

Supplimentary Material

Exploring the chemistry of backbone amino(chloro)phosphanyl-substituted imidazole-2-thiones

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1 Spectra for Compound 2a

Figure S1: ^1H NMR spectrum of **2a** in CDCl_3 (300.1 MHz, 25 °C)

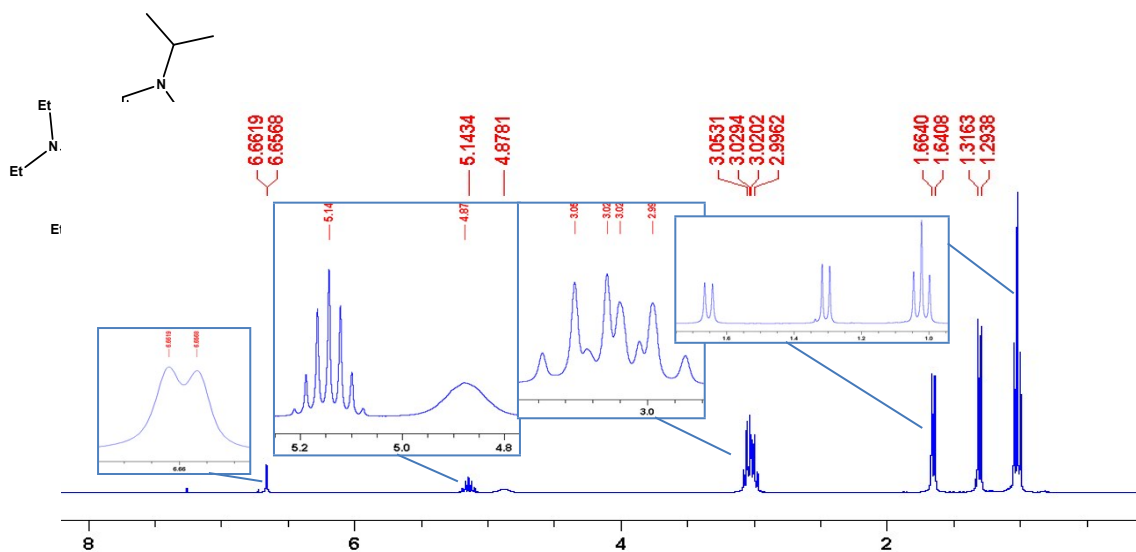


Figure S2: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **2a** in CDCl_3 (75.5 MHz, 25 °C)

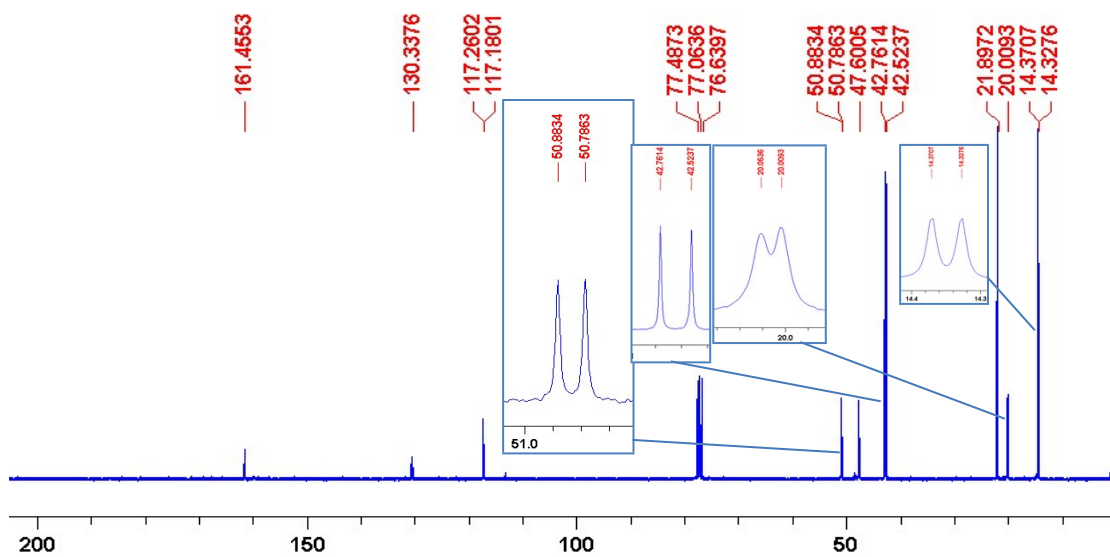


Figure S3: ^{31}P NMR spectrum of **2a** in CDCl_3 (121.5 MHz, 25 °C)

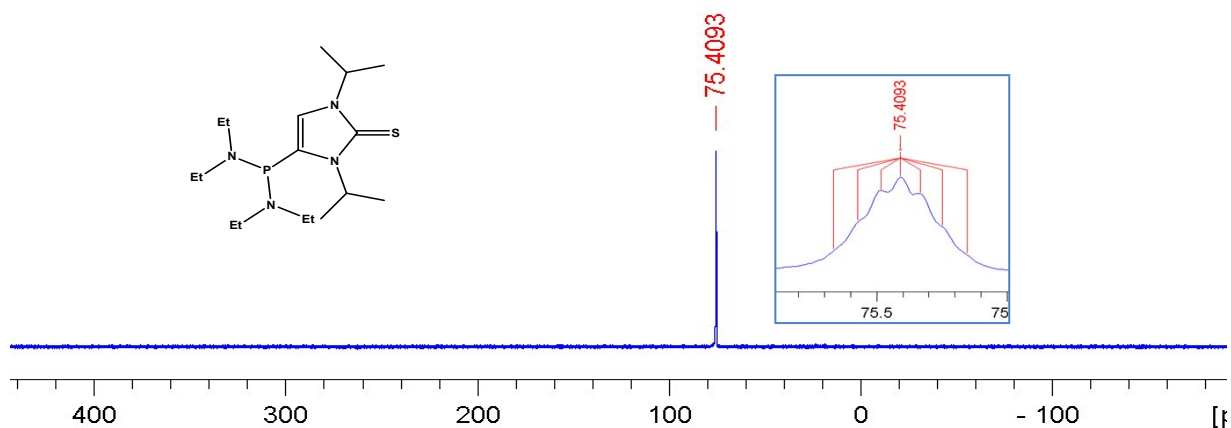
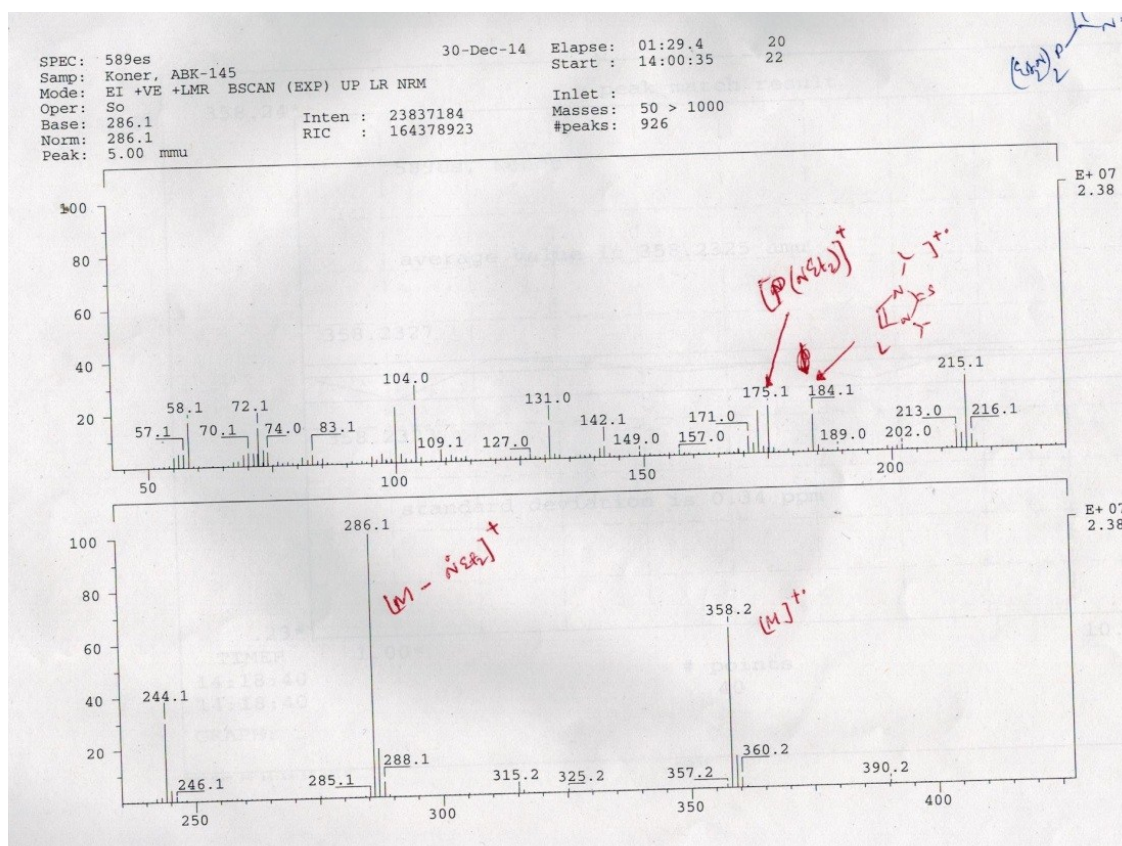


Figure S4: EI-MS spectrum of **2a**.



2 Spectra for Compound **2b**

Figure S5: ^1H NMR spectrum of **2b** in CDCl_3 (121.5 MHz, 25 °C)

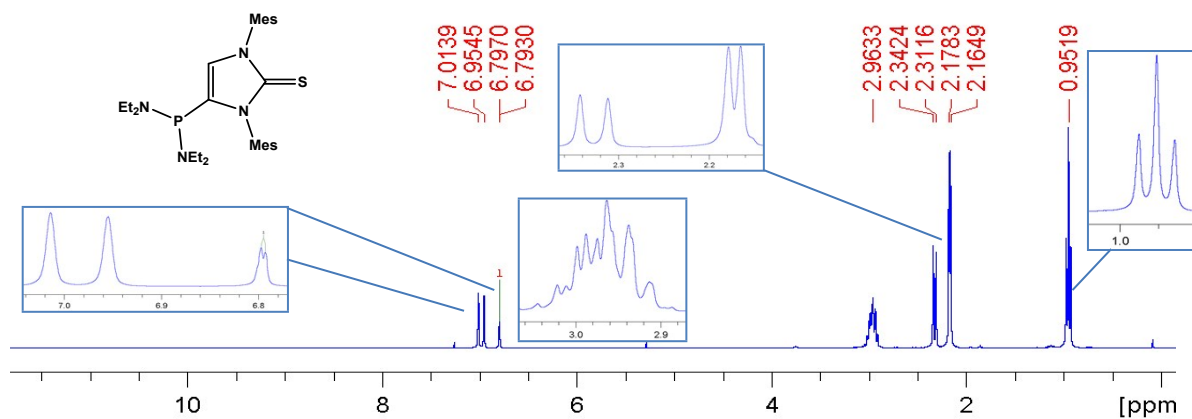


Figure S6: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **2b** in CDCl_3 (121.5 MHz, 25 °C)

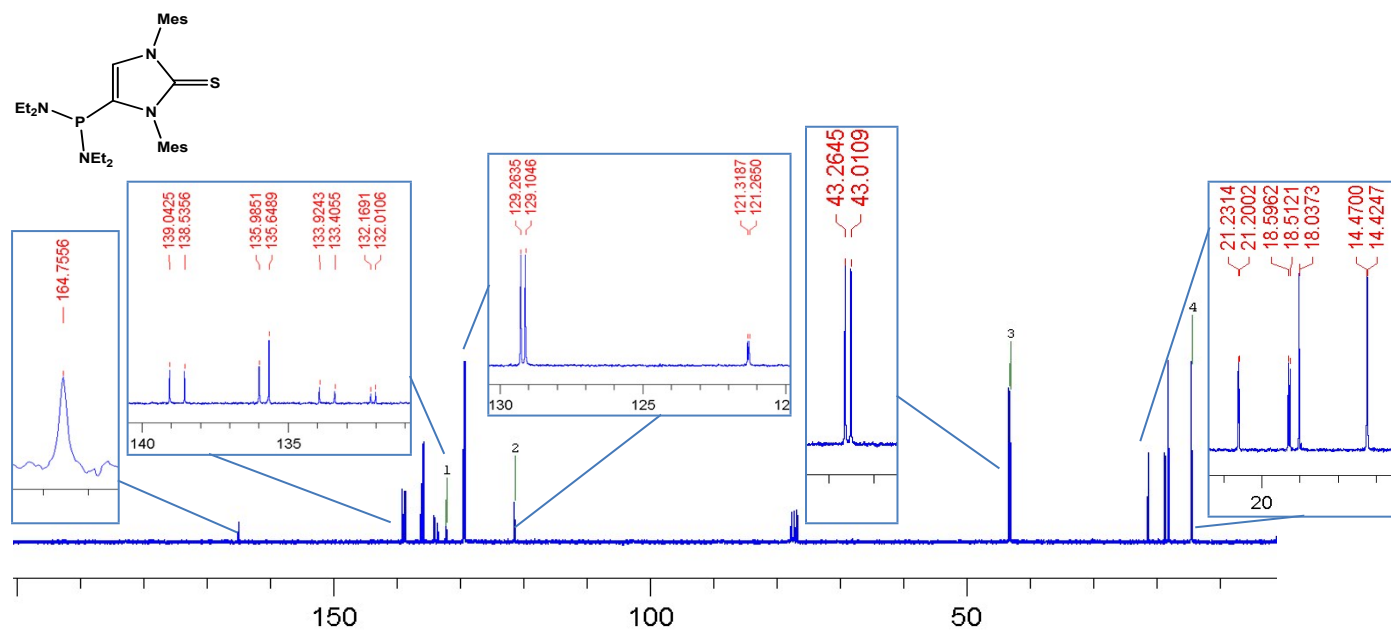


Figure S7: ^{31}P NMR spectrum of **2b** in CDCl_3 (121.5 MHz, 25 °C)

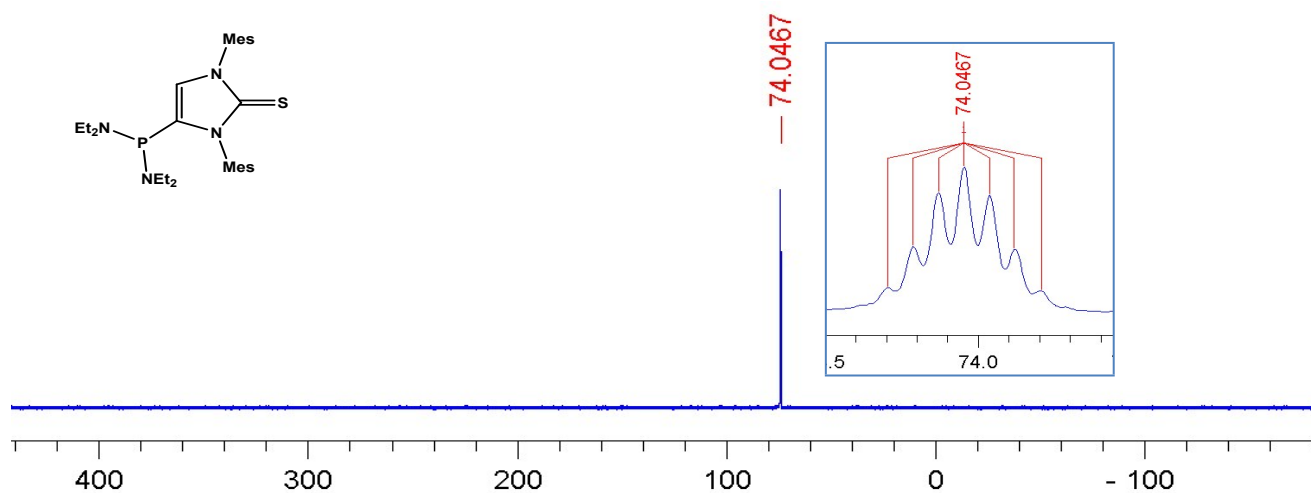
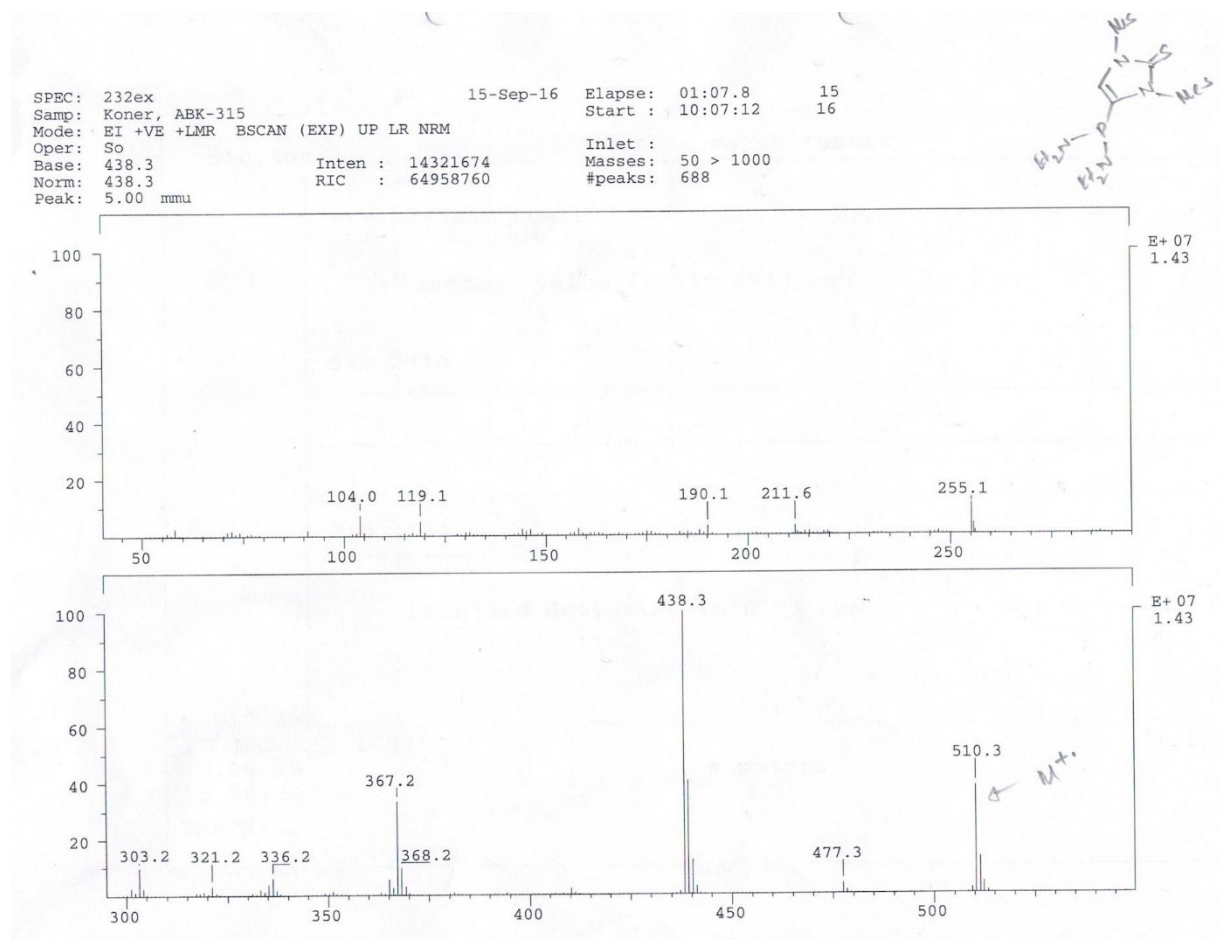


Figure S8: EI-MS spectrum of **2b**.



3 Spectra for Compound **2c**.

Figure S9: ^1H NMR spectrum of **2c** in CDCl_3 (300.1 MHz, 25 °C)

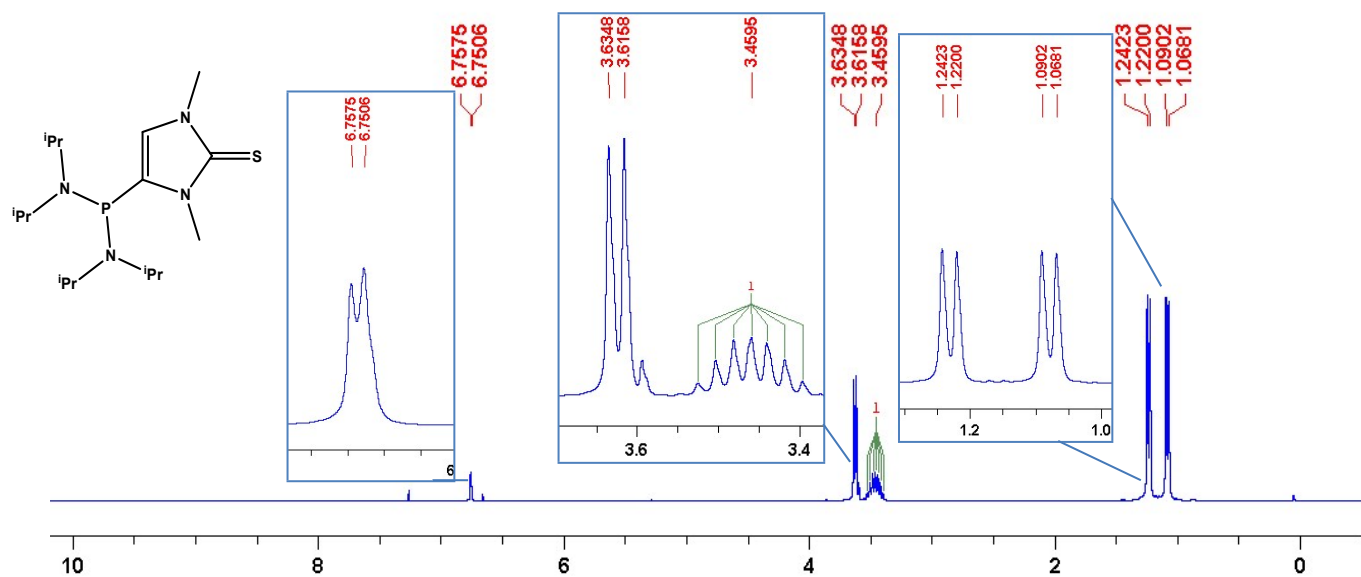


Figure S10: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **2c** in CDCl_3 (75.5 MHz, 25 °C)

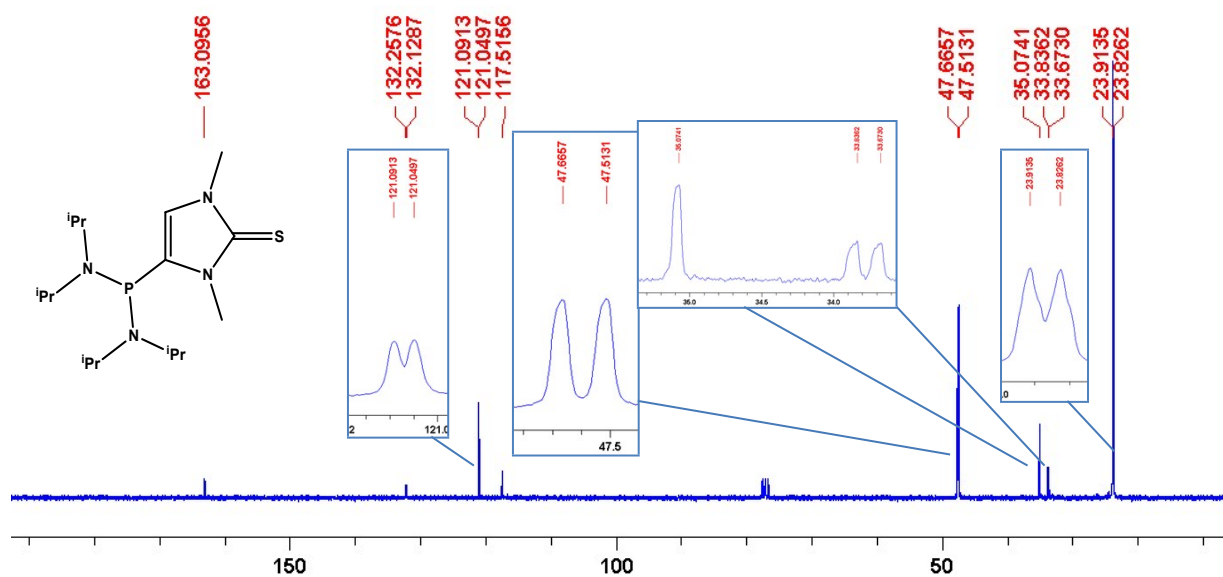


Figure S11: ^{31}P NMR spectrum of **2c** in CDCl_3 (121.5 MHz, 25 °C)

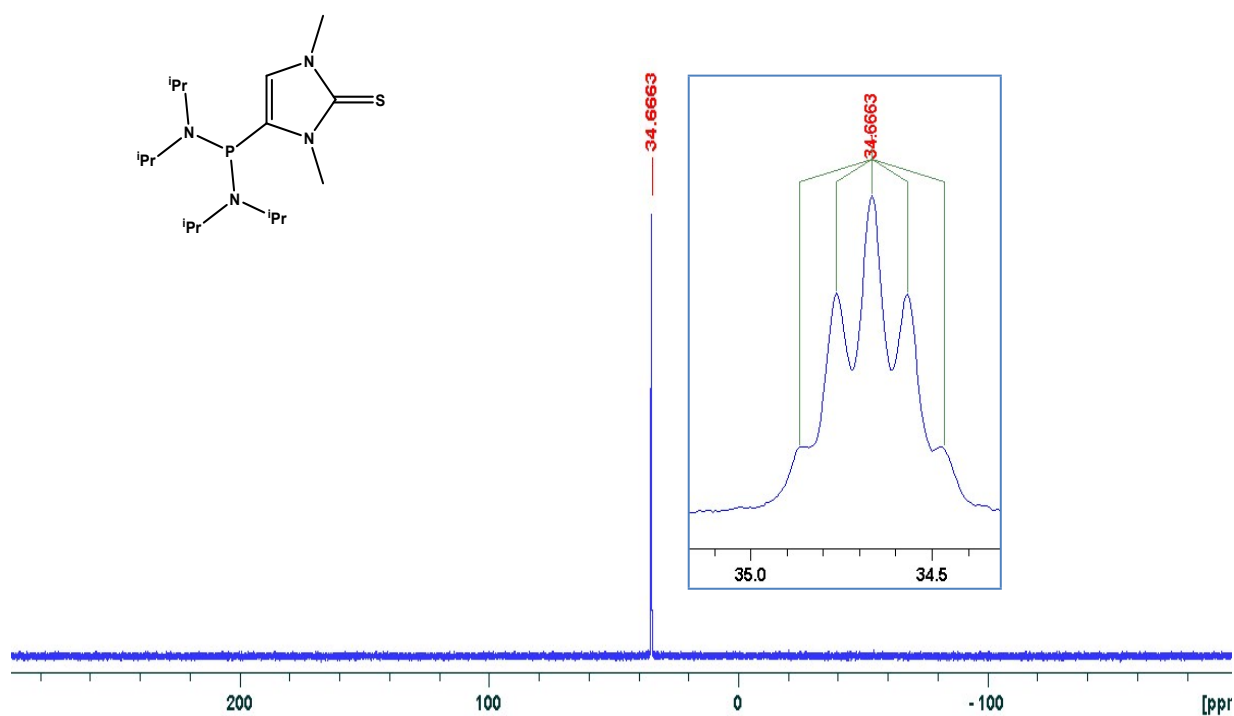
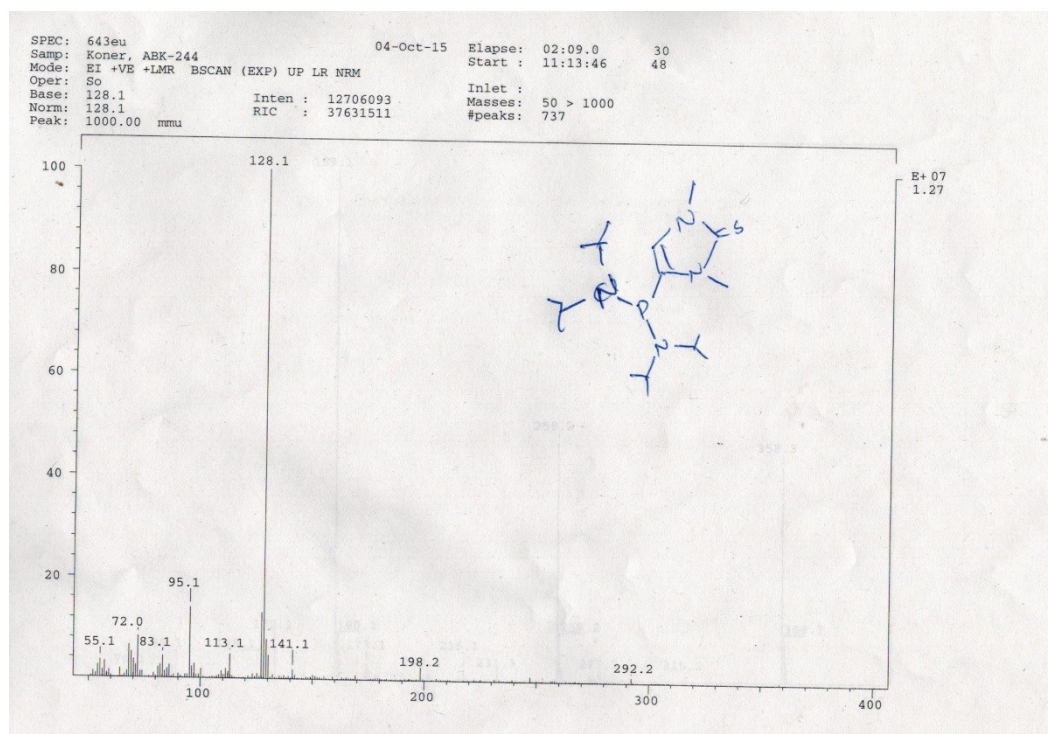


Figure S12: EI-MS spectrum of **2c**.



4 Spectra for Compound **3a**.

Figure S13: ^1H NMR spectrum of **3a** in CDCl_3 (300.1 MHz, 25 °C)

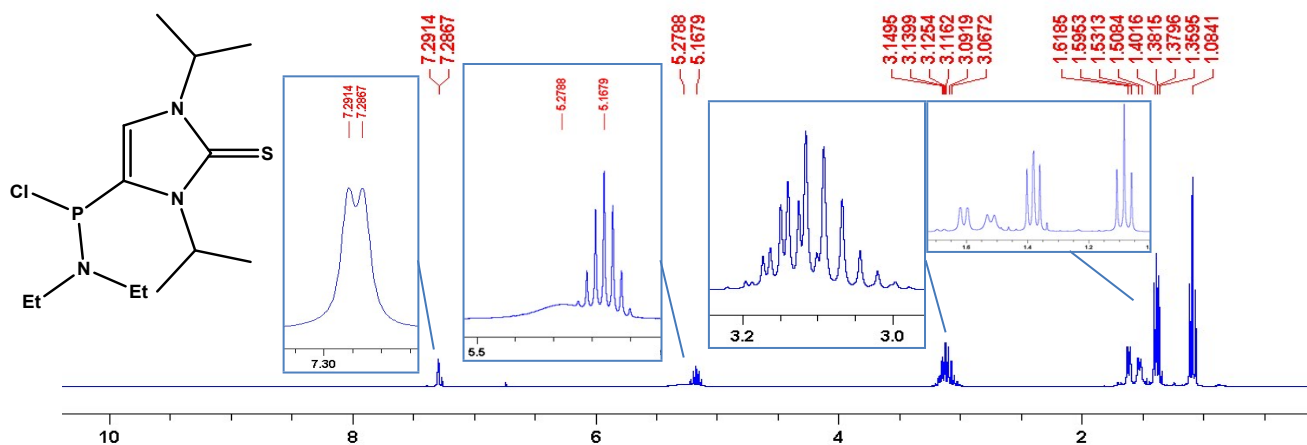


Figure S14: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **3a** in CDCl_3 (75.5 MHz, 25 °C)

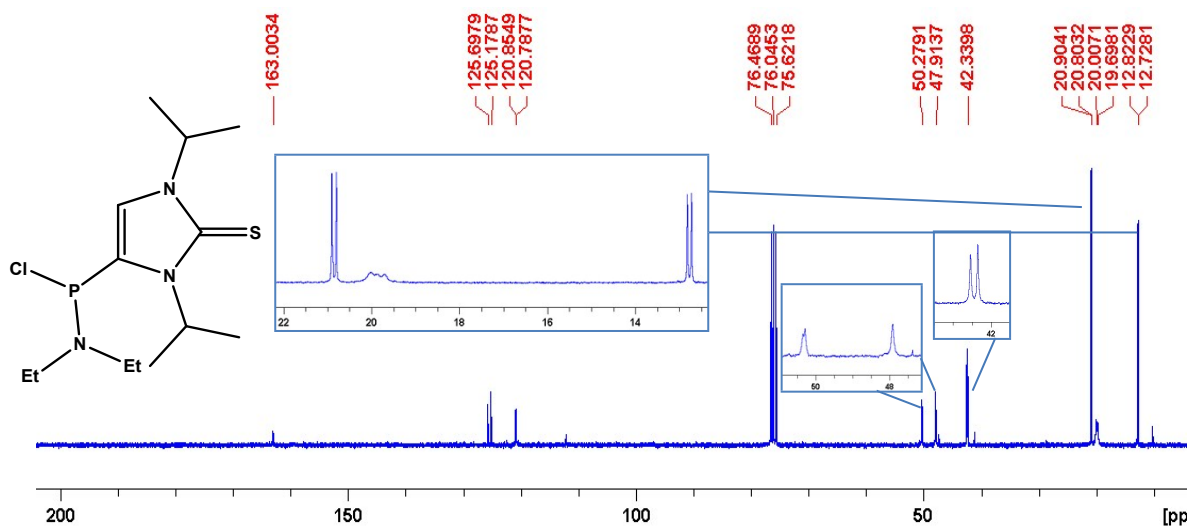


Figure S15: ^{31}P NMR spectrum of **3a** in CDCl_3 (121.5 MHz, 25 °C)

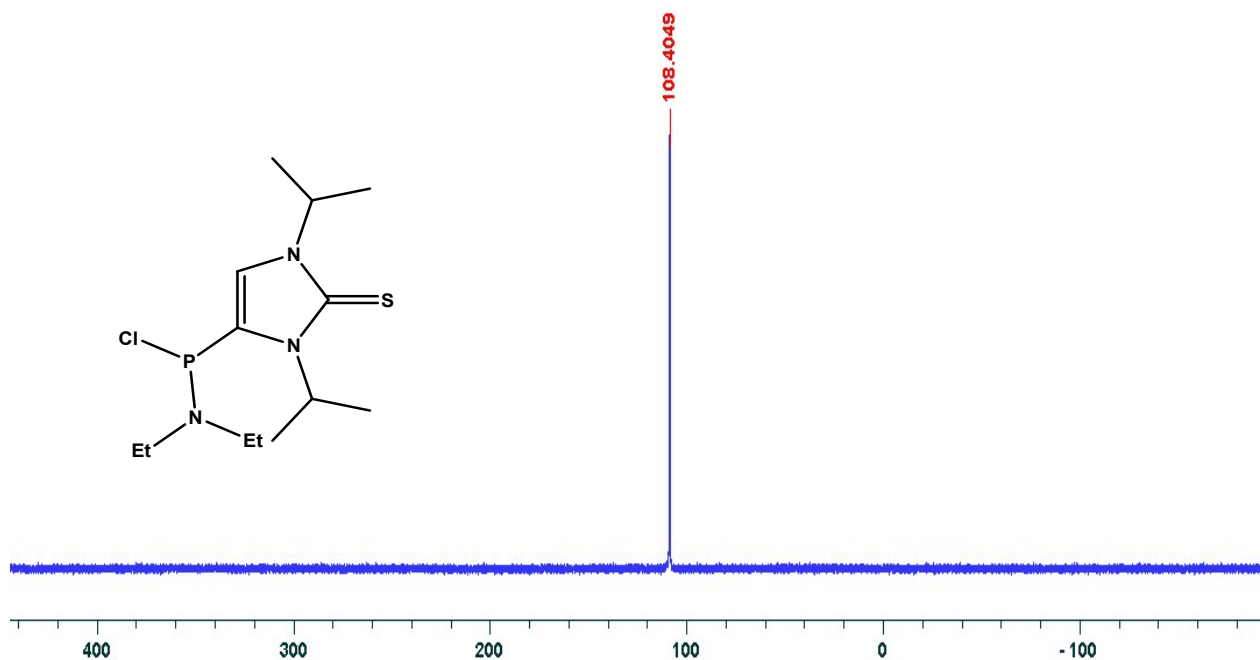
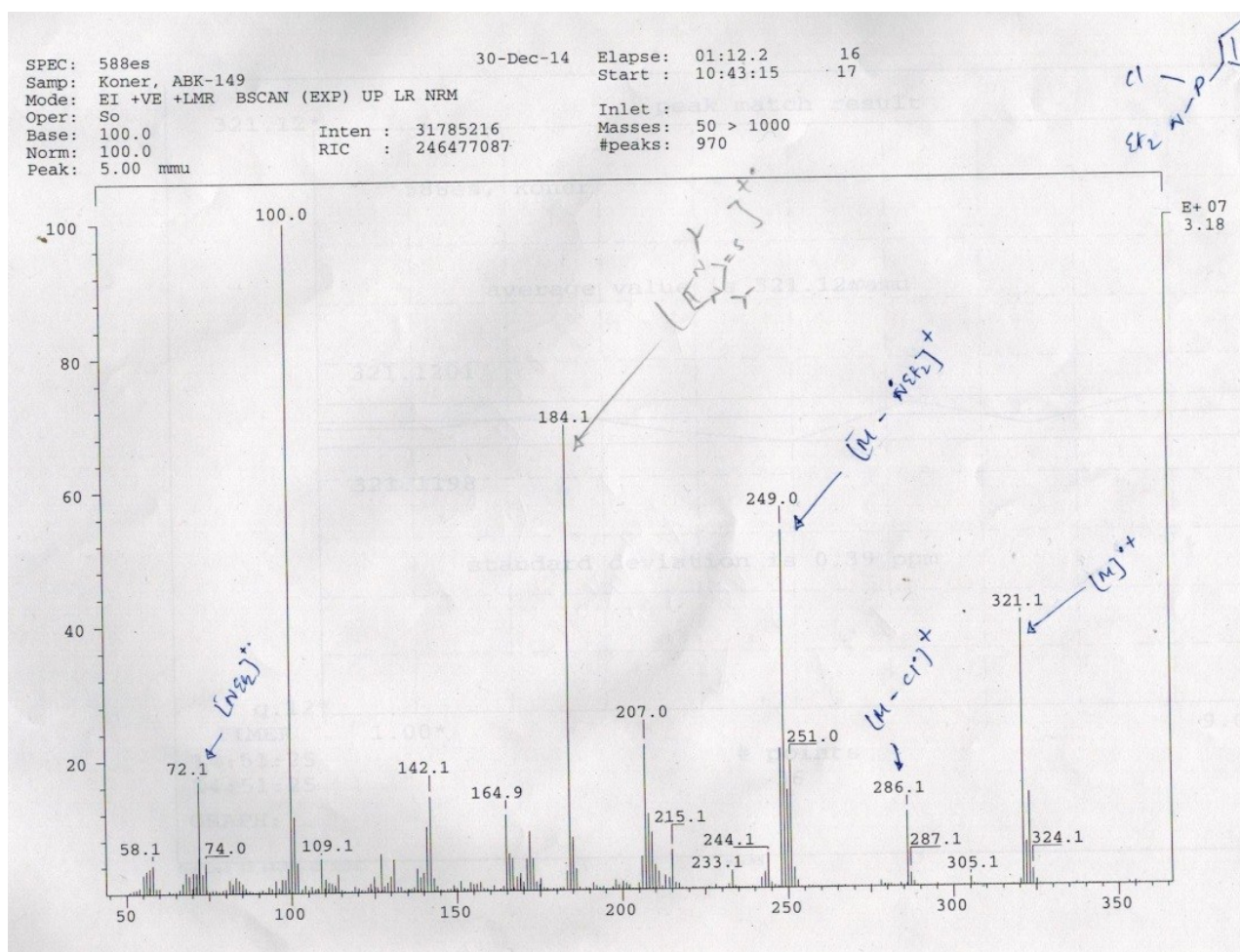


Figure S16: EI-MS spectrum of **3a**.



5 Spectra for Compound **3b**.

Figure S17: ^1H NMR spectrum of **3b** in CDCl_3 (300.1 MHz, 25 °C)

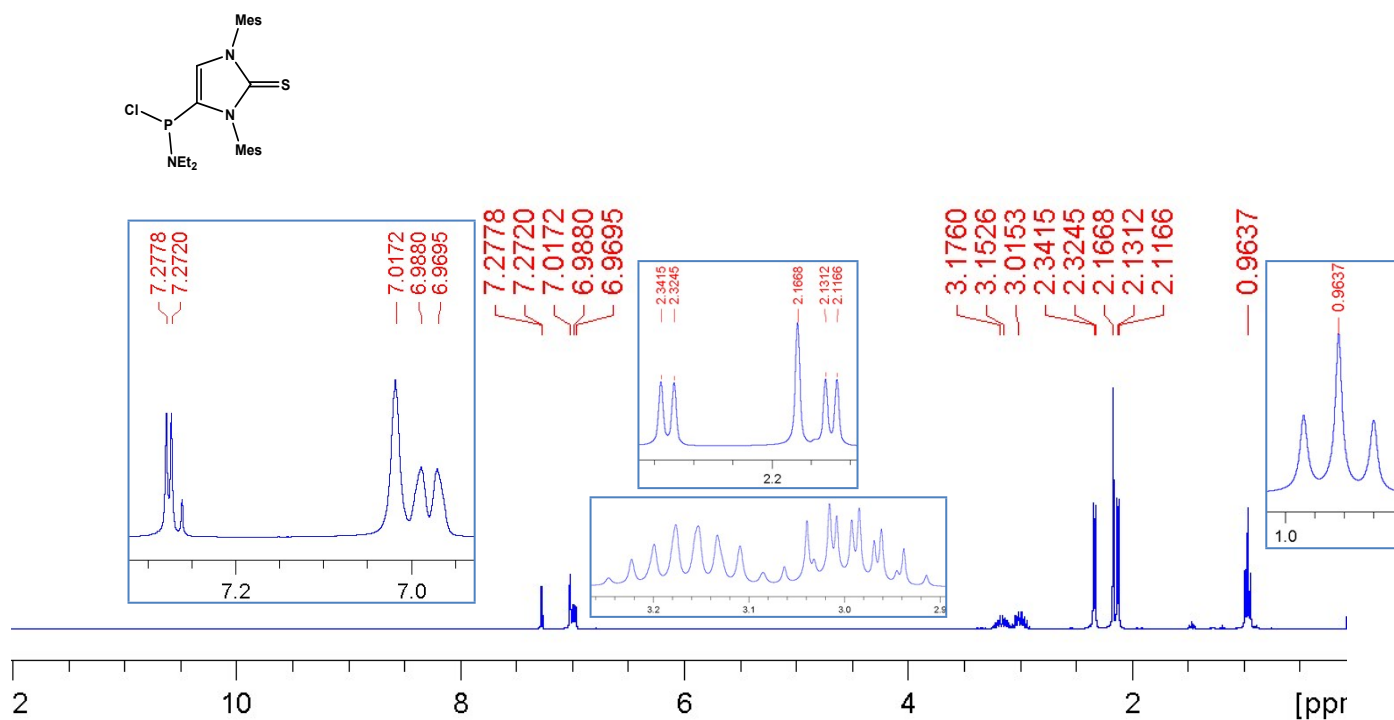


Figure S18: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3b** in CDCl_3 (75.5 MHz, 25 °C)

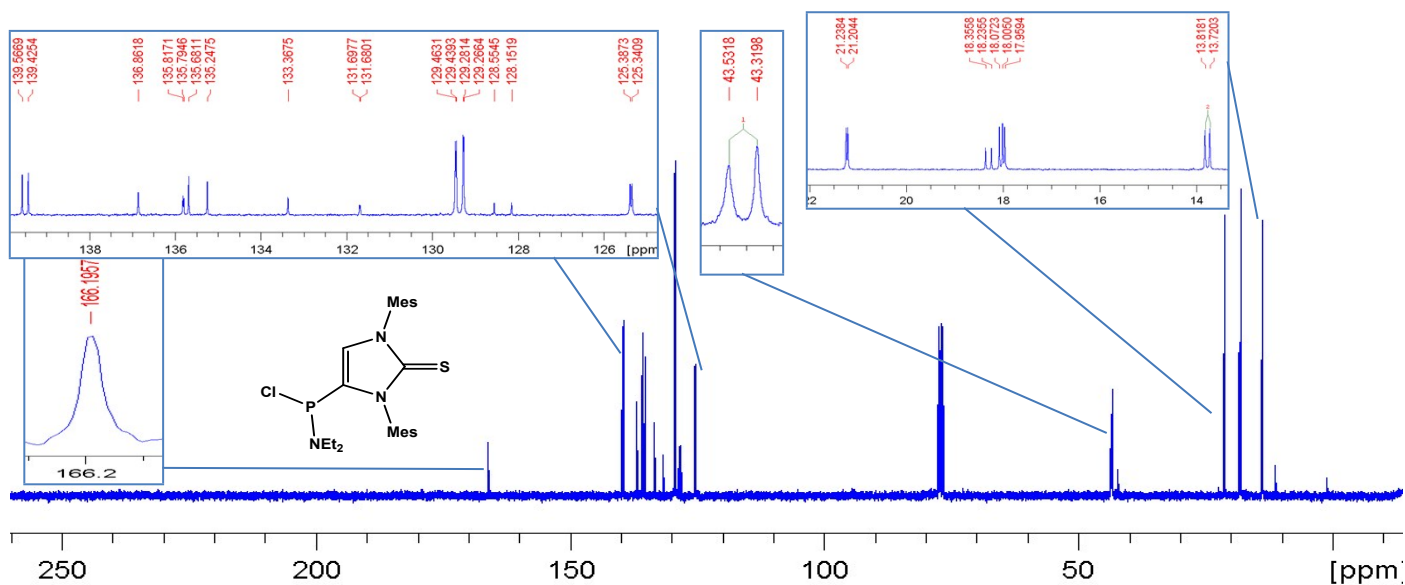


Figure S19: ^{31}P NMR spectrum of **3b** in CDCl_3 (121.5 MHz, 25 °C)

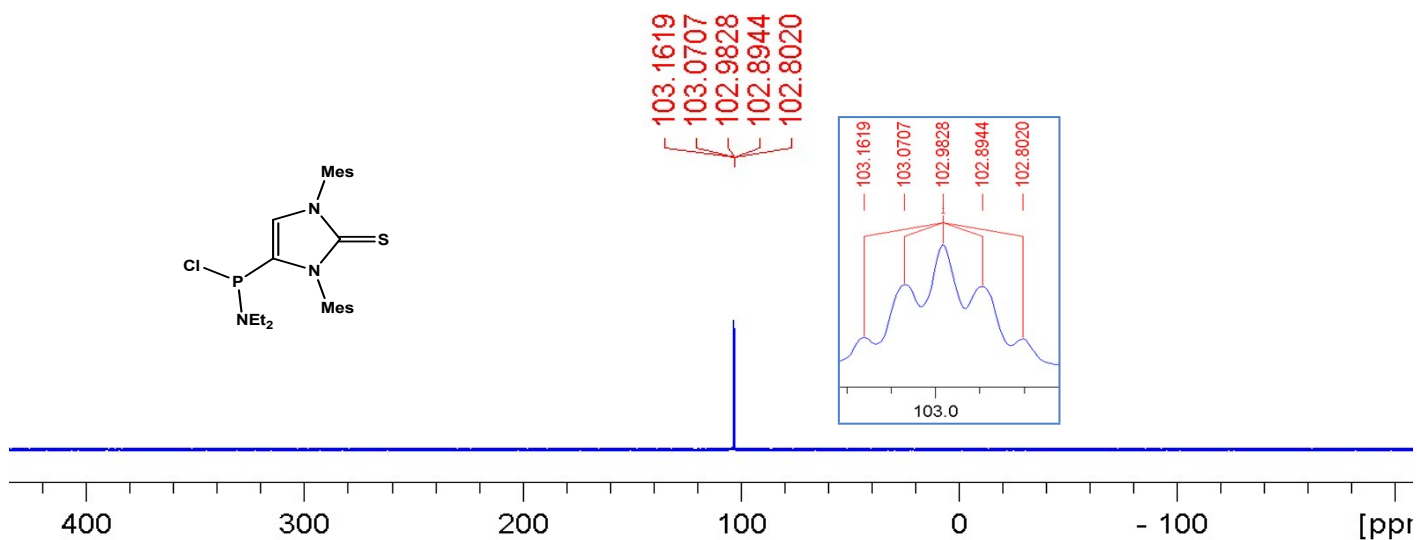
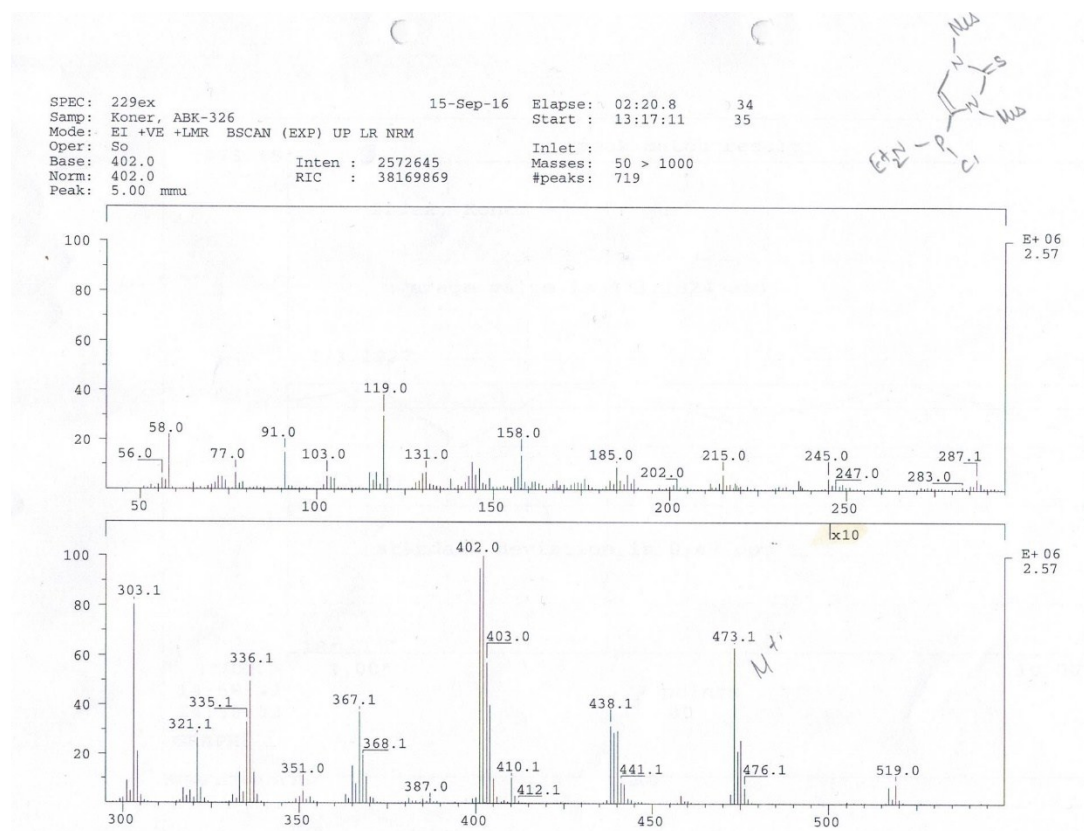


Figure S20: EI-MS spectrum of **3b**.



6 Spectra for Compound **3c**.

Figure S21: ^1H NMR spectrum of **3c** in CDCl_3 (300.1 MHz, 25 °C)

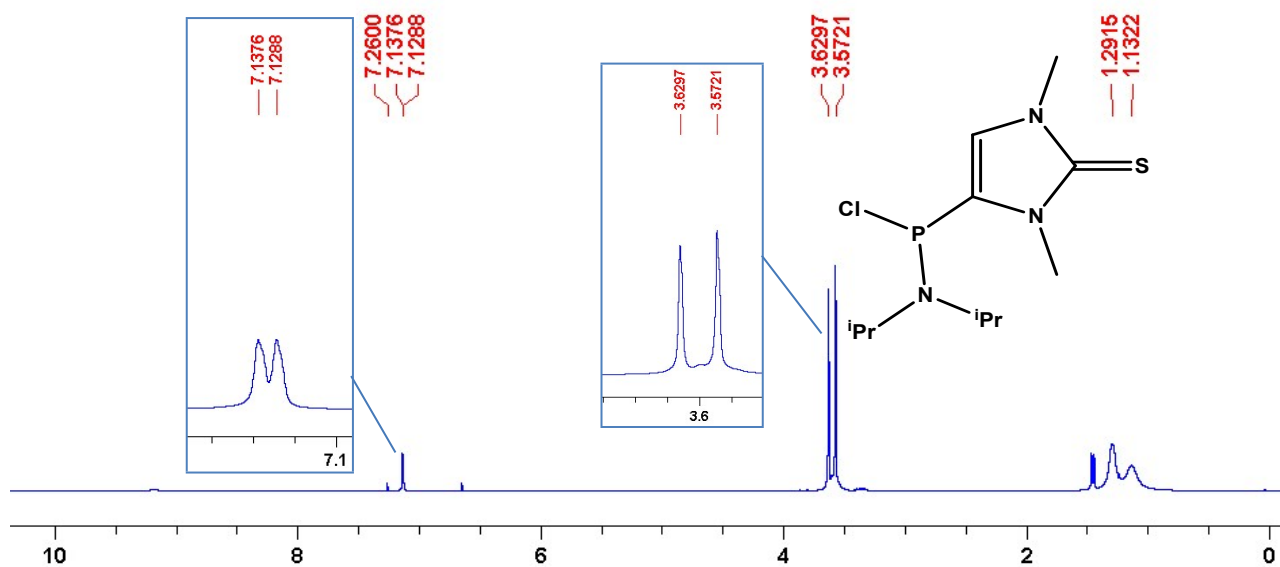


Figure S22: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **3c** in CDCl_3 (75.5 MHz, 25 °C)

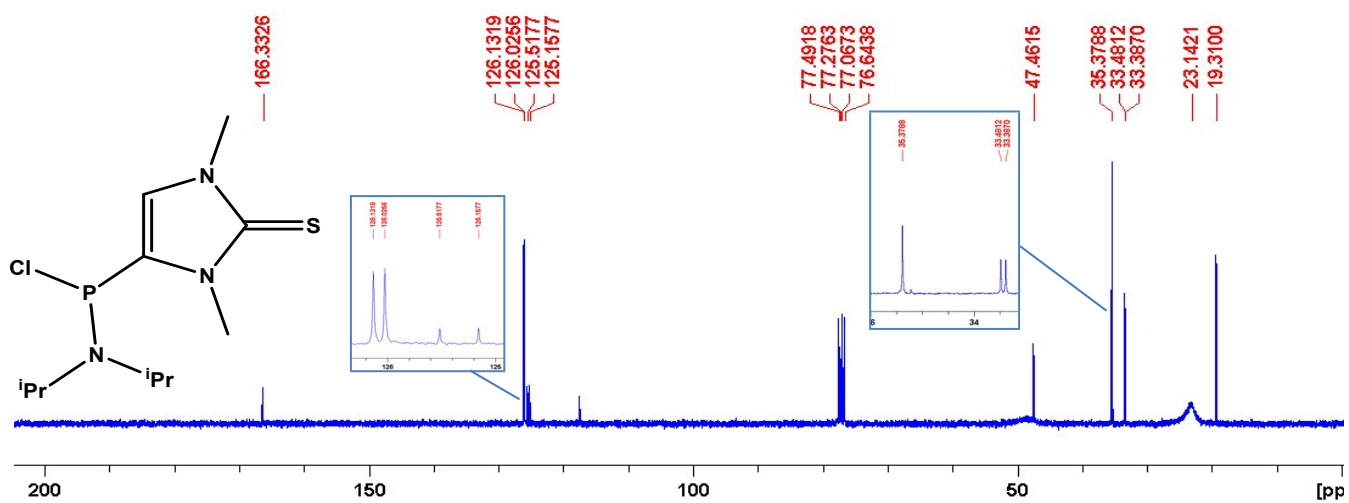


Figure S23: ^{31}P NMR spectrum of **3c** in CDCl_3 (121.5 MHz, 25 °C)

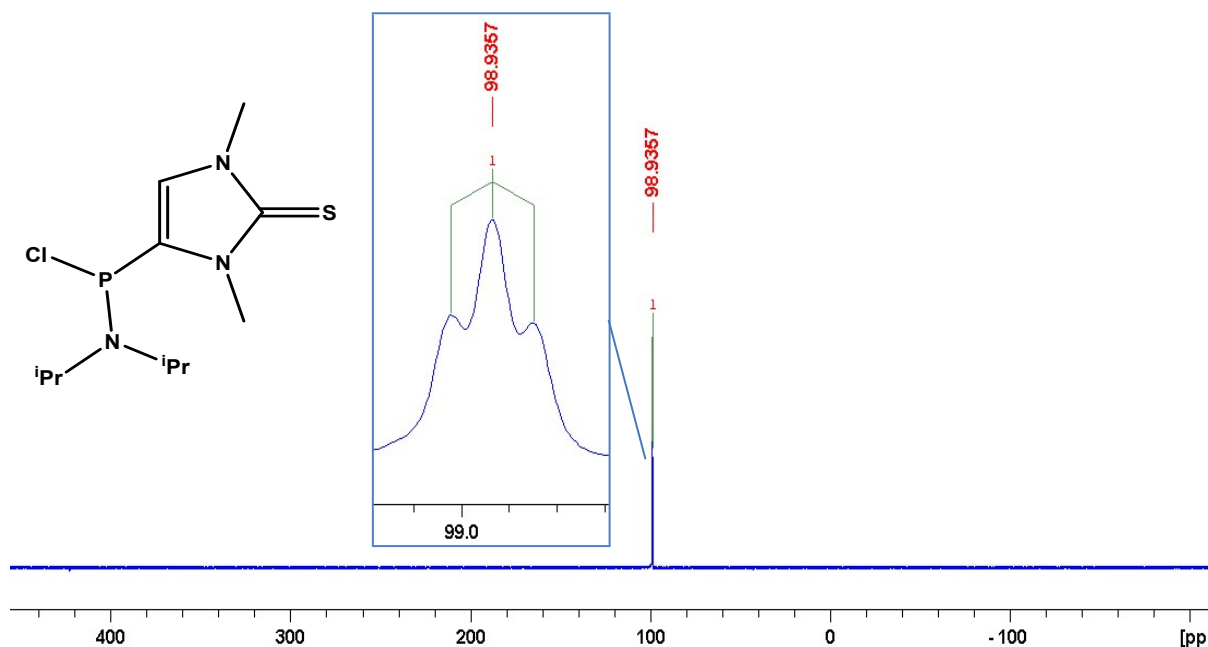
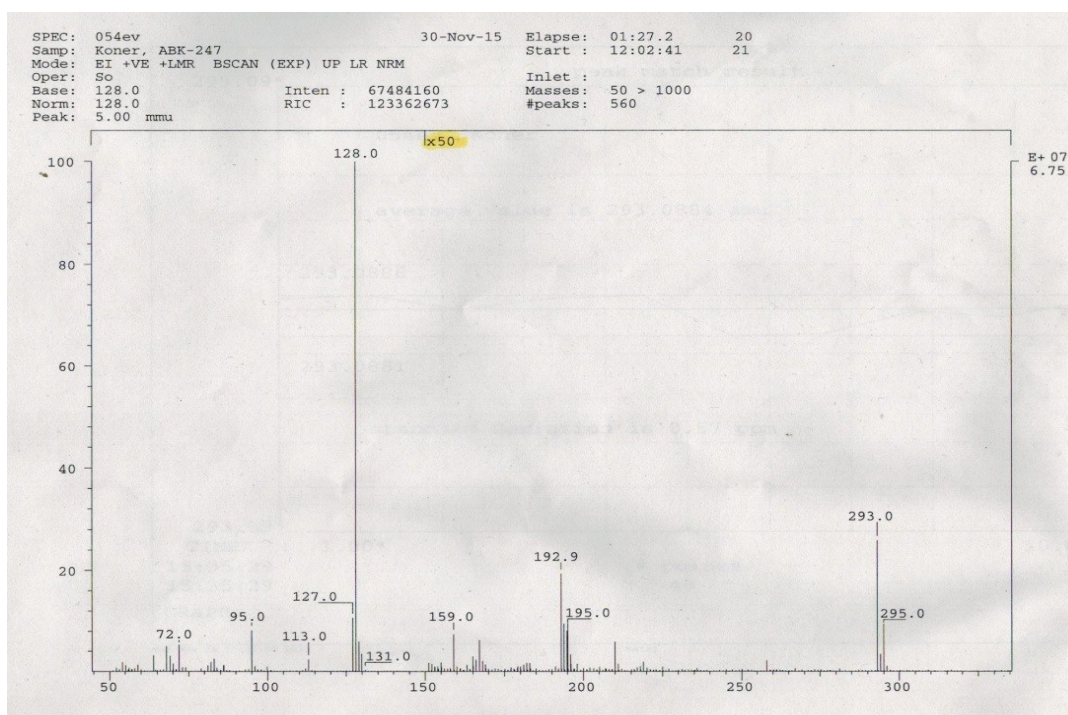


Figure S24: EI-MS spectrum of **3c**.



7 Spectra for Compound 4a.

Figure S25: ^1H NMR spectrum of **4a** in CDCl_3 (300.1 MHz, 25 °C)

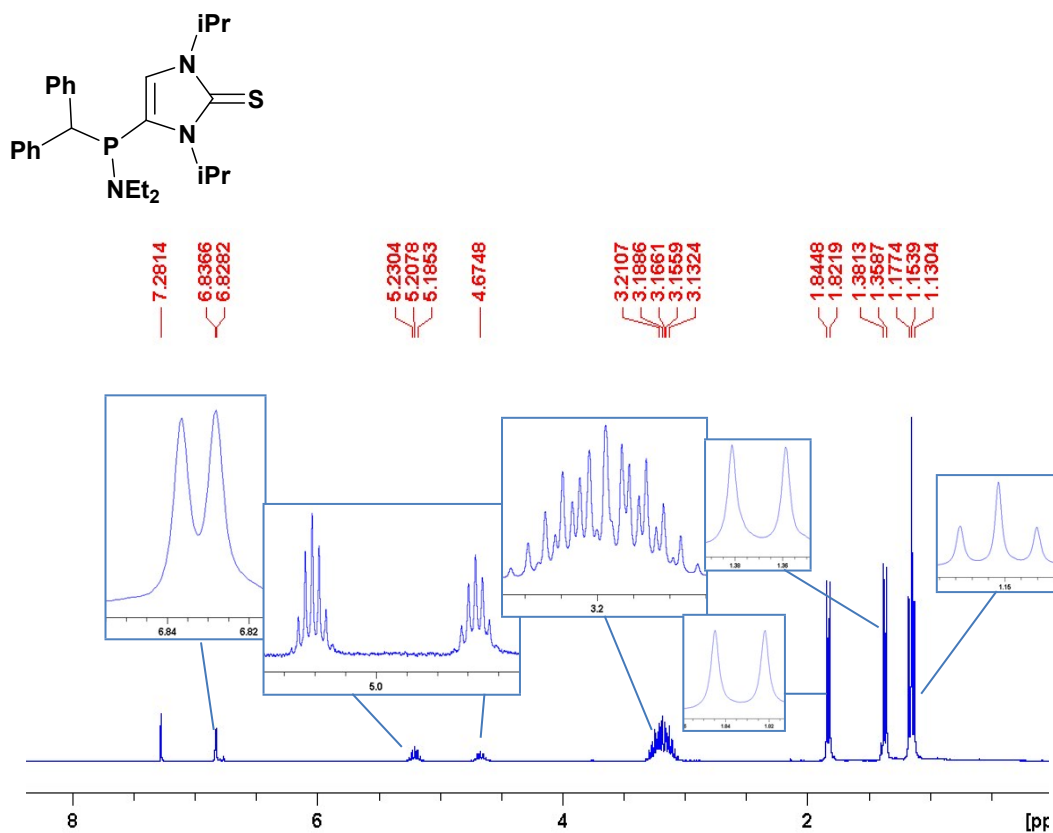


Figure S26: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **4a** in CDCl_3 (75.5 MHz, 25 °C)

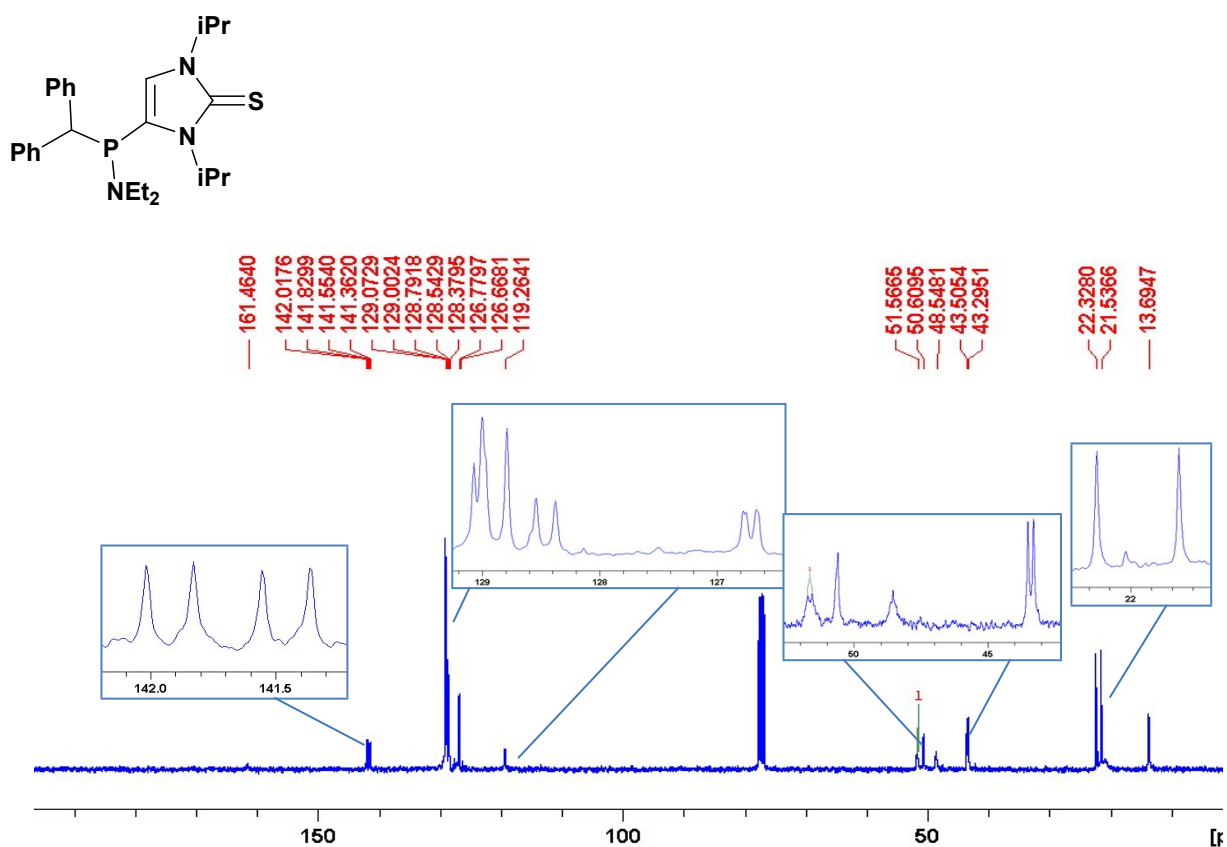


Figure S27: ^{31}P NMR spectrum of **4a** in CDCl_3 (121.5 MHz, 25 °C)

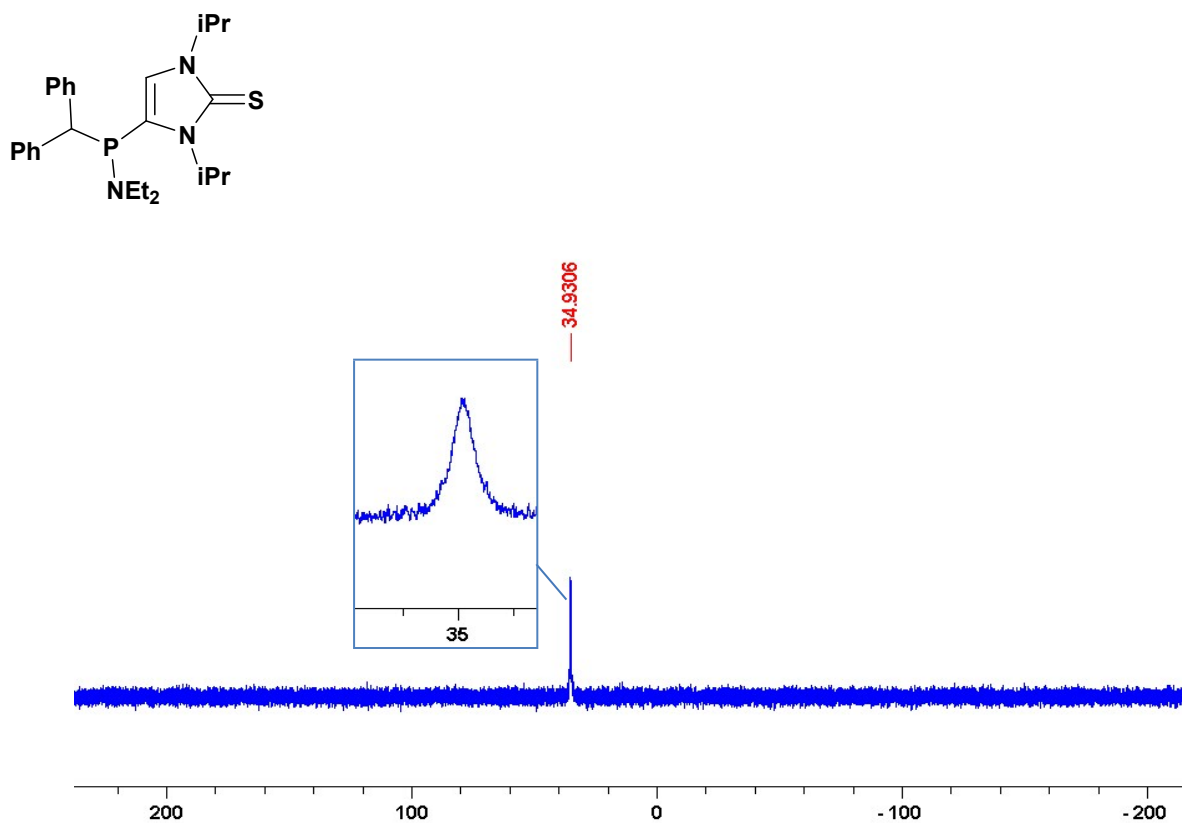
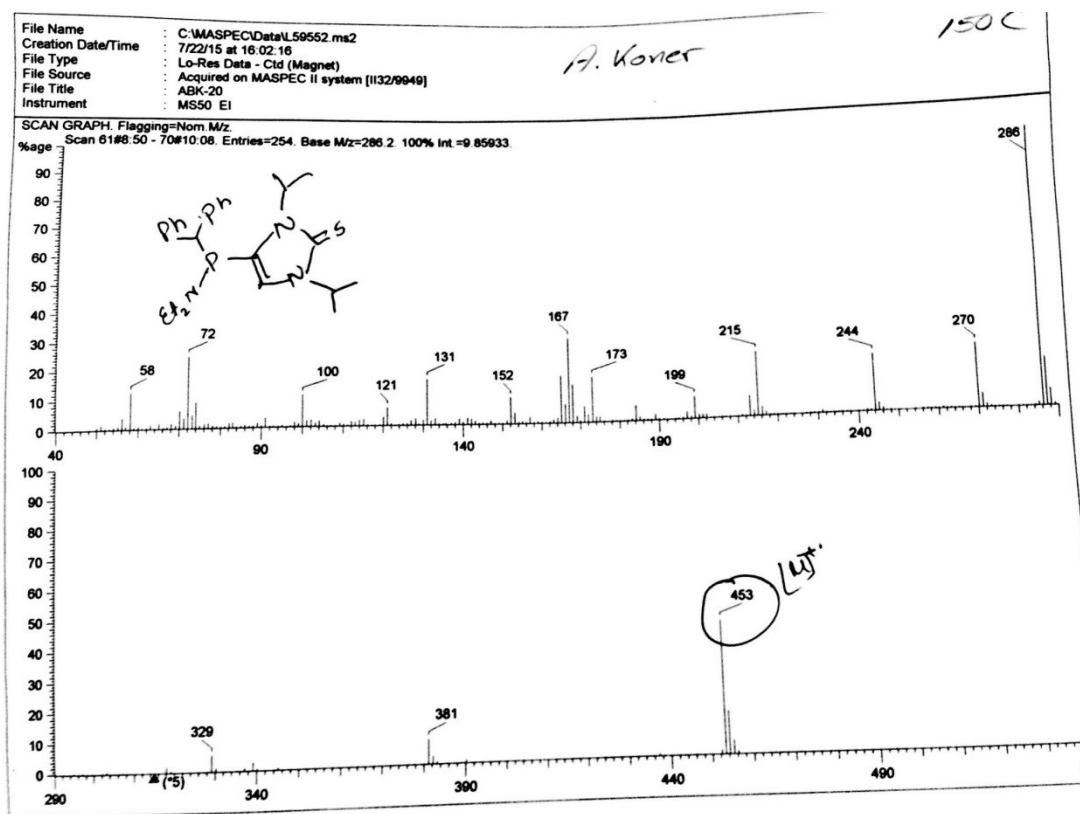


Figure S28: EI-MS spectrum of **4a**.



8 Spectra for Compound **4b**.

Figure S29: ^1H NMR spectrum of **4b** in CDCl_3 (300.1 MHz, 25 °C)

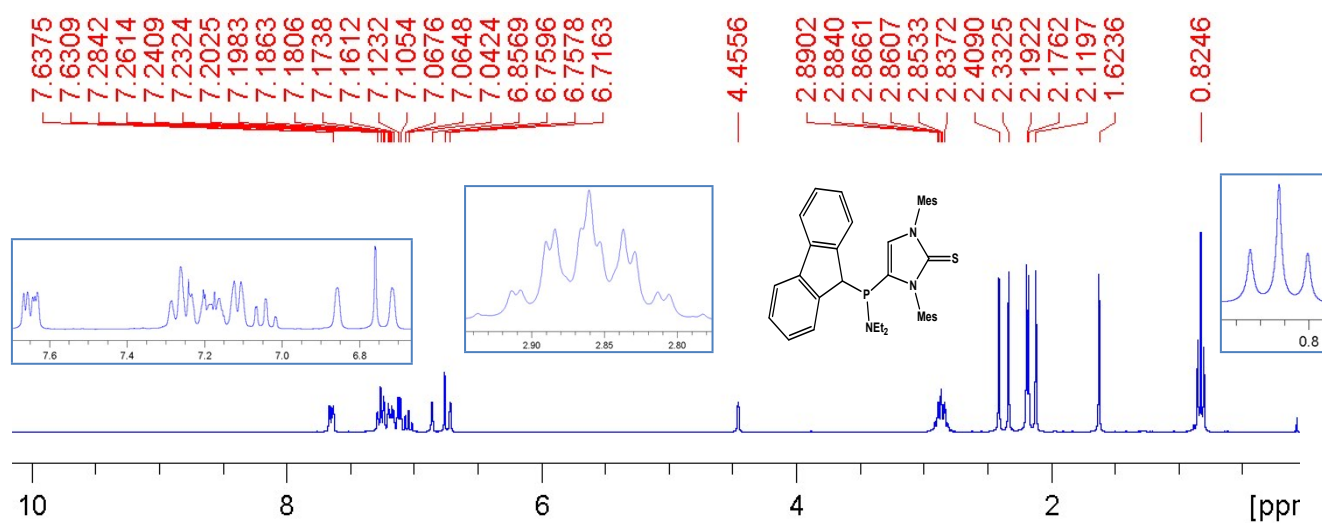


Figure S30: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **4b** in CDCl_3 (75.5 MHz, 25 °C)

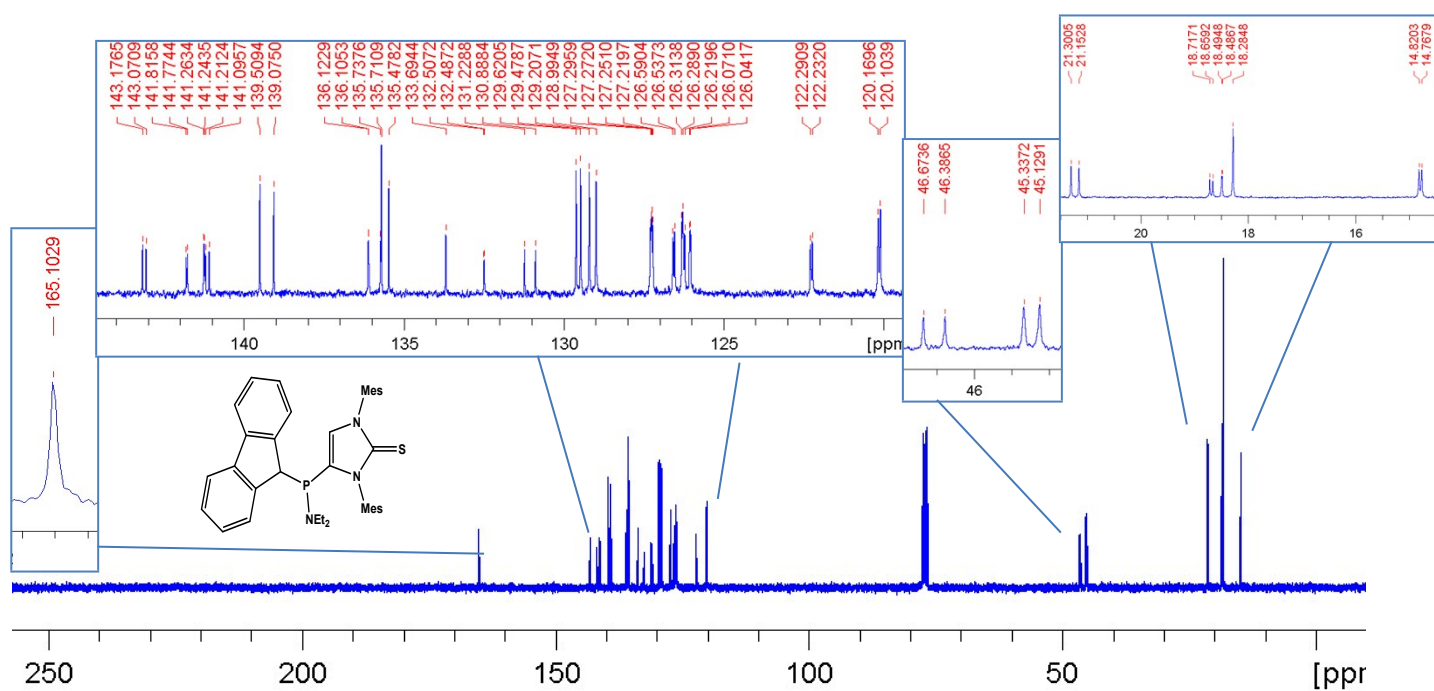


Figure S31: ^{31}P NMR spectrum of **4b** in CDCl_3 (121.5 MHz, 25 °C)

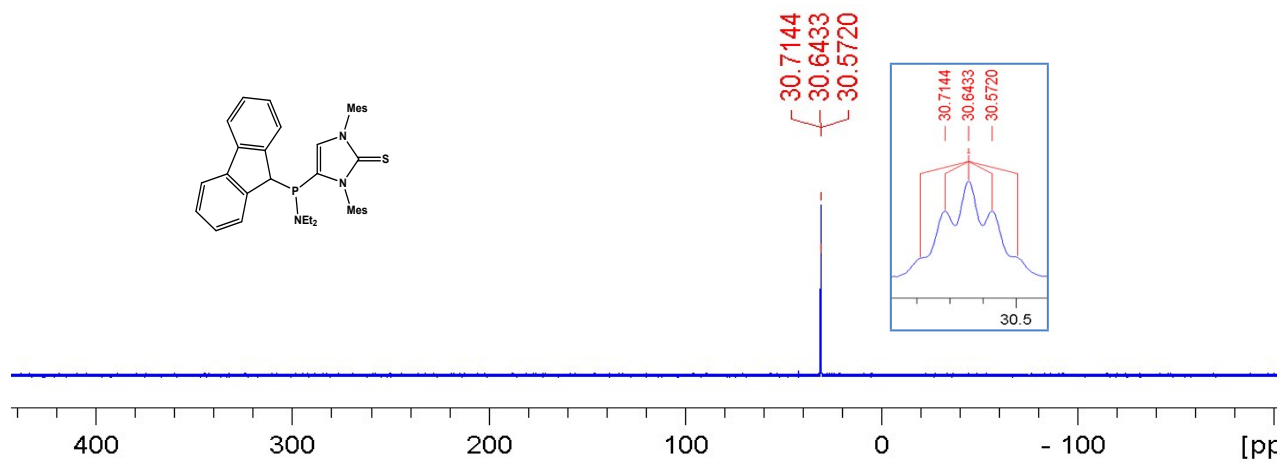
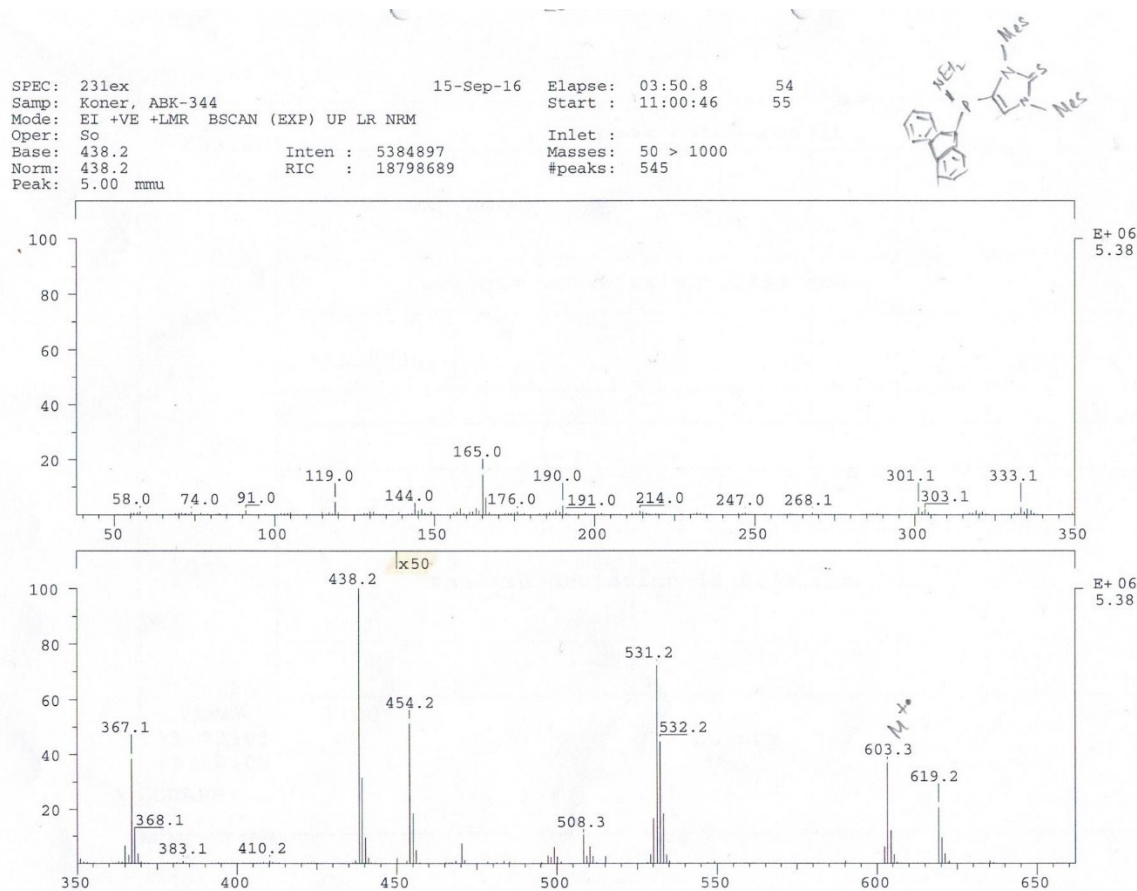


Figure 32: EI-MS spectrum of **4b**.



9 Spectra for Compound 4c.

Figure S33: ^1H NMR spectrum of **4c** in CDCl_3 (300.1 MHz, 25 °C)

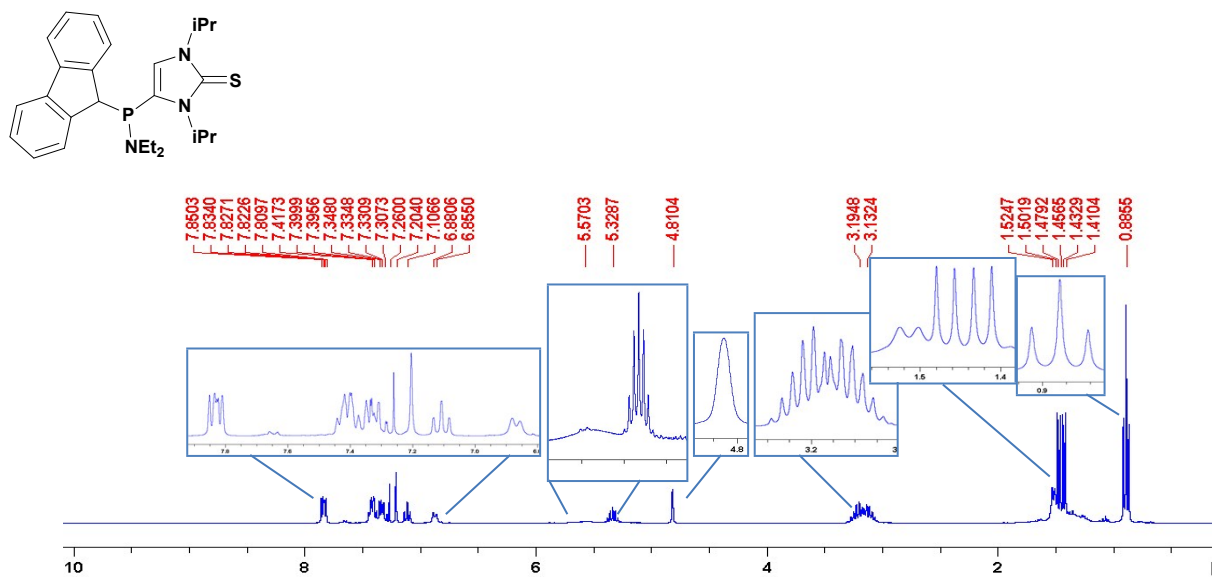
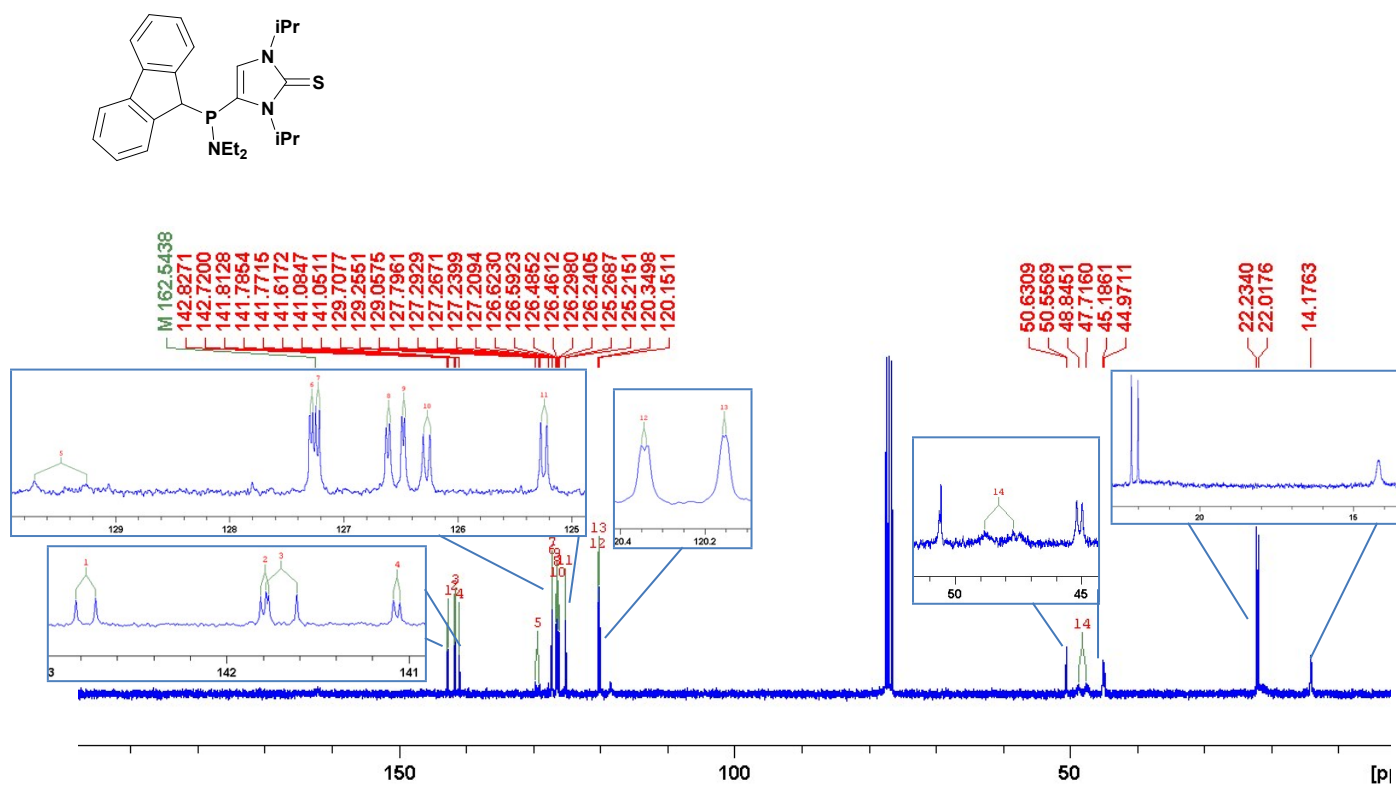


Figure S34: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **4c** in CDCl_3 (75.5 MHz, 25 °C)



10 Spectra for Compound 5.

Figure S37: ^1H NMR spectrum of **5** in CDCl_3 (300.1 MHz, 25 °C)

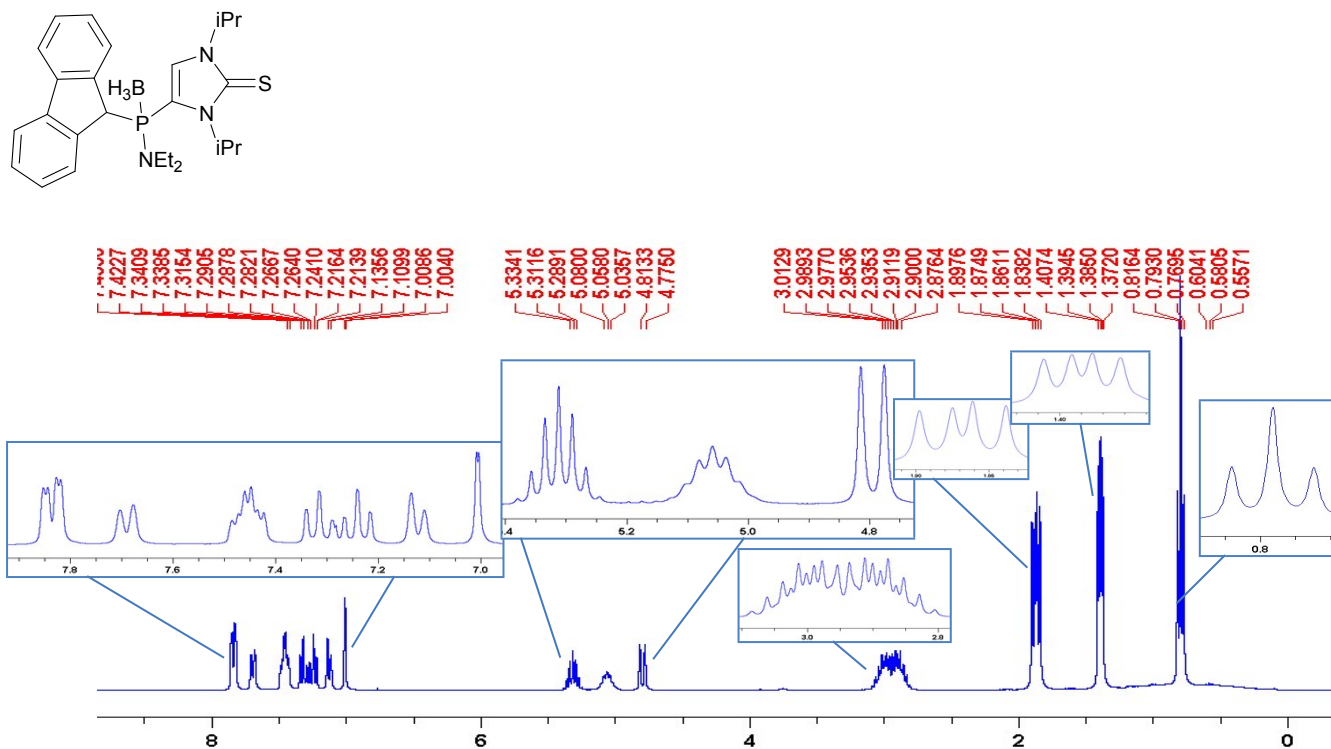


Figure S38: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **5** in CDCl_3 (75.5 MHz, 25 °C)

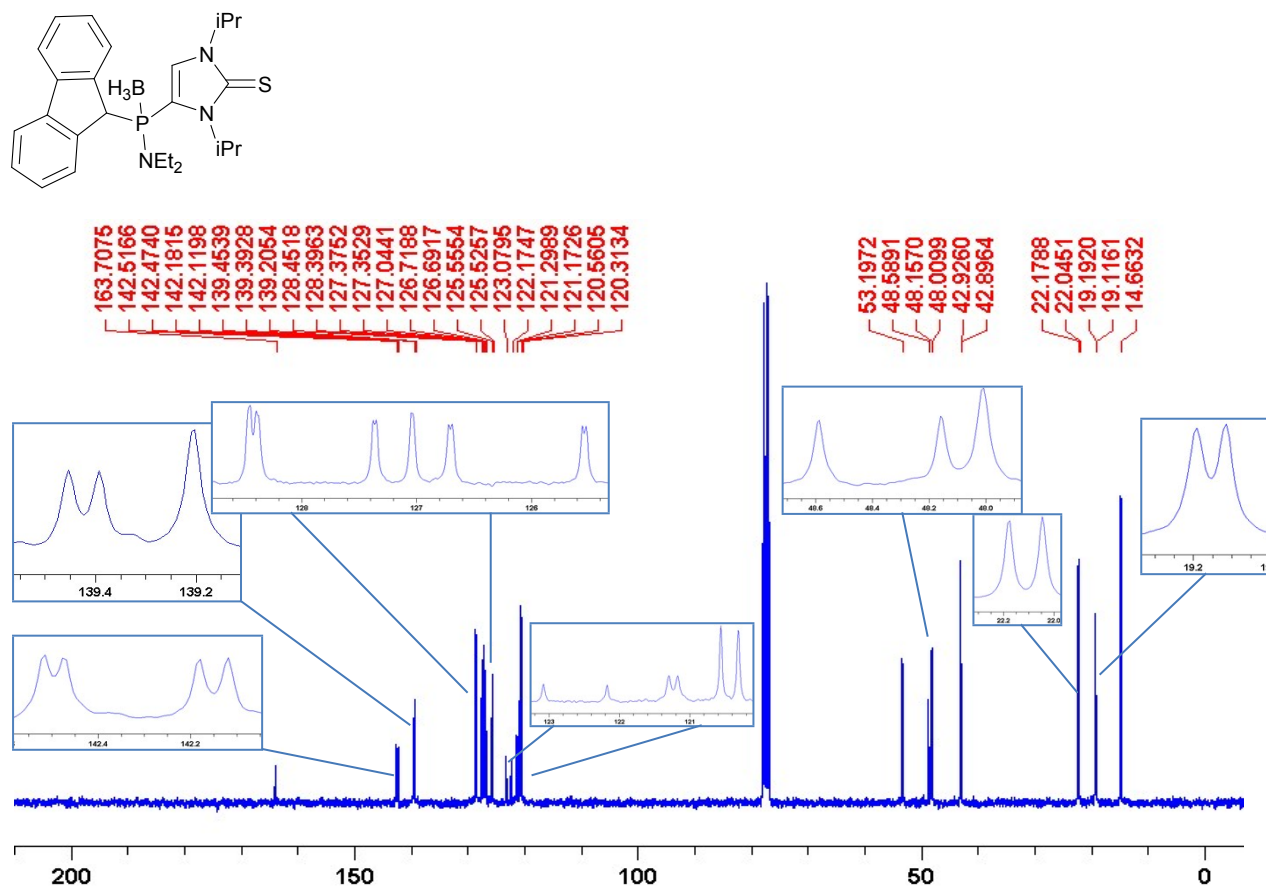


Figure S39: ^{31}P NMR spectrum of **5** in CDCl_3 (121.5 MHz, 25 °C)

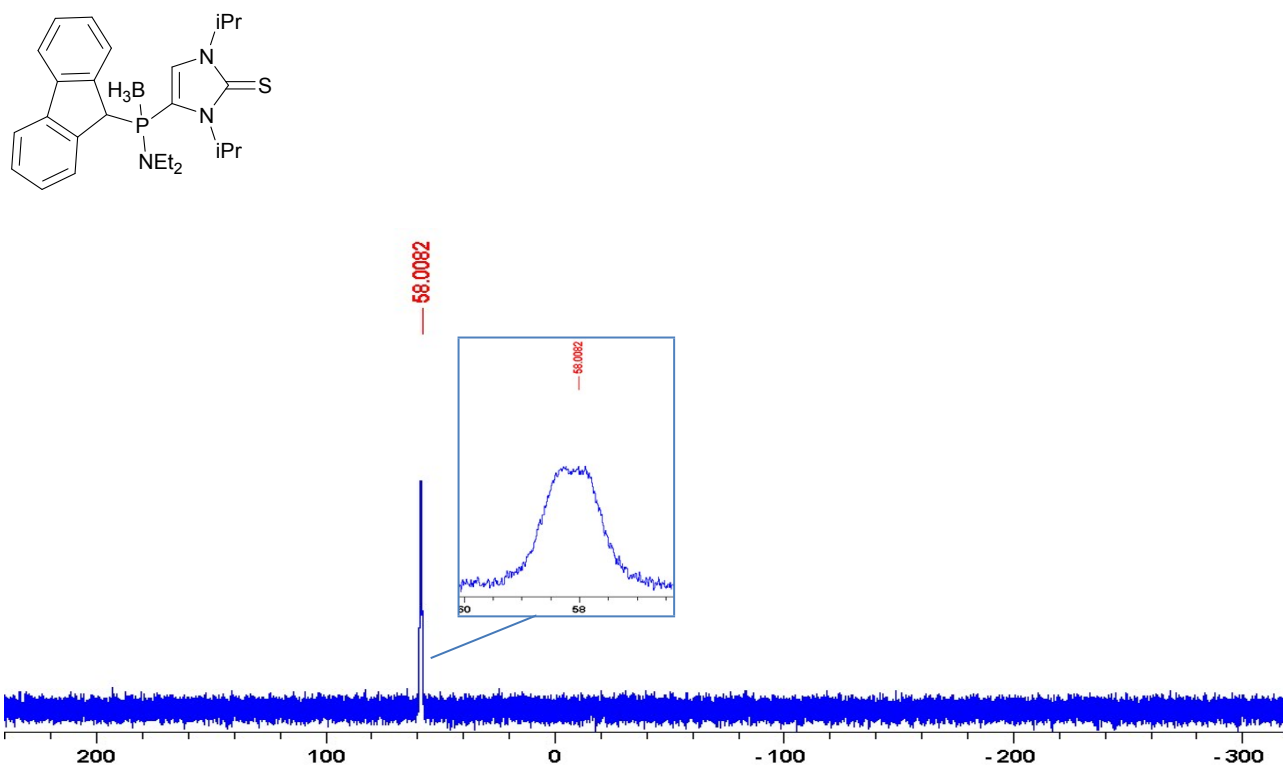
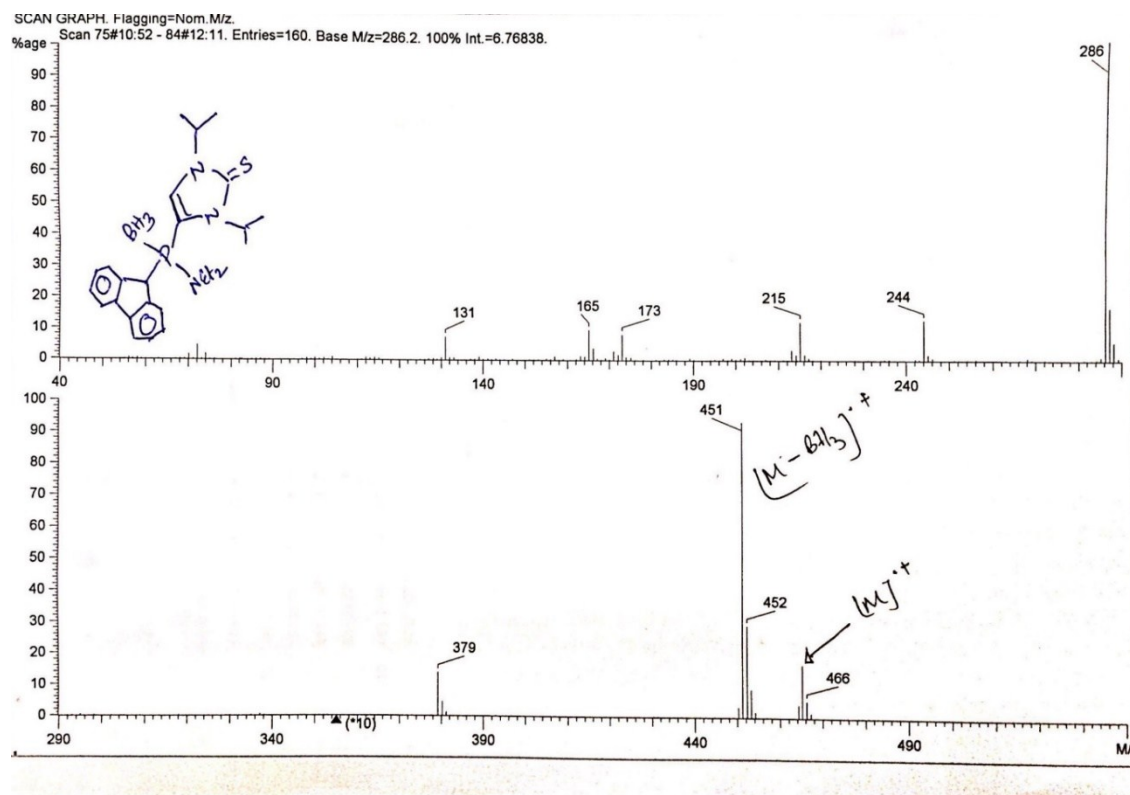


Figure 40: EI-MS spectrum of **5**.



11 Spectra for Compound 6.

Figure S41: ^1H NMR spectrum of **6** in CDCl_3 (300.1 MHz, 25 °C)

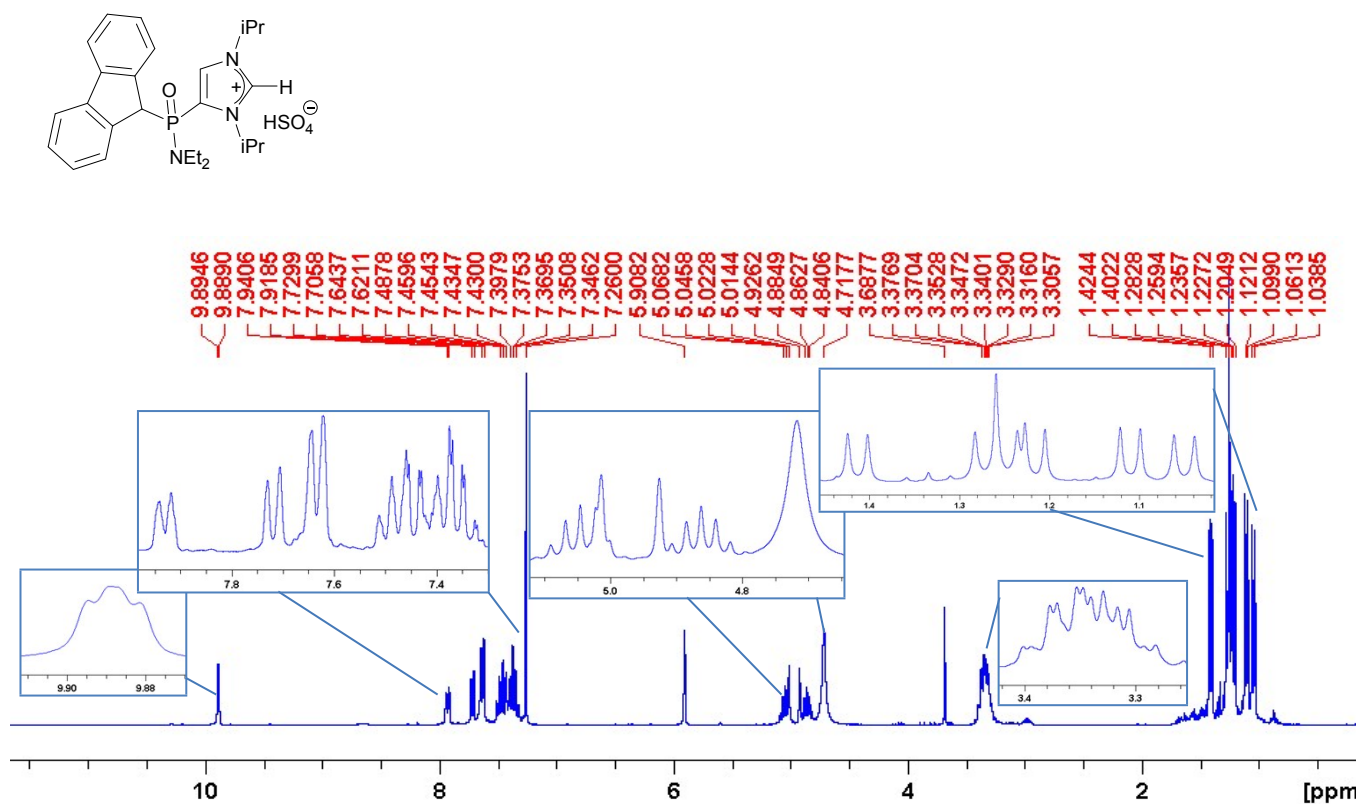


Figure S42: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **6** in CDCl_3 (75.5 MHz, 25 °C)

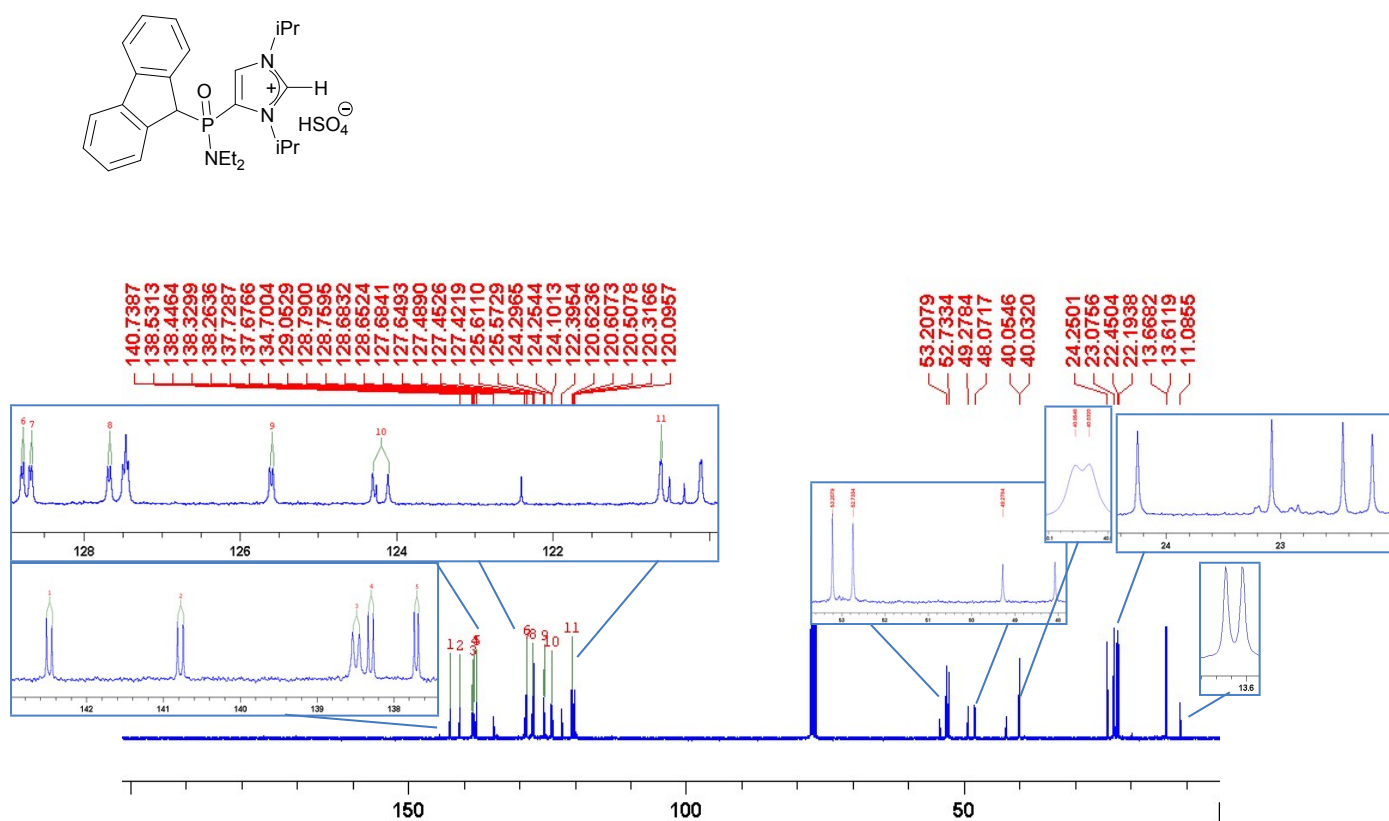


Figure S43: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **6** in CDCl_3 (121.5 MHz, 25 °C)

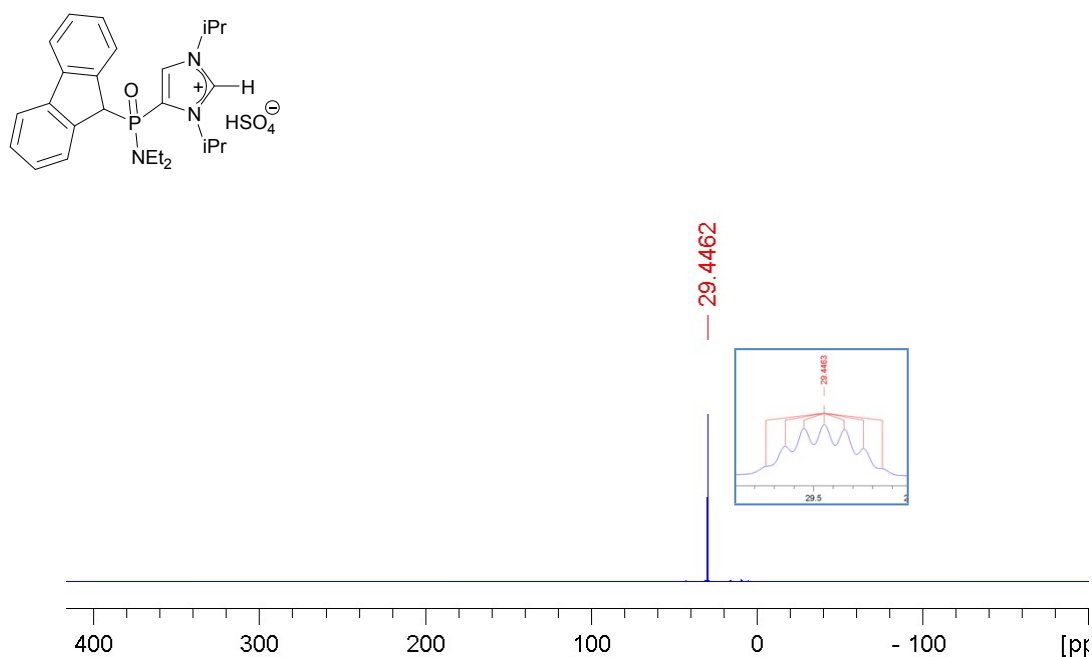
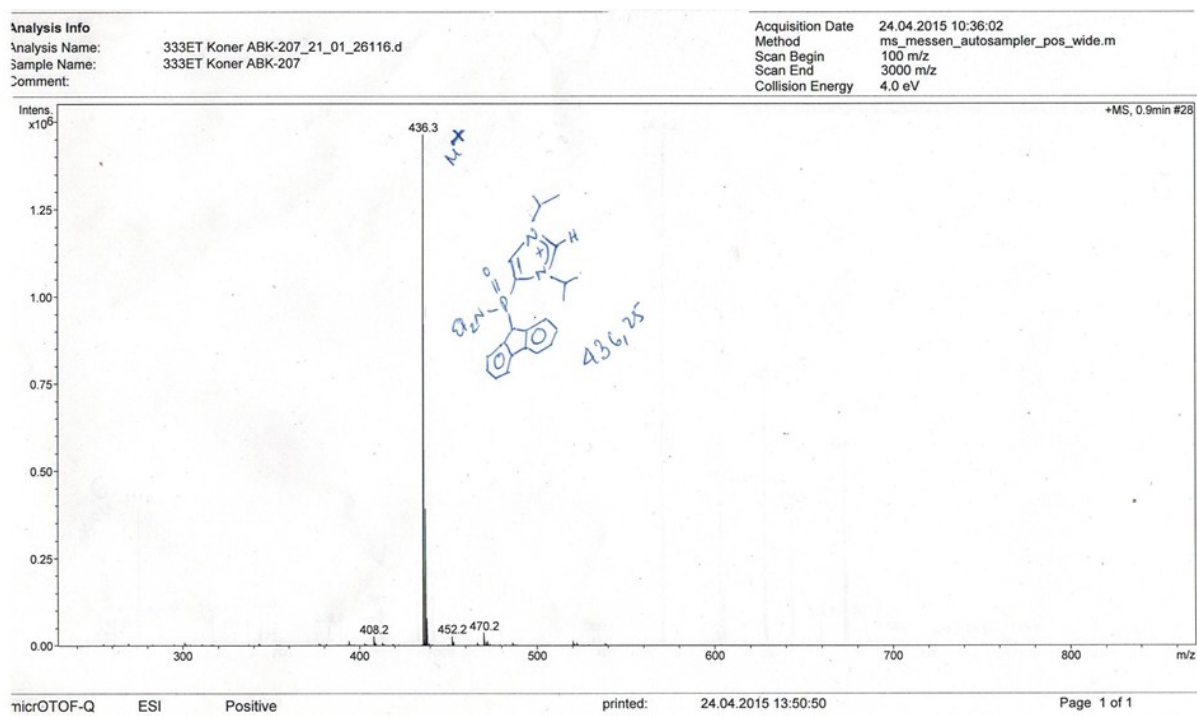


Figure 44: ESI-MS spectrum of **6**.



12 Spectra for Compound 7a.

Figure S45: ^1H NMR spectrum of **7a** in CDCl_3 (300.1 MHz, 25 °C)

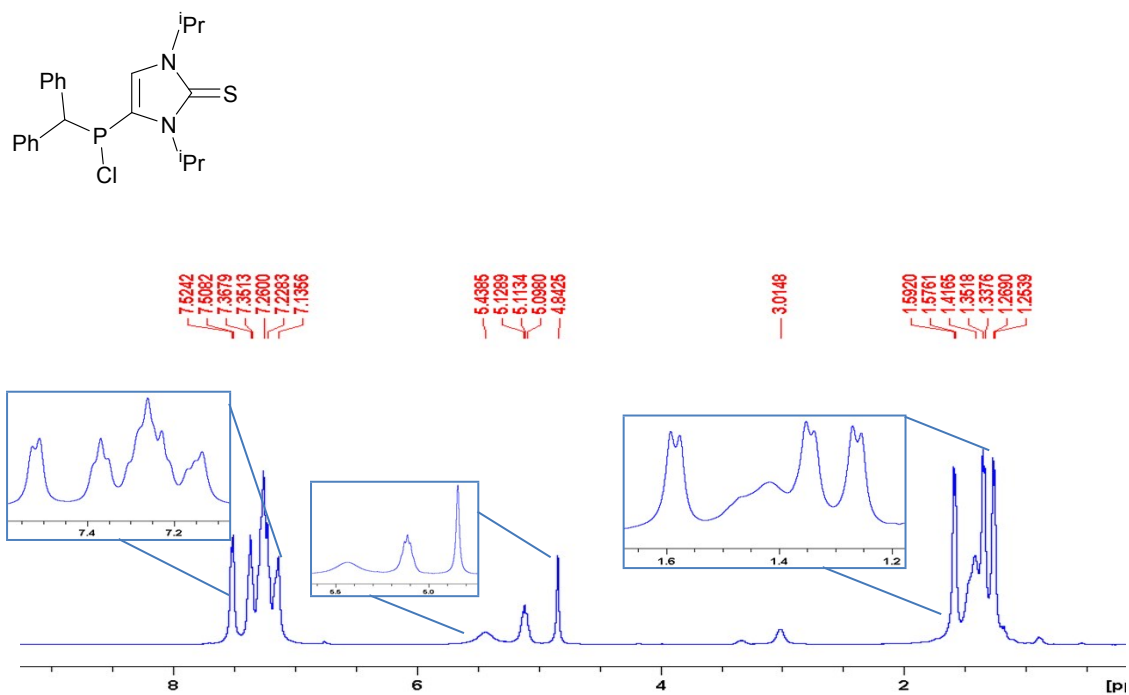


Figure S46: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **7a** in CDCl_3 (75.5 MHz, 25 °C)

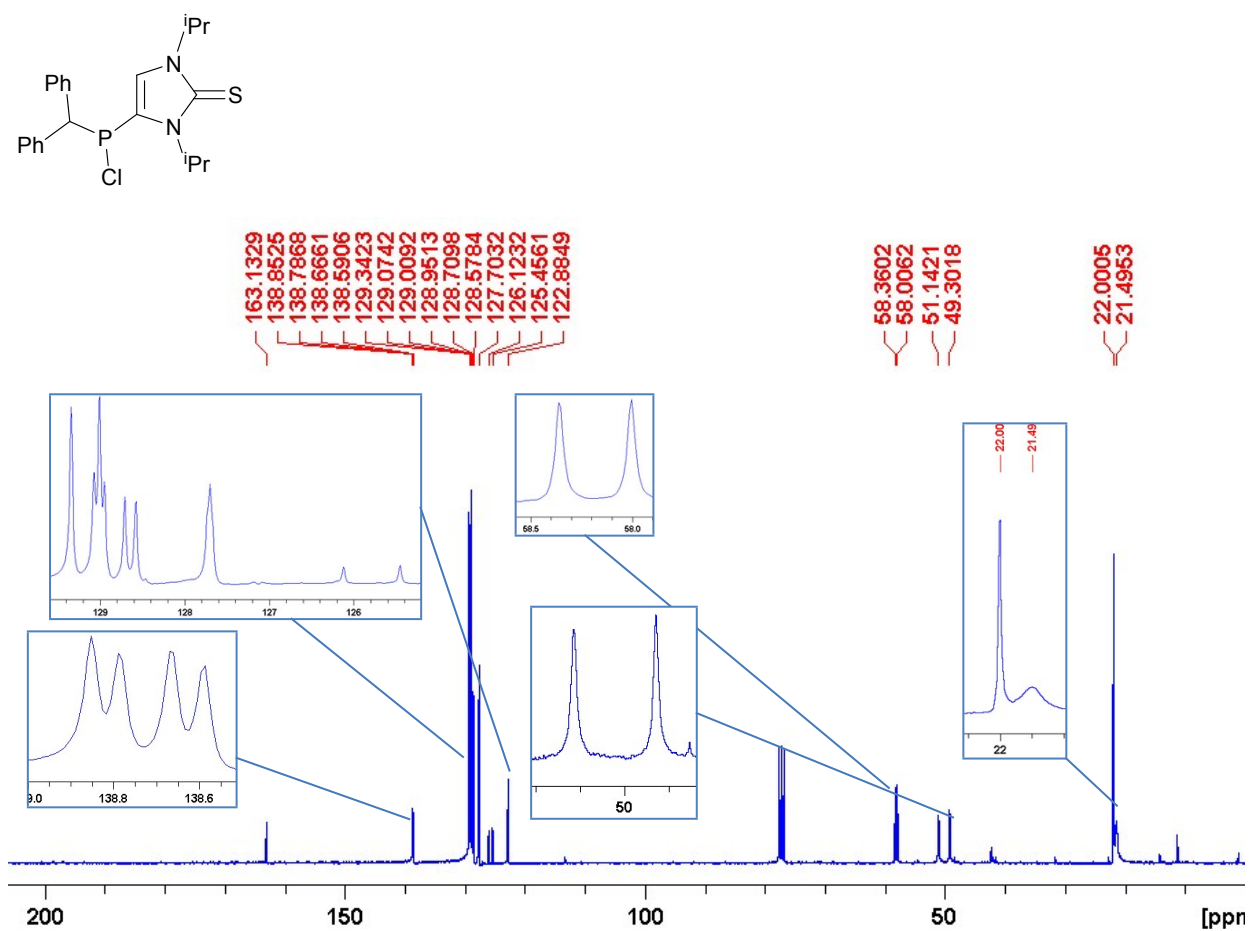


Figure S47: ^{31}P NMR spectrum of **7a** in CDCl_3 (121.5 MHz, 25 °C)

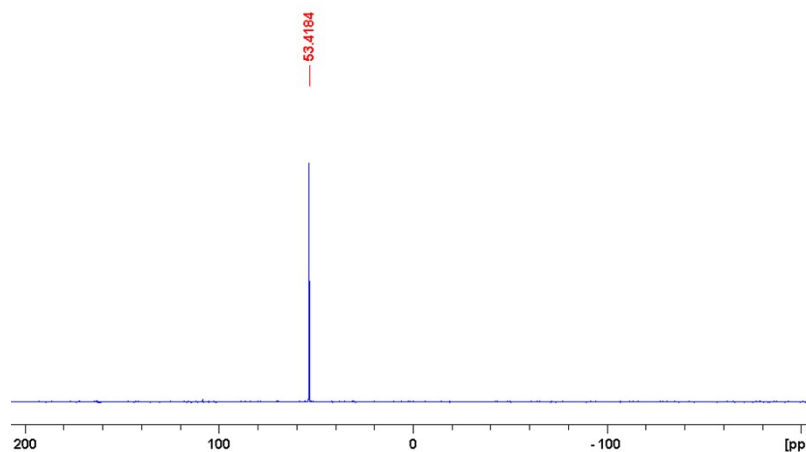
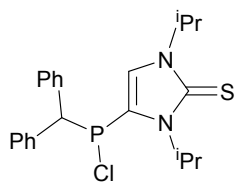
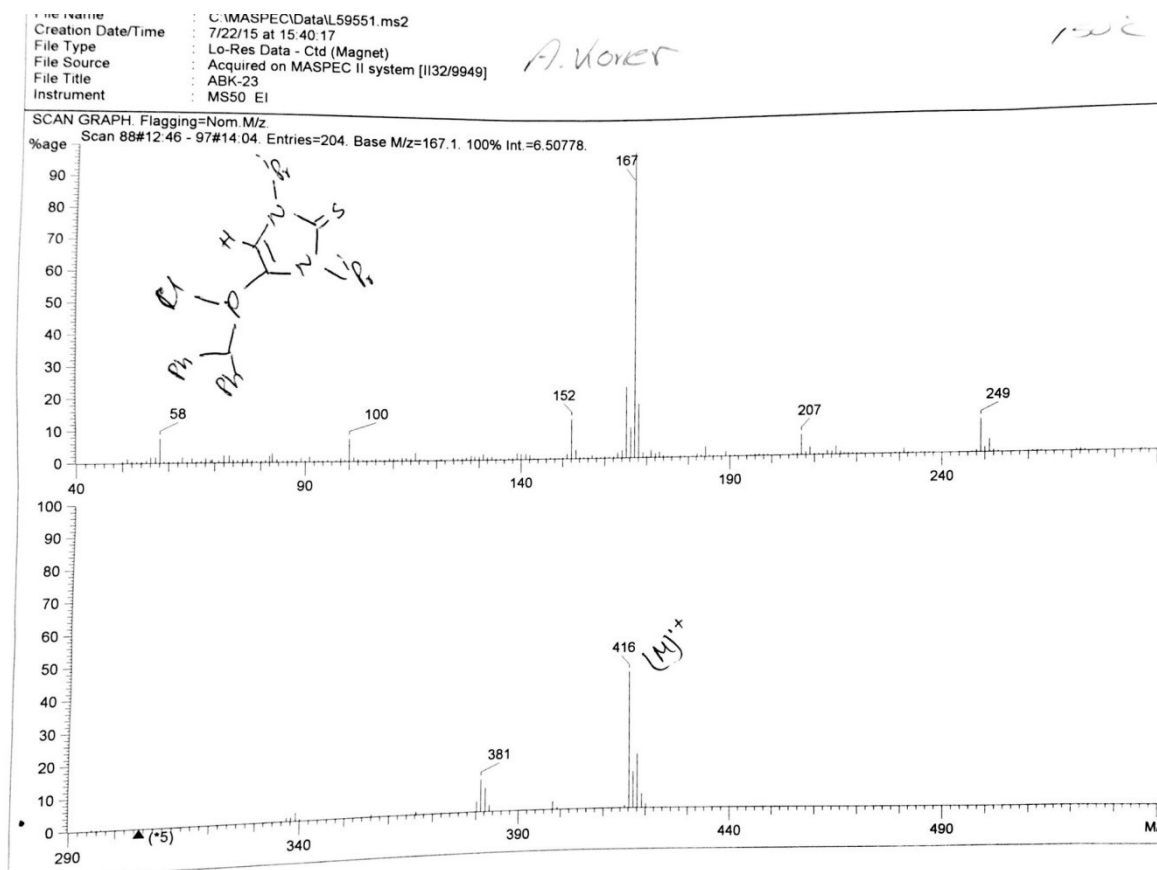


Figure 48: EI-MS spectrum of **7a**.



13 Spectra for Compound **7b**.

Figure S49: ^1H NMR spectrum of **7b** in CDCl_3 (300.1 MHz, 25 °C)

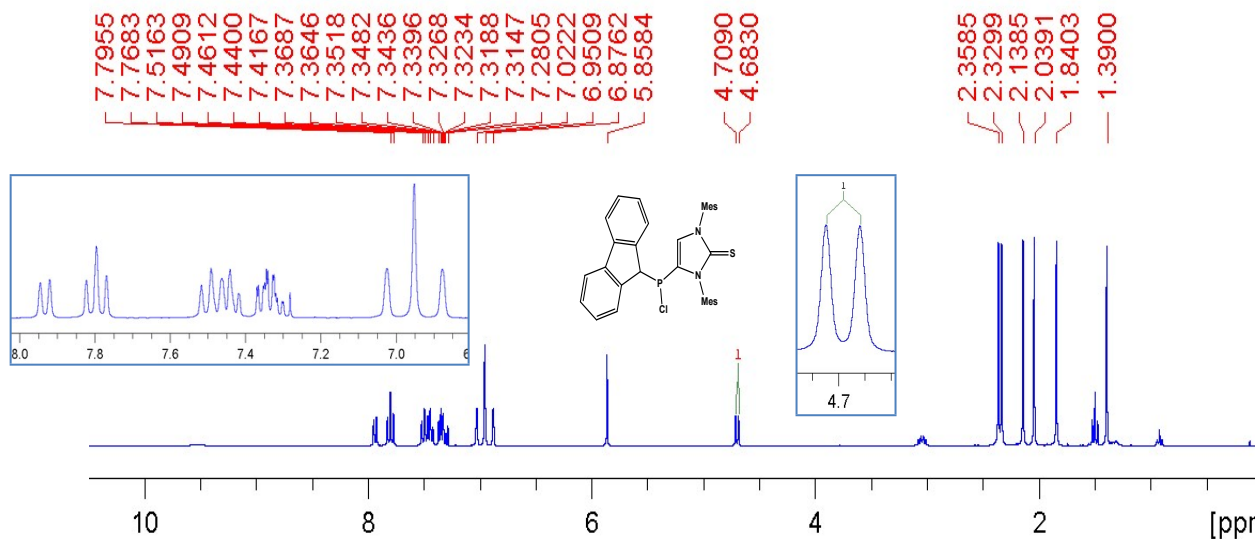


Figure S50: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **7b** in CDCl_3 (75.5 MHz, 25 °C)

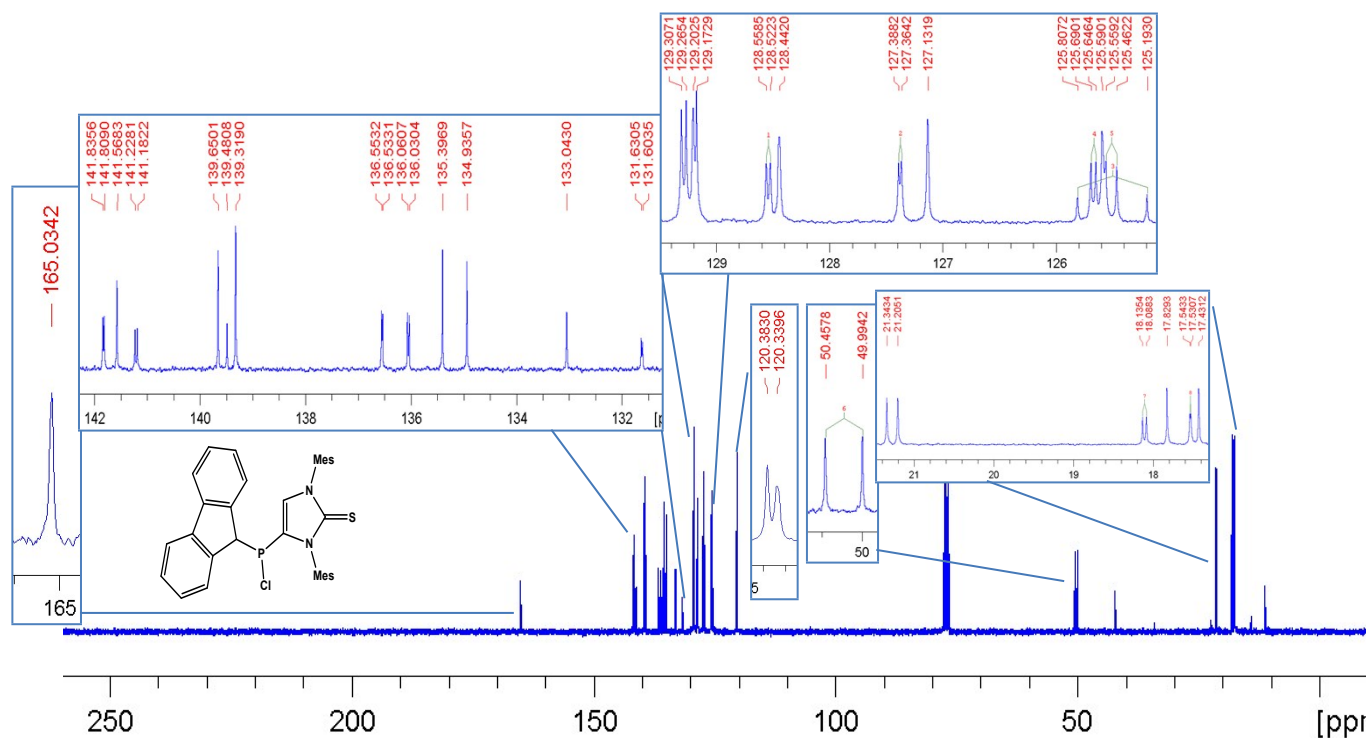


Figure S51: ^{31}P NMR spectrum of **7b** in CDCl_3 (121.5 MHz, 25 °C)

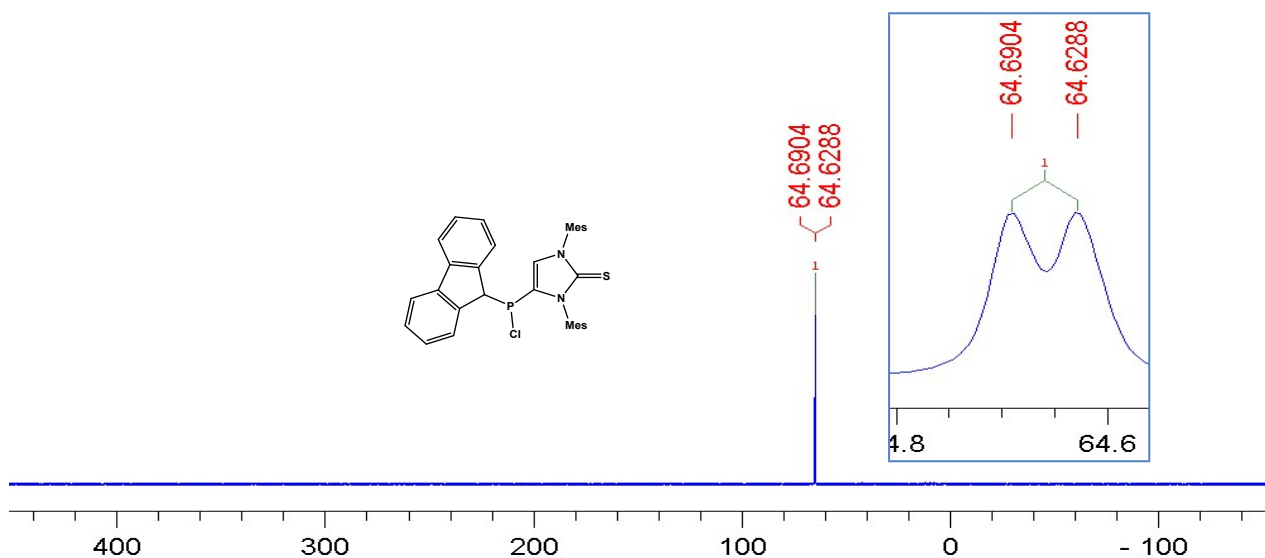
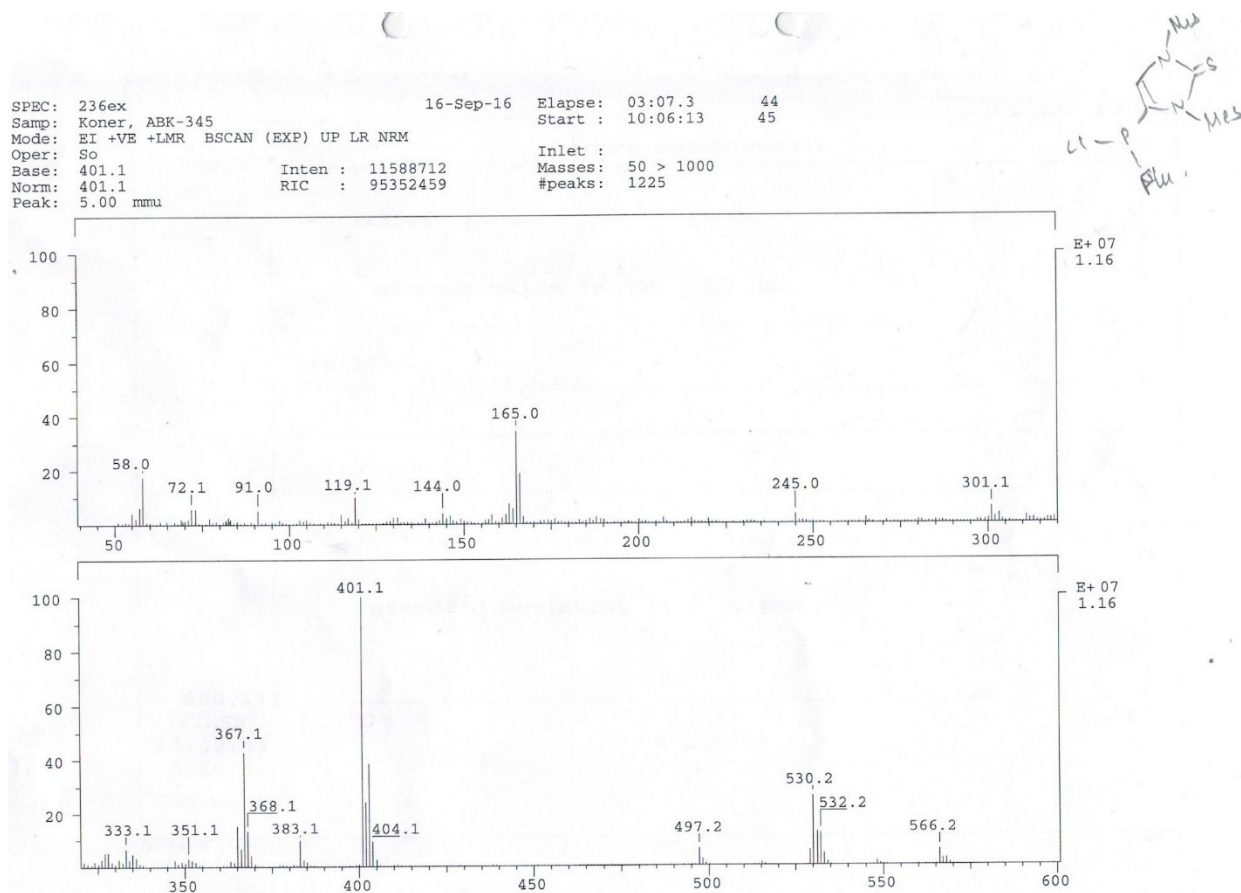


Figure 52: EI-MS spectrum of **7b**.



14 Spectra for Compound **8**.

Figure S53: ^1H NMR spectrum of **8** in CDCl_3 (300.1 MHz, 25 °C)

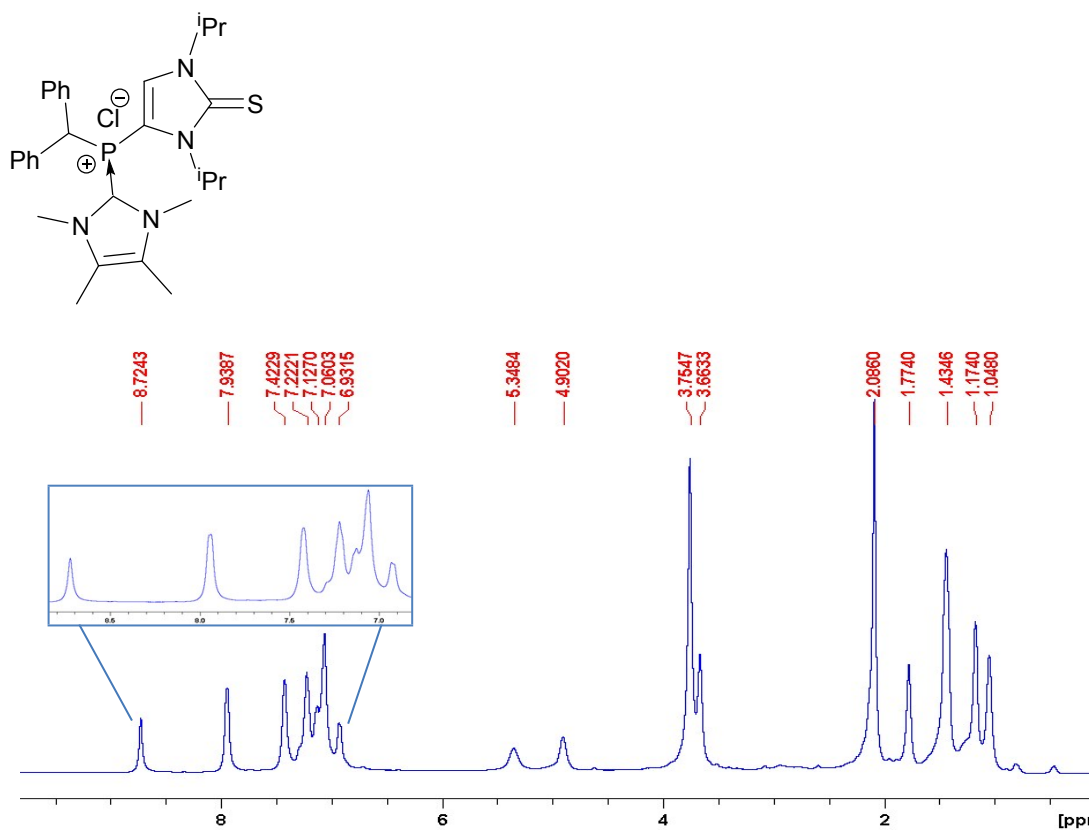


Figure S54: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **8** in CDCl_3 (75.5 MHz, 25 °C)

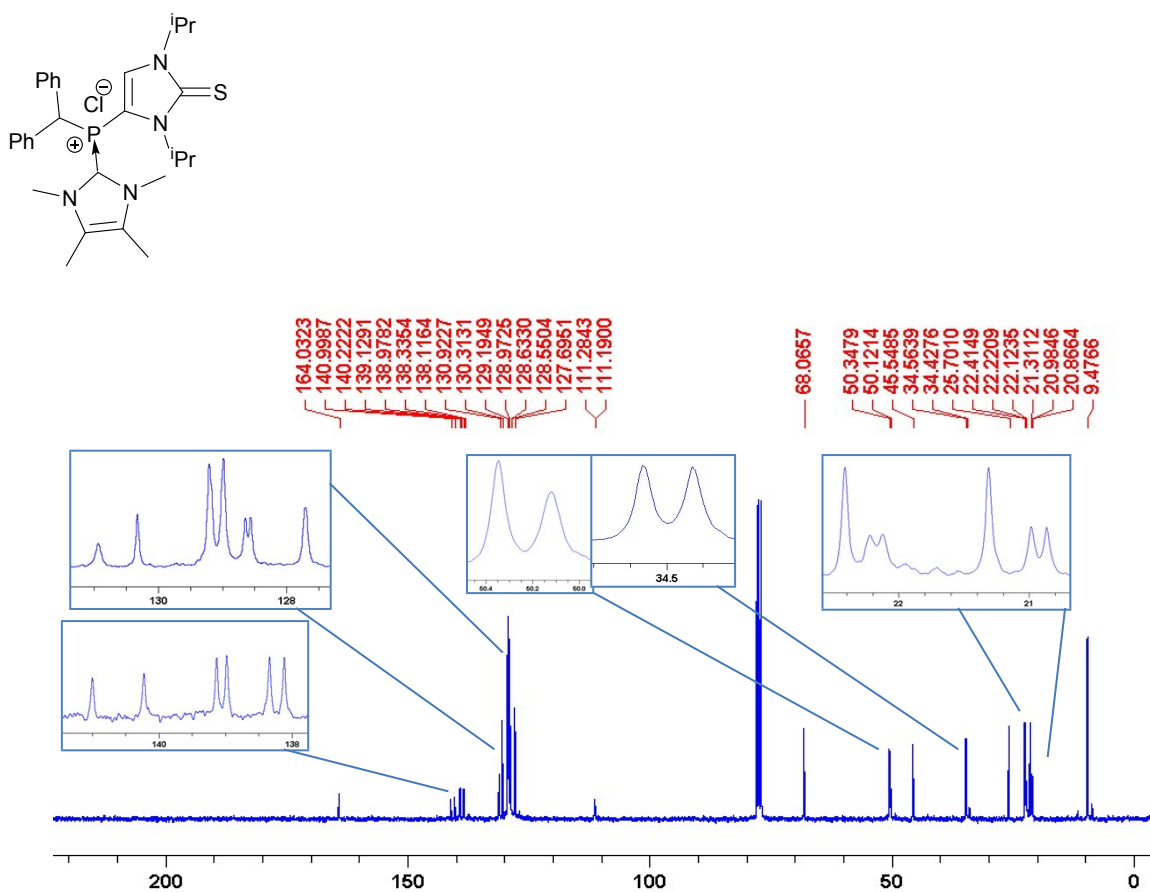


Figure S55: ^{31}P NMR spectrum of **8** in CDCl_3 (121.5 MHz, 25 °C)

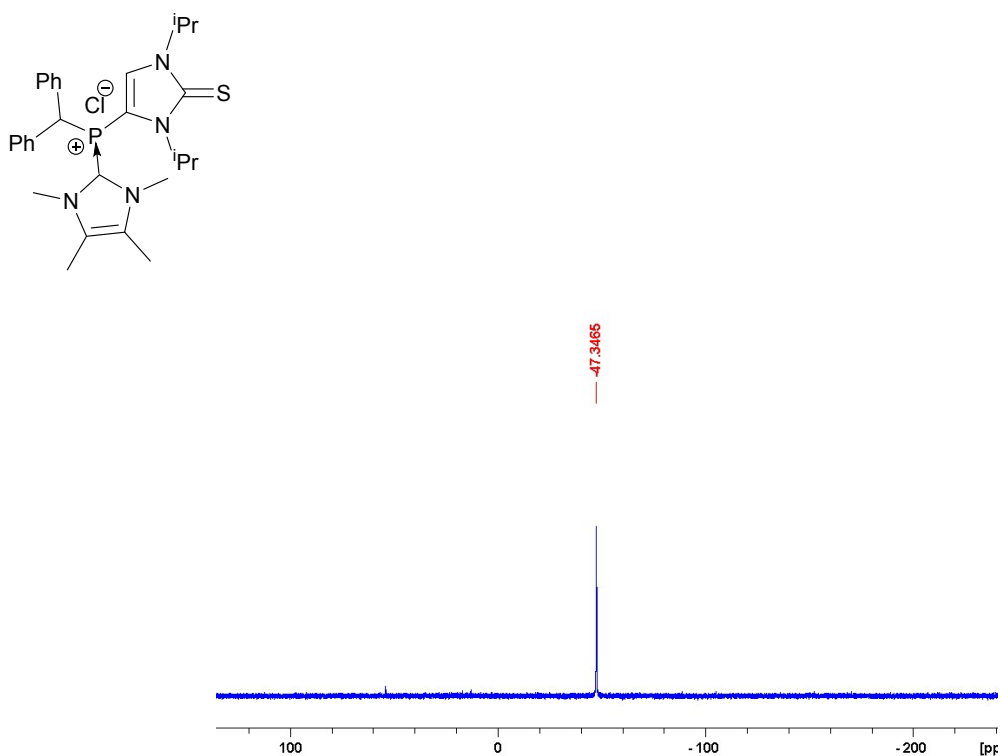
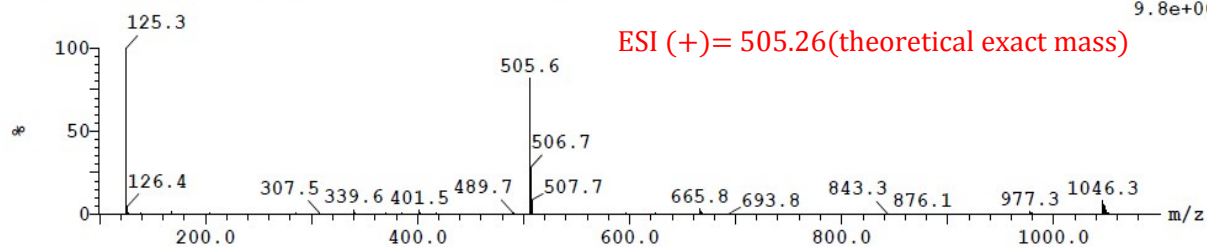


Figure 56: ESI-MS spectrum of **8**.

Sample Report (continued):

1: (Time: 1.30) Combine (49:71-(23:40+106:119))

1:MS ES+
9.8e+006



15 Spectra for Compound **11**.

Figure S57: ^1H NMR spectrum of **11** in CDCl_3 (300.1 MHz, 25 °C)

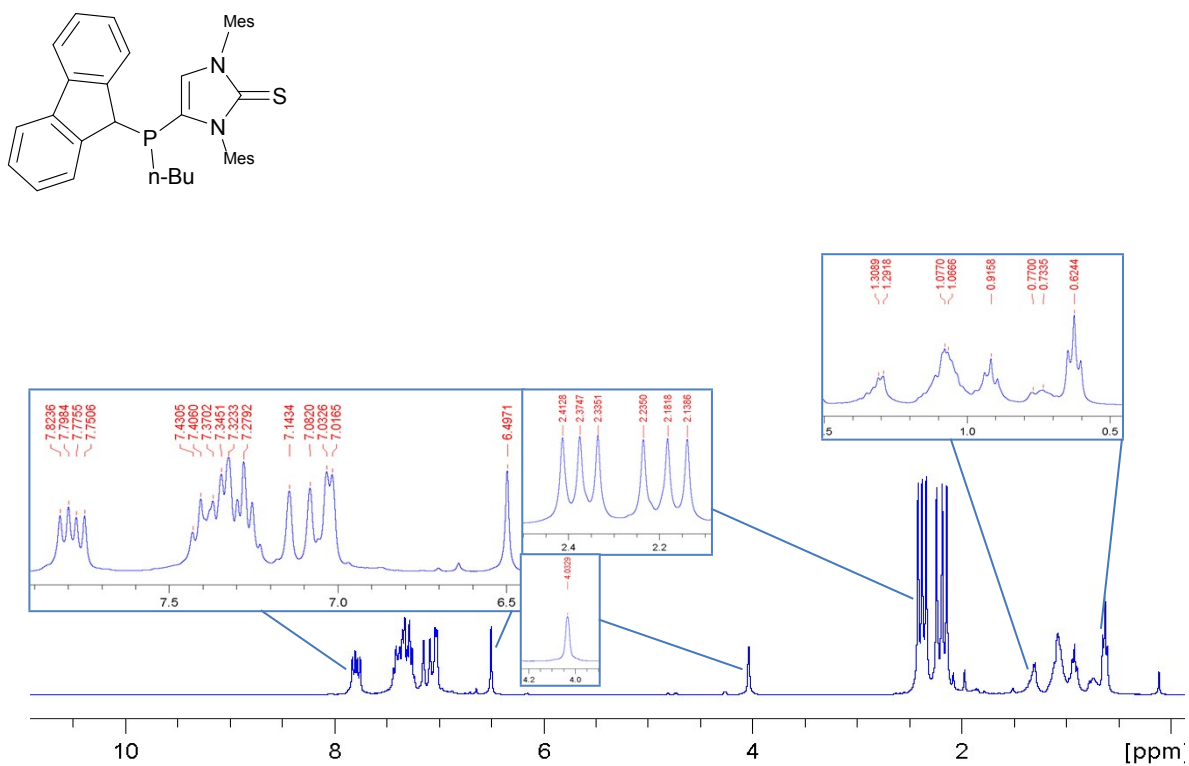


Figure S58: ^{13}C $\{^1\text{H}\}$ NMR spectrum of **11** in CDCl_3 (75.5 MHz, 25 °C)

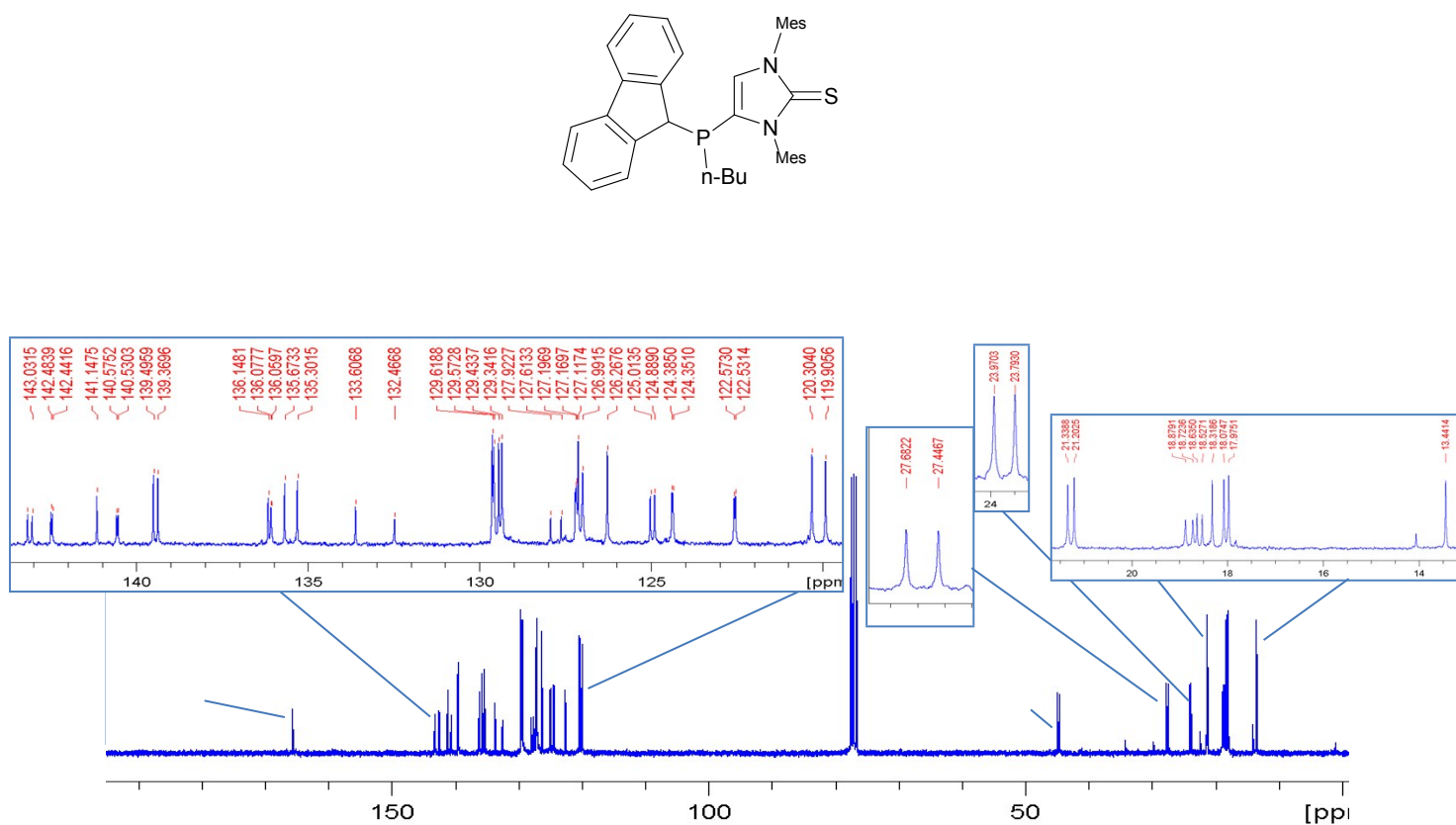


Figure S59: ^{31}P NMR spectrum of **11** in CDCl_3 (121.5 MHz, 25 °C)

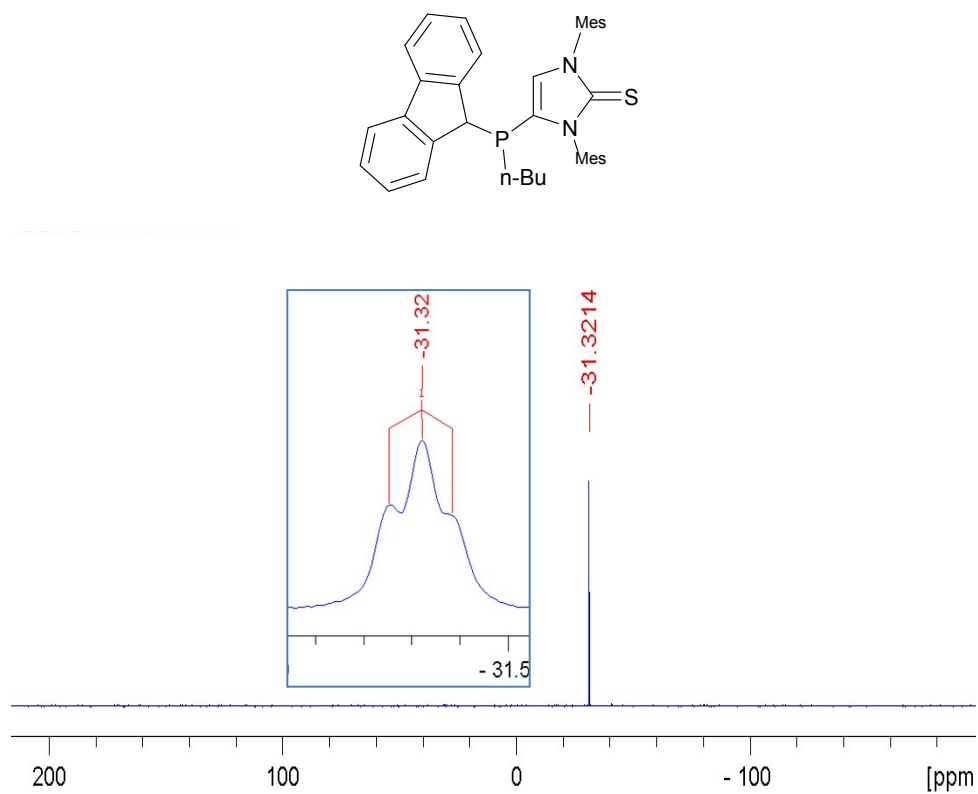


Figure 60: EI-MS spectrum of **11**.

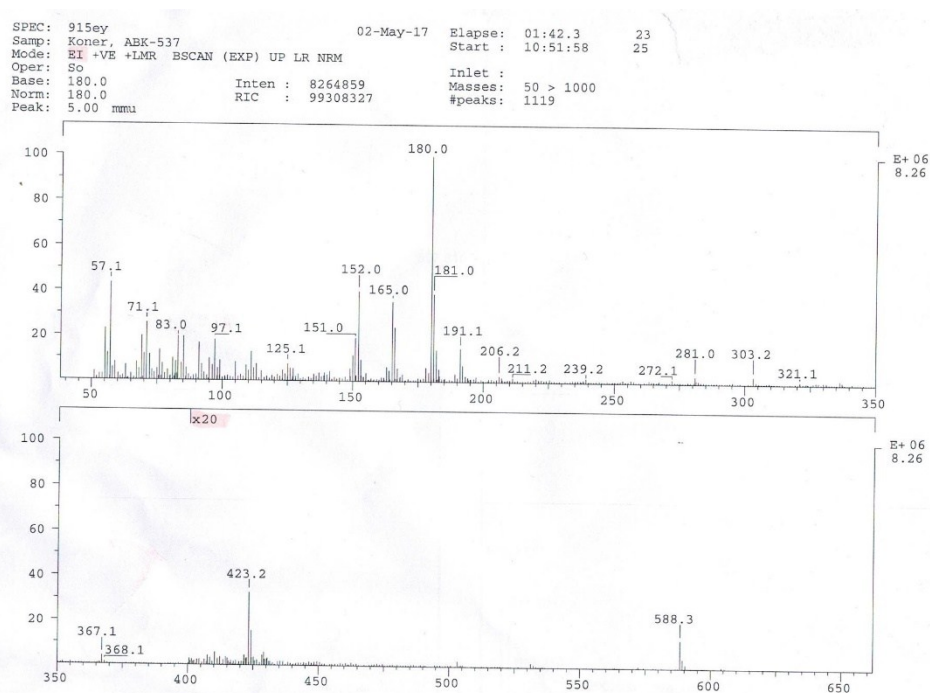


Figure 61: ESI-MS spectrum of **11**.

