Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Friedel-Crafts Alkylation Reaction with Fluorinated Alcohols as Hydrogen-Bond Donors and Solvents

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Supporting Information

General information

Thin-layer chromatography (TLC) was performed on silica gel, 60F-250 (0.26mm thickness) plates. The plates were visualized with UV light (254 nm) or with a 3.5% solution of phosphomolybdic acid in ethanol or with a solution of $KMnO_4$ in water. High-resolution mass spectra (HRMS) were obtained from waters LCT Premier (ESI/TOF). Flash chromatography (FC) was performed on Merck 60 silica gel (230 - 400 mesh). Melting points were determined on a Kofler melting point apparatus. NMR spectra were mesured on an Ultrafield AVANCE300 (^{1}H, 300 MHz; ^{13}C, 75 MHz) spectrometer. Unless otherwise stated, NMR data were obtained under ambient temperature conditions. Chemical shifts for ^{1}H NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard (dimethyl sulfoxide: δ 2.50 ppm, chloroform: δ 7.26 ppm). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard (dimethyl sulfoxide: δ 39.52 ppm, chloroform: δ 77.16 ppm). Data are reported as following: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, m = multiplet, br = broad signal), coupling constant (Hz), and integration.

Reagents: Unless otherwise noted, all commercially available aldehydes, β-nitroalkenes, indoles and arenes were purchased from various commercial sources (Acros, Aldrich) and used without further purification.

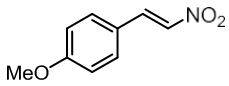
General procedures for the synthesis of *β*-nitroalkenes

General procedure for **2b** – **2l** is described as following**:** A catalytic amount of ammonium acetate (30 mol %) was added to a stirred solution of aldehydes (5 mmol) and nitromethane (20 mL) and then refluxed for 5 hours. The reaction mixture was cooled and treated with DCM (10 mL) and water (20 mL) and then extracted by DCM (20 mL × 3). The combined extraction was washed by brine, dried over anhydrous $NaSO_4$ and concentrated in vacuum. The residue was purified by silica-gel column chromatography using cyclohexane: ethyl acetate as eluant to give desired products

General procedure for **2m** – **2o** is described as following**:** To a mixture of aldehydes (20 mmol) and nitromethane (20 mmol) in methanol (5 mL) was added a solution of NaOH in H_2O (24 mmol in 2 mL) dropwise at 0 °C. Further methanol (2 mL) was added and the resulting yellow slurry was stirred at that temperature for 1 h. Water (30 mL) was added and the clear yellow solution was poured into 3N hydrochloric acid and stirred for 15 min. The aqueous mixture was extracted with DCM (20 mL × 3), the combined organic layers were dried over anhydrous $NaSO_4$ and concentrated in vacuum. The residue was purified by column chromatography using cyclohexane: ethyl acetate as eluant to give desired products

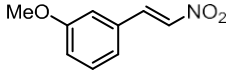
Physical data of substituted *β*-nitroalkenes

(E)-1-methoxy-4-(2-nitrovinyl)benzene (2b)



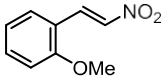
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 13.6 Hz, 1H), 7.53 - 7.48 (m, 3H), 6.95 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.1, 139.1, 135.2, 131.3, 122.7, 115.0, 55.7.

(E)-1-methoxy-3-(2-nitrovinyl)benzene (2c)



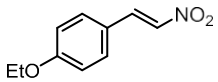
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, *J* = 13.7 Hz, 1H), 7.56 (d, *J* = 13.7 Hz, 1H), 7.36 (t, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.05 – 7.02 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.2, 139.1, 137.4, 131.4, 130.5, 121.8, 118.0, 114.1, 55.5.

(E)-1-methoxy-2-(2-nitrovinyl)benzene (2d)



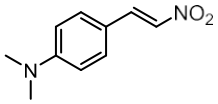
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (d, *J* = 13.6 Hz, 1H), 7.86 (d, *J* = 13.6 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.04 – 6.96 (m, 2H), 3.94 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 138.3, 135.6, 133.5, 132.5, 121.2, 119.2, 111.4, 55.7.

(E)-1-ethoxy-4-(2-nitrovinyl)benzene (2e)



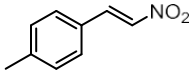
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 13.6 Hz, 1H), 7.49 – 7.47 (m, 3H), 6.93 (d, *J* = 8.7 Hz, 2H), 4.08 (q, *J* = 7.0 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 139.2, 135.0, 131.3, 122.4, 115.5, 64.0, 14.7.

(E)-N,N-dimethyl-4-(2-nitrovinyl)aniline (2f)



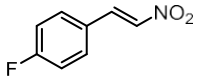
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 13.4 Hz, 1H), 7.51 – 7.41 (m, 3H), 6.70 (d, *J* = 8.9 Hz, 2H), 3.07 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.0, 140.3, 132.3, 131.6, 117.6, 112.2 , 40.3.

(E)-1-methyl-4-(2-nitrovinyl)benzene (2g)



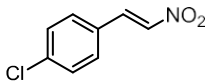
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 13.6 Hz, 1H), 7.58 (d, *J* = 13.7 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.2, 139.3, 136.4, 130.2, 129.3, 127.4, 21.8.

(E)-1-fluoro-4-(2-nitrovinyl)benzene (2h)



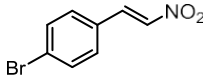
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 13.7 Hz, 1H), 7.59 – 7.51 (m, 3H), 7.15 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ165.05 (d, *J* = 253.5 Hz), 138.0, 137.0, 131.4 (d, *J* = 8.9 Hz), 126.4 (d, *J* = 3.2 Hz), 116.9 (d, *J* = 22.5 Hz).

(E)-1-chloro-4-(2-nitrovinyl)benzene (2i)



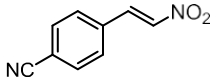
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 13.7 Hz, 1H), 7.58 – 7.41 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.5, 137.8, 137.5, 130.4, 129.9, 128.6.

(E)-1-bromo-4-(2-nitrovinyl)benzene (2j)



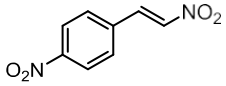
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, *J* = 13.7 Hz, 1H), 7.61 – 7.55 (m, 3H), 7.41 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.9, 137.6, 132.8, 130.5, 129.1, 126.9.

(E)-4-(2-nitrovinyl)benzonitrile (2k)



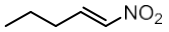
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (d, *J* = 13.8 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.67 – 7.59 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.6, 136.7, 134.5, 133.1, 129.5, 117.9, 115.3.

(E)-1-nitro-4-(2-nitrovinyl)benzene (2l)



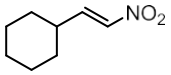
^{1}H NMR (300 MHz, DMSO) δ 8.36 (d, *J* = 13.7 Hz, 1H), 8.29 – 8.20 (m, 3H), 8.10 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, DMSO) δ 148.9, 140.9, 136.8, 136.5, 130.8, 124.0.

(E)-1-nitropent-1-ene (2m)



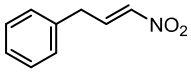
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 – 7.21 (m, 1H), 6.97 (d, *J* = 13.4 Hz, 1H), 2.28 – 2.20 (m, 2H), 1.60 – 1.48 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.6, 139.7, 30.3, 21.1, 13.5.

(E)-(2-nitrovinyl)cyclohexane (2n)



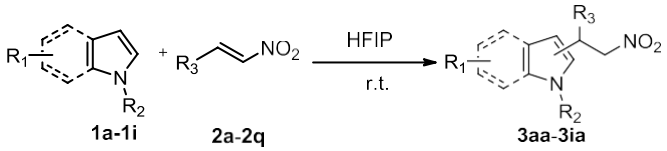
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25 – 7.18 (m, 1H), 6.92 (d, *J* = 13.5 Hz, 1H), 2.30 – 2.20 (m, 1H), 1.82 – 1.69 (m, 6H), 1.39 – 1.14 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.4, 138.4, 37.7, 31.6, 25.7, 25.6.

(E)-(3-nitroallyl)benzene (3o)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 – 7.20 (m, 6H), 6.94 (d, *J* = 13.4 Hz, 1H), 3.61 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.2, 140.5, 135.8, 129.2, 128.9, 127.5, 34.7.

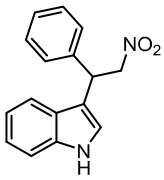
General procedures for this FC alkylation of Indoles with *β*-nitroalkenes



To a stirred solution of indoles (0.6 mmol) in HFIP (2 mL) was added *β*-nitroalkene (0.5 mmol) under air. The reaction mixture was stirred at room temperature for 2 ~ 16 h. After, the reaction mixture was evaporated under reduce pressure and the crude product was purified by column chromatography on silica gel using cyclohexane: ethyl acetate (10: 1) as the eluent to give title products.

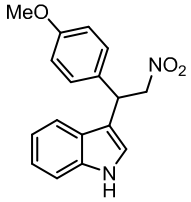
Physical data of 3aa – 3ia

3-(2-nitro-1-phenylethyl)-1H-indole (3aa) [1]



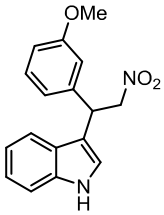
White solid; m.p. 102 - 104 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.22 (m, 7H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 2.3 Hz, 1H), 5.24 (t, *J* = 8.0 Hz, 1H), 5.13 – 5.06 (m, 1H), 5.01 – 4.94 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.3, 136.6, 129.0, 127.8, 127.6, 126.2, 122.7, 121.7, 120.0, 119.0, 114.4, 111.5, 79.6, 41.6.

3-(1-(4-methoxyphenyl)-2-nitroethyl)-1H-indole (3ab) [1]



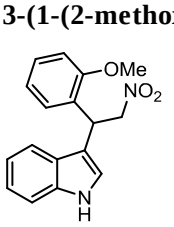
White solid; m.p. 154 - 156 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.25 – 7.17 (m, 3H), 7.07 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 1.8 Hz, 1H), 6.85 (d, *J* = 8.7 Hz, 2H), 5.14 (t, *J* = 7.9 Hz, 1H), 5.08 – 5.01 (m, 1H), 4.93 – 4.86 (m, 1H), 3.77 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 136.7, 131.3, 129.0, 126.3, 122.8, 121.6, 120.1, 119.1, 115.0, 114.4, 111.5, 79.9, 55.4, 41.0.

3-(1-(3-methoxyphenyl)-2-nitroethyl)-1H-indole (3ac) [1]



Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.28 – 7.18 (m, 2H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 2.3 Hz, 1H), 6.94 (d, *J* = 7.9 Hz, 1H), 6.88 (s, 1H), 6.82 – 6.79 (m, 1H), 5.17 (t, *J* = 7.9 Hz, 1H), 5.08 – 5.02 (m, 1H), 4.97 – 4.90 (m, 1H), 3.77 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0, 141.0, 136.6, 130.0, 126.2, 122.8, 121.7, 120.1, 120.1, 119.1, 114.4, 114.1, 112.6, 111.5, 79.6, 55.3, 41.6.

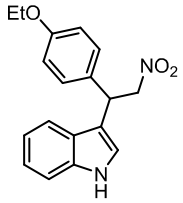
3-(1-(2-methoxyphenyl)-2-nitroethyl)-1H-indole (3ad) [2]



White solid; m.p. 92 - 94 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.26 – 7.06 (m, 5H), 6.93 (d, *J* = 8.2 Hz, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 5.62 (t, *J* = 7.5 Hz, 1H), 5.09 – 4.95 (m, 2H), 3.92 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.0, 136.5, 129.1,

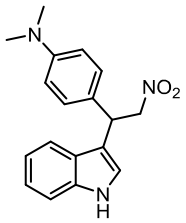
128.8, 127.4, 126.7, 122.6, 122.1, 120.9, 119.9, 119.2, 114.1, 111.4, 111.0, 78.3, 55.7, 35.7.

3-(1-(4-ethoxyphenyl)-2-nitroethyl)-1H-indole (3ae)



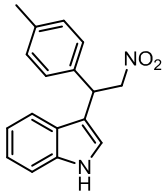
Yellow solid; m.p. 114 - 116 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.26 – 7.18 (m, 3H), 7.08 (t, *J* = 7.5 Hz, 1H), 7.00 (s, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 5.14 (t, *J* = 7.9 Hz, 1H), 5.08 – 5.01 (m, 1H), 4.93 – 4.86 (m, 1H), 4.00 (q, *J* = 7.0 Hz, 2H), 1.40 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.4, 136.6, 131.1, 128.9, 126.2, 122.7, 121.6, 120.0, 119.1, 114.9, 111.5, 110.1, 79.9, 63.5, 41.0, 14.9; HRMS calcd. for $C_{18}H_{19}N_2O_3$ $[M+H]^+$ m/z 311.1396, found 311.1389.

4-(1-(1H-indol-3-yl)-2-nitroethyl)-N, N-dimethylaniline (3af) [3]



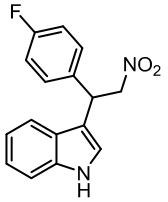
White solid; m.p. 132 - 134 ^{o}C; ^{1}H NMR (300 MHz, DMSO) δ 10.99 (s, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 8.5 Hz, 2H), 5.30 – 5.14 (m, 2H), 4.93 (t, *J* = 8.1 Hz, 1H), 2.82 (s, 6H); ^{13}C NMR (75 MHz, DMSO) δ 149.3, 136.3, 128.3, 128.0, 126.1, 121.9, 121.2, 118.5, 118.5, 114.1, 112.4, 111.4, 79.6, 40.1, 40.1.

3-(2-nitro-1-(p-tolyl)ethyl)-1H-indole (3ag) [1]



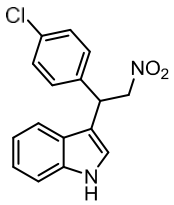
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.19 (m, 3H), 7.16 – 7.08 (m, 3H), 7.00 (d, *J* = 2.2 Hz, 1H), 5.17 (t, *J* = 7.9 Hz, 1H), 5.09 – 5.02 (m, 1H), 4.96 – 4.89 (m, 1H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.3, 136.6, 136.2, 129.7, 127.7, 126.2, 122.7, 121.7, 120.0, 119.0, 114.7, 111.5, 79.7, 41.3, 21.1.

3-(1-(4-fluorophenyl)-2-nitroethyl)-1H-indole (3ah) [1]



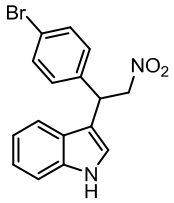
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.44 – 7.20 (m, 5H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.04 – 6.99 (m, 3H), 5.19 (t, *J* = 8.0 Hz, 1H), 5.09 – 5.03 (m, 1H), 4.94 – 4.87 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.2 (d, *J* = 244.5 Hz), 136.6, 135.0 (d, *J* = 3.0 Hz), 129.5 (d, *J* = 8.1 Hz), 126.03, 122.9, 121.5, 120.1, 118.9, 115.9 (d, *J* = 21.4 Hz), 114.3, 111.6, 79.6, 41.0.

3-(1-(4-chlorophenyl)-2-nitroethyl)-1H-indole (3ai) [1]



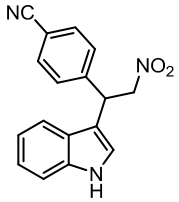
White solid; m.p. 108 - 110 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.42 – 7.19 (m, 7H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.01 (s, 1H), 5.17 (t, *J* = 7.9 Hz, 1H), 5.09 – 5.02 (m, 1H), 4.94 – 4.87 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.9, 136.6, 133.5, 129.3, 129.2, 126.0, 123.0, 121.6, 120.2, 118.9, 114.1, 111.6, 79.4, 41.1.

3-(1-(4-bromophenyl)-2-nitroethyl)-1H-indole (3aj) [1]



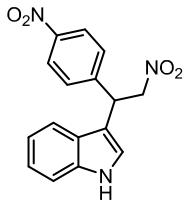
White solid; m.p. 128 - 130 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.46 – 7.35 (m, 4H), 7.26 – 7.20 (m, 3H), 7.10 (t, *J* = 7.3 Hz, 1H), 7.00 (d, *J* = 1.8 Hz, 1H), 5.16 (t, *J* = 7.9 Hz, 1H), 5.08 – 5.02 (m, 1H), 4.94 – 4.87 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.4, 136.6, 132.2, 129.6, 1260., 123.0, 121.6, 120.2, 118.9, 114.0, 111.6, 110.1, 79.3, 41.1.

4-(1-(1H-indol-3-yl)-2-nitroethyl)benzonitrile (3ak)



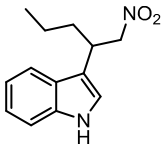
White solid; m.p. 160 - 162 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.04 (s, 1H), 5.30 – 5.22 (m, 1H), 5.12 – 5.05 (m, 1H), 4.99 – 4.92 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.9, 136.6, 132.9, 128.8, 125.8, 123.2, 121.7, 120.4, 118.7, 118.6, 113.2, 111.7, 78.9, 41.6; HRMS calcd. for $C_{17}H_{14}N_3O_2$ $[M+H]^+$ m/z 292.1086, found 292.1093.

3-(2-nitro-1-(4-nitrophenyl)ethyl)-1H-indole (3al) [4]



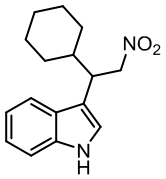
Yellow solid; m.p. 154 - 156 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 – 8.16 (m, 3H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.12 – 7.05 (m, 2H), 5.30 (t, *J* = 7.8 Hz, 1H), 5.15 – 5.08 (m, 1H), 5.03 – 4.95 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.8, 136.6, 128.9, 125.7, 124.3, 123.2, 121.7, 120.5 , 118.6, 113.1, 111.8, 110.1, 78.8, 41.4.

3-(1-nitropentan-2-yl)-1H-indole (3am) [5]



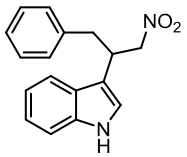
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.12 (m, 2H), 7.04 (d, *J* = 2.2 Hz, 1H), 4.72 – 4.60 (m, 2H), 3.87 – 3.77 (m, 1H), 1.95 – 1.70 (m, 2H), 1.40 – 1.26 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.6, 126.32, 122.6, 122.0, 119.9, 118.9, 114.3, 111.6, 80.7, 36.2, 34.7, 20.5, 14.0.

3-(1-cyclohexyl-2-nitroethyl)-1H-indole (3an) [6]



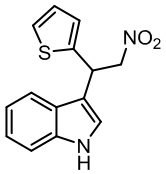
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.12 (m, 2H), 6.97 (d, *J* = 2.0 Hz, 1H), 4.86 – 4.69 (m, 2H), 3.73 – 3.65 (m, 1H), 1.87 – 1.65 (m, 6H), 1.33 – 0.89 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.4, 127.0, 122.3, 119.8, 119.2, 113.4, 111.5, 78.6, 42.0, 40.6, 31.3, 30.5, 26.4, 26.3.

3-(1-nitro-3-phenylpropan-2-yl)-1H-indole (3ao)



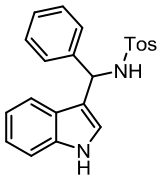
Yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.36 – 7.14 (m, 8H), 6.88 (d, *J* = 1.9 Hz, 1H), 4.77 – 4.64 (m, 2H), 4.20 – 4.10 (m, 1H), 3.29 – 3.22 (m, 1H), 3.15 – 3.08 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.5, 136.5, 129.2, 128.6, 126.7, 126.0, 122.5, 122.1, 119.9, 118.7, 113.7, 111.7, 79.2, 38.9, 38.0; HRMS calcd. for $C_{17}H_{17}N_2O_2$ $[M+H]^+$ m/z 281.1290, found 281.1292.

3-(2-nitro-1-(thiophen-2-yl)ethyl)-1H-indole (3ap) [4]



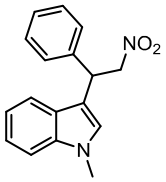
Yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.40 – 7.35 (m, 2H), 7.26 – 7.09 (m, 3H), 6.33 – 6.32 (m, 1H), 6.18 (d, *J* = 3.1 Hz, 1H), 5.27 (t, *J* = 7.8 Hz, 1H), 5.10 – 5.04 (m, 1H), 4.96 – 4.89 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.3, 142.4, 136.4, 125.8, 122.8, 122.7, 120.2, 118.8, 111.7, 110.6, 110.1, 107.5, 78.0, 35.8.

N-((1H-indol-3-yl)(phenyl)methyl)-4-methylbenzenesulfonamide (3aq) [7]



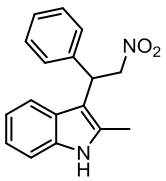
White solid; m.p. 160 - 162 °C; ^{1}H NMR (300 MHz, DMSO) δ 10.87 (s, 1H), 8.50 (d, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.26 (m, 4H), 7.17 – 7.01 (m, 6H), 6.88 (t, *J* = 7.4 Hz, 1H), 6.79 (s, 1H), 5.75 (d, *J* = 8.7 Hz, 1H), 2.26 (d, *J* = 10.8 Hz, 3H); ^{13}C NMR (75 MHz, DMSO) δ 141.8, 141.7, 138.8, 136.4, 128.9, 127.9, 127.1, 126.6, 126.4, 125.5, 123.7, 121.2, 118.9, 118.5, 115.7, 111.4, 54.5, 20.9.

1-methyl-3-(2-nitro-1-phenylethyl)-1H-indole (3ba) [8]



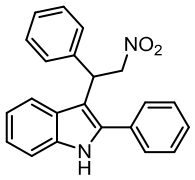
White solid; m.p. 96 - 98 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.22 (m, 7H), 7.10 (t, *J* = 7.3 Hz, 1H), 6.88 (s, 1H), 5.21 (t, *J* = 8.0 Hz, 1H), 5.10 – 5.03 (m, 1H), 4.98 – 4.91 (m, 1H), 3.75 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.5, 137.4, 129.0, 127.8, 127.6, 126.6, 126.5, 122.3, 119.5, 119.1, 112.9, 109.6, 79.6, 41.6, 32.9.

2-methyl-3-(2-nitro-1-phenylethyl)-1H-indole (3ca) [8]



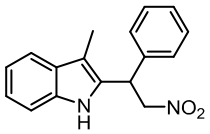
White solid; m.p. 110 - 112 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.41 – 7.25 (m, 7H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.08 – 7.03 (m, 1H), 5.28 – 5.11 (m, 3H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.6, 135.5, 133.0, 128.9, 127.4, 127.2, 127.0, 121.4, 119.8, 118.7, 110.8, 108.9, 78.7, 40.6, 12.1.

3-(2-nitro-1-phenylethyl)-2-phenyl-1H-indole (3da) [4]



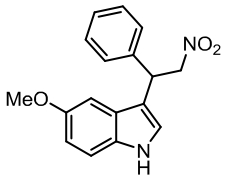
White solid; m.p. 148 - 150 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.46 (m, 5H), 7.40 -7.21 (m, 7H), 7.14 (t, *J* = 7.5 Hz, 1H), 5.36 (t, *J* = 7.8 Hz, 1H), 5.24 – 5.11 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.0, 137.1, 136.2, 132.3, 129.0, 129.0, 128.9, 128.7, 127.6, 127.3, 127.1, 122.6, 120.4, 120.0, 111.5, 109.7, 79.2, 40.9.

3-methyl-2-(2-nitro-1-phenylethyl)-1H-indole (3ea) [9]



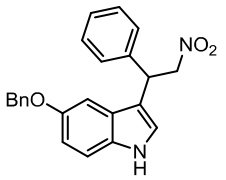
White solid; m.p. 130 - 132 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.55 (d, *J* = 7.1 Hz, 1H), 7.42 – 7.23 (m, 6H), 7.19 – 7.10 (m, 2H), 5.26 (t, *J* = 7.9 Hz, 1H), 5.12 – 5.05 (m, 1H), 4.98 – 4.92 (m, 1H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.1, 135.9, 130.7, 129.5, 129.2, 128.2, 127.4, 122.4, 119.7, 118.9, 110.9, 109.5, 77.7, 41.2, 8.8;

5-methoxy-3-(2-nitro-1-phenylethyl)-1H-indole (3fa) [4]



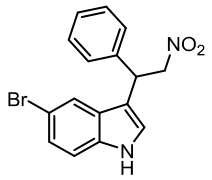
Yellow solid; m.p. 104 - 106 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.34 – 7.21 (m, 6H), 6.98 (d, *J* = 2.3 Hz, 1H), 6.88 – 6.85 (m, 2H), 5.14 (t, *J* = 7.9 Hz, 1H), 5.08 – 5,01 (m, 1H), 4.97 – 4.90 (m, 1H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.3, 139.3, 131.7, 129.0, 127.9, 127.7, 126.7, 122.4, 114.2, 112.8, 112.2, 101.0, 79.6, 56.0, 41.7.

5-(benzyloxy)-3-(2-nitro-1-phenylethyl)-1H-indole (3ga) [7]



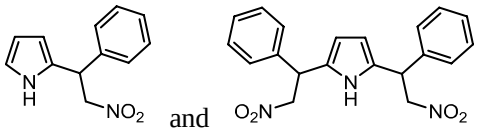
White solid; m.p. 102 - 104 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.46 – 7.21 (m, 11H), 6.95 – 6.93 (m, 3H), 5.12 (t, *J* = 8.1 Hz, 1H), 5.03 – 4.88 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.4, 139.2, 137.5, 131.8, 129.0, 128.7, 128.0, 127.8, 127.7, 127.7, 126.6, 122.4, 114.2, 113.6, 112.2, 102.6, 79.5, 71.0, 41.6.

5-bromo-3-(2-nitro-1-phenylethyl)-1H-indole (3ha) [8]



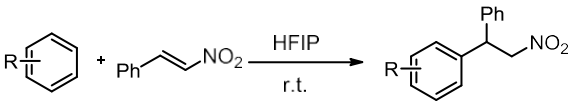
White solid; m.p. 130 - 132 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.56 (s, 1H), 7.36 – 7.18 (m, 7H), 7.04 (d, *J* = 2.0 Hz, 1H), 5.13 (t, *J* = 7.9 Hz, 1H), 5.05 – 4.99 (m, 1H), 4.95 – 4.88 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.8, 135.2, 129.2, 128.0, 127.9, 127.8, 125.8, 122.9, 121.6, 114.2, 113.4, 113.0, 79.5, 41.4.

3-(2-nitro-1-phenylethyl)-1H-pyrrole and 2,5-bis(2-nitro-1-phenylethyl)-1H-pyrrole (3ia) [4]



Yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (s, 0.77 × 1H), 7.58 (s, 0.23 × 1H), 7.39 – 7.15 (m, 0.77 × 5H + 0.23 × 10H), 6.69 (s, 0.77 × 1H), 6.18 – 6.16 (m, 0.77 × 1H), 6.10 (br, 0.77 × 1H), 6.02 – 5.99 (m, 0.23 × 2H), 5.02 – 4.70 (m, m, 0.77 × 3H + 0.23 × 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.1, 137.9, 129.6, 129.3, 129.2, 128.2, 128.0, 127.9, 127.9, 118.3, 108.8, 106.6, 106.3, 105.9, 79.3, 79.3, 43.0, 42.9.

General procedures for this FC alkylation of Indoles with *β*-nitroalkenes

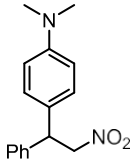


4a-4l **2a** **5a-5l**

To a stirred solution of electron-rich arenes (0.6 mmol) in HFIP (2 mL) was added *β*-nitroalkene (0.5 mmol) under air. The reaction mixture was stirred at room temperature for 16 ~ 24 h. After, the reaction mixture was evaporated under reduce pressure and the crude product was purified by column chromatography on silica gel using cyclohexane: ethyl acetate (15: 1) as the eluent to give title products.

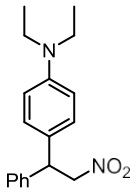
Physical data of 5a – 5l

N, N-dimethyl-4-(2-nitro-1-phenylethyl)aniline (5a) [10]



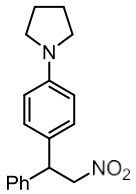
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 - 7.26 (m, 5H), 7.12 (d, *J* = 8.7 Hz, 2H), 6.70 (d, *J* = 8.7 Hz, 2H), 4.99 - 4.95 (m, 2H), 4.91 – 4.81 (m, 1H), 2.95 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.9, 140.1, 129.0, 128.4, 127.7, 127.4, 126.7, 112.9, 79.7, 48.3, 40.6.

N, N-diethyl-4-(2-nitro-1-phenylethyl)aniline (5b) [10]



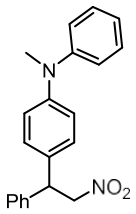
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 – 7.22 (m, 5H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.62 (d, *J* = 7.8 Hz, 2H), 5.01 – 4.88 (m, 2H), 4.81 (t, *J* = 7.8 Hz, 1H), 3.33 (q, *J* = 7.0 Hz, 4H), 1.15 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.2, 140.2, 129.0, 128.6, 127.7, 127.4, 125.6, 112.0, 79.8, 48.4, 44.4, 12.7.

1-(4-(2-nitro-1-phenylethyl)phenyl)pyrrolidine (5c) [10]



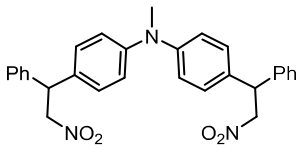
Light green solid; m.p. 90 - 92 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.21 (m, 5H), 7.09 (d, *J* = 8.6 Hz, 2H), 6.55 (d, *J* = 8.1 Hz, 2H), 5.01 – 4.89 (m, 2H), 4.82 (t, *J* = 8.1 Hz, 1H), 3.27 (t, *J* = 6.3 Hz, 4H), 2.02 – 1.98 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.1, 140.2, 129.0, 128.6, 127.7, 127.4, 126.0, 112.3, 79.8, 48.5, 48.0, 25.6.

N-methyl-4-(2-nitro-1-phenylethyl)-N-phenylaniline (5d)



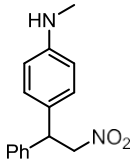
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 7H), 7.13 – 7.00 (m, 5H), 6.93 (d, *J* = 8.6 Hz, 2H), 4.98 – 4.95 (m, 2H), 4.85 (t, *J* = 7.2 Hz, 1H), 3.29 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.6, 148.4, 139.7, 131.0, 129.5, 129.1, 128.5, 127.7, 127.6, 122.6, 122.1, 119.4, 79.6, 48.5, 40.4; HRMS calcd. for $C_{21}H_{21}N_2O_2$ $[M+H]^+$ m/z 333.1603, found 333.1605.

N-methyl-4-(2-nitro-1-phenylethyl)-N-(4-(2-nitro-1-phenylethyl)phenyl)aniline (5d`)



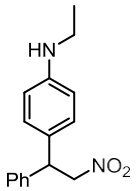
Light yellow solid; m.p. 130 - 132 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.26 (m, 10H), 7.17 (d, *J* = 8.6 Hz, 4H), 6.98 (d, *J* = 8.5 Hz, 4H), 5.00 – 4.87 (m, 6H), 3.27 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.0, 139.6, 132.1, 129.1, 128.6, 127.7, 127.6, 120.8, 79.5, 48.5, 40.2; HRMS calcd. for $C_{29}H_{28}N_3O_4$ $[M+H]^+$ m/z 482.2080, found 482.2080.

N-methyl-4-(2-nitro-1-phenylethyl)aniline (5f)



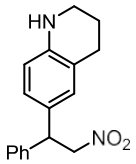
Light green solid; m.p. 94 - 96 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 – 7.23 (m, 5H), 7.06 (d, *J* = 8.4 Hz, 2H), 6.58 (d, *J* = 8.4 Hz, 2H), 4.96 – 4.88 (m, 2H), 4.81 (t, *J* = 8.1 Hz, 1H), 3.75 (s, 1H), 2.81 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.5, 140.0, 129.0, 128.6, 127.8, 127.7, 127.4, 113.0, 79.7, 48.4, 30.9; HRMS calcd. for $C_{15}H_{17}N_2O_2$ $[M+H]^+$ m/z 257.1290, found 257.1282.

N-ethyl-4-(2-nitro-1-phenylethyl)aniline (5g)



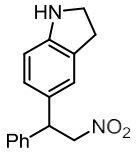
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.22 (m, 5H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 8.5 Hz, 2H), 4.99 – 4.87 (m, 2H), 4.80 (d, *J* = 7.8 Hz, 1H), 3.16 – 3.09 (m, 3H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.7, 140.0, 129.0, 128.6, 127.7, 127.4, 113.2, 79.7, 48.4, 38.6, 14.9; HRMS calcd. for $C_{16}H_{19}N_2O_2$ $[M+H]^+$ m/z 271.1447, found 271.1439.

6-(2-nitro-1-phenylethyl)-1,2,3,4-tetrahydroquinoline (5h)



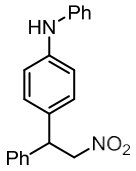
Yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 – 7.23 (m, 5H), 6.83 (m, 2H), 6.42 (d, *J* = 7.8 Hz, 1H), 4.99 – 4.87 (m, 2H), 4.77 (t, *J* = 7.8 Hz, 1H), 3.88 (s, 1H), 3.27 (t, *J* = 5.4 Hz, 2H), 2.72 (t, *J* = 6.4 Hz, 2H), 1.96 – 1.88 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.0, 140.1, 128.9, 128.8, 127.6, 127.4, 127.3, 125.9, 121.8, 114.5, 79.7, 48.5, 41.9, 27.0, 22.; HRMS calcd. for $C_{17}H_{19}N_2O_2$ $[M+H]^+$ m/z 283.1447, found 283.1439.

5-(2-nitro-1-phenylethyl)indoline (5i)



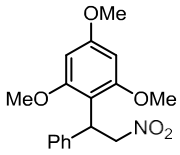
Gray liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.32 (m, 2H), 7.28 – 7.25 (m, 3H), 6.98 (s, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.60 (d, *J* = 8.0 Hz, 1H), 5.01 – 4.89 (m, 2H), 4.84 – 4.82 (m, 1H), 3.56 (t, *J* = 8.4 Hz, 3H), 3.00 (t, *J* = 8.3 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.8, 140.1, 130.5, 129.6, 129.0, 127.6, 127.441, 126.7, 124.2, 109.7, 79.8, 48.7, 47.5, 29.8; HRMS calcd. for $C_{16}H_{17}N_2O_2$ $[M+H]^+$ m/z 269.1290, found 269.1289.

4-(2-nitro-1-phenylethyl)-N-phenylaniline (5j)



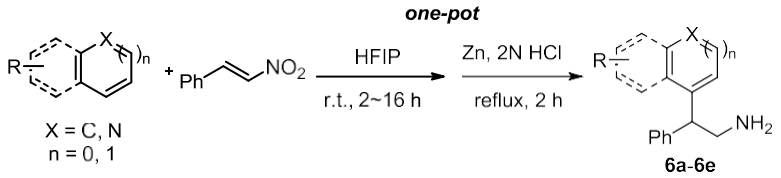
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.25 (m, 7H), 7.14 – 6.94 (m, 7H), 5.88 (s, 1H), 4.98 – 4.95 (m, 2H), 4.86 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.7, 142.63, 139.7, 131.5, 129.5, 129.1, 128.7, 127.7, 127.6, 121.7, 118.4, 117.9, 79.6, 48.5, 27.1; HRMS calcd. for $C_{20}H_{19}N_2O_2$ $[M+H]^+$ m/z 319.1447, found 319.1451.

1,3,5-trimethoxy-2-(2-nitro-1-phenylethyl)benzene (5l) [11]



White solid; m.p. 122 - 124 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 – 7.15 (m, 5H), 6.12 (s, 2H), 5.49 (t, *J* = 7.8 Hz, 1H), 5.27 – 5.20 (m, 1H), 5.16 – 5.09 (m, 1H), 3.79 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.7, 159.1, 140.6, 128.4, 127.7, 126.7, 108.8, 91.3, 78.4, 55.9, 55.4, 38.7.

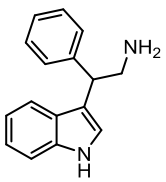
General procedures for one-pot synthesis of substituted tryptamines



To a stirred solution of indoles or electron-rich arenes (0.6 mmol) in HFIP (2 mL) was added *β*-nitroalkene (0.5 mmol) under air. The reaction mixture was stirred at room temperature for 2 ~ 16 h. Then zink power (2.0 mmol) and 2 N HCl (2.5 ml) were added and the mixture was refluxed for 2 h, cooled down to room temperature, NaOH (10%) was added to the above mixture until pH 10, then extracted with DCM (15 mL x 3). The organic layer was washed with brine, dried over anhydrous Na_2SO_4 and evaporated under reduce pressure to get crude product. Then the crude product was purified by column chromatography on silica gel using DCM : methanol (95 : 5) as the eluent to give title products.

Physical data of 6a – 6f

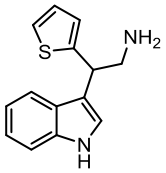
2-(1H-indol-3-yl)-2-phenylethan-1-amine (6a) [12]



White solid; m.p. 134 - 136 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.47 (d, *J* = 7.9 Hz, 1H),

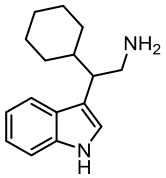
7.35 – 7.26 (m, 5H), 7.24 – 7.15 (m, 2H), 7.07 – 7.03 (m, 2H), 4.26 (t, J = 7.4 Hz, 1H), 3.48 – 3.41 (m, 1H), 3.33 – 3.26 (m, 1H), 1.61 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.1, 136.6, 128.6, 128.3, 127.1, 126.6, 122.2, 121.4, 119.5, 119.5, 117.6, 111.3, 47.4, 47.3, 47.0.

2-(1H-indol-3-yl)-2-(thiophen-2-yl)ethan-1-amine (6b) [12]



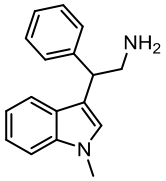
Gray solid; m.p. 126 - 128 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.36 – 7.34 (m, 2H), 7.19 (t, J = 7.5 Hz, 1H), 7.11 – 7.09 (m, 2H), 6.31 (br, 1H), 6.12 (d, J = 2.8 Hz, 1H), 4.34 (t, J = 7.0 Hz, 1H), 3.40 – 3.28 (m, 2H), 1.56 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.5, 141.5, 136.6, 126.7, 122.4, 122.3, 119.6, 119.4, 114.9, 111.4, 110.3, 106.2, 45.9, 40.9.

2-cyclohexyl-2-(1H-indol-3-yl)ethan-1-amine (6c)



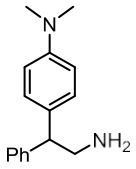
Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.36 (d, J = 8.0 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 6.97 (s, 1H), 3.04 – 2.99 (m, 2H), 2.79 – 2.72 (m, 1H), 1.93 – 1.43 (m, 8H), 1.31 – 0.89 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.7, 127.9, 122.2, 121.9, 119.7, 119.2, 116.6, 111.3, 44.2, 40.9, 31.8, 31.3, 26.7, 26.6; HRMS calcd. for $C_{16}H_{23}N_2$ $[M+H]^+$ m/z 243.1861, found 243.1856.

2-(1-methyl-1H-indol-3-yl)-2-phenylethan-1-amine (6d) [13]



Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, J = 7.9 Hz, 1H), 7.37 – 7.29 (m, 5H), 7.26 – 7.20 (m), 7.06 (t, J = 7.4 Hz, 1H), 6.93 (s, 1H), 4.30 (t, J = 7.4 Hz, 1H), 3.75 (s, 3H), 3.48 – 3.41 (m, 1H), 3.33 – 3.26 (m, 1H), 2.13 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.1, 137.3, 128.6, 128.2, 127.5, 126.5, 126.2, 121.8, 119.5, 118.9, 116.0, 109.3, 47.2, 46.6, 32.8.

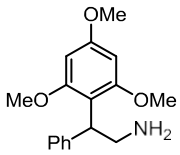
4-(2-amino-1-phenylethyl)-N,N-dimethylaniline (6e)



Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 – 7.16 (m, 5H), 7.12 (d, J = 8.7 Hz, 2H), 6.69

(d, *J* = 8.6 Hz, 2H), 3.93 (t, *J* = 7.7 Hz, 1H), 3.28 (d, *J* = 7.7 Hz, 2H), 2.93 (d, *J* = 11.1 Hz, 6H), 2.13 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.5, 143.5, 130.4, 128.8, 128.7, 128.1, 126.4, 113.0, 53.7, 47.0, 40.8; HRMS calcd. for $C_{16}H_{21}N_2$ $[M+H]^+$ m/z 241.1705, found 241.1708.

2-phenyl-2-(2,4,6-trimethoxyphenyl)ethan-1-amine (6f)



Light yellow liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.3 Hz, 2H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.14 (t, *J* = 7.1 Hz, 1H), 6.15 (s, 2H), 4.64 (t, *J* = 7.9 Hz, 1H), 3.79 (s, 3H), 3.74 (s, 6H), 3.46 (d, *J* = 7.9 Hz, 2H), 2.19 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.9, 159.4, 143.4, 128.0, 127.8, 125.5, 111.1, 91.1, 55.6, 55.2, 44.1, 44.0; HRMS calcd. for $C_{17}H_{22}NO_3$ $[M+H]^+$ m/z 288.1600, found 288.1592.

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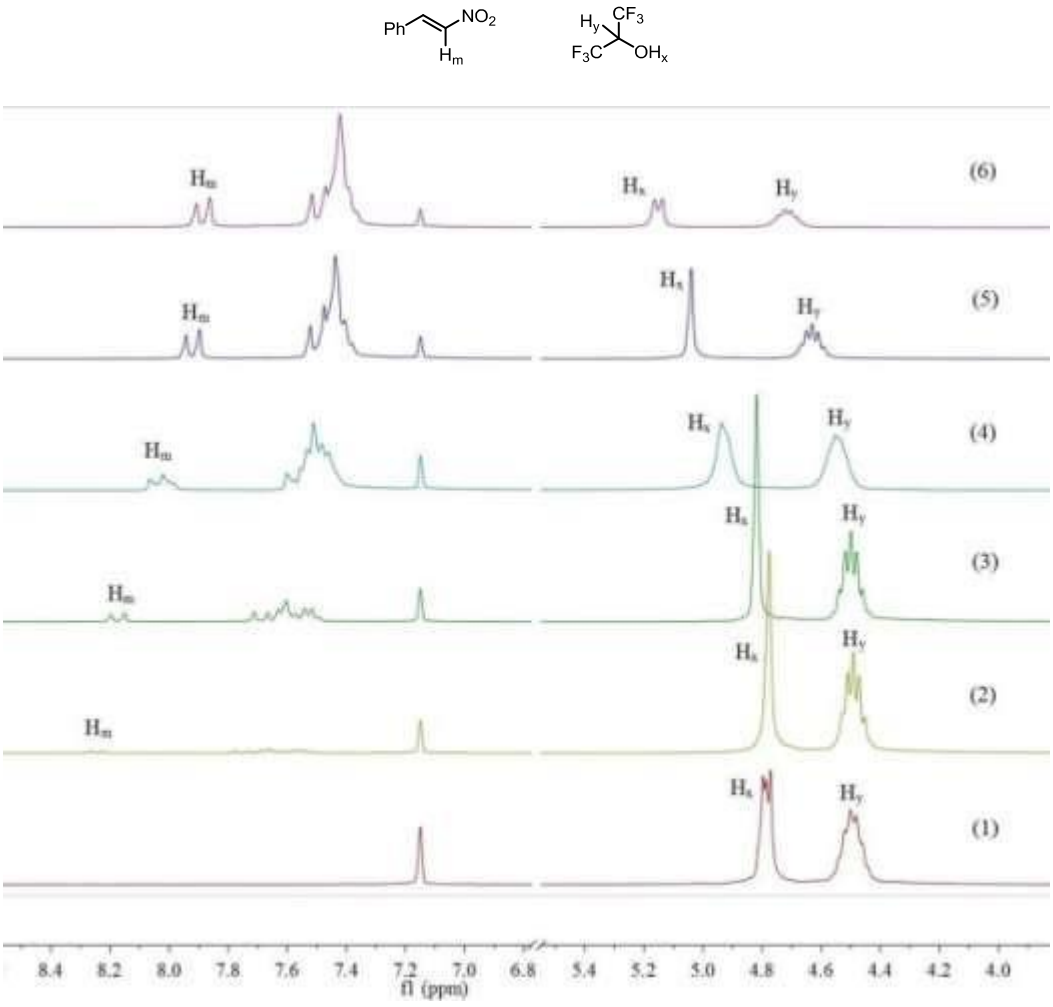
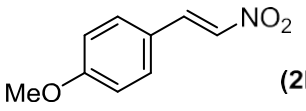
^{1}H NMR titration of a mixture of HFIP and β-nitroalkene [a]

In NMR tube, different quantities of β-nitroalkene (**2a**) were dissolved in 1.0 mmol of HFIP. After, a capillary with C_6D_6 was placed into the NMR tube (external standard), and NMR spectrum (1 to 5) were subsequently measured. A downfield shift of the OH proton (H_x) of HFIP was observed with increasing concentrations of β-nitroalkene.

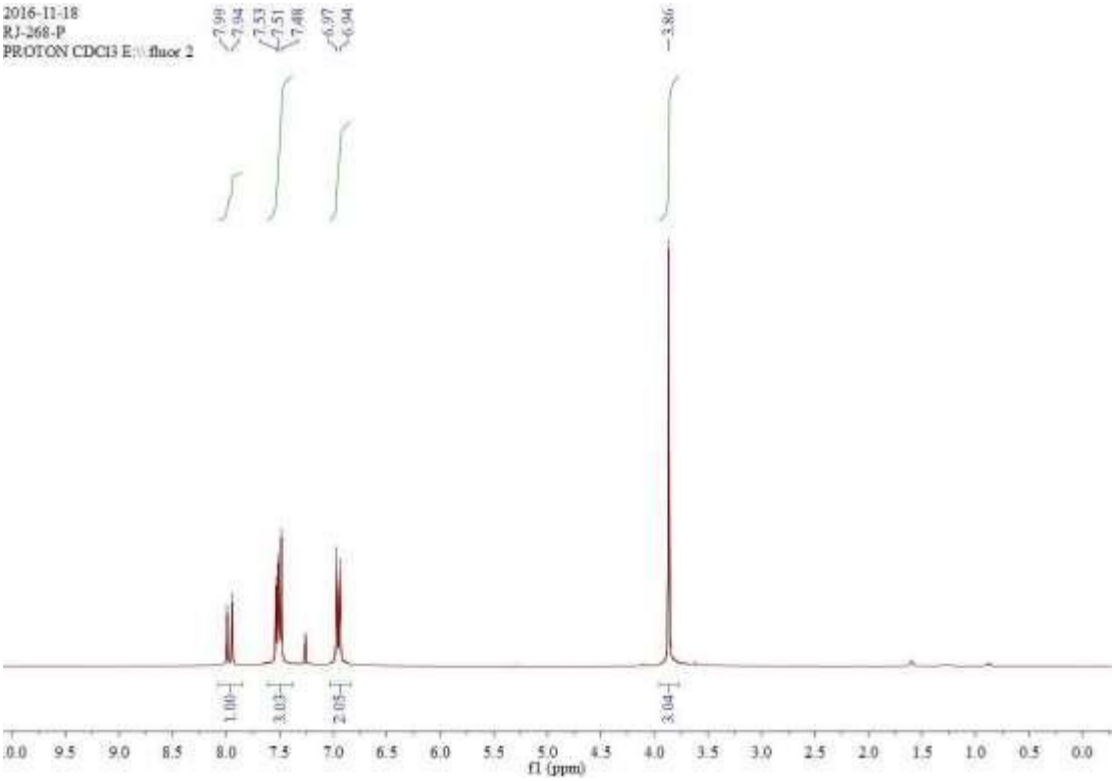


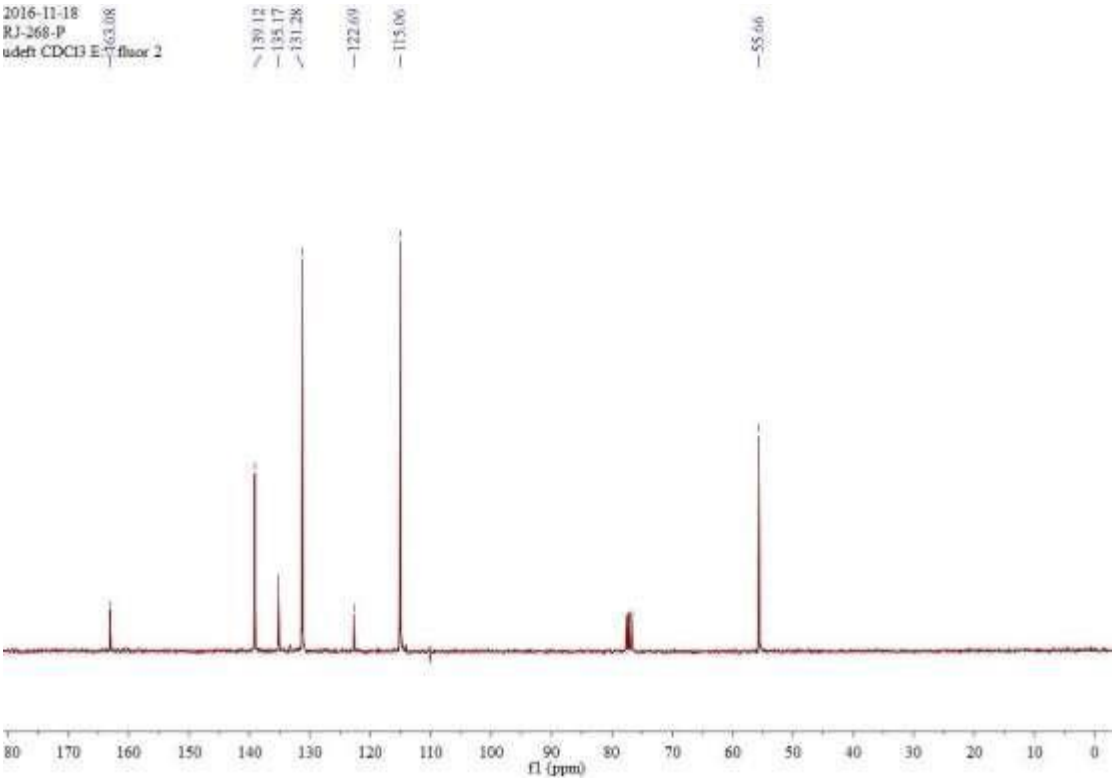
[a] Spectra were acquired in the presence of the following quantities of β-nitroalkenes: (1) 0 mol%; (2) 1 mol%; (3) 5 mol%; (4) 20 mol%; (5) 50 mol%; (6) 100 mol%. (C_6D_6 as external standard).

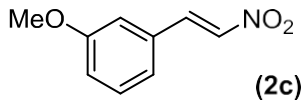
Spectra:


NO2
MeO

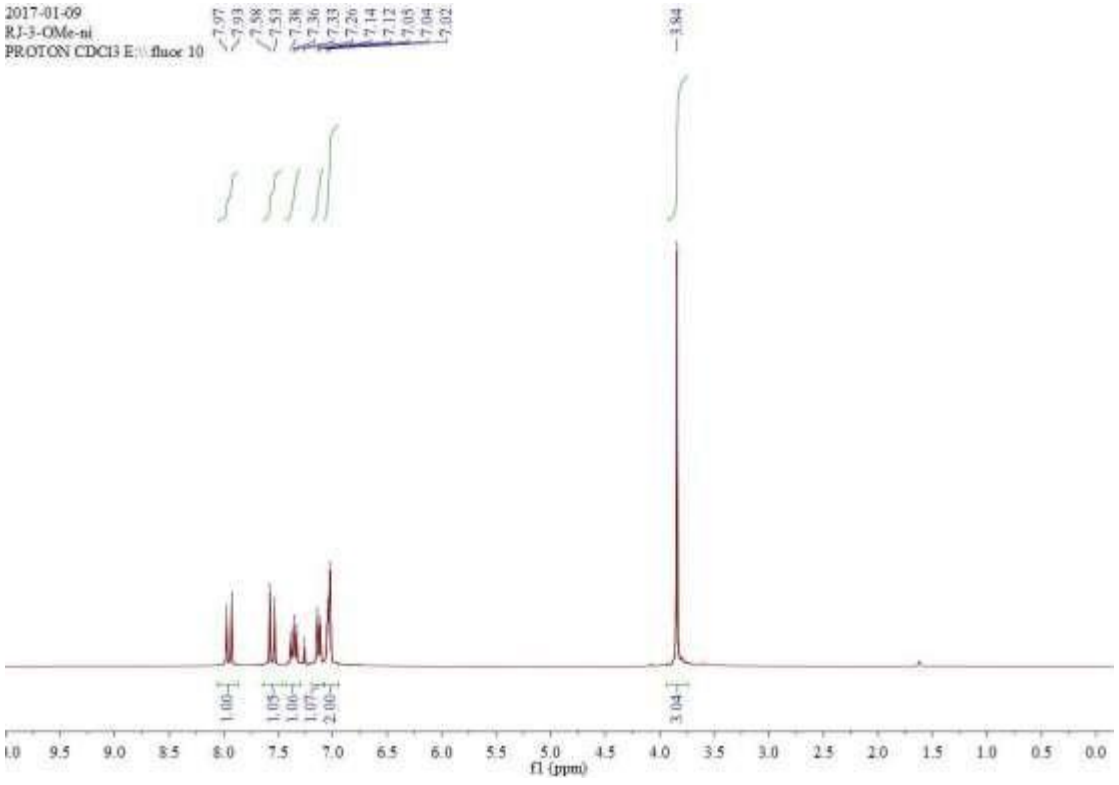
(2b)

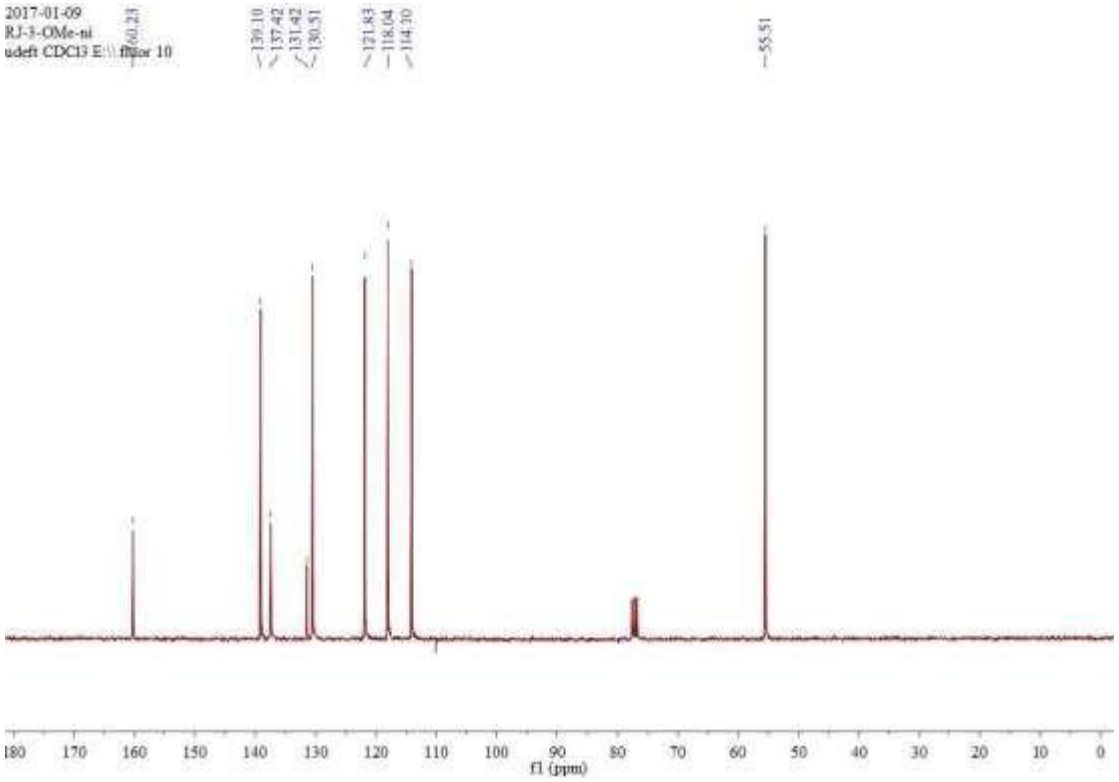

2016-11-18
RJ-268-P
PROTON CDCl3 E:\ fluor 2
7.99
7.94
7.53
7.51
7.48
6.97
6.94
3.86
1.00
3.03
2.05
3.04
f1 (ppm)

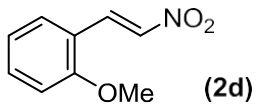

2016-11-18
RJ-268-P
udeft CDCl3 E:\ fluor 2
163.08
139.12
135.17
131.28
122.69
115.06
55.66
f1 (ppm)


MeO
NO2

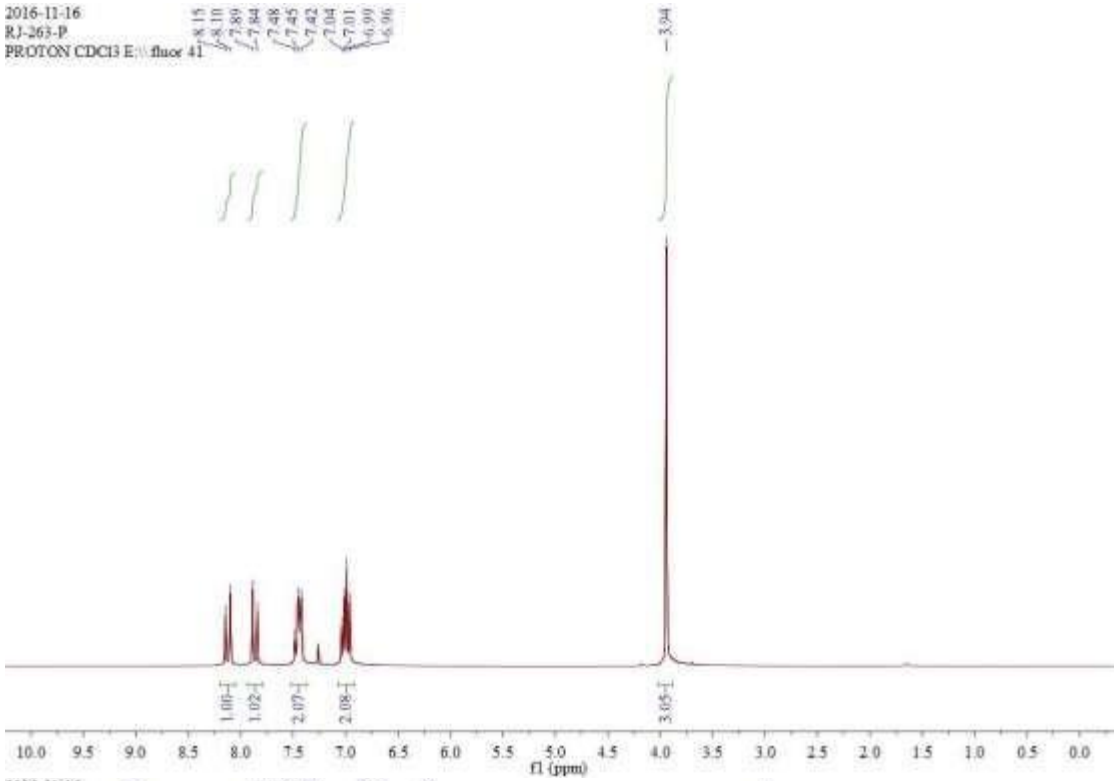
(2c)

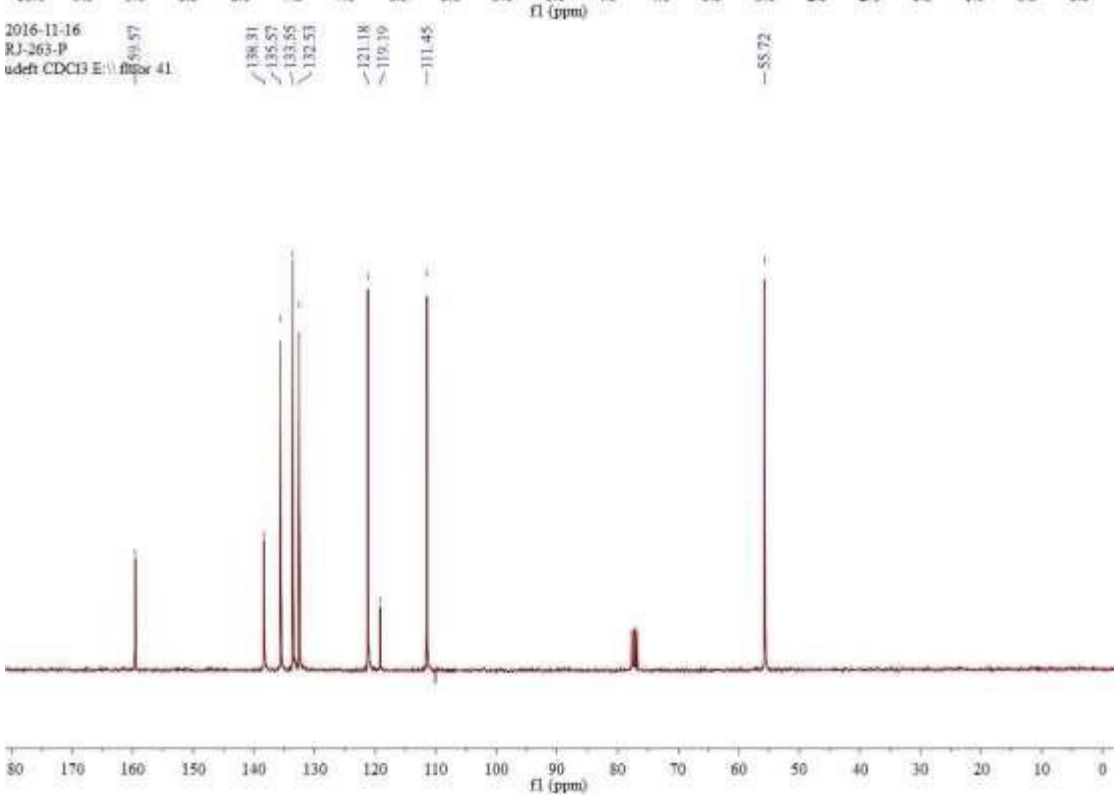

2017-01-09
RJ-3-OMe-ni
PROTON CDCl3 E:\\ fluor 10
7.97
7.93
7.58
7.53
7.38
7.36
7.33
7.26
7.14
7.12
7.05
7.04
7.02
3.84
1.00
1.05
1.00
1.07
2.00
3.04
f1 (ppm)

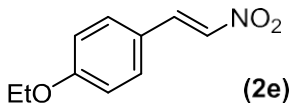

2017-01-09
RJ-3-OMe-ni
udeft CDCl3 E:\\ fluor 10
160.23
139.10
137.42
131.42
130.51
121.83
118.04
114.10
55.51
f1 (ppm)


NO2
OMe

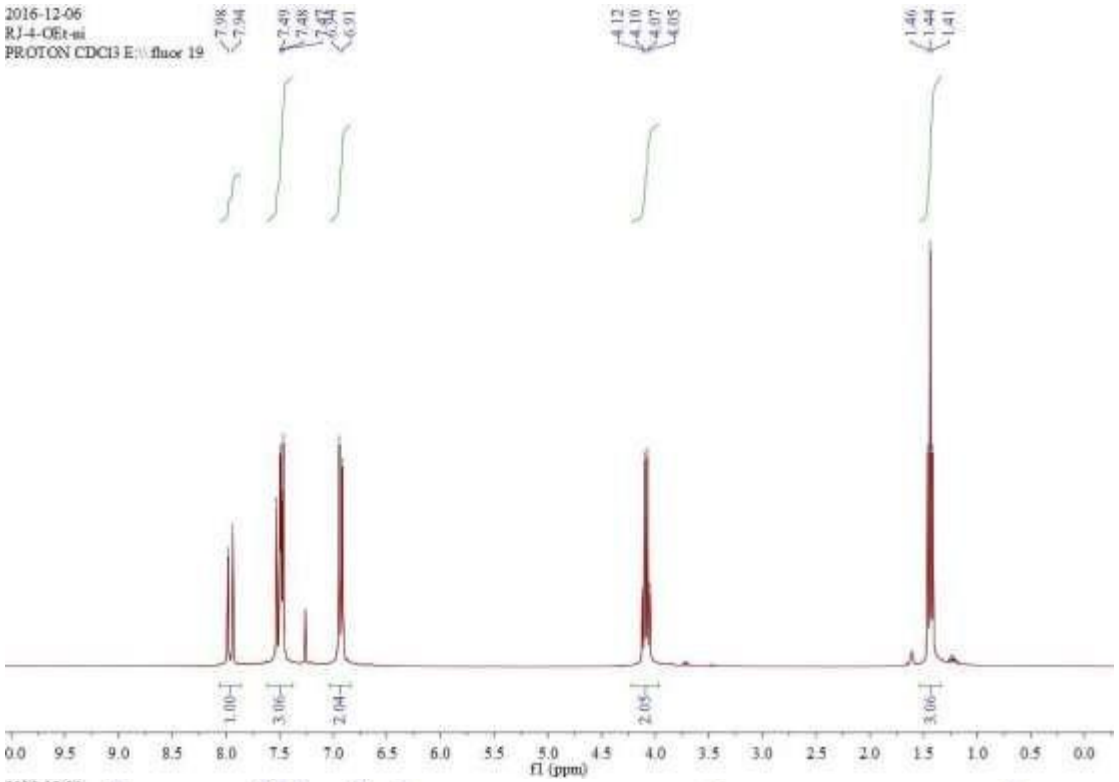
(2d)

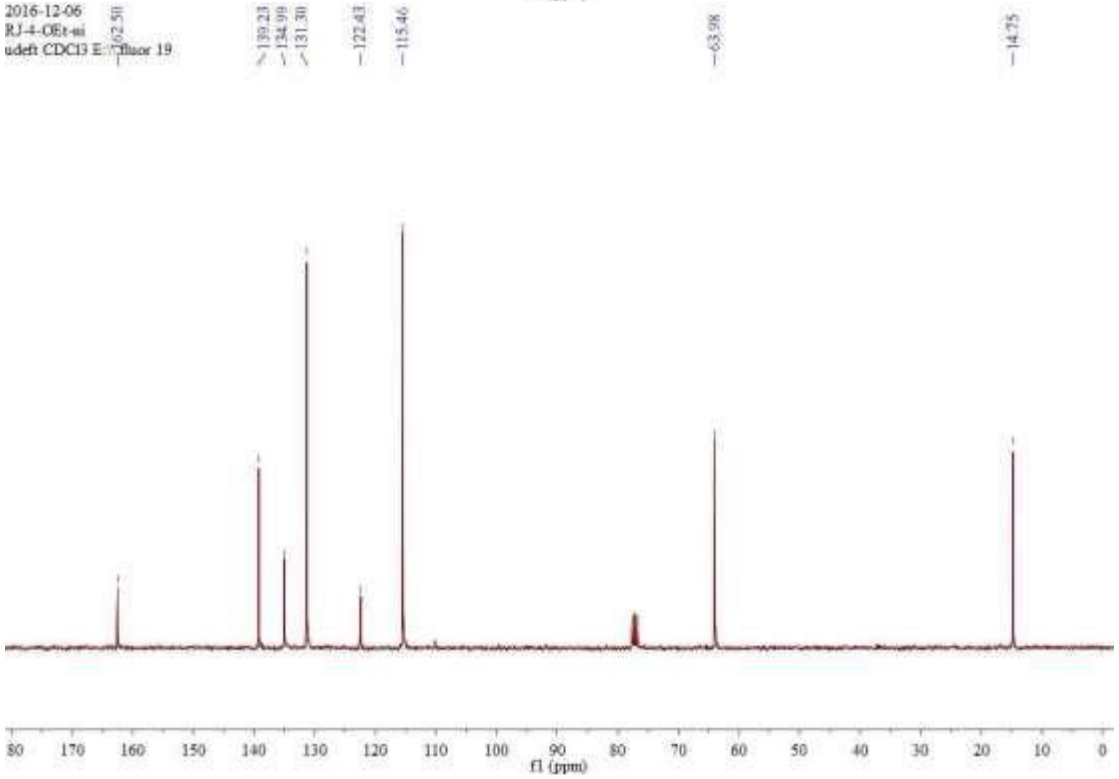

2016-11-16
RJ-263-P
PROTON CDCl3 E:\\ fluor 41
8.15
8.10
7.89
7.84
7.48
7.45
7.42
7.04
7.01
6.99
6.96
3.94
1.00
1.02
2.07
2.08
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

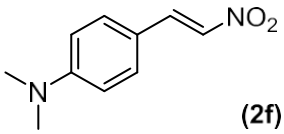

2016-11-16
RJ-263-P
udeft CDCl3 E:\\ fluor 41
159.57
138.31
135.57
133.55
132.53
121.18
119.19
111.45
55.72
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NO2
EtO

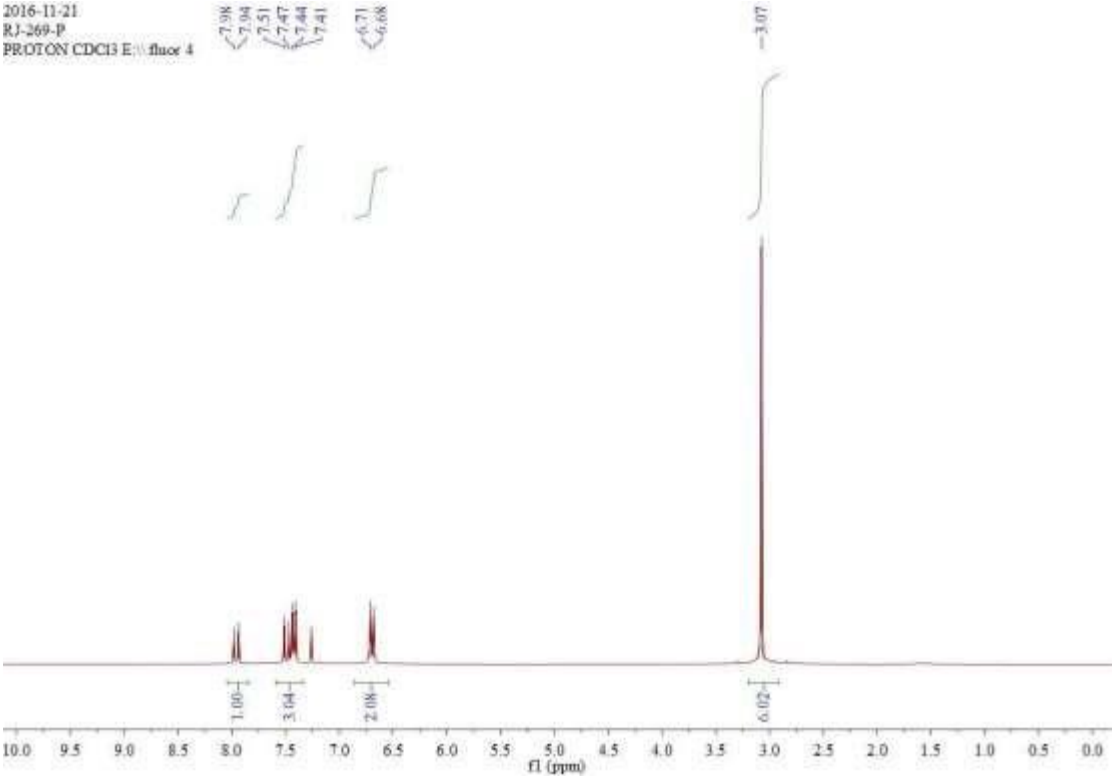
(2e)

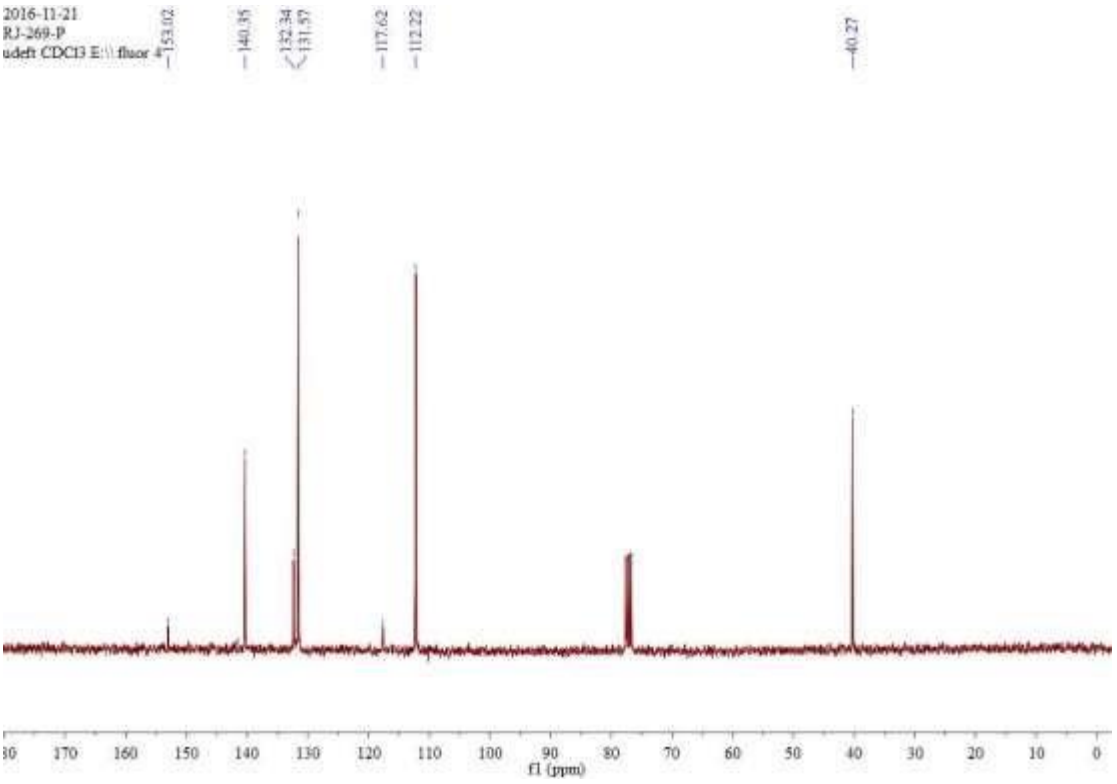

2016-12-06
RJ-4-OEt-si
PROTON CDCl3 E:\\ fluor 19
7.98
7.94
7.49
7.48
7.07
7.04
6.91
4.12
4.10
4.07
4.05
1.46
1.44
1.41
1.00
3.06
2.04
2.05
3.06
f1 (ppm)

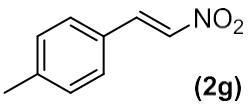

2016-12-06
RJ-4-OEt-si
udeft CDCl3 E:\\ fluor 19
162.50
139.23
134.99
131.30
122.43
115.46
63.98
14.75
f1 (ppm)


NO2
N

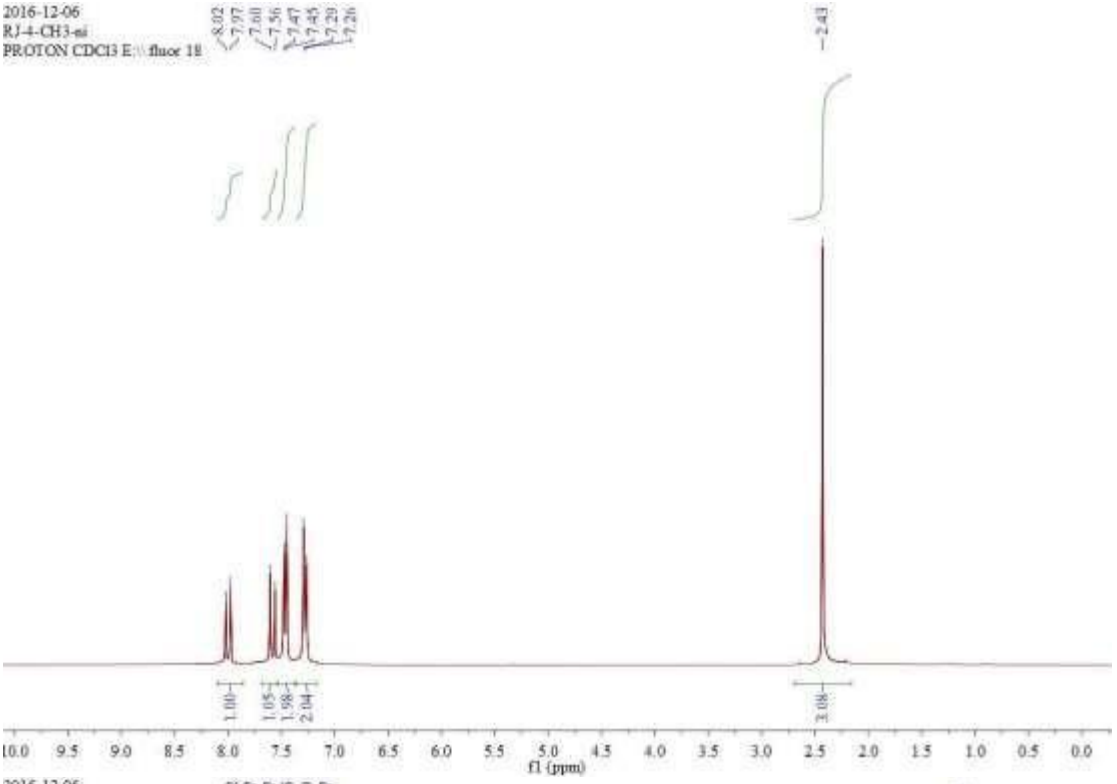
(2f)

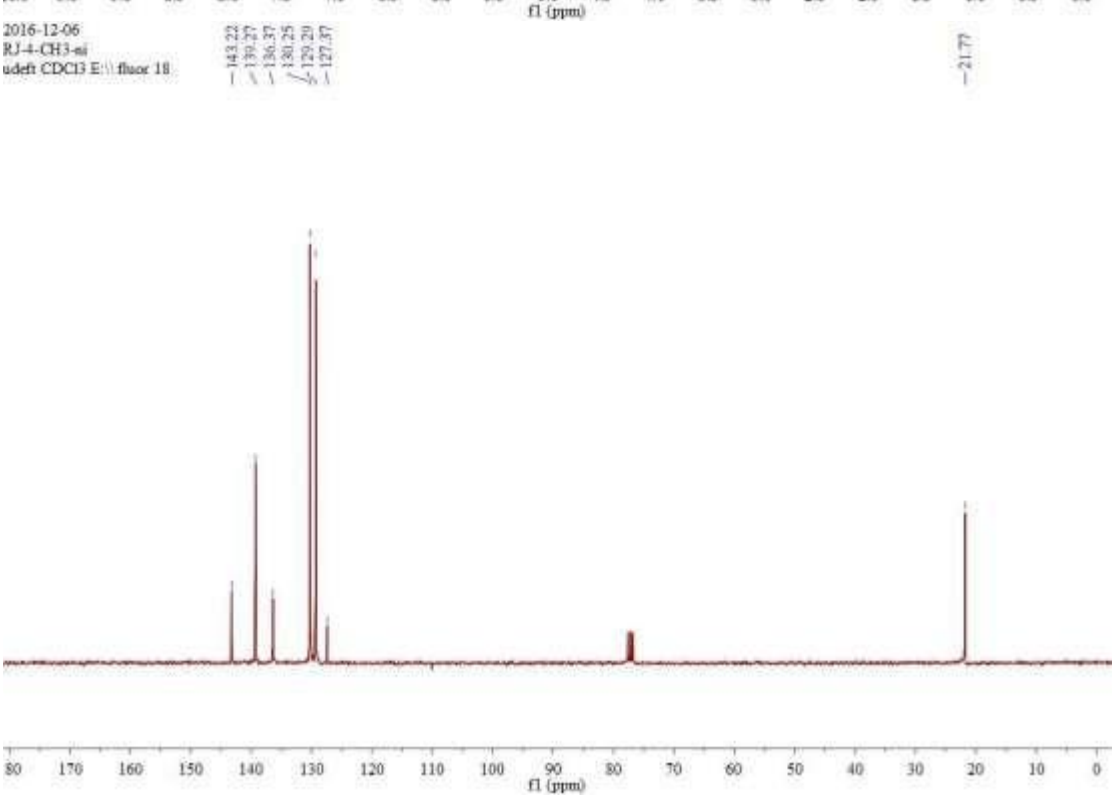

2016-11-21
RJ-269-P
PROTON CDCl3 E:\\ fluor 4
7.98
7.94
7.51
7.47
7.44
7.41
6.71
6.68
3.07
1.00
3.04
2.08
6.02
f1 (ppm)

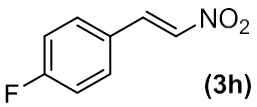

2016-11-21
RJ-269-P
udeft CDCl3 E:\\ fluor 4
153.02
140.85
132.34
131.57
117.62
112.22
40.27
f1 (ppm)


NO2

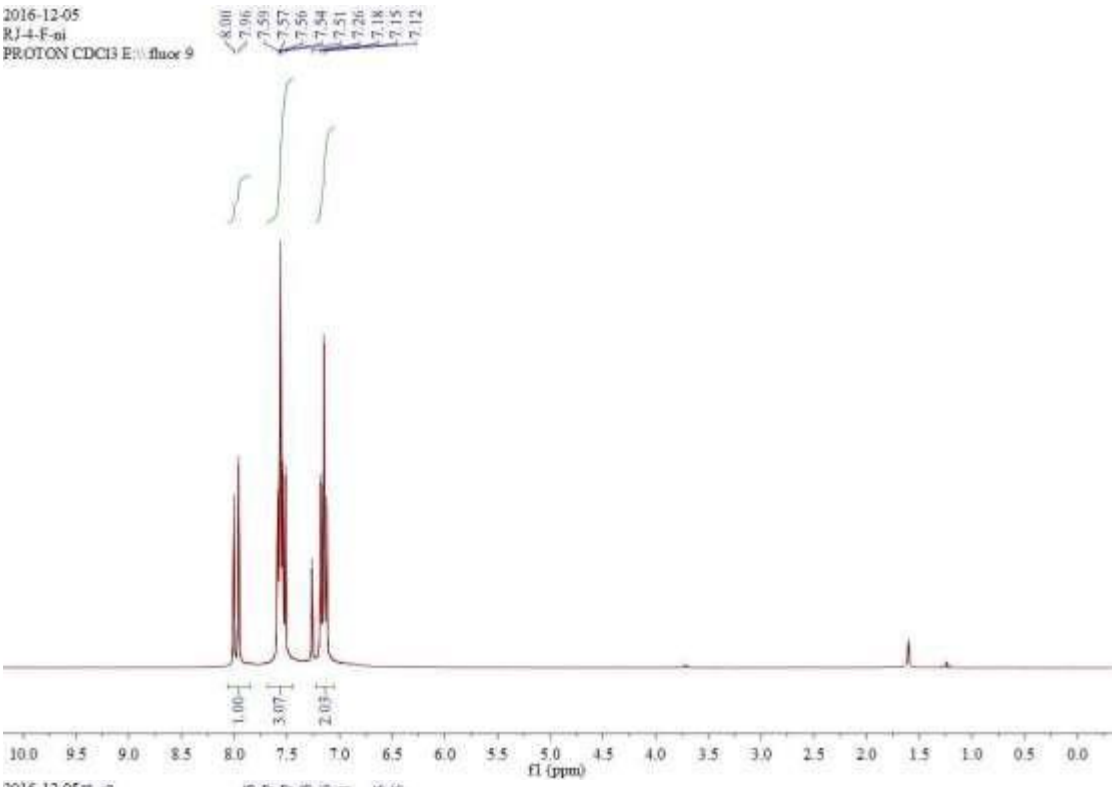
(2g)

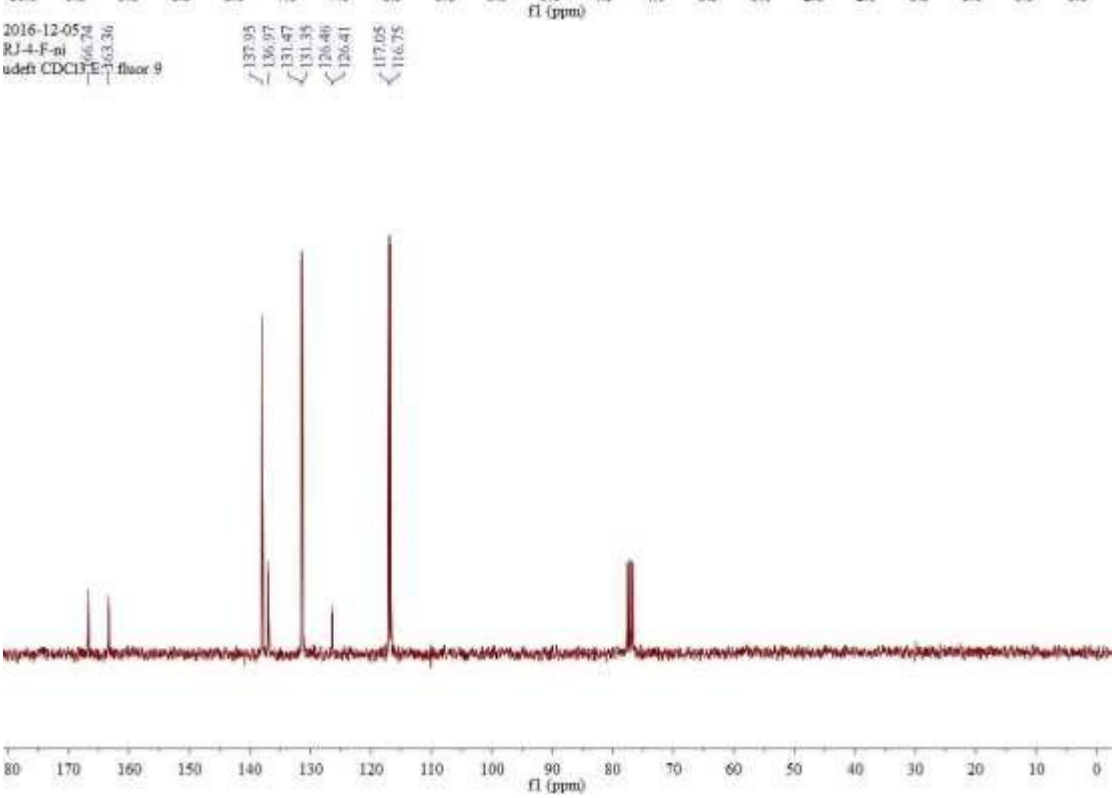

2016-12-06
RJ-4-CH3-si
PROTON CDCl3 E:\\ fluor 18
8.02
7.97
7.60
7.56
7.47
7.45
7.29
7.26
2.43
1.00
1.05
1.98
2.04
3.08
f1 (ppm)

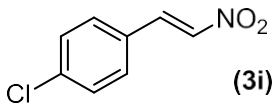

2016-12-06
RJ-4-CH3-si
udeft CDCl3 E:\\ fluor 18
143.22
139.27
136.37
130.25
129.29
127.37
21.77
f1 (ppm)


NO2
F

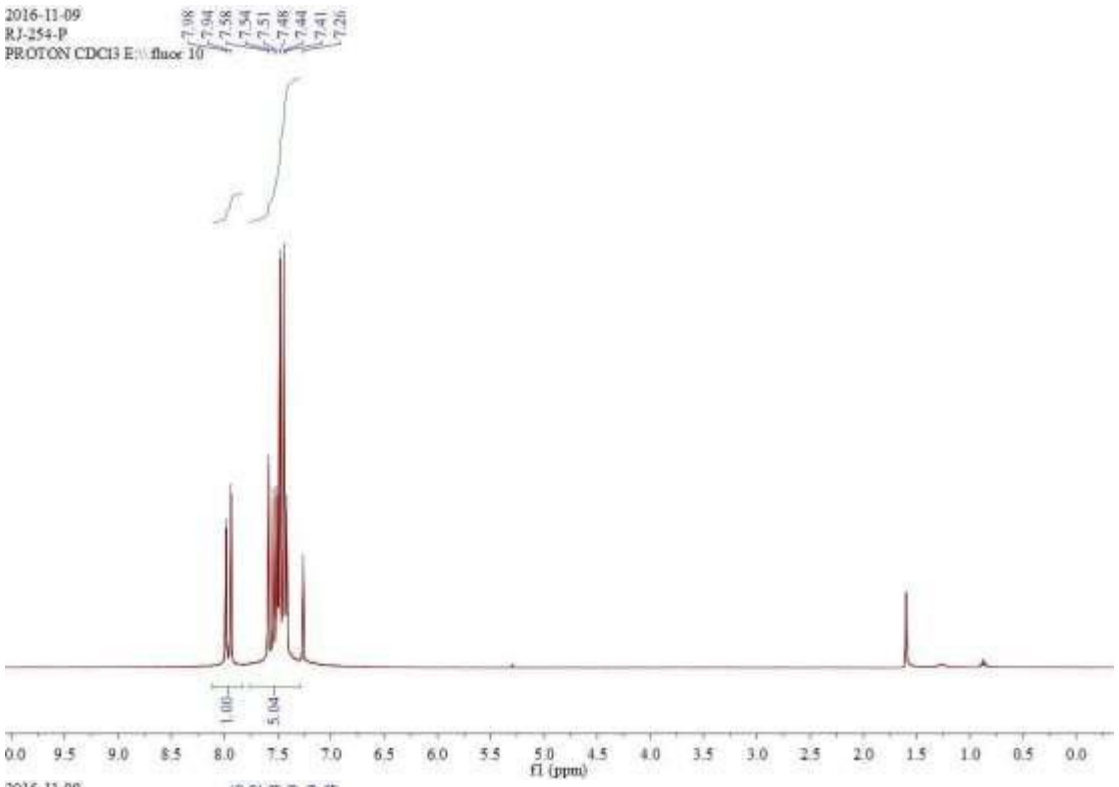
(3h)

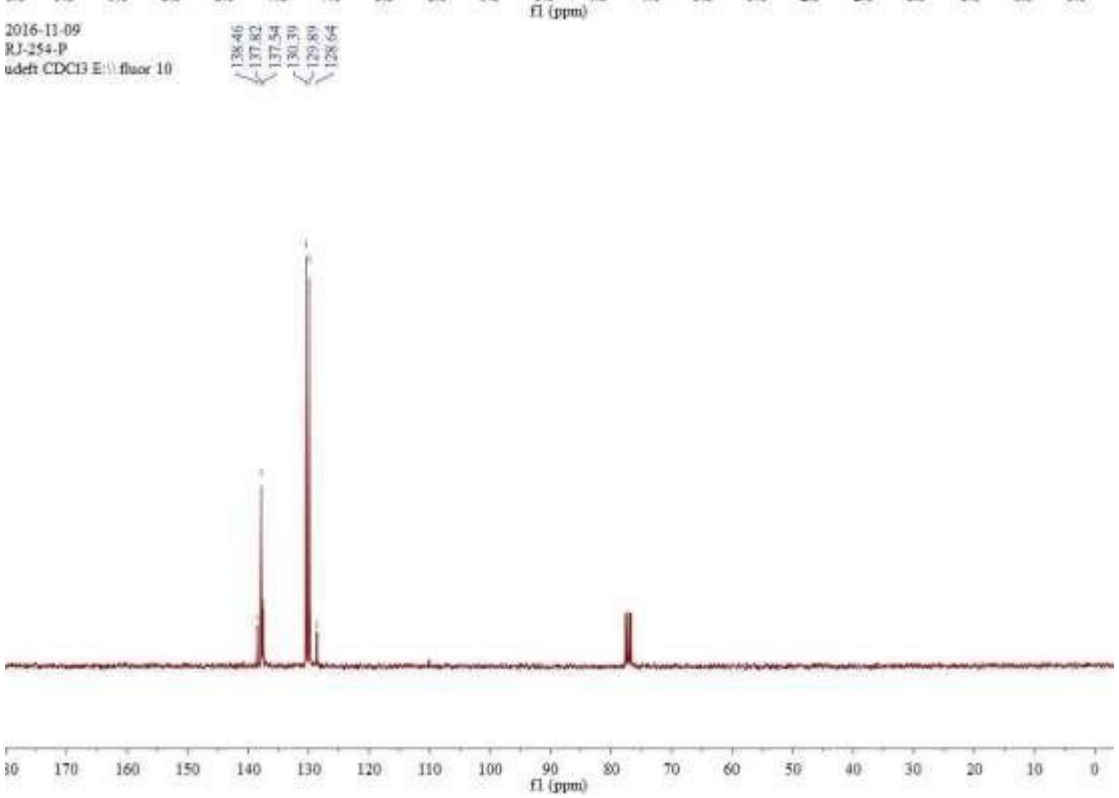

2016-12-05
RJ-4-F-ni
PROTON CDCl3 E:\ fluor 9
8.00
7.96
7.59
7.57
7.56
7.54
7.51
7.26
7.18
7.15
7.12
1.00
3.07
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

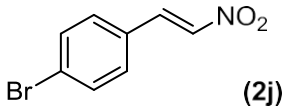

2016-12-05
RJ-4-F-ni
udeft CDCl3 E:\ fluor 9
166.74
163.36
137.95
136.97
131.47
131.35
126.46
126.41
117.05
116.75
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NO2
Cl

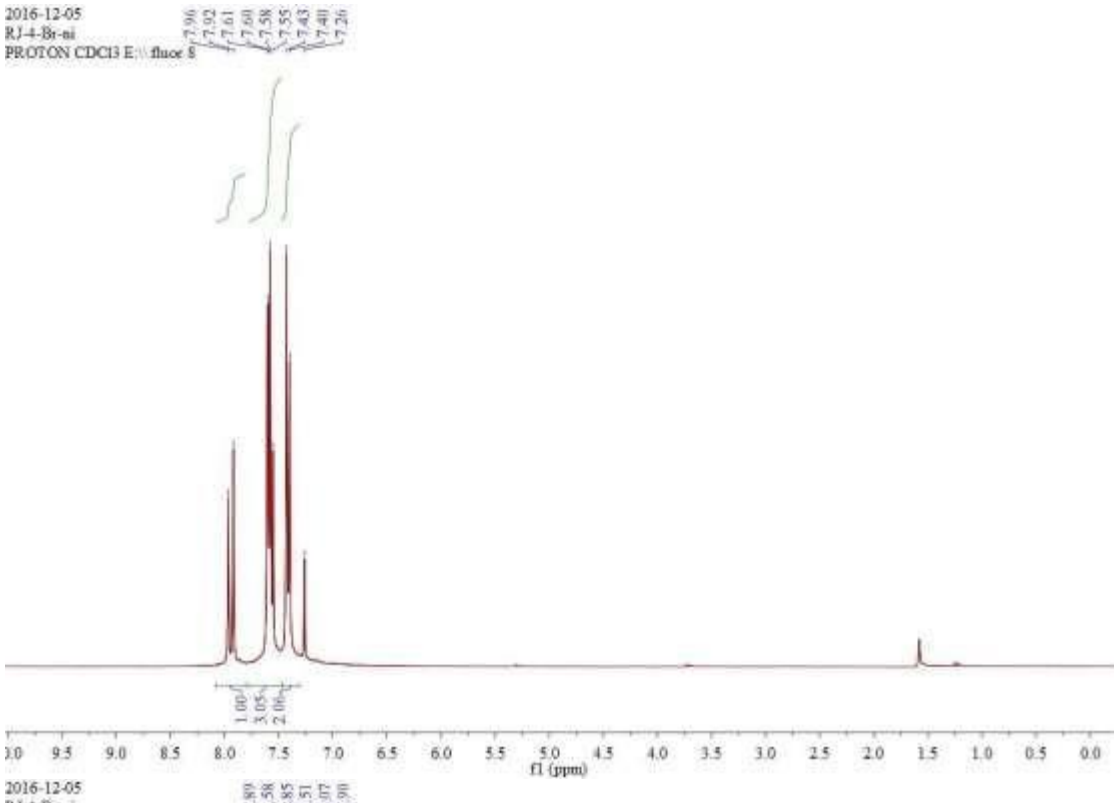
(3i)

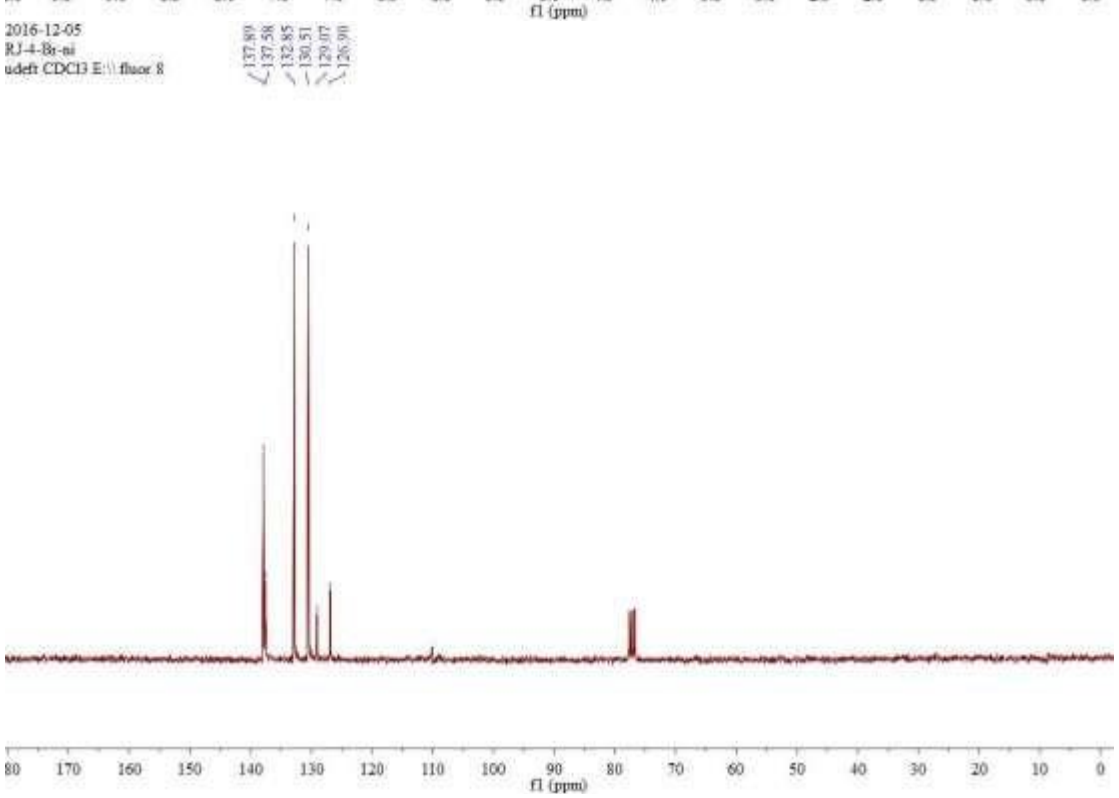

2016-11-09
RJ-254-P
PROTON CDCl3 E:\\ fluor 10
7.98
7.94
7.58
7.54
7.51
7.48
7.44
7.41
7.26
1.00
5.04
f1 (ppm)

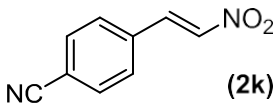

2016-11-09
RJ-254-P
udeft CDCl3 E:\\ fluor 10
138.46
137.82
137.54
130.39
129.89
128.64
f1 (ppm)


NO2
Br

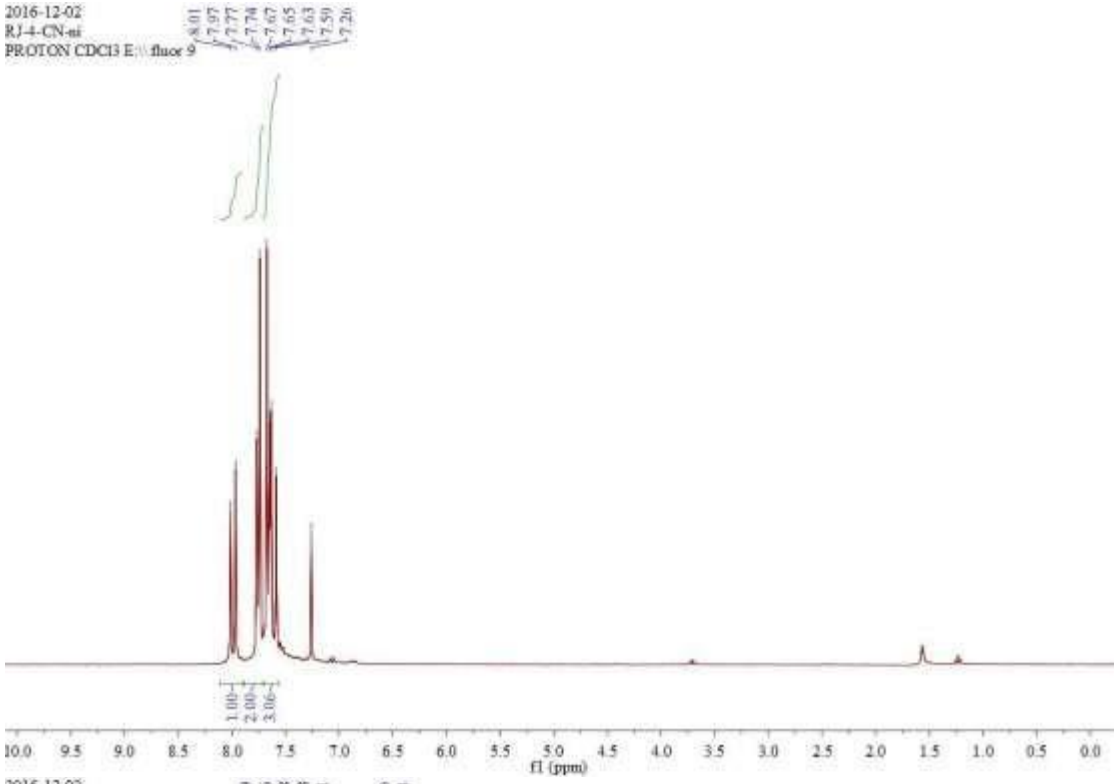
(2j)

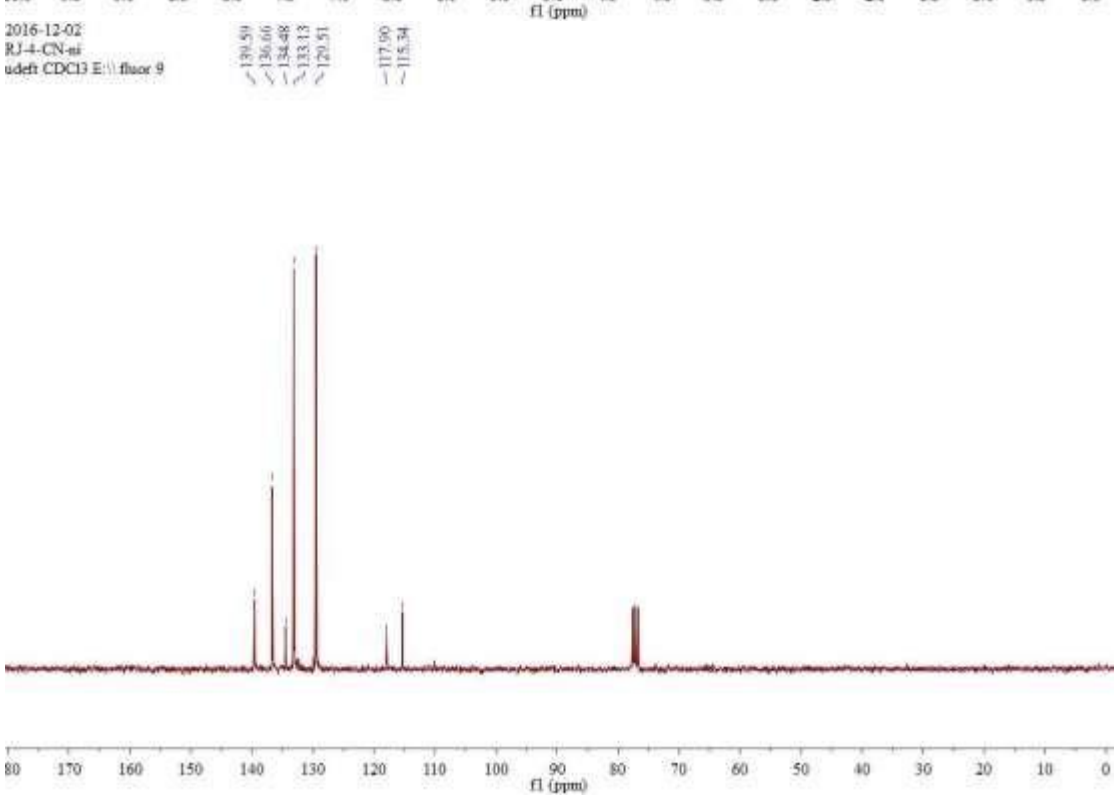

2016-12-05
RJ-4-Br-ai
PROTON CDCl3 E:\\ fluor 8
7.96
7.92
7.61
7.60
7.58
7.55
7.43
7.40
7.26
1.00
3.05
2.06
f1 (ppm)

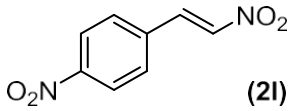

2016-12-05
RJ-4-Br-ai
udeft CDCl3 E:\\ fluor 8
137.89
137.58
132.85
130.51
129.07
126.90
f1 (ppm)


NO2
NC

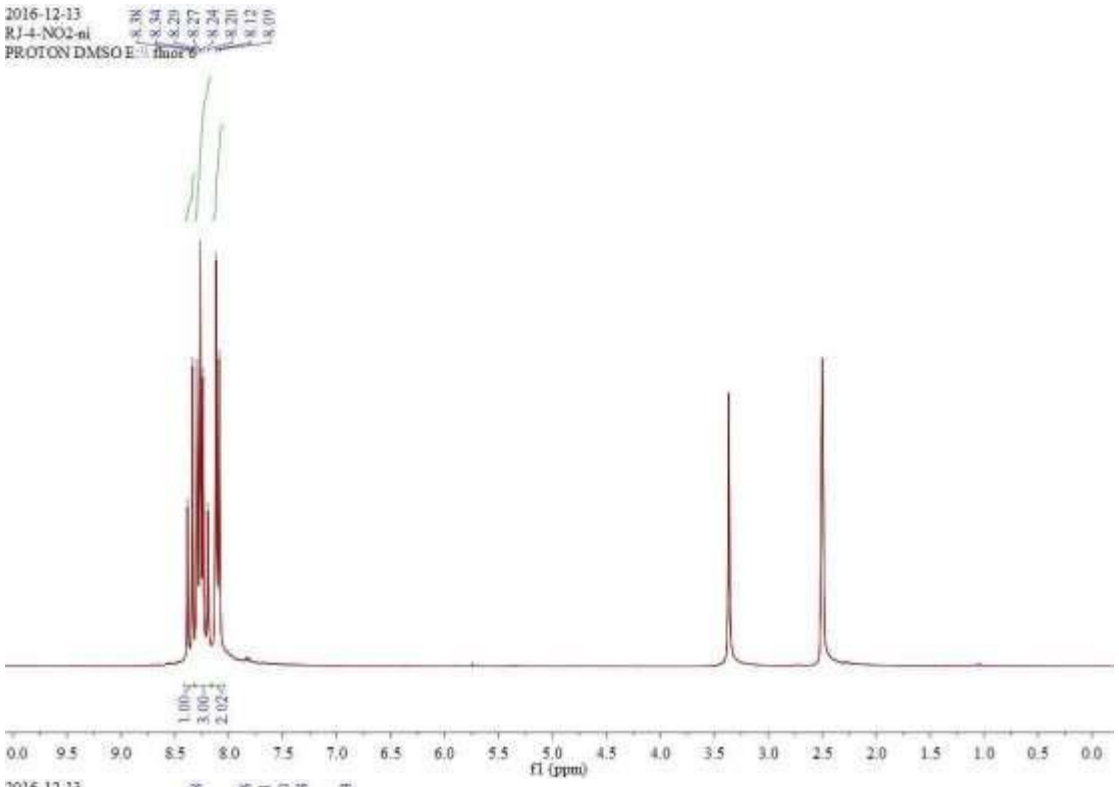
(2k)

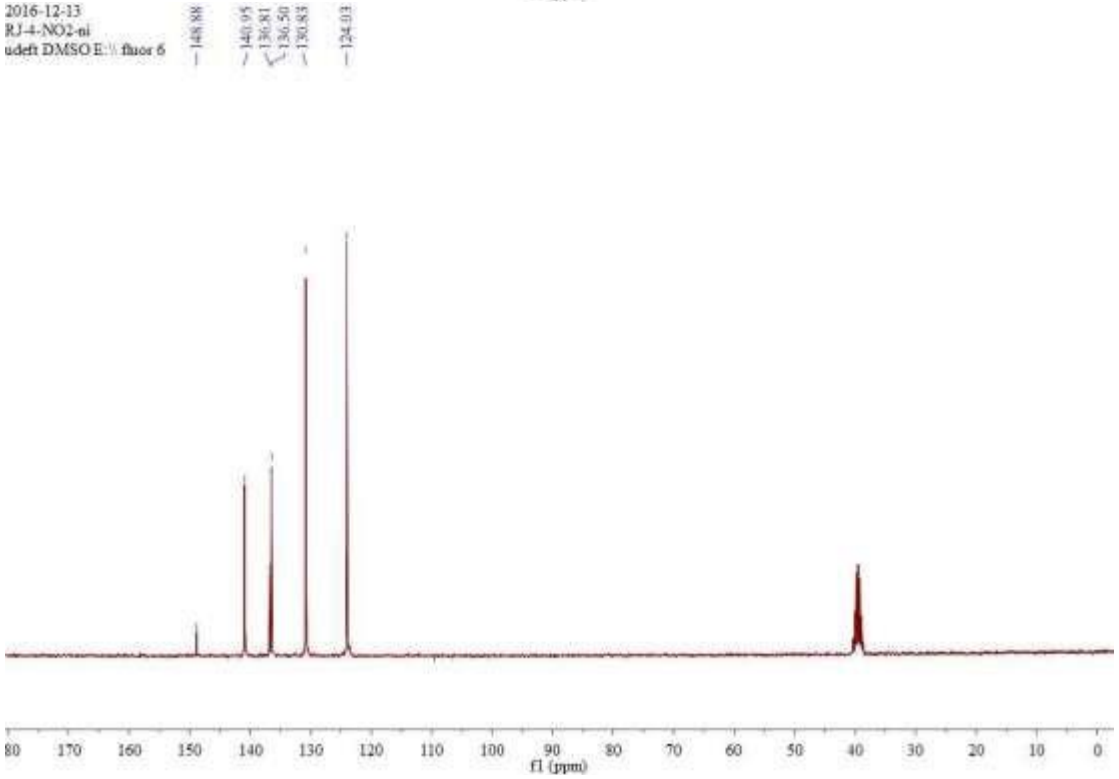

2016-12-02
RJ-4-CN-si
PROTON CDCl3 E:\\ fluor 9
8.01
7.97
7.77
7.74
7.67
7.65
7.63
7.59
7.26
1.00
2.00
3.06
f1 (ppm)

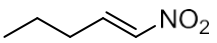

2016-12-02
RJ-4-CN-si
udeft CDCl3 E:\\ fluor 9
139.59
136.66
134.48
133.13
129.51
117.90
115.34
f1 (ppm)


NO2
O2N

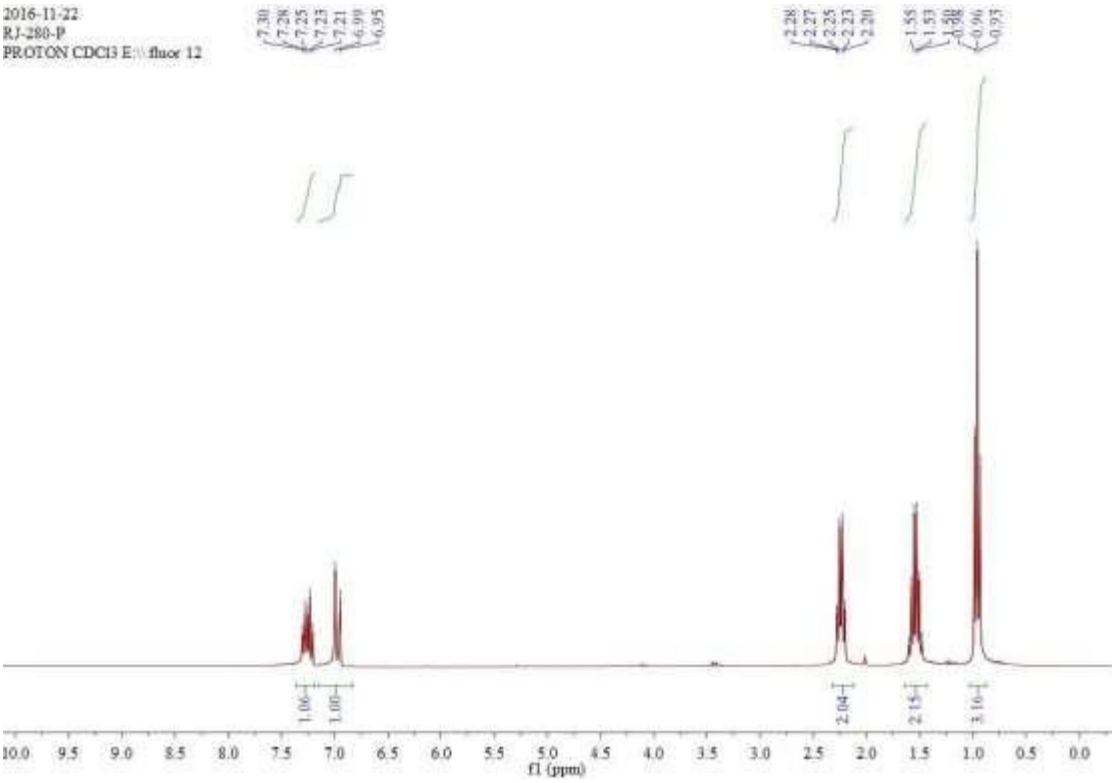
(2l)

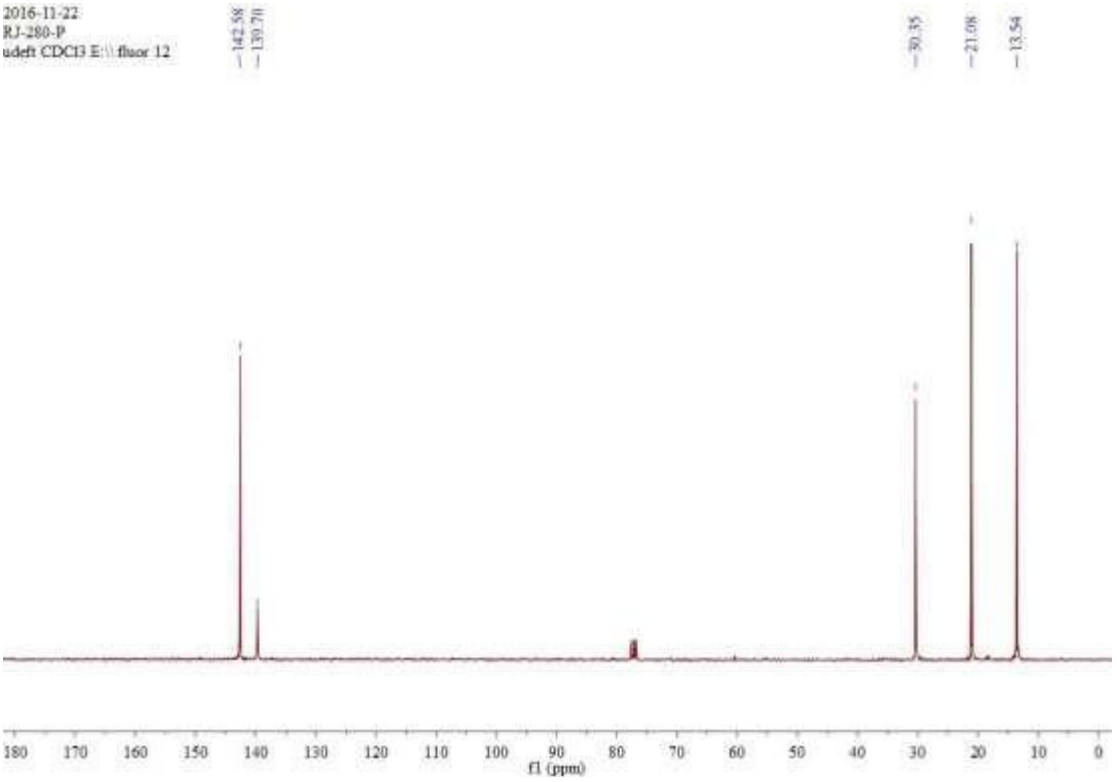

2016-12-13
RJ-4-NO2-ni
PROTON DMSO E:\ fluor 6
8.38
8.34
8.29
8.27
8.24
8.20
8.12
8.09
1.00
3.00
2.02
f1 (ppm)

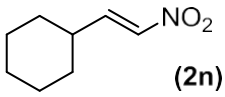

2016-12-13
RJ-4-NO2-ni
udeft DMSO E:\ fluor 6
148.88
140.95
136.81
136.50
130.83
124.03
f1 (ppm)


NO2

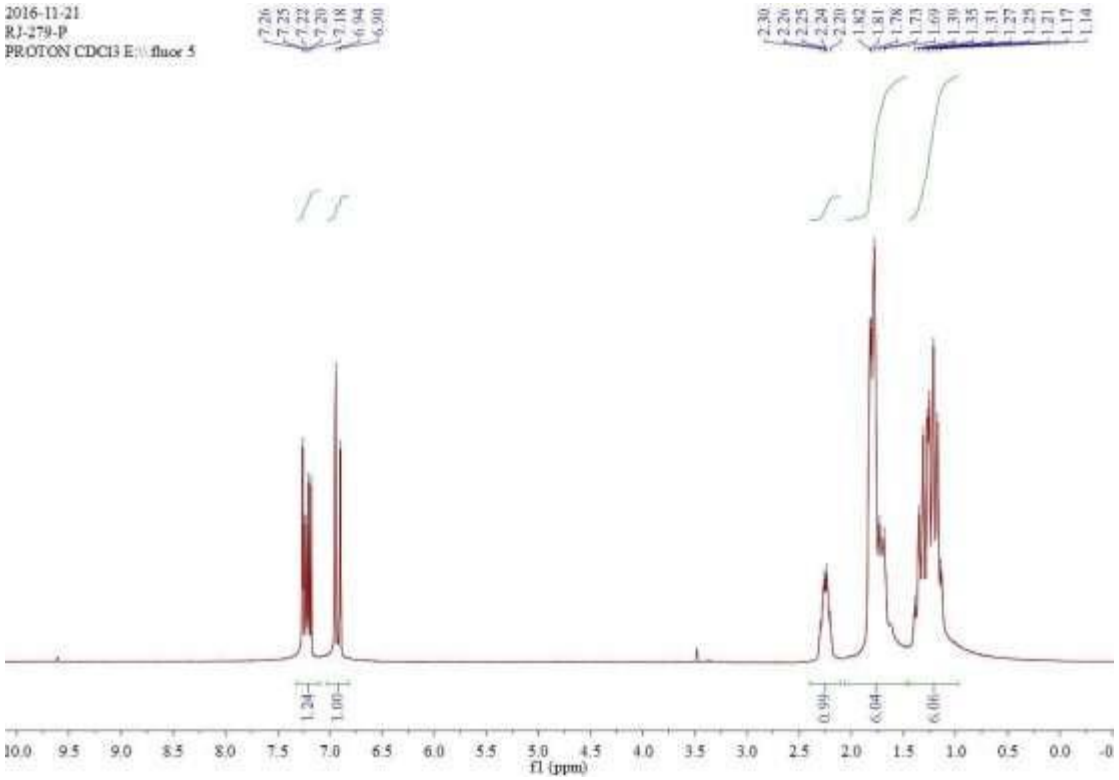
(2m)

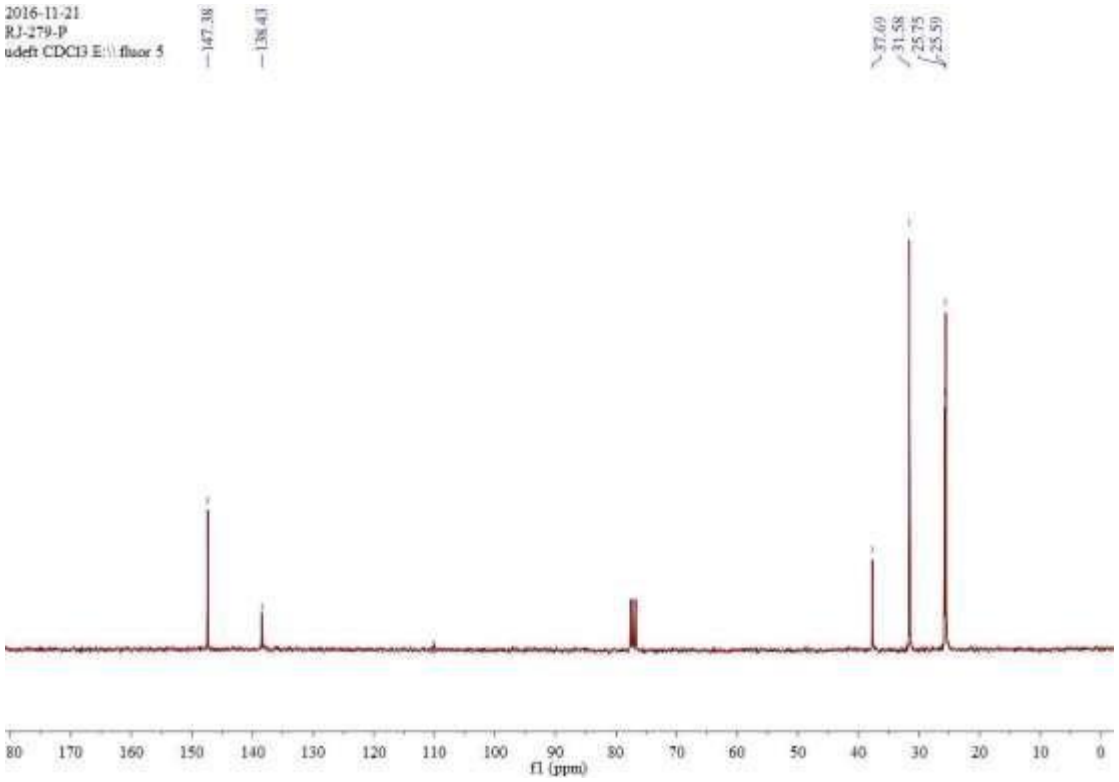

2016-11-22
RJ-280-P
PROTON CDCl3 E:\\ fluor 12
7.30
7.28
7.25
7.23
7.21
6.99
6.95
2.28
2.27
2.25
2.23
2.20
1.55
1.53
1.50
0.98
0.96
0.93
1.06
1.00
2.04
2.15
3.16
f1 (ppm)

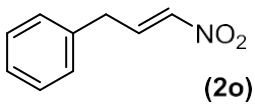

2016-11-22
RJ-280-P
udeft CDCl3 E:\\ fluor 12
142.58
139.70
30.35
21.08
13.54
f1 (ppm)


NO2

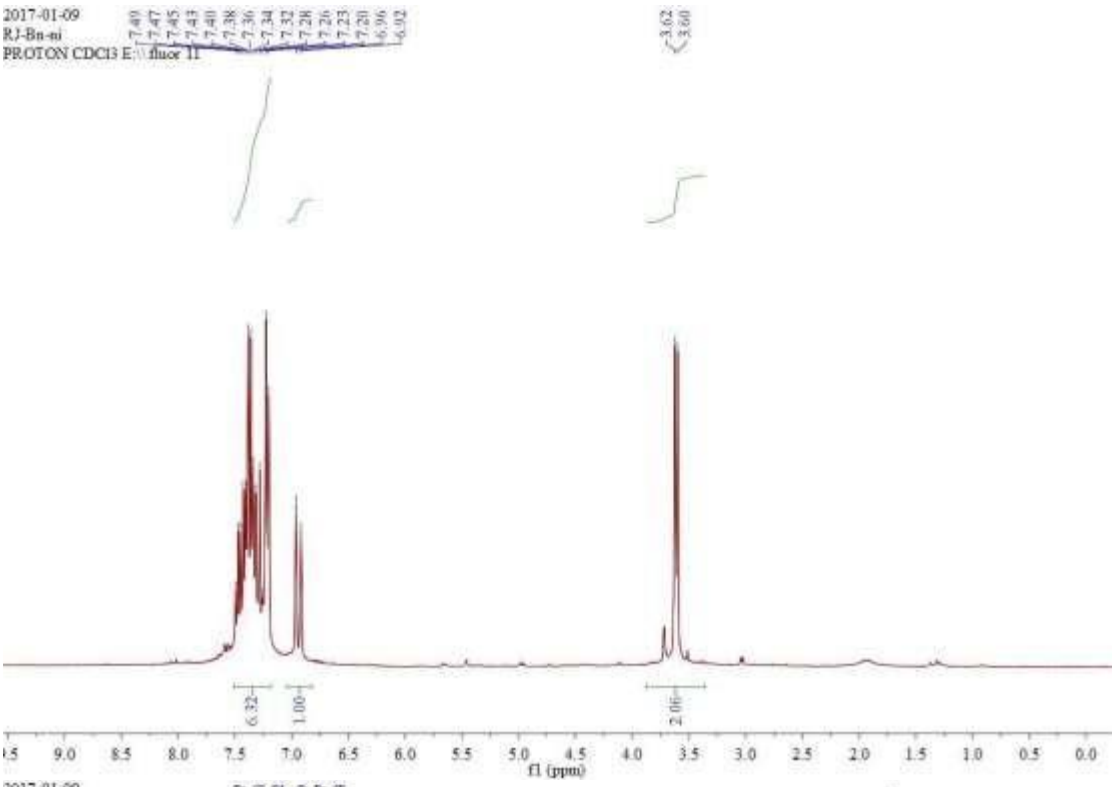
(2n)

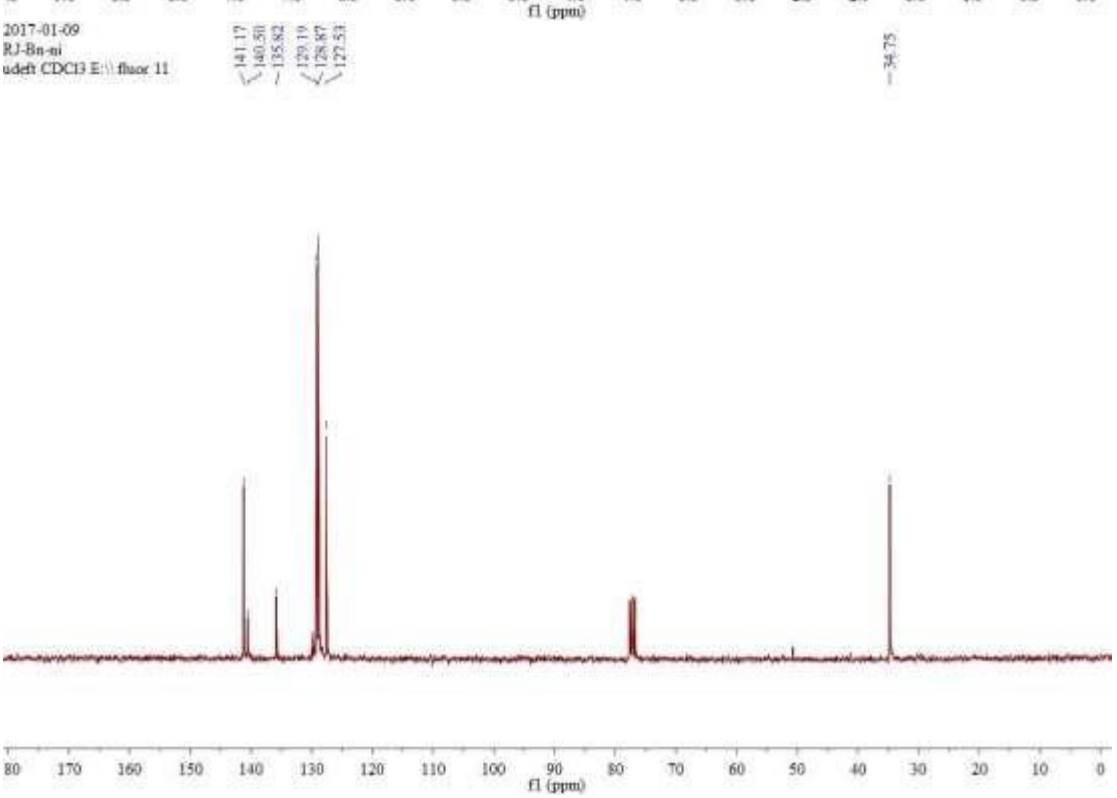

2016-11-21
RJ-279-P
PROTON CDCl3 E:\\ fluor 5
f1 (ppm)

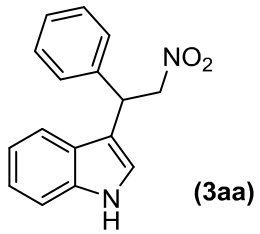

2016-11-21
RJ-279-P
udeft CDCl3 E:\\ fluor 5
f1 (ppm)


NO2

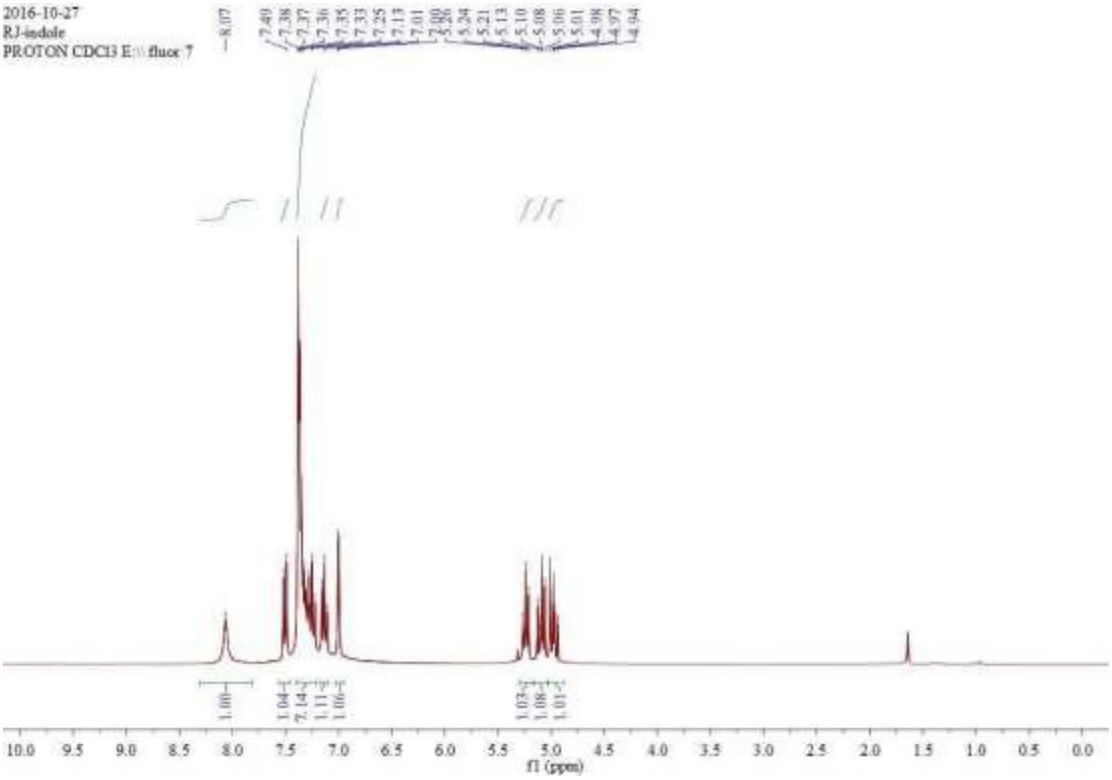
(2o)

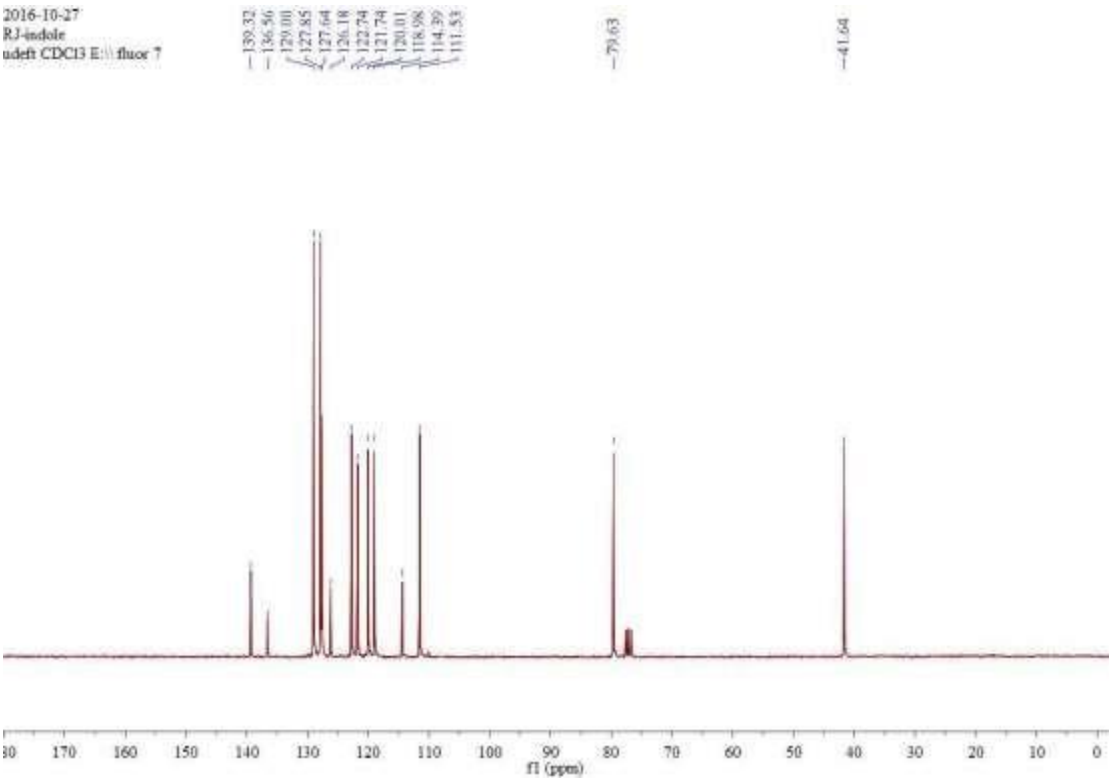

2017-01-09
RJ-Bn-ni
PROTON CDCl3 E:\\ fluor 11
7.49
7.47
7.45
7.43
7.40
7.38
7.36
7.34
7.32
7.24
7.26
7.23
7.20
6.96
6.92
3.62
3.60
6.32
1.00
2.06
f1 (ppm)

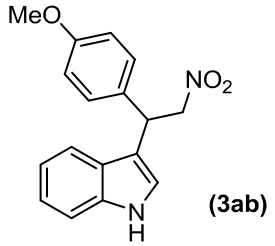

2017-01-09
RJ-Bn-ni
udeft CDCl3 E:\\ fluor 11
141.17
140.50
135.82
129.19
128.87
127.53
34.75
f1 (ppm)


NO2
N
H

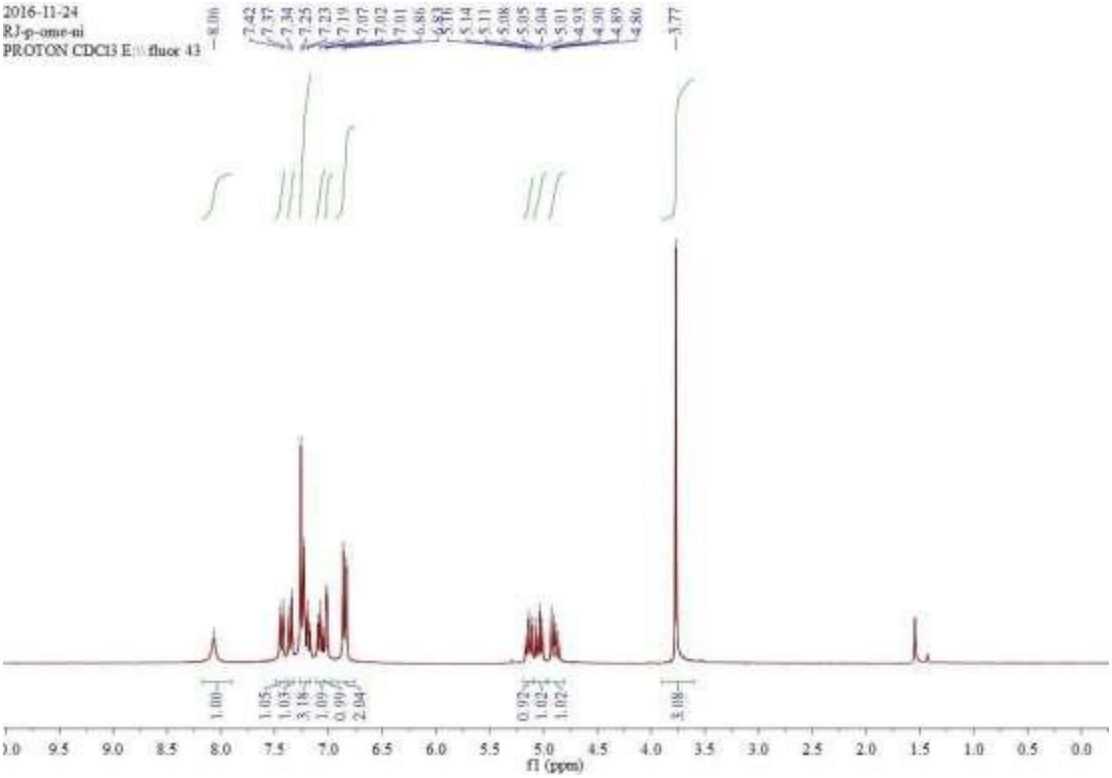
(3aa)

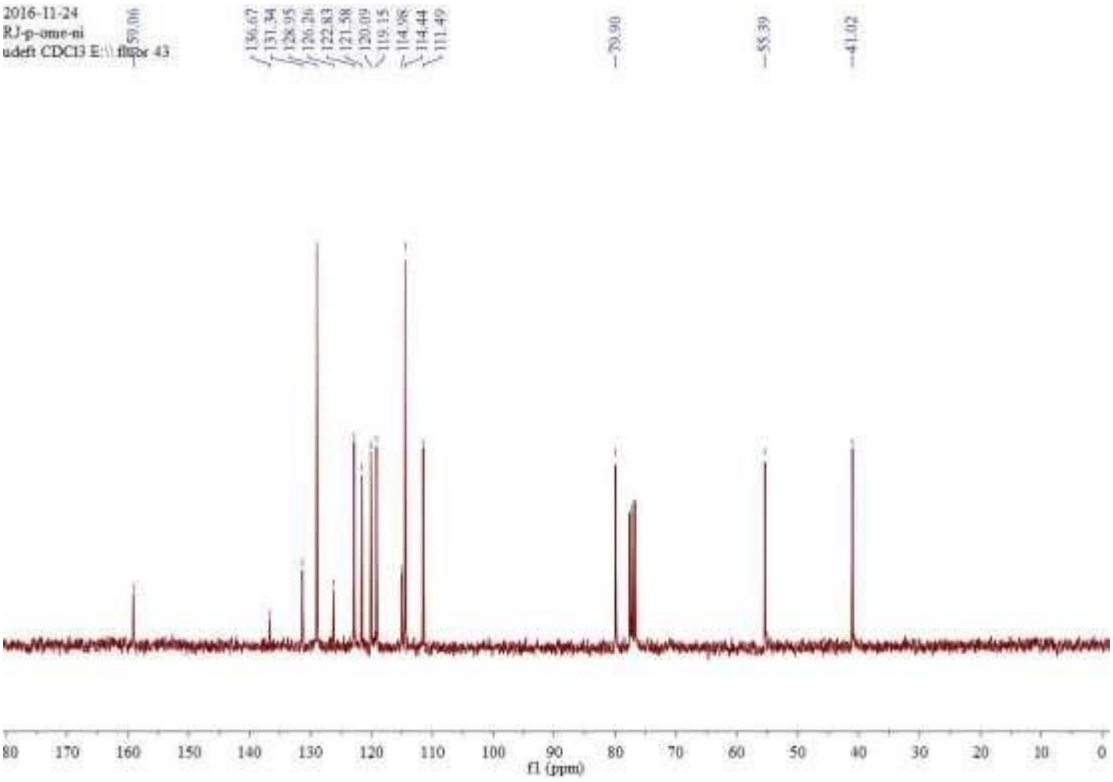

2016-10-27
RJ-indole
PROTON CDCl3 E:\\ fluor 7
f1 (ppm)

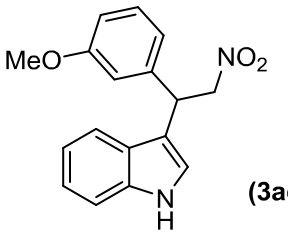

2016-10-27
RJ-indole
udeft CDCl3 E:\\ fluor 7
f1 (ppm)


MeO
NO2
N
H

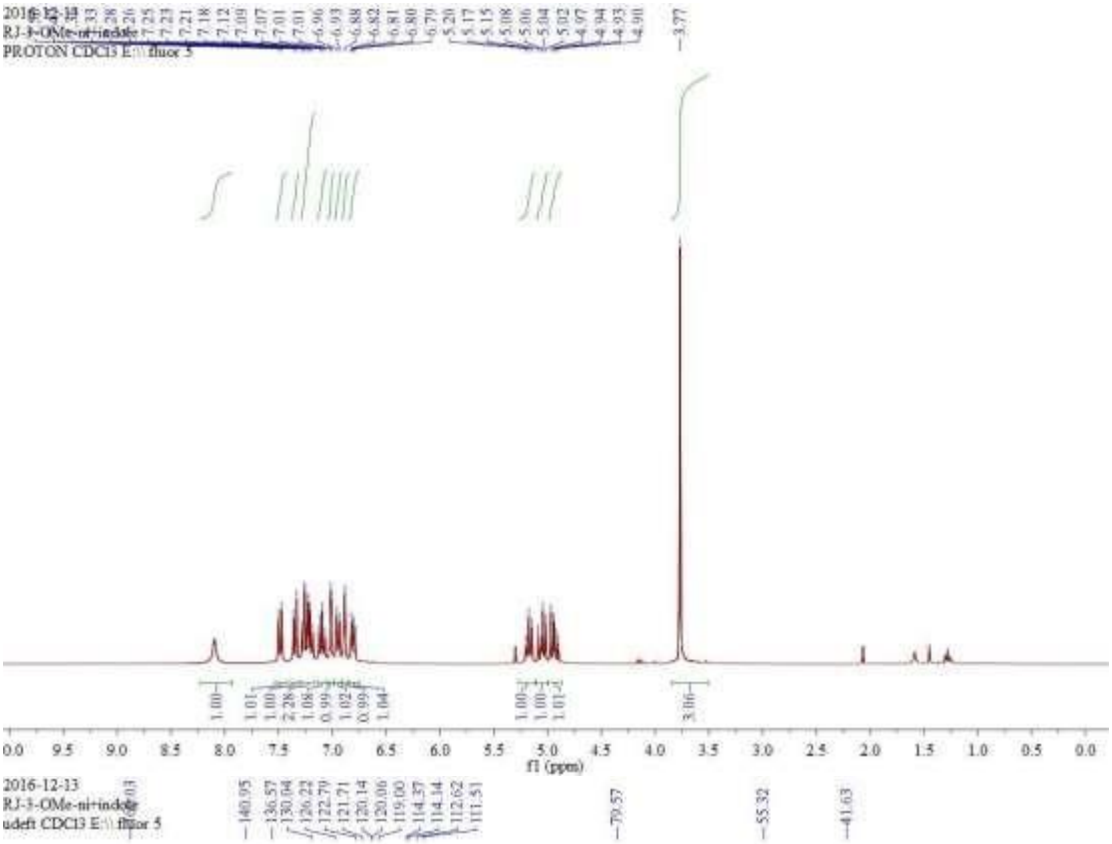
(3ab)


2016-11-24
RJ-p-ome-ni
PROTON CDCl3 E:\\ fluor 43
f1 (ppm)

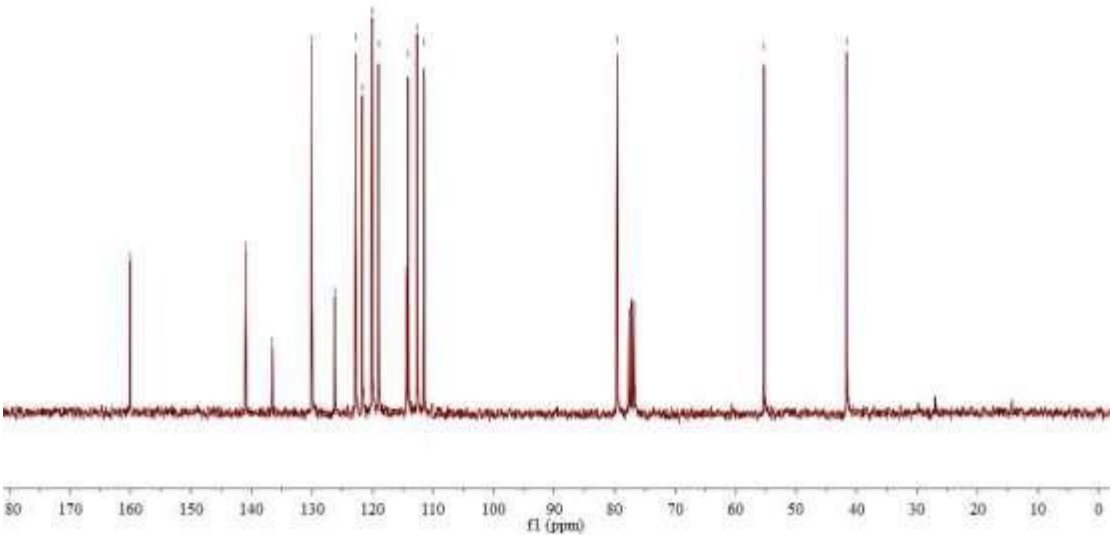

2016-11-24
RJ-p-ome-ni
udeft CDCl3 E:\\ fluor 43
f1 (ppm)

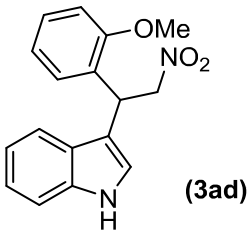

MeO
NO2
N
H

(3ac)

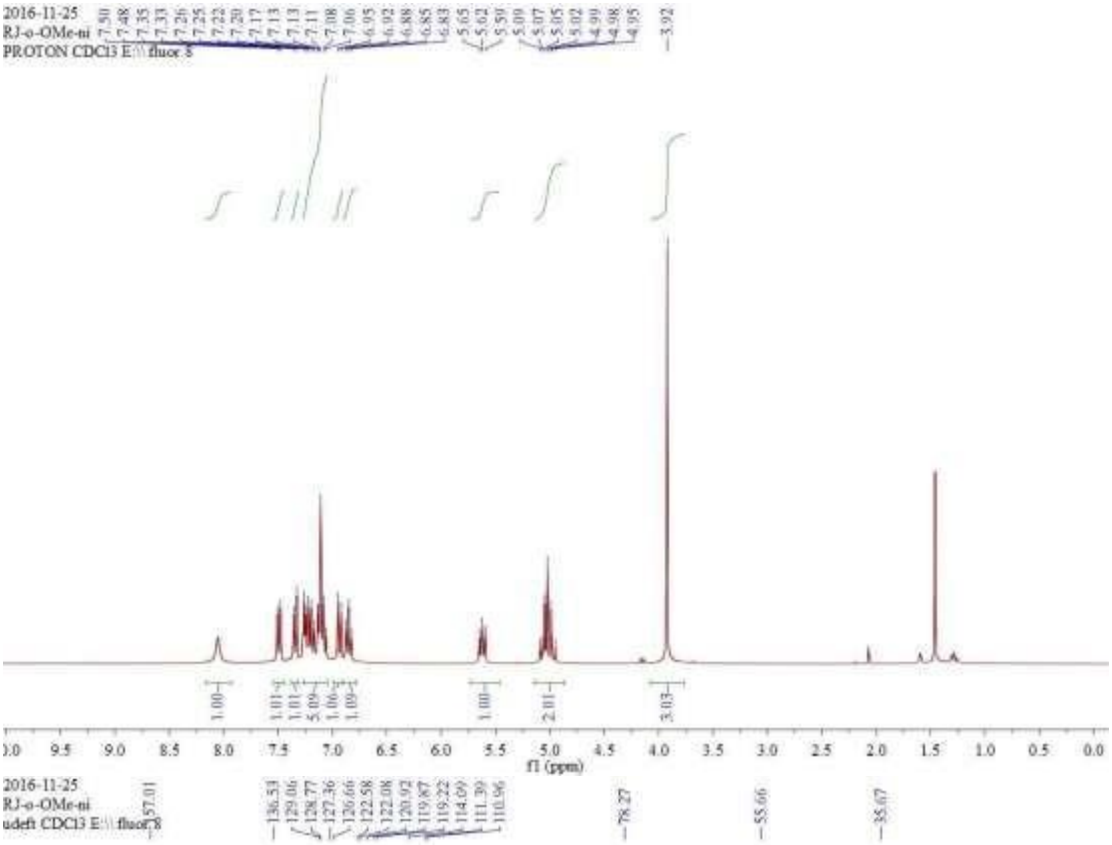

PROTON CDCl3 E:\\ fluor 5
f1 (ppm)

2016-12-13
RJ-3-OMe-ni+indole
udeft CDCl3 E:\\ fluor 5
140.95
136.57
130.04
126.22
122.79
121.71
120.14
120.06
119.00
114.37
114.14
112.62
111.51
79.57
55.32
41.63

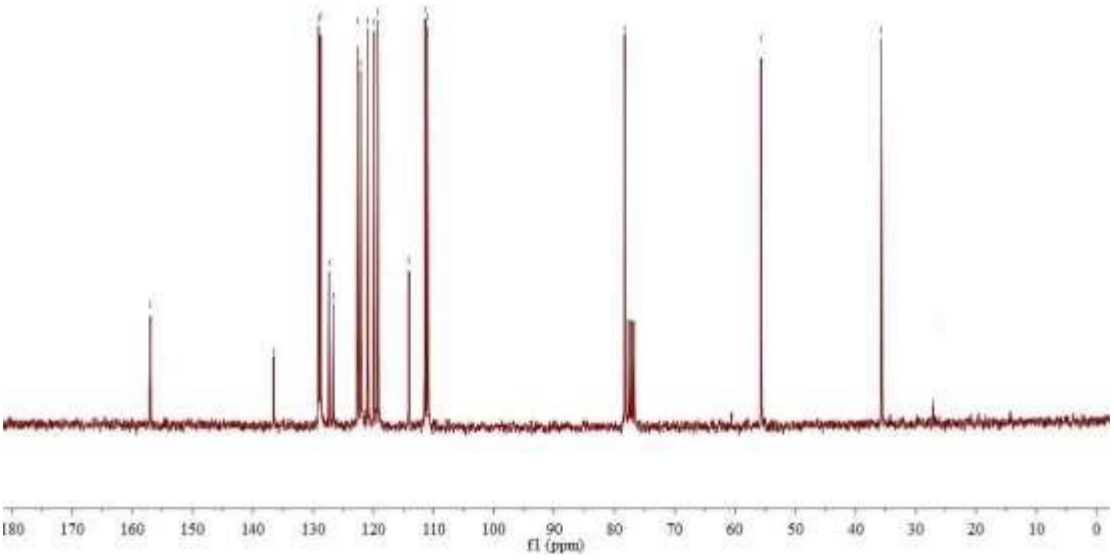

f1 (ppm)

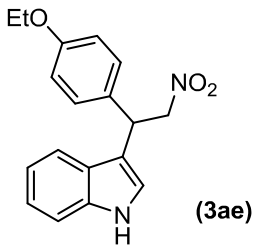

OMe
NO2
N
H

(3ad)

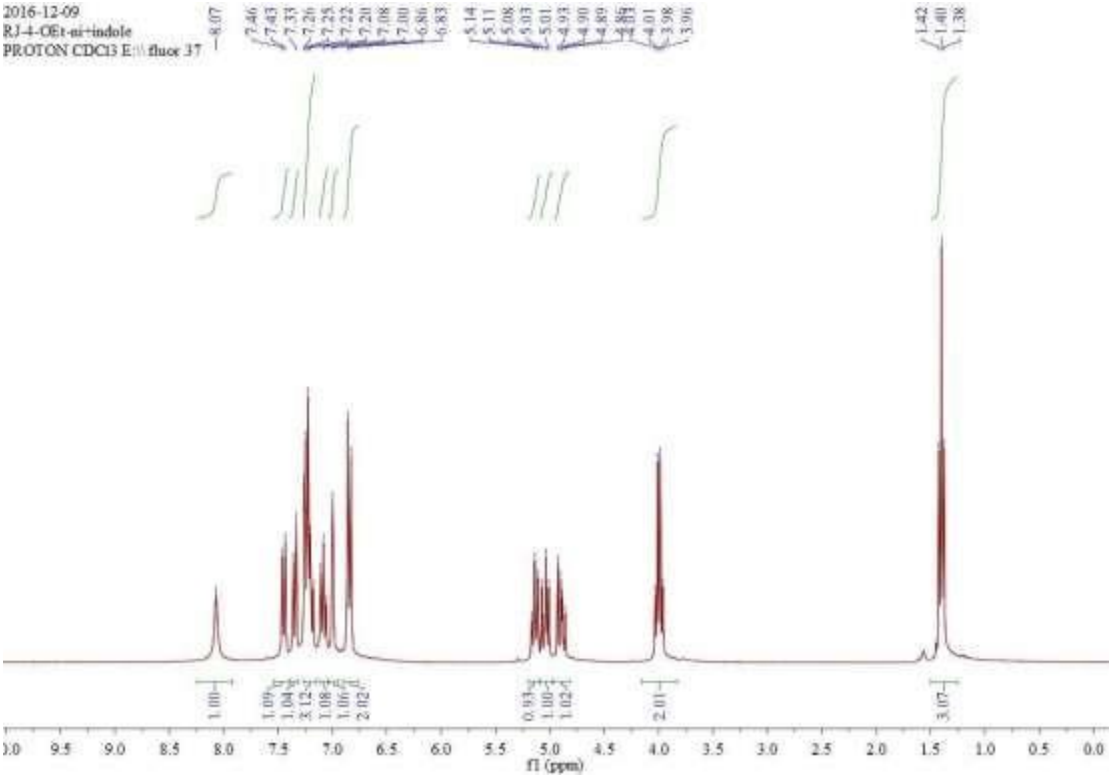

2016-11-25
RJ-o-OMe-ni
PROTON CDCl3 E:\\ fluor 8
f1 (ppm)

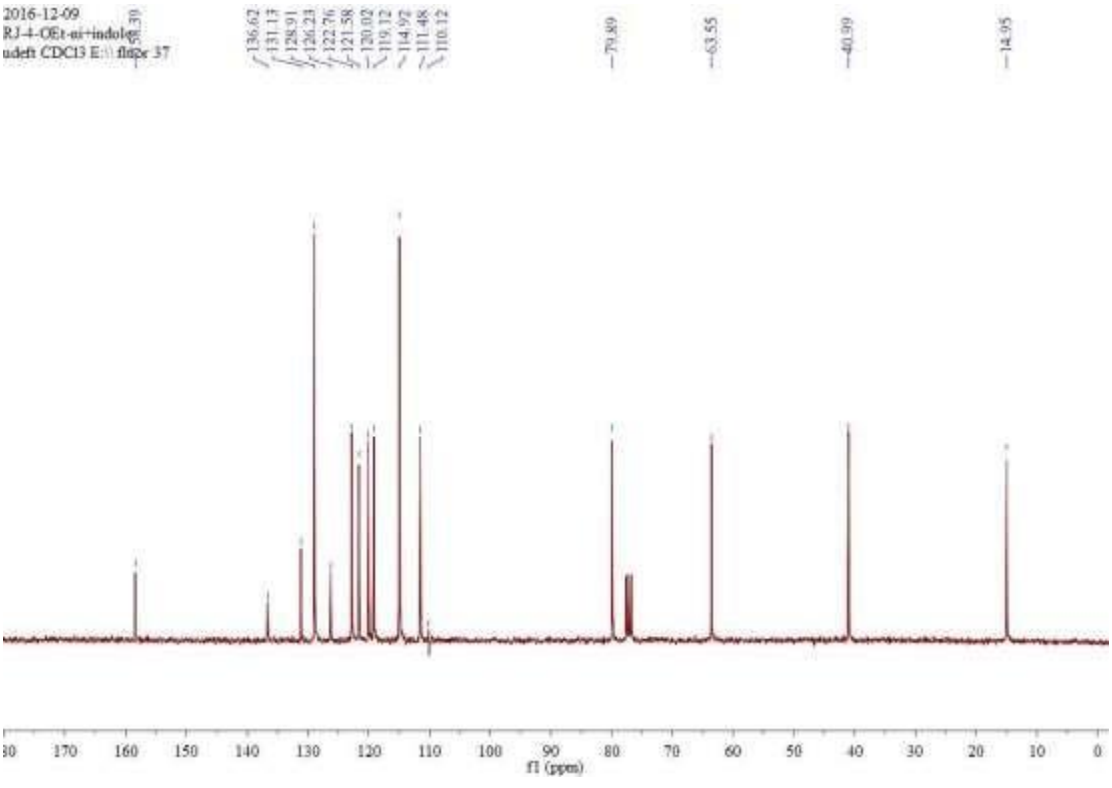
2016-11-25
RJ-o-OMe-ni
udeft CDCl3 E:\\ fluor 8

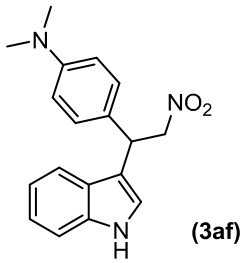

f1 (ppm)


EtO
NO2
N
H

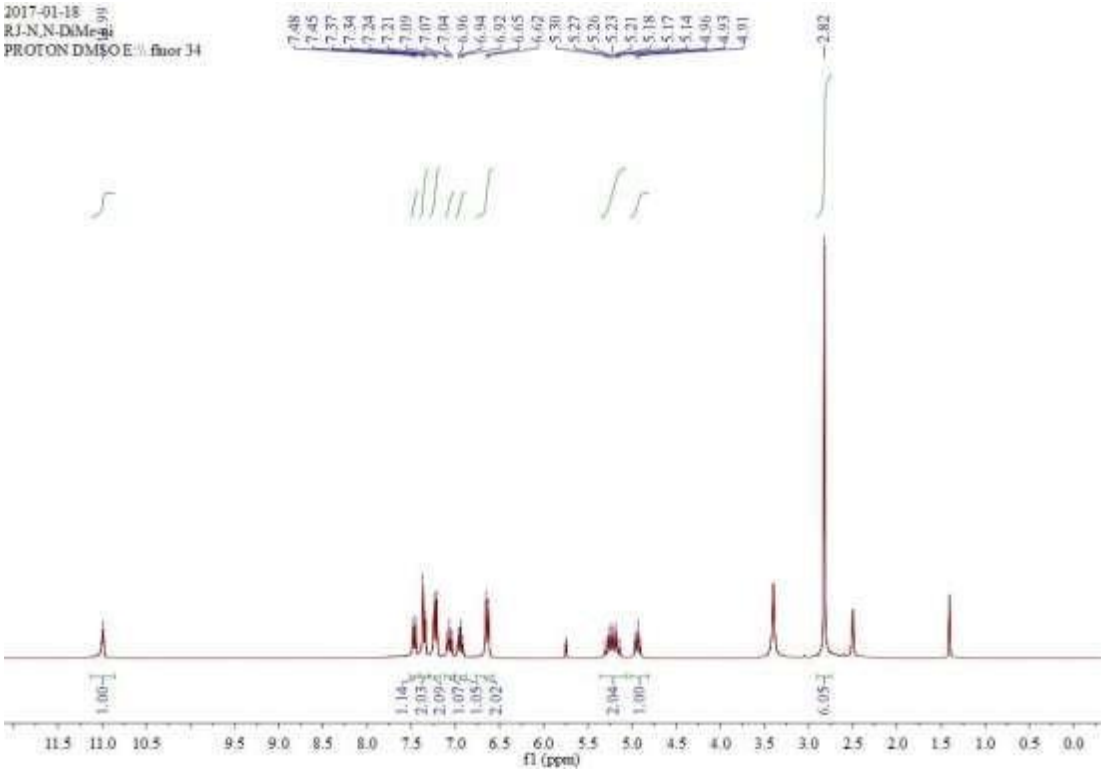
(3ae)

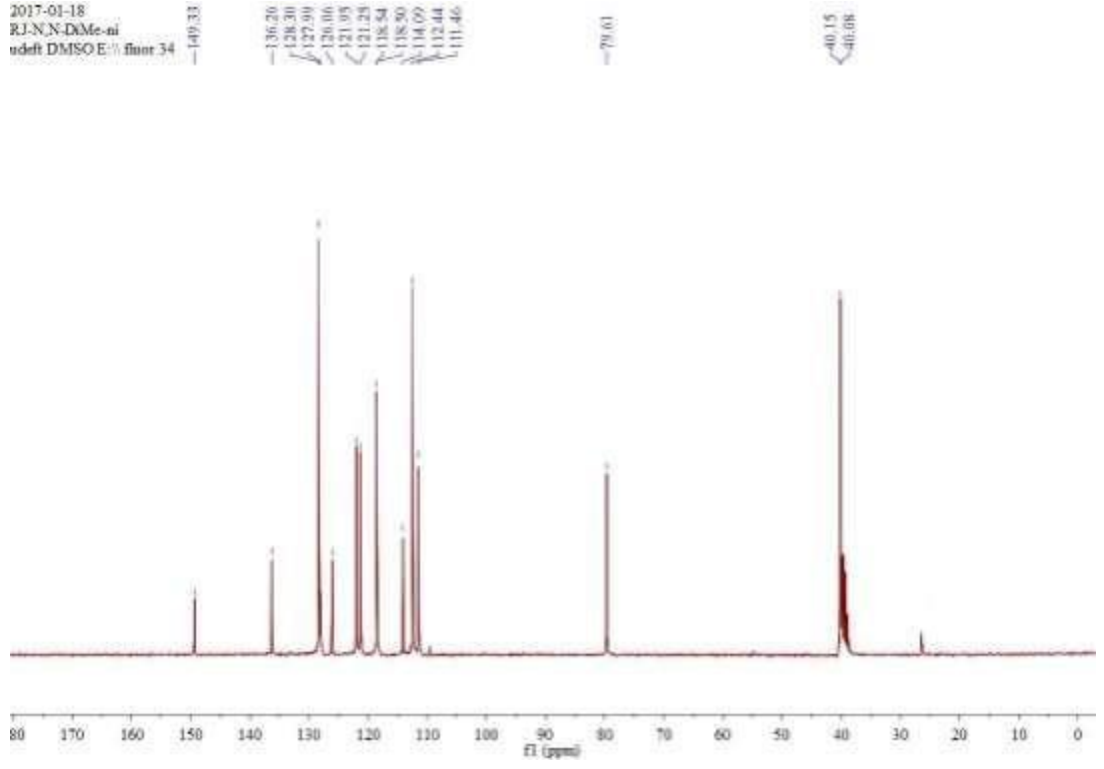

2016-12-09
RJ-4-OEt-ni+indole
PROTON CDCl3 E:\\ fluor 37
f1 (ppm)

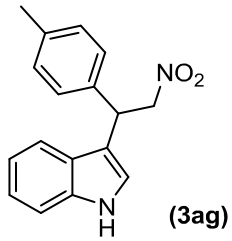

2016-12-09
RJ-4-OEt-ni+indole
udeft CDCl3 E:\\ fluor 37
f1 (ppm)


N
NO2
N
H

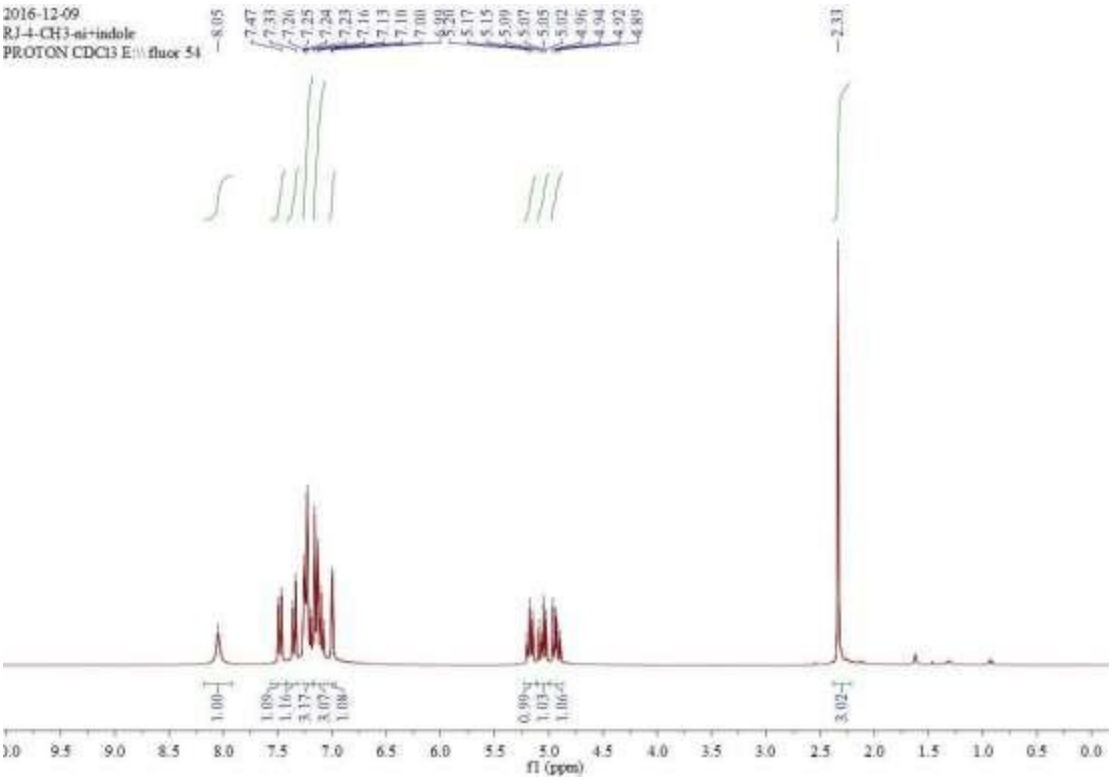
(3af)

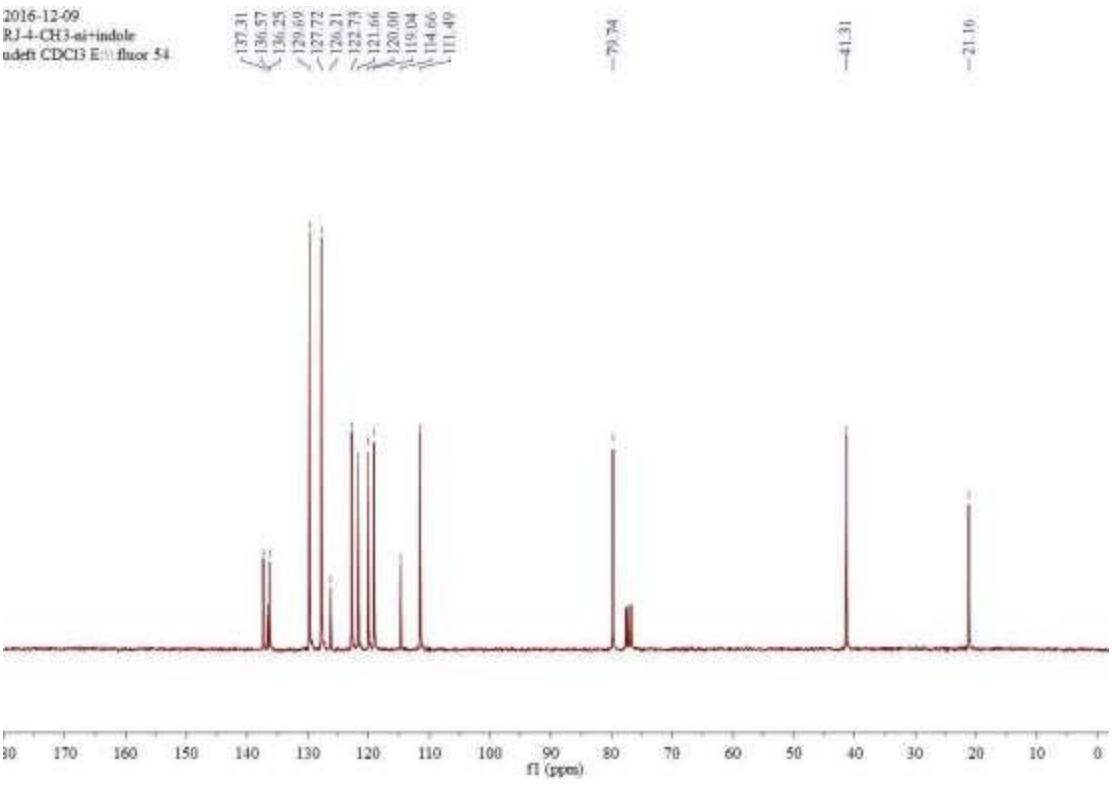

2017-01-18
RJ-N,N-DiMe-ni
PROTON DMSO E:\ fluor 34
7.48
7.45
7.37
7.34
7.24
7.21
7.09
7.07
7.04
6.96
6.94
6.92
6.65
6.62
5.30
5.27
5.26
5.23
5.21
5.18
5.17
5.14
4.96
4.93
4.91
2.82
1.00
1.14
2.03
2.09
1.07
1.05
2.02
2.04
1.00
6.05
f1 (ppm)

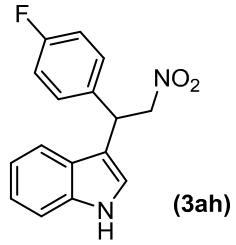

2017-01-18
RJ-N,N-DiMe-ni
udeft DMSO E:\ fluor 34
149.33
136.20
128.30
127.99
126.06
121.05
121.25
118.54
118.50
114.09
112.44
111.46
79.61
40.15
40.08
f1 (ppm)


NO2
N
H

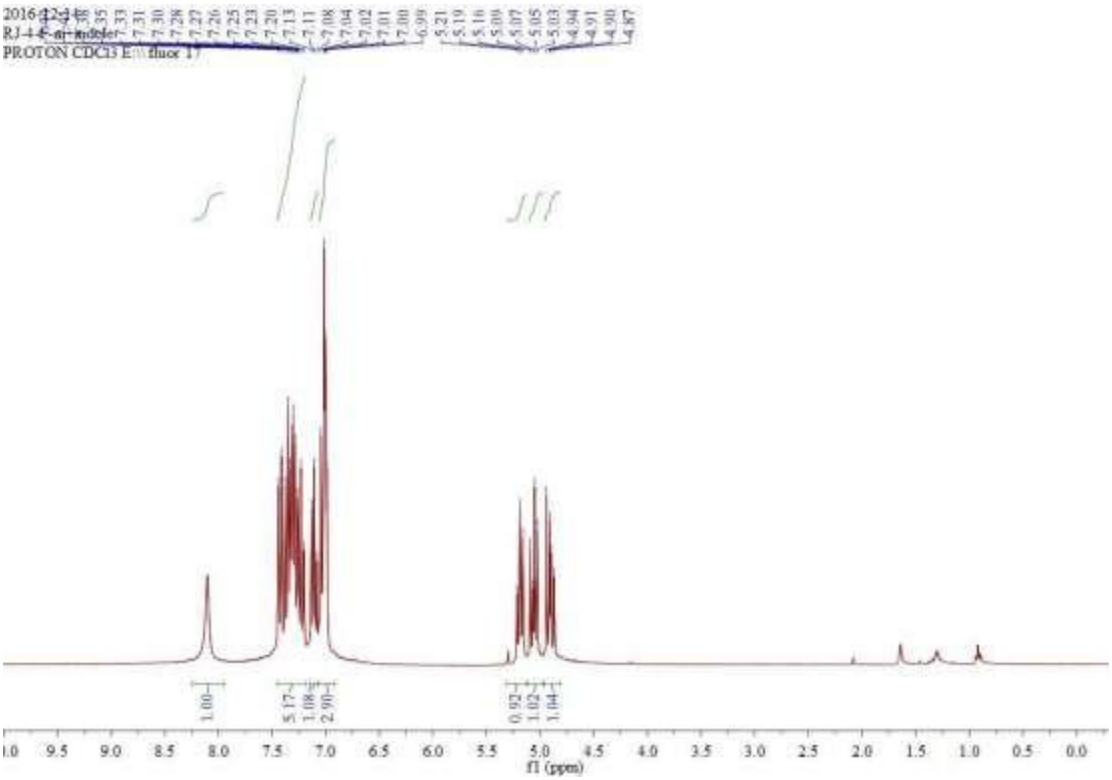
(3ag)

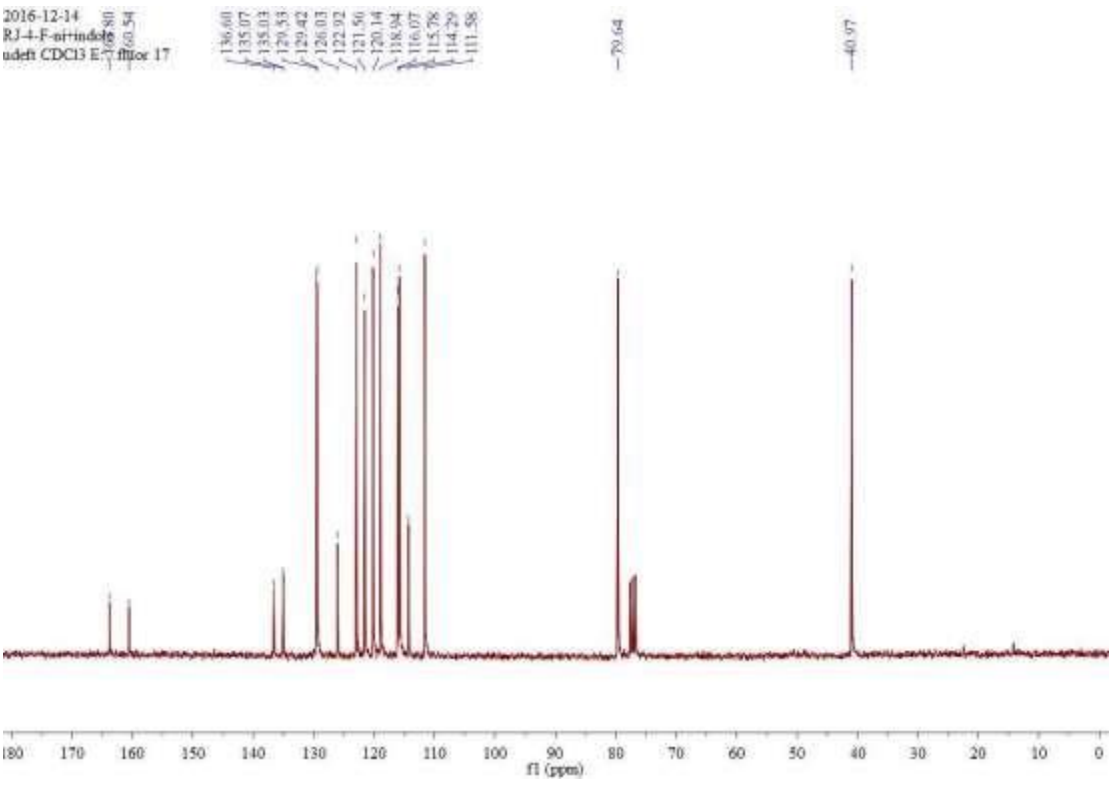

2016-12-09
RJ-4-CH3-ai+indole
PROTON CDCl3 E:\\ fluor 54
f1 (ppm)

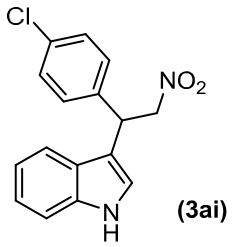

2016-12-09
RJ-4-CH3-ai+indole
udeft CDCl3 E:\\ fluor 54
f1 (ppm)


F
NO2
N
H

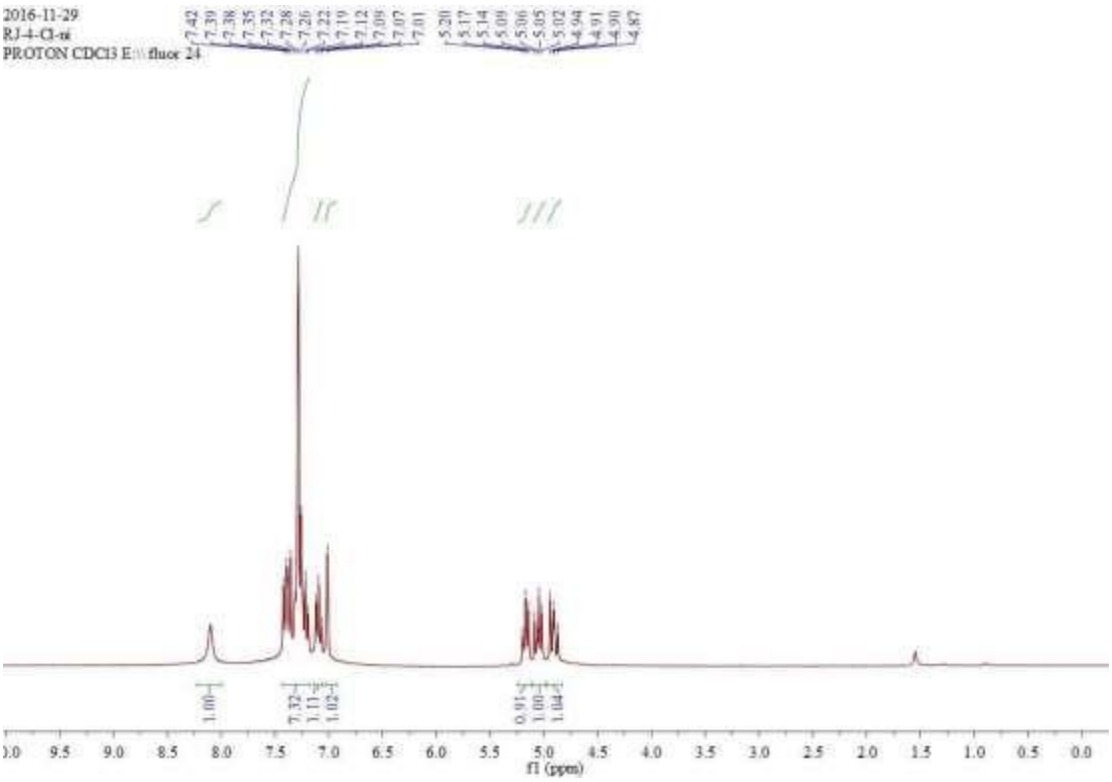
(3ah)

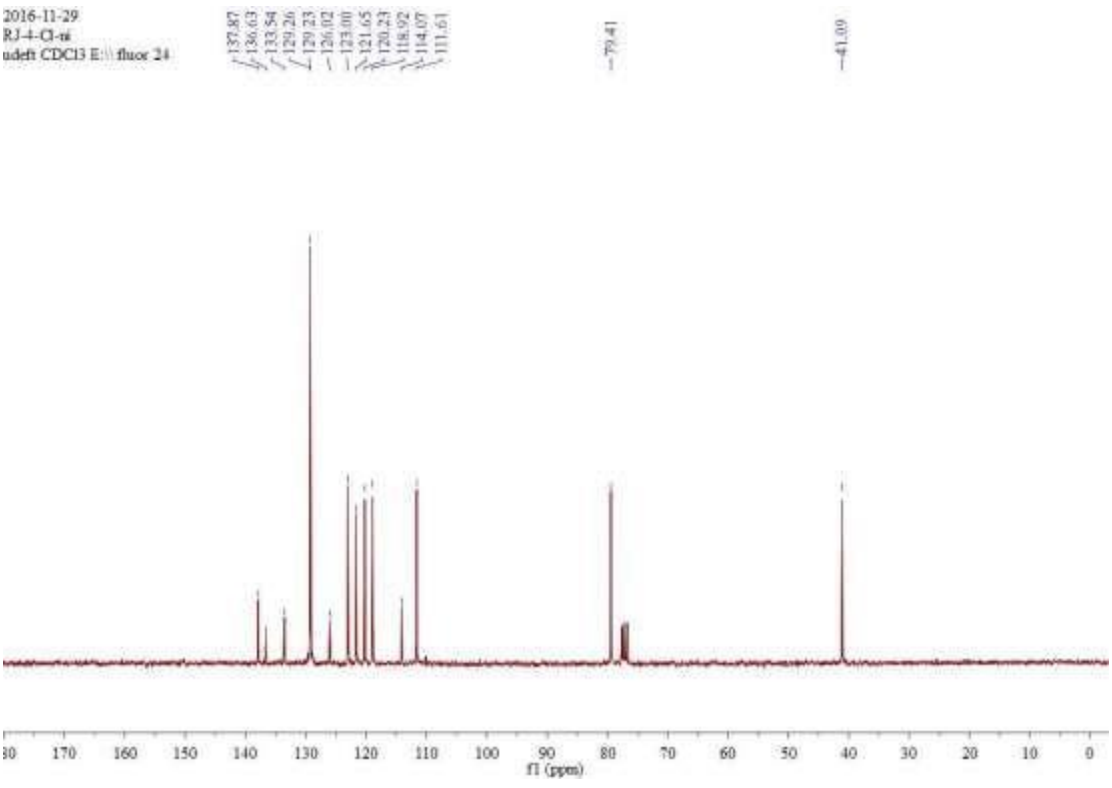

PROTON CDCl3 E:\ fluor 17
1.00
5.17
1.08
2.90
0.92
1.02
1.04
f1 (ppm)

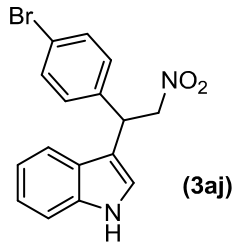

2016-12-14
RJ-4-F-nitrindole
udeft CDCl3 E:\ fluor 17
136.60
135.07
135.03
129.53
129.42
126.03
122.92
121.56
120.14
118.94
116.07
115.78
114.29
111.58
79.64
40.97
f1 (ppm)


Cl
NO2
N
H

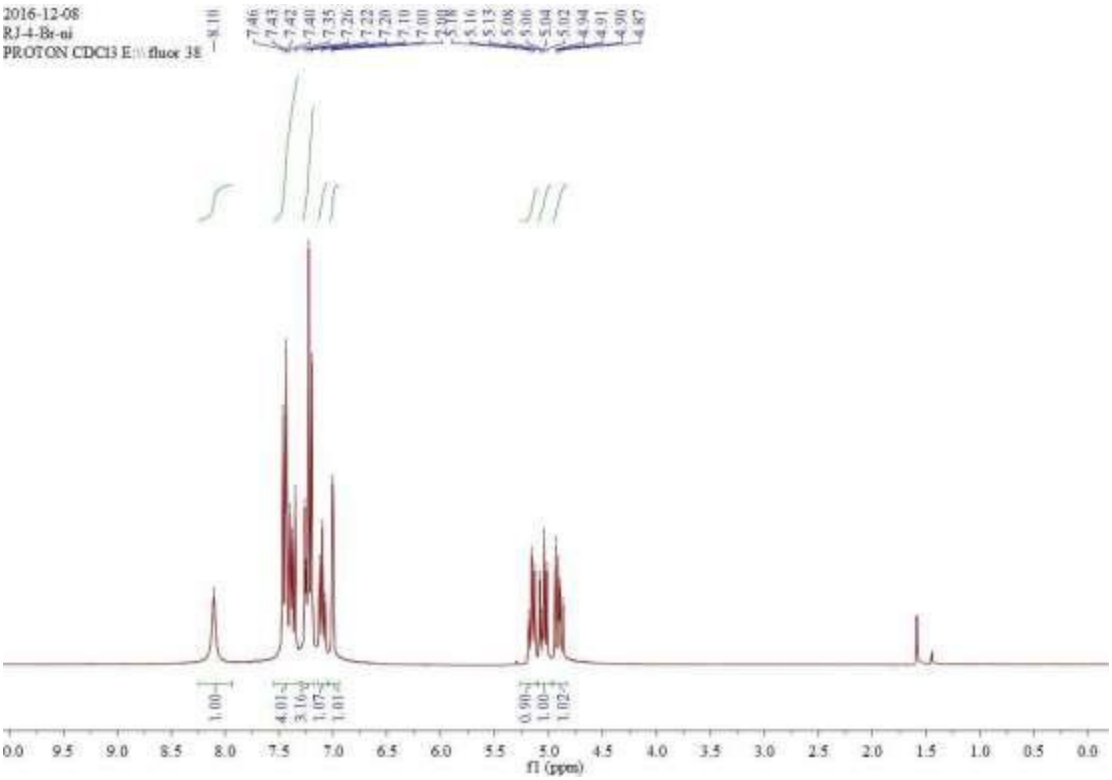
(3ai)

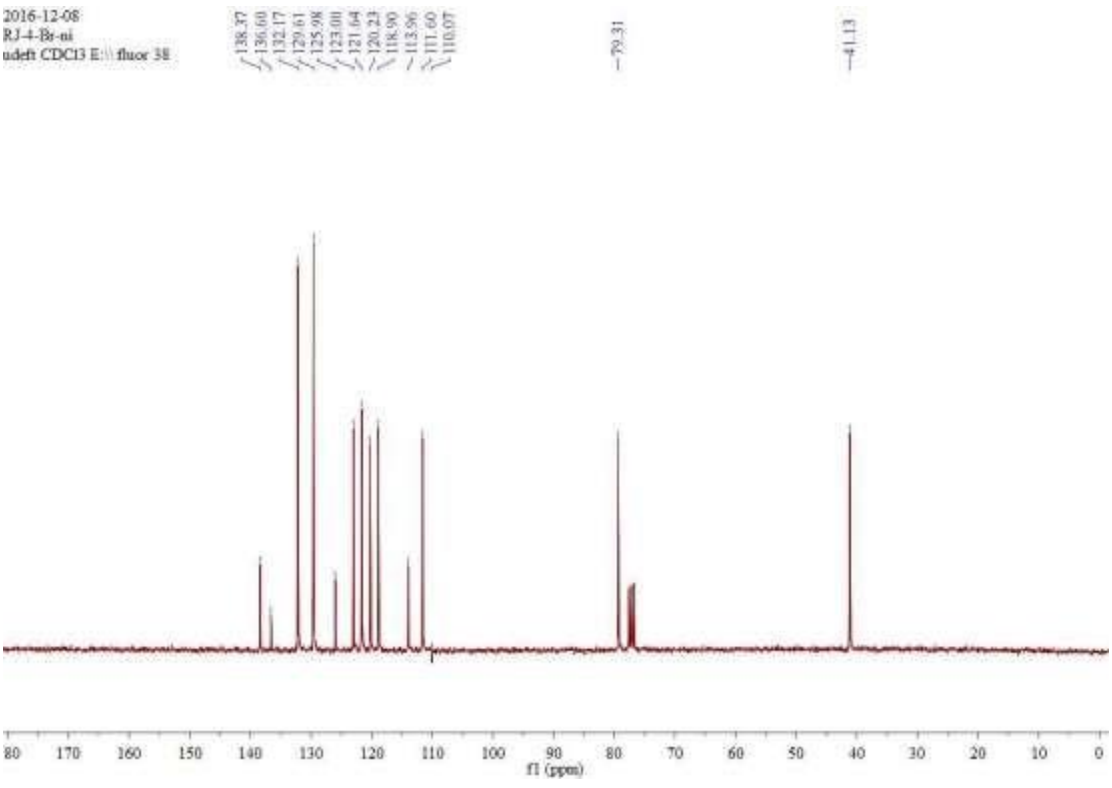

2016-11-29
RJ-4-Cl-ni
PROTON CDCl3 E:\\ fluor 24
7.42
7.39
7.38
7.35
7.32
7.28
7.26
7.22
7.19
7.12
7.09
7.07
7.01
5.20
5.17
5.14
5.09
5.06
5.05
5.02
4.94
4.91
4.90
4.87
1.00
7.32
1.11
1.02
0.91
1.00
1.04
f1 (ppm)

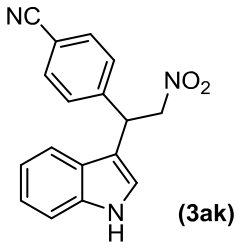

2016-11-29
RJ-4-Cl-ni
udeft CDCl3 E:\\ fluor 24
137.87
136.63
133.54
129.26
129.23
126.02
123.00
121.65
120.23
118.92
114.07
111.61
79.41
41.09
f1 (ppm)


Br
NO2
N
H

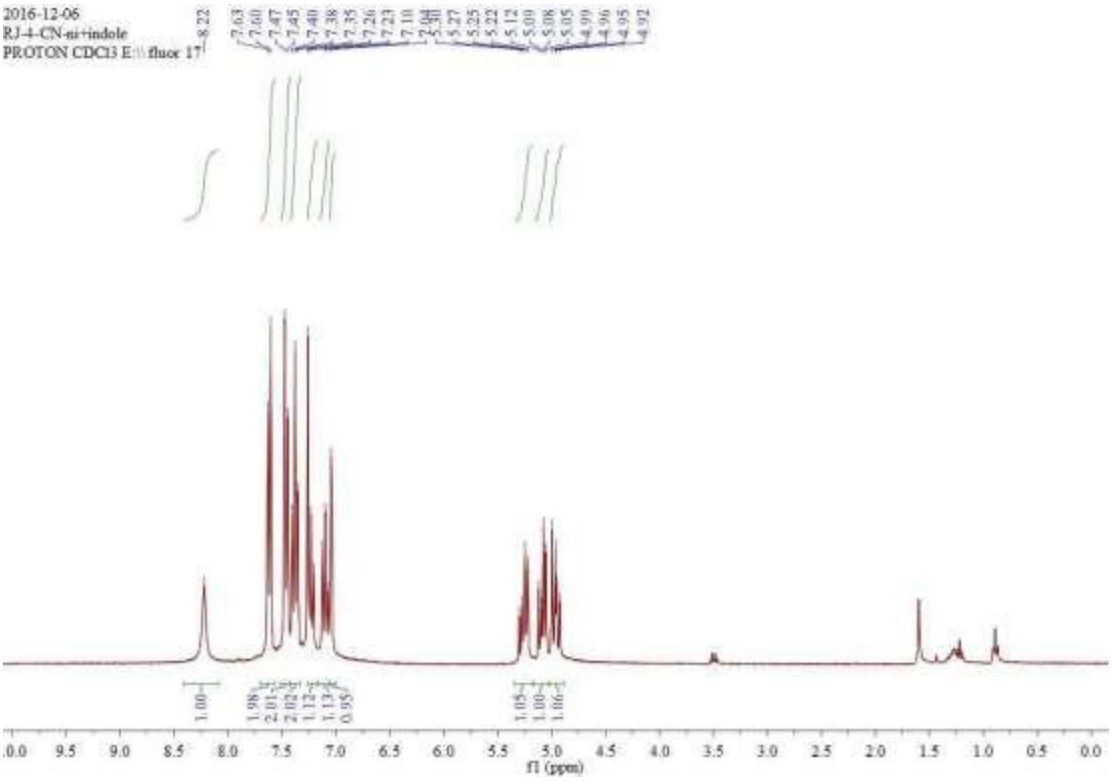
(3aj)

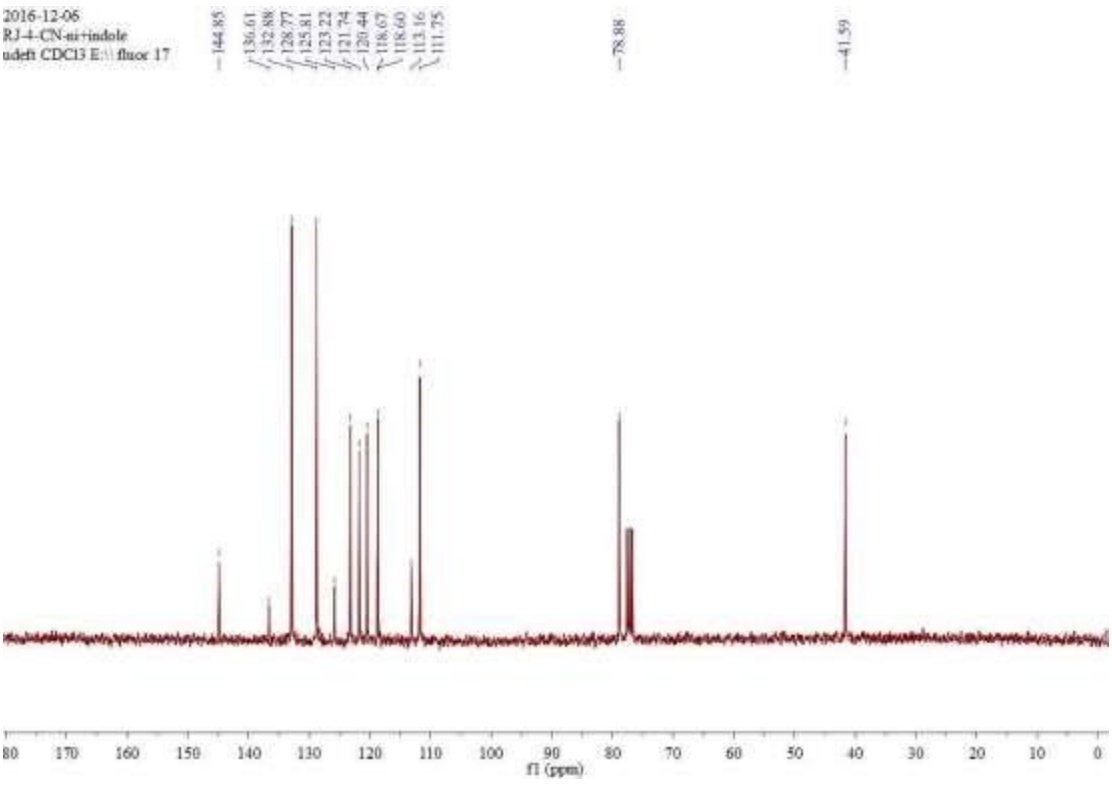

2016-12-08
RJ-4-Br-ni
PROTON CDCl3 E:\\ fluor 38
f1 (ppm)

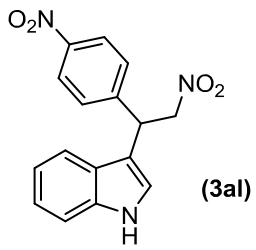

2016-12-08
RJ-4-Br-ni
udeft CDCl3 E:\\ fluor 38
f1 (ppm)


NC
NO2
N
H

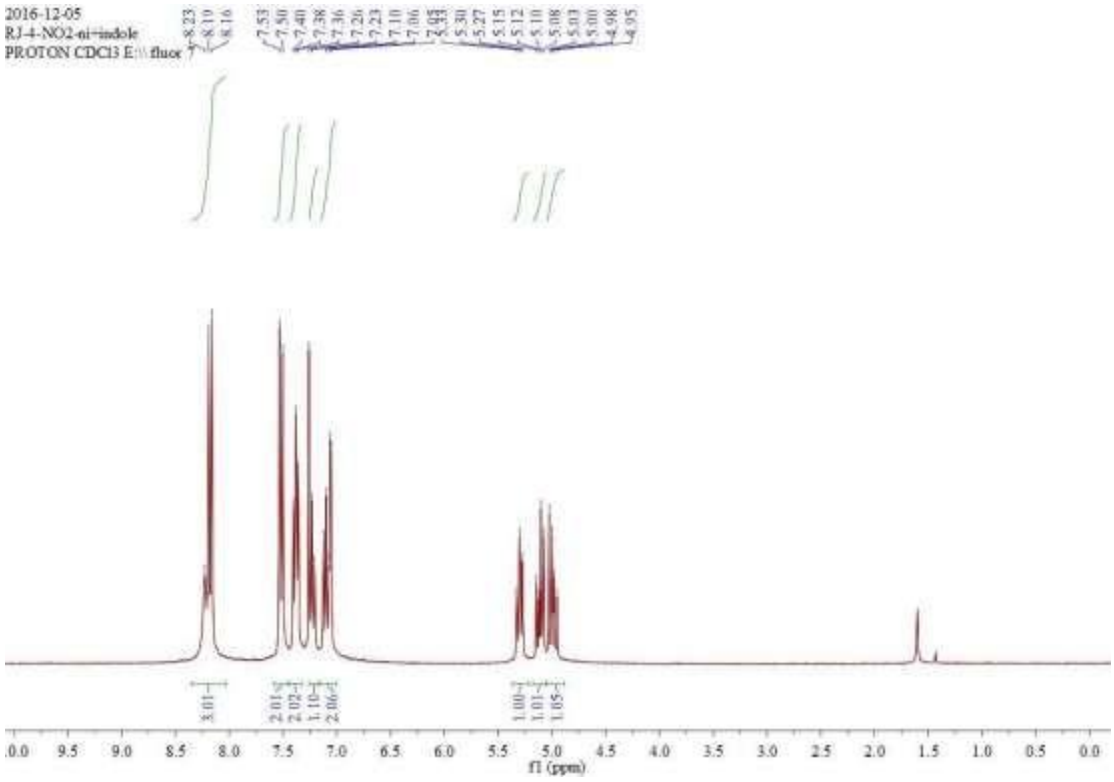
(3ak)

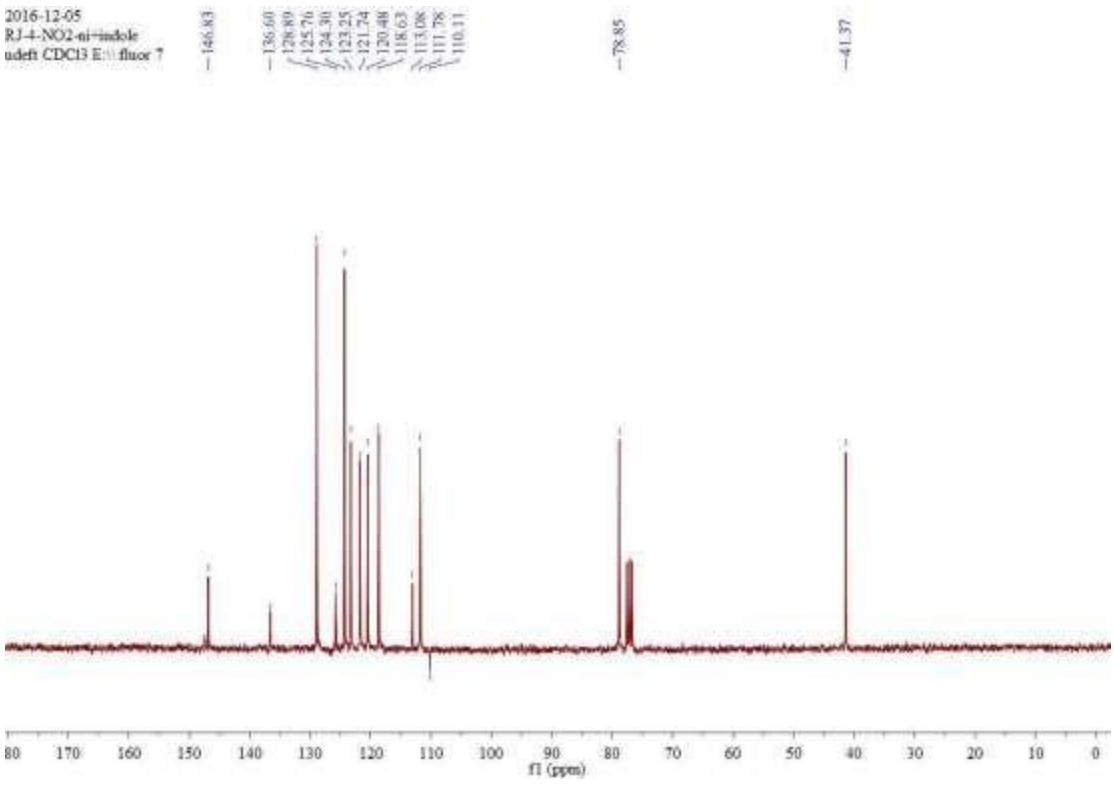

2016-12-06
RJ-4-CN-si+indole
PROTON CDCl3 E:\\ fluor 17
f1 (ppm)

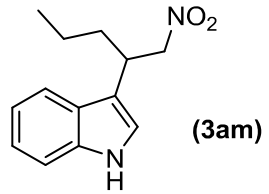

2016-12-06
RJ-4-CN-si+indole
udeft CDCl3 E:\\ fluor 17
f1 (ppm)


O_2N
NO_2
N
H

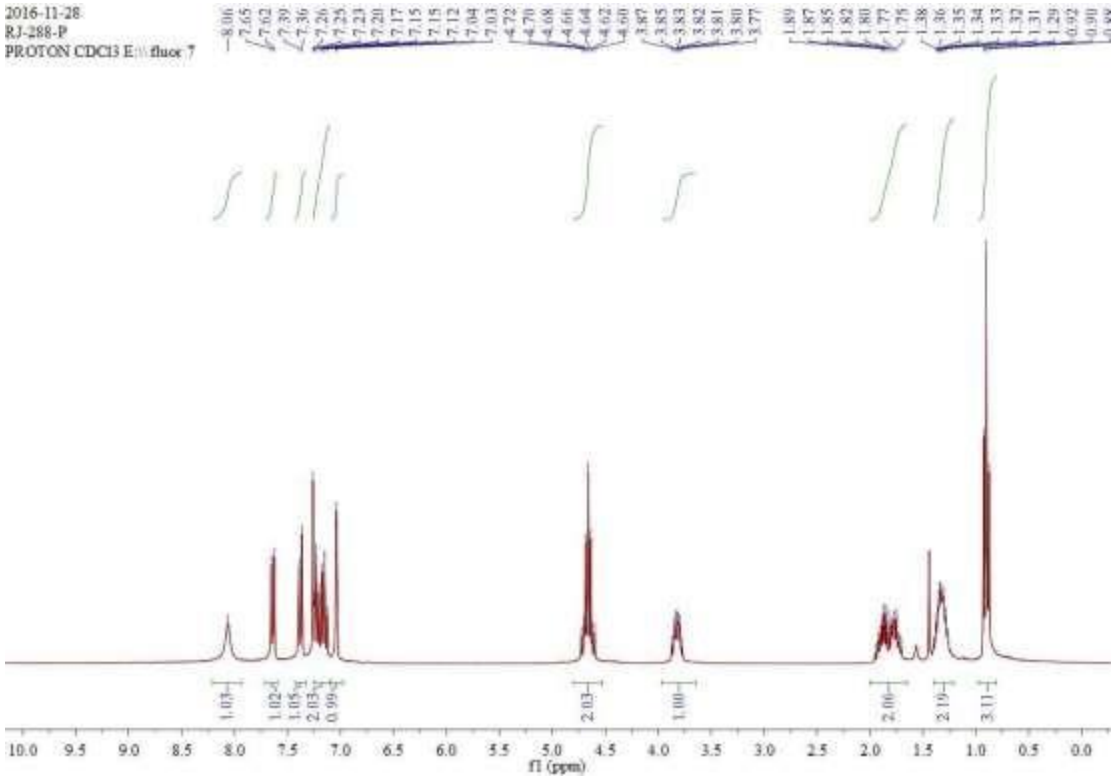
(3al)

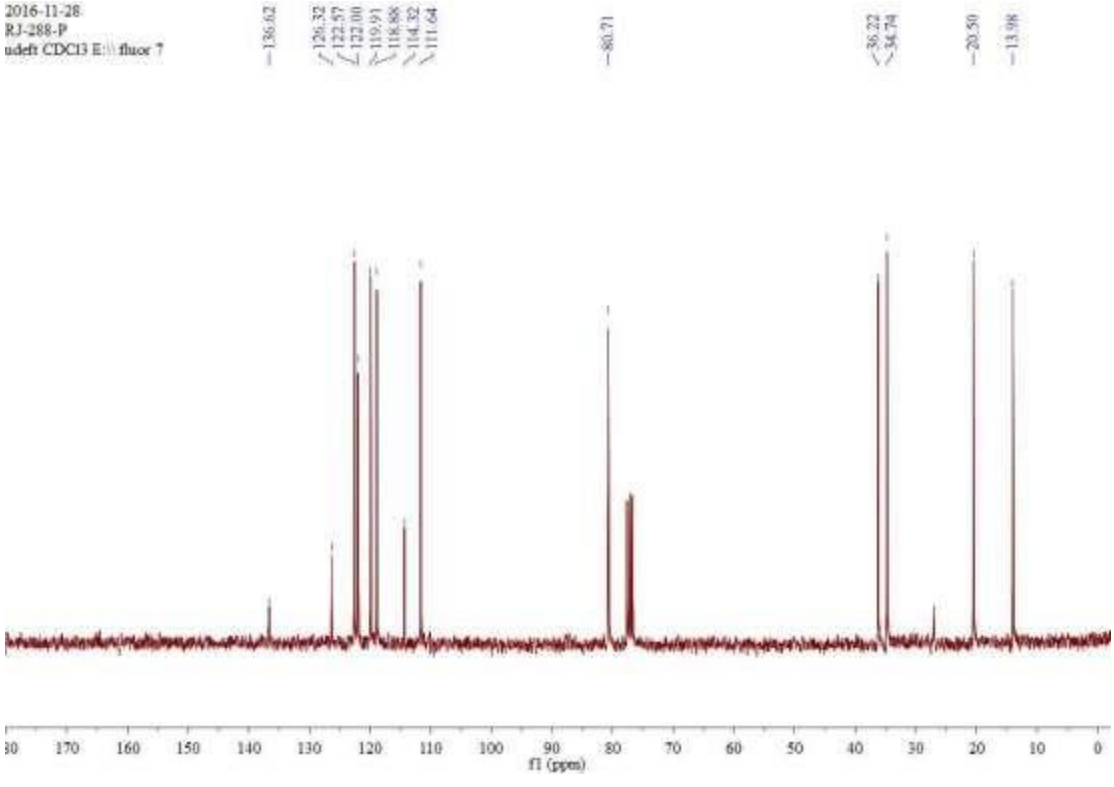

2016-12-05
RJ-4-NO2-ni-indole
PROTON CDCl3 E:\\ fluor 7
f1 (ppm)

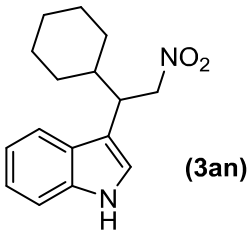

2016-12-05
RJ-4-NO2-ni-indole
udeft CDCl3 E:\\ fluor 7
f1 (ppm)


NO2
N
H

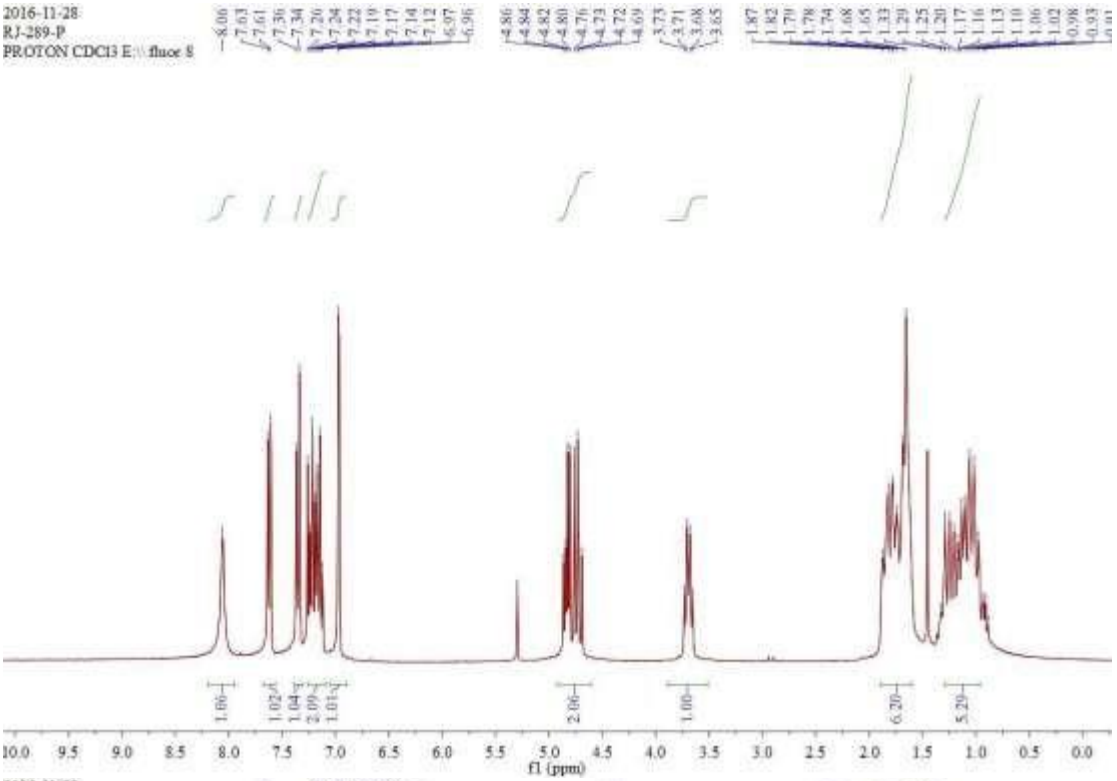
(3am)

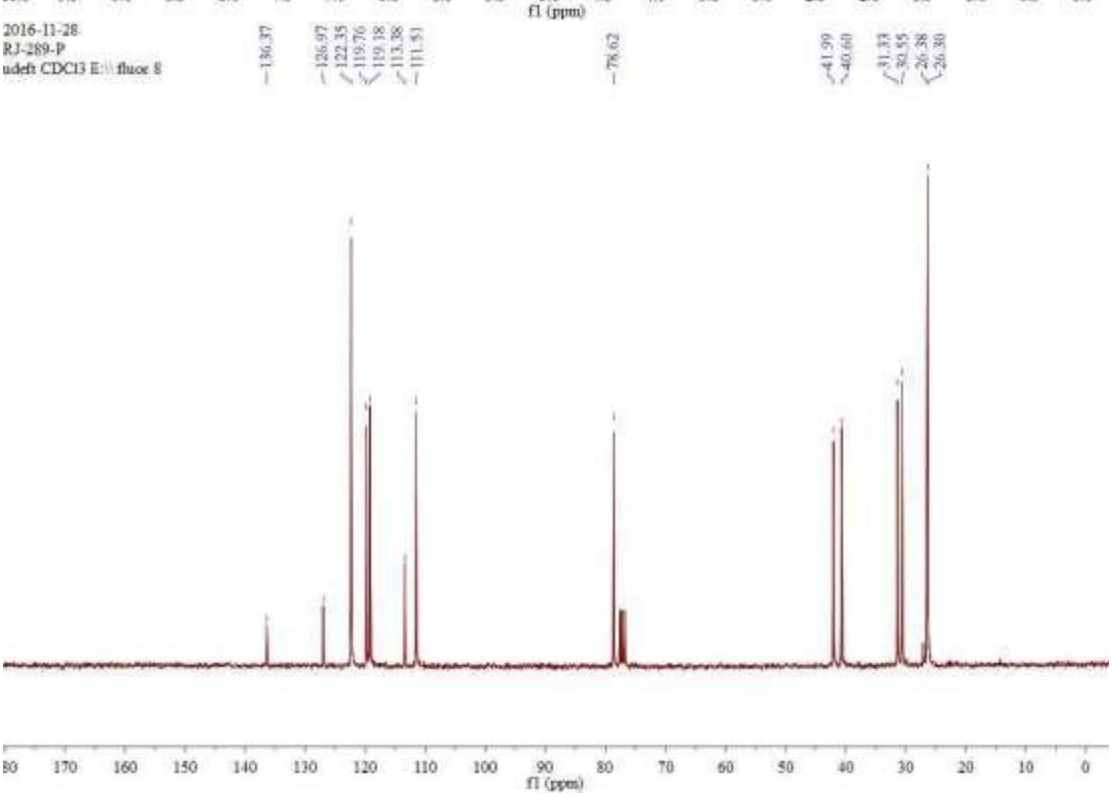

2016-11-28
RJ-288-P
PROTON CDCl3 E:\\ fluor 7
f1 (ppm)

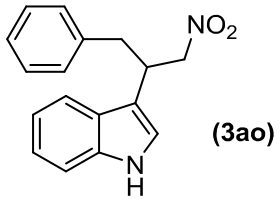

2016-11-28
RJ-288-P
udeft CDCl3 E:\\ fluor 7
f1 (ppm)


NO2
N
H

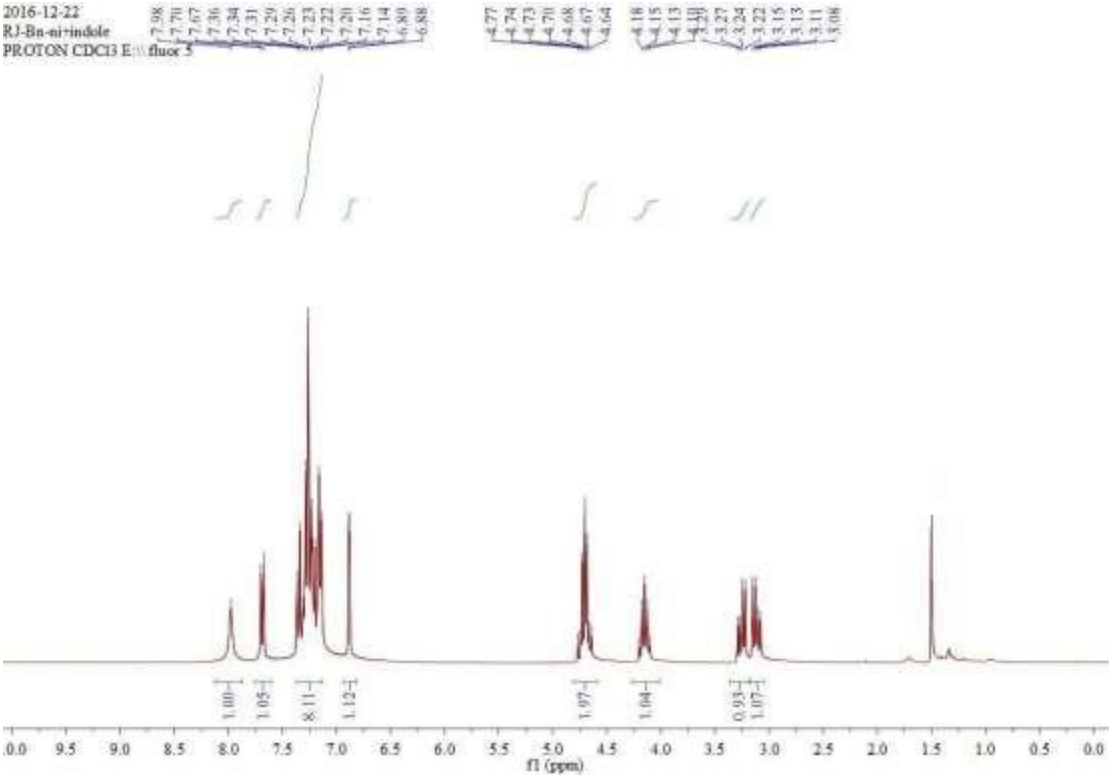
(3an)

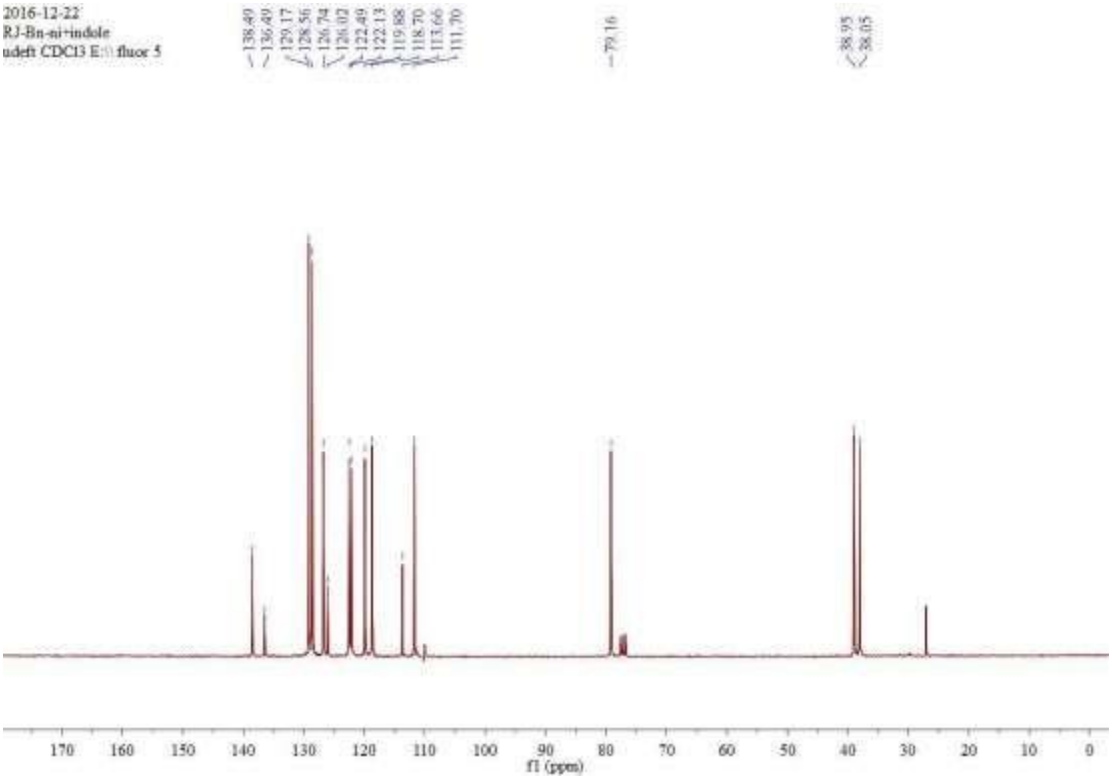

2016-11-28
RJ-289-P
PROTON CDCl3 E:\\ fluor 8
f1 (ppm)

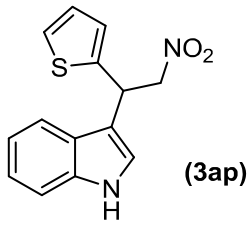

2016-11-28
RJ-289-P
udeft CDCl3 E:\\ fluor 8
f1 (ppm)


NO2
N
H

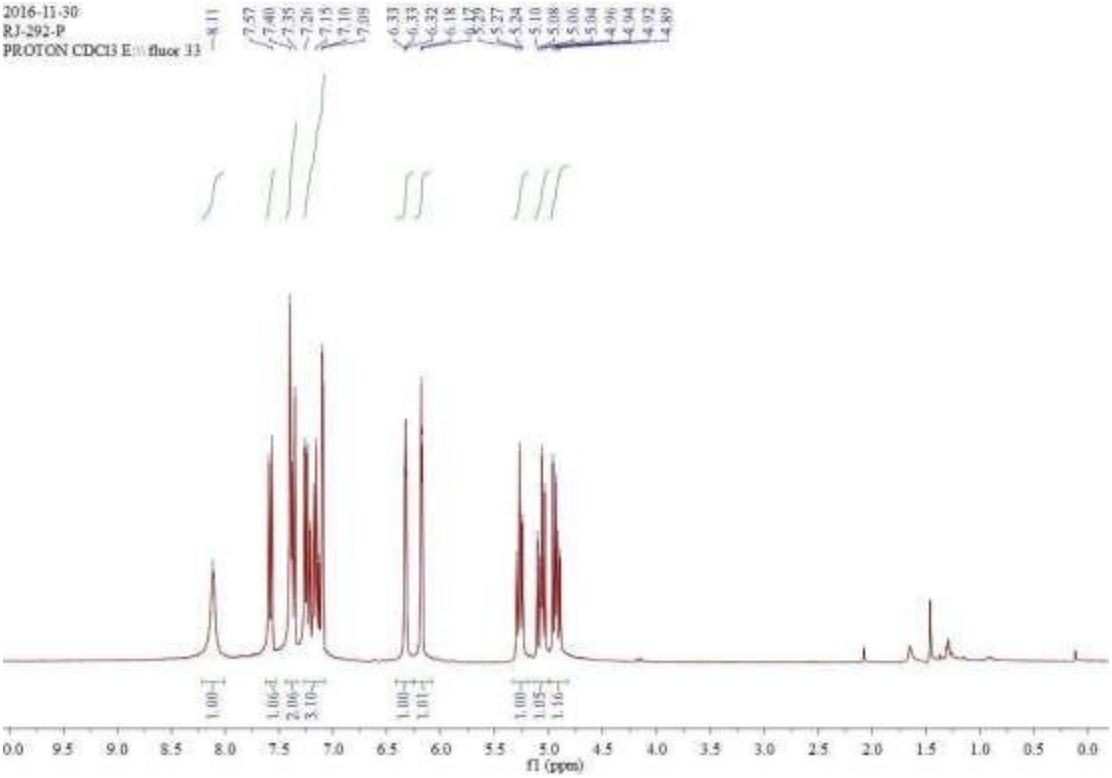
(3ao)

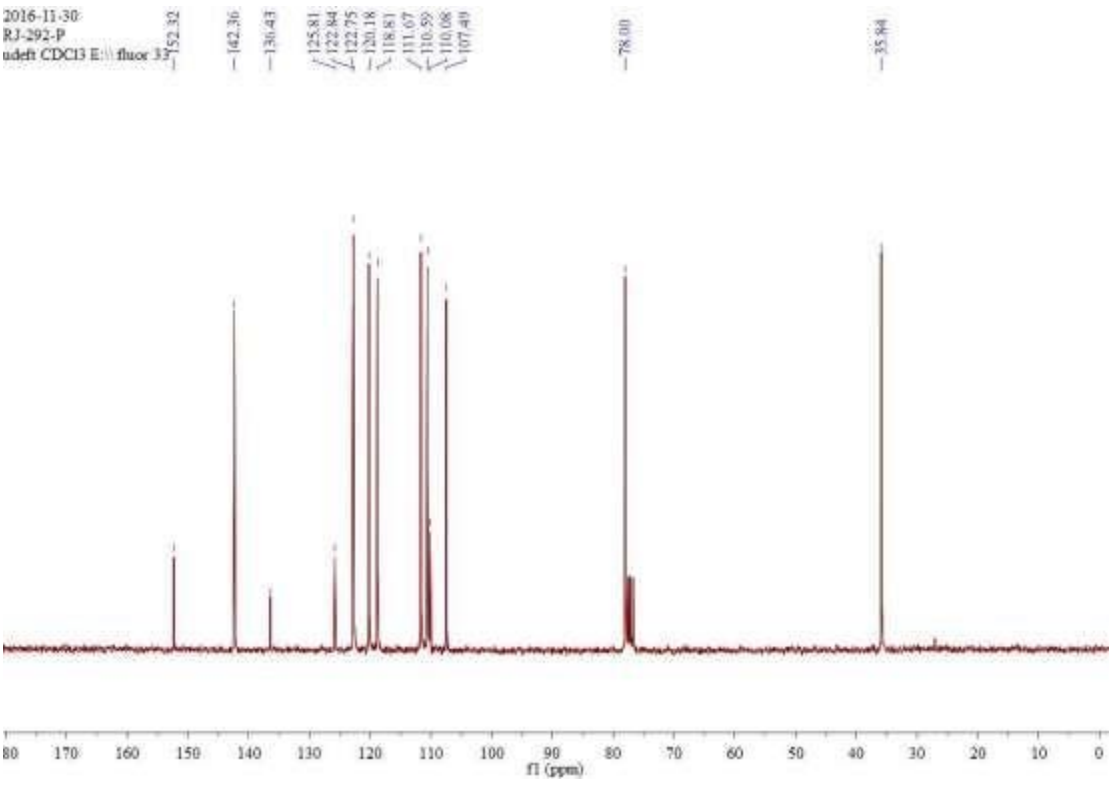

2016-12-22
RJ-Bn-ni+indole
PROTON CDCl3 E:\\ fluor 5
f1 (ppm)

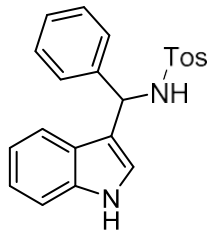

2016-12-22
RJ-Bn-ni+indole
udeft CDCl3 E:\\ fluor 5
f1 (ppm)

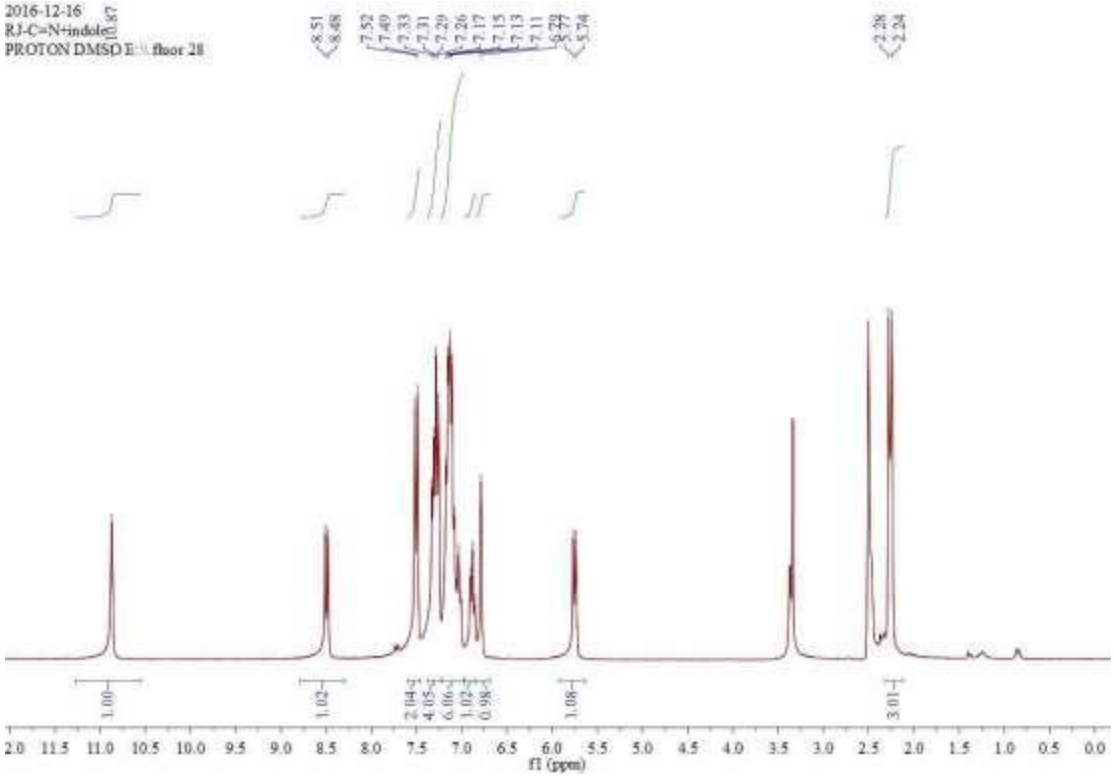

S
NO2
N
H

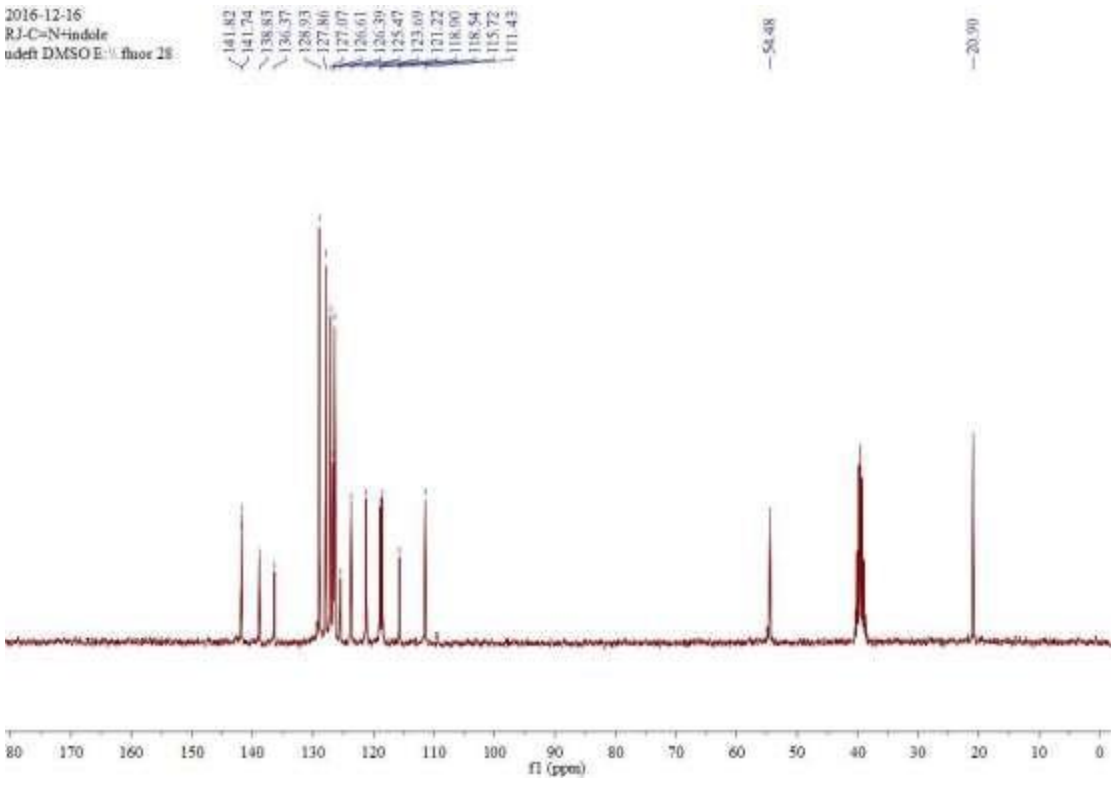
(3ap)

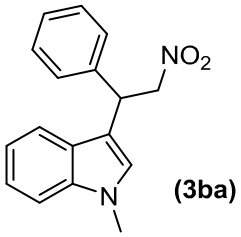

2016-11-30
RJ-292-P
PROTON CDCl3 E:\\ fluor 33
f1 (ppm)


2016-11-30
RJ-292-P
udeft CDCl3 E:\\ fluor 33
f1 (ppm)

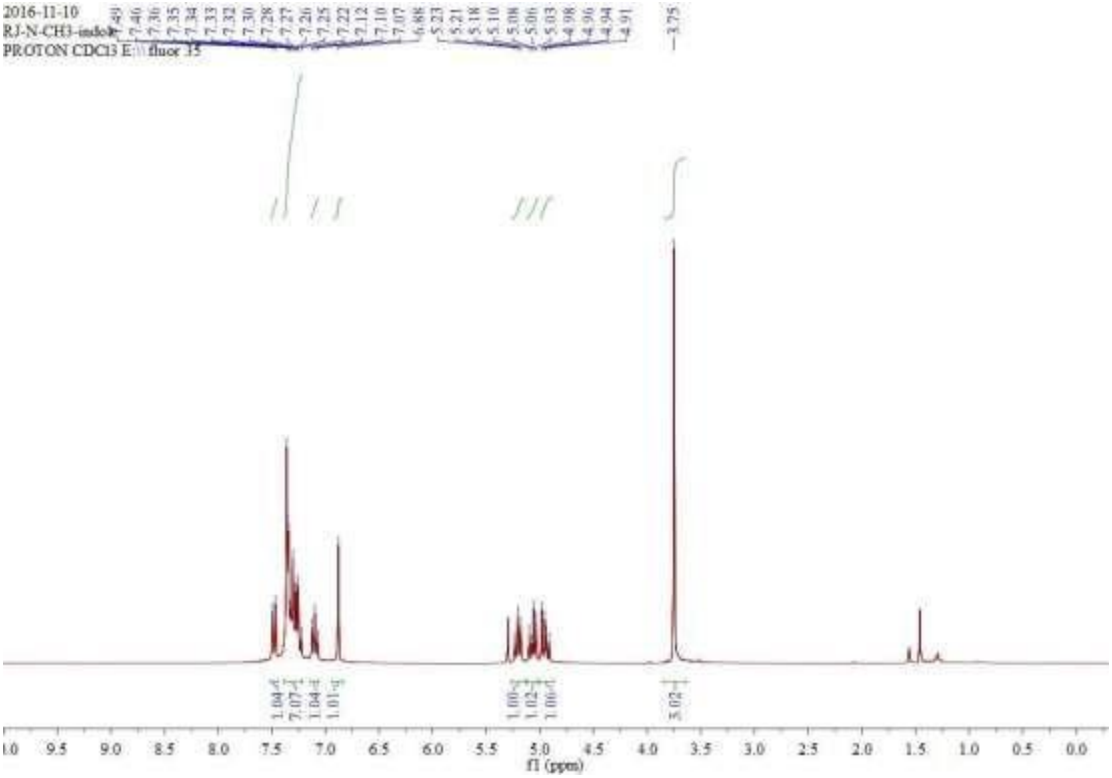

Tos
NH
N
H

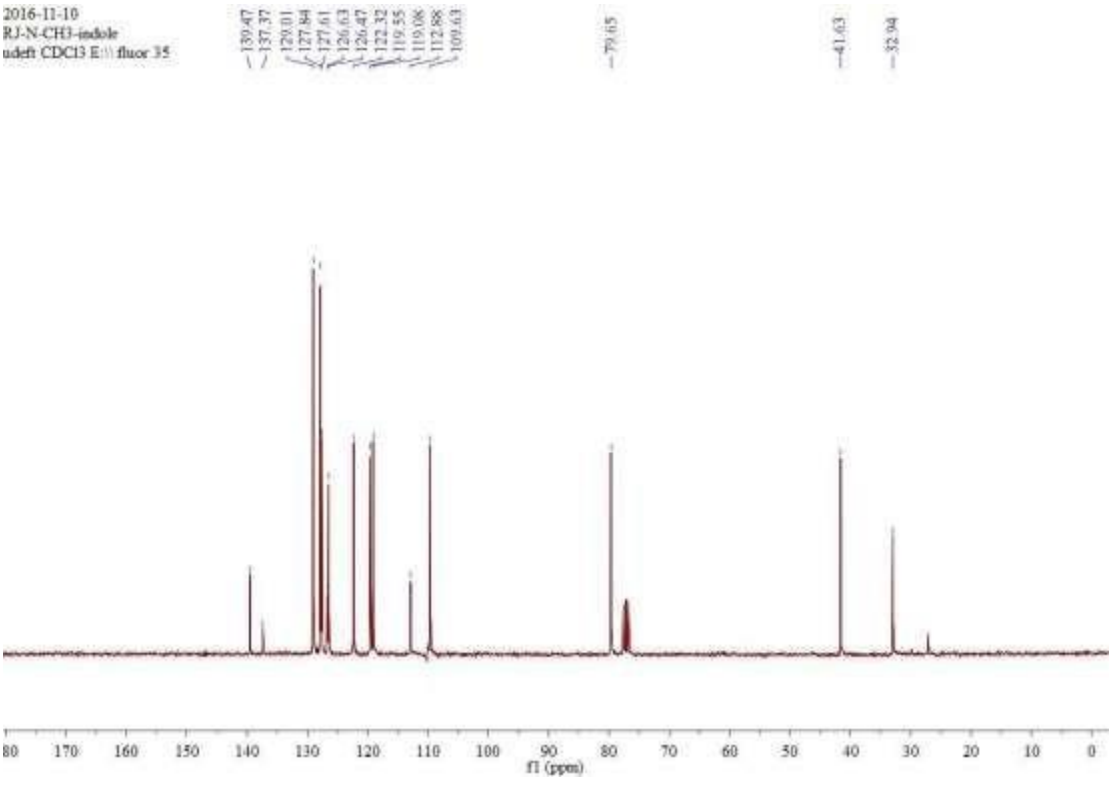

2016-12-16
RJ-C=N+indole
PROTON DMSO
fluor 28
f1 (ppm)

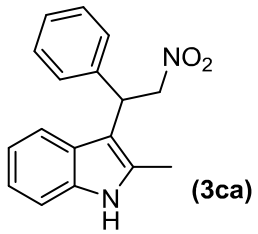

2016-12-16
RJ-C=N+indole
udeft DMSO
fluor 28
f1 (ppm)


NO2
N

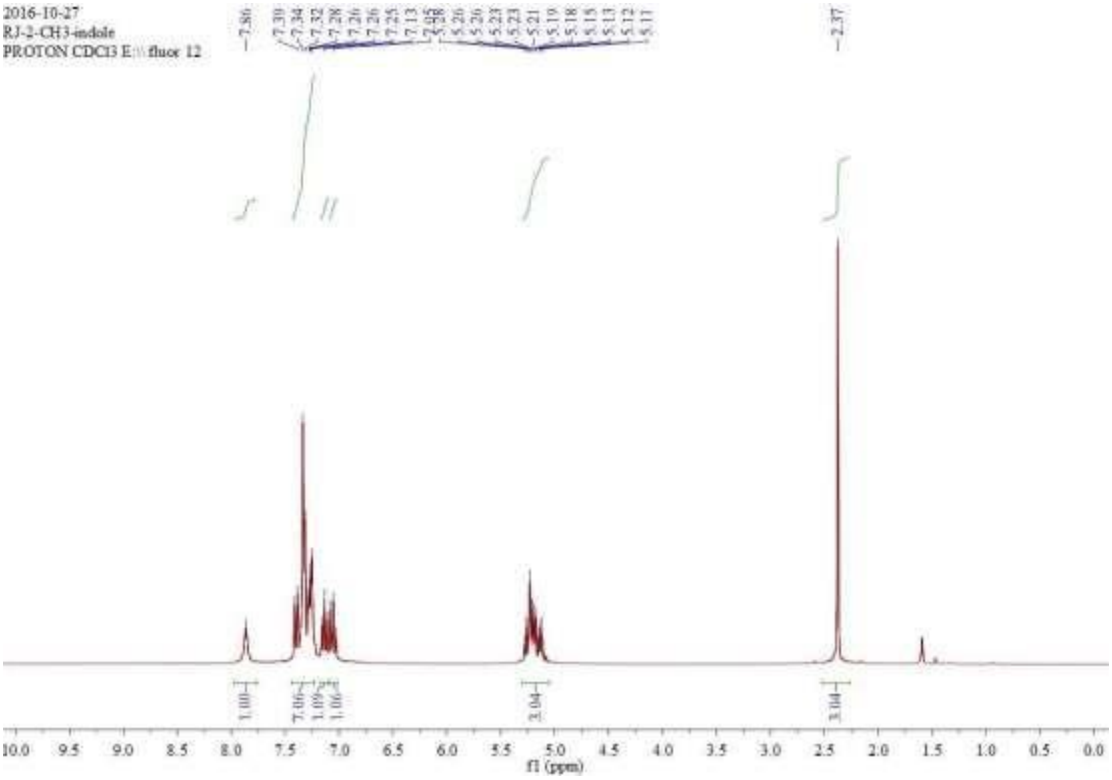
(3ba)

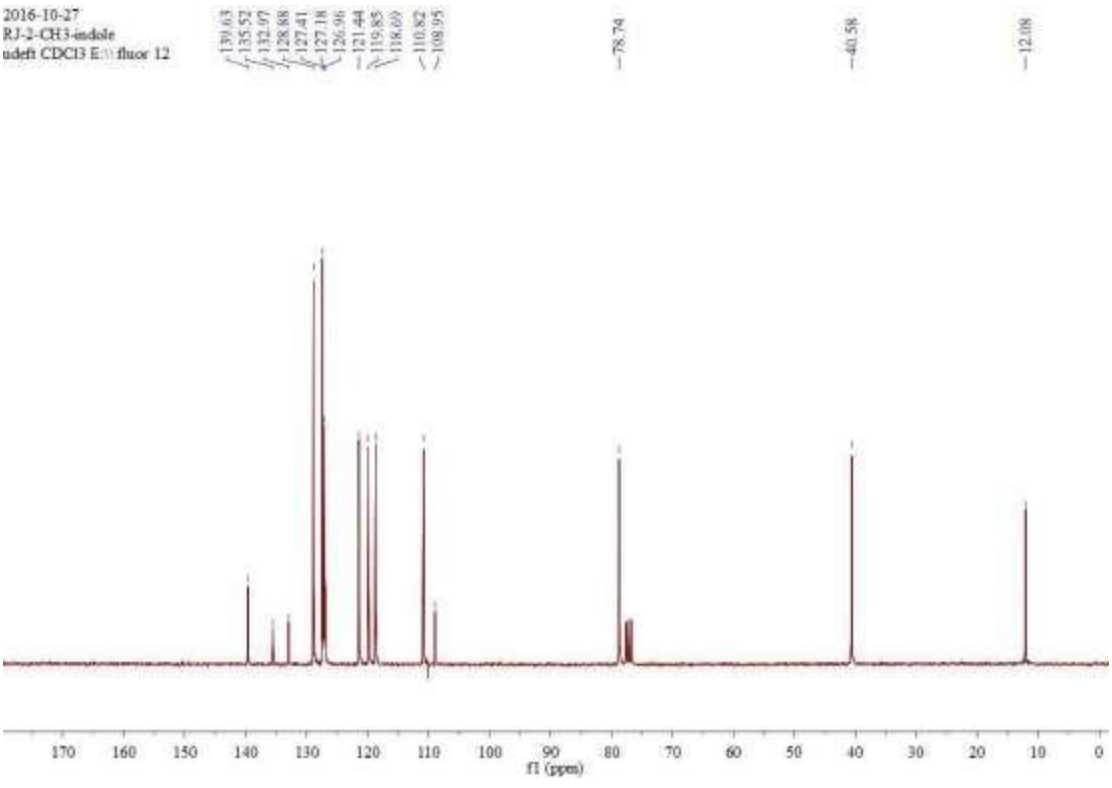

2016-11-10
RJ-N-CH3-indole
PROTON CDCl3 E:\\ fluor 35
f1 (ppm)

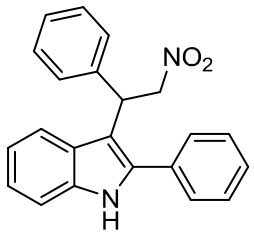

2016-11-10
RJ-N-CH3-indole
udeft CDCl3 E:\\ fluor 35
f1 (ppm)


NO2
N
H

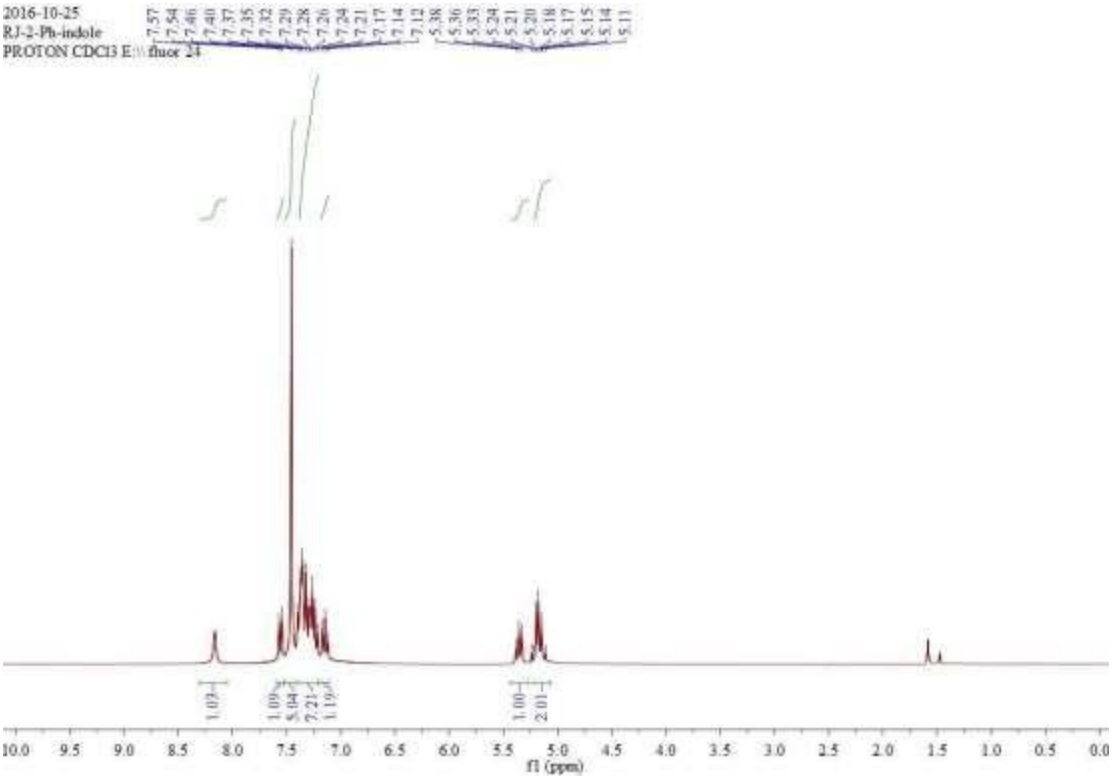
(3ca)

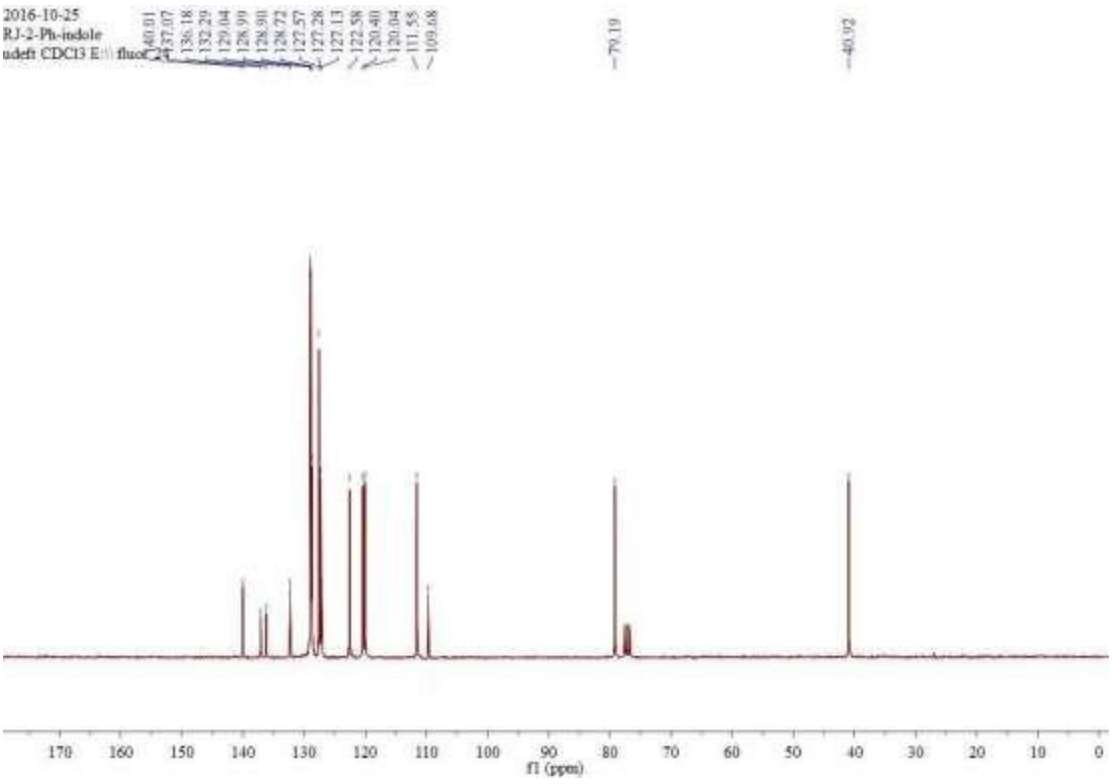

2016-10-27
RJ-2-CH3-indole
PROTON CDCl3 E:\\ fluor 12
7.86
7.39
7.34
7.32
7.28
7.26
7.26
7.25
7.13
5.26
5.26
5.23
5.23
5.21
5.19
5.18
5.15
5.13
5.12
5.11
2.37
1.00
7.06
1.09
1.06
3.04
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

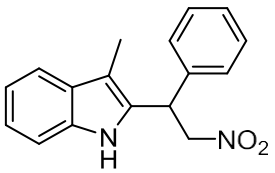

2016-10-27
RJ-2-CH3-indole
udeft CDCl3 E:\\ fluor 12
139.63
135.52
132.97
128.88
127.41
127.18
126.96
121.44
119.85
118.69
110.82
108.95
78.74
40.58
12.08
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NO2
N
H

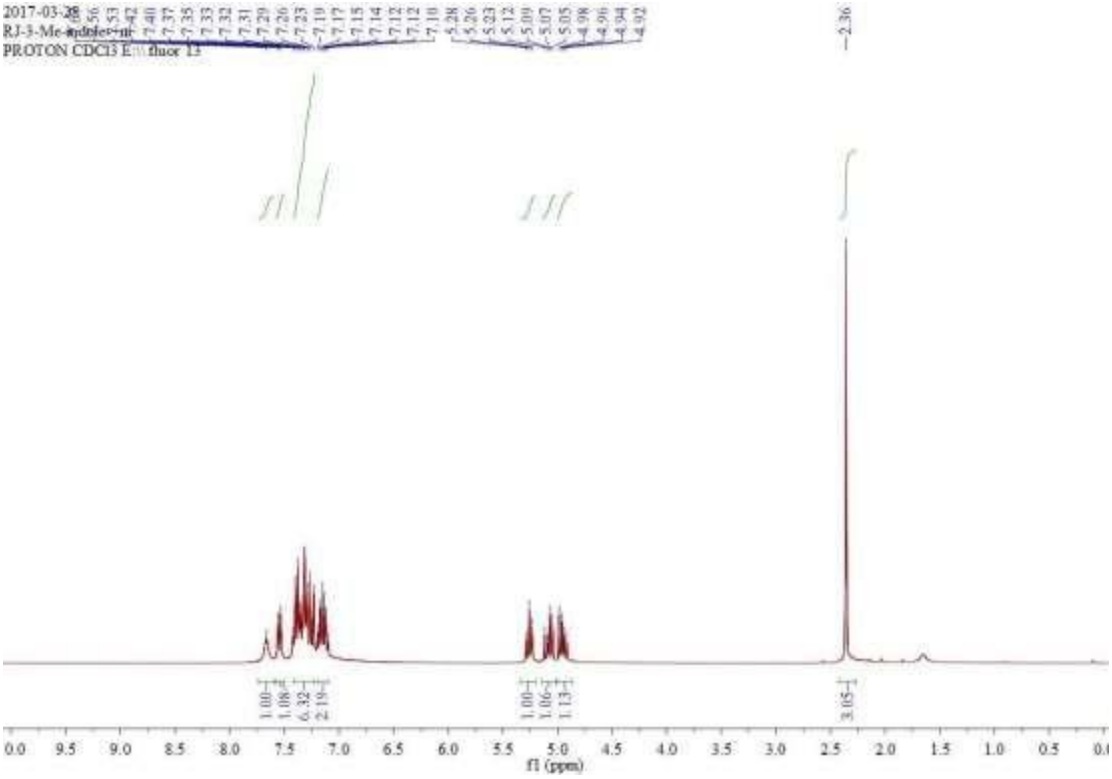
(3da)

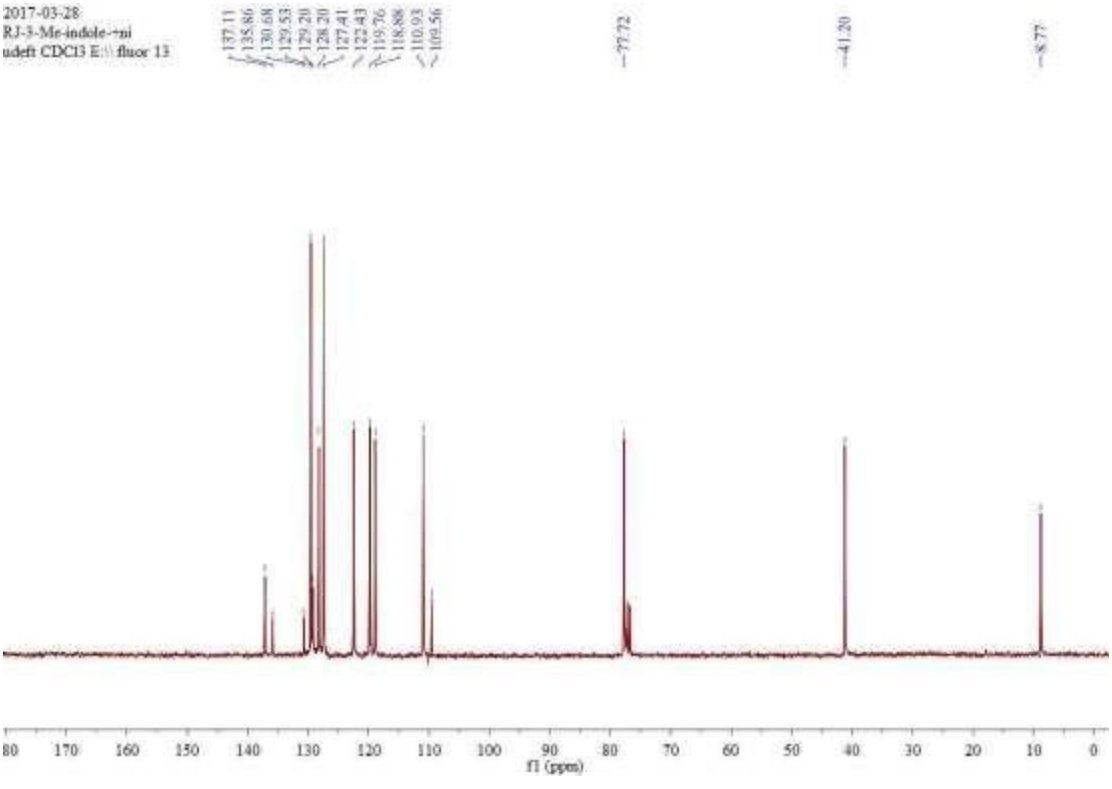

2016-10-25
RJ-2-Ph-indole
PROTON CDCl3 E:\\ fluor 24
f1 (ppm)

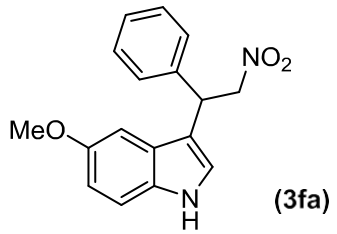

2016-10-25
RJ-2-Ph-indole
udeft CDCl3 E:\\ fluor24
f1 (ppm)


NO2
H
N

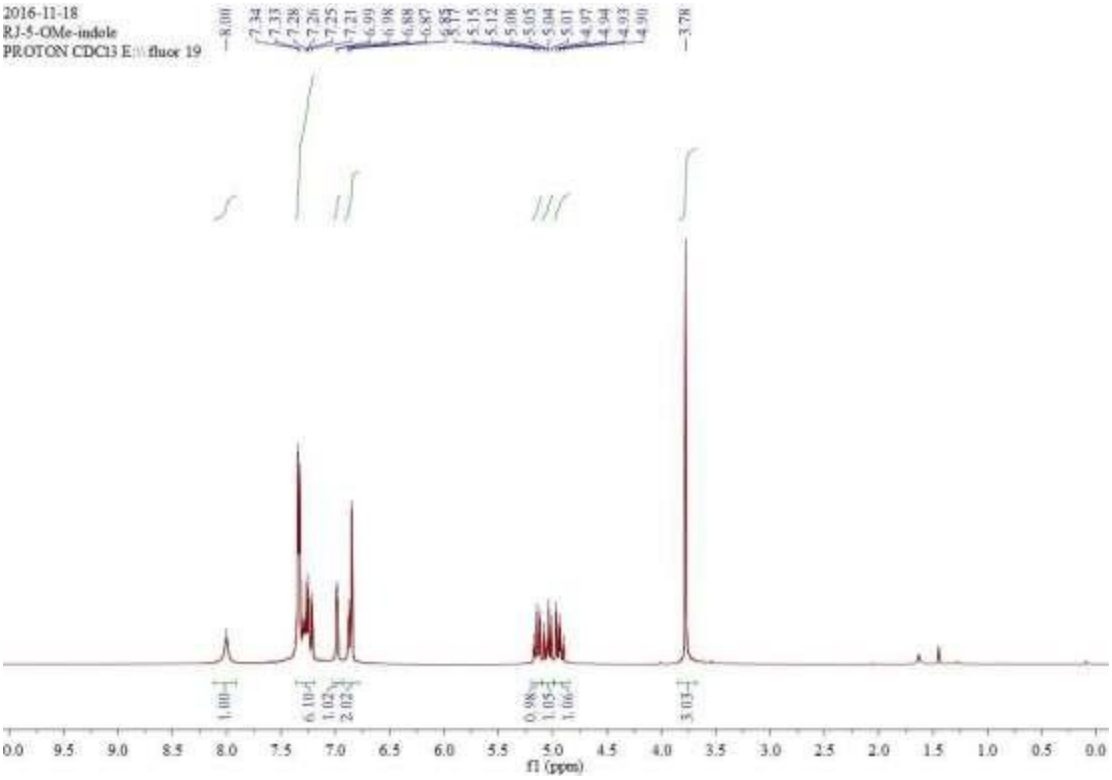
(3ea)

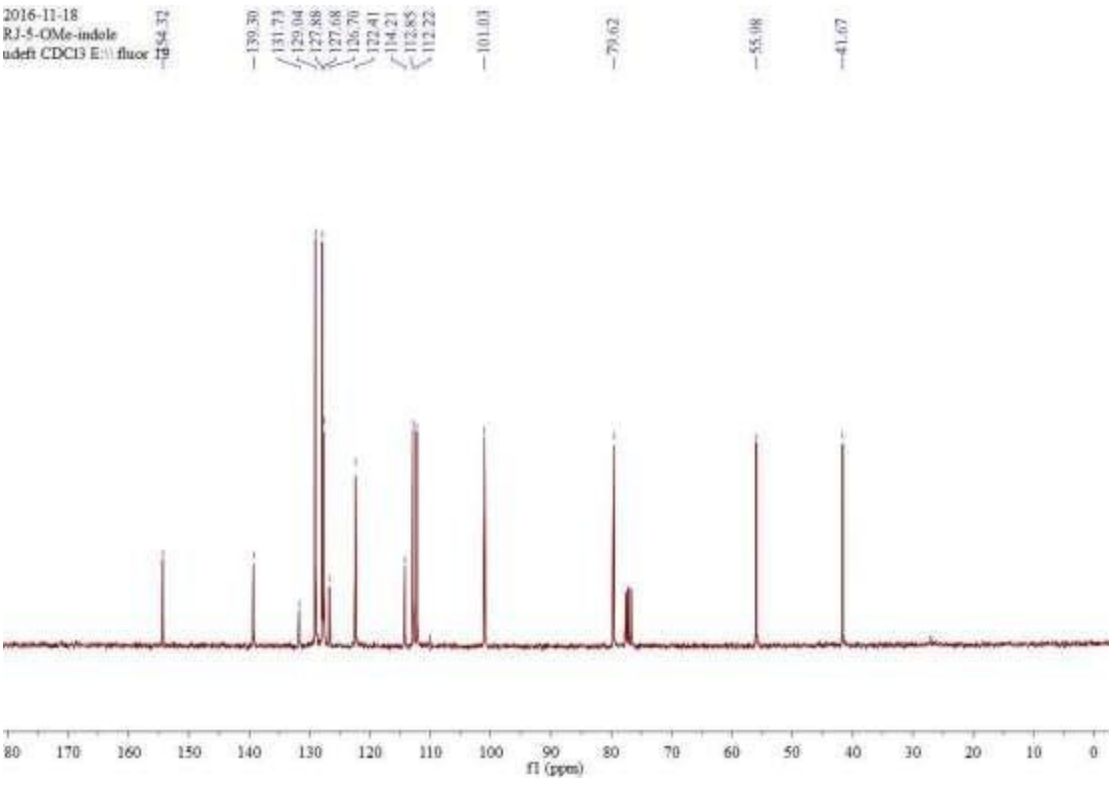

2017-03-28
RJ-3-Me-indole-+ni
PROTON CDCl3 E:\\ fluor 13
f1 (ppm)

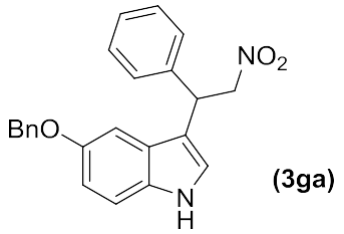

2017-03-28
RJ-3-Me-indole-+ni
udeft CDCl3 E:\\ fluor 13
f1 (ppm)


NO2
MeO
N
H

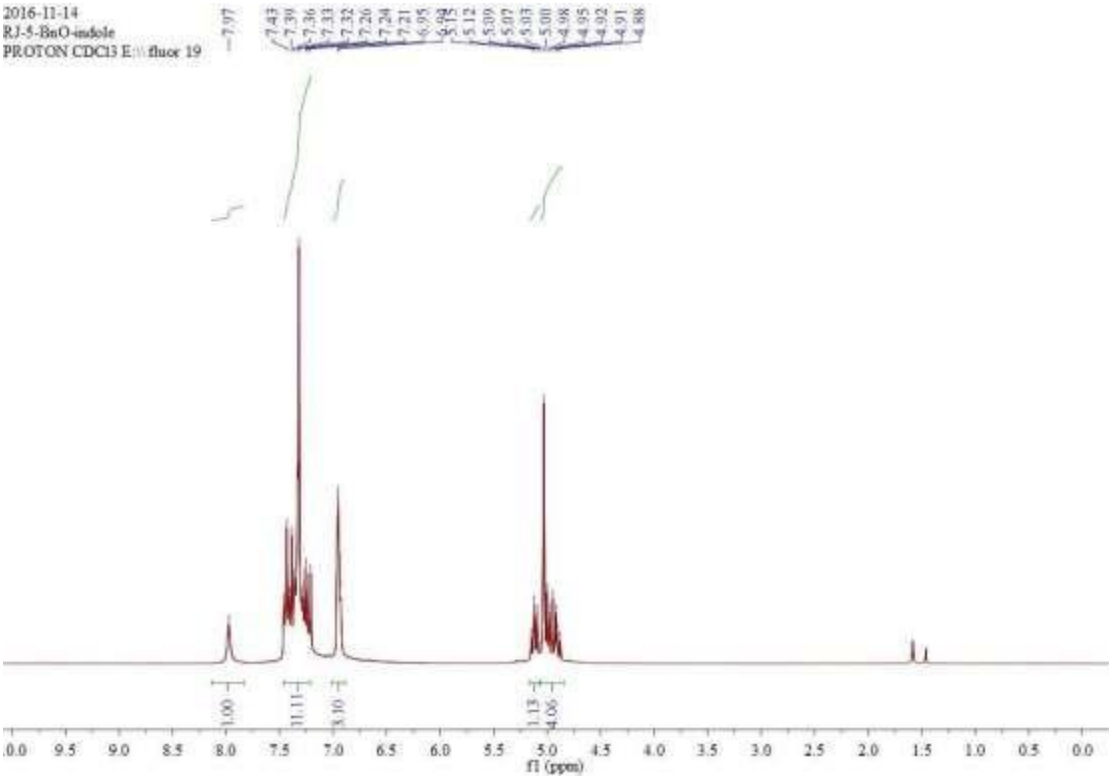
(3fa)

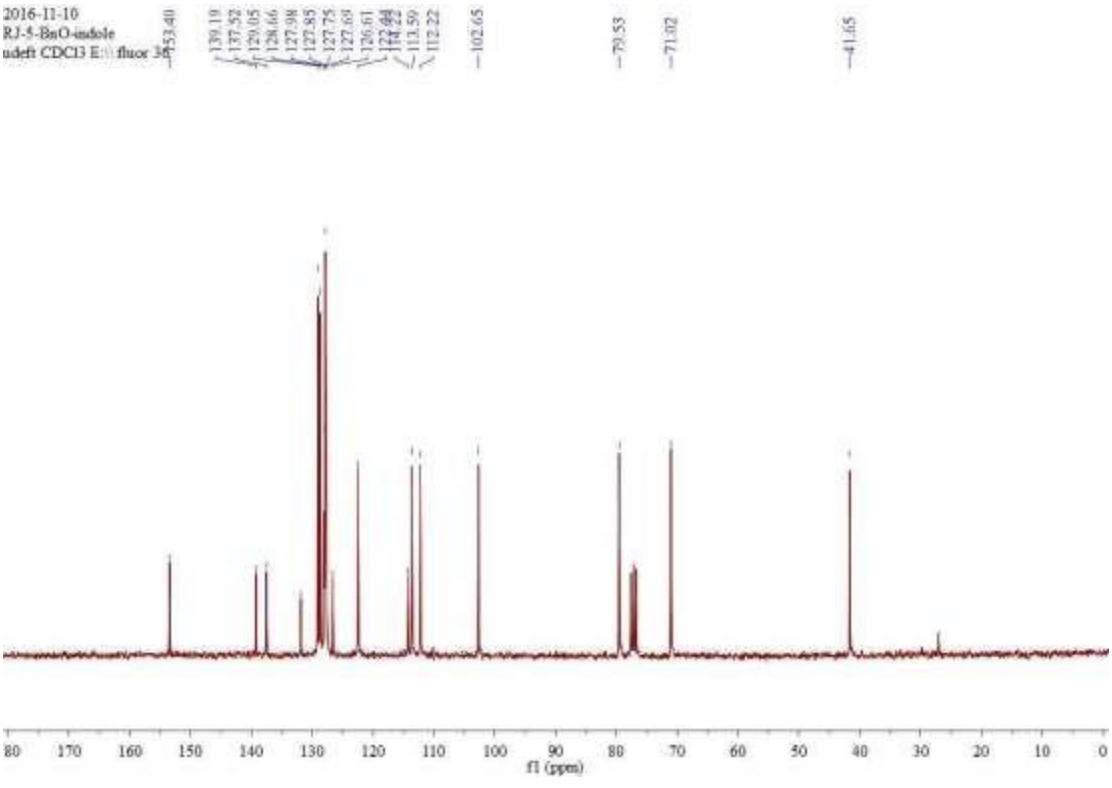

2016-11-18
RJ-5-OMe-indole
PROTON CDCl3 E:\\ fluor 19
f1 (ppm)

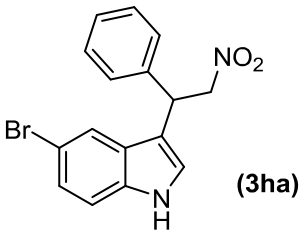

2016-11-18
RJ-5-OMe-indole
udeft CDCl3 E:\\ fluor 19
f1 (ppm)


NO2
BnO
N
H

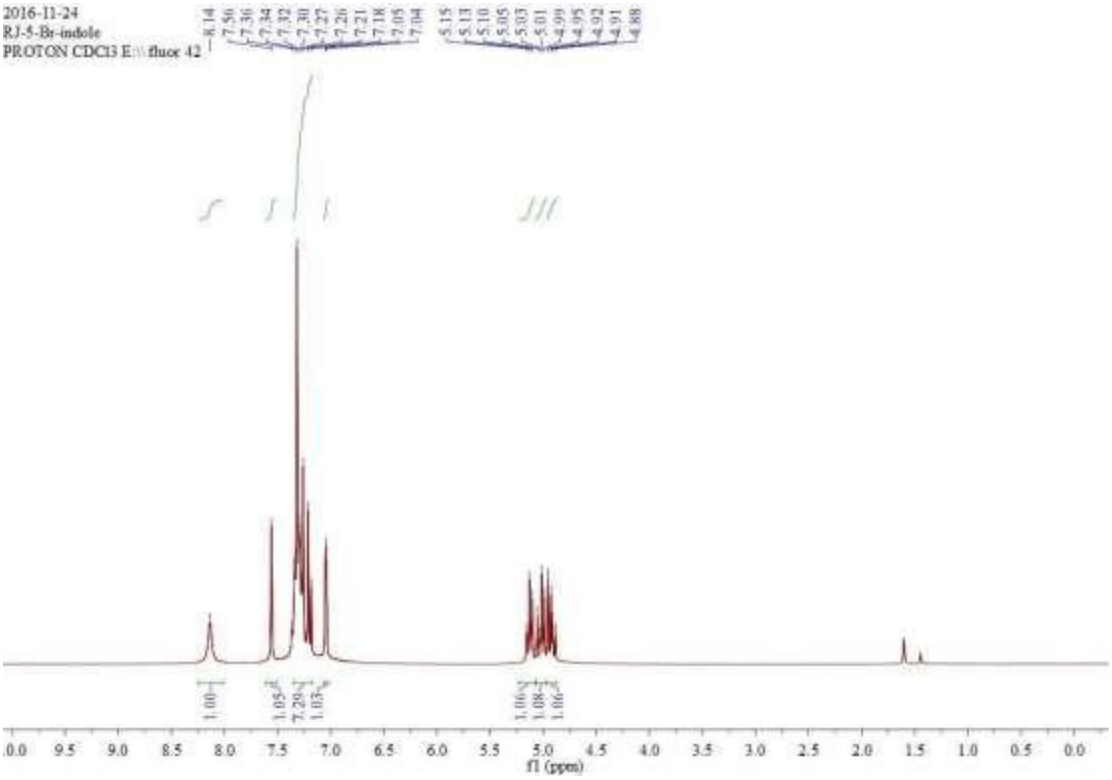
(3ga)

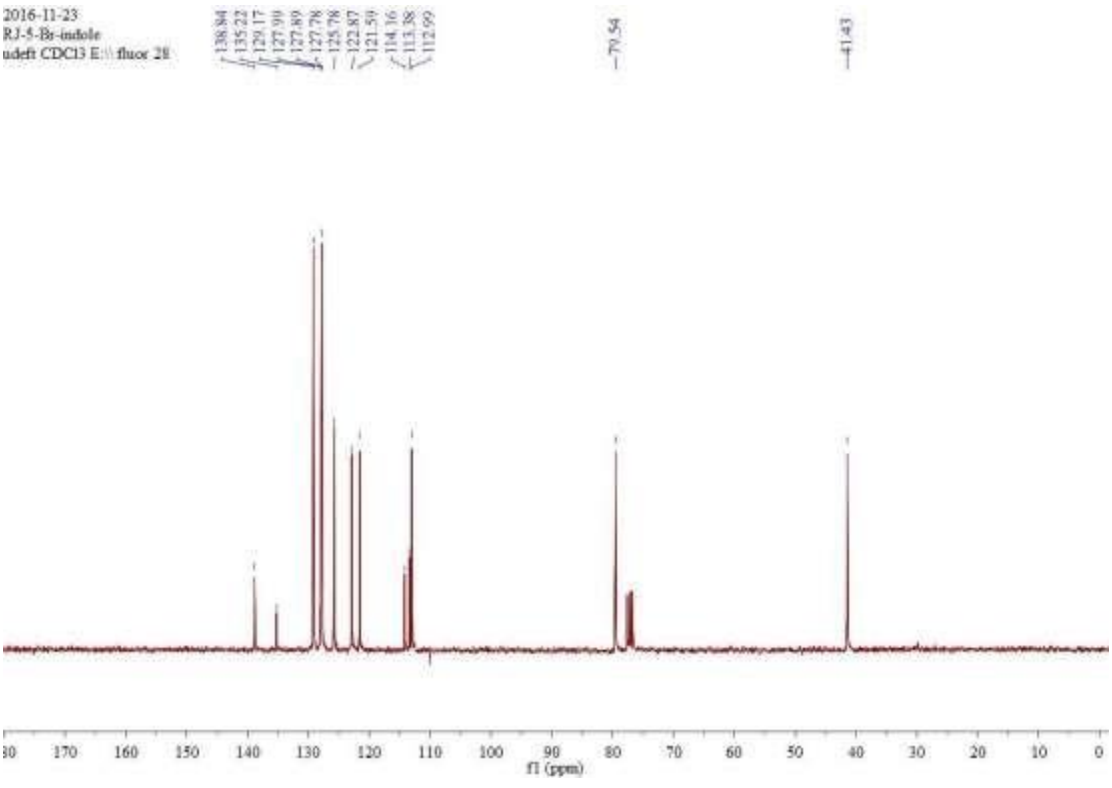

2016-11-14
RJ-5-BnO-indole
PROTON CDCl3 E:\\ fluor 19
f1 (ppm)

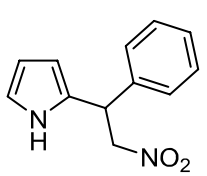

2016-11-10
RJ-5-BnO-indole
udeft CDCl3 E:\\ fluor 36
f1 (ppm)


NO2
Br
N
H

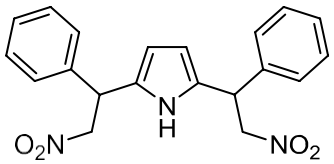
(3ha)


2016-11-24
RJ-5-Br-indole
PROTON CDCl3 E:\\ fluor 42
8.14
7.56
7.36
7.34
7.32
7.30
7.27
7.26
7.21
7.18
7.05
7.04
5.15
5.13
5.10
5.05
5.03
5.01
4.99
4.95
4.92
4.91
4.88
1.00
1.05
7.29
1.03
1.06
1.08
1.06
f1 (ppm)

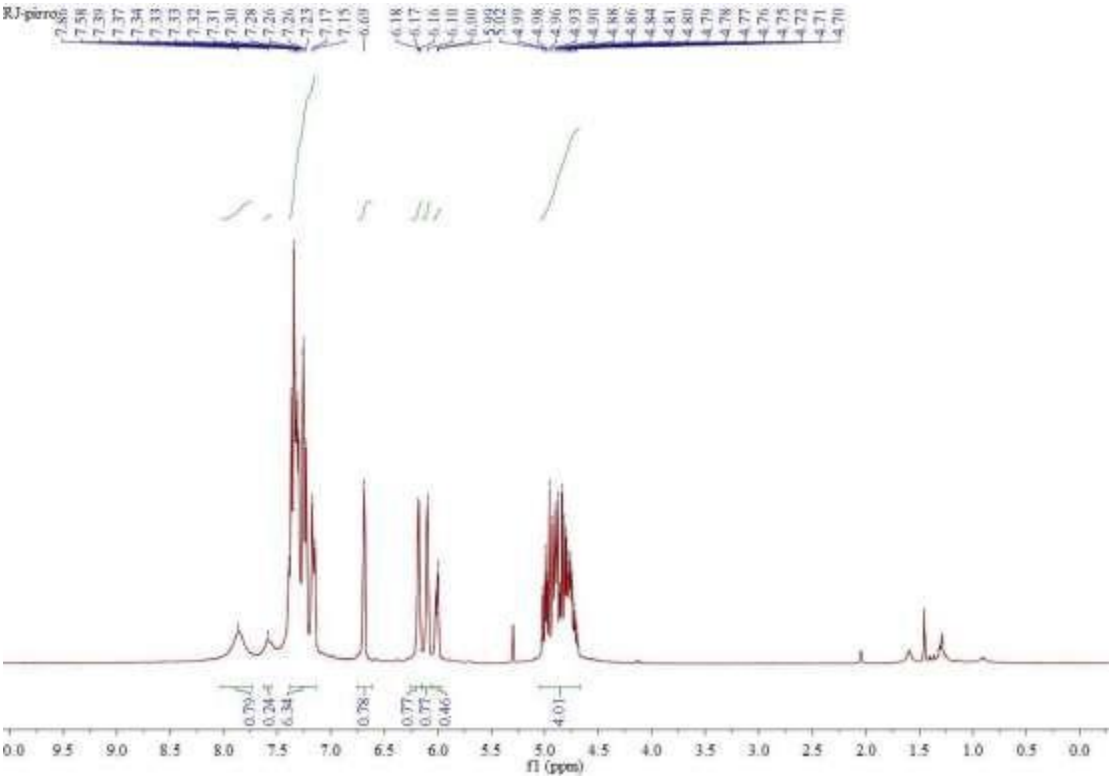

2016-11-23
RJ-5-Br-indole
udeft CDCl3 E:\\ fluor 28
138.84
135.22
129.17
127.99
127.89
127.78
125.76
122.87
121.59
114.16
113.38
112.99
79.54
41.43
f1 (ppm)

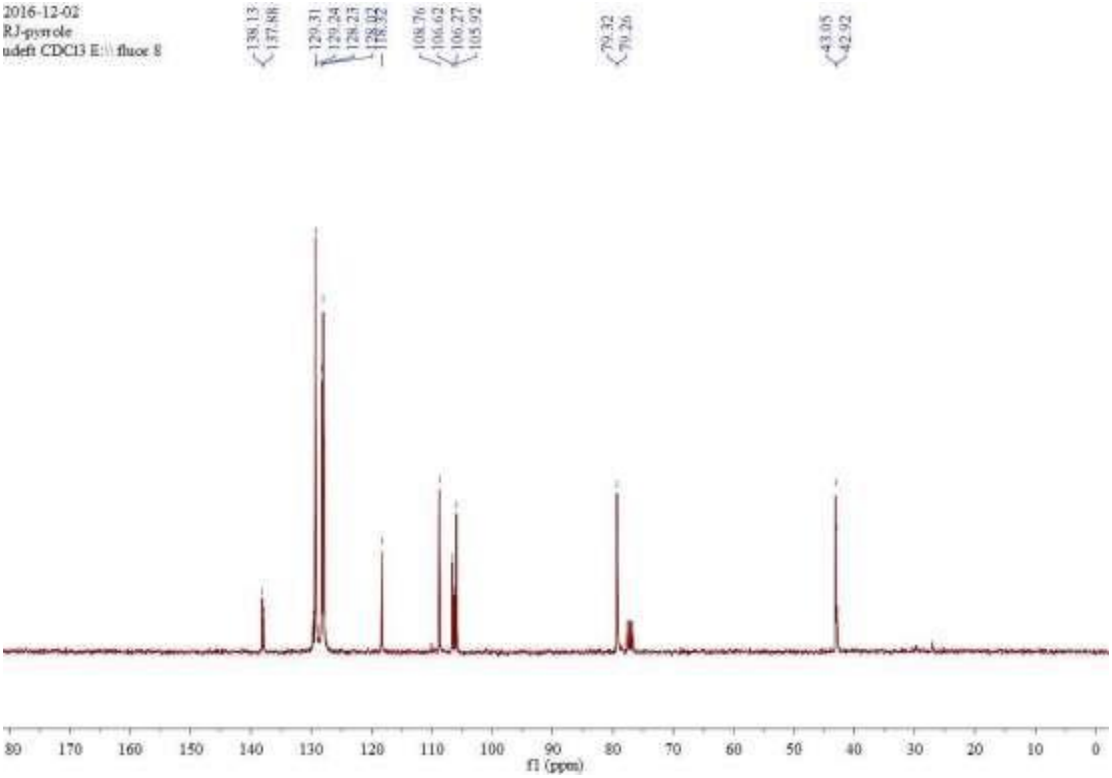

N
H
NO2

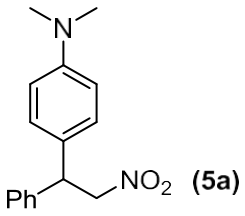
(3ia) and


O2N
N
H
NO2

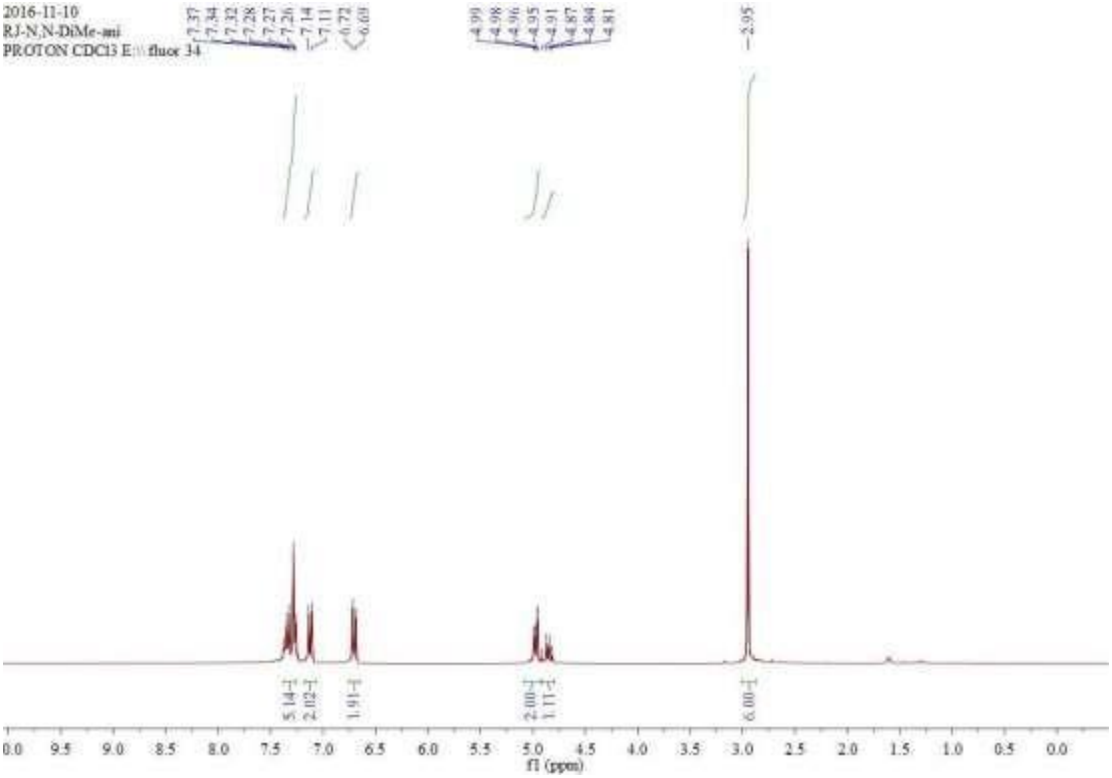
(3ia')

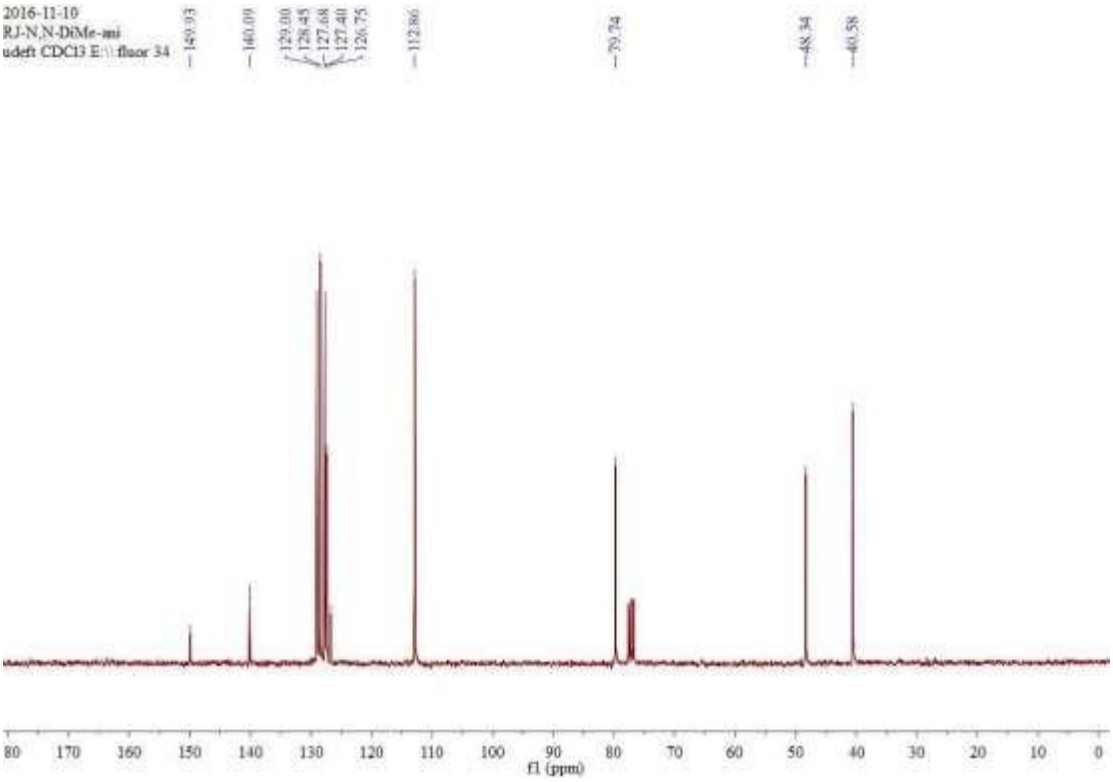

RJ-pirrole
f1 (ppm)

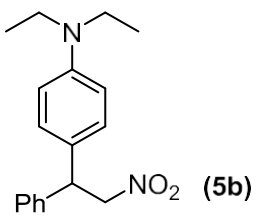

2016-12-02
RJ-pyrrole
udeft CDCl3 E:\\ fluor 8
f1 (ppm)


N
Ph
NO2

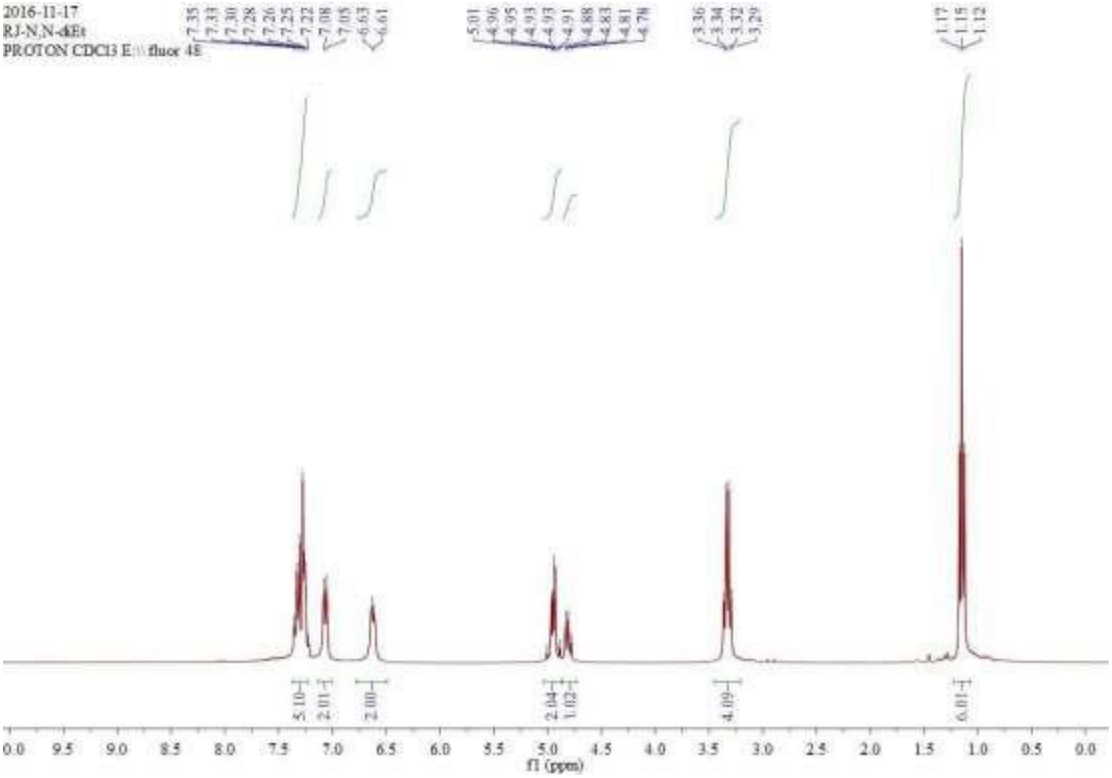
(5a)

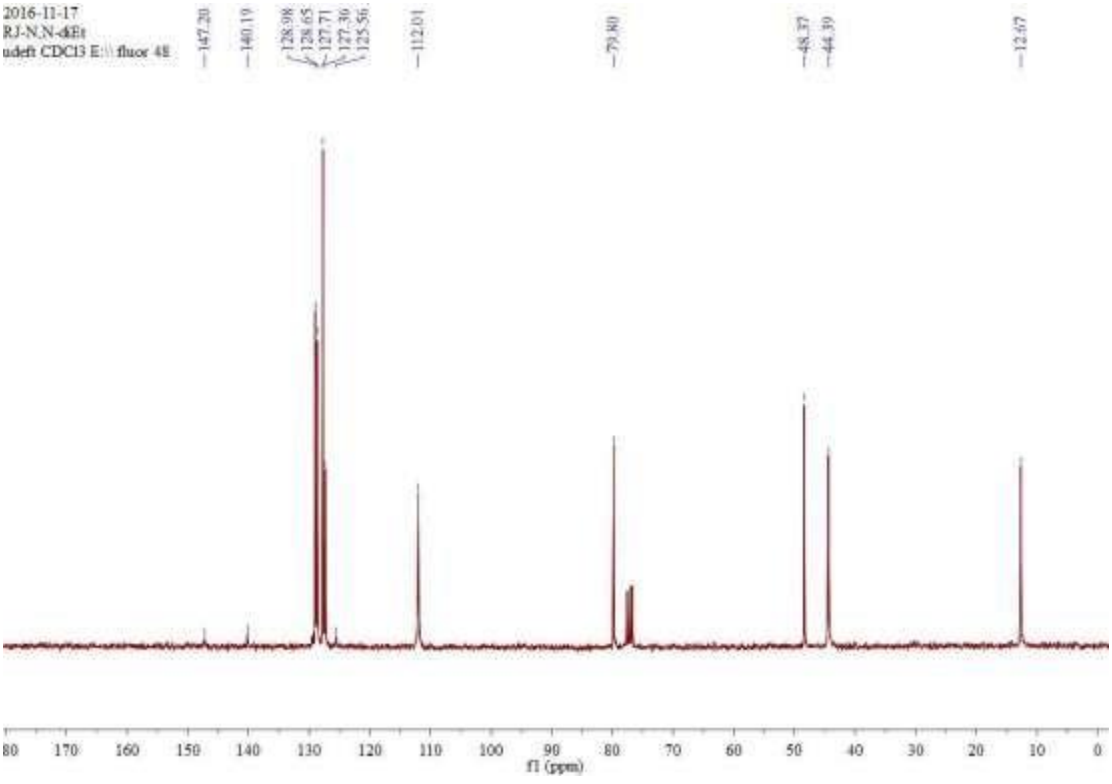

2016-11-10
RJ-N,N-DiMe-ani
PROTON CDCl3 E:\\ fluor 34
f1 (ppm)

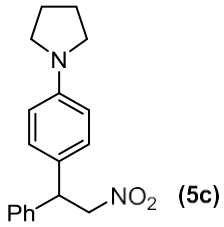

2016-11-10
RJ-N,N-DiMe-ani
udeft CDCl3 E:\\ fluor 34
f1 (ppm)


N
Ph
NO2

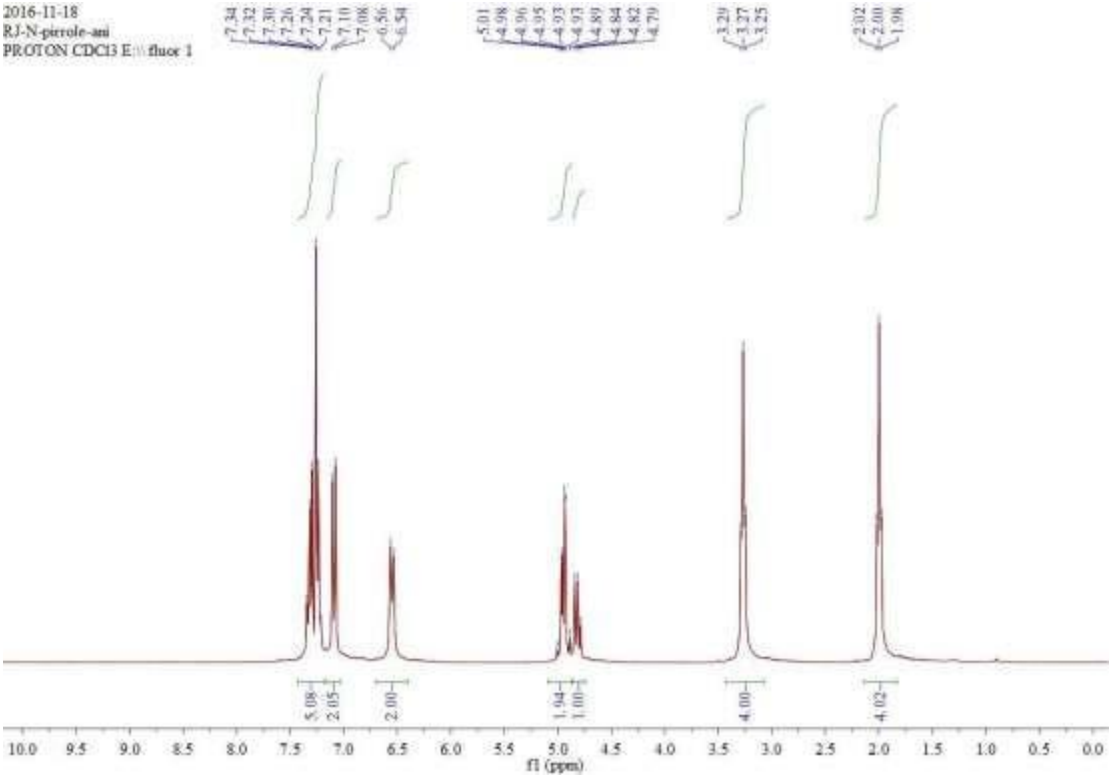
(5b)

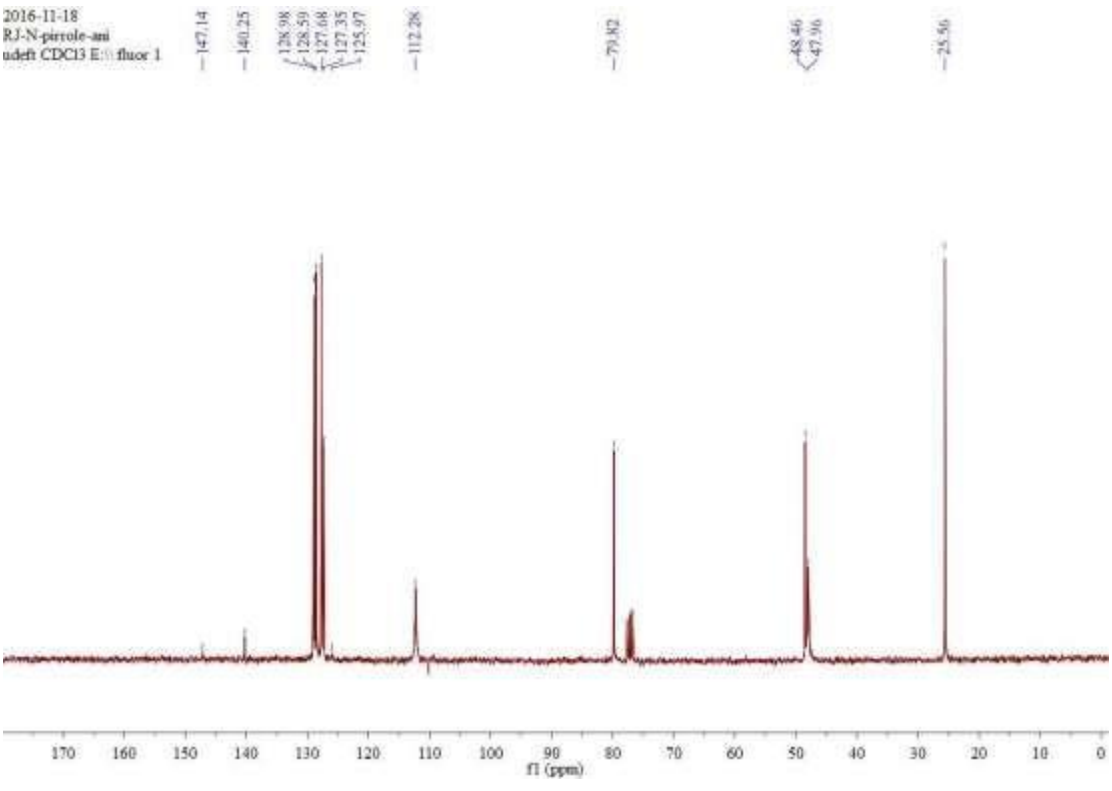

2016-11-17
RJ-N,N-diEt
PROTON CDCl3 E:\\ fluor 48
f1 (ppm)

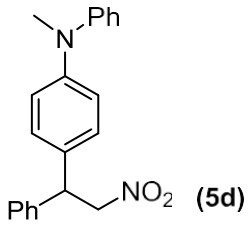

2016-11-17
RJ-N,N-diEt
udeft CDCl3 E:\\ fluor 48
f1 (ppm)


N
Ph
NO2

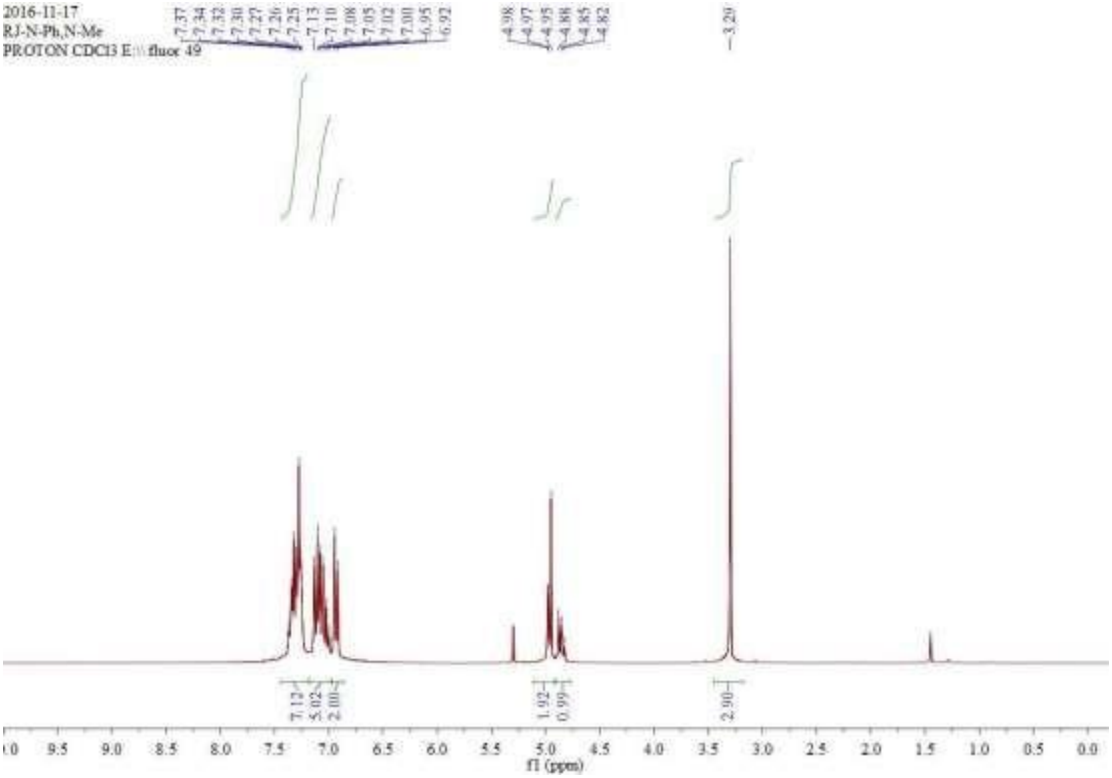
(5c)

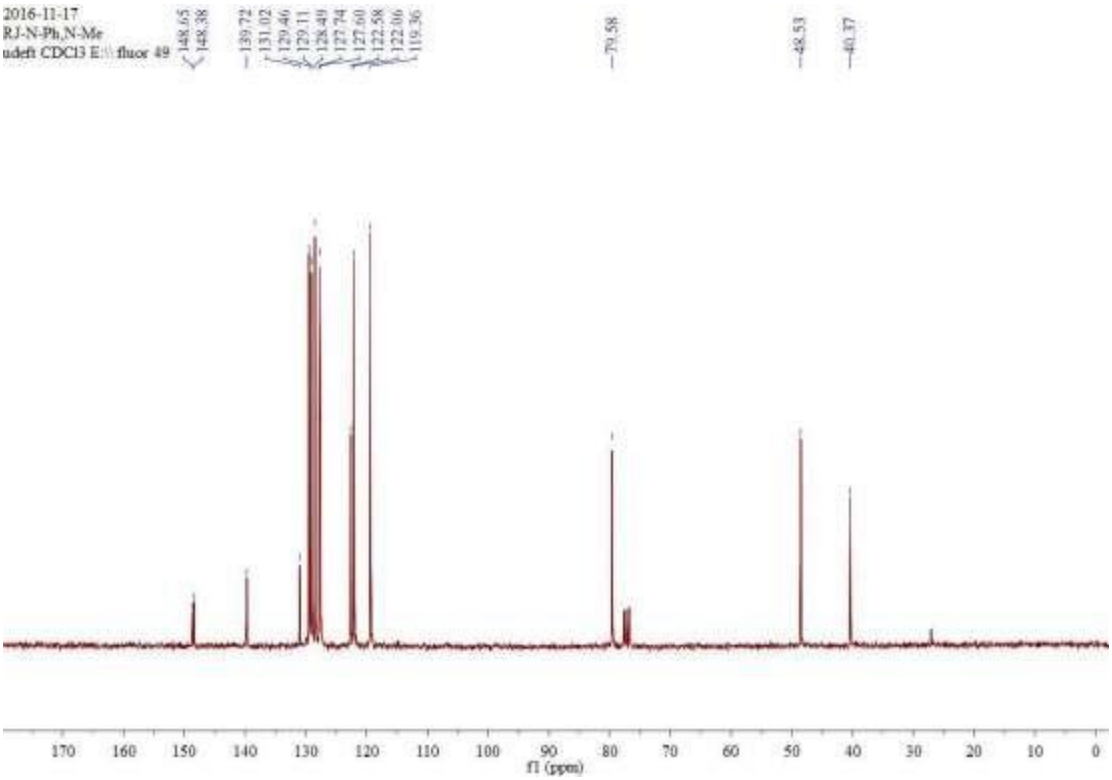

2016-11-18
RJ-N-pirrole-ani
PROTON CDCl3 E:\\ fluor 1
7.34
7.32
7.30
7.26
7.24
7.21
7.10
7.08
6.56
6.54
5.01
4.98
4.96
4.95
4.93
4.93
4.89
4.84
4.82
4.79
3.29
3.27
3.25
2.02
2.00
1.98
5.08
2.05
2.00
1.94
1.00
4.00
4.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

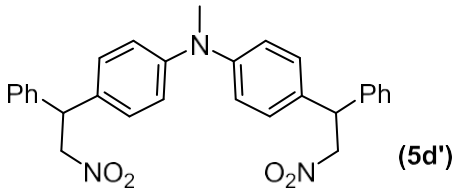

2016-11-18
RJ-N-pirrole-ani
udeft CDCl3 E:\\ fluor 1
147.14
140.25
128.98
128.59
127.68
127.35
125.97
112.26
79.82
48.46
47.96
25.56
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Ph
N
NO2
Ph

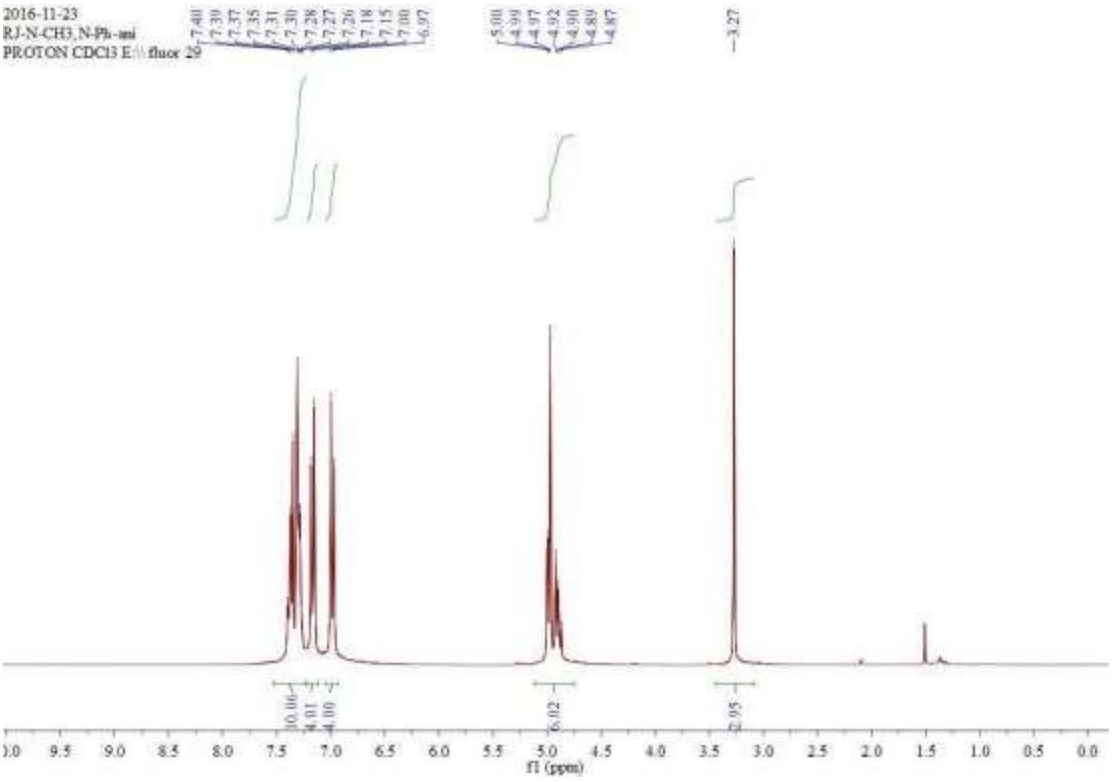
(5d)

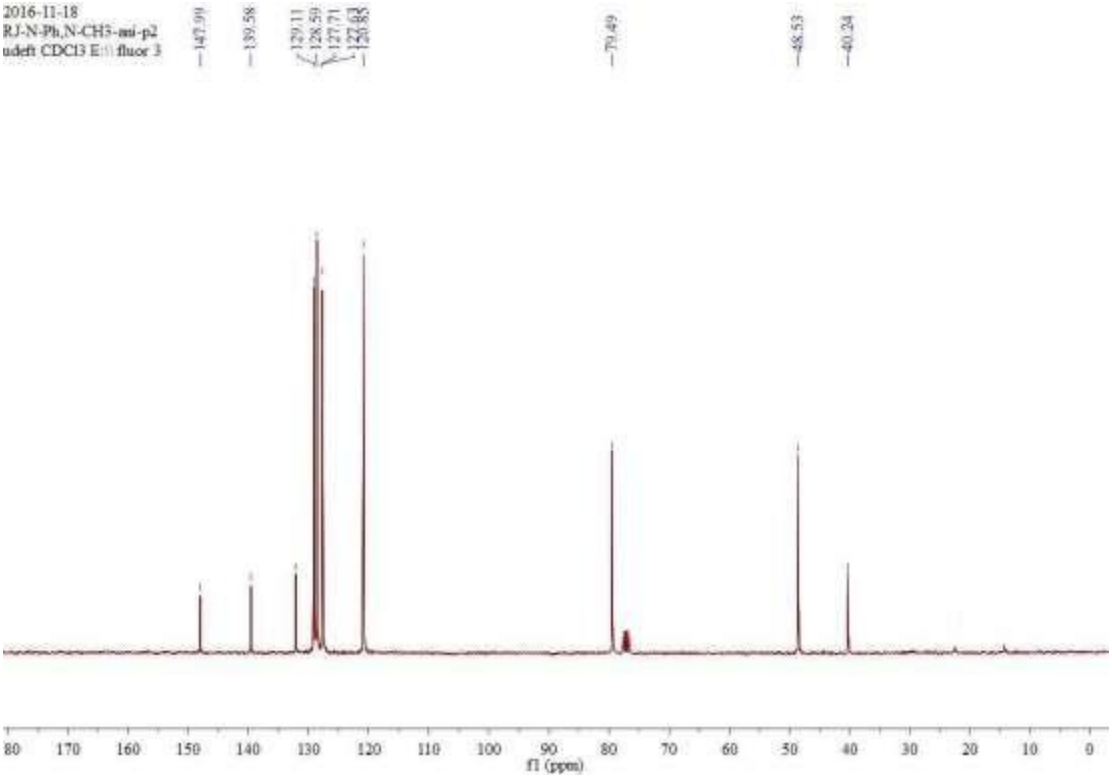

2016-11-17
RJ-N-Ph,N-Me
PROTON CDCl3 E:\\ fluor 49
7.37
7.34
7.32
7.30
7.27
7.26
7.25
7.13
7.10
7.08
7.05
7.02
7.00
6.95
6.92
4.98
4.97
4.95
4.88
4.85
4.82
3.29
7.12
5.02
2.00
1.92
0.99
2.90
f1 (ppm)

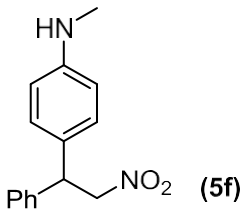

2016-11-17
RJ-N-Ph,N-Me
udeft CDCl3 E:\\ fluor 49
148.65
148.38
139.72
131.02
129.46
129.11
128.49
127.74
127.60
122.58
122.06
119.36
79.58
48.53
40.37
f1 (ppm)


N
Ph
Ph
NO2
O2N

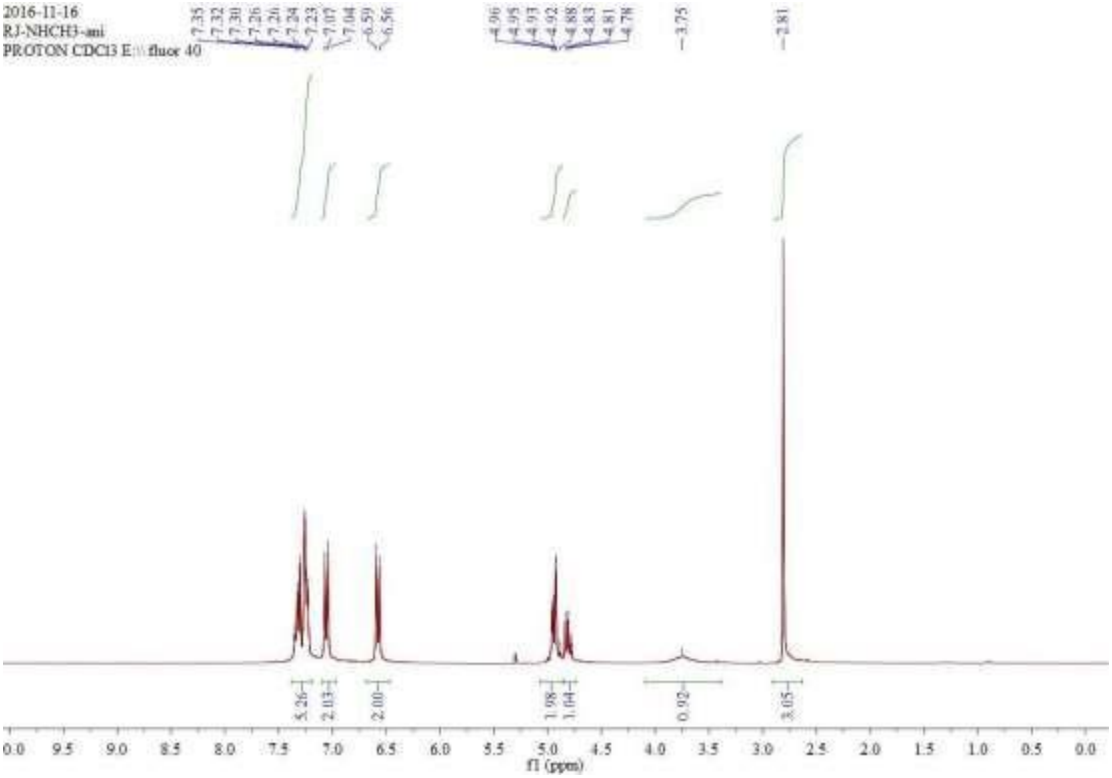
(5d')

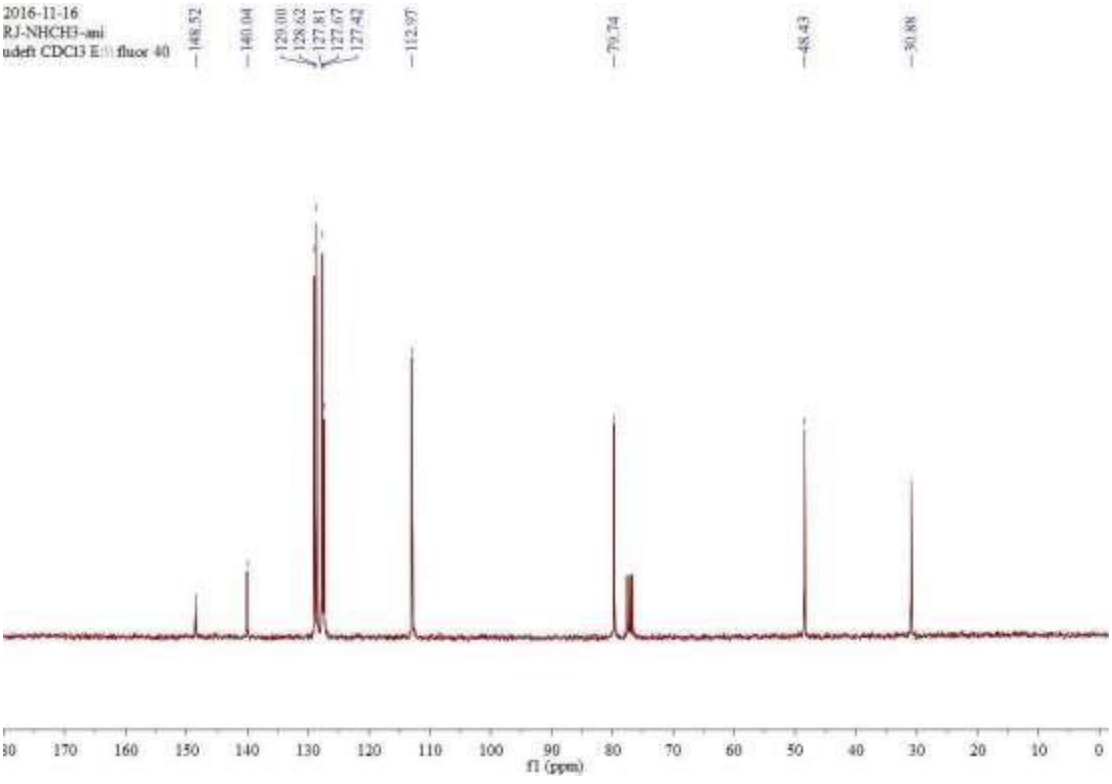

2016-11-23
RJ-N-CH3,N-Ph-ani
PROTON CDCl3 E:\\ fluor 29
7.40
7.39
7.37
7.35
7.31
7.30
7.28
7.27
7.26
7.18
7.15
7.00
6.97
5.00
4.99
4.97
4.92
4.90
4.89
4.87
3.27
10.06
4.01
4.00
6.02
2.95
f1 (ppm)

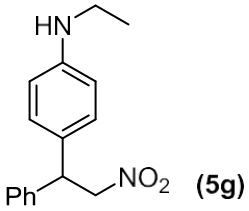

2016-11-18
RJ-N-Ph,N-CH3-ani-p2
udeft CDCl3 E:\\ fluor 3
147.99
139.58
129.11
128.59
127.71
120.85
79.49
48.53
40.24
f1 (ppm)


HN
Ph
NO2

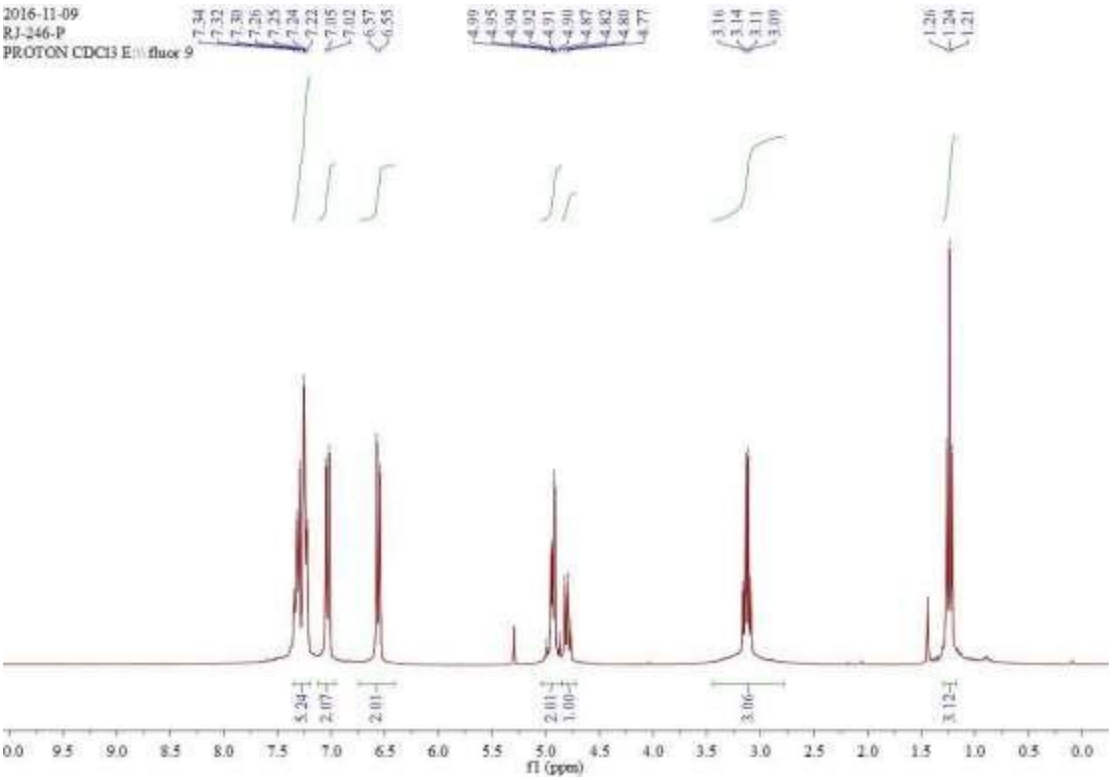
(5f)

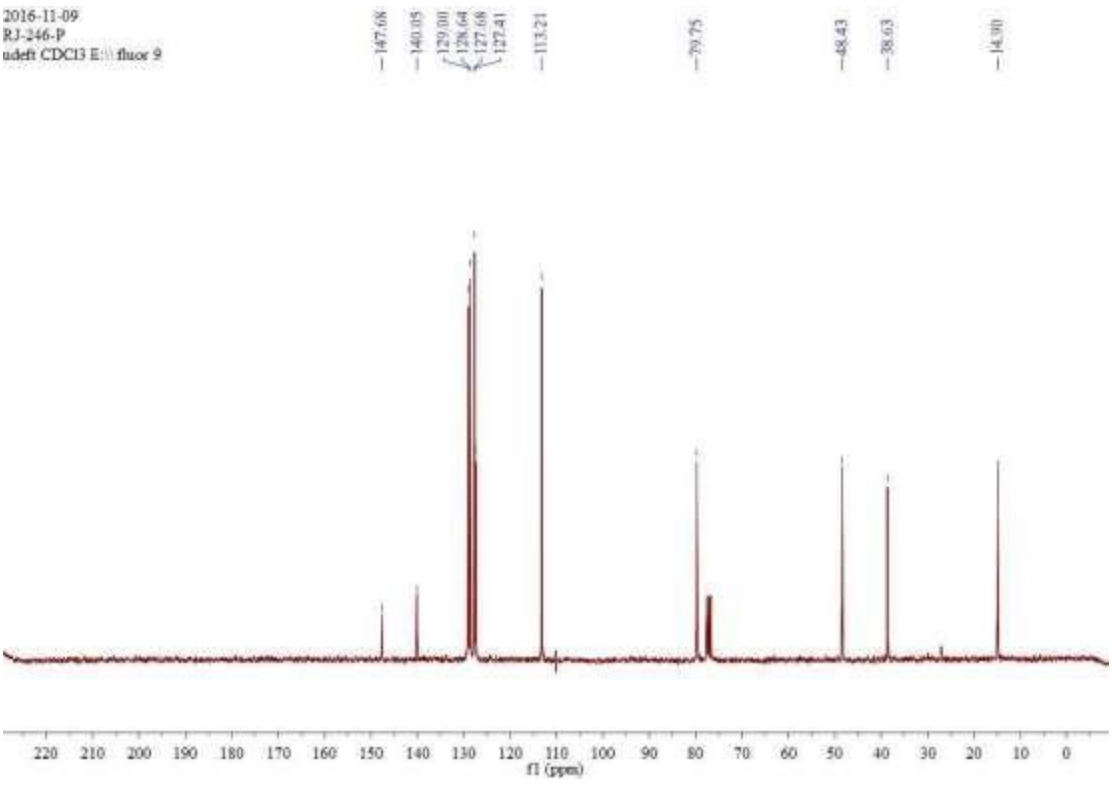

2016-11-16
RJ-NHCH3-ani
PROTON CDCl3 E:\\ fluor 40
7.35
7.32
7.30
7.26
7.24
7.23
7.07
7.04
6.59
6.56
4.96
4.95
4.93
4.92
4.88
4.83
4.81
4.78
3.75
2.81
5.26
2.03
2.00
1.98
1.04
0.92
3.05
f1 (ppm)

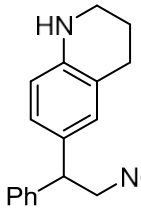

2016-11-16
RJ-NHCH3-ani
udeft CDCl3 E:\\ fluor 40
148.52
140.04
129.00
128.62
127.81
127.67
127.42
112.97
79.74
48.43
30.88
f1 (ppm)


HN
Ph
NO2

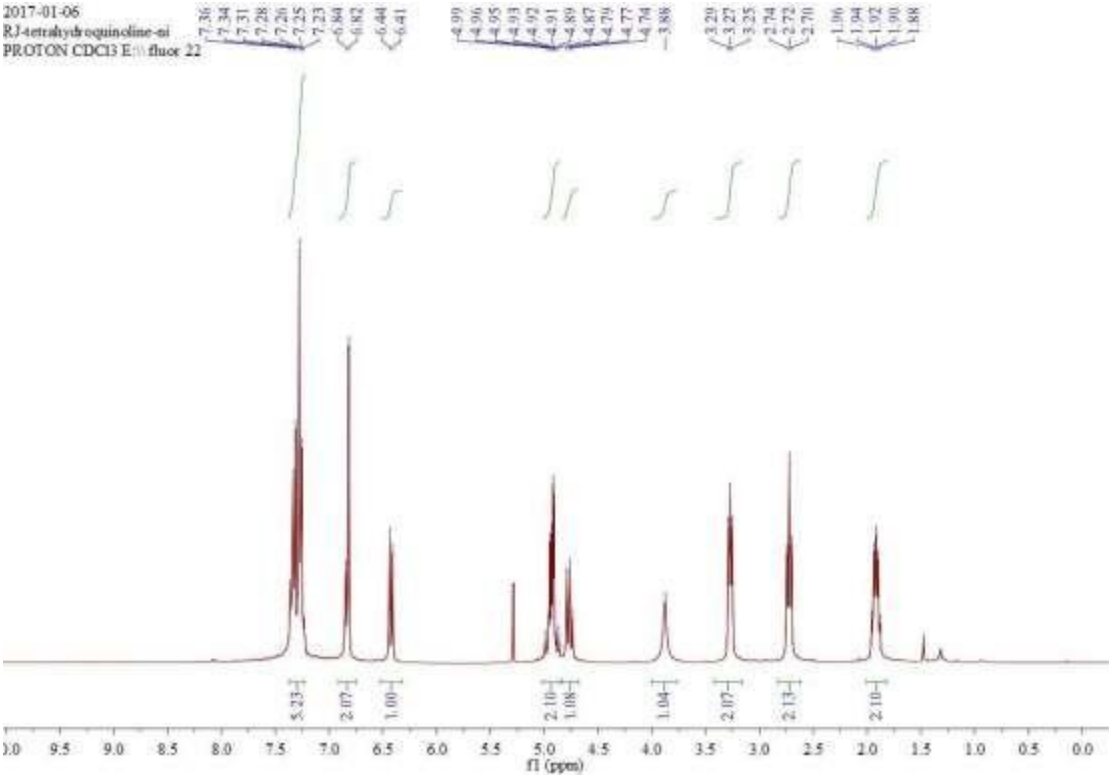
(5g)

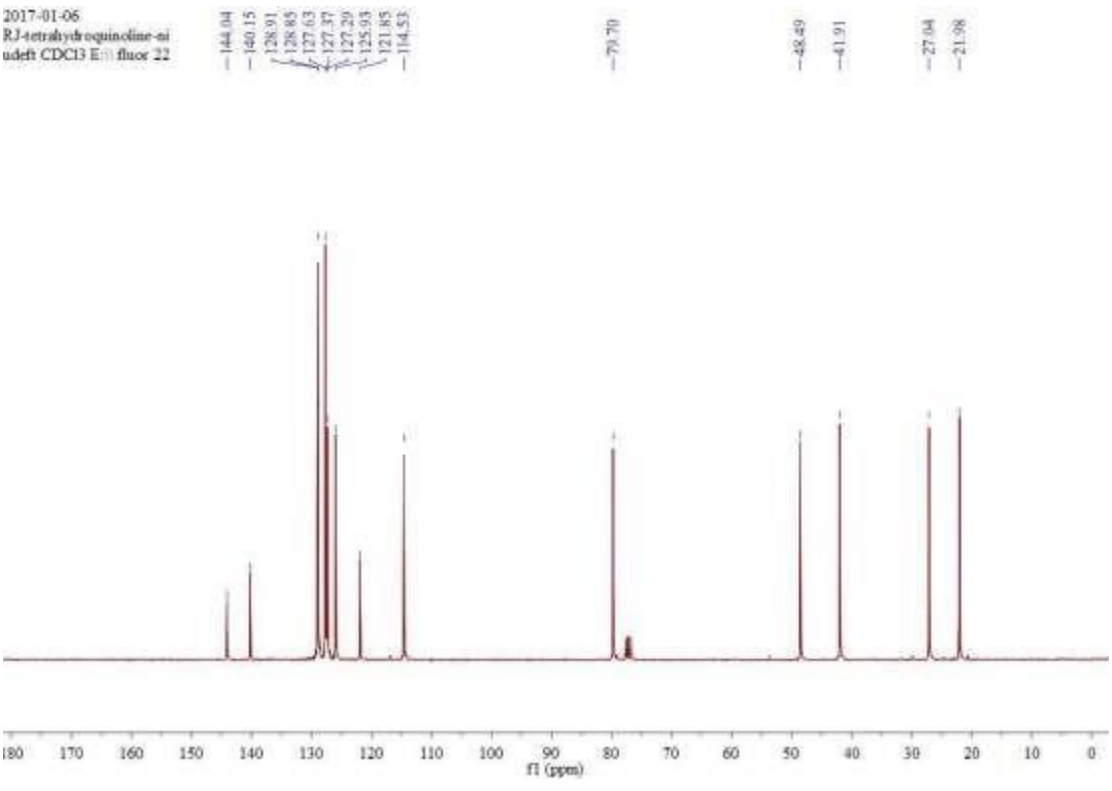

2016-11-09
RJ-246-P
PROTON CDCl3 E:\\ fluor 9
f1 (ppm)

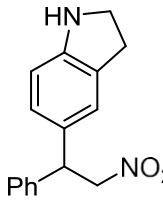

2016-11-09
RJ-246-P
udeft CDCl3 E:\\ fluor 9
f1 (ppm)


HN
NO2
Ph

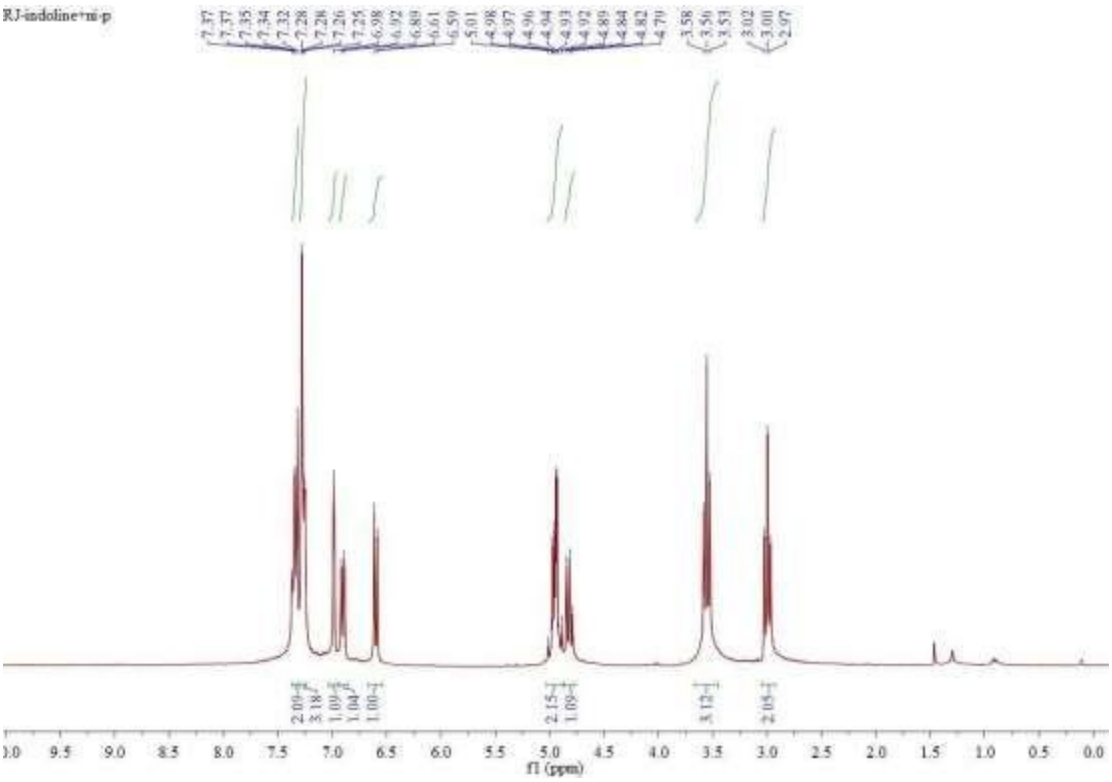
(5h)

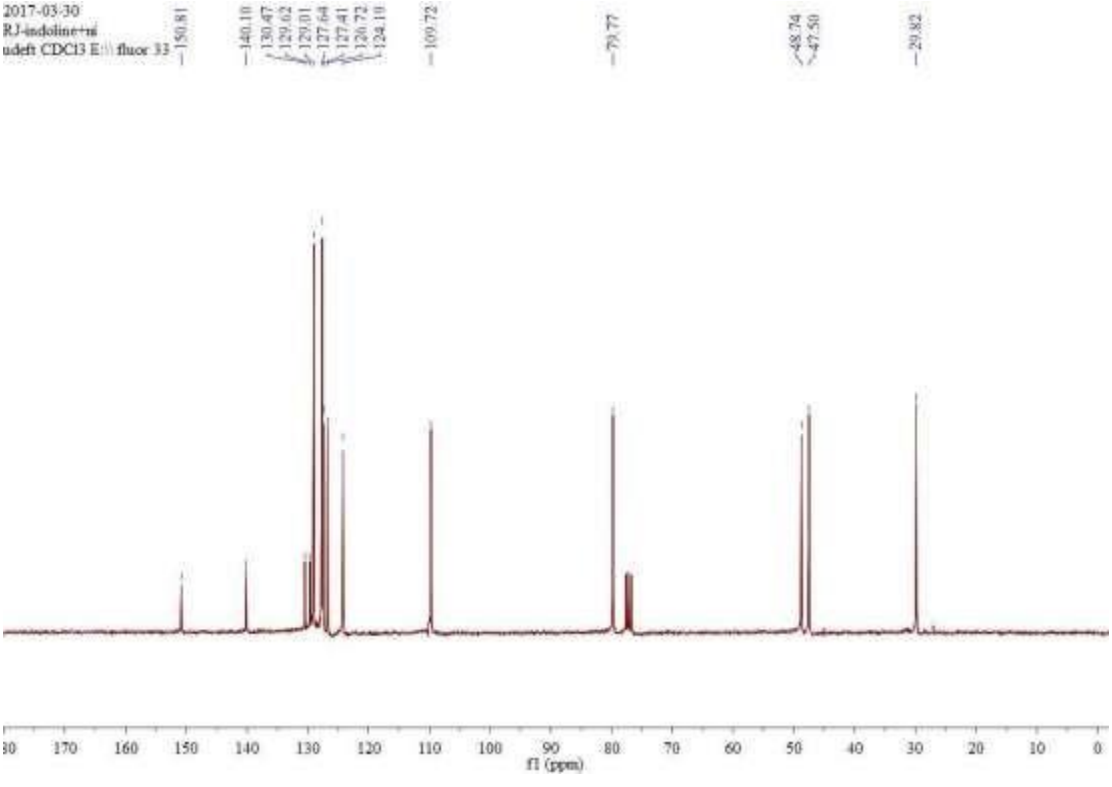

2017-01-06
RJ-tetrahydroquinoline-si
PROTON CDCl3 E:\\ fluor 22
f1 (ppm)

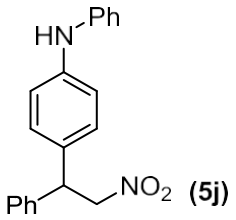

2017-01-06
RJ-tetrahydroquinoline-si
udeft CDCl3 E:\\ fluor 22
f1 (ppm)


HN
NO2
Ph

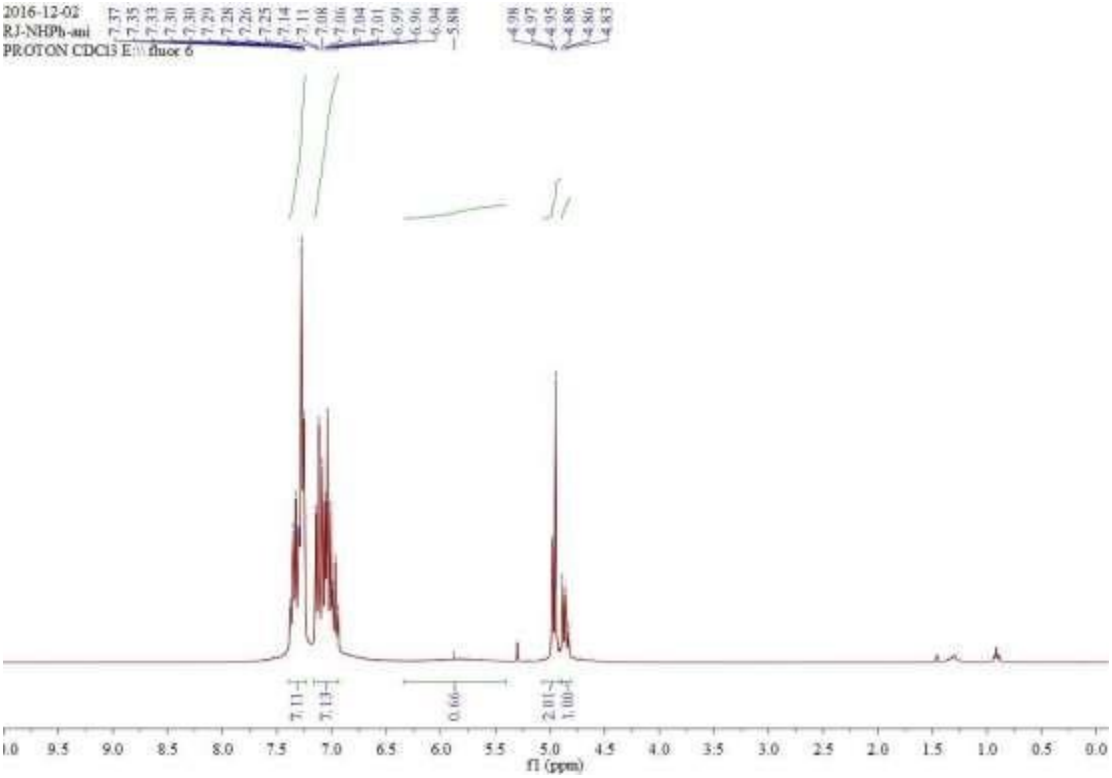
(5i)

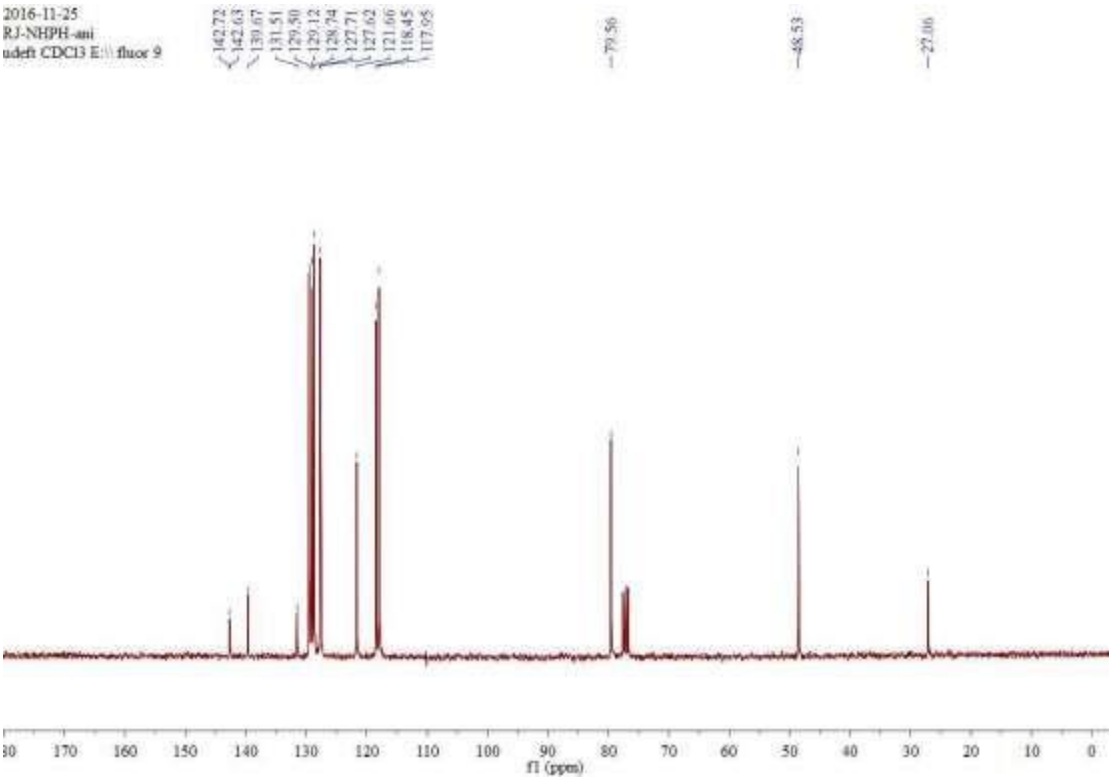

RJ-indoline+ni-p
f1 (ppm)

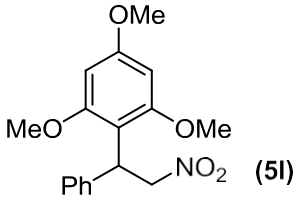

2017-03-30
RJ-indoline+ni
udeft CDCl3 E:\\ fluor 33
f1 (ppm)


HN
Ph
Ph
NO2

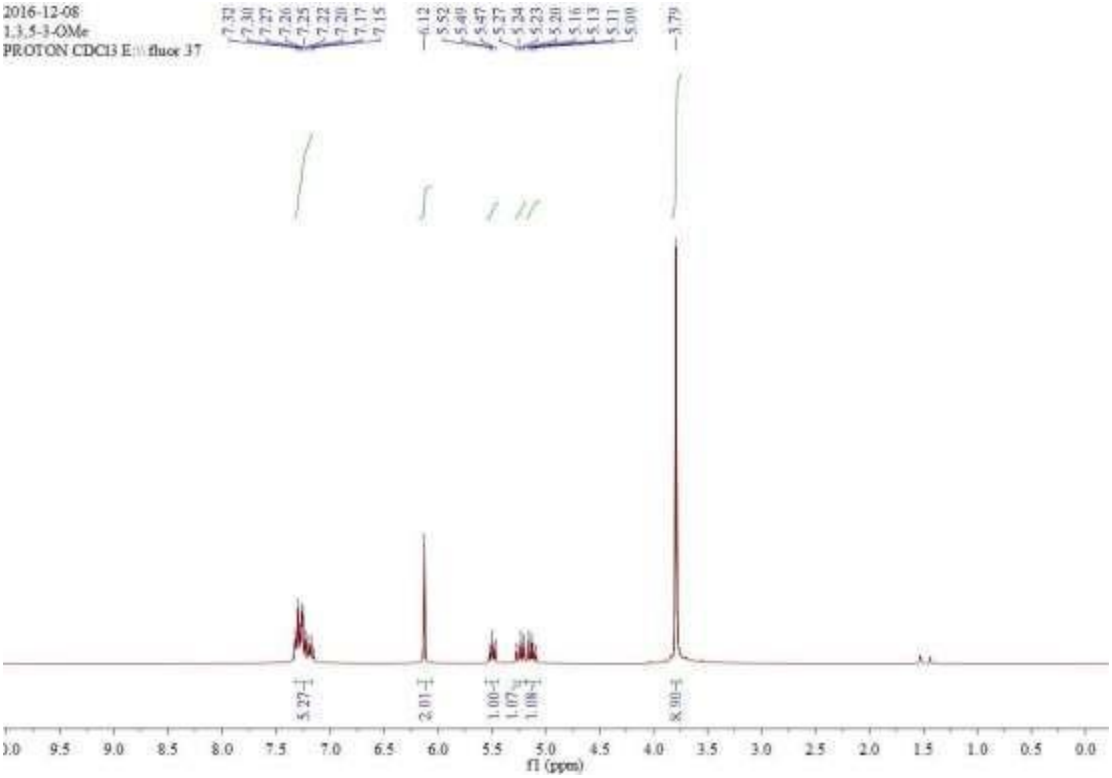
(5j)

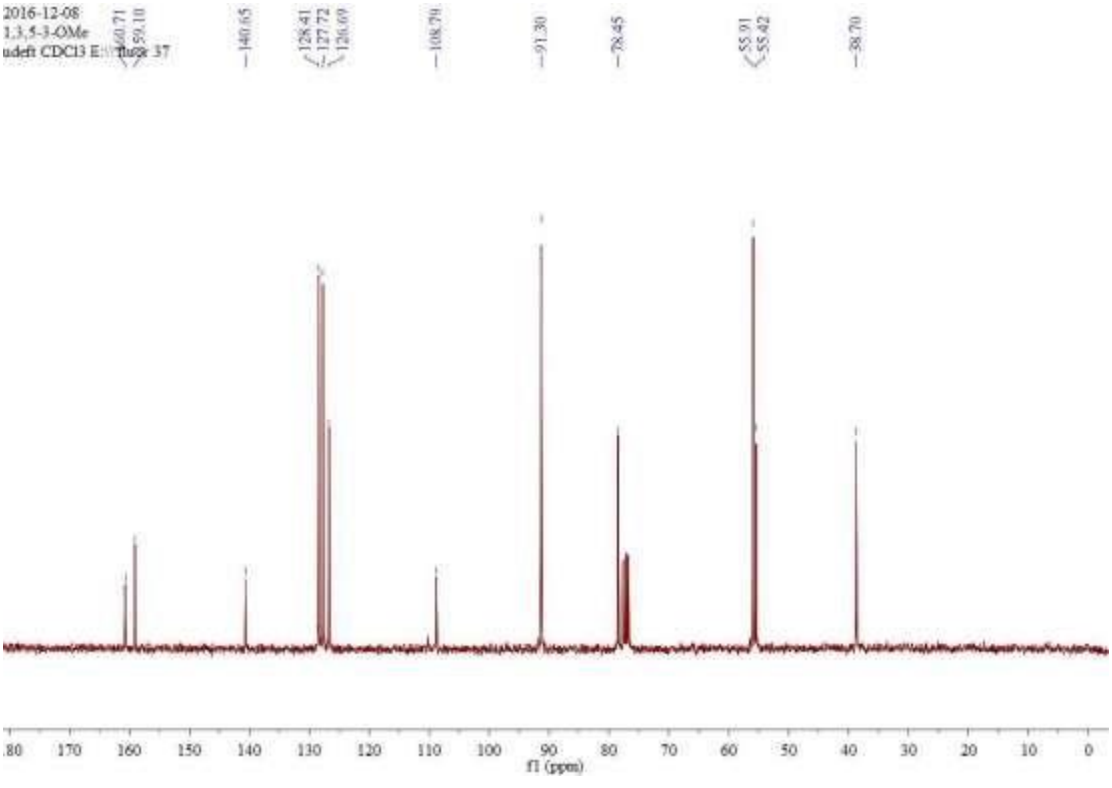

2016-12-02
RJ-NHPh-ani
PROTON CDCl3 E:\\ fluor 6
7.37
7.35
7.33
7.30
7.30
7.29
7.28
7.26
7.25
7.14
7.11
7.08
7.06
7.04
7.01
6.99
6.96
6.94
5.88
4.98
4.97
4.95
4.88
4.86
4.83
7.11
7.13
0.66
2.01
1.00
f1 (ppm)

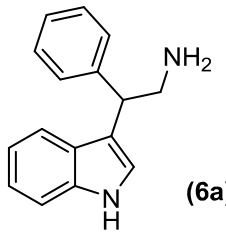

2016-11-25
RJ-NHPH-ani
udeft CDCl3 E:\\ fluor 9
142.72
142.63
139.67
131.51
129.50
129.12
128.74
127.71
127.62
121.66
118.45
117.95
79.56
48.53
27.06
f1 (ppm)


OMe
MeO
OMe
NO2
Ph

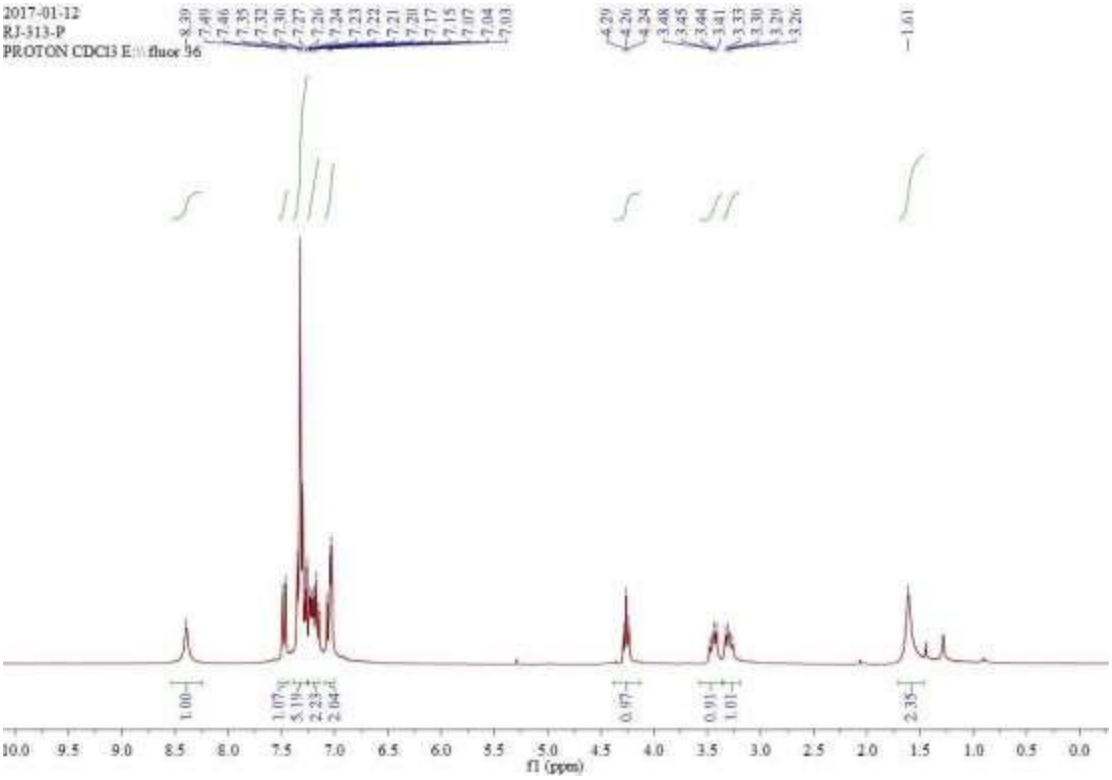
(5l)

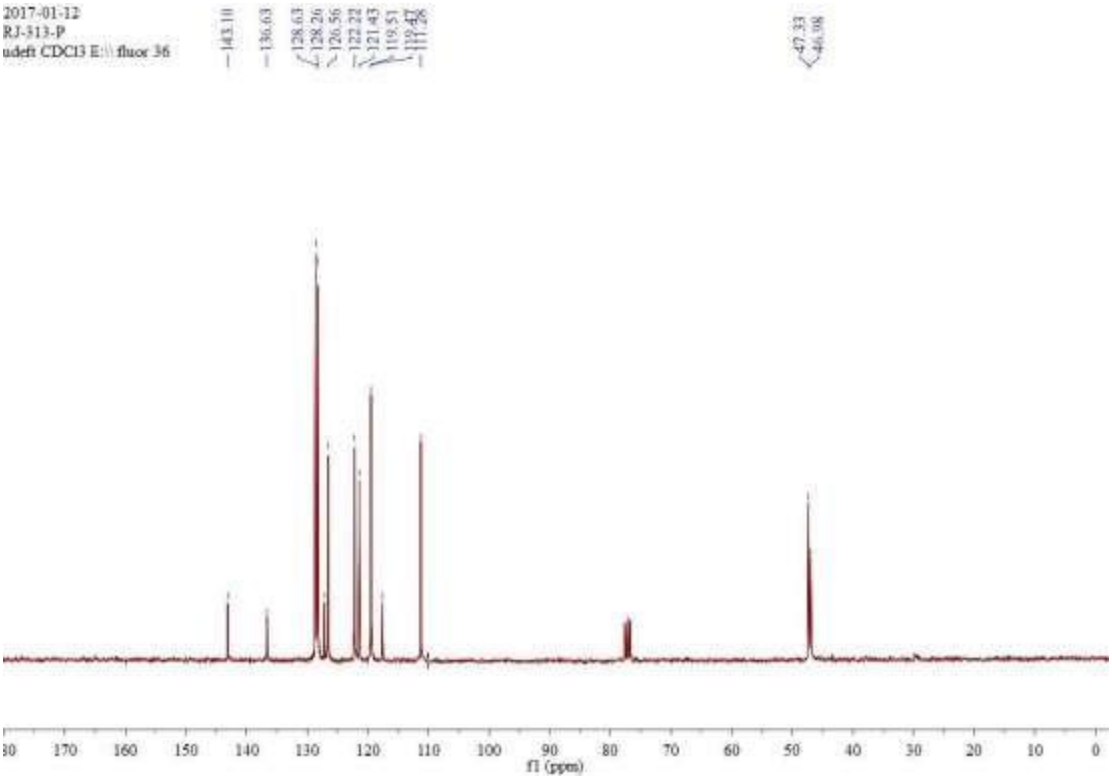

2016-12-08
1,3,5-3-OMe
PROTON CDCl3 E:\\ fluor 37
7.32
7.30
7.27
7.26
7.25
7.22
7.20
7.17
7.15
6.12
5.52
5.49
5.47
5.27
5.24
5.23
5.20
5.16
5.13
5.11
5.09
3.79
5.27
2.01
1.00
1.07
1.08
8.90
f1 (ppm)

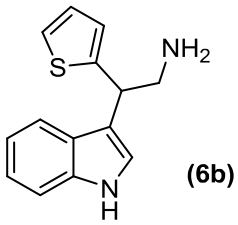

2016-12-08
1,3,5-3-OMe
udeft CDCl3 E:\\ fluor 37
160.71
159.10
140.65
128.41
127.72
126.69
108.79
91.30
78.45
55.91
55.42
38.70
f1 (ppm)


NH2
N
H

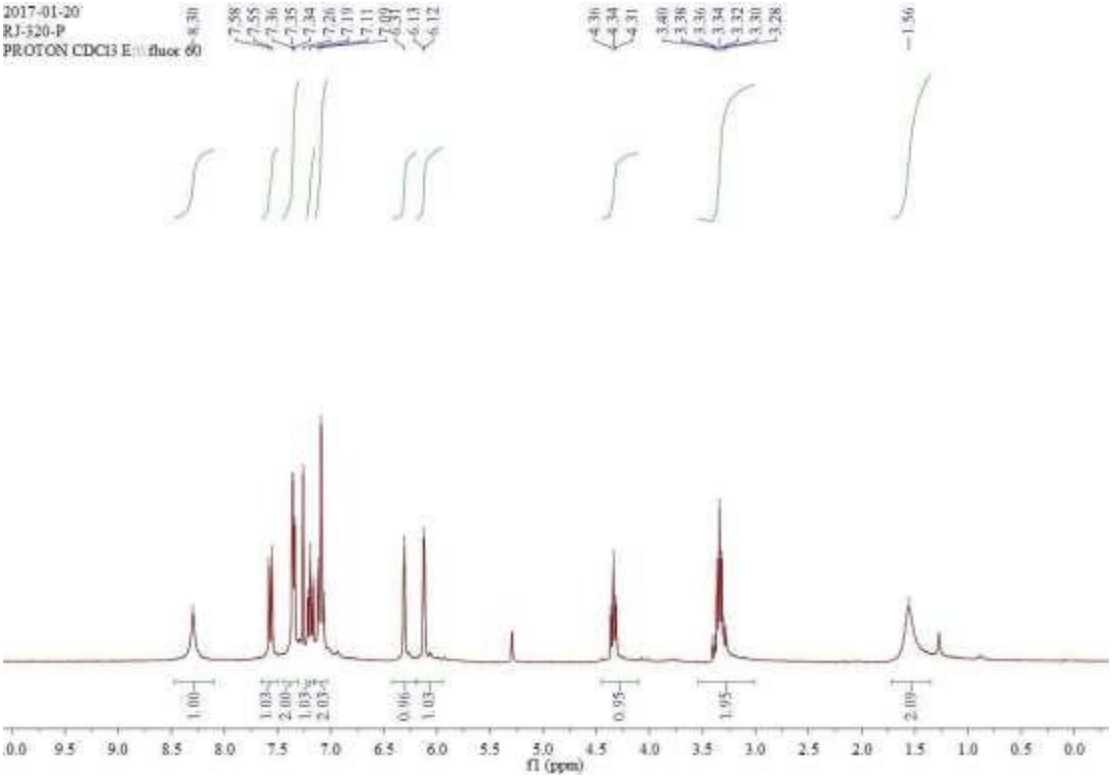
(6a)

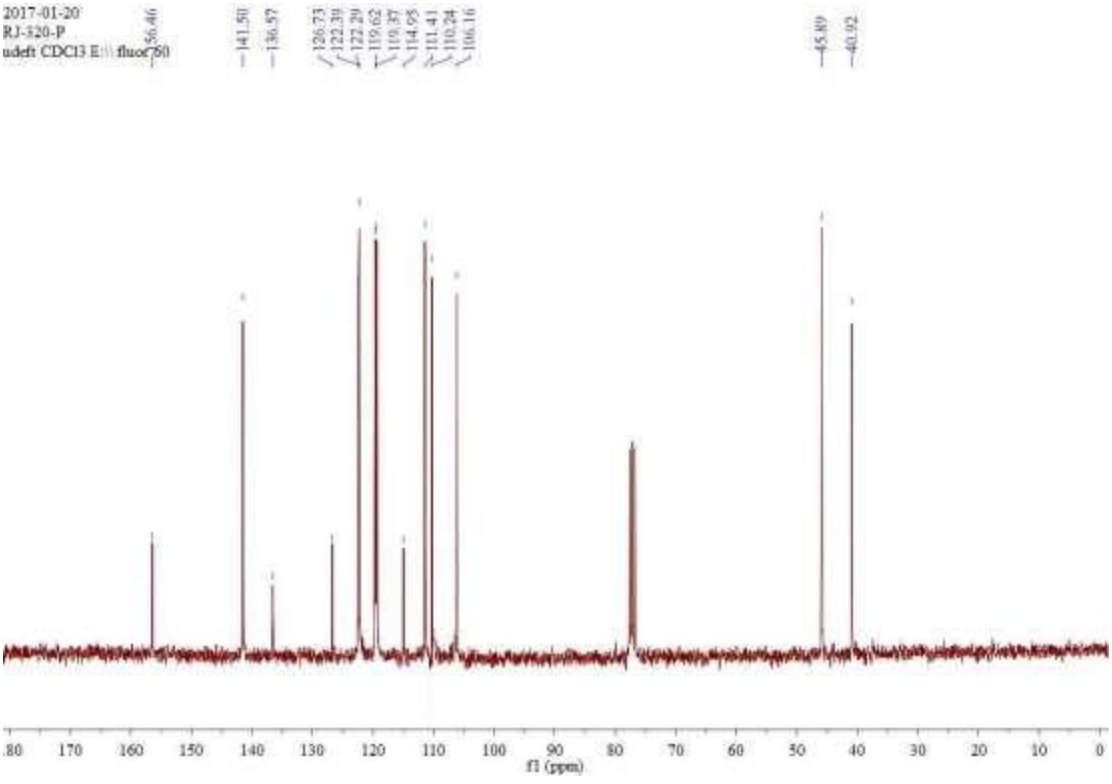

2017-01-12
RJ-313-P
PROTON CDCl3 E:\\ fluor 96
f1 (ppm)

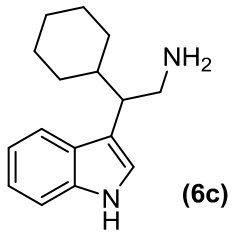

2017-01-12
RJ-313-P
udeft CDCl3 E:\\ fluor 36
f1 (ppm)


NH2
S
N
H

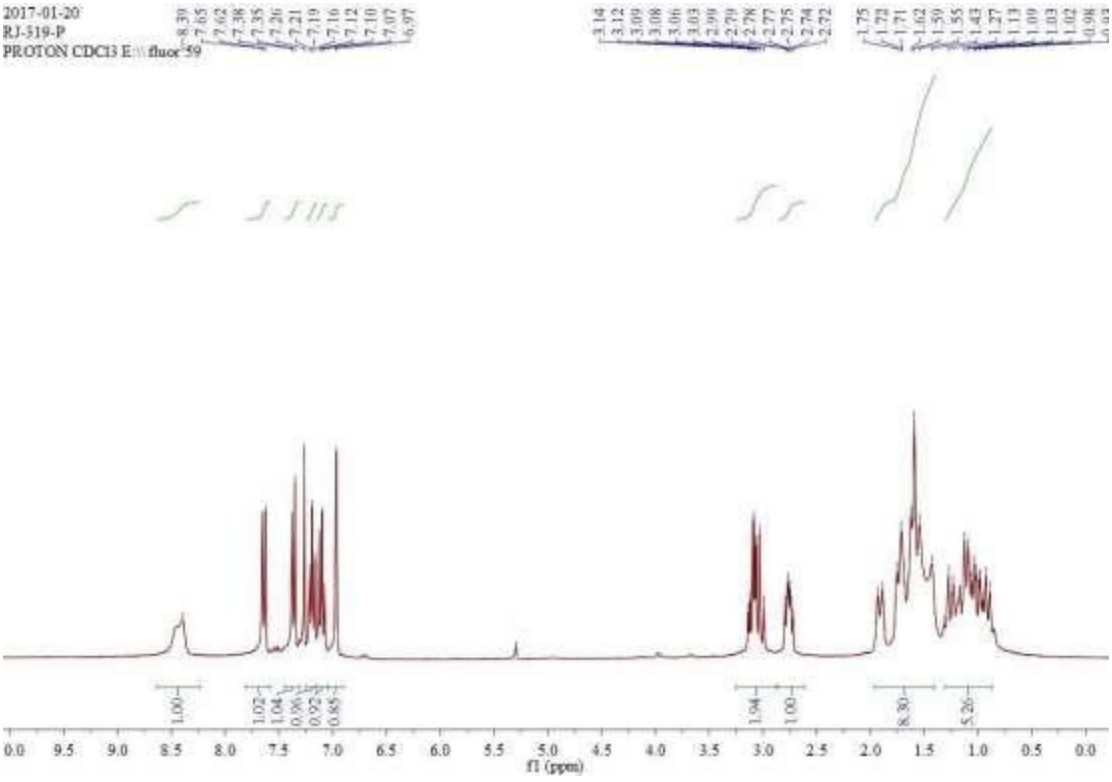
(6b)

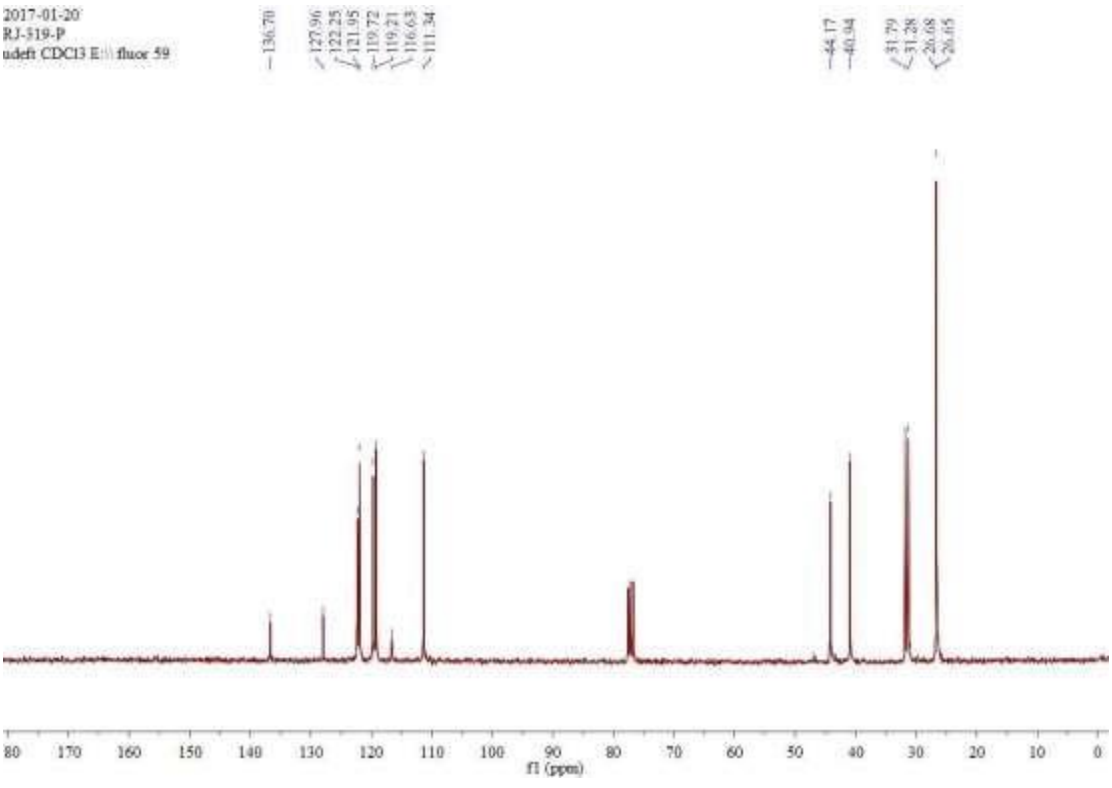

2017-01-20
RJ-320-P
PROTON CDCl3 E:\\ fluor 60
f1 (ppm)

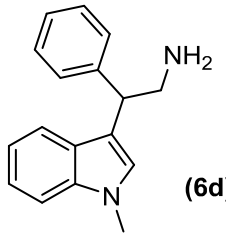

2017-01-20
RJ-320-P
udeft CDCl3 E:\\ fluor 80
f1 (ppm)


NH2
N
H

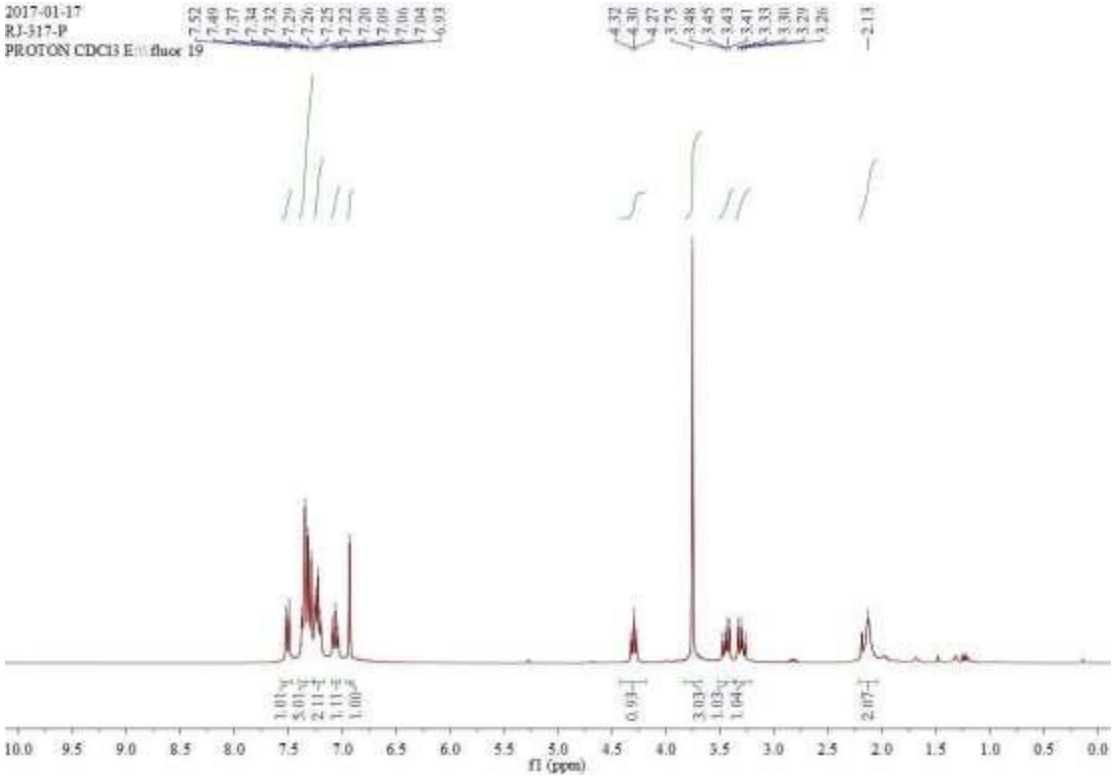
(6c)

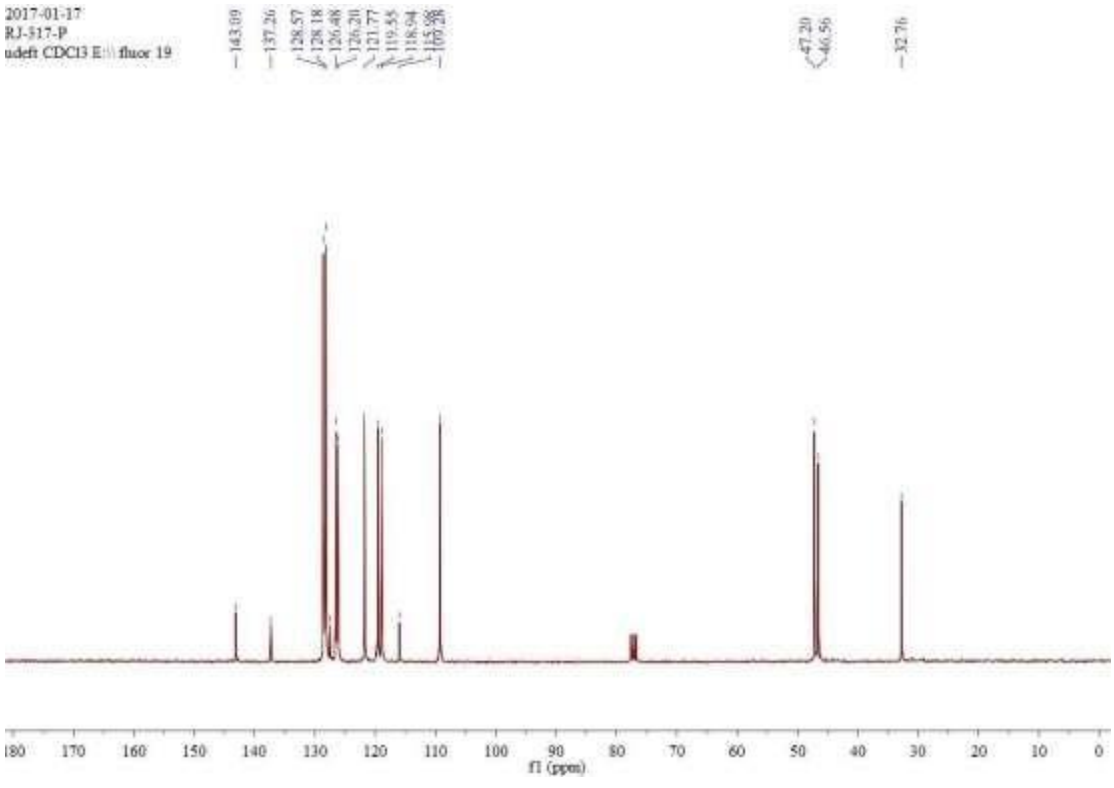

2017-01-20
RJ-519-P
PROTON CDCl3 E:\\ fluor 59
f1 (ppm)

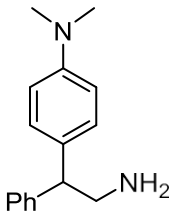

2017-01-20
RJ-519-P
udeft CDCl3 E:\\ fluor 59
f1 (ppm)


NH2
N

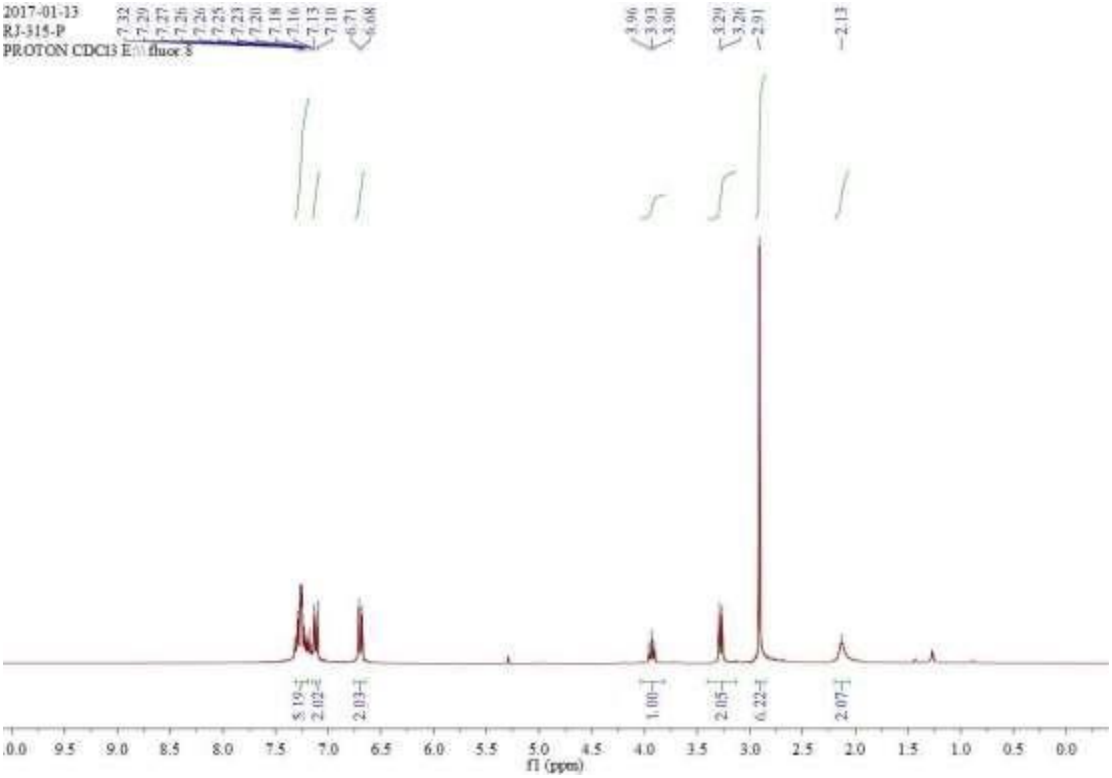
(6d)

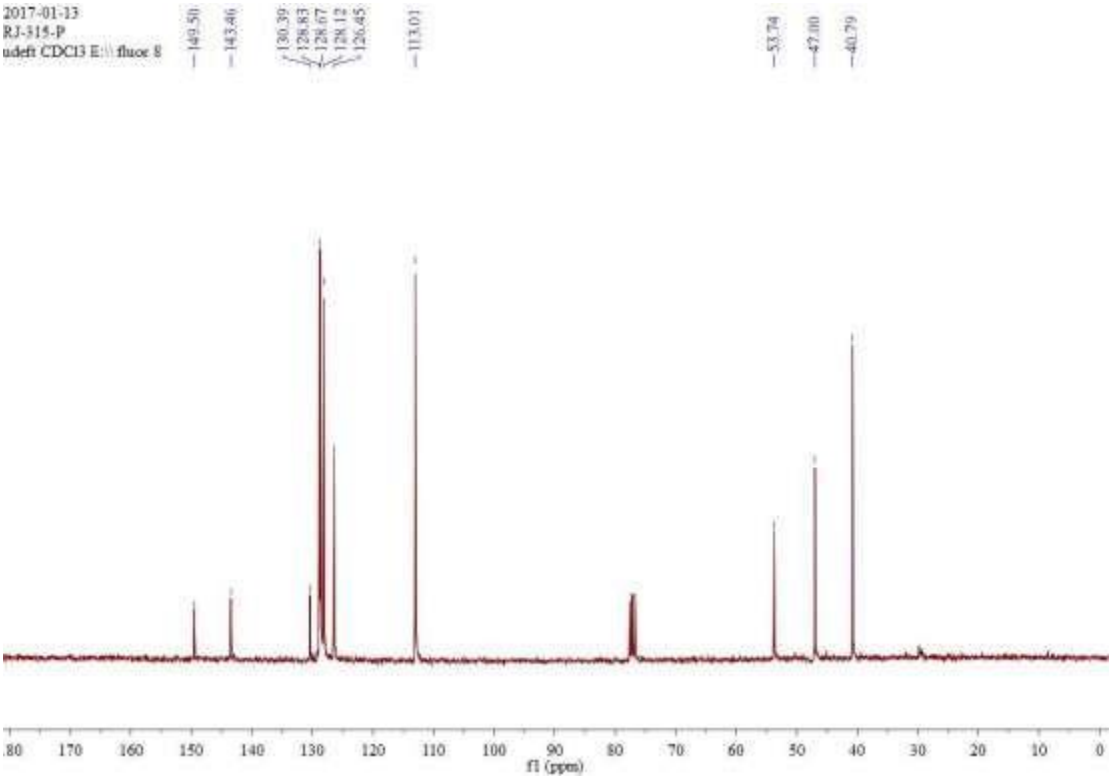

2017-01-17
RJ-317-P
PROTON CDCl3 E:\\ fluor 19
f1 (ppm)

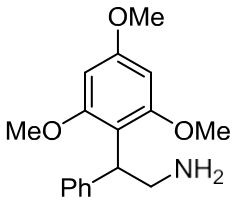

2017-01-17
RJ-317-P
udeft CDCl3 E:\\ fluor 19
f1 (ppm)


N
NH2
Ph

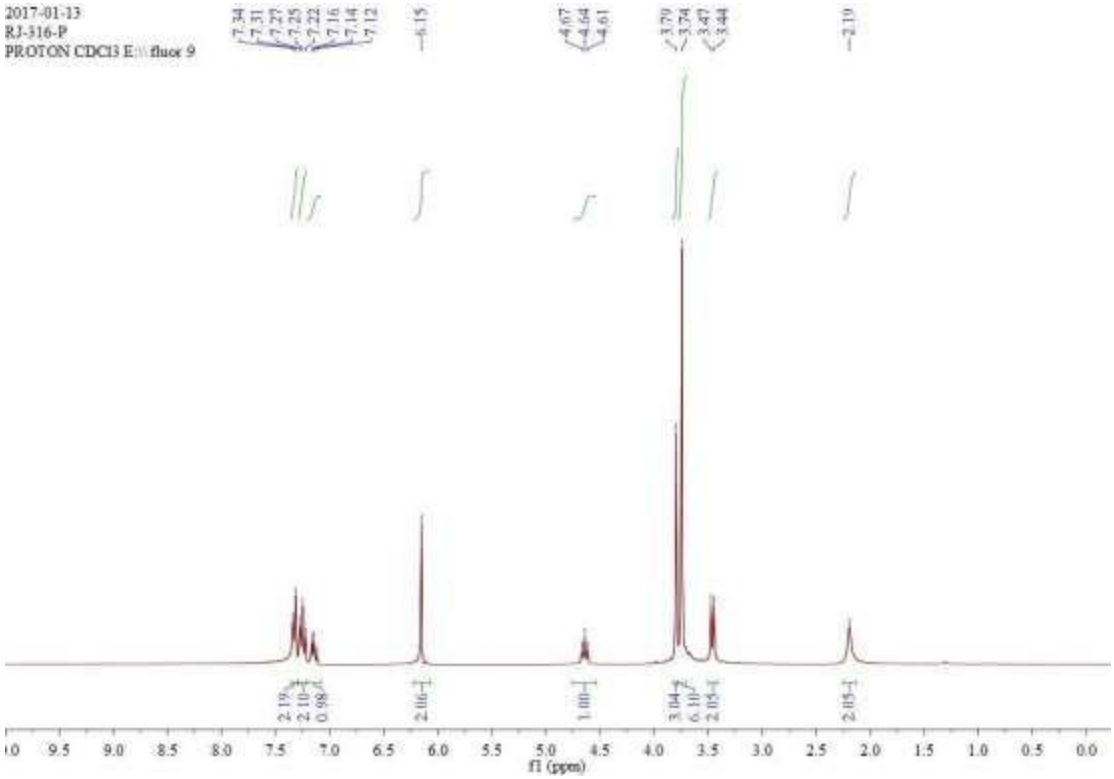
(6e)

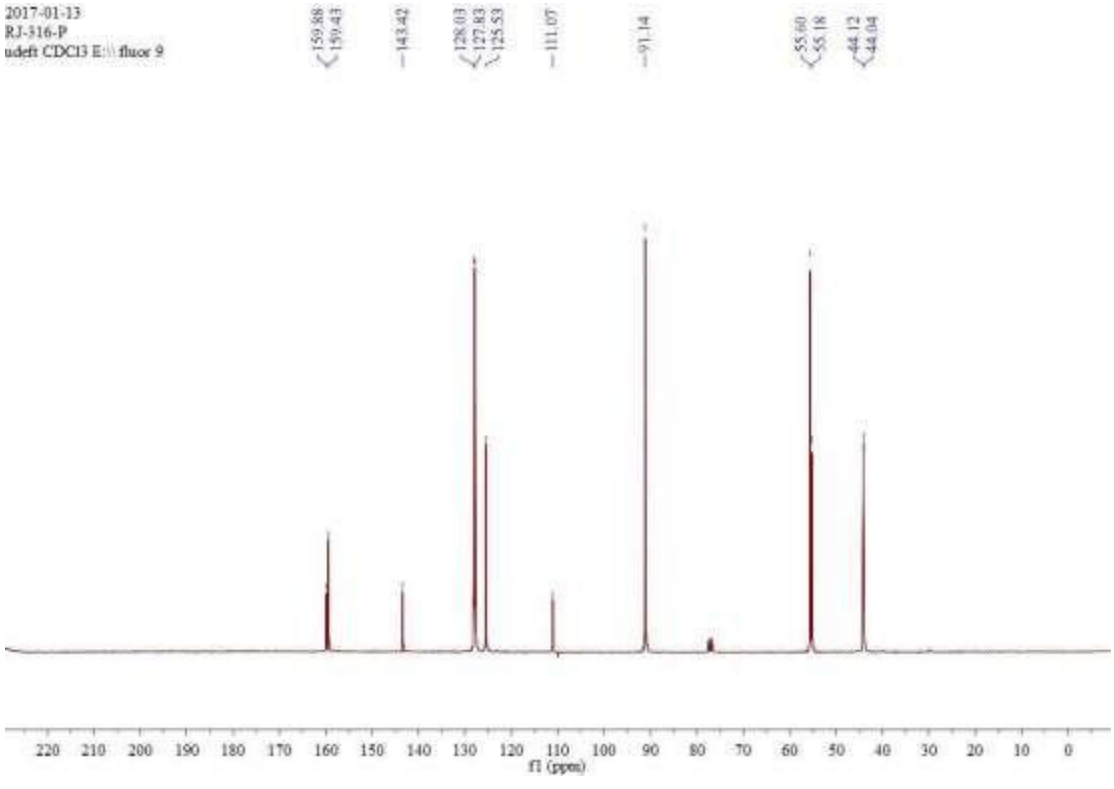

2017-01-13
RJ-315-P
PROTON CDCl3 E:\\ fluor 8
7.32
7.29
7.27
7.26
7.25
7.23
7.20
7.18
7.16
7.13
7.10
6.71
6.68
3.96
3.93
3.90
3.29
3.26
2.91
2.13
5.19
2.02
2.03
1.00
2.05
6.22
2.07
f1 (ppm)


2017-01-13
RJ-315-P
udeft CDCl3 E:\\ fluor 8
149.50
143.46
130.39
128.83
128.67
128.12
126.45
113.01
53.74
47.00
40.79
f1 (ppm)


OMe
MeO
OMe
NH2
Ph

(6f)


2017-01-13
RJ-316-P
PROTON CDCl3 E:\\ fluor 9
f1 (ppm)


2017-01-13
RJ-316-P
udeft CDCl3 E:\\ fluor 9
f1 (ppm)