Supporting Information

Cu-β-CD-Catalyzed C_{sp}-P Coupling of Alkynes with Dialkylphosphites and Phosphine oxides

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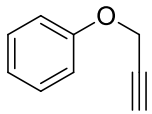
Table of Contents

Experimental Section

Procedure for the synthesis of alkynes (aryl propargyl ethers):

The aryl propargyl ethers **1** was obtained according to the literature report with slight modification [1]. Phenol derivative (3.5 mmol) was added to a mixture of K_2CO_3 (7.2 mmol) in dry DMF (22 mL) and the mixture was stirred for 15 min at 80 ^oC. Propargyl bromide (3.9 mmol) was added to the reaction mixture and the mixture was stirred for 12 h at 80 °C. After completion of the reaction (12 h), the mixture was diluted with NaOH (10%, 50 mL) and extracted with diethyl ether (3x50). The organic phase was washed with brine and dried over sodium sulfate.

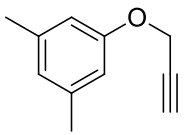
(Prop-2-yn-1-yloxy)benzene



Yellow viscous oil [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.30 (m, 2H), 7.09-6.99 (m, 3H), 4.74 (d, *J* = 2.4 Hz, 2H), 2.57 (t, *J* =2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 157.5, 129.5, 121,6, 114.9, 78.6, 75.5, 55.7.

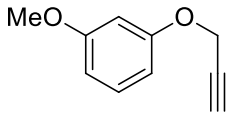
1,3-dimethyl-5-(prop-2-yn-1-yloxy)benzene



Yellow viscous oil [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.68 (s, 1H), 6.66 (s, 2H), 4.70 (d, *J* =2.4 Hz, 2H), 2.56 (t, *J* =2.4 Hz,1H), 2.35 (s, *J* =0.7 HZ, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 157.6, 139.3, 123.3, 112.6, 78.9, 75.2, 55.6, 21.4**.**

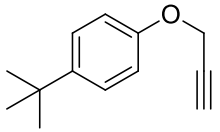
1-methoxy-3-(prop-2-yn-1-yloxy)benzene



Yellow viscous oil [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33-7.19 (m, 1H), 6.66-6.53 (m, 3H), 4.71 (d, *J* =2.4, 2H), 3.82 (s, 3H), 2.56 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 160.8, 158.8, 129.9, 107.0, 106.9, 101.4, 78.5, 75.5, 55.8, 55.3.

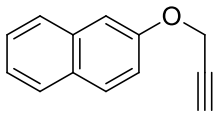
1-(tert-butyl)-4-(prop-2-yn-1-yloxy)benzene



Yellow viscous oil [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 7.8 Hz, 2H), 4.76 (d, *J* = 2.2 Hz, 2H), 2.62-2.58 (m, 1H), 1.46-1.40 (m, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 155.4, 144.3, 126.3, 114.4, 79.0, 75.4, 55.8, 34.2, 31.6.

2-(prop-2-yn-1-yloxy)naphthalene



Yellow viscous oil [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91-7.80 (m, 3H), 7.60-7.40 (m, 2H), 7.32 - 7.25 (m, 2H), 4.87 (d, *J* = 2.4 Hz, 2H), 2.65 (t, *J* = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 155.5, 134.4, 129.7, 129.4, 127.8, 127.0, 126.6, 124.1, 118.8, 107.5, 78.6,75.8, 55.9.

References:

[1] S. Keskin, M. Balci, *Org. Lett*. **2015**, *17*, 964–967.
[2] Shinde, J., Suresh, S., Kavala, V., & Yao, C. *Chem. Commun.* **2024**, 60, 3790-3793.
[3] Kaboudin, B.; Abedi, Y.; Yokomatsu, T. *Eur. J. Org. Chem.* **2011**, *2011*, 6656-6662.
[4] Liu, L. L., Wu, Y., Wang, Z., Zhu, J., & Zhao, Y. *J. Org. Chem.* **2014**, *79*, 6816-6822.

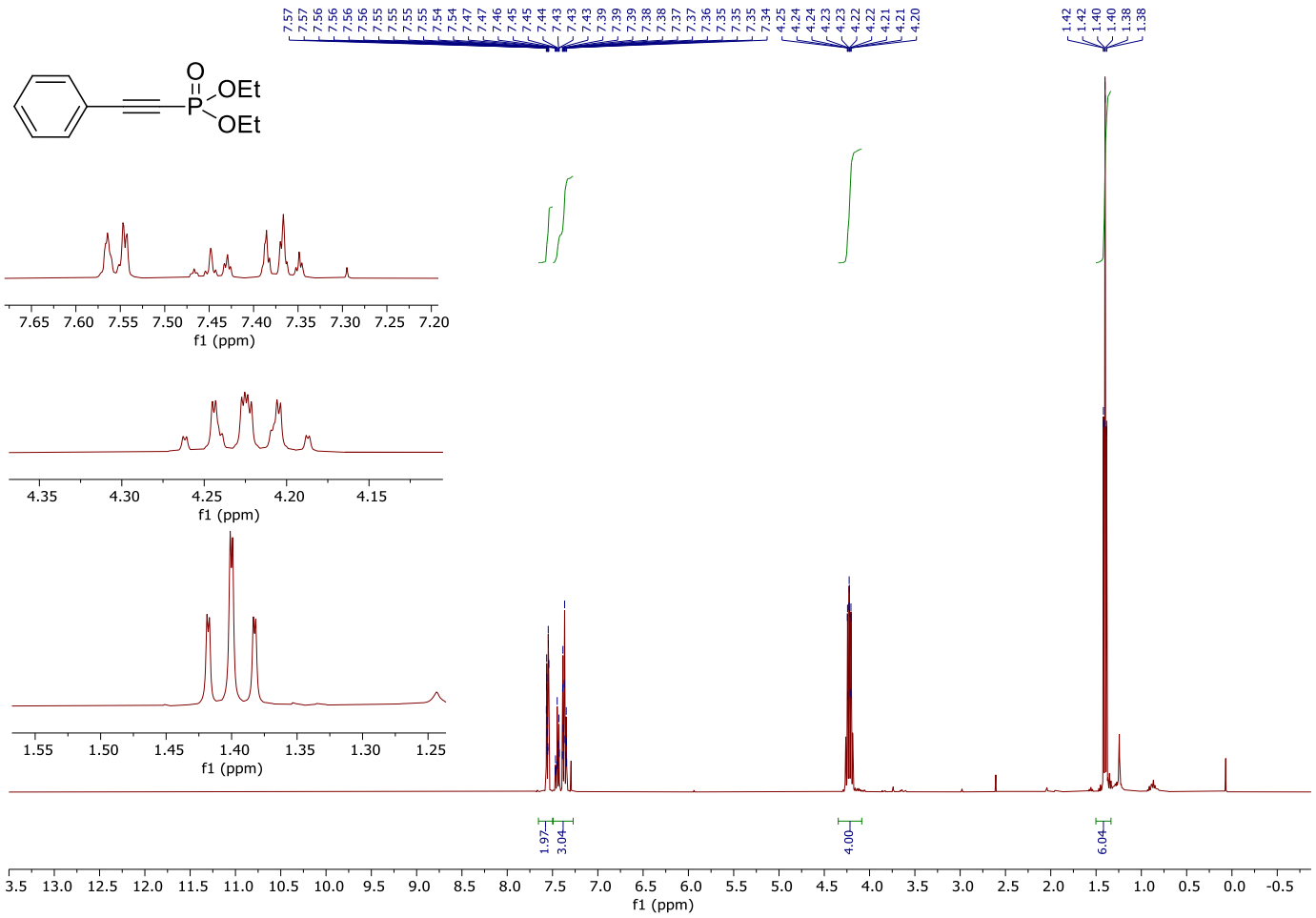


Figure S1: ^{1}H NMR Spectra of 3a

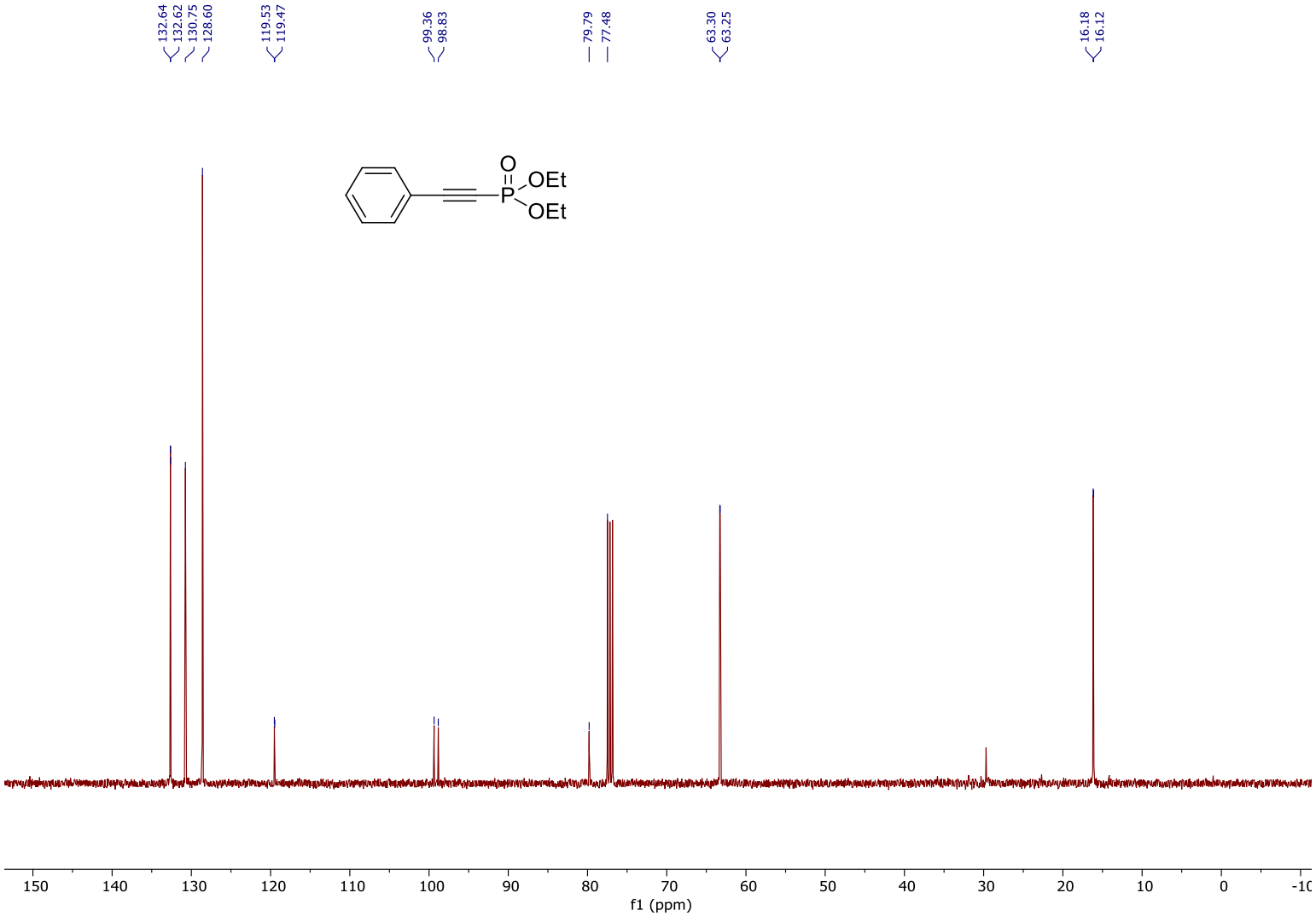


Figure S2: ^{13}C NMR Spectra of 3a

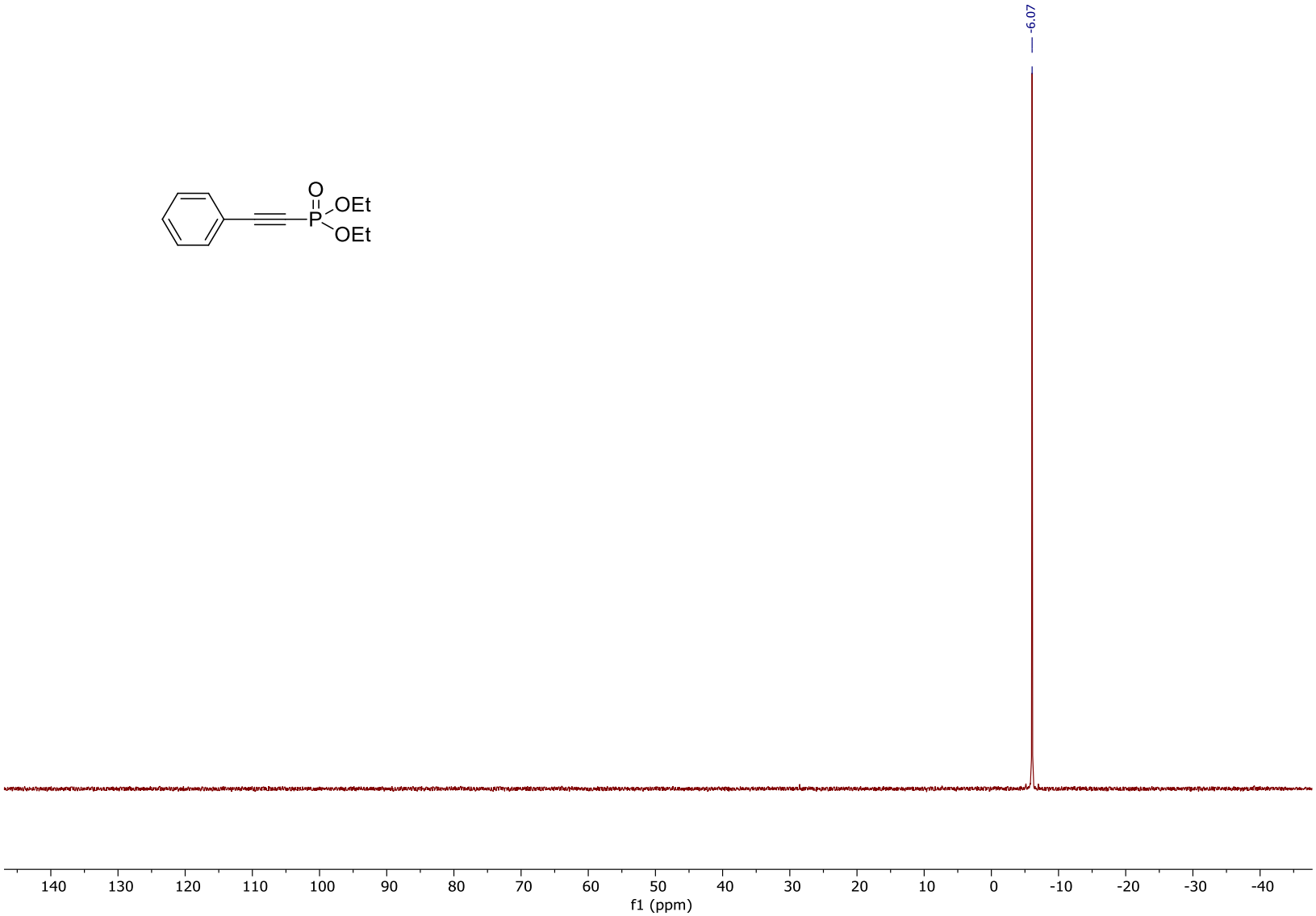


Figure S3: ^{31}P NMR Spectra of 3a

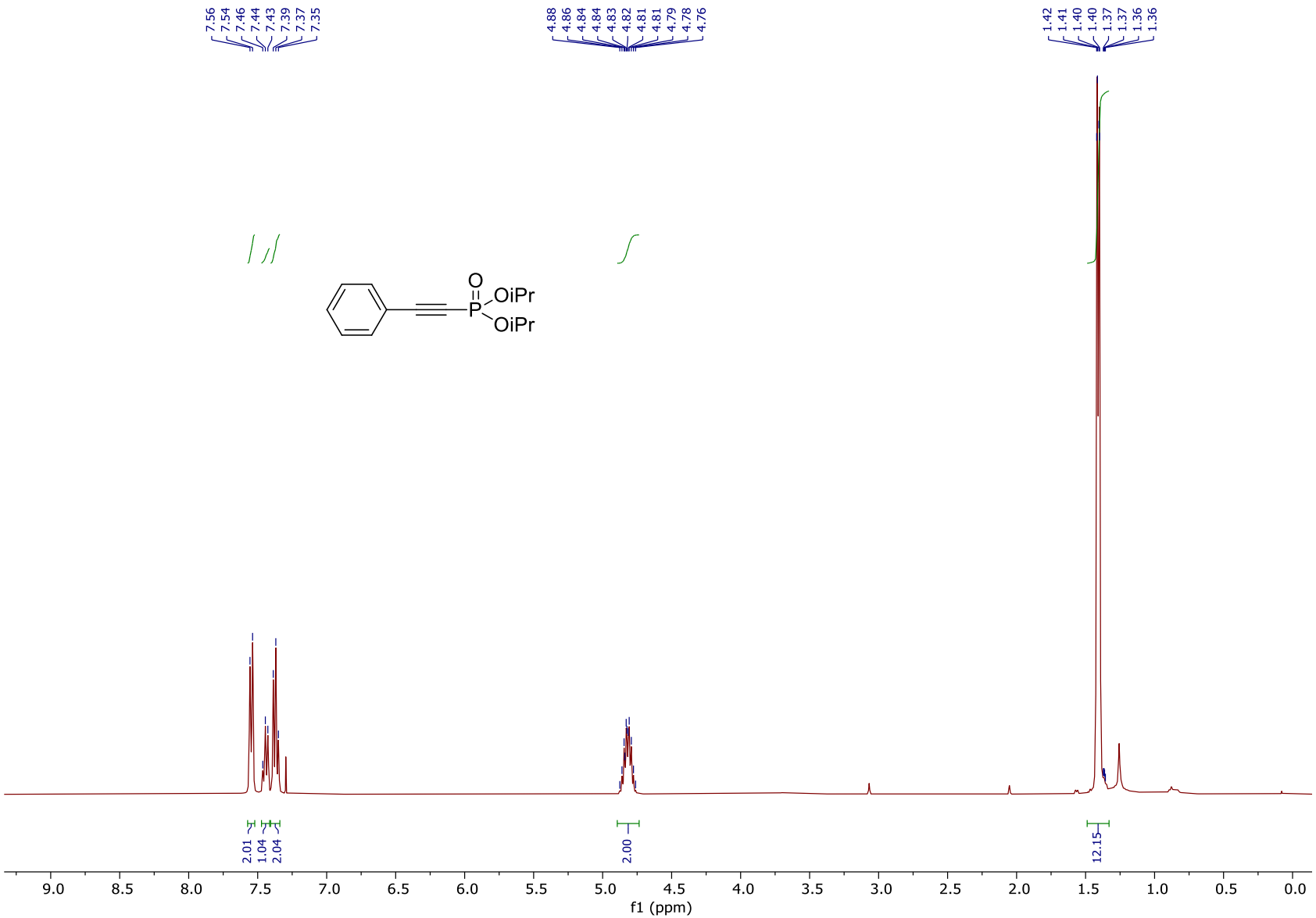


Figure S4: ^{1}H NMR Spectra of 3b

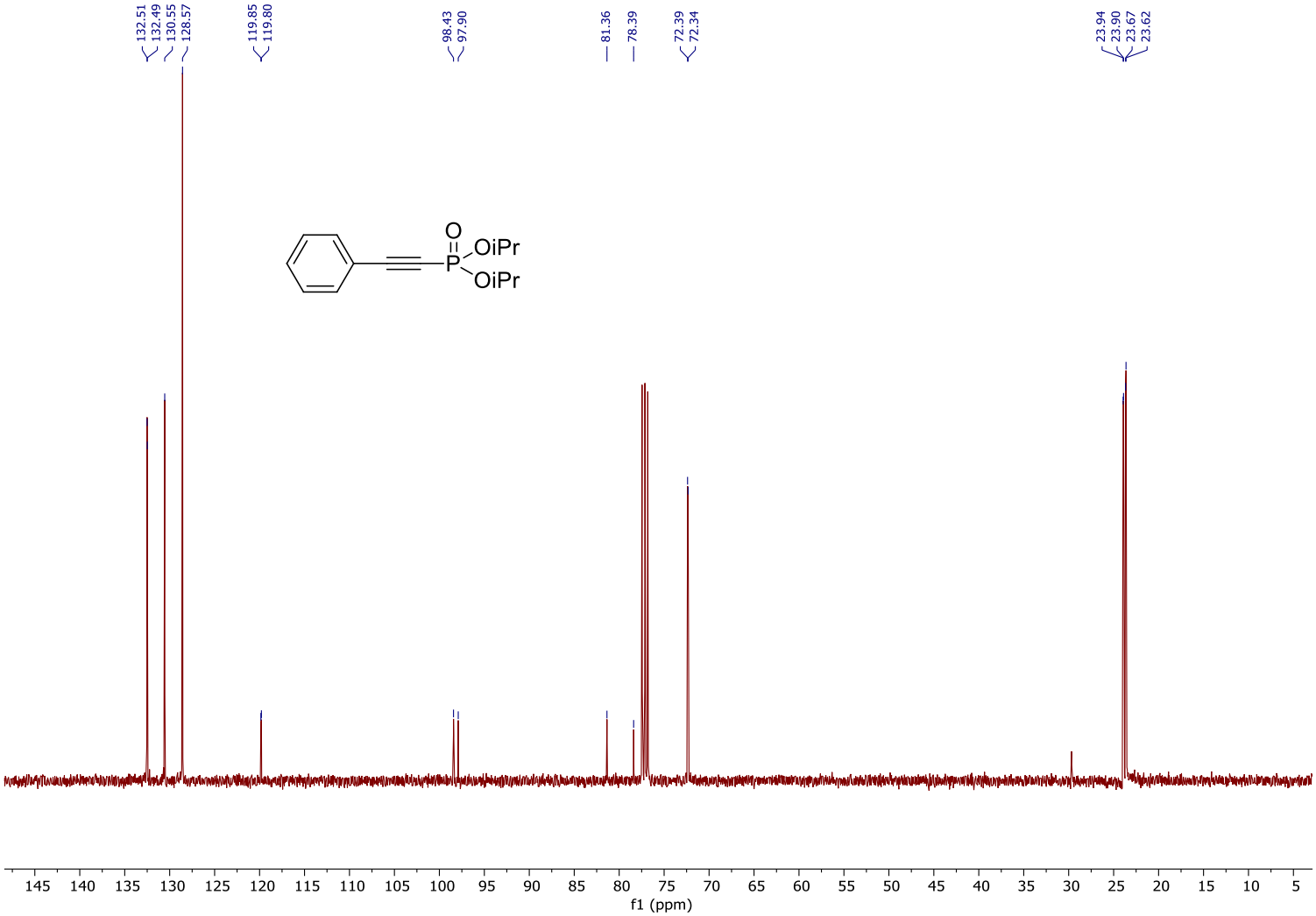


Figure S5: ^{13}C NMR Spectra of 3b

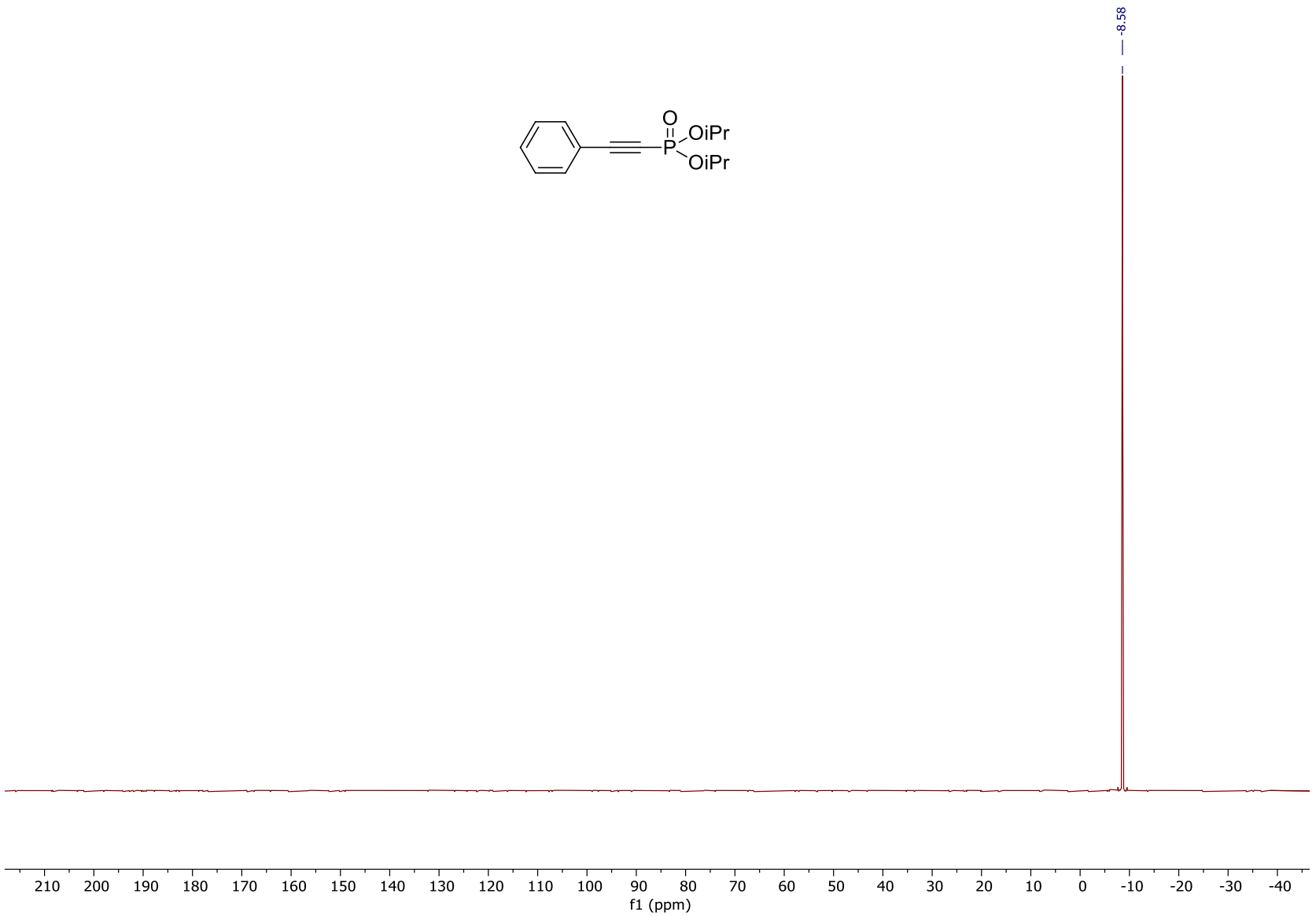


Figure S6: ^{31}P NMR Spectra of 3b

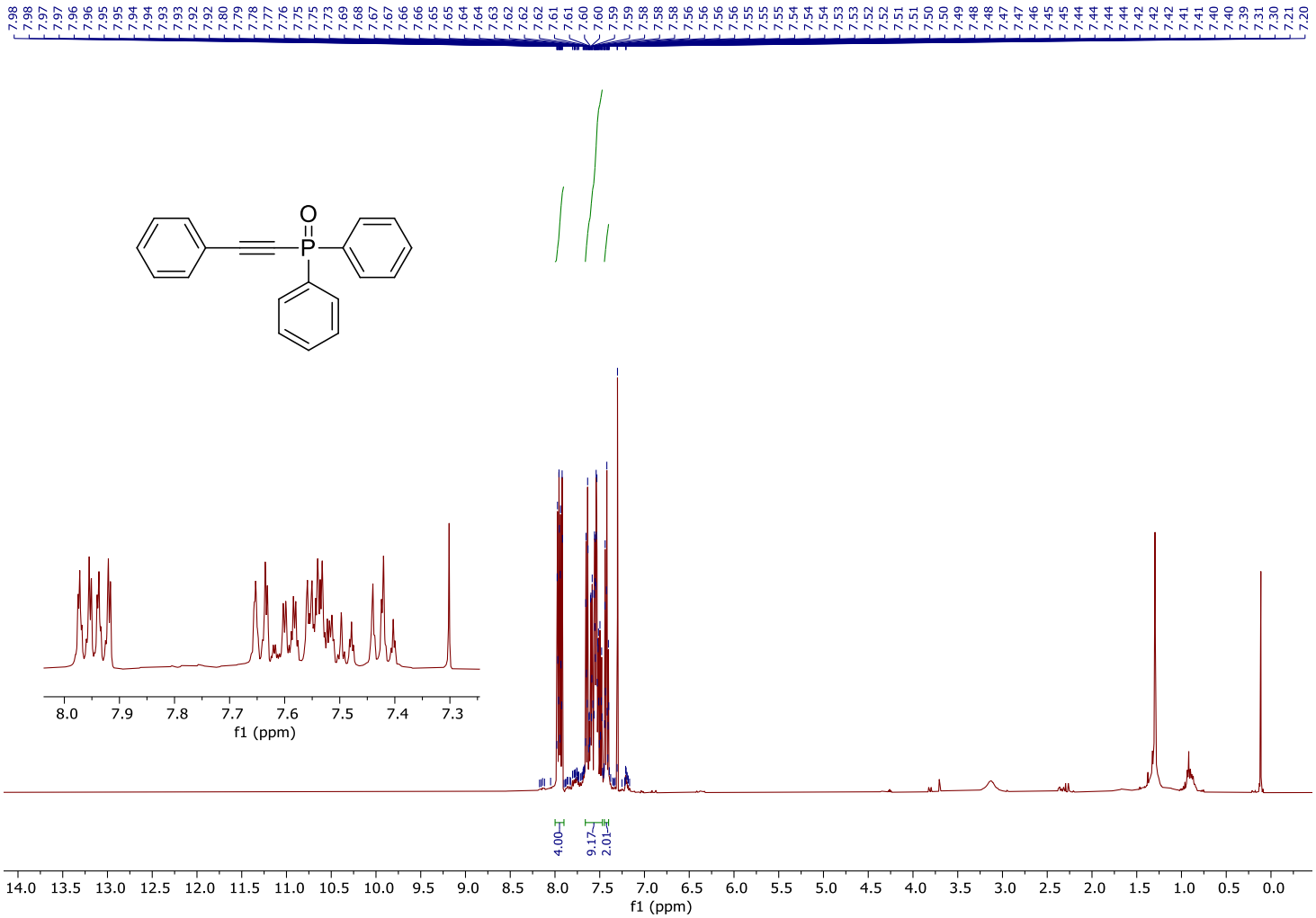


Figure S7: ^{1}H NMR Spectra of 3c

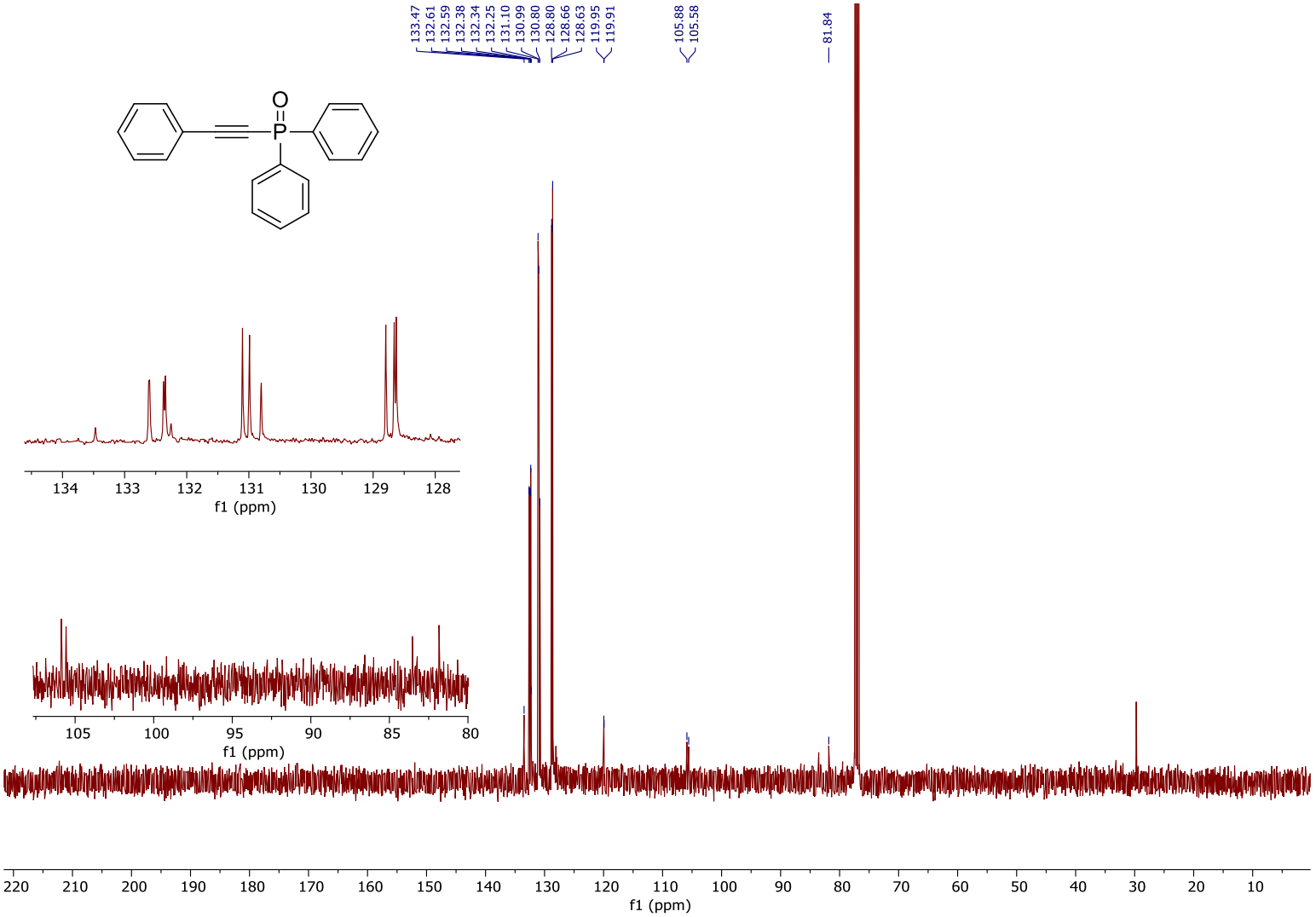


Figure S8: ^{13}C NMR Spectra of 3c

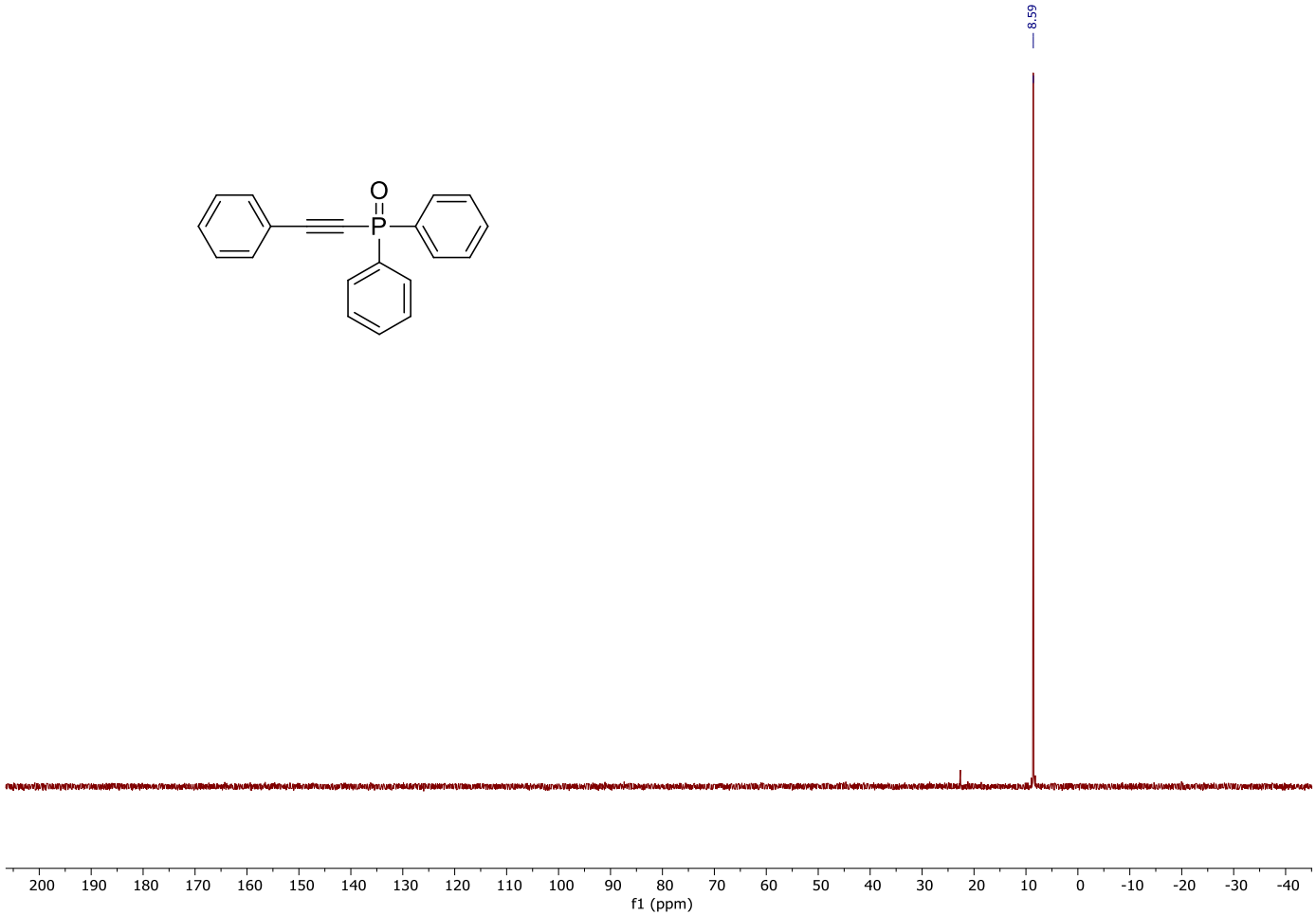


Figure S9: ^{31}P NMR Spectra of 3c

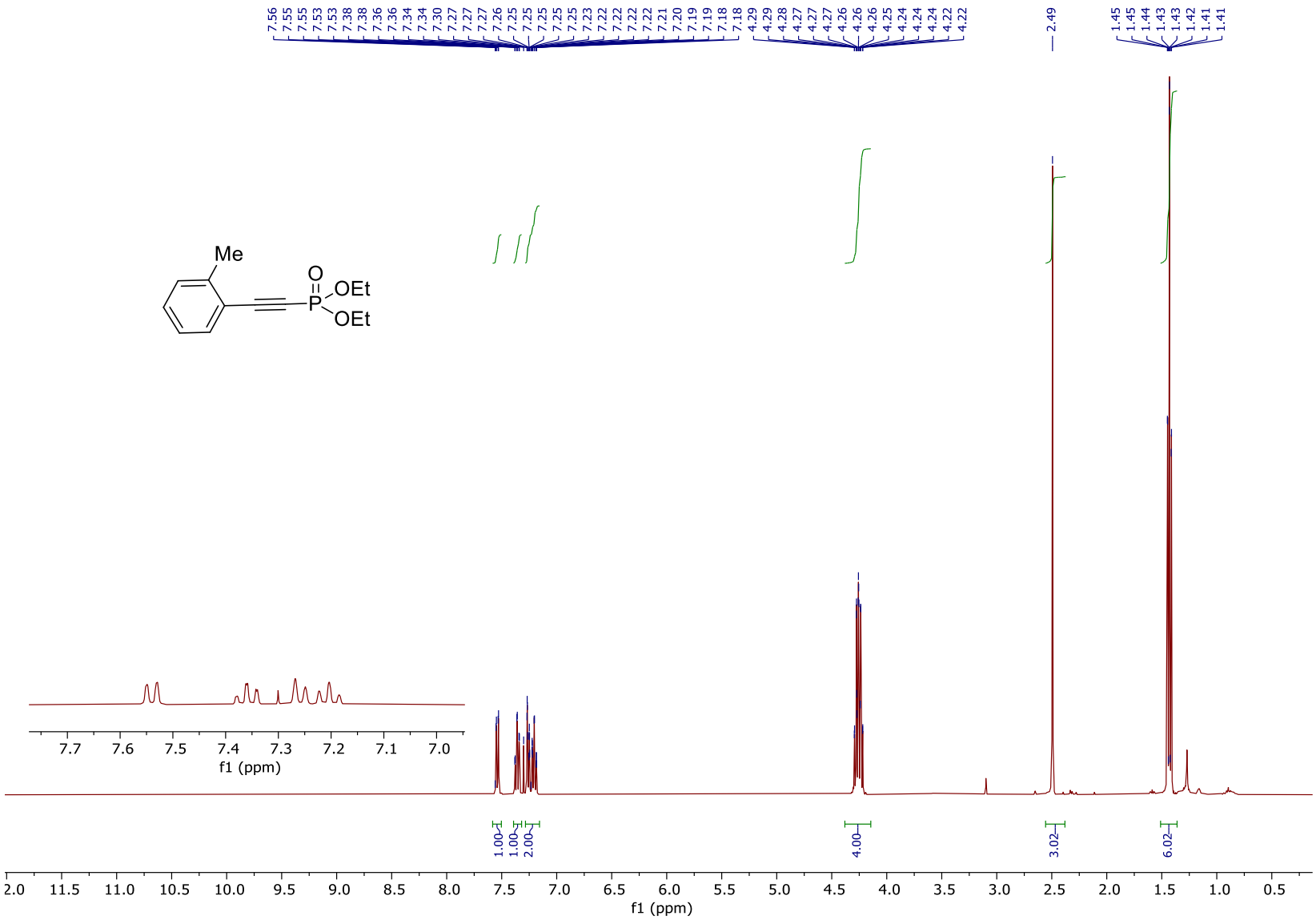


Figure S10: ^{1}H NMR Spectra of 3e

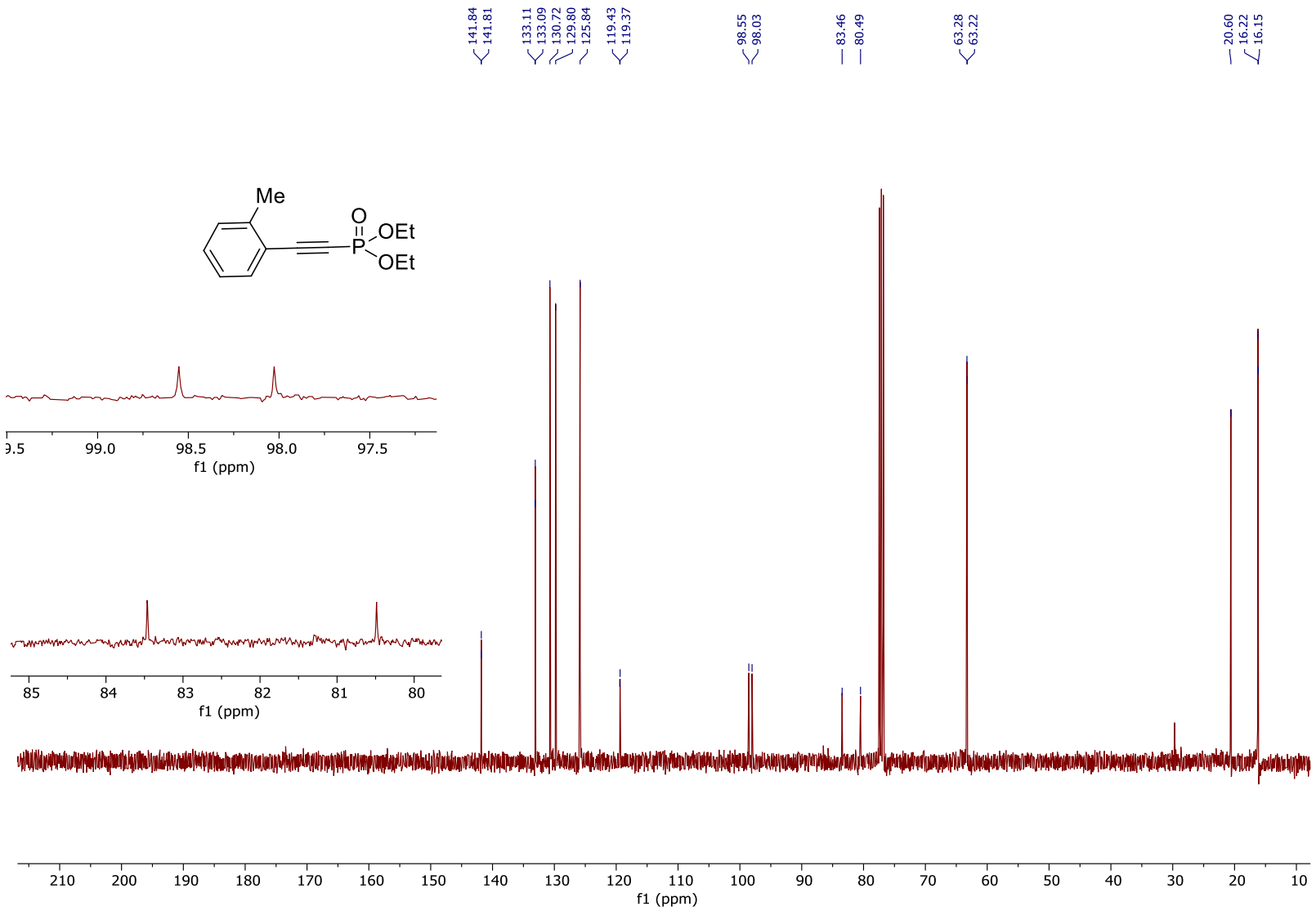


Figure S11: ^{13}C NMR Spectra of 3e

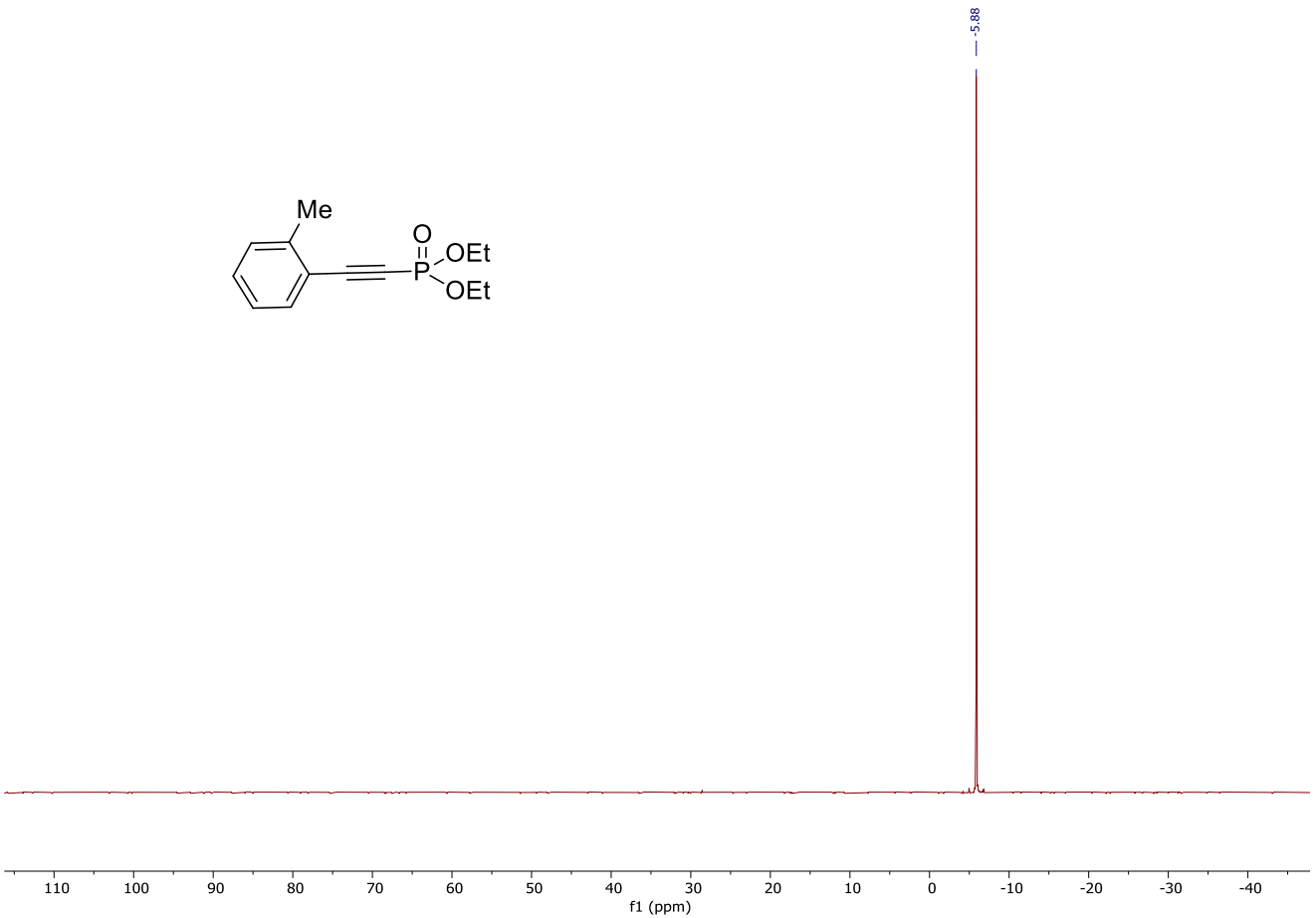


Figure S12: ^{31}P NMR Spectra of 3e

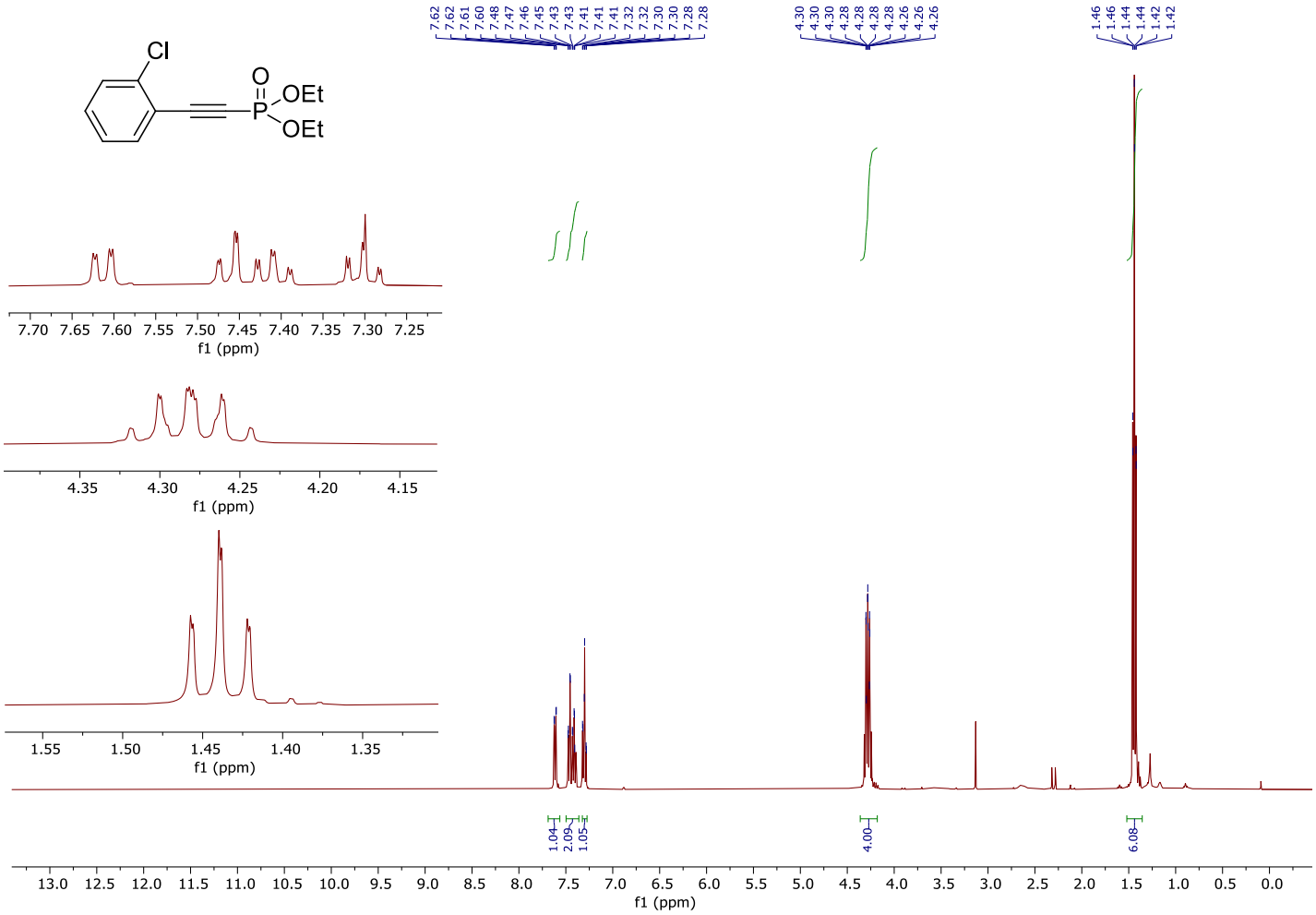


Figure S13: ^{1}H NMR Spectra of 3f

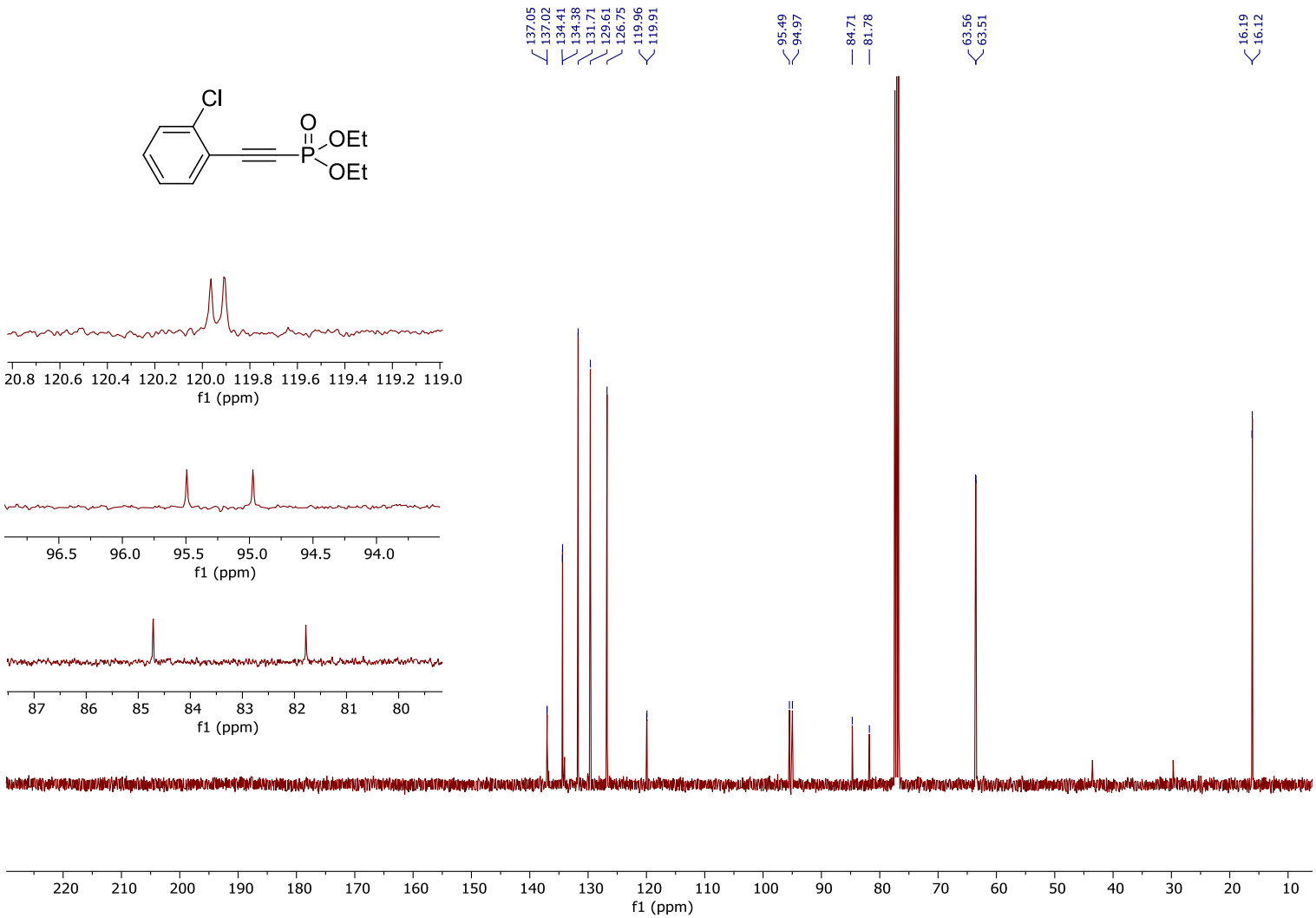


Figure S14: ^{13}C NMR Spectra of 3f

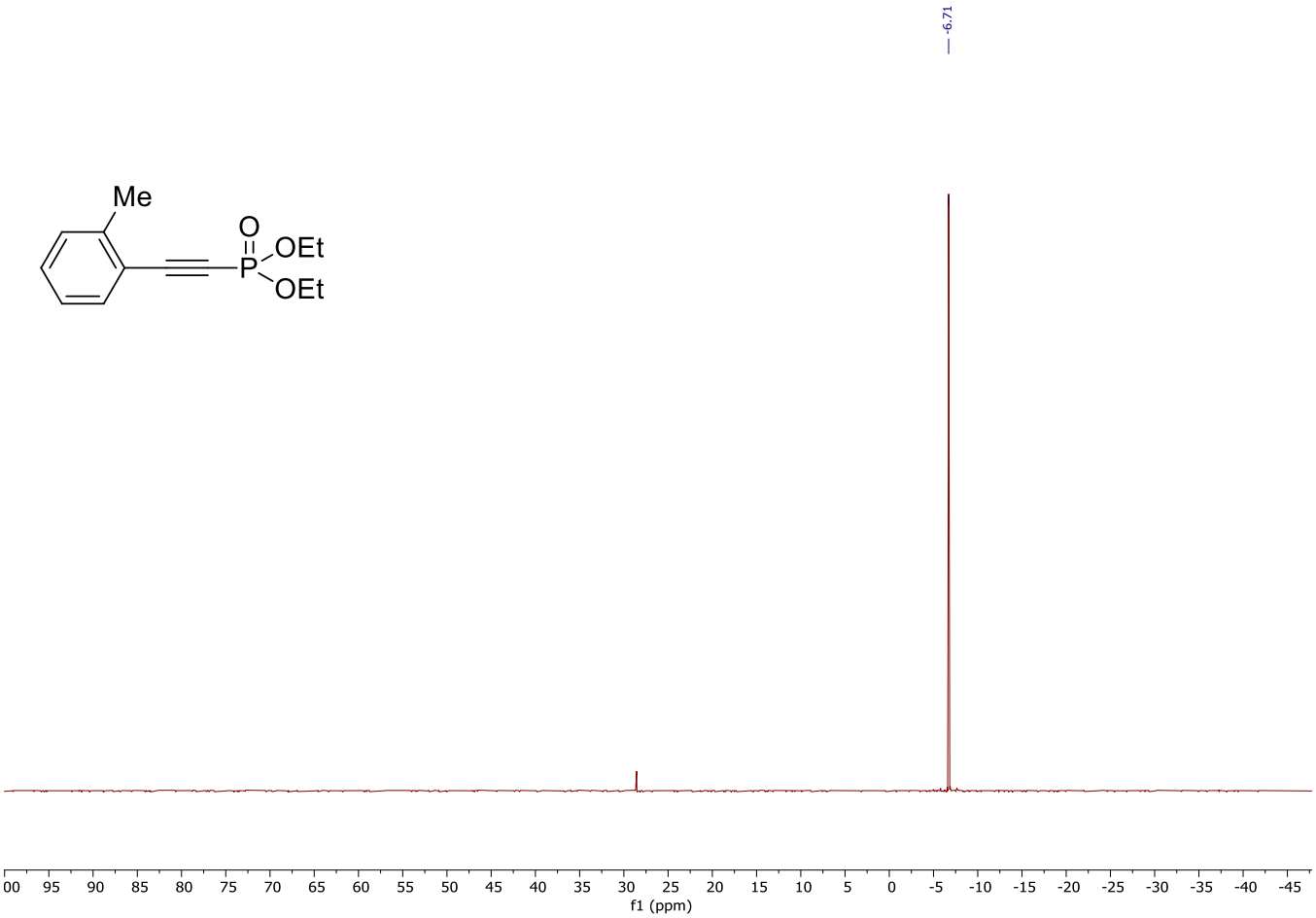


Figure S15: ^{31}P NMR Spectra of 3f

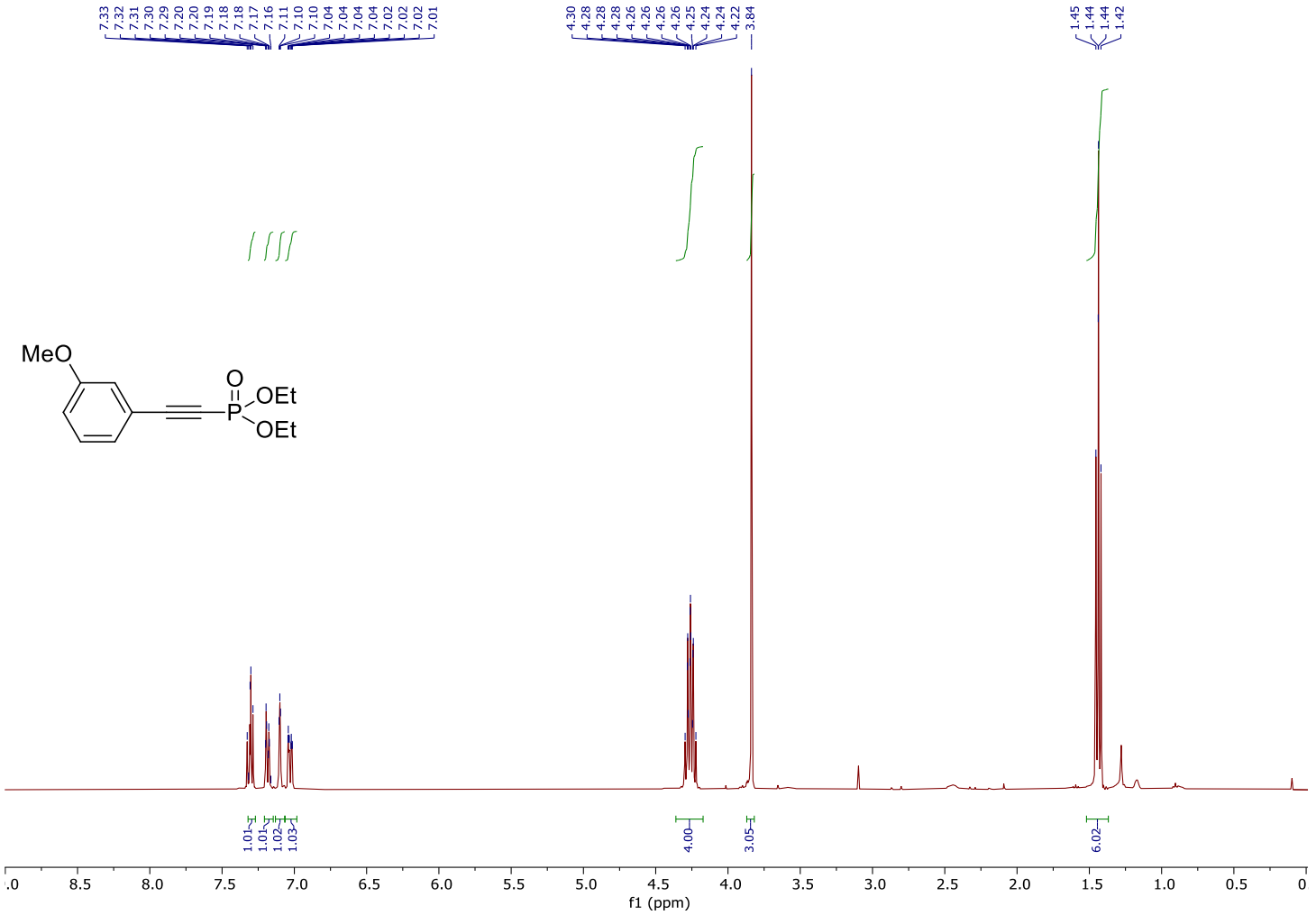


Figure S16: ^{1}H NMR Spectra of 3g

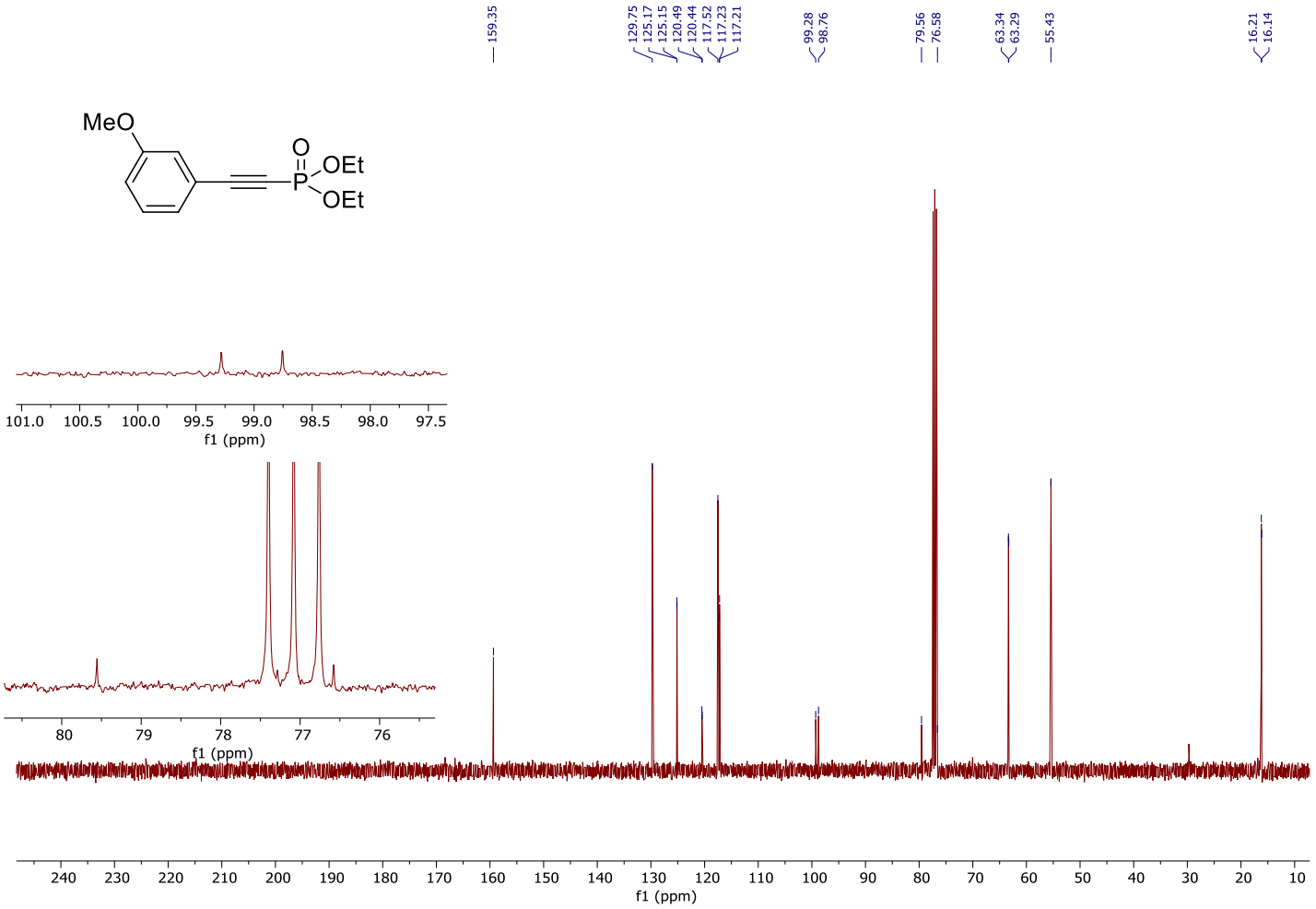


Figure S17: ^{13}C NMR Spectra of 3g

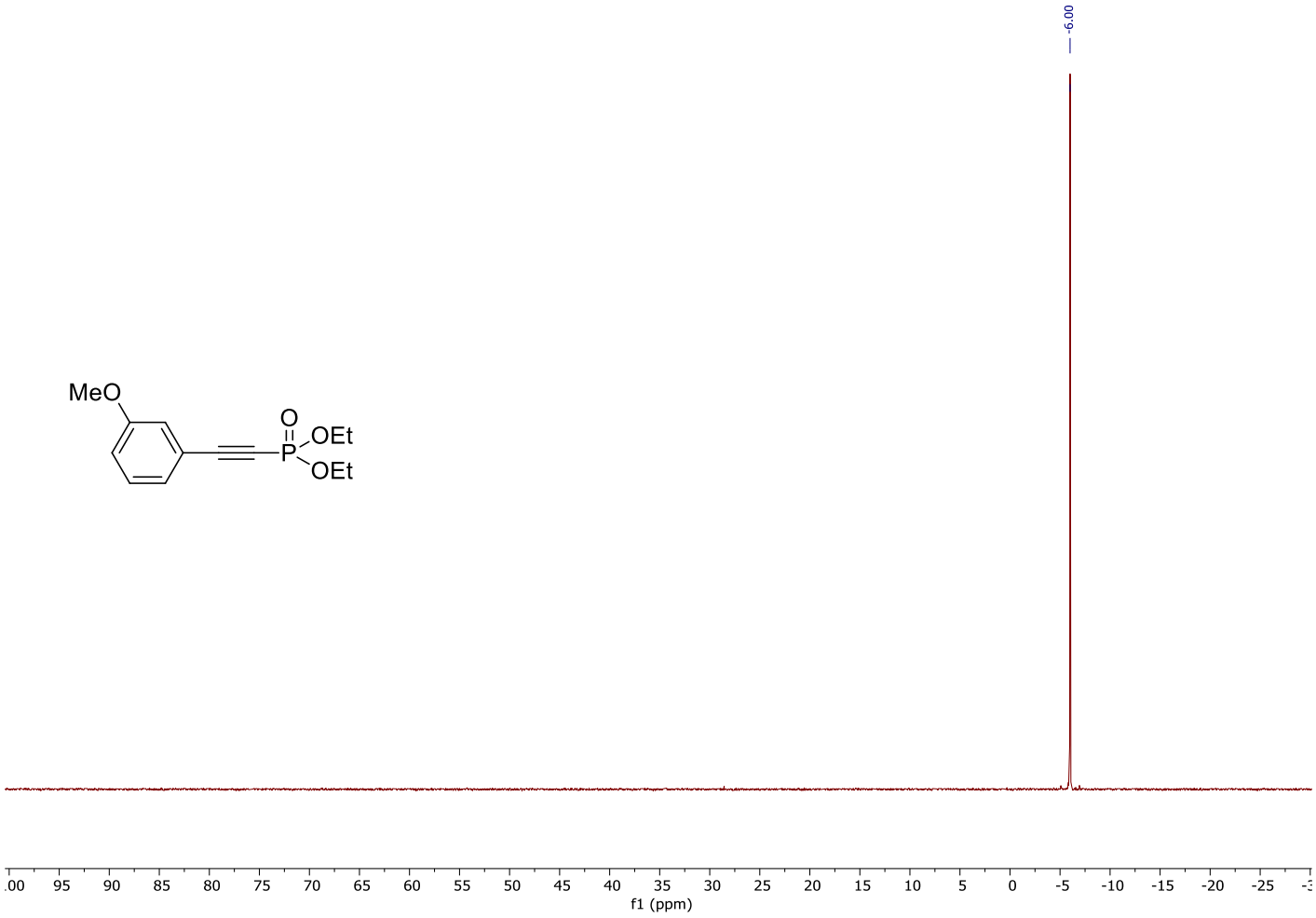


Figure S18: ^{31}P NMR Spectra of 3g

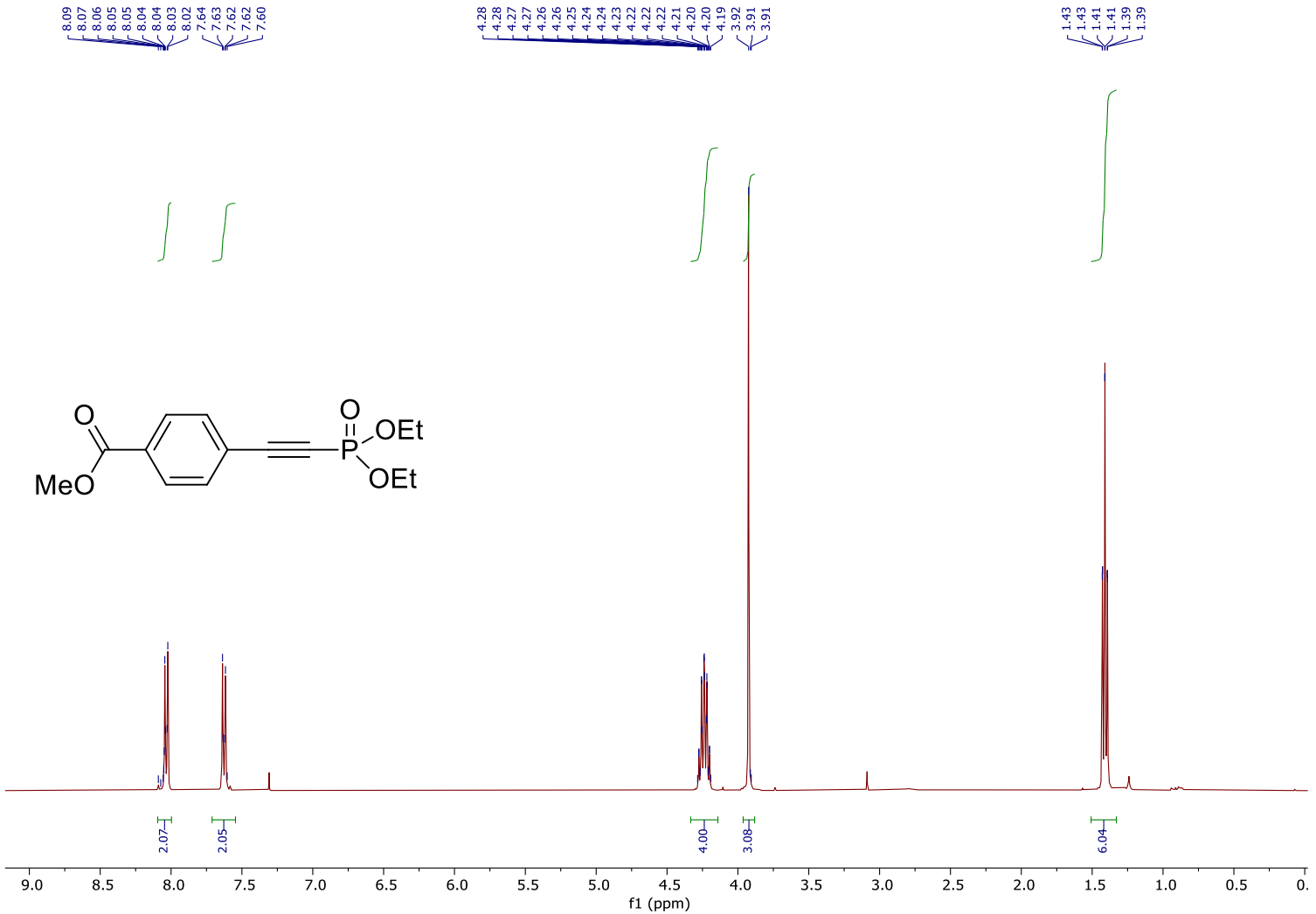


Figure S19: ^{1}H NMR Spectra of 3h

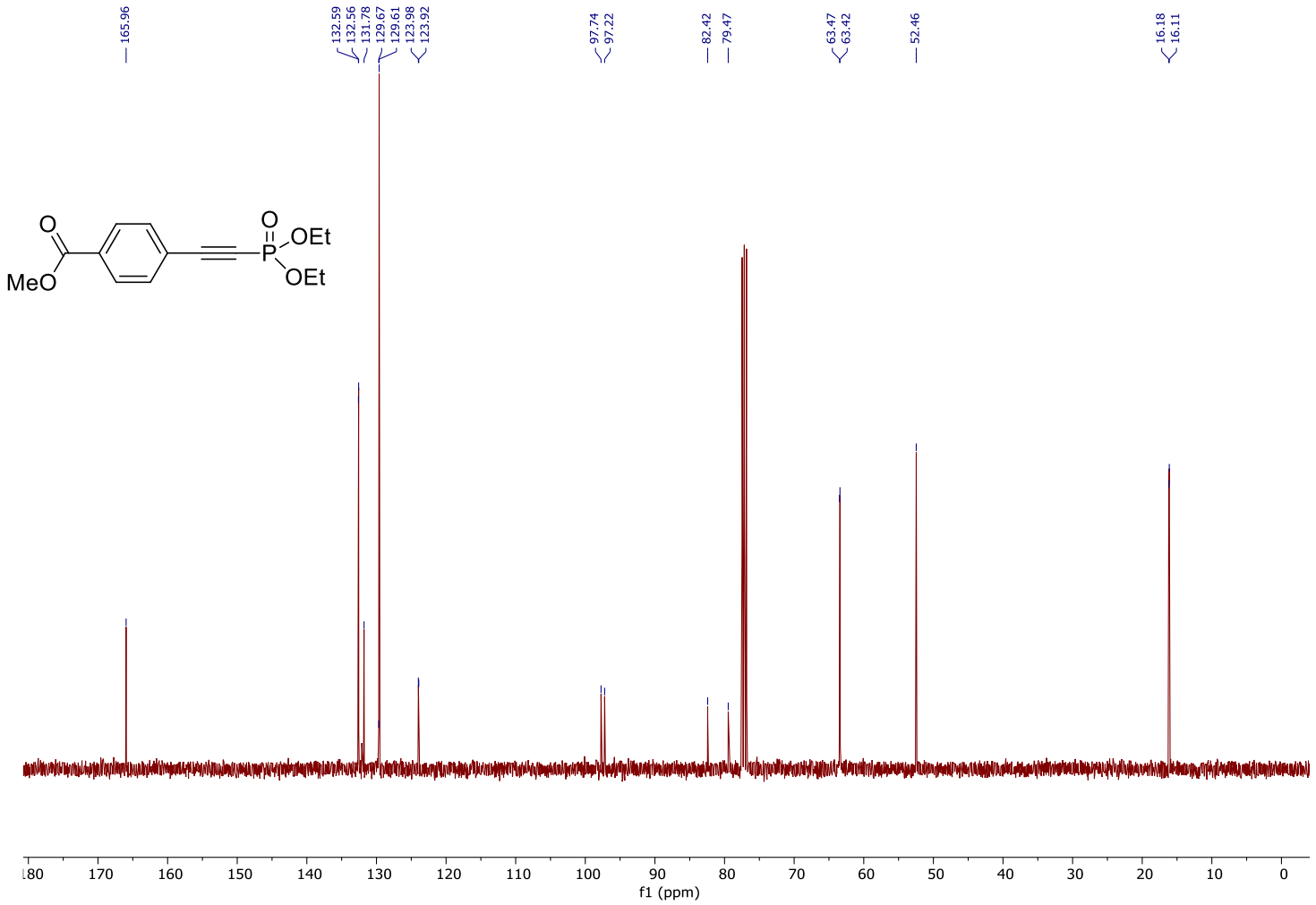


Figure S20: ^{13}C NMR Spectra of 3h

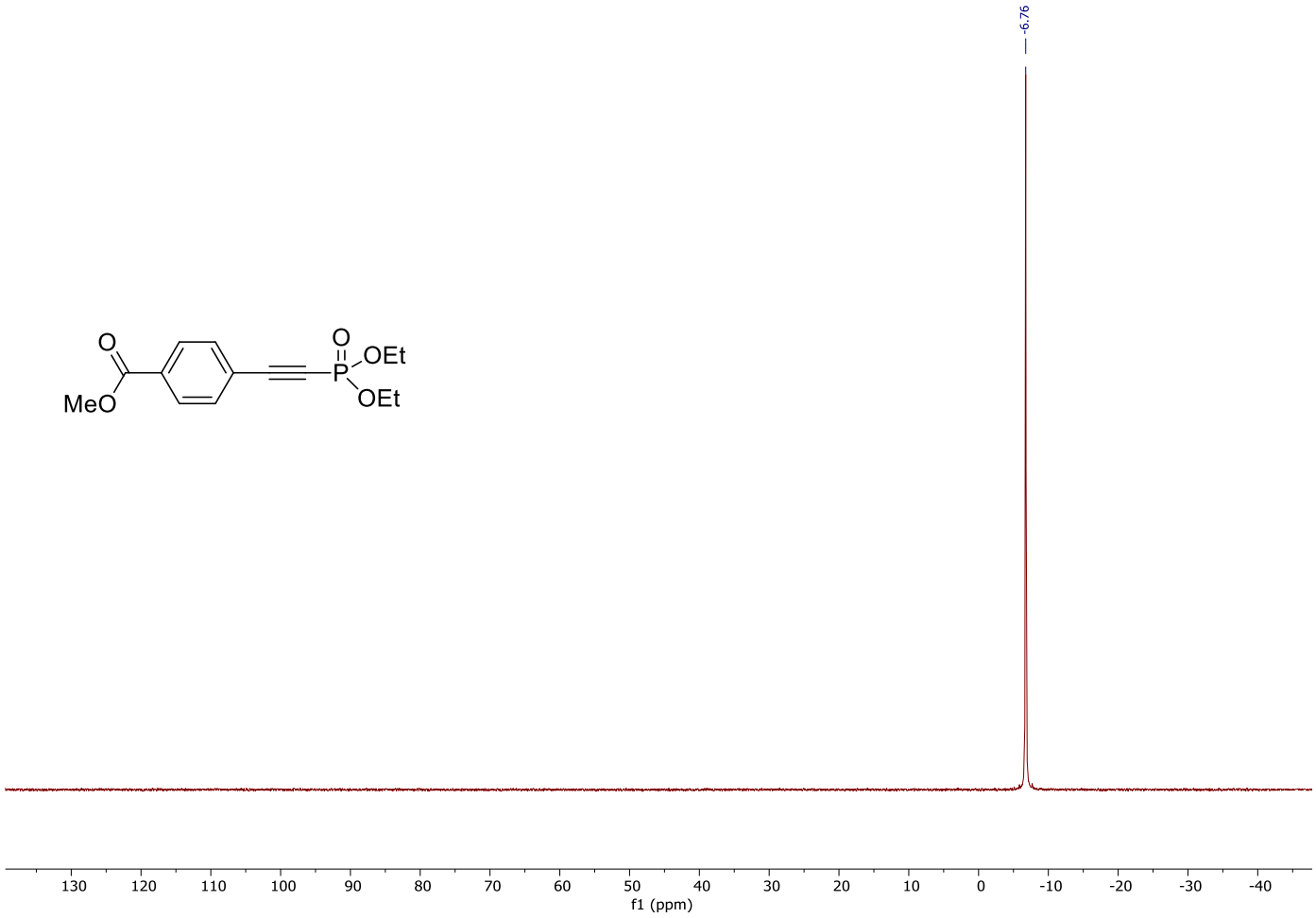


Figure S21: ^{31}P NMR Spectra of 3h

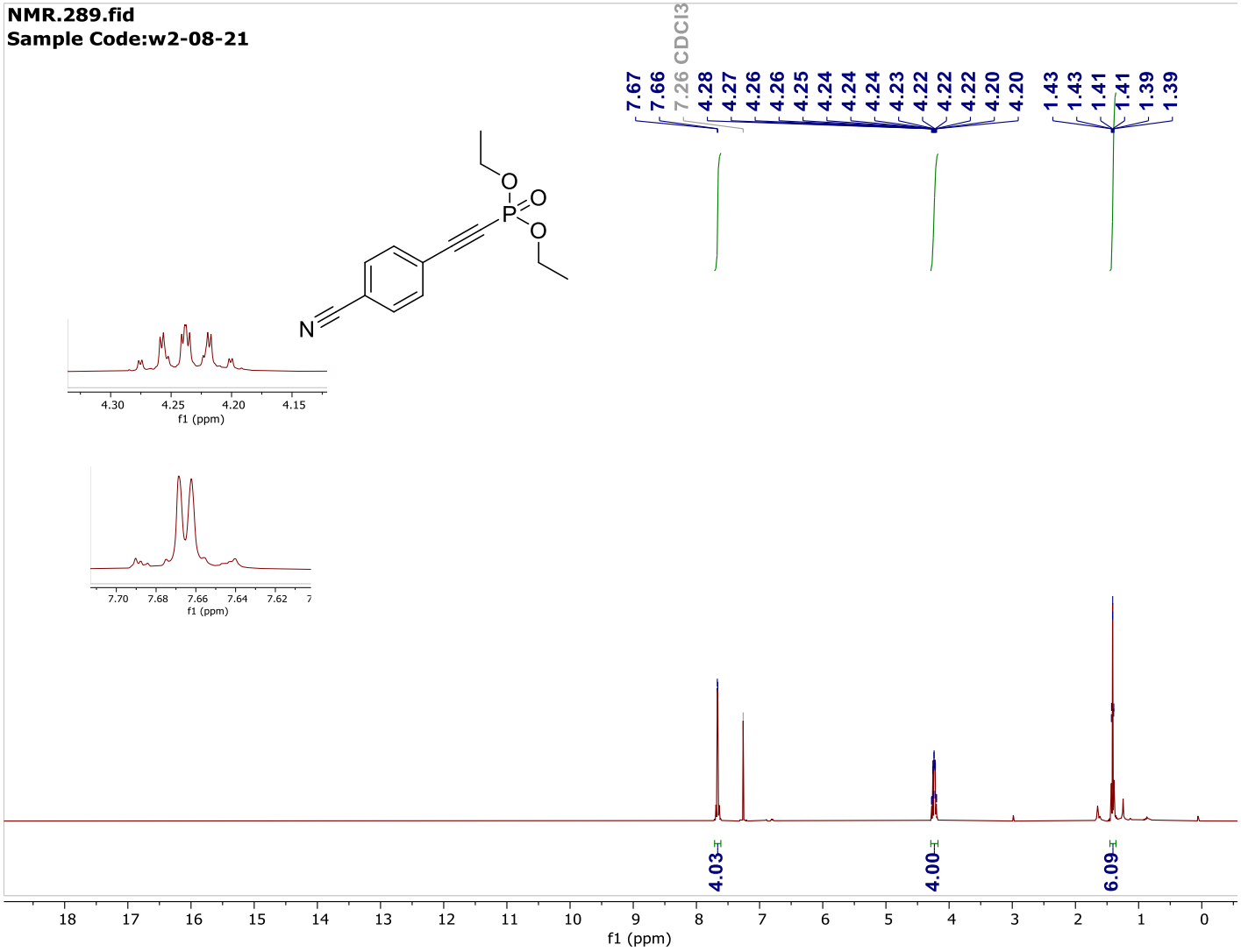


Figure S22: ^{1}H NMR Spectra of 3i

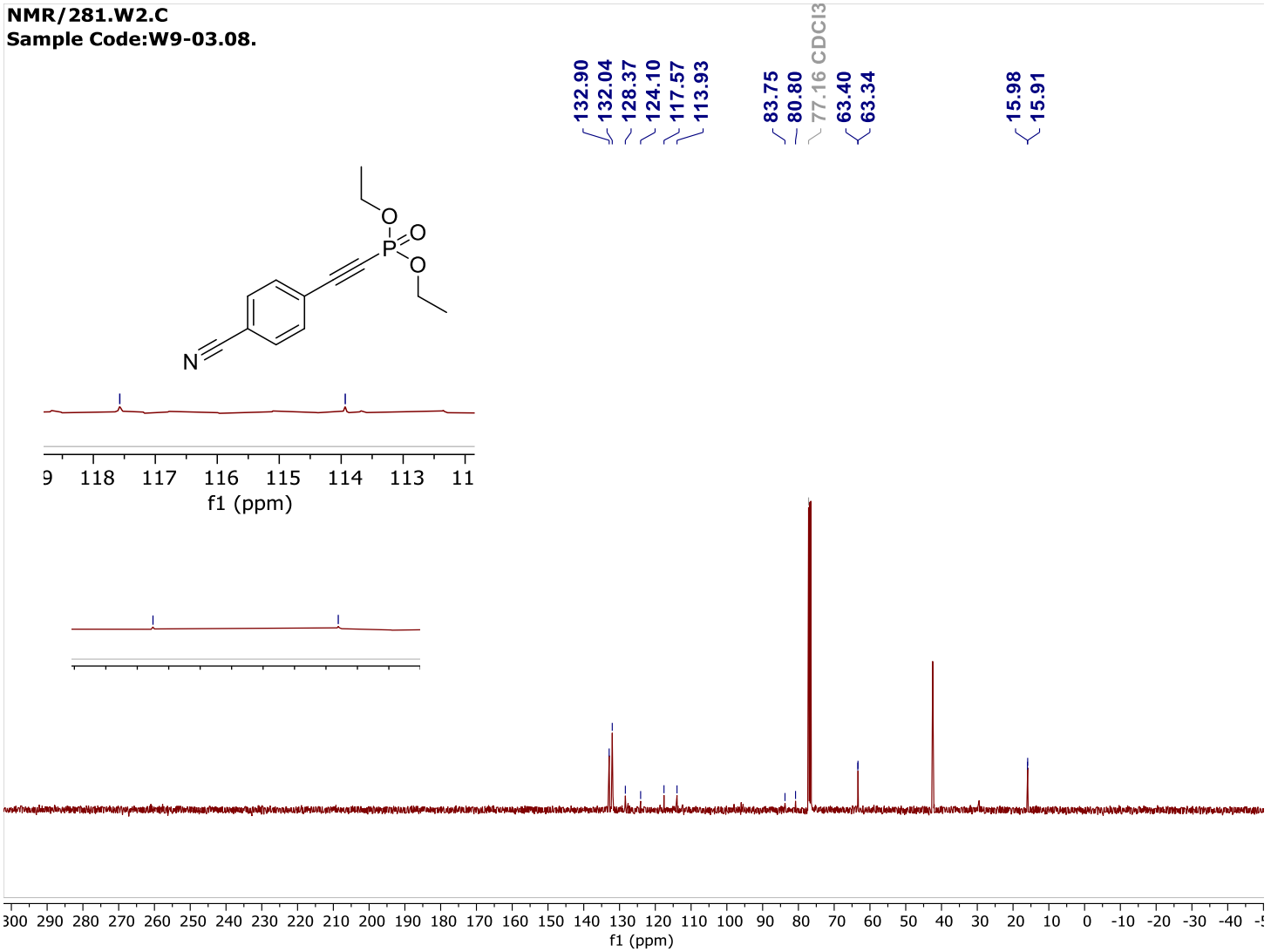


Figure S23: ^{13}C NMR Spectra of 3i

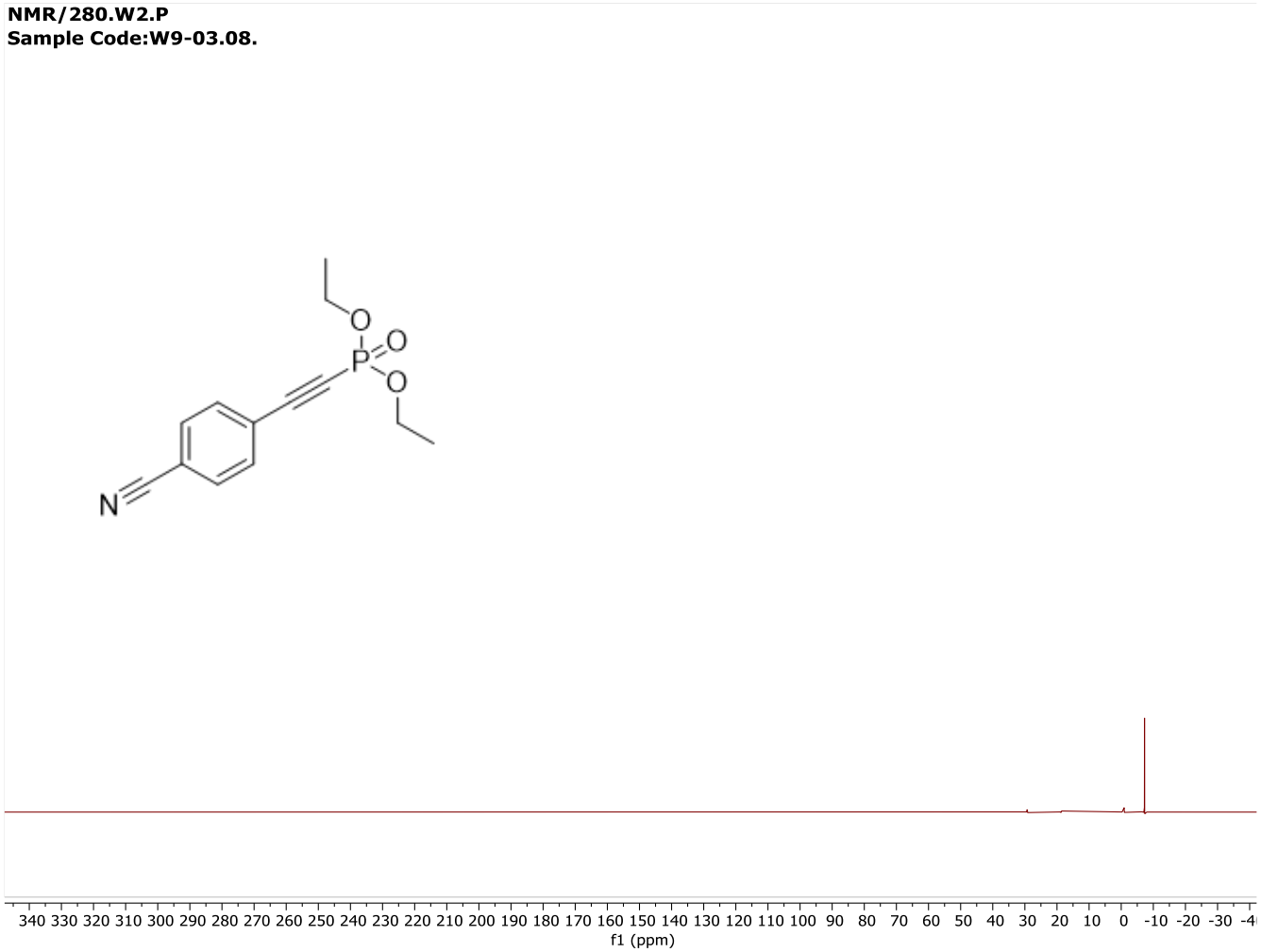


Figure S24: ^{31}P NMR Spectra of 3i

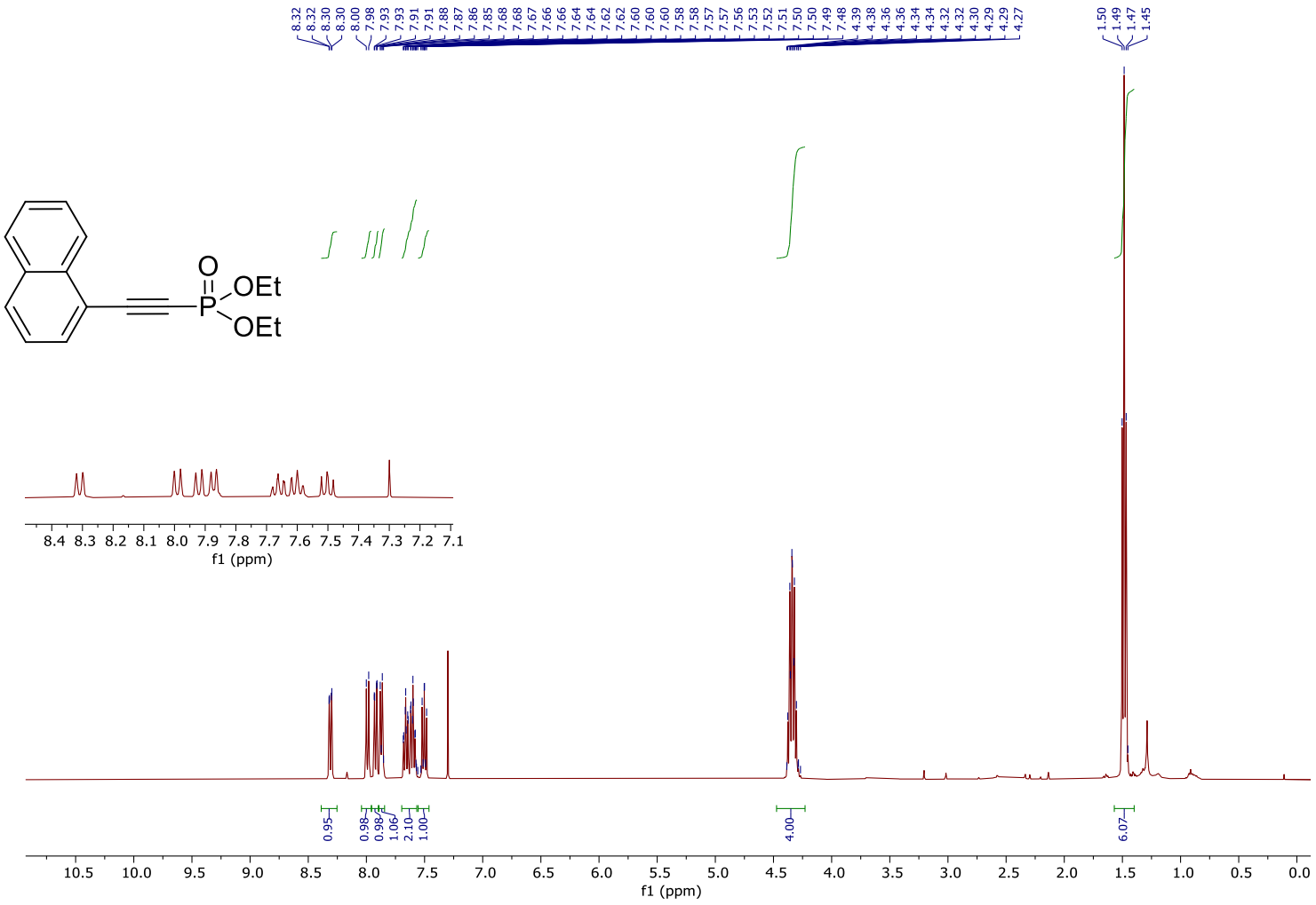


Figure S25: ^{1}H NMR Spectra of 3j

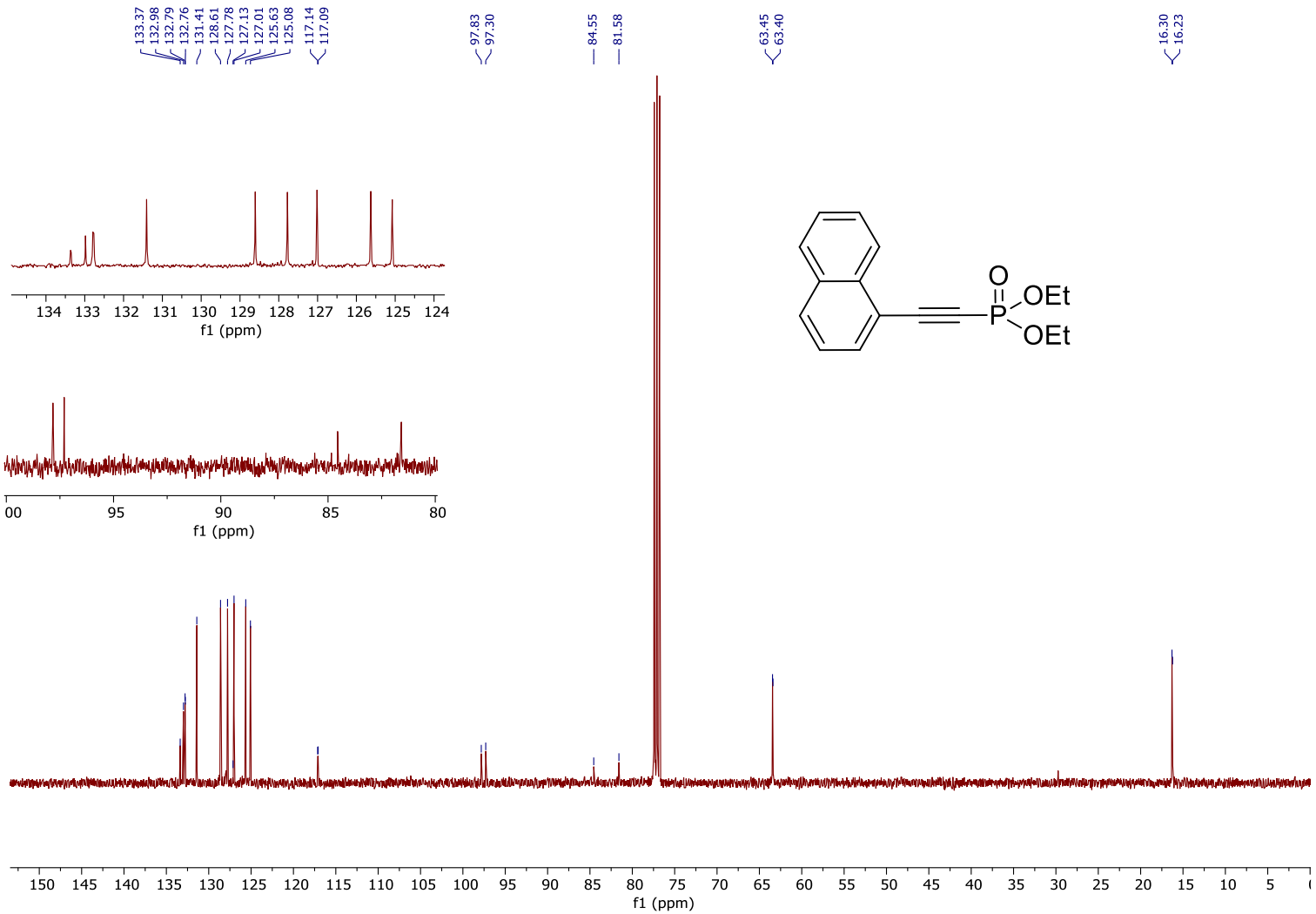


Figure S26: ^{13}C NMR Spectra of 3j

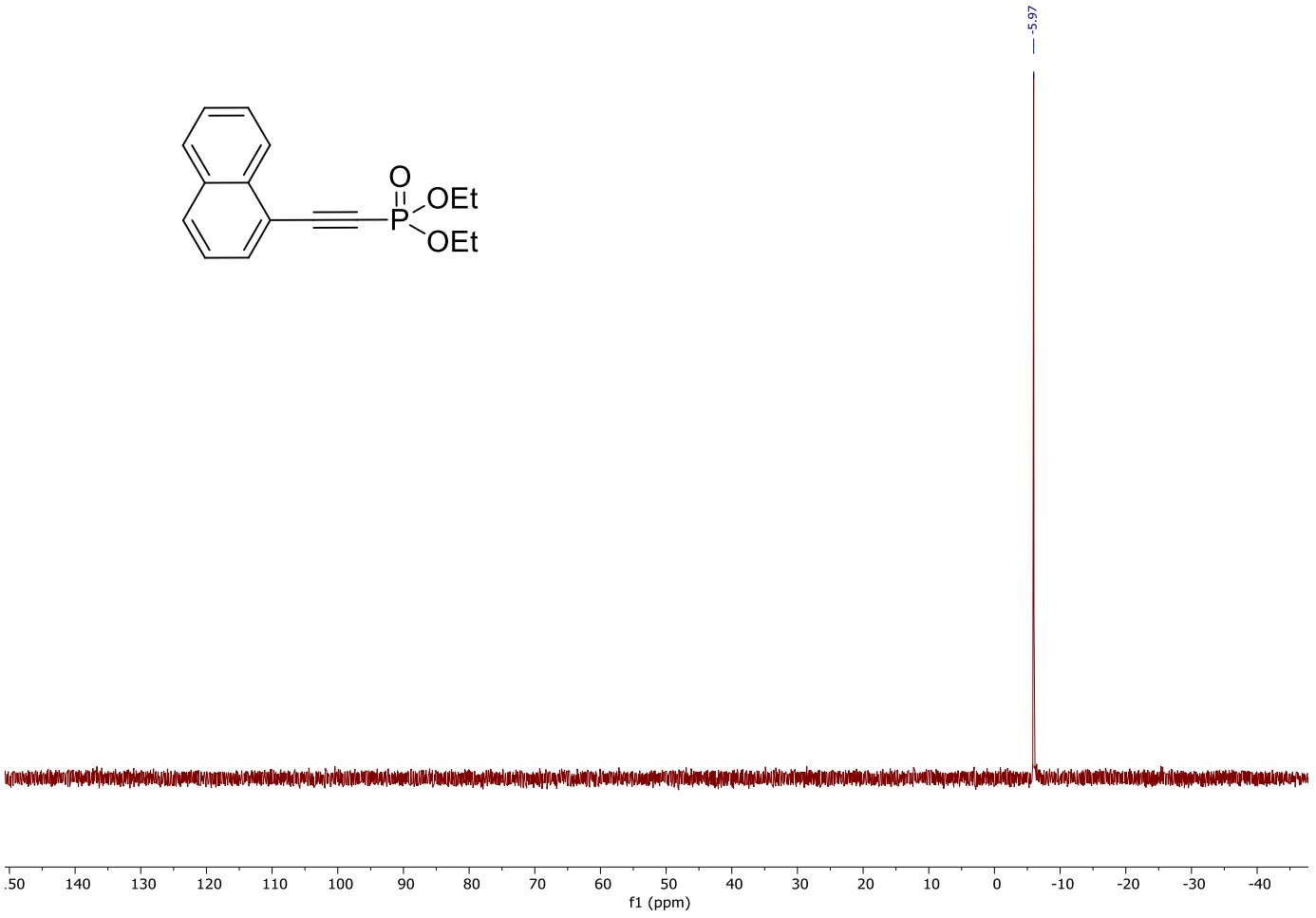


Figure S27: ^{31}P NMR Spectra of 3j

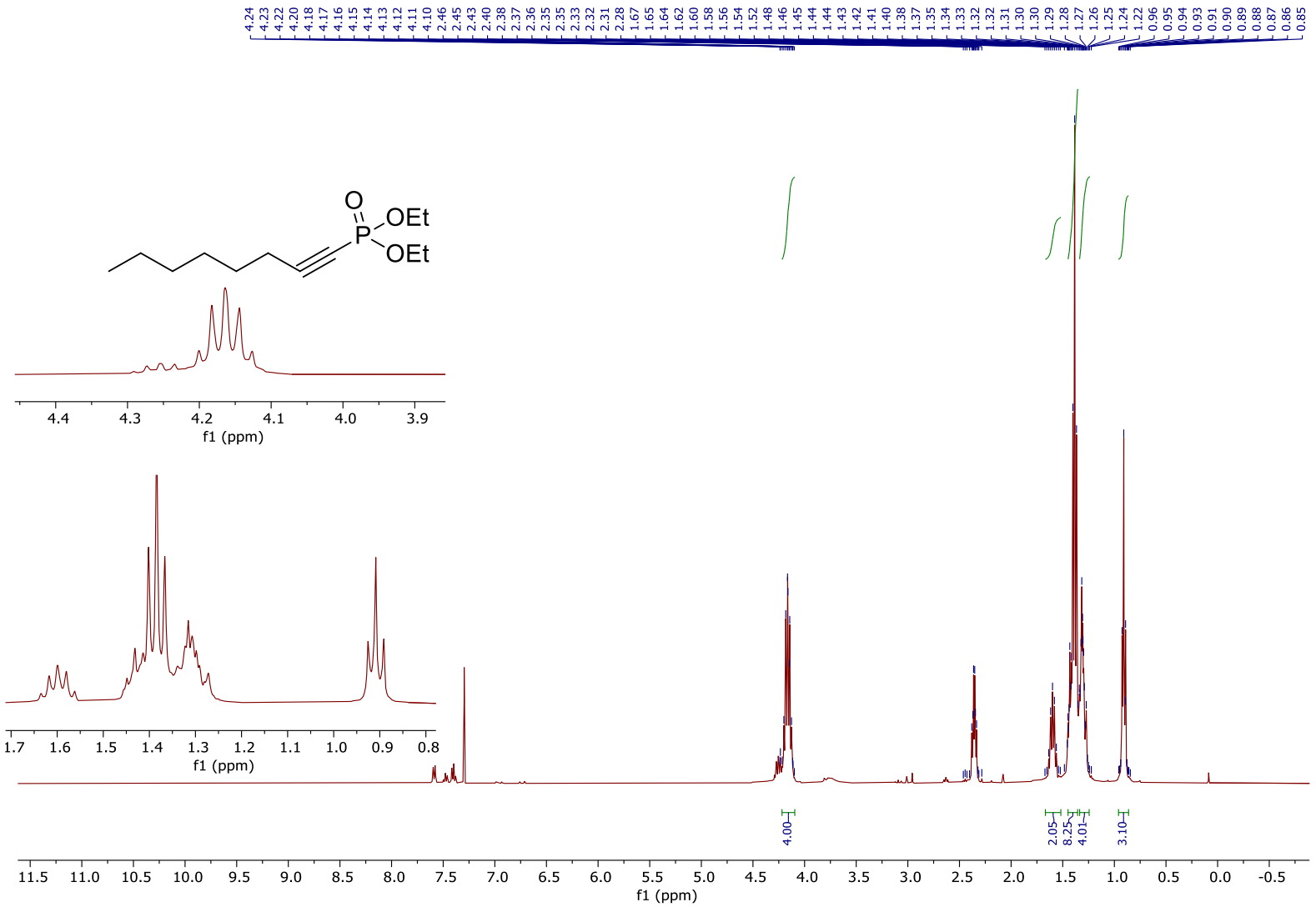


Figure S28: ^{1}H NMR Spectra of 3k

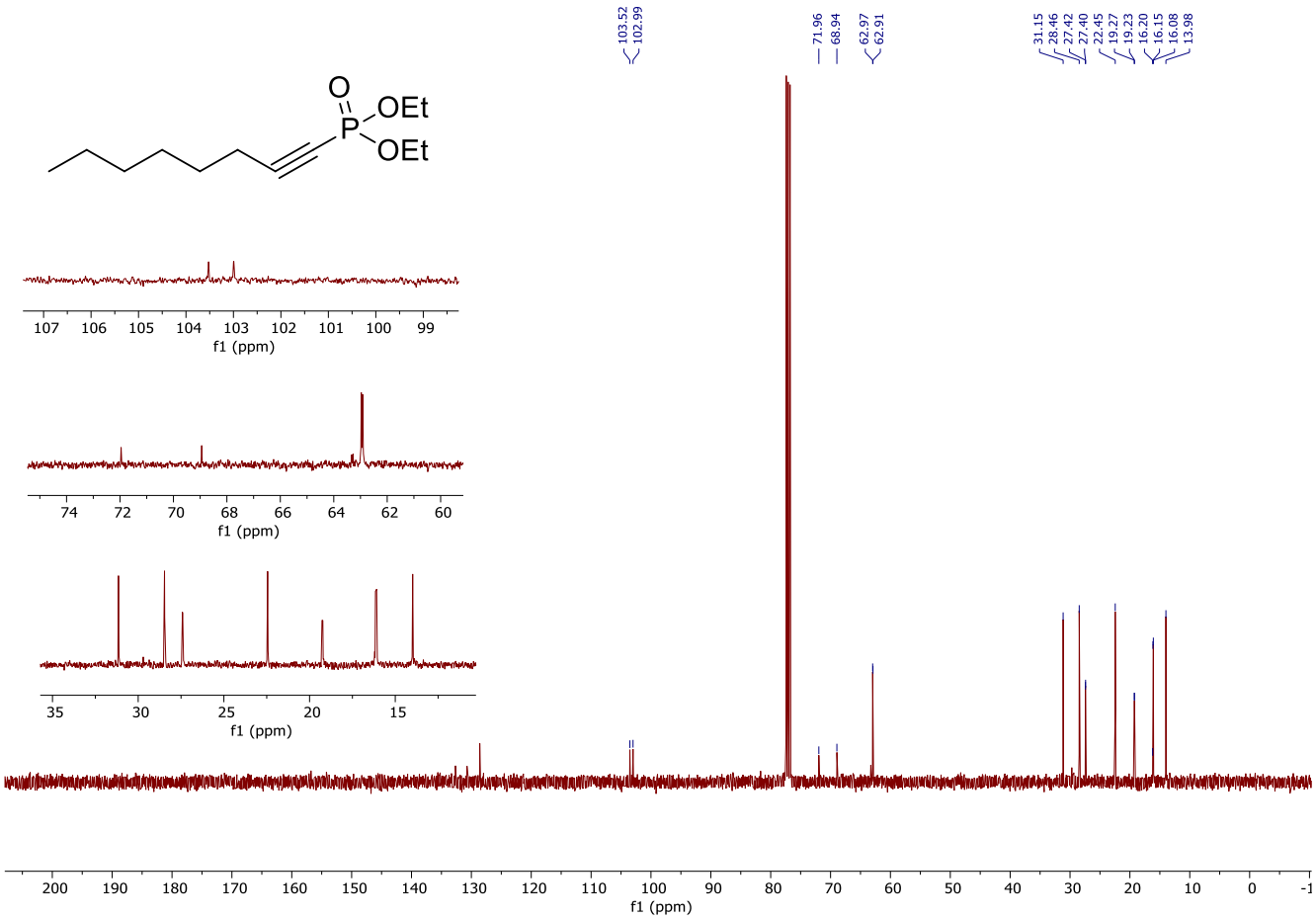


Figure S29: ^{13}C NMR Spectra of 3k

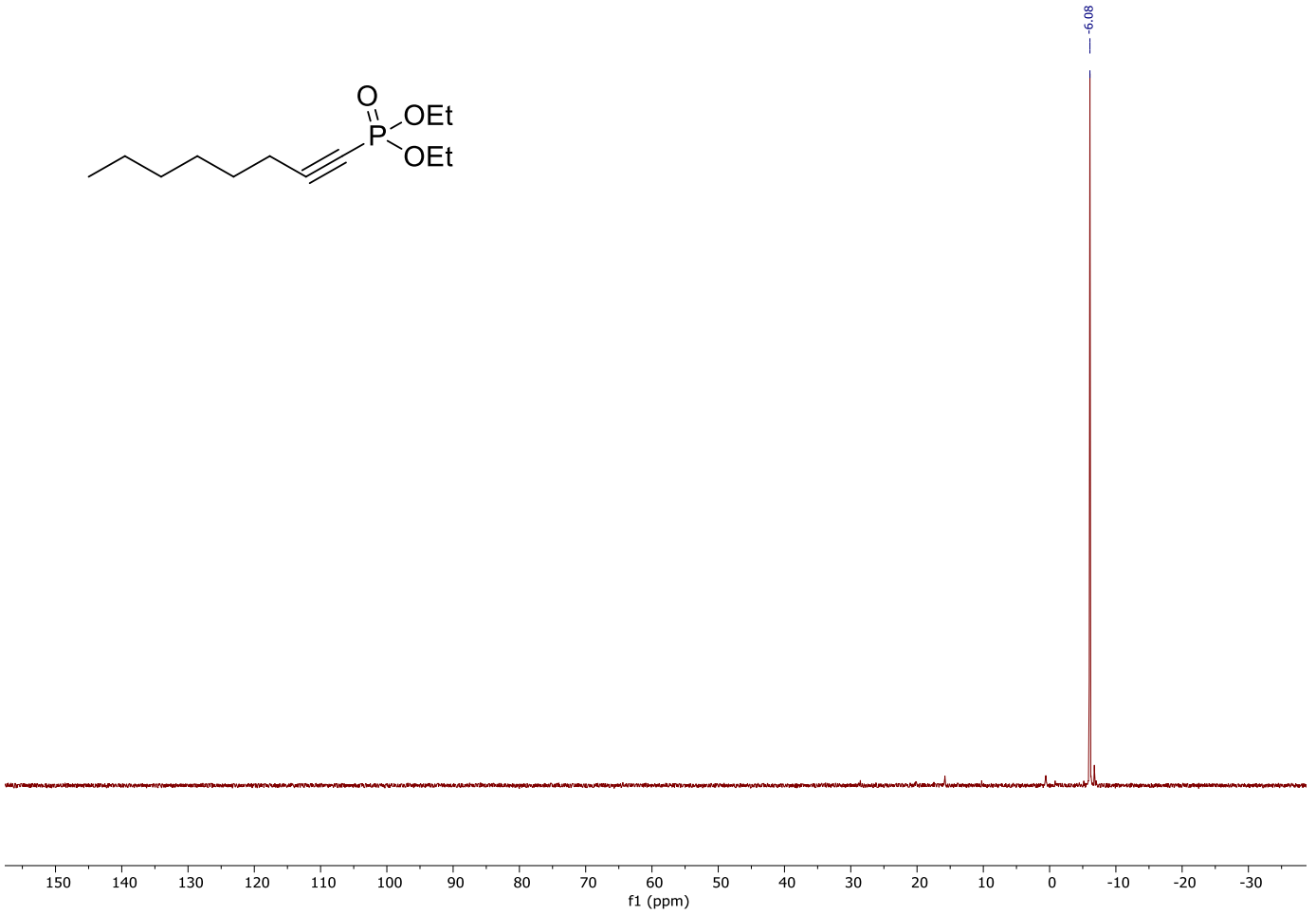


Figure S30: ^{31}P NMR Spectra of 3k

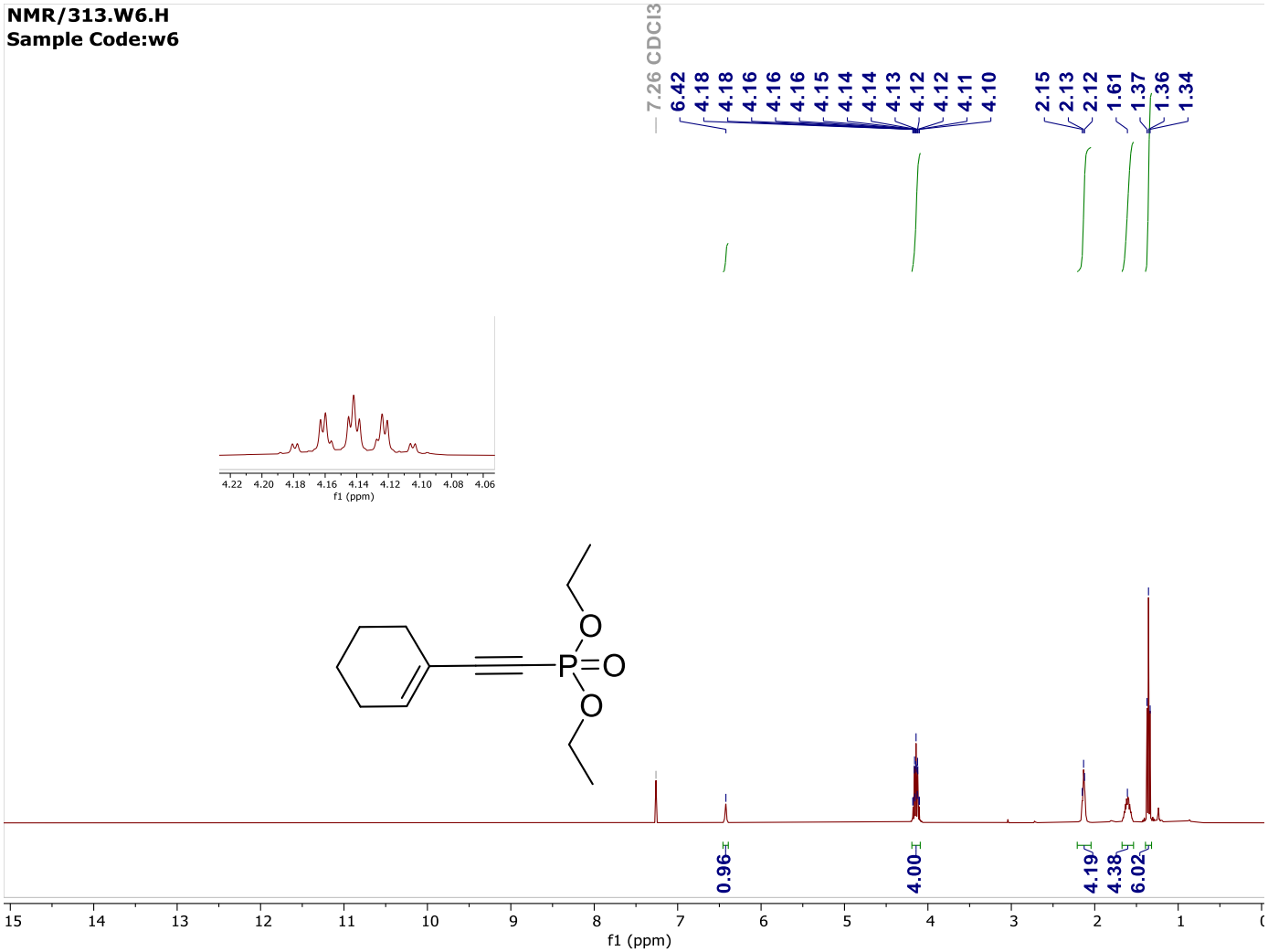


Figure S31: ^{1}H NMR Spectra of 3l

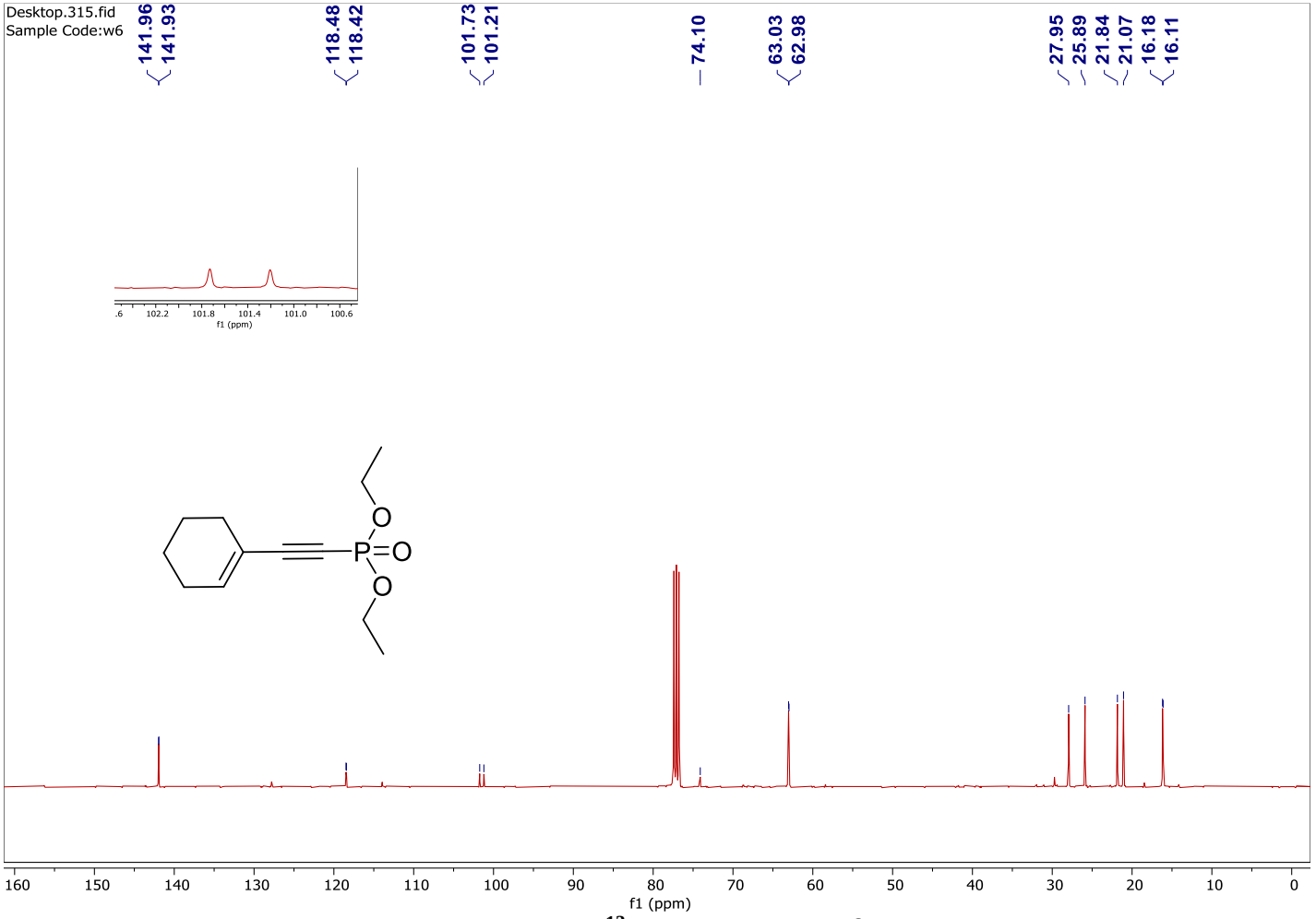


Figure S32: ^{13}C NMR Spectra of 3l

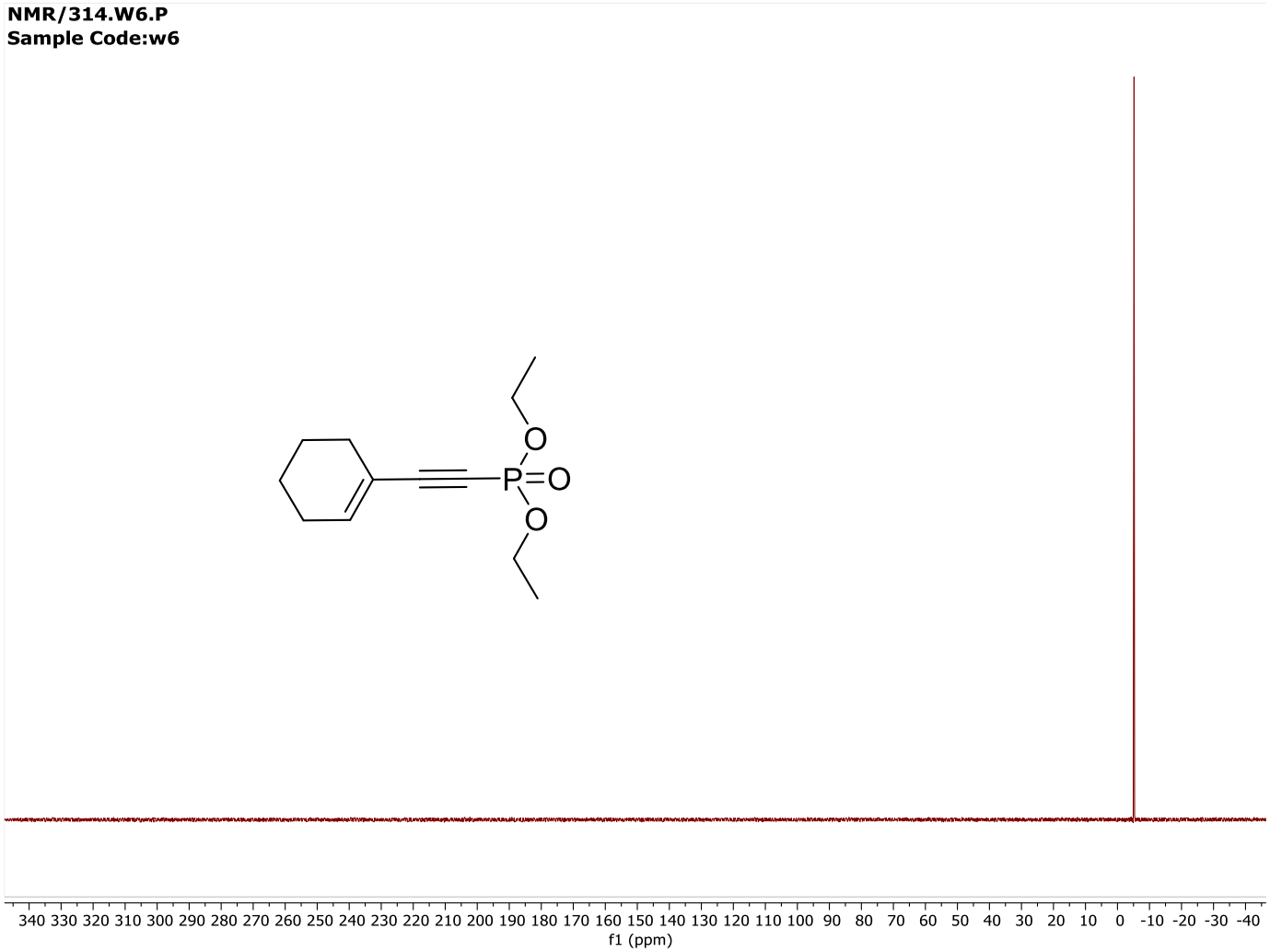


Figure S33: ^{31}P NMR Spectra of 3l

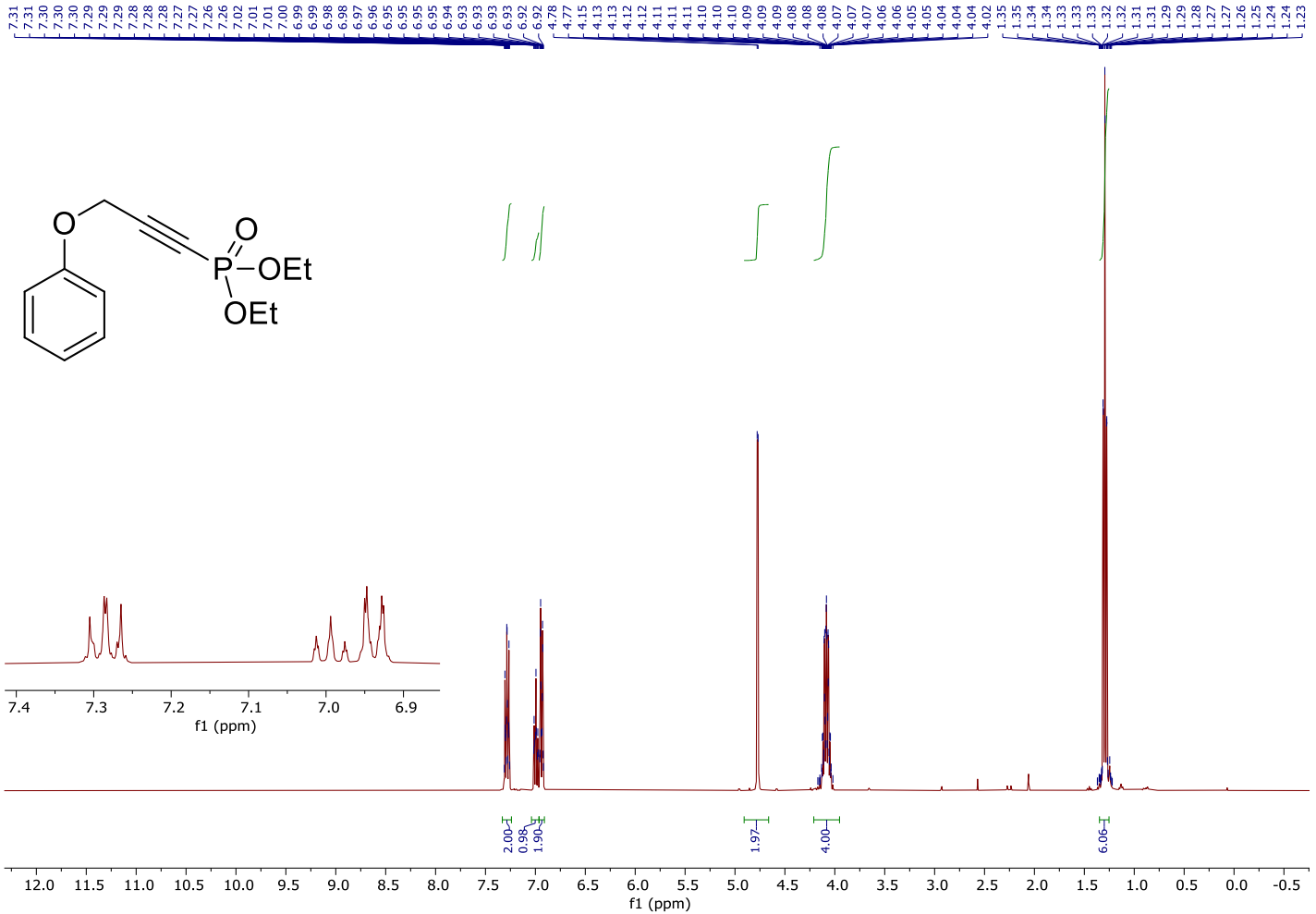


Figure S34: ^{1}H NMR Spectra of 3m

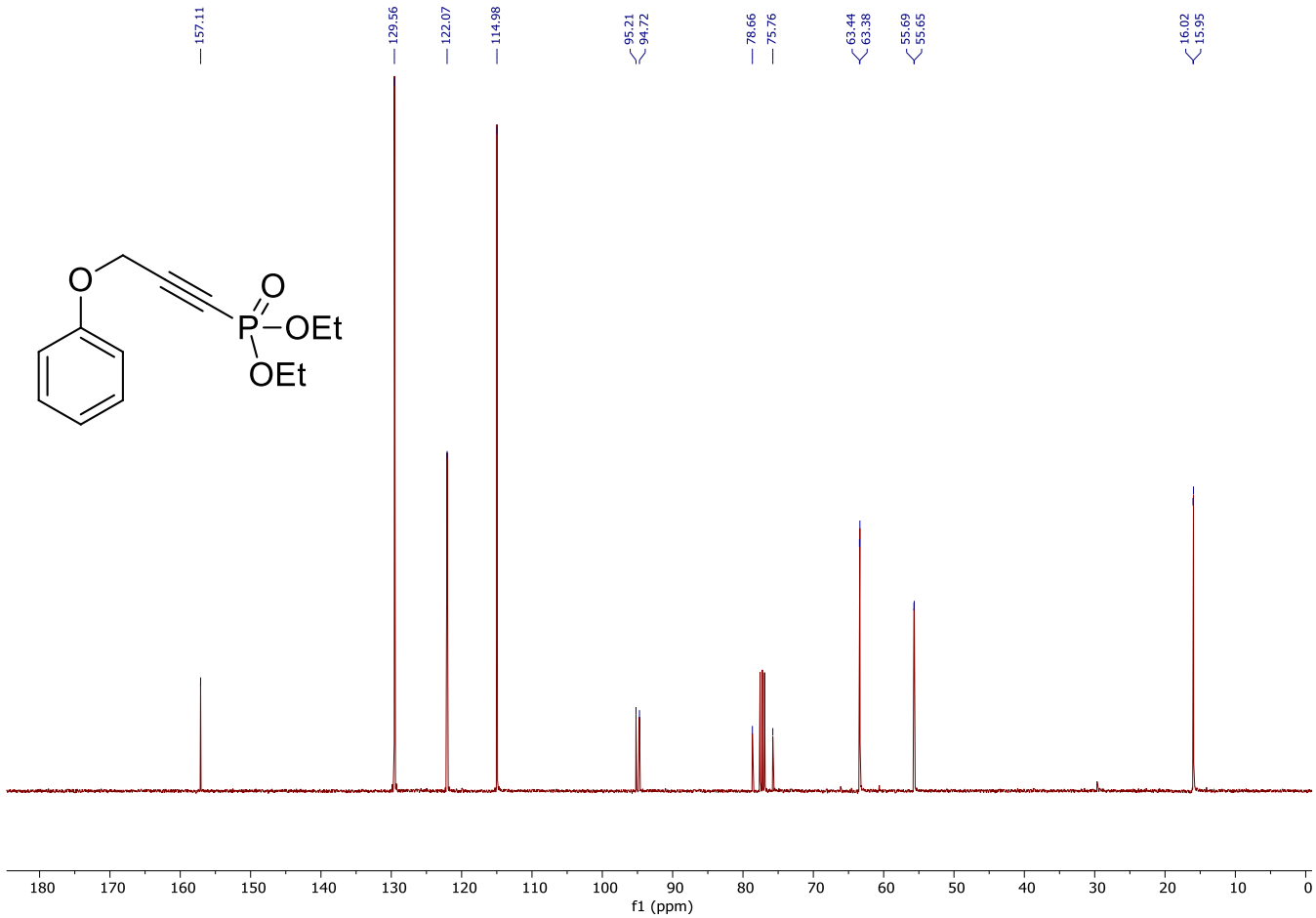


Figure S35: ^{13}C NMR Spectra of 3m

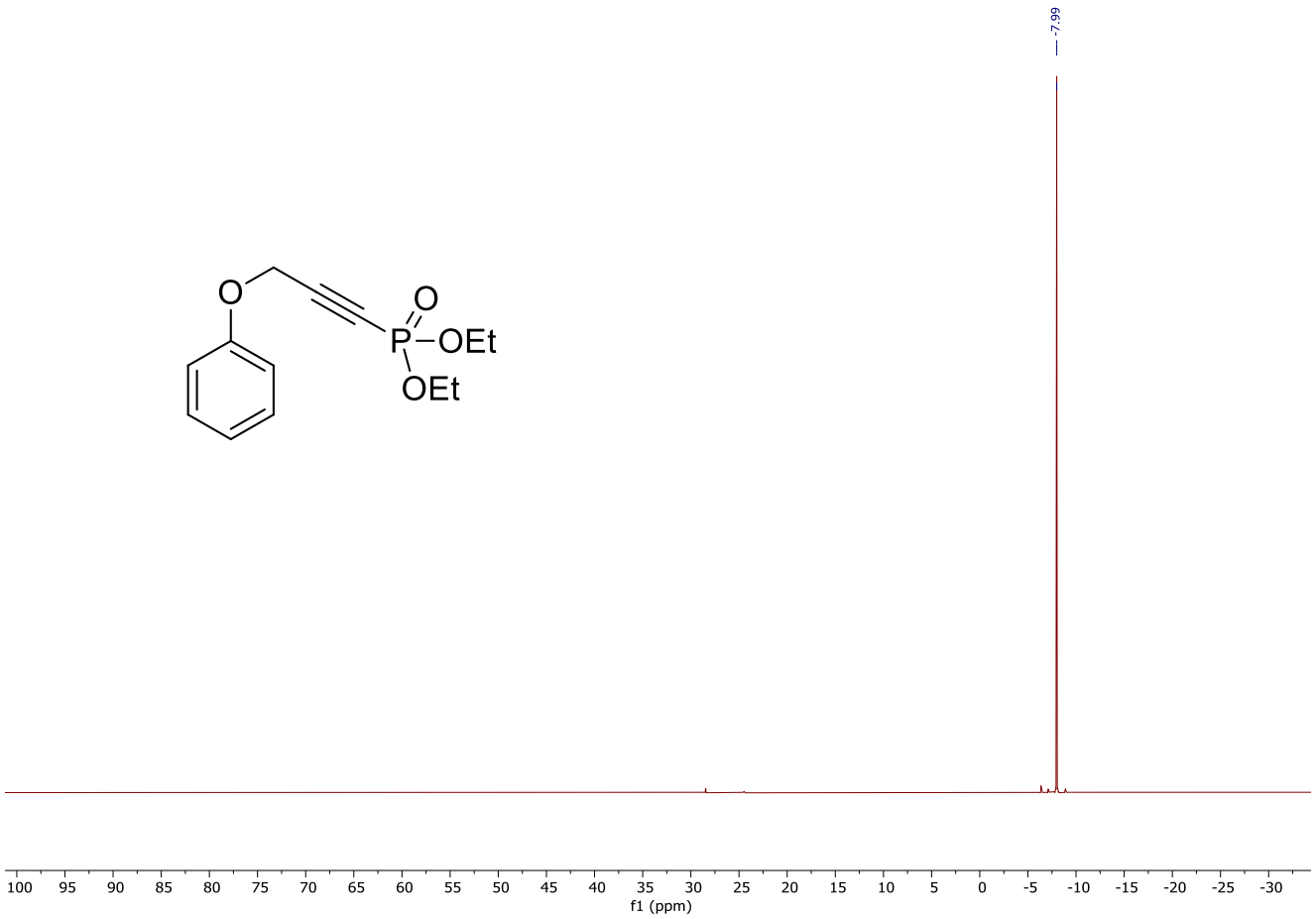


Figure S36: ^{31}P NMR Spectra of 3m

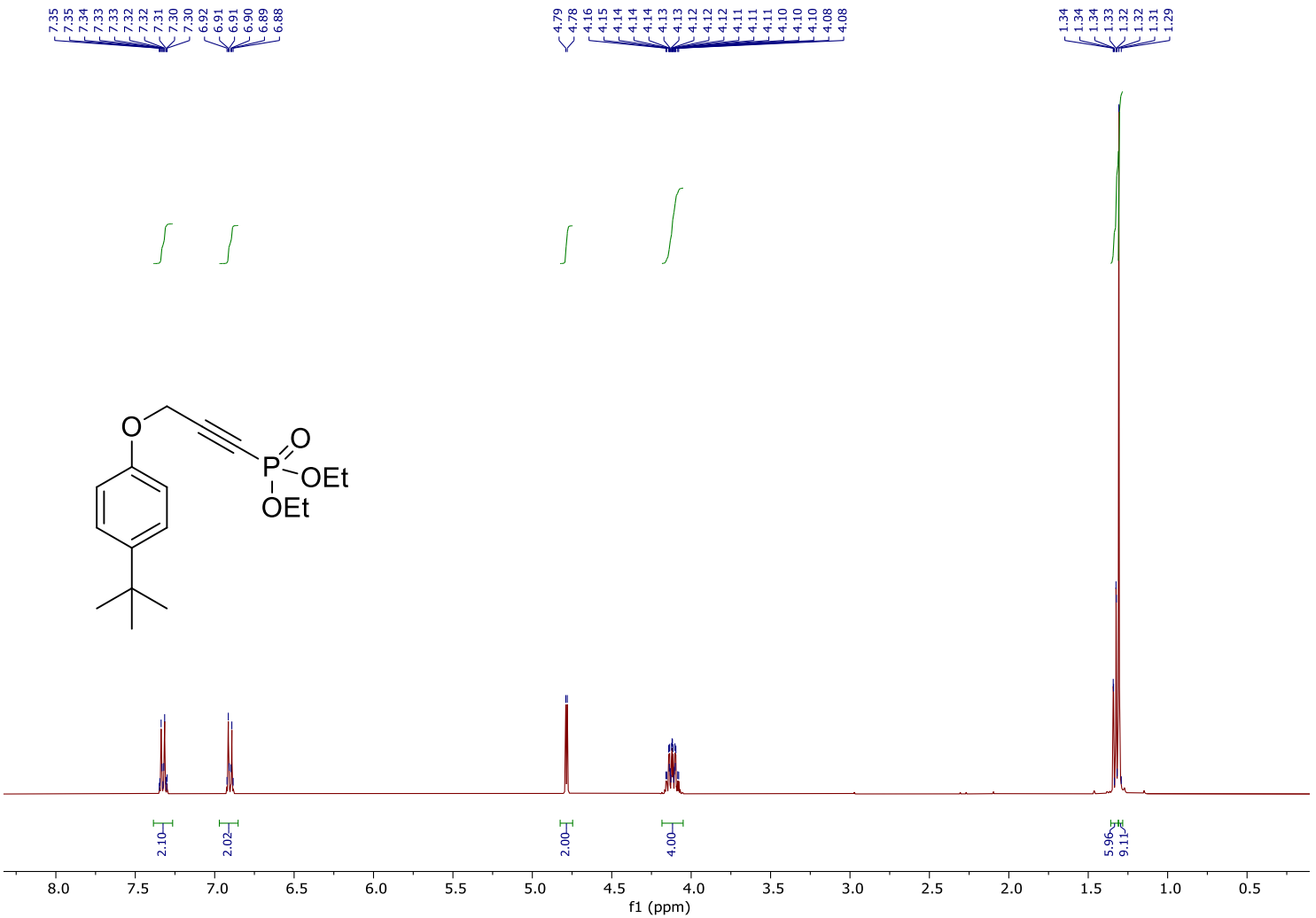


Figure S37: ^{1}H NMR Spectra of 3n

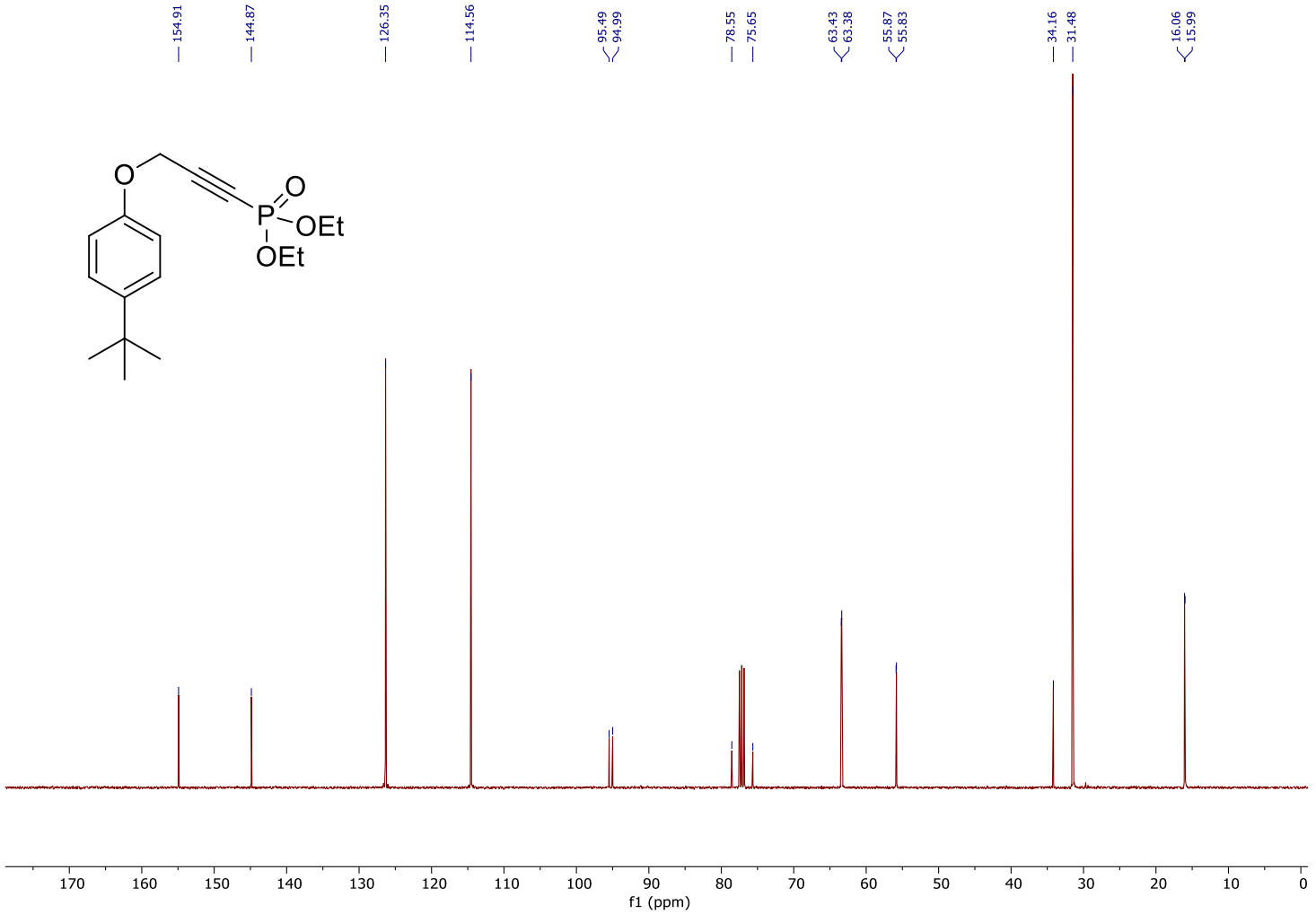


Figure S38: ^{13}C NMR Spectra of 3n

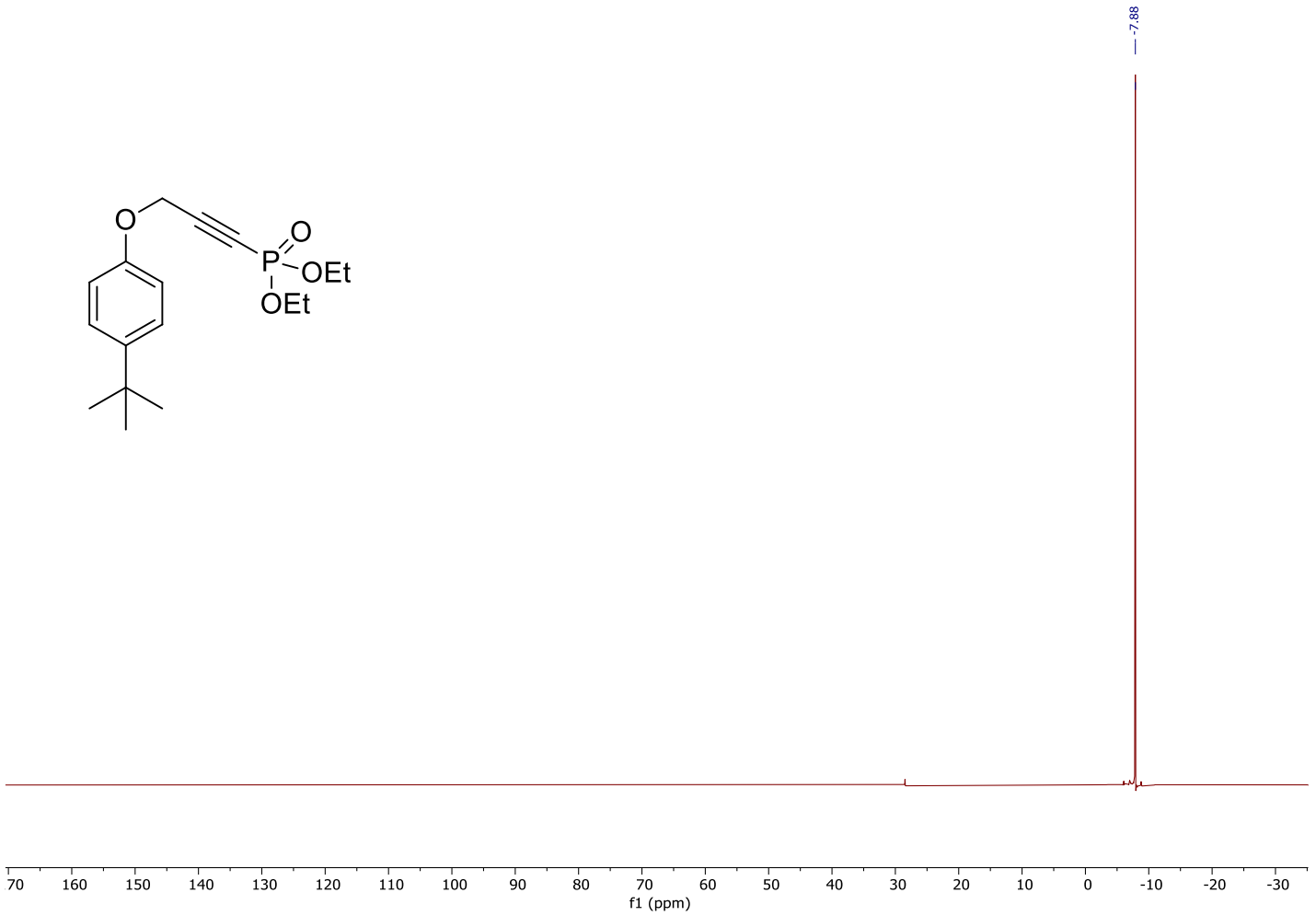


Figure S39: ^{31}P NMR Spectra of 3n

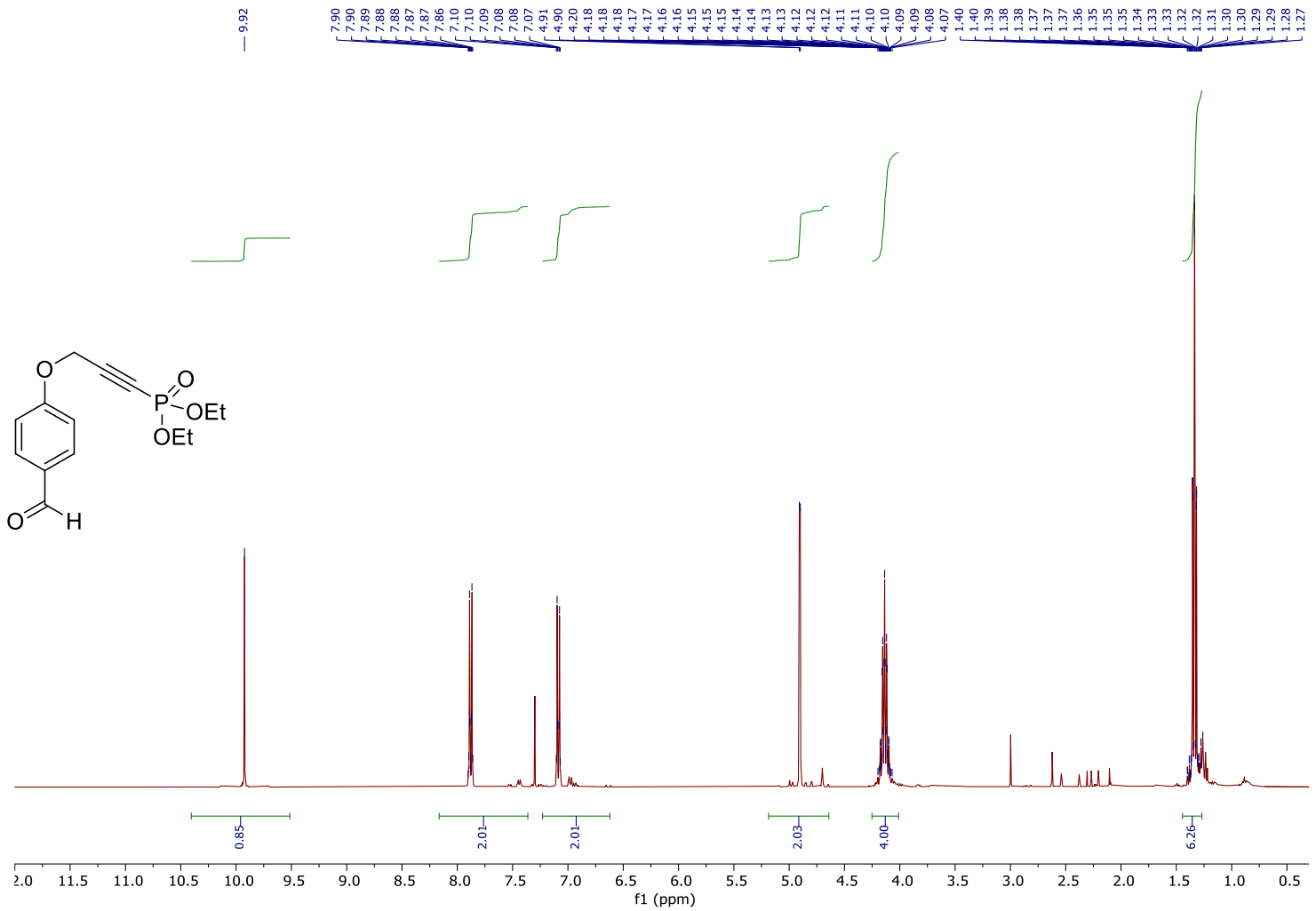
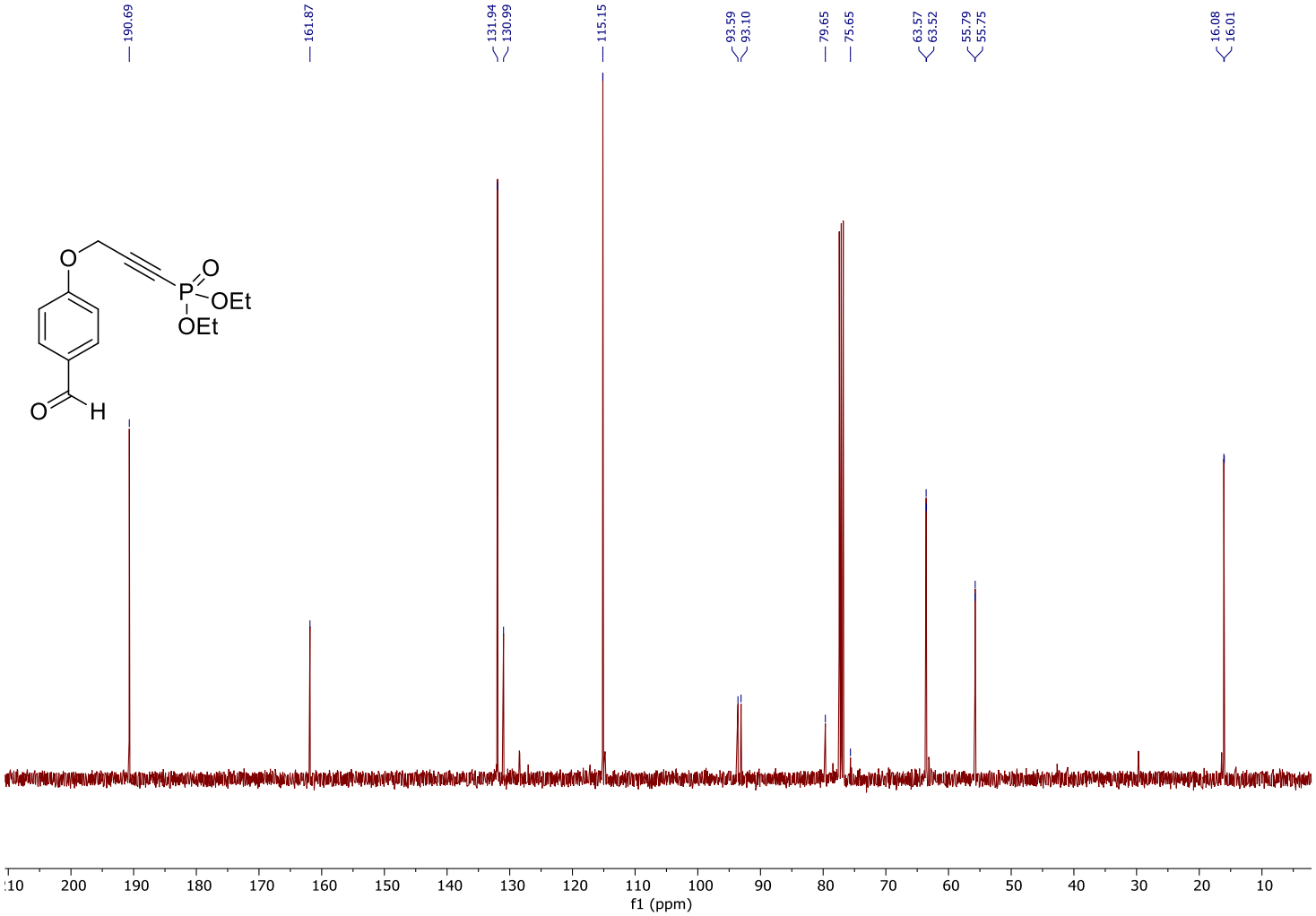


Figure S40: ^{1}H NMR Spectra of 3o

F Figure S44: ^{13}C NMR Spectra of 3o



igure S41: ^{13}C NMR Spectra of 3o

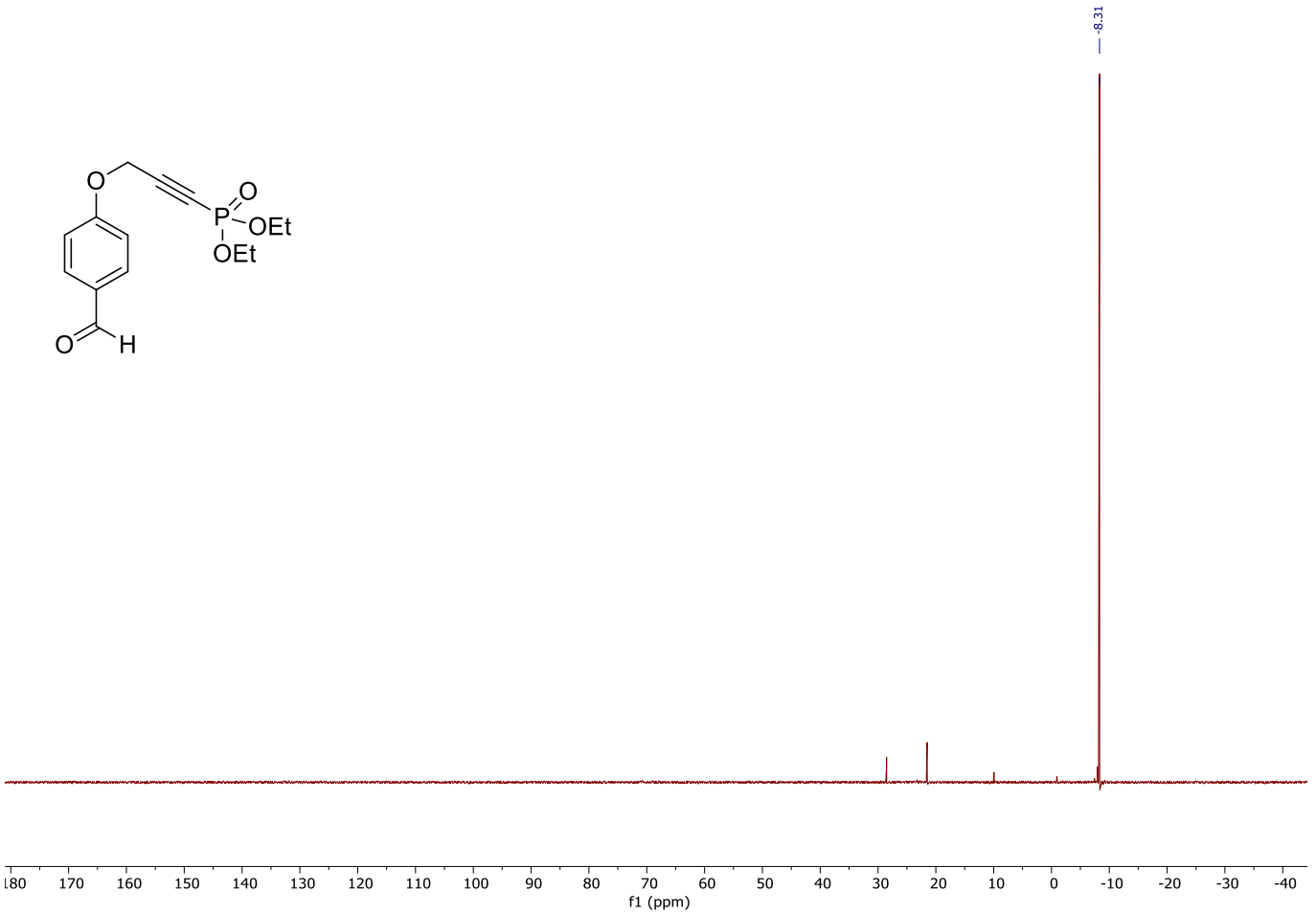


Figure S42: ^{31}P NMR Spectra of 3o

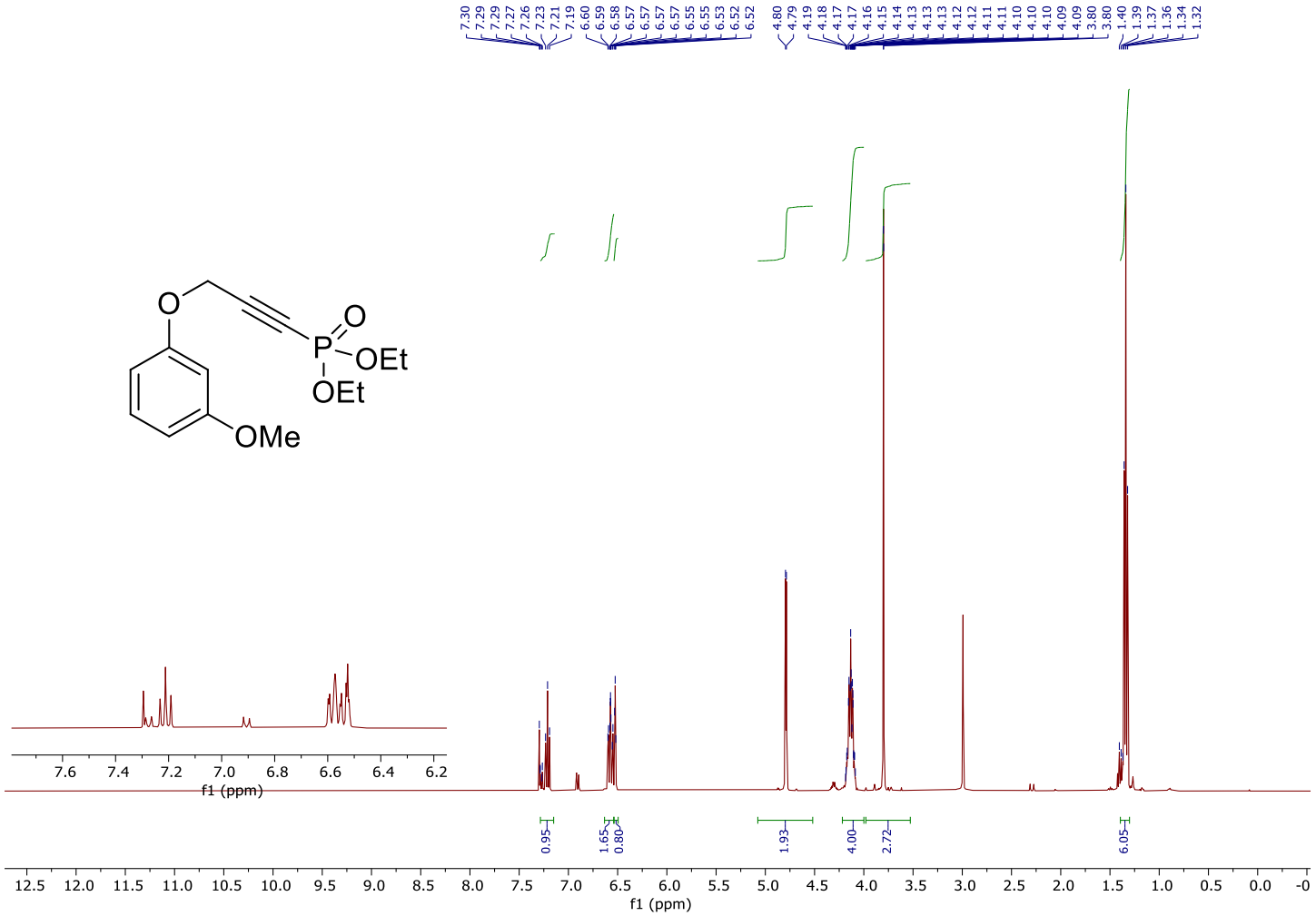


Figure S43: ^{1}H NMR Spectra of 3p

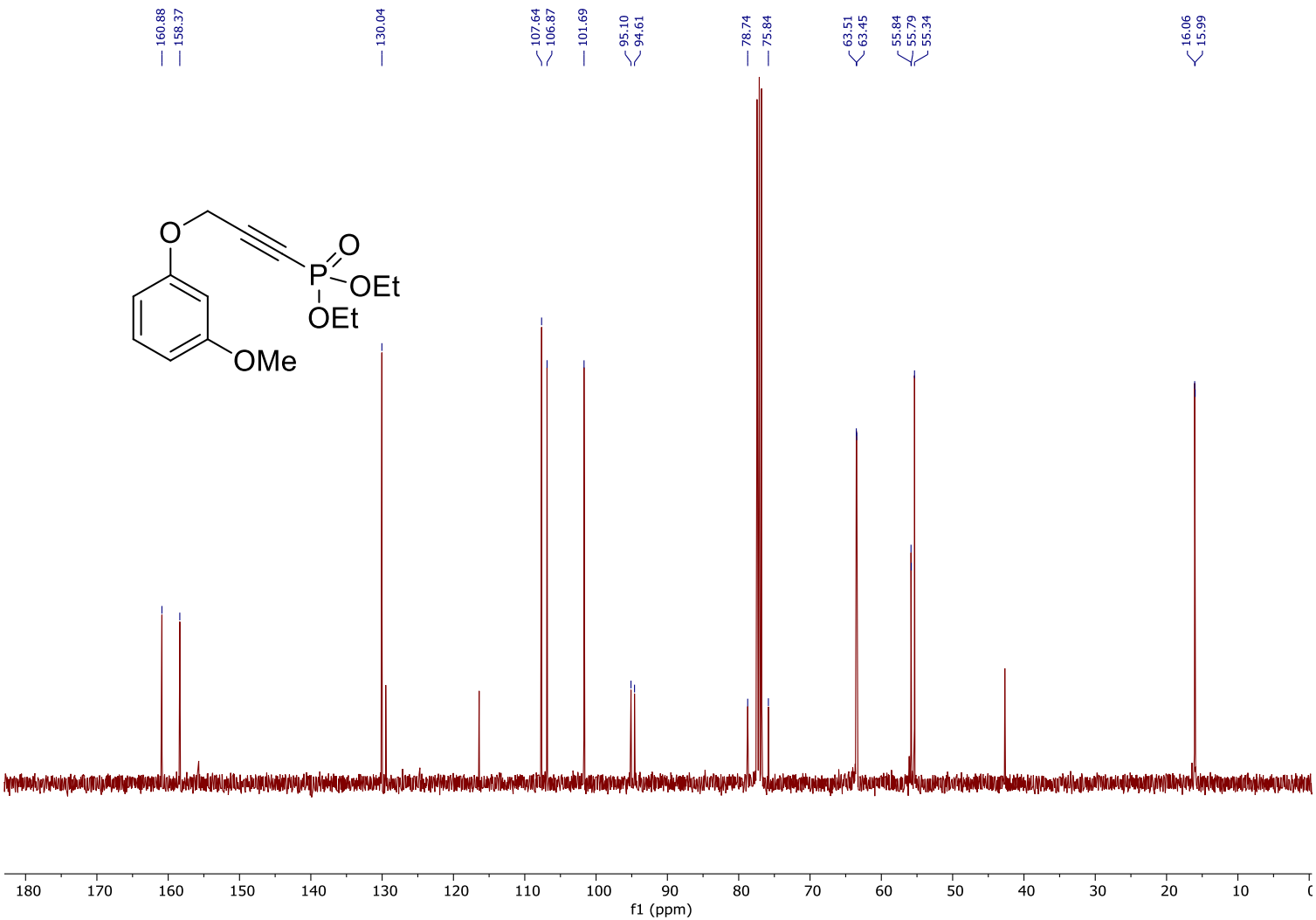


Figure S44: ^{13}C NMR Spectra of 3p

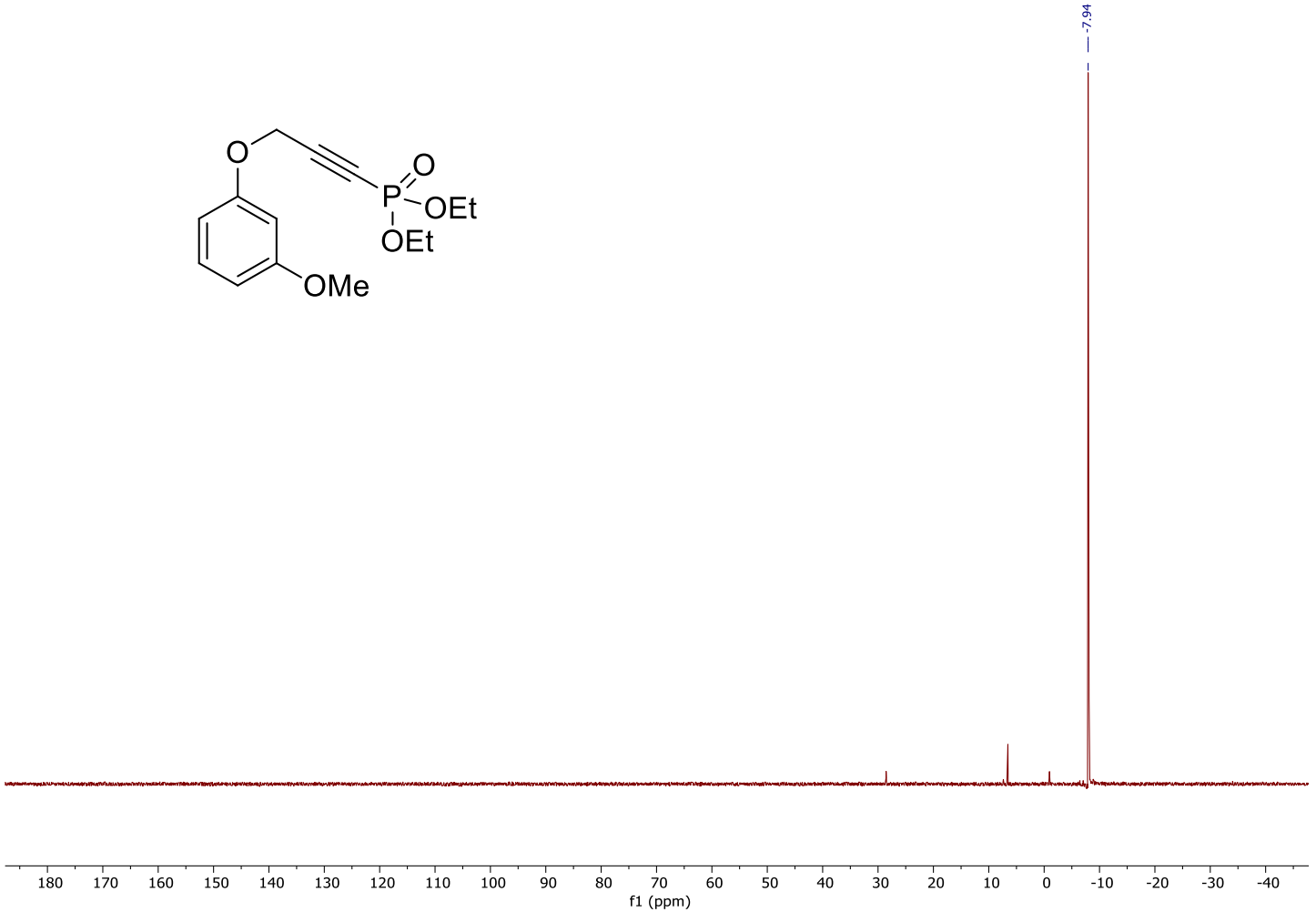


Figure S45: ^{31}P NMR Spectra of 3p

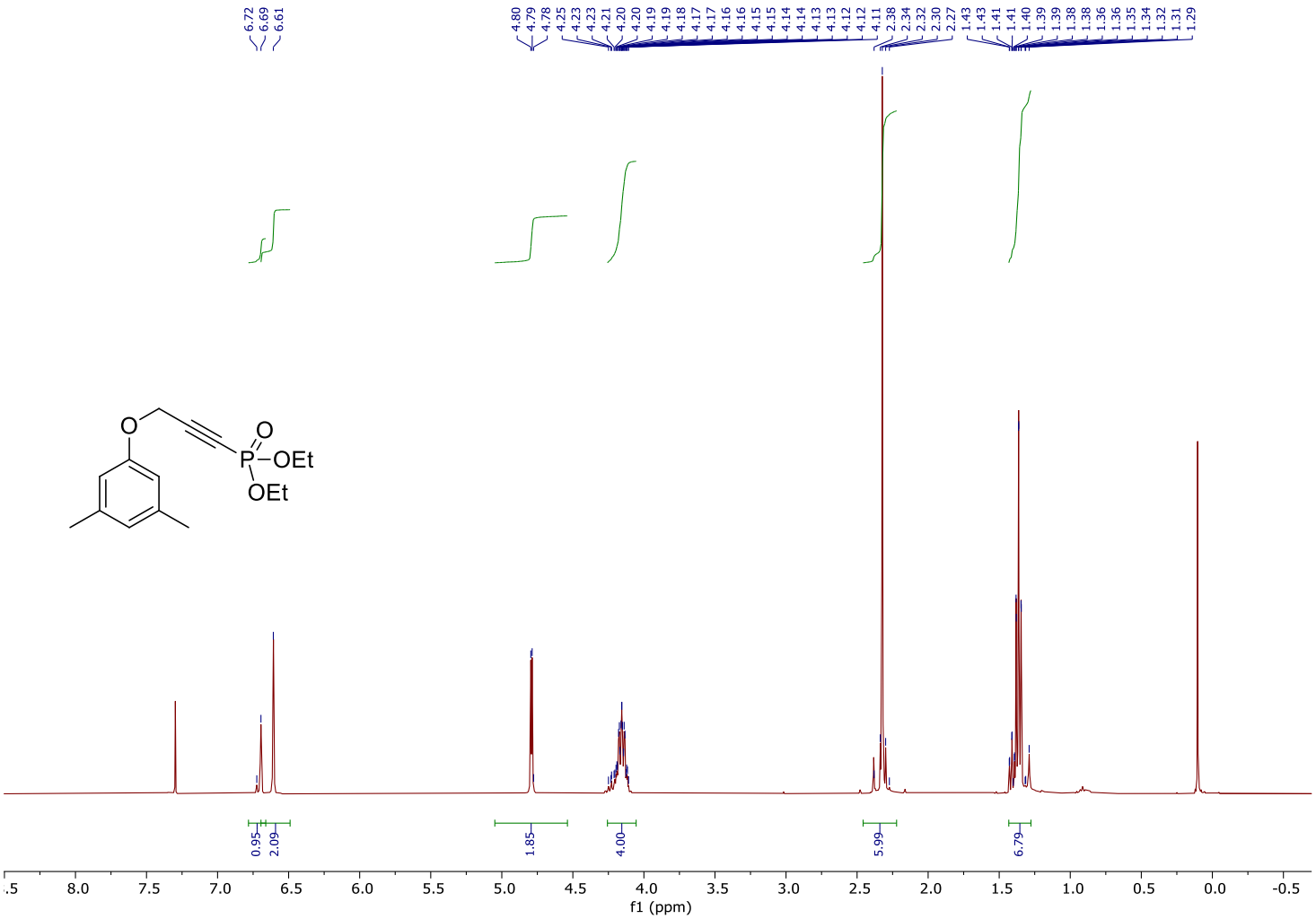


Figure S46: ^{1}H NMR Spectra of 3q

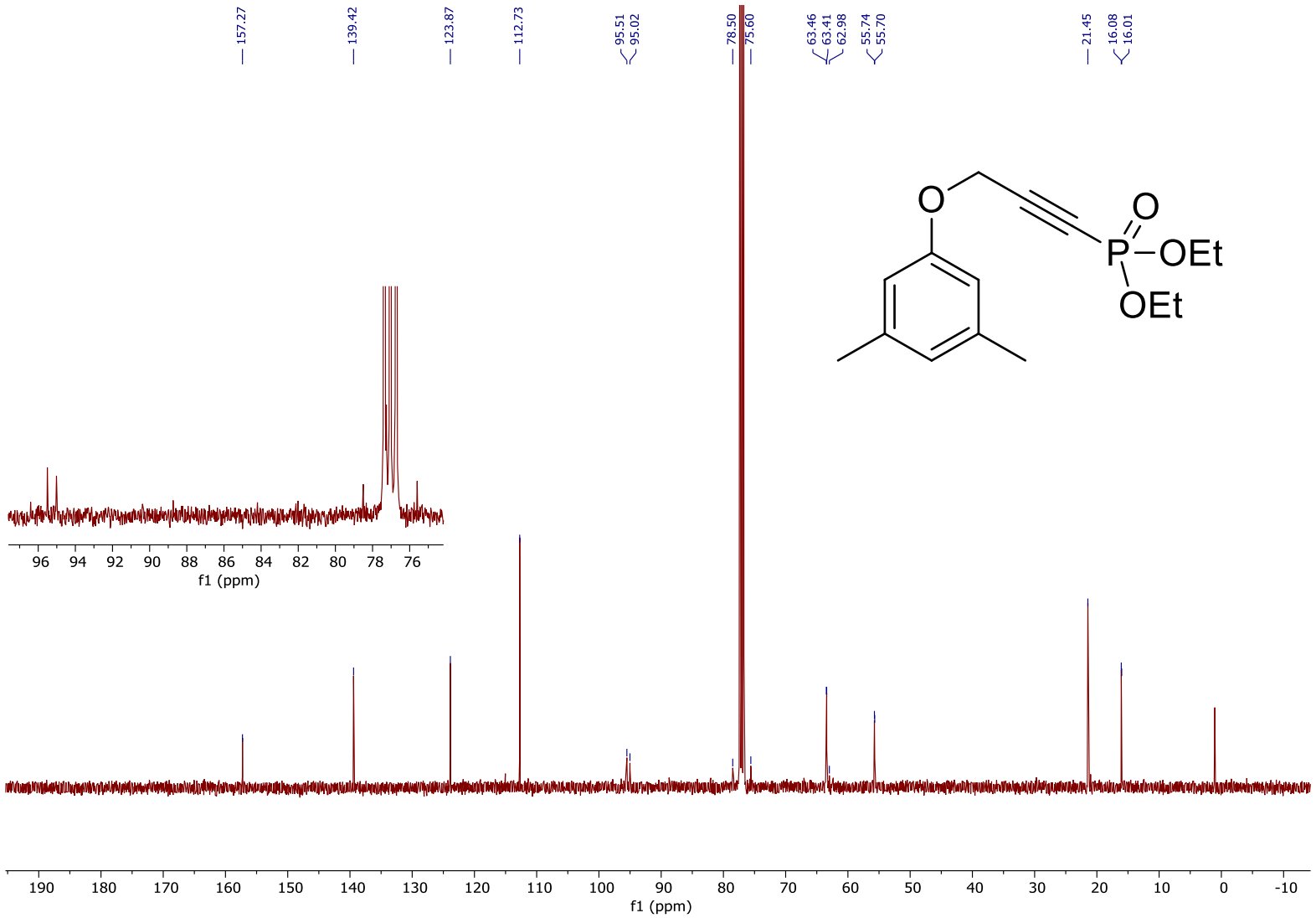


Figure S47: ^{13}C NMR Spectra of 3q

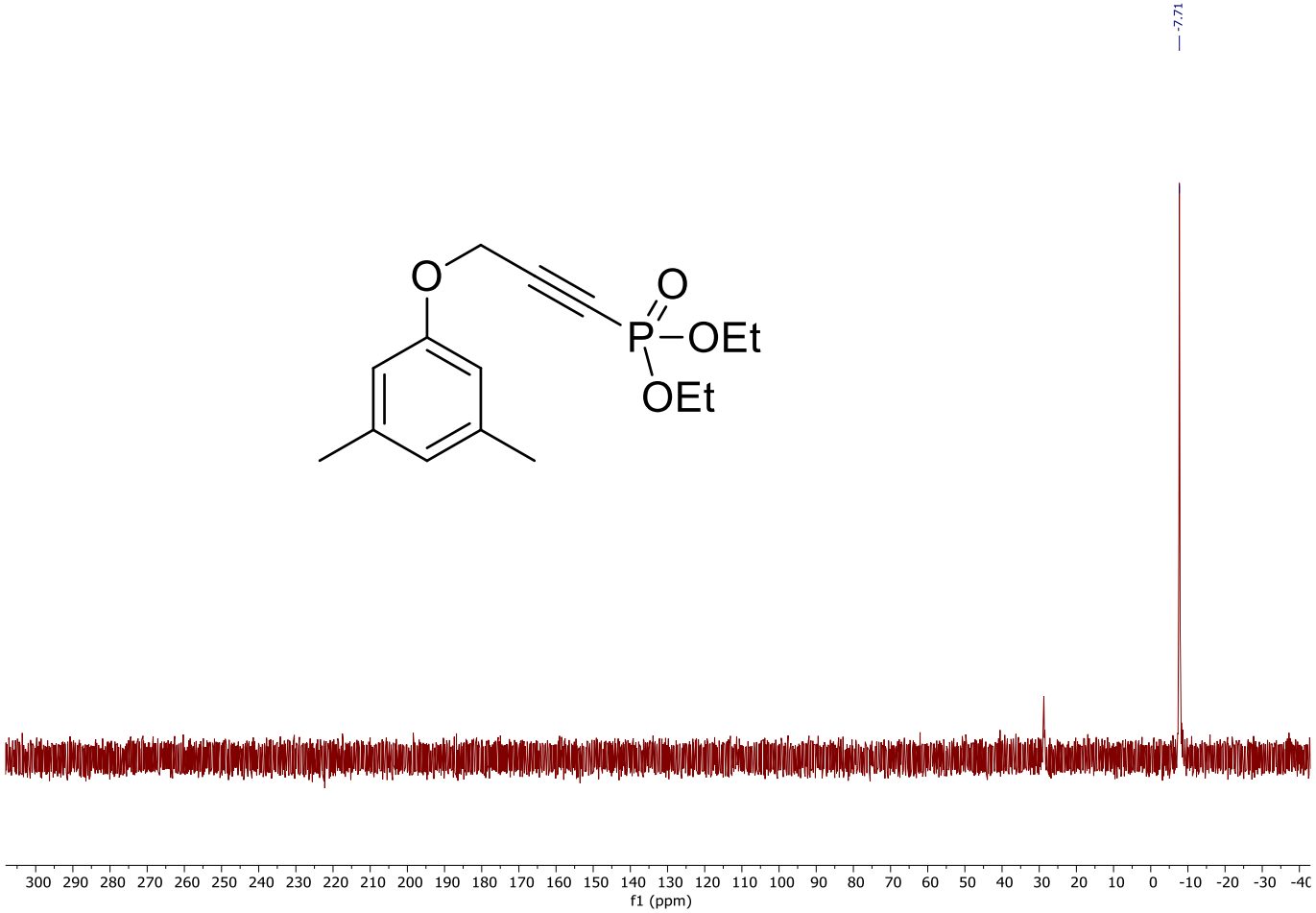


Figure S48: ^{31}P NMR Spectra of 3q

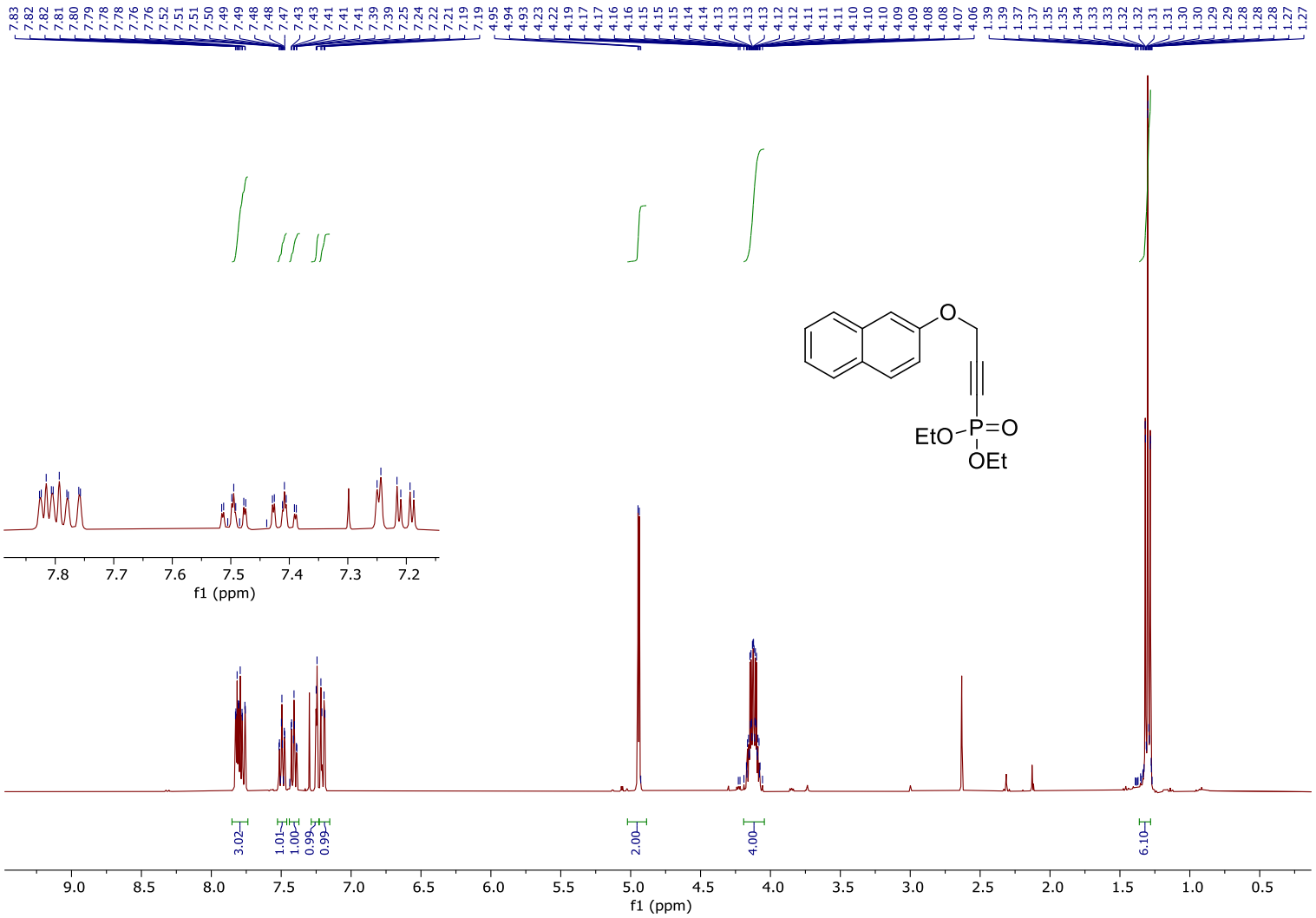


Figure S49: ^{1}H NMR Spectra of 3r

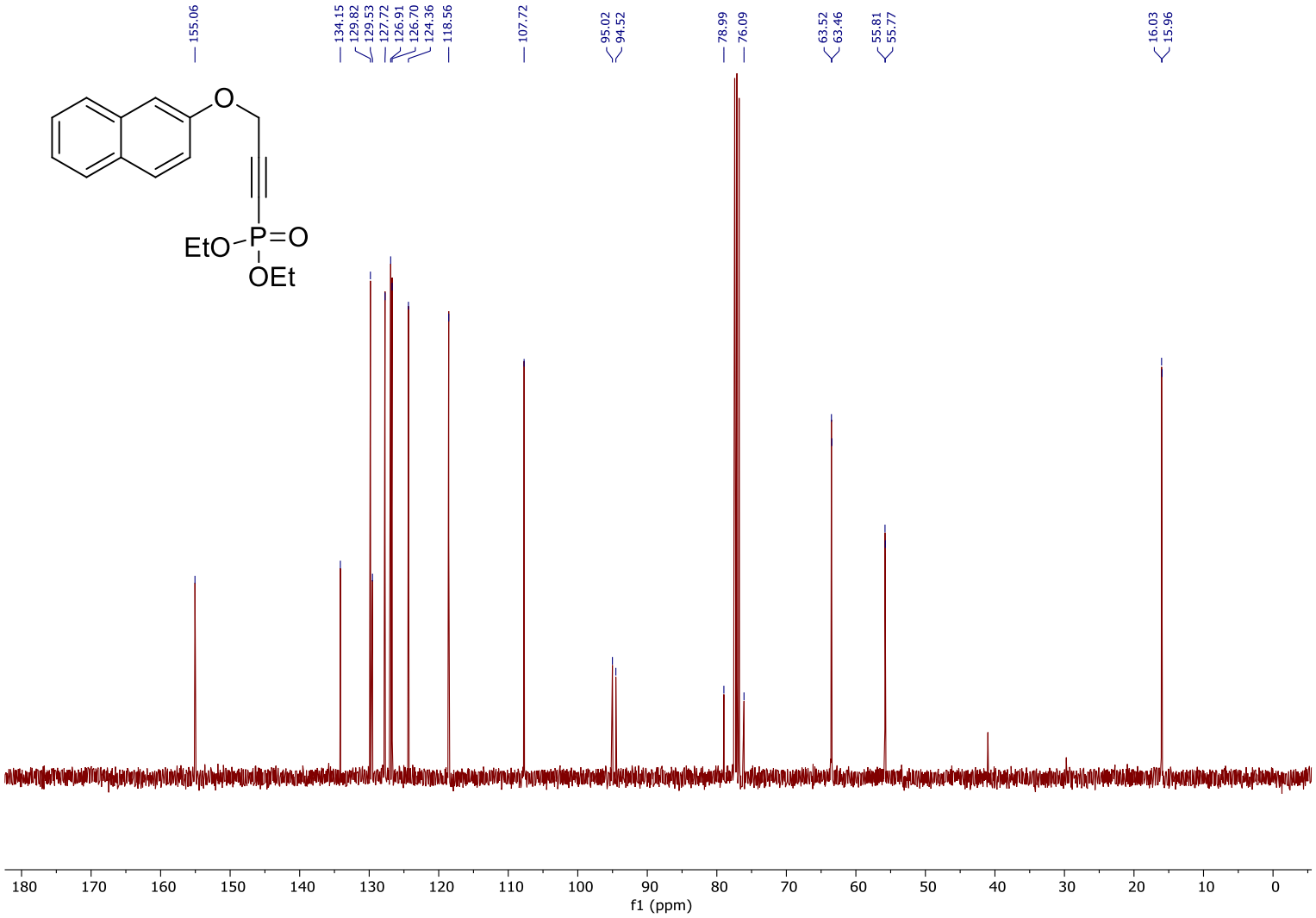


Figure S50: ^{13}C NMR Spectra of 3r

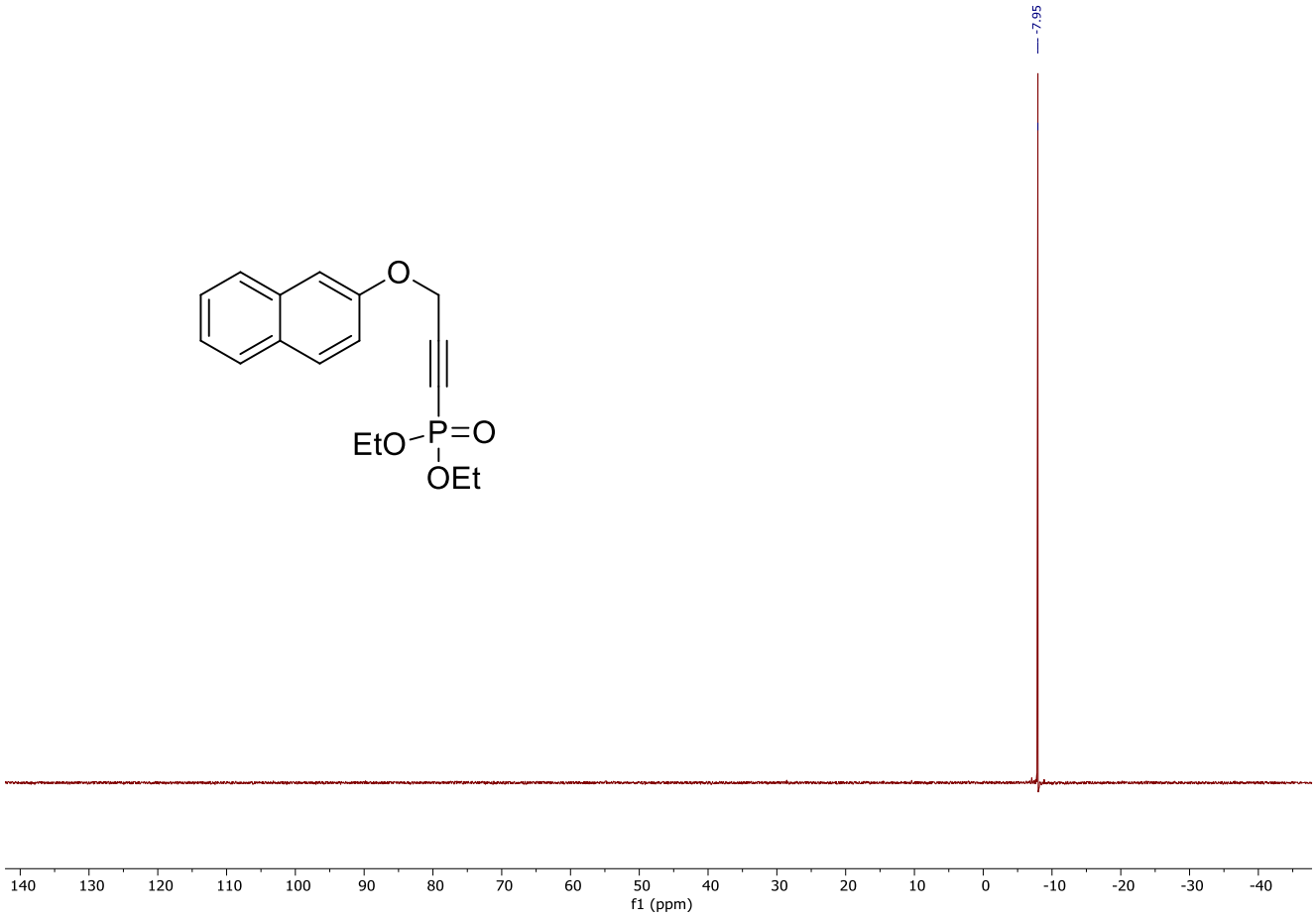


Figure S51: ^{31}P NMR Spectra of 3r

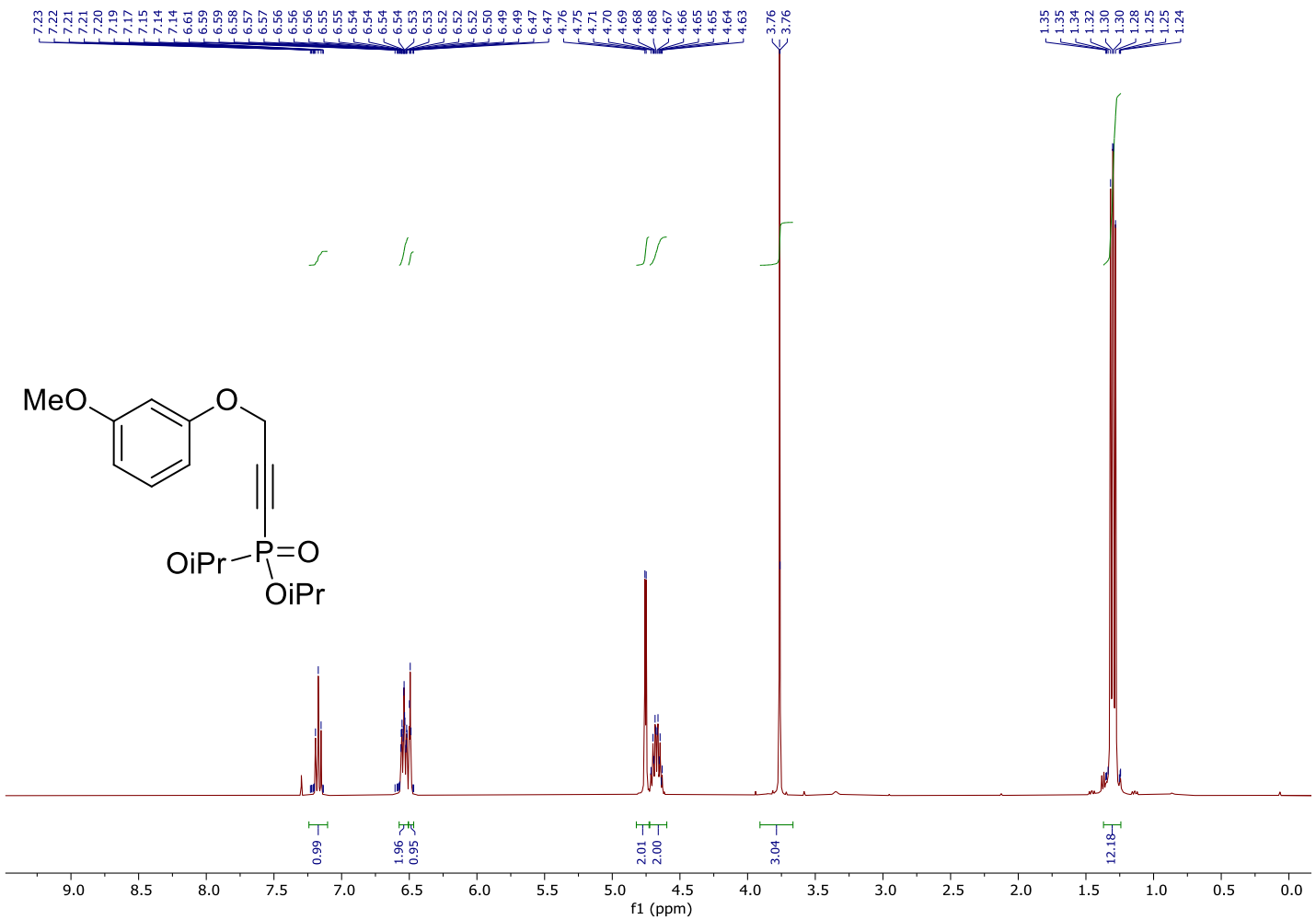


Figure S52: ^{1}H NMR Spectra of 3s

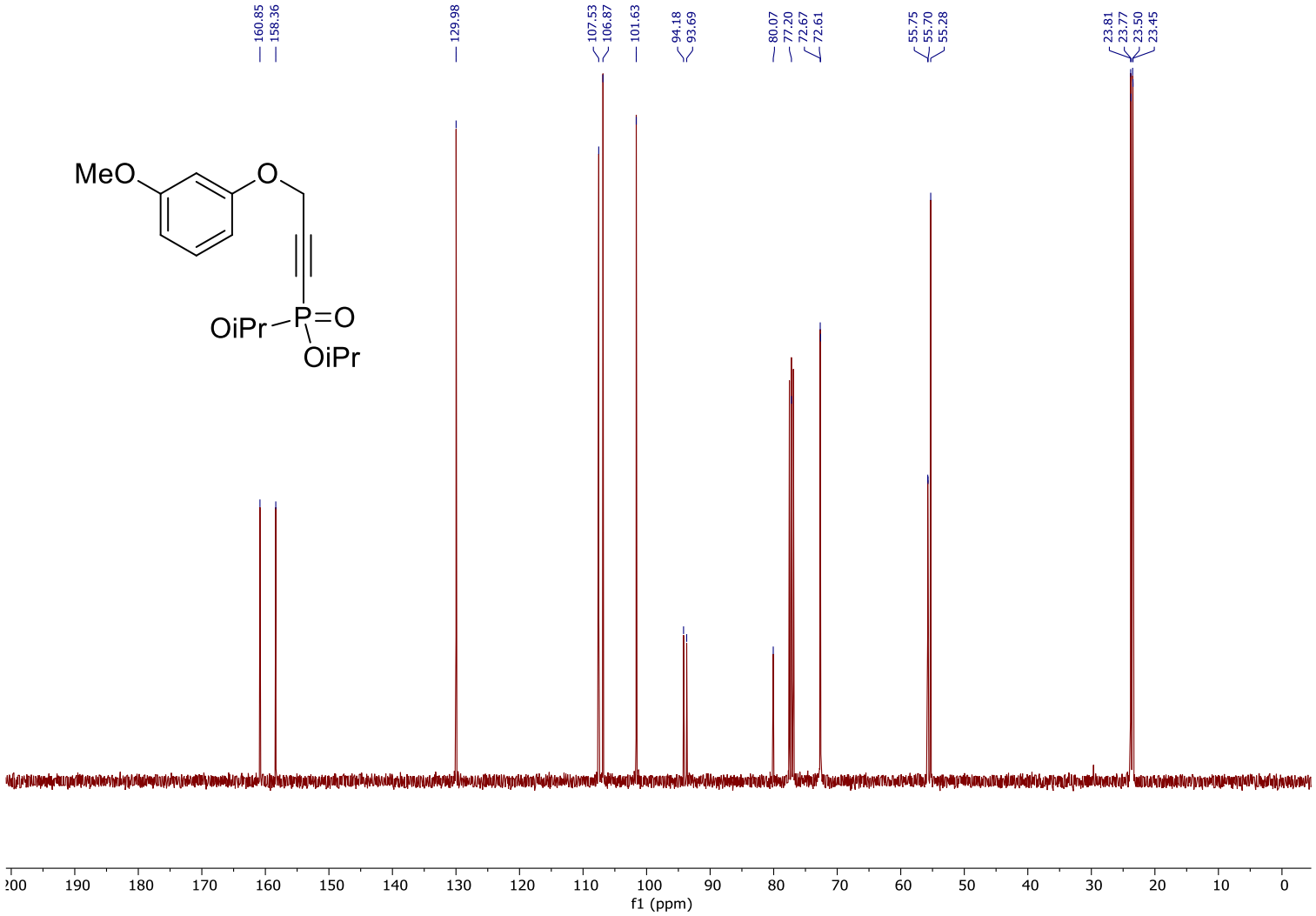


Figure S53: ^{13}C NMR Spectra of 3s

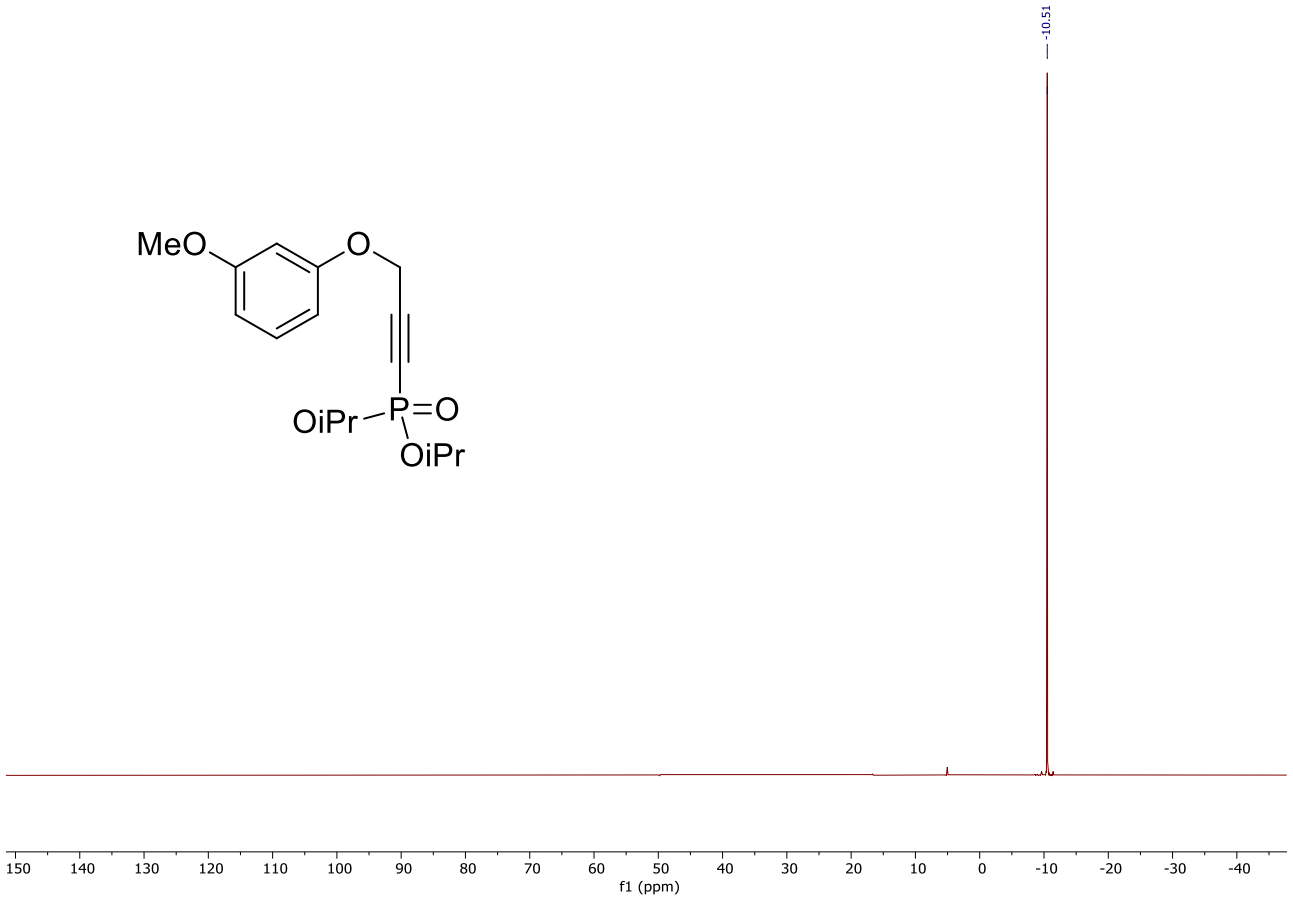


Figure S54: ^{31}P NMR Spectra of 3s

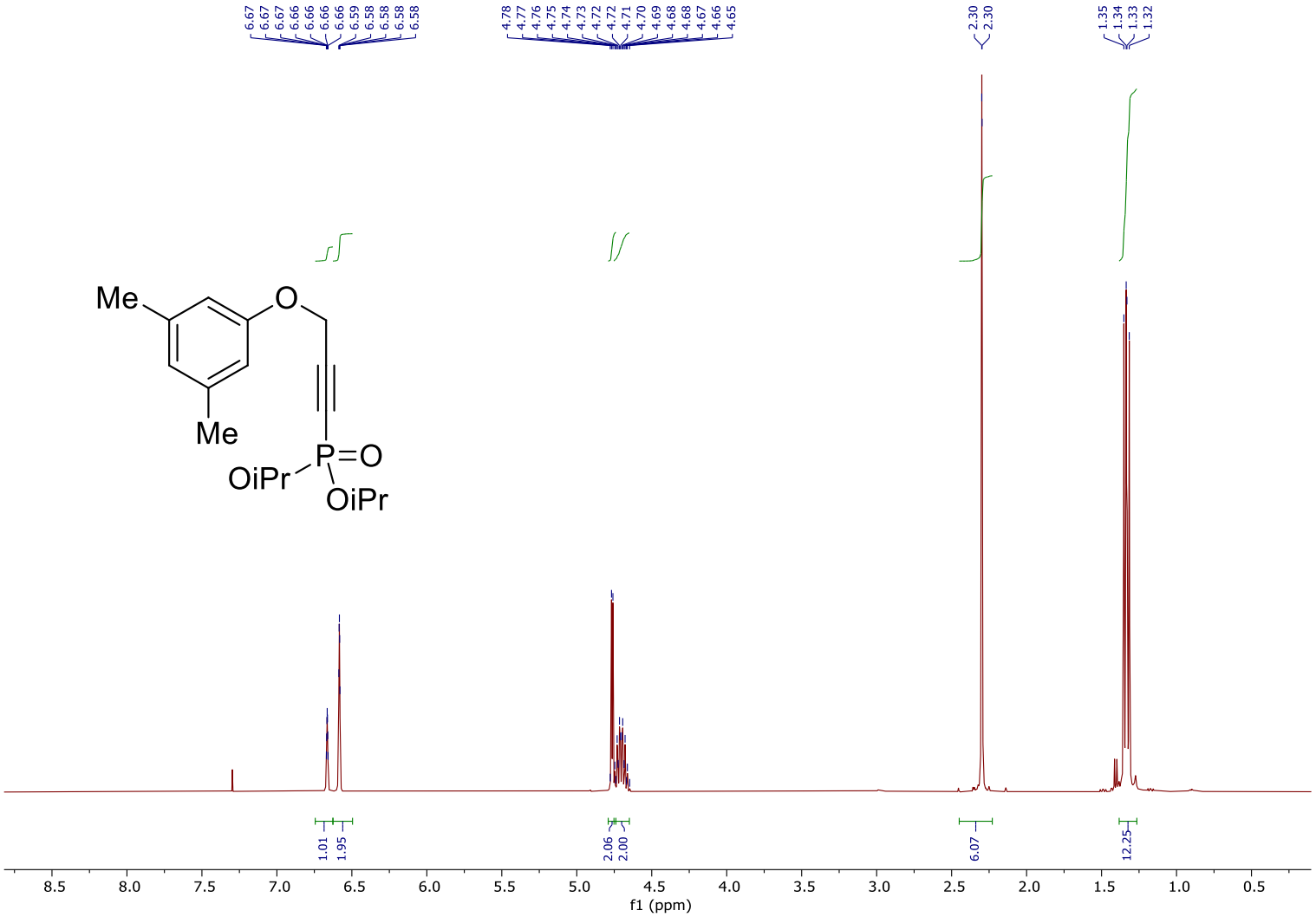


Figure S55: ^{1}H NMR Spectra of 3t

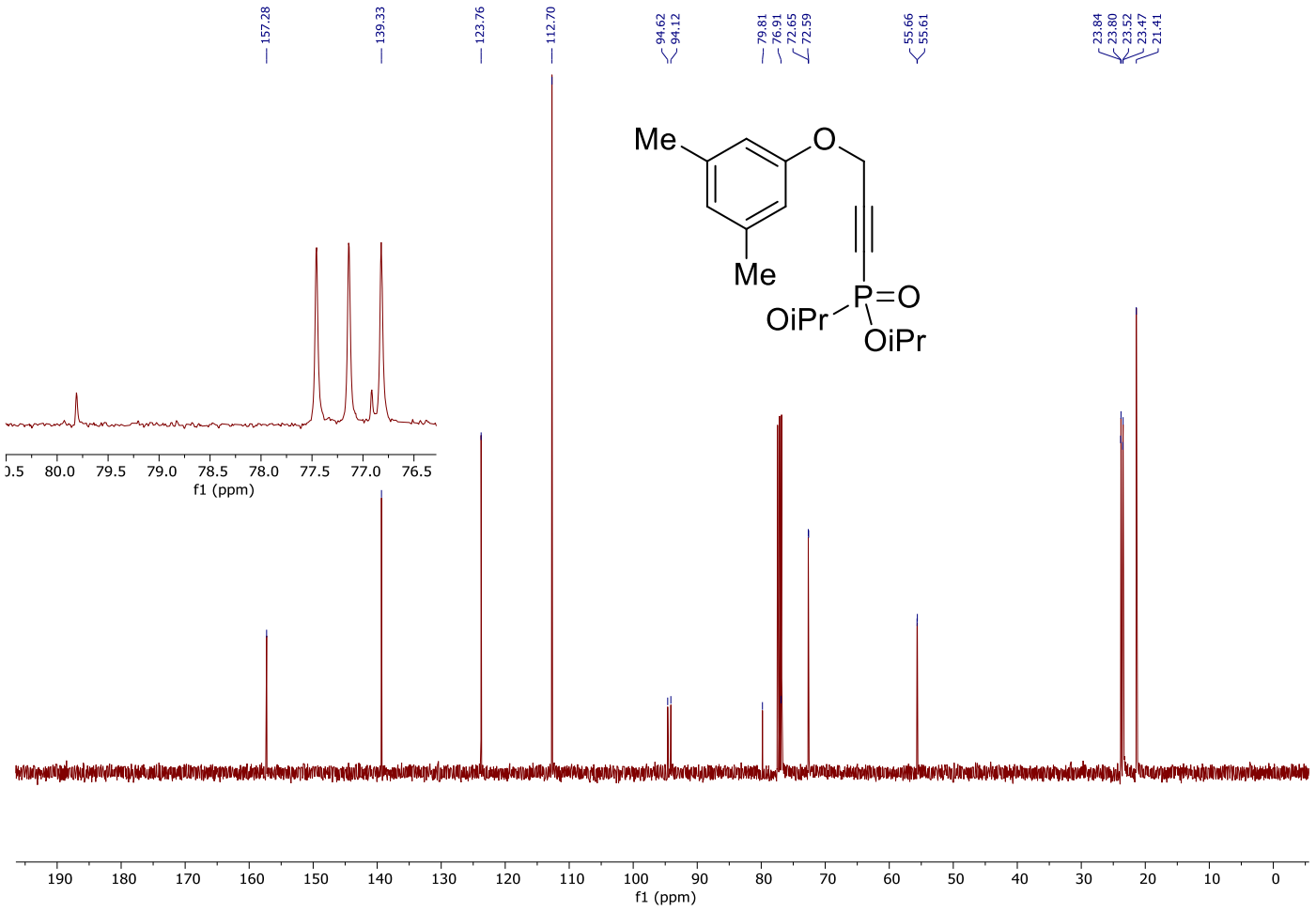


Figure S56: ^{13}C NMR Spectra of 3t

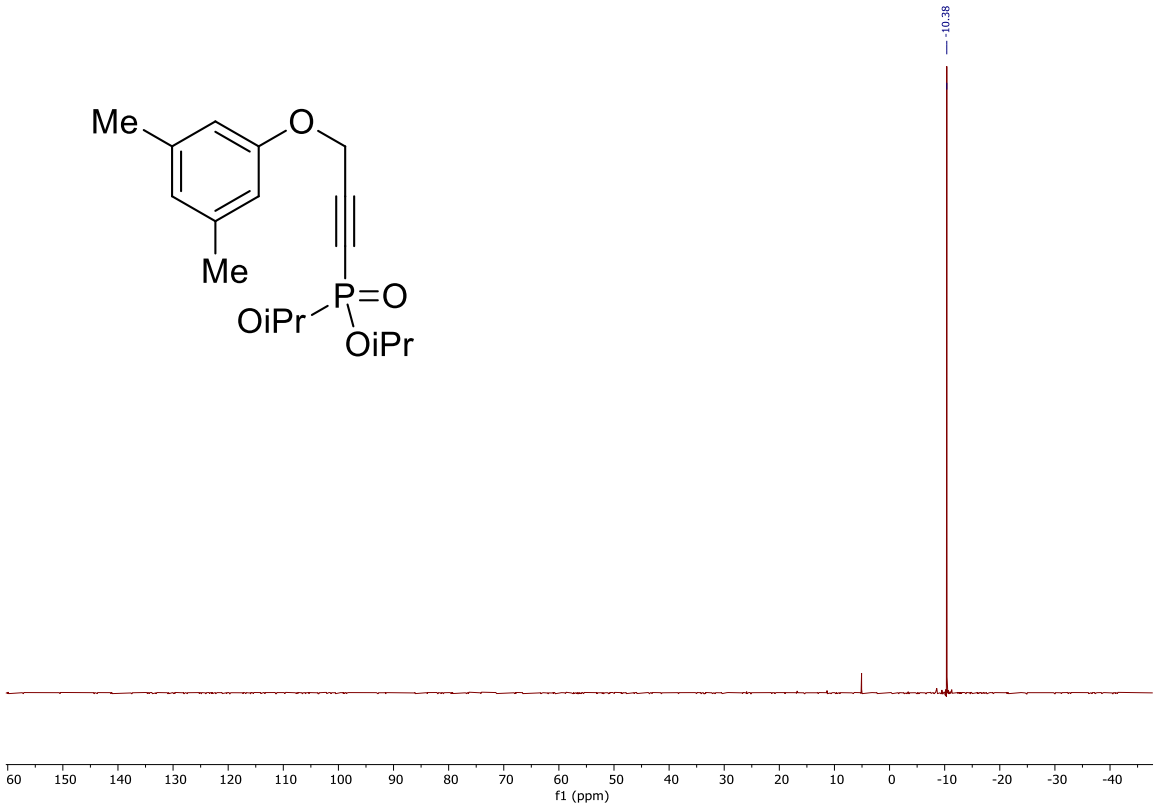


Figure S57: ^{31}P NMR Spectra of 3t