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SUPPLEMENTARY MATERIAL

Synthesis and Oxidative Desulfurization of P(V)-Functionalized Imidazole-2-thiones: Easy Access to P-Functional Ionic Liquids

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Figure S1: ^{1}H NMR spectrum of **1d** in $CDCl_3$ (300.1 MHz, 25 °C)

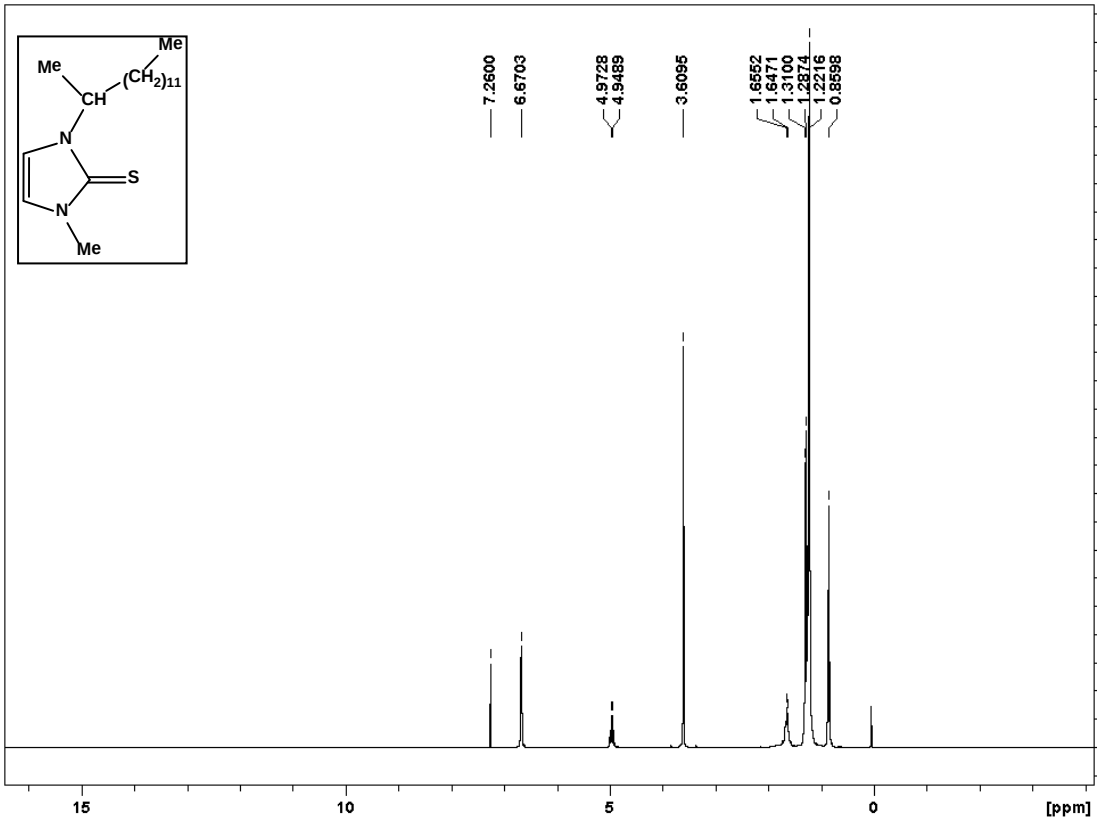

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **1d** in $CDCl_3$ (75.5 MHz, 25 °C)

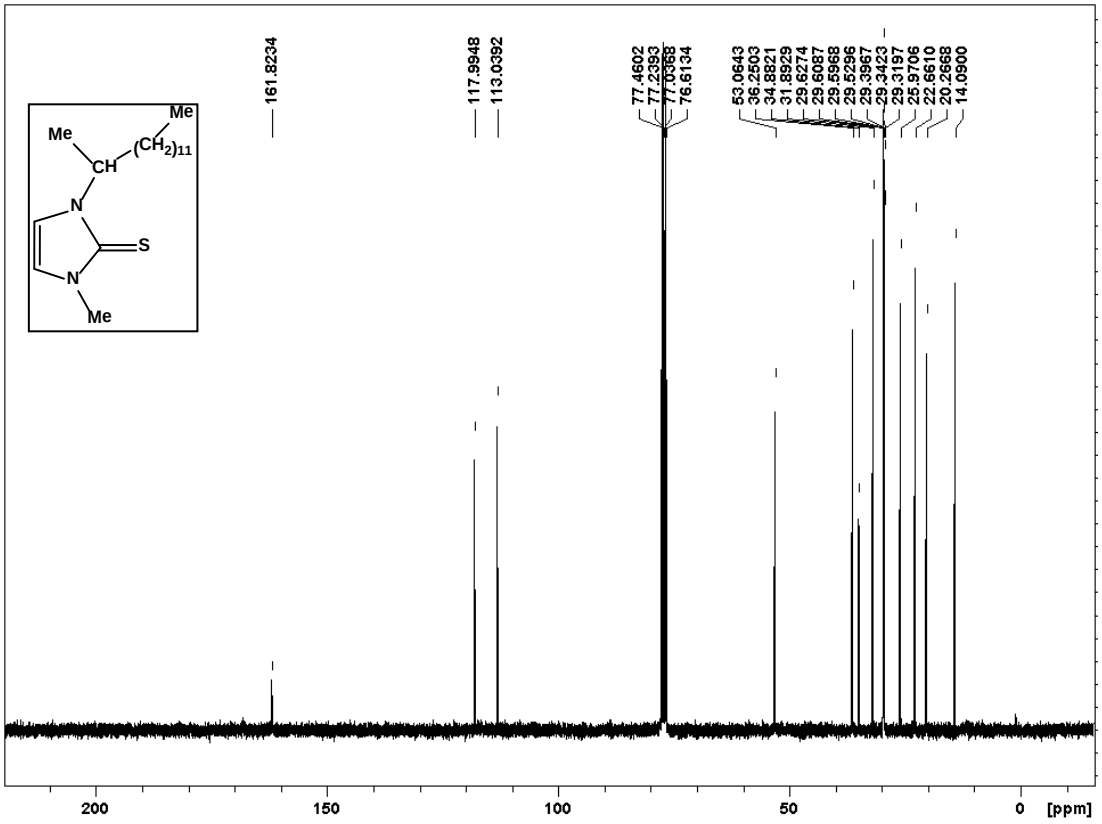

Figure S3: ^{1}H NMR spectrum of **2d** in $CDCl_3$ (300.1 MHz, 25 °C)

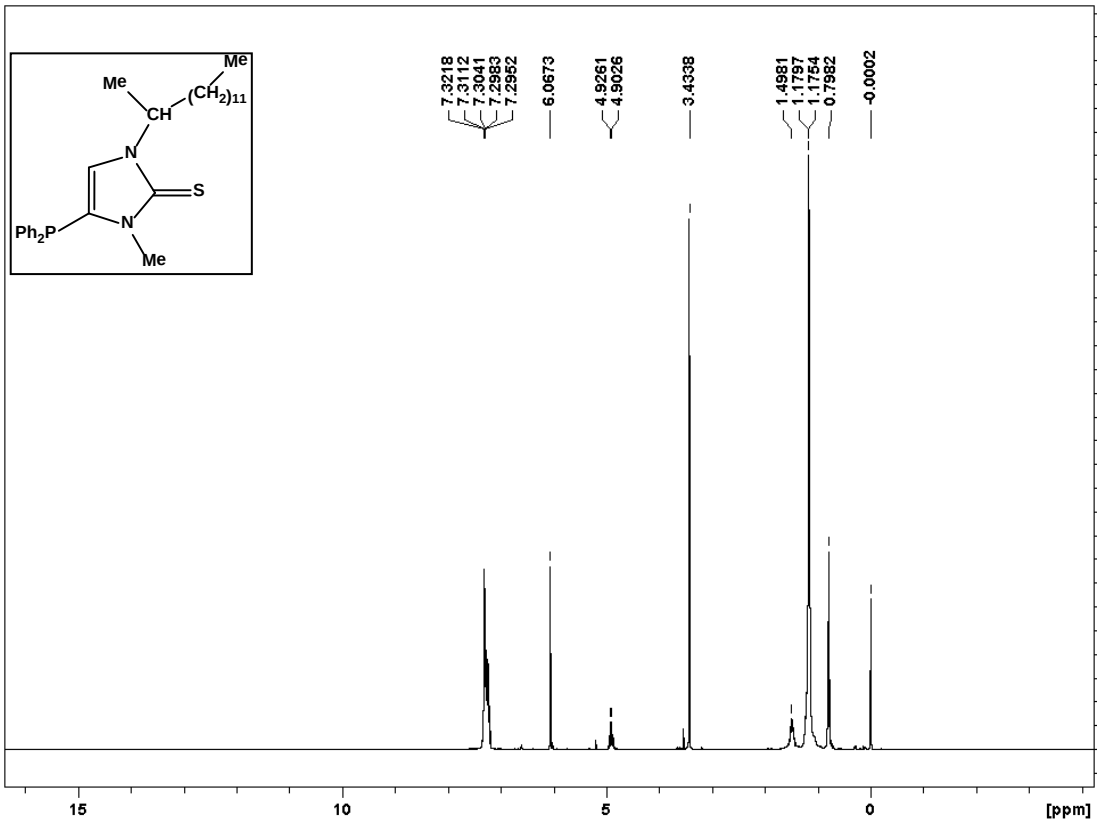

Figure S4: $^{13}C\{^{1}H\}$ NMR spectrum of **2d** in $CDCl_3$ (75.5 MHz, 25 °C)

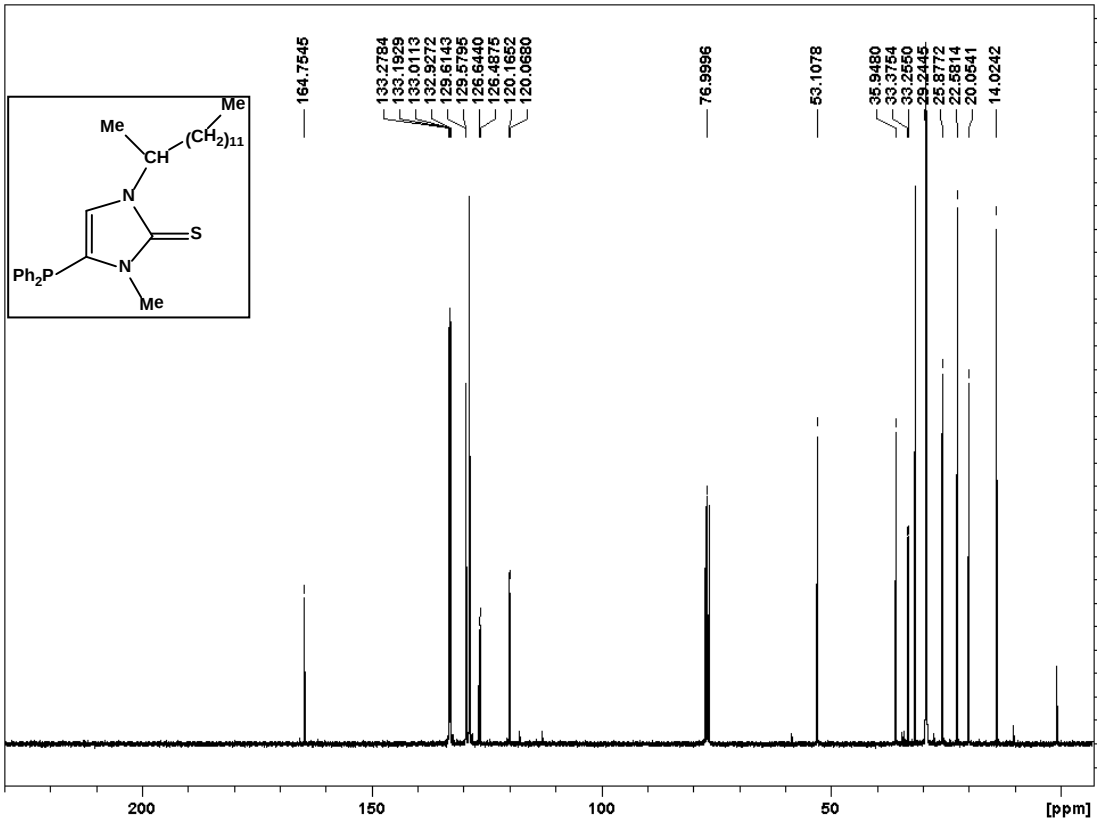

Figure S5: $^{31}P\{^{1}H\}$ NMR spectrum of **2d** in $CDCl_3$ (121.5 MHz, 25 °C)

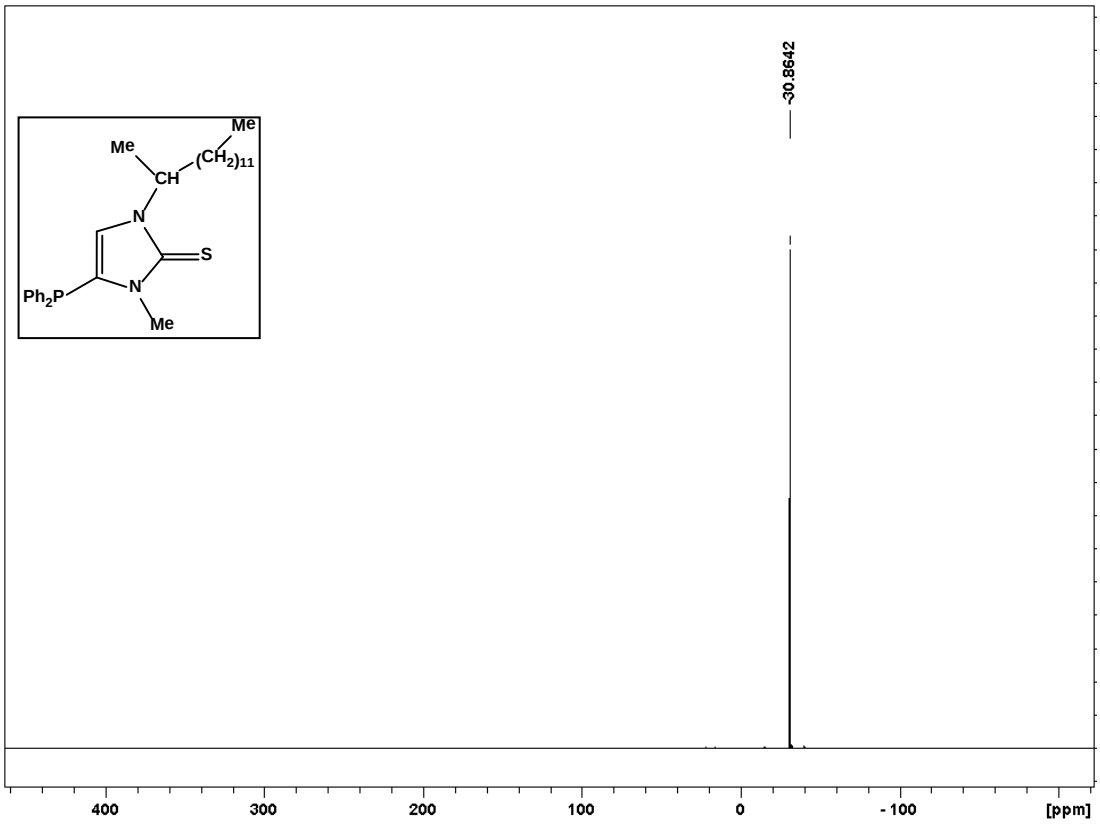

Figure S6: ^{1}H NMR spectrum of **3a** in CD_2Cl_2 (300.1 MHz, 25 °C)

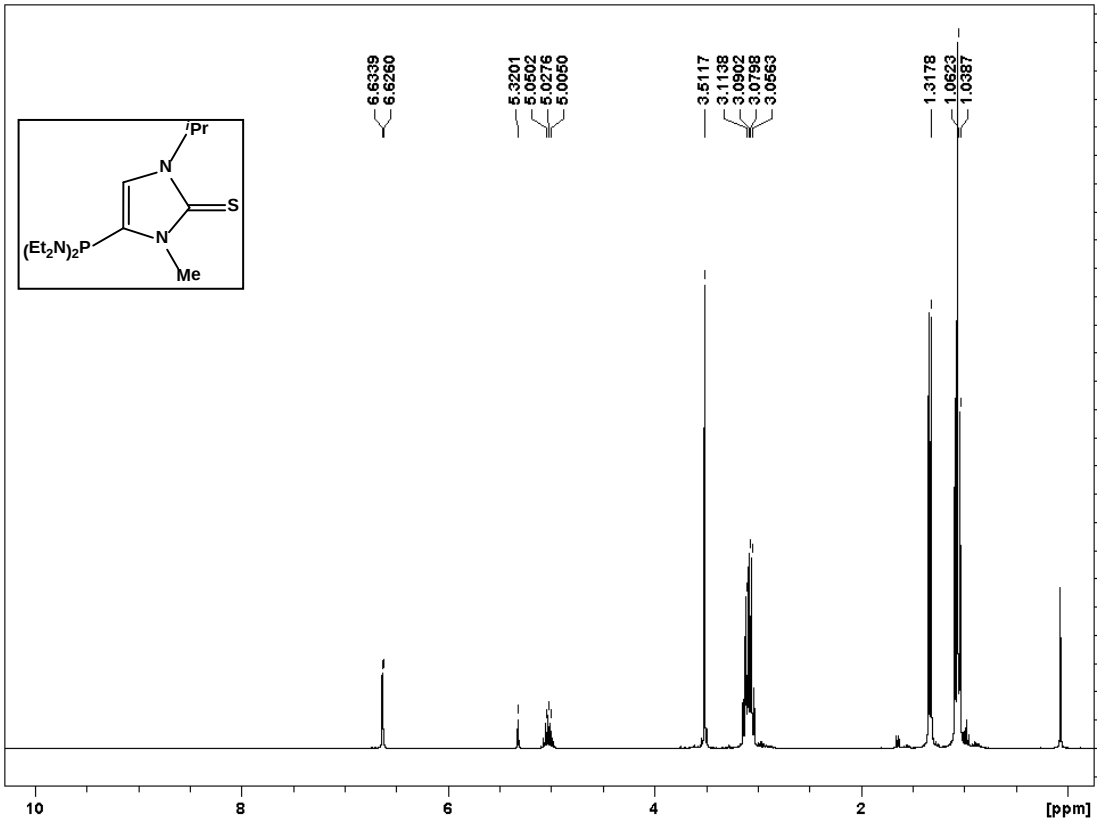

Figure S7: $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in CD_2Cl_2 (75.5 MHz, 25 °C)

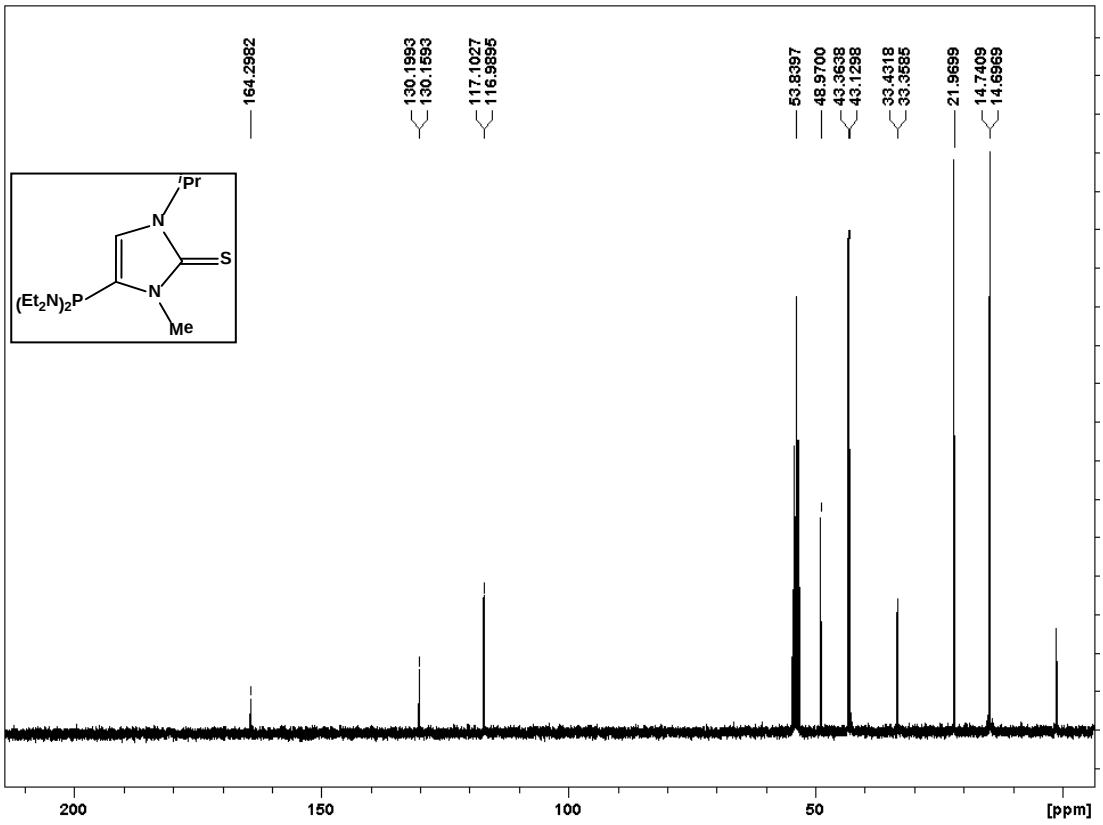

Figure S8: $^{31}P\{^{1}H\}$ NMR spectrum of **3a** in CD_2Cl_2 (121.5 MHz, 25 °C)

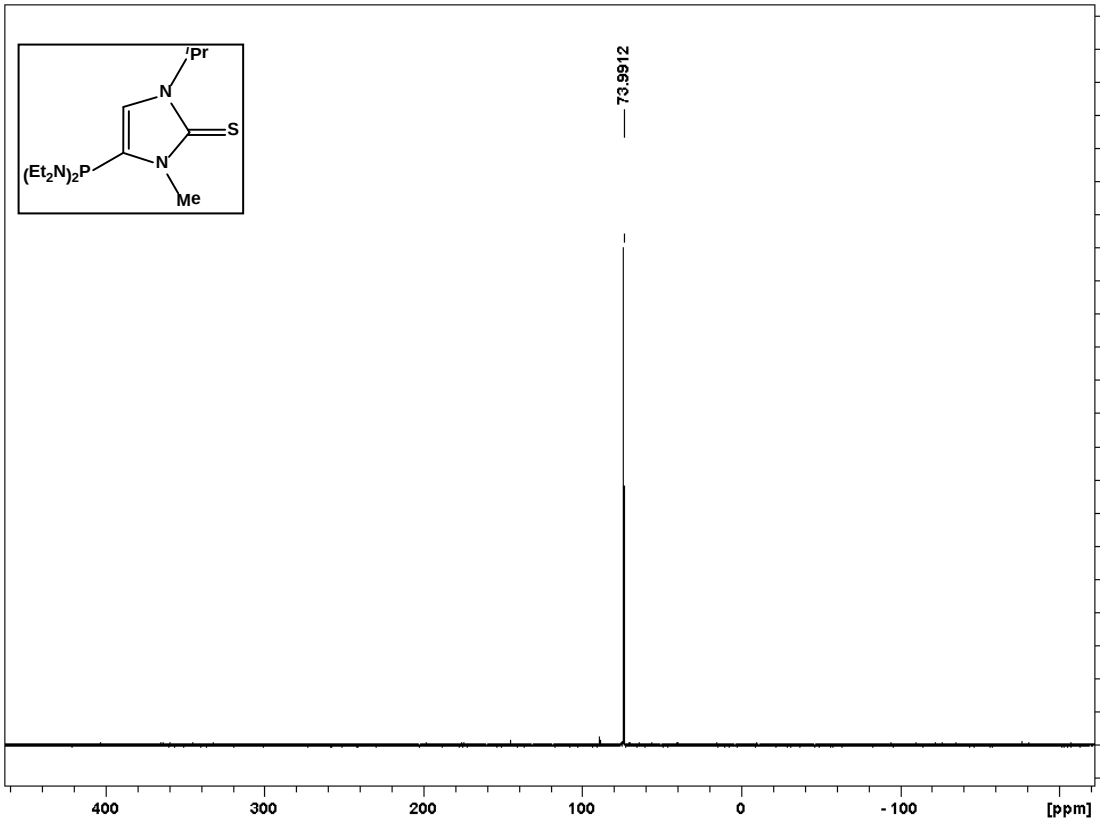

Figure S9: ^{1}H NMR spectrum of **3b(b')** in $CDCl_3$ (300.1 MHz, 25 °C)

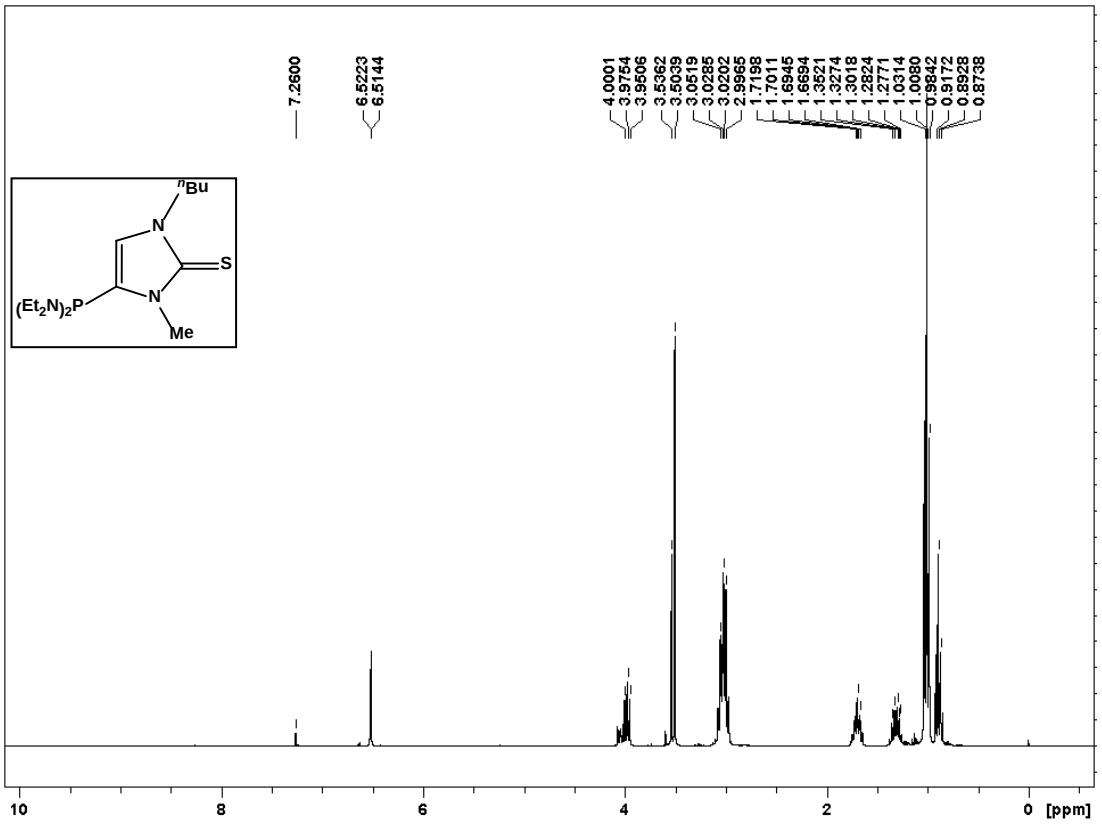

Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of **3b(b')** in $CDCl_3$ (75.5 MHz, 25 °C)

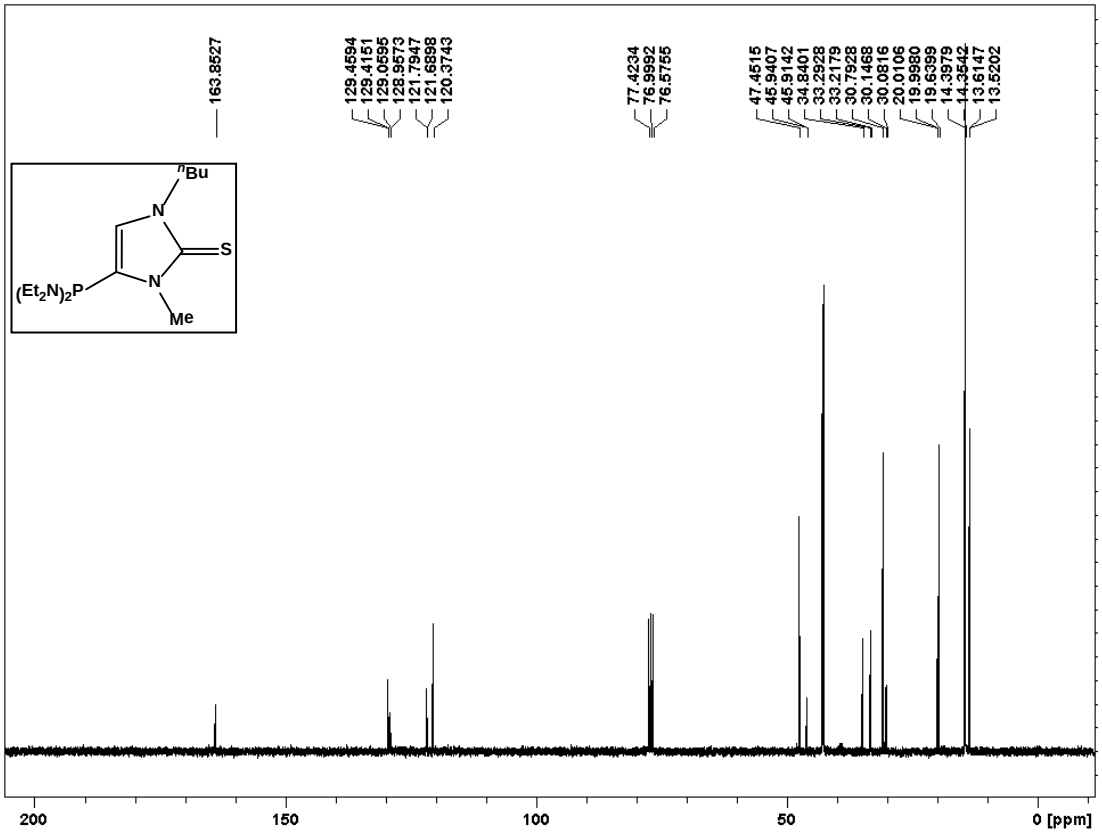

Figure S11: $^{31}P\{^{1}H\}$ NMR spectrum of **3b(b')** in $CDCl_3$ (121.5 MHz, 25 °C)

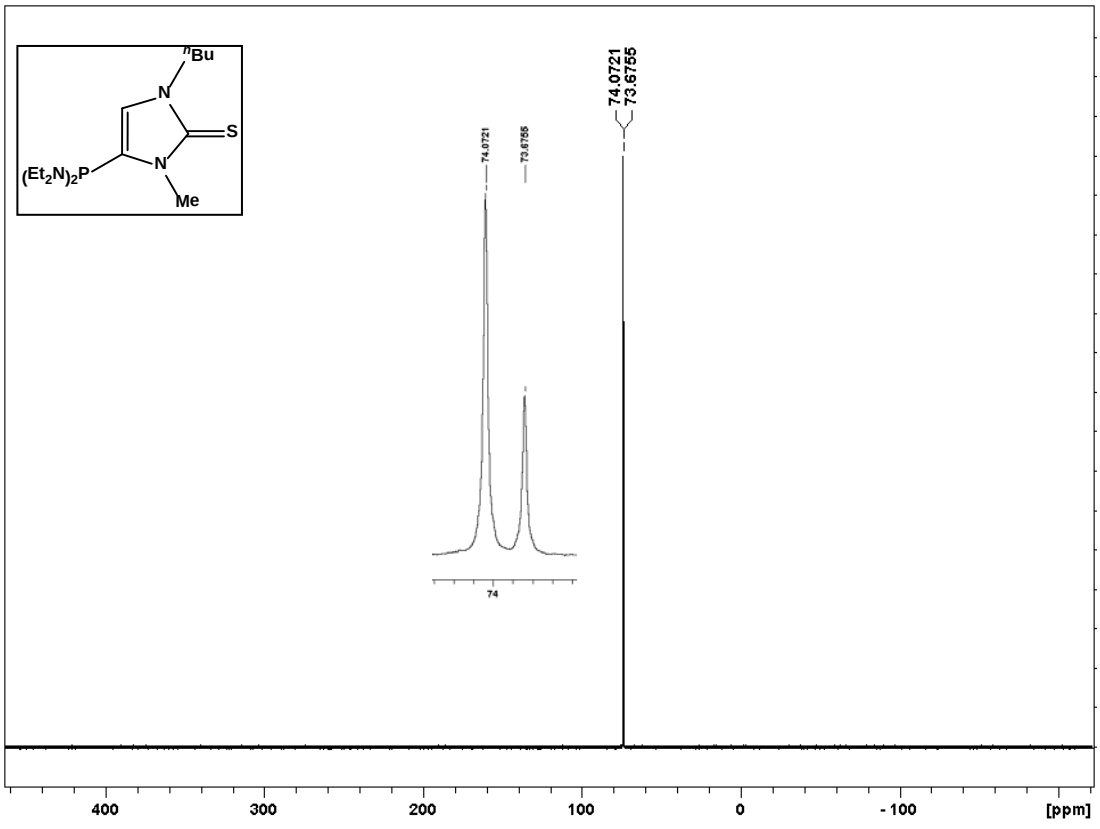

Figure S12: $^{31}P\{^{1}H\}$ NMR spectrum of **3c(c')** in thf (121.5 MHz, 25 °C)

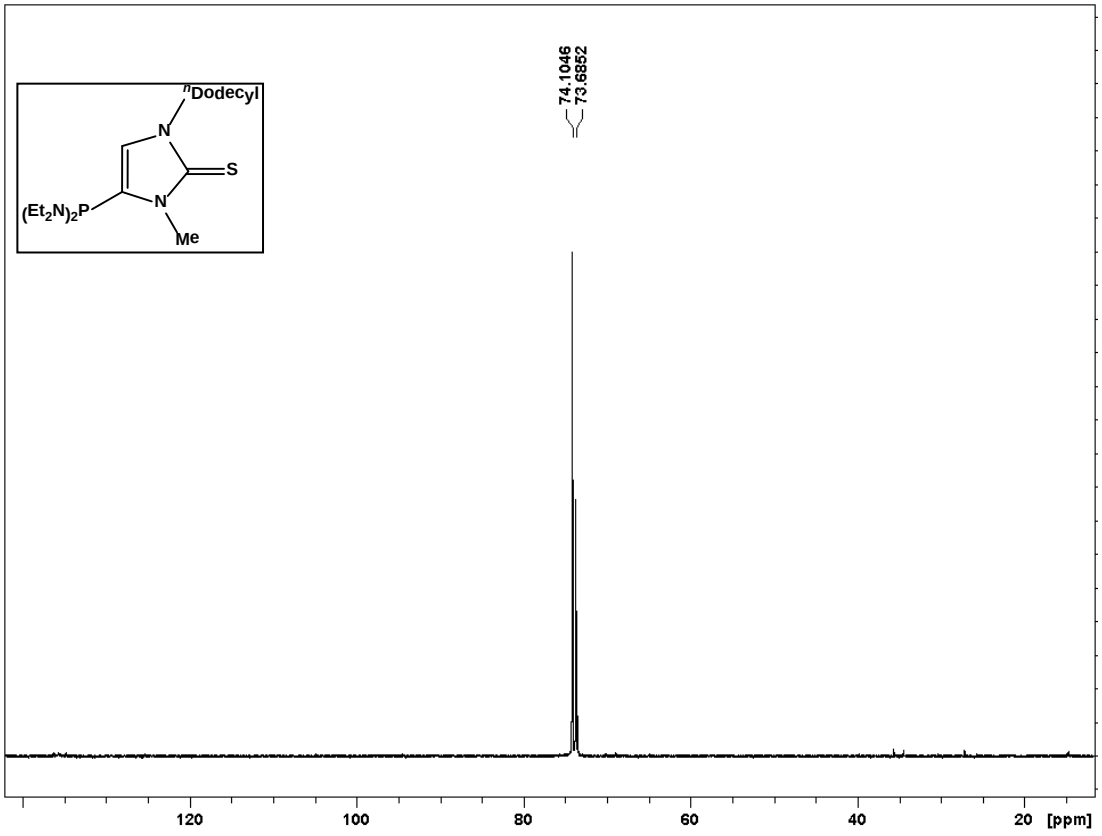

Figure S13: $^{31}P\{^{1}H\}$ NMR spectrum of **3d** in thf (121.5 MHz, 25 °C)

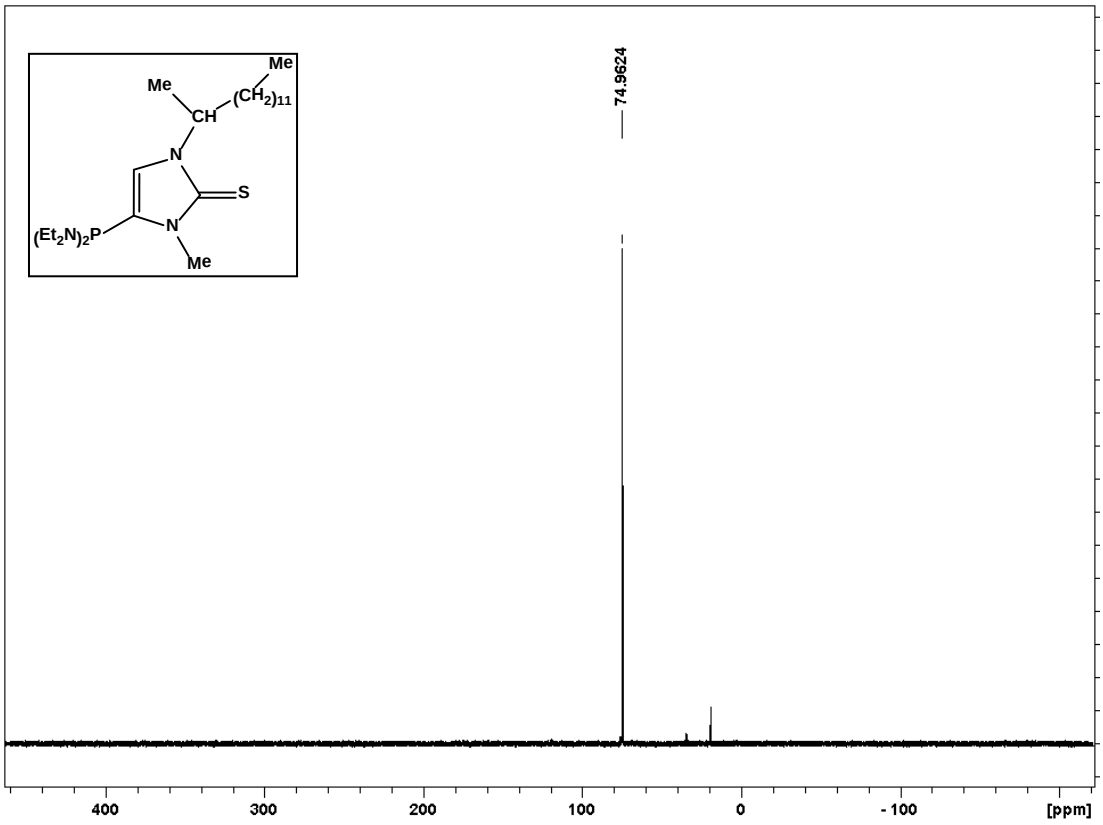

Figure S14: ^{1}H NMR spectrum of **4a** in $CDCl_3$ (300.1 MHz, 25 °C)

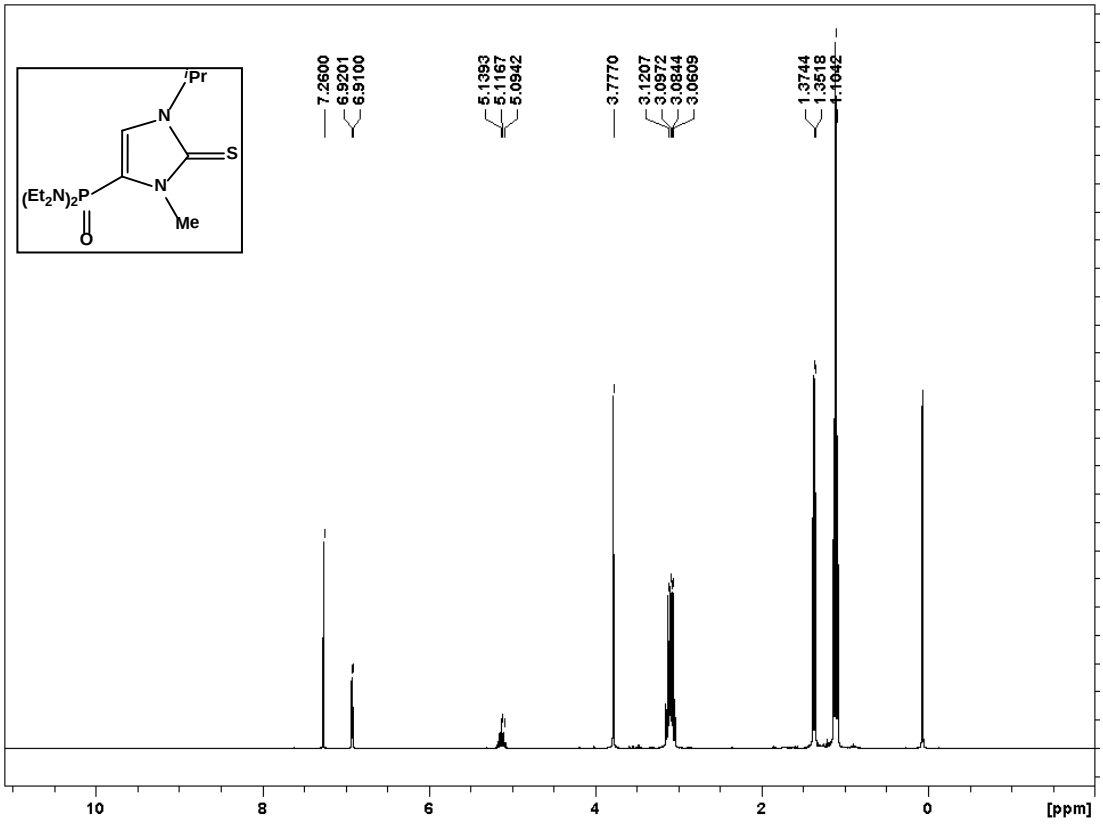

Figure S15: $^{13}C\{^{1}H\}$ NMR spectrum of **4a** in $CDCl_3$ (75.5 MHz, 25 °C)

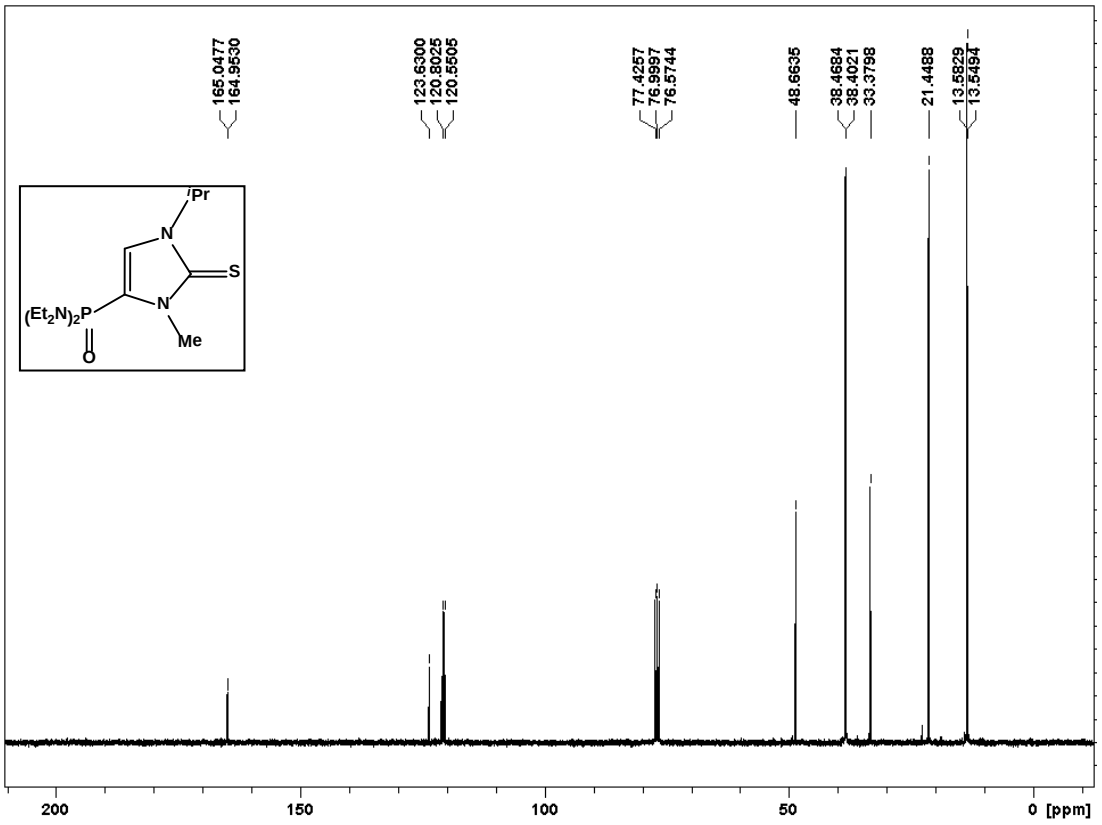

Figure S16: $^{31}P\{^{1}H\}$ NMR spectrum of **4a** in thf (121.5 MHz, 25 °C)

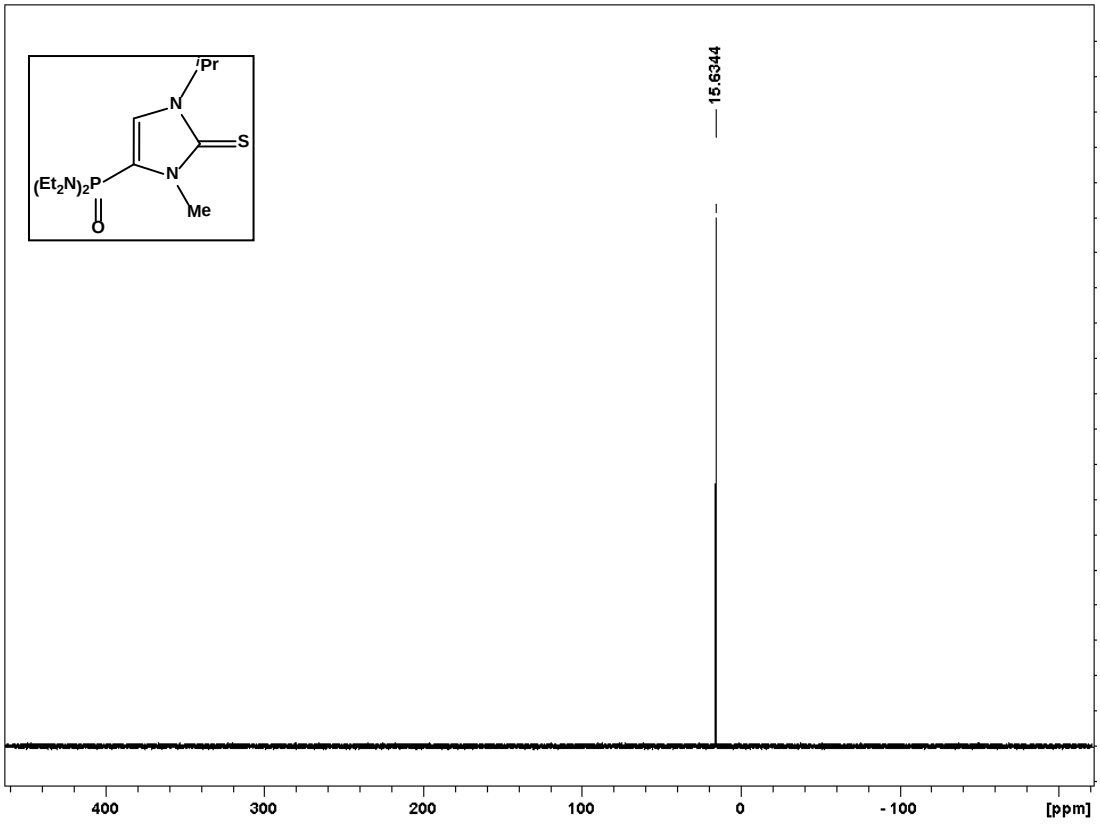

Figure S17: ^{1}H NMR spectrum of **4b(b')** in $CDCl_3$ (300.1 MHz, 25 °C)

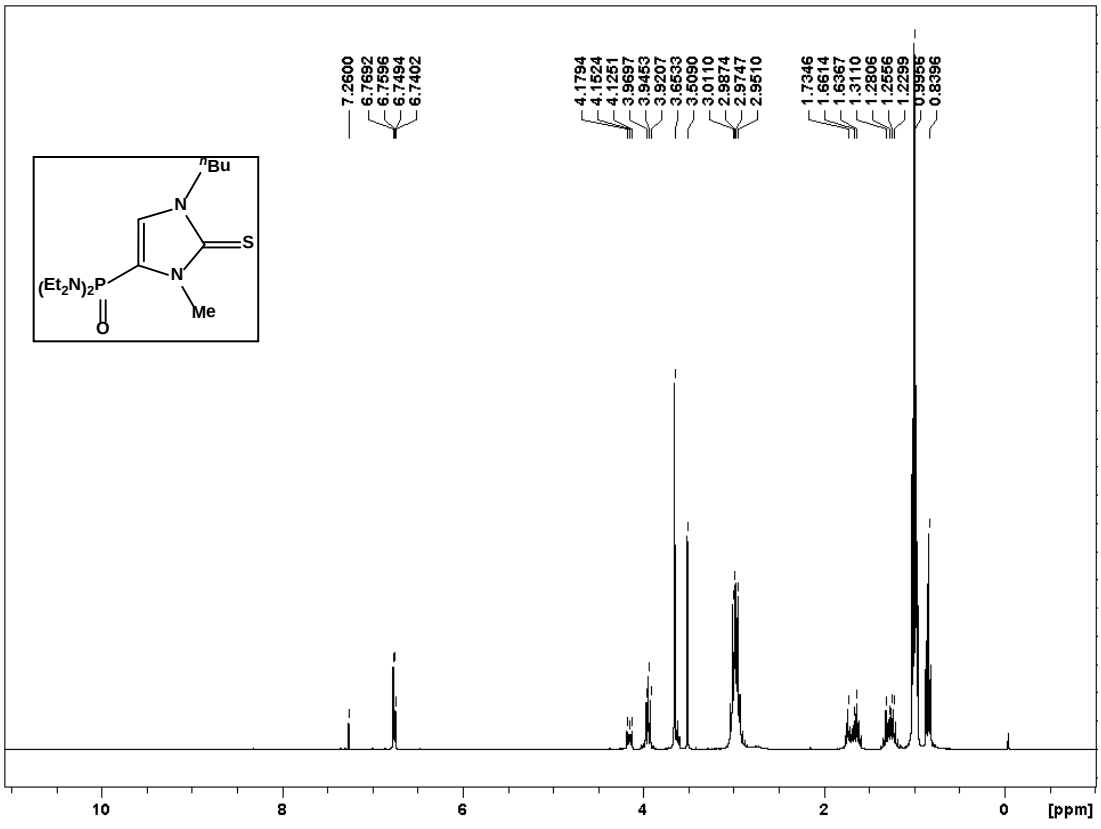

Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum of **4b(b')** in $CDCl_3$ (75.5 MHz, 25 °C)

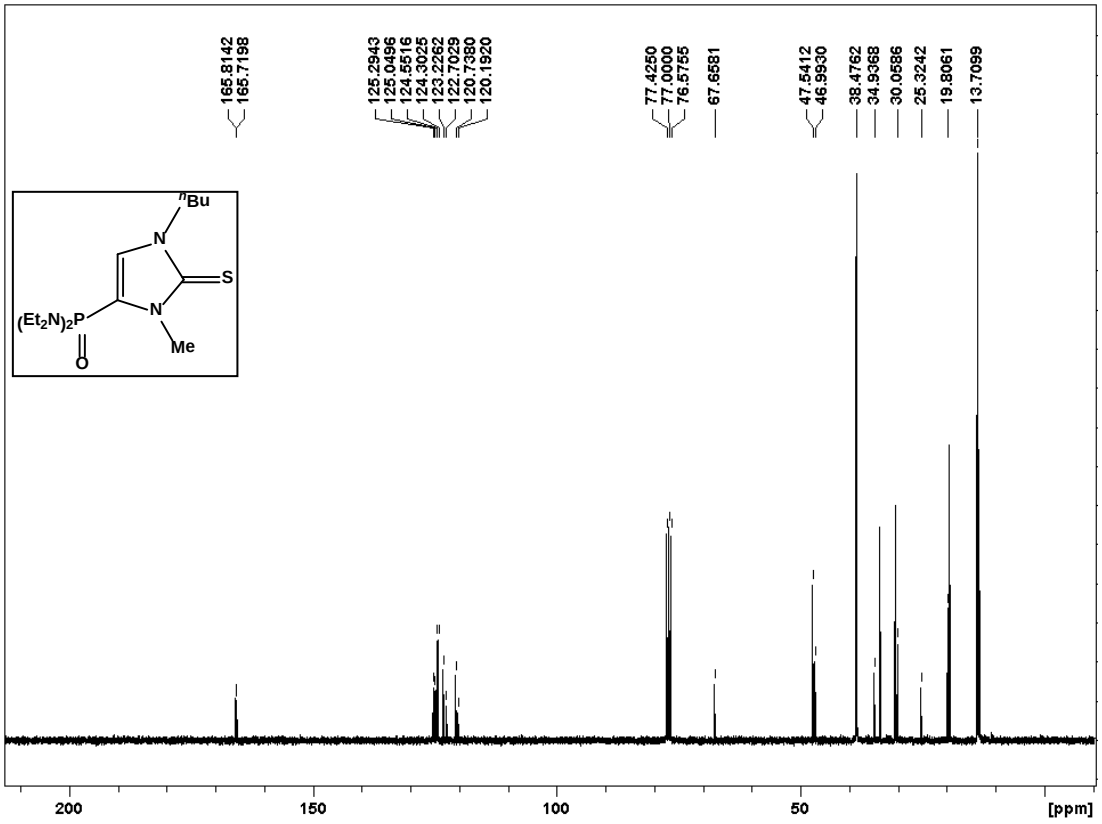

Figure S19: $^{31}P\{^{1}H\}$ NMR spectrum of **4b(b')** in thf (121.5 MHz, 25 °C)

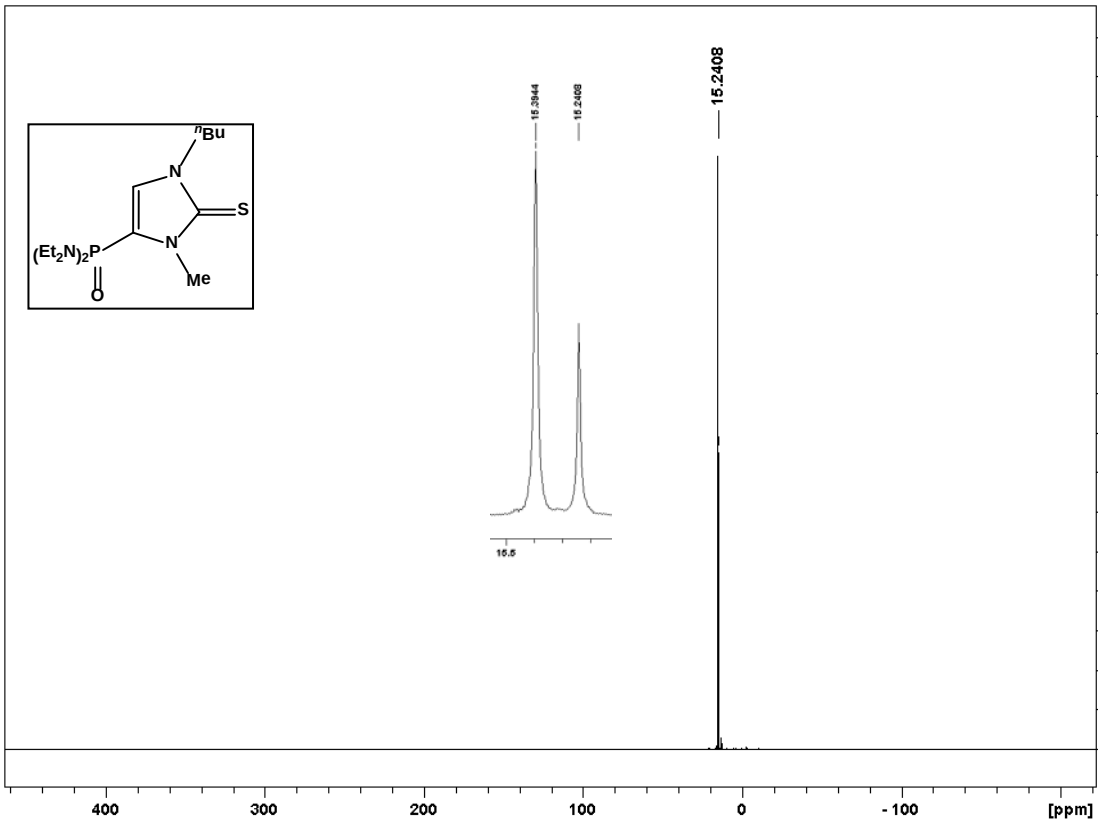

Figure S20: $^{31}P\{^{1}H\}$ NMR spectrum of **4c(c')** in $CDCl_3$ (121.5 MHz, 25 °C)

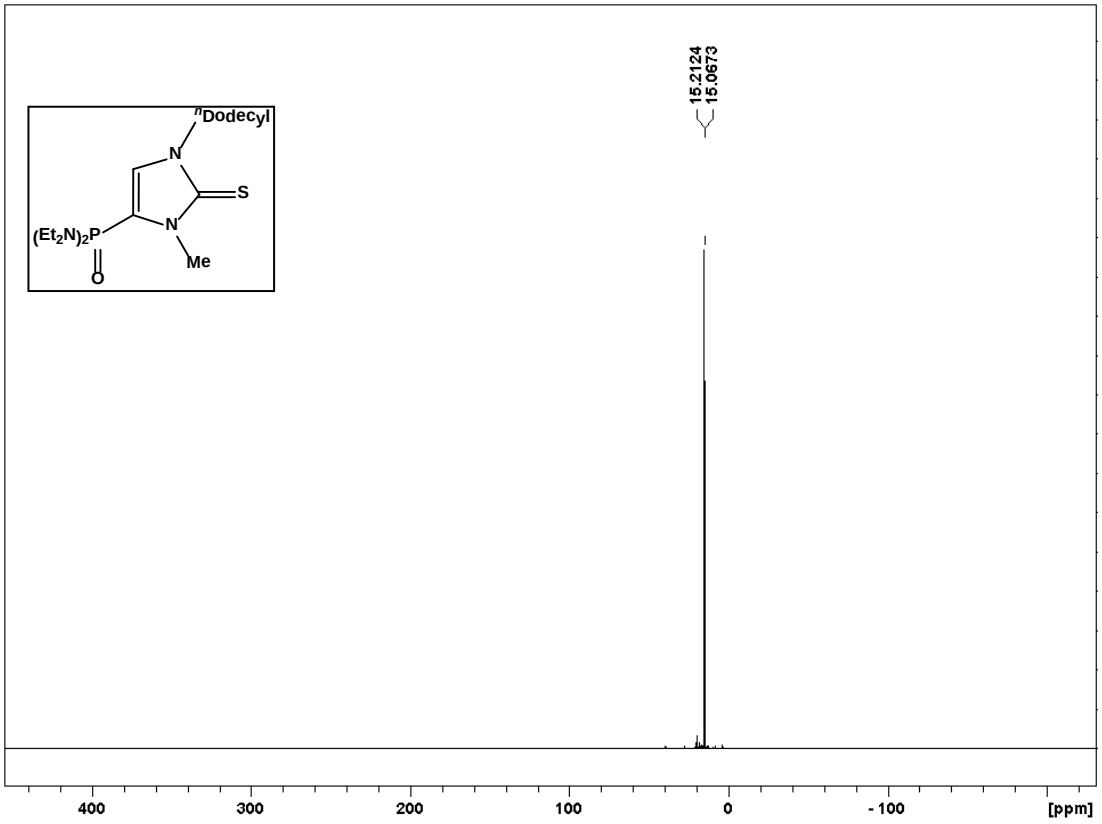

Figure S21: $^{31}P\{^{1}H\}$ NMR spectrum of **4d** in $CDCl_3$ (121.5 MHz, 25 °C)

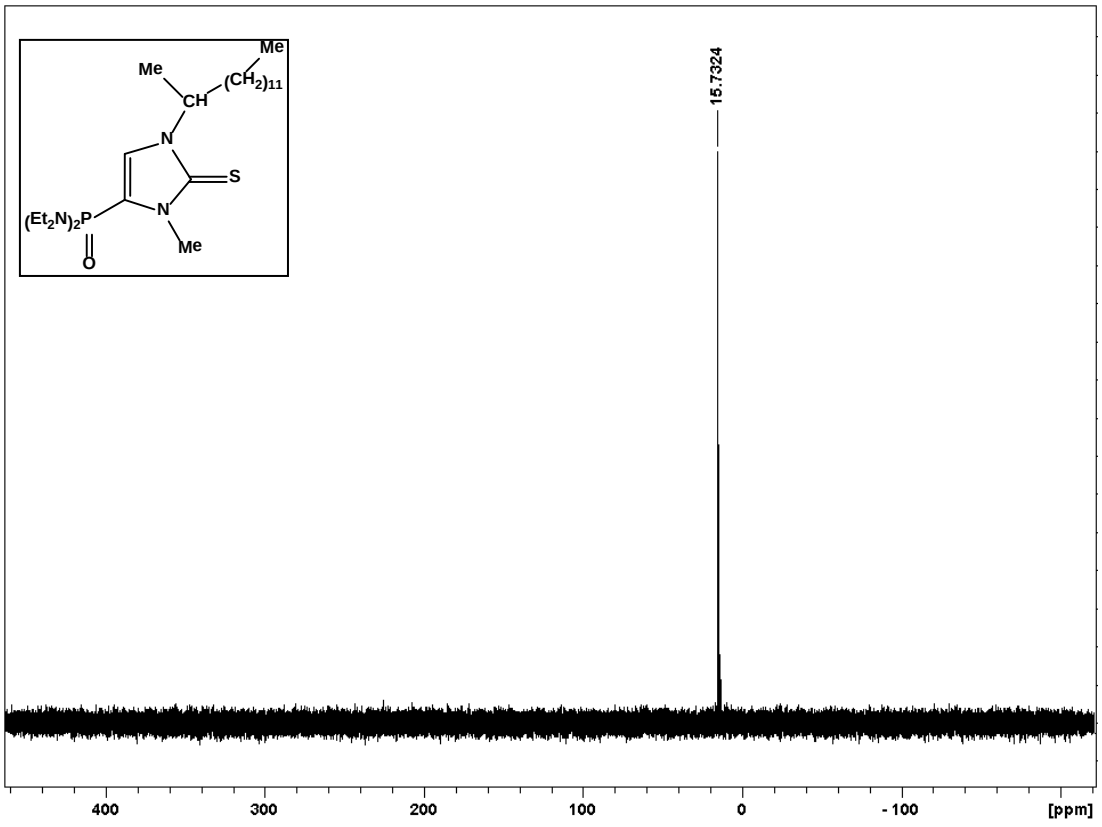

Figure S22: ^{1}H NMR spectrum of **5a** in $CDCl_3$ (300.1 MHz, 25 °C)

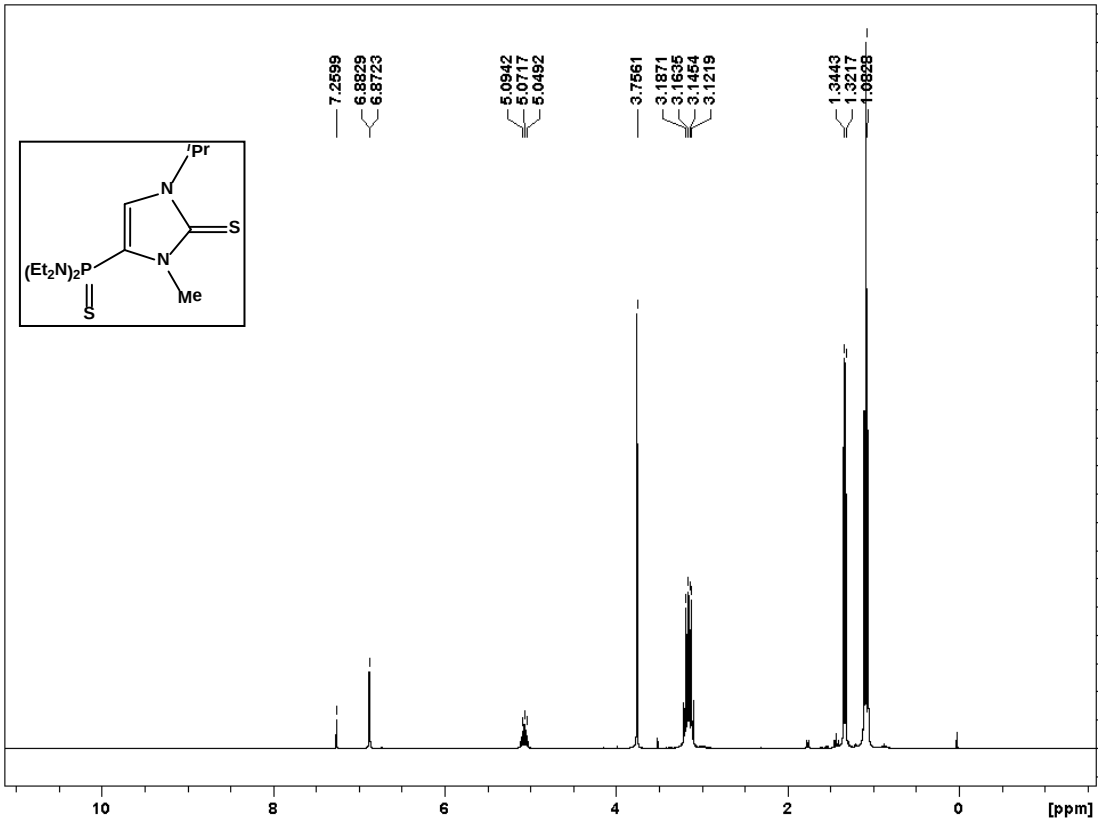

Figure S23: $^{13}C\{^{1}H\}$ NMR spectrum of **5a** in $CDCl_3$ (75.5 MHz, 25 °C)

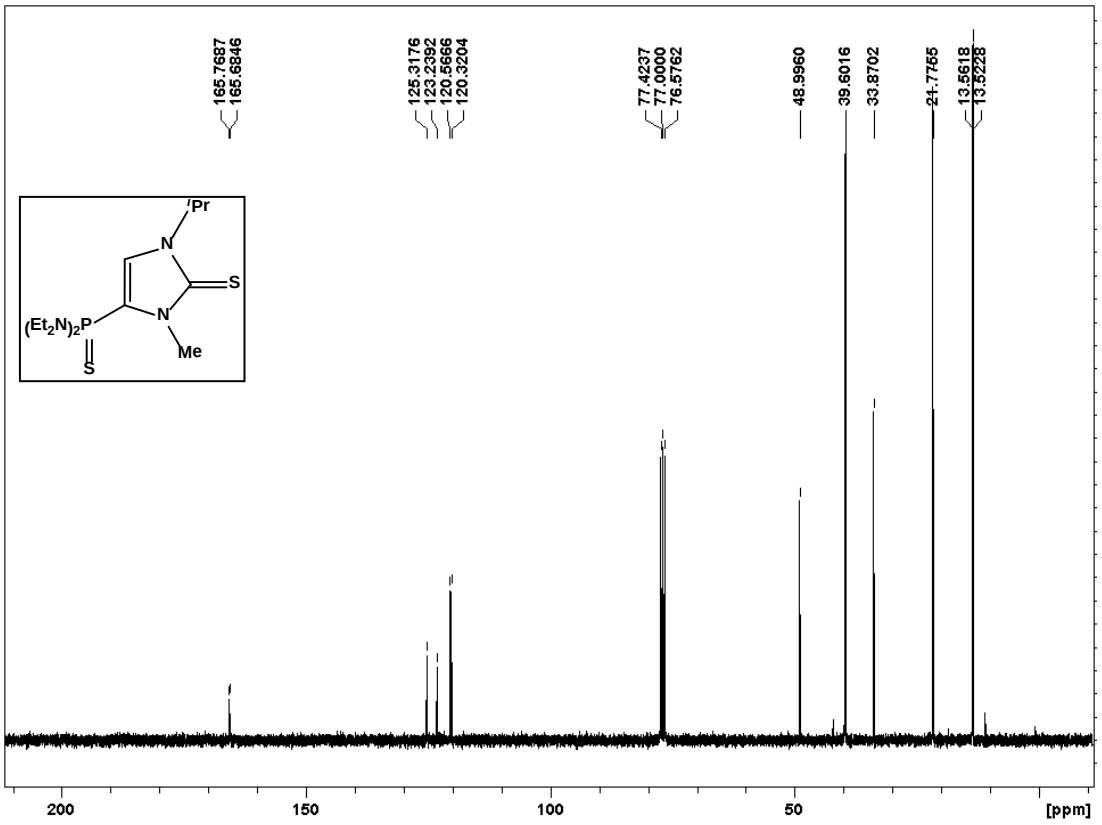

Figure S24: $^{31}P\{^{1}H\}$ NMR spectrum of **5a** in $CDCl_3$ (121.5 MHz, 25 °C)

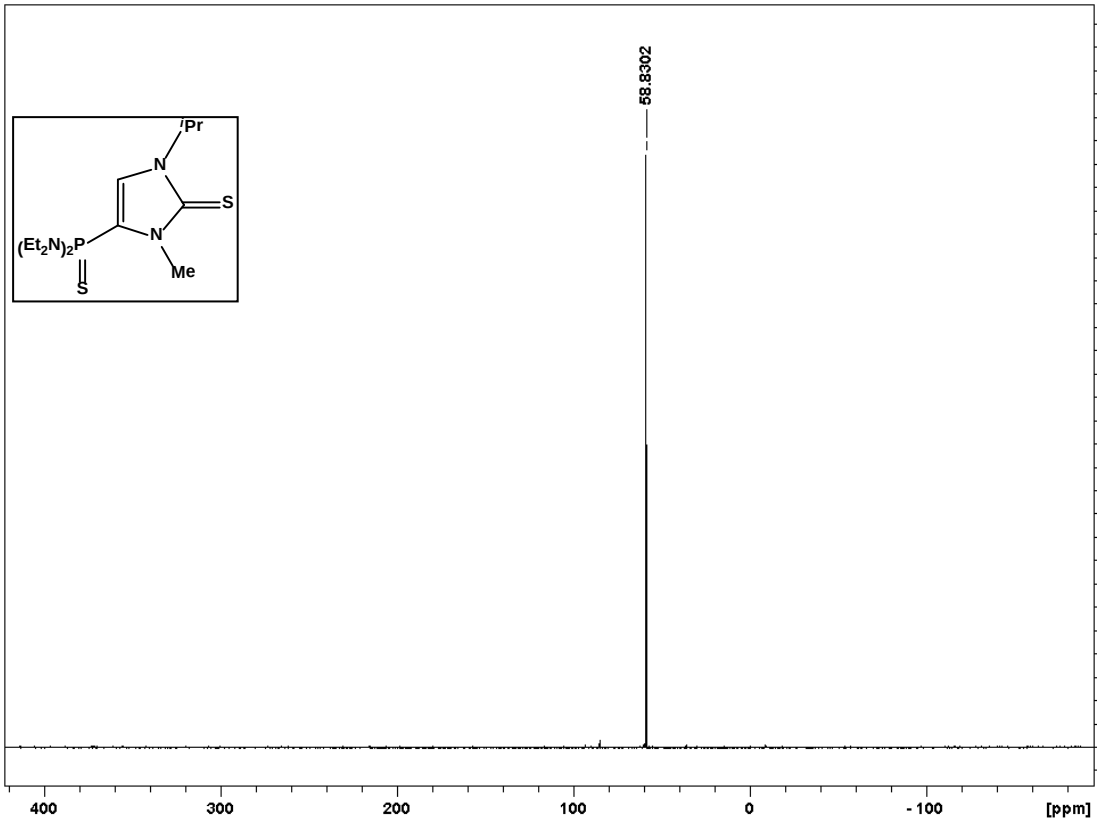

Figure S25: $^{31}P\{^{1}H\}$ NMR spectrum of **6b(b')** in thf (121.5 MHz, 25 °C)

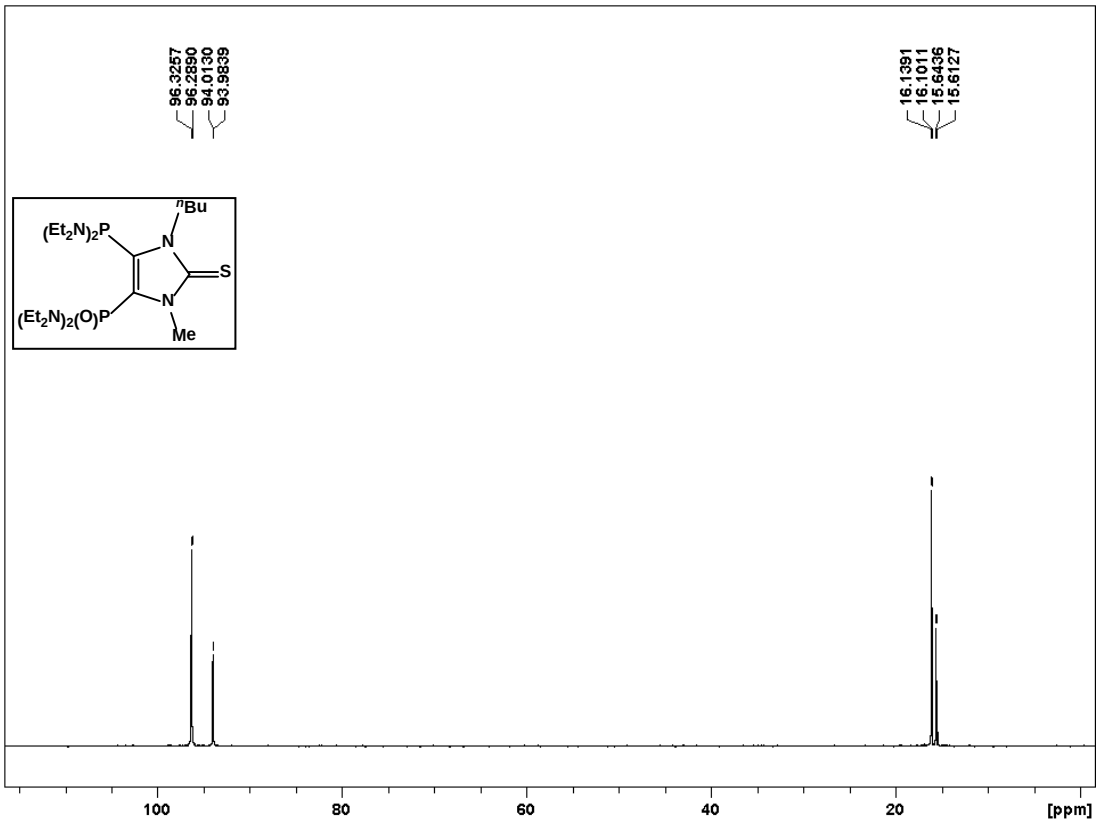

Figure S26: $^{31}P\{^{1}H\}$ NMR spectrum of **6c(c')** in thf (121.5 MHz, 25 °C)

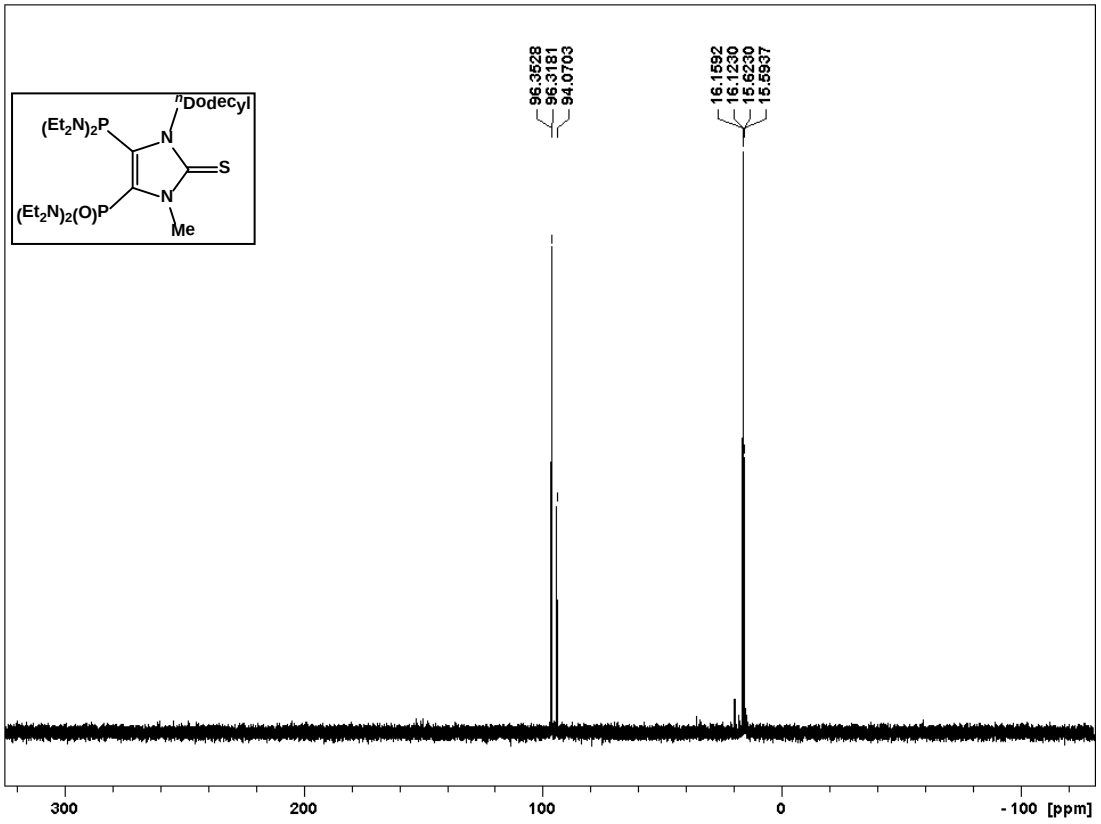

Figure S27: ^{1}H NMR spectrum of **7b** in $CDCl_3$ (300.1 MHz, 25 °C)

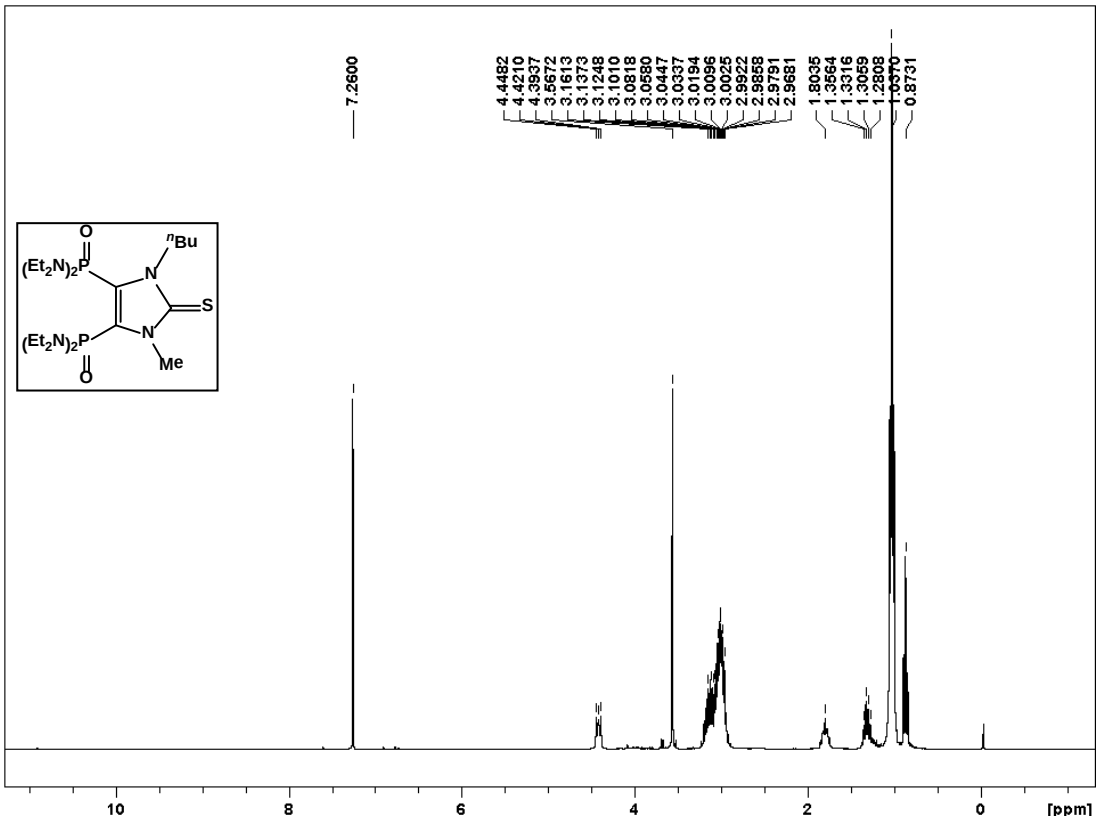

Figure S28: $^{13}C\{^{1}H\}$ NMR spectrum of **7b** in $CDCl_3$ (75.5 MHz, 25 °C)

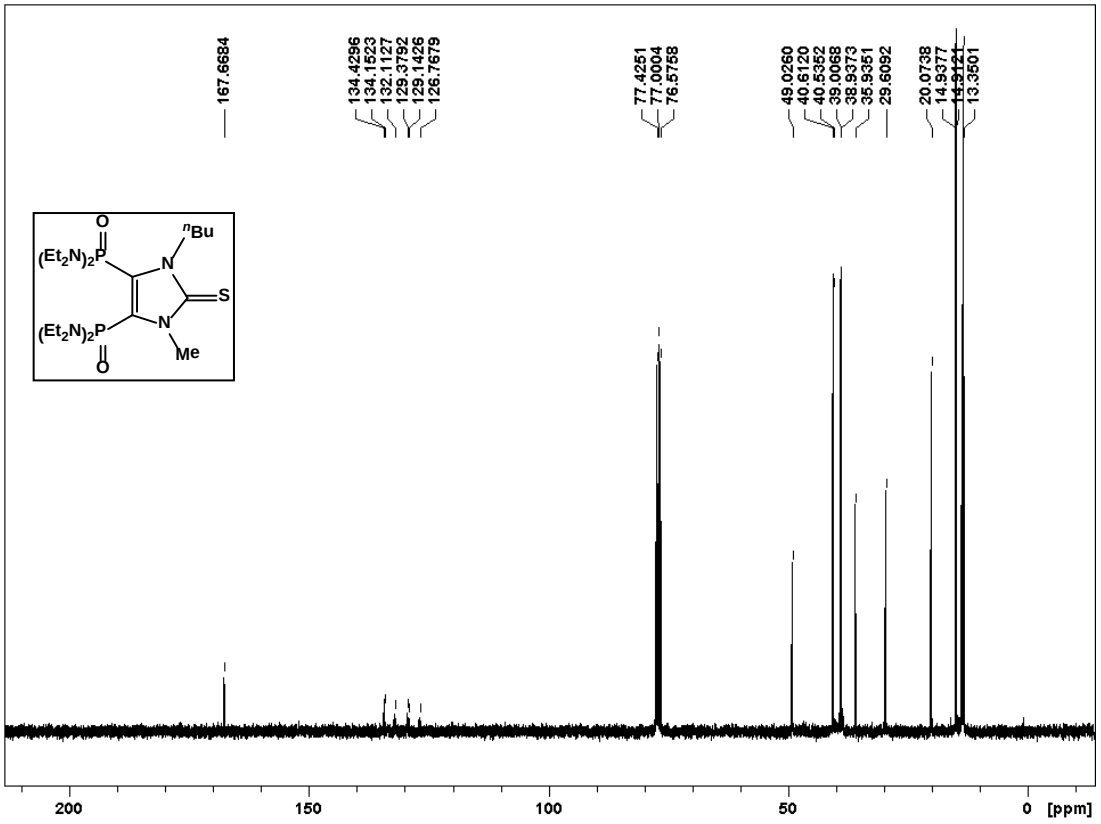

Figure S29: $^{31}P\{^{1}H\}$ NMR spectrum of **7b** in thf (121.5 MHz, 25 °C)

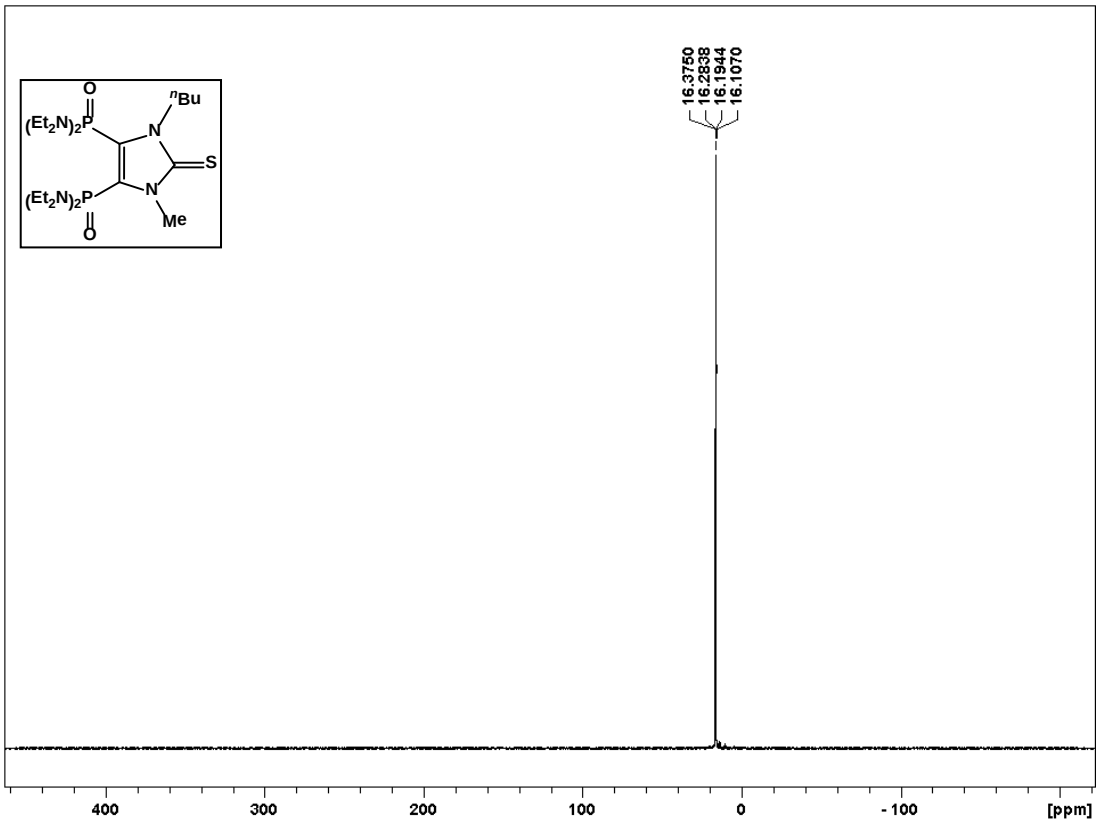

Figure S30: ^{1}H NMR spectrum of **7c** in $CDCl_3$ (300.1 MHz, 25 °C)

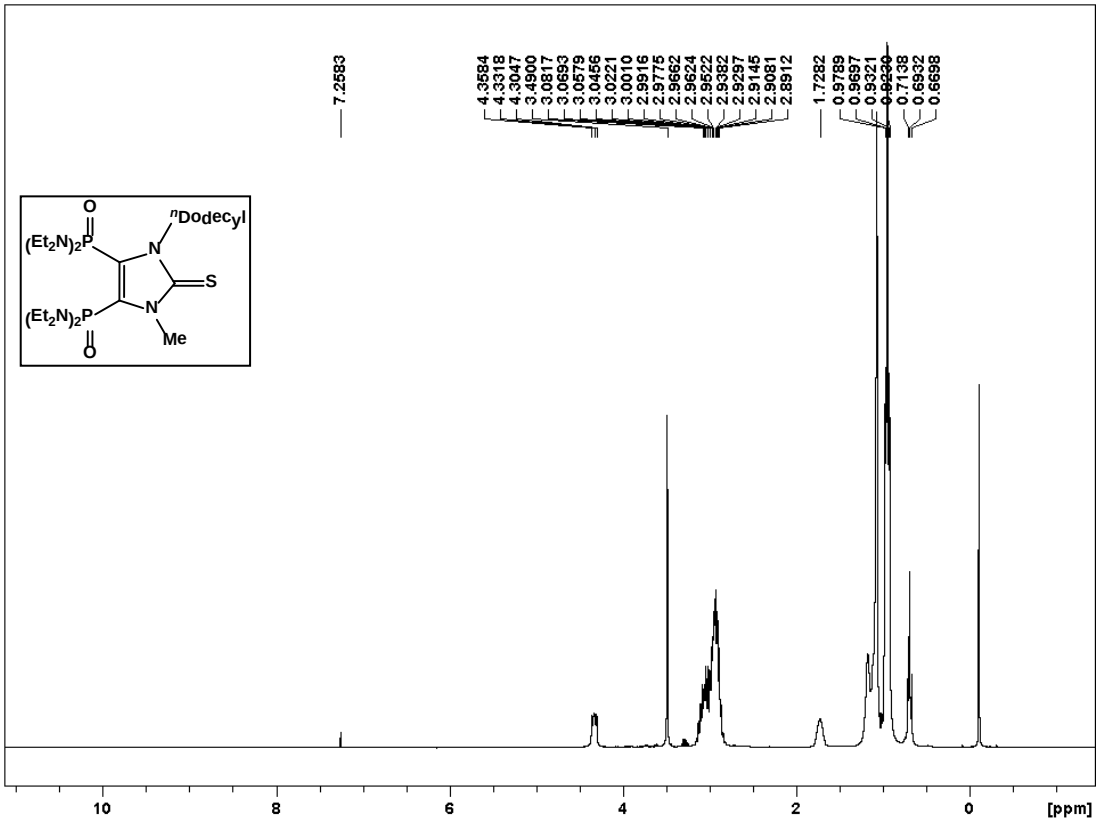

Figure S31: $^{13}C\{^{1}H\}$ NMR spectrum of **7c** in $CDCl_3$ (75.5 MHz, 25 °C)

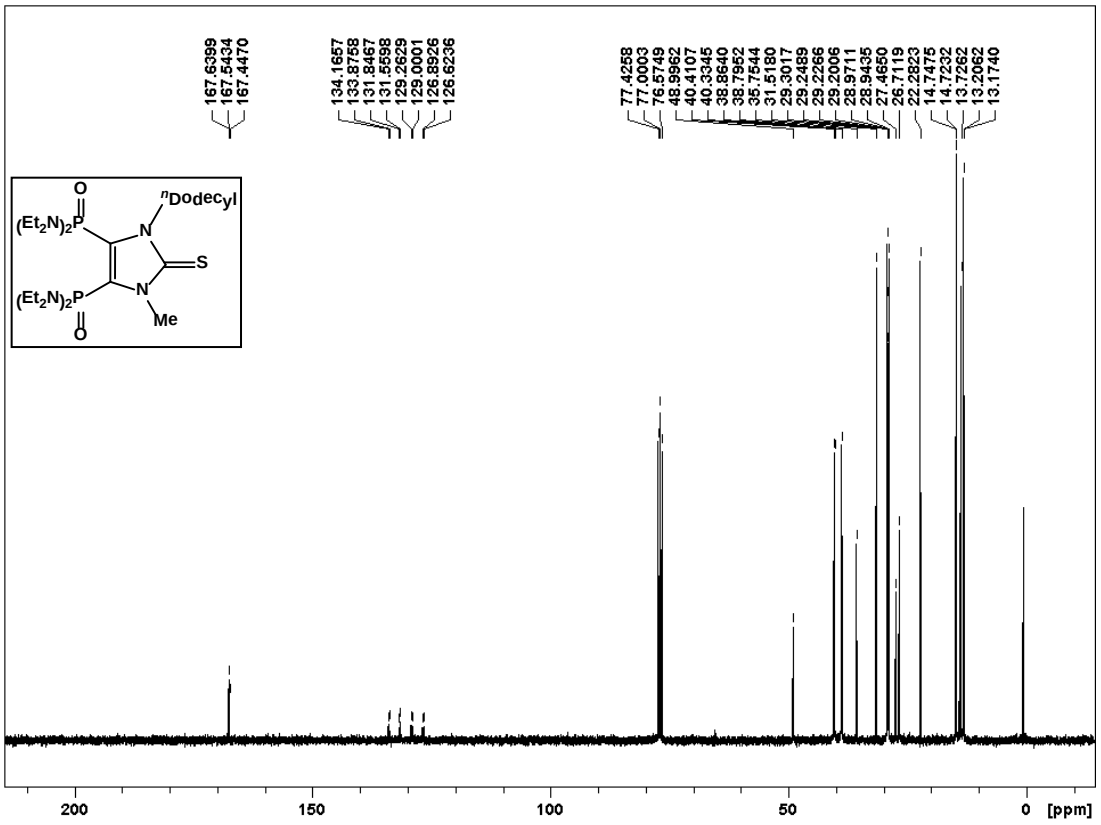

Figure S32: $^{31}P\{^{1}H\}$ NMR spectrum of **7c** in $CDCl_3$ (121.5 MHz, 25 °C)

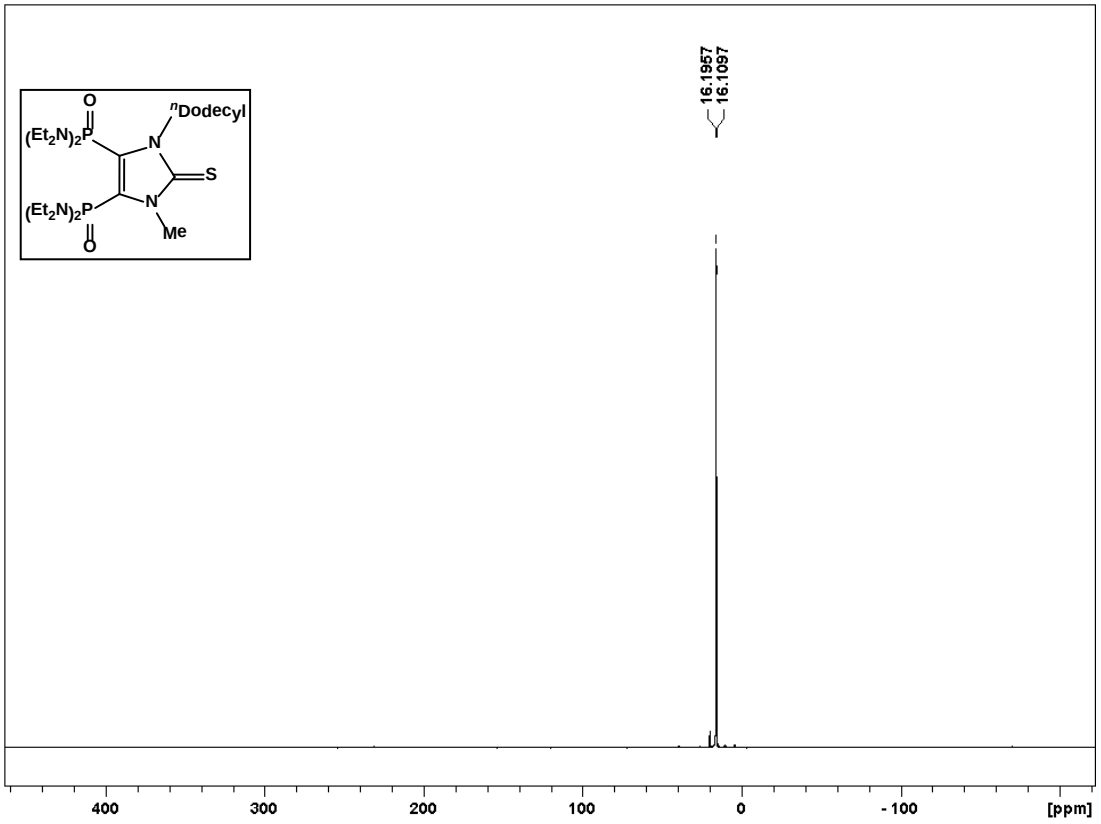

Figure S33: ^{1}H NMR spectrum of **8d** in $CDCl_3$ (300.1 MHz, 25 °C)

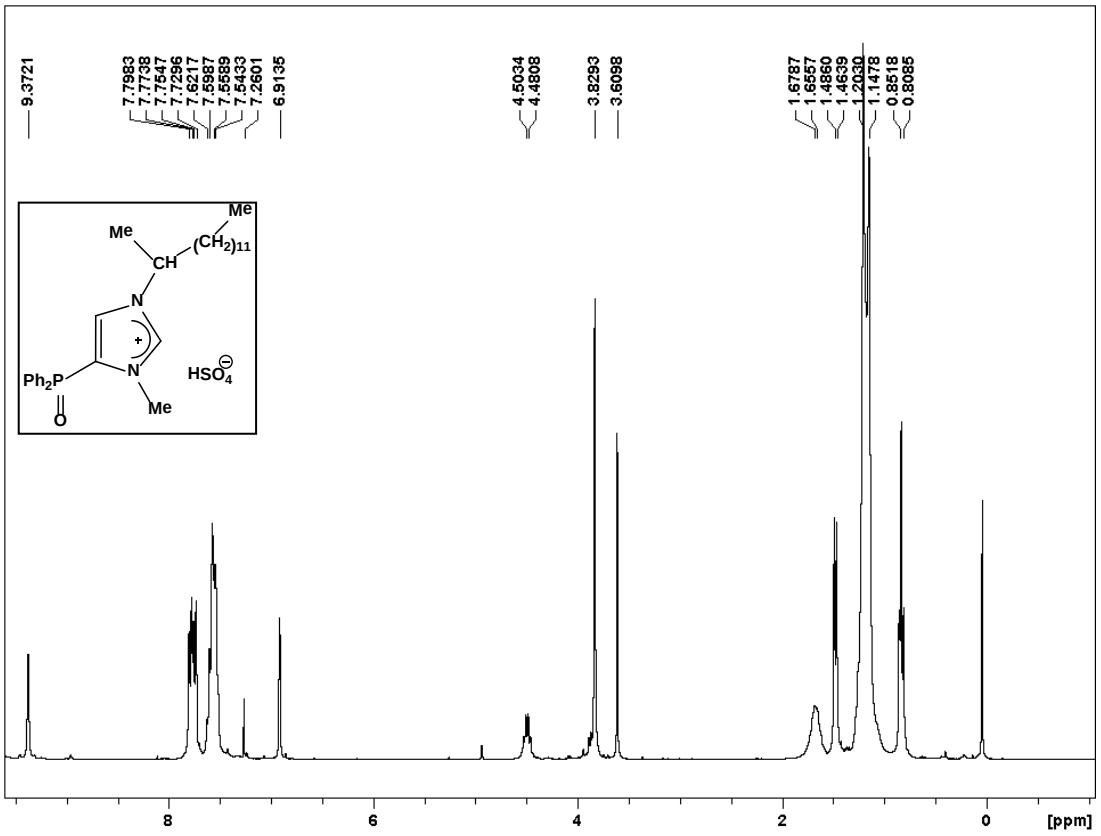

Figure S34: $^{13}C\{^{1}H\}$ NMR spectrum of **8d** in $CDCl_3$ (75.5 MHz, 25 °C)

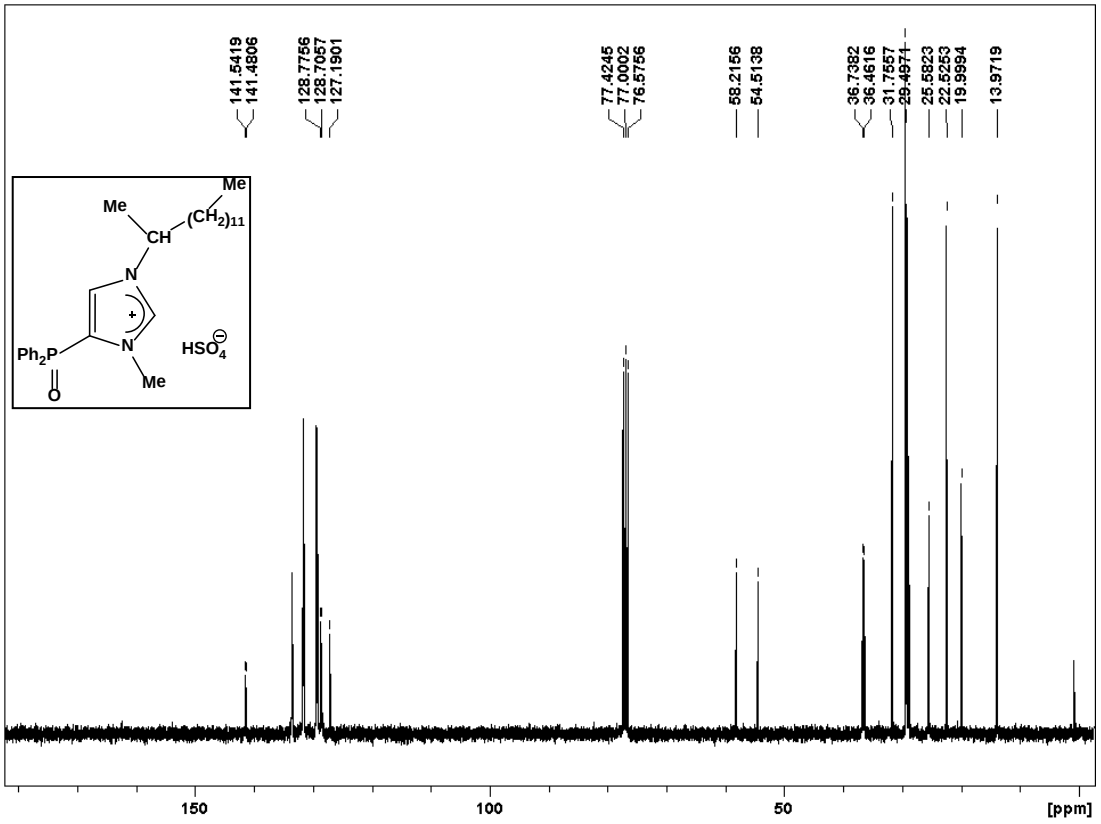

Figure S35: $^{31}P\{^{1}H\}$ NMR spectrum of **8d** in $CDCl_3$ (121.5 MHz, 25 °C)

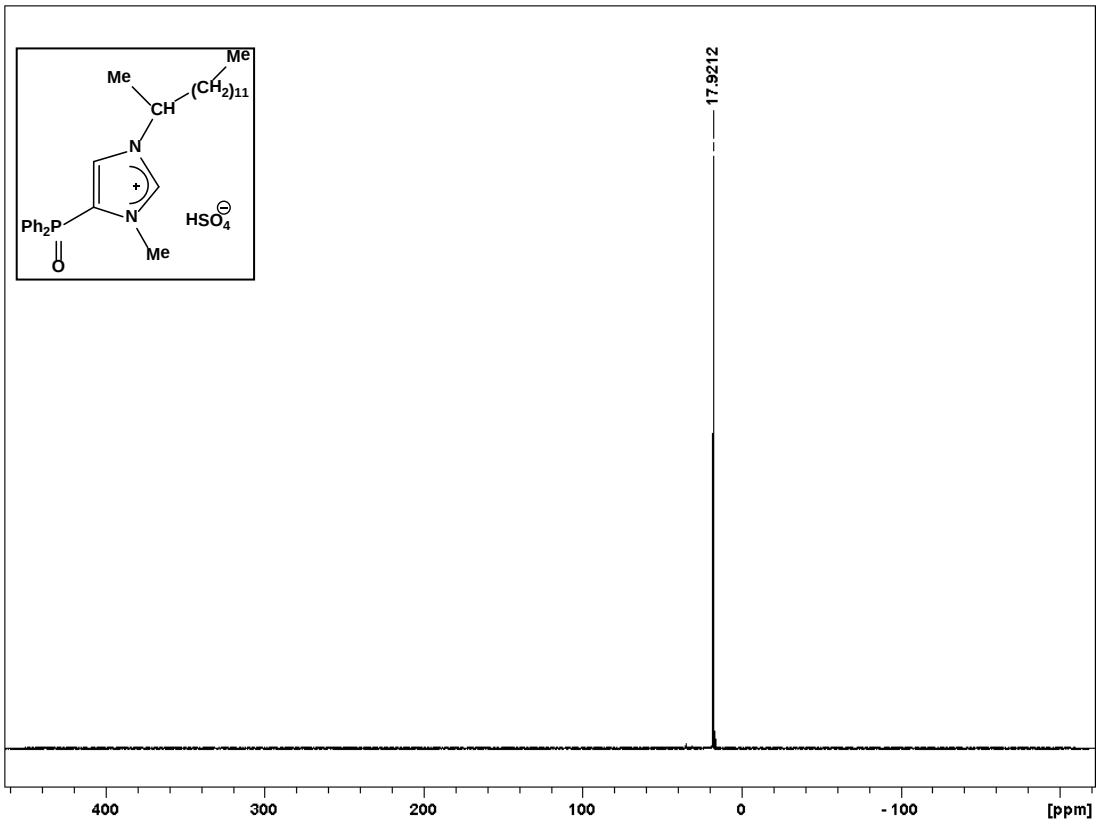

Figure S36: ^{1}H NMR spectrum of **9a** in $CDCl_3$ (300.1 MHz, 25 °C)

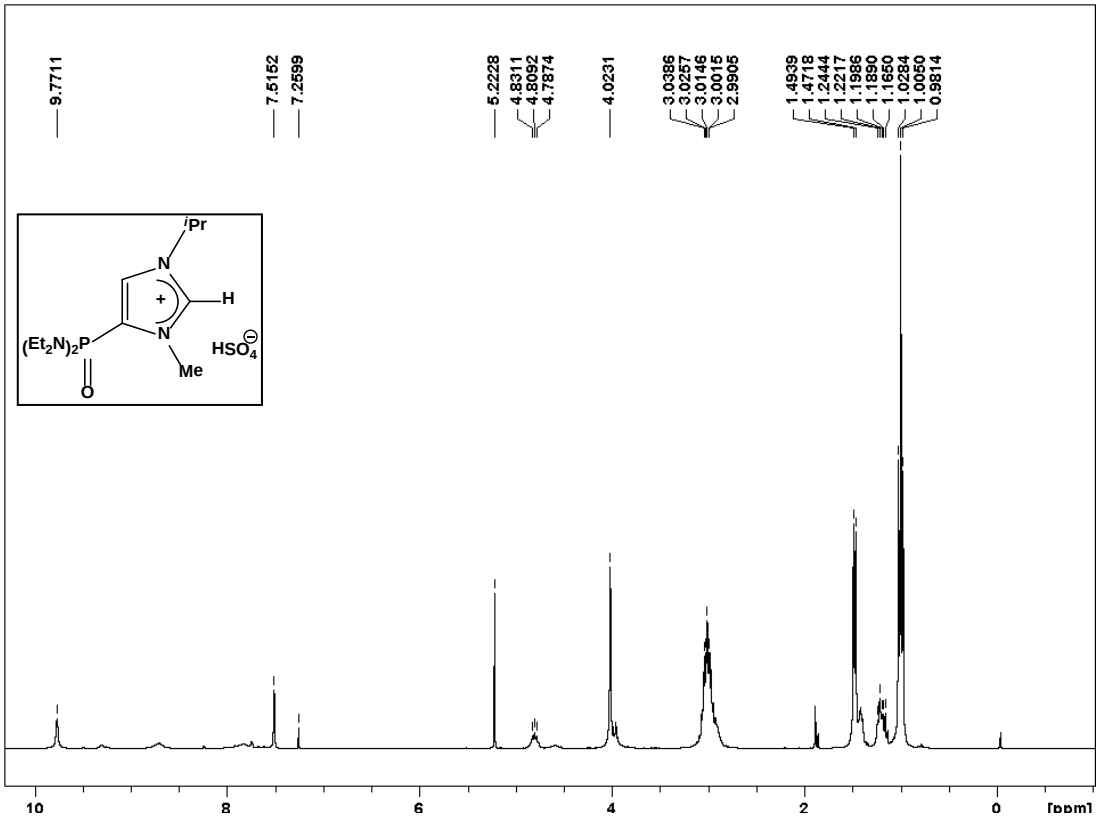

Figure S37: $^{13}C\{^{1}H\}$ NMR spectrum of **9a** in $CDCl_3$ (75.5 MHz, 25 °C)

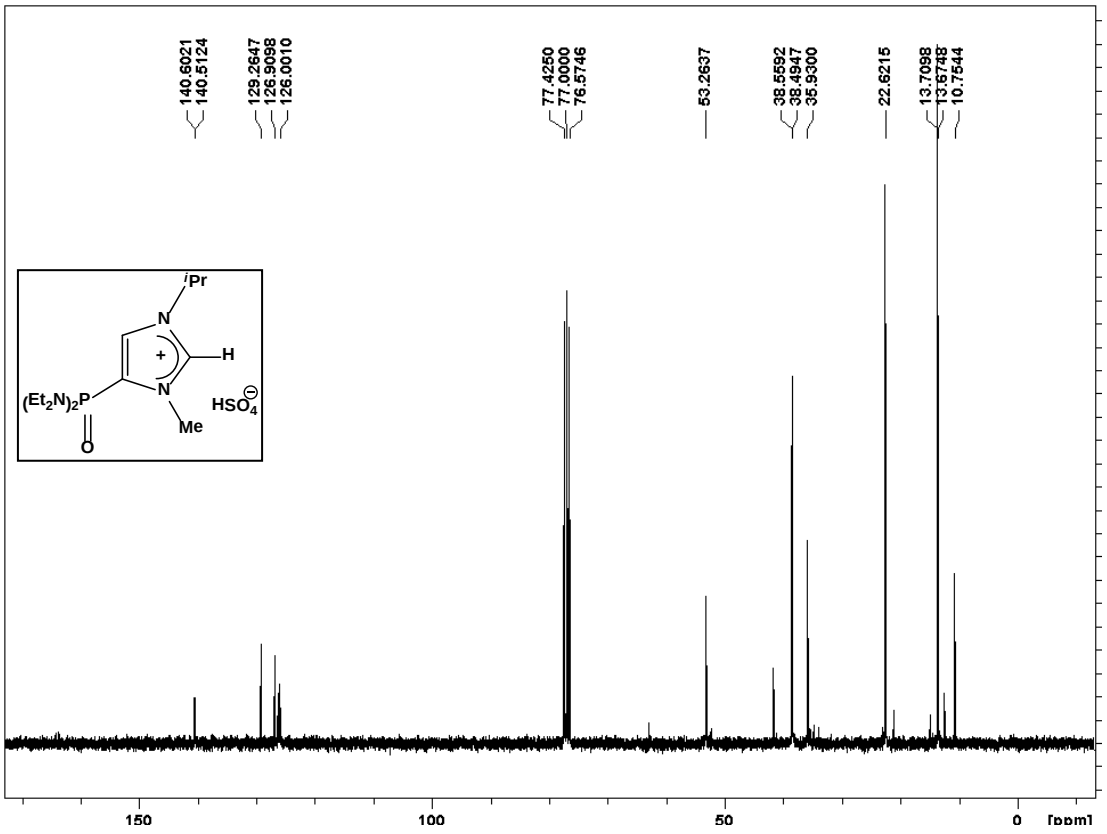

Figure S38: $^{31}P\{^{1}H\}$ NMR spectrum of **9a** in $CDCl_3$ (121.5 MHz, 25 °C)

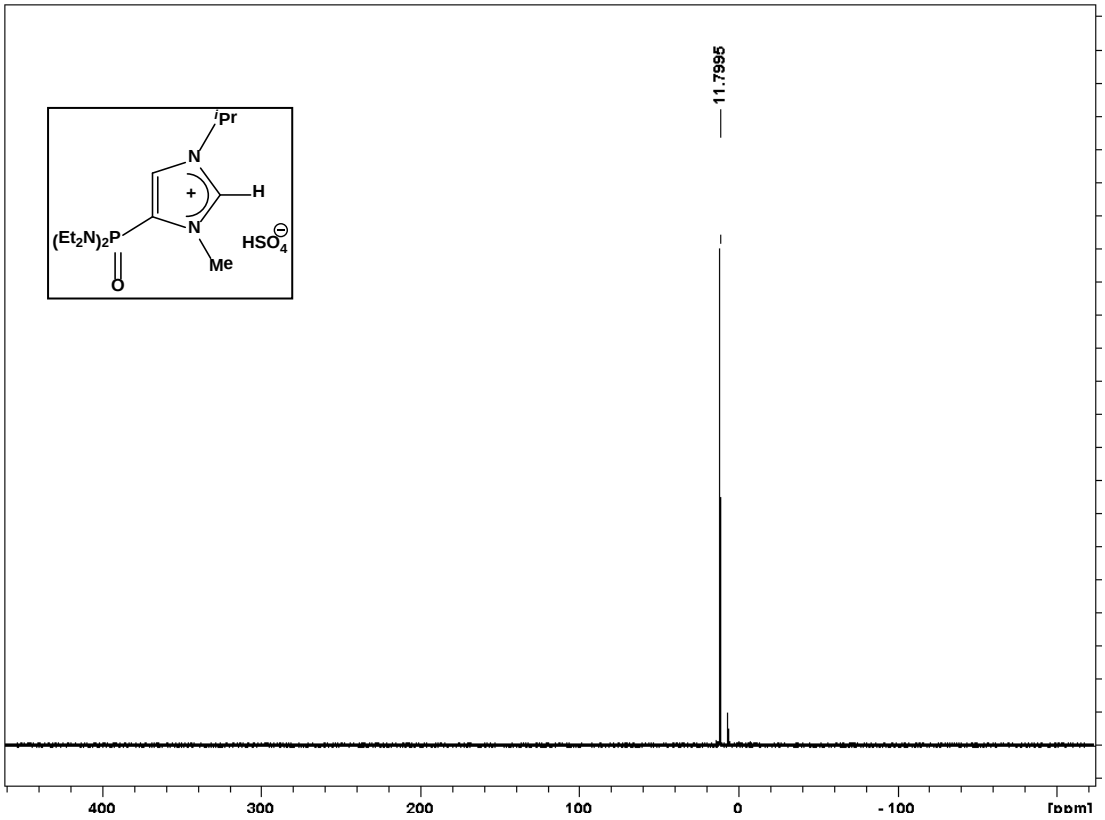

Figure S39: ^{1}H NMR spectrum of **9d** in $CDCl_3$ (300.1 MHz, 25 °C)

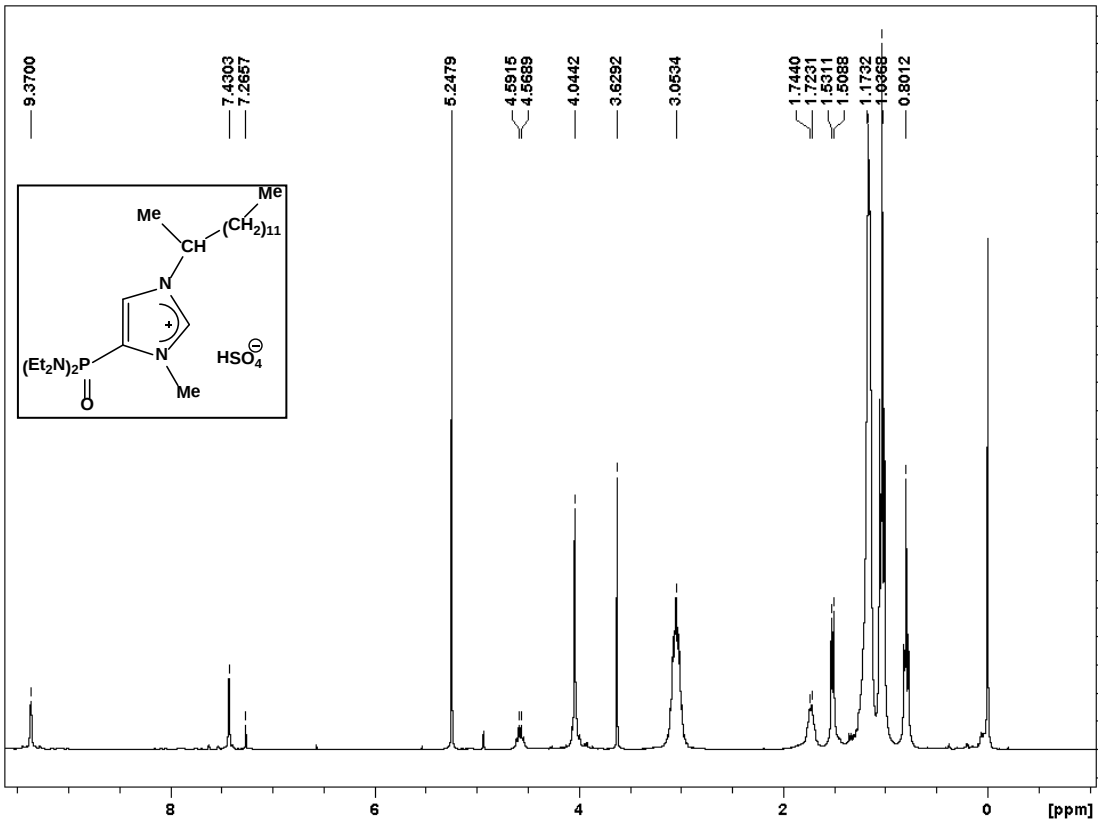

Figure S40: $^{13}C\{^{1}H\}$ NMR spectrum of **9d** in $CDCl_3$ (75.5 MHz, 25 °C)

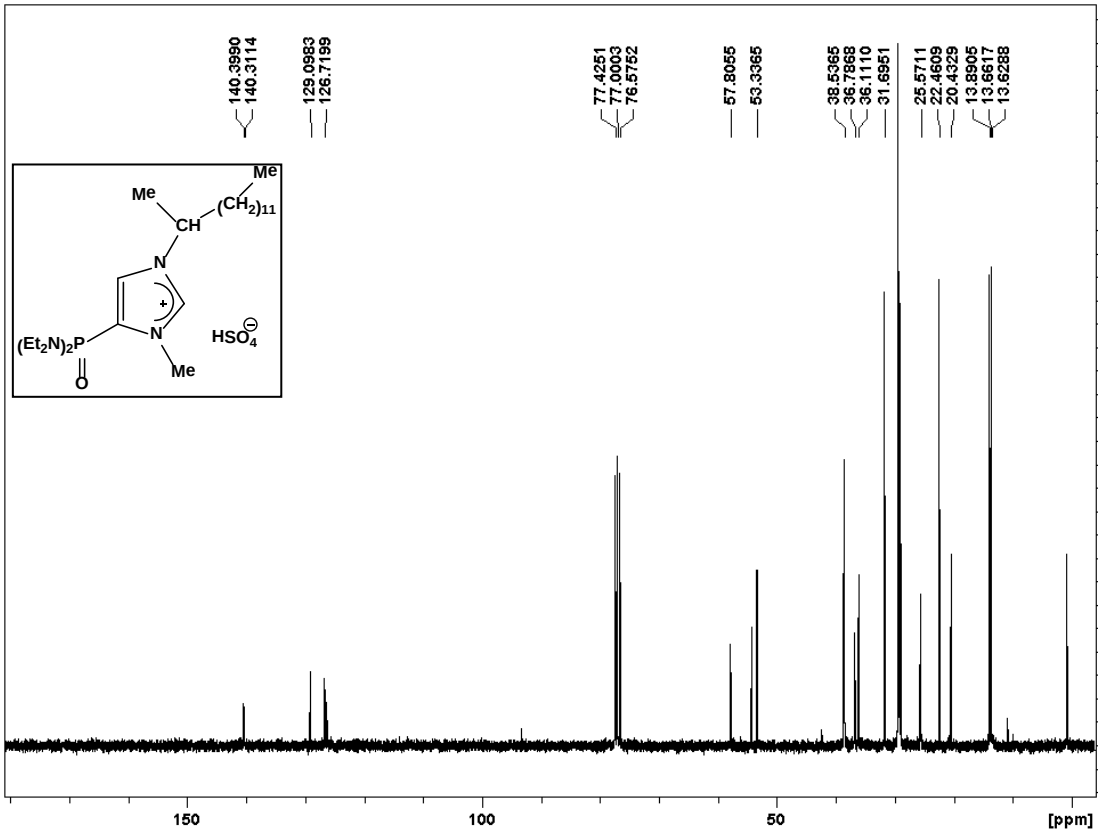

Figure S41: $^{31}P\{^{1}H\}$ NMR spectrum of **9d** in $CDCl_3$ (121.5 MHz, 25 °C)

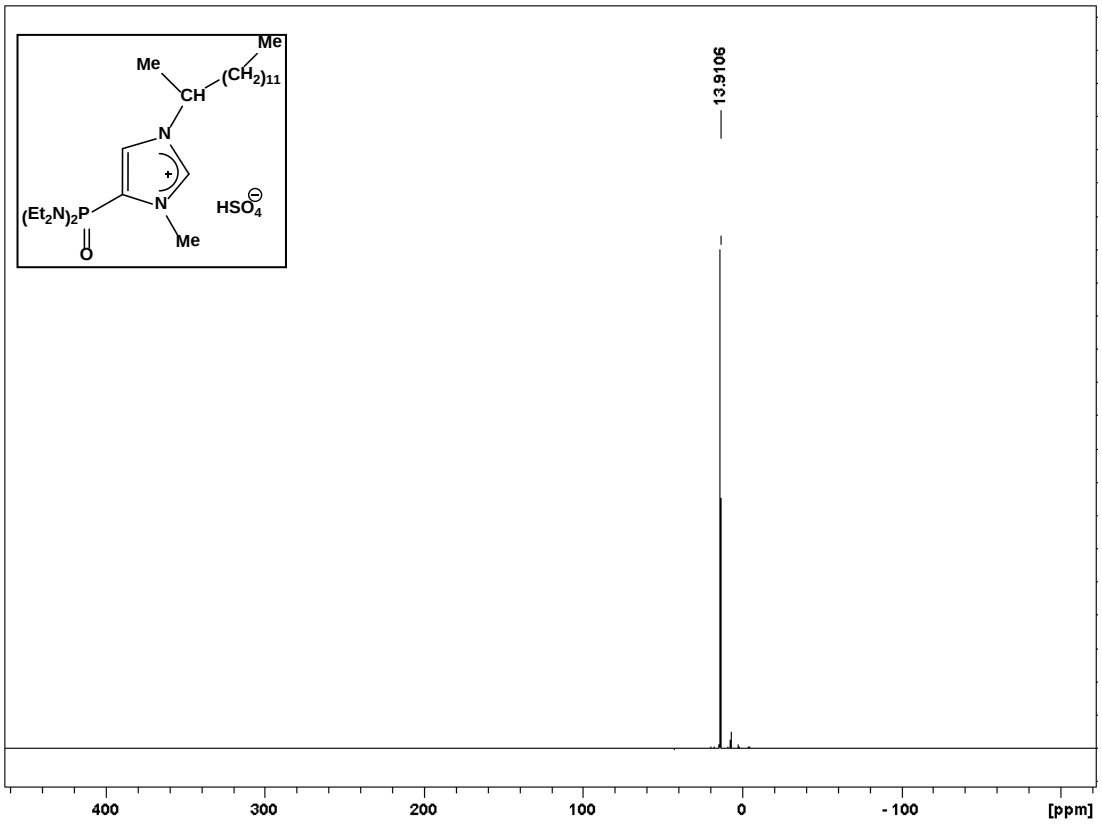

Figure S42: ^{1}H NMR spectrum of **10b** in DMSO-d6 (300.1 MHz, 25 °C)

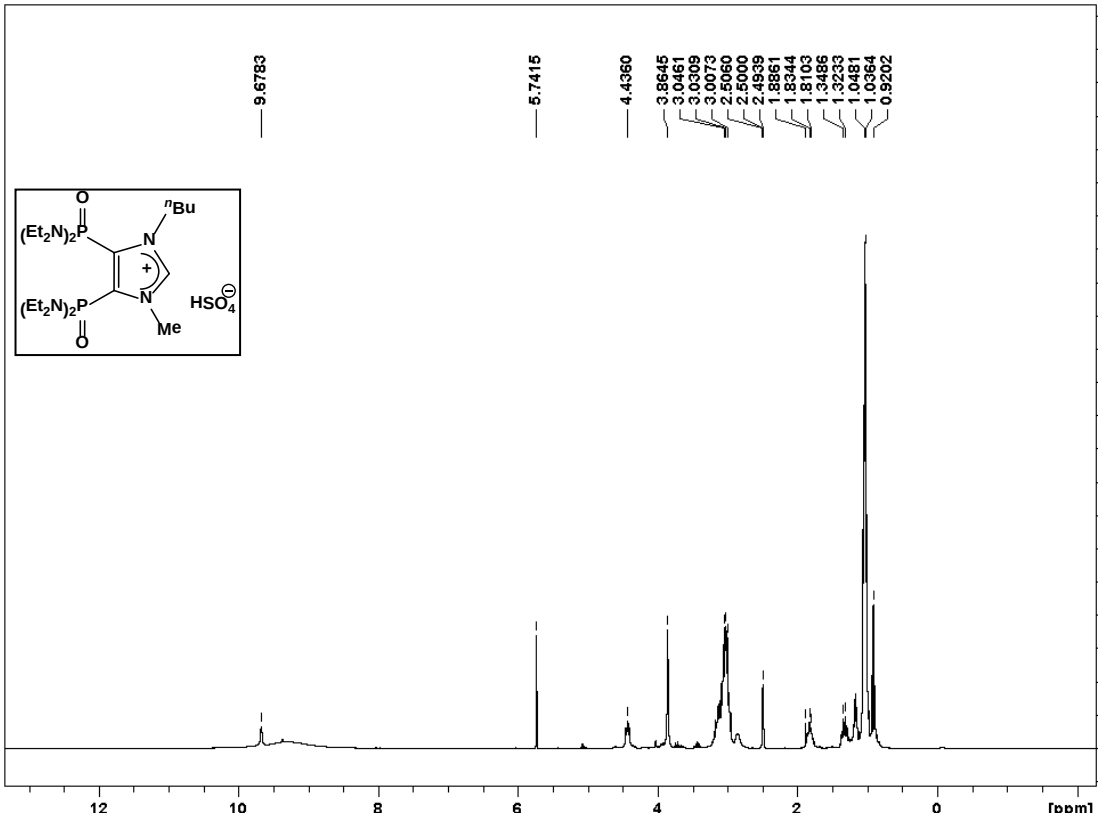

Figure S43: ^{13}C{^{1}H} NMR spectrum of **10b** in DMSO-d6 (75.5 MHz, 25 °C)

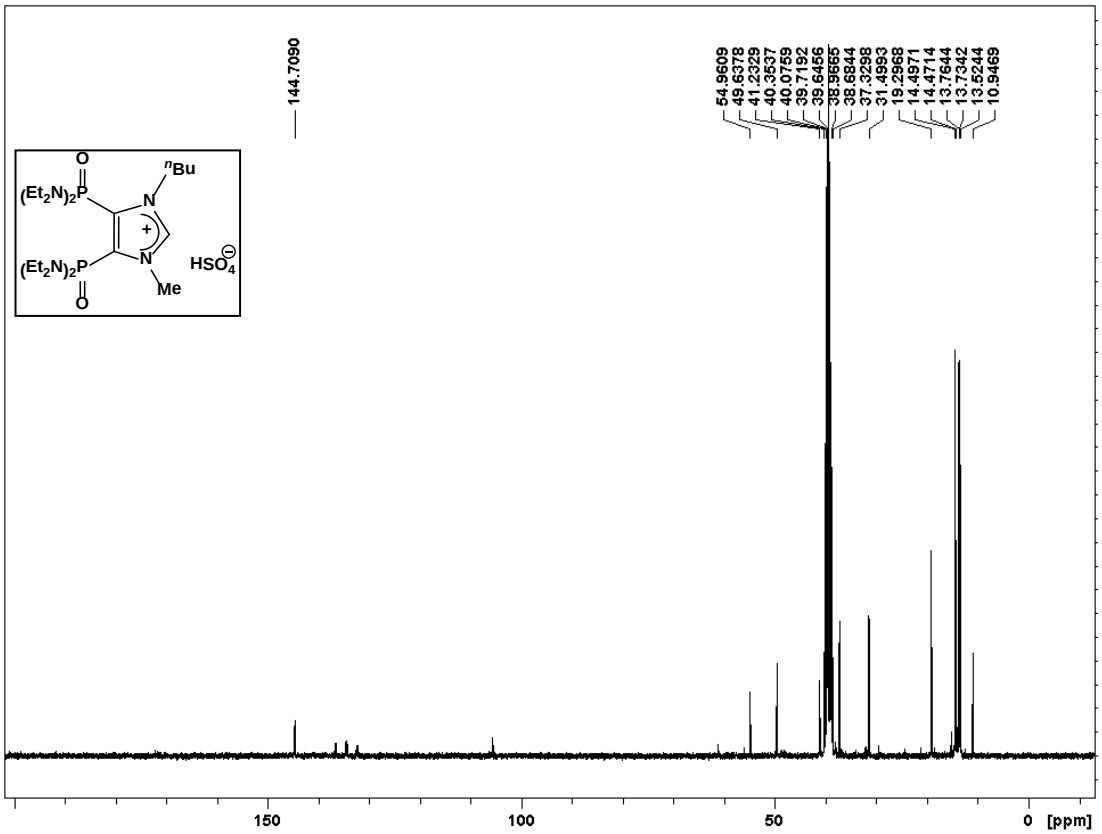

Figure S44: $^{31}P\{^{1}H\}$ NMR spectrum of **10b** in DMSO-d6 (121.5 MHz, 25 °C)

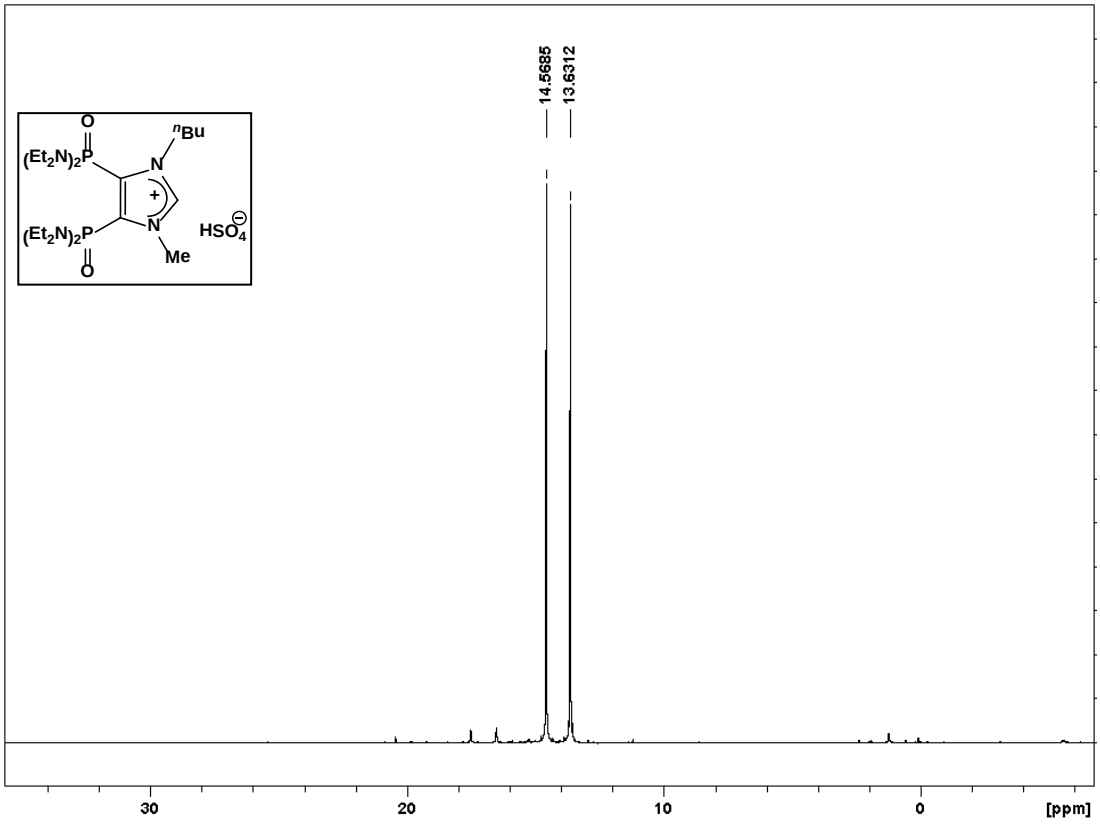

Figure S45: ^{1}H NMR spectrum of **10c** in CD_2Cl_2 (300.1 MHz, 25 °C)

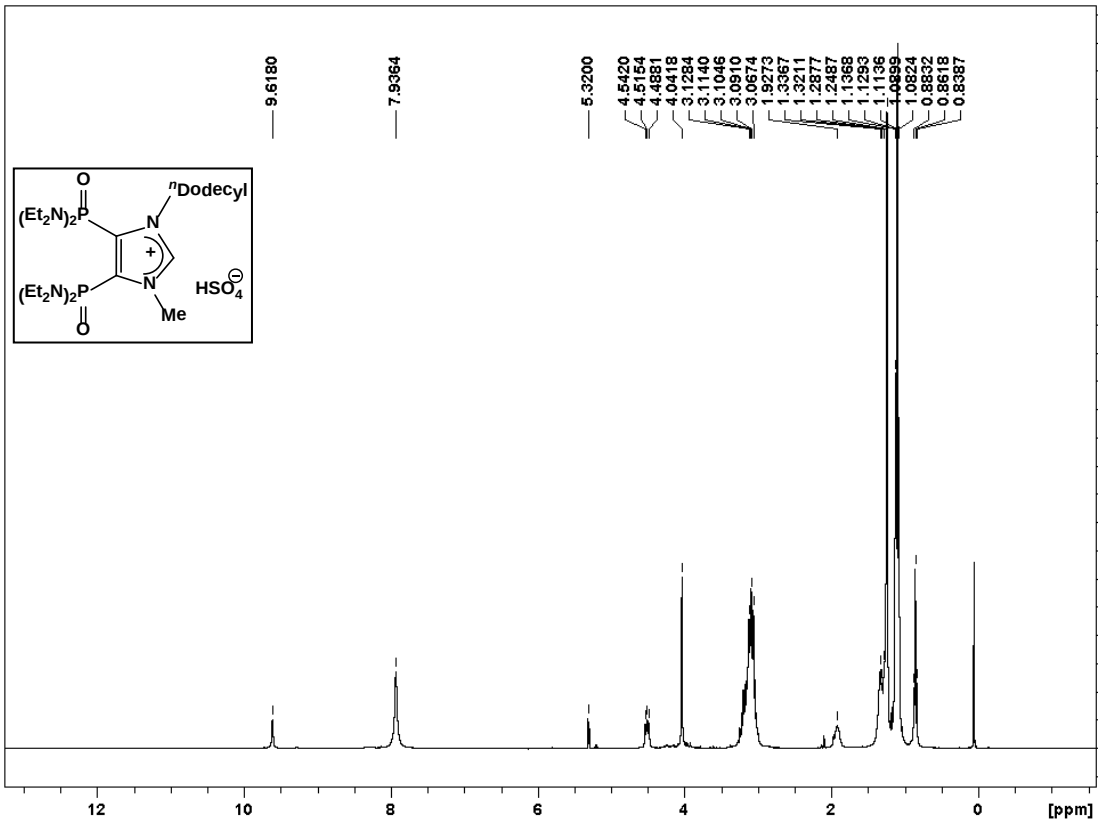

Figure S46: $^{31}P\{^{1}H\}$ NMR spectrum of **10c** in CD_2Cl_2 (121.5 MHz, 25 °C)

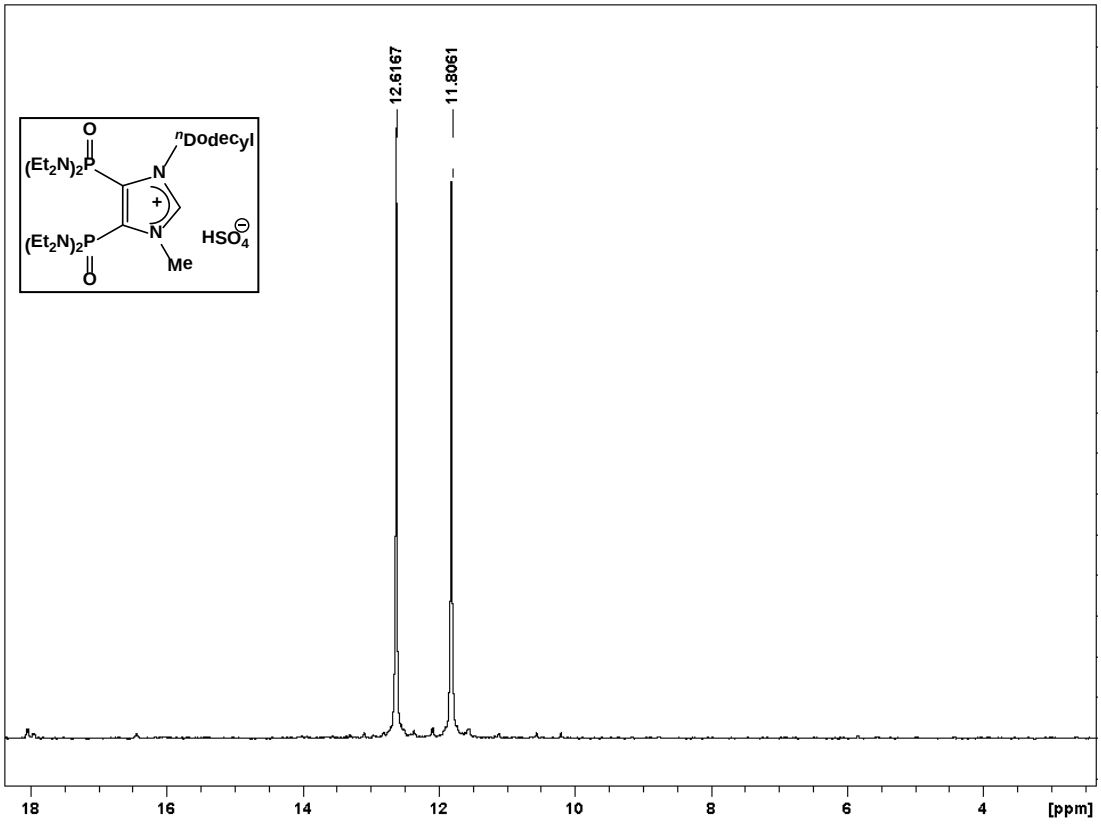

Figure S47: ^{1}H NMR spectrum of **11a** in DMSO-d6 (300.1 MHz, 25 °C)

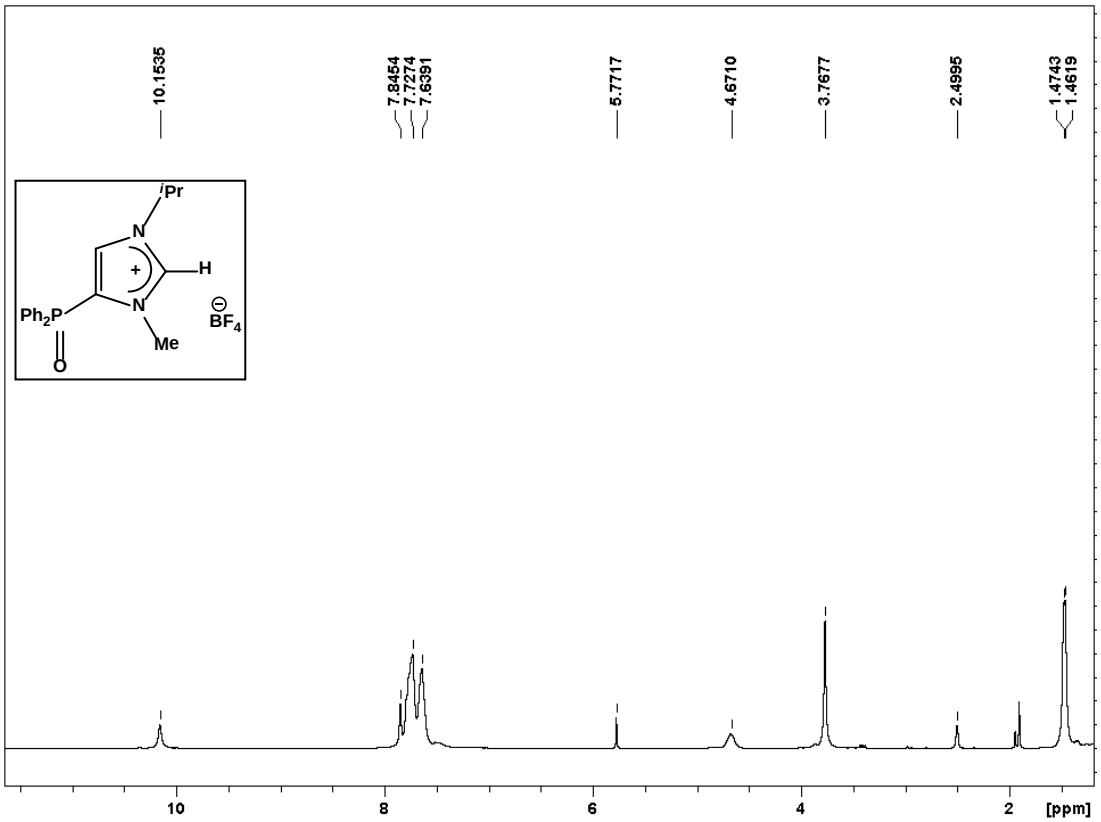

Figure S48: $^{13}C\{^{1}H\}$ NMR spectrum of **11a** in DMSO-d6 (75.5 MHz, 25 °C)

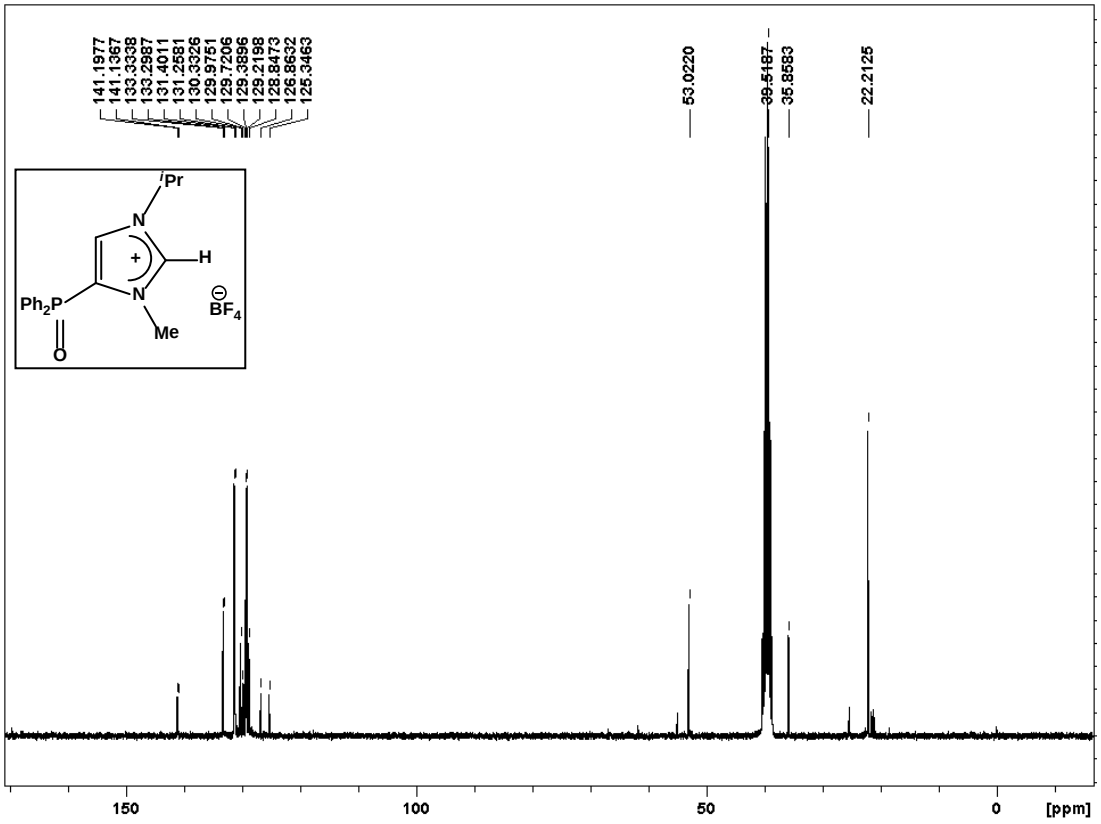

Figure S49: $^{31}P\{^{1}H\}$ NMR spectrum of **11a** in DMSO-d6 (121.5 MHz, 25 °C)

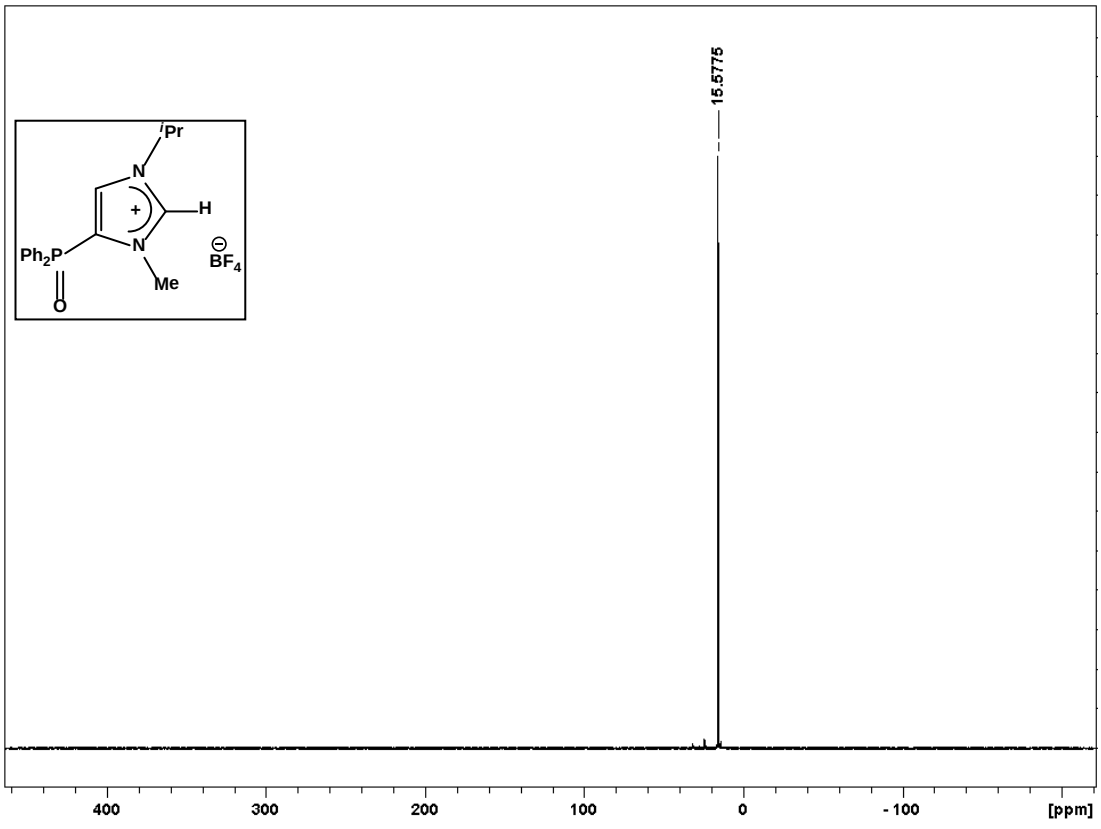

Figure S50: ^{1}H NMR spectrum of **12a** in d mso-d6 (300.1 MHz, 25 °C)

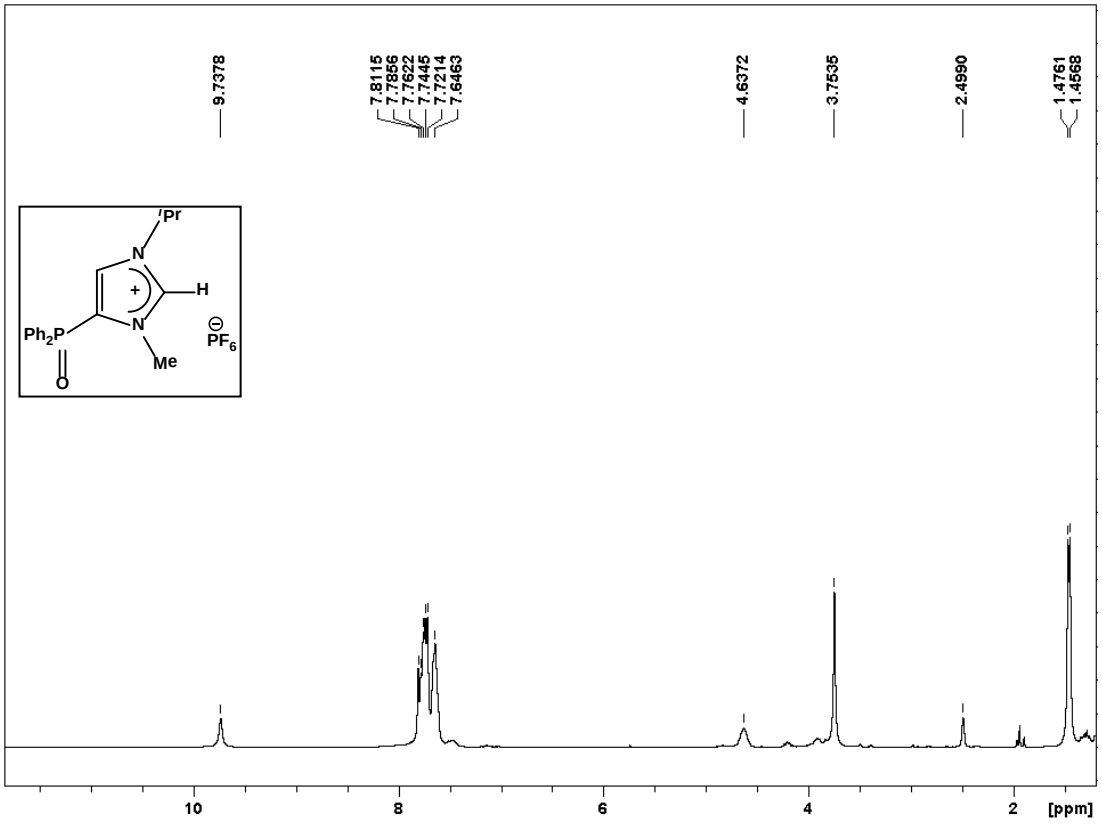

Figure S51: ^{13}C{^{1}H} NMR spectrum of **12a** in DMSO-d6 (75.5 MHz, 25 °C)

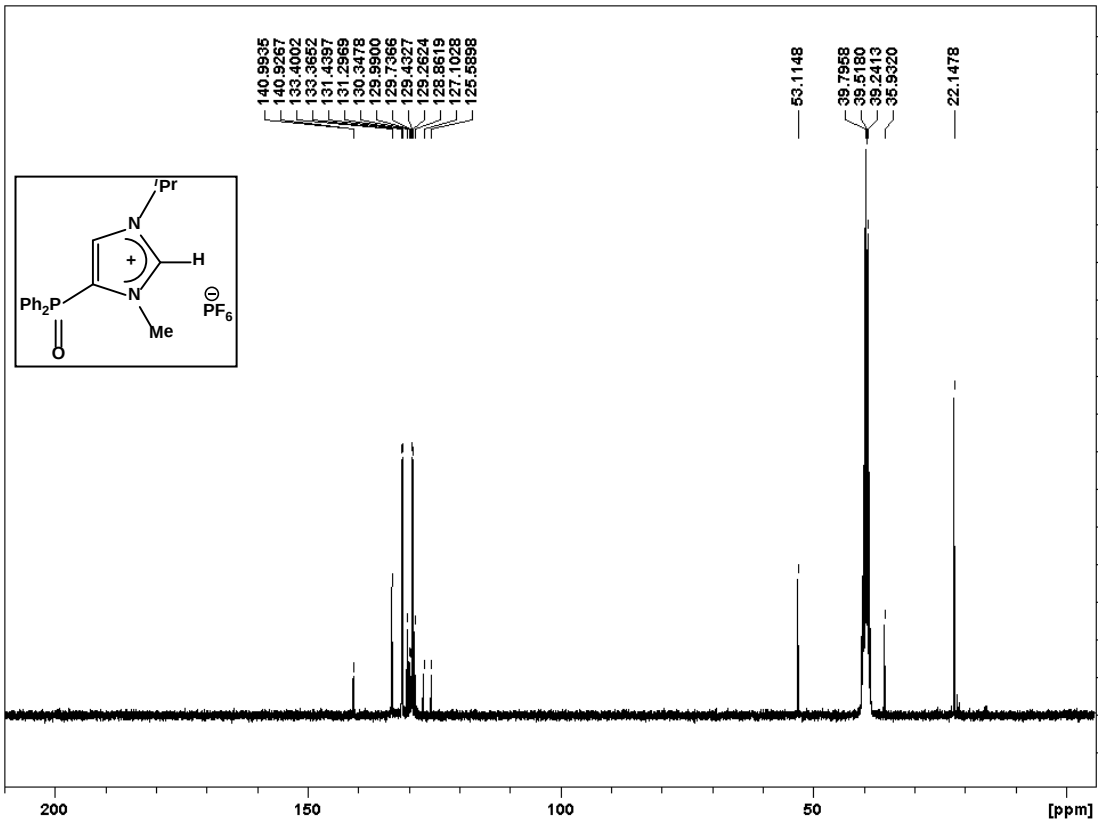

Figure S52: $^{31}P\{^{1}H\}$ NMR spectrum of **12a** in DMSO-d6 (121.5 MHz, 25 °C)

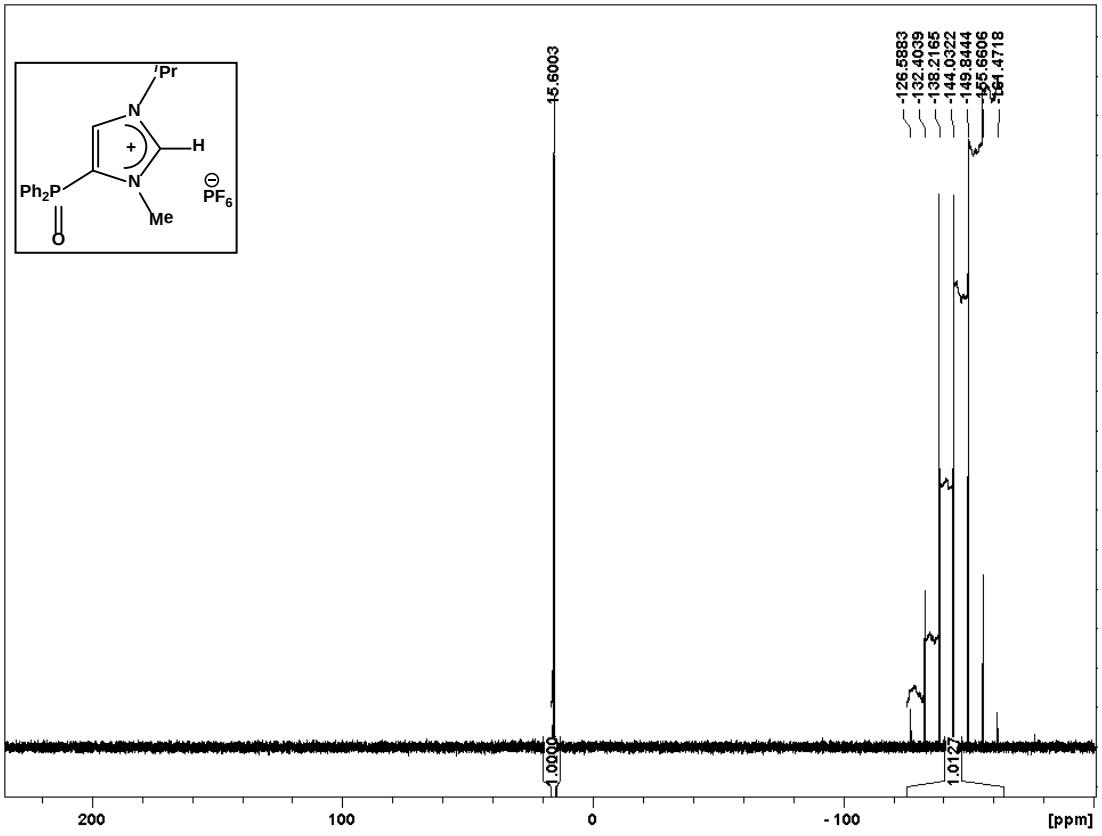

Figure S53: ^{1}H NMR spectrum of **13d** in $CDCl_3$ (300.1 MHz, 25 °C)

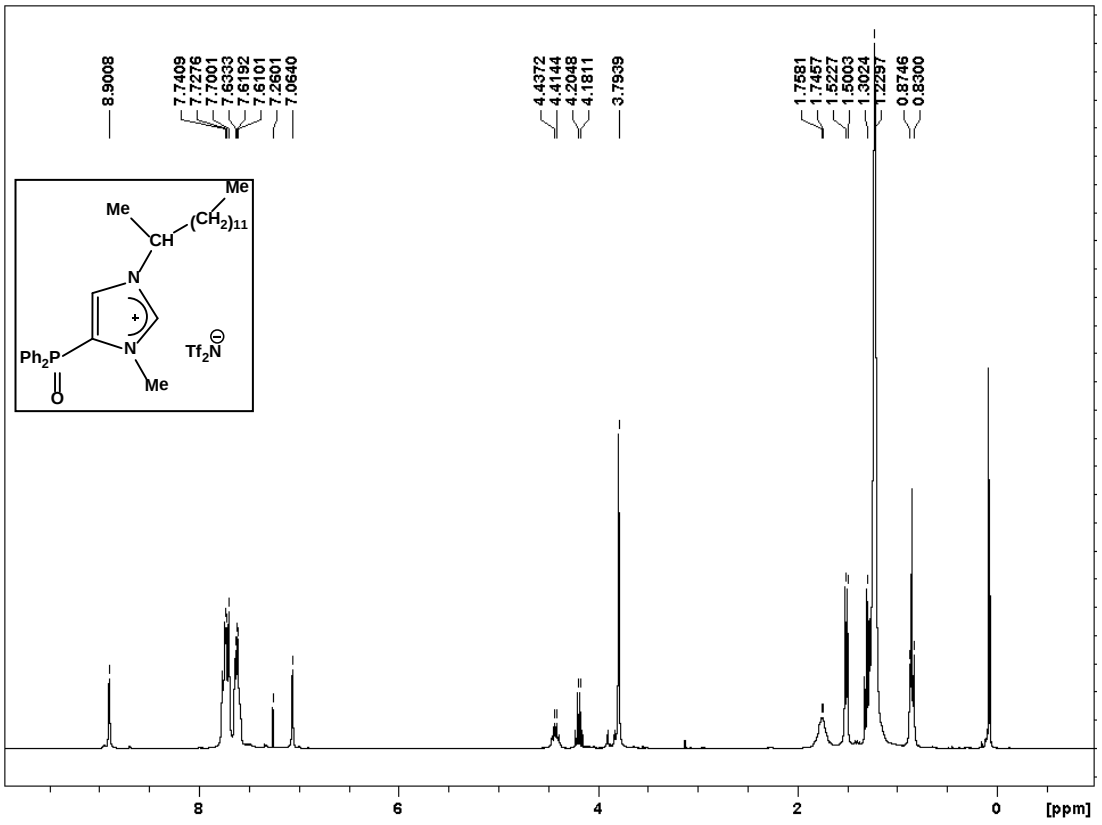

Figure S54: $^{13}C\{^{1}H\}$ NMR spectrum of **13d** in $CDCl_3$ (75.5 MHz, 25 °C)

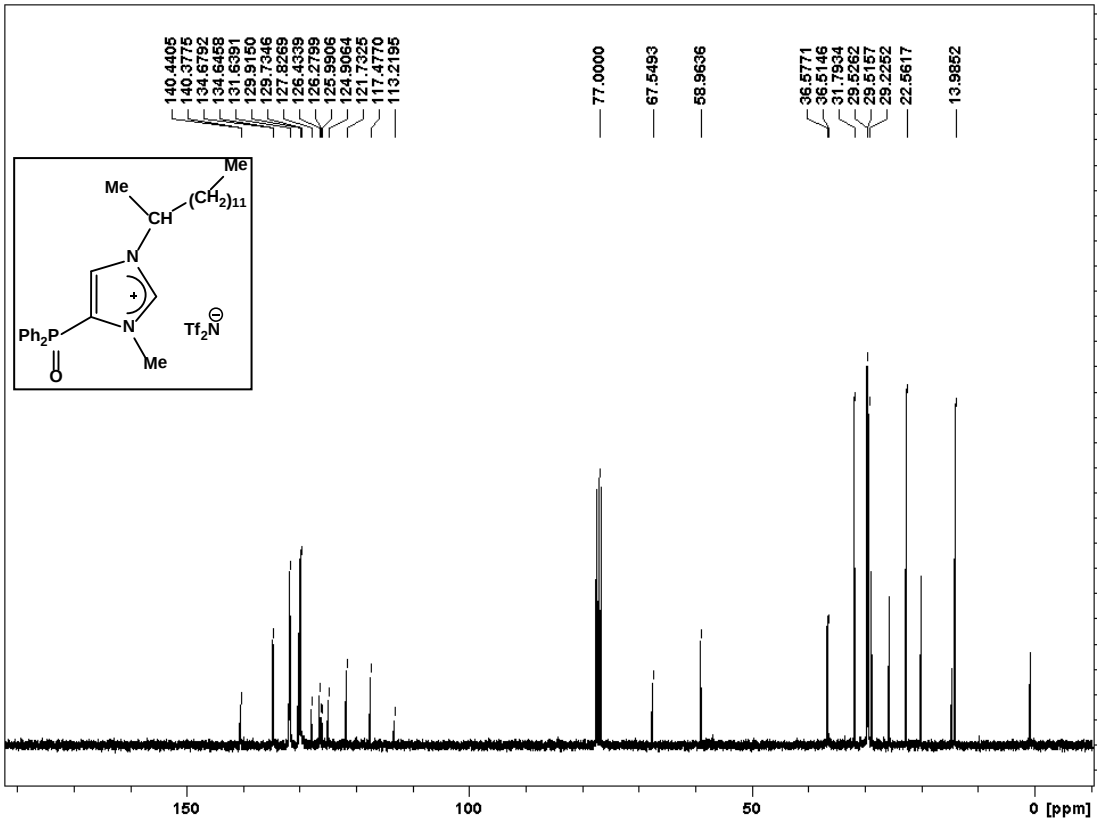

Figure S55: $^{31}P\{^{1}H\}$ NMR spectrum of **13d** in $CDCl_3$ (121.5 MHz, 25 °C)

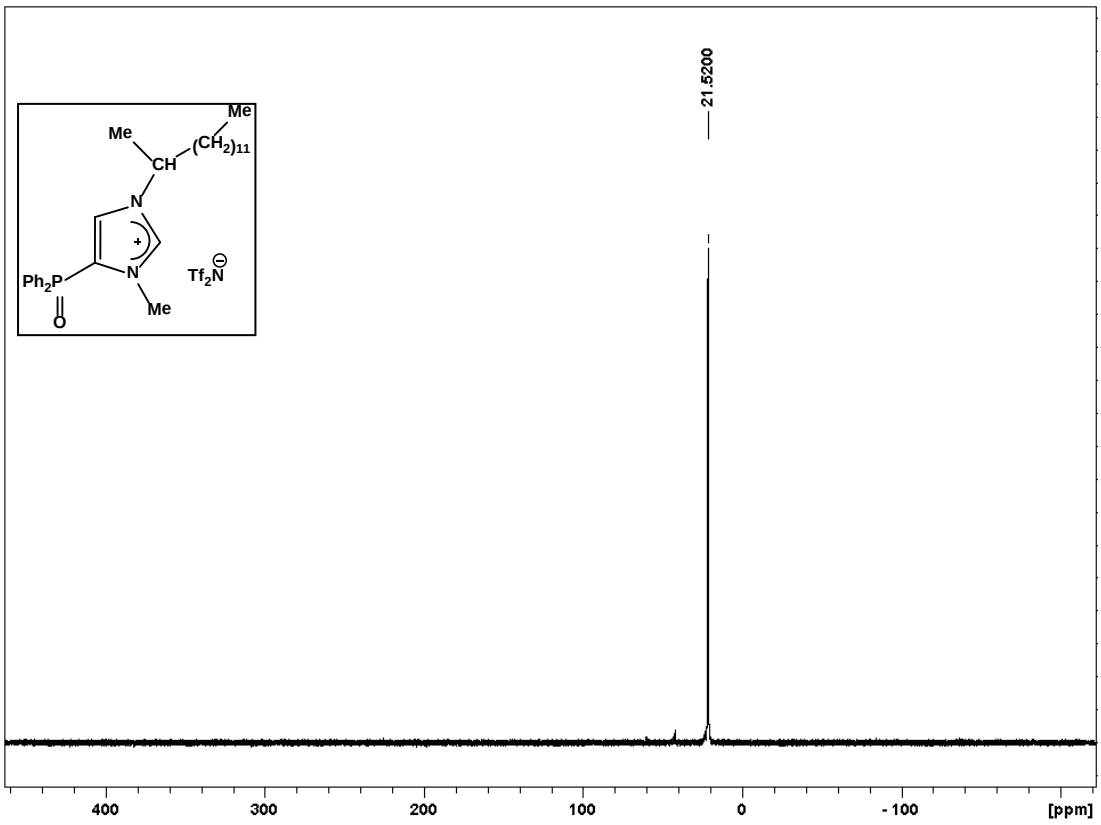

Figure S56: ^{1}H NMR spectrum of **15b** in DMSO-d6 (300.1 MHz, 25 °C)

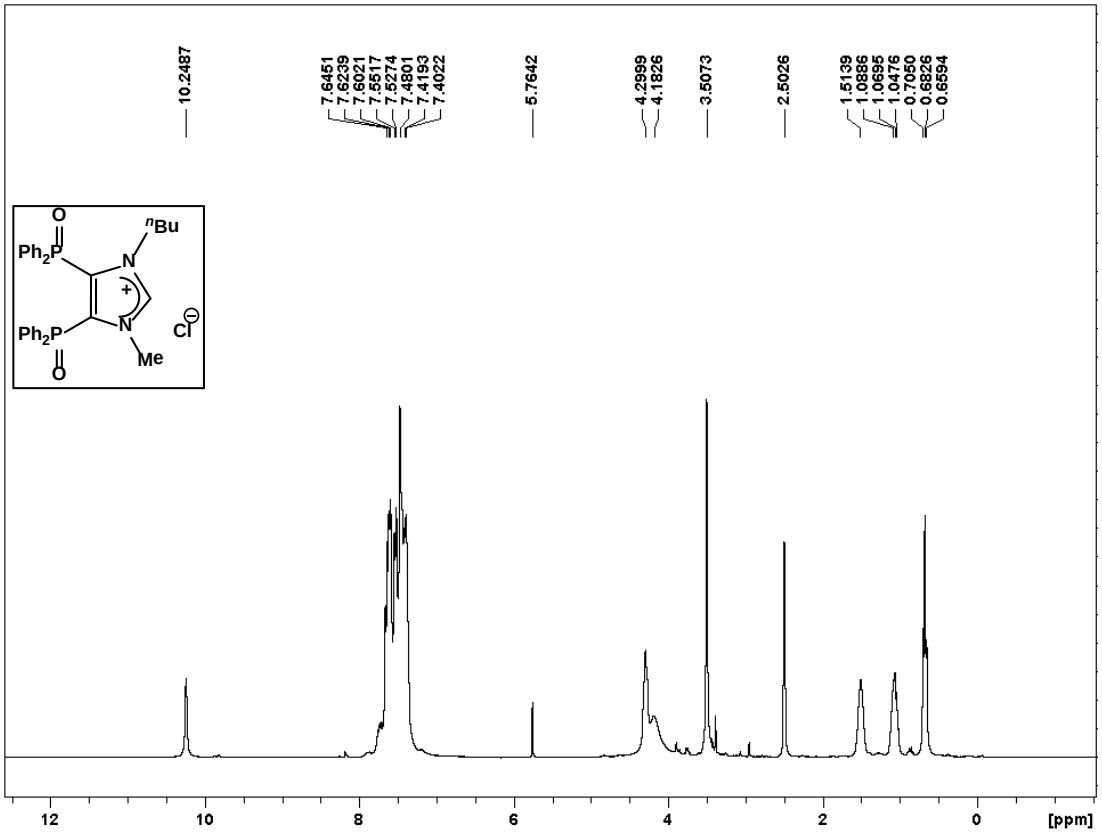

Figure S57: ^{13}C{^{1}H} NMR spectrum of **15b** in DMSO-d6 (75.5 MHz, 25 °C)

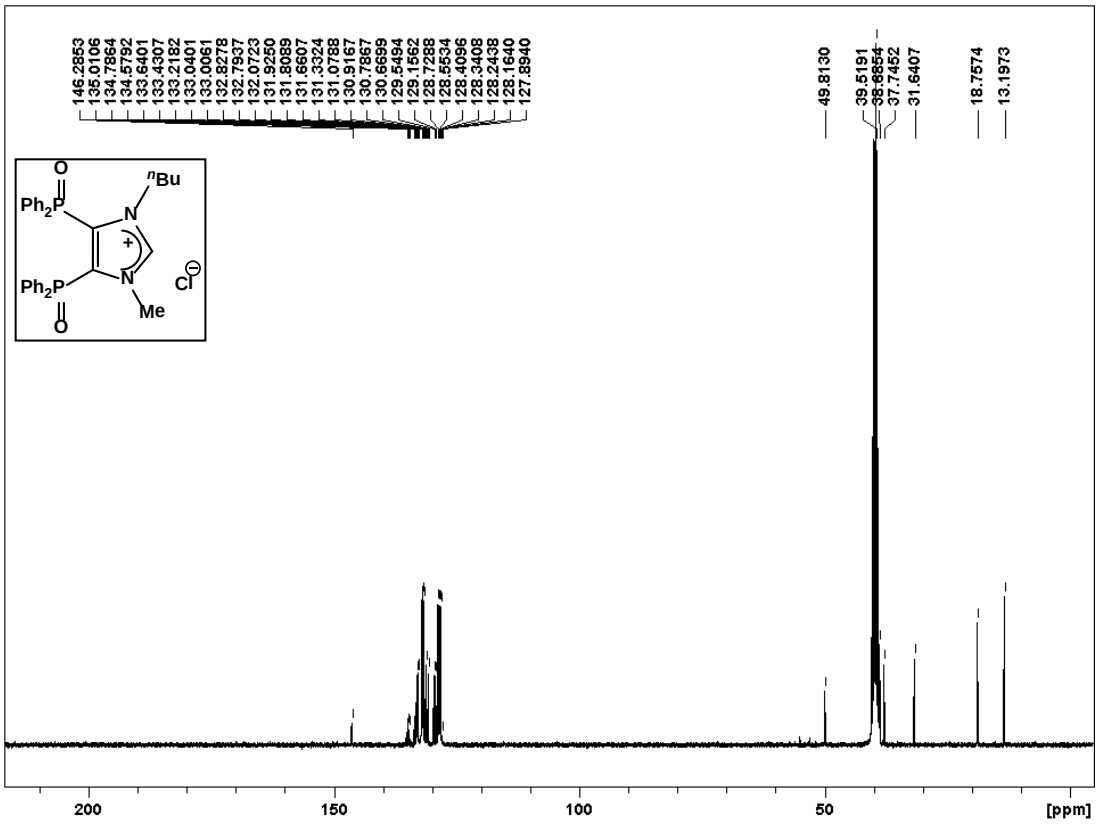

Figure S58: $^{31}P\{^{1}H\}$ NMR spectrum of **15b** in DMSO-d6 (121.5 MHz, 25 °C)

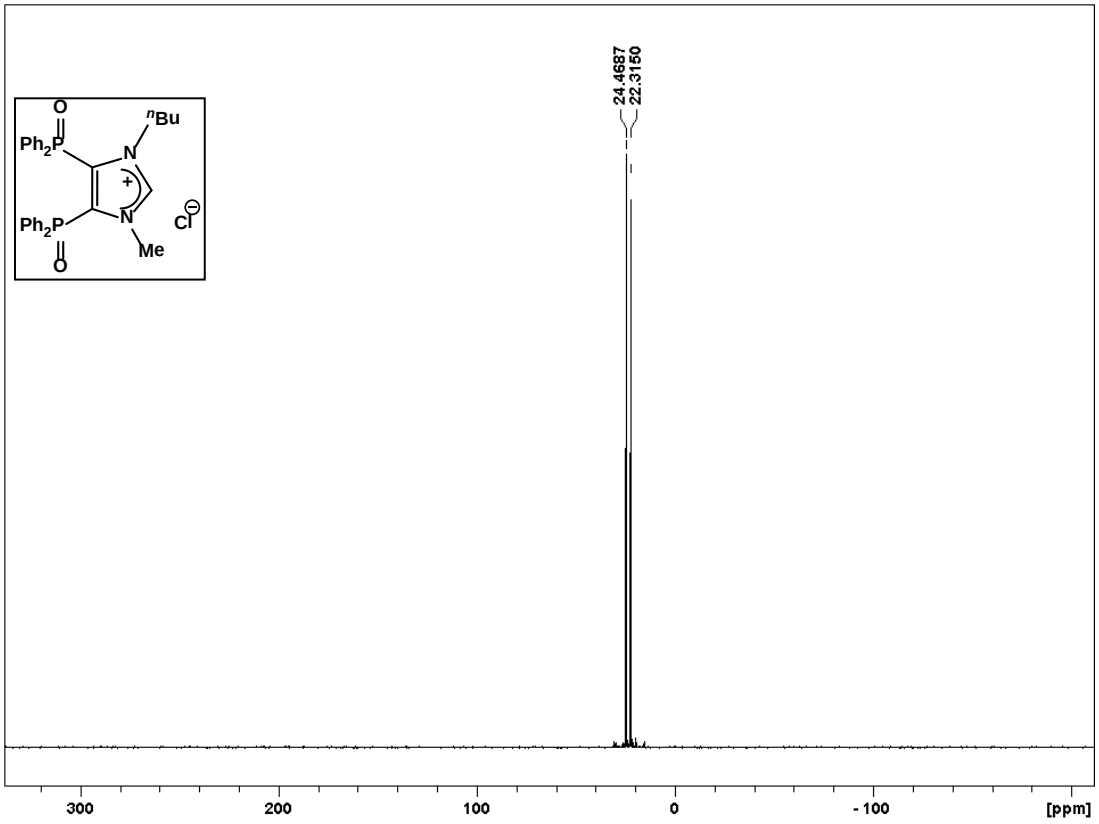

Figure S59: ^{1}H NMR spectrum of **16b** in CD_2Cl_2 (300.1 MHz, 25 °C)

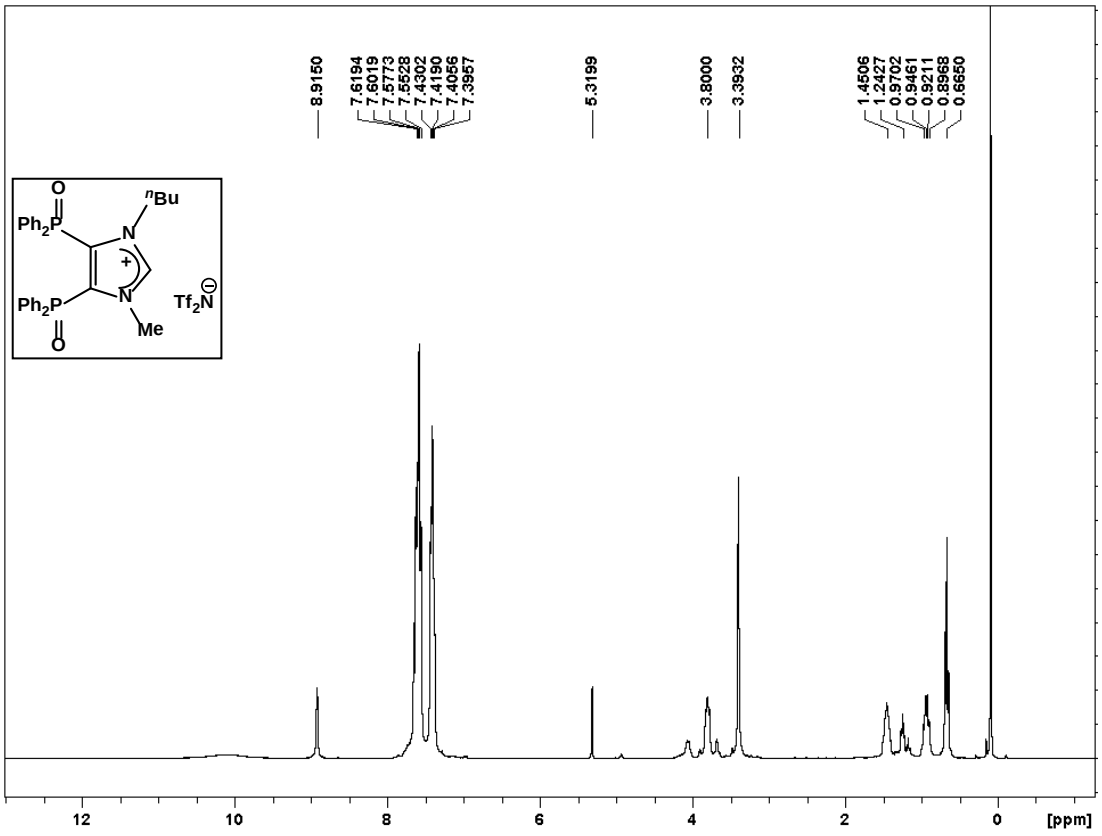

Figure S60: $^{13}C\{^{1}H\}$ NMR spectrum of **16b** in CD_2Cl_2 (75.5 MHz, 25 °C)

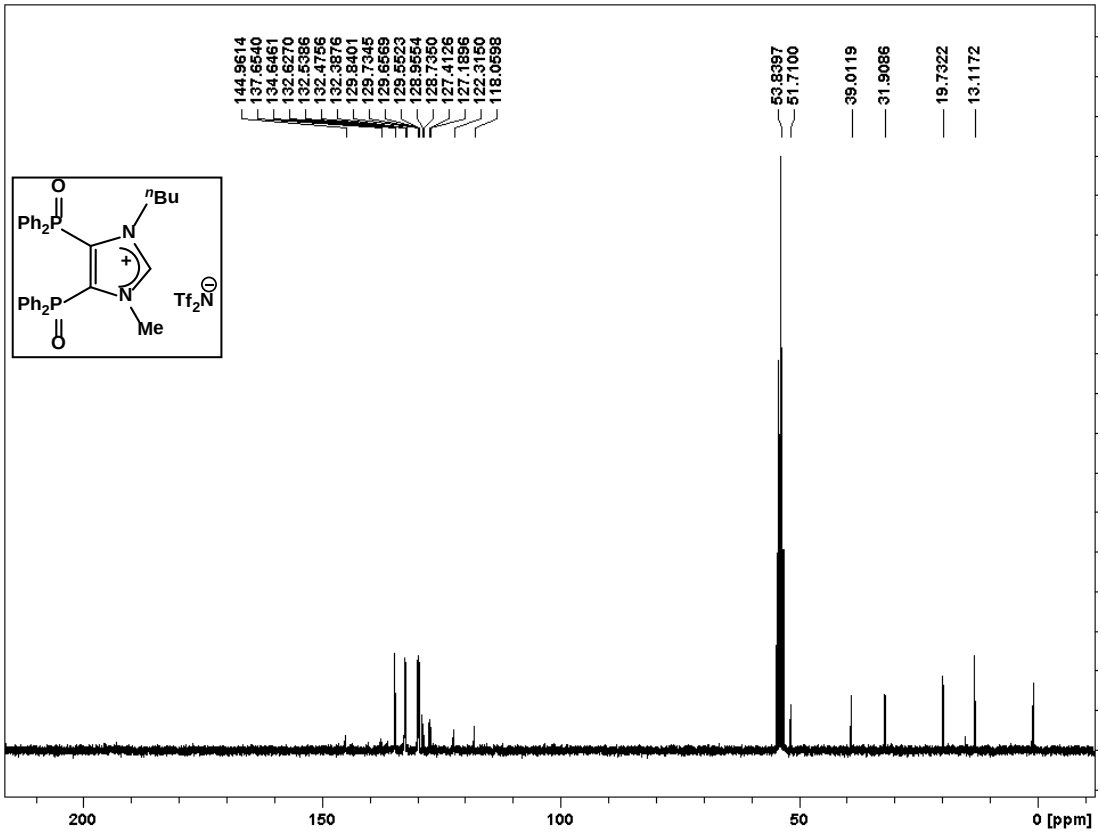

Figure S61: $^{31}P\{^{1}H\}$ NMR spectrum of **16b** in CD_2Cl_2 (121.5 MHz, 25 °C)

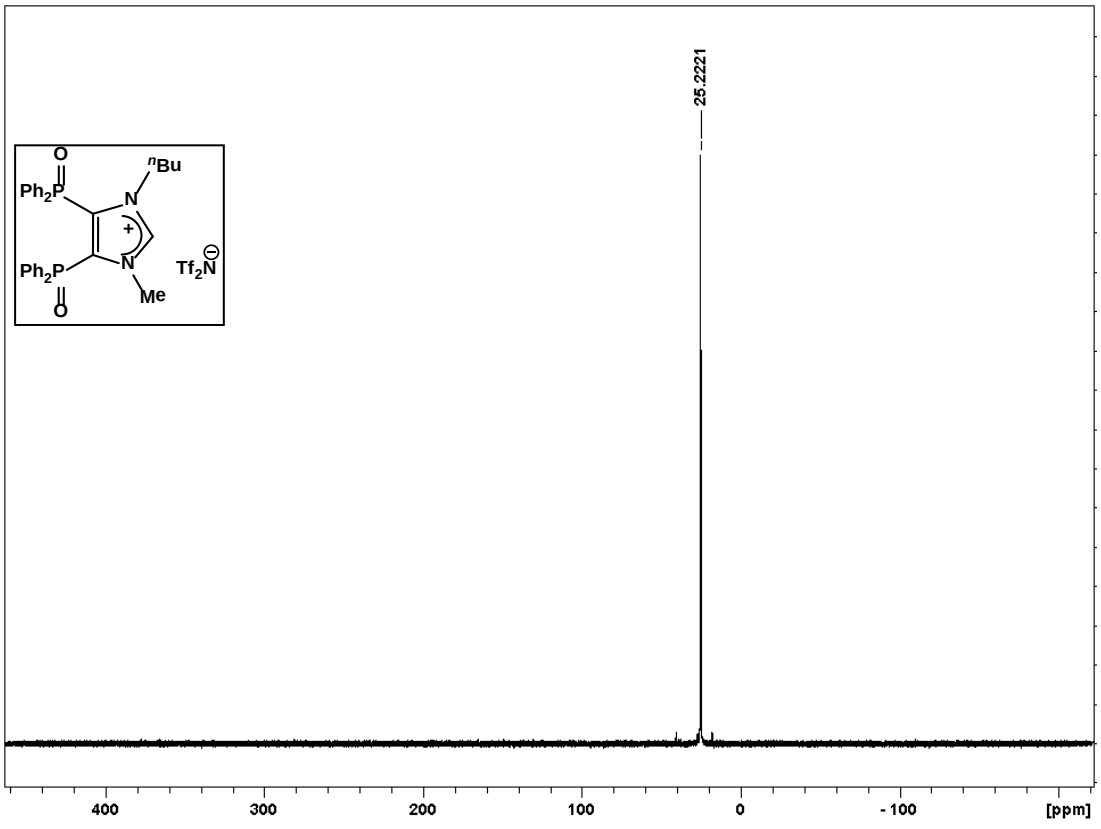

Figure S62: ^{1}H NMR spectrum of **17b** in CD_2Cl_2 (300.1 MHz, 25 °C)

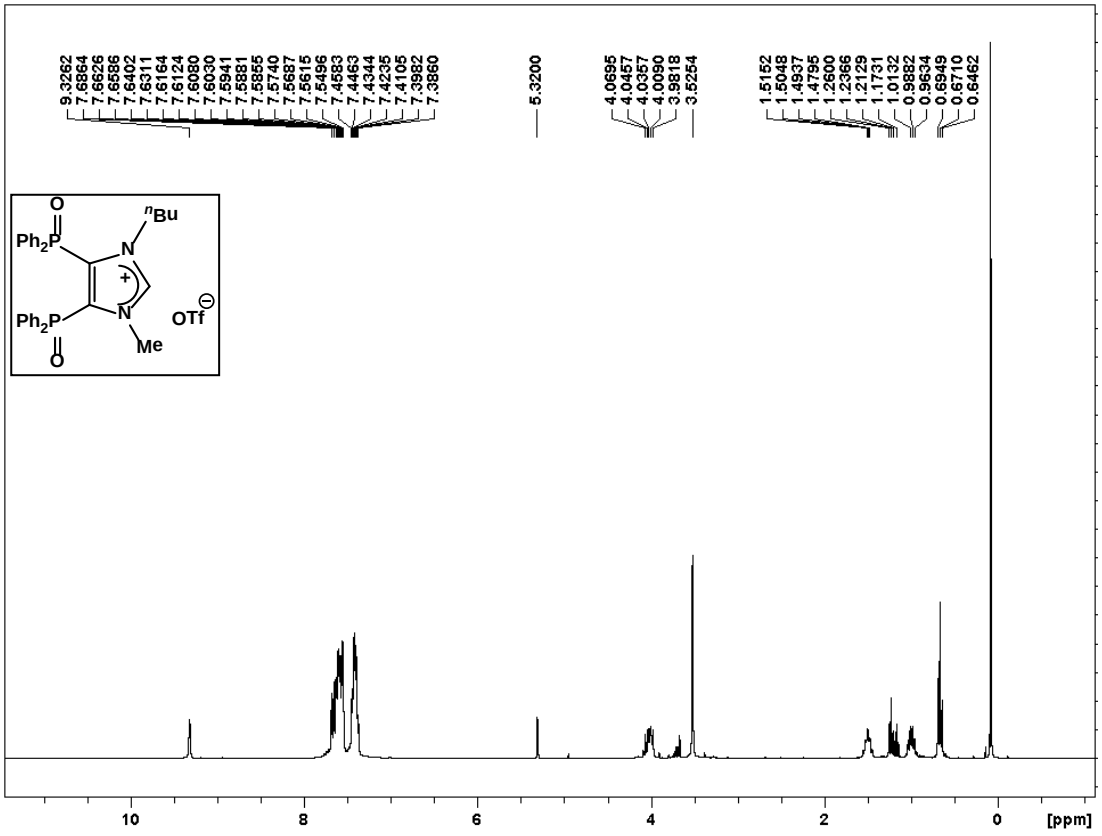

Figure S63: $^{13}C\{^{1}H\}$ NMR spectrum of **17b** in CD_2Cl_2 (75.5 MHz, 25 °C)

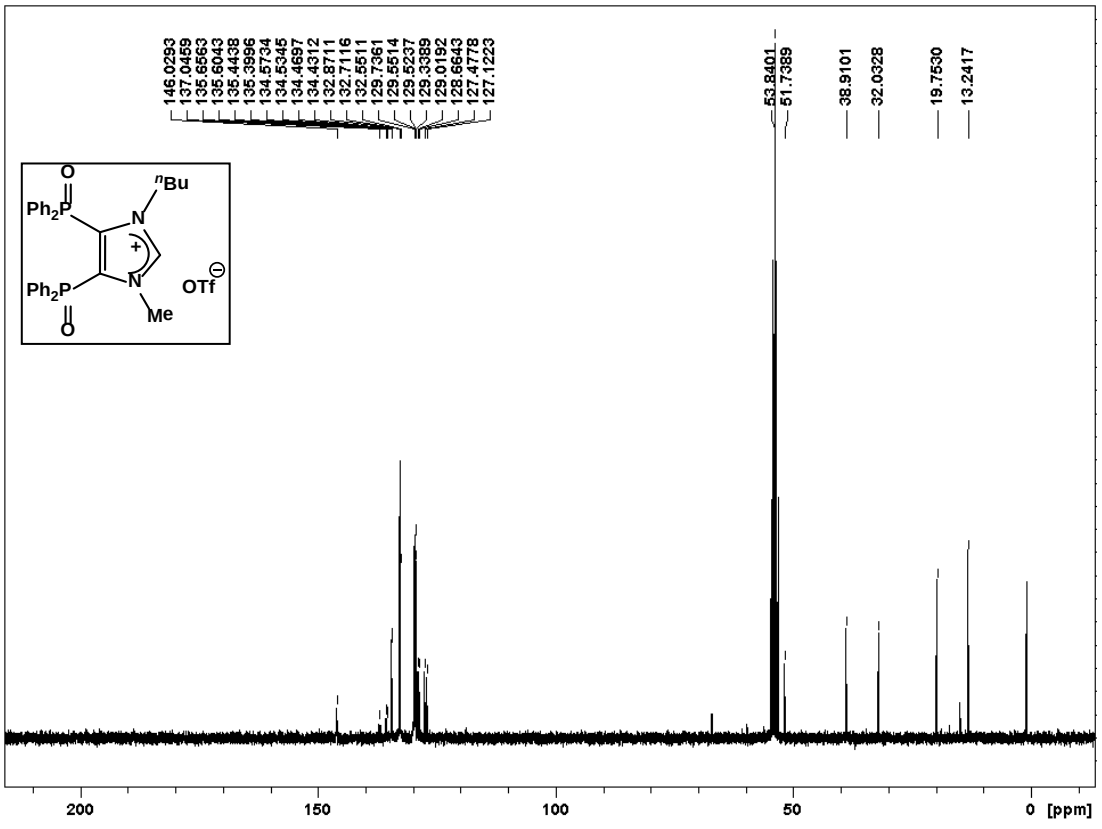

Figure S64: $^{31}P\{^{1}H\}$ NMR spectrum of **17b** in CD_2Cl_2 (121.5 MHz, 25 °C)

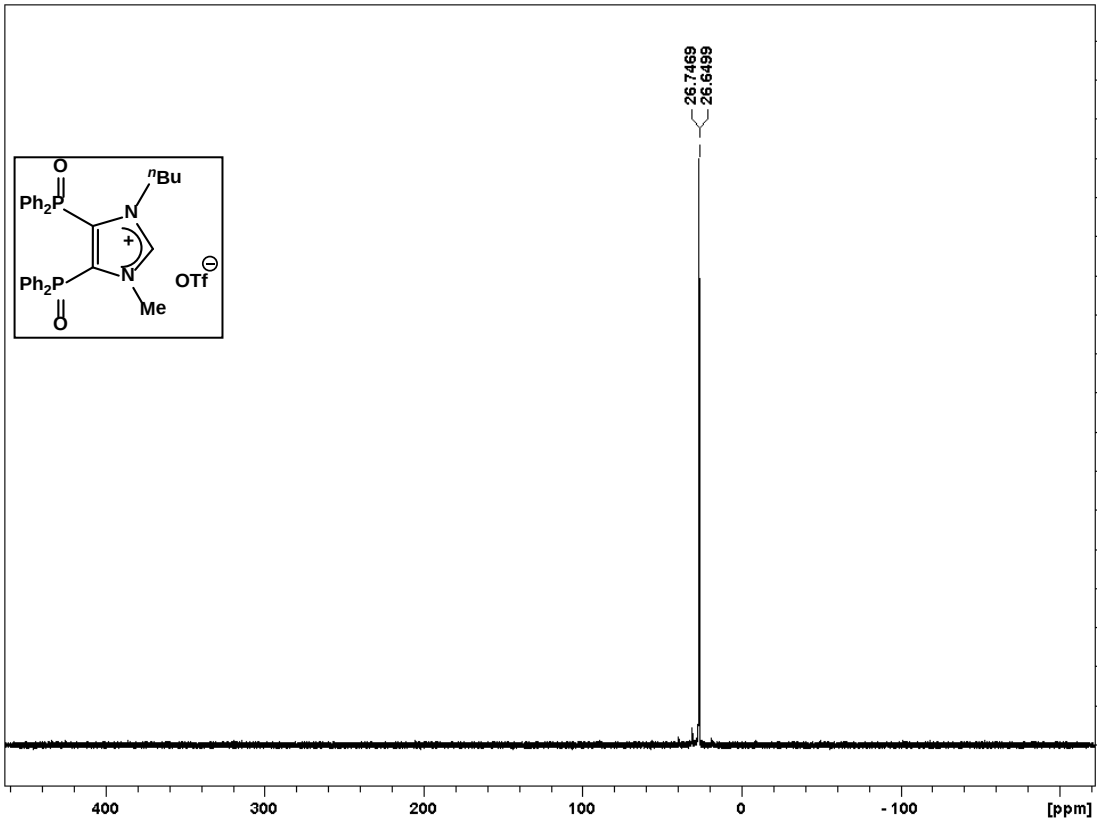

Table S1: Crystal data and structure refinement for 5a

Device Type	Bruker X8-KappaApexII	
Empirical formula	$C_{15}H_{31}N_4PS_2$	
Moiety formula	$C_{15}H_{31}N_4PS_2$	
Formula weight	362.53	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/c$	
Unit cell dimensions	a = 15.3458(6) Å	α = 90°
	b = 8.7341(3) Å	β = 117.549(2)°
	c = 16.5299(6) Å	γ = 90°
Volume	1964.32(12) $Å^3$	
Z	4	
Calculated density	1.226 mg/m^3	
Absorption coefficient	0.355 mm^{-1}	
F(000)	784	
Crystal size	0.24 × 0.20 × 0.08 mm	
Theta range for data collection	3.53 to 28.00°	
Limiting indices	$-20 \le h \le 20$, $-11 \le k \le 11$, $-21 \le l \le 21$	
Reflections collected / unique	54312 / 4681 [R(int) = 0.0322]	
Completeness to theta = 28.00	98.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9071 and 0.8259	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4681 / 2 / 206	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R_1 = 0.0262, wR_2 = 0.0657	
R indices (all data)	R_1 = 0.0314, wR_2 = 0.0688	
Largest diff. peak and hole	0.365 and -0.256 $e.Å^{-3}$	