

Supporting Information

Synthesis of Thermally Stable Geminal Dicationic Ionic Liquids and Related Ionic Compounds: An Examination of Physicochemical Properties by Structural Modification

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Methods of Analysis:

The monocationic ionic liquids and dicationic ionic liquids were characterized by electrospray ionization mass spectrometry (ESI-MS) for molecular weight. ESI-MS spectra were acquired by using a Finnigan LXQ (Thermo Fisher Scientific, San Jose, CA). ^1H NMR, ^{13}C NMR and ^{31}P NMR experiments were performed on 500 MHz JEOL Eclipse Plus 500 instrument for spectral analysis. Thermogravimetric analysis were performed using Shimadzu TGA-51 Thermogravimetric Analyzer (Kyoto, Kyoto Prefecture, Japan) for the stability testing. Samples (~10 mg) were placed in the platinum pans, and heated at $10\text{ }^\circ\text{C min}^{-1}$ from room temperature to $600\text{ }^\circ\text{C}$ in a nitrogen atmosphere (flow – 30 mL min^{-1}). The decomposition temperature were determined at 1%, 5% and 15% weight loss. 5% weight loss of the sample which corresponds to 95% w value was considered as measure of thermal stability. The GC thermal stability measurements were made using Agilent 6890N Gas Chromatograph equipped with flame ionization detector (FID). The studies were performed ramping the column oven temperature from $100\text{ to }450\text{ }^\circ\text{C}$ at $1\text{ }^\circ\text{C min}^{-1}$ and using helium as carrier gas at flow rate of 1 mL min^{-1} . The injector and FID temperatures were set at $250\text{ }^\circ\text{C}$ and $400\text{ }^\circ\text{C}$ respectively. The DSC measurements were carried out on a Shimadzu DSC-60 (Kyoto, Kyoto Prefecture, Japan) differential scanning calorimeter (DSC). The samples (~ 10 mg) were sealed in aluminum pans, and then heated at rate of $10\text{ }^\circ\text{C min}^{-1}$ up to $500\text{ }^\circ\text{C}$. Melting points were determined using a *Mel-Temp* apparatus (Laboratory Devices, Cambridge, MA). Density was measured using 10 mL Kimble specific gravity pycnometer at $22\text{ }^\circ\text{C}$. Heptane was used as an immiscible solvent for these measurements. Kinematic viscosity was determined using a Cannon-Manning semi-micro viscometer. All compounds synthesized in this study were tested for solubility with polar (water) and non-polar (heptane) solvent. This study was performed by placing a small amount (60-100 mg) of the compound in the solvent (15 mL) and through observation of whether the solute was miscible or immiscible in the solvent.

Synthesis of monocationic ILs:

Compounds **IL1**, **IL2**, **IL3**, **IL4**, **IL5**, **IL6**, **IL7**, and **IL8** were made through metathesis reactions of 1 molar equivalents of tributyltetradecylphosphonium chloride salt with 1 molar equivalents of bis(trifluoromethane)sulfonimide lithium (LiNTf_2), bis(pentafluoromethane)sulfonimide lithium (LiNPF_2), heptadecafluorooctanesulfonic acid

potassium salt (KPFOS), Iron (III) chloride(FeCl_3), tris(pentafluoroethyl)trifluorophosphate hydride (FAP), bis(2-ethylhexyl) sulfosuccinate sodium (NaAOT), 1-octanesulfonic acid sodium salt (NaOS), and potassium dodecafluoro-closo-dodecaborate ($\text{KB}_{12}\text{F}_{12}$), respectively. The reactions for all ILs were performed in water at room-temperature for 12 h with the exception of heptadecafluorooctanesulfonic acid potassium salt (KPFOS), which was performed at elevated temperature (110 °C) with oil-bath. Dichloromethane was added to the resulting solution to dissolve the target product. The aqueous layer was then removed and the organic layer washed three times with water to remove any starting material. Dichloromethane was then removed by rotary evaporation followed by vacuum drying over phosphorous pentoxide at 40 °C for 24 h. The procedure resulted in the pure monocationic ionic liquid.

Synthesis of dicationic ionic liquids:

Synthesis of dicationic ionic liquids involved two steps. First step involved a nucleophilic substitution reaction of imidazoles / pyrrolidones / phosphines with corresponding terminal dibromoalkanes to obtain bromide salt of dication. Second step was metathesis dibromodicationic salt with LiNTf_2 and KPFOS. In metathesis step bromide ions were exchanged by NTf_2^- or PFOS^- anions to obtain final product ILs and LiBr and KBr as side products.

Synthesis of imidazolium based Ionic Liquids

Procedure 1:

Step 1) **IL9, IL21 and IL 33** were made by refluxing 2 molar equivalents of 1-butyl-2-methylimidazole with 1 molar equivalent of 1, 6-dibromohexane, 1, 9-dibromononane and 1, 12-dibromododecane respectively in acetonitrile at 80 °C for 72 h.(Scheme 1) Rotary evaporation of solvent yielded the crude dibromodicationic salt. The salt was then dissolved in water and transferred to a separatory funnel and washed with dichloromethane (3×50 ml) to remove excess starting material. The aqueous layer containing dibromodications was then dried by rotary evaporation of water. Further, vacuum drying over phosphorous pentoxide at 40 °C for 24h resulted in the pure dibromodicationic salts. The products were then verified by mass spectrometry analysis.

Step 2) For the synthesis of final products, the dibromodications synthesized in the first step were dissolved in water and reacted with 2 molar equivalents of (LiNTf₂) (Scheme 2). The solution was stirred for 24 h at room temperature. The metathesis process resulted in exchange of bromide anions with NTf₂⁻ anions. Following that, dichloromethane (40 mL) was added to the solution to extract NTf₂⁻ salt of the ionic liquid that has phase separated from the water. The lithium bromide and excess NTf₂⁻ were removed from the dichloromethane phase with successive extraction with water (3x40mL). Removal of dichloromethane through rotary evaporation followed by vacuum drying over P₂O₅ at 40 °C for 24 h resulted in the pure dicationic 1-butyl-2-methylimidazolium ILs with NTf₂⁻ counter anion.

Procedure 2:

For the synthesis of **IL15**, **IL27** and **IL 39** with PFOS⁻ anion; dibromodications and heptadecafluorooctanesulfonic acid potassium salt (KPFOS) were dissolved in a mixture of methanol and water (1:1) and stirred for 12 h. (Scheme 2) The solvents were evaporated using rotary evaporation method and similar protocol as mentioned in Step 2 of procedure 1 was followed for the rest of the reaction workup.

Procedure 3:

For the synthesis of **IL10**, **IL22**, **IL34**, **IL15**, **IL28** and **IL40** similar protocol as procedure 1 and 2 was followed except 2 moles of 1, 2-dimethylimidazole used instead of 1-butyl-2-methylimidazole.

Synthesis of pyrrolidinium based Ionic Liquids:

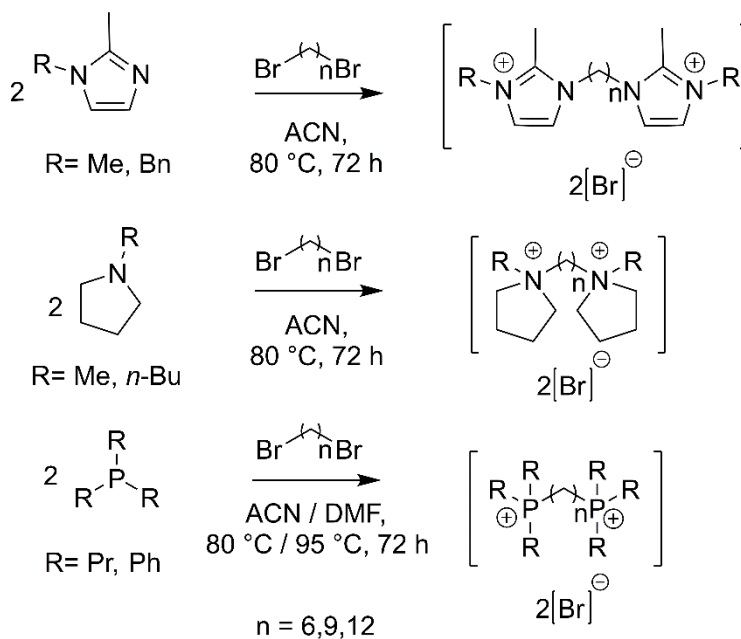
Procedure 4:

For the synthesis of **IL11**, **IL23**, **IL35**, **IL17**, **IL29** and **IL41** similar protocol as procedure 1 and 2 was followed except 2 moles of 1-butylpyrrolidine was used instead of 1-butyl-2-methylimidazole.

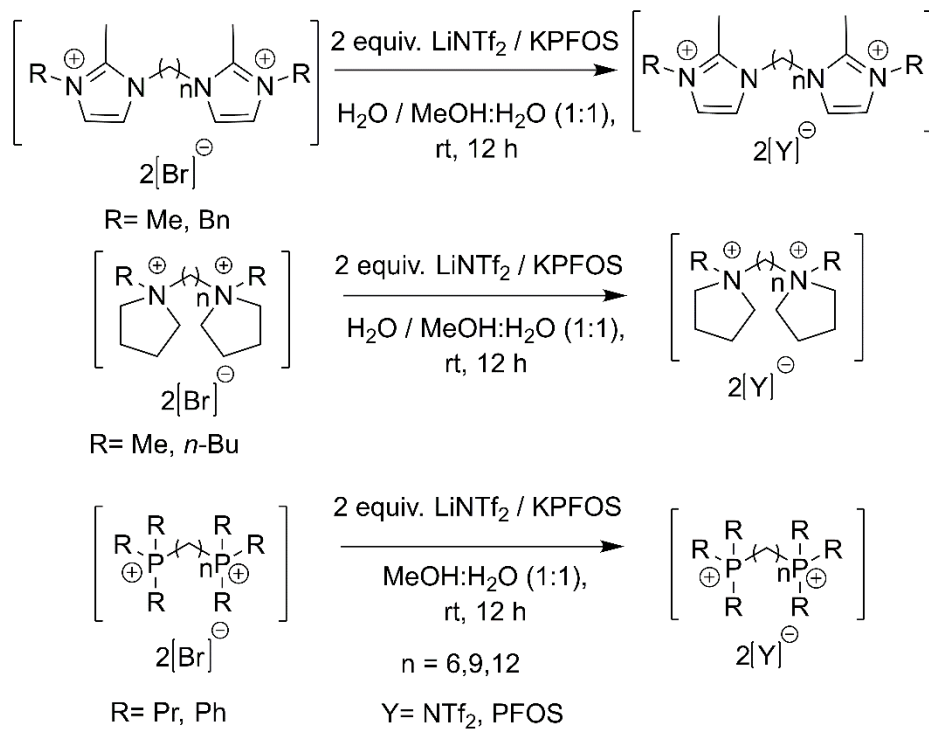
Procedure 5:

For the synthesis of **IL12**, **IL24**, **IL36**, **IL18**, **IL30** and **IL42** similar protocol as procedure 1 and 2 was followed except 2 moles of N-methylpyrrolidine was used instead of 1-butyl-2-methylimidazole.

Scheme: 1 Synthesis of bromide salt of dication



Scheme: 2 Metathesis of bromide salts to synthesize dicationic ILs



Synthesis of phosphonium based ionic liquids:

Procedure 6:

Step 1) **IL13, IL25, IL37, IL19, IL31** and **IL43** were made by refluxing 2 molar equivalents of tripropylphosphine with 1 molar equivalent of 1,6-dibromohexane, 1,9-dibromononane and 1,12-dibromododecane respectively in acetonitrile at 80 °C for 72 h.(Scheme 1) The reaction was performed under inert argon condition to prevent oxidation of tripropylphosphine. Rotary evaporation of solvent yielded the crude dibromodicationic salt. Similar protocol as mentioned in Procedure 1 and 2 was followed for the rest of the reaction workup.

Procedure 7:

Step 1) Compounds **IL14, IL26** and **IL38** were synthesized by refluxing 2 molar equivalents of triphenylphosphine with 1 molar equivalent of 1,6-dibromohexane, 1,9-dibromononane and 1,12-dibromododecane respectively in N,N-Dimethylformamide at 95 °C for 72 h.(Scheme 1) Rotary evaporation of solvent yielded the crude dibromodicationic salt. The salt was then washed with five aliquots of ethyl acetate (3×50 mL) to remove unreacted starting material. The rotary evaporation of solvent and further vacuum drying over phosphorous pentoxide resulted in the pure dibromodicationic salts. Obtained products then verified by mass spectrometry analysis.

Step 2) For the synthesis of final products, the dibromodications synthesized in the first step were dissolved in methanol and water (1:1) and reacted with 2 molar equivalents of (LiNTf₂). The solution was stirred for 24 h at room temperature.(Scheme 2) This metathesis process resulted in final IL with bromide anions exchanged with NTf₂⁻ anions. The solvents were evaporated using rotary evaporation method. The crude NTf₂⁻ salt was dissolved in dichloromethane. The lithium bromide and excess NTf₂⁻ were removed from the dichloromethane phase with successive extractions with water (3x40 mL). Removal of dichloromethane through rotary evaporation followed by vacuum drying over P₂O₅ at 40 °C for 24 h resulted in the pure dicationic triphenylphosphonium ILs with NTf₂⁻ counter anion.

Procedure 8:

To synthesize compounds **IL20, IL32** and **IL44**; dibromodications and heptadecafluorooctanesulfonic acid potassium salt (KPFOS) were dissolved in a mixture of methanol and water (1:1) and stirred for 24 h. The solvents were evaporated using rotary evaporation method and similar protocol as mentioned in Step 2 of Procedure 7 was followed for the rest of the reaction workup.

Characterization of ILs:

Characterization IL 9:

^1H NMR (500Hz; DMSO; ppm): δ 1.29 (br. s, 4H); δ 1.72 (m, 4H); δ 2.61 (s, 6H); δ 4.09 (t, $J_{\text{H-H}} = 7.45$ Hz, 4H); δ 5.40 (s, 4H); δ 7.31 (m, 4H); δ 7.40 (m, 6H); δ 7.72 (dd, $J_{\text{H-H}} = 1.72$ Hz, $J_{\text{H-H}} = 15.42$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.34; 25.02; 28.68; 47.87; 50.92; 118.12; 120.68; 121.48; 121.64; 127.64; 128.44; 128.94; 134.44; 143.99. ESI-MS: m/z (+) 214.08; m/z (-) 279.89

Characterization IL 10:

^1H NMR (500Hz; DMSO; ppm): δ 1.28 (br. s, 4H); δ 1.68 (m, 4H); δ 2.56 (s, 6H); δ 3.74 (s, 6H); δ 4.09 (t, $J_{\text{H-H}} = 7.29$ Hz, 4H), δ 7.61 (dd, $J_{\text{H-H}} = 2.19$ Hz, $J_{\text{H-H}} = 2.79$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.35; 25.30; 29.22; 34.91; 47.63; 115.99; 118.46; 121.03; 121.07; 122.58; 144.47. ESI-MS: m/z (+) 138.12; m/z (-) 279.80

Characterization IL 11:

^1H NMR (300Hz; DMSO; ppm): δ 0.90 (t, $J_{\text{H-H}} = 7.29$ Hz, 6H); δ 1.30 (m, 8H); δ 1.58 (m, 8H); δ 2.02 (br. s, 8H); δ 3.16 (m, 8H); δ 3.42 (m, 8H). ^{13}C NMR (300Hz; DMSO; ppm): δ 13.94; 19.73; 21.88; 22.88; 24.97; 25.88; 59.01; 62.64; 117.88; 122.15. ESI-MS: m/z (+) 169.17; m/z (-) 279.80

Characterization IL 12:

^1H NMR (500Hz; DMSO; ppm): δ 1.33 (br. s, 4H); δ 1.71 (m, 4H); δ 2.08 (m, 8H); δ 2.98 (s, 6H); δ 3.27 (m, 4H); 3.48 (m, 8H). ^{13}C NMR (500Hz; DMSO; ppm): δ 21.36; 23.06; 25.75; 47.78; 63.20; 63.73; 115.98; 118.51; 121.07; 123.65. ESI-MS: m/z (+) 127.14; m/z (-) 279.85

Characterization IL 13:

^1H NMR (300Hz; DMSO; ppm): δ 0.99 (dt, $J_{\text{H-H}} = 1.11$ Hz, $J_{\text{H-H}} = 7.19$ Hz 18H); δ 1.47 (m, 20H); δ 2.13 (m, 16H). ^{13}C NMR (300Hz; DMSO; ppm): δ 15.17; 15.22; 15.60; 15.82; 17.77; 18.40; 19.76; 20.38; 21.01; 29.82; 30.02; 117.89; 122.15. ESI-MS: m/z (+) 202.25; m/z (-) 279.83

Characterization IL 14:

^1H NMR (300Hz; DMSO; ppm): δ 1.45 (br. s, 8H); δ 3.48 (m, 4H); δ 7.76 (m, 24H); δ 7.87 (m, 6H). ^{13}C NMR (300Hz; DMSO; ppm): δ 20.98; 22.00; 22.06; 29.33; 29.55; 117.89; 118.44; 119.57; 122.15; 130.68; 130.86; 134.02; 134.15; 135.45. ESI-MS: m/z (+) 304.25; m/z (-) 279.85

Characterization IL 15:

^1H NMR (500Hz; DMSO; ppm): δ 1.29 (br. s, 4H); δ 1.72 (m, 4H); δ 2.59 (s, 6H); δ 4.09 (t, $J_{\text{H-H}} = 7.45$ Hz, 4H); δ 5.41 (s, 4H); δ 7.40 (m, 10H); δ 7.73 (dd, $J_{\text{H-H}} = 2.25$ Hz, $J_{\text{H-H}} = 7.45$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.67; 25.32; 28.99; 48.00; 51.02; 121.80; 121.94; 127.98; 128.71; 129.23; 134.78; 144.33. ESI-MS: m/z (+) 214.15; m/z (-) 498.89

Characterization IL 16:

^1H NMR (300Hz; DMSO; ppm): δ 1.23 (br. s, 4H); δ 1.66 (m, 4H); δ 2.54 (s, 6H); δ 3.74 (s, 6H); δ 4.06 (t, $J_{\text{H-H}} = 7.30$ Hz, 4H), δ 7.60 (dd, $J_{\text{H-H}} = 2.04$ Hz, $J_{\text{H-H}} = 4.8$ Hz, 4H). ^{13}C NMR (300Hz; DMSO; ppm): δ 9.67; 25.56; 29.49; 35.18; 47.88; 121.35; 122.84; 144.77. ESI-MS: m/z (+) 138.17; m/z (-) 498.84

Characterization IL 17:

^1H NMR (300Hz; DMSO; ppm): δ 0.88 (t, $J_{\text{H-H}} = 7.24$ Hz, 6H); δ 1.29 (m, 8H); δ 1.57 (m, 8H); δ 2.02 (br. s, 8H); δ 3.16 (m, 8H); δ 3.43 (m, 8H). ^{13}C NMR (300Hz; DMSO; ppm): δ 14.22; 20.09; 22.25; 23.21; 25.36; 26.21; 59.40; 63.00. ESI-MS: m/z (+) 169.18; m/z (-) 498.84

Characterization IL 18:

^1H NMR (300Hz; DMSO; ppm): δ 1.32 (br. s, 4H); δ 1.68 (m, 4H); δ 2.05 (m, 8H); δ 2.94 (s, 6H); δ 3.25 (m, 4H); 3.42 (m, 8H). ^{13}C NMR (300Hz; DMSO; ppm): δ 21.58; 23.26; 25.97; 48.00; 63.40; 63.93. ESI-MS: m/z (+) 127.17; m/z (-) 498.89

Characterization IL 19:

^1H NMR (300Hz; DMSO; ppm): δ 0.98 (dt, $J_{\text{H-H}} = 0.90$ Hz, $J_{\text{H-H}} = 7.24$ Hz 18H); δ 1.47 (m, 20H); δ 2.13 (m, 16H). ^{13}C NMR (500Hz; DMSO; ppm): δ 15.19; 15.22; 15.70; 15.83; 18.21; 19.88; 20.25; 21.01; 21.04; 29.93. ESI-MS: m/z (+) 202.25; m/z (-) 498.85

Characterization IL 20:

^1H NMR (300Hz; DMSO; ppm): δ 1.45 (br. s, 8H); δ 3.48 (m, 4H); δ 7.75 (m, 24H); δ 7.86 (m, 6H). ^{13}C NMR (300Hz; DMSO; ppm): δ 20.27; 20.93; 22.00; 29.29; 29.51; 118.44; 119.58; 130.67; 130.84; 134.01; 134.15. ESI-MS: m/z (+) 304.23; m/z (-) 498.89

Characterization IL 21:

^1H NMR (300Hz; DMSO; ppm): δ 1.22 (br. s, 10H); δ 1.69 (m, 4H); δ 2.56 (s, 6H); δ 4.06 (t, $J_{\text{H-H}} = 7.38$ Hz, 4H); δ 5.38 (s, 4H); δ 7.29 (m, 4H); δ 7.38 (m, 6H); δ 7.70 (dd, $J_{\text{H-H}} = 2.11$ Hz, $J_{\text{H-H}} = 5.35$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.69; 25.91; 28.68; 29.01; 29.24; 47.97; 50.92; 115.94; 118.51; 121.07; 121.84; 121.98; 123.62; 127.98; 128.77; 129.29; 134.79; 144.32. ESI-MS: m/z (+) 235.39; m/z (-) 279.85

Characterization IL 22:

^1H NMR (500Hz; DMSO; ppm): δ 1.26 (br. s, 10H); δ 1.68 (m, 4H); δ 2.56 (s, 6H); δ 3.74 (s, 6H); δ 4.08 (t, $J_{\text{H-H}} = 7.45$ Hz, 4H), δ 7.61 (dd, $J_{\text{H-H}} = 2.02$ Hz, $J_{\text{H-H}} = 10.57$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.39; 25.91; 28.78; 29.08; 29.51; 34.95; 47.84; 115.99; 118.55; 121.10; 121.15; 122.63; 123.66; 144.51. ESI-MS: m/z (+) 159.23; m/z (-) 279.79

Characterization IL 23:

^1H NMR (500Hz; DMSO; ppm): δ 0.93 (t, $J_{\text{H-H}} = 7.42$ Hz, 6H); δ 1.30 (m, 14H); δ 1.60 (m, 8H); δ 2.04 (br. s, 8H); δ 3.17 (m, 8H); δ 3.45 (m, 8H). ^{13}C NMR (500Hz; DMSO; ppm): δ 13.77; 19.80; 21.68; 22.77; 24.75; 26.20; 28.79; 58.74; 58.96; 62.39; 118.48; 121.08. ESI-MS: m/z (+) 190.17; m/z (-) 279.85

Characterization IL 24:

^1H NMR (500Hz; DMSO; ppm): δ 1.30 (br. s, 10H); δ 1.69 (m, 4H); δ 2.08 (m, 8H); δ 2.96 (s, 6H); δ 3.28 (m, 4H); 3.44 (m, 8H). ^{13}C NMR (500Hz; DMSO; ppm): δ 21.35; 23.25; 26.19; 28.74; 28.93; 47.77; 63.44; 63.73; 115.98; 118.54; 121.09; 123.65. ESI-MS: m/z (+) 148.25; m/z (-) 279.85

Characterization IL 25:

^1H NMR (500Hz; DMSO; ppm): δ 1.01 (t, $J_{\text{H-H}} = 7.42$ Hz, 18H); δ 1.28 (br. s, 6H); δ 1.37 (m, 4H); δ 1.50 (m, 16H); δ 2.15 (m, 16H). ^{13}C NMR (500Hz; DMSO; ppm): δ 15.03; 15.07; 15.52; 15.65; 17.82; 18.19; 19.75; 20.13; 21.00; 28.63; 28.98; 30.49; 30.61; 115.97; 121.14; 123.70. ESI-MS: m/z (+) 223.35; m/z (-) 279.85

Characterization IL 26:

^1H NMR (500Hz; DMSO; ppm): δ 1.18 (m, 6H); δ 1.46 (m, 8H); δ 3.53 (m, 4H); δ 7.82 (m, 30H). ^{13}C NMR (500Hz; DMSO; ppm): δ 20.29; 20.69; 22.05; 28.36; 28.75; 30.08; 30.20; 118.55; 119.22; 121.09; 130.50; 130.59; 133.86; 133.93; 135.19. ESI-MS: m/z (+) 325.25; m/z (-) 279.83

Characterization IL 27:

^1H NMR (300Hz; DMSO; ppm): δ 1.22 (br. s, 10H); δ 1.69 (m, 4H); δ 2.59 (s, 6H); δ 4.08 (t, $J_{\text{H-H}} = 7.38$ Hz, 4H); δ 5.39 (s, 4H); δ 7.33 (m, 10H); δ 7.72 (dd, $J_{\text{H-H}} = 2.20$ Hz, $J_{\text{H-H}} = 3.55$ Hz, 4H). ^{13}C NMR (300Hz; DMSO; ppm): δ 9.99; 26.14; 28.92; 29.27; 29.50; 48.19; 51.12; 122.10; 122.22; 128.26; 128.98; 129.51; 135.09; 144.59. ESI-MS: m/z (+) 235.35; m/z (-) 498.89

Characterization IL 28:

^1H NMR (500Hz; DMSO; ppm): δ 1.26 (br. s, 10H); δ 1.68 (m, 4H); δ 2.56 (s, 6H); δ 3.74 (s, 6H); δ 4.08 (t, $J_{\text{H-H}} = 7.21$ Hz, 4H), δ 7.62 (dd, $J_{\text{H-H}} = 2.30$ Hz, $J_{\text{H-H}} = 9.70$ Hz, 4H). ^{13}C NMR

(500Hz; DMSO; ppm): δ 9.43; 25.93; 28.81; 29.10; 29.53; 34.98; 47.86; 121.15; 122.63; 123.66; 144.53. ESI-MS: m/2z (+) 159.29; m/z (-) 498.89

Characterization IL 29:

ESI-MS: m/2z (+) 190.17; m/z (-) 498.89

Characterization IL 30:

ESI-MS: m/2z (+) 148.26; m/z (-) 498.86

Characterization IL 31:

ESI-MS: m/2z (+) 223.37; m/z (-) 498.85

Characterization IL 32:

^1H NMR (300Hz; DMSO; ppm): δ 1.14 (m, 6H); δ 1.42 (m, 8H); δ 3.51 (m, 4H); δ 7.78 (m, 30H). ^{13}C NMR (300Hz; DMSO; ppm): δ 20.33; 20.99; 22.24; 28.56; 28.95; 30.20; 30.42; 118.52; 119.66; 130.65; 130.82; 134.02; 134.16; 135.38. ESI-MS: m/2z (+) 325.23; m/z (-) 498.89

Characterization IL 33:

ESI-MS: m/2z (+) 256.25; m/z (-) 279.86

Characterization IL 34:

^1H NMR (500Hz; DMSO; ppm): δ 1.24 (br. s, 16H); δ 1.68 (m, 4H); δ 2.56 (s, 6H); δ 3.74 (s, 6H); δ 4.08 (t, $J_{\text{H-H}} = 7.45$ Hz, 4H), δ 7.61 (dd, $J_{\text{H-H}} = 1.97$ Hz, $J_{\text{H-H}} = 13.02$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.37; 25.92; 28.84; 29.21; 29.27; 29.50; 34.93; 47.81; 115.98; 118.52; 121.07; 121.13; 122.59; 123.66; 144.48. ESI-MS: m/2z (+) 180.17; m/z (-) 279.83

Characterization IL 35:

ESI-MS: m/2z (+) 211.25; m/z (-) 279.86

Characterization IL 36:

^1H NMR (500Hz; DMSO; ppm): δ 1.29 (br. s, 16H); δ 1.69 (m, 4H); δ 2.08 (m, 8H); δ 2.96 (s, 6H); δ 3.28 (m, 4H); 3.44 (m, 8H). ^{13}C NMR (500Hz; DMSO; ppm): δ 21.34; 23.24; 26.21; 28.82; 29.13; 29.22; 47.76; 63.48; 63.73; 115.98; 118.55; 121.10; 123.66. ESI-MS: m/2z (+) 169.18; m/z (-) 279.86

Characterization IL 37:

^1H NMR (500Hz; DMSO; ppm): δ 1.01 (t, $J_{\text{H-H}} = 7.42$ Hz, 18H); δ 1.26 (m, 12H); δ 1.37 (m, 4H); δ 1.50 (m, 16H); δ 2.14 (m, 16H). ^{13}C NMR (500Hz; DMSO; ppm): δ 14.96; 15.00; 15.47;

15.60; 17.73; 18.11; 19.68; 20.05; 20.90; 28.59; 29.14; 29.34; 30.42; 30.55; 115.95; 118.52; 121.07; 123.50. ESI-MS: m/2z (+) 244.25; m/z (-) 279.80

Characterization IL 38:

ESI-MS: m/2z (+) 346.25; m/z (-) 279.84

Characterization IL 39:

ESI-MS: m/2z (+) 256.25; m/z (-) 498.84

Characterization IL 40:

^1H NMR (300Hz; DMSO; ppm): δ 1.25 (br. s, 16H); δ 1.70 (m, 4H); δ 2.58 (s, 6H); δ 3.76 (s, 6H); δ 4.10 (t, $J_{\text{H-H}} = 7.38$ Hz, 4H), δ 7.63 (dd, $J_{\text{H-H}} = 2.07$ Hz, $J_{\text{H-H}} = 7.89$ Hz, 4H). ^{13}C NMR (500Hz; DMSO; ppm): δ 9.19; 25.75; 28.68; 29.05; 29.11; 29.36; 34.75; 47.63; 120.96; 122.42; 144.35. ESI-MS: m/2z (+) 180.15; m/z (-) 498.89

Characterization IL 41:

ESI-MS: m/2z (+) 211.26; m/z (-) 498.86

Characterization IL 42:

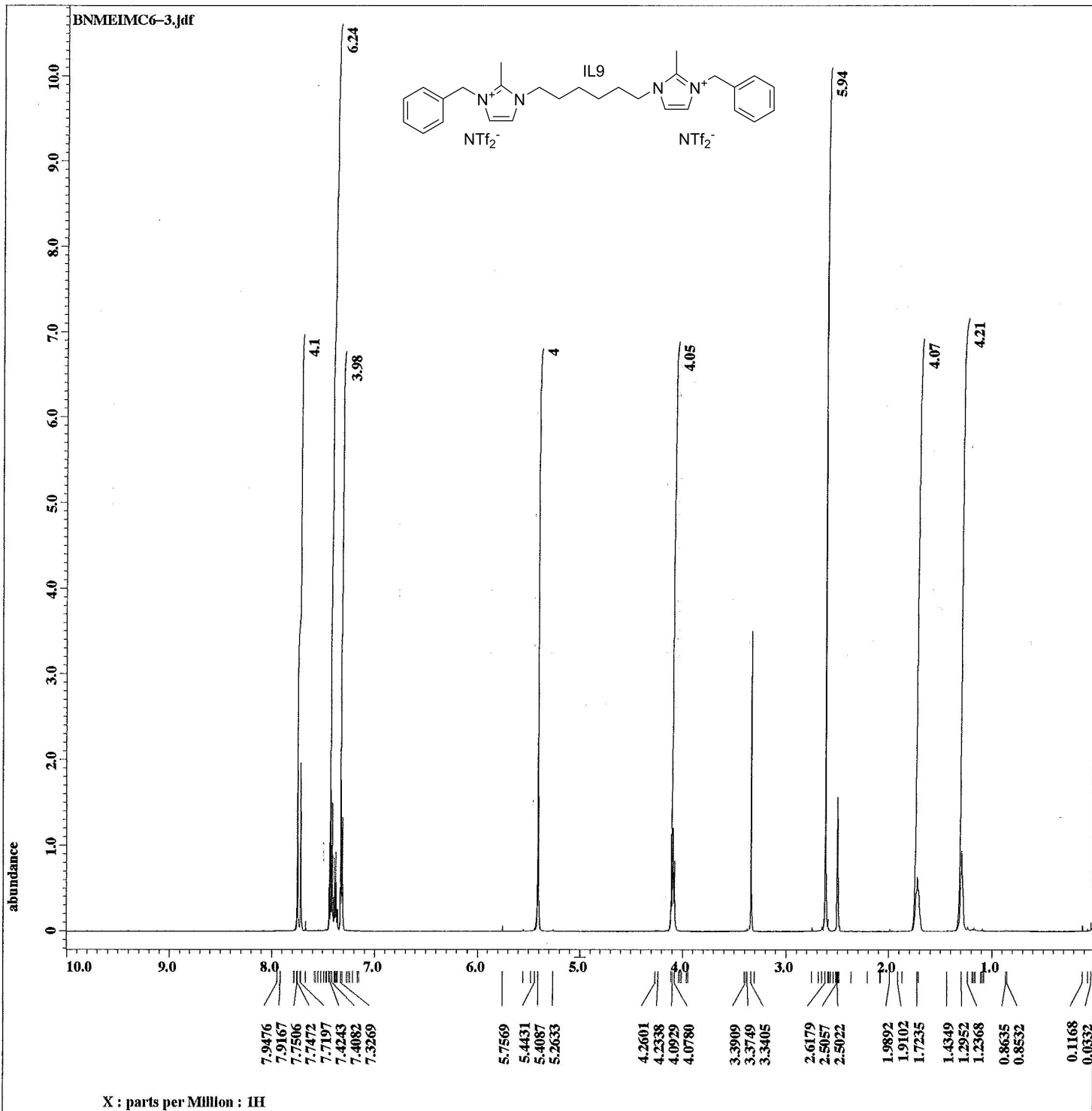
ESI-MS: m/2z (+) 169.17; m/z (-) 498.86

Characterization IL 43:

ESI-MS: m/2z (+) 244.37; m/z (-) 498.85

Characterization IL 44:

ESI-MS: m/2z (+) 346.235; m/z (-) 498.89



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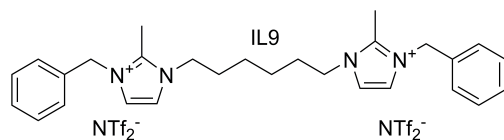
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 10
 Total_scans = 10

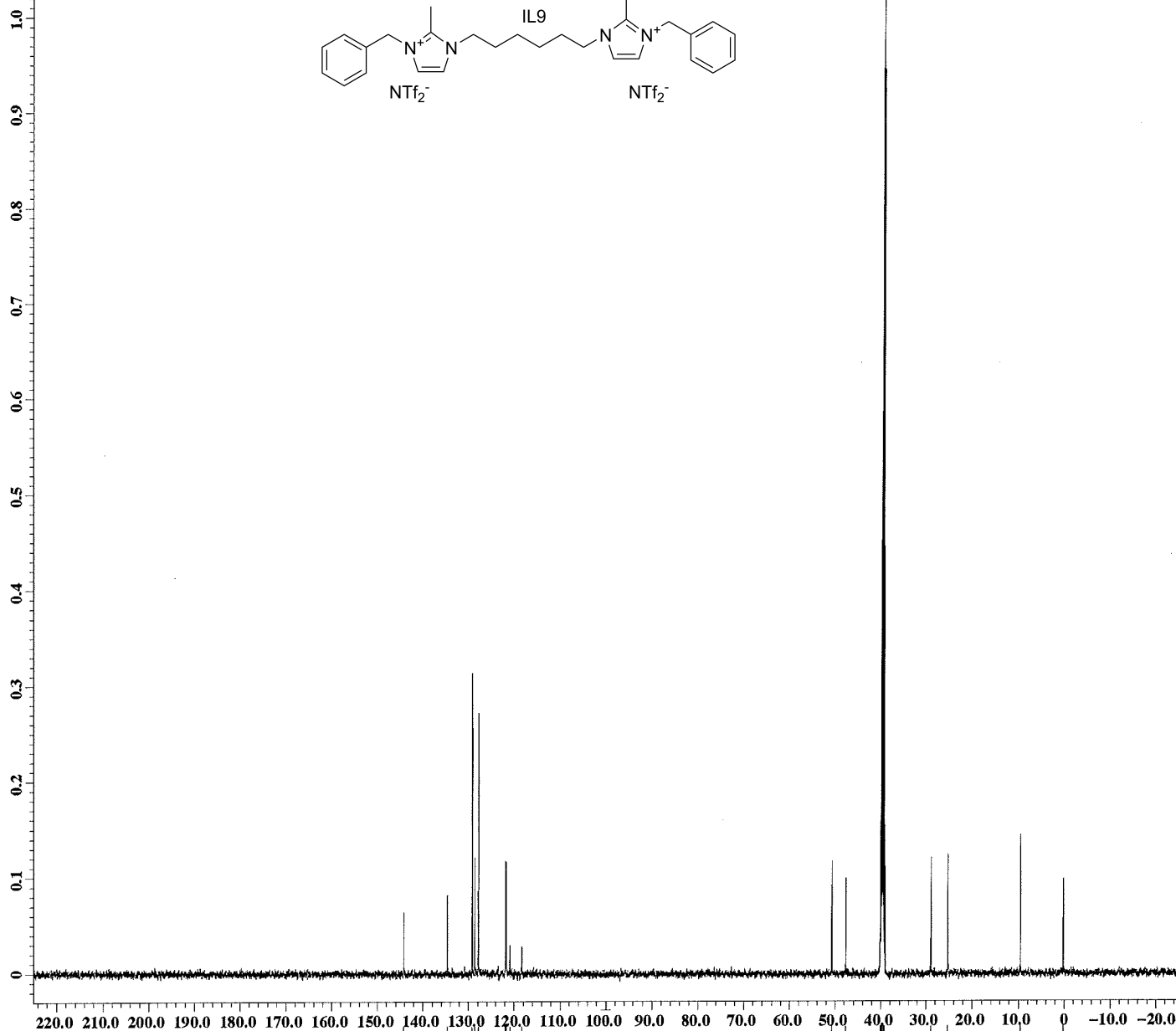
X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 21.2[dC]

X : parts per Million : 1H

BNMEIMC6CNT-2.jdf



abundance



144.2197
134.6718
129.1777
128.6722
127.8710
121.8714
121.7092
120.9175
118.3517

40.1661
39.9944
39.8322
39.6606
39.4984
39.3267
39.1646
28.9109
25.2577

9.5767
0.2291

X : parts per Million : 13C

```

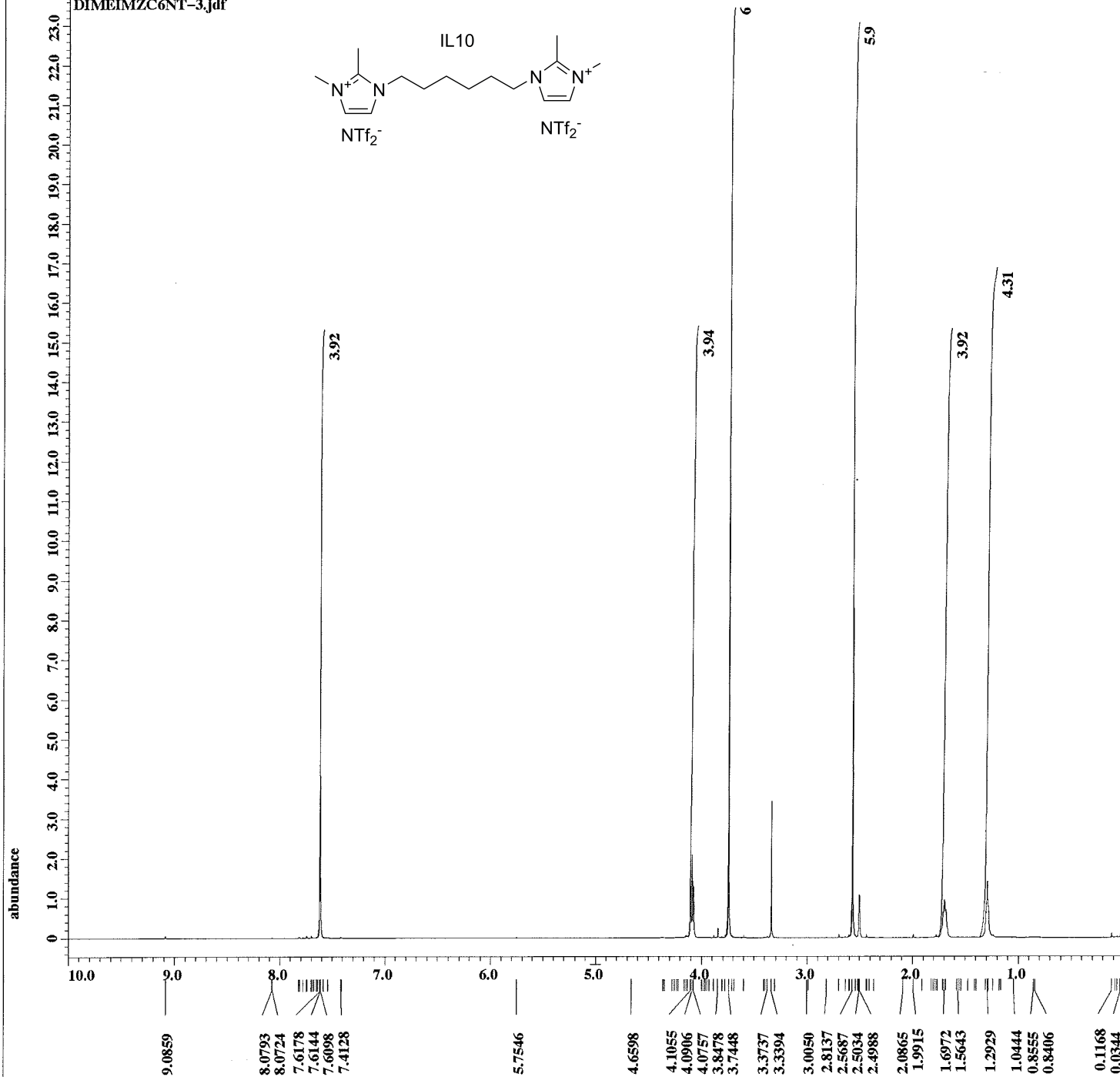
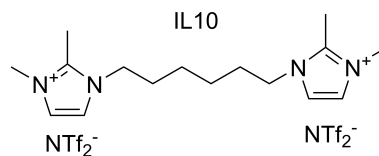
Filename      = BNMEIMC6CNT-2.jdf
Author        = delta
Experiment     = single_pulse_dec
Sample_id     = S#373612
Solvent       = DMSO-D6
Creation time  = 27-NOV-2015 00:05:53
Revision time  = 1-DEC-2015 11:35:57
Current_time   = 1-DEC-2015 11:36:06

Comment       = single pulse decouple
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq        = 125.76529768[MHz]
X_offset      = 100[ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.19959034[Hz]
X_sweep       = 39.3081761[kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521[MHz]
Irr_offset    = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 740
Total_scans   = 740

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[dB]
Irr_atn_noe   = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 0.2[s]
Recvr_gain    = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get      = 21.7[dC]
    
```

DIMEIMZC6NT-3.jdf



X : parts per Million : 1H

```

Filename      = DIMEIMZC6NT-3.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#387568
Solvent      = DMSO-D6
Creation_time = 27-NOV-2015 00:20:05
Revision_time = 1-DEC-2015 11:17:12
Current_time  = 1-DEC-2015 11:17:53

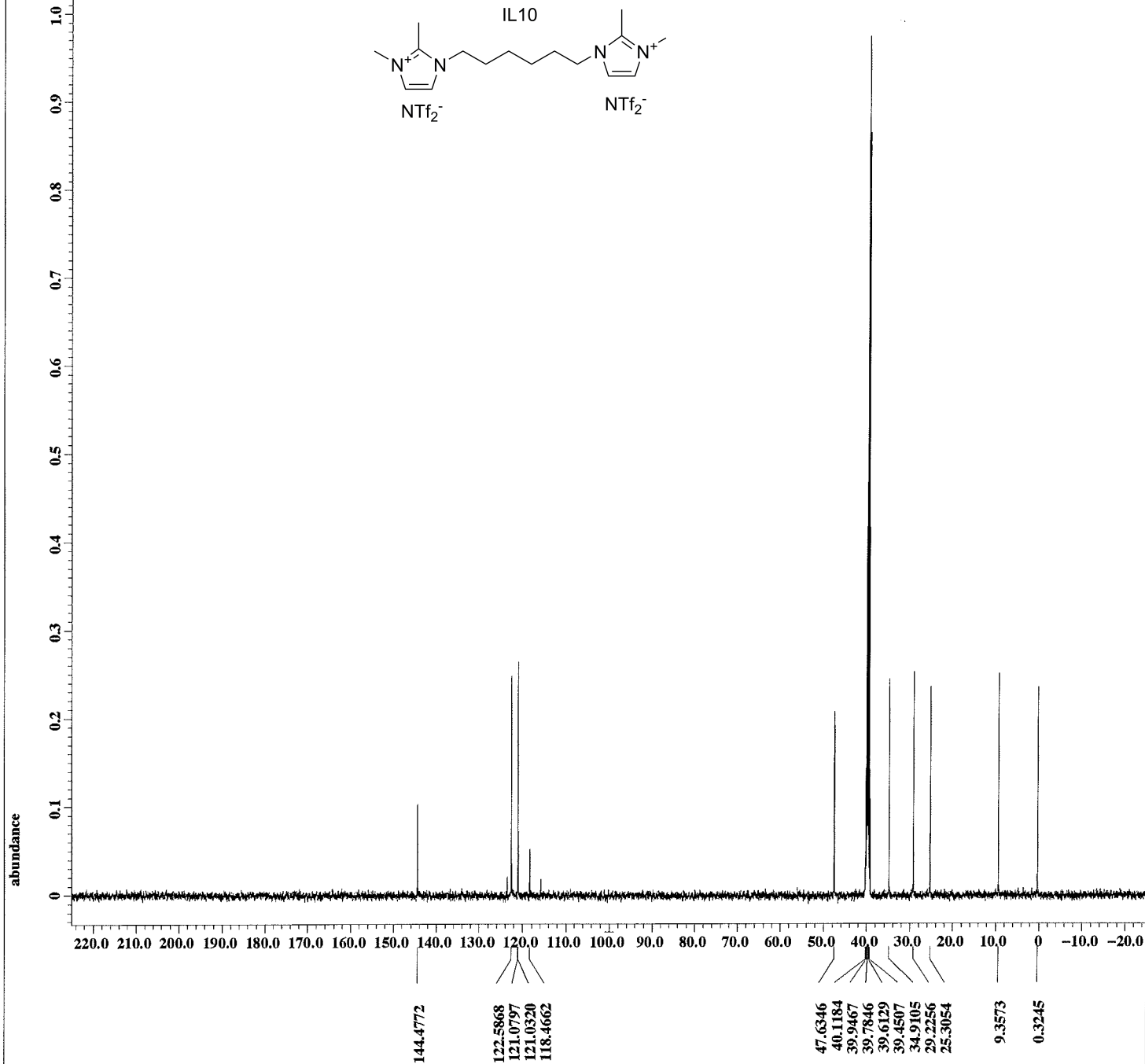
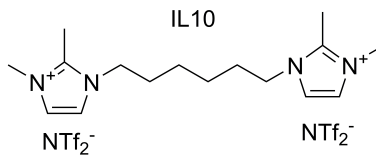
Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq        = 500.15991521[MHz]
X_offset      = 5.0[ppm]
X_points      = 16384
X_prescans    = 0
X_resolution  = 0.57277737 [Hz]
X_sweep       = 9.38438438 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521[MHz]
Irr_offset    = 5.0[ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521[MHz]
Tri_offset    = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 14
Total_scans   = 14

X_90_width    = 12.54[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_preset  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 34
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get      = 21.2[dC]
    
```

DIMEIMZC6NTC-2.jdf

IL10



X : parts per Million : 13C

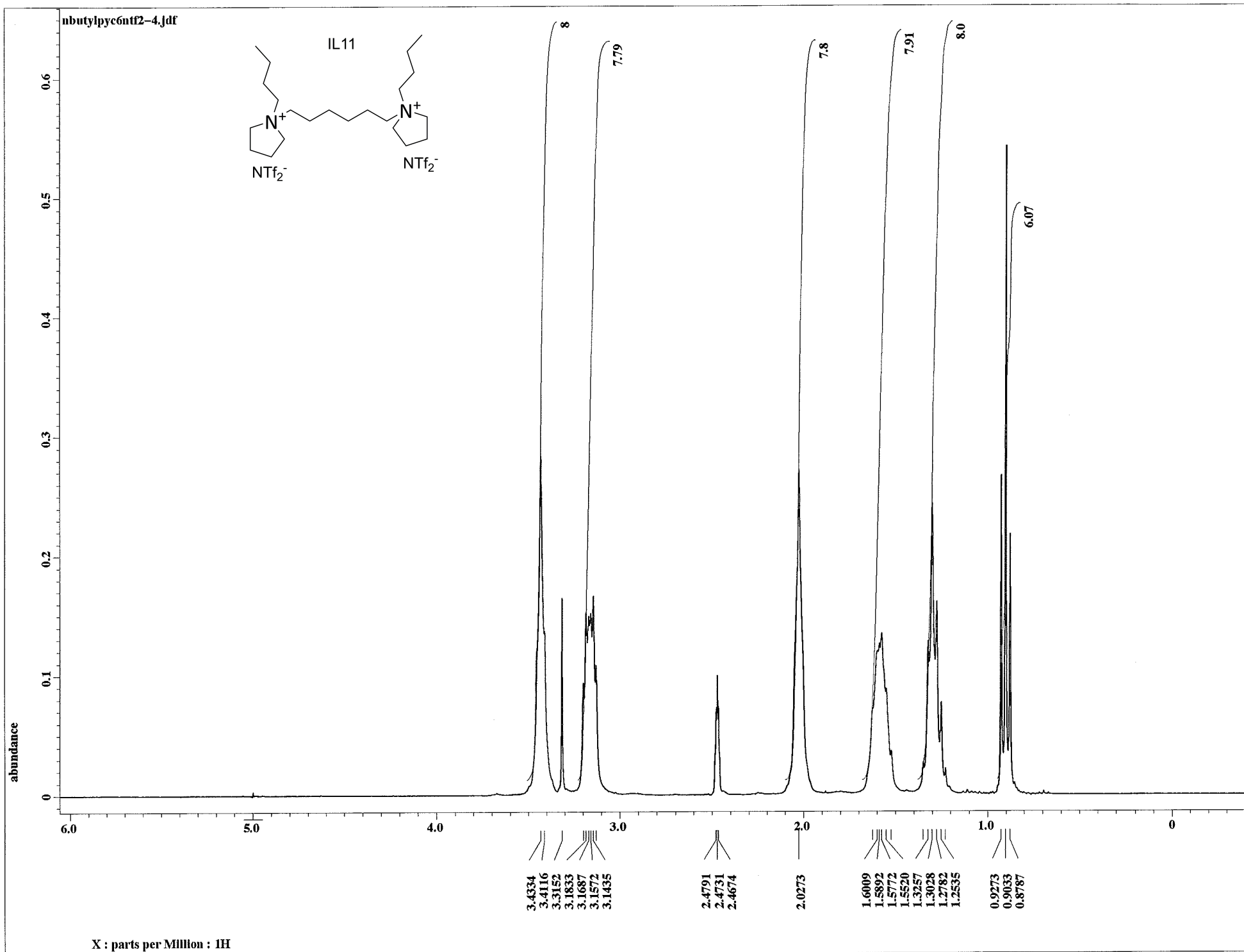
```

Filename      = DIMEIMZC6NTC-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#390373
Solvent      = DMSO-D6
Creation time = 27-NOV-2015 00:30:02
Revision time = 1-DEC-2015 11:39:16
Current_time = 1-DEC-2015 11:39:23

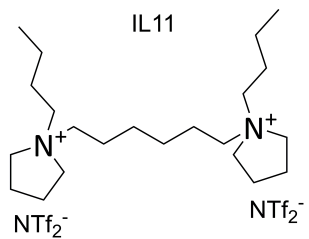
Comment      = single_pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain      = 13C
X_freq       = 125.76529768[MHz]
X_offset     = 100[ppm]
X_points     = 32768
X_prescans   = 4
X_resolution = 1.19959034[Hz]
X_sweep      = 39.3081761[kHz]
Irr_domain   = 1H
Irr_freq     = 500.15991521[MHz]
Irr_offset   = 5.0[ppm]
Clipped     = FALSE
Mod_return   = 10
Scans        = 520
Total_scans  = 520

X_90_width   = 10.73[us]
X_acq_time   = 0.83361792[s]
X_angle      = 30[deg]
X_atn        = 9[db]
X_pulse     = 3.57666667[us]
Irr_atn_dec  = 20[db]
Irr_atn_noe  = 20[db]
Irr_noise    = WALTZ
Decoupling   = TRUE
Initial_wait = 1[s]
Noe          = TRUE
Noe_time     = 0.2[s]
Recvr_gain   = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get     = 21.6[dC]
    
```



nbutylpyc6ntf2c-3.jdf



abundance

0.4
0.3
0.2
0.1
0

170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

122.1520

117.8880

62.6466

59.0135

40.3129

40.0357

39.7584

25.8859

24.9777

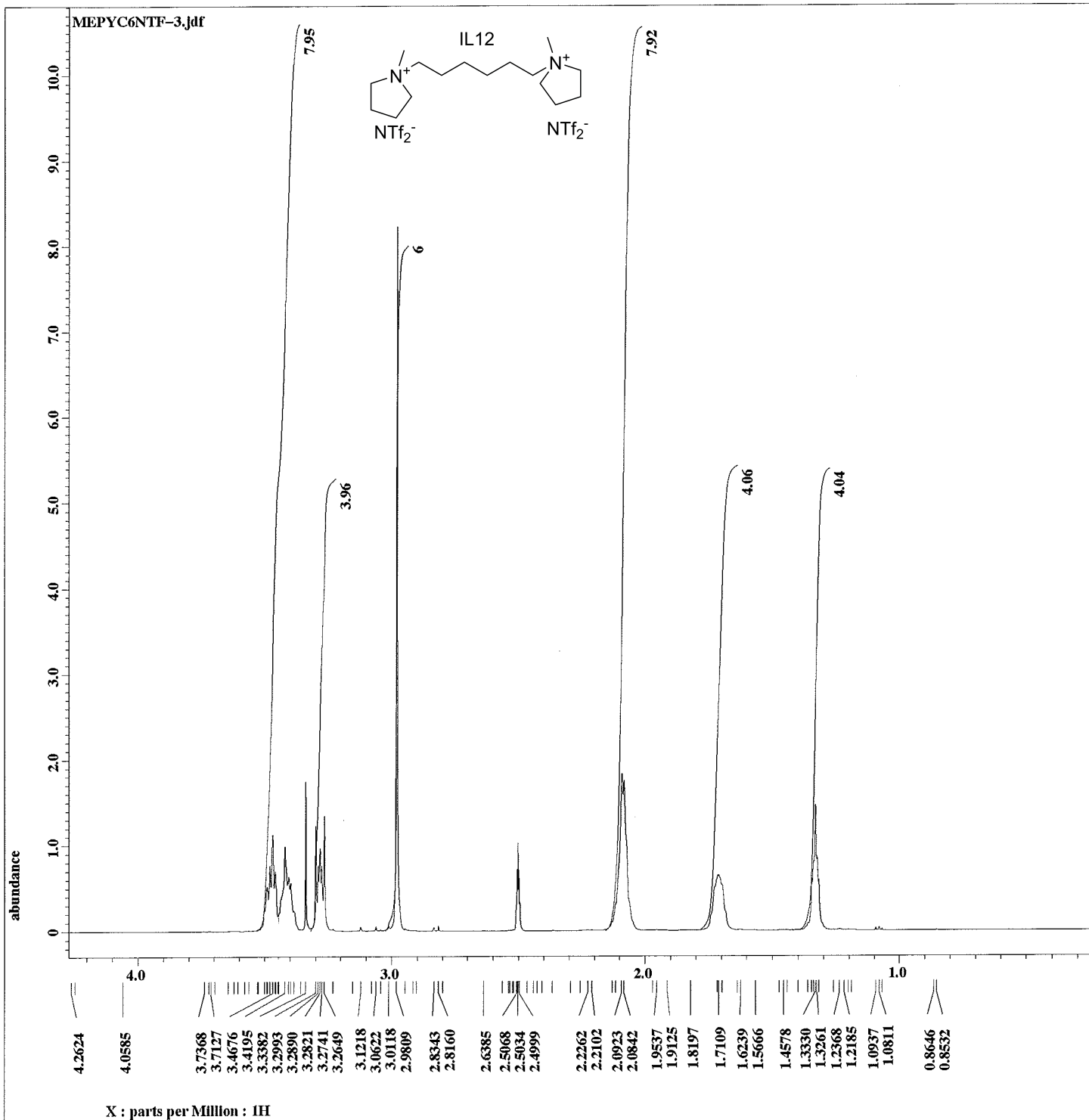
22.8839

21.8800

19.7384

13.9447

X : parts per Million : 13C



```

Filename      = MEPYC6NTF-3.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#401237
Solvent      = DMSO-D6
Creation time = 27-NOV-2015 00:42:51
Revision time = 1-DEC-2015 11:25:00
Current_time = 1-DEC-2015 11:25:37

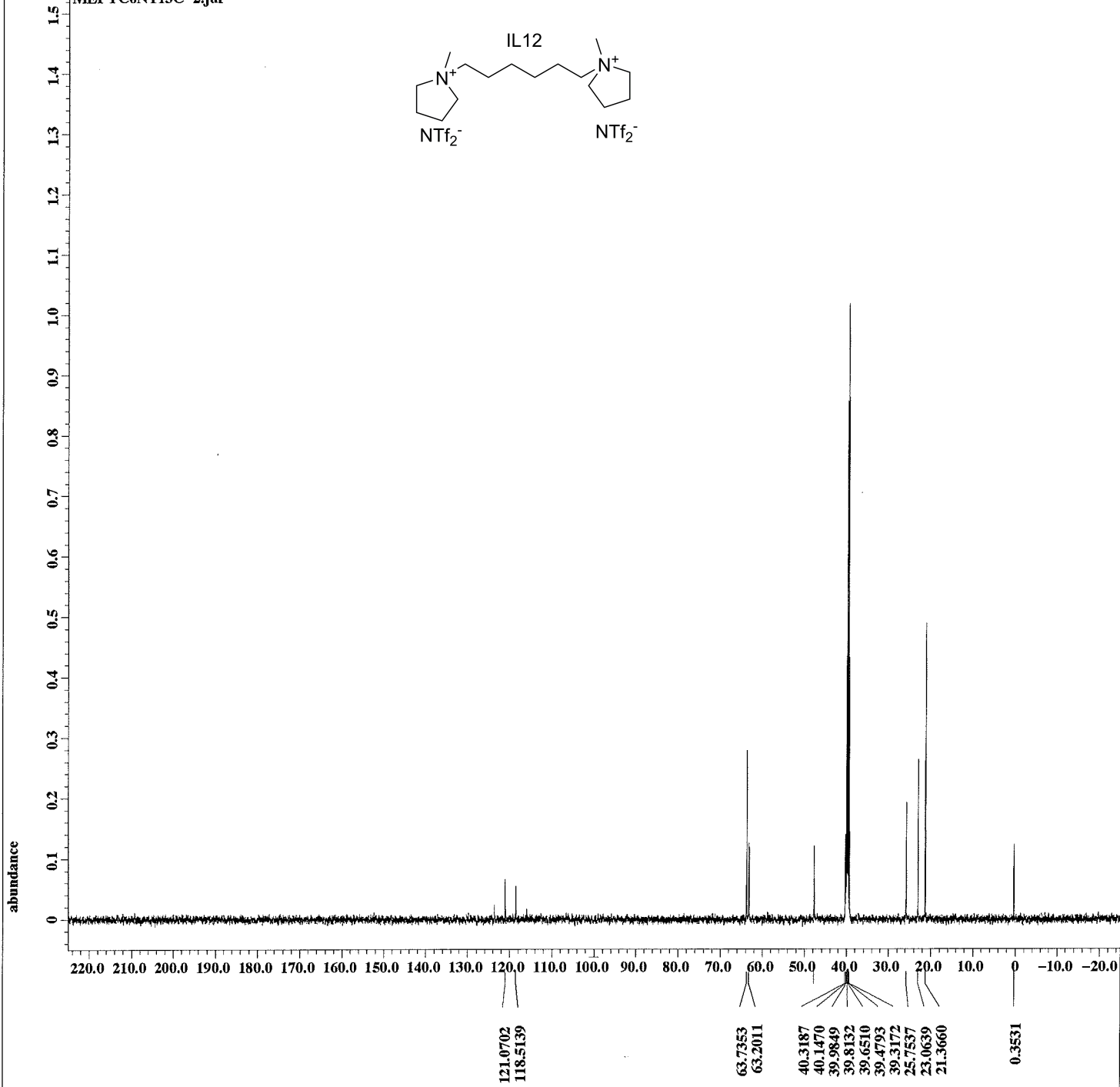
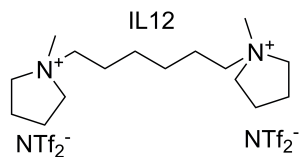
Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site        = ECA 500
Spectrometer = JNM-ECA500

Field strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans    = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain    = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain    = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 14
Total_scans   = 14

X_90_width    = 12.54[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 32
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get      = 21.2[dC]

```

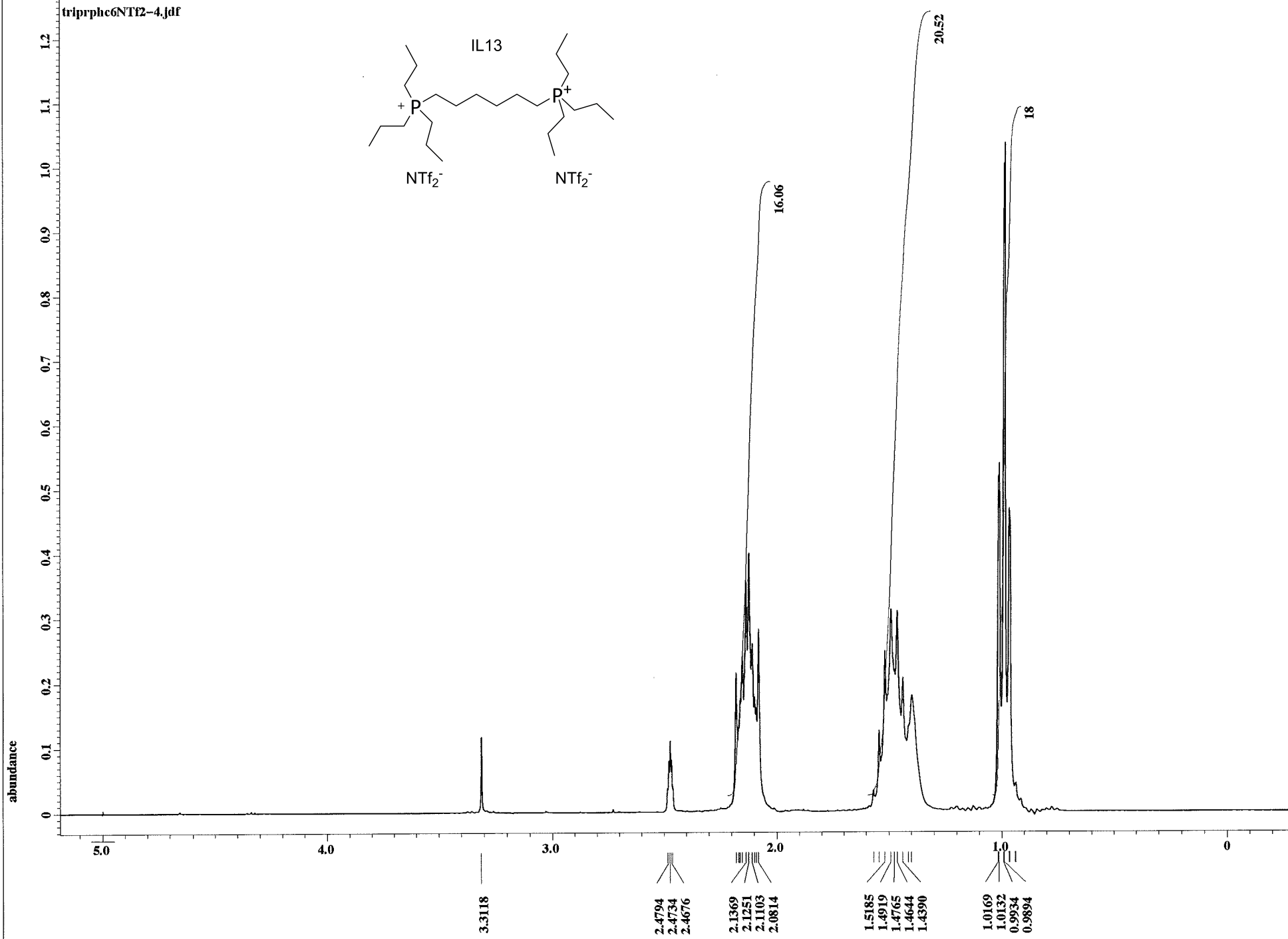
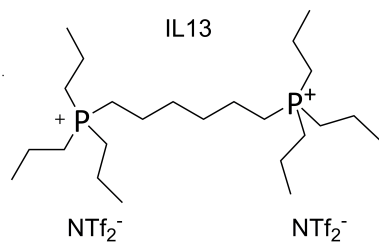
MEPYC6NT13C-2.jdf



X : parts per Million : 13C

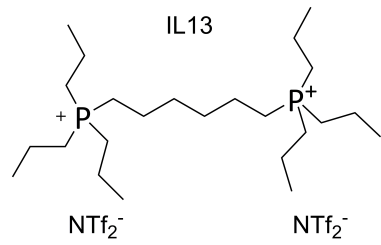
Filename = MEPYC6NT13C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#404718
Solvent = DMSO-D6
Creation_time = 27-NOV-2015 00:49:18
Revision_time = 1-DEC-2015 11:42:19
Current_time = 1-DEC-2015 11:42:23
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.3081761[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 10
Scans = 250
Total_scans = 250
X_90_width = 10.73[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 3.57666667[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.2[s]
Recvr_gain = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get = 21.6[dC]

triprphc6NTf2-4.jdf



X : parts per Million : 1H

triprphc6ntf2e-3.jdf



abundance

0.4
0.3
0.2
0.1
0

170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

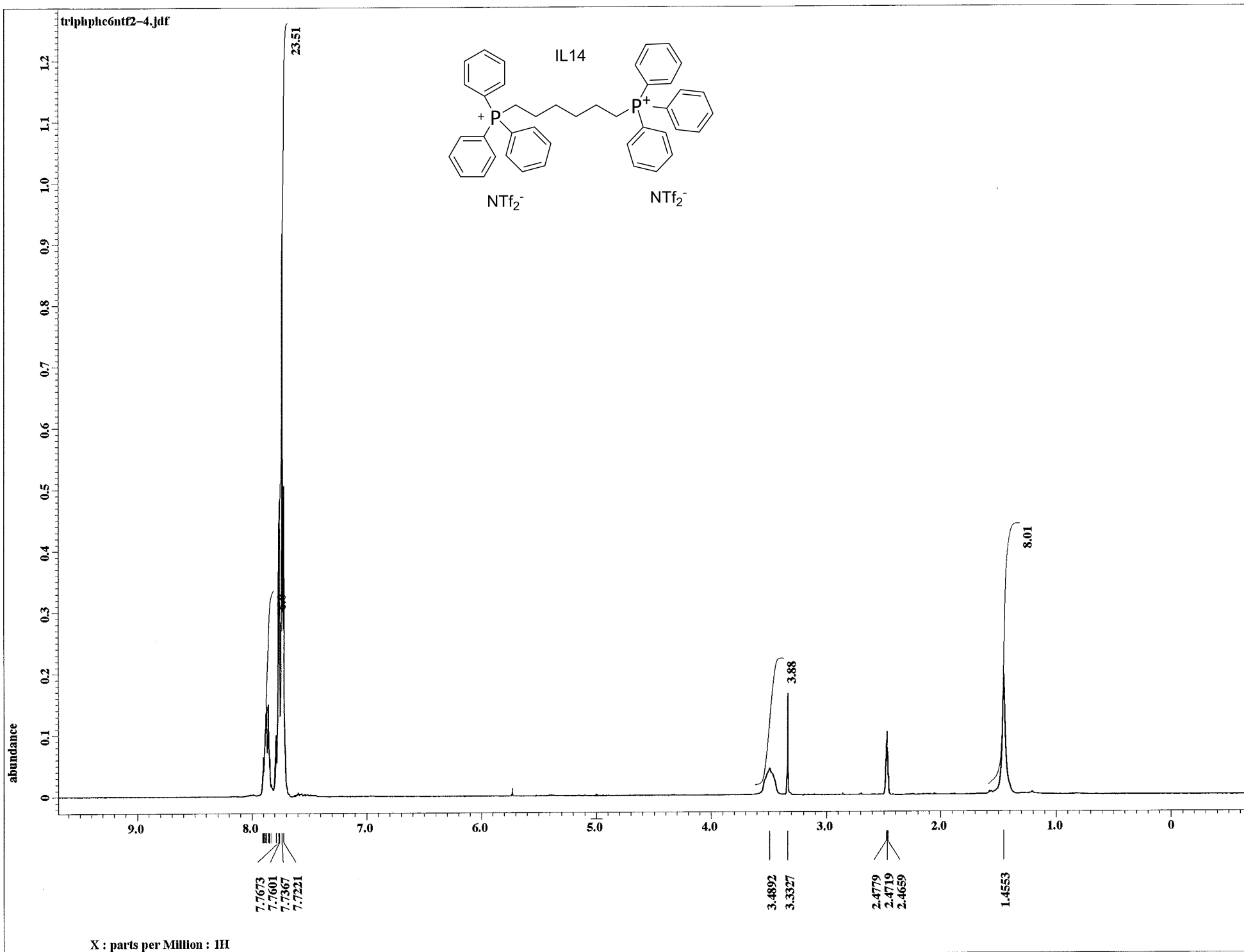
122.1520
117.8975

40.3129
40.0357
39.7584

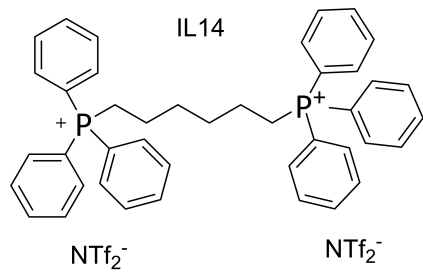
30.0257
29.8249

20.3886
19.7671
15.8281
15.6082
15.2258
15.1780

X : parts per Million : ¹³C



tripphc6ntf2c-4.jdf



abundance

0.4
0.3
0.2
0.1
0

180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

135.4509
134.1506
134.0263
130.8617
130.6897

122.1520
119.5706
118.4425
117.8975

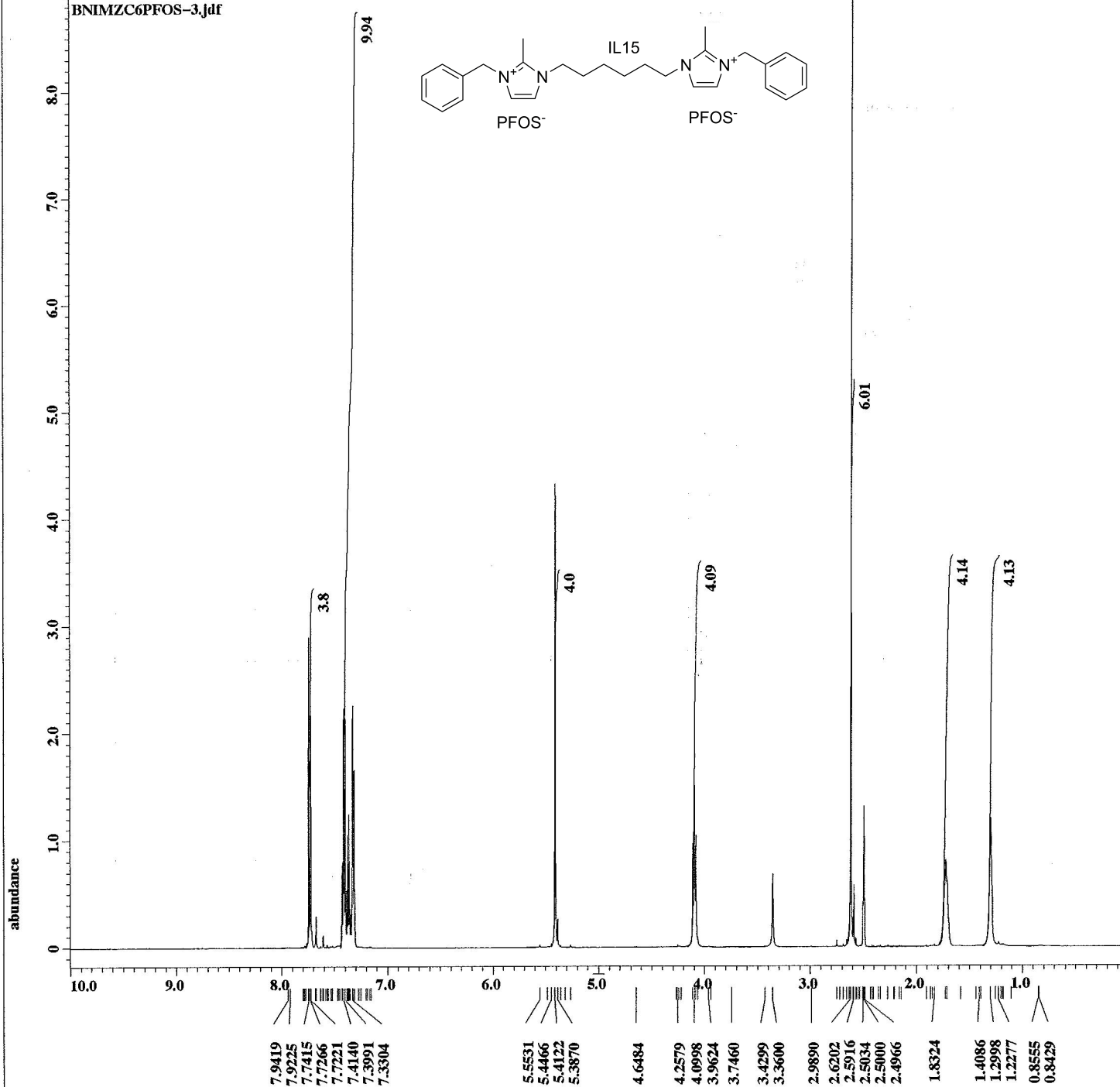
40.3225
40.0452
39.7680

29.5572
29.3373

22.0617
22.0043
20.9813

X : parts per Million : 13C

BNIMZC6PFOS-3.jdf



```

Filename      = BNIMZC6PFOS-3.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#447219
Solvent      = DMSO-D6
Creation time = 1-DEC-2015 01:58:52
Revision time = 30-NOV-2015 12:33:36
Current_time = 30-NOV-2015 12:34:50

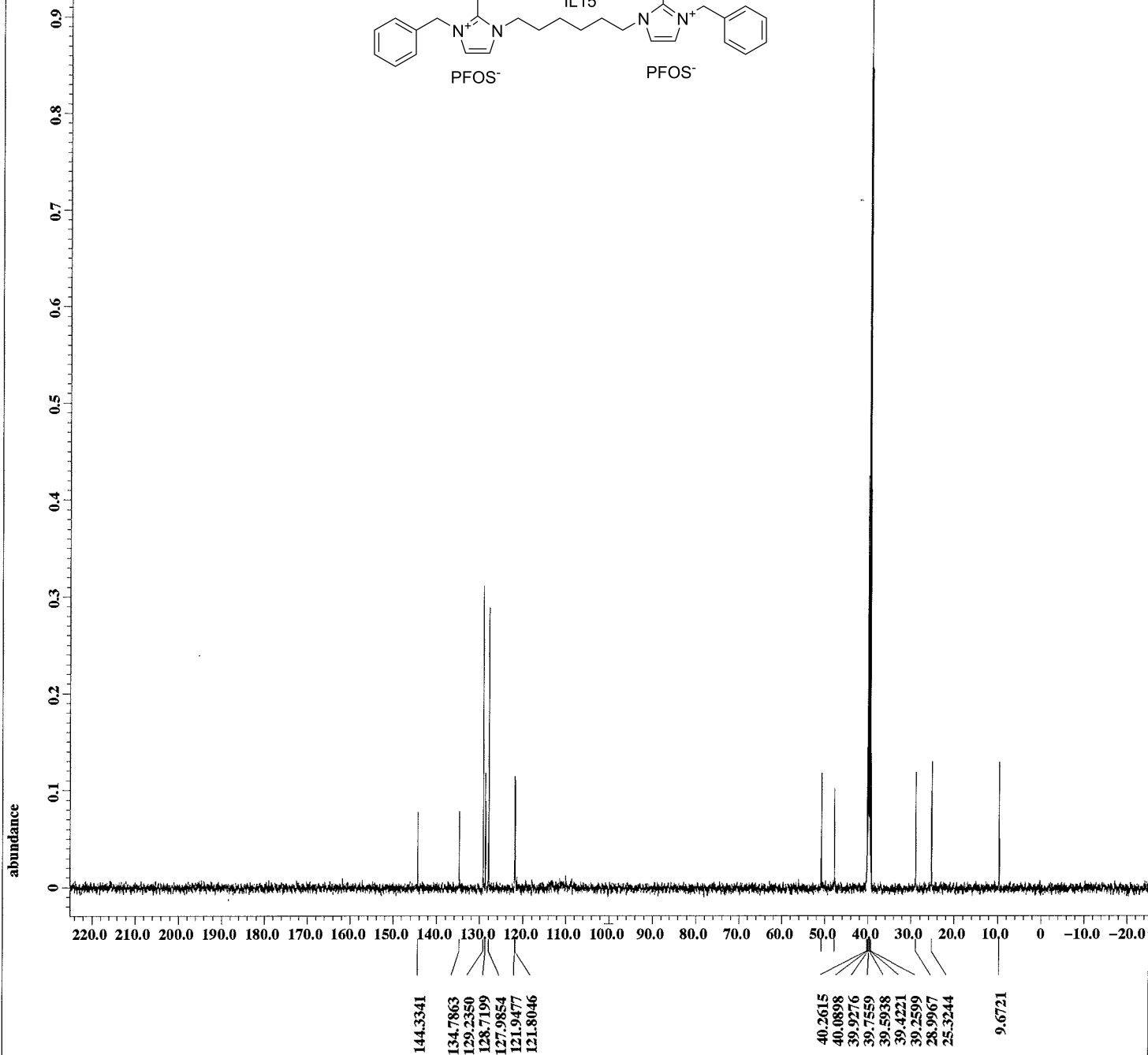
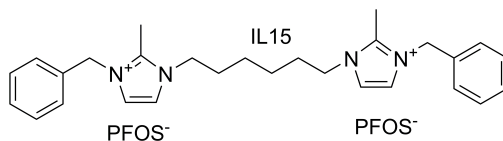
Comment      = single_pulse
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 10
Total_scans    = 10

X_90_width    = 12.54[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_preset  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 34
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get      = 21.2[dC]
    
```

X : parts per Million : 1H

BNMEIMZC6PFOSC-2.jdf



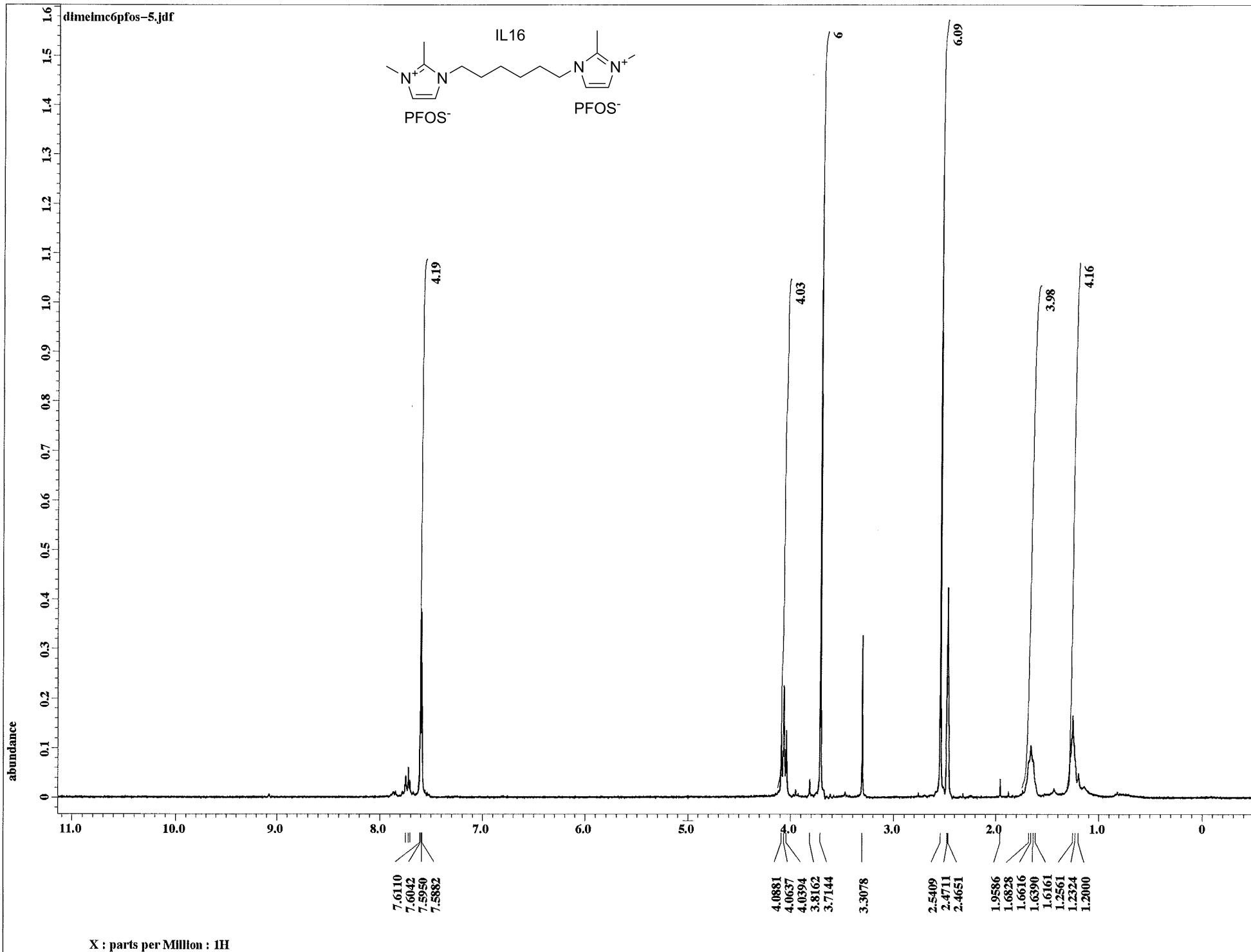
X : parts per Million : 13C

Filename = BNMEIMZC6PFOSC-2.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#449555
 Solvent = DMSO-D6
 Creation_time = 1-DEC-2015 02:05:54
 Revision_time = 1-DEC-2015 11:36:54
 Current_time = 1-DEC-2015 11:37:04

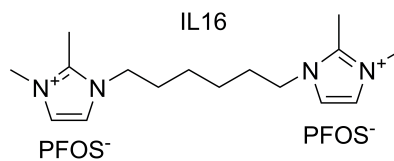
Comment = single_pulse_decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 350
 Total_scans = 350

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 0.2[s]
 Recvr_gain = 50
 Relaxation_delay = 0.2[s]
 Repetition_time = 1.03361792[s]
 Temp_get = 21.7[dC]



dlmelmc6pfosc-3.jdf



abundance

0.4
0.3
0.2
0.1
0

190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

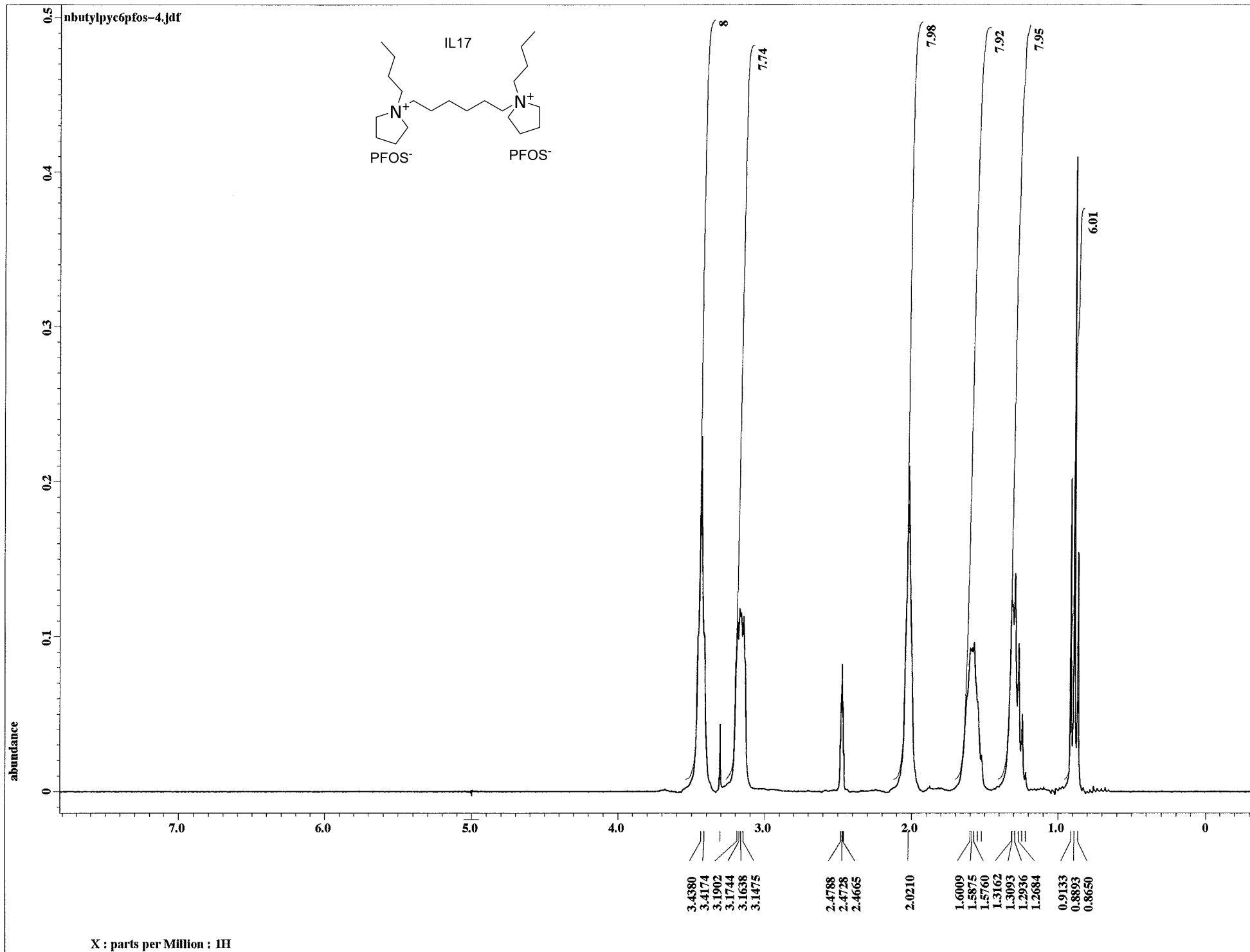
144.7725

122.8499
121.3585

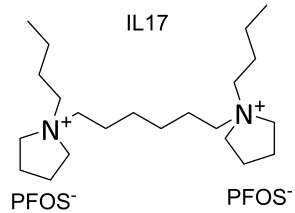
47.8850
40.8770
40.5998
40.3225
40.0452
39.7680
39.4907
39.2135
35.1884
29.4999
25.5609

9.6711

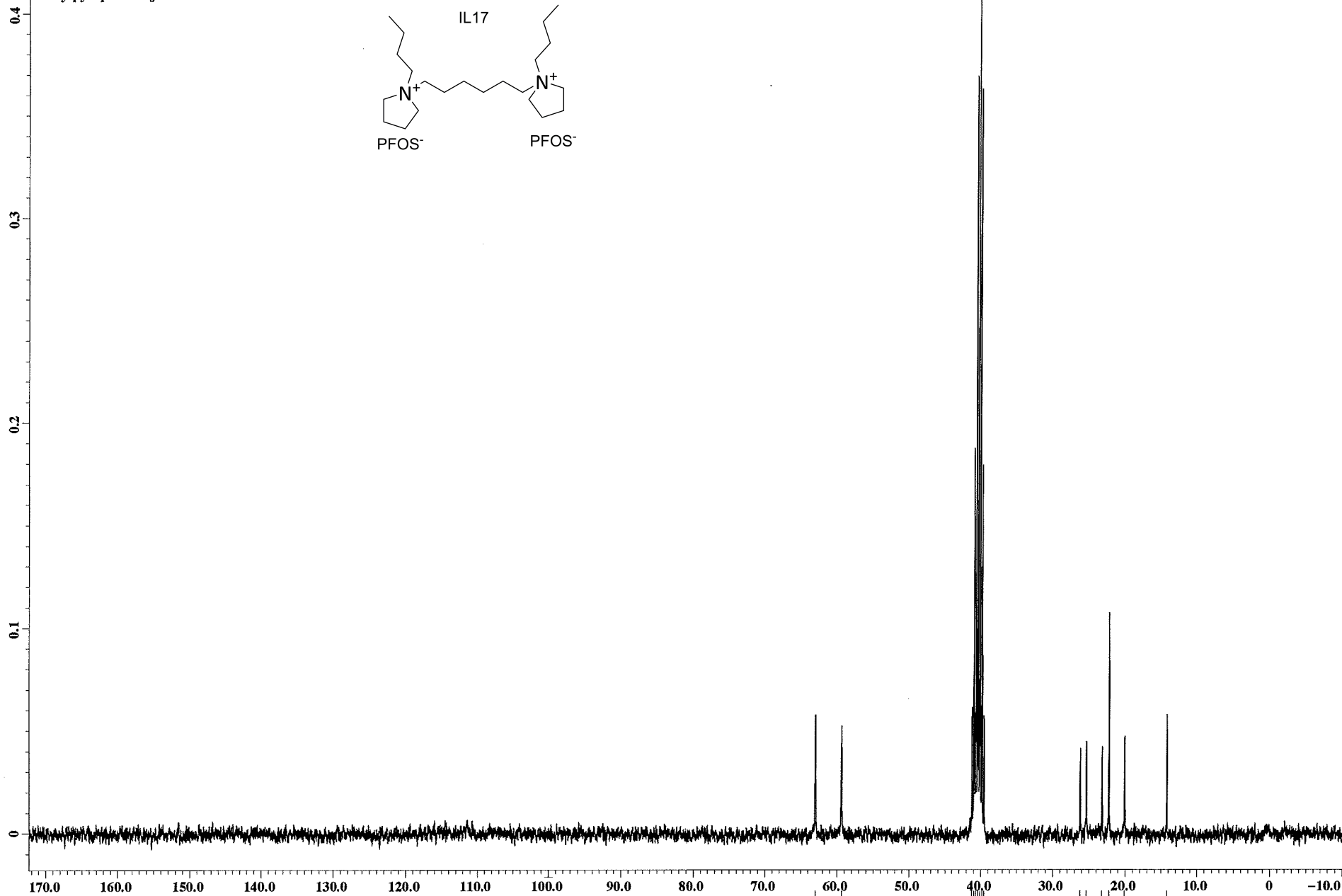
X : parts per Million : 13C



nbutylpyc6pfosc-3.jdf



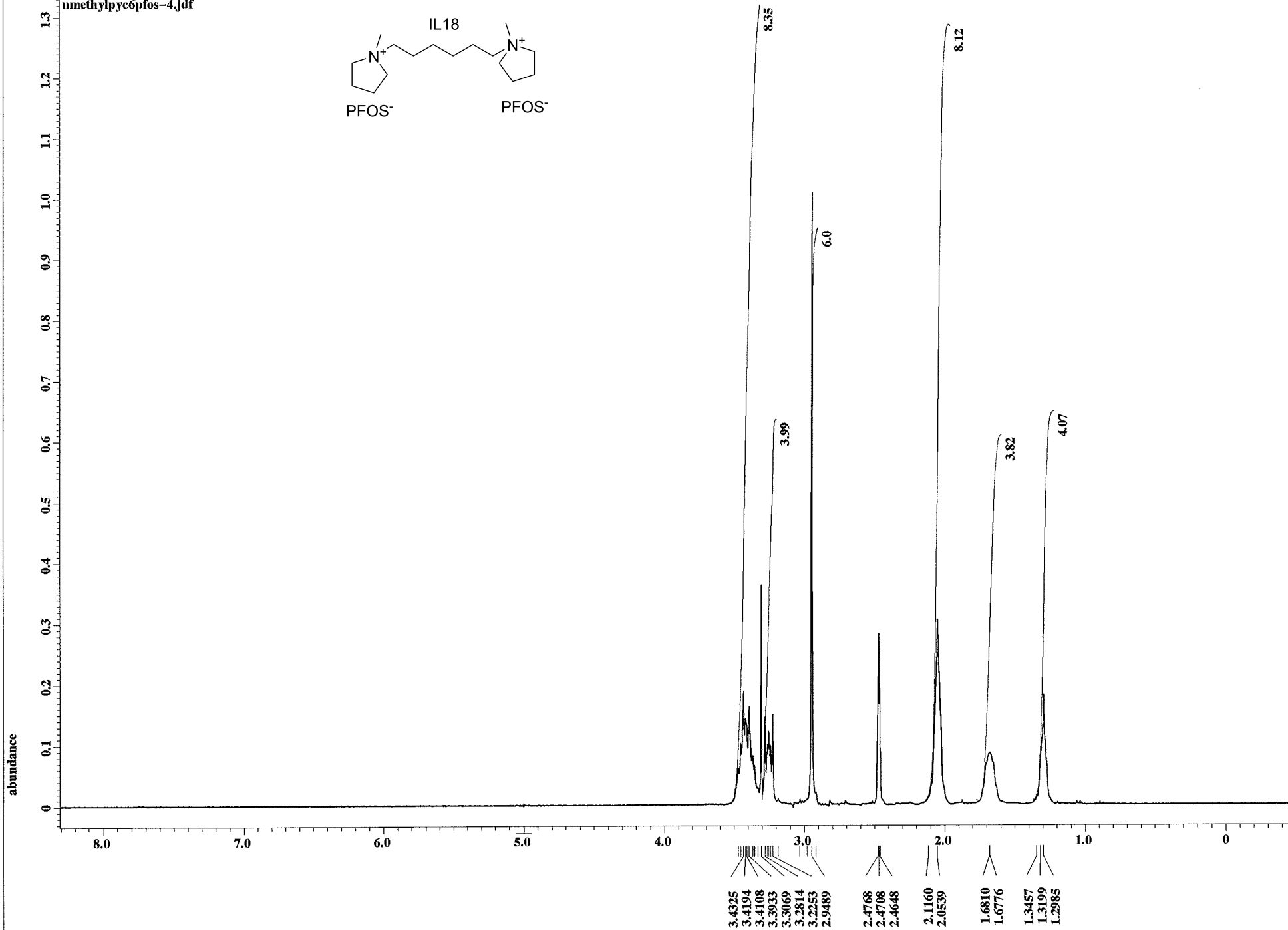
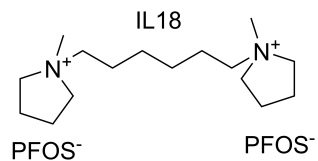
abundance



- 63.0003
- 59.4055
- 40.7049
- 40.4181
- 40.1408
- 26.2110
- 25.3601
- 23.2185
- 22.2529
- 20.0922
- 14.2220

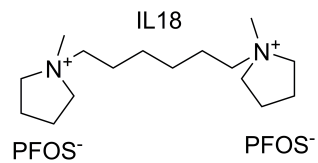
X : parts per Million : 13C

nmethylp6fos-4.jdf



X : parts per Million : 1H

nmethylpypfosc-3.jdf



abundance

0.4

0.3

0.2

0.1

160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

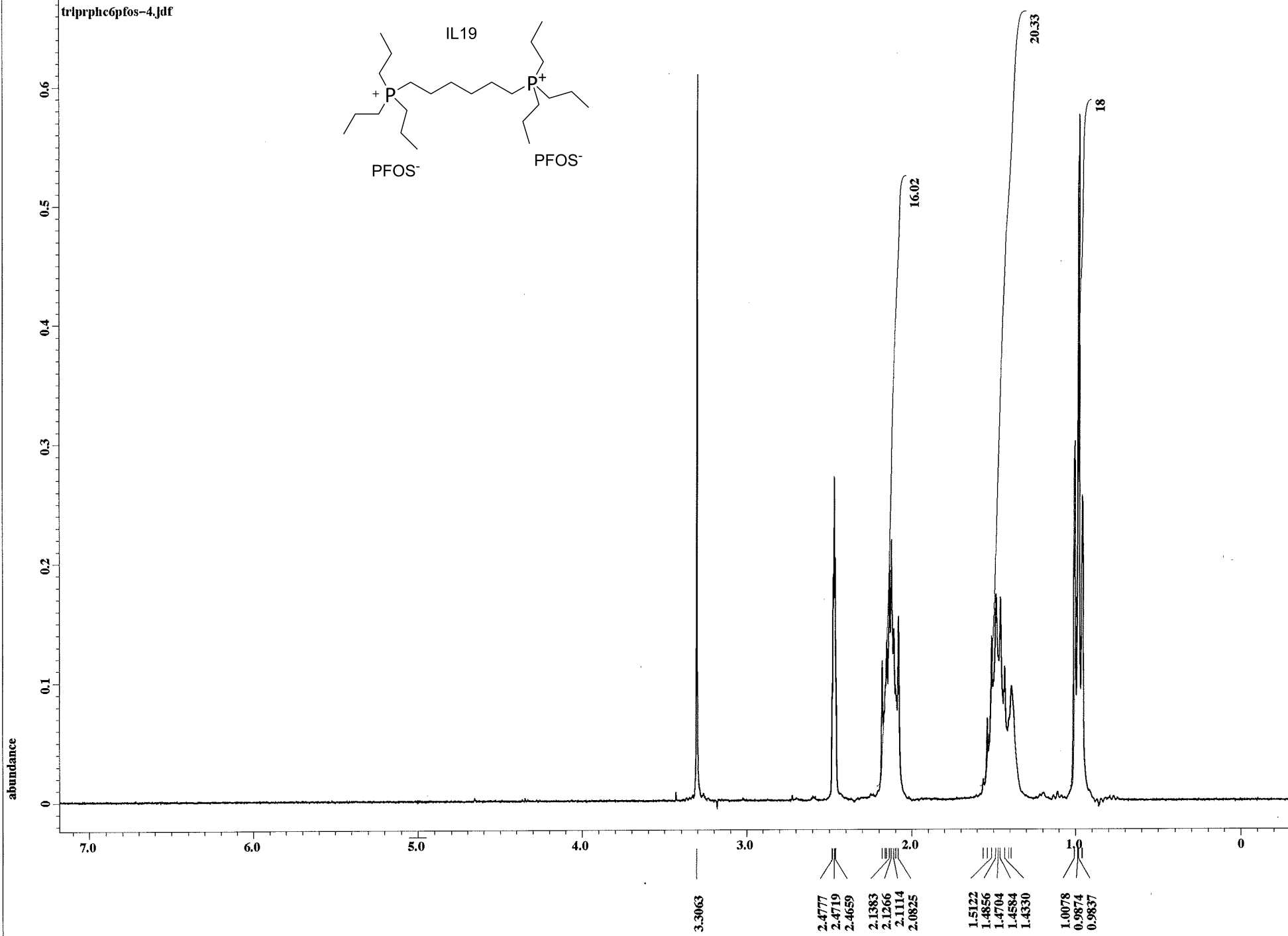
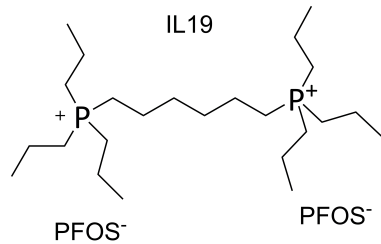
63.9373
63.4019

40.3129
40.0357
39.7584

25.9720
23.2663
21.5836

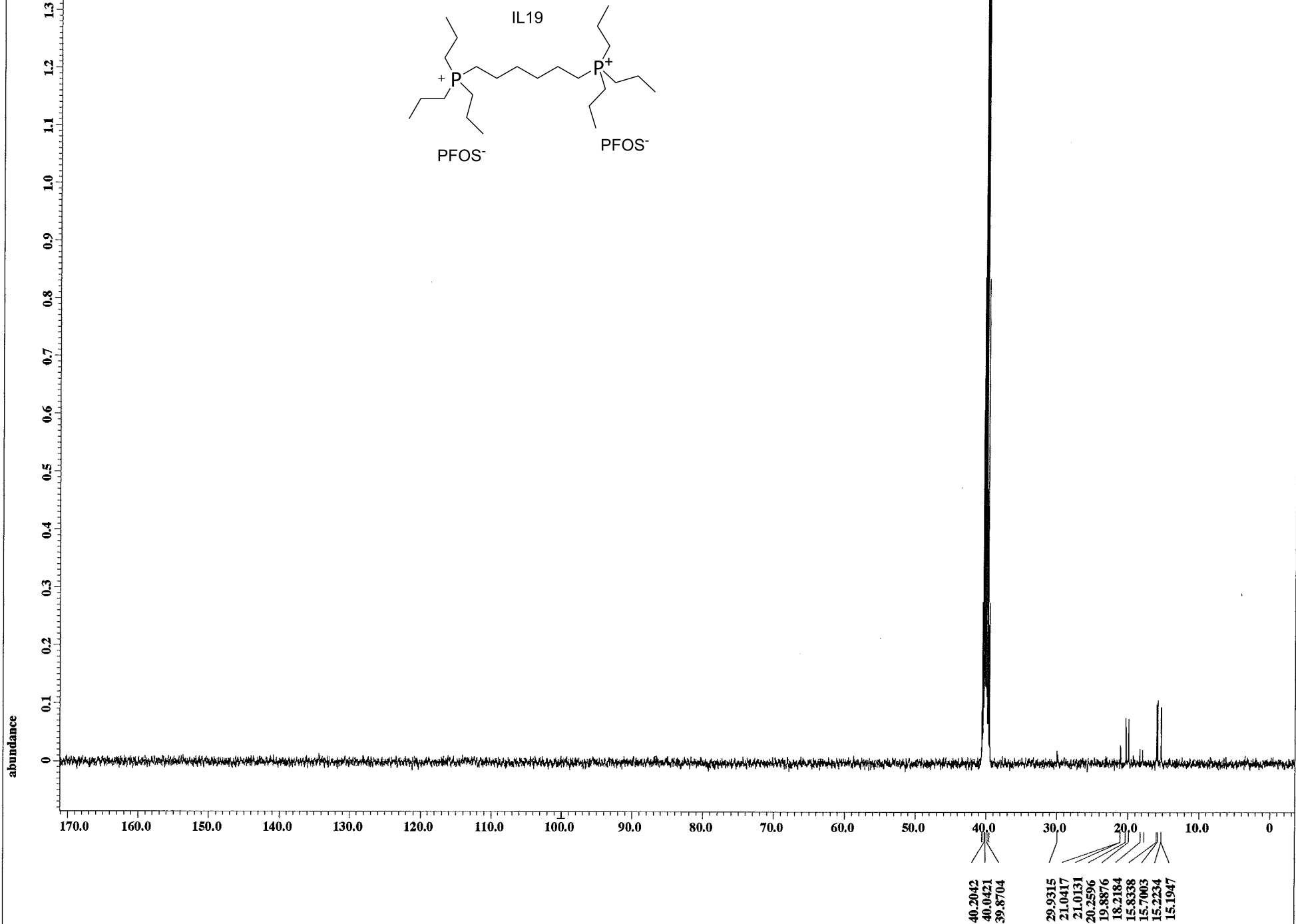
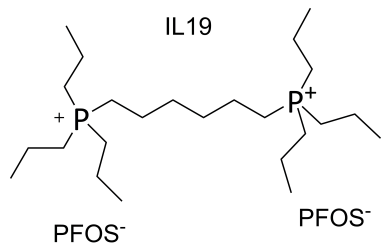
X : parts per Million : 13C

tr1prphc6pfos-4.jdf

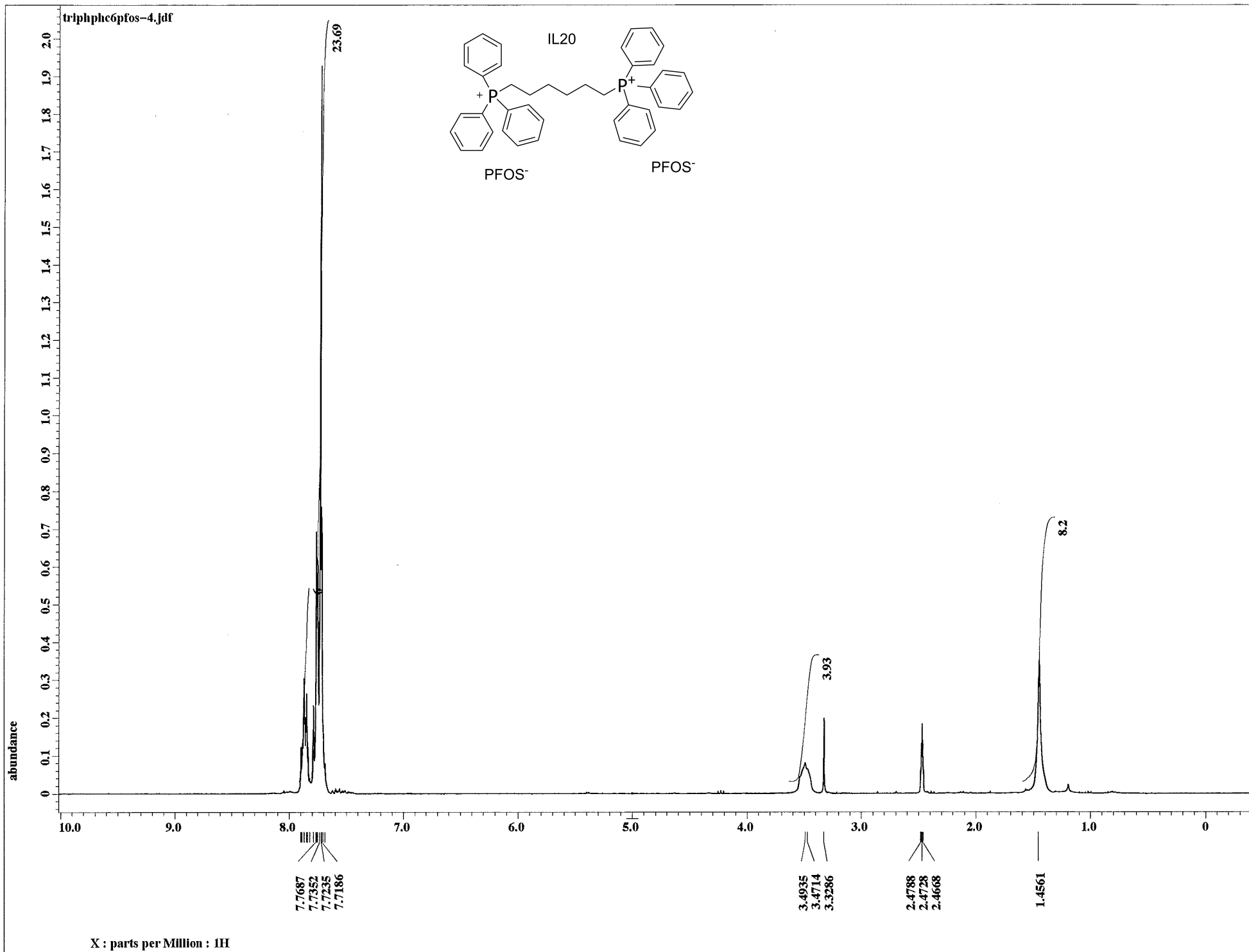


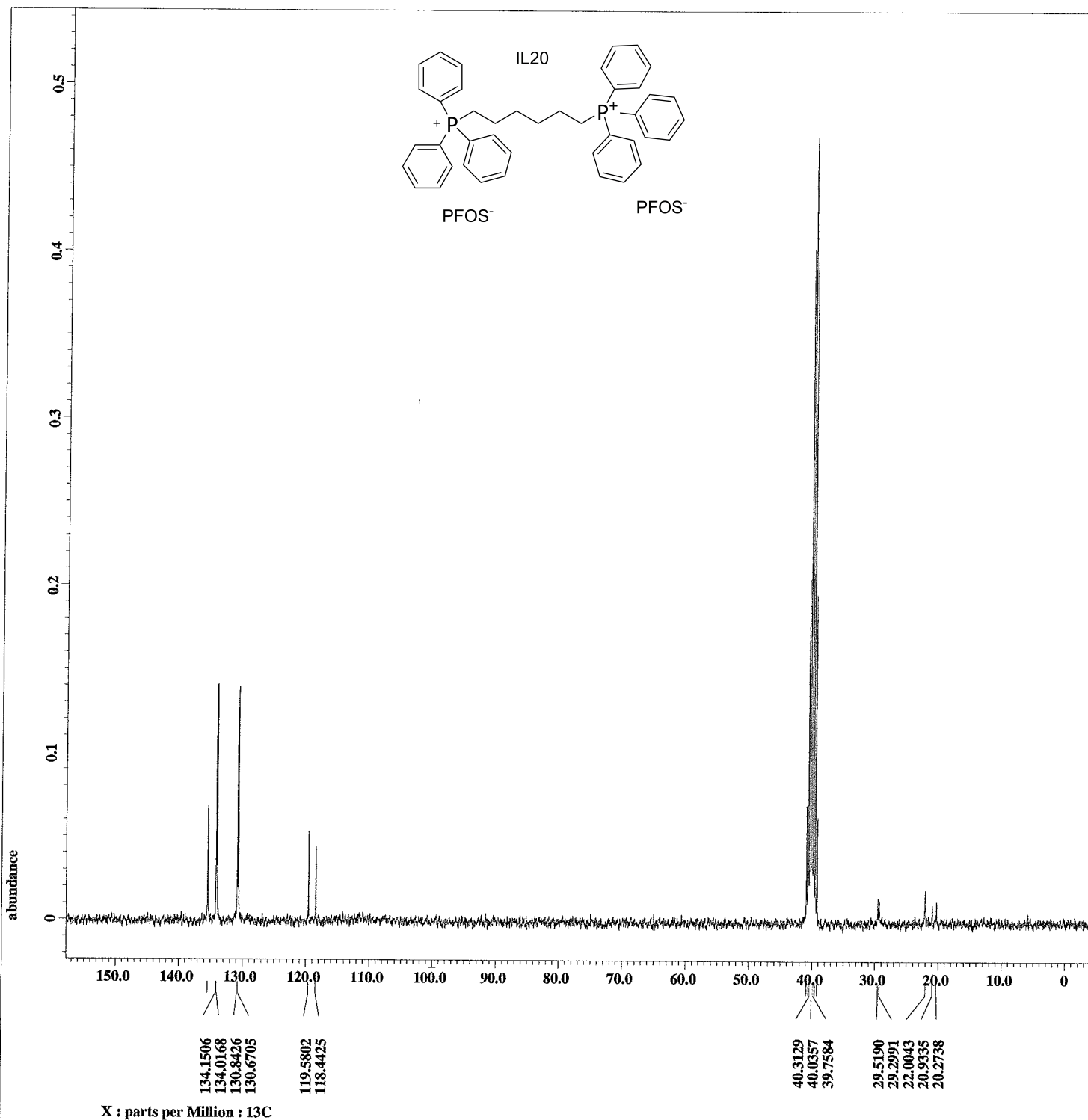
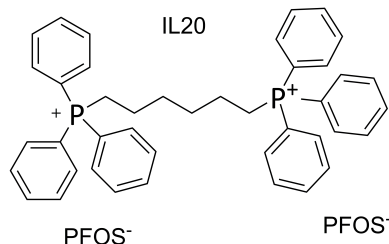
X : parts per Million : 1H

triprphc6pfosc-4.jdf



X : parts per Million : 13C





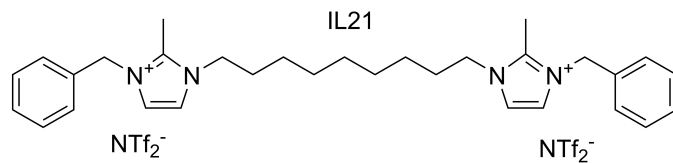
Filename = triphphc6pfosc-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#829699
 Solvent = DMSO-D6
 Creation_time = 21-MAR-2016 20:30:58
 Revision_time = 25-MAR-2016 16:47:34
 Current_time = 25-MAR-2016 16:49:21

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

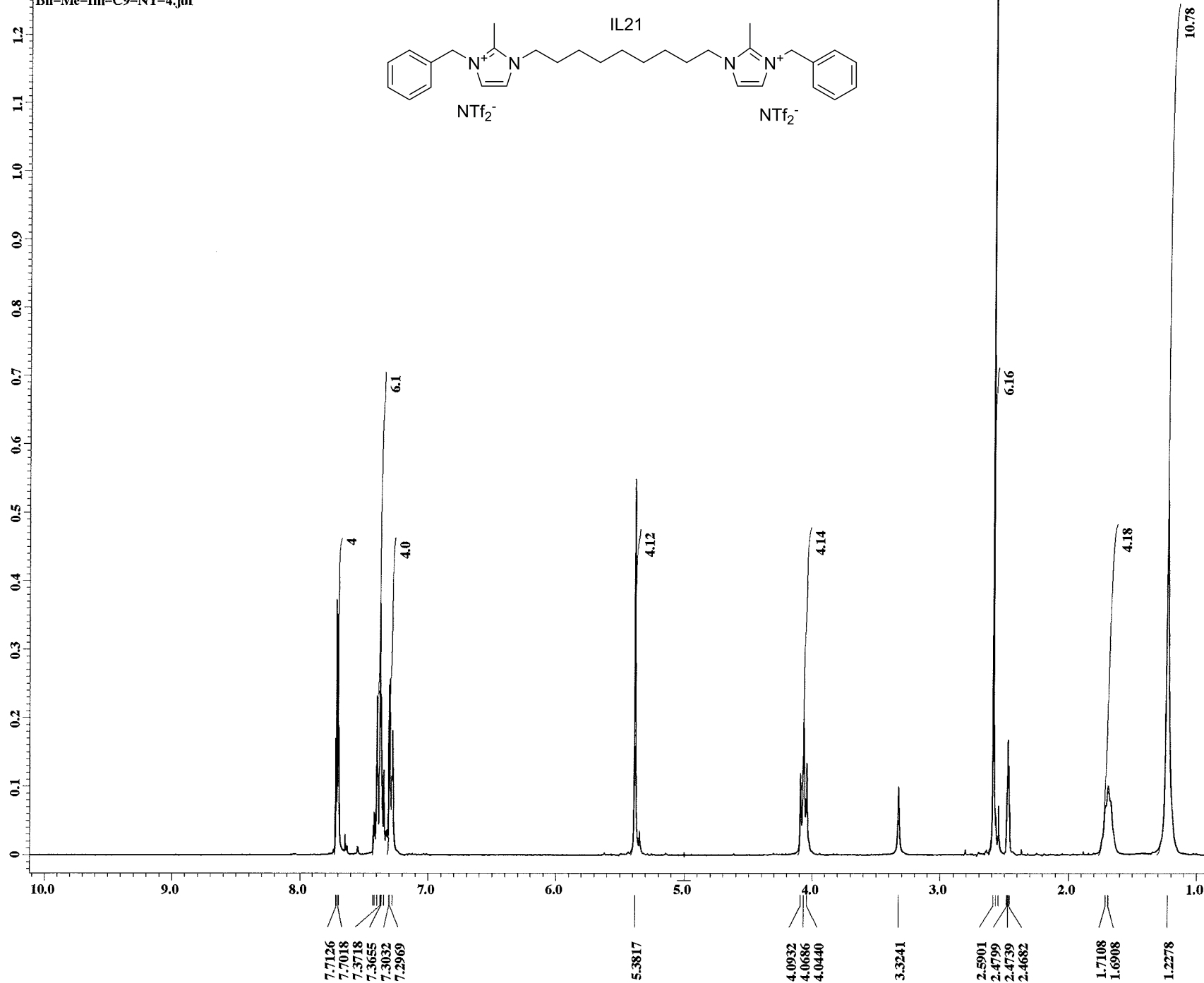
Field_strength = 7.0586013 [T] (300 [MHz])
 X_acq_duration = 1.38412032 [s]
 X_domain = 13C
 X_freq = 75.56823426 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.72248054 [Hz]
 X_sweep = 23.67424242 [kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 310
 Total_scans = 310

X_90_width = 9.75 [us]
 X_acq_time = 1.38412032 [s]
 X_angle = 30 [deg]
 X_atn = 8 [dB]
 X_pulse = 3.25 [us]
 Irr_atn_dec = 25 [dB]
 Irr_atn_noe = 25 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 50
 Relaxation_delay = 2 [s]
 Repetition_time = 3.38412032 [s]
 Temp_get = 21.5 [dC]

Bu-Me-Im-C9-NT-4.jdf



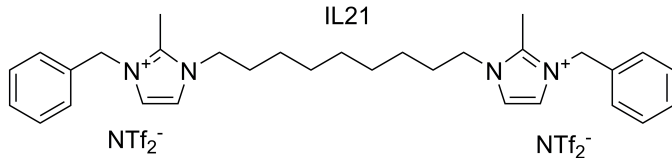
abundance



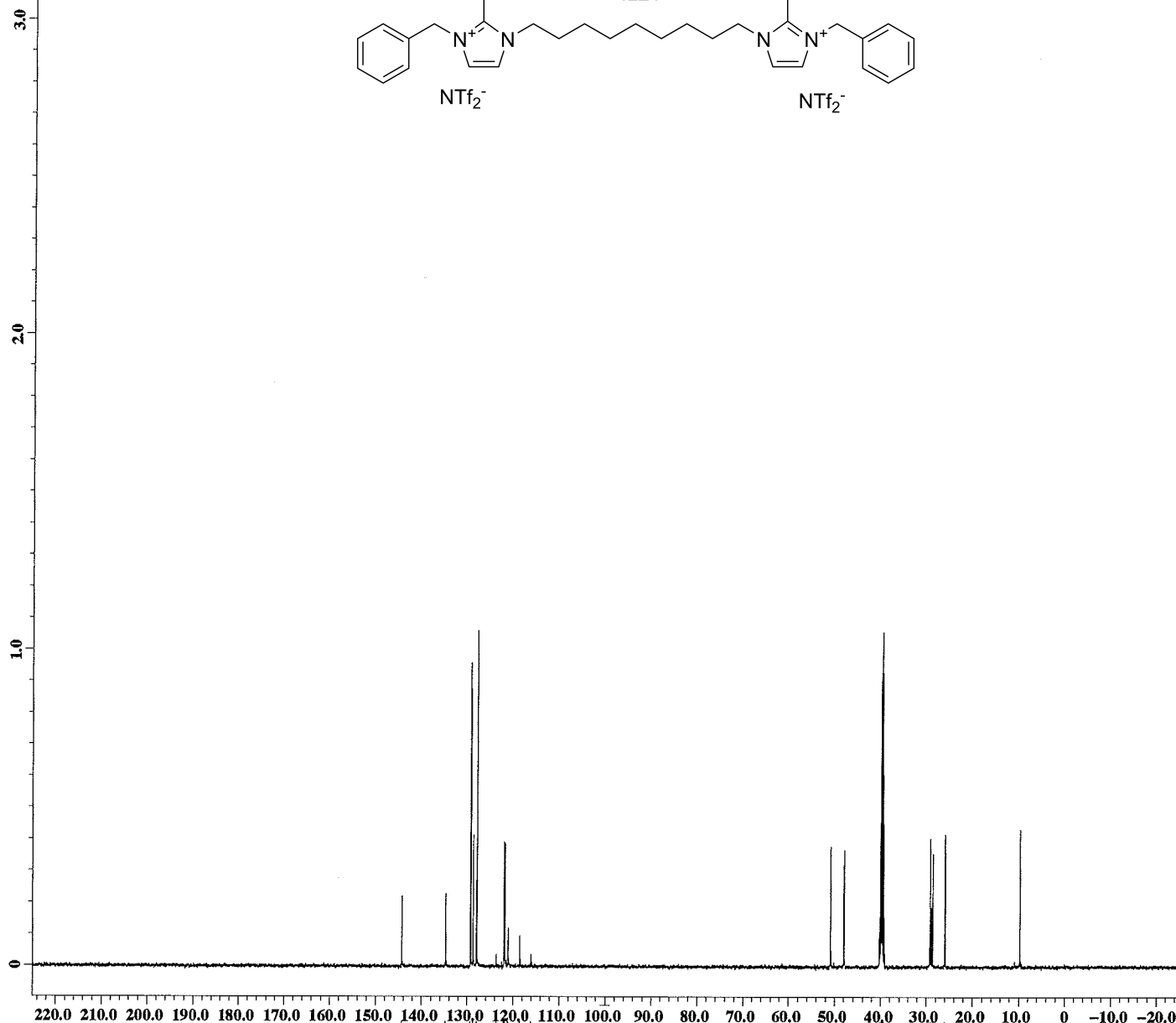
X : parts per Million : 1H

BzMeImzc9Nt-2.jdf

IL21



abundance



144.3246
134.7958
129.2922
128.7771
127.9854
123.6264
121.9858
121.8428
121.0702
118.5139

50.9253
40.1375
39.9658
39.8036
39.6319
39.4698
29.2447
28.6819
25.9158

9.6911

X : parts per Million : 13C

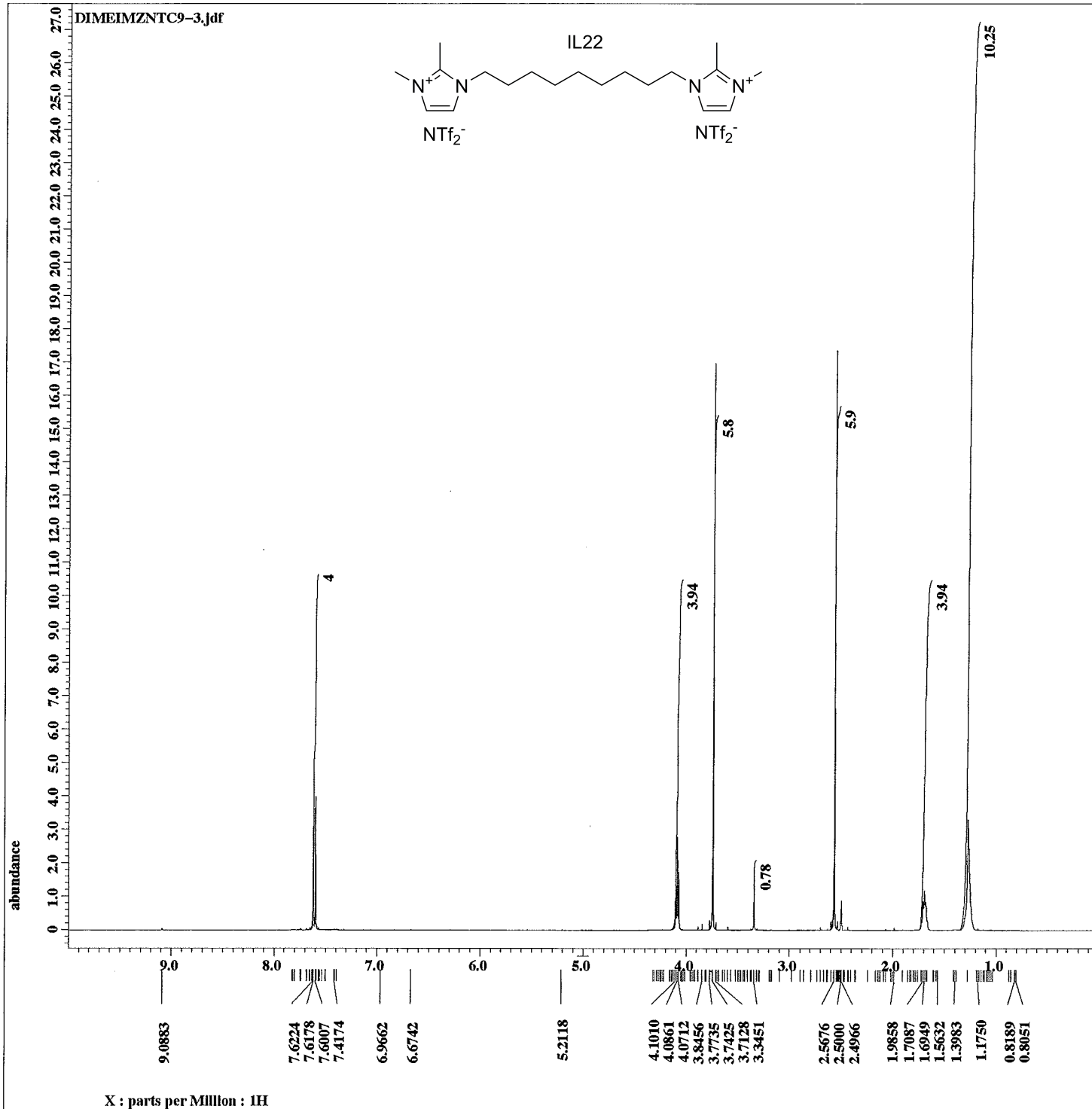
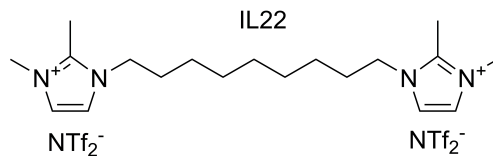
```

Filename      = BzMeImzc9Nt-2.jdf
Author        = delta
Experiment    = single_pulse_dec
Sample_id     = S#469337
Solvent       = DMSO-D6
Creation_time  = 10-OCT-2015 01:54:47
Revision_time = 9-OCT-2015 13:11:16
Current_time  = 9-OCT-2015 13:11:28

Comment       = single pulse decouple
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 440
Total_scans    = 440

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[db]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[db]
Irr_atn_noe   = 20[db]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 0.2[s]
Recvr_gain    = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get      = 22[dc]
    
```



```

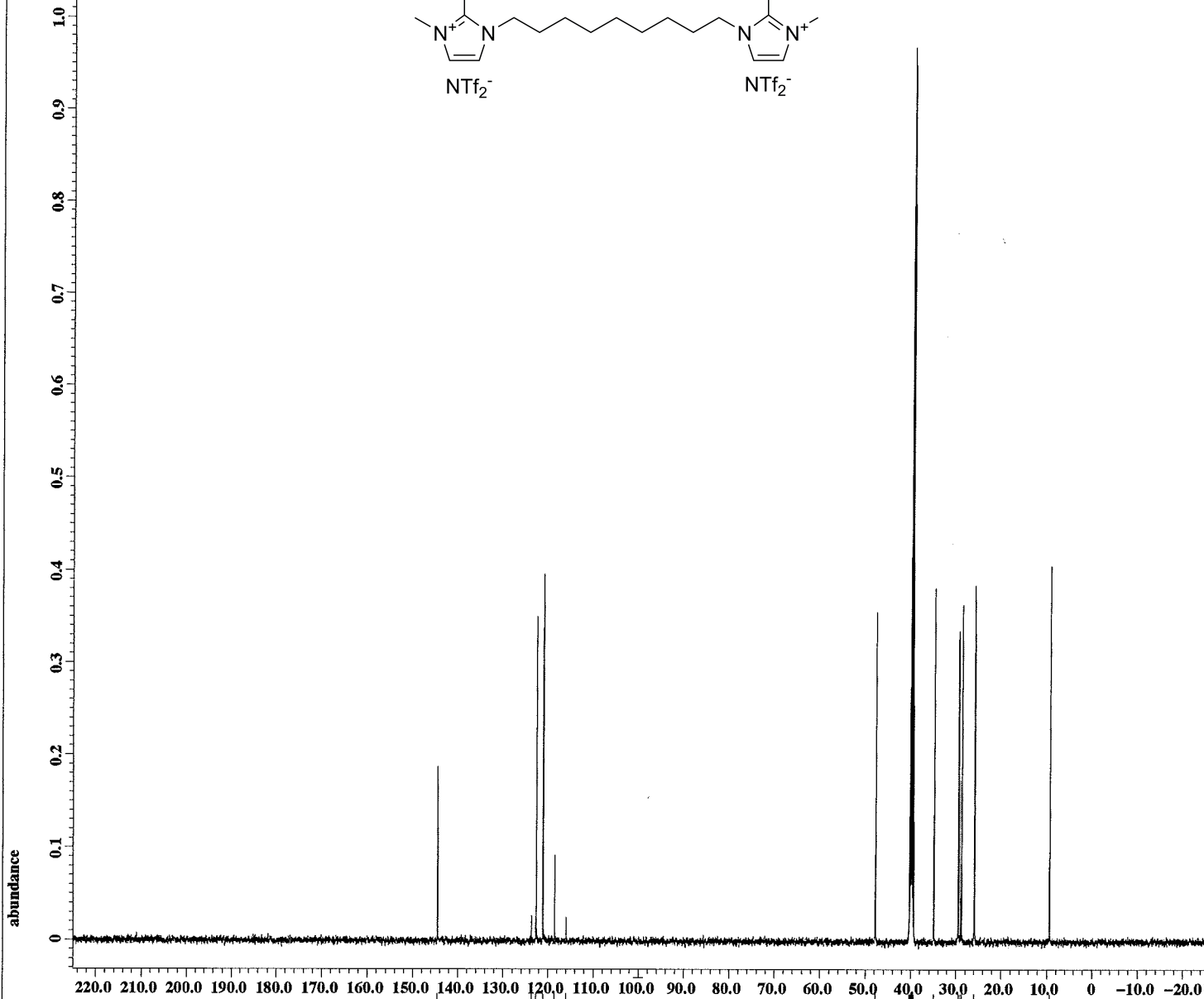
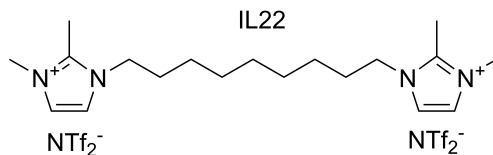
Filename      = DIMEIMZNTC9-3.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#687509
Solvent      = DMSO-D6
Creation_time = 7-OCT-2015 07:53:36
Revision_time = 6-OCT-2015 19:14:21
Current_time  = 6-OCT-2015 19:14:54

Comment      = single_pulse
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH]
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 12
Total_scans    = 12

X_90_width    = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 30
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get      = 21.4[dC]
    
```

DIMEIMZNTC9C-2.jdf



Filename = DIMEIMZNTC9C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#689799
Solvent = DMSO-D6
Creation_time = 7-OCT-2015 08:06:46
Revision_time = 6-OCT-2015 19:22:47
Current_time = 6-OCT-2015 19:23:55

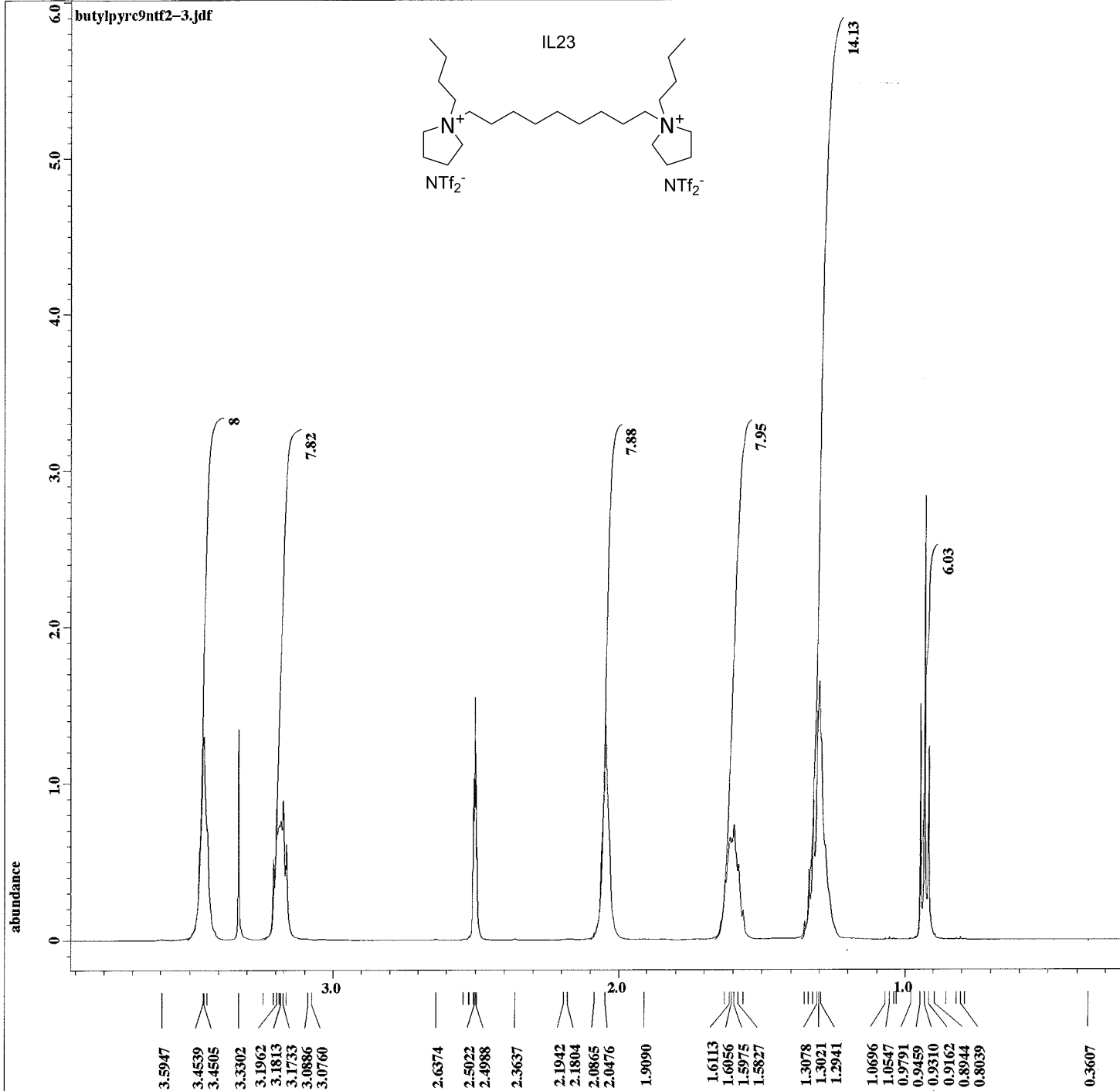
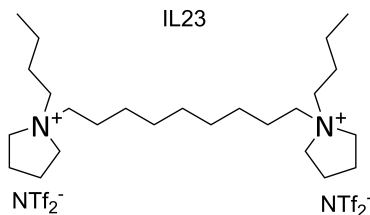
Comment = single pulse decouple
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.3081761[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 10
Scans = 710
Total_scans = 710

X_90_width = 10.73[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 3.57666667[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.2[s]
Recvr_gain = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get = 21.9[degC]

X : parts per Million : 13C

butylpyrc9ntf2-3.jdf



X : parts per Million : 1H

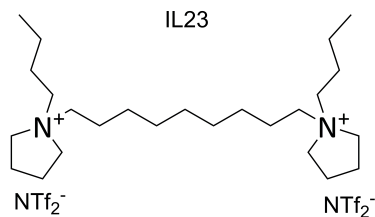
Filename = butylpyrc9ntf2-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#456875
 Solvent = DMSO-D6
 Creation time = 26-NOV-2015 02:15:09
 Revision time = 1-DEC-2015 11:09:09
 Current_time = 1-DEC-2015 11:10:00

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 12
 Total_scans = 12

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 21[dc]

Butylpyrc9NTf2C-3.jdf



abundance

0.3

0.2

0.1

0

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0

121.0892
118.4853

62.3904
58.9661
58.7467

40.3187
40.1565
39.9849
39.8227
39.6510
39.4889
39.3172
22.7777
21.6808
13.7735

0.3817

X : parts per Million : 13C

```

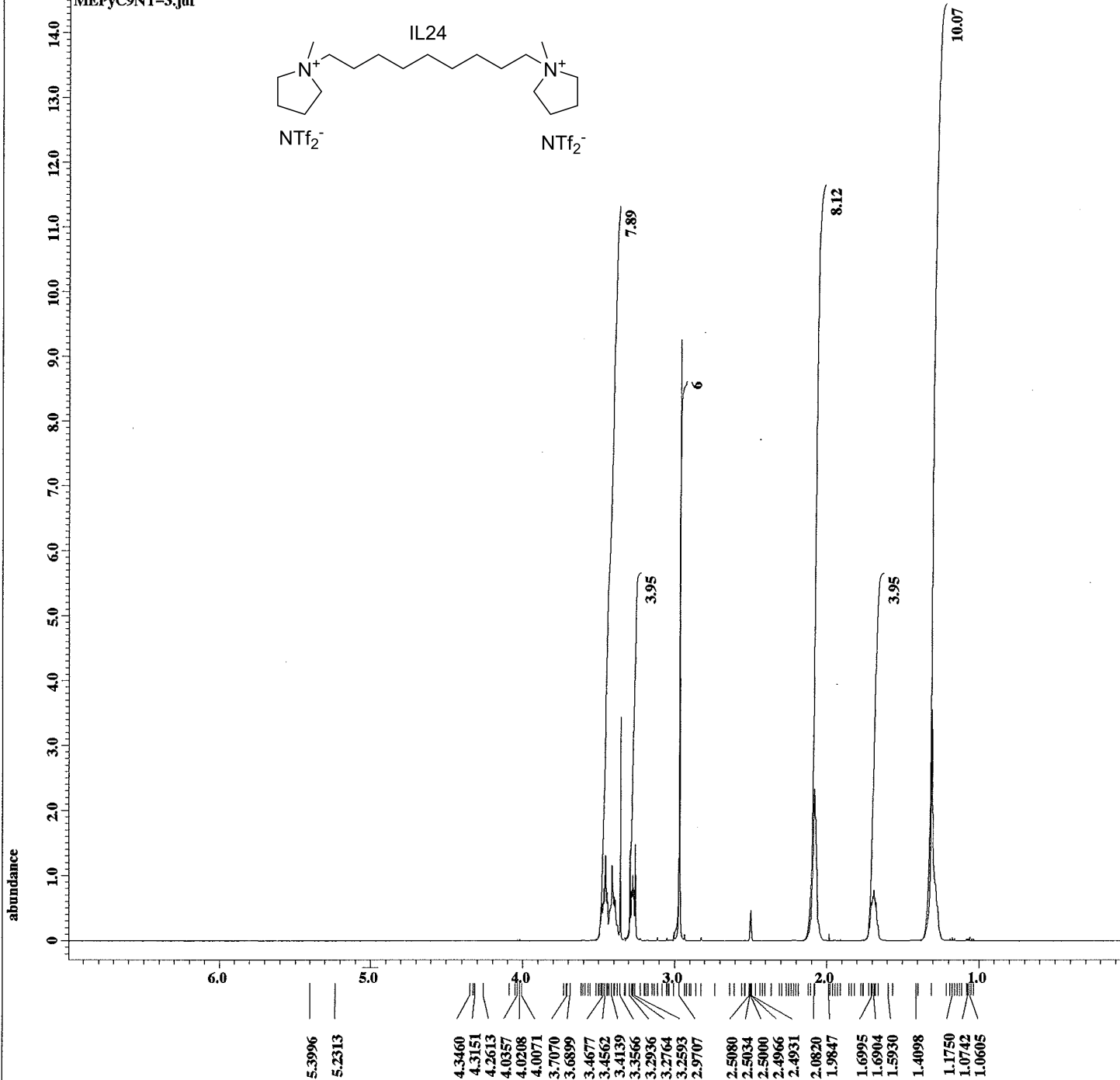
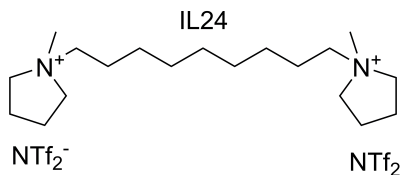
Filename      = Butylpyrc9NTf2C-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#459713
Solvent      = DMSO-D6
Creation time = 26-NOV-2015 02:31:35
Revision time = 1-DEC-2015 11:37:50
Current_time = 1-DEC-2015 11:38:13

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 870.0
Total_scans    = 870.0

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[dB]
Irr_atn_noe   = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 0.2[s]
Recvr_gain    = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get      = 21.5[dC]
    
```

MEPyC9NT-3.jdf



X : parts per Million : 1H

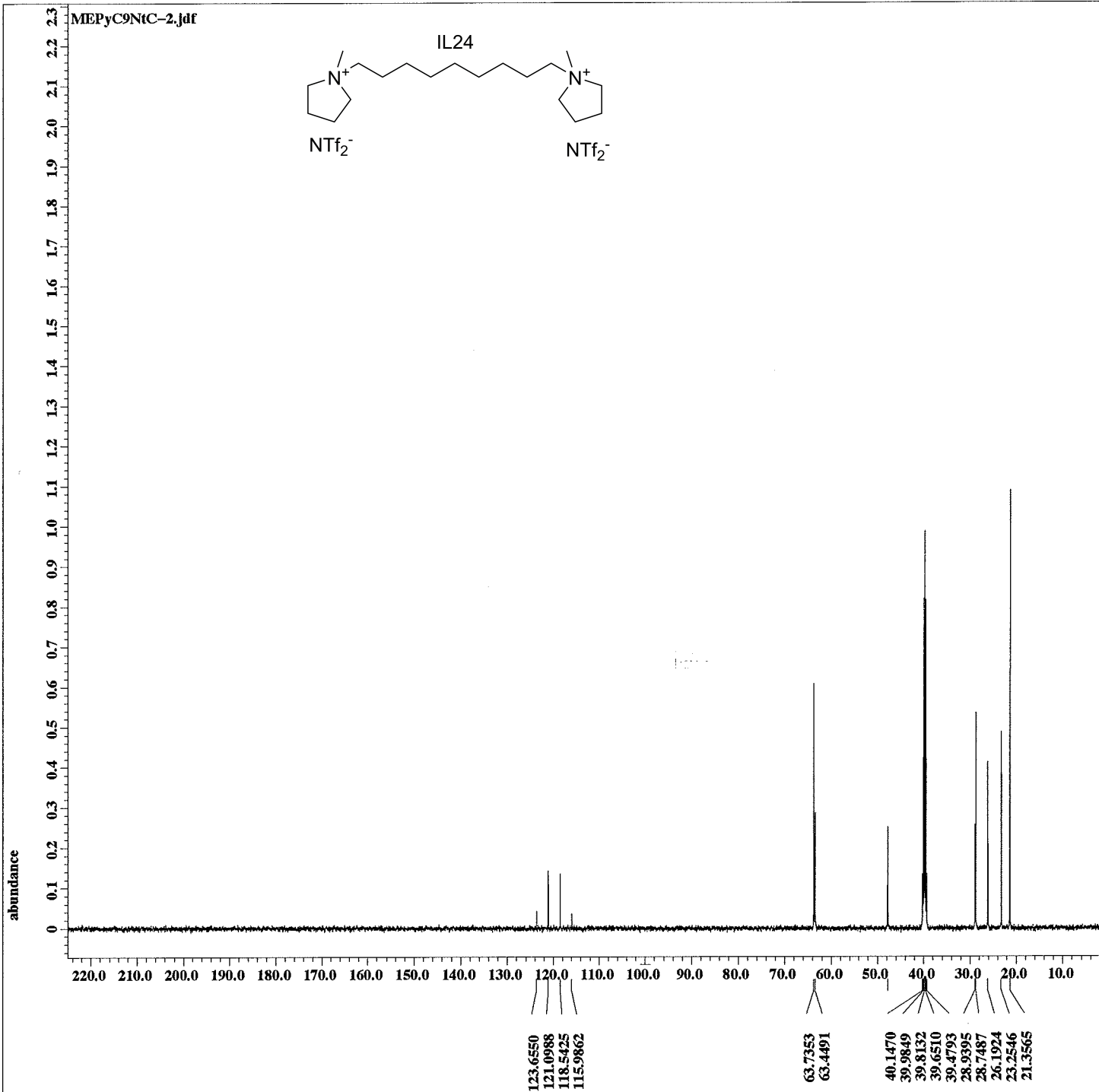
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sexp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: MEPyC9NT-1.jdf

Filename = MEPyC9NT-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#717231
 Solvent = DMSO-D6
 Creation_time = 8-OCT-2015 08:43:58
 Revision_time = 7-OCT-2015 20:03:55
 Current_time = 7-OCT-2015 20:04:48

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 14
 Total_scans = 14

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 26
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 21.4[dC]



```

Filename      = MEPyC9NtC-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#720379
Solvent      = DMSO-D6
Creation time = 8-OCT-2015 08:51:03
Revision time = 7-OCT-2015 20:09:04
Current_time = 7-OCT-2015 20:09:35

Comment      = single_pulse_decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

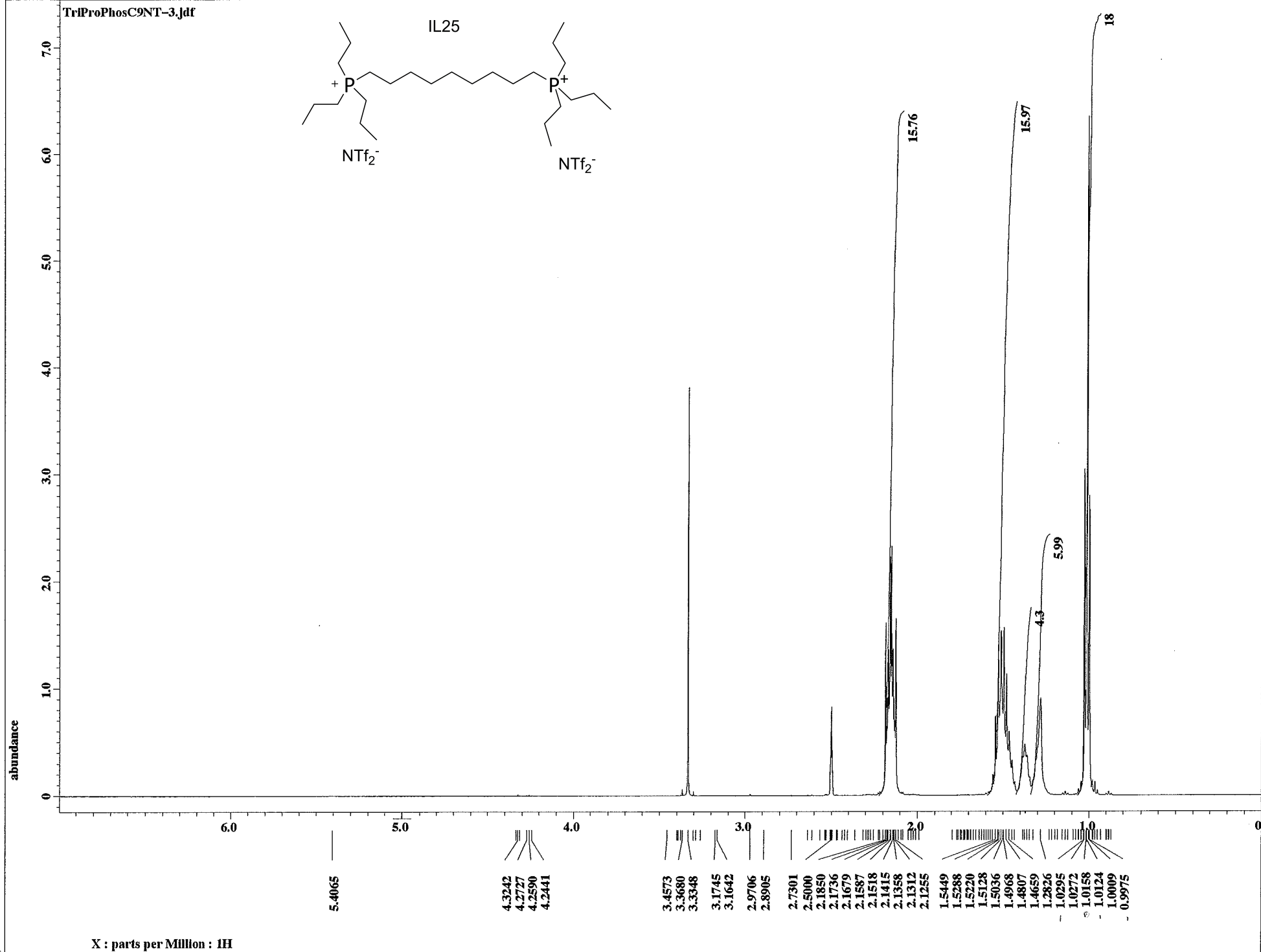
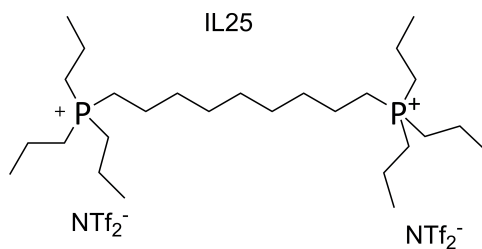
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset      = 100[ppm]
X_points       = 32768
X_prescans    = 4
X_resolution  = 1.19959034[Hz]
X_sweep       = 39.3081761[kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521[MHz]
Irr_offset    = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 320
Total_scans   = 320

X_90_width   = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec  = 20[dB]
Irr_atn_noe  = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 0.2[s]
Recvr_gain    = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get      = 21.9[dC]

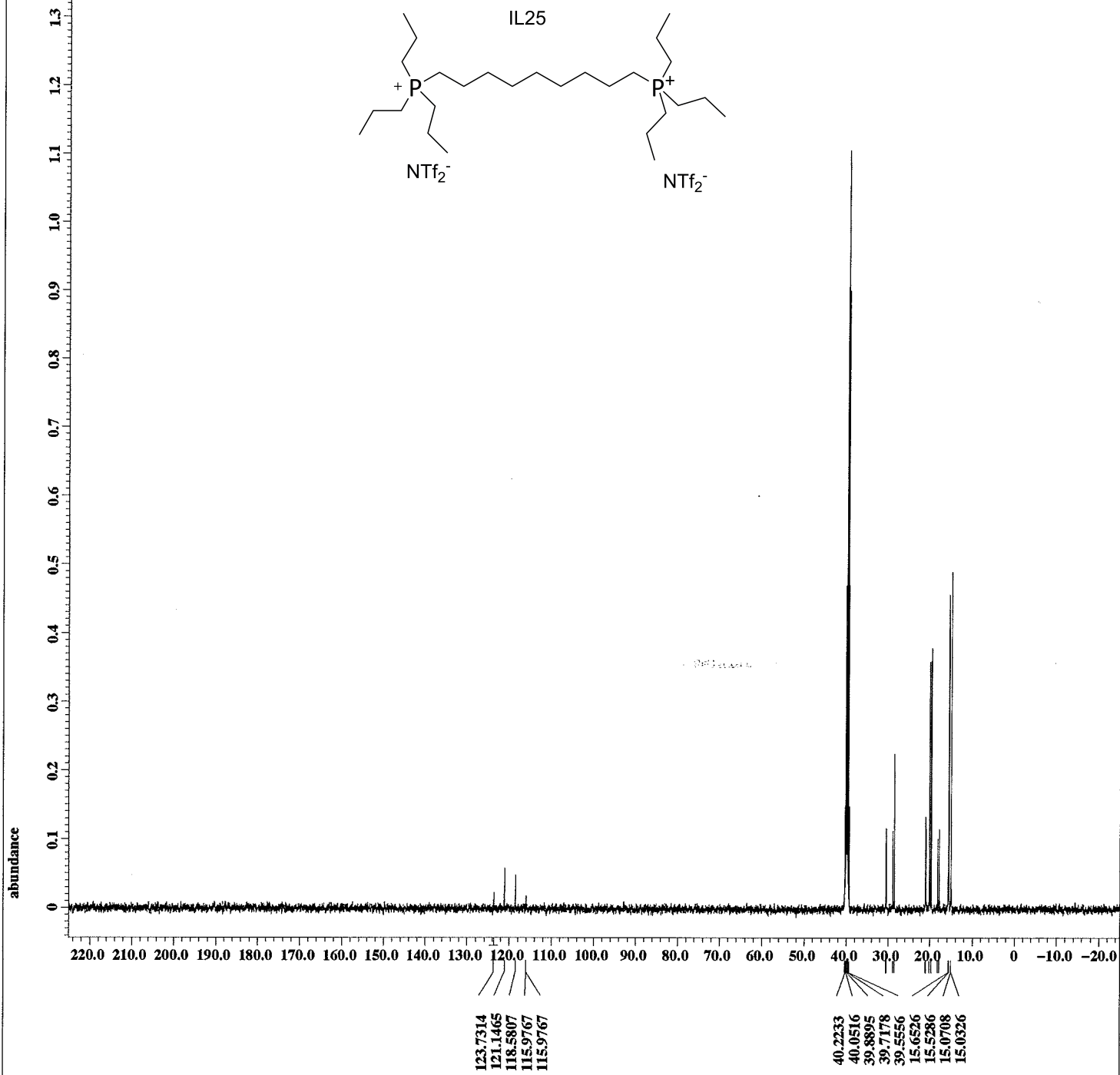
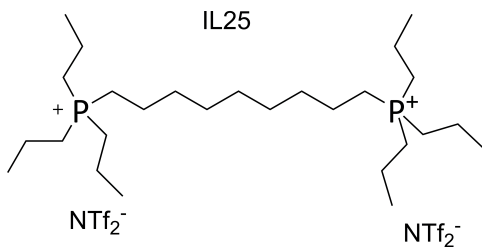
```

X: parts per Million : 13C

TriProPhosC9NT-3.jdf



TriPROPHOSC9NTC-4.jdf



X : parts per Million : 13C

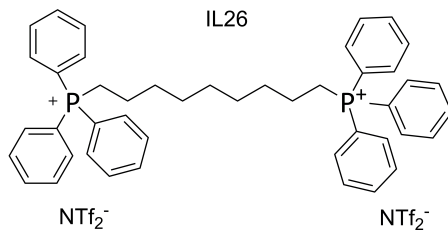
Filename = TriPROPHOSC9NTC-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#735356
 Solvent = DMSO-D6
 Creation_time = 8-OCT-2015 09:16:11
 Revision_time = 7-OCT-2015 20:35:52
 Current_time = 7-OCT-2015 20:36:05

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 330
 Total_scans = 330

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 0.2[s]
 Recvr_gain = 50
 Relaxation_delay = 0.2[s]
 Repetition_time = 1.03361792[s]
 Temp_get = 21.9[dc]

TRIPHEPHOSC9NT-3.jdf



abundance

5.0
4.0
3.0
2.0
1.0
0

12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0

7.8068
7.8034
7.7828
7.7782
7.7621

4.3266
4.2567
3.5375
3.5341
3.3497
2.9833
2.5034
2.5000
2.1393
1.4980
1.4315
1.4167
1.2288
1.2151

3.95
8.17
6.2

30

Filename = TRIPHEPHOSC9NT-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#707219
 Solvent = DMSO-D6
 Creation_time = 7-OCT-2015 08:27:15
 Revision_time = 6-OCT-2015 19:50:05
 Current_time = 6-OCT-2015 19:52:06

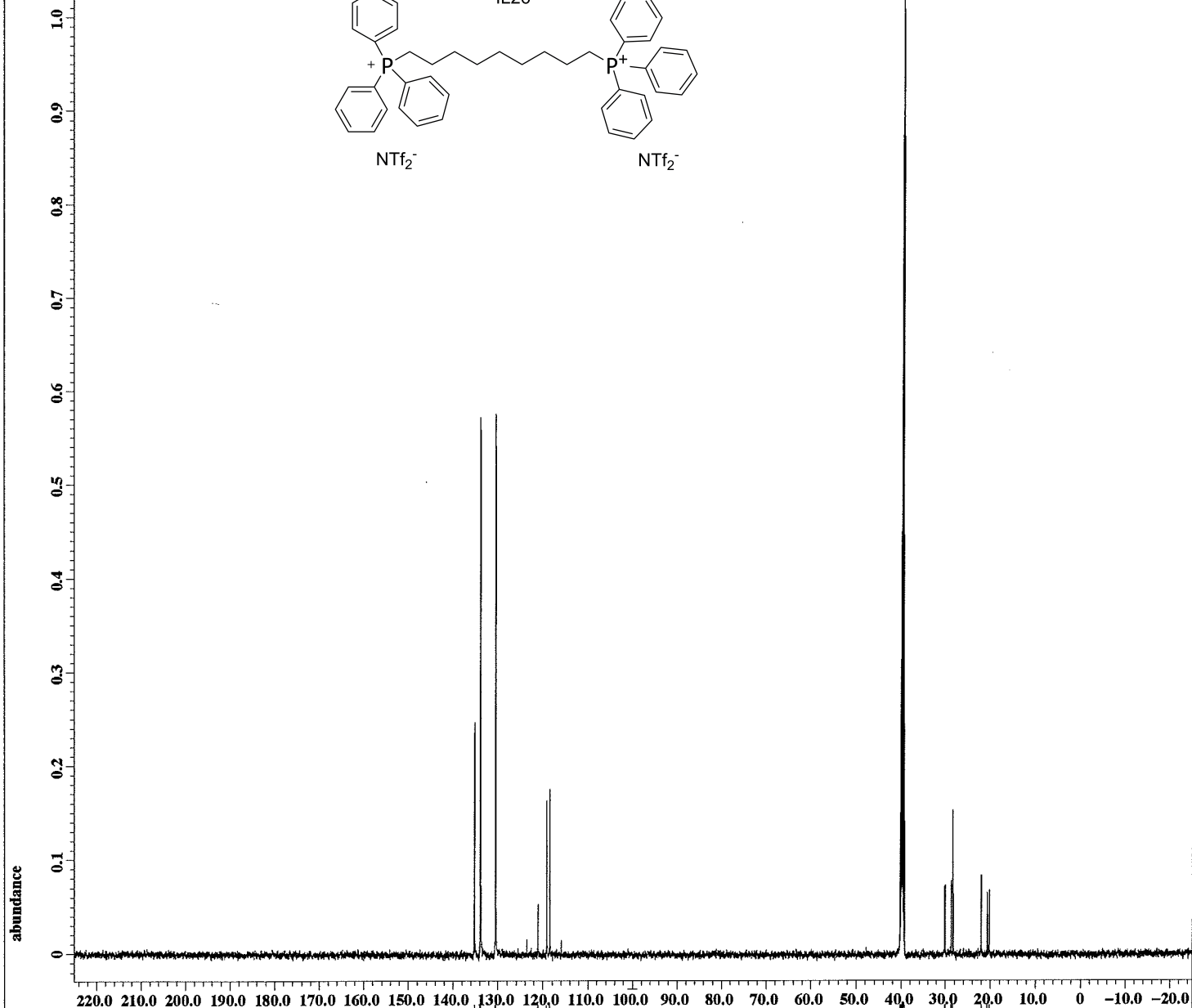
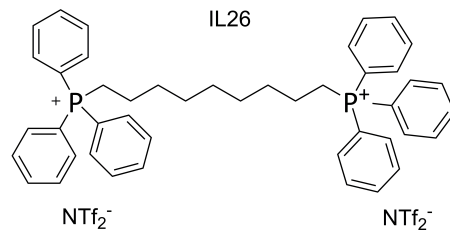
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 14
 Total_scans = 14

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 32
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 21.4[degC]

X : parts per Million : 1H

TRIPHEPHOSC9NTC-2.jdf



135.1964
133.9374
133.8611
130.5990
130.5036
119.2293
118.5520

40.3568
40.1852
40.0230
39.8513
39.6892
39.5175
39.3553
28.3672

X : parts per Million : 13C

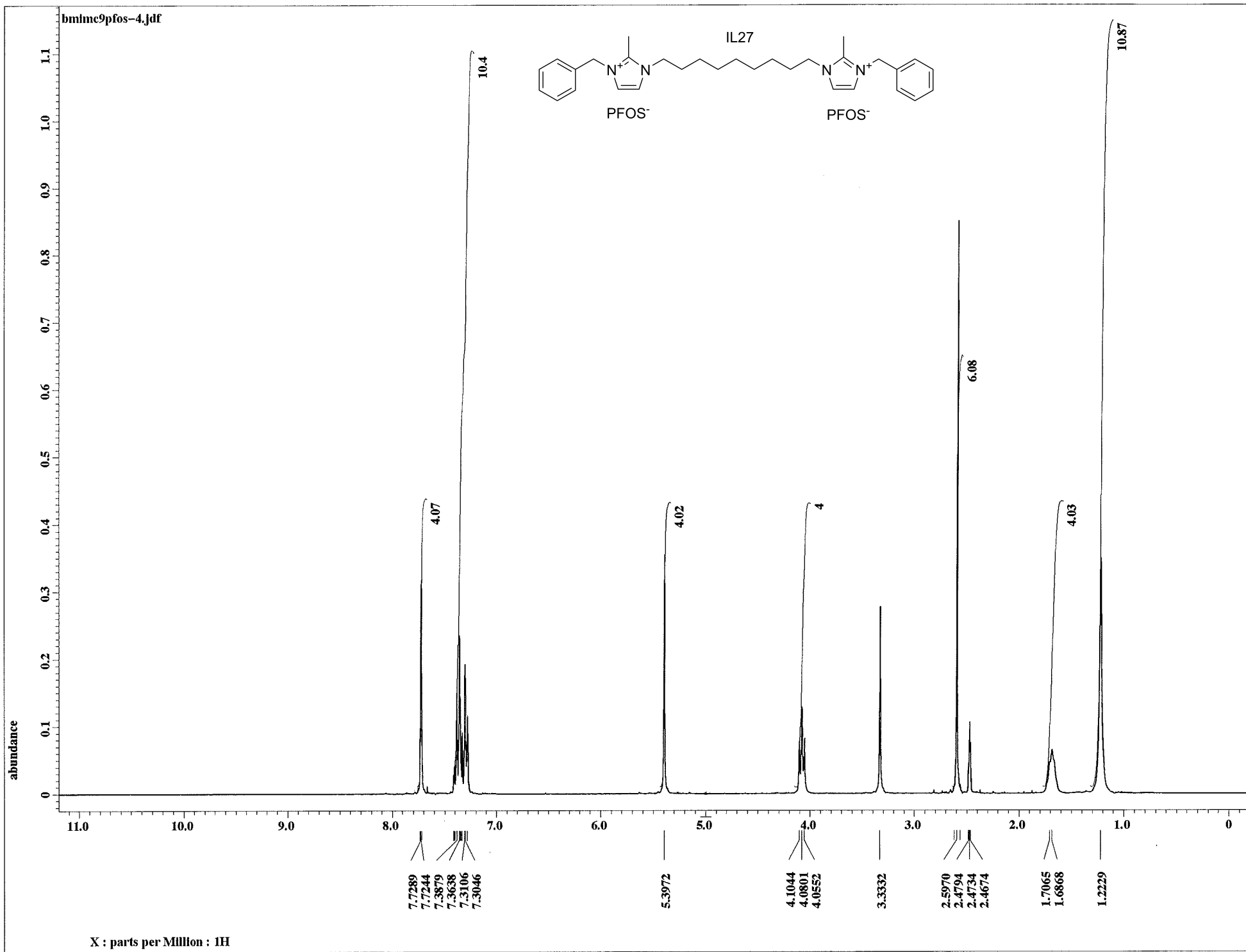
```

Filename      = TRIPHEPHOSC9NTC-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = s#709980
Solvent      = DMSO-D6
Creation_time = 7-OCT-2015 08:41:05
Revision_time = 6-OCT-2015 19:57:57
Current_time  = 6-OCT-2015 19:58:03

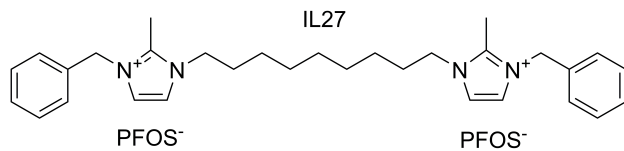
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 750
Total_scans    = 750

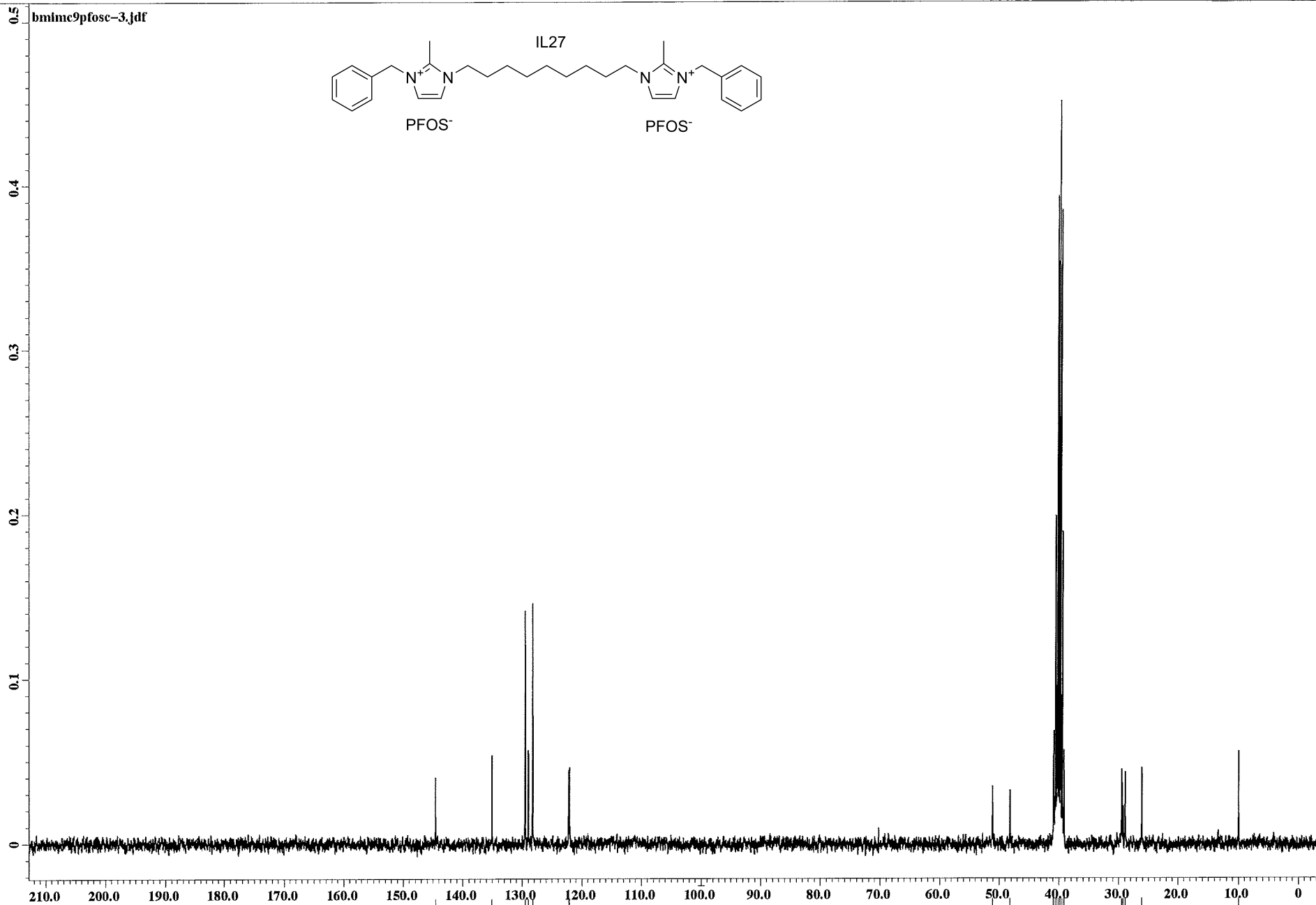
X_90_width     = 10.73[us]
X_acq_time     = 0.83361792[s]
X_angle        = 30[deg]
X_atn          = 9[dB]
X_pulse        = 3.57666667[us]
Irr_atn_dec    = 20[dB]
Irr_atn_noe    = 20[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 0.2[s]
Recvr_gain     = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get       = 21.9[dC]
    
```



bmimc9pfosc-3.jdf



abundance



144.5908

135.0971

129.5137

128.9879

128.2612

122.2285

122.1042

51.1260

48.1909

40.8675

40.5902

40.3129

40.0357

39.7584

39.4812

39.1943

29.5094

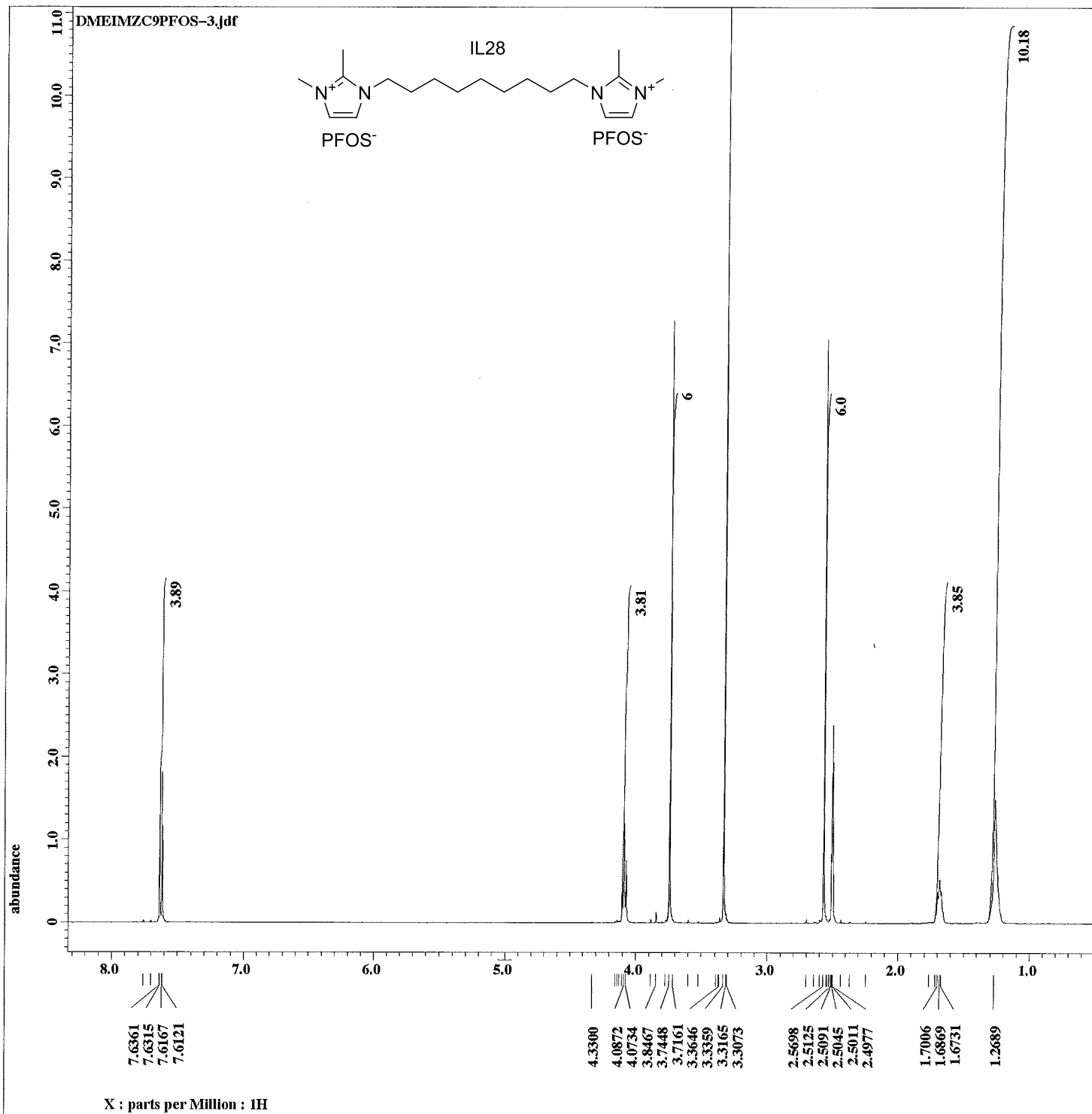
29.2704

28.9262

26.1441

9.9962

X : parts per Million : 13C



```

Filename      = DMEIMZC9PFOS-3.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#411651
Solvent      = DMSO-D6
Creation_time = 1-DEC-2015 00:59:12
Revision_time = 1-DEC-2015 11:21:04
Current_time  = 1-DEC-2015 11:22:13

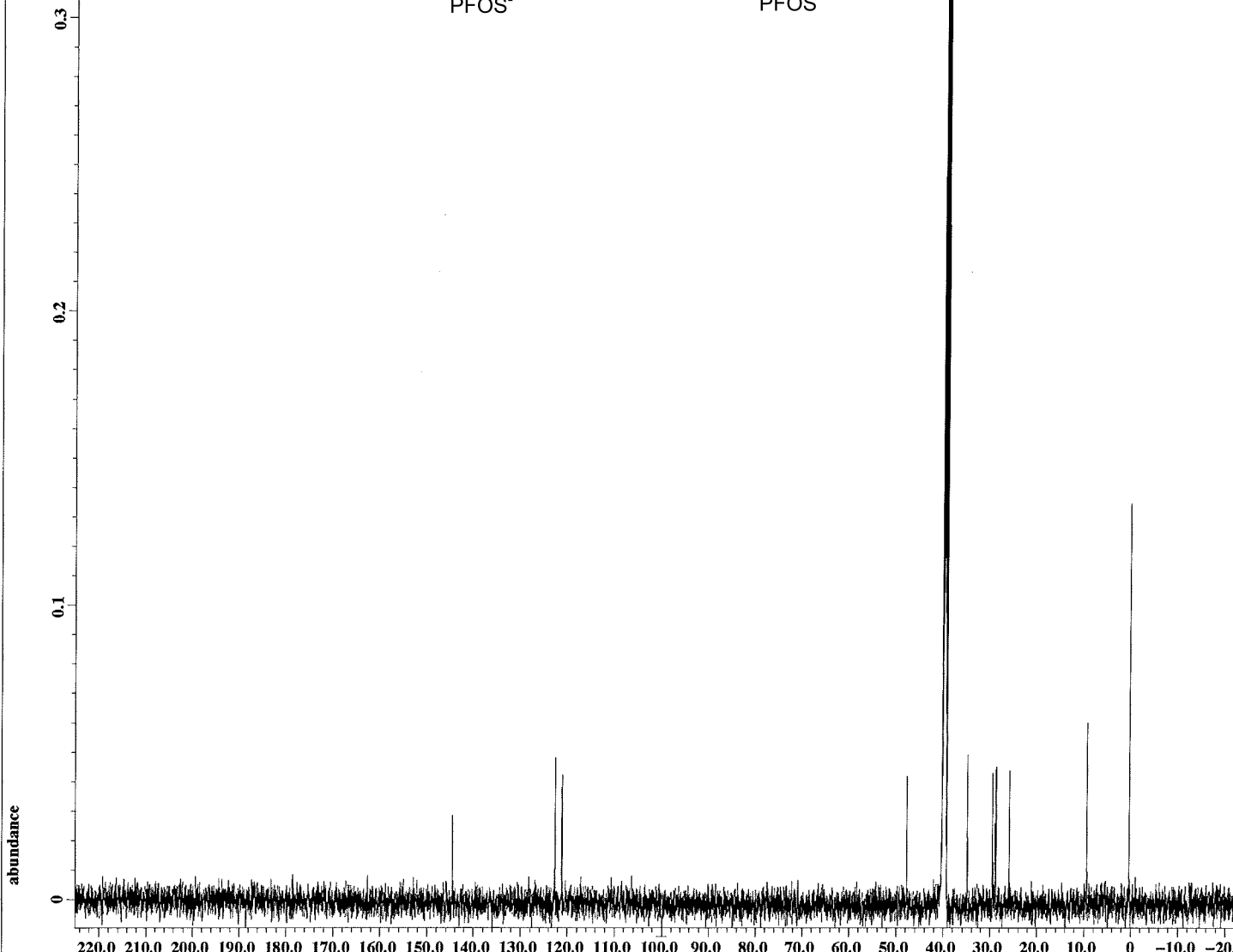
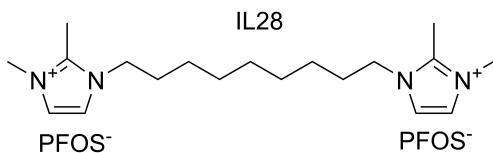
Comment      = single_pulse
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.27[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 40
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get       = 21.1[dc]

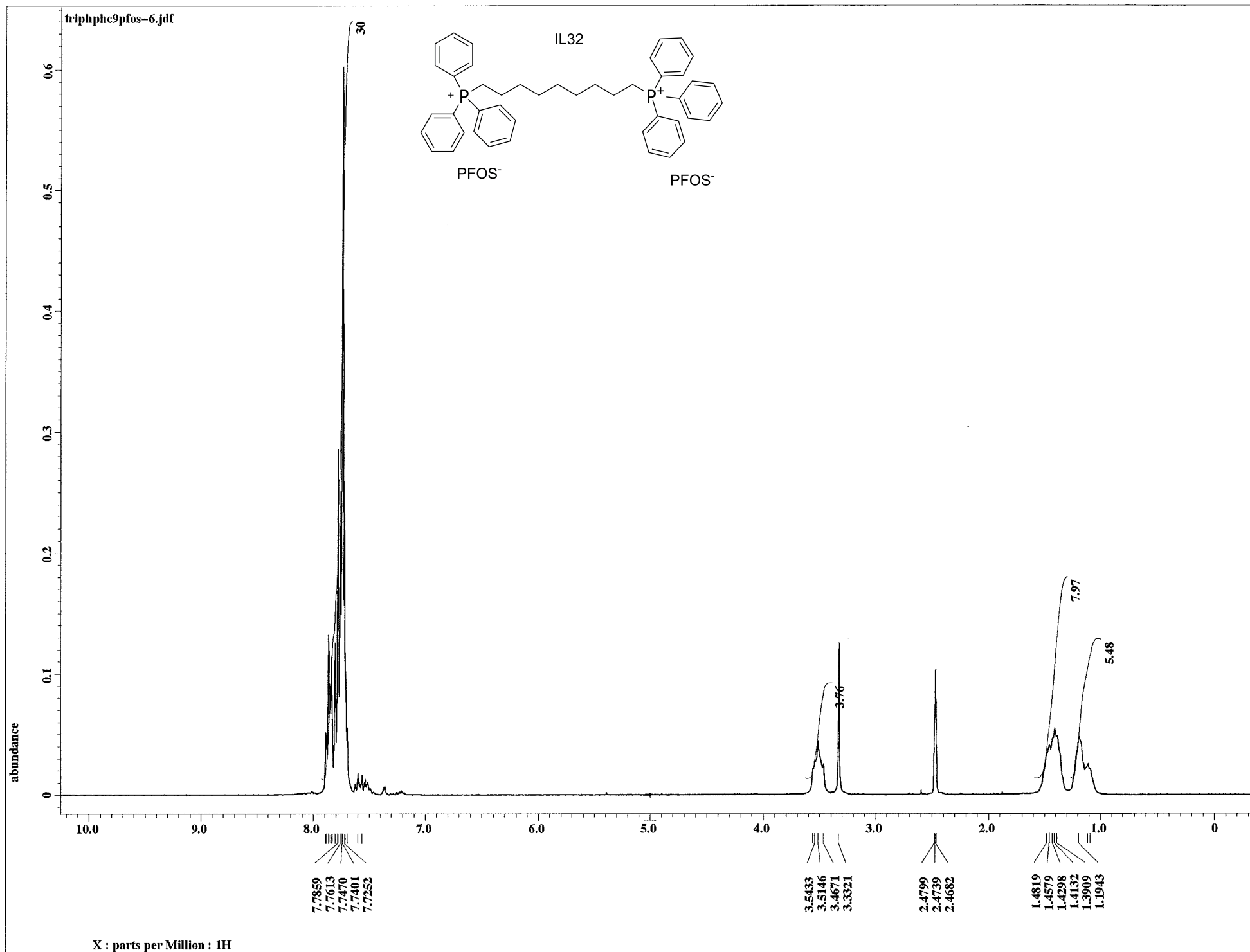
```

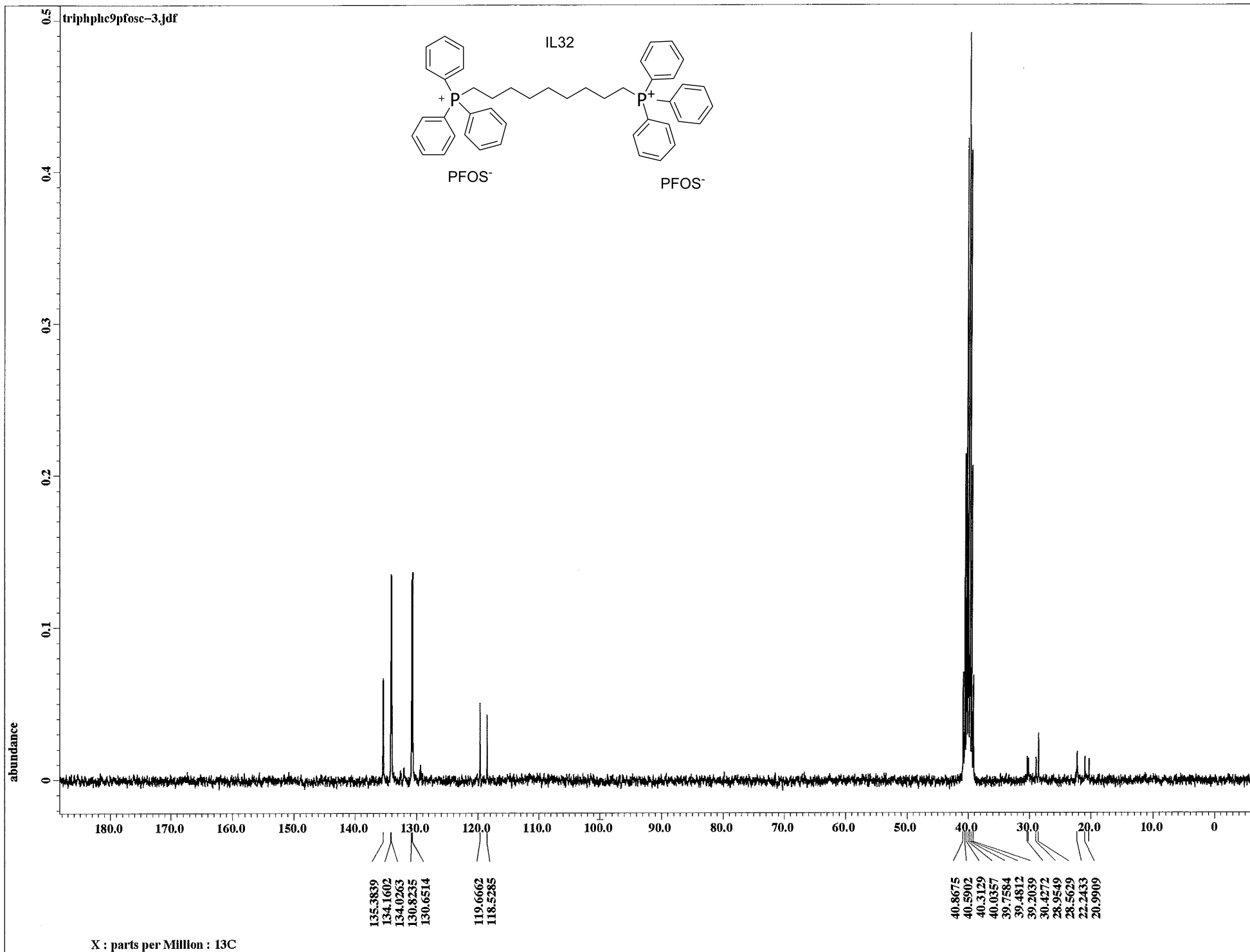
DIMEIMZC9PFOSC-2.jdf

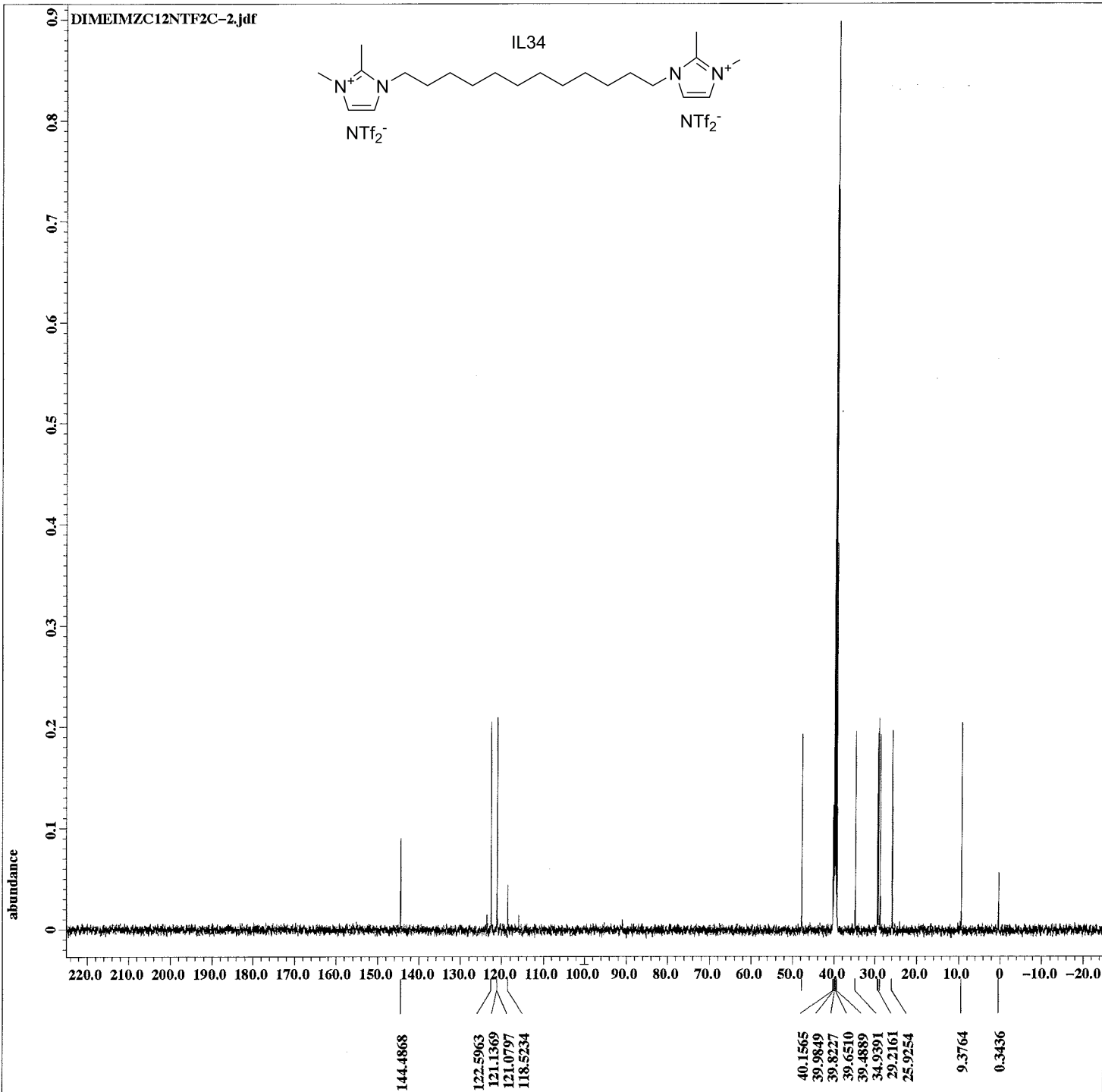


Filename = DIMEIMZC9PFOSC-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#413697
Solvent = DMSO-D6
Creation_time = 1-DEC-2015 01:14:24
Revision_time = 1-DEC-2015 11:41:07
Current_time = 1-DEC-2015 11:41:42
Comment = single pulse decouple
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500
Field_strength = 11.7473579 [T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.3081761[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 10
Scans = 300
Total_scans = 300
X_90_width = 10.73[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 3.57666667[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 21.5[dc]

X : parts per Million : 13C







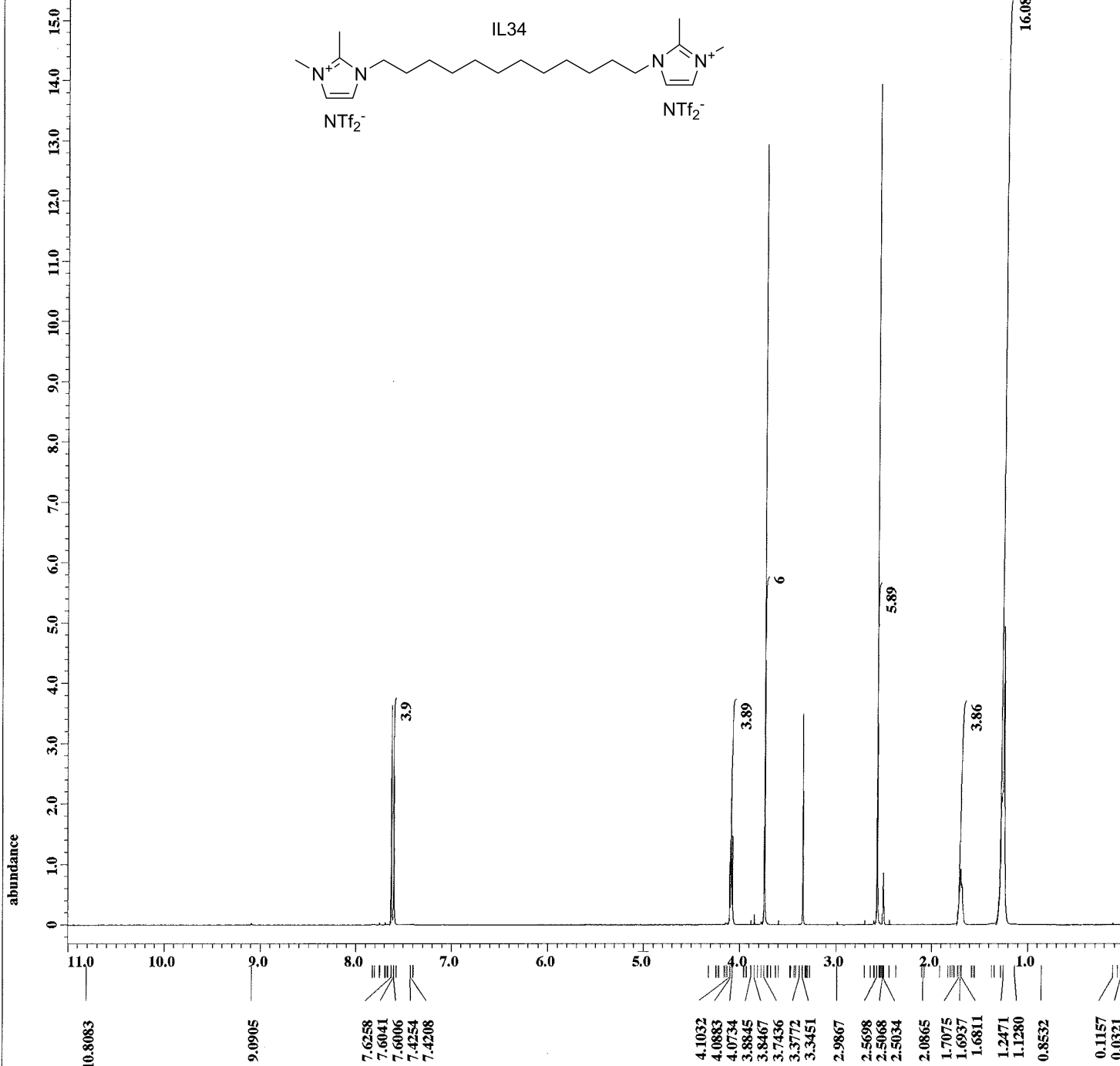
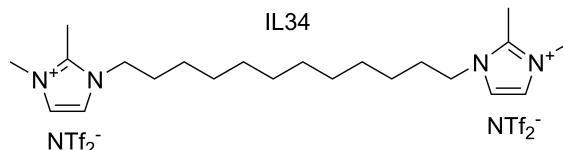
Filename = DIMEIMZC12NTF2C-2.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#392050
 Solvent = DMSO-D6
 Creation_time = 2-DEC-2015 00:29:45
 Revision_time = 1-DEC-2015 11:38:37
 Current_time = 1-DEC-2015 11:38:39

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 330
 Total_scans = 330

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 0.2[s]
 Recvr_gain = 50
 Relaxation_delay = 0.2[s]
 Repetition_time = 1.03361792[s]
 Temp_get = 21.5[dC]

X : parts per Million : 13C



X : parts per Million : 1H

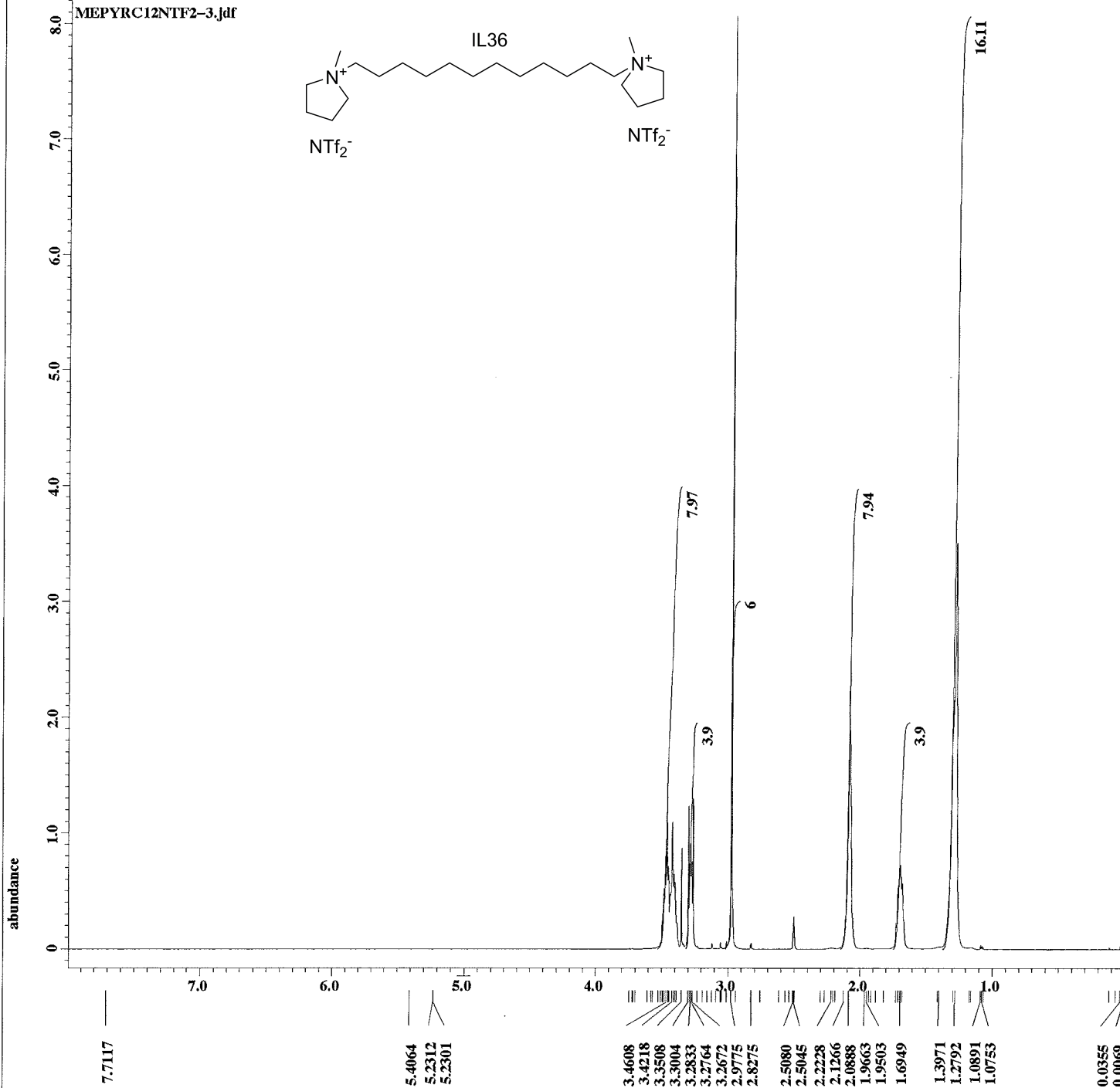
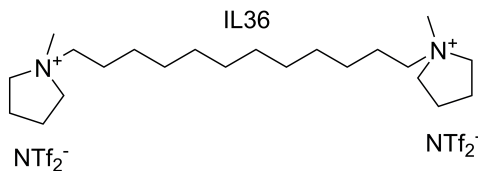
Filename = DIMEIMZC12NTF2-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#389630
 Solvent = DMSO-D6
 Creation_time = 2-DEC-2015 00:22:55
 Revision_time = 1-DEC-2015 10:56:03
 Current_time = 1-DEC-2015 10:56:41

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 12
 Total_scans = 12

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 21.1[dC]

MEPYRC12NTF2-3.jdf



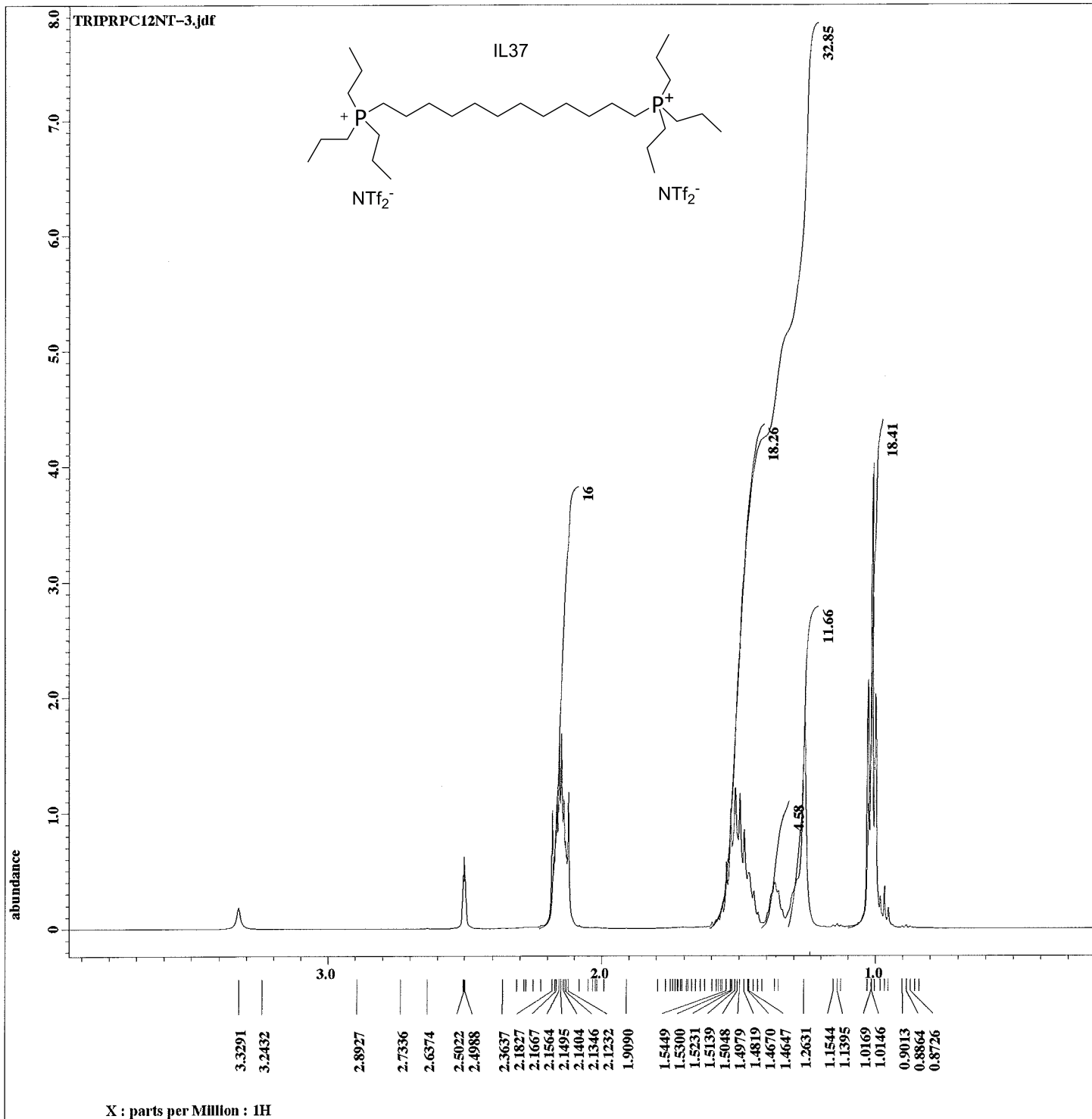
X : parts per Million : 1H

Filename = MEPYRC12NTF2-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#379847
 Solvent = DMSO-D6
 Creation_time = 2-DEC-2015 00:06:37
 Revision_time = 1-DEC-2015 10:40:39
 Current_time = 1-DEC-2015 10:41:06

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 22
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 21[dC]



```

Filename      = TRIPRPC12NT-3.jdf
Author       = delta
Experiment    = single_pulse.ex2
Sample_id    = S#413107
Solvent      = DMSO-D6
Creation time = 27-NOV-2015 01:02:15
Revision time = 1-DEC-2015 11:33:04
Current_time  = 1-DEC-2015 11:33:33

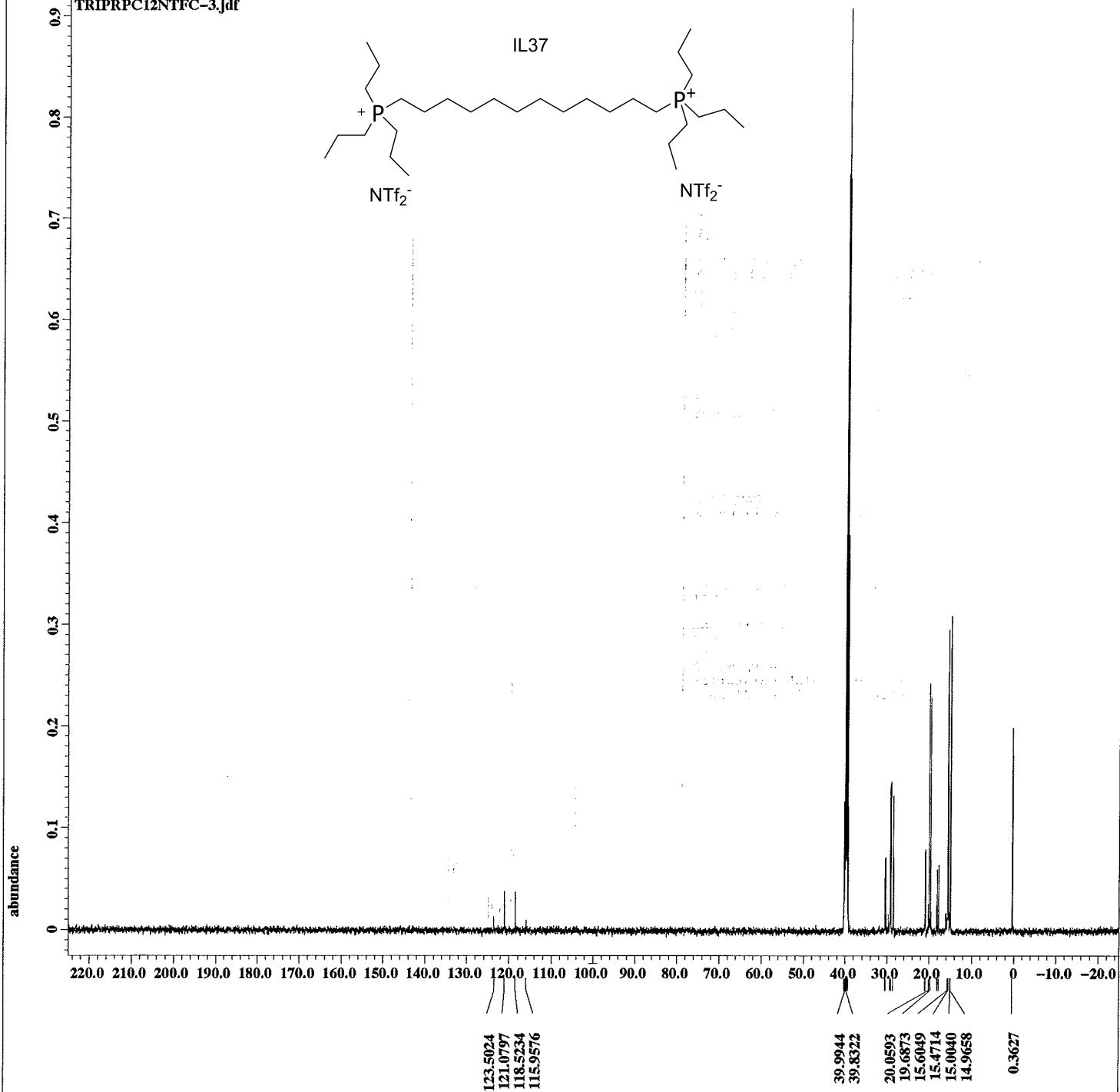
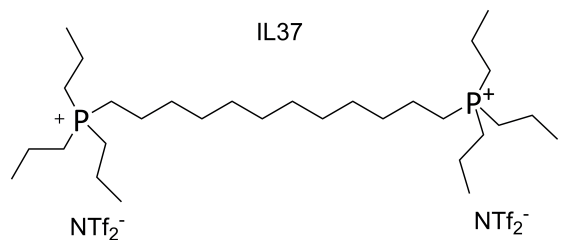
Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped       = FALSE
Mod_return     = 1
Scans          = 14
Total_scans   = 14

X_90_width    = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.27[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_preset  = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 30
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get       = 21.2[dc]

```

TRIPRPC12NTFC-3.jdf



X : parts per Million : 13C

```

Filename      = TRIPRPC12NTFC-3.jdf
Author        = delta
Experiment    = single_pulse_dec
Sample_id     = S#415624
Solvent       = DMSO-D6
Creation_time = 27-NOV-2015 01:20:24
Revision_time = 26-NOV-2015 11:56:15
Current_time  = 26-NOV-2015 11:56:26

Comment       = single pulse decouple
Data_format   = 1D_COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 1000
Total_scans    = 1000

X_90_width     = 10.73[us]
X_acq_time     = 0.83361792[s]
X_angle        = 30[deg]
X_atn          = 9[dB]
X_pulse        = 3.57666667[us]
Irr_atn_dec    = 20[dB]
Irr_atn_noe    = 20[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 0.2[s]
Recvr_gain     = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.03361792[s]
Temp_get       = 21.7[dC]
    
```

