Supporting Information

For

An operationally simple, palladium catalysed dehydrogenative cross-coupling reaction of pyridine *N*-oxides and thiazoles "on water".

Nicky J. Willis[a] and James M. Smith[b]*

[a]*School of Biological and Chemical Sciences, Joseph Priestley Building, Queen Mary, University of London, Mile End Road, E3 4NS;*
[b] *Cancer Research Technology Ltd., Discovery Laboratories, Jonas Webb Building, Babraham Research Campus, Cambridge, CB22 3AT (UK).*

e-mail: n.j.willis@qmul.ac.uk[a] and jsmith@cancertechnology.com[b].

Table of Contents:

I.	Materials and Instrumentation	S2
II.	Representative Procedure For Initial Solvent Screen	S3
III.	Representative Procedure For Calculation of ^{1}H NMR Conversion	S4
IV.	General Experimental Procedure A	S5
V.	General Experimental Procedure B	S5
VI.	Determination of Kinetic Isotope Effect	S6
VII.	Compound Data	S7-11
VIII.	NMR Spectra and HRMS Data	S12-27

I. Materials and Instrumentation. Unless otherwise stated, commercially available reagents were used as supplied. All reactions requiring anhydrous conditions were conducted in dried apparatus under an atmosphere of nitrogen. Thermal heating was conducted in 10 ml thick walled microwave vials (Biotage) fitted with crimp top teflon seals. Analytical thin-layer chromatography (TLC) was performed on silica gel plates (0.25 mm) precoated with a fluorescent indicator. Standard flash chromatography procedures were performed using Kieselgel 60 (40-63 μm) or with a TeleDyne Isco CombiFlash Rf automated purification system.

Infrared spectra were recorded in the range 4000-600 cm^{-1}, using a Bruker Tensor 37 FTIR machine equipped with a PIKE MIRacle ATR accessory. ^{1}H NMR spectra recorded during the optimisation study using an Oxford Instruments AS400 9.4 Tesla 400MHz magnet with a 5 mm BBO BB−^{1}H probe and an AVANCE/DPX400 console and final ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded using a Bruker AV400 NMR. Chemical shifts δ are reported in ppm (relative to δ_H $CHCl_3$ (7.27) and δ_C $CDCl_3$ (77.0) unless otherwise stated) and multiplicity of signals are denoted s = singlet, d = doublet, t = triplet and m = multiplet respectively, with coupling constants (*J*) reported in hertz (Hz). Structural interpretations and assignments were made based upon COSY, HSQC, HMQC, DEPT 135, DEPT 90 and NOESY experiments. High resolution mass spectra (HRMS) were obtained by the EPSRC National Mass Service (Swansea) using a double focussing mass spectrometer **(**Finnigan MAT 95 XP).

II. Representative Procedure For Initial Solvent Screen

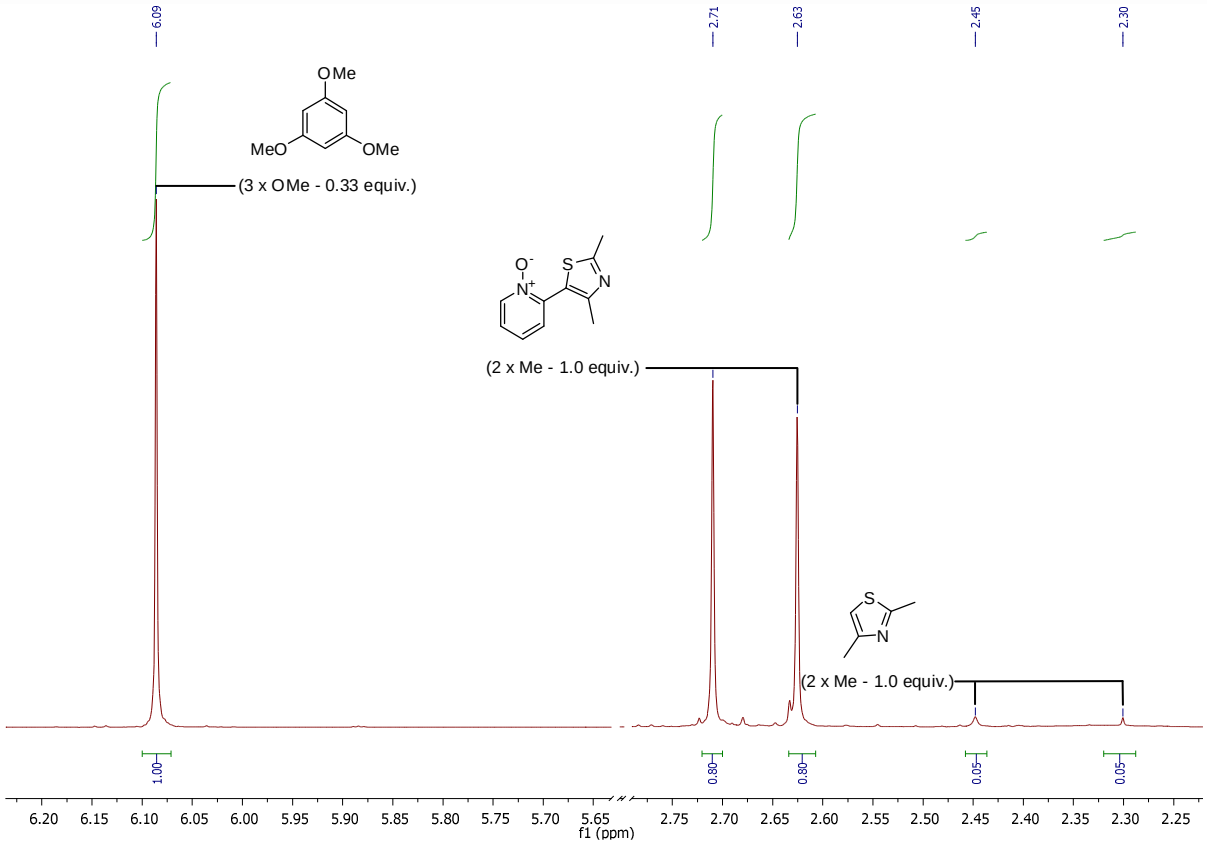
Pyridine *N*-oxide (285 mg, 3.00 mmol, 4.0 equiv.), 2,4-dimethyl-thiazole (80 µl, 0.75 mmol, 1.0 equiv.), Ag_2CO_3 (476 mg, 1.73 mmol, 2.3 equiv.), $Pd(OAc)_2$ (16.8 mg, 10 mol%), tetrabutylammonium bromide (48 mg, 0.15 mmol, 0.2 equiv.), Pyridine (242 µl, 3.00 mmol, 4.0 equiv.) and DMF (3.00 ml) were charged into a 10 ml biotage microwave vial containing a magnetic stirrer bar. The vial was then sealed with a "crimp-cap" and the mixture was stirred at 135 ^{o}C (calibrated external temperature) for 22 h.

The mixture was then diluted with EtOAc (25ml), the organics were then filtered through phase-separating filter paper, washing with further EtOAc (2 x 10ml)before concentration under reduced pressure. An internal standard (1,3,5-trimethoxybenzene, 42 mg, 0.25mmol, 0.33 equiv.) and the crude mixture was dissolved in $CDCl_3$ (5ml) and a ^{1}H NMR was recorded to determine conversion of starting material upon integration of the signals highlighted as in **III** (overleaf).

III. Representative Procedure For Calculation of ^{1}H NMR Conversion:

Pyridine *N*-oxide (428 mg, 4.50 mmol, 6.0 equiv.), 2,4-dimethyl-thiazole (80 µl, 0.75 mmol, 1.0 equiv.), Ag_2CO_3 (620mg, 2.25 mmol, 3.0 equiv.), $Pd(OAc)_2$ (4.5mg, 2.6 mol%), and tetrabutylammonium bromide (TBAB, 48 mg, 0.15 mmol, 0.2 equiv.), 2-Dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (36 mg, 0.075mmol, 10 mol%), Pyridine (116 µl, 1.50 mmol, 2.0 equiv.) and distilled de-ionised water (1.00ml, 55.55mmol) were charged into a 10 ml biotage microwave vial. The vial was then sealed with a "crimp-cap" and the mixture was stirred at 100 ^{o}C (calibrated external temperature) for 22 h.

The mixture was then diluted with sat. aq. sodium citrate solution (25ml) and CH_2Cl_2 (25ml) and the organics were then separated, filtered through phase-separating filter paper before concentration under reduced pressure. An internal standard (1,3,5-trimethoxybenzene, 42 mg, 0.25mmol, 0.33 equiv.) and the crude mixture was dissolved in $CDCl_3$ (5ml) and a ^{1}H NMR was recorded to determine conversion of starting material upon integration of the signals highlighted below (80%).



IV General Experimental Procedure A:

Pyridine *N*-oxide (4.50 mmol, 6.0 equiv.), thiazole (0.75 mmol, 1.0 equiv.), Ag_2CO_3 (620mg, 2.25 mmol), $Pd(OAc)_2$ (4.5mg, 2.6 mol%), and tetrabutylammonium bromide (TBAB, 48 mg, 0.15 mmol, 0.2 equiv.), 2-Dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (36 mg, 0.075mmol, 10 mol%), Pyridine (116 μl, 1.50 mmol, 2.0 equiv.) and distilled de-ionised water (1.00ml, 55.55mmol) were charged into a 10 ml biotage microwave vial. The vial was then sealed with a "crimp-cap" and the mixture was stirred at 100 ^oC (calibrated external temperature) for 22 h.

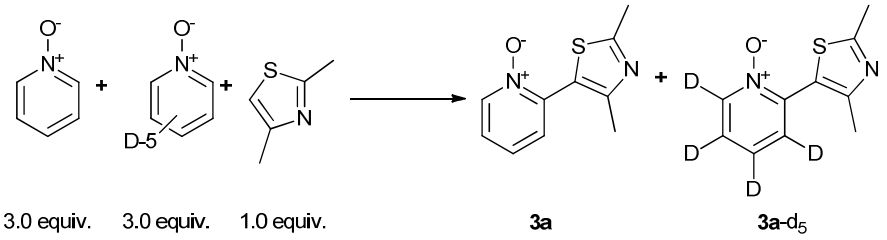
The mixture was then diluted with sat. aq. sodium citrate solution (25ml) and CH_2Cl_2 (25ml) and the organics were then separated, filtered through phase-separating filter paper before concentration under reduced pressure. The crude residue was then purified by silica gel chromatography (CH_2Cl_2:MeOH).

V General Experimental Procedure B:

Pyridine N-oxide (4.50 mmol, 6.0 equiv.), thiazole (0.75 mmol, 1.0 equiv.), Ag_2CO_3 (620mg, 2.25 mmol), $Pd(OAc)_2$ (17 mg, 10 mol%), and tetrabutylammonium bromide (TBAB, 48 mg, 0.15 mmol, 0.2 equiv.), 2-Dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (36 mg, 0.075mmol, 10 mol%), Pyridine (116 μl, 1.50 mmol, 2.0 equiv.) and distilled de-ionised water (1.00ml, 55.55 mmol) were charged into a 10 ml biotage microwave vial. The vial was then sealed with a "crimp-cap" and the mixture was stirred at 100 ^oC (calibrated external temperature) for 48 h.

The mixture was then diluted with sat. aq. sodium citrate solution (25ml) and CH_2Cl_2 (25ml) and the organics were then separated, filtered through phase-separating filter paper before concentration under reduced pressure. The crude residue was then purified by silica gel chromatography (CH_2Cl_2:MeOH).

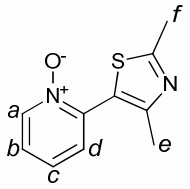
VI Determination of Kinetic Isotope Effect



Pyridine-d_5 N-oxide (230mg, 2.30 mmol, 3 equiv.), pyridine *N*-oxide (219mg, 2.30 mmol, 3 equiv.), 4-Methyl-2-phenylthiazole (130 mg, 0.75 mmol, 1.0 equiv.), Ag_2CO_3 (620mg, 2.25 mmol), $Pd(OAc)_2$ (4.5mg, 2.6 mol%), and tetrabutylammonium bromide (TBAB, 48 mg, 0.15 mmol, 0.2 equiv.), 2-Dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (36 mg, 0.075mmol, 10 mol%), Pyridine (116 µl, 1.50 mmol, 2.0 equiv.) and distilled de-ionised water (1.00ml, 55.55 mmol) were charged into a 10 ml biotage microwave vial. The vial was then sealed with a "crimp-cap" and the mixture was stirred at 100 ^{o}C (calibrated external temperature) for 22 h.

The mixture was then diluted with sat. aq. sodium citrate solution (25ml) and CH_2Cl_2 (25ml) and the organics were then separated, filtered through phase-separating filter paper before concentration under reduced pressure. The crude residue was then purified by silica gel chromatography (0 – 5 % MeOH in CH_2Cl_2) to afford a mixture of 2-(4-Methyl-2-phenyl-thiazol-5-yl)-pyridine-d_4 1-oxide and 2-(4-Methyl-2-phenyl-thiazol-5-yl)-pyridine 1-oxide as a yellow solid. The ratio of **3a** to **3a**-d_5 was determined by ^{1}H NMR to be 3.5:1.

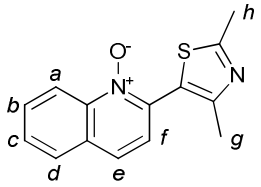
2-(2,4-Dimethyl-thiazol-5-yl)-pyridine 1-oxide (**3a**)



The titled compound was prepared from 2,4-dimethyl-thiazole and pyridine *N*-oxide according to **general procedure A**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3a** as a pale yellow solid (119 mg, 0.58 mmol, 77%).

R_f = 0.33 (CH_2Cl_2:MeOH,19:1); mp 57-58 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.30 (dd, 1H, *J* = 6.5, 0.9 Hz, H_a), 7.59 (dd, 1H, *J* = 8.1, 1.9 Hz, H_d), 7.32-7.26 (m, 1H, H_c), 7.17 (ddd, *J* = 7.0, 6.5, 2.0 Hz, H_b), 2.71 (s, 3H, H_e), 2.63 (s, 3H, H_f); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 153.4, 143.0, 139.7, 126.0, 125.5, 123.6, 120.6, 18.6, 18.4; HRMS calculated for $[C_{10}H_{11}N_2OS]^+$ = 207.0587, found = 207.0585; FT-IR (film, cm^{-1}) 3349, 3089, 1656, 1480, 1423, 1256, 1031, 836, 763;

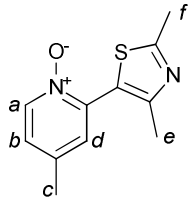
2-(2,4-Dimethyl-thiazol-5-yl)-quinoline 1-oxide (**3b**)



The titled compound was prepared from 2,4-dimethyl-thiazole and quinoline-*N*-oxide, according to **general procedure A**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3b** as a pale yellow solid (123 mg, 0.48 mmol, 64%).

R_f = 0.43 (CH_2Cl_2:MeOH,19:1); mp 108-109 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.81 (d, 1H, *J* = 8.8 Hz, H_a), 7.87 (dd, 1H, *J* = 8.1, 1.3 Hz, H_f), 7.83-7.73 (m, 3H, H_b, H_c and H_d), 7.65 (ddd, 1H, *J* = 8.1, 6.9, 1.3 Hz, H_e), 2.74 (s, 6H, H_g and H_h); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.3, 154.3, 141.5, 139.4, 130.9, 128.5, 128.5, 128.0, 125.1, 121.9, 121.4, 120.0, 19.1, 18.7; HRMS calculated for $[C_{14}H_{13}N_2OS]^+$ = 257.0743, found = 257.0743; FT-IR (film, cm^{-1}) 3055, 2922, 1598, 1451, 1370, 1322, 1295, 809, 748.

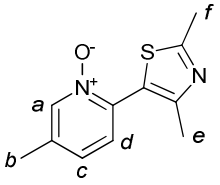
2-(2,4-Dimethyl-thiazol-5-yl)-4-methyl-pyridine 1-oxide (**3c**)



The titled compound was prepared from 2,4-dimethyl-thiazole and 4-Picoline *N*-oxide according to **general procedure B**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3c** as a pale yellow solid (119 mg, 0.54 mmol, 72%).

R_f = 0.30 (CH_2Cl_2:MeOH,19:1); mp 138-139 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, 1H, J = 6.7 Hz, H_a), 7.40 (d, 1H, J = 2.3 Hz, H_d), 7.01 (dd, 2H, J = 6.7, 2.3 Hz, H_b), 2.70 (s, 3H, H_f), 2.62 (s, 3H, H_e), 2.41 (s, 3H, H_c); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 153.3, 142.4, 139.2, 137.0, 126.6, 124.8, 120.9, 20.8, 18.9, 18.6; HRMS calculated for $[C_{11}H_{13}N_2OS]^+$ = 221.0743, found = 221.0743; FT-IR (film, cm^{-1}) 3050, 2919, 1646, 1509, 1439, 1242, 821, 784.

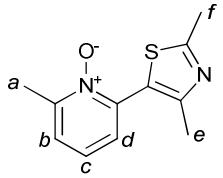
2-(2,4-Dimethyl-thiazol-5-yl)-5-methyl-pyridine 1-oxide (**3d**)



The titled compound was prepared from 2,4-dimethyl-thiazole and 3-Picoline *N*-oxide according to **general procedure B**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3d** as a pale yellow solid (97 mg, 0.44 mmol, 59%).

R_f = 0.32 (CH_2Cl_2:MeOH,19:1); mp 111 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 1H, H_a), 7.50 (d, 1H, J = 8.2 Hz, H_d), 7.16 (d, 1H, J = 8.2 Hz, H_c), 2.70 (s, 3H, H_f), 2.60 (s, 3H, H_e), 2.35 (s, 3H, H_b); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 153.1, 140.7, 139.8, 134.9, 127.4, 125.7, 121.1, 19.0, 18.6, 18.5; HRMS calculated for $[C_{11}H_{13}N_2OS]^+$ = 221.0743, found = 221.0742; FT-IR (film, cm^{-1}) 3390, 3054, 1653, 1517, 1491, 1391, 1266, 1201, 1020, 824, 625.

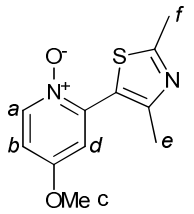
2-(2,4-Dimethyl-thiazol-5-yl)-6-methyl-pyridine 1-oxide (**3e**)



The titled compound was prepared from 2,4-dimethyl-thiazole and 2-Picoline *N*-oxide according to **general procedure B**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3e** as a colourless solid (95 mg, 0.44 mmol, 58%).

R_f = 0.32 (CH_2Cl_2:MeOH,19:1); mp 62 ^oC; ^1H NMR (400 MHz, CD_3CN): δ 7.62 (dd, 1H, J = 7.6, 2.3 Hz, H_d), 7.33-7.25 (m, 2H, H_b and H_c), 2.62 (s, 3H, H_f), 2.55 (s, 3H, H_e), 2.45 (s, 3H, H_a); ^{13}C NMR (100 MHz, CD_3CN): δ 167.2, 154.0, 149.8, 143.1, 125.2, 125.2, 124.7, 122.2, 18.6, 18.5, 18.5; HRMS calculated for $[C_{11}H_{13}N_2OS]^+$ = 221.0743, found = 221.0742; FT-IR (film, cm^{-1}) 3340, 1655, 1564, 1446, 1379, 1222, 792.

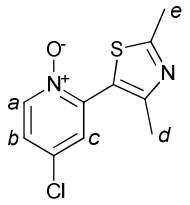
2-(2,4-Dimethyl-thiazol-5-yl)-4-methoxy-pyridine 1-oxide (**3f**)



The titled compound was prepared from 2,4-dimethyl-thiazole and 4-Methoxypyridine *N*-oxide, according to **general procedure A**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3f** as a pale yellow solid (115 mg, 0.49 mmol, 65%).

R_f = 0.27 (CH_2Cl_2:MeOH,19:1); mp 79-80 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, 1H, J = 7.4 Hz, H_a), 7.14 (d, 1H, J = 3.2 Hz, H_d), 6.78 (dd, 1H, J = 7.4, 3.2 Hz, H_b), 3.90 (s, 3H, H_c), 2.70 (s, 3H, H_f), 2.65 (s, 3H, H_e); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 157.3, 153.5, 140.4, 122.4, 120.8, 110.9, 110.1, 56.2, 18.7, 18.5; HRMS calculated for $[C_{11}H_{13}N_2O_2S]^+$ = 237.0692, found = 237.0692; FT-IR (film, cm^{-1}) 3075, 2921, 1620, 1507, 1482, 1296, 1216, 1016, 780.

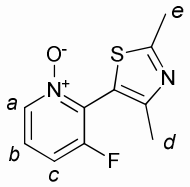
4-Chloro-2-(2,4-dimethyl-thiazol-5-yl)-pyridine 1-oxide (**3g**)



The titled compound was prepared from 2,4-dimethyl-thiazole and 4-Methoxypyridine *N*-oxide, according to **general procedure B**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3g** as a pale yellow semi-crystalline solid (47 mg, 0.20 mmol, 26%).

R_f = 0.36 (CH_2Cl_2:MeOH,19:1); mp 160-161 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, 1H, J = 6.9 Hz, H_a), 7.57 (d, 1H, J = 2.8 Hz, H_d), 7.14 (dd, 1H, J = 6.9, 2.8 Hz, H_b), 2.67 (s, 3H, H_f), 2.61 (s, 3H, H_e); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 154.3, 143.9, 140.3, 131.4, 125.4, 123.6, 119.7, 18.7, 18.6; HRMS calculated for $[C_{10}H_{10}N_2ClS]^+$ = 241.0197 found = 241.0198; FT-IR (film, cm^{-1}) 3078, 1470, 1258, 1239, 1124, 821, 677.

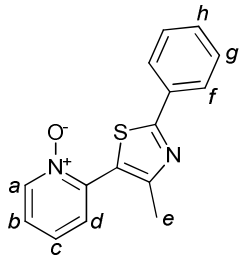
2-(2,4-Dimethyl-thiazol-5-yl)-3-fluro-pyridine 1-oxide (**3h**)



The titled compounds were prepared from 2,4-dimethyl-thiazole and 4-Methoxypyridine *N*-oxide, according to **general procedure B**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3h** as a colourless crystalline solid (52 mg, 0.29 mmol, 31%).

R_f = 0.40 (CH_2Cl_2:MeOH,19:1); mp 82-83 ^oC; ^1H NMR (400 MHz, $CDCl_3$): 8.22 (d, 1H, J = 7.1 Hz, H_a), 7.28-7.20 (m, 1H, H_b), 7.15 (dd, 1H, J = 7.5, 0.7, H_c), 2.74 (s, 3H, H_e), 2.35 (d, J = 2.6 Hz, 3H, H_d); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.1, 158.4 (d, J = 253.2 Hz), 155.4, 136.7, 124.1, 124.0, 114.7 (d, J = 2.5 Hz), 113.4 (d, J = 22.6 Hz), 19.3, 17.2 (d, J = 5.9 Hz); ^{19}F (282 MHz, $CDCl_3$): δ = -112.1; HRMS calculated for $[C_{10}H_{10}N_2OFS]^+$ = 225.0492, found = 225.0492; FT-IR (film, cm^{-1}) 3031, 1543, 1438, 1242, 1174, 1043, 821, 722.

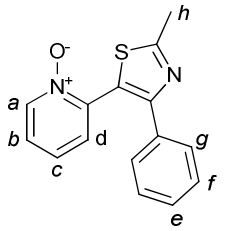
2-(4-Methyl-2-phenyl-thiazol-5-yl)-pyridine 1-oxide (**3i**)



The titled compound was prepared from 4-Methyl-2-phenylthiazole and pyridine *N*-oxide according to **general procedure A**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3i** as a colourless solid (127 mg, 0.47 mmol, 63%).

R_f = 0.43 (CH_2Cl_2:MeOH,19:1); mp 82-83 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.39 (dd, 1H, *J* = 6.5, 1.2 Hz, H_a), 8.05-8.00 (m, 2H, H_f), 7.75 (dd, 1H, *J* = 8.1, 1.9 Hz, H_d), 7.44 (m, 3H, H_g and H_h), 7.37 (ddd, 1H, *J* = 8.1, 7.6, 1.2 Hz, H_c), 7.23 (ddd, 1H, *J* = 7.6, 6.5, 2.0 Hz, H_b), 2.75 (s, 3H, H_e); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 154.9, 143.1, 139.8, 133.5, 130.3, 129.0, 126.8, 125.8, 125.6, 123.6, 121.3, 19.0; HRMS calculated for $[C_{15}H_{13}N_2OS]^+$ = 269.0743 found = 269.0744; FT-IR (film, cm^{-1}) 3043, 1651, 1478, 1428, 1240, 1014, 758, 685.

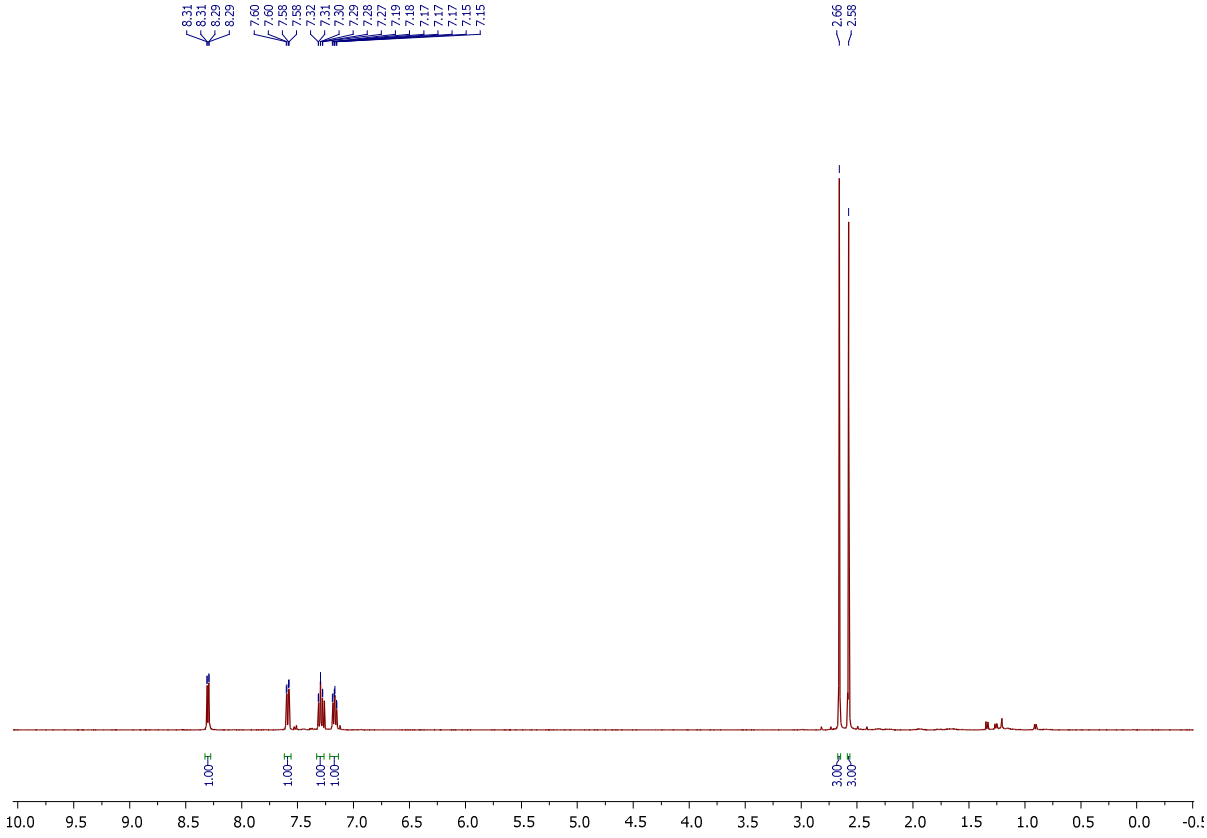
2-(2-Methyl-4-phenyl-thiazol-5-yl)-pyridine 1-oxide (**3j**)



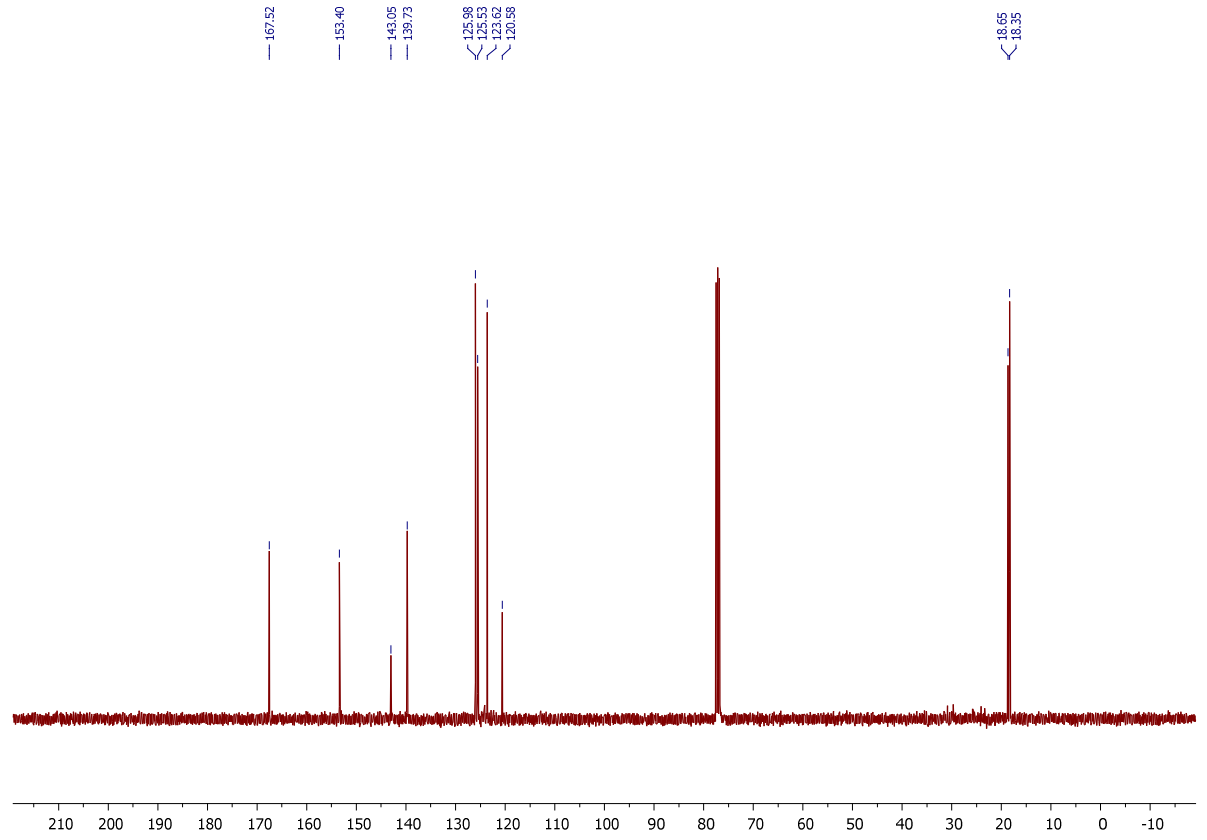
The titled compound was prepared from 2-Methyl-4-phenylthiazole and pyridine *N*-oxide according to **general procedure A**. Purified by silica gel chromatography using elution with 0 – 5 % MeOH in CH_2Cl_2 to afford **3j** as a pale orange oil (142 mg, 0.53 mmol, 71%).

R_f = 0.43 (CH_2Cl_2:MeOH,19:1);; ^1H NMR (400 MHz, $CDCl_3$): δ 8.33 (dd, 1H, *J* = 6.5, 1.3 Hz, H_a), 7.55-7.50 (m, 2H, H_g), 7.42-7.36 (m, 3H, H_e and H_f), 7.19 (dd, 1H, *J* = 8.1, 2.0 Hz, H_d), 7.12 (ddd, 1H, *J* = 7.5 6.5, 2.0 Hz, H_b), 6.99 (ddd, 1H, *J* = 8.1, 7.5, 1.3 Hz, H_c), 2.78 (s, 3H, H_h); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 156.7, 143.3, 139.7, 135.5, 129.4, 129.0, 128.9, 127.0, 125.1, 123.9, 121.2, 18.9; HRMS calculated for $[C_{15}H_{13}N_2OS]^+$ = 269.0743, found = 269.043; FT-IR (film, cm^{-1}) 3061, 1493, 1481, 1276, 881, 762, 701.

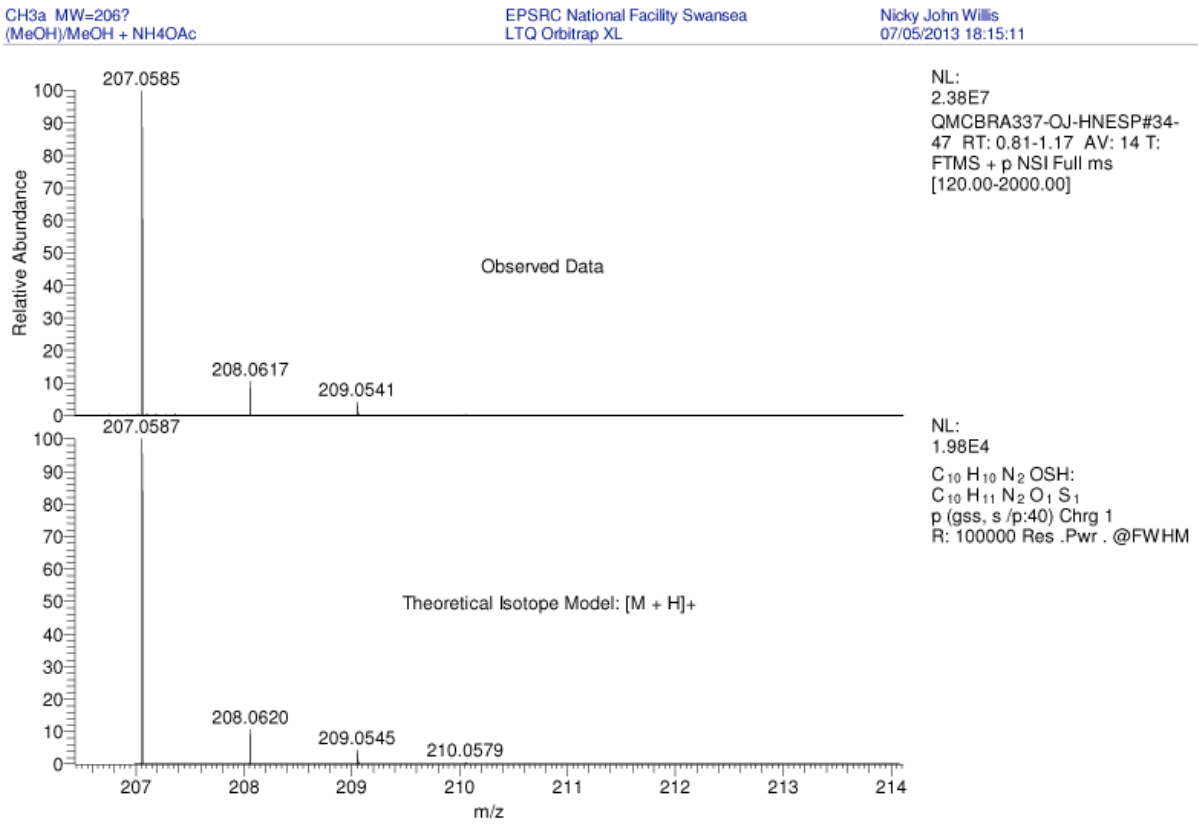
3a ^{1}H Spectrum



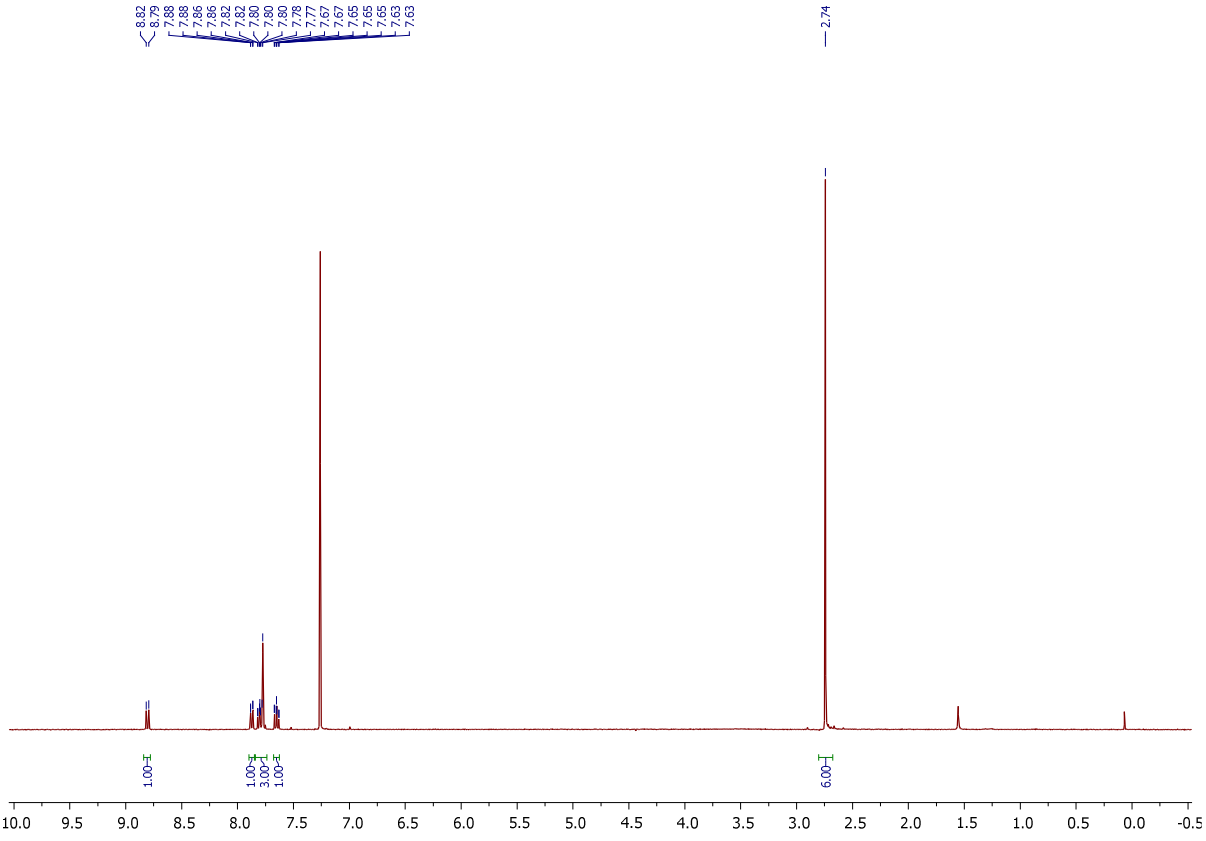
3a ^{13}C Spectrum



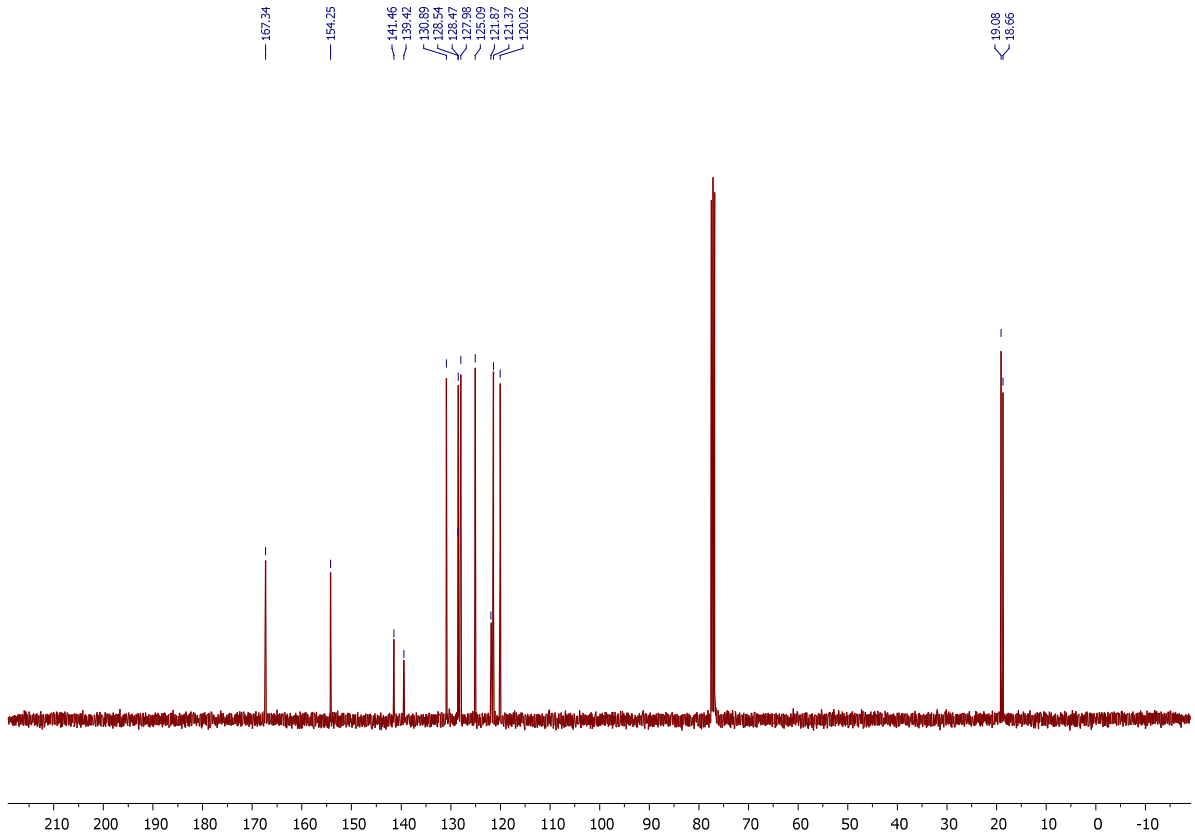
3a HRMS



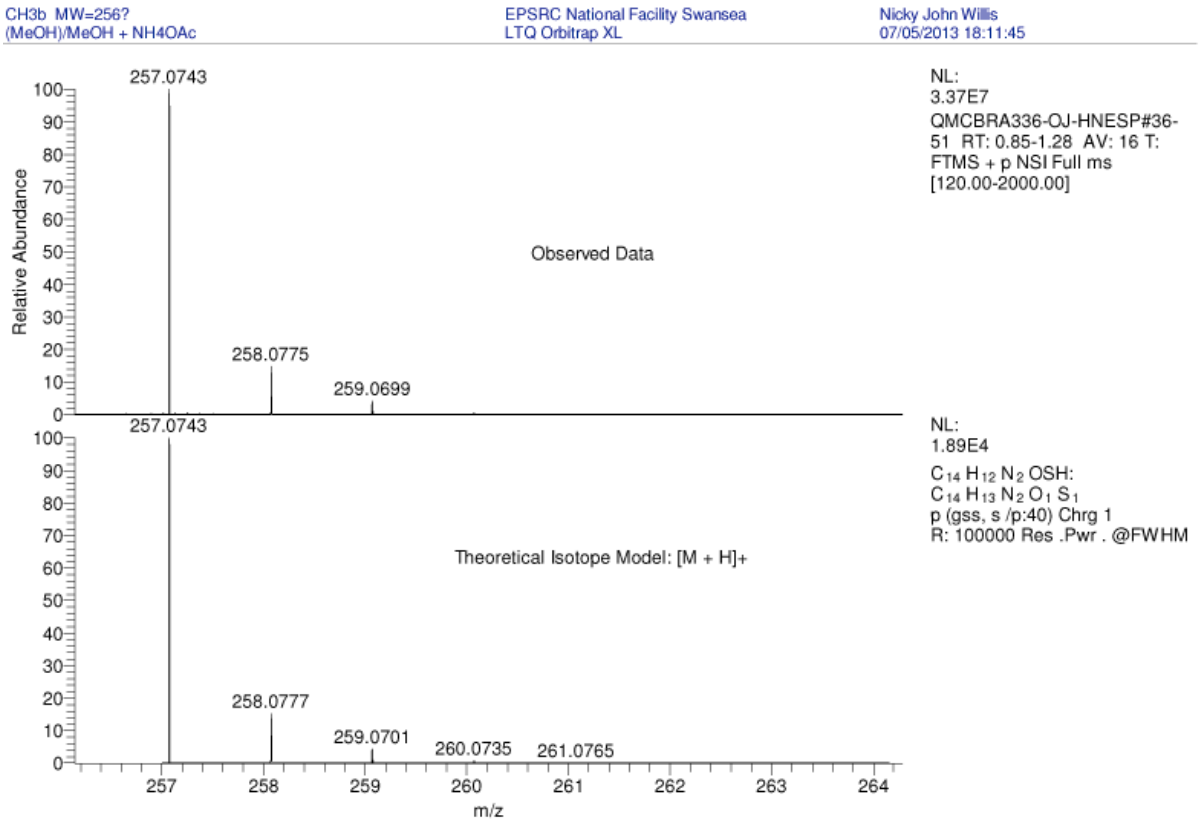
3b ^{1}H Spectrum



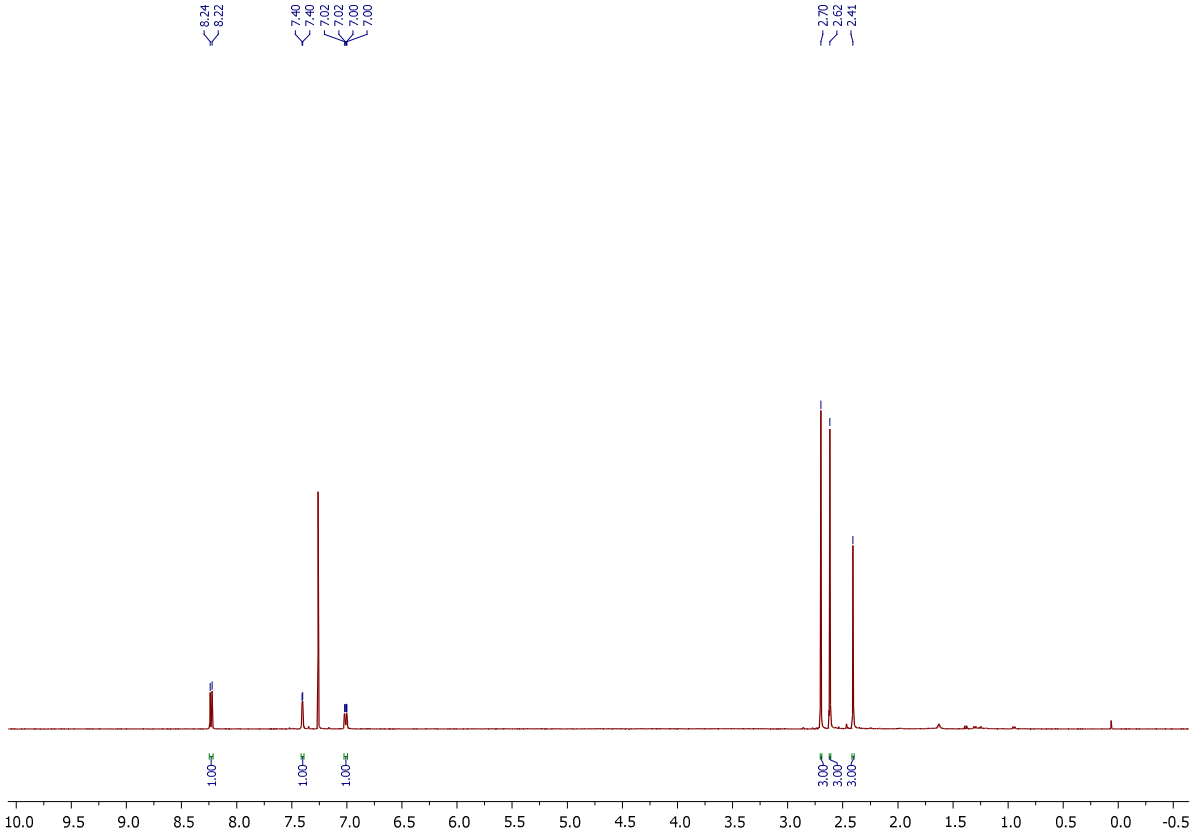
3b ^{13}C Spectrum



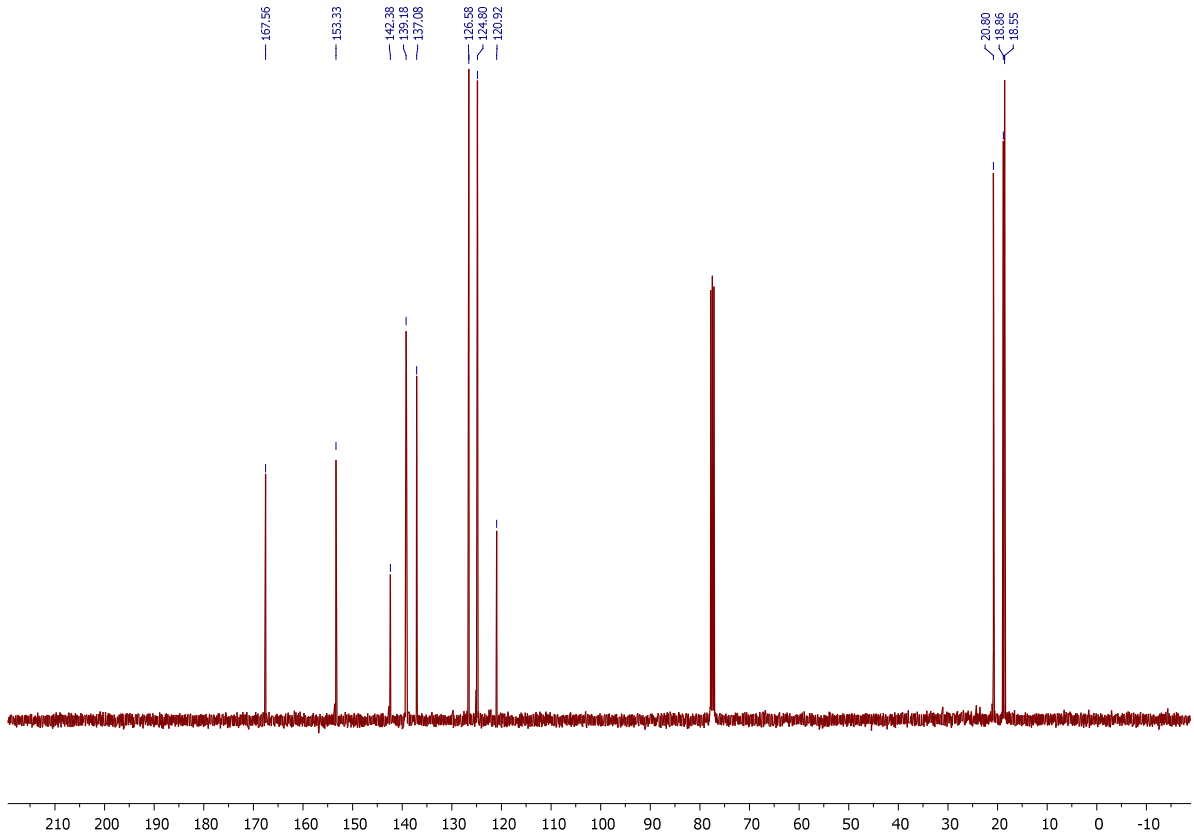
3b HRMS



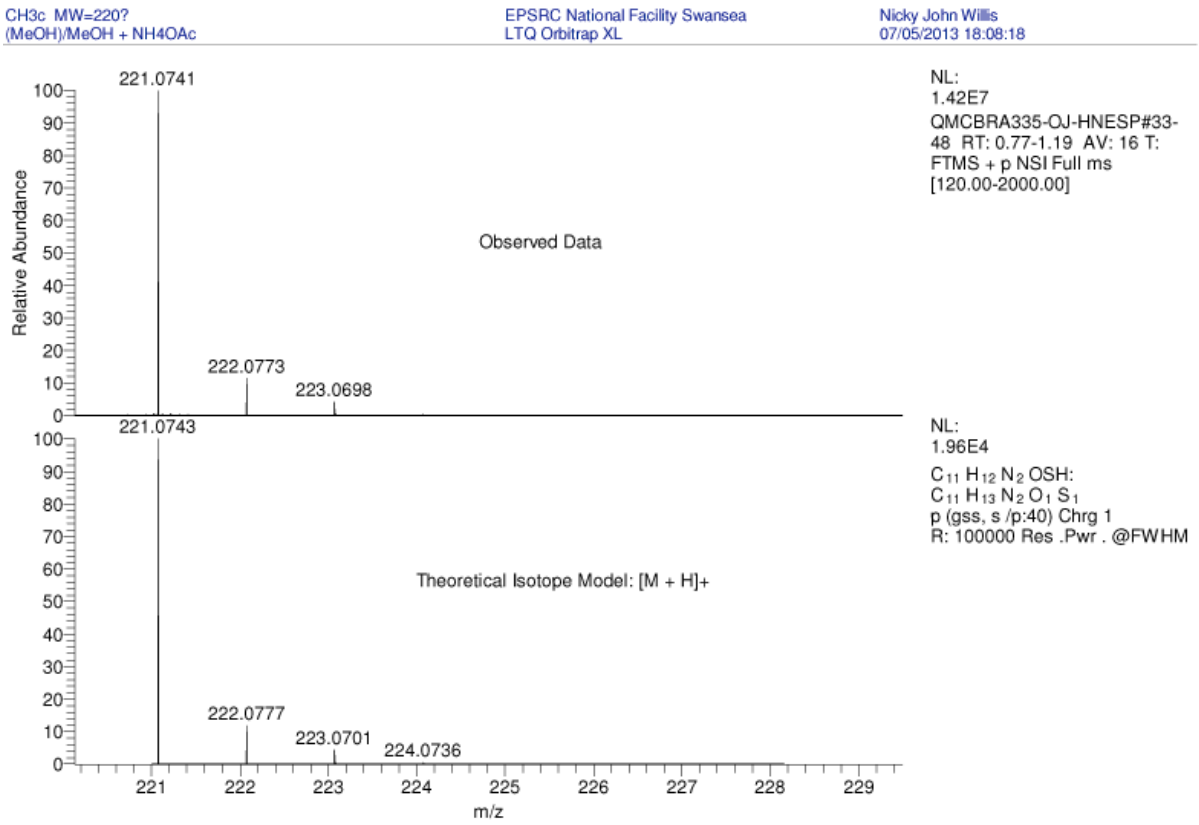
3c ^{1}H Spectrum



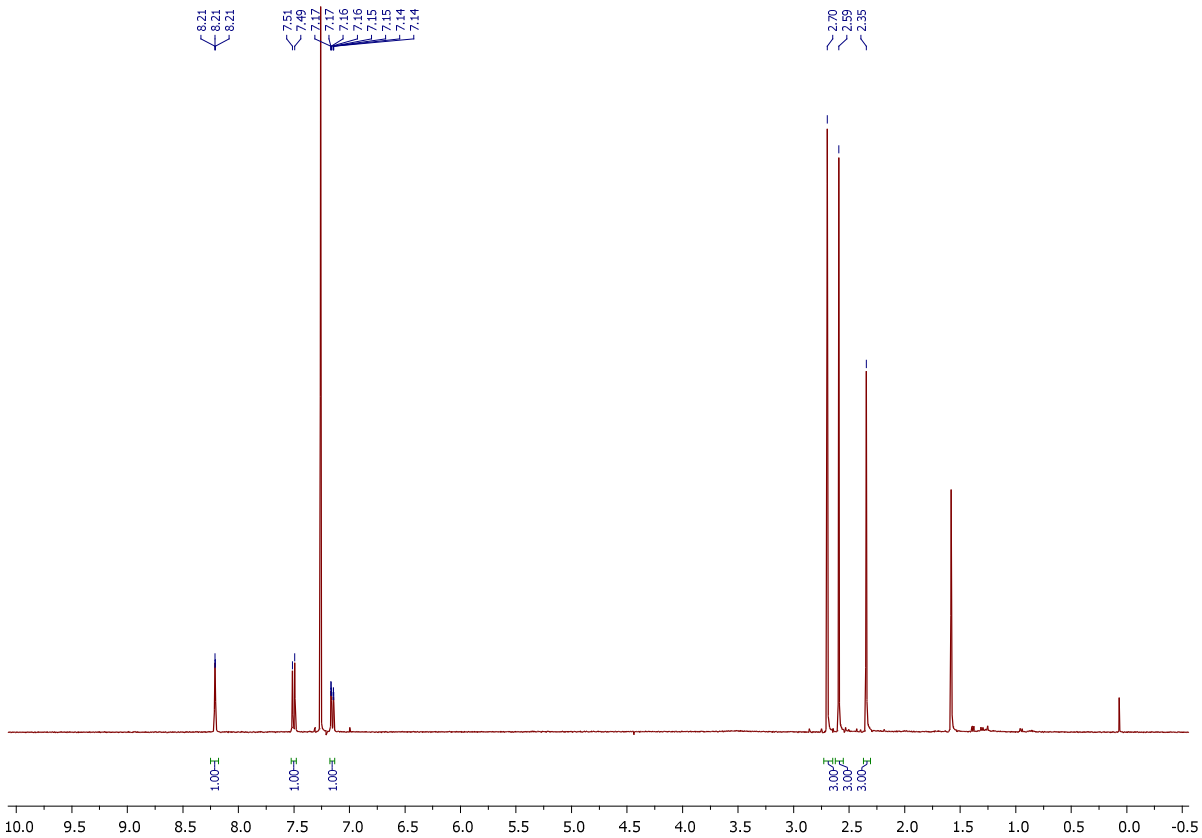
3c ^{13}C Spectrum



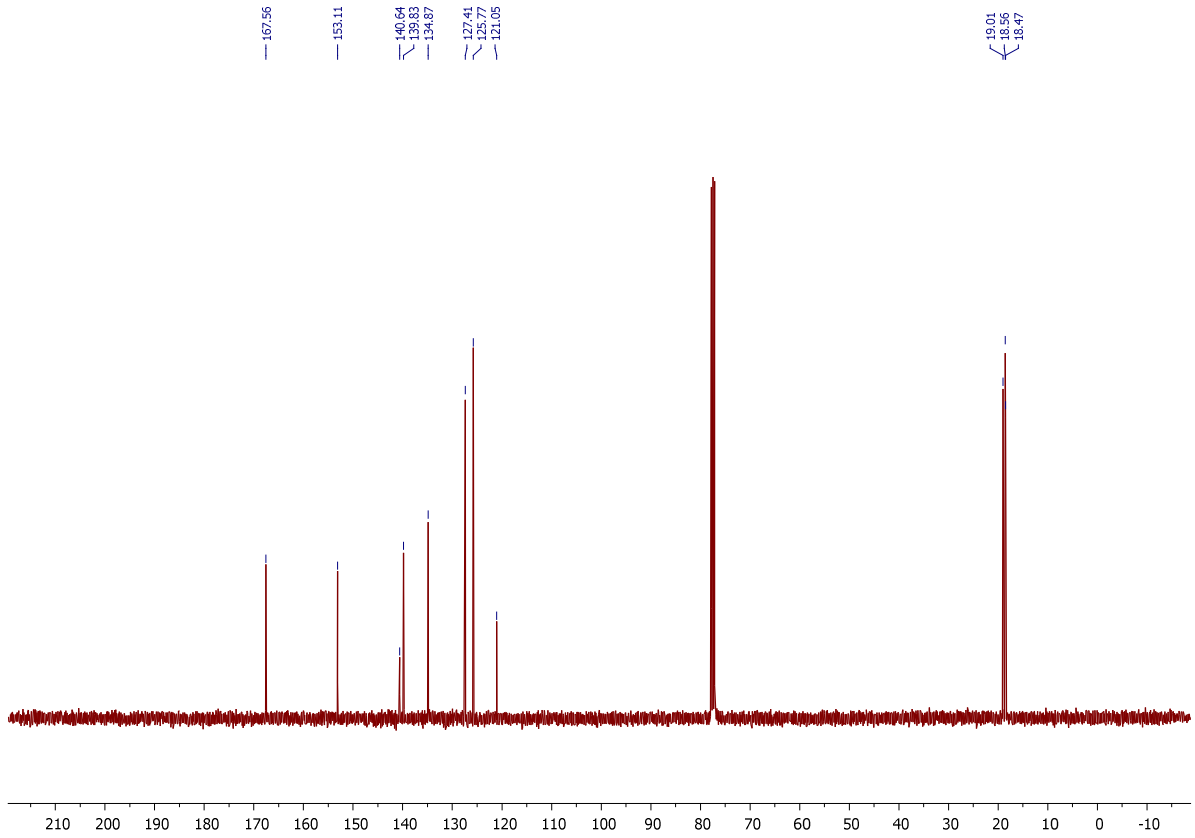
3c HRMS



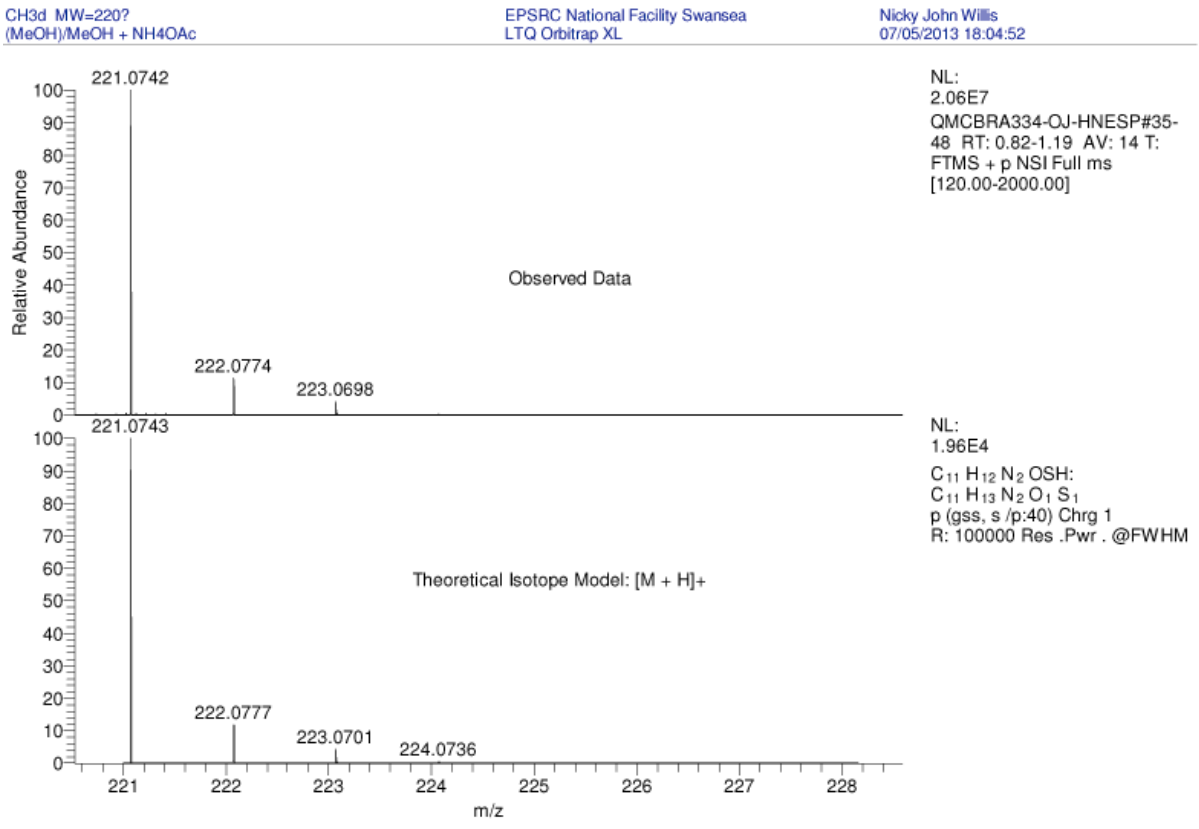
3d ^{1}H Spectrum



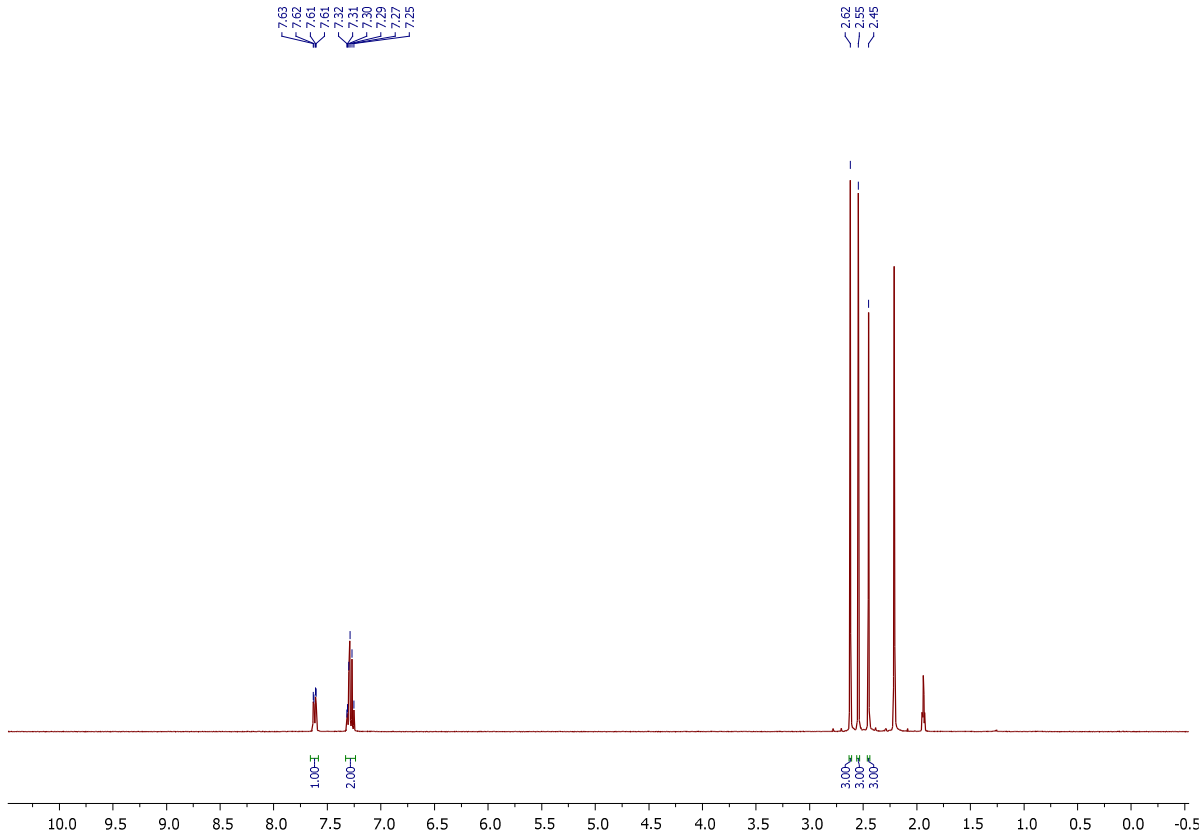
3d ^{13}C Spectrum



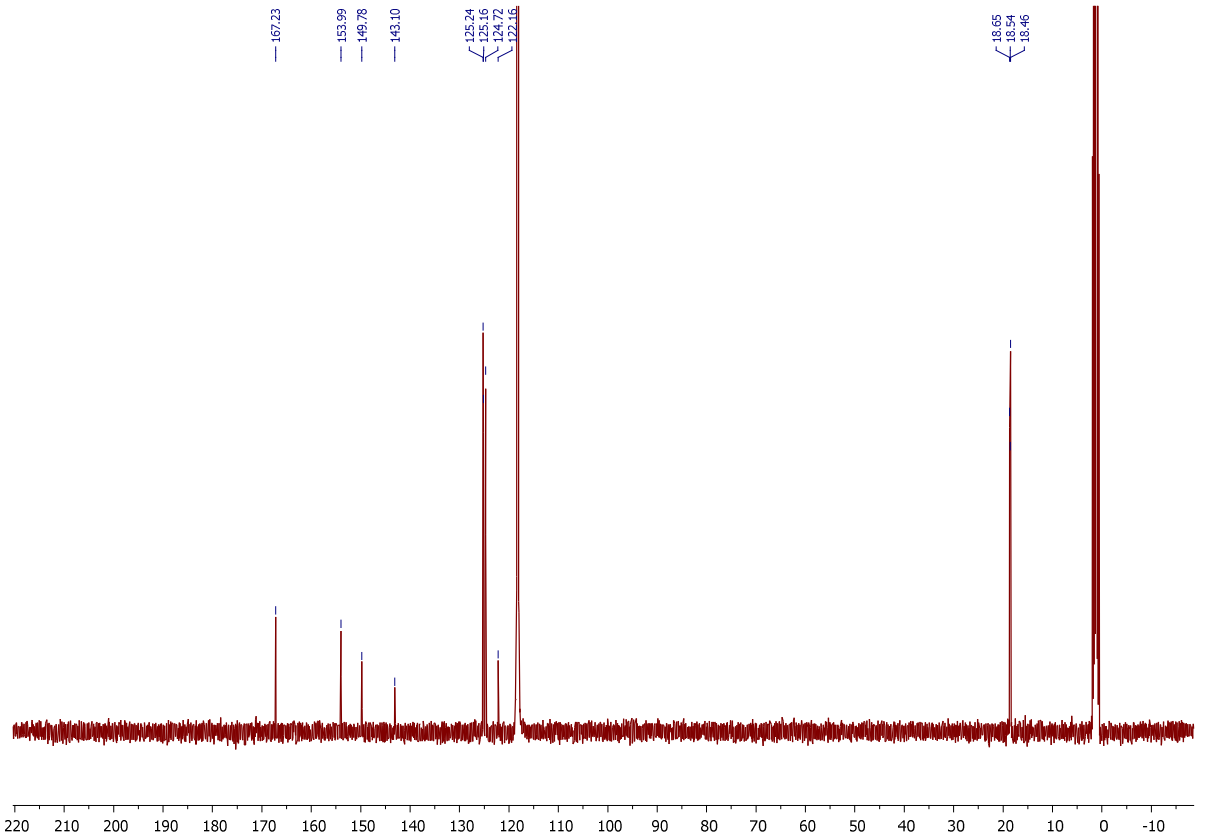
3d HRMS



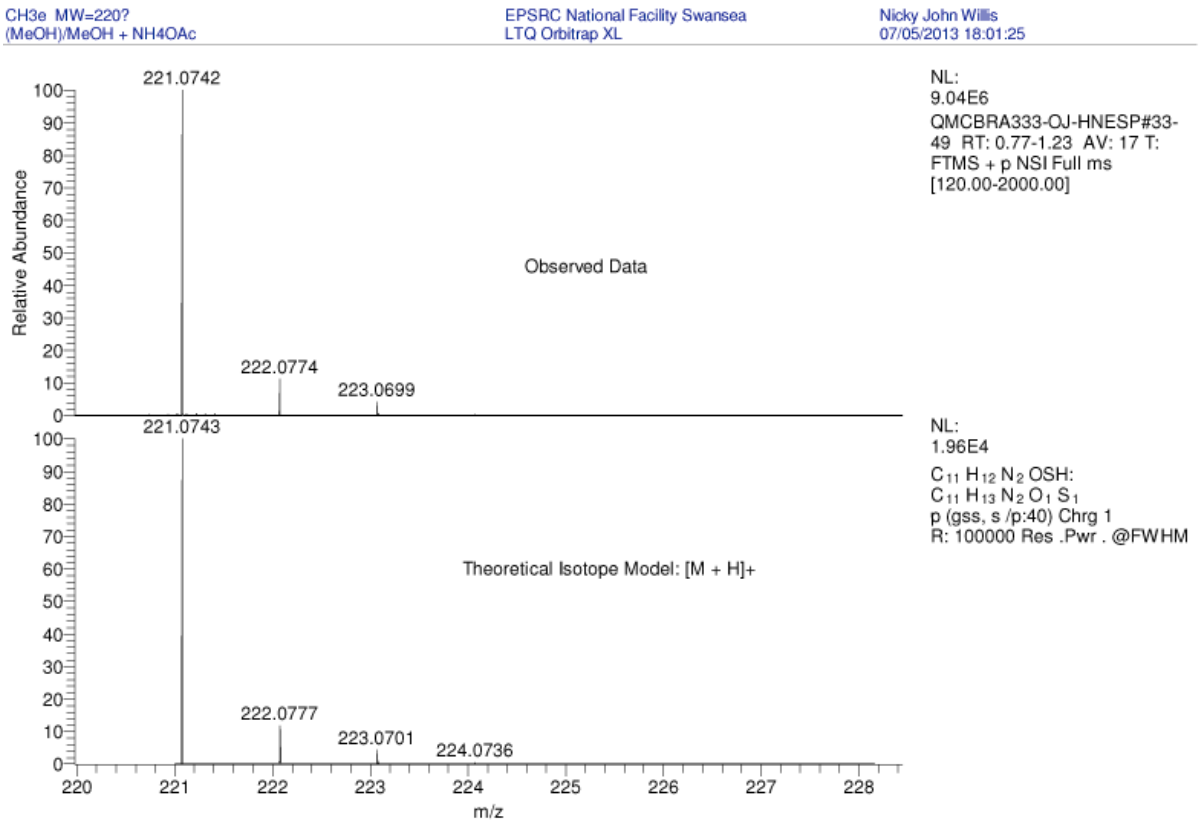
3e ^{1}H Spectrum



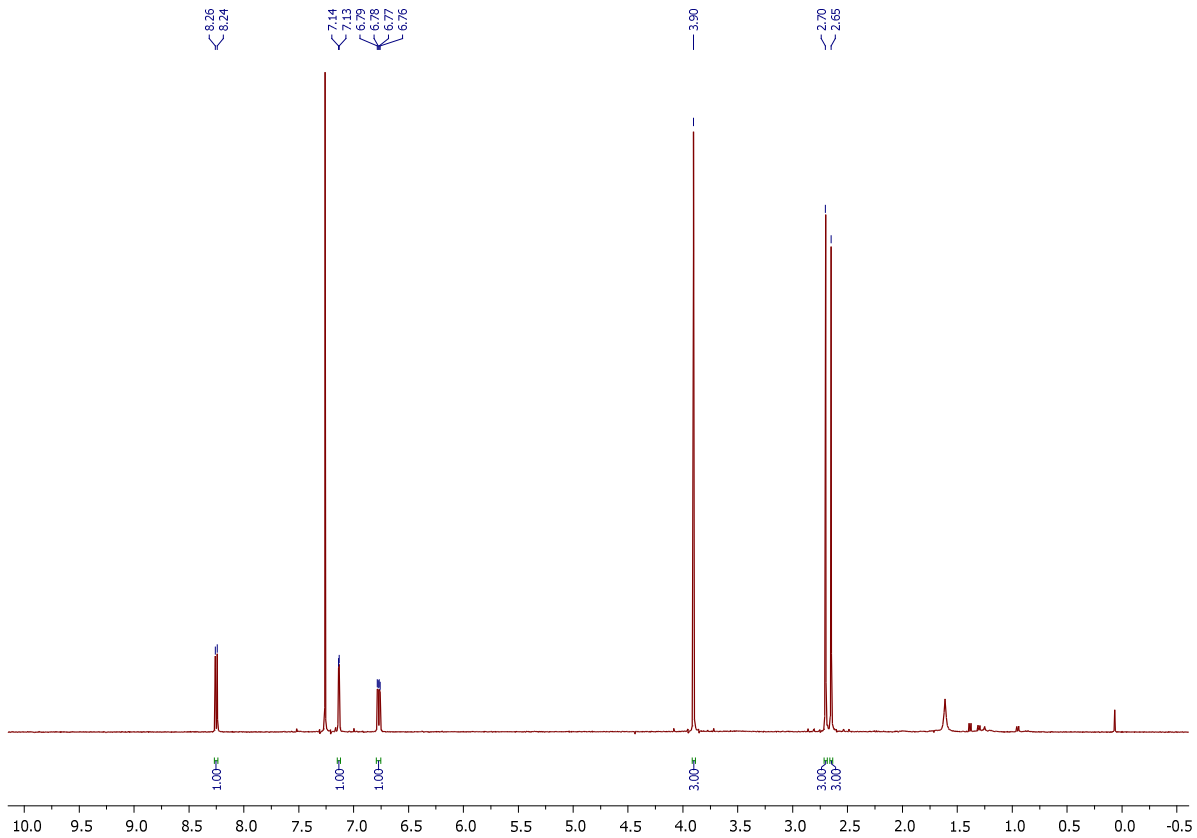
3e ^{13}C Spectrum



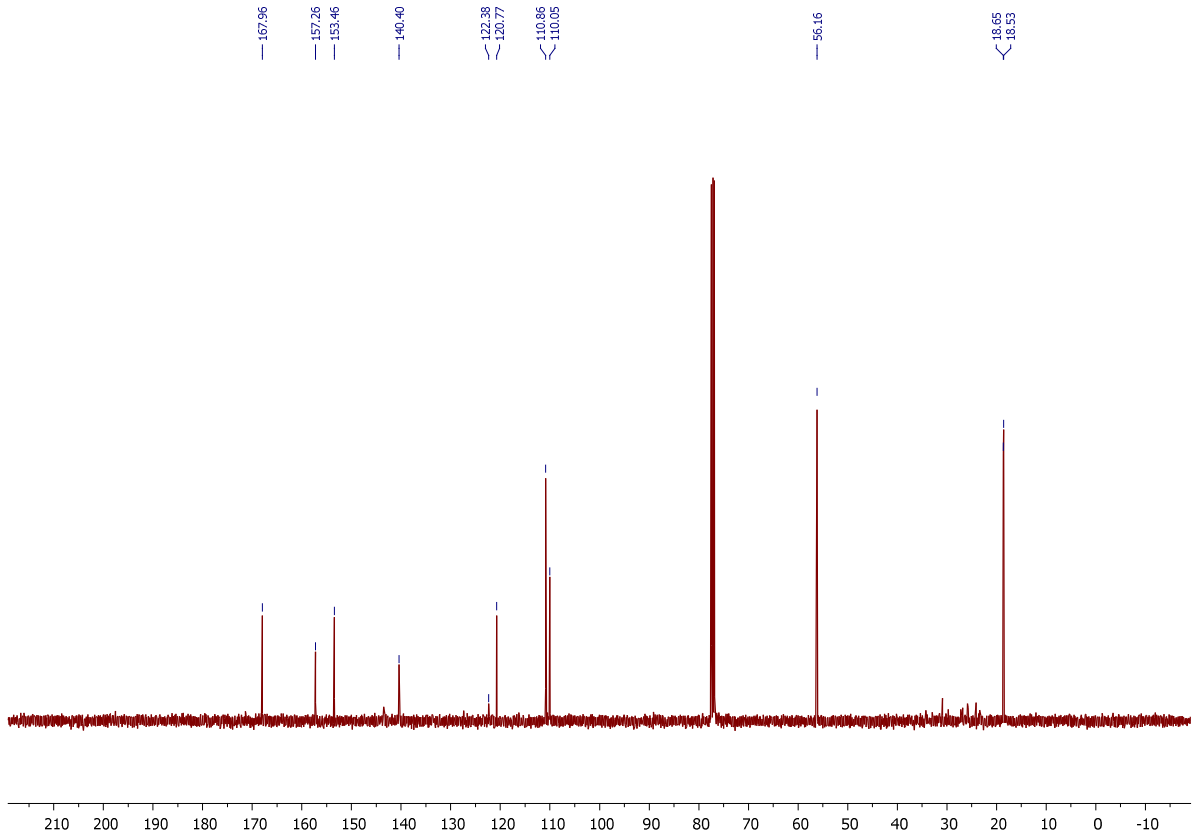
3e HRMS



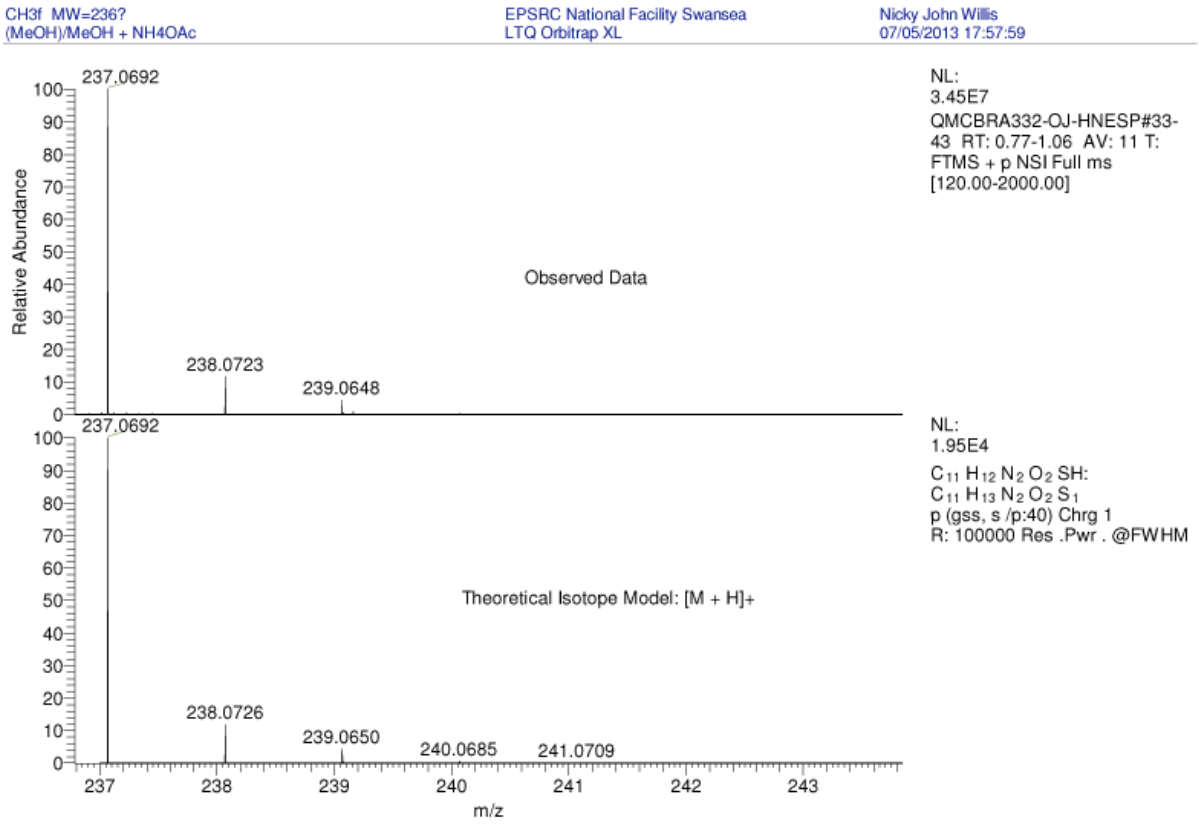
3f ^{1}H Spectrum



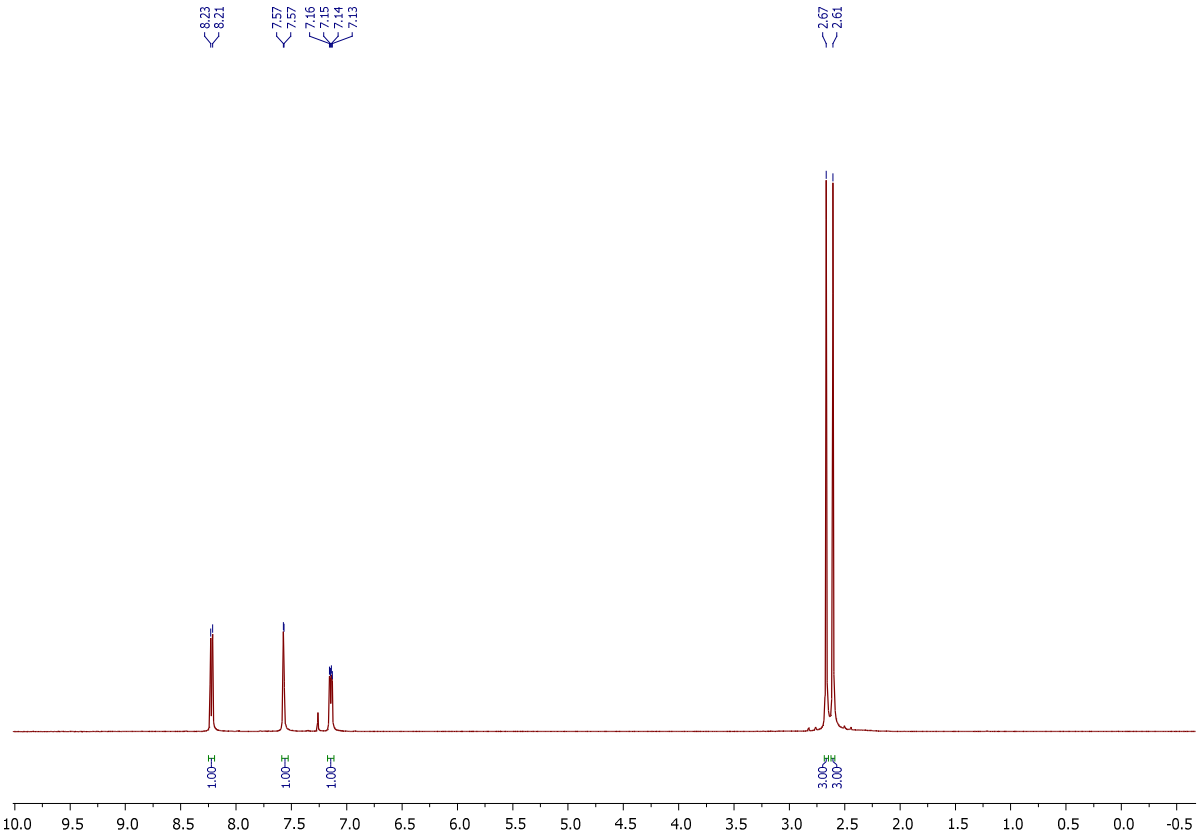
3f ^{13}C Spectrum



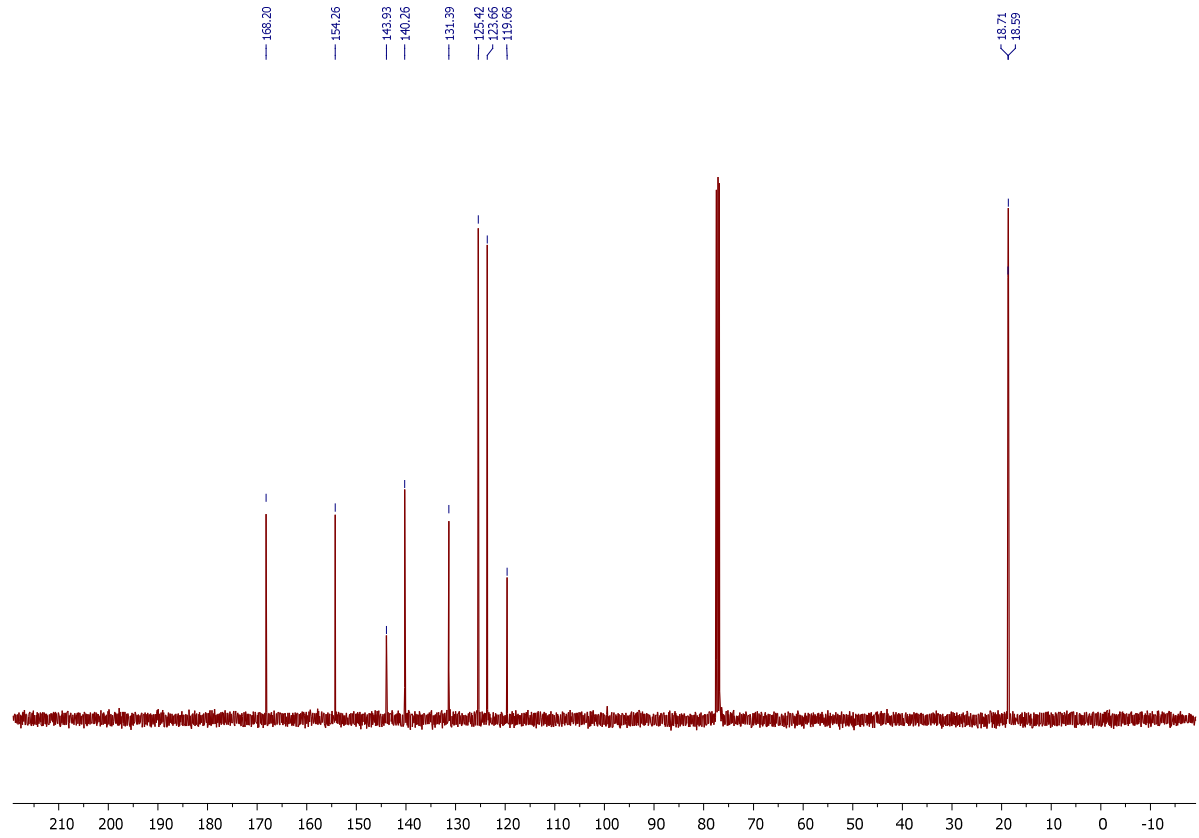
3f HRMS



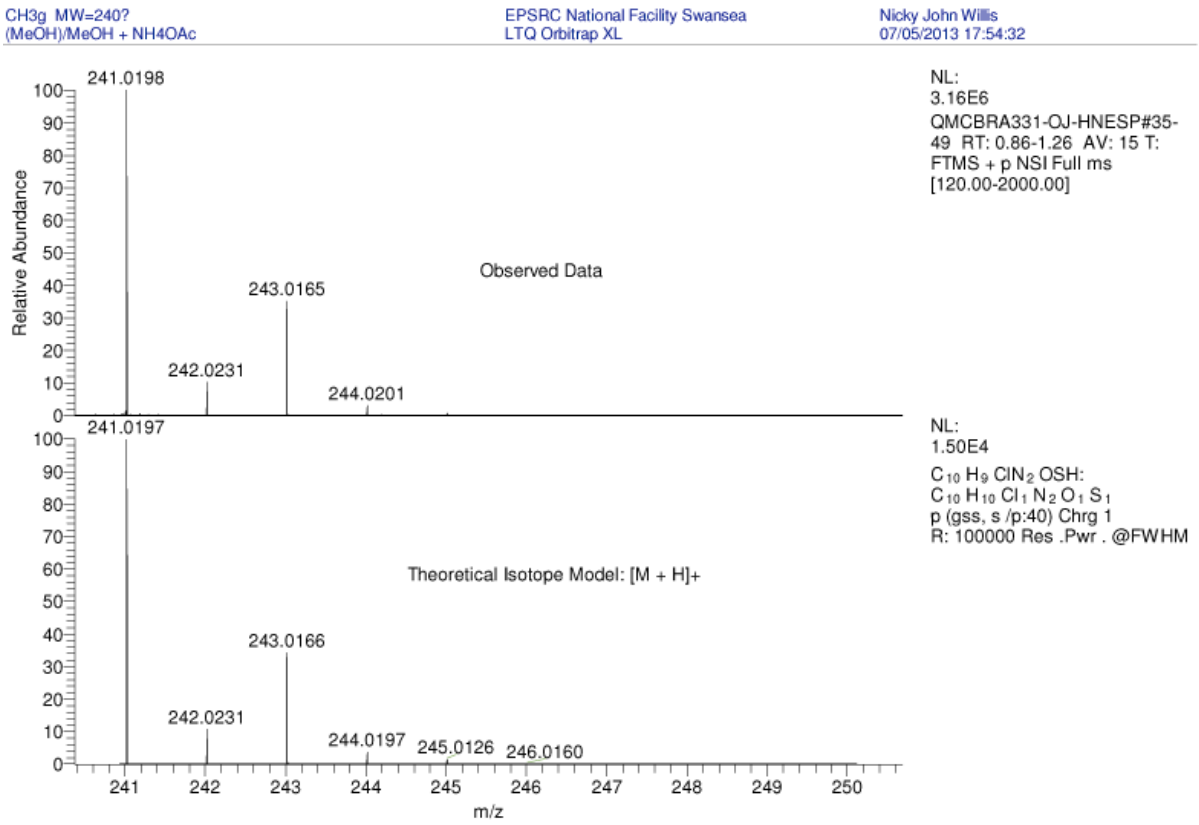
3g ^{1}H Spectrum



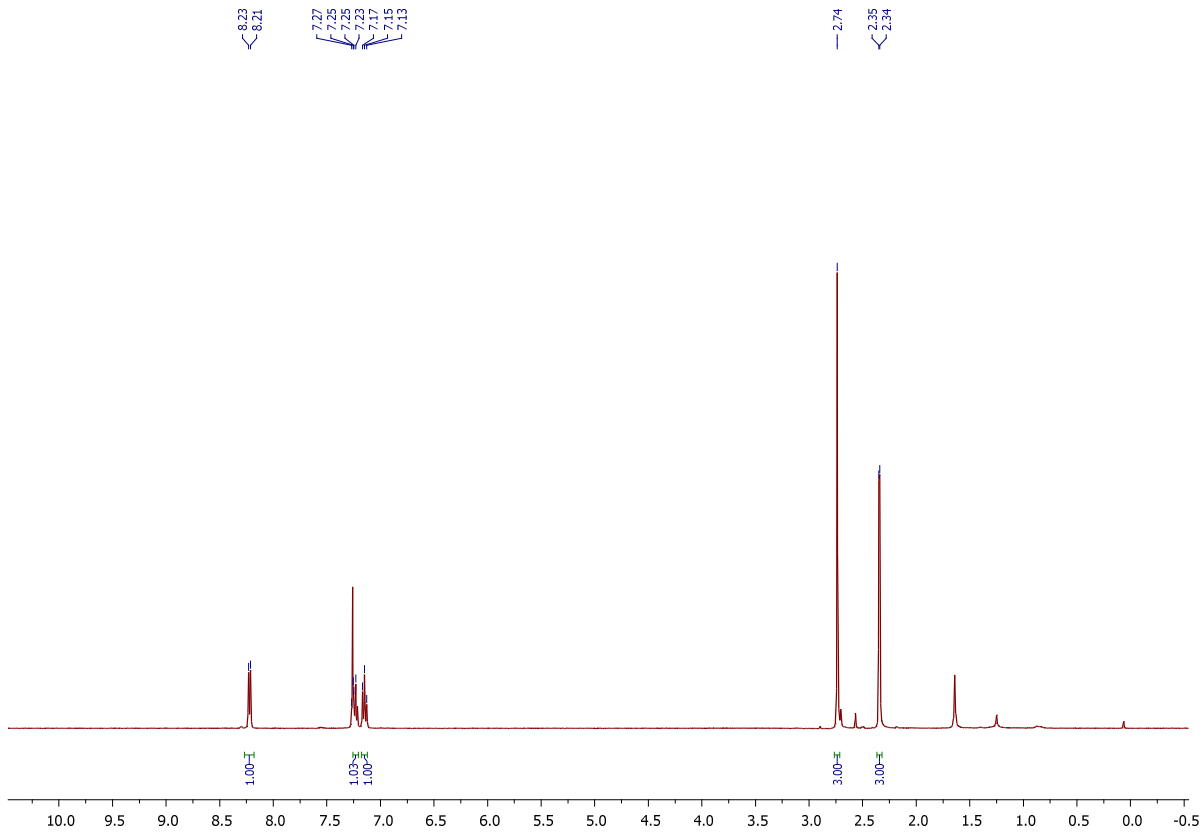
3g ^{13}C Spectrum



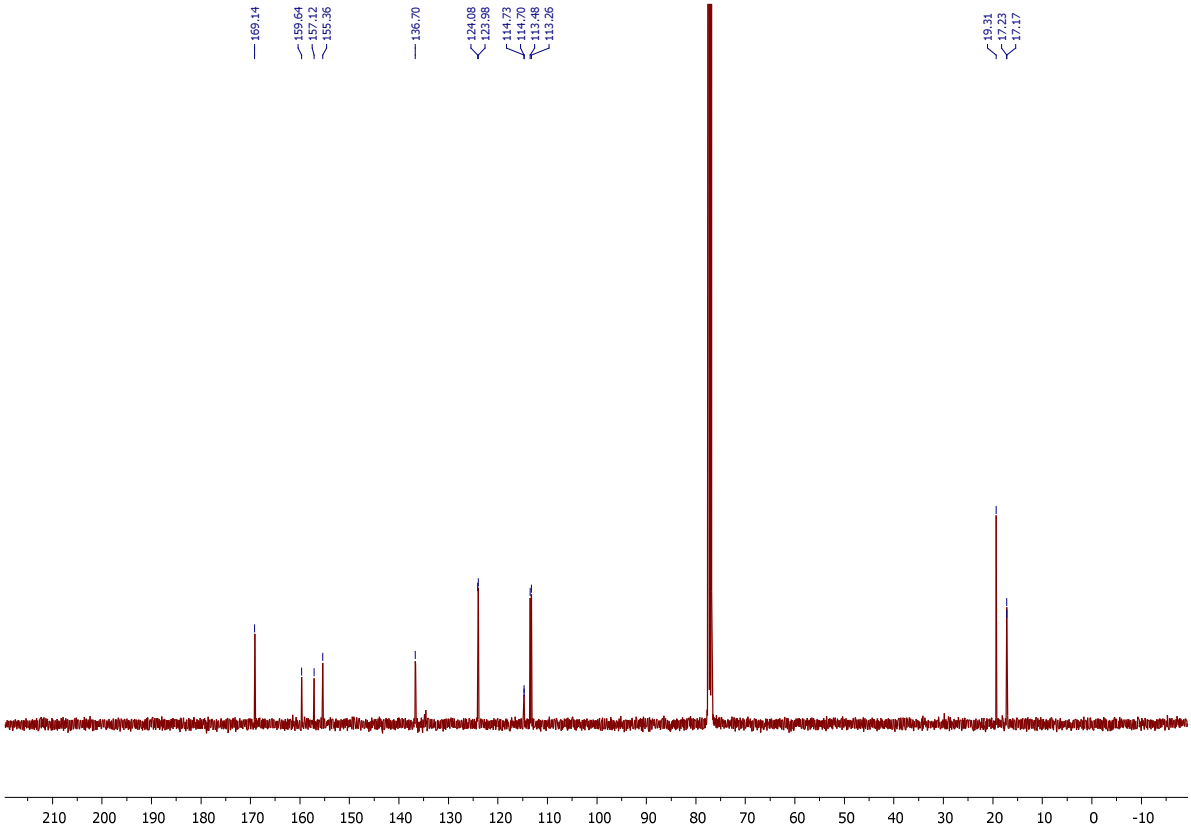
3g HRMS



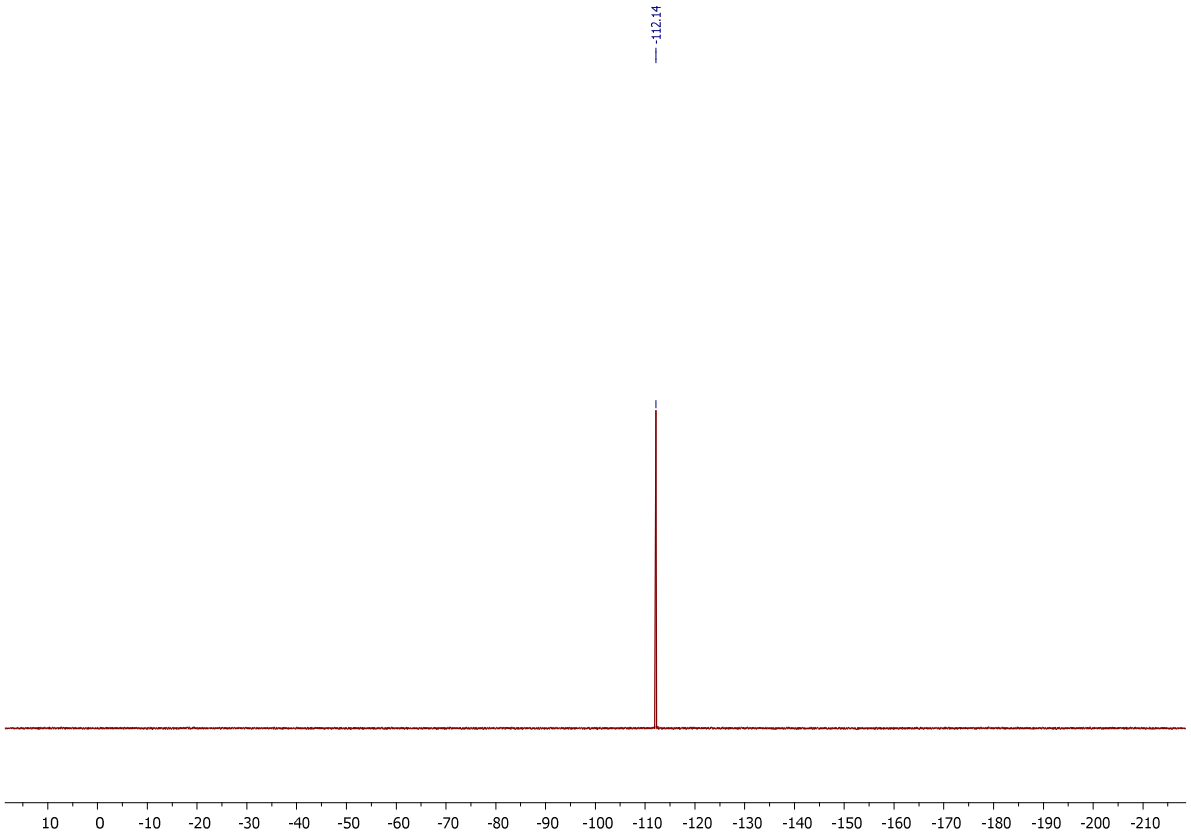
3h ^{1}H Spectrum



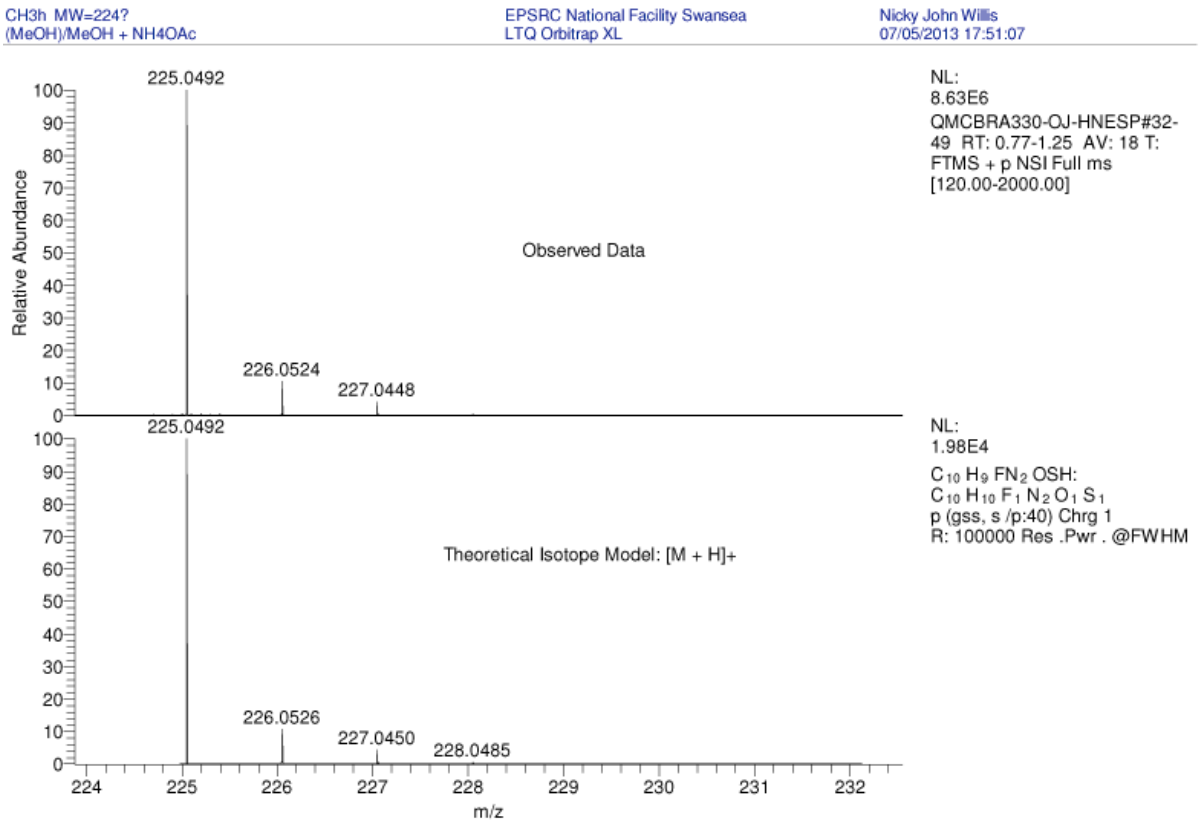
3h ^{13}C Spectrum



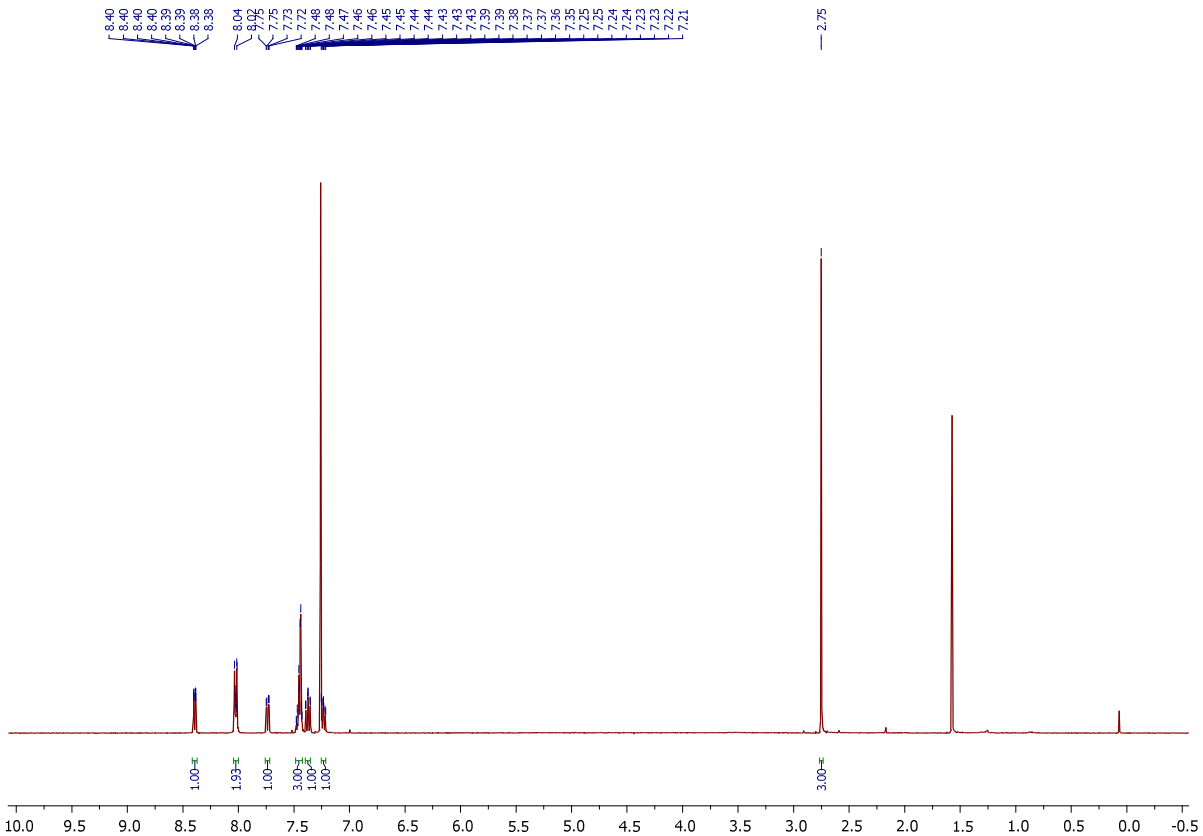
3h ^{19}F Spectrum



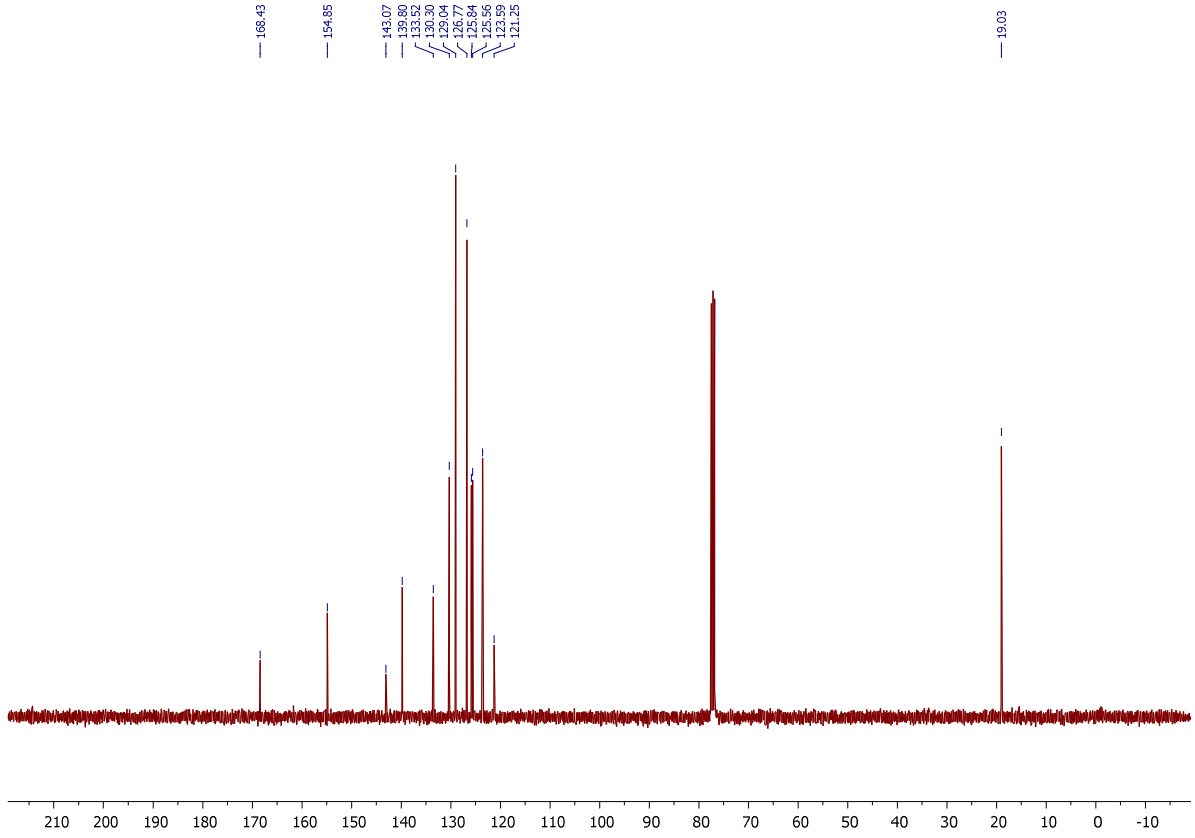
3h HRMS



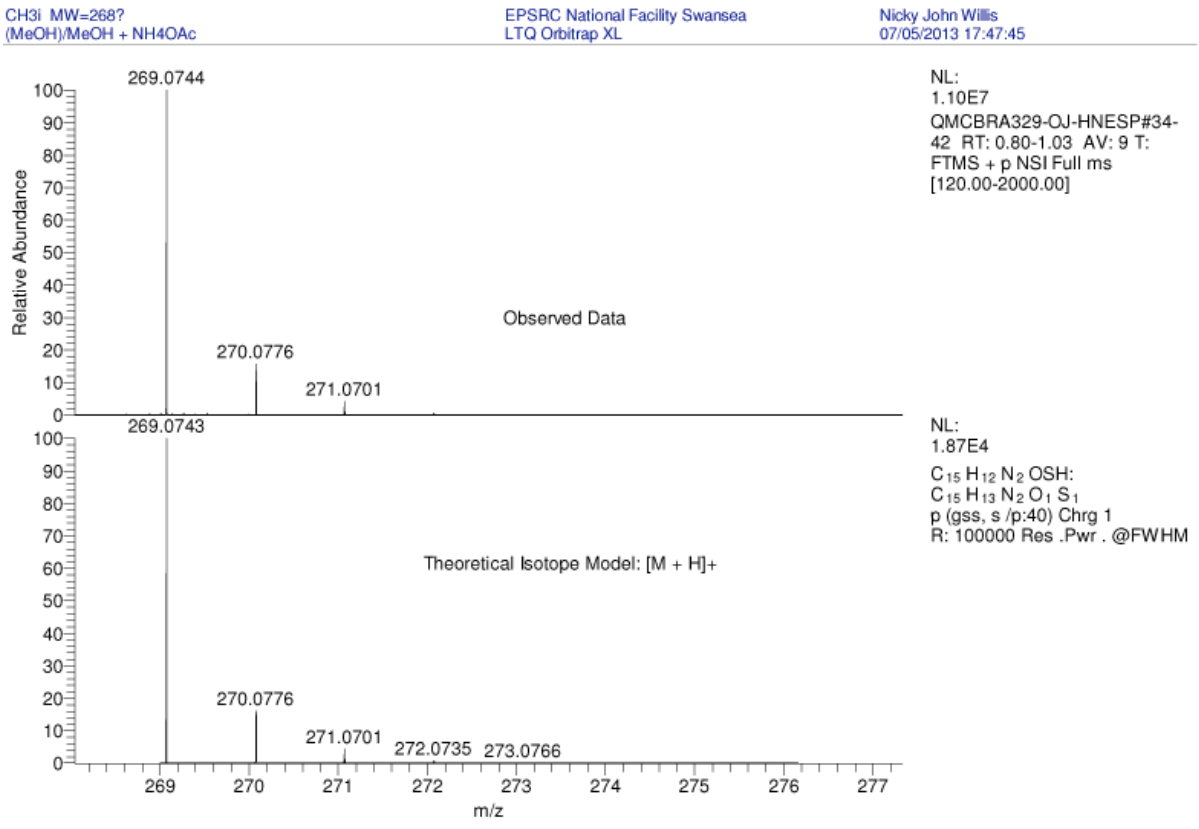
3i ^{1}H Spectrum



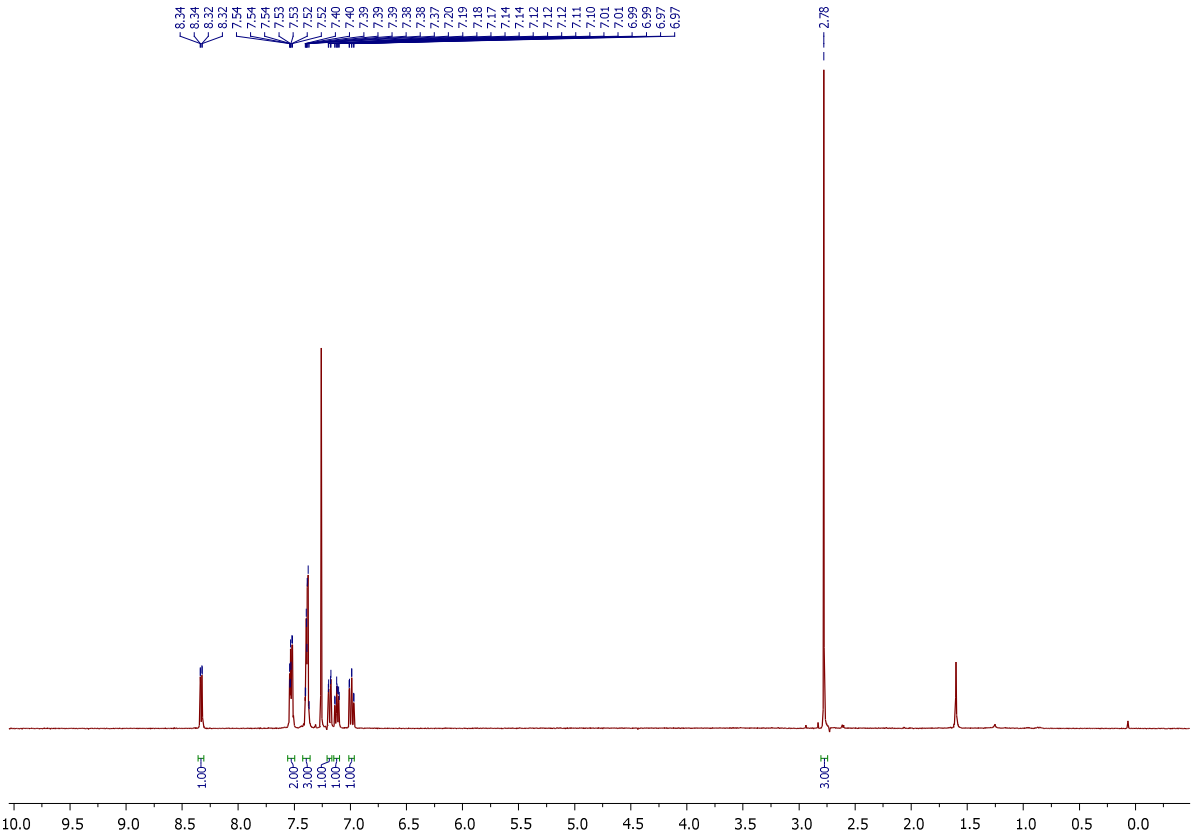
3i ^{1}H Spectrum



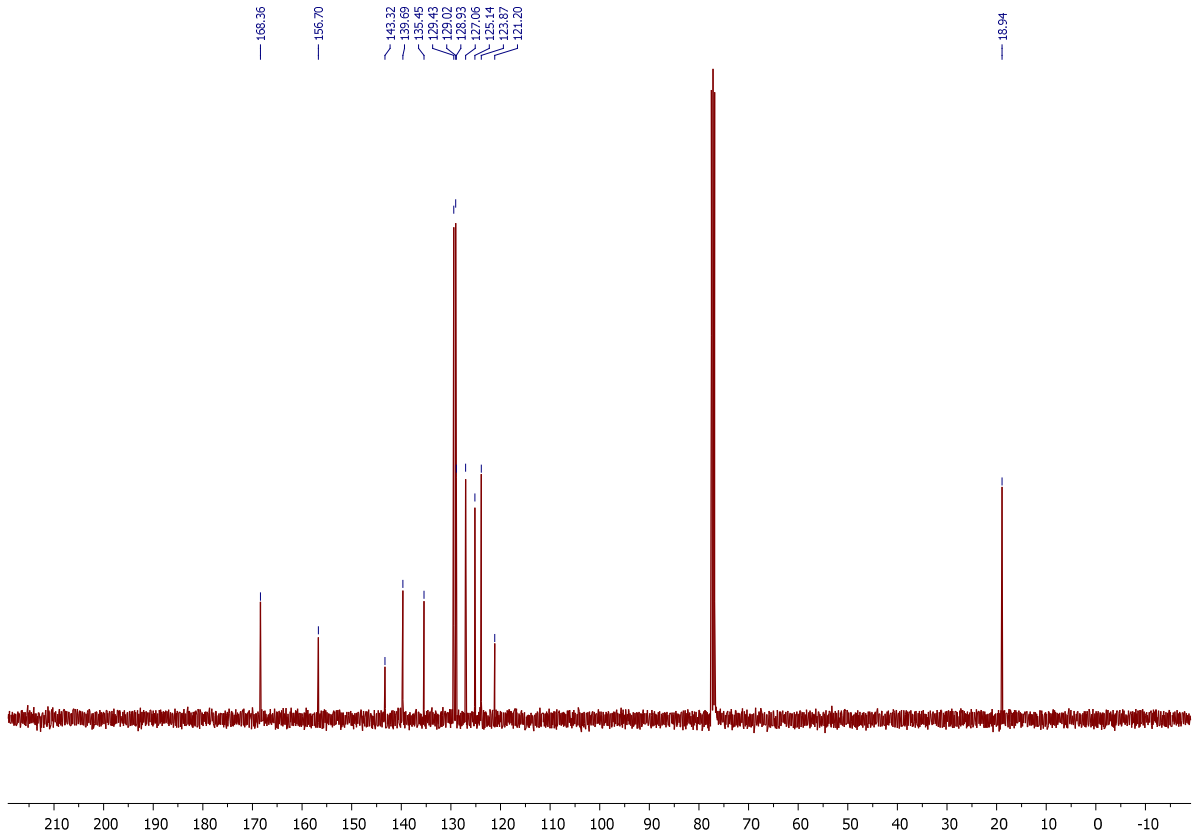
3i HRMS



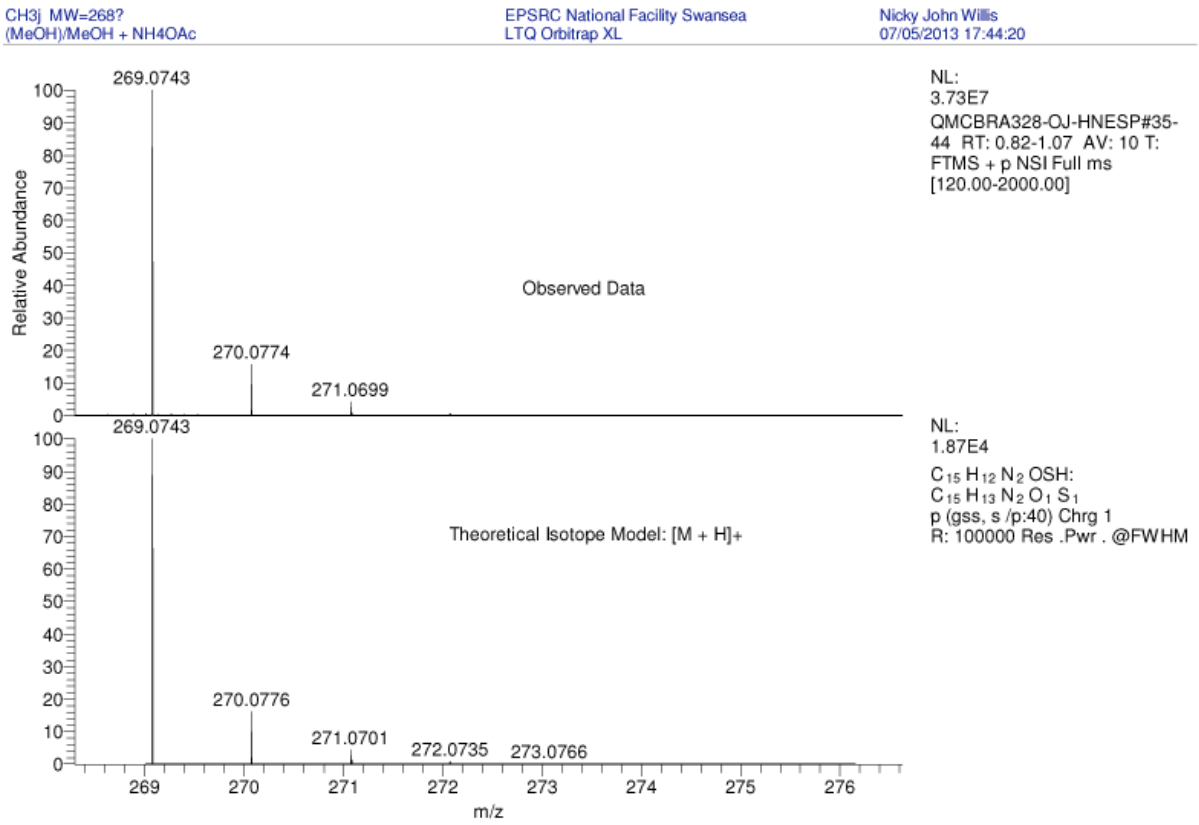
3j ^{1}H Spectrum



3j ^{13}C Spectrum



3j HRMS


CH3j MW=268?
(MeOH)/MeOH + NH4OAc
EPSRC National Facility Swansea
LTQ Orbitrap XL
Nicky John Willis
07/05/2013 17:44:20
NL:
3.73E7
QMCBRA328-OJ-HNESP#35-44 RT: 0.82-1.07 AV: 10 T: FTMS + p NSI Full ms [120.00-2000.00]
Observed Data
269.0743
270.0774
271.0699
NL:
1.87E4
C15 H12 N2 OSH:
C15 H13 N2 O1 S1
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM
Theoretical Isotope Model: [M + H]+
269.0743
270.0776
271.0701
272.0735
273.0766
Relative Abundance
m/z