Electronic Supplementary Information

Synthesis of unsymmetrical N'CN and PCN pincer palladacycles and their catalytic evaluation compared with a related SCN pincer palladacycle

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Table 1 - X-ray crystal structure data for palladacycle (**5a**)

Crystal data and structure refinement details.

Identification code	**2013ncs0430aa**	
Empirical formula	$C_{14}H_{15}ClN_2Pd$	
Formula weight	353.13	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	*Pc*	
Unit cell dimensions	a = **9.4647(7) Å**	α = **90°**
	b = **12.7252(9) Å**	β = **108.6240(10)°**
	c = **11.5908(8) Å**	γ = **90°**
Volume	1322.90(16) Å^3	
Z	4	
Density (calculated)	1.773 Mg / m^3	
Absorption coefficient	1.587 mm^{-1}	
F(000)	704	
Crystal	Block; Pale Yellow	
Crystal size	0.090 × 0.050 × 0.040 mm^3	
θ range for data collection	2.910 — 27.480°	
Index ranges	$-12 \le h \le 12$, $-16 \le k \le 16$, $-14 \le l \le 15$	
Reflections collected	17067	
Independent reflections	5364 [R_{int} = 0.0337]	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Semi—empirical from equivalents	
Max. and min. transmission	1.000 and 0.821	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5364 / 2 / 329	
Goodness-of-fit on F^2	1.097	
Final R indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0331, *wR2* = 0.0883	
R indices (all data)	*R1* = 0.0332, *wR2* = 0.0884	
Absolute structure parameter	0.034(16)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.203 and —0.700 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with VHF *Varimax* optics (70µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27 (Rigaku, 2013).* **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 3.1 b27 (Rigaku, 2013).* **Structure solution**: *SUPERFLIP* (Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790). **Structure refinement**: *SHELXL-2012* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *OLEX2* (Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Cryst. 42, 339-341).

Table 2 - X-ray crystal structure data for palladacycle (**5b**)

Crystal data and structure refinement details.

Identification code	**2013ncs0882aa**	
Empirical formula	$C_{16}H_{19}Cl_1N_2Pd_1$	
Formula weight	381.18	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P121/c1$	
Unit cell dimensions	a = **9.6575(7) Å**	α = **90°**
	b = **11.6750(8) Å**	β = **92.0790(10)°**
	c = **26.2578(18) Å**	γ = **90°**
Volume	2958.7(4) Å^3	
Z	8	
Density (calculated)	1.711 Mg / m^3	
Absorption coefficient	1.426 mm^{-1}	
F(000)	1536	
Crystal	Block; Colorless	
Crystal size	0.14 × 0.07 × 0.06 mm^3	
θ range for data collection	2.574 – 27.485°	
Index ranges	$-12 \le h \le 12, -15 \le k \le 14, -34 \le l \le 34$	
Reflections collected	20832	
Independent reflections	6748 [R_{int} = 0.0348]	
Completeness to θ = 27.500°	99.2 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.686	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6748 / 0 / 365	
Goodness-of-fit on F^2	1.067	
Final R indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0229, *wR2* = 0.0604	
R indices (all data)	*R1* = 0.0257, *wR2* = 0.0616	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.455 and –0.568 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27* (Rigaku, 2013). **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 3.1 b27 (Rigaku, 2013).* **Structure solution**: *SUPERFLIP* (Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790). **Structure refinement**: *SHELXL-2012* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *OLEX2* (Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Cryst. 42, 339-341).

Table 3 - X-ray crystal structure data for palladacycle (**5c**)

Crystal data and structure refinement details.

Identification code	**2013ncs0828r1a**	
Empirical formula	$C_{16}H_{17}Cl_1N_2O_1Pd_1$	
Formula weight	395.18	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P121/n1$	
Unit cell dimensions	a = **6.9704(5) Å**	α = **90°**
	b = **17.1706(11) Å**	β = **97.943(2)°**
	c = **12.2014(9) Å**	γ = **90°**
Volume	1446.33(18) Å^3	
Z	4	
Density (calculated)	1.815 Mg / m^3	
Absorption coefficient	1.467 mm^{-1}	
F(000)	792	
Crystal	Block; Colourless	
Crystal size	0.09 × 0.06 × 0.04 mm^3	
θ range for data collection	2.372 – 27.484°	
Index ranges	$-9 \le h \le 8, -21 \le k \le 22, -15 \le l \le 15$	
Reflections collected	9733	
Independent reflections	3305 [R_{int} = 0.0246]	
Completeness to θ = 27.500°	99.8 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.796	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3305 / 0 / 190	
Goodness-of-fit on F^2	1.187	
Final R indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0229, *wR2* = 0.0556	
R indices (all data)	*R1* = 0.0249, *wR2* = 0.0562	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.480 and –0.628 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with VHF *Varimax* optics (70µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27 (Rigaku, 2013).* **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 3.1 b27 (Rigaku, 2013).* **Structure solution**: *SUPERFLIP* (Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790).. **Structure refinement**: *SHELXL-2014* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *OLEX2* (Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Cryst. 42, 339-341).

Table 4 - X-ray crystal structure data for palladacycle (**7a**)

. Crystal data and structure refinement details.

Identification code	**2014ncs0269a**	
Empirical formula	$C_{24}H_{19}ClNOPPd$	
Formula weight	510.22	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P121/n1$	
Unit cell dimensions	a = **12.2800(8) Å**	α = **90°**
	b = **9.9230(6) Å**	β = **109.746(2)°**
	c = **17.4483(12) Å**	γ = **90°**
Volume	2001.1(2) Å^3	
Z	4	
Density (calculated)	1.694 Mg / m^3	
Absorption coefficient	1.157 mm^{-1}	
F(000)	1024	
Crystal	Shard; Yellow	
Crystal size	0.14 × 0.08 × 0.04 mm^3	
θ range for data collection	2.474 – 27.526°	
Index ranges	$-15 \le h \le 15, -12 \le k \le 12, -19 \le l \le 22$	
Reflections collected	13519	
Independent reflections	4570 [R_{int} = 0.0389]	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.742	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4570 / 0 / 262	
Goodness-of-fit on F^2	1.070	
Final R indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0329, *wR2* = 0.0813	
R indices (all data)	*R1* = 0.0385, *wR2* = 0.0856	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.002 and –0.602 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27* (Rigaku, 2013). **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 2.1 b31 (Rigaku, 2014)*. **Structure solution**: *SUPERFLIP* (Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790). **Structure refinement**: *SHELXL-2014* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *OLEX2* (Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Cryst. 42, 339-341).

Table 5 - X-ray crystal structure data for palladacycle (**7b**)

Crystal data and structure refinement details.

Identification code	**2014ncs0361a**	
Empirical formula	$C_{23}H_{17}ClNOPPd$	
Formula weight	496.20	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = **9.0914(6) Å**	α = **91.511(3)°**
	b = **9.7126(6) Å**	β = 10**8.195(3)°**
	c = **12.7482(8) Å**	γ = **112.221(2)°**
Volume	976.53(11) Å^3	
Z	2	
Density (calculated)	1.688 Mg / m^3	
Absorption coefficient	1.183 mm^{-1}	
F(000)	496	
Crystal	Block; Colorless	
Crystal size	0.13 × 0.12 × 0.07 mm^3	
θ range for data collection	2.551 – 27.509°	
Index ranges	$-11 \le h \le 11$, $-12 \le k \le 12$, $-16 \le l \le 16$	
Reflections collected	13193	
Independent reflections	4472 [R_{int} = 0.0431]	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.657	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4472 / 0 / 253	
Goodness-of-fit on F^2	1.039	
Final R indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0275, *wR2* = 0.0738	
R indices (all data)	*R1* = 0.0294, *wR2* = 0.0750	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.904 and –0.650 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27* (Rigaku, 2013). **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 2.1 b31 (Rigaku, 2014)*. **Structure solution**: *SUPERFLIP* (Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790). **Structure refinement**: *SHELXL-2014* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *OLEX2* (Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Cryst. 42, 339-341).

Figure 1 - ^{1}H NMR of 3-(pyridin-3-yl)benzaldehyde (**1**)

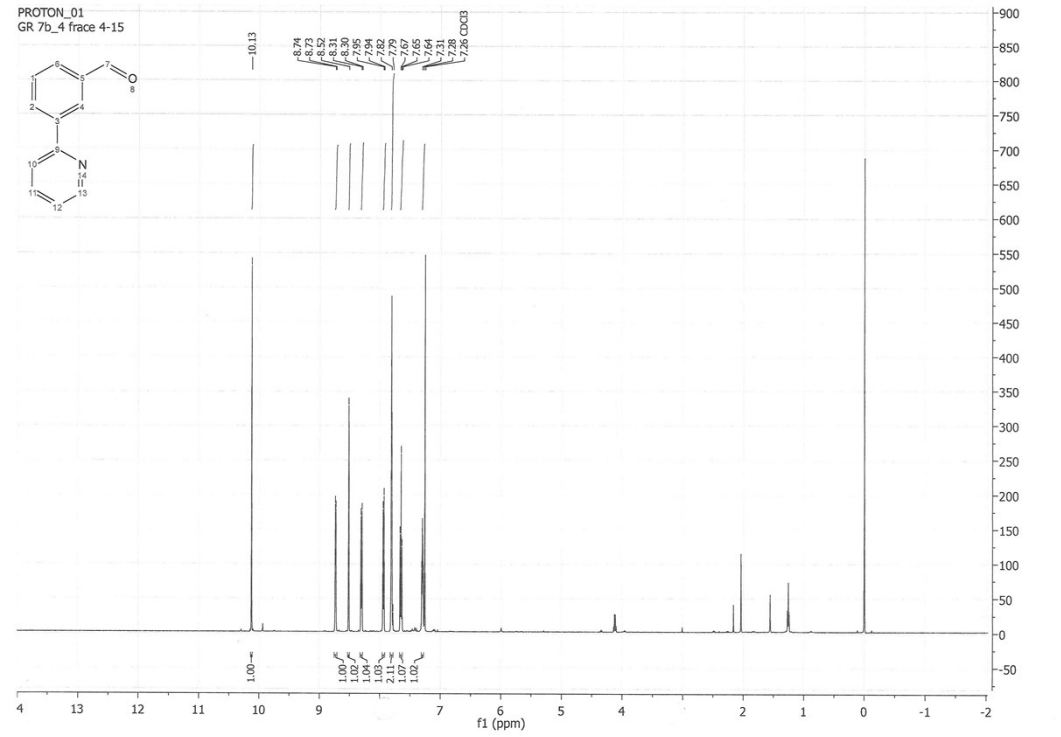
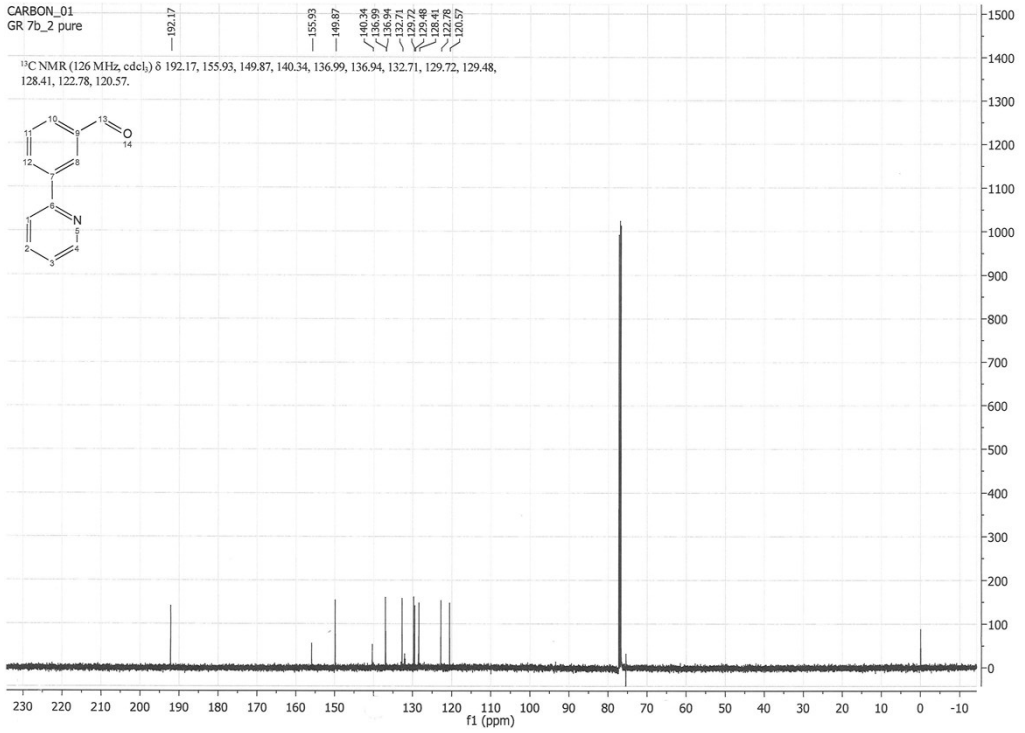
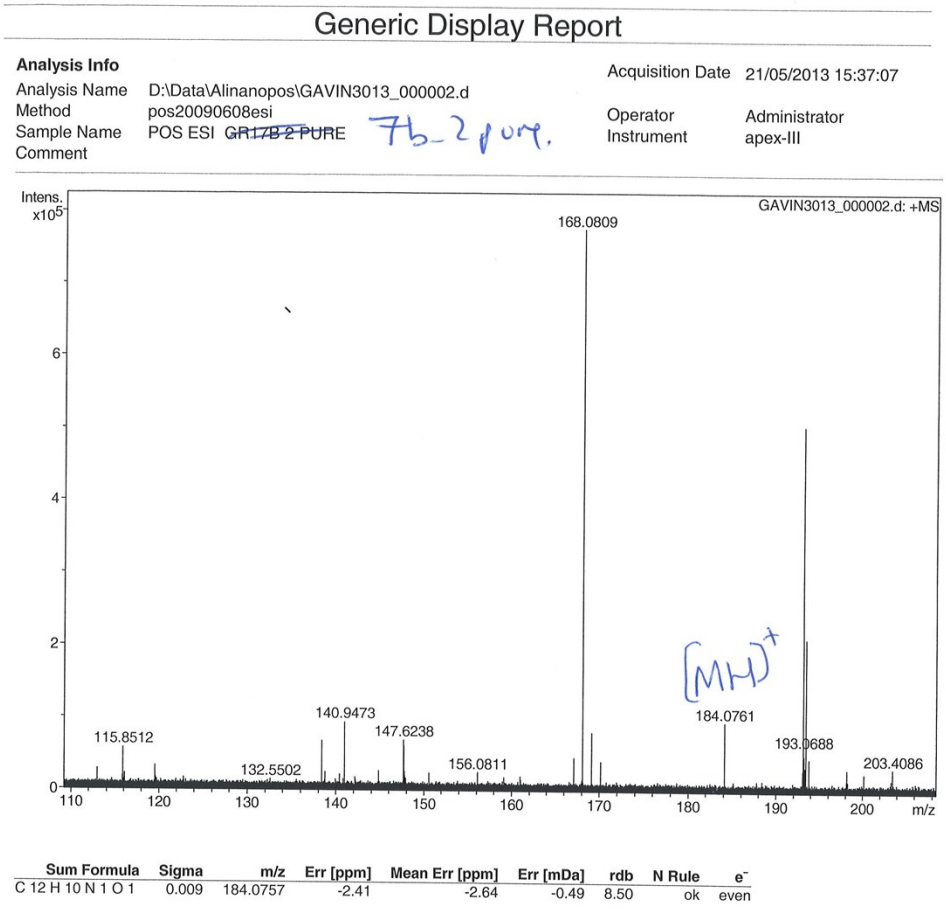


Figure 2 – ^{13}C NMR of 3-(Pyridin-



yl)benzaldehyde (**1**)

Figure 3 – HRMS of 3-(Pyridin-2-yl)benzaldehyde (**1**)



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Comment		Instrument	apex-III

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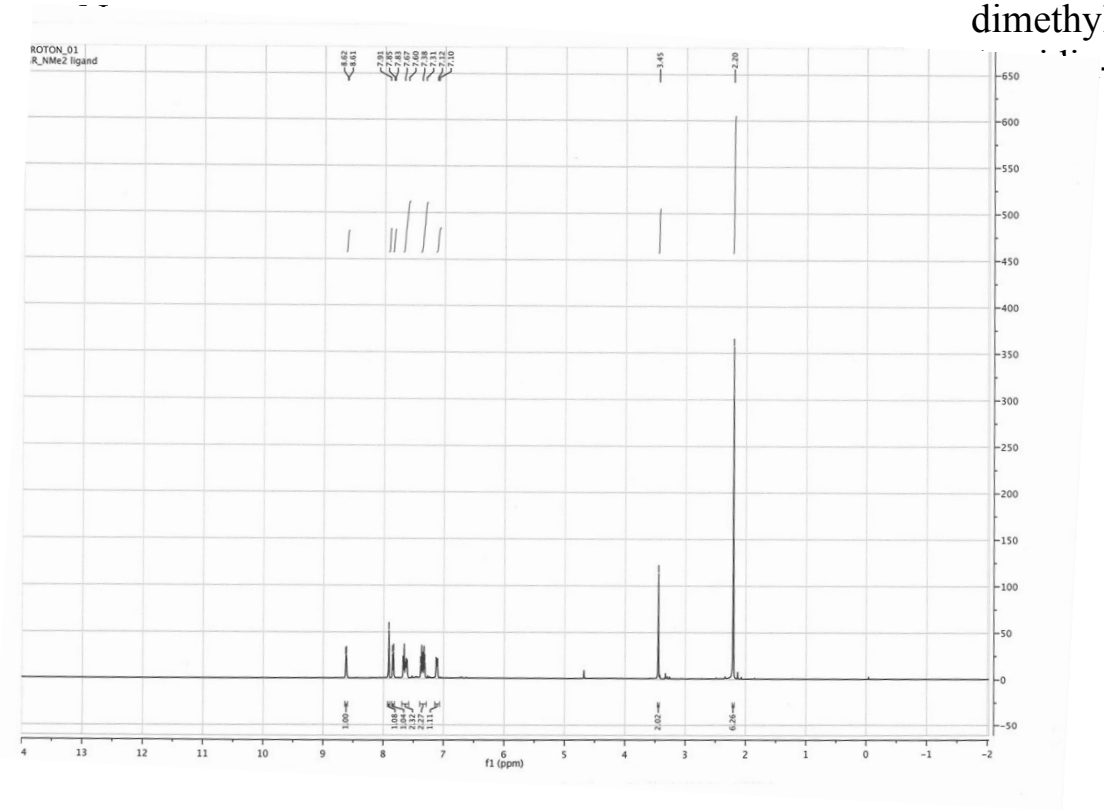
Figure 4 – ^{1}H NMR of dimethyl-[redacted]-2-



yl)phenyl)methanamine (**2a**)

Figure 5 – ^{13}C NMR of N,N-dimethyl-1-(3-(pyridin-2-yl)phenyl)methanamine (**2a**)

Figure 6 – HRMS of N,N-dimethyl-1-(3-(pyridin-2-yl)phenyl)methanamine (**2a**)

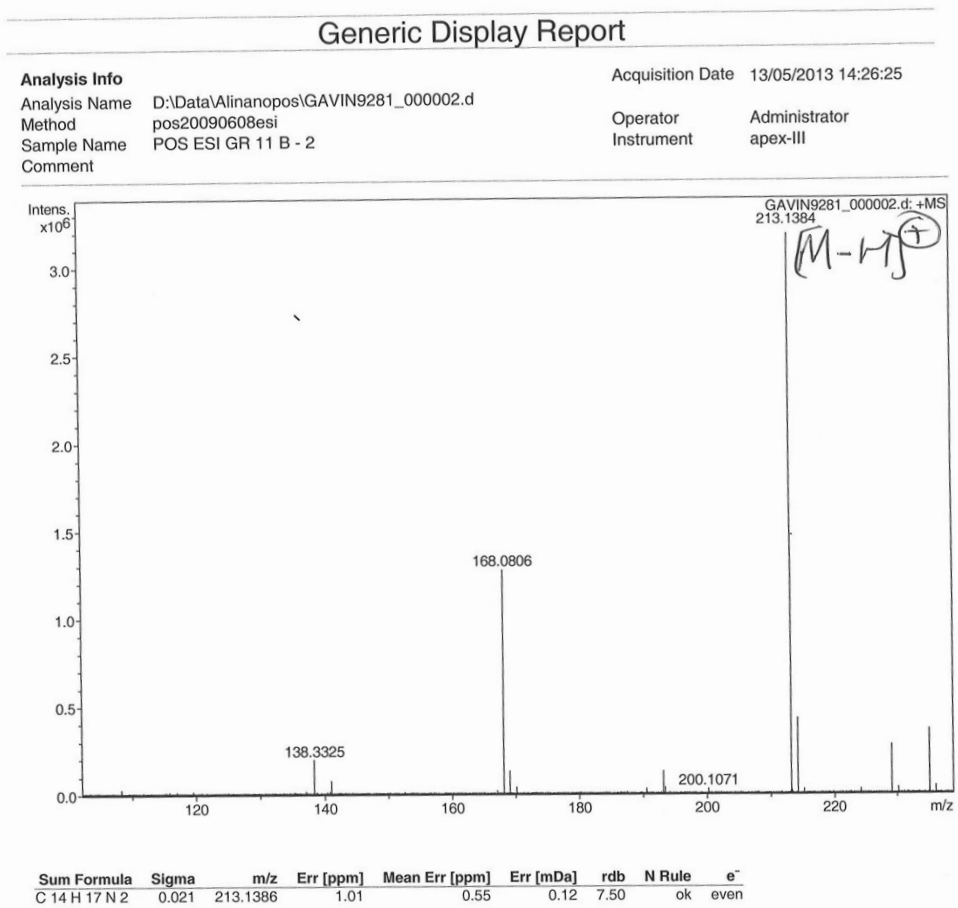


Figure 7 – ^{1}H NMR of N,N-Diethyl-1-(3-(pyridin-2-yl)phenyl)methanamine (**2b**)

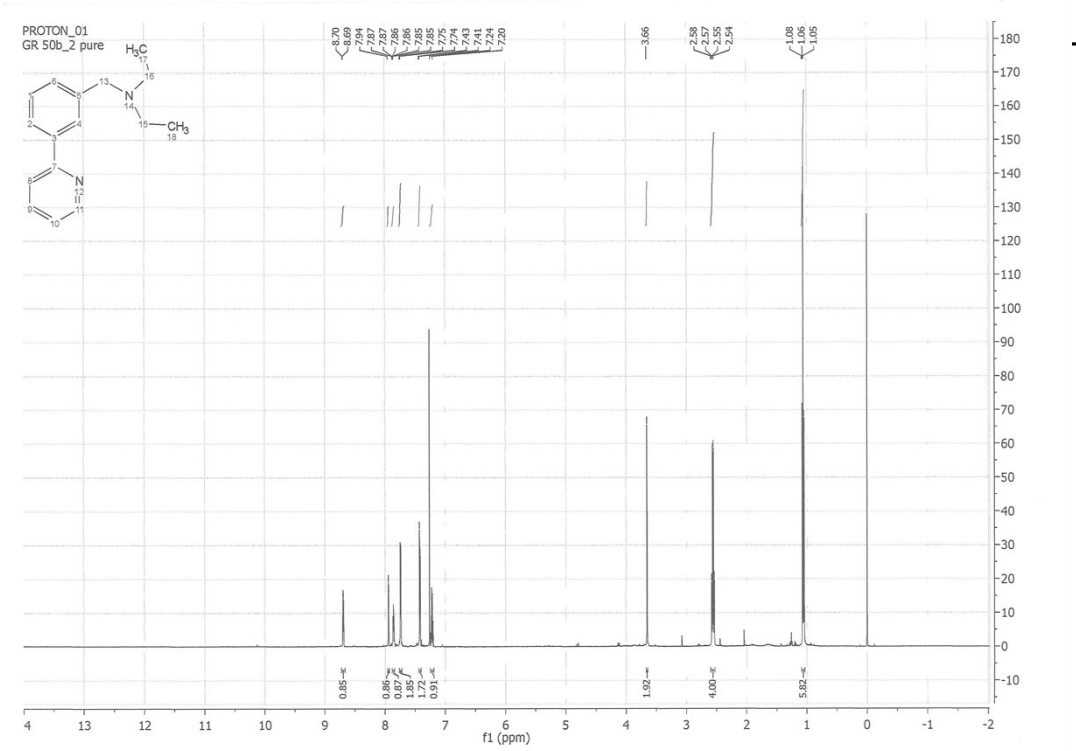
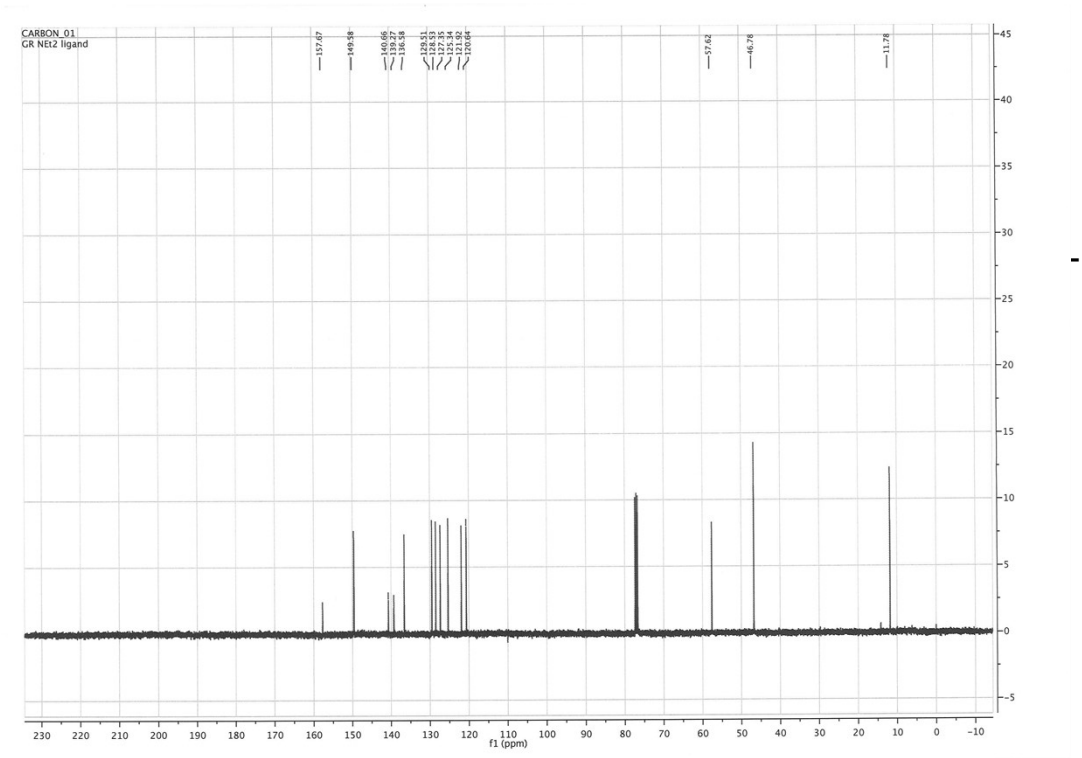


Figure 8 – ^{13}C NMR of N,N-Diethyl-1-(3-(pyridin-2-yl)phenyl)methanamine (**2b**)



-

yl)phenyl)methanamine (**2b**)

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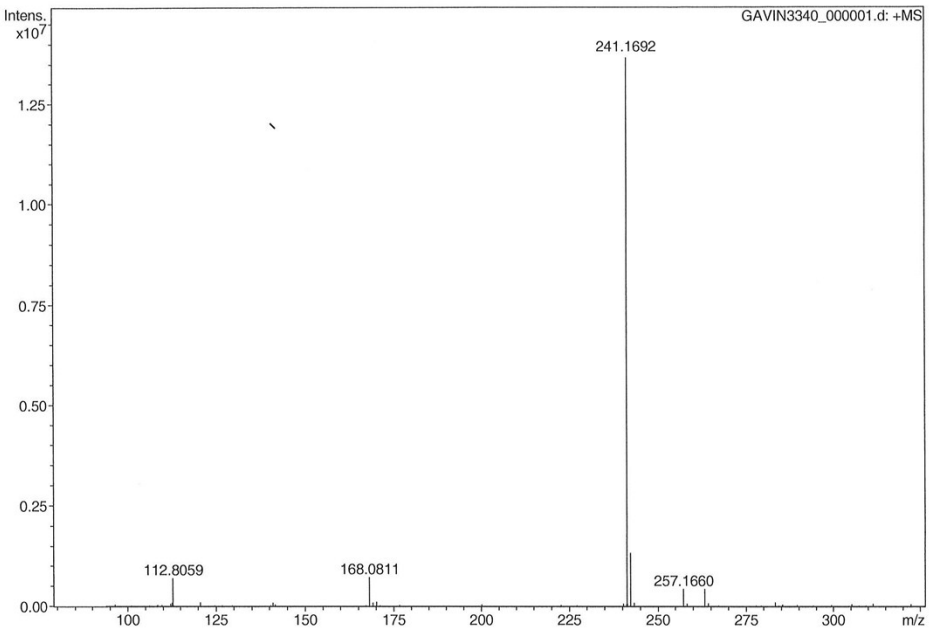

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 16 H 21 N 2	0.039	241.1699	3.13	4.05	0.98	7.50	ok	even

Figure 10 – ^{1}H NMR of 4-(3-(pyridin-2-yl)benzyl)morpholine (**2c**)

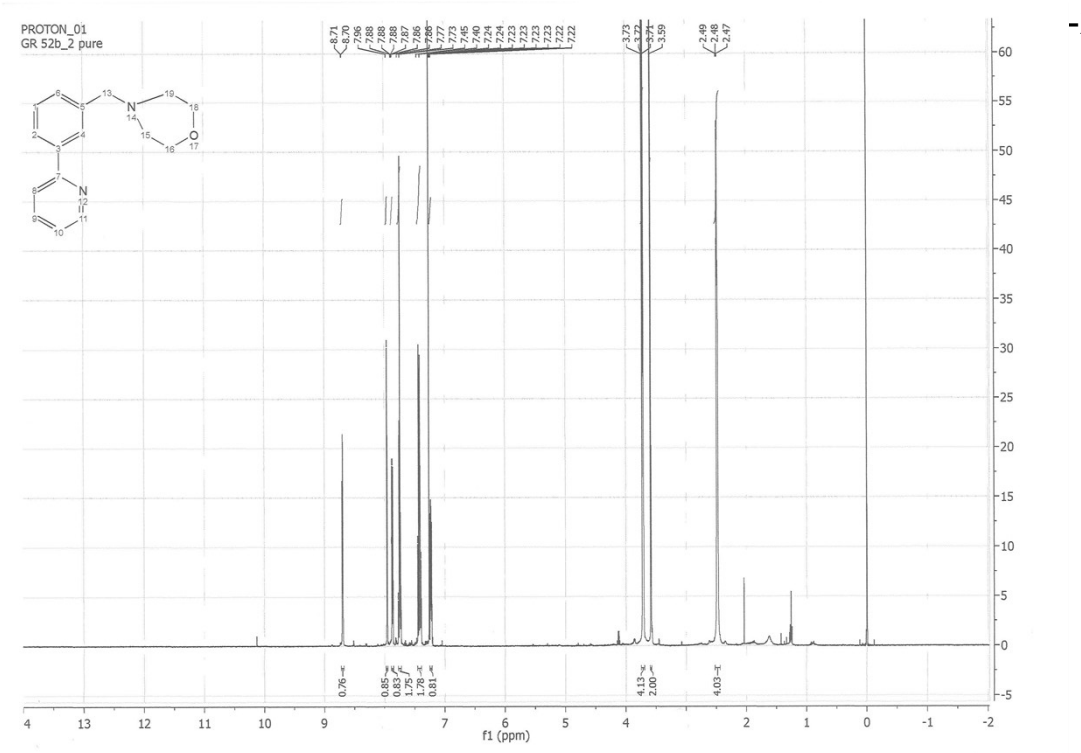

Figure 11 – ^{13}C of 4-(3-(Pyridin-2-yl)benzyl)morpholine (**2c**)

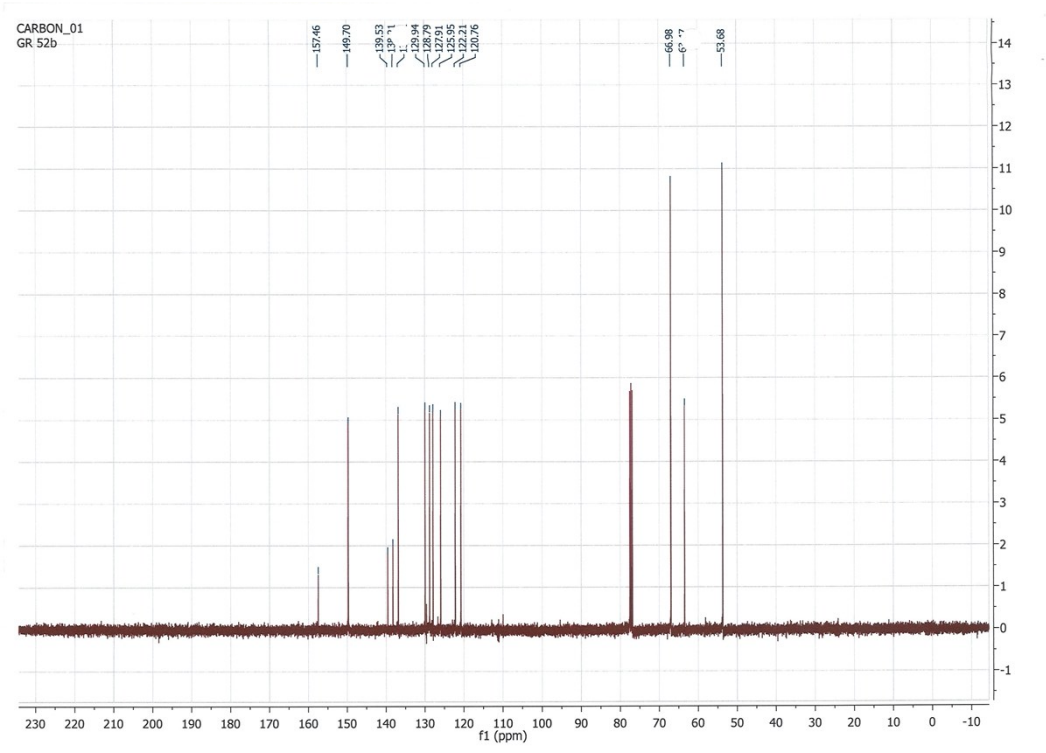

Figure 12 - HRMS of 4-(3-(Pyridin-2-yl)benzyl)morpholine (**2c**)

Generic Display Report

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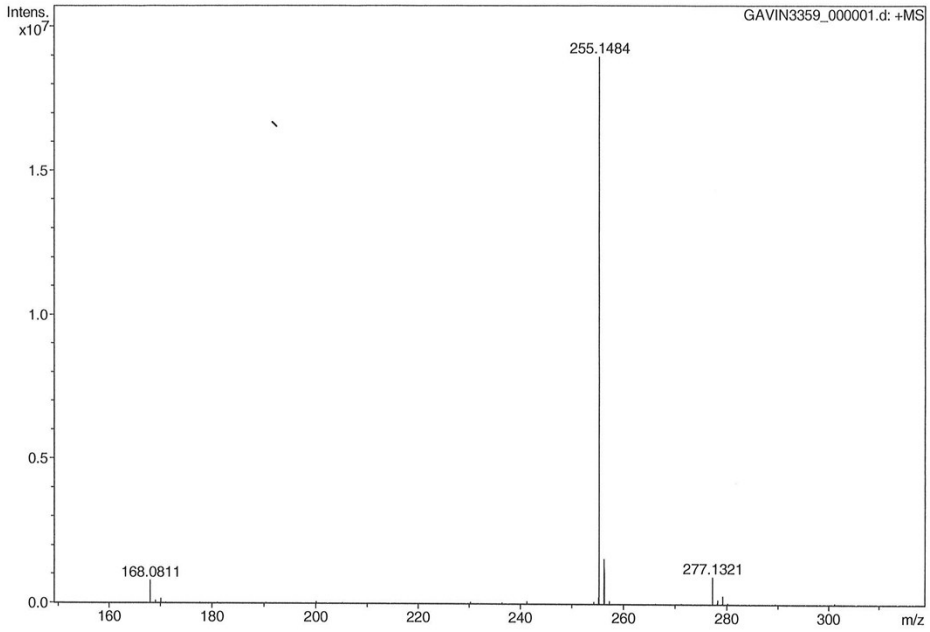
Comment			



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 16 H 19 N 2 O 1	0.046	255.1492	3.13	1.20	0.31	8.50	ok	even

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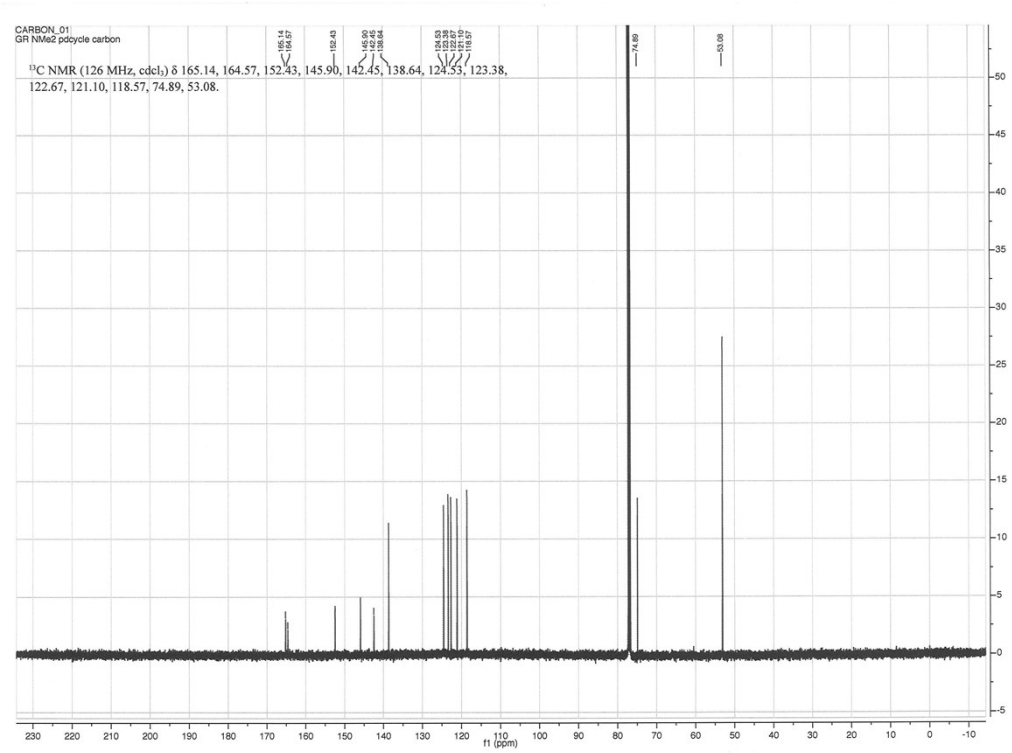
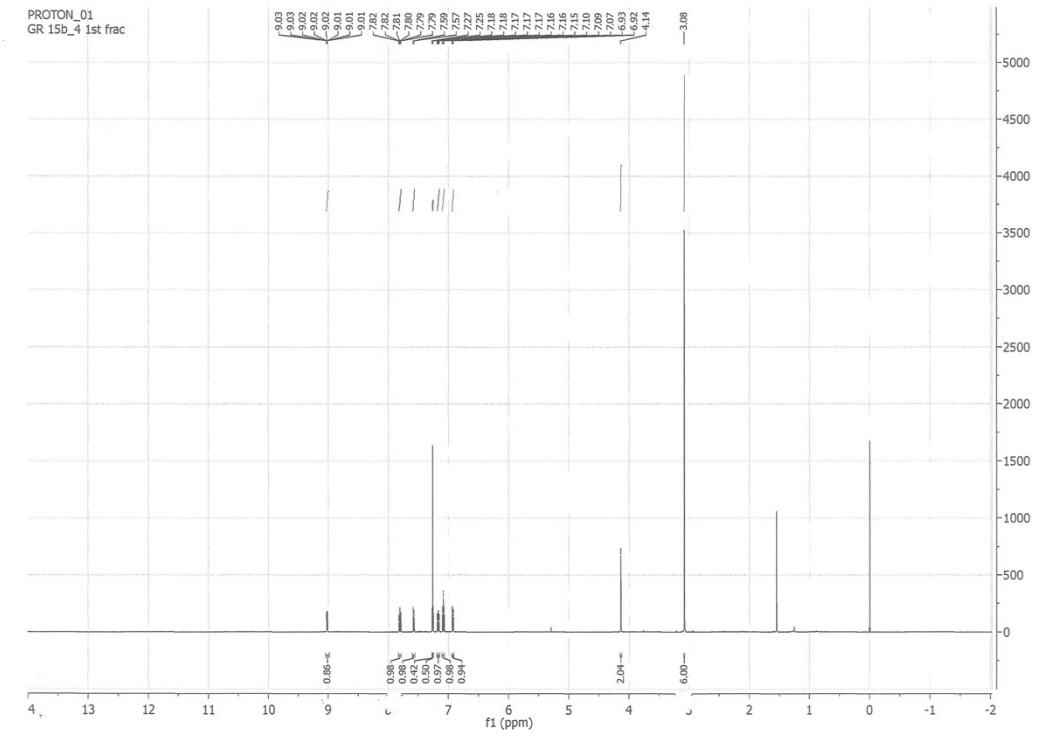
Figure 13 - ^{1}H NMR of palladacycle (**5a**)





palladacycle (**5a**)

Figure 15 – HRMS of palladacycle (**5a**)

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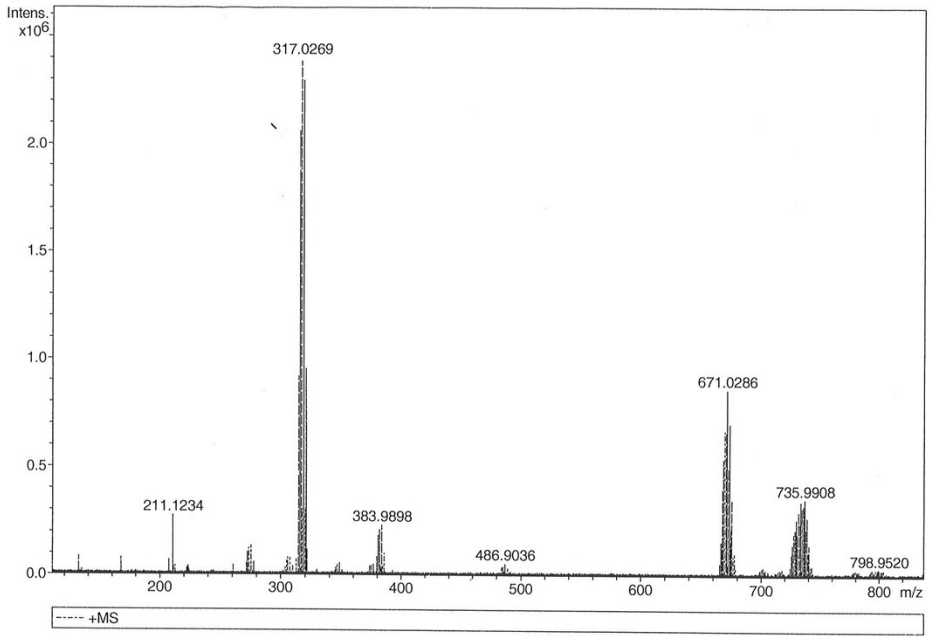

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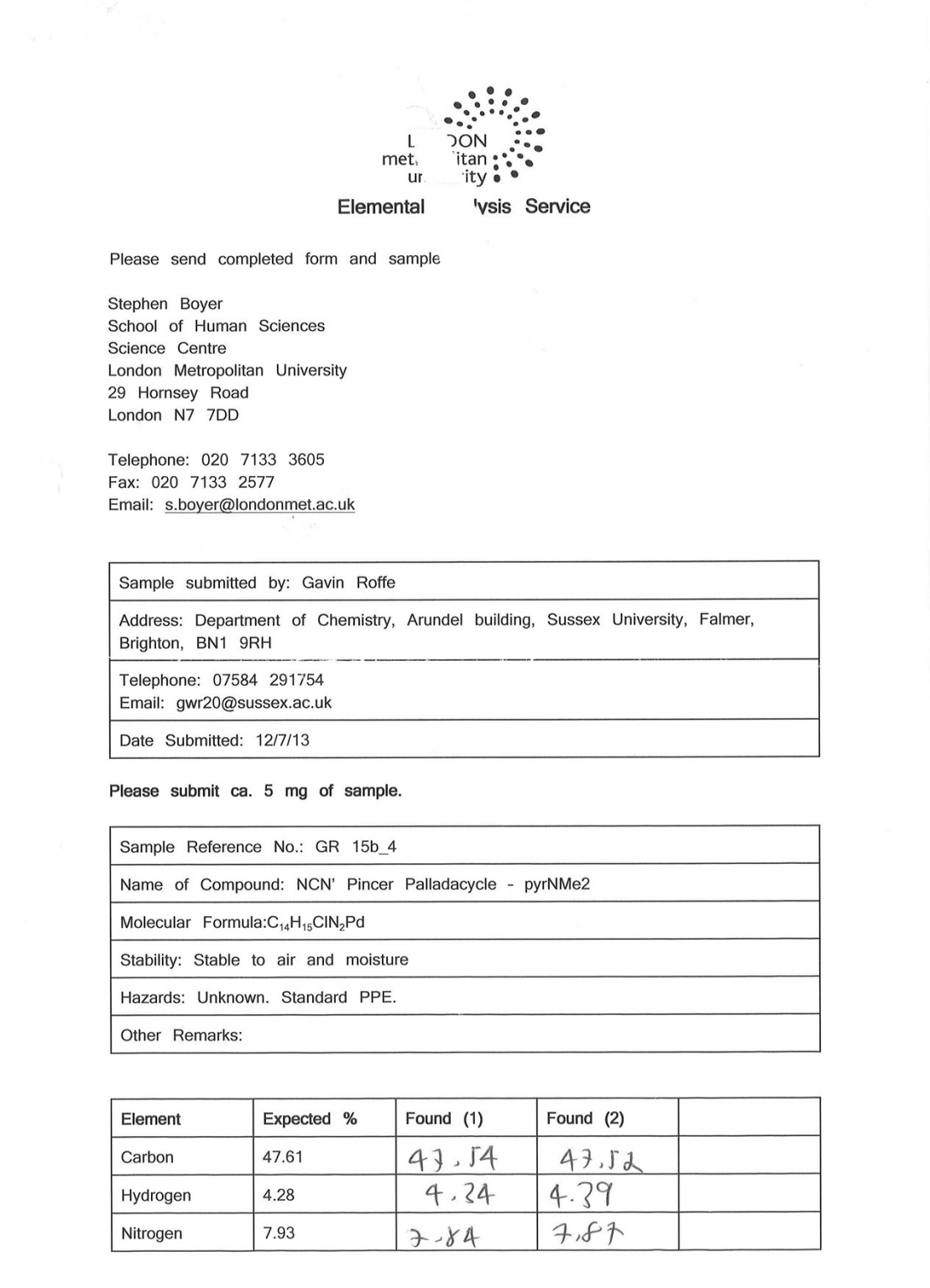
GR12b.

Figure 16 – Elemental Analysis of palladacycle (**5a**)



Elemental Analysis Service

Please send completed form and sample

Stephen Boyer
School of Human Sciences
Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

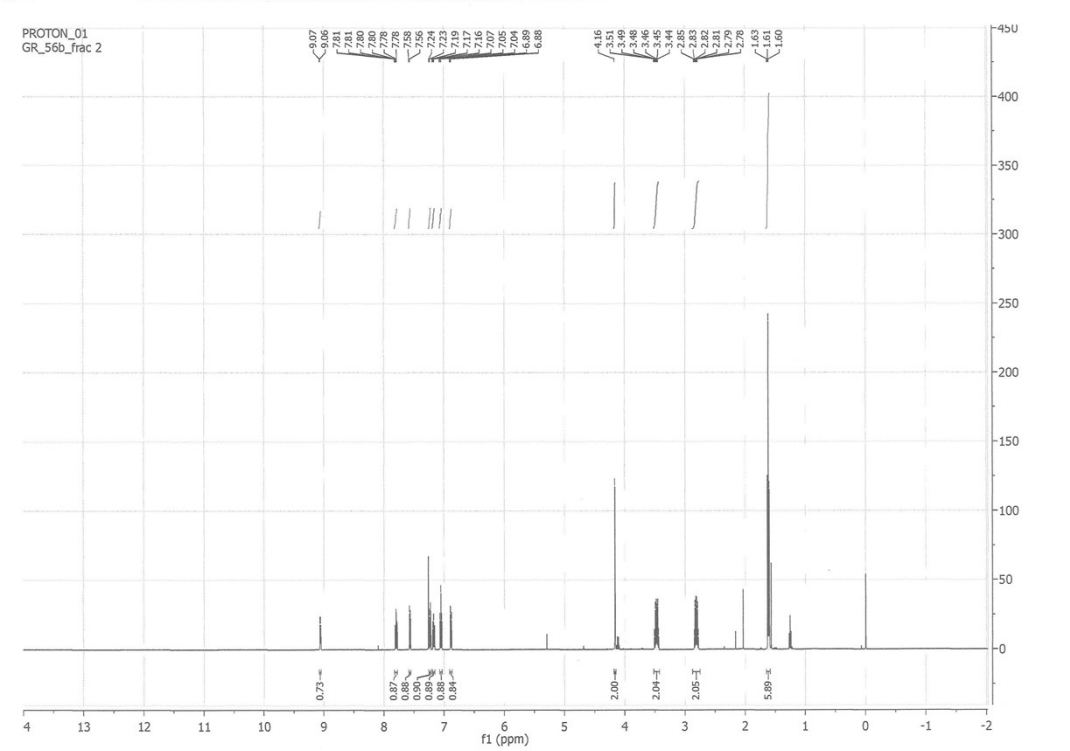
Sample submitted by: Gavin Roffe
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584 291754 Email: gwr20@sussex.ac.uk
Date Submitted: 12/7/13

Please submit ca. 5 mg of sample.

Sample Reference No.: GR 15b_4
Name of Compound: NCN' Pincer Palladacycle - pyrNMe2
Molecular Formula: $C_{14}H_{15}ClN_2Pd$
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	47.61	47.54	47.52	
Hydrogen	4.28	4.24	4.39	
Nitrogen	7.93	7.84	7.87	

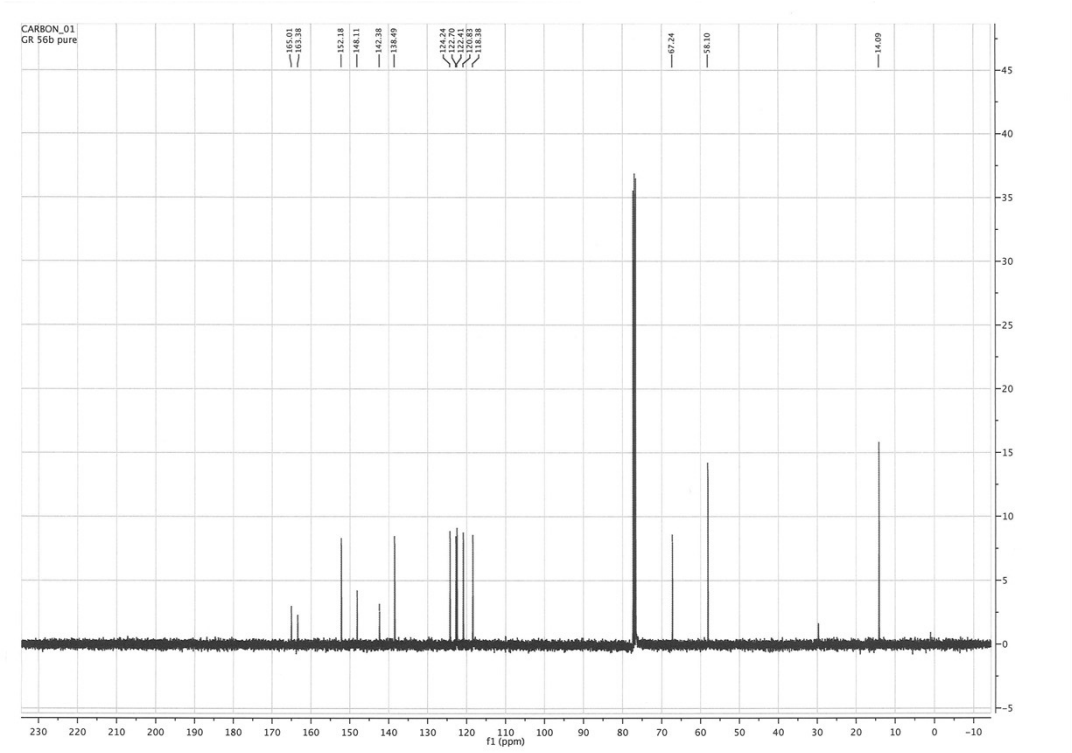
Figure 17 – ^{1}H NMR of



palladacycle (**5b**)

Figure 18 – ^{13}C NMR of palladacycle (**5b**)

Figure 19 – HRMS of palladacycle (**5b**)



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Method	pos20090608esi		
Sample Name	POS ESI GR 56 B	Operator	Administrator
Comment		Instrument	apex-III

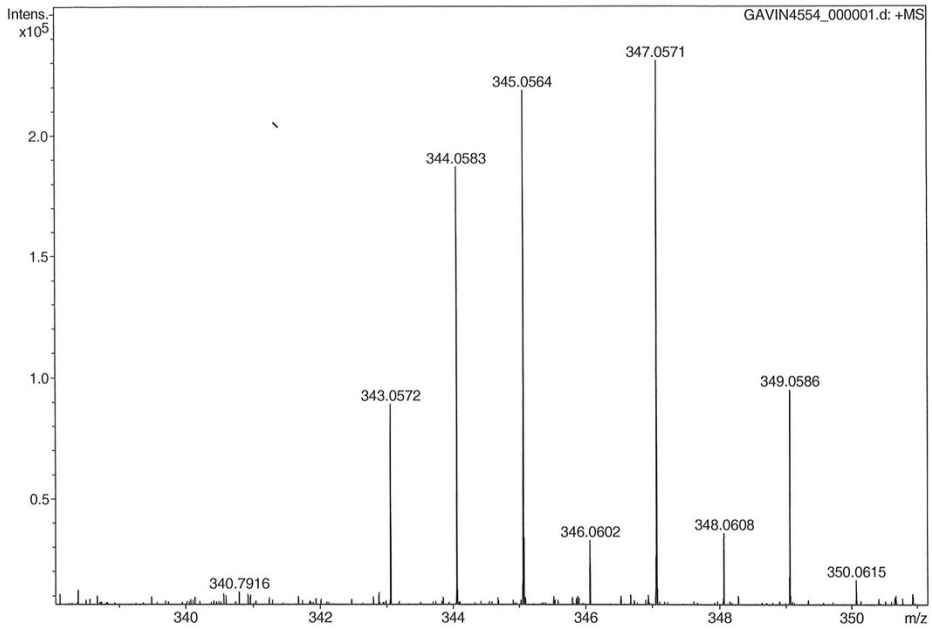
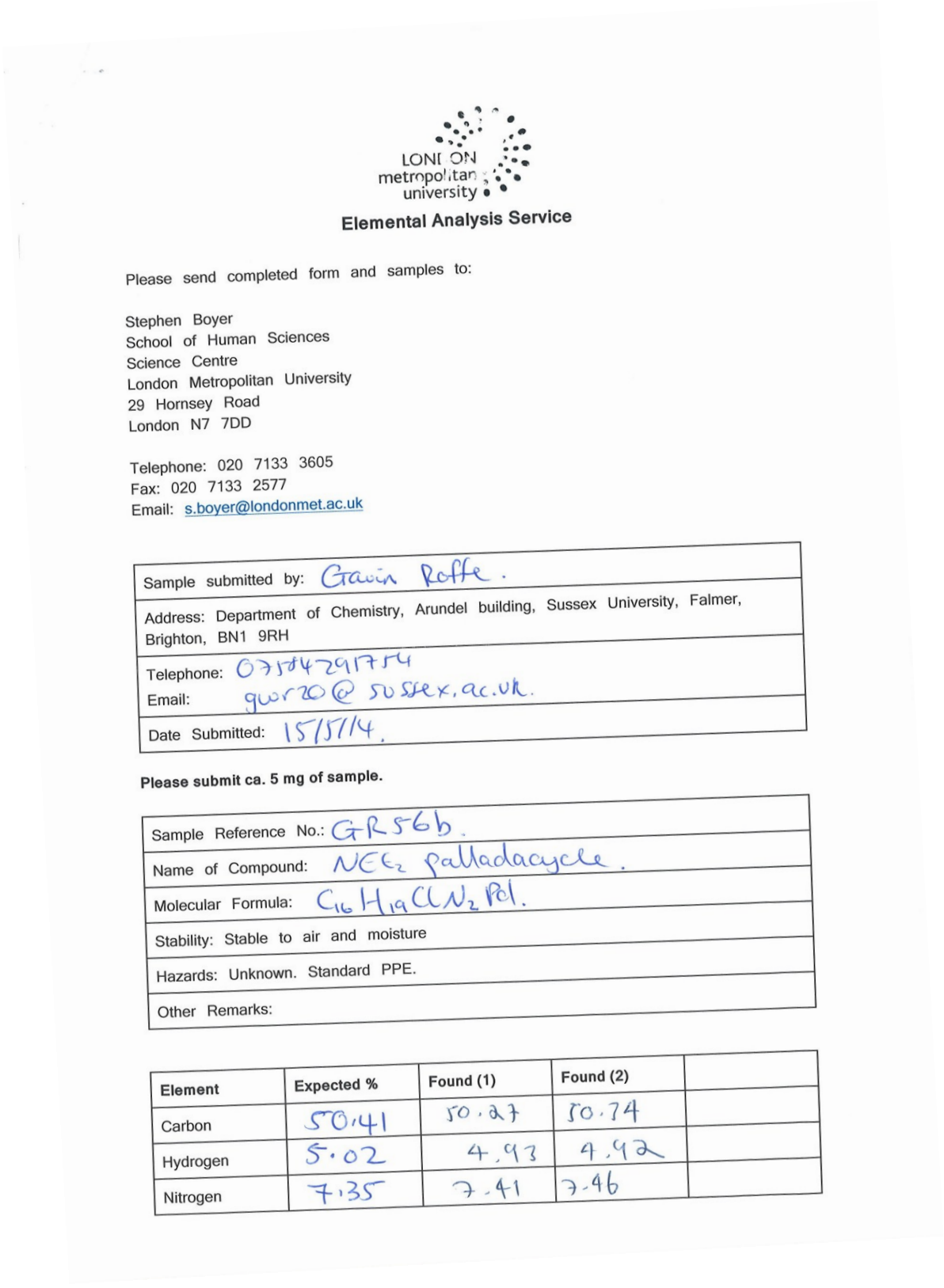


Table 'GenFormulaResults' could not be found in this analysis

Figure 20 – Elemental analysis of palladacycle (**5b**)



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Elemental Analysis Service

Please send completed form and samples to:

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Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

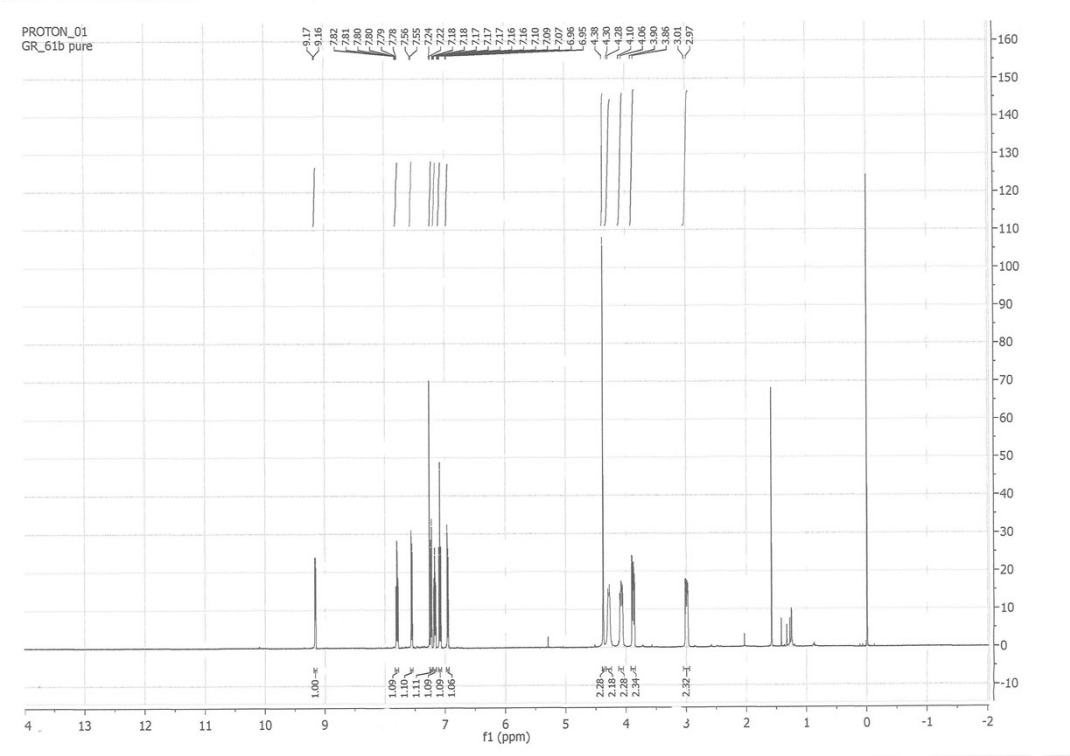
Sample submitted by: Gavin Roffe.
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584291754 Email: gwr20@sussex.ac.uk.
Date Submitted: 15/5/14.

Please submit ca. 5 mg of sample.

Sample Reference No.: GR56b.
Name of Compound: NEt_2 palladacycle.
Molecular Formula: $C_{16}H_{19}ClN_2Pd$.
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	50.41	50.27	50.74	
Hydrogen	5.02	4.93	4.92	
Nitrogen	7.35	7.41	7.46	

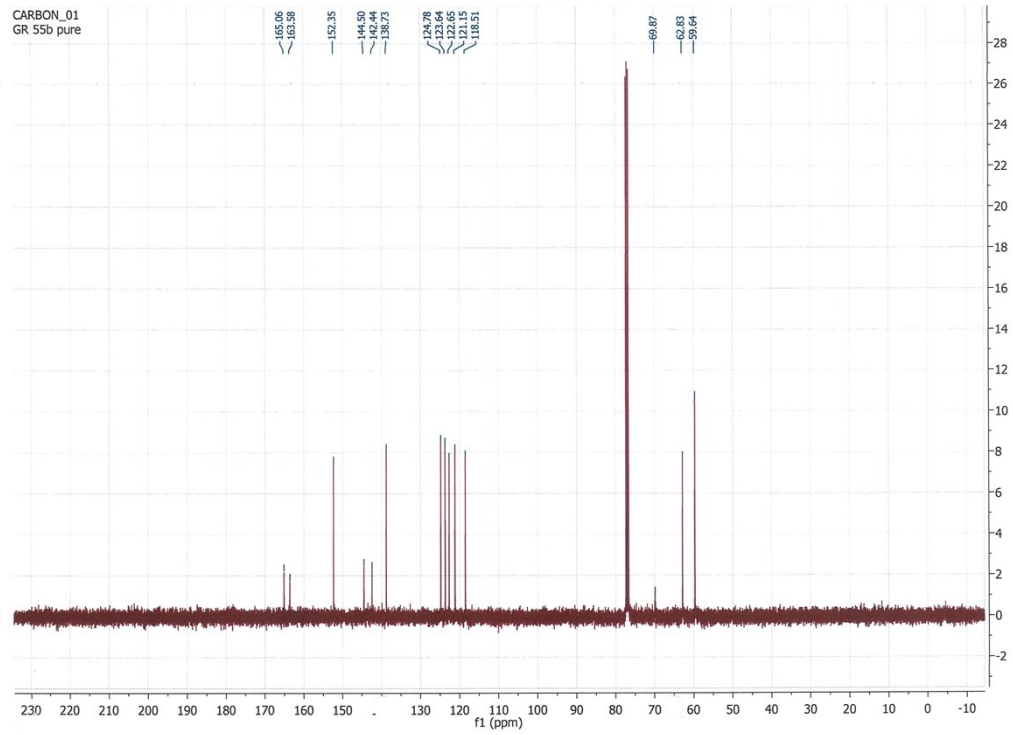
Figure 21 – ^{1}H NMR of



palladacycle (**5c**)

Figure 22 – ^{13}C NMR of palladacycle (**5c**)

Figure 23 – HRMS of palladacycle (**5c**)



Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN4555_000001.d	Acquisition Date	18/08/2014 19:02:12
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR 55 B	Instrument	apex-III
Comment			

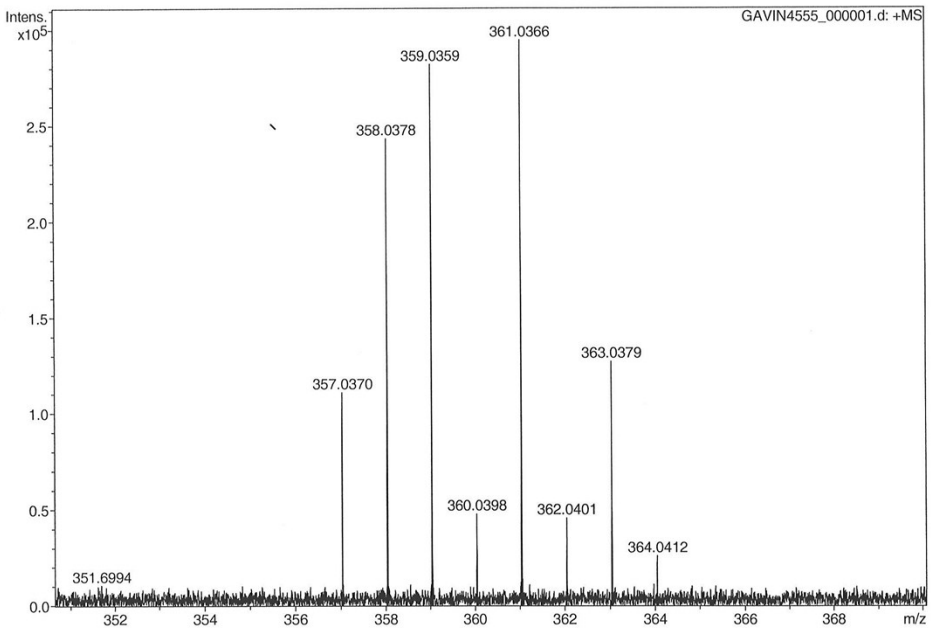


Table 'GenFormulaResults' could not be found in this analysis

Bruker Daltonics DataAnalysis 3.4 printed: 19/08/2014 11:59:57 Page 1 of 1

Figure 24 – Elemental Analysis of palladacycle (**5c**)

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Telephone: 020 7133 3605
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Email: s.boyer@londonmet.ac.uk

Sample submitted by: Gavin Roffe
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584291754 Email: gwr20@sussex.ac.uk
Date Submitted: 4/4/14

Please submit ca. 5 mg of sample.

Sample Reference No.: GR 65b
Name of Compound: Morph palladacycle
Molecular Formula: $C_{16}H_{17}ClN_2OPd$
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	48.63	48.51	48.39	
Hydrogen	4.34	4.38	4.42	
Nitrogen	7.09	6.85	6.97	

Figure 25 – ^{1}H of 3-(pyridin-2-yl)phenol (**6**)

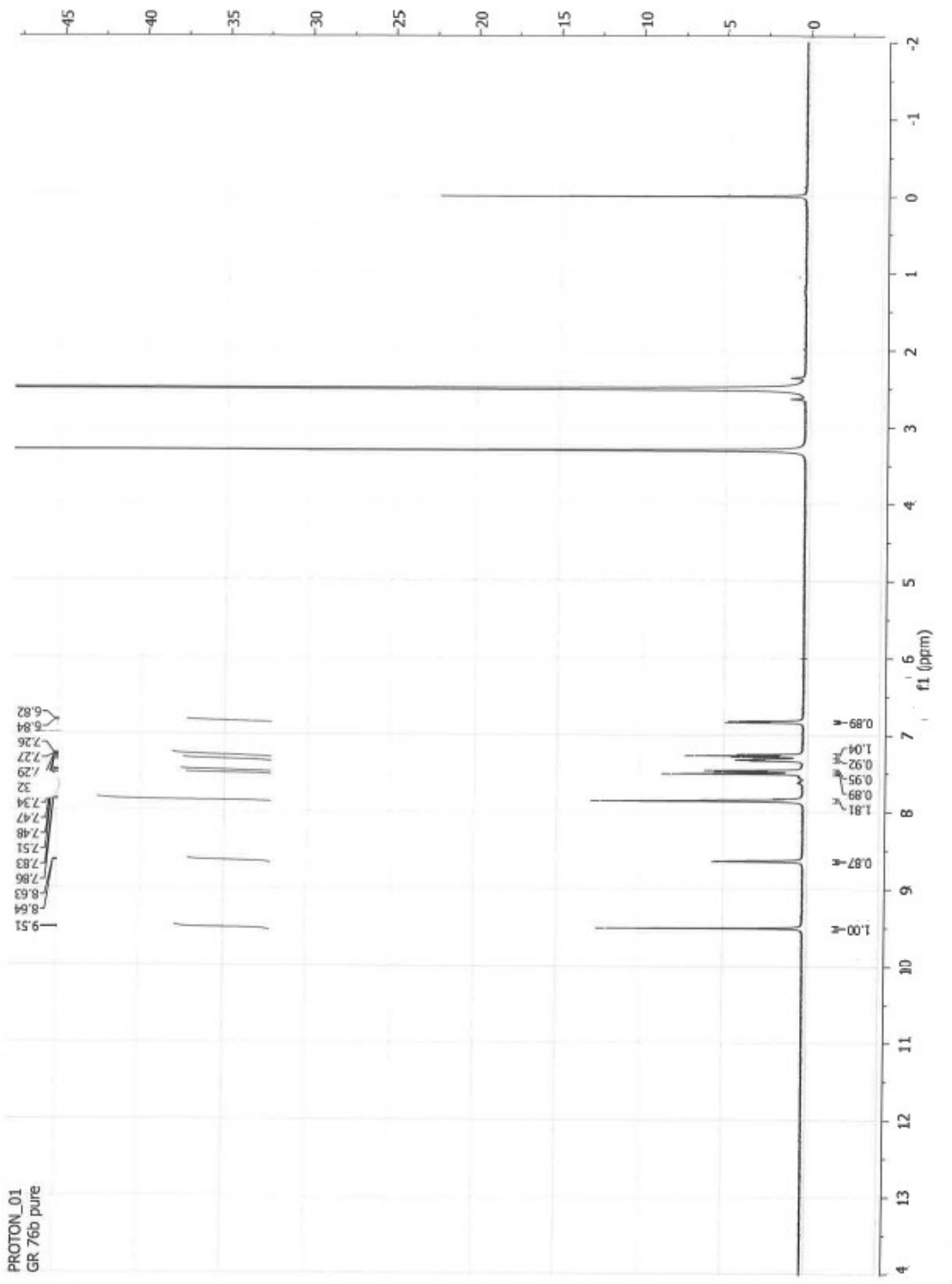

PROTON_01
GR 76b pure
f1 (ppm)
9.51
8.64
8.63
7.86
7.83
7.51
7.48
7.47
7.34
7.32
7.29
7.27
7.26
6.84
6.82
1.00
0.87
1.81
0.89
0.95
0.92
1.04
0.89

Figure 26 – ^{13}C NMR of 3-(pyridin-2-yl)phenol (**6**)

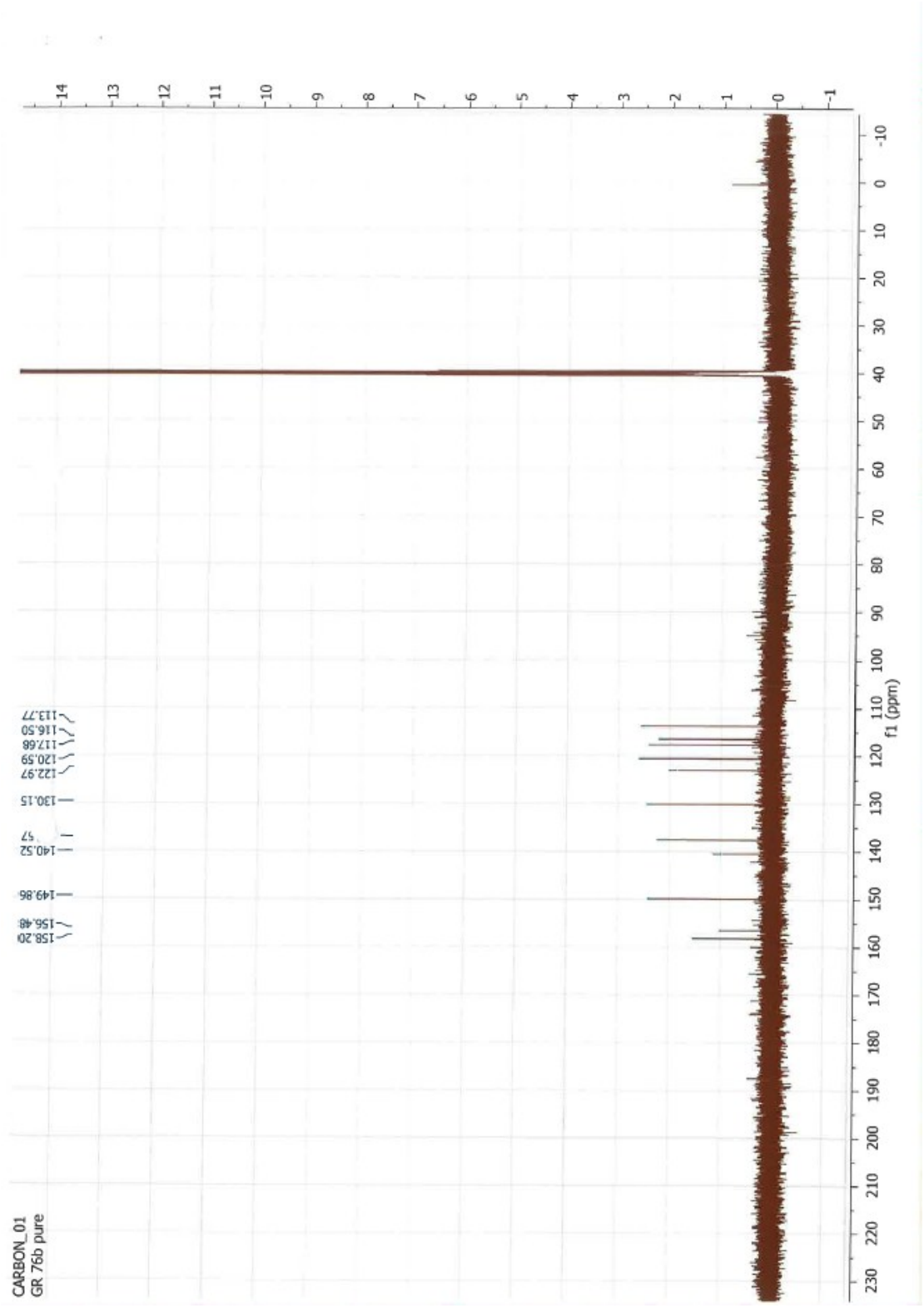


Figure 27 – HRMS of 3-(pyridin-2-yl)phenol (**6**)

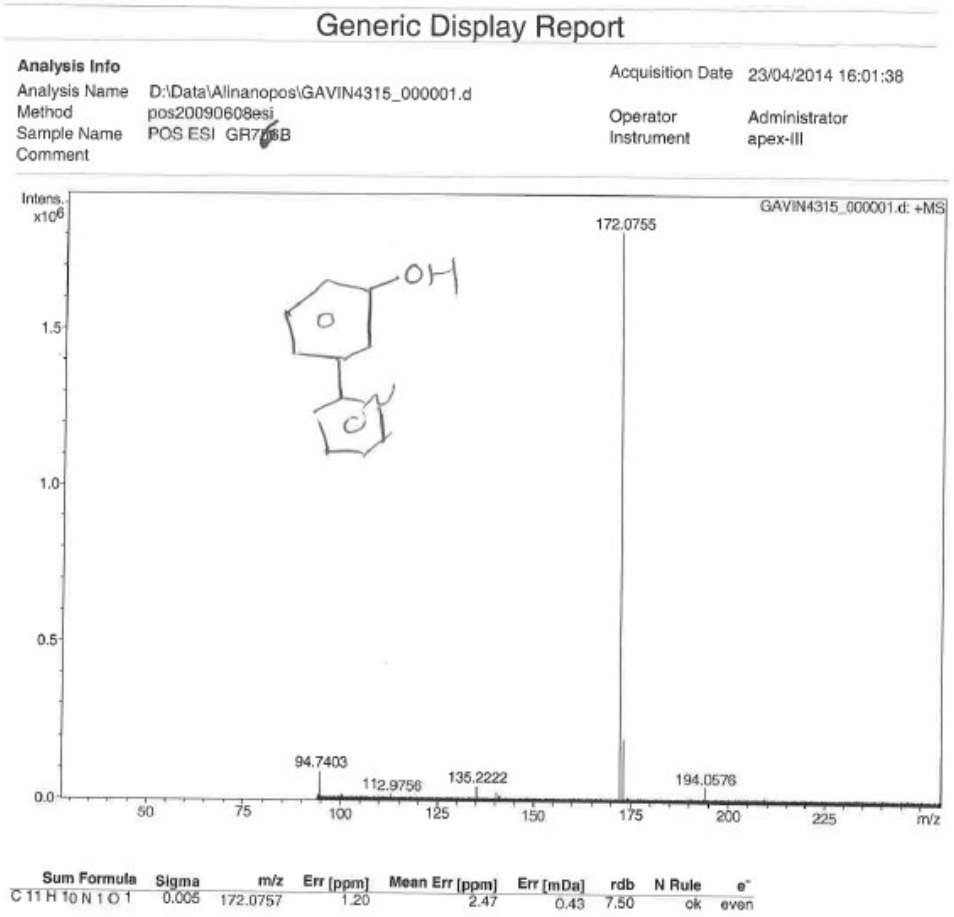


Figure 28 – ^{1}H NMR of palladacycle (**7a**)

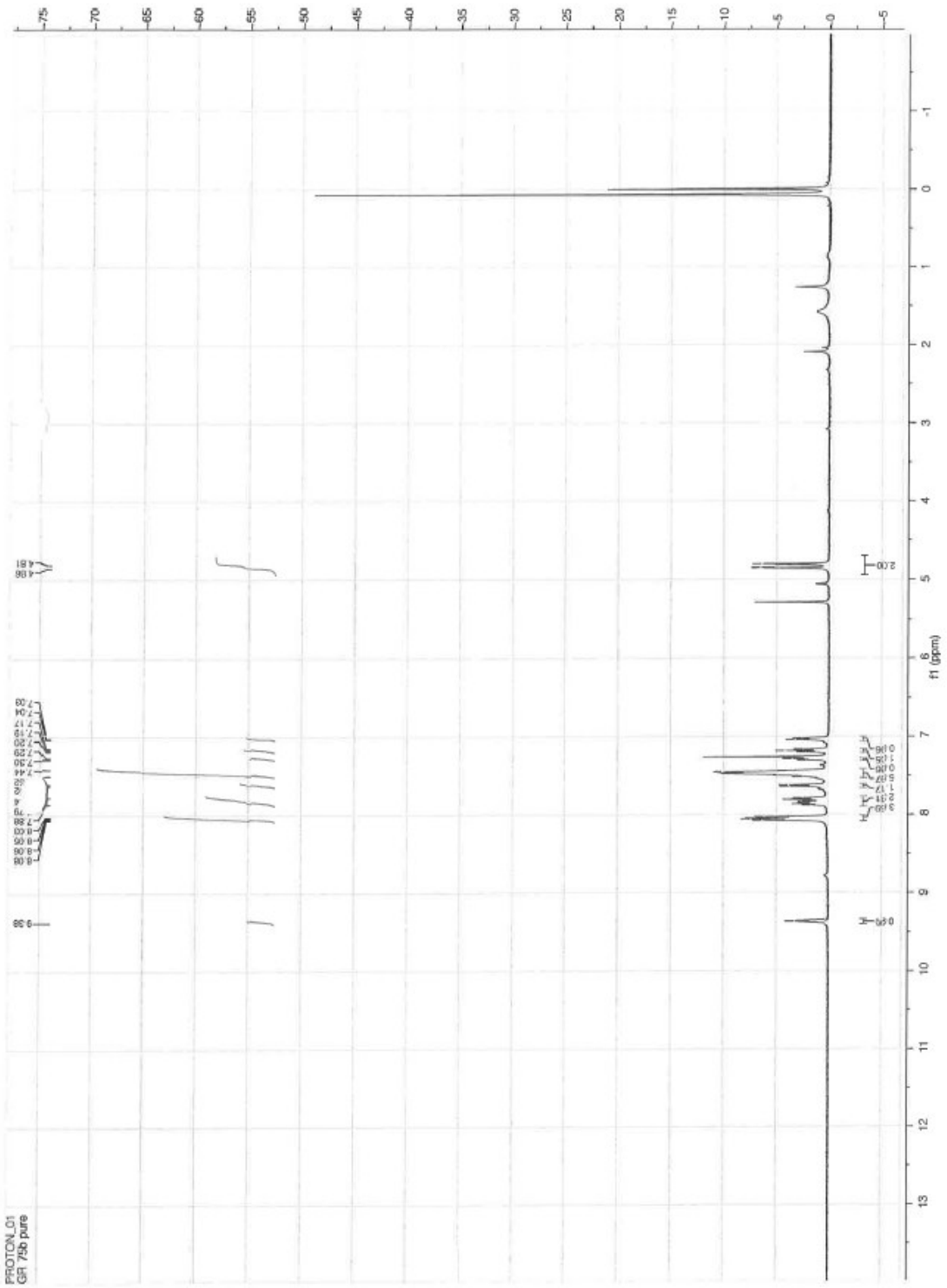


Figure 29 – ^{13}C NMR of palladacycle (**7a**)

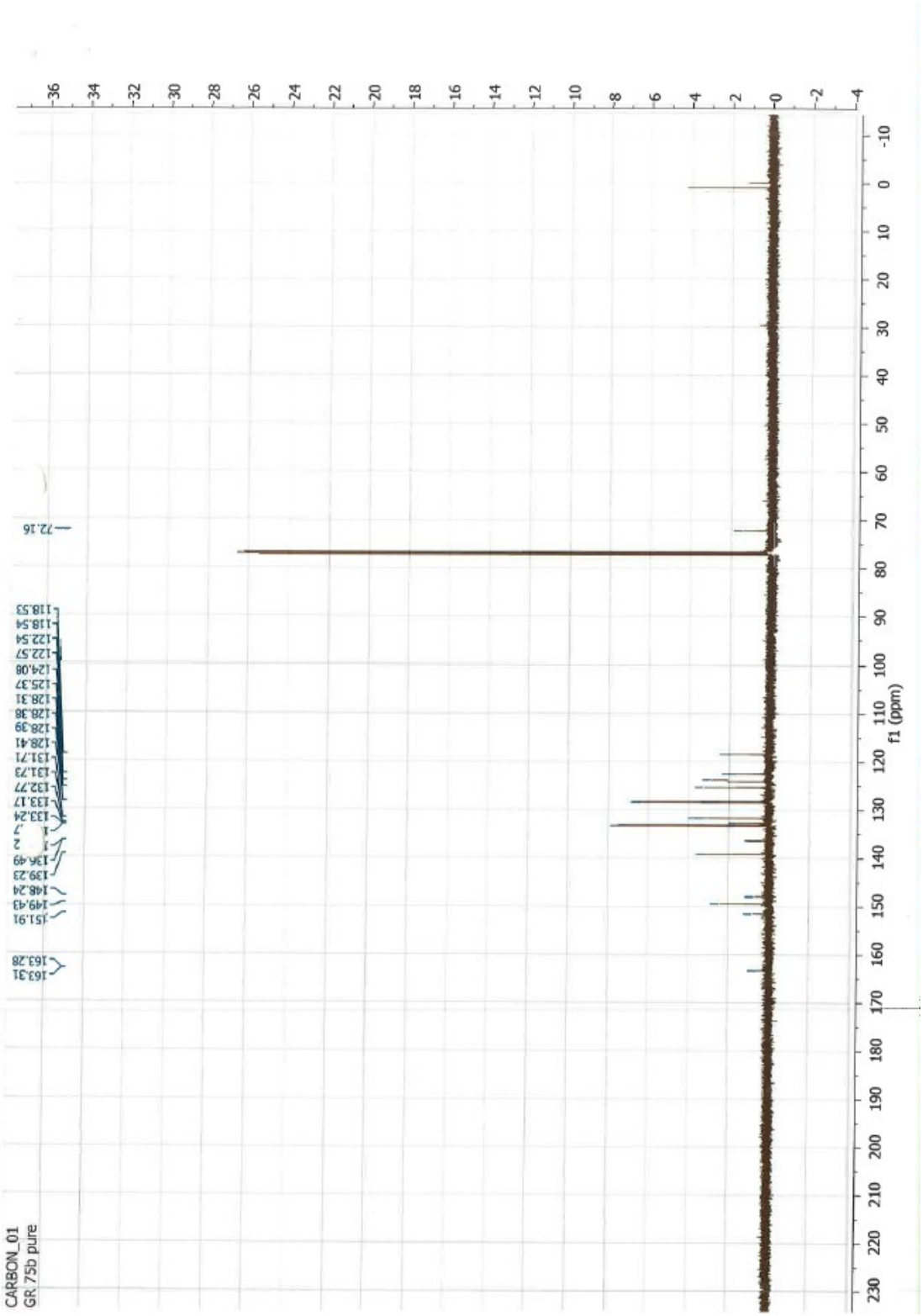


Figure 30 – ^{31}P NMR of palladacycle (**7a**)

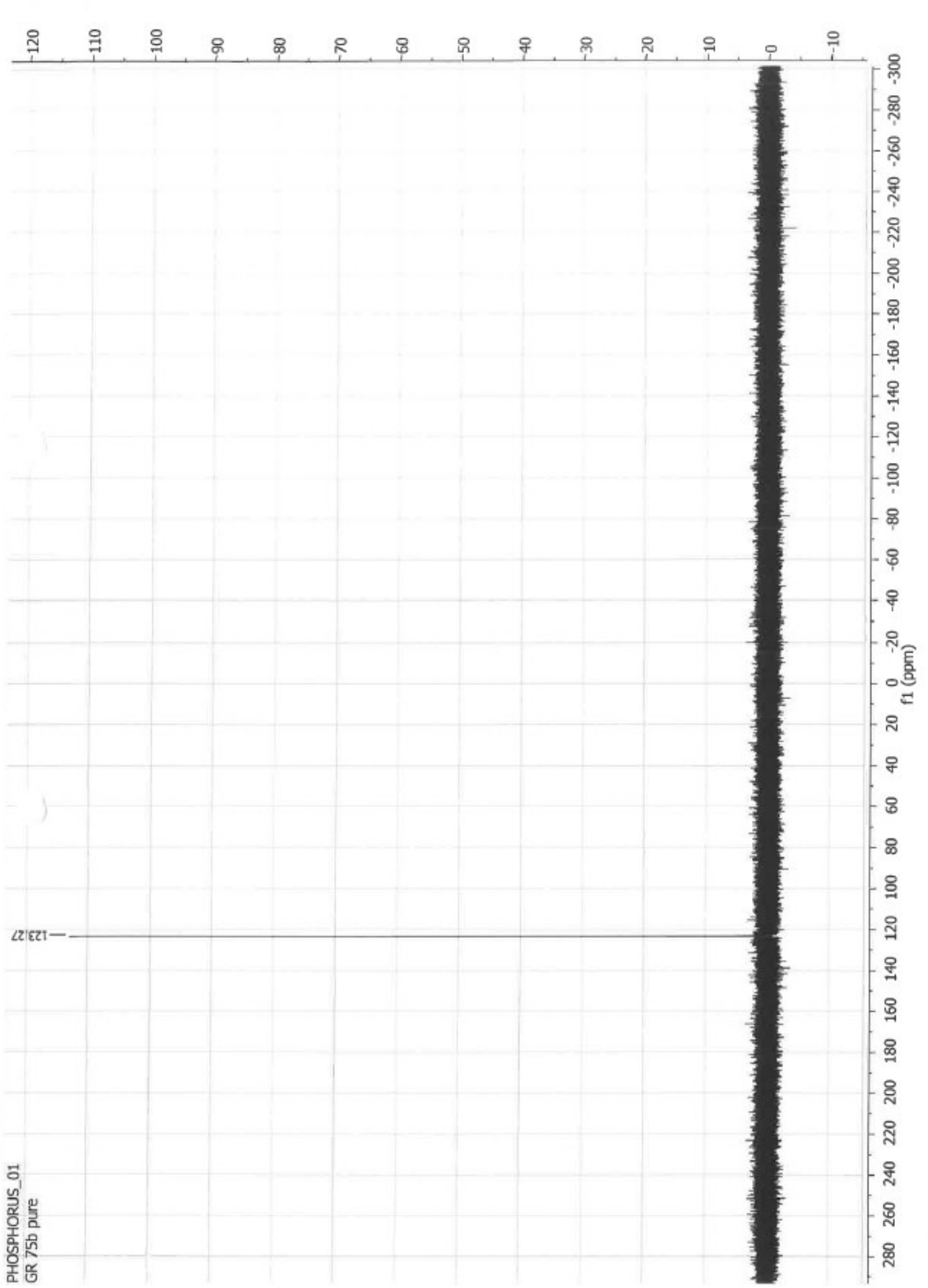
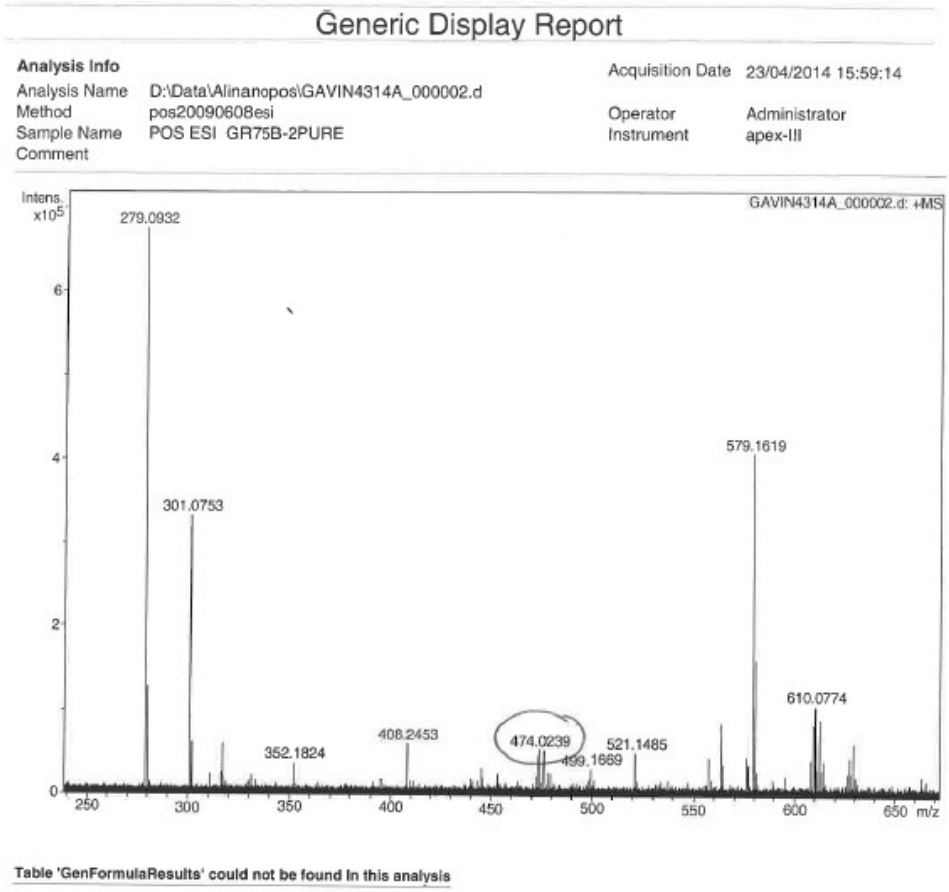


Figure 31 – HRMS of palladacycle (**7a**)



Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN4314A_000002.d	Acquisition Date	23/04/2014 15:59:14
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR75B-2PURE	Instrument	apex-III
Comment			

Table 'GenFormulaResults' could not be found in this analysis

Figure 32 – Elemental analysis of palladacycle (**7a**)

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London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

Sample submitted by: Gavin Roffe
Address: Uni of Sussex, Chemistry, BN1 9QJ
Telephone: Email:gwr20@sussex.ac.uk
Date Submitted: 4-4-14

Please submit ca. 5 mg of sample.

Sample Reference No.: GR 75b
Name of Compound: CH_2OPPh_2pyr
Molecular Formula: $C_{24}H_{19}ClNOPPd$
Stability: **ok**
Hazards:none
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	56.49	56.48	56.48	
Hydrogen	3.75	3.82	3.88	
Nitrogen	2.75	2.83	2.87	

Authorising Signature:

Date Completed: 03/04/14 Signature:
Comments:

Figure 33 – ^{1}H NMR of palladacycle (**7b**)

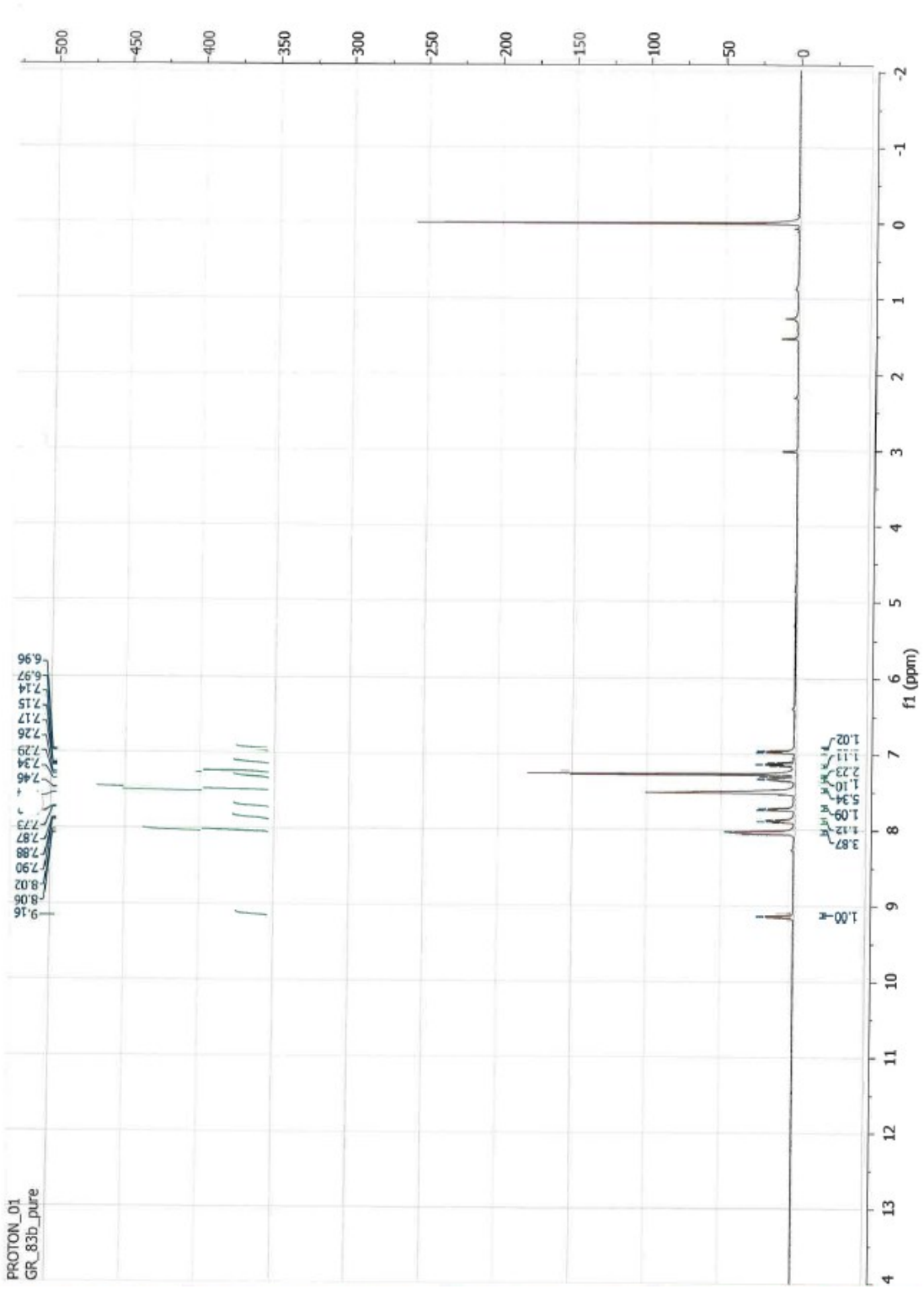

Figure 34 – ^{13}C NMR of palladacycle (**7b**)

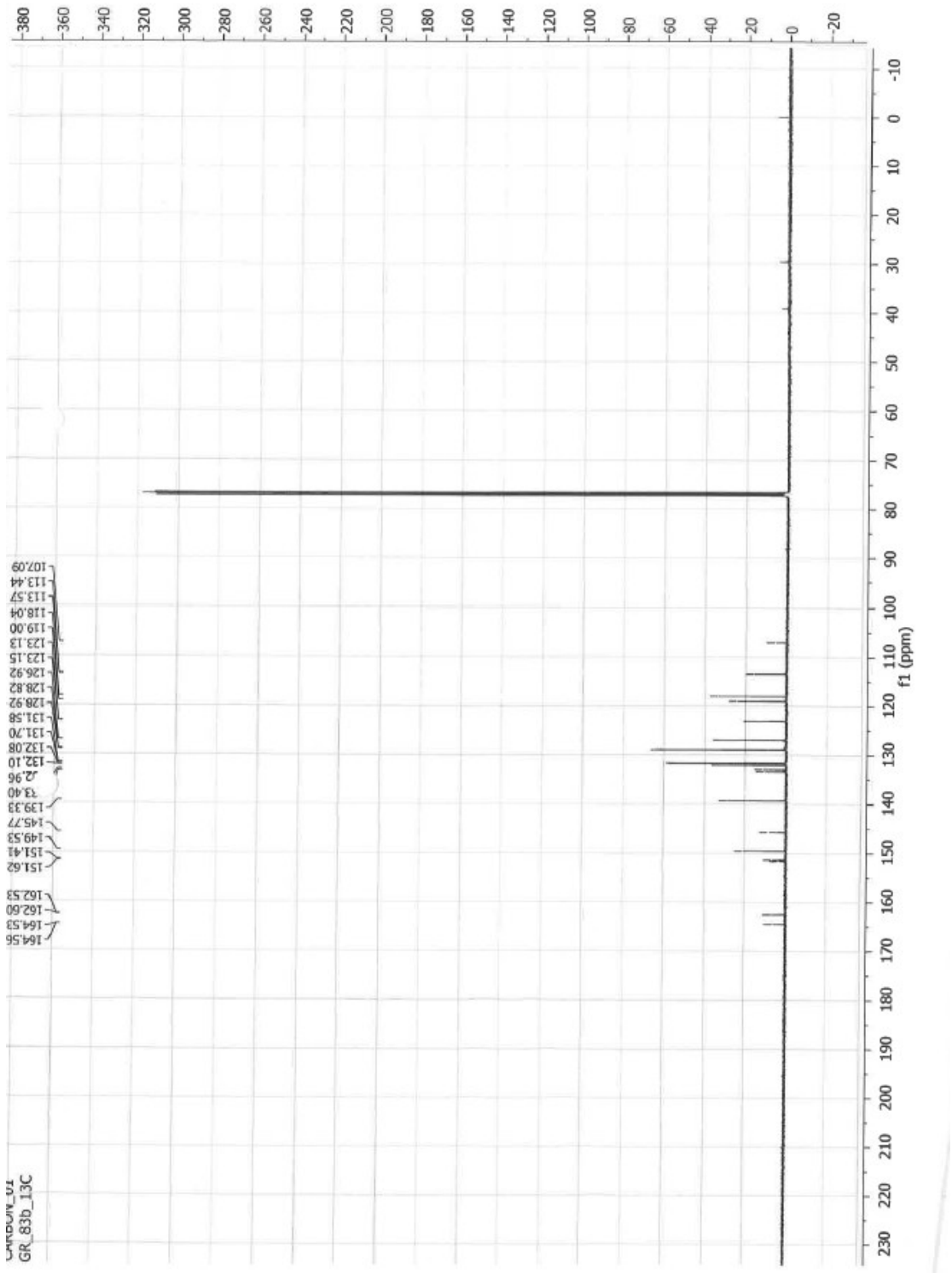

Figure 35 – ^{31}P NMR of palladacycle (**7b**)

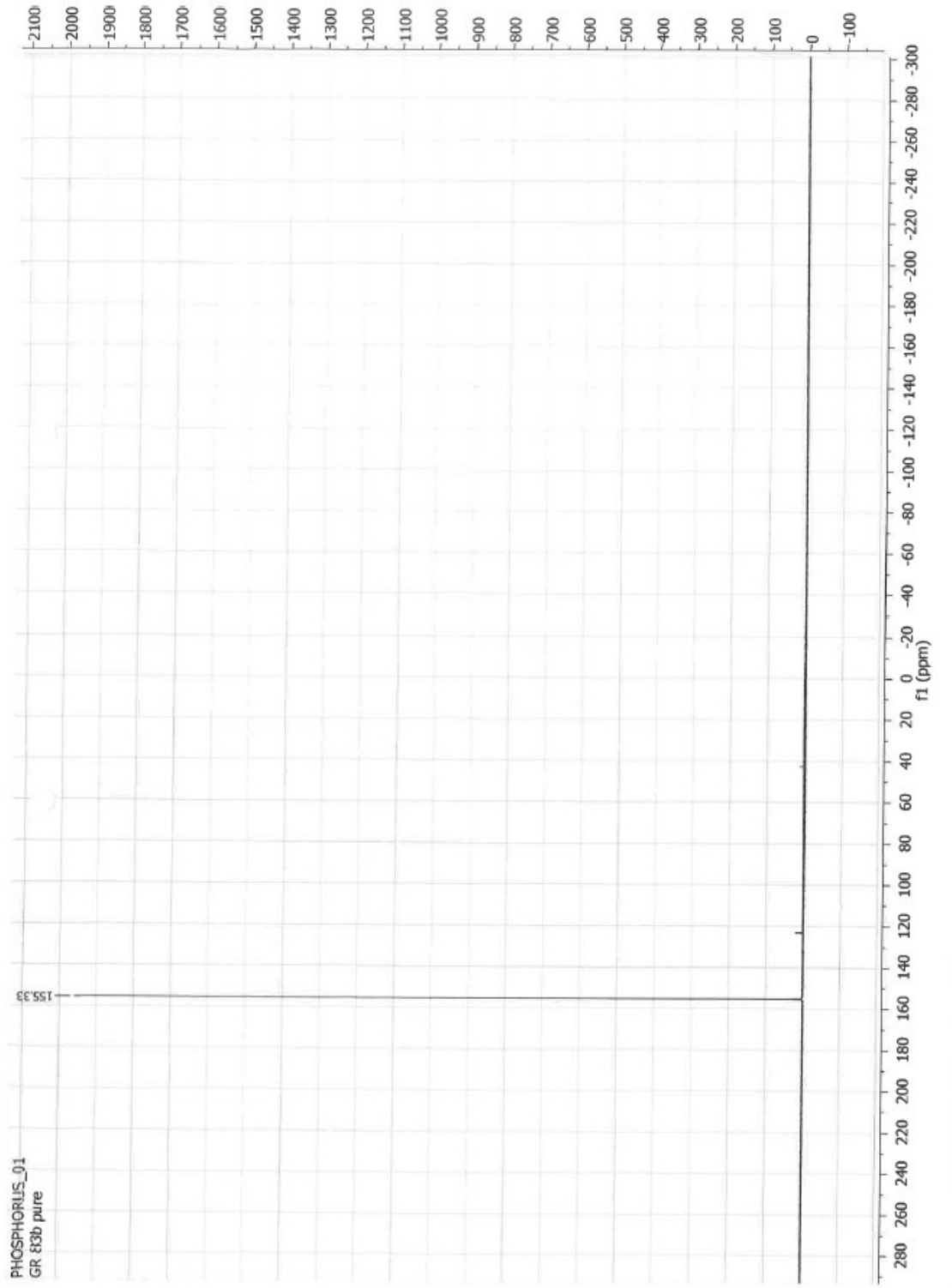

Figure 35 – HRMS of palladacycle (**7b**)

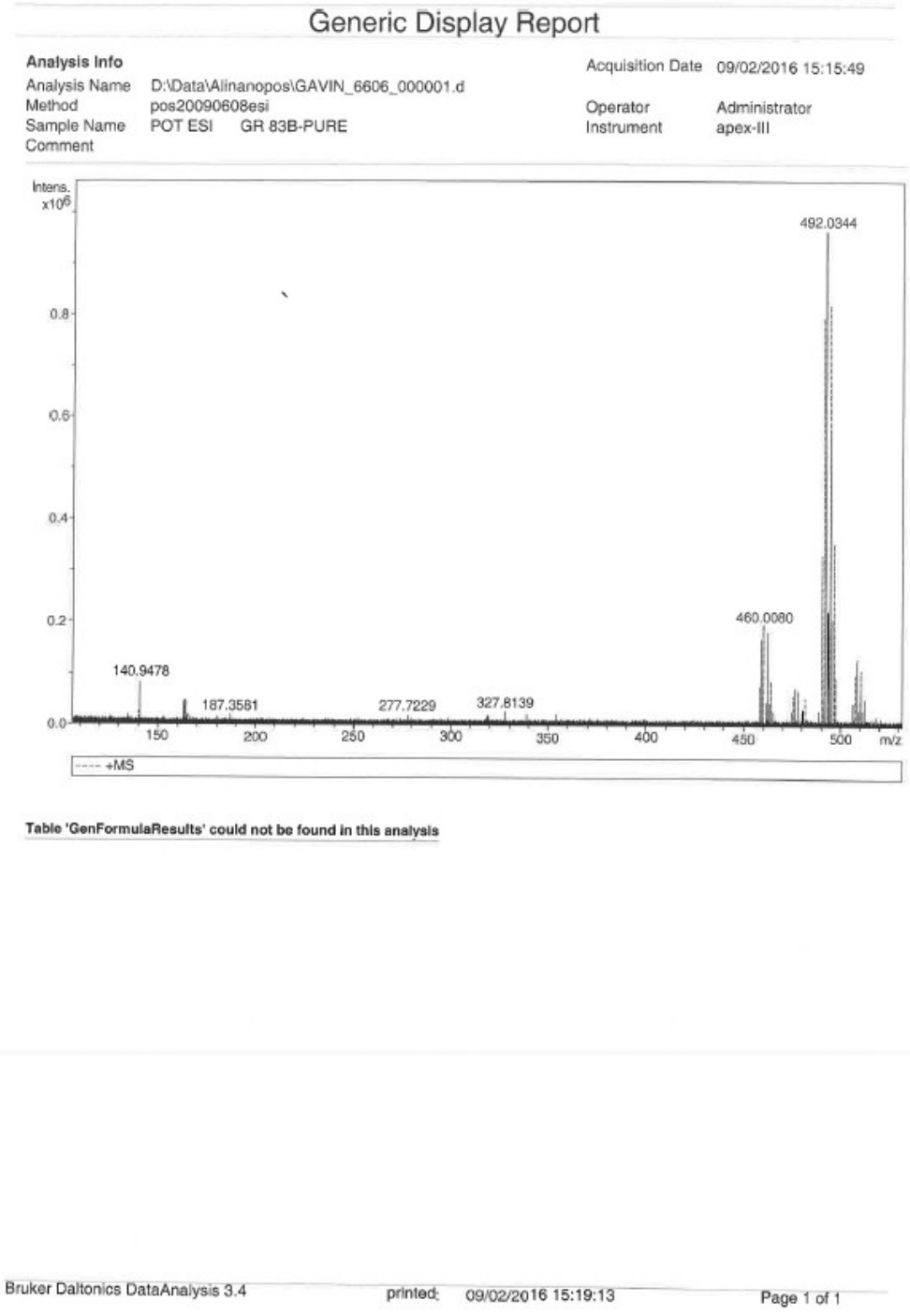

Figure 36 – Elemental analysis of palladacycle (**7b**)

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London Metropolitan University
29 Hornsey Road
London N7 7DD

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Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

Sample submitted by:	Gavin Roffe.
Address:	Life Science Stores, Uni of Sussex, Falmer, Brighton, BN1 9QG
Telephone: / Email:	07584 291754 / gwr20@sussex.ac.uk
Date Submitted:	9/2/16

Please submit ca. 5 mg of sample.

Sample Reference No.:	GR83b.
Name of Compound:	Pyr-OPPh2 chloro pallacycle.
Molecular Formula:	$C_{23}H_{17}ClNOPdP$
Stability:	
Hazards:	
Other Remarks:	

Element	Expected %	Found (1)	Found (2)	
Carbon	55.67	55.76	55.81	
Hydrogen	3.45	3.58	3.57	
Nitrogen	2.82	2.84	2.92	

Figure 37 – Aldol condensation cis/trans mixture ^{1}H NMR. Performed using **5c** achieving a *trans/cis* ratio of 58/42, using the peaks at 5.10 and 4.65 ppm.

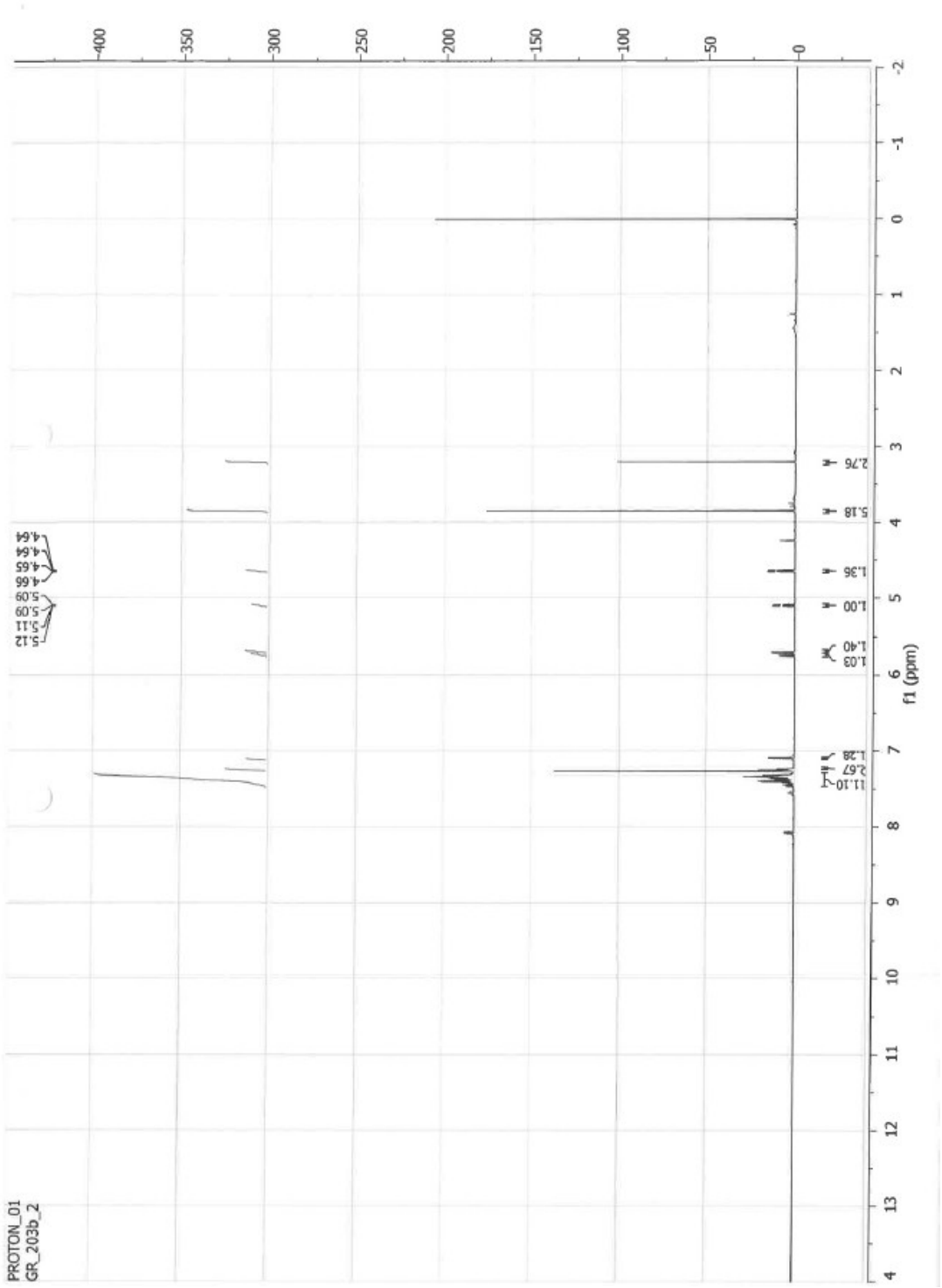

Figure 38 - Aldol condensation cis/trans mixture ^{13}C NMR

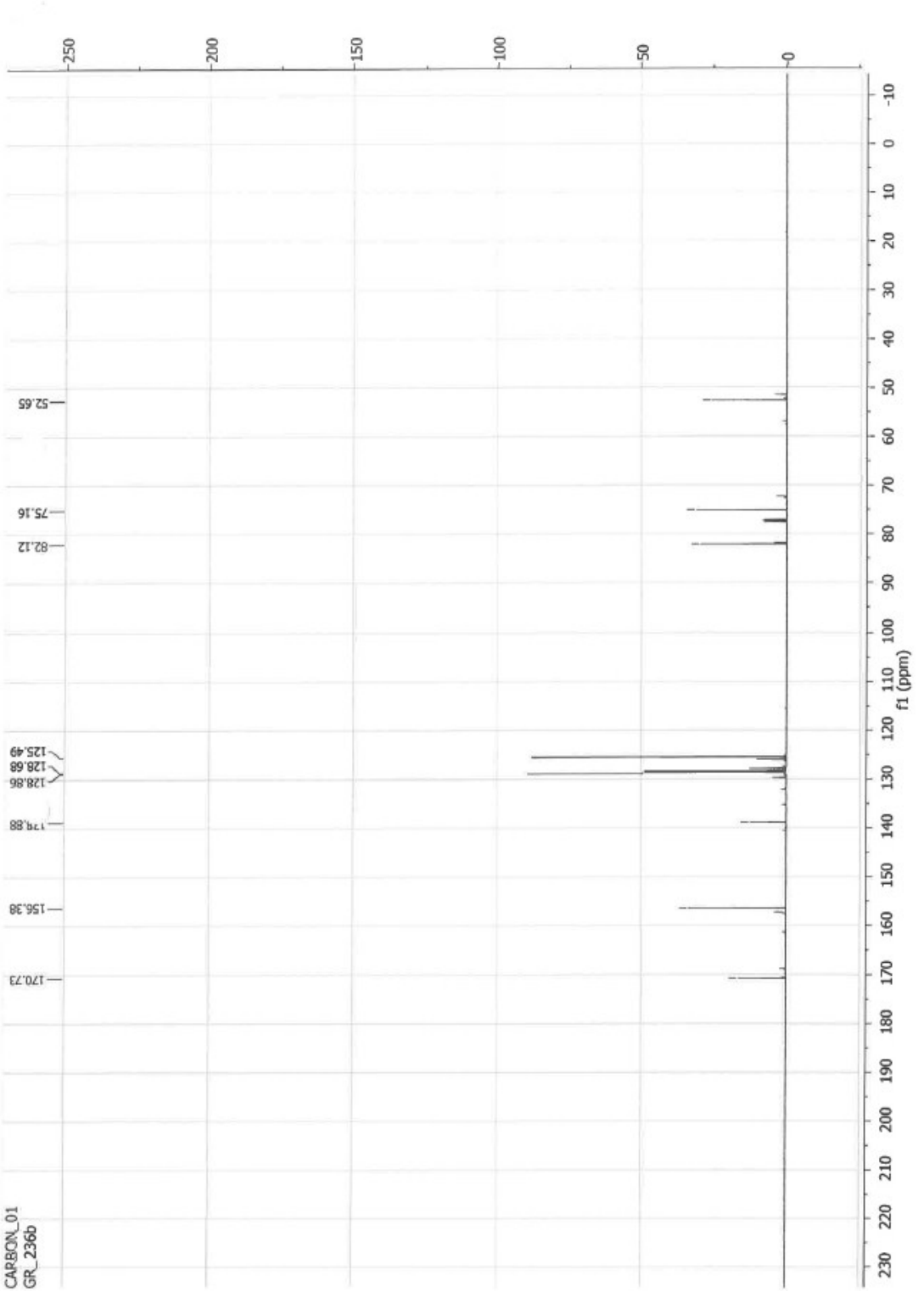

Figure 39 - Aldol condensation cis/trans mixture MS

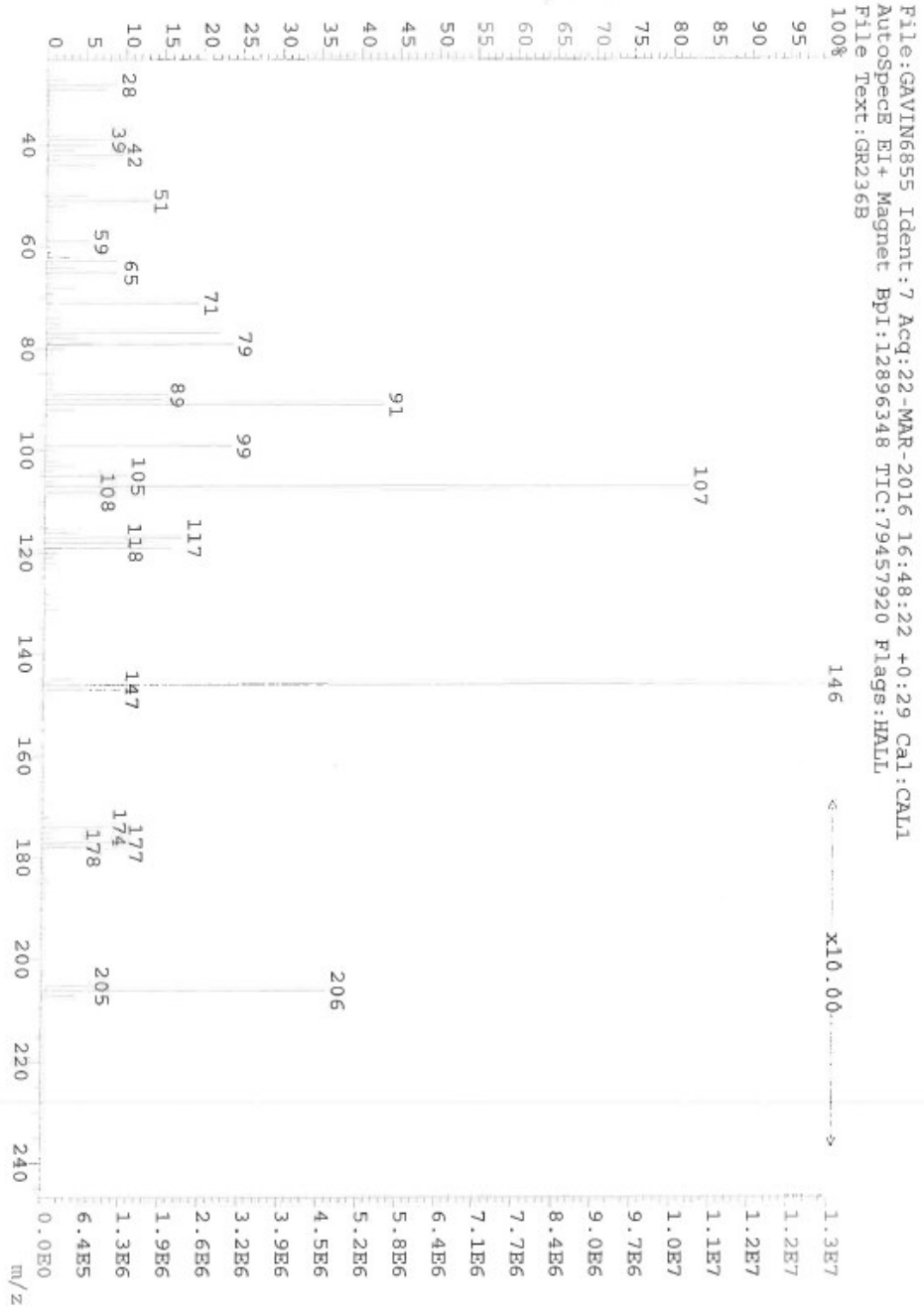

Figure 40 – V
NMR. Perforr
using peaks at

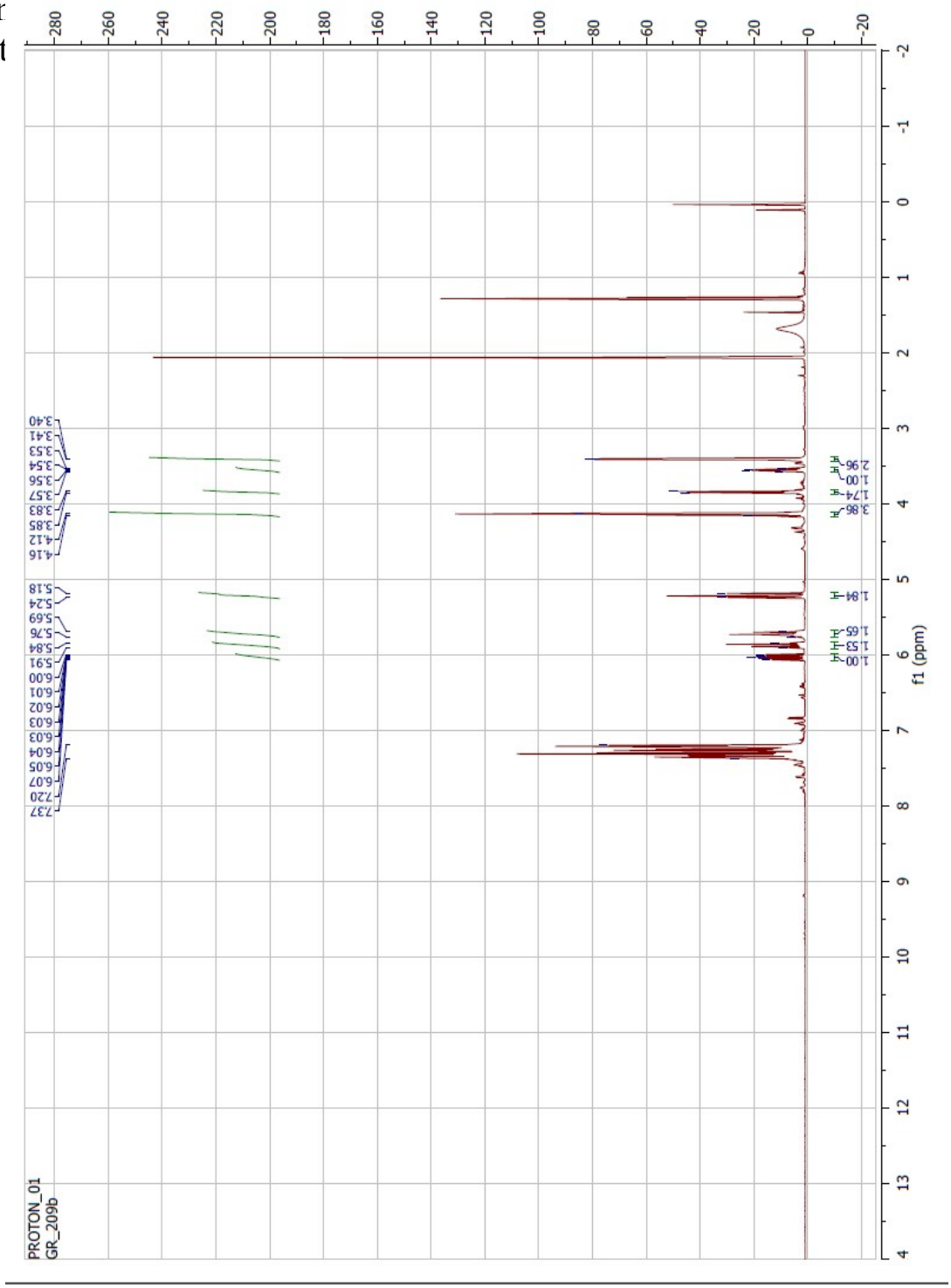

Figure 41 – Vinyl epoxide coupling linear/branched mixture ^{13}C NMR

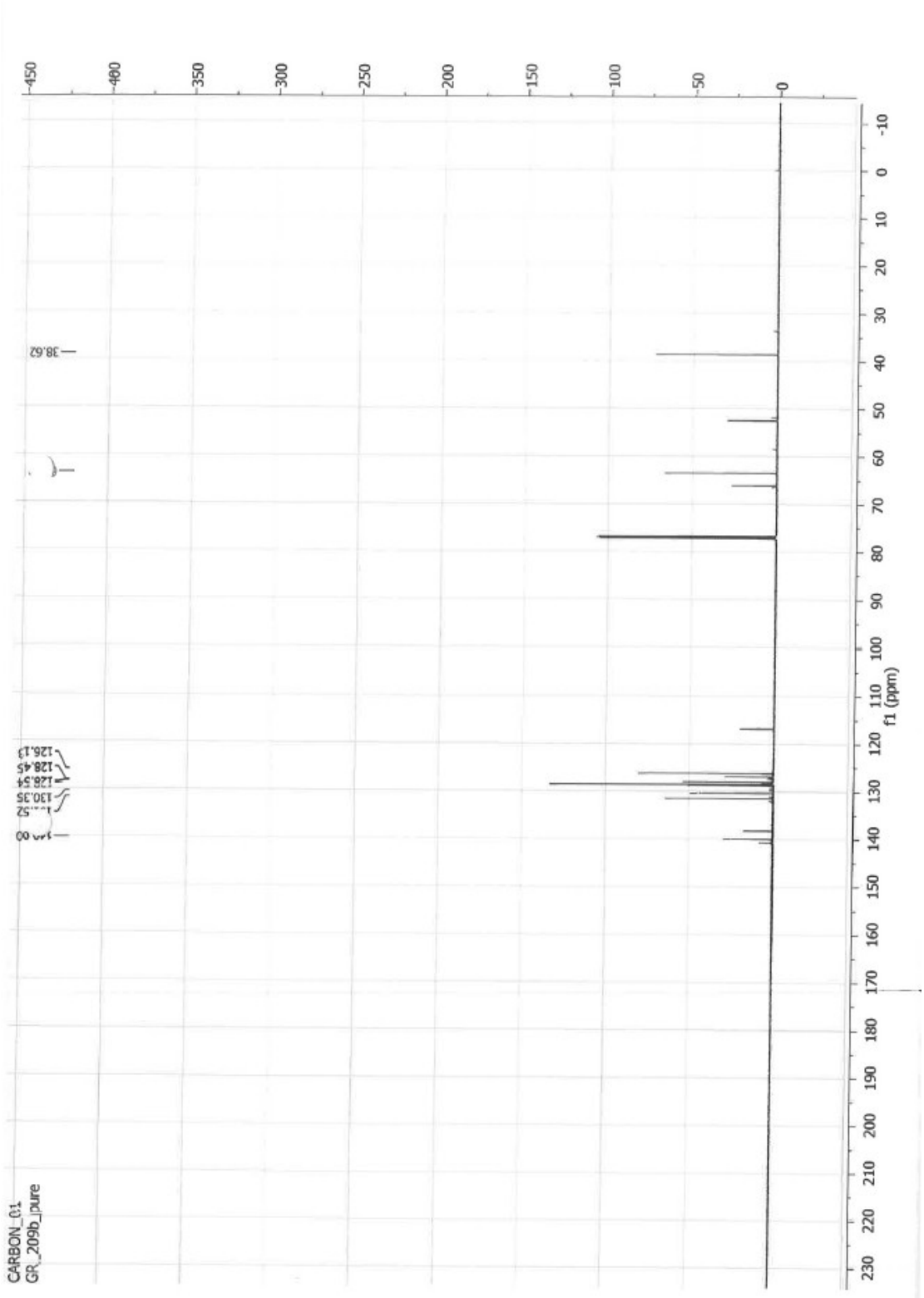

Figure 42 – Vinyl epoxide coupling linear/branched mixture MS