Supporting Information

Highly Efficient Carbazolyl-Derived Phosphine Ligands:

Application to Sterically Hindered Biaryl Couplings

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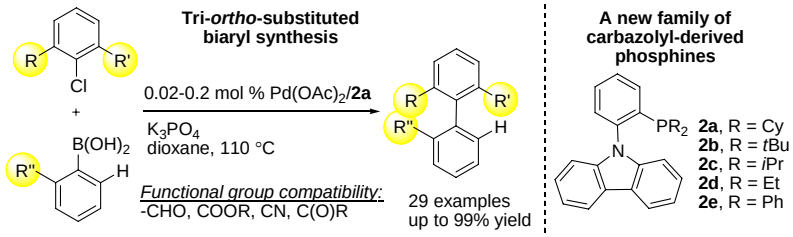

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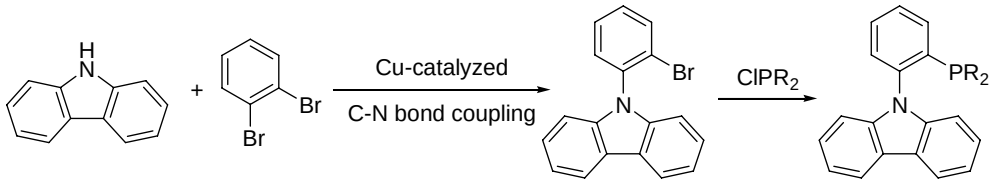
1. General considerations

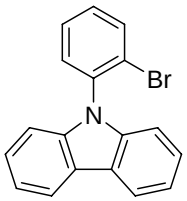
Unless otherwise noted, all reagents were purchased from commercial suppliers without purification. All Suzuki-Miyaura reactions were performed in Rotaflo® (England) resealable screw-cap Schlenk flasks (approx. 20 mL volume) in the presence of Teflon-coated magnetic stir bar (4 mm × 10 mm). Toluene, tetrahydrofuran (THF) and dioxane were distilled from sodium and sodium benzophenone ketyl under nitrogen.[1] Chlorodiphenylphosphine was distilled under vacuum prior to use. Commercially available aryl chlorides (liquid form only) were purified by passing through a short plug (0.5 cm width × 4 cm height) of neutral alumina. Most commercially available arylboronic acids were used as received. Some arylboronic acids may require further recrystallization depending on the received conditions. New bottle of *n*-butyllithium was used (*Note*: since the concentration of *n*-BuLi from old bottle may vary, we recommend performing a titration prior to use). $Pd(OAc)_2$ and $Pd_2(dba)_3$ were purchased from Strem Chemical. K_3PO_4 was purchased from Fluka. 4-Chloro-3,5-dimethylanisole[2] and 2-methoxynaphthalen-1-ylboronic acid[3] were synthesized according to the literature methods. Thin layer chromatography was performed on Merck precoated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Büchi Melting Point B-545 instrument. ^{1}H NMR spectra were recorded on a Bruker (400 MHz) or Varian (400 MHz or 500 MHz) spectrometer. Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to

$CDCl_3$ (δ 77.0 ppm, the middle peak). ^{31}P NMR spectra were referenced to 85% H_3PO_4 externally. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Brüker APEX 47e FT-ICR mass spectrometer (ESIMS). GC-MS analyses were conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 6890 GC-FID system. All yields reported refer to the isolated yield of compounds. Compounds described in the literature were characterized by comparison of their ^{1}H, and/or ^{13}C NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

2. Preparation of new carbazolyl phosphine ligands



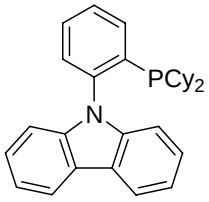
9-(2-Bromophenyl)-9H-carbazole (1)[4]



General procedures for Cu-catalyzed C-N bond coupling: 9-Carbazole (8.35 g, 50 mmol), 1,2-dibromobenzene (12 mL, 100 mmol), copper(I) oxide (1.43 g, 10 mmol), *N*,*N*'-dimethylethylenediamine (2.15 mL, 20 mmol) and anhydrous potassium phosphate (23.35 g, 110 mmol) were mixed in toluene (40 mL) and heated at 120 ℃ for 3 days.[5] After the completion of the reaction, the crude reaction mixtures were poured into 1.0 M $NH_4OH_{(aq)}$ and then extracted with DCM. The organic phase was separated and the aqueous layer was further extracted with DCM (2 x 200 mL). The combined organic phases were concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (230-400 mesh). The desired product 9-(2-bromophenyl)-9H-carbazole was dried under vacuum (9.33 g, 58%) and formed as a white solid upon standing. Hexane:DCM = 30:1, R_f=0.25; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.0 Hz, 2H), 7.35-7.56 (m, 7H), 7.91 (dd, *J* = 8.0 Hz and 1 Hz, 1H), 8.23 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 110.1, 120.1, 120.4, 123.4, 123.9, 126.0, 128.9, 130.2, 131.2, 134.3, 136.8, 140.9; MS

(EI) *m/z* (relative intensity) 321 (M^+, 100), 241 (80), 120 (40).

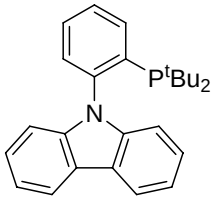
9-(2-(Dicyclohexylphosphino)phenyl)-9H-carbazole (**2a**)



General procedures for synthesis of carbazolyl dialkylphosphine or diarylphosphine: 9-(2-Bromophenyl)-9H-carbazole (3.21 g, 10 mmol) was dissolved in freshly distilled THF (50 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 ℃ using a dry ice/acetone bath. Titrated *n*-BuLi (10.5 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78℃, chlorodicyclohexylphosphine (2.6 mL, 12 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was successively washed with MeOH. The product was then dried under vacuum. 9-(2-(Dicyclohexylphosphino)phenyl)-9H-carbazole was obtained as a white solid (3.2 g, 73%). Melting point 186.3-186.8 ℃; ^{1}H NMR (400 MHz, C_6D_6) δ 0.94-1.11 (m, 10H), 1.50-1.68 (m, 12H), 7.00-7.02 (m, 1H), 7.10-7.14 (m, 3H), 7.18-7.19 (m, 1H), 7.23 (t, *J* = 6.8 Hz, 2H), 7.35 (t, *J* = 6.8 Hz, 2H), 7.55 (d, *J* = 7.6 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, C_6D_6) δ 26.3, 27.0, 27.1, 27.2, 29.6, 29.7, 30.1, 30.3, 33.9, 34.1, 110.7, 120.0, 120.3, 123.5, 125.3, 127.5, 127.8, 128.3, 130.0, 133.9, 137.9, 138.2, 142.6, 143.9, 144.1 (unresolved C-P couplings were observed); ^{31}P NMR (162 MHz, $CDCl_3$) δ -14.44; IR (cm^{-1}) 3414.3, 3059.6, 3047.0, 3018.5, 2920.3, 2844.3, 2648.0, 2363.1, 2331.4, 1926.1, 1590.5, 1451.2, 1229.6, 745.1, 720.0;

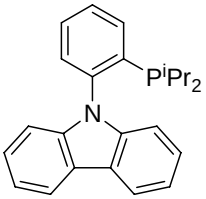
MS (EI) *m/z* (relative intensity) 438 (M^+, 100), 356 (40), 272 (100), 241 (20); HRMS: calcd. for $C_{30}H_{34}NPH^+$: 440.2507, found 440.2520.

9-(2-(Di-*tert*-butylphosphino)phenyl)-9H-carbazole (**2b**)



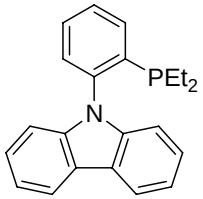
The general synthetic procedures for synthesis of the carbazolyl dialkylphosphine or diarylphosphine were followed. 9-(2-Bromophenyl)-9H-carbazole (3.21 g, 10 mmol) and di-*tert*-butylchlorophosphine (2.6 mL, 12 mmol) were used to yield the desired product (1.9 g, 50%) as a white solid. Melting point 153.0-153.6 ℃; ^{1}H NMR (400 MHz, C_6D_6) δ 0.99 (s, 9H), 1.02 (s, 9H), 6.95-6.98 (m, 1H), 7.06-7.14 (m, 4H), 7.21 (t, *J* = 6.8 Hz, 2H), 7.30 (t, *J* = 6.8 Hz, 2H), 7.89 (d, *J* = 7.6 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, C_6D_6) δ 30.7, 30.8, 31.8, 32.1, 111.2, 119.5, 120.2, 123.5, 125.0, 125.9, 127.1, 127.6, 128.3, 130.5, 136.6, 138.8, 139.2, 142.7, 144.5, 144.8 (unresolved C-P couplings were observed); ^{31}P NMR (162 MHz, C_6D_6) δ 17.79; IR (cm^{-1}) 3051.1, 2974.5, 2953.9, 2933.3, 2886.2, 2853.7, 1592.7, 1463.1, 1451.3, 1312.8, 1230.3, 747.1, 720.6; MS (EI) *m/z* (relative intensity) 387 (M^+, 30), 330 (30), 274 (100), 241 (15); HRMS: calcd. for $C_{26}H_{30}NPH^+$: 388.2194, found 388.2193.

9-(2-(Di-*iso*-propylphosphino)phenyl)-9H-carbazole (**2c**)



The general synthetic procedures for synthesis of the carbazolyl dialkylphosphine or diarylphosphine were followed. 9-(2-Bromophenyl)-9H-carbazole (3.21 g, 10 mmol) and chlorodi-*iso*-propylphosphine (1.9 mL, 12 mmol) were used to yield the desired product (1.4 g, 40%) as a white solid. Melting point 146.5-147.1 ℃; ^{1}H NMR (400 MHz, C_6D_6) δ 0.76 (q, *J* = 7.6 Hz, 6H), 0.84 (dd, *J* = 7.2 Hz and 4.4 Hz, 6H), 1.68-1.71 (m, 2H), 6.97-7.00 (m, 1H), 7.06-7.13 (m, 3H), 7.13-7.17 (m, 1H), 7.22 (t, *J* = 6.8 Hz, 2H), 7.32 (t, *J* = 6.8 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 1H), 8.07 (d, *J* = 8 Hz, 2H); ^{13}C NMR (100 MHz, C_6D_6) δ 19.5, 19.8, 24.0, 24.2, 110.7, 119.6, 120.2, 123.5, 125.0, 127.6, 127.8, 129.9, 130.5, 138.8, 139.2, 142.6, 143.8, 144.0 (unresolved C-P couplings were observed); ^{31}P NMR (162 MHz, C_6D_6) δ -6.53; IR (cm^{-1}) 3054.1, 2953.9, 2921.5, 2892.0, 2859.6, 2358.8, 2332.3, 1625.2, 1589.8, 1469.0, 1448.4, 1312.8, 1230.3, 747.2, 723.6; MS (EI) *m/z* (relative intensity) 358 (M^+, 100), 272 (70), 241 (15); HRMS: calcd. for $C_{24}H_{26}NPH^+$: 360.1881, found 360.1884.

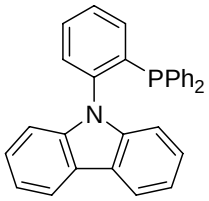
9-(2-(Diethylphosphino)phenyl)-9H-carbazole (**2d**)



The general synthetic procedures for synthesis of the carbazolyl dialkylphosphine or diarylphosphine were followed. 9-(2-Bromophenyl)-9H-carbazole (3.21 g, 10 mmol) and chlorodiethylphosphine (1.4 mL, 12 mmol) were used to yield the desired product (1.7 g, 52%) as a white solid. Melting point 119.8-120.8 ℃; ^{1}H NMR (400 MHz, C_6D_6) δ 0.65-0.72 (m, 6H), 1.16-1.31 (m, 4H), 6.93-6.96 (m, 1H), 7.08 (t, *J* = 7.6 Hz, 3H), 7.16-7.24 (m, 3H),

7.30 (t, J = 7.6 Hz, 2H), 7.39-7.41 (m, 1H), 8.06 (d, J = 8 Hz, 2H); ^{13}C NMR (100 MHz, C_6D_6) δ 9.3, 9.4, 18.9, 19.1, 110.3, 119.7, 120.3, 123.5, 125.7, 127.6, 128.5, 129.8, 131.5, 140.5, 142.3 (unresolved C-P couplings were observed); ^{31}P NMR (162 MHz, C_6D_6) δ -28.23; IR (cm^{-1}) 3051.1, 2956.9, 2924.4, 2868.5, 2815.4, 1622.2, 1592.7, 1469.0, 1451.3, 1312.8, 1230.3, 747.2, 726.3; MS (EI) *m/z* (relative intensity) 330 (M^+, 100), 274 (50), 241 (15); HRMS: calcd. for $C_{22}H_{22}NPH^+$: 332.1568, found 332.1581.

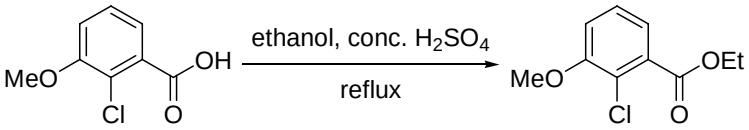
9-(2-(Diphenylphosphino)phenyl)-9H-carbazole (**2e**)



The general synthetic procedures for synthesis of the carbazolyl dialkylphosphine or diarylphosphine were followed. 9-(2-Bromophenyl)-9H-carbazole (3.21 g, 10 mmol) and chlorodiphenylphosphine (2.2 mL, 12 mmol) were used to yield the desired product (2.9 g, 70%) as a white solid. Melting point 137.9-138.8 ℃; ^{1}H NMR (400 MHz, C_6D_6) δ 6.87-6.95 (m, 9H), 7.01 (d, J = 6.8 Hz, 2H), 7.11-7.16 (m, 4H), 7.17-7.22 (m, 4H), 7.33-7.40 (m, 1H), 8.00-8.02 (m, 2H); ^{13}C NMR (100 MHz, C_6D_6) δ 110.4, 119.6, 120.1, 123.5, 125.5, 127.6, 128.3, 130.1, 133.8, 134.8, 136.6, 138.8, 140.5, 144.5, 141.8 (unresolved C-P couplings were observed); ^{31}P NMR (162 MHz, C_6D_6) δ -16.22; IR (cm^{-1}) 3048.2, 1622.2, 1595.7, 1581.0, 1469.0, 1448.4, 1312.8, 1230.3, 744.2, 697.1; MS (EI) *m/z* (relative intensity) 426 (M^+, 100), 272 (40), 241 (15); HRMS: calcd. for $C_{30}H_{22}NPH^+$: 428.1568, found 428.1574.

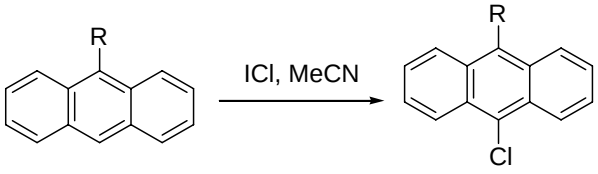
3. Preparation of aryl chlorides

Synthesis of ethyl 2-chloro-3-methoxybenzoate



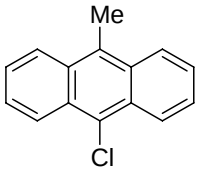
2-Chloro-3methoxybenzoic acid (1.86 g, 10 mmol), absolute ethanol (50 mL) and concentrated H_2SO_4 (0.5 mL) were mixed and refluxed for overnight.[6] The alcohol was removed under reduced pressure. Then, the mixture was poured into 1.0 M $Na_2CO_{3(aq)}$ and then extracted with diethyl ether. The organic phase was separated and the aqueous layer was further extracted with diethyl ether (2 x 50 mL). The combined organic phases were concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (230-400 mesh). The desired product ethyl 2-chloro-3-methoxybenzoate was dried under vacuum (1.39 g, 65%) and yielded a pale yellow liquid. Hexane:EA = 20:1, R_f=0.25; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.41 (t, *J* = 7.2 Hz, 3H), 3.93 (s, 3H), 4.41 (q, *J* = 7.2 Hz, 2H), 7.05 (dd, *J* = 8.4 Hz and 1.2 Hz, 1H), 7.27 (t, *J* = 8 Hz, 1H), 7.33 (dd, *J* = 7.6 Hz and 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 56.5, 61.6, 114.4, 121.8, 122.2, 127.1, 132.7, 155.7, 166.1; MS (EI) *m/z* (relative intensity) 214 (M^+, 40), 186 (25), 169 (100); HRMS: calcd. for $C_{10}H_{11}O_3ClNa^+$: 237.0294, found 237.0303.

Synthesis of 9-substituted-10-chloroanthracene



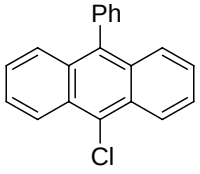
General procedures for the synthesis of 9-substituted-10-chloroanthracene: 9-Substituted-10-chloroanthracene (3 mmol) was dissolved in MeCN (100 mL). After added ICl (4.5 mmol), the mixture was stirred at room temperature for 24 h.[7] The reaction was quenched by bubbling acetylene gas. The solvent was removed under reduced pressure. Then, the mixture was poured into 1.0 M $Na_2S_2O_{3(aq)}$ and then extracted with ether. The organic phase was separated and the aqueous layer was further extracted with ether (2 x 50 mL). The combined organic phases were concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh). The residue was dissolved by minimal amount of DCM and recrystallized by methanol, and then washed with cold methanol to afford the corresponding aryl chlorides.

10-Chloro-9-methylanthracene[8]



Pure Hexane, R_f=0.65; yield=40%; yellow solid;^{1}H NMR (400 MHz, $CDCl_3$) δ 3.06 (s, 3H), 7.52-7.62 (m, 4H), 8.29 (d, *J* = 9.2 Hz, 2H), 8.56 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 125.0, 125.5, 126.3, 127.2, 128.5, 130.0, 130.6; MS (EI) *m/z* (relative intensity) 226 (M^+, 100), 191 (50), 94 (25).

10-Chloro-9-phenylanthracene[7]

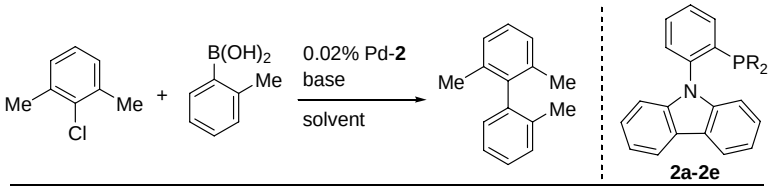


Pure Hexane, R_f=0.65; yield=40%; yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.43 (m, 4H), 7.56-7.62 (m, 5H), 7.68 (d, *J* = 8.8 Hz, 2H), 8.60 (d, *J* = 8.8 Hz,

2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.9, 125.6, 126.6, 127.3, 127.7, 128.5, 128.6, 130.8, 131.3, 136.8, 138.4; MS (EI) *m/z* (relative intensity) 288 (M^+, 100), 252 (70), 126 (35).

4. General procedures for initial ligand and reaction condition screenings

General procedures for Suzuki-Miyaura coupling of hindered aryl chlorides: A stock solution of $Pd(OAc)_2$ (2.2 mg, 0.01 mmol) with ligand (0.03 mmol) in freshly distilled dioxane (50.0 mL) was initially prepared with continuous stirring at room temperature. Phenylboronic acid (1.0 mg, as reducing agent) and magnetic stirrer bar (4 mm × 10 mm) were charged to the Schlenk tube. Each tube was carefully evacuated and backfilled with nitrogen (3 cycles). Stock solution of palladium complex (1.0 mL), base (3.0 equiv.), 1-chloro-2,6-dimethylbenzene (1.0 mmol) and *o*-tolylboronic acid (1.5 equiv.) were added to Schlenk tube. The liquid substrates were added by a syringe. Further solvent was added up to final volume 3.0 mL. This batch of Schlenk tubes was resealed and then placed into a preheated oil bath (110 °C) and stirred for the time as indicated. The reactions were allowed to reach room temperature. Diethylether (~15 mL), dodecane (227 μL, internal standard) and water were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.



entry	ligand **2**	base	solvent	yield %[b]
1	**2a**	$K_3PO_4 \bullet H_2O$	dioxane	98 (95)[c]
2	**2b**	$K_3PO_4 \bullet H_2O$	dioxane	20
3	**2c**	$K_3PO_4 \bullet H_2O$	dioxane	89
4	**2d**	$K_3PO_4 \bullet H_2O$	dioxane	11
5	**2e**	$K_3PO_4 \bullet H_2O$	dioxane	9
6	**2a**	K_2CO_3	dioxane	17
7	**2a**	K_3PO_4	dioxane	54

8	**2a**	Cs_2CO_3	dioxane	3
9	**2a**	$K_3PO_4 \bullet H_2O$	THF	76
10	**2a**	$K_3PO_4 \bullet H_2O$	toluene	65

[a]Reaction conditions: $Pd(OAc)_2$ (0.02 mol %), ligand **2** (0.06 mol %), ArCl (1.0 mmol), $ArB(OH)_2$ (1.5 mmol), $PhB(OH)_2$ (1 mg), base (3.0 mmol), solvent (3.0 mL) were stirred for 24 h at 110 °C under nitrogen. [b]Calibrated GC yields were reported using dodecane as the internal standard. [c]Isolated yield in parenthesis.

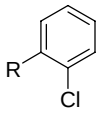
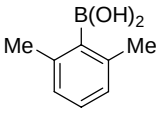
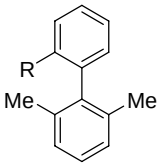
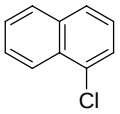
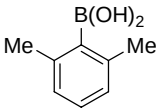
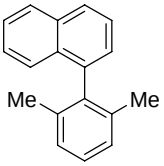
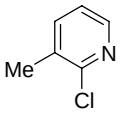
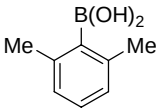
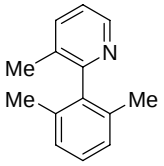
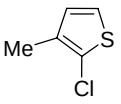
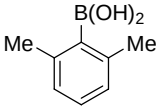
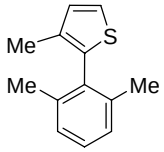
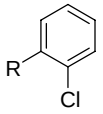
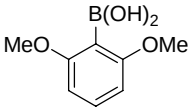
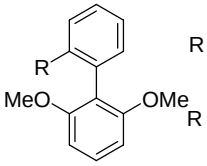
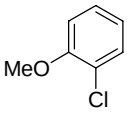
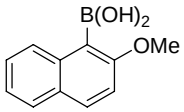
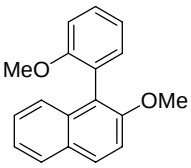
5. General procedures for Suzuki-Miyaura reaction of aryl chlorides

General procedures for Suzuki-Miyaura coupling of hindered aryl chlorides: A stock solution of $Pd(OAc)_2$ (2.2 mg, 0.01 mmol) with ligand **2a** (13.1 mg, 0.03 mmol) in freshly distilled dioxane (5.0 to 50.0 mL) was initially prepared with continuous stirring at room temperature. Phenylboronic acid (1.0 mg) and magnetic stirrer bar (4 mm × 10 mm) were charged to Schlenk tube. Each tube was carefully evacuated and backfilled with nitrogen (3 cycles). Stock solution of palladium complex (1.0 mL), hydrated potassium phosphate (3.0 mmol), aryl chlorides (1.0 mmol) and arylboronic acid (1.5 mmol) were added to Schlenk tube. The liquid substrates were added by a syringe. Further solvent was added up to final volume 3.0 mL. This batch of Schlenk tubes was resealed and then placed into a preheated oil bath (110 °C) and stirred for the time as indicated. The reactions were allowed to reach room temperature. The reactions were quenched with water and diluted with diethylether. After the completion of reaction was judged by GC or TLC analysis, the organic layer was concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

General procedures for Suzuki-Miyaura coupling of hindered arylboronic acids: A stock solution of $Pd(OAc)_2$ (2.2 mg, 0.01 mmol) with ligand **2a** (13.1 mg, 0.03 mmol) in freshly distilled dioxane (5.0 to 10.0 mL) was initially prepared with continuous stirring at room temperature. Phenylboronic acid (1.0 mg) and magnetic stirrer bar (4 mm × 10 mm) were charged to Schlenk tube. Each tube was carefully evacuated and backfilled with nitrogen (3 cycles). Stock solution of palladium

complex (1.0 mL), anhydrous potassium phosphate (3.0 mmol), aryl chlorides (1.0 mmol) and arylboronic acid (3.0 mmol) were added to Schlenk tube. The liquid substrates were added by syringe. Further solvent was added up to final volume 3.0 mL. This batch of Schlenk tubes was resealed and then placed into a preheated oil bath (110 °C) and stirred for the time as indicated. The reactions were allowed to reach room temperature. The reactions were quenched with water and diluted with diethylether. After the completion of reaction was judged by GC or TLC analysis, the organic layer was concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

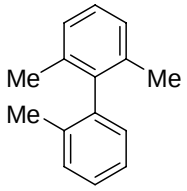
6. Palladium-Catalyzed Suzuki-Miyaura Coupling of 2,6-Disubstituted Arylboronic Acids (Table 4)[a]

entry	ArCl	$Ar'B(OH)_2$	product	Pd loading	%yield[b]
1			 R = Me	0.1%	76
2			R = OMe	0.2%	83
3[c]				0.1%	84
4				0.2%	81
5[d]				0.2%	75
6			 R = Me	0.2%	64
7			R = OMe	0.2%	58
8				0.2%	58

[a]Reaction conditions: ArCl (1.0 mmol), $ArB(OH)_2$ (3.0 mmol), $Pd(OAc)_2$ (mol % as indicated), ligand (Pd/**2a**, 1:3), $PhB(OH)_2$ (1 mg), K_3PO_4 (3.0 mmol), dioxane (3.0 mL) were stirred for 24 h at 110 °C under nitrogen. [b]Isolated yields are reported. [c]Technical grade (85% purity) 1-chloronaphthalene was used. [d]Reaction at 120 °C.

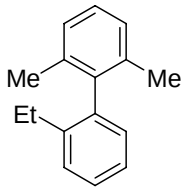
7. Characterization data of coupling products

2,2',6-Trimethylbiphenyl (Table 2, entry 1; Table 4, entry 1)[9]



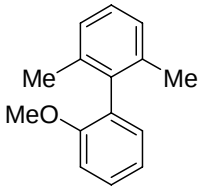
Pure Hexane, R_f=0.6; colourless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 6H), 1.99 (s, 3H), 7.02-7.04 (m, 1H), 7.11-7.13 (m, 2H), 7.16-7.20 (m, 1H), 7.25-7.30 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.4, 20.3, 126.1, 126.9, 127.0, 127.2, 128.9, 130.0, 135.6, 135.9, 140.6, 141.1; MS (EI) *m/z* (relative intensity) 196 (M^+, 60), 181 (100), 165 (40).

2'-Ethyl-2,6-dimethylbiphenyl (Table 2, entry 2)[10]



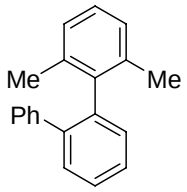
Pure Hexane, R_f=0.6; colourless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.06 (t, *J* = 7.6 Hz, 3H), 1.98 (s, 6H), 2.30 (q, *J* = 7.6 Hz, 2H), 7.01 (d, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 6.8 Hz, 2H), 7.17-7.21 (m, 1H), 7.24-7.28 (m, 1H), 7.30-7.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.6, 20.6, 25.8, 126.0, 126.9, 127.2, 128.2, 129.1, 136.1, 140.0, 141.0, 141.5; MS (EI) *m/z* (relative intensity) 210 (M^+, 75), 195 (100), 165 (60).

2'-Methoxy-2,6-dimethylbiphenyl (Table 2, entry 3; Table 4, entry 2)[11]



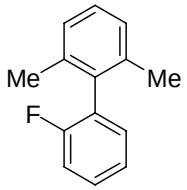
Hexane:EA = 9:1, R_f=0.6; pale yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.04 (s, 6H), 3.76 (s, 3H), 7.01 (d, *J* = 8.0 Hz, 1H), 7.03-7.07 (m, 2H), 7.13 (d, *J* = 7.2 Hz, 2H), 7.19 (dd, *J* = 8.8 Hz and 6.4 Hz, 1H), 7.34-7.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 55.5, 111.0, 120.7, 127.1, 128.4, 129.5, 130.7, 136.6, 138.2, 156.5; MS (EI) *m/z* (relative intensity) 212 (M^+, 100), 197 (40), 165 (40).

2,6-Dimethyl-2'-phenylbiphenyl (Table 2, entry 4)[12]



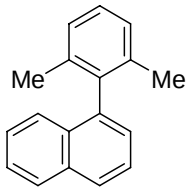
Pure Hexane, R_f=0.5; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 6H), 6.98 (d, *J* = 7.6 Hz, 2H), 7.07-7.12 (m, 3H), 7.15-7.21 (m, 4H), 7.39-7.51 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 126.6, 127.0, 127.2, 127.4, 127.5, 127.6, 128.8, 130.2, 130.4, 136.1, 139.0, 140.8, 141.3; MS (EI) *m/z* (relative intensity) 258 (M^+, 100), 243 (60), 228 (40).

2'-fluoro-2,6-dimethylbiphenyl (Table 2, entry 5)[13]



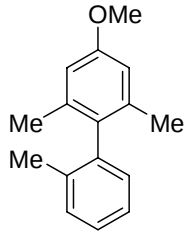
Pure Hexane, R_f=0.6; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.11 (s, 6H), 7.17-7.28 (m, 6H), 7.37-7.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 115.6, 115.8, 124.2, 127.3, 127.8, 128.0, 190.0, 131.4, 135.3, 136.7, 158.4, 160.8; MS (EI) *m/z* (relative intensity) 200 (M^+, 100), 185 (70), 165 (40).

1-(2,6-Dimethylphenyl)naphthalene (Table 2, entry 6; Table 4, entry 3)[14]



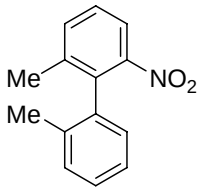
Pure Hexane, R_f=0.5; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 6H), 7.23 (d, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 6.8 Hz, 2H), 7.40 (d, *J* = 4.0 Hz, 2H) , 7.50-7.55 (m, 1H), 7.60 (t, *J* = 6.8 Hz, 1H), 7.91-7.97 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 125.4, 125.8, 126.1, 126.5, 127.2, 127.3, 127.4, 128.3, 131.8, 133.8, 137.1, 138.8, 139.7; MS (EI) *m/z* (relative intensity) 232 (M^+, 100), 217 (70), 202 (40).

4-Methoxy-2,2',6-trimethylbiphenyl (Table 2, entry 7)



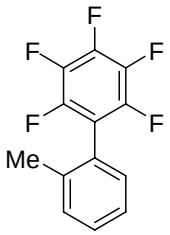
Hexane:EA = 50:1, R_f=0.4; orange solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 6H), 2.00 (s, 3H), 3.86 (s, 3H), 6.71 (s, 2H), 7.03-7.05 (m, 1H), 7.24-7.32 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.5, 20.6, 55.1, 112.6, 126.0, 127.0, 129.6, 129.9, 133.7, 136.3, 137.3, 140.4, 158.3; MS (EI) *m/z* (relative intensity) 226 (M^+, 100), 211 (70), 196 (40); HRMS: calcd. for $C_{16}H_{18}O^+$: 226.1358, found 226.1364.

6,6'-Dimethyl-2-nitrobiphenyl (Table 2, entry 8)[15]



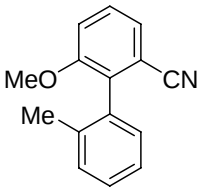
Hexane:EA = 20:1, R_f=0.5; yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.04 (s, 3H), 2.06 (s, 3H), 6.99 (d, *J* = 7.6 Hz, 1H), 7.20-7.24 (m, 1H), 7.28-7.30 (m, 2H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.6, 20.1, 121.2, 126.0, 127.8, 128.0, 128.2, 130.0, 133.8, 135.2, 135.7, 136.1, 139.3; MS (EI) *m/z* (relative intensity) 227 (M^+, 20), 197 (70), 180 (100).

2,3,4,5,6-Pentafluoro-2'-methyl biphenyl (Table 2, entry 9)[16]



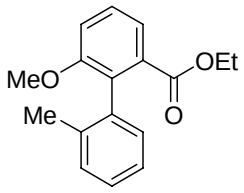
Pure Hexane, R_f=0.7; pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.19 (s, 3H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.28-7.32 (m, 1H), 7.34-7.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.6, 115.4, 125.9, 126.0, 129.6, 130.5, 130.6, 136.4, 137.4, 138.9, 142.8, 145.3; MS (EI) *m/z* (relative intensity) 258 (M^+, 100), 237 (50), 219 (25).

3-Methoxy-2-(*o*-tolyl)benzonitrile (Table 2, entry 10)



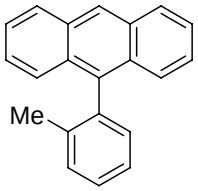
Hexane:EA = 20:1, R_f=0.25; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.12 (s, 3H), 3.78 (s, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.28-7.37 (m, 4H), 7.43 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.6, 55.9, 114.4, 115.1, 117.8, 124.6, 125.8, 128.7, 129.2, 129.7, 130.1, 134.3, 134.7, 136.7, 151.1; MS (EI) *m/z* (relative intensity) 223 (M^+, 100), 208 (50), 180 (40); HRMS: calcd. for $C_{15}H_{13}NOH^+$: 224.1075, found 224.1070.

Ethyl 2-*o*-tolyl-3-methoxybenzoate (Table 2, entry 11)



Hexane:EA = 20:1, R_f=0.3; pale red solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7 Hz, 3H), 2.10 (s, 3H), 3.75 (s, 3H), 3.97 (q, *J* = 6.8 Hz, 2H), 7.01 (d, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.16-7.20 (m, 1H), 7.24-7.26 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.5, 19.6, 55.9, 60.7, 113.6, 121.5, 125.1, 127.3, 128.4, 129.1, 130.8, 133.3, 136.9, 137.0, 157.0, 168.1; MS (EI) *m/z* (relative intensity) 270 (M^+, 70), 224 (100), 181 (40); HRMS: calcd. for $C_{17}H_{18}O_3Na^+$: 293.1154, found 293.1163.

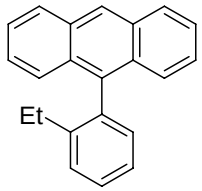
9-*o*-Tolylanthracene (Table 3, entry 1)[17]



Pure Hexane, R_f=0.5; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.88 (s, 3H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.33-7.42 (m, 3H), 7.44.7.49 (m, 4H), 7.52 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 8.4 Hz, 2H), 8.51 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 125.1, 125.5,

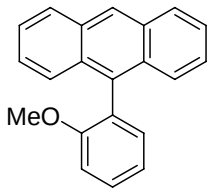
125.8, 126.4, 126.5, 127.9, 130.0, 131.2, 131.5, 136.4, 137.8, 138.2; MS (EI) *m/z* (relative intensity) 268 (M^+, 100), 252 (35), 126 (20).

9-(2-Ethylphenyl)anthracene (Table 3, entry 2)[18]



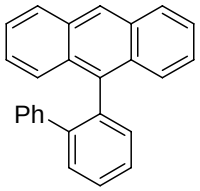
Pure Hexane, R_f=0.5; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.87 (t, *J* = 7.4 Hz, 3H), 2.19 (q, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.32-7.41 (m, 3H), 7.41-7.54 (m, 6H), 8.06 (d, *J* = 8.8 Hz, 2H), 8.51 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 26.3, 125.1, 125.3, 125.8, 126.4, 126.8, 128.1, 128.3, 128.4, 130.3, 131.4, 136.3, 137.6, 143.8; MS (EI) *m/z* (relative intensity) 282 (M^+, 100), 265 (40), 132 (15).

9-(2-Methoxyphenyl)anthracene (Table 3, entry 3)[19]



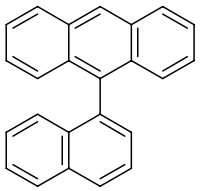
Hexane:EA = 20:1, R_f=0.5; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (s, 3H), 7.18-7.24 (m, 2H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.37-7.41 (m, 2H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 111.4, 120.8, 125.1, 125.3, 126.6, 126.8, 127.4, 128.5, 129.4, 130.5, 131.5, 132.9, 133.8, 158.1; MS (EI) *m/z* (relative intensity) 284 (M^+, 100), 268 (40), 119 (10).

9-(2-Biphenyl)anthracene (Table 3, entry 4)[20]



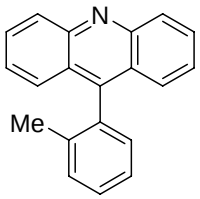
Pure Hexane, R_f=0.3; yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83-6.90 (m, 3H), 6.99-7.02 (m, 2H), 7.31-7.35 (m, 2H), 7.38-7.45 (m, 3H), 7.55-7.59 (m, 1H), 7.63-7.70 (m, 4H), 7.96 (d, *J* = 7.6 Hz, 2H), 8.38 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.9, 125.4, 126.5, 126.6, 126.9, 127.3, 127.4, 128.2, 128.4, 128.5, 130.3, 130.5, 131.2, 132.5, 136.2, 137.0, 141.2, 143.2; MS (EI) *m/z* (relative intensity) 330 (M^+, 100), 252 (40), 157 (15).

9-(1-Naphthalenyl)anthracene (Table 3, entry 5)[21]



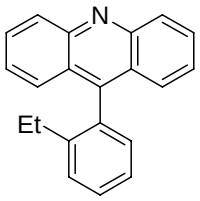
Pure Hexane, R_f=0.4; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 7.6 Hz, 1H), 7.21-7.31 (m, 3H), 7.46-7.53 (m, 5H), 7.57-7.59(m, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 8.04-8.15 (m, 4H), 8.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 125.3, 125.6, 126.0, 126.3, 127.0, 128.2, 128.3, 128.5, 129.2, 131.1, 131.5, 133.6, 133.8, 135.0, 136.6; MS (EI) *m/z* (relative intensity) 304 (M^+, 100), 150 (25), 138 (10).

9-*o*-Tolylacridine (Table 3, entry 6)[22]



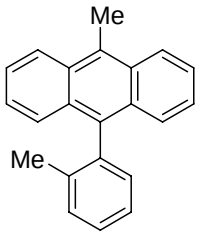
Hexane:EA = 9:1, R_f=0.4; pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.87 (s, 3H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.38-7.51 (m, 5H), 7.54 (d, *J* = 7.6 Hz, 2H), 7.78 (t, *J* = 8 Hz, 2H), 8.32 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 118.7, 125.1, 125.8, 125.9, 126.6, 128.7, 129.5, 130.2, 135.5, 136.9, 148.6; MS (EI) *m/z* (relative intensity) 269 (M^+, 100), 254 (30), 133 (10).

9-(2-Ethylphenyl)acridine (Table 3, entry 7)



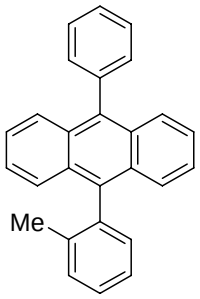
Hexane:EA = 9:1, R_f=0.35; yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.86 (t, *J* = 7.6 Hz, 3H), 2.17 (q, *J* = 7.6 Hz, 2H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.37-7.43 (m, 3H), 7.49-7.57 (m, 4H), 7.77 (t, *J* = 7.6 Hz, 2H), 8.30 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.0, 26.3, 125.5, 125.7, 125.8, 12.8, 128.5, 128.9, 129.5, 130.2, 130.4, 134.9, 143.0, 148.7; MS (EI) *m/z* (relative intensity) 283 (M^+, 100), 268 (80), 133 (20); HRMS: calcd. for $C_{21}H_{17}NH^+$: 284.1439, found 284.1452.

10-Methyl-9-*o*-tolylanthracene (Table 3, entry 8)



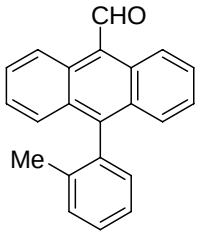
Pure Hexane, R_f=0.5; pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.89 (s, 3H), 3.20 (s, 3H), 7.27 (d, *J* = 8 Hz, 1H), 7.34-7.42 (m, 3H), 7.45-7.48 (m, 2H), 7.51-7.56 (m, 4H), 8.38 (d, *J* = 8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 19.8, 124.9, 125.1, 125.9, 127.3, 127.8, 129.9, 130.0, 131.5, 135.0, 138.0, 138.7; MS (EI) *m/z* (relative intensity) 282 (M^+, 100), 265 (35), 126 (20); HRMS: calcd. for $C_{22}H_{18}^+$: 282.1409, found 282.1415.

10-Phenyl-9-*o*-tolylanthracene (Table 3, entry 9)[23]



Pure Hexane, R_f=0.4; pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 3H), 7.33-7.37 (m, 5H), 7.42-7.45 (m, 1H), 7.49-7.64 (m, 9H), 7.72-7.74 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.9, 125.1, 125.2, 125.9, 126.7, 127.1, 127.5, 127.9, 128.4, 129.7, 130.0, 130.1, 131.4, 136.5, 138.0, 138.5, 139.1; MS (EI) *m/z* (relative intensity) 344.1 (M^+, 100), 265.1 (25), 163 (15).

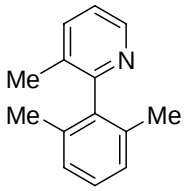
9-*o*-Tolylanthracene-10-carbaldehyde (Table 3, entry 10)



Hexane:EA = 20:1, R_f=0.4; yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 (s, 3H), 7.00-7.03 (m, 3H), 7.17-7.19 (m, 2H), 7.22-7.26 (m, 3H), 7.58 (d, *J* = 8.8 Hz, 2H),

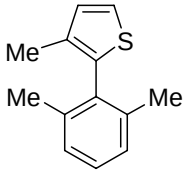
8.94 (d, *J* = 8.8 Hz, 2H), 11.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 123.7, 125.0, 125.8, 126.0, 127.6, 128.4, 128.7, 129.7, 130.2, 130.5, 131.8, 137.2, 137.7, 145.2, 193.4; MS (EI) *m/z* (relative intensity) 296 (M^+, 100), 252 (45), 126 (25); HRMS: calcd. for $C_{22}H_{16}OH^+$: 297.1279, found 297.1284.

2-(2,6-Dimethylphenyl)-3-methylpyridine (Table 4, entry 4)[24]



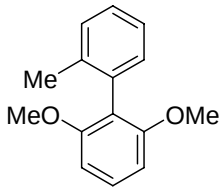
Hexane:EA = 10:1, R_f=0.25; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 (s, 6H), 2.01 (s, 3H), 7.08 (d, *J* = 7.6 Hz, 2H), 7.15-7.19 (m, 2H), 7.58 (d, *J* = 7.6 Hz, 1H), 8.54 (d, *J* = 4.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4, 19.6, 122.1, 127.5, 127.7, 131.7, 135.3, 137.6, 139.6, 147.3, 159.3; MS (EI) *m/z* (relative intensity) 197 (M^+, 25), 182 (100), 167 (30).

2-(2,6-Dimethylphenyl)-3-methylthiophene (Table 4, entry 5)



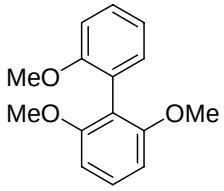
Pure Hexane, R_f=0.6; colourless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.98 (s, 3H), 2.13 (s, 3H), 6.98 (d, *J* = 5.2 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 2H), 7.20-7.24 (m, 1H), 7.30 (d, *J* = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 20.5, 123.9, 127.2, 128.1, 129.6, 133.4, 133.9, 135.8, 138.8; MS (EI) *m/z* (relative intensity) 202 (M^+, 100), 187 (85), 172 (35); HRMS: calcd. for $C_{13}H_{14}S^+$: 202.0816, found 202.0818,.

2',6'-Dimethoxy-2-methylbiphenyl (Table 4, entry 6)[25]



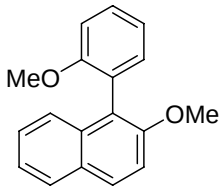
Hexane:EA = 50:1, R_f=0.3; white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.09 (s, 3H), 3.73 (s, 6H), 6.66 (d, *J* = 7.6 Hz, 2H), 7.14-7.17 (m, 1H), 7.24-7.34 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 55.9, 104.0, 119.0, 125.2, 127.2, 128.7, 129.5, 130.8, 134.2, 137.4, 157.8; MS (EI) *m/z* (relative intensity) 228 (M^+, 100), 213 (25), 197 (40).

2,2',6'-Trimethoxybiphenyl (Table 4, entry 7)[26]



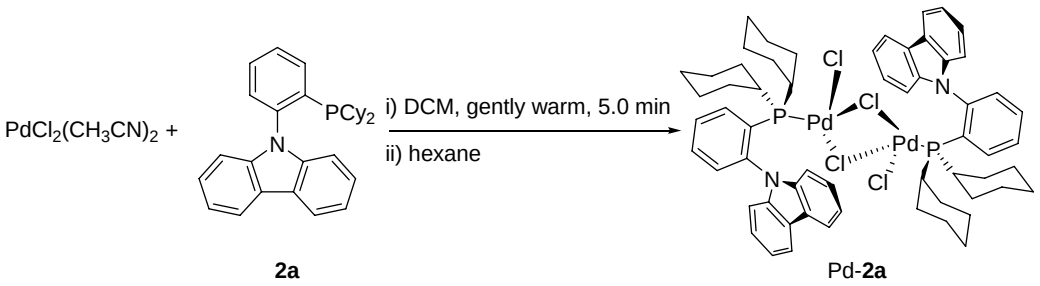
Hexane:EA = 10:1, R_f=0.3; pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (s, 6H), 3.76 (s, 3H), 6.67 (d, *J* = 8.0 Hz, 2H), 7.00-7.05 (m, 2H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.28-7.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.9, 56.1, 104.3, 111.3, 120.3, 123.6, 128.5, 128.7, 132.2, 157.5, 158.1; MS (EI) *m/z* (relative intensity) 244 (M^+, 100), 213 (20), 198 (25).

2-Methoxy-1-(2-methoxyphenyl)naphthalene (Table 4, entry 8)[27]



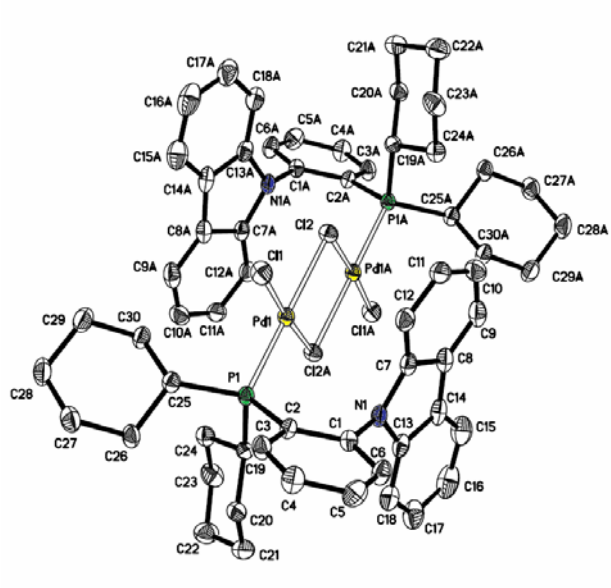
Hexane:EA = 20:1, R_f=0.3; purple solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71 (s, 3H), 3.86 (s, 3H), 7.08-7.13 (m, 2H), 7.23-7.26 (m, 1H), 7.32-7.36 (m, 2H), 7.38-7.43 (m, 2H), 7.43-7.47 (m, 1H), 7.82-7.85(m, 1H), 7.90 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 57.0, 111.4, 114.2, 120.6, 123.4, 125.3, 125.4, 126.1, 127.9, 128.9, 129.1, 132.5, 133.7, 154.3, 157.8; MS (EI) *m/z* (relative intensity) 264 (M^+, 100), 249 (15), 218 (30).

8. Preparation of Pd-2a complex



2a Pd-**2a**

Bis(acetonitrile)dichloropalladium(II) (12.9 mg, 0.05 mmol) and **2a** (22 mg, 0.05 mmol) were dissolved in freshly distilled dichloromethane (0.5 mL) under nitrogen at room temperature. The yellow solution was warmed to 40 °C for 5 minutes. Anhydrous hexane (1.0 mL) was slowly added and yellow single crystals were obtained.



Full X-ray data (cif) were reported in Section 8.

9. X-ray crystallographic data of Pd-2a complex

Table 1. Crystal data and structure refinement for Pd-**2a** complex (4 Oct 2010).

Identification code	tsc9	
Empirical formula	$[PdCl(mu\text{-}Cl)C_{30}H_{34}NP]_2 .2(CH_2Cl_2)$	
Formula weight	701.78	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.7713(6) Å	α= 96.295(3)°.
	b = 11.8421(6) Å	β= 106.772(3)°.
	c = 12.6198(6) Å	γ = 109.775(3)°.
Volume	1542.49(13) $Å^3$	
Z	2	
Density (calculated)	1.511 Mg/m^3	
Absorption coefficient	1.022 mm^{-1}	
F(000)	716	
Crystal size	0.40 x 0.18 x 0.01 mm^3	
Theta range for data collection	1.73 to 27.55°.	
Index ranges	-15<=h<=15, -15<=k<=15, -16<=l<=16	
Reflections collected	32764	
Independent reflections	7059 [R(int) = 0.0864]	
Completeness to theta = 27.55°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9899 and 0.6853	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7059 / 4 / 340	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.1454	
R indices (all data)	R1 = 0.1051, wR2 = 0.1706	
Largest diff. peak and hole	0.860 and -0.755 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for tsc9. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5156(1)	6546(1)	5310(1)	40(1)
Cl(1)	4421(1)	7762(1)	4239(1)	57(1)
Cl(2)	4120(1)	4775(1)	3709(1)	44(1)
P(1)	6113(1)	8207(1)	6757(1)	39(1)
N(1)	8325(2)	7904(3)	5979(3)	49(1)
C(1)	8439(3)	9148(4)	6300(3)	45(1)
C(2)	7445(3)	9407(3)	6530(3)	40(1)
C(3)	7543(3)	10609(4)	6644(3)	55(1)
C(4)	8590(4)	11537(4)	6582(4)	63(1)
C(5)	9578(4)	11275(4)	6400(4)	66(1)
C(6)	9490(3)	10089(4)	6261(3)	58(1)
C(7)	7837(3)	7260(4)	4846(3)	49(1)
C(8)	8163(3)	6237(4)	4751(3)	55(1)
C(9)	7779(4)	5487(4)	3695(4)	69(1)
C(10)	7115(4)	5774(5)	2767(4)	75(2)
C(11)	6803(4)	6788(4)	2858(4)	64(1)
C(12)	7151(3)	7557(4)	3877(3)	57(1)
C(13)	9056(3)	7336(4)	6614(3)	52(1)
C(14)	8935(3)	6286(4)	5897(4)	61(1)
C(15)	9531(4)	5520(4)	6360(4)	79(2)
C(16)	10251(5)	5858(5)	7503(5)	97(2)
C(17)	10390(4)	6928(5)	8185(4)	90(2)
C(18)	9791(4)	7682(5)	7744(4)	68(1)
C(19)	6895(3)	7874(3)	8109(3)	43(1)
C(20)	7930(4)	8983(4)	9048(3)	58(1)
C(21)	8584(4)	8557(5)	10047(4)	71(2)
C(22)	7619(4)	7720(5)	10500(4)	78(2)
C(23)	6601(4)	6660(4)	9584(4)	72(1)
C(24)	5908(3)	7069(4)	8568(3)	53(1)
C(25)	4972(3)	8911(3)	6925(3)	45(1)
C(26)	5368(3)	9820(4)	8052(4)	56(1)
C(27)	4399(4)	10424(4)	7996(4)	70(1)
C(28)	3057(4)	9469(5)	7721(4)	77(2)

C(29)	2649(4)	8539(4)	6633(4)	69(1)
C(30)	3616(3)	7929(4)	6678(4)	54(1)
C(31)	7534(11)	13936(14)	8593(11)	189(8)
Cl(3)	8692(4)	13288(4)	8858(4)	134(1)
Cl(4)	6926(5)	13676(6)	9649(5)	184(2)
C(31')	6779(8)	13504(11)	8686(8)	91(3)
Cl(3')	8323(6)	14239(6)	8885(5)	201(2)
Cl(4')	6512(3)	13493(3)	9909(3)	105(1)

Table 3. Bond lengths [Å] and angles [°] for tsc9.

Pd(1)-P(1)	2.2352(9)
Pd(1)-Cl(1)	2.2904(11)
Pd(1)-Cl(2)#1	2.3286(10)
Pd(1)-Cl(2)	2.4257(9)
Cl(2)-Pd(1)#1	2.3286(10)
P(1)-C(2)	1.843(3)
P(1)-C(19)	1.844(4)
P(1)-C(25)	1.852(4)
N(1)-C(7)	1.394(5)
N(1)-C(13)	1.397(5)
N(1)-C(1)	1.434(5)
C(1)-C(6)	1.375(5)
C(1)-C(2)	1.403(5)
C(2)-C(3)	1.376(6)
C(3)-C(4)	1.375(5)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.373(6)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.360(7)
C(5)-H(5A)	0.9300
C(6)-H(6A)	0.9300
C(7)-C(8)	1.393(6)
C(7)-C(12)	1.410(6)
C(8)-C(9)	1.375(6)
C(8)-C(14)	1.452(6)
C(9)-C(10)	1.355(7)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.372(7)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.356(6)
C(11)-H(11A)	0.9300
C(12)-H(12A)	0.9300
C(13)-C(18)	1.367(5)
C(13)-C(14)	1.395(6)
C(14)-C(15)	1.402(7)
C(15)-C(16)	1.378(7)

C(15)-H(15A)	0.9300
C(16)-C(17)	1.382(8)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.383(7)
C(17)-H(17A)	0.9300
C(18)-H(18A)	0.9300
C(19)-C(24)	1.535(5)
C(19)-C(20)	1.535(5)
C(19)-H(19A)	0.9800
C(20)-C(21)	1.510(6)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-C(22)	1.529(6)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(23)	1.487(6)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.531(6)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(26)	1.530(5)
C(25)-C(30)	1.540(4)
C(25)-H(25A)	0.9800
C(26)-C(27)	1.528(6)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-C(28)	1.511(6)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-C(29)	1.502(6)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(29)-C(30)	1.533(6)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700

C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(31)-Cl(4)	1.696(13)
C(31)-Cl(3)	1.750(13)
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(31')-Cl(3')	1.656(10)
C(31')-Cl(4')	1.662(10)
C(31')-H(31C)	0.9700
C(31')-H(31D)	0.9700

P(1)-Pd(1)-Cl(1)	86.47(4)
P(1)-Pd(1)-Cl(2)#1	96.99(3)
Cl(1)-Pd(1)-Cl(2)#1	176.31(4)
P(1)-Pd(1)-Cl(2)	178.64(4)
Cl(1)-Pd(1)-Cl(2)	92.31(3)
Cl(2)#1-Pd(1)-Cl(2)	84.21(3)
Pd(1)#1-Cl(2)-Pd(1)	95.79(3)
C(2)-P(1)-C(19)	103.83(15)
C(2)-P(1)-C(25)	106.89(17)
C(19)-P(1)-C(25)	110.24(18)
C(2)-P(1)-Pd(1)	111.35(12)
C(19)-P(1)-Pd(1)	112.64(12)
C(25)-P(1)-Pd(1)	111.50(11)
C(7)-N(1)-C(13)	107.5(3)
C(7)-N(1)-C(1)	122.4(3)
C(13)-N(1)-C(1)	126.1(3)
C(6)-C(1)-C(2)	119.9(4)
C(6)-C(1)-N(1)	118.4(4)
C(2)-C(1)-N(1)	121.4(3)
C(3)-C(2)-C(1)	117.2(3)
C(3)-C(2)-P(1)	121.4(3)
C(1)-C(2)-P(1)	121.3(3)
C(4)-C(3)-C(2)	122.2(4)
C(4)-C(3)-H(3A)	118.9
C(2)-C(3)-H(3A)	118.9
C(5)-C(4)-C(3)	119.9(4)
C(5)-C(4)-H(4A)	120.1

C(3)-C(4)-H(4A)	120.1
C(6)-C(5)-C(4)	119.0(4)
C(6)-C(5)-H(5A)	120.5
C(4)-C(5)-H(5A)	120.5
C(5)-C(6)-C(1)	121.8(4)
C(5)-C(6)-H(6A)	119.1
C(1)-C(6)-H(6A)	119.1
C(8)-C(7)-N(1)	110.4(4)
C(8)-C(7)-C(12)	121.2(4)
N(1)-C(7)-C(12)	128.3(4)
C(9)-C(8)-C(7)	119.3(4)
C(9)-C(8)-C(14)	135.3(4)
C(7)-C(8)-C(14)	105.3(4)
C(10)-C(9)-C(8)	119.3(5)
C(10)-C(9)-H(9A)	120.4
C(8)-C(9)-H(9A)	120.4
C(9)-C(10)-C(11)	121.5(4)
C(9)-C(10)-H(10A)	119.2
C(11)-C(10)-H(10A)	119.2
C(12)-C(11)-C(10)	121.8(4)
C(12)-C(11)-H(11A)	119.1
C(10)-C(11)-H(11A)	119.1
C(11)-C(12)-C(7)	116.9(5)
C(11)-C(12)-H(12A)	121.5
C(7)-C(12)-H(12A)	121.5
C(18)-C(13)-C(14)	122.3(4)
C(18)-C(13)-N(1)	129.1(4)
C(14)-C(13)-N(1)	108.5(3)
C(13)-C(14)-C(15)	118.9(4)
C(13)-C(14)-C(8)	108.0(4)
C(15)-C(14)-C(8)	133.1(4)
C(16)-C(15)-C(14)	118.5(5)
C(16)-C(15)-H(15A)	120.7
C(14)-C(15)-H(15A)	120.7
C(15)-C(16)-C(17)	121.1(5)
C(15)-C(16)-H(16A)	119.4
C(17)-C(16)-H(16A)	119.4
C(16)-C(17)-C(18)	121.0(5)

C(16)-C(17)-H(17A)	119.5
C(18)-C(17)-H(17A)	119.5
C(13)-C(18)-C(17)	118.0(5)
C(13)-C(18)-H(18A)	121.0
C(17)-C(18)-H(18A)	121.0
C(24)-C(19)-C(20)	110.8(3)
C(24)-C(19)-P(1)	112.0(2)
C(20)-C(19)-P(1)	116.7(3)
C(24)-C(19)-H(19A)	105.4
C(20)-C(19)-H(19A)	105.4
P(1)-C(19)-H(19A)	105.4
C(21)-C(20)-C(19)	110.5(4)
C(21)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20A)	109.5
C(21)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	108.1
C(20)-C(21)-C(22)	112.0(4)
C(20)-C(21)-H(21A)	109.2
C(22)-C(21)-H(21A)	109.2
C(20)-C(21)-H(21B)	109.2
C(22)-C(21)-H(21B)	109.2
H(21A)-C(21)-H(21B)	107.9
C(23)-C(22)-C(21)	111.5(4)
C(23)-C(22)-H(22A)	109.3
C(21)-C(22)-H(22A)	109.3
C(23)-C(22)-H(22B)	109.3
C(21)-C(22)-H(22B)	109.3
H(22A)-C(22)-H(22B)	108.0
C(22)-C(23)-C(24)	112.5(4)
C(22)-C(23)-H(23A)	109.1
C(24)-C(23)-H(23A)	109.1
C(22)-C(23)-H(23B)	109.1
C(24)-C(23)-H(23B)	109.1
H(23A)-C(23)-H(23B)	107.8
C(23)-C(24)-C(19)	109.6(3)
C(23)-C(24)-H(24A)	109.8
C(19)-C(24)-H(24A)	109.8

C(23)-C(24)-H(24B)	109.8
C(19)-C(24)-H(24B)	109.8
H(24A)-C(24)-H(24B)	108.2
C(26)-C(25)-C(30)	108.8(3)
C(26)-C(25)-P(1)	117.3(2)
C(30)-C(25)-P(1)	111.9(3)
C(26)-C(25)-H(25A)	106.0
C(30)-C(25)-H(25A)	106.0
P(1)-C(25)-H(25A)	106.0
C(27)-C(26)-C(25)	110.4(3)
C(27)-C(26)-H(26A)	109.6
C(25)-C(26)-H(26A)	109.6
C(27)-C(26)-H(26B)	109.6
C(25)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	108.1
C(28)-C(27)-C(26)	111.2(4)
C(28)-C(27)-H(27A)	109.4
C(26)-C(27)-H(27A)	109.4
C(28)-C(27)-H(27B)	109.4
C(26)-C(27)-H(27B)	109.4
H(27A)-C(27)-H(27B)	108.0
C(29)-C(28)-C(27)	111.3(4)
C(29)-C(28)-H(28A)	109.4
C(27)-C(28)-H(28A)	109.4
C(29)-C(28)-H(28B)	109.4
C(27)-C(28)-H(28B)	109.4
H(28A)-C(28)-H(28B)	108.0
C(28)-C(29)-C(30)	111.2(3)
C(28)-C(29)-H(29A)	109.4
C(30)-C(29)-H(29A)	109.4
C(28)-C(29)-H(29B)	109.4
C(30)-C(29)-H(29B)	109.4
H(29A)-C(29)-H(29B)	108.0
C(29)-C(30)-C(25)	110.5(3)
C(29)-C(30)-H(30A)	109.6
C(25)-C(30)-H(30A)	109.6
C(29)-C(30)-H(30B)	109.6
C(25)-C(30)-H(30B)	109.6

H(30A)-C(30)-H(30B)	108.1
Cl(4)-C(31)-Cl(3)	103.0(8)
Cl(4)-C(31)-H(31A)	111.2
Cl(3)-C(31)-H(31A)	111.2
Cl(4)-C(31)-H(31B)	111.2
Cl(3)-C(31)-H(31B)	111.2
H(31A)-C(31)-H(31B)	109.1
Cl(3')-C(31')-Cl(4')	111.9(5)
Cl(3')-C(31')-H(31C)	109.2
Cl(4')-C(31')-H(31C)	109.2
Cl(3')-C(31')-H(31D)	109.2
Cl(4')-C(31')-H(31D)	109.2
H(31C)-C(31')-H(31D)	107.9

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for tsc9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	43(1)	35(1)	46(1)	8(1)	18(1)	18(1)
Cl(1)	73(1)	58(1)	57(1)	20(1)	22(1)	42(1)
Cl(2)	52(1)	35(1)	44(1)	7(1)	13(1)	19(1)
P(1)	38(1)	33(1)	48(1)	6(1)	20(1)	13(1)
N(1)	45(1)	55(2)	60(2)	13(1)	26(1)	27(1)
C(1)	47(2)	50(2)	45(2)	13(2)	21(1)	22(1)
C(2)	37(1)	39(2)	48(2)	12(1)	19(1)	16(1)
C(3)	54(2)	43(2)	72(2)	8(2)	32(2)	17(2)
C(4)	66(2)	44(2)	85(3)	21(2)	36(2)	18(2)
C(5)	52(2)	62(3)	82(3)	23(2)	33(2)	11(2)
C(6)	49(2)	59(2)	73(2)	21(2)	34(2)	20(2)
C(7)	47(1)	49(2)	62(2)	13(2)	32(1)	20(2)
C(8)	56(2)	48(2)	76(2)	15(2)	40(2)	23(2)
C(9)	70(2)	49(2)	96(3)	4(2)	51(2)	17(2)
C(10)	63(2)	72(3)	68(3)	-10(2)	29(2)	3(2)
C(11)	54(2)	74(3)	56(2)	9(2)	23(2)	16(2)
C(12)	50(2)	62(2)	67(2)	17(2)	32(2)	22(2)
C(13)	50(1)	66(2)	63(2)	31(2)	35(1)	32(2)
C(14)	61(2)	57(2)	93(2)	29(2)	51(2)	33(2)
C(15)	89(2)	65(3)	115(3)	38(2)	55(2)	46(2)
C(16)	117(3)	121(3)	124(3)	77(3)	72(2)	90(2)
C(17)	93(2)	143(4)	81(3)	59(3)	40(2)	81(2)
C(18)	68(2)	85(3)	77(3)	30(2)	38(2)	45(2)
C(19)	42(1)	41(2)	45(2)	4(2)	16(1)	16(1)
C(20)	55(2)	51(2)	60(2)	2(2)	23(2)	13(2)
C(21)	57(2)	86(3)	56(2)	13(2)	12(2)	19(2)
C(22)	71(2)	94(4)	58(3)	22(2)	17(2)	22(3)
C(23)	90(2)	71(3)	66(2)	29(2)	42(2)	28(2)
C(24)	56(2)	43(2)	59(2)	11(2)	27(2)	14(2)
C(25)	44(2)	36(2)	59(2)	9(2)	21(1)	15(1)
C(26)	57(2)	44(2)	71(2)	4(2)	31(2)	22(2)
C(27)	74(2)	63(3)	82(3)	2(2)	37(2)	35(2)
C(28)	68(2)	75(3)	104(3)	2(2)	43(2)	39(2)

C(29)	49(2)	75(3)	87(3)	12(2)	29(2)	25(2)
C(30)	42(2)	50(2)	71(2)	4(2)	27(2)	14(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for tsc9.

	x	y	z	U(eq)
H(3A)	6880	10799	6766	66
H(4A)	8629	12341	6664	76
H(5A)	10298	11900	6371	79
H(6A)	10158	9911	6136	69
H(9A)	7974	4790	3618	83
H(10A)	6864	5272	2052	90
H(11A)	6340	6952	2203	76
H(12A)	6946	8249	3935	68
H(15A)	9442	4799	5906	95
H(16A)	10651	5358	7822	117
H(17A)	10895	7144	8951	109
H(18A)	9885	8402	8202	82
H(19A)	7345	7365	7920	51
H(20A)	8564	9460	8750	69
H(20B)	7536	9511	9296	69
H(21A)	9191	9271	10651	85
H(21B)	9064	8114	9817	85
H(22A)	8069	7414	11098	93
H(22B)	7221	8194	10826	93
H(23A)	5977	6183	9890	86
H(23B)	6989	6131	9326	86
H(24A)	5446	7532	8801	63
H(24B)	5288	6350	7975	63
H(25A)	4883	9381	6335	55
H(26A)	5411	9388	8663	67
H(26B)	6216	10450	8211	67
H(27A)	4653	10984	8722	84
H(27B)	4400	10901	7419	84
H(28A)	3034	9051	8338	93
H(28B)	2457	9875	7650	93
H(29A)	2578	8944	6003	83
H(29B)	1808	7912	6503	83

H(30A)	3347	7356	5958	65
H(30B)	3637	7468	7269	65
H(31A)	7922	14812	8634	227
H(31B)	6871	13534	7851	227
H(31C)	6488	12661	8267	109
H(31D)	6283	13900	8232	109

Table 6. Torsion angles [°] for tsc9.

P(1)-Pd(1)-Cl(2)-Pd(1)#1	152.1(14)
Cl(1)-Pd(1)-Cl(2)-Pd(1)#1	178.76(4)
Cl(2)#1-Pd(1)-Cl(2)-Pd(1)#1	0.0
Cl(1)-Pd(1)-P(1)-C(2)	-68.63(13)
Cl(2)#1-Pd(1)-P(1)-C(2)	110.09(13)
Cl(2)-Pd(1)-P(1)-C(2)	-41.9(14)
Cl(1)-Pd(1)-P(1)-C(19)	175.20(13)
Cl(2)#1-Pd(1)-P(1)-C(19)	-6.08(13)
Cl(2)-Pd(1)-P(1)-C(19)	-158.1(14)
Cl(1)-Pd(1)-P(1)-C(25)	50.65(14)
Cl(2)#1-Pd(1)-P(1)-C(25)	-130.63(14)
Cl(2)-Pd(1)-P(1)-C(25)	77.4(14)
C(7)-N(1)-C(1)-C(6)	-81.6(4)
C(13)-N(1)-C(1)-C(6)	73.2(5)
C(7)-N(1)-C(1)-C(2)	91.5(4)
C(13)-N(1)-C(1)-C(2)	-113.7(4)
C(6)-C(1)-C(2)-C(3)	3.7(5)
N(1)-C(1)-C(2)-C(3)	-169.3(3)
C(6)-C(1)-C(2)-P(1)	-172.8(3)
N(1)-C(1)-C(2)-P(1)	14.2(5)
C(19)-P(1)-C(2)-C(3)	-108.7(3)
C(25)-P(1)-C(2)-C(3)	7.8(3)
Pd(1)-P(1)-C(2)-C(3)	129.8(3)
C(19)-P(1)-C(2)-C(1)	67.5(3)
C(25)-P(1)-C(2)-C(1)	-175.9(3)
Pd(1)-P(1)-C(2)-C(1)	-53.9(3)
C(1)-C(2)-C(3)-C(4)	-2.6(6)
P(1)-C(2)-C(3)-C(4)	173.9(3)
C(2)-C(3)-C(4)-C(5)	0.1(6)
C(3)-C(4)-C(5)-C(6)	1.2(6)
C(4)-C(5)-C(6)-C(1)	-0.1(6)
C(2)-C(1)-C(6)-C(5)	-2.4(6)
N(1)-C(1)-C(6)-C(5)	170.8(4)
C(13)-N(1)-C(7)-C(8)	4.2(4)
C(1)-N(1)-C(7)-C(8)	163.1(3)
C(13)-N(1)-C(7)-C(12)	-173.3(3)

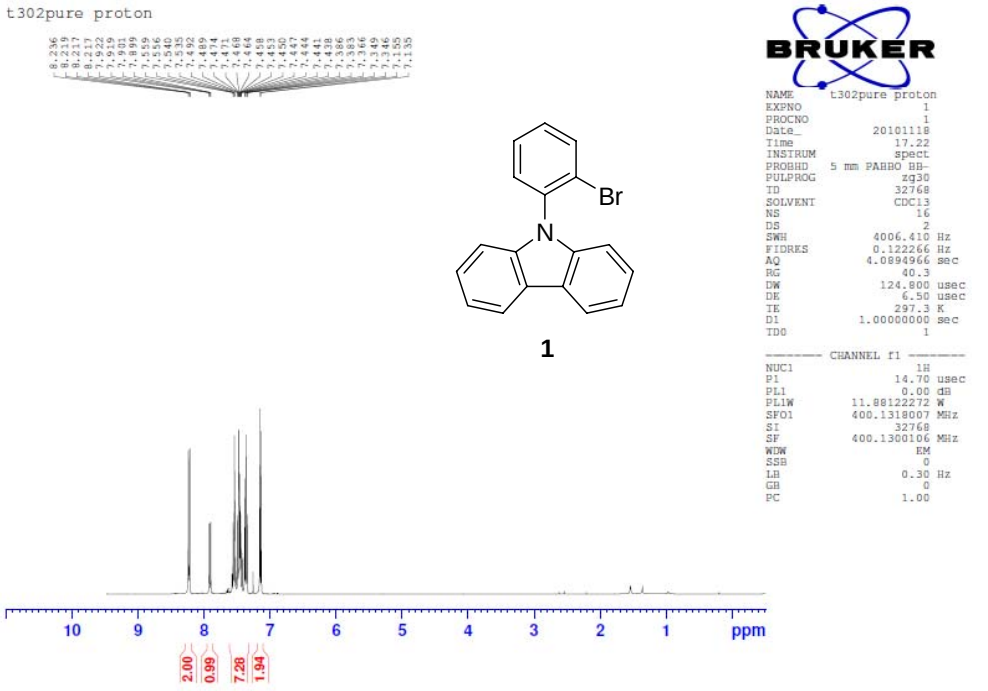
C(1)-N(1)-C(7)-C(12)	-14.4(5)
N(1)-C(7)-C(8)-C(9)	-179.4(3)
C(12)-C(7)-C(8)-C(9)	-1.6(5)
N(1)-C(7)-C(8)-C(14)	-1.9(4)
C(12)-C(7)-C(8)-C(14)	175.8(3)
C(7)-C(8)-C(9)-C(10)	1.3(6)
C(14)-C(8)-C(9)-C(10)	-175.2(4)
C(8)-C(9)-C(10)-C(11)	-0.8(6)
C(9)-C(10)-C(11)-C(12)	0.5(7)
C(10)-C(11)-C(12)-C(7)	-0.8(6)
C(8)-C(7)-C(12)-C(11)	1.3(5)
N(1)-C(7)-C(12)-C(11)	178.6(3)
C(7)-N(1)-C(13)-C(18)	175.1(4)
C(1)-N(1)-C(13)-C(18)	17.2(6)
C(7)-N(1)-C(13)-C(14)	-4.8(4)
C(1)-N(1)-C(13)-C(14)	-162.8(3)
C(18)-C(13)-C(14)-C(15)	3.5(6)
N(1)-C(13)-C(14)-C(15)	-176.5(3)
C(18)-C(13)-C(14)-C(8)	-176.3(4)
N(1)-C(13)-C(14)-C(8)	3.7(4)
C(9)-C(8)-C(14)-C(13)	175.7(4)
C(7)-C(8)-C(14)-C(13)	-1.1(4)
C(9)-C(8)-C(14)-C(15)	-4.1(8)
C(7)-C(8)-C(14)-C(15)	179.1(4)
C(13)-C(14)-C(15)-C(16)	-2.2(6)
C(8)-C(14)-C(15)-C(16)	177.6(4)
C(14)-C(15)-C(16)-C(17)	-0.1(7)
C(15)-C(16)-C(17)-C(18)	1.2(8)
C(14)-C(13)-C(18)-C(17)	-2.4(6)
N(1)-C(13)-C(18)-C(17)	177.6(4)
C(16)-C(17)-C(18)-C(13)	0.1(7)
C(2)-P(1)-C(19)-C(24)	169.2(3)
C(25)-P(1)-C(19)-C(24)	55.1(3)
Pd(1)-P(1)-C(19)-C(24)	-70.2(3)
C(2)-P(1)-C(19)-C(20)	40.0(3)
C(25)-P(1)-C(19)-C(20)	-74.2(3)
Pd(1)-P(1)-C(19)-C(20)	160.6(3)
C(24)-C(19)-C(20)-C(21)	56.7(5)

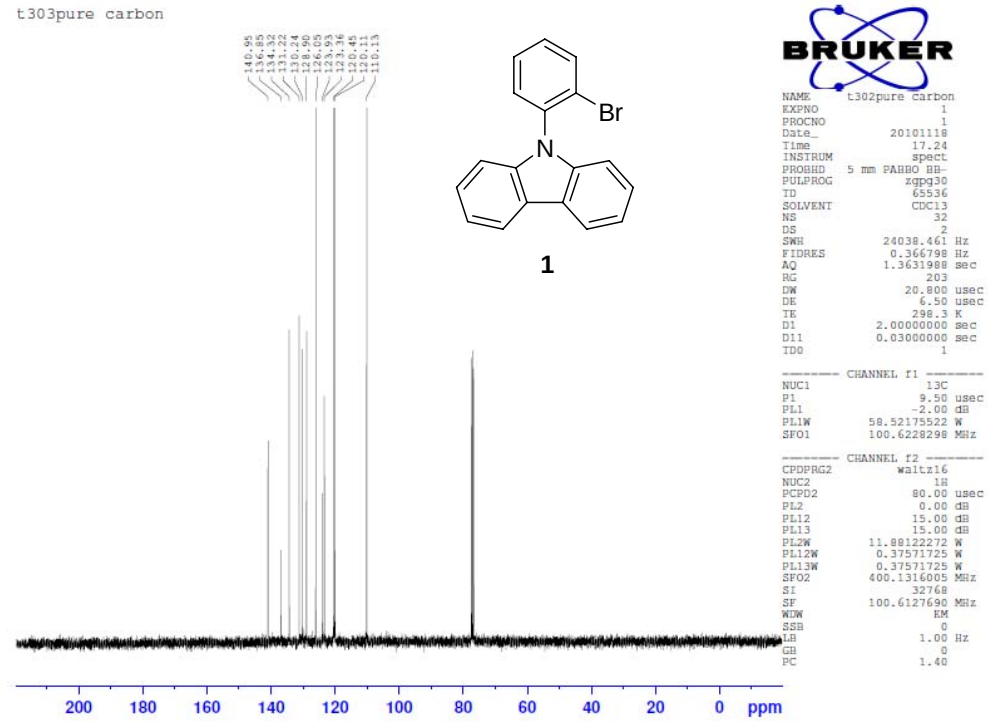
P(1)-C(19)-C(20)-C(21)	-173.6(3)
C(19)-C(20)-C(21)-C(22)	-55.0(5)
C(20)-C(21)-C(22)-C(23)	54.4(6)
C(21)-C(22)-C(23)-C(24)	-55.0(6)
C(22)-C(23)-C(24)-C(19)	56.3(5)
C(20)-C(19)-C(24)-C(23)	-56.4(5)
P(1)-C(19)-C(24)-C(23)	171.4(3)
C(2)-P(1)-C(25)-C(26)	-74.4(3)
C(19)-P(1)-C(25)-C(26)	37.8(3)
Pd(1)-P(1)-C(25)-C(26)	163.7(3)
C(2)-P(1)-C(25)-C(30)	158.8(3)
C(19)-P(1)-C(25)-C(30)	-88.9(3)
Pd(1)-P(1)-C(25)-C(30)	36.9(3)
C(30)-C(25)-C(26)-C(27)	-58.4(5)
P(1)-C(25)-C(26)-C(27)	173.4(3)
C(25)-C(26)-C(27)-C(28)	57.8(5)
C(26)-C(27)-C(28)-C(29)	-56.0(6)
C(27)-C(28)-C(29)-C(30)	55.6(6)
C(28)-C(29)-C(30)-C(25)	-57.1(5)
C(26)-C(25)-C(30)-C(29)	58.1(5)
P(1)-C(25)-C(30)-C(29)	-170.7(3)

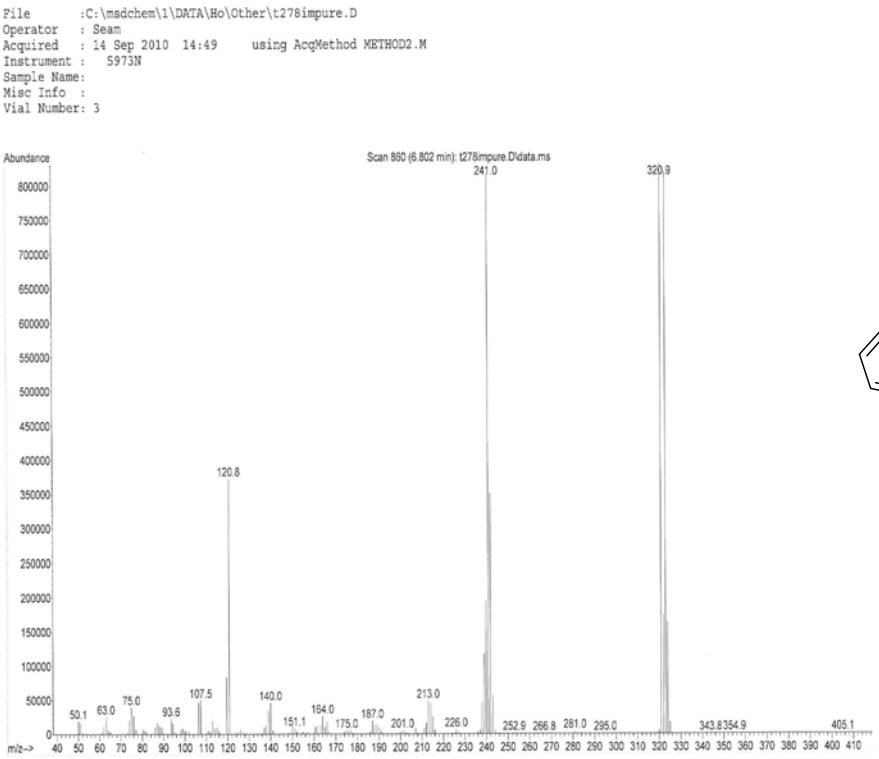
Symmetry transformations used to generate equivalent atoms:

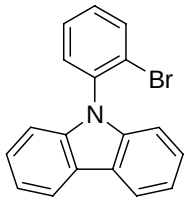
#1 -x+1,-y+1,-z+1

10. ^{1}H, ^{13}C, ^{31}P NMR, IR, MS and HRMS spectra

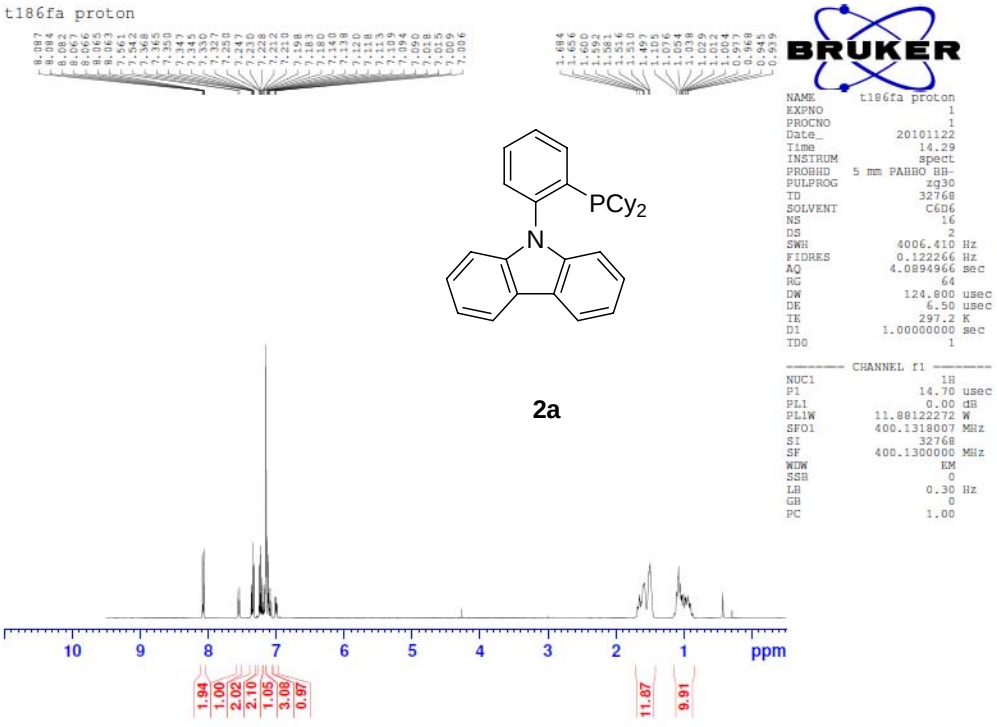




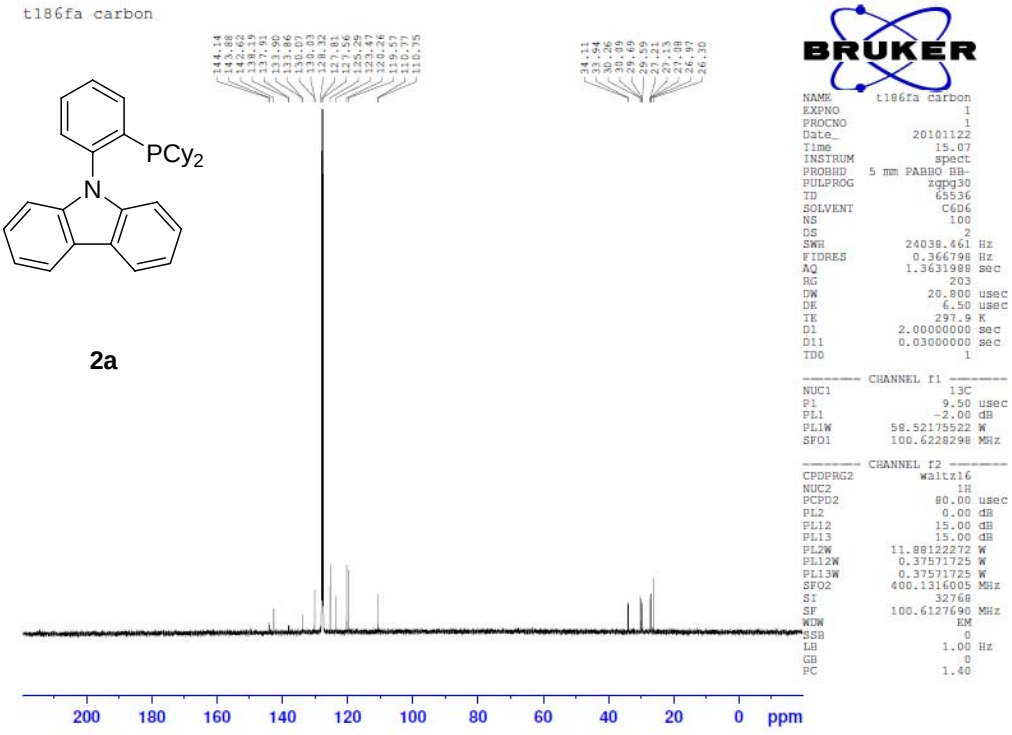

File :C:\msdchem\1\DATA\Ho\Other\t278impure.D
Operator : Seam
Acquired : 14 Sep 2010 14:49 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 860 (6.802 min): t278impure.D\data.ms
241.0
320.9
120.8
m/z-->

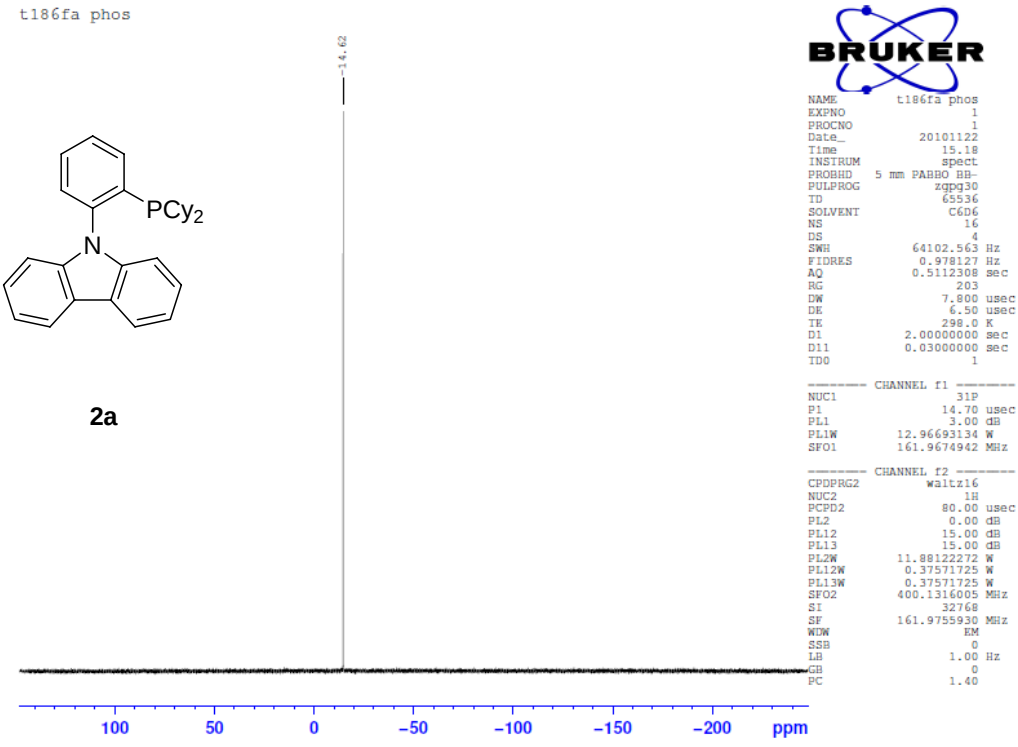

Br
N

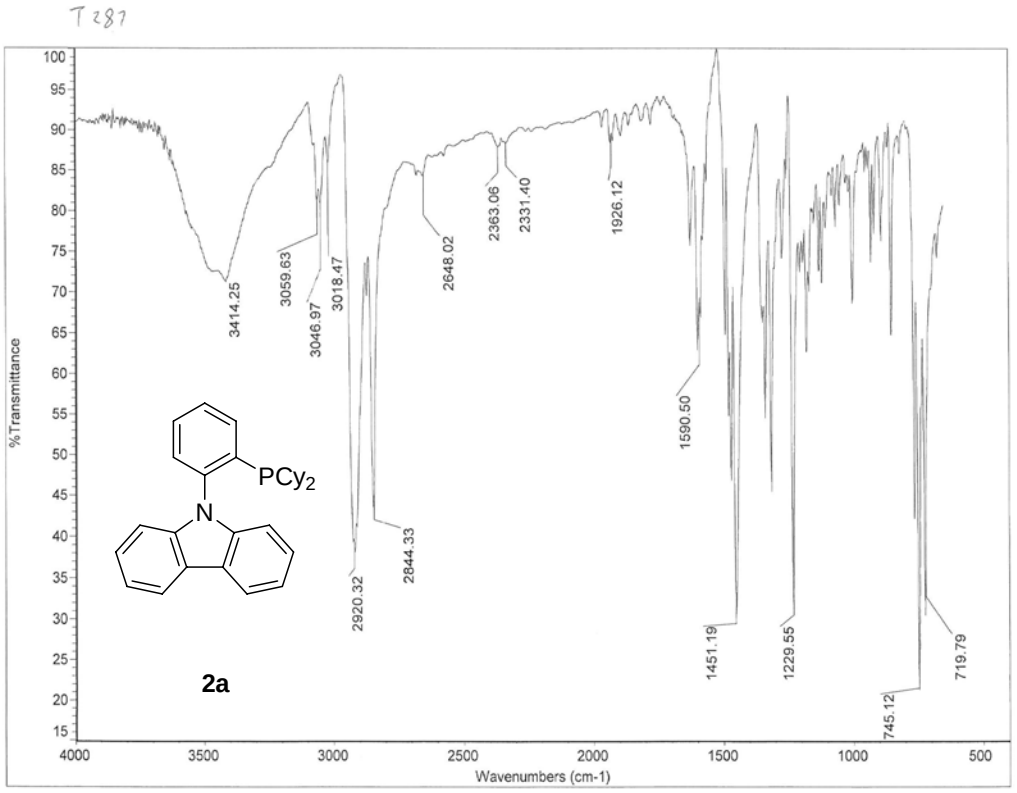
1


t186fa proton
PCy2
N
BRUKER
NAME t186fa proton
EXPNO 1
PROCNO 1
Date_ 20101122
Time 14.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT C6D6
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 124.800 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.94 1.00 2.02 2.10 1.05 3.06 0.97
11.87 9.91

2a


t186fa carbon
PCy2
N
2a
BRUKER
NAME t186fa carbon
EXPNO 1
PROCNO 1
Date_ 20101122
Time 15.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 100
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


t186fa phos
PCy2
N
2a
BRUKER
NAME t186fa phos
EXPNO 1
PROCNO 1
Date_ 20101122
Time 15.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 203
DW 7.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 31P
P1 14.70 usec
PL1 3.00 dB
PL1W 12.96693134 W
SFO1 161.9674942 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
100 50 0 -50 -100 -150 -200 ppm




```
File       :C:\msdchem\1\DATA\sean\t287ff.D
Operator   : Seam
Acquired   :  8 Oct 2010  17:36     using AcqMethod WANGJUN2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 6
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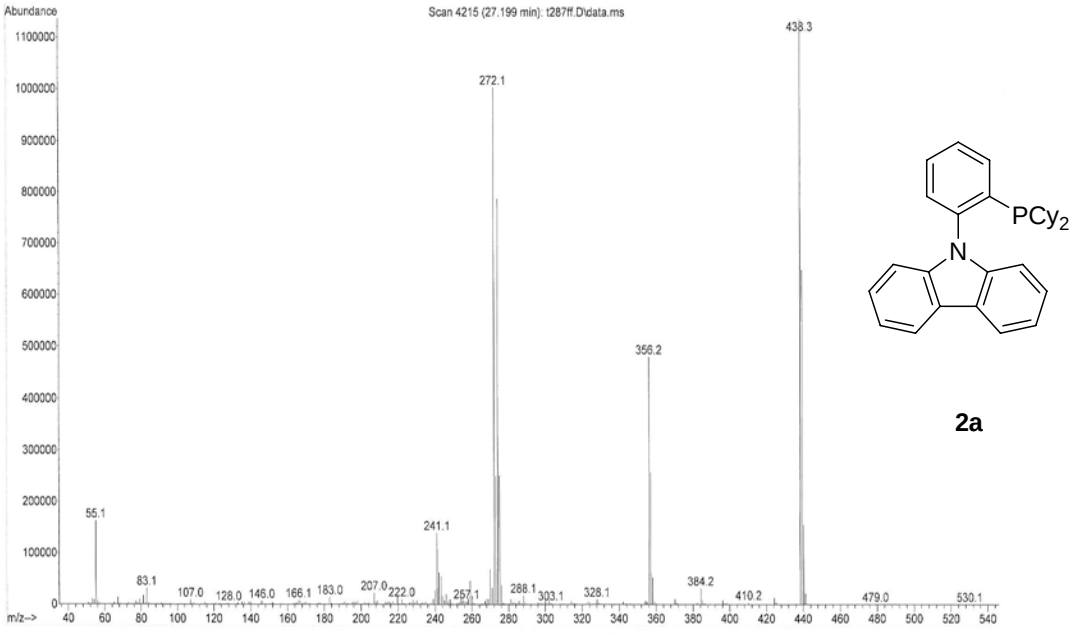
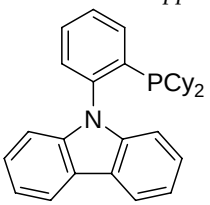




T186

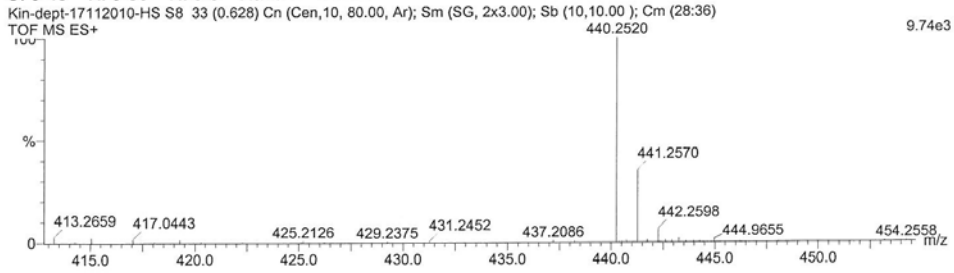
Elemental Composition Report

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

2a

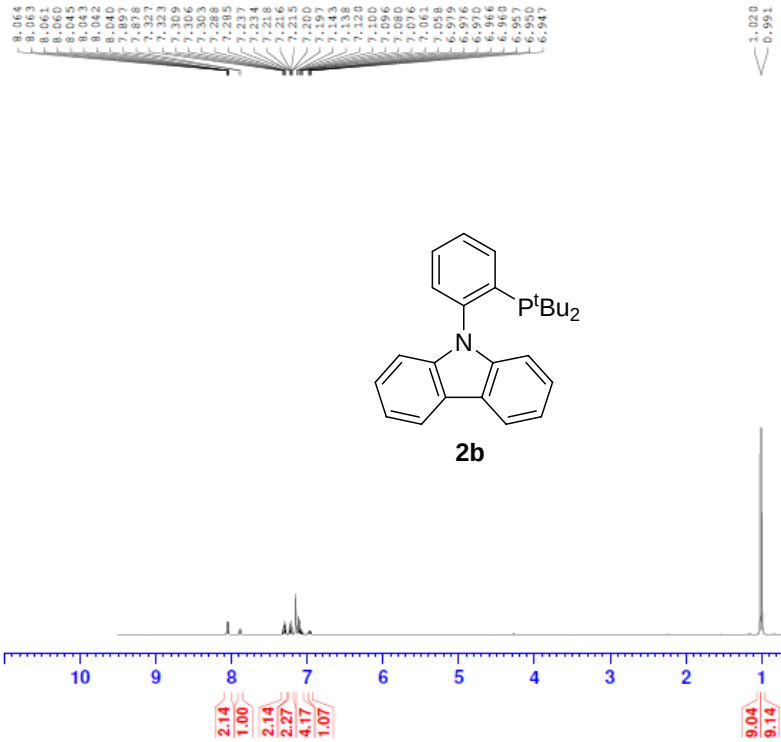
Monoisotopic Mass, Even Electron Ions
73 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-43 H: 0-35 N: 0-3 Na: 0-1 P: 0-2

Kin-dept-17112010-HS S8 33 (0.628) Cn (Cen,10, 80.00, Ar); Sm (SG, 2x3.00); Sb (10,10.00); Cm (28:36)
TOF MS ES+ 9.74e3



Minimum:				-100.0		
Maximum:		5.0	20.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
440.2520	440.2507	1.3	3.0	14.5	6.1	C30 H35 N P

t021fa proton

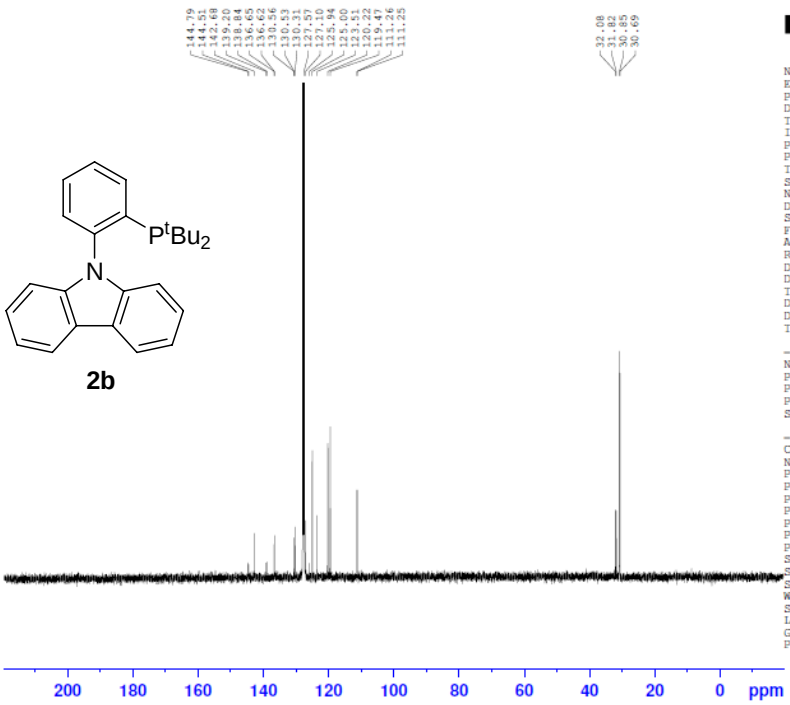


2b

BRUKER

NAME	t021fa proton
EXPNO	1
PROCNO	1
Date_	20101122
Time	15.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	C6D6
NS	16
DS	2
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	64
DW	124.800 usec
DE	6.50 usec
TE	297.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.70 usec
PL1	0.00 dB
PL1W	11.88122272 W
SFO1	400.1318007 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

t021fa carbon



2b

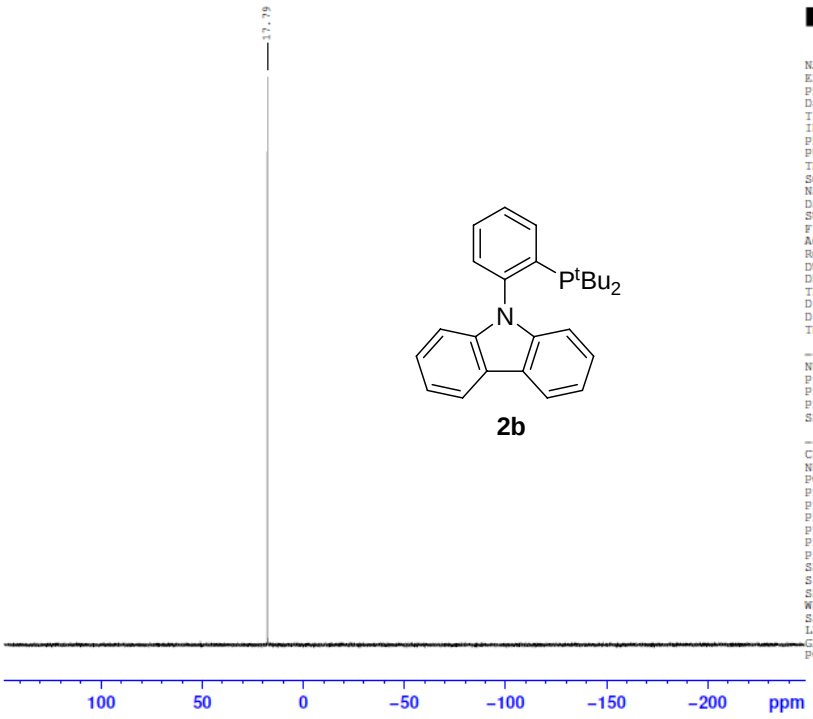
BRUKER

```
NAME            t021fa carbon
EXPNO                       1
PROCNO                      1
Date_                20101122
Time                    15.43
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  C6D6
NS                         70
DS                          2
SWH                 24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                        203
DW                     20.800 usec
DE                      6.50 usec
TE                     298.5 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.50 usec
PL1                      -2.00 dB
PL1W               58.52175522 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W               11.88122272 W
PL12W               0.37571725 W
PL13W               0.37571725 W
SFO2               400.1316005 MHz
SI                        32768
SF                 100.6127690 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

t021fa phos



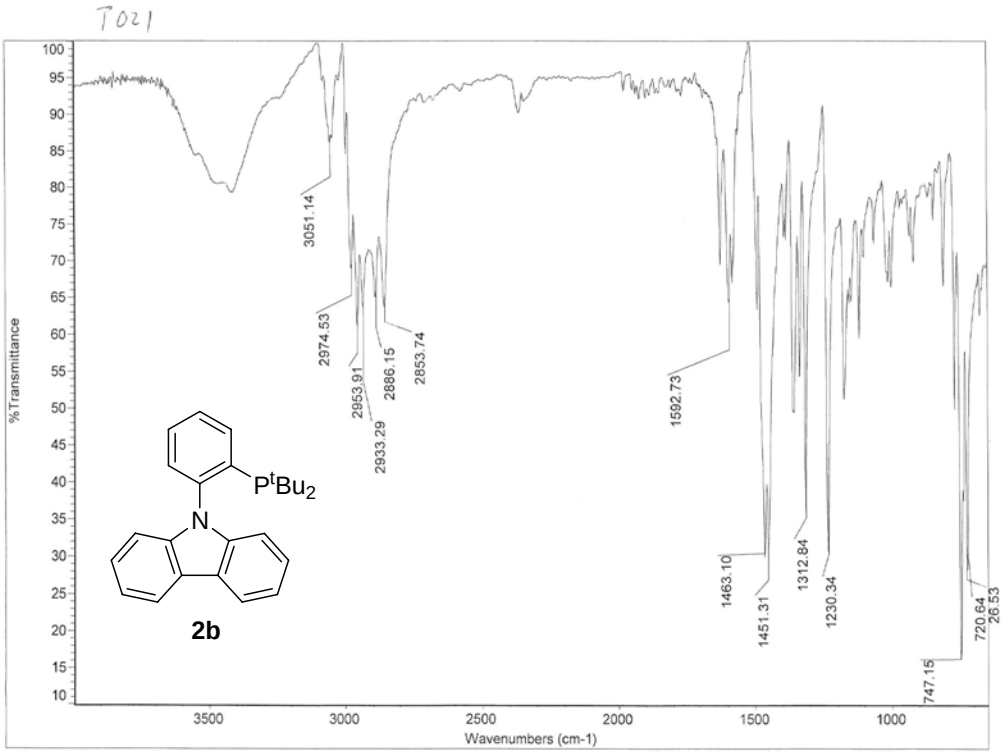
2b

BRUKER

```
NAME            t021fa phos
EXPNO                       1
PROCNO                      1
Date_                20101122
Time                    15.39
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  C6D6
NS                         16
DS                          4
SWH                 64102.563 Hz
FIDRES              0.978127 Hz
AQ                  0.5112308 sec
RG                        203
DW                      7.800 usec
DE                      6.50 usec
TE                     298.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       31P
P1                       14.70 usec
PL1                       3.00 dB
PL1W               12.96693134 W
SFO1               161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W               11.88122272 W
PL12W               0.37571725 W
PL13W               0.37571725 W
SFO2               400.1316005 MHz
SI                        32768
SF                 161.9755930 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

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Operator   :
Acquired   : 11 Jan 2010  12:41     using AcqMethod WANGJUN2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 5
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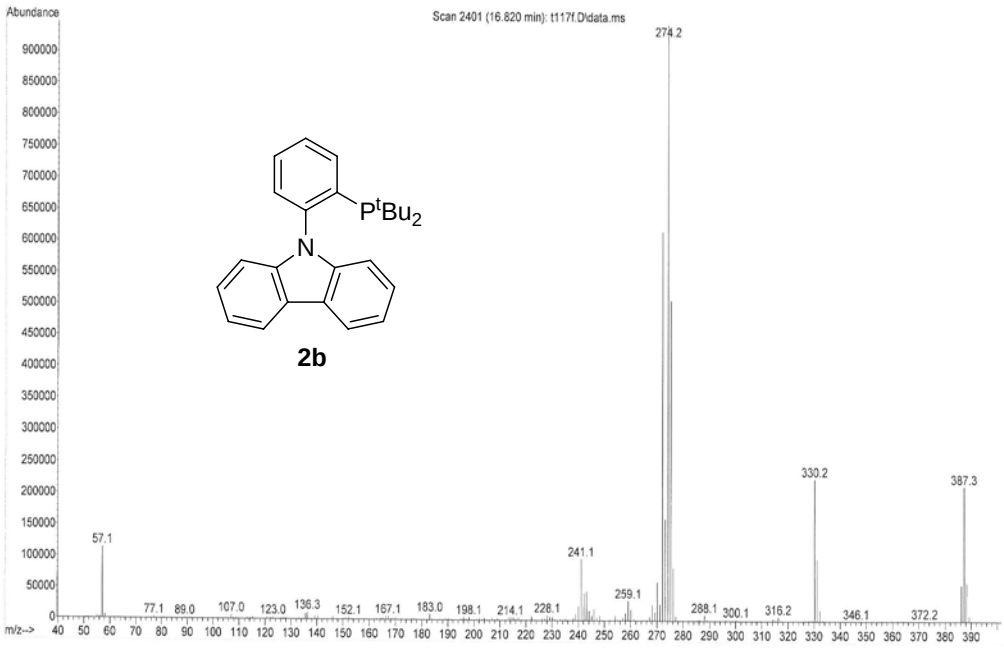
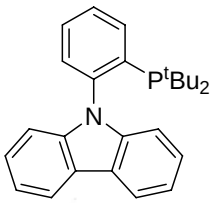




2b

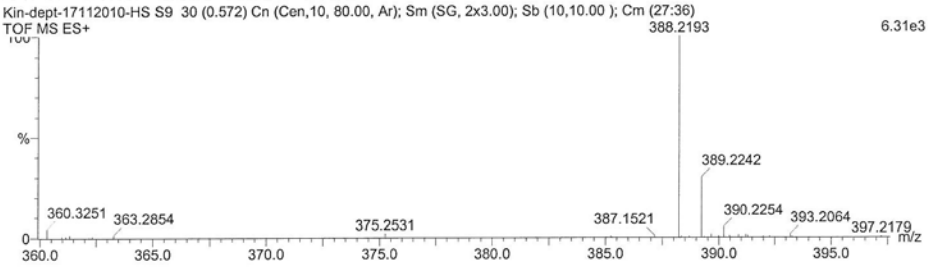
T021

Elemental Composition Report Page 1

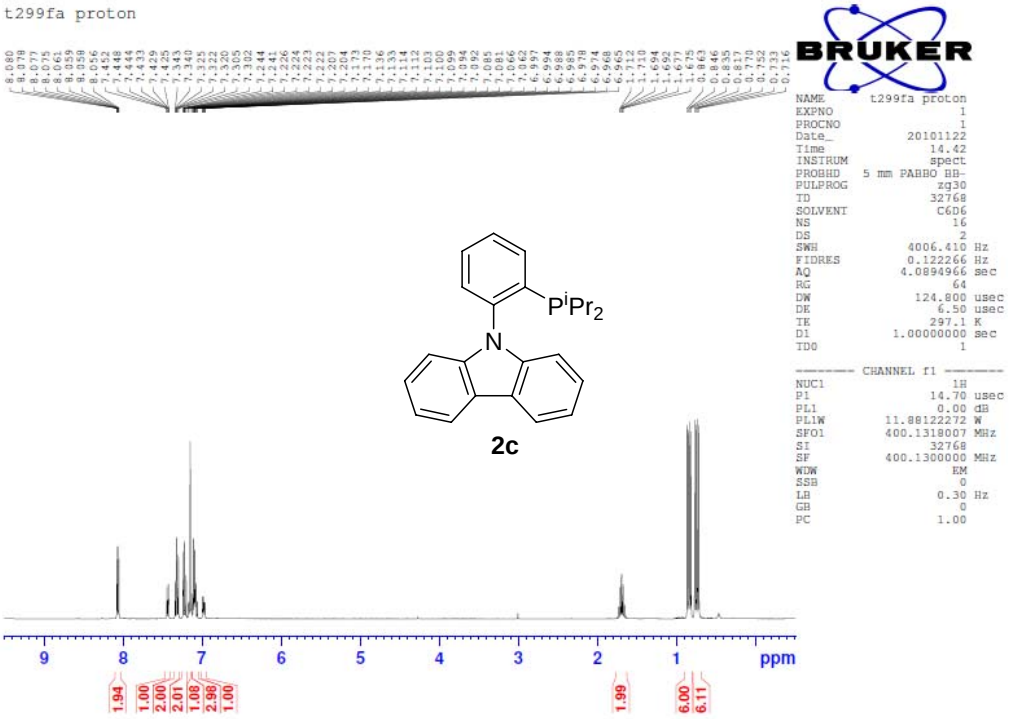
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
74 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-43 H: 0-35 N: 0-3 Na: 0-1 P: 0-2

Kin-dept-17112010-HS S9 30 (0.572) Cn (Cen,10, 80.00, Ar); Sm (SG, 2x3.00); Sb (10,10.00); Cm (27:36)
TOF MS ES+ 6.31e3



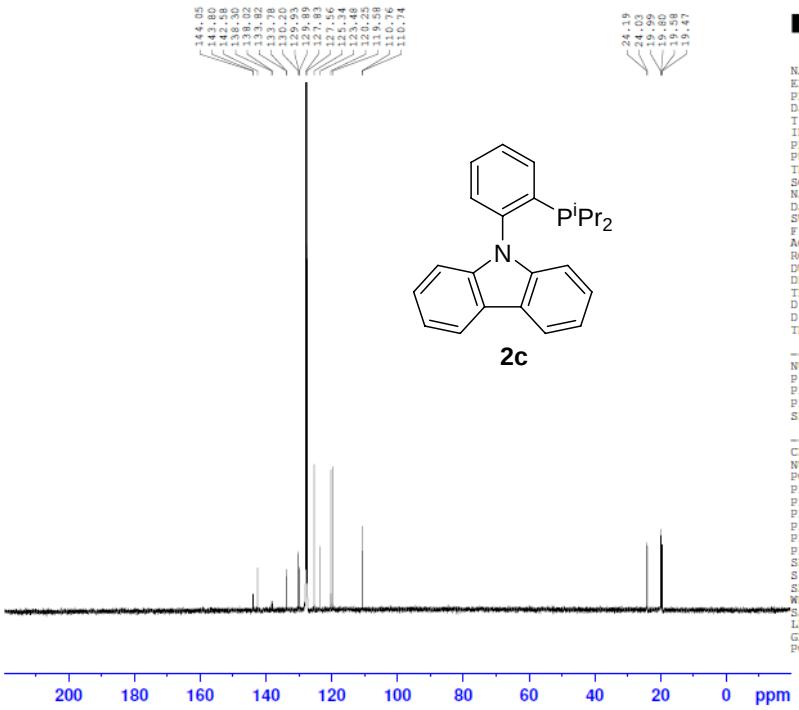
Minimum:				-100.0		
Maximum:		5.0	5.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
388.2193	388.2194	-0.1	-0.3	12.5	3.9	C26 H31 N P



NAME	t299fa proton
EXPNO	1
PROCNO	1
Date_	20101122
Time	14.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	C6D6
NS	16
DS	2
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	64
DW	124.800 usec
DE	6.50 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.70 usec
PL1	0.00 dB
PL1W	11.88122272 W
SFO1	400.1318007 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

2c

t299fa carbon



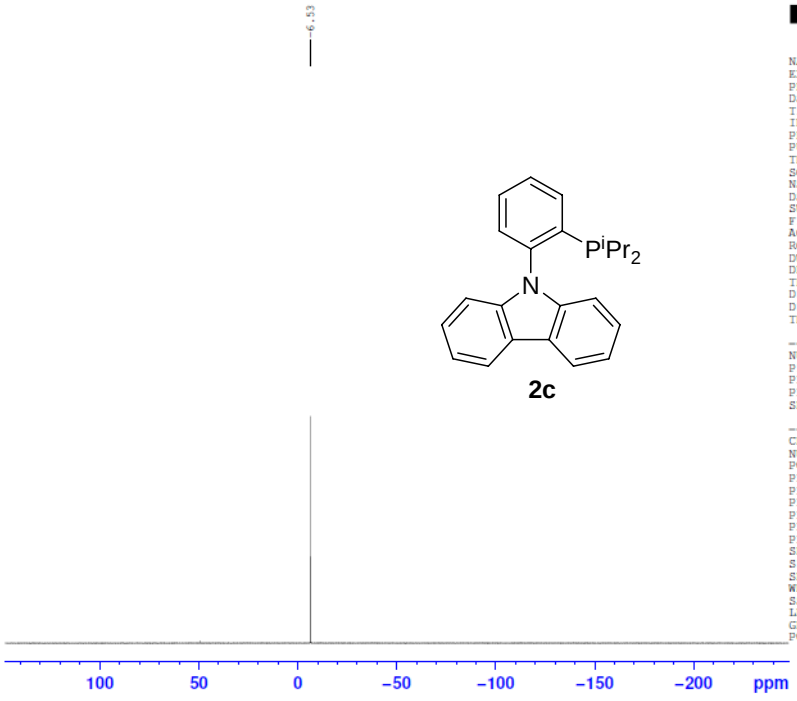
2c

```
NAME            t299fa carbon
EXPNO                       1
PROCNO                      1
Date_                20101122
Time                    14.50
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  C6D6
NS                        100
DS                          2
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                        203
DW                     20.800 usec
DE                      6.50 usec
TE                     297.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.50 usec
PL1                     -2.00 dB
PL1W               58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W               11.88122272 W
PL12W               0.37571725 W
PL13W               0.37571725 W
SFO2              400.1316005 MHz
SI                       32768
SF                100.6127690 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

t299fa phos

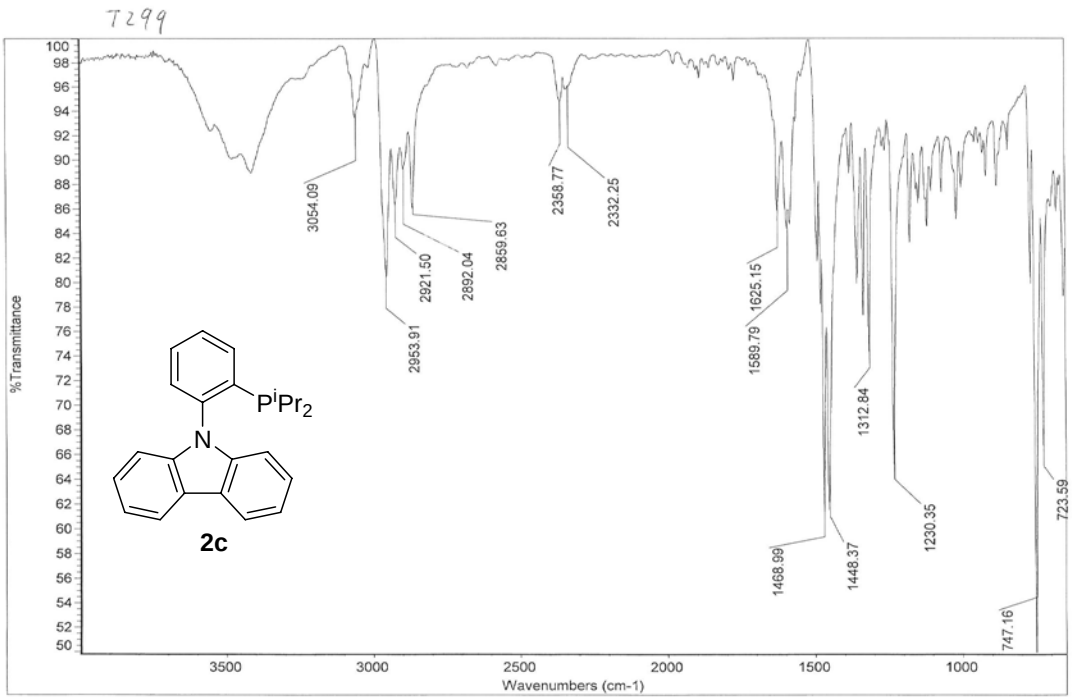


2c

```
NAME            t299fa phos
EXPNO                       1
PROCNO                      1
Date_                20101122
Time                    15.00
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  C6D6
NS                         16
DS                          4
SWH                64102.563 Hz
FIDRES             0.978127 Hz
AQ                 0.5112308 sec
RG                        203
DW                     7.800 usec
DE                      6.50 usec
TE                     298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      31P
P1                      14.70 usec
PL1                      3.00 dB
PL1W               12.96693134 W
SFO1              161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W               11.88122272 W
PL12W               0.37571725 W
PL13W               0.37571725 W
SFO2              400.1316005 MHz
SI                       32768
SF                161.9755930 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

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File       :C:\msdchem\1\DATA\tai\2010\t299.D
Operator   : Seam
Acquired   :  2 Nov 2010  19:15     using AcqMethod WANGJUN2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 2
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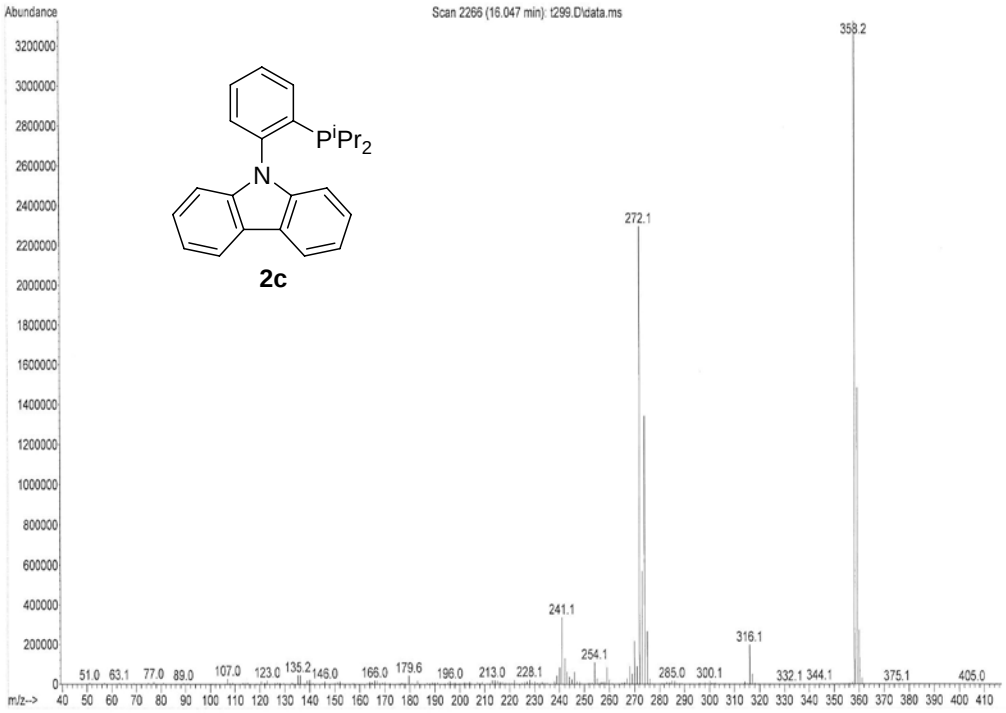
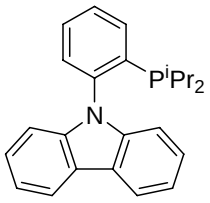




2c

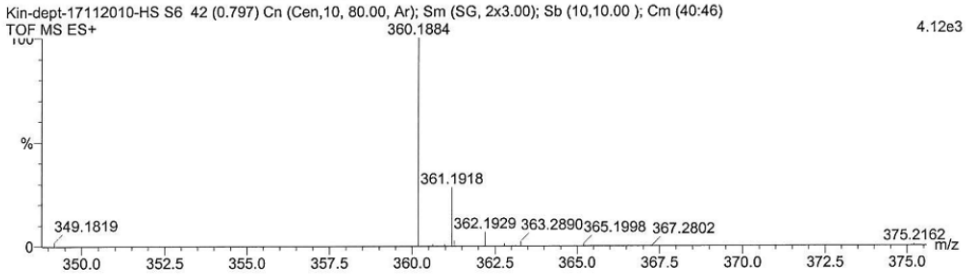
T299

Elemental Composition Report **Page 1**

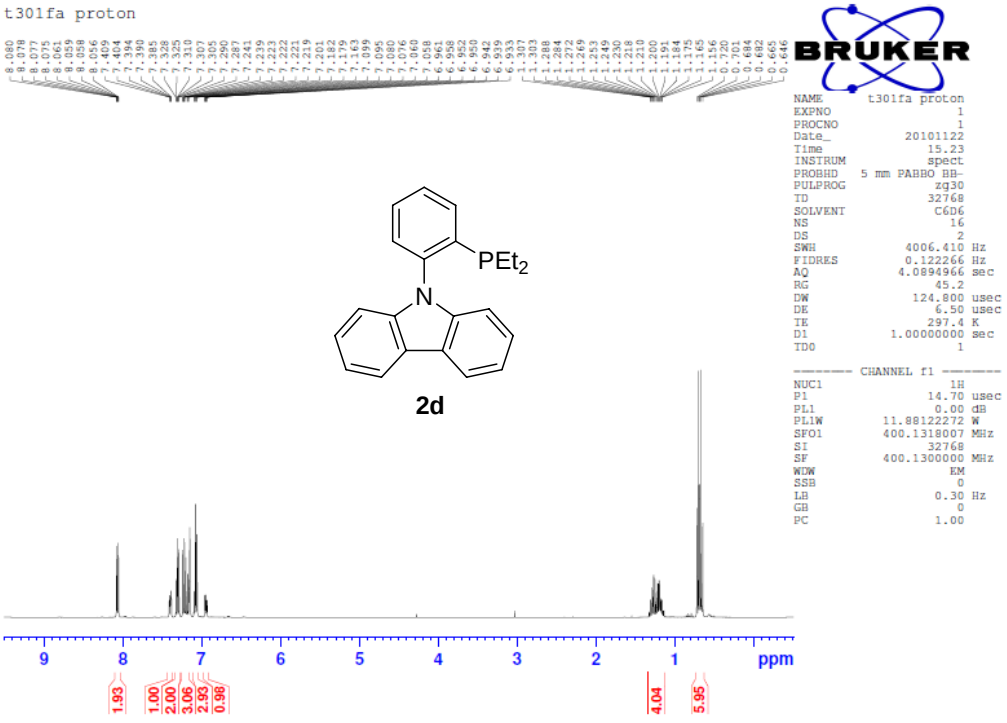
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
83 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-43 H: 0-40 N: 0-3 Na: 0-1 P: 0-2

Kin-dept-17112010-HS S6 42 (0.797) Cn (Cen,10, 80.00, Ar); Sm (SG, 2x3.00); Sb (10,10.00); Cm (40:46)



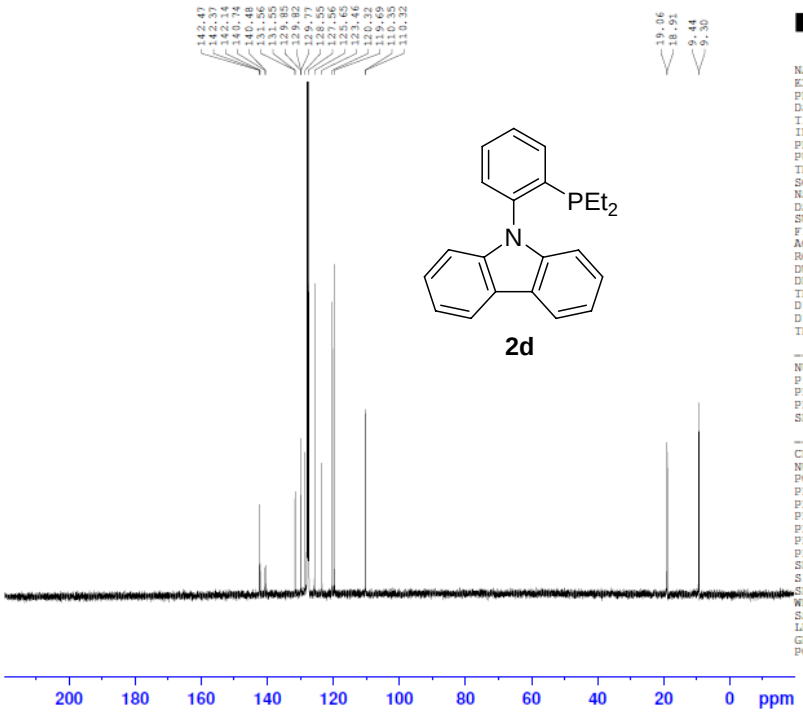
Minimum:				-100.0		
Maximum:		5.0	5.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
360.1884	360.1881	0.3	0.8	12.5	29.1	C24 H27 N P



NAME	t301fa proton
EXPNO	1
PROCNO	1
Date_	20101122
Time	15.23
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	C6D6
NS	16
DS	2
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	45.2
DW	124.800 usec
DE	6.50 usec
TE	297.4 K
D1	1.00000000 sec
TD0	1
====== CHANNEL f1 ======	
NUC1	1H
P1	14.70 usec
PL1	0.00 dB
PL1W	11.88122272 W
SFO1	400.1318007 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

2d

t301fa carbon



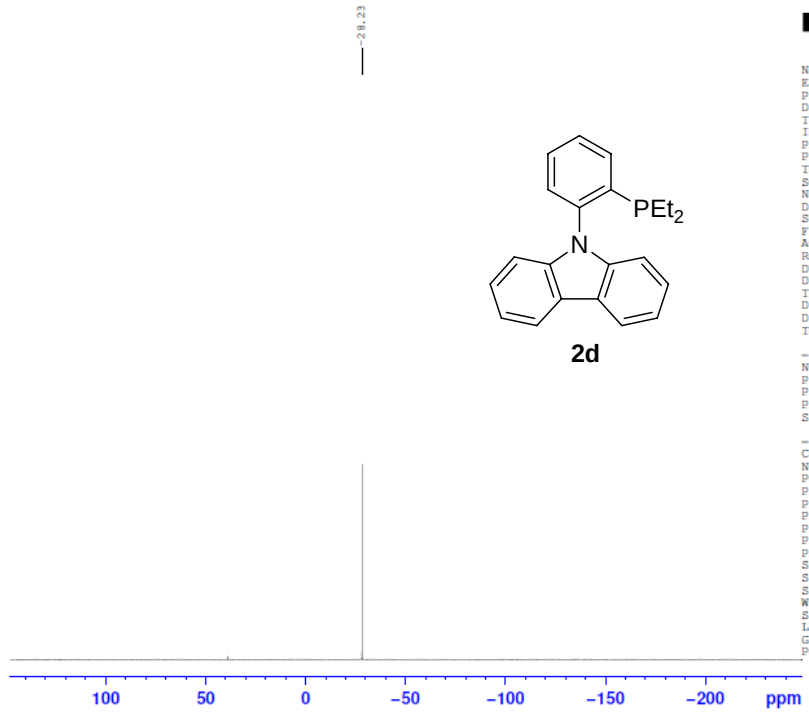
2d

```
NAME          t301fa carbon
EXPNO                    1
PROCNO                   1
Date_             20101122
Time                 15.29
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                C6D6
NS                       79
DS                        2
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                      203
DW                  20.800 usec
DE                   6.50 usec
TE                  298.8 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.50 usec
PL1                -2.00 dB
PL1W          58.52175522 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W          11.88122272 W
PL12W          0.37571725 W
PL13W          0.37571725 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                   1.00 Hz
GB                       0
PC                   1.40
```

t301fa phos

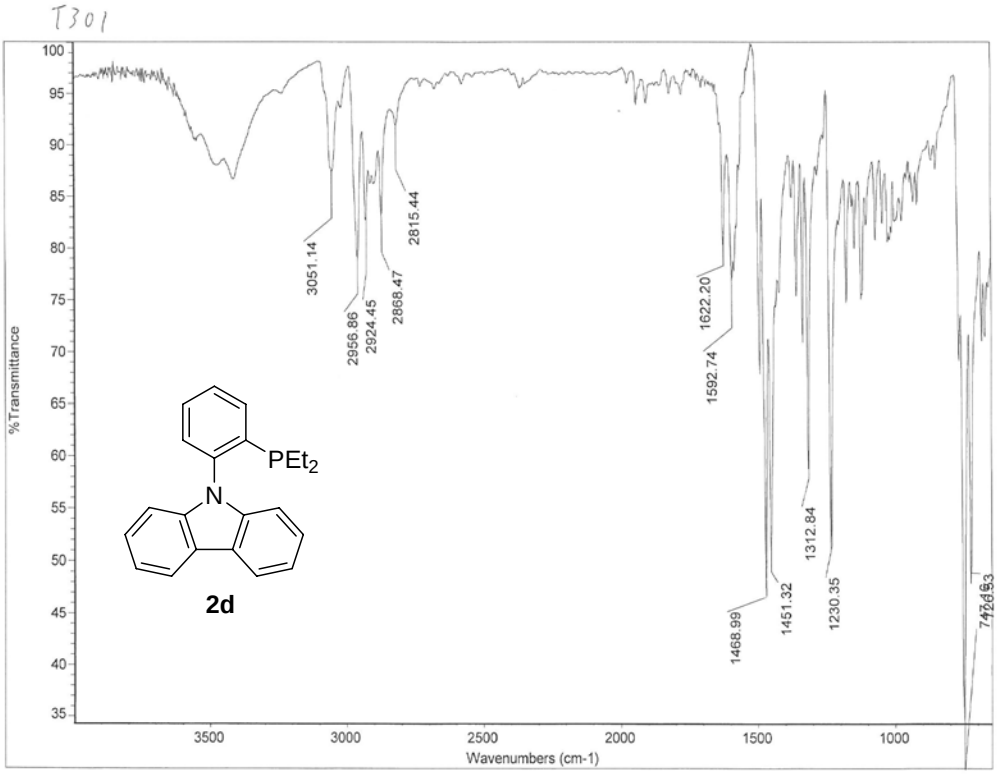


2d

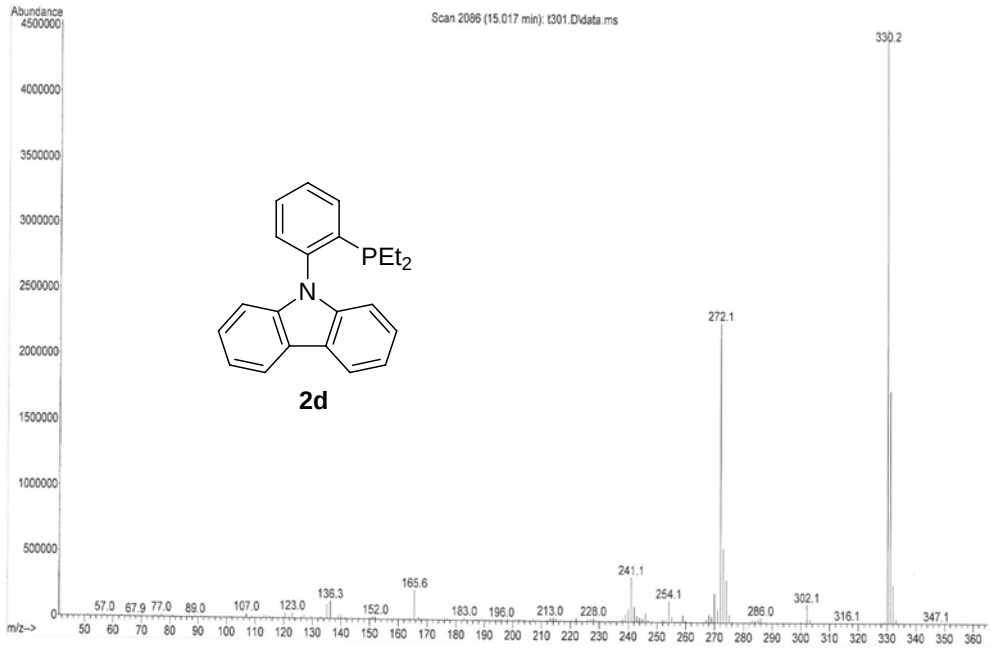
```
NAME          t301fa phos
EXPNO                    1
PROCNO                   1
Date_             20101122
Time                 15.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                C6D6
NS                       16
DS                        4
SWH              64102.563 Hz
FIDRES           0.978127 Hz
AQ               0.5112308 sec
RG                      203
DW                   7.800 usec
DE                   6.50 usec
TE                  298.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

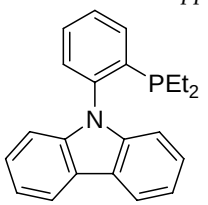
======== CHANNEL f1 ========
NUC1                   31P
P1                  14.70 usec
PL1                  3.00 dB
PL1W          12.96693134 W
SFO1         161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W          11.88122272 W
PL12W          0.37571725 W
PL13W          0.37571725 W
SFO2         400.1316005 MHz
SI                   32768
SF           161.9755930 MHz
WDW                     EM
SSB                      0
LB                   1.00 Hz
GB                       0
PC                   1.40
```




```
File       :C:\msdchem\1\DATA\chun\t301.D
Operator   : Seam
Acquired   :  2 Nov 2010  11:38     using AcqMethod WANGJUN2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 8
```





2d

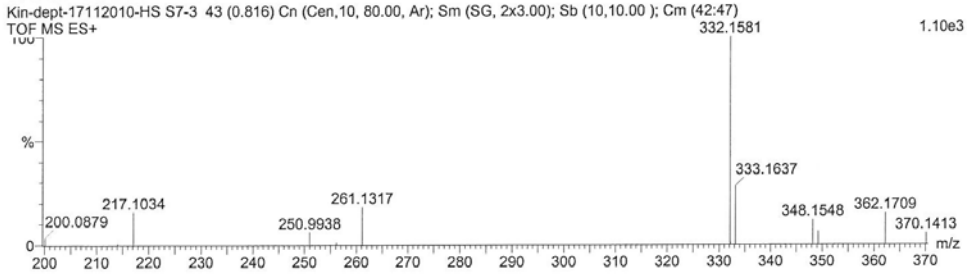
T301

Elemental Composition Report Page 1

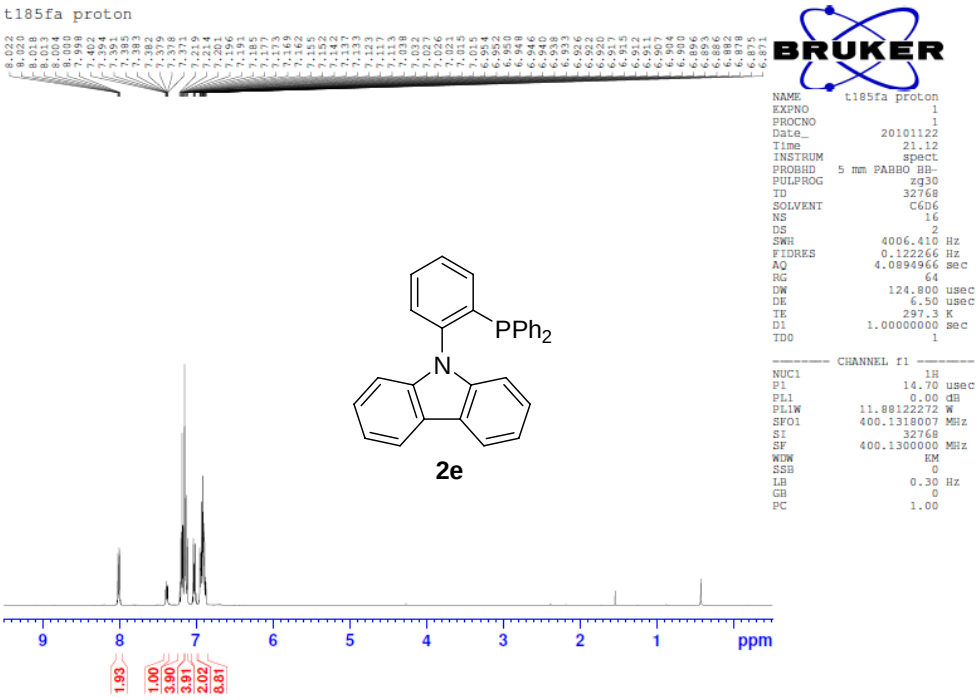
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
49 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-43 H: 0-23 N: 0-3 Na: 0-1 P: 0-2

Kin-dept-17112010-HS S7-3 43 (0.816) Cn (Cen,10, 80.00, Ar); Sm (SG, 2x3.00); Sb (10,10.00); Cm (42:47)
TOF MS ES+ 1.10e3

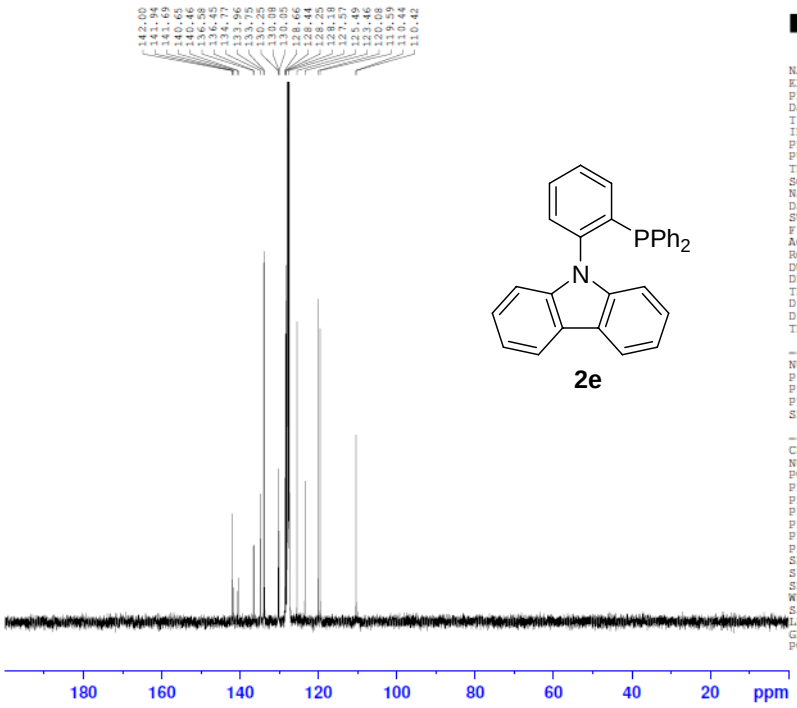


Minimum:				-100.0		
Maximum:		5.0	20.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
332.1581	332.1568	1.3	3.9	12.5	2773311.0	C22 H23 N P



2e

t185fa carbon



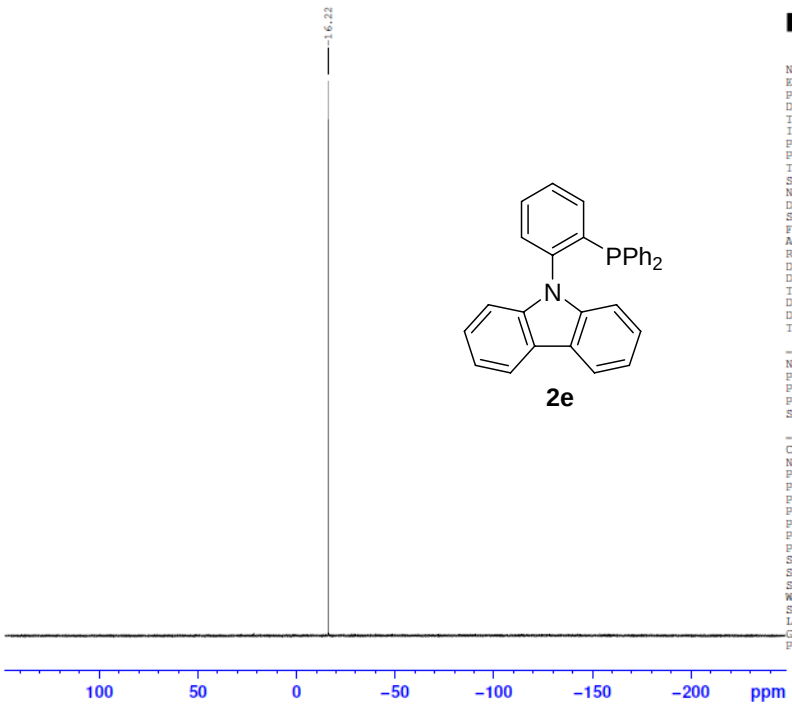
2e

```
NAME          t185fa carbon
EXPNO                    1
PROCNO                   1
Date_             20101122
Time                 21.27
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                C6D6
NS                      141
DS                        2
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                      203
DW                 20.800 usec
DE                  6.50 usec
TE                  298.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.50 usec
PL1                 -2.00 dB
PL1W           58.52175522 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W           11.88122272 W
PL12W           0.37571725 W
PL13W           0.37571725 W
SFO2          400.1316005 MHz
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

t185fa phos

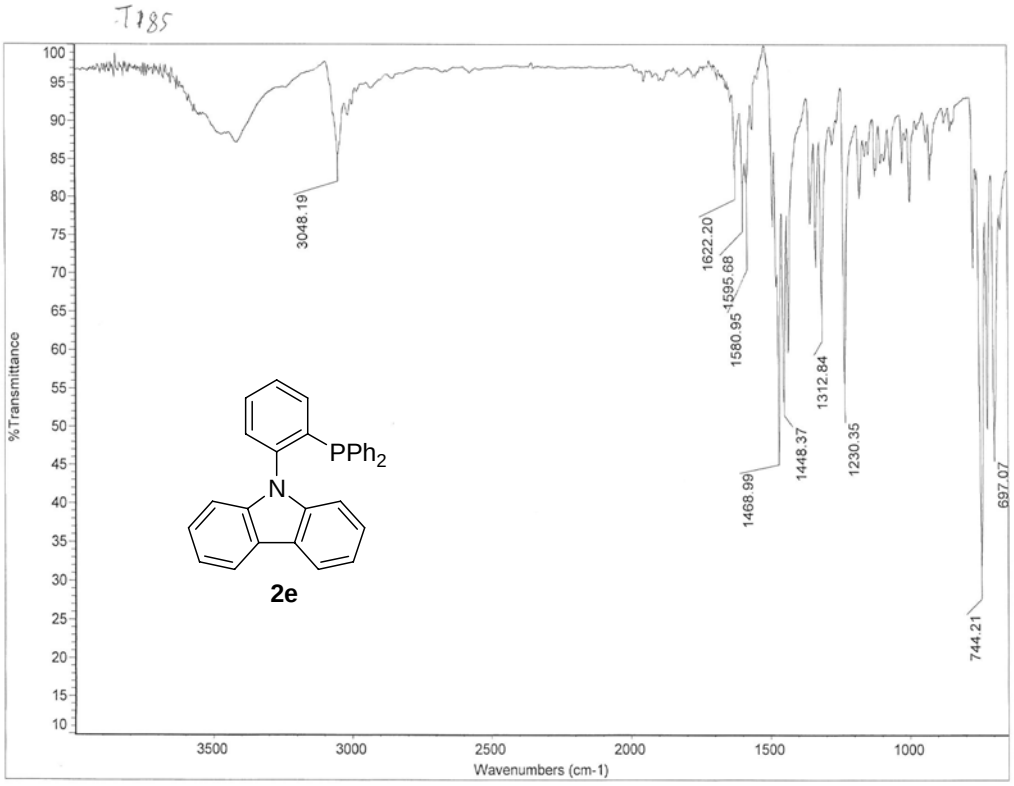


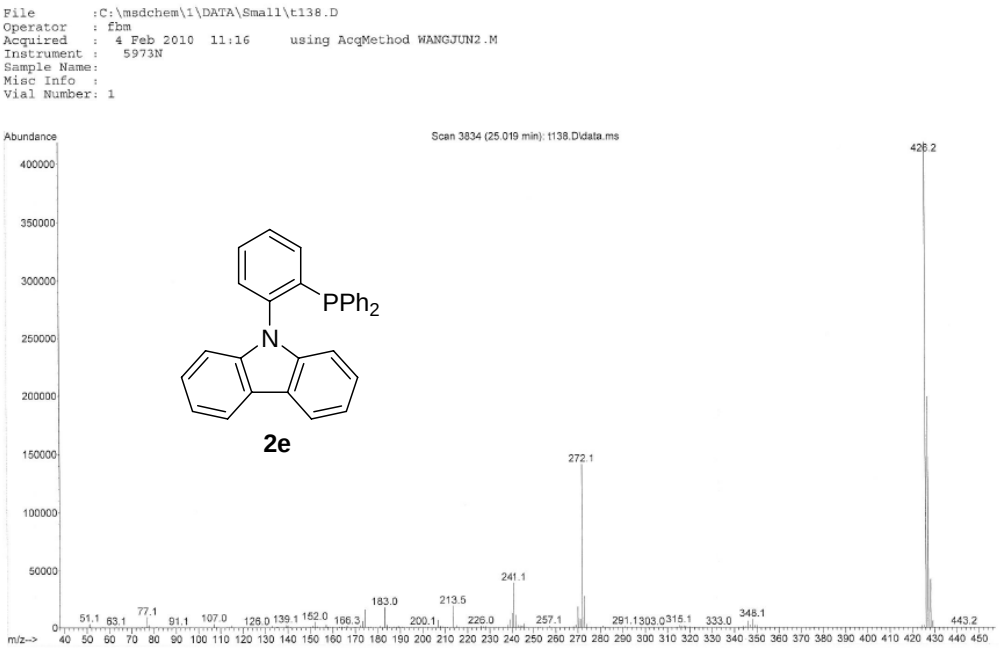
2e

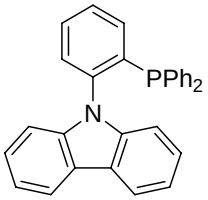
```
NAME          t185fa phos
EXPNO                    1
PROCNO                   1
Date_             20101122
Time                 21.16
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                C6D6
NS                       16
DS                        4
SWH              64102.563 Hz
FIDRES           0.978127 Hz
AQ               0.5112308 sec
RG                      203
DW                  7.800 usec
DE                  6.50 usec
TE                  297.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    31P
P1                  14.70 usec
PL1                  3.00 dB
PL1W           12.96693134 W
SFO1          161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W           11.88122272 W
PL12W           0.37571725 W
PL13W           0.37571725 W
SFO2          400.1316005 MHz
SI                    32768
SF            161.9755930 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```


T185
%Transmittance
Wavenumbers (cm-1)
3048.19
1622.20
1595.68
1580.95
1468.99
1448.37
1312.84
1230.35
744.21
697.07
PPh2
N
2e


File :C:\msdchem\1\DATA\Small\t138.D
Operator : fbm
Acquired : 4 Feb 2010 11:16 using AcqMethod WANGJUN2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1
Abundance
Scan 3834 (25.019 min): 1138.D\data.ms
426.2
272.1
241.1
PPh2
N
2e
m/z-->



2e

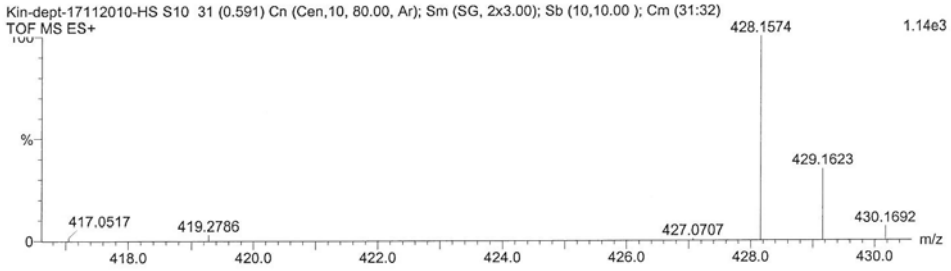
T185

Elemental Composition Report

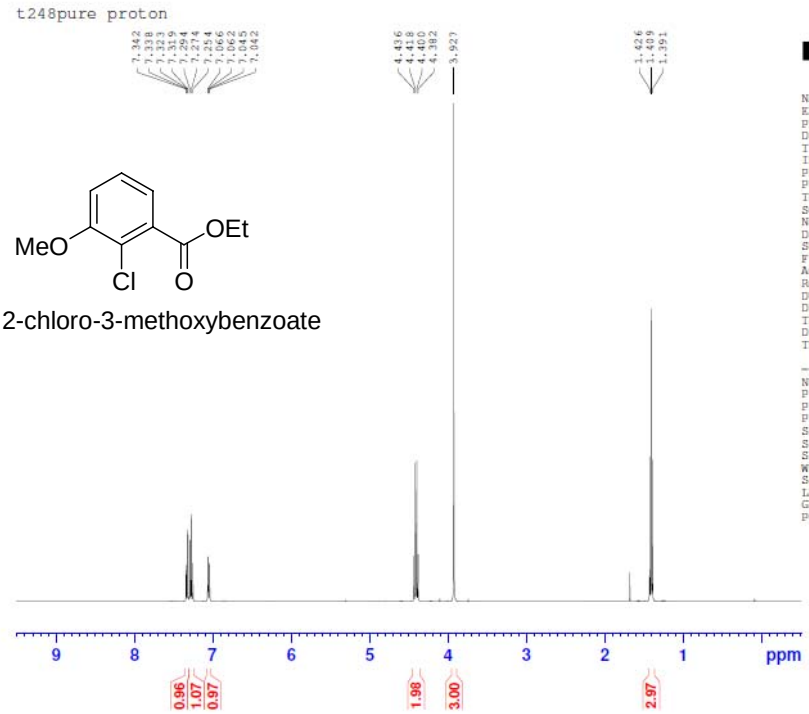
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
73 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-43 H: 0-35 N: 0-3 Na: 0-1 P: 0-2

Kin-dept-17112010-HS S10 31 (0.591) Cn (Cen,10, 80.00, Ar); Sm (SG, 2x3.00); Sb (10,10.00); Cm (31:32)
TOF MS ES+



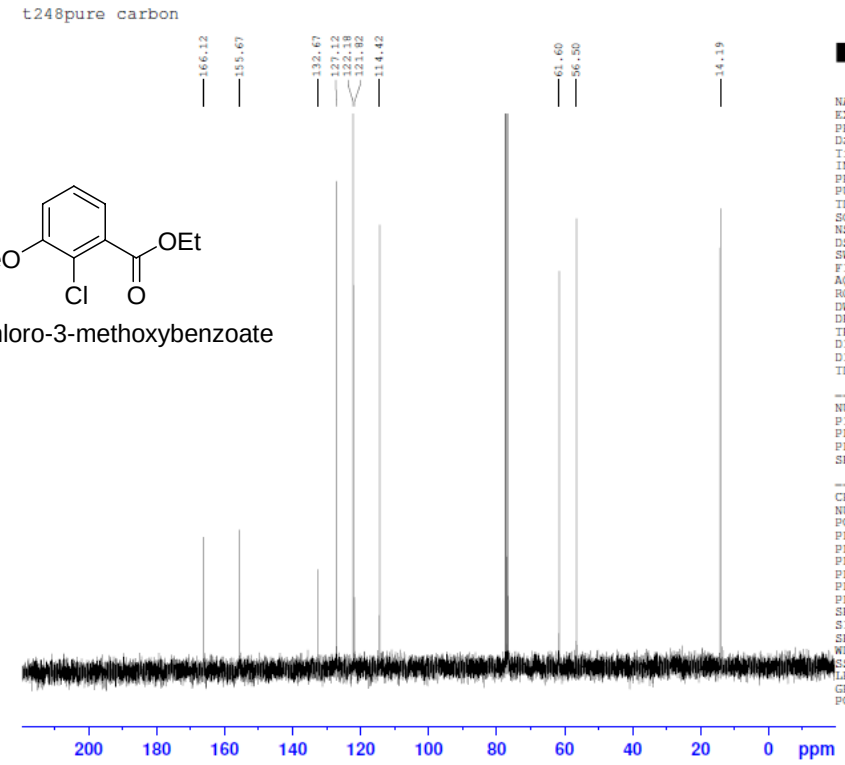
Minimum:				-100.0		
Maximum:		5.0	5.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1574	428.1568	0.6	1.4	20.5	1.1	C30 H23 N P



ethyl 2-chloro-3-methoxybenzoate

```
NAME          t248pure proton
EXPNO                      1
PROCNO                     1
Date_               20100610
Time                   18.06
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                4006.410 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                      50.8
DW                   124.800 usec
DE                     6.50 usec
TE                   296.4 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.70 usec
PL1                     0.00 dB
PL1W              11.88122272 W
SFO1              400.1318007 MHz
SI                       32768
SF                400.1300000 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                      1.00
```



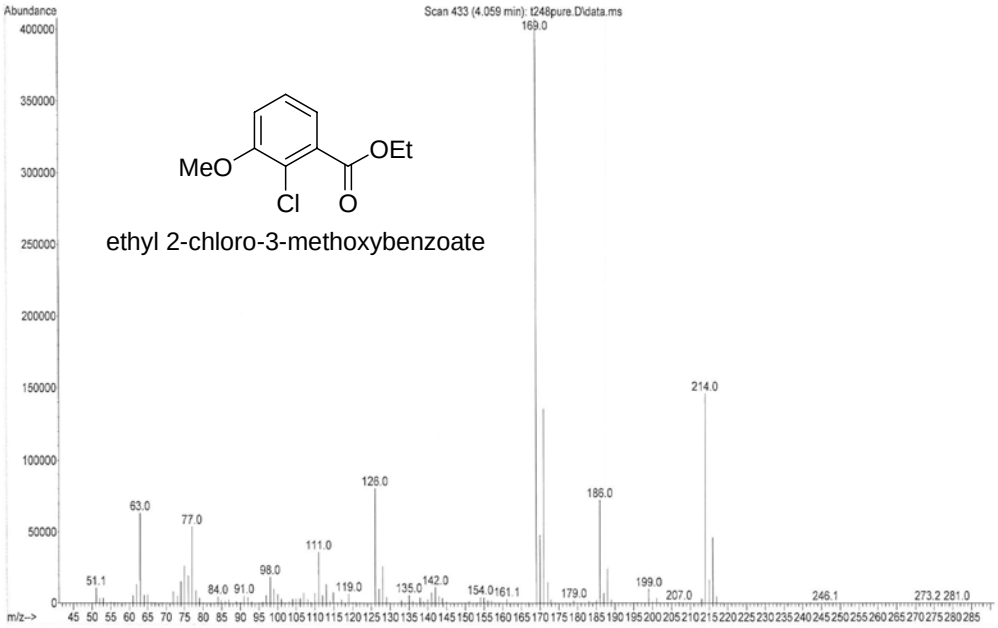
ethyl 2-chloro-3-methoxybenzoate

```
NAME          t248pure carbon
EXPNO                      1
PROCNO                     1
Date_               20100610
Time                   18.10
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       32
DS                        2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      161
DW                   20.800 usec
DE                     6.50 usec
TE                   297.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

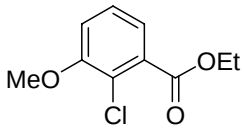
======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                    -2.00 dB
PL1W              58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.00 dB
PL12                   15.00 dB
PL13                   15.00 dB
PL2W              11.88122272 W
PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2              400.1316005 MHz
SI                       32768
SF                100.6127690 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                      1.40
```

```
File       :C:\msdchem\1\DATA\Ho\Other\t248pure.D
Operator   : fbm
Acquired   : 10 Jun 2010  19:45     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 5
```



ethyl 2-chloro-3-methoxybenzoate



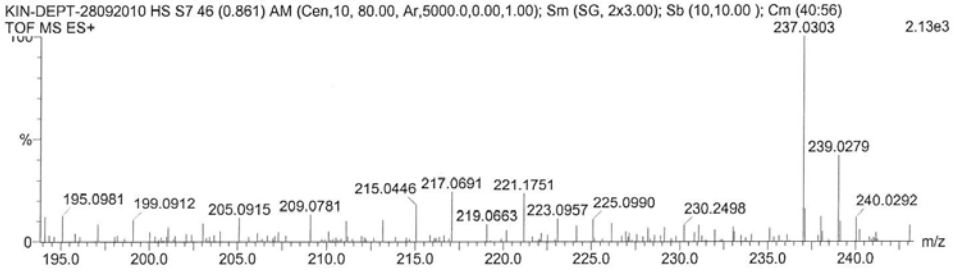
ethyl 2-chloro-3-methoxybenzoate

Elemental Composition Report T248 **Page 1**

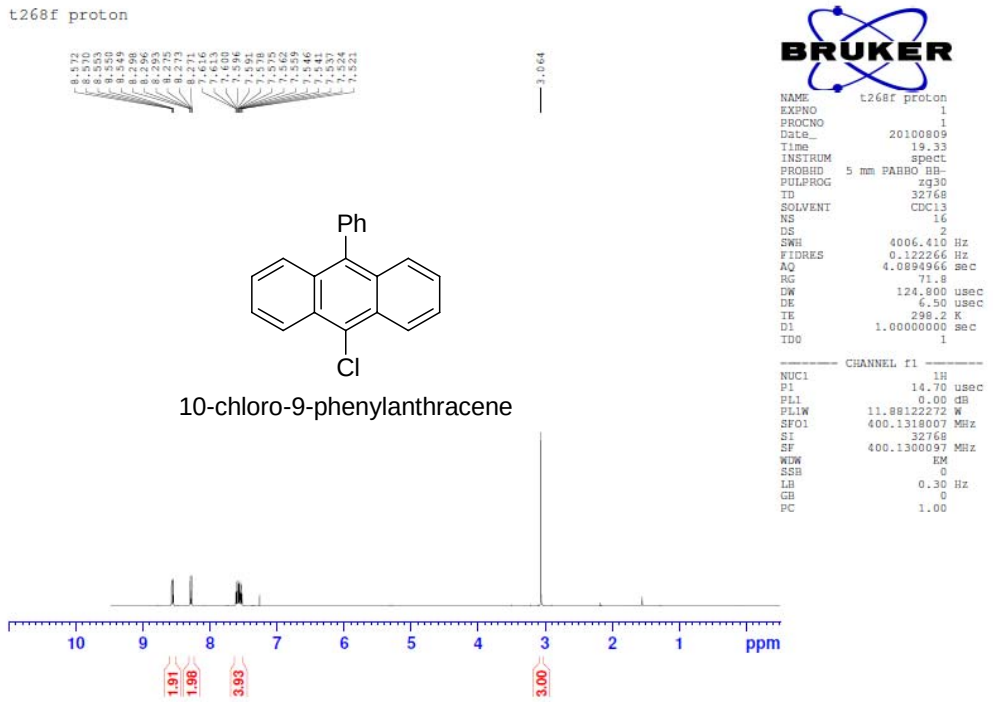
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

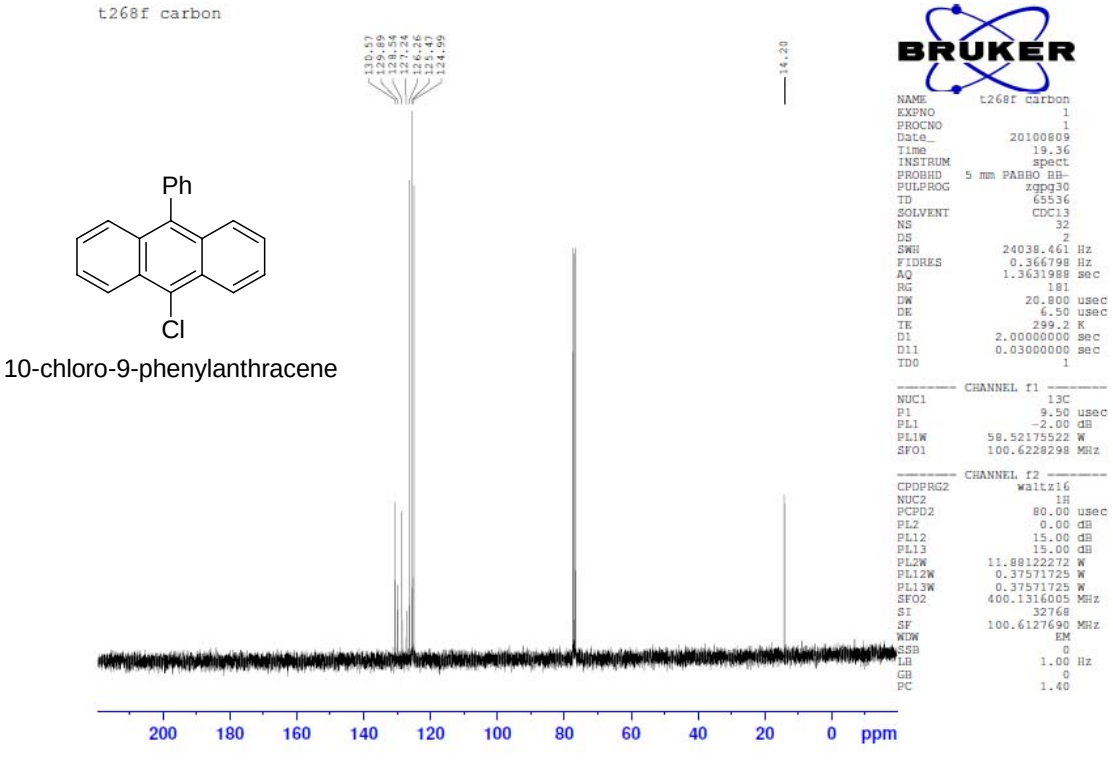
Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-18 O: 0-6 Na: 0-1 Cl: 0-1

KIN-DEPT-28092010 HS S7 46 (0.861) AM (Cen,10, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Sb (10,10.00); Cm (40:56)

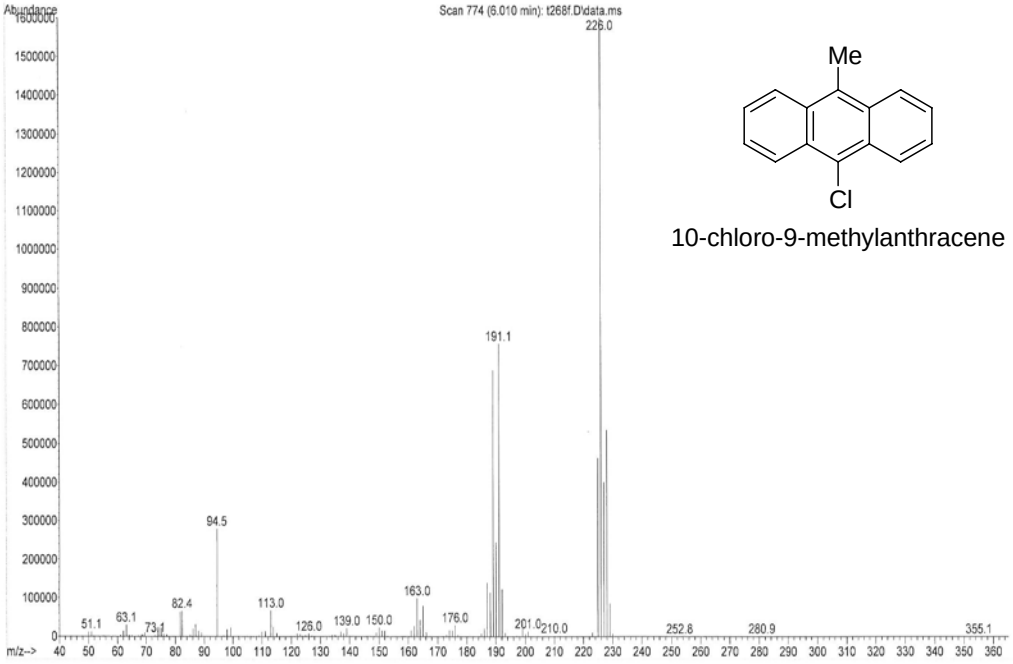


Minimum:				-100.0		
Maximum:		5.0	5.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
237.0303	237.0294	0.9	3.8	4.5	15.3	C10 H11 O3 Na Cl


t268f proton
Ph
Cl
10-chloro-9-phenylanthracene
BRUKER
NAME t268f proton
EXPNO 1
PROCNO 1
Date_ 20100809
Time 19.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.8
DW 124.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.91
1.98
3.93
3.00

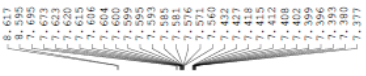

t268f carbon
Ph
Cl
10-chloro-9-phenylanthracene
BRUKER
NAME t268f carbon
EXPNO 1
PROCNO 1
Date_ 20100809
Time 19.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

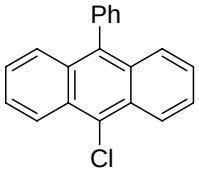
```
File       :C:\msdchem\1\DATA\arwo\t268f.D
Operator   : CM SO
Acquired   :  9 Aug 2010  18:31     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 4
```



10-chloro-9-methylanthracene

t263fa proton

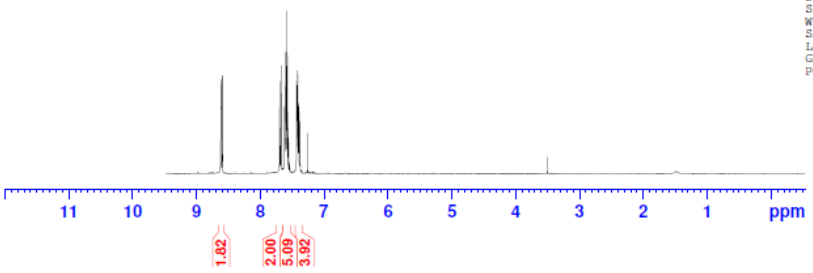


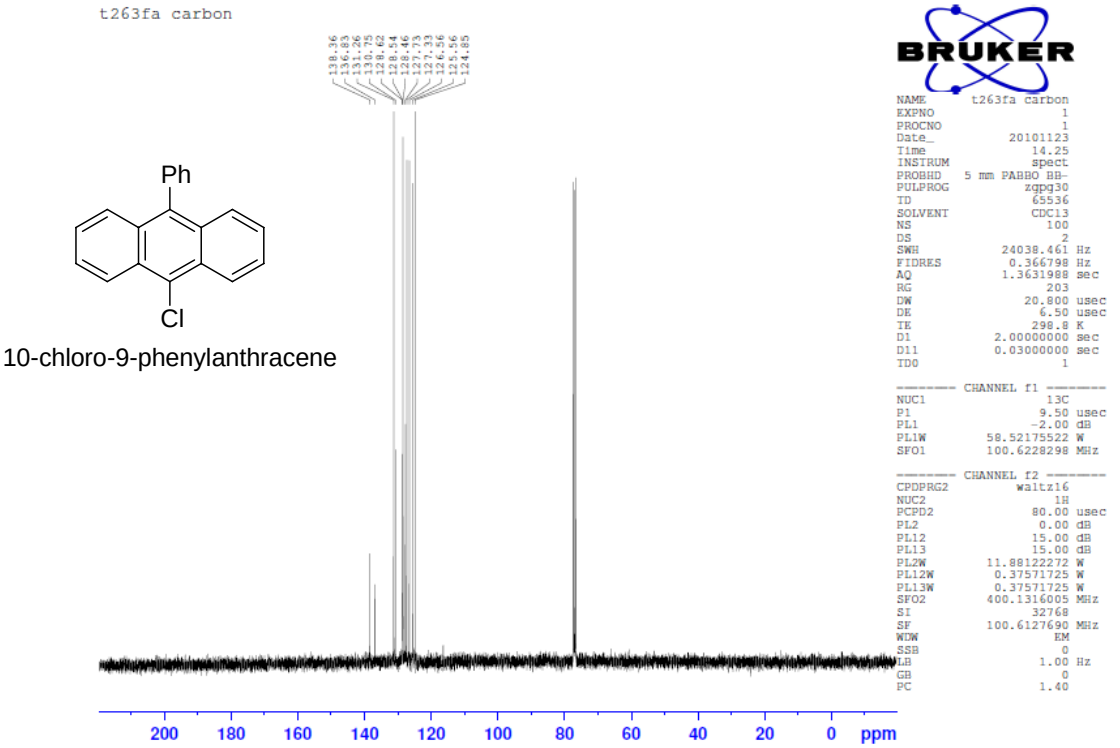


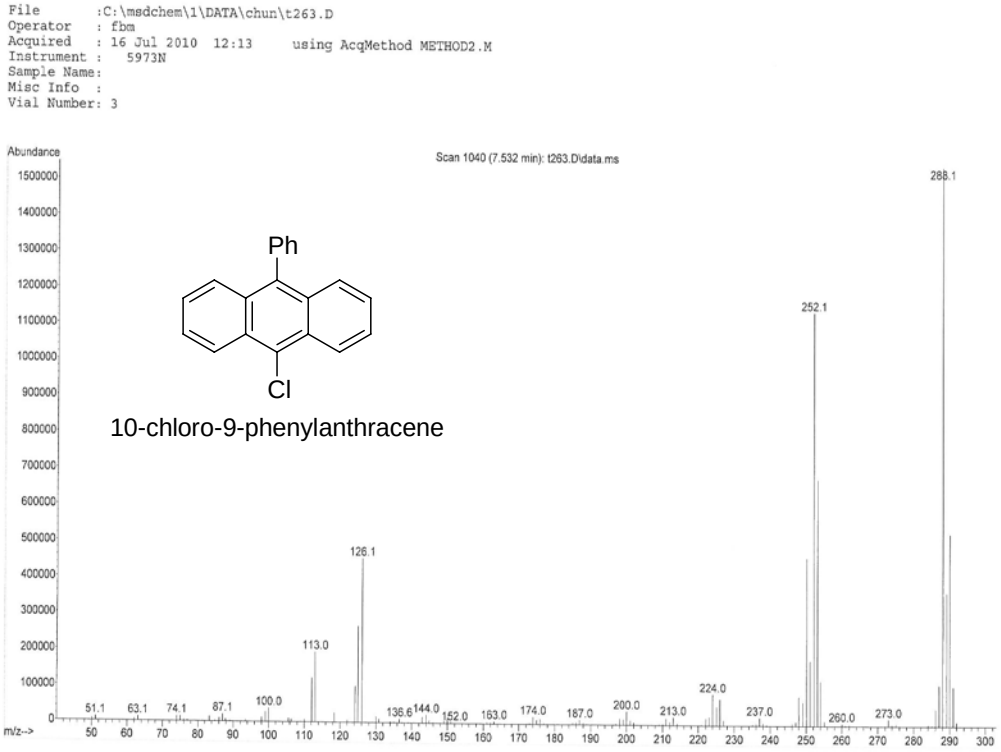
10-chloro-9-phenylanthracene

```
NAME          t263fa proton
EXPNO                    1
PROCNO                   1
Date_             20101123
Time                 14.19
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      16
DS                       2
SWH              4006.410 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                      64
DW               124.800 usec
DE                 6.50 usec
TE                 297.3 K
D1               1.00000000 sec
TD0                      1

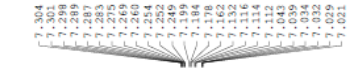
======== CHANNEL f1 ========
NUC1                    1H
P1                 14.70 usec
PL1                 0.00 dB
PL1W         11.88122272 W
SFO1         400.1318007 MHz
SI                  32768
SF           400.1300101 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```




t263fa carbon
138.36
136.83
135.26
133.75
128.62
128.54
128.46
127.73
127.33
126.56
125.56
124.85
Ph
Cl
10-chloro-9-phenylanthracene
BRUKER
NAME t263fa carbon
EXPNO 1
PROCNO 1
Date_ 20101123
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


File :C:\msdchem\1\DATA\chun\t263.D
Operator : fbm
Acquired : 16 Jul 2010 12:13 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 1040 (7.532 min): t263.D\data.ms
Ph
Cl
10-chloro-9-phenylanthracene
288.1
252.1
126.1
113.0
224.0
m/z-->

t253f proton



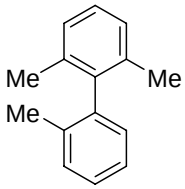
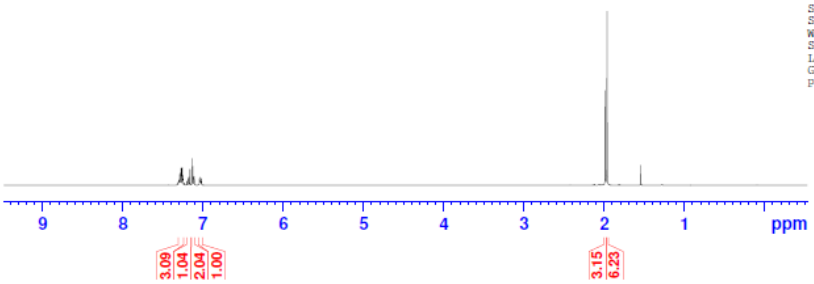


Table 2, entry 1;
Table 4, entry 1



BRUKER

```
NAME            t253f proton
EXPNO                      1
PROCNO                     1
Date_               20100629
Time                   14.58
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                 4006.410 Hz
FIDRES              0.122266 Hz
AQ                  4.0894966 sec
RG                      71.8
DW                    124.800 usec
DE                      6.50 usec
TE                    297.8 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.70 usec
PL1                     0.00 dB
PL1W              11.88122272 W
SFO1              400.1318007 MHz
SI                       32768
SF                400.1300099 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```

t253f carbon

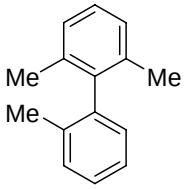


Table 2, entry 1;
Table 4, entry 1

BRUKER

```
NAME            t253f carbon
EXPNO                      1
PROCNO                     1
Date_               20100629
Time                   15.01
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                        32
DS                         2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       203
DW                    20.800 usec
DE                      6.50 usec
TE                    298.8 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                    -2.00 dB
PL1W              58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.00 dB
PL12                   15.00 dB
PL13                   15.00 dB
PL2W              11.88122272 W
PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2              400.1316005 MHz
SI                       32768
SF                100.6127690 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

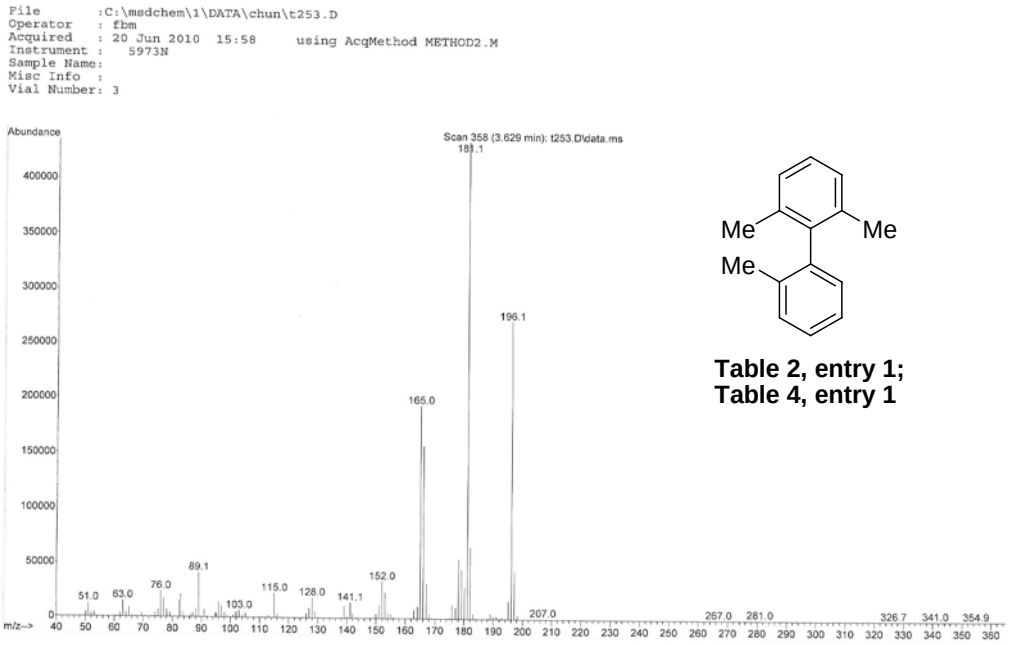


Table 2, entry 1;
Table 4, entry 1

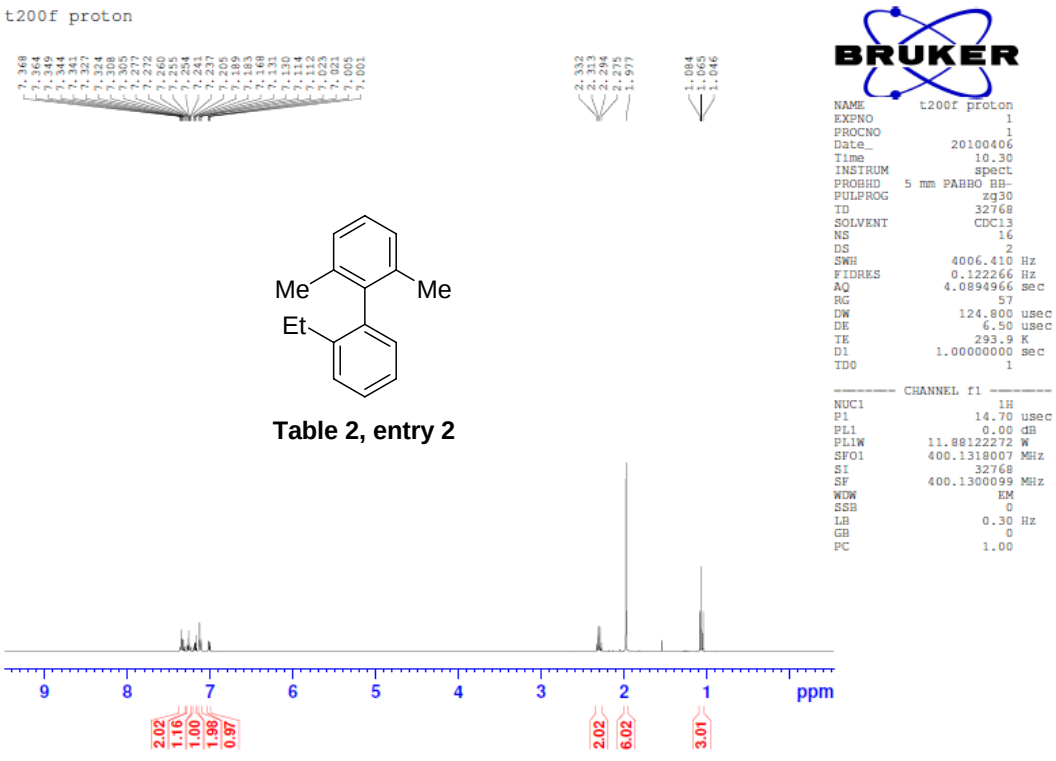


Table 2, entry 2

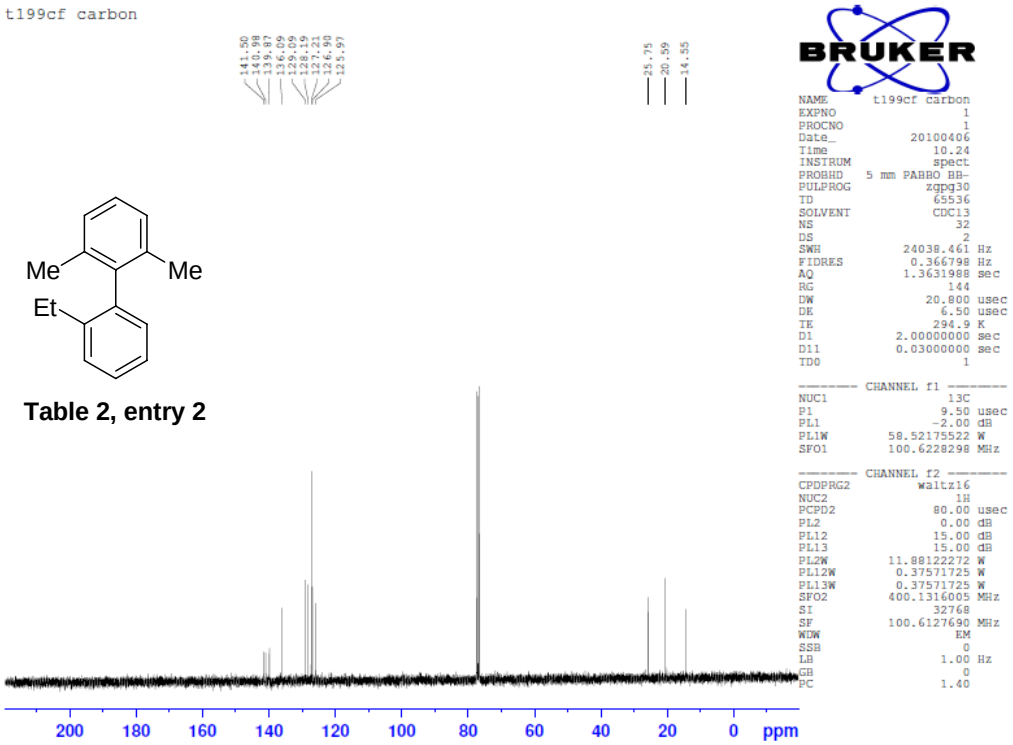


Table 2, entry 2

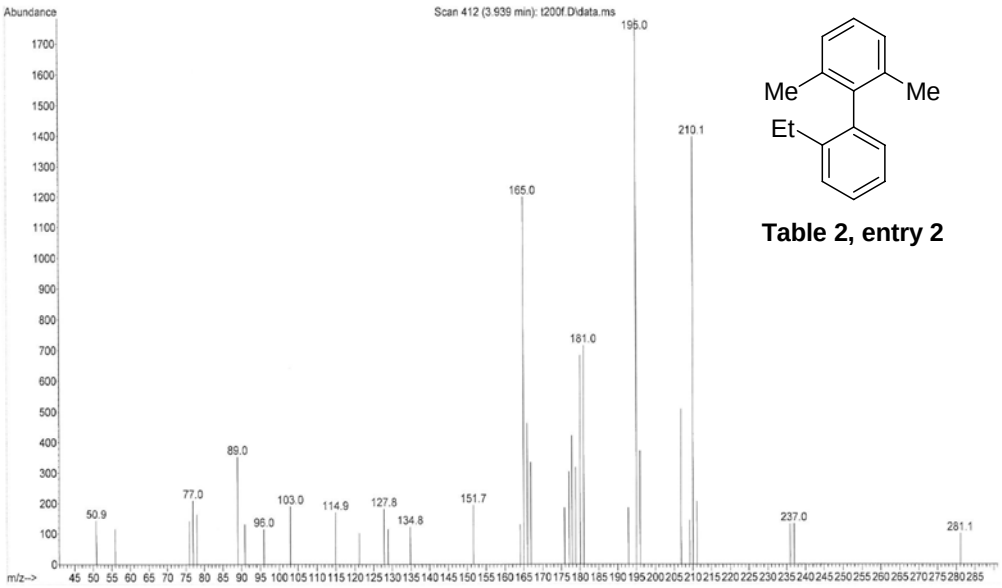


Table 2, entry 2

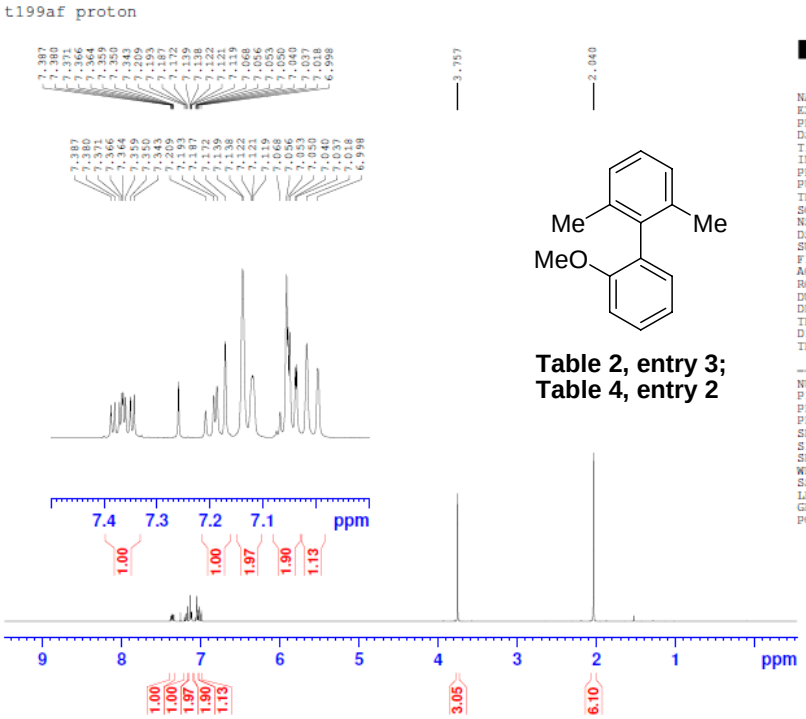


Table 2, entry 3;
Table 4, entry 2

BRUKER

```
NAME          t199af proton
EXPNO                    1
PROCNO                   1
Date_             20100406
Time                 10.06
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              4006.410 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                     57
DW                124.800 usec
DE                  6.50 usec
TE                 293.6 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.70 usec
PL1                 0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI                  32768
SF            400.1300099 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

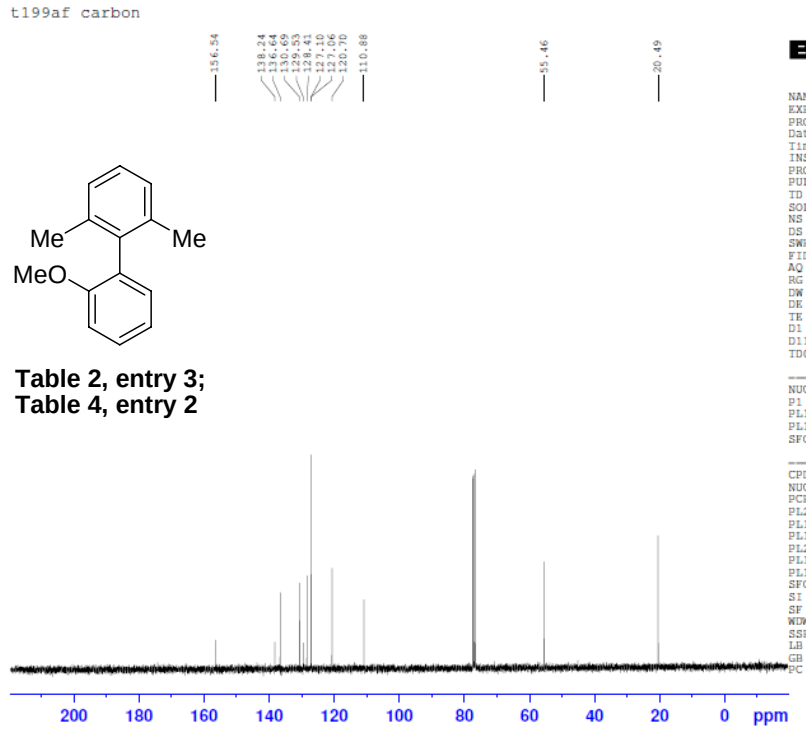


Table 2, entry 3;
Table 4, entry 2

BRUKER

```
NAME          t199af carbon
EXPNO                    1
PROCNO                   1
Date_             20100406
Time                 10.12
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    144
DW                20.800 usec
DE                  6.50 usec
TE                 294.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.50 usec
PL1                -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.00 dB
PL13               15.00 dB
PL2W          11.88122272 W
PL12W          0.37571725 W
PL13W          0.37571725 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 1.40
```

```
File       :C:\msdchem\1\DATA\chun\t199af.D
Operator   : fbm
Acquired   :  6 Apr 2010  10:06     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 1
```

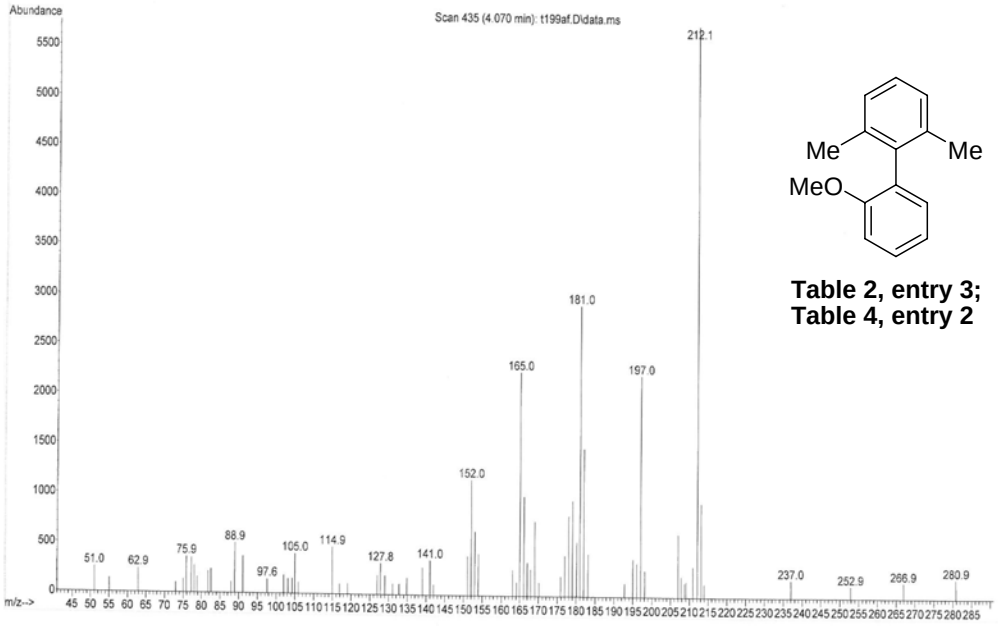


Table 2, entry 3;
Table 4, entry 2

t241dpure proton

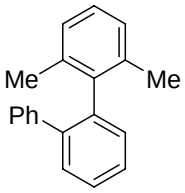
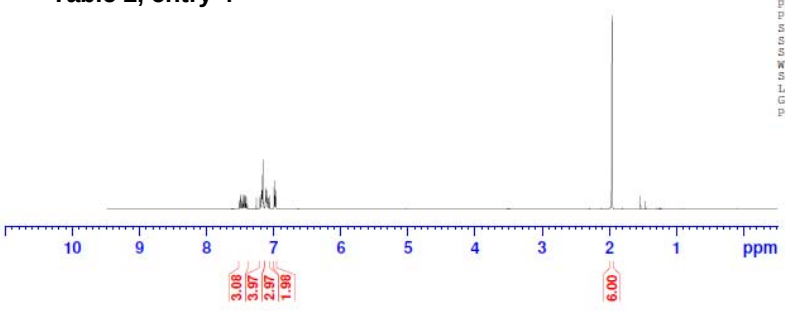


Table 2, entry 4

```
NAME          t241dpure proton
EXPNO                        1
PROCNO                       1
Date_                 20100605
Time                     18.49
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                          16
DS                           2
SWH                 4006.410 Hz
FIDRES              0.122266 Hz
AQ                  4.0894966 sec
RG                          57
DW                     124.800 usec
DE                       6.50 usec
TE                      295.1 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.70 usec
PL1                       0.00 dB
PL1W               11.88122272 W
SFO1              400.1318007 MHz
SI                       32768
SF                400.1300098 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



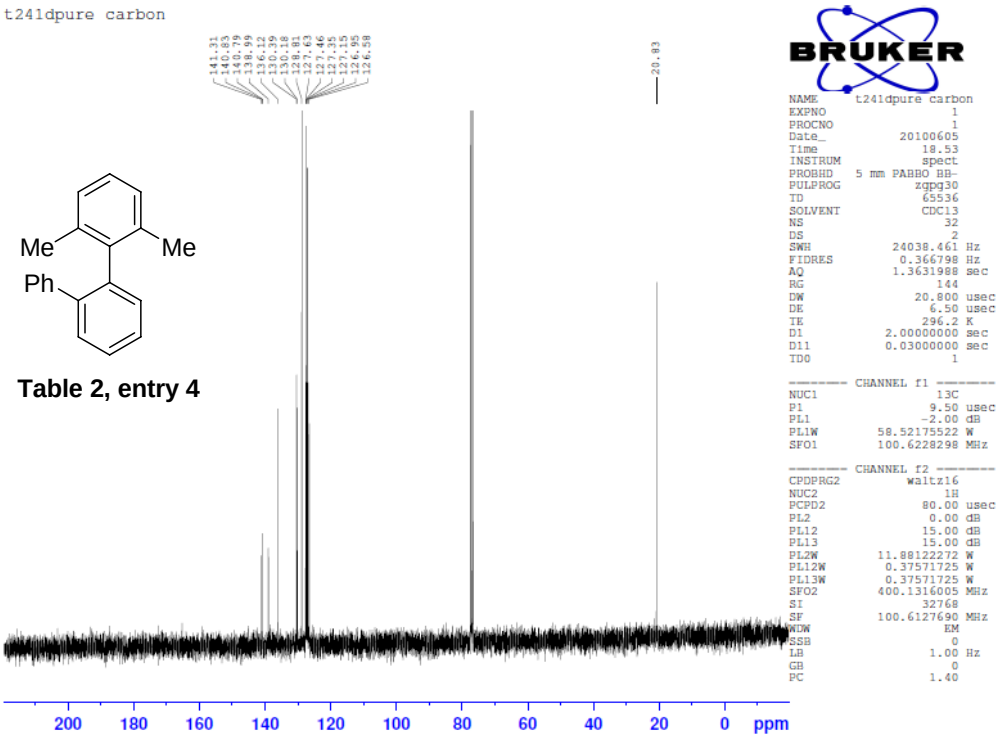


Table 2, entry 4

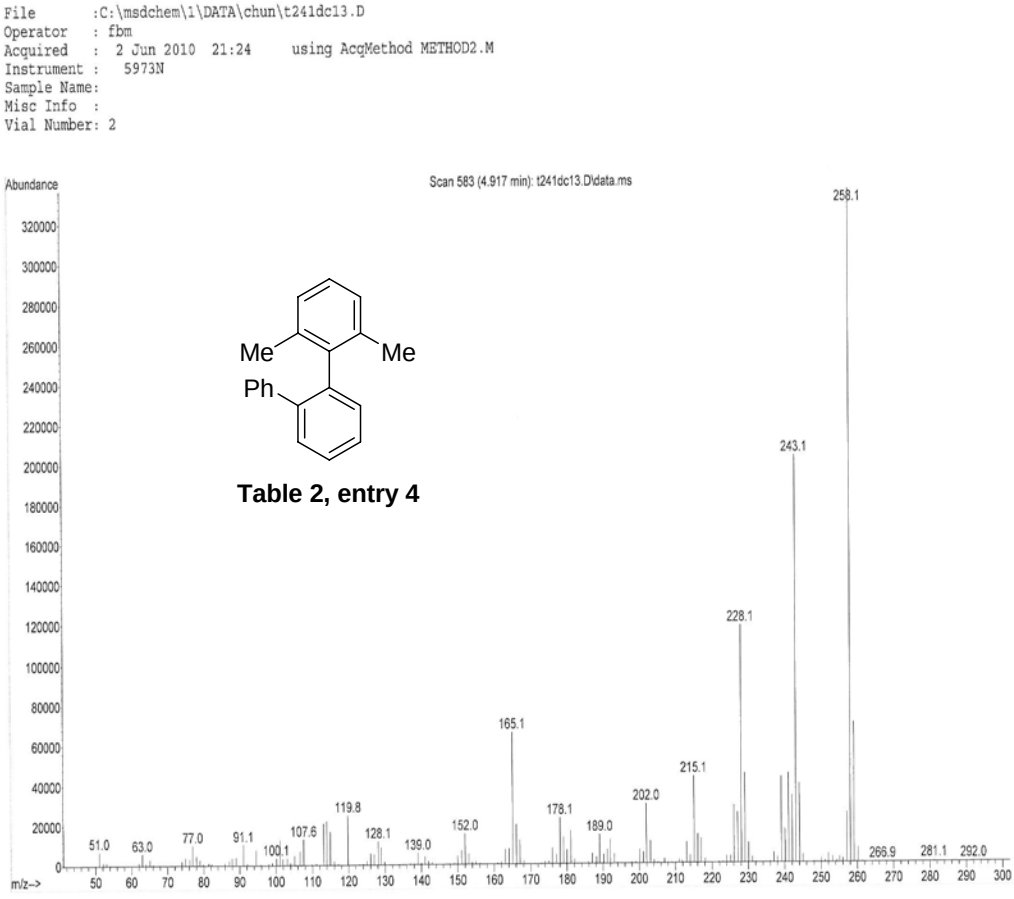
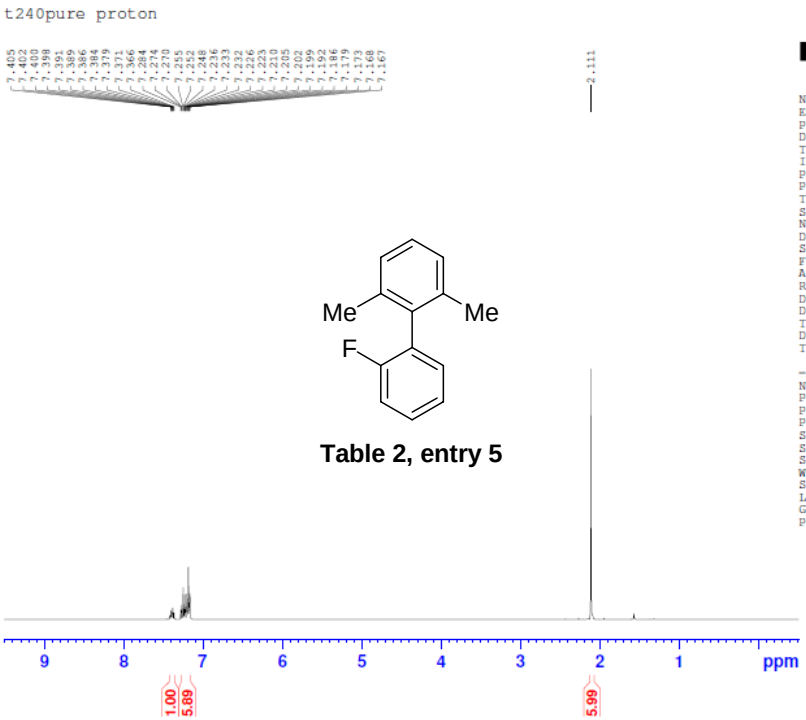


Table 2, entry 4



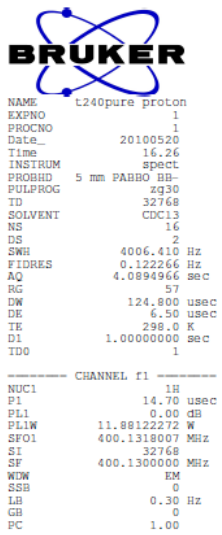
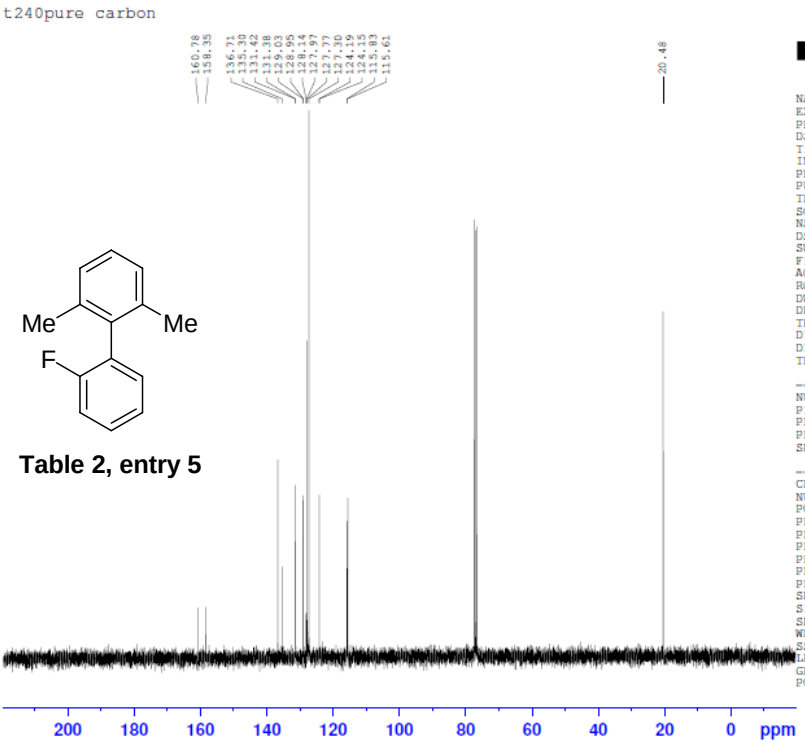


Table 2, entry 5



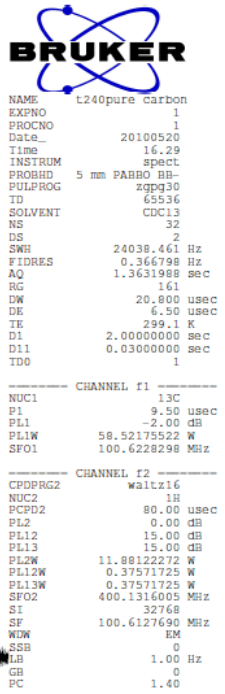


Table 2, entry 5

```
File       :C:\msdchem\1\DATA\chun\t240fpure.D
Operator   : fbm
Acquired   : 20 May 2010  16:12     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 7
```

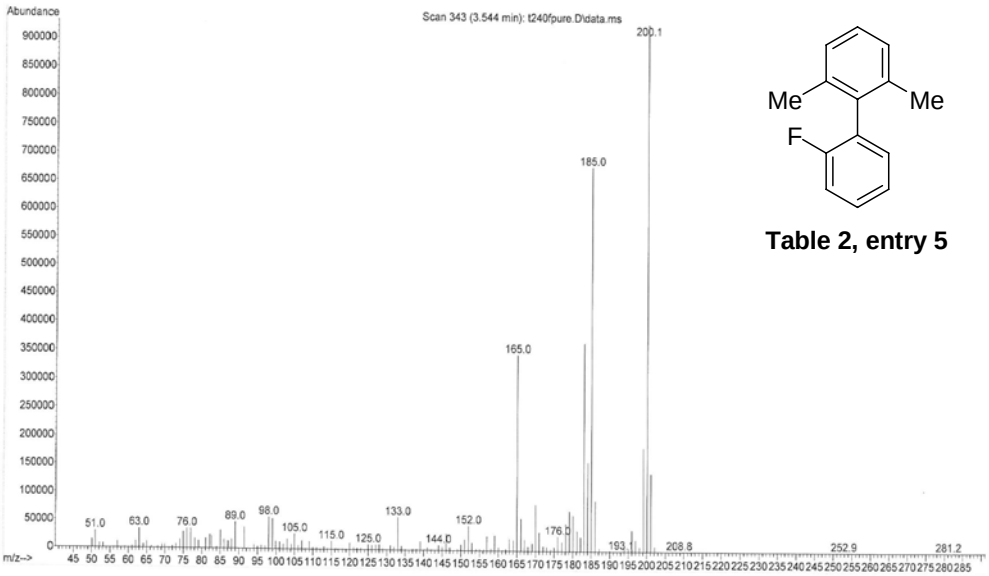
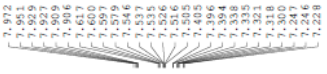


Table 2, entry 5

t199bf proton




```
NAME          t199bf proton
EXPNO                    1
PROCNO                   1
Date_             20100403
Time                 23.38
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              4006.410 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                    50.8
DW               124.800 usec
DE                 6.50 usec
TE                 291.9 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.70 usec
PL1                 0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI                   32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

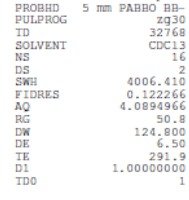
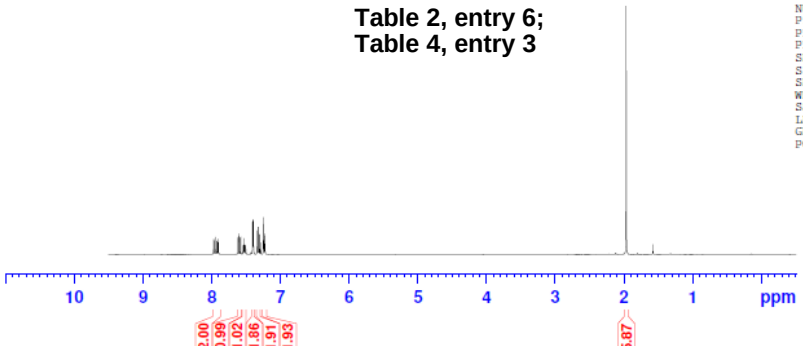


Table 2, entry 6;
Table 4, entry 3



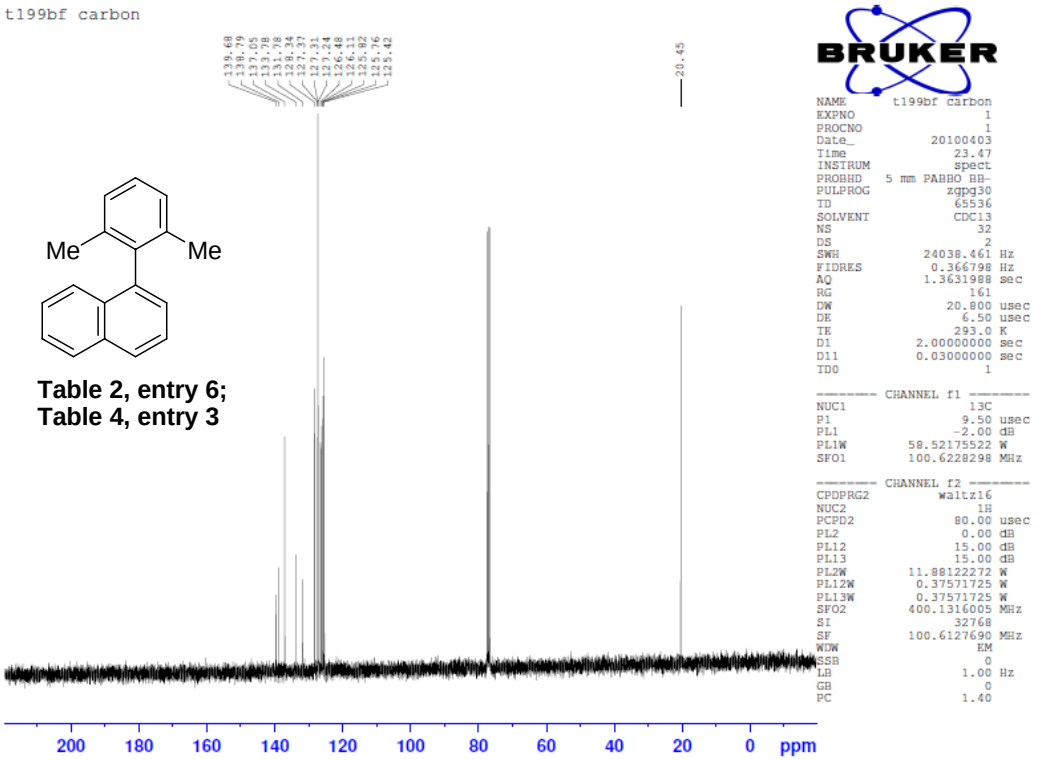


Table 2, entry 6;
Table 4, entry 3

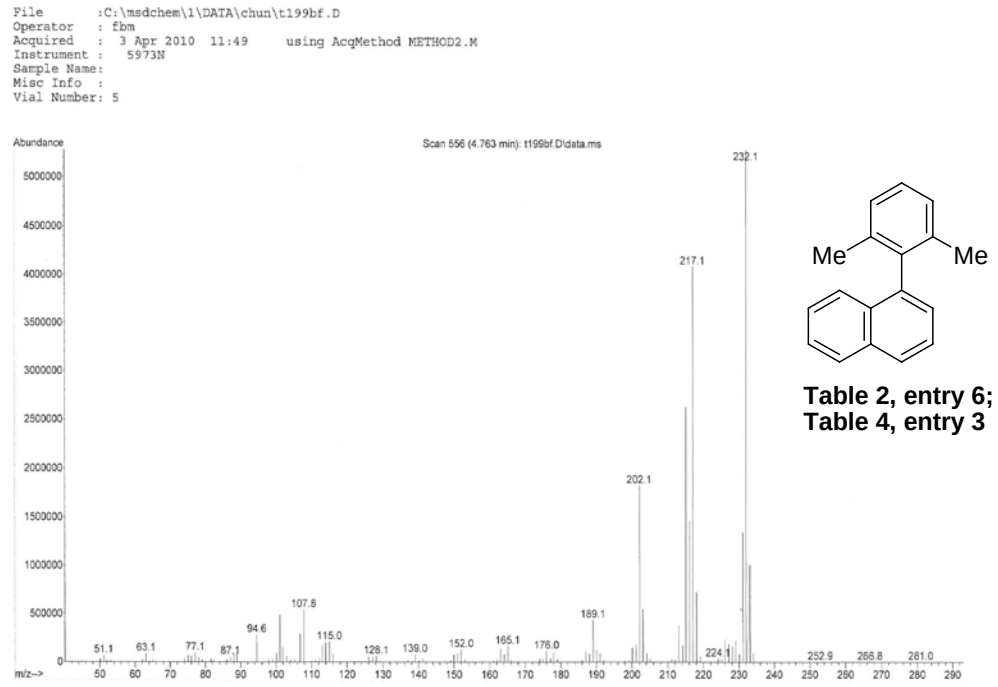


Table 2, entry 6;
Table 4, entry 3

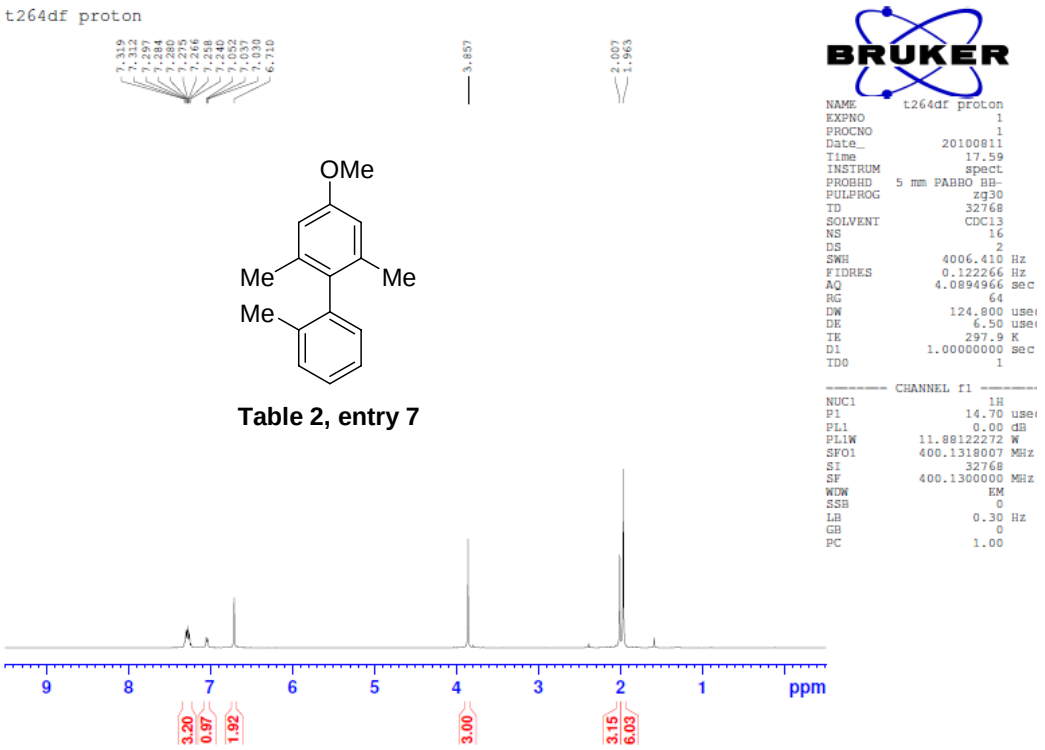


Table 2, entry 7

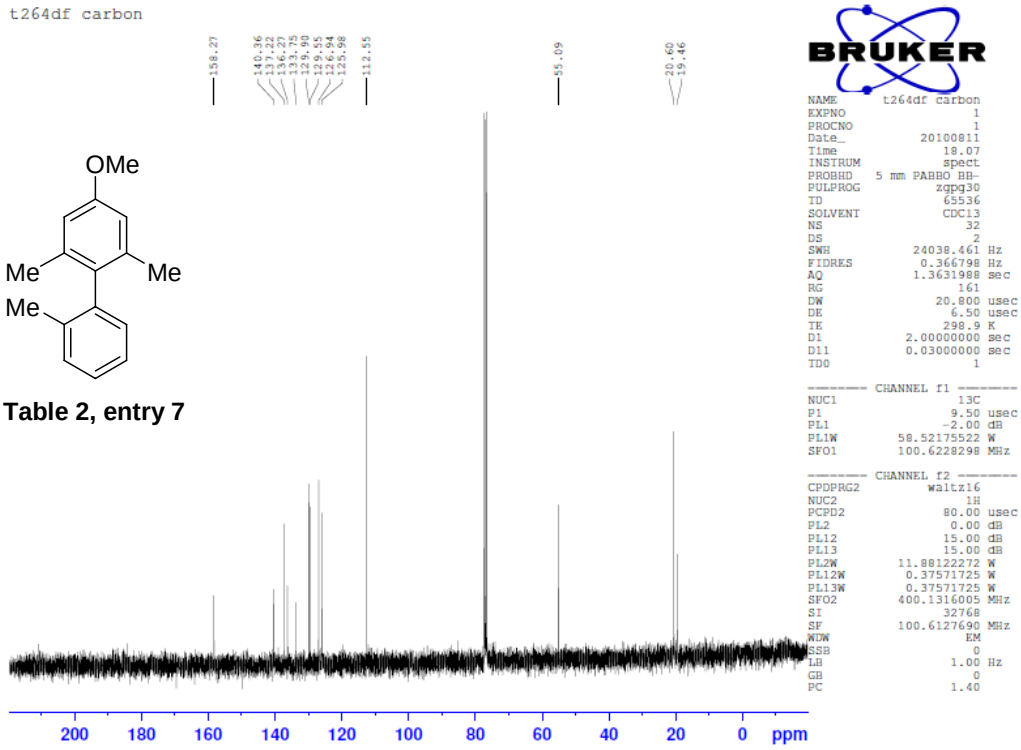


Table 2, entry 7

```
File       :C:\msdchem\1\DATA\Ho\Other\t264df.D
Operator   : Seam
Acquired   : 11 Aug 2010  20:53     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 5
```

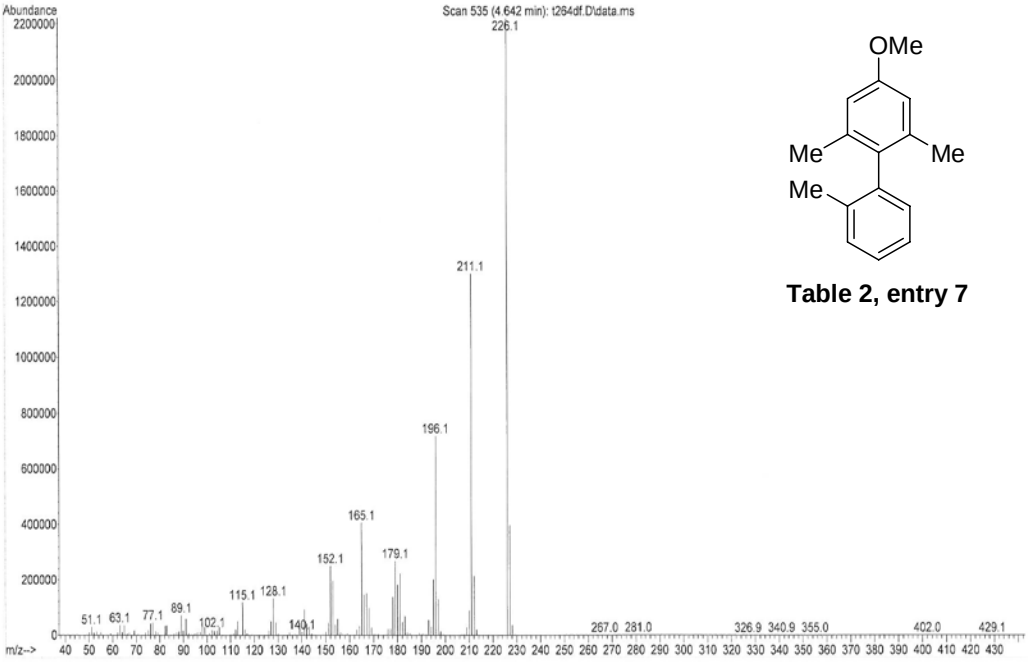


Table 2, entry 7

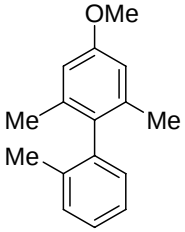


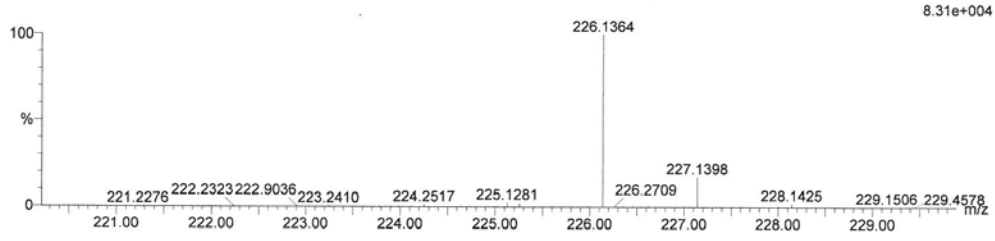
Table 2, entry 7

T264d

Elemental Composition Report **Page 1**

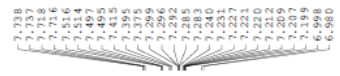
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-20 O: 0-1
Kin-dept-04112010 S5 HS 12 (0.200) Cm (12:21)
TOF MS EI+



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
226.1364	226.1358	0.6	2.7	8.0	16.8	C16 H18 O

t272f proton



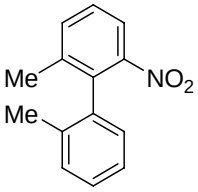
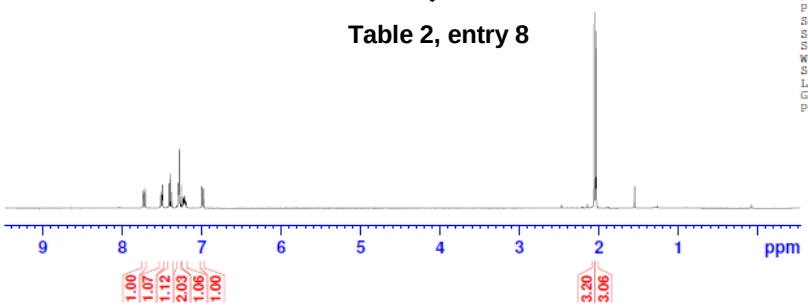


Table 2, entry 8




```
NAME          t272f proton
EXPNO                    1
PROCNO                   1
Date_             20100819
Time                 17.44
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               4006.410 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                    80.6
DW                  124.800 usec
DE                    6.50 usec
TE                  298.4 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.70 usec
PL1                   0.00 dB
PL1W         11.88122272 W
SFO1         400.1318007 MHz
SI                   32768
SF           400.1300106 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

t272f carbon

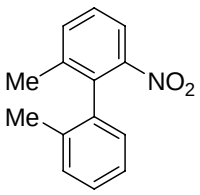


Table 2, entry 8


```
NAME          t272f carbon
EXPNO                    1
PROCNO                   1
Date_             20100819
Time                 17.46
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      32
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     203
DW                  20.800 usec
DE                    6.50 usec
TE                  299.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.50 usec
PL1                  -2.00 dB
PL1W         58.52175522 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.00 dB
PL13                 15.00 dB
PL2W         11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

```
File       :C:\msdchem\1\DATA\Ho\Other\t272f.D
Operator   : Seam
Acquired   : 19 Aug 2010  17:45     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 2
```

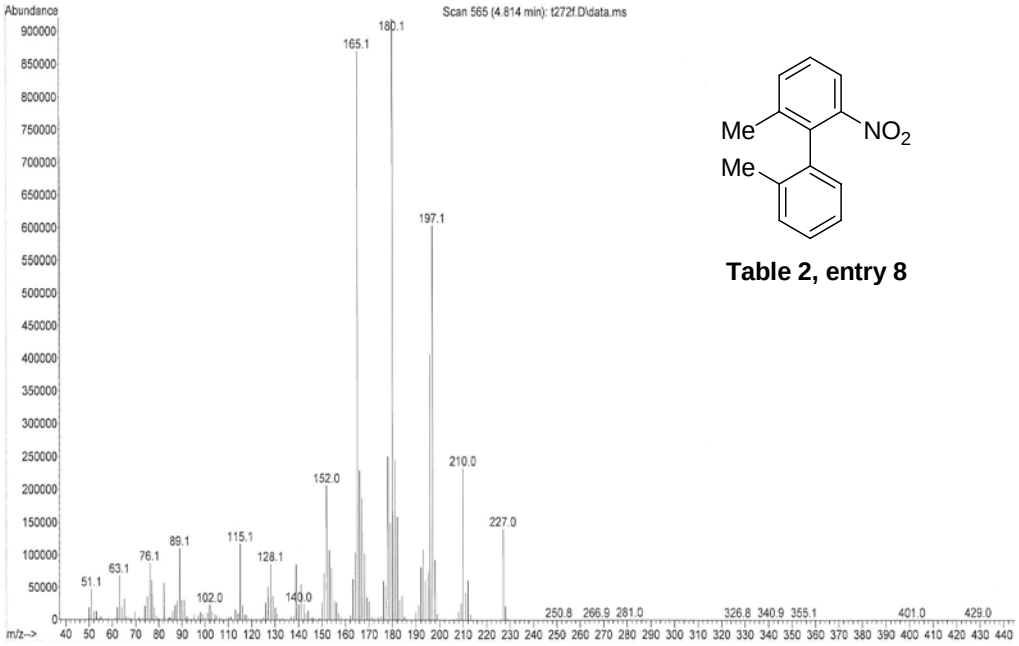


Table 2, entry 8

t187fa proton

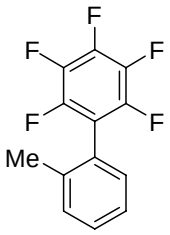
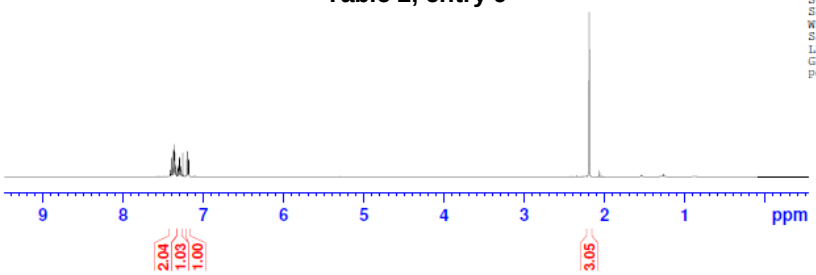


Table 2, entry 9

```
NAME          t187fa proton
EXPNO                    1
PROCNO                   1
Date_             20101124
Time                 11.14
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      16
DS                       2
SWH              4006.410 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                    90.5
DW                 124.800 usec
DE                   6.50 usec
TE                  297.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.70 usec
PL1                 0.00 dB
PL1W         11.88122272 W
SFO1        400.1318007 MHz
SI                   32768
SF          400.1300100 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```



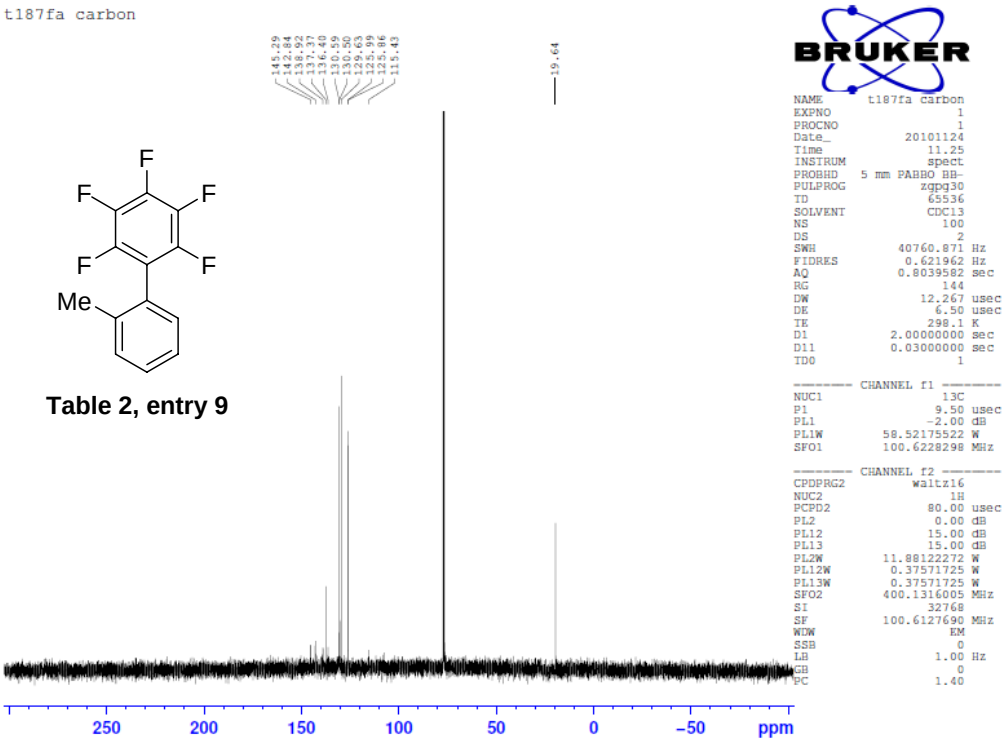


Table 2, entry 9

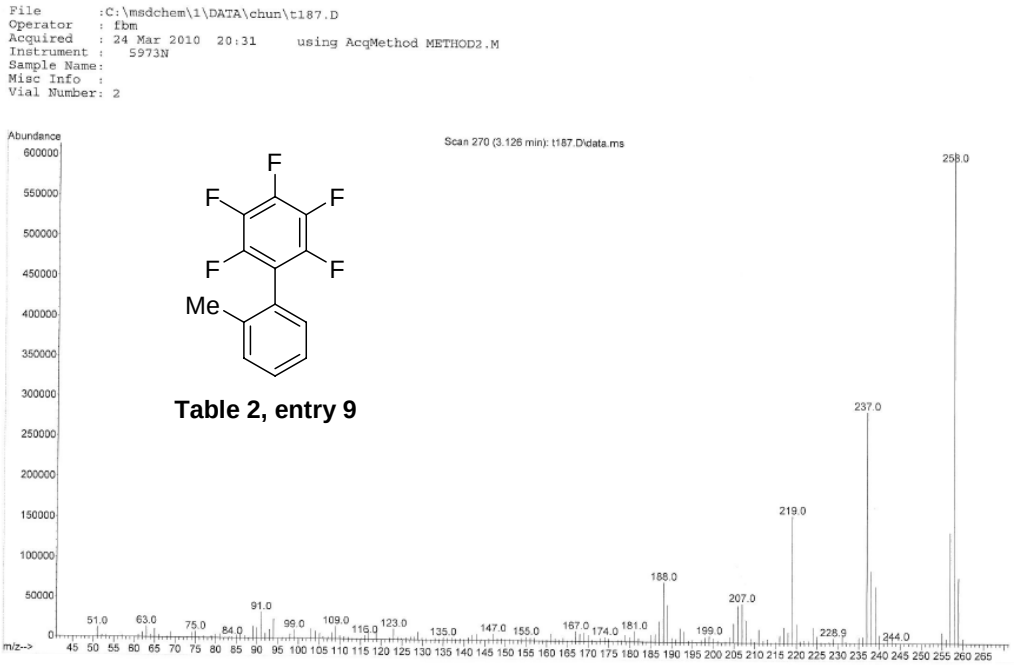


Table 2, entry 9

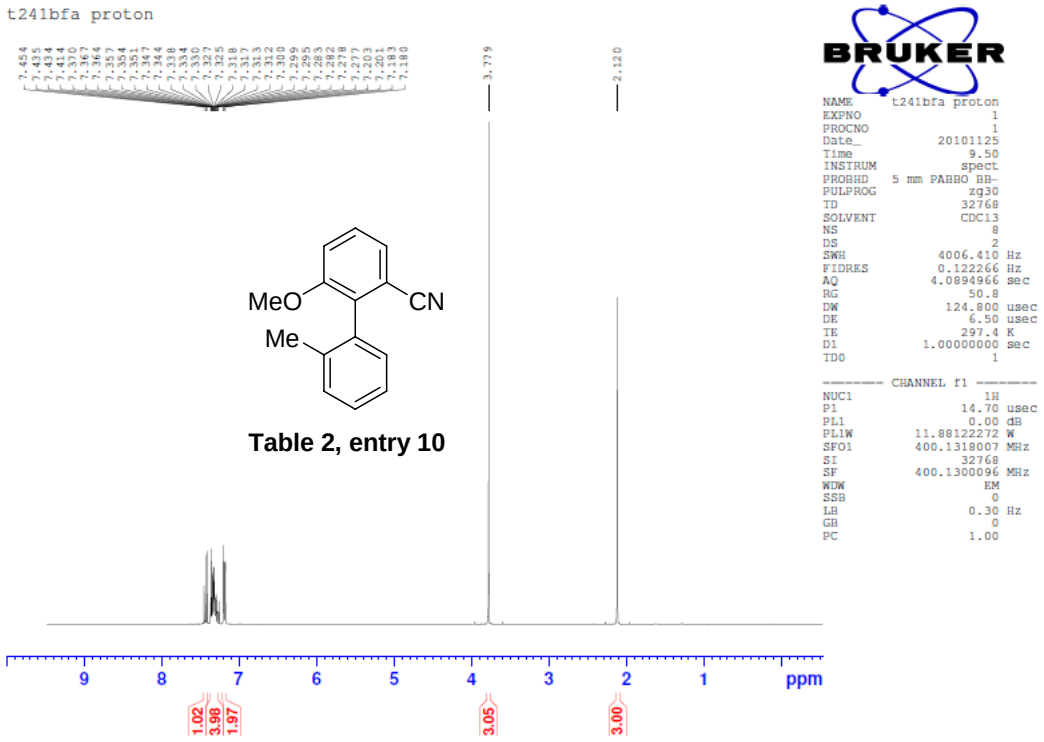


Table 2, entry 10

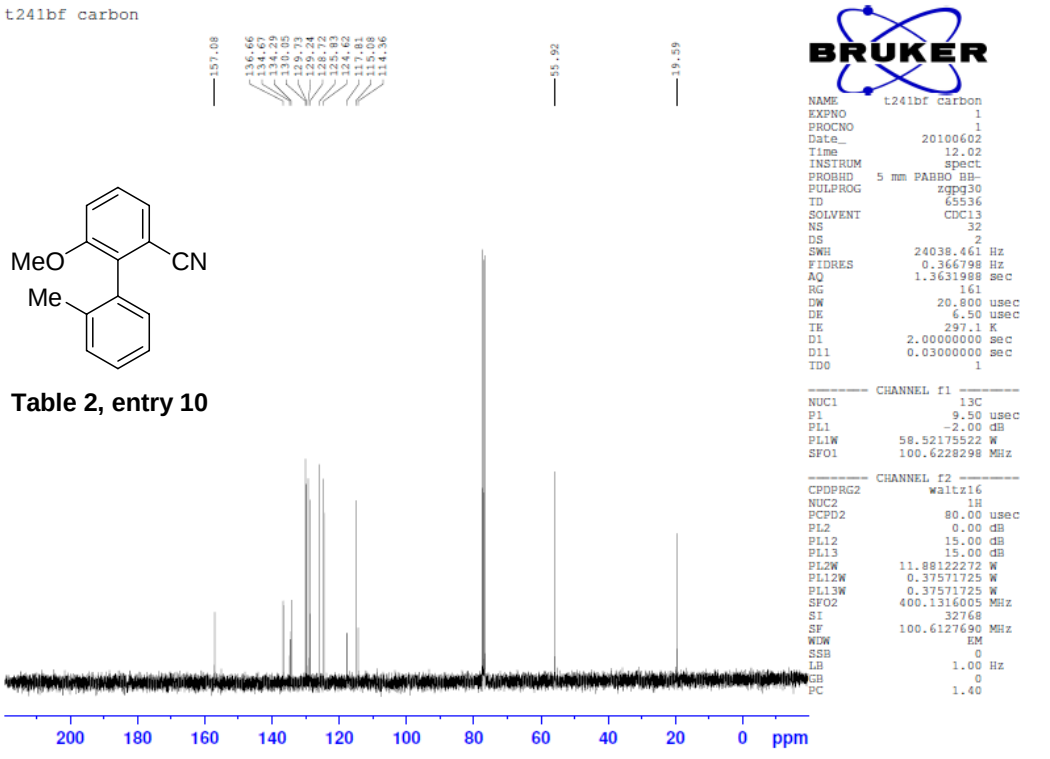


Table 2, entry 10

```
File       :C:\msdchem\1\DATA\chun\t241bf.D
Operator   : fbm
Acquired   :  1 Jun 2010  20:21     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 4
```

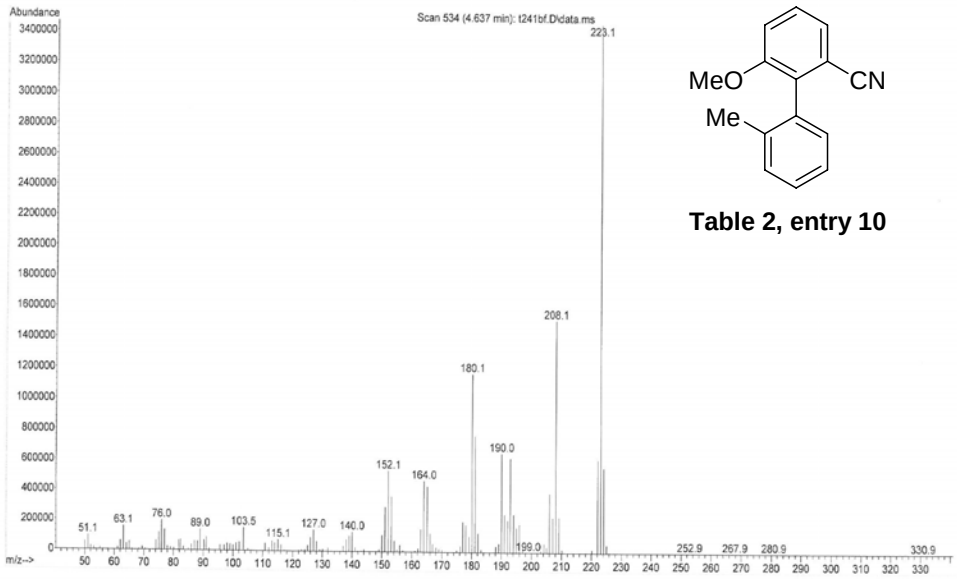
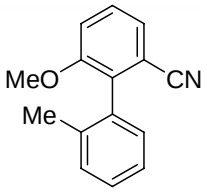


Table 2, entry 10

T241b

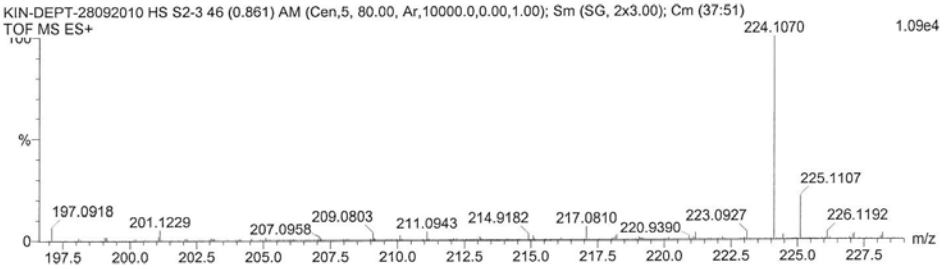


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -100.0, max = 1000.0 **Table 2, entry 10**
Selected filters: None

Monoisotopic Mass, Even Electron Ions
108 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-29 N: 0-2 O: 0-6 Na: 0-1

KIN-DEPT-28092010 HS S2-3 46 (0.861) AM (Cen,5, 80.00, Ar,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (37:51)
TOF MS ES+ 1.09e4



Minimum:				-100.0		
Maximum:		5.0	5.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.1070	224.1075	-0.5	-2.2	9.5	102.5	C15 H14 N O

t257af proton

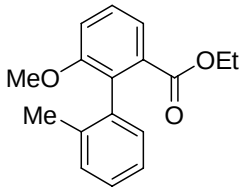
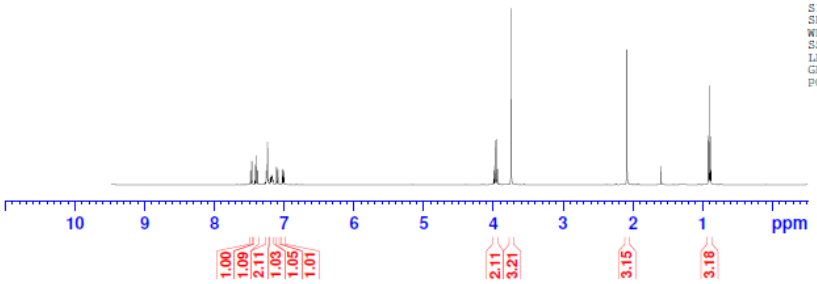


Table 2, entry 11




```
NAME          t257af proton
EXPNO                    1
PROCNO                   1
Date_             20100726
Time                 15.05
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             4006.410 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                   50.8
DW                124.800 usec
DE                  6.50 usec
TE                 298.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.70 usec
PL1                  0.00 dB
PL1W            11.88122272 W
SFO1           400.1318007 MHz
SI                   32768
SF             400.1300103 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

t257af carbon

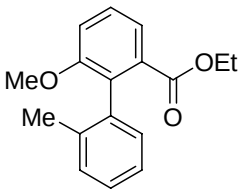


Table 2, entry 11


```
NAME          t257af carbon
EXPNO                    1
PROCNO                   1
Date_             20100726
Time                 15.07
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                  6.50 usec
TE                 299.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.50 usec
PL1                 -2.00 dB
PL1W            58.52175522 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W            11.88122272 W
PL12W            0.37571725 W
PL13W            0.37571725 W
SFO2           400.1316005 MHz
SI                   32768
SF             100.6127690 MHz
WDW                     EM
SSB                      0
LB                   1.00 Hz
GB                       0
PC                    1.40
```

```
File       :C:\msdchem\1\DATA\chun\t257af.D
Operator   : fbm
Acquired   : 26 Jul 2010  12:05     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 1
```

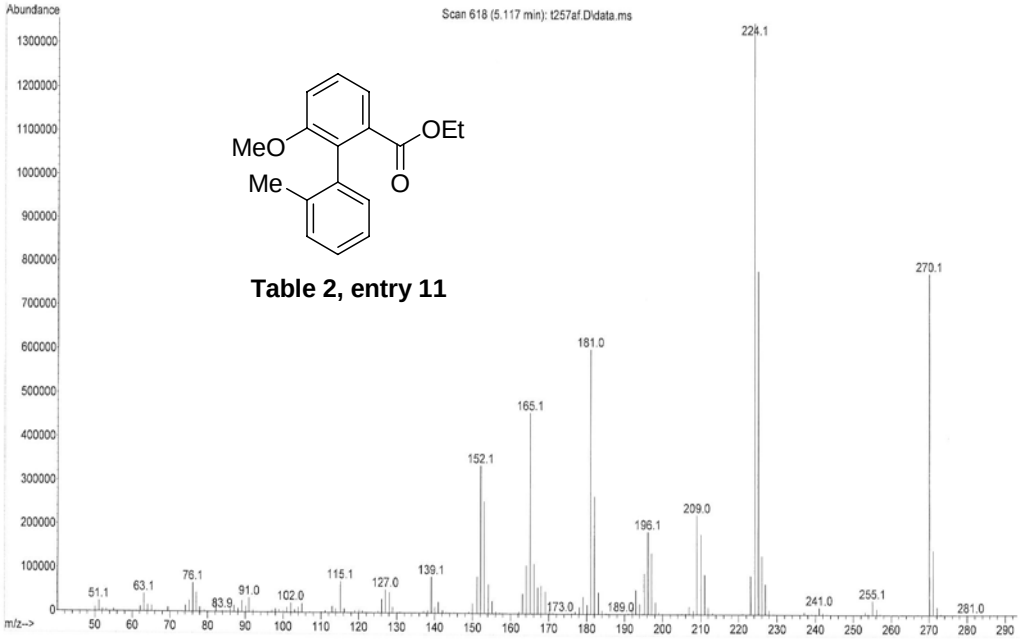
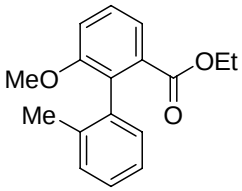


Table 2, entry 11

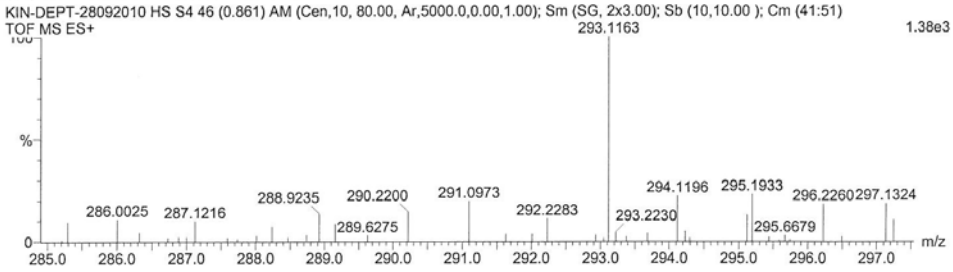


Elemental Composition Report T257a **Page 1**

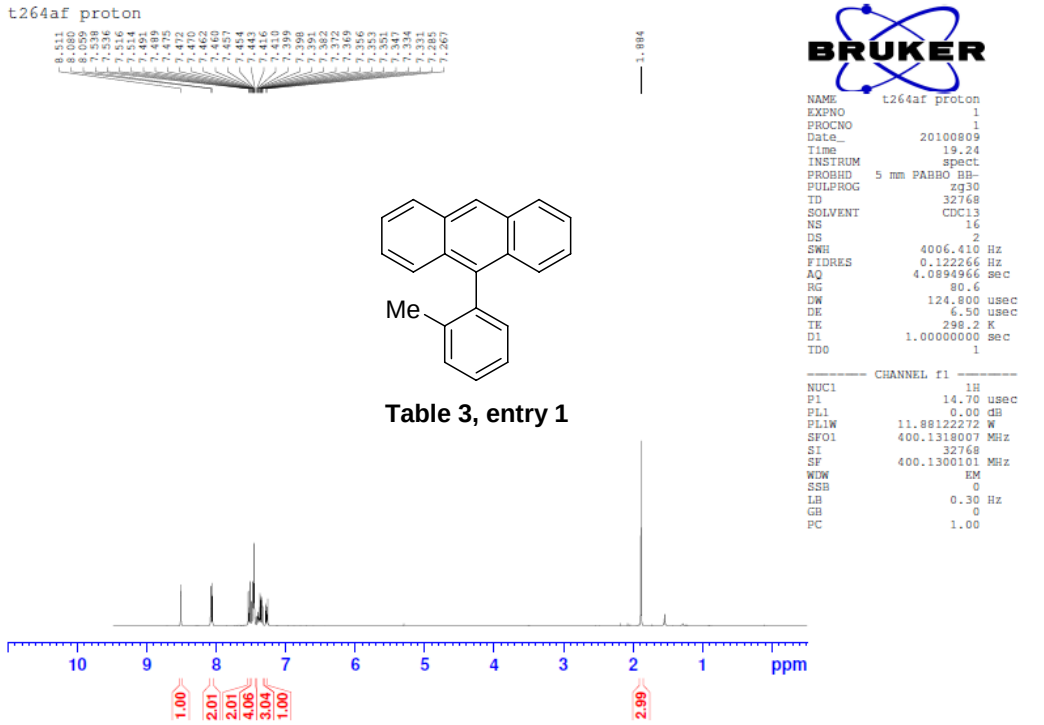
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

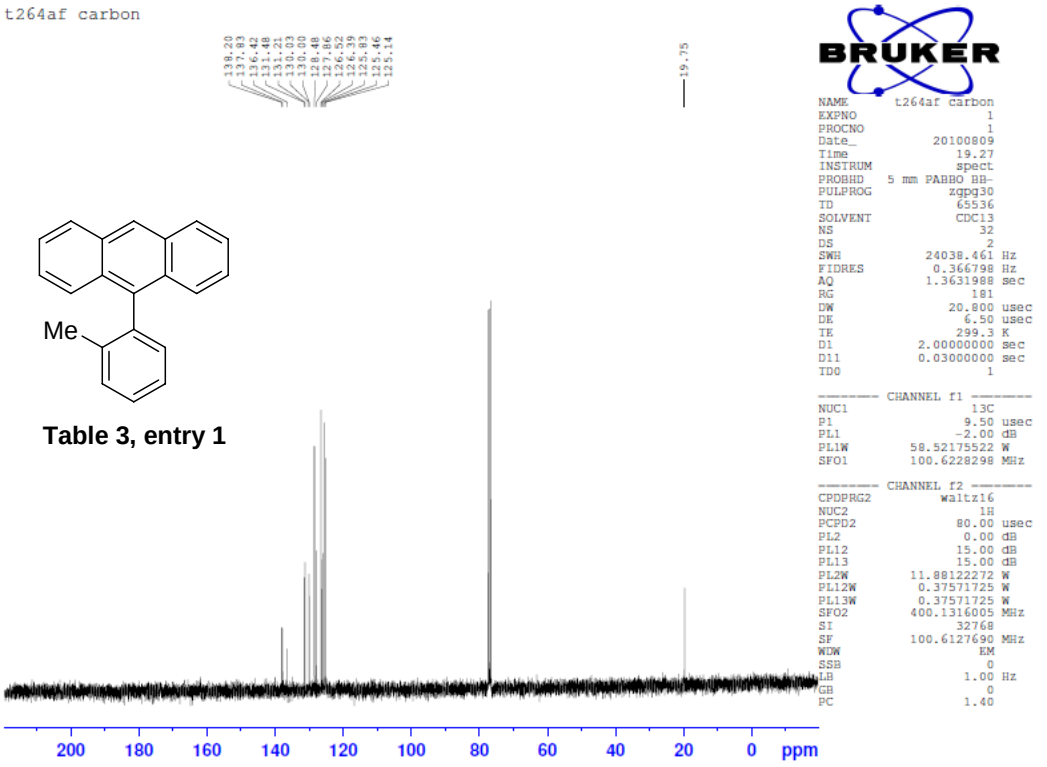
Table 2, entry 11

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-18 O: 0-6 Na: 0-1
KIN-DEPT-28092010 HS S4 46 (0.861) AM (Cen,10, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Sb (10,10.00); Cm (41:51)



Minimum:				-100.0		
Maximum:		5.0	20.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
293.1163	293.1154	0.9	3.1	8.5	61.1	C17 H18 O3 Na


t264af proton
Me
Table 3, entry 1
NAME t264af proton
EXPNO 1
PROCNO 1
Date_ 20100809
Time 19.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 80.6
DW 124.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 2.01 2.01 4.06 3.04 1.00 2.99


t264af carbon
Me
Table 3, entry 1
NAME t264af carbon
EXPNO 1
PROCNO 1
Date_ 20100809
Time 19.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

```
File       :C:\msdchem\1\DATA\arwo\t264af.D
Operator   : CM SO
Acquired   :  9 Aug 2010  17:58     using AcqMethod METHOD2.M
Instrument :
  5973N
Sample Name:
Misc Info  :
Vial Number: 2
```

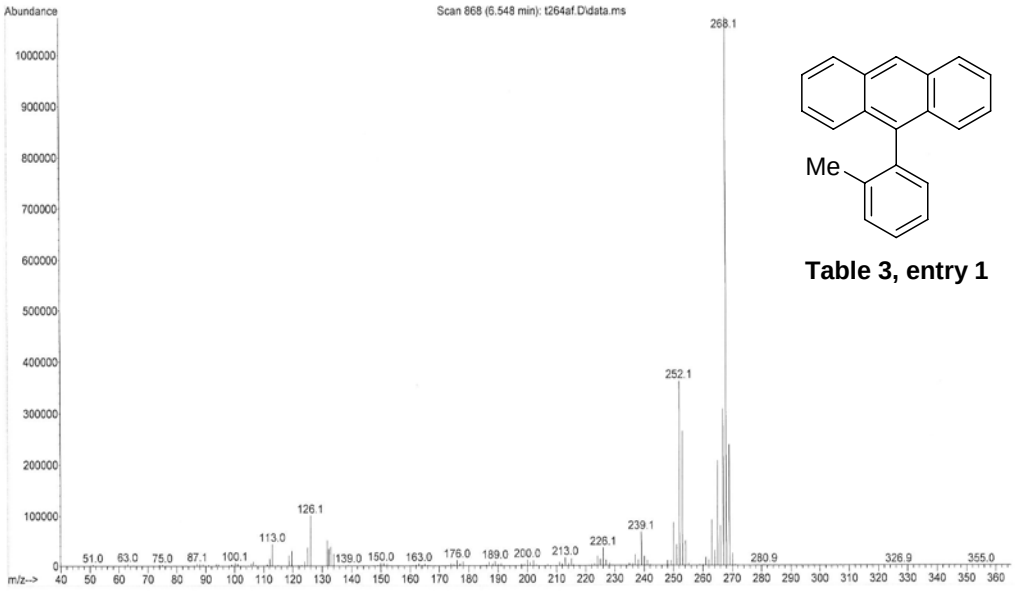


Table 3, entry 1

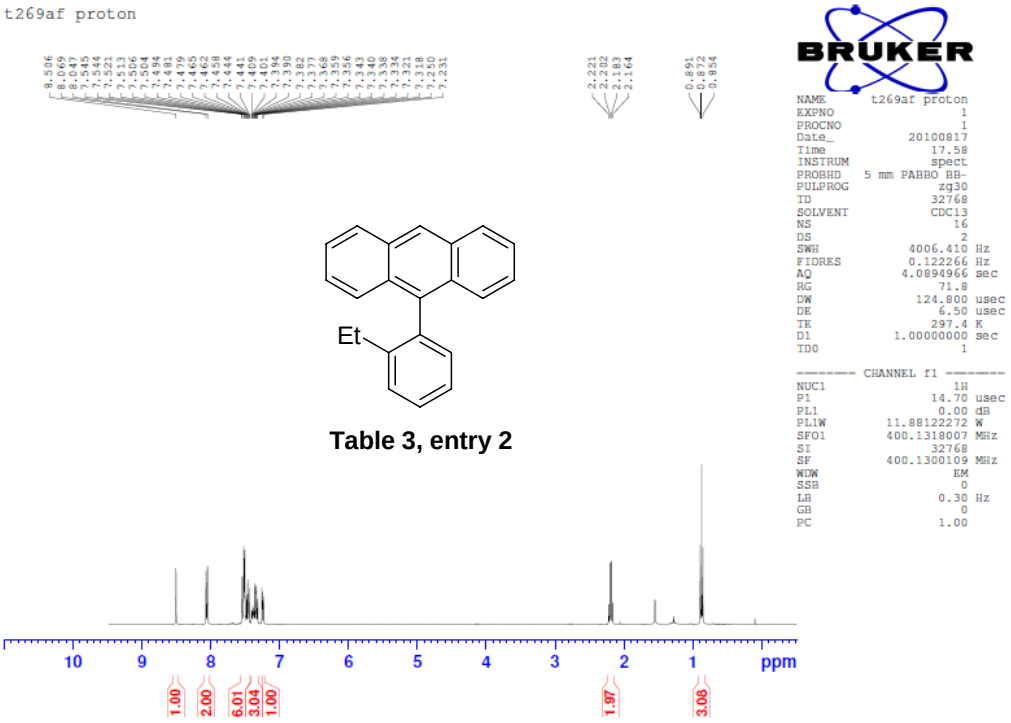


Table 3, entry 2

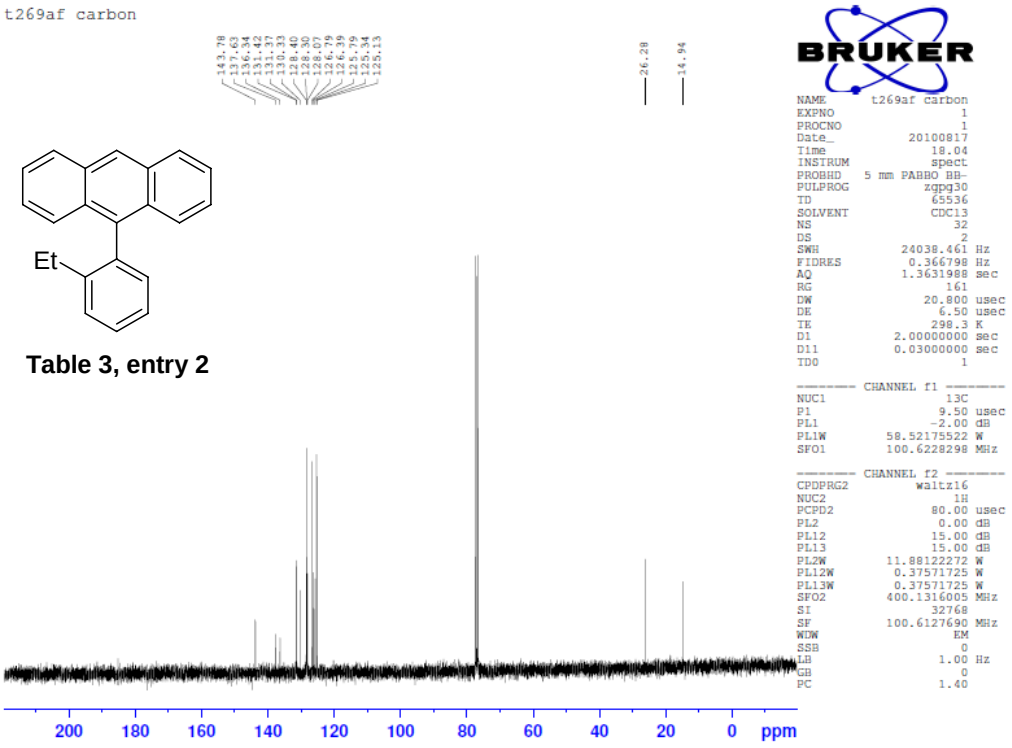


Table 3, entry 2

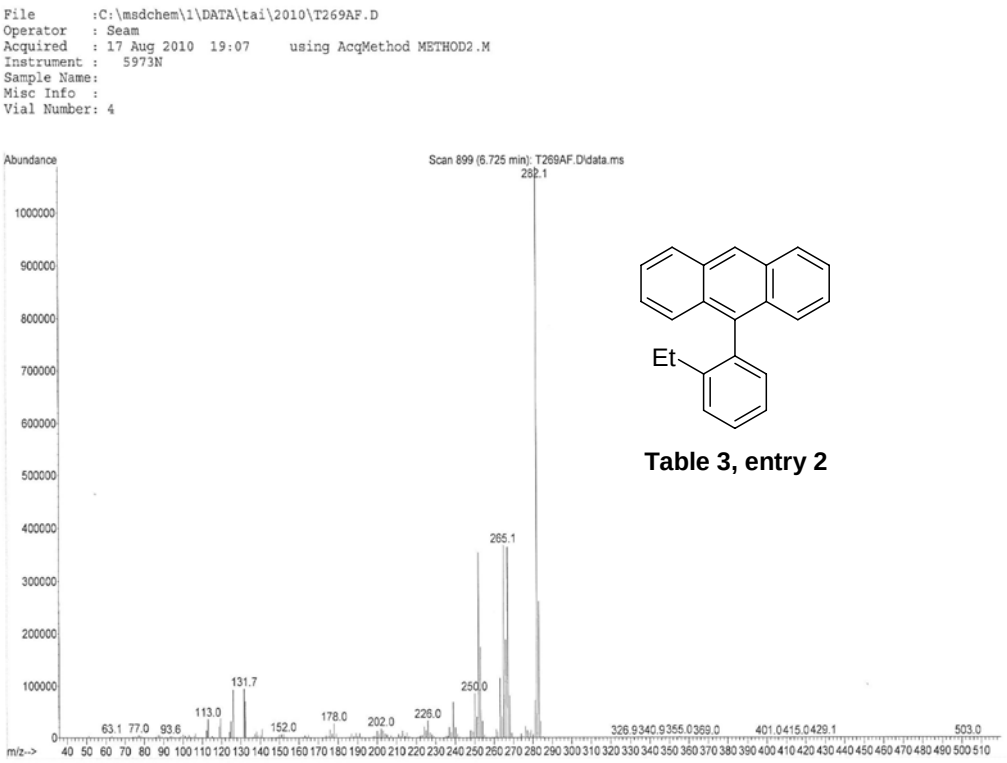


Table 3, entry 2

t275f proton

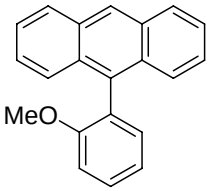
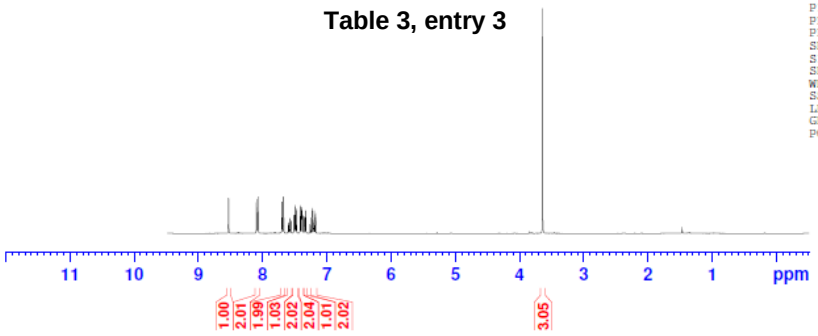


Table 3, entry 3




```
NAME            t275f proton
EXPNO                      1
PROCNO                     1
Date_               20100826
Time                   16.28
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                4006.410 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                      45.2
DW                   124.800 usec
DE                     6.50 usec
TE                   297.5 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.70 usec
PL1                      0.00 dB
PL1W               11.88122272 W
SFO1              400.1318007 MHz
SI                        32768
SF                400.1300094 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

t275f carbon

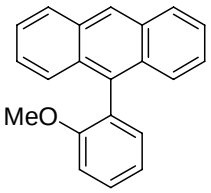
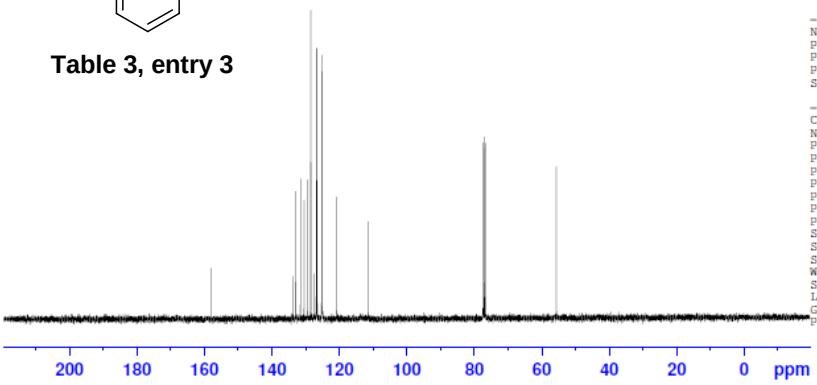


Table 3, entry 3




```
NAME            t275f carbon
EXPNO                      1
PROCNO                     1
Date_               20100826
Time                   16.33
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                        32
DS                         2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       203
DW                   20.800 usec
DE                     6.50 usec
TE                   298.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                     -2.00 dB
PL1W               58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                      0.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W               11.88122272 W
PL12W               0.37571725 W
PL13W               0.37571725 W
SFO2              400.1316005 MHz
SI                        32768
SF                100.6127690 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

```
File          :C:\madchem\1\DATA\Ho\Othex\t265.D
Operator      : Seam
Acquired      : 19 Aug 2010   16:17       using AcqMethod METHOD2.M
Instrument    :
   5973N
Sample Name:
Misc Info     :
Vial Number:  3
```

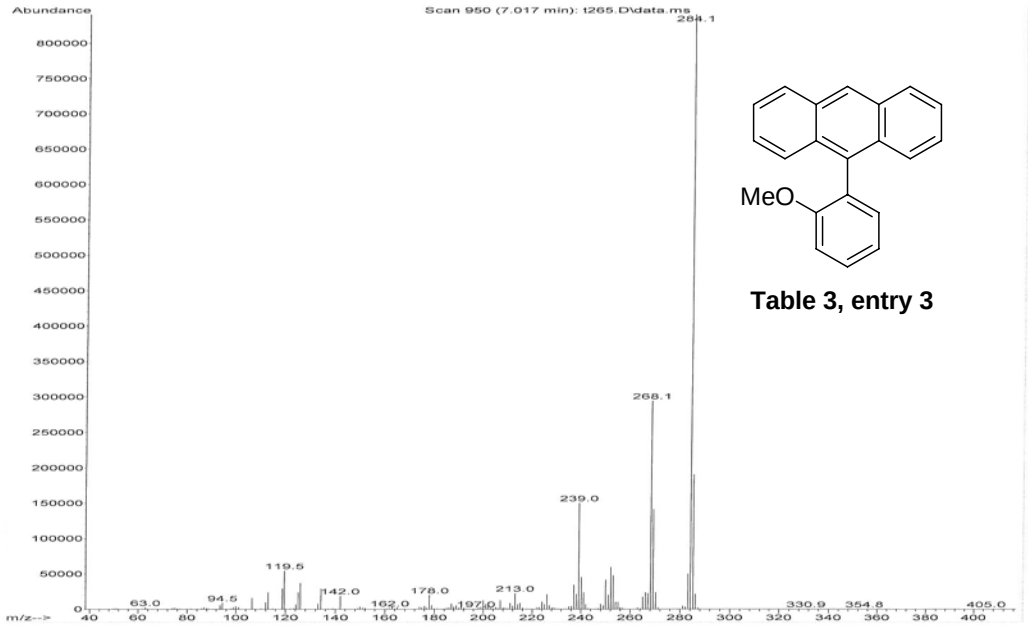
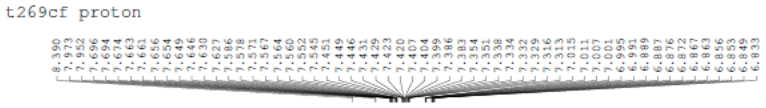


Table 3, entry 3



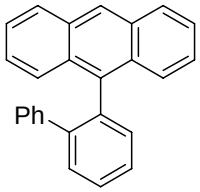
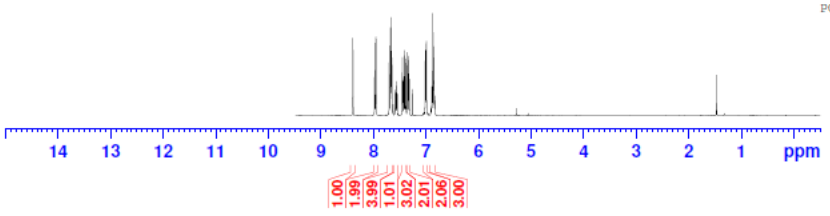


Table 3, entry 4

BRUKER

```
NAME            t269cf proton
EXPNO                       1
PROCNO                      1
Date_                20100817
Time                    18.18
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                      32768
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  4006.410 Hz
FIDRES               0.122266 Hz
AQ                   4.0894966 sec
RG                        50.8
DW                     124.800 usec
DE                       6.50 usec
TE                      297.4 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.70 usec
PL1                      0.00 dB
PL1W                11.88122272 W
SFO1               400.1318007 MHz
SI                      32768
SF                 400.1300098 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```



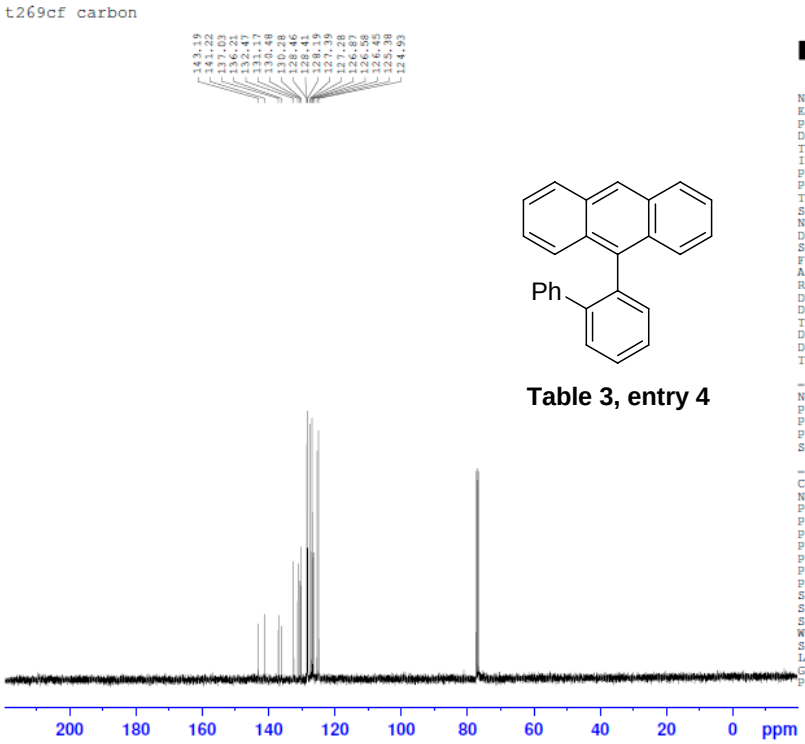


Table 3, entry 4

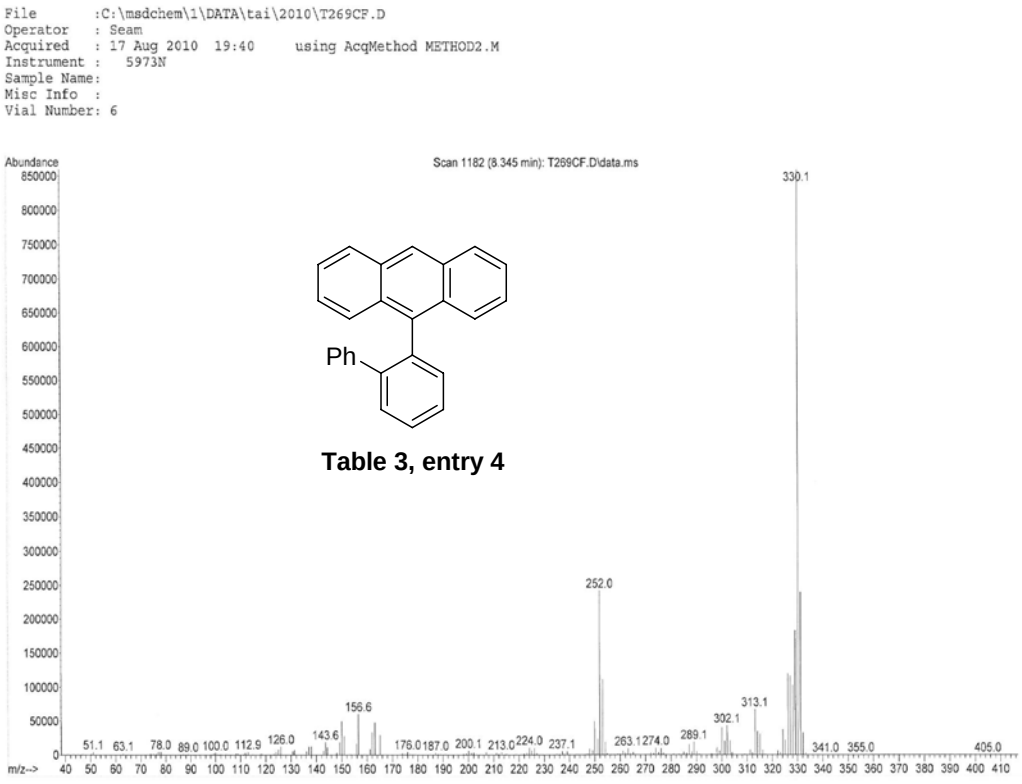
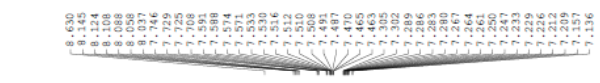


Table 3, entry 4

t269bf proton



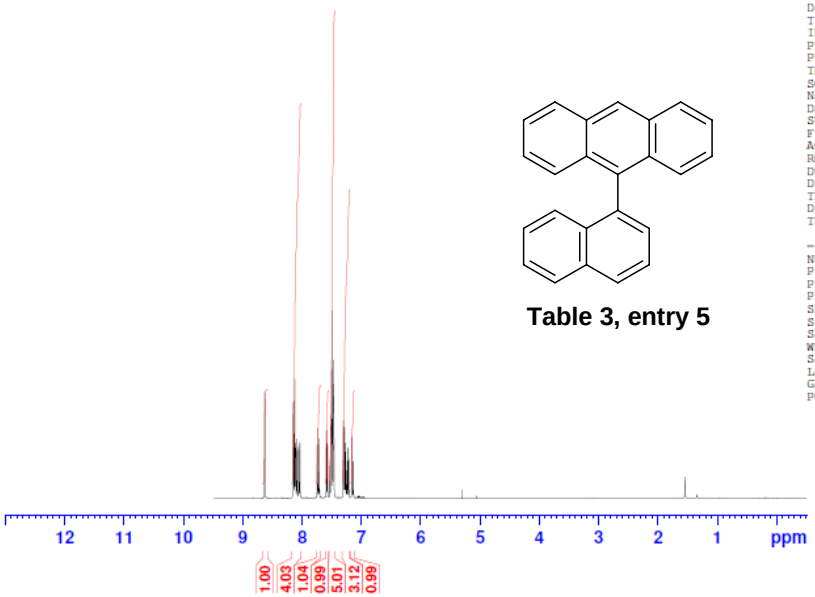


Table 3, entry 5

```
NAME          t269bf proton
EXPNO                    1
PROCNO                   1
Date_             20100817
Time                 18.09
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      16
DS                       2
SWH              4006.410 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                    45.2
DW                124.800 usec
DE                  6.50 usec
TE                 297.3 K
D1            1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.70 usec
PL1                   0.00 dB
PL1W         11.88122272 W
SFO1         400.1318007 MHz
SI                   32768
SF           400.1300093 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

t269bf carbon

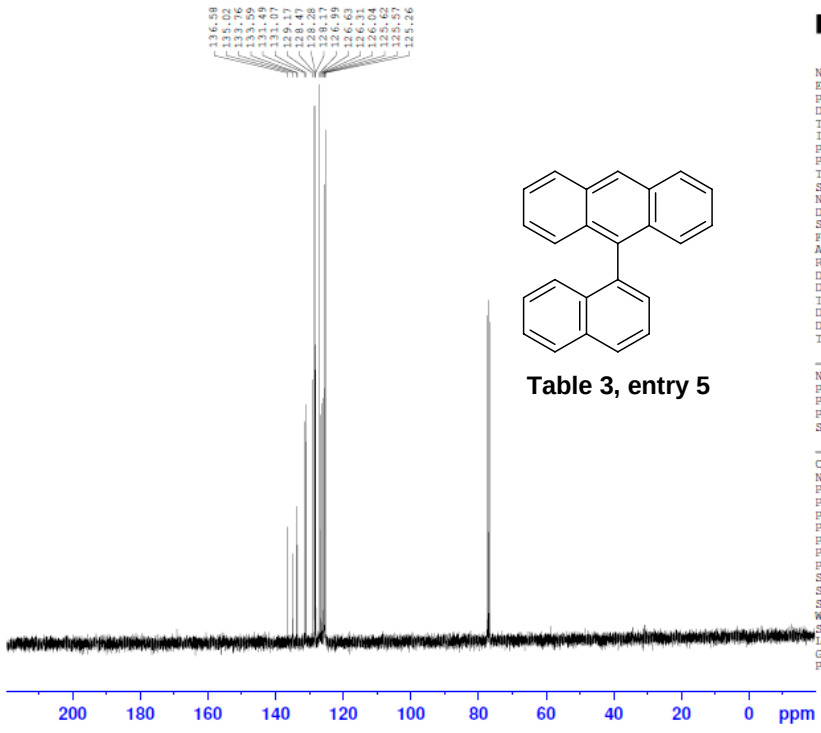


Table 3, entry 5

```
NAME          t269bf carbon
EXPNO                    1
PROCNO                   1
Date_             20100817
Time                 18.11
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                      32
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     144
DW                 20.800 usec
DE                  6.50 usec
TE                 298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.50 usec
PL1                  -2.00 dB
PL1W         58.52175522 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.00 dB
PL13                 15.00 dB
PL2W         11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

```
File       :C:\msdchem\1\DATA\tai\2010\T269BF.D
Operator   : Seam
Acquired   : 17 Aug 2010  19:24     using AcqMethod METHOD2.M
Instrument :
   5973N
Sample Name:
Misc Info  :
Vial Number: 5
```

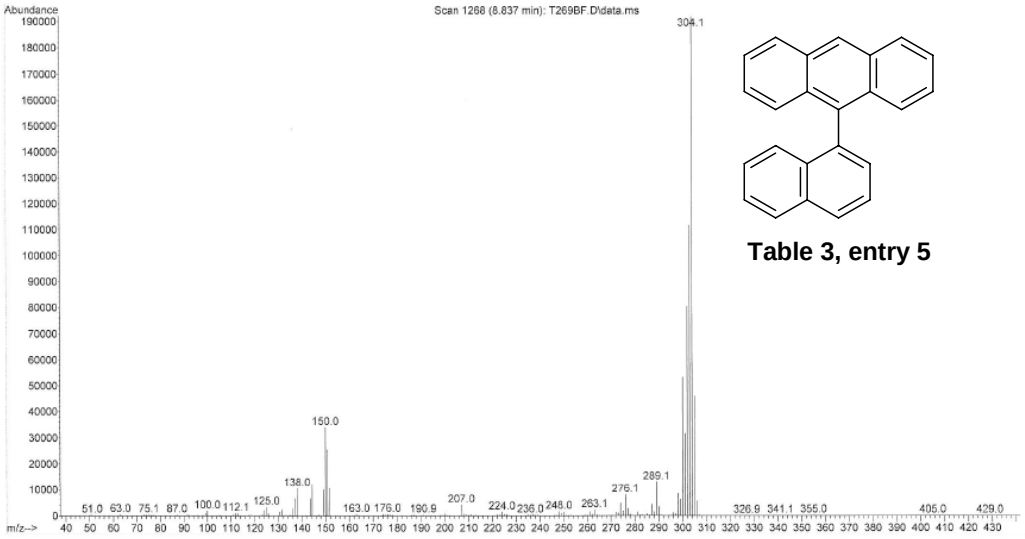
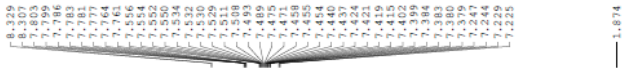


Table 3, entry 5

t210afa proton




```
NAME          t210afa proton
EXPNO                      1
PROCNO                     1
Date_               20101124
Time                   16.14
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                4006.410 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                       161
DW                 124.800 usec
DE                   6.50 usec
TE                   297.3 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                   14.70 usec
PL1                   0.00 dB
PL1W             11.88122272 W
SFO1             400.1318007 MHz
SI                    32768
SF               400.1300107 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

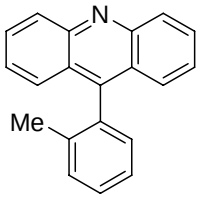
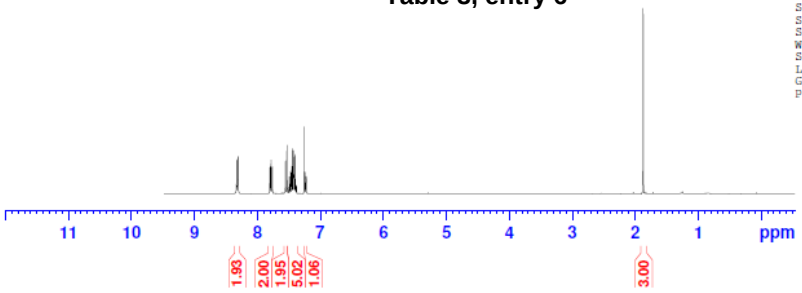
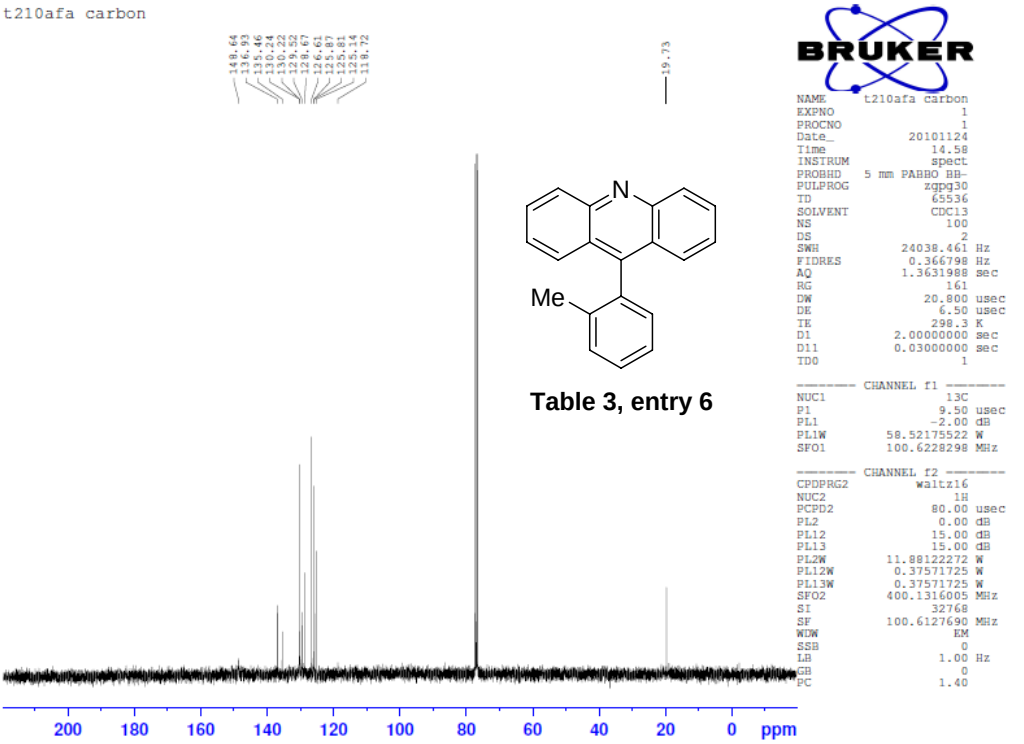
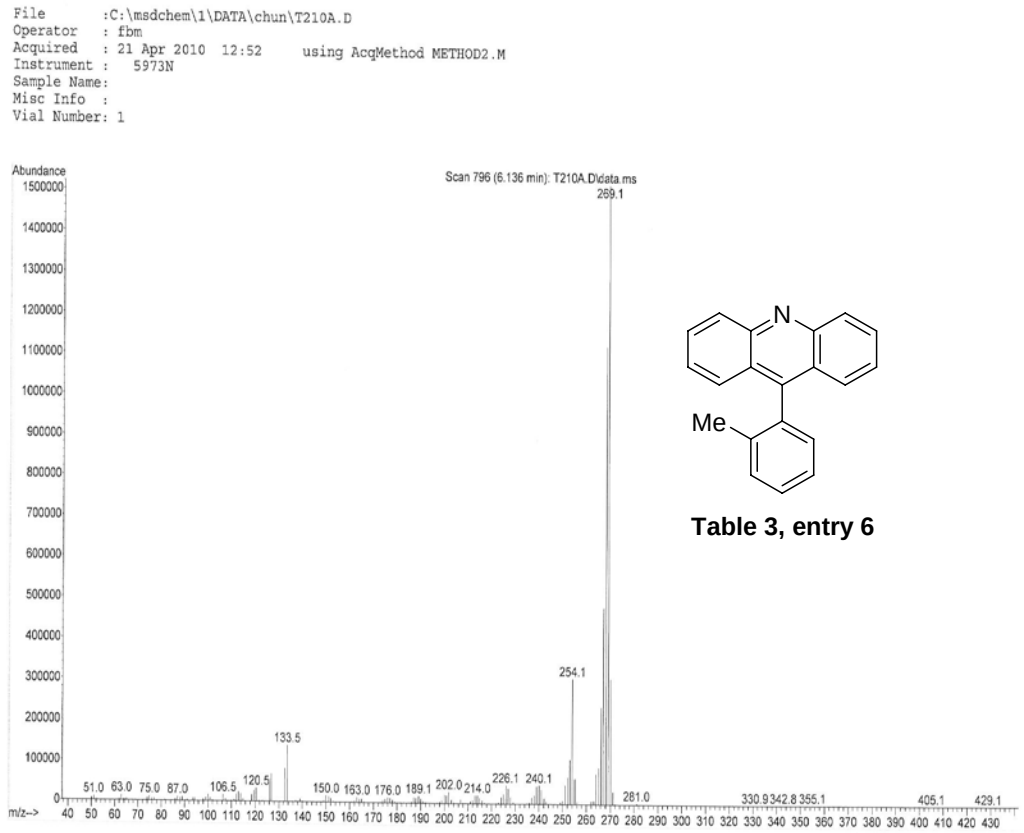


Table 3, entry 6




t210afa carbon
148.64
136.93
135.46
130.24
130.22
129.52
128.67
126.61
125.88
125.81
125.14
118.72
19.73
N
Me
Table 3, entry 6
BRUKER
NAME t210afa carbon
EXPNO 1
PROCNO 1
Date_ 20101124
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 100
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 161
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


File :C:\msdchem\1\DATA\chun\T210A.D
Operator : fbm
Acquired : 21 Apr 2010 12:52 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1
Abundance
Scan 796 (6.136 min): T210A.D\data.ms
269.1
254.1
133.5
N
Me
Table 3, entry 6
m/z-->

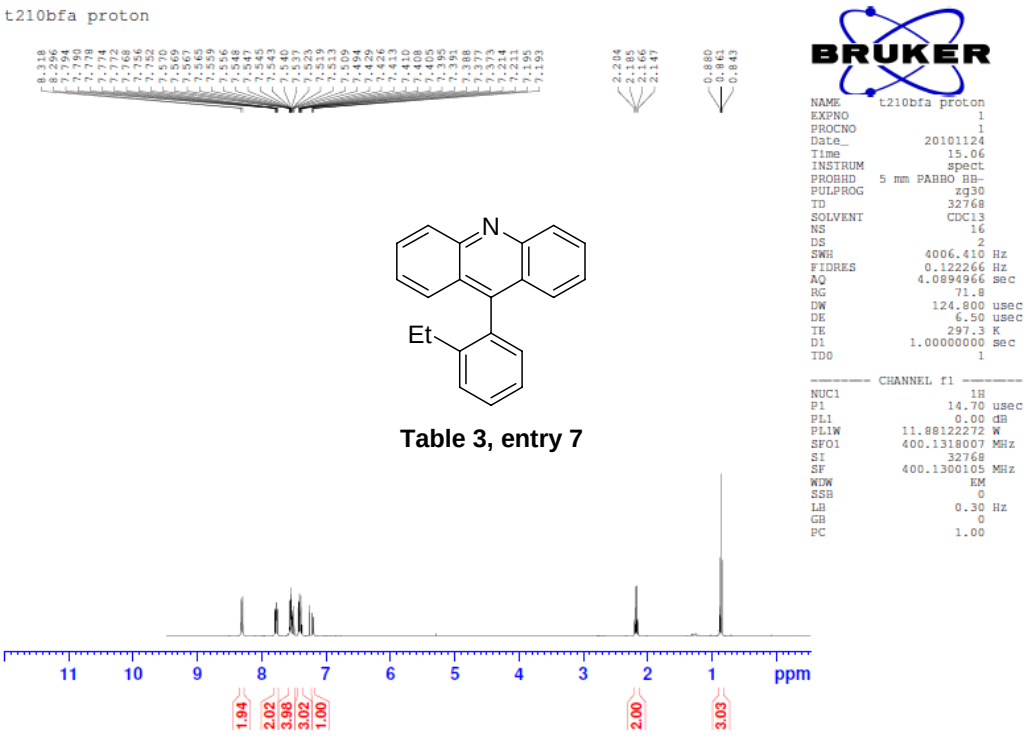


Table 3, entry 7

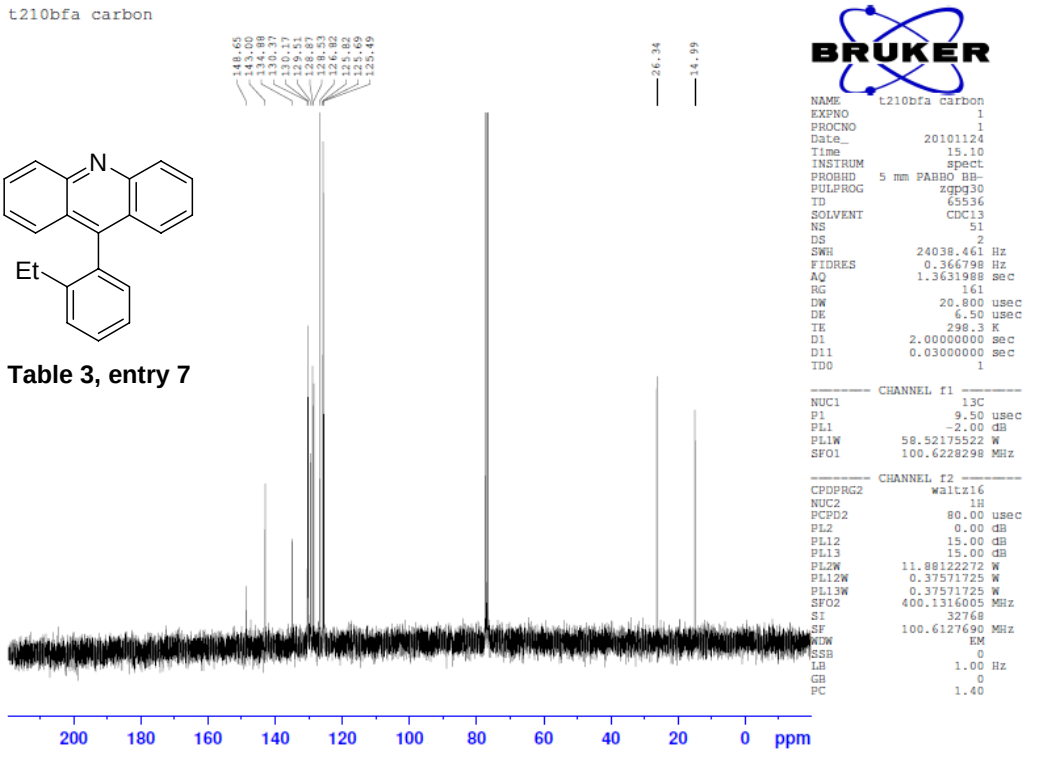


Table 3, entry 7

```
File       :C:\msdchem\1\DATA\chun\T210B.D
Operator   : fbm
Acquired   : 21 Apr 2010  13:08     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 2
```

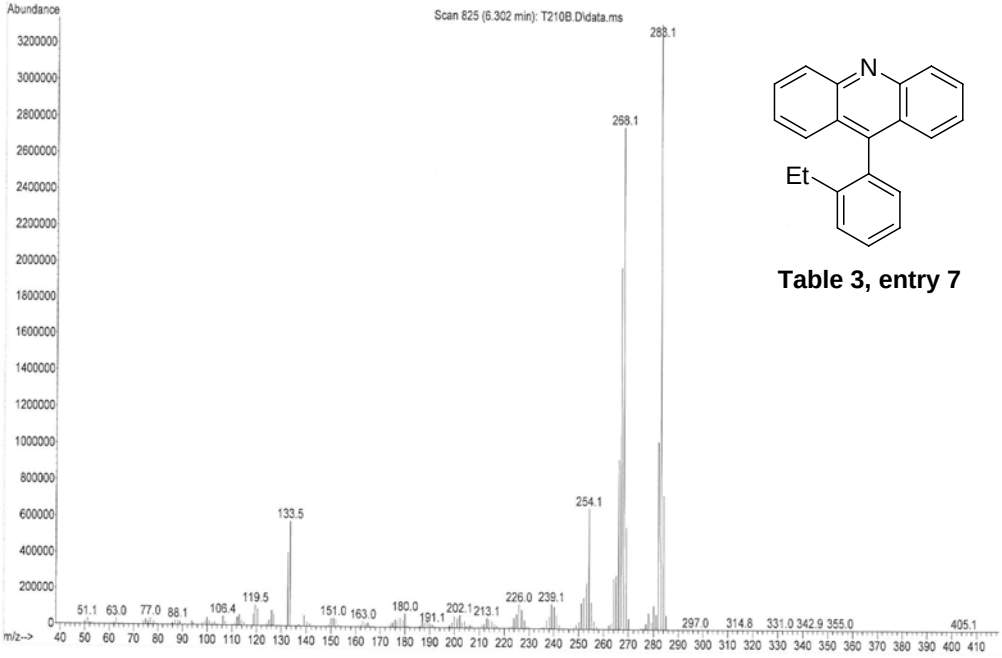


Table 3, entry 7

T210b

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

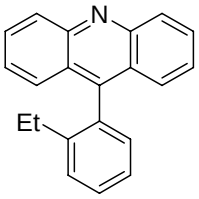
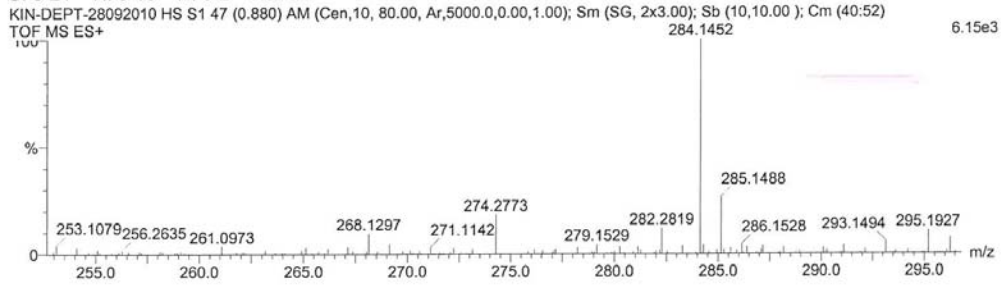
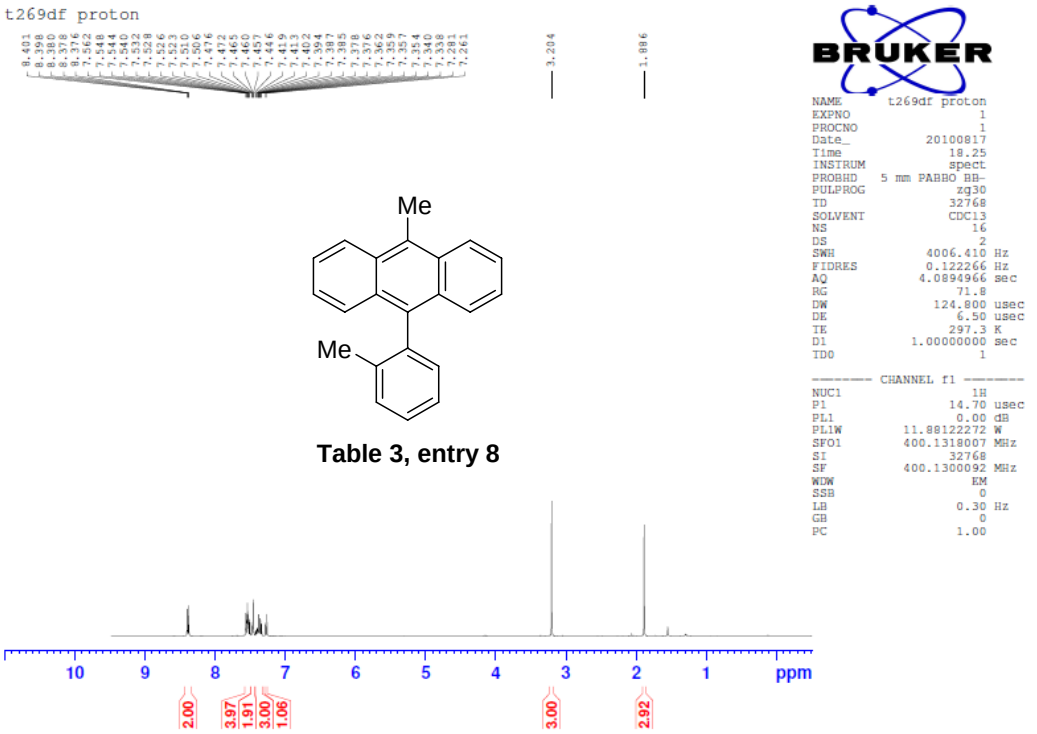


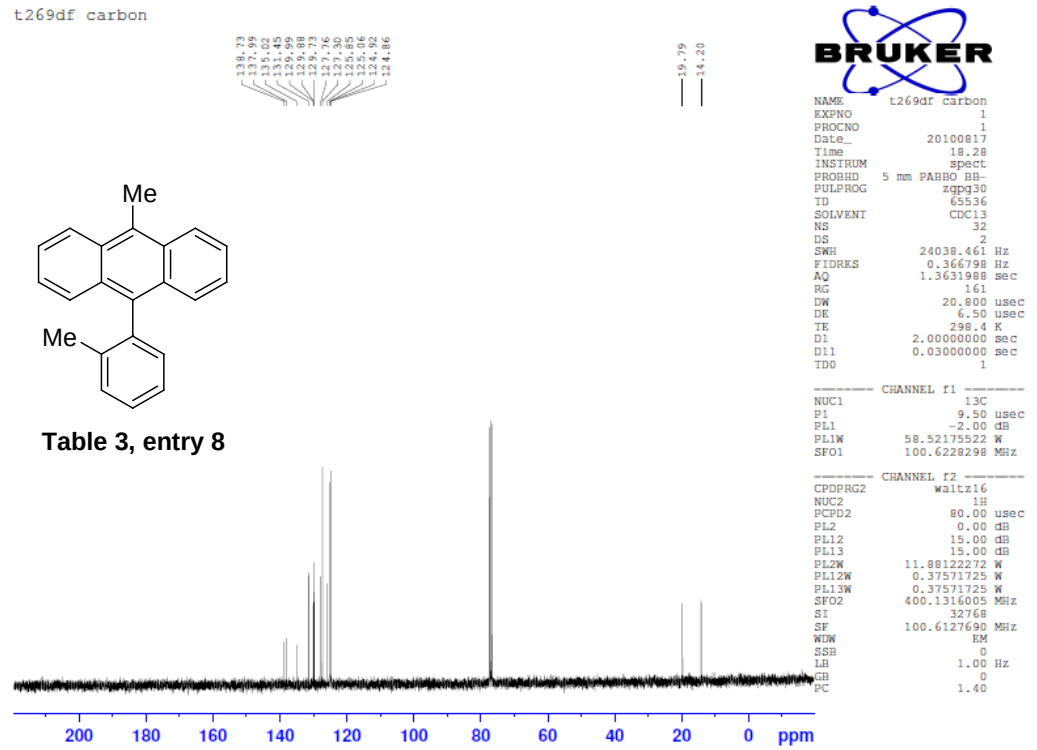
Table 3, entry 7

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-18 N: 0-2 Na: 0-1
KIN-DEPT-28092010 HS S1 47 (0.880) AM (Cen,10, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Sb (10,10.00); Cm (40:52)
TOF MS ES+ 6.15e3



Minimum:				-100.0		
Maximum:		5.0	20.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
284.1452	284.1439	1.3	4.6	13.5	20.4	C21 H18 N


t269df proton
Me
Me
Table 3, entry 8
NAME t269df proton
EXPNO 1
PROCNO 1
Date_ 20100817
Time 18.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.8
DW 124.800 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
2.00 3.97 1.91 3.00 1.06 3.00 2.92


t269df carbon
Me
Me
Table 3, entry 8
NAME t269df carbon
EXPNO 1
PROCNO 1
Date_ 20100817
Time 18.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 161
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

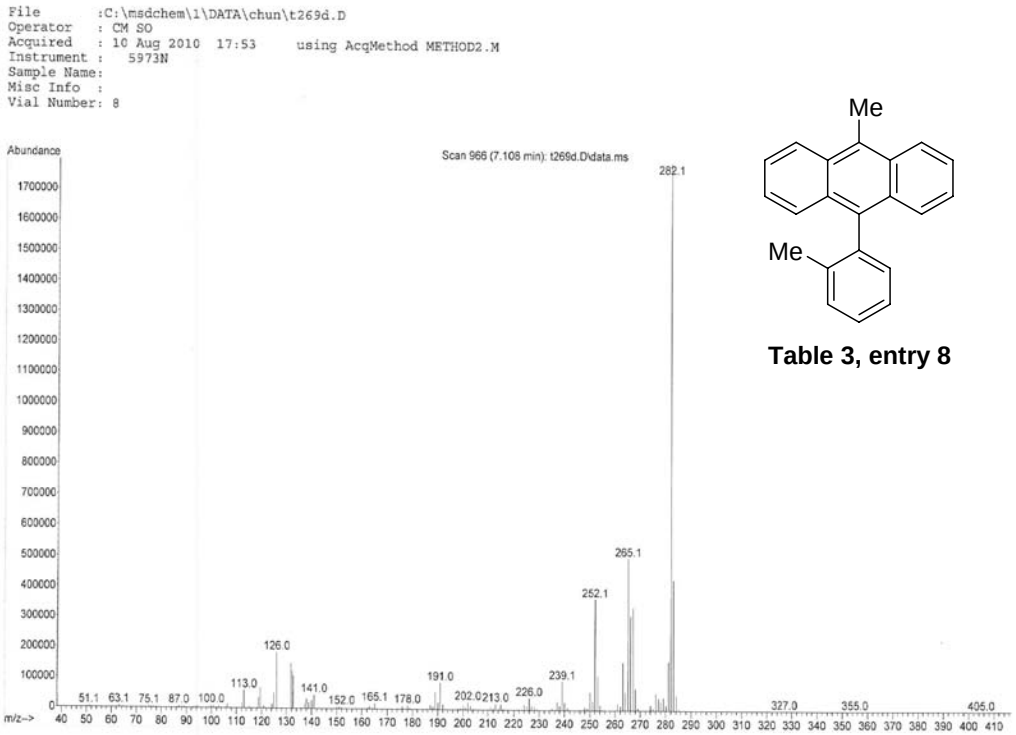


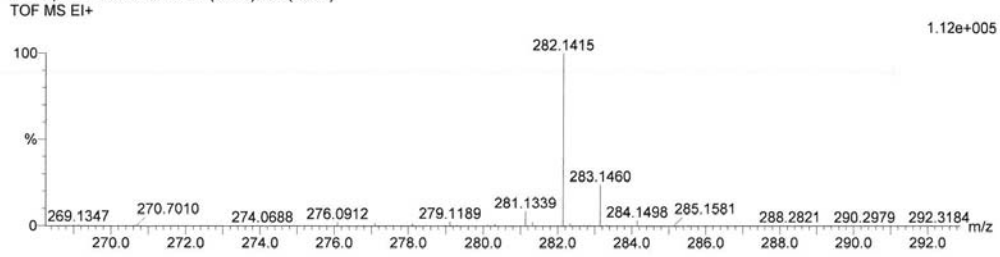
Table 3, entry 8

T269d

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-20
Kin-dept-04112010 S6 HS 47 (0.783) Cm (23:47)
TOF MS EI+



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
282.1415	282.1409	0.6	2.1	14.0	27.0	C22 H18

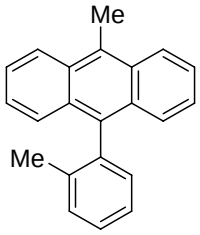
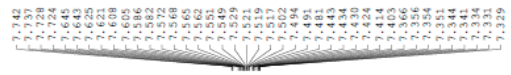


Table 3, entry 8

t264cfa proton



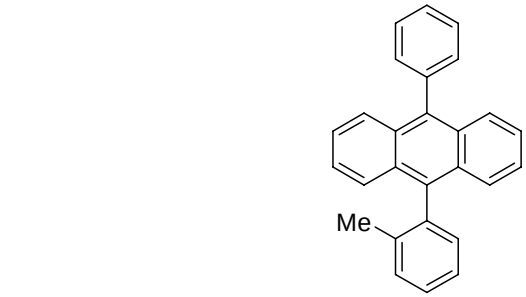
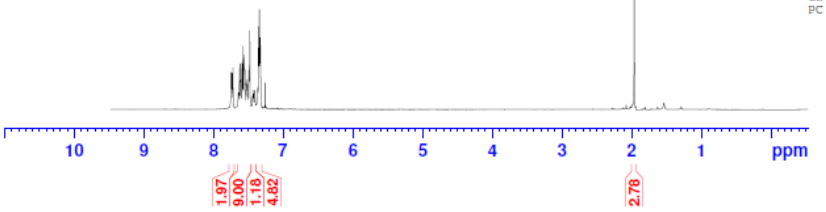


Table 3, entry 9




```
NAME          t264cfa proton
EXPNO                      1
PROCNO                     1
Date_               20101125
Time                   20.12
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                4006.410 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                      71.8
DW                 124.800 usec
DE                   6.50 usec
TE                   297.8 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.70 usec
PL1                     0.00 dB
PL1W             11.88122272 W
SFO1             400.1318007 MHz
SI                       32768
SF               400.1300101 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

t264cf carbon

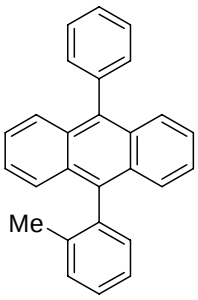
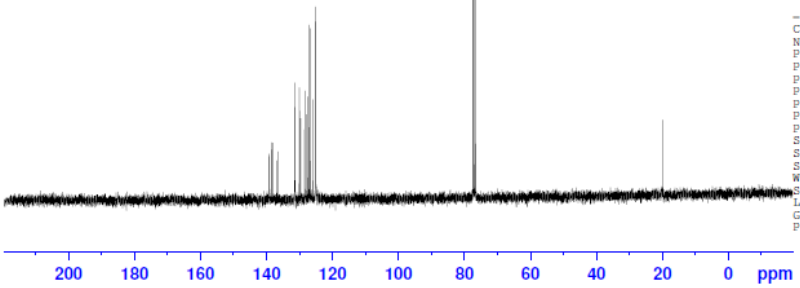


Table 3, entry 9




```
NAME          t264cf carbon
EXPNO                      1
PROCNO                     1
Date_               20100809
Time                   19.19
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                        32
DS                        2
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      203
DW                  20.800 usec
DE                   6.50 usec
TE                   299.4 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.50 usec
PL1                    -2.00 dB
PL1W             58.52175522 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                80.00 usec
PL2                     0.00 dB
PL12                   15.00 dB
PL13                   15.00 dB
PL2W             11.88122272 W
PL12W             0.37571725 W
PL13W             0.37571725 W
SFO2             400.1316005 MHz
SI                       32768
SF               100.6127690 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

```
File       :C:\msdchem\1\DATA\arwo\t264cf.D
Operator   : CM SO
Acquired   :  9 Aug 2010  18:14     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 3
```

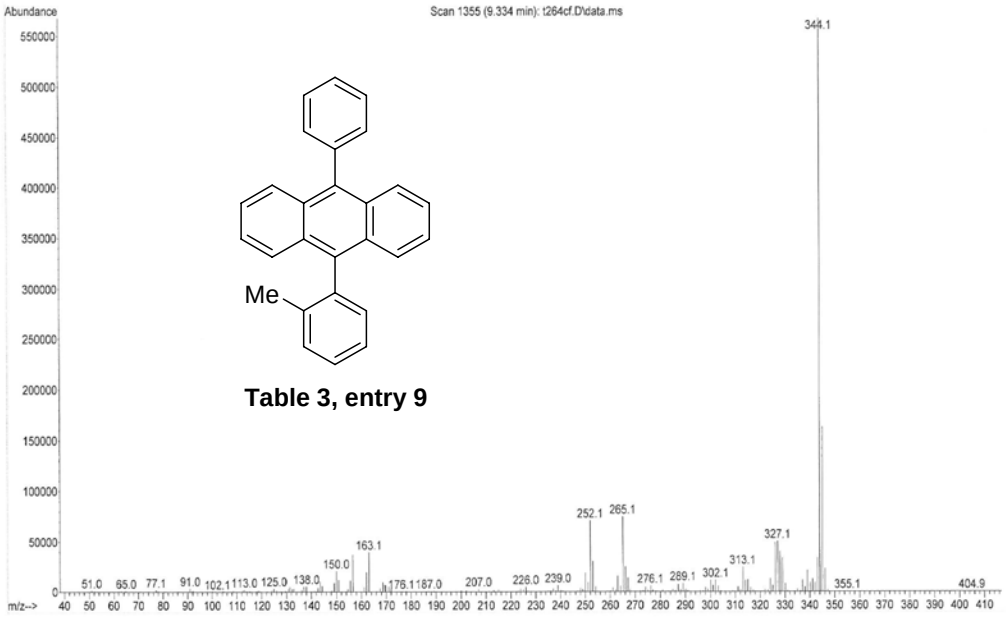


Table 3, entry 9

t244af1 proton

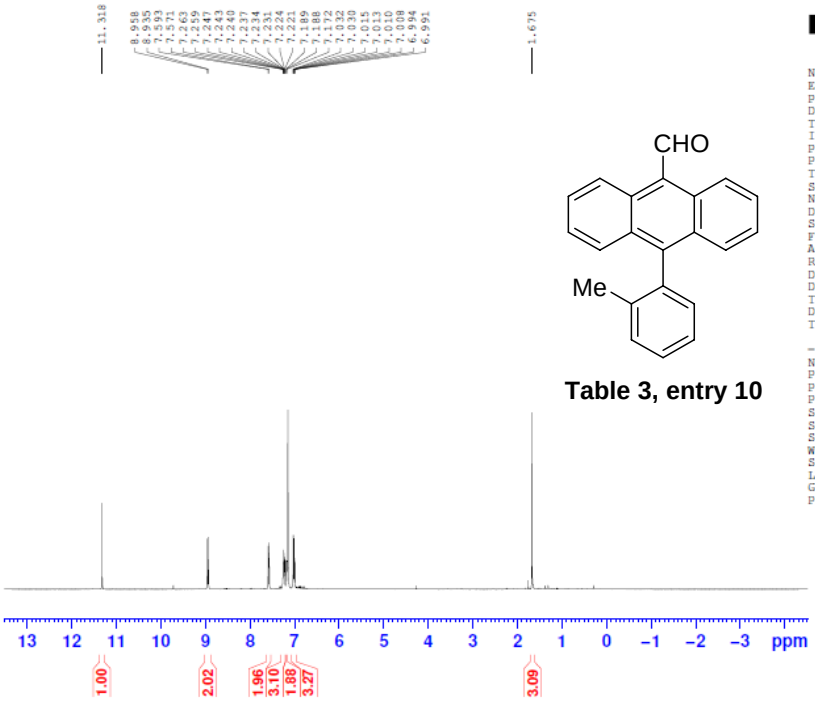


Table 3, entry 10

BRUKER

```
NAME          t244af1 proton
EXPNO                      1
PROCNO                     1
Date_               20100604
Time                   17.00
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               C6D6
NS                      16
DS                       2
SWH               7211.539 Hz
FIDRES            0.220079 Hz
AQ                2.2719646 sec
RG                     80.6
DW                69.333 usec
DE                   6.50 usec
TE                  295.5 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.70 usec
PL1                  0.00 dB
PL1W            11.88122272 W
SFO1           400.1318007 MHz
SI                    32768
SF             400.1300000 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```

t261bf carbon

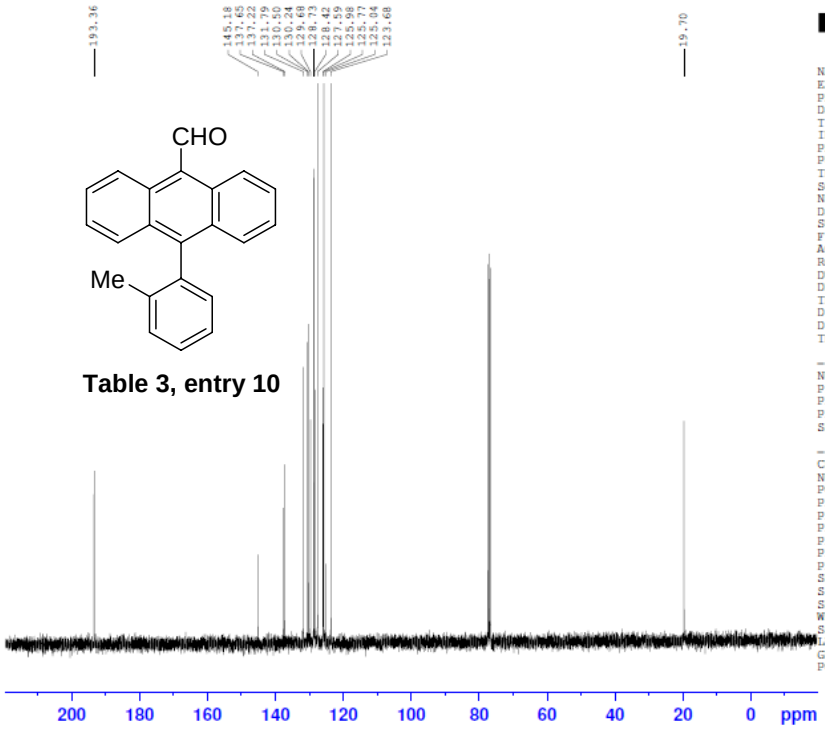


Table 3, entry 10

BRUKER

```
NAME          t261bf carbon
EXPNO                      1
PROCNO                     1
Date_               20100713
Time                   21.47
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      32
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     203
DW                20.800 usec
DE                   6.50 usec
TE                  299.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.50 usec
PL1                  -2.00 dB
PL1W            58.52175522 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W            11.88122272 W
PL12W            0.37571725 W
PL13W            0.37571725 W
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127690 MHz
WDW                      EM
SSB                       0
LB                 1.00 Hz
GB                        0
PC                     1.40
```

```
File       :C:\msdchem\1\DATA\chun\t261b.D
Operator   : fbm
Acquired   : 13 Jul 2010  12:59     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 2
```

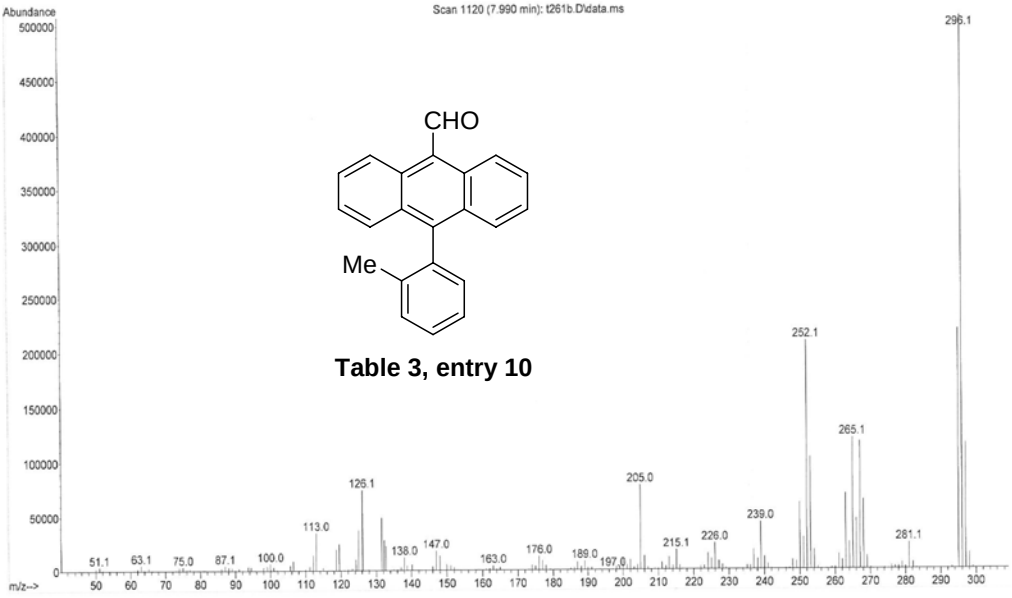


Table 3, entry 10

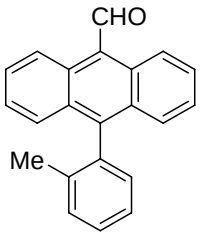
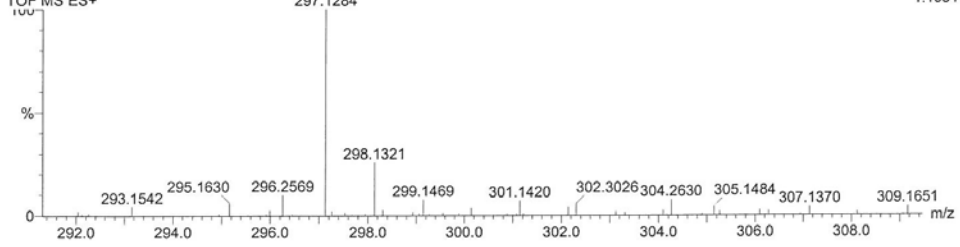


Table 3, entry 10

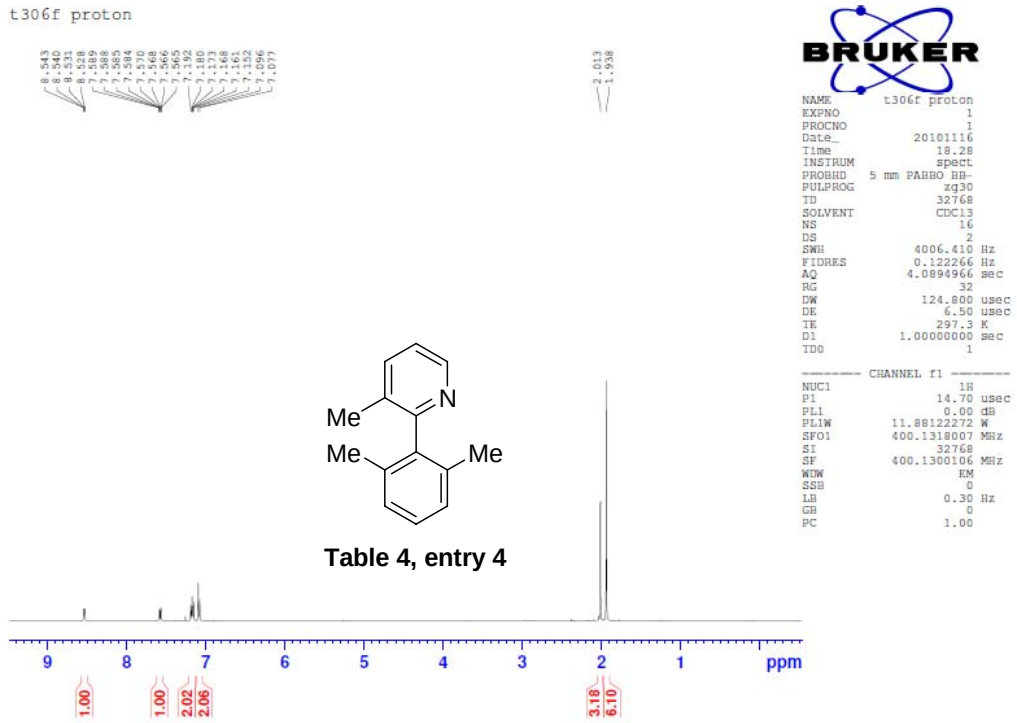
Elemental Composition Report T261b **Page 1**

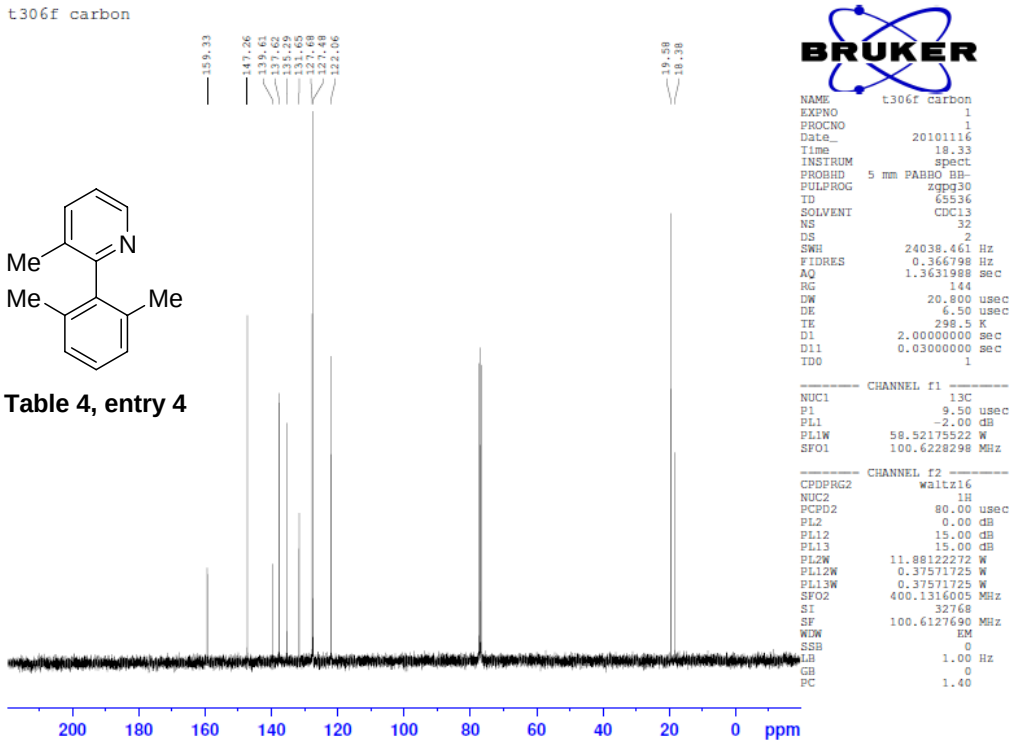
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-29 N: 0-2 O: 0-6 Na: 0-1
KIN-DEPT-28092010 HS S3-2 46 (0.861) Cn (Cen,10, 80.00, Ar); Sm (SG, 2x3.00); Sb (10,10.00); Cm (41:53)
TOF MS ES+ 1.10e4



Minimum:				-100.0		
Maximum:		5.0	5.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
297.1284	297.1279	0.5	1.7	14.5	146.1	C22 H17 O


t306f proton
BRUKER
NAME t306f proton
EXPNO 1
PROCNO 1
Date_ 20101116
Time 18.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 32
DW 124.800 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GH 0
PC 1.00
Me
Me
Me
N
Table 4, entry 4
ppm
1.00
1.00
2.02
2.06
3.18
6.10


t306f carbon
BRUKER
NAME t306f carbon
EXPNO 1
PROCNO 1
Date_ 20101116
Time 18.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
159.33
147.26
139.61
137.62
135.29
131.65
127.68
127.48
122.06
19.58
18.38
Me
Me
Me
N
Table 4, entry 4
ppm

```
File       :C:\msdchem\1\DATA\chun\T234F.D
Operator   : fbm
Acquired   : 23 May 2010  20:49     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 2
```

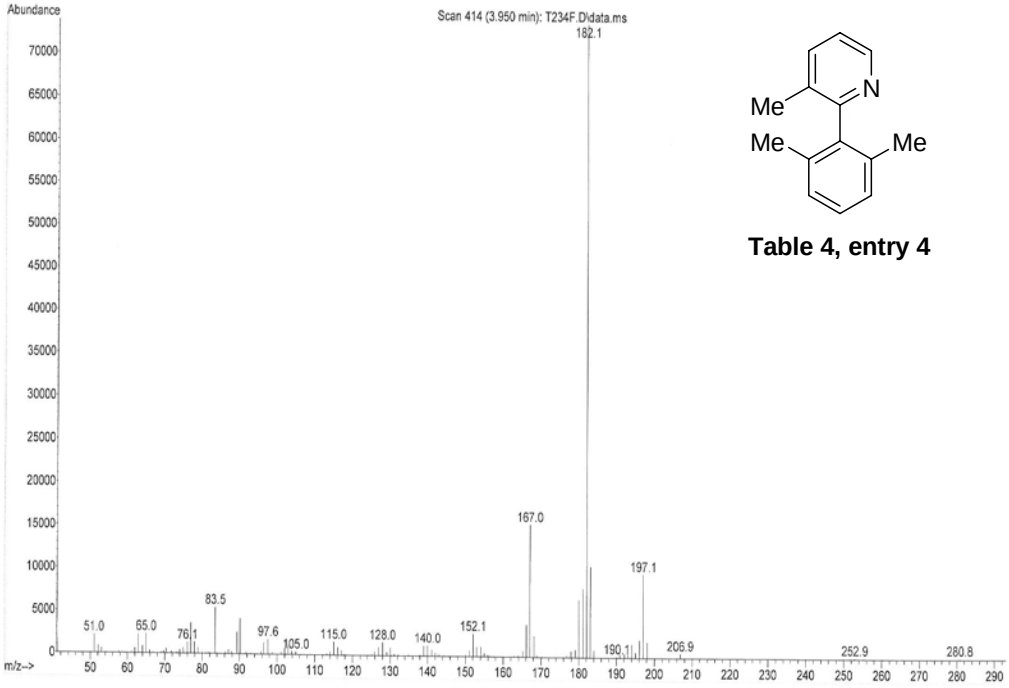


Table 4, entry 4

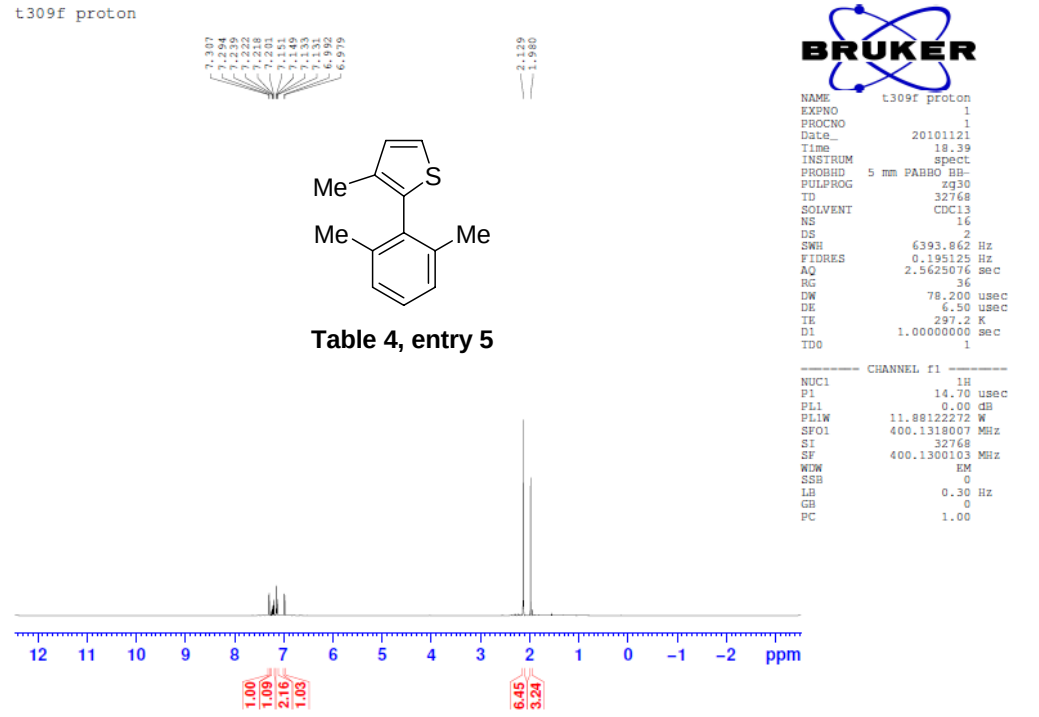


Table 4, entry 5

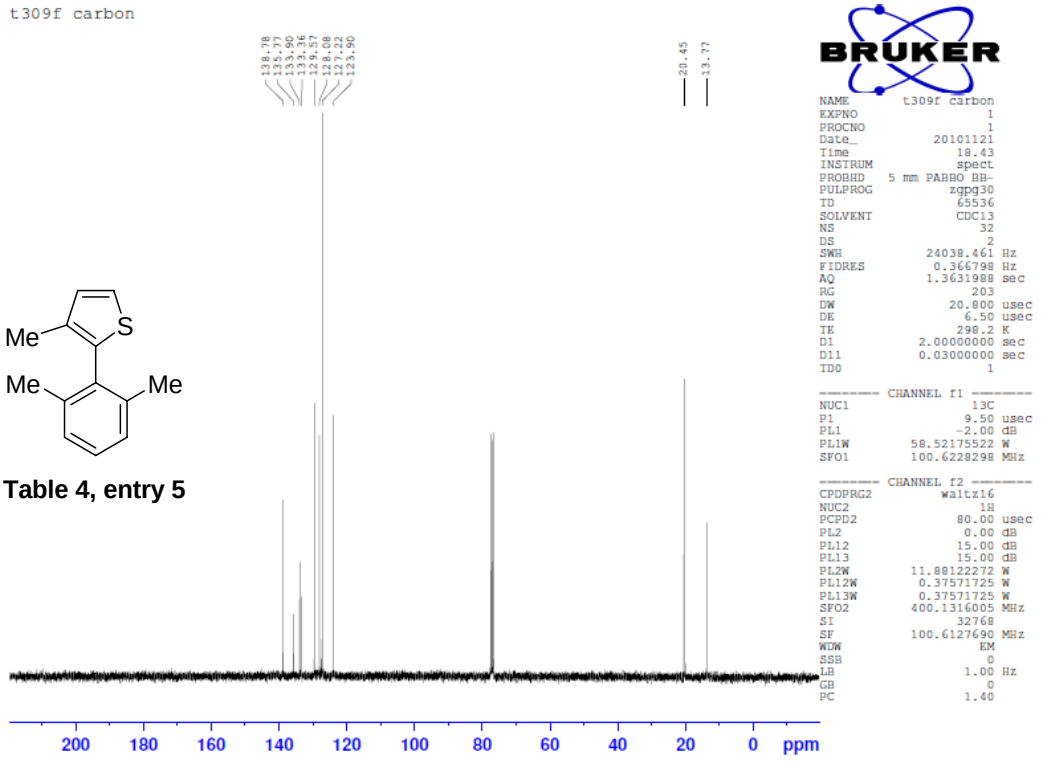


Table 4, entry 5

```
File       :C:\msdchem\1\DATA\wzx\wzx047\t309.D
Operator   : Seam
Acquired   : 21 Nov 2010  16:00     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 1
```

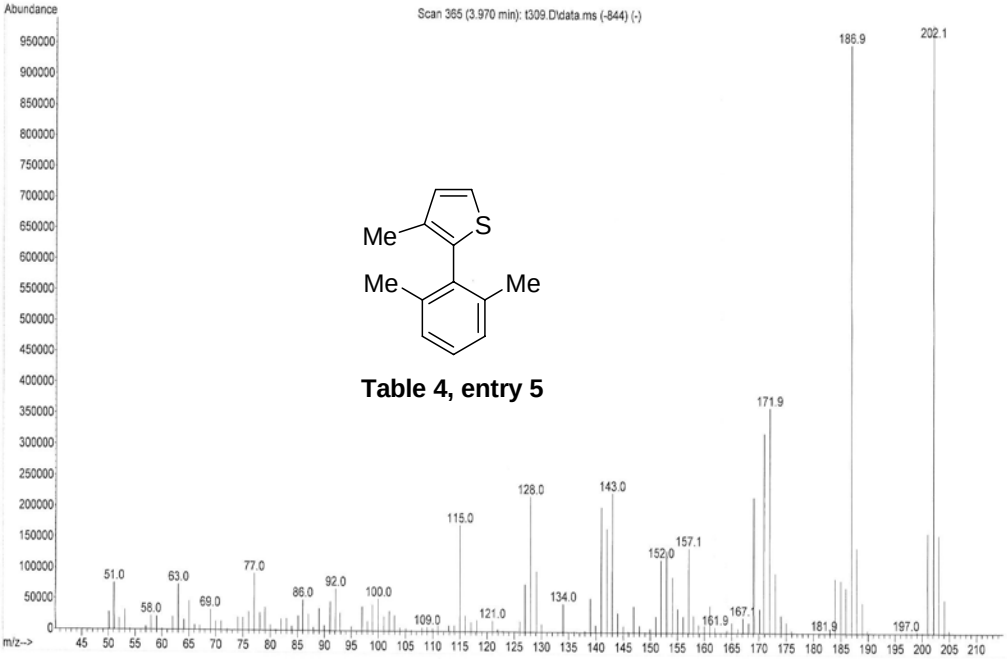


Table 4, entry 5

T309

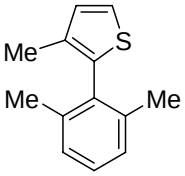


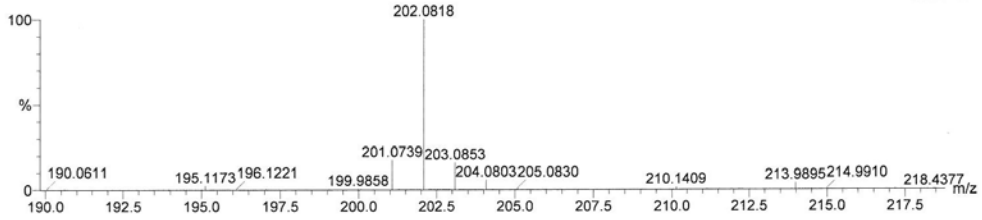
Table 4, entry 5

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

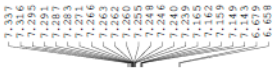
Monoisotopic Mass, Odd and Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-18 H: 0-15 S: 0-6
Kin-dept-26112010 HS S2 64 (1.067) Cm (63:72)
TOF MS EI+

8.58e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
202.0818	202.0816	0.2	1.0	7.0	6.2	C13 H14 S

t239fa proton



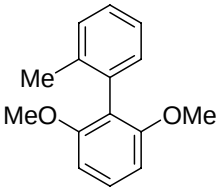
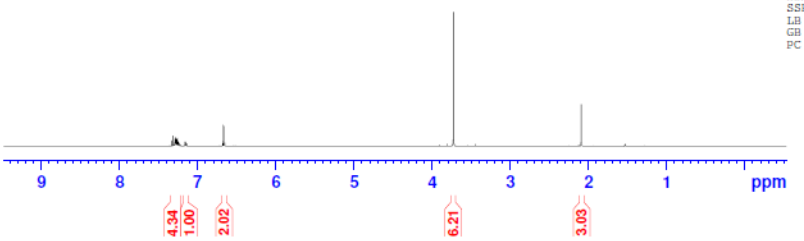


Table 4, entry 6




```
NAME          t239fa proton
EXPNO                    1
PROCNO                   1
Date_             20101124
Time                 12.03
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDC13
NS                     16
DS                      2
SWH             4006.410 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                   71.8
DW                124.800 usec
DE                  6.50 usec
TE                 297.1 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.70 usec
PL1                  0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI                  32768
SF            400.1300095 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

t239fa carbon

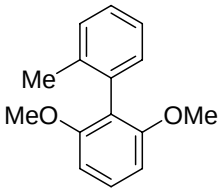


Table 4, entry 6


```
NAME          t239fa carbon
EXPNO                    1
PROCNO                   1
Date_             20101124
Time                 12.07
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDC13
NS                     60
DS                      2
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                   161
DW                 20.800 usec
DE                  6.50 usec
TE                 298.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.50 usec
PL1                -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W          11.88122272 W
PL12W          0.37571725 W
PL13W          0.37571725 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

```
File       :C:\msdchem\1\DATA\chun\T239F.D
Operator   : fbm
Acquired   : 25 May 2010  16:03     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 4
```

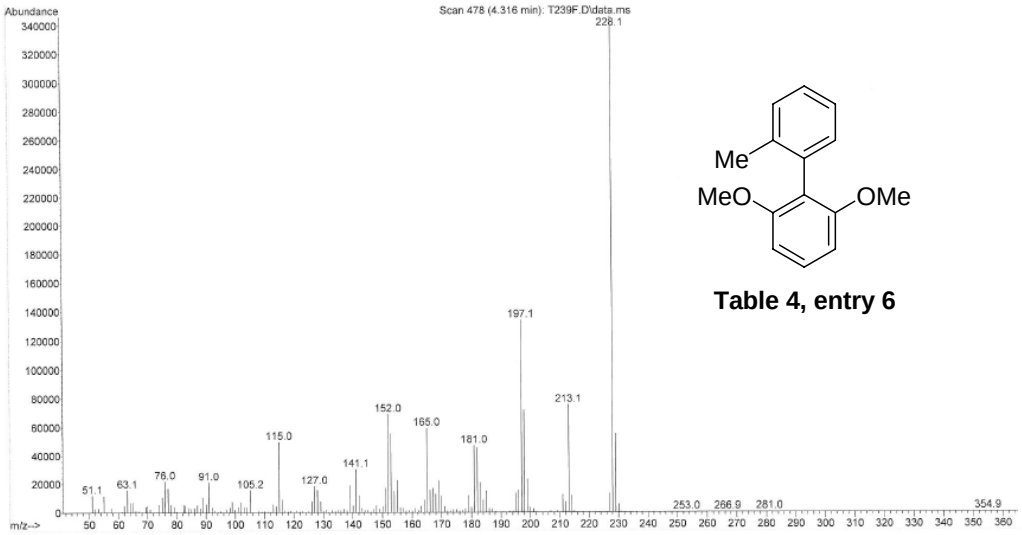


Table 4, entry 6

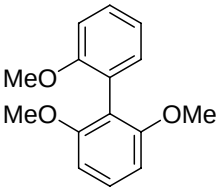
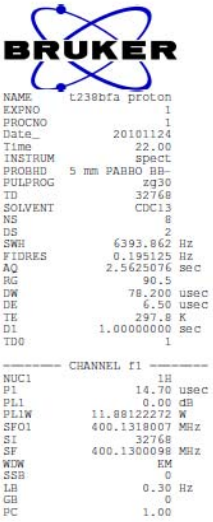
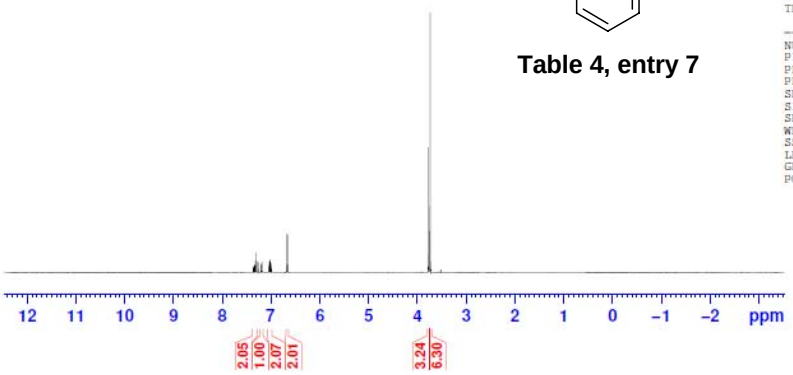


Table 4, entry 7





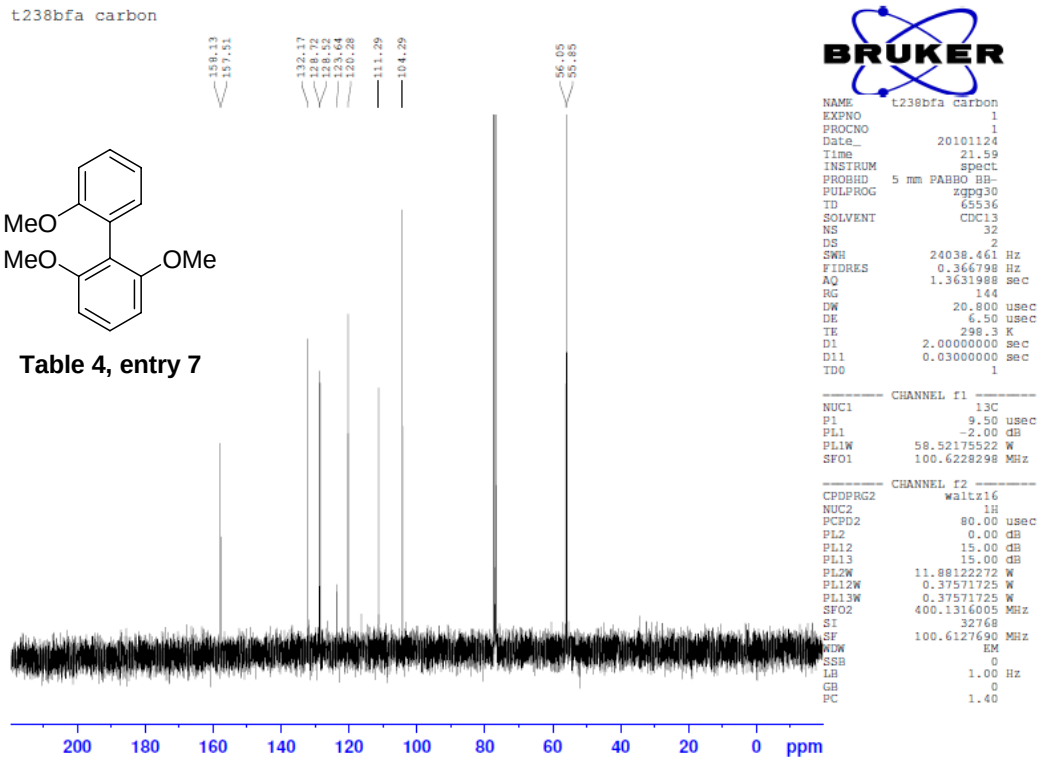


Table 4, entry 7

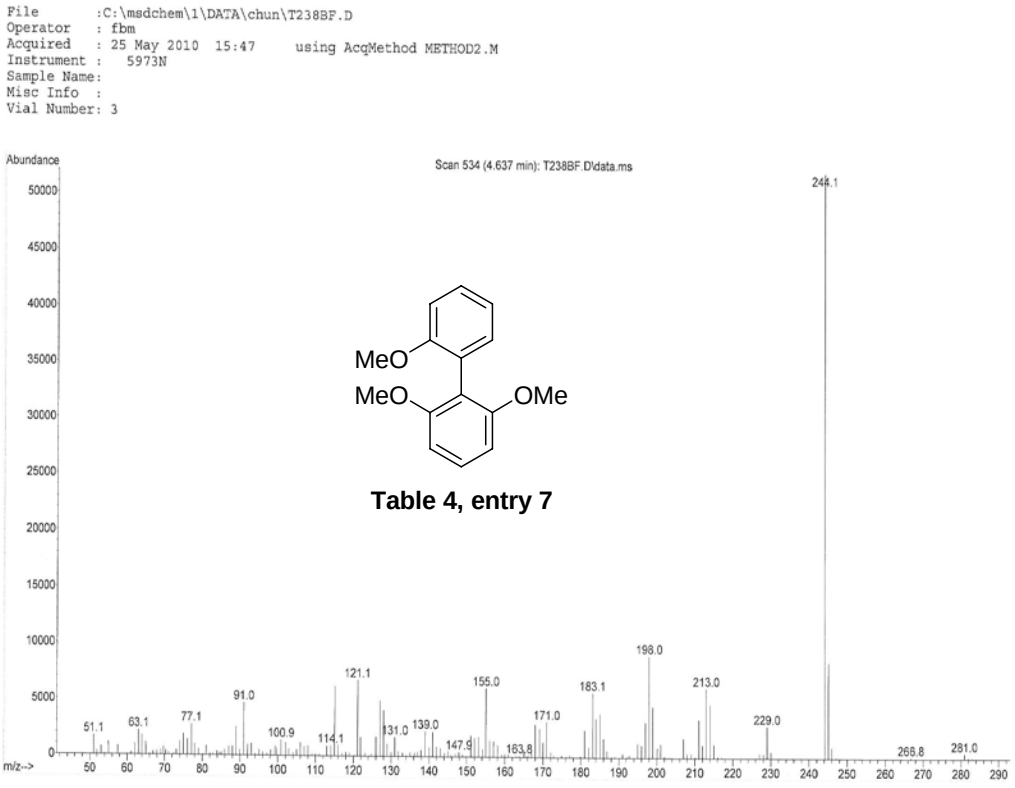


Table 4, entry 7

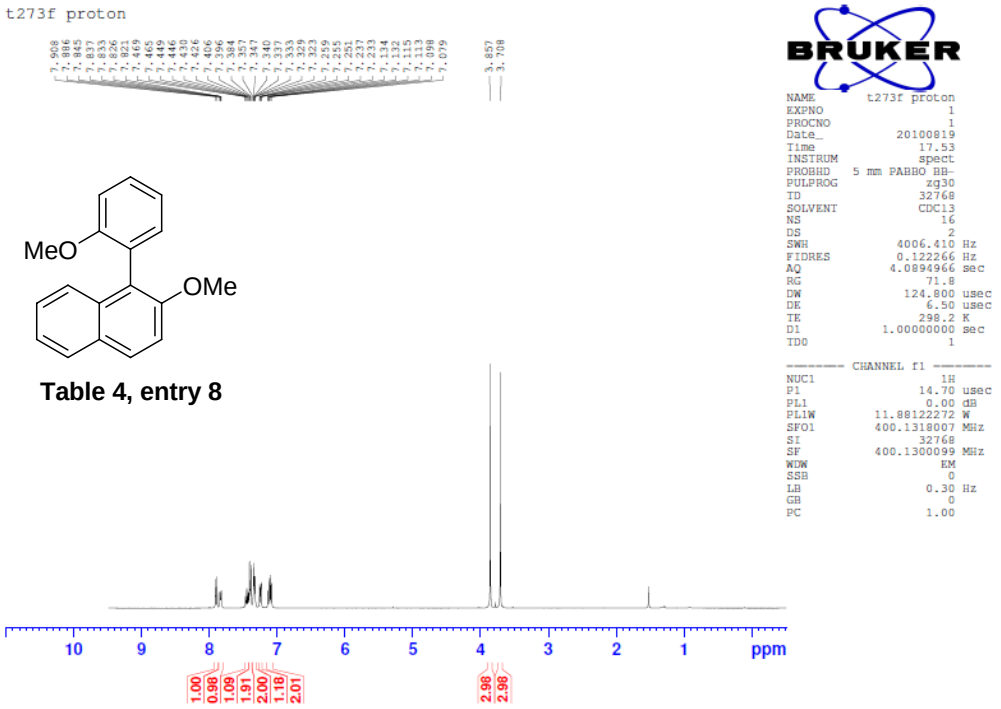


Table 4, entry 8

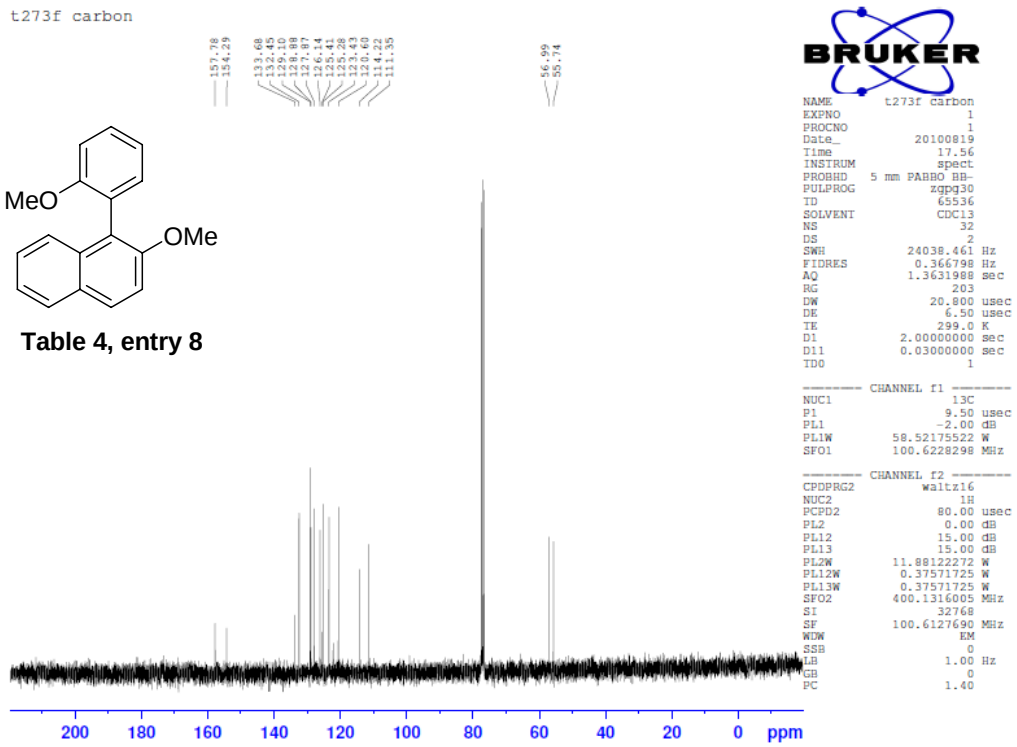


Table 4, entry 8

```
File       :C:\msdchem\1\DATA\Ho\Other\t273f.D
Operator   : Seam
Acquired   : 19 Aug 2010  18:01     using AcqMethod METHOD2.M
Instrument :   5973N
Sample Name:
Misc Info  :
Vial Number: 3
```

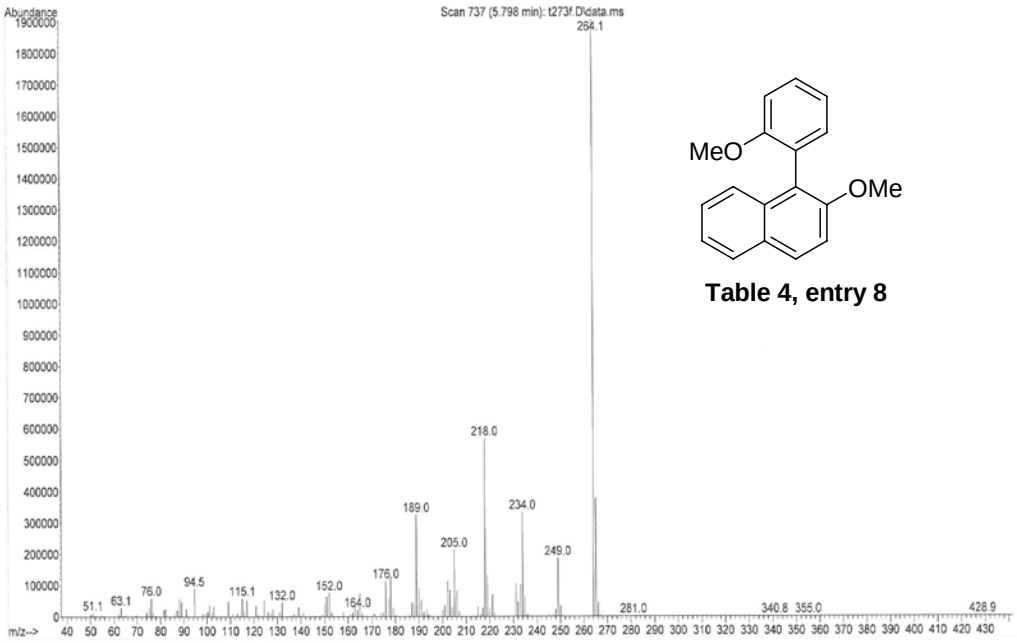


Table 4, entry 8

11. References

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