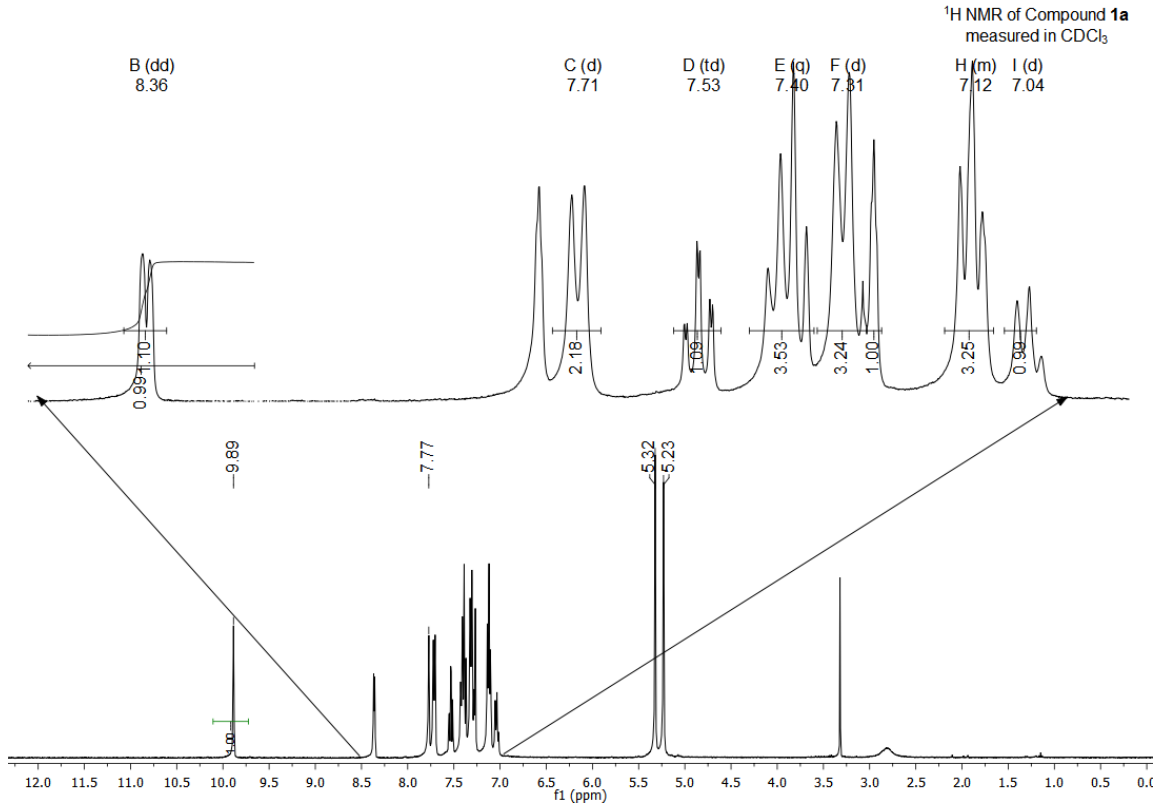
Electronic Supplementary Information (ESI)

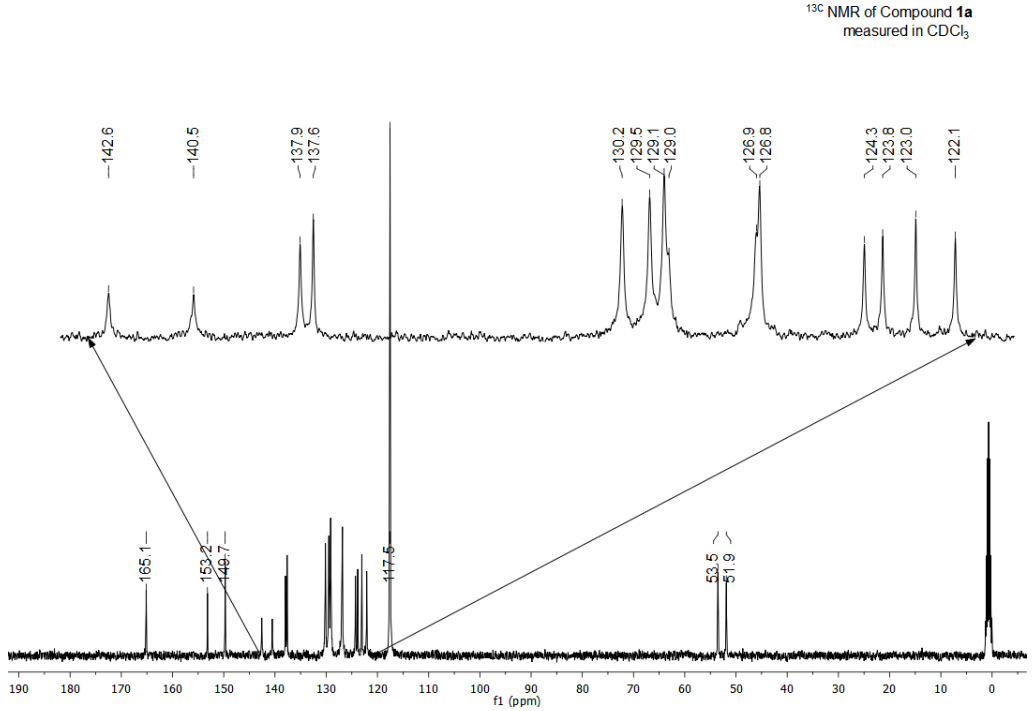
Table **S1**. Structural data and refinement parameters of (**4a**) and (**3b**).

	4a·$(PF_6)_2$	**3b**·$(PF_6)_2$·CH_2Cl_2
Formula	$C_{47}H_{44}F_{12}N_7OP_3Ru$	$C_{40}H_{39}F_{12}N_6OP_3Ru$
Formula weight	1144.87	1112.65
T (K)	223(2)	296(2)
Crystal size [mm]	0.34 × 0.32 × 0.15	0.42 × 0.38 × 0.31
Crystal system	Triclinic	Orthorhombic
Space group, (Z)	P-1, (2)	P2(1)2(1)2(1), (4)
a (Å)	12.1842(6)	11.6726(7)
b (Å)	13.2317(8)	18.6442(11)
c (Å)	16.7148(8)	21.5813(13)
α (°)	84.6250(10)	90.00
β (°)	76.0910(10)	90.00
γ (°)	71.8680(10)	90.00
V (Å^3)	2485.3(2)	4696.7(5)
λ (Å)	0.71073	0.71073
Dcalc (mg/m^3)	1.530	1.574
Abs coeff (mm^{-1})	0.501	0.637
θ min, max	1.26, 26.50	1.44, 25.04
Reflections number, total/unique	18346/ 10220 [R_{int}=0.0252]	13978 / 8260 [R_{int} = 0.0367]
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	10220 / 0 / 643	8260 / 0 / 586
Goodness-of-fit on F^2	1.056	1.031
Final R [I > 2σ(I)]	R_1 = 0.0491, wR^2 = 0.1378	R_1 = 0.0519, wR^2 = 0.1251
R indices (all data)	R_1 = 0.0603, wR^2 = 0.1493	R_1 = 0.0818, wR^2 = 0.1444
Largest diff. peak and hole (e.A^{-3})	1.238 and –0.723	0.742 and –0.512

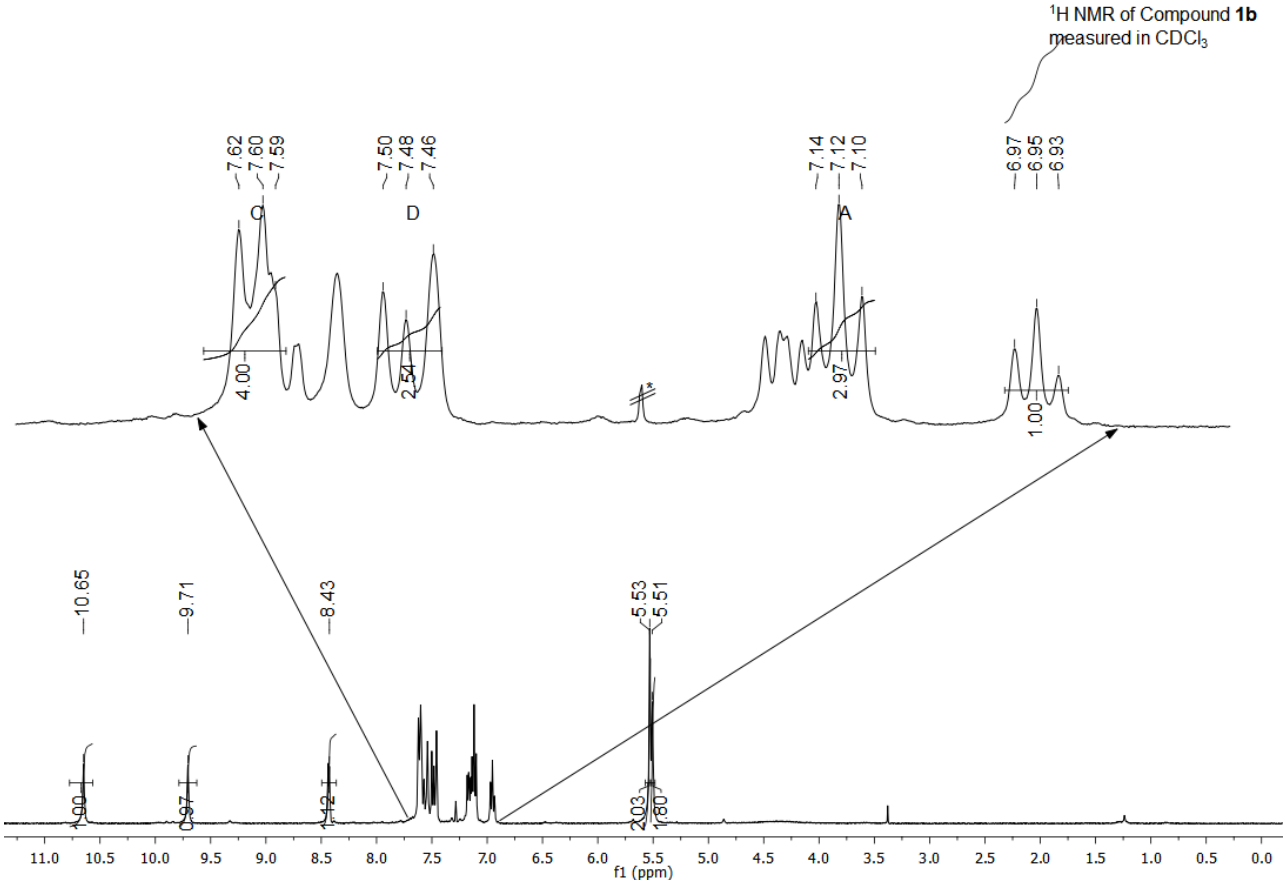
NMR Spectra of compounds reported

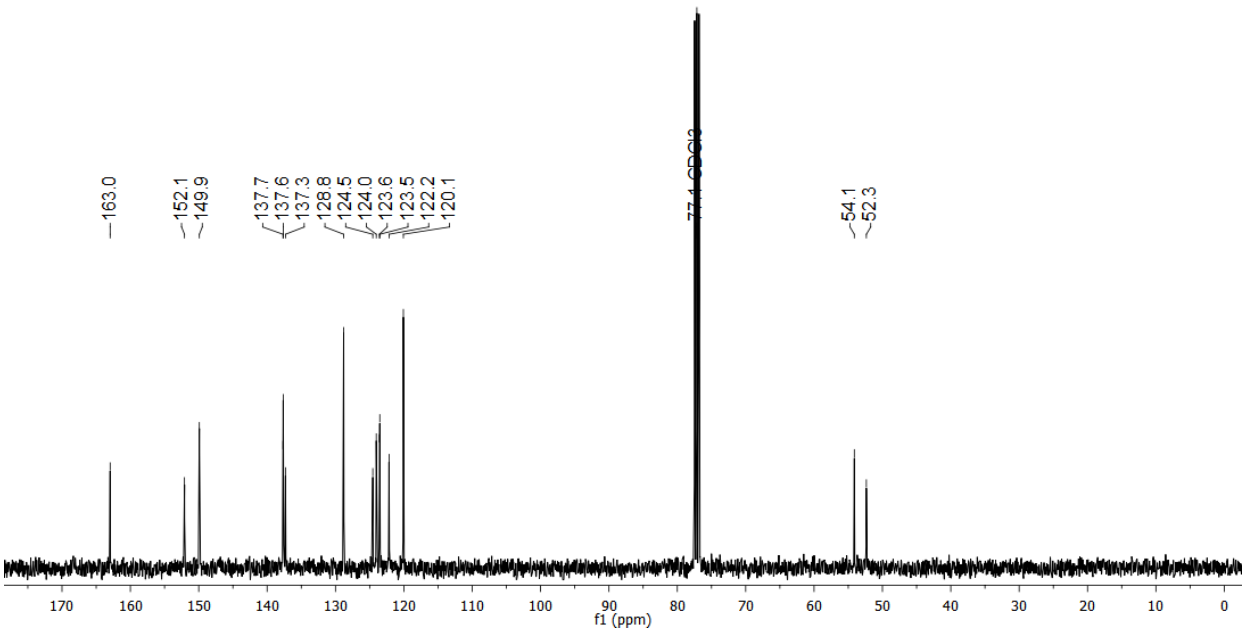
Compound 1a.





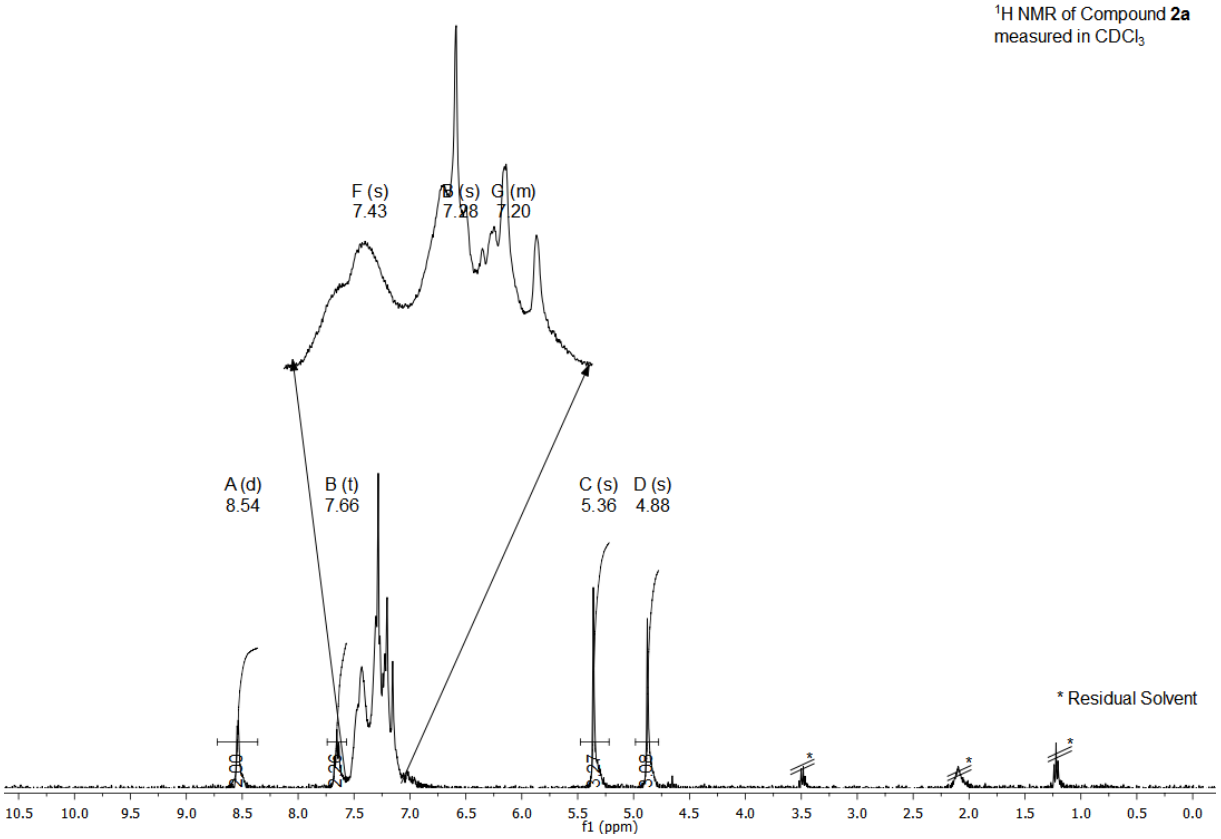
Compound 1b.



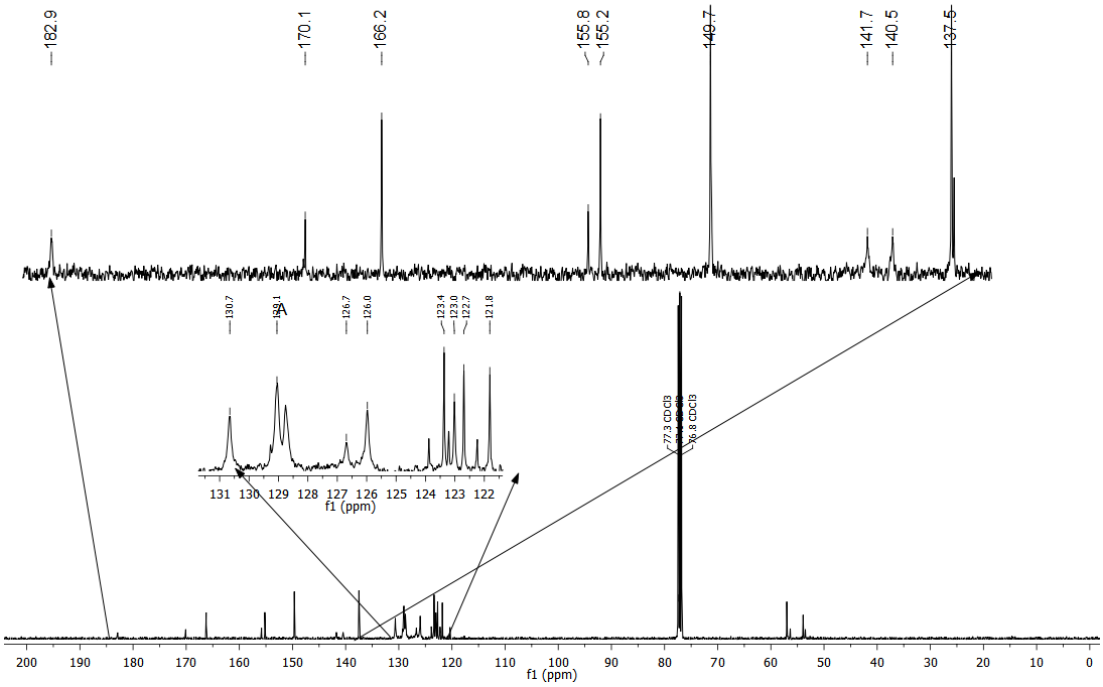


Compound 2a.

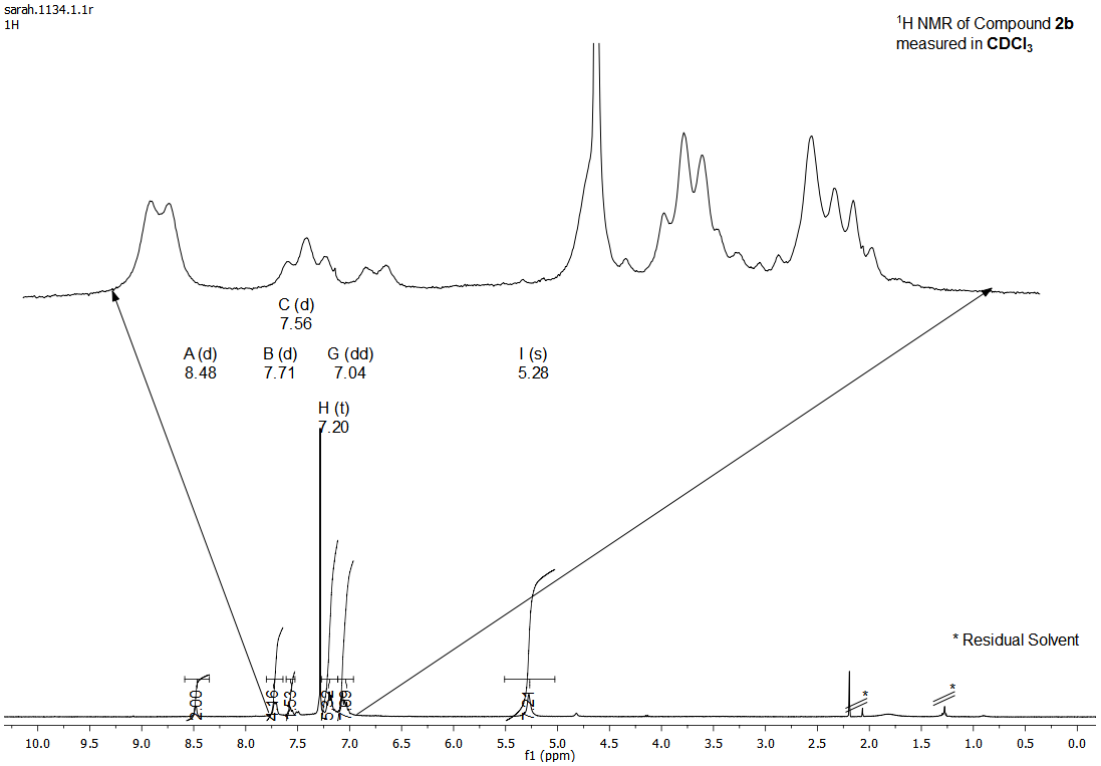
^{1}H NMR of Compound **2a** measured in $CDCl_3$

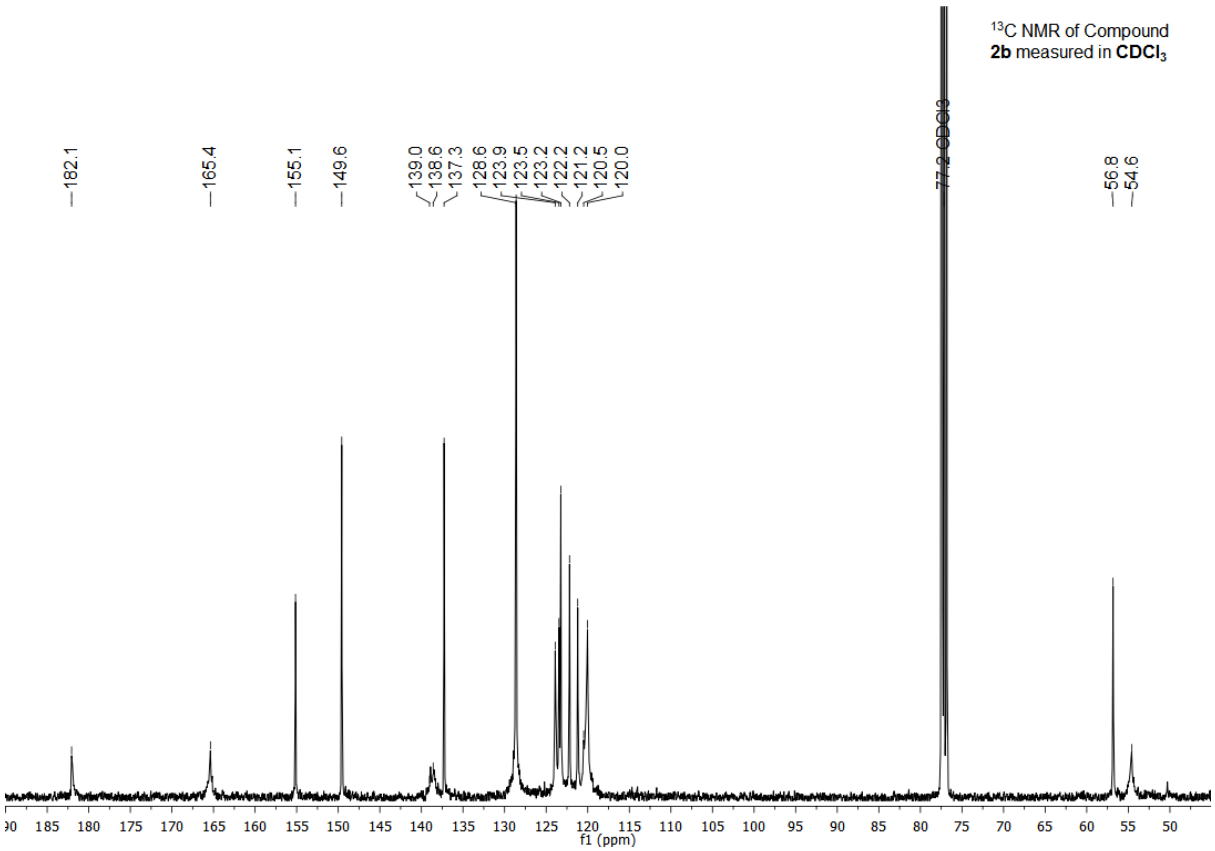


^{13}C NMR of Compound **2a** measured in **$CDCl_3$**

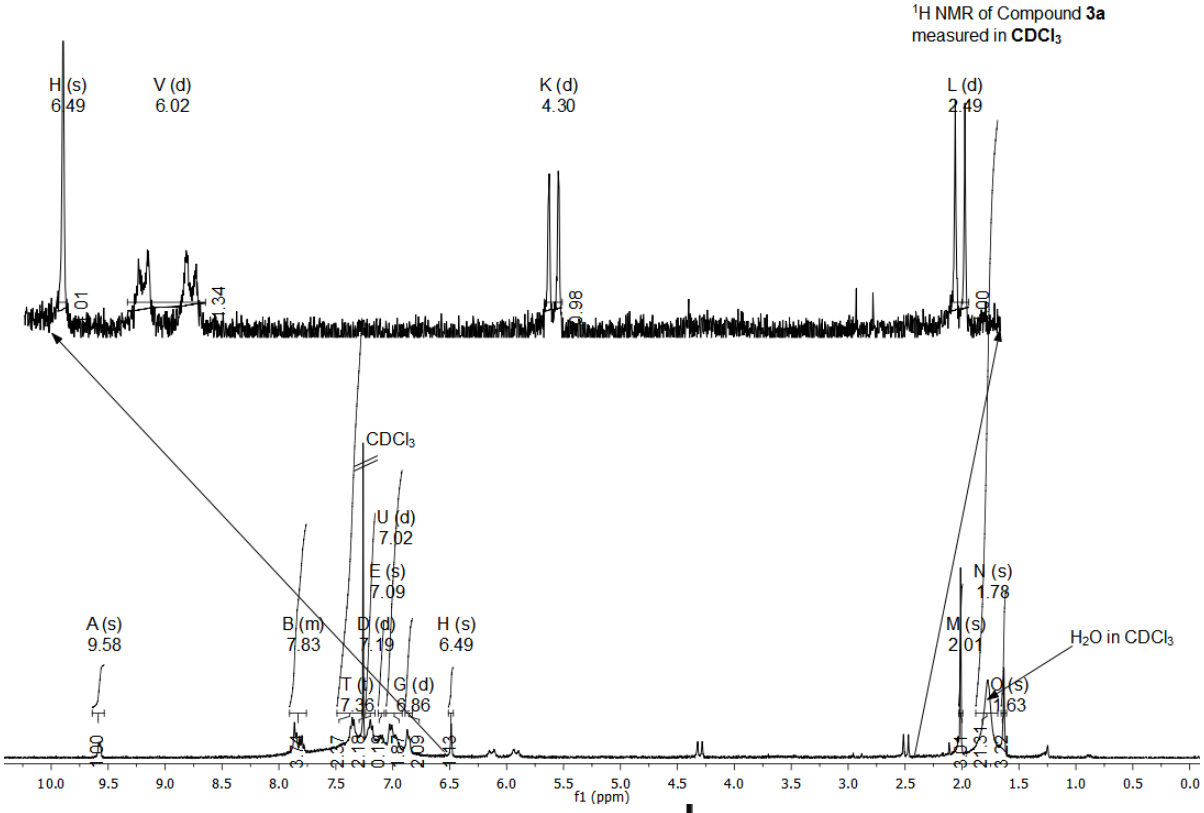


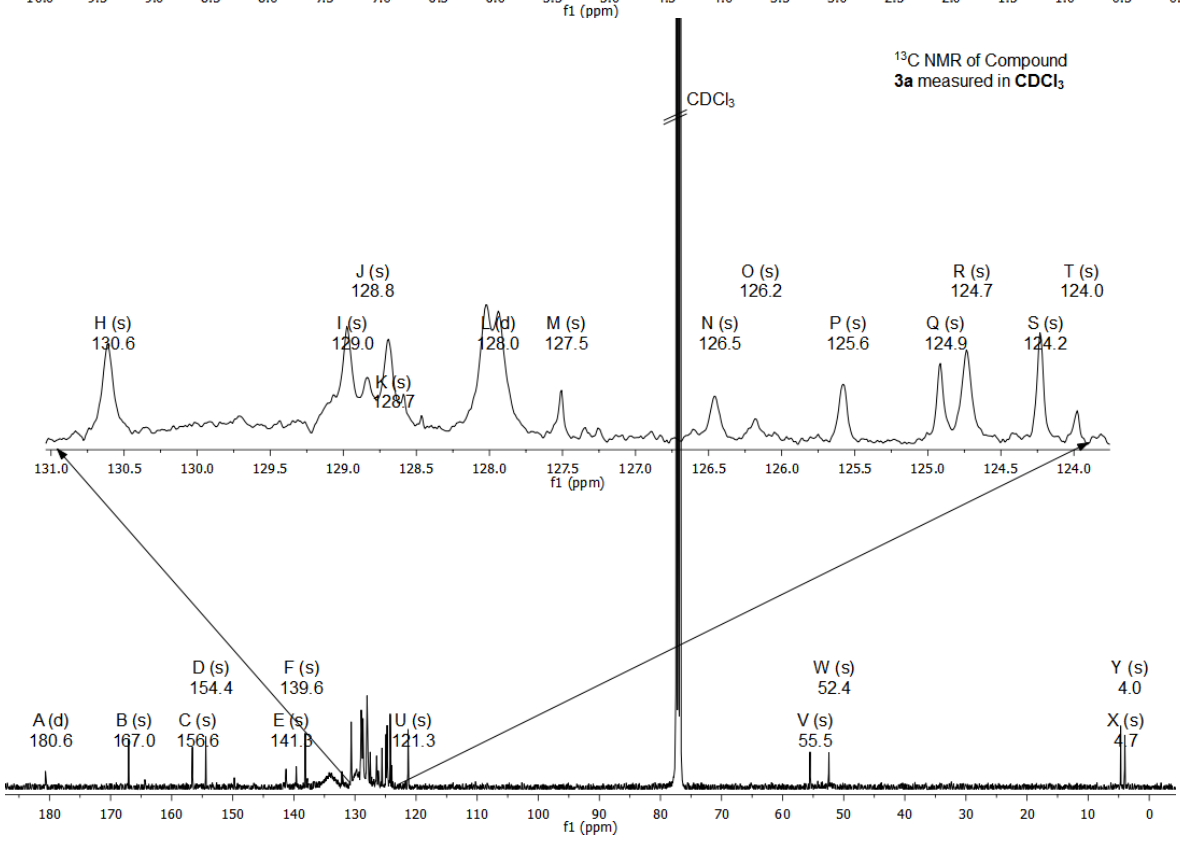
Compound 2b.


sarah.1134.1.1r
1H
^{1}H NMR of Compound **2b** measured in **CDCl$_3$**
C (d)
7.56
A (d)
8.48
B (d)
7.71
G (dd)
7.04
I (s)
5.28
H (t)
7.20
* Residual Solvent
f1 (ppm)

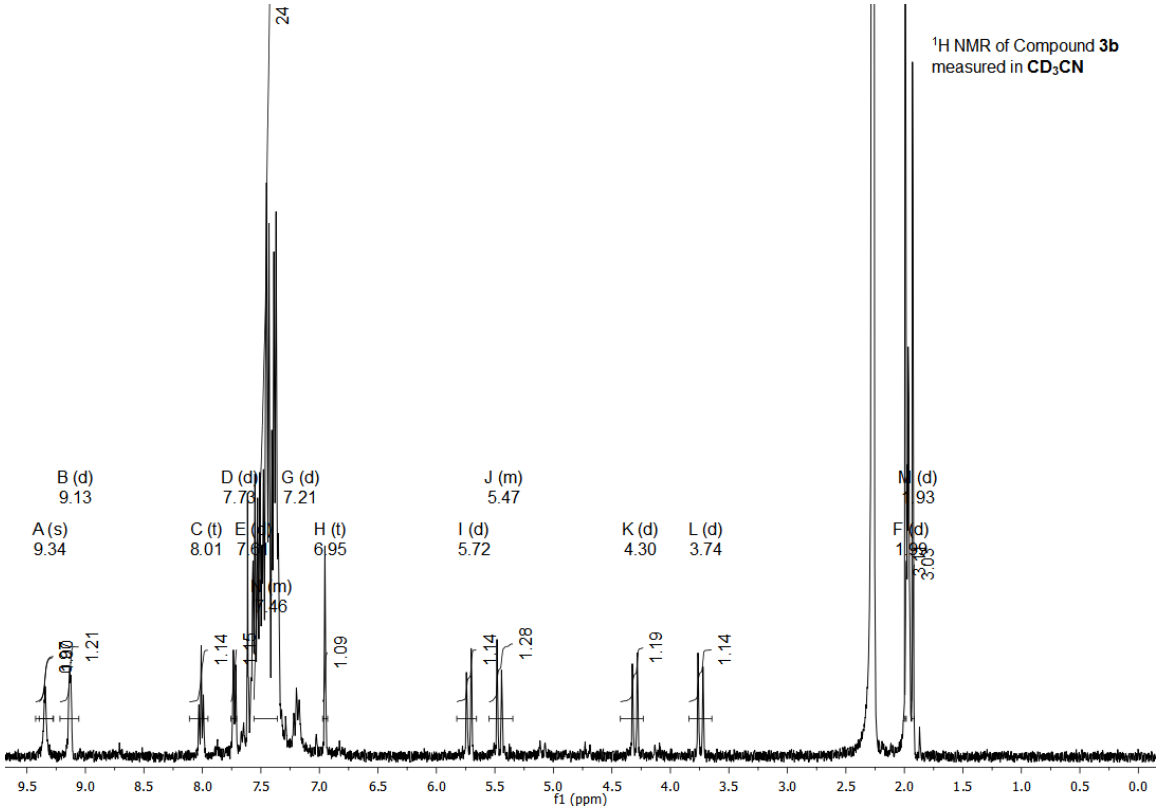

^{13}C NMR of Compound **2b** measured in **CDCl$_3$**
182.1
165.4
155.1
149.6
139.0
138.6
137.3
128.6
123.9
123.5
123.2
122.2
121.2
120.5
120.0
77.2 CDCl3
56.8
54.6
f1 (ppm)

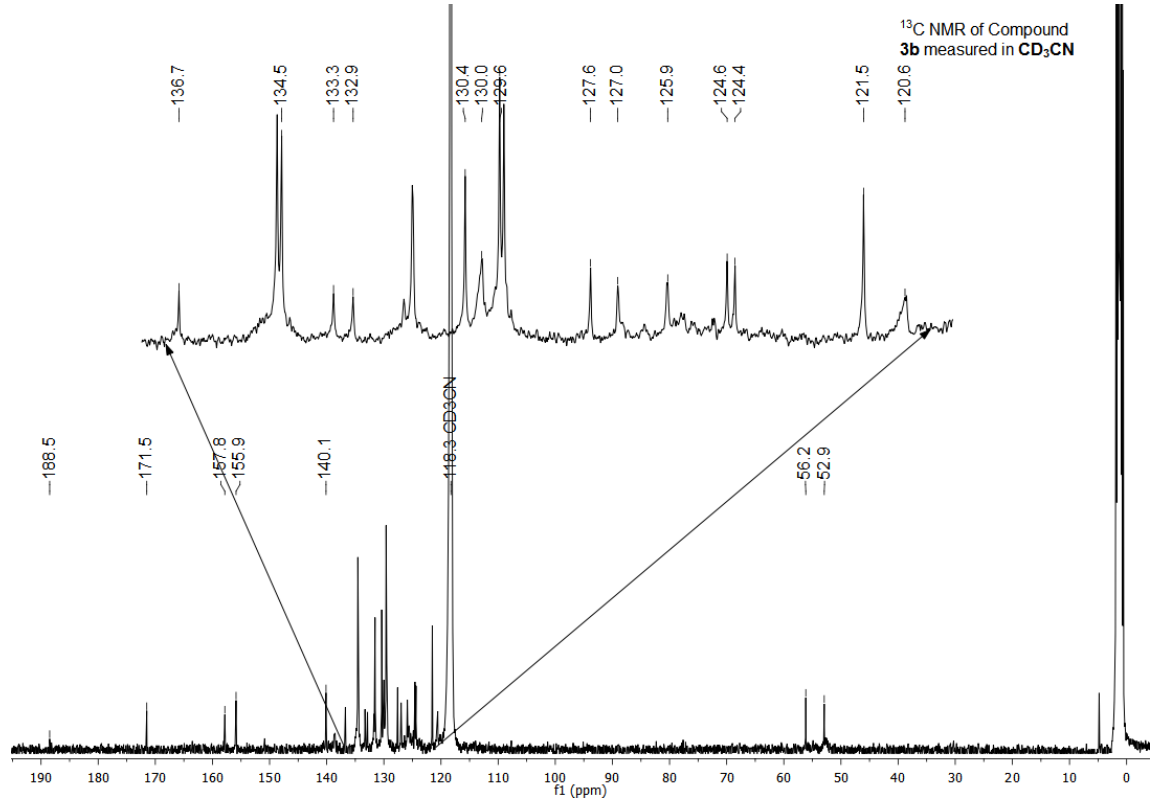
Compound 3a.

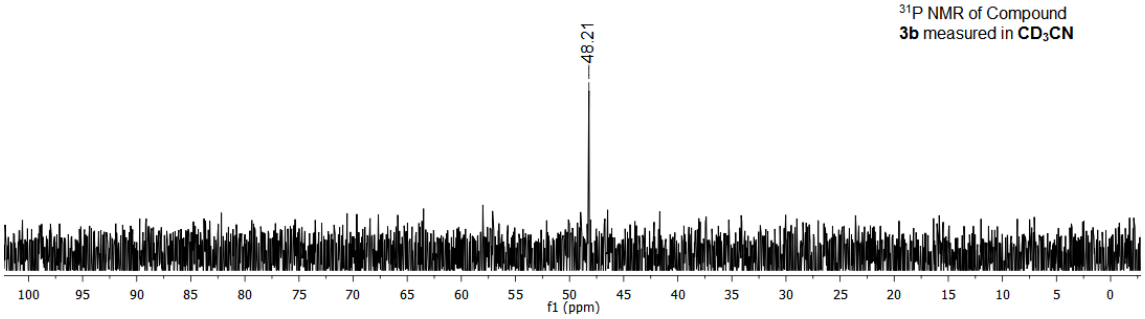

^{1}H NMR of Compound **3a** measured in **CDCl$_3$**
H (s) 6.49
V (d) 6.02
K (d) 4.30
L (d) 2.49
CDCl$_3$
U (d) 7.02
E (s) 7.09
N (s) 1.78
A (s) 9.58
B (m) 7.83
D (d) 7.19
H (s) 6.49
M (s) 2.01
H$_2$O in CDCl$_3$
T (t) 7.36
G (d) 6.86
O (s) 1.63
f1 (ppm)


^{13}C NMR of Compound **3a** measured in **CDCl$_3$**
CDCl$_3$
J (s) 128.8
O (s) 126.2
R (s) 124.7
T (s) 124.0
H (s) 130.6
I (s) 129.0
L (d) 128.0
M (s) 127.5
N (s) 126.5
P (s) 125.6
Q (s) 124.9
S (s) 124.2
K (s) 128.7
D (s) 154.4
F (s) 139.6
W (s) 52.4
Y (s) 4.0
A (d) 180.6
B (s) 167.0
C (s) 156.6
E (s) 141.3
U (s) 121.3
V (s) 55.5
X (s) 4.7
f1 (ppm)

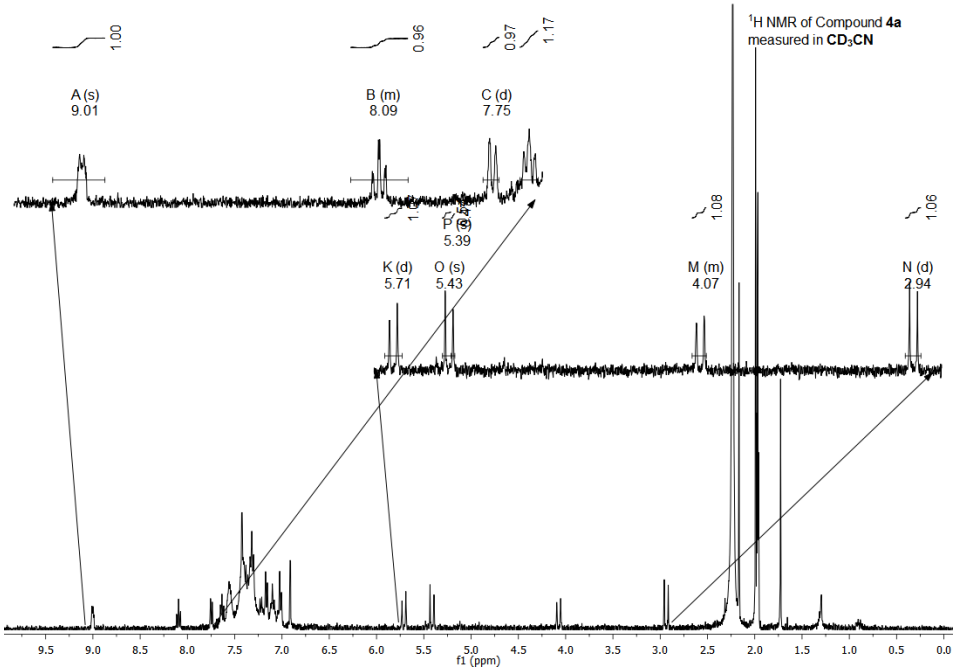
Compound 3b.

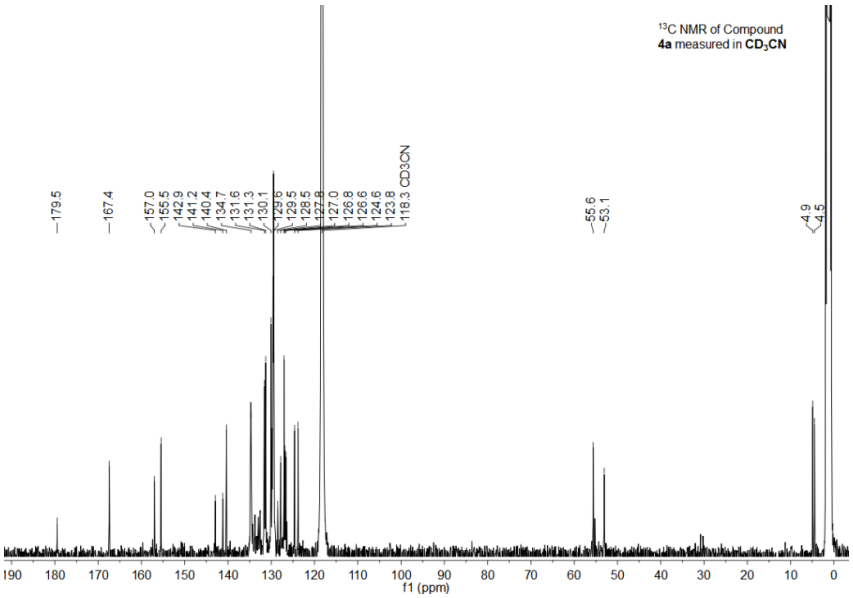

^{1}H NMR of Compound **3b** measured in **CD$_3$CN**
B (d) 9.13
A (s) 9.34
C (t) 8.01
H (t) 6.95
I (d) 5.72
J (m) 5.47
K (d) 4.30
L (d) 3.74
f1 (ppm)


^{13}C NMR of Compound **3b** measured in **CD$_3$CN**
136.7
134.5
133.3
132.9
130.4
130.0
129.6
127.6
127.0
125.9
124.6
124.4
121.5
120.6
188.5
171.5
157.8
155.9
140.1
118.3 CD3CN
56.2
52.9
f1 (ppm)


31P NMR of Compound
3b measured in CD3CN
48.21
f1 (ppm)

Compound 4a.


1H NMR of Compound 4a
measured in CD3CN
1.00
0.96
0.97
1.17
A (s)
9.01
B (m)
8.09
C (d)
7.75
P (s)
5.39
K (d)
5.71
O (s)
5.43
M (m)
4.07
N (d)
2.94
1.08
1.06
f1 (ppm)


13C NMR of Compound
4a measured in CD3CN
179.5
167.4
157.0
155.5
142.9
141.2
140.4
134.7
131.6
131.3
130.1
129.6
129.5
128.5
127.8
127.0
126.8
126.6
124.6
123.8
118.3 CD3CN
55.6
53.1
4.9
4.5
f1 (ppm)