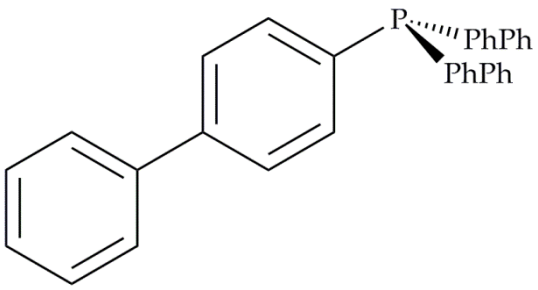
Accompanying Material

This document includes relevant spectral data for all of the compounds presented in the Experimental chapter.

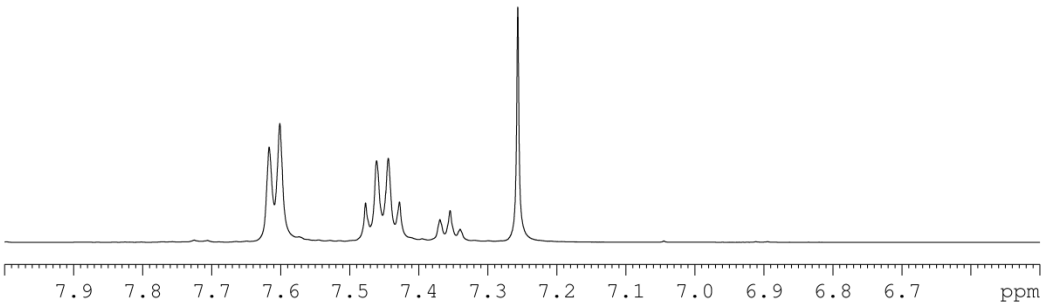
1.1 Tris(4-biphenyl)phosphine



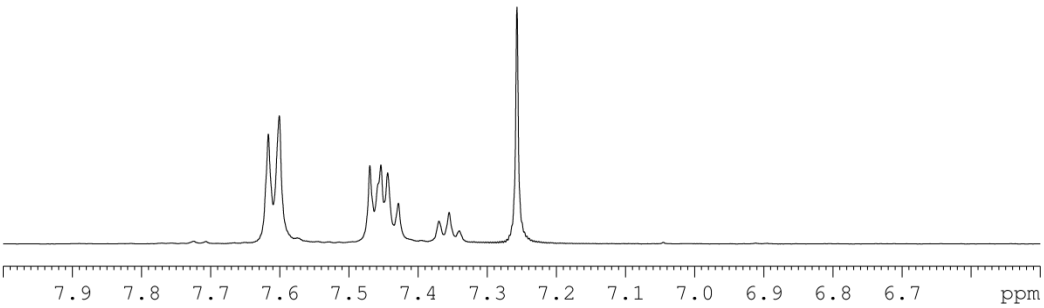
Compound reference kma-3-48

1.1.1 NMR spectra

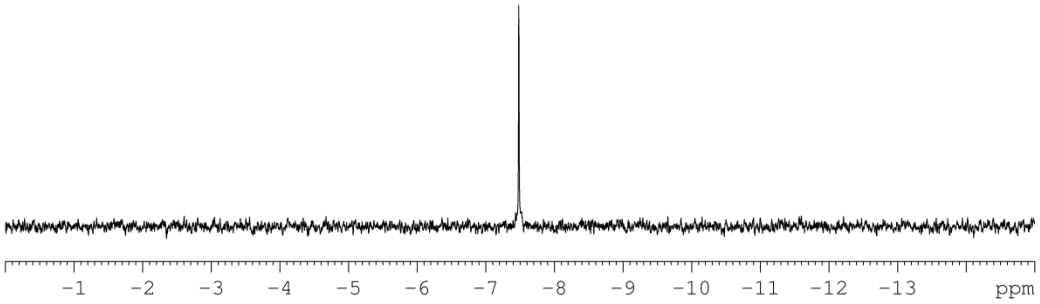
^{1}H



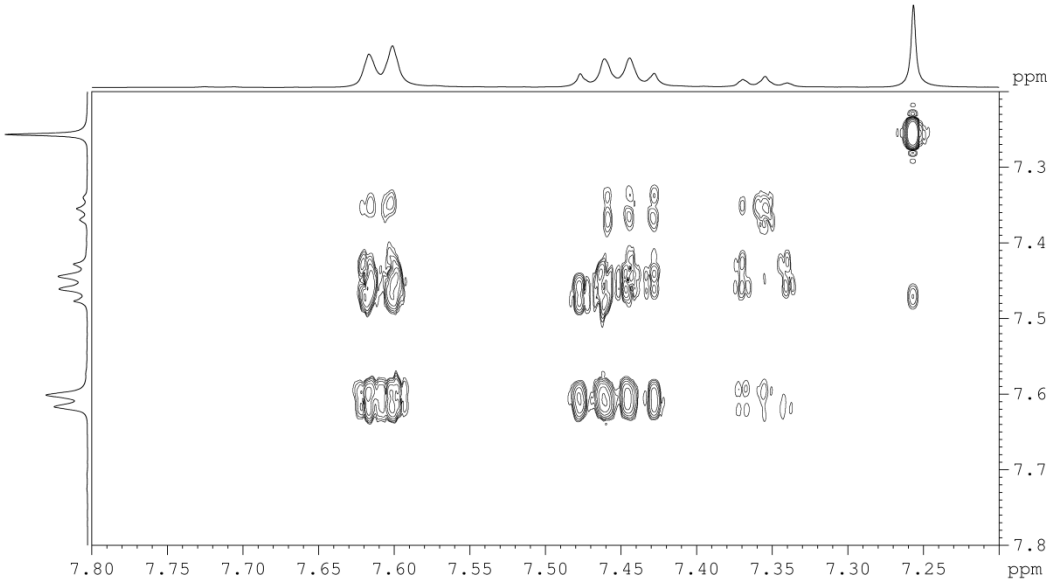
^{1}H {^{31}P}



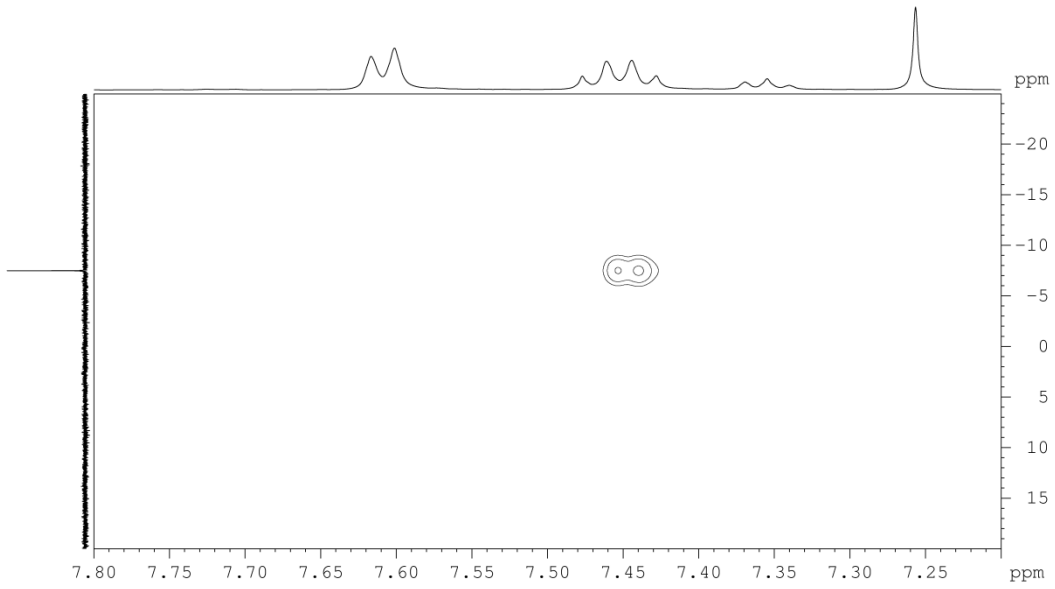
$^{31}P\ \{^{1}H\}$



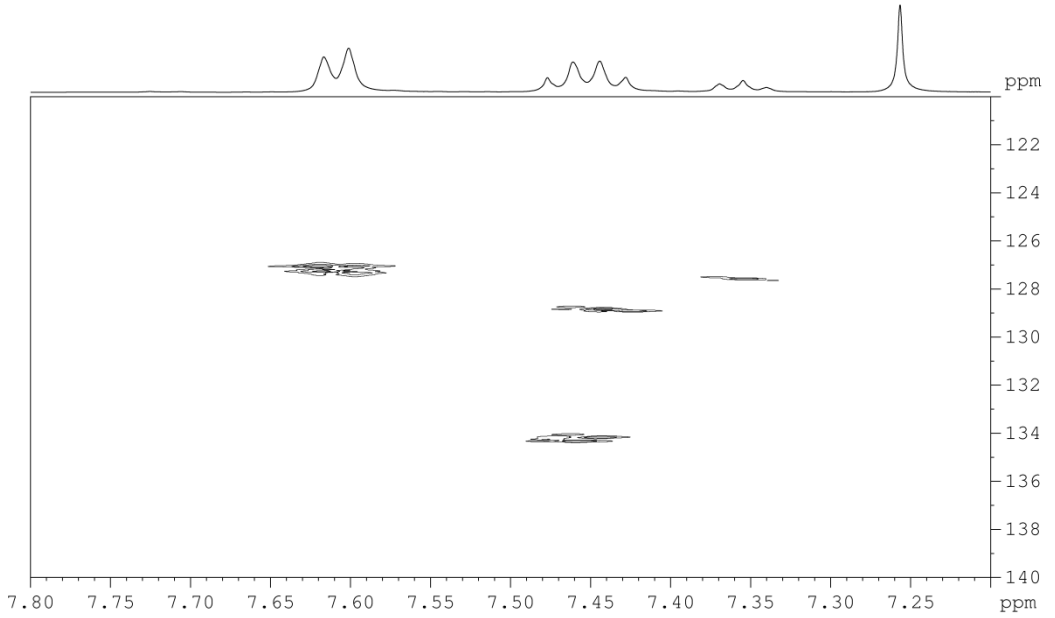
COSY



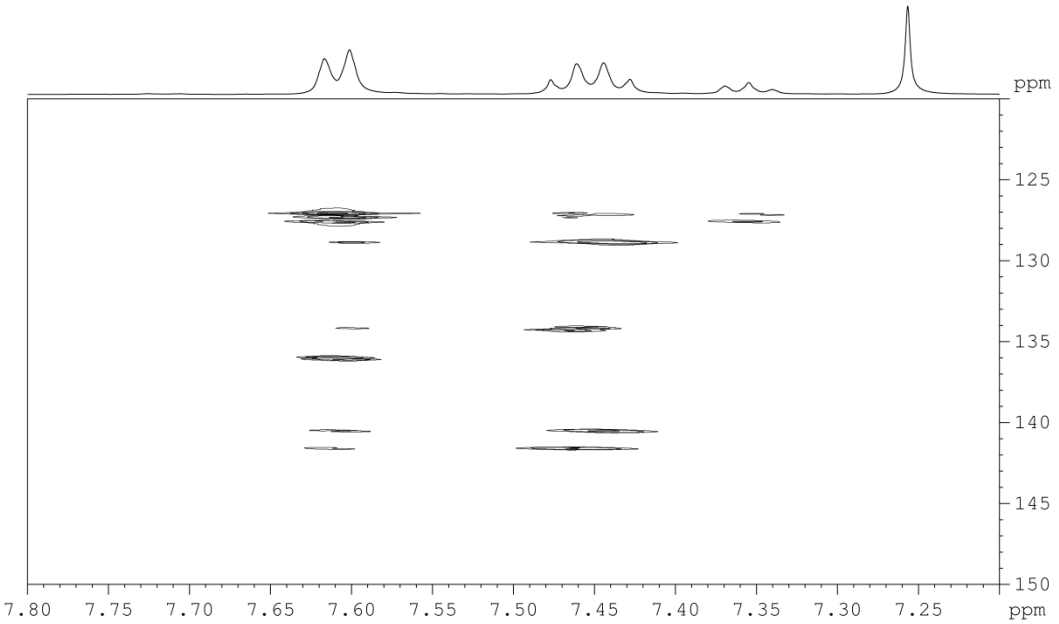
^{31}P-optimised HMQC using a coupling of 12 Hz



^{13}C-optimised HMQC using a coupling of 145 Hz

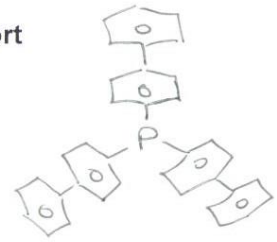


^{13}C-optimised HMQC using a coupling constant of 12 Hz



kma-3-48

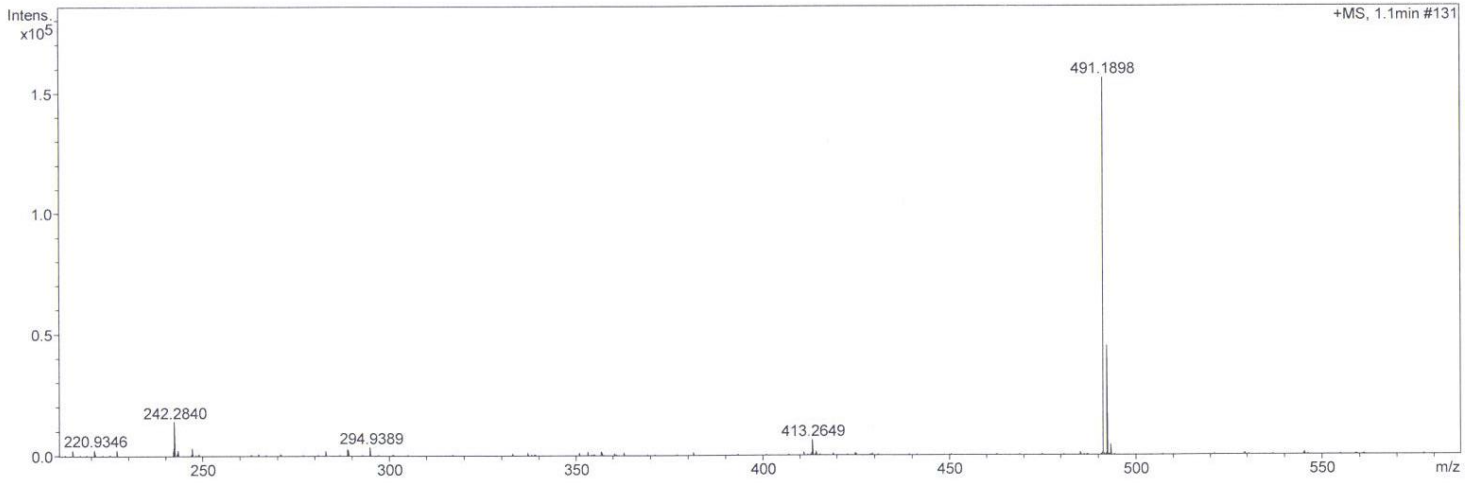
York - Chemistry - Mass Spectrometry Service Report



Analysis Information

Analysis Filename	sbd54757ka_P1-C-7_01_61121.d
Method	600p_meoh1260_2c1s.m
Submission Name	sbd54757ka
Instrument	micrOTOF
ESI	Positive

Acquisition Date 23/09/2015 13:15:18



Meas. m/z	#	Formula	m/z	err [ppm]	err [mDa]	mSigma	Mean err [ppm]
491.1898	1	C 36 H 28 P	491.1923	5.2	2.6	56.2	4.8

1.1.3 CHN elemental analysis

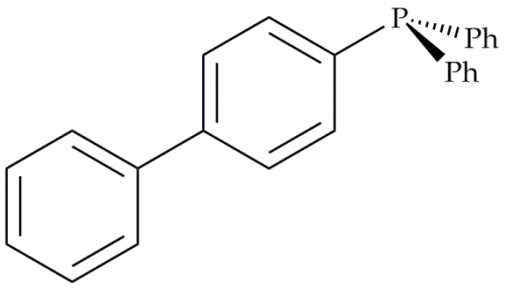
CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma-3-48 P(PhPh)3

Element	% C	% H	% N	% Rest
Observed 1	87.35	5.52	–	7.13
Observed 2	87.25	5.47	–	7.28
Mean	87.300	5.495	–	–
Calc (theory)	88.14	5.55	–	6.31

Comments: Check std within specified limits YES / NO. Counter/run no: 21023

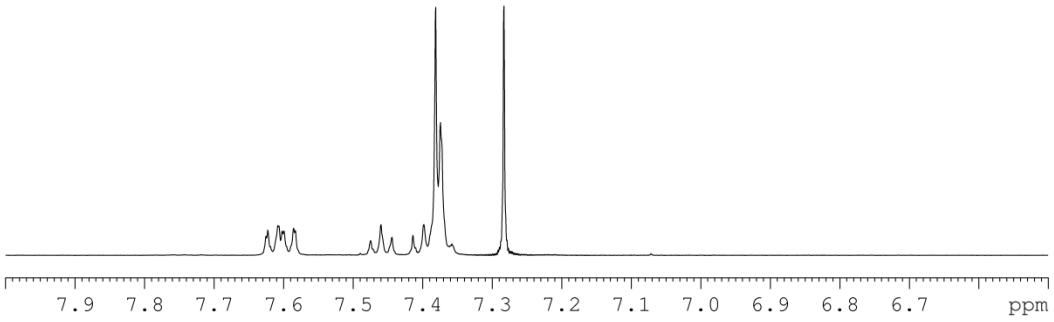
1.2 (4-biphenyl)diphenylphosphine



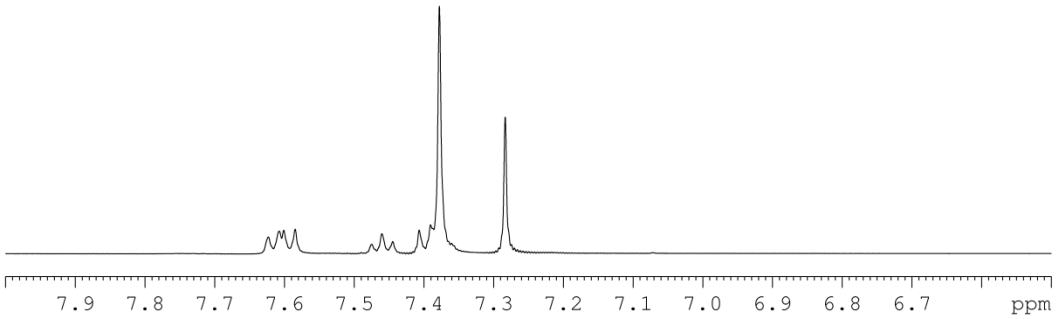
Compound reference kma-3-10

1.2.1 NMR spectra

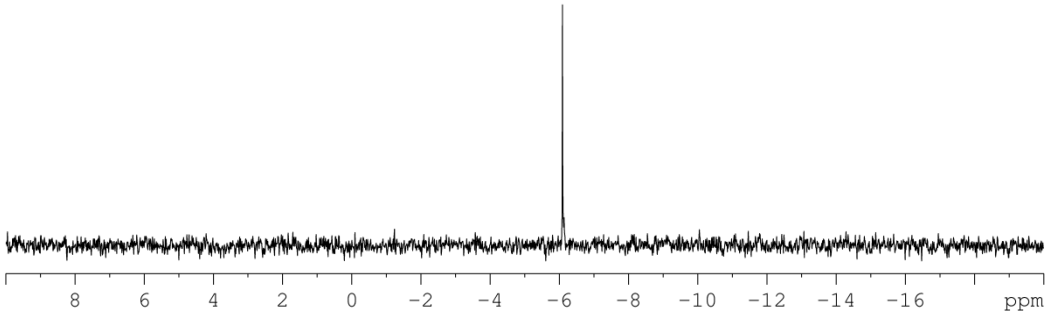
^{1}H



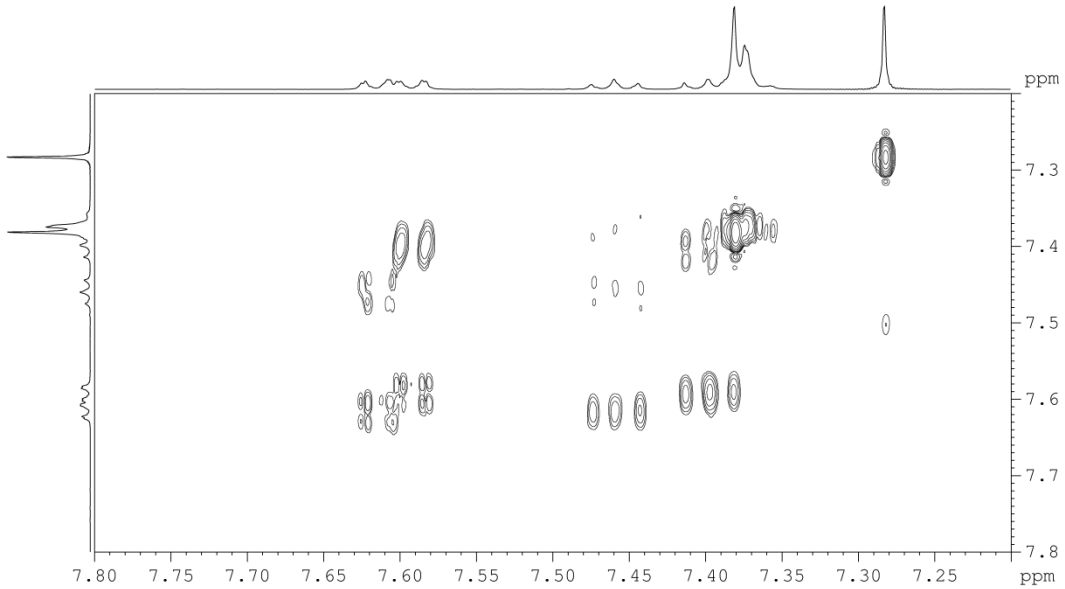
^{1}H $\{^{31}P\}$



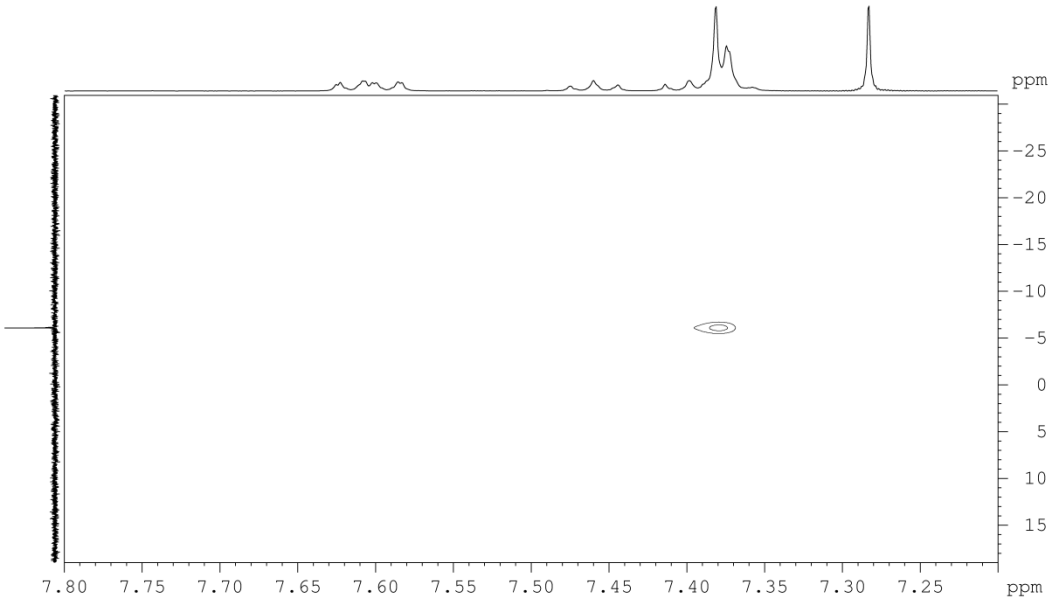
^{31}P $\{^{1}H\}$



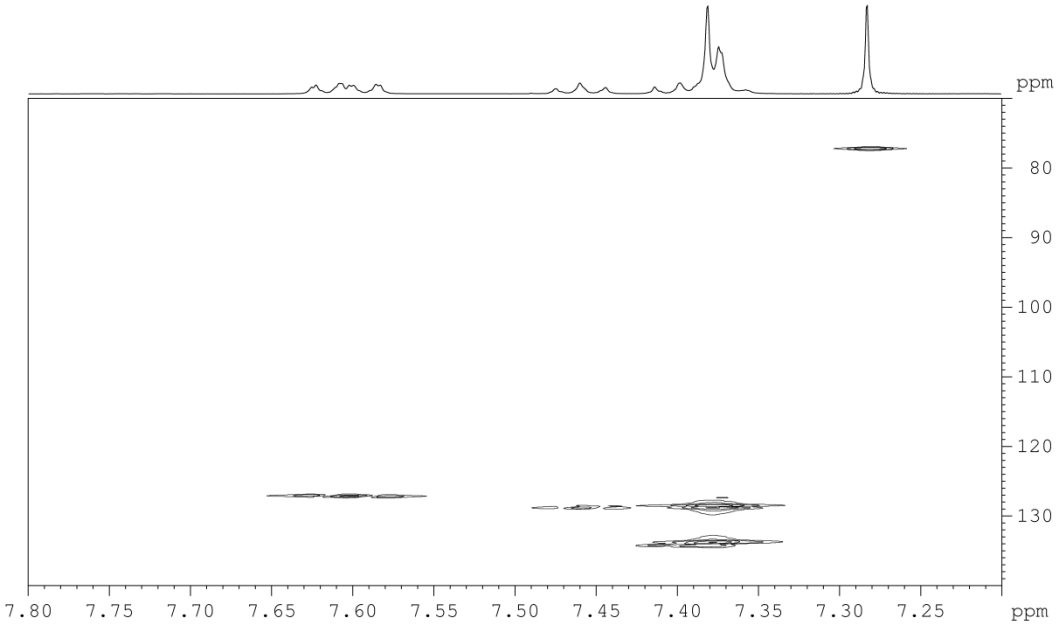
COSY



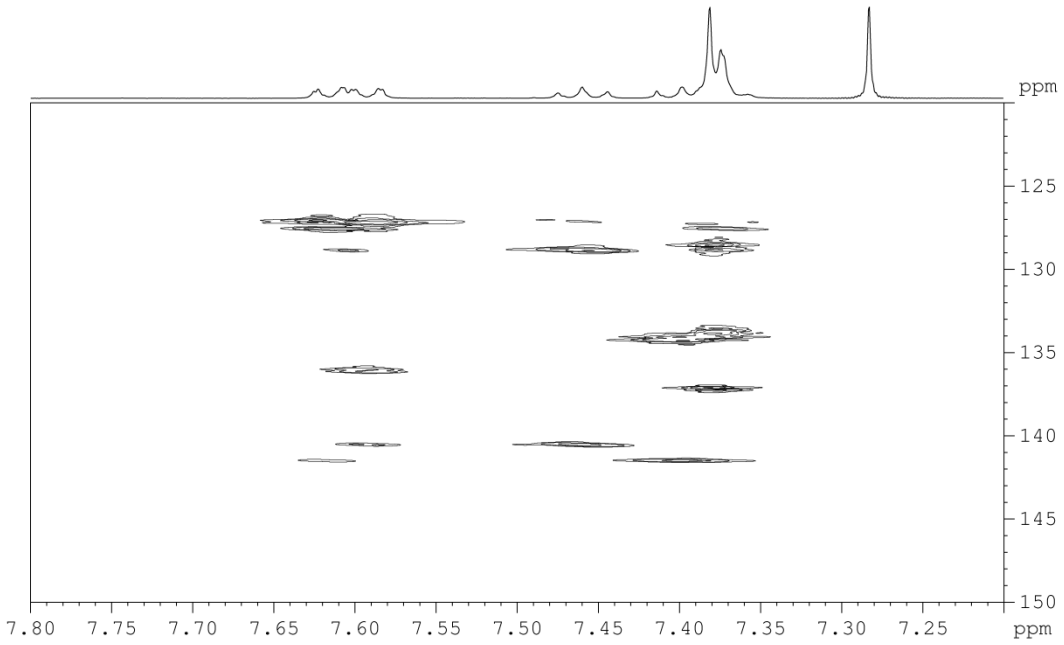
^{31}P-optimised HMQC with a coupling of 12 Hz



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz


ppm
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130
135
140
145
150
7.80
7.75
7.70
7.65
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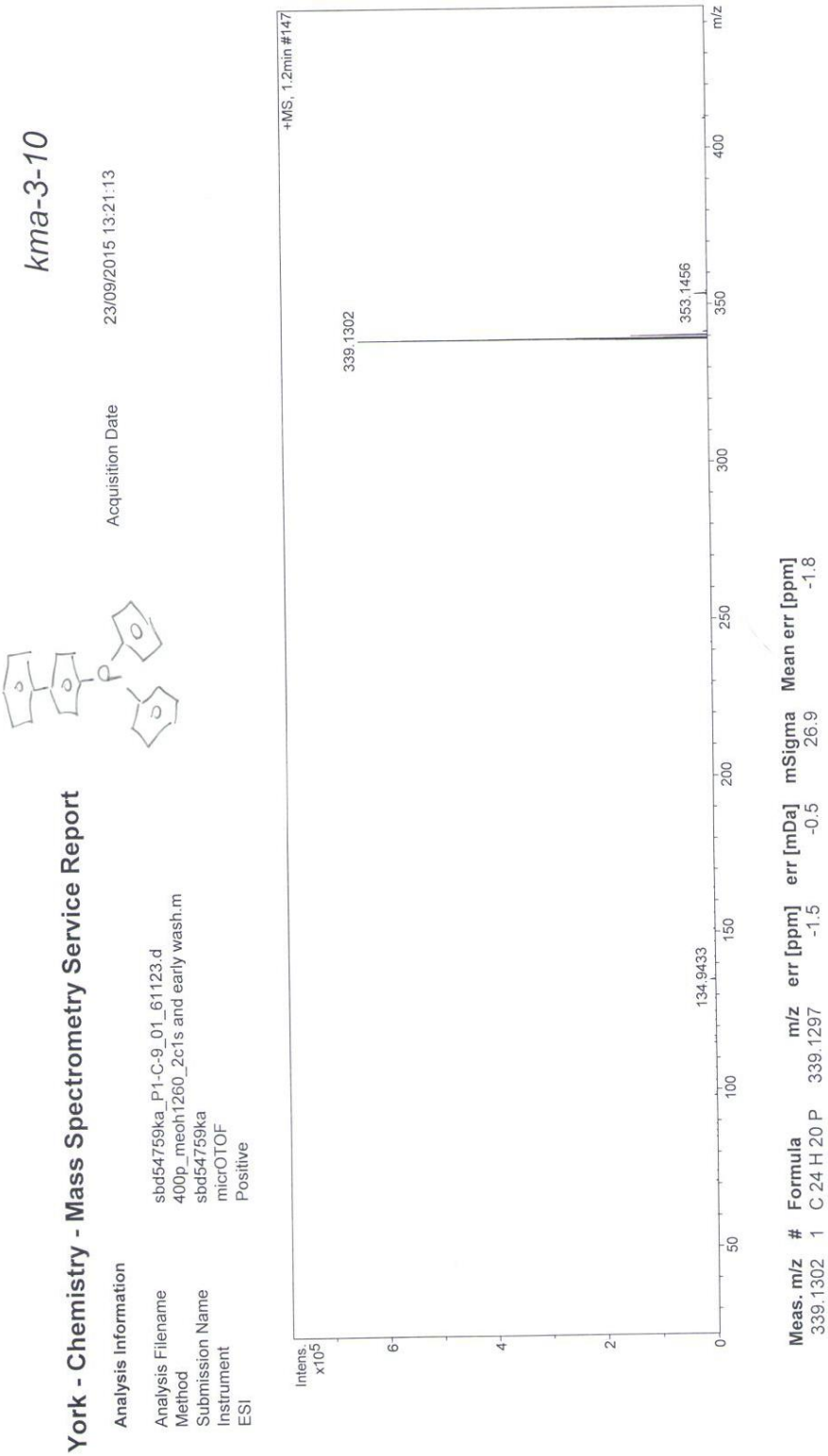
7.55
7.50
7.45
7.40
7.35
7.30
7.25
ppm

1.2.2 Mass Spectra



1.2.3 CHN elemental analysis

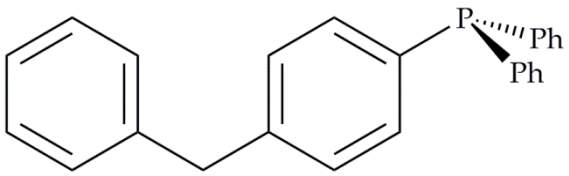
CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma -3-10 $PPh_2(APh)$

Element	% C	% H	% N	% Rest
Observed 1	84.10	5.69	–	10.20
Observed 2	84.63	5.75	–	9.62
Mean	84.368	5.723	–	–
Calc (theory)	85.19	5.66	–	9.15

Comments: Check std within specified limits YES / NO. Counter/run no: 21023

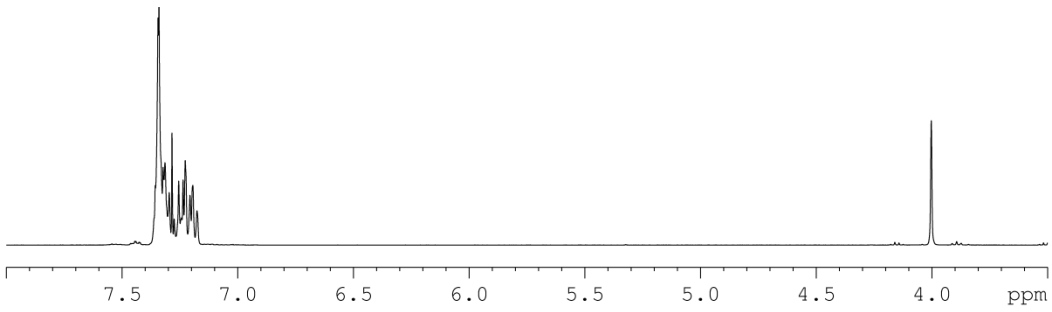
1.3 (4-benzylbenzene)diphenylphosphine



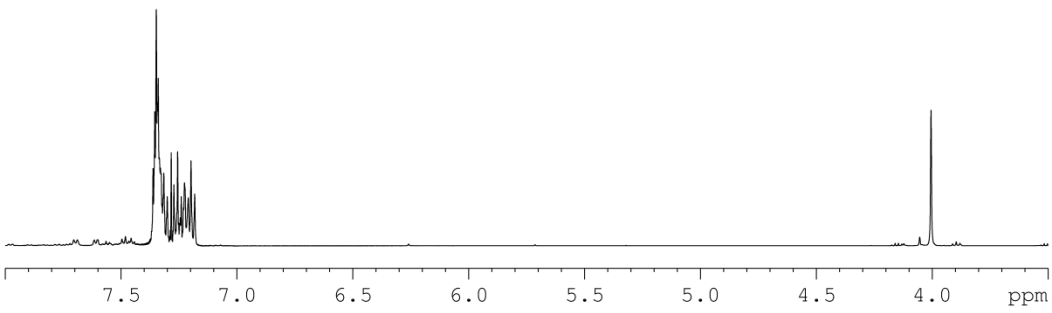
Compound reference kma-3-20

1.3.1 NMR spectra

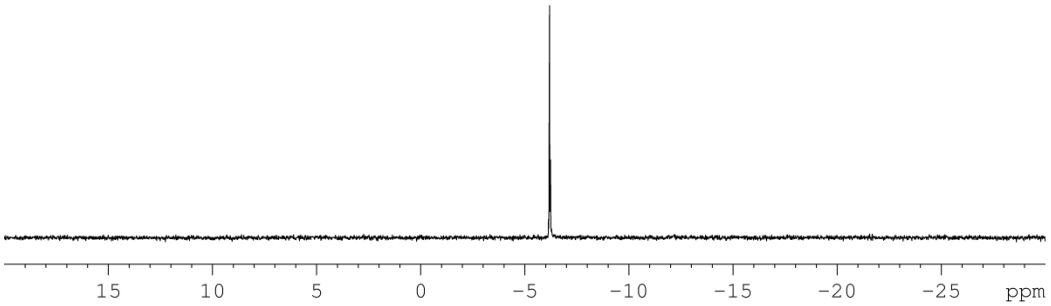
^{1}H



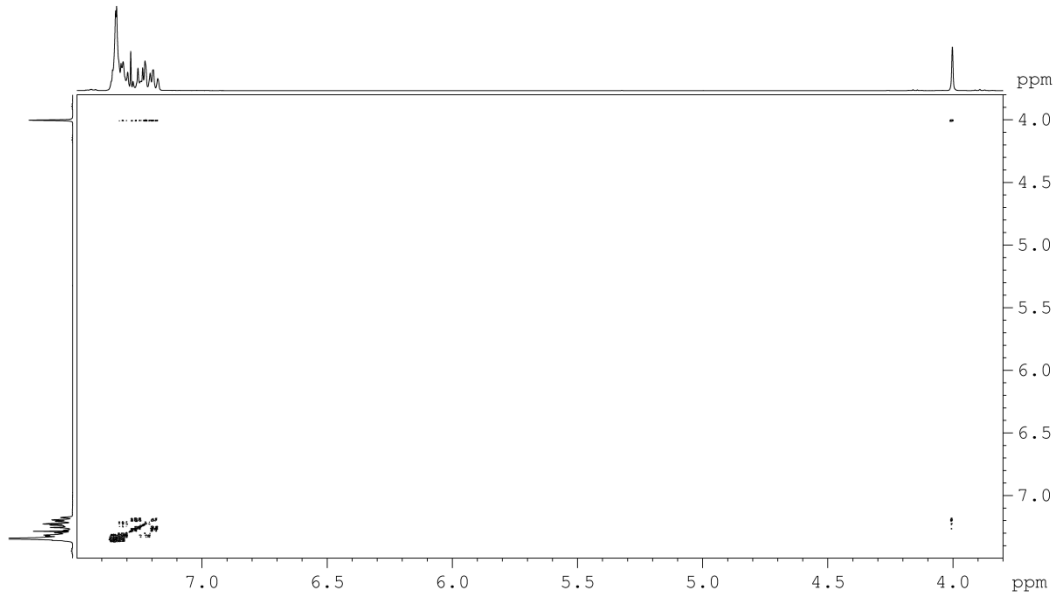
$^{1}H\{^{31}P\}$



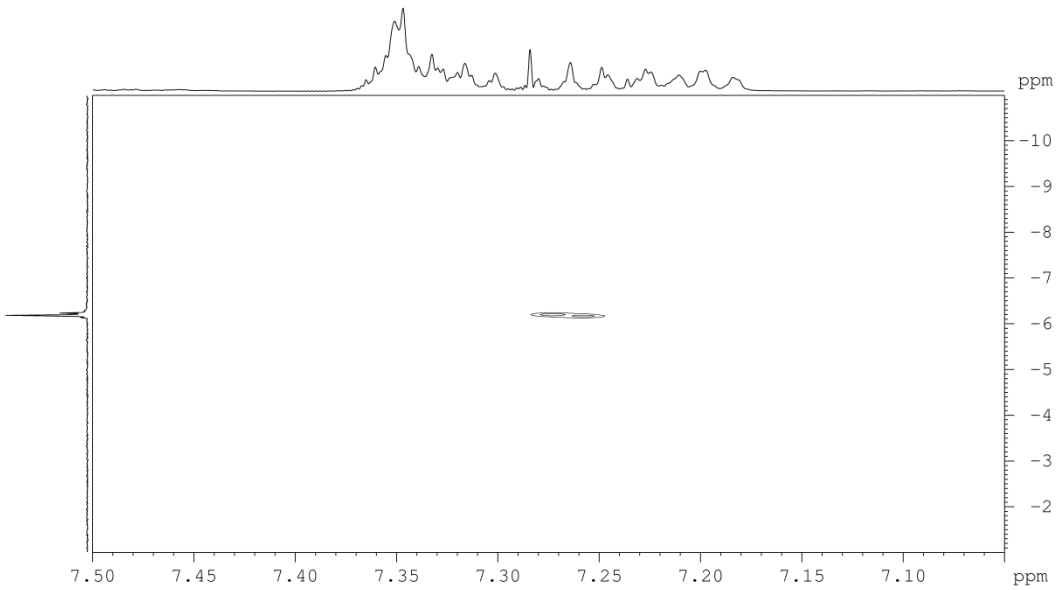
$^{31}P\ \{^{1}H\}$



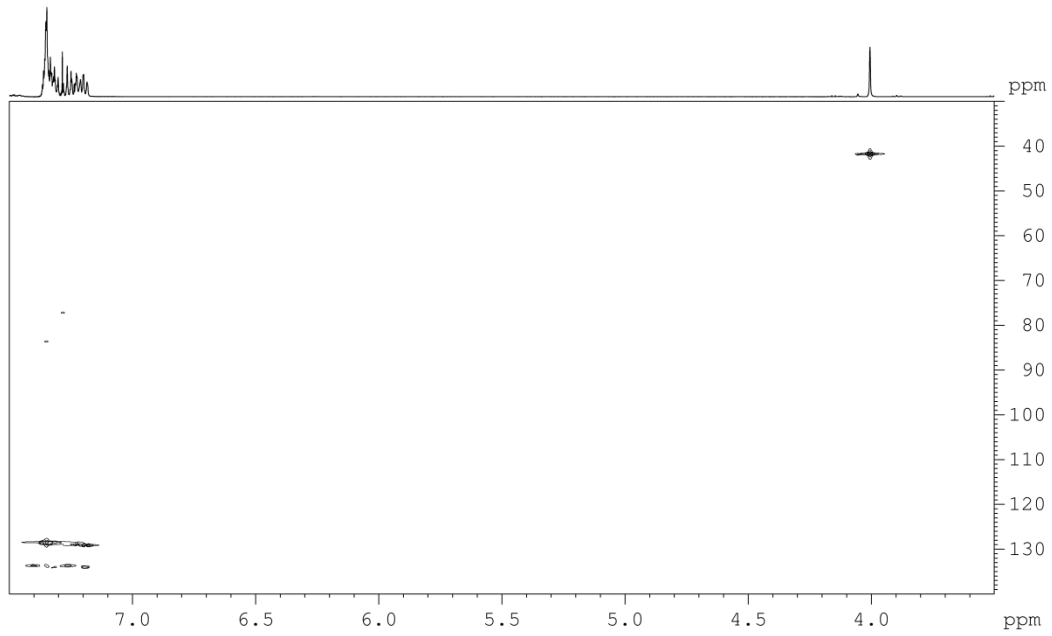
COSY



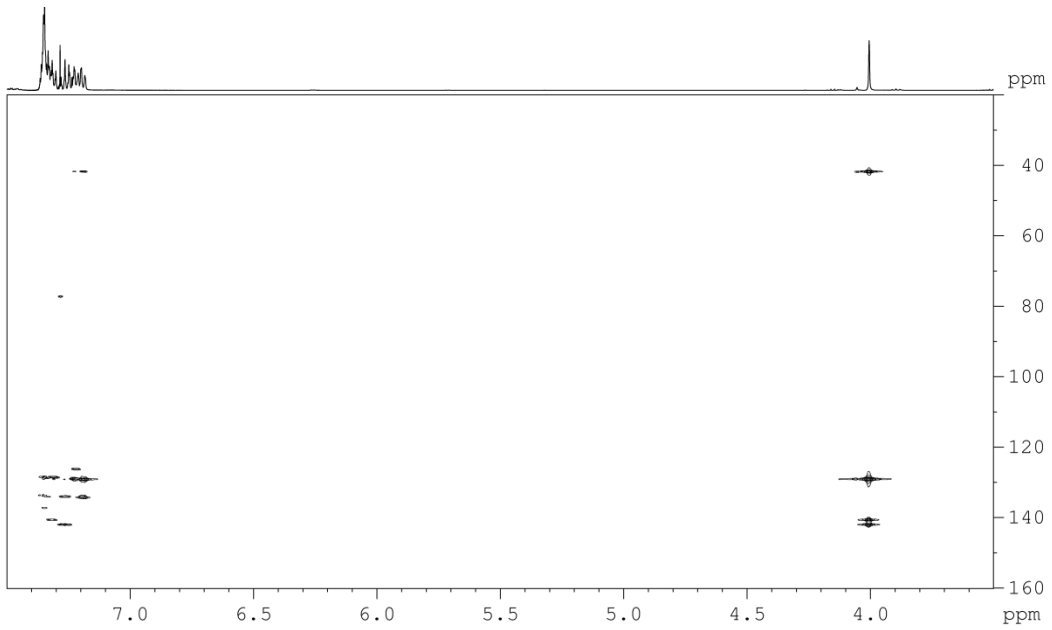
^{31}P-optimised HMQC with a coupling of 14 Hz



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.3.2 Mass spectra

1.3.3 CHN elemental analysis

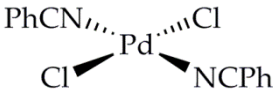
CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma-3-20 $PPh_2(PhCH_2Ph)$

Element	% C	% H	% N	% Rest
Observed 1	84.84	6.20	-	8.96
Observed 2	85.11	6.25	-	8.64
Mean	84.976	6.222	-	-
Calc (theory)	85.20	6.01	-	8.79

Comments: Check std within specified limits YES / NO. Counter/run no: 21023

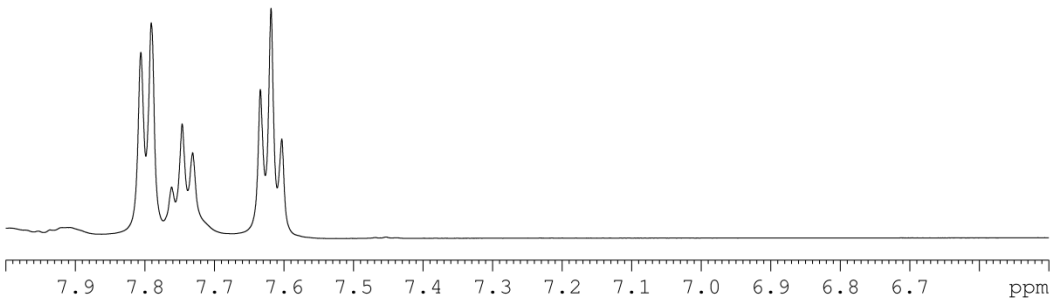
1.4 $[Pd(Cl)_2(C_6H_5CN)_2]$



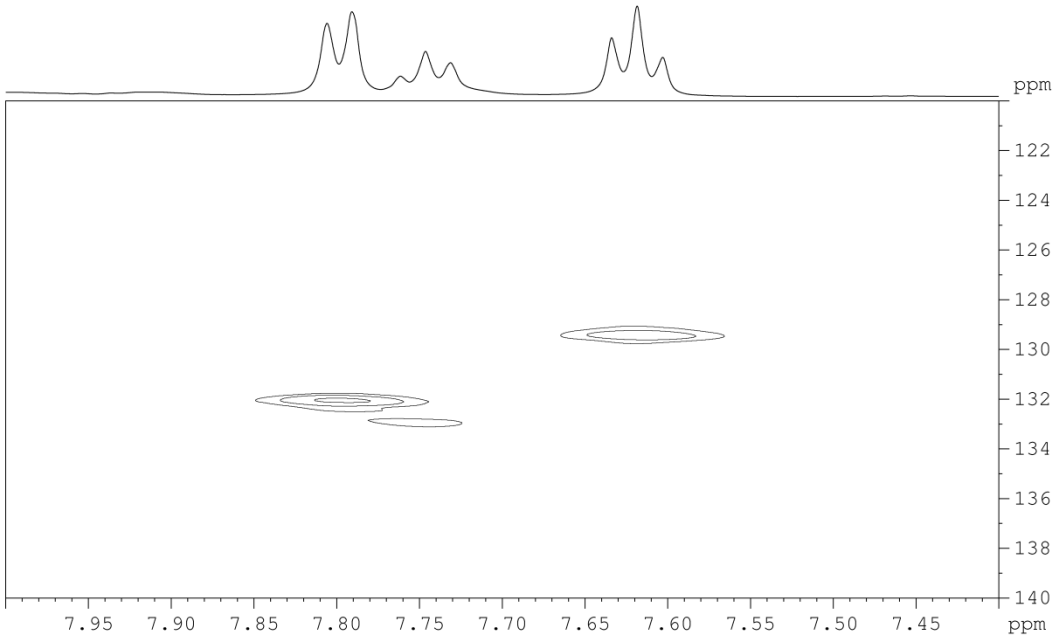
Compound reference kma-2-26

1.4.1 NMR spectra

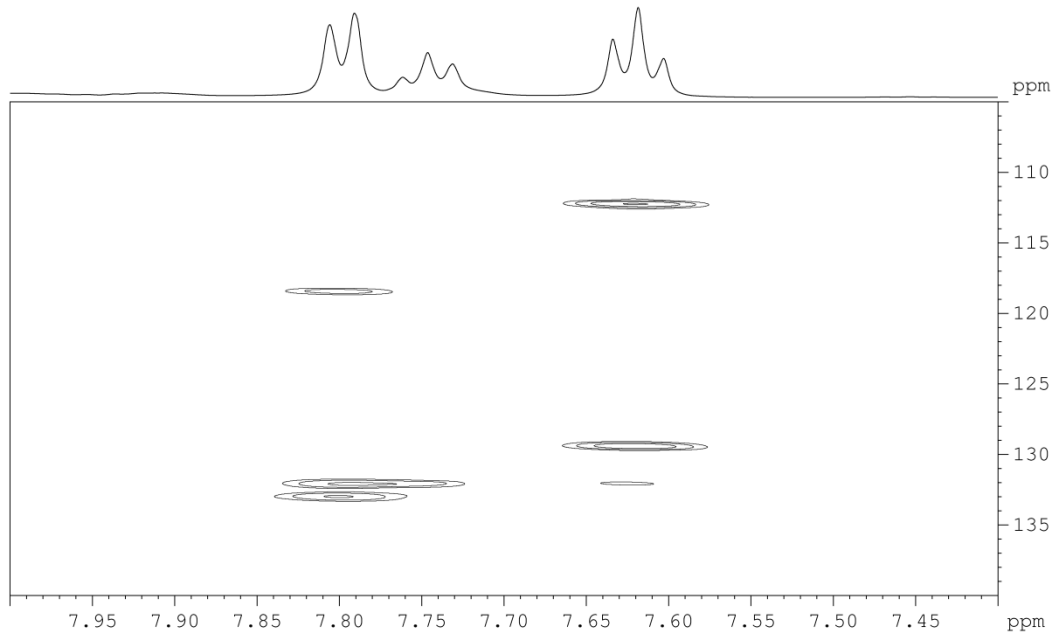
^1H



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



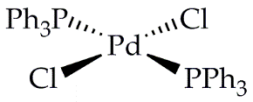
1.4.2 CHN elemental analysis

CHN Microanalytical Service Results

Name	K. APPLEBY	Compound ID	kma-2-26 [Pd Cl2 (NC Ph)2]	
Element	**% C**	**% H**	**% N**	**% Rest**
Observed 1	44.44	2.57	7.29	45.70
Observed 2	44.44	2.48	7.32	45.76
Mean	44.433	2.526	7.306	–
Calc (theory)	43.84	2.63	7.30	46.23

Comments: Check std within specified limits YES / NO. Counter/run no: 1618

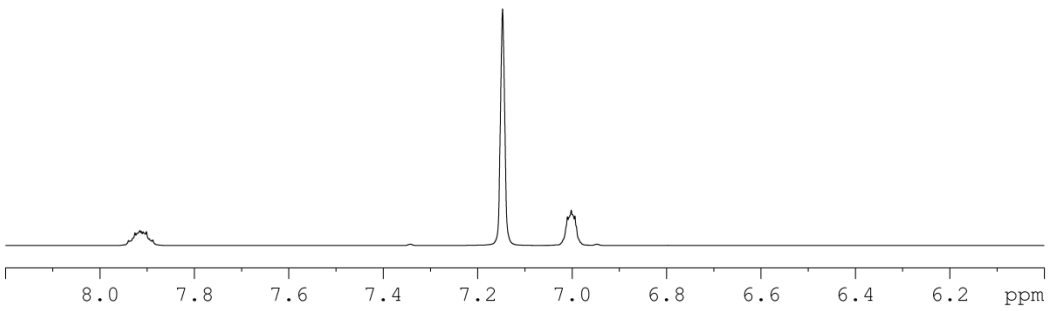
1.5 $[Pd(Cl_2)(PPh_3)_2]$



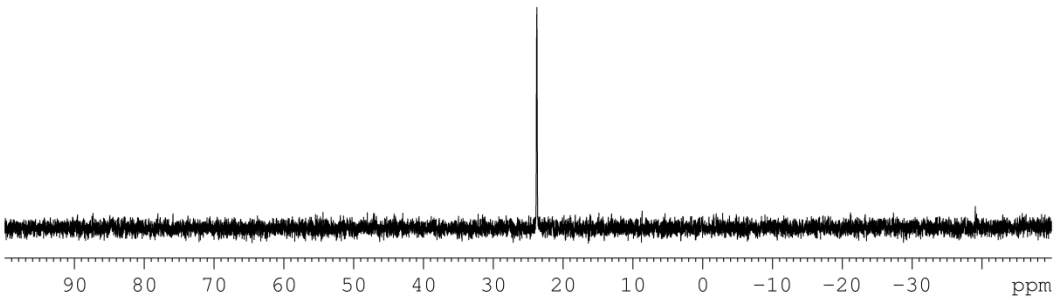
Compound reference kma-1-23

1.5.1 NMR spectra

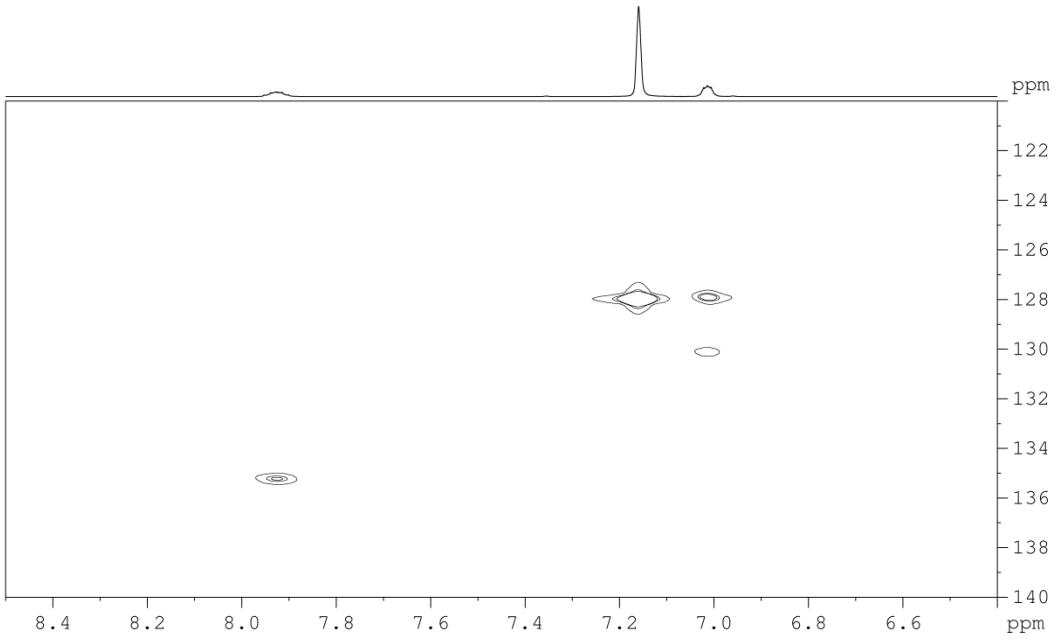
^{1}H



$^{31}P\ \{^{1}H\}$



^{13}C-optimised HMQC with a coupling of 145 Hz



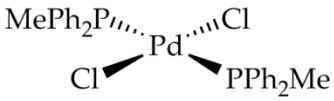
1.5.2 CHN elemental analysis

CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	[Pd(Cl)$_2$(PPh$_3$)$_2$]	
Element	**% C**	**% H**	**% N**	**% Rest**
Observed 1	61.80	4.31	–	33.89
Observed 2	61.64	4.26	–	34.10
Mean	61.717	4.287	–	–
Calc (theory)	61.60	4.31	–	34.09

Comments: Check std within specified limits YES / NO. Counter/run no: 20461

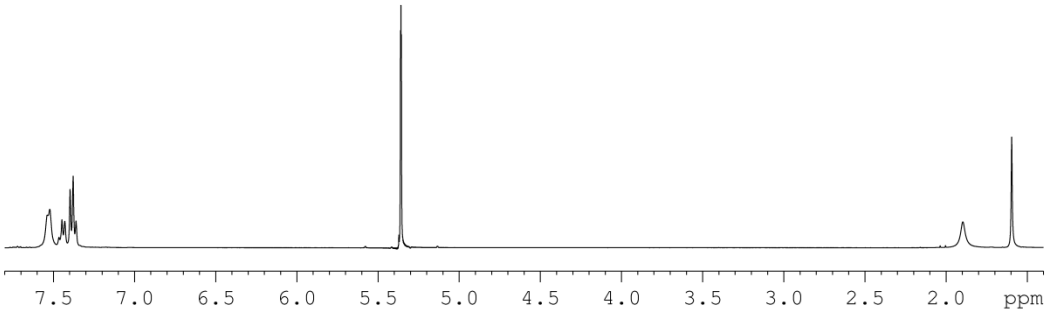
1.6 [Pd(Cl$_2$)(PPh$_2$Me)$_2$]



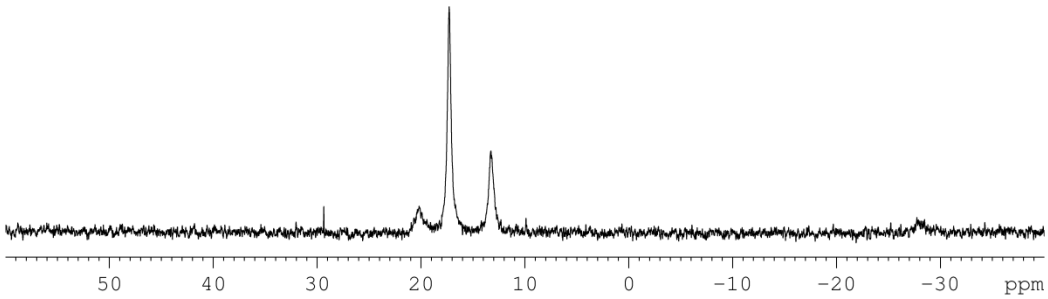
Compound reference kma-3-110

1.6.1 NMR spectra

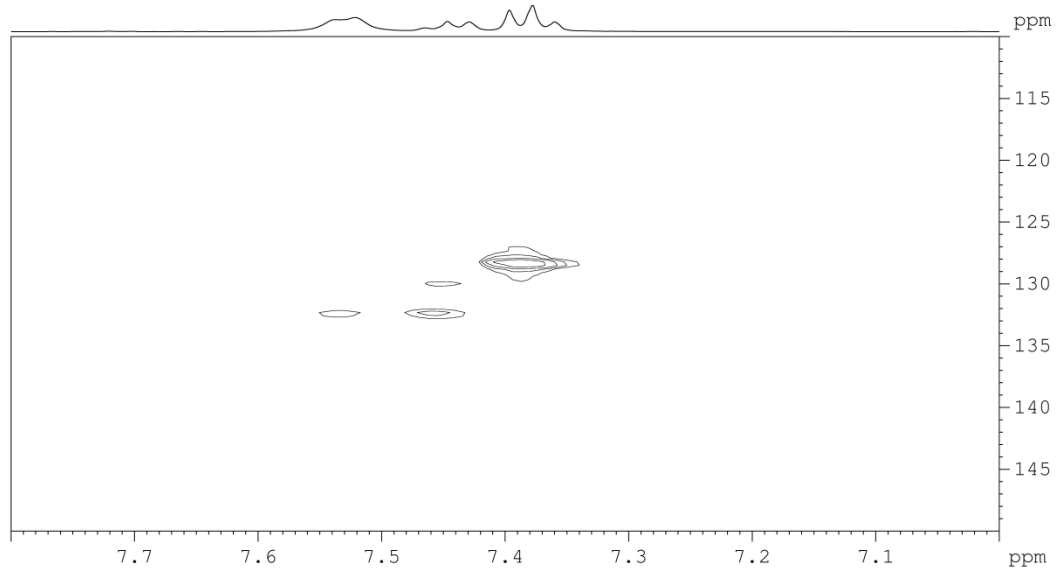
^{1}H



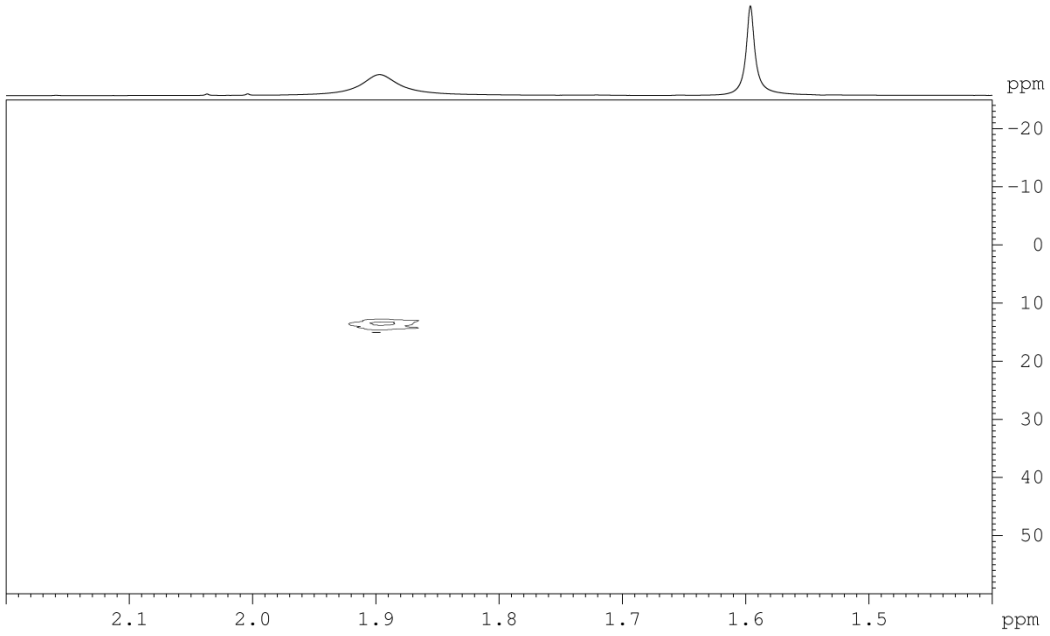
^{31}P $\{^{1}H\}$



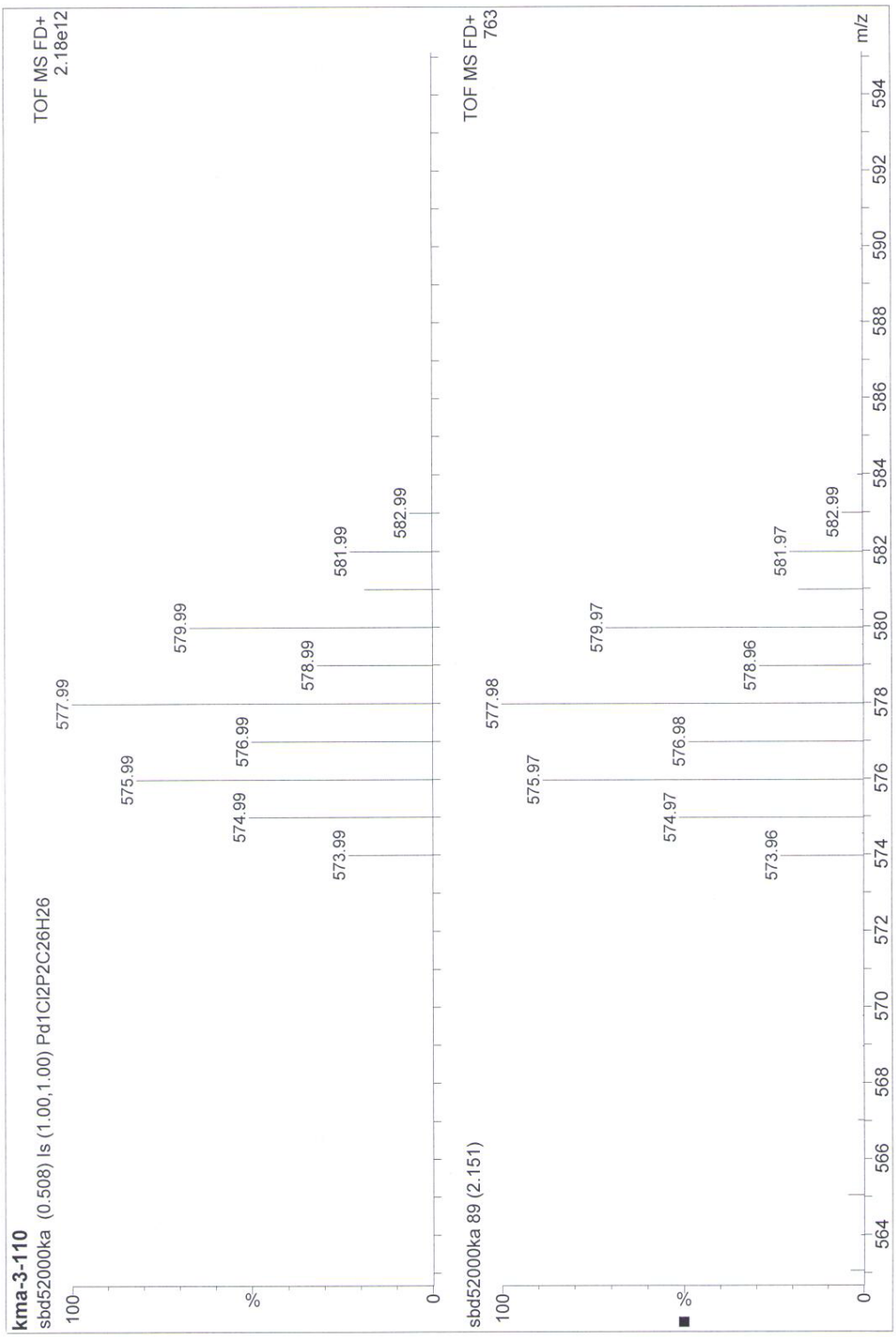
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 145 Hz



1.6.2 Mass spectra



kma-3-110 APCI inf

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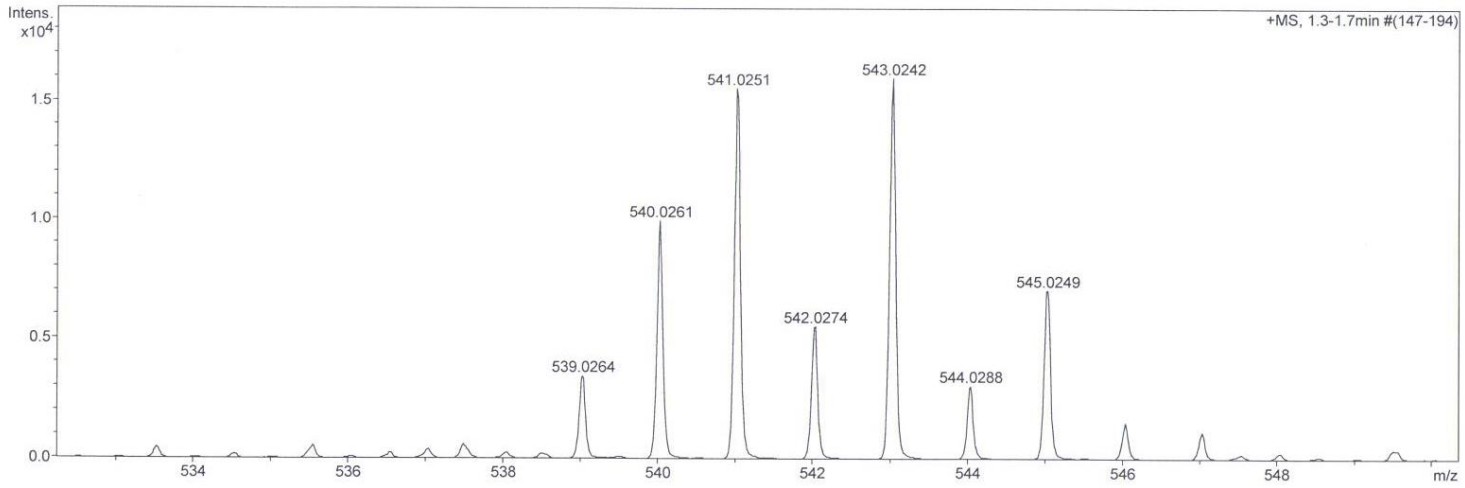
Analysis Information

Acquisition Date 20/04/2015 10:43:04

Analysis Filename	sbd52000ka APCI inf.d
Method	APCI_KH400_1260.m
Submission Name	sbd52000ka APCI inf
Instrument	micrOTOF
APCI	Positive



Meas. m/z	#	Formula	m/z	err [ppm]	err [mDa]	mSigma	Mean err [ppm]
541.0251	1	C 26 H 26 Cl P 2 Pd	541.0234	-3.1	-1.7	75.9	-2.8

1.6.3 CHN elemental analysis

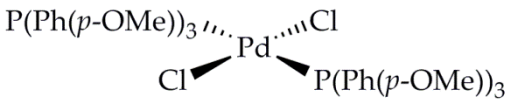
CHN Microanalytical Service Results $[Pd(Cl)_2(PPh_2Me)_2]$

Name	Kate Appleby	Compound ID	kma-4-19

Element	% C	% H	% N	% Rest
Observed 1	58.75	4.96	–	36.29
Observed 2	58.50	4.90	–	36.60
Mean	58.629	4.932	–	–
Calc (theory)	54.05	4.54	–	41.41

Comments: Check std within specified limits YES / NO. Counter/run no: 20461

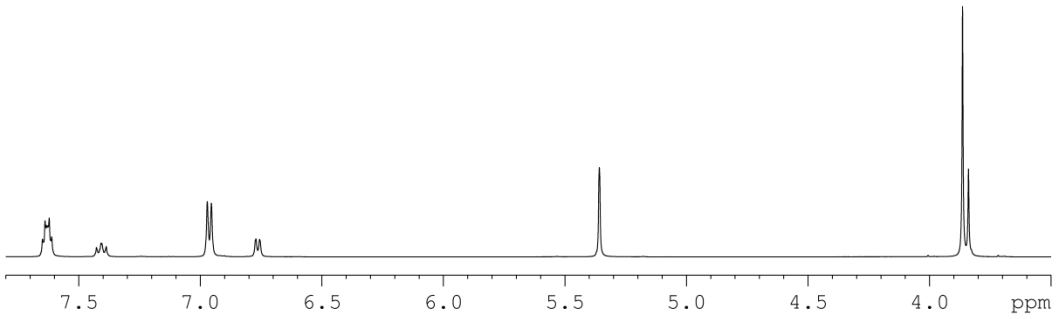
1.7 $[Pd(Cl)_2(P(Ph(p\text{-}OMe))_3)_2]$



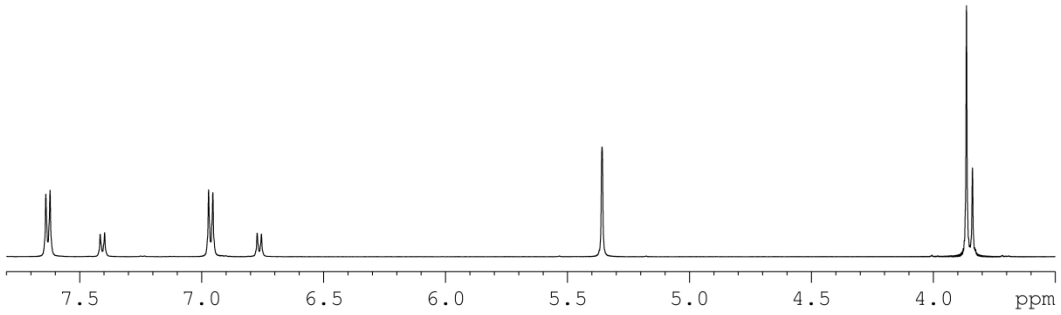
Compound reference kma-3-38

1.7.1 NMR spectra

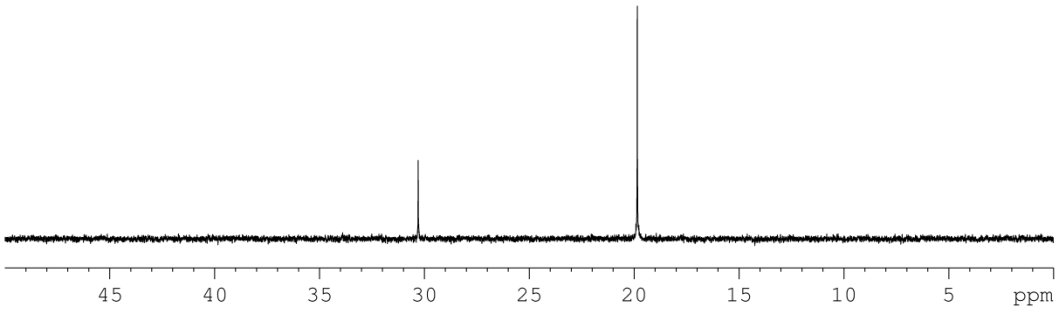
^{1}H



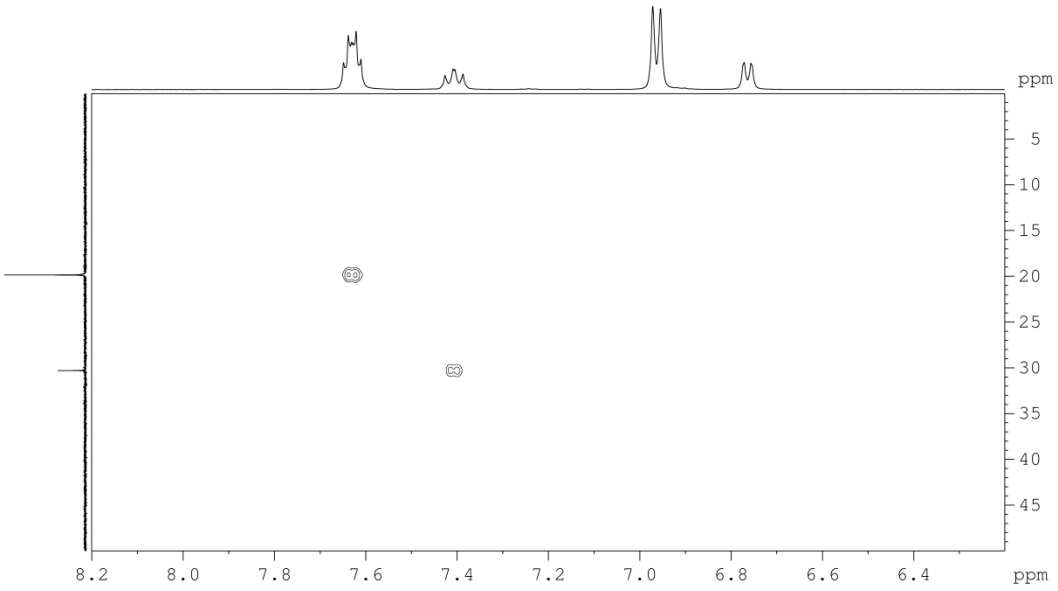
$^{1}H\ \{^{31}P\}$



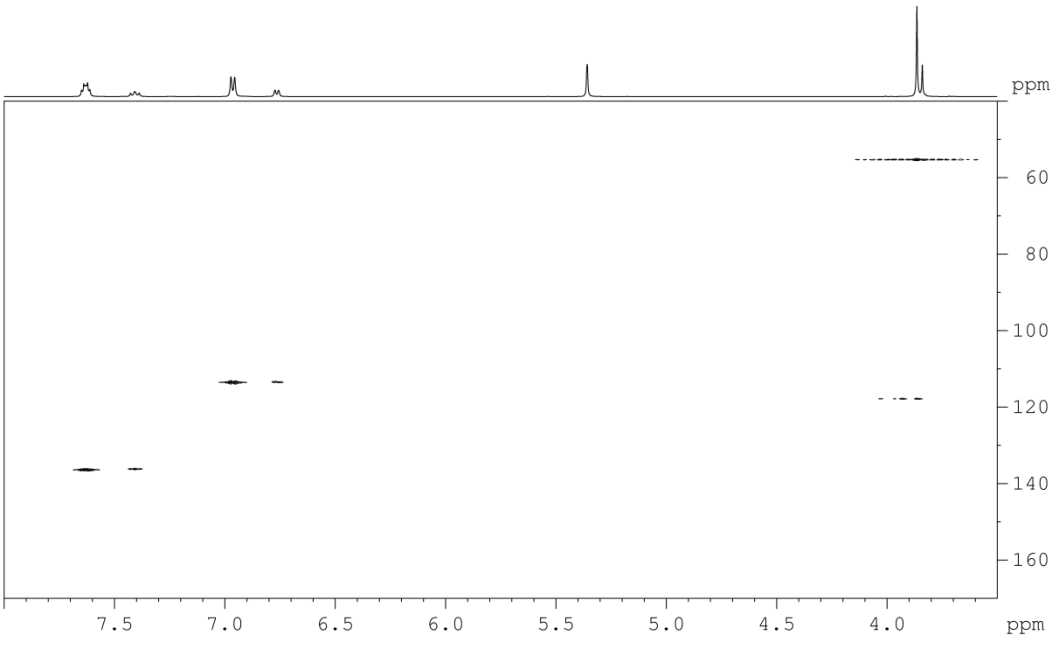
^{31}P {^{1}H}



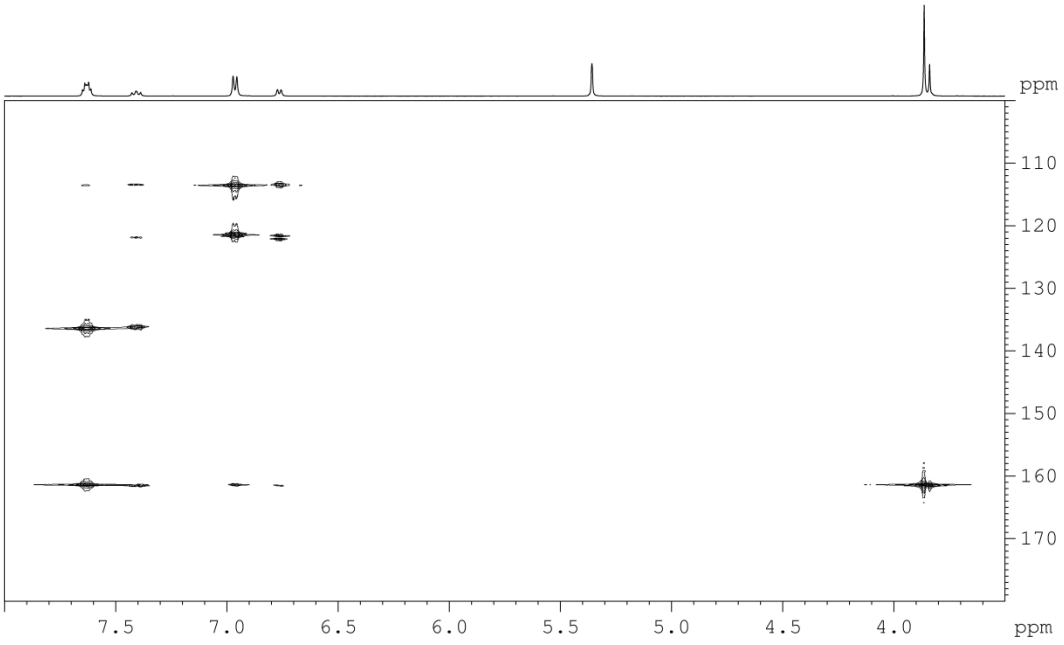
^{31}P-optimised HMQC with a coupling of 12 Hz



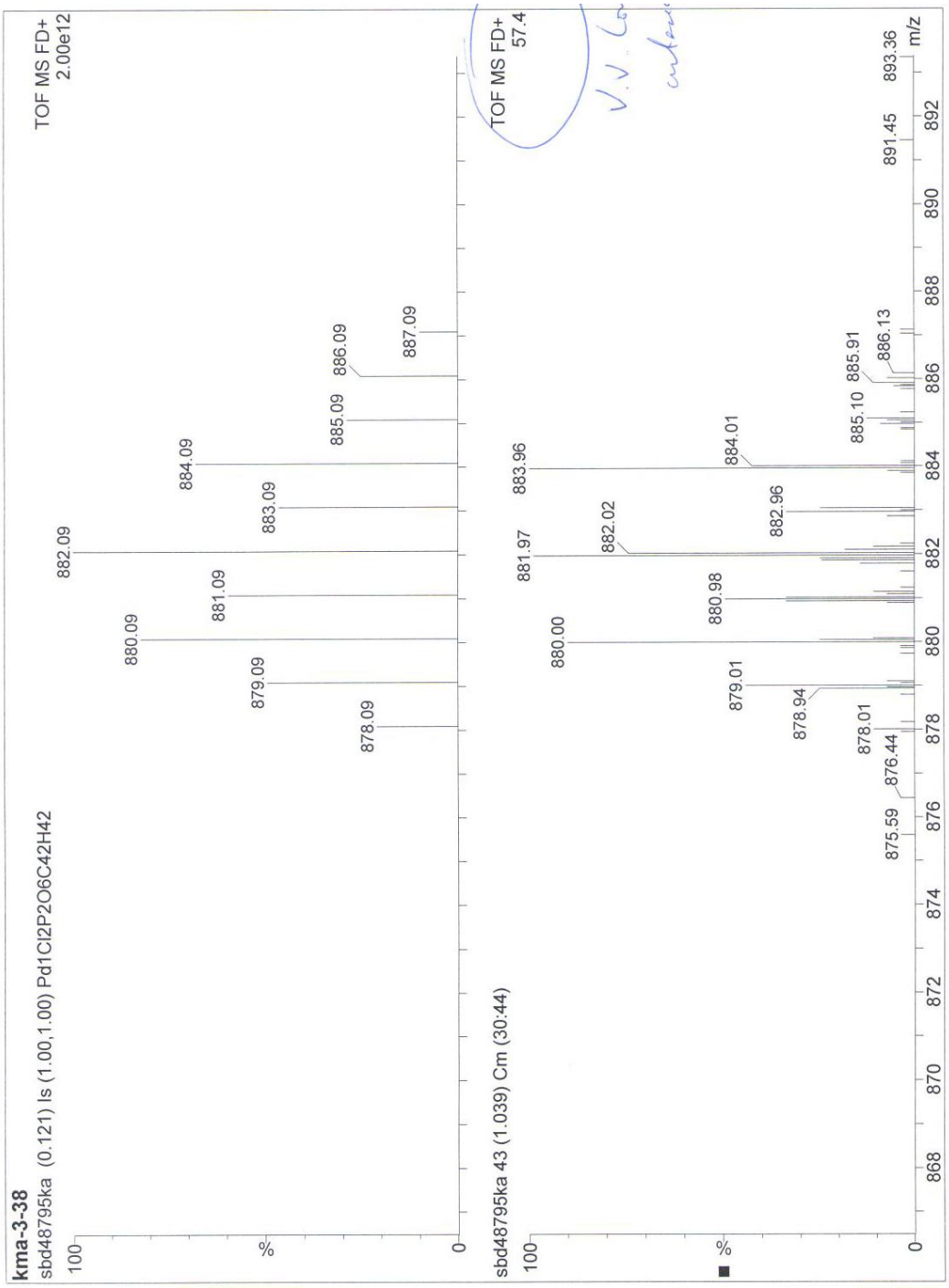
^{31}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.7.2 Mass spectra



1.7.3 CHN elemental analysis

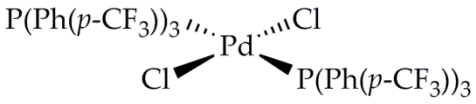
CHN Microanalytical Service Results $[Pd(Cl)_2(P(PhOMe)_3)_2]$

Name	Kate Appleby	Compound ID	kma-3-38

Element	% C	% H	% N	% Rest
Observed 1	56.52	4.69	-	38.78
Observed 2	56.73	4.70	-	38.57
Mean	56.626	4.692	-	-
Calc (theory)	57.19	4.80	-	38.01

Comments: Check std within specified limits YES / NO. Counter/run no: 20471

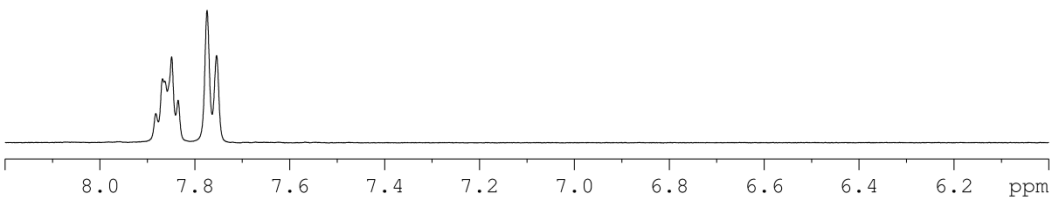
1.8 $[Pd(Cl)_2(P(Ph(p\text{-}CF_3))_3)_2]$



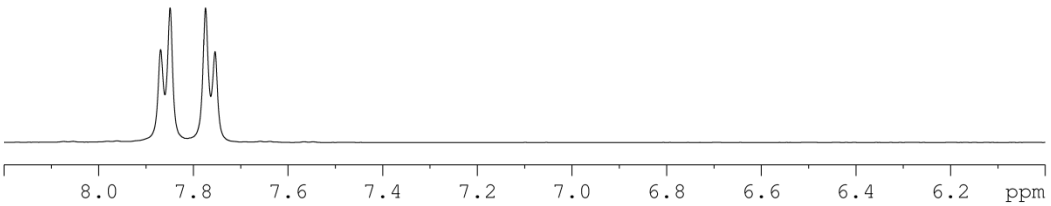
Compound reference kma-3-39

1.8.1 NMR spectra

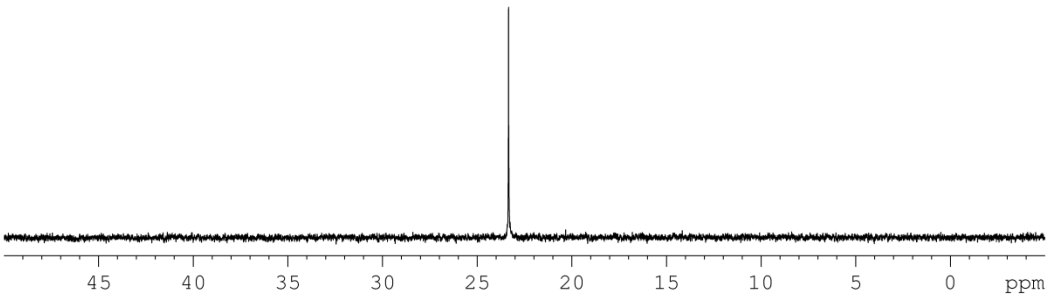
^{1}H



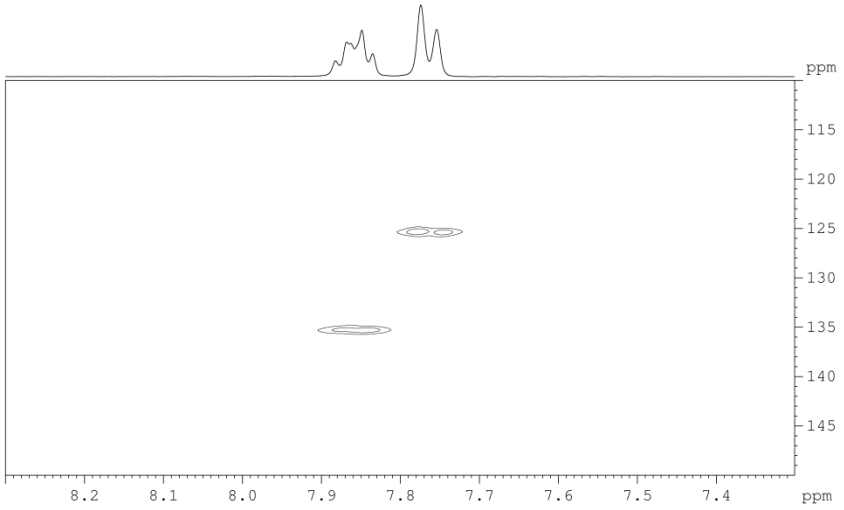
$^{1}H\ \{^{31}P\}$



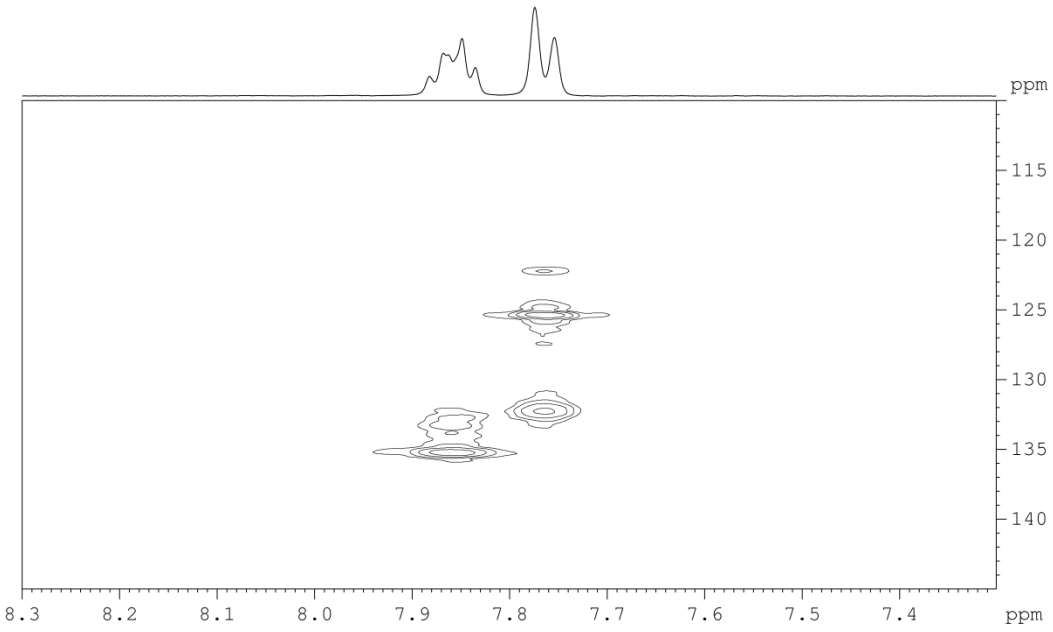
^{31}P {^{1}H}



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.8.2 CHN elemental analysis

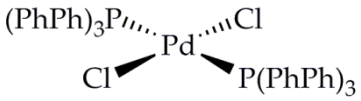
CHN Microanalytical Service Results $[Pd(Cl)_2(P(PhCF_3)_3)_2]$

Name	Kate Appleby	Compound ID	kma-3-39

Element	% C	% H	% N	% Rest
Observed 1	44.74	2.13	-	53.13
Observed 2	44.61	2.07	-	53.32
Mean	44.677	2.101	-	-
Calc (theory)	45.45	2.18	-	52.37

Comments: Check std within specified limits YES / NO. Counter/run no: 20477

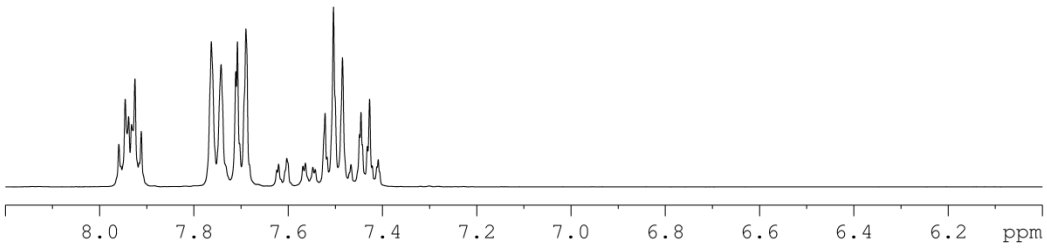
1.9 $[Pd(Cl)_2(P(PhPh)_3)_2]$



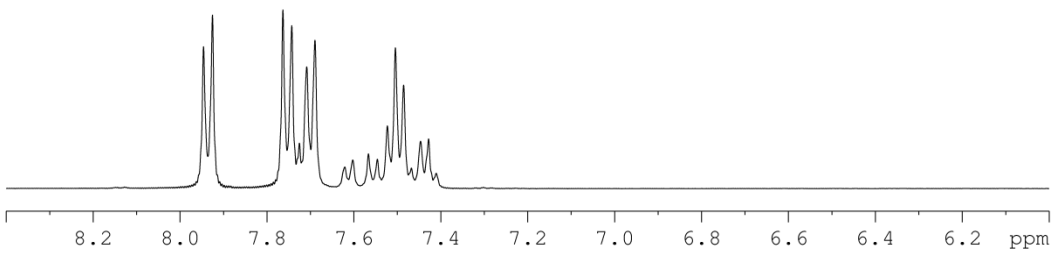
Compound reference kma-3-49

1.9.1 NMR spectra

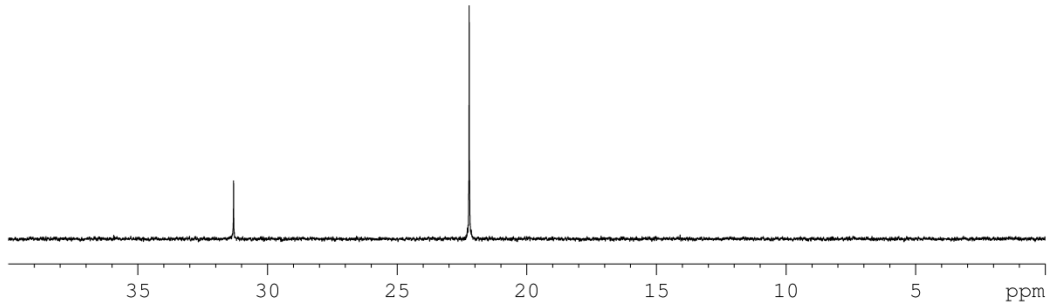
^{1}H



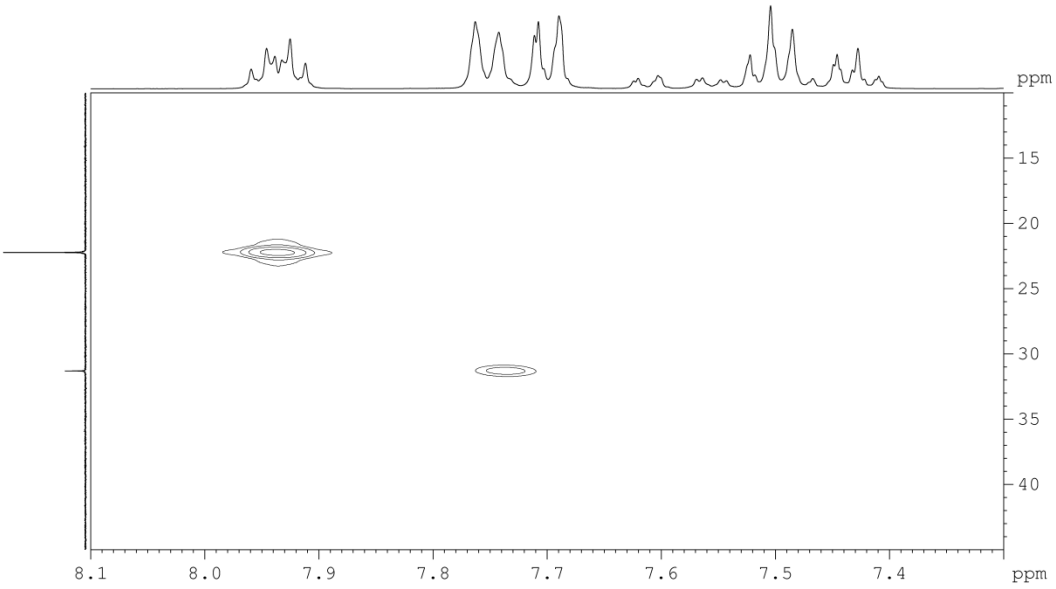
^{1}H $\{^{31}P\}$



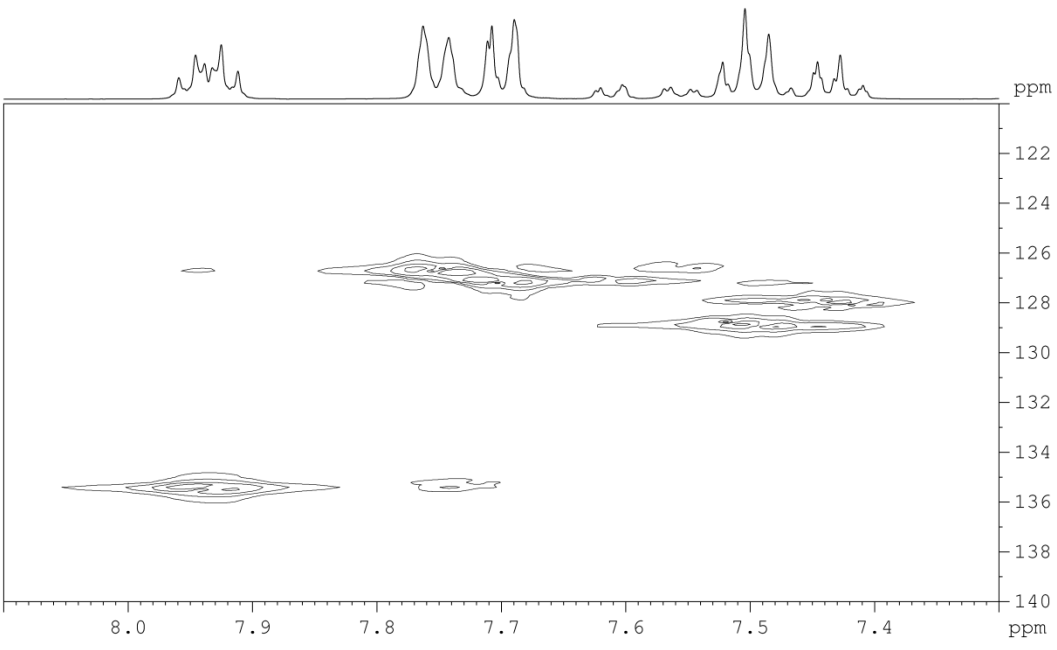
^{31}P {^{1}H}



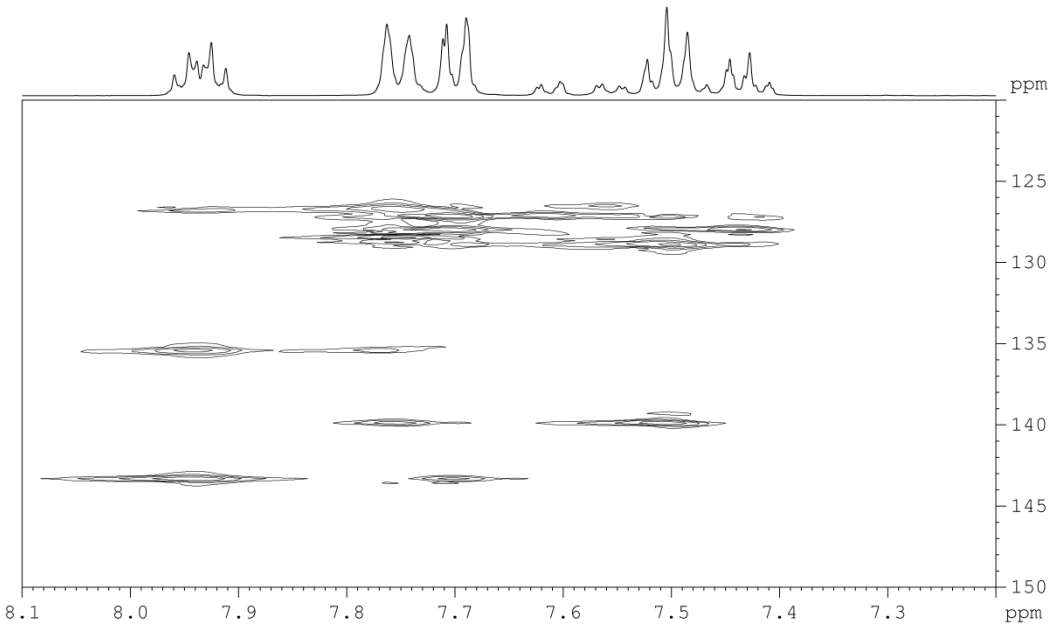
^{31}P-optimised HMQC with a coupling of 12 Hz



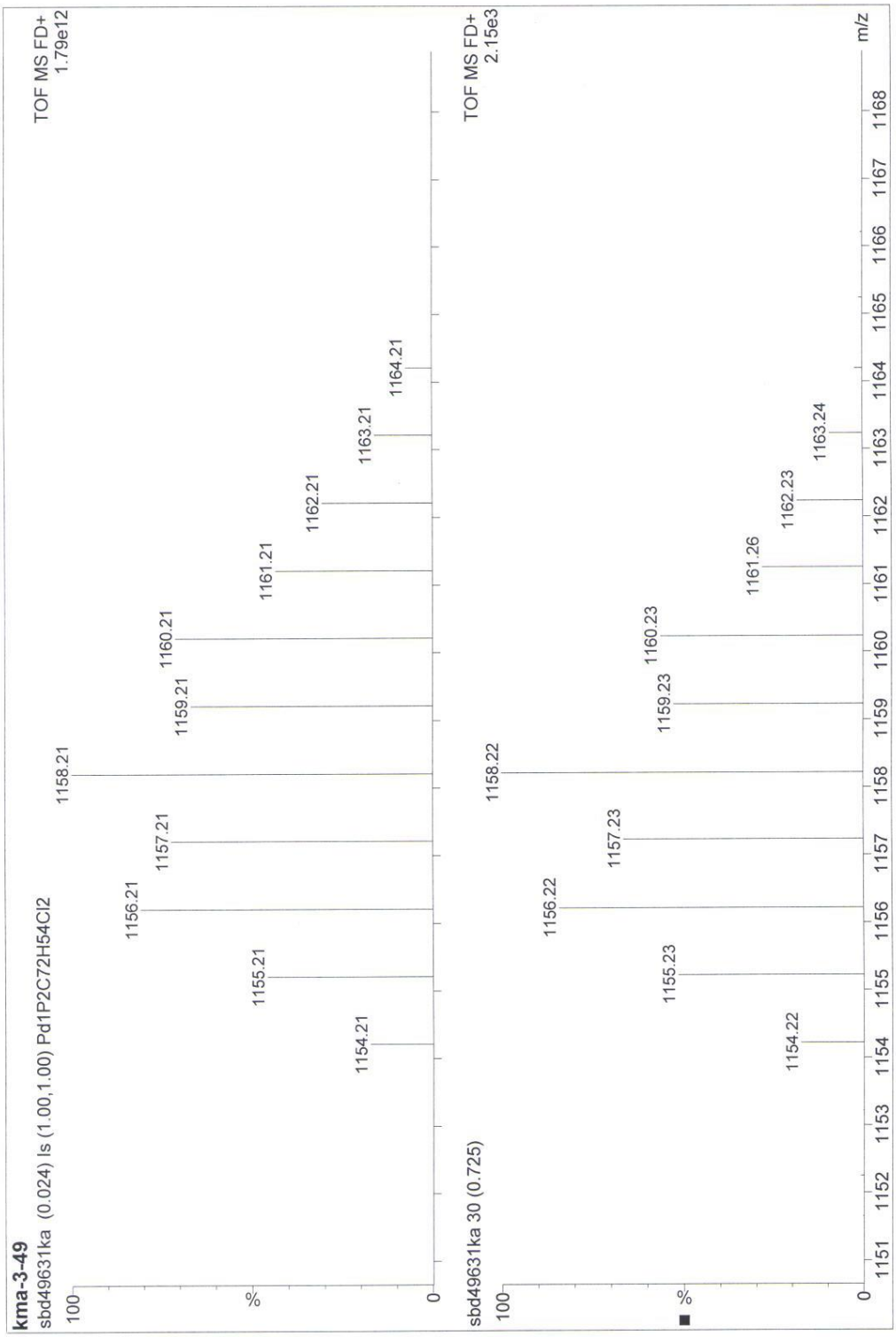
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.9.2 Mass spectra



1.9.3 CHN elemental analysis

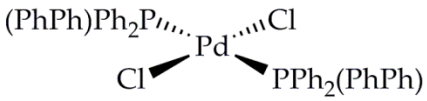
CHN Microanalytical Service Results $[Pd(Cl)_2(P(APh)_3)_2]$

Name	Kate Appleby	Compound ID	kma-3-49

Element	% C	% H	% N	% Rest
Observed 1	74.08	4.69	-	21.23
Observed 2	74.07	4.65	-	21.28
Mean	74.075	4.670	-	-
Calc (theory)	74.65	4.70	-	20.65

Comments: Check std within specified limits YES / NO. Counter/run no: 20461

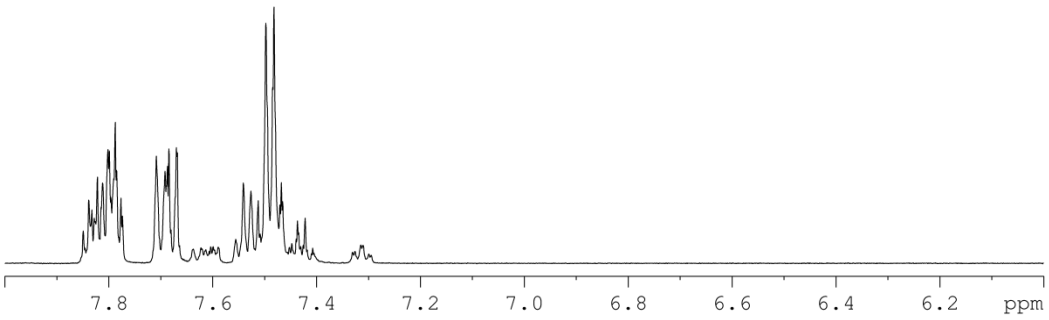
1.10 $[Pd(Cl)_2(PPh_2(PhPh))_2]$



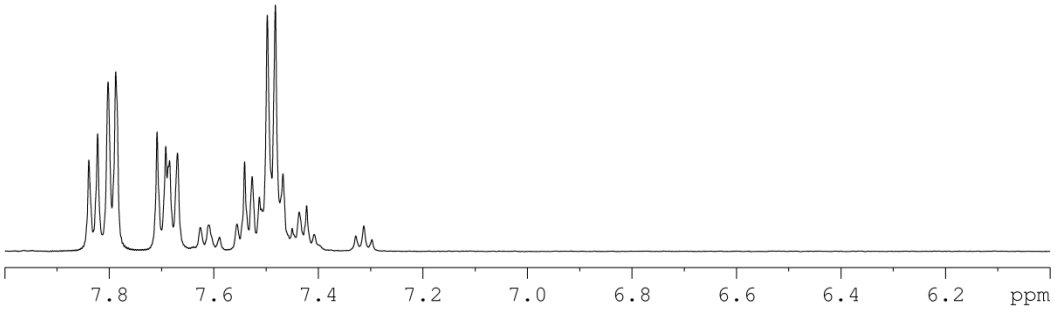
Compound reference kma-3-11

1.10.1 NMR spectra

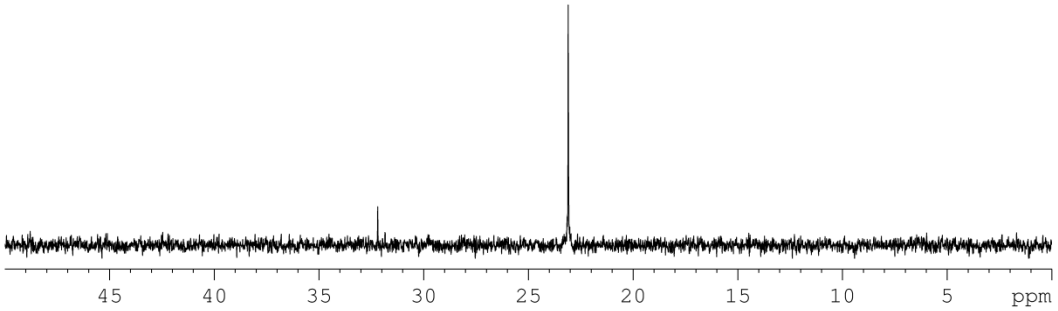
^{1}H



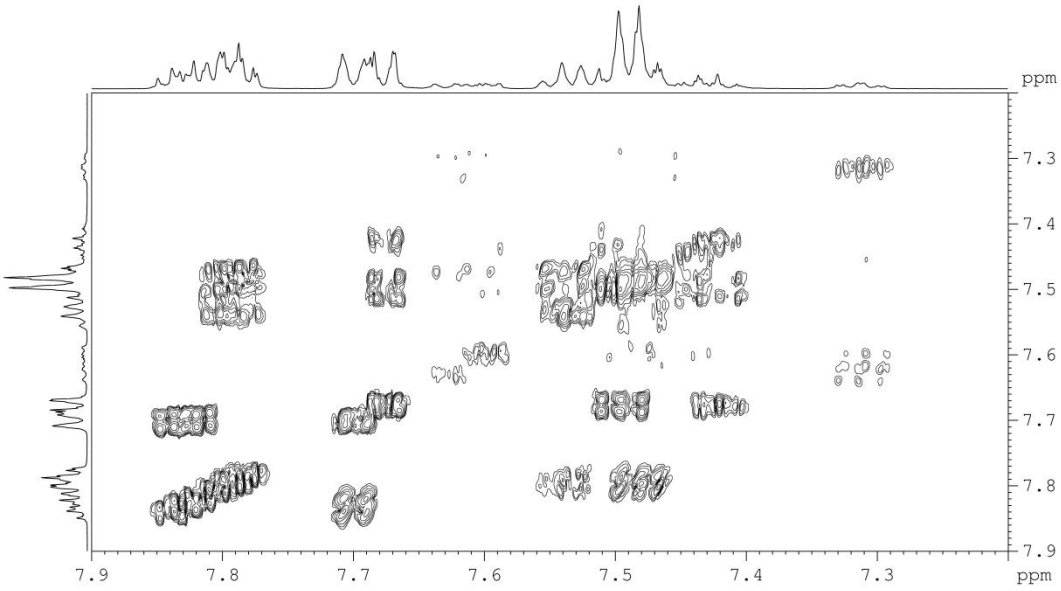
$^{1}H\ \{^{31}P\}$



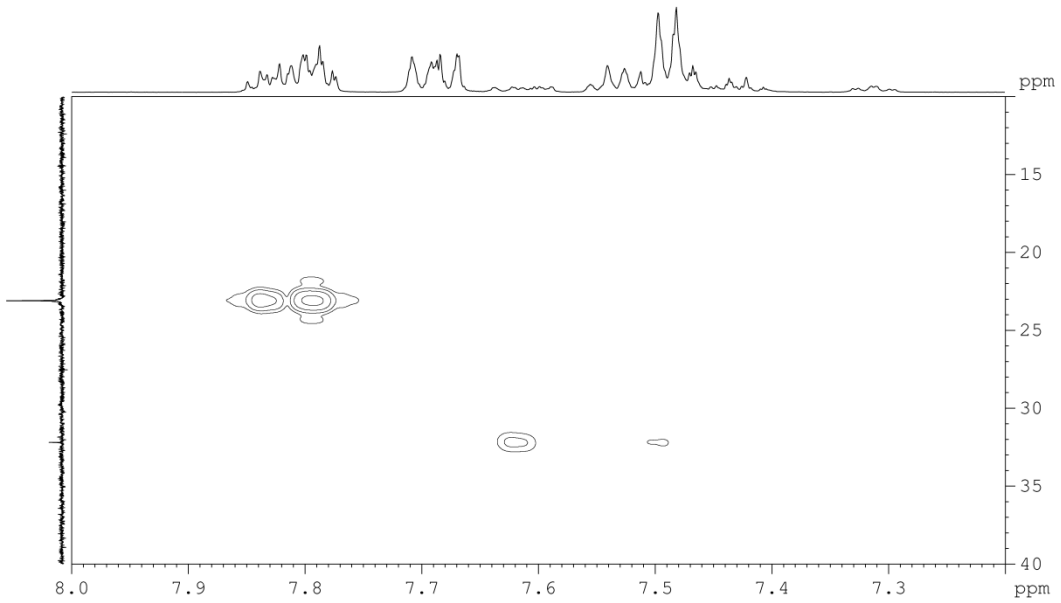
$^{31}P\ \{^{1}H\}$



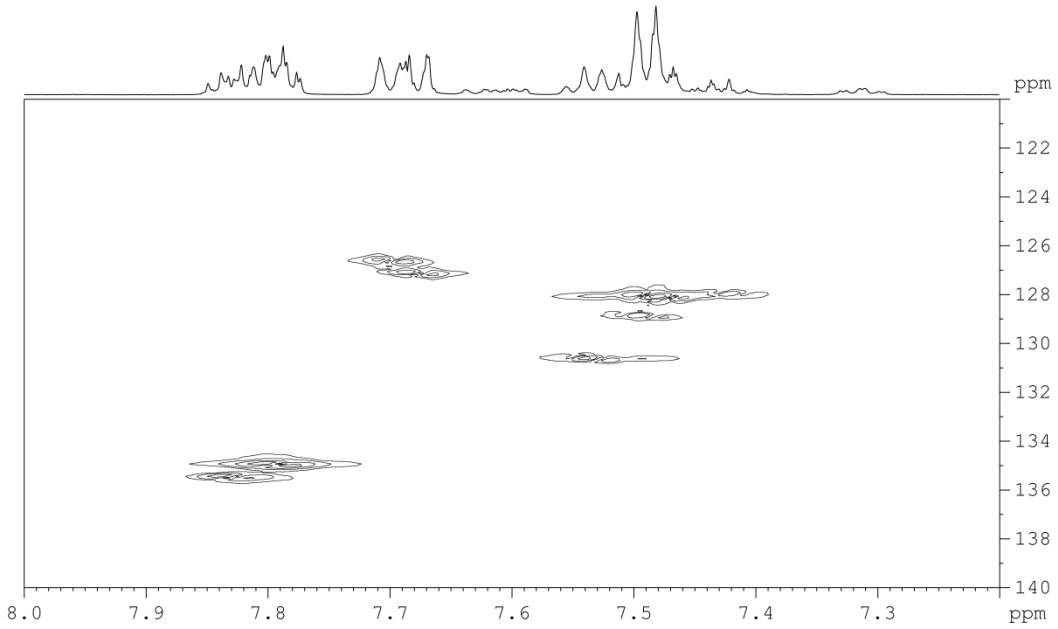
COSY



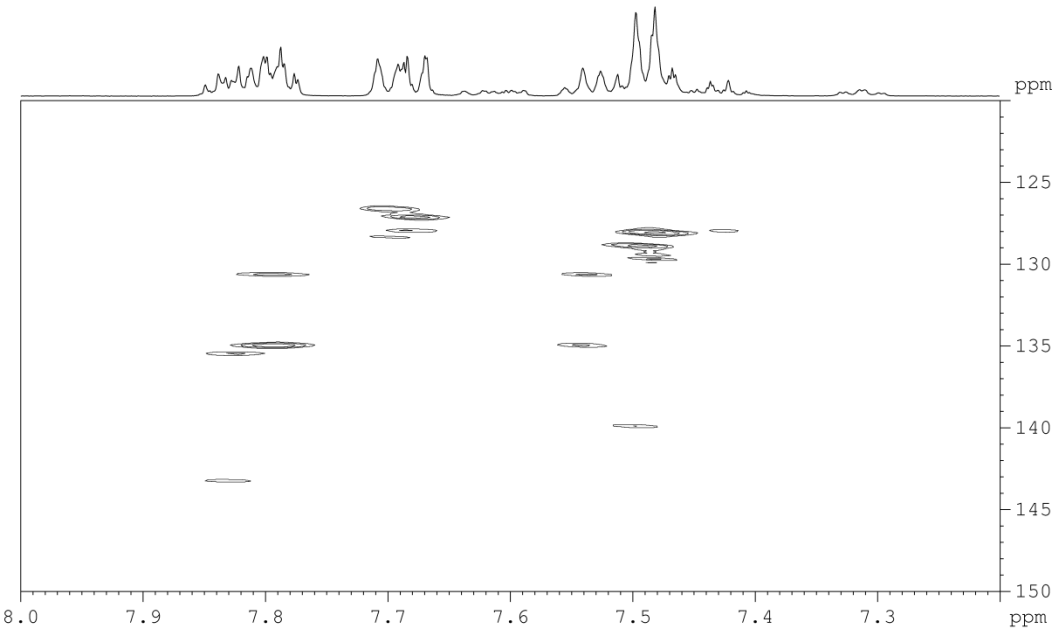
^{31}P-optimised HMQC with a coupling of 12 Hz



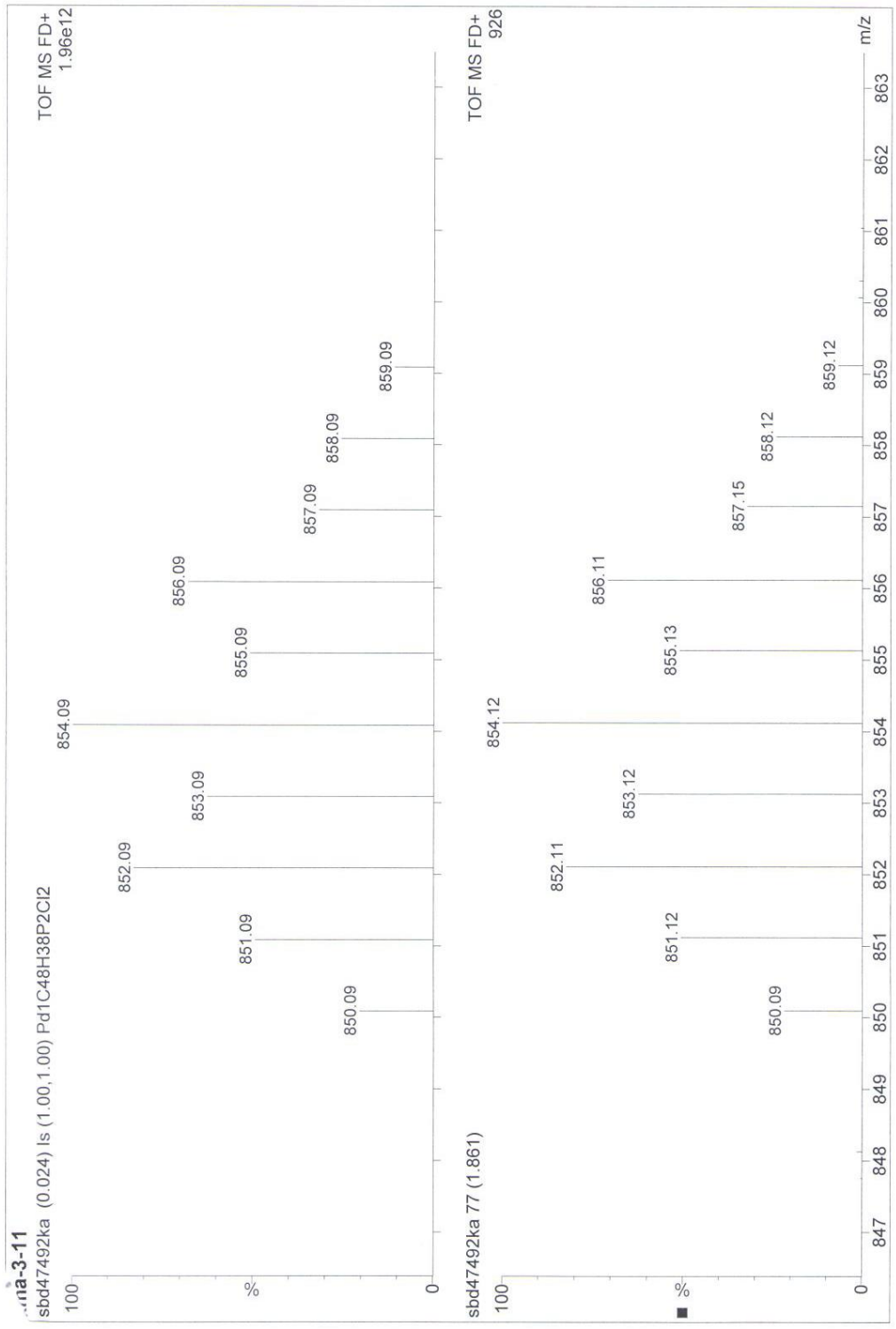
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.10.2 Mass spectra



1.10.3 CHN elemental analysis

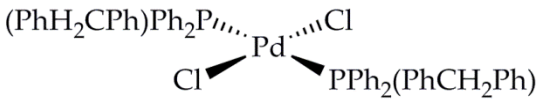
CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma-3-11 $[Pd(Cl)_2(PPh_2(PhPh))_2]$

Element	% C	% H	% N	% Rest
Observed 1	67.15	4.42	–	28.43
Observed 2	67.20	4.43	–	28.37
Mean	67.171	4.424	–	–
Calc (theory)	67.50	4.48	–	28.02

Comments: Check std within specified limits YES / NO. Counter/run no: 18633

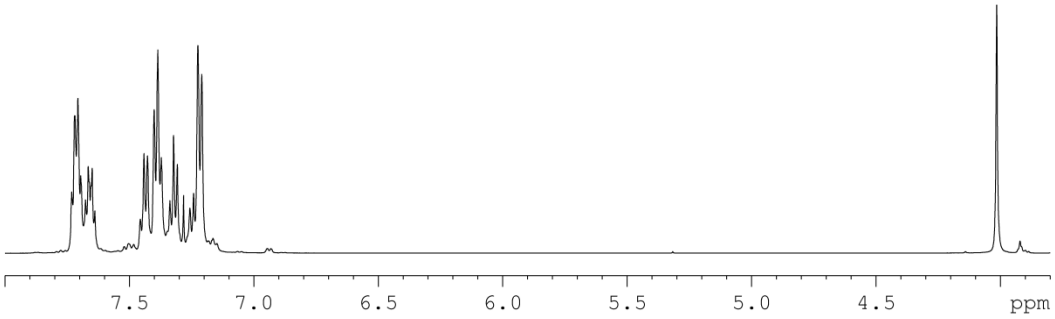
1.11 $[Pd(Cl)_2(PPh_2(PhCH_2Ph))_2]$



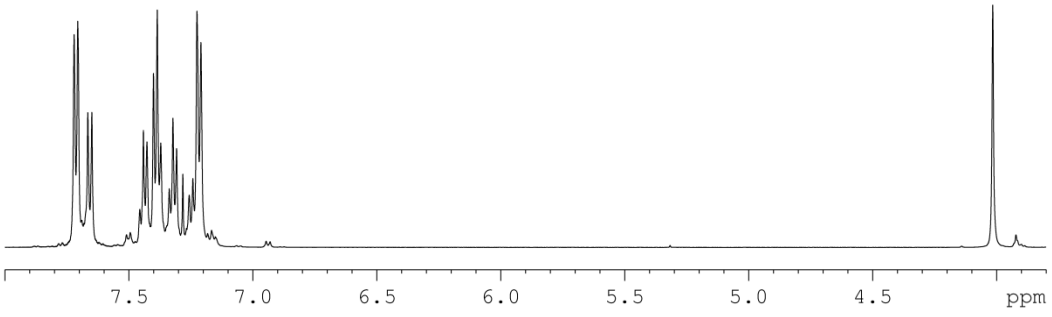
Compound reference kma-3-24

1.11.1 NMR spectra

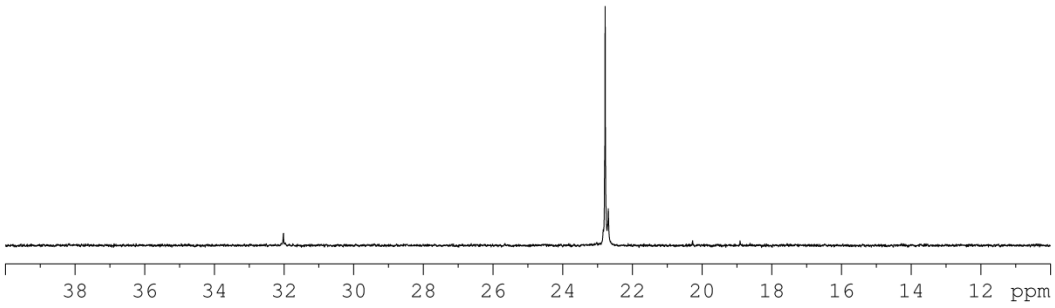
^{1}H



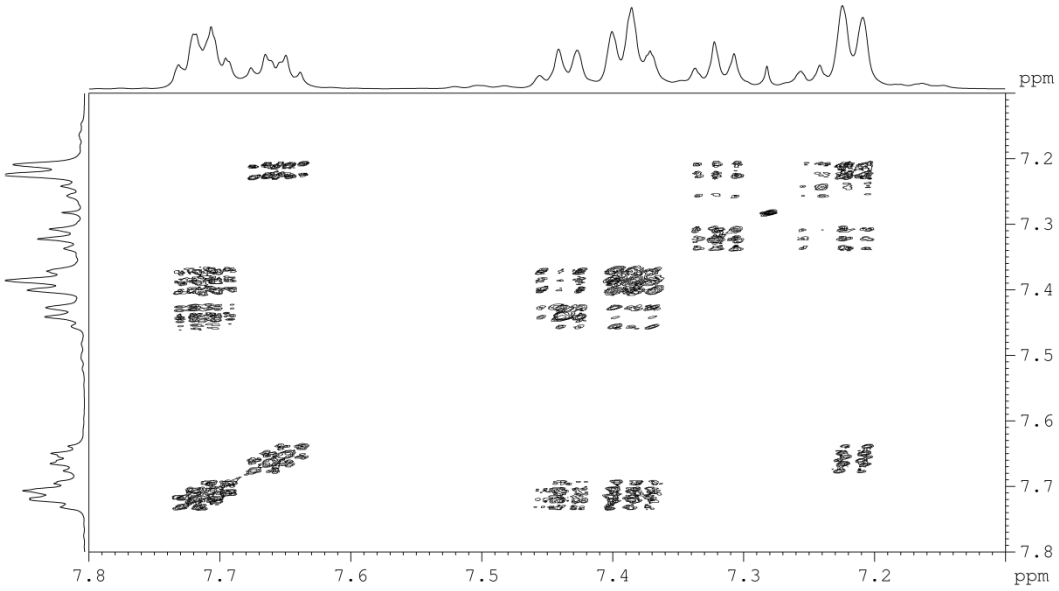
$^{1}H\ \{^{31}P\}$



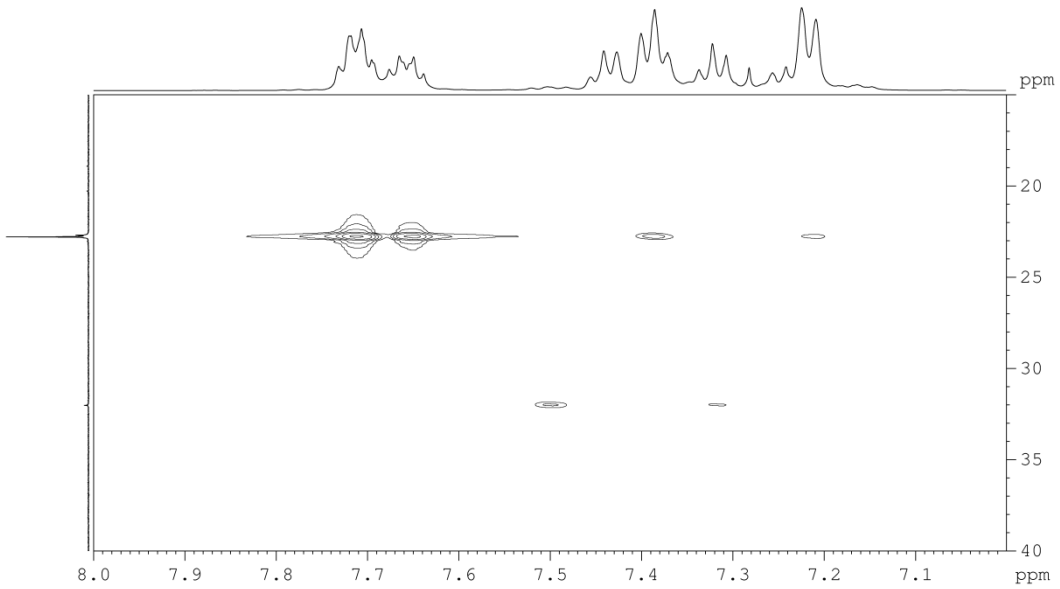
$^{31}P\ \{^{1}H\}$



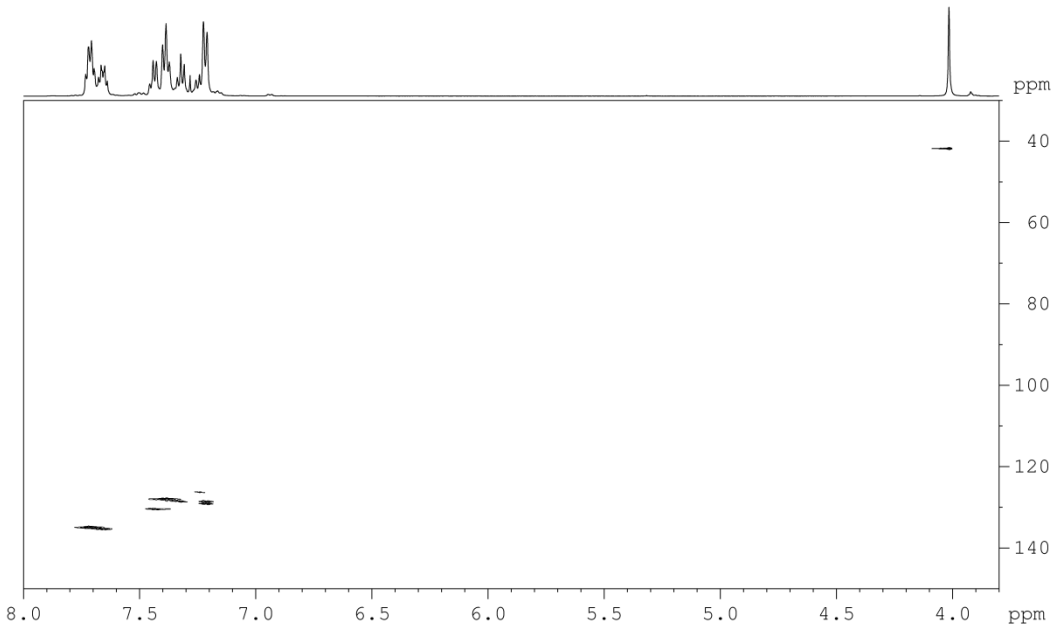
COSY



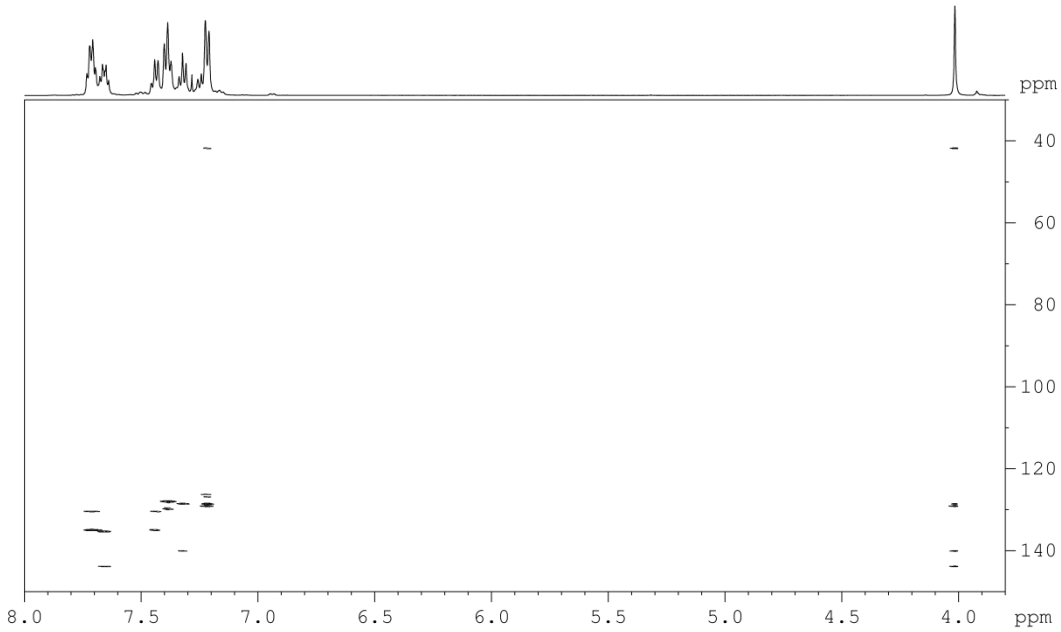
^{31}P-optimised HMQC with a coupling of 12 Hz



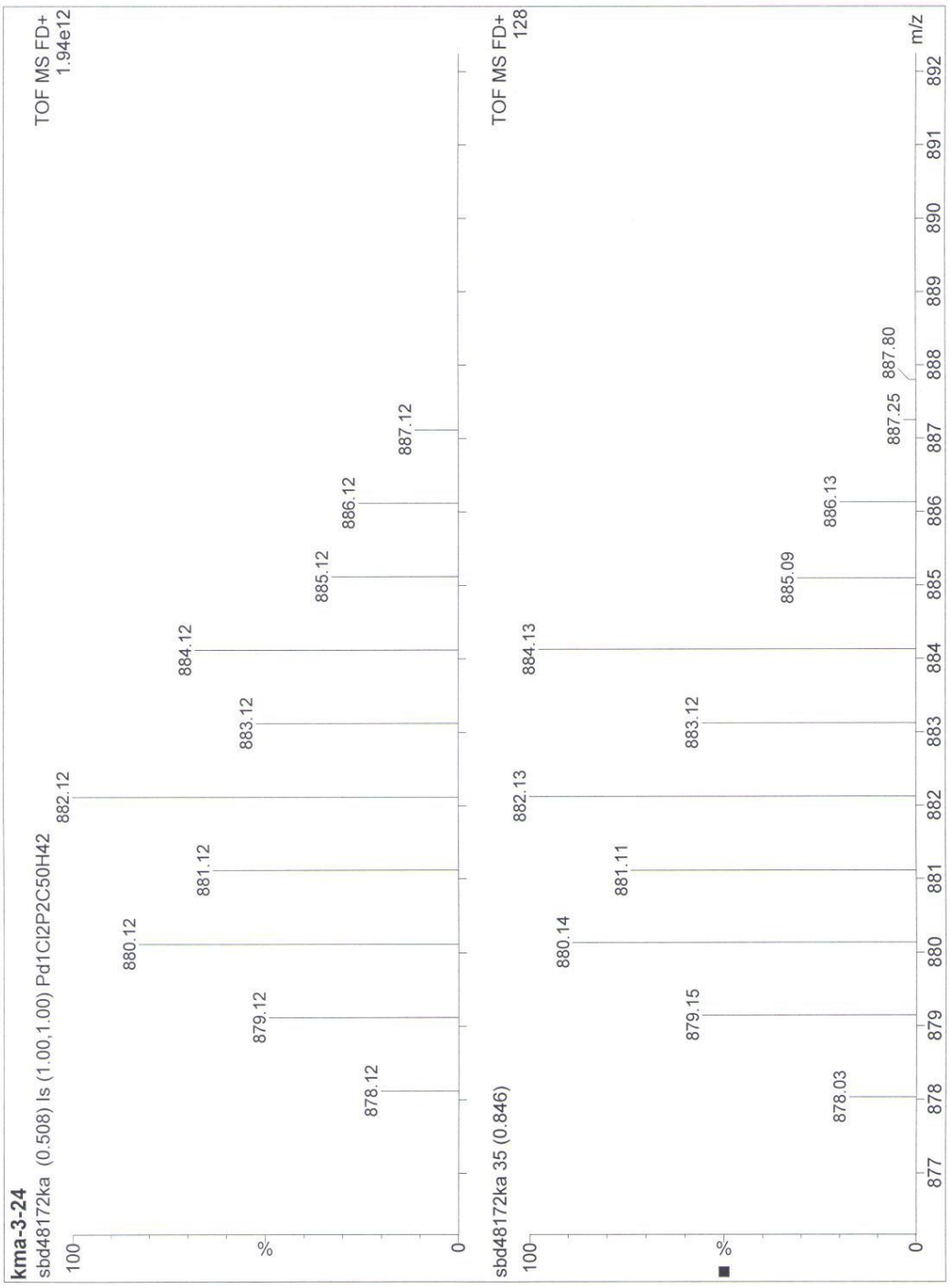
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.11.2 Mass spectra



1.11.3 CHN elemental analysis

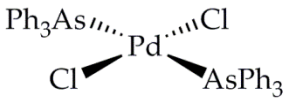
CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma - 3-24 $[Pd(Cl)_2(P(Ph_2(AsCH_3Ph))_3)_2]$

Element	% C	% H	% N	% Rest
Observed 1	68.21	5.06	-	26.73
Observed 2	68.16	4.98	-	26.86
Mean	68.185	5.023	-	-
Calc (theory)	68.08	4.80	-	27.12

Comments: Check std within specified limits YES / NO. Counter/run no: 18633

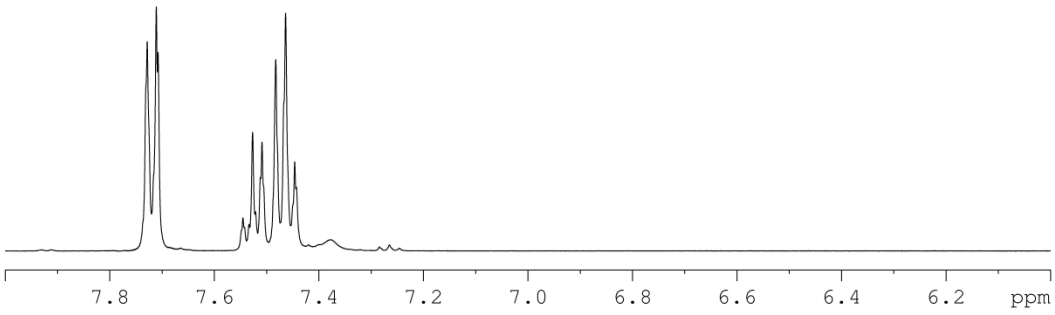
1.12 $[Pd(Cl)_2(AsPh_3)_2]$



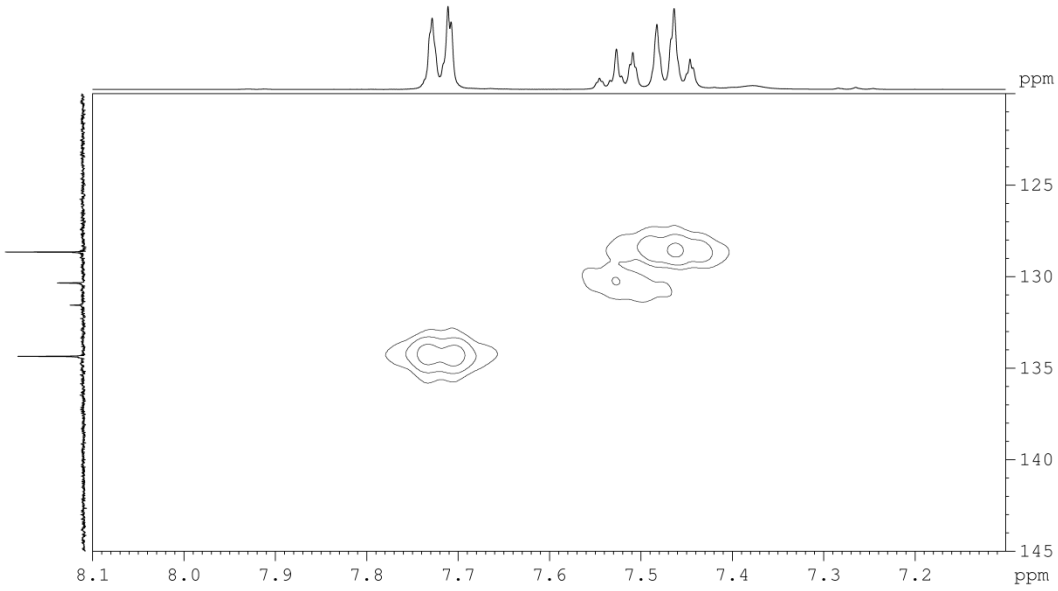
Compound reference kma-3-79

1.12.1 NMR spectra

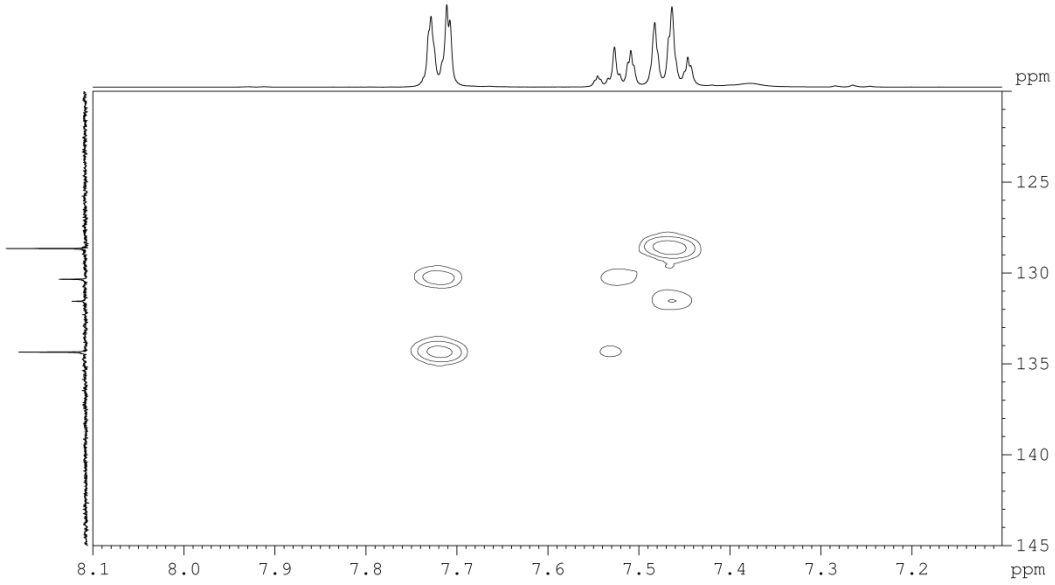
^{1}H



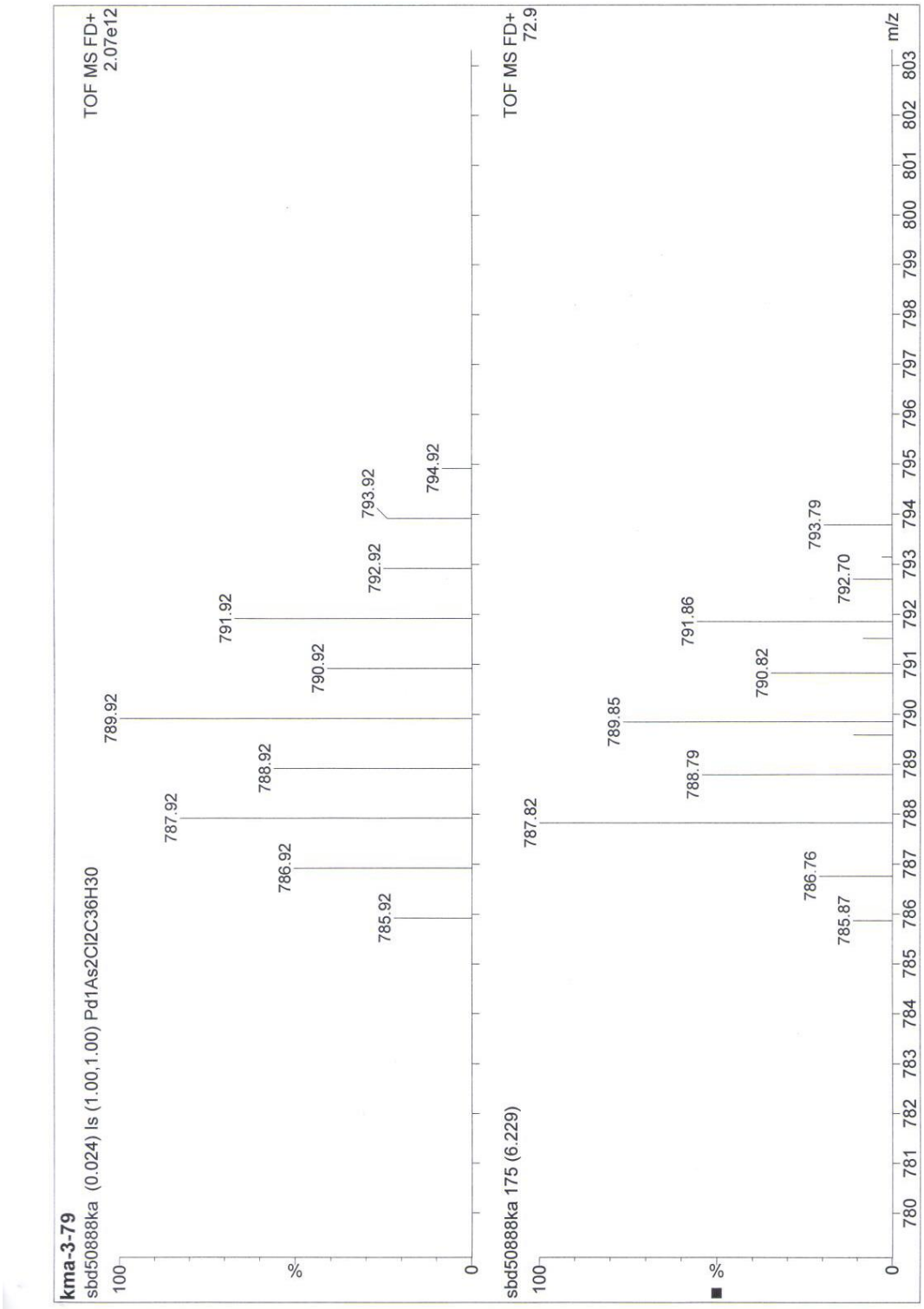
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



1.12.2 Mass spectra



1.12.3 CHN elemental analysis

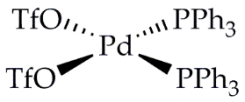
CHN Microanalytical Service Results $[Pd(Cl)_2(AsPh_3)_2]$

Name	Kate Appleby	Compound ID	kma-4-25

Element	% C	% H	% N	% Rest
Observed 1	54.21	3.78	–	42.01
Observed 2	54.20	3.76	–	42.04
Mean	54.209	3.768	–	–
Calc (theory)	54.75	3.83	–	41.42

Comments: Check std within specified limits YES / NO. Counter/run no: 20461

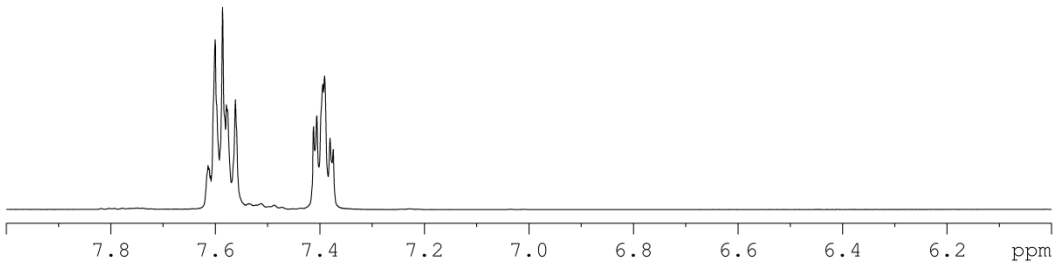
1.13 $[Pd(PPh_3)_2(OTf)_2]$



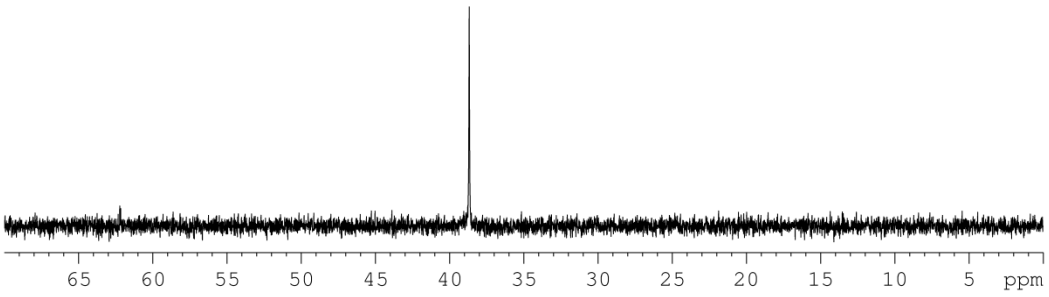
Compound reference kma-1-51

1.13.1 NMR spectra

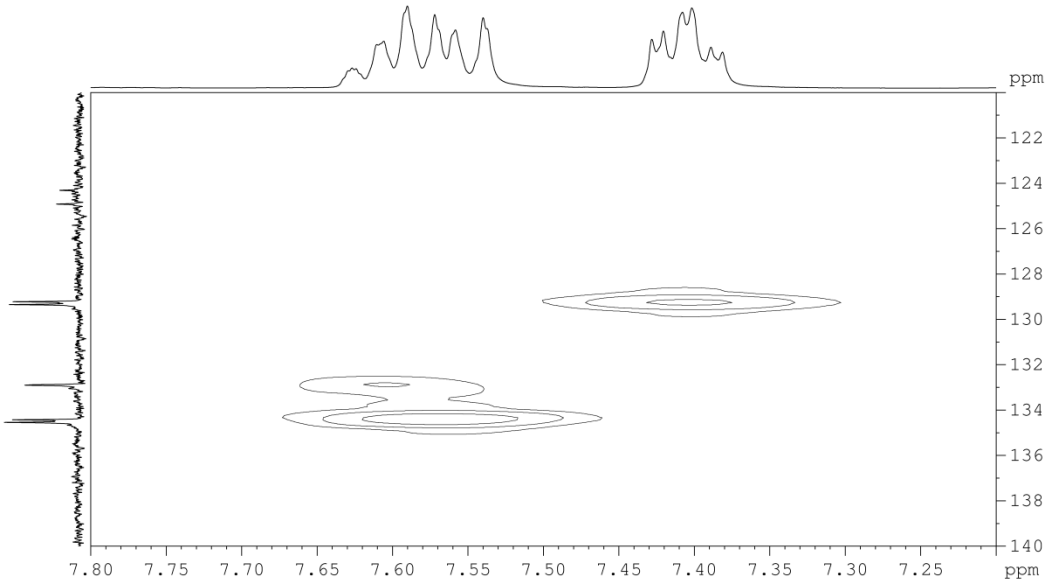
^{1}H



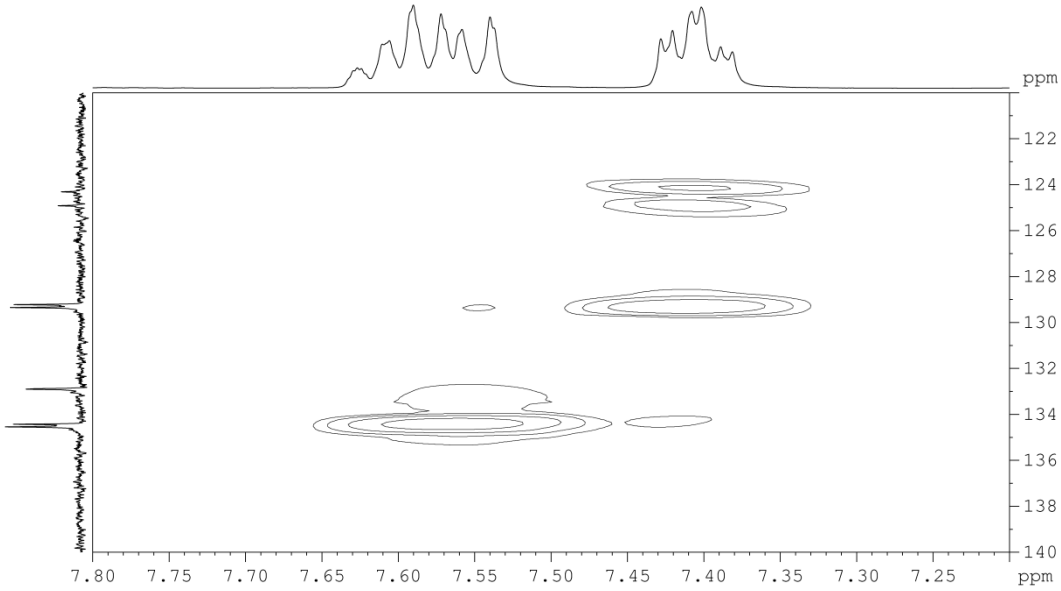
$^{31}P\ \{^{1}H\}$



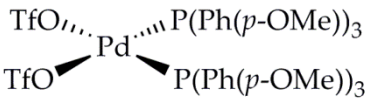
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



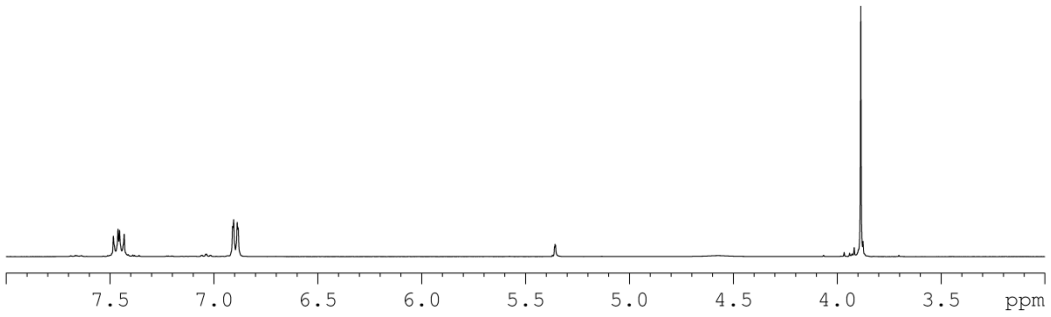
1.14 [Pd(OTf)$_2$(P(Ph(*p*-OMe)$_3$)$_3$)$_2$]



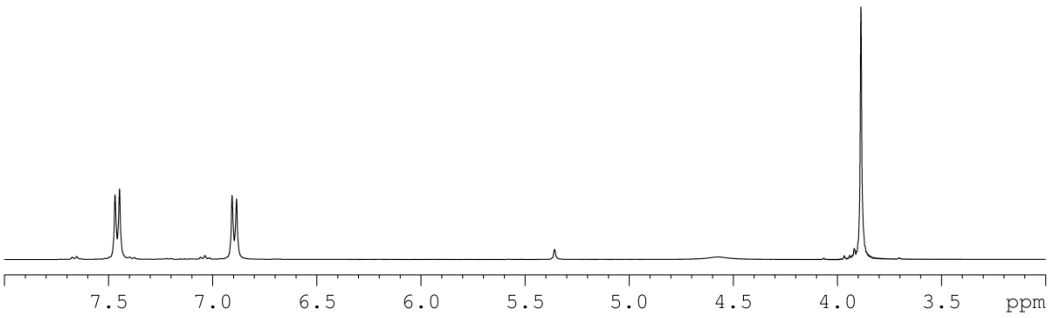
Compound reference kma-3-41

1.14.1NMR spectra

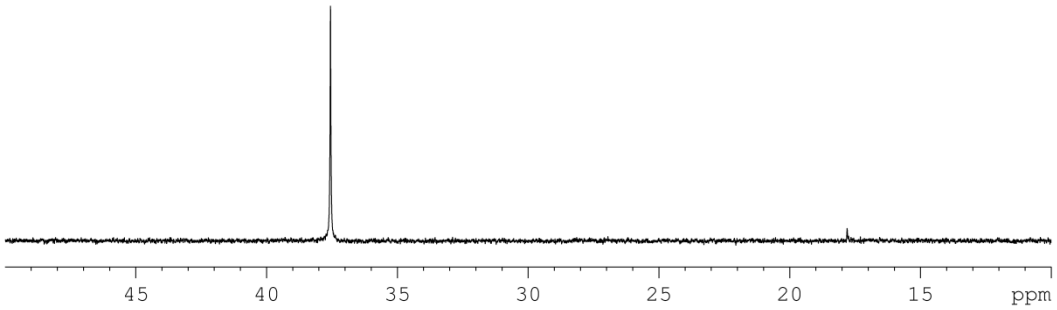
^{1}H



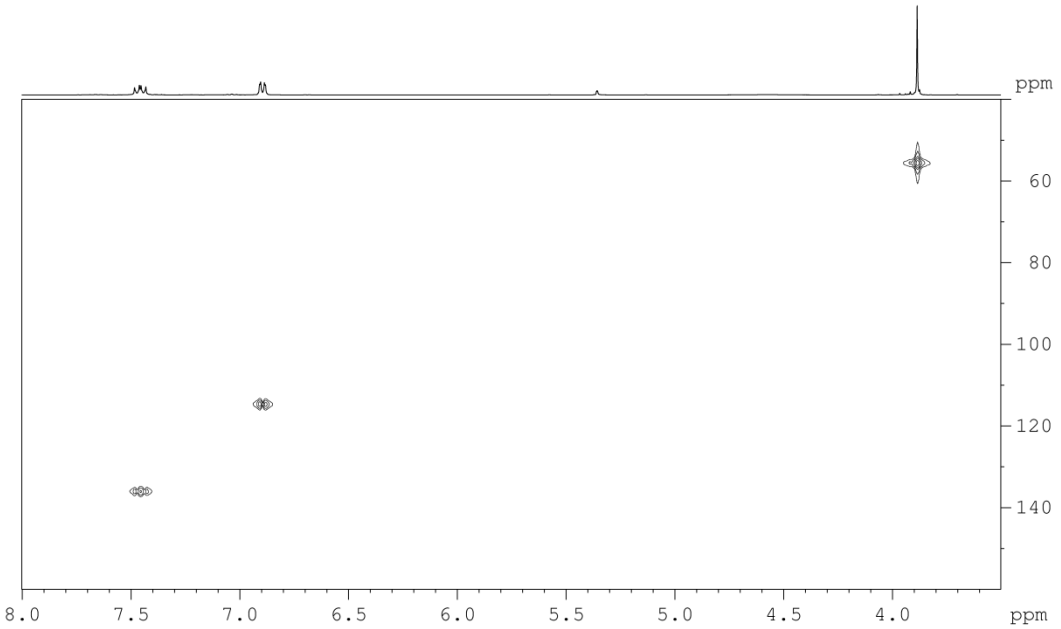
^{1}H {^{31}P}



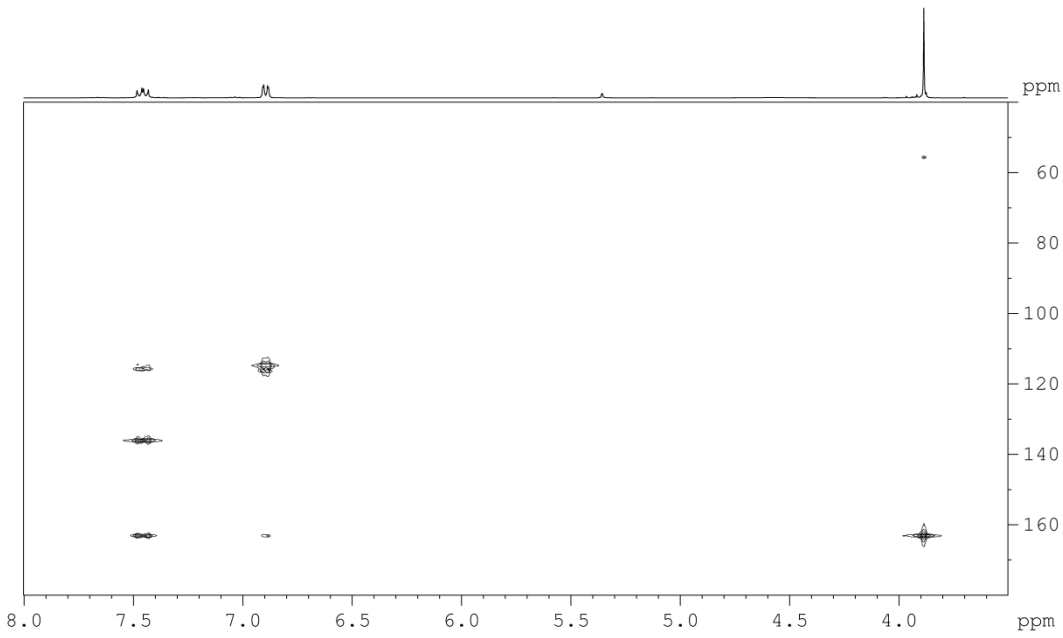
^{31}P {^{1}H}



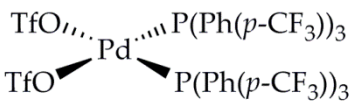
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



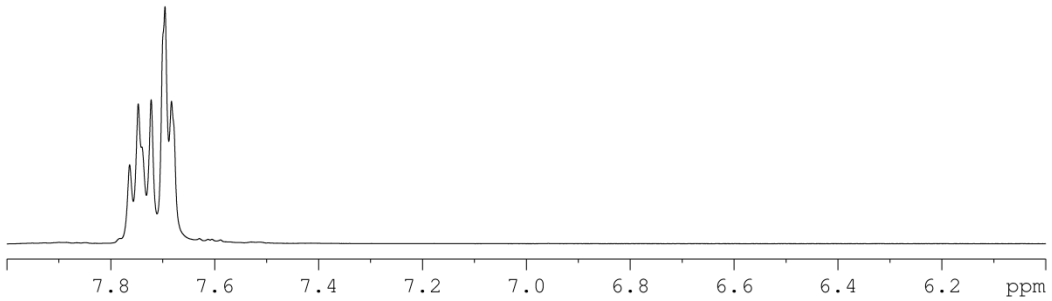
1.15 $[Pd(OTf)_2(P(Ph(p\text{-}CF_3))_3)_2]$



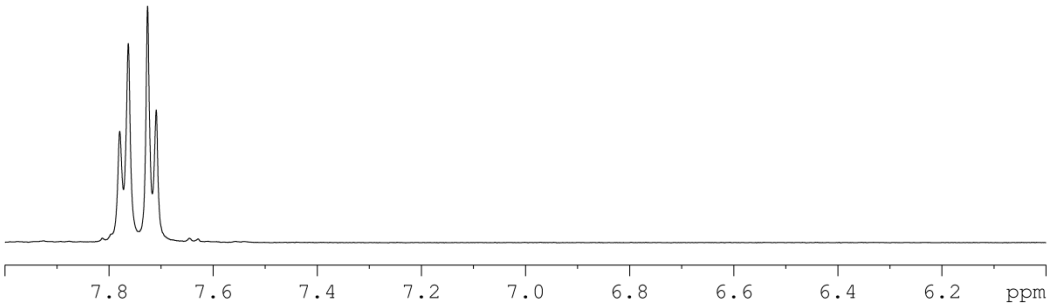
Compound reference kma-3-44

1.15.1NMR spectra

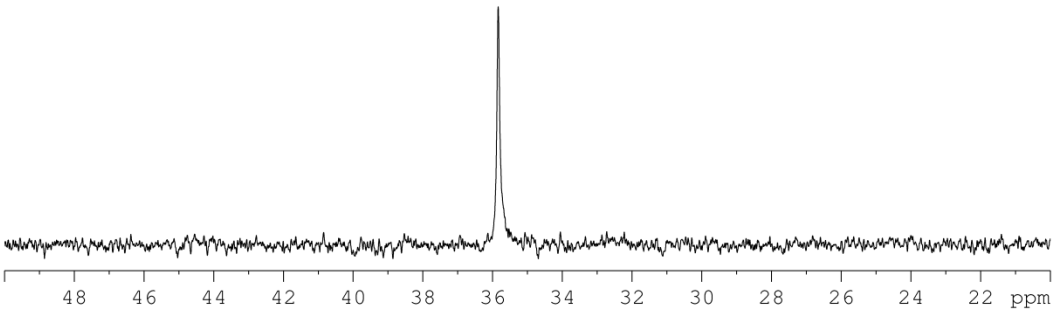
^{1}H



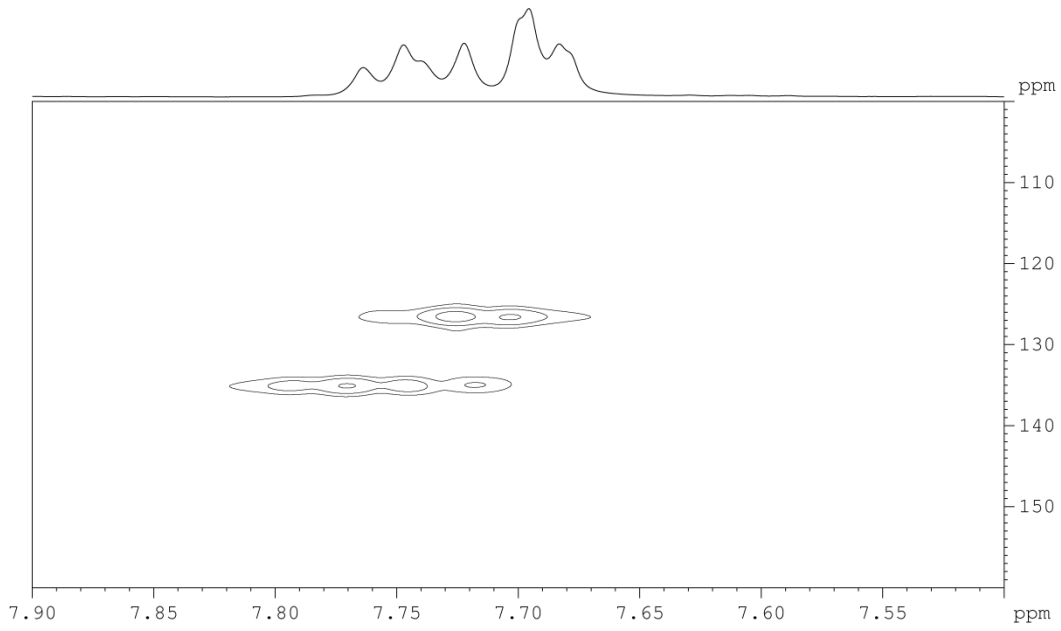
^{1}H {^{31}P}



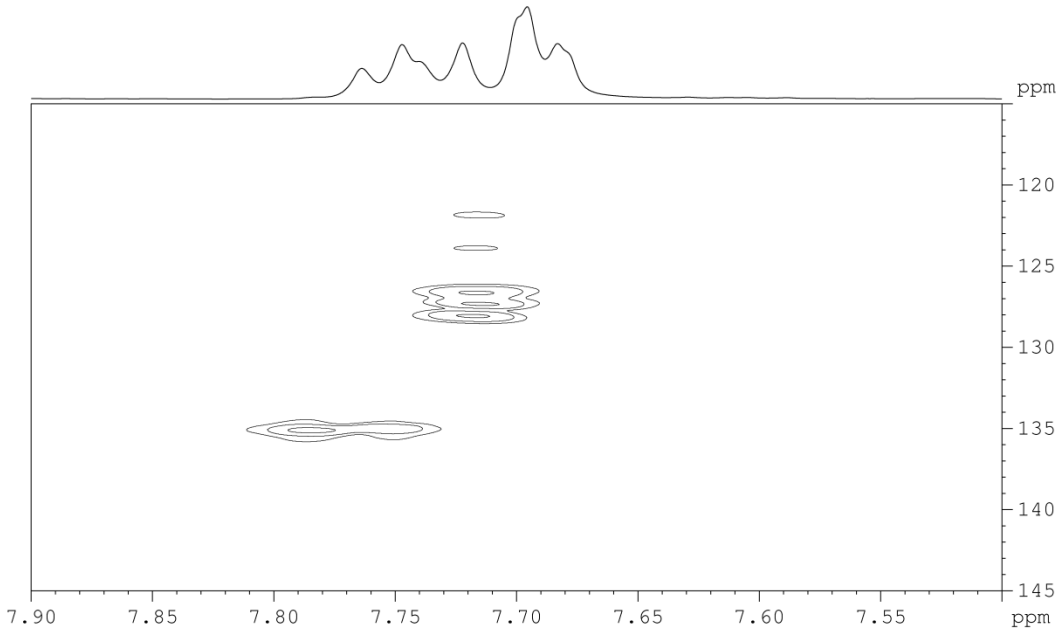
^{31}P {^{1}H}



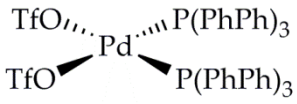
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



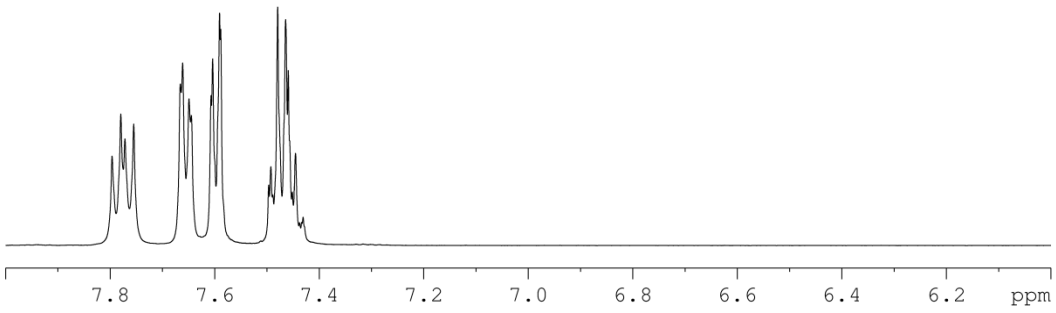
1.16 [Pd(OTf)$_2$(P(PhPh)$_3$)$_2$]



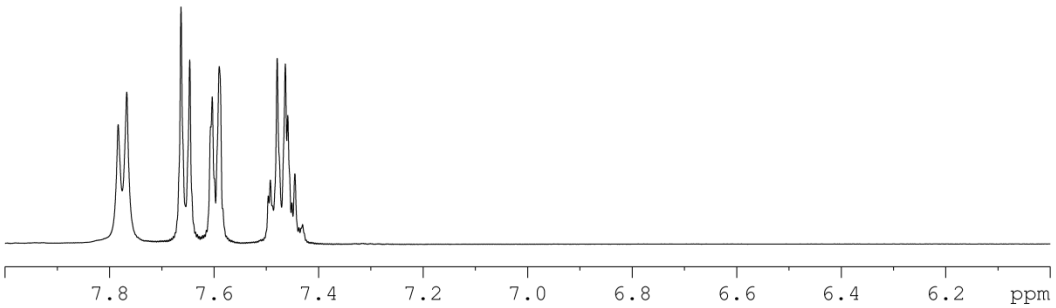
Compound reference kma-3-51

1.16.1NMR spectra

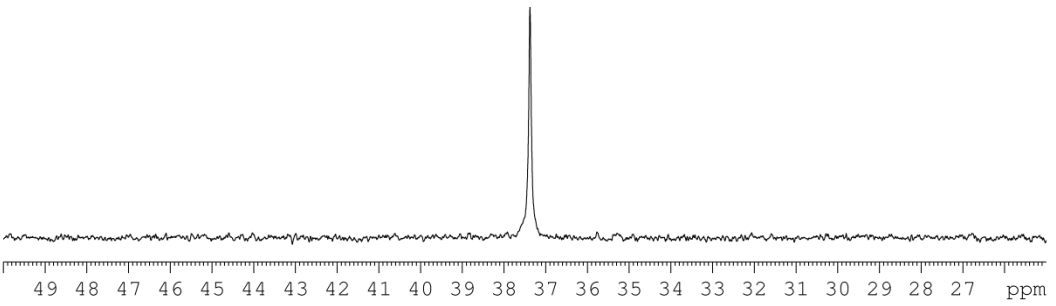
^{1}H



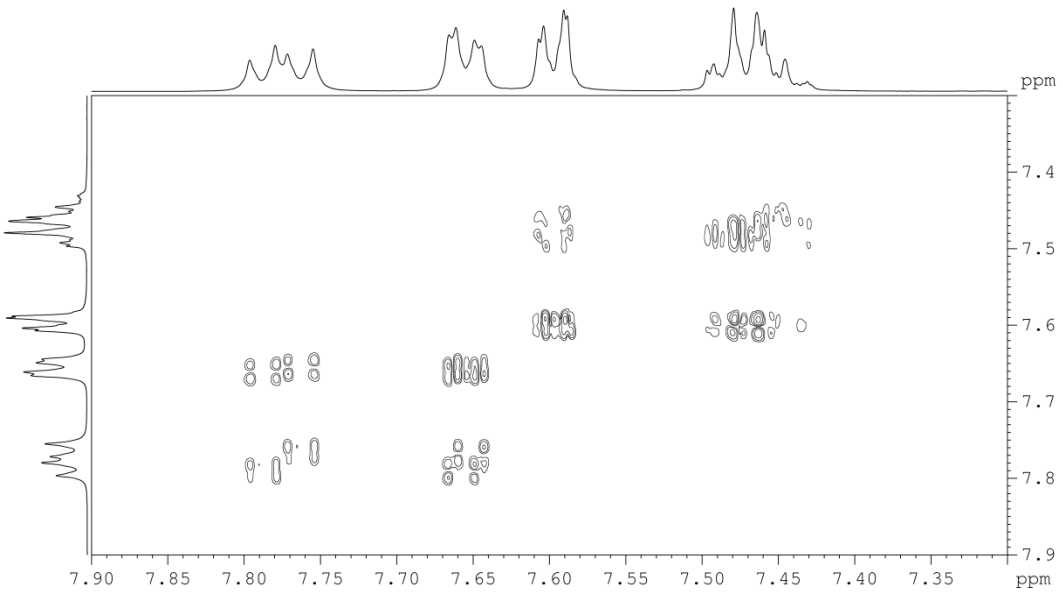
^{1}H {^{31}P}



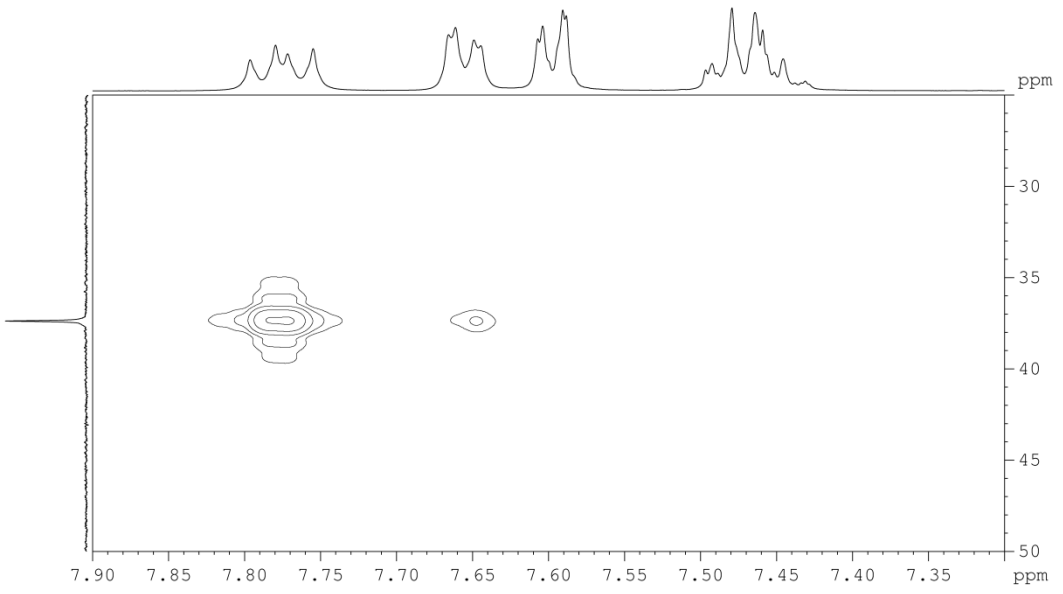
^{31}P {^{1}H}



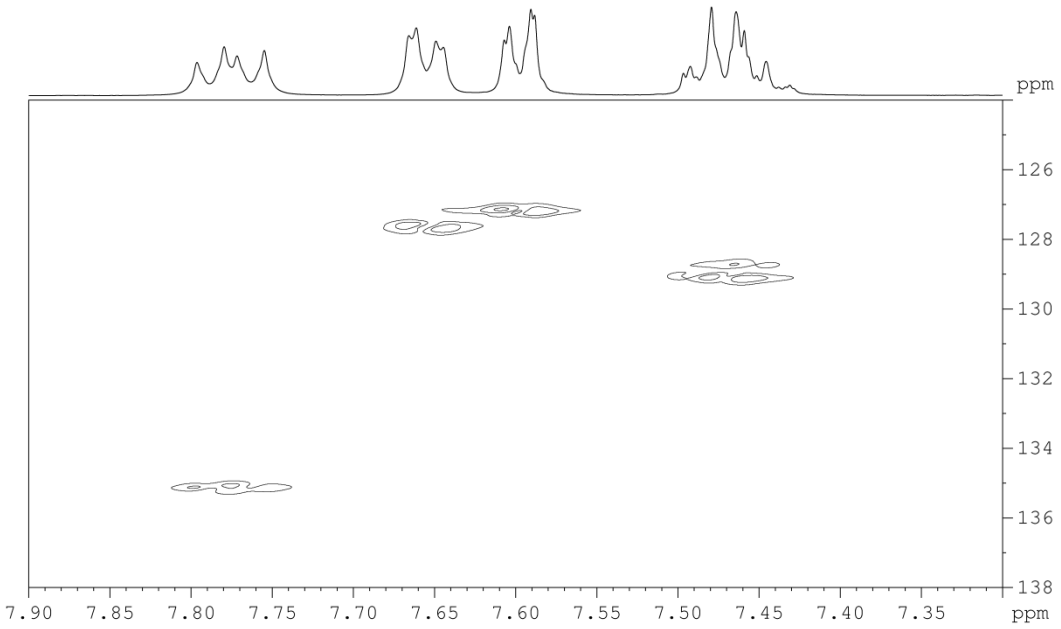
COSY



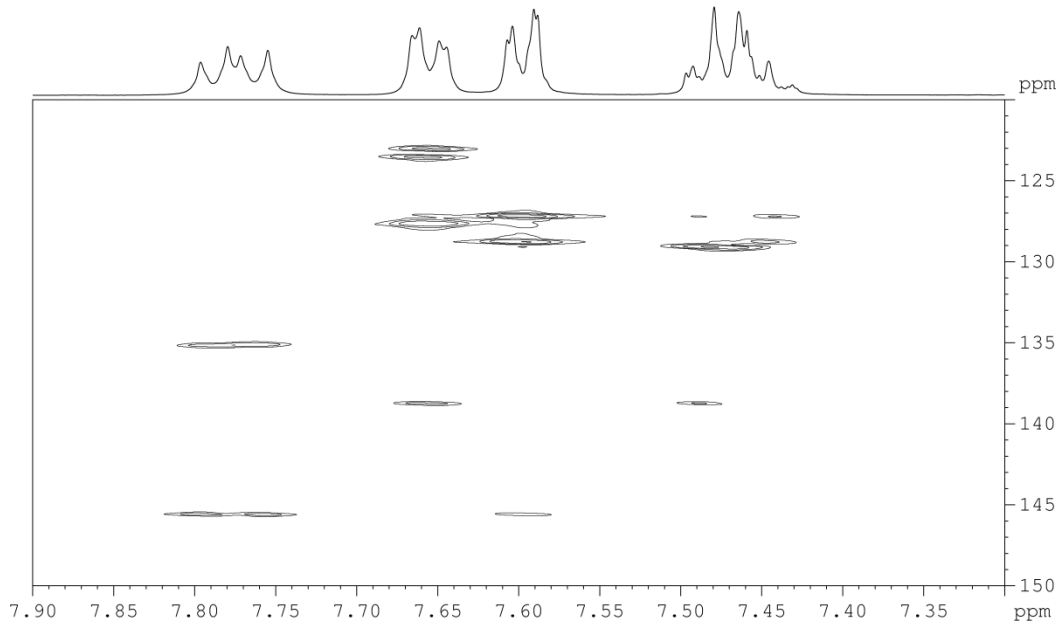
^{31}P-optimised HMQC with a coupling of 12 Hz



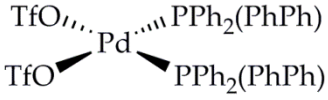
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



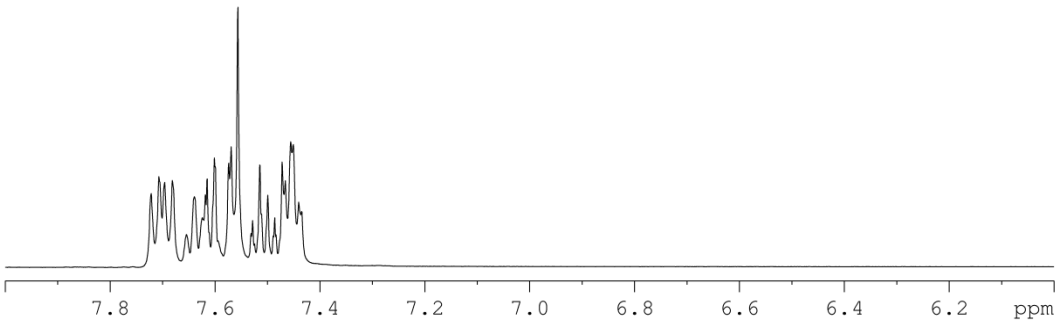
1.17 [Pd(OTf)$_2$(PPh$_2$(PhPh))$_2$]



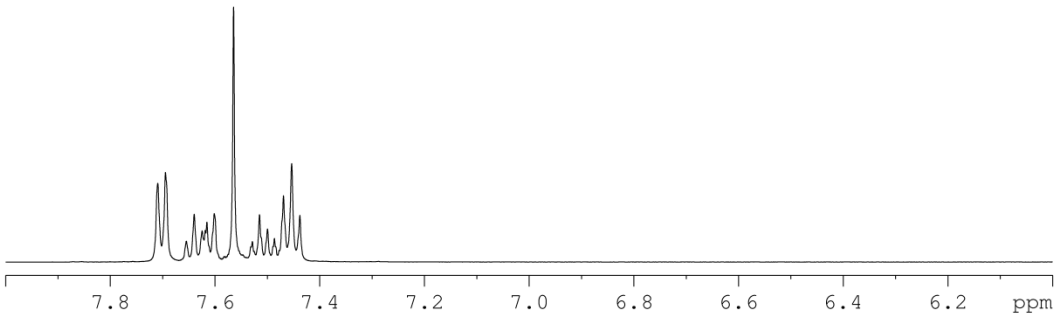
Compound reference kma-3-13

1.17.1NMR spectra

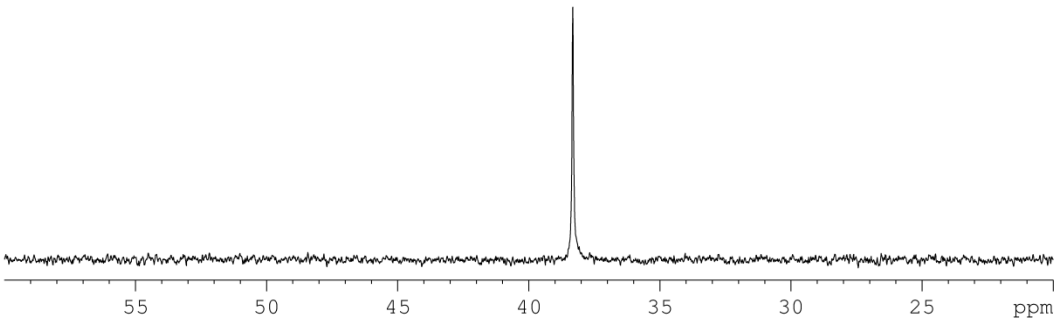
^{1}H



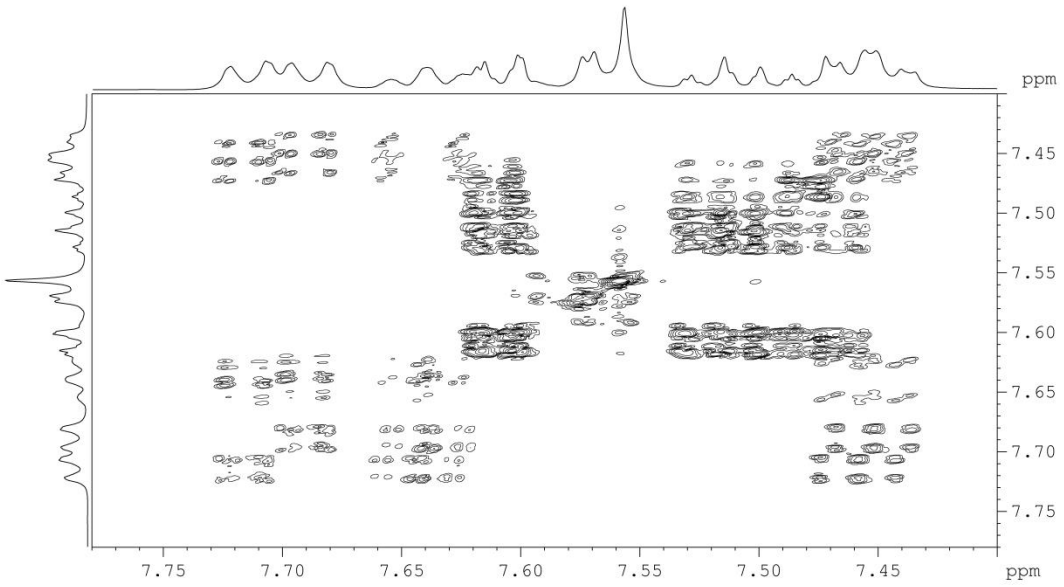
^{1}H {^{31}P}



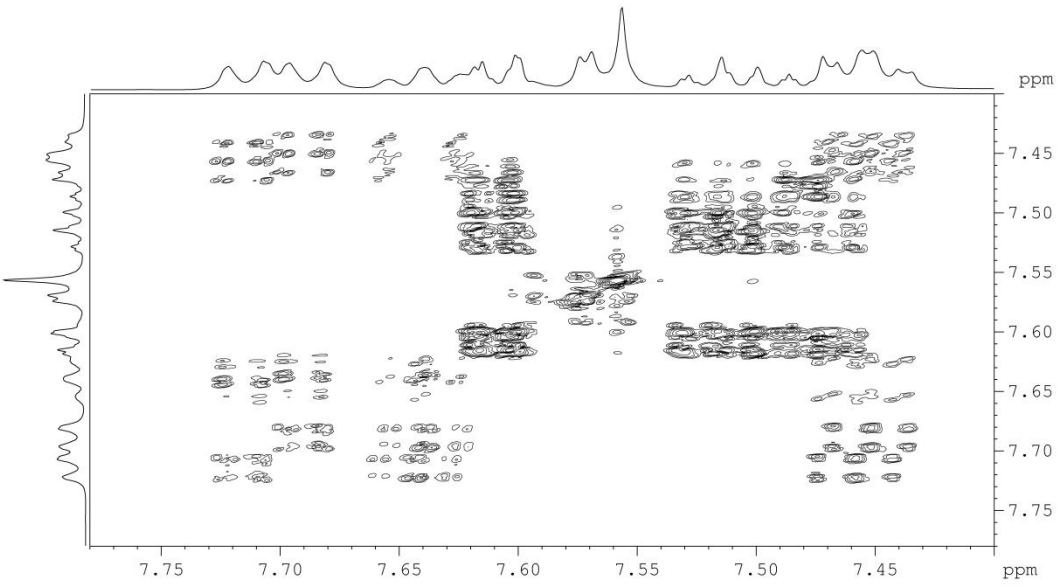
^{31}P {^{1}H}



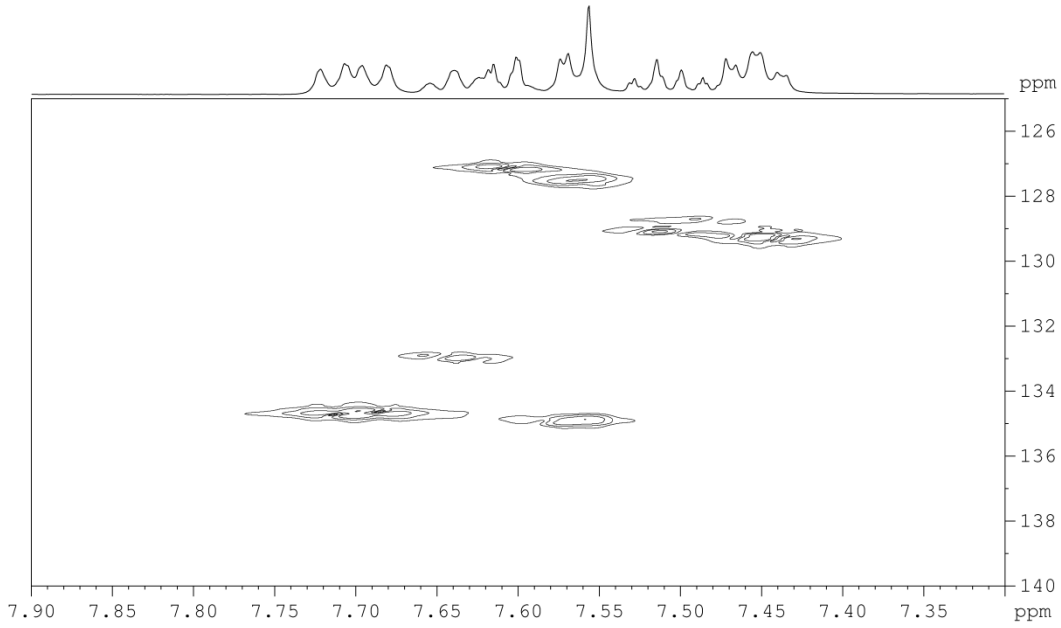
COSY



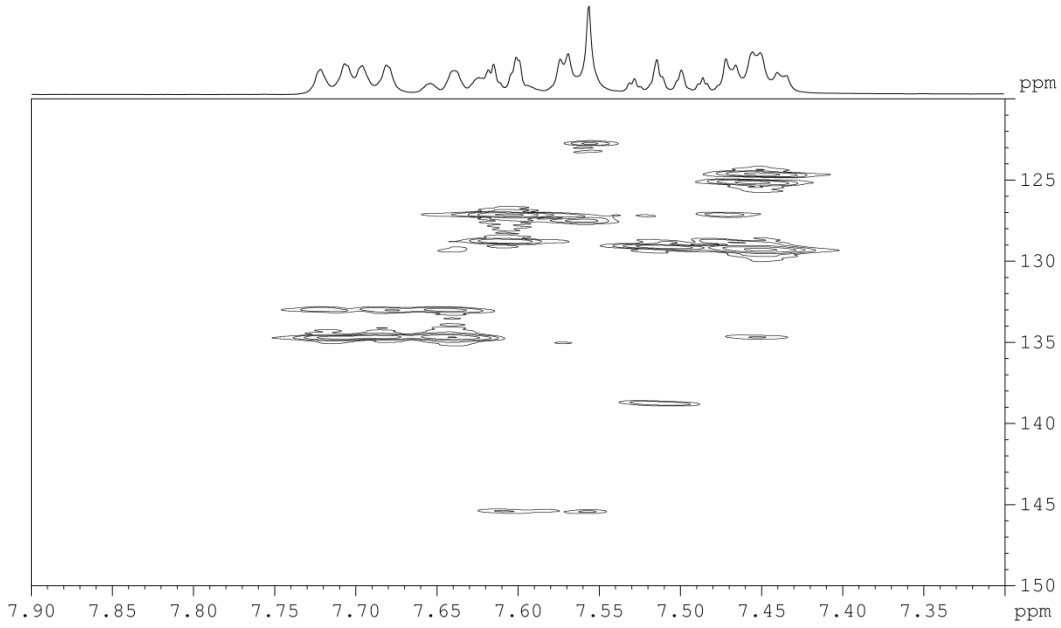
^{31}P-optimised HMQC with a coupling of 12 Hz



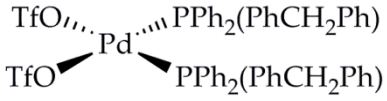
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



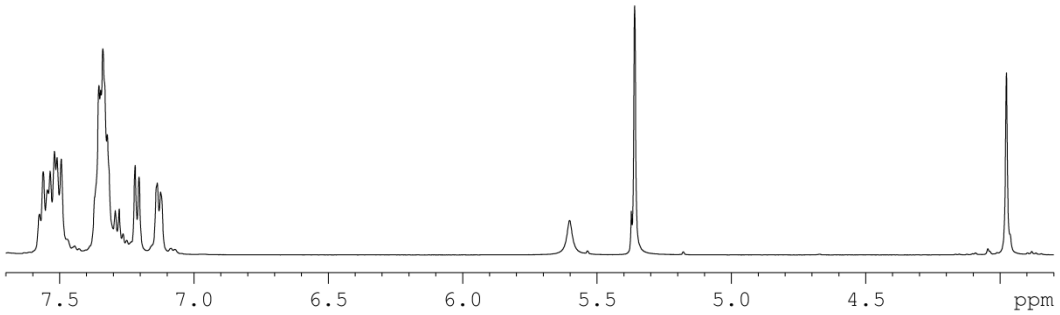
1.18 [Pd(OTf)$_2$(PPh$_2$(PhCH$_2$Ph))$_2$]



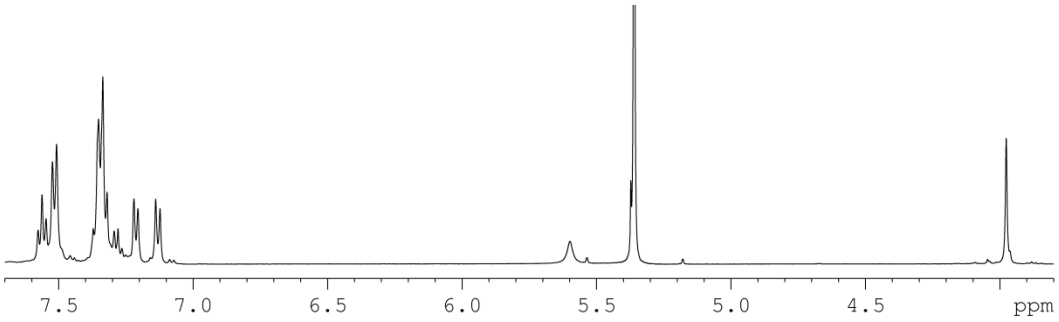
Compound reference kma-3-28

1.18.1NMR spectra

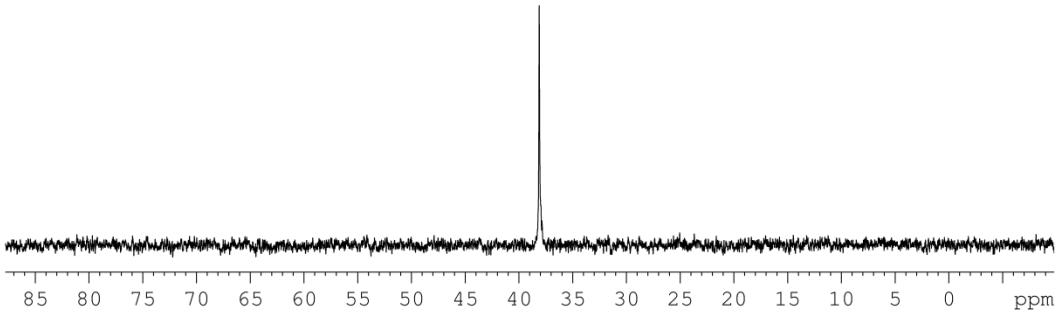
^{1}H



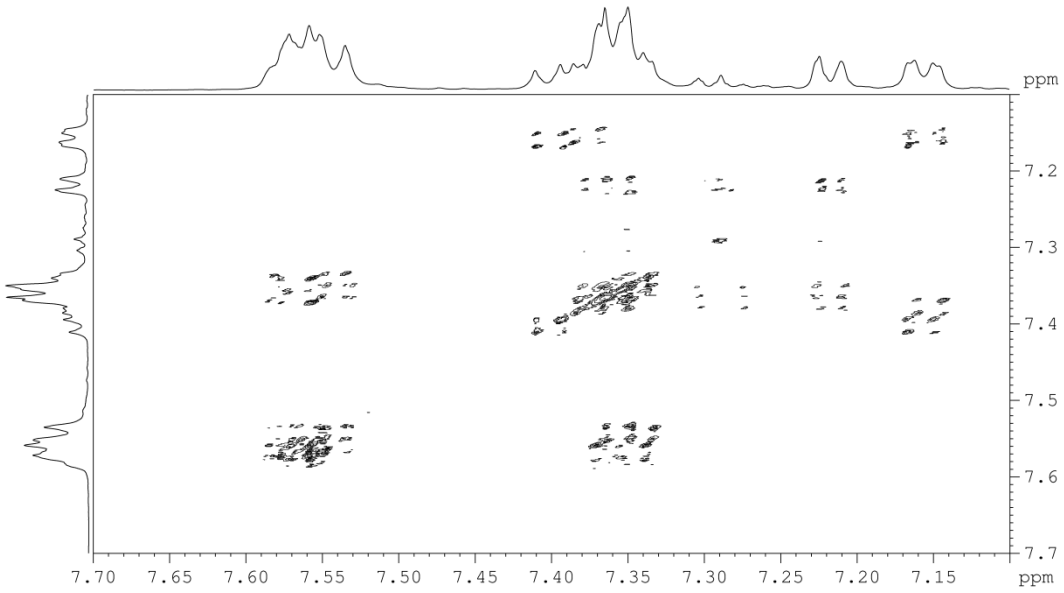
^{1}H {^{31}P}



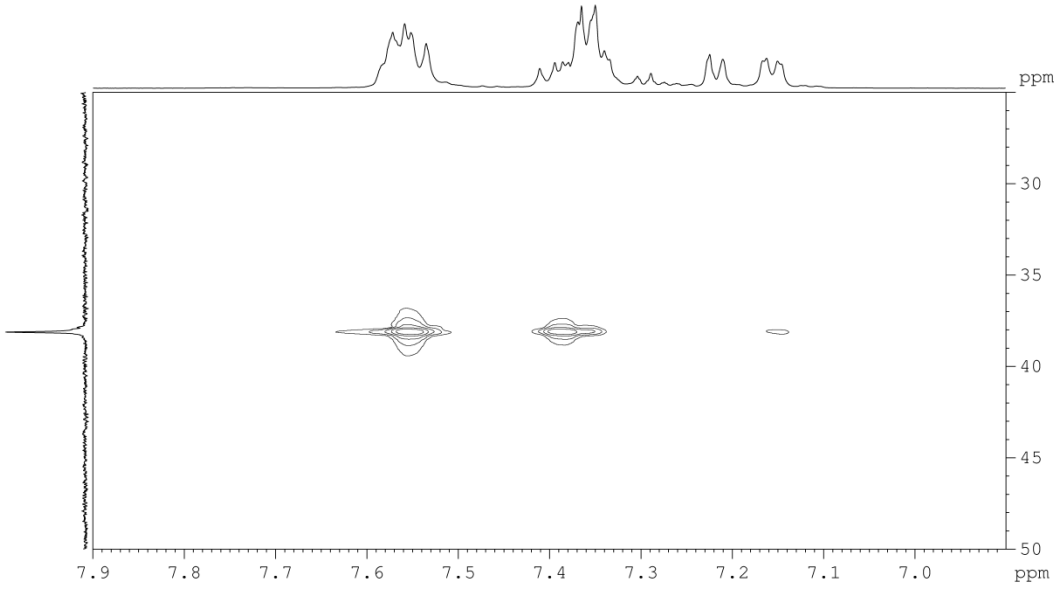
^{31}P {^{1}H}



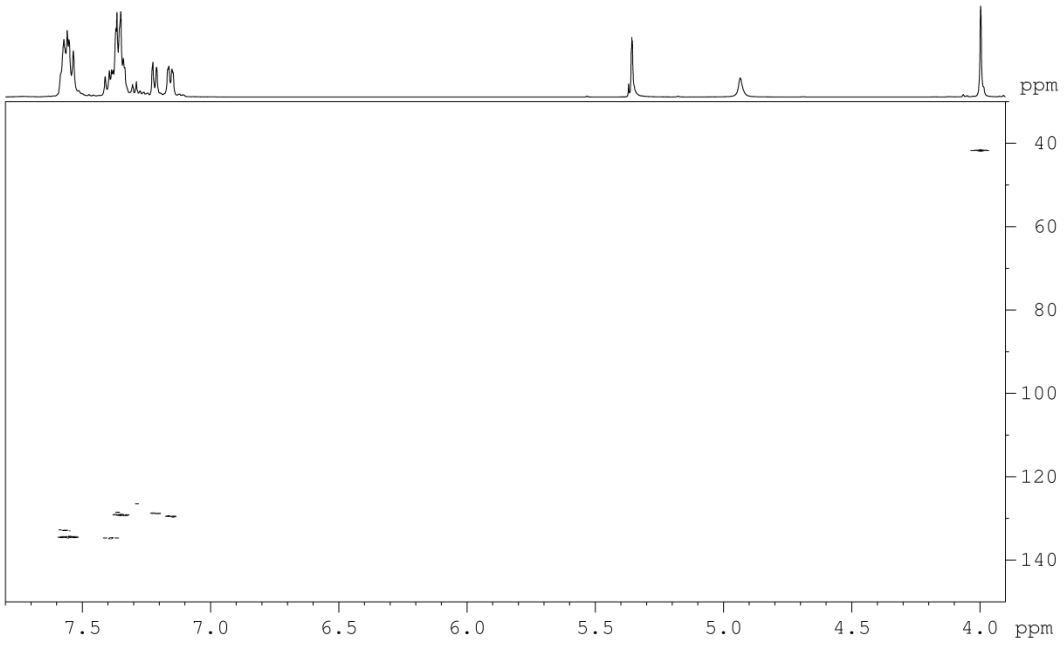
COSY



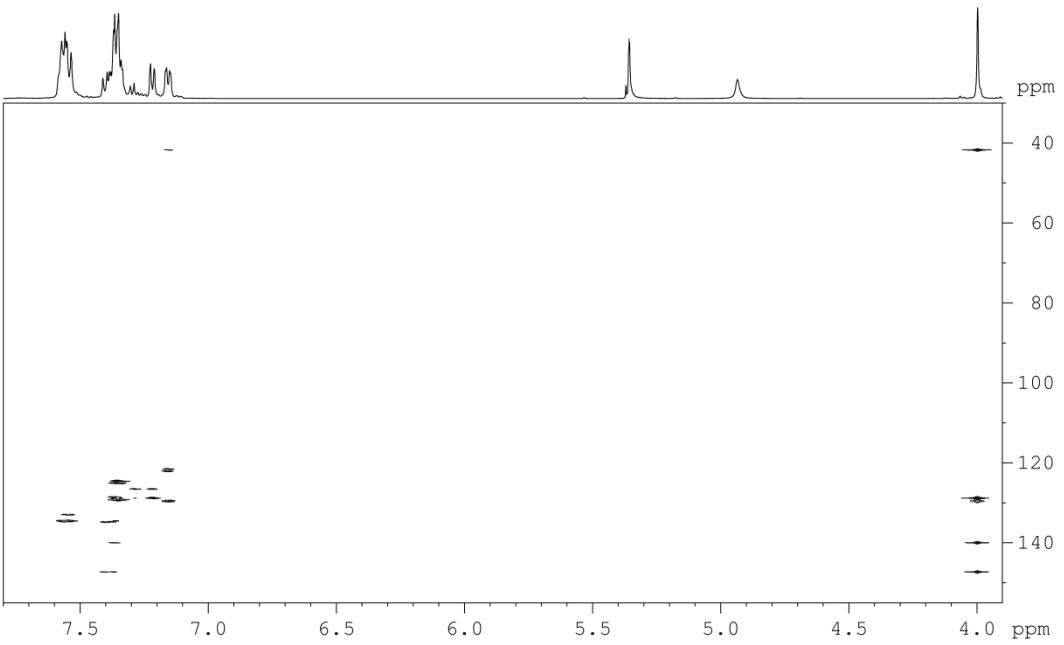
^{31}P-optimised HMQC with a coupling of 12 Hz



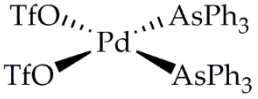
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



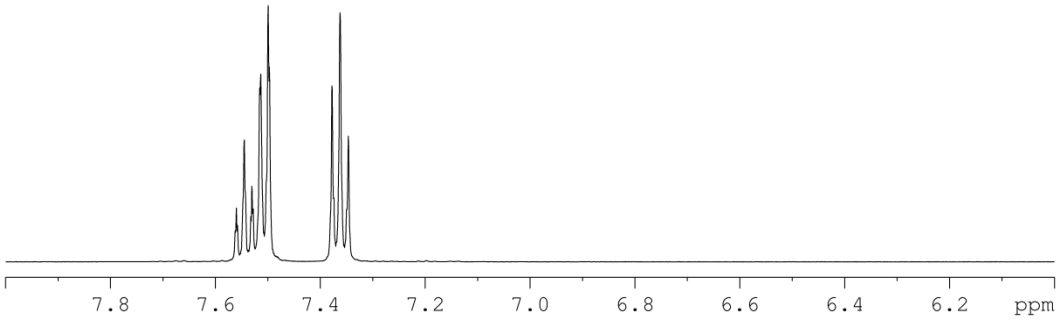
1.19 $[Pd(OTf)_2(AsPh_3)_2]$



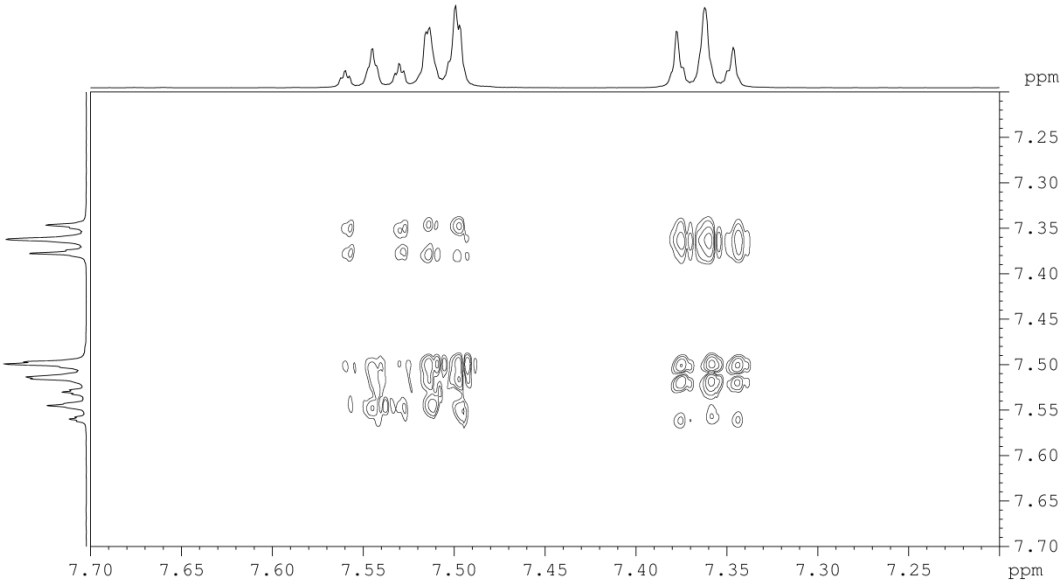
Compound reference kma-3-82

1.19.1NMR spectra

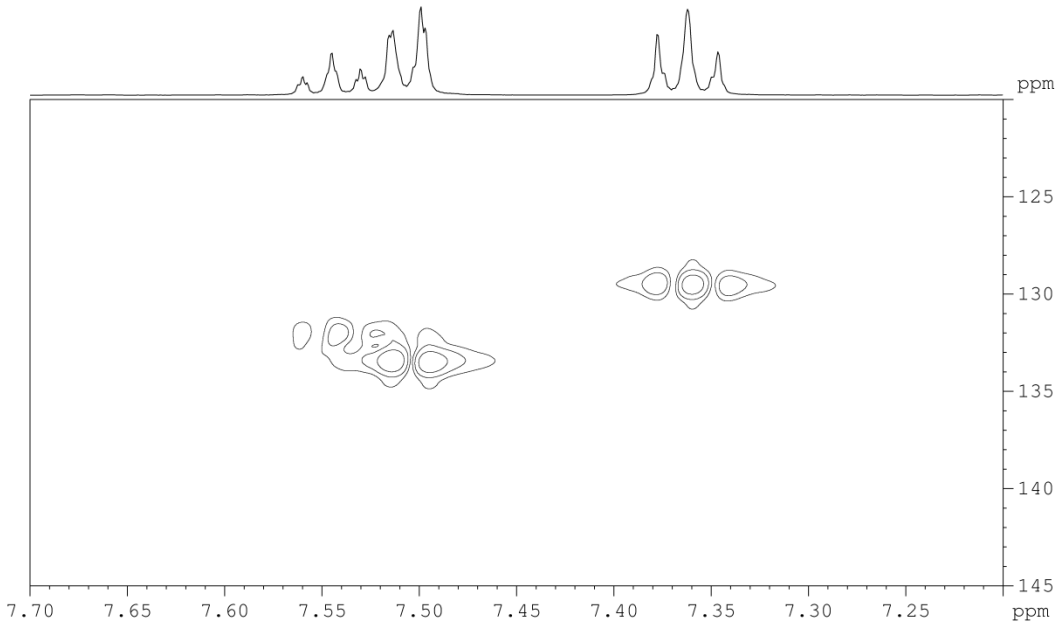
^{1}H



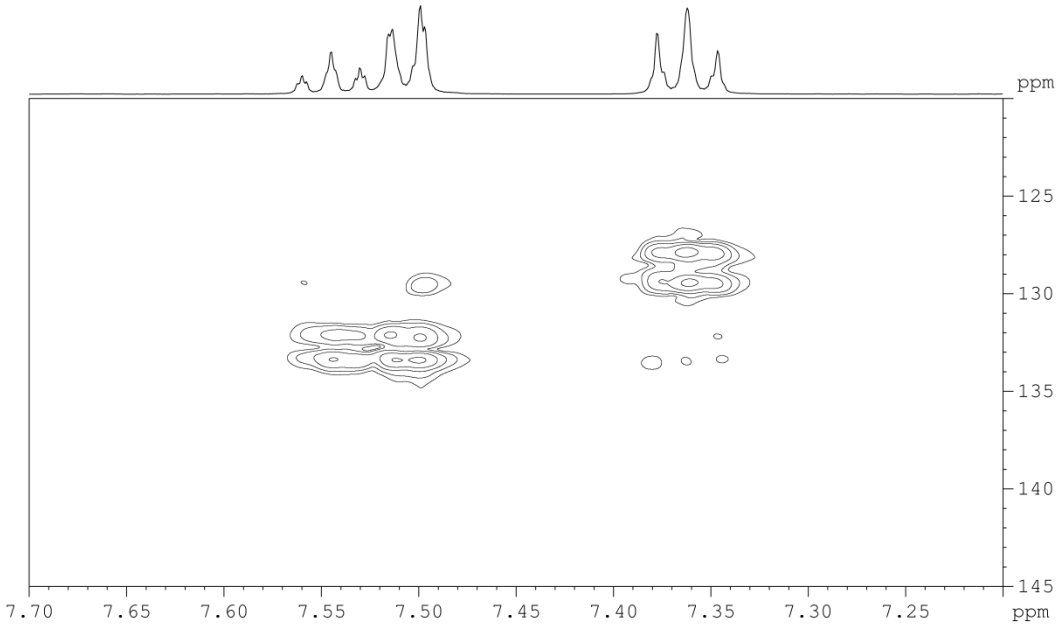
COSY



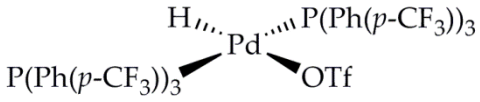
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



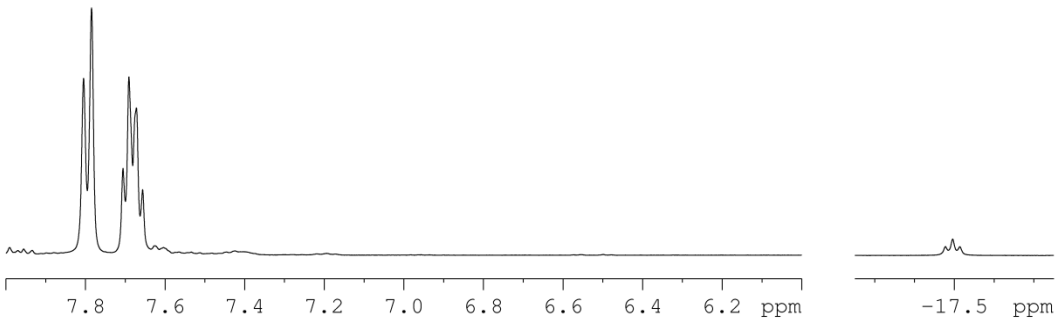
1.20 [Pd(H)(OTf)(P(Ph(*p*-CF_3))$_3$)$_2$]



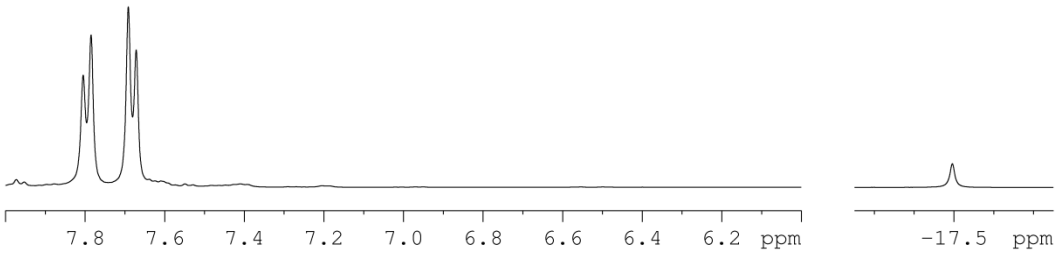
Compound reference kma-3-45

1.20.1NMR spectra

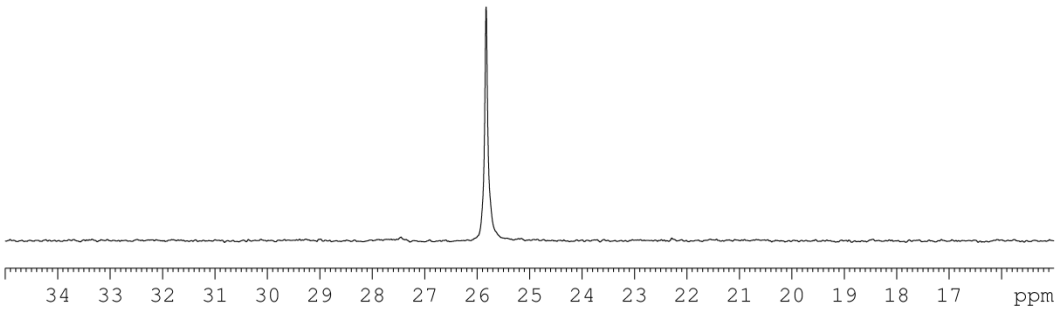
^{1}H



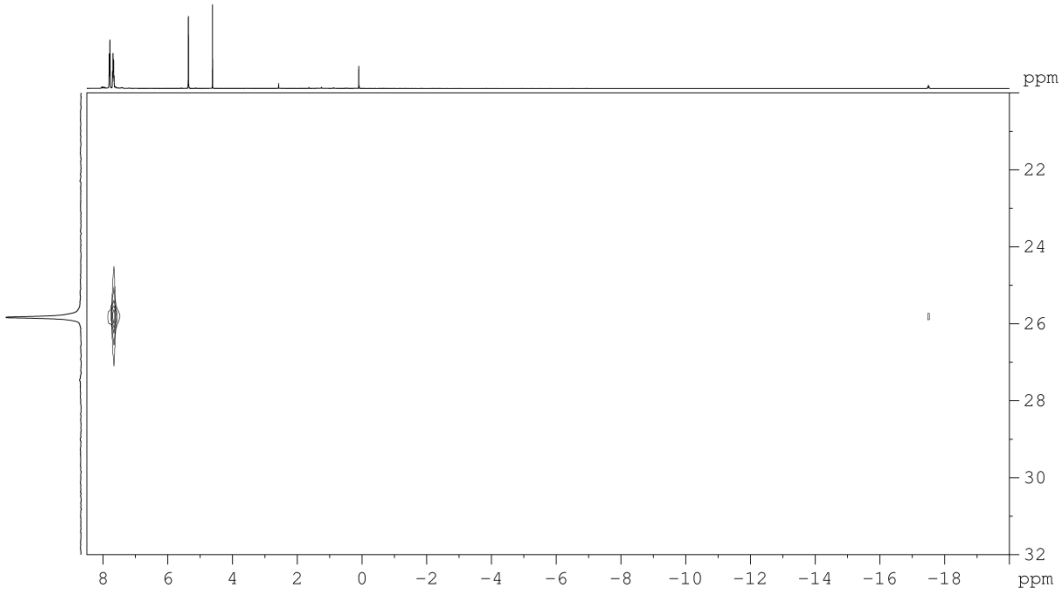
^{1}H {^{31}P}



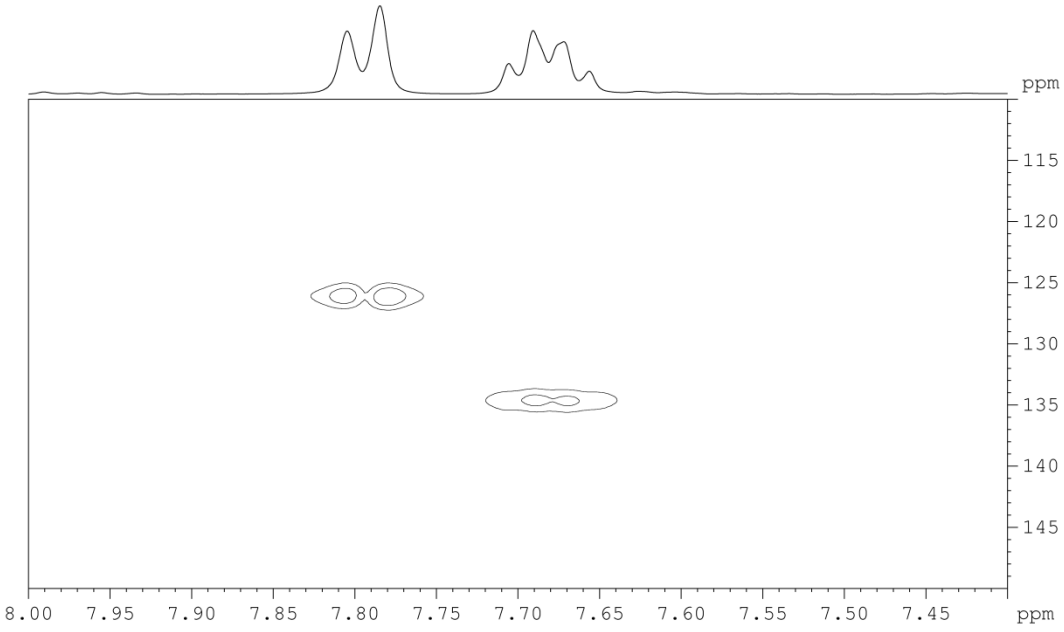
^{31}P {^{1}H}



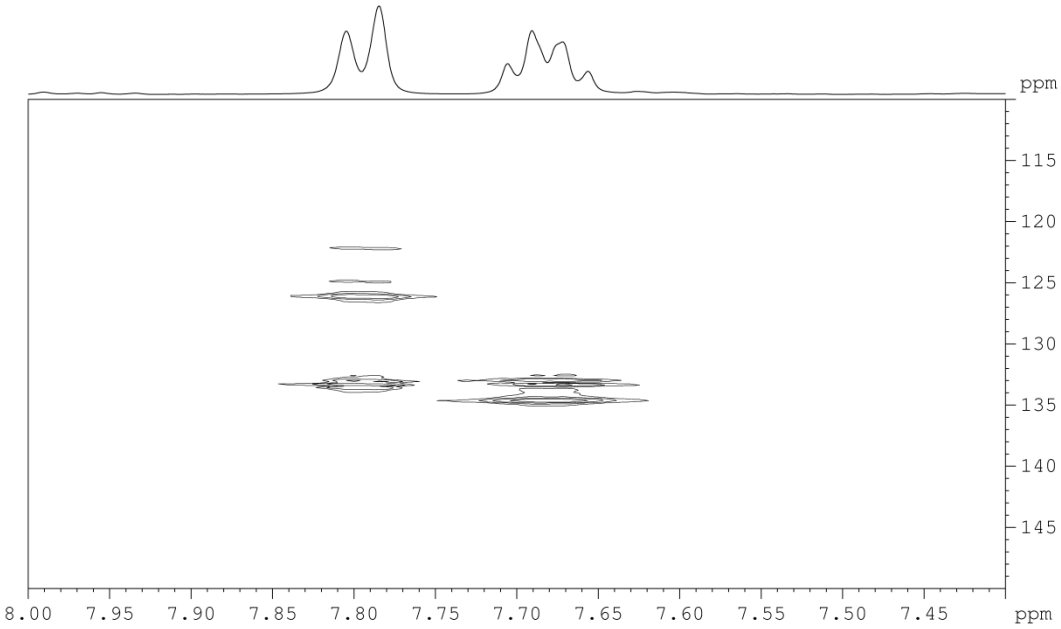
^{31}P-optimised HMQC with a coupling of 12 Hz



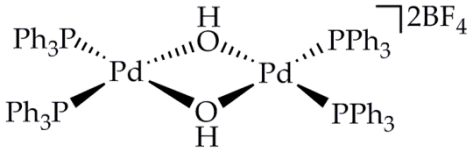
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



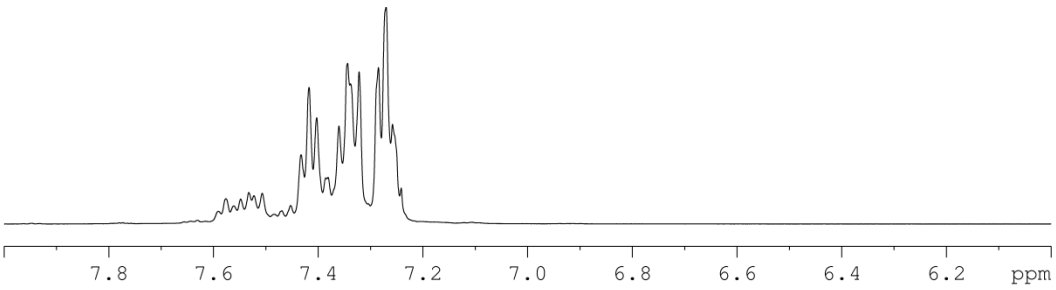
1.21 $[Pd(\mu\text{-}OH)(PPh_3)_2]_2[BF_4]_2$



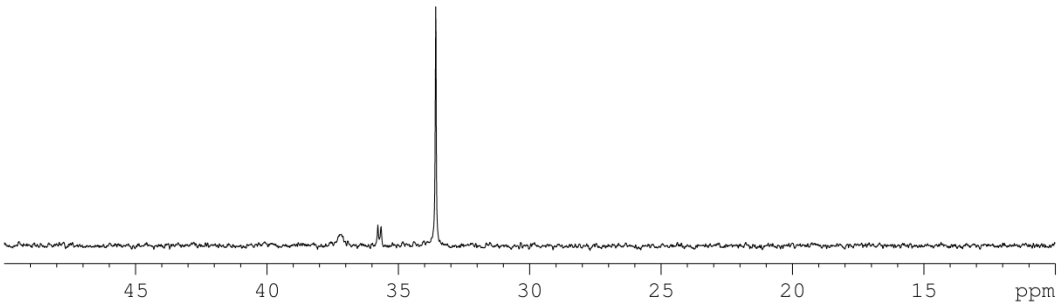
Compound reference kma-4-04

1.21.1NMR spectra

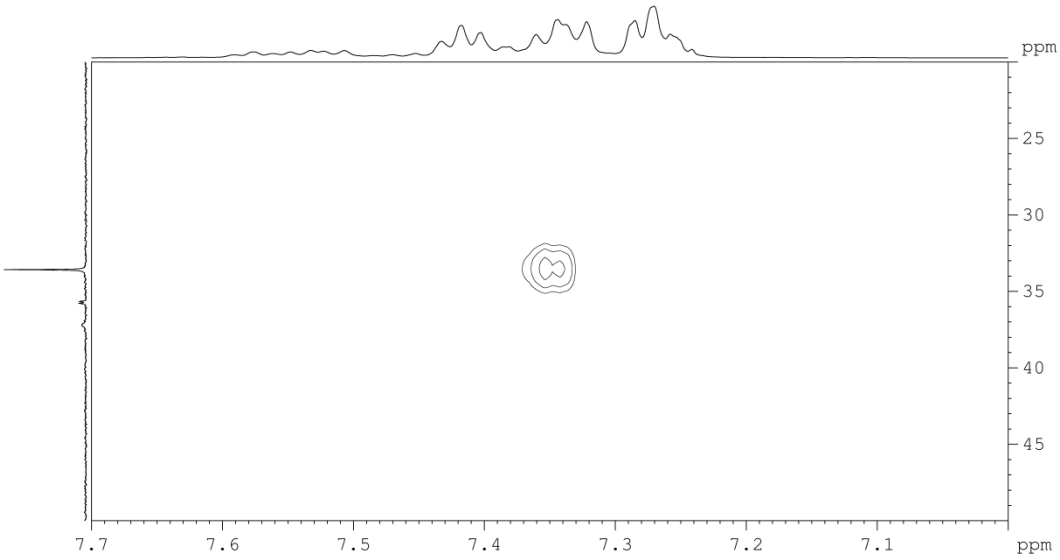
^{1}H



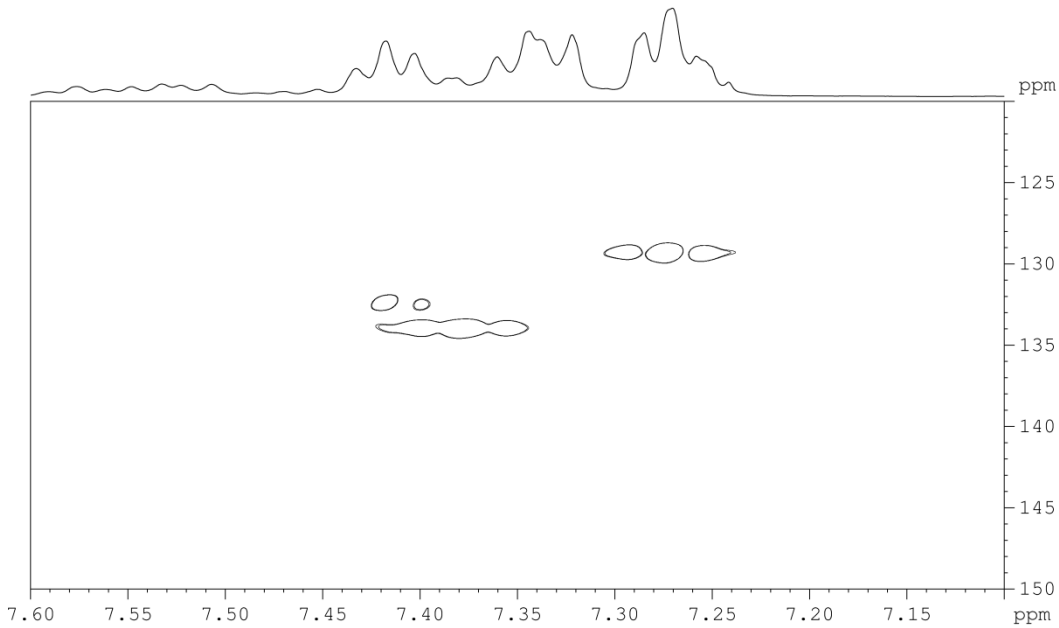
$^{31}P\ \{^{1}H\}$



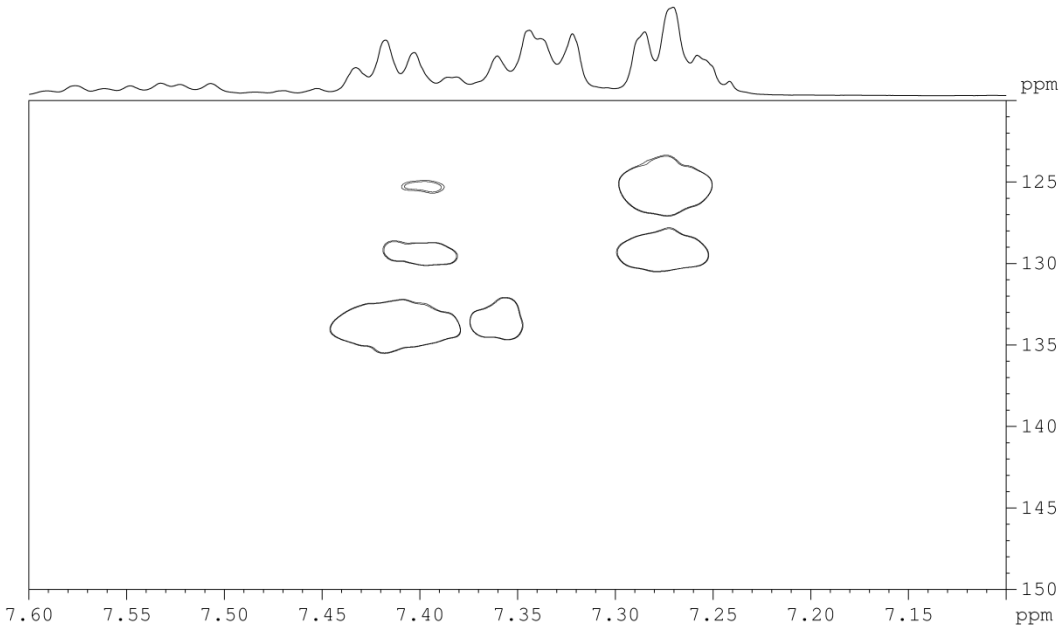
^{31}P-optimised HMQC with a coupling of 12 Hz



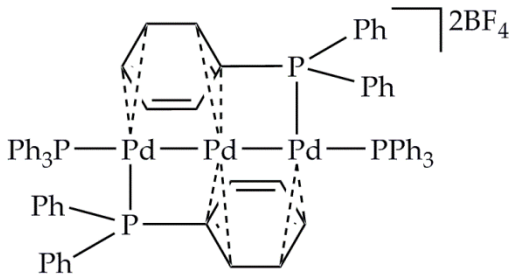
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



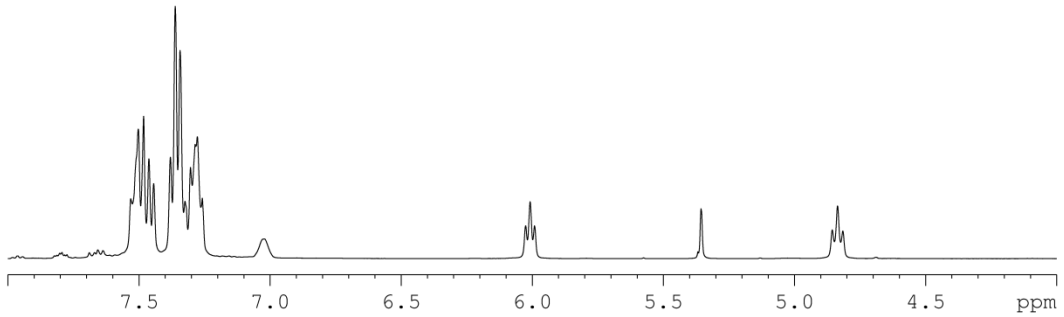
1.22 $[Pd_3(PPh_3)_4][BF_4]_2$



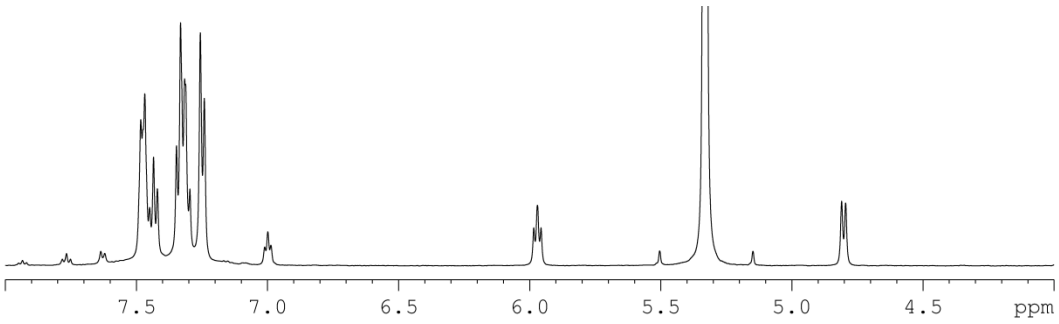
Compound reference kma-4-35

1.22.1NMR spectra

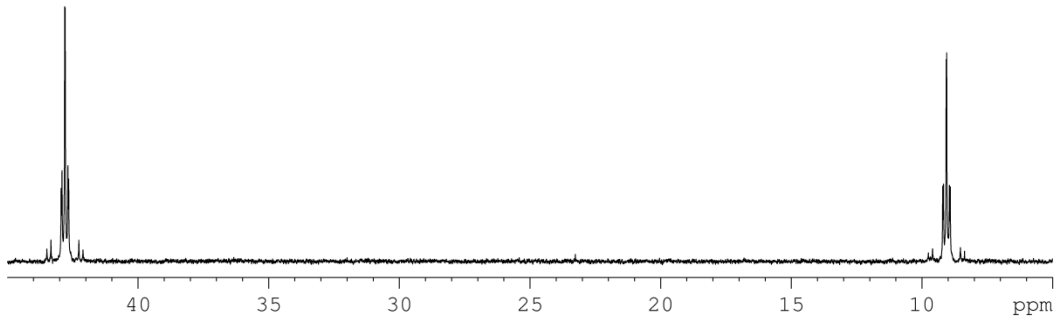
^{1}H



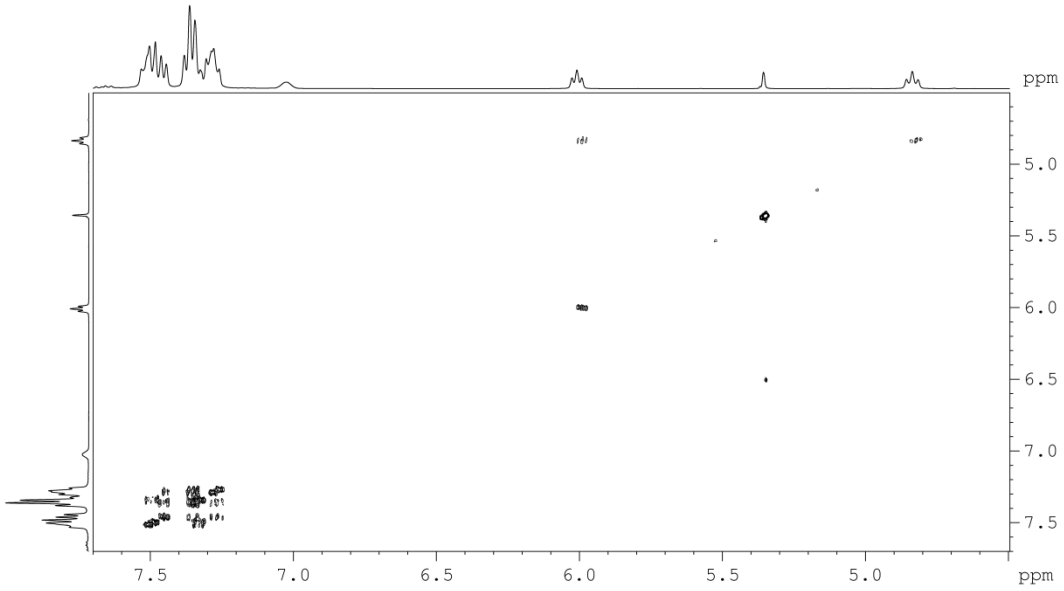
^{1}H $\{^{31}P\}$



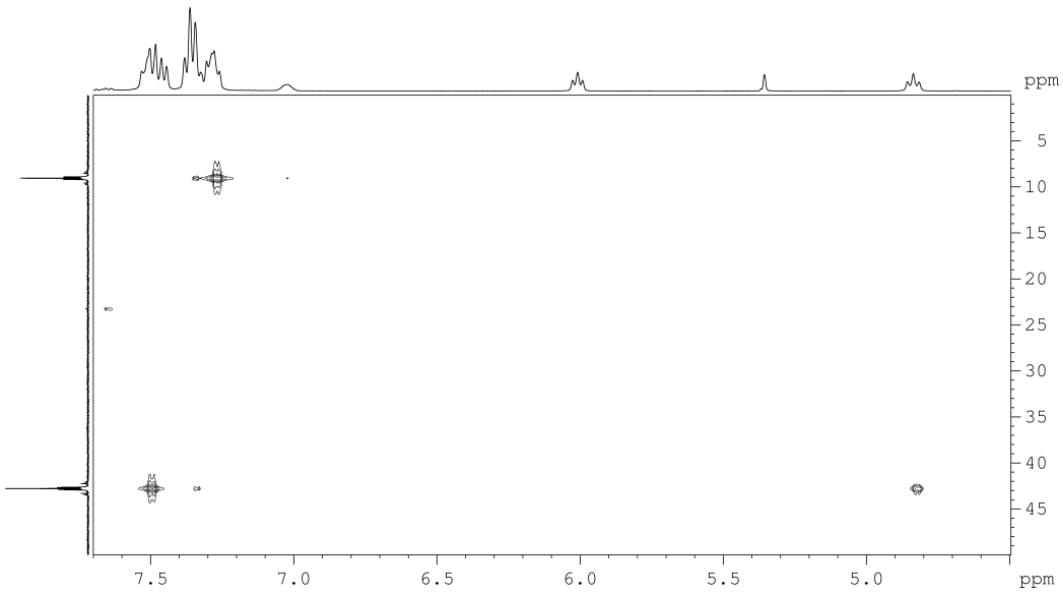
^{31}P $\{^{1}H\}$



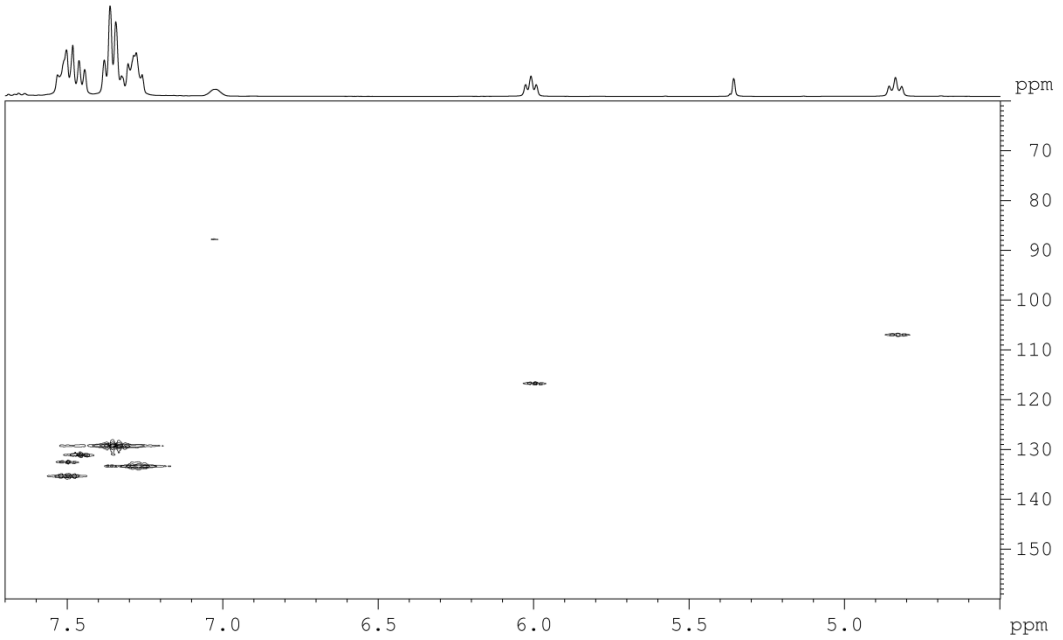
COSY



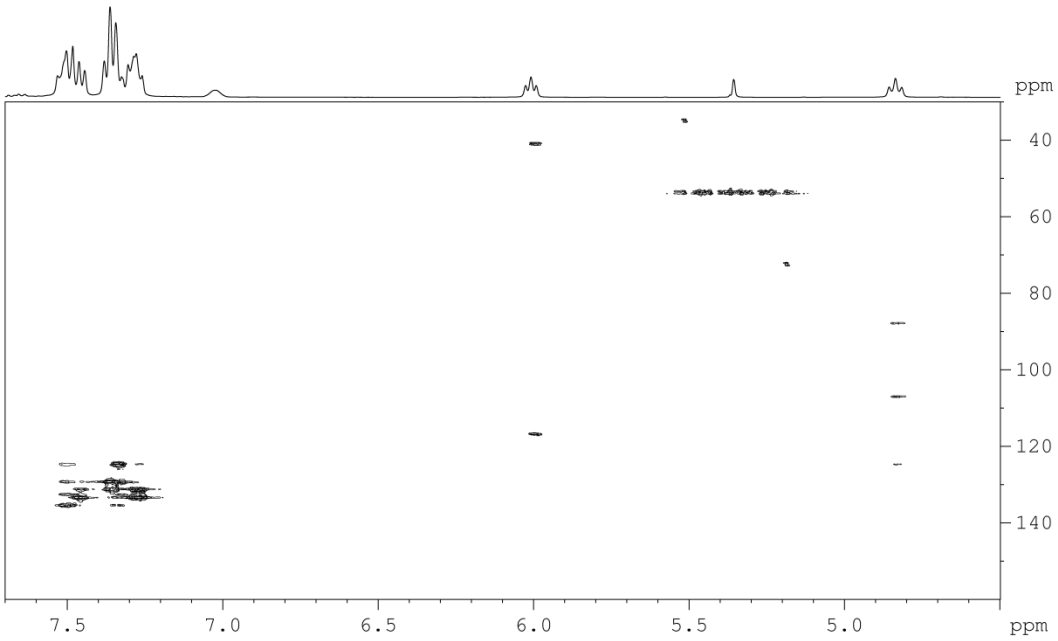
^{31}P-optimised HMQC with a coupling of 12 Hz



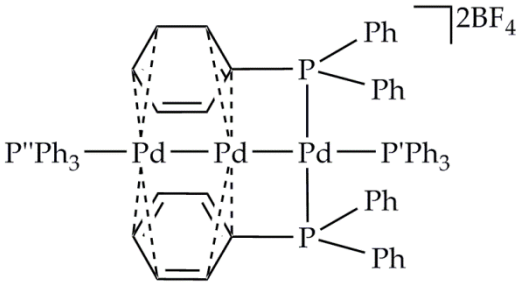
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



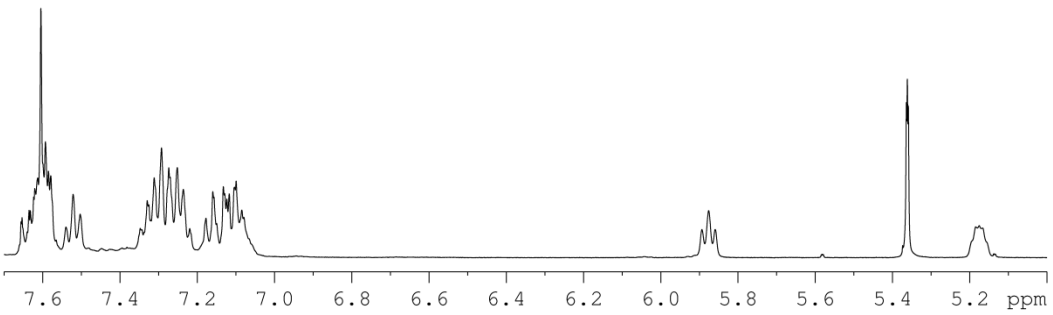
1.23 $[Pd_3(PPh_3)_4][BF_4]_2$ (photoisomer)



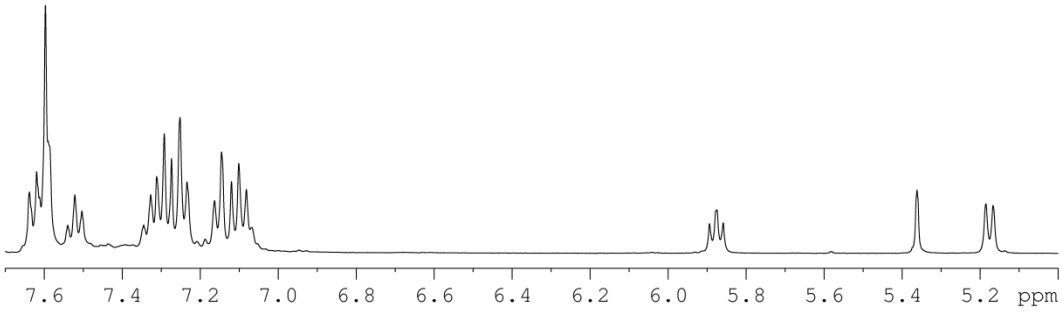
Compound reference kma-4-22

1.23.1NMR spectra

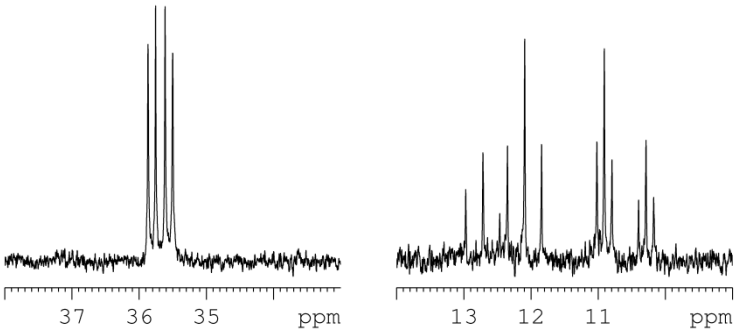
^{1}H



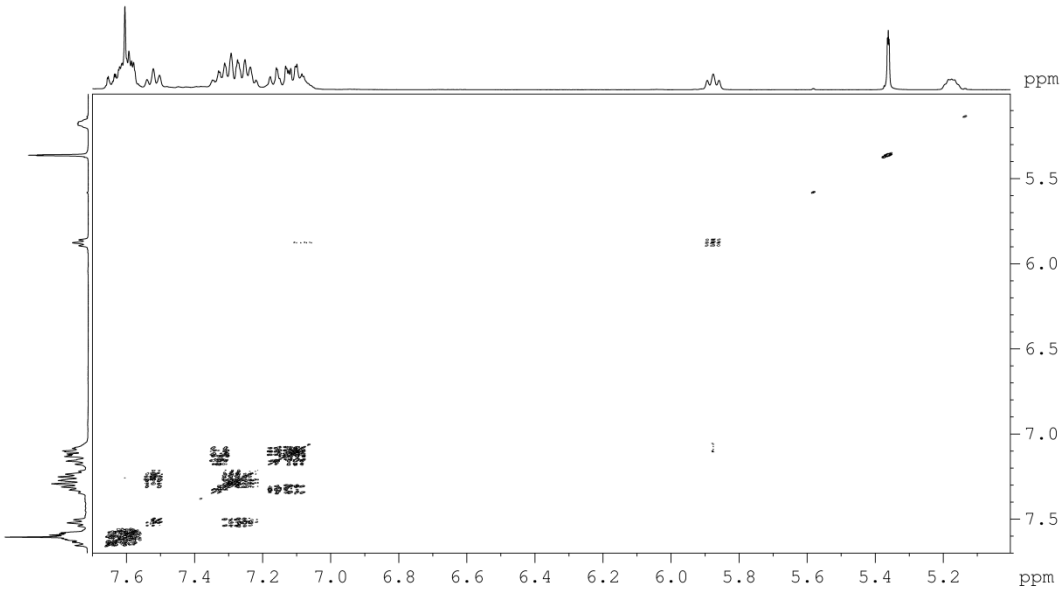
^{1}H {^{31}P}



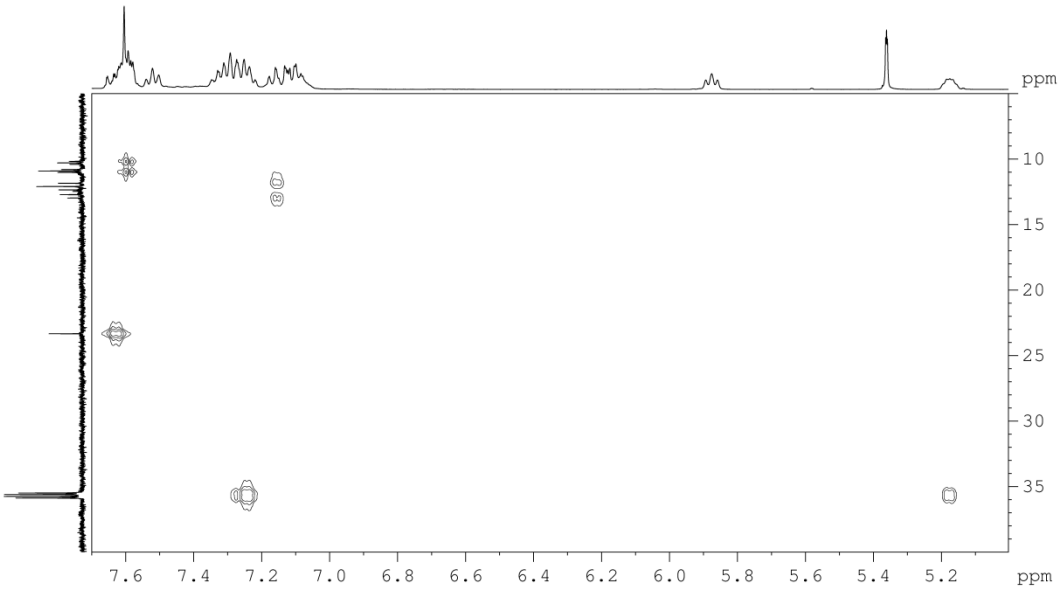
^{31}P {^{1}H}



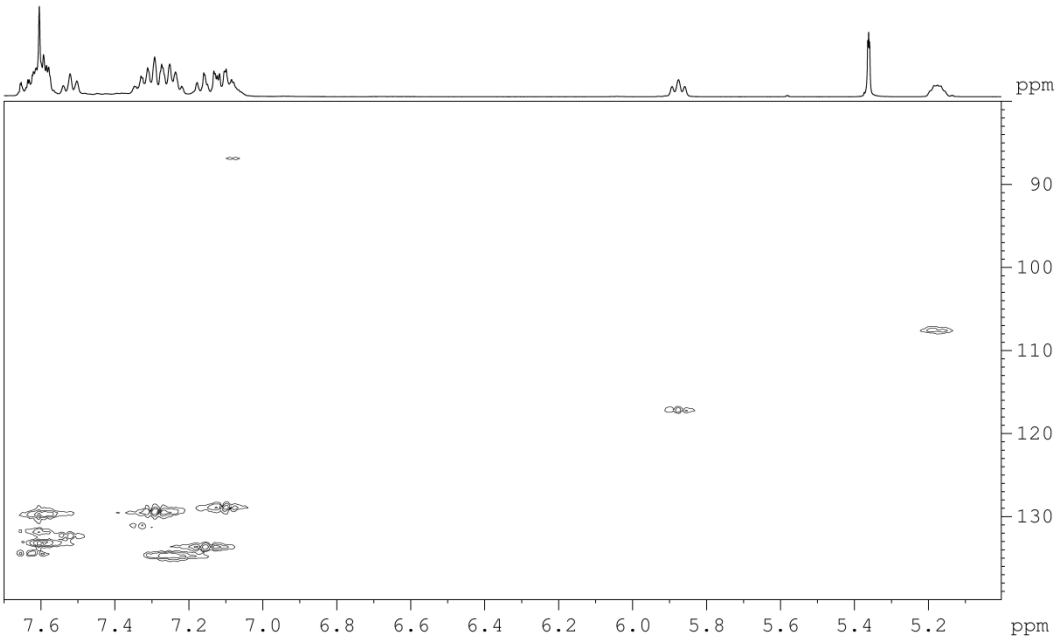
COSY



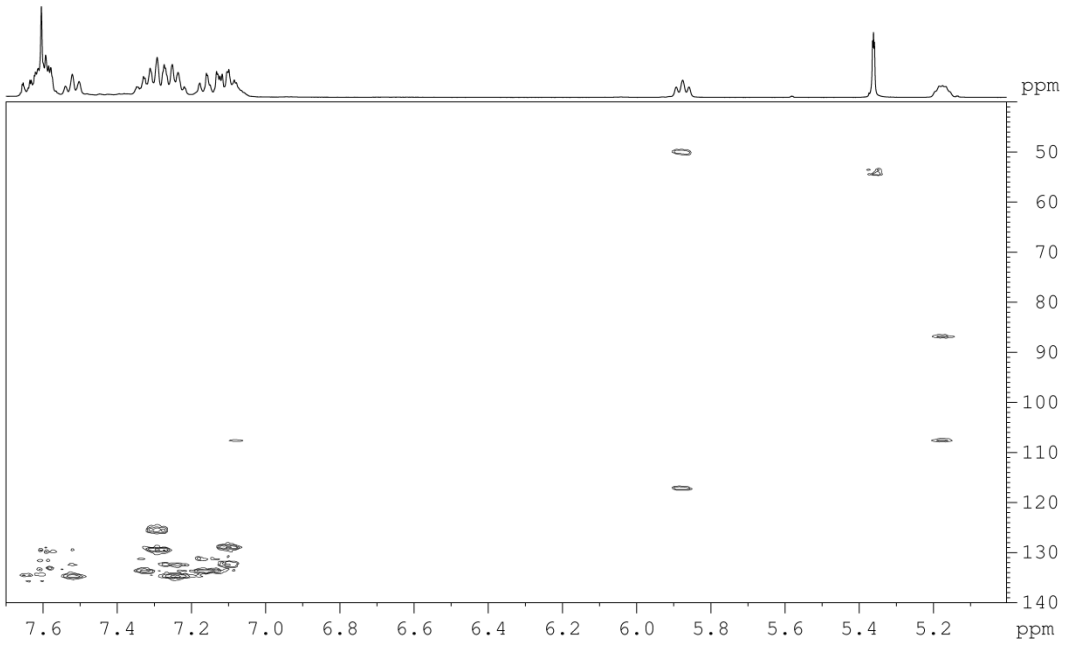
^{31}P-optimised HMQC with a coupling of 12 Hz



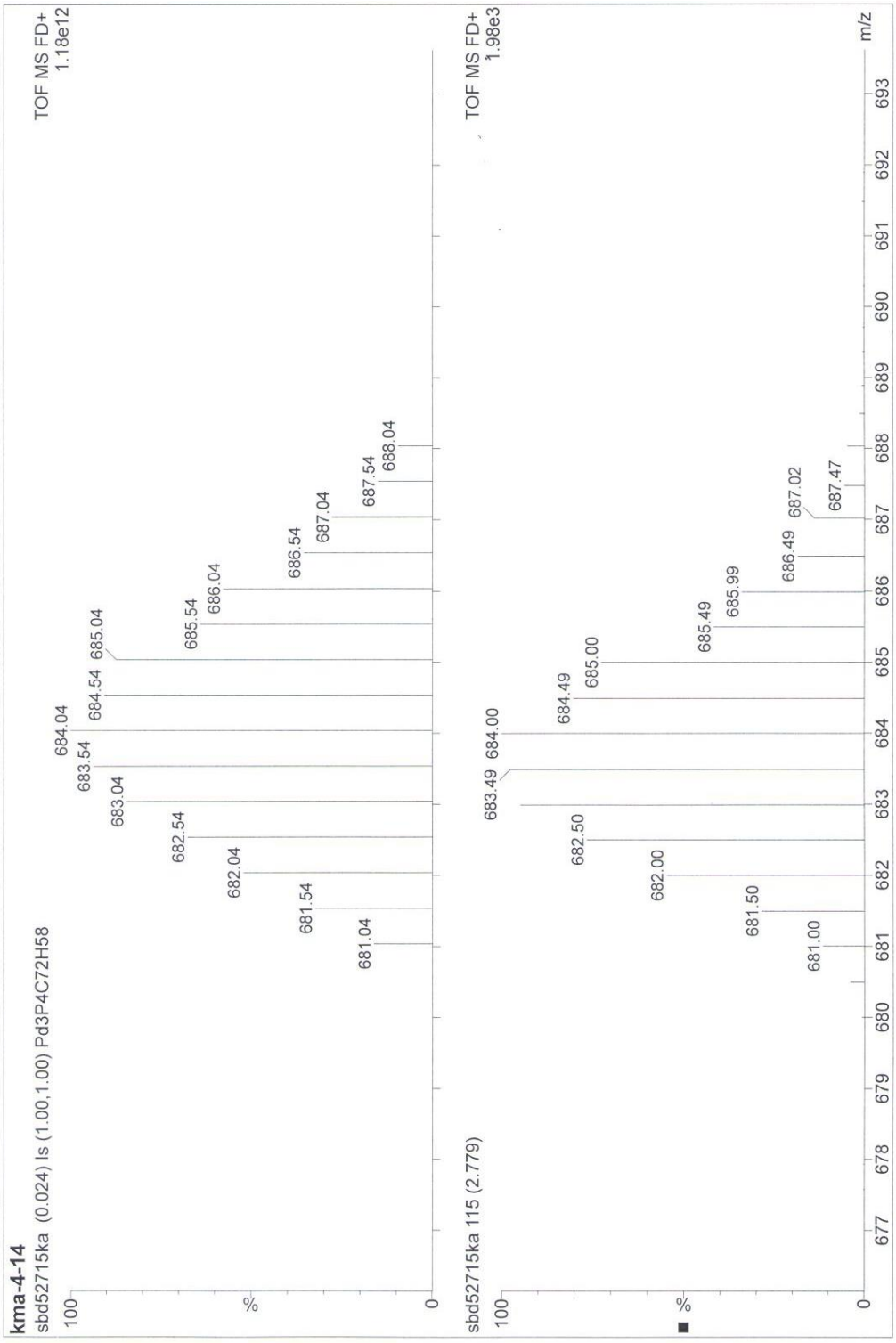
^{13}C-optimised HMQC with a coupling of 145 Hz



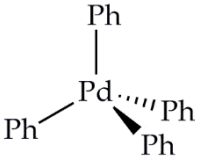
^{13}C-optimised HMQC with a coupling of 12 Hz



1.23.2 Mass spectra

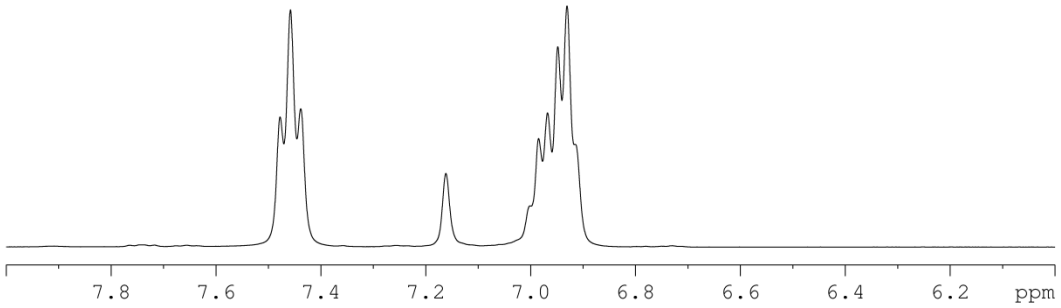


1.24 $[Pd(PPh_3)_4]$

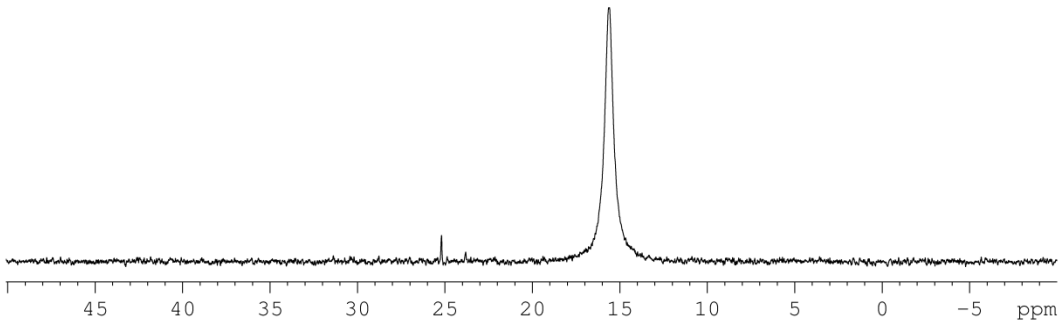


1.24.1NMR spectra

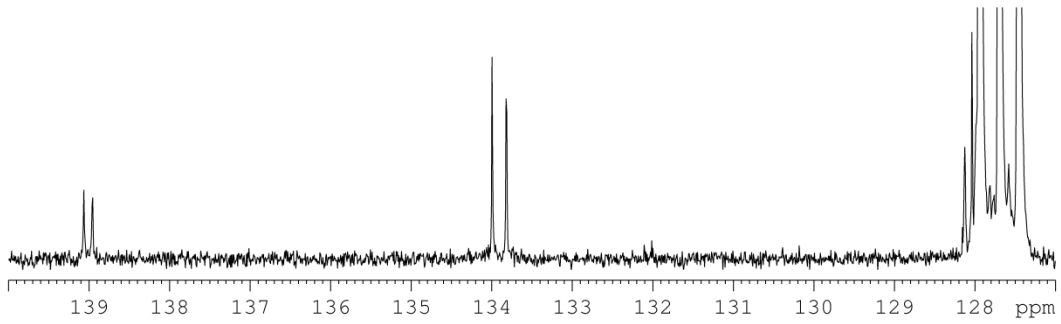
^{1}H



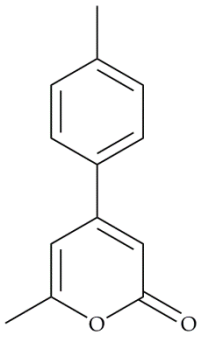
$^{31}P\ \{^{1}H\}$



$^{13}C\ \{^{1}H\}$



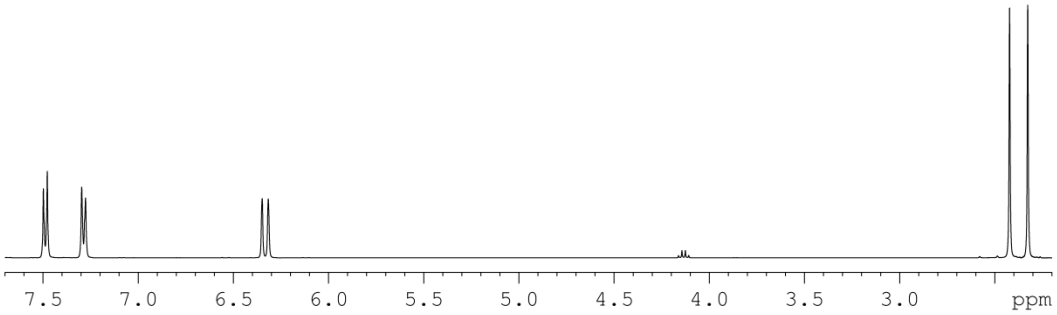
1.25 6-methyl-4-(4-methylphenyl)-pyran-2-one



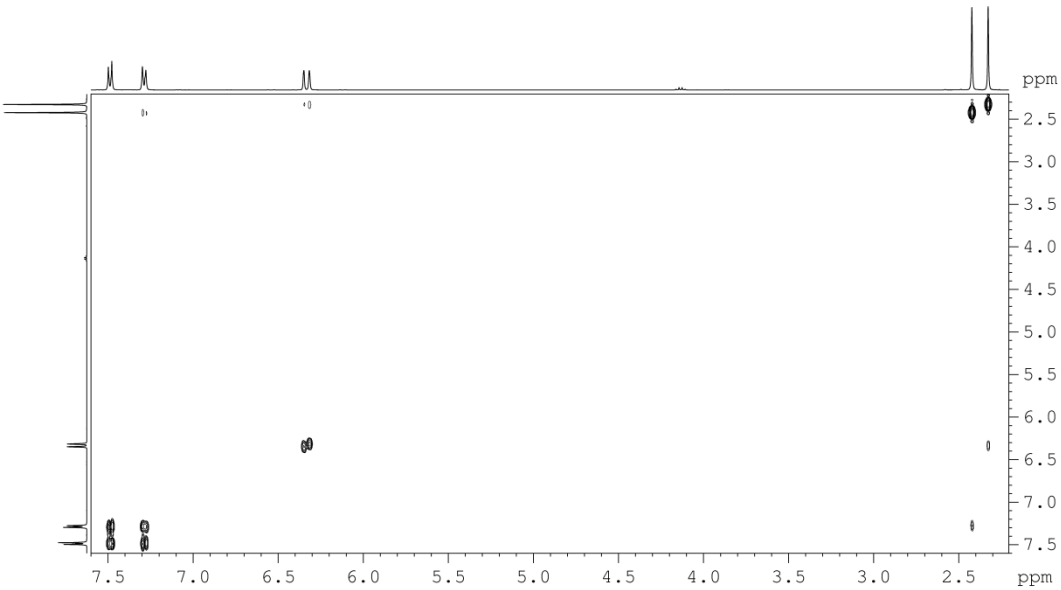
Compound reference kma-3-93

1.25.1NMR spectra

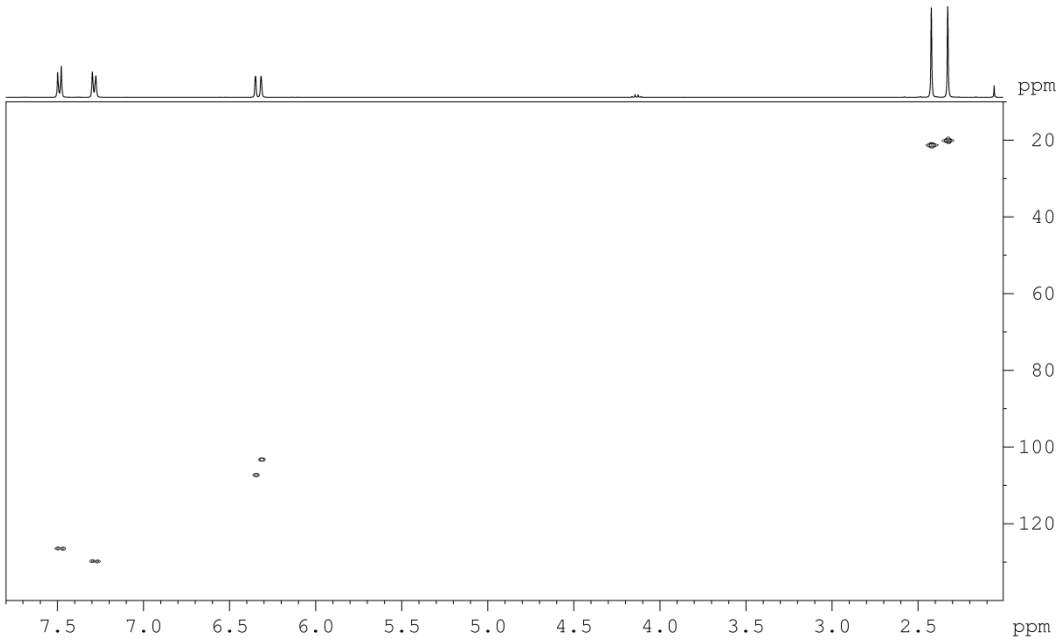
^{1}H



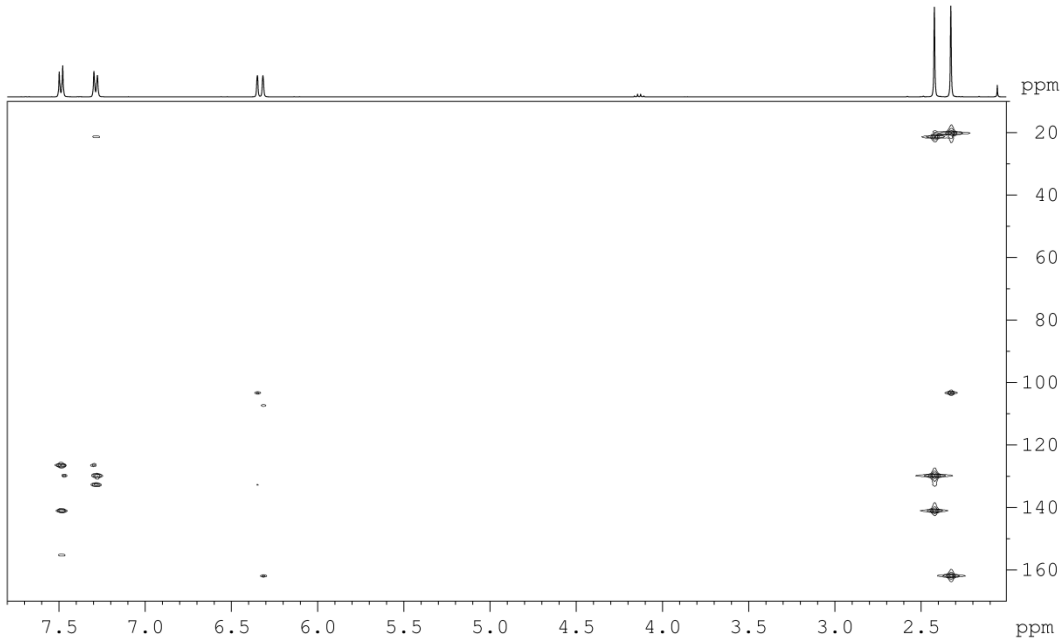
COSY



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



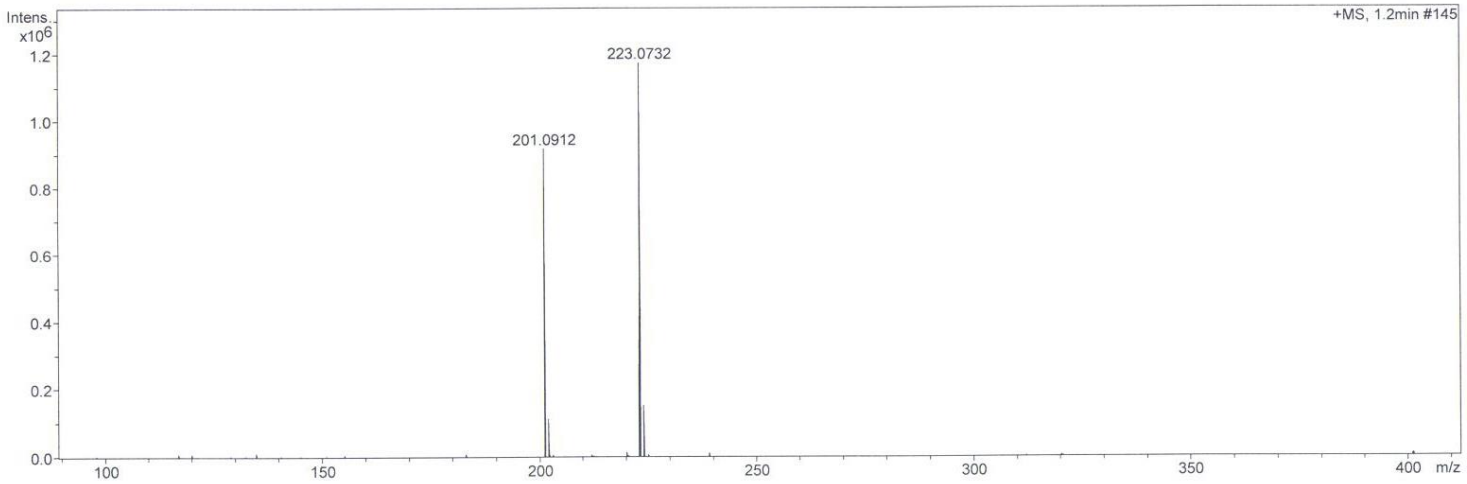
kma-3-93

York - Chemistry - Mass Spectrometry Service Report

Analysis Information

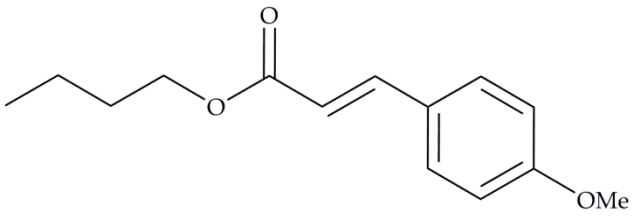
Acquisition Date 29/09/2015 14:26:39

Analysis Filename	sbd54813ka_P1-F-1_01_61203.d
Method	400p_meoh1260_2c1s.m
Submission Name	sbd54813ka
Instrument	micrOTOF
ESI	Positive



Meas. m/z	#	Formula	m/z	err [ppm]	err [mDa]	mSigma	Mean err [ppm]
201.0912	1	C 13 H 13 O 2	201.0910	-1.1	-0.2	11.4	-0.8
223.0732	1	C 13 H 12 Na O 2	223.0730	-1.3	-0.3	7.6	-0.9

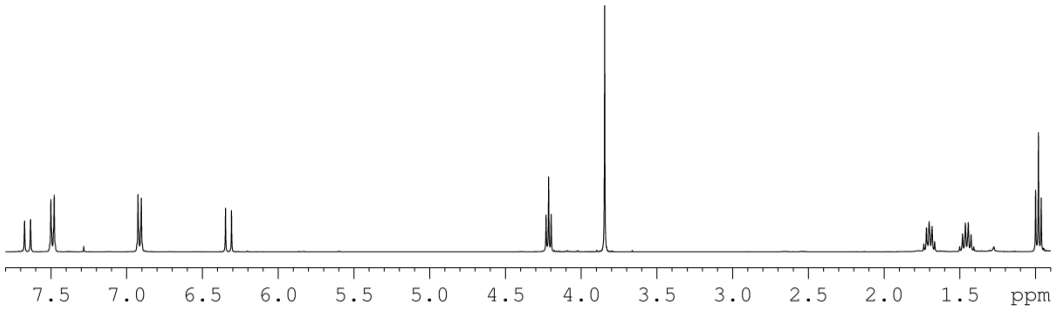
1.26 butyl (2*E*)-3-(4-methoxyphenyl)acrylate



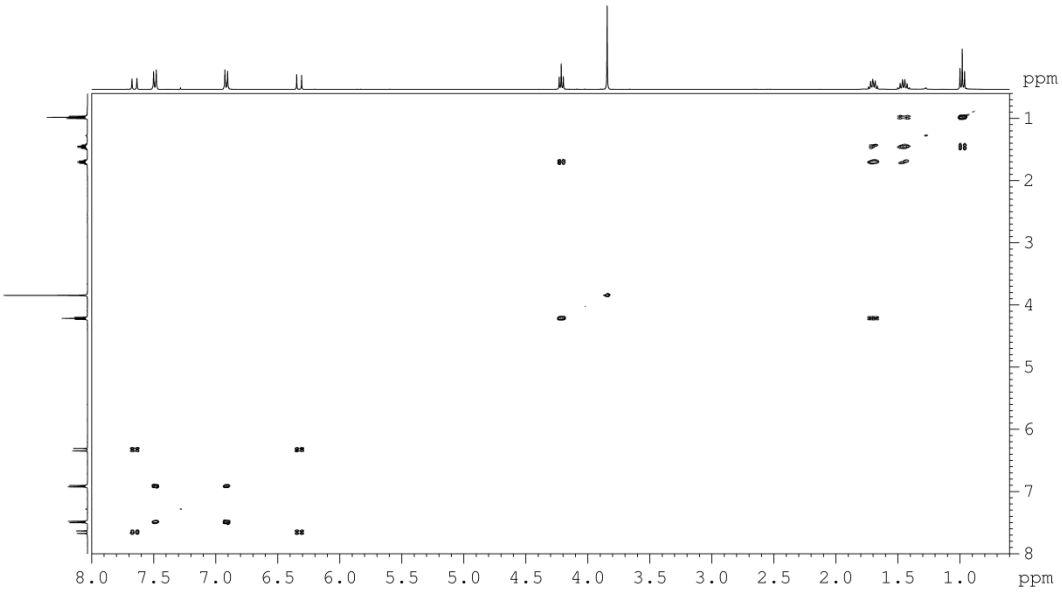
Compound reference kma-4-61

1.26.1NMR spectra

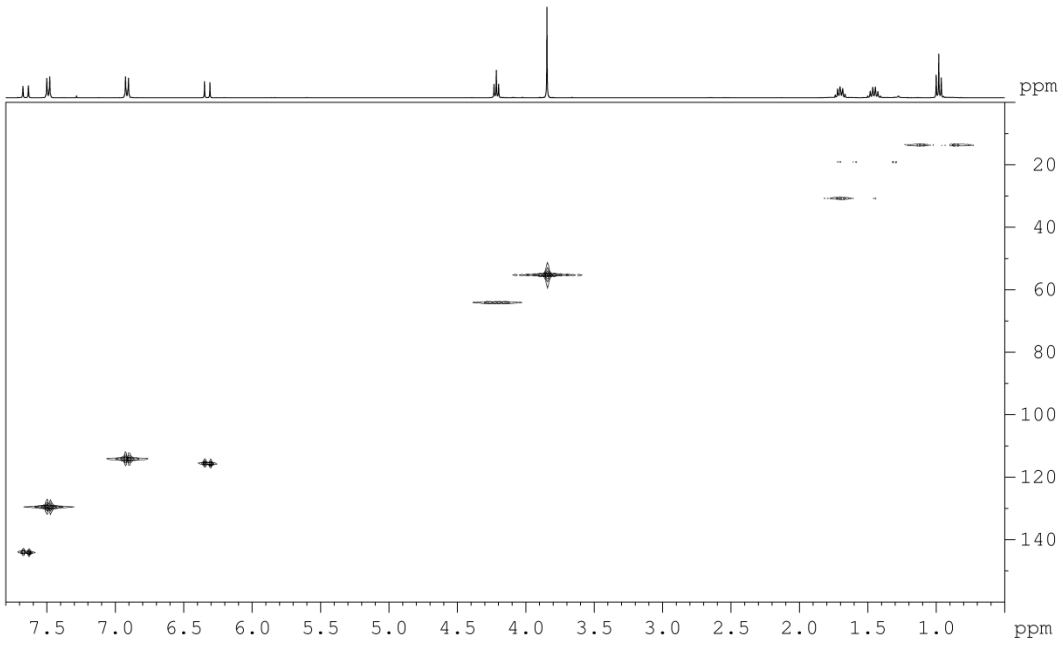
^{1}H



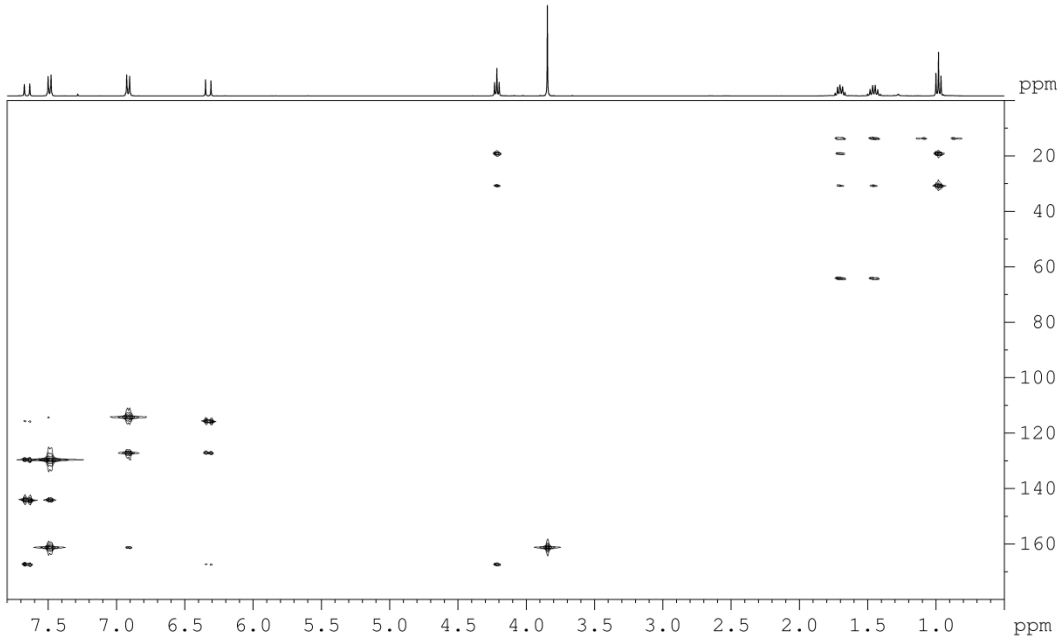
COSY



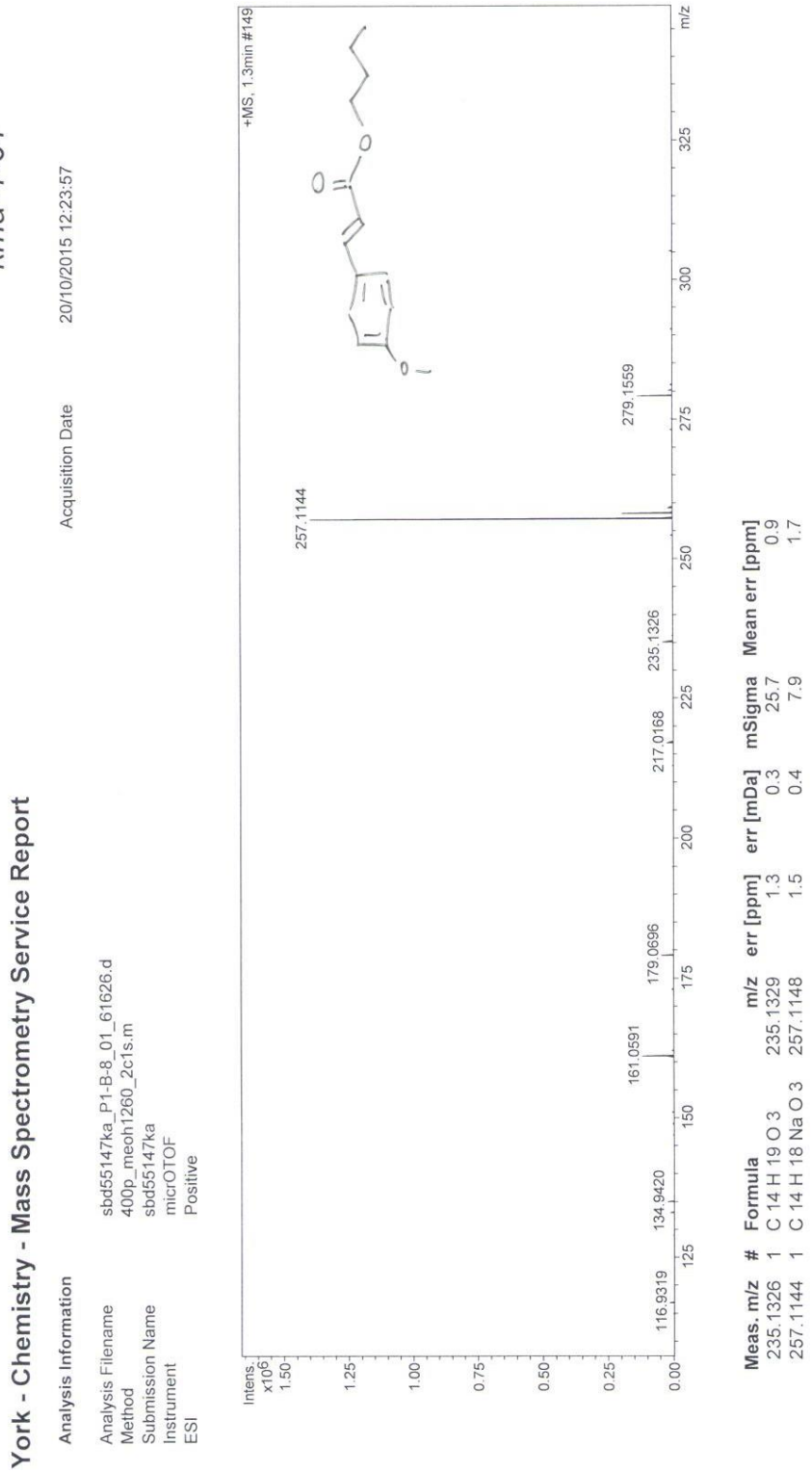
^{13}C-optimised HMQC with a coupling of 145 Hz



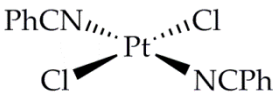
^{13}C-optimised HMQC with a coupling of 12 Hz



1.26.2 Mass spectra



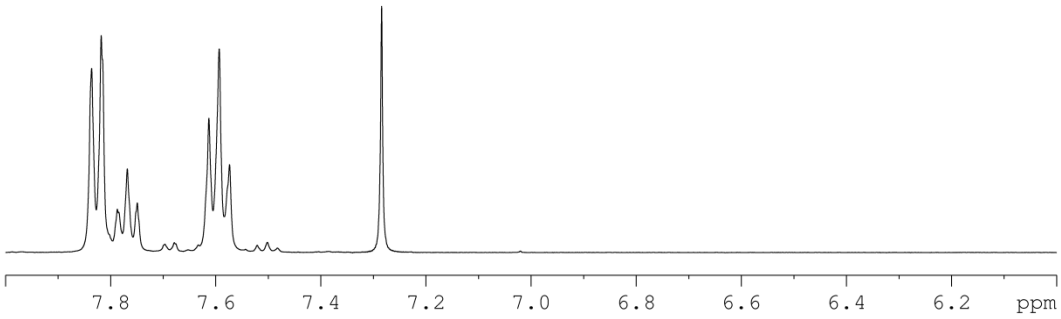
1.27 $[Pt(Cl)(C_6H_5CN)_2]$



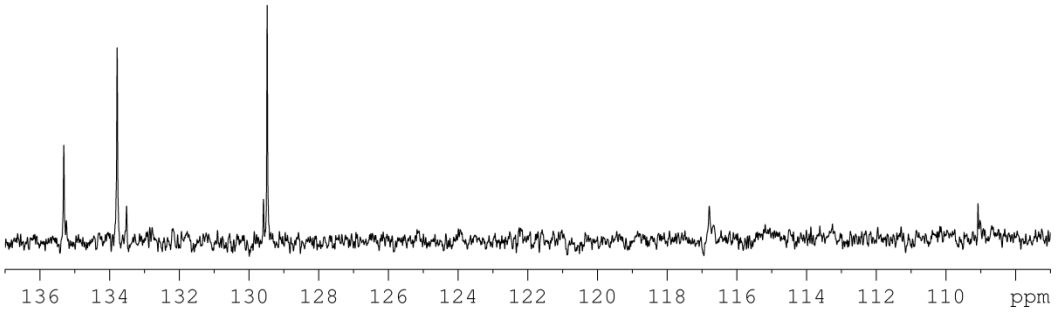
Compound reference kma-3-56

1.27.1NMR spectra

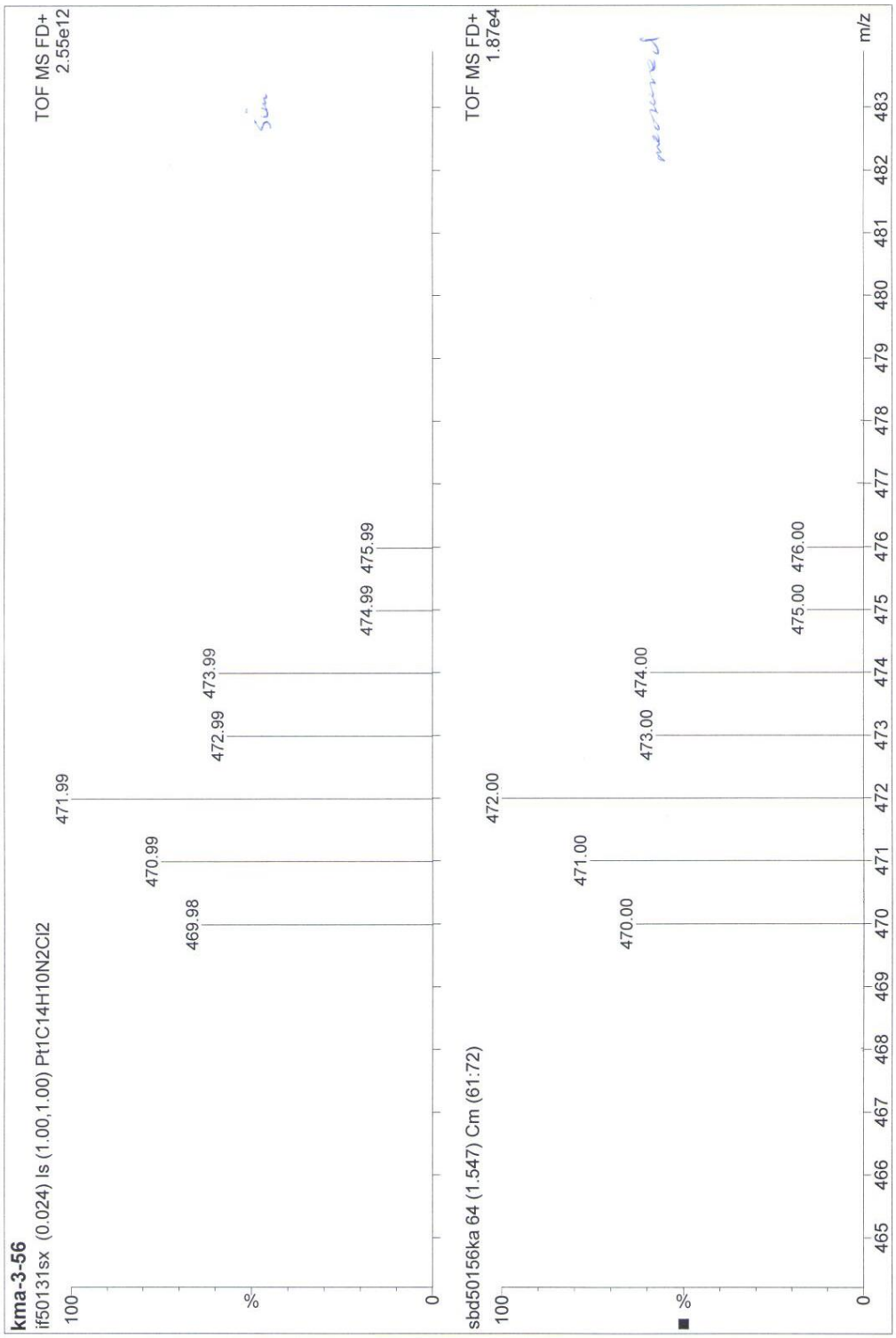
^{1}H



^{13}C {^{1}H}



1.27.2 Mass spectra



1.27.3 CHN elemental analysis

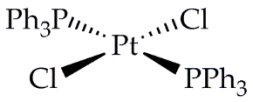
CHN Microanalytical Service Results $[PtCl_2(NCPh)_2]$

Name	Kate Appleby	Compound ID	kma-3-58

Element	% C	% H	% N	% Rest
Observed 1	36.14	2.12	6.02	55.72
Observed 2	36.14	2.05	5.92	55.89
Mean	36.142	2.085	5.971	–
Calc (theory)	35.61	2.13	5.93	56.33

Comments: Check std within specified limits YES / NO. Counter/run no: 21033

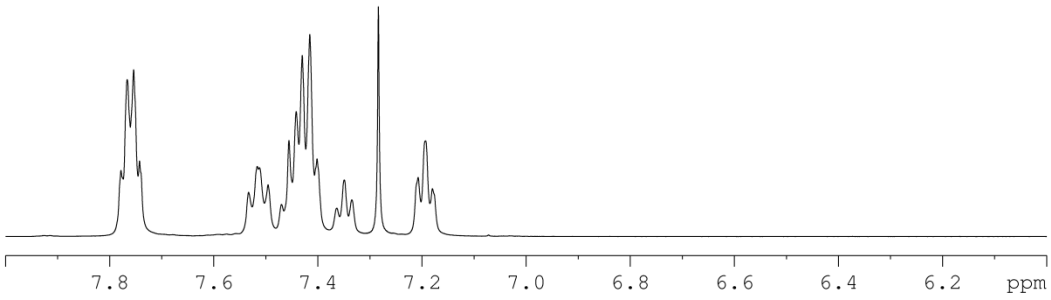
1.28 $[Pt(Cl)_2(PPh_3)_2]$



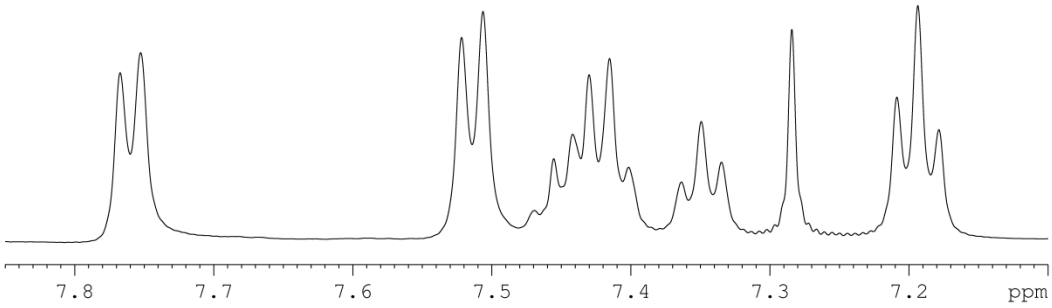
Compound reference kma-3-58

1.28.1 NMR spectra

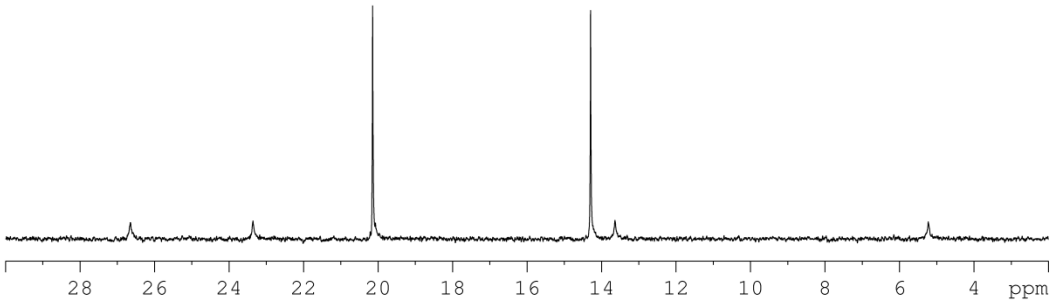
^{1}H



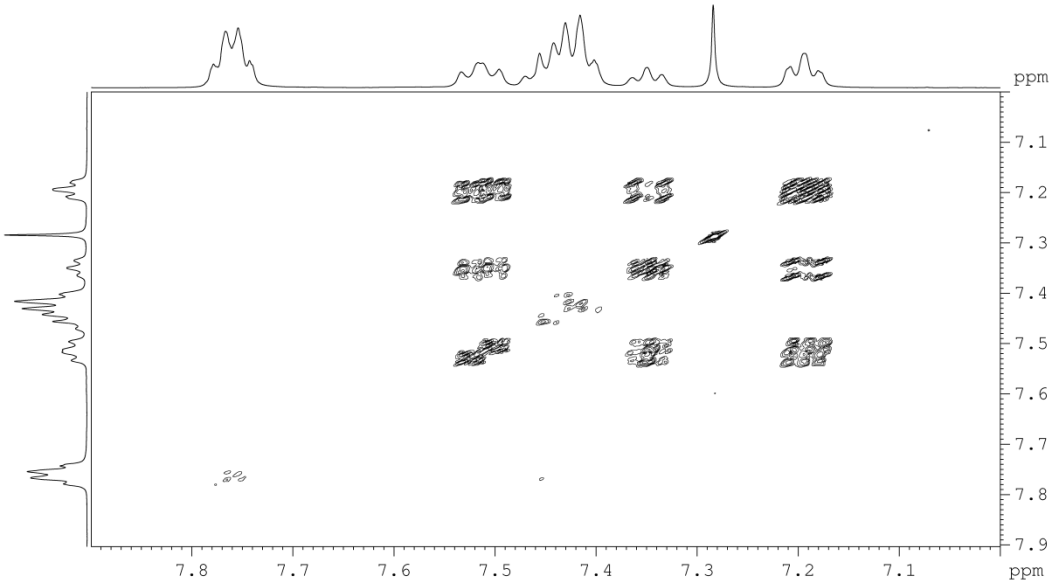
$^{1}H\ \{^{31}P\}$



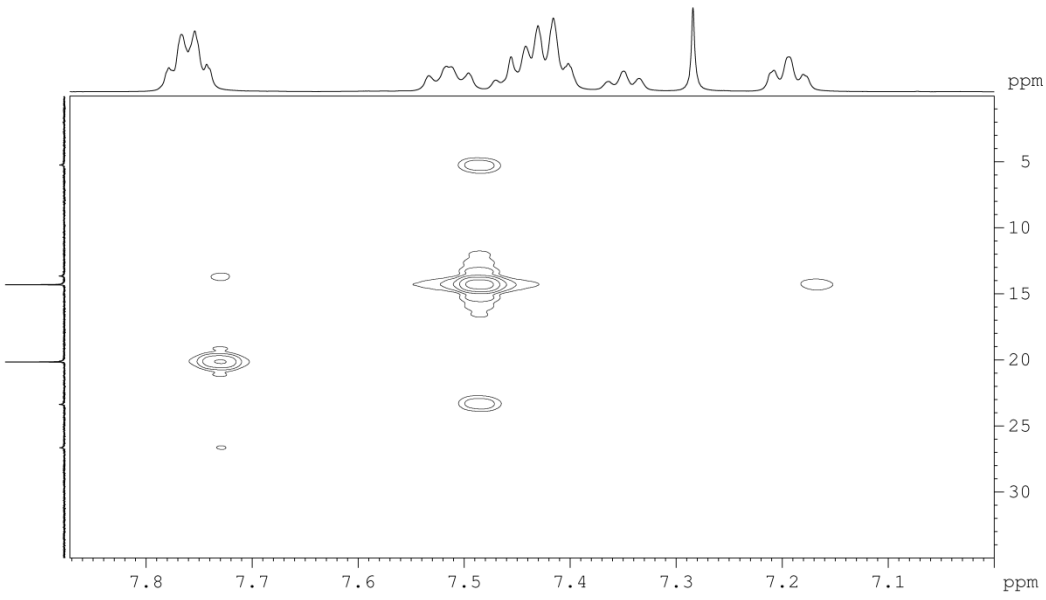
$^{31}P\ \{^{1}H\}$



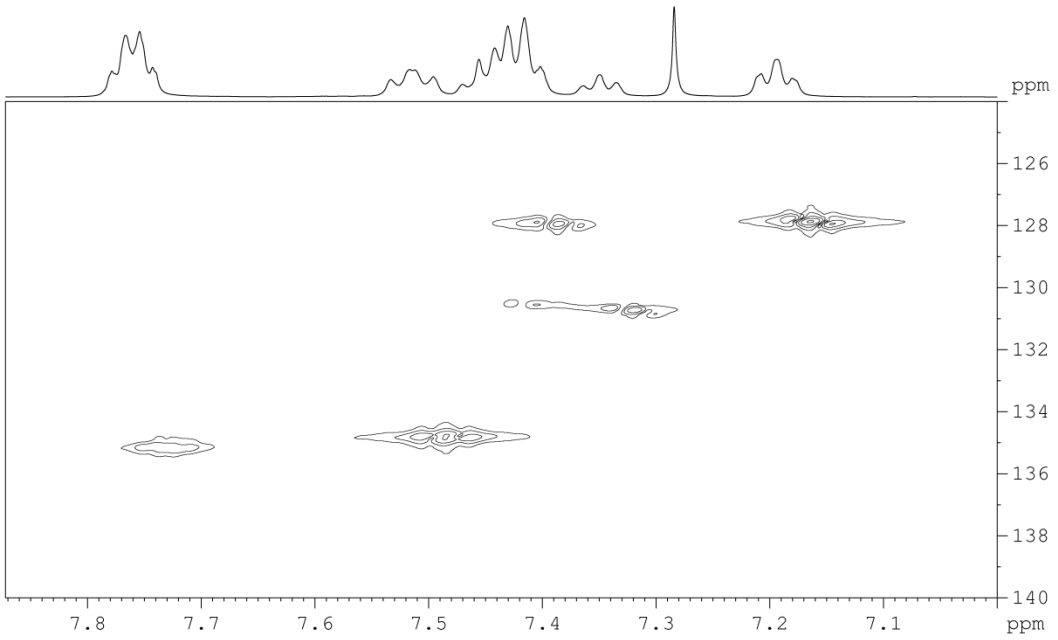
COSY



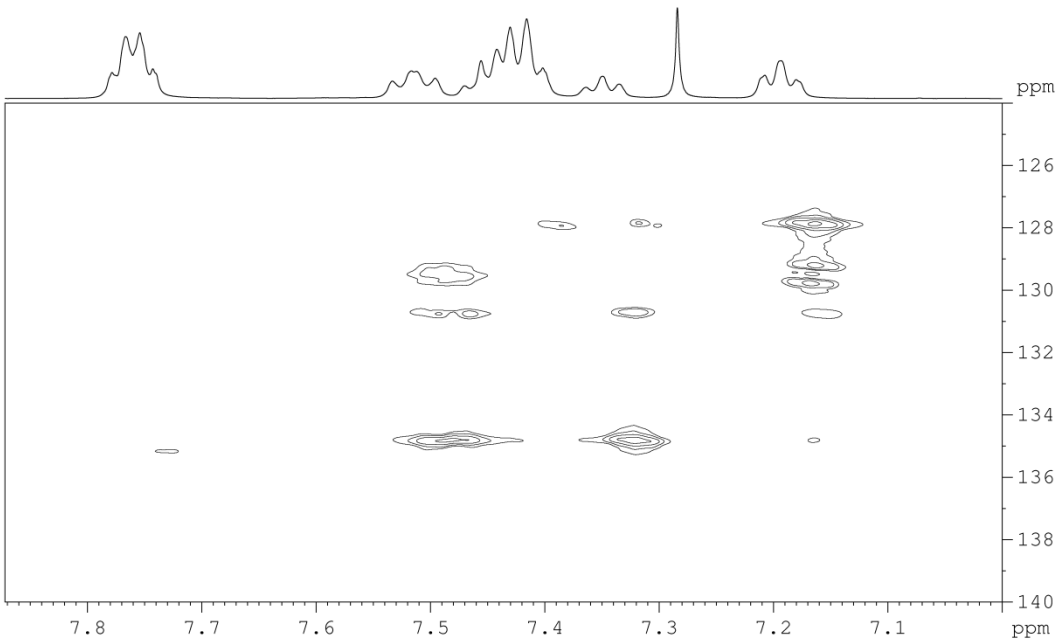
^{31}P-optimised HMQC with a coupling of 12 Hz



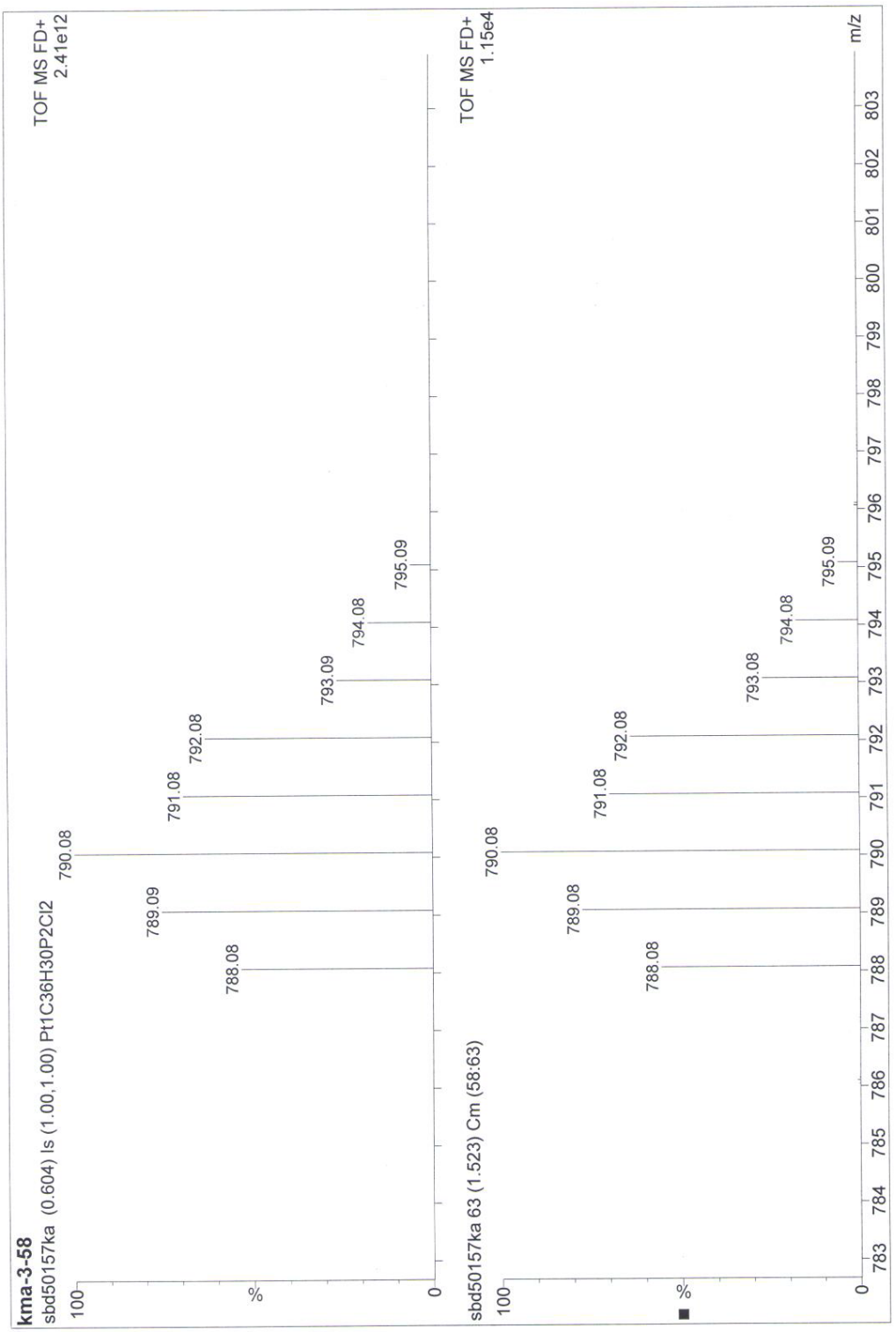
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling constant of 12 Hz



1.28.2 Mass spectra



1.28.3 CHN elemental analysis

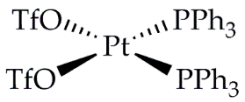
CHN Microanalytical Service Results $[PtCl_2(PPh_3)_2]$

Name	Kate Appleby	Compound ID	kma-3-58

Element	% C	% H	% N	% Rest
Observed 1	54.66	3.81	–	41.53
Observed 2	54.69	3.80	–	41.50
Mean	54.677	3.806	–	–
Calc (theory)	~~69.00~~ 54.70	~~4.83~~ 3.83	–	~~26.17~~ 41.47

Comments: Check std within specified limits YES / NO. Counter/run no: 21033

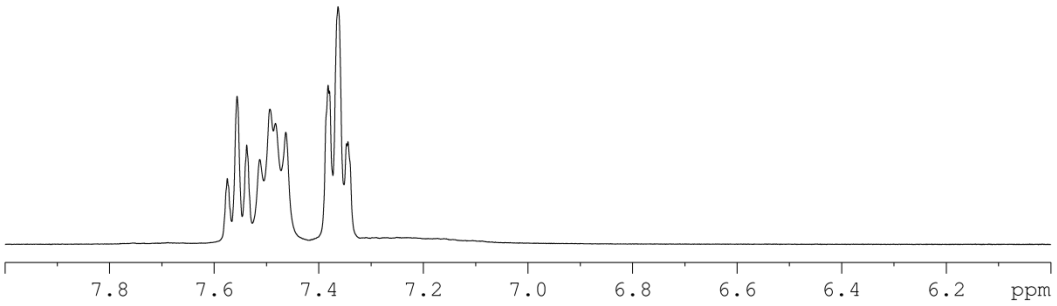
1.29 $[Pt(OTf)_2(PPh_3)_2]$



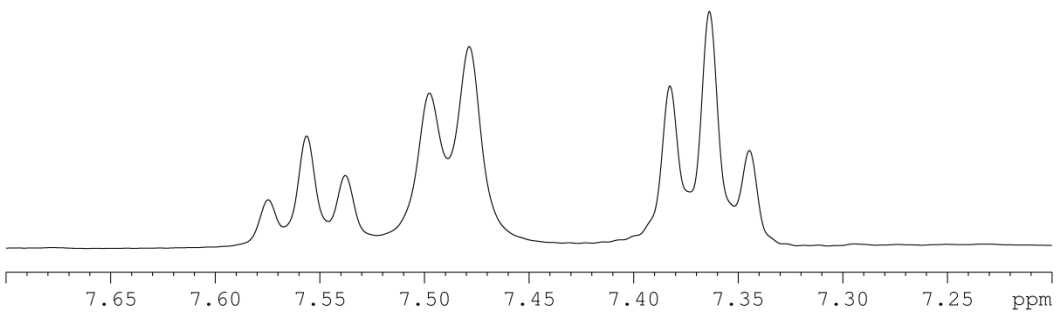
Compound reference kma-3-63

1.29.1 NMR spectra

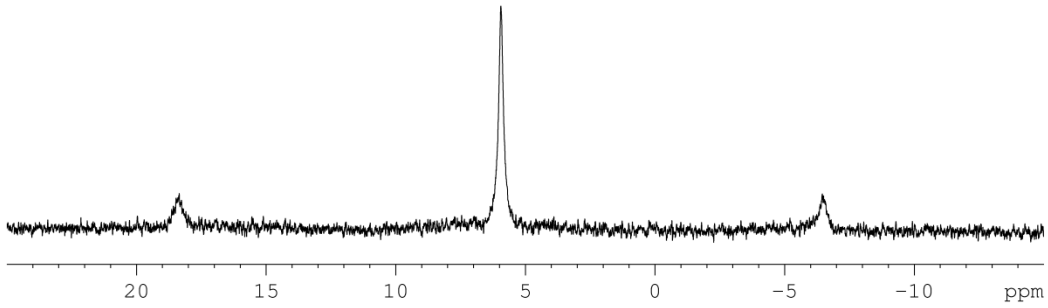
^{1}H



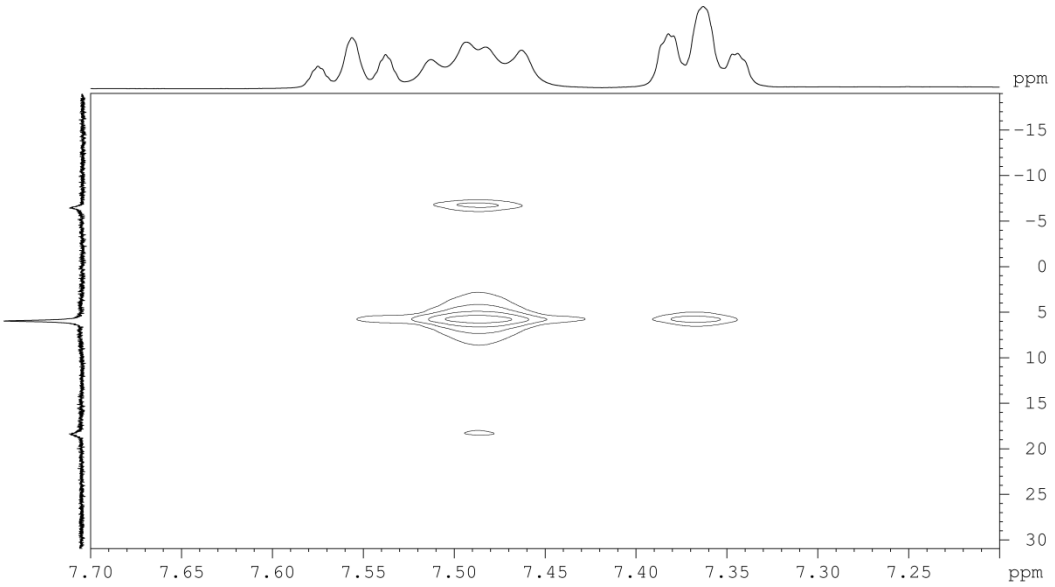
$^{1}H\ \{^{31}P\}$



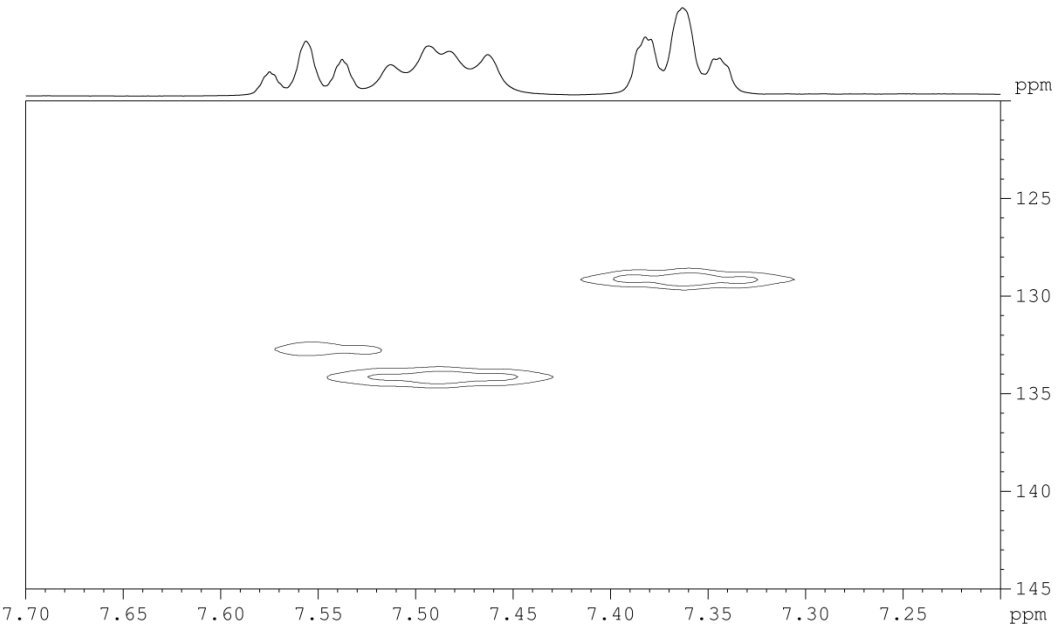
^{31}P {^{1}H}



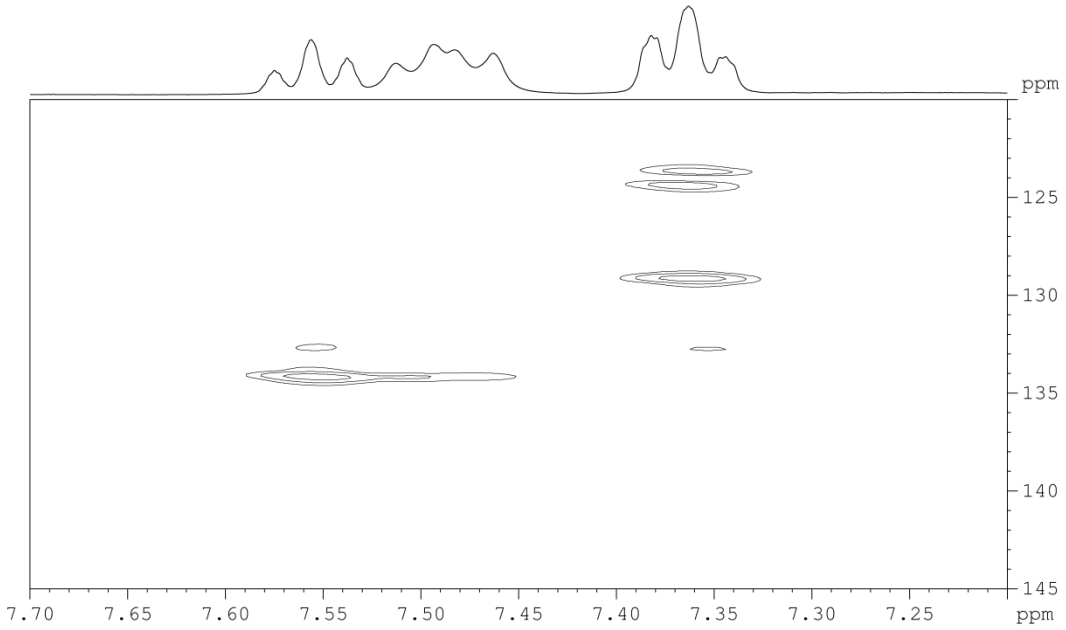
^{31}P-optimised HMQC with a coupling of 12 Hz



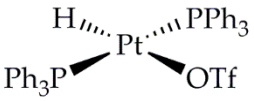
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



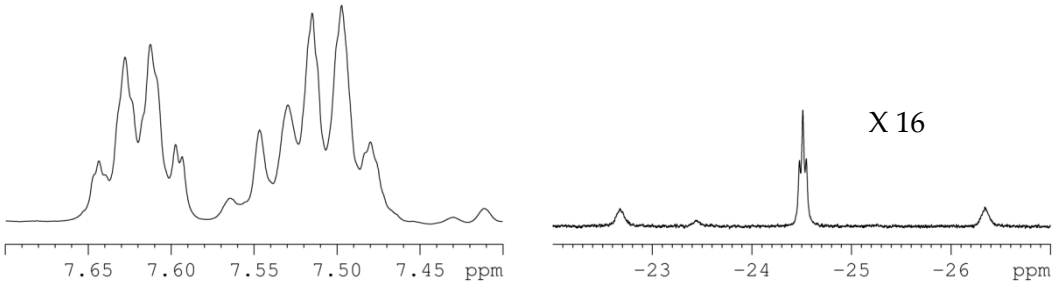
1.30 [Pt(H)(OTf)(PPh$_3$)$_2$]



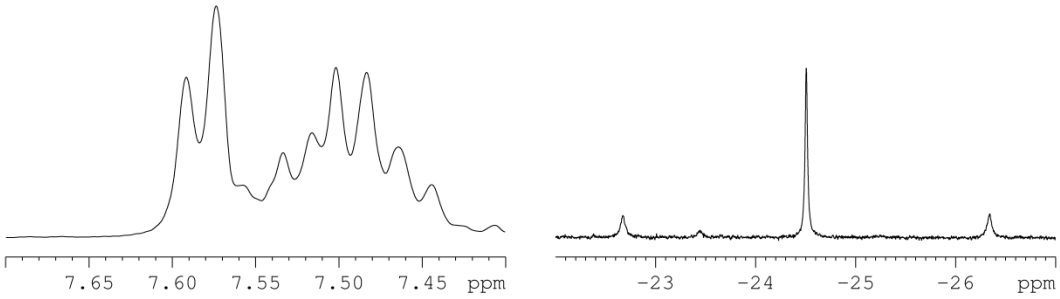
Compound reference kma-3-66

1.30.1NMR spectra

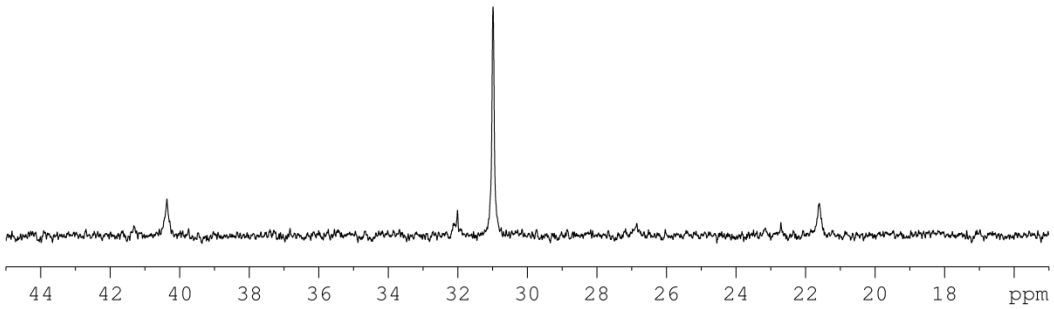
^{1}H



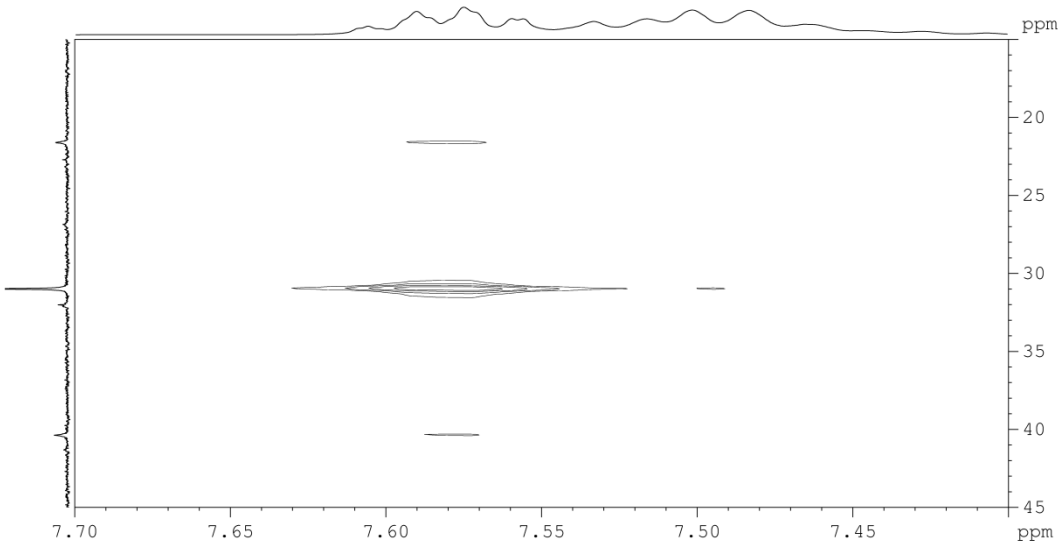
^{1}H {^{31}P}



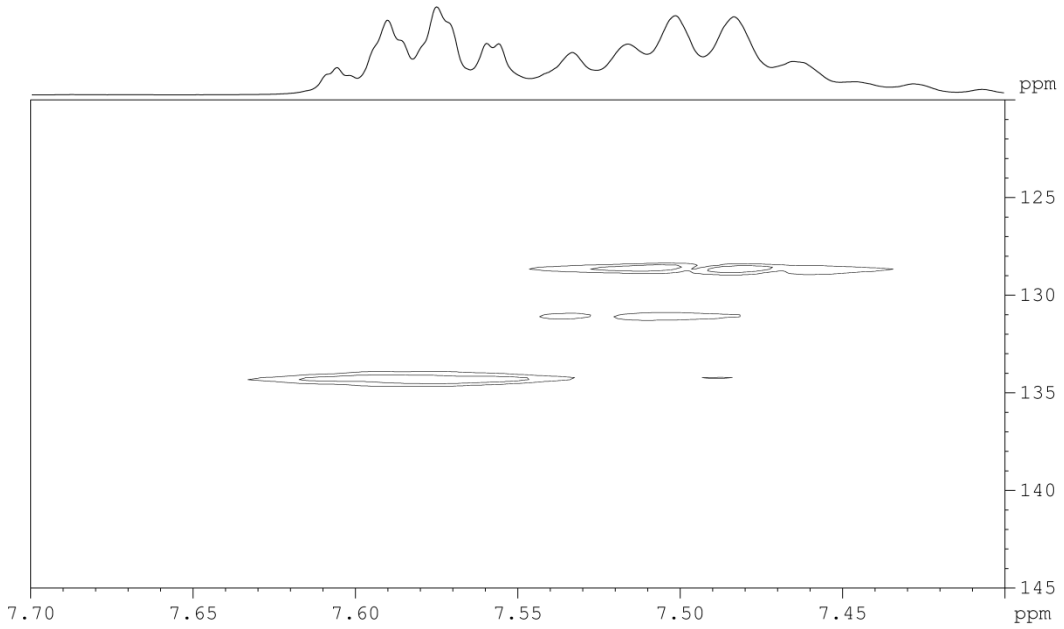
^{31}P



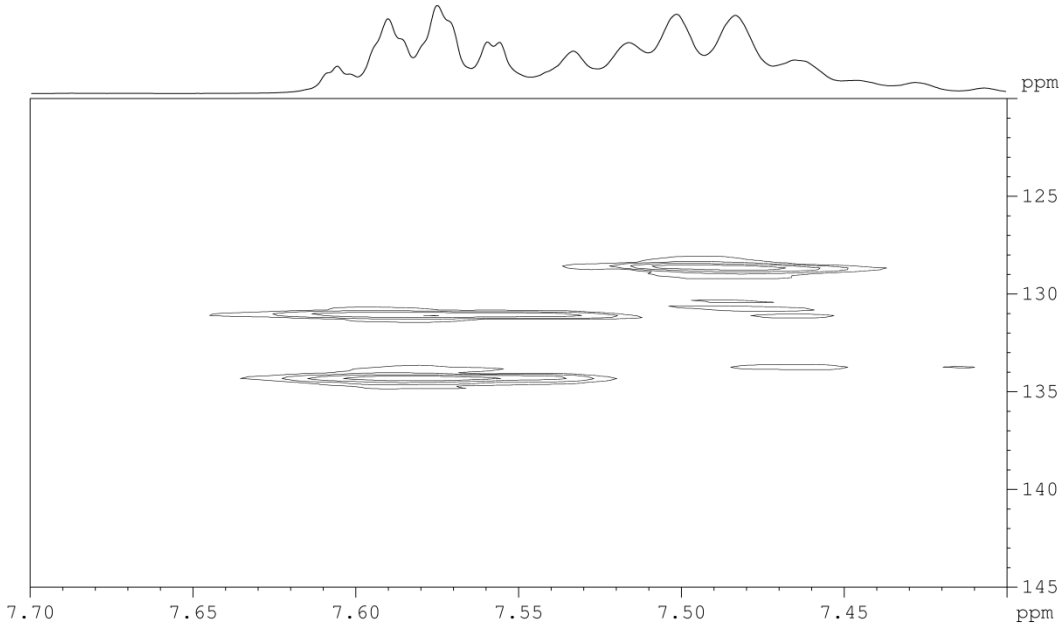
^{31}P-optimised HMQC with a coupling of 12 Hz



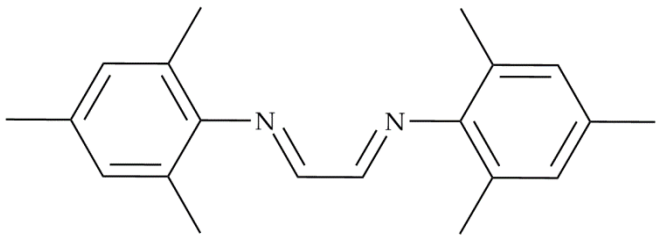
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz

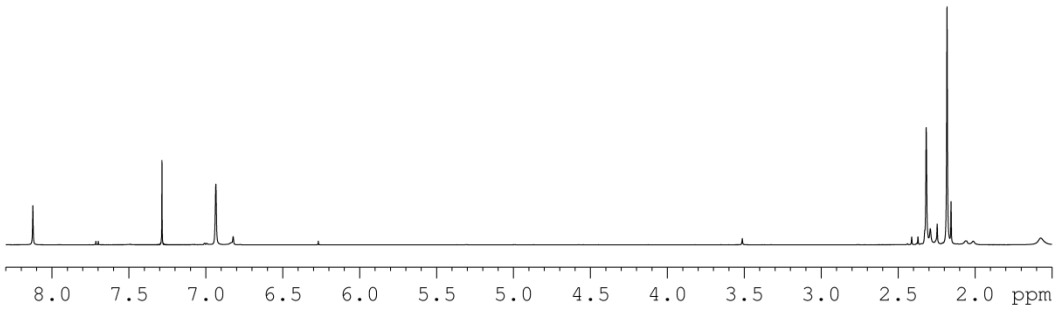


1.31 1,4-Bis-(2,4,6-trimethylphenyl)-1,4-diaza-butadiene

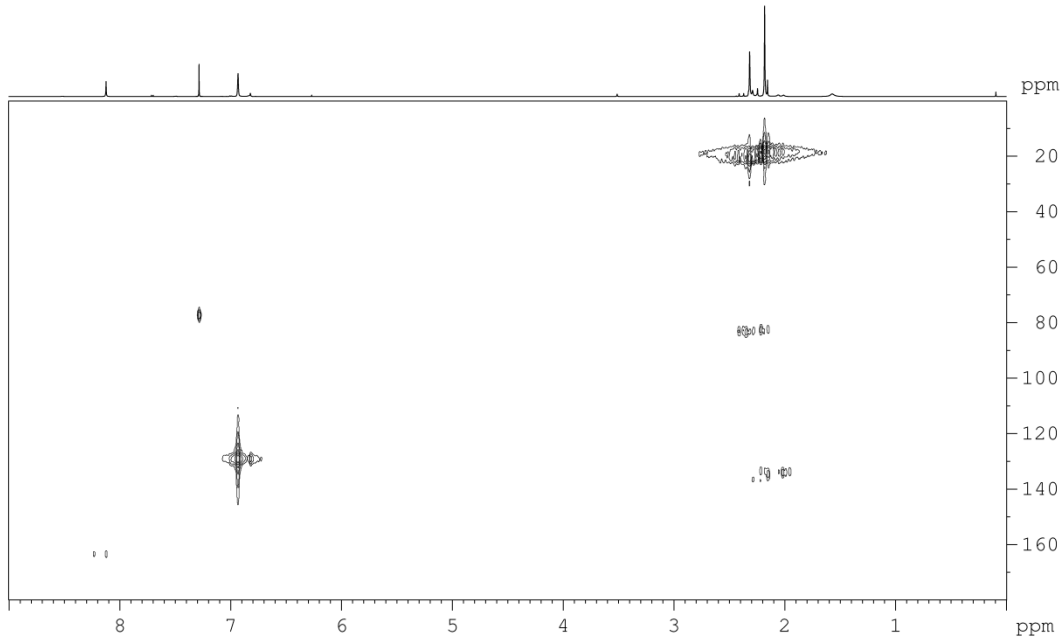


1.31.1NMR spectra

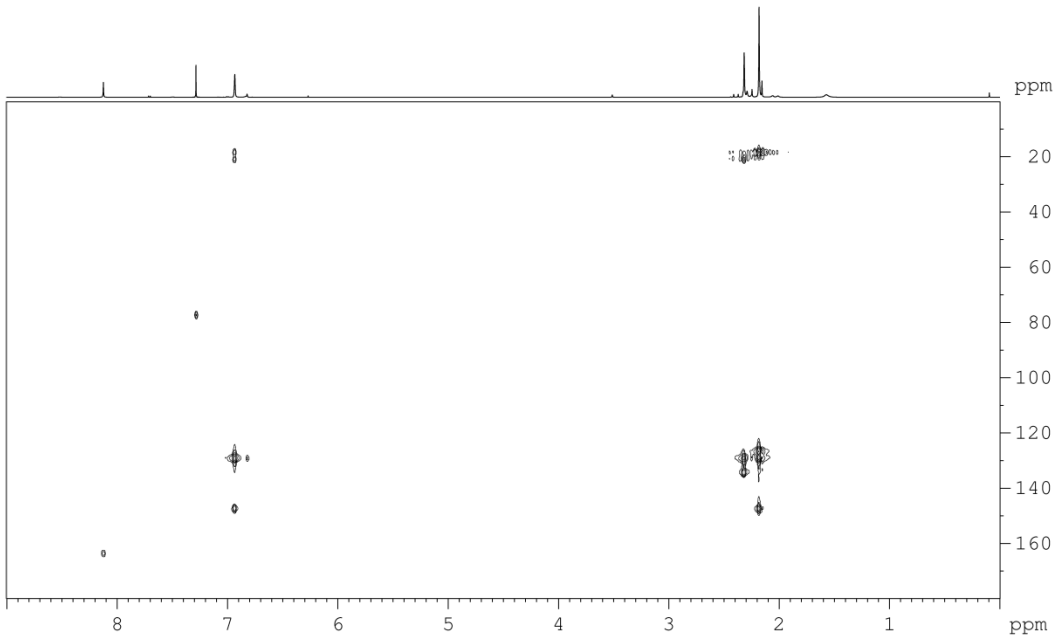
^{1}H



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



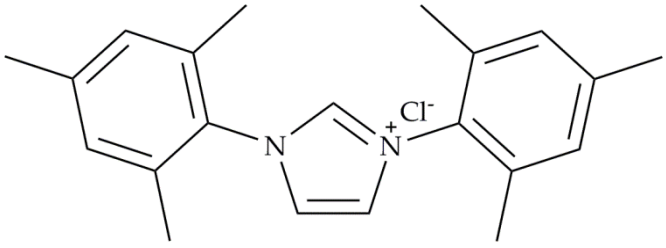
1.31.2 CHN elemental analysis

CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma-2-25 IMes (i)	
Element	**% C**	**% H**	**% N**	**% Rest**
Observed 1	82.17	8.26	9.57	–
Observed 2	82.19	8.25	9.56	–
Mean	82.179	8.255	9.566	–
Calc (theory)	82.15	8.27	9.58	–

Comments: Check std within specified limits YES / NO. Counter/run no: 21033

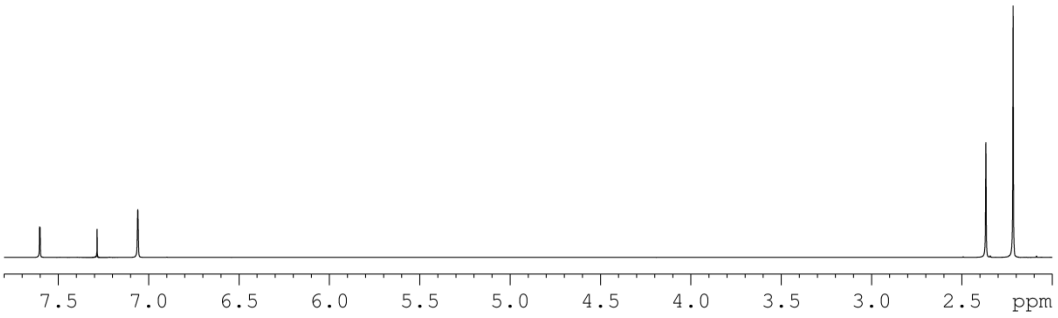
1.32 1,3-Bis-(2,4,6-trimethylphenyl)-imidazolium chloride



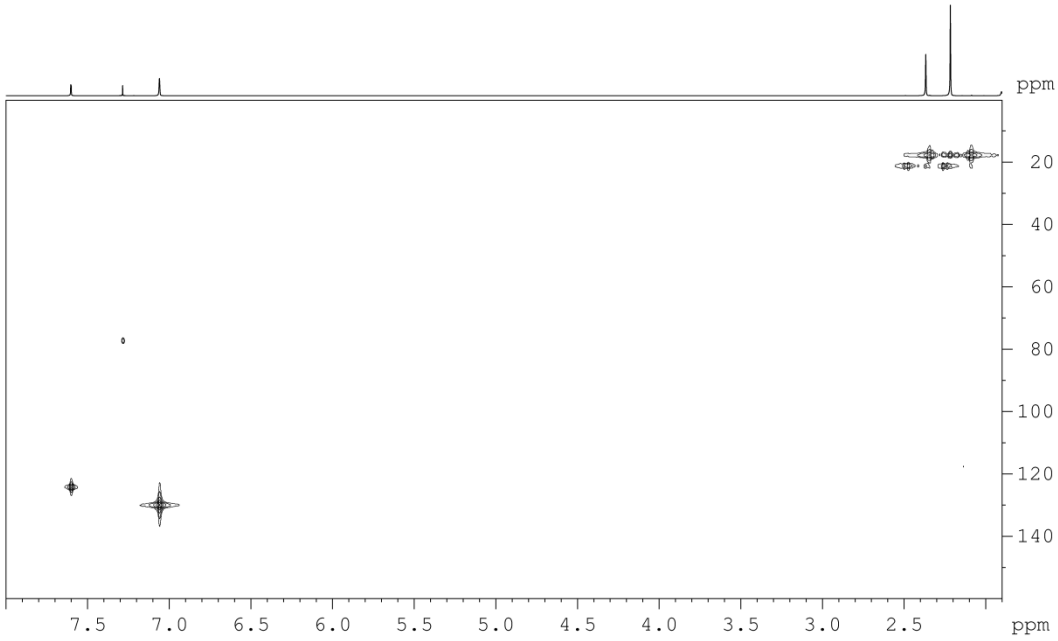
Compound reference kma-2-33

1.32.1NMR spectra

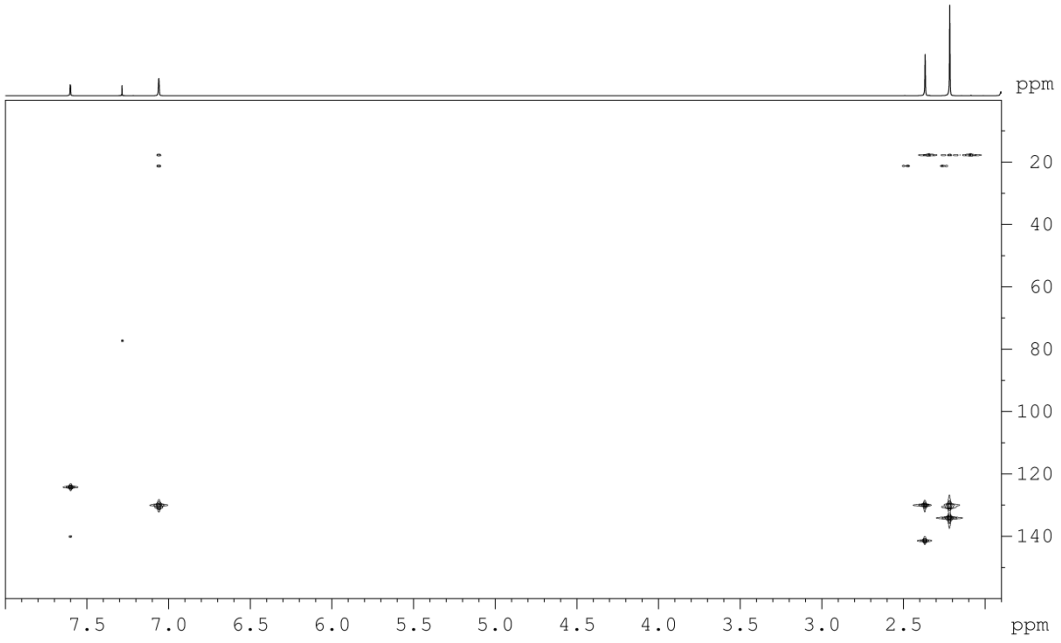
^{1}H



^{13}C-optimised HMQC with a coupling constant of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



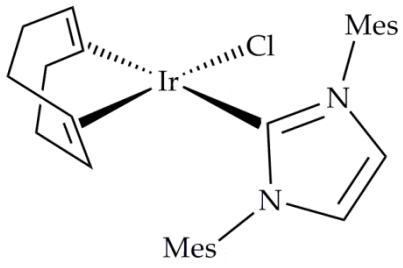
1.32.2 CHN elemental analysis

CHN Microanalytical Service Results

Name	Kate Appleby	Compound ID	kma-2-33 iMes (2)	
Element	**% C**	**% H**	**% N**	**% Rest**
Observed 1	70.26	7.55	7.73	14.46
Observed 2	70.15	7.55	7.74	14.56
Mean	70.206	7.551	7.731	-
Calc (theory)	73.99	7.39	8.22	10.40

Comments: Check std within specified limits YES / NO. Counter/run no: 21023

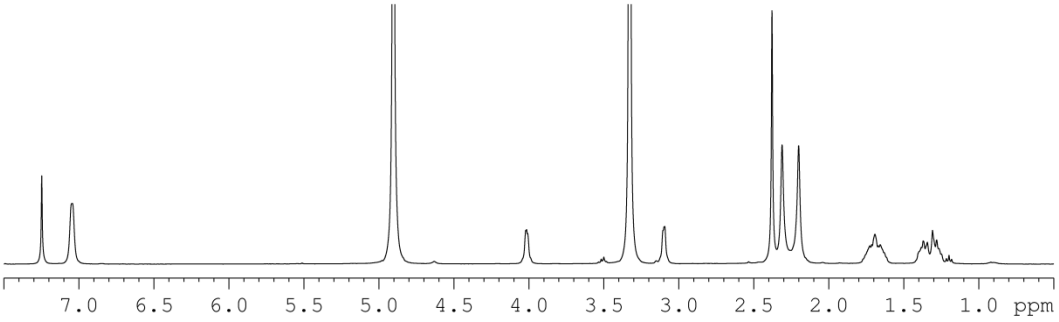
1.33 [IrCl(COD)(IMes)]



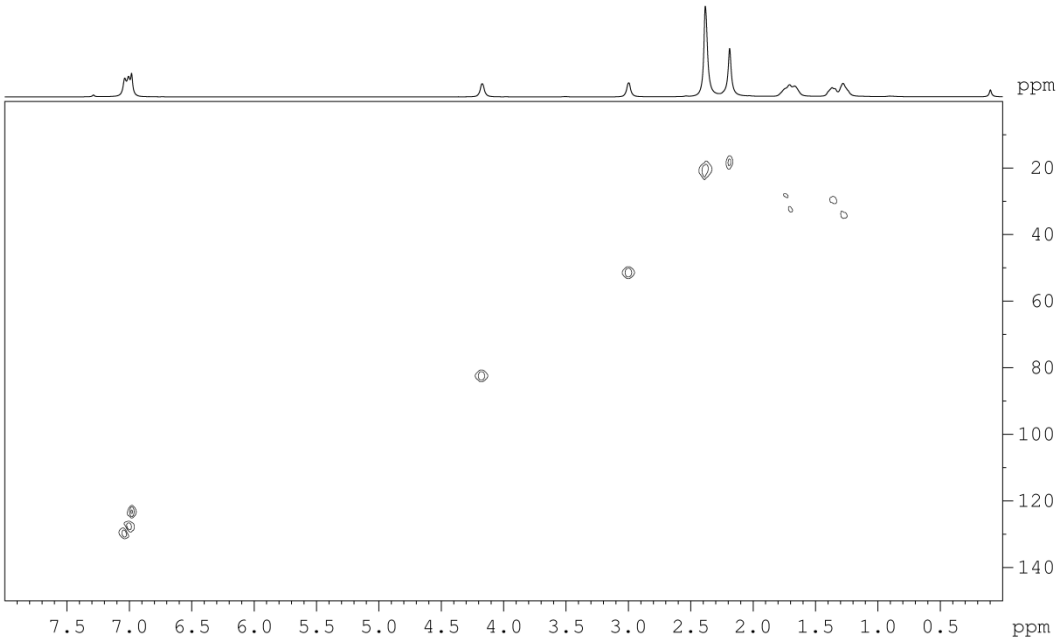
Compound reference kma-2-40

1.33.1NMR spectra

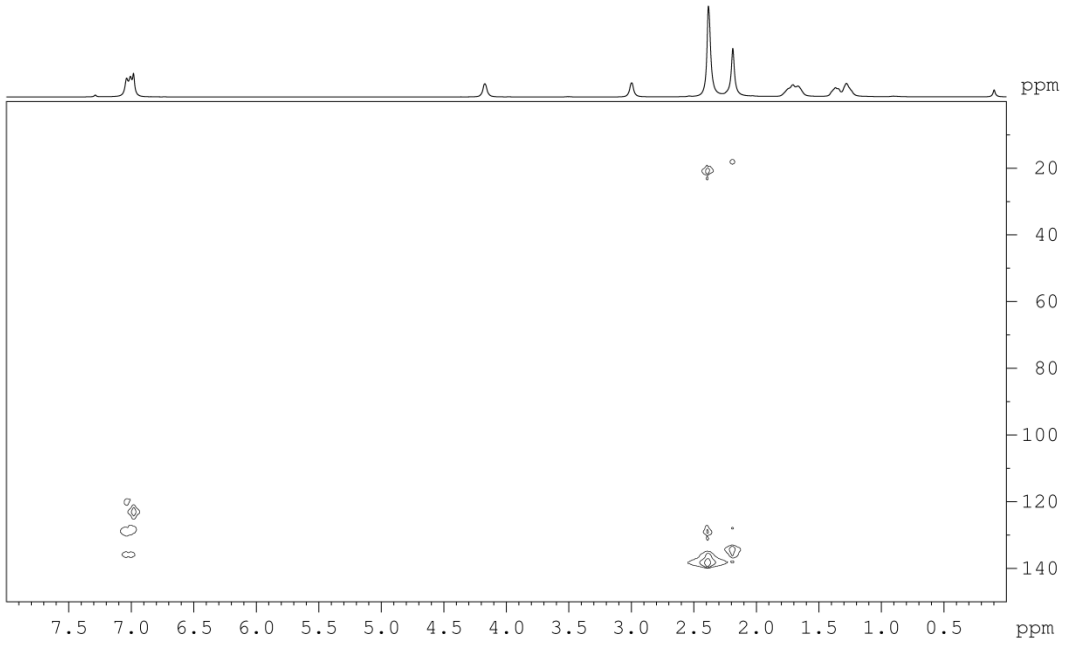
^{1}H



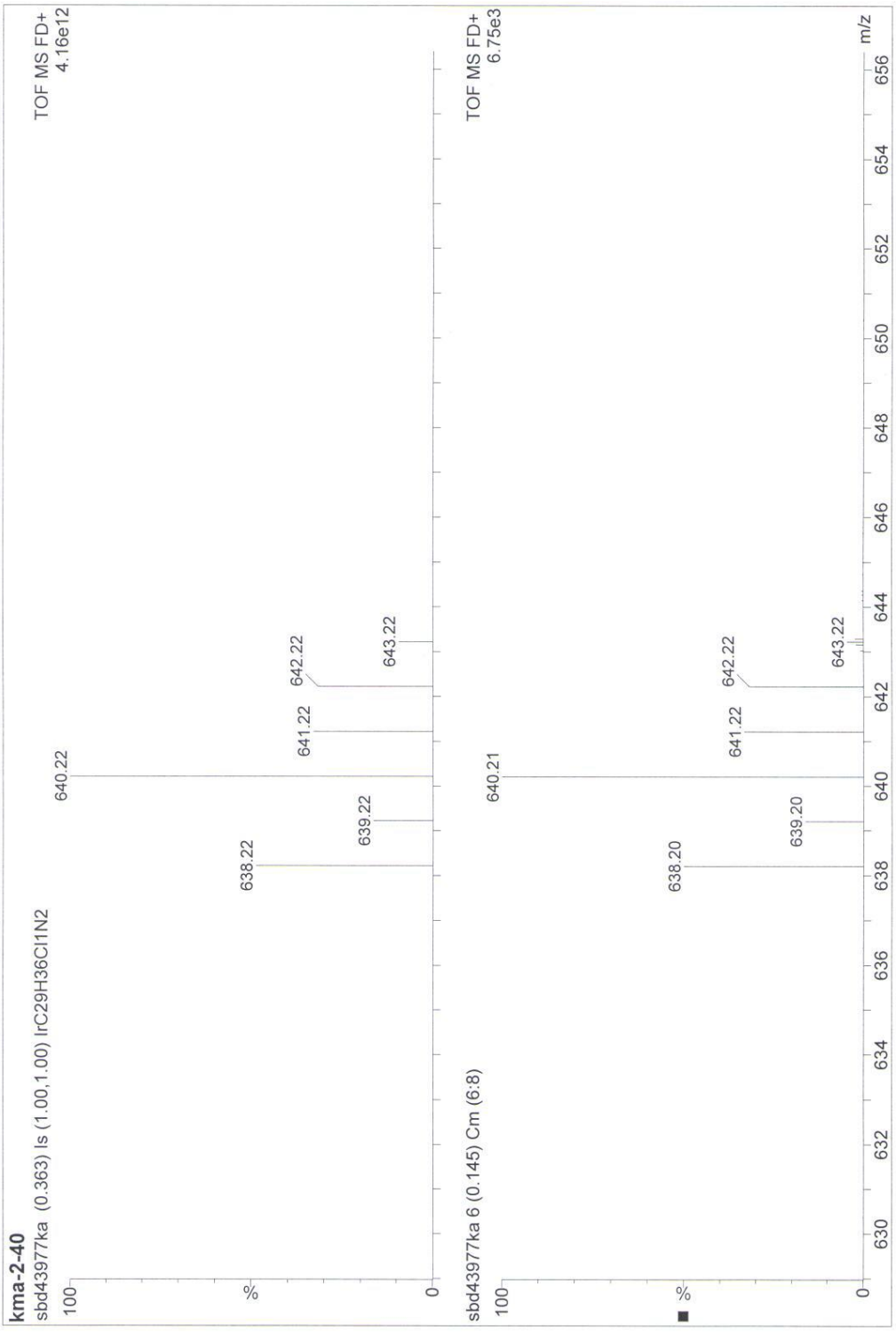
^{13}C-optimised HMQC with a coupling of 145 Hz



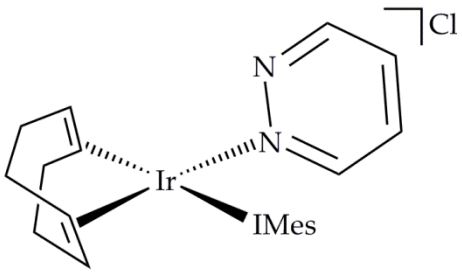
^{13}C-optimised HMQC with a coupling of 12 Hz



1.33.2Mass spectra



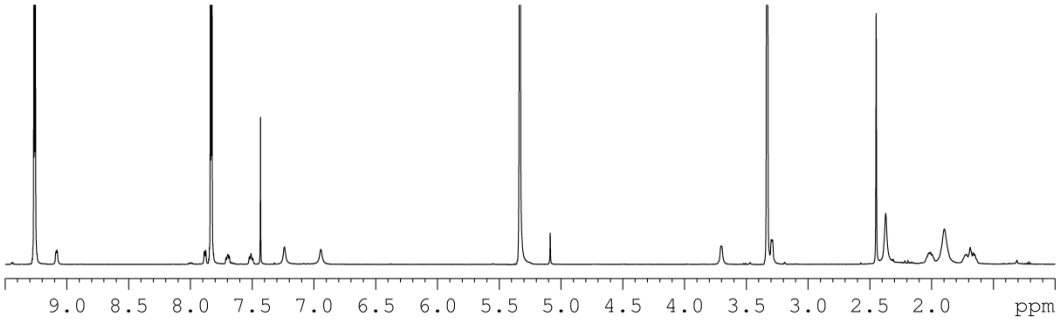
1.34 [Ir(COD)(IMes)(pdz)]Cl



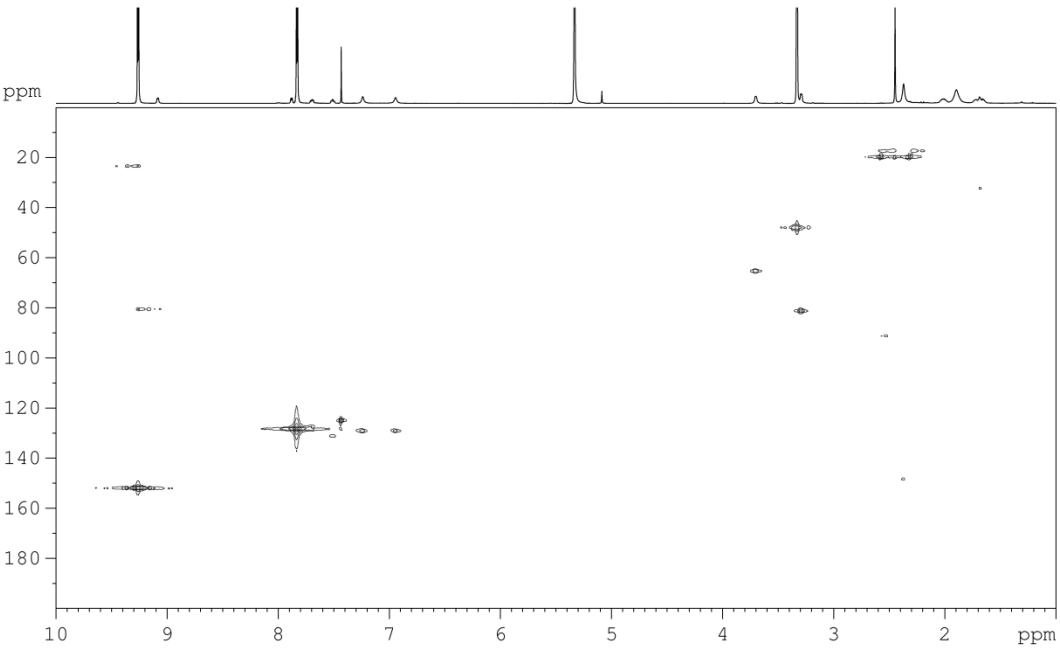
Compound reference kma-2-48

1.34.1 NMR spectra

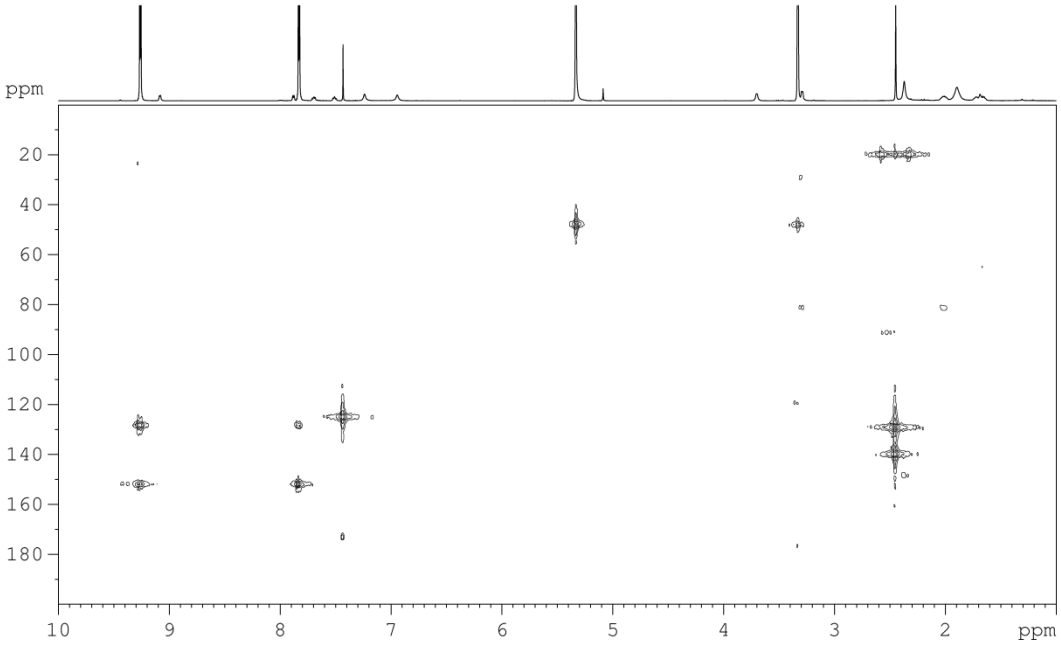
^{1}H



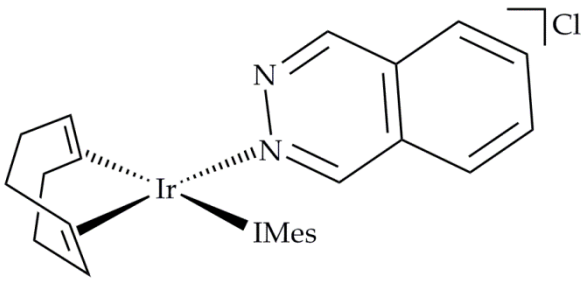
^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



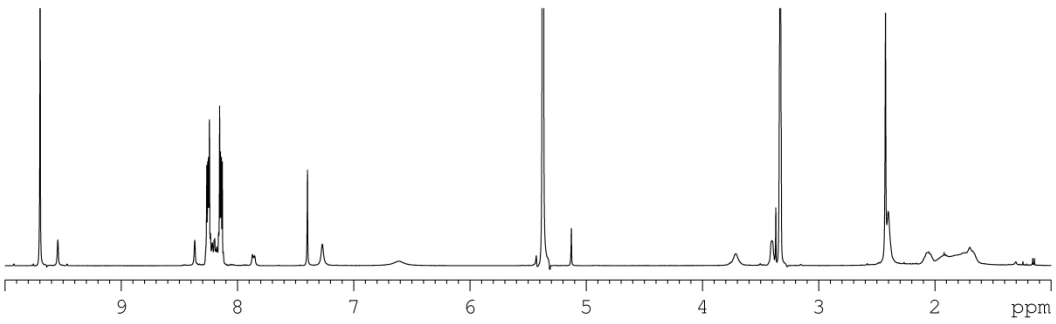
1.35 [Ir(COD)(IMes)(phth)]Cl



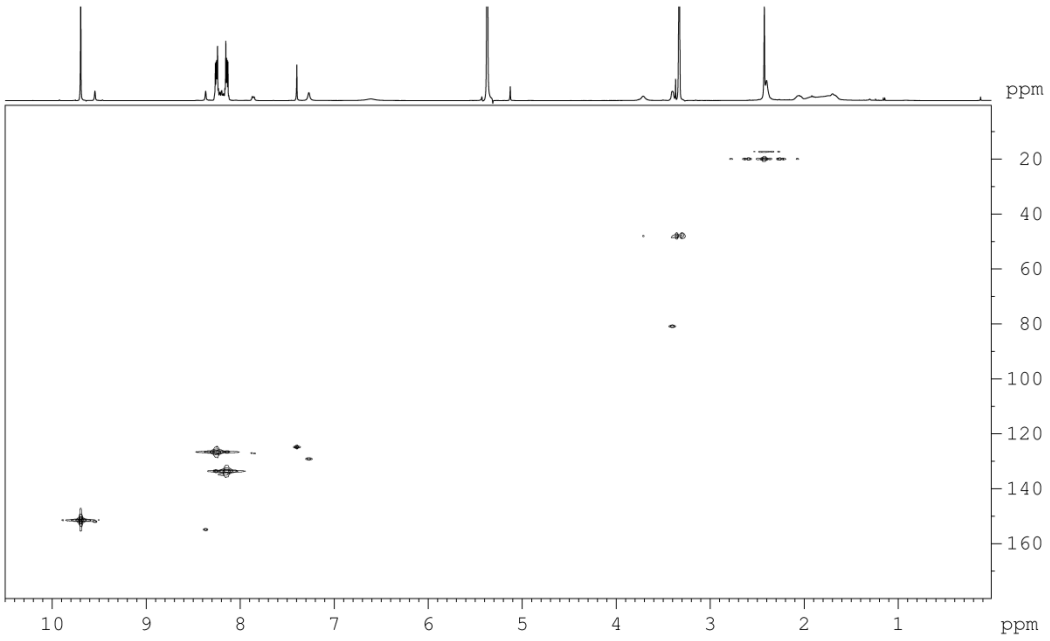
Compound reference kma-2-54

1.35.1 NMR spectra

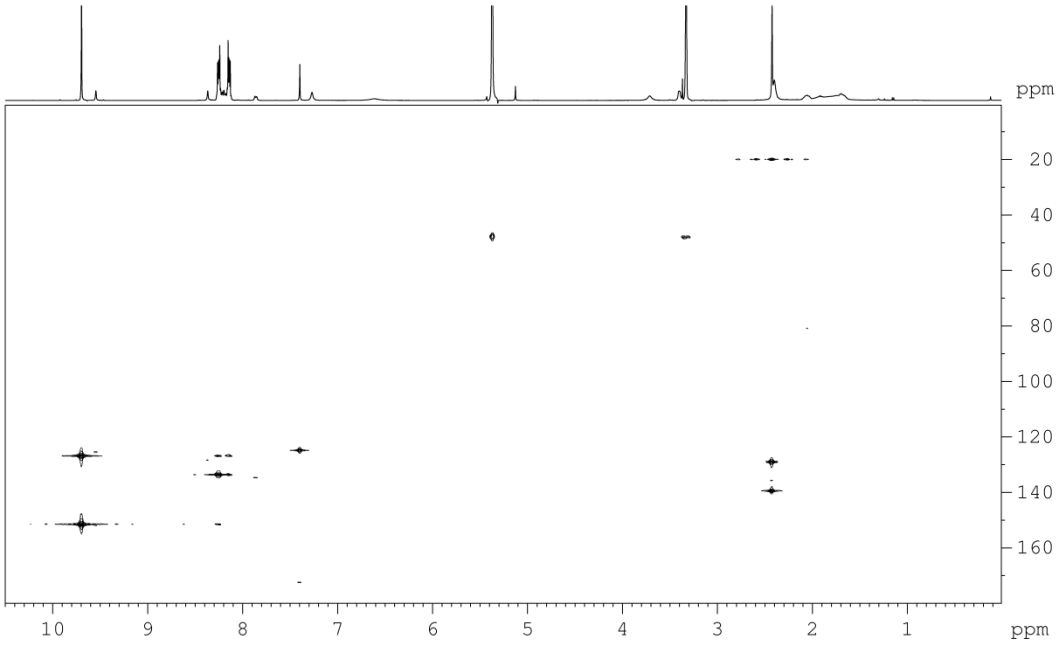
^{1}H



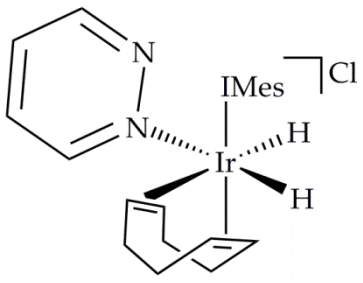
^{13}C-optimised HMQC with a coupling constant of 145 Hz



^{13}C-optimised HMQC with a coupling constant of 12 Hz

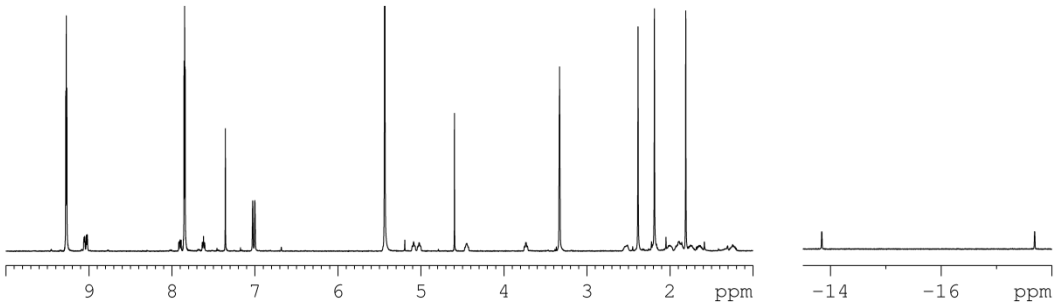


1.36 [Ir(H)$_2$(COD)(IMes)(pdz)]Cl

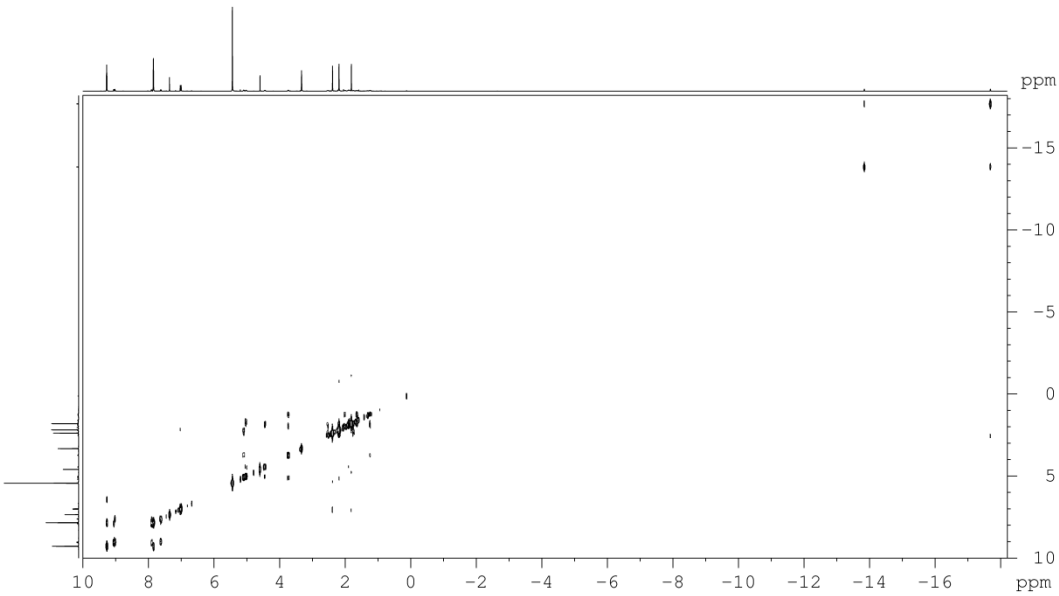


1.36.1NMR spectra

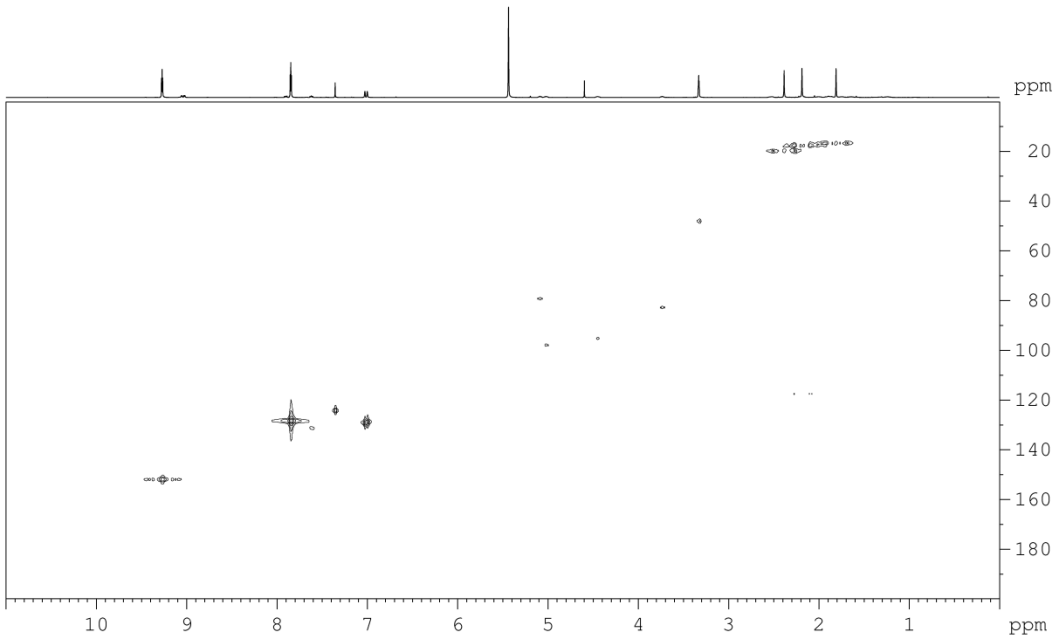
^{1}H



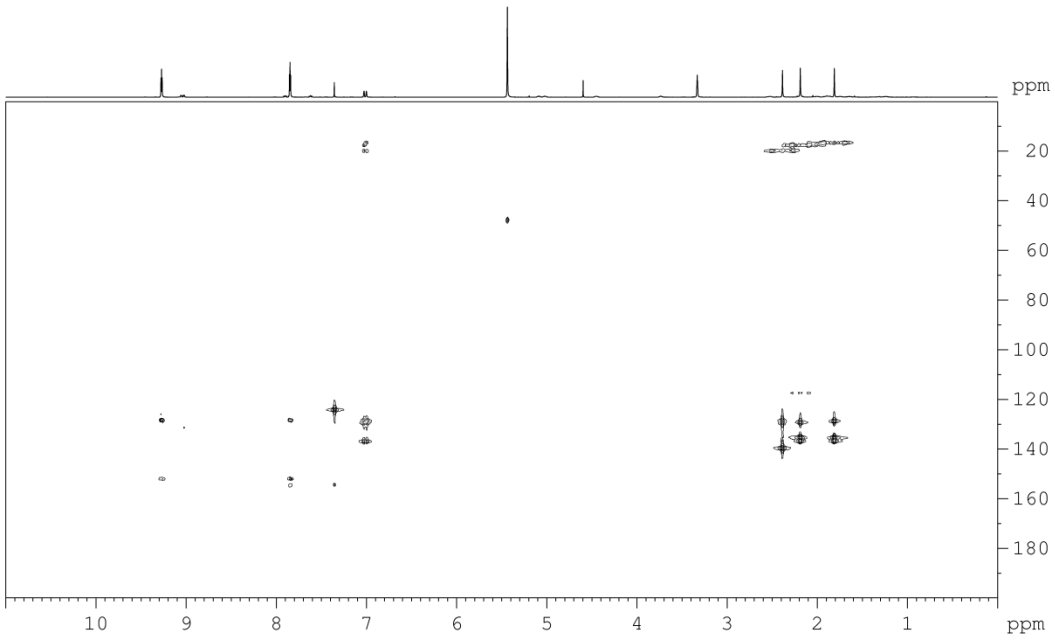
COSY



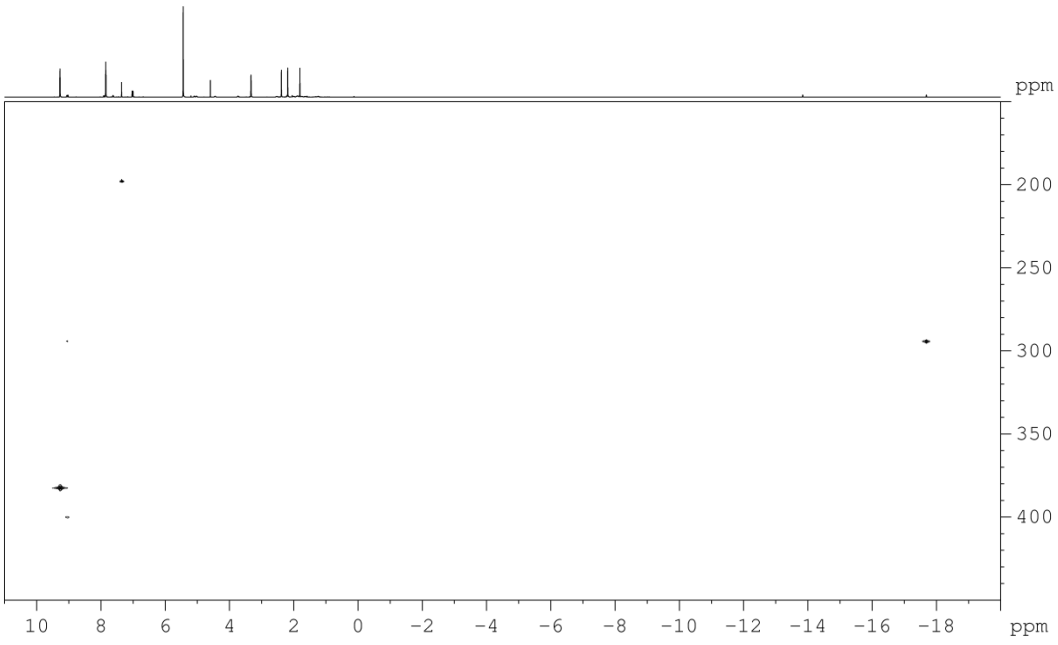
^{13}C-optimised HMQC with a coupling of 145 Hz



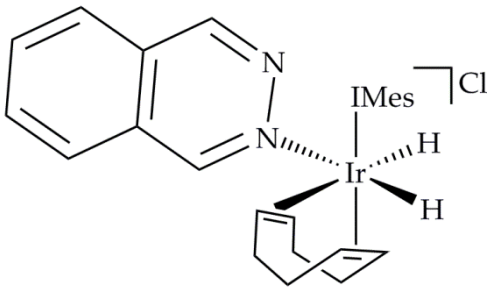
13C-optimised HMQC with a coupling of 12 Hz



^{15}N-optimised HMQC with a coupling of 17 Hz



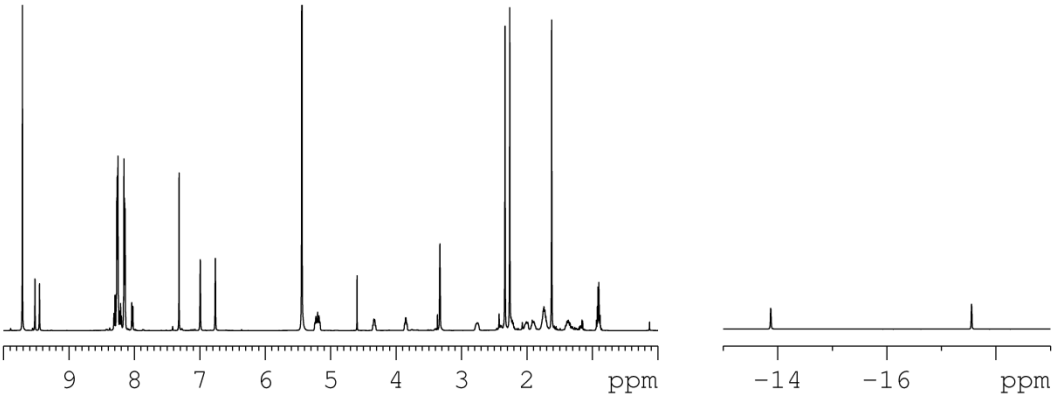
1.37 [Ir(H)$_2$(COD)(IMes)(phth)]Cl



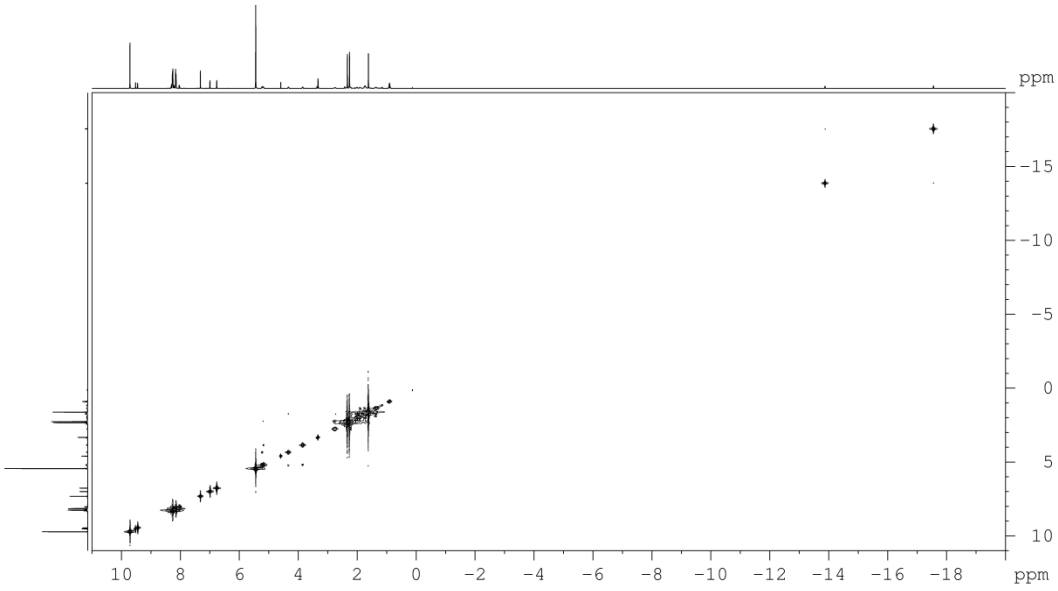
Compound reference kma-2-65

1.37.1NMR spectra

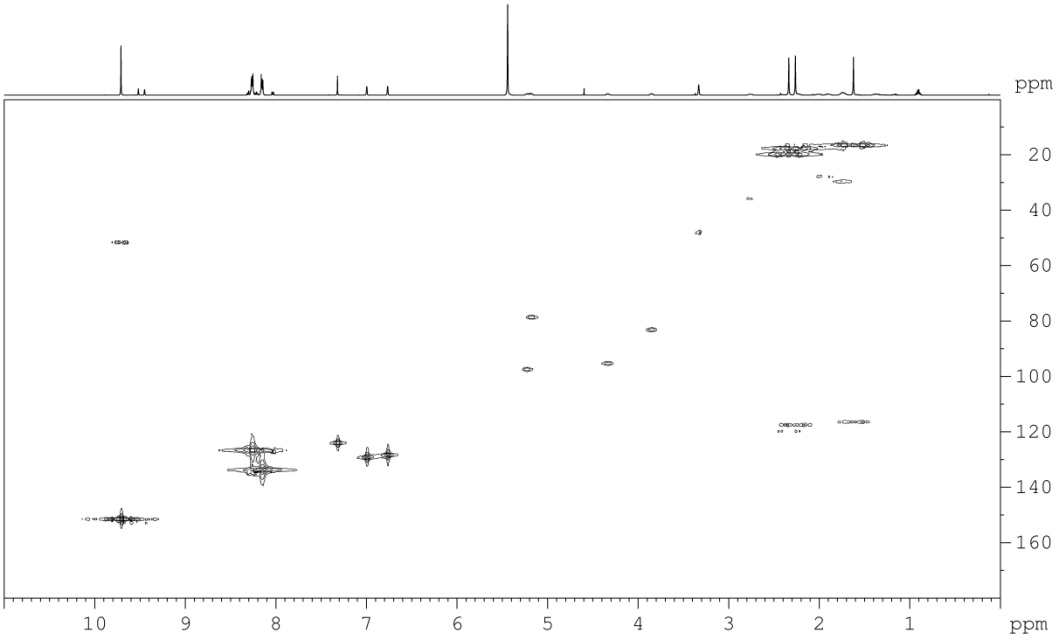
^{1}H



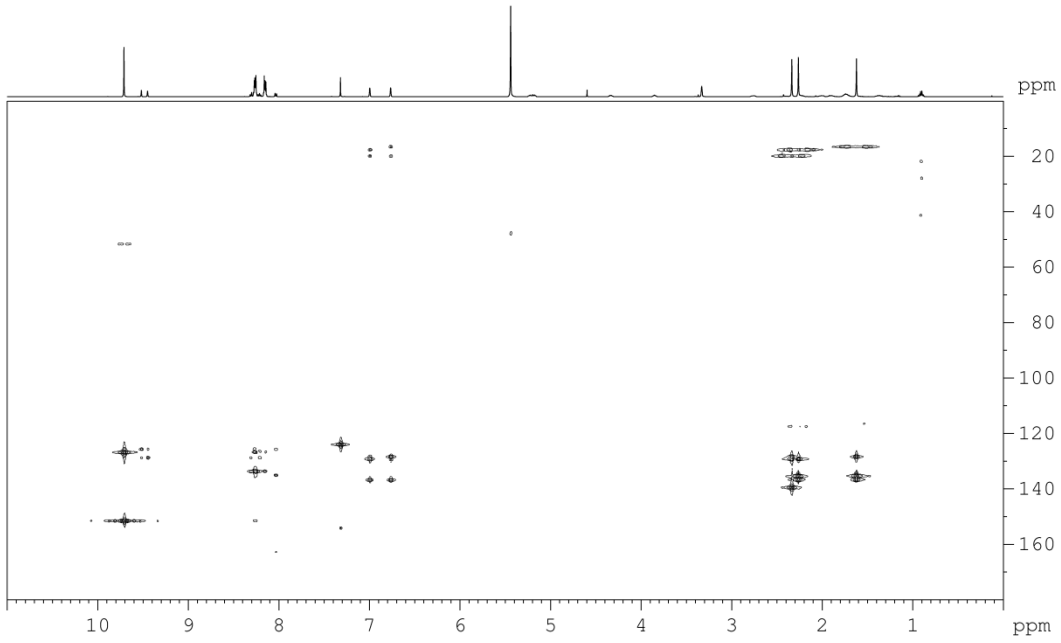
COSY



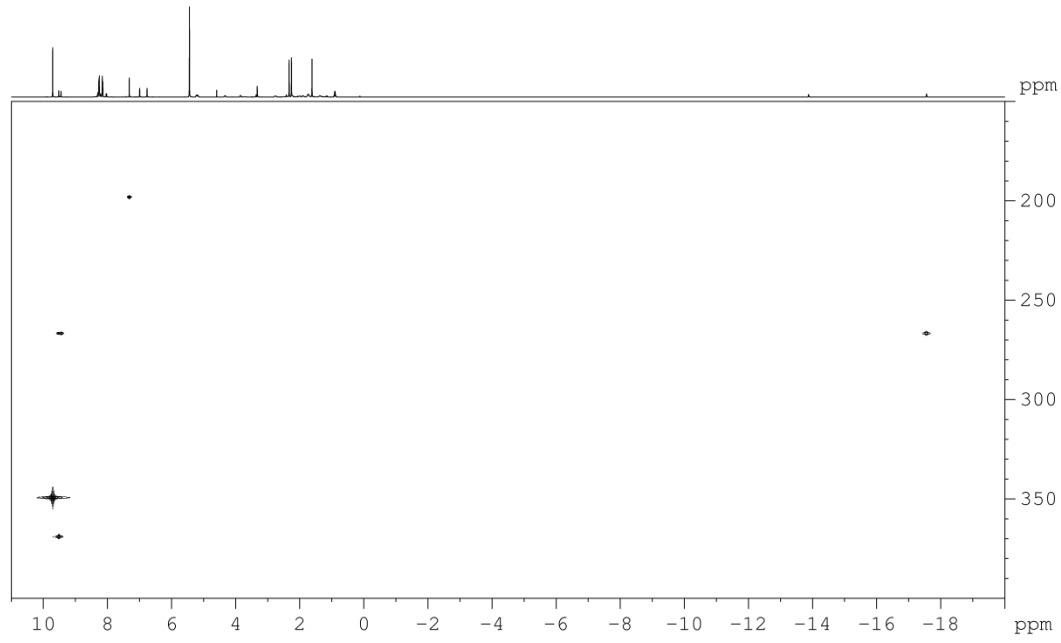
^{13}C-optimised HMQC with a coupling of 145 Hz



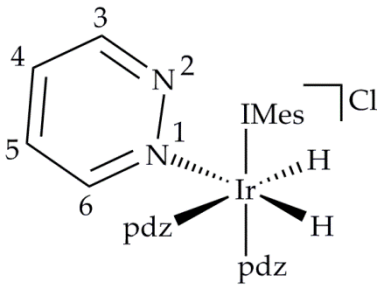
^{13}C-optimised HMQC with a coupling of 12 Hz



^{15}N-optimised HMQC with a coupling of 17 Hz



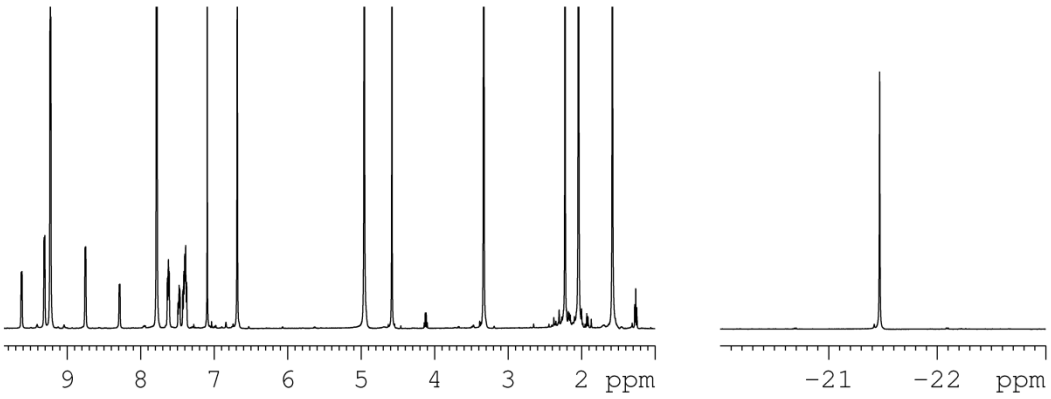
1.38 $[Ir(H)_2(IMes)(pdz)_3]Cl$



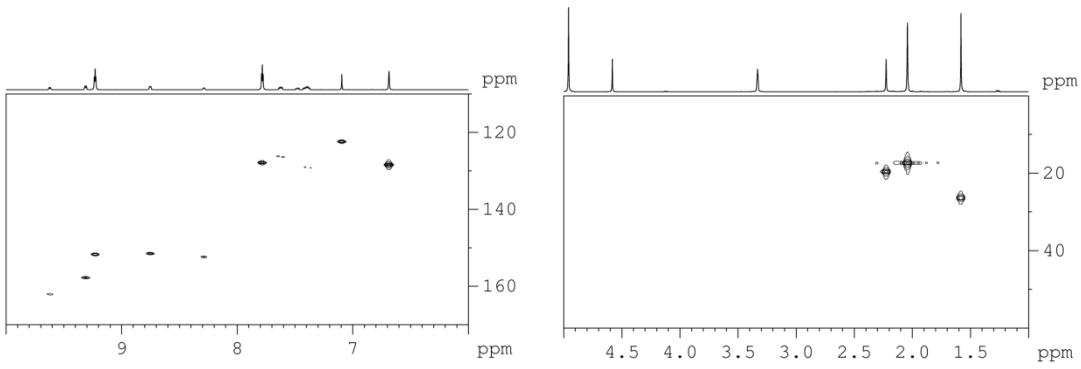
Compound reference kma-1-56

1.38.1 NMR spectra

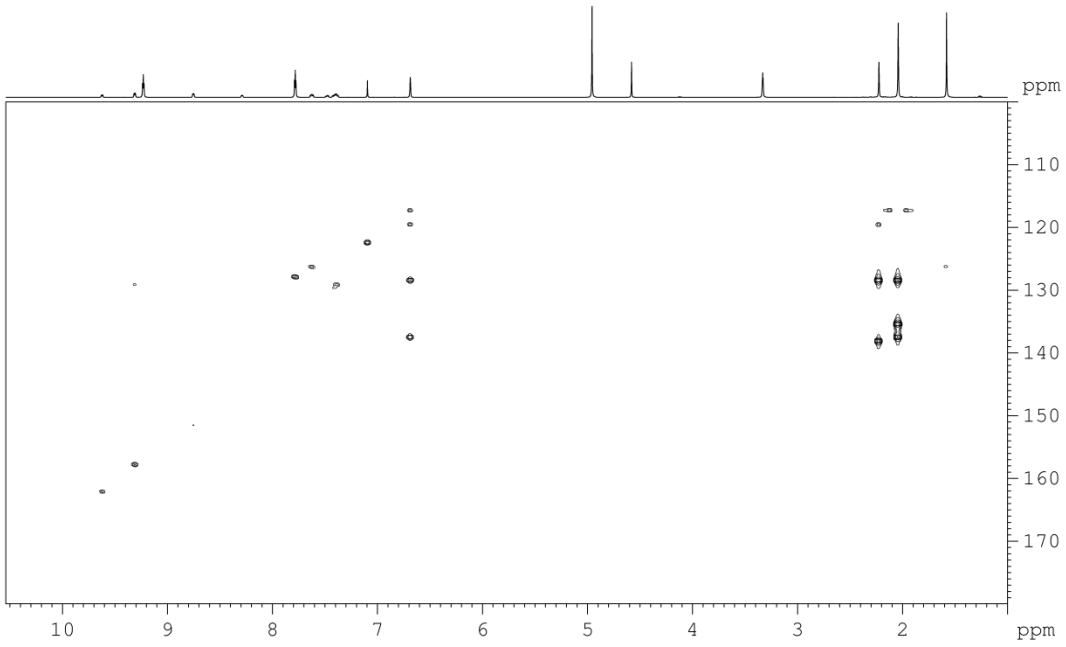
^{1}H



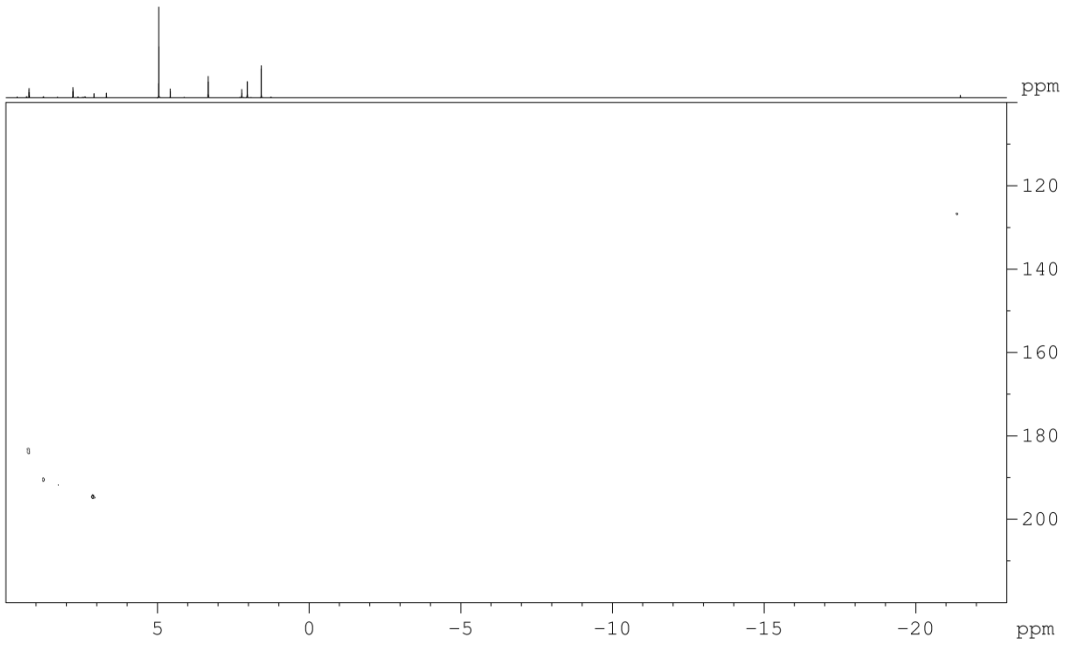
^{13}C-optimised HMQC with a coupling of 145 Hz



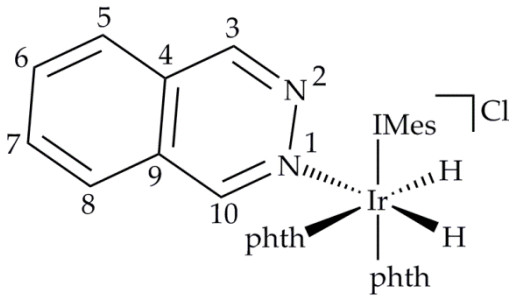
^{13}C-optimised HMQC with a coupling of 12 Hz



^{15}N-optimised HMQC with a coupling of 17 Hz



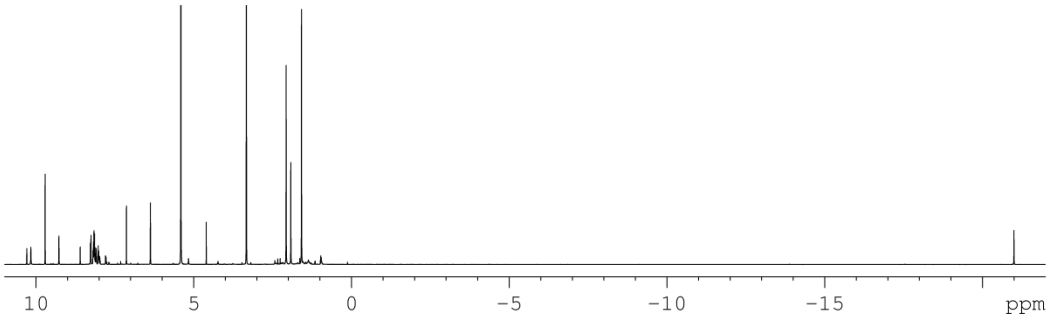
1.39 $[Ir(H)_2(IMes)(phth)_3]Cl$



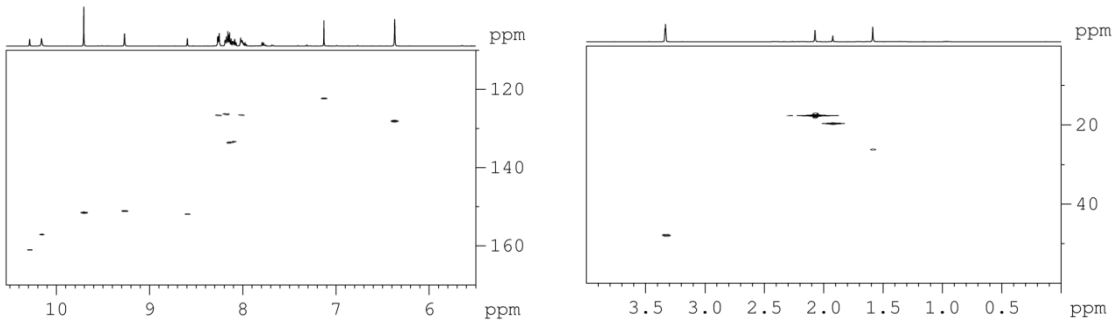
Compound reference kma-1-26

1.39.1 NMR spectra

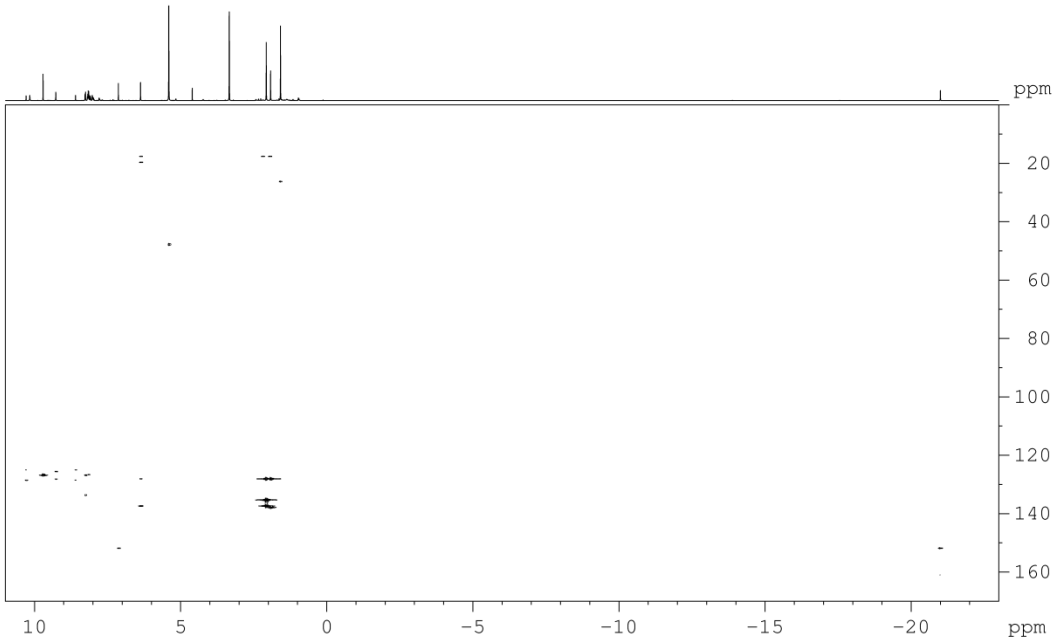
^{1}H



^{13}C-optimised HMQC with a coupling of 145 Hz



^{13}C-optimised HMQC with a coupling of 12 Hz



^{15}N-optimised HMQC with a coupling of 17 Hz