This ESI for Org. Chem. Front DOI 10.1039/C8QO00938D, originally published on 22nd Oct 2018, was updated on 4th January 2019. The carbon NMR spectra for some compounds were updated for clarity and improvement.

Metal-Free Cross-Coupling of π-Conjugated Triazenes with Unactivated Arenes via Photoactivation

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General Information

All photochemical reactions were carried out in quartz tubes using a Rayonet photochemical reactor with 350 nm UV lamps. All commercially obtained reagents were used as received. Solvents were dried, degassed and obtained from a JC Meyer company solvent purification system. Heating was accomplished by either a heating mantle or silicone oil bath. Purification of reaction products was carried out by flash column chromatography using silica gel 60 (230-400 mesh). TLC visualization was accompanied with UV light. Concentration in vacuo refers to the removal of volatile solvent using a rotary evaporator attached to a dry diaphragm pump (10-15 mm Hg) followed by pumping to a constant weight with an oil pump (<300 mTorr).

^{1}H NMR spectra were recorded at 500 MHz and are reported relative to $CDCl_3$ (δ 7.26) or DMSO (δ 2.50). ^{1}H NMR coupling constants (J) are reported in Hertz (Hz) and multiplicities are indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet). Proton-decoupled ^{13}C NMR spectra were recorded at 125 MHz and reported relative to $CDCl_3$ (δ 77.0) or DMSO (δ 39.52). IR experiments were recorded with neat samples on a Bruker Alpha instruments fitted with diamond ATR sample plate. High-resolution (HR) mass spectra were recorded at the Shimadzu Center Laboratory for Biological Mass Spectrometry at UTA.

List of Known Biaryl Compounds

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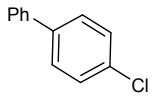
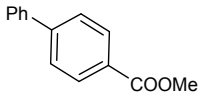
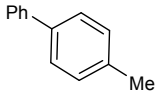
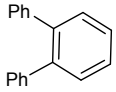
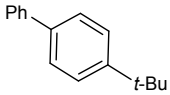
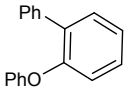
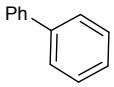
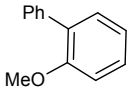
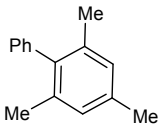
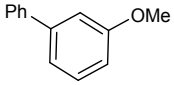
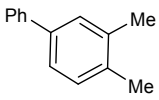
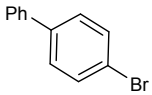
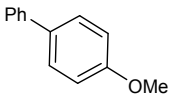
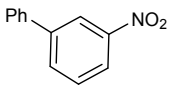
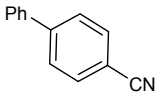
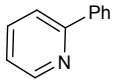
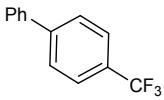
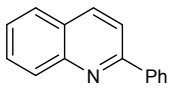
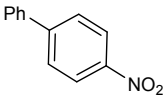
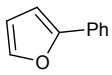
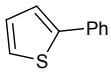
4a		S1	**4k**		S6
4b		S2	**4l**		S7
4c		S3	**4m**		S8
4d		S2	**4n**		S9
4e		S4	**4o**		S10
4f		S5	**4p**		S6
4g		S6	**4q**		S1
4h		S6	**4r**		S11
4i		S2	**4s**		S12
4j		S6	**4t**		S13
			4u		S14

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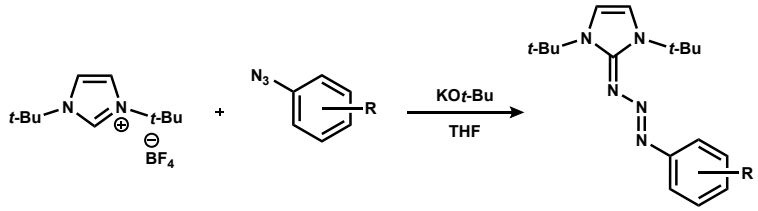
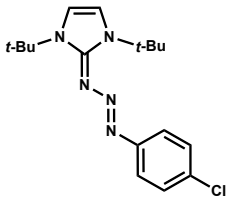
General Methods for the Preparation of Triazenes (3)

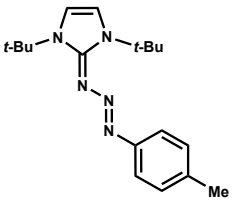


Method A. To a flask containing 1,3-di*tert*-butylimidazolium tetrafluoroborate (1.1 mmol), potassium *tert*-butoxide (1.3 mmol) and dry THF was added (10 mL) under Ar. The resulting suspension was stirred for 15 minutes, followed by dropwise addition of aromatic azide (1.1 mmol). The resulting mixture was left stirring at room temperature for 12 h. After this time, hexanes (10 mL) were added and the resulting solid precipitate filtered. The filtered solid was dissolved in DCM (20 mL) and the precipitated salts filtered. The resulting solution was then concentrated *in vacuo* and dried under high vacuum, affording the pure triazene.

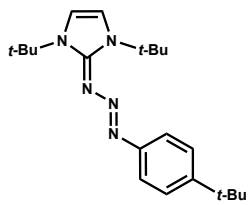
Method B. Same procedure for method A but using NaH instead of potassium *tert*-butoxide. This method was used to prepare triazenes **3e** and **3g**.



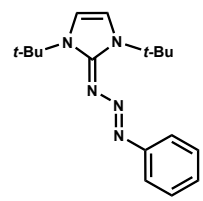
(*E*)-2-((4-chlorophenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3a**): Prepared from 4-chloroazidobenzene (169 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (242 mg, 66%). IR (neat) ν 3095, 1473, 1449, 1257, 699 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.48 (d, J = 8.6 Hz, 2H), 7.25 (d, J = 8.6 Hz, 2H), 6.92 (s, 2H), 1.63 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 153.95, 151.51, 128.97, 128.52, 121.71, 112.65, 59.35, 30.19; HRMS (ESI) *m/z* 334.1798, calcd for $C_{17}H_{25}N_5Cl$ $[M + H]^+$ 334.1793.



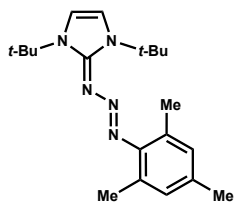
(*E*)-2-((4-methylphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3b**): Prepared from 4-methylazidobenzene (149 mg, 1.1 mmol) according to the general procedure A, obtained as an orange solid (228 mg, 48%). IR (neat) ν 3088, 1491, 1448, 1266, 694 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.44 (d, J = 8.6 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 6.85 (s, 2H), 2.31 (s, 3H), 1.63 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 153.97, 150.51, 133.57, 129.07, 120.58, 112.24, 58.99, 30.10, 20.93; HRMS (ESI) *m/z* 314.2335, calcd for $C_{18}H_{28}N_5$ $[M + H]^+$ 314.2339.



(*E*)-2-((4-*tert*-butylphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3c**): Prepared from 4-*tert*-butylazidobenzene (193 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (348 mg, 89%). IR (neat) ν 3032, 1493, 1447, 1260, 687 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.49 (d, J = 8.6 Hz, 2H), 7.32 (d, J = 8.6 Hz, 2H), 6.86 (s, 2H), 1.64 (s, 18H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 153.98, 150.26, 146.84, 125.35, 120.22, 112.29, 59.05, 34.31, 31.46, 30.15; HRMS (ESI) *m/z* 356.2812, calcd for $C_{21}H_{34}N_5$ $[M + H]^+$ 356.2809.

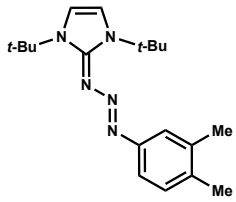


(*E*)-2-((phenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3d**): Prepared from azidobenzene (131 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (287 mg, 87%). IR (neat) ν 3179, 1475, 1449, 1263, 693 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.53 (dd, J = 8.6 Hz, J = 1.2 Hz, 2H), 7.31-7.28 (m, 2H), 7.09-7.06 (m, 1H), 6.85 (s, 2H), 1.64 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 154.05, 152.78, 128.44, 124.05, 120.70, 112.44, 59.17, 30.16; HRMS (ESI) *m/z* 300.2178, calcd for $C_{17}H_{26}N_5$ $[M + H]^+$ 300.2183.

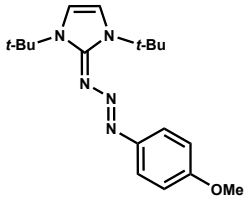


(*E*)-2-((2,4,6-trimethylphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3e**): Prepared from 2,4,6-trimethylazidobenzene (177 mg, 1.1 mmol) according to the general procedure B, obtained as a yellow solid (327 mg, 87%). IR (neat) ν 3132, 1477, 1427, 1265, 674 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ 7.12 (s, 2H), 6.75 (s, 2H), 2.18 (s, 3H), 1.60 (s, 6H), 1.50 (s, 18H); ^{13}C NMR (DMSO-d_6, 125

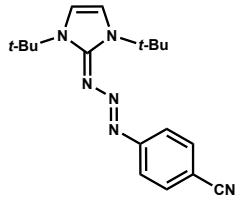
MHz): δ 154.01, 148.68, 131.45, 128.62, 120.47, 113.14, 58.23, 29.35, 20.43, 18.62; HRMS (ESI) *m/z* 342.2655, calcd for $C_{20}H_{32}N_5$ $[M + H]^+$ 342.2658.



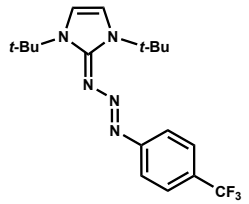
(*E*)-2-((3,4-dimethylphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3f**): Prepared from 3,4-dimethylazidobenzene (162 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (223 mg, 62%). IR (neat) ν 3077, 1478, 1433, 1261, 650 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.34 (s, 1H), 7.28-7.27 (m, 1H), 7.05 (d, J = 8.0 Hz, 1H), 6.80 (s, 2H), 2.24 (s, 6H), 1.63 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 153.85, 150.59, 136.40, 132.35, 129.65, 122.19, 117.91, 112.25, 59.01, 30.10, 19.97, 19.27; HRMS (ESI) *m/z* 328.2499, calcd for $C_{19}H_{30}N_5$ $[M + H]^+$ 328.2501.



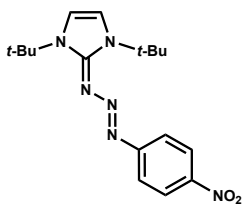
(*E*)-2-((4-methoxyphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3g**): Prepared from 4-methoxyazidobenzene (164 mg, 1.1 mmol) according to the general procedure B, obtained as a yellow solid (254 mg, 70%). IR (neat) ν 3091, 1491, 1434, 1267, 698 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.47 (d, J = 9.2 Hz, 2H), 6.85 (d, J = 9.2 Hz, 2H), 6.78 (s, 2H), 3.79 (s, 3H), 1.63 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 156.87, 153.71, 146.29, 121.55, 113.80, 112.28, 59.04, 55.38, 30.28; HRMS (ESI) *m/z* 330.2285, calcd for $C_{18}H_{26}N_5O$ $[M + H]^+$ 330.2288.



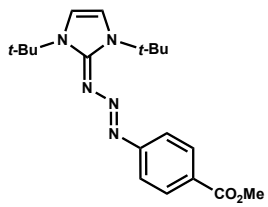
(*E*)-2-((4-cyanophenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3h**): Prepared from 4-cyanoazidobenzene (159 mg, 1.1 mmol) according to the general procedure A, obtained as an orange solid (264 mg, 74%). IR (neat) ν 3099, 1481, 1444, 1254, 670 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.51 (s, 4H), 6.94 (s, 2H), 1.61 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 156.73, 153.62, 132.75, 120.50, 120.27, 113.34, 105.47, 59.80, 30.19; HRMS (ESI) *m/z* 325.2132, calcd for $C_{18}H_{25}N_6$ $[M + H]^+$ 325.2135.



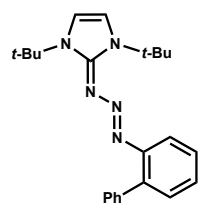
(*E*)-2-((4-trifluorophenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3i**): Prepared from 4-(trifluoromethyl)azidobenzene (206 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (430 mg, 94%). IR (neat) ν 3094, 1488, 1450, 1249, 678 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.56-7.50 (m, 4H), 6.88 (s, 2H), 1.63 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 155.84, 153.95, 124.84 (m), 125.66 (q, J_{CF} = 3.6 Hz), 125.05 (m), 120.26, 112.97, 59.56, 30.20; HRMS (ESI) *m/z* 368.2052, calcd for $C_{18}H_{25}N_6F_3$ $[M + H]^+$ 368.2057.



(*E*)-2-((4-nitrophenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3j**): Prepared from 4-nitroazidobenzene (181 mg, 1.1 mmol) according to the general procedure A, obtained as a red solid (341 mg, 90%). IR (neat) ν 3099, 1492, 1454, 1238, 697 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.15 (d, J = 9.2 Hz, 2H), 7.62 (d, J = 9.2 Hz, 2H), 7.09 (s, 2H), 1.63 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 158.94, 153.24, 143.23, 124.87, 119.80, 113.60, 60.02, 30.21; HRMS (ESI) *m/z* 345.2030, calcd for $C_{17}H_{25}N_6O_2$ $[M + H]^+$ 345.2034.

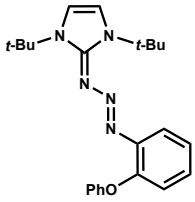


(*E*)-2-((4-)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3k**): Prepared from methyl 4-azidobenzoate (195 mg, 1.1 mmol) according to the general procedure A, obtained as a red solid (271 mg, 69%). IR (neat) ν 3164, 1711, 1480, 1451, 1271, 697 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.94 (d, J = 8.6 Hz, 2H), 7.51 (d, J = 8.6 Hz, 2H), 6.90 (s, 2H), 3.85 (s, 3H), 1.61 (s, 18H) ; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.40, 157.05, 153.81, 130.33, 124.68, 119.98, 113.02, 59.56, 51.65, 30.15; HRMS (ESI) *m/z* 358.2240, calcd for $C_{19}H_{28}N_5O_2$ $[M + H]^+$ 358.2238.

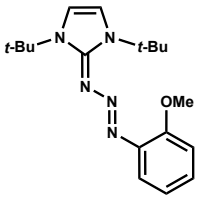


(*E*)-2-((2-phenylphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3l**): Prepared from 2-phenylazidobenzene (215 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (409 mg, 99%). IR (neat) ν 3088, 1497, 1470, 1236 692 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.51 (d, J = 7.5 Hz, 2H), 7.38-7.35 (m, 2H), 7.32-7.29 (m, 2H), 7.27-7.20 (m, 2H), 7.16 (t, J = 7.5 Hz, 1H), 6.82 (s, 2H), 1.62 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 152.34, 149.53, 140.42, 136.57,

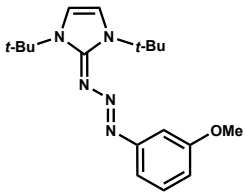
130.93, 130.42, 127.67, 127.53, 126.28, 125.42, 118.55, 116.29, 35.63, 30.01; HRMS (ESI) *m/z* 376.2491, calcd for $C_{23}H_{30}N_5$ $[M + H]^+$ 376.2496.



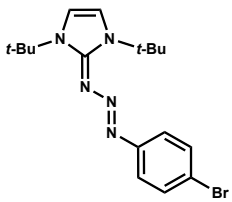
(*E*)-2-((2-phenyloxyphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3m**): Prepared from 2-phenyloxyazidobenzene (232 mg, 1.1 mmol) according to the general procedure A, obtained as a brown solid (332 mg, 77%). IR (neat) ν 3066, 1488, 1448, 1235, 688 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.42-7.40 (m, 1H), 7.21-7.18 (m, 2H), 7.06-7.01 (m, 2H), 6.98-6.91 (m, 4H), 6.81 (s, 2H), 1.56 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.04, 154.29, 149.28, 145.49, 129.01, 124.54, 123.99, 121.46, 120.96, 119.47, 117.86, 112.57, 59.22, 30.09; HRMS (ESI) *m/z* 392.2447, calcd for $C_{23}H_{30}N_5O$ $[M + H]^+$ 392.2445.



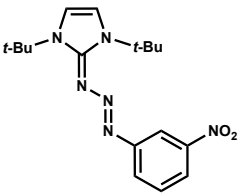
(*E*)-2-((2-methoxyphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3n**): Prepared from 2-methoxyazidobenzene (164 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (185 mg, 51%). IR (neat) ν 3097, 1480, 1433, 1256, 676 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ 7.20-7.18 (m, 3H), 6.99-6.95 (m, 2H), 6.81-6.78 (m, 1H), 3.78 (s, 3H), 1.55 (s, 18H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ 153.14, 152.74, 142.21, 124.46, 120.47, 116.75, 113.61, 112.39, 58.64, 55.49, 29.51; HRMS (ESI) *m/z* 330.2293, calcd for $C_{18}H_{28}N_5O$ $[M + H]^+$ 330.2294.



(*E*)-2-((3-methoxyphenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3o**): Prepared from 3-methoxyazidobenzene (164 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (359 mg, 99%). IR (neat) ν 3090, 1494, 1433, 1270, 675 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ 7.23 (s, 2H), 7.15 (t, *J* = 8.0 Hz, 1H), 6.89-6.88 (m, 2H), 6.59-6.57 (m, 1H), 3.71 (s, 3H), 1.56 (s, 18H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ 154.18, 153.35, 142.25, 124.76, 120.25, 117.61, 112.28, 111.57, 59.14, 55.69, 30.21; HRMS (ESI) *m/z* 330.2296, calcd for $C_{18}H_{28}N_5O$ $[M + H]^+$ 330.2294.



(*E*)-2-((2-bromophenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3p**): Prepared from 4-bromoazidobenzene (218 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (370 mg, 89%). IR (neat) ν 3092, 1496, 1435, 1260, 641 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.45 (d, *J* = 8.9 Hz, 2H), 7.39 (d, *J* = 8.9 Hz, 2H), 6.97 (s, 2H), 1.62 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 153.91, 151.99, 131.40, 122.10, 116.76, 112.66, 59.31, 30.15; HRMS (ESI) *m/z* 378.1291, calcd for $C_{17}H_{25}BrN_5$ $[M + H]^+$ 378.1293.

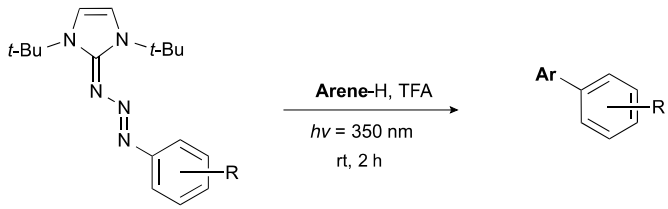


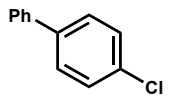
(*E*)-2-((3-nitrophenyl)triaz-2-en-1-ylidene)-1,3-di-*tert*-butyl-2,3-dihydro-1*H*-imidazole (**3q**): Prepared from 3-nitroazidobenzene (181 mg, 1.1 mmol) according to the general procedure A, obtained as a yellow solid (367 mg, 97%). IR (neat) ν 3096, 1496, 1435, 1256, 678 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 8.30 (t, *J* = 2.0 Hz, 1H), 7.86-7.82 (m, 2H), 7.41 (t, *J* = 8.0 Hz, 1H), 6.94 (s, 2H), 1.64 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 154.44, 153.70, 148.91, 129.02, 127.76, 117.75, 113.21, 113.16, 59.69, 30.16; HRMS (ESI) *m/z* 345.2036, calcd for $C_{17}H_{25}N_6O_2$ $[M + H]^+$ 345.2039.

General Method for the Preparation of Biaryl Compounds (4)

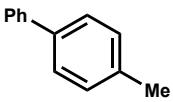
To a quartz tube containing triazene (0.2 mmol) was added aromatic solvent (2 mL). Then, the tube was capped and TFA (1.0 mmol) was added with a syringe. Next, the mixture was left to stir inside a photoreactor under UV irradiation (350 nm) for 2 h. After 2 h the resulting mixture was concentrated *in vacuo*. Purification by flash chromatography (SiO_2, EtOAc/hexanes mixtures) provided the pure biaryl compound.

Sunlight Reactions Variation: Conditions are identical as for the general method but using natural sunlight as radiation source instead of photoreactor. Reactions were exposed to natural sunlight for 9 h.

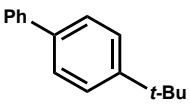




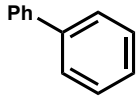
4-chlorodiphenyl (**4a**): Prepared from triazene **3a** (67 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (17 mg, 38%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.57-7.52 (m, 4H), 7.47-7.41 (m, 4H), 7.38-7.37 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 139.97, 139.64, 133.35, 128.89, 128.86, 128.37, 127.57, 126.97.



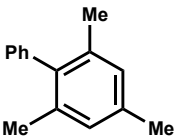
4-methyldiphenyl (**4b**): Prepared from triazene **3b** (73 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (16 mg, 40%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.60 (d, J = 7.5 Hz, 2H), 7.51 (d, J = 8.6 Hz, 2H), 7.44 (t, J = 7.5 Hz, 2H), 7.34 (t, J = 7.5 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 141.13, 138.32, 136.99, 129.45, 128.69, 126.97, 126.95 (2C), 21.08.



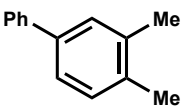
4-*tert*-butyldiphenyl (**4c**): Prepared from triazene **3c** (71 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (25 mg, 48%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.61 (d, J = 7.5 Hz, 2H), 7.56 (d, J = 8.0 Hz, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.44 (m, 2H), 7.34 (t, J = 7.5 Hz, 1H), 1.39 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 150.22, 141.03, 138.29, 128.67, 127.00, 126.95, 126.76, 125.68, 34.51, 31.35.



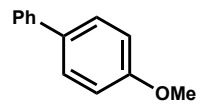
Biphenyl (**4d**): Prepared from triazene **3d** (69 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (21 mg, 59%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.70 (d, J = 8.0 Hz, 4H), 7.54 (t, J = 8.0 Hz, 4H), 7.45 (t, J = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 141.18, 128.72, 127.21, 127.12. Sunlight: (15 mg, 43%).



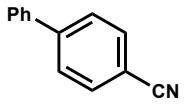
2,4,6-trimethyldiphenyl (**4e**): Prepared from triazene **3e** (68 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (9 mg, 20%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.42 (t, J = 7.5 Hz, 2H), 7.32 (t, J = 7.5 Hz, 1H), 7.15-7.13 (m, 2H), 6.95 (s, 2H), 2.34 (s, 3H), 2.00 (s, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 141.05, 139.03, 136.53, 135.95, 129.27, 128.33, 128.01, 126.47, 21.00, 20.71.



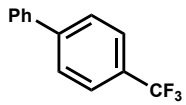
3,4-dimethyldiphenyl (**4f**): Prepared from triazene **3f** (65 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (13 mg, 31%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.59 (d, J = 6.9 Hz, 2H), 7.45-7.42 (m, 2H), 7.39 (s, 1H), 7.36-7.32 (m, 2H), 7.22 (d, J = 7.5 Hz, 1H), 2.35 (s, 3H), 2.32 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 141.26, 138.84, 136.88, 135.69, 130.03, 128.64, 128.42, 126.98, 126.87, 124.49, 19.93, 19.43.



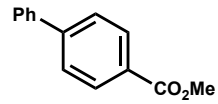
4-methoxydiphenyl (**4g**): Prepared from triazene **3g** (66 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (13 mg, 30%). ^{1}H NMR ($CDCl_3$, 500 MHz):7.58-7.53 (m, 4H), 7.43 (m, 2H), 7.32 (t, J = 7.5 Hz, 1H), 6.99 (d, J = 8.6 Hz, 2H), 3.86 (s, 3H); δ; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.11, 140.80, 133.74, 128.70, 128.14, 126.71, 126.64, 114.17, 55.32.



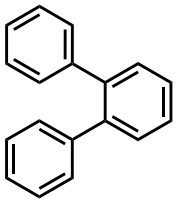
4-cyanodiphenyl (**4h**): Prepared from triazene **3h** (65 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (4 mg, 10%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.73 (d, *J* = 8.6 Hz, 2H), 7.69 (d, *J* = 8.6 Hz, 2H), 7.59 (d, *J* = 6.9 Hz, 2H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 145.67, 139.17, 132.59, 129.10, 128.65, 127.73, 127.22, 118.95, 110.89.



4-(trifluoromethyl)diphenyl (**4i**): Prepared from triazene **3i** (73 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (15 mg, 28%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.70 (s, 4H), 7.62-7.60 (m, 2H), 7.50-7.47 (m, 2H), 7.43-7.39 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 144.71, 139.75, 129.31 (m), 128.97, 128.16, 127.41, 127.27, 125.69 (q, J_{CF} = 3.6 Hz), 124.29 (m)

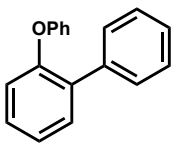


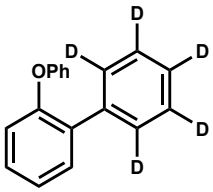
Methyl 4-phenylbenzoate (**4k**): Prepared from triazene **3k** (71 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (13 mg, 26%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.11 (d, *J* = 8.6 Hz, 2H), 7.67-7.62 (m, 4H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.41-7.39 (m, 1H), 3.95 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.99, 145.61, 139.98, 130.08, 128.90, 128.86, 128.12, 127.26, 127.03, 52.12.



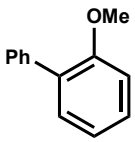
1,2-diphenylbenzene (**4l**): Prepared from triazene **3l** (87 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (18 mg, 34%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.46-7.44 (m, 4H), 7.25-7.21 (m, 6H), 7.17-7.16 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 141.48, 140.54, 130.58, 129.87, 127.83, 127.45, 126.42.

2-phenoxydiphenylbenzene (**4m**): Prepared from triazene **3m** (78 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (33 mg, 57%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.55 (d, *J* = 6.8 Hz, 2H), 7.47 (dd *J* = 7.5 Hz, *J* = 1.72 Hz, 1H), 7.38-7.35 (m, 3H), 7.31-7.25 (m, 3H), 7.23-7.20 (m, 1H), 7.02-7.00 (m, 2H), 6.94 (dd, *J* = 8.6 Hz, *J* = 1.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 157.77, 153.56, 137.70, 133.66, 131.26, 129.57, 129.18, 128.65, 128.09, 127.17, 124.01, 122.60, 120.09, 118.15.

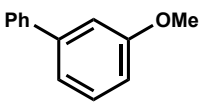




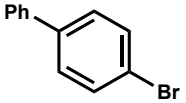
2'-phenoxy-1-1'-biphenyl-2,3,4,5,6-*d*$_5$ (**4m'**): Prepared from triazene **3m** (78 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (25 mg, 50%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.48 (dd *J* = 8.0 Hz, *J* = 1.7 Hz, 1H), 7.33-7.20 (m, 4 H), 7.05-7.02 (m, 2H), 6.96-6.94 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 157.78, 153.57, 137.51, 133.63, 131.25, 129.57, 128.76 (t, J_{CD} = 24.0 Hz), 128.64, 127.57 (t, J_{CD} = 24.0 Hz), 126.66 (t, J_{CD} = 24.0 Hz), 124.02, 122.59, 120.11, 118.14.



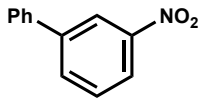
2-methoxydiphenylbenzene (**4n**): Prepared from triazene **3n** (76 mg, 0.2 mmol) according to the general procedure, obtained as a yellow oil (8 mg, 18%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.55-7.53 (m, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.35-7.32 (m, 3H), 7.06-6.99 (m, 2H), 3.82 (s, 3H); ^{13}C NMR $CDCl_3$, 125 MHz): δ 156.43, 138.50, 130.87, 130.68, 129.52, 128.58, 127.95, 126.90, 120.79, 111.18, 55.52.



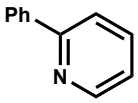
3-methoxydiphenylbenzene (**4o**): Prepared from triazene **3o** (76 mg, 0.2 mmol) according to the general procedure, obtained as a yellow oil (18 mg, 41%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.61 (d, *J* = 7.5 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.39-7.36 (m, 2H), 7.21-7.19 (m, 1H), 7.15-7.14 (m, 1H), 6.93-6.91 (m, 1H), 3.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.91, 142.75, 141.08, 129.73, 128.71, 127.39, 127.18, 119.67, 112.87, 112.65, 55.28.



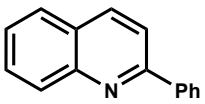
4-bromodiphenylbenzene (**4p**): Prepared from triazene **3p** (76 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (24 mg, 44%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.58-7.55 (m, 4H), 7.48-7.44 (m, 4H), 7.39-7.36 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 140.11, 139.97, 131.84, 128.88, 128.73, 127.62, 126.92, 121.52.



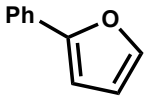
3-nitrodiphenylbenzene (**4q**): Prepared from triazene **3q** (80 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (6 mg, 13%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.47-8.46 (m, 1H), 8.22-8.20 (m, 1H), 7.92 (d, J = 7.5 Hz, 1H), 7.64-7.60 (m, 3H), 7.52-7.44 (m, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 148.72, 142.87, 138.67, 133.04, 129.70, 129.16, 128.53, 127.15, 122.03, 121.96



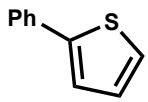
2-phenylpyridine (**4r**): Prepared from triazene **3d** (69 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (13 mg, 35%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.72 (d, J = 4.6 Hz, 1H), 8.00 (d, J = 6.9 Hz, 2H), 7.81-7.74 (m, 2H), 7.51-7.42 (m, 3H), 7.28-7.26 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 157.22, 149.16, 137.29, 129.50, 129.18, 128.81, 127.01, 122.23, 120.89.



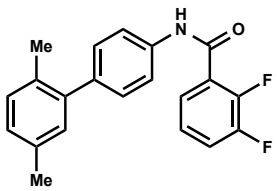
2-phenylquinoline (**4s**): Prepared from triazene **3d** (69 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (7 mg, 15%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.24 (d, J = 8.6 Hz, 1H), 8.18 (d, J = 6.9 Hz, 3H), 7.89 (d, J = 8.6 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.74 (t, J = 8.6 Hz, 1H), 7.54 (t, J = 7.5 Hz, 3H), 7.48 (t, J = 7.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 157.28, 148.86, 139.64, 136.97, 129.87, 129.47, 129.12, 128.87, 127.68, 127.47, 127.15, 126.43, 119.10.



2-phenylfuran (**4t**): Prepared from triazene **3d** (69 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (9 mg, 28%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.68 (d, J = 8.3 Hz, 2H), 7.47 (d, J = 1.2 Hz, 1H), 7.38 (t, J = 8.0 Hz, 2H), 7.27-7.22 (m, 1H), 6.66 (d, J = 3.4 Hz, 1H), 6.48-6.47 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 154.12, 142.03, 130.86, 128.64, 127.30, 123.76, 111.61, 104.92.



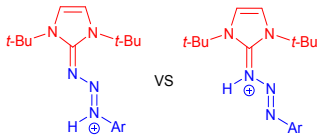
2-phenylthiophene (**4u**): Prepared from triazene **3d** (69 mg, 0.2 mmol) according to the general procedure, obtained as a colorless solid (16 mg, 42%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.64-7.60 (m, 2H), 7.40-7.37 (m, 2H), 7.33-7.27 (m, 3H), 7.10-7.08 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 144.37, 134.20, 128.86, 128.74, 127.98, 127.44, 125.94, 123.06.



***N*-(2',5'-dimethyl-[1,1'-biphenyl]-4-yl)-2,3-difluorobenzamide** (**5**): Prepared from triazene **3p** (180 mg, 0.5 mmol), obtained as a pale-yellow solid (54 mg, 32%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.33 (d, J = 13.2 Hz, 1H), 7.94-7.91 (m, 1H), 7.70 (d, J = 8.6 Hz, 2H), 7.39-7.34 (m, 4H), 7.17 (d, J = 7.5 Hz, 1H), 7.09-7.06 (m, 2H), 2.36 (s, 3H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.28 (m), 150.64 (m), 148.81 (m), 140.95, 138.96, 136.01, 135.27, 132.21, 130.49, 130.32, 129.91, 128.03, 126.66 (d, J_{CF} = 3.6 Hz), 124.87 (m), 123.62 (d, J_{CF} = 9.6 Hz), 120.62 (m), 120.24, 20.92, 19.98.

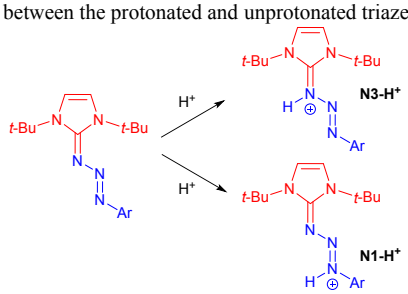
Computational Data Tables

Table S1 PCM ground state energy difference between N1-H$^+$ and N3-H$^+$, calculated using DFT-B3LYP and RI-MP2 (Basis set: 6-31+G* and cc-pVTZ basis set, respectively)



Compound	B3LYP (kcal/mol)	RI-MP2 (kcal/mol)
3a	-4.5	-3.2
3b	-5.0	-3.7
3c	-14.9	-10.7
3d	-14.9	-10.3
3e	-14.2	-8.4
3f	-5.2	-3.9
3g	-14.6	-11.5
3h	-4.9	-3.4
3i	-5.0	-3.6
3j	-5.0	-3.2
3k	-5.5	-3.7
3l	-16.2	-11.4
3m	-7.9	-4.9
3n	-16.4	-9.9
3o	-5.6	-4.0
3p	-4.4	-3.2
3q	-4.3	-3.8

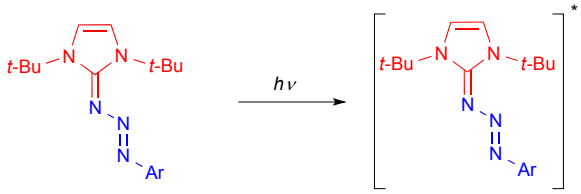
Table S2 Electronic energy difference between the protonated and unprotonated triazenes at the PCM ground electronic state



Compound	N1-H$^+$ (kcal/mol)	N3-H$^+$ (kcal/mol)
3a	17.8	22.2
3b	14.5	19.4
3c	14.2	29.2
3d	15.3	30.1
3e	13.3	27.5
3f	13.8	19.0
3g	14.3	28.9
3h	21.2	26.0
3i	19.6	24.7
3j	22.9	27.9
3k	18.1	23.7
3l	14.0	30.3
3m	13.5	21.3
3n	11.2	27.7
3o	14.3	19.9
3p	17.9	22.3
3q	21.1	25.5

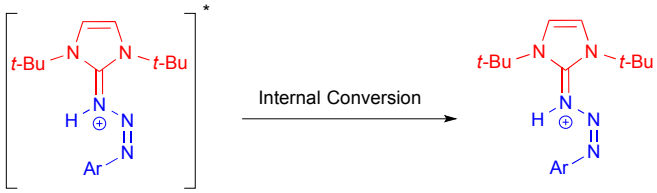
In summary: The title reaction has a positive reaction energy. However, it is acid dependent. Here was calulated for TFA.

Table S3 Calculated absorption wavelength for the first bright state



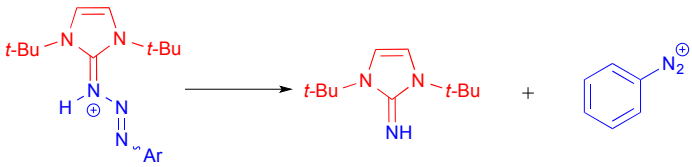
Compound	N1-H$^+$(nm)	N3-H$^+$ (nm)	Unprotonated (nm)
3a	357	319	400
3b	358	316	395
3c	356	332	396
3d	349	318	396
3e	358	348	391
3f	357	321	395
3g	376	352	395
3h	354	324	420
3i	347	319	407
3j	376	339	477
3k	356	325	420
3l	370	336	401
3m	393	399	403
3n	379	340	402
3o	375	359	393
3p	354	323	400
3q	356	329	529

Table S4 Electronic coupling between the ground and first bright excited state, calculated at the Frank-Condon geometry (absorption) for the 1-*Z* configuration of N3-H$^+$



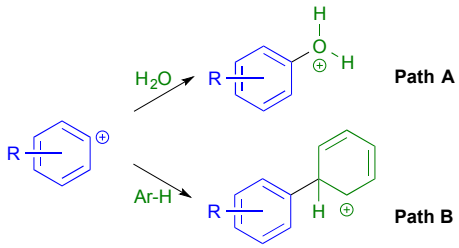
Compound	Coupling (cm^{-1})
3a	14
3b	37
3c	146
3d	514
3e	53
3f	2713
3g	5
3h	35
3i	9
3j	24
3k	5
3l	9
3m	520
3n	6
3o	2000
3p	7
3q	9

Table S5 Energy of dissociation reaction between 1-*E* and 1-*Z* of N3-H$^+$



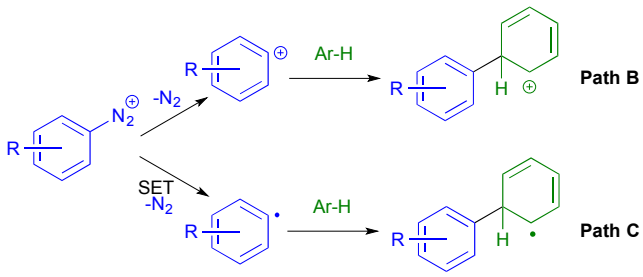
Compound	1-*E* (kcal/mol)	1-*Z* (kcal/mol)
3a	31.6	-20.5
3b	26.8	-26.0
3c	16.2	-26.7
3d	19.8	-32.5
3e	8.7	-38.4
3f	25.3	-26.9
3g	13.2	-32.7
3h	37.3	-17.7
3i	35.8	-17.4
3j	39.6	-25.0
3k	32.8	-26.3
3l	15.4	-28.3
3m	23.5	-34.6
3n	14.5	-40.4
3o	28.9	-39.8
3p	31.5	-31.6
3q	38.7	-28.5

Table S6 Difference of binding energy (BE) between path A and B. The difference is BE(pathA)- BE(pathB)



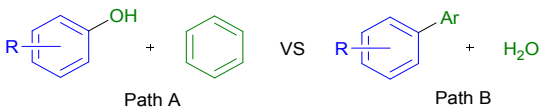
Aryldiazonium Salt	BE Difference(kcal/mol)
3a	4.4
3b	8.3
3c	-2.5
3d	2.7
3e	-2.0
3f	1.6
3g	2.2
3h	5.9
3i	5.2
3j	7.4
3k	4.2
3l	0.2
3m	3.0
3n	2.4
3o	2.4
3p	4.3
3q	6.8

Table S7 Binding energy (BE) between path B and C. The difference is BE(pathB)-BE(pathC)



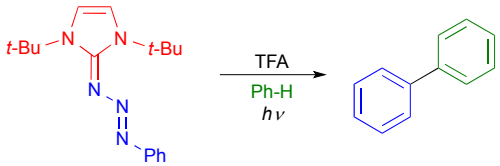
Compound	Energy Difference(kcal/mol)
3a	-61.0
3b	-60.2
3c	-48.5
3d	-55.2
3e	-42.5
3f	-51.3
3g	-56.8
3h	-63.6
3i	-62.3
3j	-66.3
3k	-58.6
3l	-50.0
3m	-44.7
3n	-62.3
3o	-52.9
3p	-60.7
3q	-66.6

Table S8 Energy difference between final products of path A and B. The difference is E(pathA)-E(pathB)



Compound	Energy Difference (kcal/mol)
3a	6.0
3b	6.1
3c	5.9
3d	5.6
3e	2.0
3f	6.0
3g	7.2
3h	4.7
3i	4.9
3j	4.3
3k	4.6
3l	2.4
3m	3.2
3n	6.2
3o	5.4
3p	5.9
3q	5.7

Table S9 Relative free energies and enthalpies for species involved in the Ar-Ar-Cross-coupling of triazene **3d**

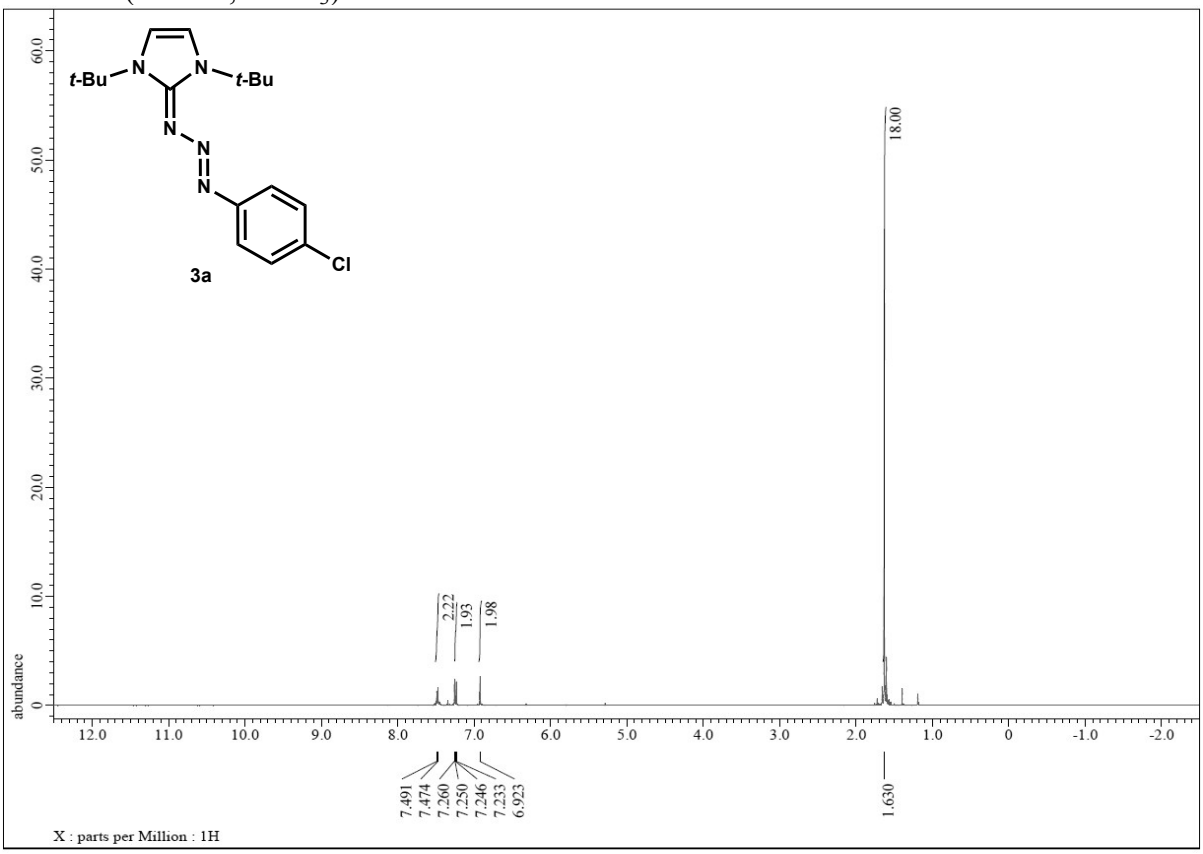


Compound	ΔG (kcal/mol)	ΔH (kcal/mol)
3d-*E* *S0(min)*	0.0	0.0
3d-*E* (N1-H$^+$) *S0(min)*	16.8	0.0
3d-*E* (N3-H$^+$) *S0(min)*	31.7	-0.3
3d-*E* *S1*	71.9	0.0
3d-*E* (N1-H$^+$) *S1*	98.0	-0.1
3d-*E* (N3-H$^+$) *S1*	121.3	-0.3
3d-*Z* (N3-H$^+$) *S1(min)*	76.1	-3.3
3d-E (N1-H$^+$) *S1(min)*	65.5	-0.1
3d-E *S1(min)*	43.6	0.0
3d-*Z* (N3-H$^+$) *S0*	73.8	-3.3
3d-E (N1-H$^+$) *S0*	58.6	-0.1
3d-E *S0*	38.3	0.0
6	36.3	-2.8
7 (H_2O)	18.9	-2.3
7 (C_6H_6)	15.9	-3.3
10	34.3	-5.5
4d	-64.2	-1.2
4d'	-59.5	-0.9

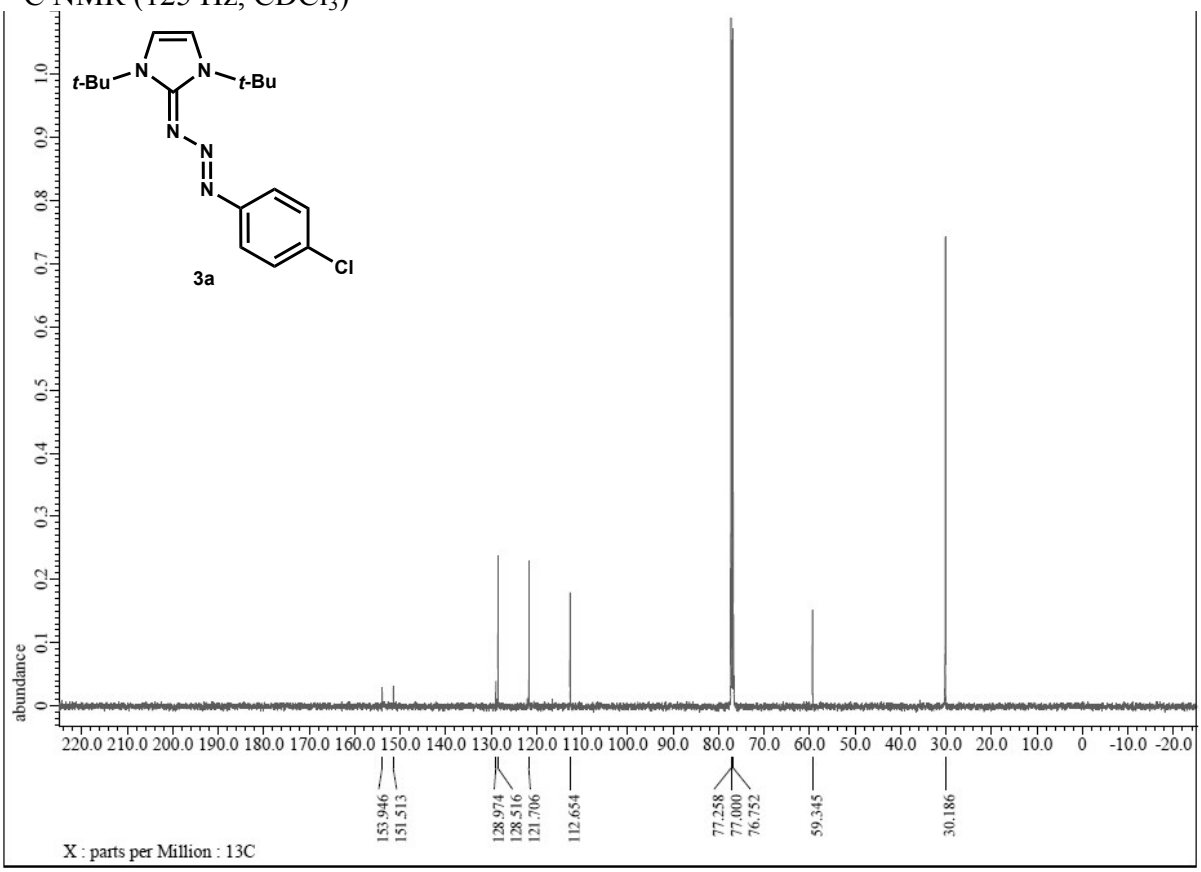
min = minima

^{1}H and ^{13}C NMR Spectra

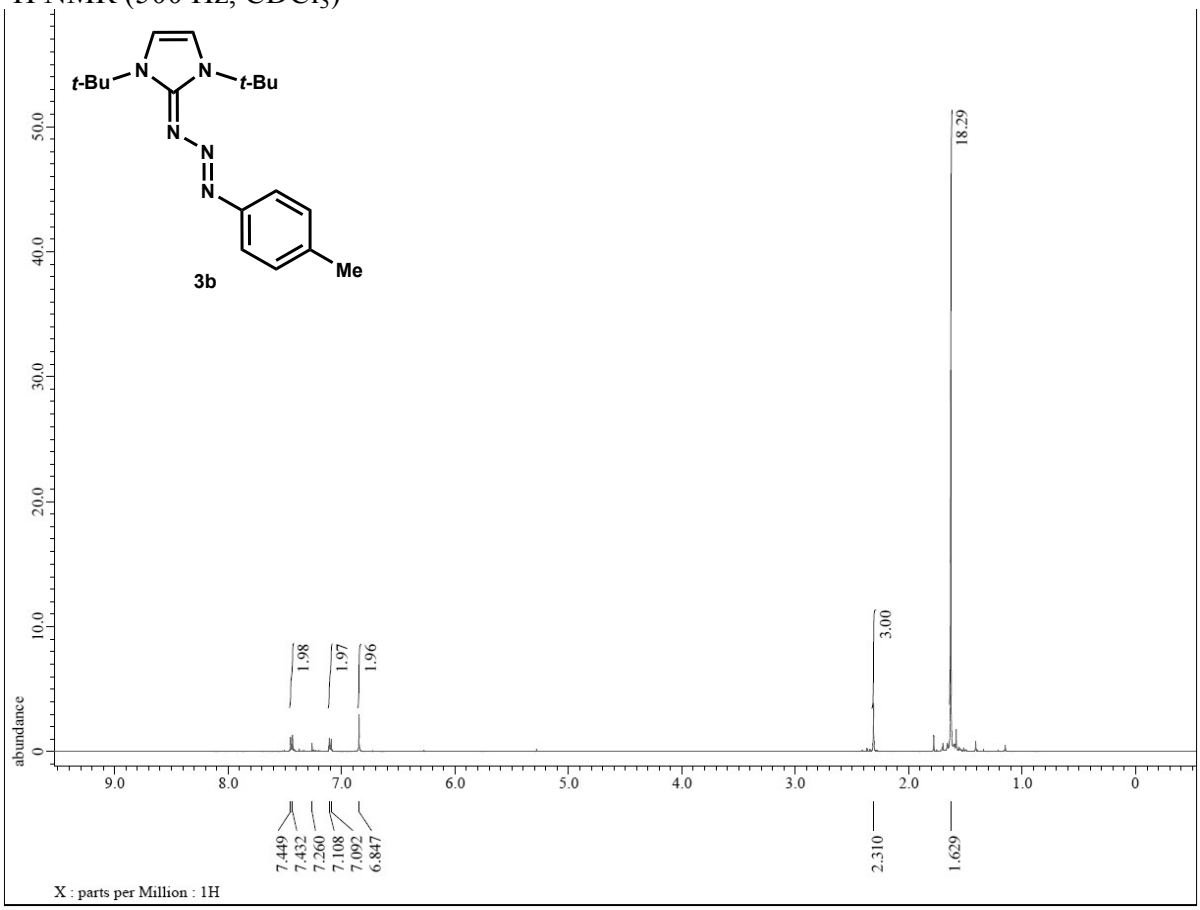
^{1}H NMR (500 Hz, $CDCl_3$)



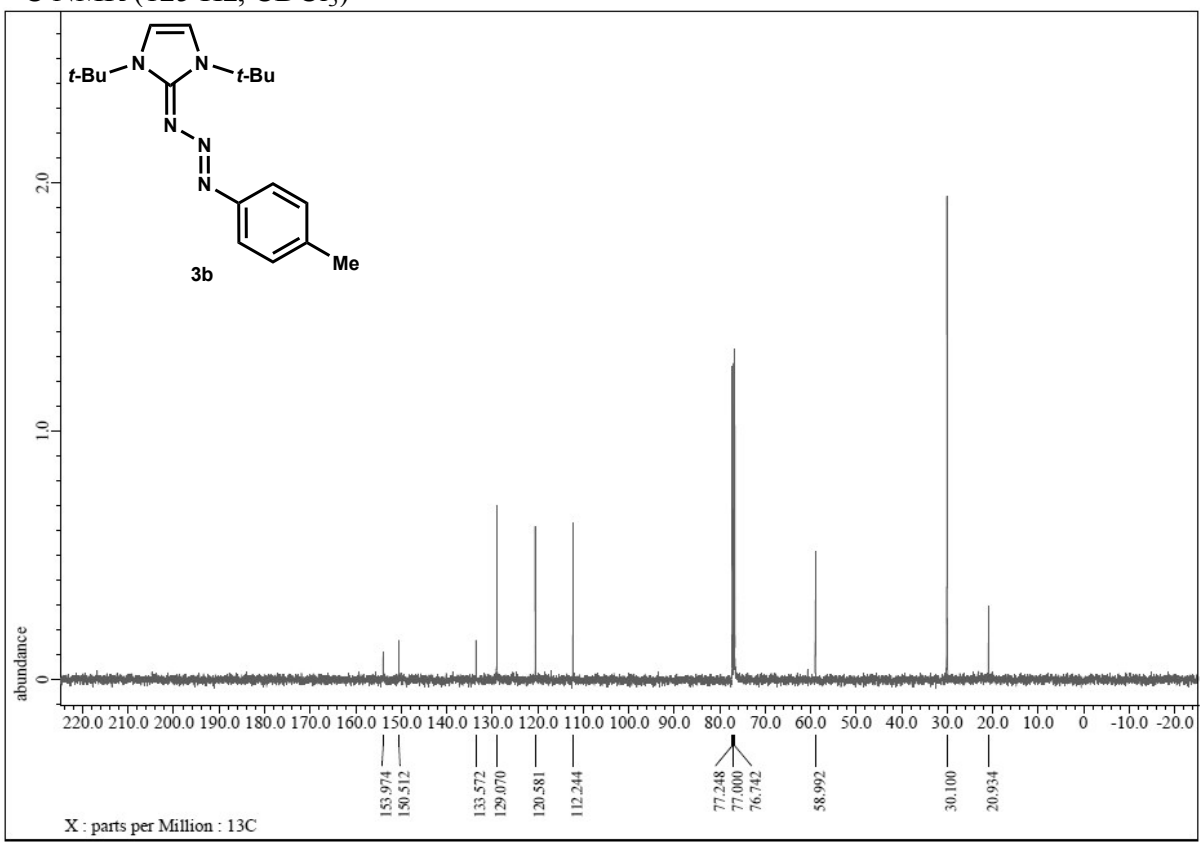
^{13}C NMR (125 Hz, $CDCl_3$)



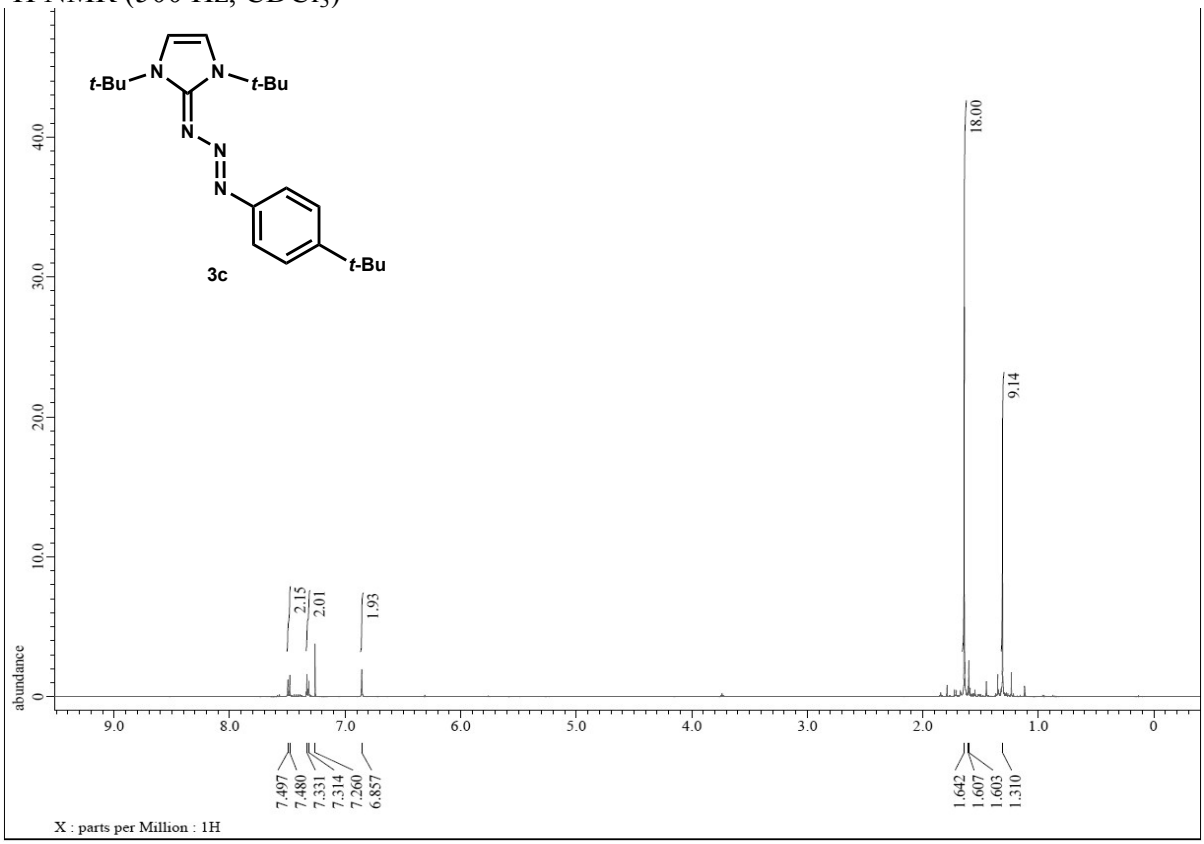
^{1}H NMR (500 Hz, $CDCl_3$)



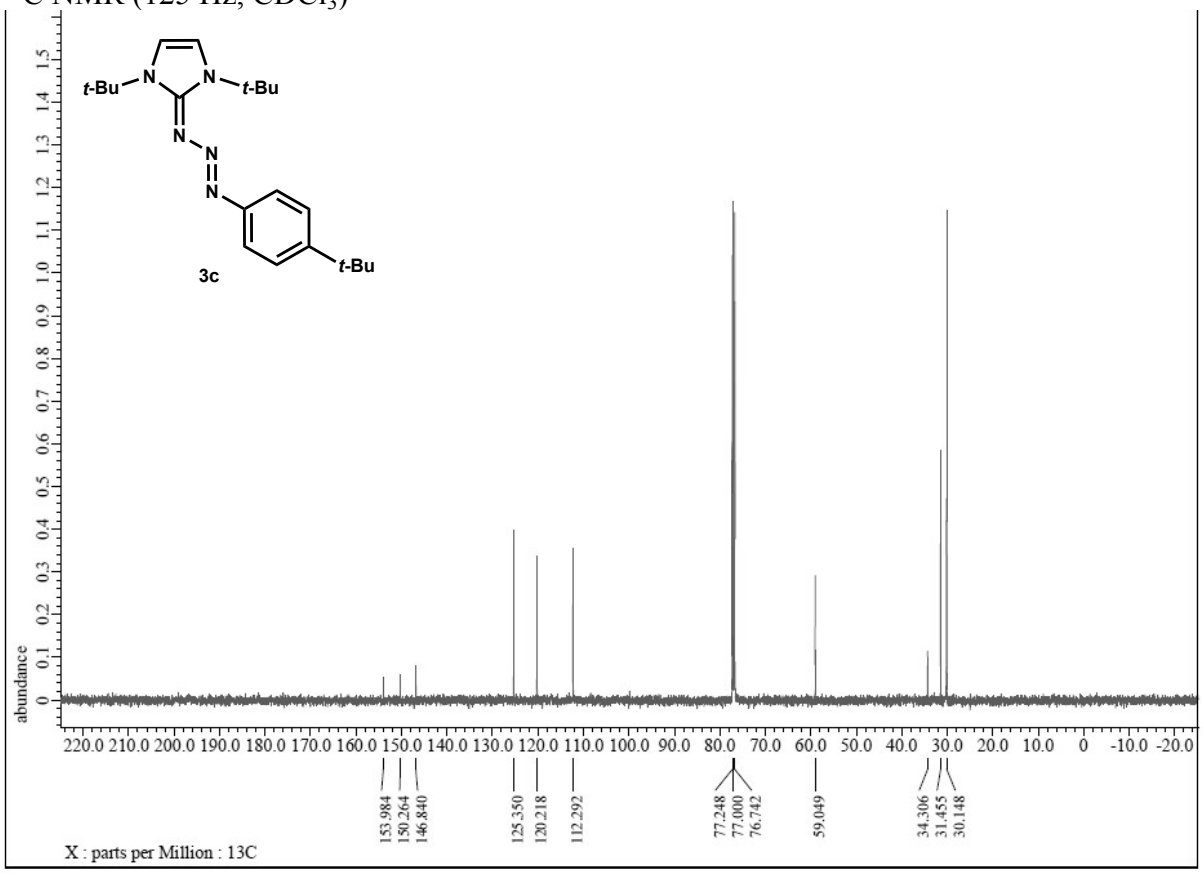
^{13}C NMR (125 Hz, $CDCl_3$)



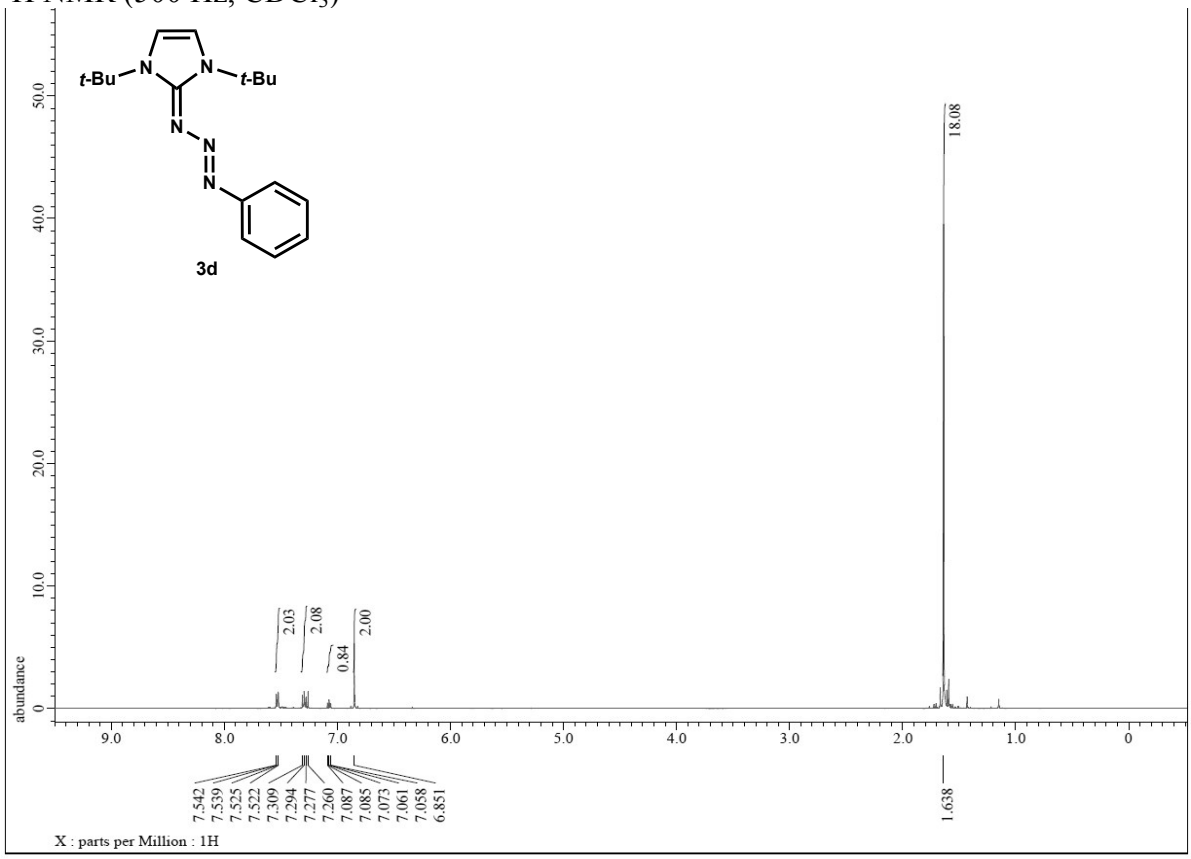
^{1}H NMR (500 Hz, $CDCl_3$)



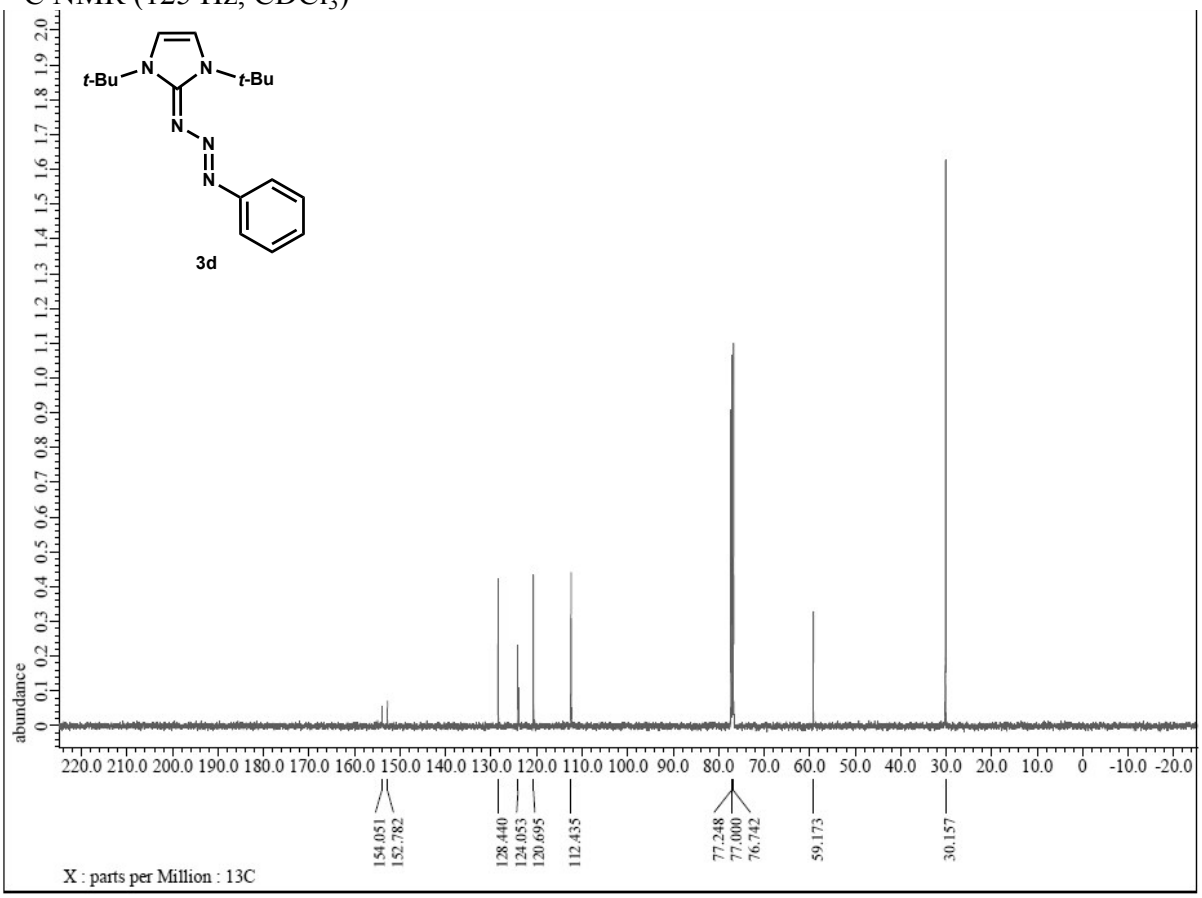
^{13}C NMR (125 Hz, $CDCl_3$)



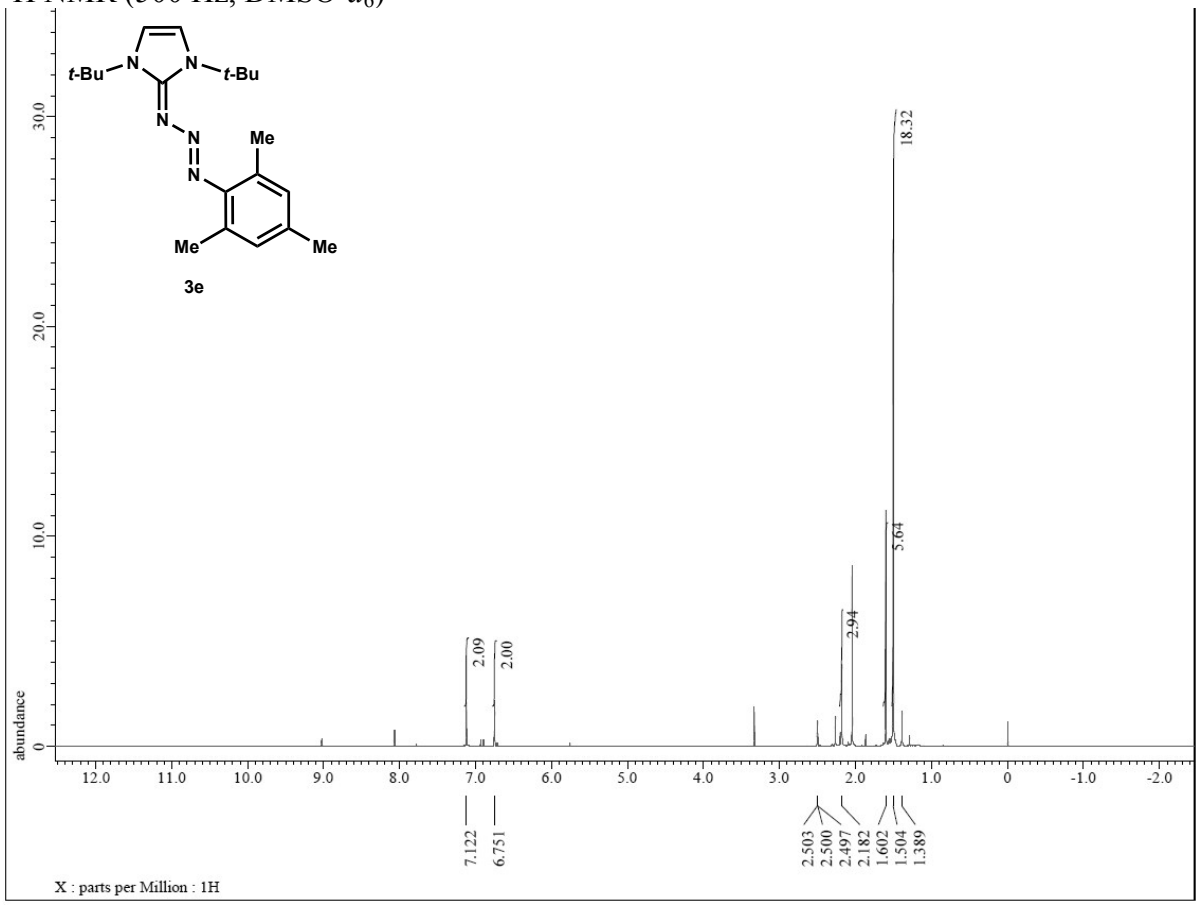
^{1}H NMR (500 Hz, $CDCl_3$)



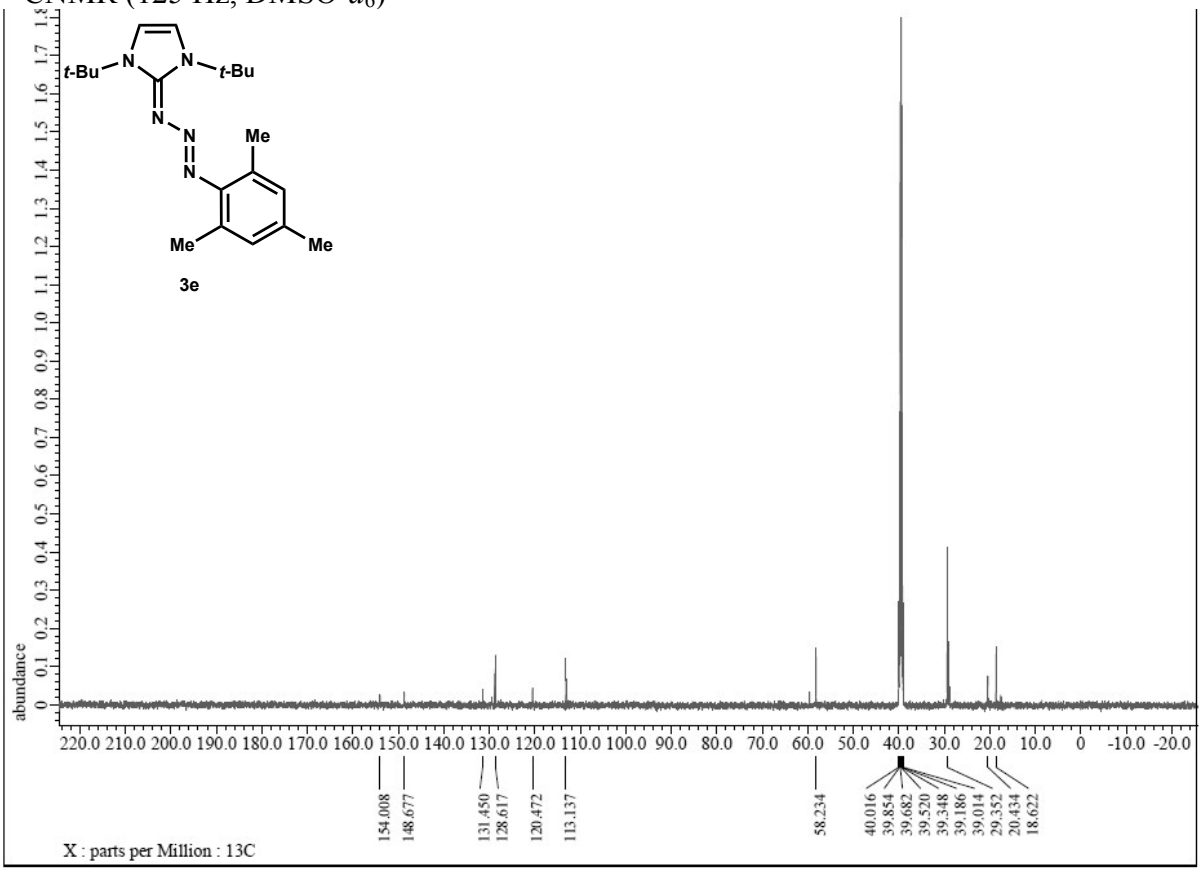
^{13}C NMR (125 Hz, $CDCl_3$)



^{1}H NMR (500 Hz, DMSO-d_6)



^{13}CNMR (125 Hz, DMSO-d_6)



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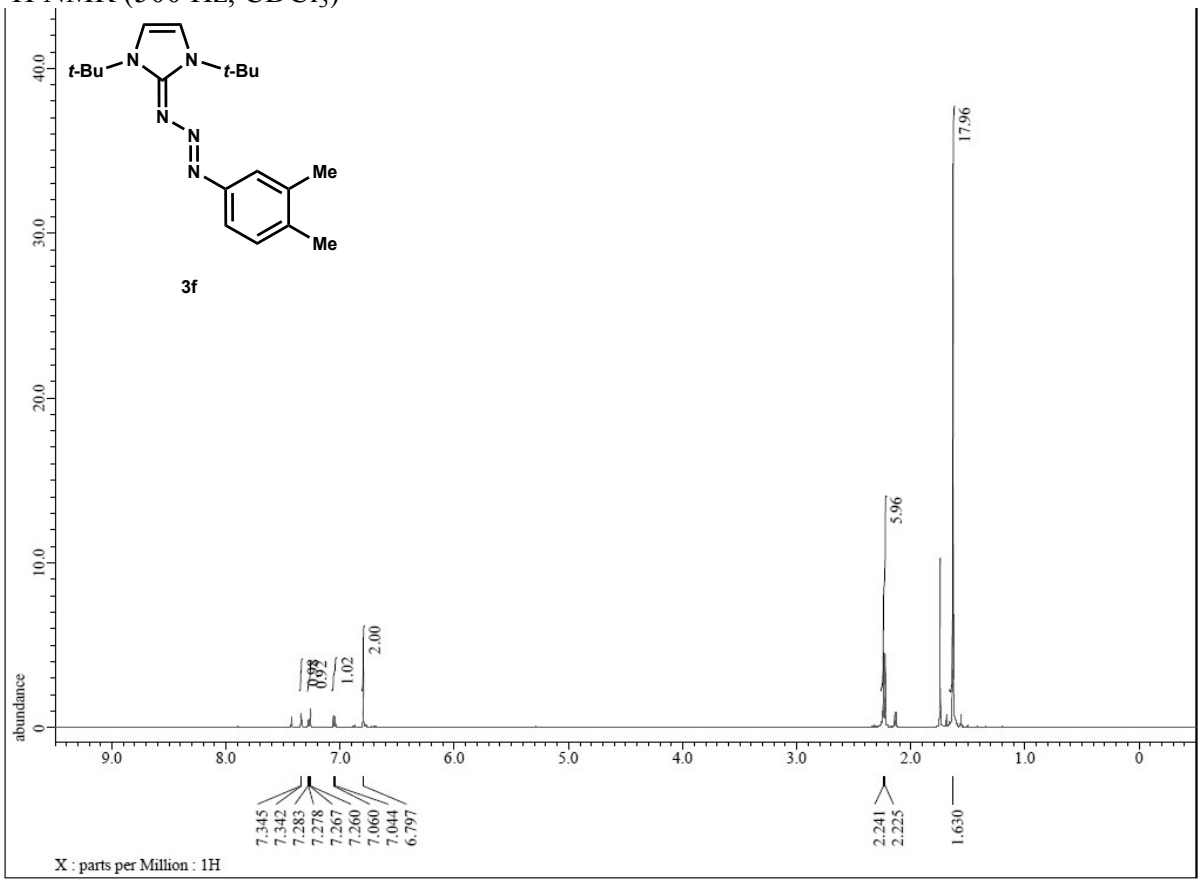

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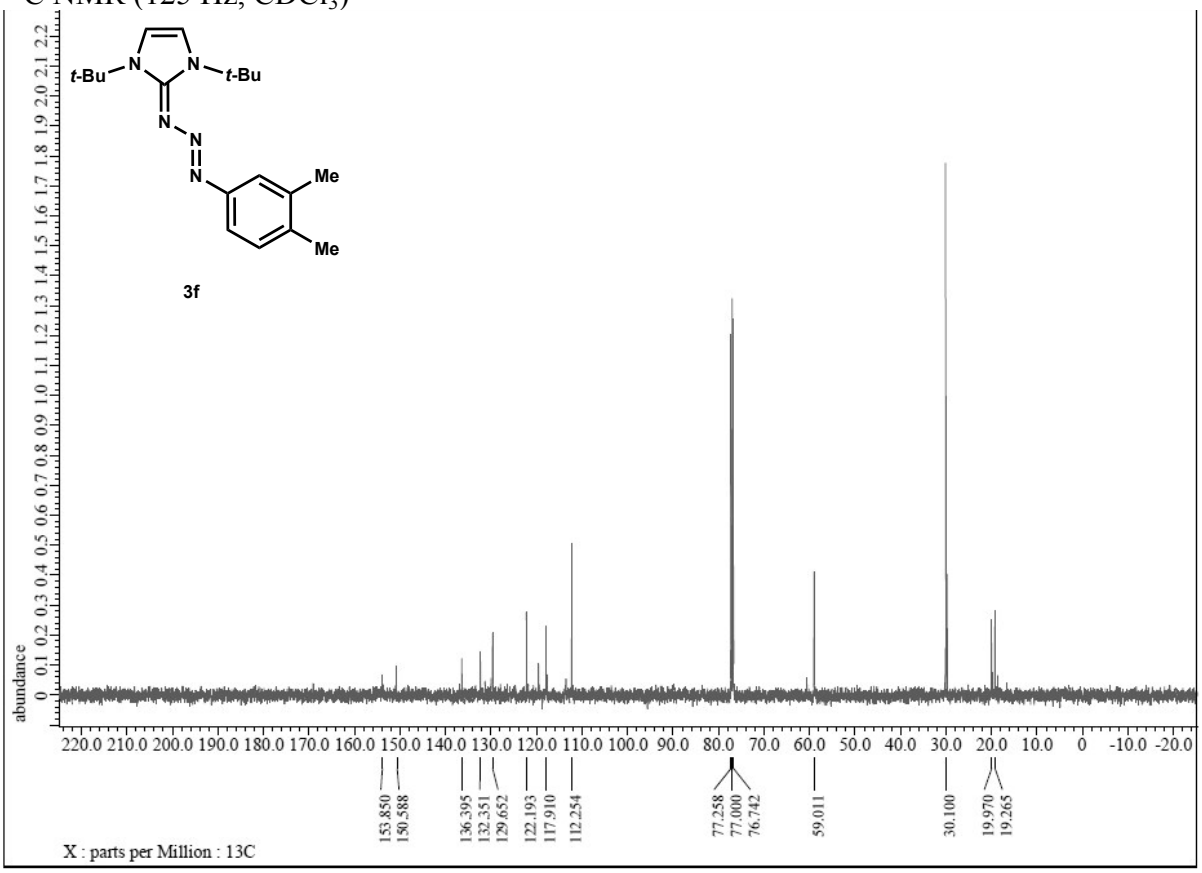

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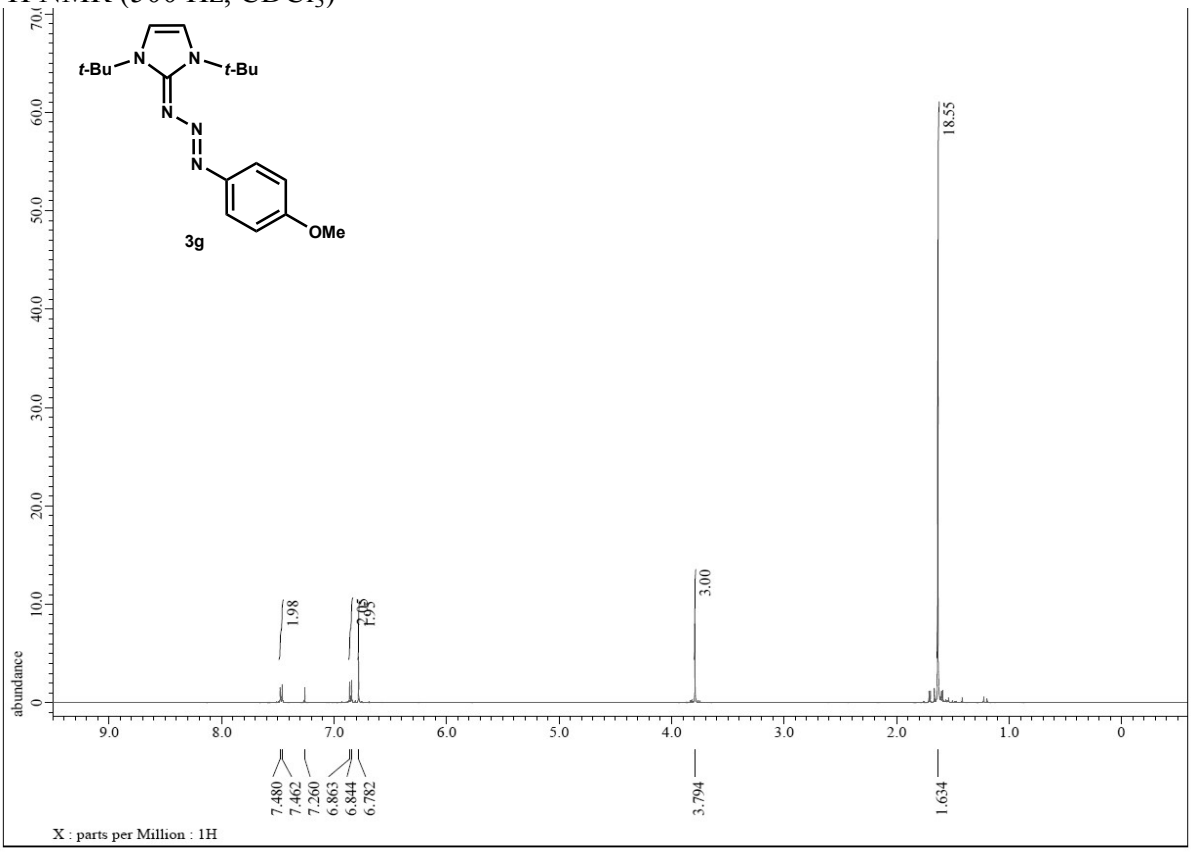

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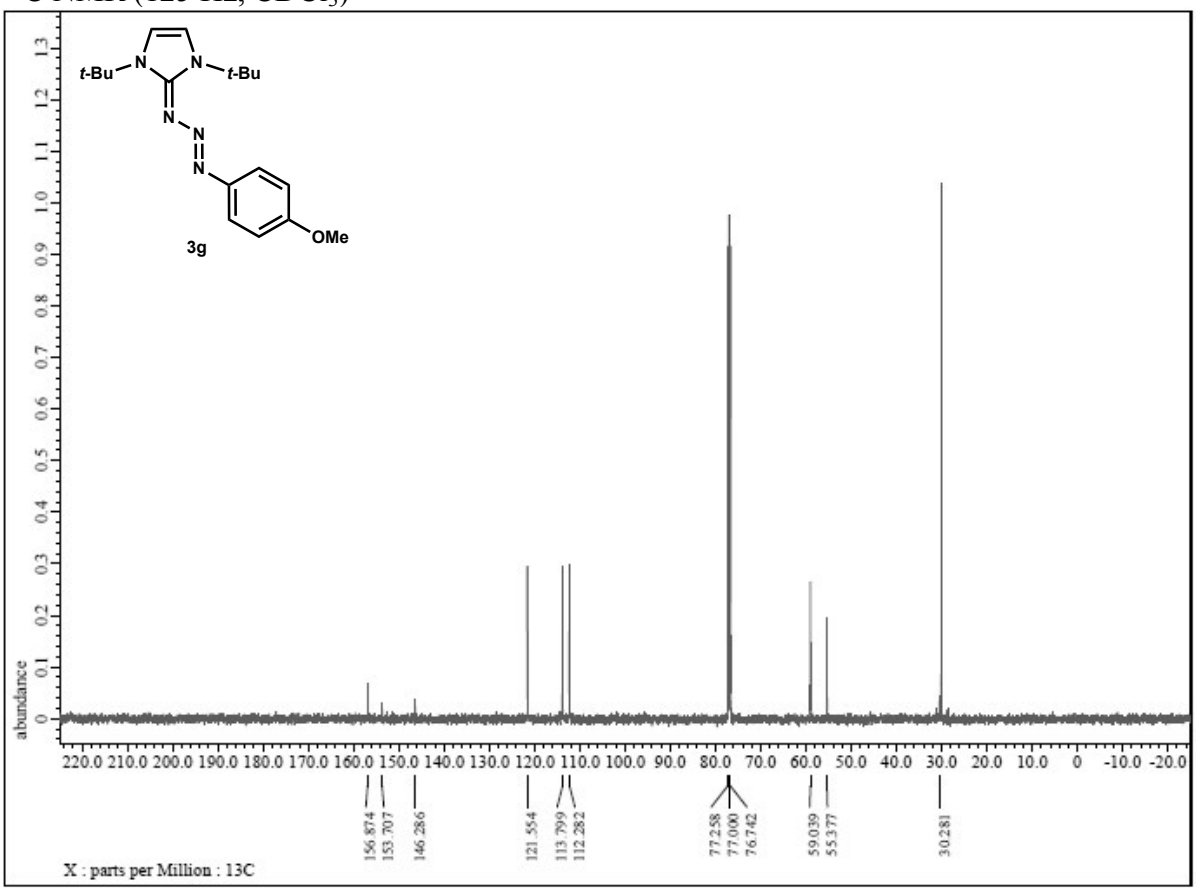

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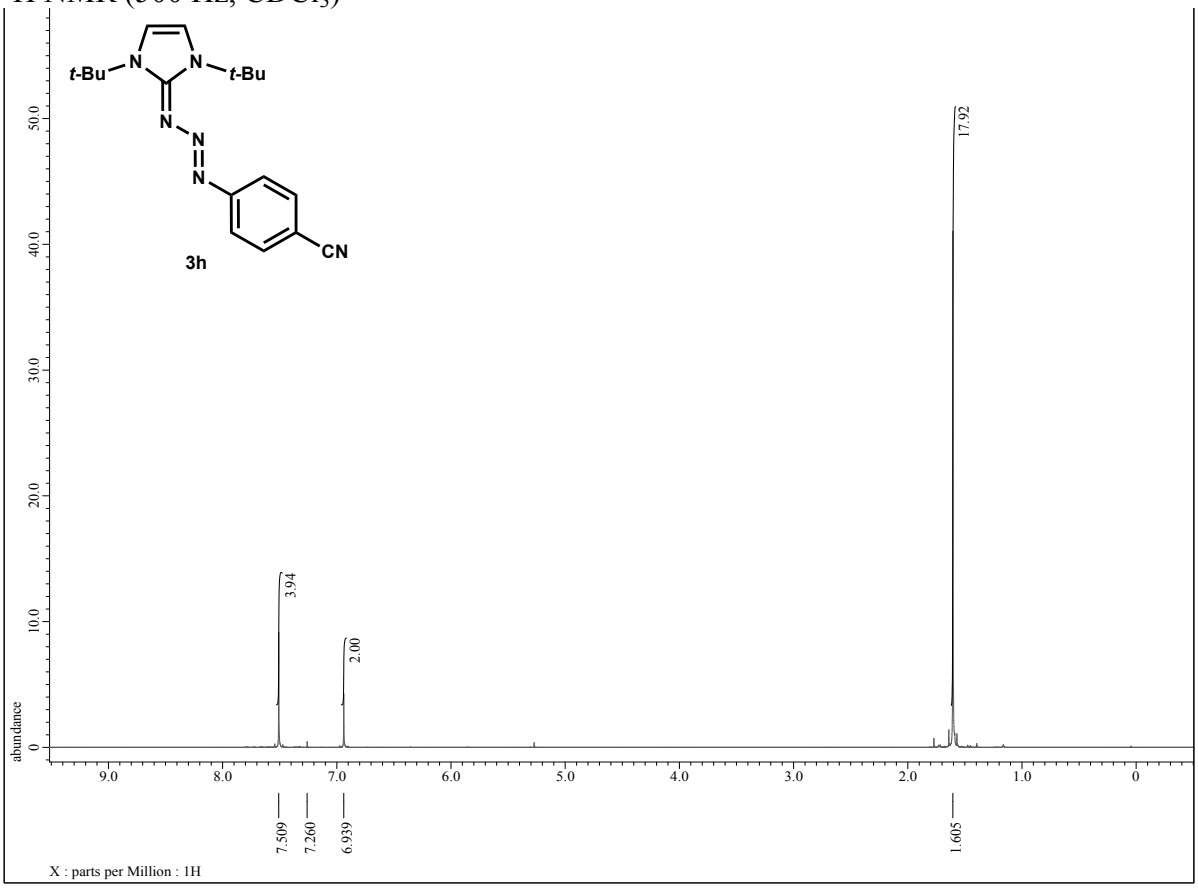

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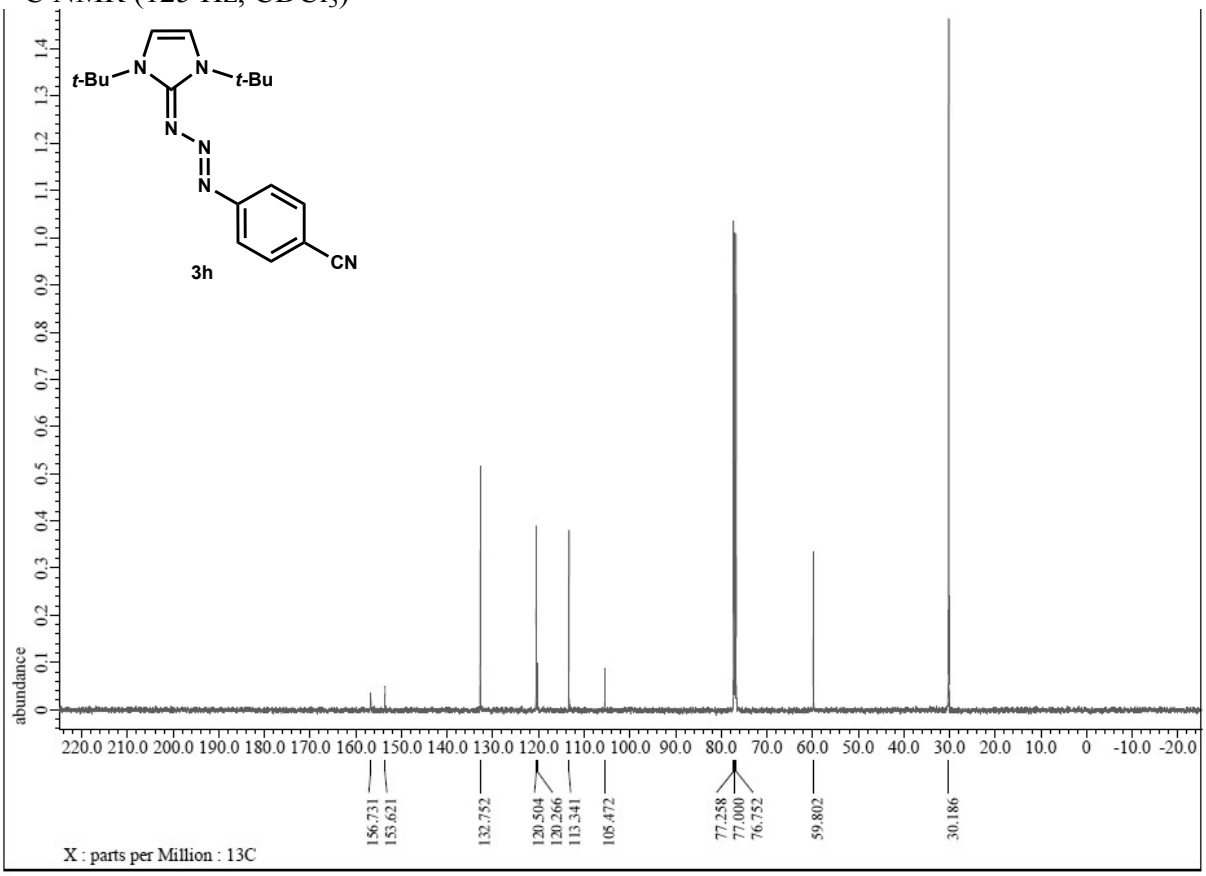

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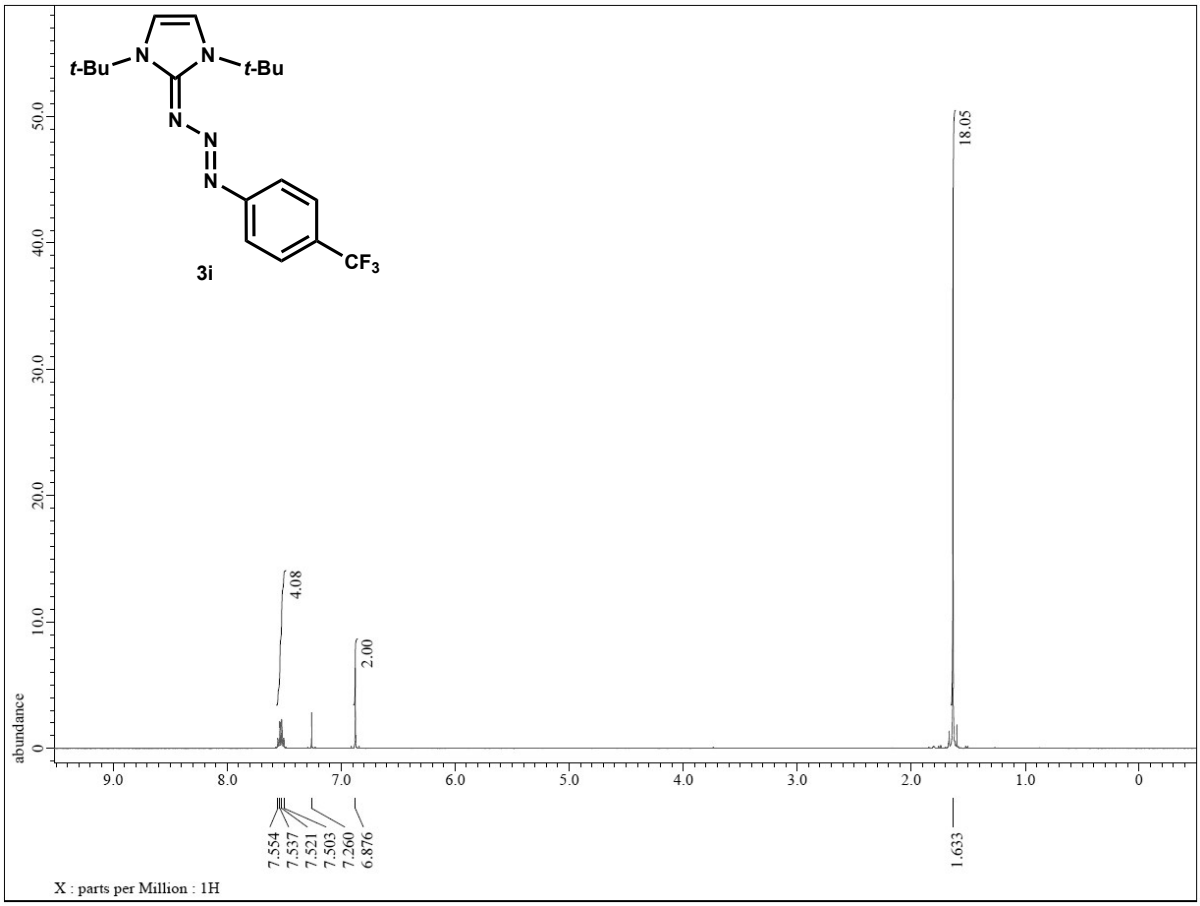

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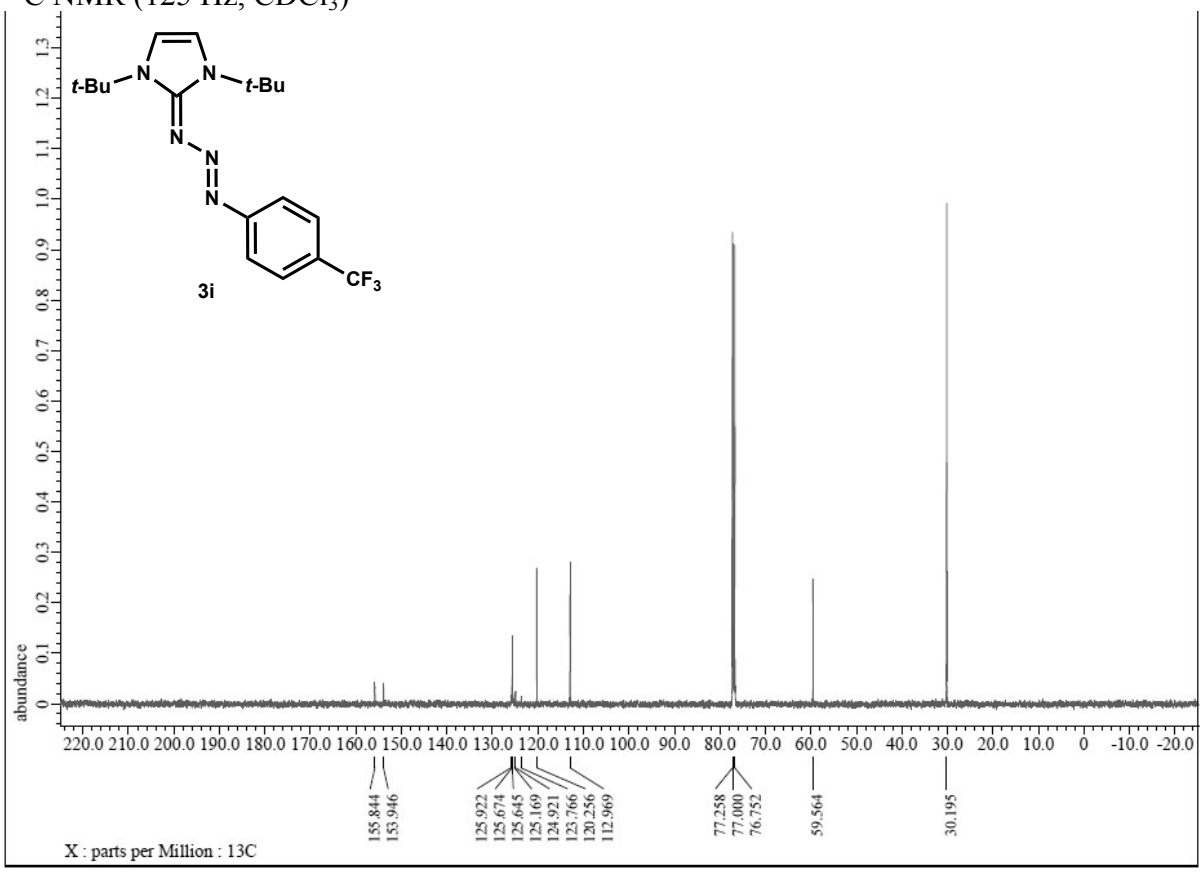

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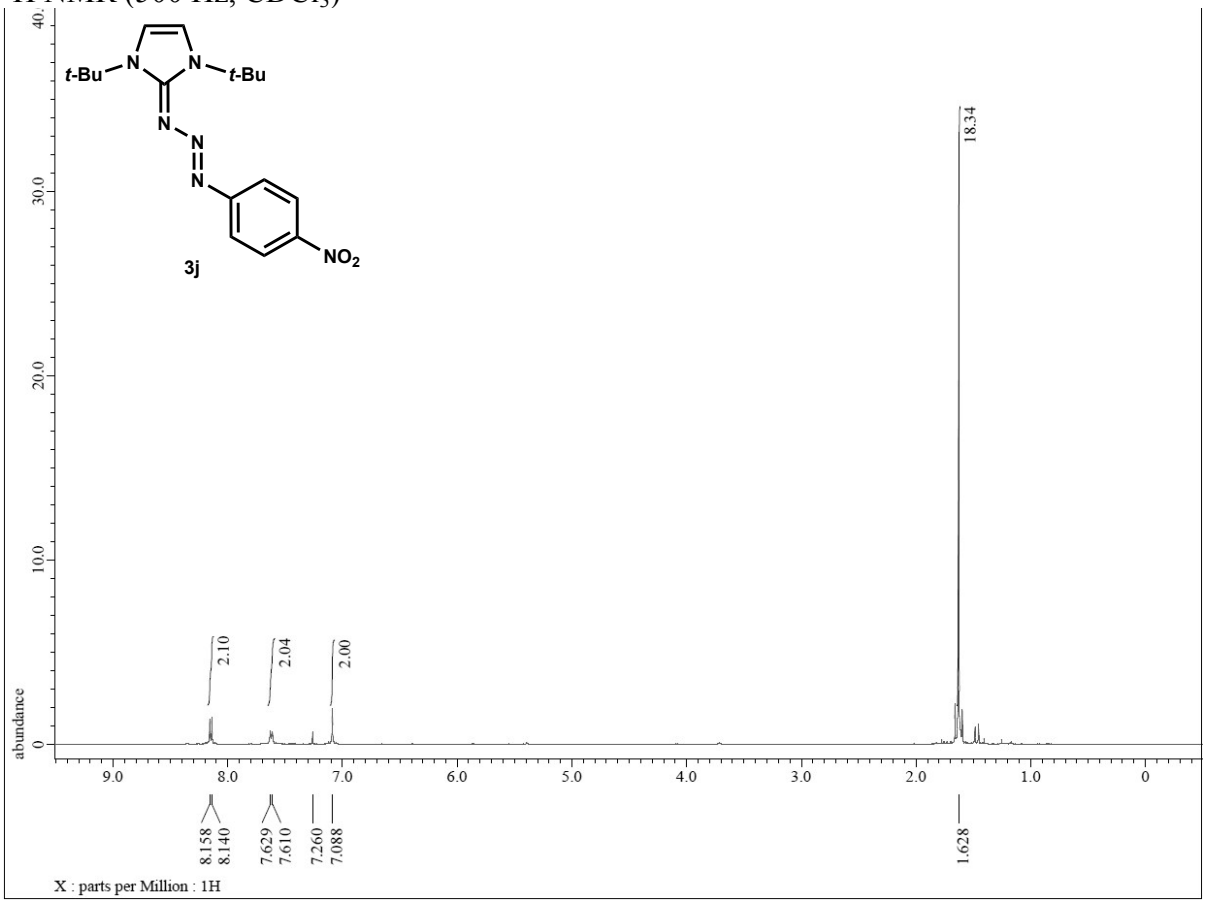

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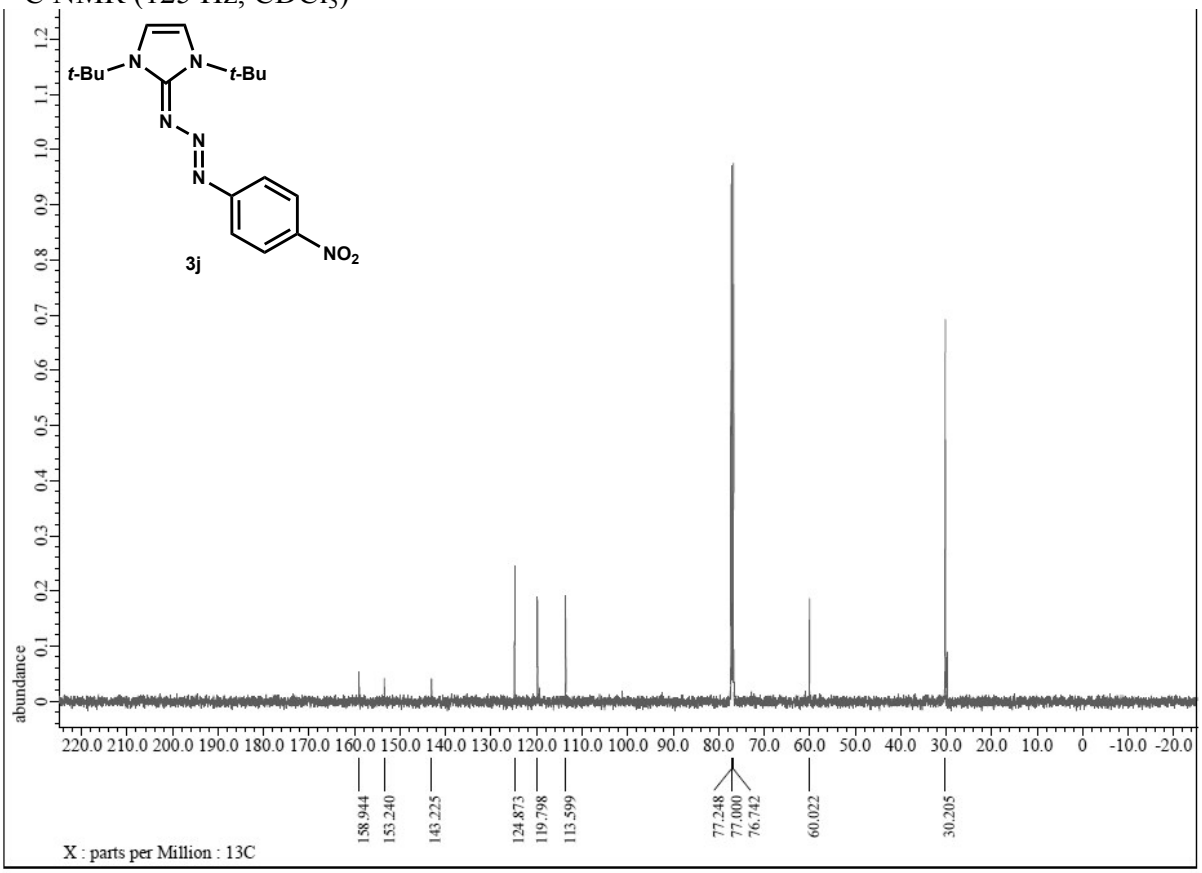

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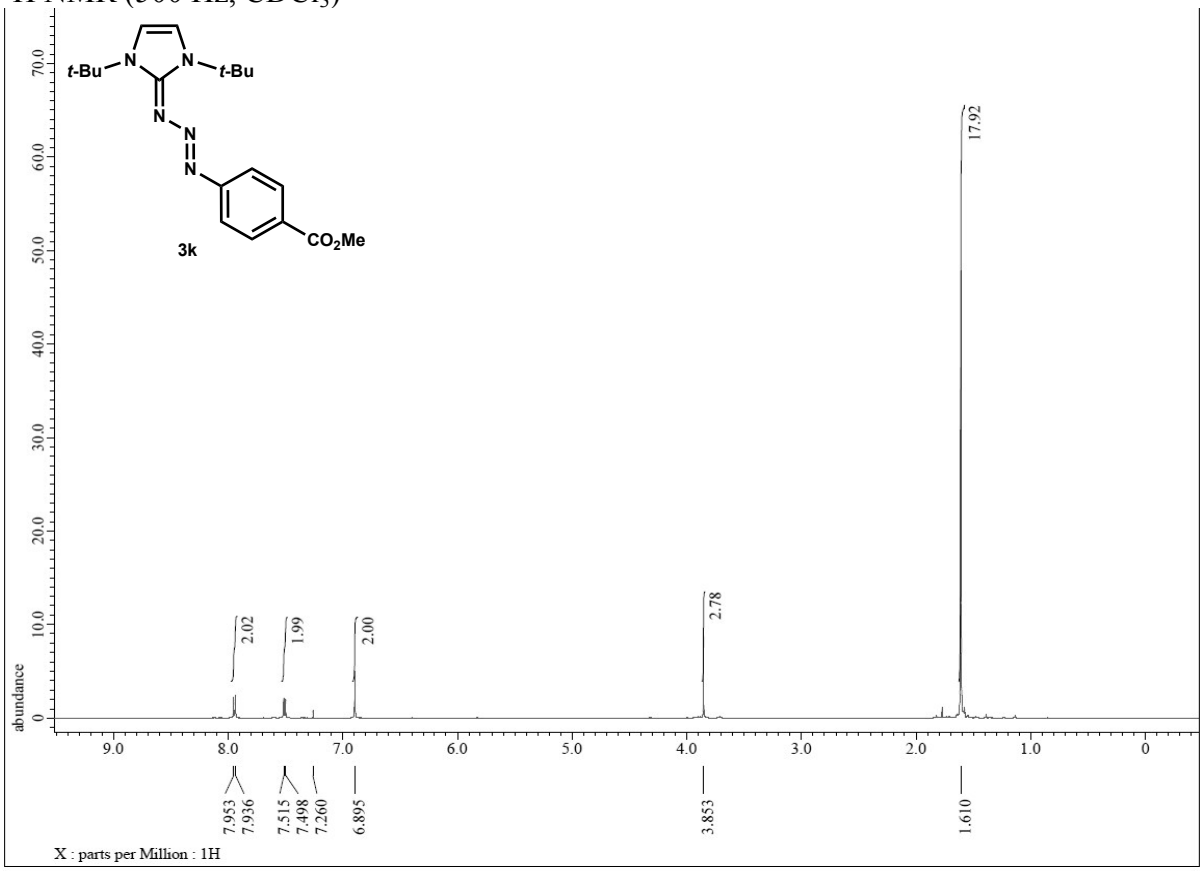

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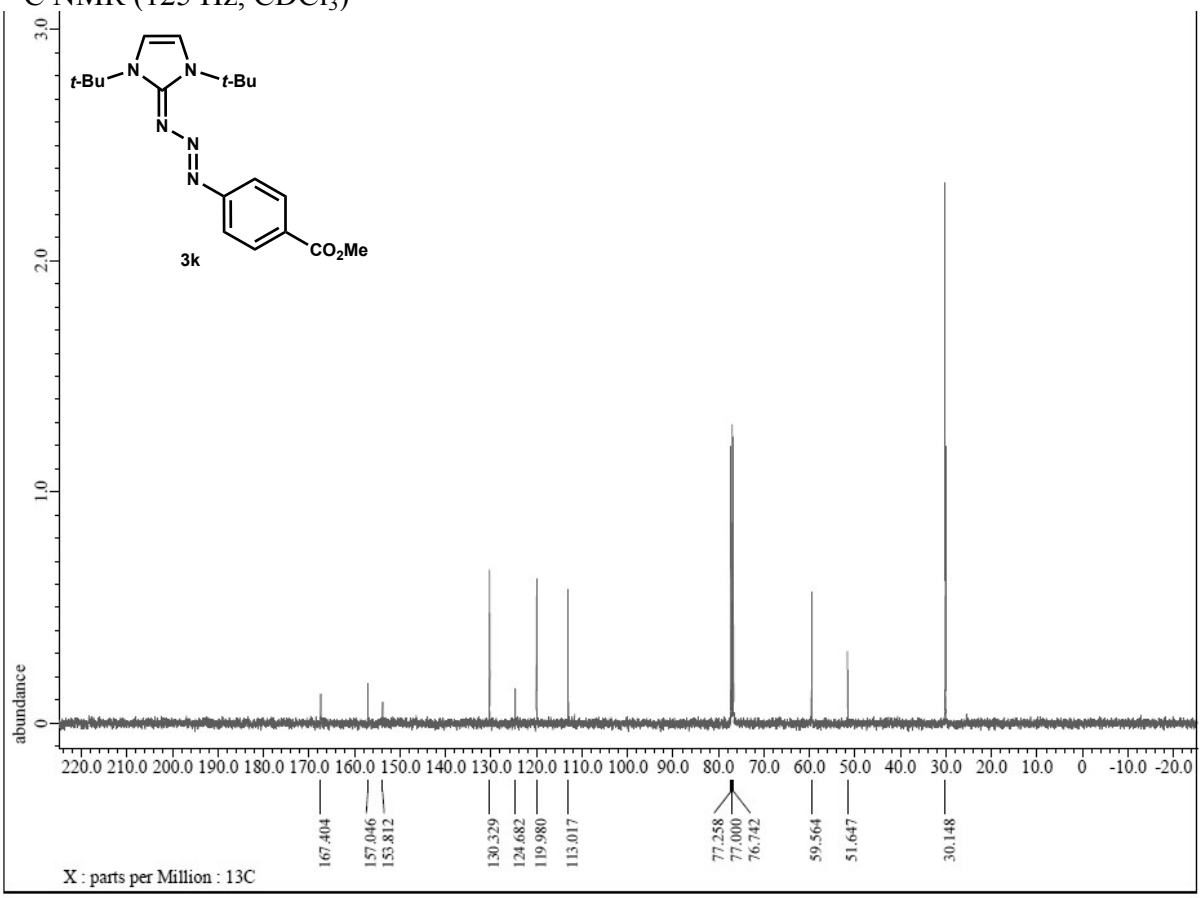

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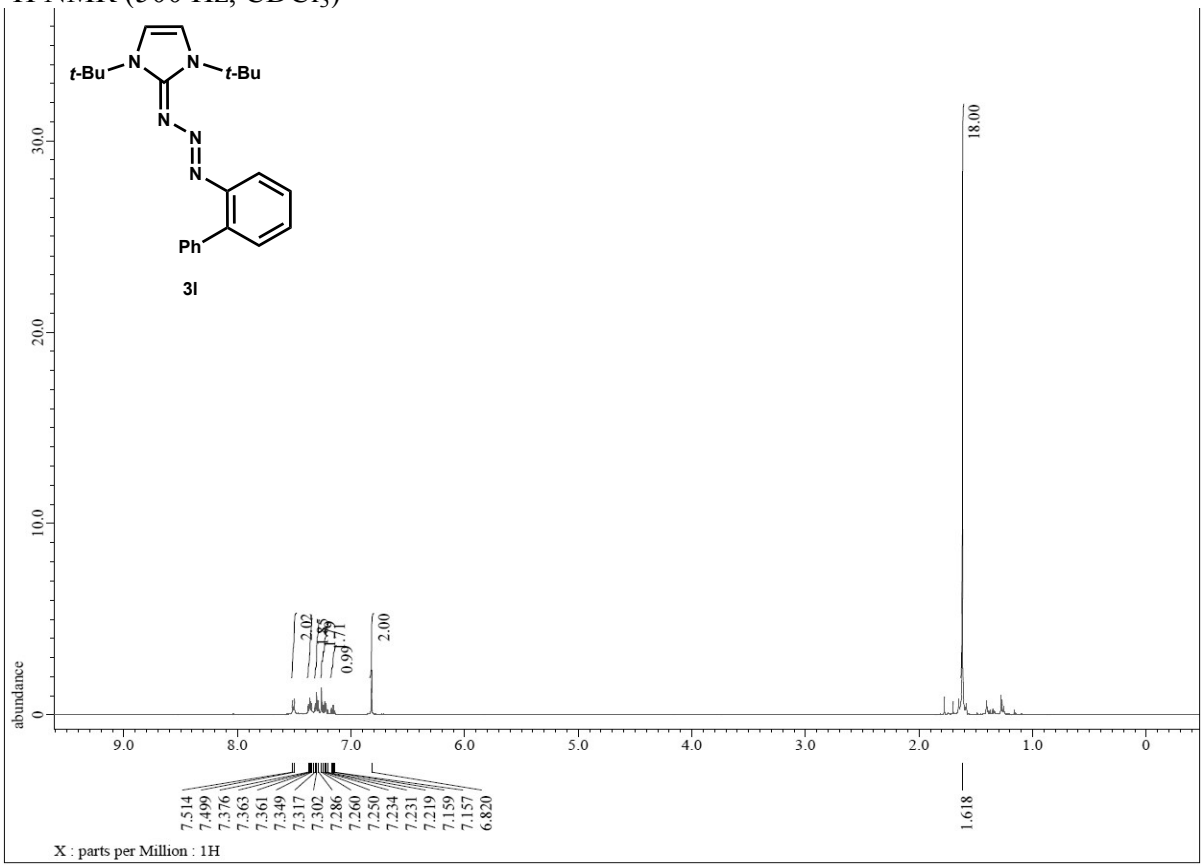

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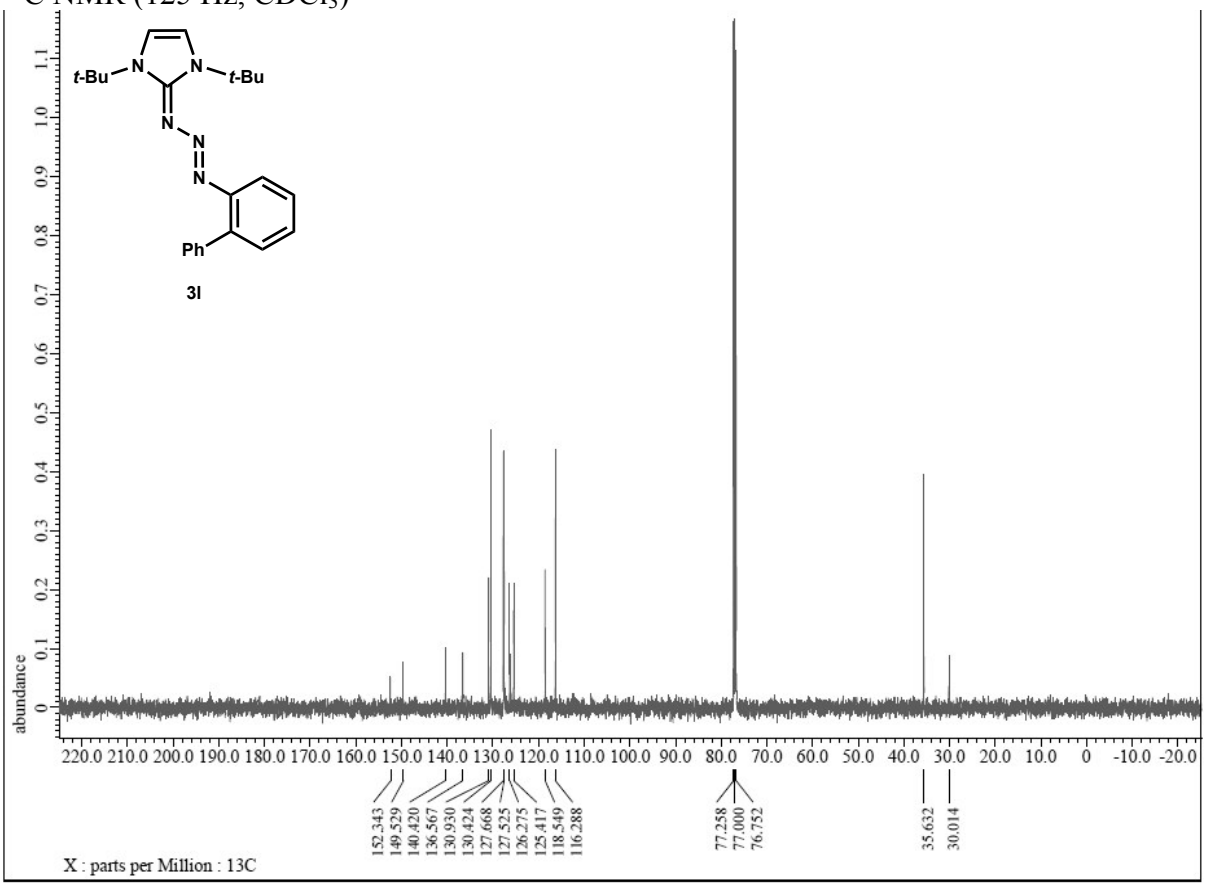

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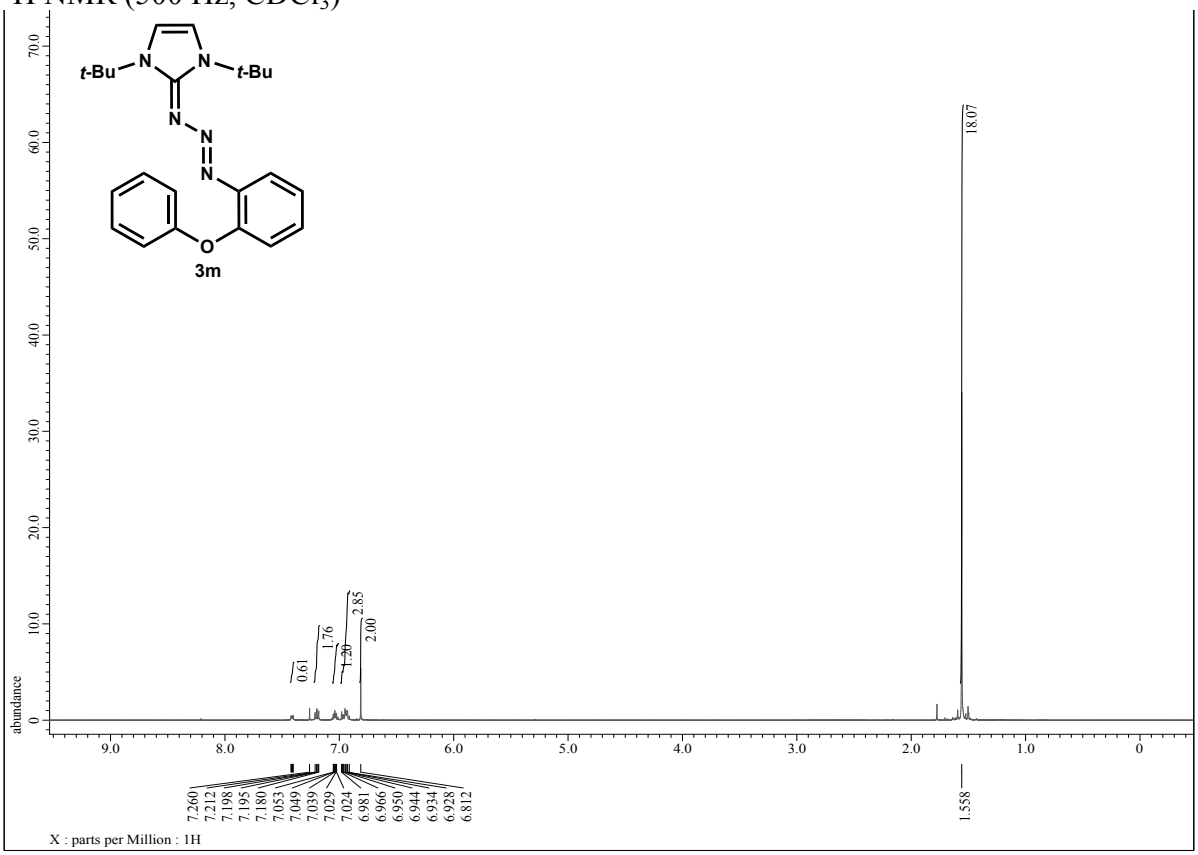

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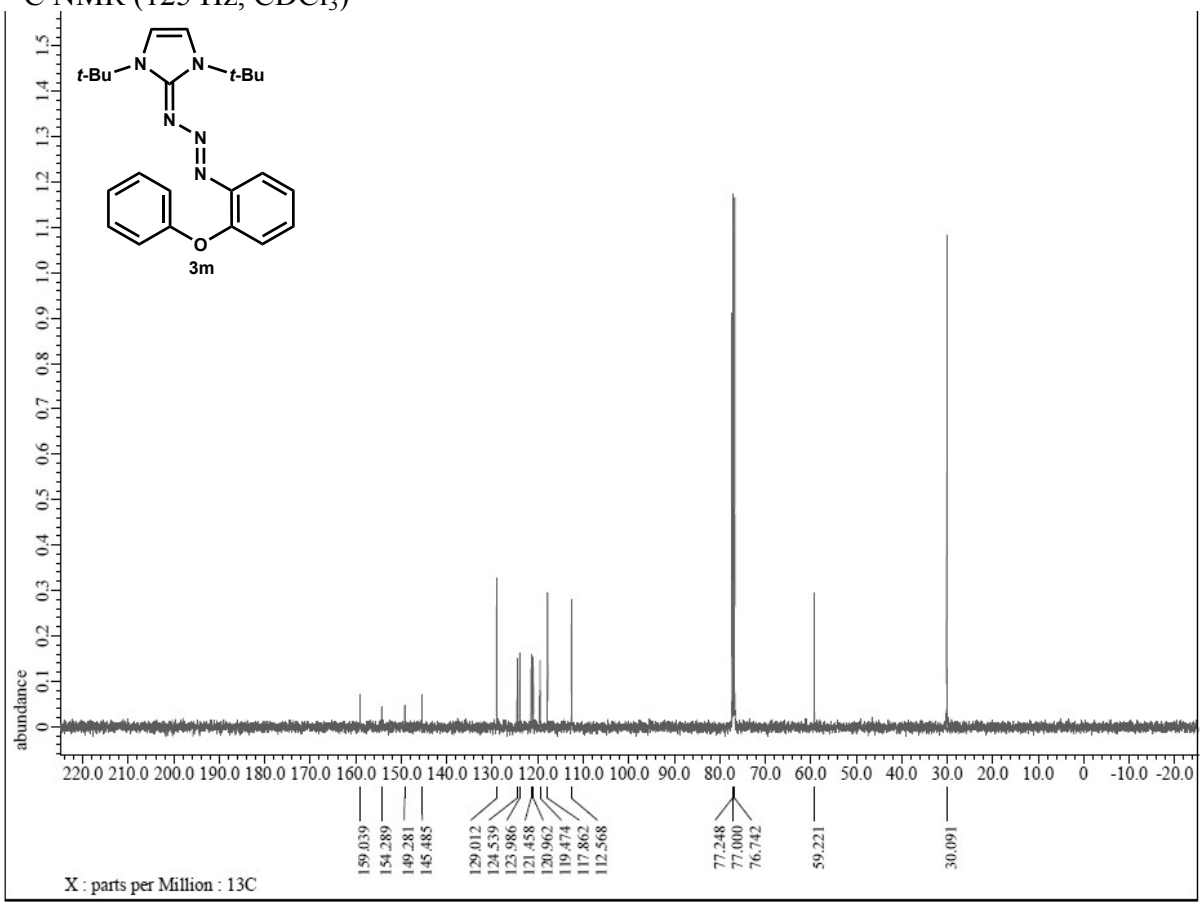

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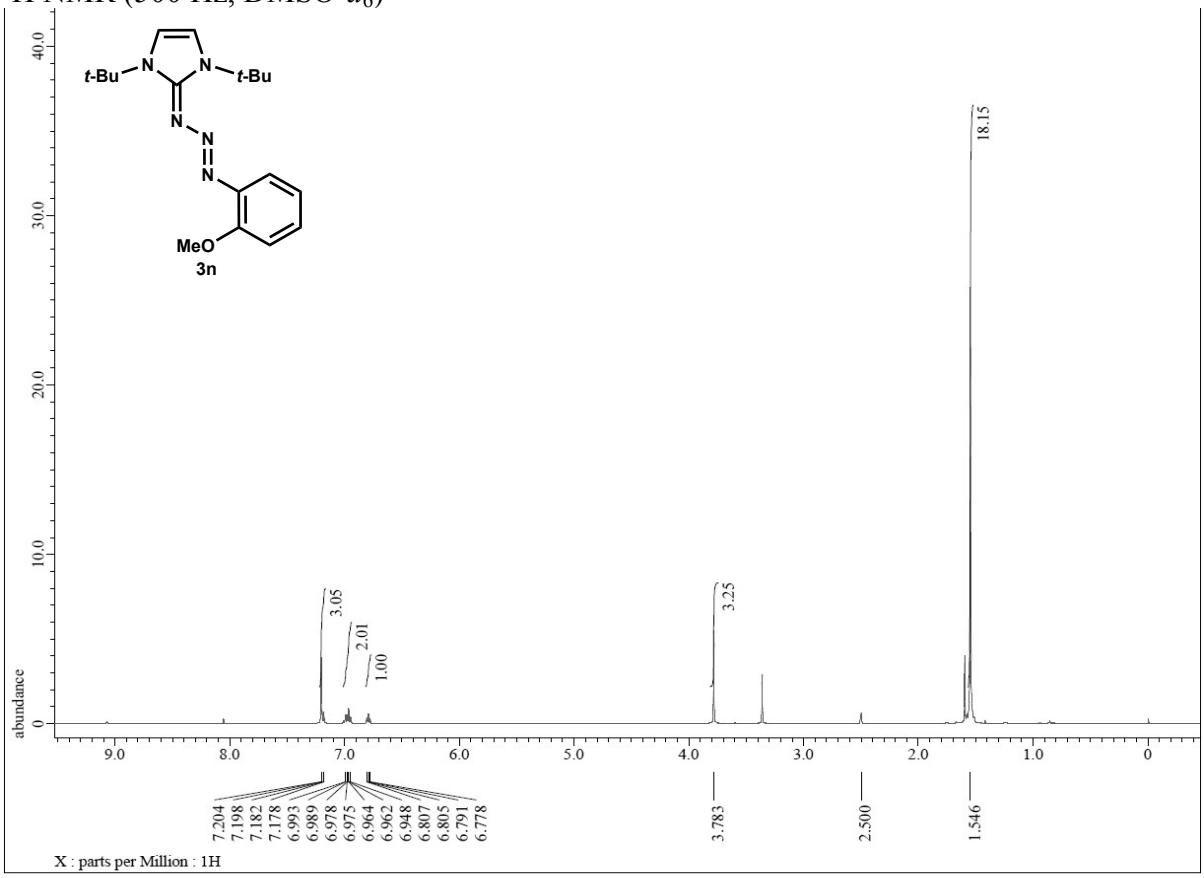

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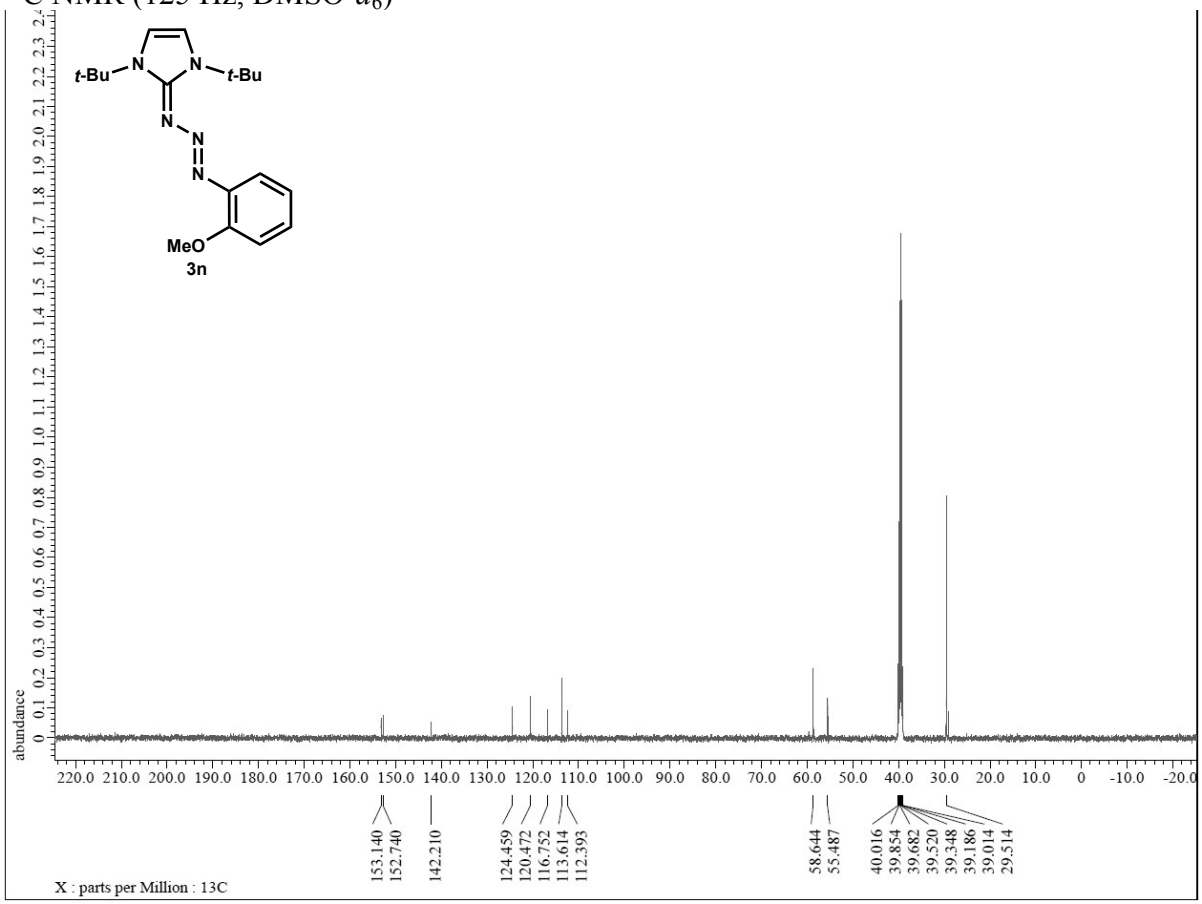

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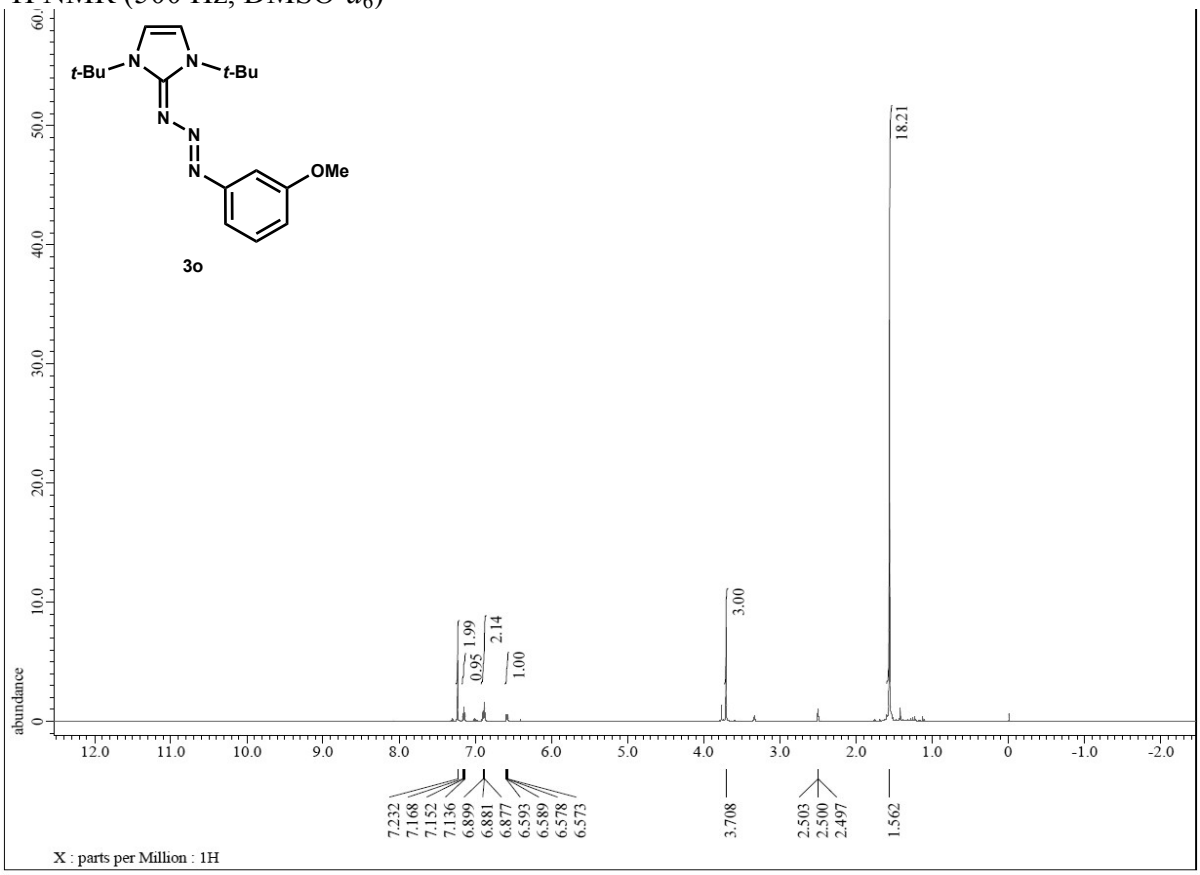

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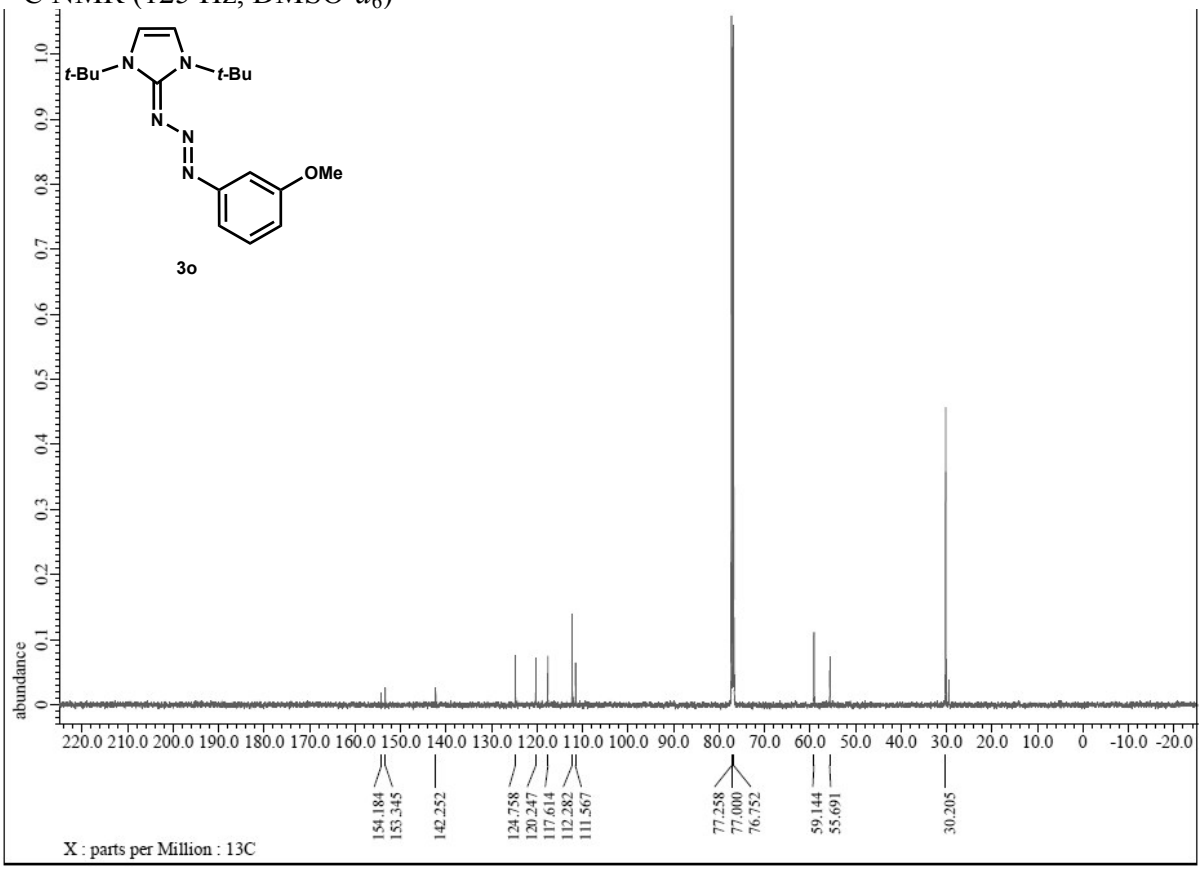

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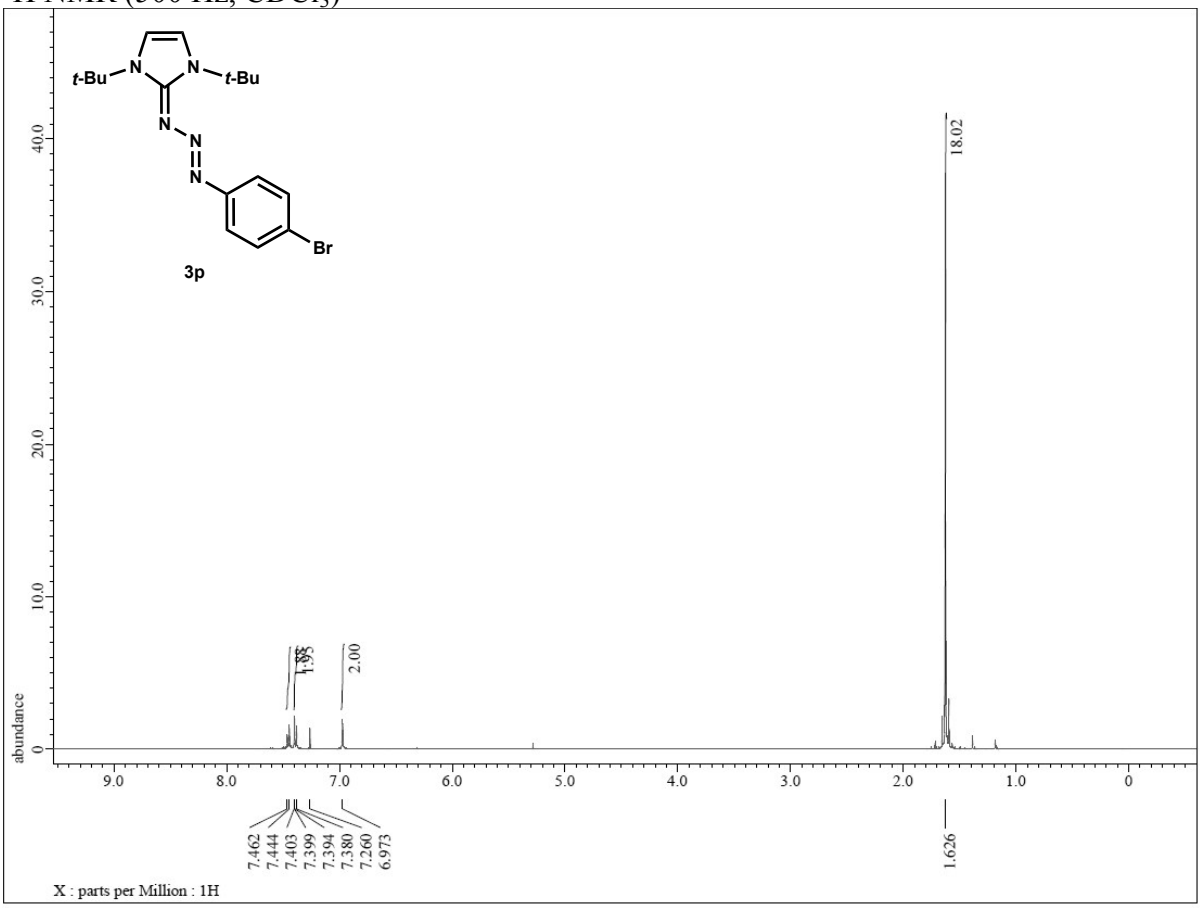

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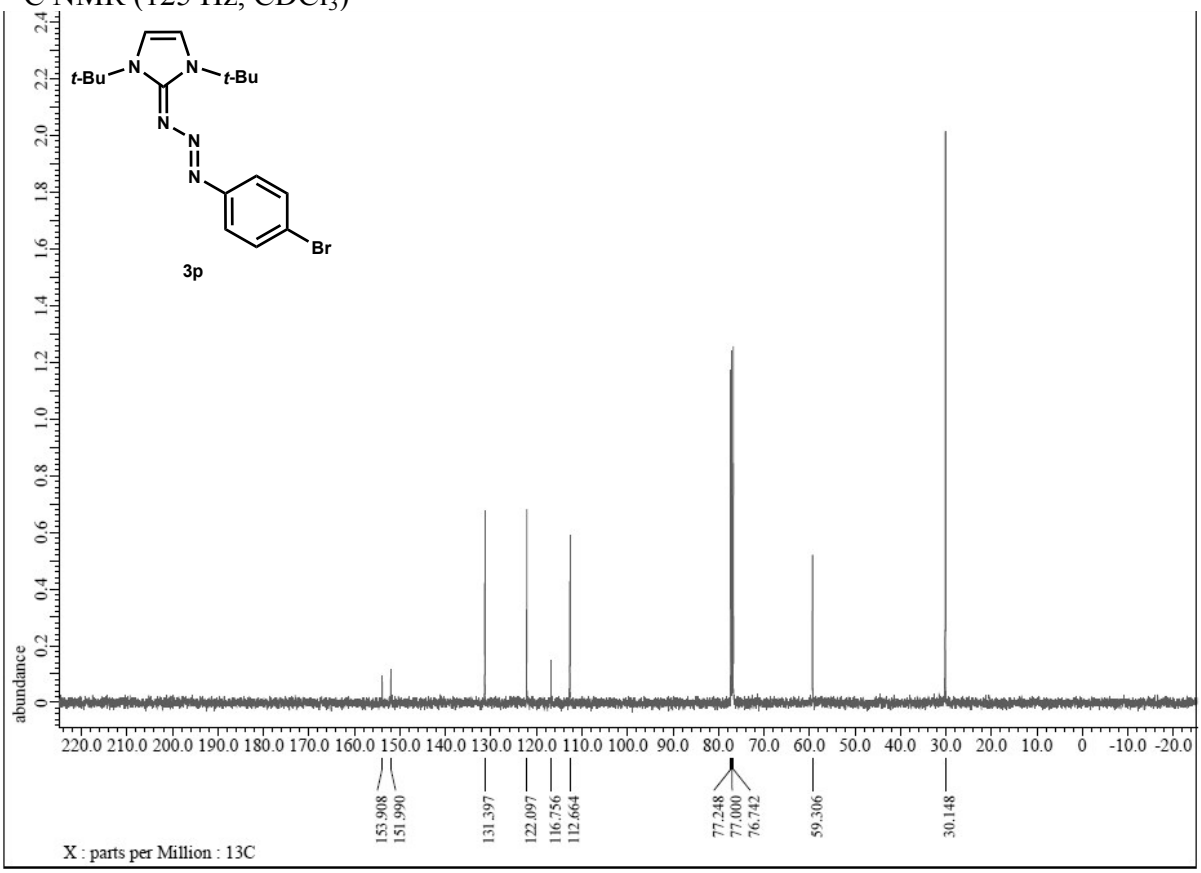

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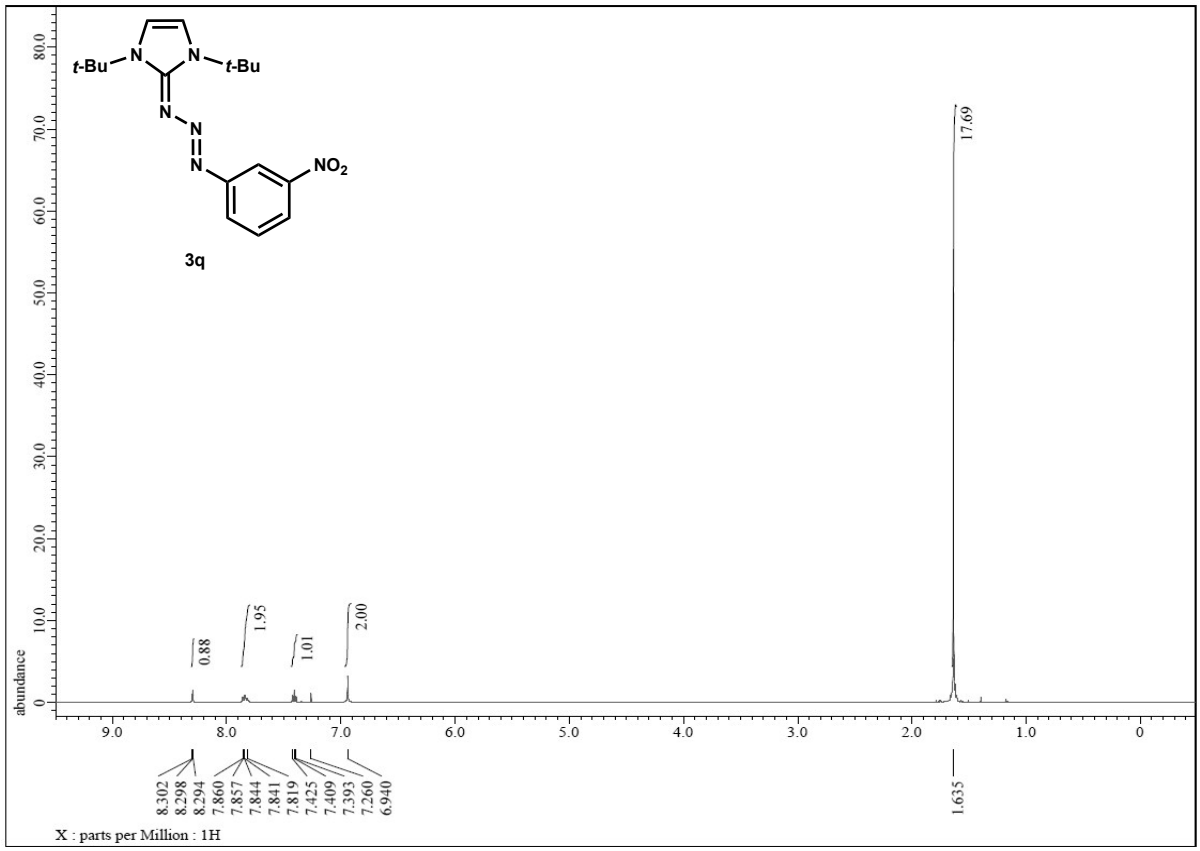

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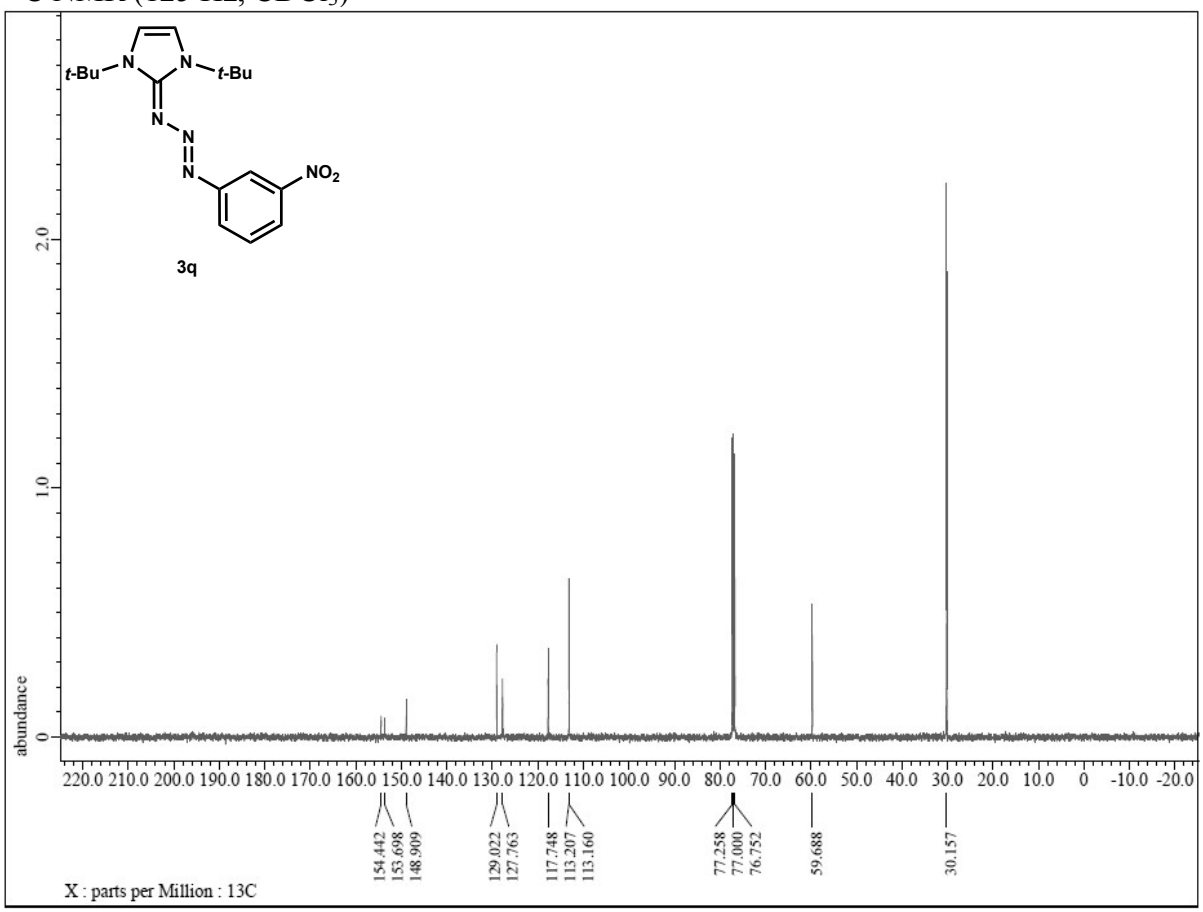

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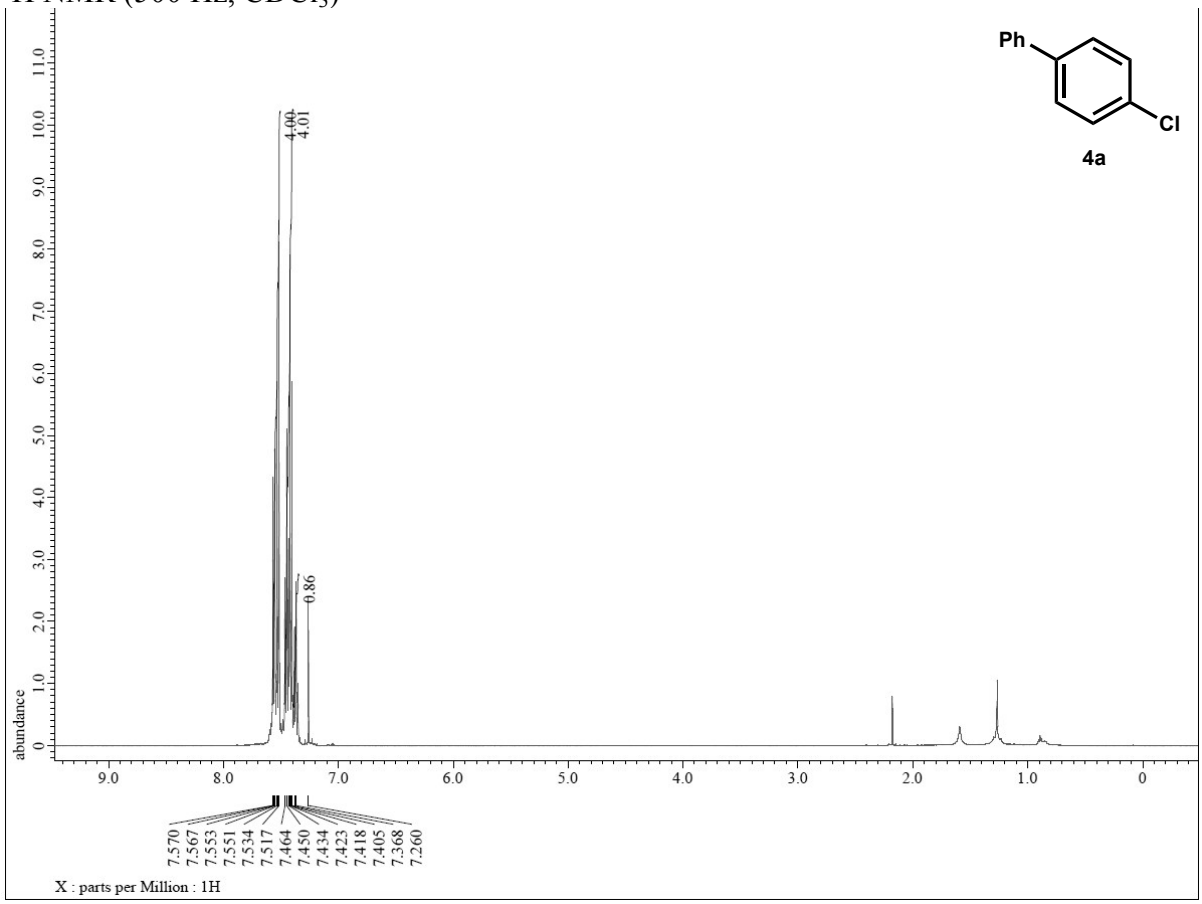

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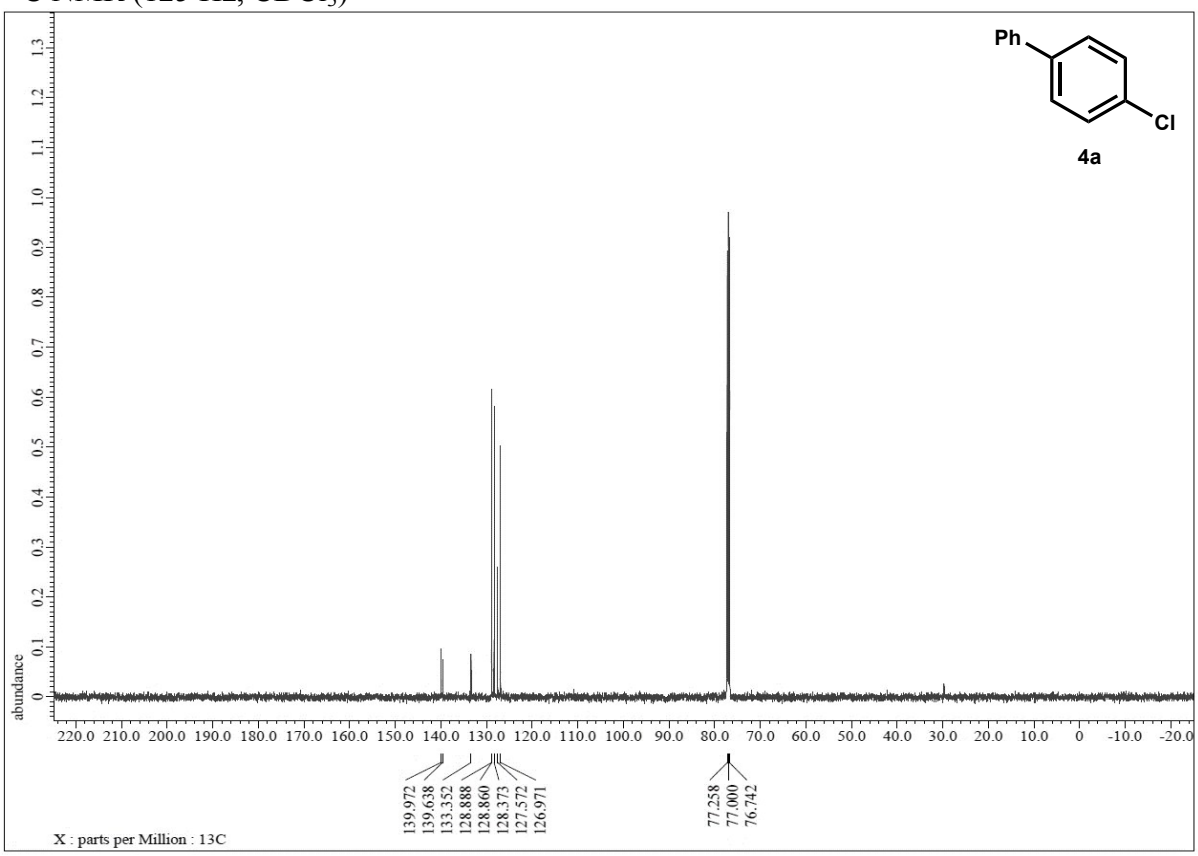

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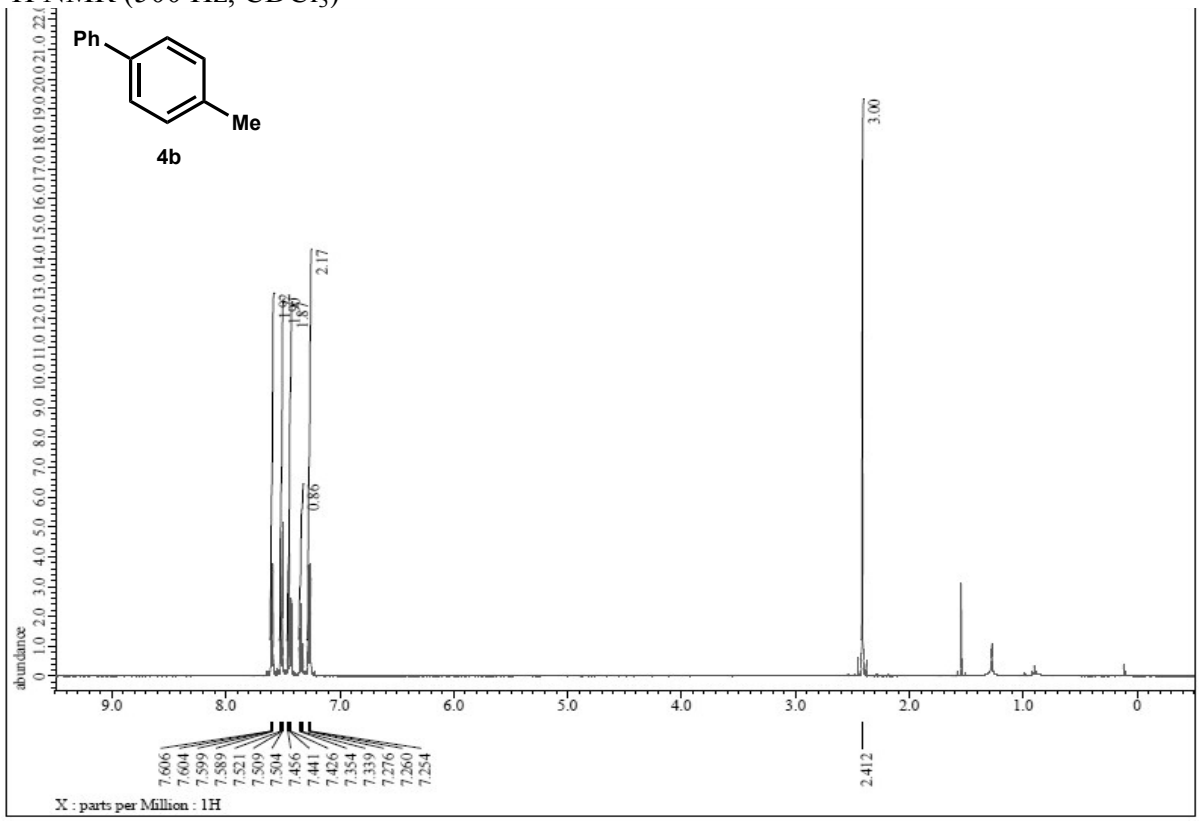

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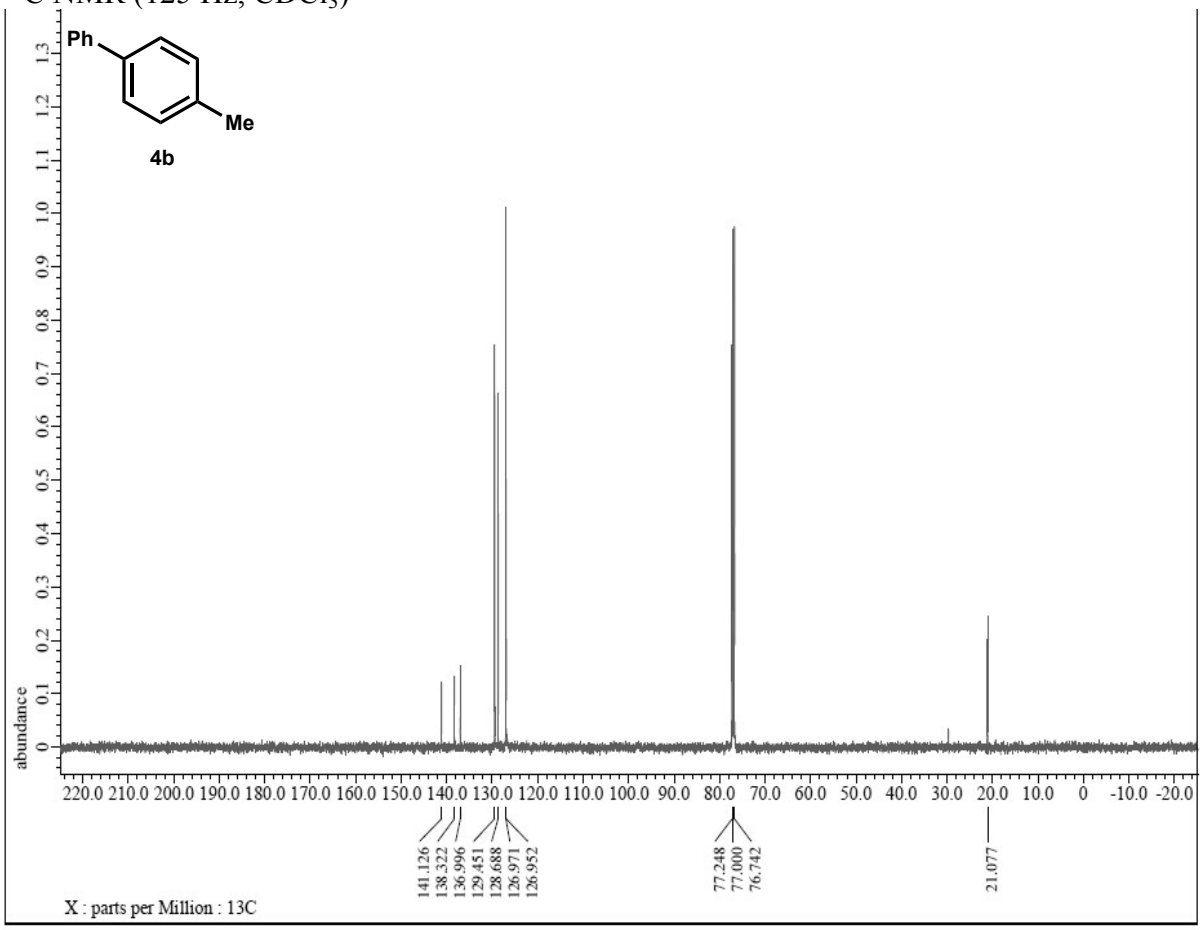

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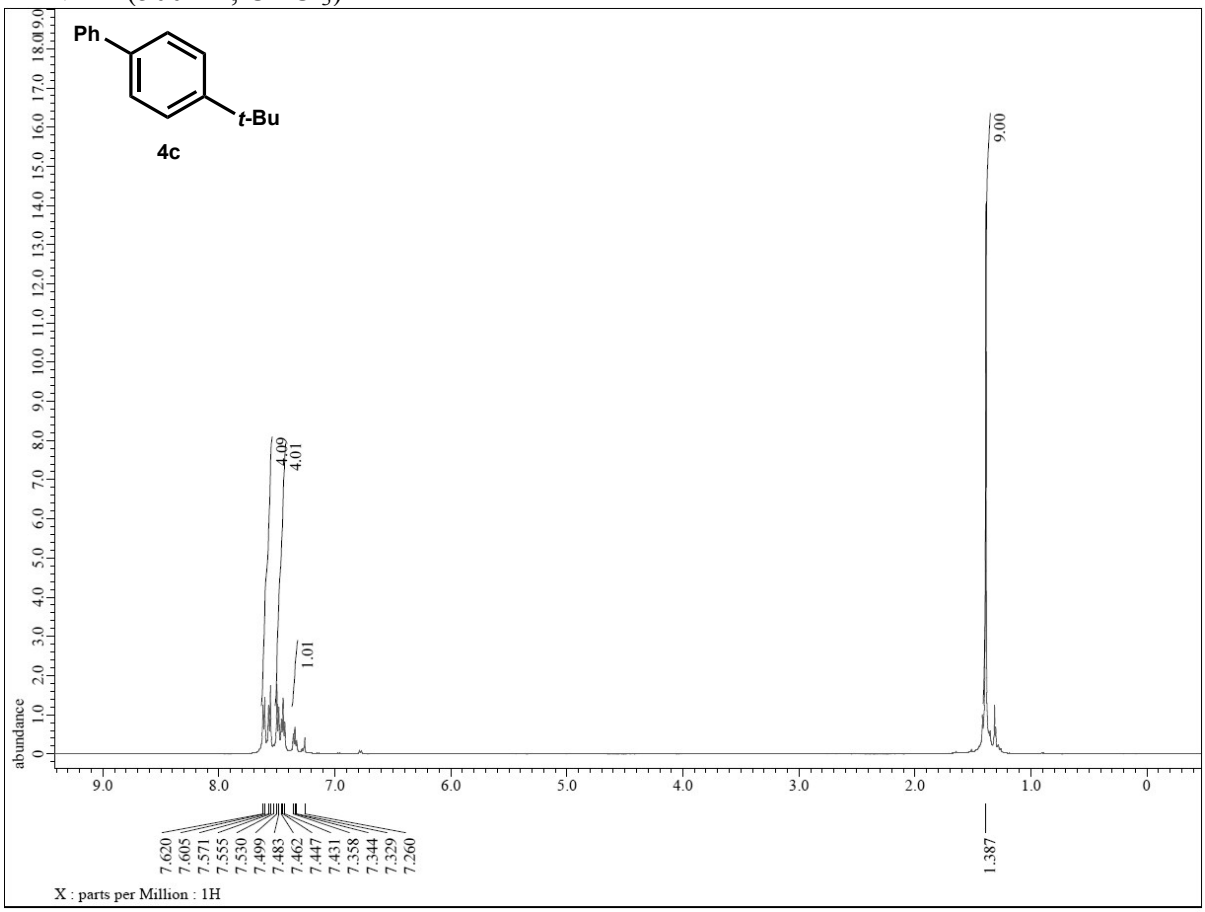

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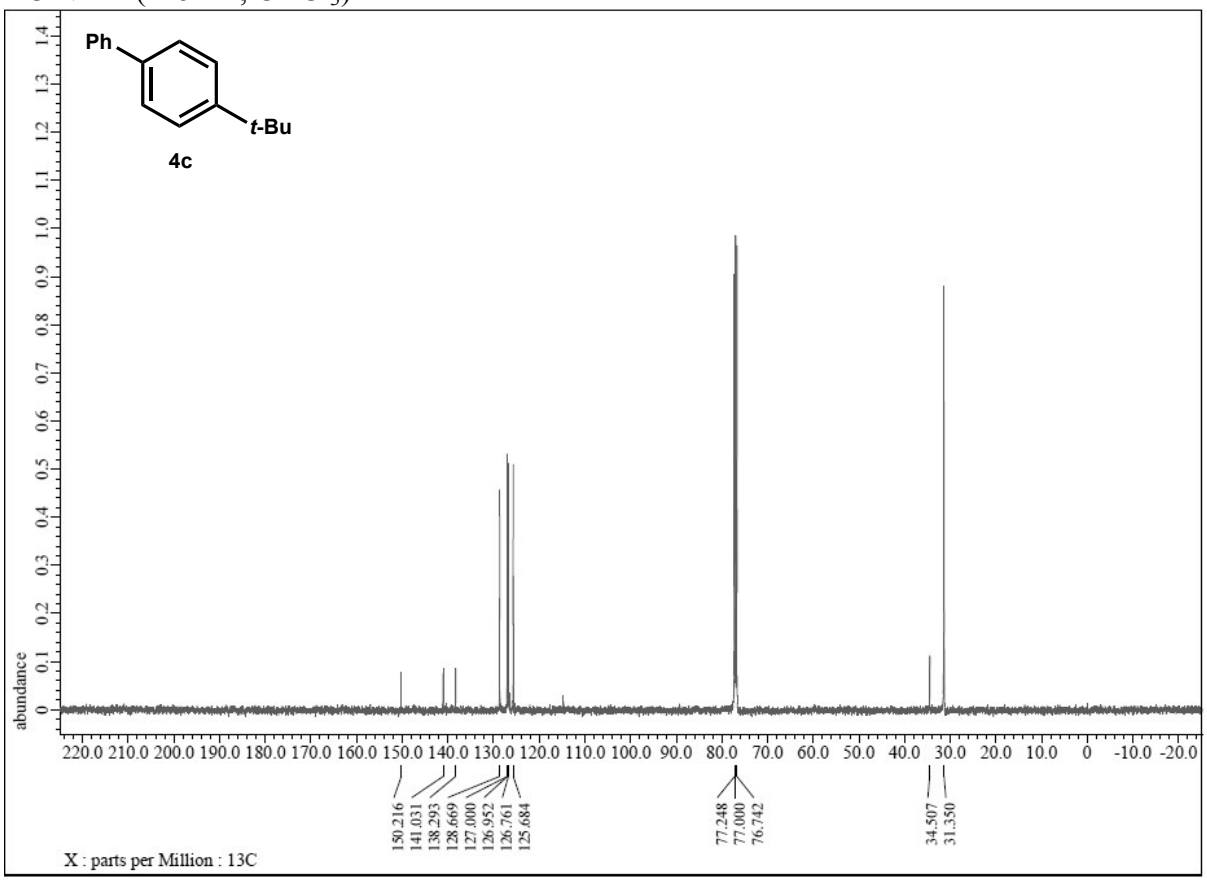

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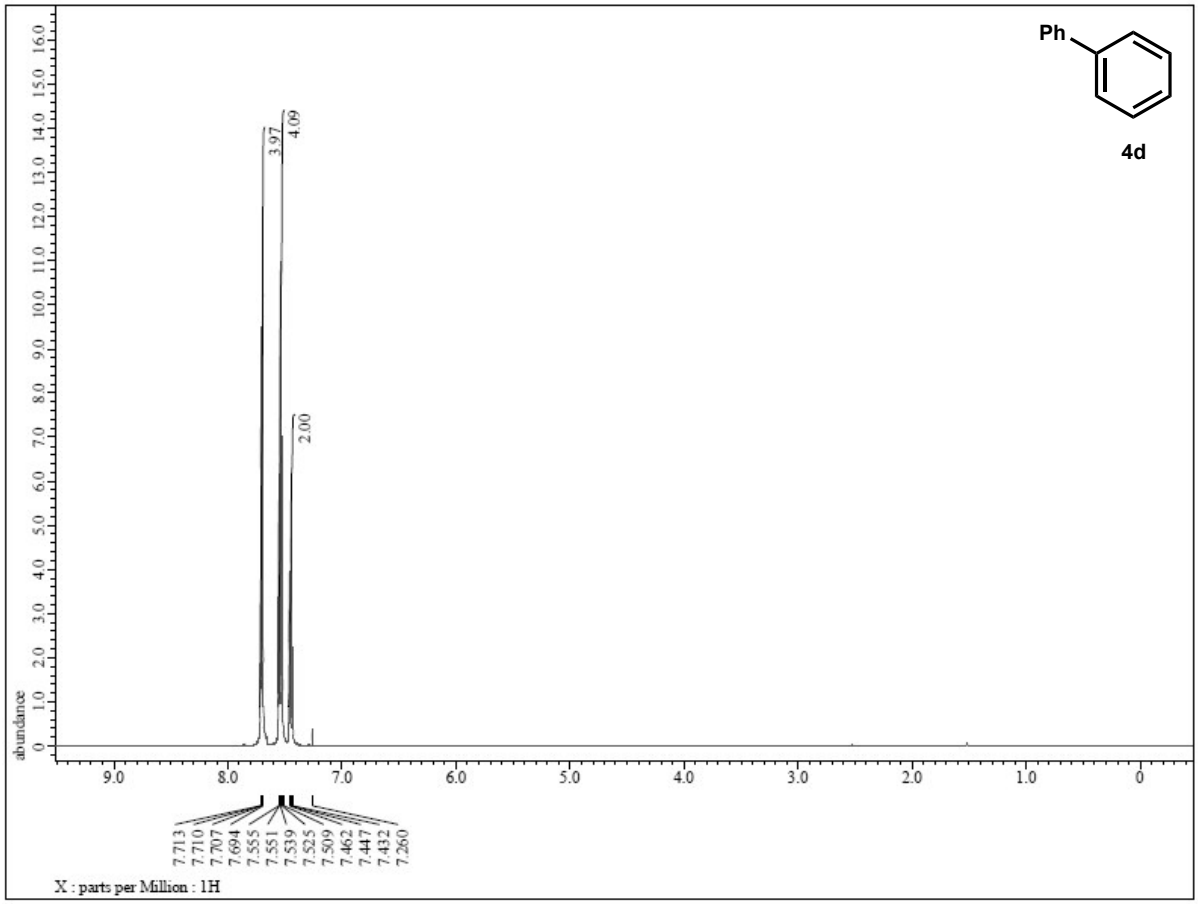

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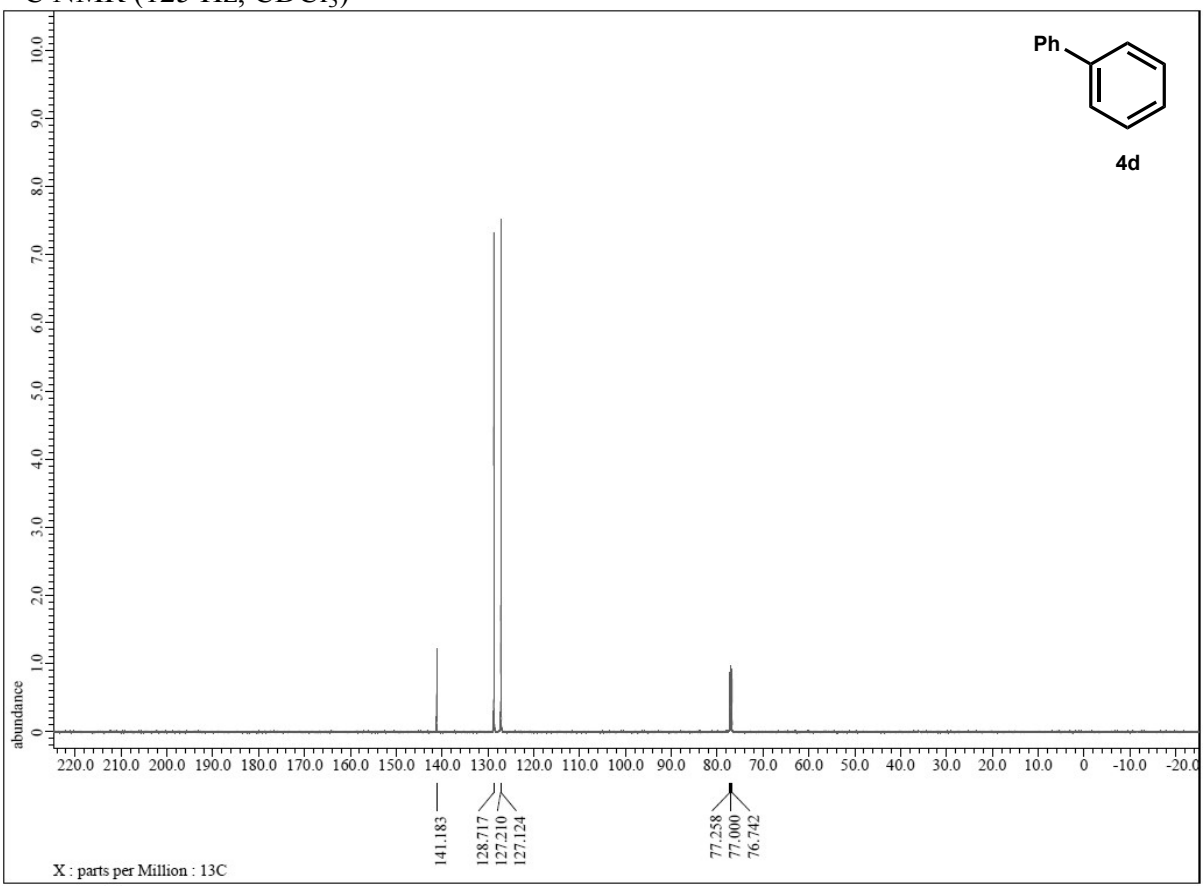

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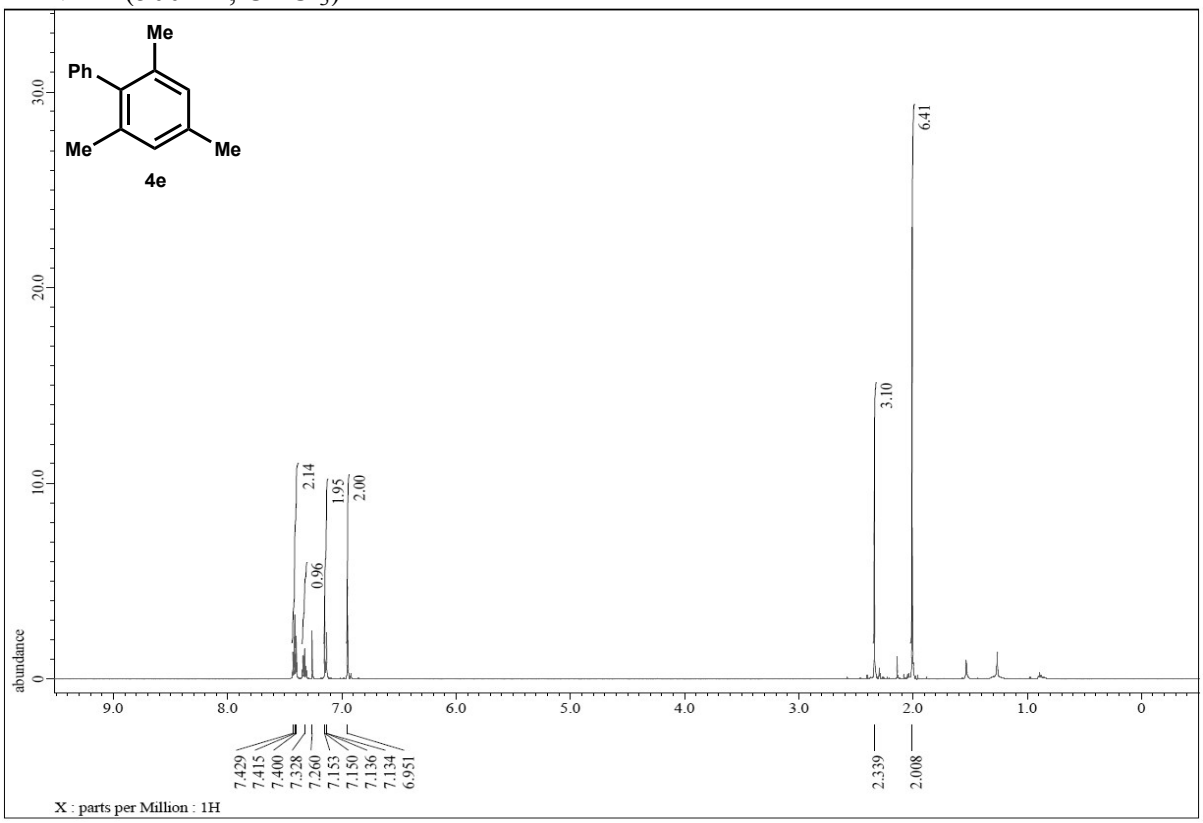

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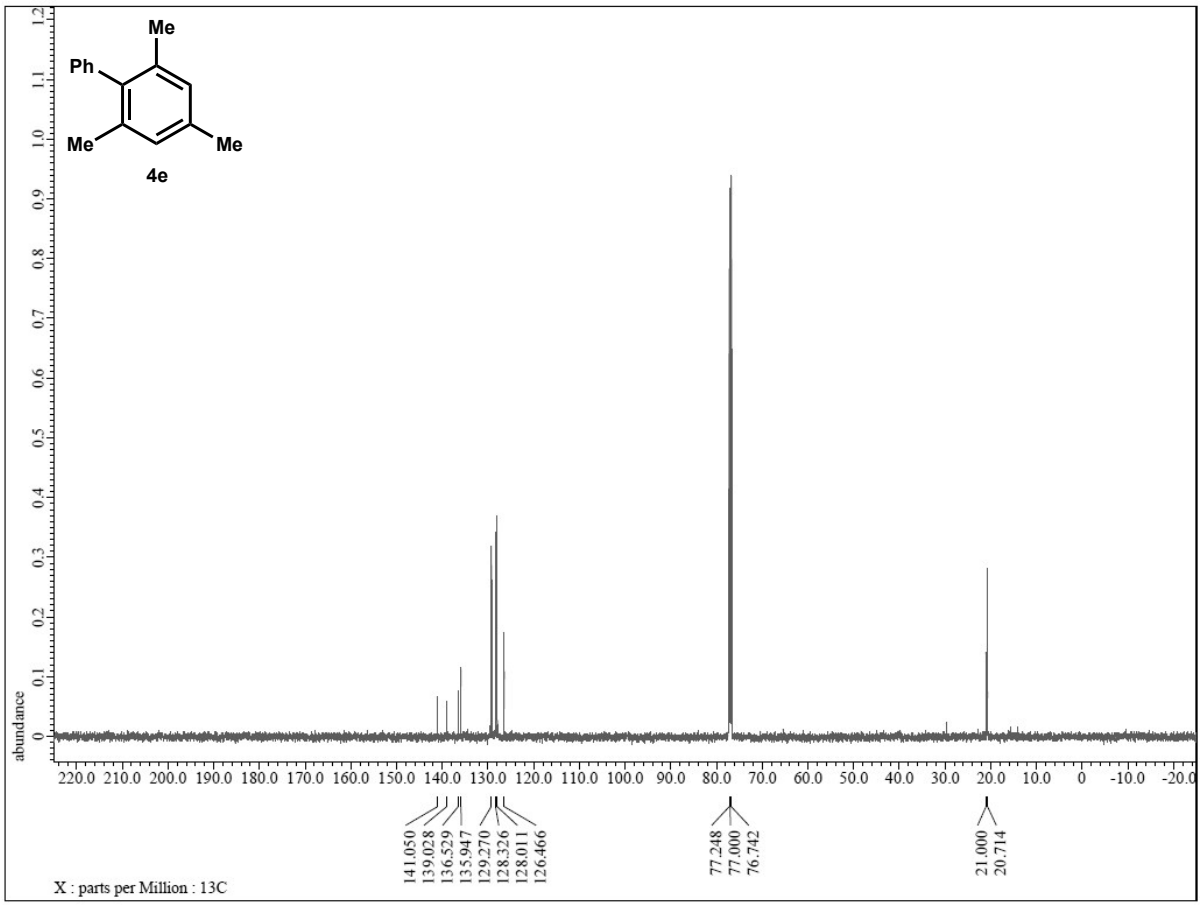

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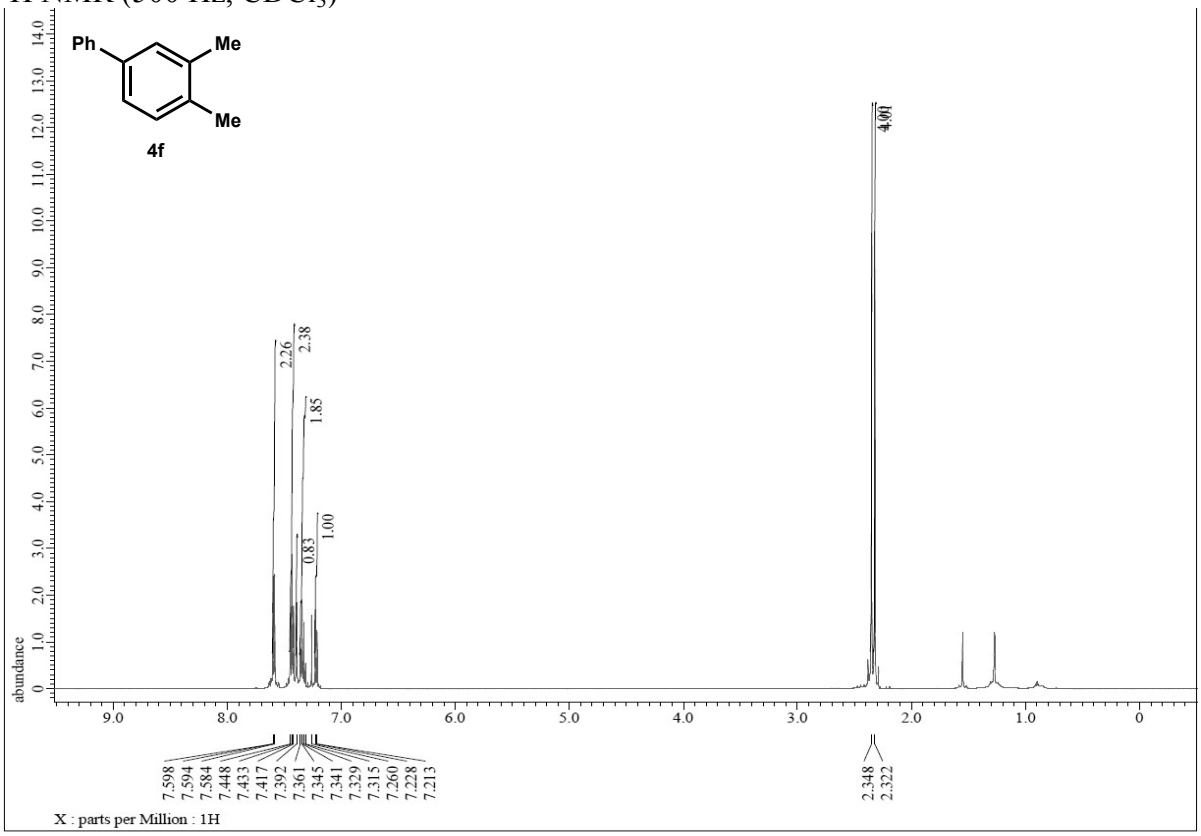

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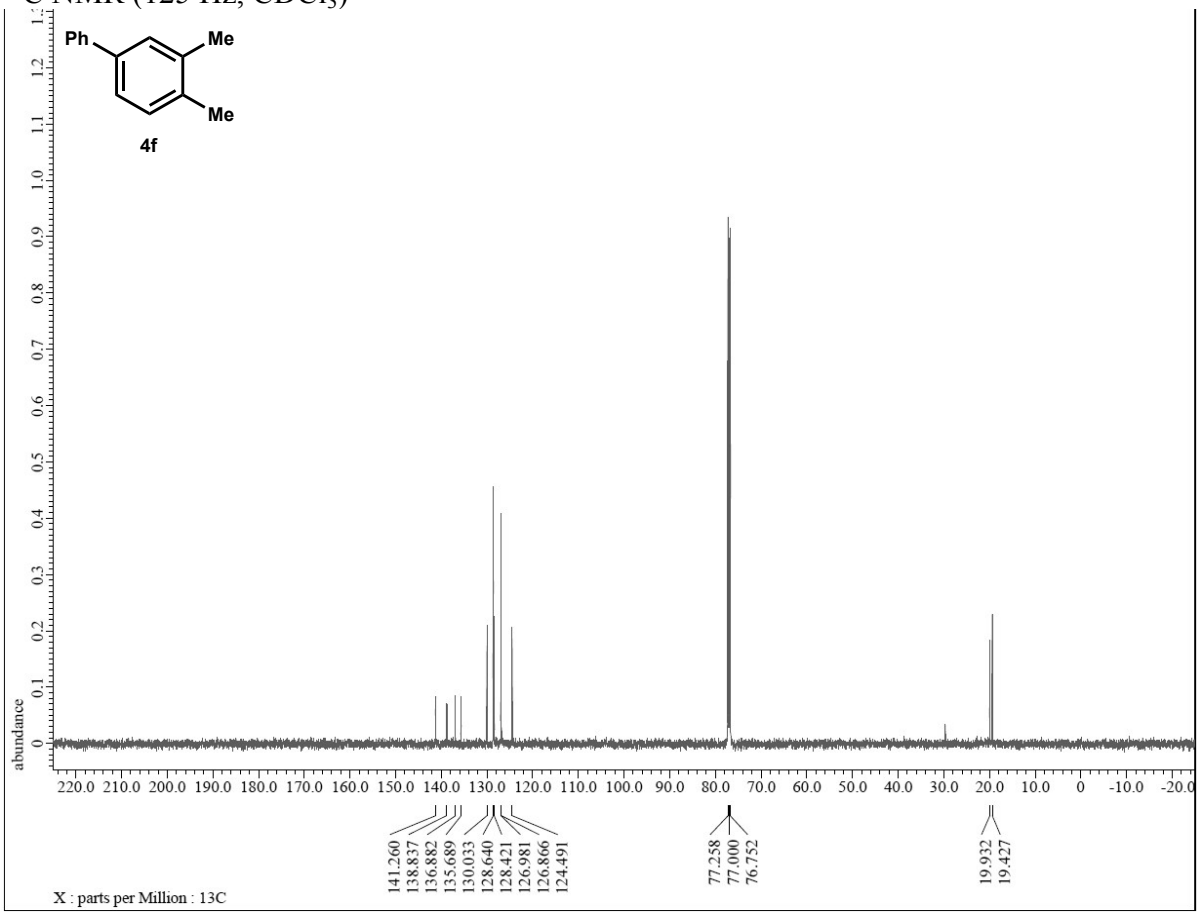

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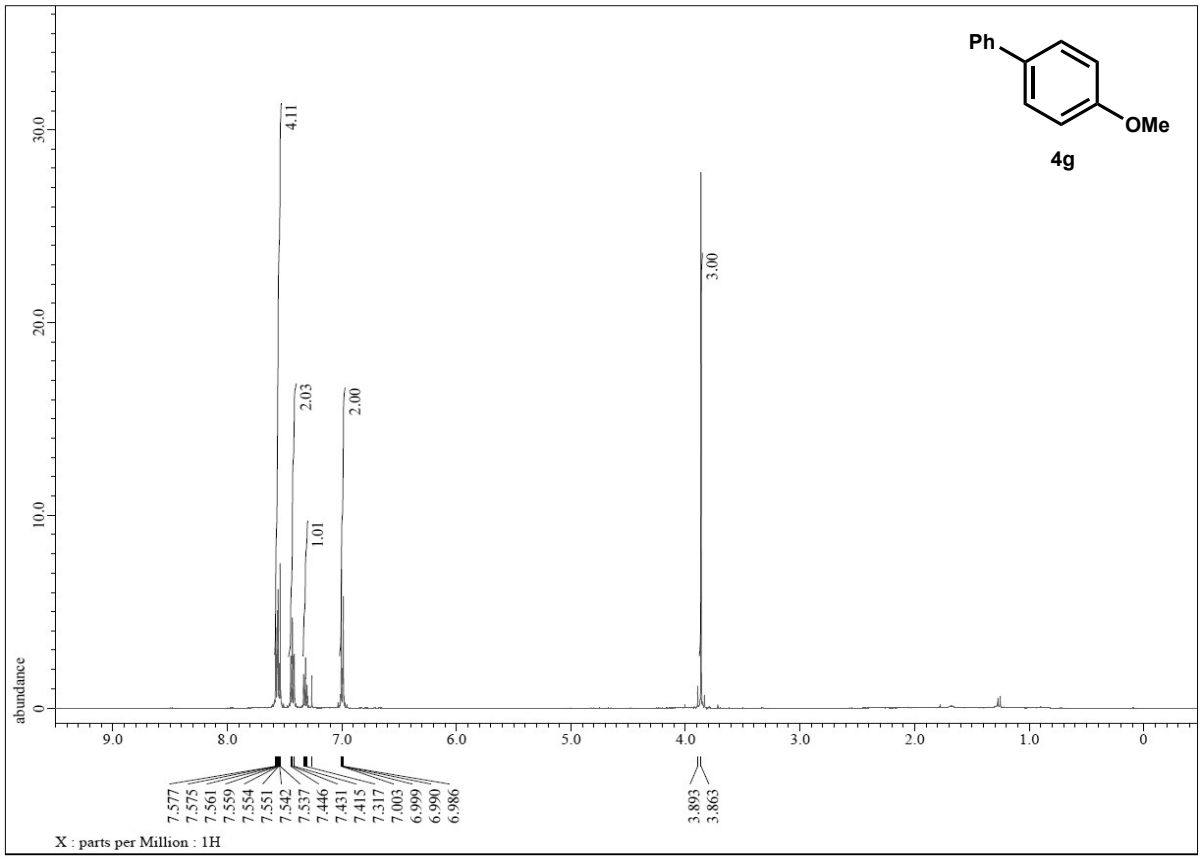

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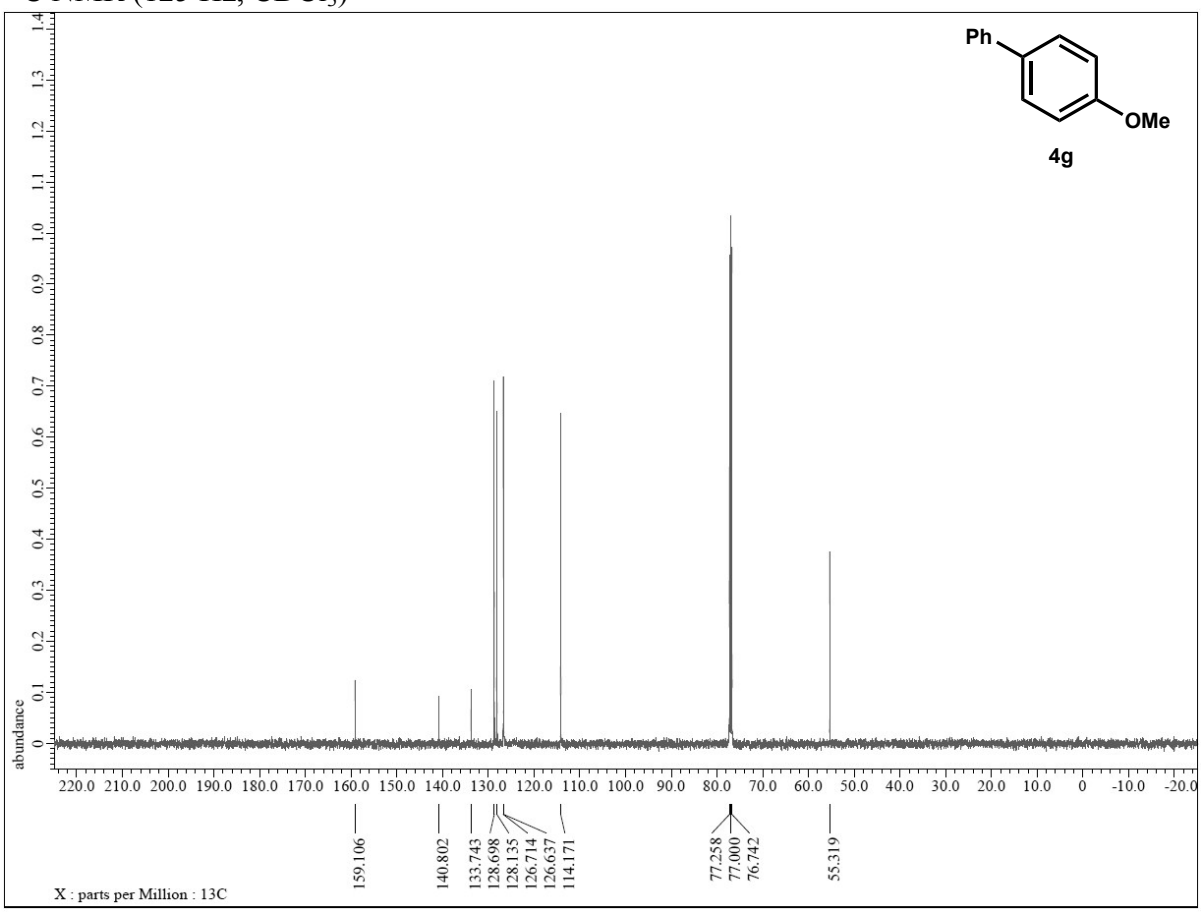

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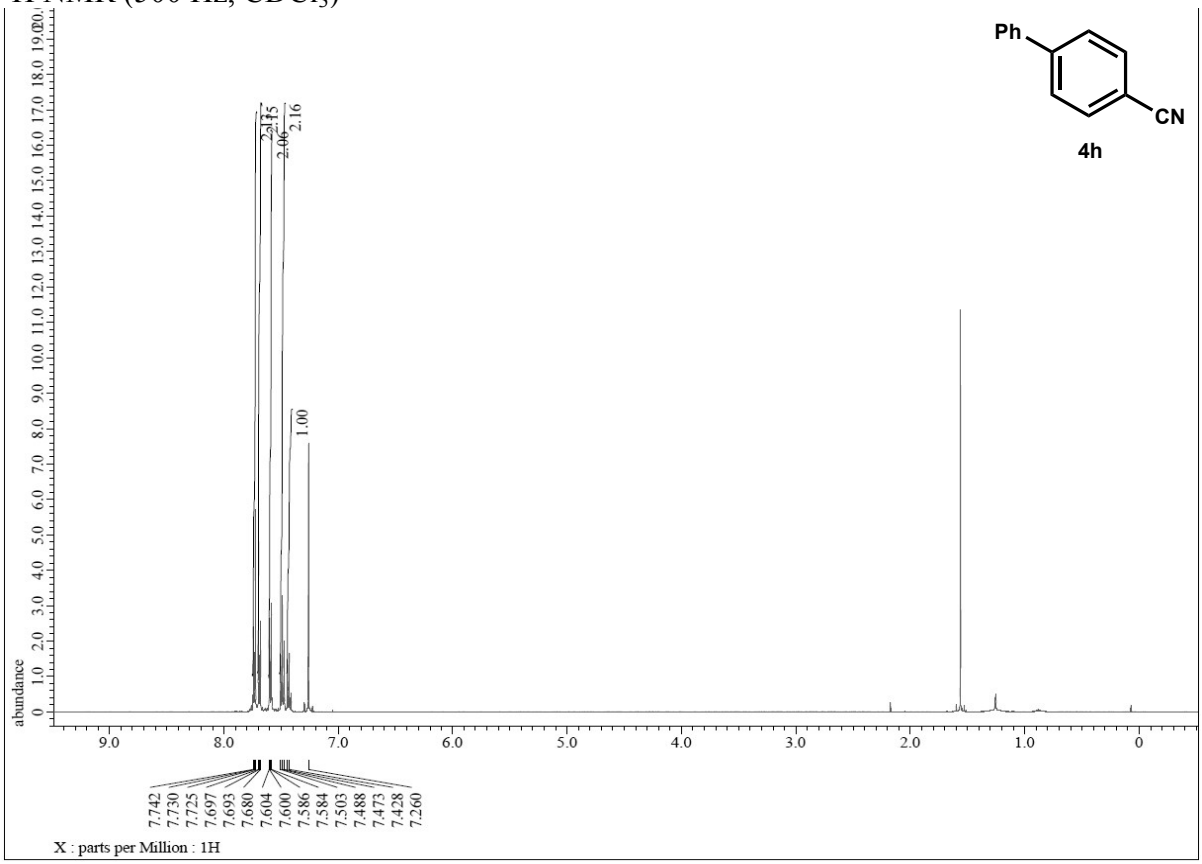

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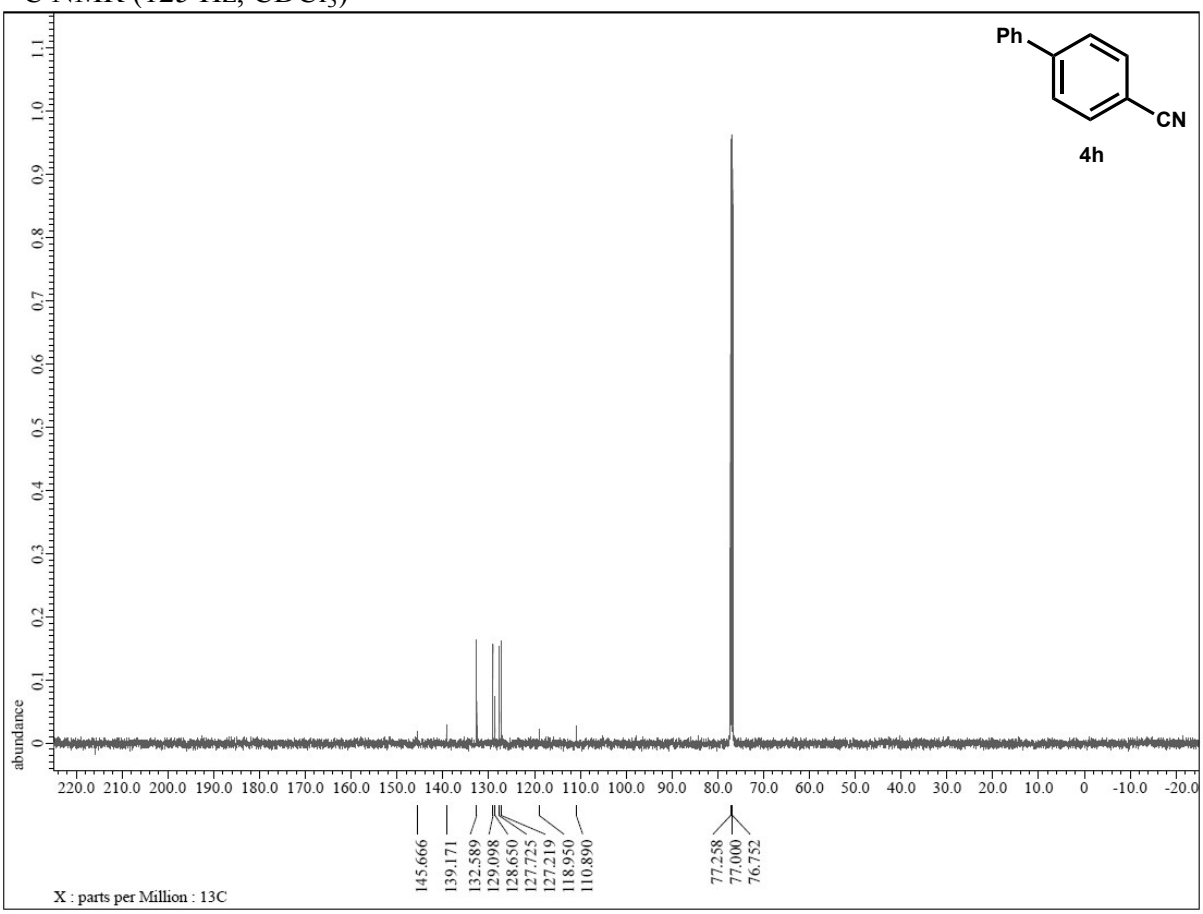

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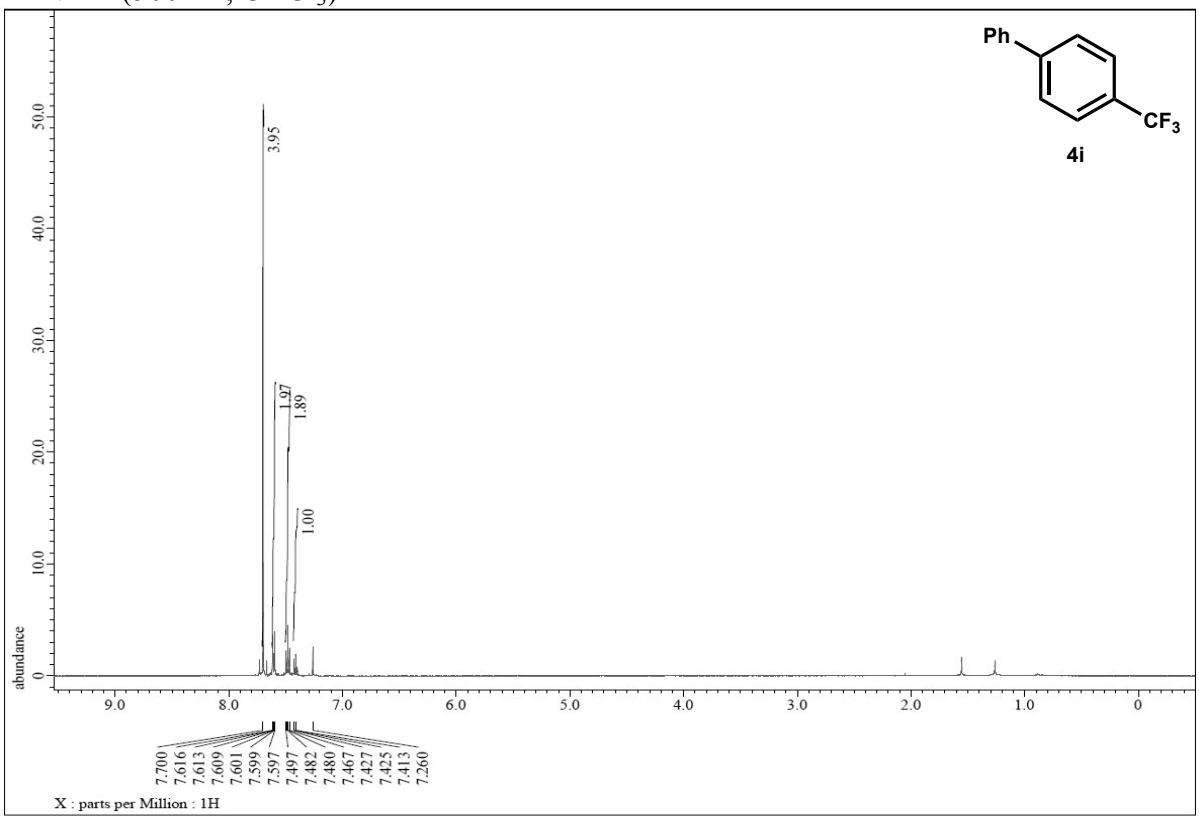

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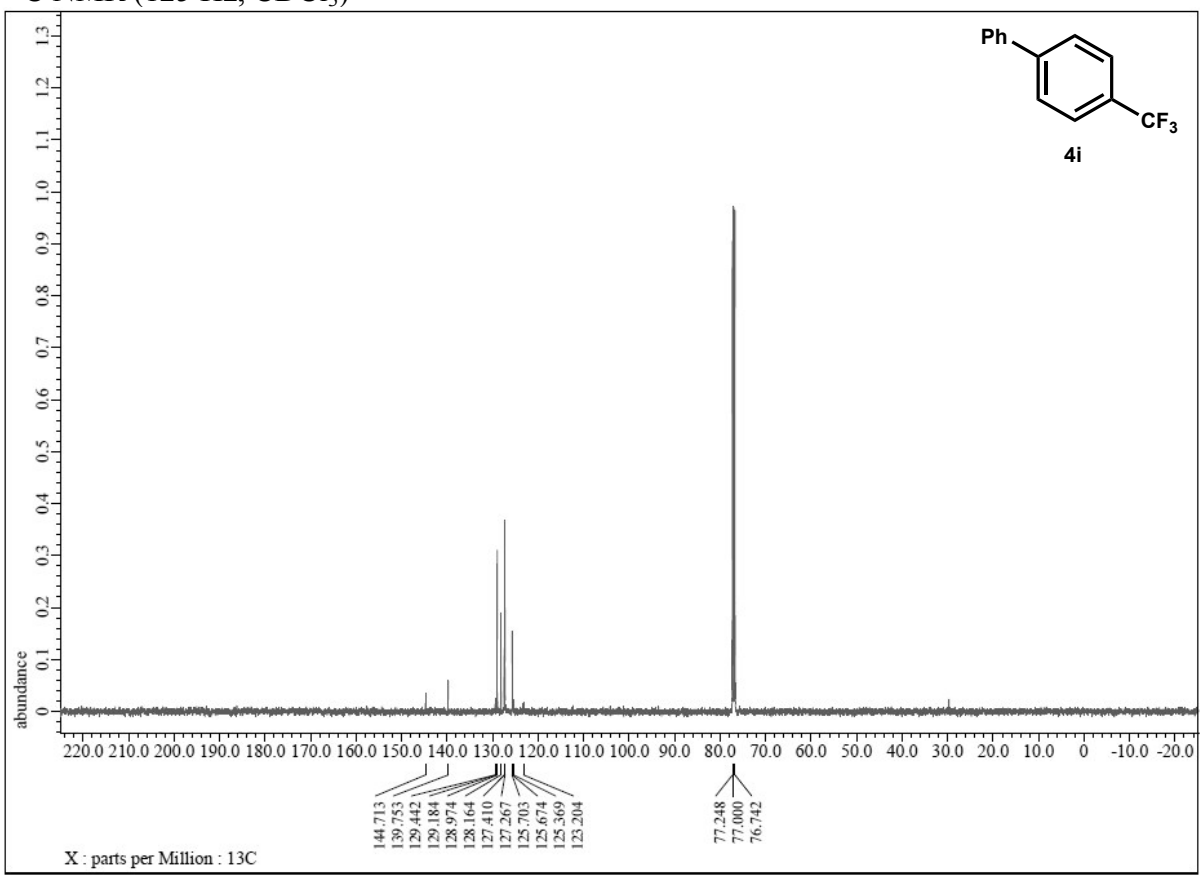

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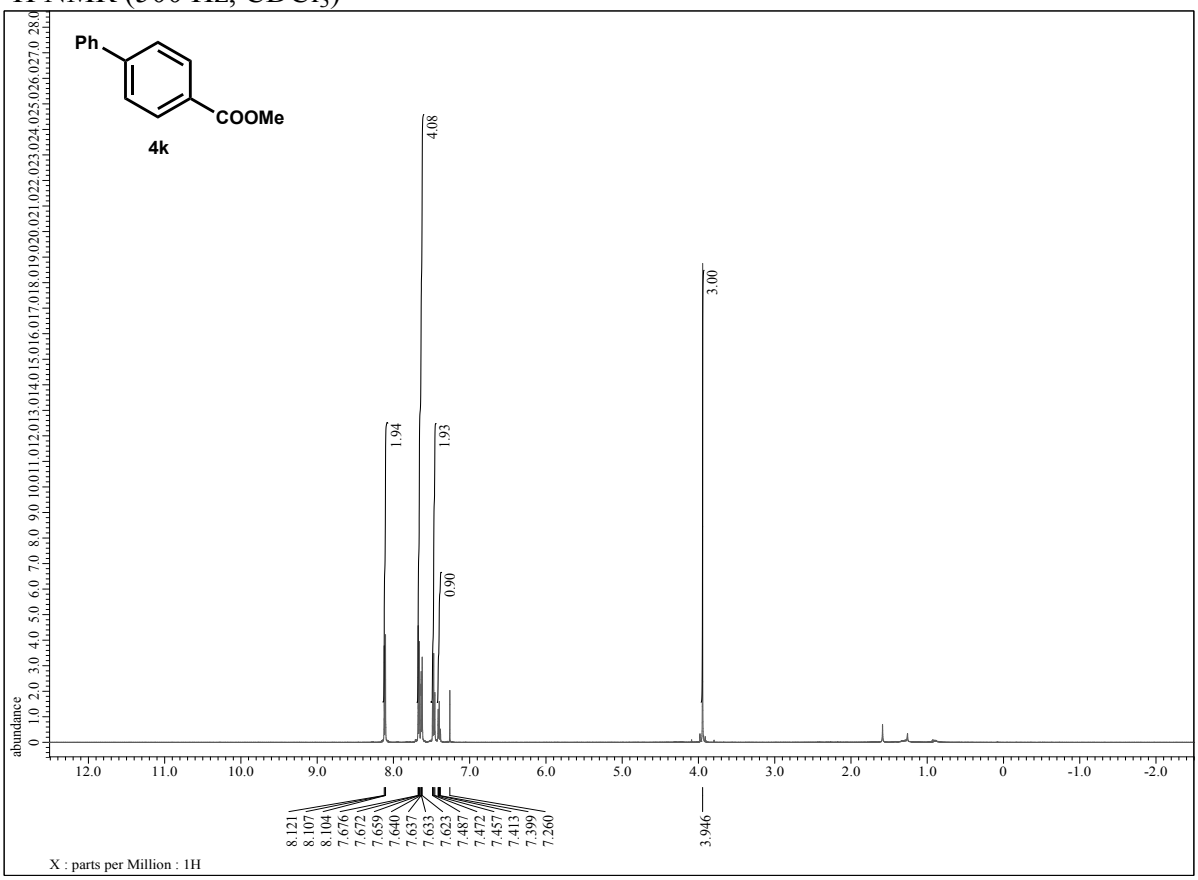

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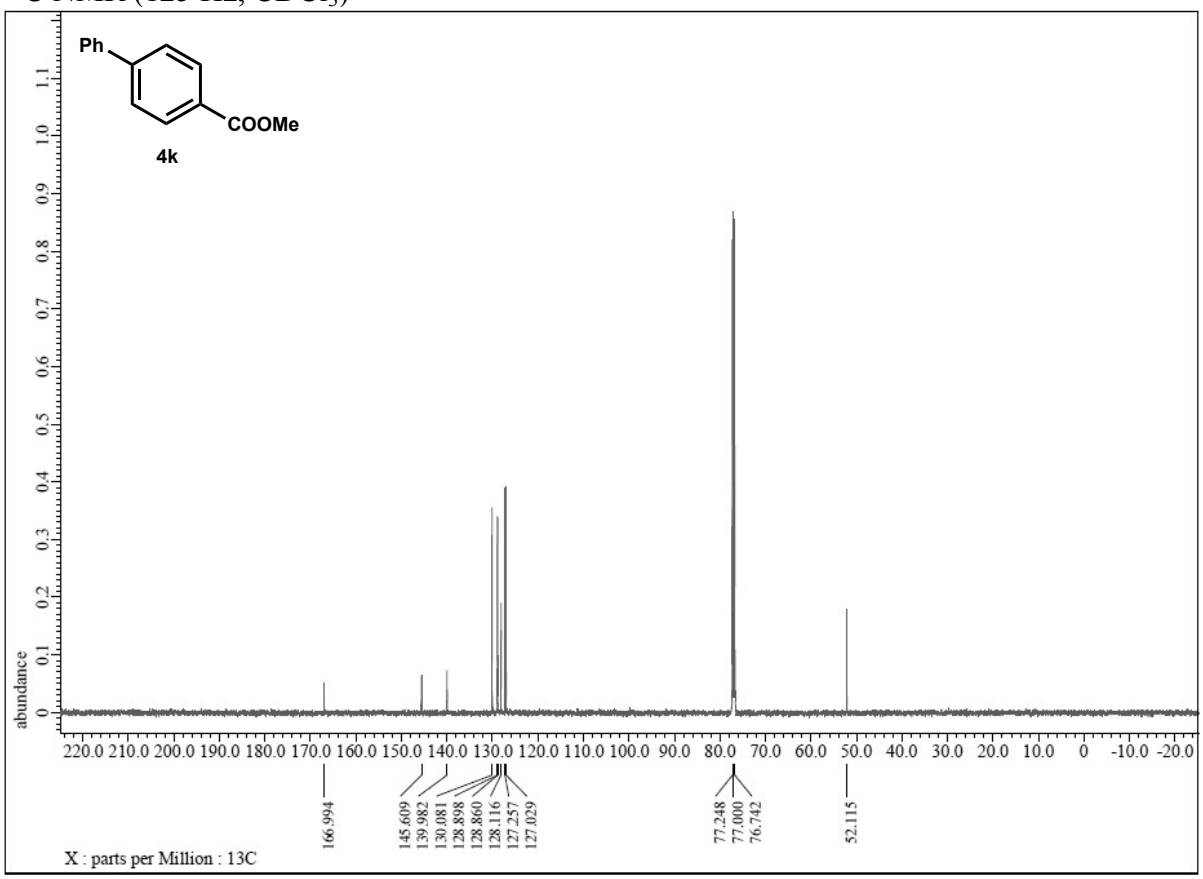

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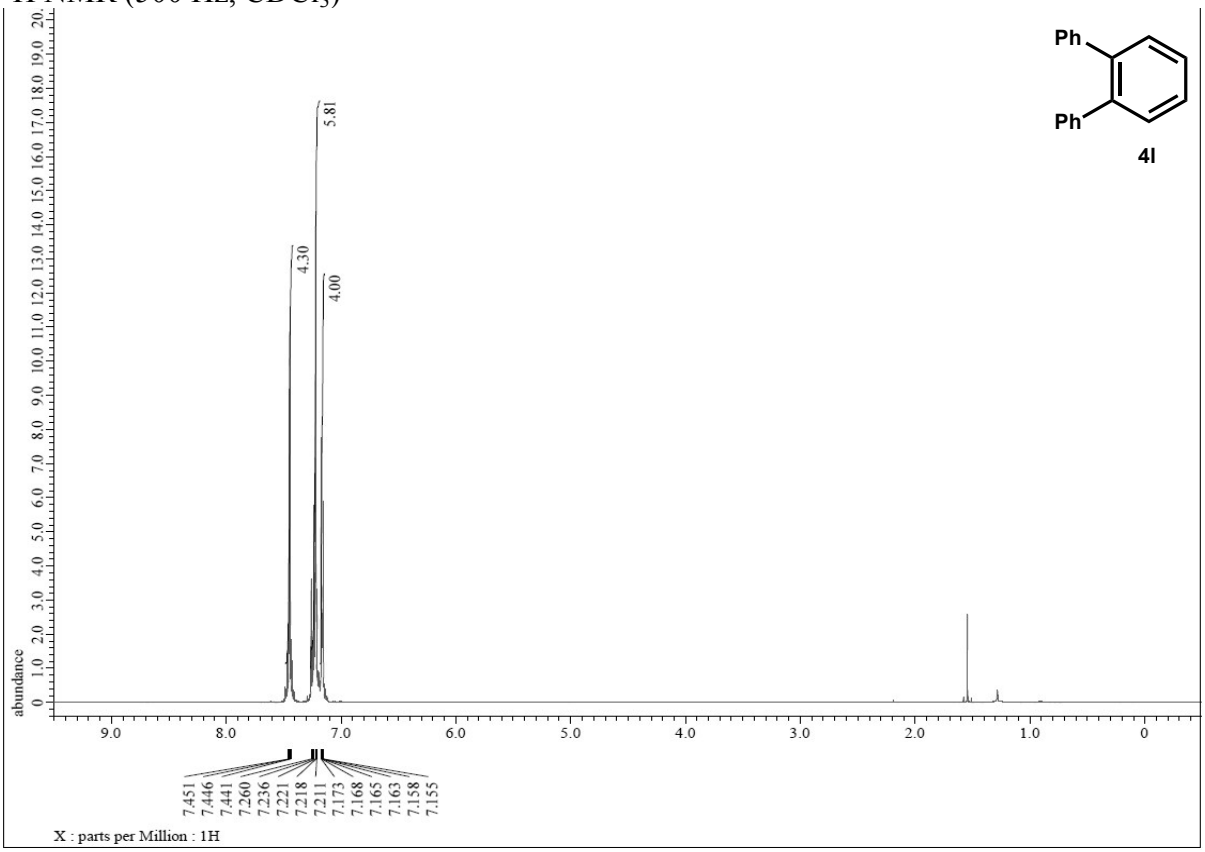

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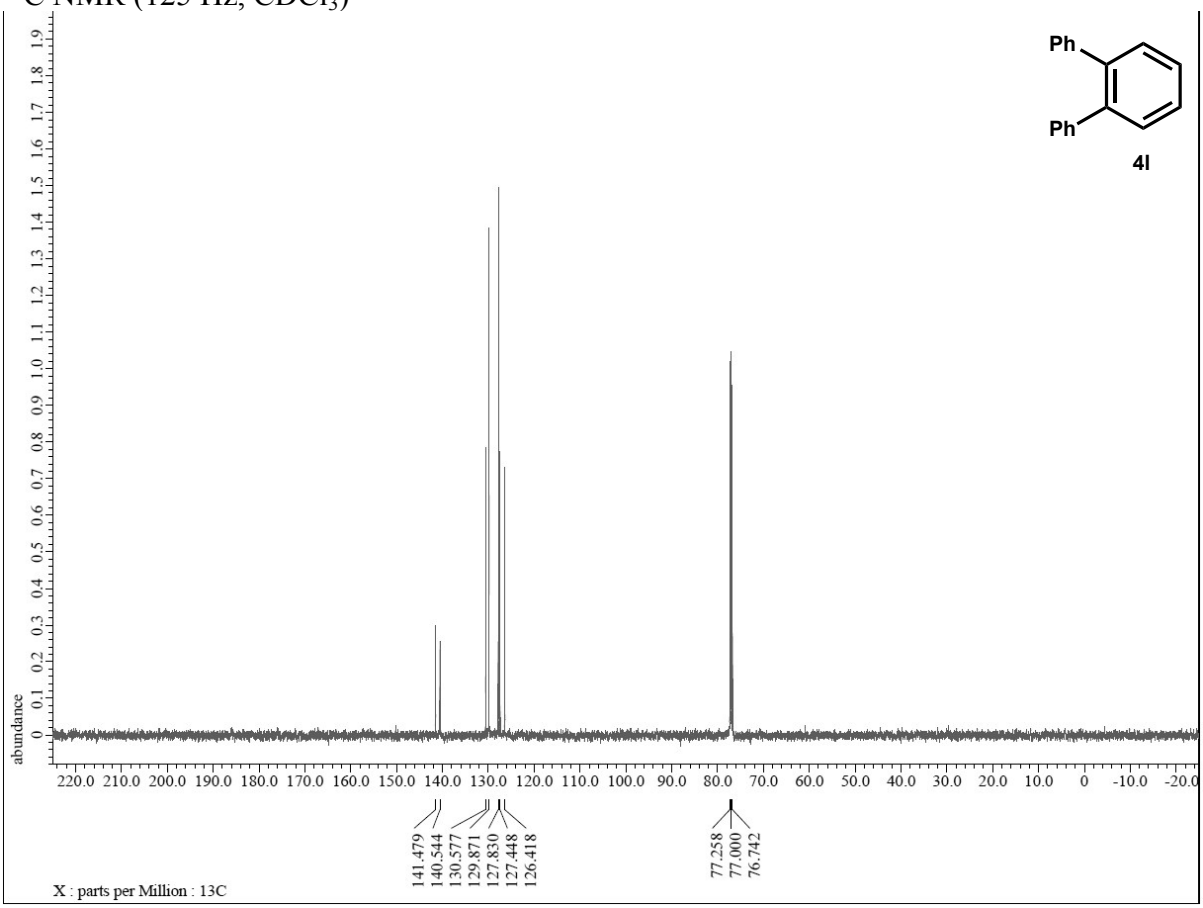

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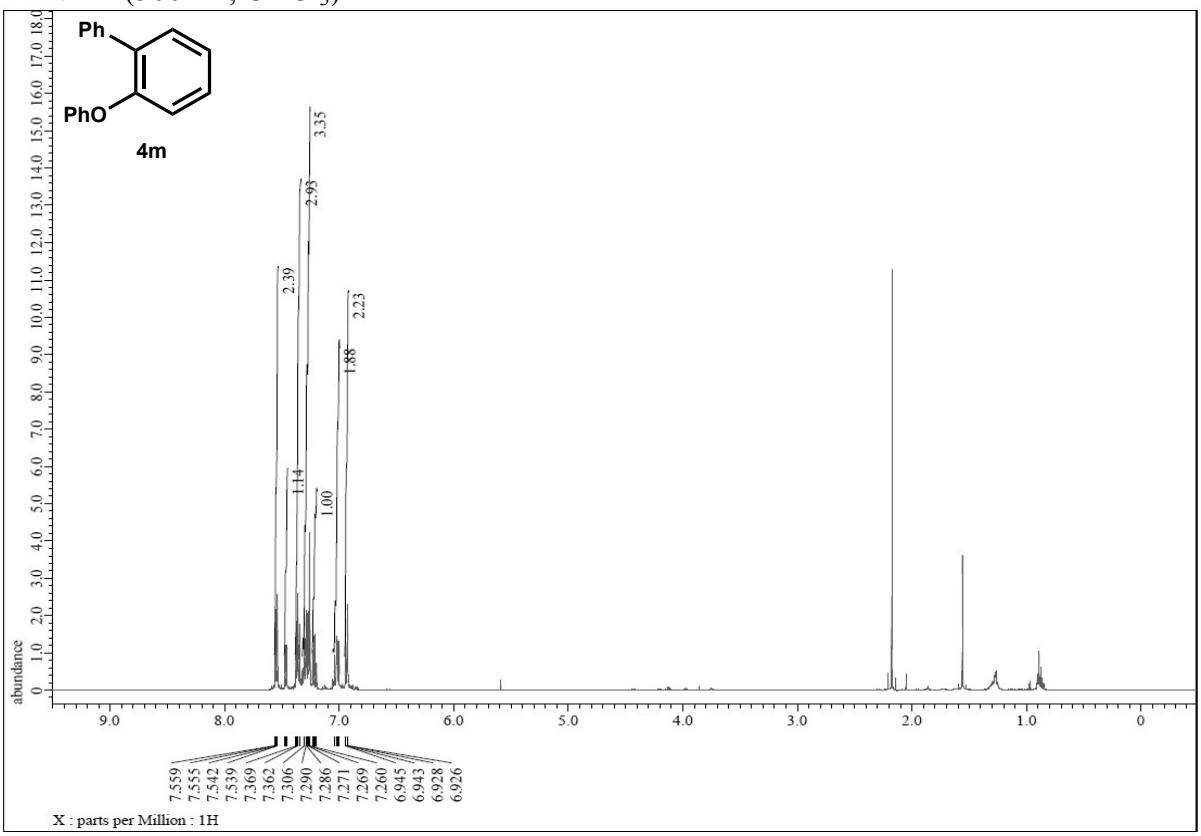

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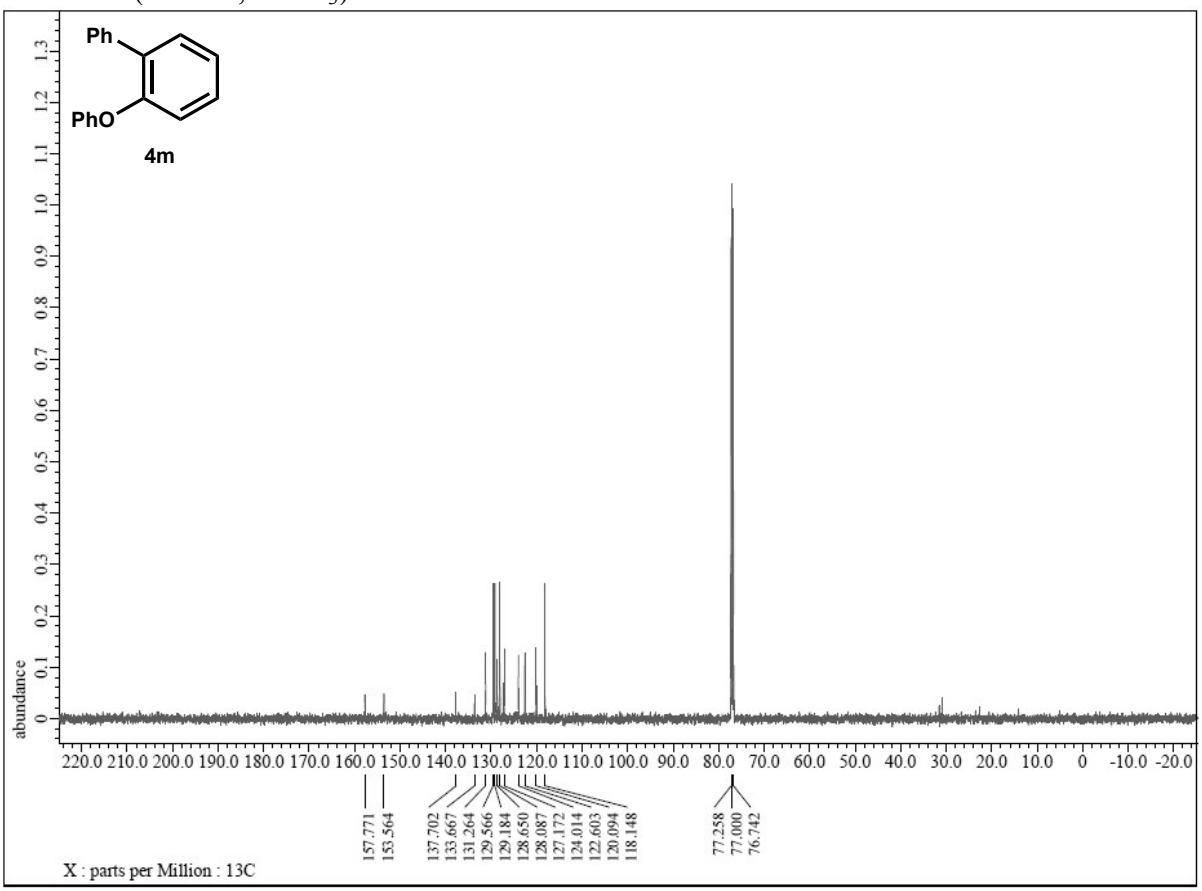

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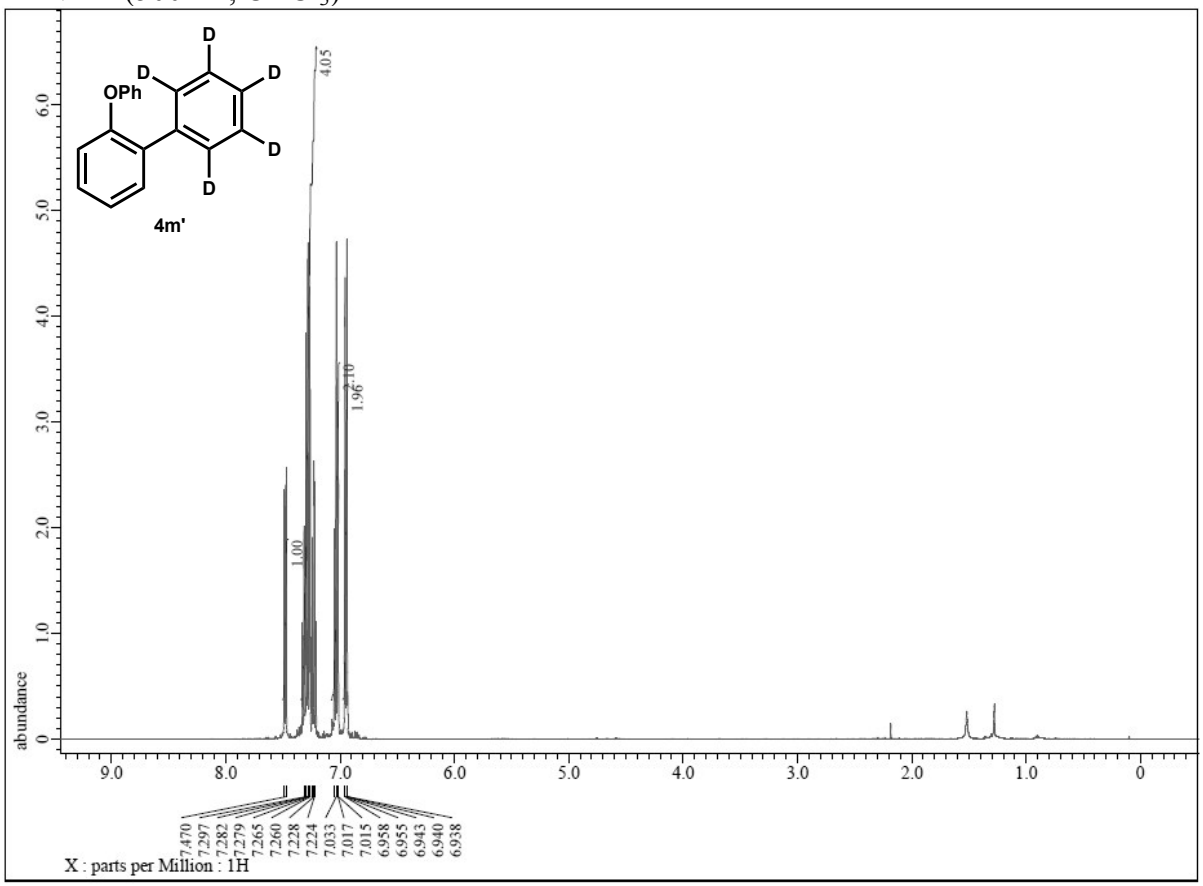

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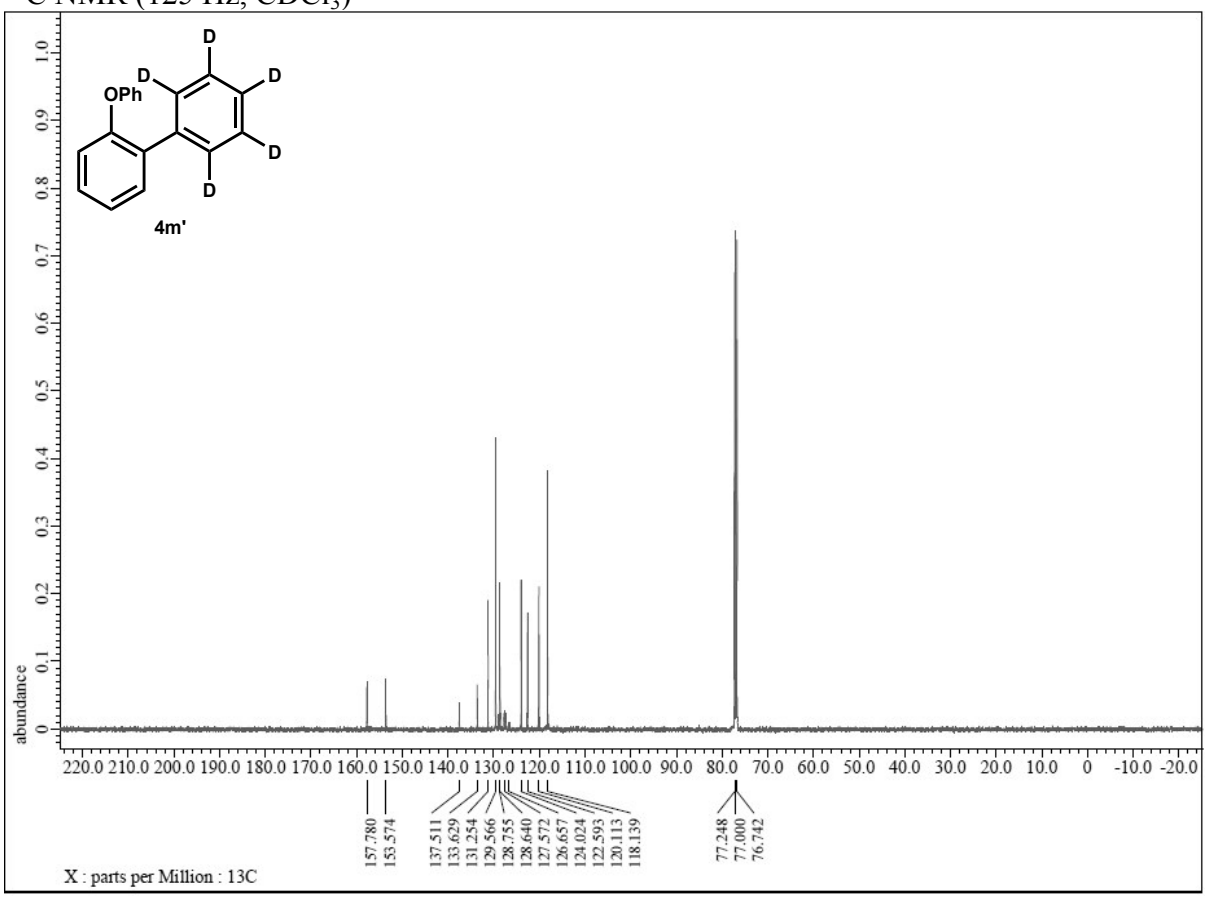

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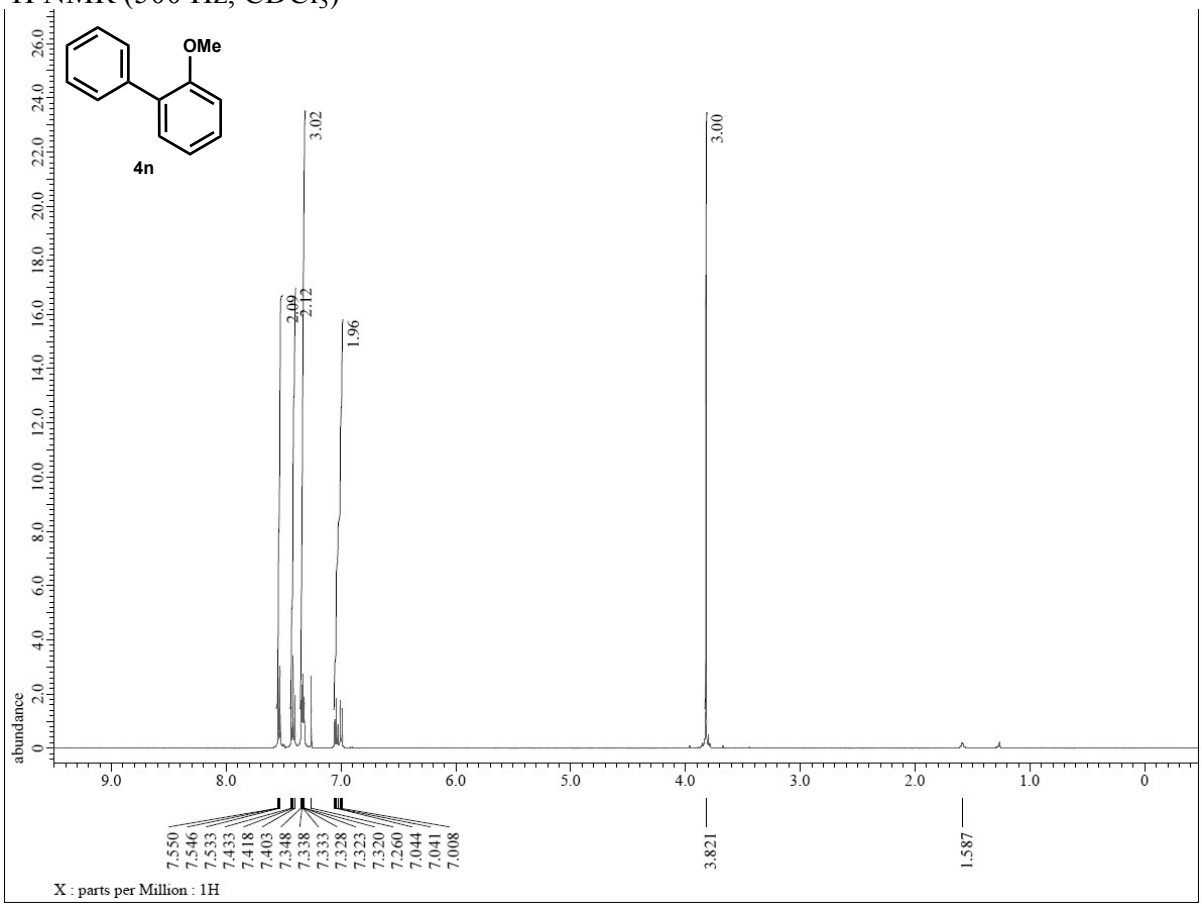

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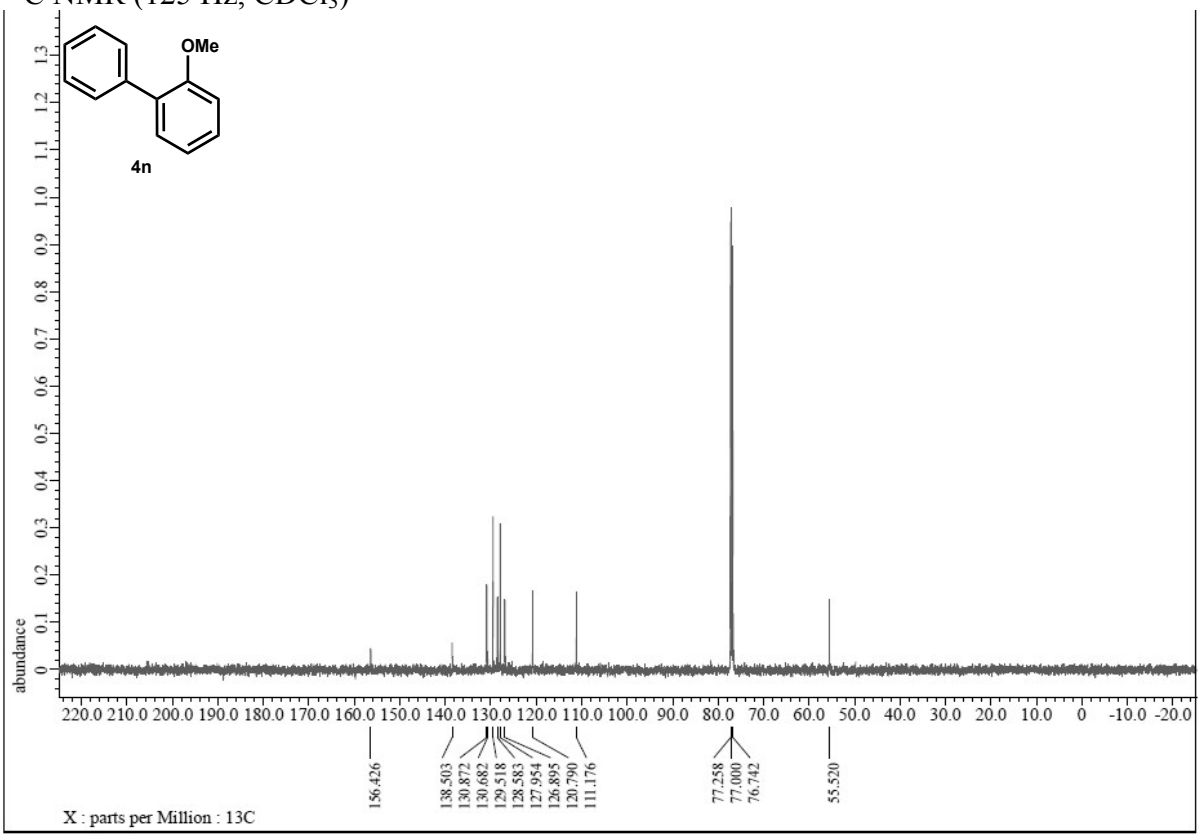
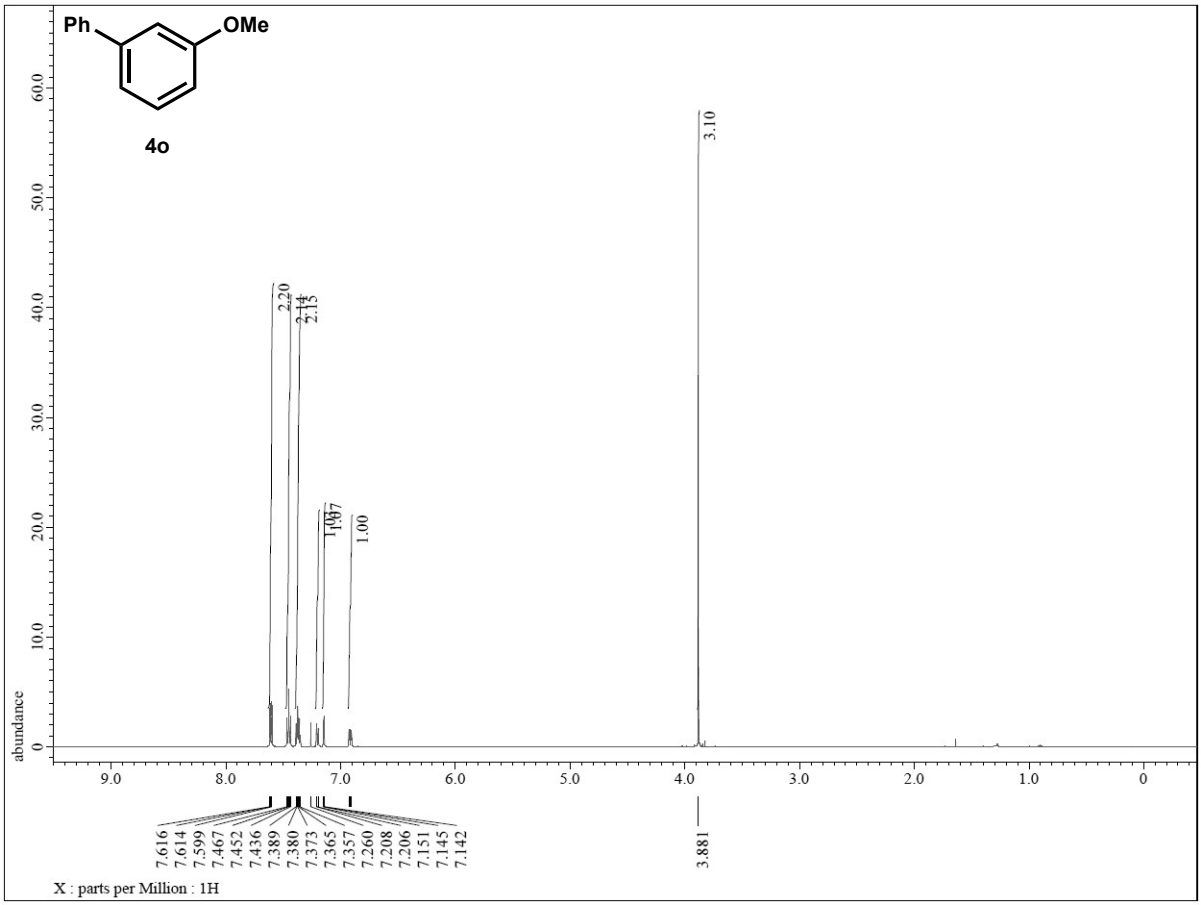
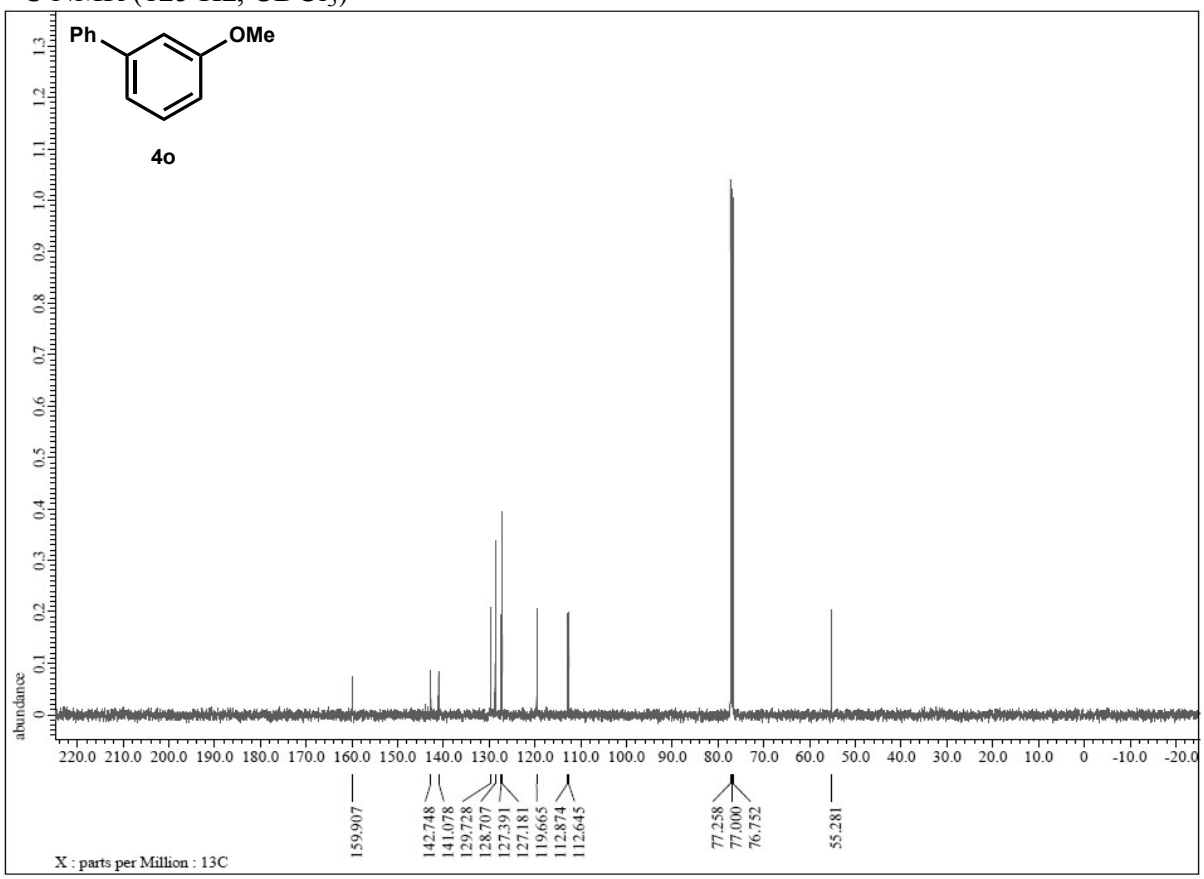


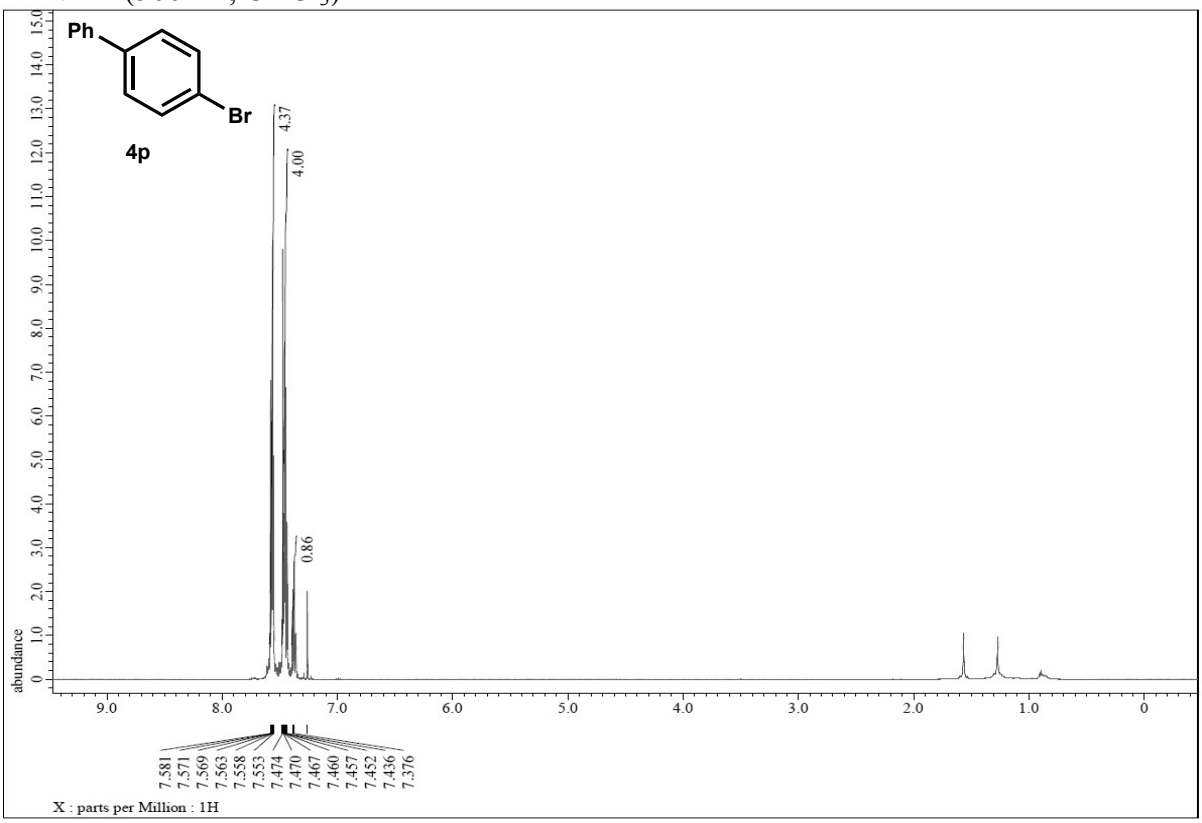
^{1}H NMR (500 Hz, $CDCl_3$)



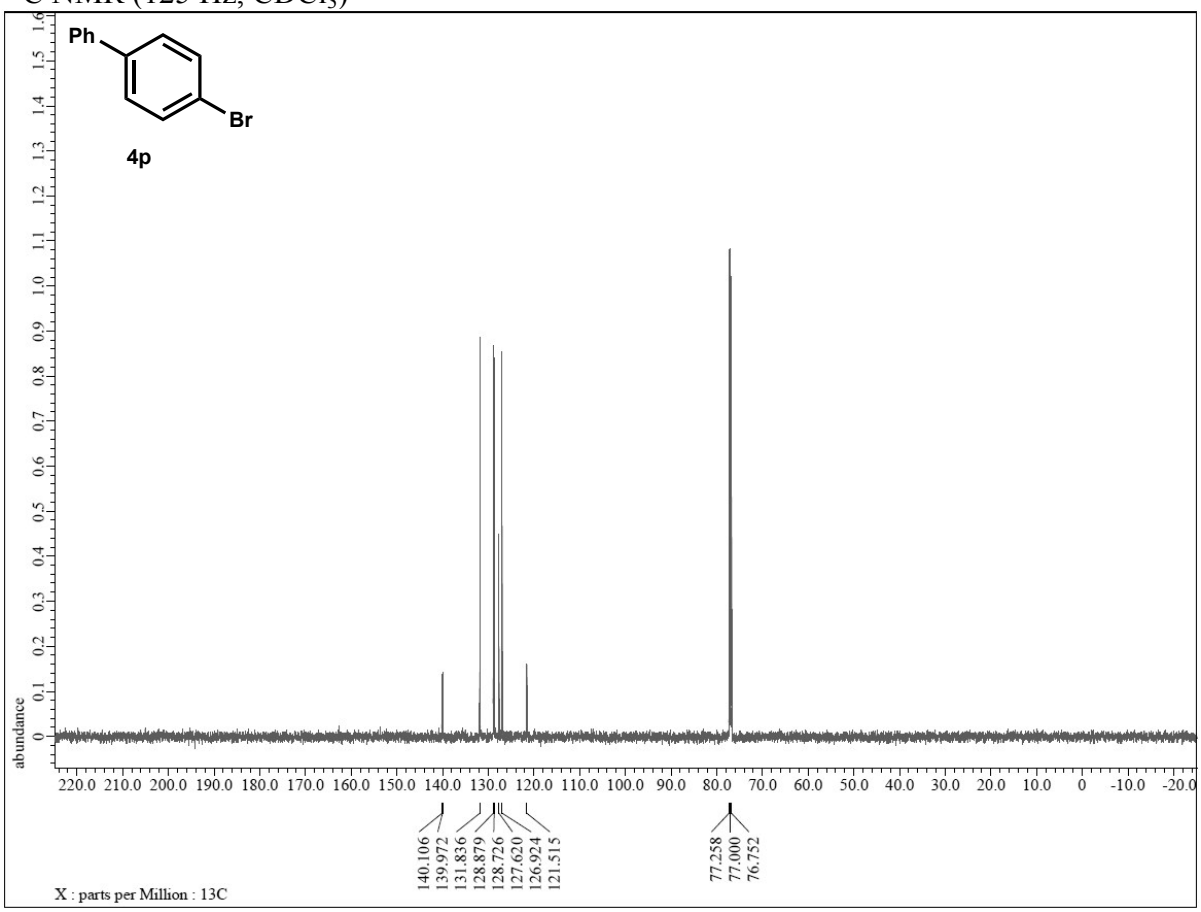
^{13}C NMR (125 Hz, $CDCl_3$)



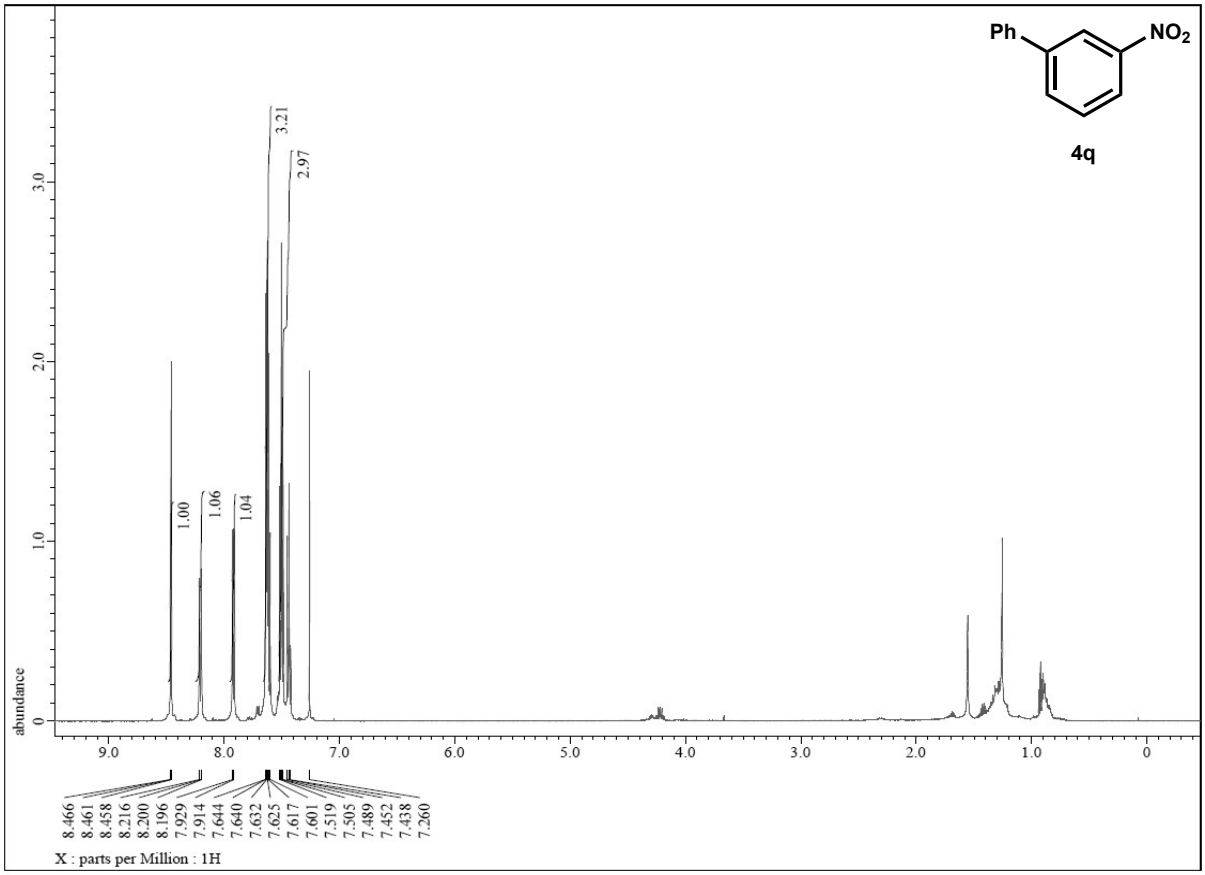
^{1}H NMR (500 Hz, $CDCl_3$)



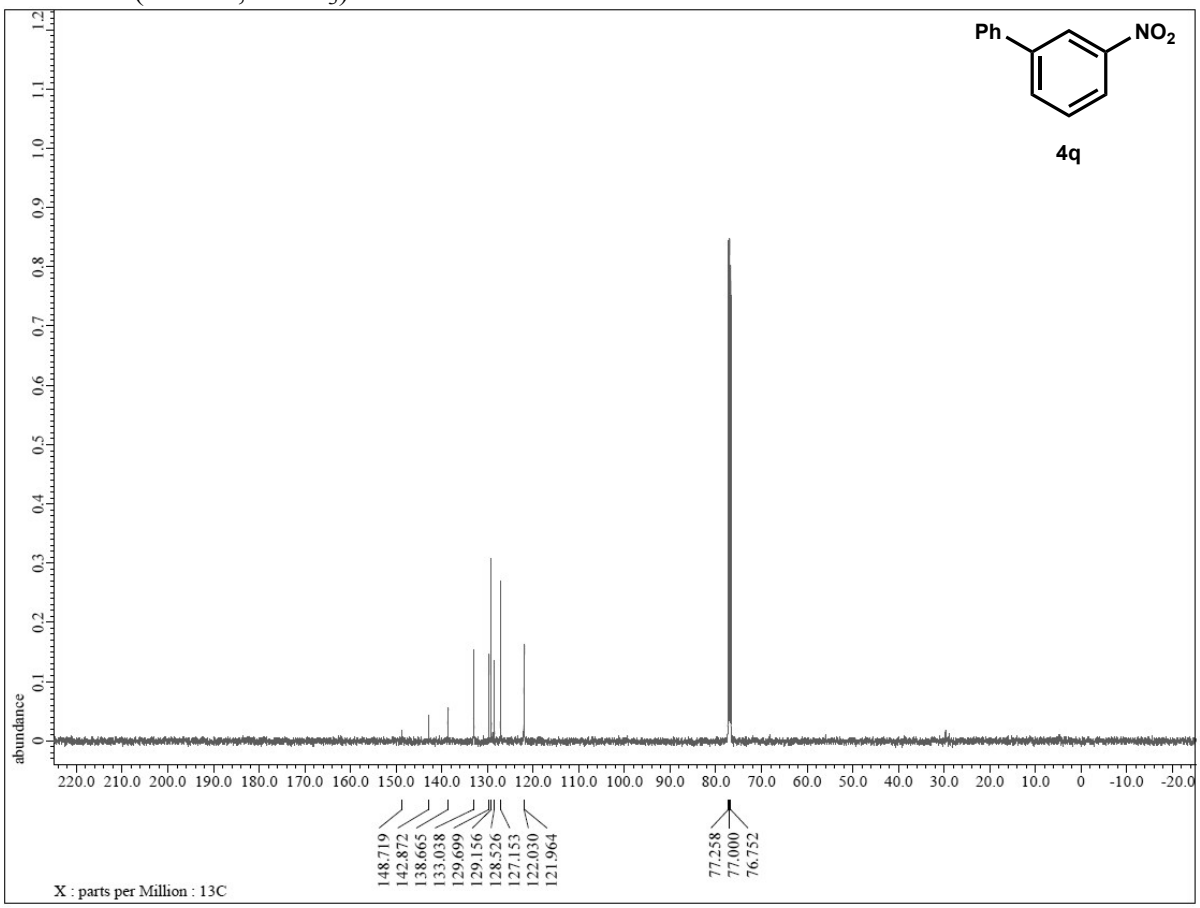
^{13}C NMR (125 Hz, $CDCl_3$)



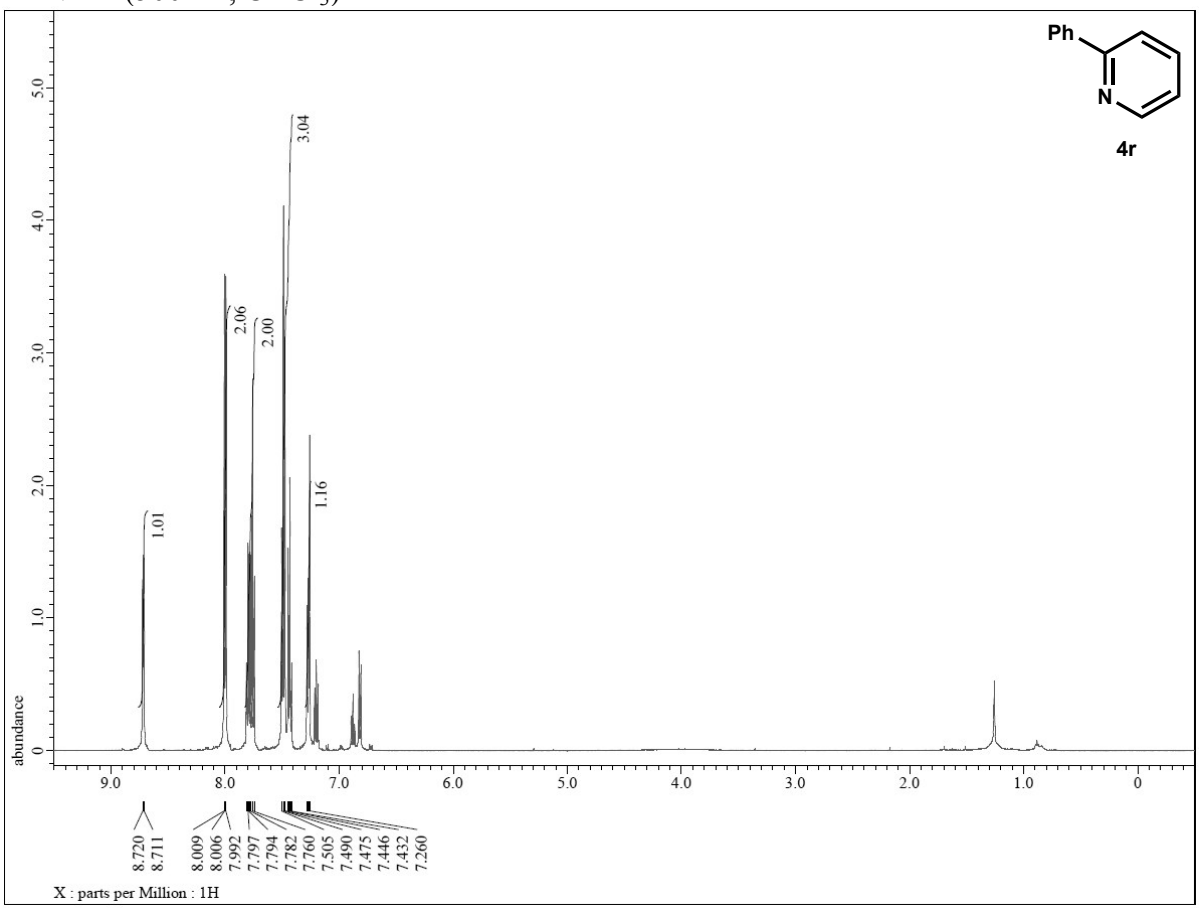
^{1}H NMR (500 Hz, $CDCl_3$)



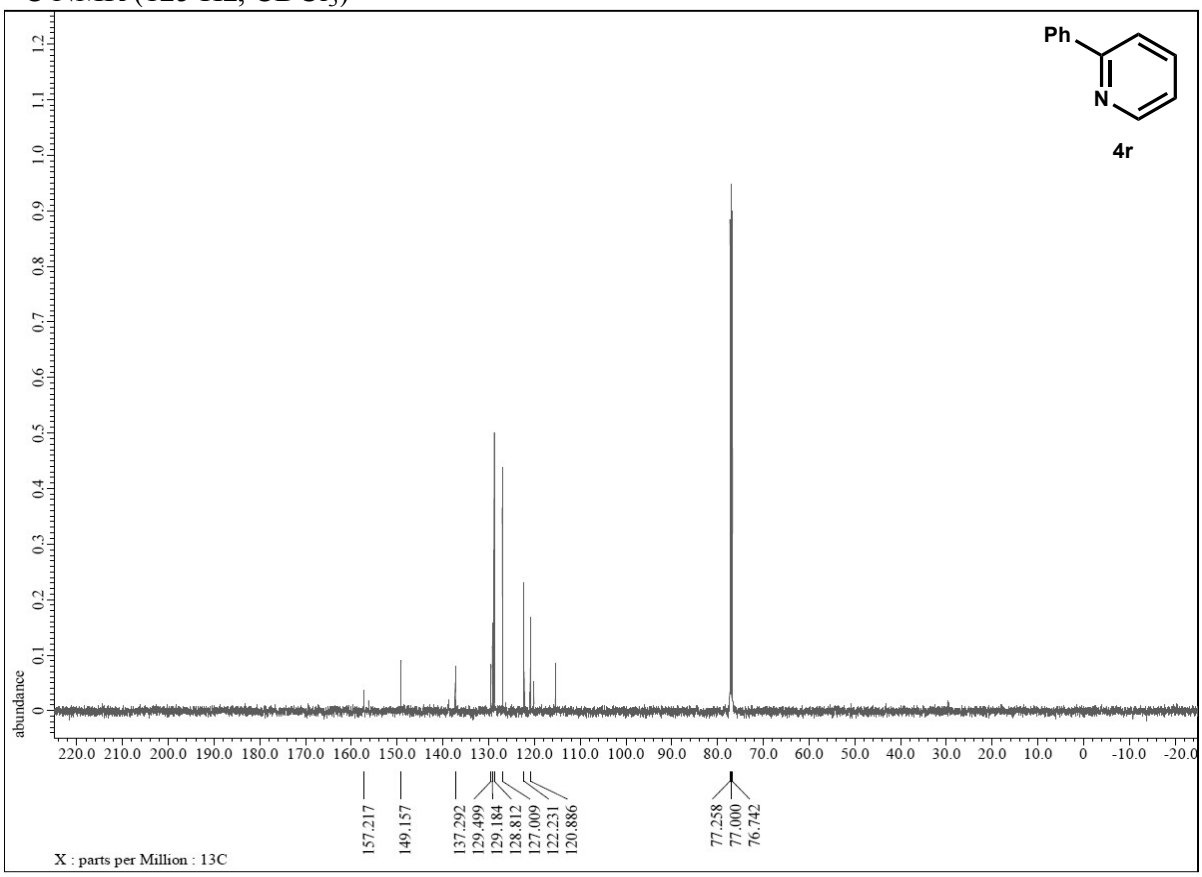
^{13}C NMR (125 Hz, $CDCl_3$)



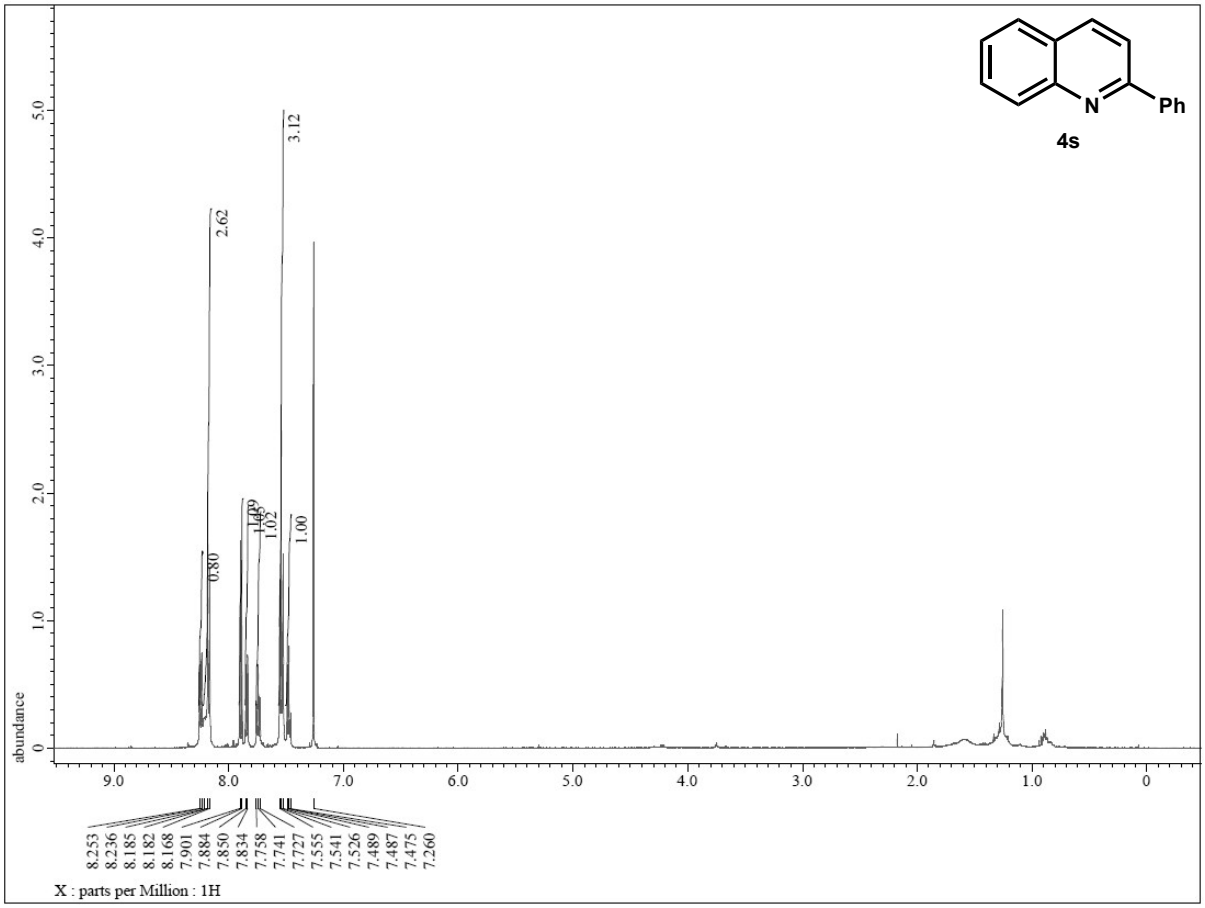
^{1}H NMR (500 Hz, $CDCl_3$)



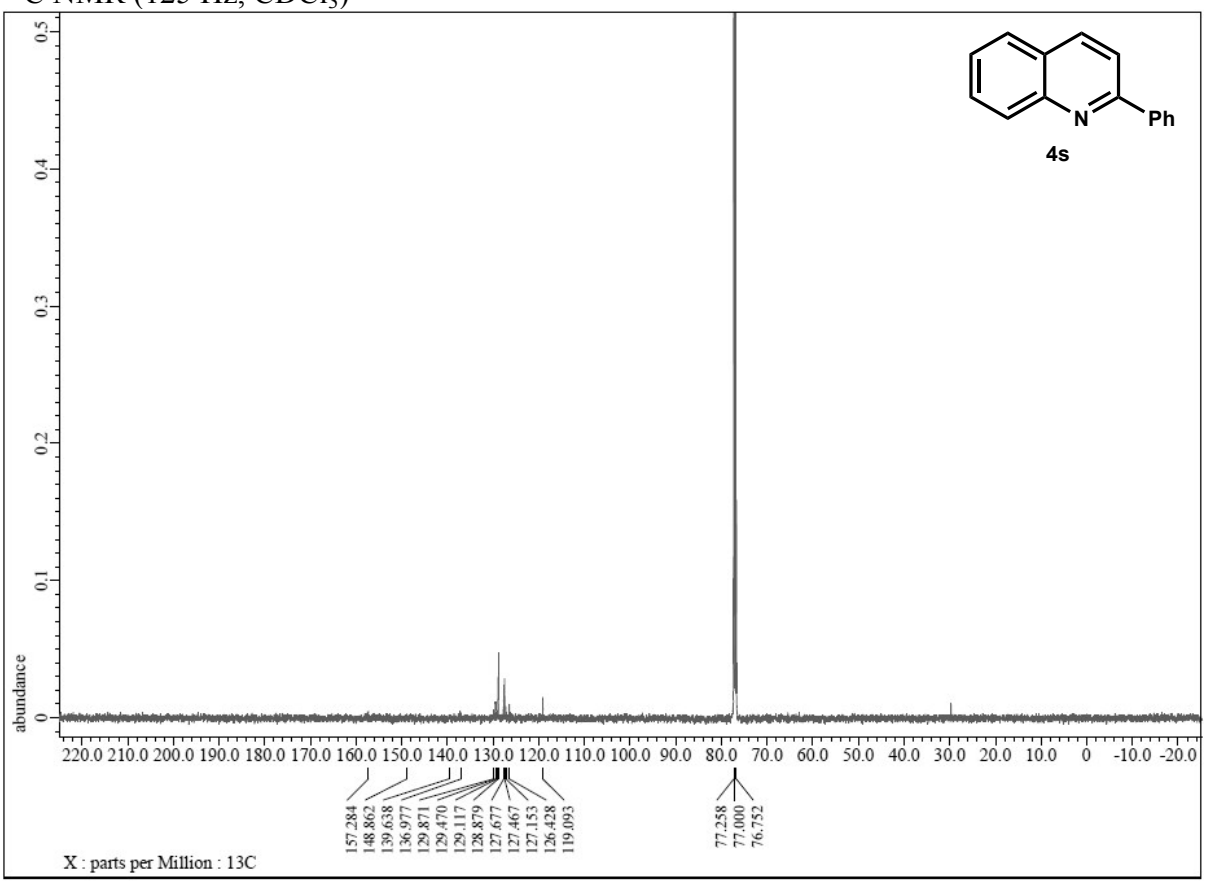
^{13}C NMR (125 Hz, $CDCl_3$)



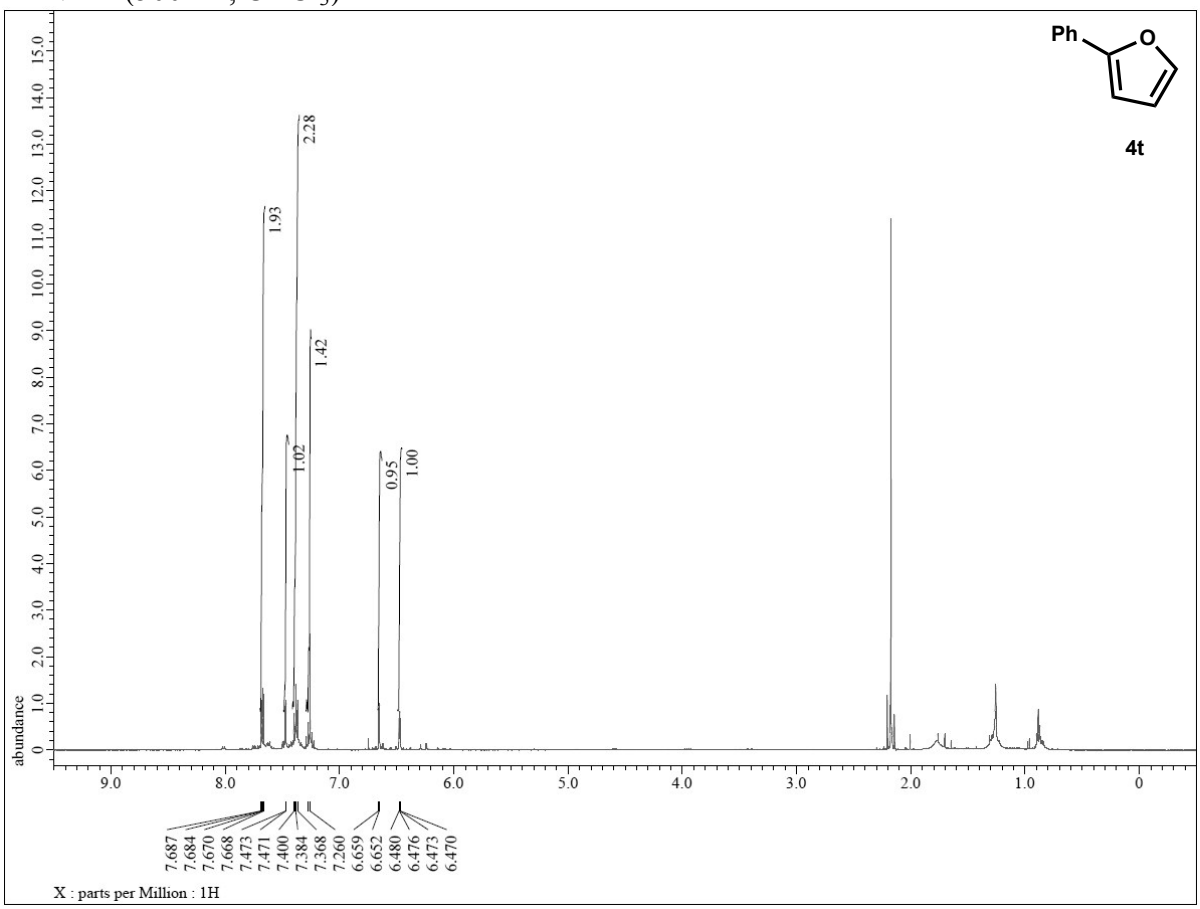
^{1}H NMR (500 Hz, $CDCl_3$)



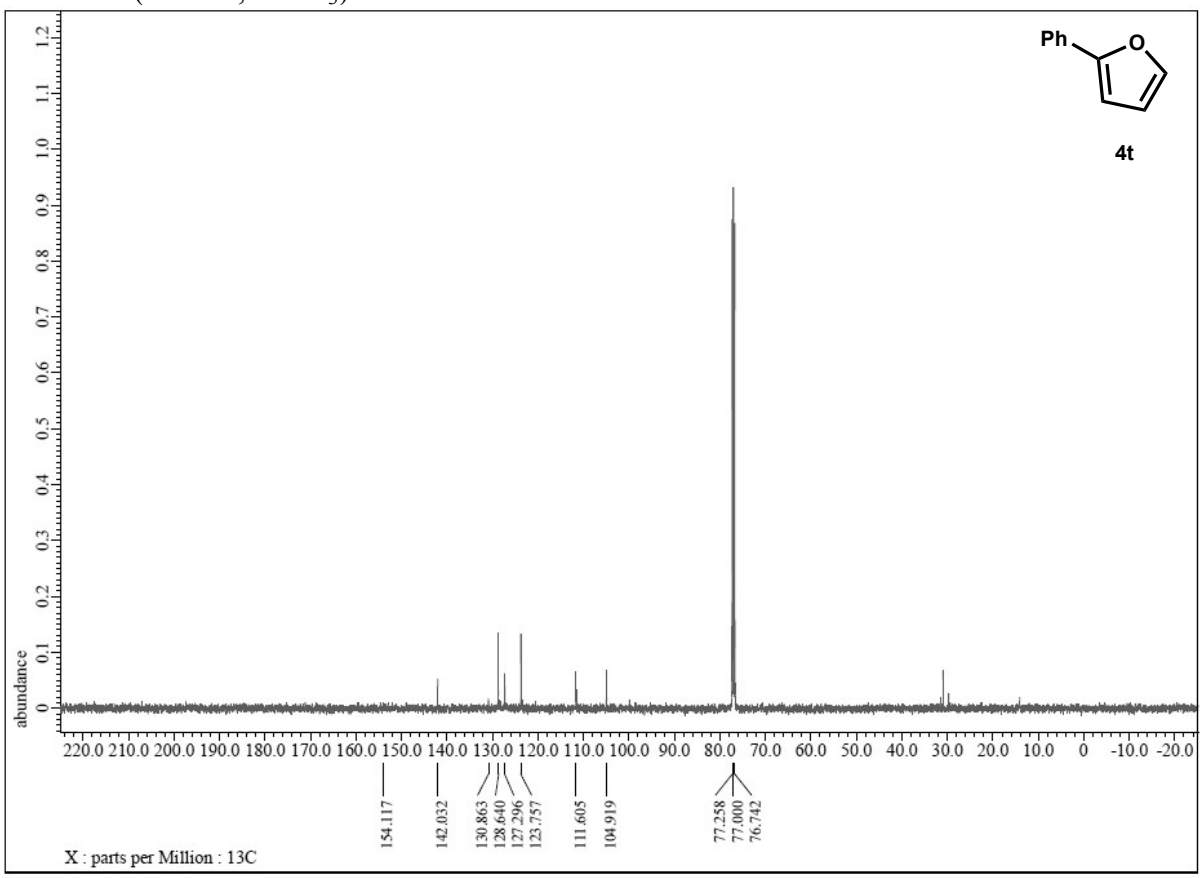
^{13}C NMR (125 Hz, $CDCl_3$)



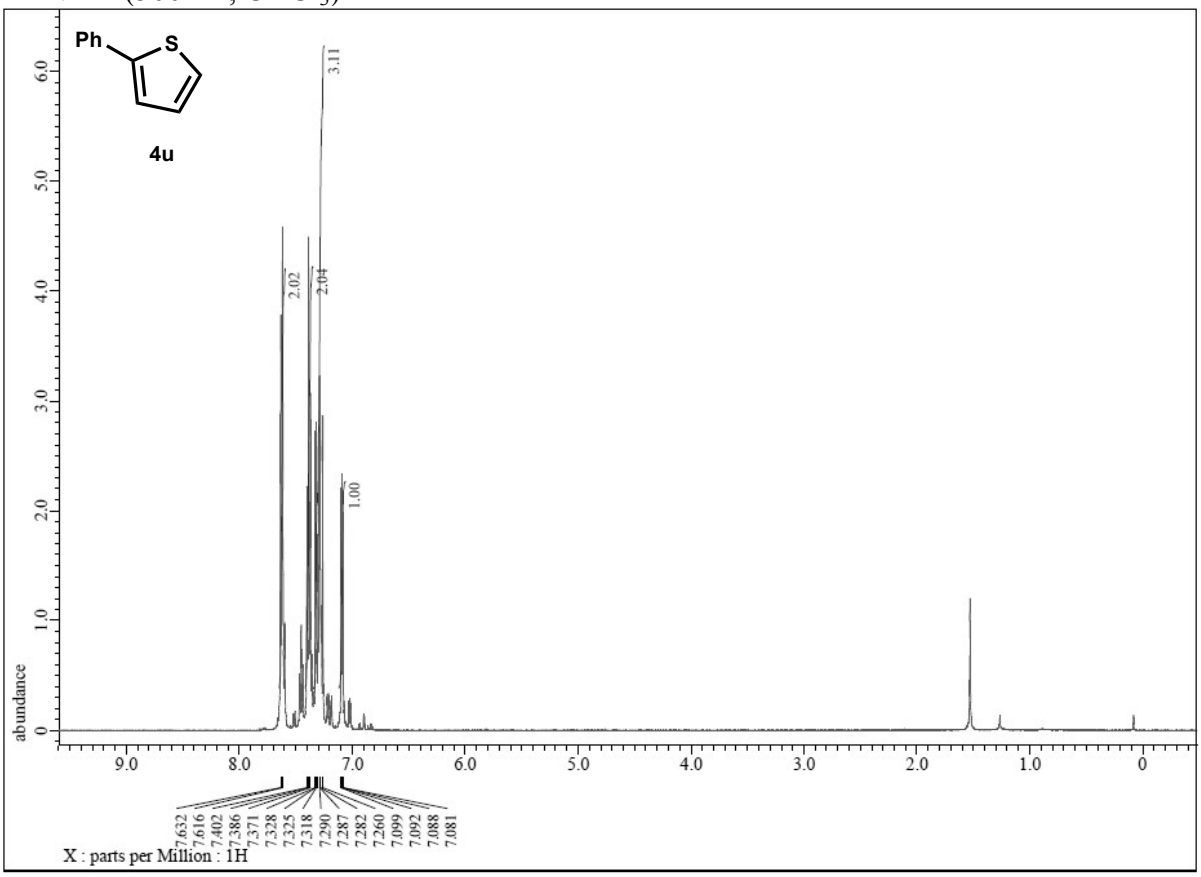
^{1}H NMR (500 Hz, $CDCl_3$)



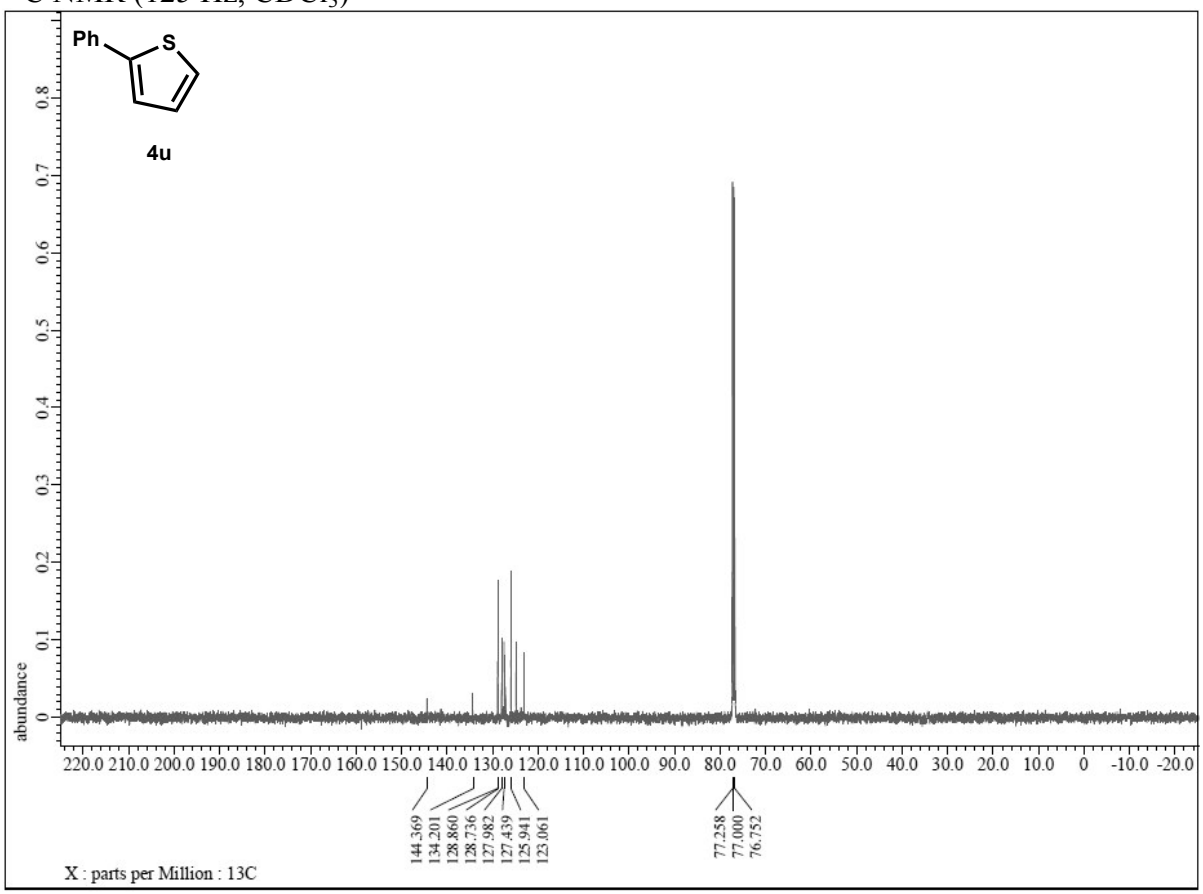
^{13}C NMR (125 Hz, $CDCl_3$)



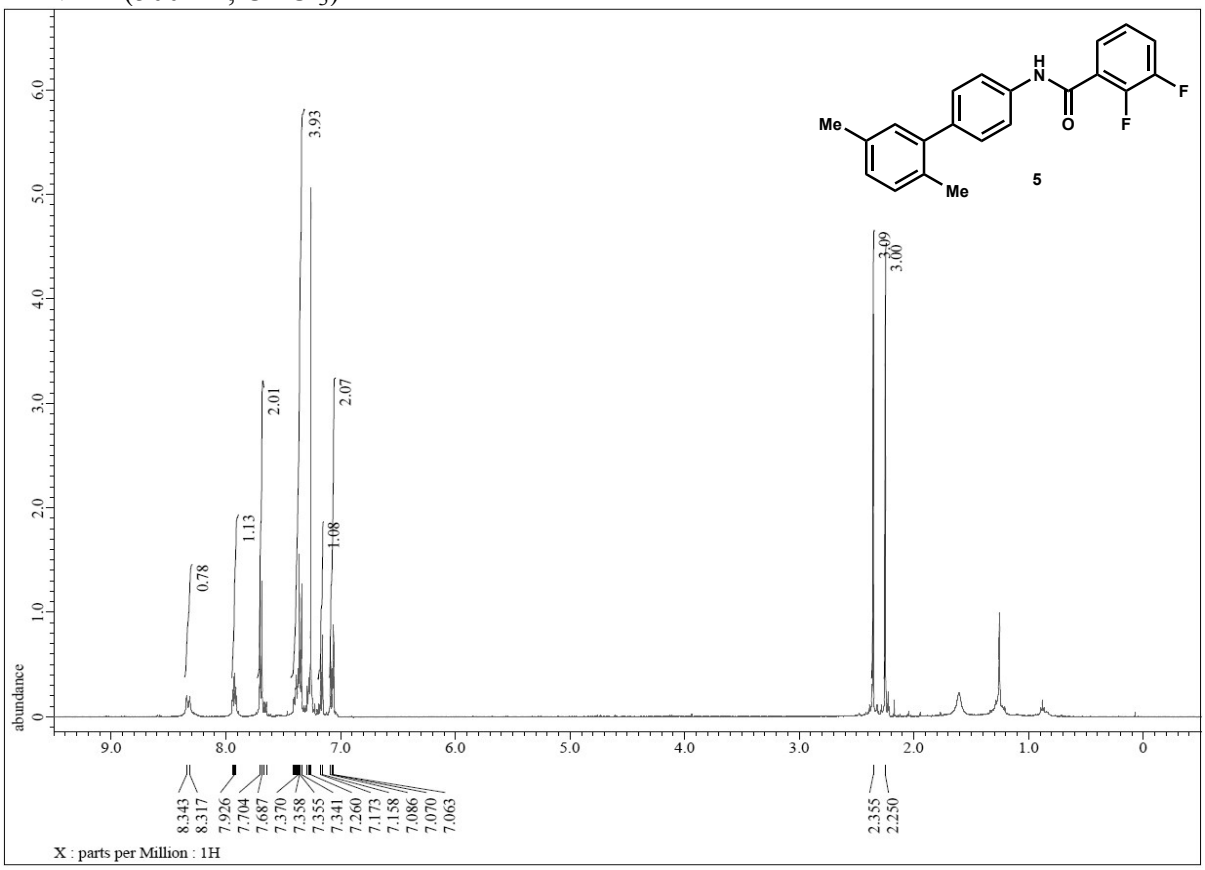
^{1}H NMR (500 Hz, $CDCl_3$)



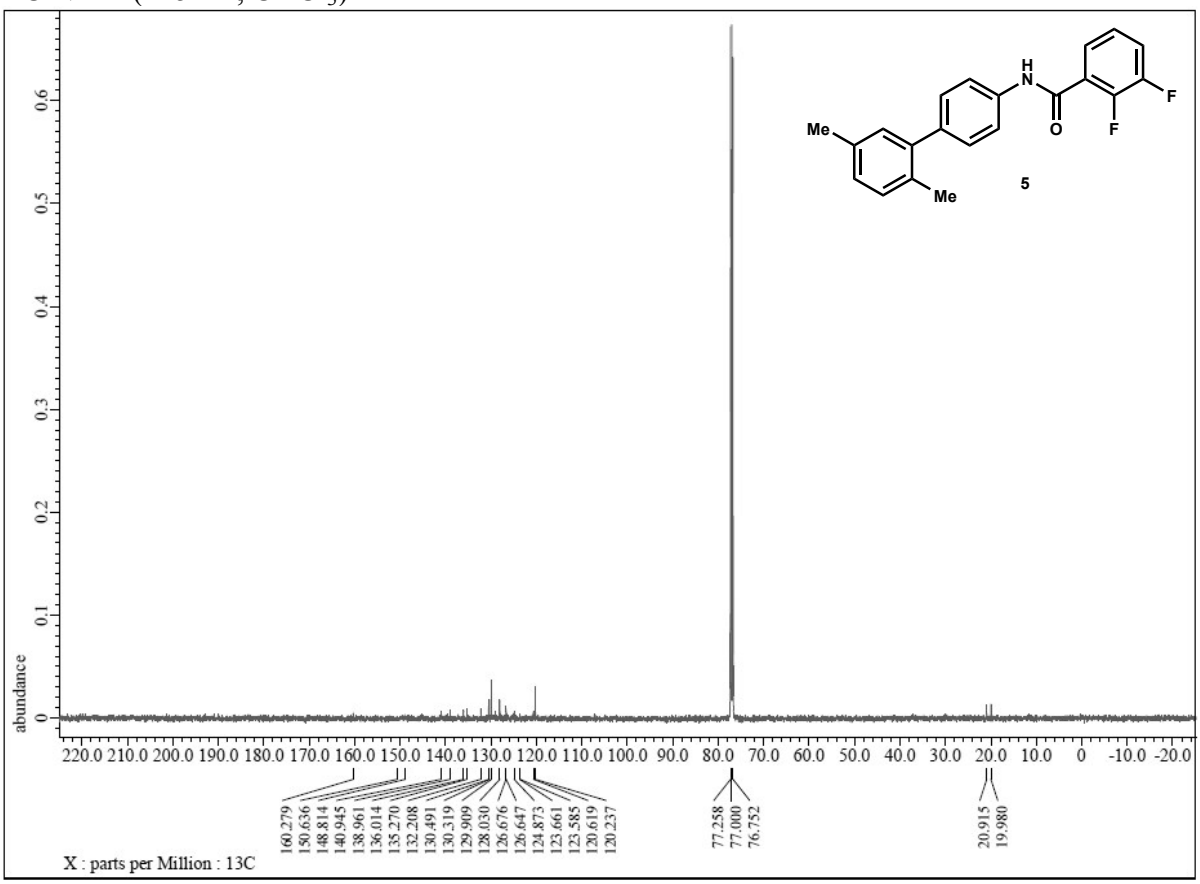
^{13}C NMR (125 Hz, $CDCl_3$)



^{1}H NMR (500 Hz, $CDCl_3$)



^{13}C NMR (125 Hz, $CDCl_3$)



XYZ Coordinates

Diazonium salt N	0.00000	0.00000	0.00000
N	0.00000	0.00000	1.11354
C	0.00089	0.00000	-1.37446
C	-1.16631	0.43312	-2.03514
H	-2.03508	0.75509	-1.47178
C	-1.14307	0.42504	-3.42144
H	-2.01933	0.75009	-3.97190
C	0.00462	-0.00034	-4.10573
H	0.00570	-0.00014	-5.19134
C	1.15052	-0.42579	-3.41865
H	2.02801	-0.75171	-3.96658
C	1.16981	-0.43315	-2.03229
H	2.03670	-0.75543	-1.46613
Aryl cation + Benzene			
C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.39761
H	0.93808	0.00000	1.94740
C	-1.21225	0.00175	2.09069
H	-1.20841	0.00169	3.17672
C	-2.42055	0.00405	1.39141
H	-3.36180	0.00554	1.93311
C	-2.41818	0.00385	-0.00567
H	-3.35551	0.00520	-0.55430
C	-1.21088	0.00151	-0.70438
H	-1.21294	0.00102	-1.79174
C	1.32734	-0.00037	-0.78859
H	2.12765	0.00820	-0.01272
C	1.55243	1.24560	-1.55312
H	1.37694	2.18391	-1.03454
C	1.97918	1.22748	-2.85644
H	2.14616	2.14836	-3.40492
C	2.18807	-0.01532	-3.49188
H	2.51611	-0.02123	-4.52870
C	1.99059	-1.25093	-2.83921
H	2.16617	-2.17775	-3.37487
C	1.56429	-1.25522	-1.53545
H	1.39801	-2.18835	-1.00411
Aryl cation + water			
C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.38090
H	0.92518	0.00000	1.94660
C	-1.11798	0.00035	-0.81392
H	-1.04207	-0.00011	-1.89692
C	-2.35602	0.00240	-0.16489
H	-3.26540	0.00333	-0.75695
C	-2.42002	0.00243	1.23173
H	-3.38748	0.00363	1.72378
C	-1.25357	0.00064	2.00087
H	-1.30975	0.00090	3.08455
O	1.34767	0.00000	-0.63491
H	1.51852	0.78991	-1.19718
H	1.53823	-0.81215	-1.15797
Aryl cation			
C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.32640
H	0.81417	0.00000	2.04132
C	-0.71778	0.00009	-1.11544
H	-0.42026	0.00047	-2.15731

C	-1.39121	-0.00009	1.67485
H	-1.60818	-0.00073	2.74054
C	-2.39149	0.00023	0.70290
H	-3.43205	0.00092	1.00897
C	-2.07635	-0.00003	-0.65576
H	-2.83543	-0.00037	-1.43455

Phenol

C	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.36852
H	0.91739	0.00000	1.68914
C	1.18033	0.00744	-0.75326
H	2.14382	0.01344	-0.24753
C	1.11025	0.00595	-2.14819
H	2.03132	0.01099	-2.72545
C	-0.12583	-0.00236	-2.79895
H	-0.17507	-0.00404	-3.88403
C	-1.29919	-0.00938	-2.03762
H	-2.26799	-0.01557	-2.53076
C	-1.24378	-0.00792	-0.64422
H	-2.14935	-0.01299	-0.04440

Biphenyl

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.40639
H	0.94513	0.00000	1.94234
C	-1.19597	-0.02935	2.12435
H	-1.16977	-0.03692	3.21103
C	-2.42057	-0.05940	1.45250
H	-3.35220	-0.08317	2.01151
C	-2.43676	-0.05928	0.05538
H	-3.38306	-0.07479	-0.47928
C	-1.24058	-0.02925	-0.66200
H	-1.26927	-0.00566	-1.74795
C	1.27415	0.02999	-0.76582
C	2.37547	0.77793	-0.31232
H	2.28836	1.36130	0.60015
C	3.56989	0.80498	-1.03296
H	4.40481	1.39653	-0.66619
C	3.69061	0.08508	-2.22443
H	4.62097	0.10640	-2.78563
C	2.60498	-0.66235	-2.68781
H	2.68879	-1.23242	-3.60956
C	1.41110	-0.68957	-1.96648
H	0.58212	-1.29275	-2.32639

Aryl radical + Benzene

C	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.08725
C	1.20533	0.00000	-0.70612
H	2.15303	-0.00038	-0.17327
C	-1.21441	-0.00872	-0.69181
H	-2.15211	-0.01133	-0.14186
C	-1.22393	-0.01064	-2.08899
H	-2.16904	-0.01609	-2.62612
C	-0.01806	-0.00570	-2.79531
H	-0.02430	-0.00682	-3.88236
C	1.19598	-0.00142	-2.10377
H	2.13426	0.00017	-2.65274
H	2.09753	0.82125	2.42376
C	2.17280	1.66707	3.10228
C	1.77849	2.93784	2.74145
C	1.84035	4.05878	3.54132

H	1.51348	5.03768	3.20006
C	2.68064	1.51088	4.40323
H	3.00671	0.52927	4.73974
C	2.76742	2.61230	5.26018
H	3.16132	2.48233	6.26454
C	2.35212	3.87896	4.83770
H	2.42325	4.73042	5.51063

Aryl radical

C	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.08666
C	1.21474	0.00000	-0.69249
H	2.15569	0.00076	-0.14703
C	-1.21482	-0.00047	-0.69242
H	-2.15561	0.00042	-0.14665
C	-1.22717	-0.00158	-2.09787
H	-2.16494	-0.00200	-2.64759
C	-0.00018	-0.00197	-2.72586
C	1.22687	-0.00100	-2.09796
H	2.16447	-0.00163	-2.64801

Benzene

C	0.54966	0.00000	-2.46186
C	-0.60726	-0.35495	-1.76324
C	1.70658	0.35495	-1.76324
H	-1.50724	-0.63107	-2.30683
H	2.60656	0.63107	-2.30683
C	-0.60726	-0.35495	-0.36582
C	1.70658	0.35495	-0.36582
H	-1.50724	-0.63107	0.17777
H	2.60656	0.63107	0.17777
C	0.54966	0.00000	0.33281
H	0.54966	0.00000	1.41988
H	0.54966	0.00000	-3.54894

CF3COO

F	0.00072	-0.00256	0.00084
C	-0.00024	-0.00036	1.33707
F	1.25814	0.00084	1.78914
F	-0.61993	1.10557	1.77386
C	-0.73830	-1.24483	1.85802
O	-0.54943	-1.71699	3.00354
O	-1.60545	-1.85015	1.18513

CF3COO-

C	0.00067	-0.00127	-2.89787
F	-0.26969	1.22614	-2.38654
F	-0.92087	-0.84750	-2.35754
F	1.20465	-0.37310	-2.37558
C	0.00640	-0.06375	-4.46794
O	-0.17655	1.02628	-5.04655
O	0.20409	-1.21952	-4.90060

CF3COOH

F	0.03554	0.01874	0.00080
C	0.00002	-0.00204	1.34466
F	1.25162	-0.02080	1.80722
F	-0.62172	-1.12970	1.73294
C	-0.74745	1.23722	1.88415
O	-0.24976	2.03618	2.63497
O	-1.99058	1.26690	1.39595
H	-2.43790	2.05827	1.75648

Water

O	-0.02087	0.00000	-1.22941
H	-0.02087	0.76002	-0.62725

H	-0.02087	-0.76002	-0.62725

Guanidine byproduct

N	-1.64194	-0.79980	-0.26061
N	-3.23690	0.86341	-1.13826
N	-3.87692	-0.51290	0.49142
C	-2.79051	-0.18851	-0.32367
C	-4.56848	1.15753	-0.80778
H	-5.13039	1.93423	-1.29595
C	-4.95136	0.32297	0.17648
H	-5.90010	0.25702	0.67940
C	-2.42611	1.55182	-2.17964
C	-3.87367	-1.59131	1.52087
C	-3.27478	2.64397	-2.85175
H	-3.59906	3.40795	-2.13747
H	-2.66615	3.13844	-3.61506
H	-4.15741	2.22742	-3.34825
C	-1.20637	2.23376	-1.52391
H	-0.56199	1.52647	-0.99655
H	-0.60404	2.73670	-2.28808
H	-1.53890	2.98483	-0.79894
C	-2.00706	0.53964	-3.26718
H	-1.42382	-0.29227	-2.86556
H	-2.89536	0.12066	-3.75216
H	-1.40147	1.04011	-4.03032
C	-2.79970	-1.28143	2.58201
H	-2.78203	-2.07725	3.33574
H	-1.81426	-1.20943	2.11843
H	-3.02397	-0.33508	3.08817
C	-3.59917	-2.94660	0.84038
H	-2.63908	-2.92397	0.32212
H	-3.58017	-3.74262	1.59337
H	-4.38929	-3.17788	0.11639
C	-5.24807	-1.64769	2.20679
H	-6.05115	-1.87591	1.49739
H	-5.22917	-2.44560	2.95571
H	-5.48774	-0.71214	2.72417
H	-0.98825	-0.41346	-0.93288

3d-E(N1-H+) S0min

N	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.36153
N	1.28568	0.00000	1.79760
C	2.11078	-0.03492	0.68846
H	3.18350	-0.05816	0.76256
C	1.32256	-0.03677	-0.41494
H	1.60672	-0.05415	-1.45186
N	-1.07311	0.13782	2.22769
N	-1.90412	-0.84029	2.20063
N	-2.92652	-0.66544	2.98720
H	-2.97389	0.20980	3.51522
C	-3.94180	-1.63452	3.15536
C	-5.03436	-1.28854	3.95825
H	-5.08215	-0.30701	4.42306
C	-6.06011	-2.21230	4.15246
H	-6.90752	-1.94339	4.77582
C	-5.99920	-3.47036	3.55021
H	-6.79958	-4.18775	3.70324
C	-4.90028	-3.80401	2.75265
H	-4.84346	-4.78297	2.28596
C	-3.86375	-2.89520	2.55147
H	-3.00556	-3.15825	1.94414

C	1.75504	0.04151	3.24353
C	-1.18809	0.11887	-0.94799
C	3.28994	-0.00283	3.26185
H	3.61445	0.03468	4.30521
H	3.73409	0.85563	2.74798
H	3.68141	-0.92823	2.82677
C	-1.91617	-1.23293	-1.02034
H	-2.35160	-1.51120	-0.05940
H	-2.72115	-1.16326	-1.75903
H	-1.22973	-2.02508	-1.33724
C	1.27497	1.35844	3.87559
H	0.18606	1.43416	3.87702
H	1.62488	1.40139	4.91182
H	1.68941	2.21870	3.33946
C	-0.65667	0.47928	-2.34528
H	-1.51869	0.62869	-3.00074
H	-0.05287	-0.32253	-2.78096
H	-0.07656	1.40760	-2.33826
C	1.20633	-1.18805	3.98653
H	0.11789	-1.17139	4.06503
H	1.61664	-1.19559	5.00097
H	1.51182	-2.11341	3.48739
C	-2.11041	1.25425	-0.47184
H	-2.59277	1.04058	0.48233
H	-2.89747	1.39345	-1.21874
H	-1.55641	2.19444	-0.38187

3d-E(N1-H+) S1min

N	-0.25177	0.10194	0.28160
C	0.07708	-0.39246	1.57908
N	1.31449	0.21893	1.92631
C	1.65782	1.07287	0.94572
H	2.53855	1.69175	0.97422
C	0.71239	0.99087	-0.06515
H	0.72482	1.50848	-1.00833
N	-0.44399	-1.20235	2.43076
N	-1.68355	-1.80751	2.30290
N	-2.64015	-1.01402	2.79694
H	-2.37847	-0.13061	3.22987
C	-3.96430	-1.44438	2.92444
C	-4.89309	-0.56109	3.50363
H	-4.57293	0.42417	3.83548
C	-6.21955	-0.95863	3.65627
H	-6.93191	-0.27430	4.10856
C	-6.63234	-2.22802	3.23365
H	-7.66660	-2.53554	3.35604
C	-5.70183	-3.09777	2.65354
H	-6.01359	-4.08573	2.32553
C	-4.36886	-2.71844	2.49202
H	-3.64728	-3.39715	2.05175
C	2.10160	-0.01160	3.20793
C	-1.30502	-0.38805	-0.72041
C	3.36875	0.85616	3.15522
H	3.94109	0.66367	4.06692
H	3.14069	1.92775	3.13313
H	4.01392	0.60429	2.30616
C	-1.25568	-1.92299	-0.78261
H	-1.54422	-2.38834	0.16051
H	-1.95895	-2.25578	-1.55273
H	-0.25479	-2.26827	-1.06501
C	1.25023	0.41869	4.41673

H	0.39186	-0.23791	4.56261
H	1.87621	0.37365	5.31358
H	0.90137	1.45125	4.30069
C	-0.95398	0.16467	-2.11381
H	-1.68393	-0.24528	-2.81710
H	0.03940	-0.14936	-2.45229
H	-1.03307	1.25553	-2.17098
C	2.50540	-1.49526	3.28338
H	1.63531	-2.14915	3.34649
H	3.11578	-1.64023	4.18061
H	3.10741	-1.77938	2.41307
C	-2.68275	0.15648	-0.31809
H	-3.01217	-0.20765	0.65303
H	-3.41695	-0.16509	-1.06381
H	-2.67425	1.25199	-0.30152

N2

N	0.00000	0.00000	-0.00005
N	0.00000	0.00000	1.10528

3d-E(N3-H+) S0min

N	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.01903
C	1.18843	0.00000	-0.70392
N	1.75432	-1.10433	-1.25853
N	1.98084	1.07418	-0.96885
C	2.91275	-0.71371	-1.88681
H	3.55748	-1.40027	-2.40613
C	3.05248	0.62947	-1.70858
H	3.83653	1.28052	-2.05215
N	-1.15957	0.36723	-0.67958
N	-2.21501	0.51343	-0.03500
C	-2.27485	0.29866	1.38570
C	-2.45000	1.40648	2.22436
H	-2.47477	2.40425	1.79663
C	-2.59844	1.20957	3.59773
H	-2.72562	2.06858	4.25022
C	-2.60074	-0.08206	4.13041
H	-2.72909	-0.22933	5.19860
C	-2.45438	-1.18428	3.28473
H	-2.47360	-2.19130	3.69146
C	-2.28968	-1.00155	1.91075
H	-2.19854	-1.85411	1.24378
C	1.23067	-2.53742	-1.19915
C	1.74977	2.53387	-0.57714
C	2.25302	-3.45704	-1.88284
H	1.87341	-4.48011	-1.81871
H	2.37891	-3.22024	-2.94385
H	3.22798	-3.43246	-1.38572
C	3.05385	3.30891	-0.82189
H	2.89694	4.33764	-0.48778
H	3.32049	3.35059	-1.88193
H	3.88980	2.89298	-0.25053
C	-0.10395	-2.60800	-1.95802
H	-0.88333	-2.00508	-1.48959
H	-0.44157	-3.64899	-1.97113
H	0.02027	-2.27676	-2.99404
C	0.63309	3.10322	-1.46667
H	-0.31670	2.58462	-1.31990
H	0.49048	4.15889	-1.21452
H	0.90895	3.03742	-2.52402
C	1.08634	-2.95311	0.27388

H	0.31441	-2.38096	0.79132
H	0.80081	-4.00877	0.31065
H	2.03550	-2.83925	0.80811
C	1.39536	2.62027	0.91741
H	0.39407	2.24729	1.13753
H	1.41819	3.67299	1.21352
H	2.12548	2.08246	1.53129

3d-E(N3-H+) S1min

N	0.47000	0.11558	0.33889
H	0.81598	0.25036	1.28987
C	1.40881	0.07805	-0.69052
N	1.79732	-1.06171	-1.31494
N	2.07293	1.12920	-1.24139
C	2.72423	-0.72307	-2.27404
H	3.20532	-1.44759	-2.90838
C	2.88640	0.62911	-2.23433
H	3.52809	1.25361	-2.83120
N	-0.76684	0.64346	0.04657
N	-1.33283	1.19294	1.12568
C	-2.07698	0.49377	1.99624
C	-2.68422	1.23765	3.06433
H	-2.51263	2.30891	3.10120
C	-3.46903	0.60115	4.00668
H	-3.92104	1.17585	4.81023
C	-3.68911	-0.78720	3.92835
H	-4.30919	-1.28288	4.66908
C	-3.11341	-1.53127	2.88112
H	-3.30012	-2.59998	2.81764
C	-2.32302	-0.91723	1.92496
H	-1.89843	-1.49285	1.11122
C	1.29174	-2.47477	-1.03834
C	1.96222	2.61997	-0.90941
C	2.13292	-3.46643	-1.85614
H	1.78719	-4.47459	-1.61061
H	2.00236	-3.33201	-2.93481
H	3.19815	-3.40915	-1.60888
C	3.24017	3.31560	-1.40741
H	3.18812	4.36286	-1.09699
H	3.32526	3.30939	-2.49834
H	4.14362	2.87744	-0.96911
C	-0.17646	-2.55594	-1.48570
H	-0.81077	-1.85199	-0.94477
H	-0.54423	-3.56945	-1.29543
H	-0.26646	-2.35167	-2.55766
C	0.73578	3.18495	-1.64513
H	-0.18619	2.70046	-1.31663
H	0.66035	4.25714	-1.43388
H	0.83915	3.05633	-2.72802
C	1.46177	-2.77719	0.46079
H	0.80595	-2.16490	1.08425
H	1.20408	-3.82675	0.63267
H	2.49973	-2.62704	0.77822
C	1.85815	2.81722	0.61281
H	0.88705	2.52787	1.01846
H	1.98522	3.88359	0.82319
H	2.65371	2.27764	1.13973

3d-E S0min

N	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.38500
N	0.98286	0.00000	2.29711

N	2.04702	0.76204	2.02082
N	3.00627	0.57011	2.84505
N	-1.31392	-0.11147	1.78603
C	-2.12304	-0.14950	0.65948
H	-3.19479	-0.22117	0.71451
C	-1.32653	-0.07219	-0.42736
H	-1.60017	-0.06706	-1.46662
C	4.08644	1.46088	2.65920
C	5.33456	1.03825	3.14841
H	5.39999	0.05697	3.61024
C	6.45864	1.85334	3.03070
H	7.41749	1.50457	3.40637
C	6.35508	3.11509	2.43759
H	7.22919	3.75526	2.35282
C	5.11181	3.55335	1.97018
H	5.01716	4.54176	1.52629
C	3.98456	2.74134	2.08128
H	3.01533	3.09327	1.74396
C	-1.79268	-0.15783	3.21213
C	1.17439	-0.09940	-0.94788
C	-3.32732	-0.22850	3.21973
H	-3.66059	-0.26641	4.26068
H	-3.70010	-1.12838	2.71925
H	-3.78278	0.65364	2.75710
C	1.83062	1.28161	-1.11448
H	2.21650	1.64274	-0.16095
H	2.65807	1.20667	-1.82920
H	1.10527	2.00409	-1.50641
C	-1.22988	-1.41910	3.89287
H	-0.13881	-1.41023	3.89000
H	-1.58065	-1.45688	4.92998
H	-1.58168	-2.32194	3.38043
C	-1.34896	1.12256	3.94378
H	-0.26154	1.19818	3.98028
H	-1.73547	1.10176	4.96863
H	-1.75204	2.01081	3.44404
C	2.17116	-1.15720	-0.43714
H	2.65543	-0.86776	0.49385
H	2.95050	-1.29318	-1.19398
H	1.66758	-2.11875	-0.28869
C	0.66213	-0.56563	-2.32470
H	1.52987	-0.70447	-2.97569
H	0.01500	0.17700	-2.80245
H	0.12862	-1.52041	-2.26688

3d-E S1min

N	-0.01310	-0.21845	-0.23079
C	0.27713	-0.09116	1.13667
N	1.39174	-0.04316	1.86705
N	2.57854	-0.10572	1.29954
N	3.60213	-0.12699	2.24161
N	-0.95093	-0.00944	1.79673
C	-1.96224	-0.08379	0.85626
H	-3.00535	-0.04129	1.11540
C	-1.39955	-0.21044	-0.36733
H	-1.88884	-0.29588	-1.32065
C	4.06857	1.06719	2.62713
C	5.18372	1.05110	3.53813
H	5.57049	0.08227	3.84018
C	5.73454	2.22603	4.01370
H	6.57323	2.18934	4.70455

C	5.22064	3.47128	3.60288
H	5.65941	4.39307	3.97392
C	4.13956	3.51607	2.70273
H	3.75133	4.47962	2.38057
C	3.56686	2.35311	2.21633
H	2.74163	2.40111	1.51661
C	-1.15566	0.13927	3.27856
C	0.92459	-0.36338	-1.40566
C	-2.66493	0.19932	3.57238
H	-2.79338	0.30852	4.65345
H	-3.18254	-0.71684	3.26717
H	-3.14711	1.05922	3.09359
C	1.81119	0.89086	-1.51557
H	2.44978	0.99907	-0.63773
H	2.45056	0.80324	-2.40158
H	1.18899	1.78689	-1.62908
C	-0.56055	-1.08078	4.00825
H	0.51671	-1.14920	3.84904
H	-0.75243	-0.98689	5.08320
H	-1.03100	-2.00632	3.65580
C	-0.51076	1.45292	3.76130
H	0.56879	1.44465	3.60622
H	-0.71037	1.57894	4.83139
H	-0.94127	2.30945	3.22899
C	1.74841	-1.65568	-1.25396
H	2.36580	-1.62875	-0.35456
H	2.40790	-1.76589	-2.12280
H	1.08393	-2.52726	-1.21528
C	0.10063	-0.47394	-2.70279
H	0.80518	-0.57710	-3.53355
H	-0.50353	0.42036	-2.89136
H	-0.54786	-1.35676	-2.71131