Supporting Information

Nickel-catalyzed C-N bond activation: Activated primary amines as alkylating reagent in reductive cross-couplings

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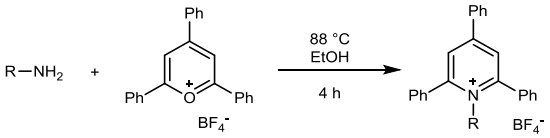
1. General Information

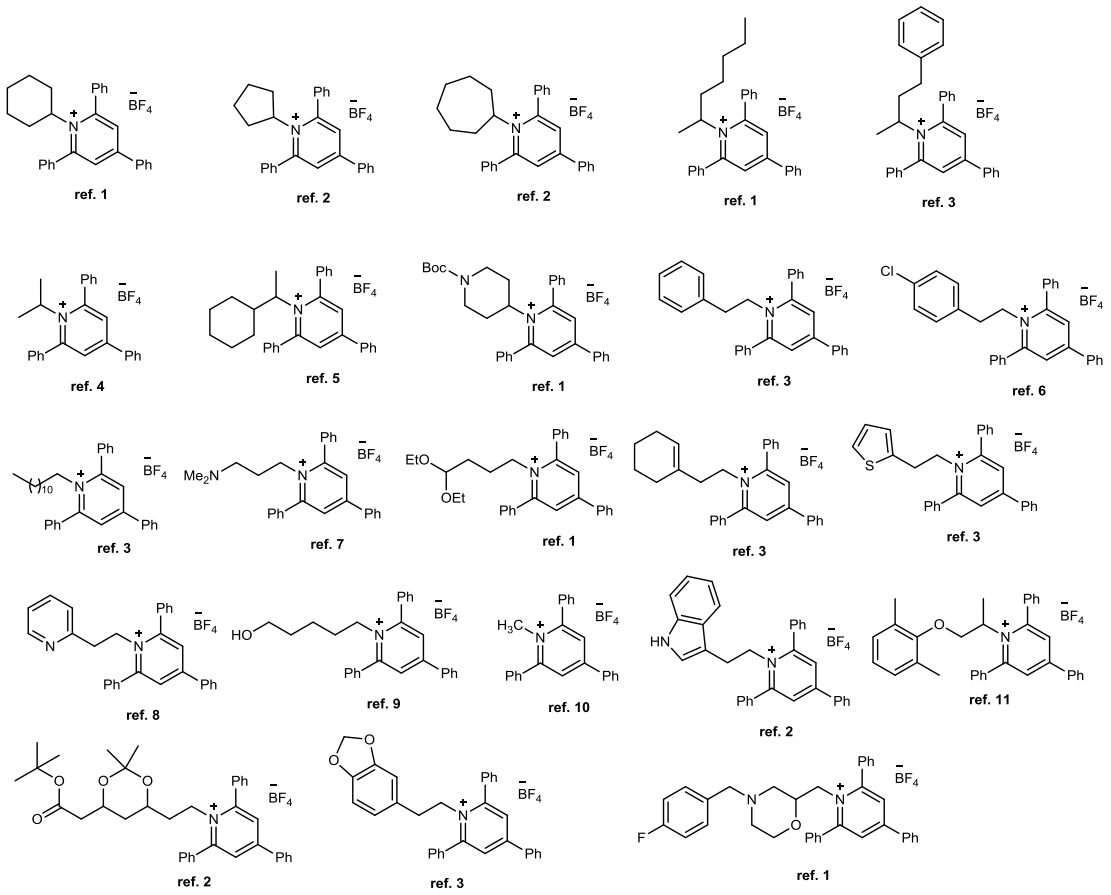
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were technical grade and freshly distilled prior to use. DMA used in reactions was purchased from J&K, bubbled for 30 min with Ar, and stored at room temperature. All other solvent used in reaction optimization were acquired from SPS. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with F-254 indicator, visualized by irradiation with UV light, in some cases stained with PMA. Column chromatography was performed using silica gel (Macherey Nagel, particle size 0.040-0.063 mm). ^{1}H-NMR and ^{13}C-NMR were recorded on a Varian AV300, AV400 or AV600 spectrometer in $CDCl_3$ and are reported relative to the solvent residual peaks. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), bs (broad singlet), d (doublet), t (triplet), m (multiplet); coupling constants (*J*) are in Hertz (Hz). IR spectra were recorded on a Perkin Elmer-100 spectrometer and are reported in terms of frequency of absorption (cm^{-1}). Mass spectra (EI-MS, 70 eV) were conducted on a Finnigan SSQ 7000 spectrometer. HRMS were recorded on a Thermo Scientific LTQ Orbitrap XL spectrometer. Gas chromatography (GC) was performed on a Shimadzu GC-2010 chromatograph.

2. Substrates Synthesis

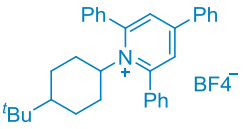
General Procedure for Preparation of Pyridinium Salts from Ammonium Salts



The Katritzky pyridinium salts were synthesized according to the procedure described previously in the literature.[1-11] 2,4,6-Triphenylpyrylium tetrafluoroborate (4.0 mmol, 1.0 equiv.) was suspended in absolute EtOH (4 mL). Subsequently, primary amine (4.8 mmol, 1.2 equiv.) was added and the reaction mixture was refluxed at 88 °C for 4 h. After this time, the mixture was cooled to room temperature and diluted with Et_2O (20 mL). The resulting precipitate was filtered off, washed with Et_2O, and dried under vacuum to afford the Katritzky salt. If the product failed to precipitate after addition of Et_2O, the reaction mixture was concentrated in vacuo and purified by column chromatography (acetone/CH_2Cl_2).

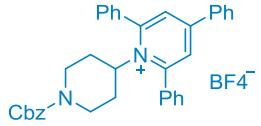


1-(4-(tert-butyl)cyclohexyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate



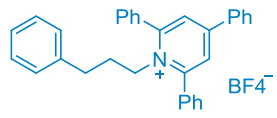
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.64 (m, 8H), 7.64 – 7.53 (m, 6H), 7.51 – 7.43 (m, 3H), 4.54 (t, *J* = 12.2 Hz, 1H), 2.14 (d, *J* = 7.4 Hz, 2H), 1.60 (d, *J* = 12.0 Hz, 2H), 1.47 (q, *J* = 12.3 Hz, 2H), 0.60 (s, 9H), 0.53 – 0.35 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 155.0, 134.0, 131.8, 130.8, 129.5, 129.3, 128.8, 128.2, 128.1, 72.1, 46.5, 33.3, 31.9, 27.4, 27.2.

1-(1-((benzyloxy)carbonyl)piperidin-4-yl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate



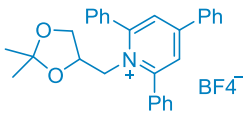
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.66 (m, 7H), 7.62 – 7.40 (m, 8H), 7.35 – 7.10 (m, 6H), 6.76 (s, 1H), 5.11 – 4.88 (m, 2H), 4.82 – 4.71 (m, 1H), 4.17 – 3.89 (m, 2H), 2.33 – 2.00 (m, 4H), 1.73 – 1.51 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 155.5, 154.7, 136.2, 133.8, 133.6, 132.1, 131.1, 129.6, 129.2, 129.0, 128.5, 128.3, 128.1, 127.8, 69.5, 67.2, 44.2, 32.4.

2,4,6-triphenyl-1-(3-phenylpropyl)pyridin-1-ium tetrafluoroborate



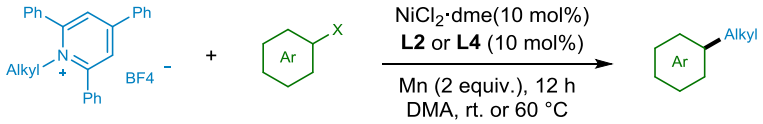
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.61 (m, 8H), 7.59 – 7.39 (m, 9H), 7.11 – 6.96 (m, 3H), 6.61 (dd, *J* = 6.0, 2.6 Hz, 2H), 4.41 – 4.28 (m, 2H), 2.06 (t, *J* = 7.1 Hz, 2H), 1.77 (dt, *J* = 15.6, 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 155.8, 138.7, 134.1, 132.6, 132.0, 131.0, 129.6, 129.2, 128.9, 128.5, 128.1, 127.7, 126.7, 126.2, 54.2, 32.3, 30.6.

1-((2,2-dimethyl-1,3-dioxolan-4-yl)methyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 – 7.71 (m, 8H), 7.66 – 7.51 (m, 9H), 4.99 (d, *J* = 13.4 Hz, 1H), 4.85 – 4.72 (m, 1H), 3.88 – 3.78 (m, 1H), 3.62 – 3.51 (m, 1H), 3.19 – 3.10 (m, 1H), 1.13 (s, 3H), 0.95 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.5, 155.9, 133.7, 133.0, 132.4, 131.2, 129.8, 129.7, 129.4, 128.1, 126.6, 110.4, 73.3, 66.9, 57.3, 25.7, 25.1.

3. General Procedure for the Catalytic Reactions



A dry reaction tube equipped with a Teflon-coated magnetic stir bar was charged with aryl halide (0.2 mmol, 1 equiv., if solid), Katritzky salt (0.3 mmol, 1.5 equiv.), $NiCl_2$·dme (4.4 mg, 0.02 mmol, 10 mol%), 2,2'-bipyridine **L2** (3.1 mg, 0.02 mmol, 10 mol%, for secondary alkyl Katritzky salts) or 4,4',4''-Tri-*tert*-Butyl-2,2':6',2''-terpyridine **L4** (8.0 mg, 0.02 mmol, 10 mol%, for primary alkyl Katritzky salts) and Mn (22 mg, 0.4 mmol, 2 equiv.). It was capped with a rubber septum, evacuated and backfilled with argon (3 times). Then, degassed DMA (1.0 mL), aryl halide (0.2 mmol, 1 equiv., if liquid) were added via syringe. The reaction mixture was stirred at room temperature (for secondary alkyl Katritzky salts) or 60 °C (for primary alkyl Katritzky salts) for 12 h. Upon completion, the mixture was purified by column chromatography on silica gel using hexane/EtOAc or hexane/toluene as eluent to get the corresponding pure product.

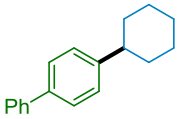
4. Gram Scale Reaction

A dry 100 mL flask equipped with a teflon-coated magnetic stir bar was charged with 4-iodobiphenyl (1.40 g, 5 mmol, 1 equiv.), 1-cyclohexyl-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (3.58 g, 7.5 mmol, 1.5 equiv.), $NiCl_2$·dme (55 mg, 0.25 mmol, 5 mol%), 2,2'-bipyridine **L2** (38.8 mg, 0.25 mmol, 5 mol%) and Mn (550 mg, 10 mmol, 2 equiv.). It was capped with a rubber septum, evacuated and backfilled with argon (3 times). Then, degassed DMA (25 mL) were added via syringe. The reaction mixture was stirred at room temperature for 12 h. Upon completion, the solution was diluted with H_2O (50 mL) and EtOAc (50 mL). The layers were separated, then the aqueous layer was extracted with EtOAc. The combined organic layer was washed with H_2O (50 mL) and brine (50 mL). The organic layer was dried with anhydrous Na_2SO_4, then concentrated under vacuum and purified by column chromatography on silica gel using pure hexane as eluent to get the product (96%, 1.13 g). The by-product 2,4,6-triphenylpyridine (85%, 1.96 g) was obtained via purification by column chromatography on silica gel using hexane:EtOAc = 50:1 as eluent.

Figure S1: Isolated organic base 2,4,6-triphenylpyridine

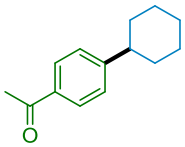
5. Spectroscopic Data of the Products

4-cyclohexyl-1,1'-biphenyl (3b)



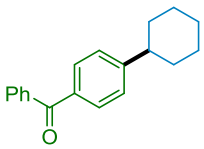
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 95% yield (44.8 mg) for 4-iodobiphenyl and 78% yield (37.1 mg) for 4-bromobiphenyl. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 – 7.52 (m, 4H), 7.50 – 7.40 (m, 2H), 7.39 – 7.28 (m, 3H), 2.67 – 2.50 (m, 1H), 2.05 – 1.81 (m, 5H), 1.59 – 1.36 (m, 5H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.3, 141.2, 138.8, 128.7, 127.3, 127.1, 127.0, 127.0, 44.3, 34.5, 27.0, 26.2. Data in accordance with the literature.[12]

1-(4-cyclohexylphenyl)ethan-1-one (3c)



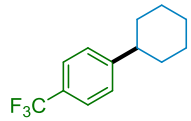
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 80:1 hexane: EtOAc) in 92% yield (37.1 mg) for 4′-iodoacetophenone and 90% yield (36.3 mg) for 4′-bromoacetophenone. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 2.56 (s, 4H), 1.90 – 1.79 (m, 4H), 1.79 – 1.70 (m, 1H), 1.48 – 1.32 (m, 4H), 1.29 – 1.20 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 153.7, 135.0, 128.5, 127.0, 44.7, 34.1, 26.7, 26.5, 26.0. Data in accordance with the literature.[1]

(4-cyclohexylphenyl)(phenyl)methanone (3d)



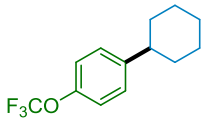
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 2:1 hexane: toluene) in 92% yield (48.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.69 (m, 4H), 7.59 – 7.51 (m, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 2.64 – 2.52 (m, 1H), 1.97 – 1.81 (m, 4H), 1.80 – 1.71 (m, 1H), 1.51 – 1.34 (m, 4H), 1.32 – 1.23 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.4, 153.1, 138.0, 135.2, 132.1, 130.4, 129.9, 128.2, 126.8, 44.7, 34.1, 26.7, 26.0. IR (ATR): $\tilde{\upsilon}$ = 3057, 2924, 2852, 2321, 2102, 1994, 1931, 1656, 1602, 1448, 1278, 1122, 928, 842, 746, 700 cm^{-1}. HRMS (ESI) for $C_{19}H_{20}O$: calculated for $[M+Na]^+$ 287.14064, found 287.14120.

1-cyclohexyl-4-(trifluoromethyl)benzene (3e)



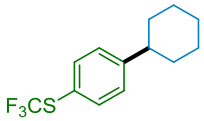
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: hexane) in 66% yield (30.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 2.55 (tt, *J* = 8.3, 3.5 Hz, 1H), 1.93 – 1.80 (m, 4H), 1.79 – 1.71 (m, 1H), 1.49 – 1.32 (m, 4H), 1.32 – 1.20 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 128.0 (q, *J* = 32.3 Hz), 127.1, 125.2 (q, *J* = 3.8 Hz), 124.38 (q, *J* = 271.6 Hz), 44.5, 34.2, 26.7, 26.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.30. Data in accordance with the literature.[13]

1-cyclohexyl-4-(trifluoromethoxy)benzene (3f)



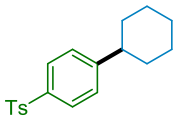
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: hexane) in 84% yield (41.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.8 Hz, 2H), 7.11 (d, *J* = 8.6 Hz, 2H), 2.50 (tt, *J* = 8.6, 3.2 Hz, 1H), 1.91 – 1.79 (m, 4H), 1.79 – 1.70 (m, 1H), 1.45 – 1.32 (m, 4H), 1.30 – 1.20 (m, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 147.2 (d, *J* = 1.8 Hz), 146.7, 127.9, 120.8, 120.5 (q, *J* = 256.3 Hz), 43.9, 34.4, 26.8, 26.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.96. Data in accordance with the literature.[14]

(4-cyclohexylphenyl)(trifluoromethyl)sulfane (3g)



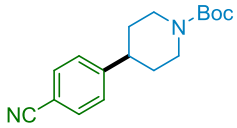
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: hexane) in 77% yield (40.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 2H), 2.53 (tt, *J* = 8.9, 3.0 Hz, 1H), 1.96 – 1.79 (m, 4H), 1.79 – 1.71 (m, 1H), 1.47 – 1.32 (m, 4H), 1.31 – 1.19 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 136.4, 129.68 (q, *J* = 307.9 Hz), 128.0, 121.1 (d, *J* = 2.1 Hz), 44.3, 34.2, 26.7, 26.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.1. IR (ATR): $\tilde{\nu}$ = 3467, 2926, 2854, 1449, 1383, 1121, 1016, 824, 535 cm^{-1}. HRMS (EI) for $C_{13}H_{15}F_3S$: calculated for $[M]^+$ 260.08411, found 260.08417.

1-cyclohexyl-4-tosylbenzene (3h)



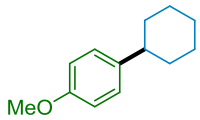
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 100:1 to 10:1 hexane: EtOAc) in 32% yield (20.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 8.3, 1.6 Hz, 4H), 7.27 (t, *J* = 7.9 Hz, 4H), 2.51 (tt, *J* = 8.7, 3.4 Hz, 1H), 2.37 (s, 3H), 1.87 – 1.69 (m, 5H), 1.42 – 1.29 (m, 4H), 1.27 – 1.18 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7, 143.9, 139.2, 139.0, 129.8, 127.7, 127.6, 127.6, 44.5, 34.0, 26.6, 25.9, 21.5. IR (ATR): $\tilde{\nu}$ = 3056, 2922, 2849, 1594, 1491, 1446, 1408, 1313, 1150, 1106, 1073, 1013, 822, 732, 706 cm^{-1}. HRMS (ESI) for $C_{19}H_{22}O_2S$: calculated for $[M+Na]^+$ 337.12327, found 337.12384.

tert-butyl 4-(4-cyanophenyl)piperidine-1-carboxylate (3i)



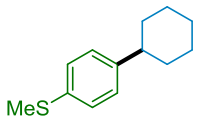
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 5:1 hexane: EtOAc) in 99% yield (56.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 4.22 (s, 2H), 2.87 – 2.61 (m, 3H), 1.78 (d, *J* = 12.9 Hz, 2H), 1.64 -1.50 (m, 2H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 151.1, 132.4, 127.6, 118.9, 110.2, 79.6, 44.1, 42.8, 32.7, 28.4. Data in accordance with the literature.[15]

1-cyclohexyl-4-methoxybenzene (3j)



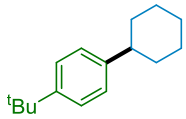
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 64% yield (24.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, *J* = 8.5 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 3.77 (s, 3H), 2.43 (tt, *J* = 8.2, 3.8 Hz, 1H), 1.89 – 1.78 (m, 4H), 1.76 – 1.69 (m, 1H), 1.43 – 1.30 (m, 4H), 1.28 – 1.18 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 140.4, 127.6, 113.6, 55.2, 43.7, 34.7, 26.9, 26.2. Data in accordance with the literature.[16]

(4-cyclohexylphenyl)(methyl)sulfane (3k)



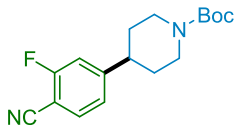
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 77% yield (31.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.3 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 2.46 (s, 4H), 1.83 (s, 4H), 1.77 – 1.68 (m, 1H), 1.44 – 1.30 (m, 4H), 1.29 – 1.17 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 135.0, 127.4, 127.2, 44.0, 34.4, 26.9, 26.1, 16.4. Data in accordance with the literature.[17]

1-(tert-butyl)-4-cyclohexylbenzene (3l)



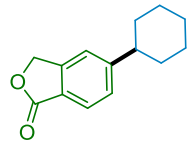
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 51% yield (22.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 2.52 – 2.41 (m, 1H), 1.94 – 1.78 (m, 4H), 1.78 – 1.69 (m, 1H), 1.47 – 1.35 (m, 4H), 1.34 – 1.20 (m, 10H).^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 145.0, 126.4, 125.1, 44.0, 34.5, 34.3, 31.4, 27.0, 26.2. Data in accordance with the literature.[13]

Tert-butyl 4-(4-cyano-3-fluorophenyl)piperidine-1-carboxylate (3m)



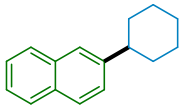
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 5:1 hexane: EtOAc) in 99% yield (60.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.9, 6.8 Hz, 1H), 7.12 – 6.98 (m, 2H), 4.24 (s, 2H), 2.84 – 2.64 (m, 3H), 1.79 (d, *J* = 12.8 Hz, 2H), 1.56 (td, *J* = 12.6, 4.2 Hz, 2H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.3 (d, J = 258.9 Hz), 154.6, 154.45 (d, *J* = 7.2 Hz), 133.5, 123.4, 114.77 (d, *J* = 19.4 Hz), 114.0, 99.18 (d, *J* = 15.5 Hz), 79.7, 43.9, 42.8, 32.5, 28.4. Data in accordance with the literature.[18]

5-cyclohexylisobenzofuran-1(3H)-one (3n)



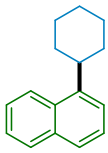
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 hexane: EtOAc) in 79% yield (34.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.29 (s, 1H), 5.26 (s, 2H), 2.62 (t, *J* = 9.9 Hz, 1H), 1.86 (s, 4H), 1.76 (d, *J* = 13.7 Hz, 1H), 1.49 – 1.33 (m, 4H), 1.32 – 1.19 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 155.2, 147.1, 128.3, 125.6, 123.5, 120.1, 69.5, 45.1, 34.3, 26.6, 25.9. IR (ATR): $\tilde{\upsilon}$ = 2922, 2851, 1752, 1687, 1610, 1446, 1354, 1212, 1040, 997, 925, 888, 842, 773, 691 cm^{-1}. HRMS (ESI) for $C_{14}H_{16}O_2$: calculated for $[M+Na]^+$ 239.10425, found 239.10464.

2-cyclohexylnaphthalene (3o)



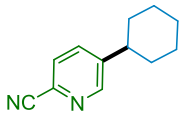
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: hexane) in 61% yield (25.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.73 (m, 3H), 7.64 (s, 1H), 7.51 – 7.30 (m, 3H), 2.67 (tt, *J* = 11.8, 3.4 Hz, 1H), 2.05 – 1.84 (m, 4H), 1.84 – 1.74 (m, 1H), 1.60 – 1.39 (m, 4H), 1.37 – 1.25 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 133.7, 132.1, 127.7, 127.6, 127.5, 126.2, 125.7, 125.0, 124.5, 44.7, 34.4, 26.9, 26.2. Data in accordance with the literature.[19]

1-cyclohexylnaphthalene (3p)



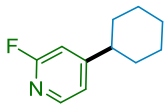
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: hexane) in 71% yield (30.1 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 – 8.11 (m, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.64 – 7.35 (m, 4H), 3.43 – 3.26 (m, 1H), 2.16 – 1.78 (m, 5H), 1.69 – 1.49 (m, 4H), 1.47 – 1.29 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.8, 133.9, 131.4, 128.9, 126.2, 125.7, 125.6, 125.2, 123.2, 122.3, 39.3, 34.2, 27.3, 26.6. Data in accordance with the literature.[20]

5-cyclohexylpicolinonitrile (3q)



According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 50:1 to 5:1 hexane: EtOAc) in 64% yield (23.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 7.60 (s, 2H), 2.59 (t, *J* = 9.1 Hz, 1H), 1.86 (d, *J* = 8.7 Hz, 4H), 1.76 (d, *J* = 12.8 Hz, 1H), 1.47 – 1.32 (m, 4H), 1.31 – 1.18 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.5, 147.1, 134.8, 131.3, 128.3, 117.5, 42.1, 33.7, 26.4, 25.7. Data in accordance with the literature.[21]

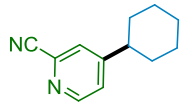
4-cyclohexyl-2-fluoropyridine (3r)



According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 50:1 to 10:1 hexane: EtOAc) in 67% yield (24.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 5.2 Hz, 1H), 6.98 (d, *J* = 5.2 Hz, 1H), 6.72 (s, 1H), 2.58 – 2.45 (m, 1H), 1.91 – 1.78 (m, 4H), 1.78 – 1.70 (m, 1H), 1.44 – 1.30 (m, 4H), 1.28 – 1.20 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.2 (d, *J* = 237.8 Hz), 162.7 (d, *J* = 7.5 Hz), 147.2 (d, *J* = 15.3 Hz), 120.2 (d, *J* = 3.7 Hz), 107.4 (d, *J* = 36.7 Hz), 43.7, 33.4, 26.3, 25.8. ^{19}F NMR (376 MHz,

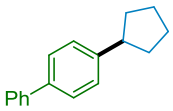
$CDCl_3$) δ -69.17. Data in accordance with the literature.[22]

4-cyclohexylpicolinonitrile (3s)



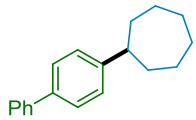
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 50:1 to 10:1 hexane: EtOAc) in 72% yield (26.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.52 (s, 1H), 7.32 (d, *J* = 4.2 Hz, 1H), 2.54 (s, 1H), 1.86 (d, *J* = 8.0 Hz, 4H), 1.76 (d, *J* = 13.0 Hz, 1H), 1.49 – 1.31 (m, 4H), 1.30 – 1.19 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 150.9, 133.9, 127.3, 125.6, 117.5, 43.5, 33.3, 26.2, 25.6. IR (ATR): $\tilde{\nu}$ = 3467, 3053, 2928, 2854, 2236, 1595, 1449, 1407, 992, 925, 848, 498 cm^{-1}. HRMS (ESI) for $C_{12}H_{14}N_2$: calculated for $[M+Na]^+$ 209.10492, found 209.10521.

4-cyclopentyl-1,1'-biphenyl (4a)



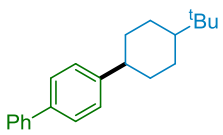
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 99% yield (44.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.59 (m, 2H), 7.58 – 7.53 (m, 2H), 7.50 – 7.41 (m, 2H), 7.40 – 7.31 (m, 3H), 3.13 – 3.00 (m, 1H), 2.20 – 2.08 (m, 2H), 1.93 – 1.81 (m, 2H), 1.80 – 1.61 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.7, 141.2, 138.7, 128.7, 127.6, 127.0, 127.0, 127.0, 45.7, 34.7, 25.6. Data in accordance with the literature.[23]

4-cycloheptyl-1,1'-biphenyl (4b)



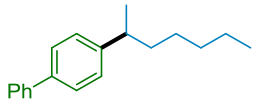
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 62% yield (31.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.56 (m, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 2H), 2.73 (tt, *J* = 10.5, 3.7 Hz, 1H), 2.01 – 1.92 (m, 2H), 1.88 – 1.79 (m, 2H), 1.76 – 1.55 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 141.2, 138.5, 128.7, 127.1, 127.0, 127.0, 126.9, 46.7, 36.8, 28.0, 27.2. IR (ATR): $\tilde{\nu}$ = 3025, 2920, 2854, 1597, 1484, 1452, 1405, 828, 759, 728, 692 cm^{-1}. HRMS (EI) for $C_{19}H_{22}$: calculated for $[M]^+$ 250.17160, found 250.17182.

4-(4-(tert-butyl)cyclohexyl)-1,1'-biphenyl (4c)



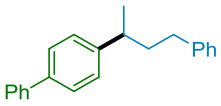
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 88% yield (51.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.51 (m, 4H), 7.51 – 7.26 (m, 5H), 3.11 (s, 0.46H), 2.52 (tt, *J* = 12.2, 3.4 Hz, 0.74H), 2.32 (d, *J* = 14.3 Hz, 1H), 1.99 (dd, *J* = 30.5, 11.0 Hz, 2H), 1.88 – 1.76 (m, 1H), 1.65 (d, *J* = 10.2 Hz, 1H), 1.58 – 1.45 (m, 1H), 1.32 – 1.12 (m, 3H), 0.94 (s, 5.47H), 0.86 (s, 3.53H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0 (144.5), 141.2 (141.1), 138.8 (138.0), 128.7, 128.2, 127.3 (127.2), (127.1) 127.0, 126.84 (126.80), (48.3) 47.8, (44.2) 36.2, 34.8 (30.8), (32.7) 32.5, (27.7) 27.6, 22.8. IR (ATR): $\tilde{\nu}$ = 3026, 2934, 2855, 1481, 1447, 1365, 1234, 1005, 900, 844, 758, 732, 694 cm^{-1}. HRMS (EI) for $C_{22}H_{28}$: calculated for $[M]^+$ 292.21855, found 292.21919.

4-(heptan-2-yl)-1,1'-biphenyl (4d)



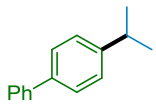
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 82% yield (41.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.59 (m, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.31 (m, 1H), 7.28 (d, *J* = 8.2 Hz, 2H), 2.80 – 2.68 (m, 1H), 1.69 – 1.55 (m, 2H), 1.35 – 1.21 (m, 9H), 0.95 – 0.84 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.2, 141.2, 138.7, 128.7, 127.4, 127.0, 126.9, 39.6, 38.4, 32.0, 27.4, 22.6, 22.3, 14.1. IR (ATR): $\tilde{\nu}$ = 3028, 2956, 2858, 2326, 2091, 1907, 1682, 1602, 1485, 1456, 1374, 1007, 835, 763, 731, 696 cm^{-1}. HRMS (EI) for $C_{19}H_{24}$: calculated for $[M]^+$ 252.18725, found 252.18677.

4-(4-phenylbutan-2-yl)-1,1'-biphenyl (4e)



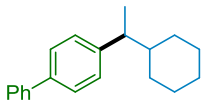
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 79% yield (45.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.58 (m, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.38 – 7.25 (m, 5H), 7.23 – 7.12 (m, 3H), 2.84 – 2.72 (m, 1H), 2.56 (td, *J* = 7.8, 7.3, 2.1 Hz, 2H), 2.05 – 1.88 (m, 2H), 1.32 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 142.5, 141.1, 138.9, 128.7, 128.4, 128.3, 127.5, 127.1, 127.0, 125.7, 39.9, 39.2, 33.9, 22.5. Data in accordance with the literature.[24]

4-isopropyl-1,1'-biphenyl (4f)



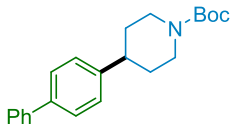
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: hexane) in 88% yield (34.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.2 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 3H), 2.98 (hept, *J* = 6.9 Hz, 1H), 1.32 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 141.2, 138.8, 128.7, 127.1, 127.0, 127.0, 126.9, 33.8, 24.0. Data in accordance with the literature.[25]

4-(1-cyclohexylethyl)-1,1'-biphenyl (4g)



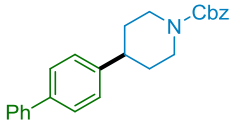
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 72% yield (38.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 8.3 Hz, 2H), 2.50 (p, *J* = 7.2 Hz, 1H), 1.91 (d, *J* = 12.7 Hz, 1H), 1.76 (dt, *J* = 12.5, 3.1 Hz, 1H), 1.71 – 1.58 (m, 2H), 1.55 – 1.39 (m, 2H), 1.27 (d, *J* = 7.0 Hz, 3H), 1.19 – 1.07 (m, 2H), 1.02 – 0.81 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.3, 141.2, 138.5, 128.7, 128.1, 127.0, 126.9, 126.7, 45.6, 44.2, 31.5, 30.6, 26.6, 18.8. IR (ATR): $\tilde{\nu}$ = 3036, 2915, 2849, 1599, 1486, 1450, 1406, 1008, 835, 760, 726, 687 cm^{-1}. HRMS (EI) for $C_{20}H_{24}$: calculated for $[M]^+$ 264.18725, found 264.18786.

Tert-butyl 4-([1,1'-biphenyl]-4-yl)piperidine-1-carboxylate (4h)



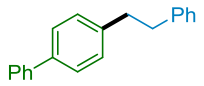
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 10:1 hexane: EtOAc) in 94% yield (63.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.50 (m, 4H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.36 – 7.30 (m, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 4.27 (s, 2H), 2.82 (t, *J* = 12.0 Hz, 2H), 2.69 (tt, *J* = 12.1, 3.4 Hz, 1H), 1.86 (d, *J* = 12.8 Hz, 2H), 1.73 – 1.60 (m, 2H), 1.50 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9, 144.9, 140.9, 139.3, 128.7, 127.2, 127.2, 127.1, 127.0, 79.4, 44.4, 42.4, 33.2, 28.5. IR (ATR): $\tilde{\nu}$ = 29025, 2854, 1706, 1675, 1609, 1448, 1420, 1368, 1274, 1171, 1114, 1008, 844, 762, 703 cm^{-1}. HRMS (ESI) for $C_{22}H_{27}O_2N$: calculated for $[M+Na]^+$ 360.19340, found 360.19394.

Benzyl 4-([1,1'-biphenyl]-4-yl)piperidine-1-carboxylate (4i)



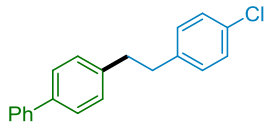
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 10:1 hexane: EtOAc) in 96% yield (71.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.53 (m, 4H), 7.50 – 7.31 (m, 8H), 7.28 (d, *J* = 8.2 Hz, 2H), 5.20 (s, 2H), 4.39 (s, 2H), 2.92 (s, 2H), 2.73 (tt, *J* = 12.1, 3.4 Hz, 1H), 1.89 (d, *J* = 12.5 Hz, 2H), 1.70 (d, *J* = 10.9 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 144.6, 140.9, 139.4, 136.9, 128.8, 128.5, 128.0, 127.9, 127.3, 127.2, 127.2, 127.0, 67.1, 44.6, 42.3, 33.1. IR (ATR): $\tilde{\nu}$ = 3028, 2923, 2852, 1692, 1483, 1430, 1364, 12286, 1219, 1111, 1072, 1016, 836, 757, 697 cm^{-1}. HRMS (ESI) for $C_{25}H_{25}O_2N$: calculated for $[M+Na]^+$ 394.17775, found 394.17831.

4-phenethyl-1,1'-biphenyl (4j)



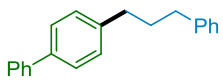
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 74% yield (38.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.1 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.40 – 7.21 (m, 8H), 3.00 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 141.1, 140.9, 138.9, 128.9, 128.8, 128.5, 128.4, 127.1, 127.1, 127.0, 126.0, 37.9, 37.6. Data in accordance with the literature.[26]

4-(4-chlorophenethyl)-1,1'-biphenyl (4k)



According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 65% yield (38.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.8 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.29 – 7.19 (m, 4H), 7.12 (d, *J* = 8.4 Hz, 2H), 2.94 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 140.4, 140.1, 139.0, 131.7, 129.9, 128.9, 128.7, 128.4, 127.1, 127.0, 37.4, 37.1. Data in accordance with the literature.[27]

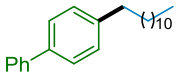
4-(3-phenylpropyl)-1,1'-biphenyl (4l)



According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 78% yield (42.3

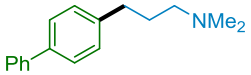
mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.60 (m, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.18 (m, 8H), 2.73 (td, *J* = 7.8, 3.0 Hz, 4H), 2.09 – 1.99 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 141.4, 141.1, 138.7, 128.9, 128.7, 128.5, 128.4, 127.1, 127.0, 125.8, 35.5, 35.1, 32.9. Data in accordance with the literature.[28]

4-dodecyl-1,1'-biphenyl (4m)



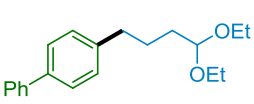
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 92% yield (59.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.57 (m, 2H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.31 (m, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 2.71 – 2.62 (m, 2H), 1.68 (p, *J* = 7.5 Hz, 2H), 1.34 – 1.27 (m, 18H), 0.91 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.7, 141.1, 138.7, 128.8, 128.7, 127.05, 127.01, 62.9, 35.6, 32.7, 31.3, 25.5. Data in accordance with the literature.[29]

3-([1,1'-biphenyl]-4-yl)-*N, N*-dimethylpropan-1-amine (4n)



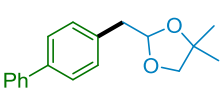
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 10:1 to 1:1 hexane: EtOAc) in 72% yield (34.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 2.71 – 2.65 (m, 2H), 2.36 – 2.30 (m, 2H), 2.24 (s, 6H), 1.83 (p, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 141.1, 138.7, 128.8, 128.7, 127.1, 127.0, 59.3, 45.5, 33.3, 29.5. IR (ATR): $\tilde{\nu}$ = 3027, 2939, 2766, 1728, 1484, 1457, 1265, 1037, 1009, 963, 834, 759, 696 cm^{-1}. HRMS (ESI) for $C_{17}H_{22}N$: calculated for $[M+H]^+$ 240.17468, found 240.17487.

4-(4,4-diethoxybutyl)-1,1'-biphenyl (4o)



According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 4:1 to 1:1 hexane: toluene) in 53% yield (31.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.4 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 2H), 4.51 (t, *J* = 5.2 Hz, 1H), 3.73 – 3.38 (m, 4H), 2.68 (t, *J* = 7.3 Hz, 2H), 1.85 – 1.61 (m, 4H), 1.20 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 141.1, 138.7, 128.8, 128.7, 127.2, 127.03, 126.97, 102.8, 61.0, 35.3, 33.2, 26.6, 15.4. IR (ATR): $\tilde{\nu}$ = 34465, 3028, 2922, 1728, 1602, 1485, 1449, 1382, 1125, 1064, 838, 761, 697, 502 cm^{-1}. HRMS (ESI) for $C_{20}H_{26}O_2$: calculated for $[M+Na]^+$ 321.18250, found 321.18304.

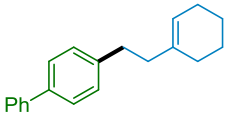
2-([1,1'-biphenyl]-4-ylmethyl)-4,4-dimethyl-1,3-dioxolane (4p)



According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 100:1 hexane: EtOAc) in 56% yield (30.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 17.9, 7.7 Hz, 4H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.31 (dd, *J* = 20.4, 7.8 Hz, 3H), 4.41 – 4.32 (m, 1H), 4.01 (dd, *J* = 8.0, 6.0 Hz, 1H), 3.72 – 3.63 (m, 1H), 3.04 (dd, *J* = 13.7, 6.3 Hz, 1H), 2.82 (dd, *J* = 13.7, 6.9 Hz, 1H), 1.46 (s, 3H), 1.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9, 139.5, 136.7, 129.6, 128.7, 127.2, 127.1,

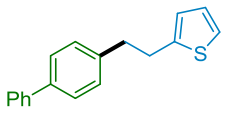
127.0, 109.2, 69.0, 39.8, 27.0, 25.7. IR (ATR): $\tilde{\nu}$ = 3030, 2985, 2932, 2328, 2088, 1719, 1601, 1484, 1373, 12218, 1154, 1060, 1006, 916, 832, 758, 696 cm^{-1}. HRMS (ESI) for $C_{18}H_{20}O_2$: calculated for $[M+Na]^+$ 291.13555, found 291.13589.

4-(2-(cyclohex-1-en-1-yl)ethyl)-1,1'-biphenyl (4q)



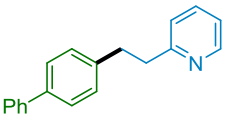
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 81% yield (42.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 5.48 (s, 1H), 2.81 – 2.73 (m, 2H), 2.33 – 2.24 (m, 2H), 2.07 – 1.97 (m, 4H), 1.72 – 1.54 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 141.2, 138.6, 137.3, 128.8, 128.7, 127.0, 127.0, 121.3, 40.0, 34.1, 28.6, 25.3, 23.0, 22.6. IR (ATR): $\tilde{\nu}$ = 3029, 2926, 2838, 1485, 1446, 1406, 1131, 1005, 912, 832, 754, 690 cm^{-1}. HRMS (EI) for $C_{20}H_{22}$: calculated for $[M]^+$ 262.17160, found 262.17230.

2-(2-([1,1'-biphenyl]-4-yl)ethyl)thiophene (4r)



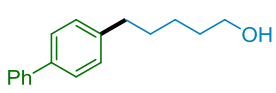
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 100:1 hexane: EtOAc) in 40% yield (21.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.1 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.13 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.92 (dd, *J* = 5.1, 3.4 Hz, 1H), 6.83 – 6.76 (m, 1H), 3.22 – 3.13 (m, 2H), 3.07 – 2.99 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 141.0, 140.2, 139.1, 128.8, 128.7, 127.1, 127.1, 127.0, 126.7, 124.4, 123.1, 37.7, 31.8. IR (ATR): $\tilde{\nu}$ = 3030, 2922, 2852, 2324, 2081, 1485, 1450, 1234, 833, 763, 686 cm^{-1}. HRMS (EI) for $C_{18}H_{16}S$: calculated for $[M]^+$ 264.09672, found 264.09682.

2-(2-([1,1'-biphenyl]-4-yl)ethyl)pyridine (4s)



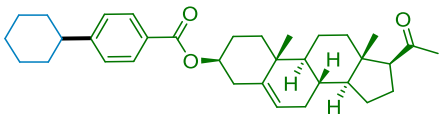
According to the general procedure, the title compound was isolated as a slight yellow solid after flash chromatography on silica gel (eluent: 50:1 to 5:1 hexane: EtOAc) in 17% yield (8.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.3 Hz, 1H), 7.56 (d, *J* = 7.2 Hz, 3H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.08 (m, 2H), 3.17 – 3.06 (m, *J* = 4.3 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0, 149.0, 141.0, 140.5, 138.9, 136.7, 128.9, 128.7, 127.1, 127.0, 127.0, 123.2, 121.3, 39.9, 35.6.

5-([1,1'-biphenyl]-4-yl)pentan-1-ol (4t)



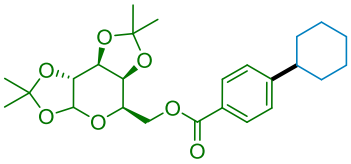
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 10:1 hexane: EtOAc) in 74% yield (35.3 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 – 7.58 (m, 2H), 7.57 – 7.50 (m, 2H), 7.49 – 7.40 (m, 2H), 7.39 – 7.31 (m, 1H), 7.27 (d, *J* = 8.3 Hz, 2H), 3.67 (t, *J* = 6.3 Hz, 2H), 2.74 – 2.64 (m, 2H), 1.77 – 1.58 (m, 4H), 1.52 – 1.40 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.7, 141.1, 138.7, 128.8, 128.7, 127.0, 127.0, 62.9, 35.6, 32.7, 31.3, 25.5. Data in accordance with the literature.[30]

(3S,8S,9S,10R,13S,14S,17S)-17-acetyl-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-cyclohexylbenzoate (5a)



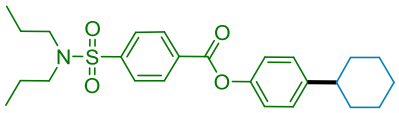
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 100:1 to 20:1 hexane: EtOAc) in 56% yield (56.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 5.39 (d, *J* = 4.2 Hz, 1H), 4.87 – 4.78 (m, 1H), 2.60 – 2.38 (m, 4H), 2.24 – 0.96 (m, 33H), 0.62 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 209.5, 166.0, 153.3, 139.7, 129.6, 128.3, 126.8, 122.4, 74.1, 63.7, 56.8, 49.9, 44.7, 44.0, 38.8, 38.2, 37.0, 36.6, 34.1, 31.8, 31.5, 27.8, 26.7, 26.0, 24.5, 22.8, 21.0, 19.3, 13.2. IR (ATR): $\tilde{\nu}$ = 2928, 2852, 1706, 1444, 1355, 1271, 1182, 1113, 1016, 948, 843, 757, 704 cm^{-1}. HRMS (ESI) for $C_{34}H_{46}O_3$: calculated for $[M+Na]^+$ 525.33392, found 525.33466.

((5R,5aS,8aS,8bR)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 4-cyclohexylbenzoate (5b)



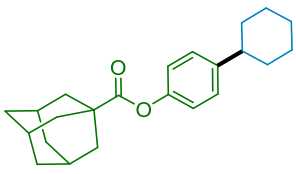
According to the general procedure, the title compound was isolated as a colorless oil after flash chromatography on silica gel (eluent: 100:1 to 20:1 hexane: EtOAc) in 95% yield (85.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.3 Hz, 2H), 5.54 (d, *J* = 4.9 Hz, 1H), 4.62 (dd, *J* = 7.9, 2.5 Hz, 1H), 4.49 (dd, *J* = 11.4, 5.1 Hz, 1H), 4.38 (dd, *J* = 11.5, 7.4 Hz, 1H), 4.35 – 4.25 (m, 2H), 4.20 – 4.11 (m, 1H), 2.60 – 2.45 (m, 1H), 1.91 – 1.67 (m, 5H), 1.55 – 1.13 (m, 17H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 153.5, 129.8, 127.6, 126.8, 109.6, 108.7, 96.3, 71.1, 70.7, 70.5, 66.1, 63.6, 44.7, 34.1, 26.7, 26.00, 25.95, 25.0, 24.5. IR (ATR): $\tilde{\nu}$ = 2896, 2926, 2854, 1718, 1609, 1450, 1377, 1271, 1211, 1173, 1068, 1003, 894, 855, 759, 705 cm^{-1}. HRMS (ESI) for $C_{25}H_{34}O_7$: calculated for $[M+Na]^+$ 469.21967, found 469.22018.

4-cyclohexylphenyl 4-(*N*, *N*-dipropylsulfamoyl)benzoate (5c)



According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 100:1 to 20:1 hexane: EtOAc) in 84% yield (74.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 7.11 (d, *J* = 8.6 Hz, 2H), 3.16 – 3.03 (m, 4H), 2.52 (tt, *J* = 8.3, 3.5 Hz, 1H), 1.92 – 1.79 (m, 4H), 1.78 – 1.69 (m, 1H), 1.55 (dq, *J* = 14.9, 7.2 Hz, 4H), 1.39 (t, *J* = 10.4 Hz, 4H), 1.29 – 1.21 (m, 1H), 0.87 (t, *J* = 7.4 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.0, 148.5, 146.1, 144.8, 133.0, 130.7, 127.9, 127.1, 121.1, 49.9, 44.0, 34.5, 26.8, 26.1, 21.9, 11.1. IR (ATR): $\tilde{\nu}$ = 2924, 2851, 1740, 1508, 1452, 1331, 1262, 1154, 1074, 990, 874, 855, 802, 744, 687 cm^{-1}. HRMS (ESI) for $C_{25}H_{33}O_4NS$: calculated for $[M+Na]^+$ 466.20284, found 466.20337.

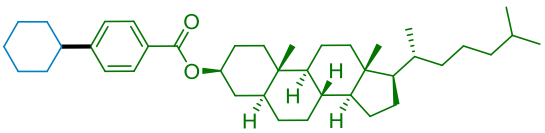
4-cyclohexylphenyl (3r,5r,7r)-adamantane-1-carboxylate (5d)



According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 5:1 to 2:1 hexane: toluene) in 83% yield (56.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ

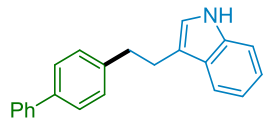
7.18 (d, *J* = 8.5 Hz, 2H), 6.94 (d, *J* = 8.5 Hz, 2H), 2.48 (tt, *J* = 11.7, 3.1 Hz, 1H), 2.16 – 1.94 (m, 9H), 1.91 – 1.69 (m, 11H), 1.45 – 1.31 (m, 4H), 1.28 – 1.17 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.3, 149.0, 145.2, 127.6, 121.1, 44.0, 41.0, 38.8, 36.5, 34.5, 27.9, 26.9, 26.1. IR (ATR): $\tilde{\upsilon}$ = 2909, 2850, 1743, 1506, 1448, 1193, 1053, 846, 798, 729, 678 cm^{-1}. HRMS (ESI) for $C_{23}H_{30}O_2$: calculated for $[M+Na]^+$ 361.21411, found 361.21429.

(3S,5S,8R,9S,10S,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)hexadecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-cyclohexylbenzoate (5e)



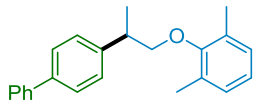
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 5:1 to 2:1 hexane: toluene) in 87% yield (100.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 8.3 Hz, 2H), 4.97 – 4.86 (m, 1H), 2.58 – 2.48 (m, 1H), 2.05 – 0.74 (m, 53H), 0.65 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 153.1, 129.6, 128.5, 126.7, 74.0, 56.4, 56.3, 54.2, 44.7, 44.7, 42.6, 40.0, 39.5, 36.8, 36.2, 35.8, 35.5, 34.2, 32.0, 28.6, 28.2, 28.0, 27.6, 26.7, 26.0, 24.2, 23.9, 22.8, 22.6, 21.2, 18.7, 12.3, 12.1. IR (ATR): $\tilde{\upsilon}$ = 2925, 2854, 1707, 1609, 1449, 1378, 1274, 1178, 1112, 1003, 846, 766, 706 cm^{-1}. HRMS (ESI) for $C_{40}H_{62}O_2$: calculated for $[M+Na]^+$ 597.46420, found 597.46503.

3-(2-([1,1'-biphenyl]-4-yl)ethyl)-1H-indole (5f)



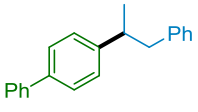
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 10:1 hexane: EtOAc) in 61% yield (36.0 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.77 – 7.07 (m, 13H), 6.96 (s, 1H), 3.24 – 3.03 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.6, 141.2, 138.8, 136.3, 129.0, 128.8, 127.1, 122.0, 121.4, 119.3, 118.9, 116.1, 111.2, 36.1, 27.3. IR (ATR): $\tilde{\upsilon}$ = 3401, 3028, 2910, 2327, 1598, 1484, 1454, 1091, 1005, 824, 741, 690 cm^{-1}. HRMS (ESI) for $C_{22}H_{19}N$: calculated for $[M+Na]^+$ 320.14097, found 320.14169.

4-(1-(2,6-dimethylphenoxy)propan-2-yl)-1,1'-biphenyl (5g)



According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 84% yield (53.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.56 (m, 4H), 7.51 – 7.40 (m, 4H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.02 (d, *J* = 7.4 Hz, 2H), 6.97 – 6.90 (m, 1H), 3.98 – 3.84 (m, 2H), 3.35 (h, *J* = 6.9 Hz, 1H), 2.24 (s, 6H), 1.55 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 143.2, 141.1, 139.5, 131.0, 128.82, 128.76, 127.9, 127.14, 127.06, 123.8, 77.3, 40.5, 18.3, 16.3. IR (ATR): $\tilde{\upsilon}$ = 3465, 3028, 2920, 2866, 1597, 1478, 1381, 1263, 1201, 1092, 1008, 912, 836, 766, 697 cm^{-1}. HRMS (ESI) for $C_{23}H_{24}O$: calculated for $[M+Na]^+$ 339.17194, found 339.17252.

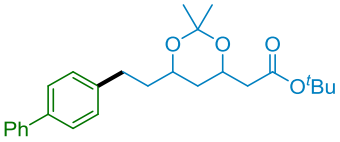
4-(1-phenylpropan-2-yl)-1,1'-biphenyl (5h)



According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: hexane) in 74% yield (40.1

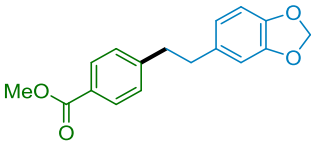
mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.1 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.28 (t, *J* = 8.1 Hz, 4H), 7.20 (t, *J* = 7.3 Hz, 1H), 7.14 (d, *J* = 6.9 Hz, 2H), 3.13 – 2.98 (m, 2H), 2.87 – 2.78 (m, 1H), 1.30 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.2, 141.1, 140.8, 138.9, 129.2, 128.7, 128.1, 127.5, 127.0, 127.0, 125.9, 45.0, 41.5, 21.2. IR (ATR): $\tilde{\nu}$ = 3030, 2920, 2852, 1486, 1452, 1009, 841, 821, 760, 691 cm^{-1}. HRMS (EI) for $C_{21}H_{20}$: calculated for $[M]^+$ 272.15595, found 272.15644.

Tert-butyl 2-(6-(2-([1,1'-biphenyl]-4-yl)ethyl)-2,2-dimethyl-1,3-dioxan-4-yl)acetate (5i)



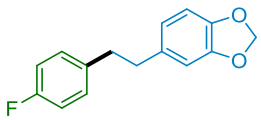
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 200:1 to 50:1 hexane: EtOAc) in 74% yield (60.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 2H), 4.27 – 4.18 (m, 1H), 3.89 – 3.79 (m, 1H), 2.83 – 2.65 (m, 2H), 2.44 (dd, *J* = 15.1, 7.0 Hz, 1H), 2.30 (dd, *J* = 15.1, 6.2 Hz, 1H), 1.92 – 1.81 (m, 1H), 1.77 – 1.69 (m, 1H), 1.56 (dt, *J* = 12.7, 2.3 Hz, 2H), 1.49 – 1.38 (m, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 141.1, 138.7, 129.0, 128.7, 127.0, 127.0, 127.0, 98.7, 80.5, 67.7, 66.3, 42.7, 37.8, 36.6, 30.7, 30.2, 28.1, 19.8. IR (ATR): $\tilde{\nu}$ = 2939, 1716, 1486, 1372, 1288, 1260, 1173, 990, 944, 840, 758, 732, 686 cm^{-1}. HRMS (ESI) for $C_{26}H_{34}O_4$: calculated for $[M+Na]^+$ 433.23493, found 433.23572.

Methyl 4-(2-(benzo[d][1,3]dioxol-5-yl)ethyl)benzoate (5j)



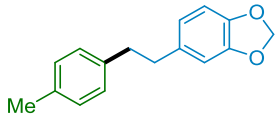
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 2:1 hexane: toluene) in 94% yield (53.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 2H), 6.69 (d, *J* = 7.9 Hz, 1H), 6.63 (d, *J* = 1.7 Hz, 1H), 6.55 (dd, *J* = 7.9, 1.7 Hz, 1H), 5.90 (s, 2H), 3.88 (s, 3H), 2.96 – 2.79 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 147.5, 147.0, 145.8, 134.9, 129.7, 128.5, 127.9, 121.2, 108.8, 108.1, 100.8, 52.0, 38.1, 37.1. IR (ATR): $\tilde{\nu}$ = 2919, 2857, 1713, 1607, 1489, 1437, 1276, 1178, 1099, 1033, 925, 854, 801, 758, 700 cm^{-1}. HRMS (ESI) for $C_{17}H_{16}O_4$: calculated for $[M+Na]^+$ 307.09408, found 307.09464.

5-(4-fluorophenethyl)benzo[d][1,3]dioxole (5k)



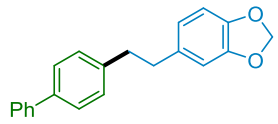
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 5:1 hexane: toluene) in 66% yield (32.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (dd, *J* = 8.4, 5.5 Hz, 2H), 6.94 (t, *J* = 8.7 Hz, 2H), 6.71 (d, *J* = 7.9 Hz, 1H), 6.64 (d, *J* = 1.5 Hz, 1H), 6.57 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.91 (s, 2H), 2.87 – 2.77 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3 (d, *J* = 243.2 Hz), 147.5, 145.7, 137.1, 135.2, 129.8 (d, *J* = 7.7 Hz), 121.2, 115.0 (d, *J* = 21.0 Hz), 108.9, 108.1, 100.8, 37.7, 37.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.60 (ddd, *J* = 14.0, 8.9, 5.6 Hz). IR (ATR): $\tilde{\nu}$ = 2925, 2858, 2110, 1601, 1490, 1442, 1239, 1036, 923, 817, 746 cm^{-1}. HRMS (EI) for $C_{15}H_{13}O_2F$: calculated for $[M]^+$ 244.08941, found 244.08945.

5-(4-methylphenethyl)benzo[d][1,3]dioxole (5l)



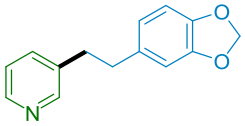
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 5:1 hexane: toluene) in 67% yield (32.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 – 6.98 (m, 4H), 6.78 – 6.66 (m, 2H), 6.62 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.92 (s, 2H), 2.83 (s, 4H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 145.6, 138.6, 135.8, 135.3, 129.0, 128.3, 121.2, 108.9, 108.1, 100.7, 37.8, 37.7, 21.0. Data in accordance with the literature.[1]

5-(2-([1,1'-biphenyl]-4-yl)ethyl)benzo[d][1,3]dioxole (5m)



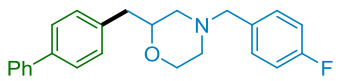
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 5:1 hexane: toluene) in 51% yield (31.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.1 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 2H), 6.77 – 6.68 (m, 2H), 6.64 (dd, *J* = 7.9, 1.6 Hz, 1H), 5.92 (s, 2H), 2.96 – 2.82 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 145.7, 141.0, 140.7, 138.9, 135.6, 128.9, 128.7, 127.1, 127.0, 127.0, 121.2, 108.9, 108.1, 100.8, 37.8, 37.6. IR (ATR): $\tilde{\upsilon}$ = 3032, 2922, 2857, 1481, 1246, 1187, 1041, 1003, 923, 822, 751, 689 cm^{-1}. HRMS (ESI) for $C_{21}H_{18}O_2$: calculated for $[M+Na]^+$ 325.11990, found 325.12054.

3-(2-(benzo[d][1,3]dioxol-5-yl)ethyl)pyridine (5n)



According to the general procedure, the title compound was isolated as a light yellow oil after flash chromatography on silica gel (eluent: 50:1 to 2:1 hexane: EtOAc) in 67% yield (30.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 4.8 Hz, 1H), 8.38 (s, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.16 (dd, *J* = 7.7, 4.9 Hz, 1H), 6.68 (d, *J* = 7.9 Hz, 1H), 6.61 (s, 1H), 6.54 (d, *J* = 7.9 Hz, 1H), 5.89 (s, 2H), 2.89 – 2.78 (m, *J* = 4.3 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.9, 147.6, 147.4, 145.9, 136.7, 136.0, 134.5, 123.2, 121.3, 108.8, 108.2, 100.8, 37.1, 35.1. Data in accordance with the literature.[31]

2-([1,1'-biphenyl]-4-ylmethyl)-4-(4-fluorobenzyl)morpholine (5o)

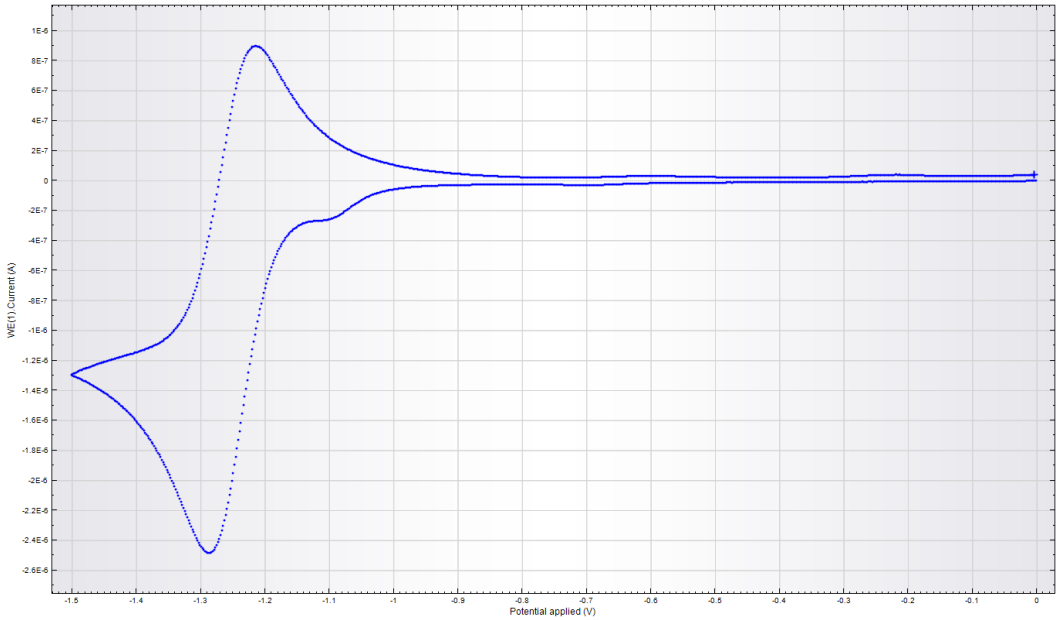


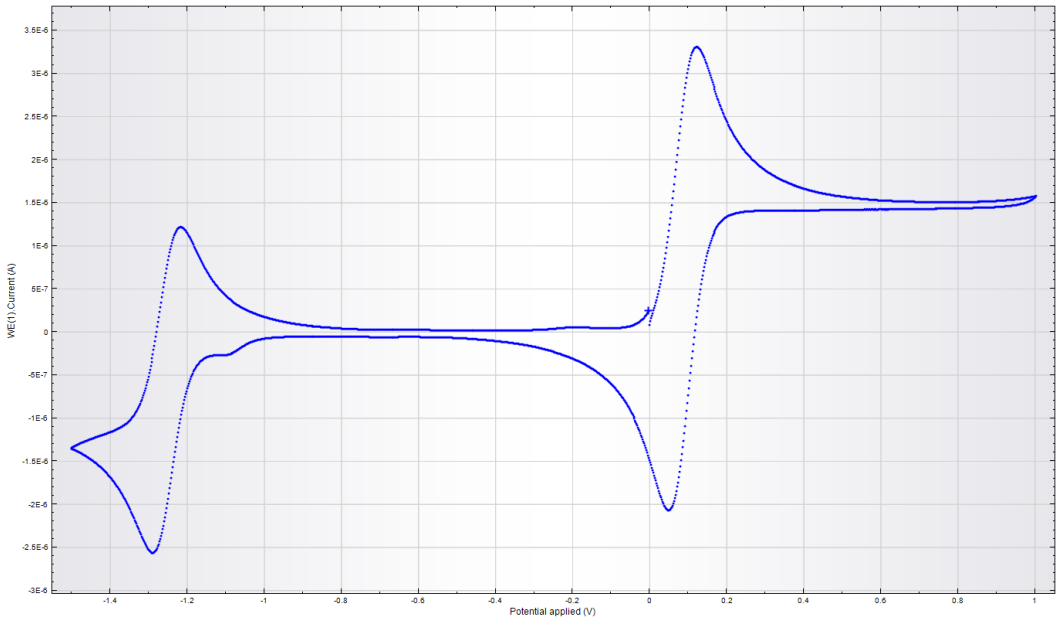
According to the general procedure, the title compound was isolated as a white solid after flash chromatography on silica gel (eluent: 50:1 to 5:1 hexane: EtOAc) in 25% yield (18.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.54 (m, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.16 (m, 5H), 6.98 (t, *J* = 8.7 Hz, 2H), 3.89 – 3.72 (m, 2H), 3.62 (td, *J* = 11.3, 2.3 Hz, 1H), 3.53 – 3.33 (m, 2H), 2.86 (dd, *J* = 13.9, 7.3 Hz, 1H), 2.80 – 2.66 (m, 2H), 2.59 (d, *J* = 11.2 Hz, 1H), 2.13 (td, *J* = 11.3, 3.1 Hz, 1H), 1.97 (t, *J* = 10.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.0 (d, *J* = 244.8 Hz), 141.0, 139.2, 137.2, 133.5 (d, *J* = 3.0 Hz), 130.6 (d, *J* = 7.8 Hz), 129.6, 128.7, 127.0, 127.0, 115.0 (d, *J* = 21.2 Hz), 76.5, 66.9, 62.4, 58.4, 52.7, 39.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.75. IR (ATR): $\tilde{\upsilon}$ = 3032, 2960, 2857, 1725, 1672, 1508, 1447, 1260, 1220, 1094, 1027, 804, 756, 694 cm^{-1}. HRMS (ESI) for $C_{24}H_{24}ONF$: calculated for $[M+H]^+$ 362.19147, found 362.19174.

6. Cyclic Voltammetry Measurement of Katritzky Salt

Cyclic voltammograms were taken on PGSTAT101 from Metrohm Autolab using a platinum working electrode, a Ag^{+}(0.01 M $AgNO_3$, 0.1 M NBu_4PF_6, CH_3CN)/Ag as reference electrode, a platinum wire counter electrode and 0.1 M NBu_4PF_6 as supporting electrolyte. The solution was prepared in CH_3CN and degassed with argon bubbling for 20 min prior to voltammetric studies. The scan rate was 50 mV/s. The potentials were given relative to the Fc/Fc^{+} redox couple with ferrocene as internal standard. For conversion to SCE as reference, it is known that SCE is 400 mV more negative than Fc/Fc^{+} in MeCN with NBu_4PF_6 as supporting electrolyte.[32]

We chose 1-cyclohexyl-2,4,6-triphenylpyridin-1-ium tetrafluoroborate salt as model Katritzky salt. The concentration of it was 10 mM. The scan direction was negative. We first measured the CV of our substrate alone, then measured the CV of our substrate together with internal standard ferrocene.





The reversible peaks at -1.29 V and -1.22 V correspond to the reduction of Katritzky salt. The reversible peaks at 0.12 V and 0.05 V correspond to the Fc/Fc^+ couples.
$E_{1/2}$(substrate) = -1.25 V
$E_{1/2}(Fc/Fc^+)$ = +0.085 V

E_{red}(substrate) = -1.34 V v. Fc/Fc^+
E_{red}(substrate) = -0.94 V v. SCE

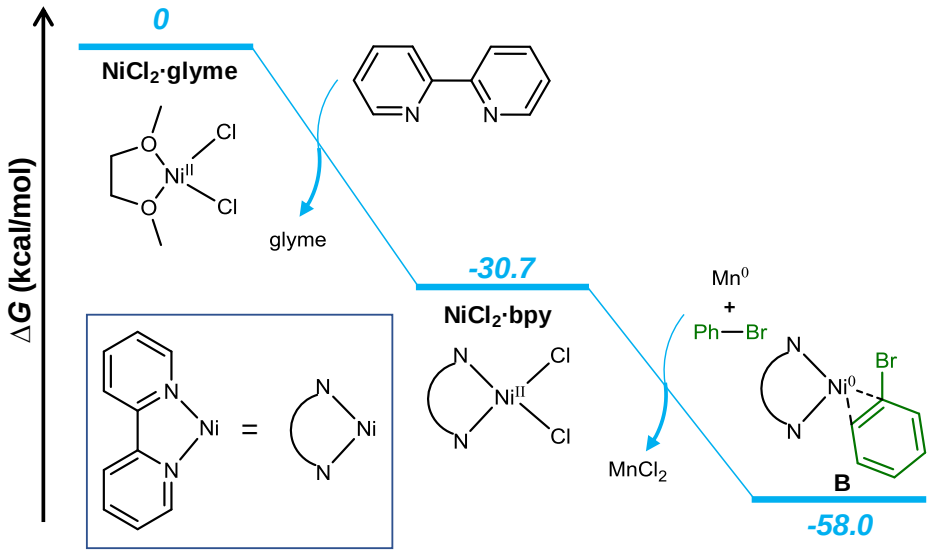
7. Computational Methods and Details

7.1 Computational methods

All DFT-calculations were performed using Gaussian 09, Revision D.01.[33] The geometry optimization and frequency analysis were performed using meta-hybrid-GGA DFT functional ωB97xD.[34] The split-valence plus one polarization function Def2-SVP basis set was used for non-metal atoms and the triple-ζ basis set Def2-TZVP was used for metals (Ni and Mn).[35] In all cases, the default integral grid (Fine Grid) was employed. Frequency calculations were performed in order to obtain thermal corrections (298 K) and to confirm the nature of the stationary points (minima with no imaginary frequency or transition states with one imaginary frequency). All transition states were optimized using the default Berny algorithm implemented in the Gaussian 09 code.[33] For transition state structures, IRC calculations were undertaken to confirm that the transition states were connected to the correct minima. For further validation of energetics, single-point calculations were performed on the ωB97xD/Def2-SVP optimized geometries using meta-hybrid GGA functional M06[36] employing a valence quadruple-ζ-type of basis set Def2-QZVPP[35] for all atoms. The solvent effects (n,n-DiMethylAcetamide (DMA): ε=37.781) were evaluated implicitly by a self-consistent reaction field (SCRF) approach for all the intermediates and transition states, using the SMD continuum solvation model.[37] Unless specified otherwise, ΔG was used throughout the text. The ΔG value was obtained by augmenting the E_{el} energy terms at M06(SMD-DMA)/Def2-QZVPP with the respective free energy corrections at the ωB97xD/Def2-TZVP(Ni,Mn)/Def2-SVP(non-metal) level in gas phase. The wavefunction analysis were performed using Multiwfn 3.6 dev.b.[38] VMD was used to visualize the orbitals.[39] The geometries were realized using CYLview, 1.0b.[40]

7.2 Generation of Ni^0 active catalyst B

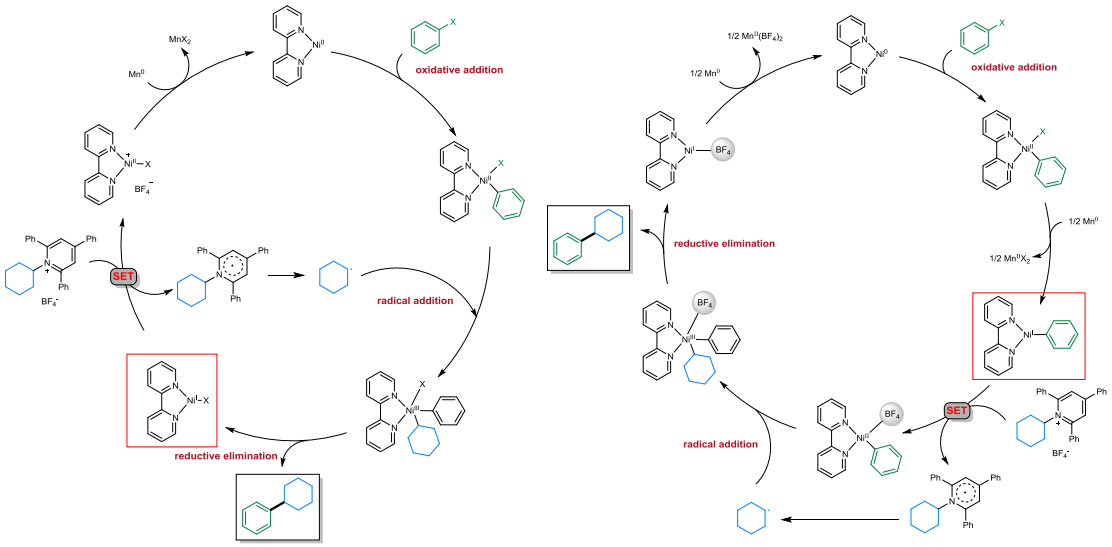
In this reaction, Ni^{II} pre-catalyst $NiCl_2$·glyme was used. First, it complexes with ligand bpy and glyme is liberated with a free energy gain of 30.7 kcal/mol. Next, the Ni^{II} complex is reduced by Mn to form the Ni^0 active catalyst H3 with a free energy gain of 58.0 kcal/mol.



Scheme S1: Generation of Ni^0 active catalyst B

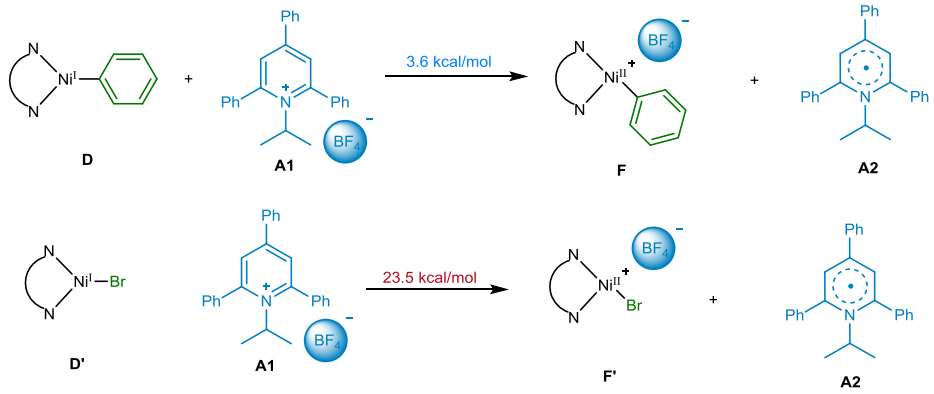
7.3 SET reduction of Katritzky salt

Two possible mechanisms were initially proposed (**Scheme S2**).



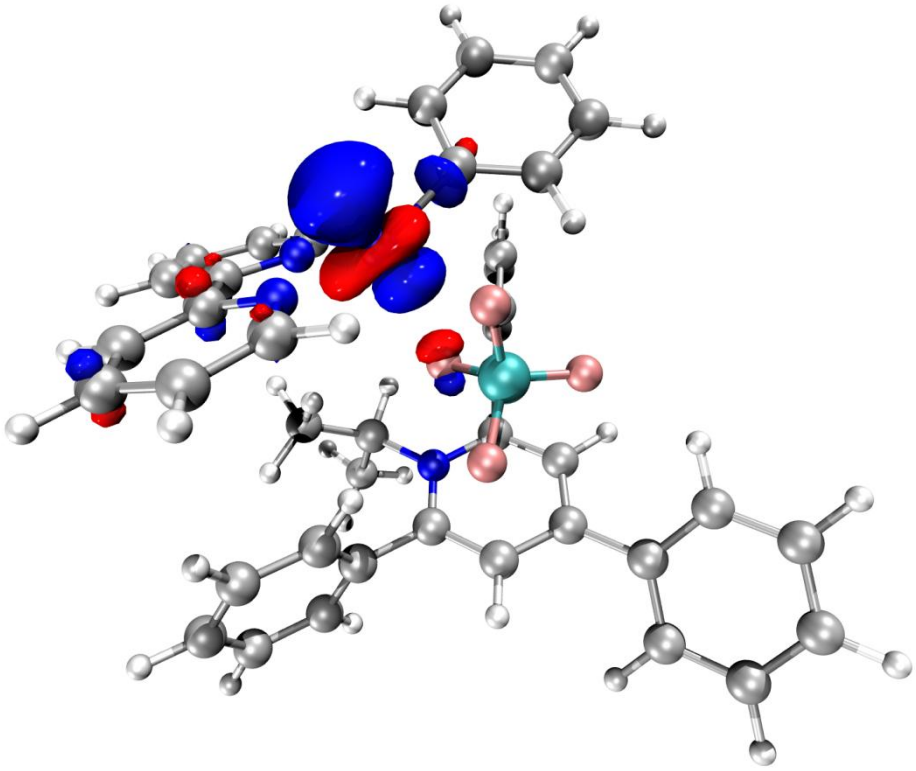
Scheme S2: Two possible catalytic cycles

The main difference was the SET reduction of Katritzky salt. In order to figure out this process, DFT calculations were performed for both possible pathways (**Scheme S3**). The results showed that the SET reduction of Katritzky salt by Ni^{I}-aryl is clearly favored.

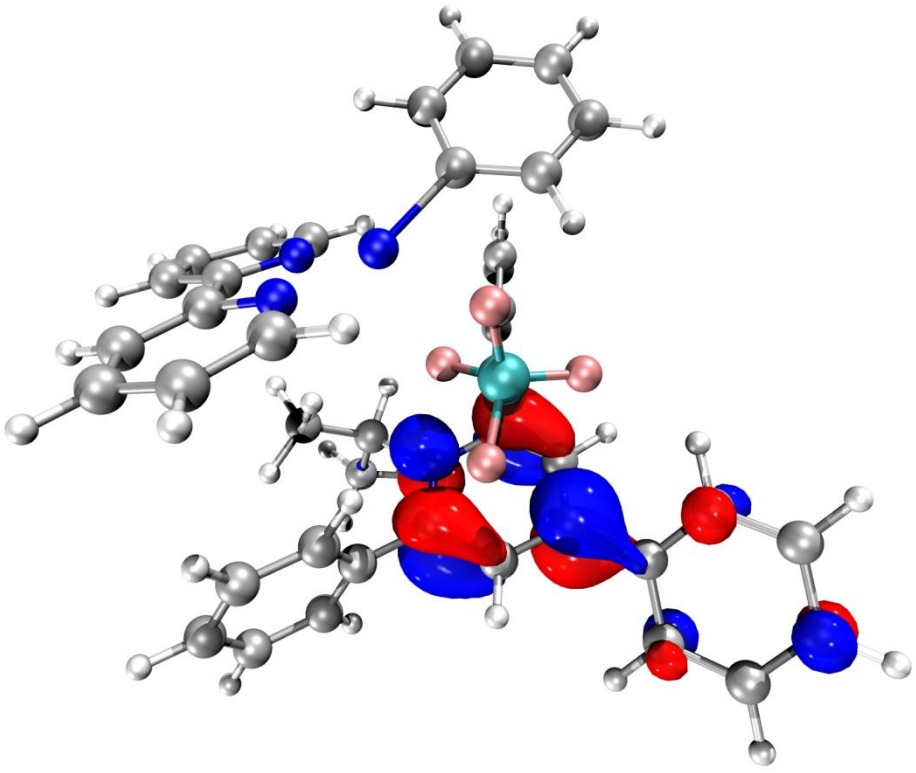


Scheme S3: SET reduction of Katritzky salt by Ni^{I}-aryl or Ni^{I}-Br

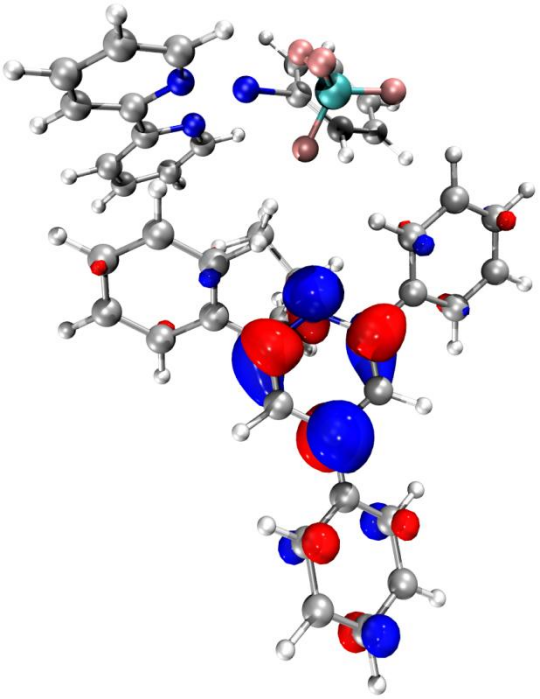
7.4 Molecular orbital plots of E and Eb



SOMO of E

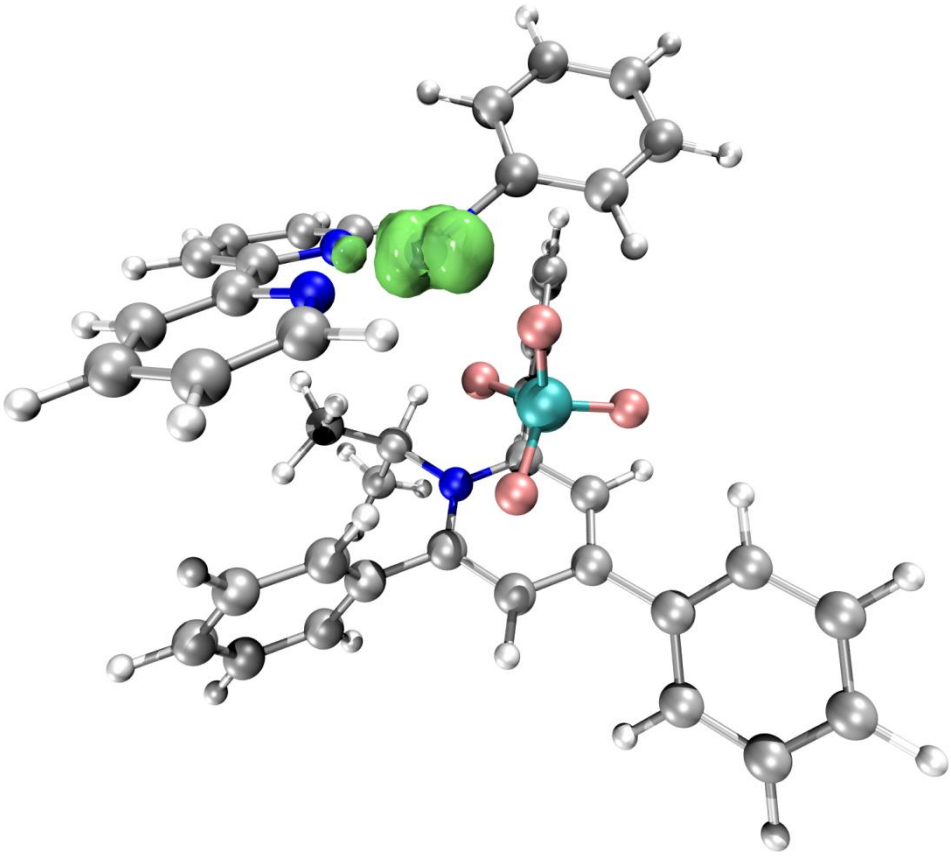


LUMO of E

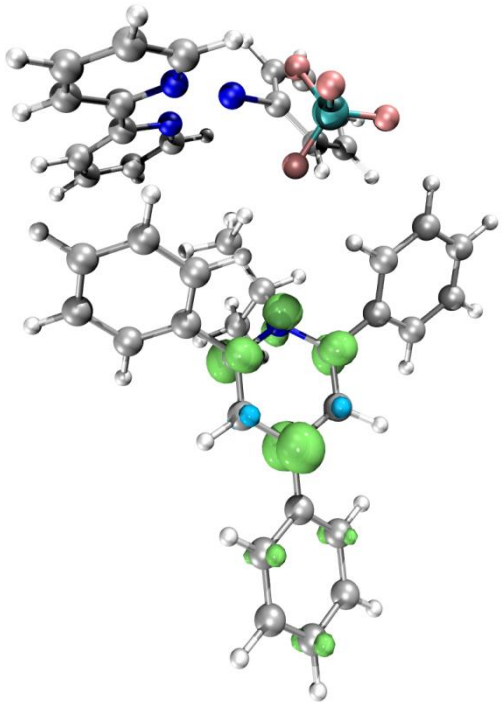


SOMO of Eb

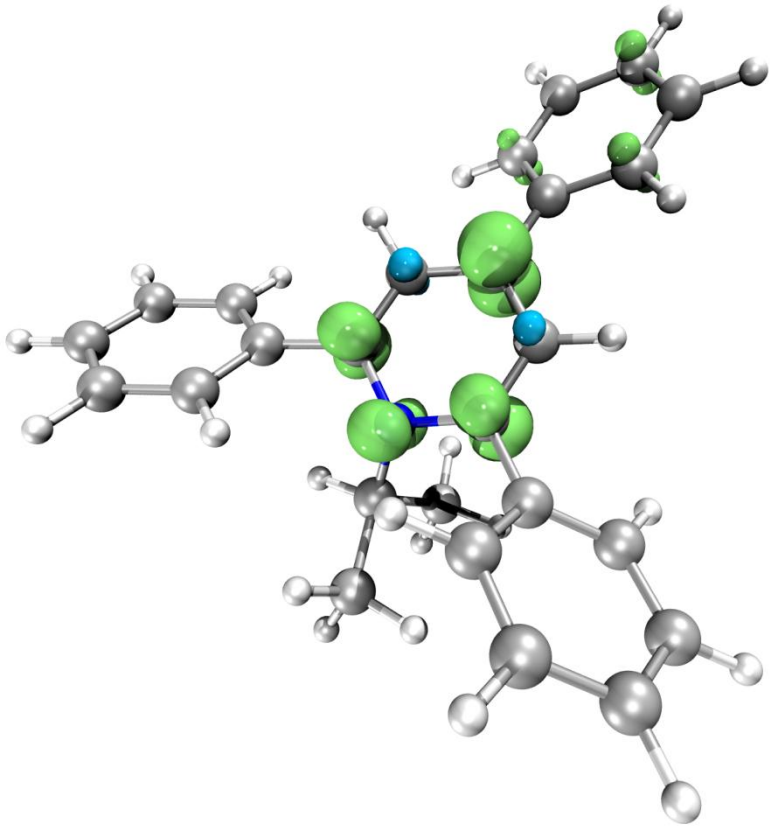
7.5 Spin density plots of E, Eb and A2TS



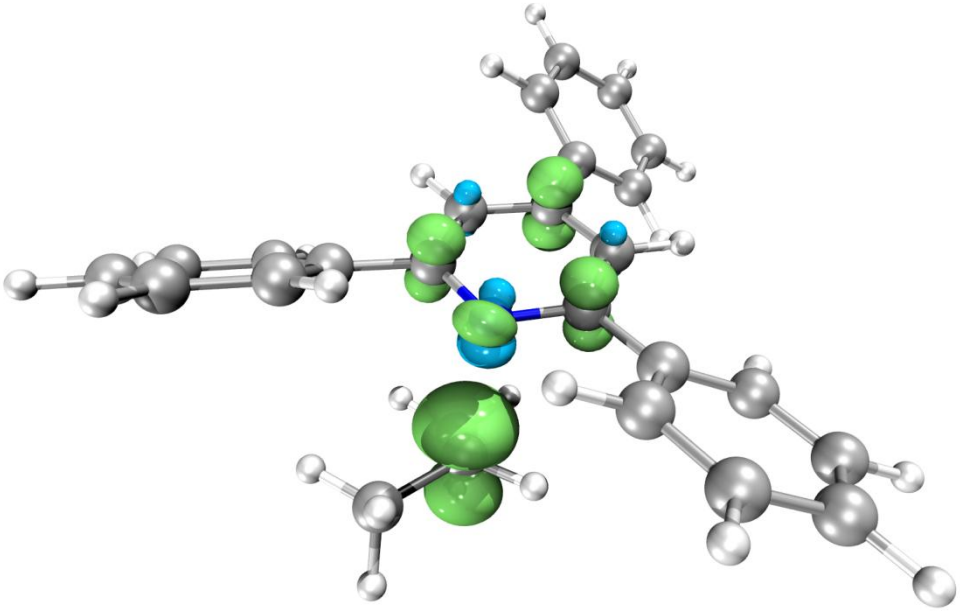
Spin density of E



Spin density of Eb

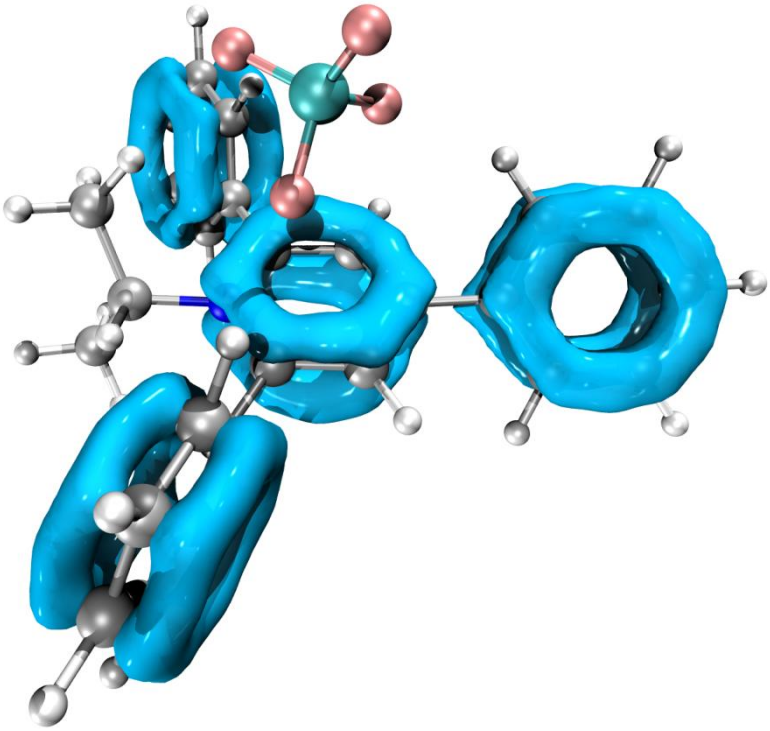


Spin density of A2

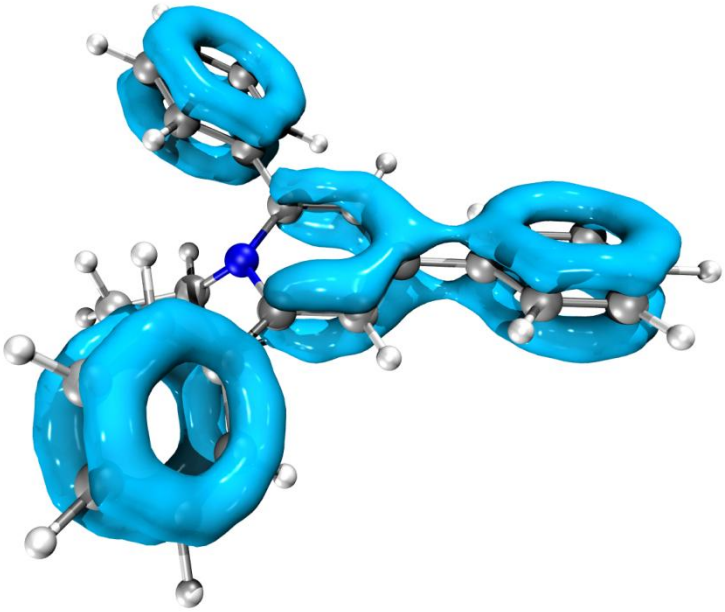


Spin density of A2TS

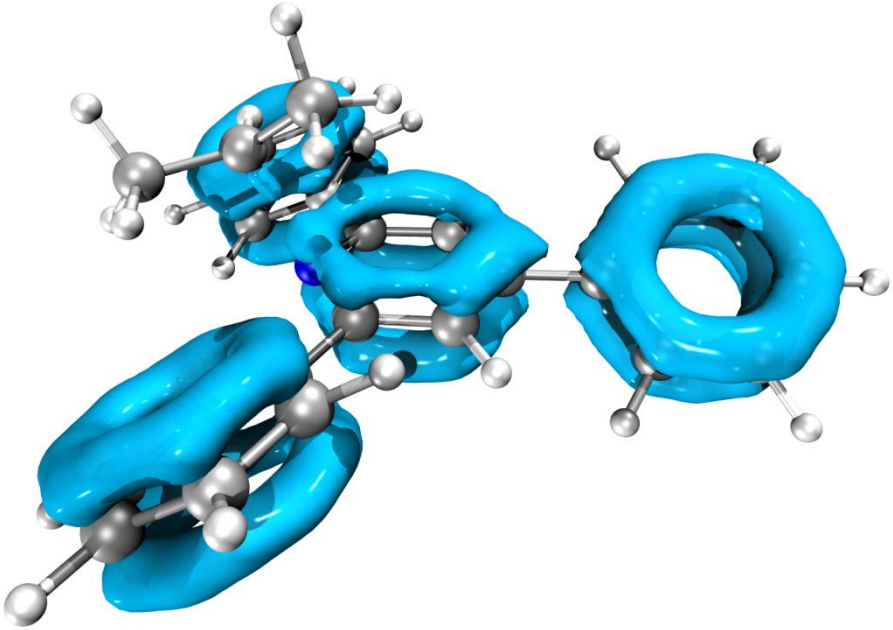
7.6 Localized orbital locator (LOL) – π plots of A1, A2, A2TS, and A3



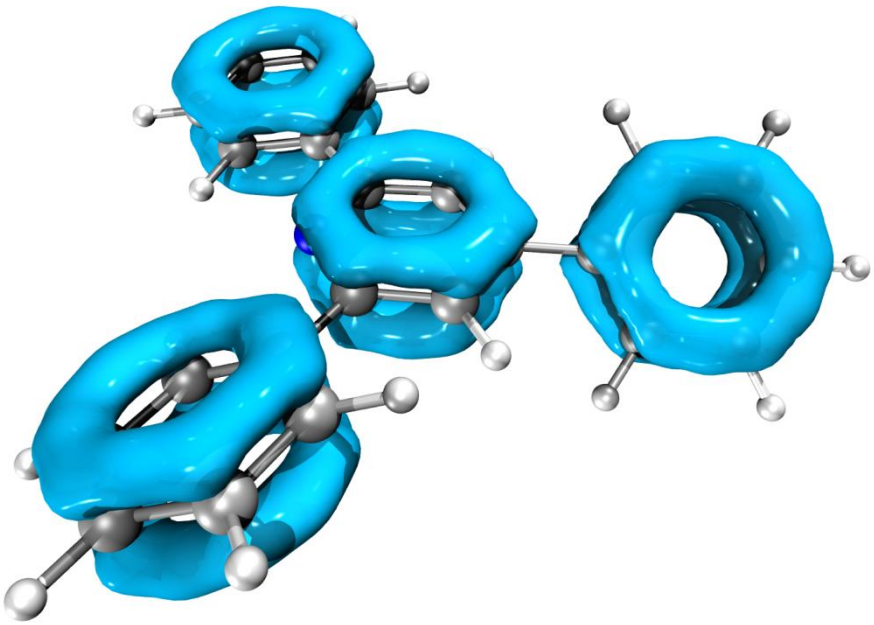
LOL – π plots of A1 (iso=0.4)



LOL – π plots of A2 (iso=0.4)



LOL – π plots of A2TS (iso=0.4)



LOL – π plots of A3 (iso=0.4)

7.7 Multi-center bond order of the central nitrogen-containing aromatic ring from A1, A2, A2TS and A3

```
 Input atom indices, e.g. 3,4,7,8,10   (2~12 centers)
 Input -3/-4/-5/-6 can search all possible three/four/five/six-center bonds
 Input 0 can return to upper level menu
16,10,12,13,11,9
 The multicenter bond order:    0.0526046522
 The normalized multicenter bond order:    0.6121211126
```

Multicenter bond order of A1: 0.053

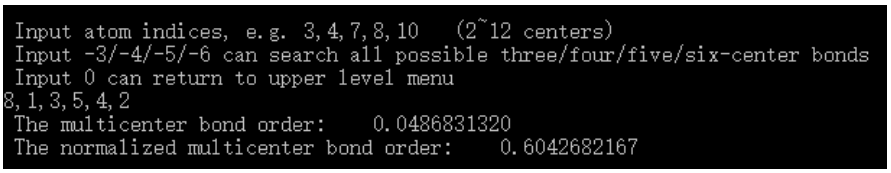
```
 Input atom indices, e.g. 3,4,7,8,10   (2~12 centers)
 Input -3/-4/-5/-6 can search all possible three/four/five/six-center bonds
 Input 0 can return to upper level menu
16,9,11,13,12,10
 The multicenter bond order from alpha density matrix:   -0.0000001
 The multicenter bond order from beta density matrix:     0.0005176
 The sum of multicenter bond order from alpha and beta parts:        0.0005174
 Above result in normalized form:    0.2833416
 The multicenter bond order from mixed alpha&beta density matrix:    0.0000451
 Above result in normalized form:    0.1886906
```

Multicenter bond order of A2: 0.00005

```
Please wait...

 Input atom indices, e.g. 3,4,7,8,10   (2~12 centers)
 Input -3/-4/-5/-6 can search all possible three/four/five/six-center bonds
 Input 0 can return to upper level menu
16,10,12,13,11,9
 The multicenter bond order from alpha density matrix:   -0.0004250
 The multicenter bond order from beta density matrix:     0.0215291
 The sum of multicenter bond order from alpha and beta parts:        0.0211041
 Above result in normalized form:    0.5256877
 The multicenter bond order from mixed alpha&beta density matrix:    0.0102500
 Above result in normalized form:    0.4660728
```

Multicenter bond order of A2TS: 0.01



Multicenter bond order of A3: 0.049

8. References

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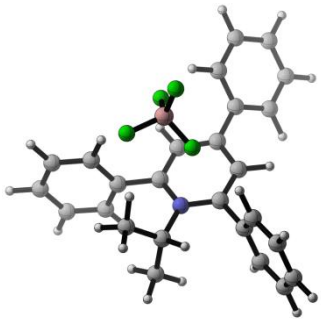
9. Cartesian Coordinates and Energies of Calculated Structures

A1:



E_{el} = -1484.184714
Zero-point correction = 0.450472
Thermal correction to Energy = 0.478675
Thermal correction to Enthalpy = 0.479619
Thermal correction to Gibbs Free Energy = 0.389735

C	3.04012700	-0.71817300	0.83380800
C	2.58671800	0.25314700	-0.25056000
C	3.42456100	0.20285800	-1.52181200
H	3.29218800	-1.70925500	0.43775400
H	2.28047100	-0.82463400	1.62104500
H	3.42513000	-0.79686100	-1.97430600
H	3.07796800	0.93526800	-2.26509900
H	2.70456500	1.25238000	0.17452300
C	0.42729100	1.37915300	-0.55644500
C	0.43390400	-0.96924900	-0.72460100
C	-0.94571400	1.40478100	-0.71448000
C	-0.94545600	-0.96323200	-0.83241200
C	-1.67631500	0.22244300	-0.80419800
H	-1.44709600	2.37146900	-0.66978900
H	-1.44880300	-1.92406100	-0.92773700
N	1.11161600	0.20004500	-0.55632900
C	1.11487900	-2.29141700	-0.81183700
C	1.04385200	-3.17176700	0.27384200
C	1.71093700	-2.69919200	-2.00898100
C	1.61960400	-4.43524100	0.16675600
H	0.57828500	-2.84025200	1.20477400
C	2.28303800	-3.96594400	-2.10773700
H	1.71577800	-2.02897500	-2.87188400
C	2.24445100	-4.83172900	-1.01573000
H	1.58009500	-5.11450300	1.02051500
H	2.75088400	-4.27957100	-3.04312600
H	2.69502100	-5.82372600	-1.09119800

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C	1.17174500	3.18480700	0.98789500
C	1.66998100	3.40190500	-1.37724600
C	1.78013600	4.41651500	1.21880100
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H	1.61124500	3.00756300	-2.39474900
C	2.33426200	5.13900600	0.16148900
H	1.81987000	4.81539000	2.23437700
H	2.70047900	5.20099800	-1.96714000
H	2.80947000	6.10415400	0.34906200
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C	-3.86283400	1.09588900	-1.65922000
C	-3.84973900	-0.66536100	0.00639100
C	-5.25478800	1.07794000	-1.66816200
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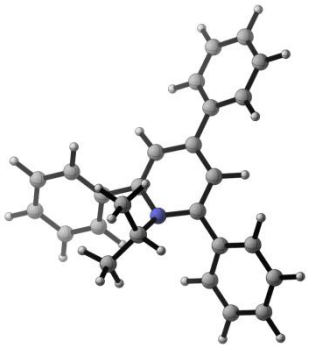
C	-5.24226500	-0.66853600	0.00115600
H	-3.28606900	-1.30058800	0.69410000
C	-5.94581200	0.19511700	-0.83801300
H	-5.80353800	1.75515600	-2.32582400
H	-5.78178500	-1.34476100	0.66713100
H	-7.03794600	0.18566400	-0.84084700
H	4.46364100	0.45198400	-1.26272100
H	3.94939400	-0.29760700	1.28766100
F	-0.03167400	0.47923900	2.00387600
B	-0.46066300	-0.68765400	2.70169400
F	-1.37099800	-1.38898700	1.87183300
F	-1.04763500	-0.34231000	3.89364500
F	0.66981100	-1.50748800	2.89589700

A2:



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Thermal correction to Enthalpy = 0.454142
Thermal correction to Gibbs Free Energy = 0.377320

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C	1.97209000	0.32000700	1.35588100
C	3.38097200	-0.20733200	1.10356000
H	1.28899400	-1.33534200	2.60373800
H	0.36134600	0.17418100	2.81146200
H	3.43278000	-1.30376300	1.12115500
H	3.77066300	0.14296300	0.13758700
H	2.06397700	1.40710000	1.47930600
C	0.18116600	1.27516800	-0.01151400
C	0.44107900	-1.10612300	0.01037300
C	-1.17880900	1.12343900	-0.10182900
C	-0.91564300	-1.25848400	-0.07800000
C	-1.80609400	-0.14950800	-0.05111600
H	-1.77368400	2.01036500	-0.32685900
H	-1.29530000	-2.26922300	-0.23495900
N	1.01569900	0.16223100	0.21896000
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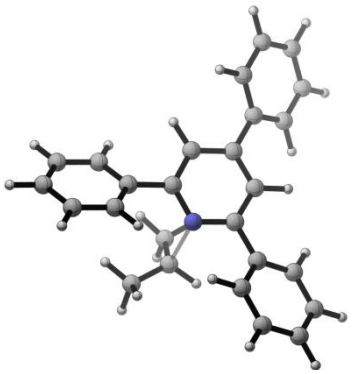
C	1.18339200	-3.45744600	0.49887100
C	2.36611300	-2.17365900	-1.16577700
C	2.02018800	-4.54523200	0.25166300
H	0.39957800	-3.52913800	1.25707100
C	3.19908200	-3.25877500	-1.41305700
H	2.49494500	-1.24088700	-1.71883600
C	3.03129400	-4.44912600	-0.70237500
H	1.88313900	-5.47265300	0.81207800
H	3.98299100	-3.17993700	-2.16955800
H	3.68816200	-5.30018100	-0.89441800
C	0.84192200	2.57966700	-0.22402600
C	0.26564600	3.77491000	0.23337200
C	2.06593200	2.65064300	-0.91038300
C	0.88437400	5.00004500	-0.00073900
H	-0.66954400	3.73919900	0.79675400
C	2.68495700	3.87512700	-1.13959300
H	2.52142000	1.72746400	-1.27458000
C	2.09685100	5.05678600	-0.68740500
H	0.42083900	5.91780500	0.36785900
H	3.63288800	3.90864500	-1.68140800
H	2.58413600	6.01769800	-0.86522700
C	-3.26519000	-0.30057700	-0.09526300
C	-4.11321700	0.73503800	0.34557900
C	-3.87692200	-1.47623600	-0.57357500
C	-5.49764800	0.60490000	0.30310100
H	-3.67958600	1.65004100	0.75456500
C	-5.26102100	-1.60609700	-0.61280000

H	-3.26173800	-2.29684700	-0.94703100
C	-6.08303300	-0.56659700	-0.17655400
H	-6.12671000	1.42477400	0.65771000
H	-5.70363200	-2.52728900	-0.99889300
H	-7.16956900	-0.67008500	-0.20950300
H	4.04564900	0.17247400	1.89431600
H	1.99889800	0.02584300	3.50480100

A2TS:



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Thermal correction to Gibbs Free Energy = 0.371684

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C	-1.98387500	0.27635400	1.68317700
C	-0.97710800	-0.30500700	2.61907700
H	-3.24650400	-1.46760100	1.49287700
H	-3.86549400	-0.00592700	0.67864400
H	-0.86350200	-1.39014300	2.46576500
H	0.00906200	0.16951300	2.49460200
H	-2.01080000	1.37045900	1.65776600
C	-0.22408300	1.23949200	-0.25188300
C	-0.39838400	-1.08470300	-0.25305300
C	1.16281900	1.15964200	-0.21980200
C	0.98347100	-1.21949400	-0.22395100
C	1.80919500	-0.08619500	-0.18020900
H	1.75468800	2.07185100	-0.31021700
H	1.42282500	-2.21742000	-0.26890900
N	-1.01217900	0.12803900	-0.18283400
C	-1.28768900	-2.26855100	-0.35086300
C	-2.47529700	-2.18783500	-1.09113800
C	-0.97795800	-3.47436500	0.29203500
C	-3.32835000	-3.28235400	-1.18654000
H	-2.72056500	-1.24557400	-1.58390500

C	-1.83485600	-4.56947900	0.20117300
H	-0.06888800	-3.54918100	0.89377200
C	-3.01328900	-4.47726100	-0.53767700
H	-4.24917300	-3.20343900	-1.76880200
H	-1.58460500	-5.49809400	0.71888400
H	-3.68750100	-5.33379400	-0.60586400
C	-0.93479100	2.53783500	-0.35938600
C	-2.22162700	2.58116000	-0.91667300
C	-0.36672200	3.73585300	0.09829900
C	-2.90996300	3.78547100	-1.02860000
H	-2.67042800	1.64915800	-1.26370900
C	-1.05654400	4.94045200	-0.01191600
H	0.61785700	3.72743700	0.57049800
C	-2.33024200	4.97157000	-0.57856500
H	-3.90711800	3.79937100	-1.47434100
H	-0.59875700	5.86074000	0.35755800
H	-2.87020200	5.91692700	-0.66491200
C	3.28499100	-0.19661900	-0.14195600
C	4.05502600	0.72563400	0.58358800
C	3.95290900	-1.22726000	-0.82177700
C	5.44294300	0.61975000	0.63015300
H	3.55671100	1.52317800	1.13976100
C	5.34009200	-1.33380400	-0.77474400
H	3.37880400	-1.94128100	-1.41646700
C	6.09194600	-0.41149400	-0.04734500
H	6.02159600	1.34296700	1.20914600
H	5.83878700	-2.14040300	-1.31688900
H	7.17995300	-0.49707200	-0.00829100
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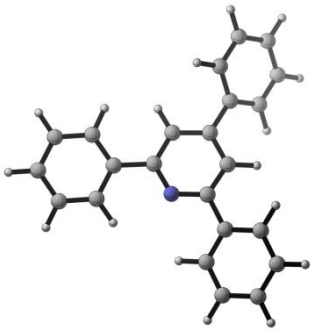
H	-1.28411000	-0.15540900	3.67106400

A4:



E_{el} = -941.159175

Zero-point correction = 0.335549

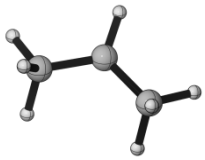
Thermal correction to Energy = 0.353545

Thermal correction to Enthalpy = 0.354490

Thermal correction to Gibbs Free Energy = 0.287195

C	0.61777200	1.16387300	-0.01161700
C	0.63072200	-1.14783200	-0.05074400
C	-0.78213500	1.19056300	0.00835100
C	-0.76770800	-1.20002400	-0.02678100
C	-1.49653200	-0.00943400	0.00426200
H	-1.32275300	2.13461300	0.07009400
H	-1.28749200	-2.15861400	-0.02640000
N	1.28893700	0.01096100	-0.03328600
C	1.45505600	-2.38989000	-0.08014200
C	2.75859000	-2.36812400	0.43261000
C	0.96358800	-3.58762700	-0.61511600
C	3.54214800	-3.51826900	0.42811200
H	3.14465700	-1.43237100	0.83913200
C	1.75043400	-4.73750500	-0.62603900
H	-0.03547400	-3.62341200	-1.05469900
C	3.04075300	-4.70807700	-0.10009300
H	4.55263100	-3.48607000	0.84153600
H	1.35378800	-5.65979900	-1.05602300
H	3.65682000	-5.61004900	-0.10638500
C	1.43564700	2.41422100	0.00339300
C	2.82296000	2.32661300	0.18284900
C	0.86519300	3.68356200	-0.16270400
C	3.61294400	3.47192400	0.20754200
H	3.26802100	1.33834400	0.29964200
C	1.65563400	4.83034500	-0.14060000
H	-0.20811100	3.79420300	-0.32476800
C	3.03287100	4.72980300	0.04734600
H	4.69160800	3.38051600	0.35266600
H	1.19015900	5.80910700	-0.27531400
H	3.65221700	5.62935800	0.06527900
C	-2.98200900	-0.01803000	0.04630200
C	-3.72381100	0.88948900	-0.72182000
C	-3.66952300	-0.93343200	0.85458700
C	-5.11613200	0.88074600	-0.68404800
H	-3.20301100	1.59491000	-1.37363700
C	-5.06165200	-0.93887800	0.89605500
H	-3.10545700	-1.63268500	1.47623300
C	-5.78947500	-0.03276100	0.12584900
H	-5.67946800	1.58775200	-1.29681500
H	-5.58162200	-1.65176300	1.53956100
H	-6.88108200	-0.03831000	0.15757300

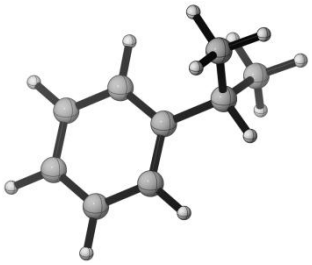
A3:



E_{el} = -118.432086
Zero-point correction = 0.088272
Thermal correction to Energy = 0.093428
Thermal correction to Enthalpy = 0.094373
Thermal correction to Gibbs Free Energy = 0.061040

C	-1.29569800	-0.19778100	0.00302200
H	-1.30562000	-1.05198500	-0.69694200
H	-1.49036200	-0.62460900	1.00866600
H	-2.14843500	0.45263900	-0.24075600
C	0.00000000	0.53393500	-0.04722600
H	0.00000000	1.61767600	0.10516000
C	1.29569800	-0.19778100	0.00302200
H	2.14843500	0.45264000	-0.24075200
H	1.49036000	-0.62461300	1.00866500
H	1.30562200	-1.05198200	-0.69694500

A5:



E_{el} = -350.072391
Zero-point correction = 0.186361
Thermal correction to Energy = 0.194873
Thermal correction to Enthalpy = 0.195817
Thermal correction to Gibbs Free Energy = 0.152868

C	-0.14067800	-0.19917300	0.00000300
C	0.74914400	-1.27793200	-0.00006400
C	0.39386900	1.09621500	0.00000300
C	2.12934100	-1.07496400	-0.00004800
H	0.35288800	-2.29733400	-0.00018300
C	1.77072700	1.30533600	0.00004600
H	-0.27716900	1.95967200	-0.00001800
C	2.64571800	0.21865700	0.00004800
H	2.80464500	-1.93378200	-0.00010700

H	2.16501000	2.32426900	0.00003200
H	3.72570100	0.38155000	0.00011100
C	-1.64274000	-0.42779800	-0.00001200
H	-1.80052200	-1.51947600	-0.00009400
C	-2.29885300	0.13139100	1.26680100
H	-1.84598500	-0.30018000	2.17163400
H	-2.18551500	1.22561700	1.32524100
H	-3.37674800	-0.09311000	1.28100000
C	-2.29885700	0.13156700	-1.26676900
H	-1.84616000	-0.30011000	-2.17163300
H	-3.37680800	-0.09270300	-1.28088000
H	-2.18536000	1.22578700	-1.32514900

Mn:

E_{el} = -1150.810406

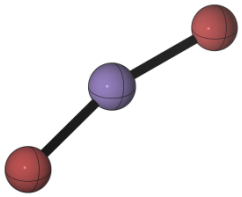
Zero-point correction = 0.000000

Thermal correction to Energy = 0.001416

Thermal correction to Enthalpy = 0.002360

Thermal correction to Gibbs Free Energy = -0.016317

$MnBr_2$:



E_{el} = -6299.192095

Zero-point correction = 0.001574

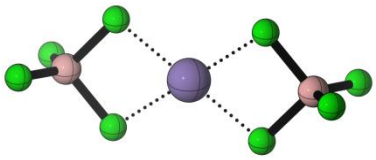
Thermal correction to Energy = 0.006069

Thermal correction to Enthalpy = 0.007014

Thermal correction to Gibbs Free Energy = -0.029808

Mn	0.00000000	0.21480900	0.00000000
Br	2.21557200	-0.08155800	0.00000000
Br	-2.21557200	-0.07187700	0.00000000

$Mn(BF_4)_2$:



E_{el} = -1999.974931

Zero-point correction = 0.031434

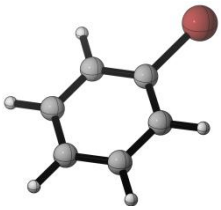
Thermal correction to Energy = 0.042720

Thermal correction to Enthalpy = 0.043664

Thermal correction to Gibbs Free Energy = -0.010427

Mn	0.00000300	0.00004900	-0.00000300
F	-1.57706800	-0.00020300	-1.11701300
B	-2.61995800	-0.00001700	-0.00003700
F	-1.57701500	0.00016100	1.11696900
F	-3.27781100	1.15239400	-0.00019200
F	-3.27783000	-1.15241300	0.00018600
B	2.61998500	-0.00002500	0.00014600
F	3.27793200	1.15231600	0.00018300
F	1.57715400	-0.00013500	1.11702800
F	1.57691200	0.00027400	-1.11696800
F	3.27770200	-1.15250600	-0.00024400

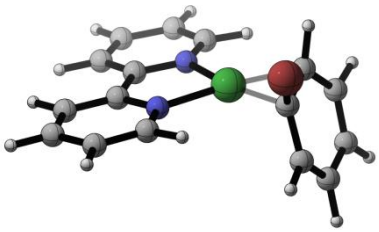
Ph-Br:



E_{el} = -2805.686887
Zero-point correction = 0.091512
Thermal correction to Energy = 0.097156
Thermal correction to Enthalpy = 0.098100
Thermal correction to Gibbs Free Energy = 0.060677

C	0.09188500	-0.00005900	-0.00000300
C	0.77856500	1.21353900	-0.00002000
C	2.17277300	1.20595200	0.00000300
C	2.87235800	0.00000100	-0.00000100
C	2.17287500	-1.20589300	-0.00000500
C	0.77856800	-1.21354500	0.00000800
H	0.22805600	2.15537500	0.00001300
H	2.71348600	2.15437600	0.00004100
H	3.96397300	0.00011100	0.00002400
H	2.71350900	-2.15436200	-0.00001600
H	0.22822100	-2.15547500	0.00000400
Br	-1.80141100	0.00000000	0.00000100

B:

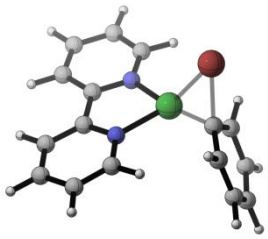


E_{el} = -4809.306149
Zero-point correction = 0.253021
Thermal correction to Energy = 0.270180
Thermal correction to Enthalpy = 0.271124
Thermal correction to Gibbs Free Energy = 0.205407

C	-2.65662400	-0.17153000	-0.10378000
C	-4.00576400	-0.52495700	-0.14203900
C	-4.35091300	-1.84251300	-0.42721400
C	-3.34010900	-2.77095100	-0.66014600
C	-2.01799700	-2.34190500	-0.60418000
N	-1.68665400	-1.07600200	-0.33908000
H	-5.40065300	-2.13988900	-0.46262800
H	-4.78161500	0.21506100	0.05324200
H	-3.56514900	-3.81510400	-0.88019800
H	-1.18359200	-3.02700200	-0.76882400
C	-2.16015800	1.19681700	0.20016000
C	-2.98653800	2.29724600	0.42839200
N	-0.81887700	1.30444400	0.23867900
C	-2.40445200	3.53212900	0.69885600
H	-4.07130000	2.19857800	0.39173200
C	-0.25928100	2.49046500	0.48926300
C	-1.01646200	3.63327200	0.72839200
H	-3.03128200	4.40713900	0.88062900
H	0.83369000	2.51336300	0.48014500
H	-0.51934700	4.58284900	0.92944800
Ni	0.14501700	-0.37909800	-0.13973600
C	2.42242100	-1.50680800	2.18665200
C	2.42020500	-0.34213800	1.47108800
C	1.99896600	-0.31694500	0.08768300
C	1.60923900	-1.58785500	-0.52903500
C	1.75678100	-2.79501000	0.24814700
C	2.10866600	-2.75861300	1.56773300
H	2.70604500	-1.48551600	3.24203200
H	2.74014900	0.59230500	1.93935400
H	1.67539000	-1.69151400	-1.61897900
H	1.60769500	-3.75884800	-0.24910100
H	2.19810500	-3.68256000	2.14353400

Br	2.90177700	1.05607300	-1.00870900

B-TS:

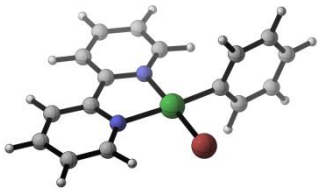


E_{el} = -4809.286882
Zero-point correction = 0.252164
Thermal correction to Energy = 0.269055
Thermal correction to Enthalpy = 0.270000
Thermal correction to Gibbs Free Energy = 0.204723

C	2.54014800	-0.18003800	-0.20642500
C	3.88361300	-0.55349500	-0.30375800
C	4.20320100	-1.86851500	-0.61661400
C	3.17040900	-2.78195400	-0.82163600
C	1.85996400	-2.33708300	-0.70786200
N	1.54820800	-1.06931000	-0.41168200
H	5.24692200	-2.17804800	-0.69601200
H	4.67512000	0.17435100	-0.12709900
H	3.37220000	-3.82579000	-1.06464200
H	1.01685100	-3.01507700	-0.85620900
C	2.08935400	1.19271500	0.12808000
C	2.95437900	2.28411700	0.24842600
N	0.76049000	1.32389300	0.29820100
C	2.42866600	3.53340100	0.55506900
H	4.02674200	2.16514100	0.09479800
C	0.25749000	2.52759700	0.58265800
C	1.05123800	3.65913900	0.72611200
H	3.08628500	4.39927500	0.65164800
H	-0.82965000	2.57573800	0.68591200
H	0.59232600	4.62006300	0.96223600
Ni	-0.28108500	-0.38599200	-0.10373900
C	-3.37801600	1.68543100	-1.00424800
C	-2.83549700	1.08793100	0.11331200
C	-2.06723700	-0.09673900	-0.05549700
C	-2.04374500	-0.77753400	-1.31418700
C	-2.60771000	-0.11533500	-2.42903900
C	-3.23928200	1.10640500	-2.28833400
H	-3.92483300	2.62610700	-0.89526700
H	-2.95448600	1.52493200	1.10726200
H	-1.81792500	-1.84307700	-1.38559600

H	-2.59152900	-0.60928700	-3.40462700
H	-3.68725600	1.59704100	-3.15470200
Br	-1.83151800	-1.41091200	1.60414300

C:

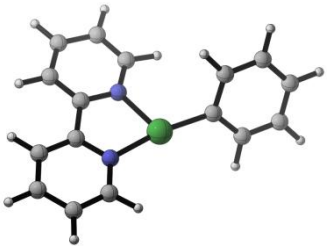


E_{el} = -4809.358426
Zero-point correction = 0.255102
Thermal correction to Energy = 0.272256
Thermal correction to Enthalpy = 0.273201
Thermal correction to Gibbs Free Energy = 0.207287

C	-1.67108100	1.73475600	-0.00014200
C	-2.17053400	3.03627400	-0.00029500
C	-1.28156700	4.10563500	-0.00044300
C	0.08208700	3.83906000	-0.00043000
C	0.50833600	2.51533800	-0.00028500
N	-0.34459400	1.48357400	-0.00015200
H	-1.65386100	5.13175400	-0.00057500
H	-3.24477700	3.21623000	-0.00032100
H	0.82217300	4.63953700	-0.00053800
H	1.56872300	2.26038100	-0.00027800
C	-2.53365500	0.52988800	0.00001600
C	-3.92766000	0.56833600	0.00029300
N	-1.85992000	-0.63245700	-0.00010200
C	-4.63199200	-0.63196500	0.00042400
H	-4.46220500	1.51752200	0.00043200
C	-2.53302400	-1.78445000	0.00001000
C	-3.92433800	-1.82870700	0.00026700
H	-5.72371800	-0.62761700	0.00066000
H	-1.90933200	-2.68432300	-0.00009600
H	-4.43421400	-2.79251400	0.00035900
Ni	0.15149600	-0.41821700	-0.00010100
Br	0.65307200	-2.66384100	-0.00018500
C	1.99854900	-0.05494500	0.00011900
C	2.69168100	0.15133100	-1.20125100
C	2.69127200	0.15131000	1.20173000
C	4.02117700	0.58010100	-1.20317300
H	2.19001000	-0.02565700	-2.15716100
C	4.02076500	0.58007900	1.20411400
H	2.18928400	-0.02569800	2.15747000

C	4.69003500	0.80293600	0.00058600
H	4.53994200	0.73545600	-2.15324700
H	4.53921300	0.73541600	2.15436400
H	5.73065700	1.13631600	0.00076900

D:

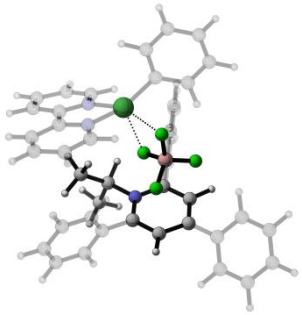


E_{el} = -2235.170751
Zero-point correction = 0.252271
Thermal correction to Energy = 0.268012
Thermal correction to Enthalpy = 0.268956
Thermal correction to Gibbs Free Energy = 0.205849

C	-1.84162700	1.14200700	-0.05648700
C	-2.58273000	2.32494400	-0.06683300
C	-1.90598600	3.53717500	-0.16720500
C	-0.51590900	3.53532700	-0.25649500
C	0.14957800	2.31294700	-0.23772100
N	-0.50295200	1.15531900	-0.13664800
H	-2.46217400	4.47652800	-0.17709200
H	-3.67048600	2.30847500	0.00131000
H	0.04870300	4.46475300	-0.33903400
H	1.23905300	2.23647800	-0.30074800
C	-2.42952800	-0.21958000	0.03421300
C	-3.79837200	-0.46990700	0.14022600
N	-1.52932100	-1.22379200	0.00363800
C	-4.24562200	-1.78472100	0.21221300
H	-4.51251000	0.35282900	0.16760100
C	-1.96394500	-2.48736600	0.07157200
C	-3.31025500	-2.81578900	0.17523300
H	-5.31222900	-1.99964900	0.29807300
H	-1.19400200	-3.26169100	0.04428100
H	-3.61256000	-3.86224000	0.22894600
Ni	0.39062200	-0.68230200	-0.06563200
C	2.33772400	-0.54071300	0.00320200
C	2.95796800	0.31762800	0.93937400
C	3.22614400	-1.23984300	-0.84342000
C	4.34364900	0.47587200	1.02680200
H	2.33653500	0.88974400	1.63987100
C	4.61411700	-1.09752400	-0.76868500

H	2.82639400	-1.92583300	-1.59868300
C	5.18203100	-0.23506000	0.16890500
H	4.77217800	1.15456900	1.77086100
H	5.25890300	-1.66404200	-1.44755500
H	6.26728100	-0.11853900	0.23159000

E:



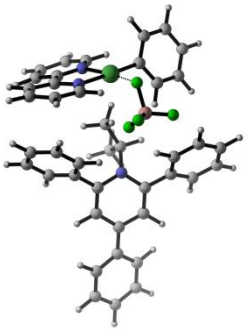
E_{el} = -3719.350453
Zero-point correction = 0.703032
Thermal correction to Energy = 0.748347
Thermal correction to Enthalpy = 0.749291
Thermal correction to Gibbs Free Energy = 0.621725

C	-3.62986700	1.25002700	-0.00173000
C	-4.53734000	1.73411200	0.97727400
C	-4.84847800	0.95820200	2.06753100
C	-4.25783500	-0.32386500	2.20270800
C	-3.41887300	-0.75881400	1.19798000
N	-3.11543700	-0.01817900	0.11989400
H	-5.54731900	1.32656100	2.82171100
H	-4.98561000	2.72148600	0.86230400
H	-4.47126200	-0.96583600	3.05751900
H	-2.95449900	-1.74816600	1.23299900
C	-3.14511700	2.00147300	-1.11972500
C	-3.44201200	3.36771000	-1.36741500
N	-2.30421700	1.31819200	-1.96919500
C	-2.87126200	4.01168600	-2.43742900
H	-4.11179400	3.90804000	-0.69774600
C	-1.74003600	1.97266300	-3.00352300
C	-1.98168800	3.29989100	-3.28206400
H	-3.09455600	5.06358300	-2.62913200
H	-1.06250200	1.37711100	-3.61938300
H	-1.50348400	3.77468300	-4.13899700
Ni	-1.94002300	-0.58624200	-1.41918400
F	0.02790000	-0.55910000	-2.95208900
B	0.91784100	-0.32091600	-1.89910000
F	1.78019700	-1.38648500	-1.70734200

F	1.59062300	0.87464300	-2.05934600
F	0.07647000	-0.20703500	-0.70613000
C	-2.06136800	-2.56808700	-1.43286900
C	-0.98441500	-3.41602200	-1.76251000
C	-3.25890600	-3.21785400	-1.07186000
C	-1.08323100	-4.80858400	-1.70825700
H	-0.02643700	-2.98149600	-2.06058800
C	-3.37638400	-4.60970400	-1.01700100
H	-4.14356400	-2.62171900	-0.82031200
C	-2.28138500	-5.41479100	-1.32999900
H	-0.21754500	-5.42575300	-1.96633300
H	-4.32797200	-5.06792000	-0.73186000
H	-2.36407000	-6.50402300	-1.28723400
C	0.35634800	1.26634500	3.97674100
C	-0.01594200	0.83042900	2.56486600
C	-1.04830800	1.73549900	1.91022900
H	0.81194300	2.26594400	3.98230400
H	1.04731900	0.55722400	4.45382500
H	-0.85724700	2.80345500	2.06322100
H	-1.13305000	1.52786400	0.83871900
H	-0.48320600	-0.15596900	2.62698100
C	1.67643700	-0.72964400	1.70923100
C	1.93926000	1.54276600	1.13599700
C	2.84877000	-1.04282100	1.04745700
C	3.12363600	1.24438400	0.48359200
C	3.61110000	-0.05977800	0.41603100
H	3.14705100	-2.08997800	1.01348200
H	3.62337900	2.05416600	-0.04689400
N	1.23695600	0.56283900	1.76981300
C	1.42789100	2.93745800	1.02153700
C	1.67912200	3.90188700	1.99963900
C	0.72596800	3.27988400	-0.14053500
C	1.17409900	5.19224100	1.84525000
H	2.26643700	3.64608300	2.88469000
C	0.22006900	4.56757200	-0.28570400
H	0.56535800	2.52686200	-0.91471800
C	0.43272600	5.52069100	0.71072900
H	1.36288600	5.94390800	2.61444500
H	-0.35158500	4.81523900	-1.18220500
H	0.02810300	6.52868200	0.59710400
C	0.86509300	-1.84650600	2.27408100
C	0.98097100	-2.25780200	3.60606900
C	0.01555300	-2.53295900	1.40088000
C	0.21893000	-3.33108900	4.06377800
H	1.66784200	-1.74440700	4.28321100

C	-0.74462400	-3.60501400	1.86262400
H	-0.05676800	-2.22460900	0.35891900
C	-0.64743300	-3.99918200	3.19658100
H	0.30863500	-3.65172200	5.10381200
H	-1.40434800	-4.12397200	1.16179100
H	-1.24143400	-4.83953000	3.56209300
C	4.84290100	-0.39151200	-0.32836000
C	4.88084400	-1.52965000	-1.14529000
C	5.97443400	0.42996500	-0.23755100
C	6.03822500	-1.84065400	-1.85313200
H	3.97932200	-2.13200400	-1.26768500
C	7.13305200	0.10812400	-0.93880900
H	5.95569500	1.31459800	0.40387200
C	7.16628400	-1.02785800	-1.74732700
H	6.05359300	-2.71832000	-2.50229600
H	8.01436400	0.74701400	-0.85369600
H	8.07383700	-1.27622600	-2.30171000
H	-2.01777100	1.49577400	2.36956700
H	-0.55938800	1.30965200	4.58319000

Eb:



E_{el} = -3719.361346

Zero-point correction = 0.703945

Thermal correction to Energy = 0.748720

Thermal correction to Enthalpy = 0.749665

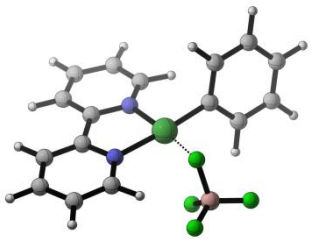
Thermal correction to Gibbs Free Energy = 0.621805

C	3.31538800	-2.06042100	1.22824300
C	3.05385500	-2.96402100	2.25311800
C	2.83903800	-2.48495900	3.54145800
C	2.90171000	-1.11586500	3.76517200
C	3.13855400	-0.26866000	2.68872500
N	3.32873700	-0.72537100	1.44583000
H	2.62330300	-3.17747600	4.35686100
H	2.99864600	-4.03123100	2.04346800
H	2.74841100	-0.68955200	4.75664900
H	3.16589400	0.81454100	2.80884400

C	3.58277300	-2.46538700	-0.16910000
C	3.79155000	-3.77740900	-0.58477400
N	3.61623500	-1.43988800	-1.03359600
C	4.00294000	-4.02149400	-1.93893000
H	3.78746000	-4.59807100	0.13135200
C	3.80938800	-1.66612300	-2.33403900
C	3.99991100	-2.95342800	-2.82971300
H	4.16311000	-5.04113700	-2.29409900
H	3.78864300	-0.79313500	-2.98875300
H	4.14751200	-3.10230700	-3.89937800
Ni	3.38746400	0.33404200	-0.15458800
F	3.36472600	1.22588700	-1.85330000
B	2.06957500	1.25554000	-2.63439700
F	1.69224900	2.55698000	-2.75613700
F	2.34258000	0.62995200	-3.82668200
F	1.17645900	0.50824600	-1.85467400
C	3.21957600	1.99895400	0.71172500
C	2.02062100	2.71249800	0.59350800
C	4.26869000	2.57651100	1.43834200
C	1.86075300	3.95496000	1.20762500
H	1.19502900	2.30883100	0.00484000
C	4.11512100	3.82535300	2.04882700
H	5.22613200	2.05428100	1.53827300
C	2.90756500	4.51386400	1.94146800
H	0.91208200	4.48750200	1.09738500
H	4.94763200	4.26387600	2.60560500
H	2.78595400	5.48851500	2.41984400
C	-2.00687300	0.21885500	2.75669600
C	-1.29817800	0.53974100	1.44158200
C	0.11358900	-0.02716600	1.39802200
H	-2.12595000	-0.86865300	2.88481400
H	-3.00600200	0.67872600	2.78625600
H	0.15842700	-1.09216900	1.67005200
H	0.56387500	0.10183300	0.40524900
H	-1.18874600	1.62968900	1.37251400
C	-3.10034200	1.17812500	-0.06759000
C	-2.59950100	-1.15221500	0.17483300
C	-4.43149700	0.87827400	-0.18245400
C	-3.93095400	-1.45450800	0.06665400
C	-4.92837600	-0.44692700	-0.02635100
H	-5.10478700	1.67434800	-0.50471400
H	-4.19786400	-2.50937100	-0.01636900
N	-2.17001300	0.18224700	0.28825200
C	-1.56657000	-2.20590600	0.05435900
C	-1.61831900	-3.37547200	0.82373800

C	-0.53625100	-2.05961300	-0.88807100
C	-0.66292100	-4.37820500	0.65718200
H	-2.40929200	-3.48978400	1.56923200
C	0.40815000	-3.06408200	-1.05937900
H	-0.47463400	-1.14892000	-1.48572600
C	0.35164400	-4.22684600	-0.28650000
H	-0.71731400	-5.28479200	1.26479300
H	1.18526600	-2.94064600	-1.81712600
H	1.08993300	-5.01961800	-0.43200300
C	-2.56172300	2.52657700	-0.35145000
C	-3.25277400	3.68108800	0.04570000
C	-1.34114500	2.67302400	-1.03116600
C	-2.74209300	4.94606800	-0.23573500
H	-4.18906700	3.58369700	0.60042200
C	-0.83133700	3.93801900	-1.31039800
H	-0.78410800	1.78788000	-1.34728800
C	-1.52950800	5.07896700	-0.91216200
H	-3.29033800	5.83440800	0.08657100
H	0.11912400	4.01628100	-1.84077800
H	-1.12547800	6.07076300	-1.12709100
C	-6.36295200	-0.74879600	-0.07641600
C	-7.31883900	0.23486100	0.24867100
C	-6.84718600	-2.02103100	-0.44197500
C	-8.68248100	-0.03640300	0.20433300
H	-6.98602200	1.22491700	0.56717600
C	-8.21072700	-2.29134100	-0.48370600
H	-6.14691900	-2.80864600	-0.72592900
C	-9.14048300	-1.30184000	-0.16225400
H	-9.39596100	0.74763600	0.46865600
H	-8.55241600	-3.28587400	-0.78052900
H	-10.21094700	-1.51463800	-0.19746500
H	0.71954100	0.54061000	2.11771600
H	-1.42456600	0.60260000	3.60794600

F:



E_{el} = -2659.739448

Zero-point correction = 0.270624

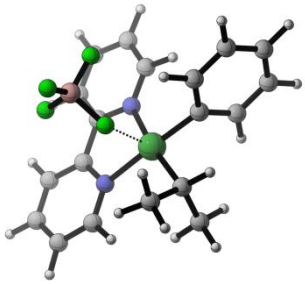
Thermal correction to Energy = 0.291470

Thermal correction to Enthalpy = 0.292414

Thermal correction to Gibbs Free Energy = 0.218661

C	-1.85016400	1.72897500	-0.15070500
C	-2.48215400	2.93598900	-0.43693000
C	-1.71121600	4.05172500	-0.74777000
C	-0.32811400	3.92400200	-0.77035700
C	0.23894900	2.69147200	-0.46572800
N	-0.50139600	1.62086400	-0.15207900
H	-2.19009100	5.00566700	-0.97537600
H	-3.56926200	3.00467800	-0.42589500
H	0.32046000	4.76406000	-1.01977500
H	1.31874200	2.54291900	-0.46261800
C	-2.57542300	0.47062700	0.14394300
C	-3.96084900	0.35007200	0.20965300
N	-1.76961100	-0.58812700	0.32635200
C	-4.50956700	-0.90601500	0.46053300
H	-4.60892200	1.21401400	0.06584200
C	-2.28664600	-1.79530600	0.55854900
C	-3.66323000	-1.99508400	0.63177900
H	-5.59274300	-1.02896400	0.51656400
H	-1.57353600	-2.61543200	0.66589700
H	-4.05291600	-2.99633100	0.81636400
Ni	0.16790300	-0.12561600	0.26469600
F	0.67592300	-1.92471900	0.66254500
B	0.77329700	-2.84767100	-0.55139600
F	2.06049700	-3.26243300	-0.64446400
F	-0.13282700	-3.85644100	-0.29846600
F	0.37050300	-2.04250700	-1.61284700
C	1.97509500	0.39428600	0.32186400
C	2.85123800	0.01738300	-0.70317900
C	2.48115000	1.13062000	1.40135500
C	4.19744400	0.38567500	-0.65675500
H	2.48591600	-0.58412100	-1.53897000
C	3.82961700	1.49327500	1.45209200
H	1.82086800	1.43210800	2.22137000
C	4.69021600	1.12511800	0.41858000
H	4.86993900	0.08083000	-1.46271200
H	4.21006900	2.06041900	2.30594500
H	5.74581700	1.40463500	0.45648600

G:

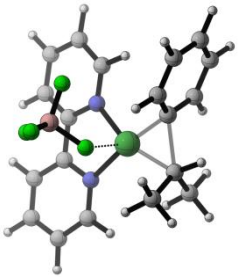


E_{el} = -2778.204600
Zero-point correction = 0.364815
Thermal correction to Energy = 0.390998
Thermal correction to Enthalpy = 0.391942
Thermal correction to Gibbs Free Energy = 0.307164

C	-2.33058000	0.22483700	-0.84026600
C	-2.46766200	-2.04128100	-0.43455700
C	-3.85374500	-2.03597900	-0.51963400
C	-4.49082400	-0.82853600	-0.78055900
C	-3.71906500	0.31367000	-0.94454100
C	-1.44529600	1.41077500	-0.97697400
C	0.73202000	2.18289100	-0.88973700
C	0.33155200	3.49290200	-1.12253500
C	-1.02276900	3.75055900	-1.28932000
C	-1.92610900	2.69615300	-1.21641100
H	-1.93477500	-2.96800900	-0.22503100
H	-4.41049600	-2.96206300	-0.37599100
H	-5.57856900	-0.77203000	-0.85138900
H	-4.20014200	1.27085400	-1.13528500
H	1.78182400	1.93256100	-0.73139700
H	1.07501600	4.28909500	-1.15452300
H	-1.38081500	4.76680800	-1.46404400
H	-2.99200500	2.88542400	-1.32749200
N	-1.72077800	-0.94732200	-0.59304500
N	-0.13486400	1.17236800	-0.83174300
Ni	0.36074000	-0.76249500	-0.25117700
C	2.87537700	0.02764200	0.84536200
C	4.23554600	-0.03876500	-1.59357800
C	4.18891000	0.49265600	0.75739100
H	2.33752100	0.08128600	1.79308500
C	4.87193300	0.46323800	-0.45909800
H	4.76162200	-0.06736500	-2.55118600
H	4.67917700	0.88807800	1.65037300
H	5.89863300	0.83066100	-0.52293900
C	2.92250000	-0.50824700	-1.50932000
H	2.44110900	-0.89855000	-2.41175700

C	2.23299700	-0.46682300	-0.29335600
C	0.99982300	-2.62542300	-0.02408800
H	2.08643200	-2.69792500	0.09211100
C	0.64743700	-3.33500200	-1.32758900
H	1.21016500	-2.91408000	-2.17572100
H	0.92494200	-4.40235400	-1.26372800
H	-0.41976500	-3.29825200	-1.59194200
C	0.38532200	-3.18850700	1.24942000
H	-0.70422700	-3.07188000	1.32506300
H	0.61206900	-4.26733900	1.32458200
H	0.80810200	-2.69024300	2.13135700
F	-0.06290700	-0.37007700	1.72948000
B	-0.58388600	0.88221300	2.35117300
F	0.30896800	1.88488600	2.00855200
F	-1.83663900	1.10515300	1.78011800
F	-0.65295600	0.65873000	3.69660700

G-TS:

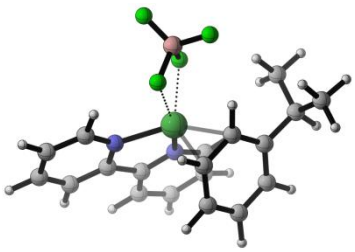


E_{el} = -2778.197820
Zero-point correction = 0.364116
Thermal correction to Energy = 0.389690
Thermal correction to Enthalpy = 0.390634
Thermal correction to Gibbs Free Energy = 0.307006

C	-2.41542400	0.15650000	-0.78581100
C	-2.43149200	-2.12897500	-0.46646600
C	-3.81954200	-2.17636400	-0.41935100
C	-4.51945700	-0.98332800	-0.56684900
C	-3.81024800	0.19645000	-0.75350600
C	-1.58046400	1.38310800	-0.93252100
C	0.56855900	2.23642700	-0.83645100
C	0.11806000	3.53498600	-1.04715500
C	-1.24607500	3.73956200	-1.21818300
C	-2.11124000	2.65133200	-1.16051100
H	-1.84123900	-3.04071500	-0.34526700
H	-4.33068700	-3.12619800	-0.26082000
H	-5.61017600	-0.96751000	-0.52505100
H	-4.34104700	1.14234900	-0.84604900

H	1.62757800	2.01541900	-0.68191000
H	0.82739600	4.36245400	-1.06358500
H	-1.64207100	4.74316800	-1.38476200
H	-3.18293700	2.80132500	-1.28069100
N	-1.74902600	-0.99958900	-0.64869200
N	-0.26274700	1.19864000	-0.79796500
Ni	0.35586300	-0.72545300	-0.30448600
C	2.84439700	-0.19650500	0.87394700
C	4.00178200	0.46209000	-1.58039900
C	3.99233300	0.58900200	0.82495500
H	2.37587000	-0.41694800	1.83410400
C	4.58049700	0.92095400	-0.39797100
H	4.44864400	0.71569100	-2.54491300
H	4.42610500	0.95739300	1.75744100
H	5.48366300	1.53400900	-0.42734100
C	2.85056200	-0.32493200	-1.54231200
H	2.41522400	-0.67477000	-2.48271500
C	2.25055800	-0.65654900	-0.31413500
C	1.49856200	-2.47892300	-0.28702000
H	2.57191000	-2.69818700	-0.27646700
C	0.97166600	-3.07607500	-1.59388800
H	1.45395600	-2.62148800	-2.47162200
H	1.20260500	-4.15464200	-1.62981000
H	-0.11579900	-2.97145500	-1.72203200
C	0.94389300	-3.11660600	0.98497400
H	-0.14602900	-3.02890400	1.08774400
H	1.20541600	-4.18893000	0.99723000
H	1.37858000	-2.65262500	1.87969000
F	-0.07455000	-0.53967900	1.70235100
B	-0.50970100	0.70744600	2.39270000
F	0.42011000	1.68036500	2.06145200
F	-1.76885800	1.01455700	1.88115300
F	-0.53912000	0.42917400	3.73142800

H:



E_{el} = -2778.269775

Zero-point correction = 0.365908

Thermal correction to Energy = 0.391799

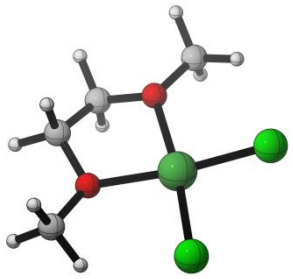
Thermal correction to Enthalpy = 0.392743

Thermal correction to Gibbs Free Energy = 0.307800

C	-2.83272800	-0.14727900	-0.02997500
C	-4.21301600	-0.05516500	0.15957500
C	-4.74512600	1.12666600	0.66616500
C	-3.89002400	2.18447800	0.96262300
C	-2.52565100	2.01350100	0.75114100
N	-2.02005300	0.87420700	0.27730900
H	-5.82156800	1.22180200	0.82031200
H	-4.87141900	-0.88681600	-0.08988100
H	-4.26885300	3.13112000	1.34951900
H	-1.79738500	2.80348300	0.95106500
C	-2.15128000	-1.33833900	-0.60892500
C	-2.83105800	-2.48652700	-1.01721600
N	-0.81778000	-1.23007000	-0.74652200
C	-2.11463900	-3.52852700	-1.59812400
H	-3.90969200	-2.57154100	-0.89091600
C	-0.13497000	-2.22153200	-1.31737600
C	-0.74117000	-3.39162200	-1.76374200
H	-2.62935600	-4.43383000	-1.92536200
H	0.93951200	-2.06776800	-1.41687900
H	-0.14007000	-4.17453700	-2.22695600
Ni	-0.01979200	0.46546900	0.09960600
C	2.43121000	-1.20884100	0.76930300
C	1.89407100	-2.41122100	1.20458800
C	1.81488600	0.00119700	1.19038700
C	0.77514400	-2.44836600	2.06241900
H	2.36138300	-3.34984500	0.89307500
C	0.69929800	-0.03143600	2.05903200
H	2.31489100	0.95132500	0.98481300
C	0.19135100	-1.27797300	2.50115500
H	0.38574800	-3.41281300	2.39731400
H	0.36226300	0.89049800	2.53985700
H	-0.65016600	-1.30286200	3.19685500
C	3.68185400	-1.16788500	-0.08944700
H	3.95162300	-2.21607200	-0.30672600
C	3.45753200	-0.44335600	-1.42105600
H	2.64185200	-0.89627500	-2.00437600
H	3.19870000	0.61326800	-1.26650200
H	4.37063800	-0.48459800	-2.03465400
C	4.84964600	-0.53726700	0.67975700
H	5.01744100	-1.04491400	1.64139700
H	5.77777000	-0.59812800	0.09101700
H	4.65587000	0.52753100	0.88226100
F	0.45345700	2.56397300	0.39117400

B	1.17430700	2.75873500	-0.86715800
F	0.72016000	3.88105200	-1.48852700
F	0.85300900	1.58080700	-1.61917800
F	2.52518600	2.77218800	-0.58520500

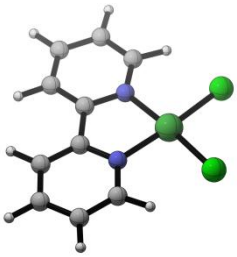
$NiCl_2$·glyme:



E_{el} = -2737.683685
Zero-point correction = 0.149071
Thermal correction to Energy = 0.161280
Thermal correction to Enthalpy = 0.162225
Thermal correction to Gibbs Free Energy = 0.109313

C	2.32544300	-0.76533100	-0.28020000
H	2.39741100	-0.76617600	-1.38282100
H	3.16190400	-1.35603300	0.12903000
C	2.37014800	0.63781500	0.26211100
H	2.45915600	0.63307700	1.36348800
H	3.23290700	1.17956300	-0.16016000
O	1.09209700	-1.32396000	0.12208300
O	1.16472900	1.26653400	-0.12067300
C	0.98632100	-2.72277200	-0.12250500
H	1.75714800	-3.24918700	0.46162200
H	-0.01964100	-3.01976400	0.18939300
H	1.11810400	-2.92990500	-1.19656800
C	1.13572100	2.66491400	0.14431900
H	1.93481700	3.15693200	-0.43184600
H	0.14839600	3.02185600	-0.16376000
H	1.27805400	2.84938600	1.22120900
Ni	-0.42745800	0.01101900	0.00007400
Cl	-1.85317300	1.59856500	-0.16717900
Cl	-1.93858200	-1.49601300	0.16333800

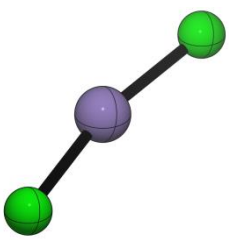
$NiCl_2$·bpy:



E_{el} = -2924.155808
Zero-point correction = 0.165863
Thermal correction to Energy = 0.178955
Thermal correction to Enthalpy = 0.179899
Thermal correction to Gibbs Free Energy = 0.124542

C	-1.58179400	0.74086100	0.00037200
C	-0.22506000	2.62022900	0.00018900
C	-1.33000500	3.46592400	0.00052300
C	-2.60374000	2.91034700	0.00081100
C	-2.73299900	1.52484100	0.00073200
C	-1.58381000	-0.73658500	0.00018900
C	-0.23219200	-2.61966400	-0.00038000
C	-1.33942600	-3.46234000	-0.00035300
C	-2.61165000	-2.90328600	-0.00001900
C	-2.73714600	-1.51745200	0.00025700
H	0.80847500	2.97829100	-0.00003100
H	-1.17837300	4.54567200	0.00056200
H	-3.49174100	3.54534300	0.00108600
H	-3.71936900	1.06263800	0.00095400
H	0.80038800	-2.98047800	-0.00060200
H	-1.19080200	-4.54250600	-0.00059600
H	-3.50134600	-3.53590400	0.00001900
H	-3.72224900	-1.05255000	0.00051100
N	-0.35150400	1.28983800	0.00012000
N	-0.35502500	-1.28893200	-0.00011100
Ni	1.13457600	-0.00155400	-0.00017300
Cl	2.65206300	-1.55248800	-0.00033700
Cl	2.65614400	1.54539500	-0.00031300

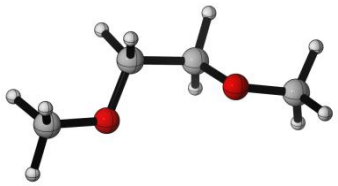
$MnCl_2$:



E_{el} = -2071.400360
Zero-point correction = 0.002111
Thermal correction to Energy = 0.006359
Thermal correction to Enthalpy = 0.007303
Thermal correction to Gibbs Free Energy = -0.026588

Mn	0.00000000	0.00000000	0.15743800
Cl	0.00000000	2.08370000	-0.11576300
Cl	0.00000000	-2.08370000	-0.11576300

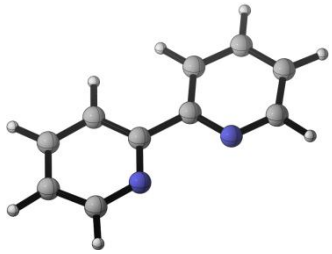
glyme:



E_{el} = -308.815210
Zero-point correction = 0.142438
Thermal correction to Energy = 0.150179
Thermal correction to Enthalpy = 0.151123
Thermal correction to Gibbs Free Energy = 0.110387

C	0.71949300	0.73357300	-0.22780400
H	0.74401600	0.65511700	-1.33391500
H	1.18353900	1.70505200	0.04468400
C	-0.71949300	0.73357300	0.22780500
H	-0.74401600	0.65511500	1.33391600
H	-1.18353800	1.70505300	-0.04468200
O	1.40365900	-0.32763900	0.36538400
O	-1.40366000	-0.32763700	-0.36538500
C	2.72368600	-0.44590700	-0.06081100
H	3.31942100	0.45938200	0.17475800
H	3.17322200	-1.30309100	0.45826100
H	2.79392800	-0.62134500	-1.15267100
C	-2.72368600	-0.44590800	0.06081200
H	-3.31942200	0.45938200	-0.17475500
H	-3.17322200	-1.30309100	-0.45826200
H	-2.79392600	-0.62134700	1.15267200

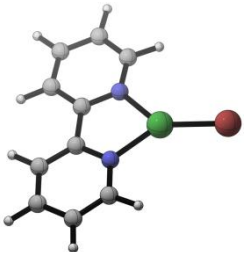
bpy:



E_{el} = -495.238858
Zero-point correction = 0.159237
Thermal correction to Energy = 0.167025
Thermal correction to Enthalpy = 0.167970
Thermal correction to Gibbs Free Energy = 0.126022

C	-0.75157000	0.02235500	-0.00000400
C	-2.67605400	-1.22603000	0.00059500
C	-3.49769500	-0.09824000	0.00005700
C	-2.88262100	1.14913600	-0.00056500
C	-1.49314300	1.21372600	-0.00059500
C	0.75156900	0.02235600	-0.00000200
C	2.67605300	-1.22603100	-0.00059400
C	3.49769600	-0.09823900	-0.00004800
C	2.88262200	1.14913600	0.00056800
C	1.49314200	1.21372600	0.00059000
H	-3.11935900	-2.22838000	0.00109700
H	-4.58420600	-0.20091800	0.00011100
H	-3.47521500	2.06671500	-0.00103800
H	-1.00357400	2.18703900	-0.00115600
H	3.11936000	-2.22838000	-0.00109700
H	4.58420600	-0.20091900	-0.00009100
H	3.47521300	2.06671600	0.00104400
H	1.00357400	2.18703900	0.00114500
N	-1.35112300	-1.17002000	0.00056400
N	1.35112400	-1.17002100	-0.00056900

D':

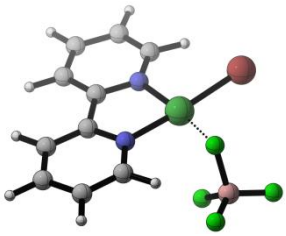


E_{el} = -4577.806295
Zero-point correction = 0.162542
Thermal correction to Energy = 0.174845
Thermal correction to Enthalpy = 0.175789

Thermal correction to Gibbs Free Energy = 0.119072

C	-1.79087400	0.75118400	0.00018100
C	-2.93846500	1.54545700	0.00067700
C	-2.79983900	2.92972200	0.00060900
C	-1.52143300	3.48273700	0.00003300
C	-0.42687500	2.62506600	-0.00041400
N	-0.56070200	1.29605000	-0.00033500
H	-3.68372800	3.57035800	0.00099800
H	-3.93018100	1.09370600	0.00116500
H	-1.36806800	4.56242200	-0.00005400
H	0.59914200	3.00142800	-0.00085000
C	-1.80081200	-0.73409200	0.00017600
C	-2.95911000	-1.51251400	0.00014800
N	-0.57800400	-1.29548100	0.00013400
C	-2.83960200	-2.89852800	0.00008200
H	-3.94449600	-1.04710900	0.00013400
C	-0.46263400	-2.62629900	0.00007600
C	-1.56886300	-3.46893800	0.00004800
H	-3.73230500	-3.52682800	0.00004200
H	0.55787000	-3.01723400	0.00005600
H	-1.43001400	-4.55058900	-0.00001100
Ni	0.95281600	-0.01045700	-0.00022800
Br	3.22499700	-0.01028800	-0.00009700

F':

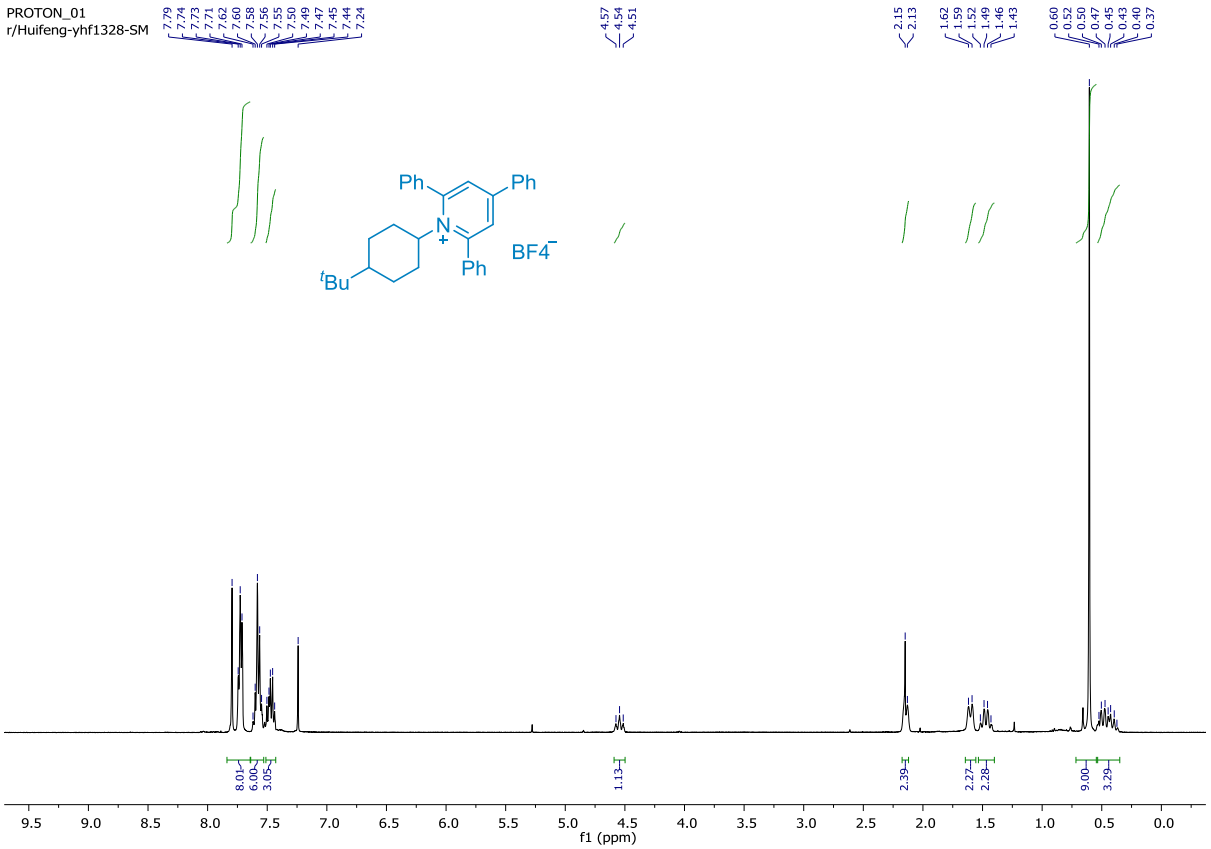


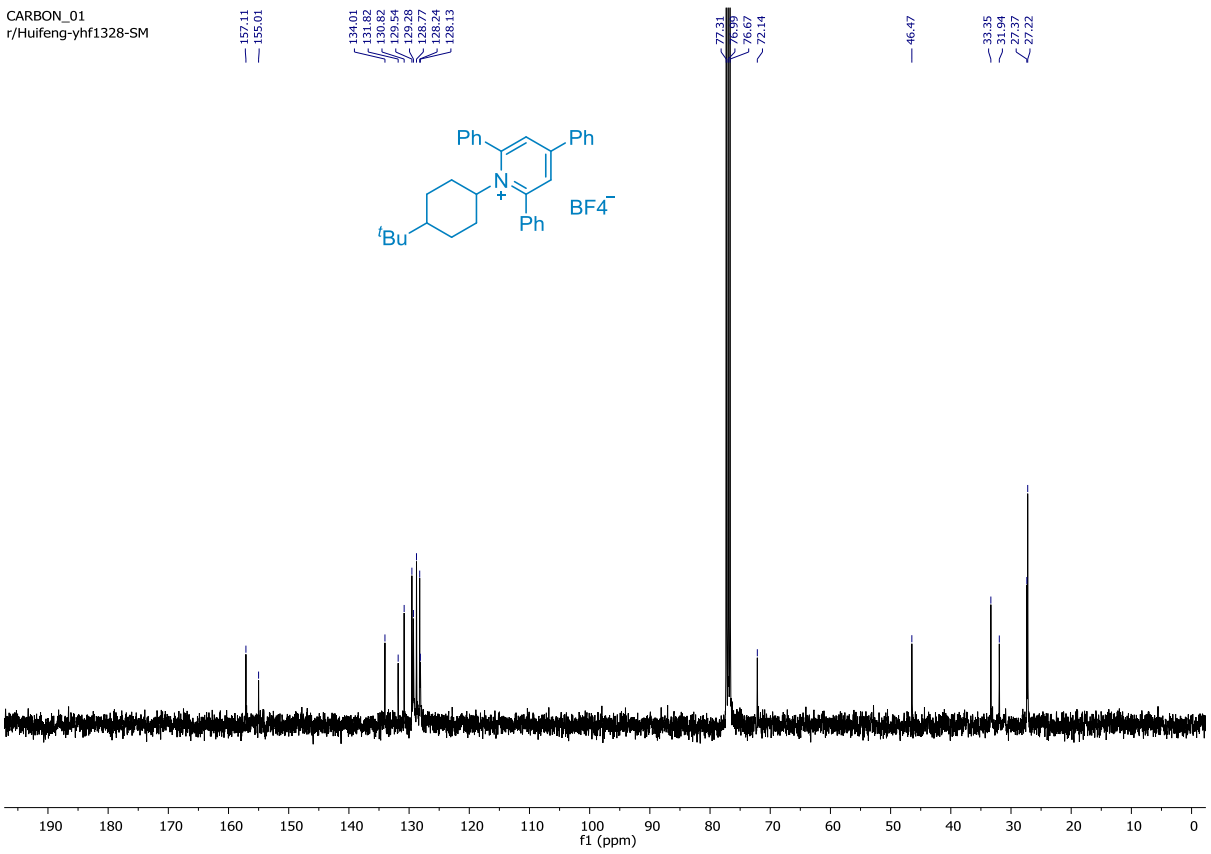
E_{el} = -5002.341503
Zero-point correction = 0.181125
Thermal correction to Energy = 0.198365
Thermal correction to Enthalpy = 0.199309
Thermal correction to Gibbs Free Energy = 0.133546

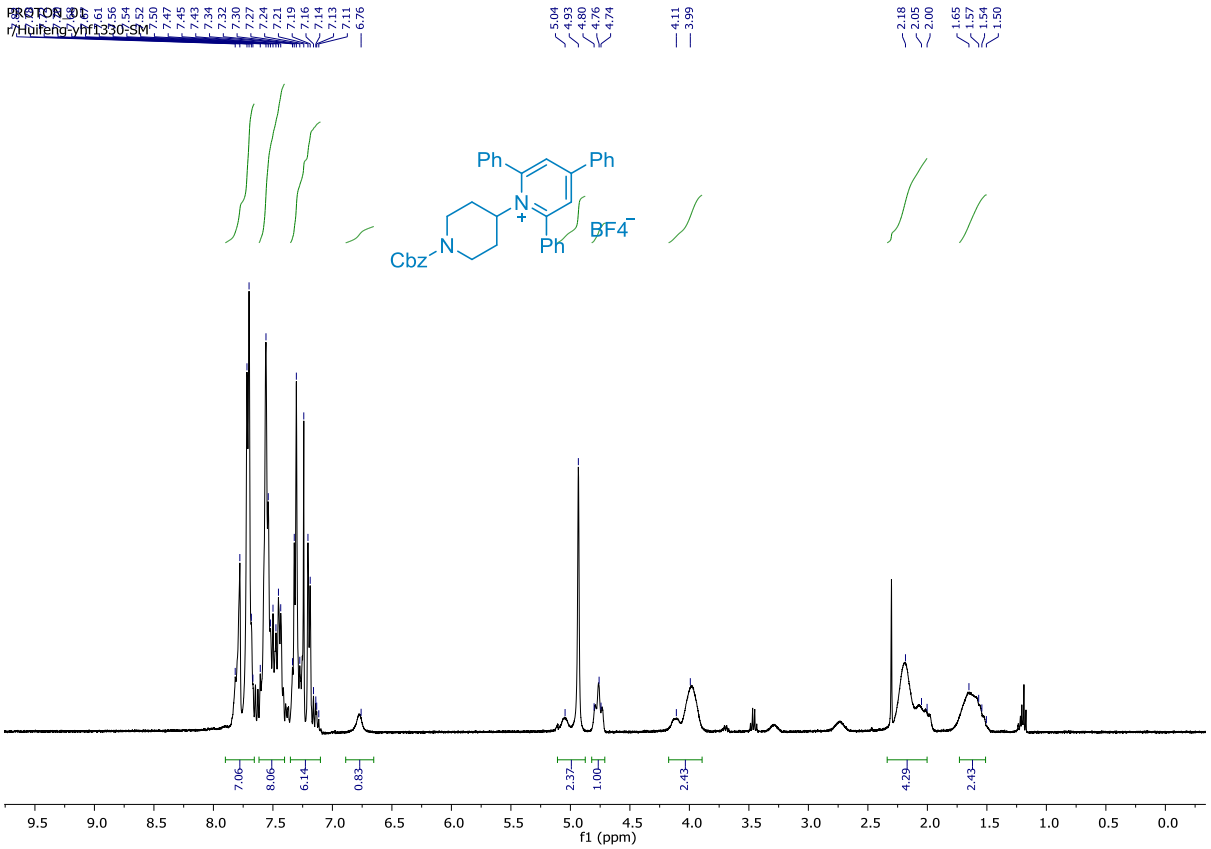
C	-2.36719500	0.20505400	0.12533900
C	-3.72116400	0.03263000	0.39262100
C	-4.20931800	-1.25112200	0.61791800
C	-3.32552400	-2.32136700	0.57192900
C	-1.98432900	-2.07921000	0.29495500
N	-1.51712700	-0.84501500	0.07246400
H	-5.26862600	-1.40807200	0.82849900

H	-4.39014600	0.89158400	0.42759900
H	-3.65695900	-3.34527100	0.74544400
H	-1.24044500	-2.87657400	0.23671900
C	-1.72863300	1.51462200	-0.11203000
C	-2.39066900	2.73725800	-0.10961200
N	-0.40353000	1.43238000	-0.33136000
C	-1.65370100	3.89717300	-0.33911200
H	-3.46372400	2.79177700	0.07013800
C	0.31071400	2.53933000	-0.54866600
C	-0.28615600	3.79691600	-0.56023800
H	-2.14921700	4.86958700	-0.33999200
H	1.38364000	2.41099900	-0.69636500
H	0.33072200	4.67827300	-0.73553800
Ni	0.31263100	-0.37293900	-0.28970600
Br	1.10557400	-2.52101400	-0.46188000
F	2.04966100	0.28638800	-0.58891500
B	2.82211900	0.80401400	0.66602700
F	3.82560700	-0.06447100	0.89969300
F	3.22536700	2.06701000	0.29404800
F	1.84112800	0.83397700	1.64234800

10. Copies of NMR Spectra



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7.47
7.45
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7.34
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7.30
7.27
7.24
7.21
7.19
7.16
7.14
7.13
7.11
5.04
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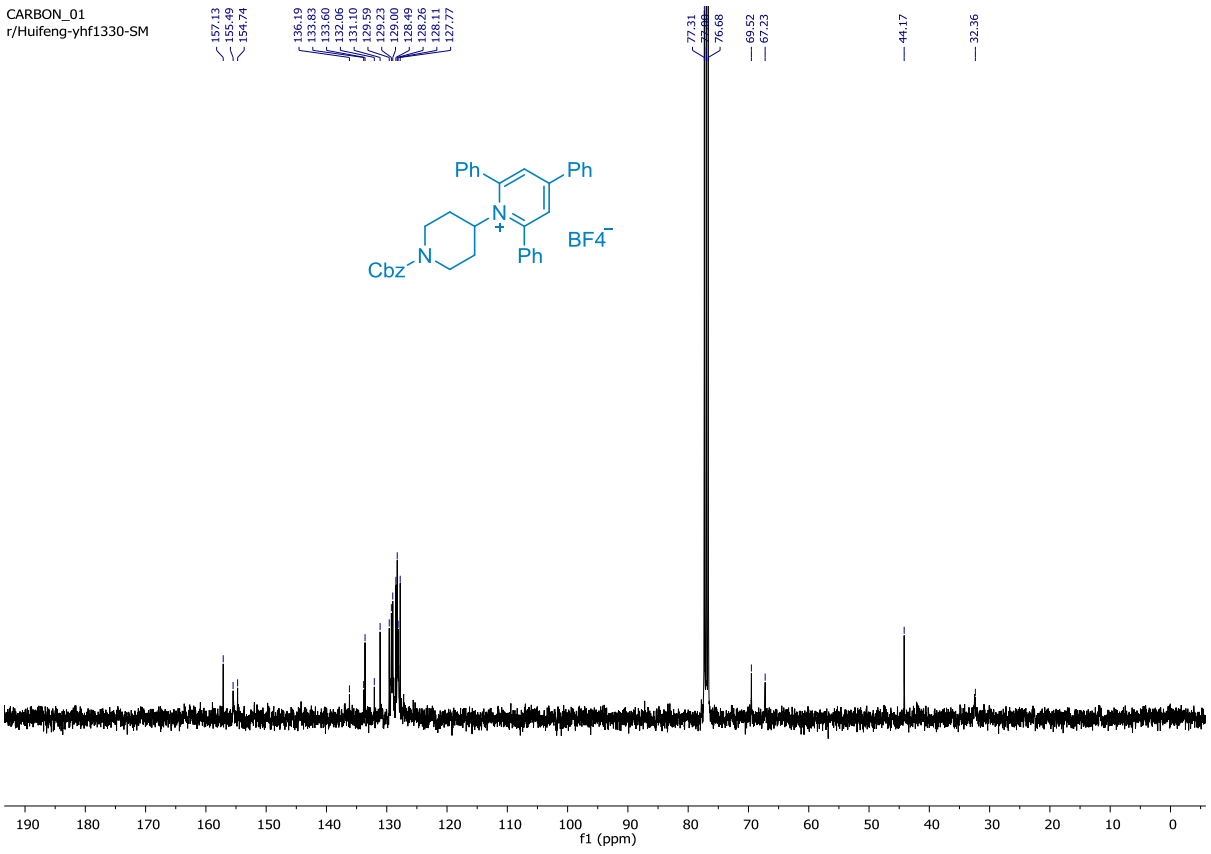
4.80
4.76
4.74
4.11
3.99
2.18
2.05
2.00
1.65
1.57
1.54
1.50
Ph
Ph
N
Ph
Cbz
N
BF4−
7.06
8.06
6.14
0.83
2.37
1.00
2.43
4.29
2.43
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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132.06
131.10
129.59
129.23
129.00
128.49
128.26
128.11
127.77
77.31
77.00
76.68
69.52
67.23
44.17
32.36
Ph
Ph
N
Ph
Cbz
N
BF4−
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

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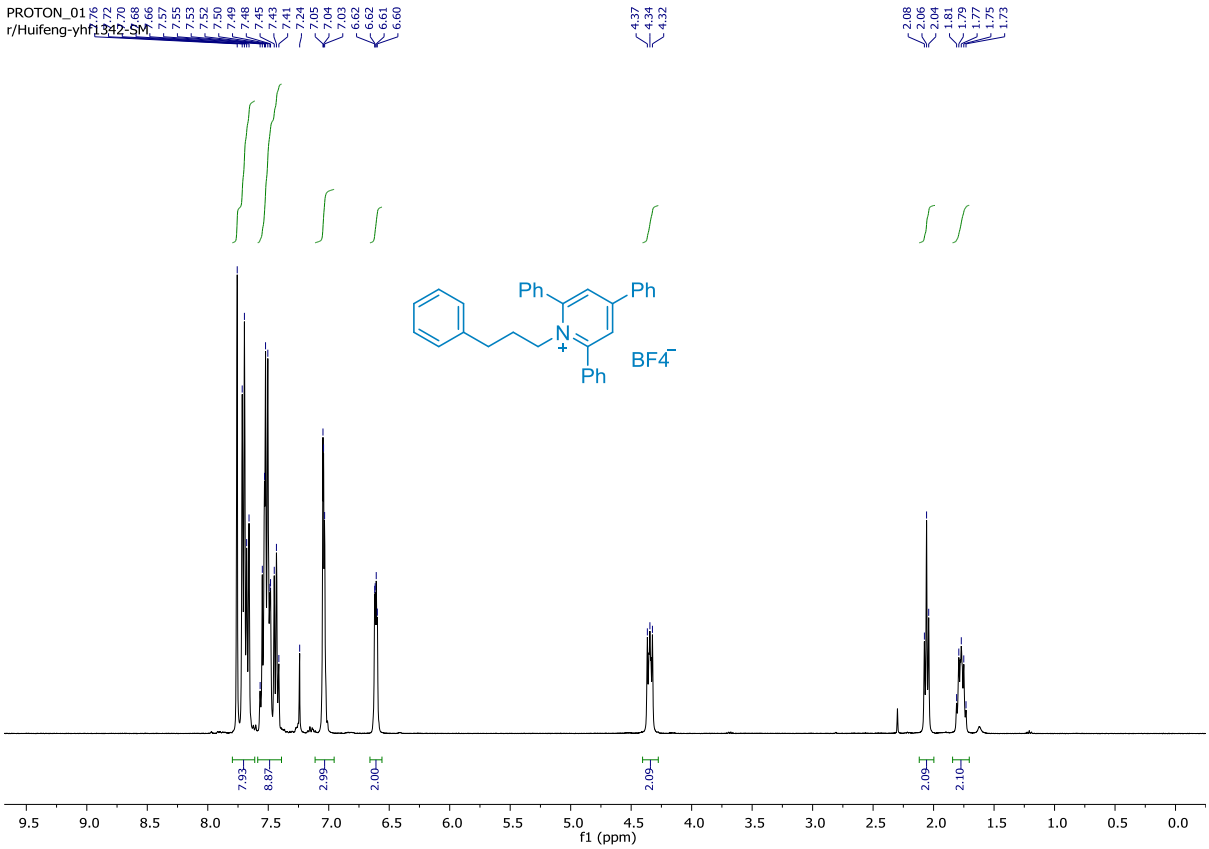

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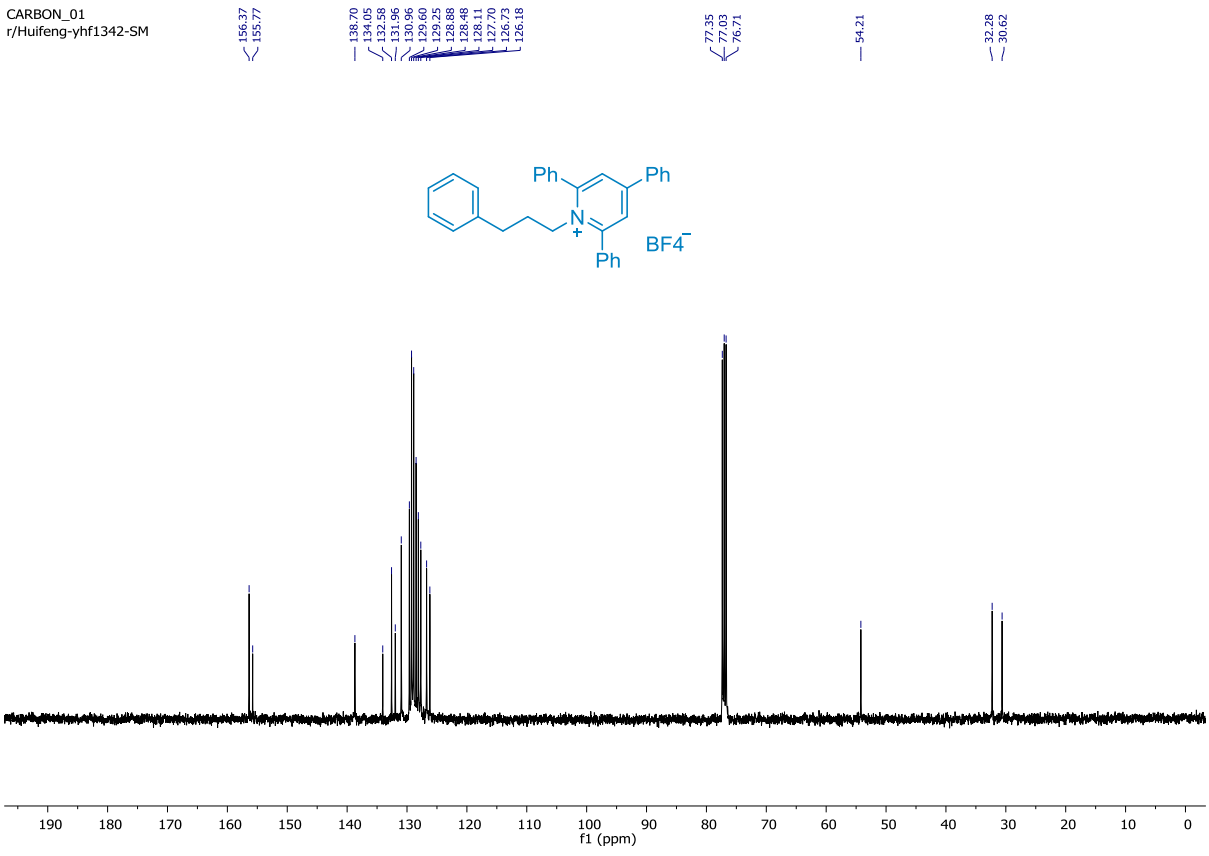

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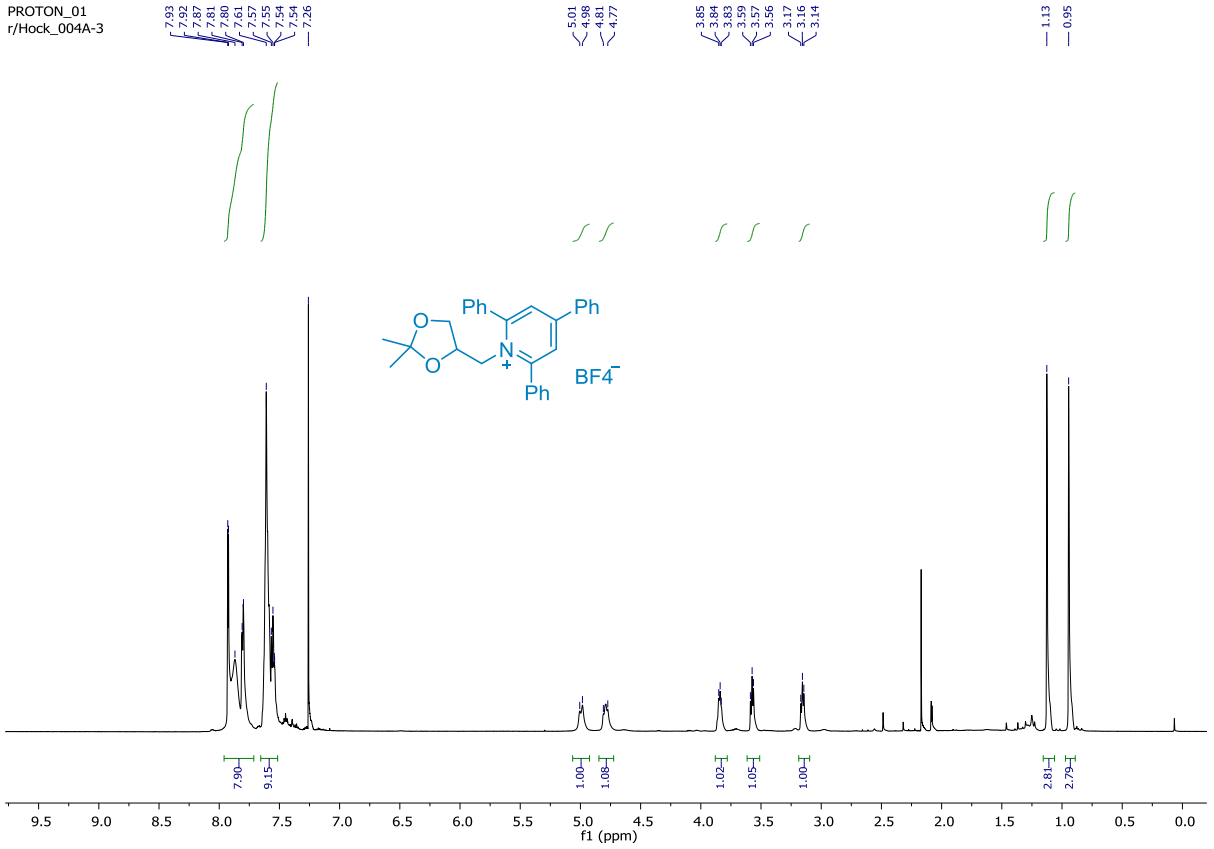

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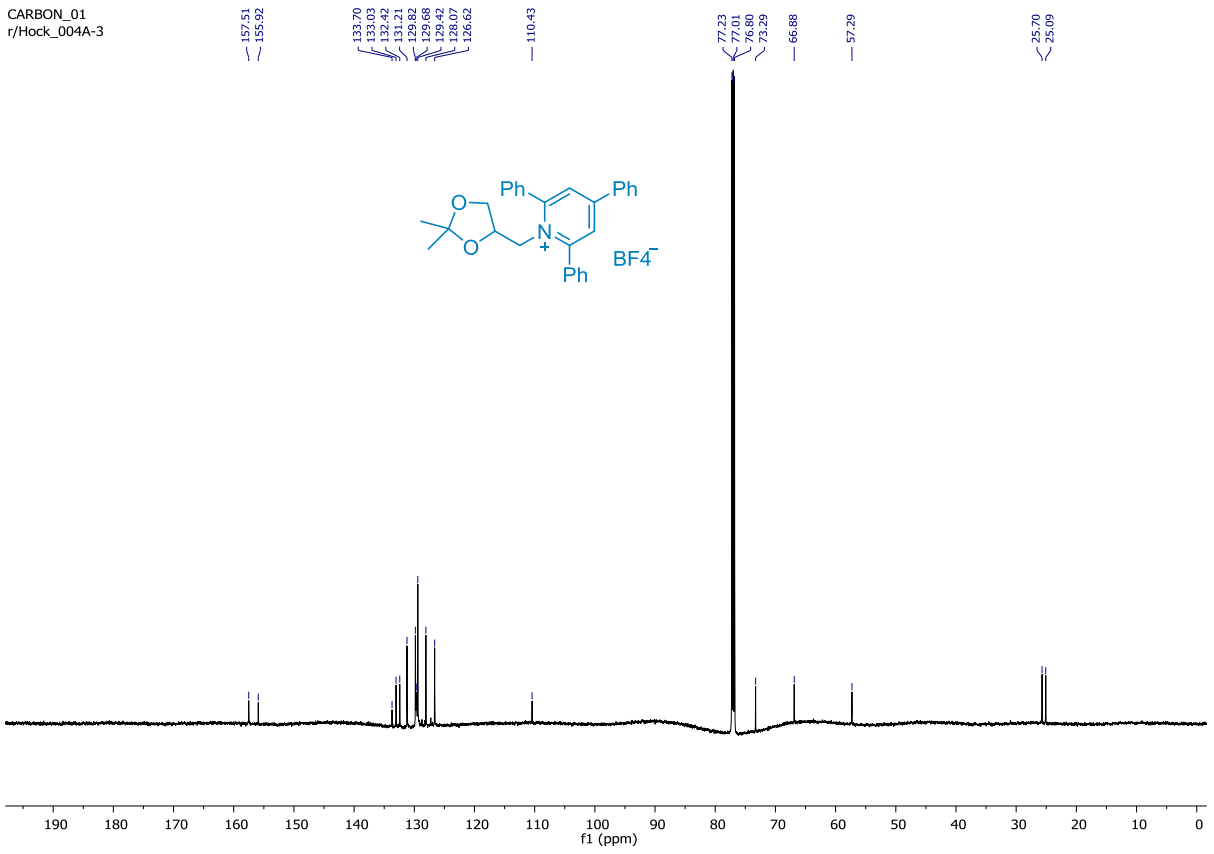

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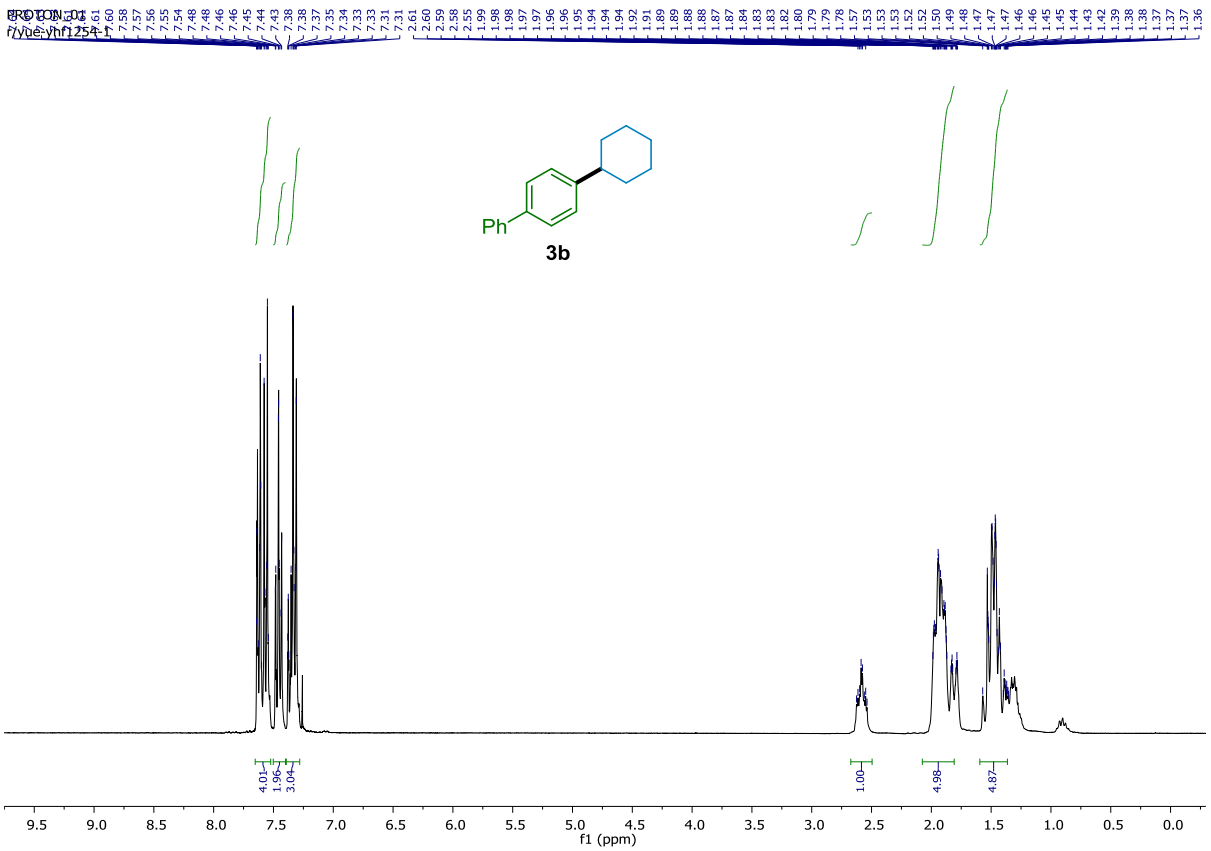

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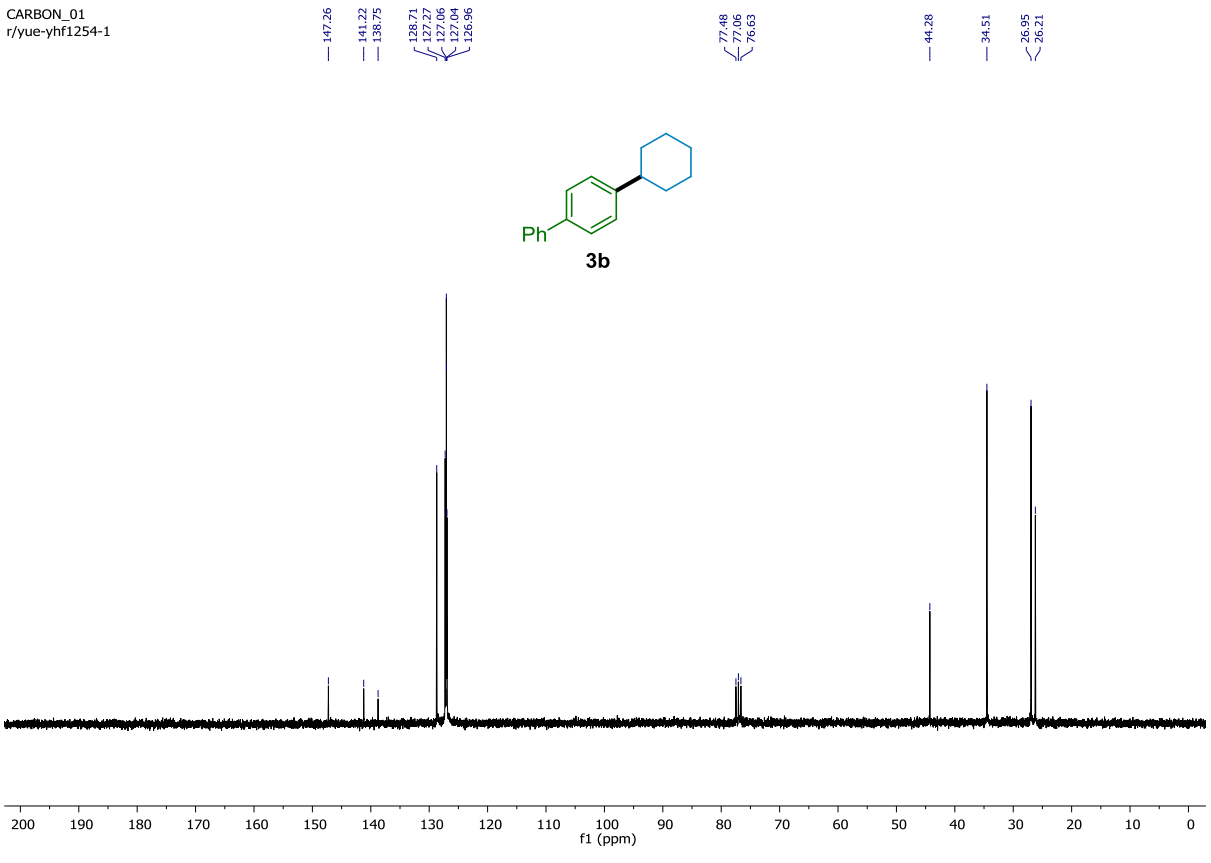

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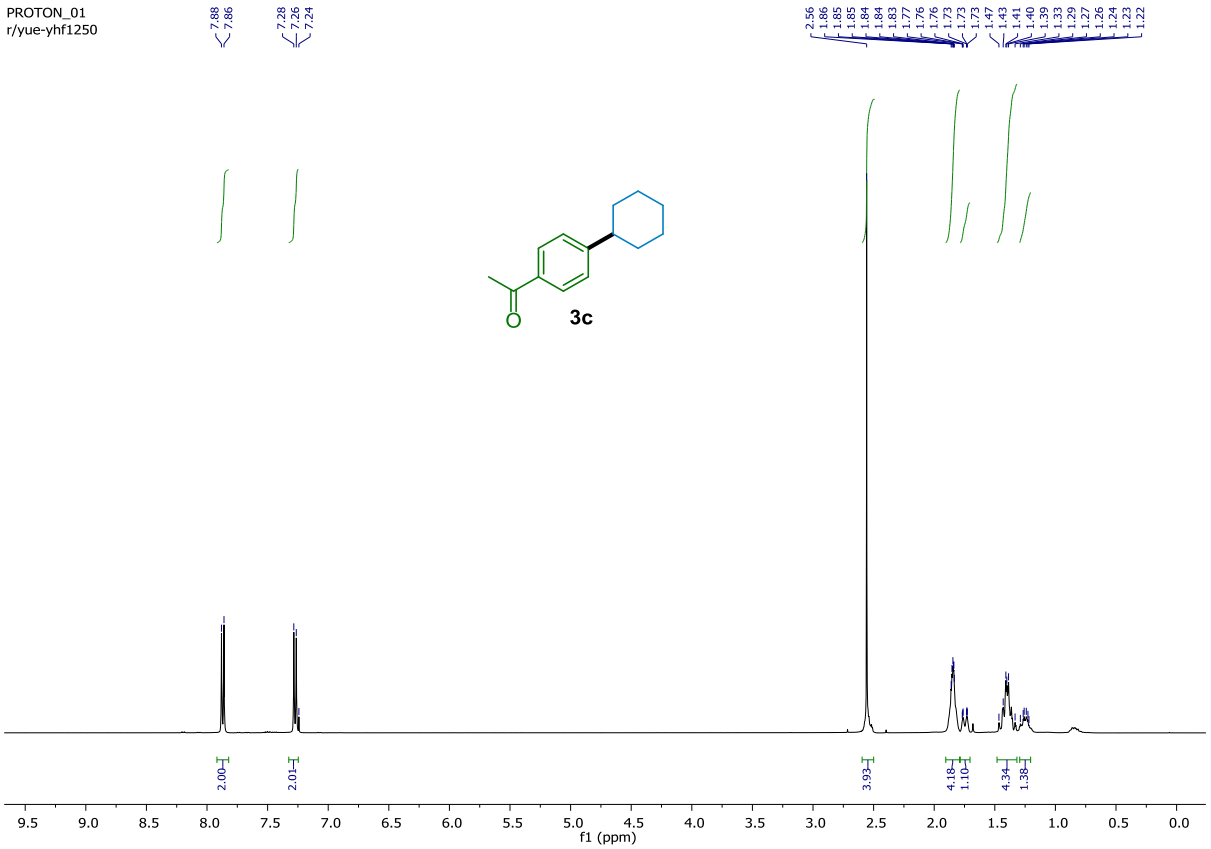

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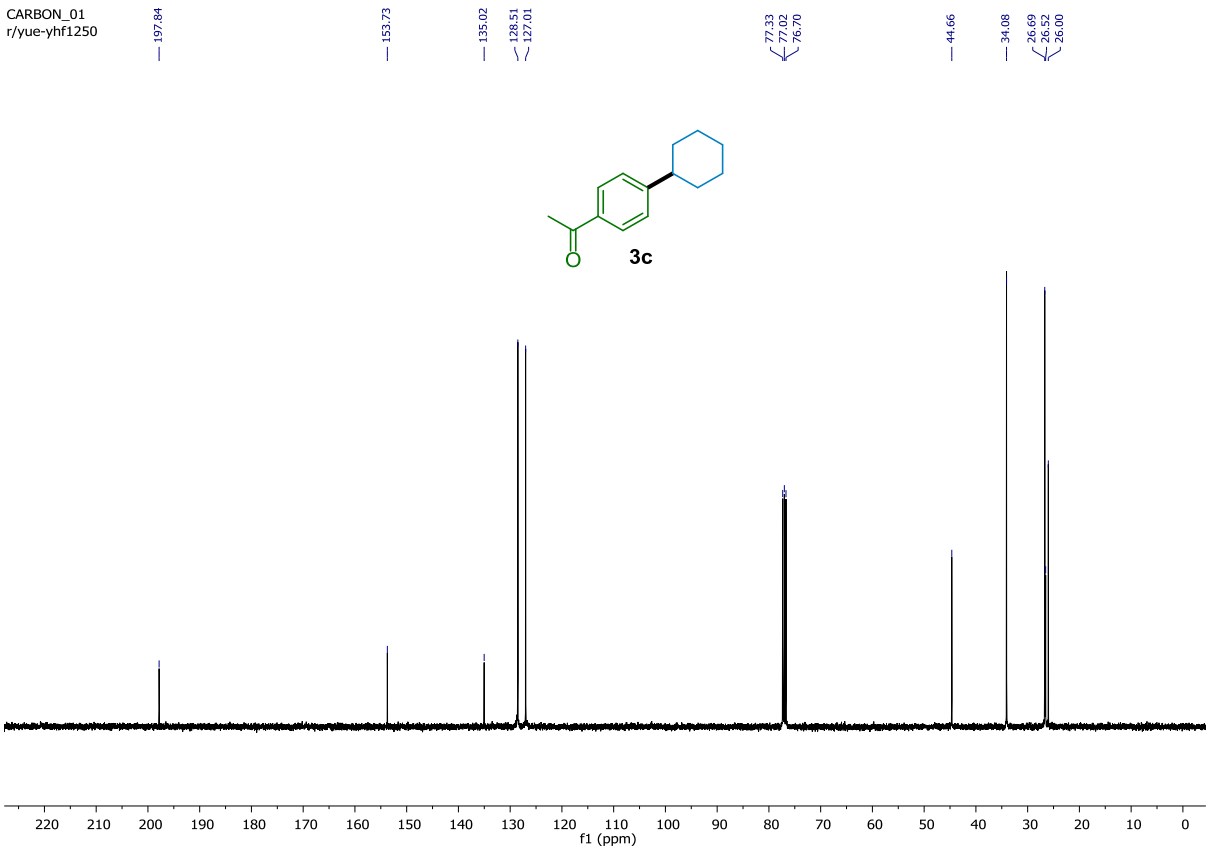

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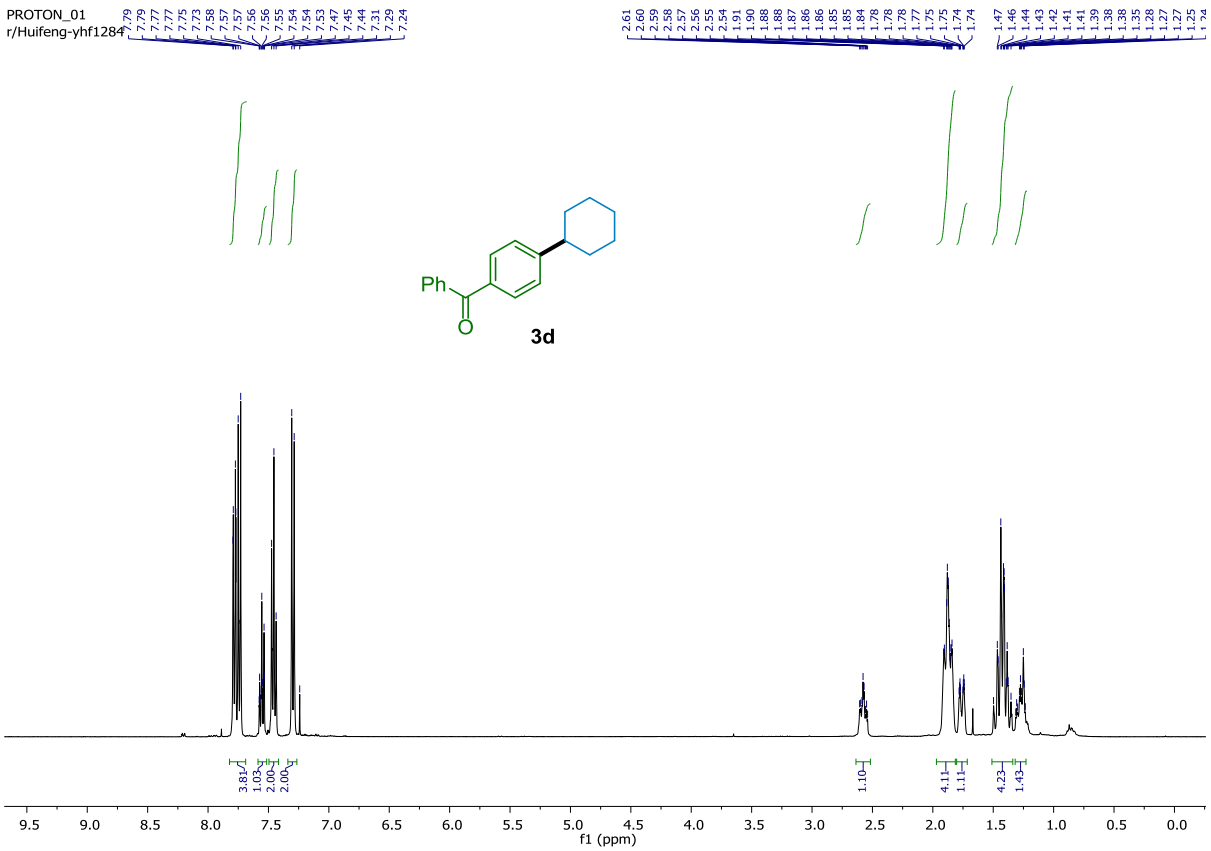

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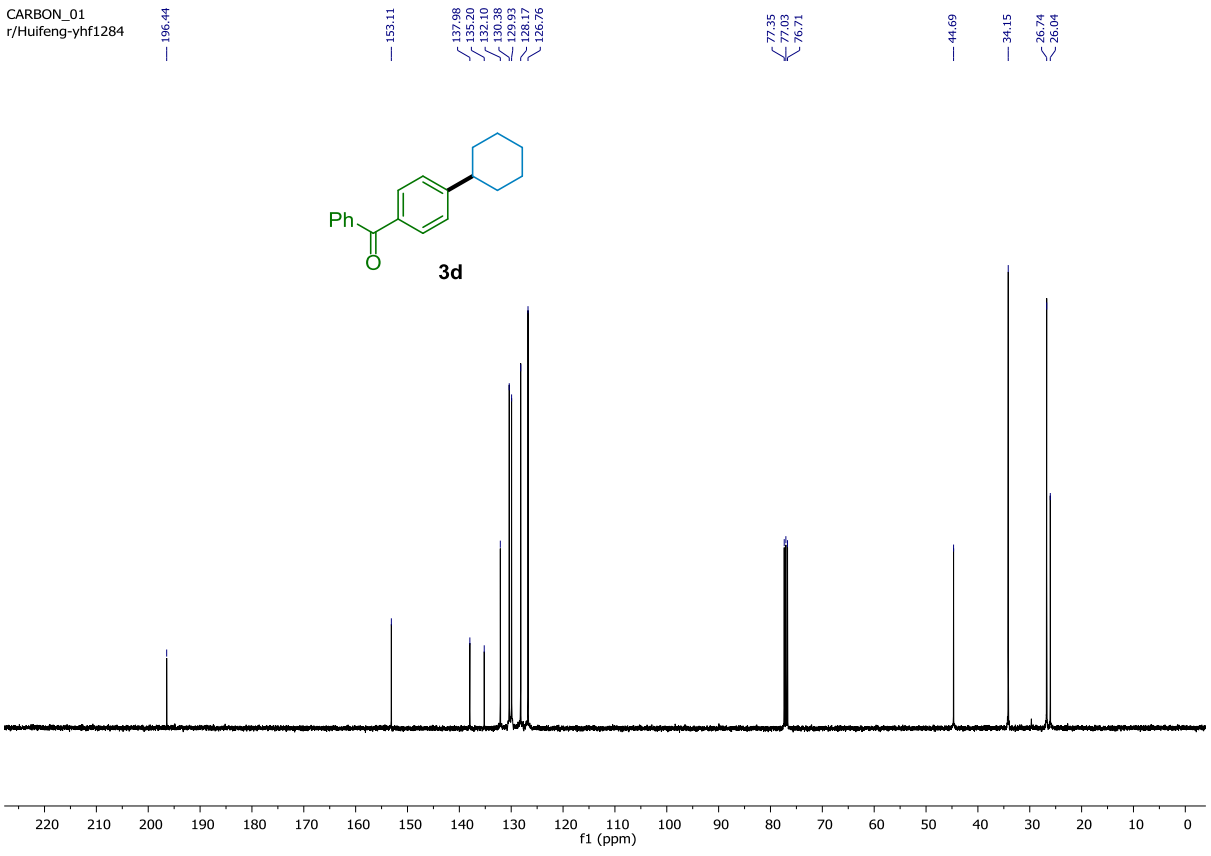

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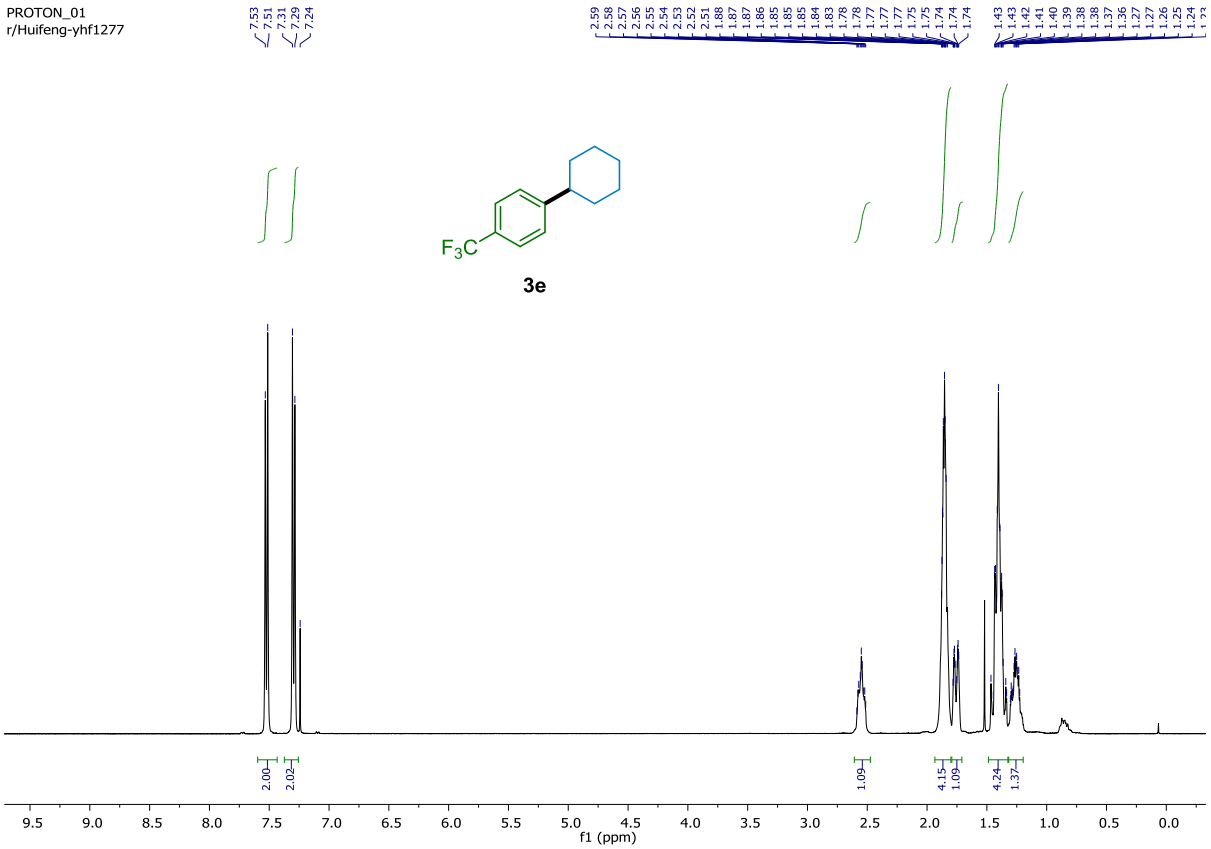

3e

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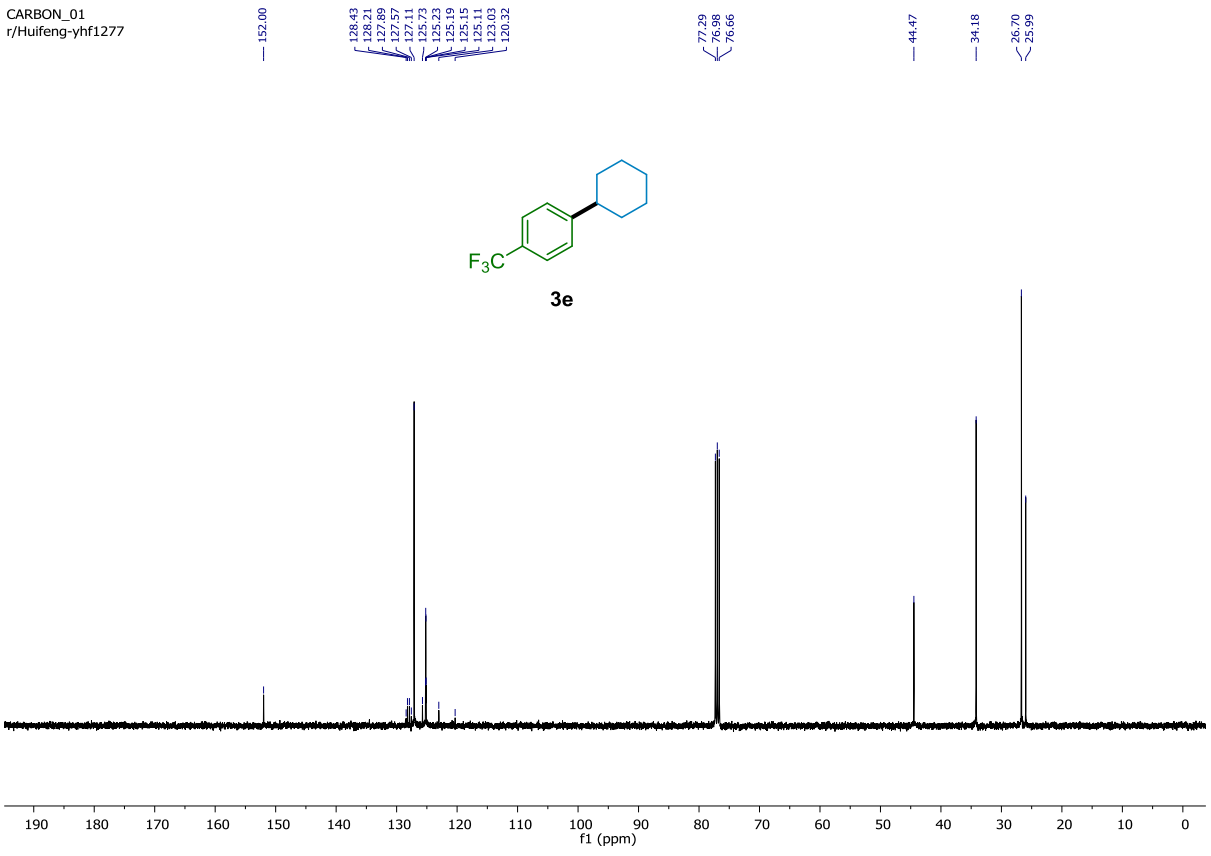
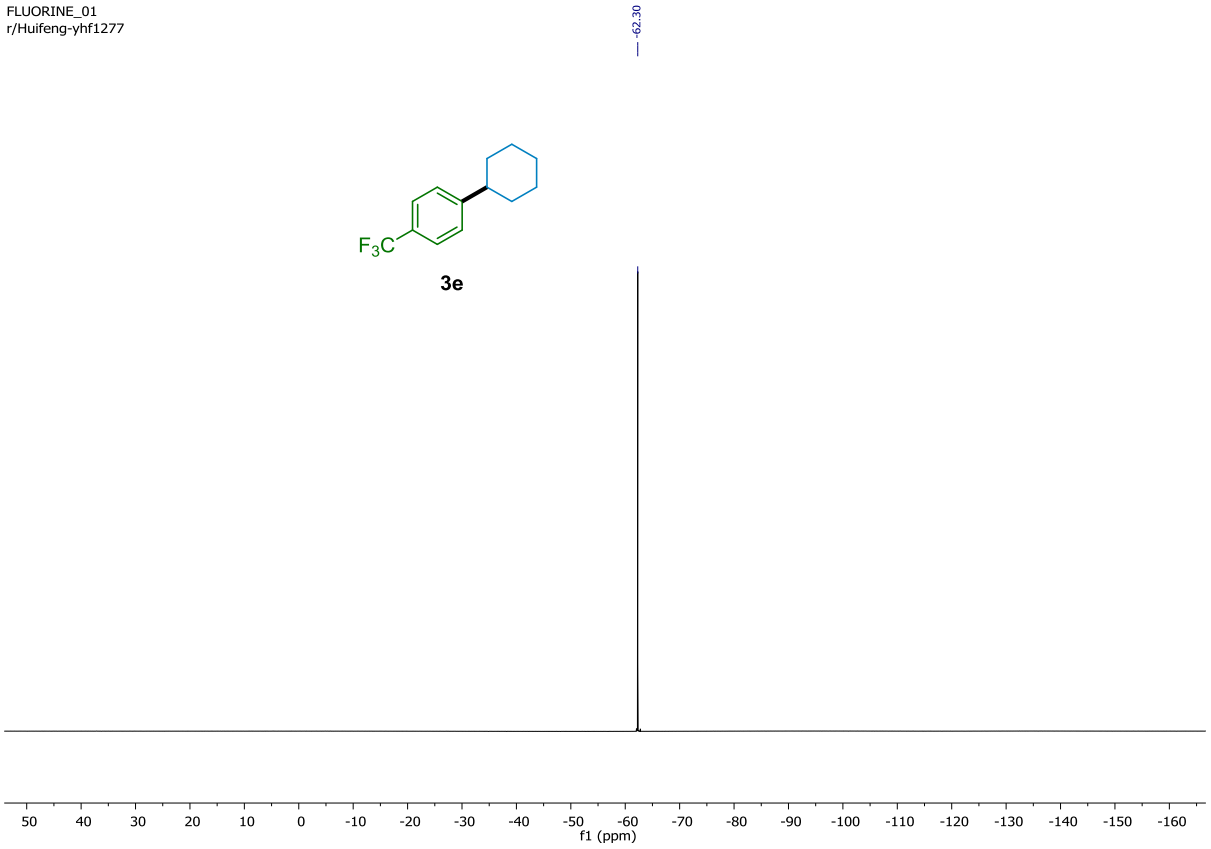


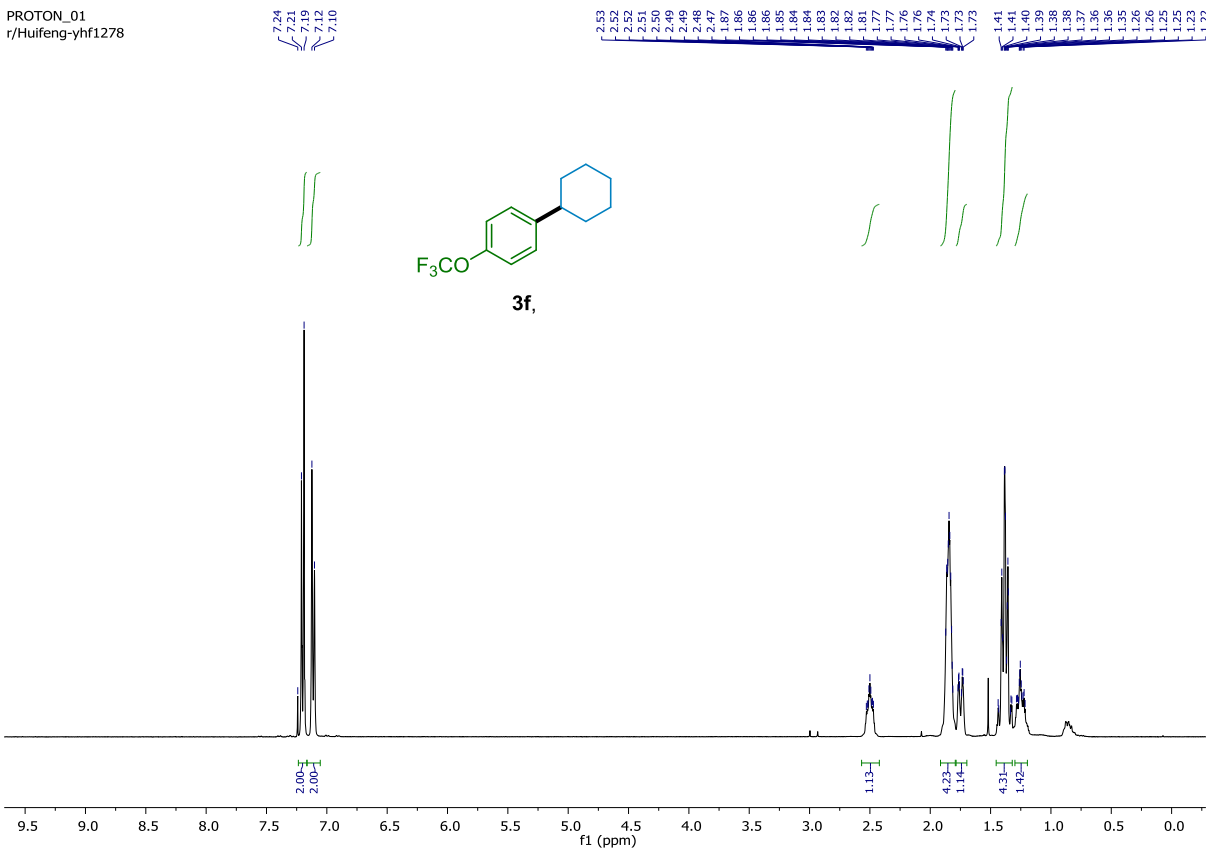
3e

FLUORINE_01
r/Huifeng-yhf1277



3e

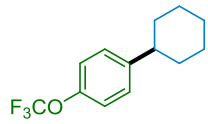
PROTON_01
r/Huifeng-yhf1278



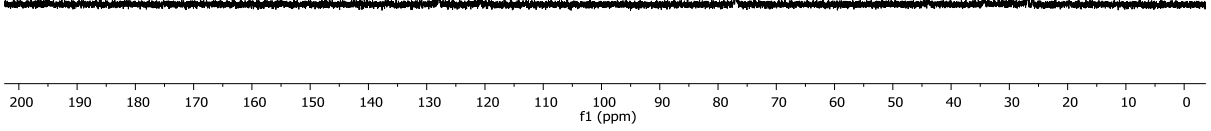
3f,

CARBON_01
r/Huifeng-yhf1278

147.24
147.22
147.20
146.70
127.94
124.35
121.80
120.75
119.25
116.70
77.39
76.97
76.65
43.94
34.43
26.76
26.02



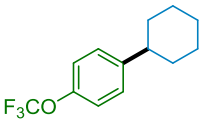
3f,



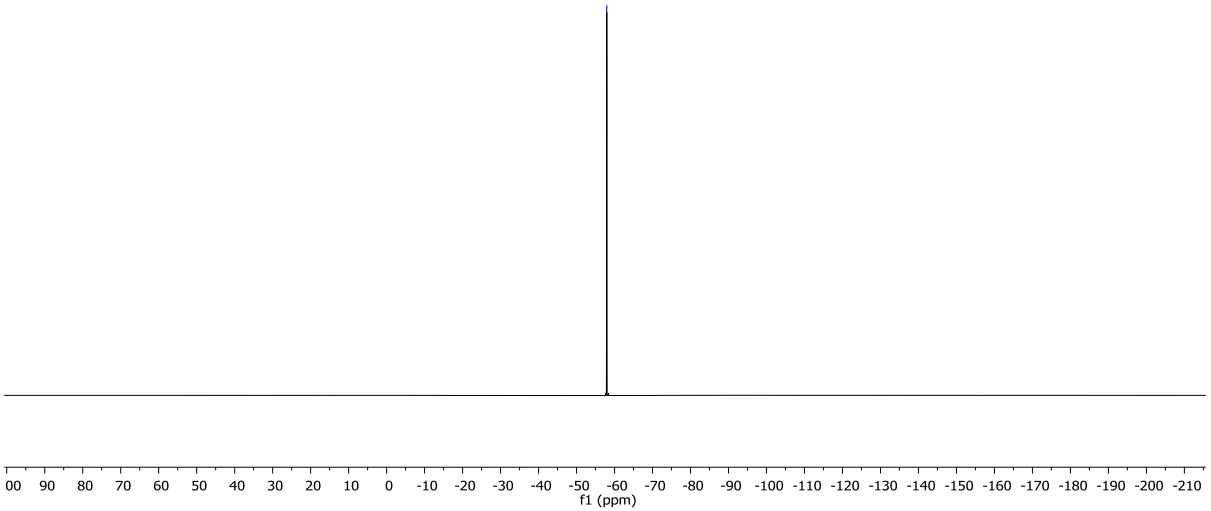
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

FLUORINE_01
r/Huifeng-yhf1278

-57.96

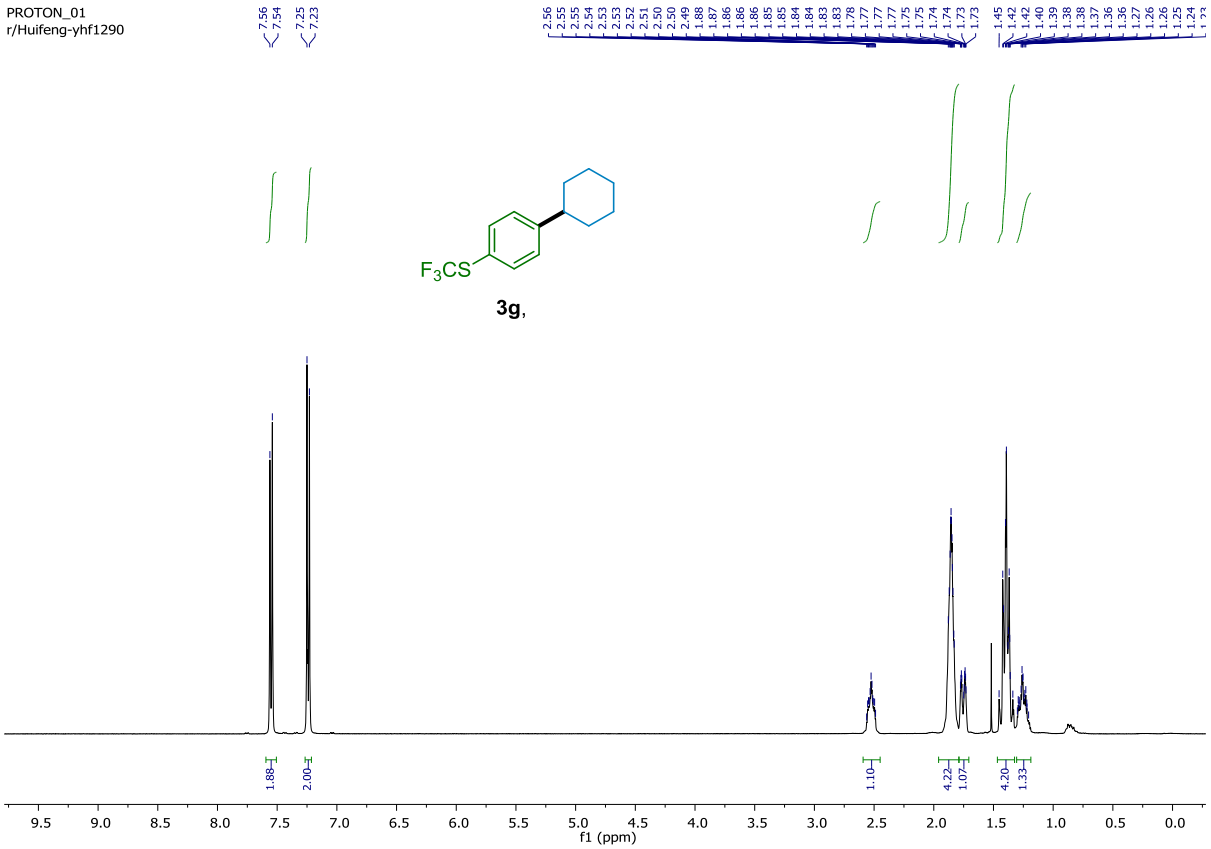


3f,



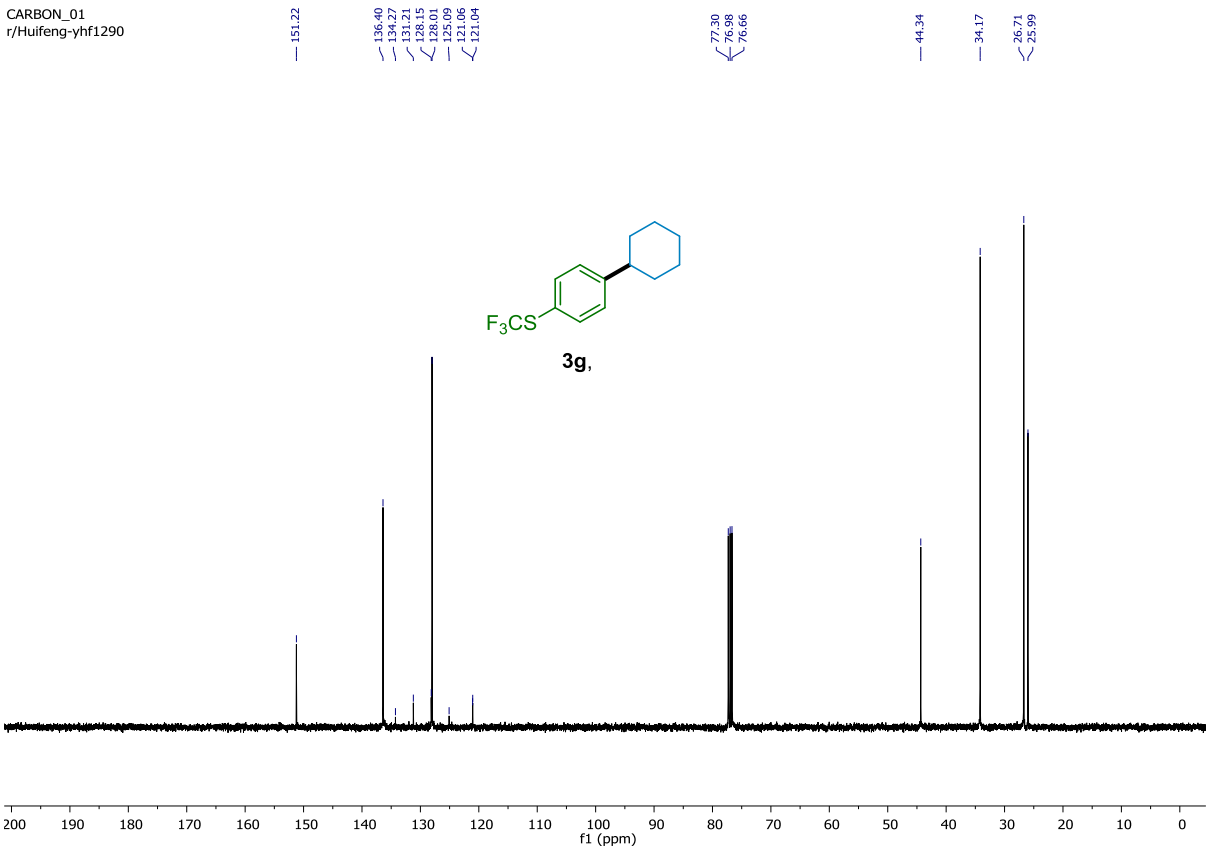
00 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

PROTON_01
r/Huifeng-yhf1290



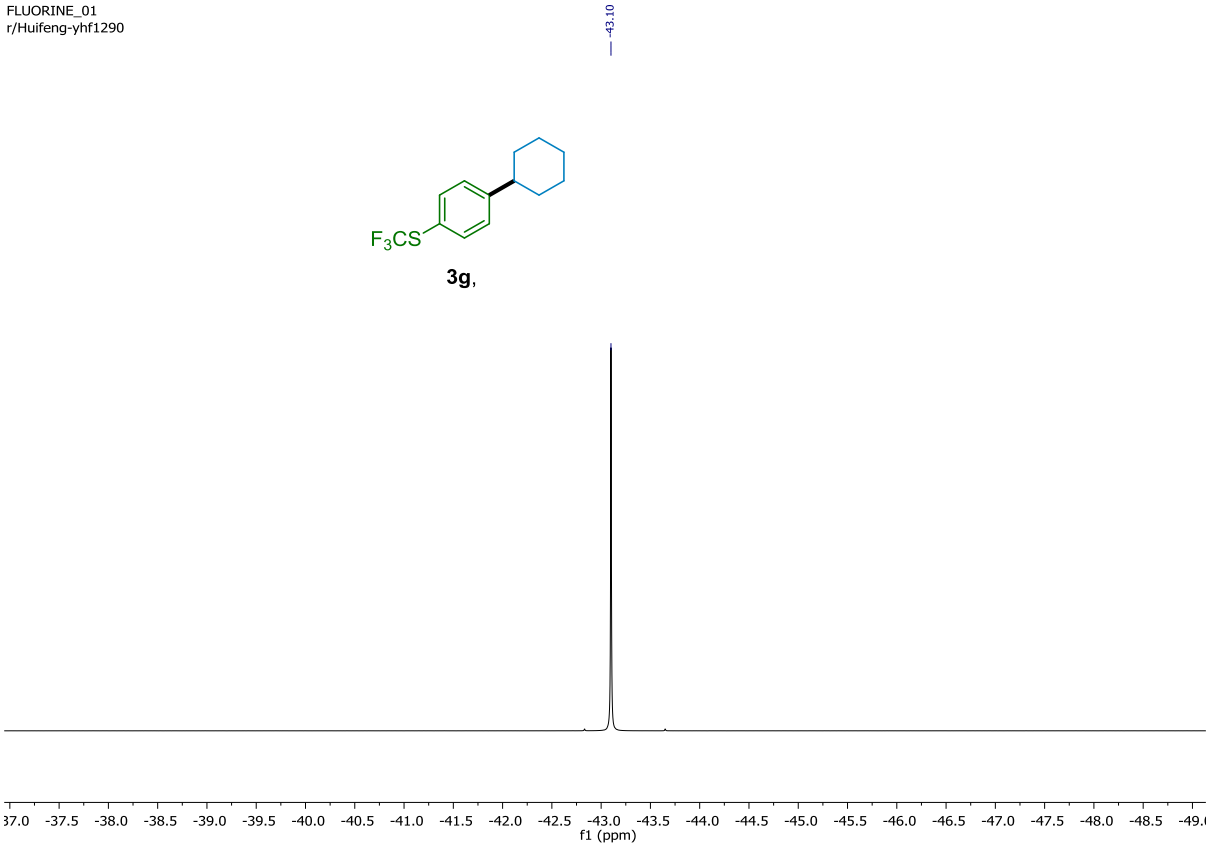
3g,

CARBON_01
r/Huifeng-yhf1290



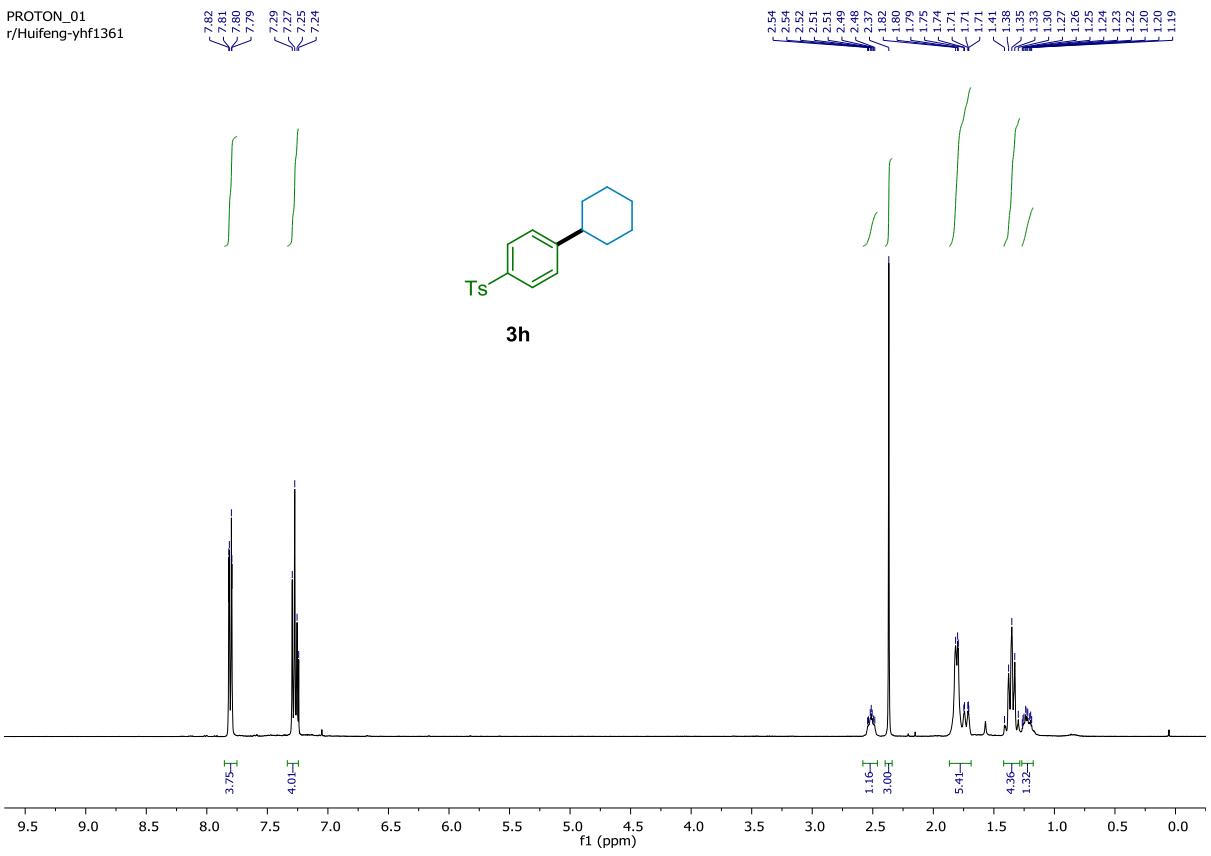
3g,

FLUORINE_01
r/Huifeng-yhf1290



3g,

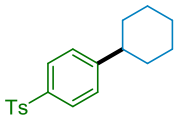
PROTON_01
r/Huifeng-yhf1361



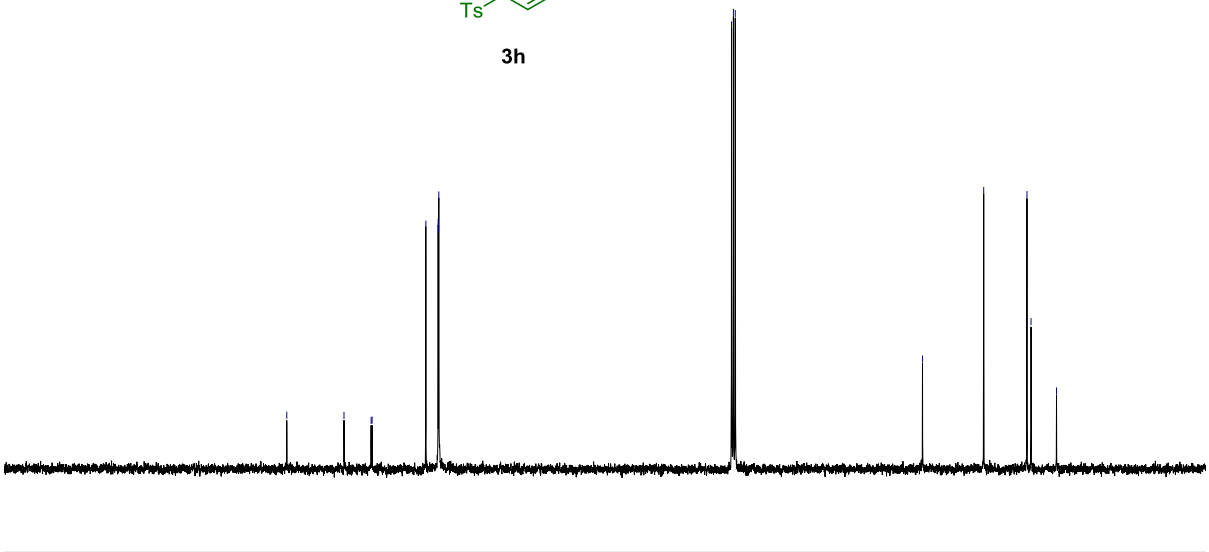
3h

CARBON_01
r/Huifeng-yhf1361

153.68
143.86
139.20
139.03
129.81
127.69
127.61
127.57
77.31
77.00
76.68
44.53
34.02
26.59
25.89
21.52



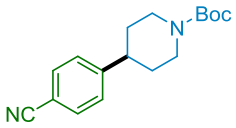
3h



200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

PROTON_01
r/Huifeng-yhf1347

7.57
7.55
7.28
7.26
7.24
4.22
2.80
2.77
2.74
2.72
2.71
2.70
2.69
2.68
2.67
2.66
2.65
2.64
1.79
1.76
1.62
1.61
1.59
1.58
1.56
1.55
1.52
1.51
1.44

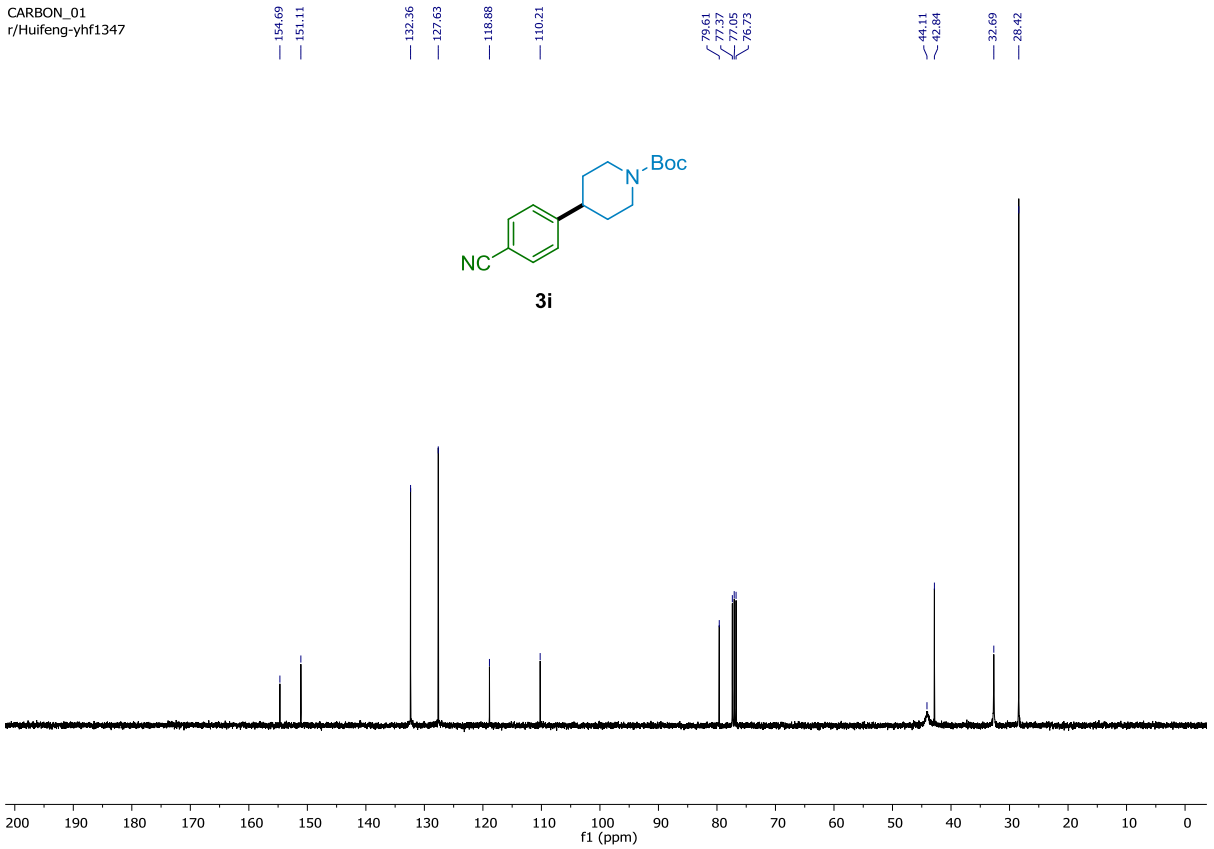


3i

2.00
2.02
2.00
3.26
2.15
2.30
9.04

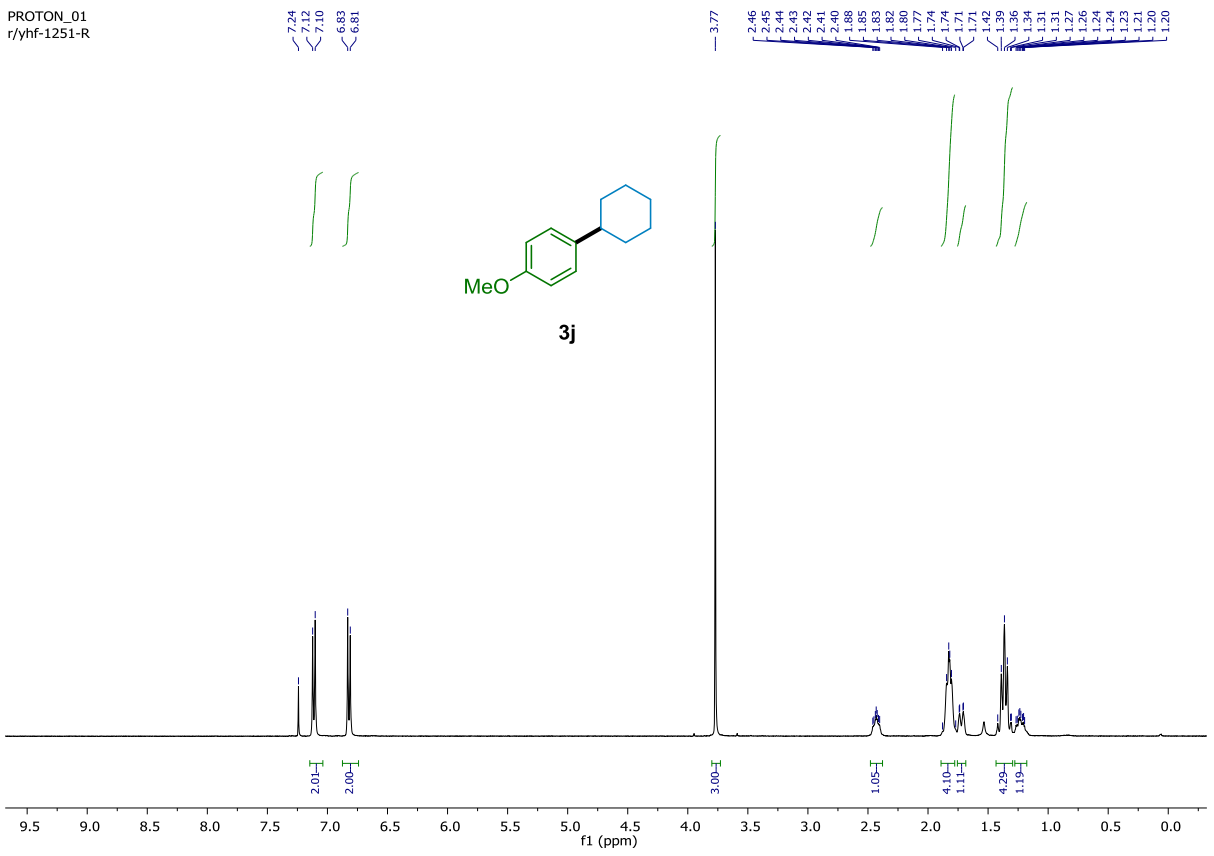
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

CARBON_01
r/Huifeng-yhf1347



3i

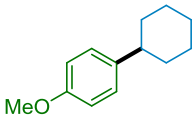
PROTON_01
r/yhf-1251-R



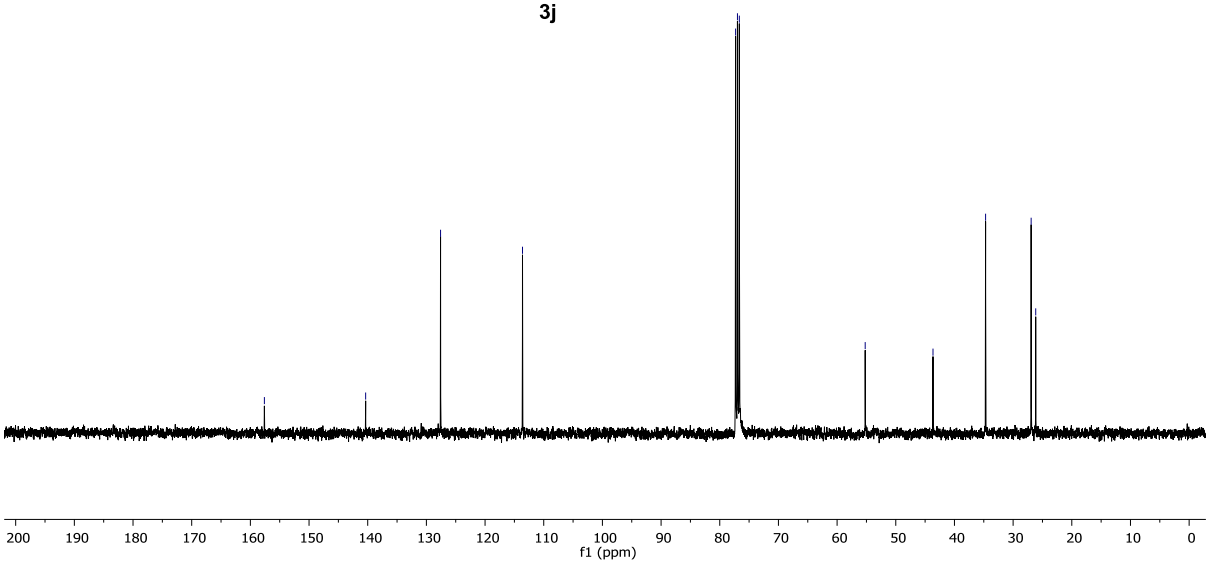
3j

CARBON_01
r/yhf-1251-R

157.61 140.35 127.59 113.62 77.30 76.98 76.66 55.21 43.66 34.69 26.93 26.15

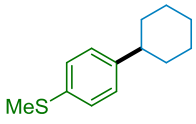


3j

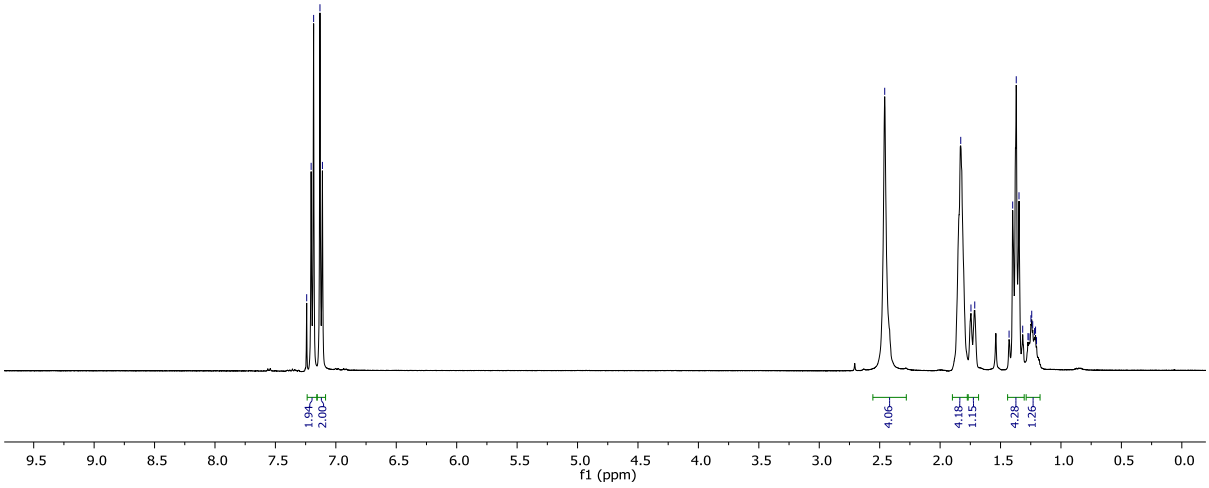


PROTON_01
r/yhf-1345-R

7.24 7.20 7.18 7.13 7.11 2.46 1.83 1.74 1.71 1.43 1.40 1.37 1.35 1.32 1.27 1.26 1.25 1.24 1.23 1.22 1.21 1.20

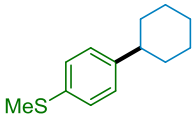


3k

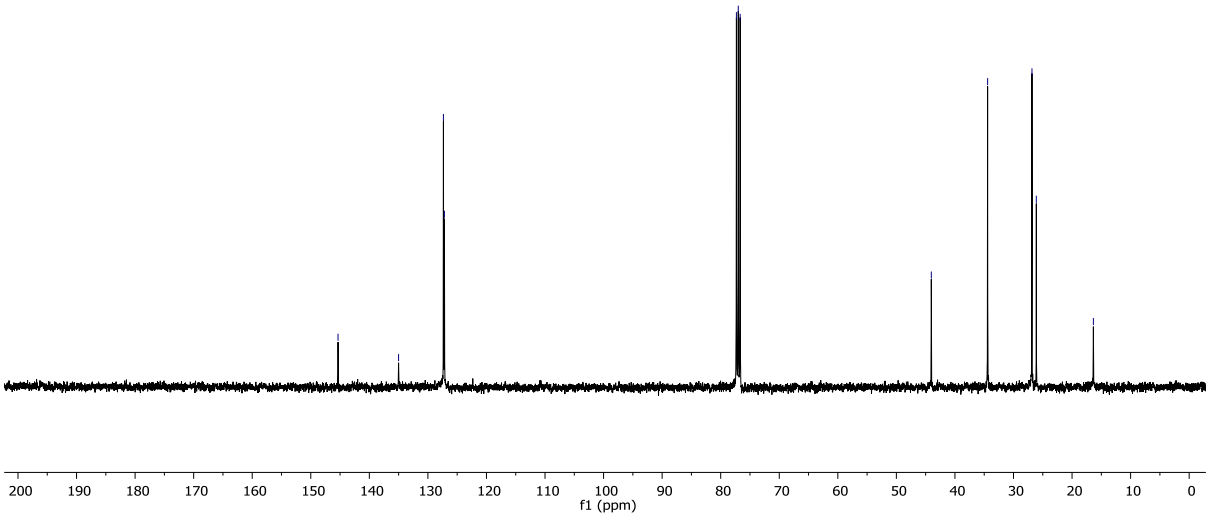


CARBON_01
r/yhf-1345-R

145.35 135.01 127.35 127.18 77.32 77.00 76.68 44.03 34.42 26.85 26.10 16.36



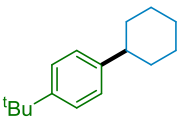
3k



PROTON_01
r/Huifeng-yhf1276

7.32 7.30 7.24 7.15 7.13

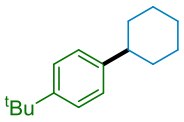
2.50 2.49 2.48 2.47 2.46 2.45 2.43 1.90 1.89 1.89 1.88 1.88 1.87 1.87 1.86 1.86 1.86 1.86 1.86 1.85 1.84 1.84 1.83 1.82 1.82 1.82 1.81 1.81 1.76 1.76 1.75 1.75 1.75 1.73 1.73 1.72 1.72 1.71 1.46 1.43 1.41 1.40 1.39 1.36 1.31 1.26 1.24 1.24 1.23



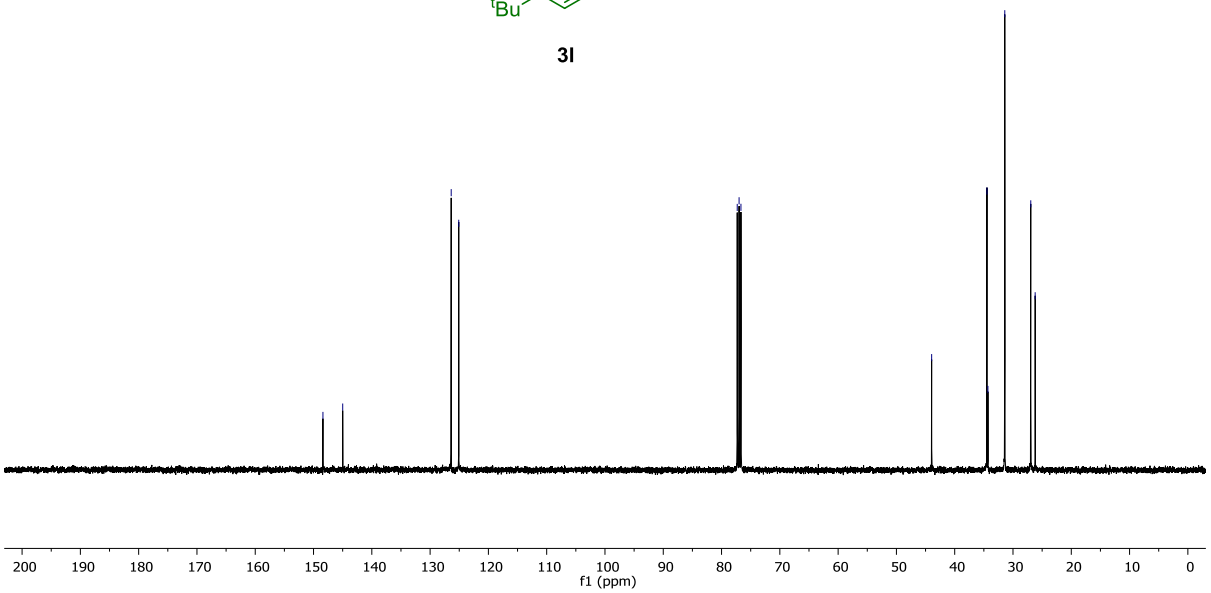
3l

CARBON_01
r/Huifeng-yhf1276

148.39
144.99
126.38
125.09
77.31
76.99
76.67
43.95
34.46
34.30
31.41
26.95
26.20

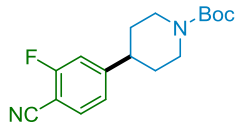


3l



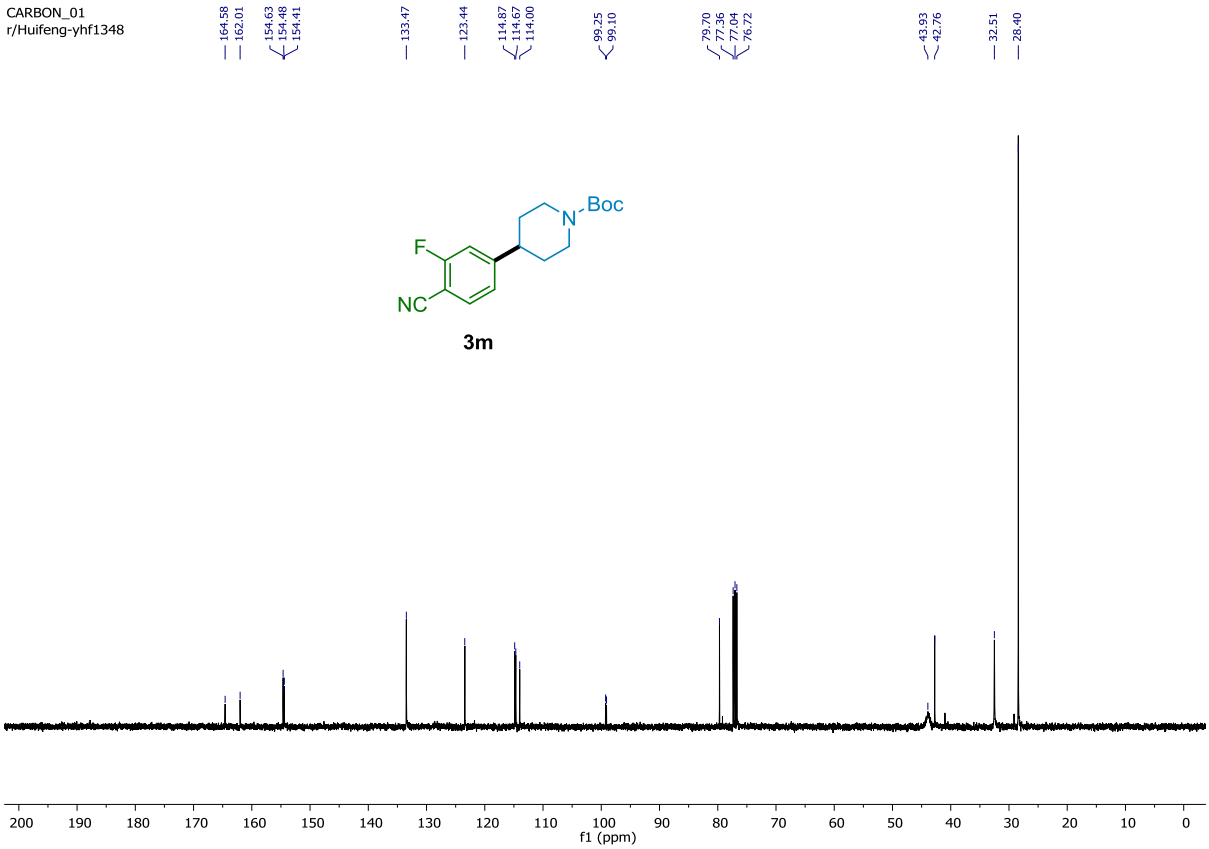
PROTON_01
r/Huifeng-yhf1348

7.54
7.52
7.52
7.50
7.24
7.08
7.08
7.06
7.06
7.03
7.01
4.24
2.79
2.76
2.73
2.72
2.70
2.69
2.68
2.67
2.66
2.65
1.80
1.77
1.59
1.58
1.56
1.55
1.53
1.52
1.44



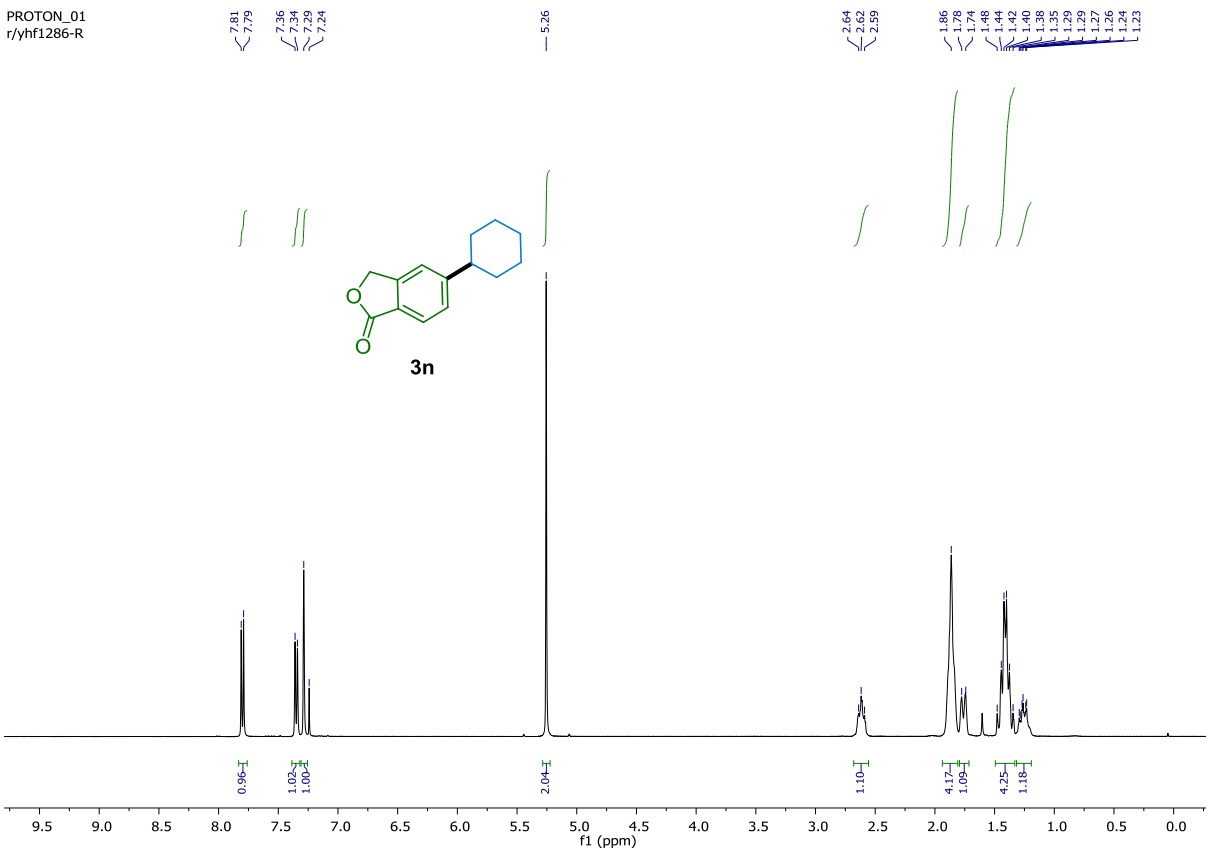
3m

CARBON_01
r/Huifeng-yhf1348

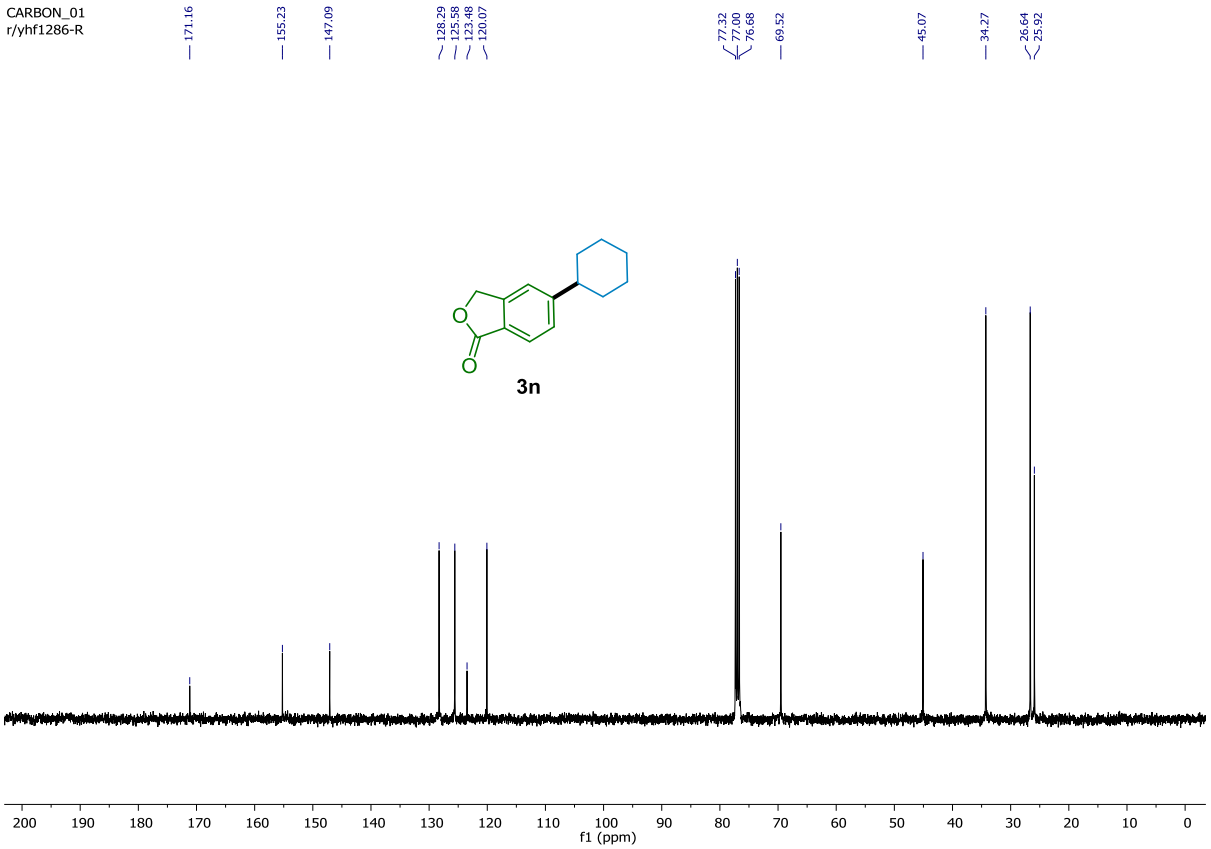


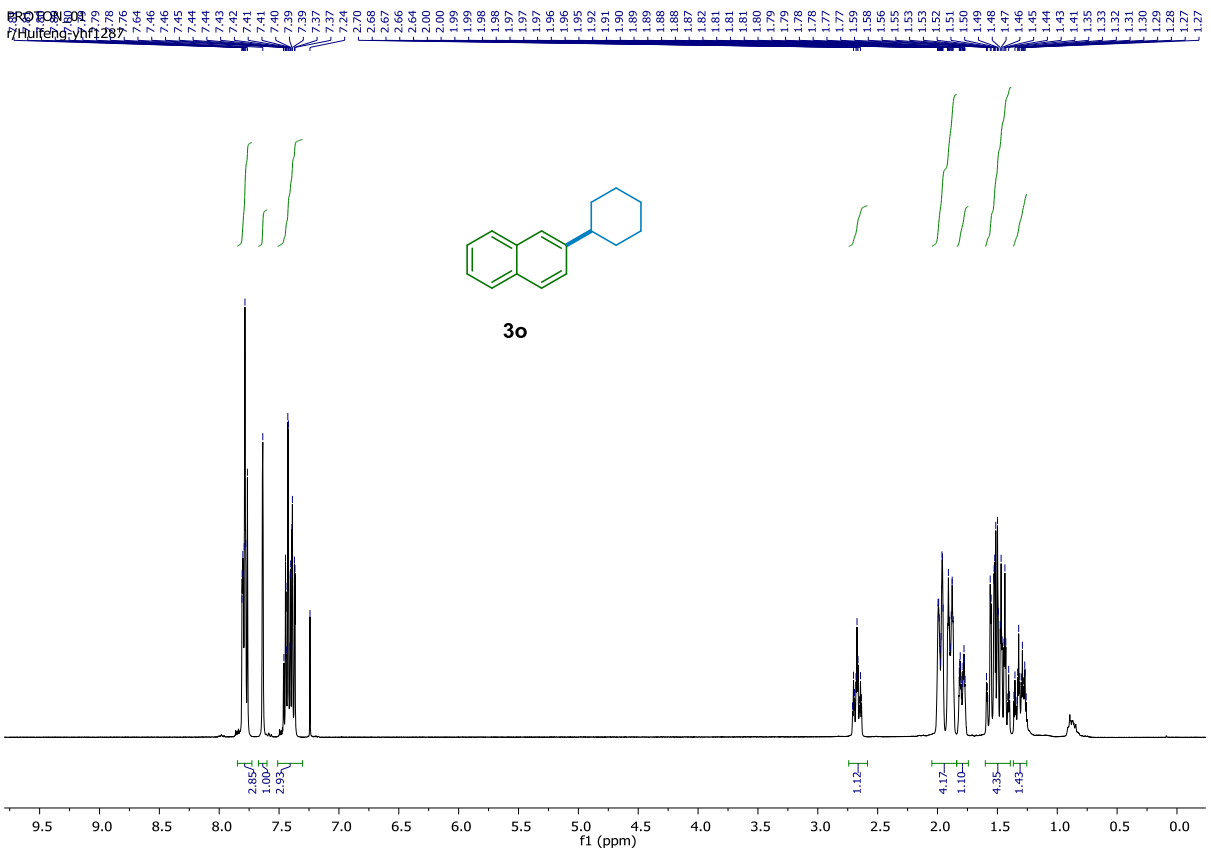
3m

PROTON_01
r/yhf1286-R



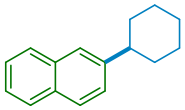
3n


CARBON_01
r/yhf1286-R
171.16
155.23
147.09
128.29
125.58
123.48
120.07
77.32
77.00
76.68
69.52
45.07
34.27
26.64
25.92
3n
f1 (ppm)

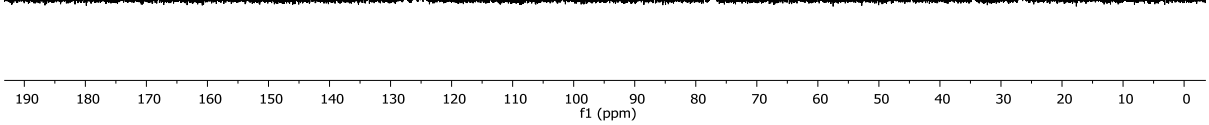

PROTON_01
r/Huifeng-yhf1287
3o
2.85
1.00
2.93
1.12
4.17
1.10
4.35
1.43
f1 (ppm)

CARBON_01
r/Huifeng-yhf1287

145.56
133.68
132.10
127.70
127.58
127.53
126.19
125.74
125.00
124.51
77.33
77.01
76.69
44.67
34.42
26.95
26.23



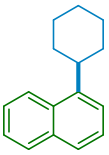
3o



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

PROTON_01
r/yue-yhf1256-1

8.16
8.13
7.89
7.86
7.73
7.70
7.56
7.55
7.55
7.54
7.53
7.53
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.40
7.40
3.38
3.35
3.33
2.08
2.05
1.93
1.89
1.85
1.85
1.66
1.62
1.58
1.55
1.53
1.51
1.43
1.42
1.40
1.39
1.38
1.36
1.35



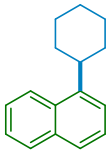
3p

1.09
0.98
0.92
3.92
1.00
5.37
4.48
1.13

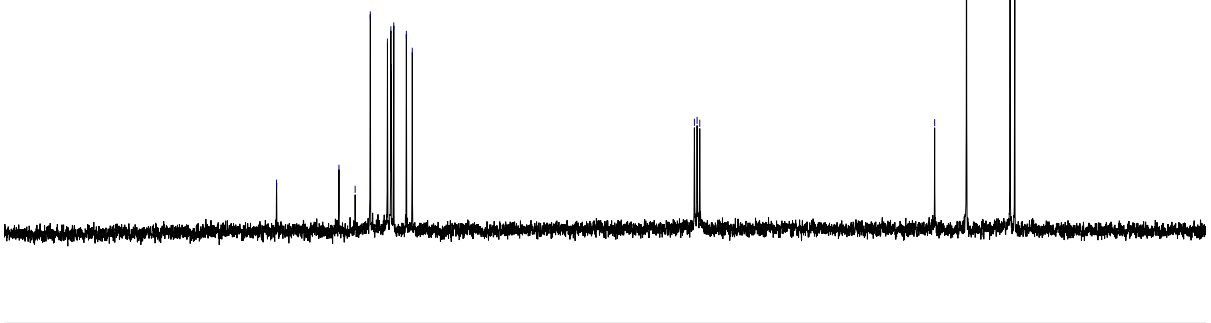
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

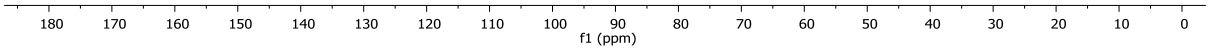
CARBON_01
r/yue-yhf1256-1

143.84
133.93
131.36
128.95
126.22
125.68
125.60
125.22
123.22
122.28
77.46
77.03
76.61
39.29
34.23
27.31
26.56



3p

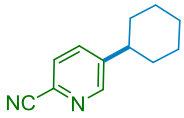




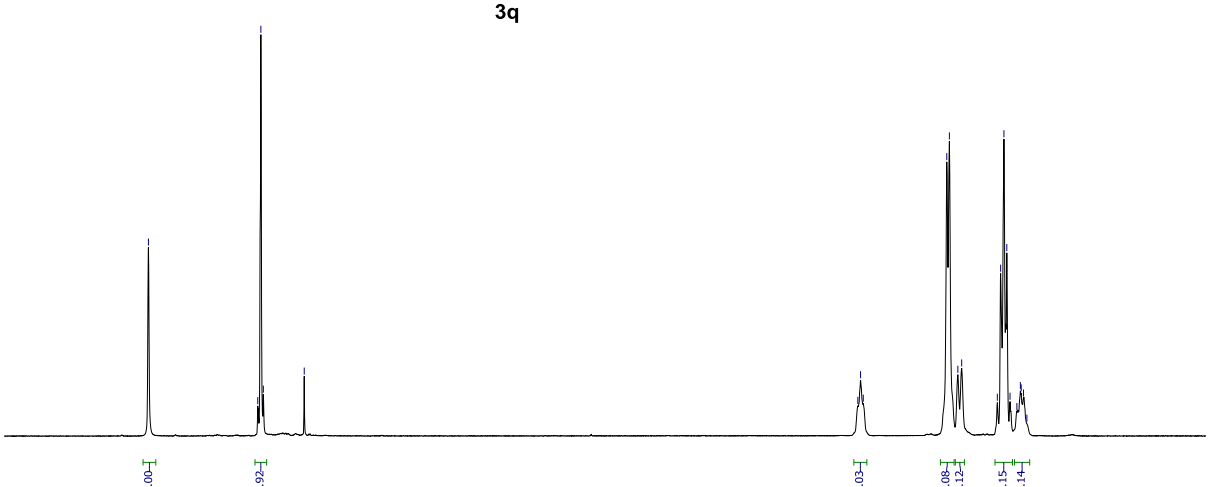
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

PROTON_01
r/yhf-1288-R

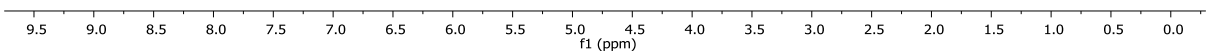
8.54
7.63
7.60
7.58
7.24
2.62
2.59
2.57
1.87
1.85
1.78
1.75
1.45
1.42
1.39
1.37
1.34
1.29
1.26
1.25
1.23
1.20



3q



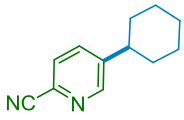
1.00
1.92
1.03
4.08
1.12
4.15
1.14



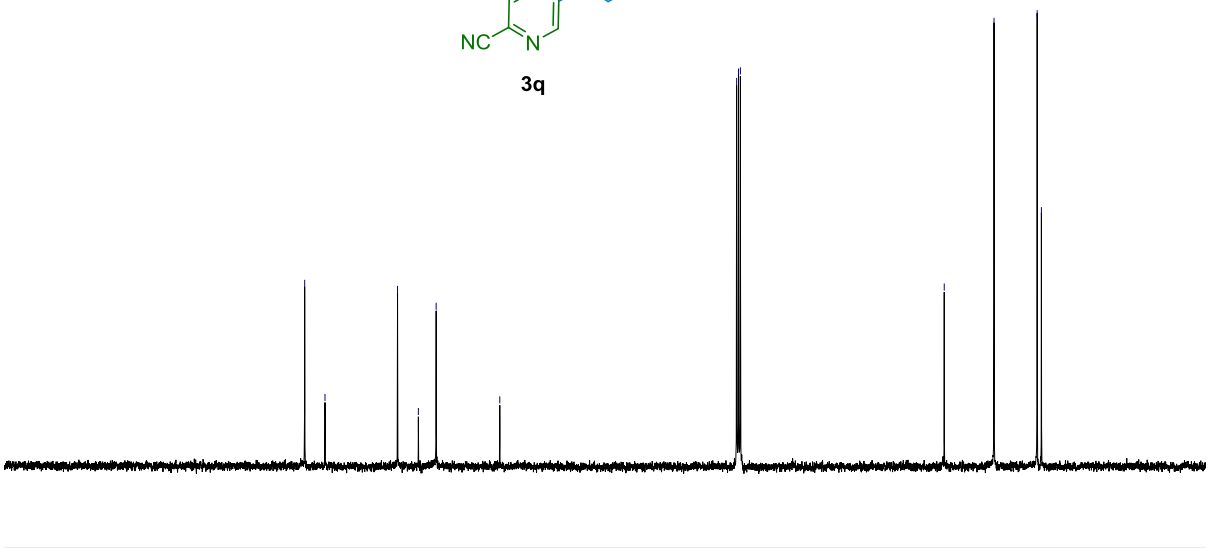
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

CARBON_01
r/yhf-1288-R

150.54
147.10
134.81
131.27
128.26
117.47
77.32
77.00
76.69
42.13
33.69
26.38
25.66

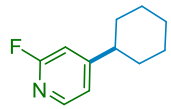


3q

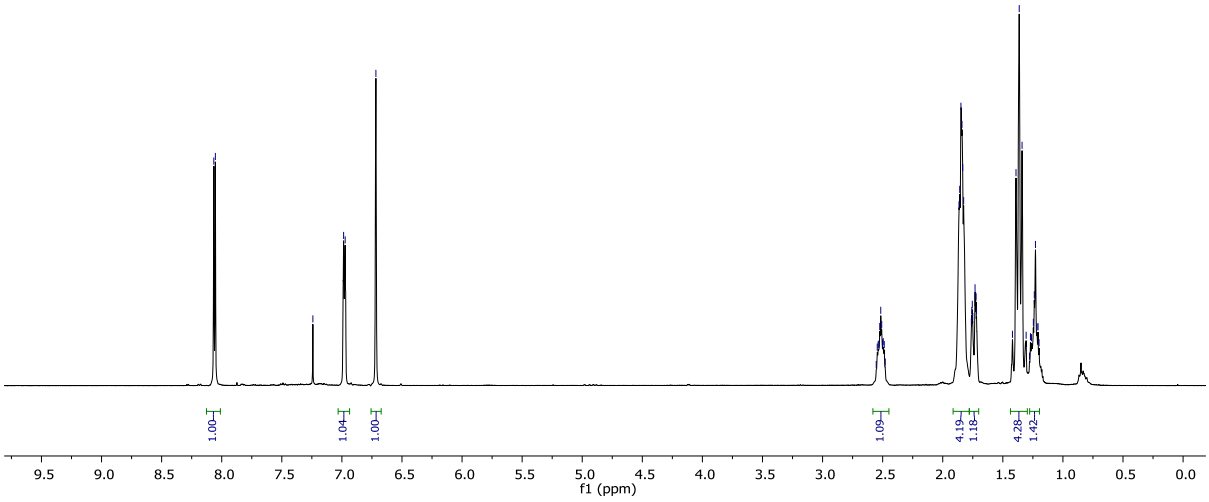


PROTON_01
r/Huifeng-yhf1365

8.07
8.05
7.24
6.99
6.97
6.72
2.55
2.55
2.54
2.54
2.53
2.52
2.52
2.52
2.51
2.50
2.50
2.49
2.48
1.86
1.86
1.85
1.84
1.84
1.83
1.83
1.76
1.76
1.75
1.75
1.73
1.73
1.72
1.72
1.42
1.39
1.36
1.34
1.31
1.28
1.27
1.26
1.25
1.24
1.23
1.22
1.21
1.20

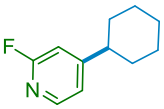


3r



CARBON_01
r/Huifeng-yhf1365

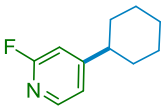
165.34
162.98
162.75
162.68
147.31
147.15
120.18
120.14
107.60
107.23
77.32
77.00
76.68
43.73
33.35
26.35
25.79



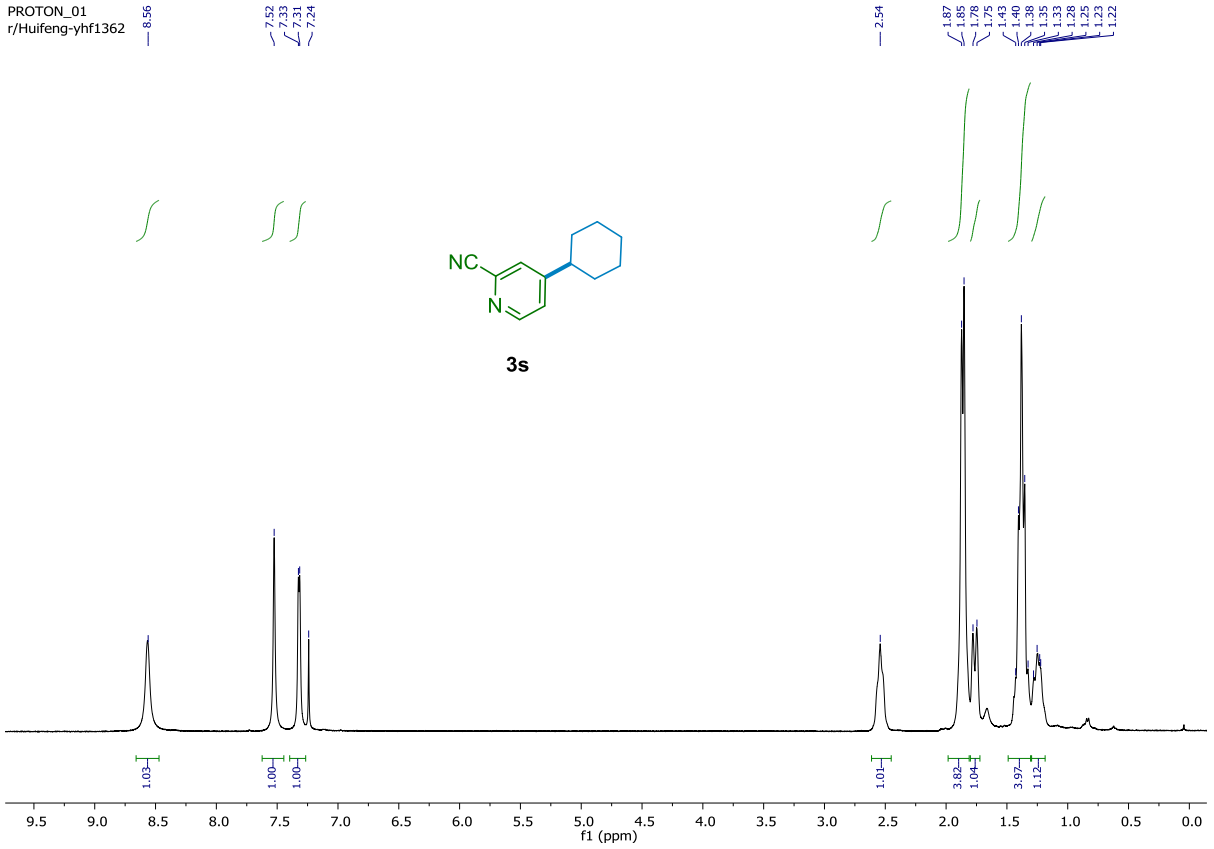
3r

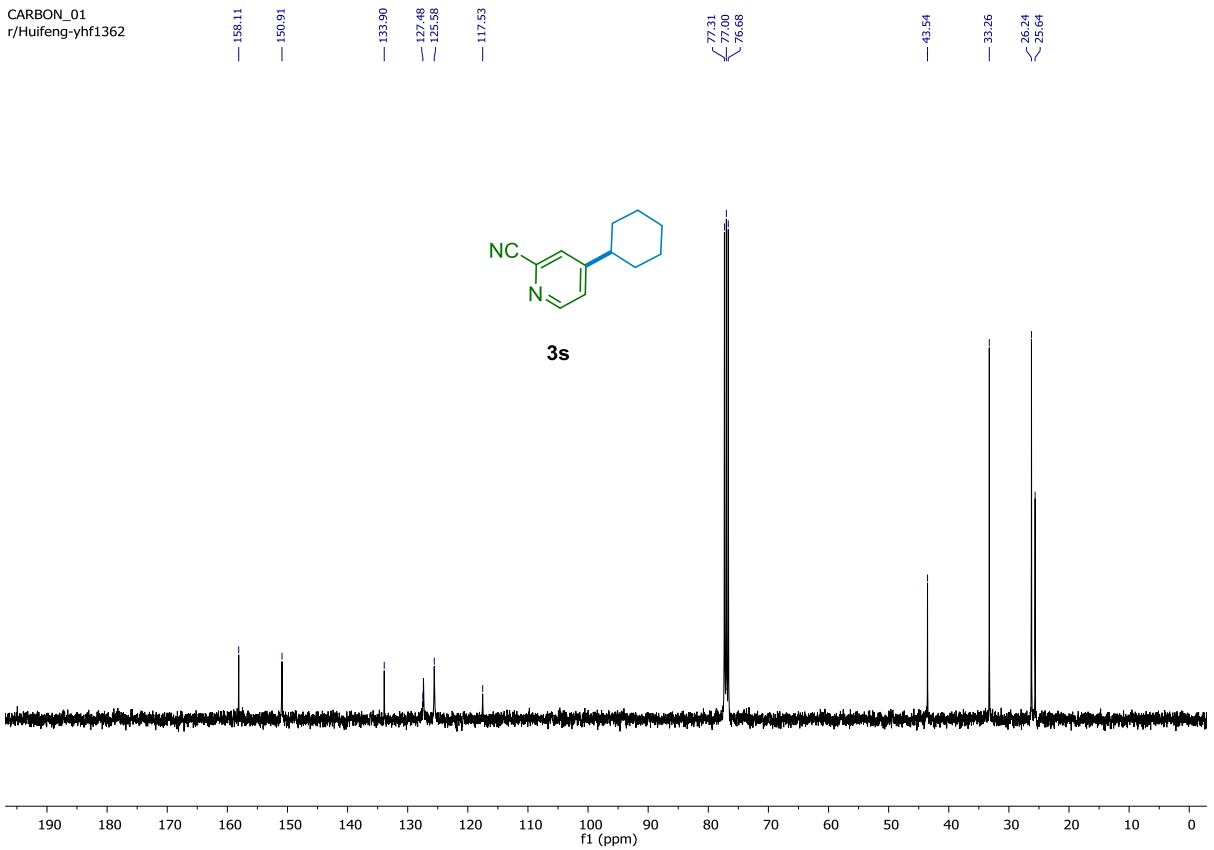
FLUORINE_01
r/Huifeng-yhf1365

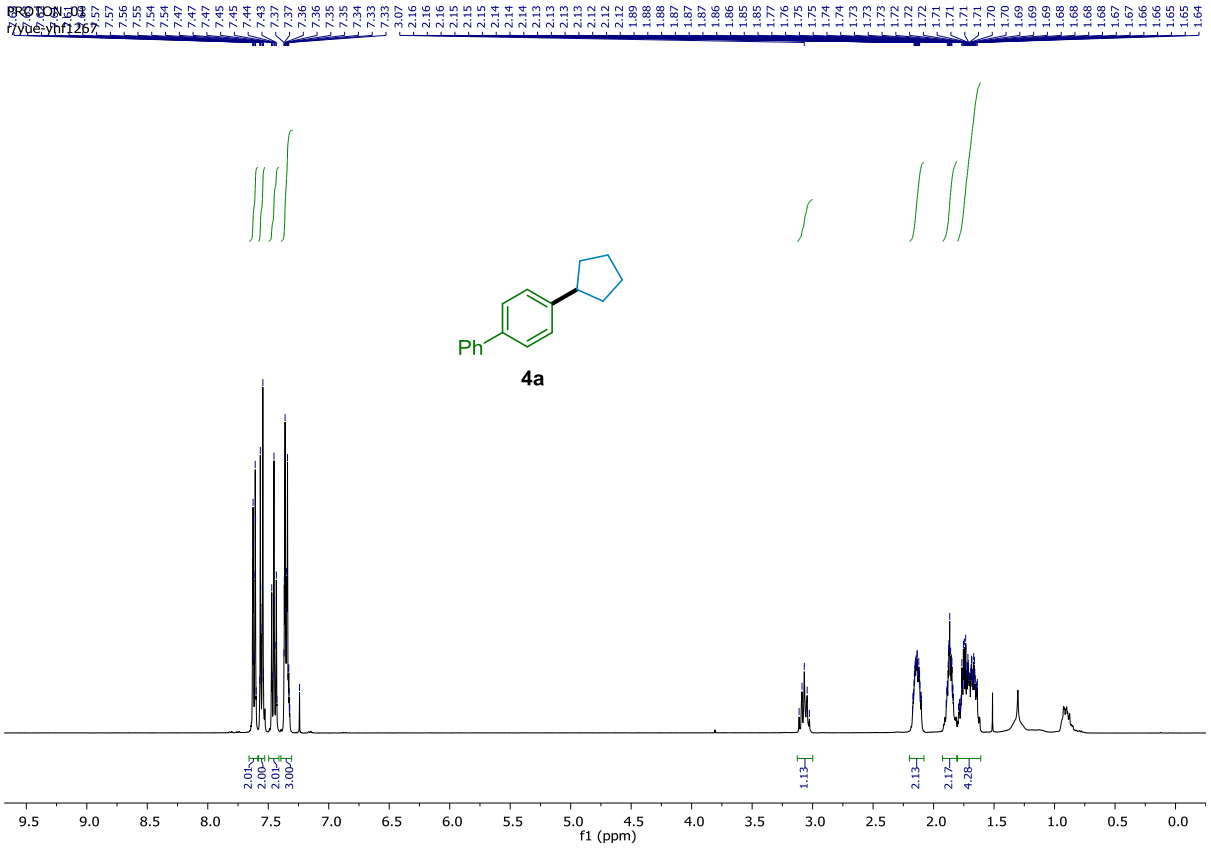
-69.17

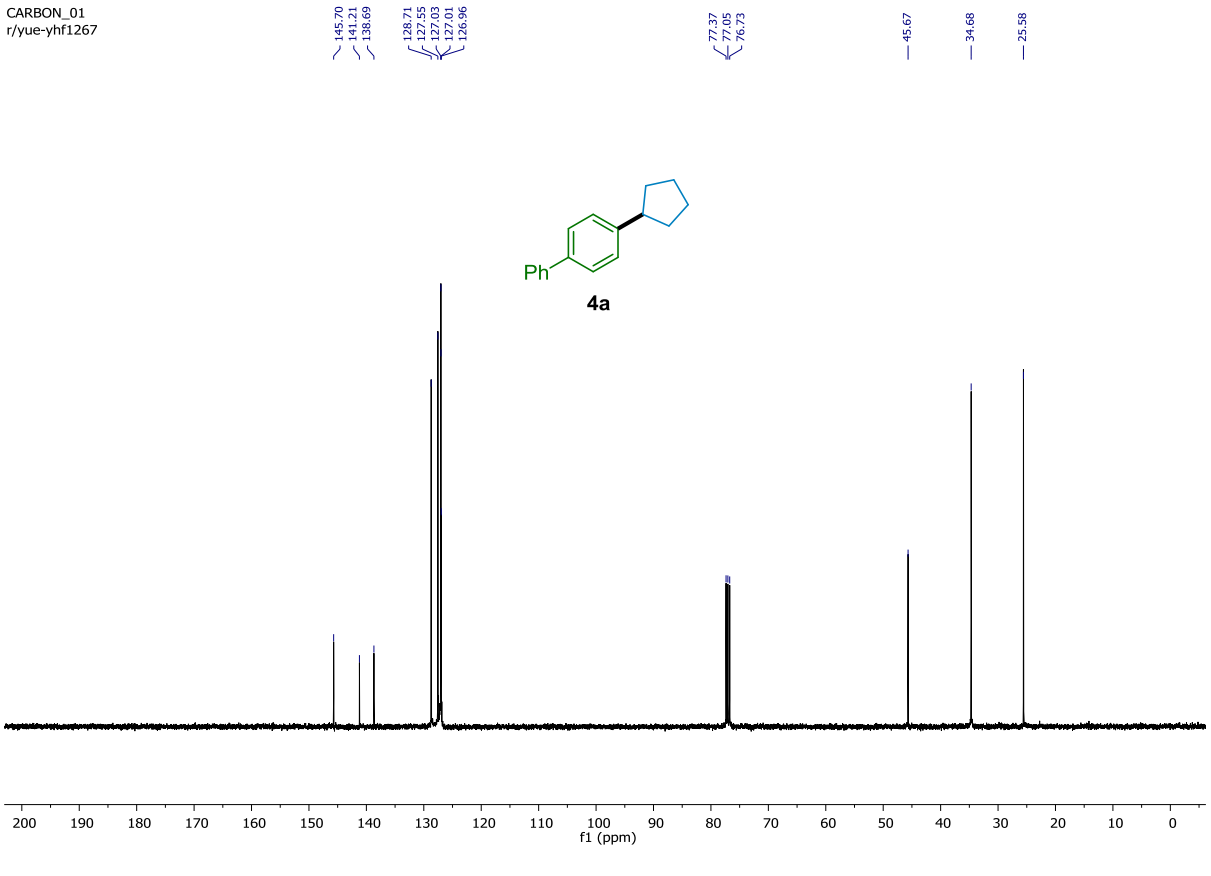


3r

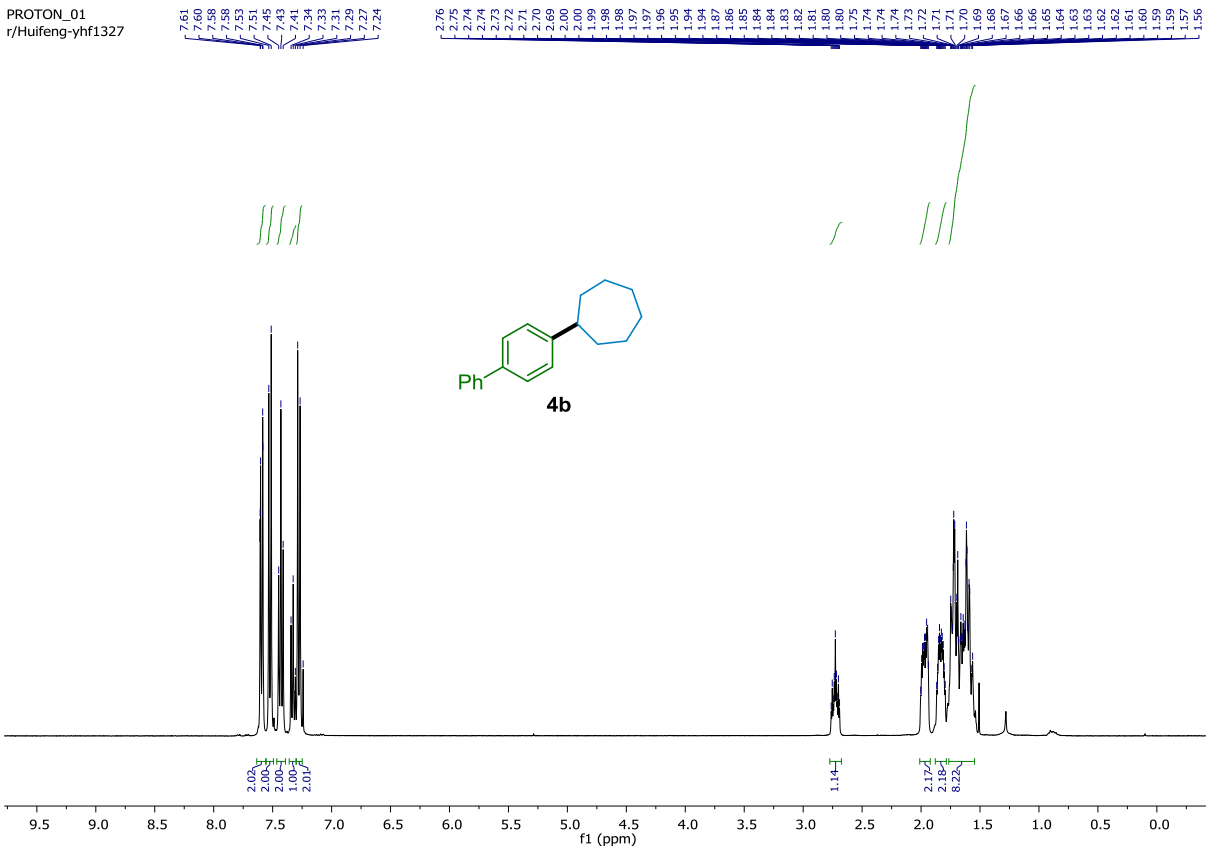

PROTON_01
r/Huifeng-yhf1362
8.56
7.52
7.33
7.31
7.24
2.54
1.87
1.85
1.78
1.75
1.43
1.40
1.38
1.35
1.33
1.28
1.25
1.23
1.22
NC
N
3s
1.03
1.00
1.00
1.01
3.82
1.04
3.97
1.12
f1 (ppm)


CARBON_01
r/Huifeng-yhf1362
158.11
150.91
133.90
127.48
125.58
117.53
77.31
77.00
76.68
43.54
33.26
26.24
25.64
NC
N
3s
f1 (ppm)

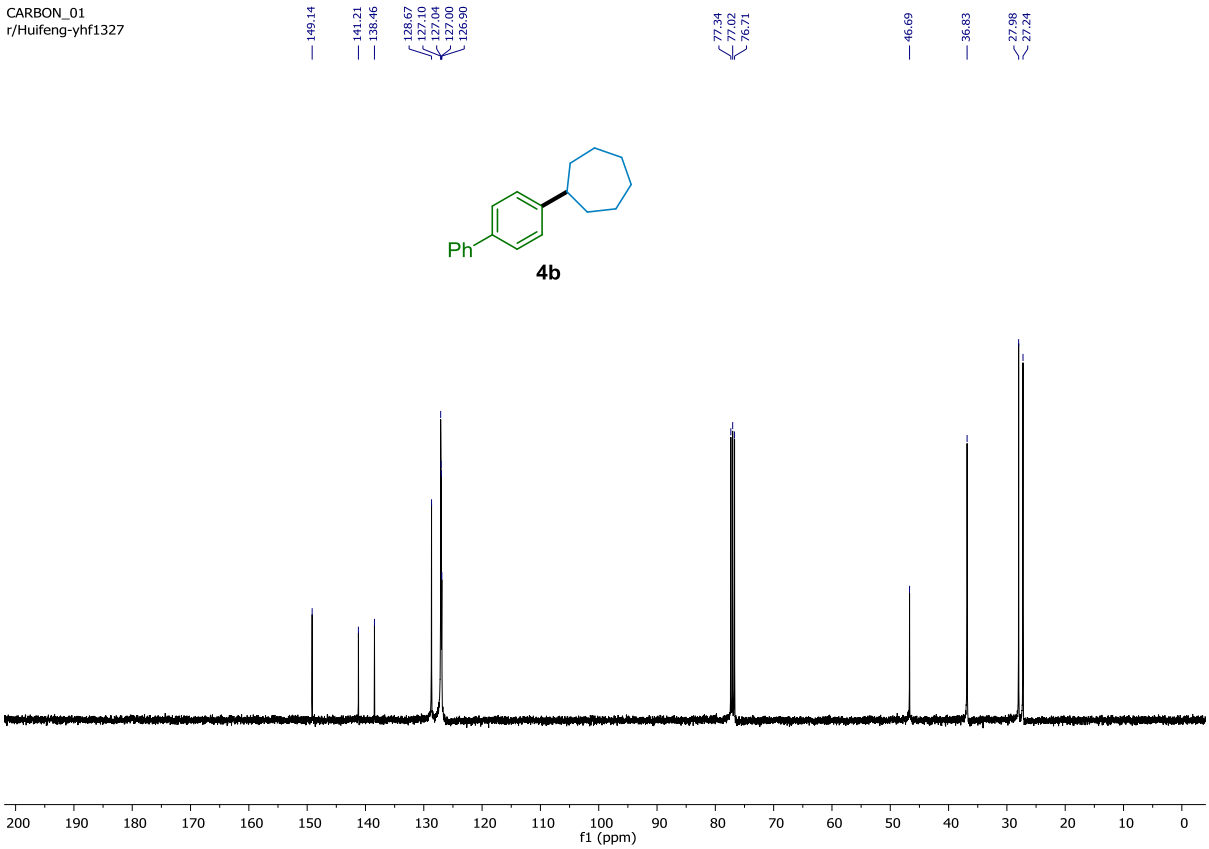

PROTON_01
r/yue-yhf1267
Ph
4a
2.01
2.00
2.01
3.00
1.13
2.13
2.17
4.28
f1 (ppm)


CARBON_01
r/yue-yhf1267
145.70
141.21
138.69
128.71
127.55
127.03
127.01
126.96
77.37
77.05
76.73
45.67
34.68
25.58
Ph
4a
f1 (ppm)

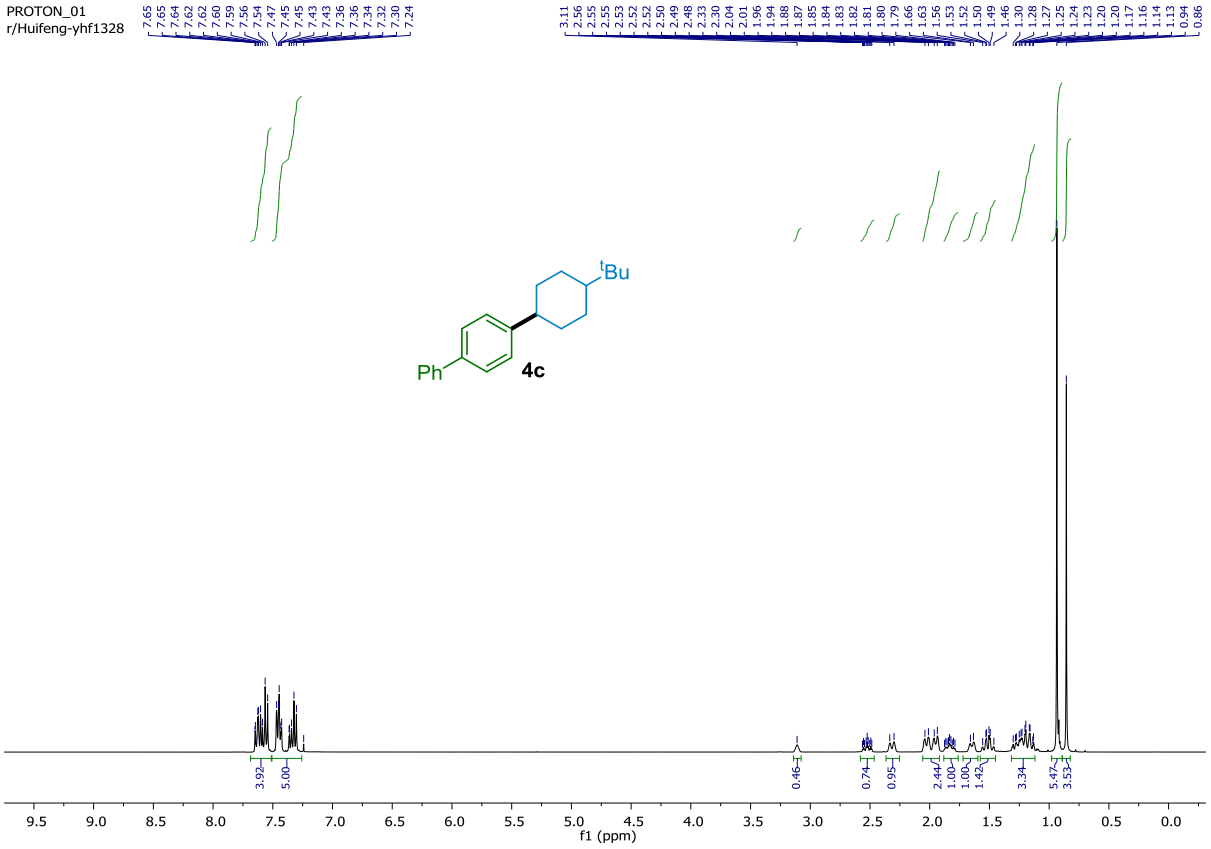
PROTON_01
r/Huifeng-yhf1327



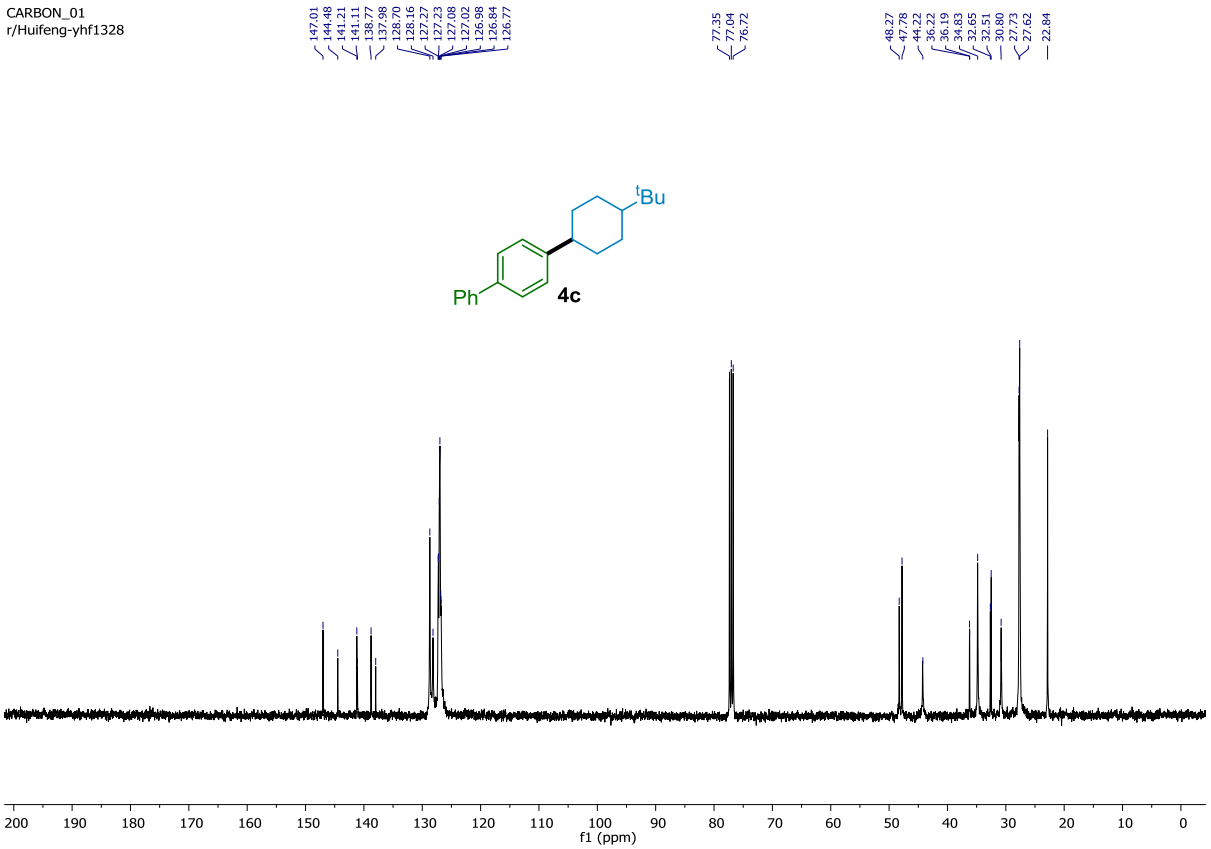
CARBON_01
r/Huifeng-yhf1327



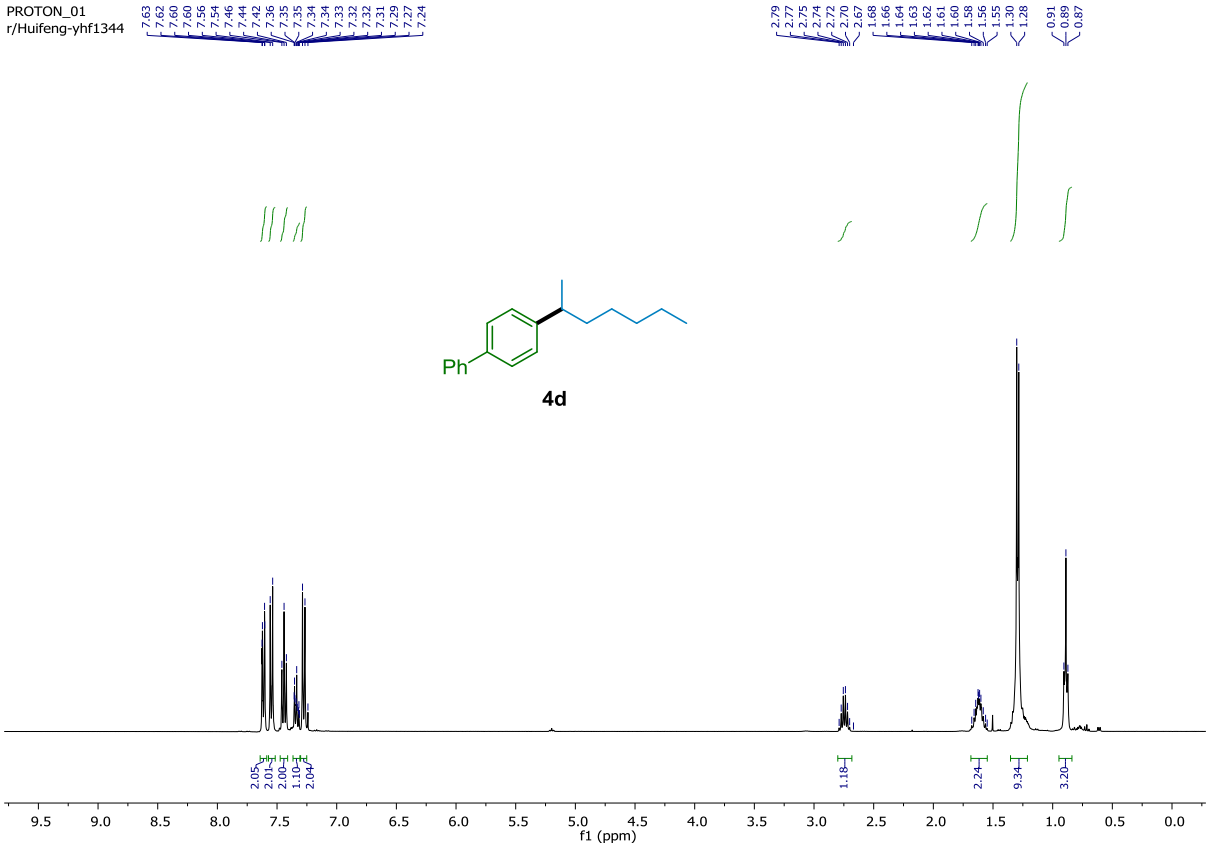
PROTON_01
r/Huifeng-yhf1328



CARBON_01
r/Huifeng-yhf1328

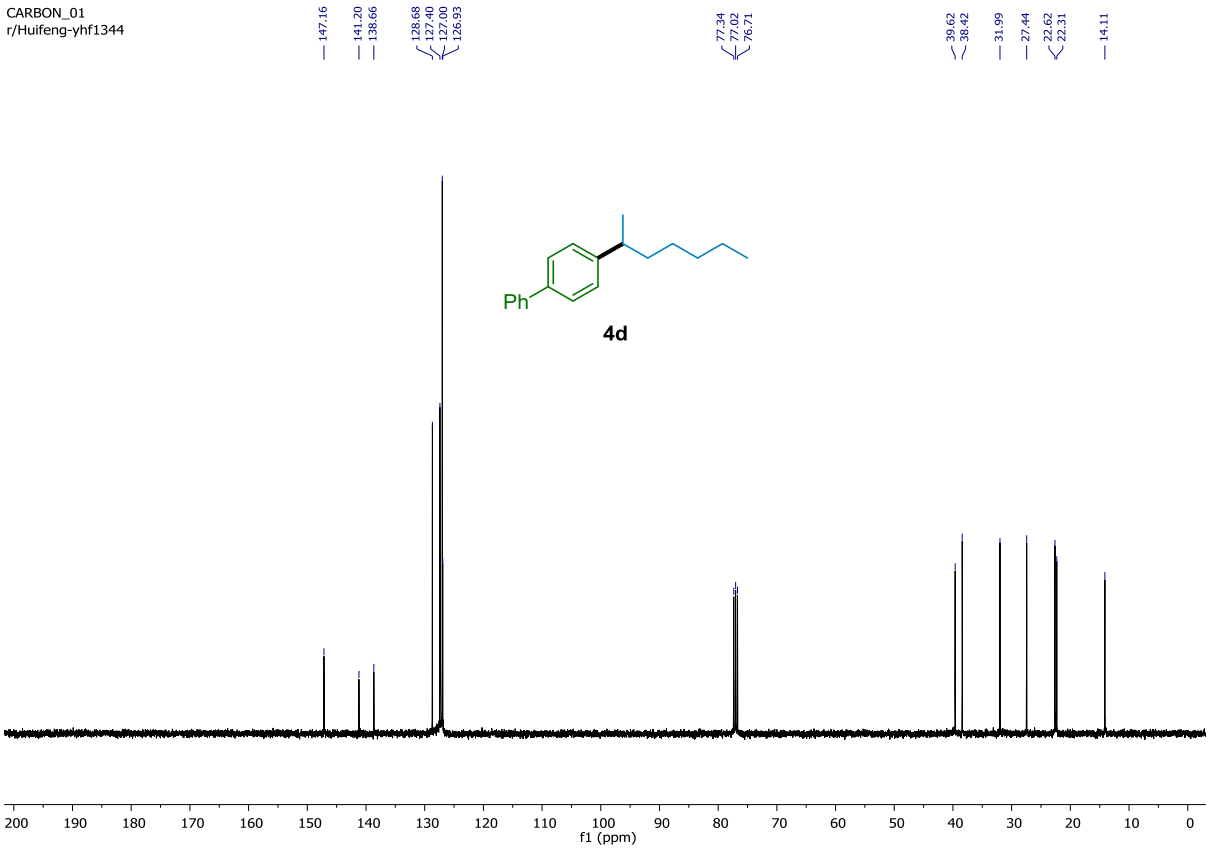


PROTON_01
r/Huifeng-yhf1344



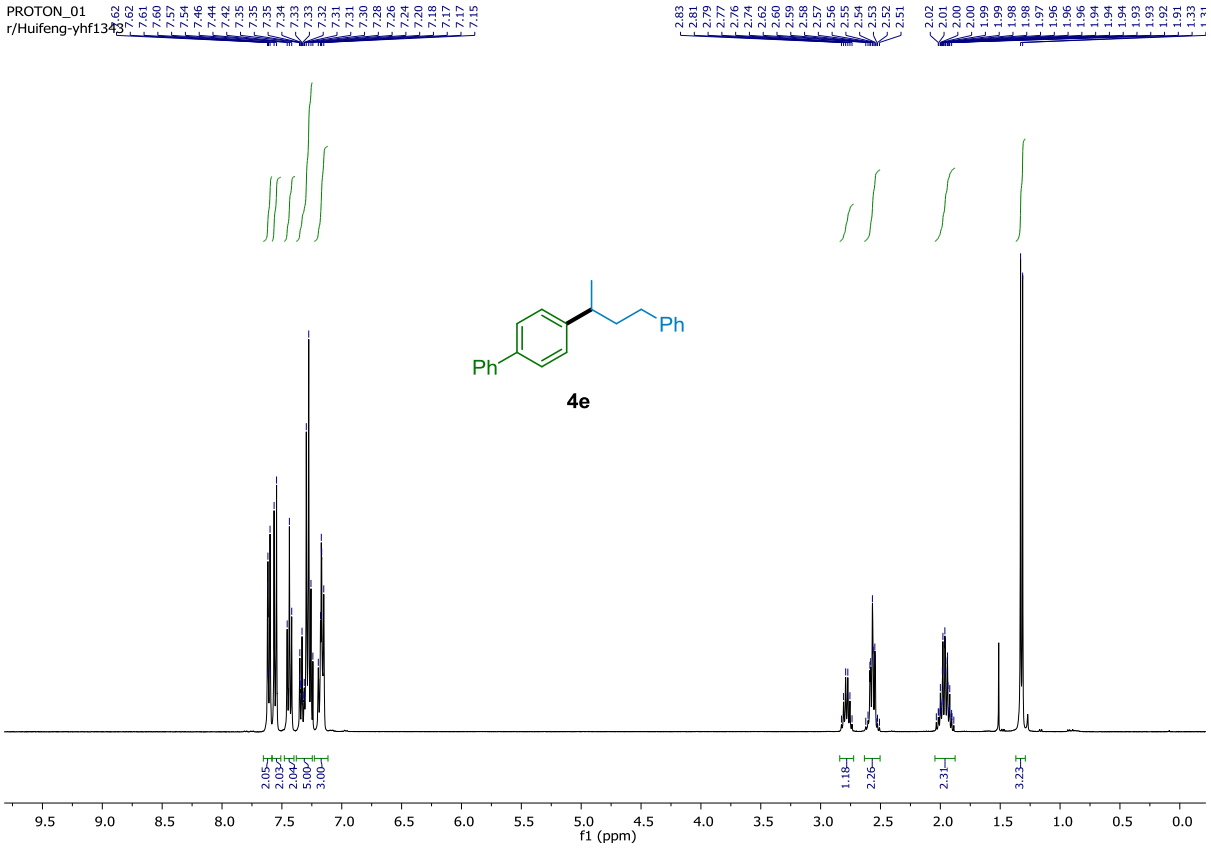
4d

CARBON_01
r/Huifeng-yhf1344



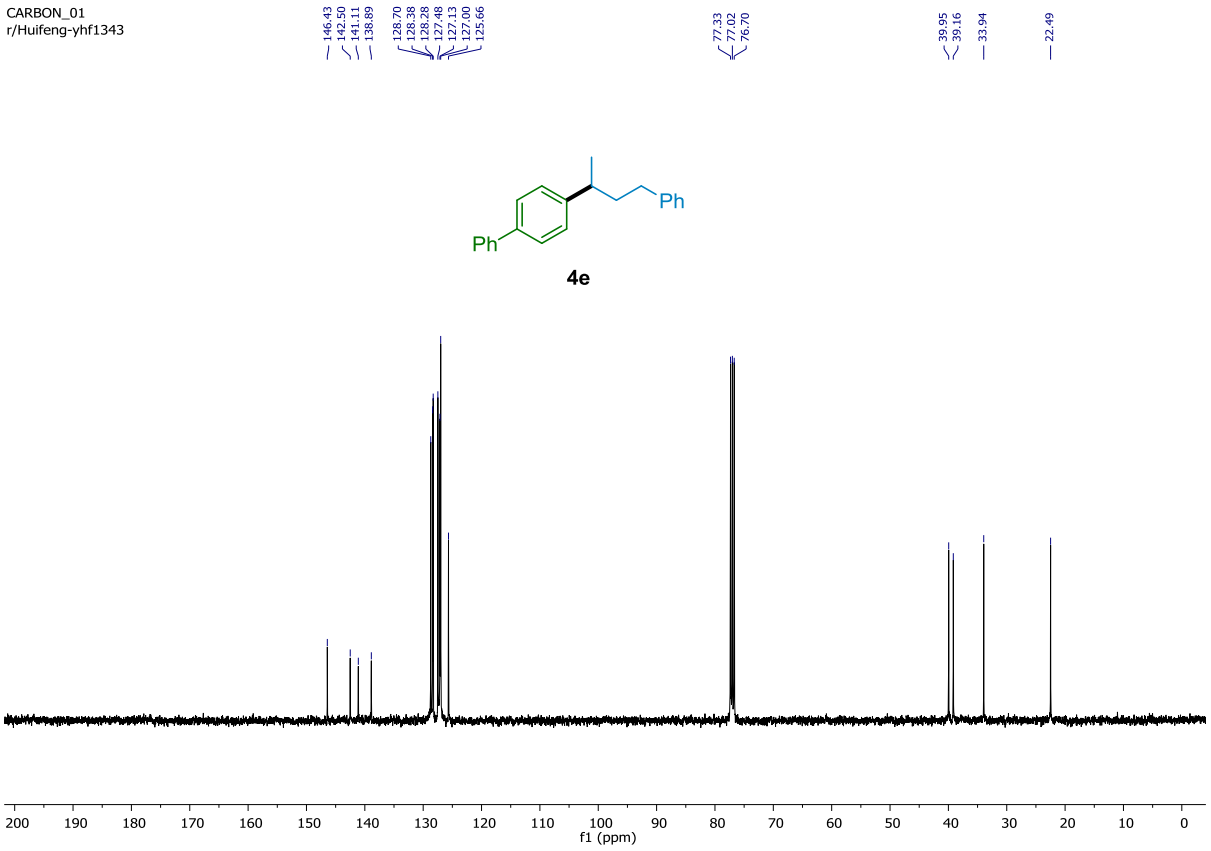
4d

PROTON_01
r/Huifeng-yhf1343



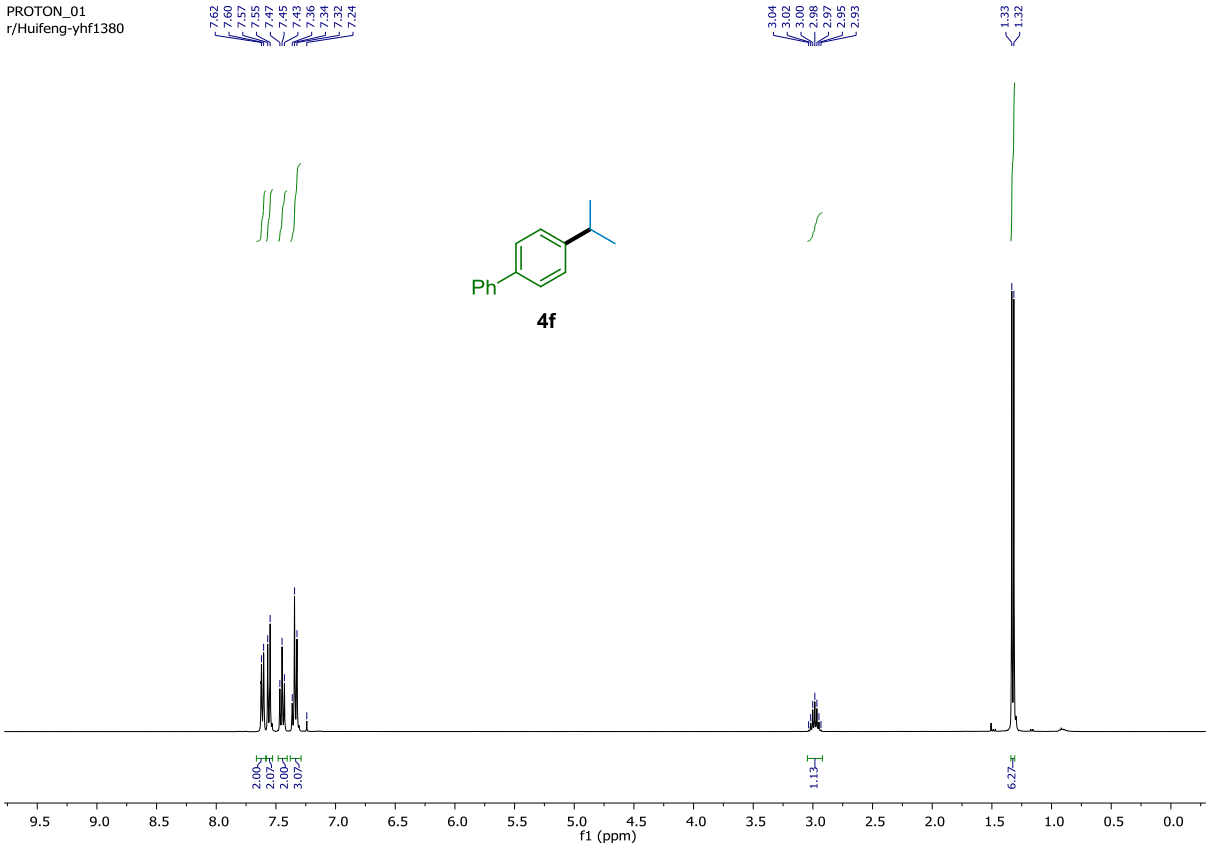
4e

CARBON_01
r/Huifeng-yhf1343



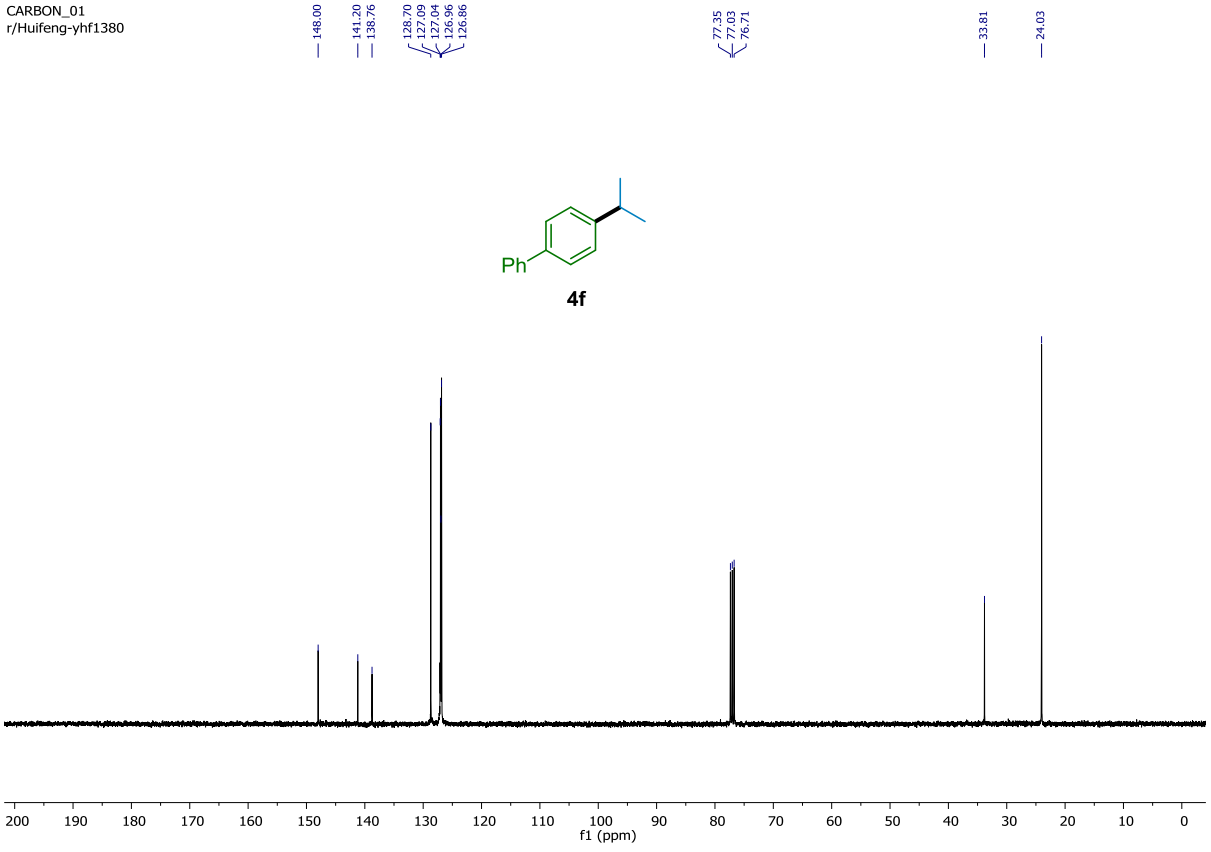
4e

PROTON_01
r/Huifeng-yhf1380



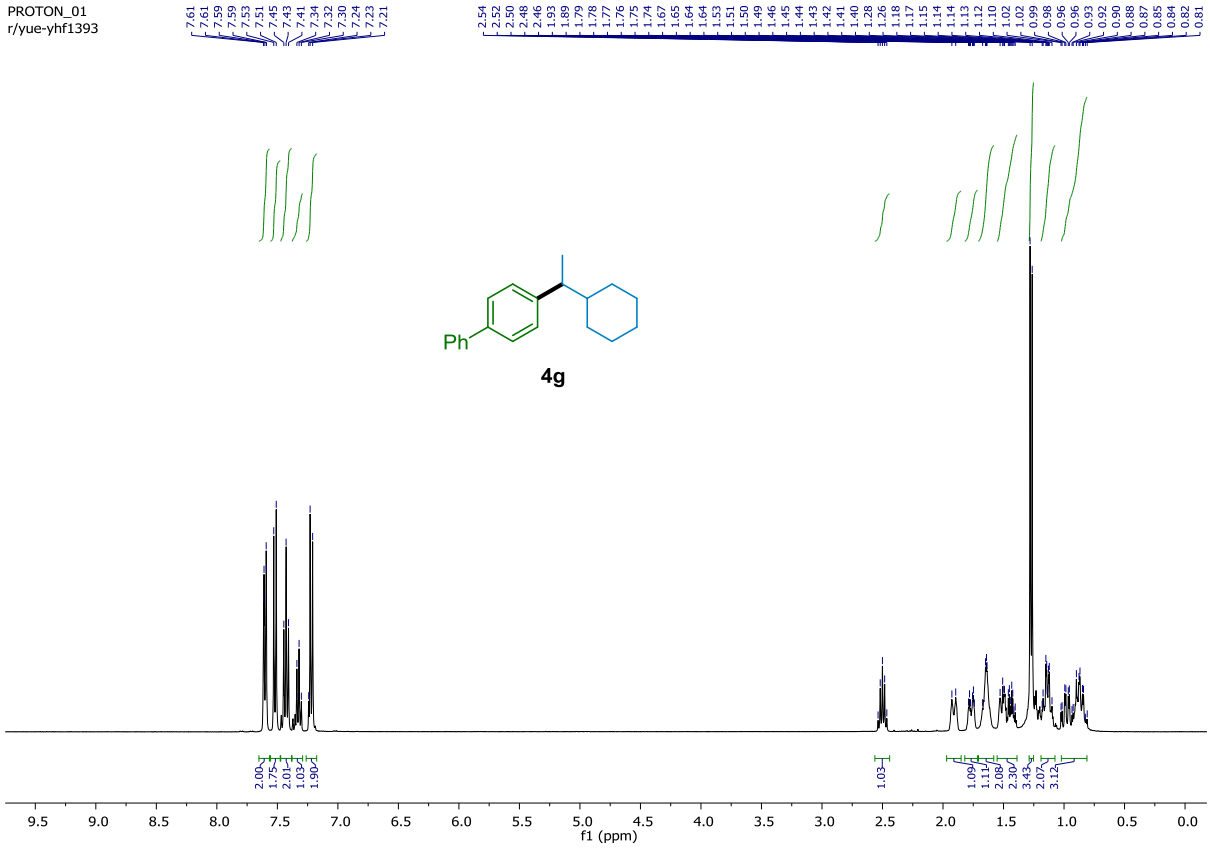
4f

CARBON_01
r/Huifeng-yhf1380



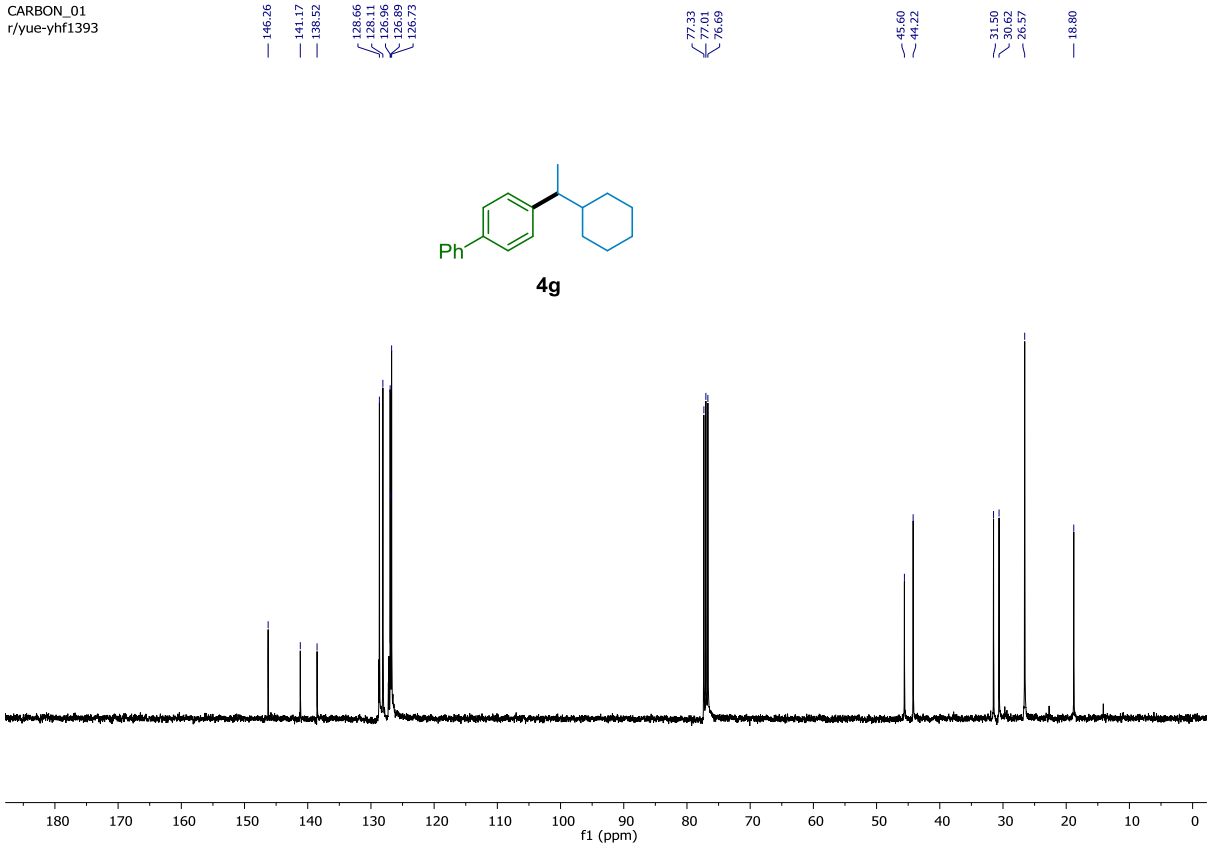
4f

PROTON_01
r/yue-yhf1393



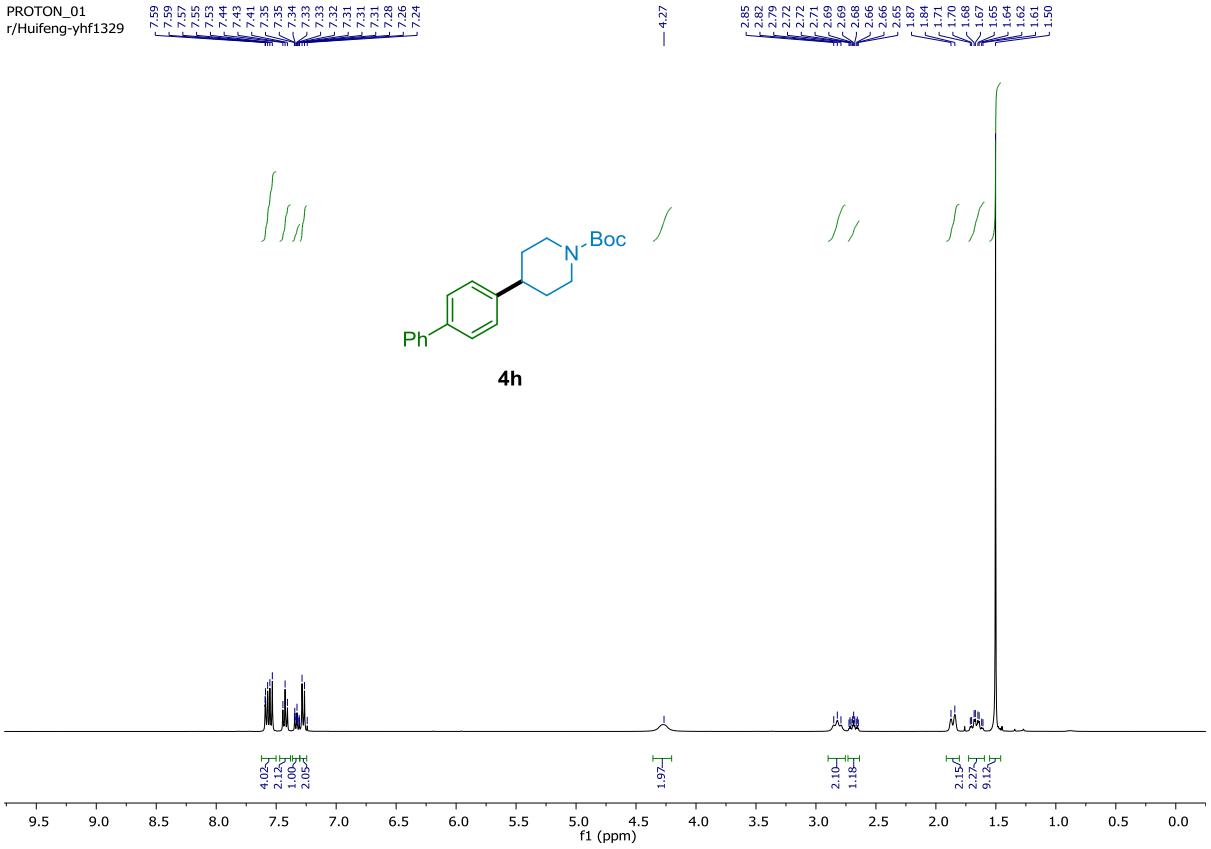
4g

CARBON_01
r/yue-yhf1393



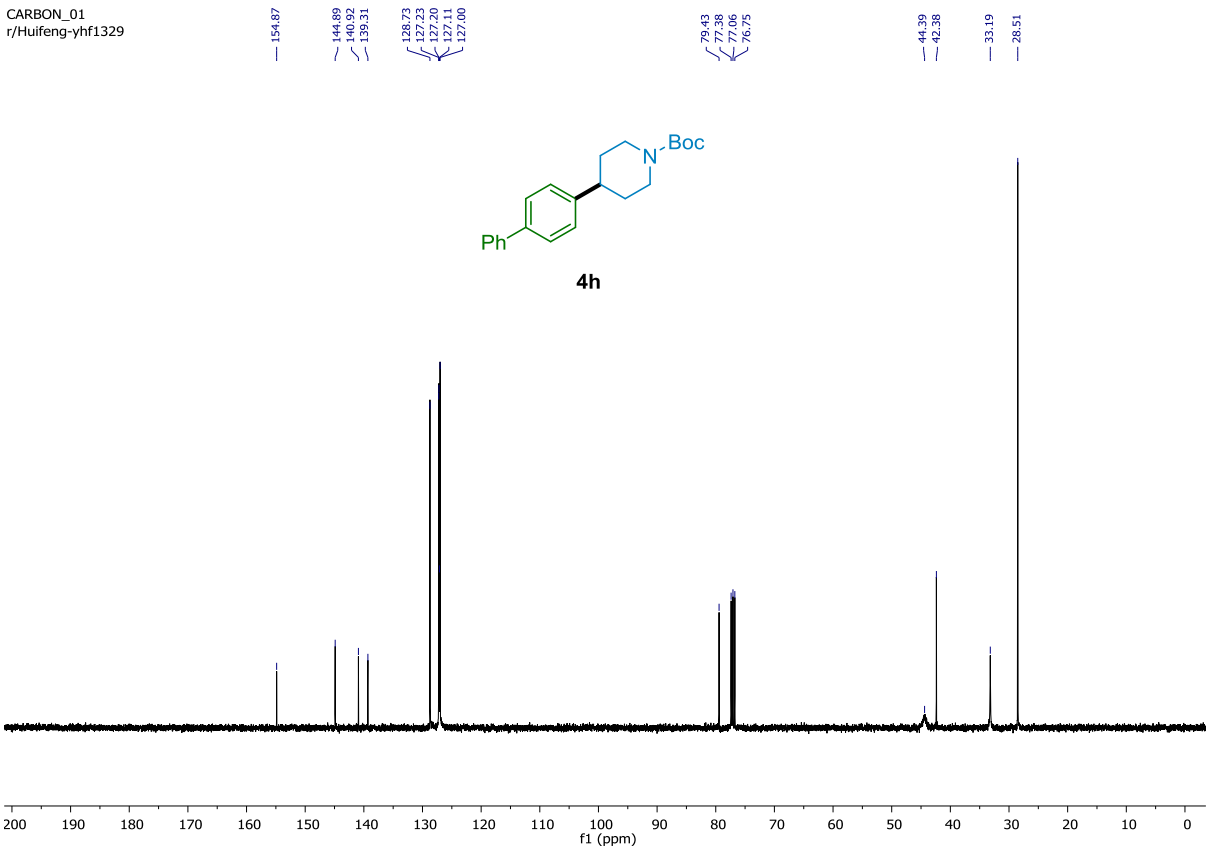
4g

PROTON_01
r/Huifeng-yhf1329



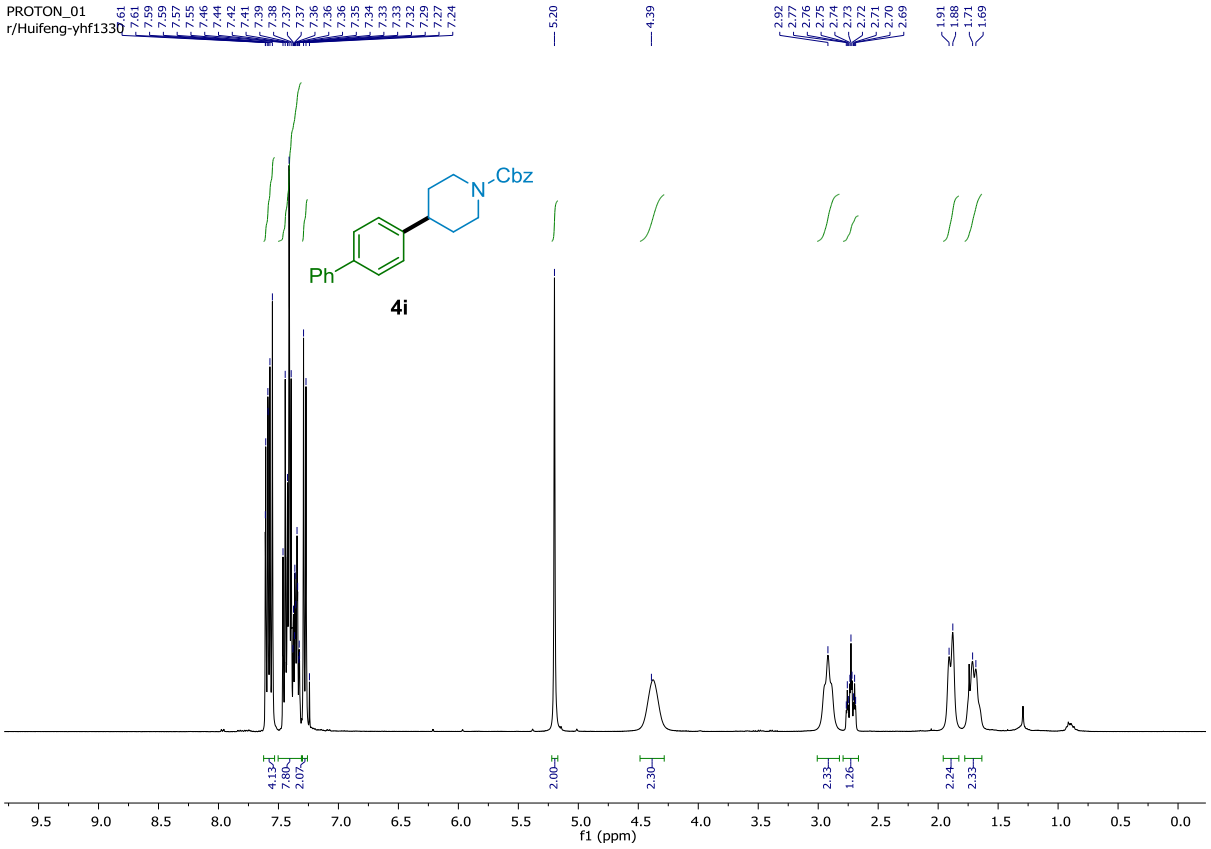
4h

CARBON_01
r/Huifeng-yhf1329

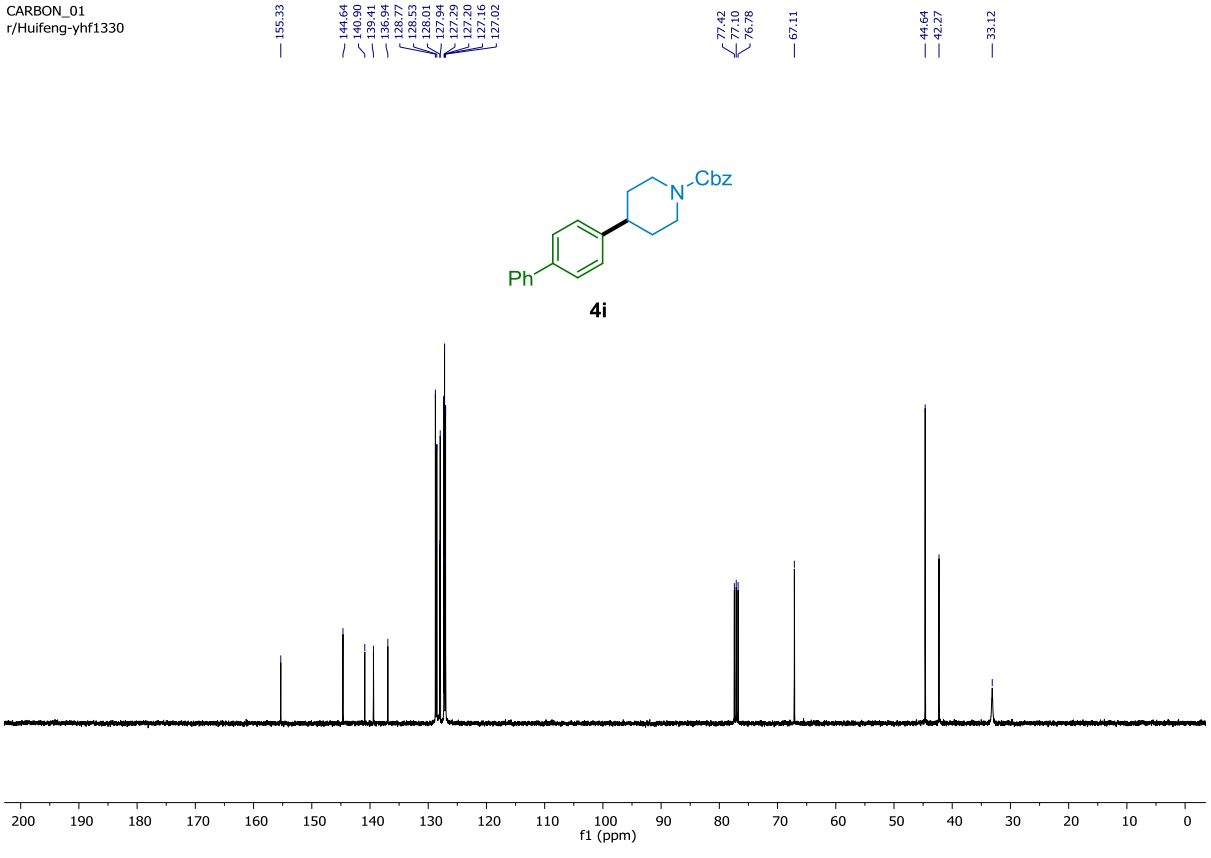


4h

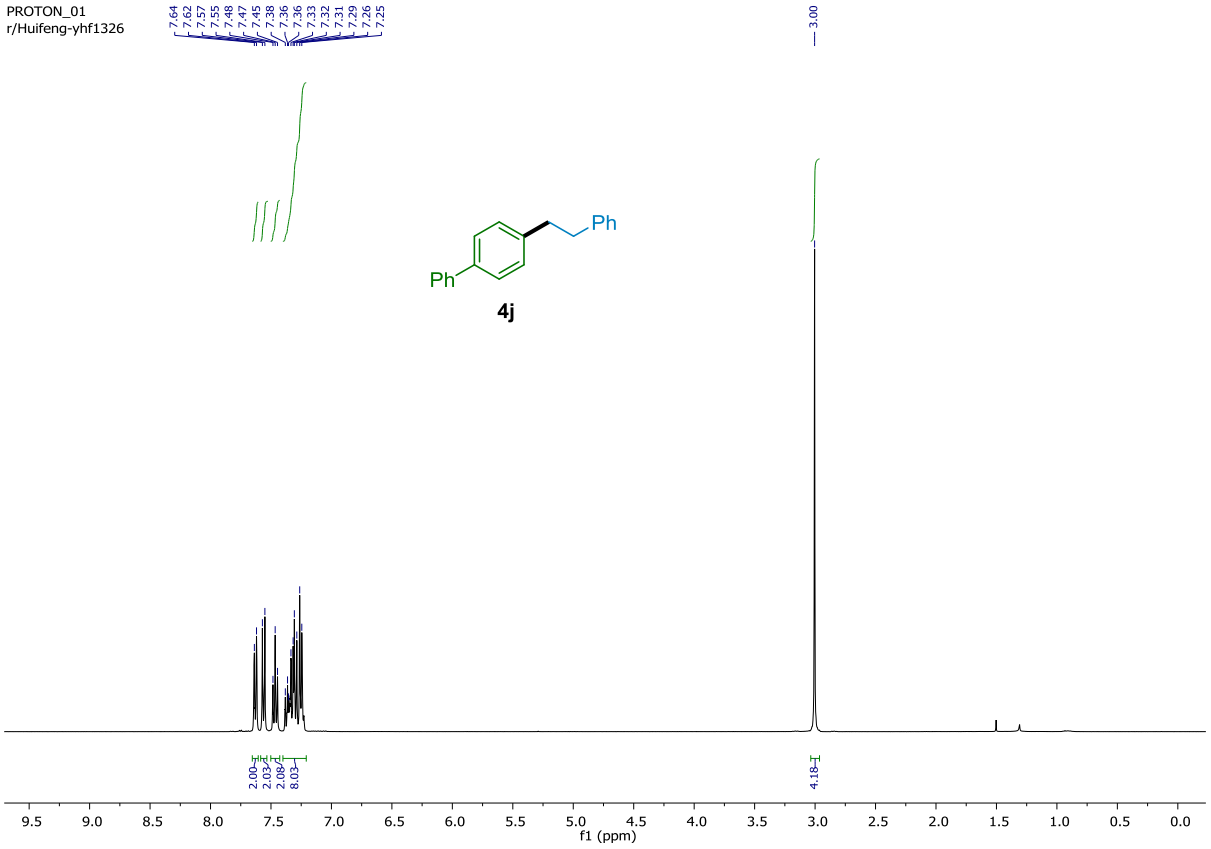
PROTON_01
r/Huifeng-yhf1330



CARBON_01
r/Huifeng-yhf1330

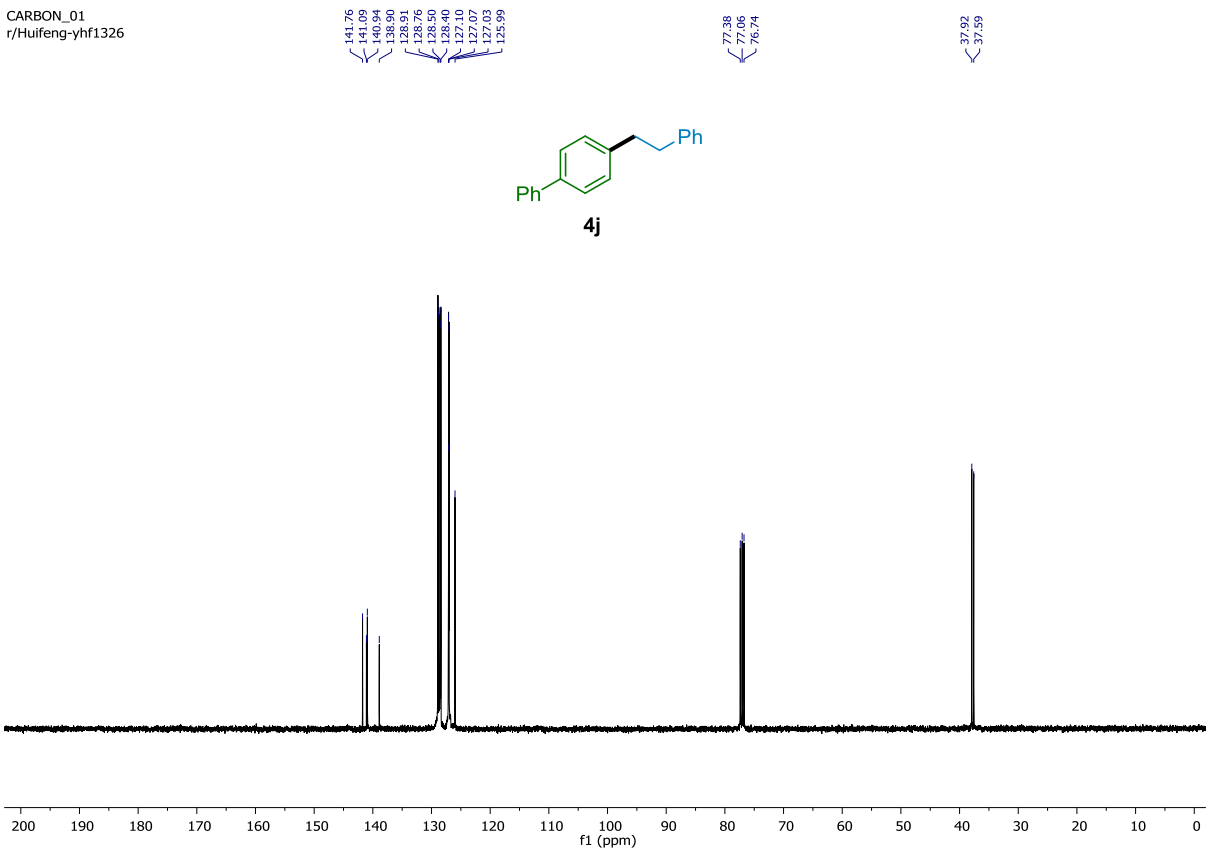


PROTON_01
r/Huifeng-yhf1326



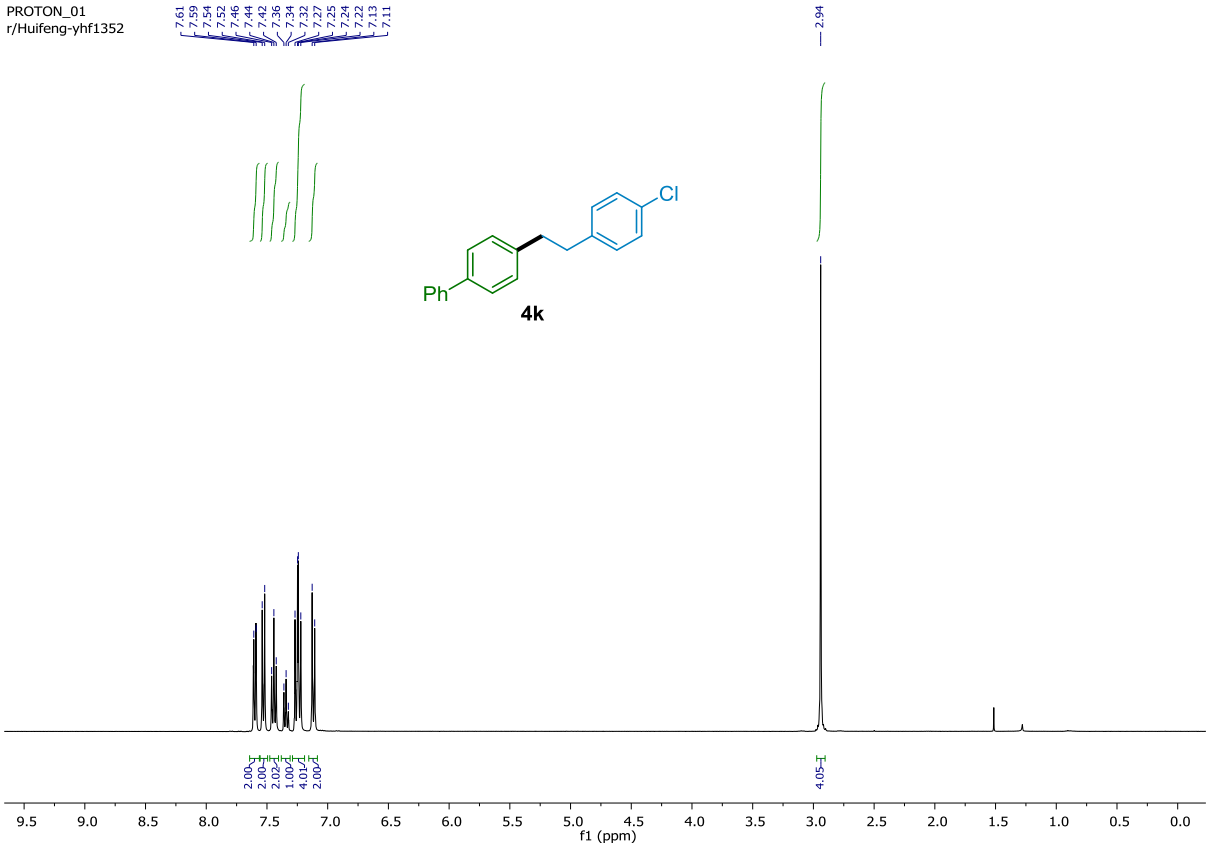
4j

CARBON_01
r/Huifeng-yhf1326

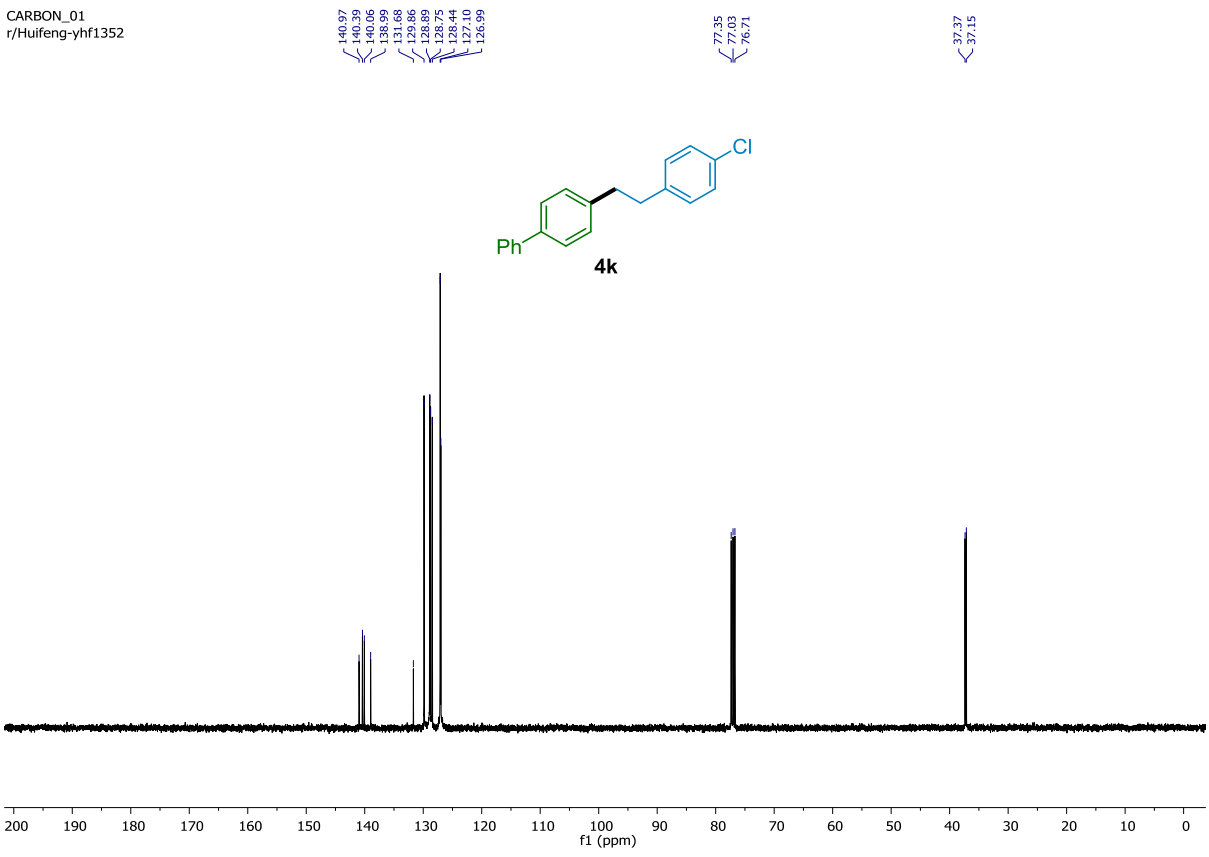


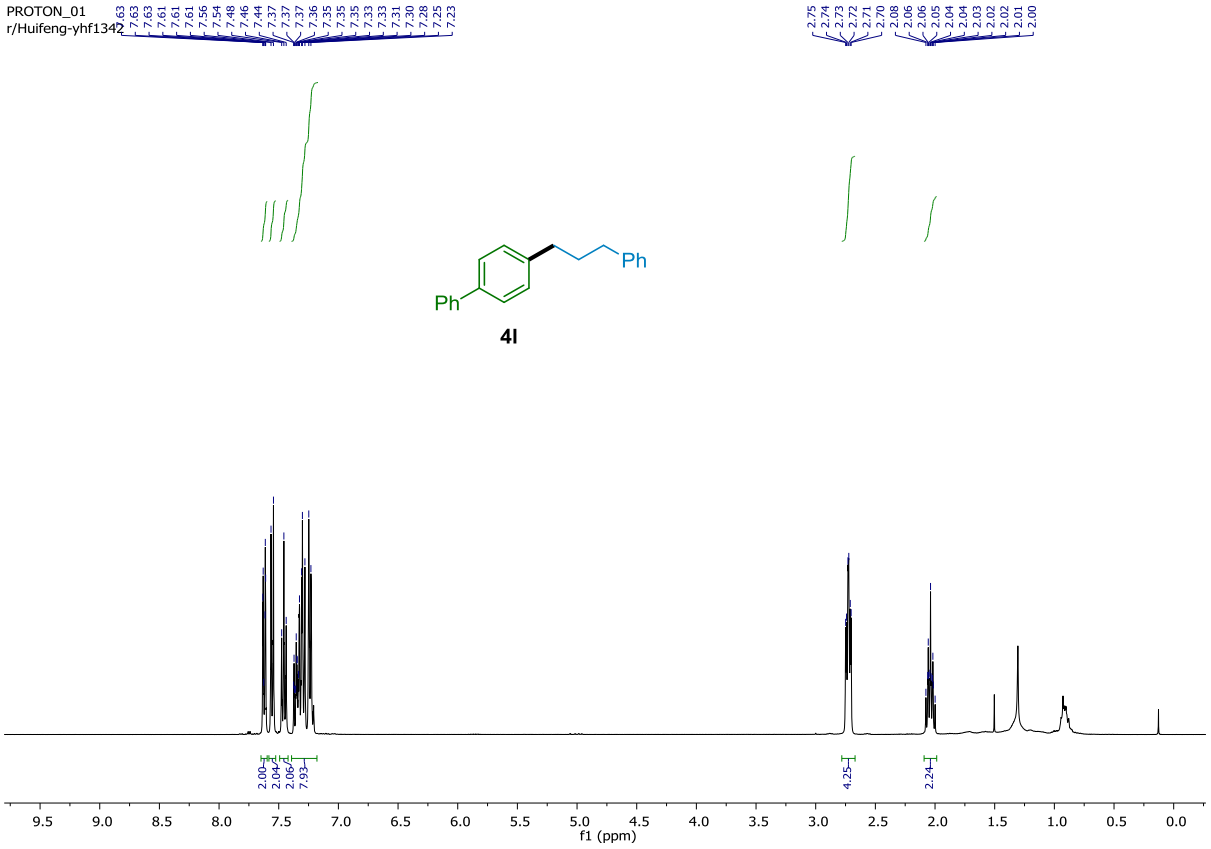
4j

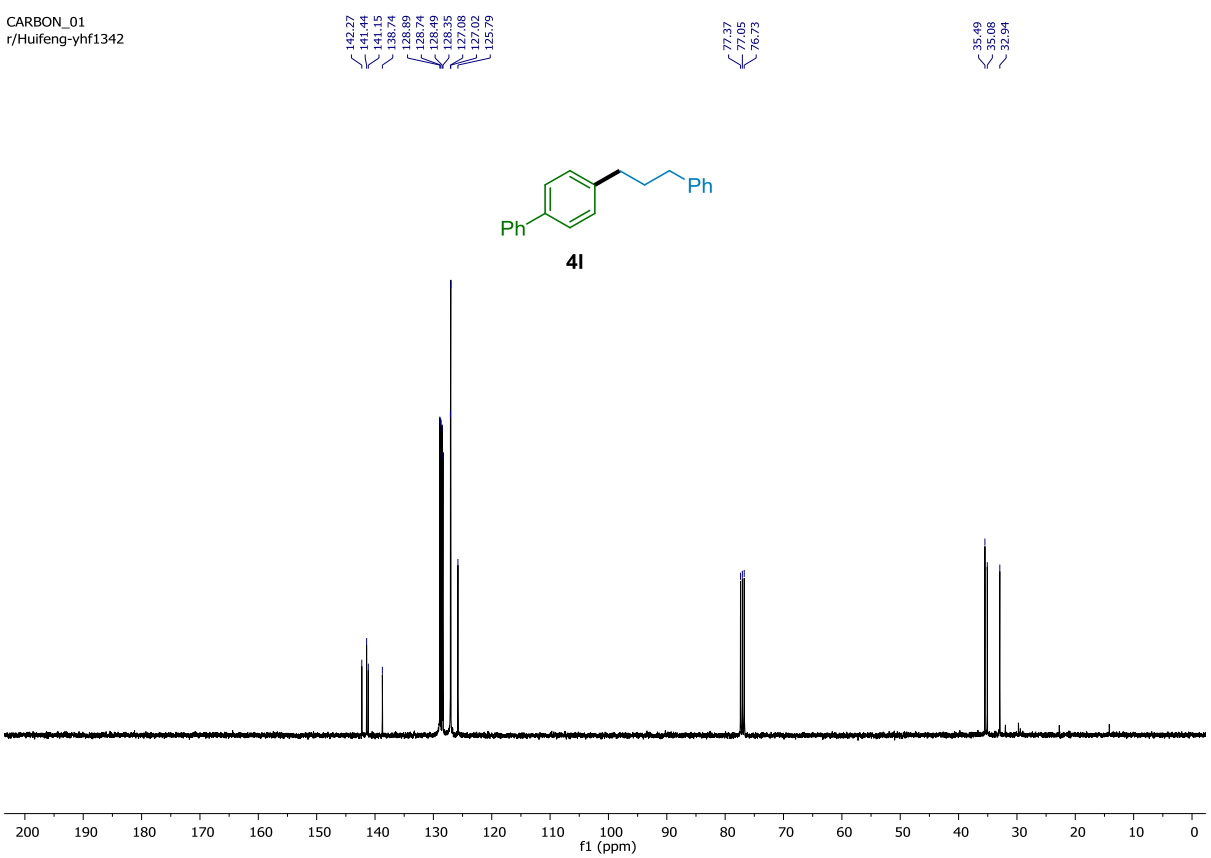
PROTON_01
r/Huifeng-yhf1352

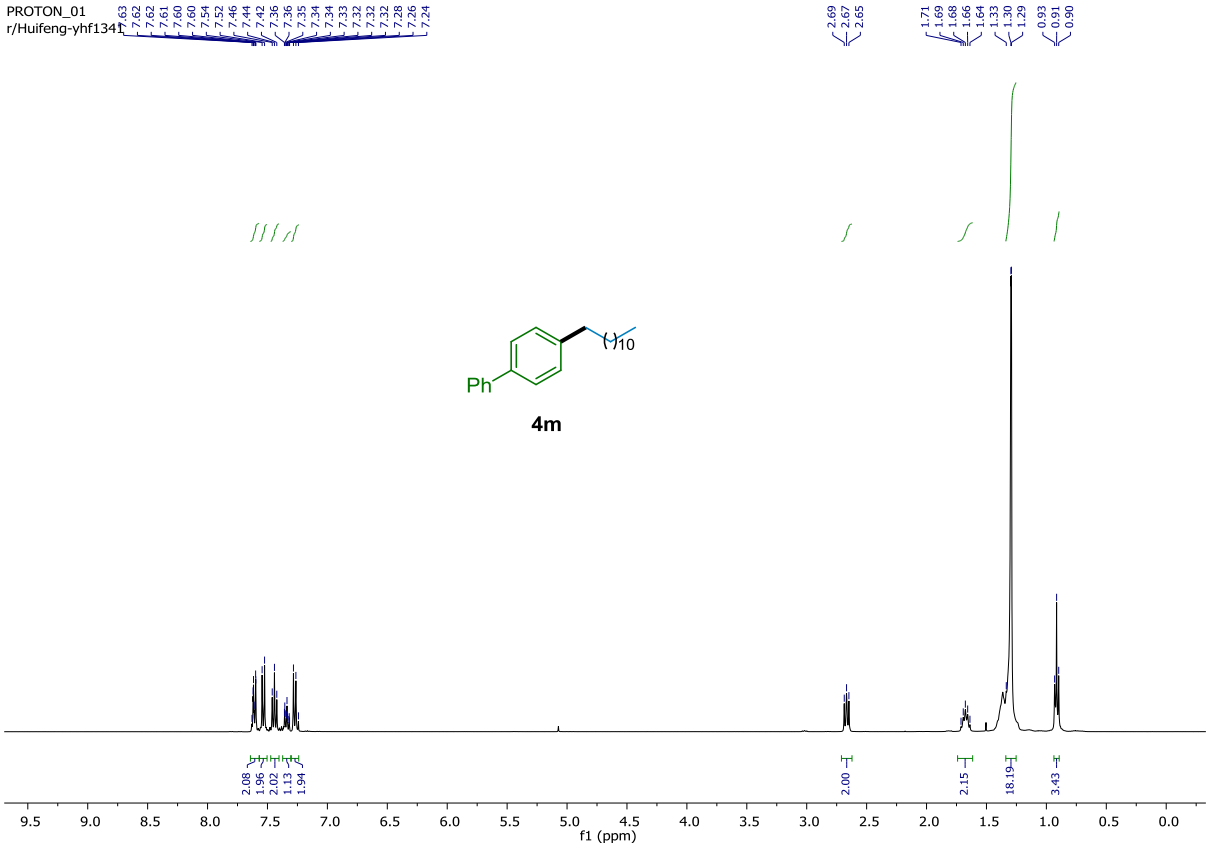


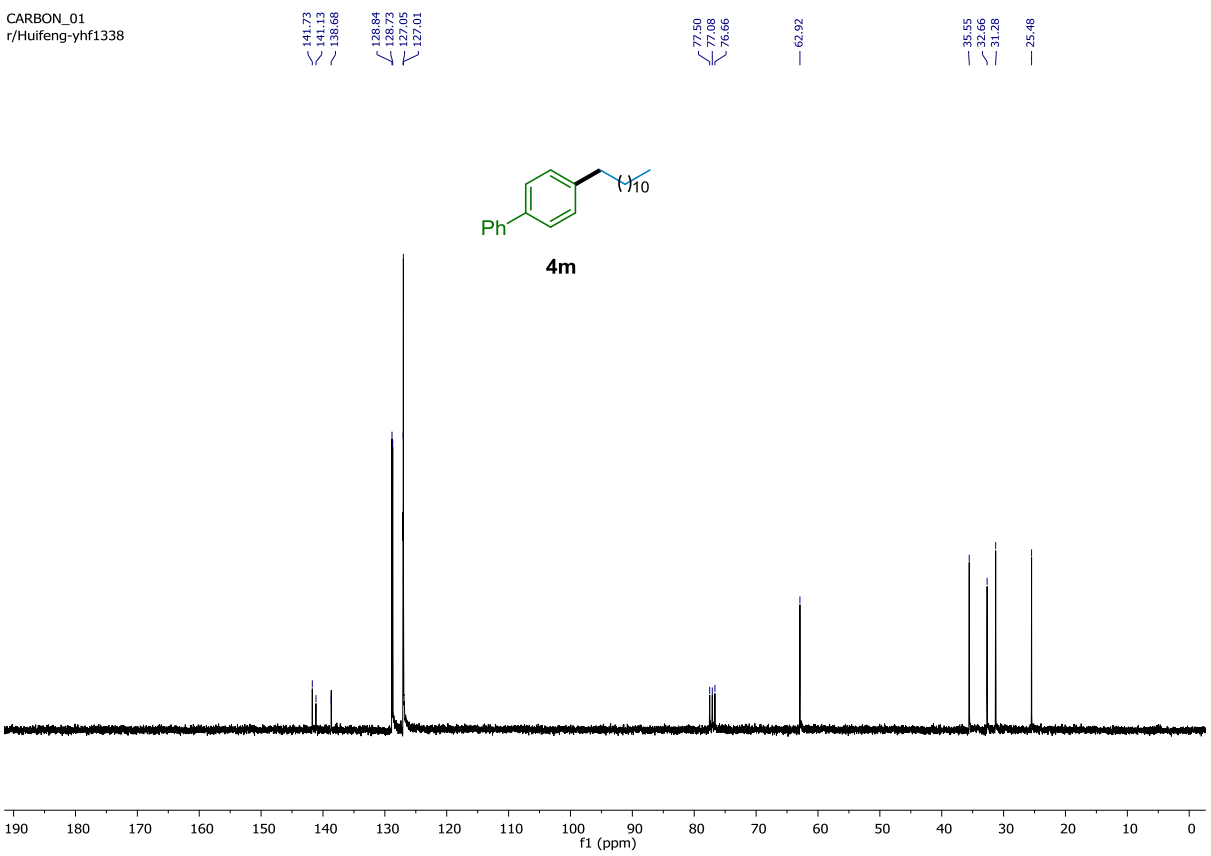
CARBON_01
r/Huifeng-yhf1352



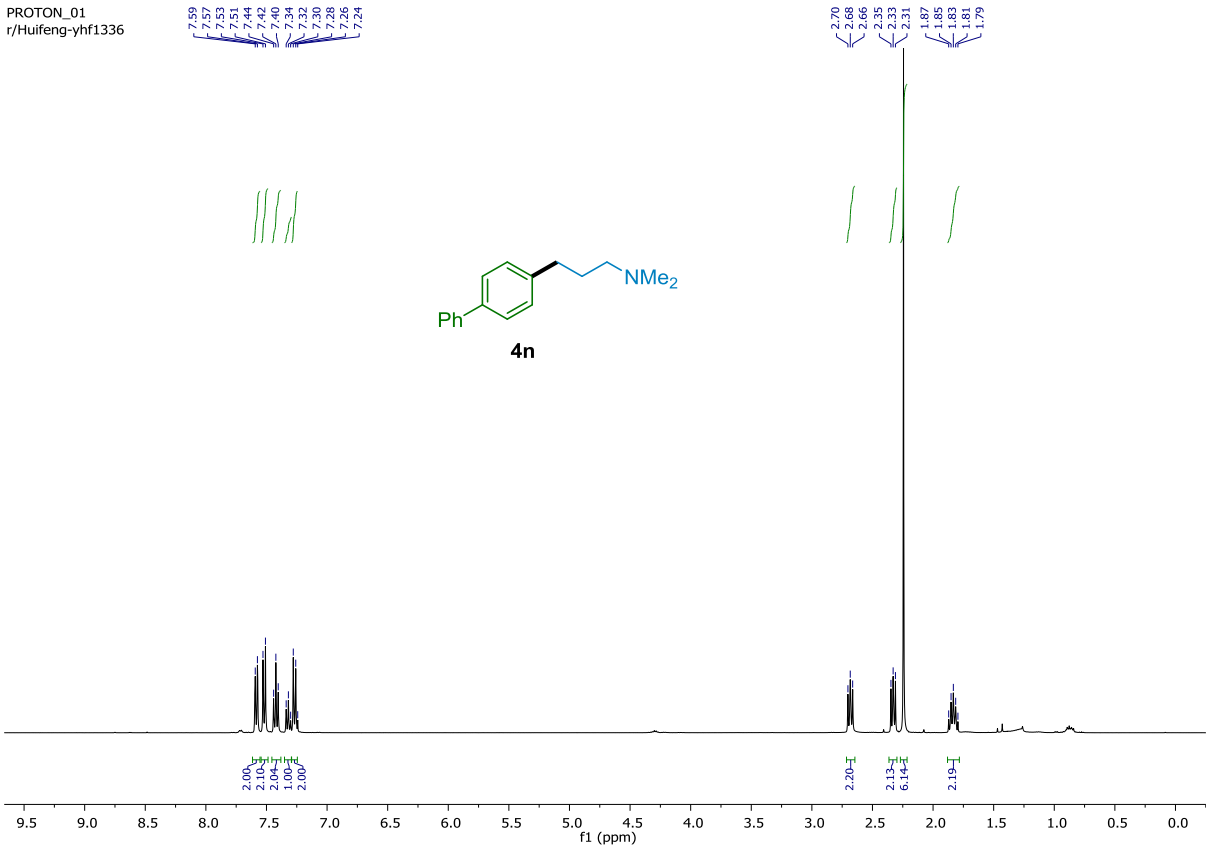

PROTON_01
r/Huifeng-yhf1342
7.63
7.63
7.63
7.61
7.61
7.61
7.56
7.54
7.48
7.46
7.44
7.37
7.37
7.37
7.36
7.35
7.35
7.35
7.33
7.33
7.31
7.30
7.28
7.25
7.23
2.75
2.74
2.73
2.72
2.71
2.70
2.08
2.06
2.06
2.05
2.04
2.04
2.03
2.02
2.02
2.01
2.00
Ph
Ph
4l
2.00
2.04
2.06
7.93
4.25
2.24
9.5
9.0
8.5
8.0
7.5
7.0
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)


CARBON_01
r/Huifeng-yhf1342
142.27
141.44
141.15
138.74
128.89
128.74
128.49
128.35
127.08
127.02
125.79
77.37
77.05
76.73
35.49
35.08
32.94
Ph
Ph
4l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON_01
r/Huifeng-yhf1341
7.63
7.62
7.62
7.61
7.60
7.60
7.54
7.52
7.46
7.44
7.42
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.32
7.32
7.28
7.26
7.24
2.69
2.67
2.65
1.71
1.69
1.68
1.66
1.64
1.33
1.30
1.29
0.93
0.91
0.90
Ph
10
4m
2.08
1.95
2.02
1.13
1.94
2.00
2.15
18.19
3.43
f1 (ppm)

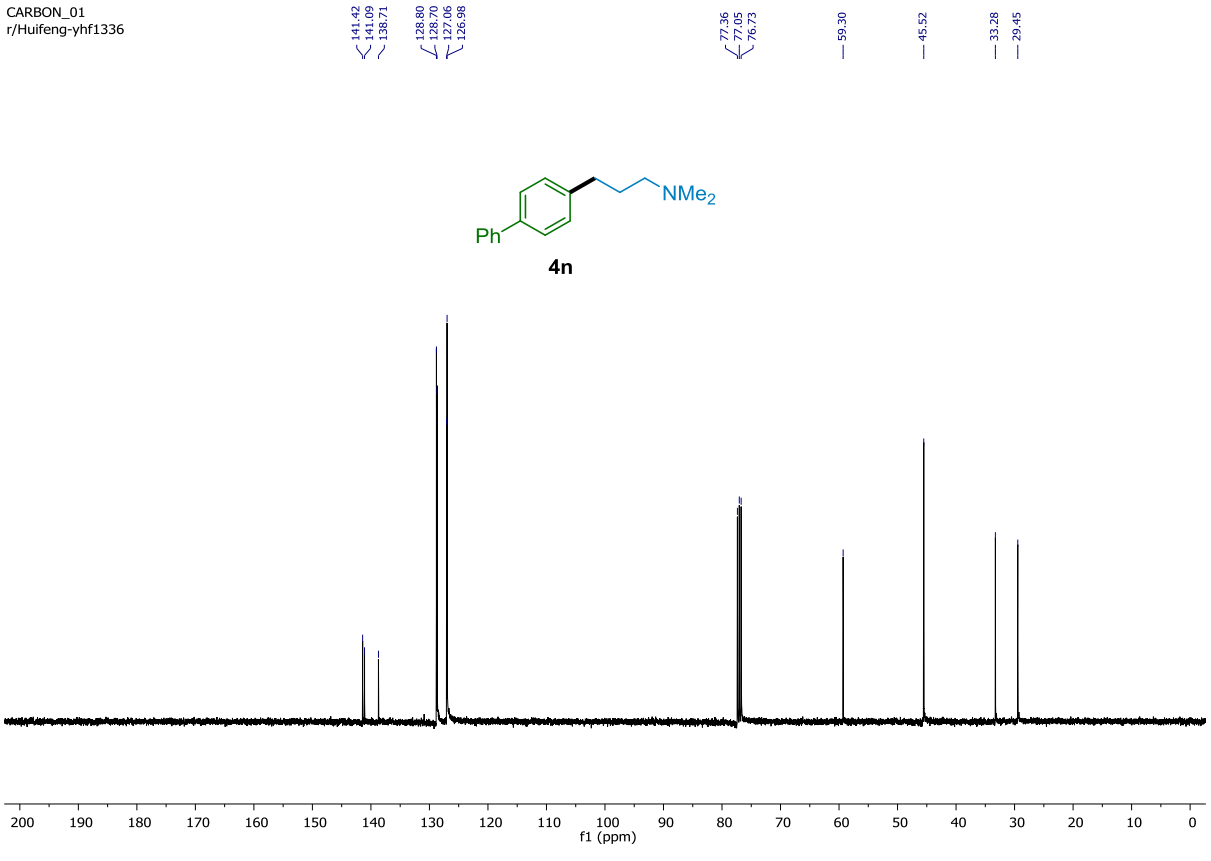

CARBON_01
r/Huifeng-yhf1338
141.73
141.13
138.68
128.84
128.73
127.05
127.01
77.50
77.08
76.66
62.92
35.55
32.66
31.28
25.48
Ph
10
4m
f1 (ppm)

PROTON_01
r/Huifeng-yhf1336



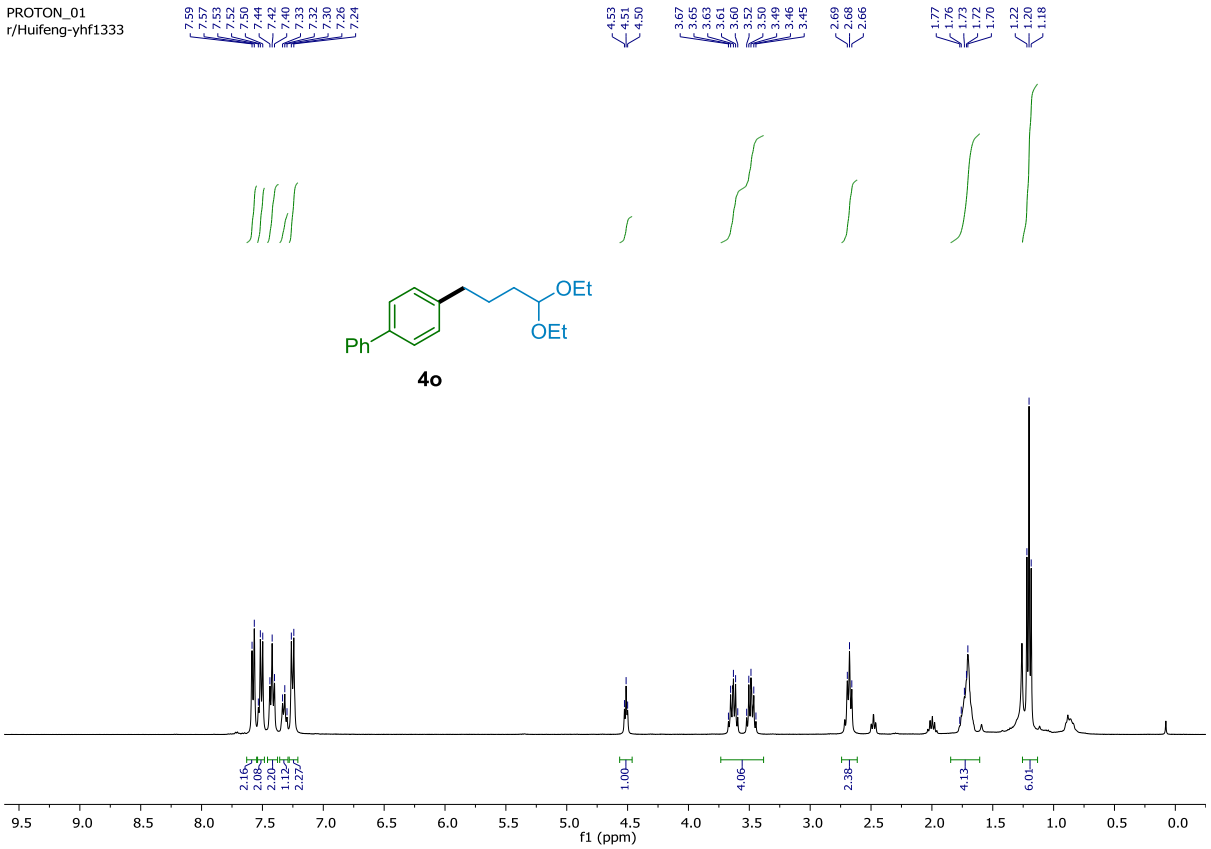
4n

CARBON_01
r/Huifeng-yhf1336



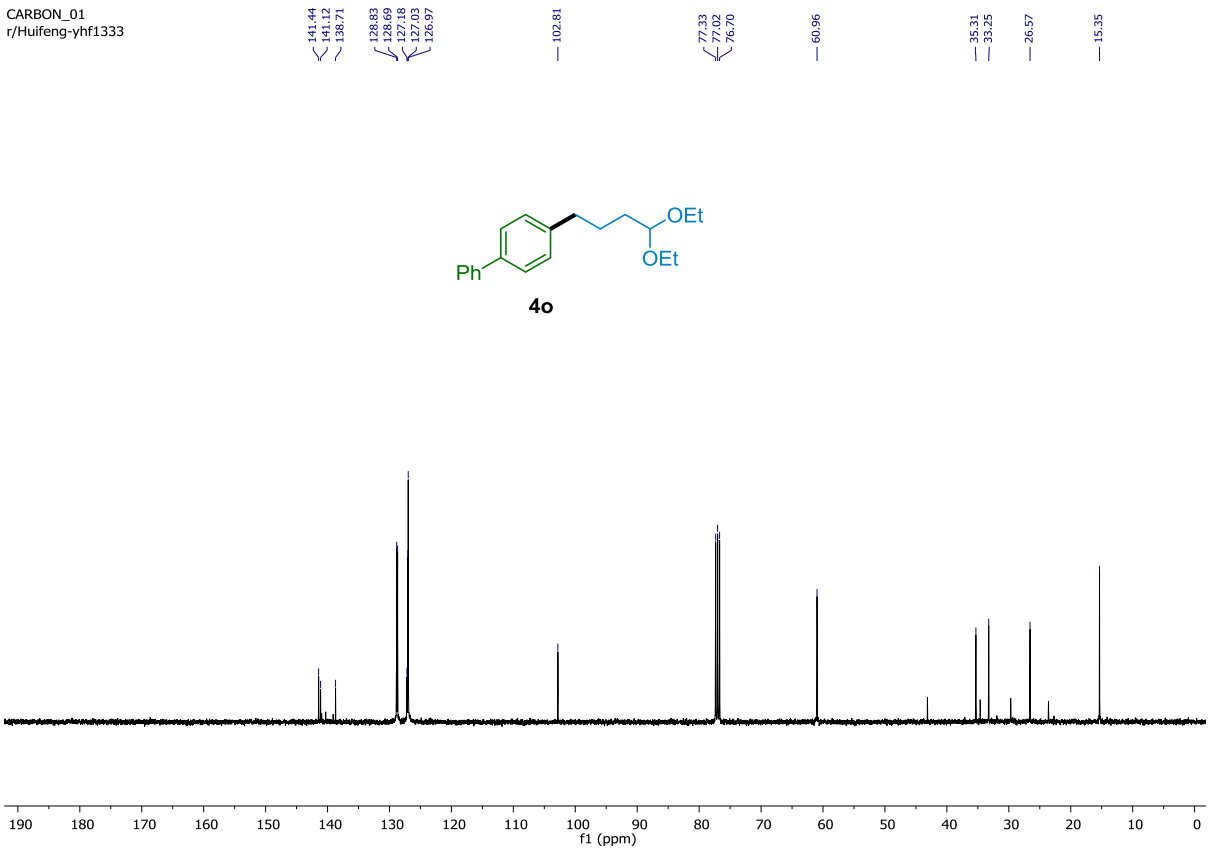
4n

PROTON_01
r/Huifeng-yhf1333



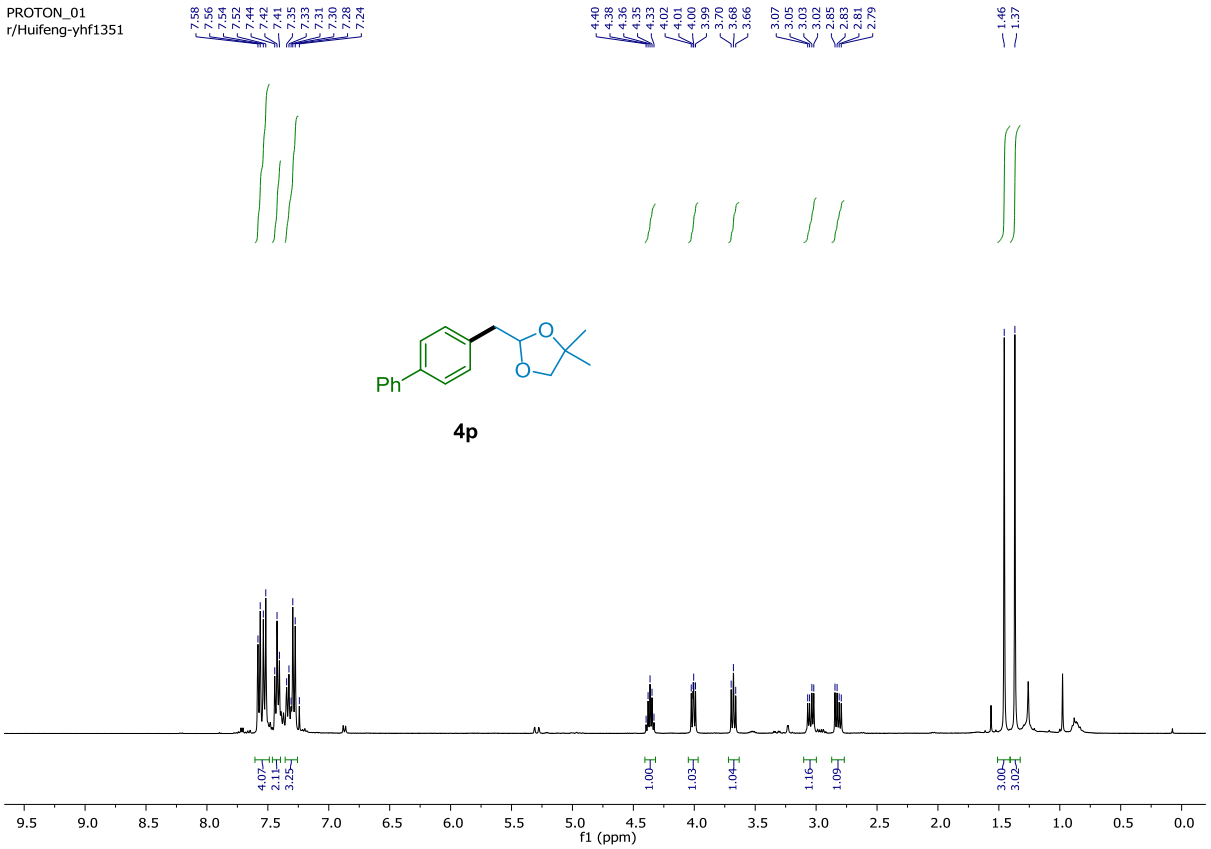
4o

CARBON_01
r/Huifeng-yhf1333



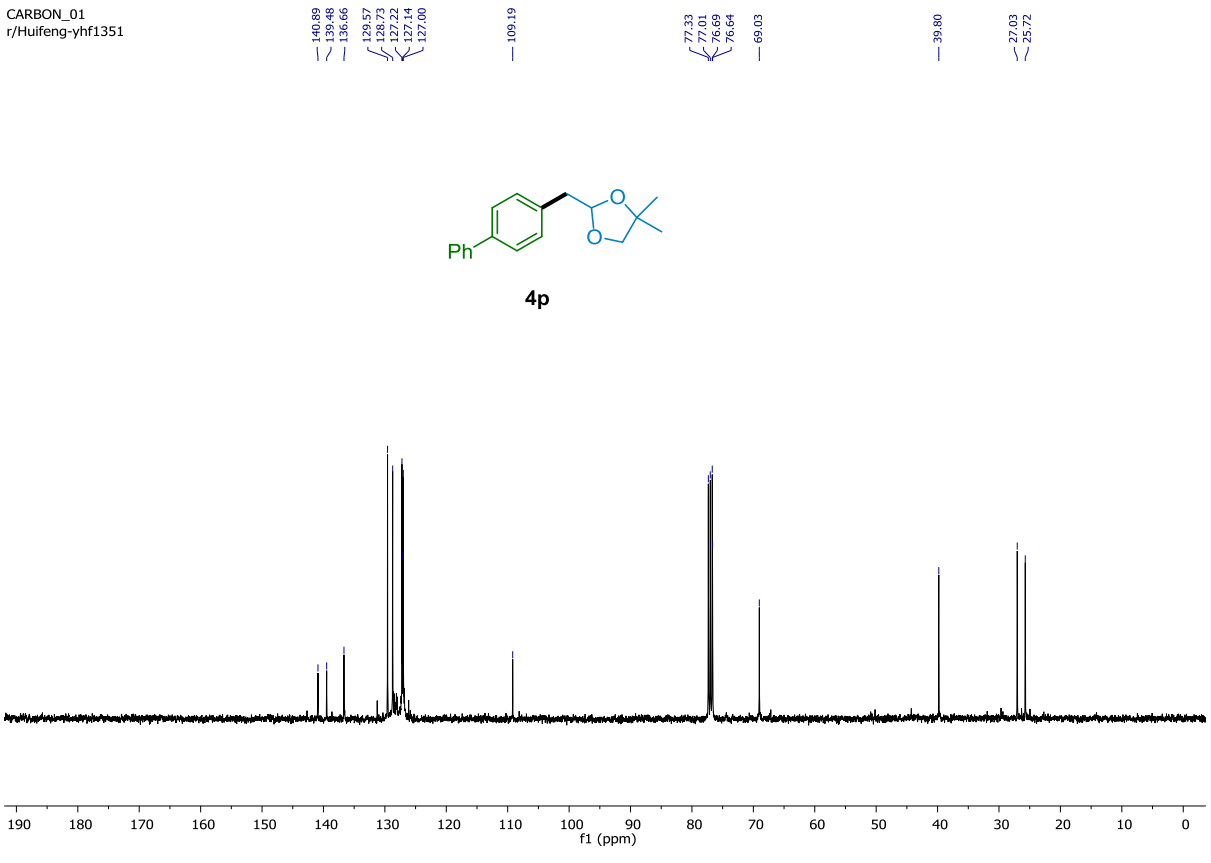
4o

PROTON_01
r/Huifeng-yhf1351



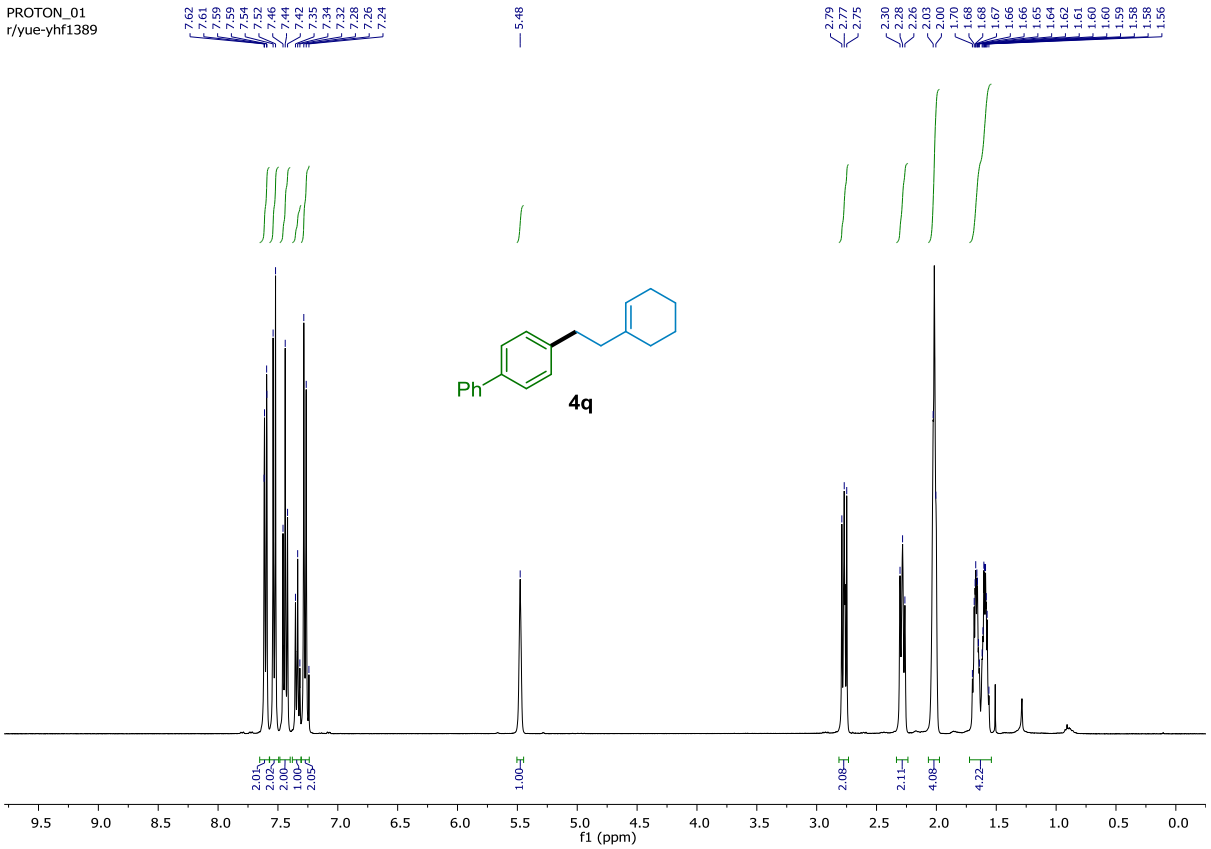
4p

CARBON_01
r/Huifeng-yhf1351

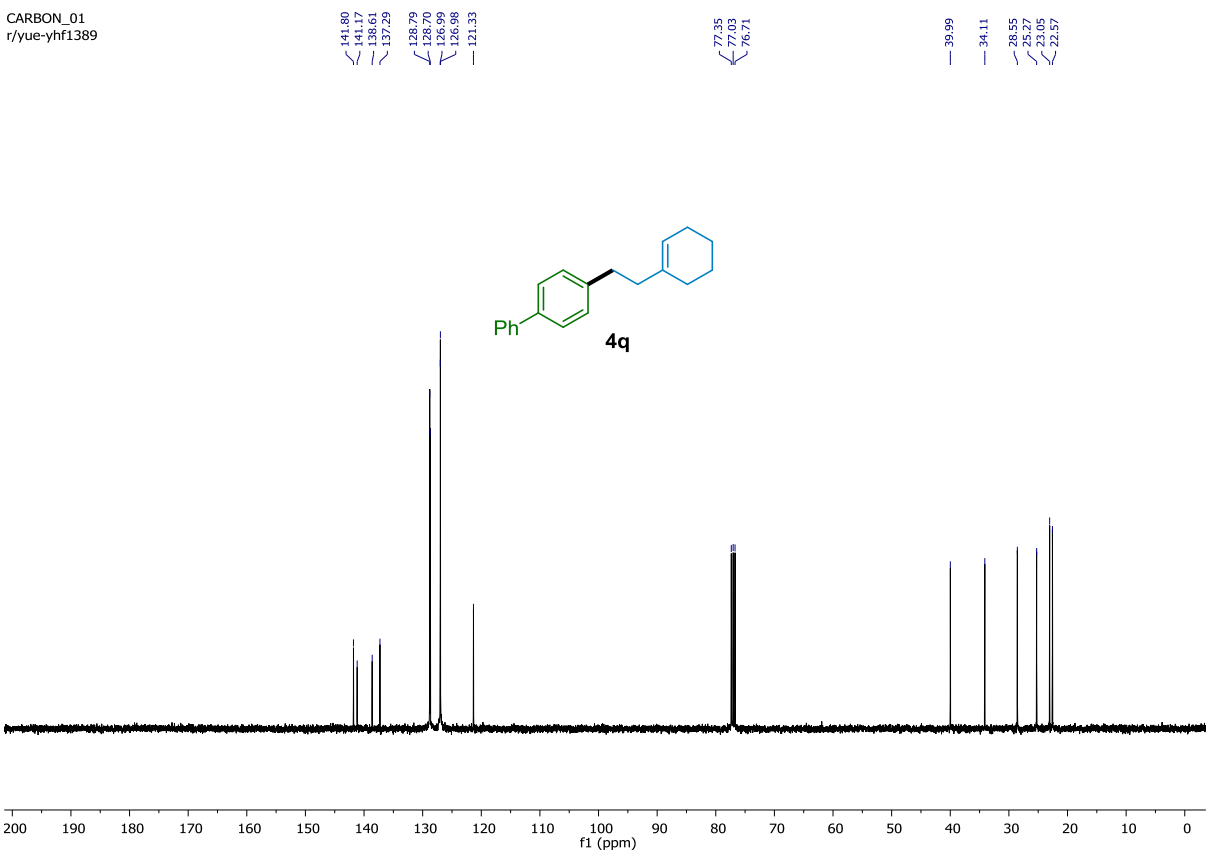


4p

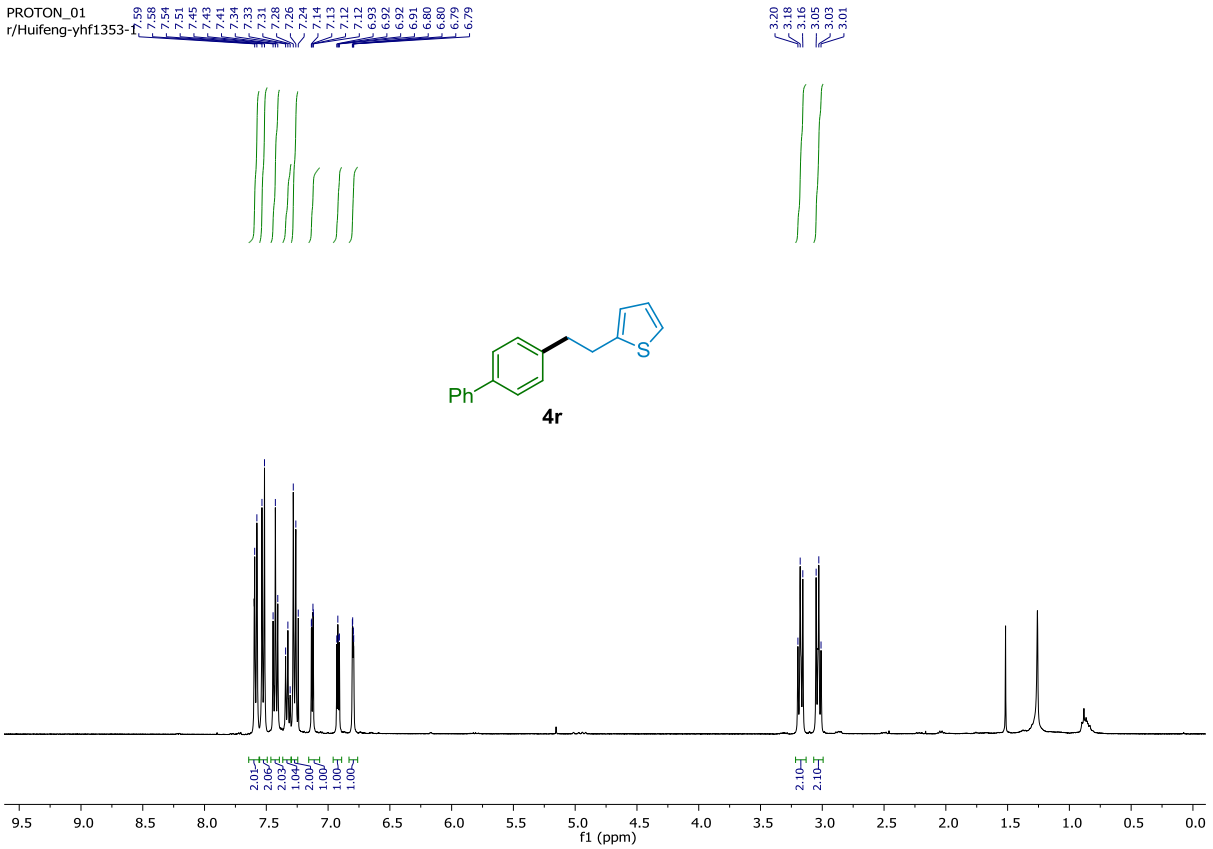
PROTON_01
r/yue-yhf1389



CARBON_01
r/yue-yhf1389

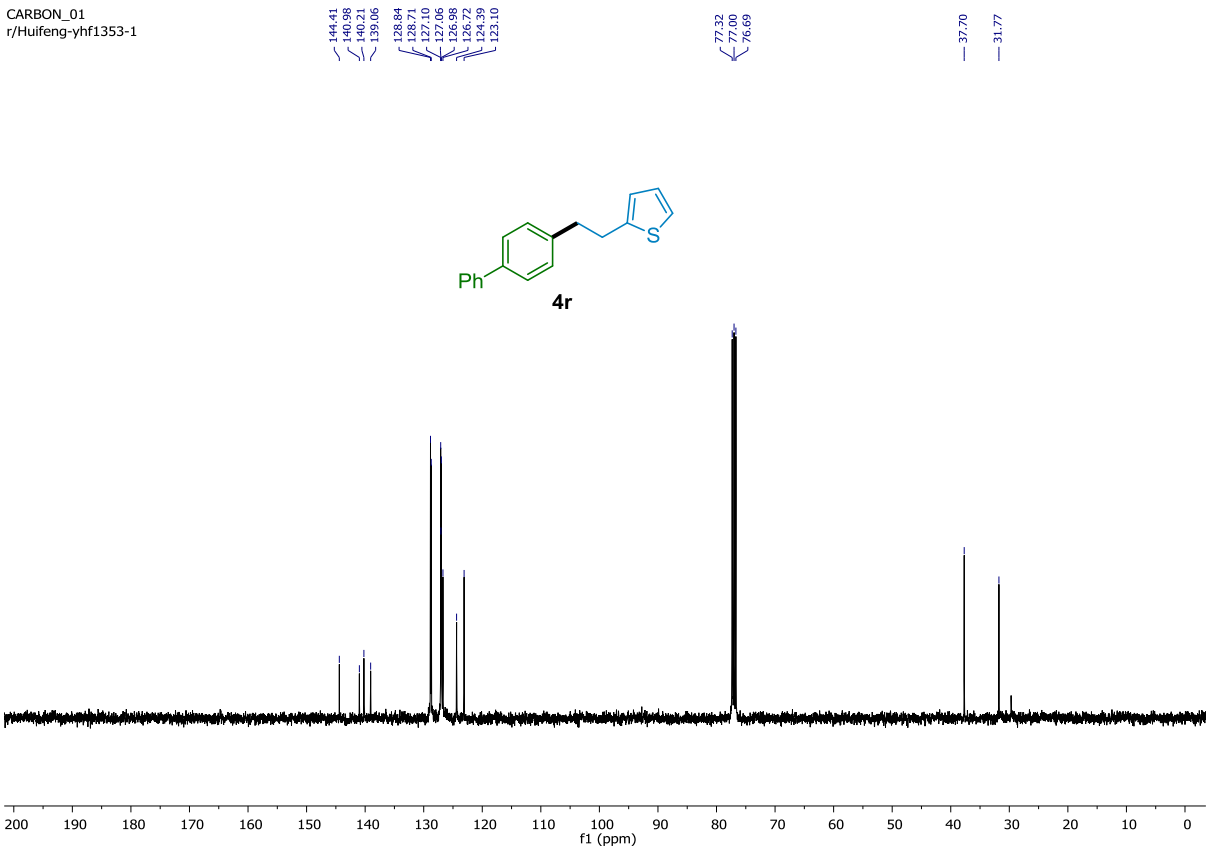


PROTON_01
r/Huifeng-yhf1353-1



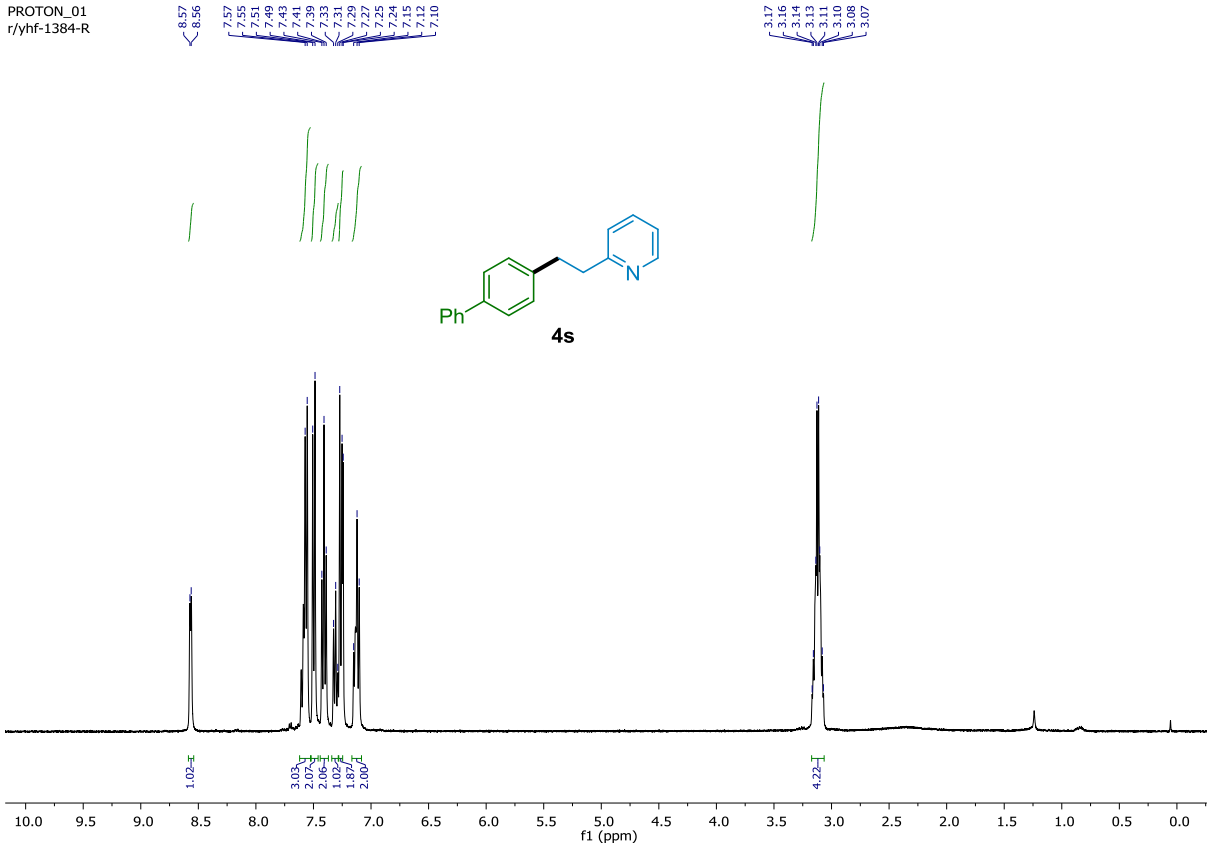
4r

CARBON_01
r/Huifeng-yhf1353-1



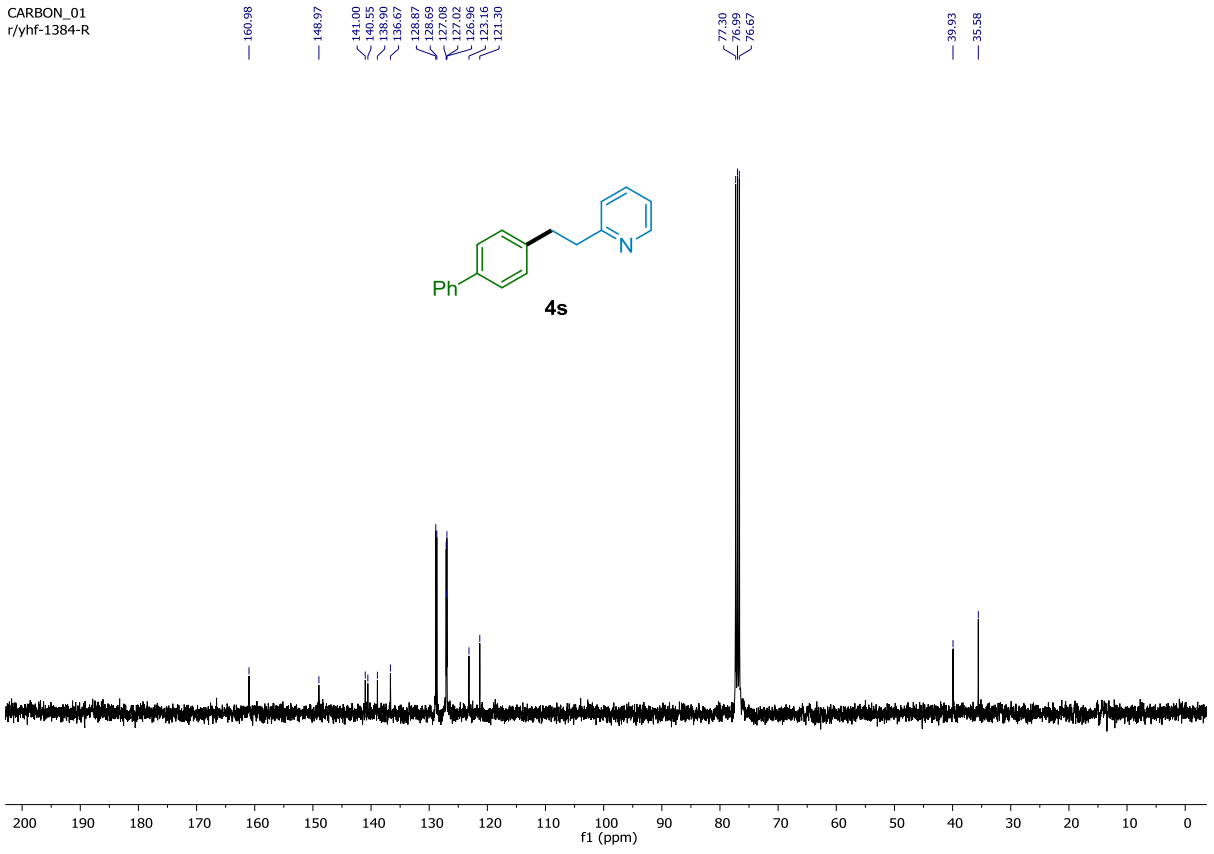
4r

PROTON_01
r/yhf-1384-R



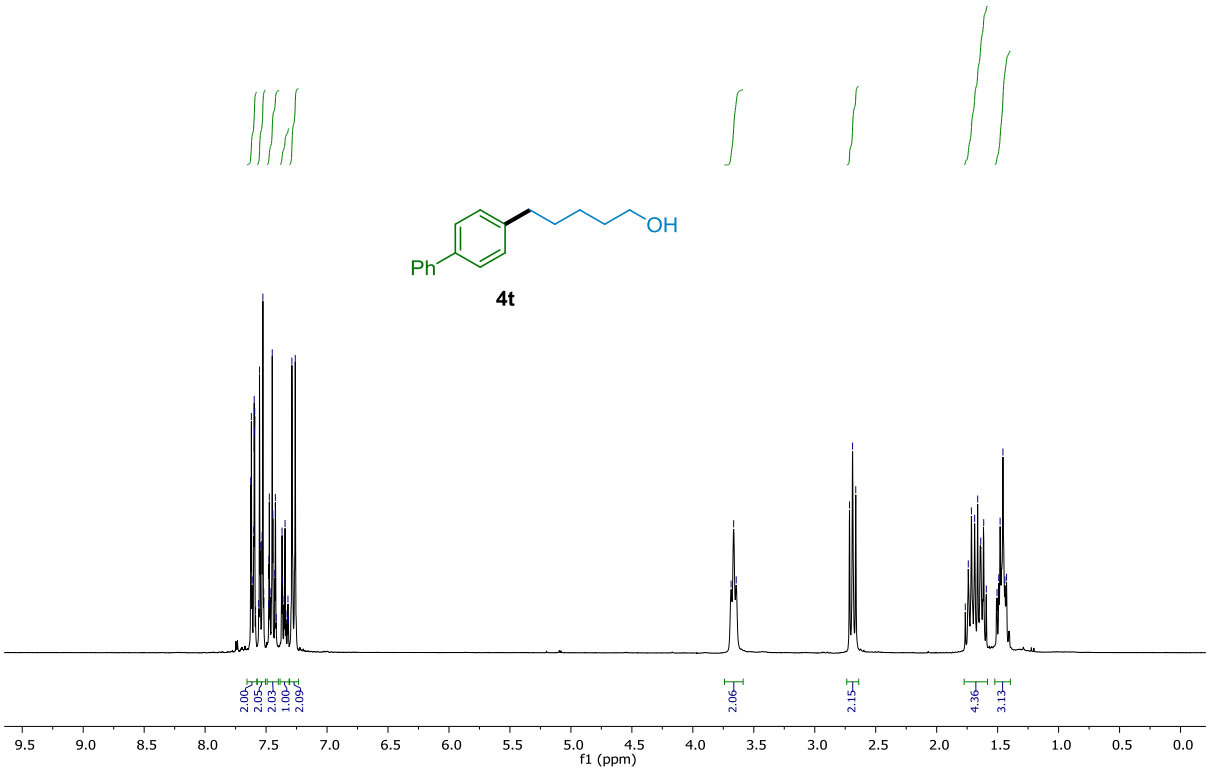
4s

CARBON_01
r/yhf-1384-R

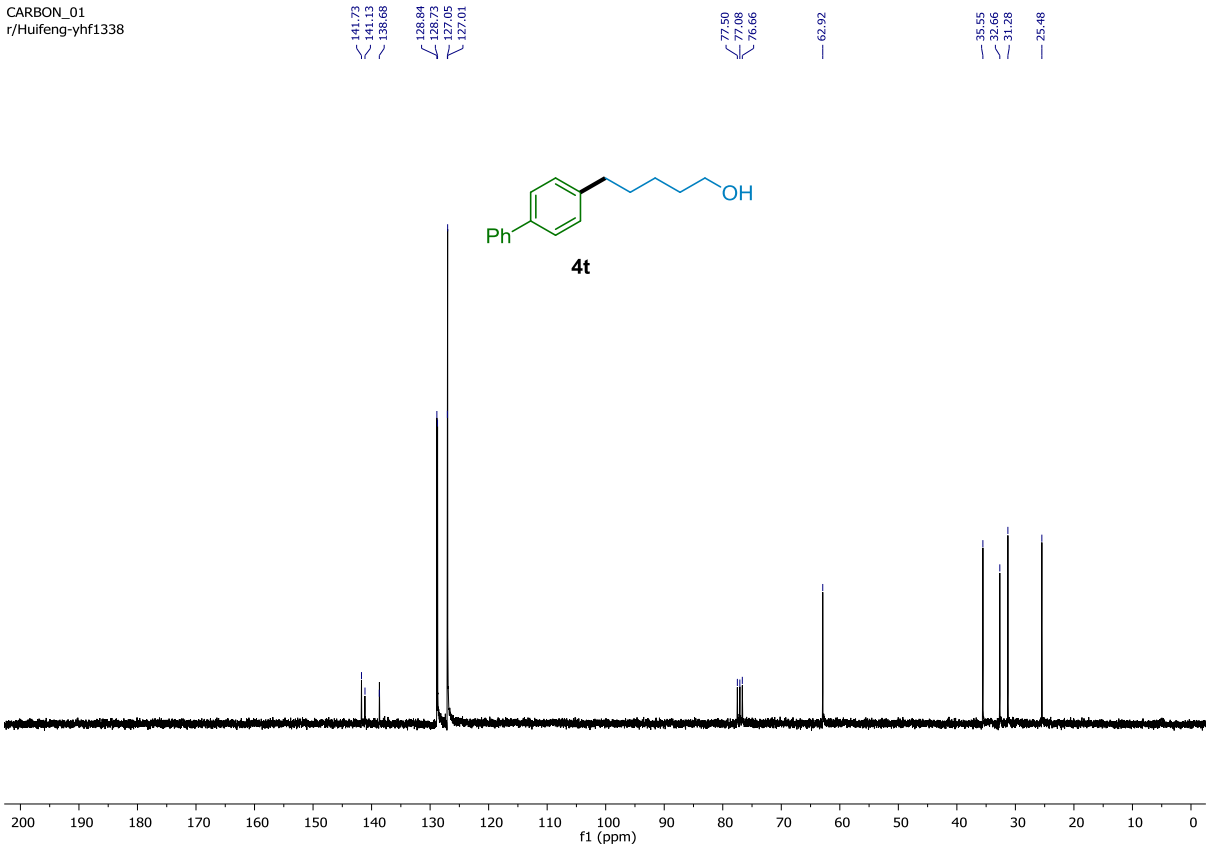


4s

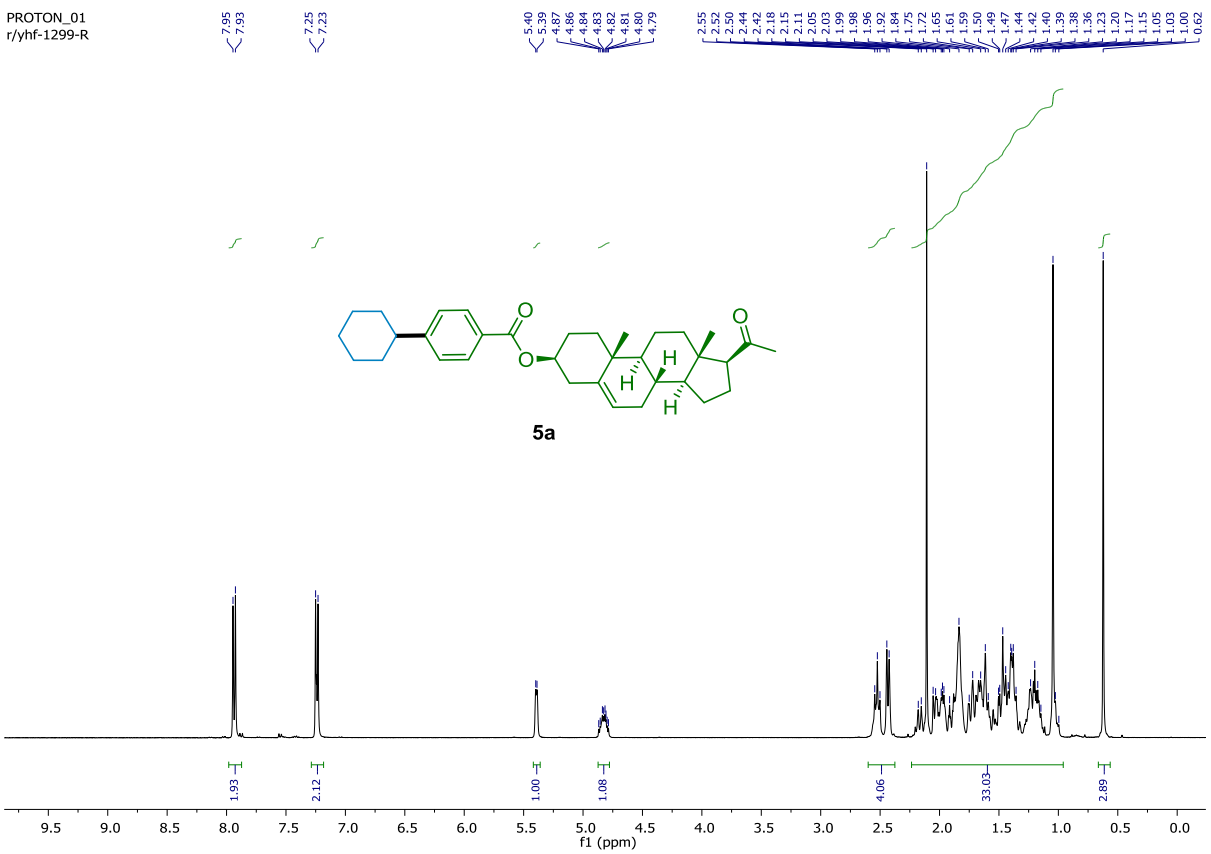
PROTON_01
r/Huifeng-yhf1338



CARBON_01
r/Huifeng-yhf1338

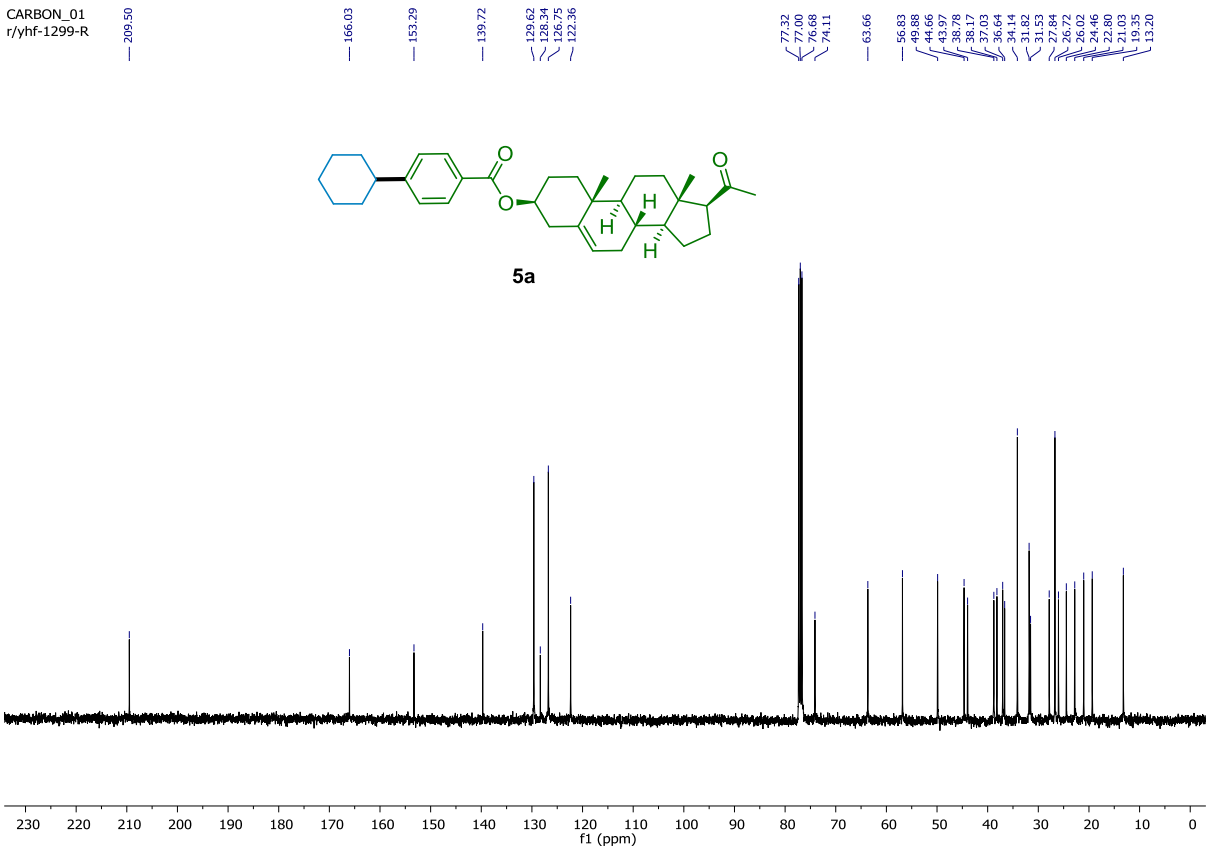


PROTON_01
r/yhf-1299-R



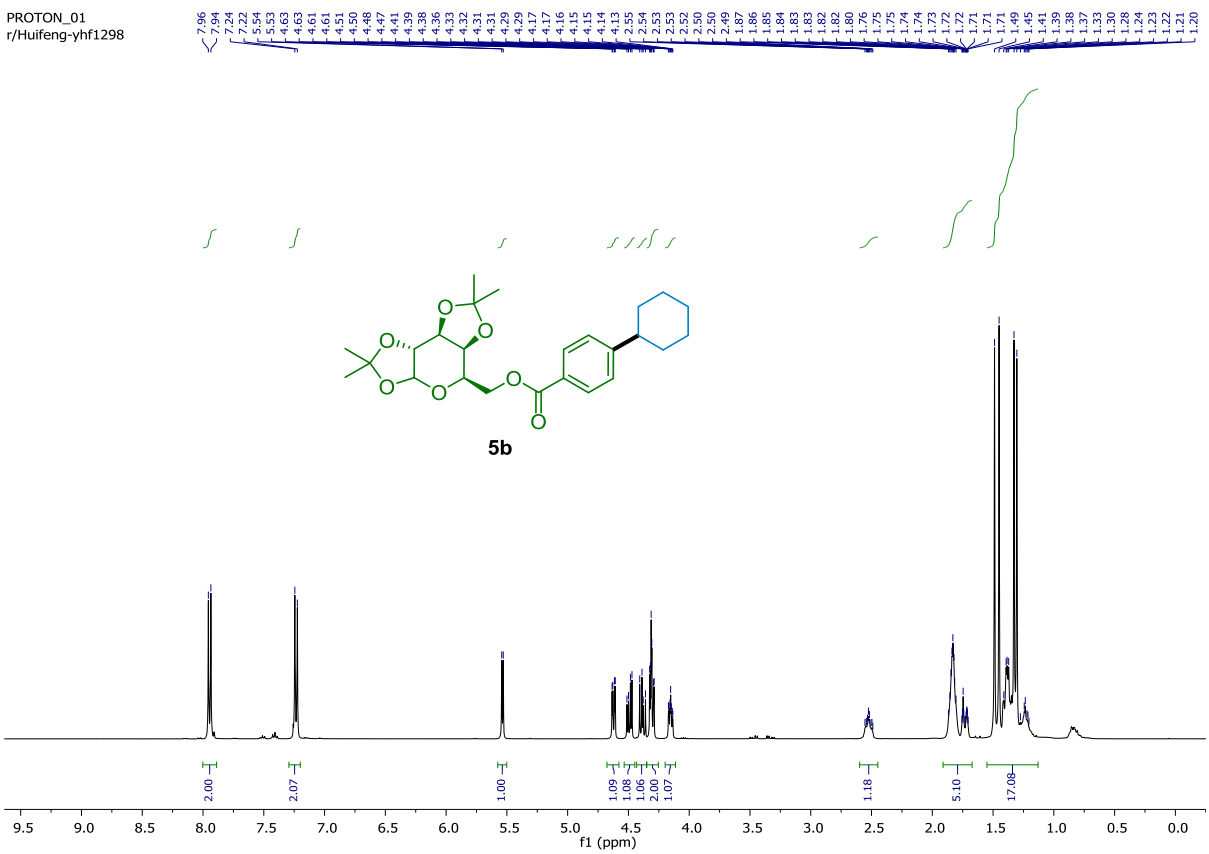
5a

CARBON_01
r/yhf-1299-R

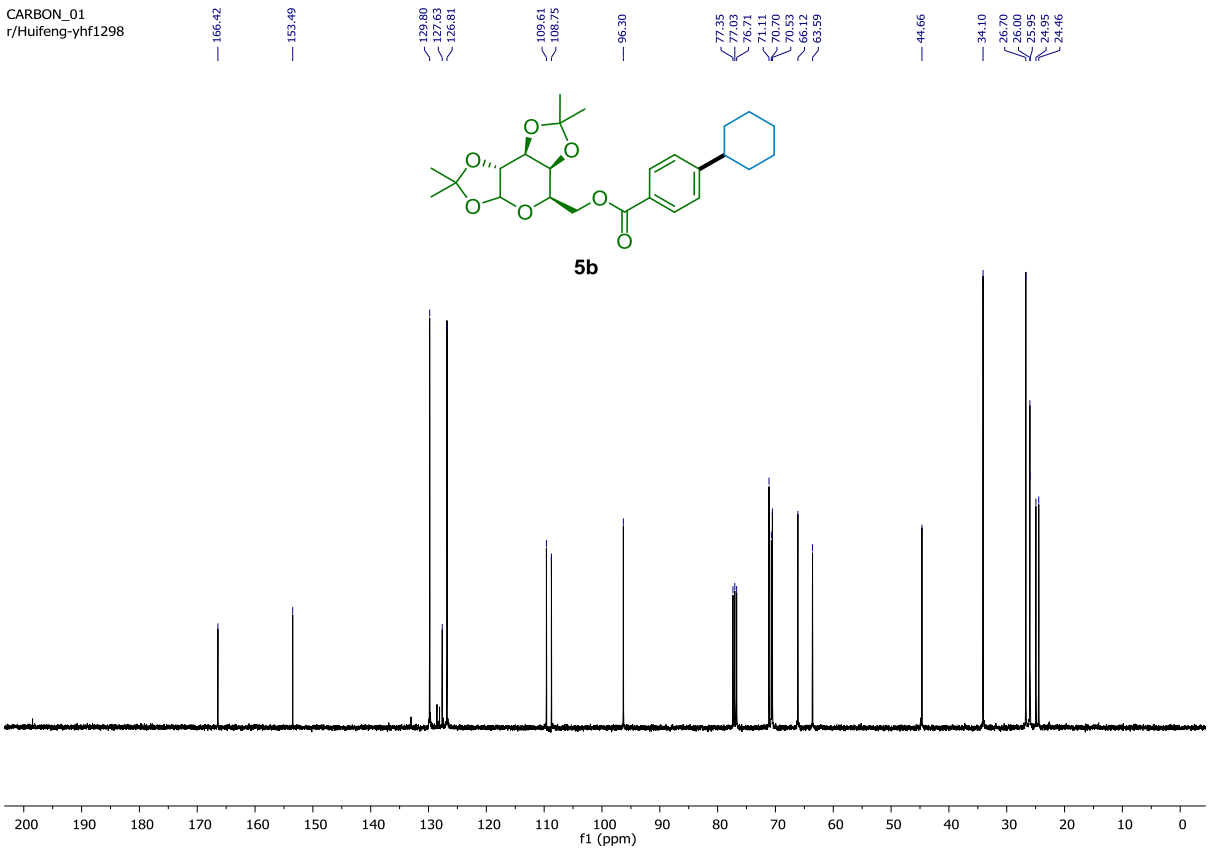


5a

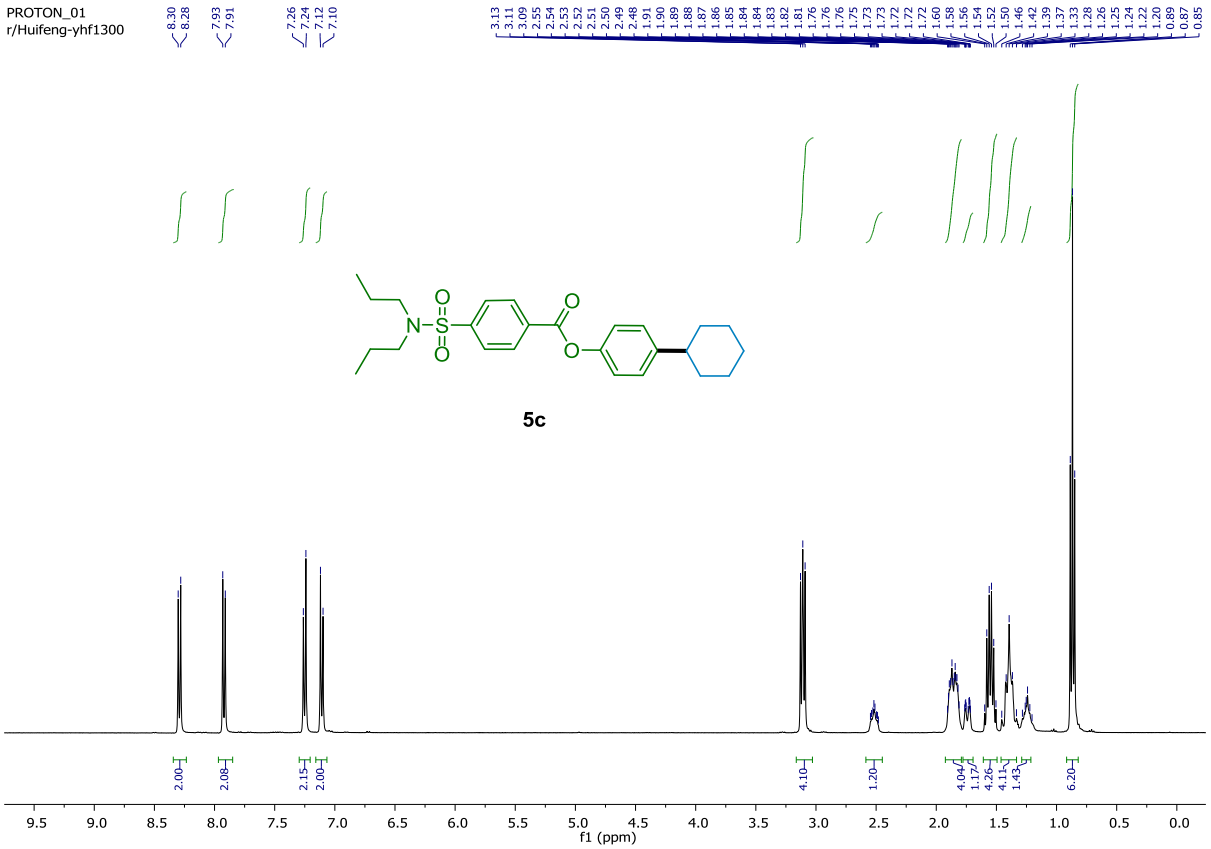
PROTON_01
r/Huifeng-yhf1298



CARBON_01
r/Huifeng-yhf1298

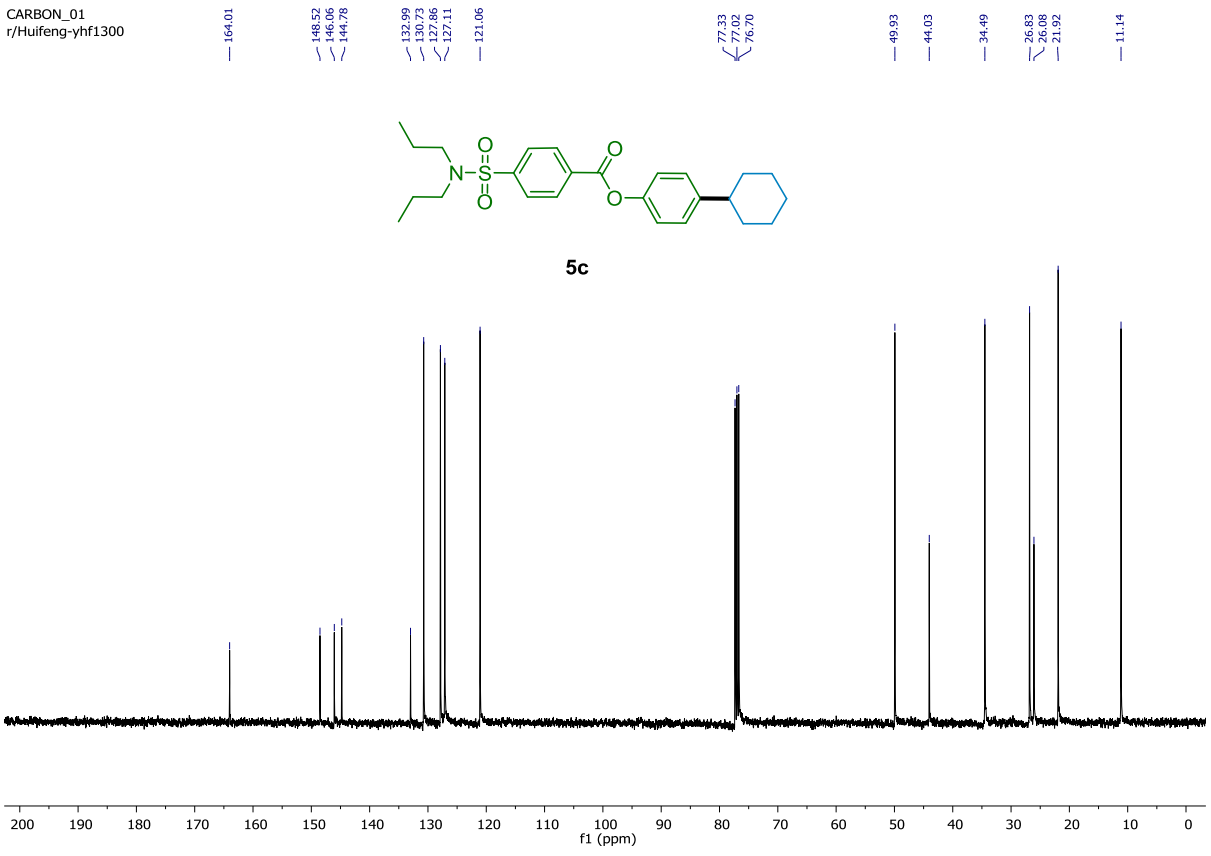


PROTON_01
r/Huifeng-yhf1300



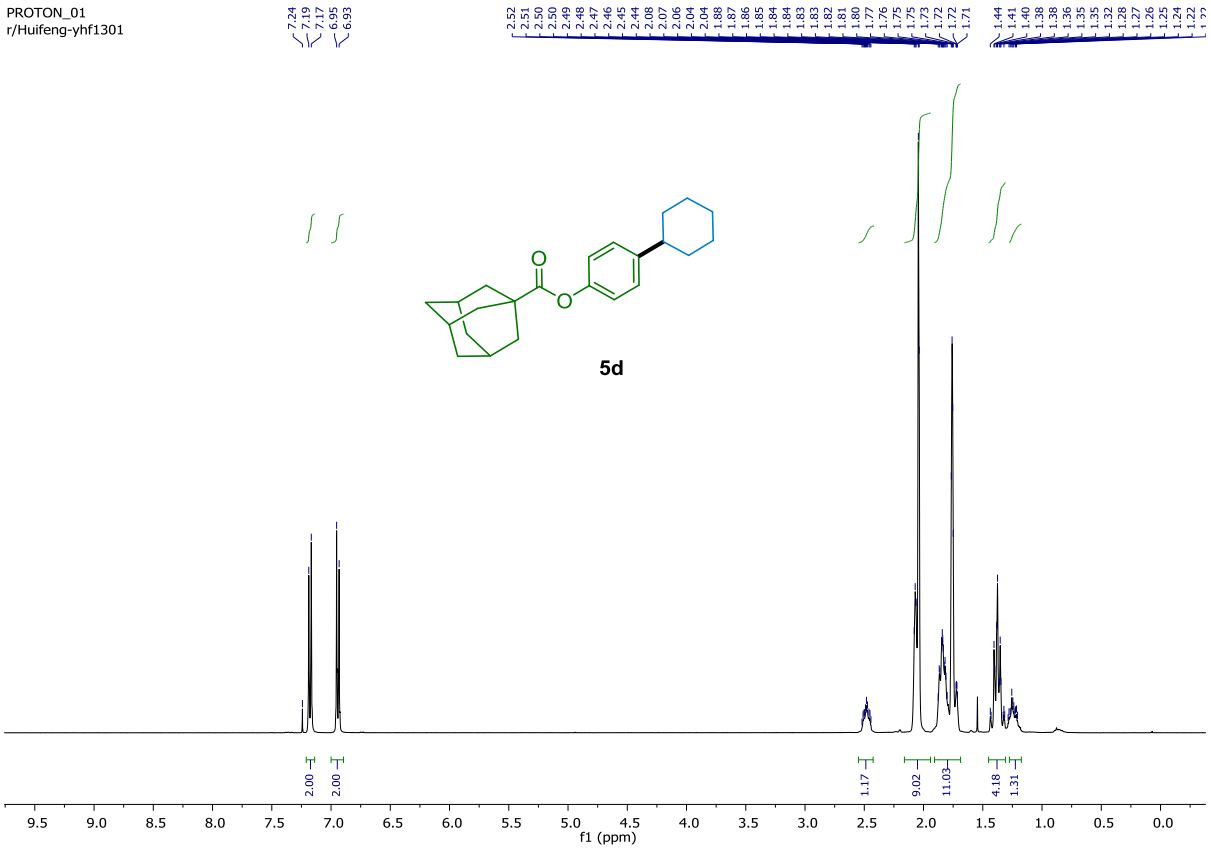
5c

CARBON_01
r/Huifeng-yhf1300

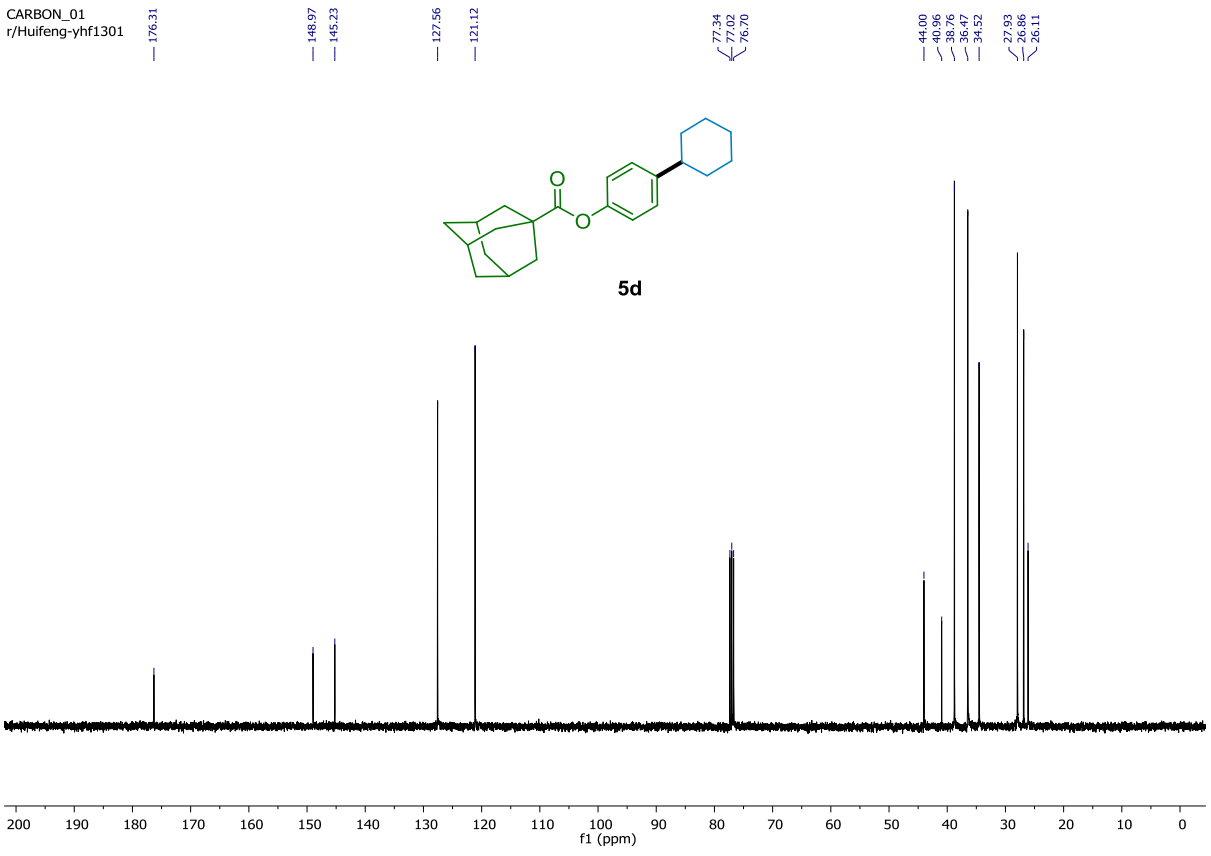


5c

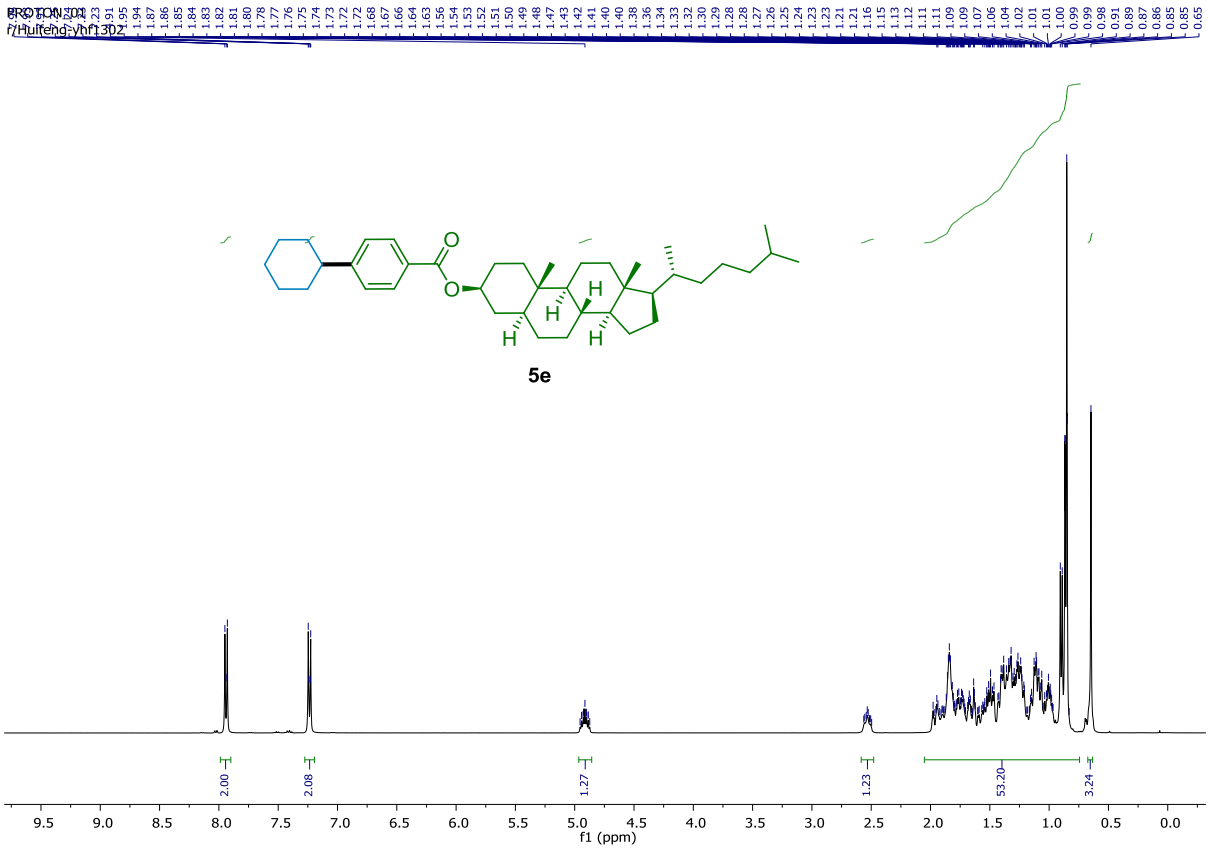
PROTON_01
r/Huifeng-yhf1301



CARBON_01
r/Huifeng-yhf1301

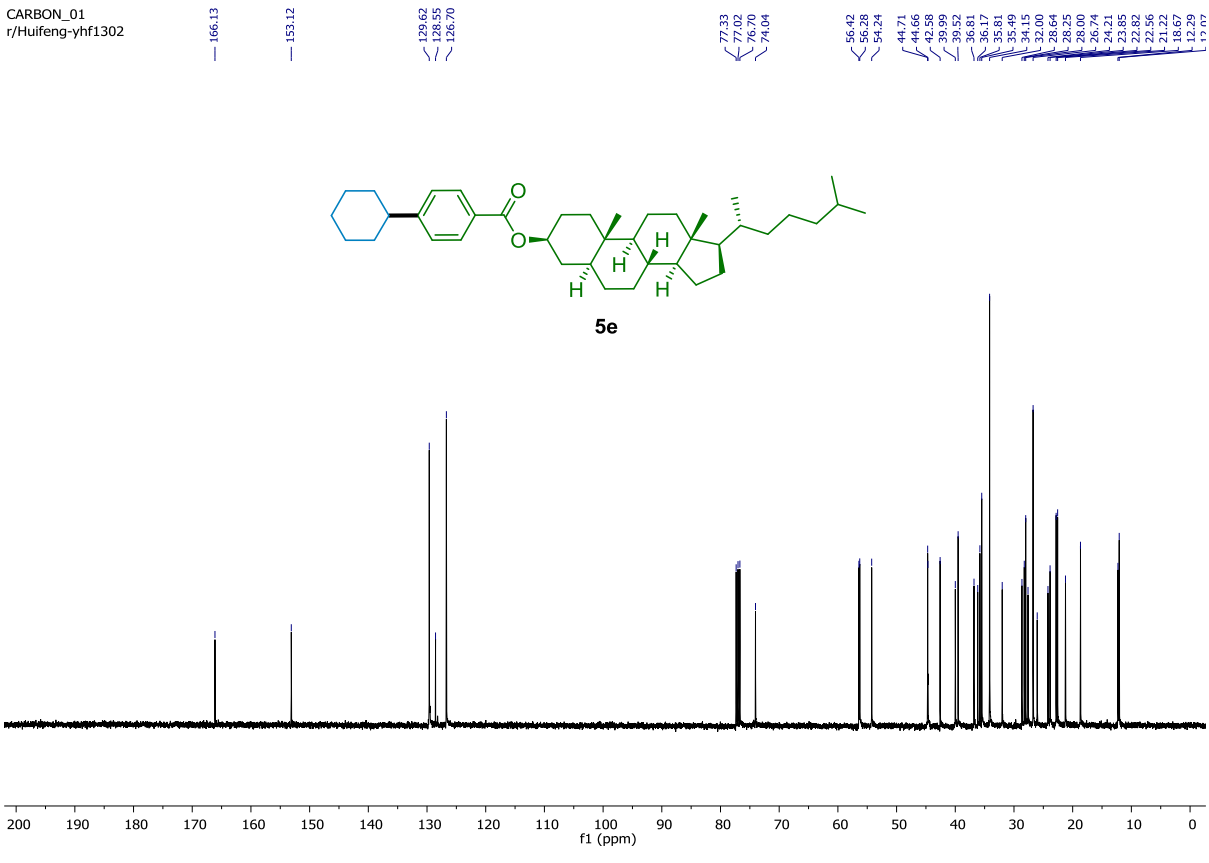


PROTON_01
r/Huifeng-yhf1302



5e

CARBON_01
r/Huifeng-yhf1302

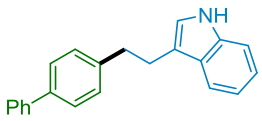


5e

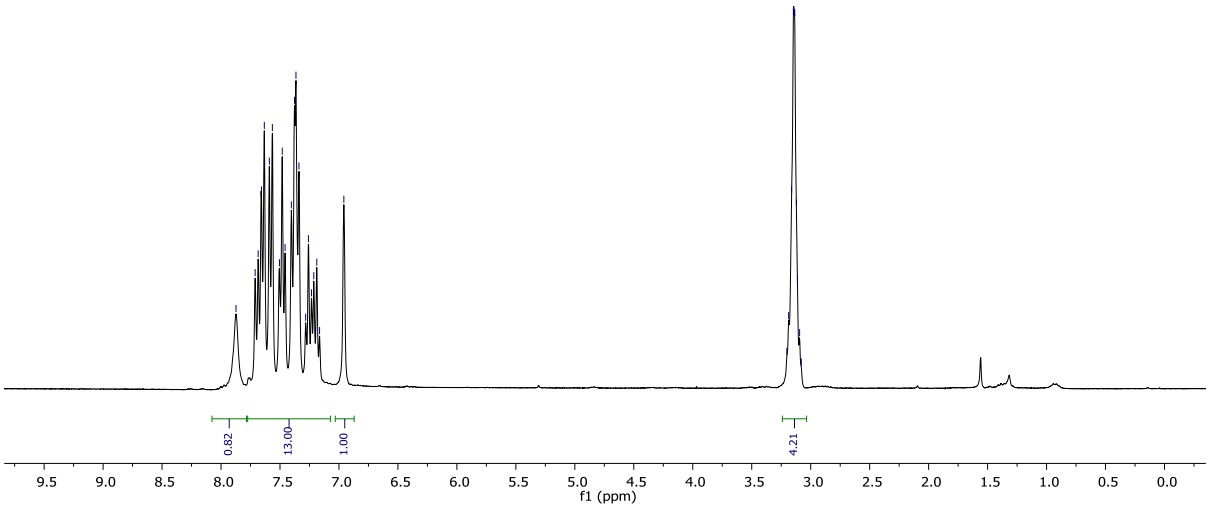
PROTON_01
r/Huifeng-yhf1339

7.87 7.71 7.69 7.66 7.63 7.59 7.56 7.50 7.48 7.46 7.40 7.38 7.36 7.34 7.28 7.26 7.23 7.21 7.19 7.16 6.96

3.20 3.19 3.16 3.15 3.14 3.12 3.11 3.09 3.08



5f



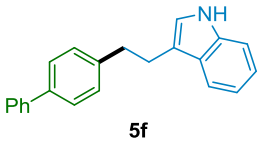
0.82 13.00 1.00 4.21

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)

CARBON_01
r/Huifeng-yhf1339

141.58 141.17 138.81 136.33 128.97 128.78 127.06 122.01 121.39 119.27 118.91 116.13 111.16 77.51 77.08 76.66 36.14 27.27

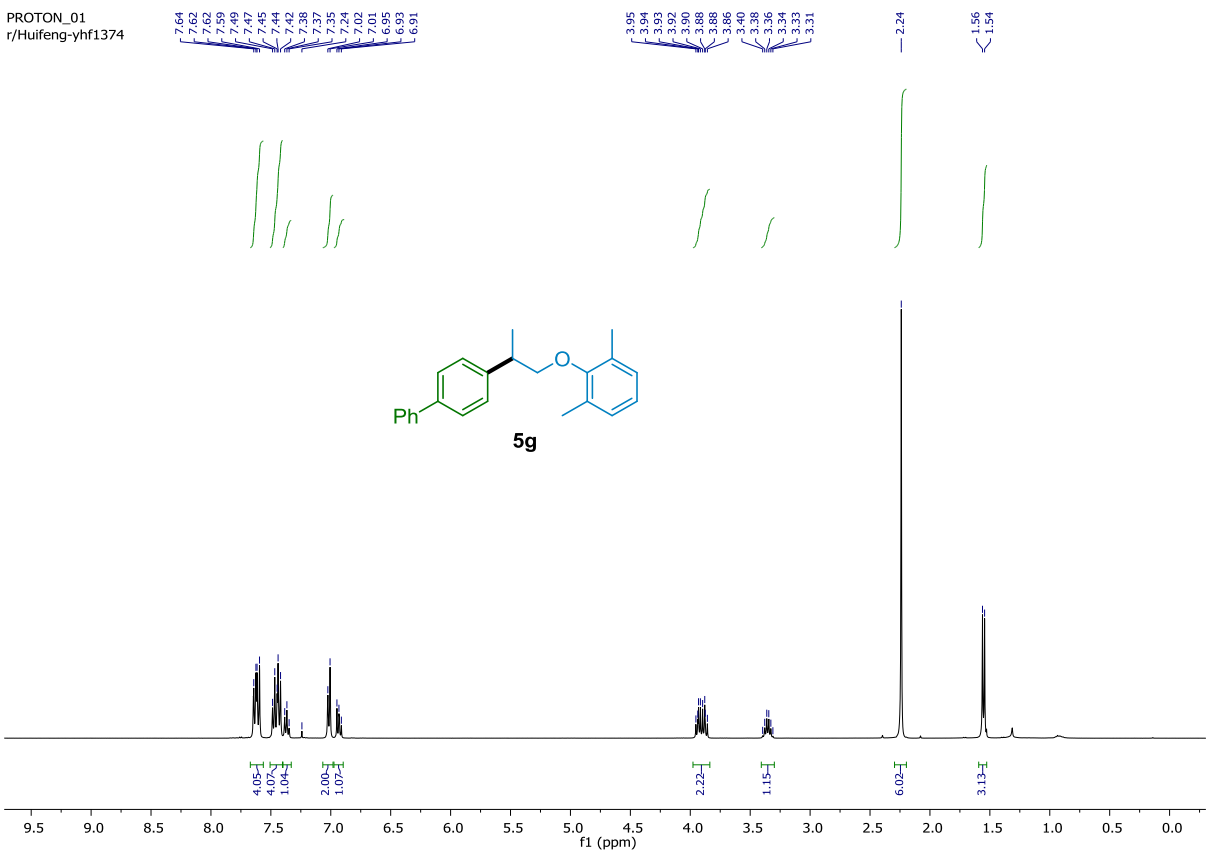


5f

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

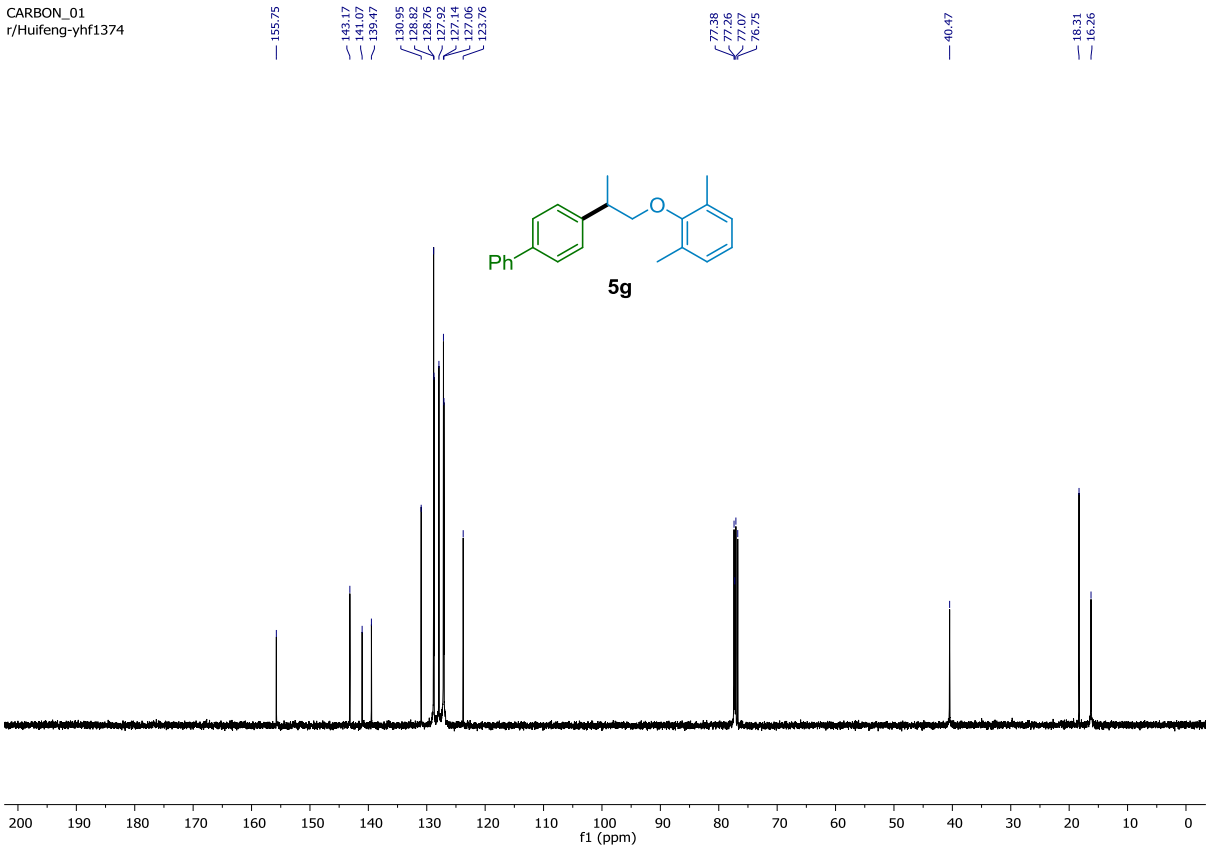
f1 (ppm)

PROTON_01
r/Huifeng-yhf1374



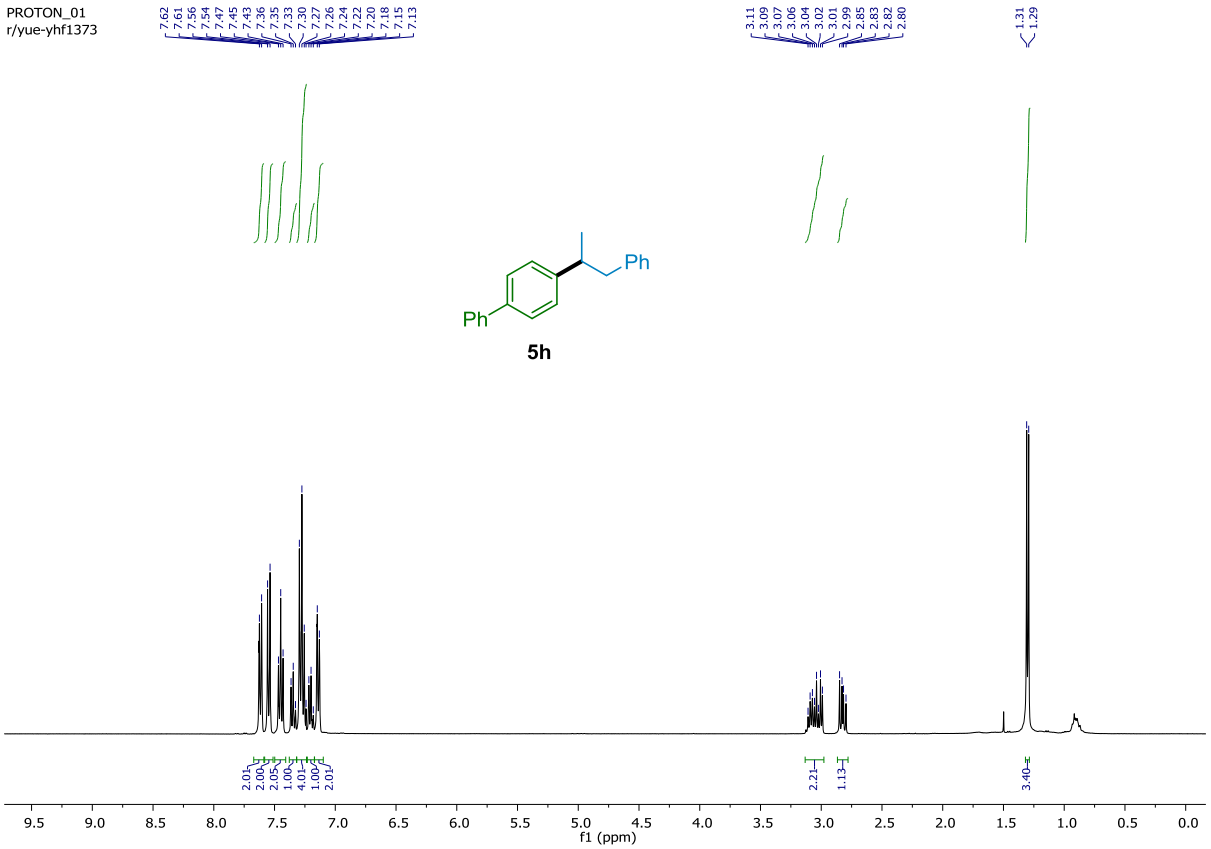
5g

CARBON_01
r/Huifeng-yhf1374



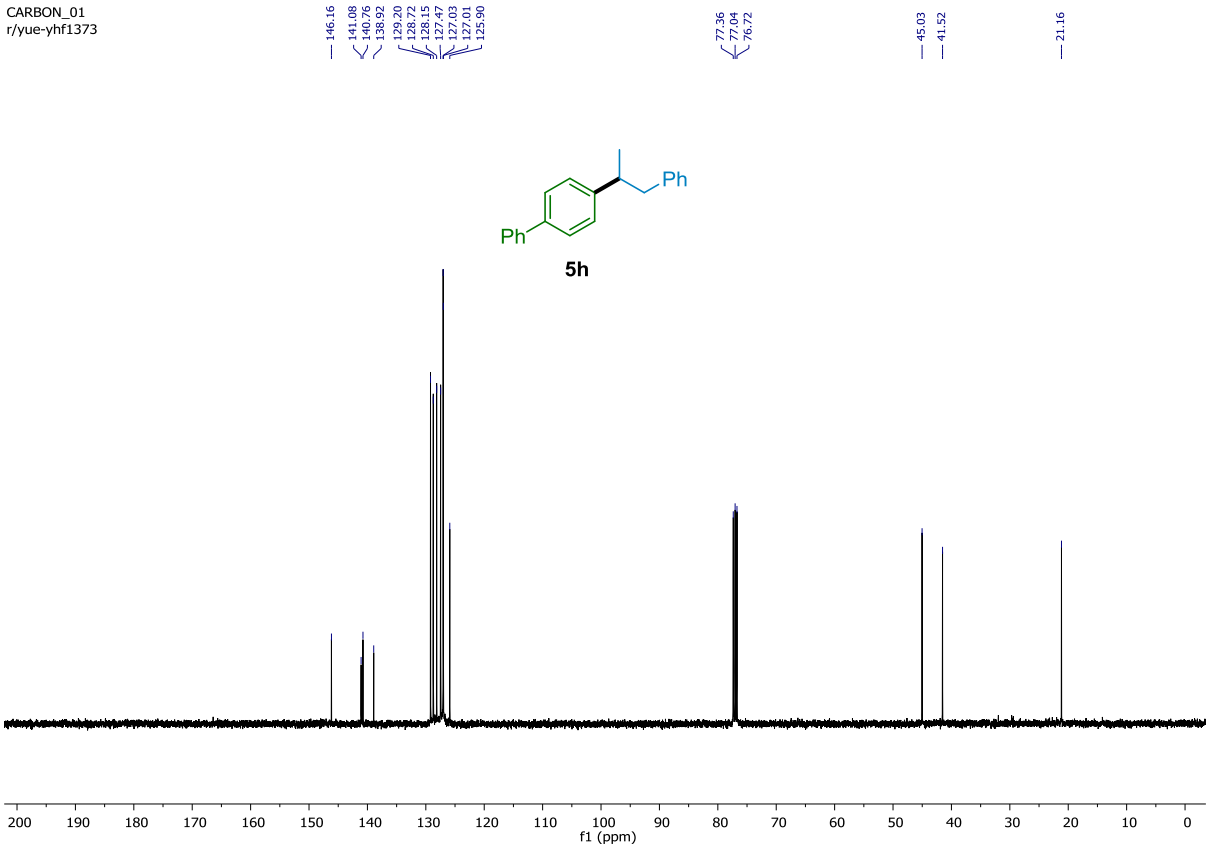
5g

PROTON_01
r/yue-yhf1373

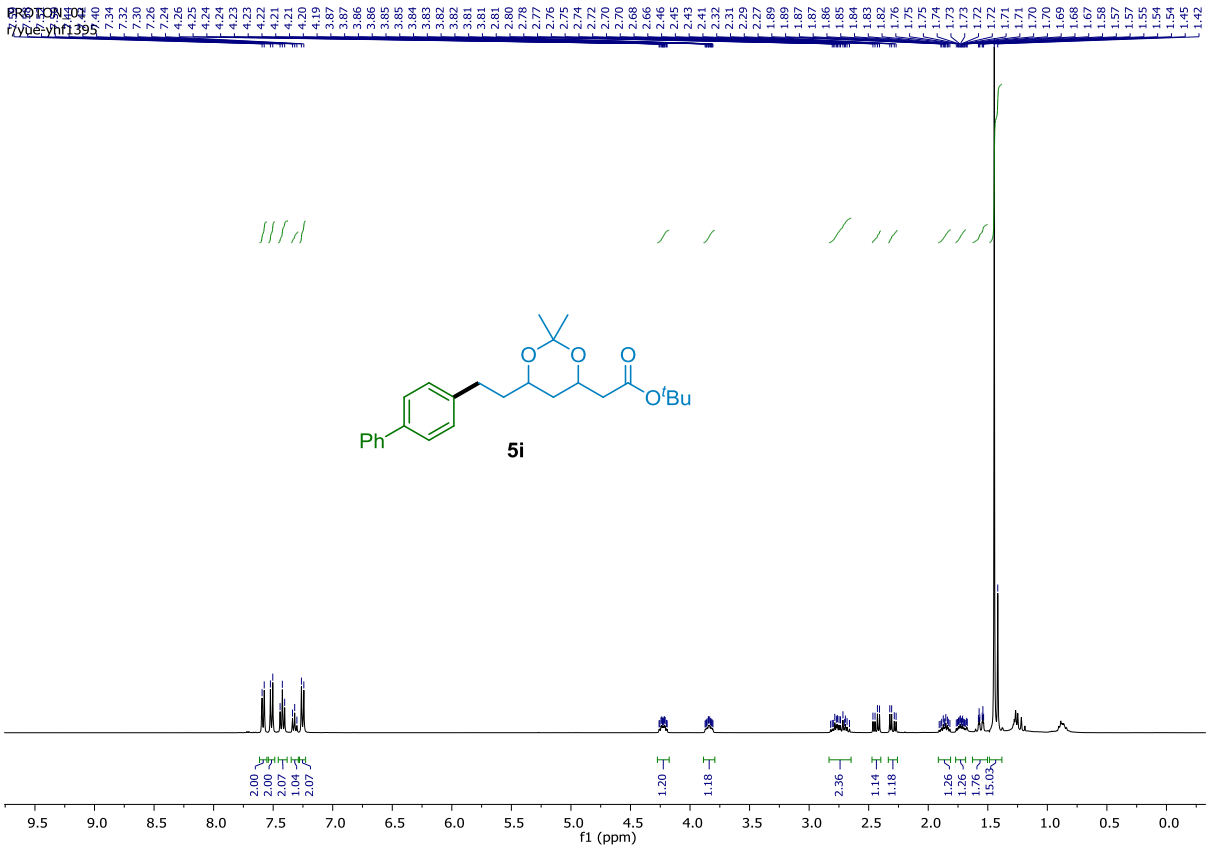


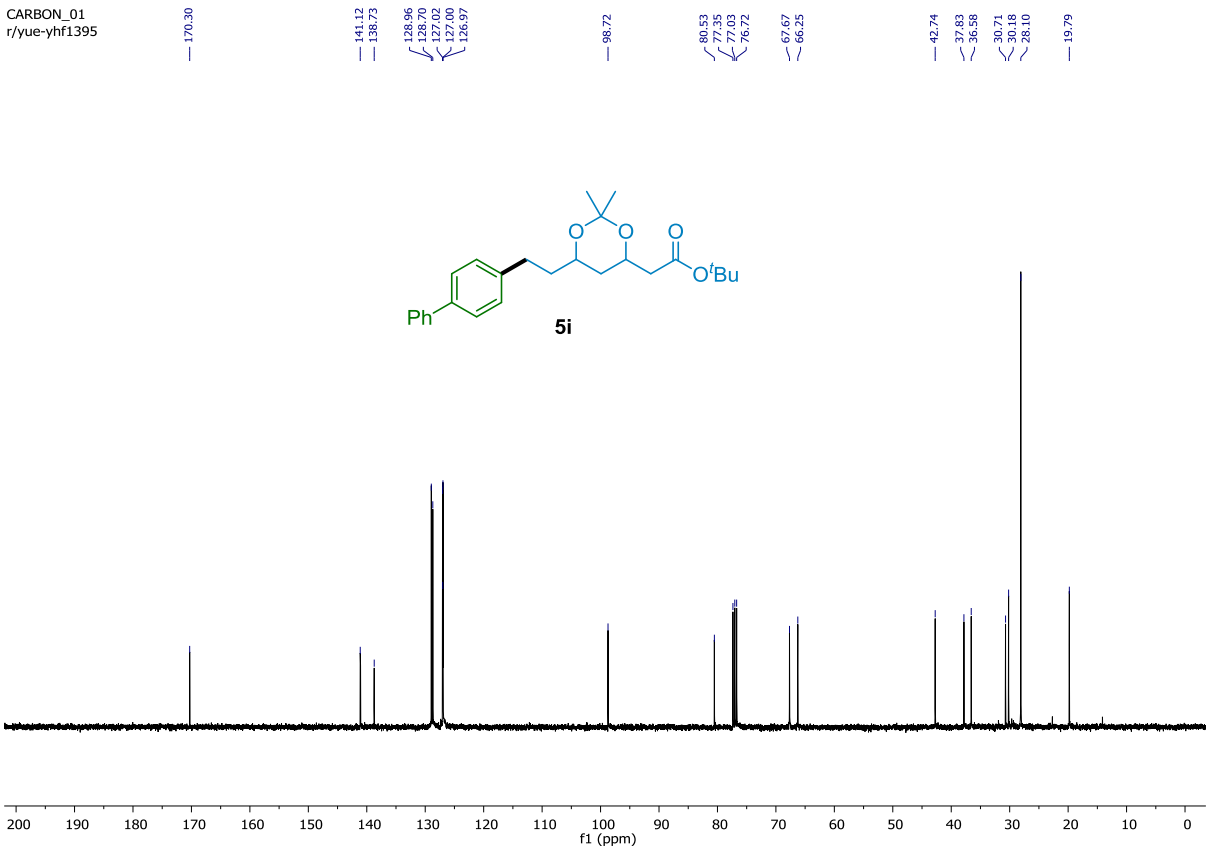
5h

CARBON_01
r/yue-yhf1373

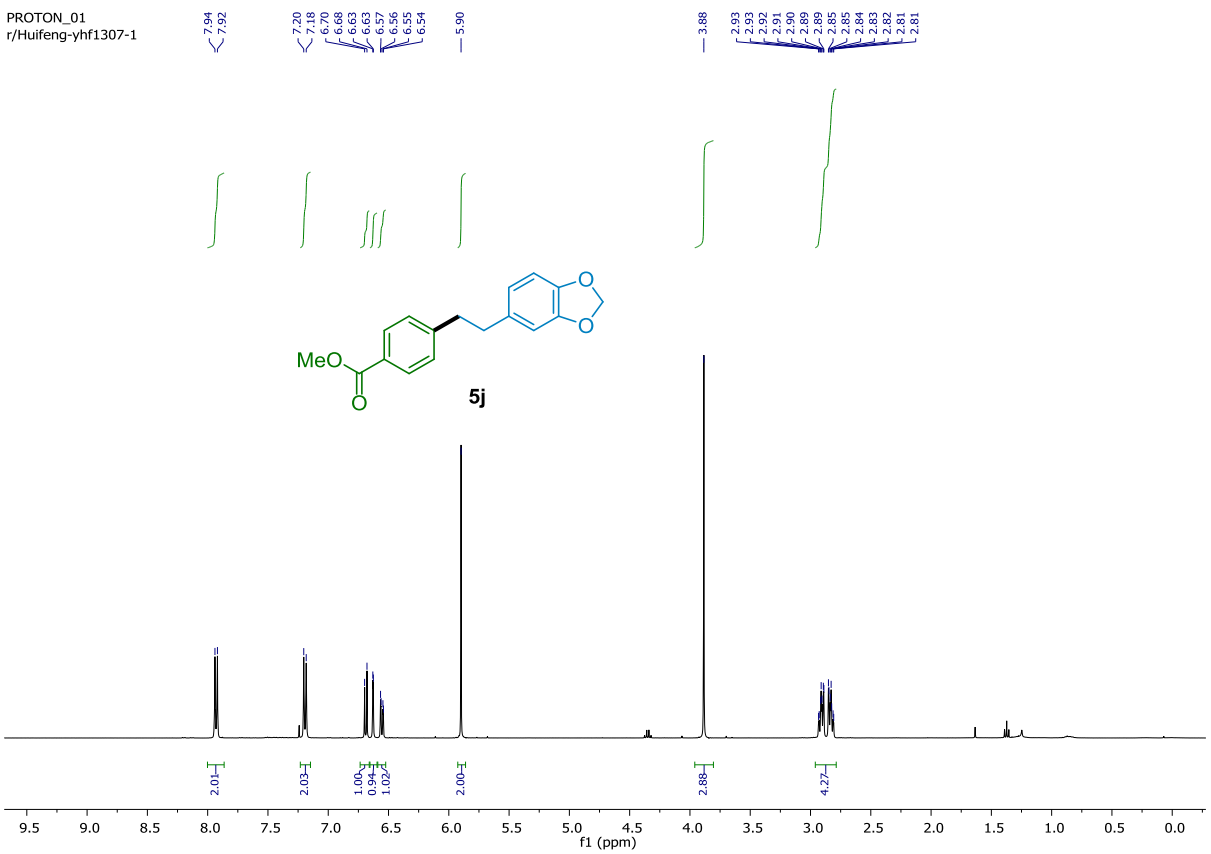


5h

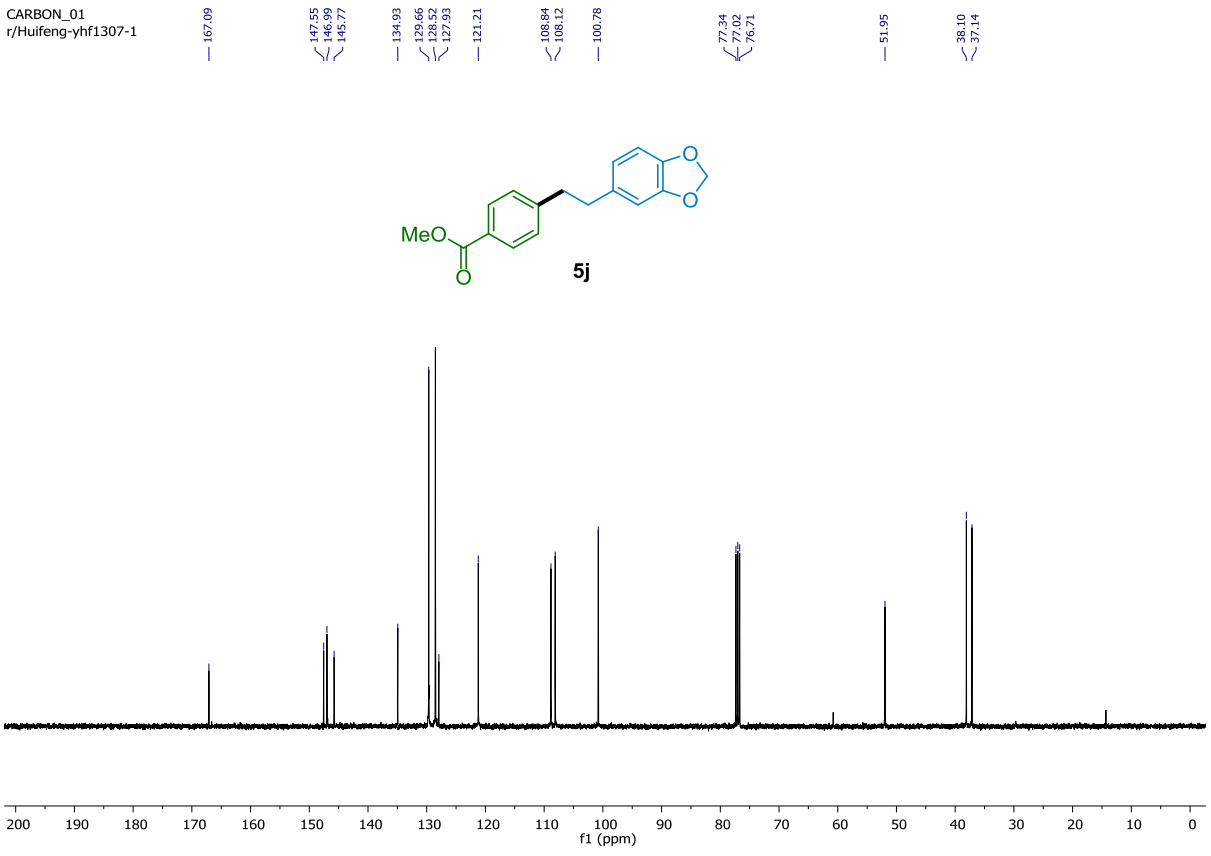

PROTON_01
r/yue-yhf1395
Ph
O
O
O
O^{t}Bu
5i
f1 (ppm)


CARBON_01
r/yue-yhf1395
Ph
O
O
O
O^{t}Bu
5i
f1 (ppm)

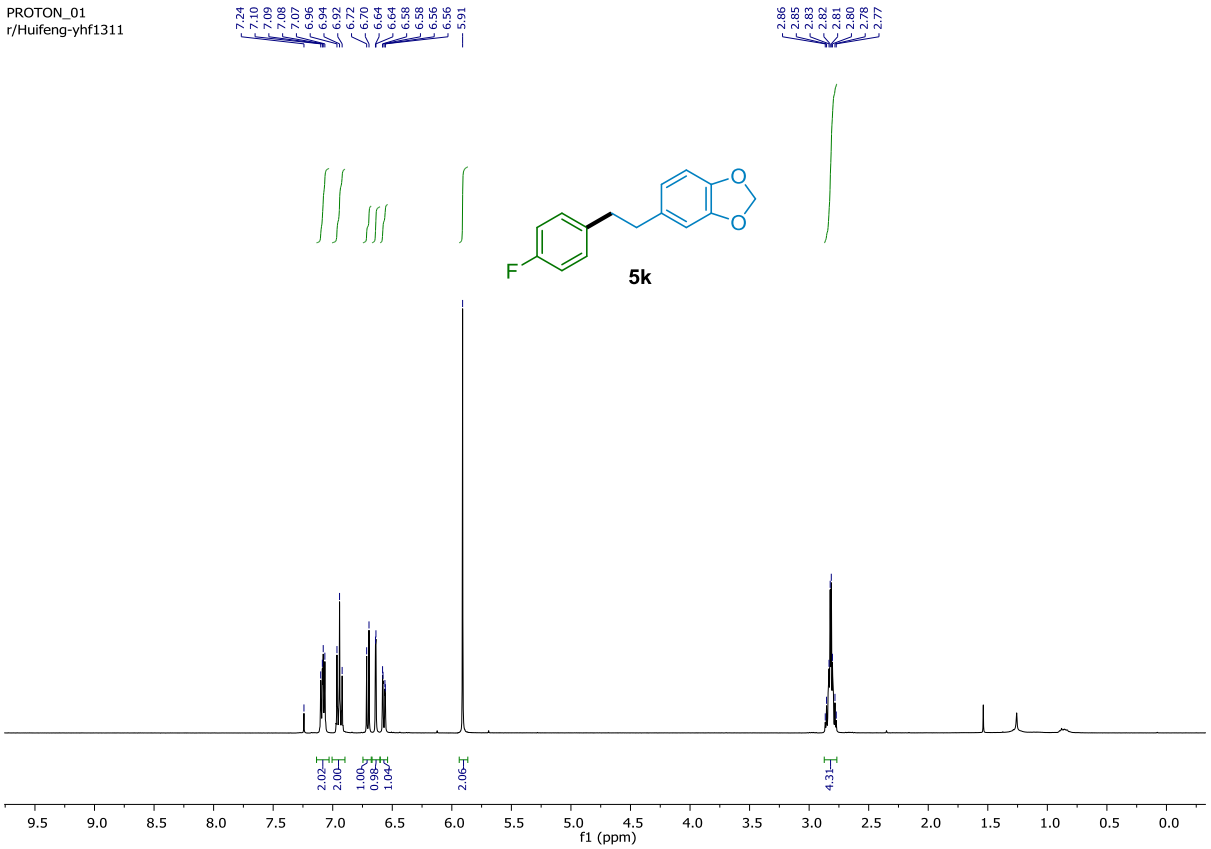
PROTON_01
r/Huifeng-yhf1307-1



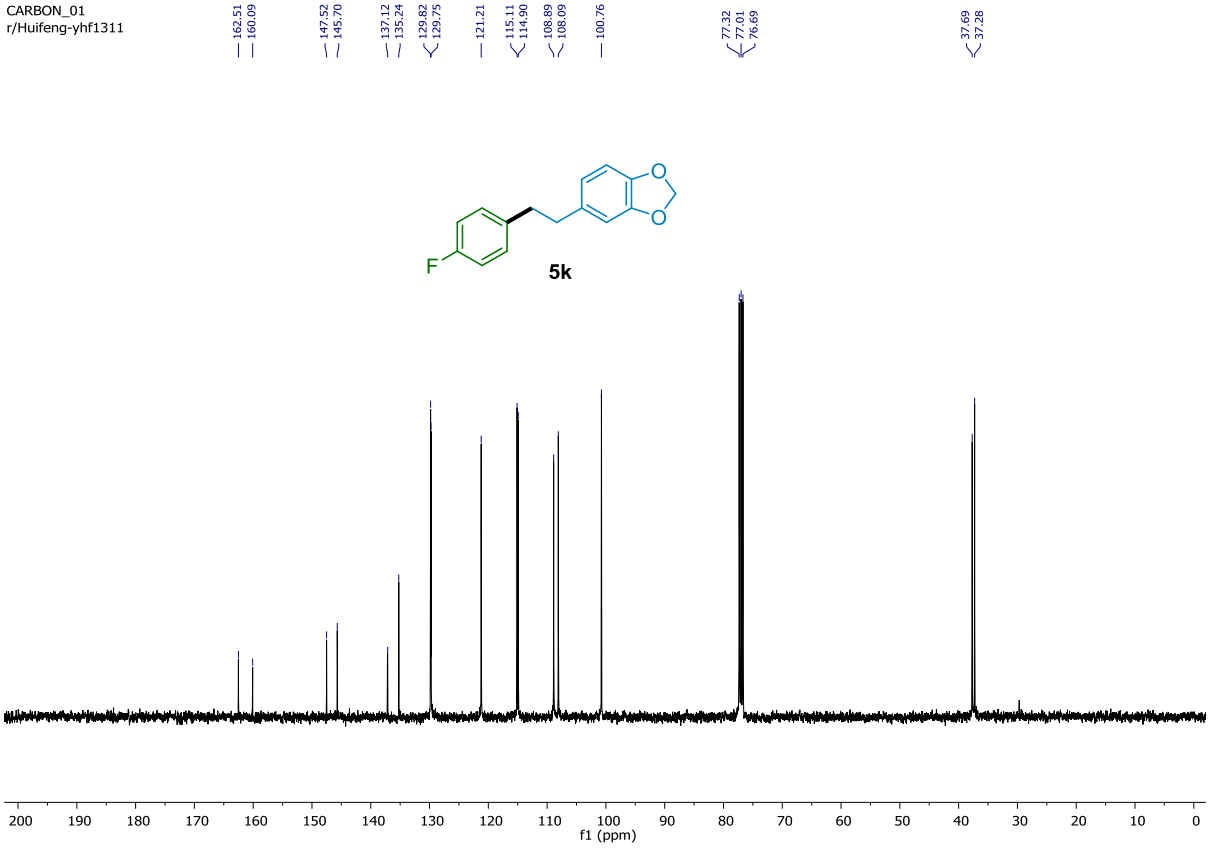
CARBON_01
r/Huifeng-yhf1307-1



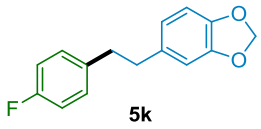
PROTON_01
r/Huifeng-yhf1311



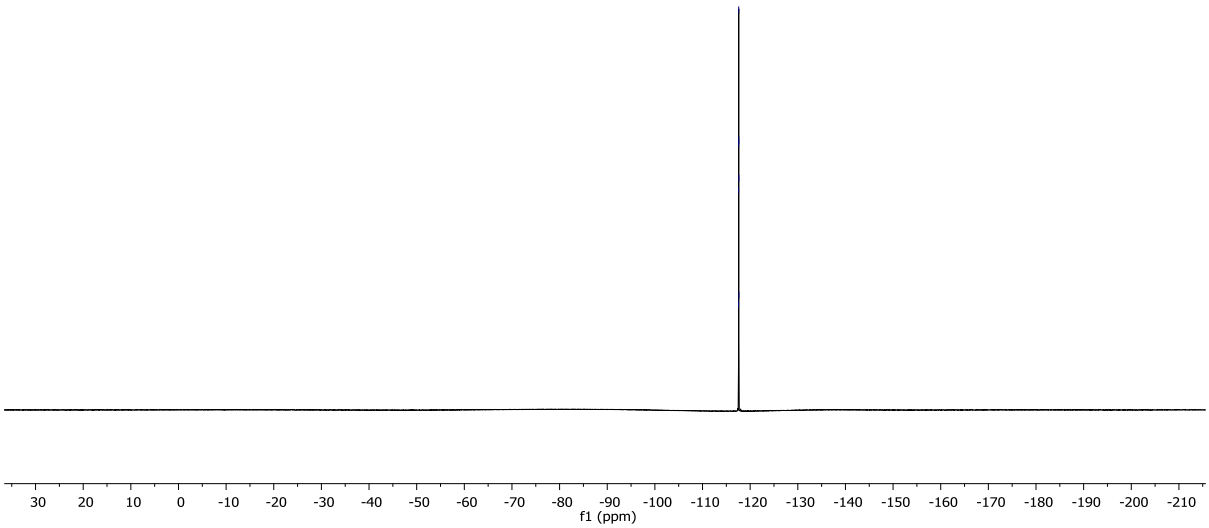
CARBON_01
r/Huifeng-yhf1311



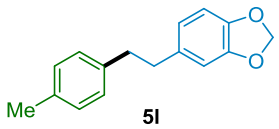
FLUORINE_01
r/Huifeng-yhf1311



5k



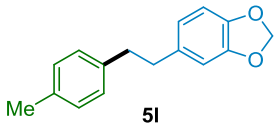
PROTON_01
r/Huifeng-yhf1308



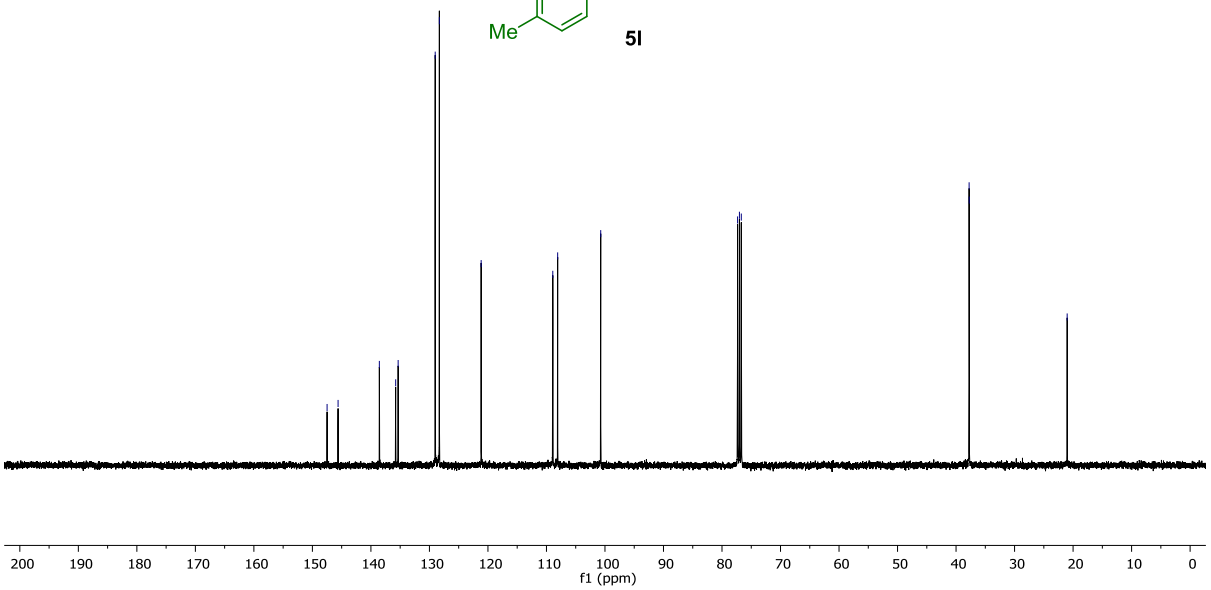
5l

CARBON_01
r/Huifeng-yhf1308

147.49
145.61
138.56
135.77
135.35
129.01
128.30
121.16
108.92
108.09
100.73
77.34
77.02
76.70
37.77
37.74
21.01

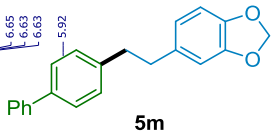


5l

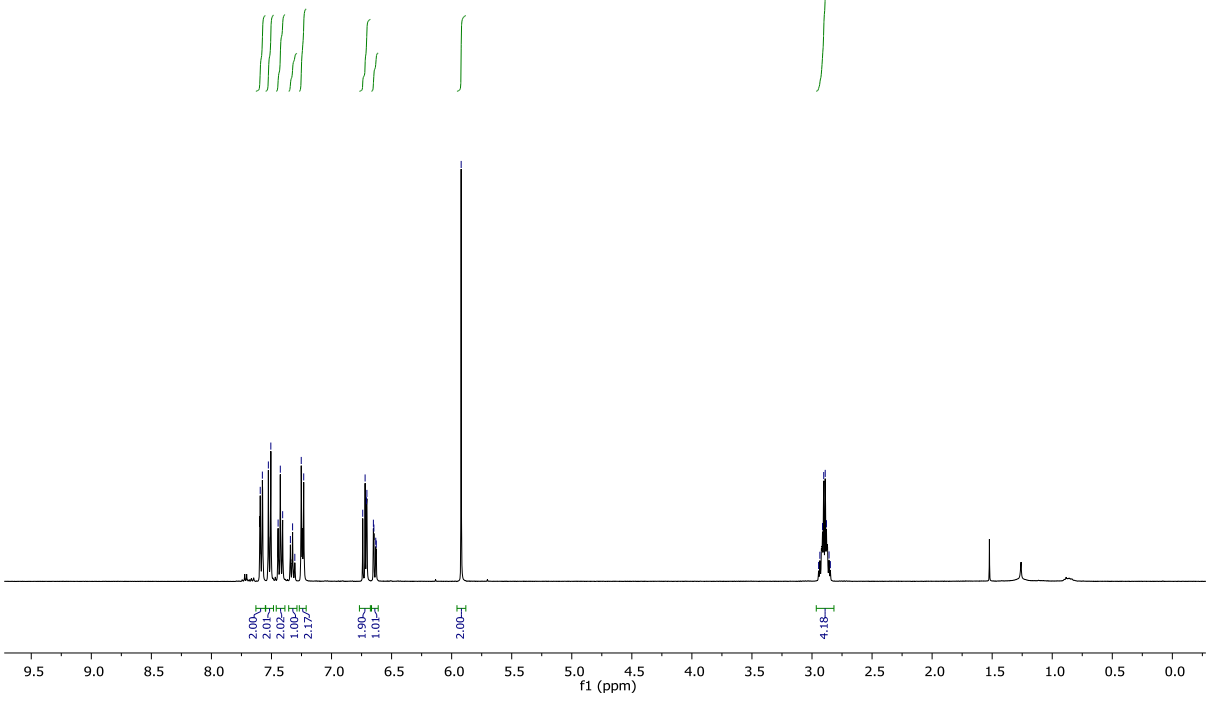


PROTON_01
r/Huifeng-yhf1325

7.59
7.58
7.53
7.51
7.44
7.43
7.41
7.34
7.32
7.31
7.25
7.23
6.74
6.72
6.71
6.71
6.65
6.65
6.63
6.63
5.92
2.95
2.93
2.91
2.90
2.89
2.88
2.86
2.85

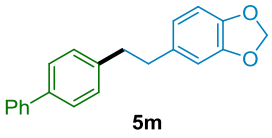


5m

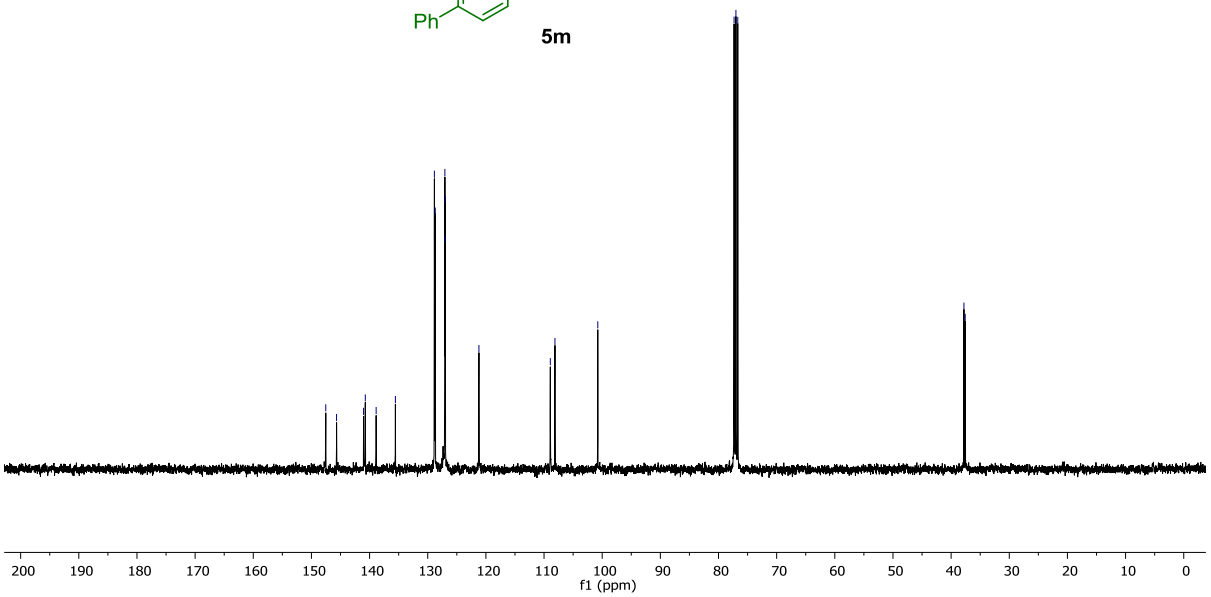


CARBON_01
r/Huifeng-yhf1325

147.53
145.68
141.04
140.74
138.87
135.56
128.85
128.71
127.05
127.03
126.98
121.20
108.92
108.12
100.76
77.32
77.01
76.69
37.80
37.58



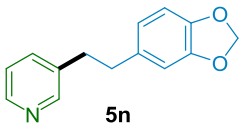
5m



200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

PROTON_01
r/zhu-cz1248

8.42
8.41
8.38
7.42
7.40
7.24
7.18
7.17
7.16
7.15
6.69
6.67
6.61
6.55
6.53
5.89
2.88
2.87
2.85
2.84
2.83
2.82
2.80
2.79



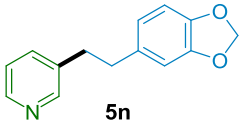
5n

0.90
0.93
1.00
1.01
0.97
0.93
1.00
2.00
4.33

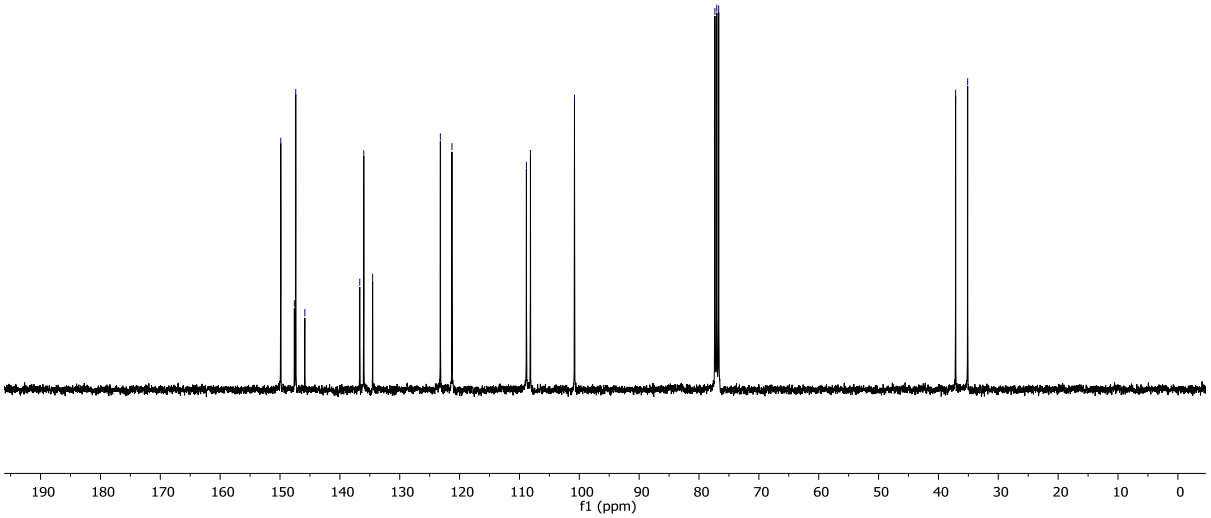
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

CARBON_01
r/zhu-cz1248

149.87
147.60
147.37
145.85
136.68
136.01
134.52
123.21
121.27
108.83
108.16
100.80
77.35
77.03
76.71
37.13
35.12

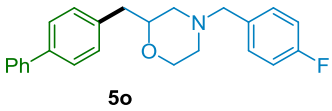


5n



PROTON_01
r/Huifeng-yhf1355

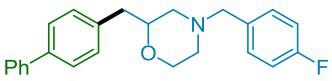
7.58
7.58
7.56
7.52
7.50
7.43
7.41
7.39
7.33
7.31
7.30
7.27
7.25
7.24
7.00
6.98
6.96
3.86
3.83
3.80
3.78
3.78
3.65
3.64
3.62
3.62
3.59
3.59
3.51
3.48
3.39
3.36
2.89
2.87
2.86
2.84
2.76
2.73
2.72
2.70
2.68
2.61
2.58
2.16
2.15
2.13
2.13
2.11
2.10
2.00
1.97
1.94



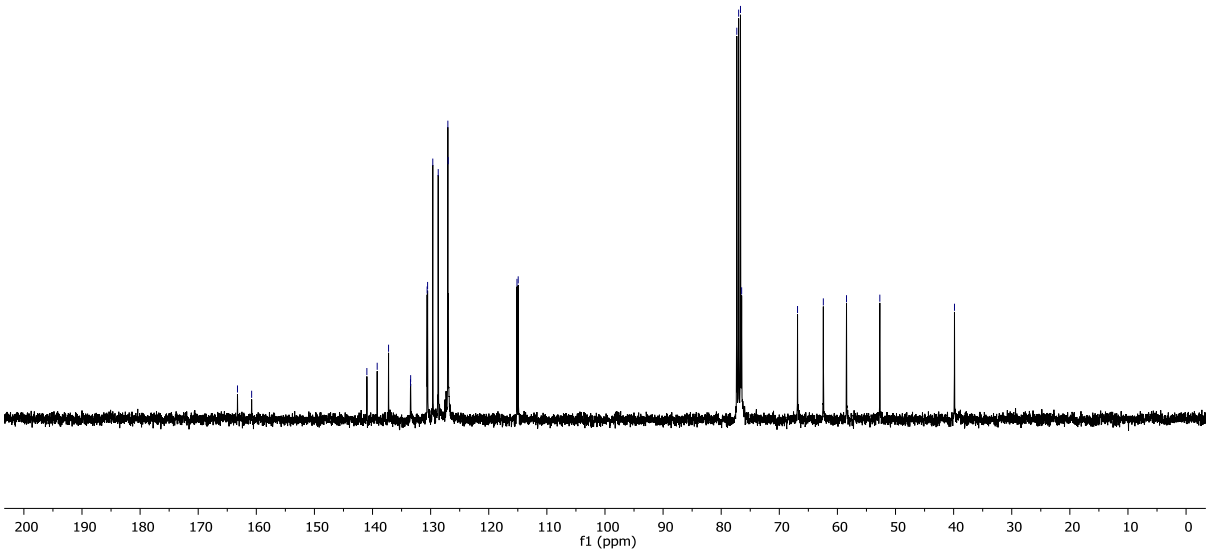
5o

CARBON_01
r/Huifeng-yhf1355

163.24
160.81
140.97
139.20
137.24
133.47
133.44
130.60
130.53
129.63
128.70
127.04
126.98
115.14
114.93
77.31
77.00
76.68
76.48
66.86
62.42
58.43
52.70
39.85

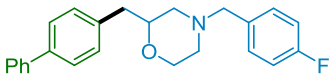


5o

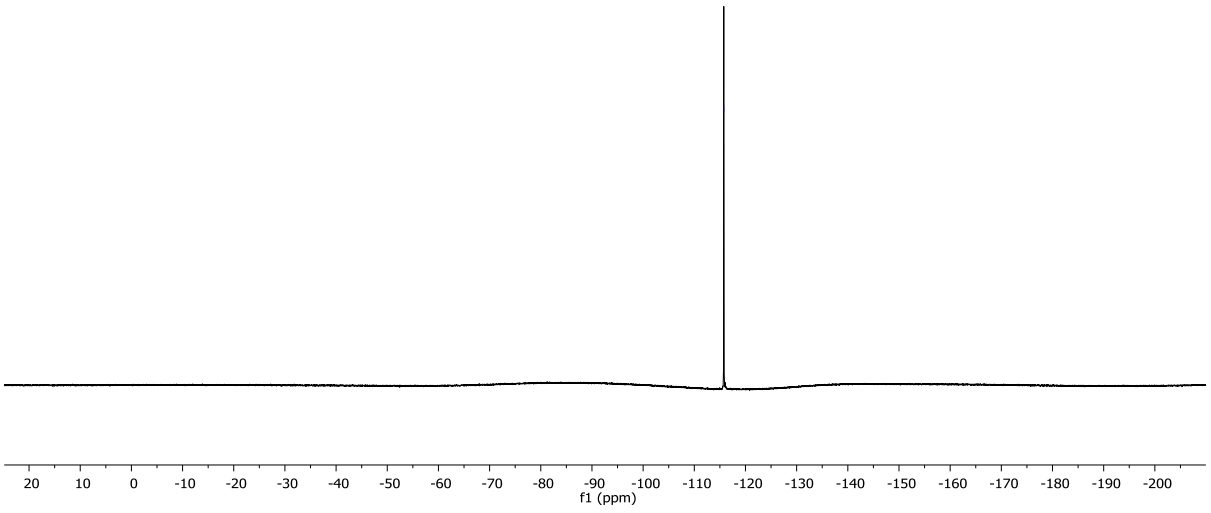


FLUORINE_01
r/Huifeng-yhf1355

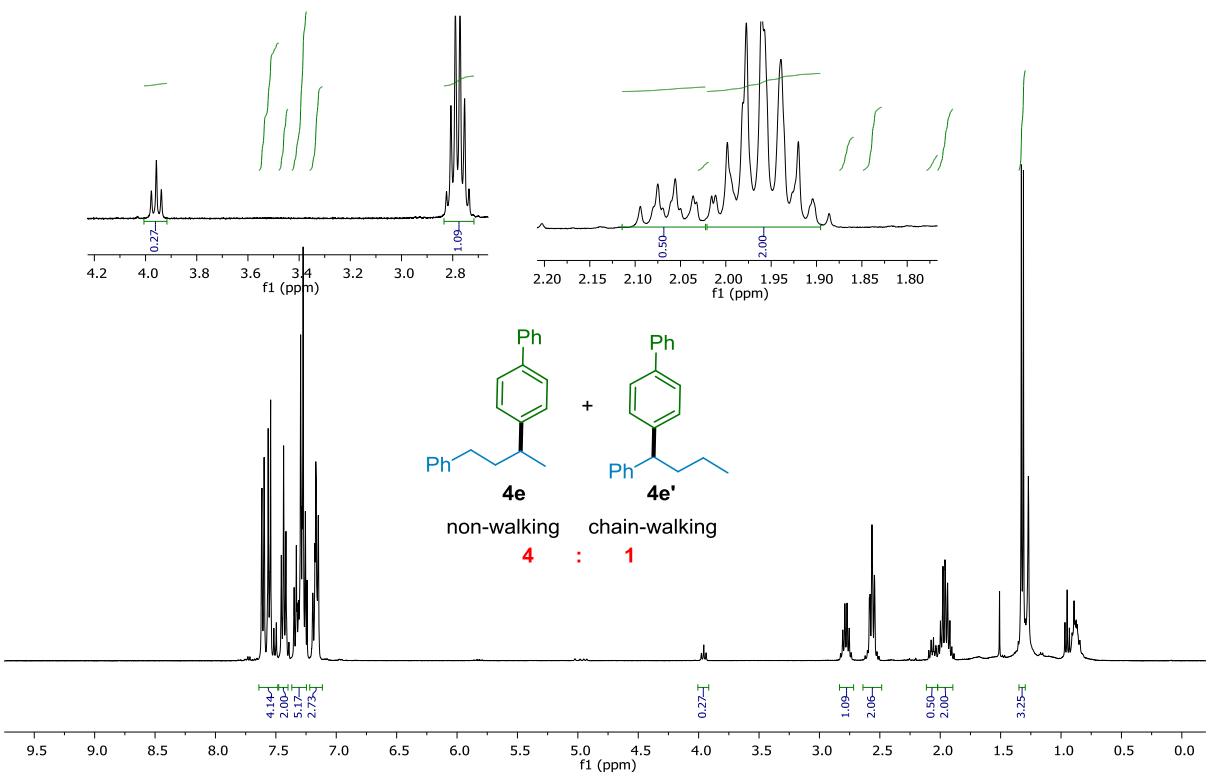
-115.75



5o



PROTON_01
r/Huifeng-yhf1378



PROTON_01
r/Huifeng-yhf1409