Supplementary Material

Bidentate [C,N] Schiff base ligand palladacycles: Synthesis, X-ray diffractometric analysis and survey of their catalytic activity

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Table 1 SI. bond lengths (Å) and angles (◦) for compounds **3a** and **4b**

Compound 3a		Compound 4b	
Bond lengths		Bond lengths	
Pd(1)-N(1)	2.118(6)	Pd(1)-N(1)	2.115(4)
Pd(1)-C(1)	2.023(8)	Pd(1)-C(1)	2.034(5)
Pd(1)-P(1)	2.260(2)	Pd(1)-P(1)	2.245(12)
Pd(1)-Cl(1)	2.364(18)	Pd(1)-P(2)	2.376(12)
Pd(2)-N(2)	2.110(6)	Pd(2)-N(2)	2.125(4)
Pd(2)-C(2)	2.017(7)	Pd(2)-C(2)	2.036(4)
Pd(2)-P(2)	2.264(19)	Pd(2)-P(3)	2.388(13)
Pd(2)-Cl(2)	2.366(19)	Pd(2)-P(4)	2.240(12)
Bond angles			
N(1)-Pd(1)-P(1)	176.50(18)	N(1)-Pd(1)-P(1)	177.90(12)
C(1)-Pd(1)-N(1)	81.9(3)	C(1)-Pd(1)-N(1)	81.25(3)
P(1)-Pd(1)-Cl(1)	90.32(7)	P(1)-Pd(1)-P(2)	78.78(4)
Cl(1)-Pd(1)-N(1)	93.11(17)	C(1)-Pd(1)-P(2)	167.85(13)
P(1)-Pd(1)-C(1)	94.7(2)	P(2)-Pd(1)-N(1)	109.34(12)
C(1)-Pd(1)-Cl(1)	171.5(2)	P(1)-Pd(1)-C(1)	97.83(14)
C(2)-Pd(2)-N(2)	81.5(3)	C(2)-Pd(2)-P(4)	97.06(12)
P(2)-Pd(2)-Cl(2)	91.97(7)	C(2)-Pd(2)-N(2)	81.08(17)
N(2)-Pd(2)-P(2)	173.17(17)	P(3)-Pd(2)-P(4)	71.89(4)
C(2)-Pd(2)-Cl(2)	170.20(2)	N(2)-Pd(2)-P(3)	110.24(12)
N(2)-Pd(2)-Cl(2)	91.83(2)	N(2)-Pd(2)-P(4)	173.97(15)
P(2)-Pd(2)-C(2)	95.4(2)	C(2)-Pd(2)-P(3)	168.43(12)

Table 2 SI. Secondary interaction lengths (Å) and angles (◦) for compounds **3a** and **4b**

D–H···A	D–H	H···A	D···A	<D–H···A
Compound (3a)				
C16–H16···F1[a]	0.95	2.447	2.873	108.58
C50–H50···F2[b]	0.95	2.550	3.139	121.28
C61–H61···Cl1[a]	0.95	2.847	3.510	128.01
C17–H17···Cl2[a]	0.95	2.886	3.577	129.11
Compound (4b)[c]				
C11–H11a···O1	0.99	2.619	3.490	146.14
C49–H49a···O2	0.99	2.615	3.517	150.94

Compound 3a. Symmetry code: (#)[a] x,1+y,z; (#)[b] 1.5-x,-1/2+y,1/2-z. Compound 4b. Symmtery code:(#)[c] -1+x,y,z.

Table 3 SI.- Crystal data and structure refinement for compound **3a.**

Identification code	compound 3a
Empirical formula	$C_{31}H_{30}ClFN_1PPd$
Formula weight	608.430
Temperature/K	100.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	25.2382(19)
b/Å	9.3553(8)
c/Å	25.294(2)
α/°	90
β/°	95.345(2)
γ/°	90
Volume/Å^3	5946.2(8)
Z	8
ρ_{calc}g/cm^3	1.362
μ/mm^{-1}	0.793
F(000)	2479.3
Crystal size/mm^3	0.14 × 0.04 × 0.02
Radiation	Mo Kα (λ = 0.71073)
θ range for data collection/°	4.36 to 53.36
Index ranges	-31 ≤ h ≤ 31, -11 ≤ k ≤ 11, -31 ≤ l ≤ 31
Reflections collected	257548
Independent reflections	12382 [R_{int} = 0.1679, R_{sigma} = 0.0581]
Data/restraints/parameters	12382/0/656
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.1041, wR_2 = 0.2718
Final R indexes [all data]	R_1 = 0.1166, wR_2 = 0.2811
Largest diff. peak/hole / e Å^{-3}	2.58/-1.28

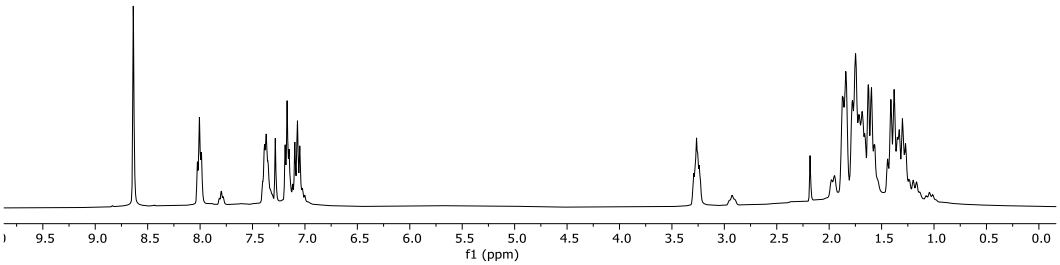
Table 4 SI.- Crystal data and structure refinement for compound **4b**

Identification code	compound 4b
Empirical formula	$C_{39}H_{40}F_6NOP_3Pd.\ 2(CH_2Cl_2)$
Formula weight	852.09
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
a/Å	12.0121(8)
b/Å	18.4207(14)
c/Å	21.3521(16)
α/°	107.573(2)
β/°	104.718(2)
γ/°	103.530(2)
Volume/Å^3	4101.6(5)
Z	4
ρ_{calc}g/cm^3	1.517
μ/mm^{-1}	0.760
F(000)	1904.0
Crystal size/mm^3	0.23 × 0.04 × 0.03
Radiation	MoKα (λ = 0.71073)
θ range for data collection/°	3.83 to 52.746
Index ranges	-15 ≤ h ≤ 15, -23 ≤ k ≤ 23, -26 ≤ l ≤ 26
Reflections collected	151568
Independent reflections	16747 [R_{int} = 0.0685, R_{sigma} = 0.0386]
Data/restraints/parameters	16747/0/946
Goodness-of-fit on F^2	1.123
Final R indexes [I>=2σ (I)]	R_1 = 0.0603, wR_2 = 0.1216
Final R indexes [all data]	R_1 = 0.0730, wR_2 = 0.1270
Largest diff. peak/hole / e Å^{-3}	1.25/-1.13

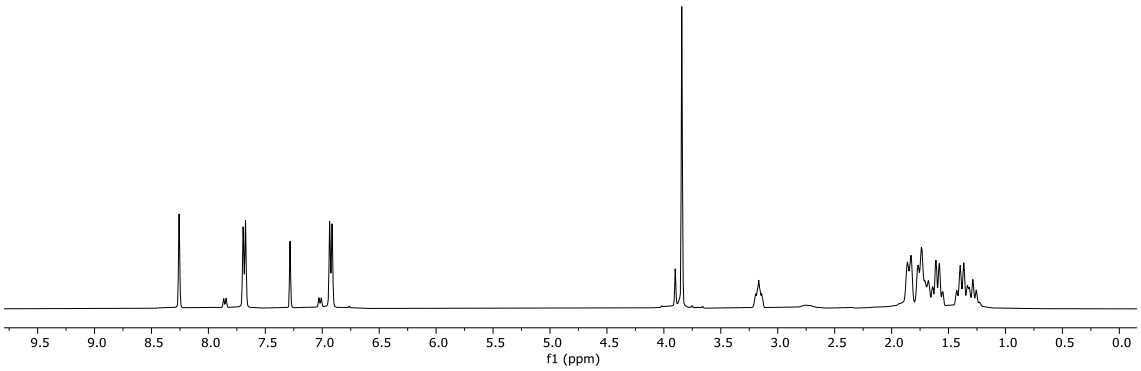
CCDC Identification numbers.

CCDC 2201142 for compound **3a**. CCDC 2201143 for compound **4b**.

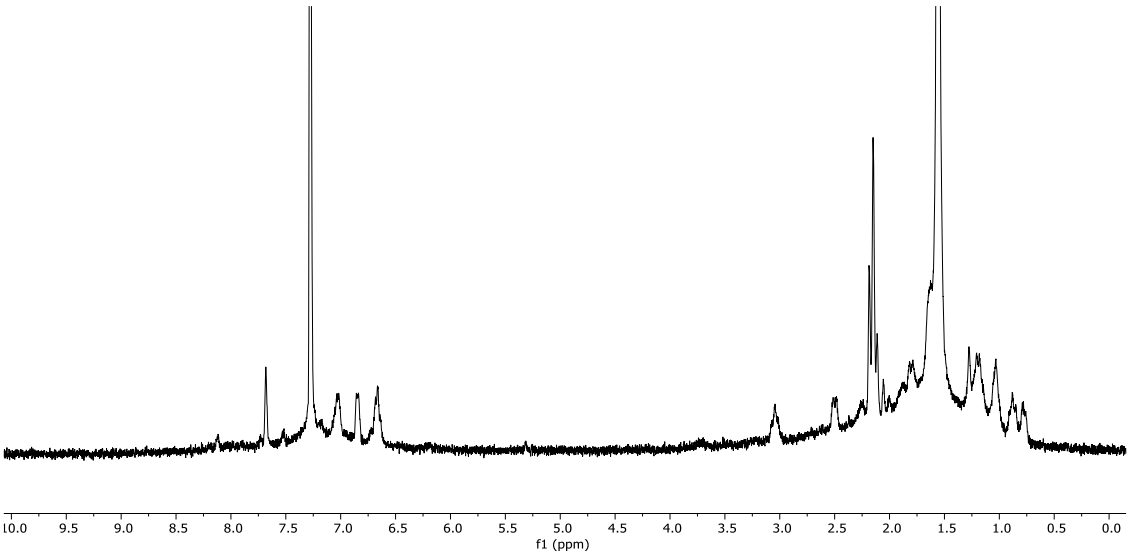
NMR SPECTRA



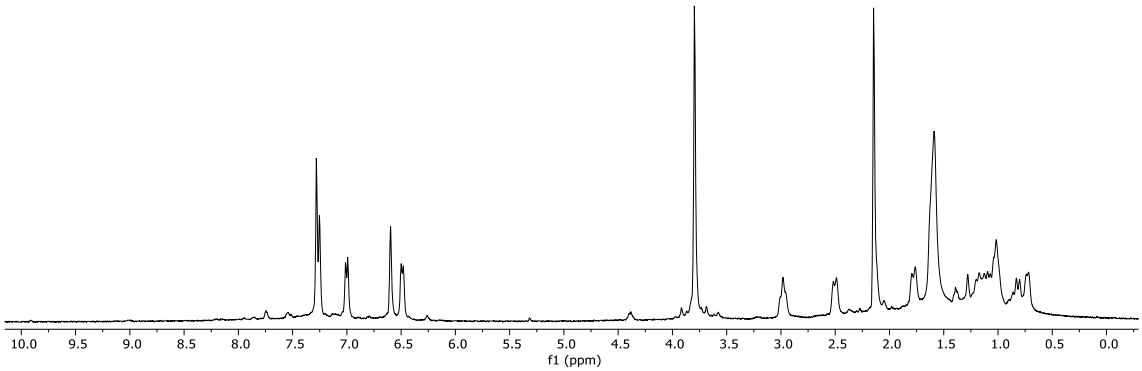
^{1}H-NMR spectrum in $CDCl_3$ of compound **a**



^{1}H-NMR spectrum in $CDCl_3$ of compound **b**



^{1}H-NMR spectrum in $CDCl_3$ of compound **1a**



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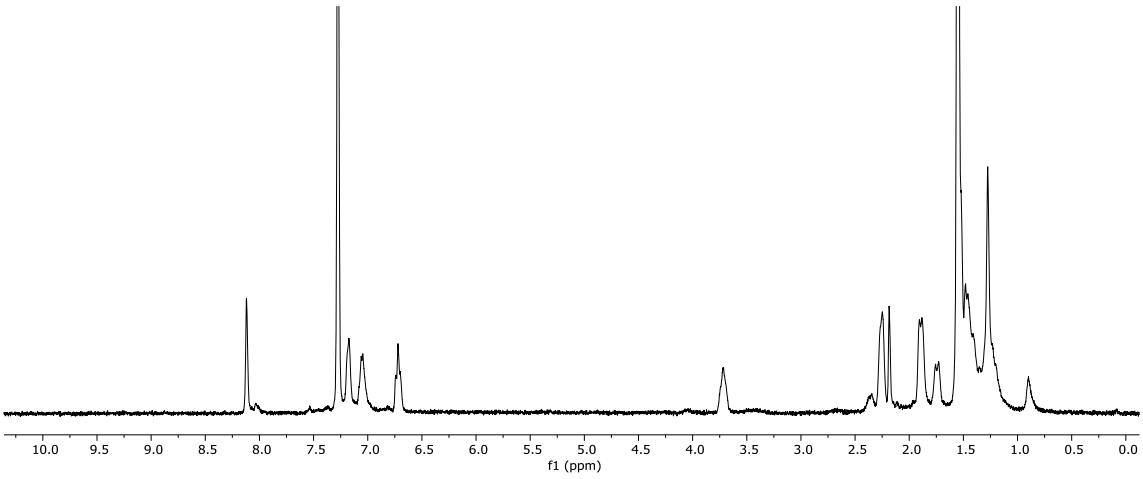
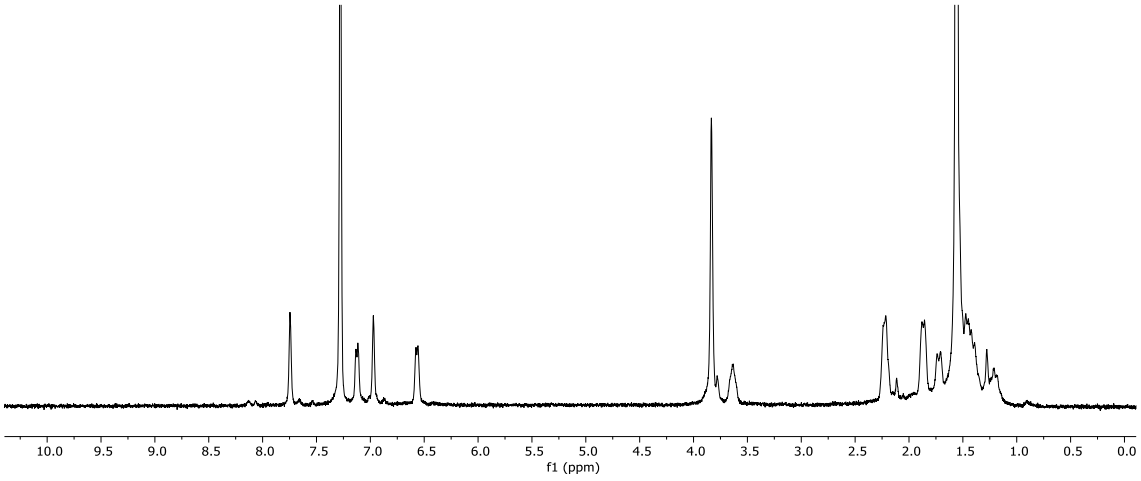
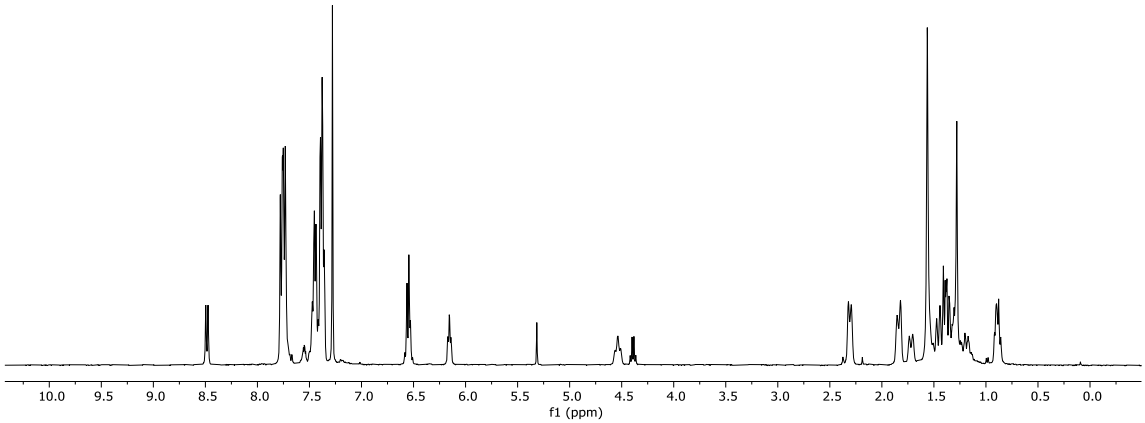


^{1}H-NMR spectrum in $CDCl_3$ of compound **2a**



^{1}H-NMR spectrum in $CDCl_3$ of compound **2b**



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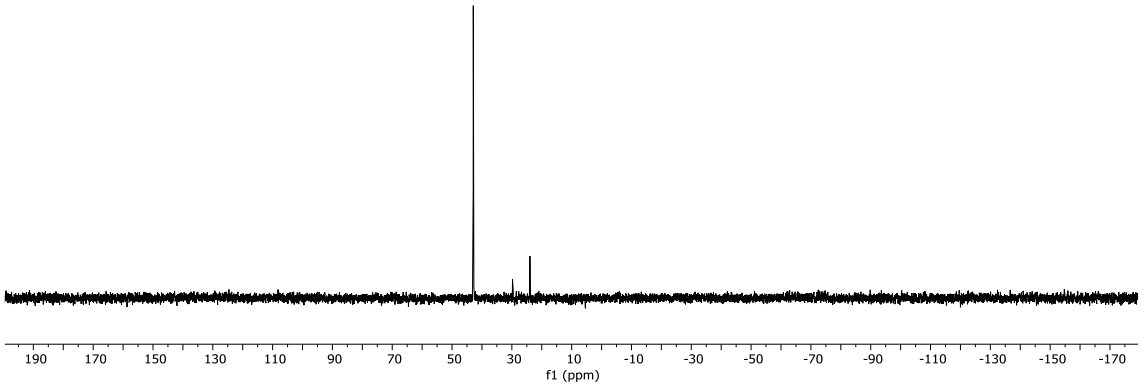
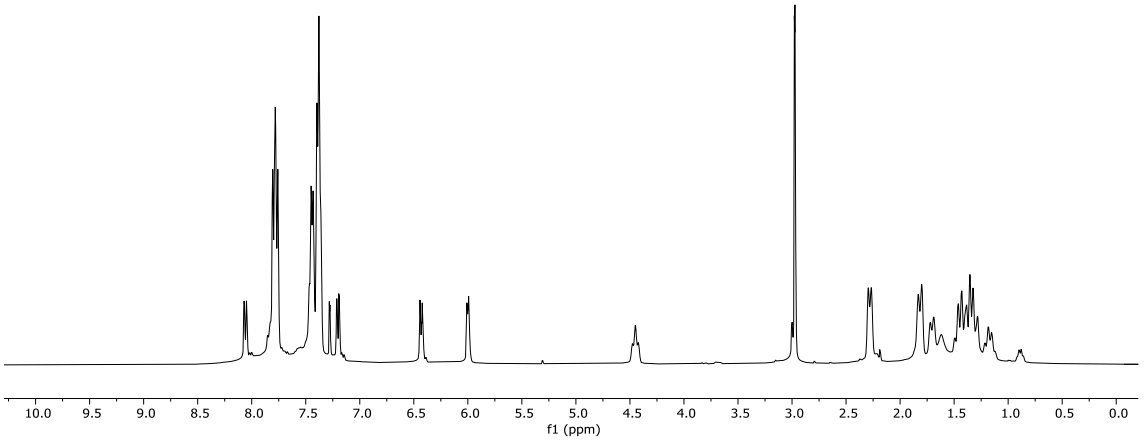


^{31}P-{^{1}H} NMR spectrum in $CDCl_3$ of compound **3a**



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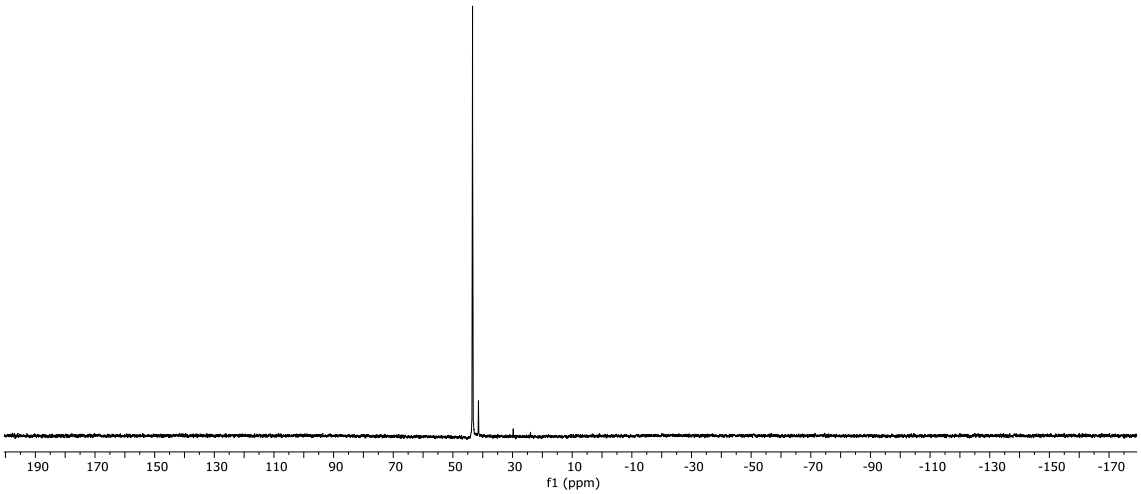
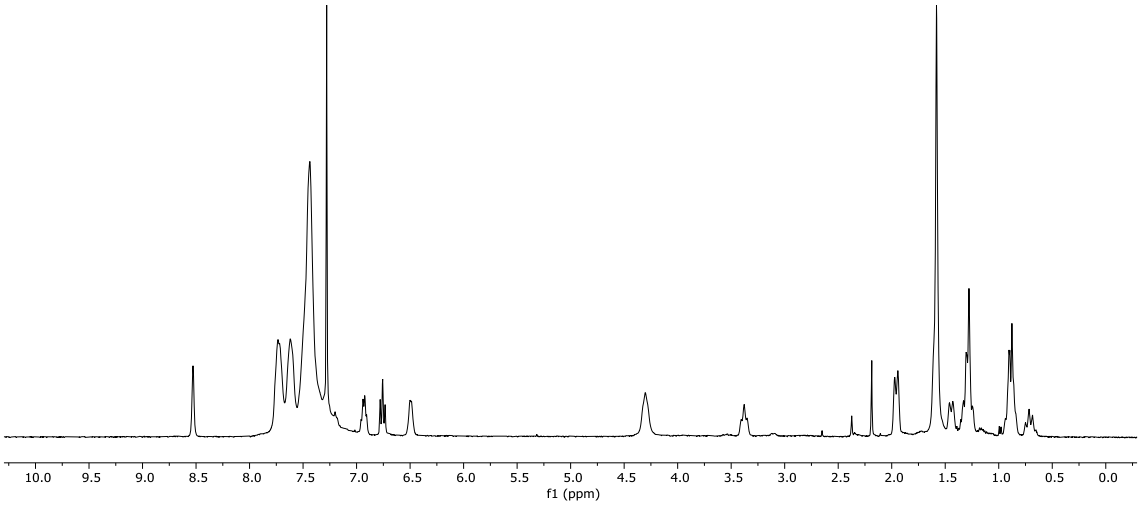
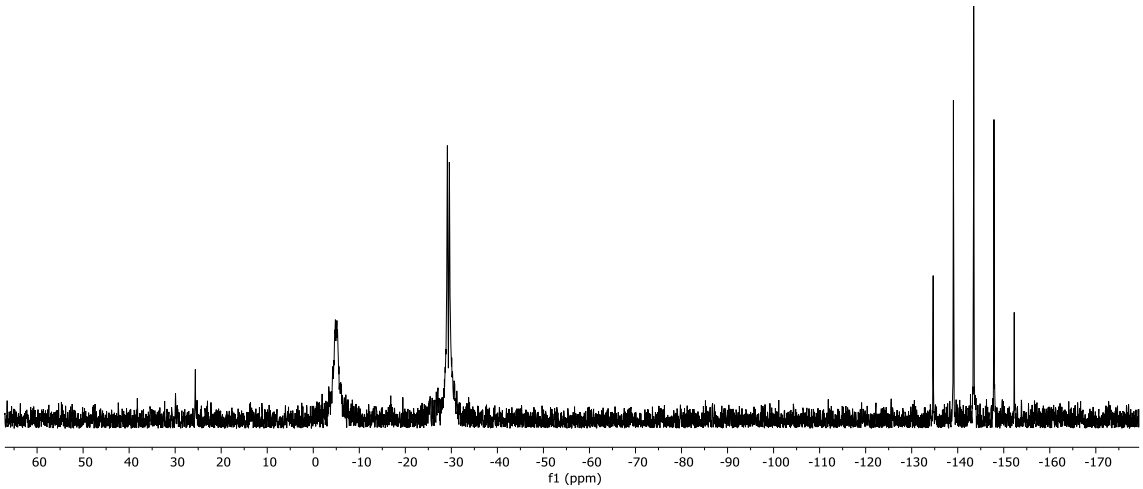


^{31}P-{^{1}H} NMR spectrum in $CDCl_3$ of compound **3b**

^{1}H-NMR spectrum in $CDCl_3$ of compound **4a**



^{1}H-NMR spectrum in $CDCl_3$ of compound **4a**



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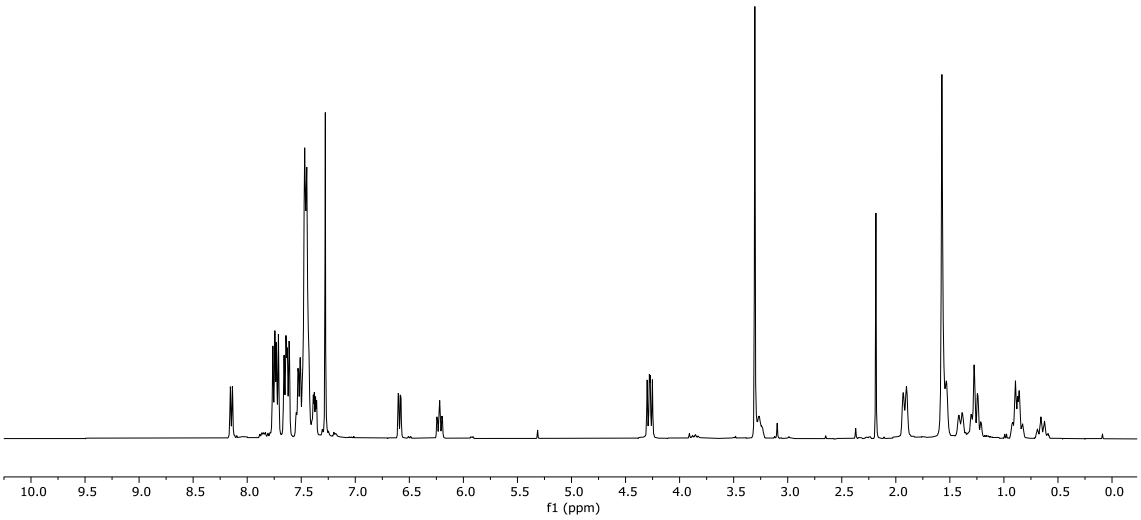
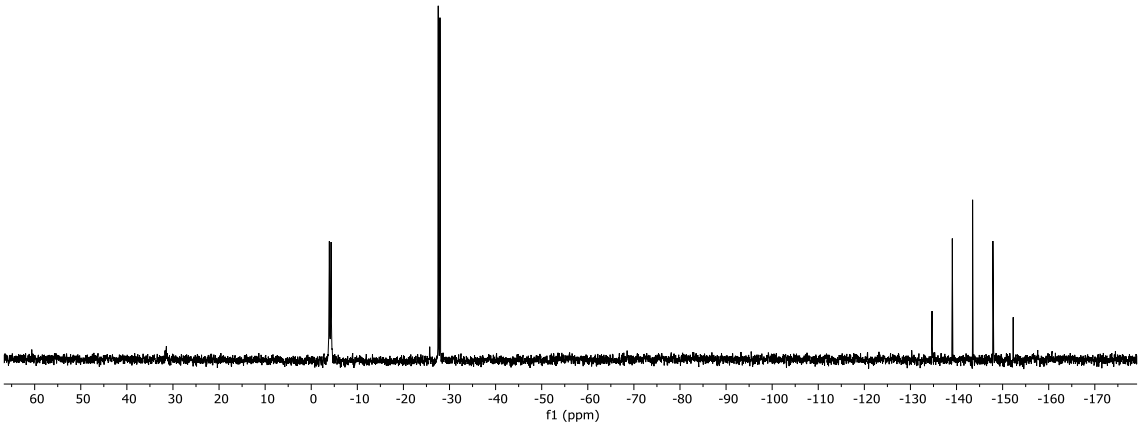


^{1}H-NMR spectrum in $CDCl_3$ of compound **4b**



^{31}P-{^{1}H} NMR spectrum in $CDCl_3$ of compound **4b**

