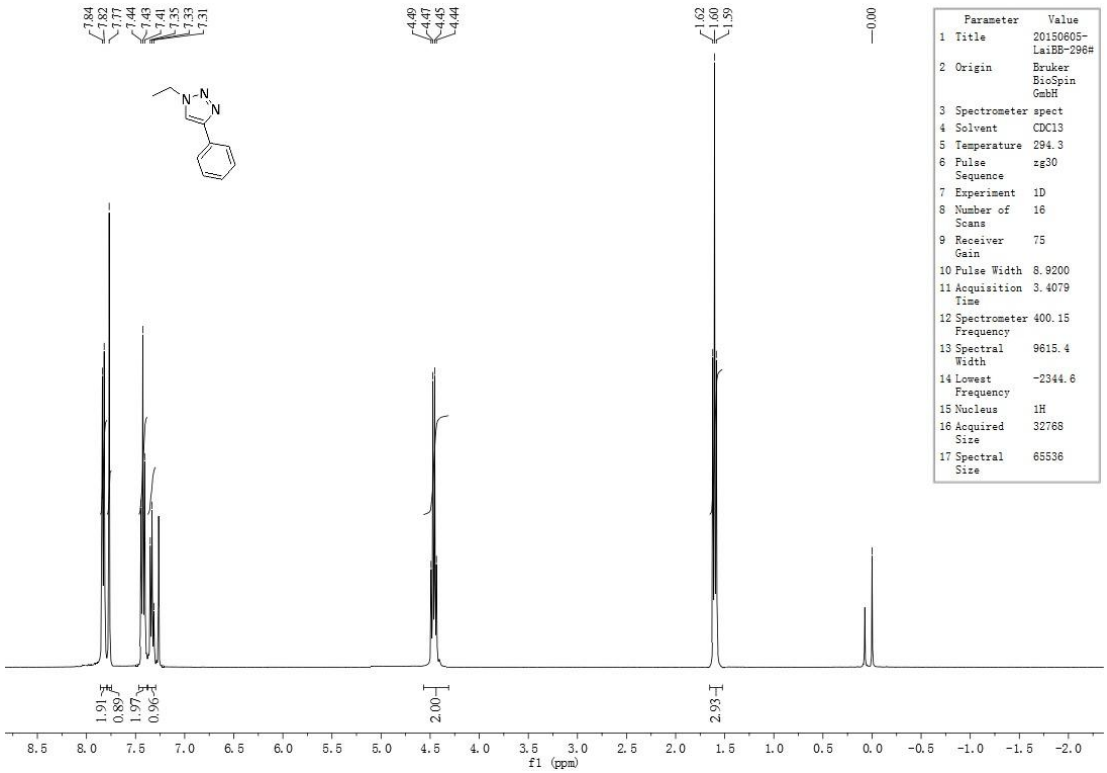

147.70
130.71
128.83
128.09
125.68
119.47
50.45
31.71
30.35
29.05
28.98
26.50
22.60
14.07
f1 (ppm)
Parameter Value
1 Title 20150604-LaiBB-291#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

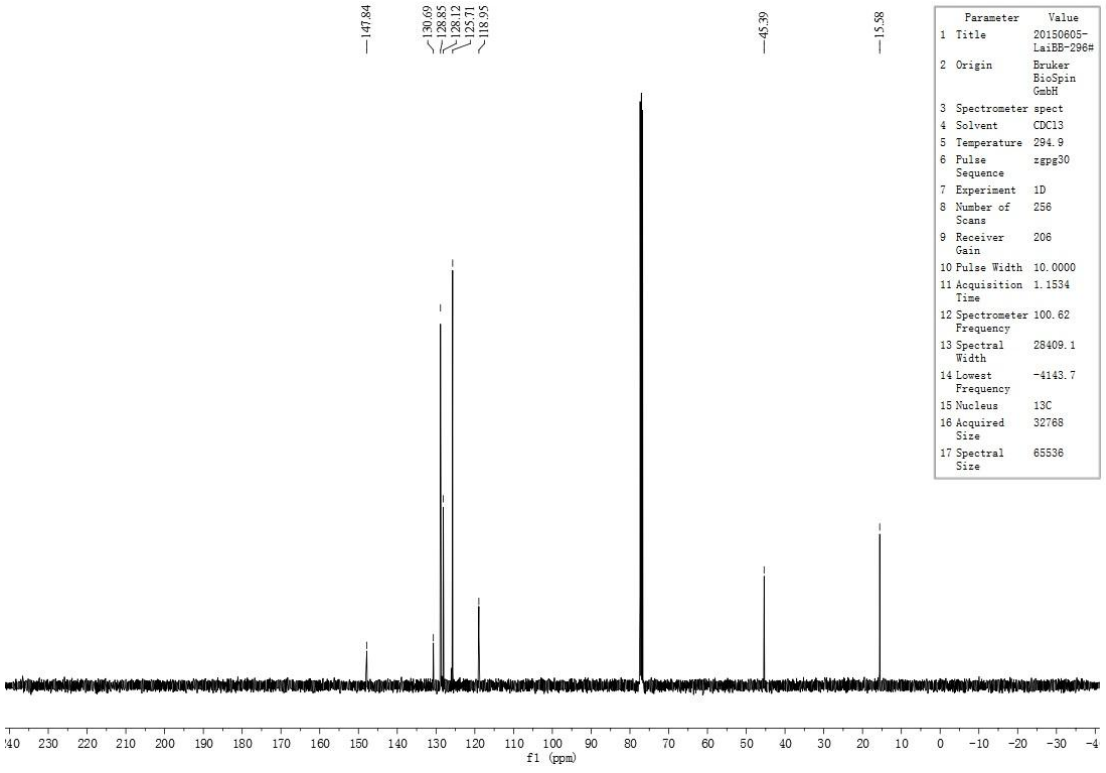

7.84
7.82
7.75
7.43
7.41
7.40
7.34
7.32
7.30
4.39
4.37
4.35
1.94
1.92
1.91
1.32
0.90
0.88
0.86
0.00
1.93
0.95
1.95
0.98
2.00
2.00
6.36
3.02
f1 (ppm)
Parameter Value
1 Title 20150604-LaiBB-292#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 22
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2343.4
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

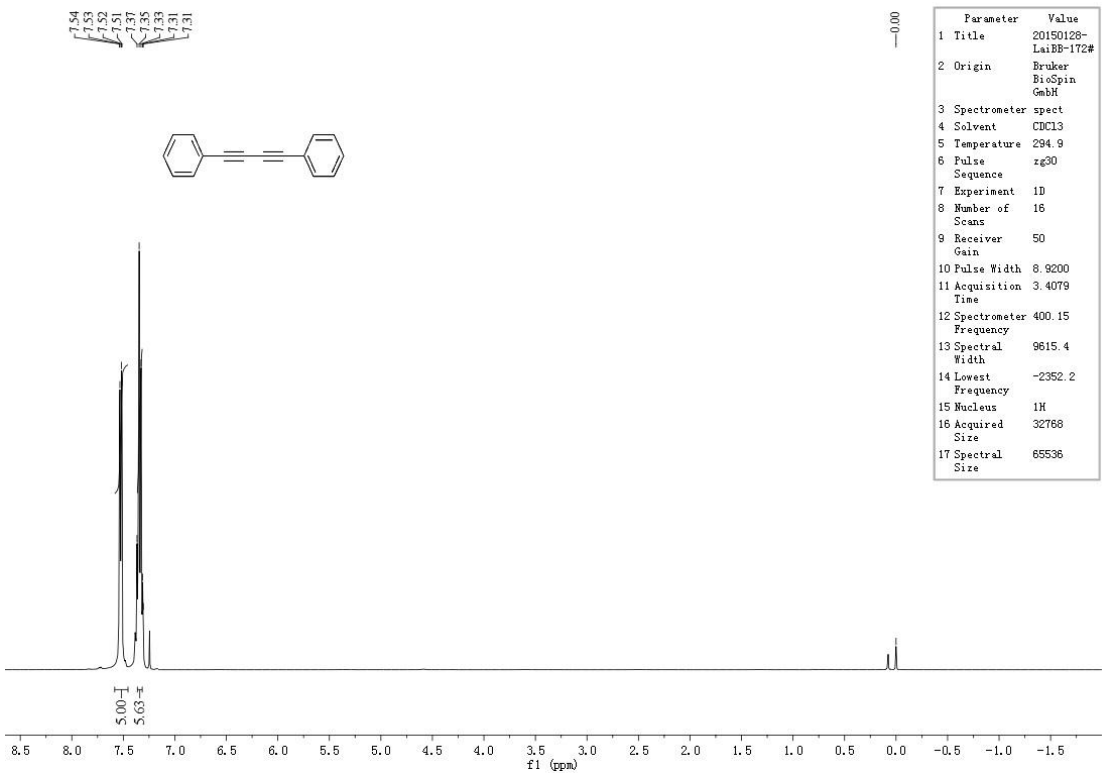

147.69
130.71
128.84
128.09
125.68
119.50
50.44
31.17
30.31
26.17
22.43
13.96
f1 (ppm)
Parameter Value
1 Title 20150604-LaiBB-292#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.76
7.75
7.47
7.41
7.39
7.37
7.32
7.30
7.29
7.27
7.26
7.25
7.24
7.12
7.10
4.62
4.60
4.58
3.24
3.22
3.21
0.00
1.89
1.02
2.05
3.92
1.85
2.00
2.00
f1 (ppm)
Parameter Value
1 Title 20150604-LaiBB-293#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 44
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2351.3
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

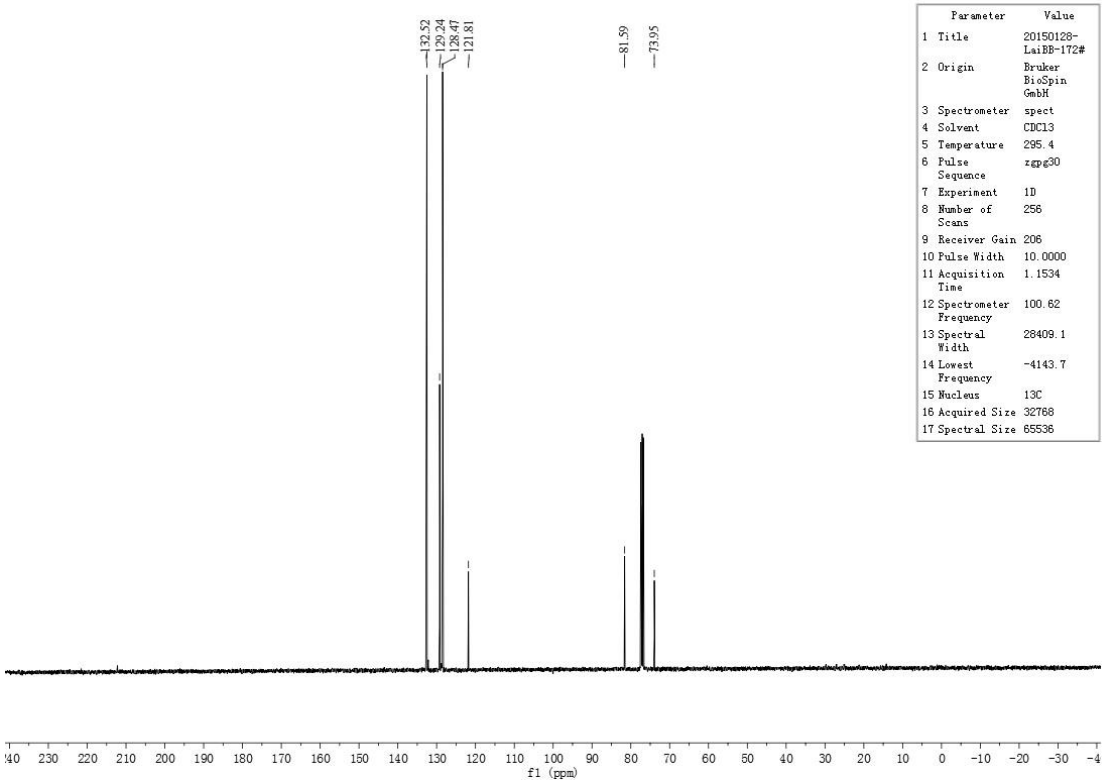

147.47
137.09
130.66
128.86
128.85
128.76
128.11
127.15
125.71
120.03
51.74
36.79
f1 (ppm)
Parameter Value
1 Title 20150604-LaiBB-293#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.84
7.82
7.77
7.44
7.43
7.41
7.35
7.33
7.31
4.49
4.47
4.45
4.44
1.62
1.60
1.59
0.00
1.91
0.89
1.97
0.96
2.00
2.93
f1 (ppm)
Parameter Value
1 Title 20150605-LaiBB-296#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 16
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2344.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

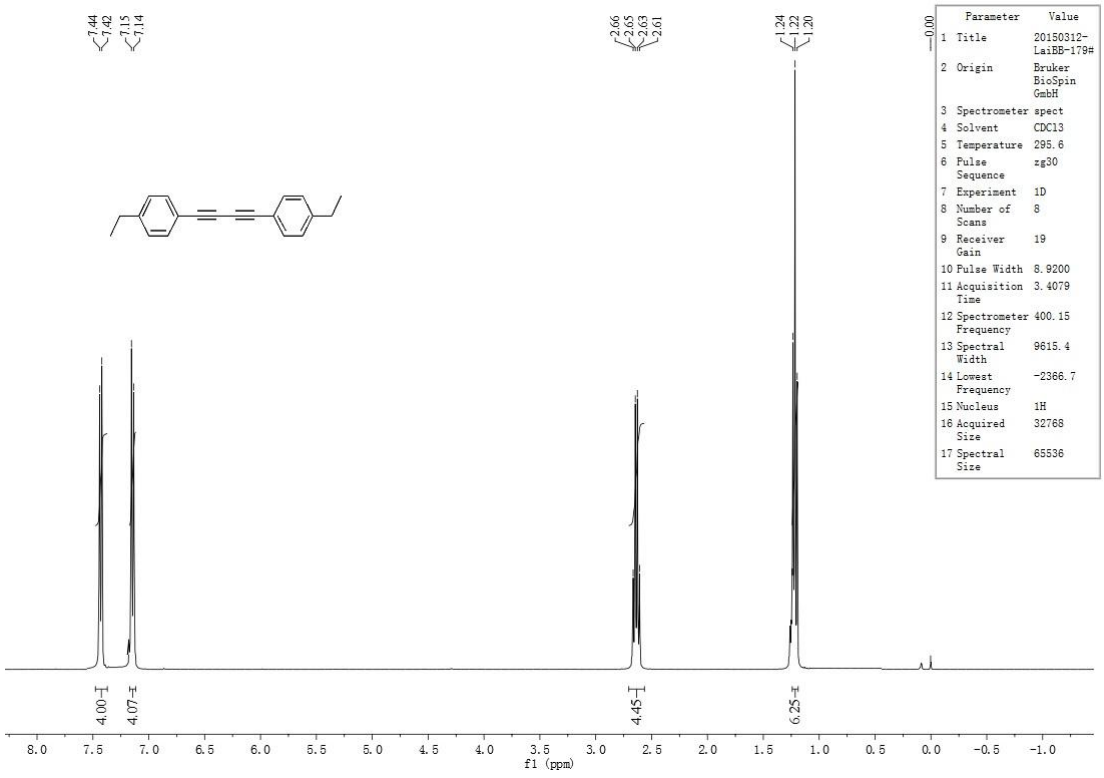

147.84
130.69
128.85
128.12
125.71
118.95
45.39
15.58
f1 (ppm)
Parameter Value
1 Title 20150605-LaiBB-296#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 256
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

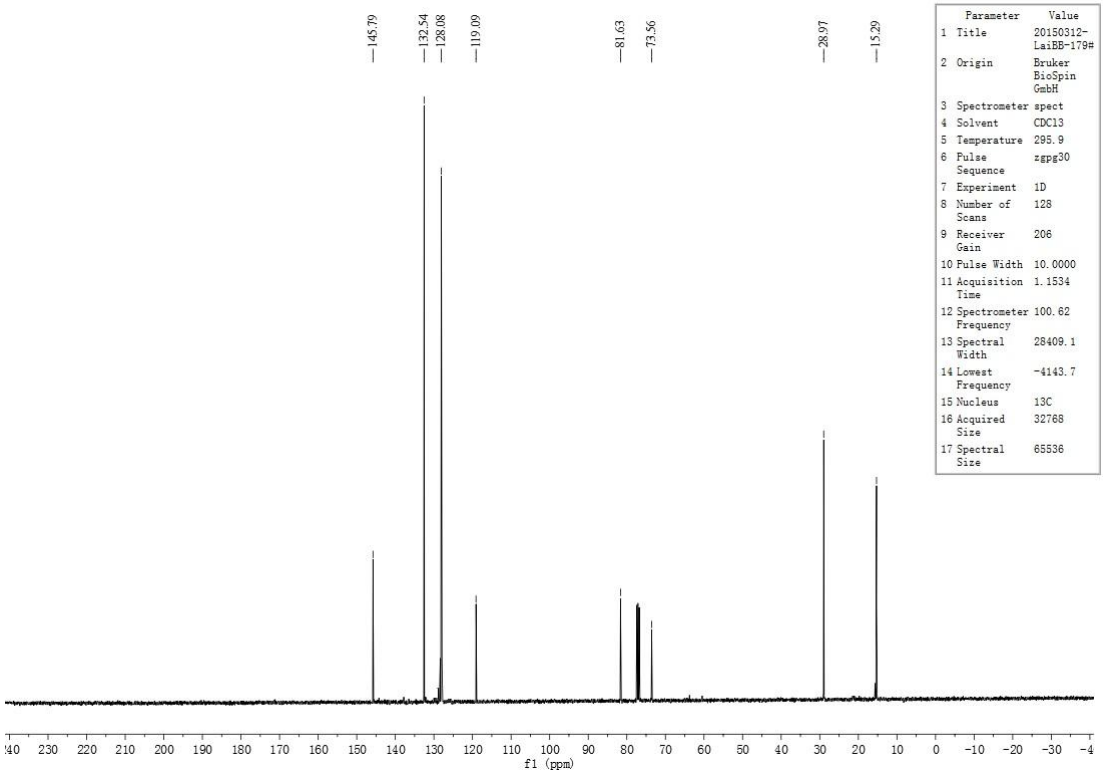


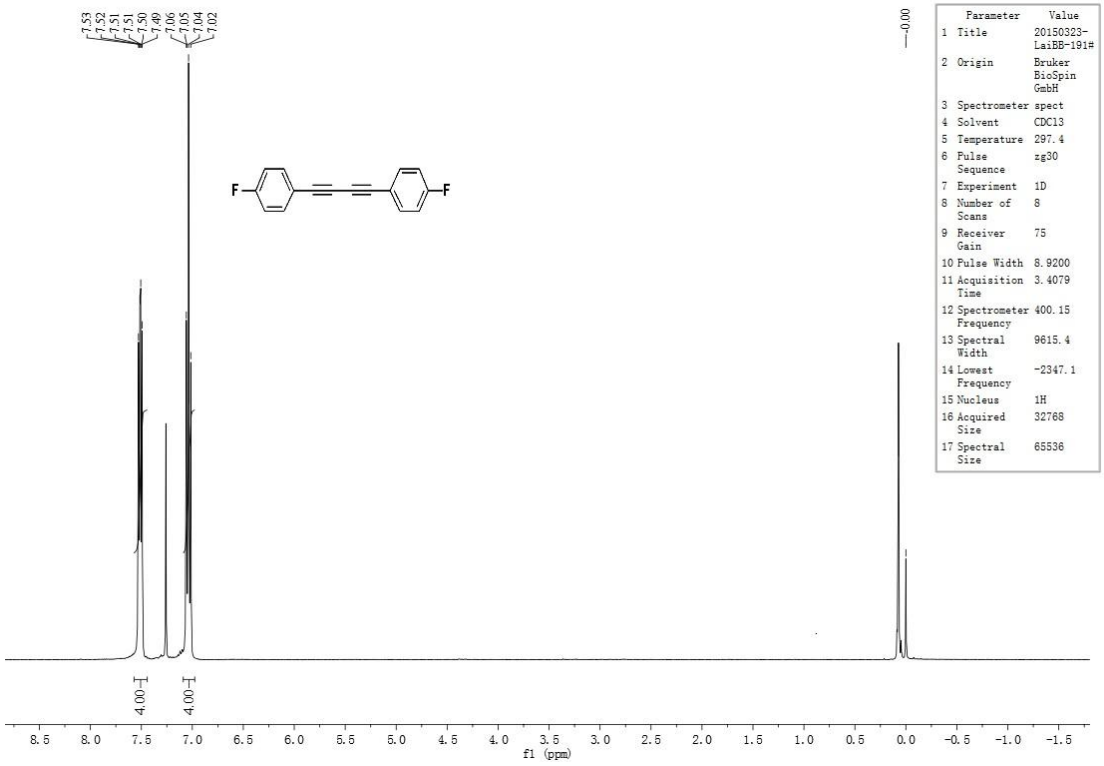
	Parameter	Value
1	Title	20150128-LaiBB-172#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	294.9
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	50
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2352.2
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



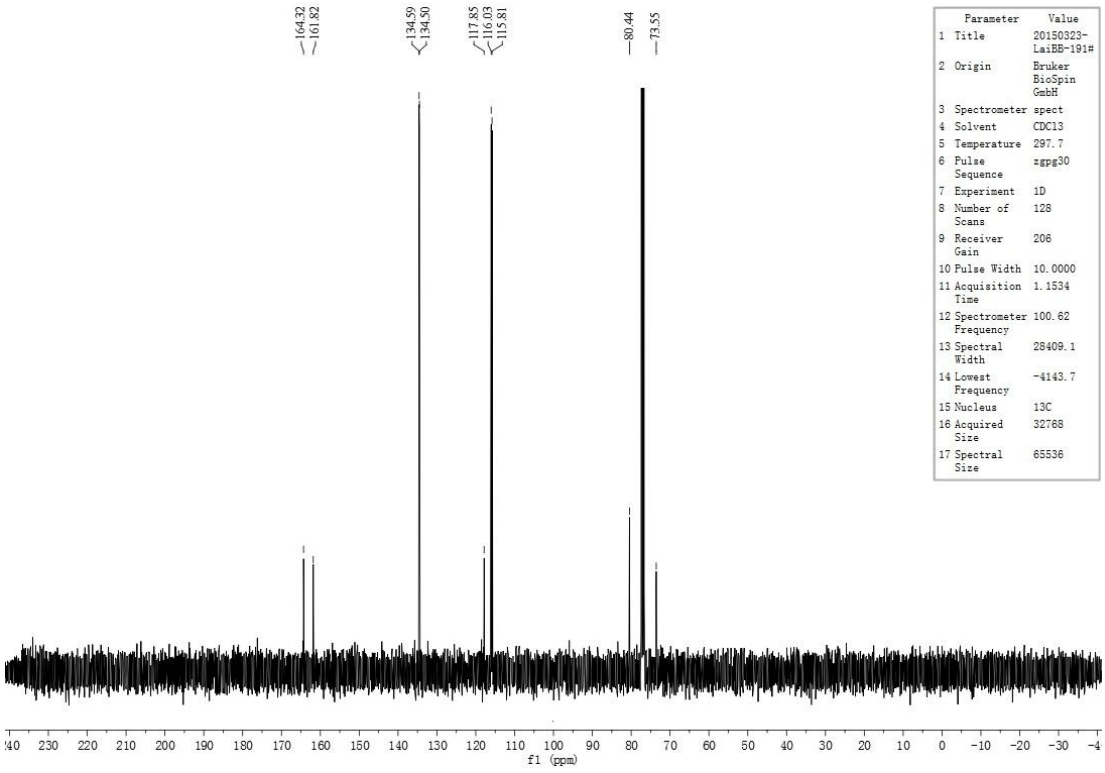
	Parameter	Value
1	Title	20150128-LaiBB-172#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.4
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	256
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536


7.44
7.42
7.15
7.14
2.66
2.65
2.63
2.61
1.24
1.22
1.20
0.00
4.00
4.07
4.45
6.25
f1 (ppm)
Parameter Value
1 Title 20150312-LaiBB-179#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.6
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 19
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2366.7
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

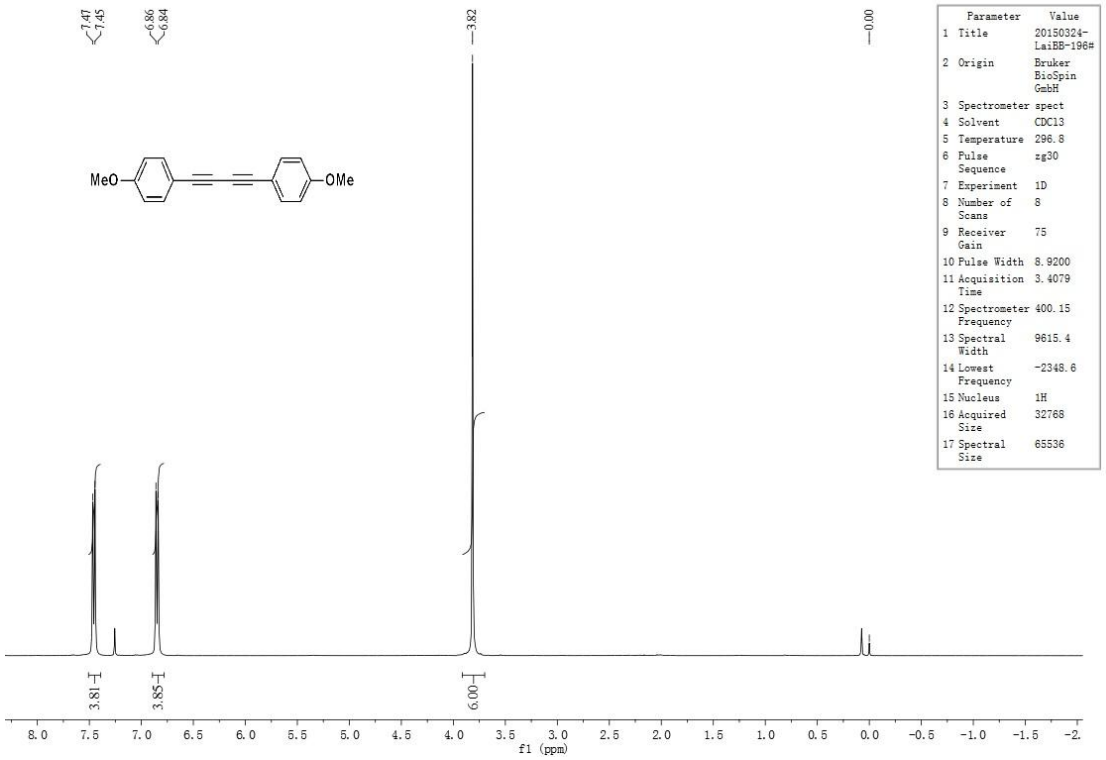

145.79
132.54
128.08
119.09
81.63
73.56
28.97
15.29
f1 (ppm)
Parameter Value
1 Title 20150312-LaiBB-179#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.9
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536



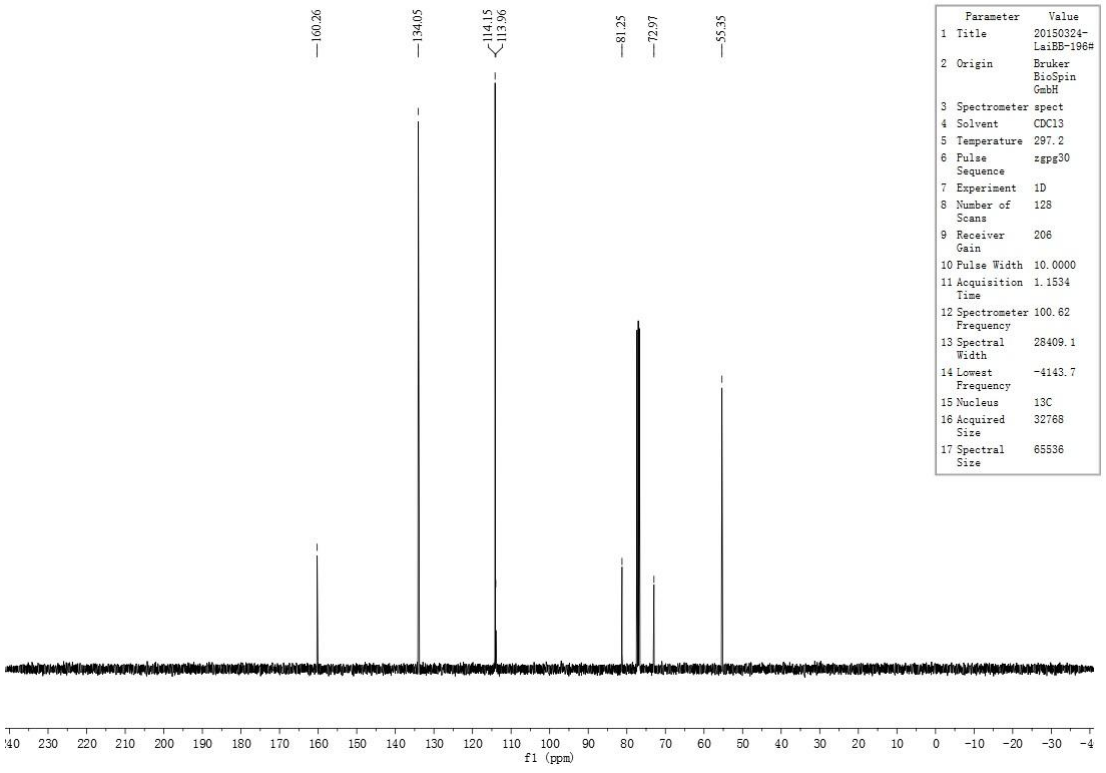
	Parameter	Value
1	Title	20150323-LaiBB-191#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	297.4
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	75
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2347.1
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



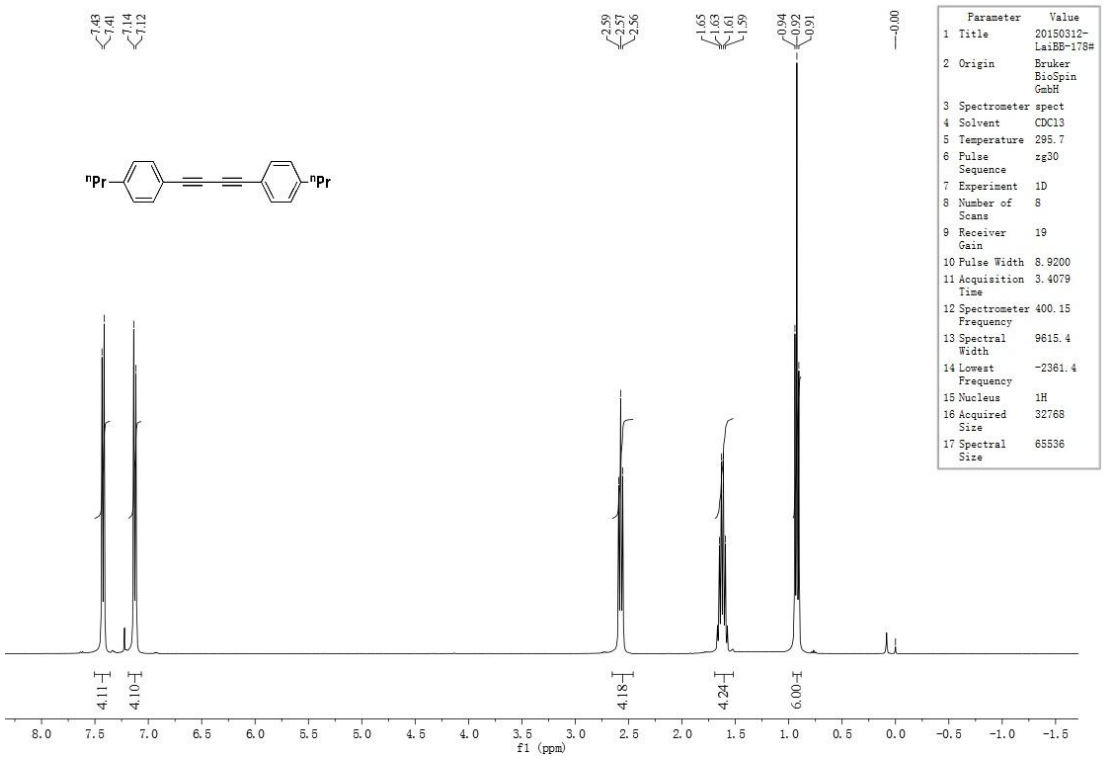
	Parameter	Value
1	Title	20150323-LaiBB-191#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	297.7
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536



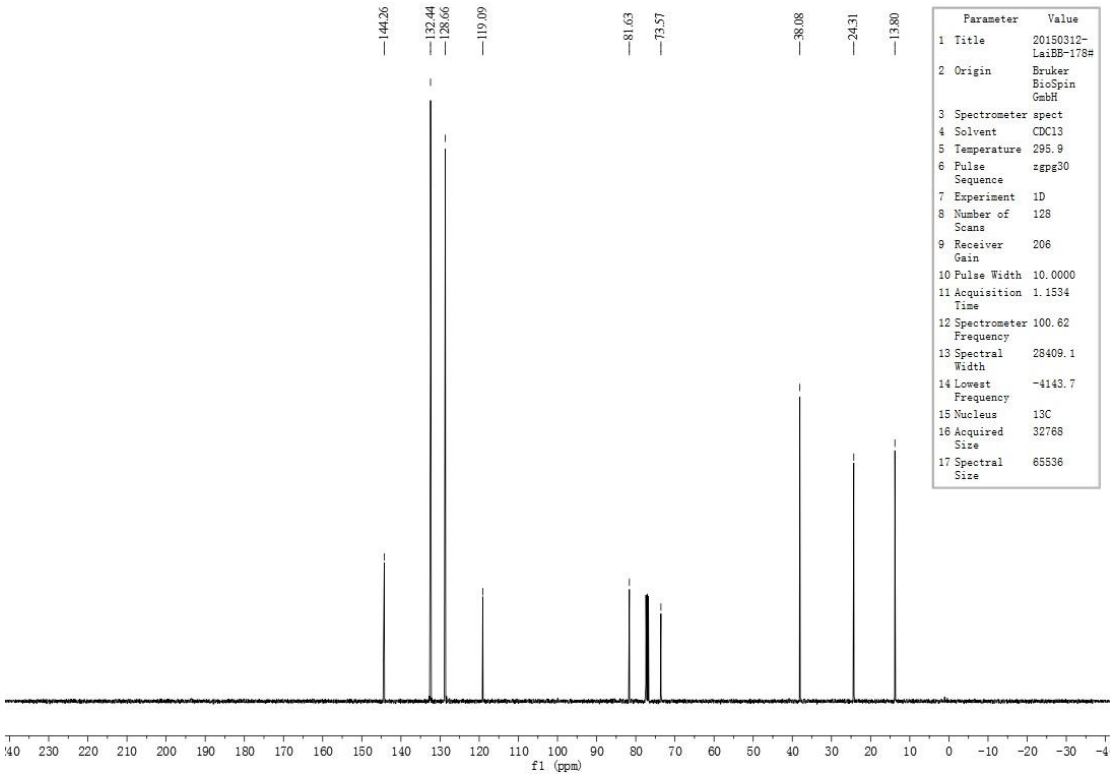
	Parameter	Value
1	Title	20150324-LaiBB-196#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	296.8
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	75
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2348.6
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



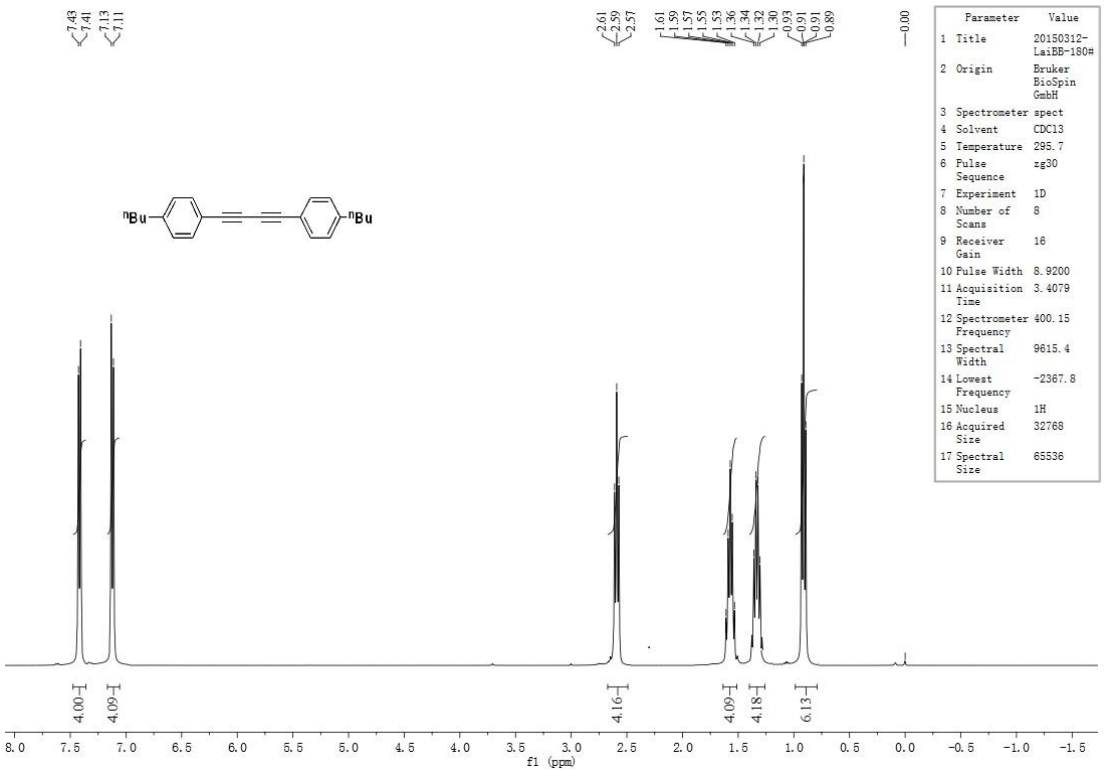
	Parameter	Value
1	Title	20150324-LaiBB-196#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

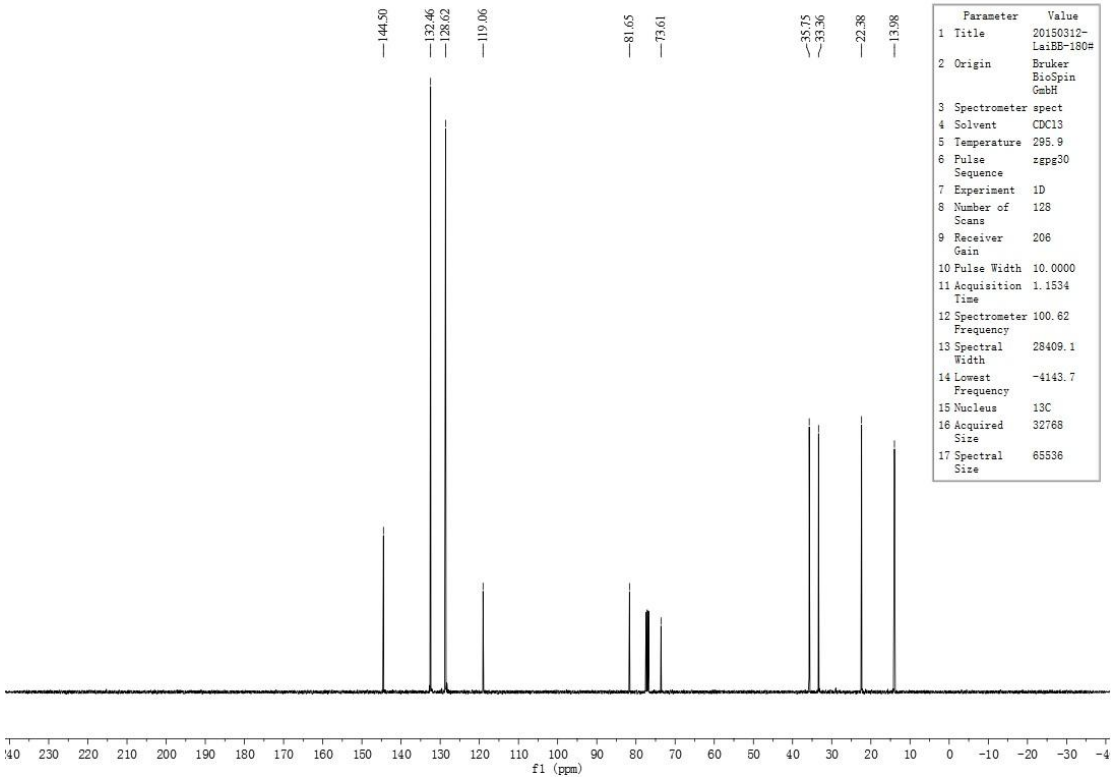


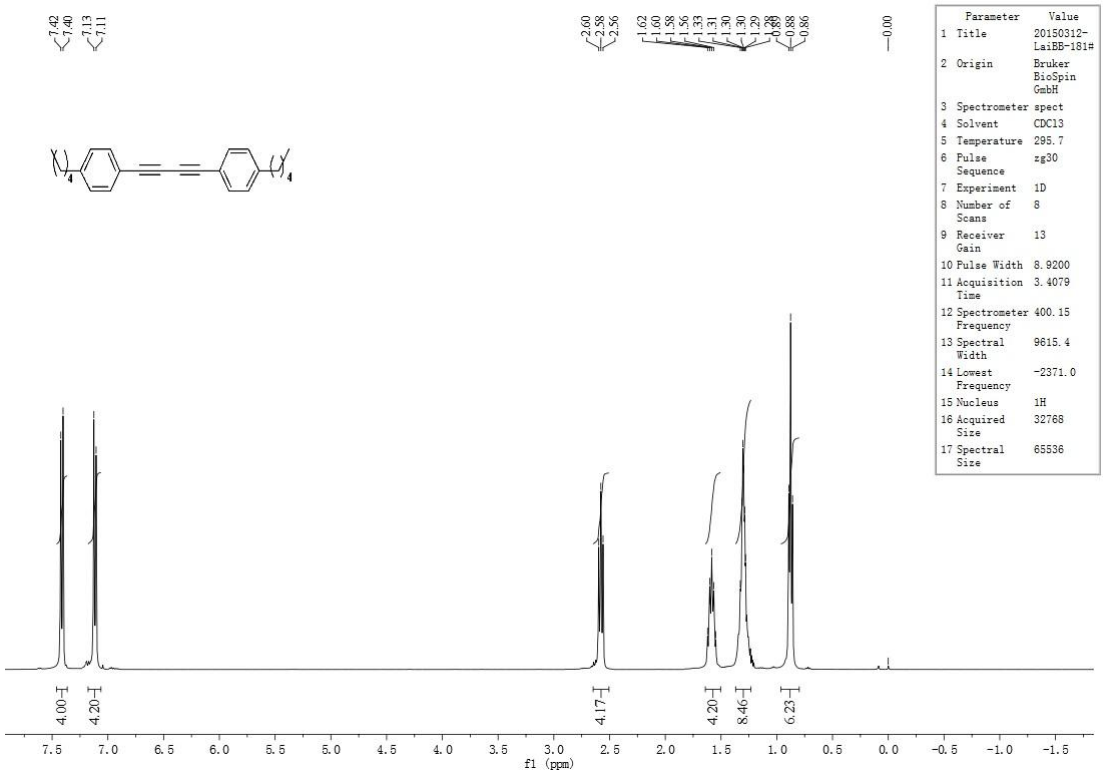
	Parameter	Value
1	Title	20150312-LaiBB-178#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.7
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	19
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2361.4
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

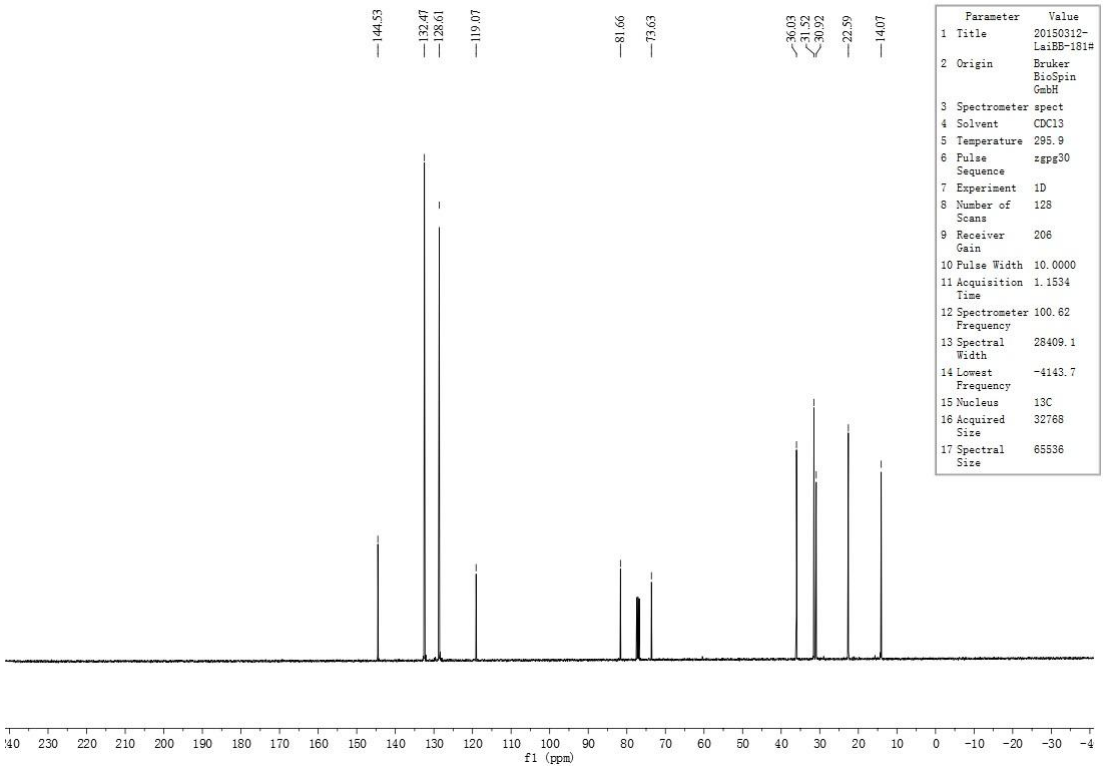


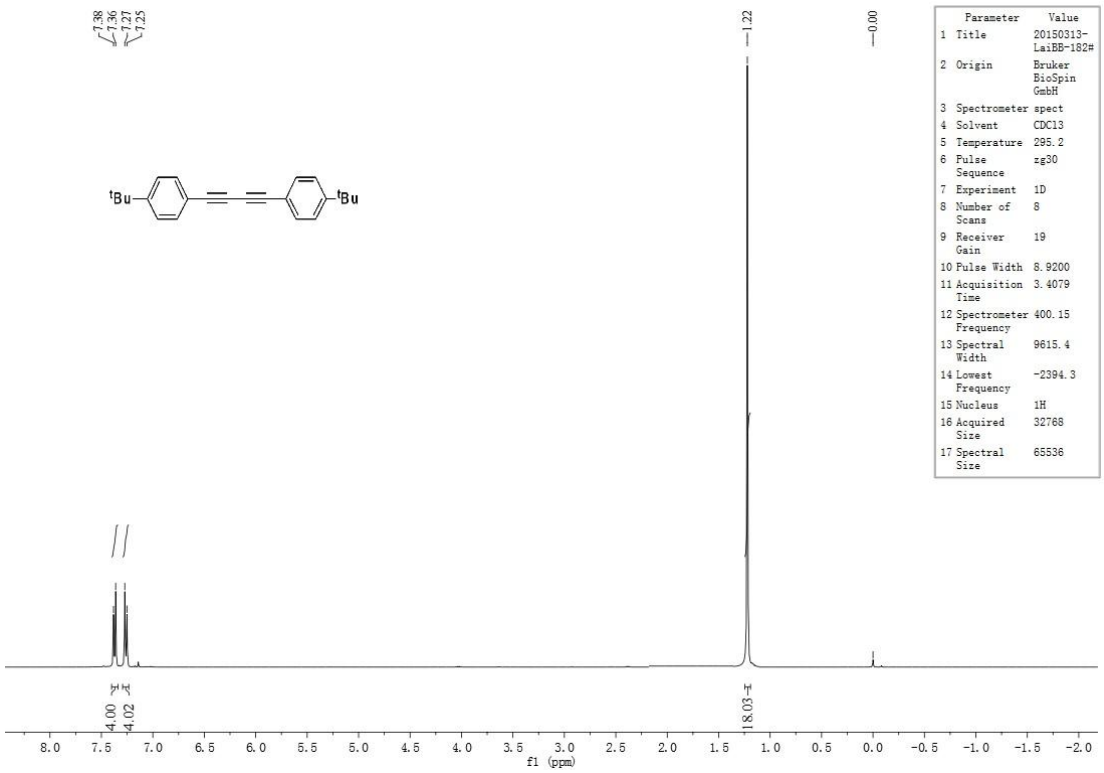
	Parameter	Value
1	Title	20150312-LaiBB-178#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.9
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536


7.43
7.41
7.13
7.11
2.61
2.59
2.57
1.61
1.59
1.57
1.55
1.53
1.36
1.34
1.32
1.30
0.93
0.91
0.91
0.89
0.00
nBu
nBu
4.00
4.09
4.16
4.09
4.18
6.13
f1 (ppm)
Parameter Value
1 Title 20150312-LaiBB-180#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.7
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 16
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2367.8
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

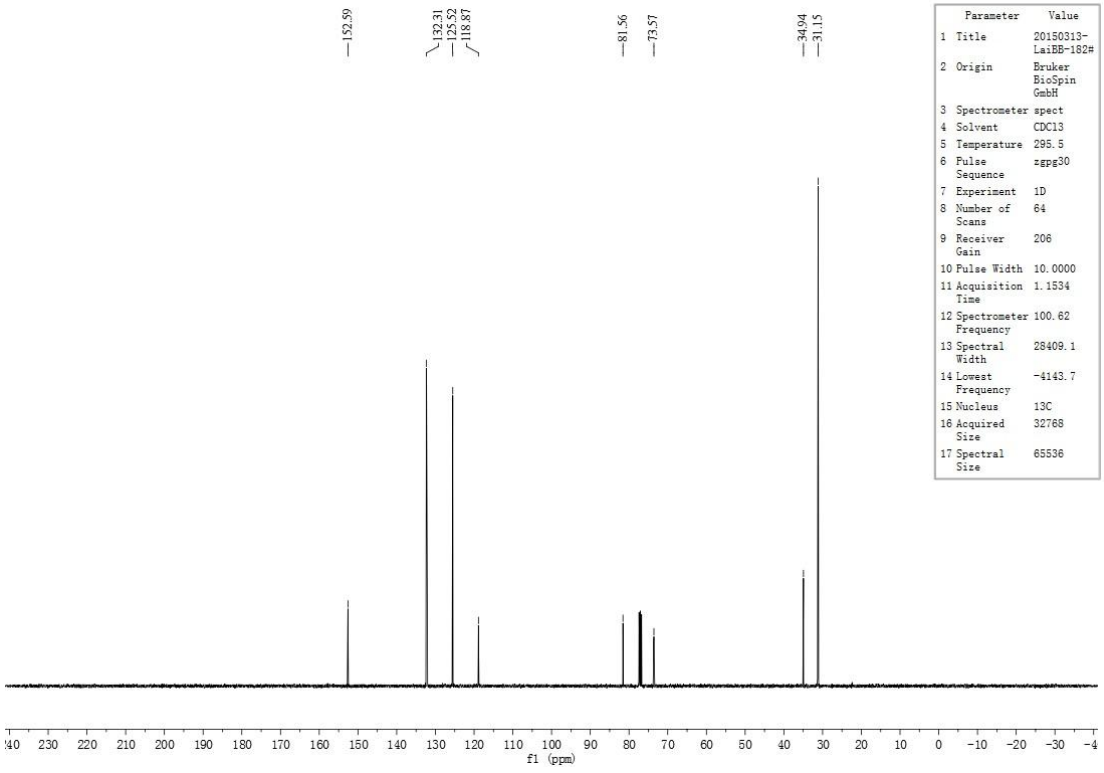

144.50
132.46
128.62
119.06
81.65
73.61
35.75
33.36
22.38
13.98
f1 (ppm)
Parameter Value
1 Title 20150312-LaiBB-180#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.9
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.42
7.40
7.13
7.11
2.60
2.58
2.56
1.62
1.60
1.58
1.56
1.33
1.31
1.30
1.30
1.29
0.88
0.86
0.00
4.00
4.20
4.17
4.20
8.46
6.23
f1 (ppm)
Parameter Value
1 Title 20150312-LaiBB-181#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.7
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 13
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2371.0
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

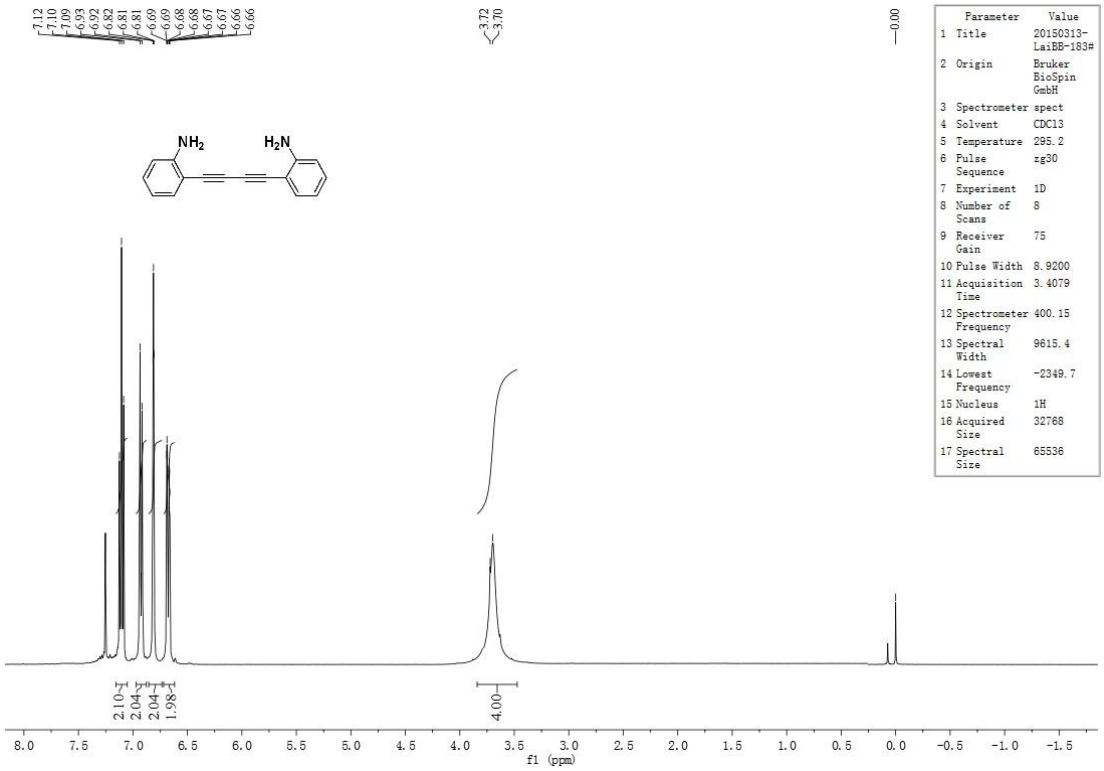

144.53
132.47
128.61
119.07
81.66
73.63
36.03
31.52
30.92
22.59
14.07
f1 (ppm)
Parameter Value
1 Title 20150312-LaiBB-181#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.9
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

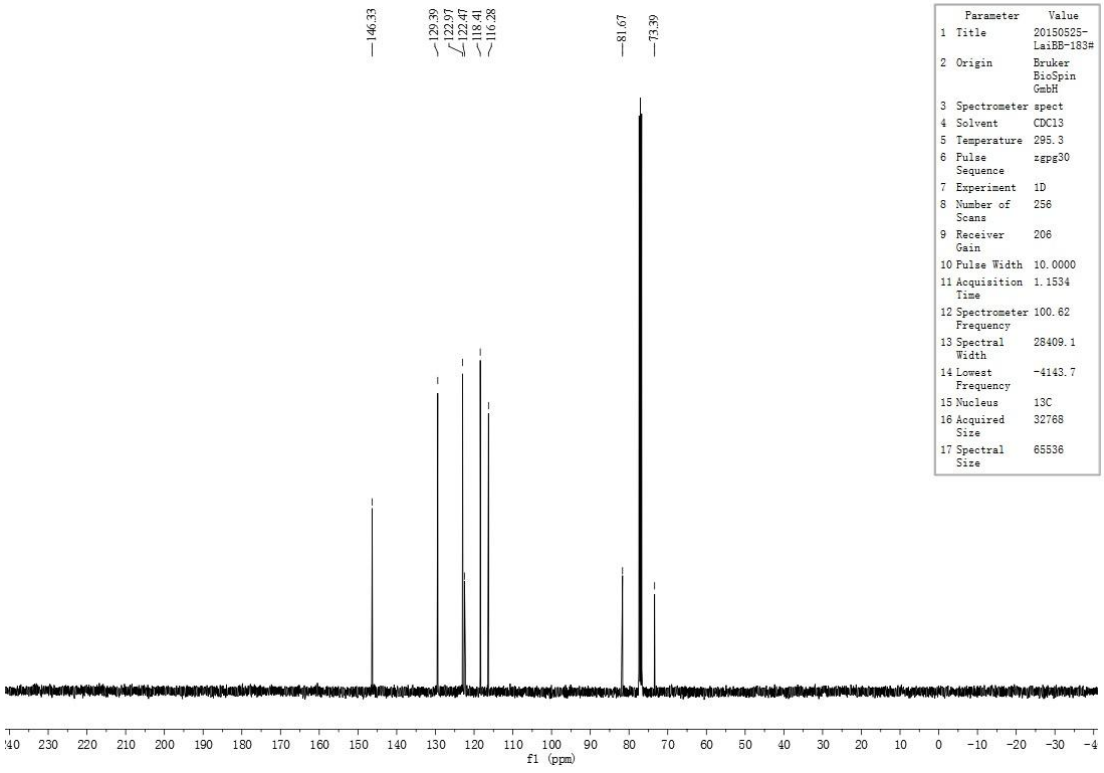


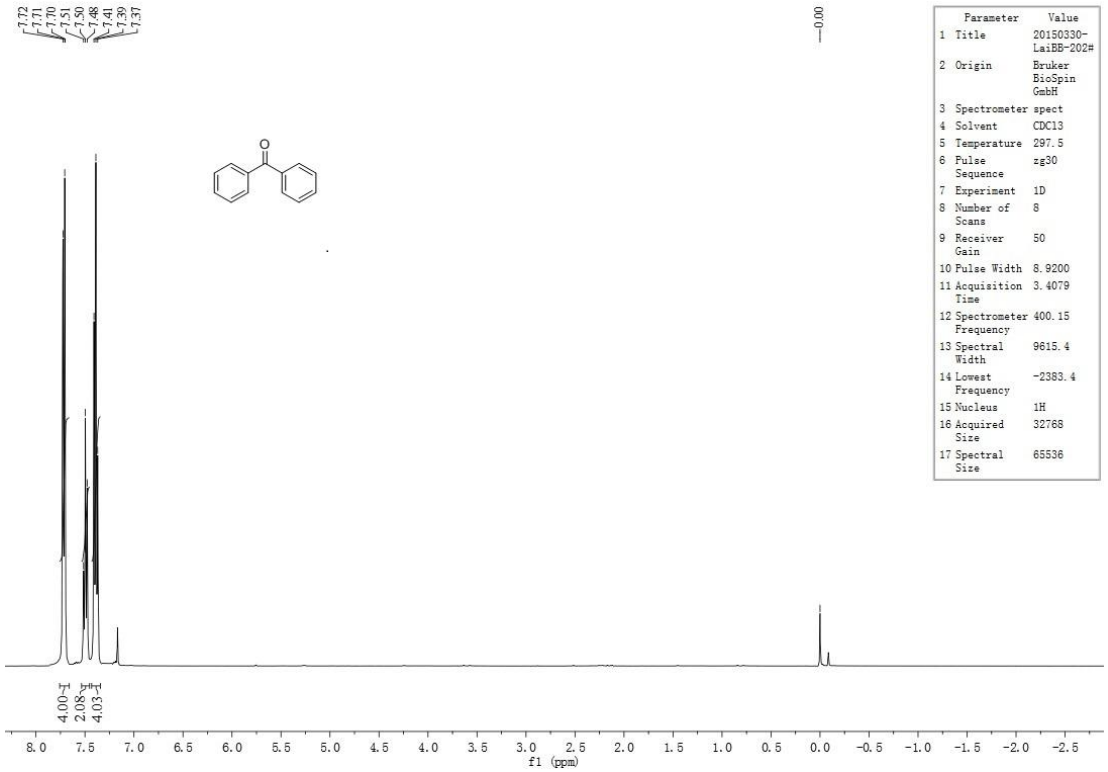
	Parameter	Value
1	Title	20150313-LaiBB-182#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	19
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2394.3
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



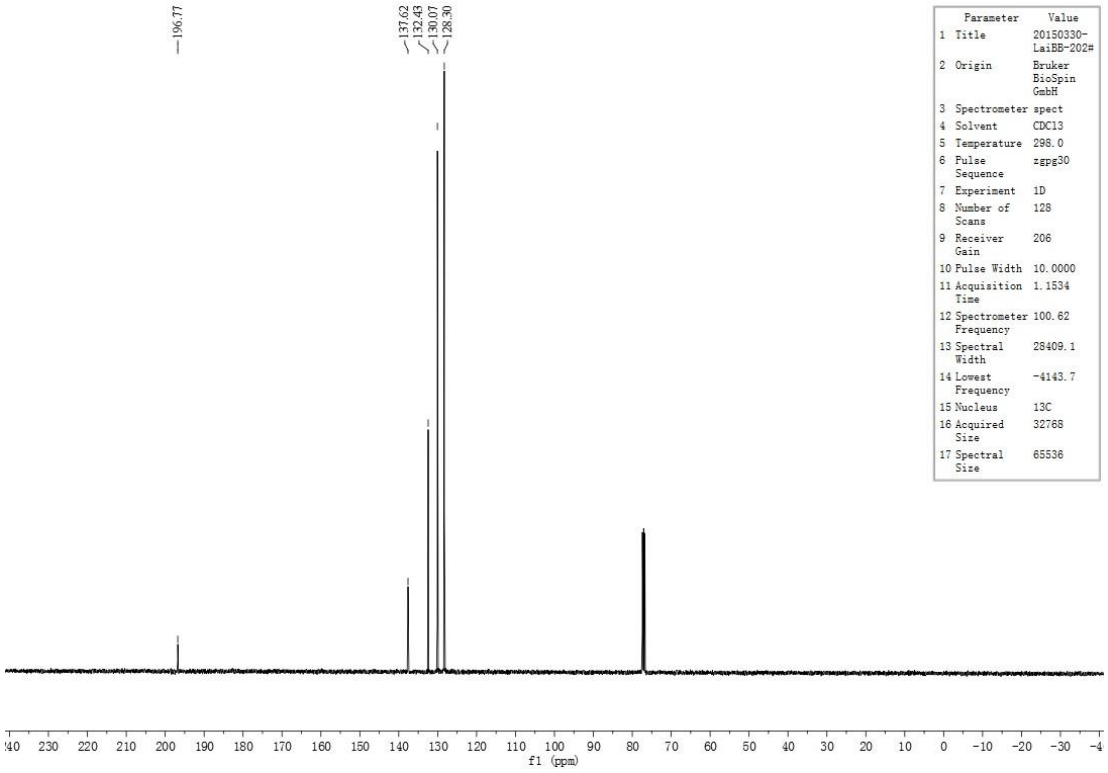
	Parameter	Value
1	Title	20150313-LaiBB-182#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.5
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	64
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536


7.12
7.10
7.09
6.93
6.92
6.82
6.81
6.81
6.69
6.69
6.68
6.68
6.67
6.67
6.66
6.66
3.72
3.70
0.00
NH2
H2N
2.10
2.04
2.04
1.98
4.00
f1 (ppm)
Parameter Value
1 Title 20150313-LaiBB-183#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2349.7
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

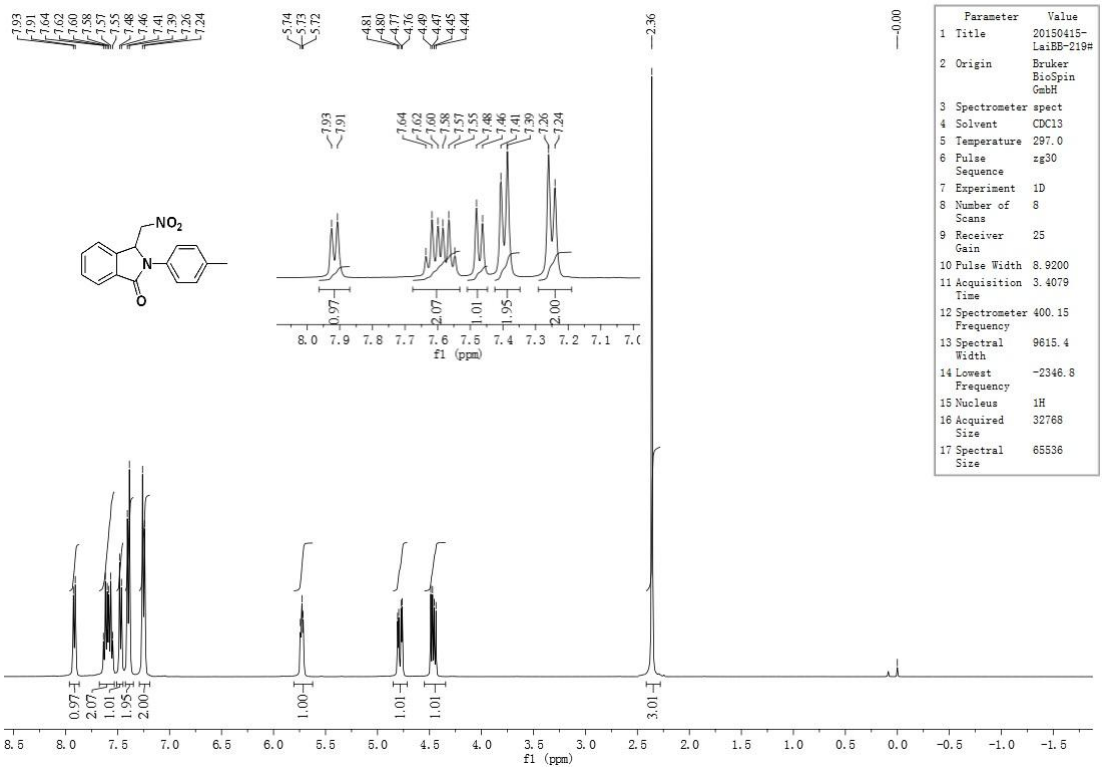

146.33
129.39
122.97
122.47
118.41
116.28
81.67
73.39
f1 (ppm)
Parameter Value
1 Title 20150525-LaiBB-183#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 256
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

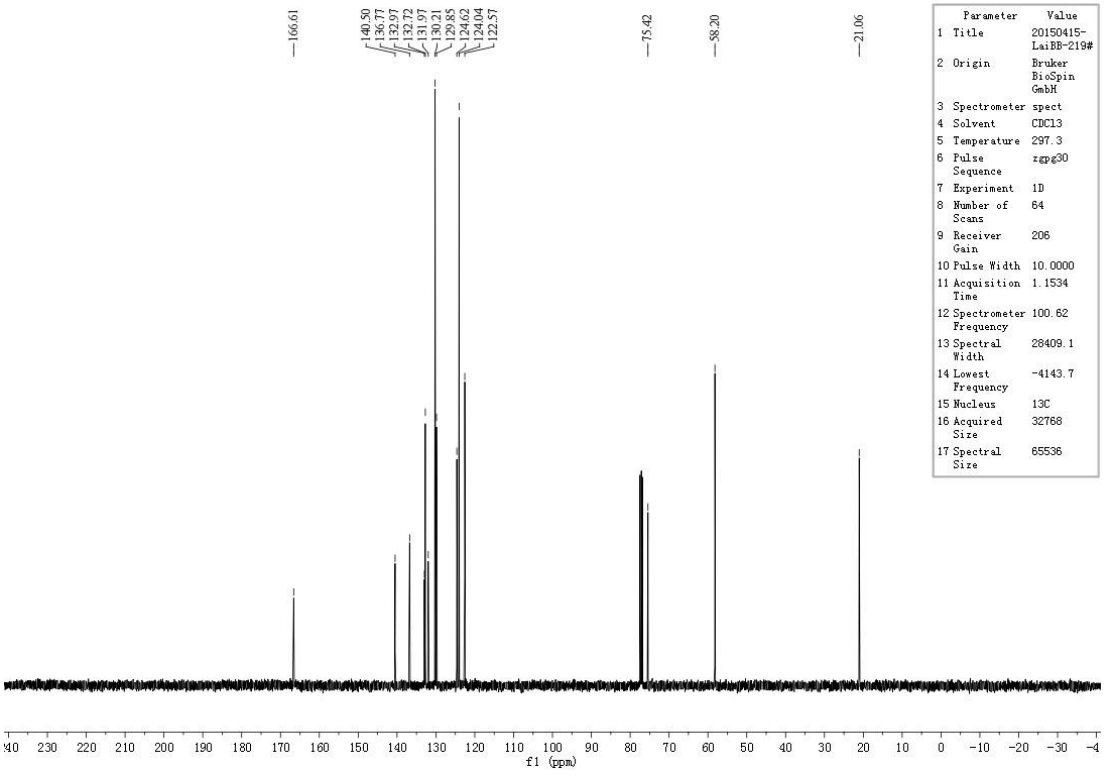


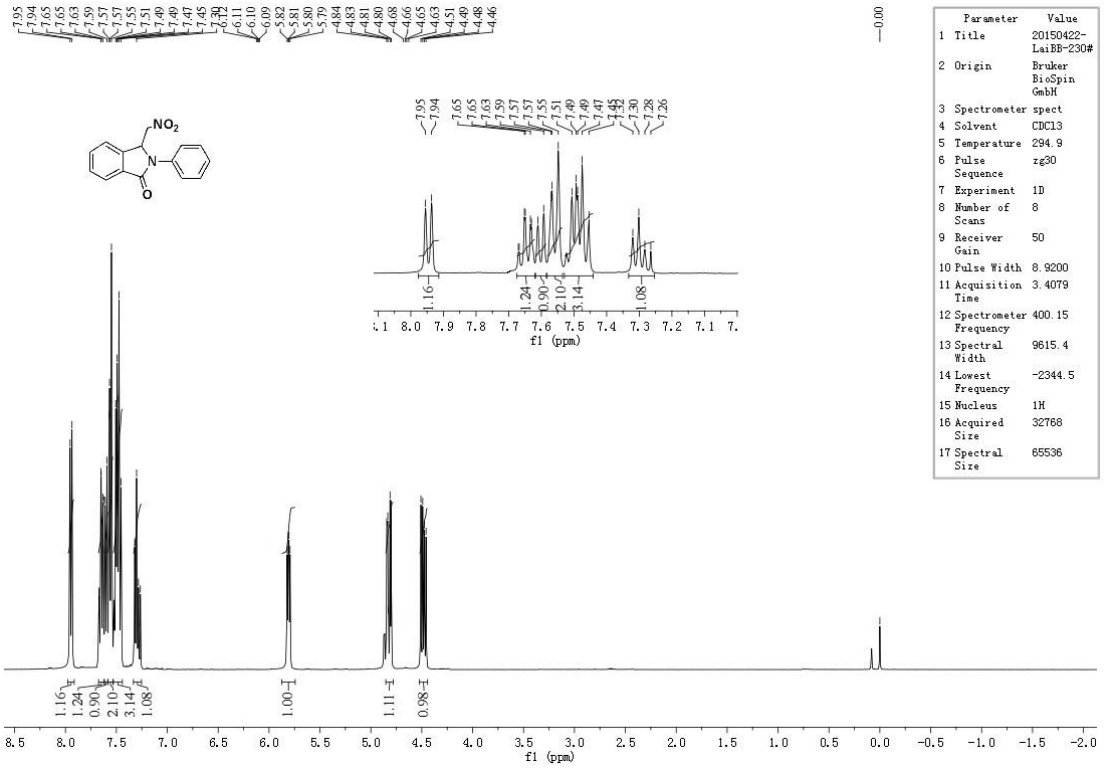
	Parameter	Value
1	Title	20150330-LaiBB-202#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	297.5
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	50
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2383.4
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



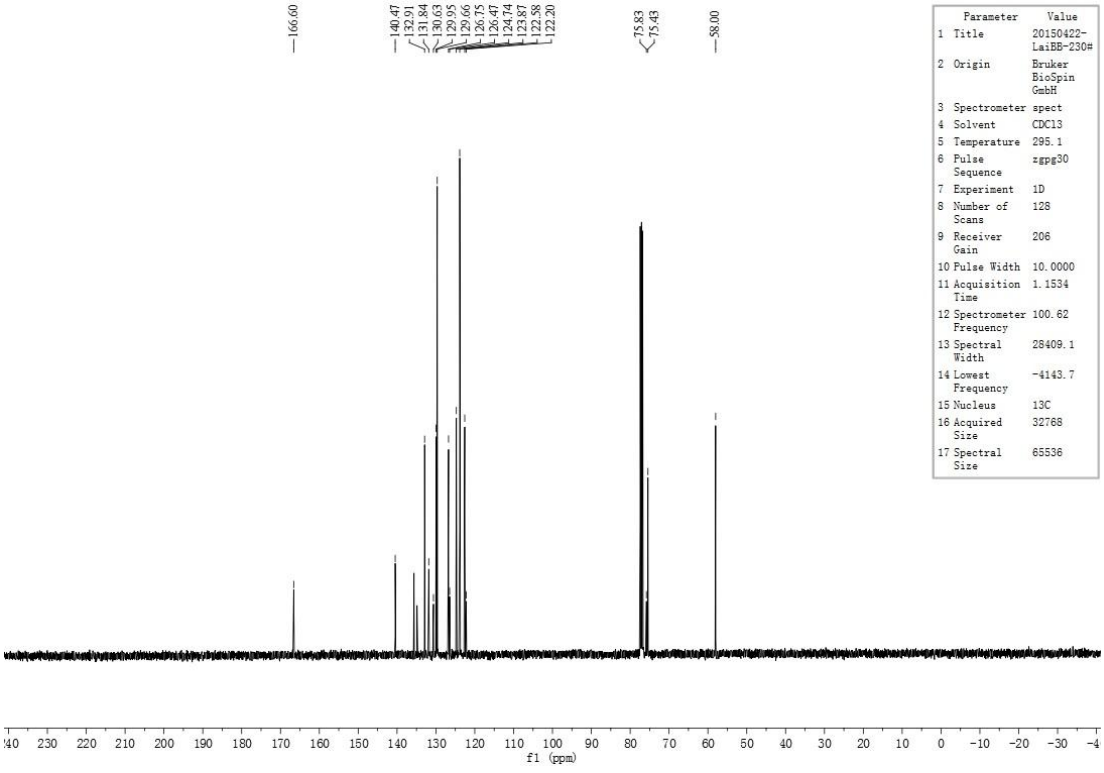
	Parameter	Value
1	Title	20150330-LaiBB-202#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	298.0
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536


7.93
7.91
7.64
7.62
7.60
7.58
7.57
7.55
7.48
7.46
7.41
7.39
7.26
7.24
5.74
5.73
5.72
4.81
4.80
4.77
4.76
4.49
4.47
4.45
4.44
2.36
0.00
NO2
N
O
0.97
2.07
1.01
1.95
2.00
1.00
1.01
1.01
3.01
f1 (ppm)
Parameter Value
1 Title 20150415-LaiBB-219#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 297.0
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 25
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2346.8
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

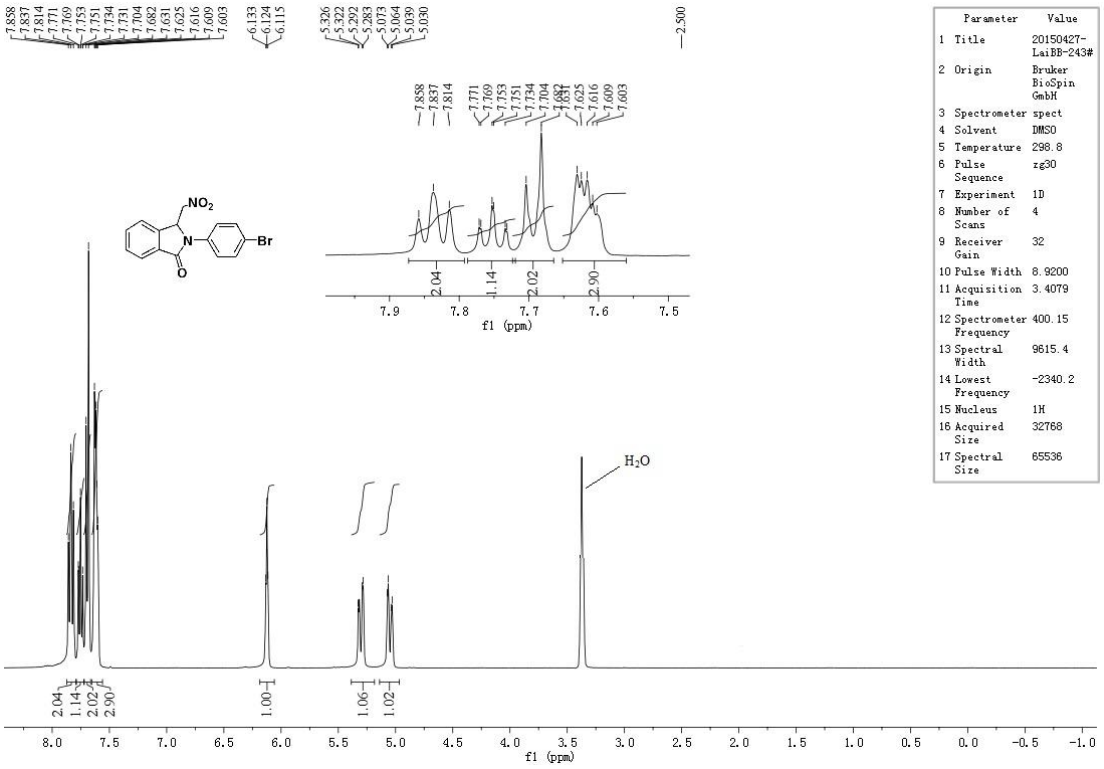

166.61
140.50
136.77
132.97
132.72
131.97
130.21
129.85
124.62
124.04
122.57
75.42
58.20
21.06
f1 (ppm)
Parameter Value
1 Title 20150415-LaiBB-219#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 297.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

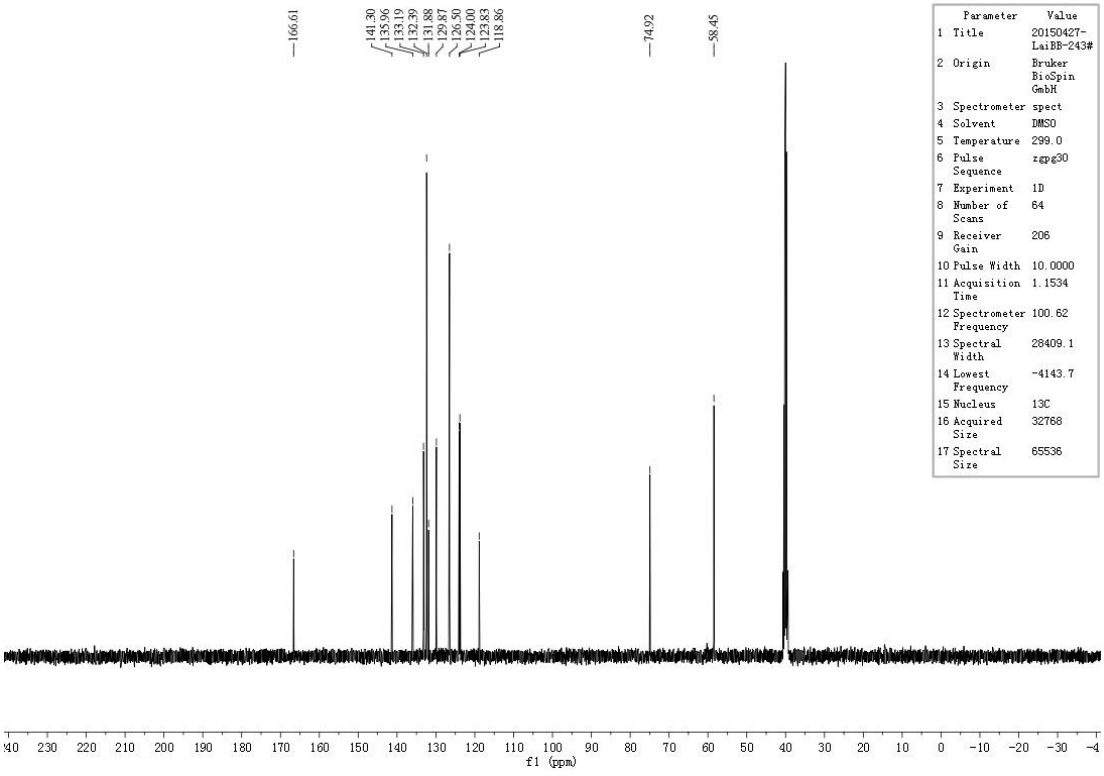


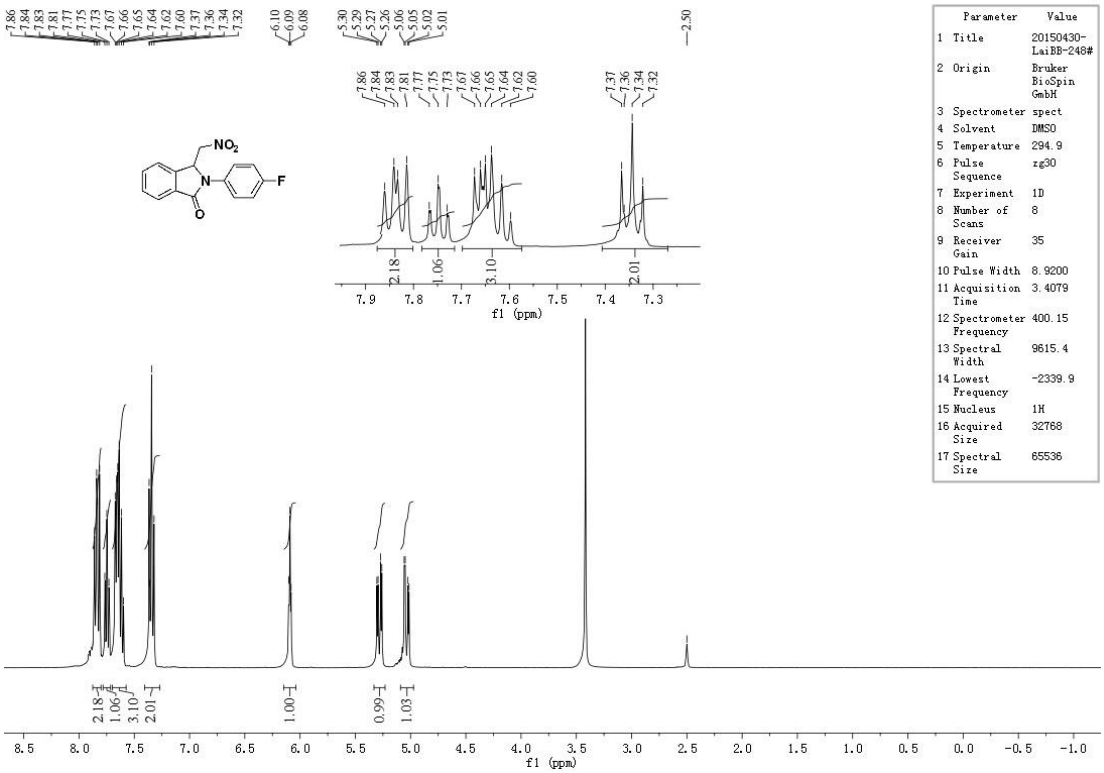
	Parameter	Value
1	Title	20150422-LaiBB-230#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	294.9
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	50
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2344.5
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



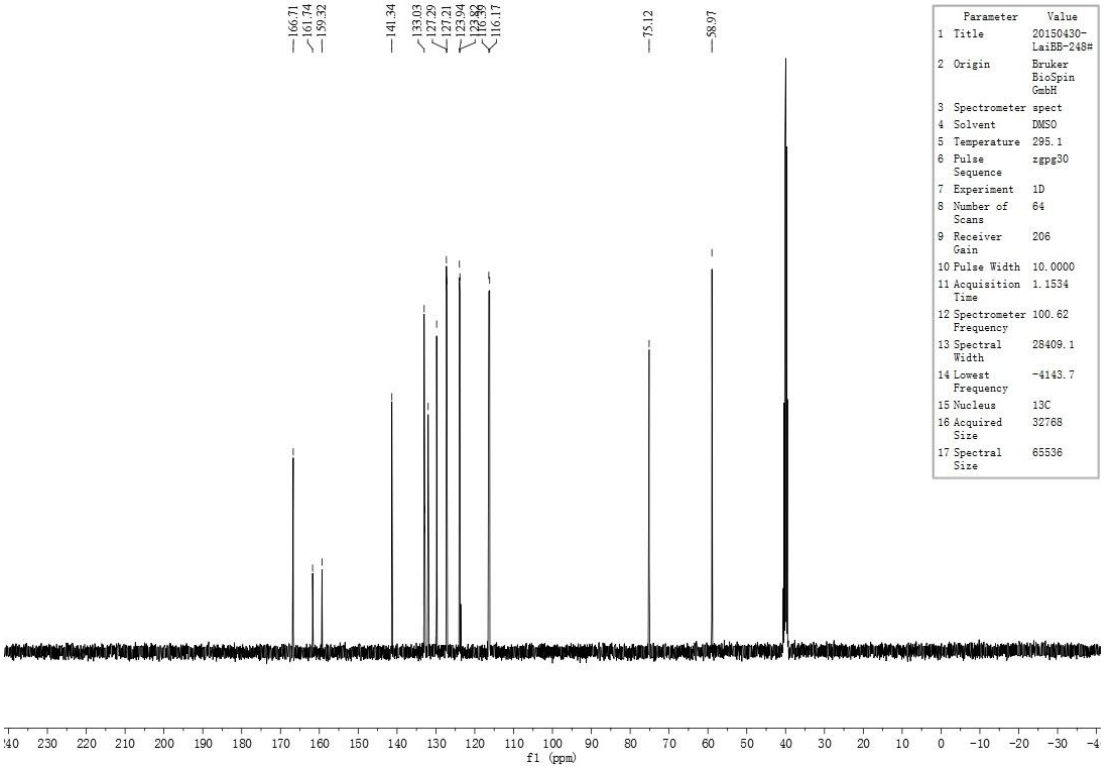
	Parameter	Value
1	Title	20150422-LaiBB-230#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536


7.858
7.837
7.814
7.771
7.769
7.753
7.751
7.734
7.731
7.704
7.682
7.631
7.625
7.616
7.609
7.603
6.133
6.124
6.115
5.326
5.322
5.292
5.283
5.073
5.064
5.039
5.030
2.500
NO2
N
Br
O
2.04
1.14
2.02
2.90
f1 (ppm)
H2O
1.00
1.06
1.02
Parameter Value
1 Title 20150427-LaiBB-243#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.8
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 32
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2340.2
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

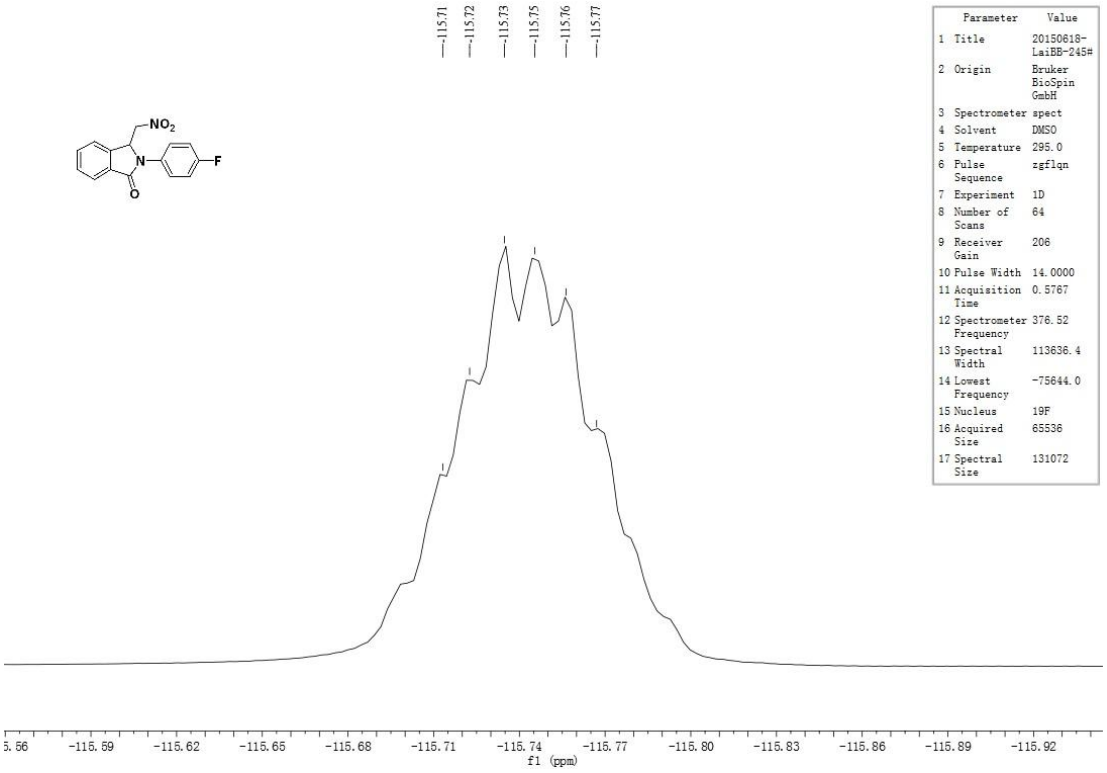

166.61
141.30
135.96
133.19
132.39
131.88
129.87
126.50
124.00
123.83
118.86
74.92
58.45
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-243#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.0
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

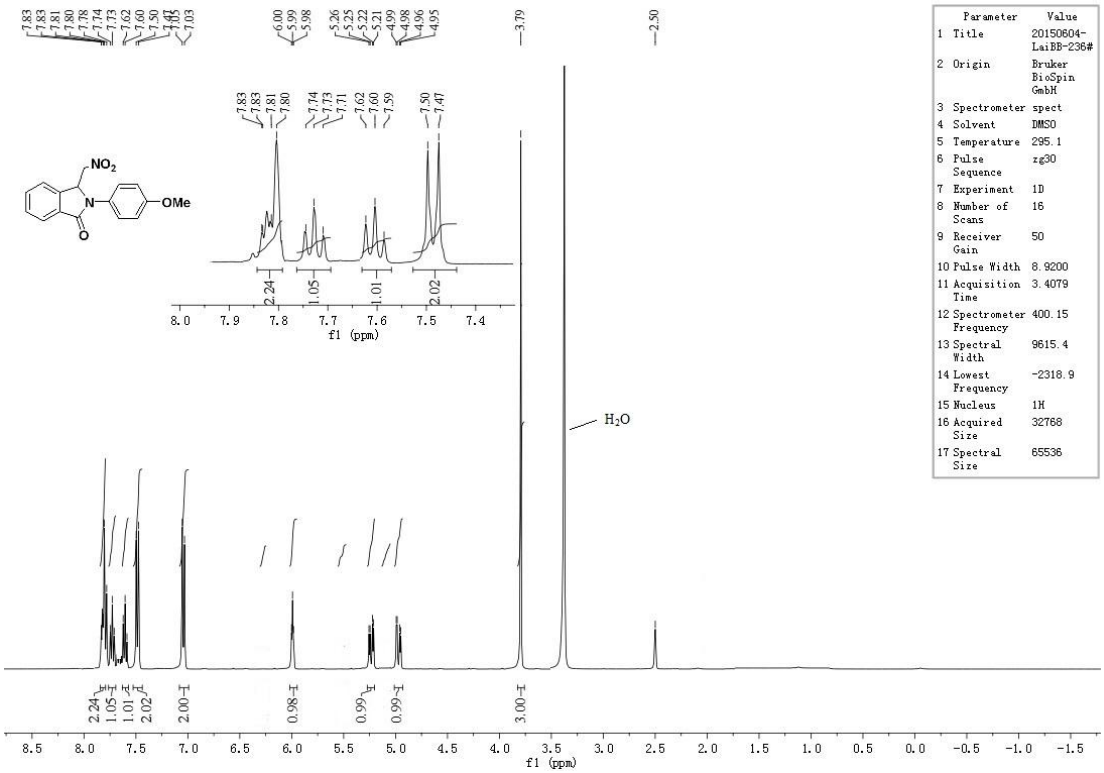


	Parameter	Value
1	Title	20150430-LaiBB-248#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	DMSO
5	Temperature	294.9
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	35
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2339.9
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

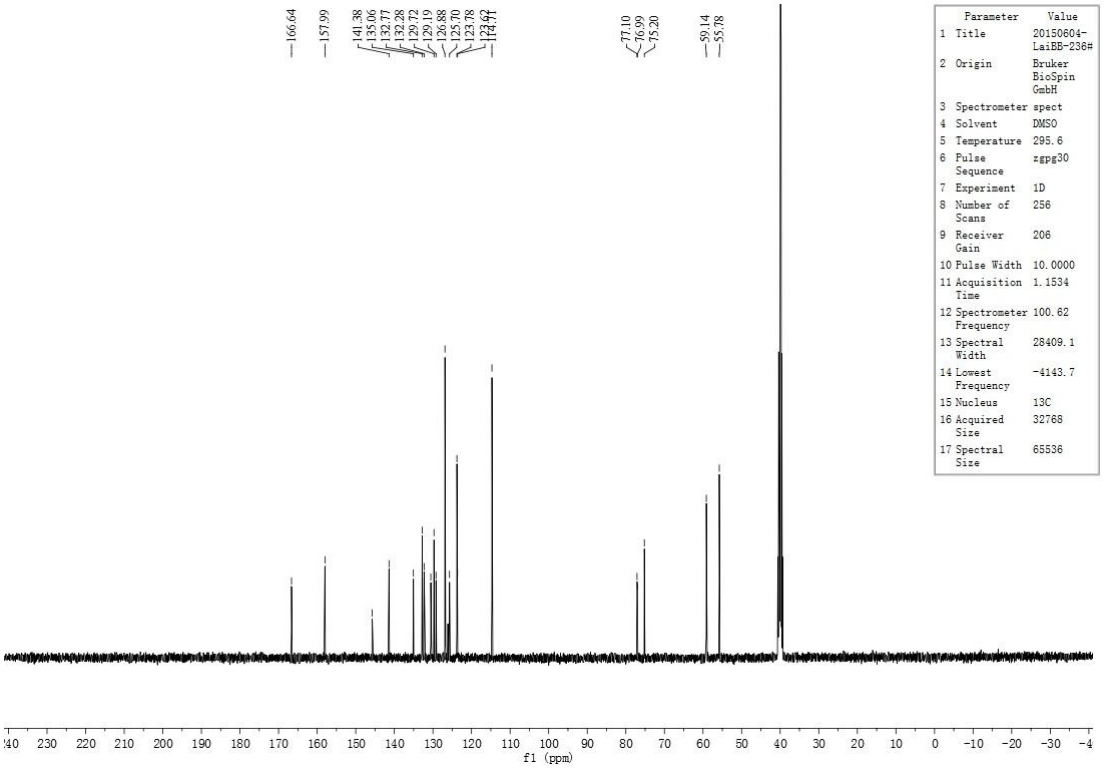


	Parameter	Value
1	Title	20150430-LaiBB-248#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	DMSO
5	Temperature	295.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	64
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

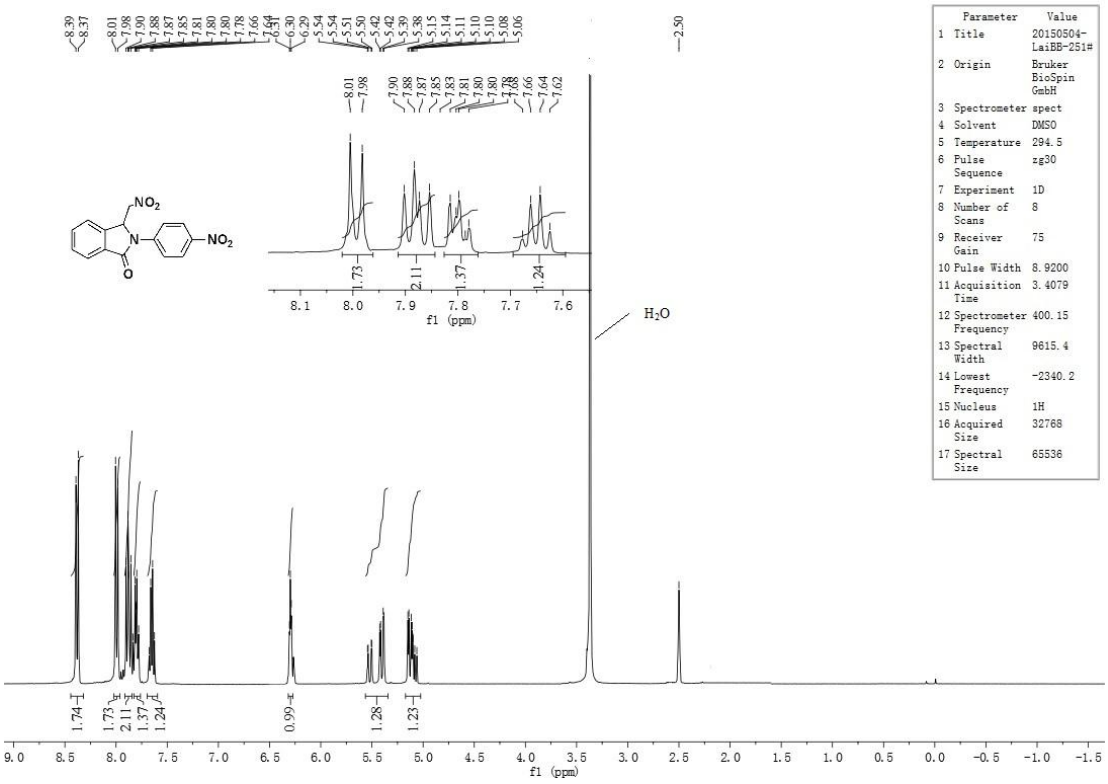

-115.71
-115.72
-115.73
-115.75
-115.76
-115.77
NO2
N
F
O
Parameter Value
1 Title 20150618-LaiBB-245#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 295.0
6 Pulse Sequence zgflqn
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 14.0000
11 Acquisition Time 0.5767
12 Spectrometer Frequency 376.52
13 Spectral Width 113636.4
14 Lowest Frequency -75644.0
15 Nucleus 19F
16 Acquired Size 65536
17 Spectral Size 131072
5.56 -115.59 -115.62 -115.65 -115.68 -115.71 -115.74 -115.77 -115.80 -115.83 -115.86 -115.89 -115.92
f1 (ppm)

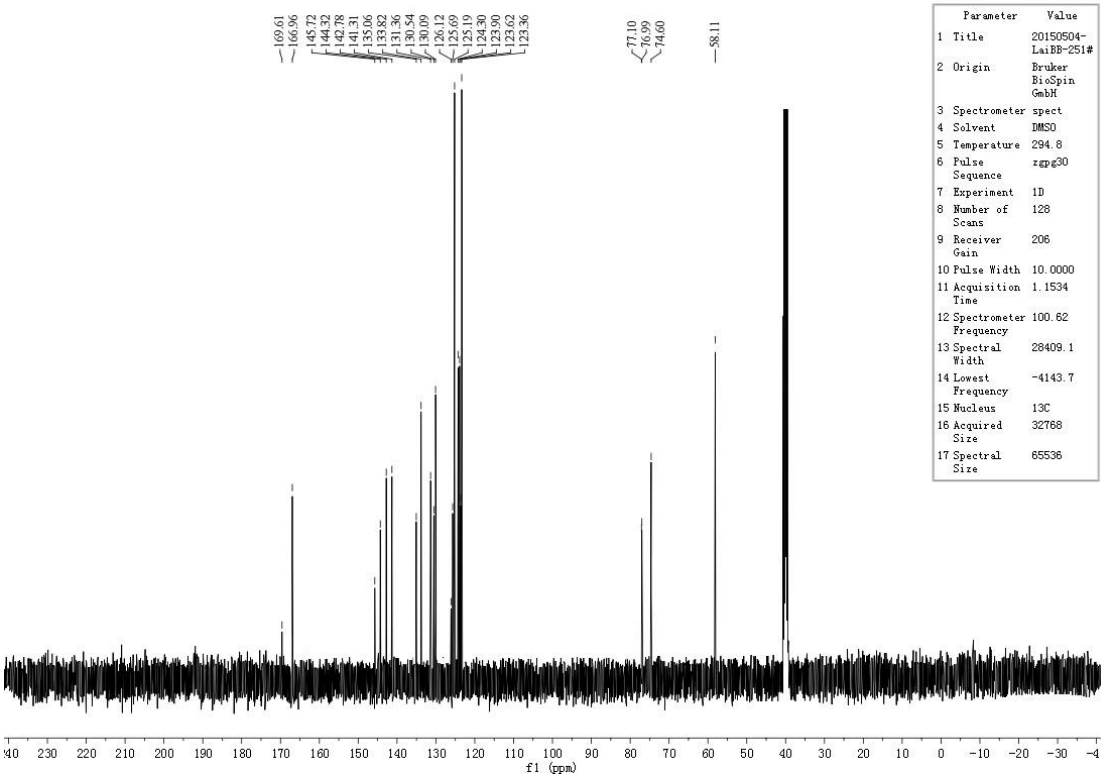


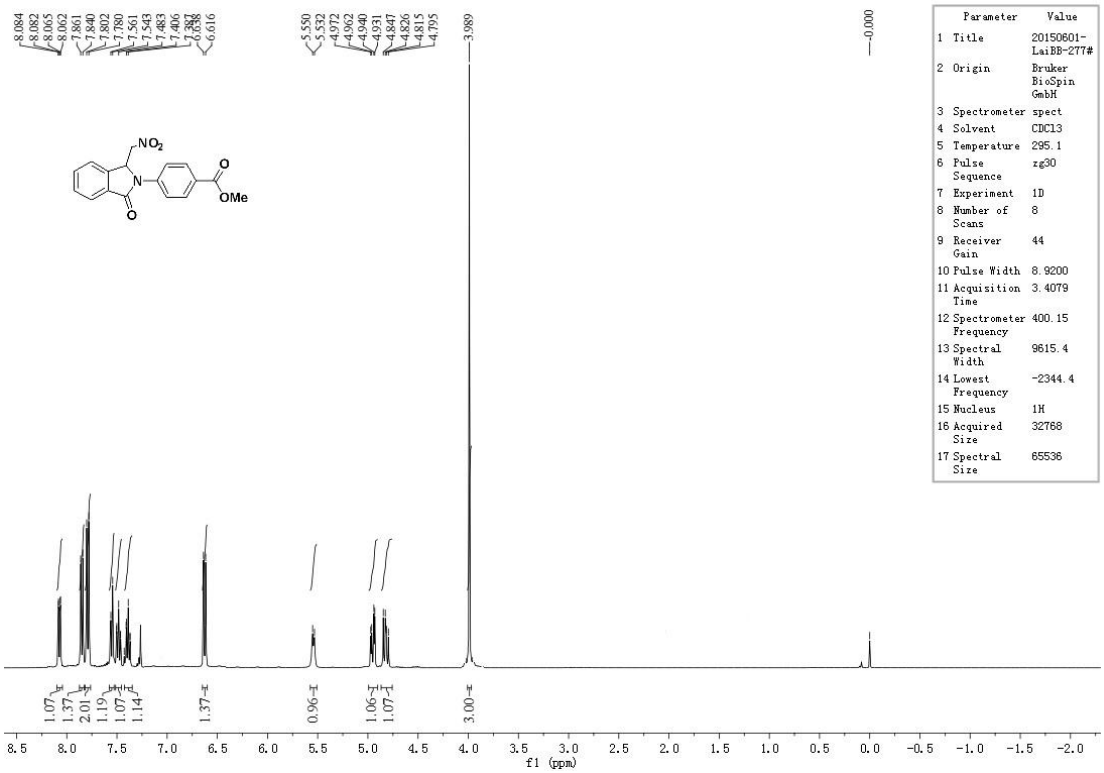
Parameter	Value
1 Title	20150604-LaiBB-236#
2 Origin	Bruker BioSpin GmbH
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	295.1
6 Pulse Sequence	zg30
7 Experiment	1D
8 Number of Scans	16
9 Receiver Gain	50
10 Pulse Width	8.9200
11 Acquisition Time	3.4079
12 Spectrometer Frequency	400.15
13 Spectral Width	9615.4
14 Lowest Frequency	-2318.9
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



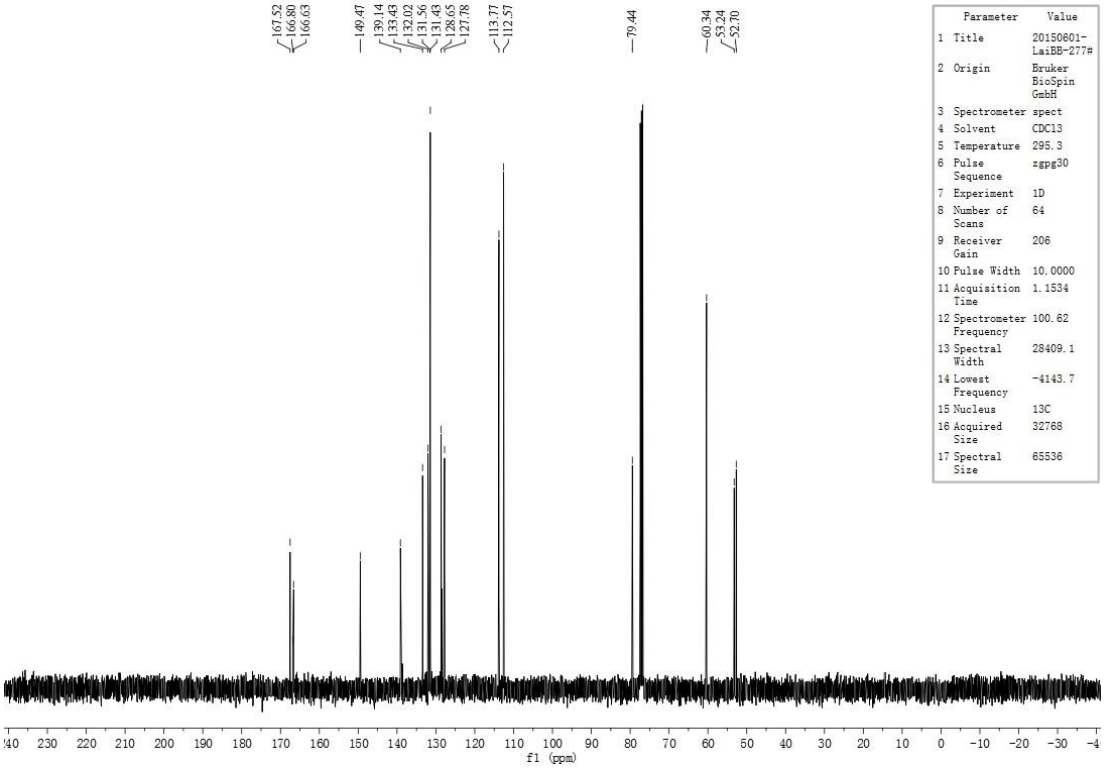
Parameter	Value
1 Title	20150604-LaiBB-236#
2 Origin	Bruker BioSpin GmbH
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	295.6
6 Pulse Sequence	zgpg30
7 Experiment	1D
8 Number of Scans	256
9 Receiver Gain	206
10 Pulse Width	10.0000
11 Acquisition Time	1.1534
12 Spectrometer Frequency	100.62
13 Spectral Width	28409.1
14 Lowest Frequency	-4143.7
15 Nucleus	13C
16 Acquired Size	32768
17 Spectral Size	65536


8.39
8.37
8.01
7.98
7.90
7.88
7.87
7.85
7.81
7.80
7.80
7.78
7.66
7.64
6.30
6.29
5.54
5.54
5.51
5.50
5.42
5.42
5.39
5.38
5.15
5.14
5.11
5.10
5.10
5.08
5.06
2.50
NO2
NO2
O
1.73
2.11
1.37
1.24
8.1
8.0
7.9
7.8
7.7
7.6
f1 (ppm)
H2O
1.74
1.73
2.11
1.37
1.24
0.99
1.28
1.23
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
-0.5
-1.0
-1.5
f1 (ppm)
Parameter Value
1 Title 20150504-LaiBB-251#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 294.5
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2340.2
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

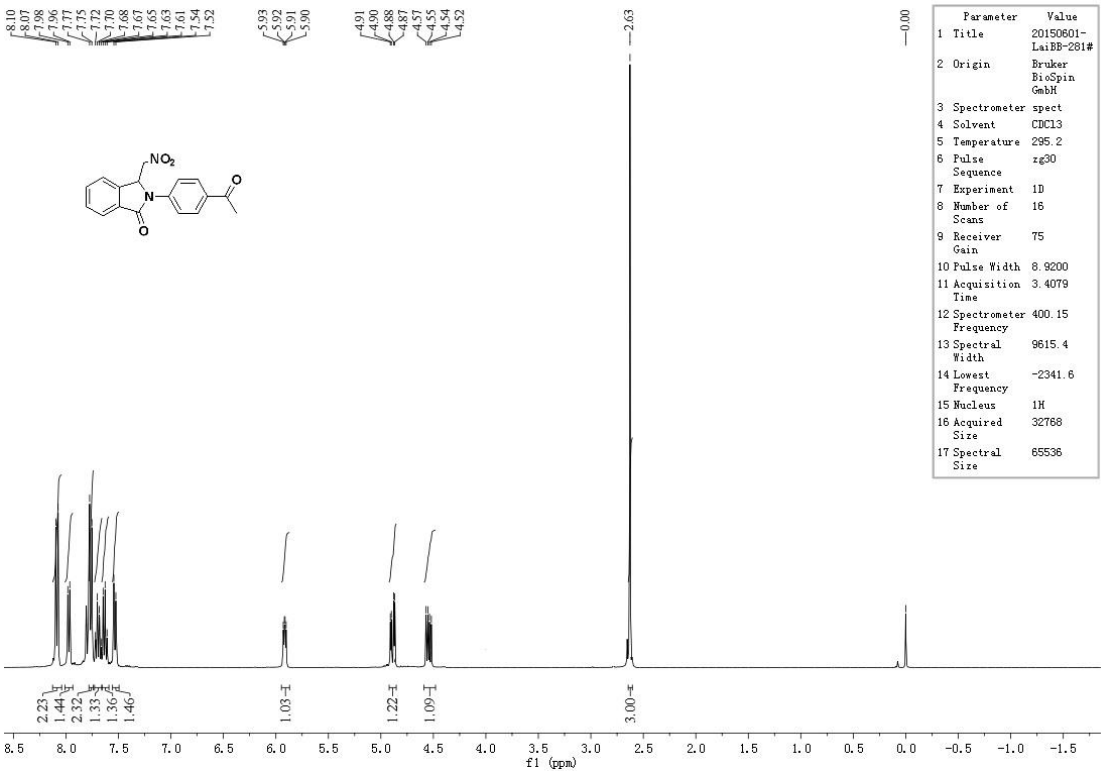

169.61
166.96
145.72
144.32
142.78
141.31
135.06
133.82
131.36
130.54
130.09
126.12
125.69
125.19
124.30
123.90
123.62
123.36
77.10
76.99
74.60
58.11
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-4
f1 (ppm)
Parameter Value
1 Title 20150504-LaiBB-251#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 294.8
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

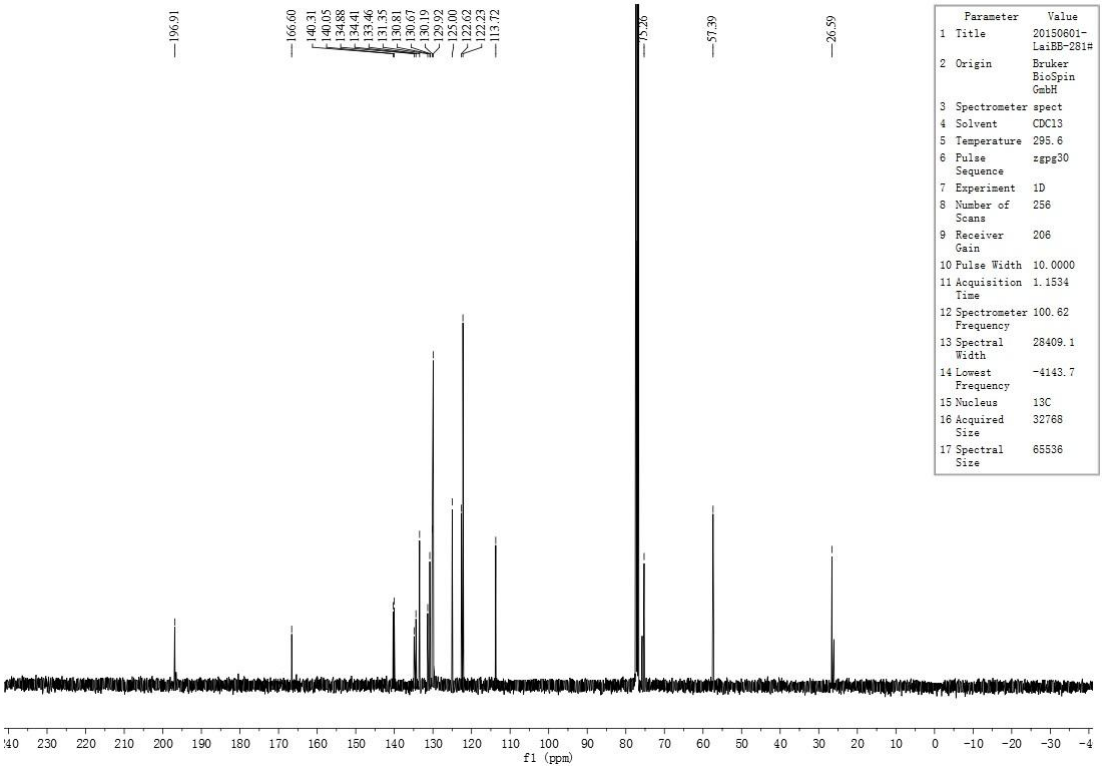


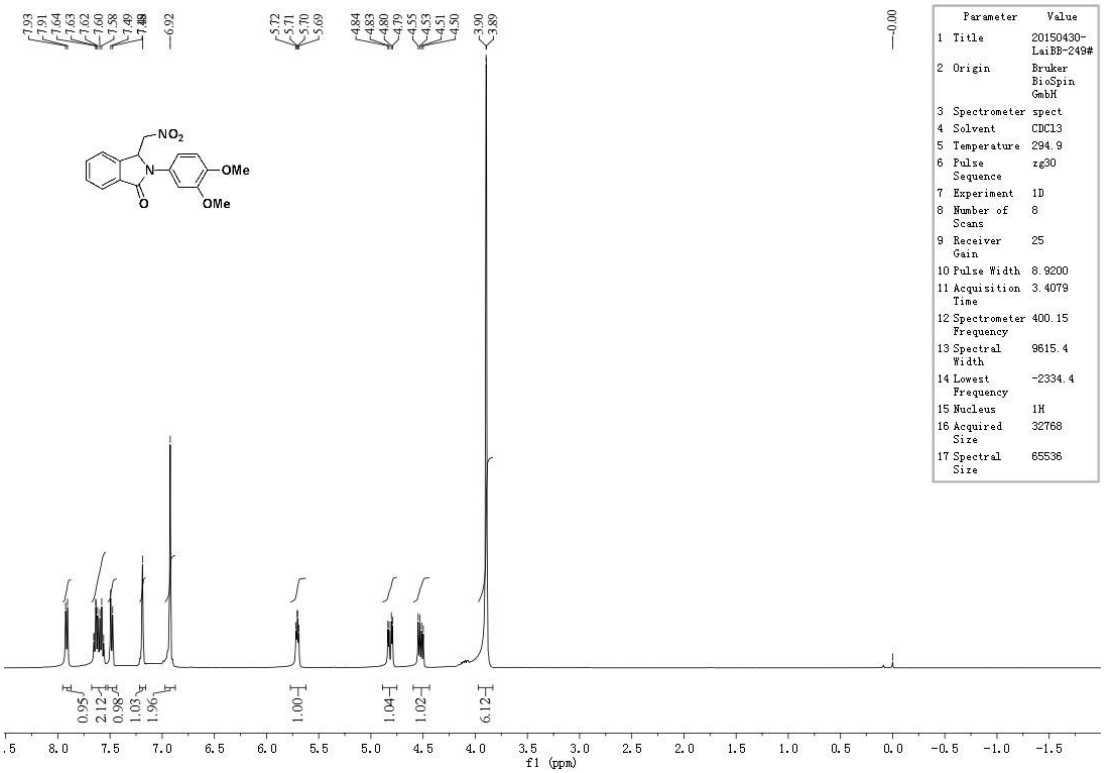
	Parameter	Value
1	Title	20150601-LaiBB-277#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	44
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2344.4
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

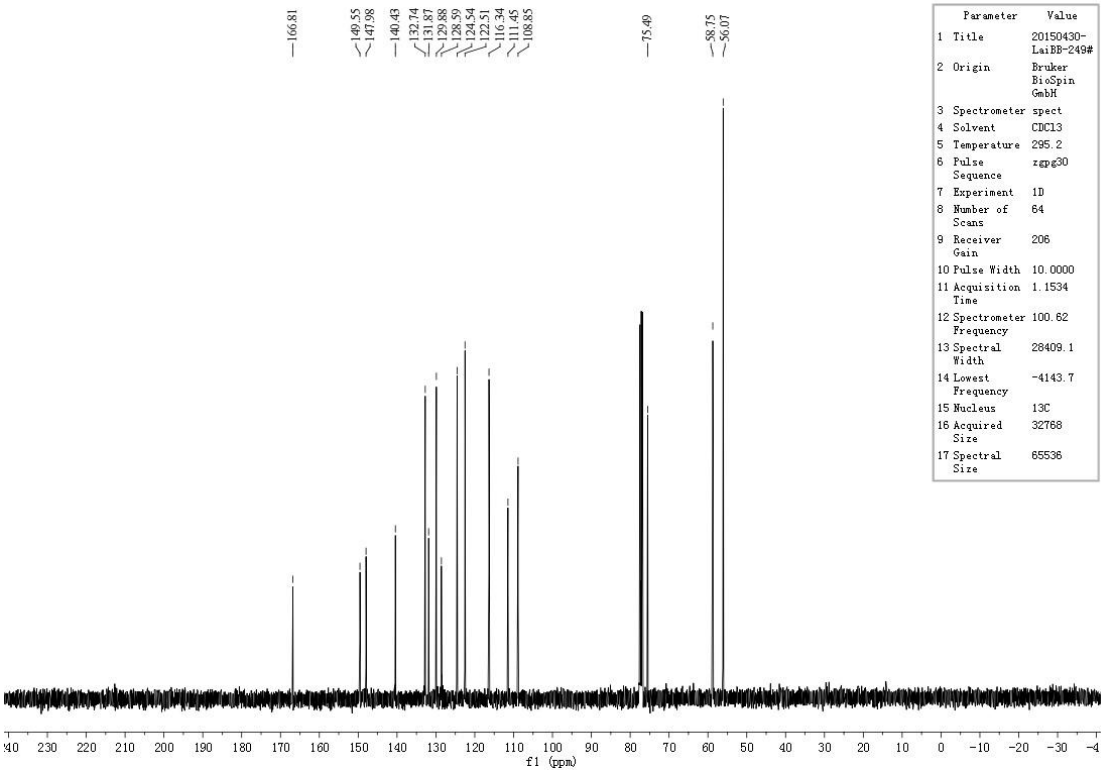


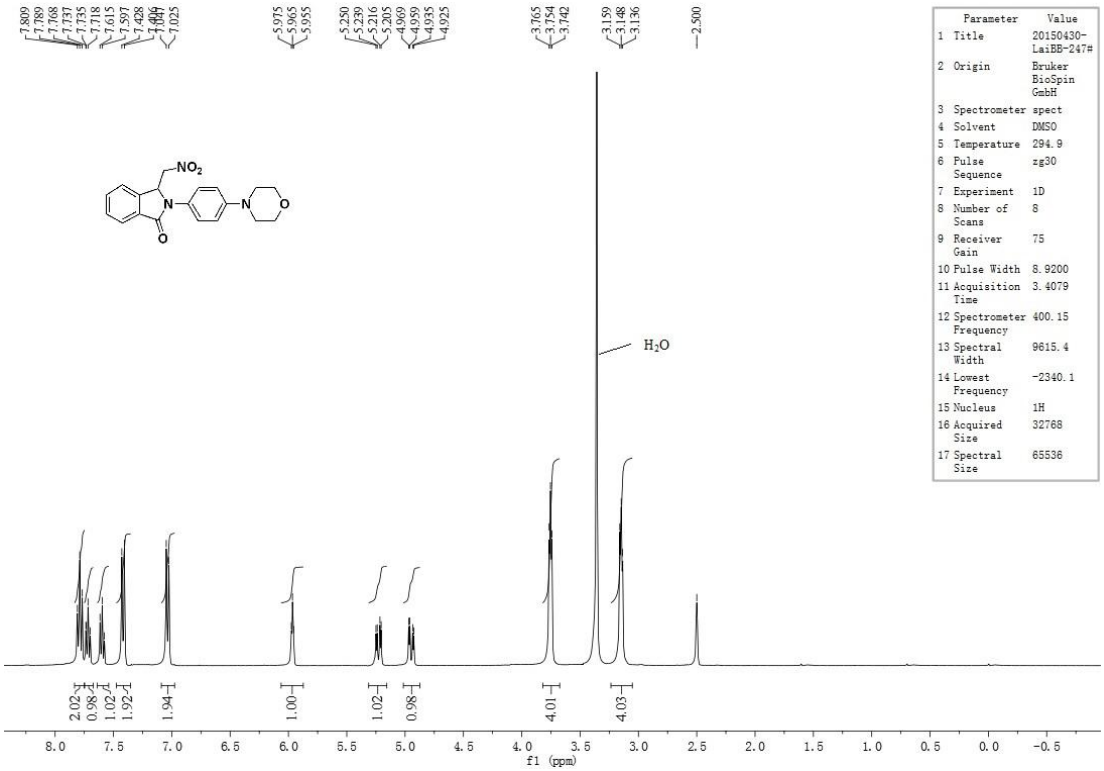
	Parameter	Value
1	Title	20150601-LaiBB-277#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.3
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	64
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

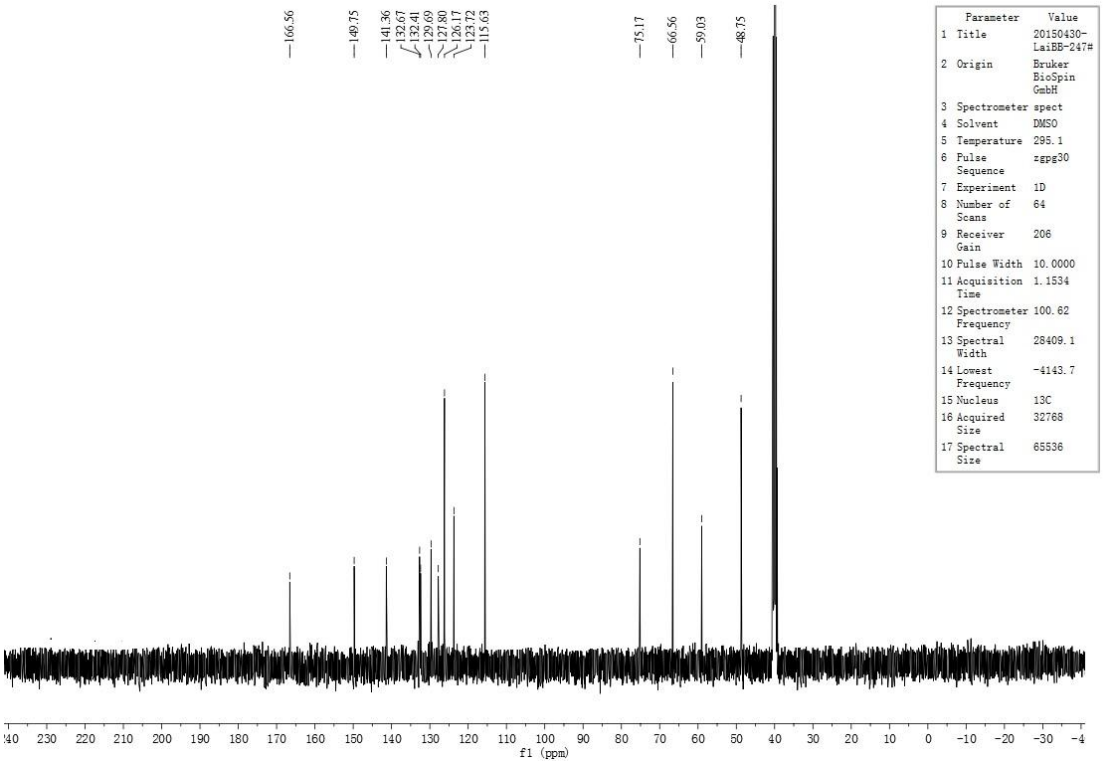

8.10
8.07
7.98
7.96
7.77
7.75
7.72
7.70
7.68
7.67
7.65
7.63
7.61
7.54
7.52
5.93
5.92
5.91
5.90
4.91
4.90
4.88
4.87
4.57
4.55
4.54
4.52
2.63
0.00
NO2
N
O
O
Parameter Value
1 Title 20150601-LaiBB-281#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 16
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2341.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
2.23
1.44
2.32
1.33
1.36
1.46
1.03
1.22
1.09
3.00
f1 (ppm)

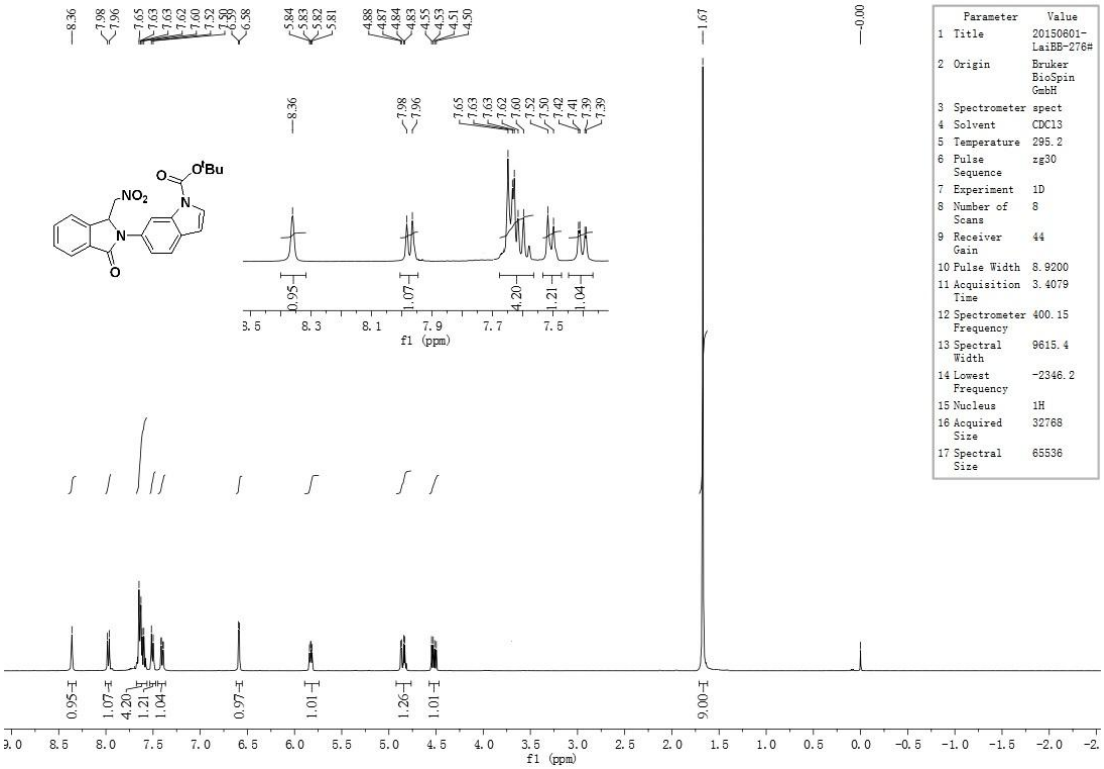

196.91
166.60
140.31
140.05
134.88
134.41
133.46
131.35
130.81
130.67
130.19
129.92
125.00
122.62
122.23
113.72
75.26
57.39
26.59
Parameter Value
1 Title 20150601-LaiBB-281#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.6
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 256
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)


7.93
7.91
7.64
7.63
7.62
7.60
7.58
7.49
7.48
6.92
5.72
5.71
5.70
5.69
4.84
4.83
4.80
4.79
4.55
4.53
4.51
4.50
3.90
3.89
0.00
NO2
OMe
OMe
O
N
0.95
2.12
0.98
1.03
1.96
1.00
1.04
1.02
6.12
f1 (ppm)
Parameter Value
1 Title 20150430-LaiBB-249#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 25
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2334.4
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

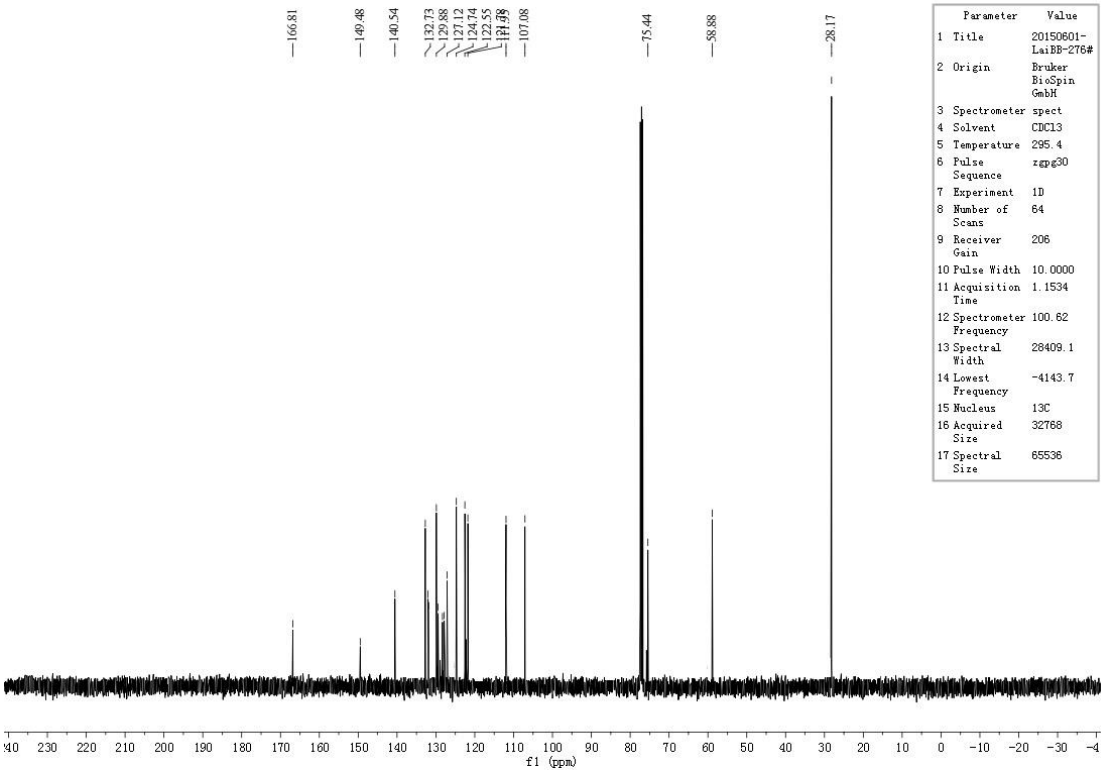

166.81
149.55
147.98
140.43
132.74
131.87
129.88
128.59
124.54
122.51
116.34
111.45
108.85
75.49
58.75
56.07
f1 (ppm)
Parameter Value
1 Title 20150430-LaiBB-249#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.809
7.789
7.768
7.737
7.735
7.718
7.615
7.597
7.428
7.406
7.047
7.025
5.975
5.965
5.955
5.250
5.239
5.216
5.205
4.969
4.959
4.935
4.925
3.765
3.754
3.742
3.159
3.148
3.136
2.500
NO2
N
N
O
O
H2O
2.02
0.98
1.02
1.92
1.94
1.00
1.02
0.98
4.01
4.03
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 -0.5
f1 (ppm)
Parameter Value
1 Title 20150430-LaiBB-247#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 294.9
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2340.1
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

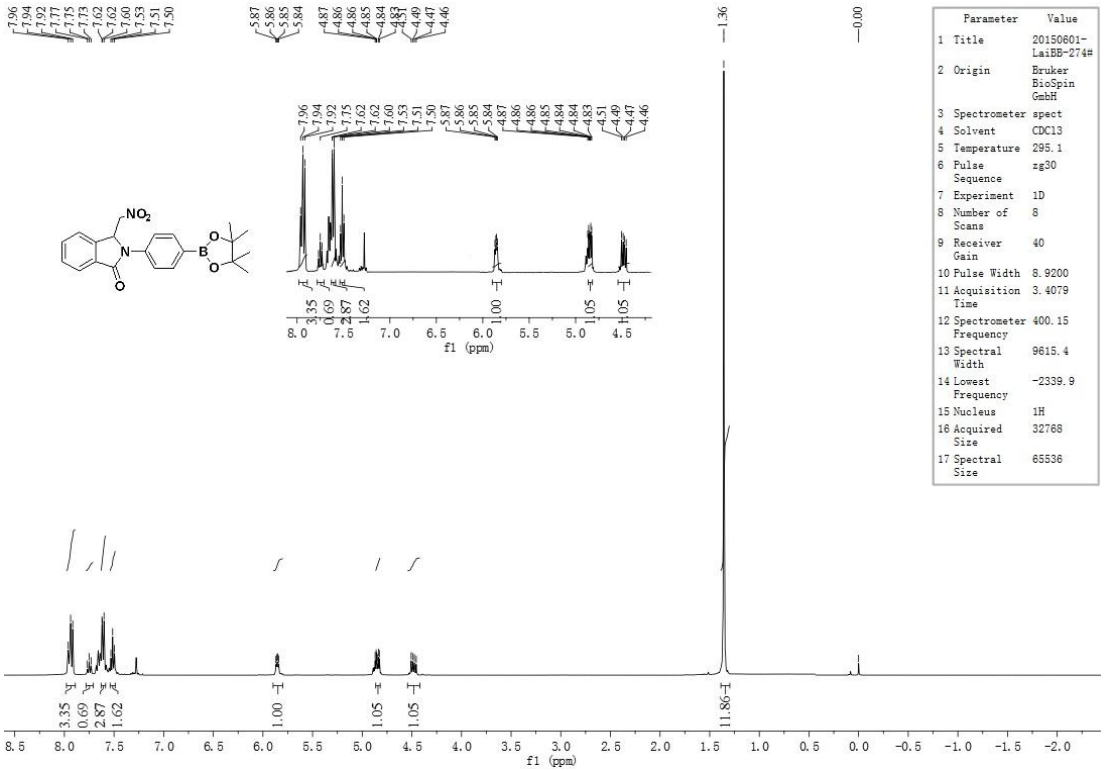

166.56
149.75
141.36
132.67
132.41
129.69
127.80
126.17
123.72
115.63
75.17
66.56
59.03
48.75
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)
Parameter Value
1 Title 20150430-LaiBB-247#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

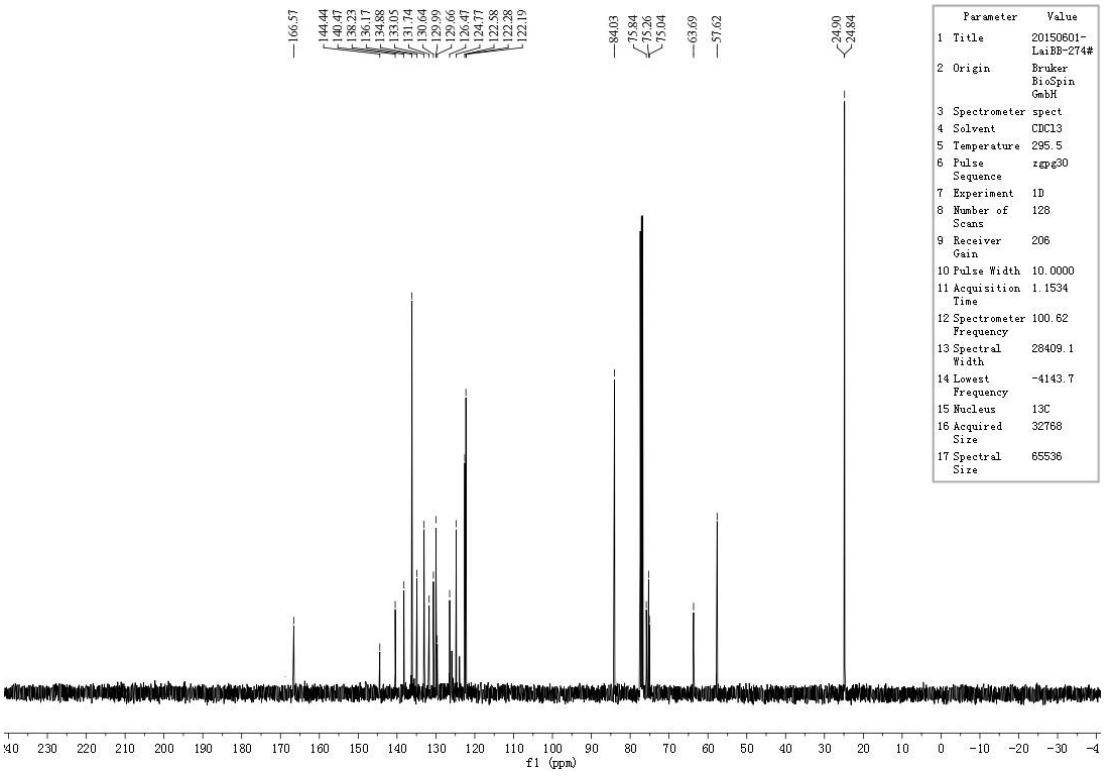


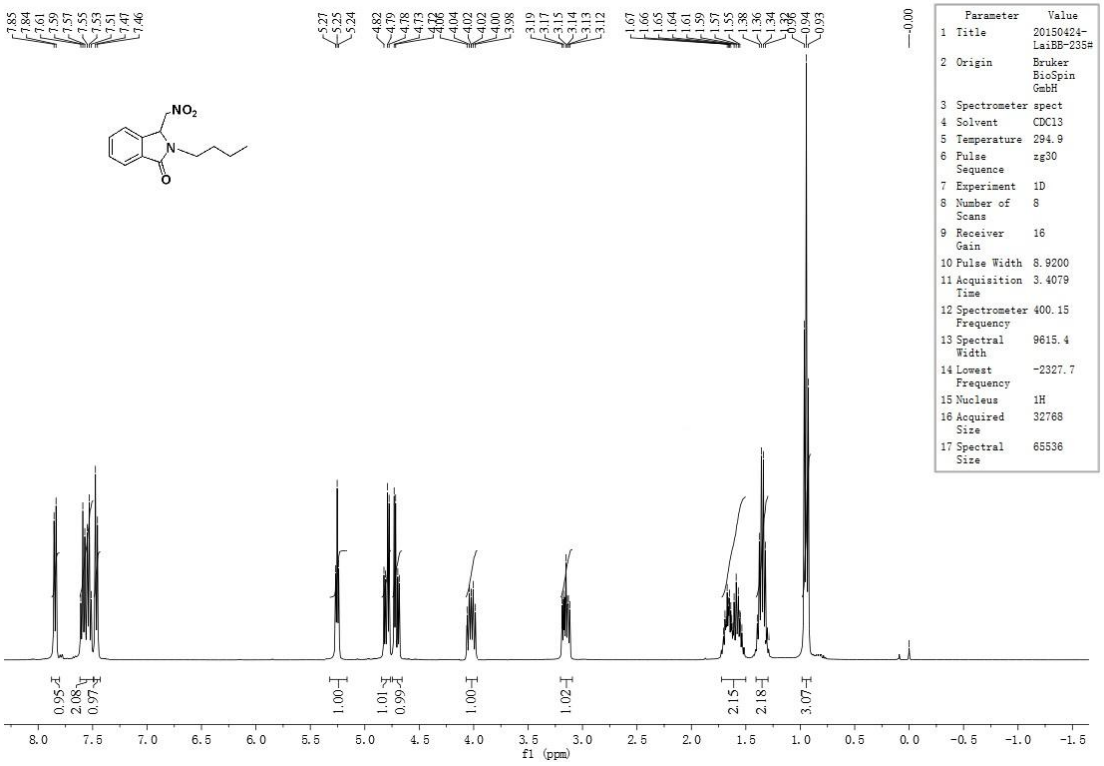
	Parameter	Value
1	Title	20150601-LaiBB-276#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	44
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2346.2
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

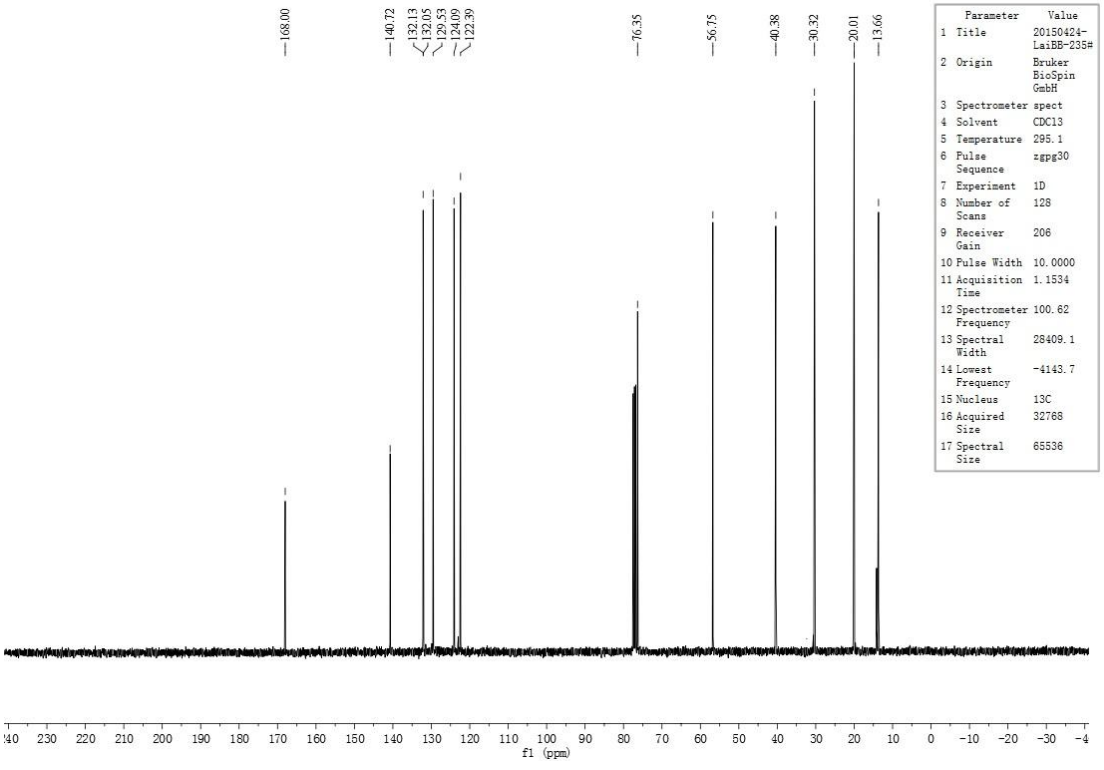


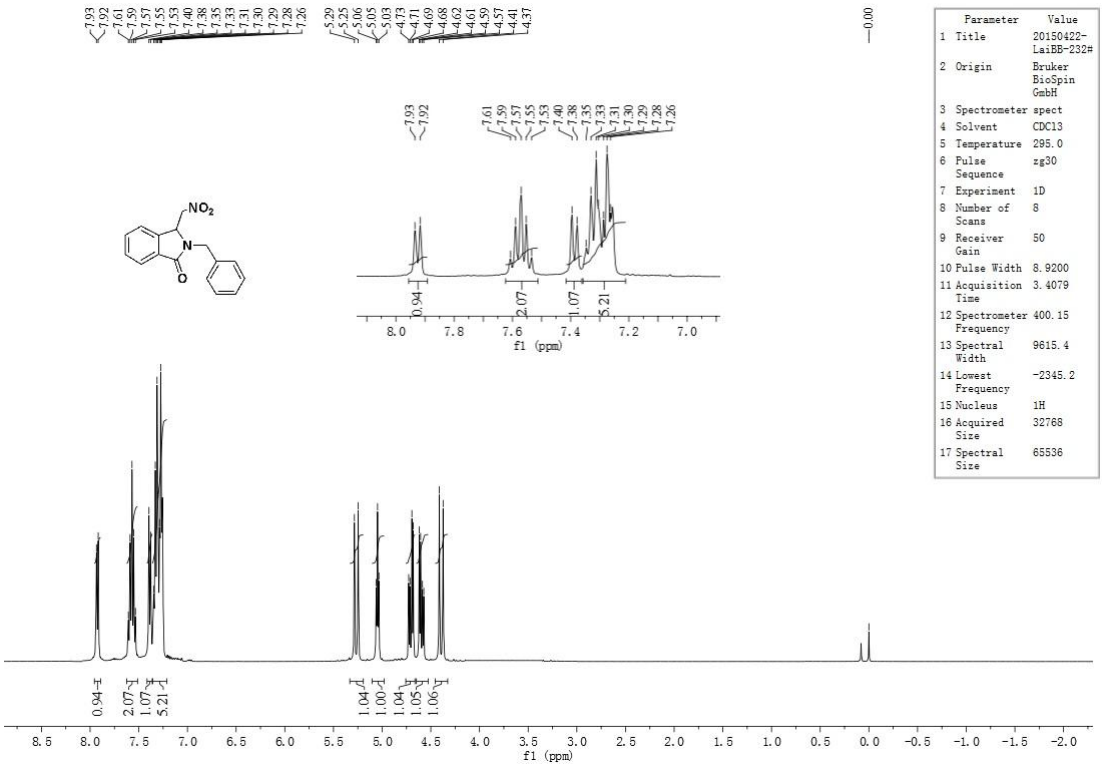
	Parameter	Value
1	Title	20150601-LaiBB-276#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.4
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	64
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536


Parameter Value
1 Title 20150601-LaiBB-274#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 40
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2339.9
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

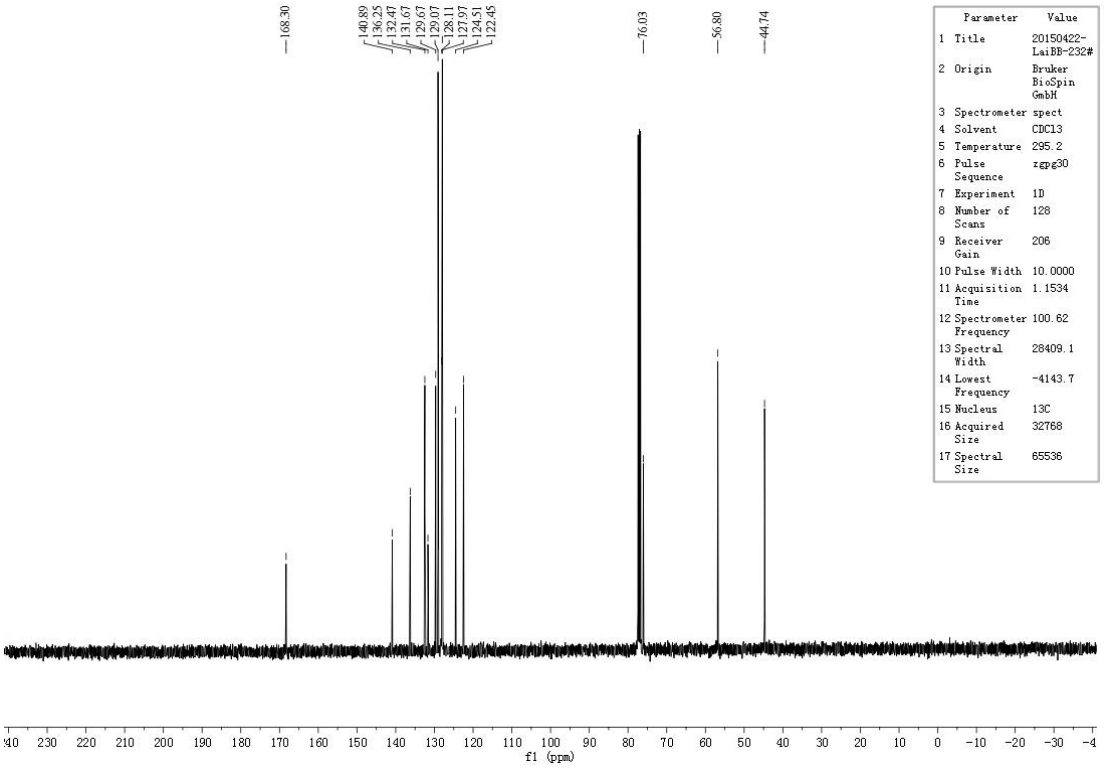

Parameter Value
1 Title 20150601-LaiBB-274#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.5
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)


7.85
7.84
7.61
7.59
7.57
7.55
7.53
7.51
7.47
7.46
5.27
5.25
5.24
4.82
4.79
4.78
4.73
4.72
4.06
4.04
4.02
4.02
4.00
3.98
3.19
3.17
3.15
3.14
3.13
3.12
1.67
1.66
1.65
1.64
1.61
1.59
1.57
1.55
1.38
1.36
1.34
1.32
0.96
0.94
0.93
0.00
NO2
N
O
0.95
2.08
0.97
1.00
1.01
0.99
1.00
1.02
2.15
2.18
3.07
f1 (ppm)
Parameter Value
1 Title 20150424-LaiBB-235#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 16
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2327.7
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

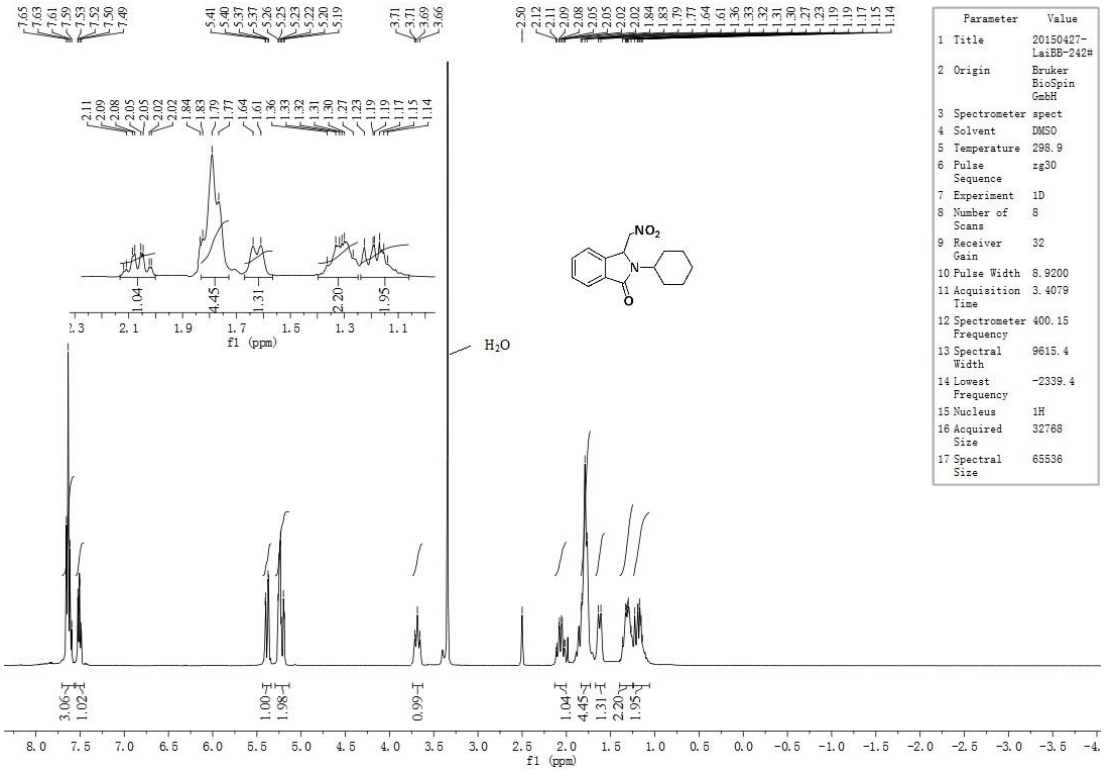

168.00
140.72
132.13
132.05
129.53
124.09
122.39
76.35
56.75
40.38
30.32
20.01
13.66
f1 (ppm)
Parameter Value
1 Title 20150424-LaiBB-235#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536



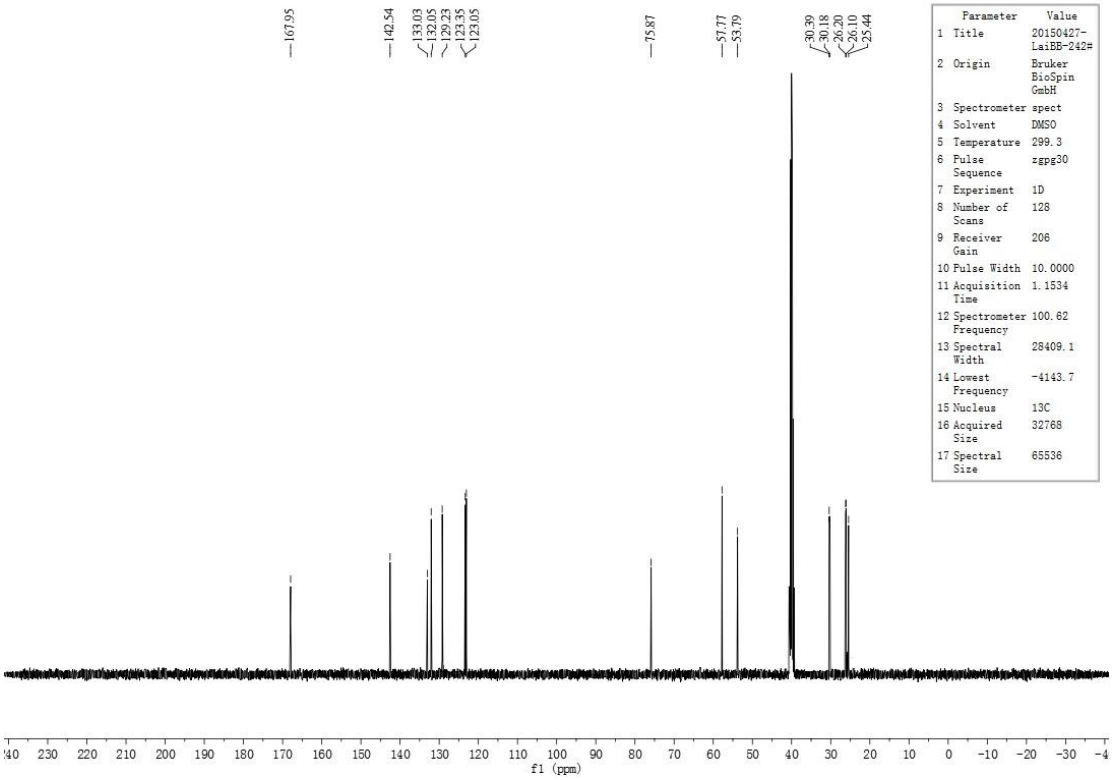
	Parameter	Value
1	Title	20150422-LaiBB-232#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.0
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	50
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2345.2
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



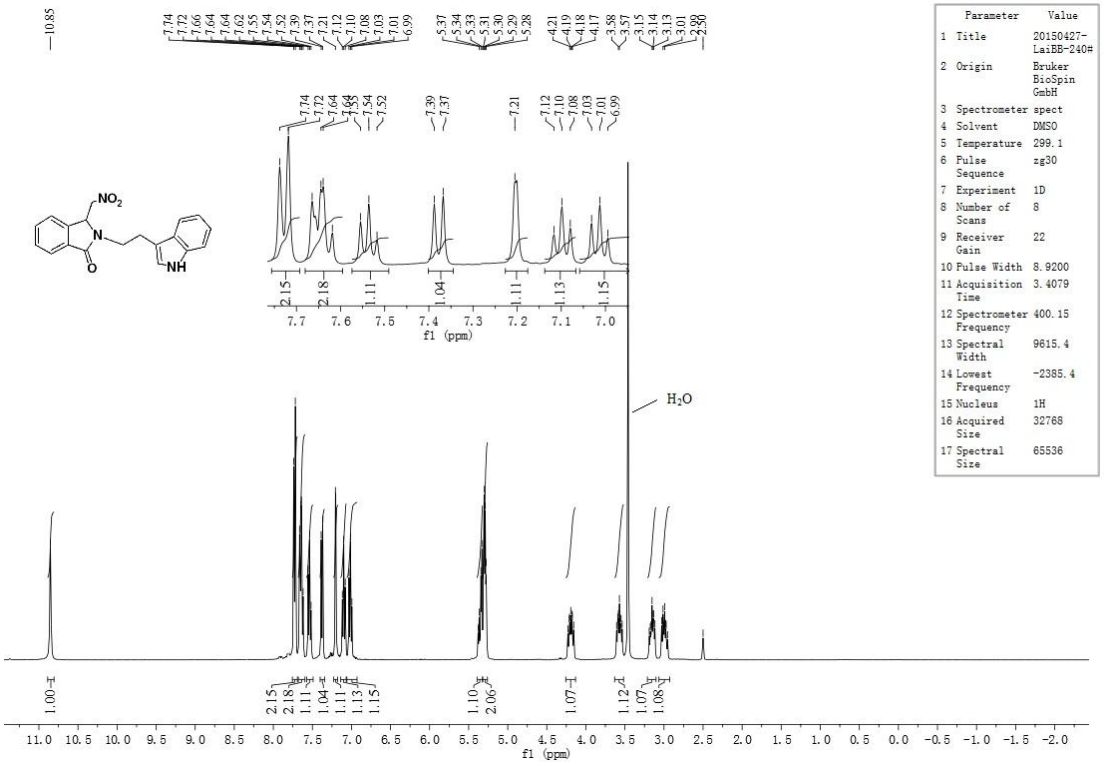
	Parameter	Value
1	Title	20150422-LaiBB-232#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	CDCl3
5	Temperature	295.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

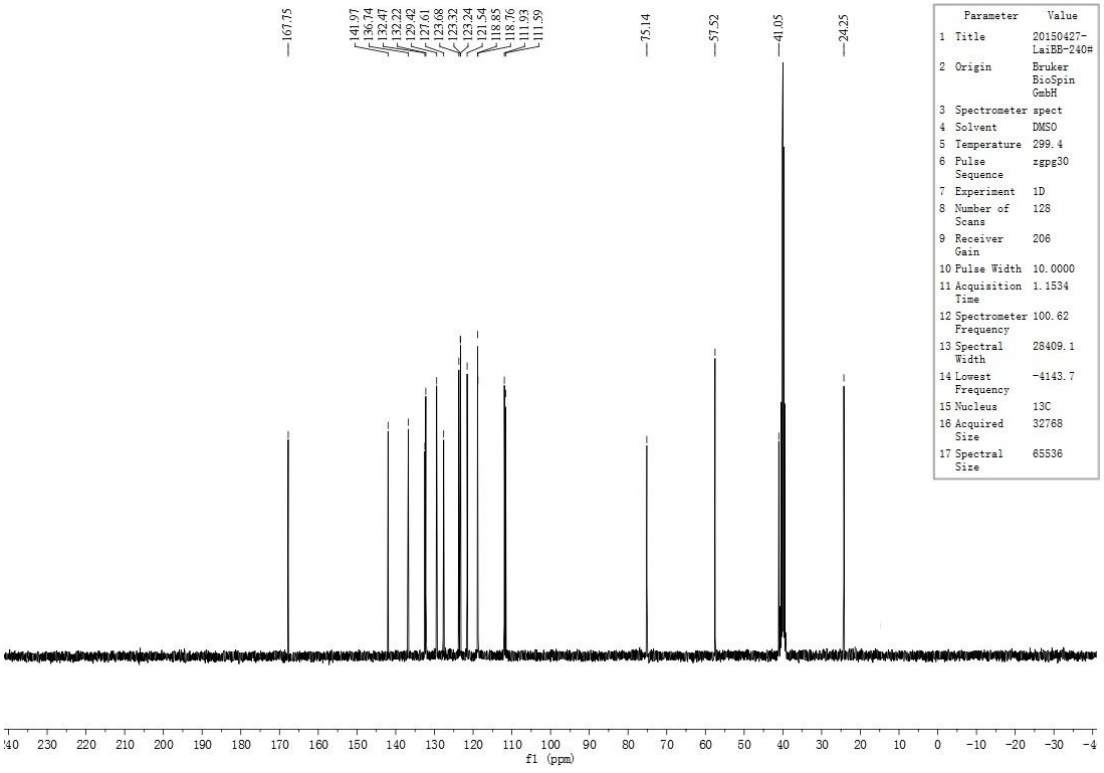


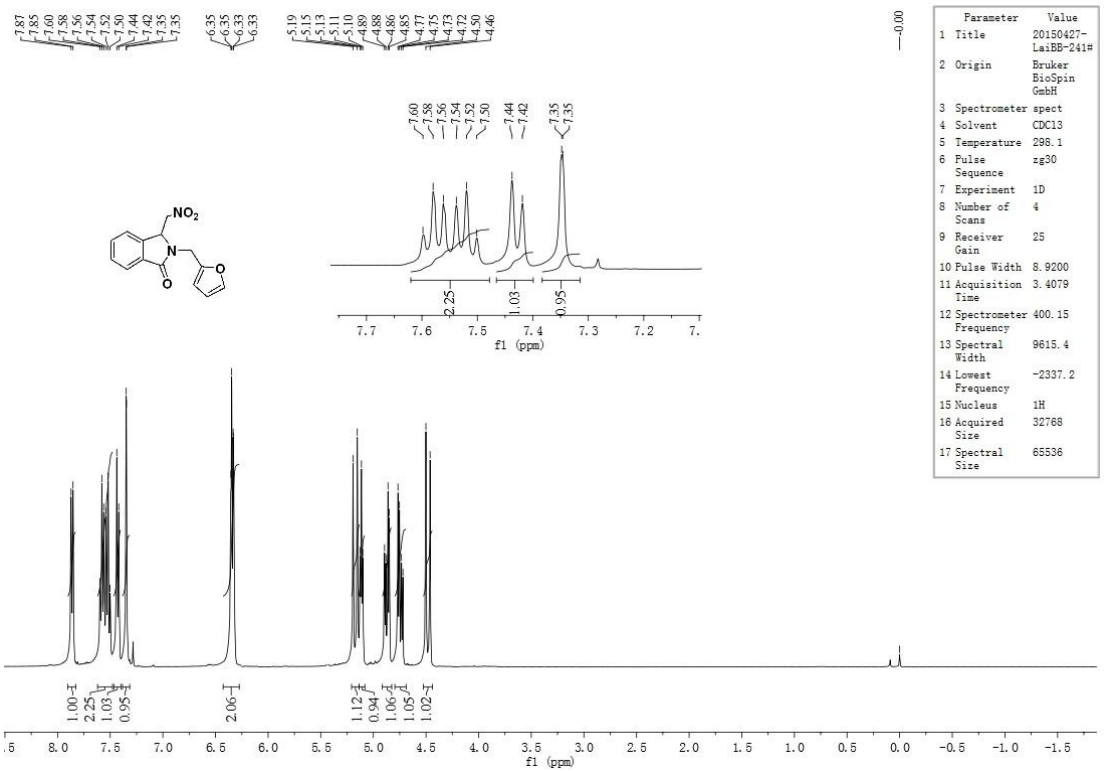
	Parameter	Value
1	Title	20150427-LaiBB-242#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	DMSO
5	Temperature	298.9
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	8
9	Receiver Gain	32
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2339.4
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536

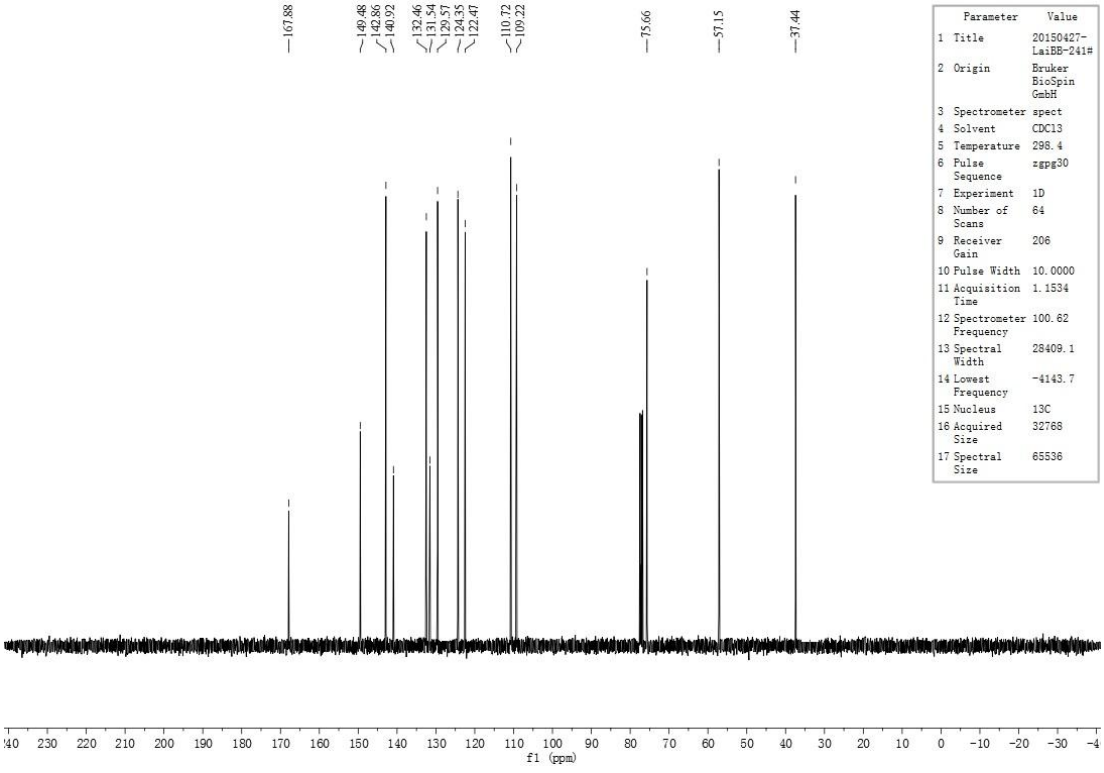


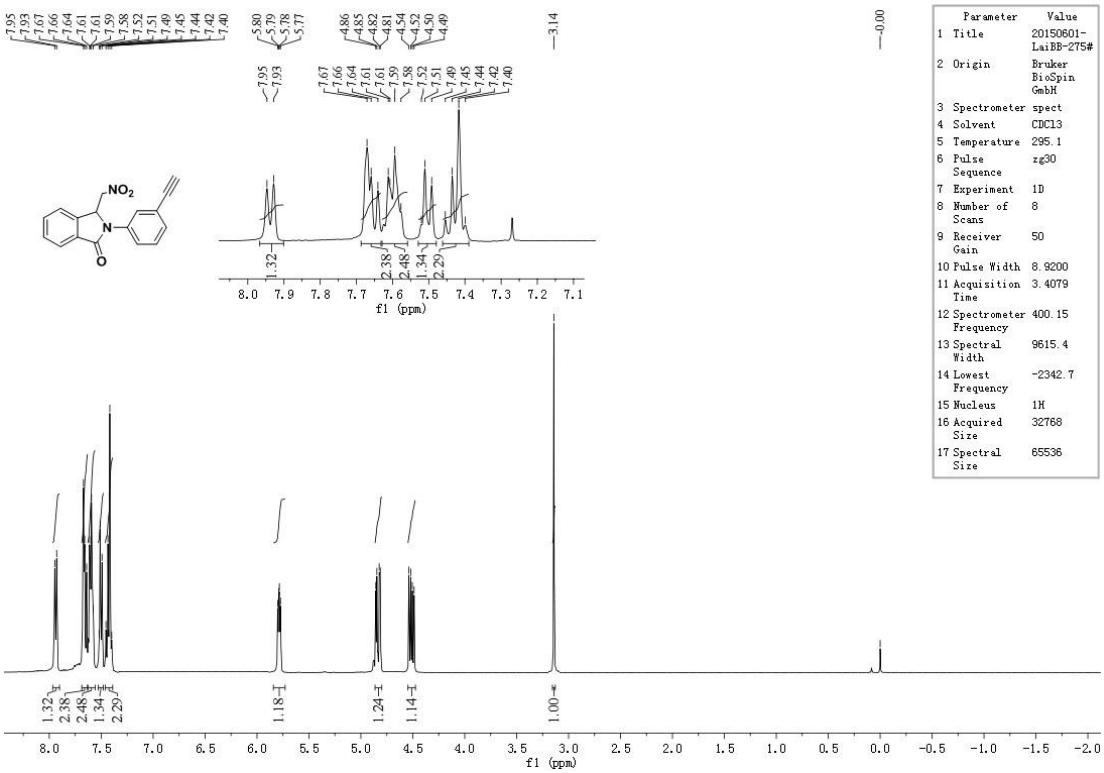
	Parameter	Value
1	Title	20150427-LaiBB-242#
2	Origin	Bruker BioSpin GmbH
3	Spectrometer	spect
4	Solvent	DMSO
5	Temperature	299.3
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	128
9	Receiver Gain	206
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.62
13	Spectral Width	28409.1
14	Lowest Frequency	-4143.7
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

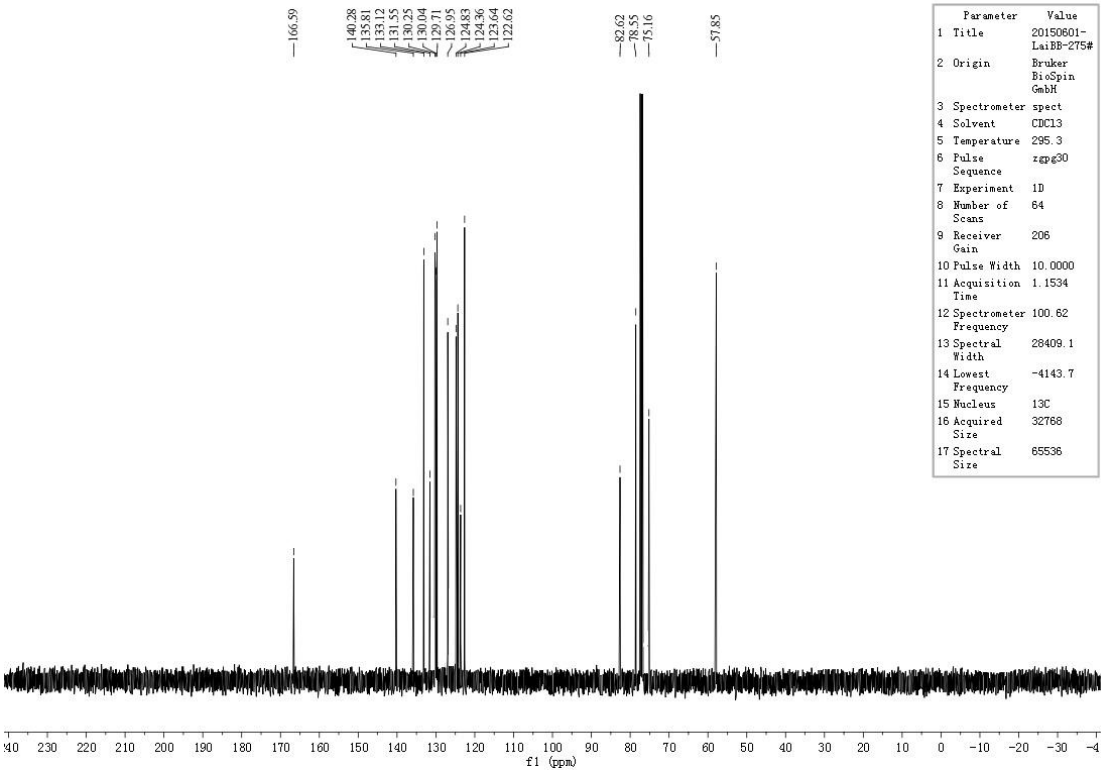

10.85
7.74
7.72
7.66
7.64
7.62
7.55
7.54
7.52
7.39
7.37
7.21
7.12
7.10
7.08
7.03
7.01
6.99
5.37
5.34
5.33
5.31
5.30
5.29
5.28
4.21
4.19
4.18
4.17
3.58
3.57
3.15
3.14
3.13
3.01
2.88
2.50
NO2
N
O
NH
H2O
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-240#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 22
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2385.4
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

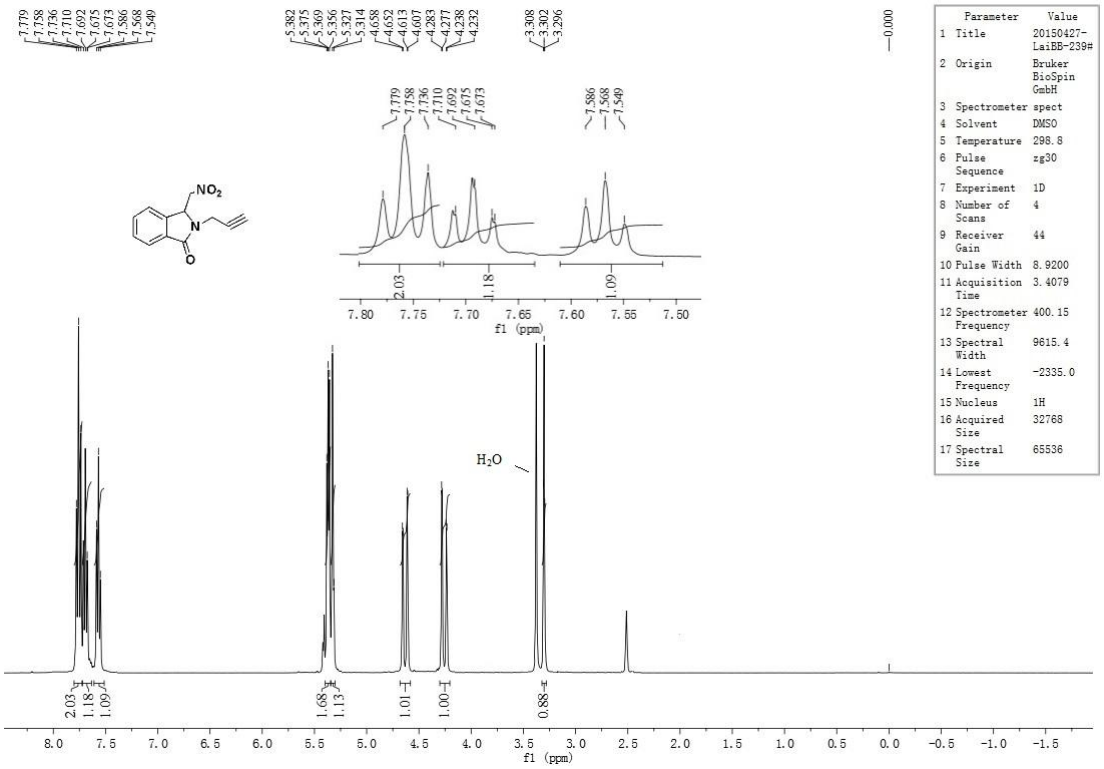

167.75
141.97
136.74
132.47
132.22
129.42
127.61
123.68
123.32
123.24
121.54
118.85
118.76
111.93
111.59
75.14
57.52
41.05
24.25
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-240#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.4
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

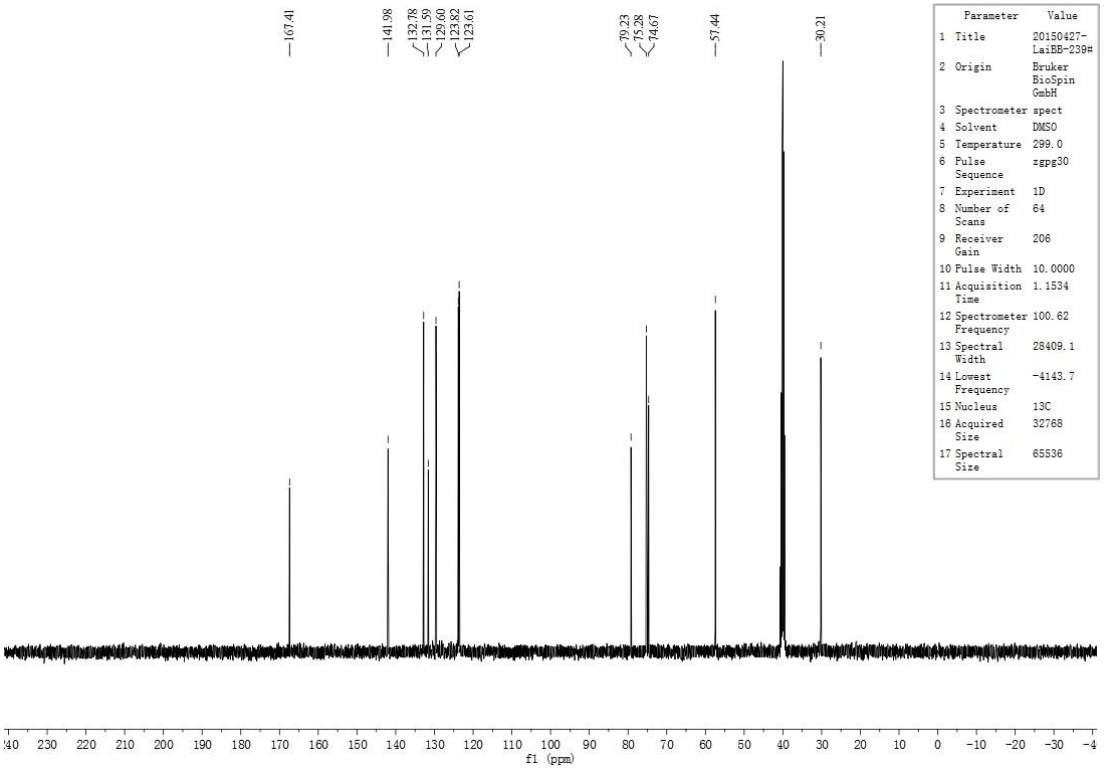

7.87 7.85 7.60 7.58 7.56 7.54 7.52 7.50 7.44 7.42 7.35 7.35
6.35 6.35 6.33 6.33
5.19 5.15 5.13 5.11 5.10 4.89 4.88 4.86 4.85 4.77 4.75 4.73 4.72 4.50 4.46
0.00
NO2
N
O
O
7.60 7.58 7.56 7.54 7.52 7.50 7.44 7.42 7.35 7.35
2.25 1.03 0.95
7.7 7.6 7.5 7.4 7.3 7.2 7.
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-241#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDC13
5 Temperature 298.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 25
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2337.2
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
1.00 2.25 1.03 0.95 2.06 1.12 0.94 1.06 1.05 1.02
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 0.0 -0.5 -1.0 -1.5
f1 (ppm)

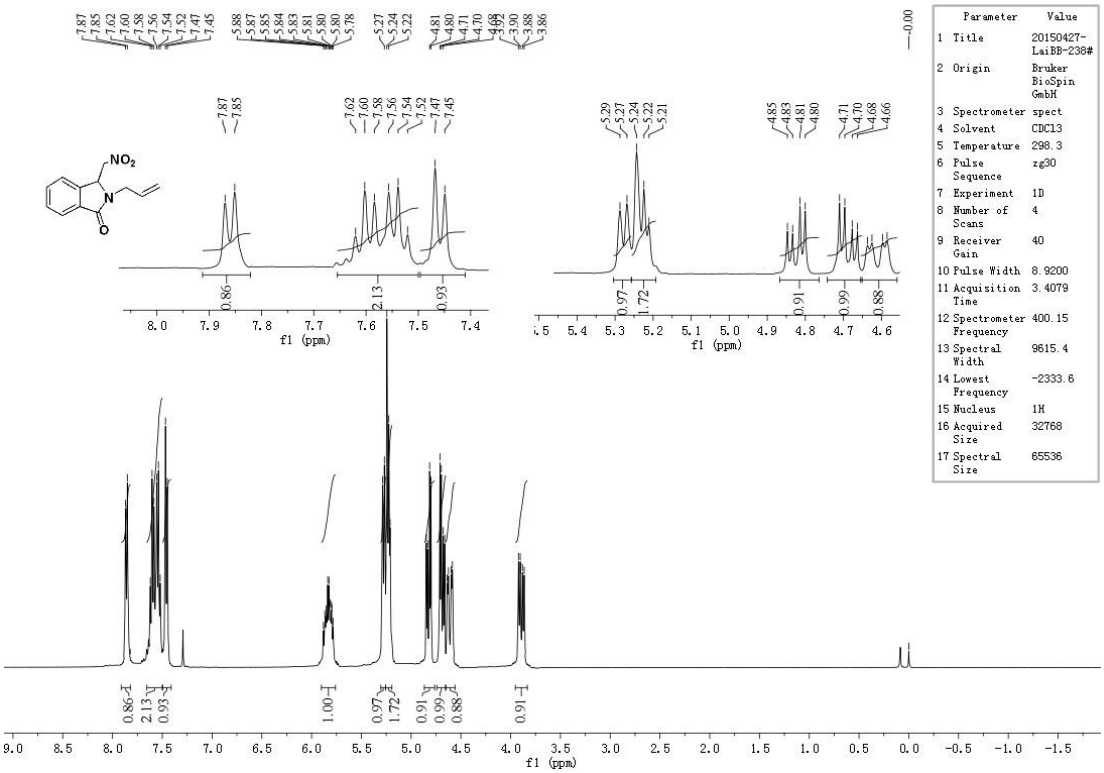

167.88
149.48 142.86 140.92
132.46 131.54 129.57 124.35 122.47
110.72 109.22
75.66
57.15
37.44
Parameter Value
1 Title 20150427-LaiBB-241#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDC13
5 Temperature 298.4
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

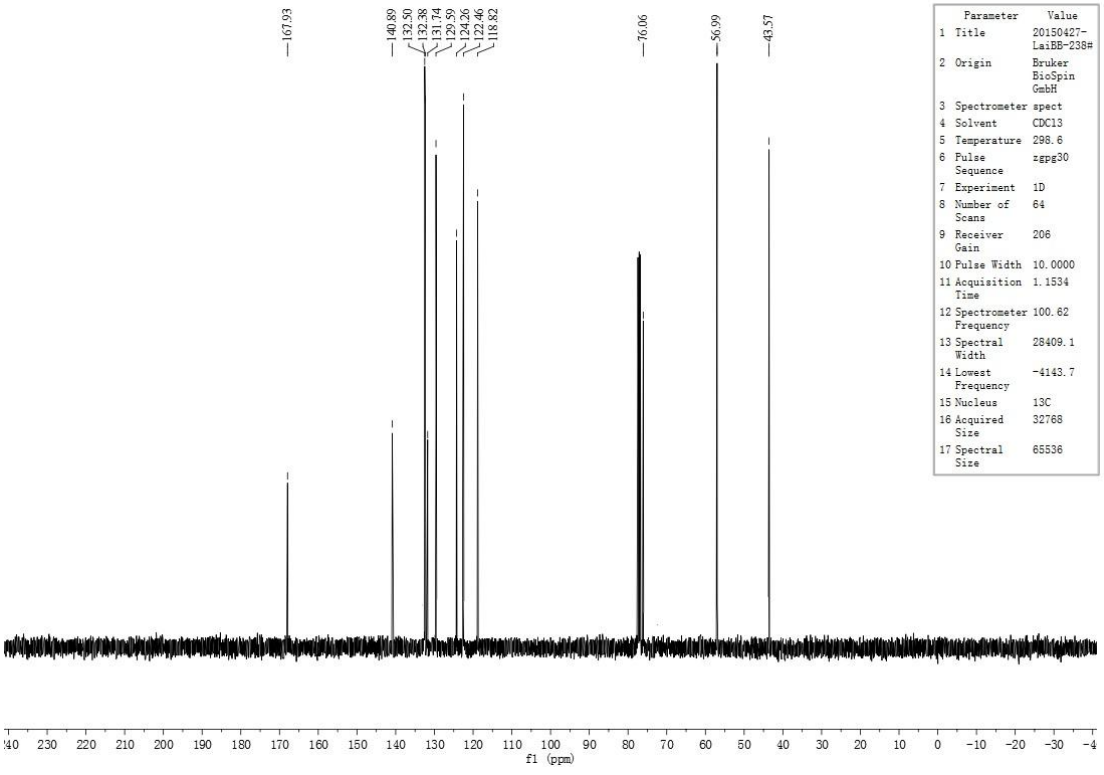

Parameter Value
1 Title 20150601-LaiBB-275#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.1
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 50
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2342.7
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

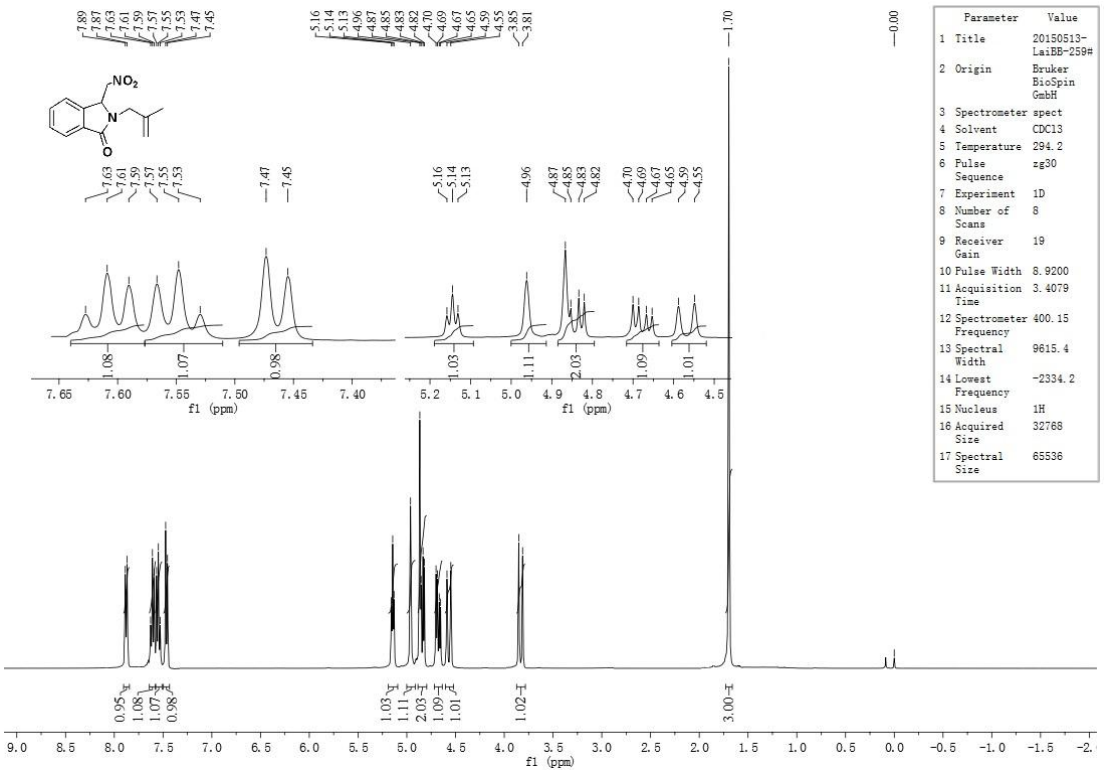

Parameter Value
1 Title 20150601-LaiBB-275#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

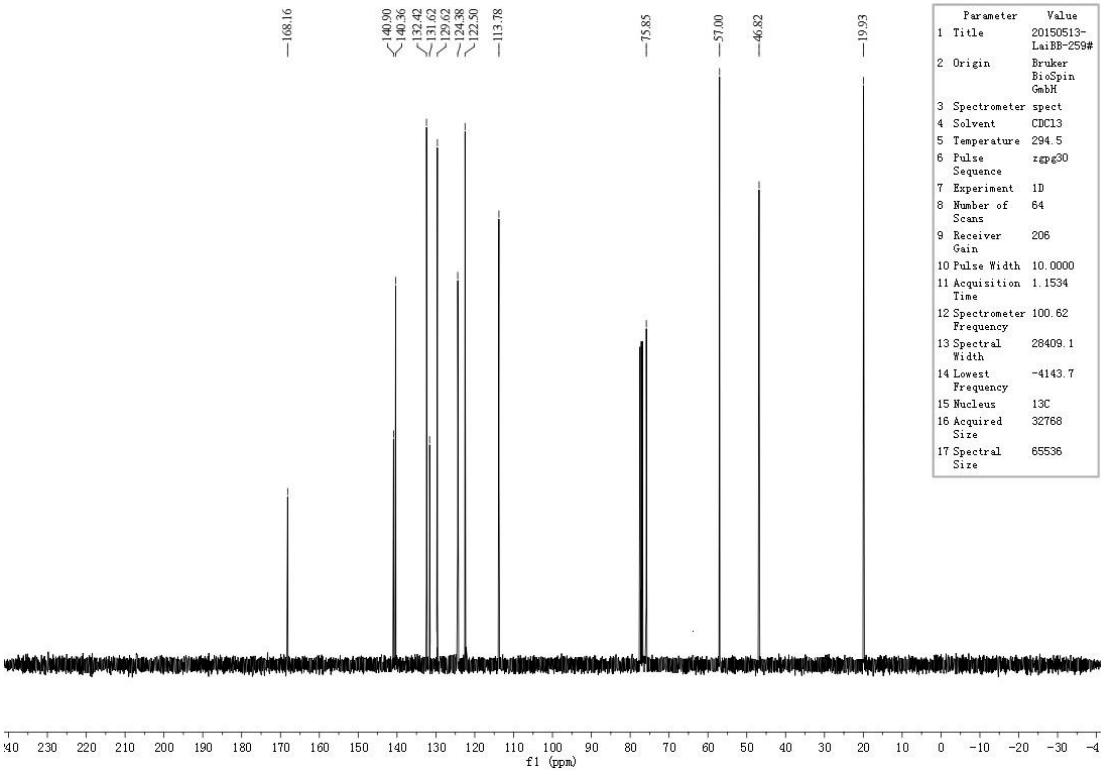

7.779
7.758
7.736
7.710
7.692
7.675
7.673
7.586
7.568
7.549
5.382
5.375
5.369
5.356
5.327
5.314
4.658
4.652
4.613
4.607
4.283
4.277
4.238
4.232
3.308
3.302
3.296
0.000
NO2
N
O
2.03
1.18
1.09
f1 (ppm)
H2O
1.68
1.13
1.01
1.00
0.88
Parameter Value
1 Title 20150427-LaiBB-239#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.8
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 44
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2335.0
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

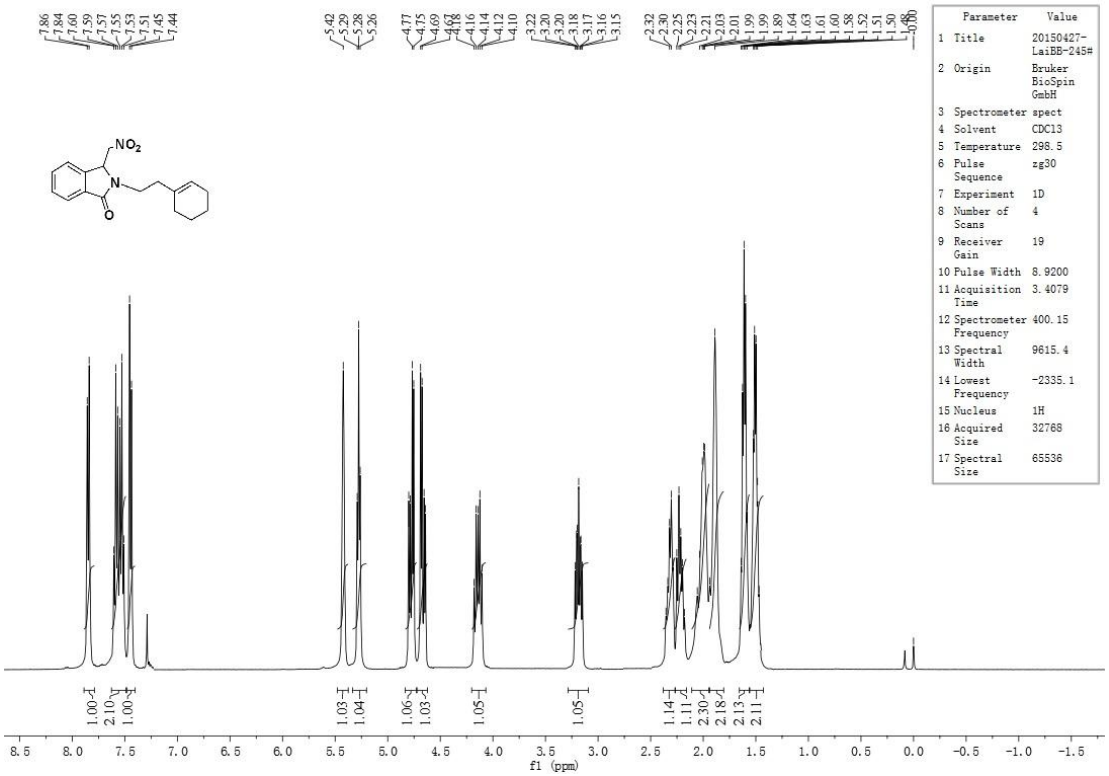

167.41
141.98
132.78
131.59
129.60
123.82
123.61
79.23
75.28
74.67
57.44
30.21
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-239#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.0
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

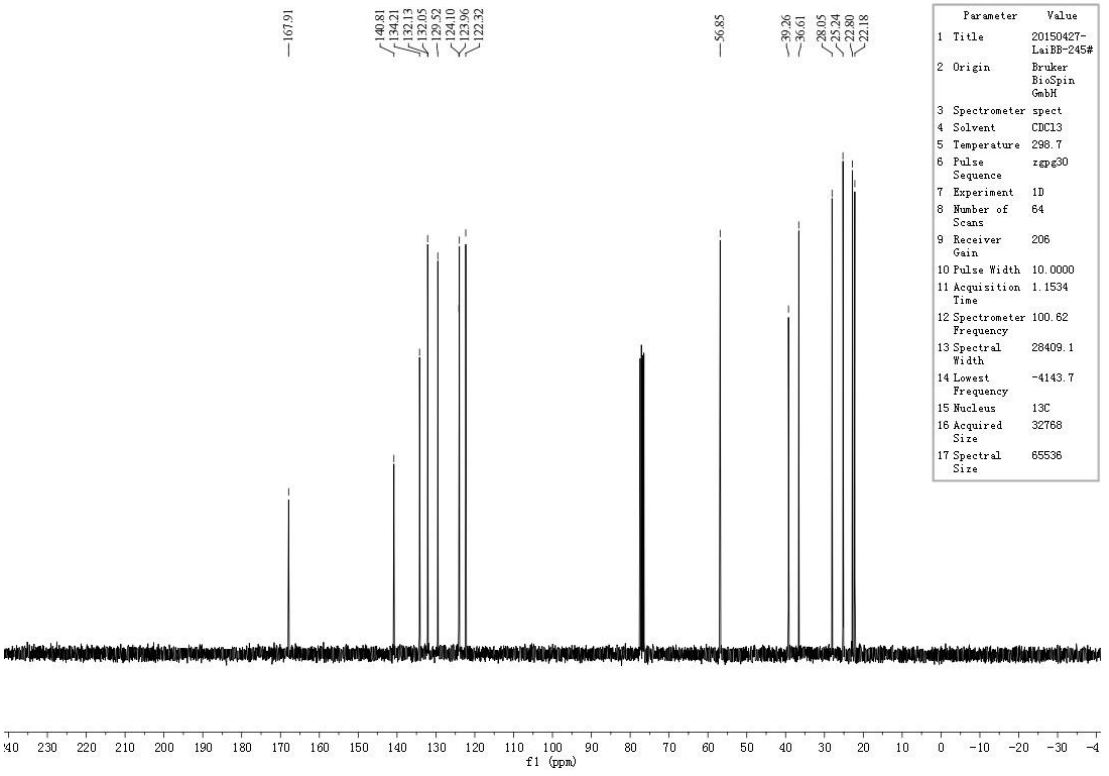

Parameter Value
1 Title 20150427-LaiBB-238#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.3
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 40
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2333.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

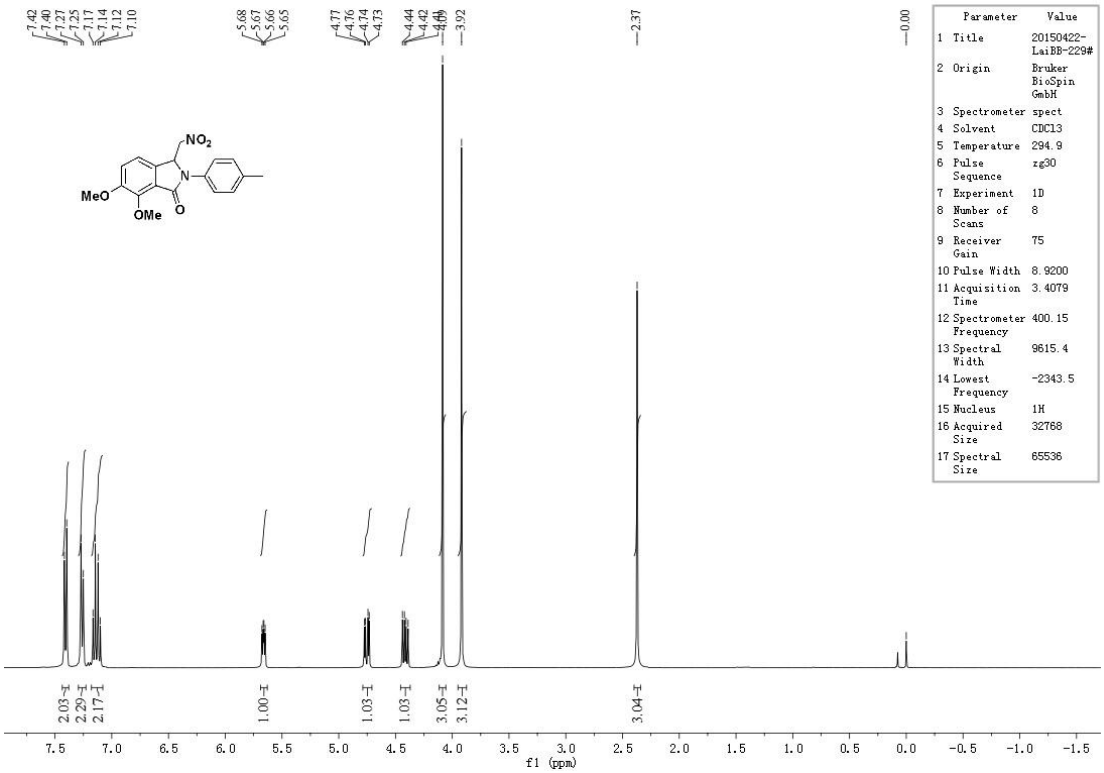

Parameter Value
1 Title 20150427-LaiBB-238#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.6
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

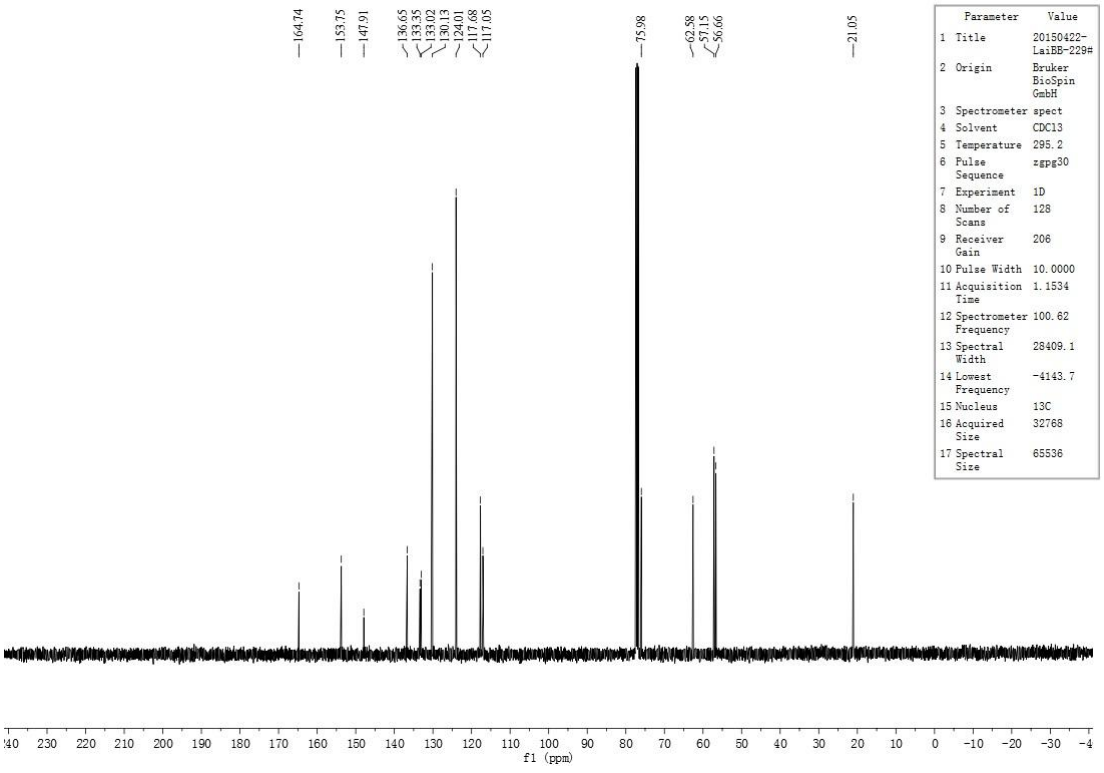

Parameter Value
1 Title 20150513-LaiBB-259#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.2
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 19
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2334.2
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

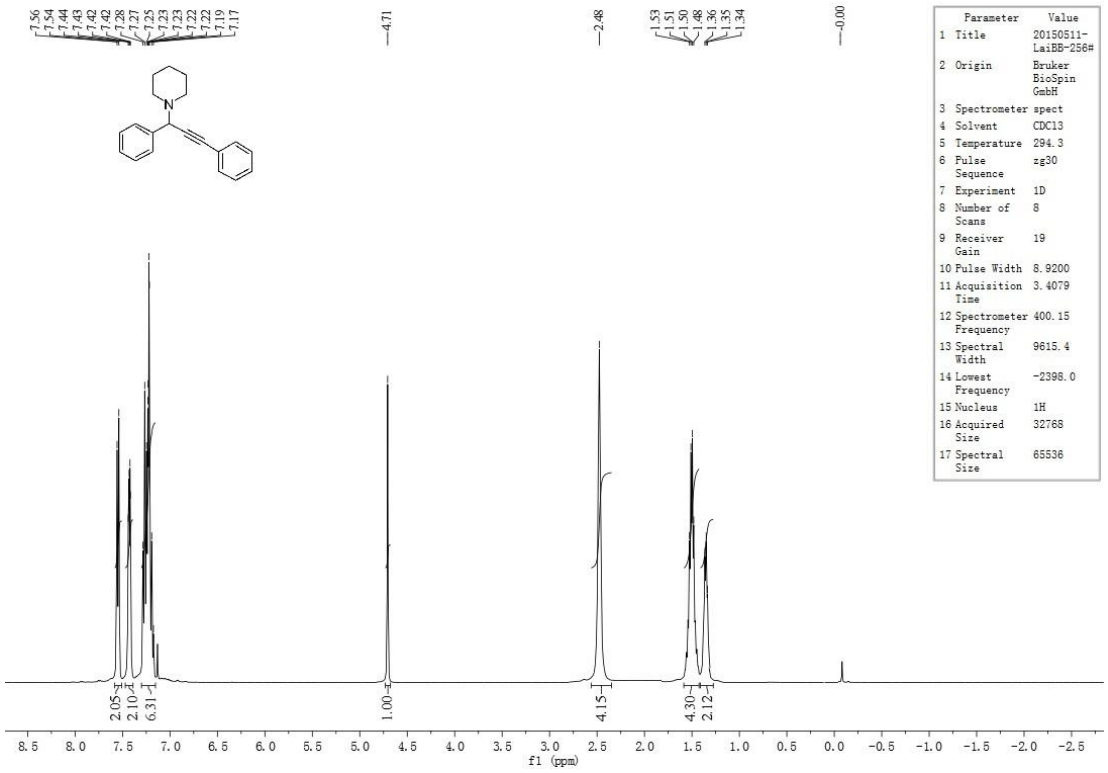

Parameter Value
1 Title 20150513-LaiBB-259#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.5
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
f1 (ppm)

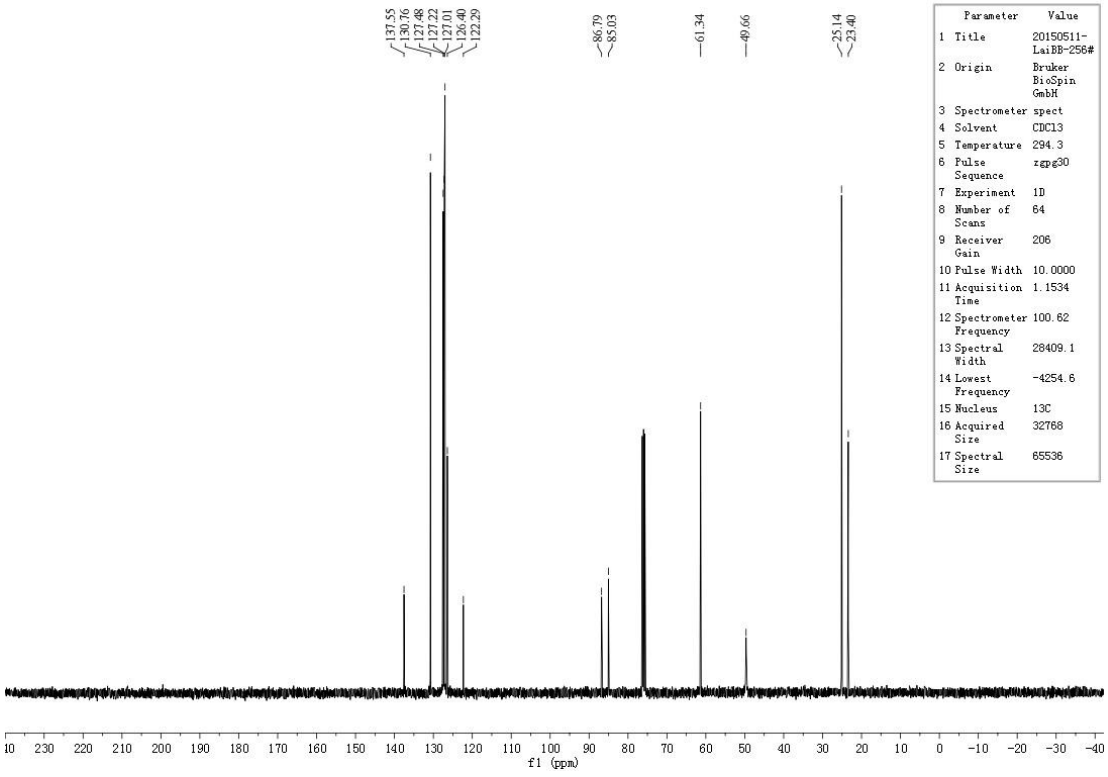

7.86
7.84
7.60
7.59
7.57
7.55
7.53
7.51
7.45
7.44
5.42
5.29
5.28
5.26
4.77
4.75
4.69
4.63
4.18
4.16
4.14
4.12
4.10
3.22
3.20
3.20
3.18
3.17
3.16
3.15
2.32
2.30
2.25
2.23
2.21
2.03
2.01
1.99
1.99
1.89
1.64
1.63
1.61
1.60
1.58
1.52
1.51
1.50
1.48
0.00
NO2
N
O
1.00
2.10
1.00
1.03
1.04
1.06
1.03
1.05
1.05
1.14
1.11
2.30
2.18
2.13
2.11
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 -0.5 -1.0 -1.5
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-245#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.5
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 19
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2335.1
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

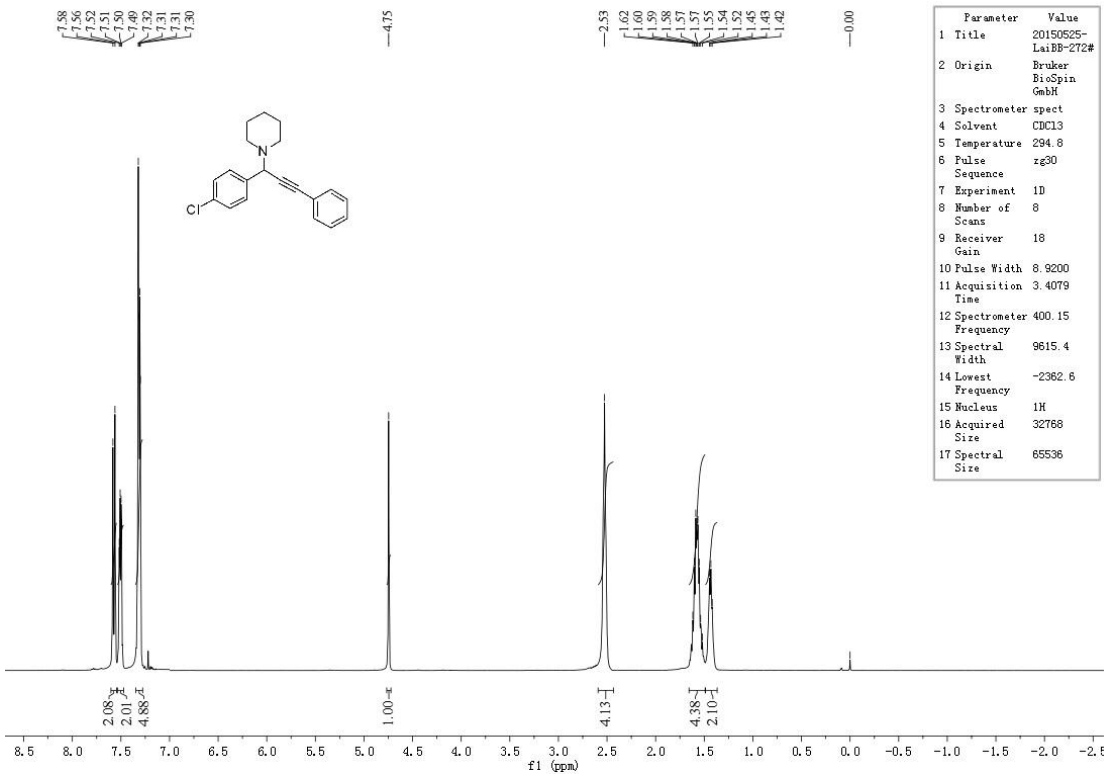

167.91
140.81
134.21
132.13
132.05
129.52
124.10
123.96
122.32
56.85
39.26
36.61
28.05
25.24
22.80
22.18
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)
Parameter Value
1 Title 20150427-LaiBB-245#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.7
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

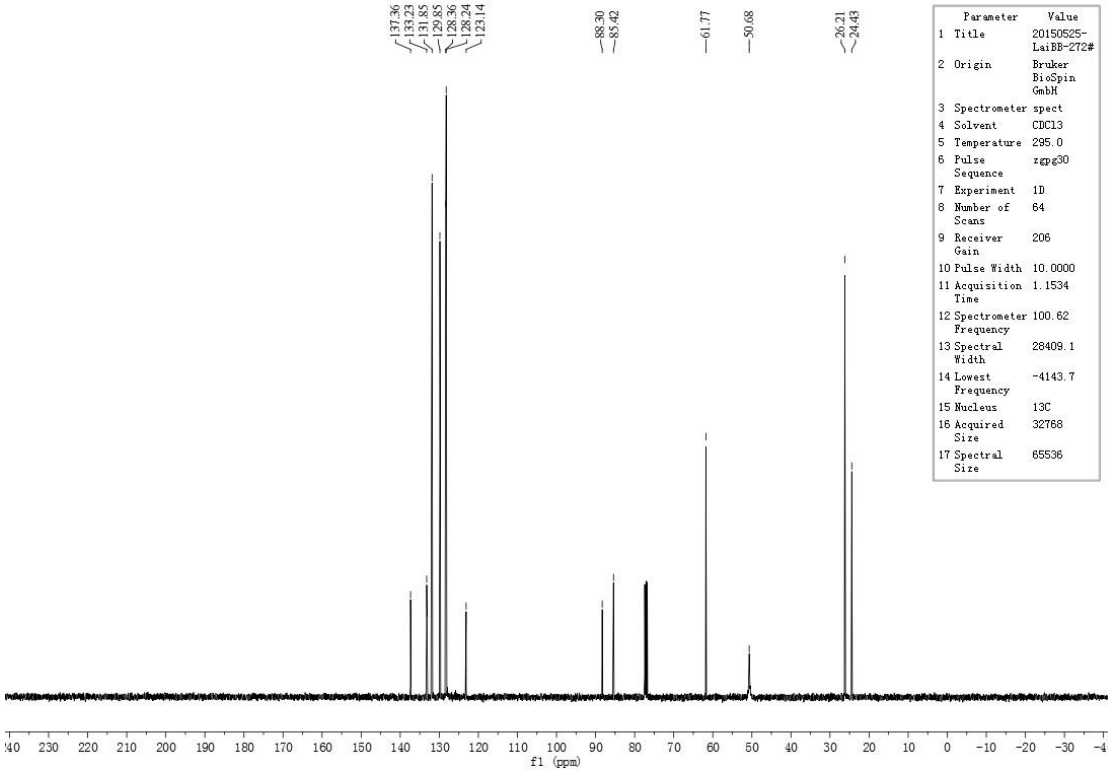

7.42
7.40
7.27
7.25
7.17
7.14
7.12
7.10
5.68
5.67
5.66
5.65
4.77
4.76
4.74
4.73
4.44
4.42
3.92
2.37
0.00
NO2
MeO
OMe
O
N
2.03
2.29
2.17
1.00
1.03
1.03
3.05
3.12
3.04
f1 (ppm)
Parameter Value
1 Title 20150422-LaiBB-229#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.9
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 75
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2343.5
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

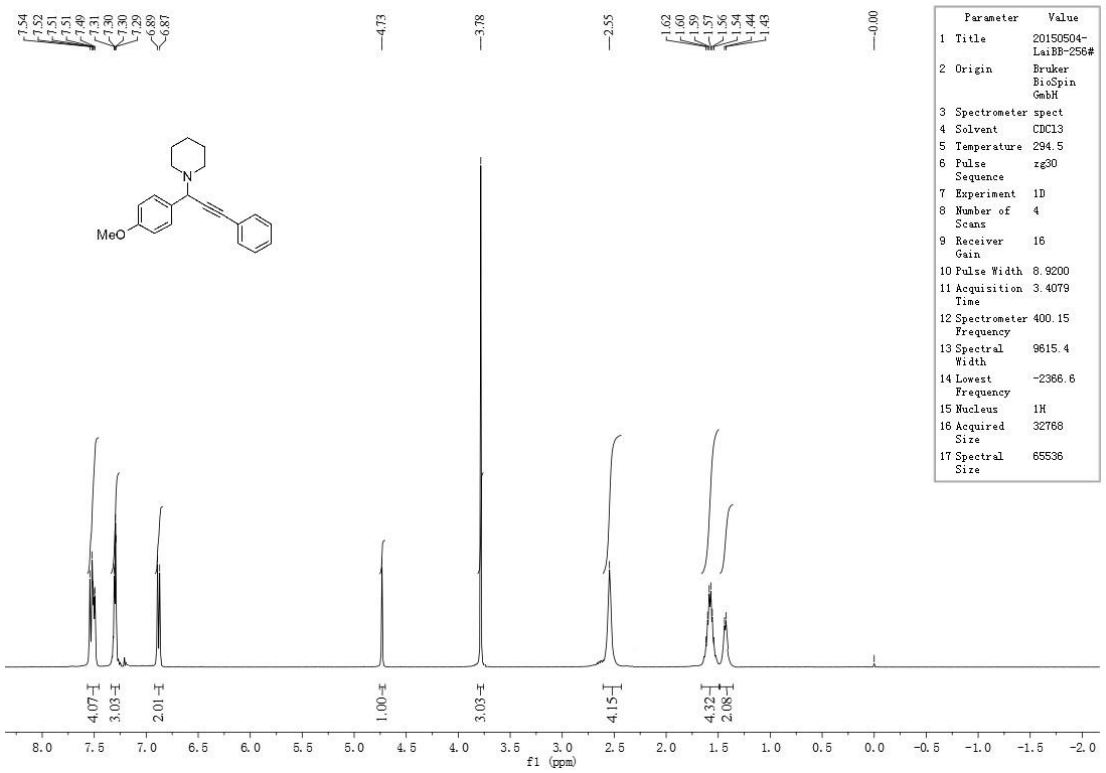

164.74
153.75
147.91
136.65
133.35
133.02
130.13
124.01
117.68
117.05
75.98
62.58
57.15
56.66
21.05
f1 (ppm)
Parameter Value
1 Title 20150422-LaiBB-229#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 128
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

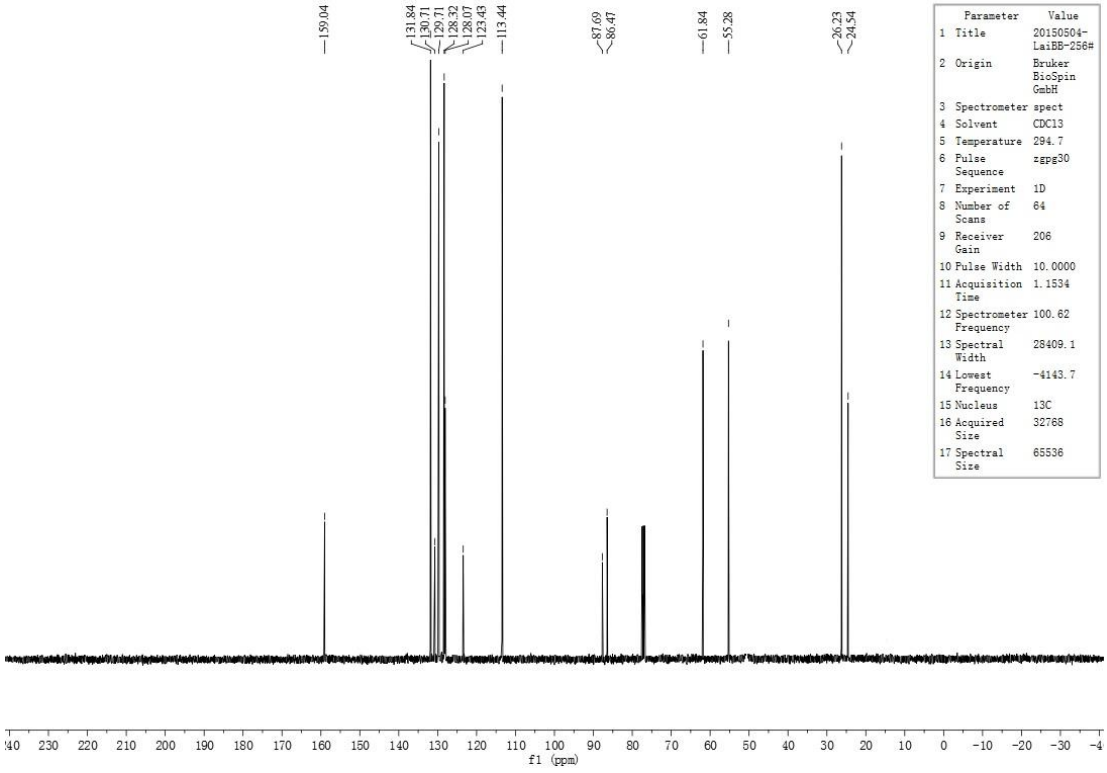

7.56
7.54
7.44
7.43
7.42
7.42
7.28
7.27
7.25
7.23
7.23
7.22
7.22
7.19
7.17
4.71
2.48
1.53
1.51
1.50
1.48
1.36
1.35
1.34
0.00
2.05
2.10
6.31
1.00
4.15
4.30
2.12
f1 (ppm)
Parameter Value
1 Title 20150511-LaiBB-256#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 19
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2398.0
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536

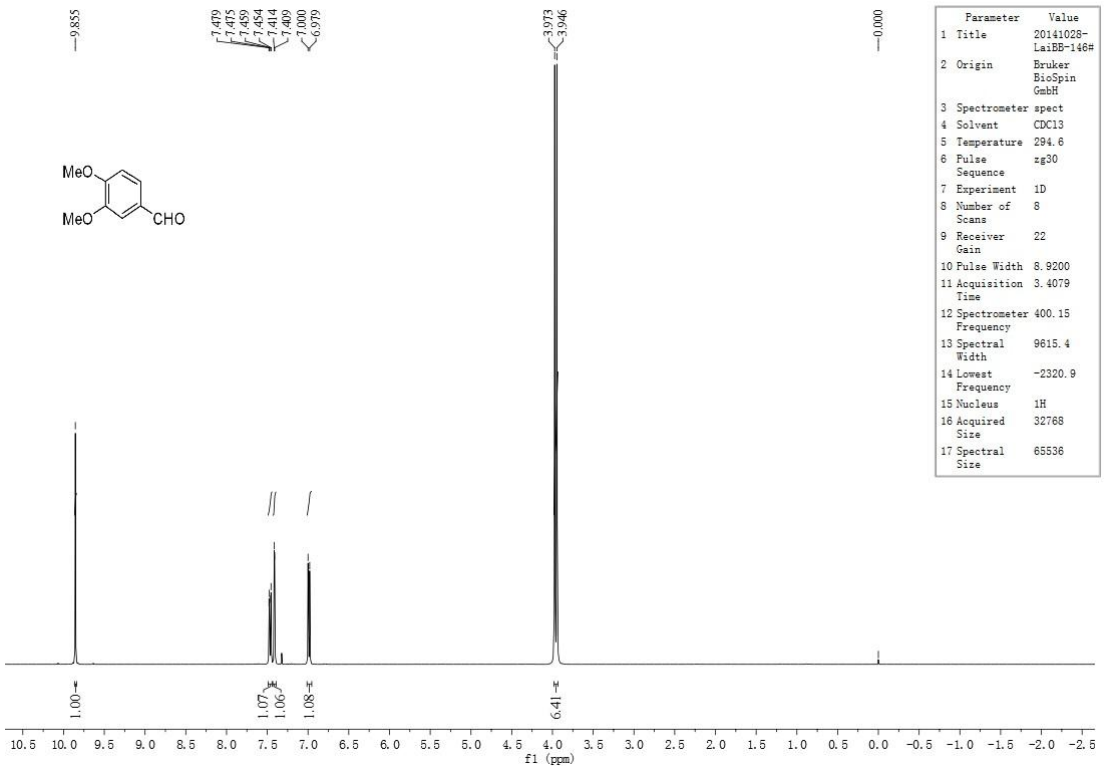

137.55
130.76
127.48
127.22
127.01
126.40
122.29
86.79
85.03
61.34
49.66
25.14
23.40
f1 (ppm)
Parameter Value
1 Title 20150511-LaiBB-256#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.3
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4254.6
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536

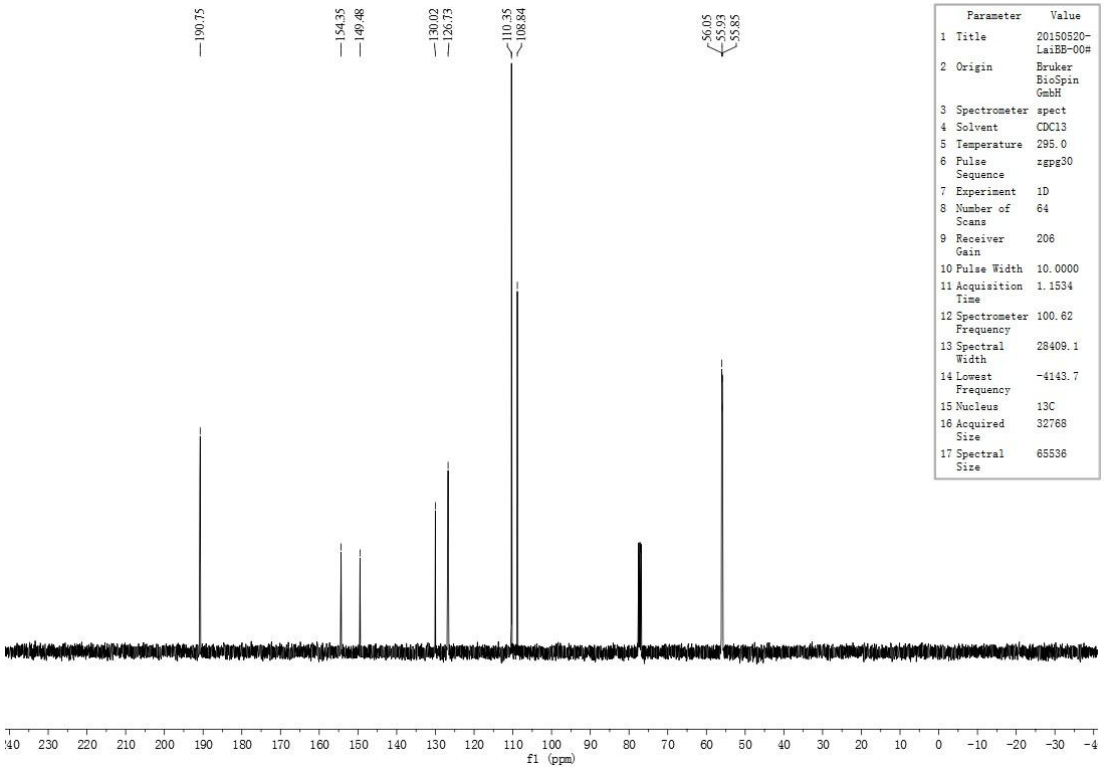

7.58
7.56
7.52
7.51
7.50
7.49
7.32
7.31
7.31
7.30
4.75
2.53
1.62
1.60
1.59
1.58
1.57
1.57
1.55
1.54
1.52
1.45
1.43
1.42
0.00
Cl
2.08
2.01
4.88
1.00
4.13
4.38
2.10
f1 (ppm)
Parameter Value
1 Title 20150525-LaiBB-272#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.8
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 8
9 Receiver Gain 18
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2362.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536


137.36
133.23
131.85
129.85
128.36
128.24
123.14
88.30
85.42
61.77
50.68
26.21
24.43
f1 (ppm)
Parameter Value
1 Title 20150525-LaiBB-272#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 295.0
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536


7.54
7.52
7.51
7.51
7.49
7.31
7.30
7.30
7.29
6.89
6.87
4.73
3.78
2.55
1.62
1.60
1.59
1.57
1.56
1.54
1.44
1.43
0.00
MeO
N
4.07
3.03
2.01
1.00
3.03
4.15
4.32
2.08
f1 (ppm)
Parameter Value
1 Title 20150504-LaiBB-256#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.5
6 Pulse Sequence zg30
7 Experiment 1D
8 Number of Scans 4
9 Receiver Gain 16
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2366.6
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536


159.04
131.84
130.71
129.71
128.32
128.07
123.43
113.44
87.69
86.47
61.84
55.28
26.23
24.54
f1 (ppm)
Parameter Value
1 Title 20150504-LaiBB-256#
2 Origin Bruker BioSpin GmbH
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 294.7
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 64
9 Receiver Gain 206
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.62
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536





7. References

[1] M. Li, J. Yang, Y. Gu, *Adv. Synth. Catal.* 2011, **353**, 1551-1564.
[2] M. Li, H. Li, T. Li, Y. Gu, *Org. Lett.* 2011, **13**, 1065.
[3] L. Huang, W. Liu, J. Wu, Y. Fu, K. Wang, C. Huo, Z. Du, *Tetrahedron Lett.* 2014, **55,** 2312-2316.

[4] J. M. Pérez, R. Cano, D. J. Ramó n, *RSC Adv*. 2014, **4**, 23943.
[5] S. Sun, R. Bai, Y. Gu, *Chem. Eur. J*. 2014, **20**, 549-558.
[6] C. Zhang, B. Huang, Y. Chen, D. -M. Cui, *New J. Chem.* 2013, **37**, 2606.
[7] X. Niu, C. Li, J. Li, X. Jia, *Tetrahedron Lett.* 2012, **53**, 5559-5561.
[8] Y. Ren, M. Li, J. Yang, J. Peng, Y.Gu, *Adv. Synth. Catal*. 2011, **353**, 3473-3484.
[9] D. –X. Liu, F. –L. Li, H. –X. Li a, J. Gao, J.-P. Lang, *Tetrahedron*, 2014**, 70**, 2416-2421.
[10] Y. Liu, C. Wang, X. Wang, J. -P. Wan, *Tetrahedron Lett*. 2013, **54**, 3953-3955.
[11] K. C. Weerasiri, A.E.V. Gorden, *Tetrahedron*. 2014, **70**, 7962-7968.
[12] B. J. Borah, S. J. Borah, L. Saikia, D.K. Dutta, *Catal. Sci. Technol.* 2014, **4**, 1047.
[13] T. X. T. Luu, T. T. Lam, T. N. Le, F. Duus, *Molecules.* 2009, **14**, 3411-3424.