Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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1 NMR Spectra

1.1 Compound 1

Figure S1: ^{1}H NMR spectra of compound **1**

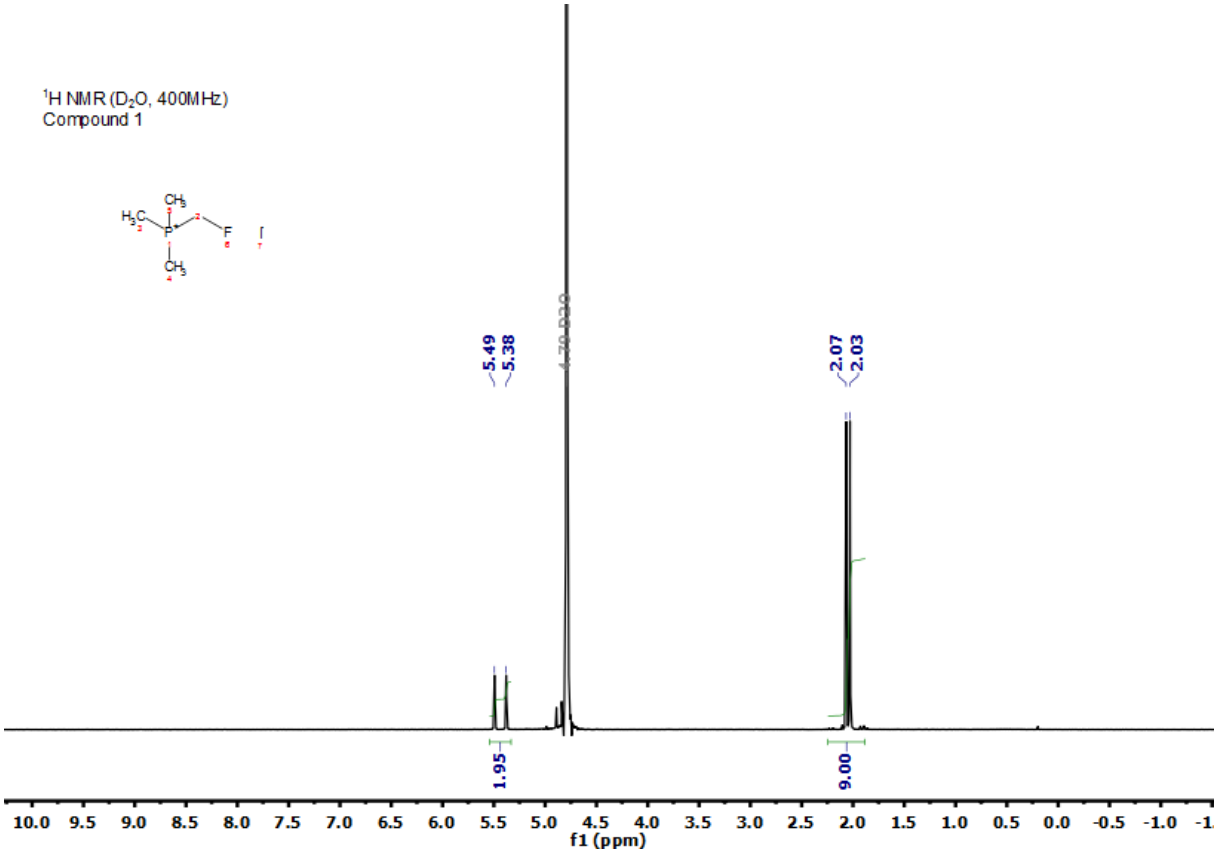


Figure S2: $^{19}F\{^{1}H\}$ NMR spectrum of compound **1**

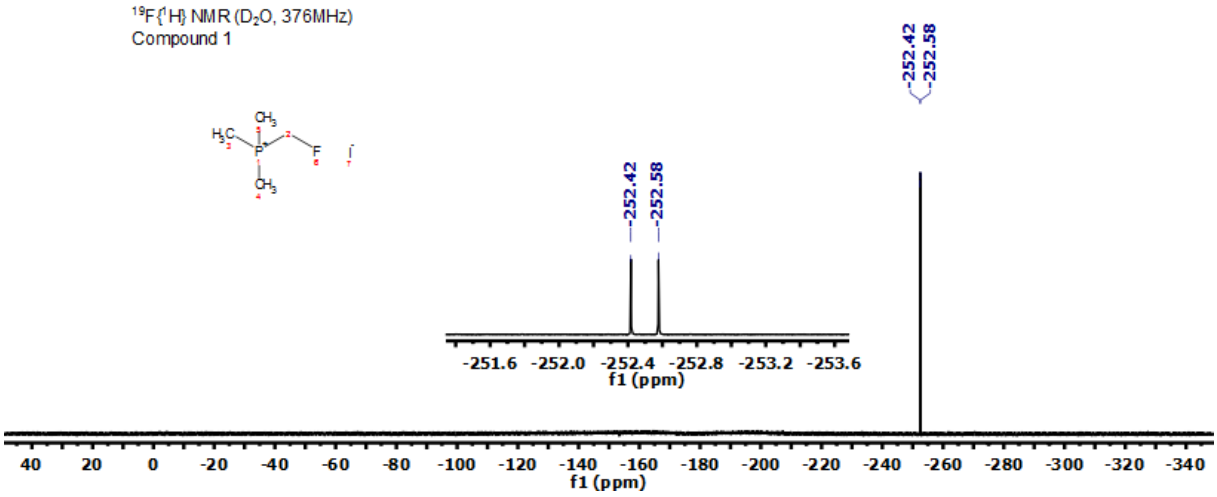


Figure S3: ^{19}F NMR spectrum of compound **1**

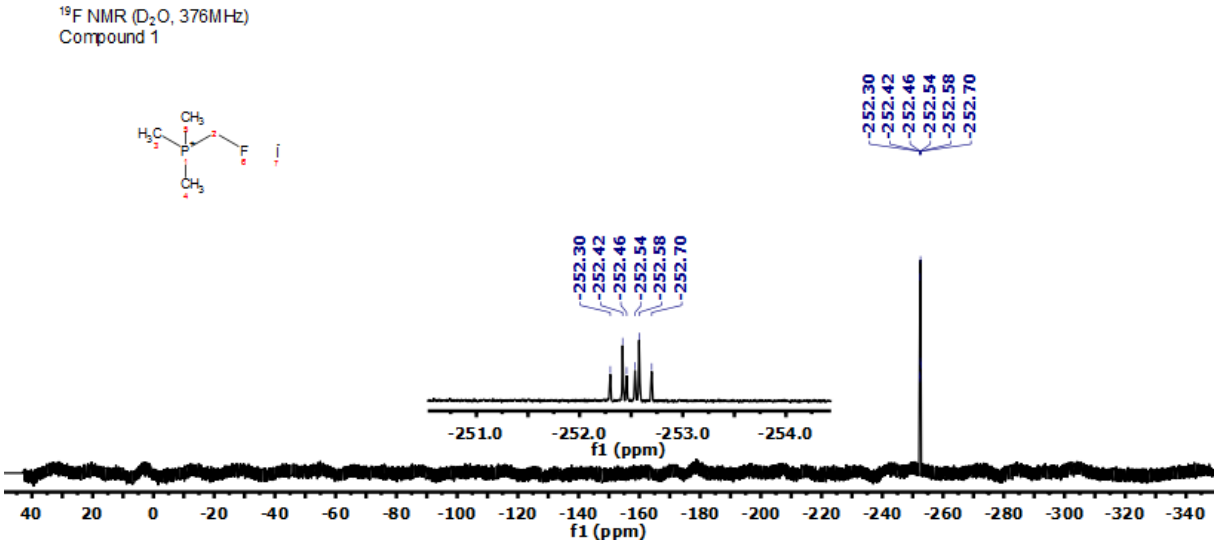


Figure S4: $^{31}P\{^{1}H\}$ NMR spectrum of compound **1**

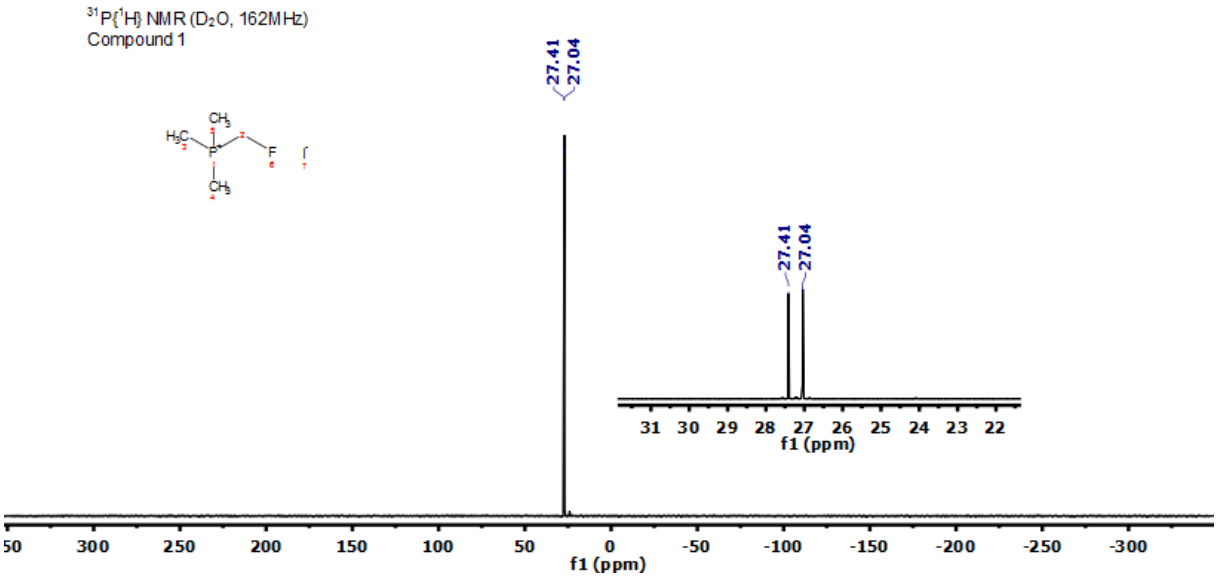


Figure S5: ^{31}P NMR spectrum of compound **1**

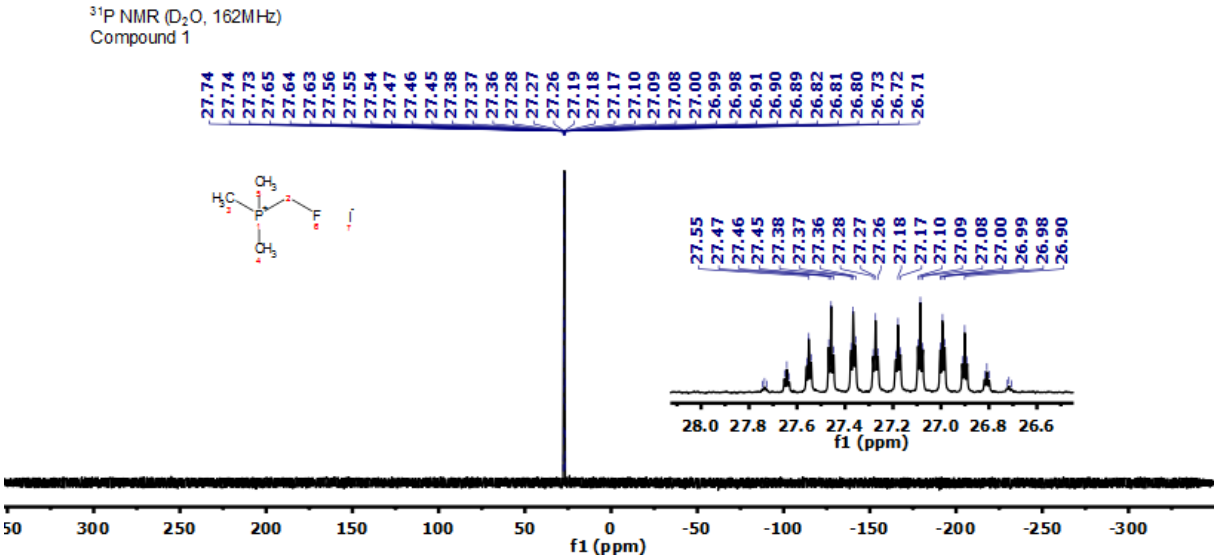
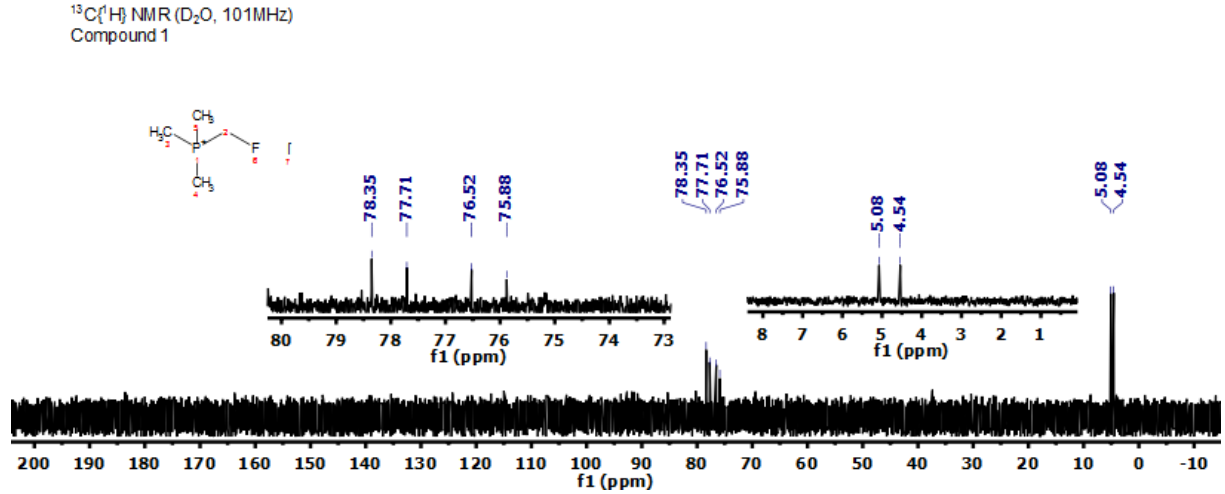


Figure S6: ^{13}C{^{1}H} NMR spectrum of compound **1**



1.2 Compound 2

Figure S7: ^{1}H NMR spectrum of compound **2**

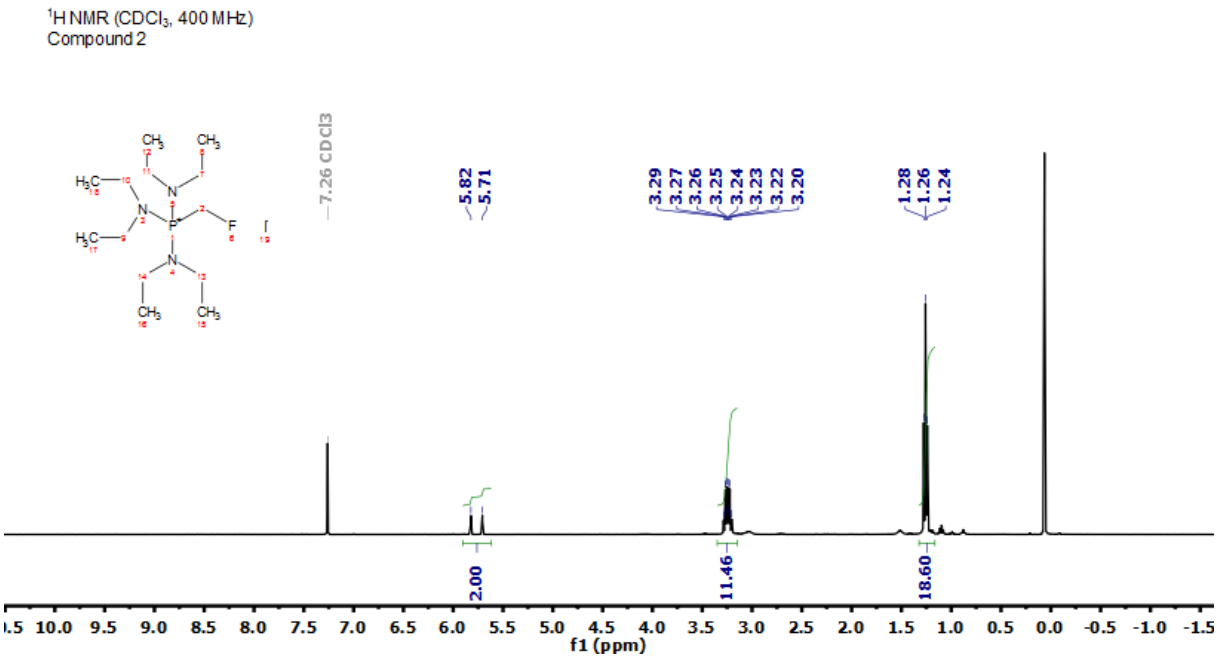


Figure S8: $^{19}F\{^{1}H\}$ NMR spectrum of compound **2**

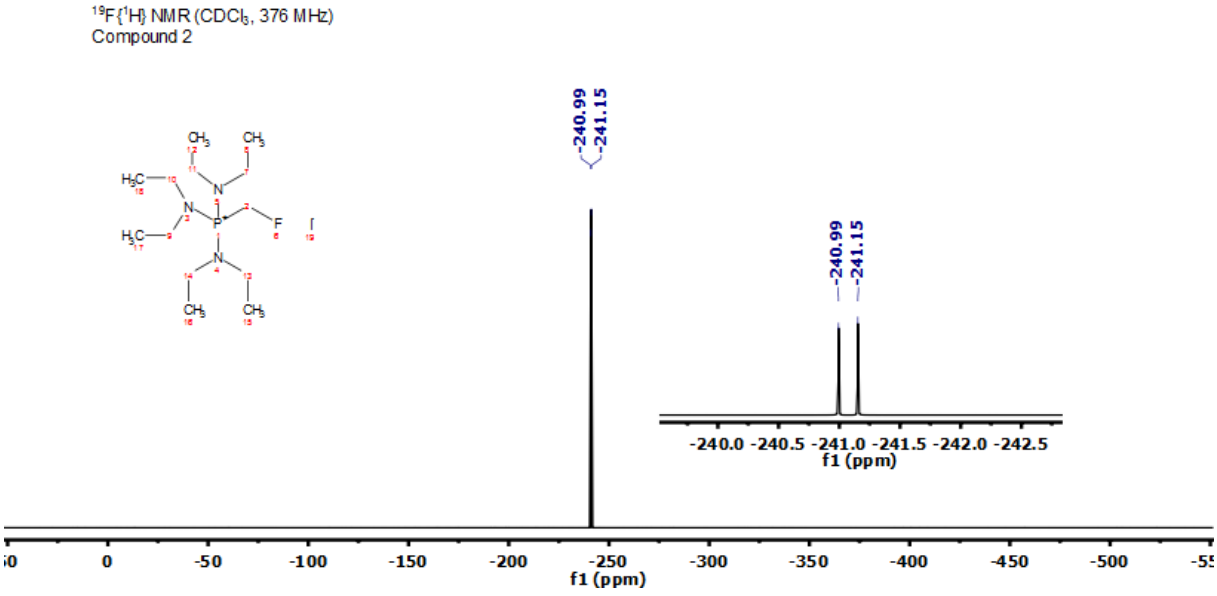


Figure S9: ^{19}F NMR spectrum of compound **2**

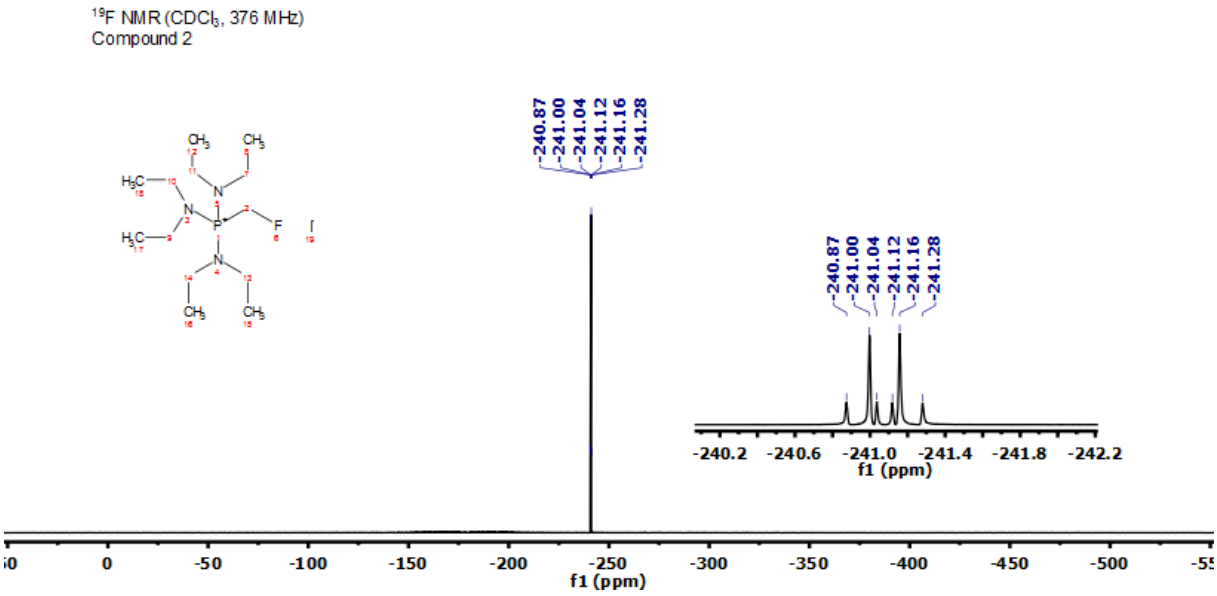


Figure S10: $^{31}P\{^{1}H\}$ NMR spectrum of compound **2**

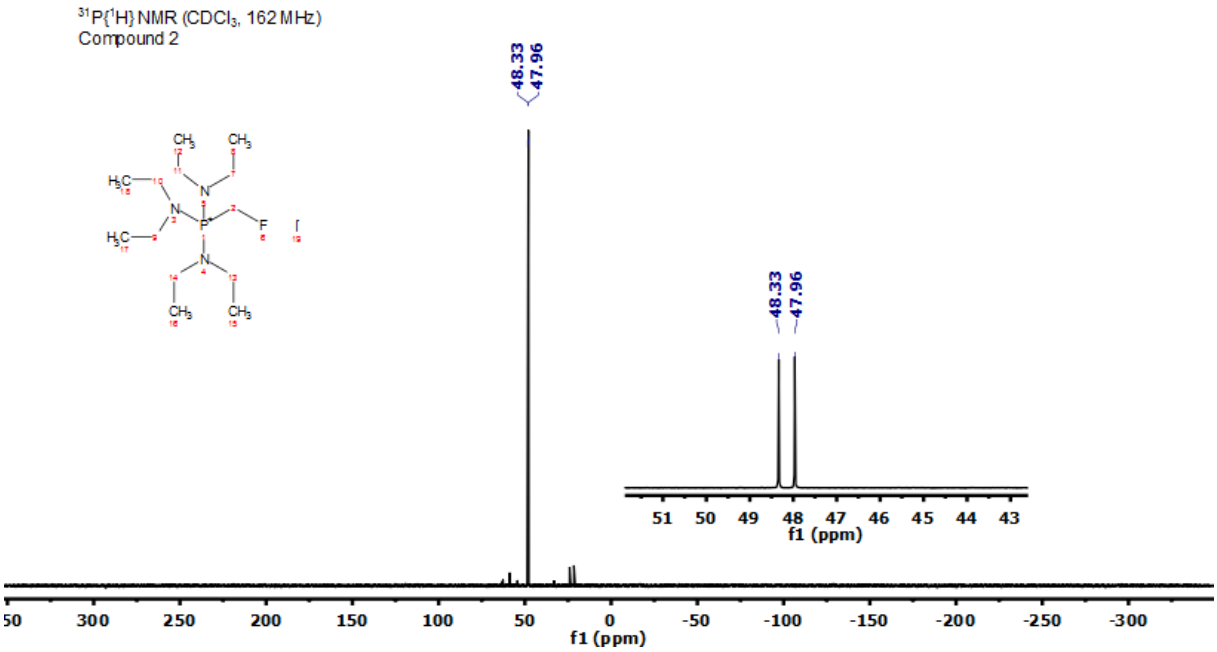


Figure S11: ^{31}P NMR spectrum of compound **2**

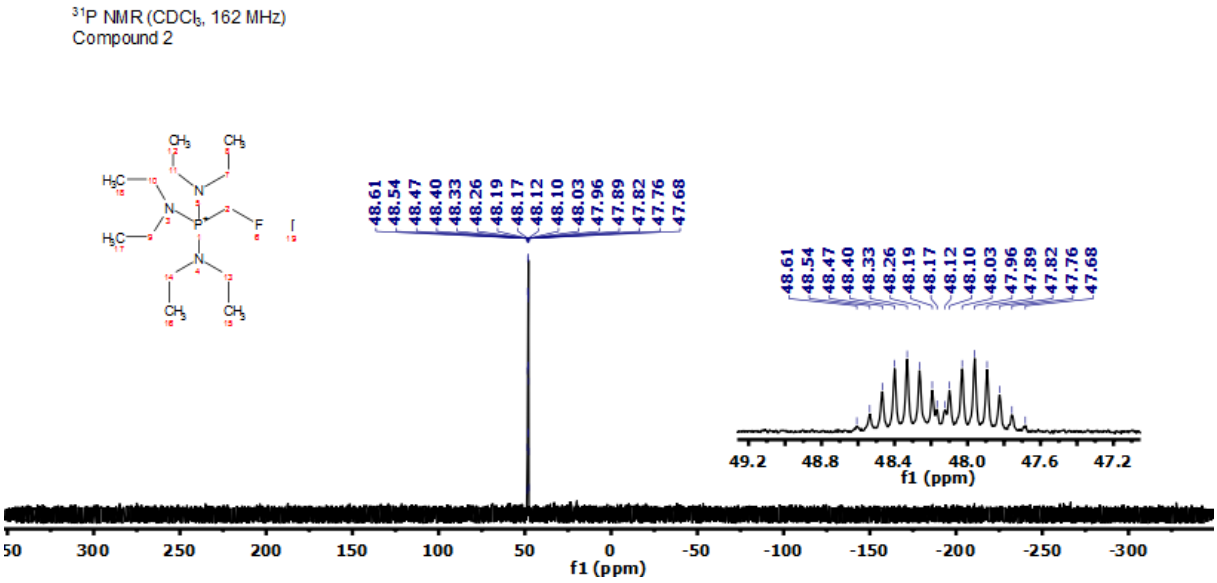
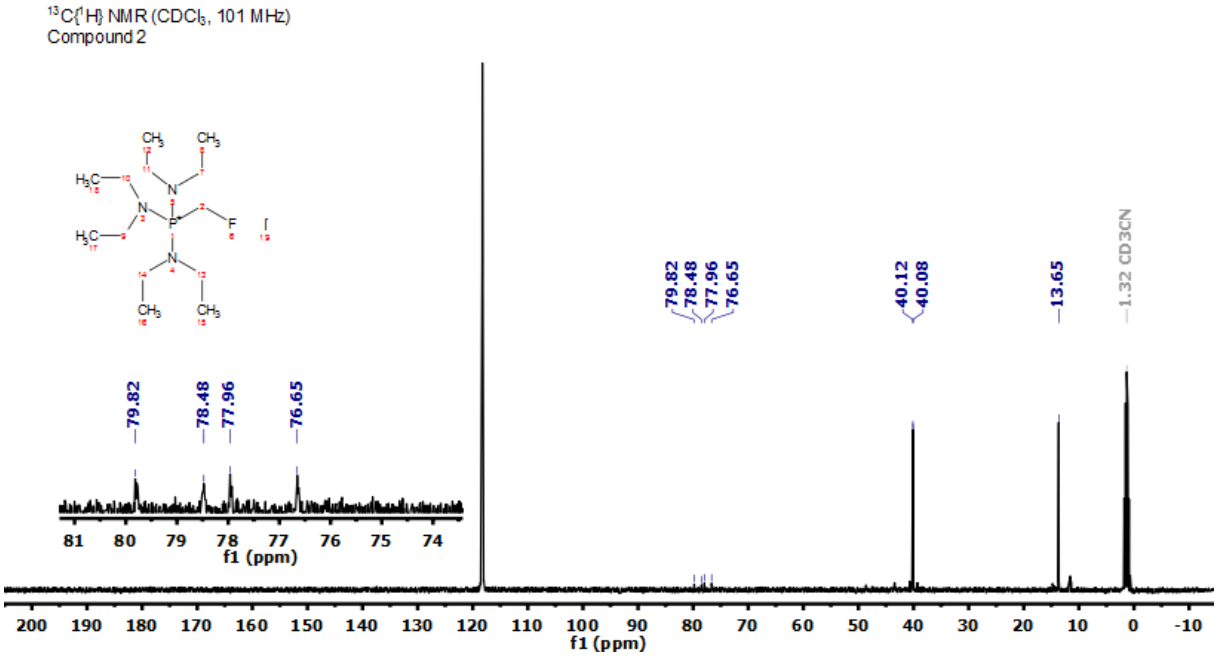


Figure S12: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2**



1.3 Compound 3

Figure S13: ^{1}H NMR spectrum of compound **3**

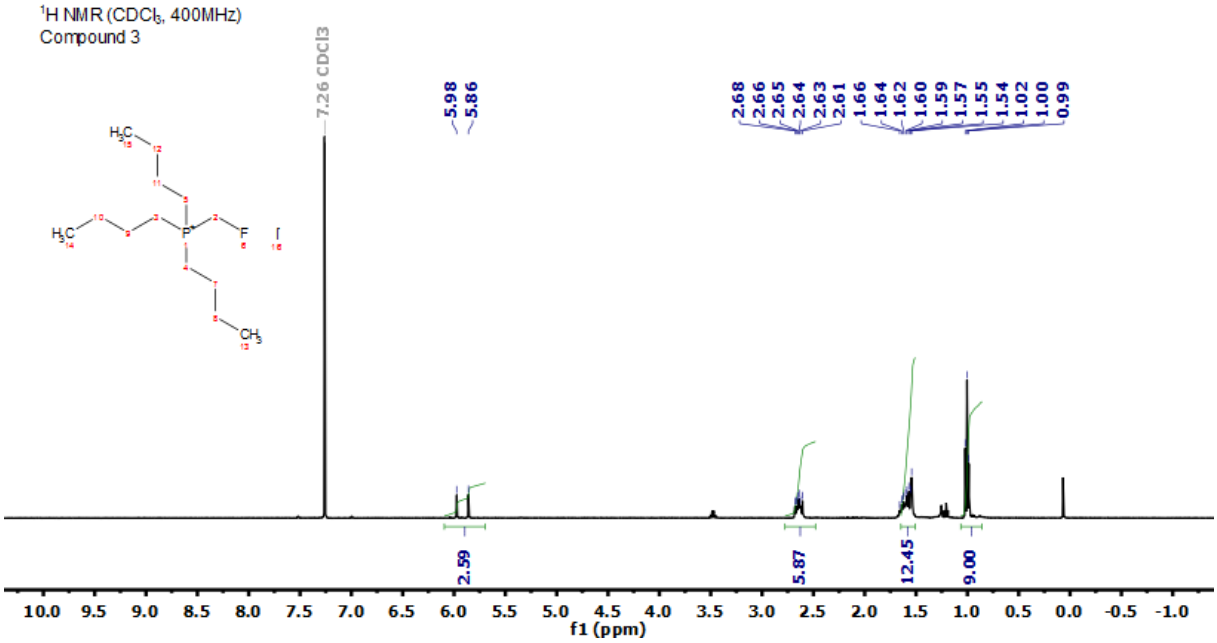


Figure S14: ^{19}F{^{1}H} NMR spectrum of compound **3**

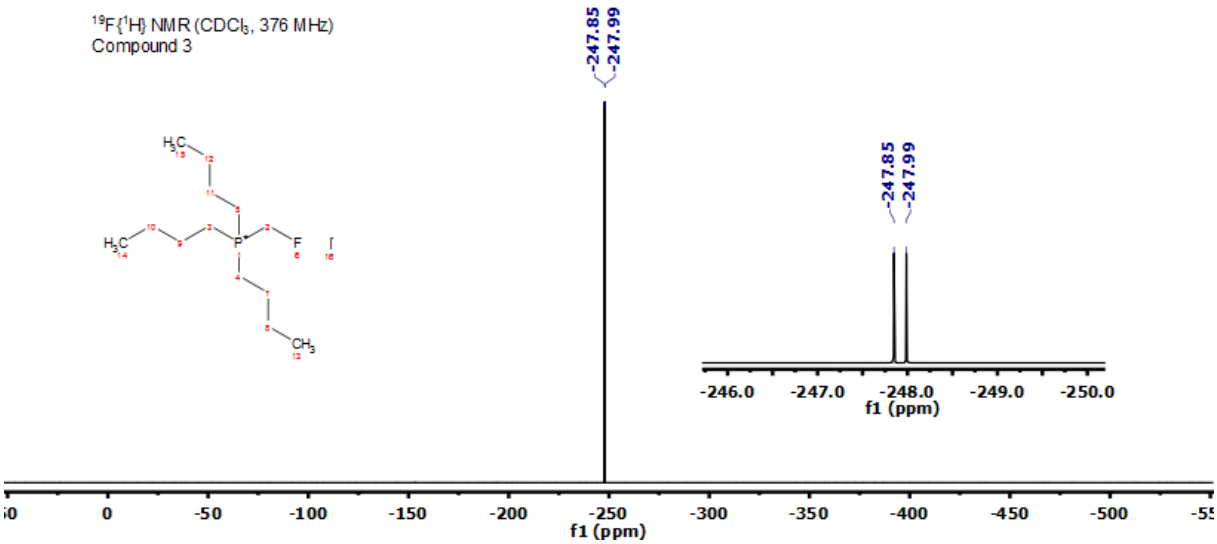


Figure S15: ^{19}F NMR spectrum of compound **3**

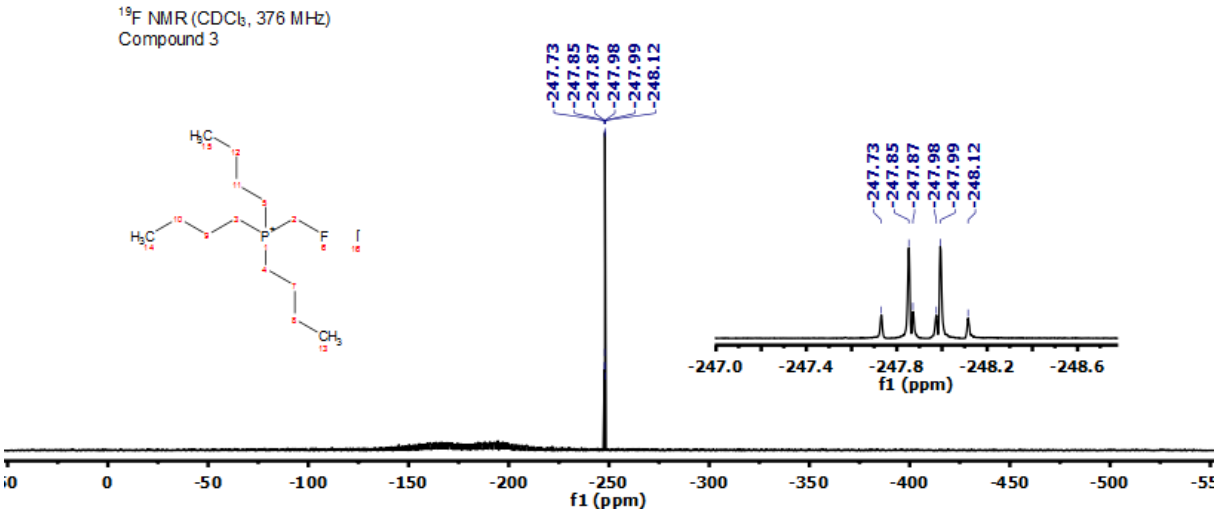


Figure S16: $^{31}P\{^{1}H\}$ NMR spectrum of compound **3**

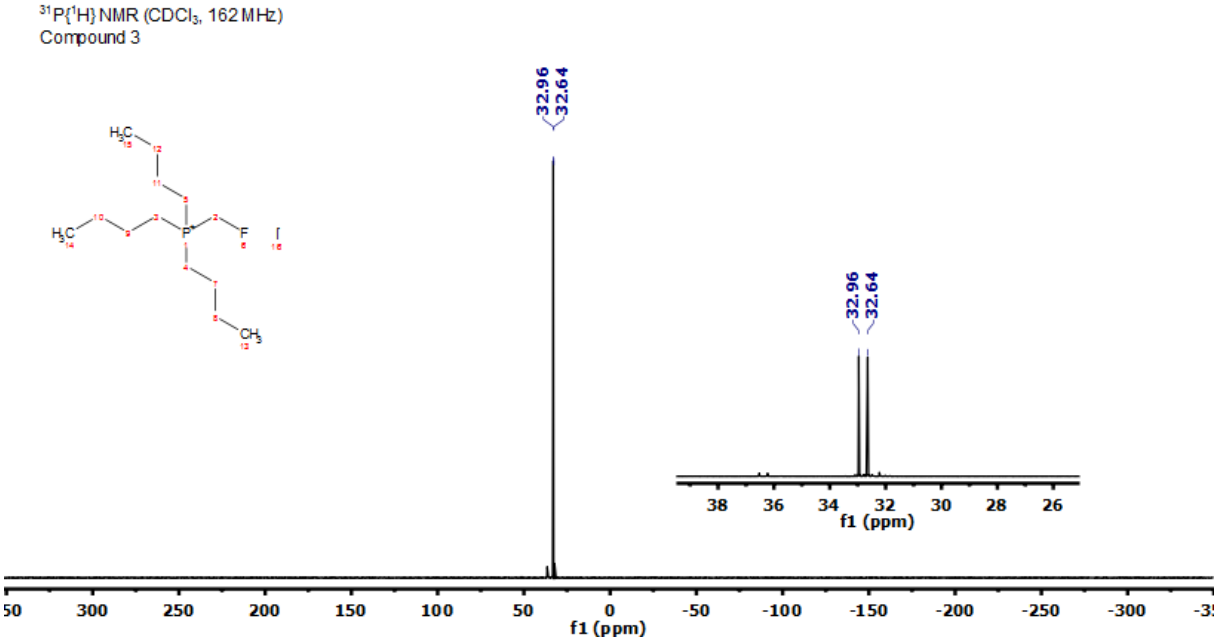


Figure S17: ^{31}P NMR spectrum of compound **3**

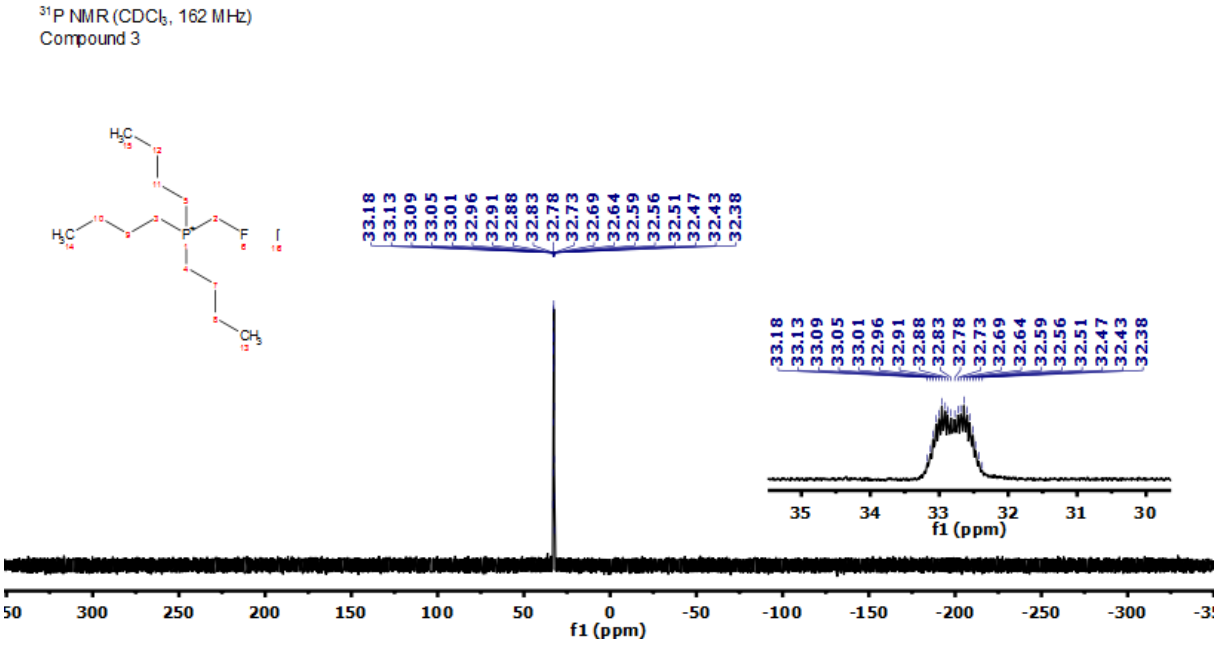
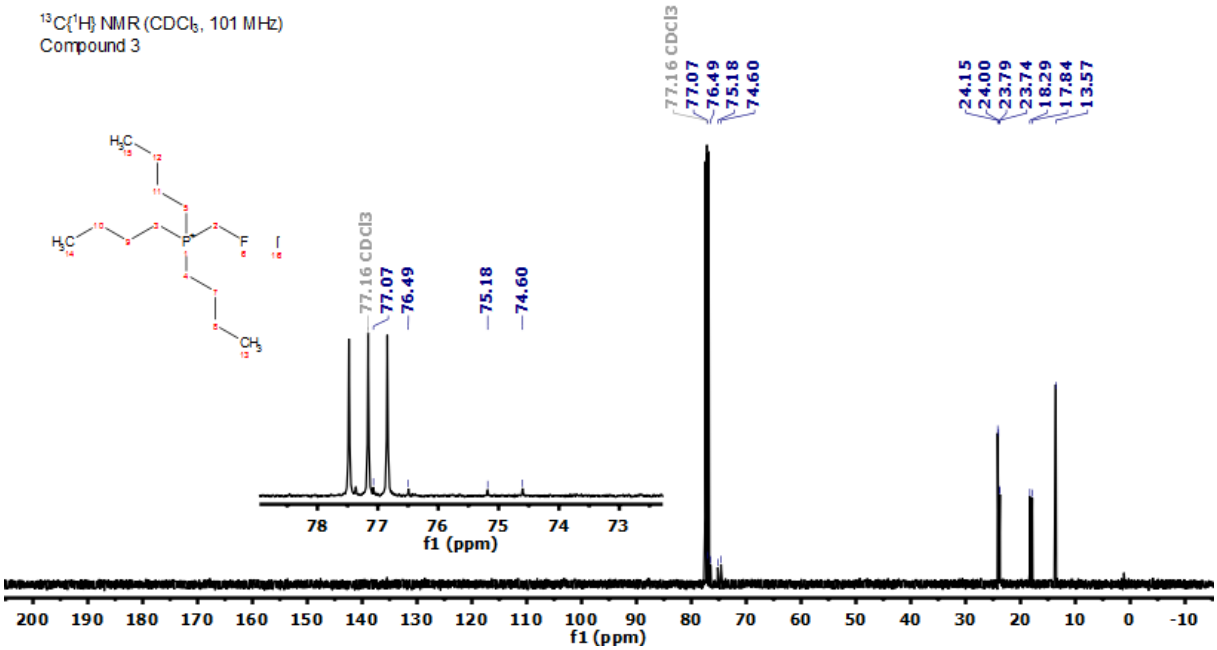


Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum of compound **3**



1.4 Compound 4

Figure S19: ^{1}H NMR spectrum of compound **4**

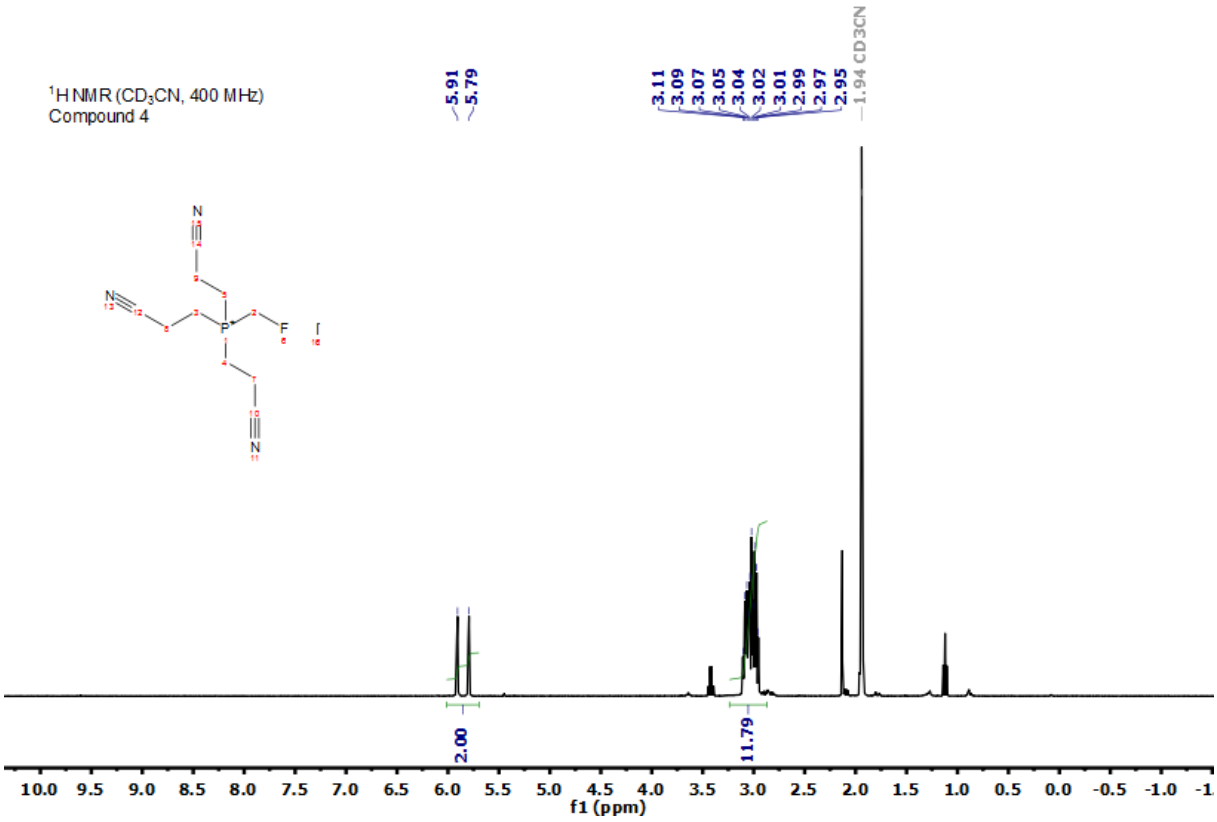


Figure S20: ^{19}F{^{1}H} NMR spectrum of compound **4**

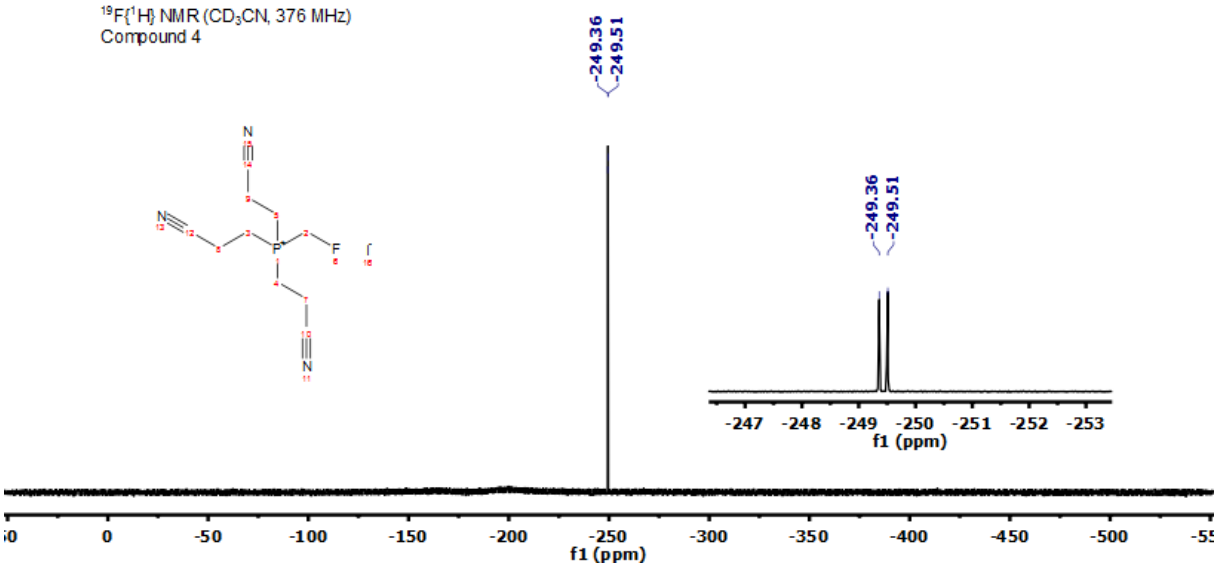


Figure S21: ^{19}F NMR spectrum of compound **4**

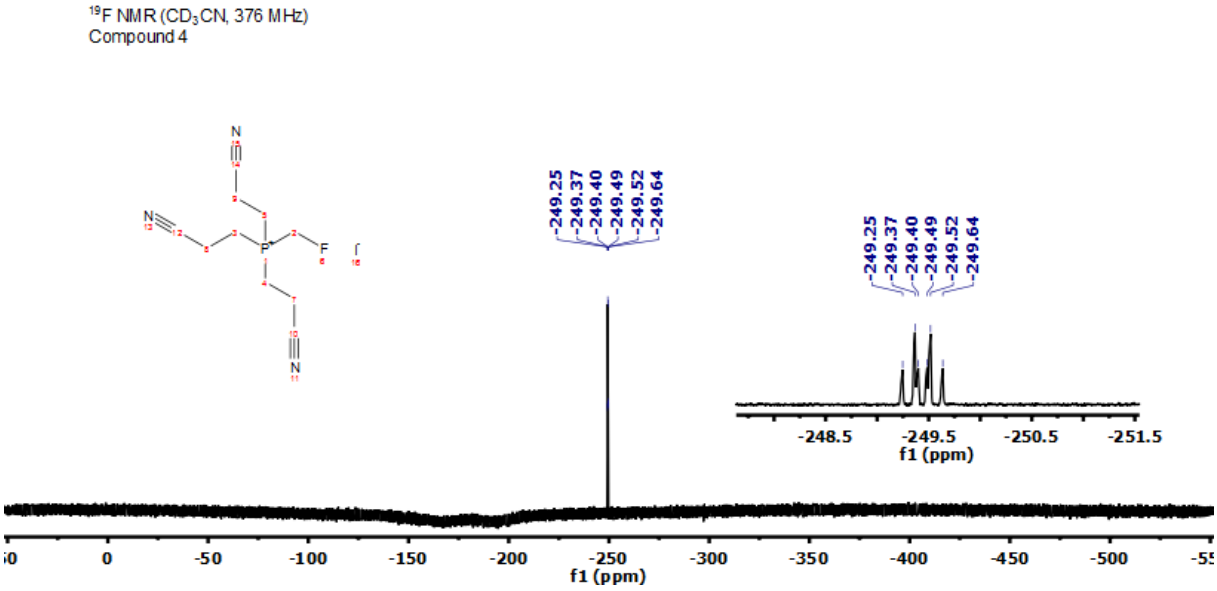


Figure S22: $^{31}P\{^{1}H\}$ NMR spectrum of compound **4**

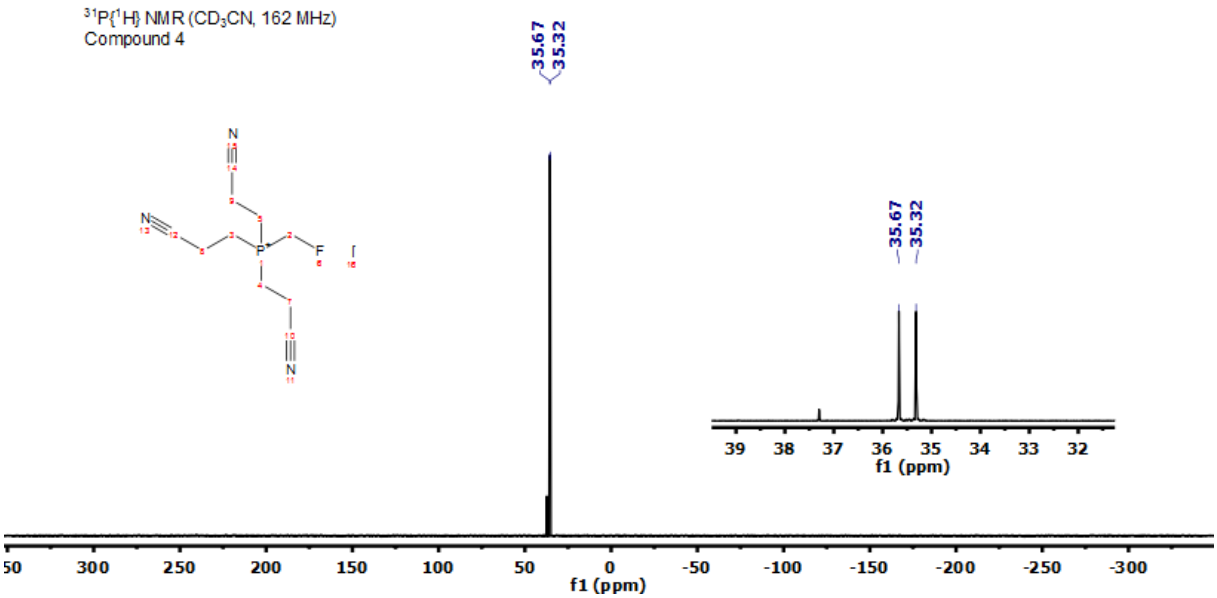


Figure S23: ^{31}P NMR spectrum of compound **4**

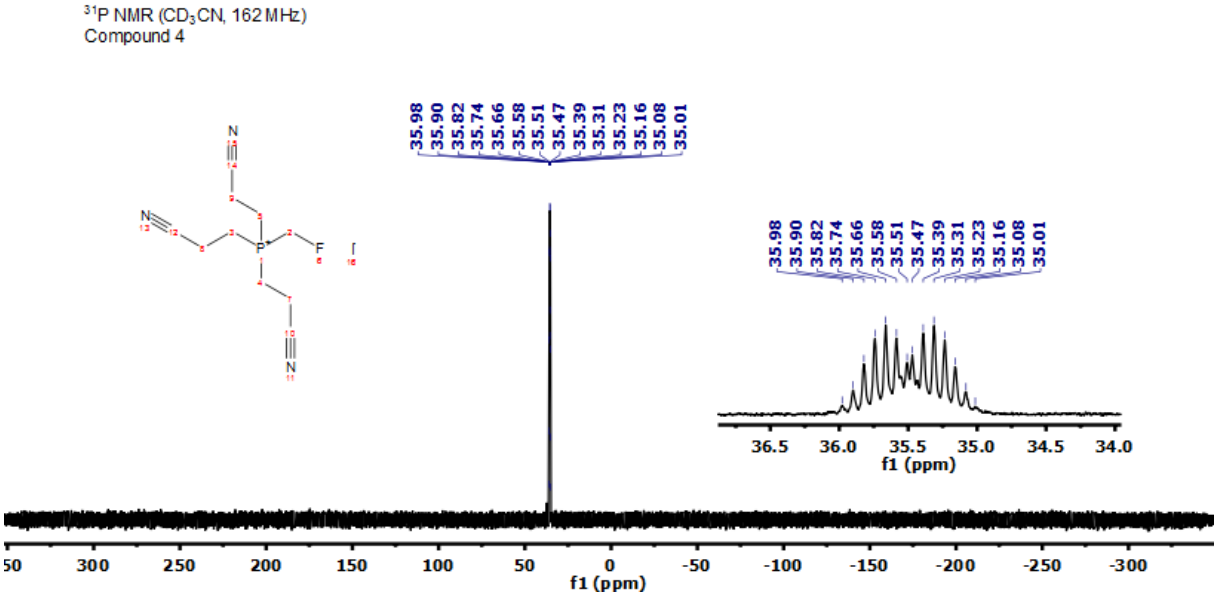
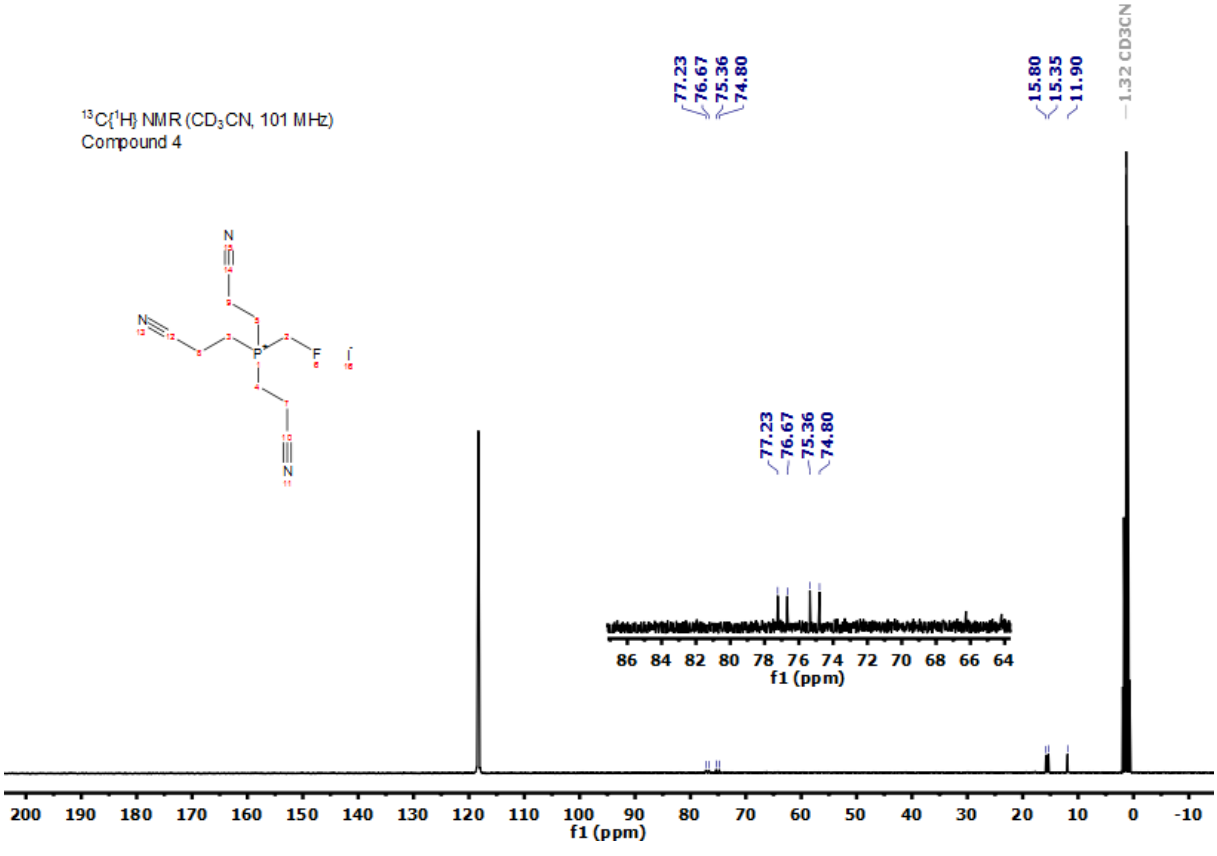


Figure S24: ^{13}C{^{1}H} NMR spectrum of compound **4**



1.5 Compound 5

Figure S25: ^{1}H NMR spectrum of compound **5**

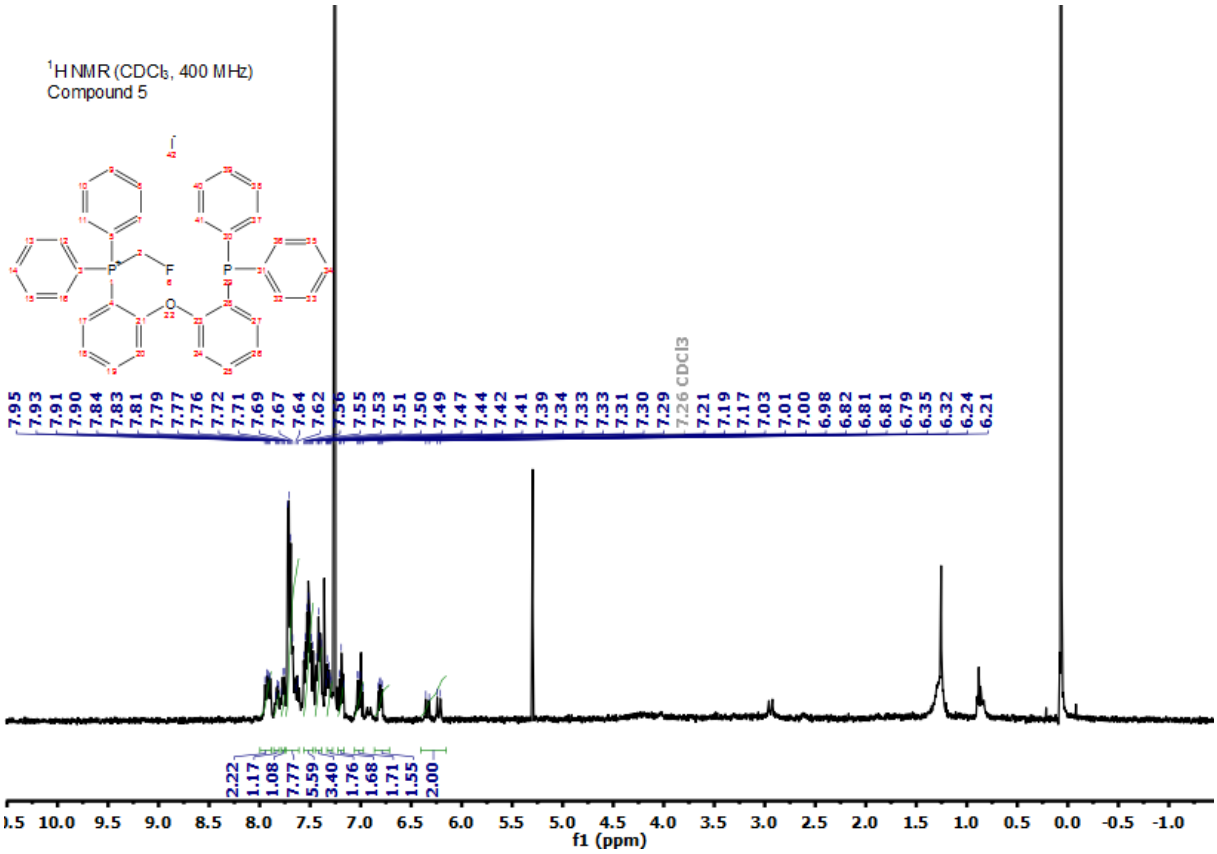


Figure S26: ^{19}F{^{1}H} NMR spectrum of compound **5**

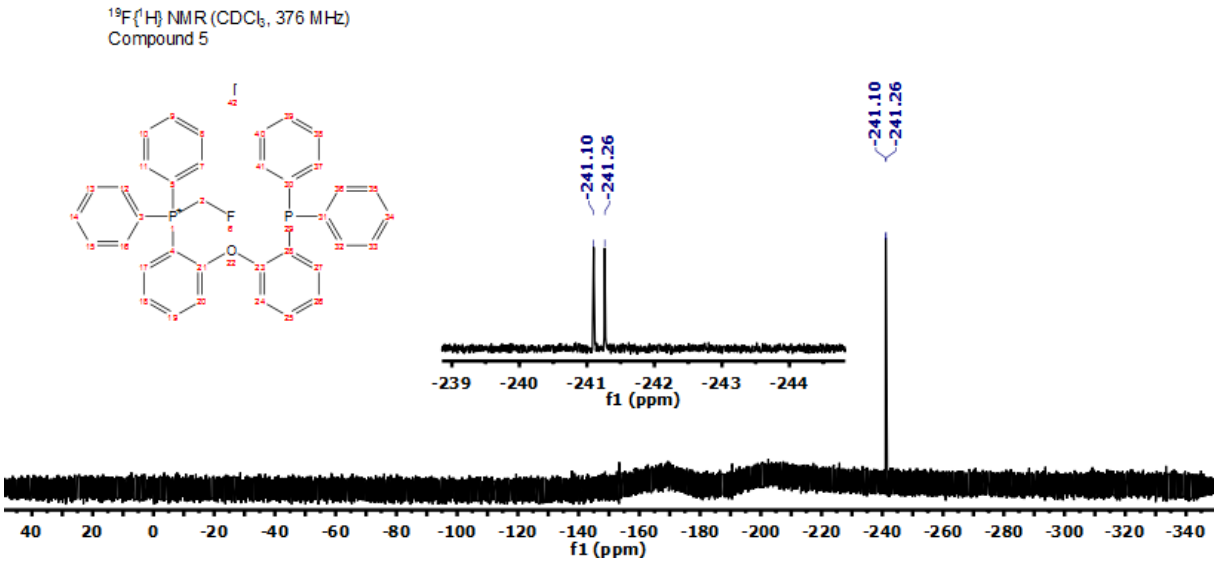


Figure S27: ^{19}F NMR spectrum of compound **5**

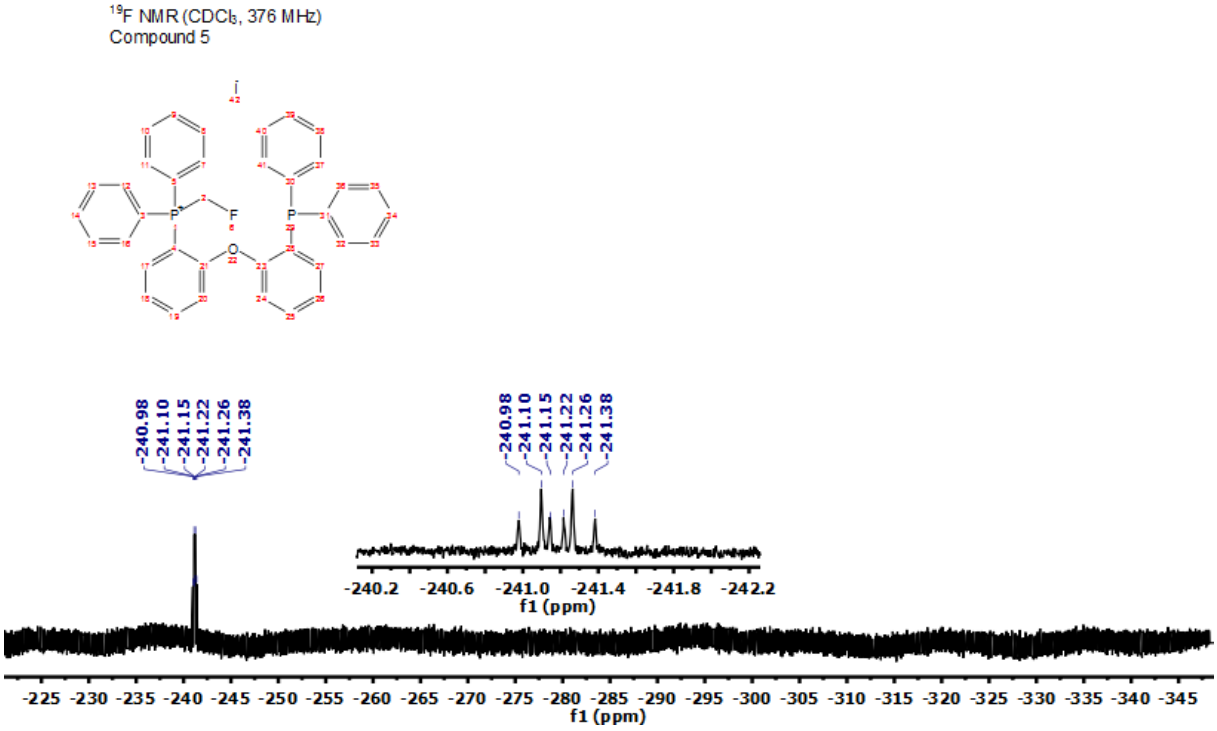


Figure S28: $^{31}P\{^{1}H\}$ NMR spectrum of compound **5**

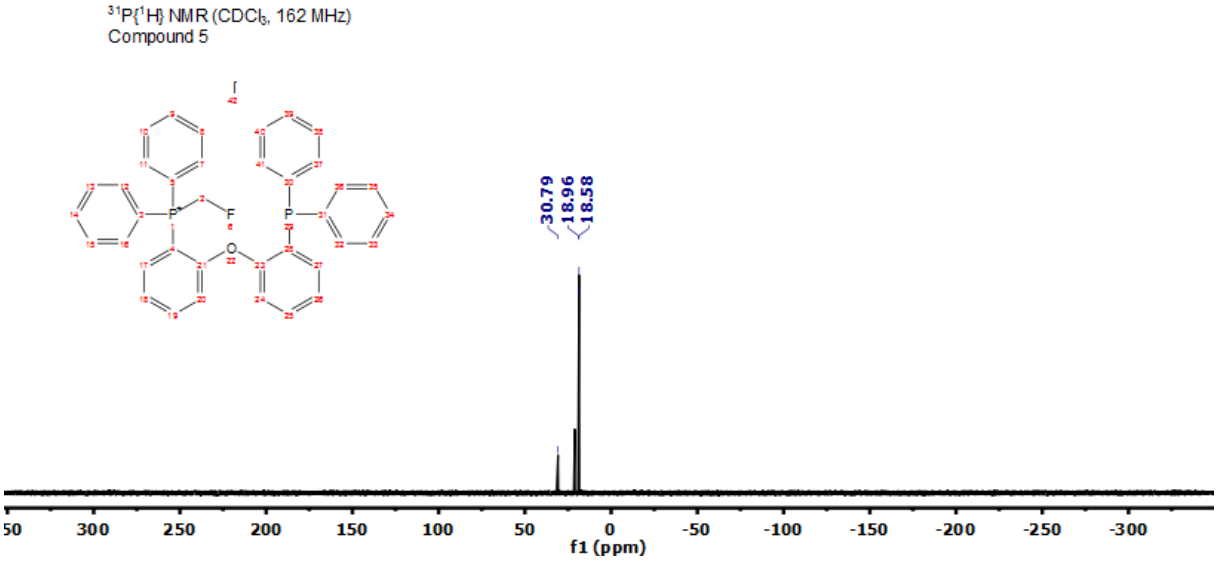


Figure S29: ^{31}P NMR spectrum of compound **5**

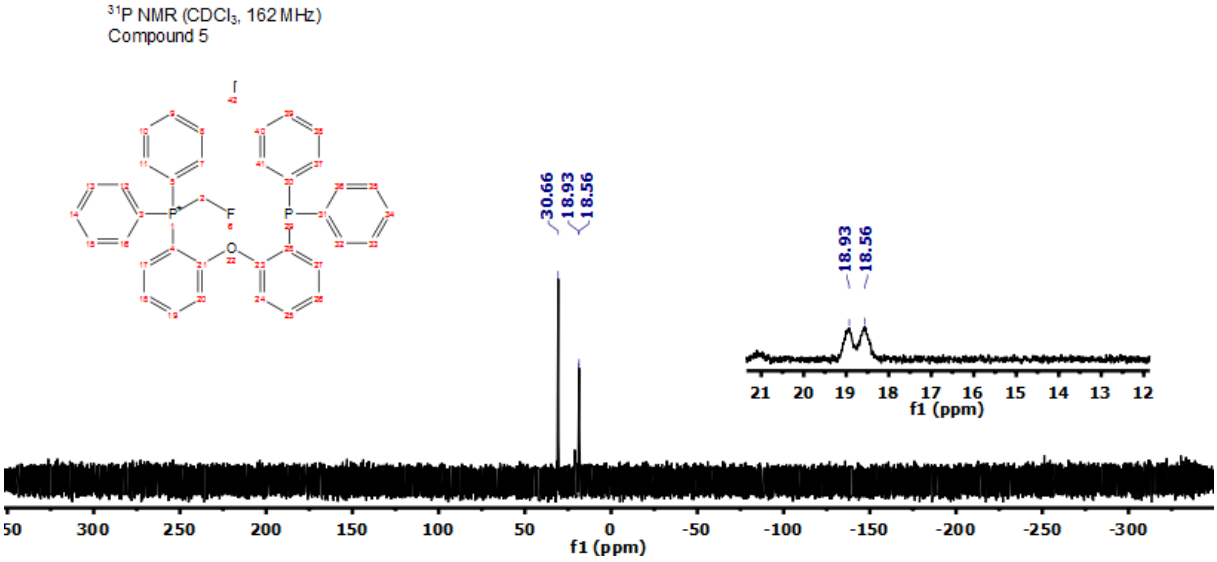
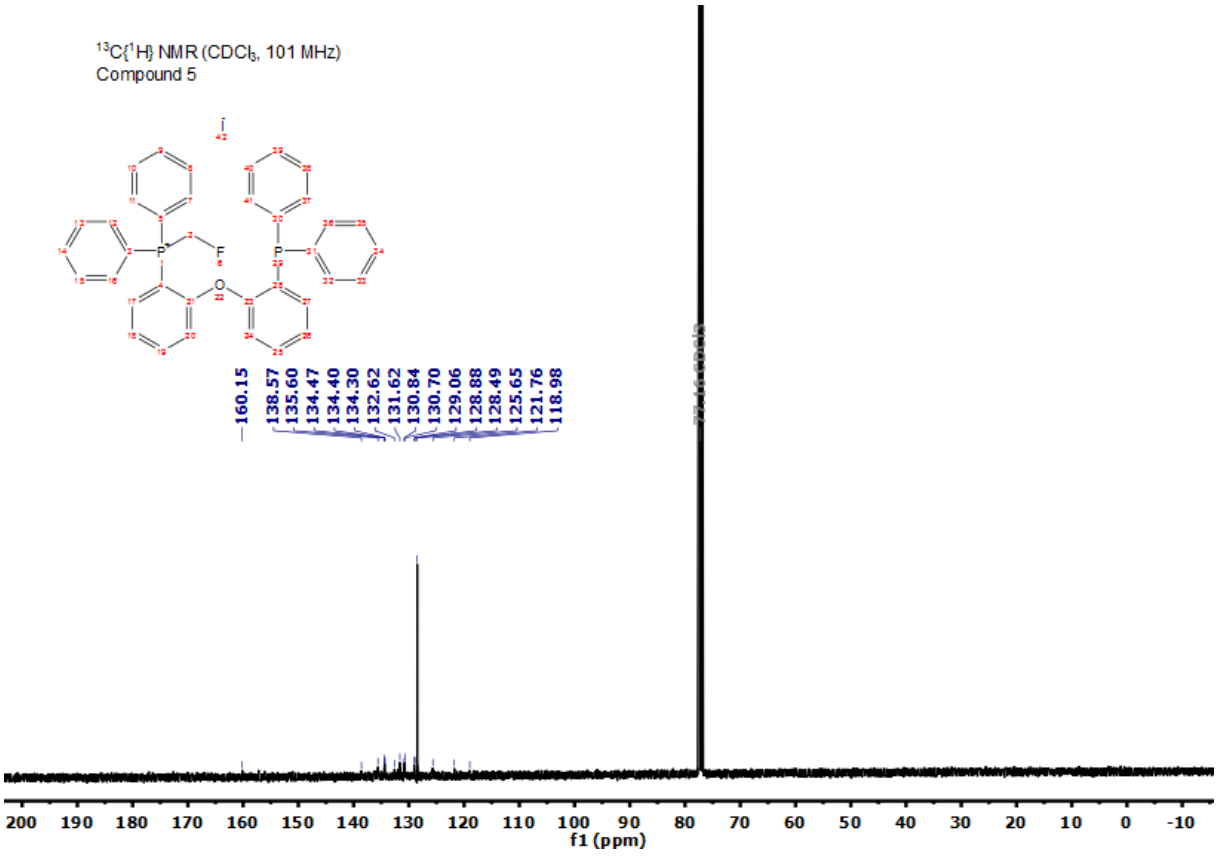


Figure S30: $^{13}C\{^{1}H\}$ NMR spectrum of compound **5**



1.6 Compound 6

Figure S31: ^{1}H NMR spectrum of compound **6**

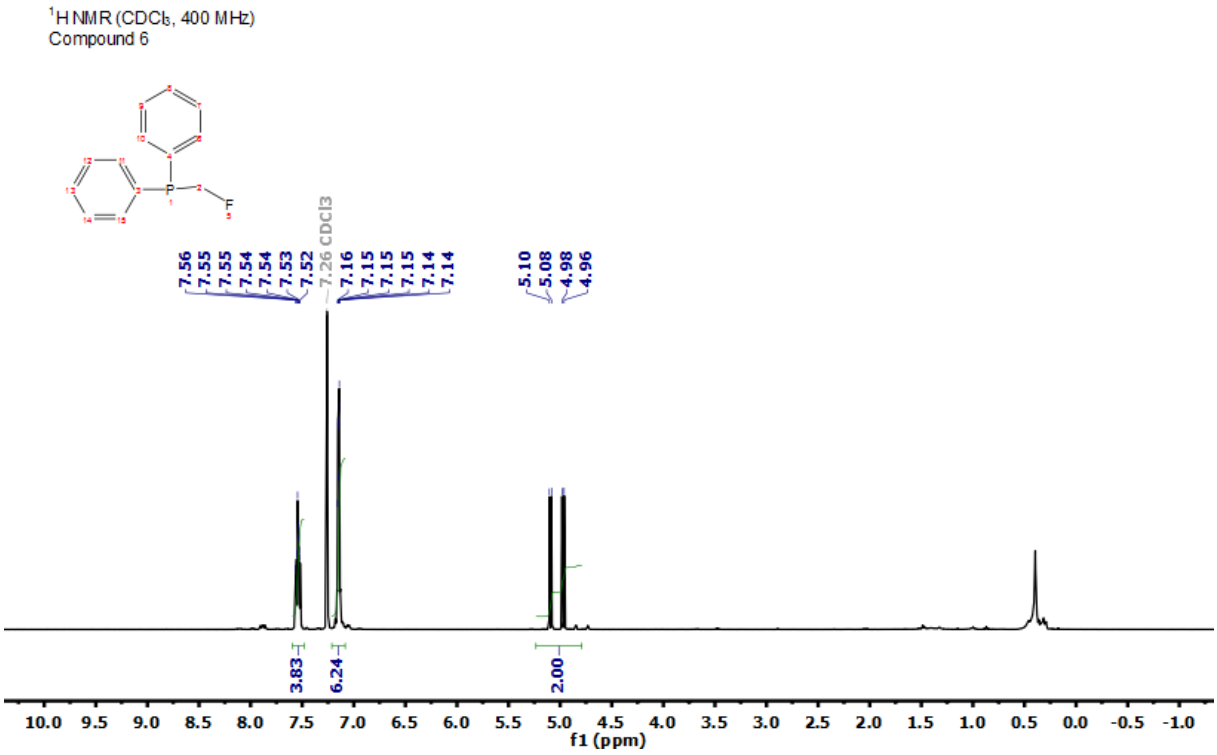


Figure S32: ^{19}F{^{1}H} NMR spectrum of compound **6**

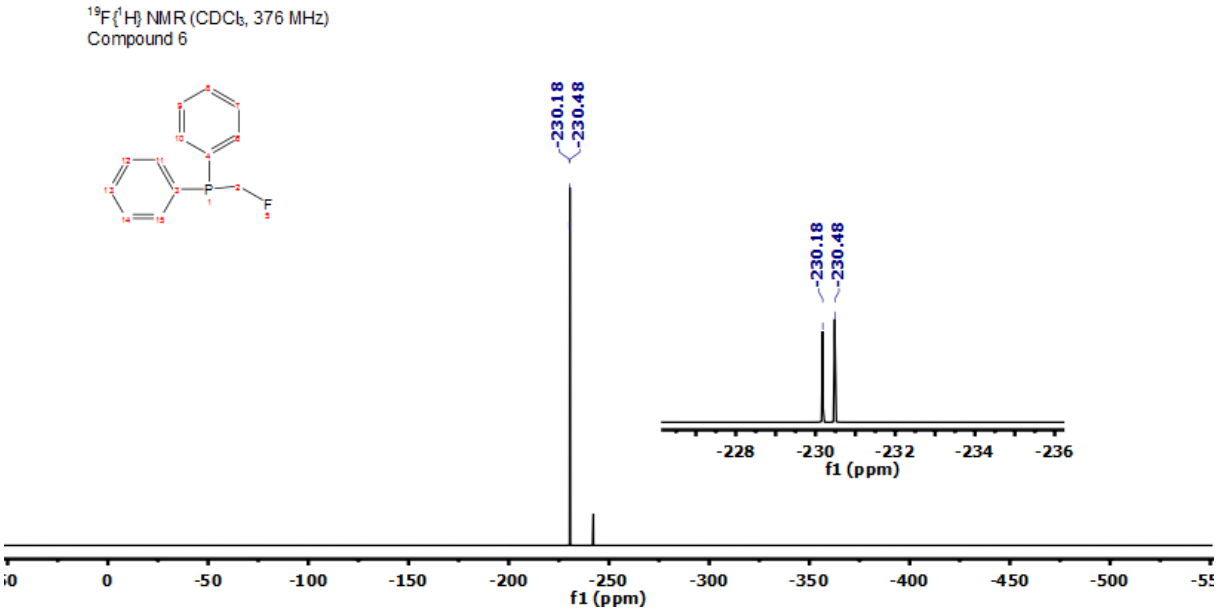


Figure S33: ^{19}F NMR spectrum of compound **6**

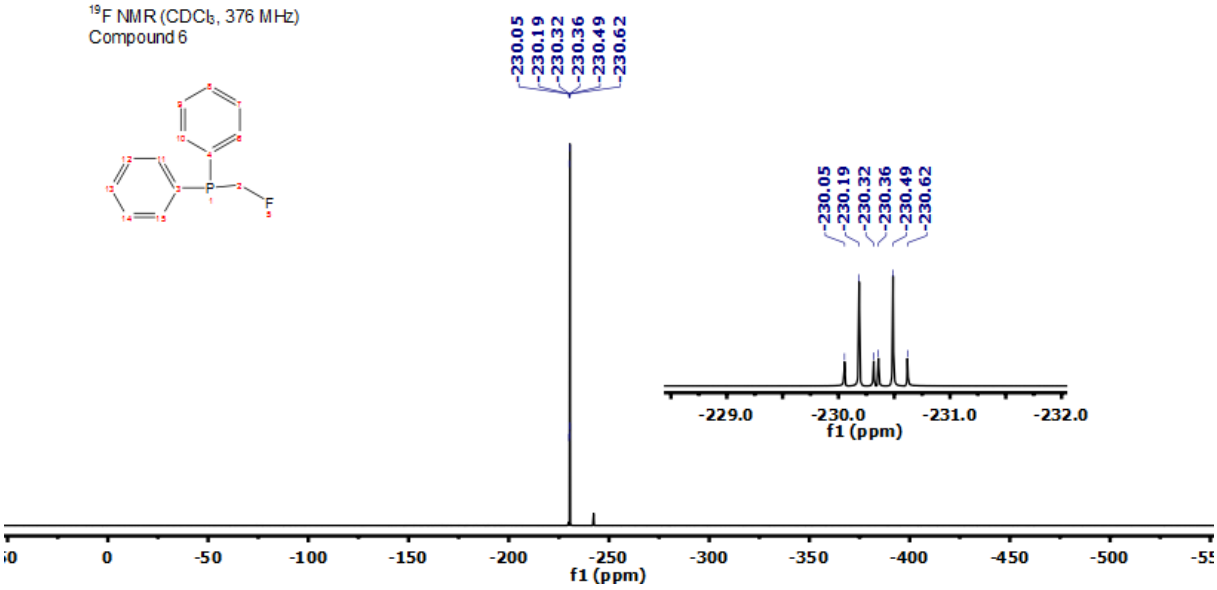


Figure S34: $^{31}P\{^{1}H\}$ NMR spectrum of compound **6**

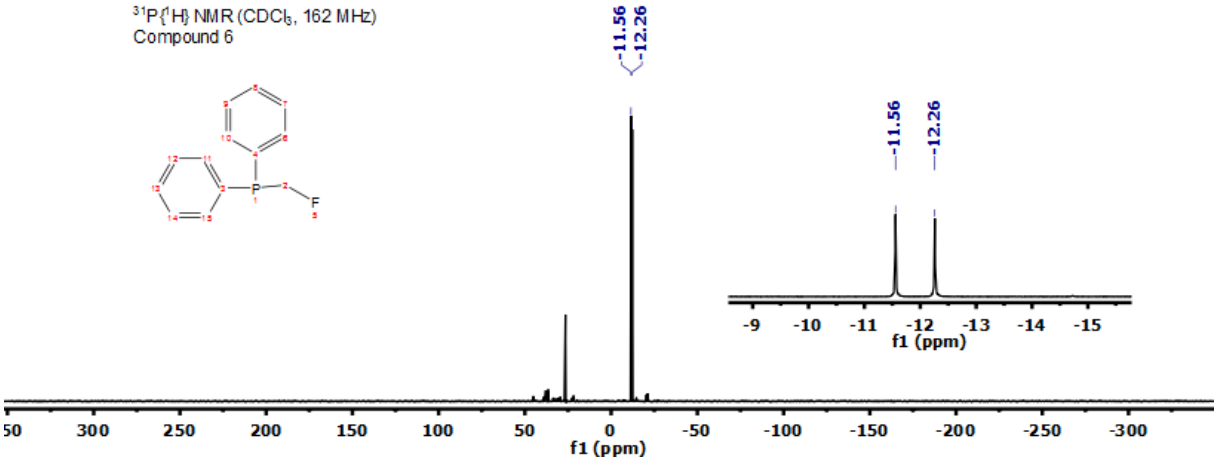


Figure S35: ^{31}P NMR spectrum of compound **6**

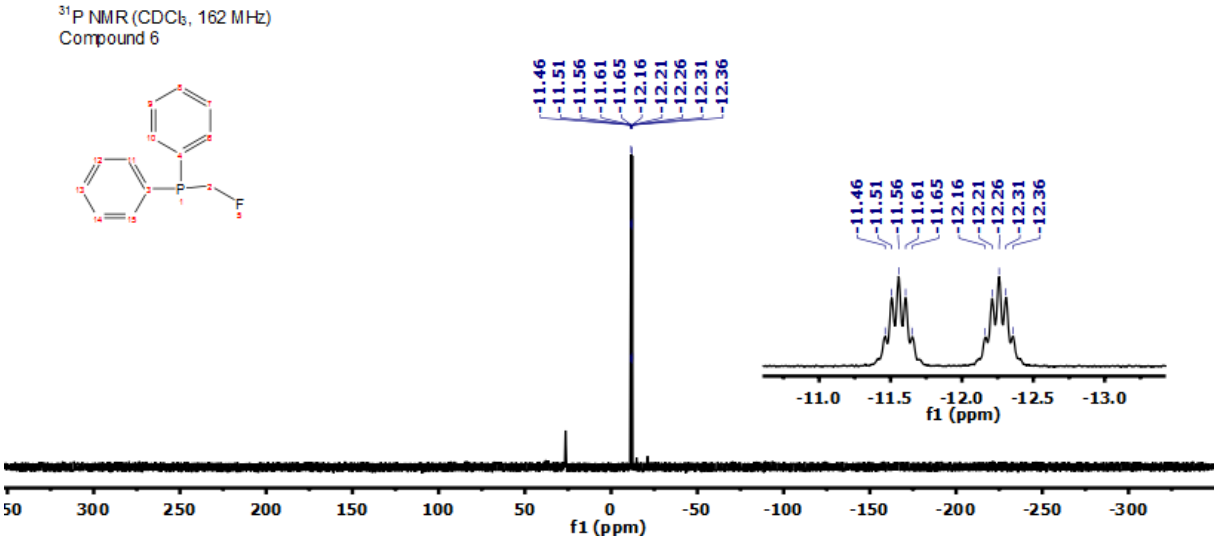
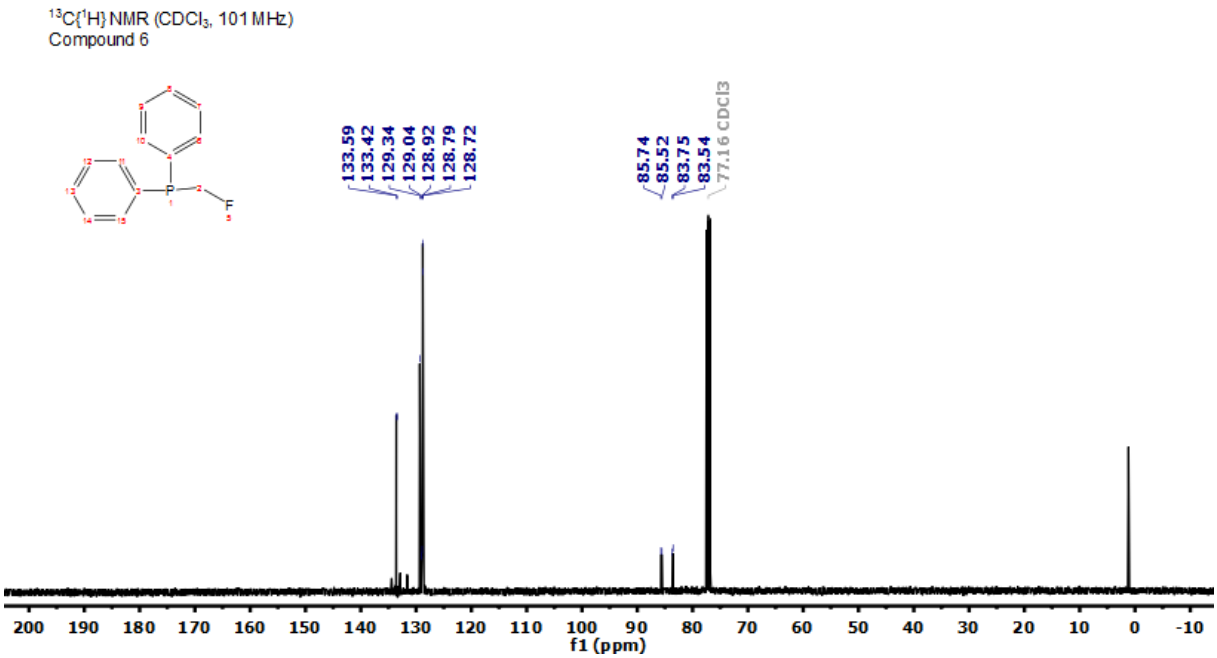


Figure S36: ^{13}C{^{1}H} NMR spectrum of compound **6**



2 Crystallographic refinement Data

2.1 Compound 1

Table S1: Crystallographic data for compound **1**

CCDC	1967513
Empirical formula	$C_4 H_{11} F I P$
Formula weight	236.00
Temperature	143(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*P*nma
Unit cell dimensions	a = 12.1430(5) Å
	b = 7.3397(3) Å
	c = 9.2655(5) Å
	α= 90°
	β= 90°
	γ = 90°
Volume	825.80(7) $Å^3$
Z	4
Density (calculated)	1.898 mg/m^3
Absorption coefficient	3.993 mm^{-1}
F(000)	448
Crystal size	0.100 x 0.050 x 0.050 mm^3
Theta range for data collection	4.356 - 30.493°
Index ranges	-17 ≤h ≤17, -10 ≤k ≤10, -13 ≤l ≤11
Reflections collected	8368
Independent reflections	1346 [R_{int} = 0.0395]
Data / restraints / parameters	1346 / 0 / 43
Goodness-of-fit on F^2	1.102
Final R indices [I>2sigma(I)]	R_1 = 0.0223, wR_2 = 0.0460
R indices (all data)	R_1 = 0.0313, wR_2 = 0.0504
Largest diff. peak and hole	1.020 and -0.573 e.$Å^{-3}$

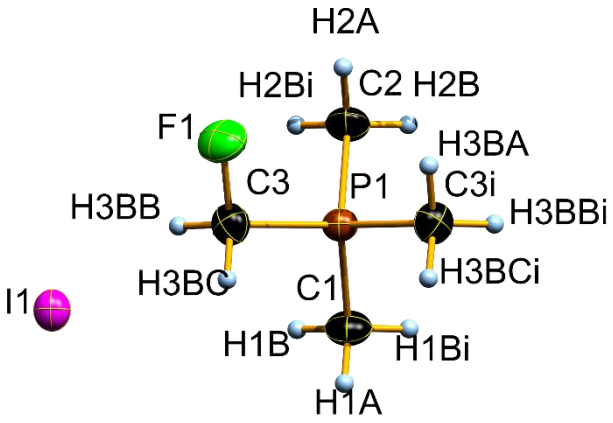


Figure S37: Molecular structure of compound **1** in the crystal; DIAMOND representation, thermal ellipsoids shown at 50 % probability level. The CH_2F group is disordered over two positions; only one of the positions is shown.

Table S2: Bond lengths [Å] and angles [°] of compound **1**.

P(1)-C(1)	1.768(3)	C(1)-P(1)-C(2)	110.0(2)	F(1)-C(3)-P(1)	108.8(2)
P(1)-C(2)	1.771(3)	C(1)-P(1)-C(3B)	109.6(2)	C(2)-P(1)-C(3)	109.8(2)
P(1)-C(3)	1.792(2)	C(2)-P(1)-C(3B)	109.8(2)	C(1)-P(1)-C(3)	109.6(2)
C(3)-F(1)	1.370(4)				

Table S3: Torsion angles [°] of product of **1**.

C(1)-P(1)-C(3)-F(1)	-176.1(2)	C(1)-(P1)-C(3)-H3BB	-60.0(2)
C(2)-P(1)-C(3)-F(1)	-55.2(3)	C(2)-(P1)-C(3)-H3BB	60.9(2)
C(3)-(P1)-C(1)-H1A	-59.3(3)	C(2)-(P1)-C(3)-H3BC	-179.2(2)
C(1)-(P1)-C(3)-H3BC	60.0(3)	C(3)-(P1)-C(1)-H1B	60.8(3)

2.2 Compound 2

Table S4: Crystallographic data for compound **2**

CCDC	1967516
Empirical formula	C_{13} H_{32} F I N_3 P
Formula weight	407.28
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	*P*-1
Unit cell dimensions	a = 10.0648(3) Å
	b = 10.1439(5) Å

	c = 18.6453(8) Å
	α= 93.292(4)°
	β= 92.580(3)°
	γ = 90.104(3)°
Volume	1898.53(14) Å^3
Z	4
Density (calculated)	1.425 mg/m^3
Absorption coefficient	1.774 mm^{-1}
F(000)	832
Crystal size	0.100 x 0.100 x 0.020 mm^3
Theta range for data collection	4.151 - 28.282°
Index ranges	-13 ≤h ≤13, -13 ≤k ≤13, -24 ≤l ≤24
Reflections collected	30663
Independent reflections	9397 [R_{int} = 0.0592]
Data / restraints / parameters	9397 / 0 / 367
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R_1 = 0.0430, wR_2 = 0.0717
R indices (all data)	R_1 = 0.0826, wR_2 = 0.0860
Largest diff. peak and hole	1.020 and -0.588 e.Å^{-3}

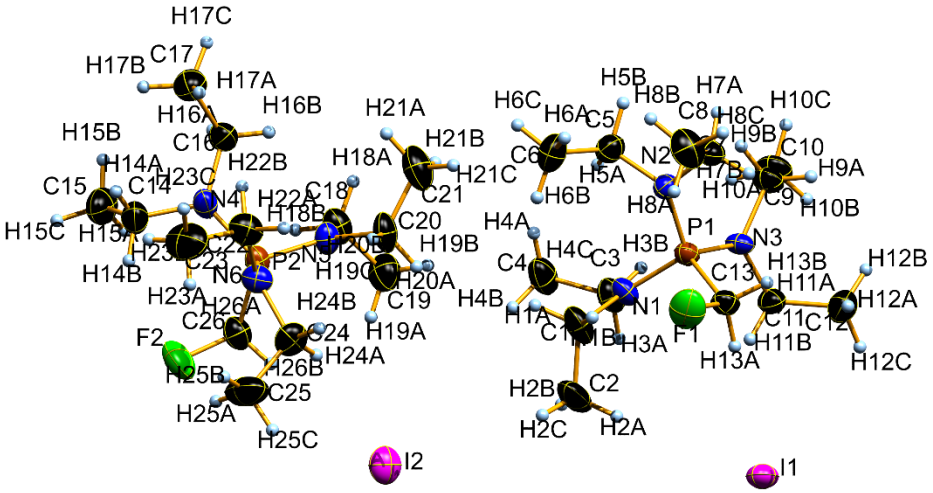


Figure S38: Molecular structure of compound **2** in the crystal, DIAMOND representation, thermal ellipsoids shown at 50 % probability level.

Table S5: Bond lengths [Å] and angles [°] of compound **2**.

P(1)-N(3)	1.612(3)	N(2)-C(5)	1.479(4)	C(11)-H(11B)	0.96(2)
P(1)-N(2)	1.620(3)	N(1)-C(3)	1.473(5)	C(16)-C(17)	1.514(5)
P(1)-N(1)	1.621(3)	N(1)-C(1)	1.479(4)	C(16)-H(16A)	0.95(2)

P(1)-C(13)	1.824(3)	C(19)-C(18)	1.506(5)	C(16)-H(16B)	0.95(2)
P(2)-N(5)	1.609(3)	C(13)-H(13A)	0.99(2)	C(2)-C(1)	1.502(5)
P(2)-N(6)	1.613(3)	C(13)-H(13B)	0.99(2)	C(26)-H(26A)	0.94(2)
P(2)-N(4)	1.616(3)	C(5)-C(6)	1.509(5)	C(26)-H(26B)	0.94(2)
P(2)-C(26)	1.813(4)	C(5)-H(5A)	0.99(2)	C(9)-C(10)	1.506(5)
N(5)-C(20)	1.486(4)	C(5)-H(5B)	0.99(2)	C(9)-H(9A)	0.98(2)
N(5)-C(18)	1.487(4)	C(7)-C(8)	1.505(5)	C(9)-H(9B)	0.98(2)
N(3)-C(9)	1.482(4)	C(7)-H(7A)	0.90(2)	C(4)-C(3)	1.516(5)
N(3)-C(11)	1.486(4)	C(7)-H(7B)	0.90(2)	C(15)-C(14)	1.510(6)
F(2)-C(26)	1.393(4)	N(4)-C(16)	1.479(4)	C(22)-C(23)	1.482(6)
N(6)-C(22)	1.483(5)	N(4)-C(14)	1.487(4)	C(14)-H(14A)	0.93(2)
N(6)-C(24)	1.500(4)	C(11)-C(12)	1.506(5)	C(14)-H(14B)	0.93(2)
F(1)-C(13)	1.378(4)	C(11)-H(11A)	0.96(2)	C(3)-H(3A)	0.95(2)
N(2)-C(7)	1.474(4)	C(24)-H(24B)	0.94(3)	C(3)-H(3B)	0.95(2)
C(11)-N(3)-P(1)	119.5(2)	N(3)-P(1)-N(2)	112.7(2)	C(18)-H(18A)	0.99(2)
C(22)-N(6)-C(24)	115.7(3)	N(3)-P(1)-N(1)	109.0(2)	C(18)-H(18B)	0.99(2)
C(22)-N(6)-P(2)	121.5(2)	N(2)-P(1)-N(1)	111.4(2)	C(20)-C(21)	1.497(5)
C(24)-N(6)-P(2)	119.4(2)	N(3)-P(1)-C(13)	106.7(2)	C(1)-H(1A)	1.00(3)
C(7)-N(2)-C(5)	116.4(3)	N(2)-P(1)-C(13)	106.4(2)	F(1)-C(13)-P(1)	112.5(2)
C(7)-N(2)-P(1)	120.6(2)	N(1)-P(1)-C(13)	110.5(2)	N(2)-C(5)-C(6)	113.1(3)
C(5)-N(2)-P(1)	121.4(2)	N(5)-P(2)-N(6)	113.4(2)	N(2)-C(7)-C(8)	114.5(3)
C(3)-N(1)-C(1)	116.5(3)	N(5)-P(2)-N(4)	109.4(2)	C(16)-N(4)-C(14)	116.1(3)
C(3)-N(1)-P(1)	123.1(2)	N(1)-C(3)-C(4)	113.7(3)	C(16)-N(4)-P(2)	123.7(2)
C(1)-N(1)-P(1)	120.4(3)	N(5)-C(18)-C(19)	112.8(3)	C(14)-N(4)-P(2)	120.2(2)
C(9)-N(3)-P(1)	123.5(2)	N(5)-C(20)-C(21)	113.1(3)	N(3)-C(11)-C(12)	113.4(3)
N(6)-P(2)-N(4)	110.8(2)	N(1)-C(1)-C(2)	113.7(4)	N(4)-C(16)-C(17)	114.2(3)
N(5)-P(2)-C(26)	105.5(2)	N(3)-C(9)-C(10)	112.8(3)	F(2)-C(26)-P(2)	112.8(3)
N(6)-P(2)-C(26)	106.8(2)	C(23)-C(22)-N(6)	113.6(3)	C(20)-N(5)-P(2)	123.5(2)
N(4)-P(2)-C(26)	110.8(2)	N(4)-C(14)-C(15)	111.9(4)	C(18)-N(5)-P(2)	120.3(2)
C(20)-N(5)-C(18)	116.1(3)	C(25)-C(24)-N(6)	114.3(3)	C(9)-N(3)-C(11)	116.0(3)
C(1)-H(1B)	1.00(3)	C(24)-C(25)	1.484(5)	C(24)-H(24A)	0.94(3)

Table S6: Torsion angles [°] of product of **2**.

N(6)-P(2)-N(5)-C(20)	-3.2(3)	N(6)-P(2)-N(4)-C(16)	110.3(3)
N(4)-P(2)-N(5)-C(20)	121.0(3)	C(26)-P(2)-N(4)-C(16)	-131.3(3)
C(26)-P(2)-N(5)-C(20)	-119.8(3)	N(5)-P(2)-N(4)-C(14)	163.8(3)
N(6)-P(2)-N(5)-C(18)	173.5(3)	N(6)-P(2)-N(4)-C(14)	-70.5(3)
N(4)-P(2)-N(5)-C(18)	-62.3(3)	C(26)-P(2)-N(4)-C(14)	47.9(4)
C(26)-P(2)-N(5)-C(18)	56.9(3)	C(9)-N(3)-C(11)-C(12)	57.9(4)
N(2)-P(1)-N(3)-C(9)	2.0(3)	P(1)-N(3)-C(11)-C(12)	-111.5(3)
N(1)-P(1)-N(3)-C(9)	126.3(3)	C(14)-N(4)-C(16)-C(17)	51.6(5)
C(13)-P(1)-N(3)-C(9)	-114.3(3)	P(2)-N(4)-C(16)-C(17)	-129.2(3)
N(2)-P(1)-N(3)-C(11)	170.6(3)	N(5)-P(2)-C(26)-F(2)	177.4(3)
N(1)-P(1)-N(3)-C(11)	-65.1(3)	N(6)-P(2)-C(26)-F(2)	56.4(3)
C(13)-P(1)-N(3)-C(11)	54.3(3)	N(4)-P(2)-C(26)-F(2)	-64.4(3)
N(5)-P(2)-N(6)-C(22)	88.7(3)	C(11)-N(3)-C(9)-C(10)	53.3(4)

N(4)-P(2)-N(6)-C(22)	-34.8(3)	P(1)-N(3)-C(9)-C(10)	-137.7(3)
C(26)-P(2)-N(6)-C(22)	-155.5(3)	C(24)-N(6)-C(22)-C(23)	-83.4(4)
N(5)-P(2)-N(6)-C(24)	-69.6(3)	P(2)-N(6)-C(22)-C(23)	117.6(4)
N(4)-P(2)-N(6)-C(24)	167.0(3)	C(16)-N(4)-C(14)-C(15)	59.9(5)
C(26)-P(2)-N(6)-C(24)	46.2(3)	P(2)-N(4)-C(14)-C(15)	-119.4(3)
N(3)-P(1)-N(2)-C(7)	-72.7(3)	C(1)-N(1)-C(3)-C(4)	51.5(4)
N(1)-P(1)-N(2)-C(7)	164.3(3)	P(1)-N(1)-C(3)-C(4)	-129.3(3)
C(13)-P(1)-N(2)-C(7)	43.8(3)	C(20)-N(5)-C(18)-C(19)	60.8(4)
N(3)-P(1)-N(2)-C(5)	91.9(3)	P(2)-N(5)-C(18)-C(19)	-116.1(3)
N(1)-P(1)-N(2)-C(5)	-31.1(3)	C(18)-N(5)-C(20)-C(21)	56.0(5)
C(13)-P(1)-N(2)-C(5)	-151.6(3)	P(2)-N(5)-C(20)-C(21)	-127.2(3)
N(3)-P(1)-N(1)-C(3)	-18.4(3)	C(3)-N(1)-C(1)-C(2)	60.7(5)
N(2)-P(1)-N(1)-C(3)	106.6(3)	P(1)-N(1)-C(1)-C(2)	-118.5(3)
C(13)-P(1)-N(1)-C(3)	-135.3(3)	C(22)-N(6)-C(24)-C(25)	90.3(4)
N(3)-P(1)-N(1)-C(1)	160.8(3)	P(2)-N(6)-C(24)-C(25)	-110.2(4)
N(2)-P(1)-N(1)-C(1)	-74.2(3)	P(1)-N(2)-C(5)-C(6)	106.7(3)
C(13)-P(1)-N(1)-C(1)	43.8(3)	C(5)-N(2)-C(7)-C(8)	79.1(4)
N(3)-P(1)-C(13)-F(1)	173.1(2)	P(1)-N(2)-C(7)-C(8)	-115.5(3)
N(2)-P(1)-C(13)-F(1)	52.6(3)	N(5)-P(2)-N(4)-C(16)	-15.4(4)
N(1)-P(1)-C(13)-F(1)	-68.5(3)	C(7)-N(2)-C(5)-C(6)	-88.1(4)

2.3 Compound 4

Table S7: Crystallographic data for compound **4**

CCDC	1967514
Empirical formula	$C_{10}H_{14}FIN_3P$
Formula weight	353.11
Temperature	143(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 8.7566(2) Å
	b = 9.3257(3) Å
	c = 17.2049(5) Å
	α= 90°
	β= 100.741(2)°
	γ = 90°
Volume	1380.36(7) $Å^3$
Z	4
Density (calculated)	1.699 mg/m^3
Absorption coefficient	2.427 mm^{-1}

F(000)	688
Crystal size	0.393 x 0.307 x 0.165 mm^3
Theta range for data collection	4.226 - 30.505°
Index ranges	-12 ≤h ≤12, -13 ≤k ≤13, -24 ≤l ≤24
Reflections collected	27409
Independent reflections	4202 [R_{int} = 0.0388]
Data / restraints / parameters	4202 / 0 / 152
Goodness-of-fit on F^2	1.021
Final R indices [I>2sigma(I)]	R_1 = 0.0241, wR_2 = 0.0497
R indices (all data)	R_1 = 0.0351, wR_2 = 0.0547
Largest diff. peak and hole	0.916 and -0.561 e.$Å^{-3}$

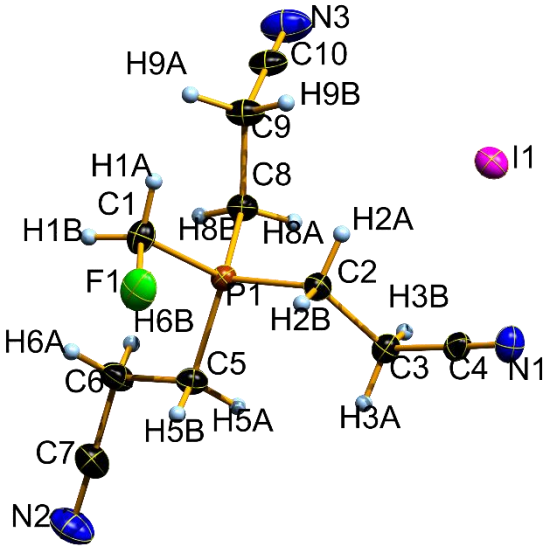


Figure S39: Molecular structure of compound **4** in the crystal; DIAMOND representation; thermal ellipsoids drawn at 50 % probability level.

Table S8: Bond lengths [Å] and angles [°] of compound **4**.

P(1)-C(2)	1.794(2)	C(2)-P(1)-C(8)	110.60(9)	C(9)-C(8)	1.531(3)
P(1)-C(5)	1.799(2)	C(5)-P(1)-C(8)	110.09(9)	C(9)-H(9A)	0.96(2)
P(1)-C(8)	1.804(2)	C(2)-P(1)-C(1)	105.84(9)	C(9)-H(9B)	0.96(2)
P(1)-C(1)	1.818(2)	C(5)-P(1)-C(1)	108.7(2)	C(5)-H(5A)	0.92(2)
C(2)-C(3)	1.532(3)	C(8)-P(1)-C(1)	111.27(9)	C(5)-H(5B)	0.92(2)
C(2)-H(2A)	0.92(2)	C(3)-C(2)-P(1)	115.9(2)	C(4)-N(1)	1.143(3)
C(2)-H(2B)	0.92(2)	C(7)-C(6)-C(5)	111.7(2)	C(4)-C(3)	1.465(3)
C(6)-C(7)	1.457(3)	N(3)-C(10)-C(9)	178.6(2)	C(8)-H(8A)	0.92(2)
C(6)-C(5)	1.535(3)	C(10)-C(9)-C(8)	109.7(2)	C(8)-H(8B)	0.92(2)
C(6)-H(6A)	0.92(2)	C(6)-C(5)-P(1)	112.7(2)	C(1)-H(1A)	0.93(2)
C(6)-H(6B)	0.92(2)	N(1)-C(4)-C(3)	176.1(2)	C(1)-H(1B)	0.93(2)

F(1)-C(1)	1.384(2)	C(9)-C(8)-P(1)	115.1(2)	C(3)-H(3A)	0.93(2)
N(2)-C(7)	1.140(3)	F(1)-C(1)-P(1)	106.9(2)	C(3)-H(3B)	0.93(2)
C(10)-N(3)	1.136(3)	C(4)-C(3)-C(2)	108.0(2)	C(2)-P(1)-C(5)	110.25(9)
C(10)-C(9)	1.469(3)	N(2)-C(7)-C(6)	178.6(3)		

Table S9: Torsion angles [°] of product of **4**.

C(5)-P(1)-C(2)-C(3)	41.2(2)	C(5)-P(1)-C(1)-F(1)	65.4(2)
C(8)-P(1)-C(2)-C(3)	-80.8(2)	C(8)-P(1)-C(1)-F(1)	-173.2(2)
C(1)-P(1)-C(2)-C(3)	158.6(2)	P(1)-C(2)-C(3)-C(4)	179.6(2)
C(7)-C(6)-C(5)-P(1)	-180.0(2)	C(2)-P(1)-C(8)-C(9)	-74.6(2)
C(2)-P(1)-C(5)-C(6)	-174.9(2)	C(5)-P(1)-C(8)-C(9)	163.3(2)
C(8)-P(1)-C(5)-C(6)	-52.6(2)	C(1)-P(1)-C(8)-C(9)	42.8(2)
C(1)-P(1)-C(5)-C(6)	69.6(1)	C(2)-P(1)-C(1)-F(1)	-53.0(2)
C(10)-C(9)-C(8)-P(1)	174.9(2)		

2.4 Compound 5

Table S10: Crystallographic data for compound **5**

CCDC	1967515
Empirical formula	$C_{37}\ H_{30.57}\ F\ I\ O_{1.28}\ P_2$
Formula weight	703.57
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	*P*-1
Unit cell dimensions	a = 11.3894(4) Å
	b = 13.0313(6) Å
	c = 13.4302(4) Å
	α= 64.227(4)°
	β= 66.641(3)°
	γ = 68.195(4)°
Volume	1599.41(13) $Å^3$
Z	2
Density (calculated)	1.461 mg/m^3
Absorption coefficient	1.136 mm^{-1}
F(000)	710
Crystal size	0.250 x 0.100 x 0.080 mm^3
Theta range for data collection	4.110 - 30.507°
Index ranges	-16 ≤h ≤16, -18 ≤k ≤18, -19 ≤l ≤19
Reflections collected	32102

Independent reflections	9734 [R_{int} = 0.0358]
Data / restraints / parameters	9734 / 3 / 422
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R_1 = 0.0410, wR_2 = 0.0929
R indices (all data)	R_1 = 0.0555, wR_2 = 0.1020
Largest diff. peak and hole	2.846 and -0.832 e.Å^{-3}

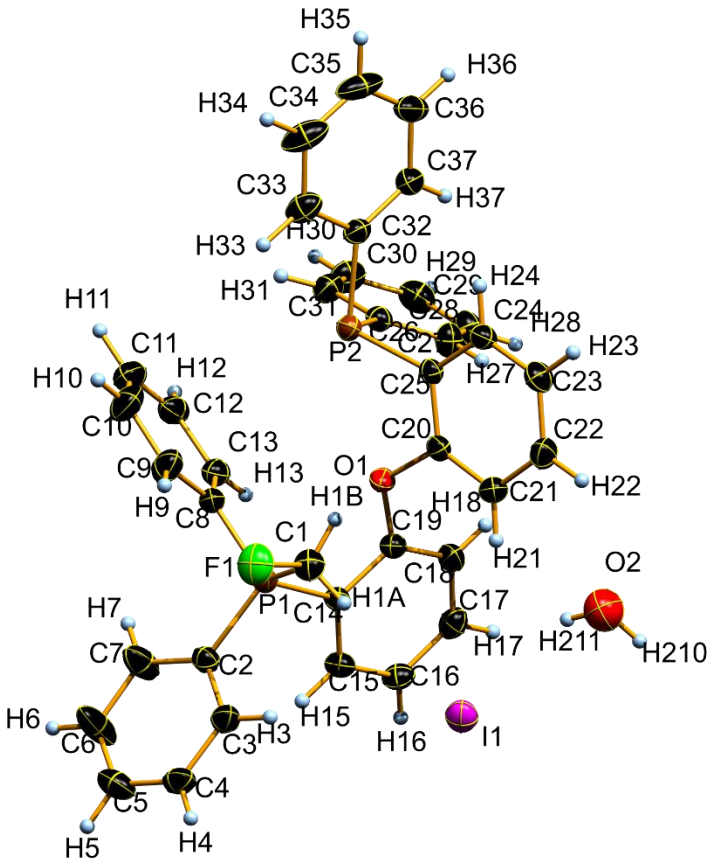


Figure S40: Molecular structure of compound **5** in the solid state, DIAMOND representation, thermal ellipsoids shown at 50 % probability level. Water position is only occupied by a third.

Table S11: Bond lengths [Å] and angles [°] of compound **5**.

P(2)-C(32)	1.829(2)	C(15)-C(16)	1.389(3)	C(23)-H(23)	0.93(3)
P(2)-C(26)	1.829(2)	C(15)-H(15)	0.95(3)	C(24)-H(24)	0.92(3)
P(2)-C(25)	1.844(2)	C(13)-C(8)	1.387(4)	C(26)-C(31)	1.390(3)
P(1)-C(2)	1.784(2)	C(13)-C(12)	1.397(4)	C(26)-C(27)	1.393(3)
P(1)-C(14)	1.784(2)	C(13)-H(13)	0.92(3)	C(18)-H(18)	0.85(3)
P(1)-C(8)	1.789(2)	C(19)-C(18)	1.383(3)	C(37)-C(36)	1.394(4)
P(1)-C(1)	1.831(3)	C(25)-C(24)	1.394(3)	C(37)-H(37)	0.94(3)
O(1)-C(19)	1.384(3)	C(25)-C(20)	1.394(3)	C(3)-C(4)	1.391(4)
O(1)-C(20)	1.393(3)	C(16)-C(17)	1.384(4)	C(3)-H(3)	0.95(3)
C(14)-C(15)	1.395(3)	C(16)-H(16)	0.86(3)	C(31)-C(30)	1.393(4)

C(14)-C(19)	1.398(3)	C(1)-F(1)	1.376(3)	C(31)-H(31)	0.93(3)
C(11)-C(12)	1.376(5)	C(1)-H(1A)	0.94(2)	C(28)-C(29)	1.381(4)
C(11)-C(10)	1.377(5)	C(1)-H(1B)	0.94(2)	C(28)-C(27)	1.388(4)
C(11)-H(11)	1.01(4)	C(20)-C(21)	1.391(3)	C(28)-H(28)	0.96(3)
C(22)-C(21)	1.386(4)	C(17)-C(18)	1.380(4)	C(7)-C(6)	1.388(4)
C(22)-C(23)	1.393(4)	C(12)-H(12)	0.90(4)	C(7)-H(7)	0.91(4)
C(22)-H(22)	0.94(3)	C(32)-C(37)	1.388(4)	C(8)-C(9)	1.397(4)
C(2)-C(7)	1.390(4)	C(32)-C(33)	1.400(4)	C(30)-C(29)	1.381(4)
C(2)-C(3)	1.396(3)	C(23)-C(24)	1.387(4)	C(30)-H(30)	0.88(4)
C(21)-H(21)	0.92(3)	C(14)-P(1)-C(8)	111.4(2)	C(27)-H(27)	0.90(3)
C(29)-H(29)	0.95(3)	C(2)-P(1)-C(1)	108.6(2)	C(23)-C(24)-C(25)	121.2(2)
C(33)-C(34)	1.380(4)	C(14)-P(1)-C(1)	107.2(2)	C(31)-C(26)-C(27)	118.6(2)
C(33)-H(33)	1.05(3)	C(8)-P(1)-C(1)	110.0(2)	C(31)-C(26)-P(2)	116.7(2)
C(4)-C(5)	1.375(4)	C(19)-O(1)-C(20)	121.7(2)	C(27)-C(26)-P(2)	124.7(2)
C(4)-H(4)	0.89(3)	C(15)-C(14)-C(19)	119.3(2)	C(17)-C(18)-C(19)	118.7(2)
C(9)-C(10)	1.391(4)	C(15)-C(14)-P(1)	122.2(2)	C(32)-C(37)-C(36)	120.3(3)
C(9)-H(9)	0.94(4)	C(19)-C(14)-P(1)	118.5(2)	C(4)-C(3)-C(2)	119.1(3)
C(36)-C(35)	1.379(5)	C(12)-C(11)-C(10)	120.8(3)	C(26)-C(31)-C(30)	120.5(2)
C(34)-C(35)	1.393(5)	C(21)-C(22)-C(23)	120.3(2)	C(29)-C(28)-C(27)	120.2(3)
C(34)-H(34)	0.99(4)	C(7)-C(2)-C(3)	120.4(2)	C(6)-C(7)-C(2)	119.7(3)
C(35)-H(35)	0.93(4)	C(7)-C(2)-P(1)	119.5(2)	C(13)-C(8)-C(9)	120.8(2)
C(5)-C(6)	1.383(5)	C(3)-C(2)-P(1)	120.0(2)	C(13)-C(8)-P(1)	120.5(2)
C(5)-H(5)	0.92(4)	C(16)-C(15)-C(14)	119.6(2)	C(9)-C(8)-P(1)	118.7(2)
C(10)-H(10)	0.92(4)	C(8)-C(13)-C(12)	119.2(3)	C(29)-C(30)-C(31)	120.1(3)
C(6)-H(6)	0.94(4)	C(18)-C(19)-O(1)	123.6(2)	C(28)-C(27)-C(26)	120.7(3)
O(2)-H(210)	0.89(2)	C(18)-C(19)-C(14)	121.1(2)	C(22)-C(21)-C(20)	118.2(2)
O(2)-H(211)	0.88(2)	O(1)-C(19)-C(14)	115.1(2)	C(30)-C(29)-C(28)	119.8(3)
C(32)-P(2)-C(26)	100.6(2)	C(24)-C(25)-C(20)	117.0(2)	C(34)-C(33)-C(32)	120.5(3)
C(32)-P(2)-C(25)	102.2(2)	C(24)-C(25)-P(2)	126.4(2)	C(5)-C(4)-C(3)	120.2(3)
C(26)-P(2)-C(25)	101.4(2)	C(20)-C(25)-P(2)	116.3(2)	C(10)-C(9)-C(8)	119.0(3)
C(2)-P(1)-C(14)	109.5(2)	C(17)-C(16)-C(15)	119.9(2)	C(35)-C(36)-C(37)	120.2(3)
C(2)-P(1)-C(8)	110.1(2)	F(1)-C(1)-P(1)	109.3(2)	C(33)-C(34)-C(35)	120.0(3)
C(37)-C(32)-C(33)	119.0(2)	C(21)-C(20)-O(1)	122.5(2)	C(36)-C(35)-C(34)	119.9(3)
C(37)-C(32)-P(2)	124.9(2)	C(21)-C(20)-C(25)	123.1(2)	C(4)-C(5)-C(6)	120.9(3)
C(33)-C(32)-P(2)	116.0(2)	O(1)-C(20)-C(25)	114.2(2)	C(11)-C(10)-C(9)	120.2(3)
C(24)-C(23)-C(22)	120.1(2)	C(18)-C(17)-C(16)	121.4(2)	C(5)-C(6)-C(7)	119.7(3)
C(11)-C(12)-C(13)	120.0(3)	H(210)-O(2)-H(211)	103(3)		

Table S12: Torsion angles [°] of product of **5**.

C(2)-P(1)-C(14)-C(15)	3.8(2)	C(15)-C(14)-C(19)-C(18)	0.1(3)
C(8)-P(1)-C(14)-C(15)	-118.2(2)	P(1)-C(14)-C(19)-C(18)	178.8(2)
C(1)-P(1)-C(14)-C(15)	121.4(2)	C(15)-C(14)-C(19)-O(1)	174.9(2)
C(2)-P(1)-C(14)-C(19)	-174.9(2)	P(1)-C(14)-C(19)-O(1)	-6.3(3)
C(8)-P(1)-C(14)-C(19)	63.1(2)	C(32)-P(2)-C(25)-C(24)	2.2(2)
C(1)-P(1)-C(14)-C(19)	-57.3(2)	C(26)-P(2)-C(25)-C(24)	105.8(2)
C(14)-P(1)-C(2)-C(7)	-95.3(2)	C(32)-P(2)-C(25)-C(20)	176.0(2)

C(8)-P(1)-C(2)-C(7)	27.5(3)	C(26)-P(2)-C(25)-C(20)	-80.3(2)
C(1)-P(1)-C(2)-C(7)	148.0(2)	C(14)-C(15)-C(16)-C(17)	-0.4(4)
C(14)-P(1)-C(2)-C(3)	82.4(2)	C(2)-P(1)-C(1)-F(1)	-50.7(2)
C(8)-P(1)-C(2)-C(3)	-154.8(2)	C(14)-P(1)-C(1)-F(1)	-168.9(2)
C(1)-P(1)-C(2)-C(3)	-34.3(2)	C(8)-P(1)-C(1)-F(1)	69.9(2)
C(19)-C(14)-C(15)-C(16)	0.1(3)	C(19)-O(1)-C(20)-C(21)	-29.9(3)
P(1)-C(14)-C(15)-C(16)	-178.6(2)	C(19)-O(1)-C(20)-C(25)	155.6(2)
C(20)-O(1)-C(19)-C(18)	-53.0(3)	C(24)-C(25)-C(20)-C(21)	1.1(3)
C(20)-O(1)-C(19)-C(14)	132.3(2)	P(2)-C(25)-C(20)-C(21)	-173.4(2)
C(26)-P(2)-C(32)-C(37)	-33.2(2)	C(24)-C(25)-C(20)-O(1)	175.6(2)
C(25)-P(2)-C(32)-C(37)	71.1(2)	P(2)-C(25)-C(20)-O(1)	1.1(3)
C(26)-P(2)-C(32)-C(33)	145.4(2)	C(15)-C(16)-C(17)-C(18)	0.4(4)
C(25)-P(2)-C(32)-C(33)	-110.4(2)	C(10)-C(11)-C(12)-C(13)	-0.8(4)
C(21)-C(22)-C(23)-C(24)	0.3(4)	C(8)-C(13)-C(12)-C(11)	1.6(4)
C(22)-C(23)-C(24)-C(25)	-0.6(4)	C(14)-P(1)-C(8)-C(13)	16.6(2)
C(20)-C(25)-C(24)-C(23)	0.0(3)	C(1)-P(1)-C(8)-C(13)	135.2(2)
P(2)-C(25)-C(24)-C(23)	173.8(2)	C(2)-P(1)-C(8)-C(9)	75.3(2)
C(32)-P(2)-C(26)-C(31)	-76.5(2)	C(14)-P(1)-C(8)-C(9)	-163.1(2)
C(25)-P(2)-C(26)-C(31)	178.6(2)	C(1)-P(1)-C(8)-C(9)	-44.4(2)
C(32)-P(2)-C(26)-C(27)	103.5(2)	C(26)-C(31)-C(30)-C(29)	1.6(4)
C(25)-P(2)-C(26)-C(27)	-1.4(2)	C(29)-C(28)-C(27)-C(26)	0.3(4)
C(16)-C(17)-C(18)-C(19)	-0.2(4)	C(31)-C(26)-C(27)-C(28)	1.7(4)
O(1)-C(19)-C(18)-C(17)	-174.4(2)	P(2)-C(26)-C(27)-C(28)	-178.3(2)
C(14)-C(19)-C(18)-C(17)	0.0(4)	C(23)-C(22)-C(21)-C(20)	0.7(4)
C(33)-C(32)-C(37)-C(36)	1.6(4)	O(1)-C(20)-C(21)-C(22)	-175.4(2)
P(2)-C(32)-C(37)-C(36)	-179.9(2)	C(25)-C(20)-C(21)-C(22)	-1.4(4)
C(7)-C(2)-C(3)-C(4)	-0.6(4)	C(31)-C(30)-C(29)-C(28)	0.5(4)
P(1)-C(2)-C(3)-C(4)	-178.3(2)	C(27)-C(28)-C(29)-C(30)	-1.4(4)
C(27)-C(26)-C(31)-C(30)	-2.6(4)	C(37)-C(32)-C(33)-C(34)	-1.2(4)
P(2)-C(26)-C(31)-C(30)	177.3(2)	P(2)-C(32)-C(33)-C(34)	-179.8(2)
C(3)-C(2)-C(7)-C(6)	-0.7(5)	C(2)-C(3)-C(4)-C(5)	1.9(4)
P(1)-C(2)-C(7)-C(6)	177.0(3)	C(13)-C(8)-C(9)-C(10)	-0.4(4)
C(12)-C(13)-C(8)-C(9)	-0.9(4)	P(1)-C(8)-C(9)-C(10)	179.2(2)
C(12)-C(13)-C(8)-P(1)	179.5(2)	C(32)-C(37)-C(36)-C(35)	-0.5(4)
C(2)-P(1)-C(8)-C(13)	-105.1(2)	C(32)-C(33)-C(34)-C(35)	-0.2(5)
C(12)-C(11)-C(10)-C(9)	-0.6(5)	C(37)-C(36)-C(35)-C(34)	-0.9(4)
C(8)-C(9)-C(10)-C(11)	1.2(5)	C(33)-C(34)-C(35)-C(36)	1.2(5)
C(4)-C(5)-C(6)-C(7)	0.7(5)	C(3)-C(4)-C(5)-C(6)	-2.0(5)
C(2)-C(7)-C(6)-C(5)	0.7(5)		

2.5 Compound 6b

Table S13: Crystallographic data for compound **6**

CCDC	1967517
Empirical formula	C_{13} H_{12} F O P
Formula weight	234.20
Temperature	143(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	*P*-1
Unit cell dimensions	a = 11.5552(17) Å
	b = 13.7077(16) Å
	c = 17.2666(11) Å
	α= 69.635(9)°
	β= 78.081(9)°
	γ = 65.391(13)°
Volume	2325.0(5) $Å^3$
Z	8
Density (calculated)	1.338 mg/m^3
Absorption coefficient	0.224 mm^{-1}
F(000)	976
Crystal size	0.200 x 0.200 x 0.100 mm^3
Theta range for data collection	4.104 - 26.372°
Index ranges	-14 ≤h ≤14, -17 ≤k ≤17, -21 ≤l ≤21
Reflections collected	34798
Independent reflections	9439 [R_{int} = 0.0508]
Data / restraints / parameters	9439 / 0 / 624
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R_1 = 0.0489, wR_2 = 0.1157
R indices (all data)	R_1 = 0.0929, wR_2 = 0.1424
Largest diff. peak and hole	0.470 and -0.289 e.$Å^{-3}$

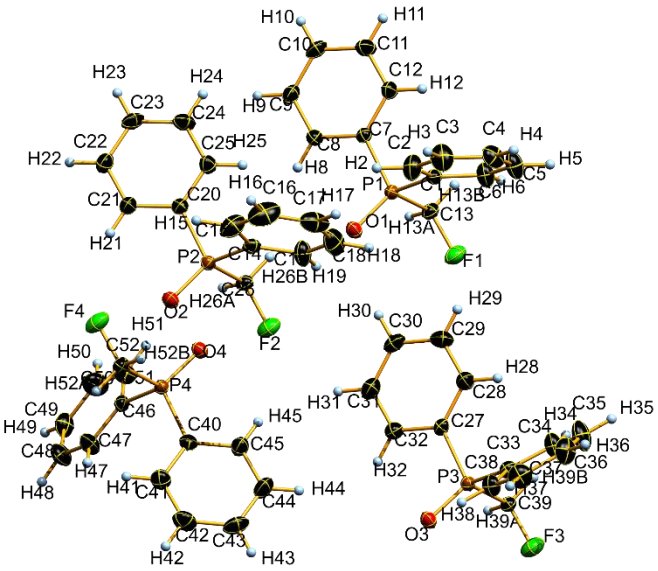


Figure S41: Molecular structure of (fluoromethyl)diphenyl phosphine oxide in the crystal. DIAMOND representation, thermal ellipsoids shown at 50 % probability level.

Table S14: Bond lengths [Å] and angles [°] of compound **6**.

P(1)-O(1)	1.489(2)	C(33)-C(34)	1.395(3)	C(48)-C(47)	1.386(3)
P(1)-C(7)	1.801(2)	C(45)-C(44)	1.391(3)	C(48)-H(48)	0.90(3)
P(1)-C(1)	1.809(2)	C(45)-H(45)	0.91(3)	C(47)-H(47)	0.87(3)
P(1)-C(13)	1.815(2)	C(52)-H(52A)	0.98(2)	C(22)-H(22)	0.95(3)
P(2)-O(2)	1.486(2)	C(52)-H(52B)	0.98(2)	C(51)-C(50)	1.391(3)
P(2)-C(20)	1.800(2)	C(6)-C(5)	1.390(3)	C(51)-H(51)	0.95(3)
P(2)-C(14)	1.812(2)	C(6)-H(6)	0.97(3)	C(34)-C(35)	1.387(3)
P(2)-C(26)	1.817(2)	C(31)-C(30)	1.377(4)	C(34)-H(34)	0.97(3)
P(3)-O(3)	1.490(2)	C(31)-C(32)	1.394(3)	C(42)-H(42)	0.95(3)
P(3)-C(33)	1.807(2)	C(31)-H(31)	0.97(3)	C(29)-C(28)	1.390(3)
P(3)-C(27)	1.807(2)	C(30)-C(29)	1.386(4)	C(29)-H(29)	0.91(3)
P(3)-C(39)	1.813(2)	C(30)-H(30)	0.93(3)	C(36)-C(35)	1.375(4)
P(4)-O(4)	1.489(2)	C(25)-C(24)	1.383(3)	C(36)-H(36)	0.97(3)
P(4)-C(40)	1.803(2)	C(25)-H(25)	0.93(2)	C(50)-H(50)	0.94(3)
P(4)-C(46)	1.816(2)	C(12)-C(11)	1.383(3)	C(15)-C(16)	1.381(4)
P(4)-C(52)	1.817(2)	C(12)-H(12)	0.92(2)	C(15)-H(15)	1.00(3)
F(2)-C(26)	1.393(2)	C(21)-C(22)	1.390(3)	C(28)-H(28)	0.94(3)
F(4)-C(52)	1.383(3)	C(21)-H(21)	0.91(3)	C(35)-H(35)	0.93(3)
F(1)-C(13)	1.398(2)	C(19)-C(18)	1.393(3)	C(44)-H(44)	0.96(3)
F(3)-C(39)	1.390(2)	C(19)-H(19)	0.94(3)	C(16)-C(17)	1.367(4)
C(1)-C(6)	1.389(3)	C(24)-C(23)	1.385(4)	C(16)-H(16)	0.93(3)
C(1)-C(2)	1.393(3)	C(24)-H(24)	0.93(3)	C(17)-C(18)	1.380(4)
C(26)-H(26A)	0.99(2)	C(32)-H(32)	0.95(2)	C(17)-H(17)	0.96(3)
C(26)-H(26B)	0.99(2)	C(37)-C(36)	1.385(4)	C(18)-H(18)	0.95(3)
C(39)-H(39A)	1.01(2)	C(37)-H(37)	0.88(3)	O(1)-P(1)-C(7)	112.2(2)
C(39)-H(39B)	1.01(2)	C(41)-C(42)	1.388(3)	O(1)-P(1)-C(1)	113.2(2)
C(40)-C(41)	1.388(3)	C(41)-H(41)	0.93(3)	C(7)-P(1)-C(1)	108.3(2)

C(40)-C(45)	1.392(3)	C(10)-C(11)	1.387(4)	O(1)-P(1)-C(13)	113.3(2)
C(20)-C(25)	1.392(3)	C(10)-H(10)	0.91(3)	C(7)-P(1)-C(13)	102.7(2)
C(20)-C(21)	1.398(3)	C(11)-H(11)	0.91(3)	C(1)-P(1)-C(13)	106.5(2)
C(9)-C(10)	1.384(3)	C(49)-C(48)	1.377(4)	O(2)-P(2)-C(20)	112.3(2)
C(9)-C(8)	1.397(3)	C(49)-C(50)	1.381(4)	O(2)-P(2)-C(14)	113.5(2)
C(9)-H(9)	0.95(3)	C(49)-H(49)	0.95(3)	C(20)-P(2)-C(14)	107.7(2)
C(46)-C(51)	1.387(3)	C(8)-H(8)	0.93(2)	O(2)-P(2)-C(26)	113.5(2)
C(46)-C(47)	1.391(3)	C(4)-C(5)	1.372(4)	C(20)-P(2)-C(26)	102.4(2)
C(14)-C(15)	1.385(3)	C(4)-C(3)	1.375(4)	C(14)-P(2)-C(26)	106.7(2)
C(14)-C(19)	1.387(3)	C(4)-H(4)	0.96(3)	O(3)-P(3)-C(33)	111.9(2)
C(27)-C(28)	1.393(3)	C(3)-C(2)	1.384(4)	O(3)-P(3)-C(27)	111.4(2)
C(27)-C(32)	1.395(3)	C(3)-H(3)	0.92(3)	C(33)-P(3)-C(27)	110.2(2)
C(13)-H(13A)	0.99(2)	C(23)-C(22)	1.387(4)	O(3)-P(3)-C(39)	113.9(2)
C(13)-H(13B)	0.98(2)	C(23)-H(23)	0.91(3)	C(33)-P(3)-C(39)	106.3(2)
C(7)-C(12)	1.391(3)	C(2)-H(2)	0.97(3)	C(27)-P(3)-C(39)	102.7(2)
C(7)-C(8)	1.395(3)	C(5)-H(5)	0.96(3)	O(4)-P(4)-C(40)	112.7(2)
C(38)-C(37)	1.394(3)	C(43)-C(44)	1.383(4)	O(4)-P(4)-C(46)	110.8(2)
C(38)-C(33)	1.396(3)	C(43)-C(42)	1.392(4)	C(40)-P(4)-C(46)	109.9(2)
C(38)-H(38)	0.93(2)	C(43)-H(43)	0.89(3)	O(4)-P(4)-C(52)	113.9(2)
C(40)-P(4)-C(52)	102.19(11)	C(7)-C(8)-C(9)	119.9(2)	C(12)-C(7)-P(1)	122.9(2)
C(46)-P(4)-C(52)	106.82(11)	C(5)-C(4)-C(3)	120.0(3)	C(8)-C(7)-P(1)	117.5(2)
C(6)-C(1)-C(2)	119.3(2)	C(4)-C(3)-C(2)	119.9(3)	C(37)-C(38)-C(33)	120.1(3)
C(6)-C(1)-P(1)	124.2(2)	C(24)-C(23)-C(22)	120.2(2)	C(34)-C(33)-C(38)	119.2(2)
C(2)-C(1)-P(1)	116.5(2)	C(3)-C(2)-C(1)	120.4(3)	C(34)-C(33)-P(3)	124.2(2)
F(2)-C(26)-P(2)	109.9(2)	C(4)-C(5)-C(6)	120.9(3)	C(38)-C(33)-P(3)	116.6(2)
F(3)-C(39)-P(3)	109.1(2)	C(44)-C(43)-C(42)	119.8(3)	C(44)-C(45)-C(40)	120.3(3)
C(41)-C(40)-C(45)	119.5(2)	C(49)-C(48)-C(47)	120.0(3)	F(4)-C(52)-P(4)	109.2(2)
C(41)-C(40)-P(4)	123.9(2)	C(49)-C(48)-H(48)	121(2)	C(1)-C(6)-C(5)	119.3(3)
C(45)-C(40)-P(4)	116.5(2)	C(47)-C(48)-H(48)	118(2)	C(30)-C(31)-C(32)	120.1(3)
C(25)-C(20)-C(21)	119.9(2)	C(48)-C(47)-C(46)	120.7(3)	C(31)-C(30)-C(29)	120.0(2)
C(25)-C(20)-P(2)	122.5(2)	C(23)-C(22)-C(21)	119.8(3)	C(24)-C(25)-C(20)	119.7(2)
C(21)-C(20)-P(2)	117.6(2)	C(46)-C(51)-C(50)	120.3(3)	C(11)-C(12)-C(7)	120.3(2)
C(10)-C(9)-C(8)	119.9(2)	C(35)-C(34)-C(33)	120.1(3)	C(22)-C(21)-C(20)	119.9(2)
C(51)-C(46)-C(47)	118.8(2)	C(41)-C(42)-C(43)	120.2(3)	C(14)-C(19)-C(18)	120.1(3)
C(51)-C(46)-P(4)	117.0(2)	C(30)-C(29)-C(28)	120.4(3)	C(25)-C(24)-C(23)	120.5(3)
C(47)-C(46)-P(4)	124.1(2)	C(35)-C(36)-C(37)	120.1(3)	C(31)-C(32)-C(27)	120.2(2)
C(15)-C(14)-C(19)	119.2(2)	C(49)-C(50)-C(51)	120.2(3)	C(36)-C(37)-C(38)	120.0(3)
C(15)-C(14)-P(2)	117.6(2)	C(16)-C(15)-C(14)	120.2(3)	C(42)-C(41)-C(40)	120.1(3)
C(19)-C(14)-P(2)	123.2(2)	C(29)-C(28)-C(27)	120.0(2)	C(9)-C(10)-C(11)	120.2(2)
C(28)-C(27)-C(32)	119.3(2)	C(36)-C(35)-C(34)	120.5(3)	C(12)-C(11)-C(10)	120.2(2)
C(28)-C(27)-P(3)	124.2(2)	C(43)-C(44)-C(45)	120.0(3)	C(48)-C(49)-C(50)	120.0(3)
C(32)-C(27)-P(3)	116.6(2)	C(17)-C(16)-C(15)	120.7(3)	C(17)-C(18)-C(19)	119.9(3)
F(1)-C(13)-P(1)	109.2(2)	C(16)-C(17)-C(18)	120.0(3)	C(12)-C(7)-C(8)	119.6(2)

Table S15: Torsion angles [°] of product of **6**.

O(1)-P(1)-C(1)-C(6)	132.0(2)	P(2)-C(20)-C(25)-C(24)	179.8(2)
C(7)-P(1)-C(1)-C(6)	-103.0(2)	C(8)-C(7)-C(12)-C(11)	0.7(4)

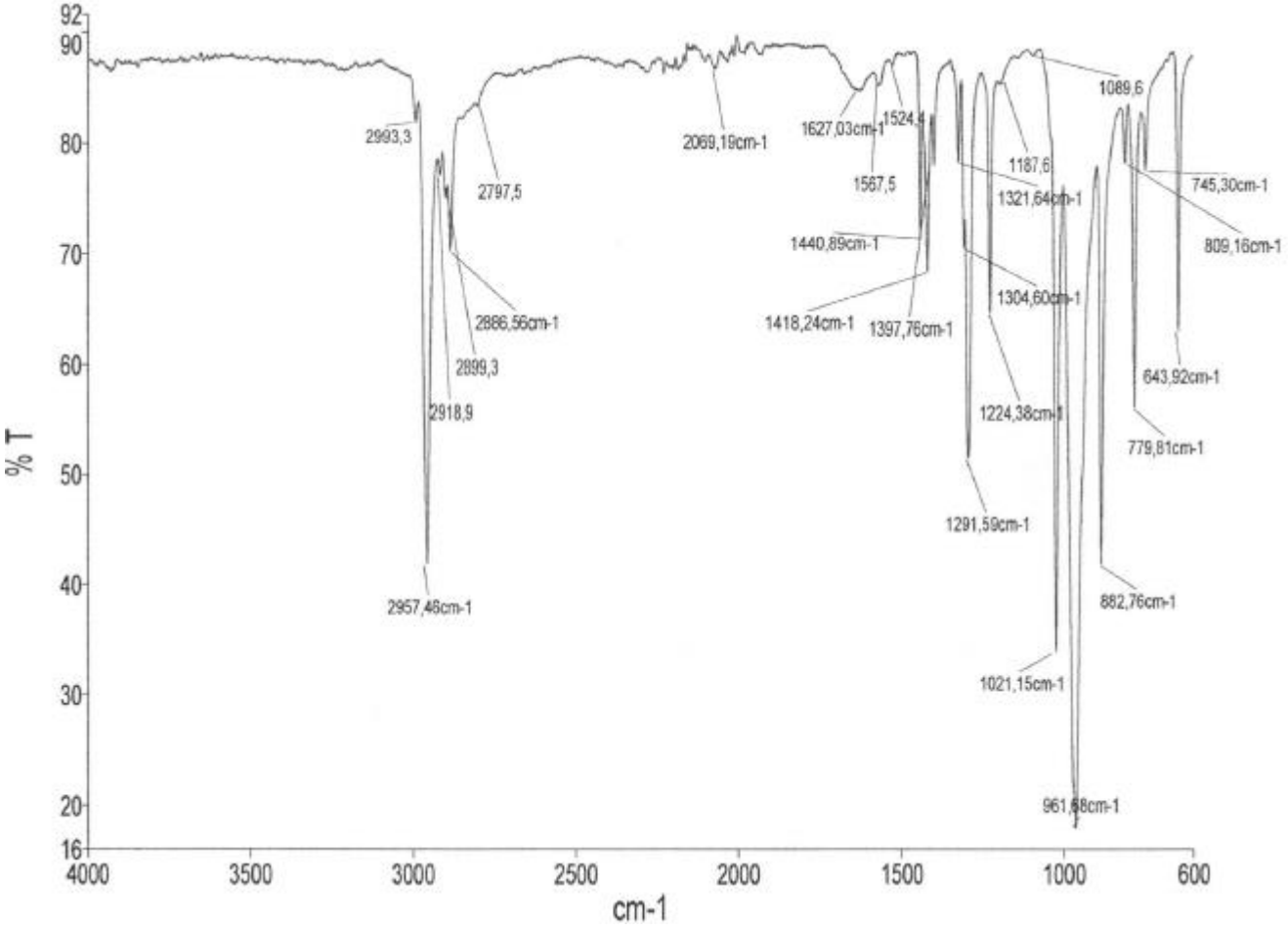
C(13)-P(1)-C(1)-C(6)	6.9(2)	P(1)-C(7)-C(12)-C(11)	-178.9(2)
O(1)-P(1)-C(1)-C(2)	-46.5(2)	C(25)-C(20)-C(21)-C(22)	-0.7(4)
C(7)-P(1)-C(1)-C(2)	78.5(2)	P(2)-C(20)-C(21)-C(22)	179.9(2)
C(13)-P(1)-C(1)-C(2)	-171.7(2)	C(15)-C(14)-C(19)-C(18)	1.9(4)
O(2)-P(2)-C(26)-F(2)	-58.0(2)	P(2)-C(14)-C(19)-C(18)	-176.8(2)
C(20)-P(2)-C(26)-F(2)	-179.3(2)	C(20)-C(25)-C(24)-C(23)	0.5(4)
C(14)-P(2)-C(26)-F(2)	67.7(2)	C(30)-C(31)-C(32)-C(27)	-0.3(4)
O(3)-P(3)-C(39)-F(3)	-61.0(2)	C(28)-C(27)-C(32)-C(31)	-0.8(4)
C(33)-P(3)-C(39)-F(3)	62.7(2)	P(3)-C(27)-C(32)-C(31)	179.5(2)
C(27)-P(3)-C(39)-F(3)	178.5(2)	C(33)-C(38)-C(37)-C(36)	-0.4(4)
O(4)-P(4)-C(40)-C(41)	170.9(2)	C(45)-C(40)-C(41)-C(42)	-2.0(4)
C(46)-P(4)-C(40)-C(41)	-64.9(2)	P(4)-C(40)-C(41)-C(42)	-179.9(2)
C(52)-P(4)-C(40)-C(41)	48.2(2)	C(8)-C(9)-C(10)-C(11)	1.5(4)
O(4)-P(4)-C(40)-C(45)	-7.1(2)	C(7)-C(12)-C(11)-C(10)	0.3(4)
C(46)-P(4)-C(40)-C(45)	117.1(2)	C(9)-C(10)-C(11)-C(12)	-1.5(4)
C(52)-P(4)-C(40)-C(45)	-129.8(2)	C(12)-C(7)-C(8)-C(9)	-0.6(4)
O(2)-P(2)-C(20)-C(25)	173.5(2)	P(1)-C(7)-C(8)-C(9)	179.0(2)
C(14)-P(2)-C(20)-C(25)	47.9(2)	C(10)-C(9)-C(8)-C(7)	-0.5(4)
C(26)-P(2)-C(20)-C(25)	-64.4(2)	C(5)-C(4)-C(3)-C(2)	0.6(4)
O(2)-P(2)-C(20)-C(21)	-7.1(2)	C(25)-C(24)-C(23)-C(22)	-1.4(4)
C(14)-P(2)-C(20)-C(21)	-132.8(2)	C(4)-C(3)-C(2)-C(1)	0.2(4)
C(26)-P(2)-C(20)-C(21)	115.0(2)	C(6)-C(1)-C(2)-C(3)	-1.5(4)
O(4)-P(4)-C(46)-C(51)	-13.2(2)	P(1)-C(1)-C(2)-C(3)	177.1(2)
C(40)-P(4)-C(46)-C(51)	-138.5(2)	C(3)-C(4)-C(5)-C(6)	-0.2(4)
C(52)-P(4)-C(46)-C(51)	111.4(2)	C(1)-C(6)-C(5)-C(4)	-1.1(4)
O(4)-P(4)-C(46)-C(47)	166.3(2)	C(50)-C(49)-C(48)-C(47)	-0.6(4)
C(40)-P(4)-C(46)-C(47)	41.1(2)	C(49)-C(48)-C(47)-C(46)	-0.2(4)
C(52)-P(4)-C(46)-C(47)	-69.0(2)	C(51)-C(46)-C(47)-C(48)	0.8(4)
O(2)-P(2)-C(14)-C(15)	-58.7(2)	P(4)-C(46)-C(47)-C(48)	-178.7(2)
C(20)-P(2)-C(14)-C(15)	66.2(2)	C(24)-C(23)-C(22)-C(21)	1.2(4)
C(26)-P(2)-C(14)-C(15)	175.5(2)	C(20)-C(21)-C(22)-C(23)	-0.2(4)
O(2)-P(2)-C(14)-C(19)	120.0(2)	C(47)-C(46)-C(51)-C(50)	-0.7(4)
C(20)-P(2)-C(14)-C(19)	-115.1(2)	P(4)-C(46)-C(51)-C(50)	178.9(2)
C(26)-P(2)-C(14)-C(19)	-5.8(2)	C(38)-C(33)-C(34)-C(35)	-2.6(4)
O(3)-P(3)-C(27)-C(28)	156.6(2)	P(3)-C(33)-C(34)-C(35)	179.5(2)
C(33)-P(3)-C(27)-C(28)	31.8(2)	C(40)-C(41)-C(42)-C(43)	0.5(4)
C(39)-P(3)-C(27)-C(28)	-81.1(2)	C(44)-C(43)-C(42)-C(41)	1.4(4)
O(3)-P(3)-C(27)-C(32)	-23.7(2)	C(31)-C(30)-C(29)-C(28)	-0.6(4)
C(33)-P(3)-C(27)-C(32)	-148.5(2)	C(38)-C(37)-C(36)-C(35)	-0.3(4)
C(39)-P(3)-C(27)-C(32)	98.6(2)	C(48)-C(49)-C(50)-C(51)	0.8(4)
O(1)-P(1)-C(13)-F(1)	-59.7(2)	C(46)-C(51)-C(50)-C(49)	-0.1(4)
C(7)-P(1)-C(13)-F(1)	179.1(2)	C(19)-C(14)-C(15)-C(16)	-0.7(4)
C(1)-P(1)-C(13)-F(1)	65.4(2)	P(2)-C(14)-C(15)-C(16)	178.1(2)
O(1)-P(1)-C(7)-C(12)	160.6(2)	C(30)-C(29)-C(28)-C(27)	-0.4(4)
C(1)-P(1)-C(7)-C(12)	35.0(2)	C(32)-C(27)-C(28)-C(29)	1.1(4)
C(13)-P(1)-C(7)-C(12)	-77.4(2)	P(3)-C(27)-C(28)-C(29)	-179.2(2)
O(1)-P(1)-C(7)-C(8)	-19.1(2)	C(37)-C(36)-C(35)-C(34)	-0.5(4)

C(1)-P(1)-C(7)-C(8)	-144.7(2)	C(33)-C(34)-C(35)-C(36)	1.9(4)
C(13)-P(1)-C(7)-C(8)	103.0(2)	C(42)-C(43)-C(44)-C(45)	-1.9(4)
C(37)-C(38)-C(33)-C(34)	1.8(4)	C(40)-C(45)-C(44)-C(43)	0.4(4)
C(37)-C(38)-C(33)-P(3)	179.9(2)	C(14)-C(15)-C(16)-C(17)	-0.8(5)
O(3)-P(3)-C(33)-C(34)	165.5(2)	C(15)-C(16)-C(17)-C(18)	1.0(5)
C(27)-P(3)-C(33)-C(34)	-70.0(2)	C(16)-C(17)-C(18)-C(19)	0.3(4)
C(39)-P(3)-C(33)-C(34)	40.6(2)	C(14)-C(19)-C(18)-C(17)	-1.7(4)
O(3)-P(3)-C(33)-C(38)	-12.5(2)	C(40)-P(4)-C(52)-F(4)	-180.0(2)
C(27)-P(3)-C(33)-C(38)	112.0(2)	C(46)-P(4)-C(52)-F(4)	-64.5(2)
C(39)-P(3)-C(33)-C(38)	-137.4(2)	C(2)-C(1)-C(6)-C(5)	1.9(4)
C(41)-C(40)-C(45)-C(44)	1.5(4)	P(1)-C(1)-C(6)-C(5)	-176.6(2)
P(4)-C(40)-C(45)-C(44)	179.6(2)	C(32)-C(31)-C(30)-C(29)	1.0(4)
O(4)-P(4)-C(52)-F(4)	58.2(2)	C(21)-C(20)-C(25)-C(24)	0.5(3)

3 IR Spectra

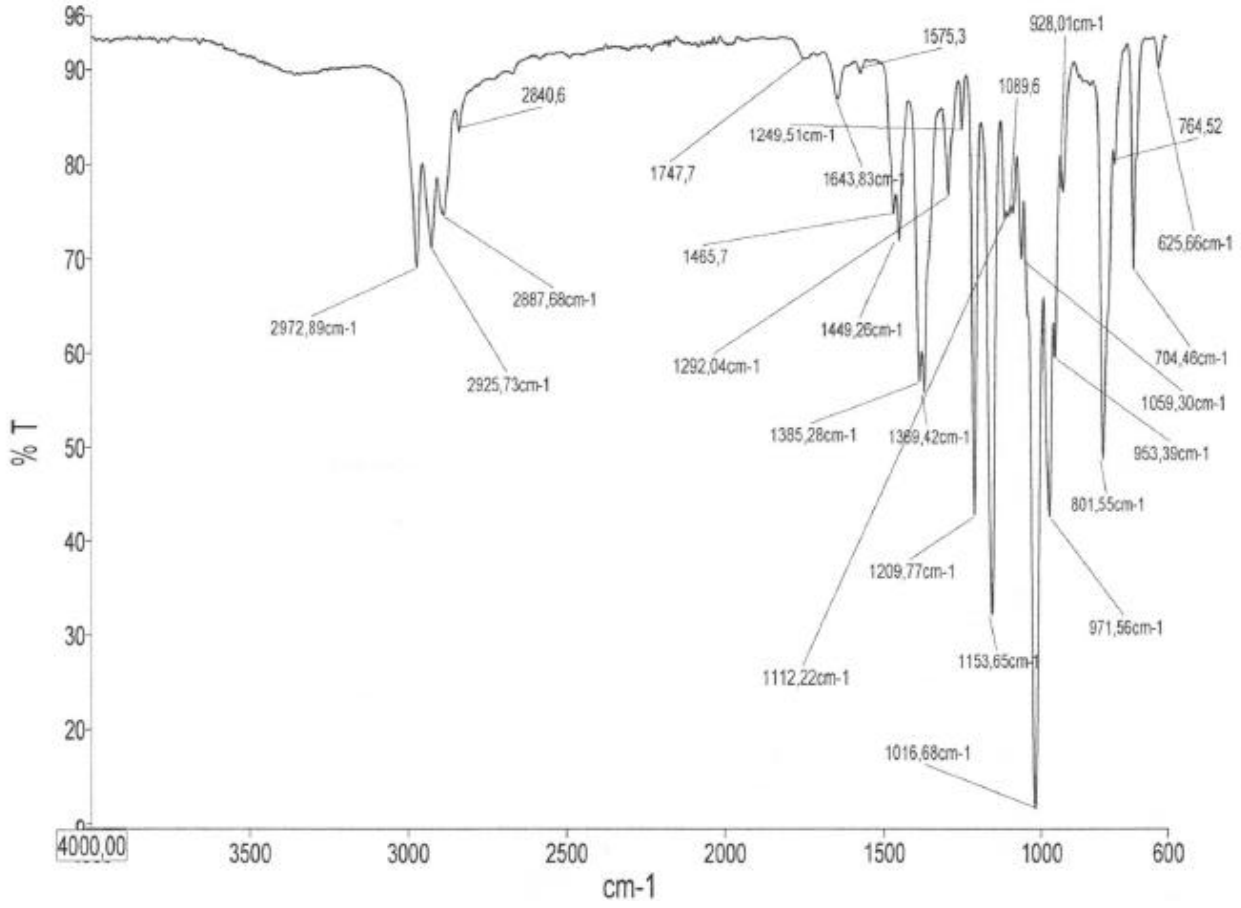
3.1 Compound 1

Figure S42: IR Spectra of compound **1**



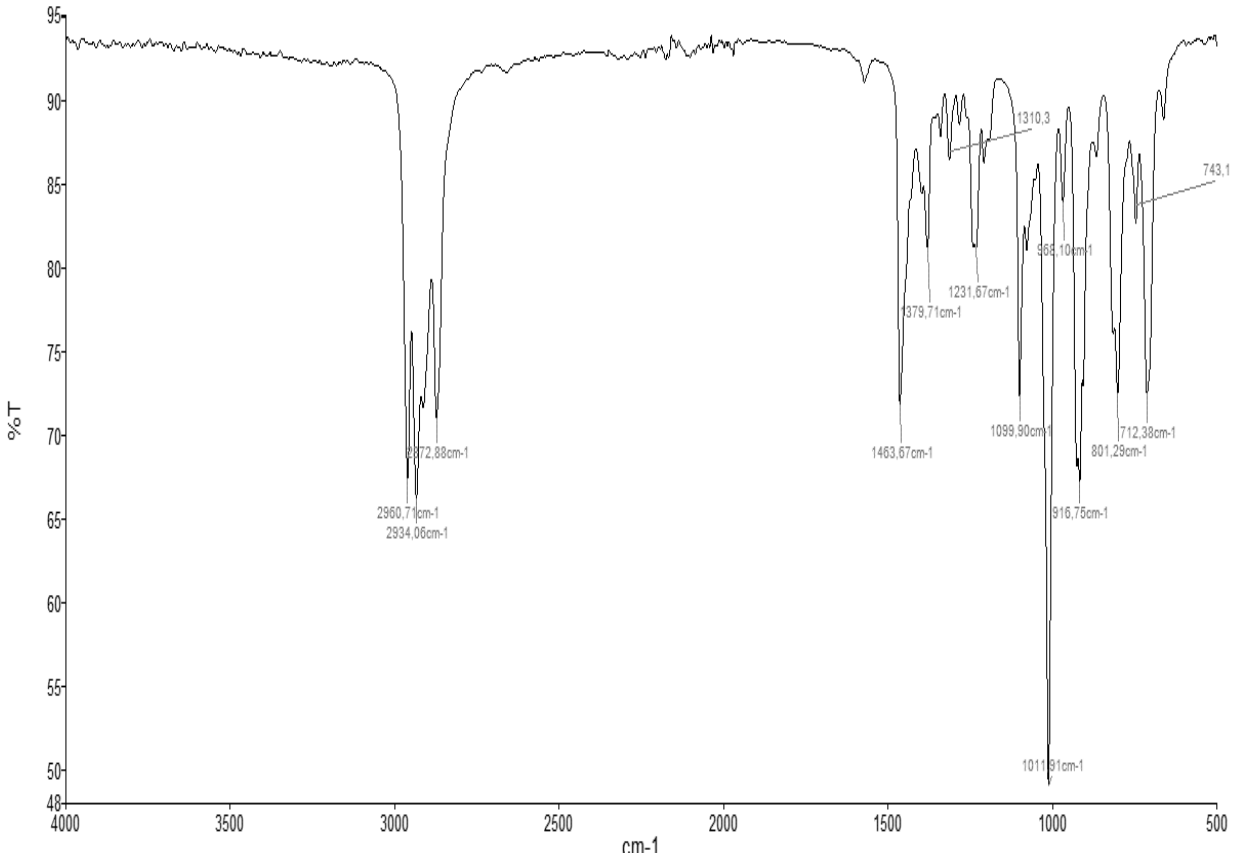
3.2 Compound 2

Figure S43: IR Spectra of compound **2**



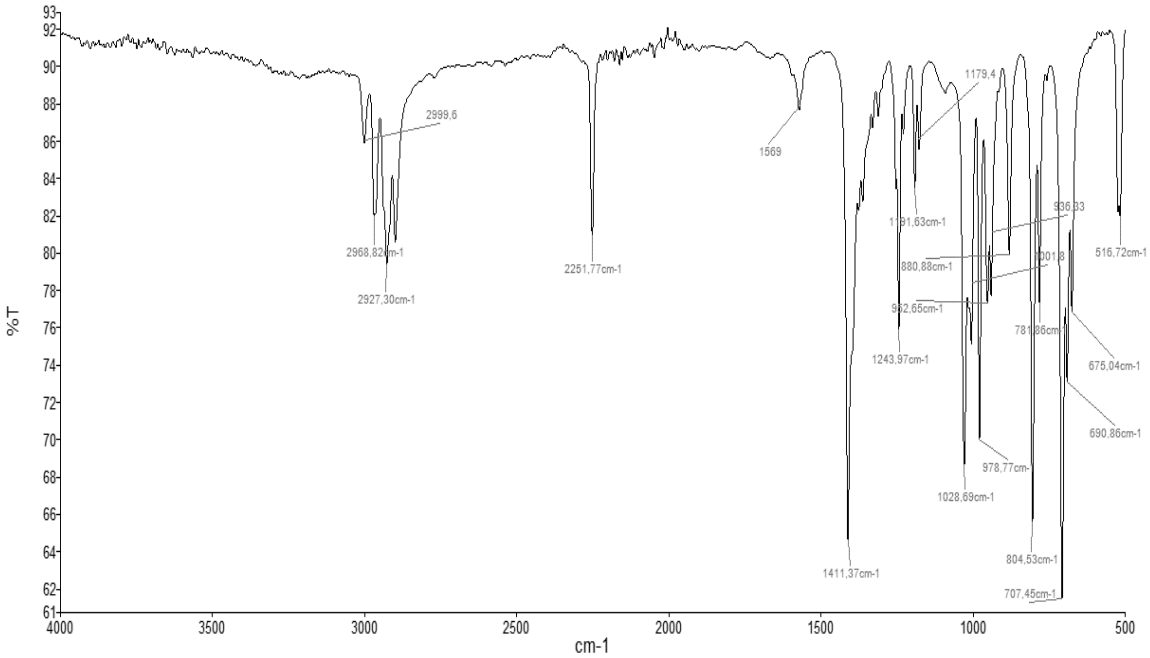
3.3 Compound 3

Figure S44: IR Spectra of compound **3**



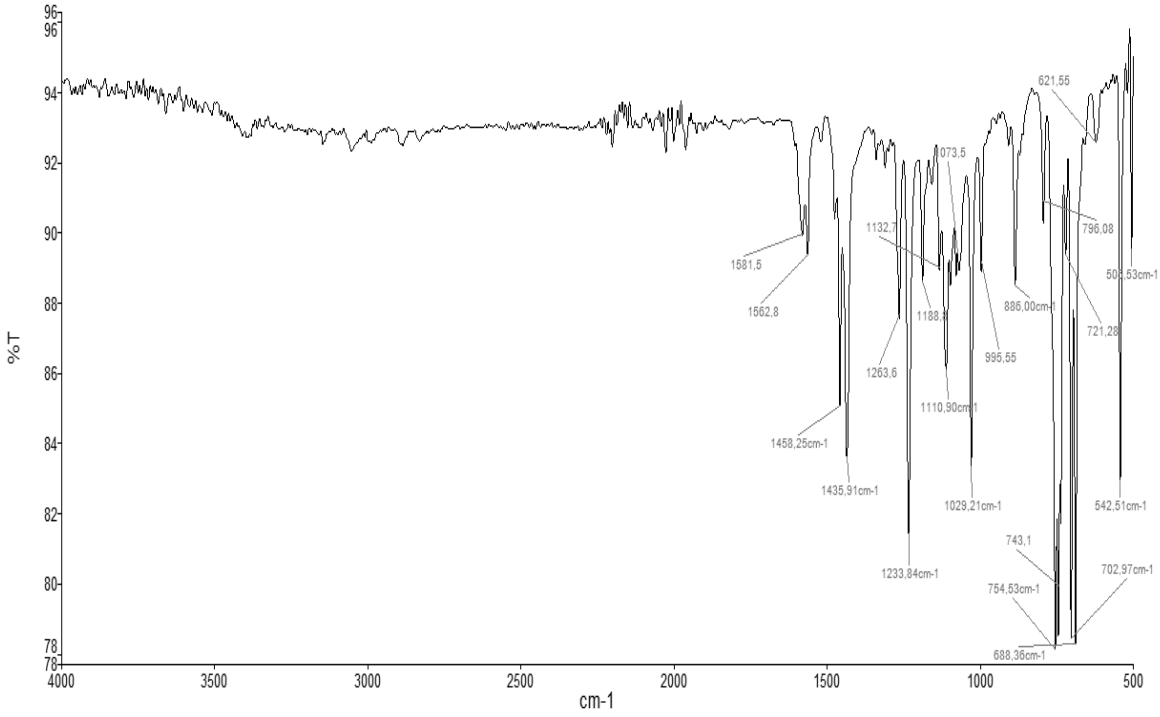
3.4 Compound 4

Figure S45: IR Spectra of compound **4**



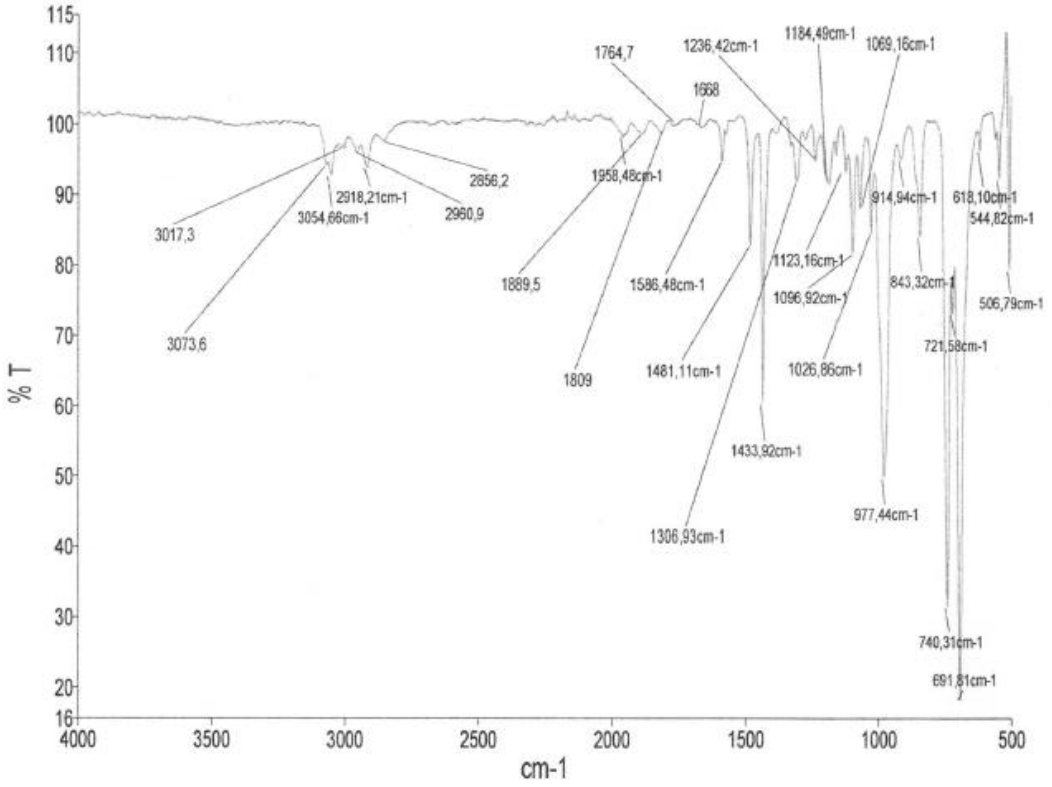
3.5 Compound 5

Figure S46: IR Spectra of compound **5**



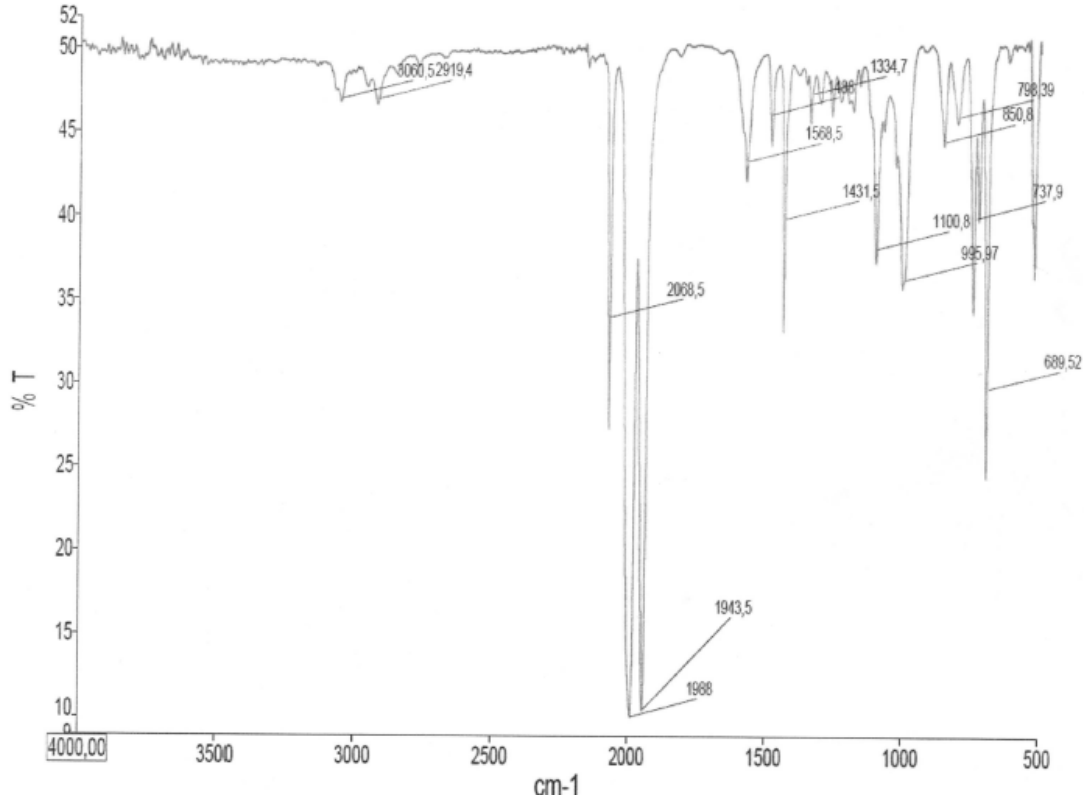
3.6 Compound 6a

Figure S47: IR Spectra of compound **6a**



IR TEP 6a

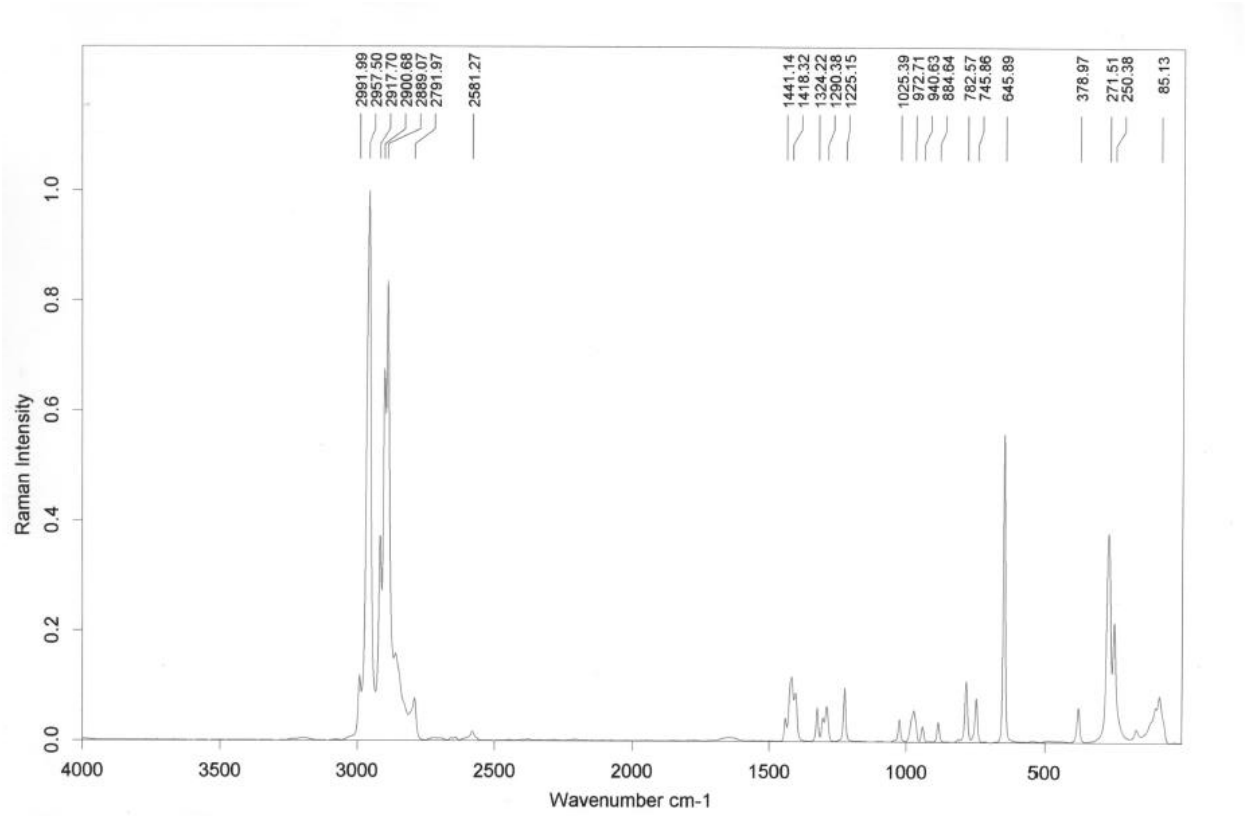
Figure S48: IR TEP **6a**



4 Raman Spectra

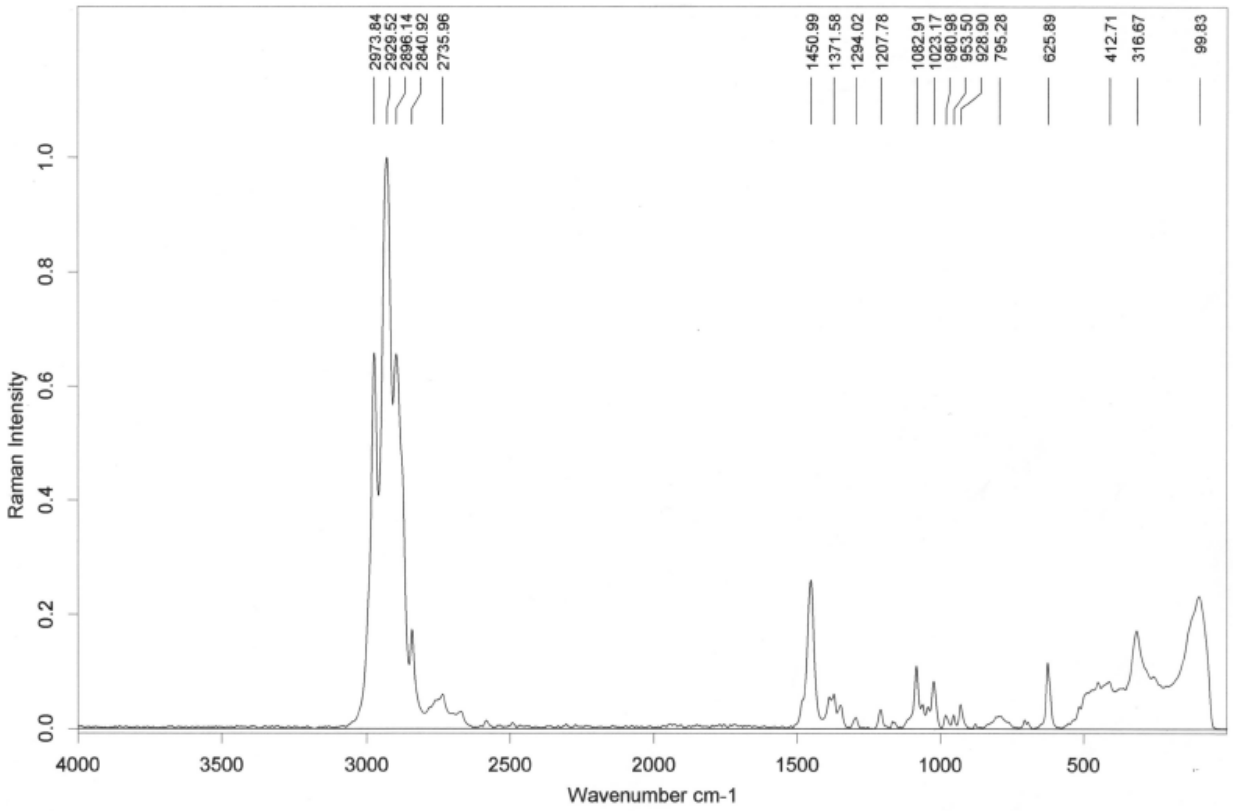
4.1 Compound 1

Figure S49: Raman Spectra of compound **1**



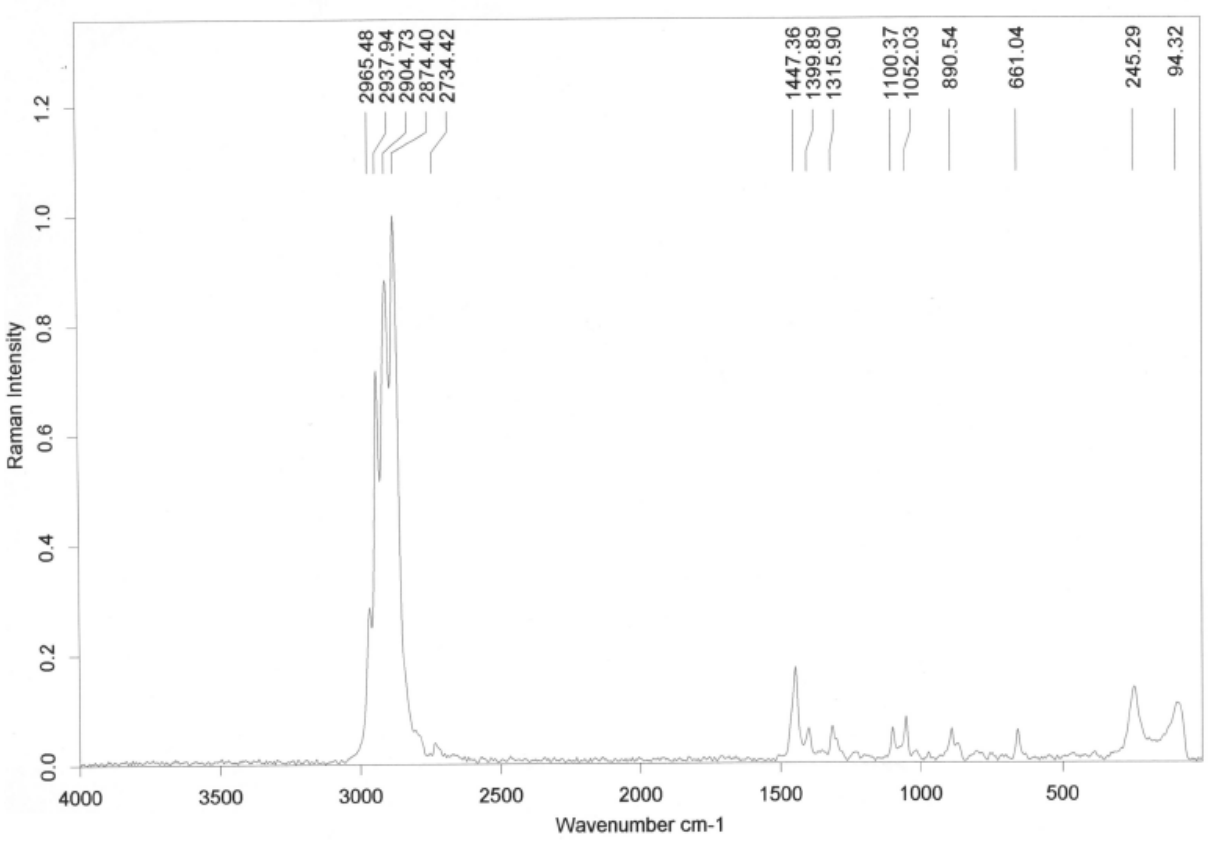
4.2 Compound 2

Figure S50: Raman Spectra of compound **2**



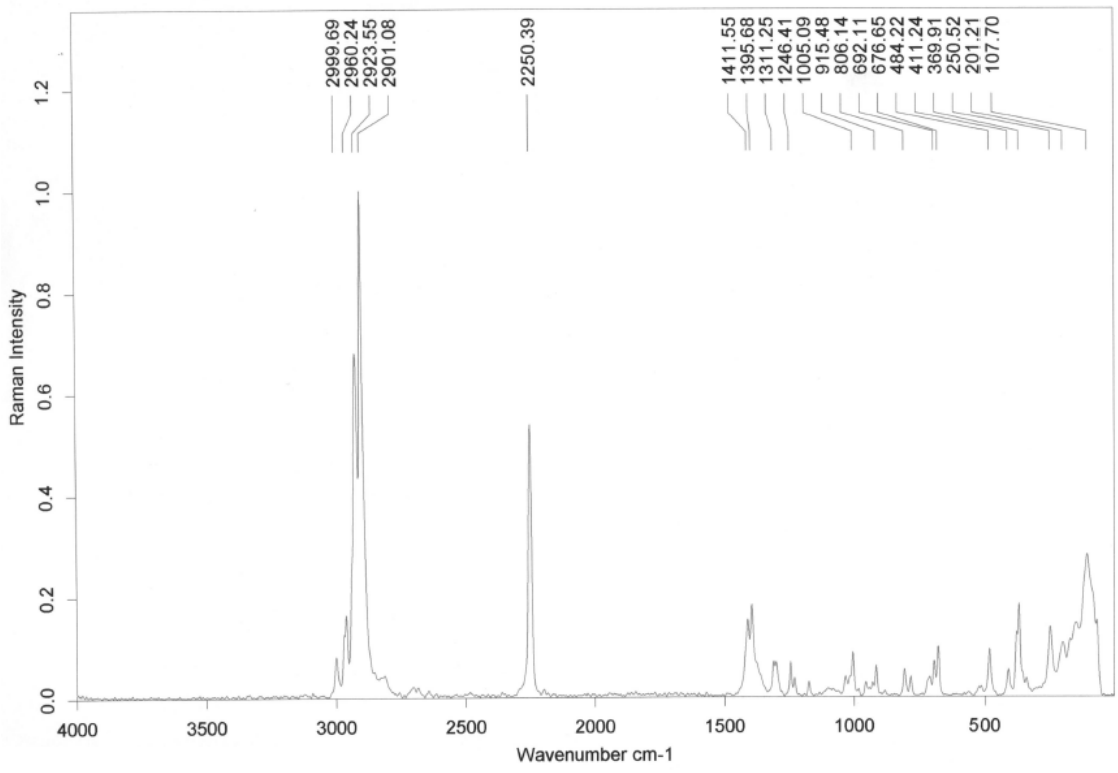
4.3 Compound 3

Figure S51: Raman Spectra of compound **3**



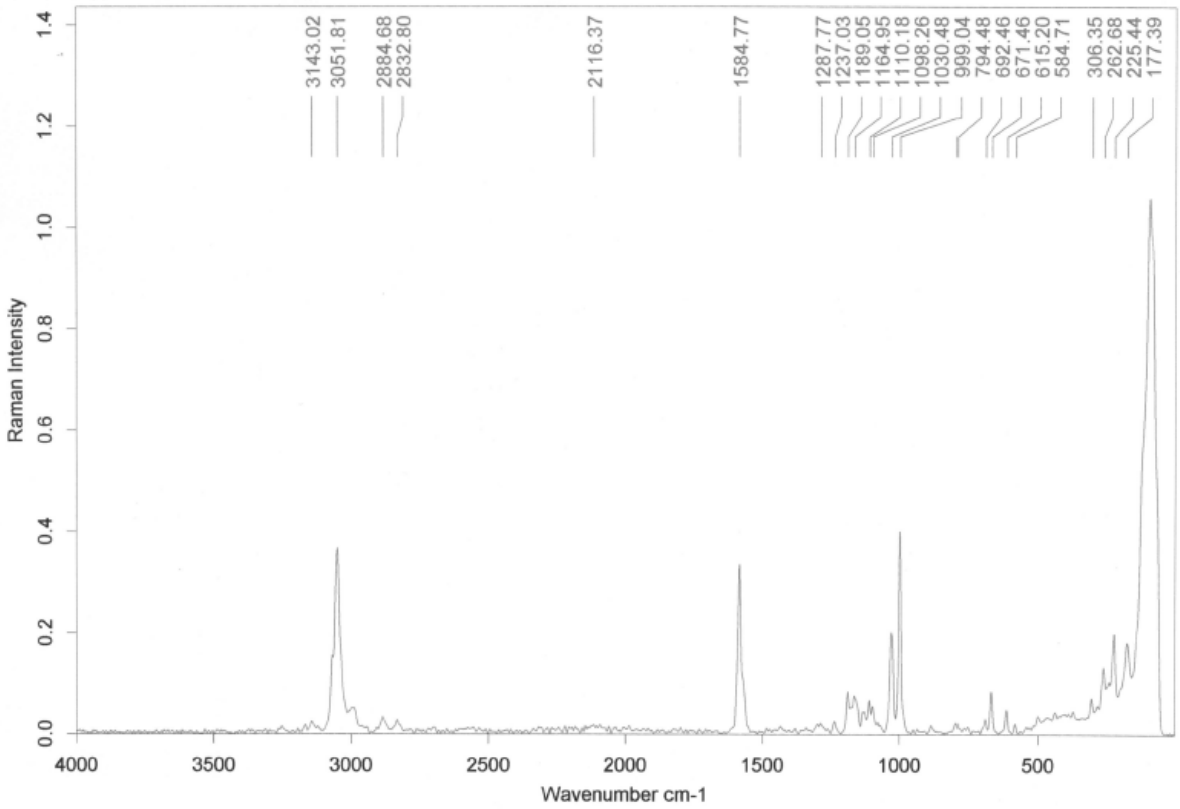
4.4 Compound 4

Figure S52: Raman Spectra of compound **4**



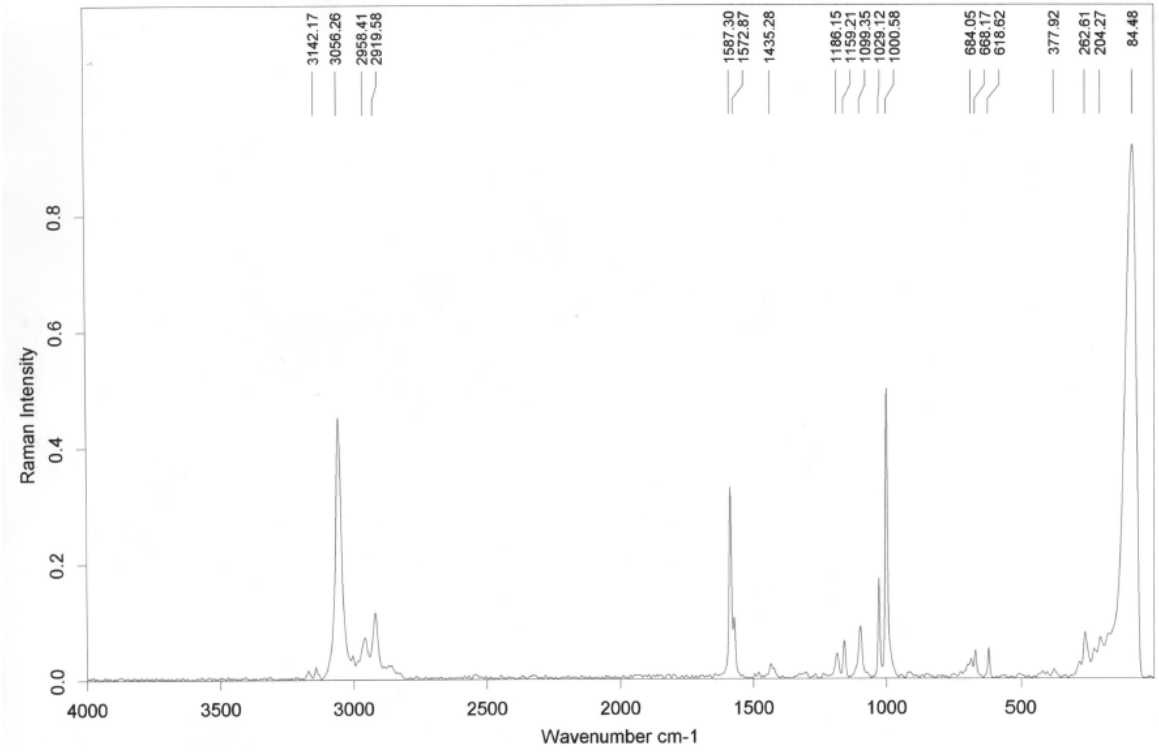
4.5 Compound 5

Figure S53: Raman Spectra of compound **5**



4.6 Compound 6a

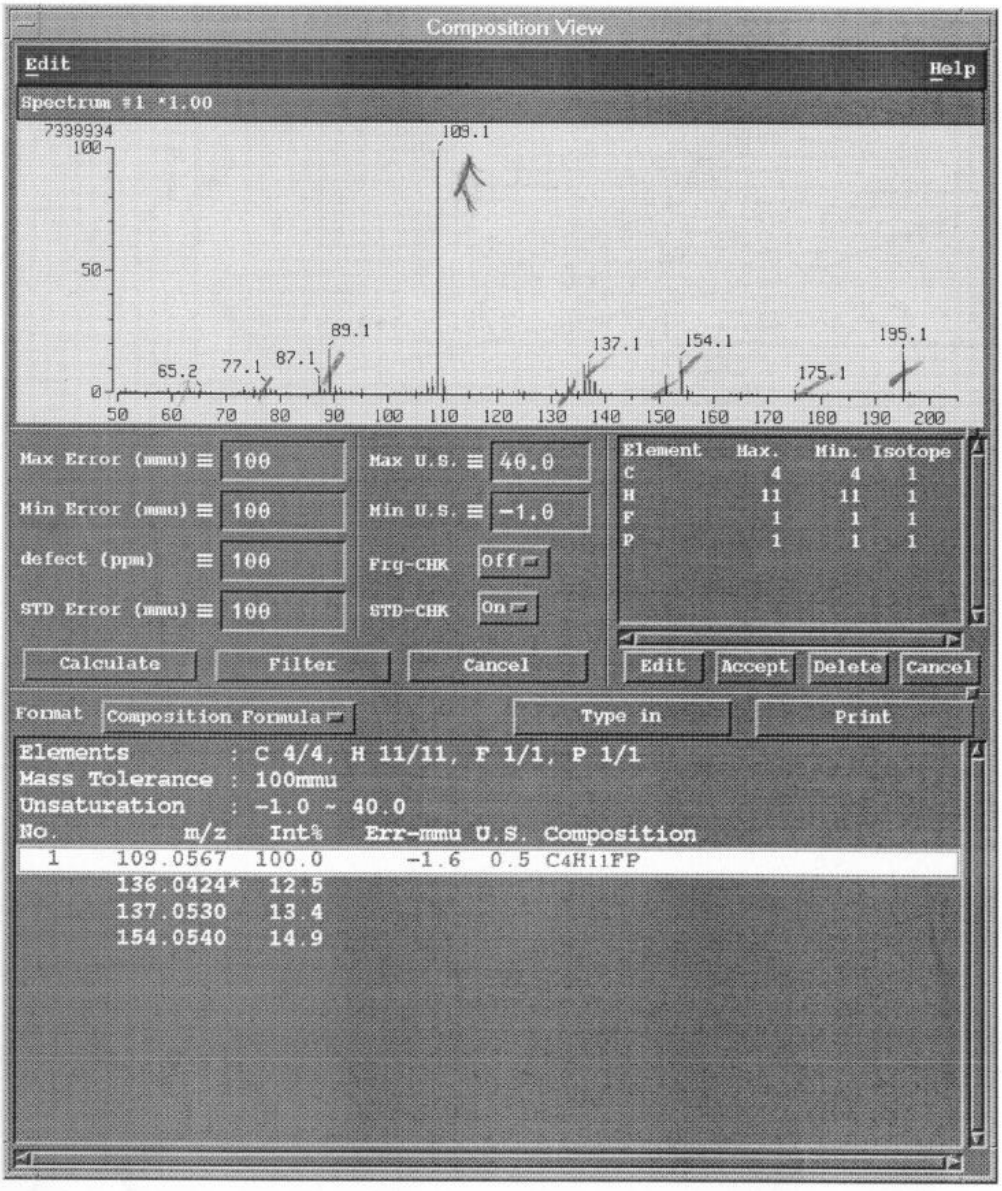
Figure S54: Raman Spectra of compound **6a**



5 Mass Spectrometry

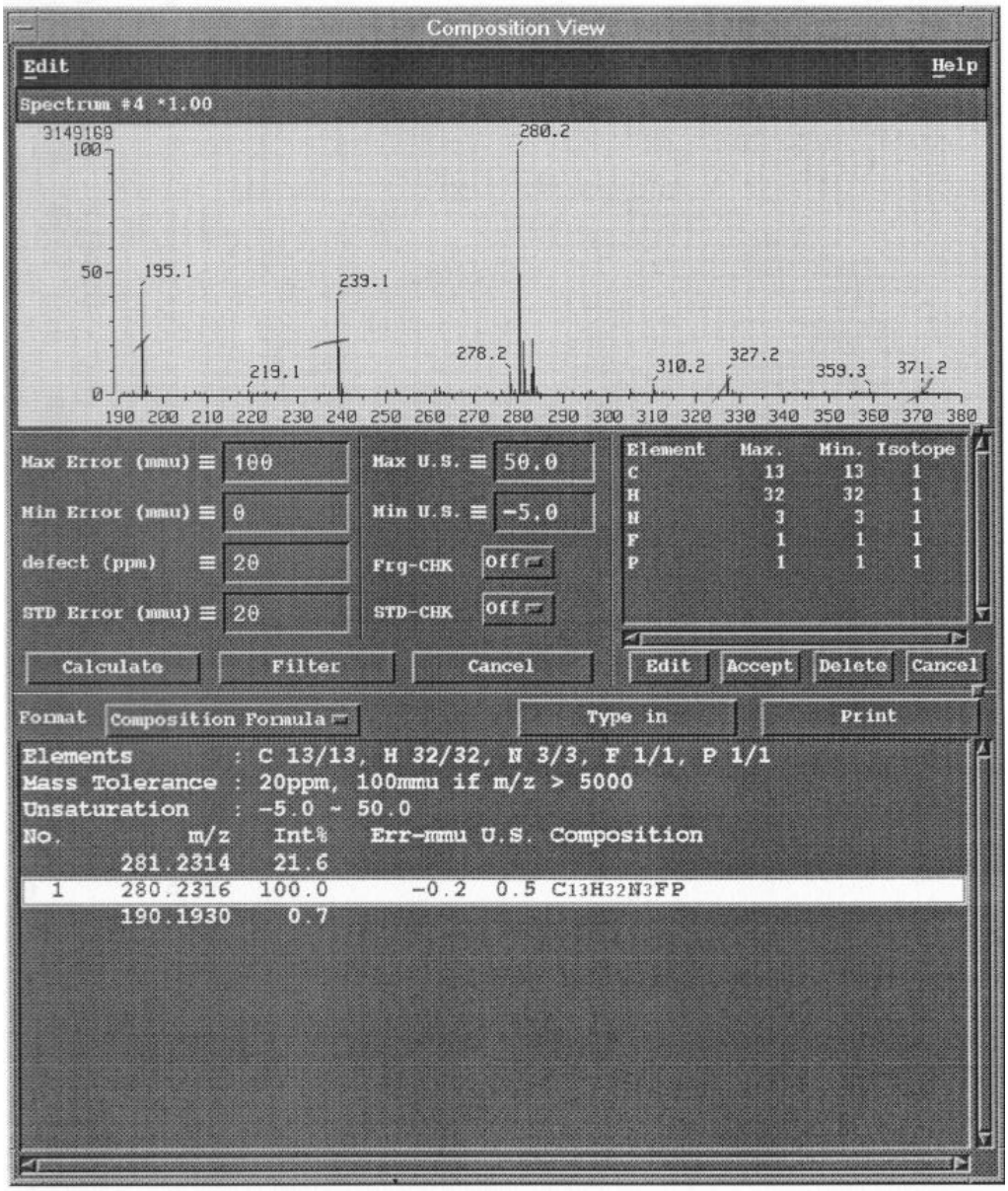
5.1 Compound 1

Figure S55: Mass Spectra of compound **1**



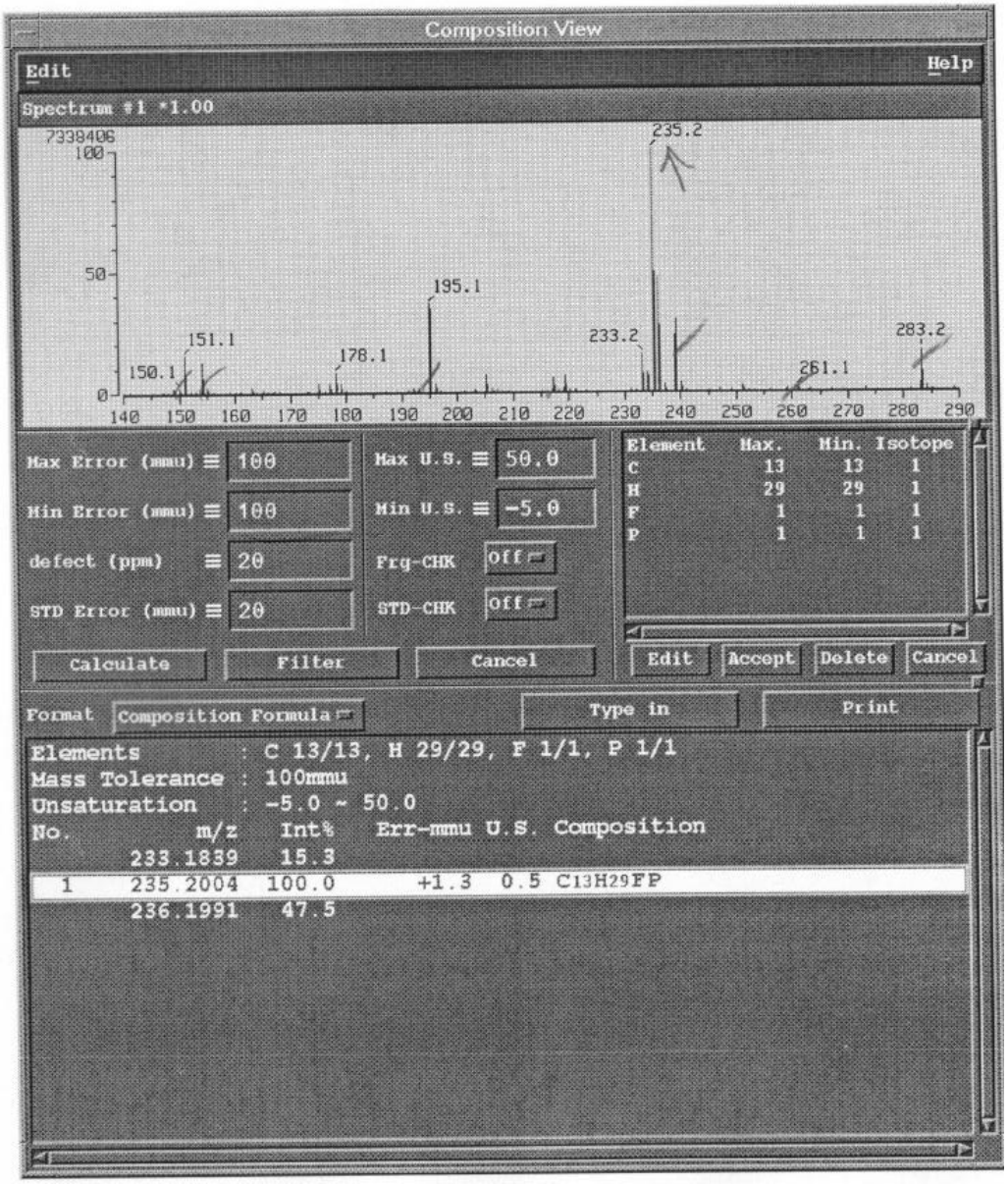
5.2 Compound 2

Figure S56: Mass Spectra of compound **2**



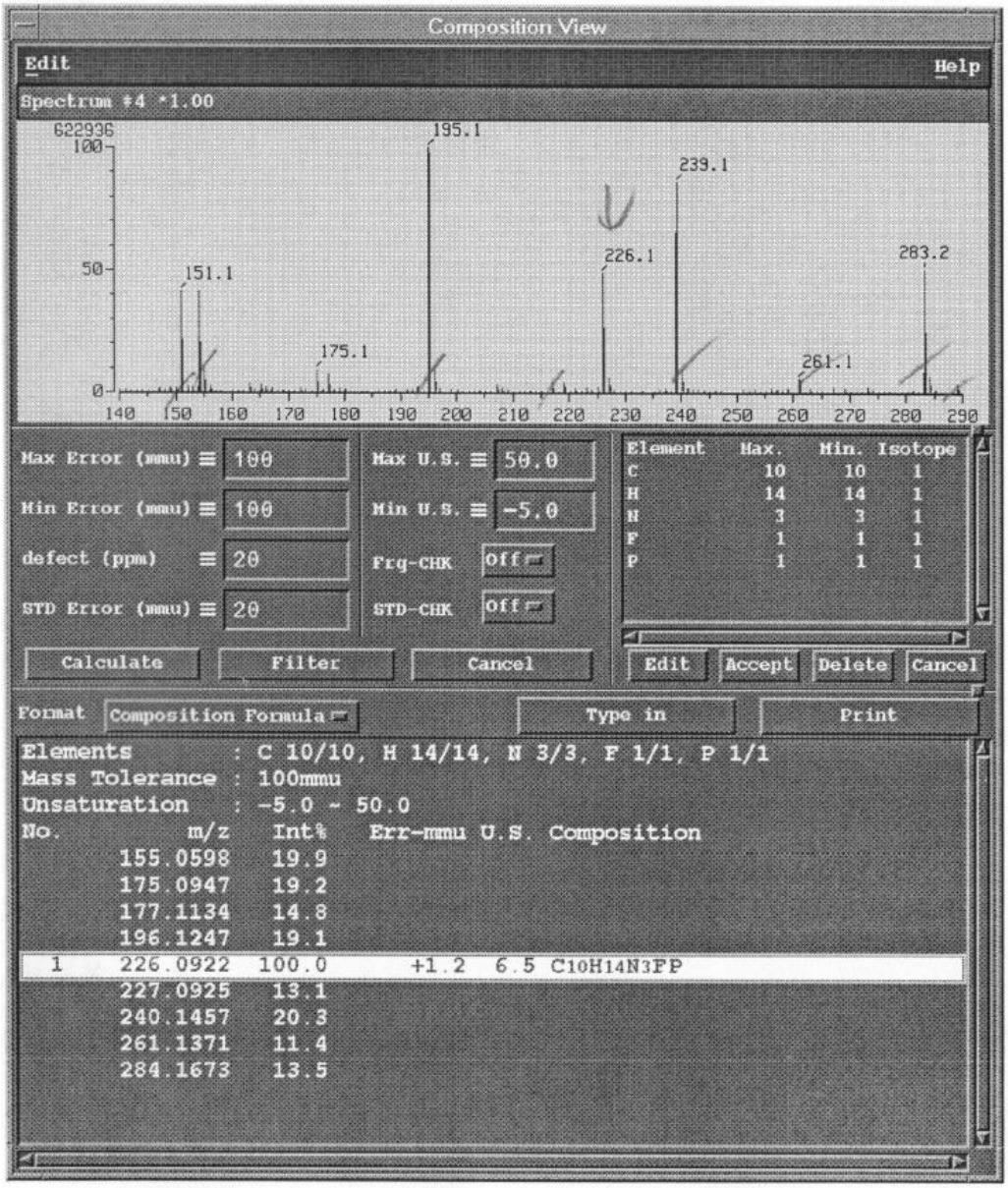
5.3 Compound 3

Figure S57: Mass Spectra of compound **3**



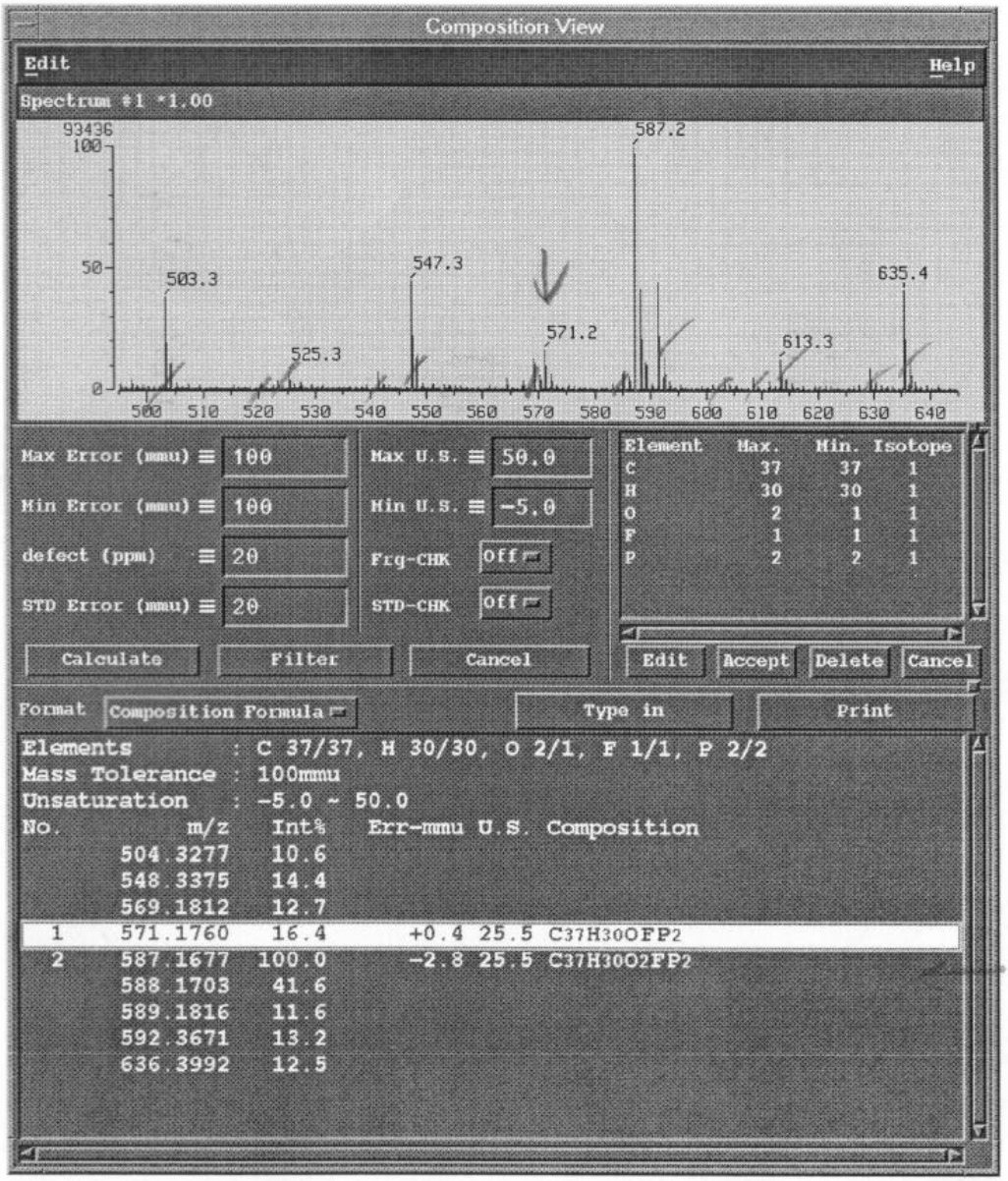
5.4 Compound 4

Figure S58: Mass Spectra of compound **4**



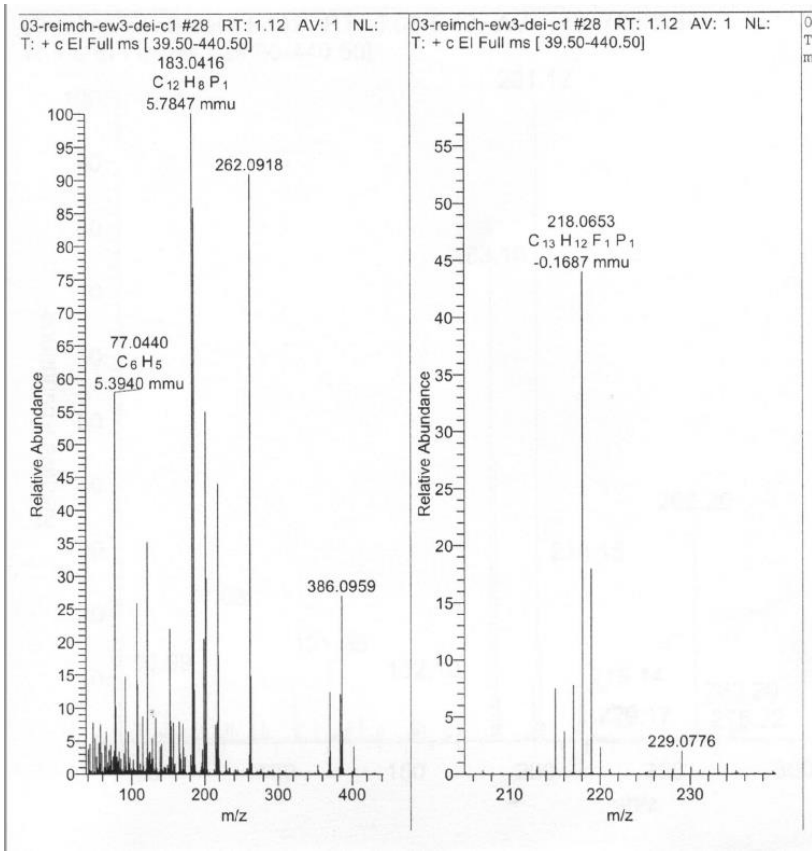
5.5 Compound 5

Figure S59: Mass Spectra of compound **5**



5.6 Compound 6a

Figure S60: Mass Spectra of compound **6a**



03-reimch-ew3-dei-c1#28 RT: 1.12
T: + c EI Full ms [39.50-440.50]
m/z= 37.50-441.77

m/z	Intensity	Relative	Flags
46.9083	3476797.0	7.77	
77.0440	25865472.0	57.79	
78.0510	4561582.0	10.19	
91.0597	6573598.0	14.69	
107.0129	11565312.0	25.84	
108.0219	6060622.0	13.54	
115.0565	3865553.0	8.64	
121.0217	15710976.0	35.10	
133.0212	3780579.0	8.45	
152.0626	9817600.0	21.93	
153.0686	3594178.0	8.03	
165.0711	3503435.0	7.83	
183.0139	24546304.0	54.84	S
183.0198	24511232.0	54.76	S
183.0416	44759040.0	100.00	S
183.0576	22828032.0	51.00	S
183.0635	22856960.0	51.07	S
184.0415	8902912.0	19.89	
185.0527	38389760.0	85.77	
186.0587	5689459.0	12.71	
199.0672	9131776.0	20.40	
201.0158	16117248.0	36.01	S
201.0223	16059648.0	35.88	S
201.0288	15964672.0	35.67	S
201.0644	24482816.0	54.70	S
201.0709	24542720.0	54.83	S
201.0774	24566272.0	54.89	S
202.0511	13278976.0	29.67	
217.0561	3472737.0	7.76	
218.0653	19671040.0	43.95	
219.0596	8025059.0	17.93	
262.0918	40662016.0	90.85	
263.0945	6591975.0	14.73	
370.1017	5530338.0	12.36	
384.1175	5371075.0	12.00	
386.0959	12056320.0	26.94	