

**Supporting Information – Part A**

**The study of *cis-trans* isomerization preference of N–alkylated peptides containing phosphorus in the side chain and backbone.**

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### Spectra's of compounds

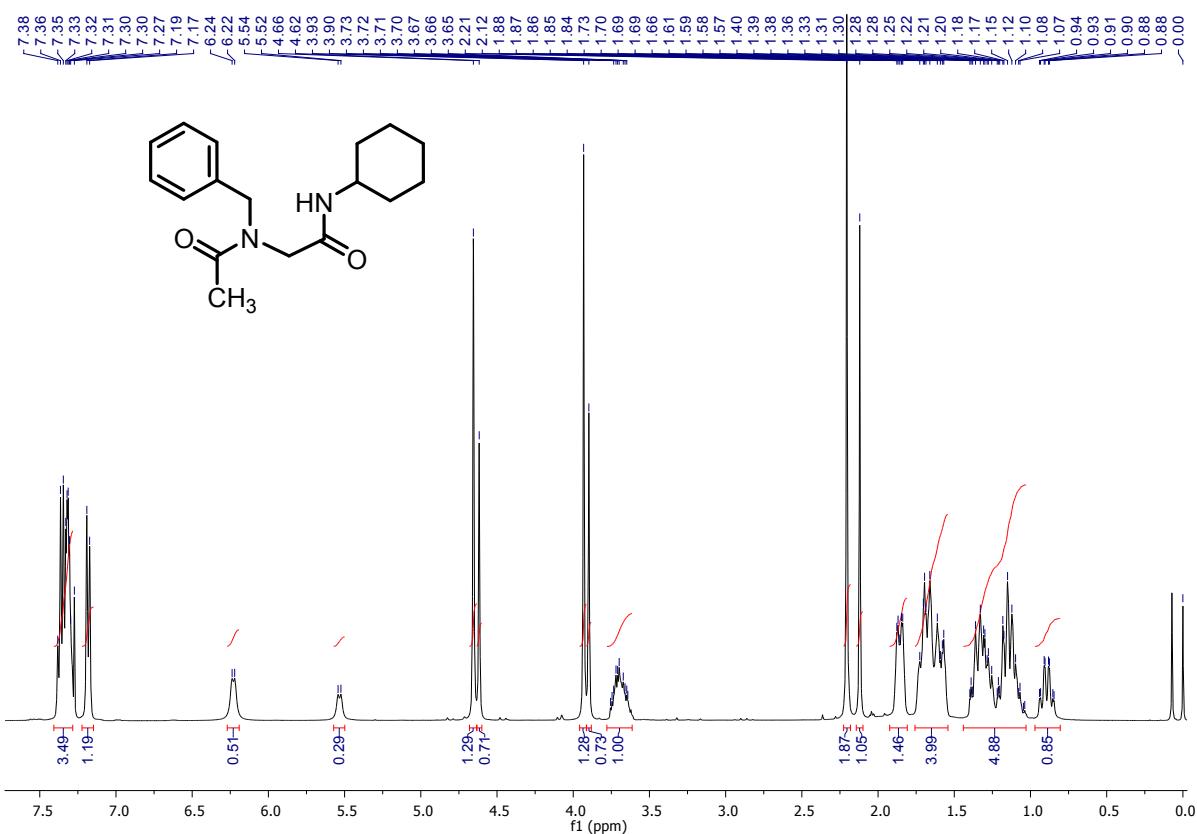


FIGURE 1. 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **1**.

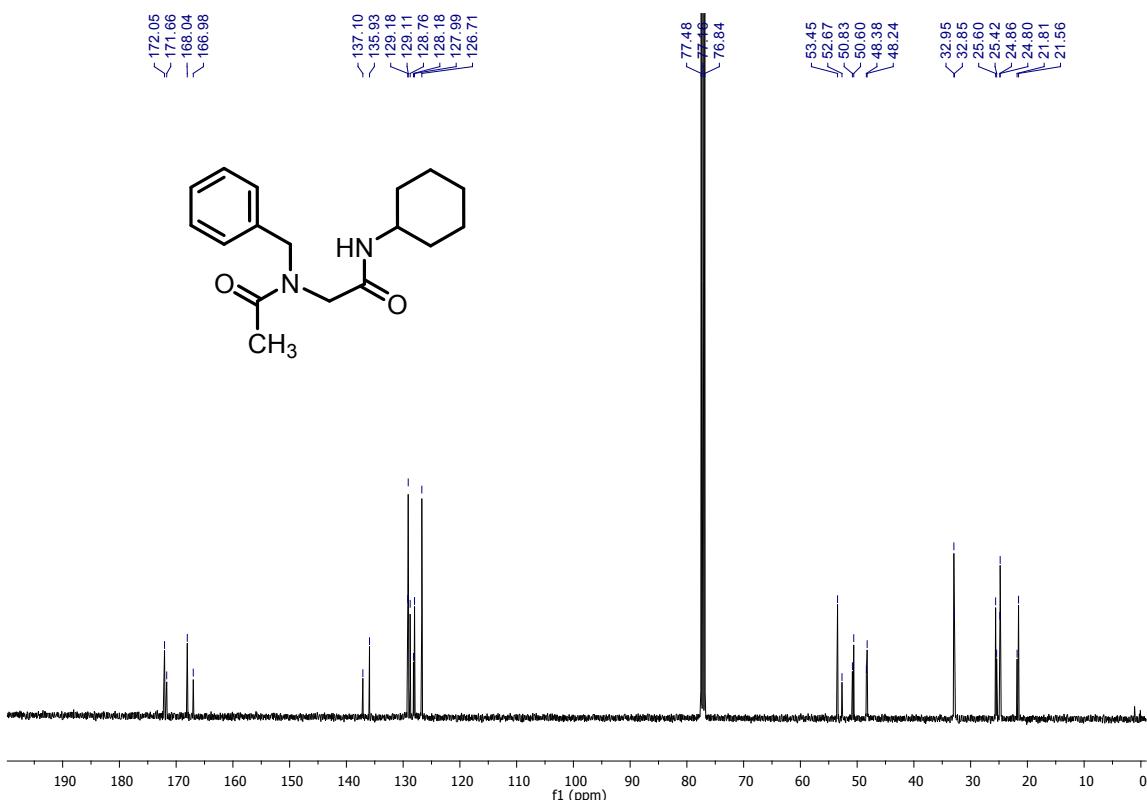


FIGURE 2: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **1**.

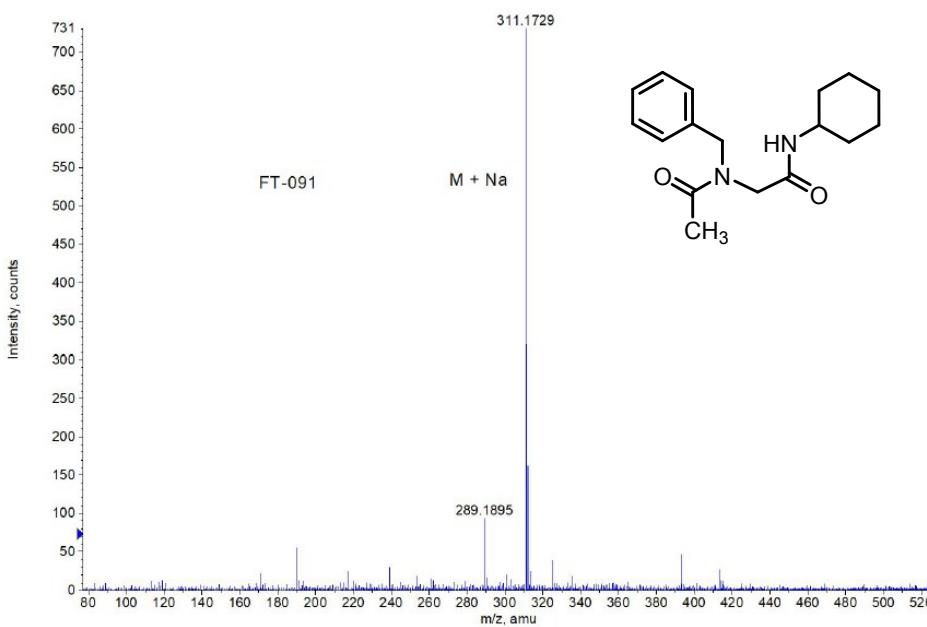
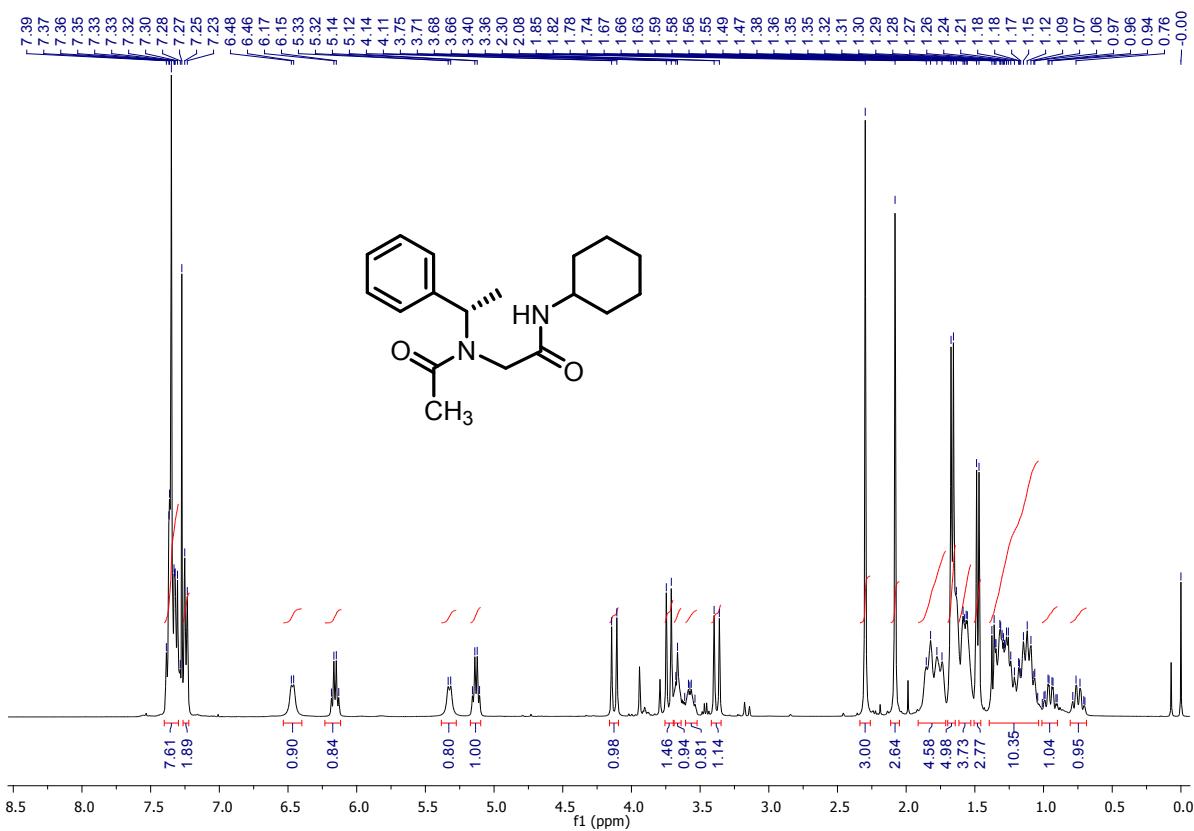


FIGURE 3- HRMS (ESI-FT-ICR)  $m/z$  spectrum of **1**.



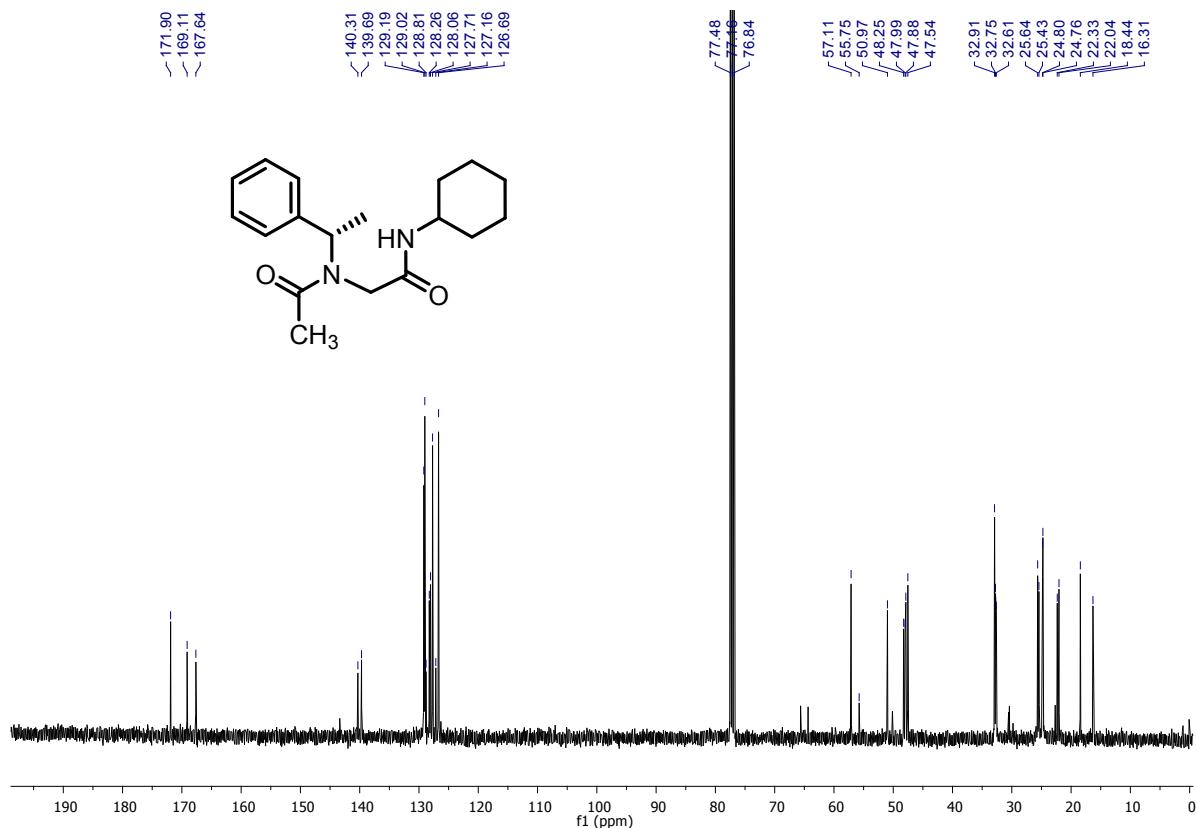


FIGURE 5: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **2**.

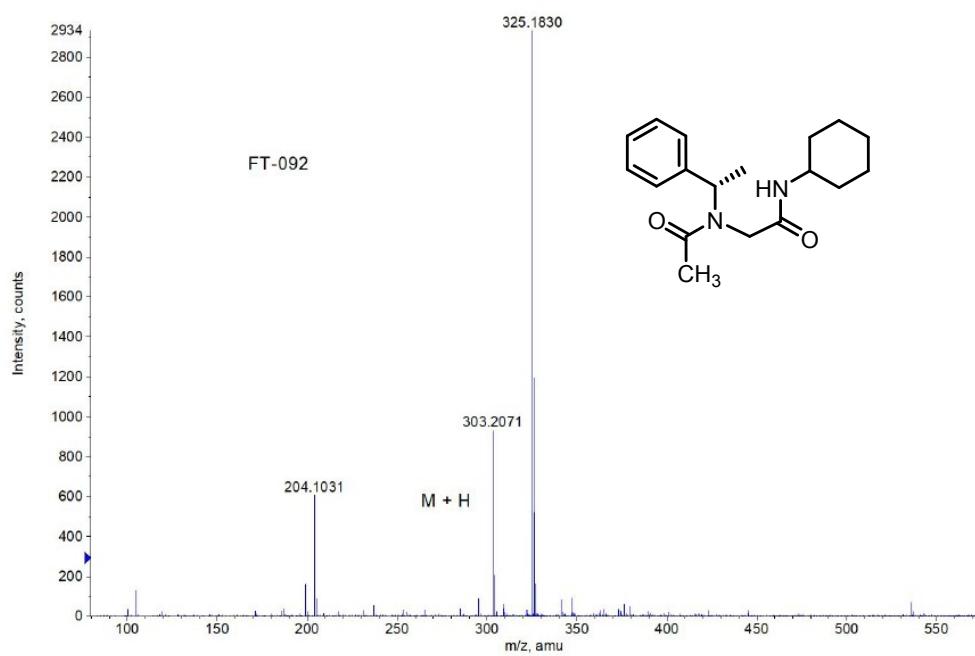


FIGURE 6- HRMS (ESI-FT-ICR)  $m/z$  spectrum of **2**.

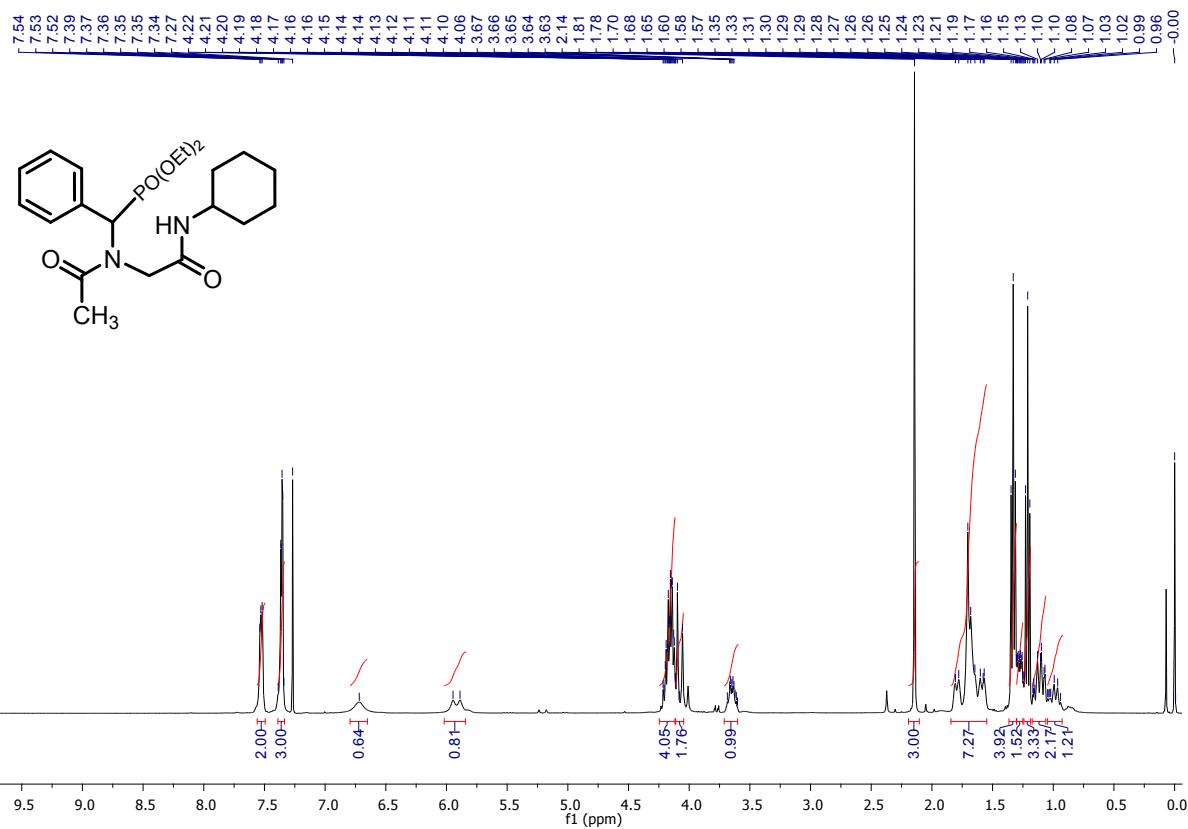


FIGURE 7: 400 MHz <sup>1</sup>H NMR spectrum in CDCl<sub>3</sub> of **3**.

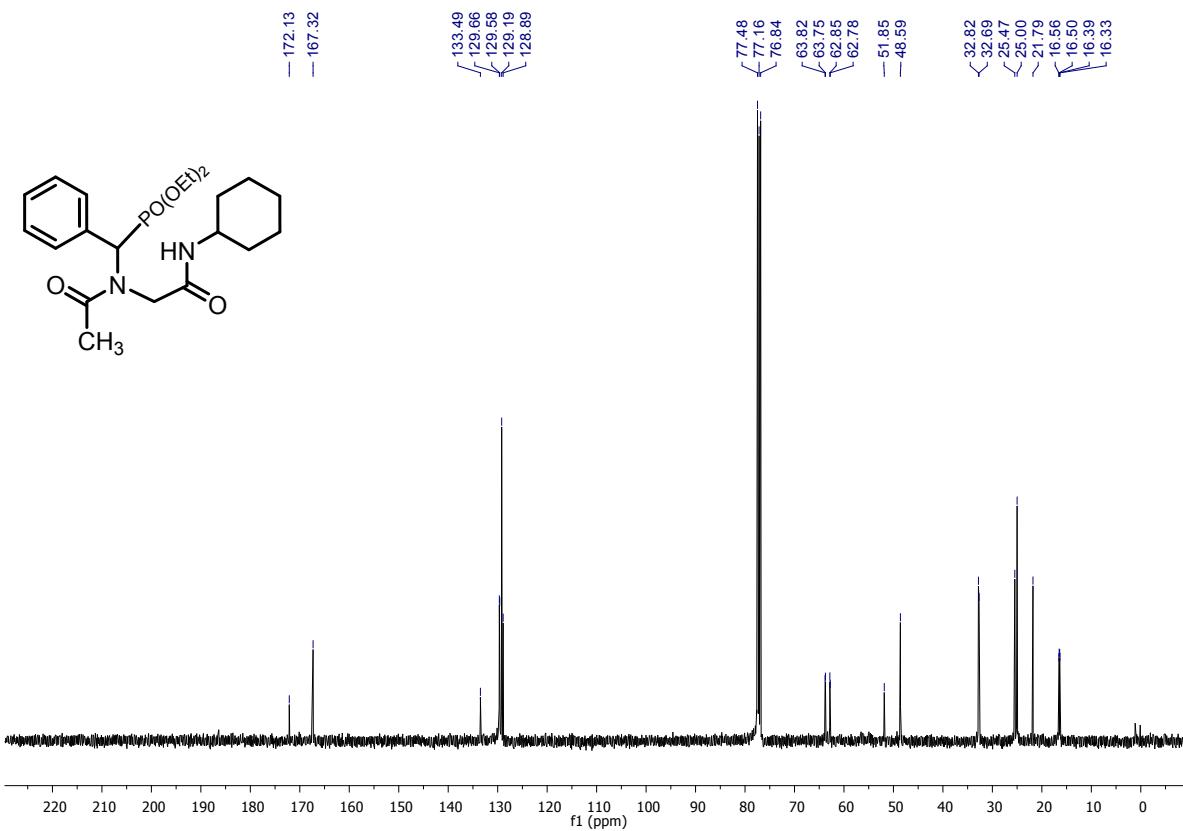


FIGURE 8: 100 MHz <sup>13</sup>C NMR spectrum in CDCl<sub>3</sub> of **3**.

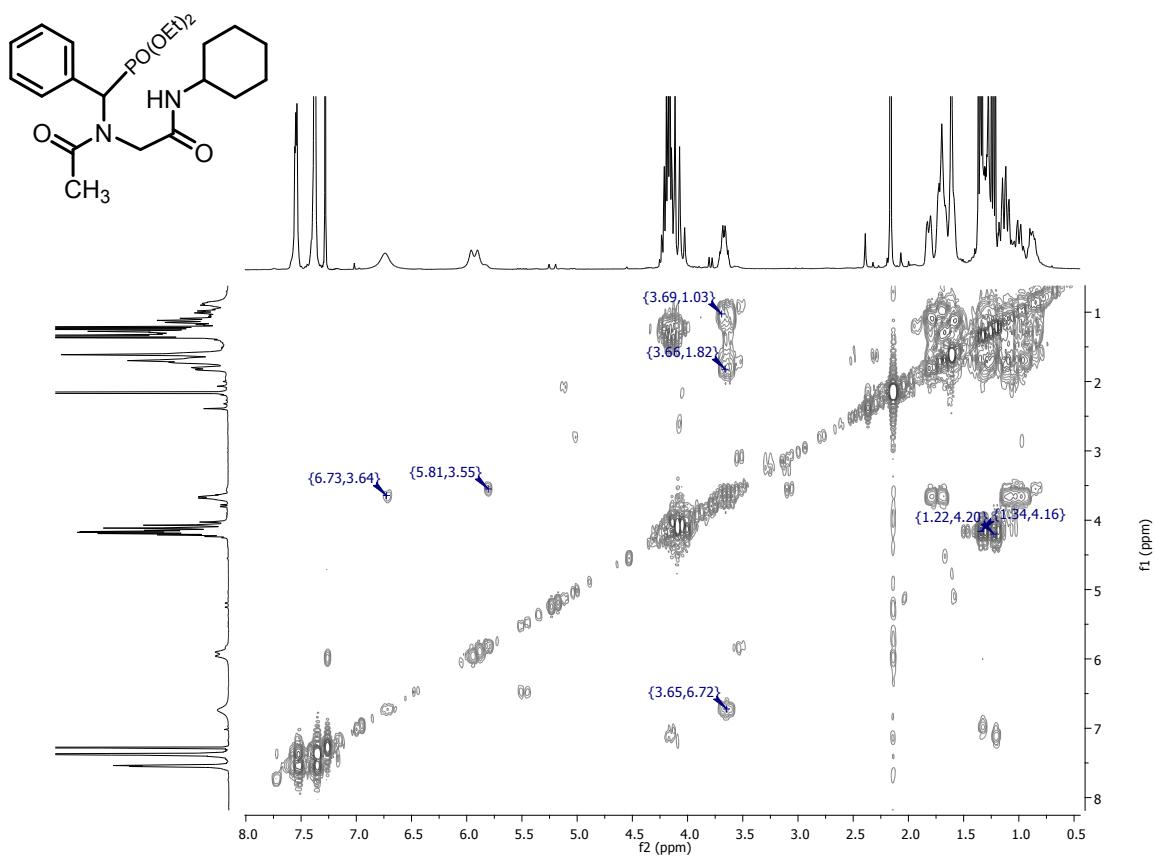


FIGURE 9: COSY spectrum in  $\text{CDCl}_3$  of **3**.

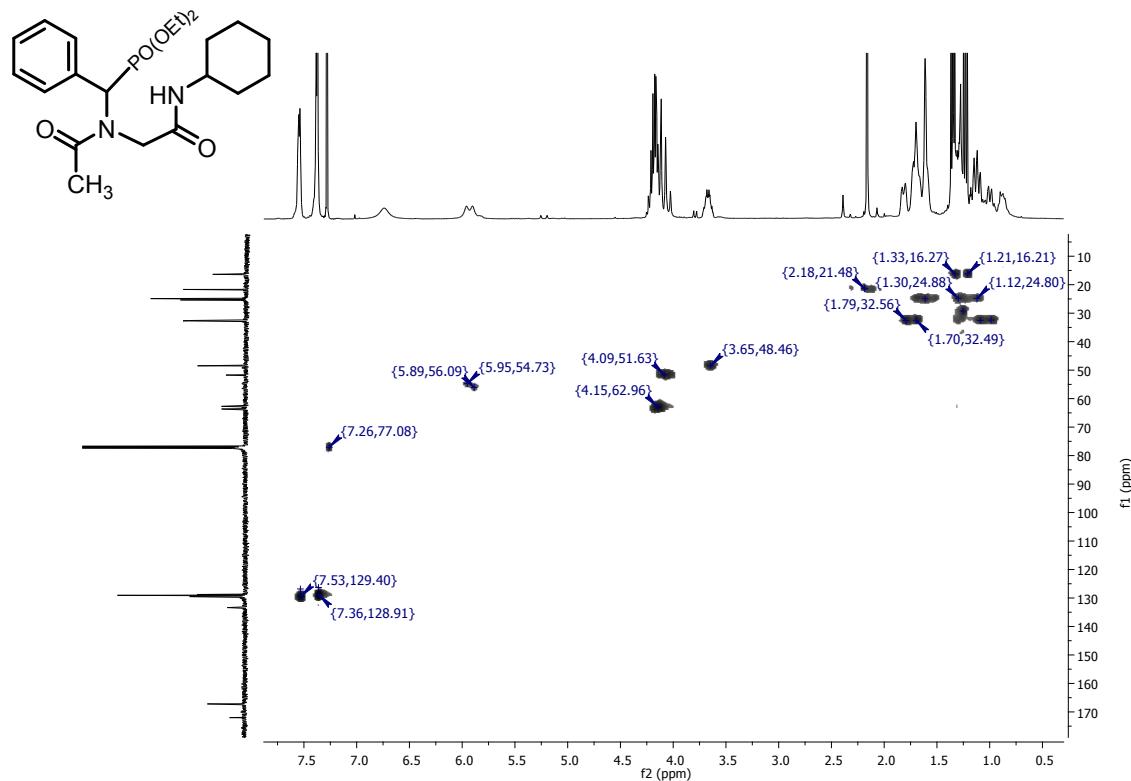


FIGURE 10: HSQC spectrum in  $\text{CDCl}_3$  of **3**.

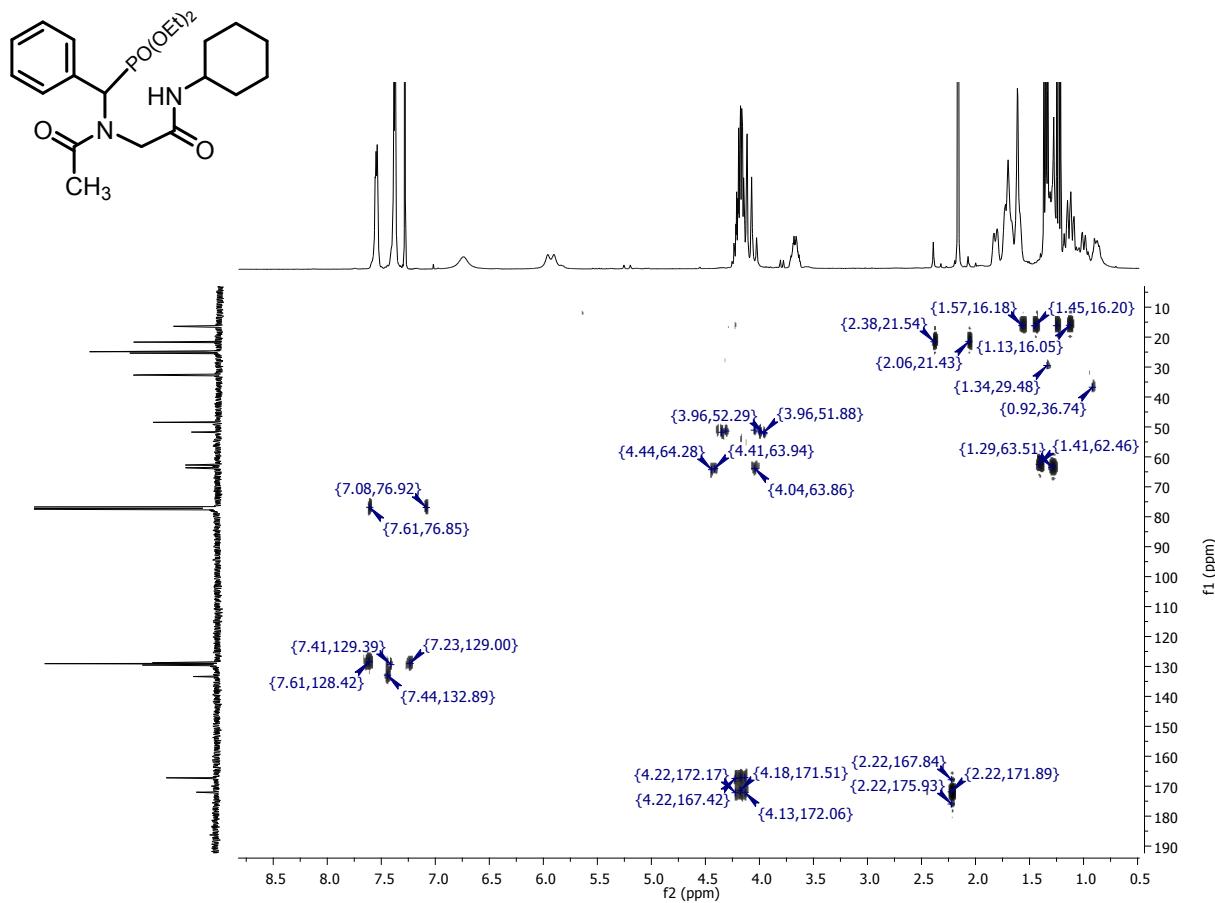


FIGURE 11: HMBC spectrum in  $\text{CDCl}_3$  of **3**.

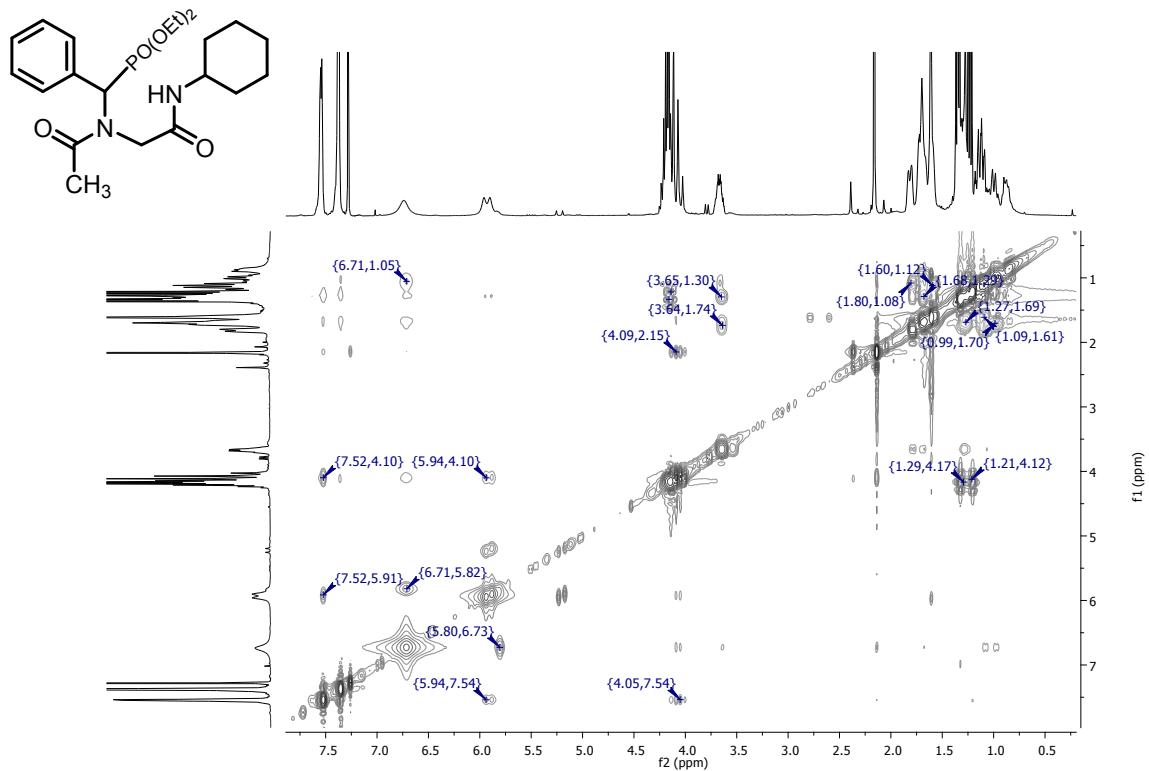


FIGURE 12: NOESY spectrum in  $\text{CDCl}_3$  of **3**.

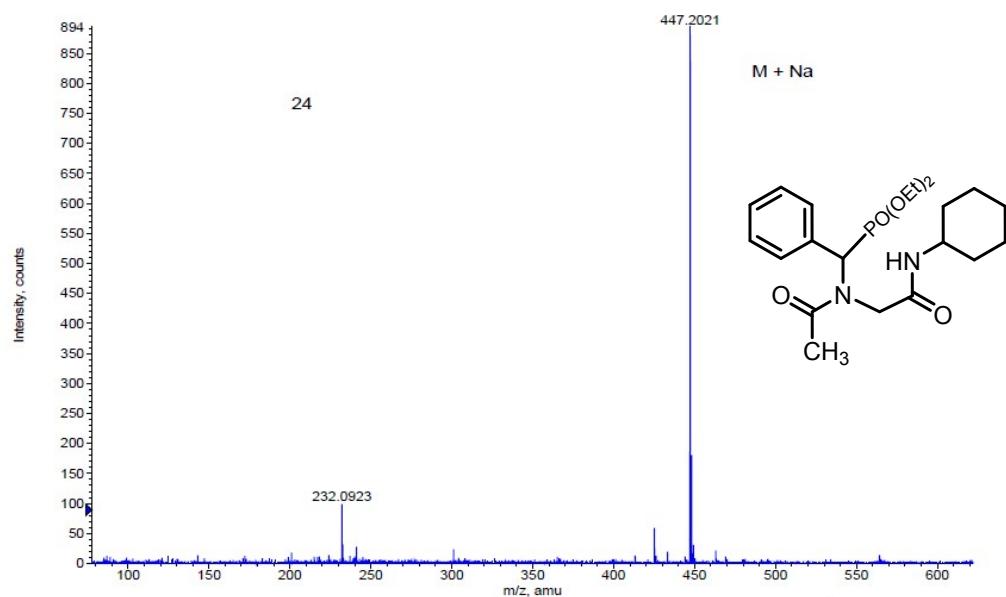


FIGURE 13- HRMS (ESI-FT-ICR)  $m/z$  spectrum of 3.

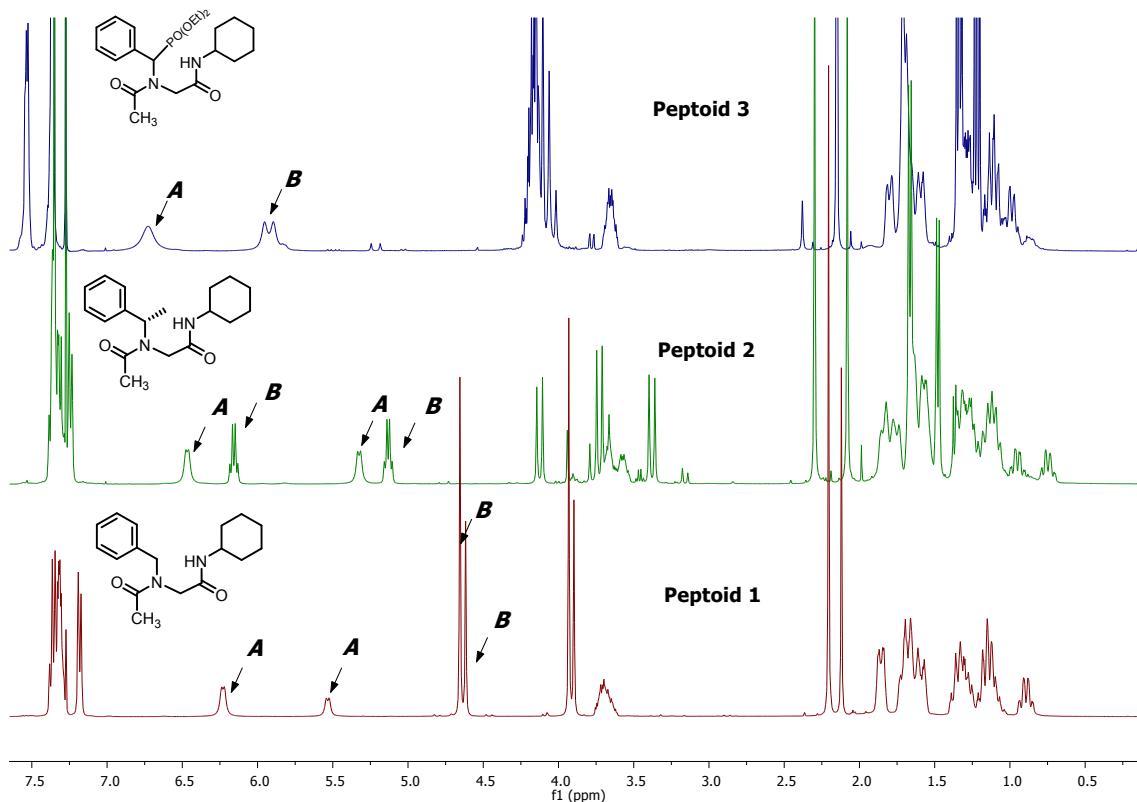


FIGURE 14- 400 MHz  $^1\text{H}$  NMR spectra in  $\text{CDCl}_3$  of compounds 1 (redline), 2 (greenline) and 3 (blueline). (A) correspond to NH of secondary amide and (B) correspond to protons of CH groups that support  $\text{R}^2$  substitutions.

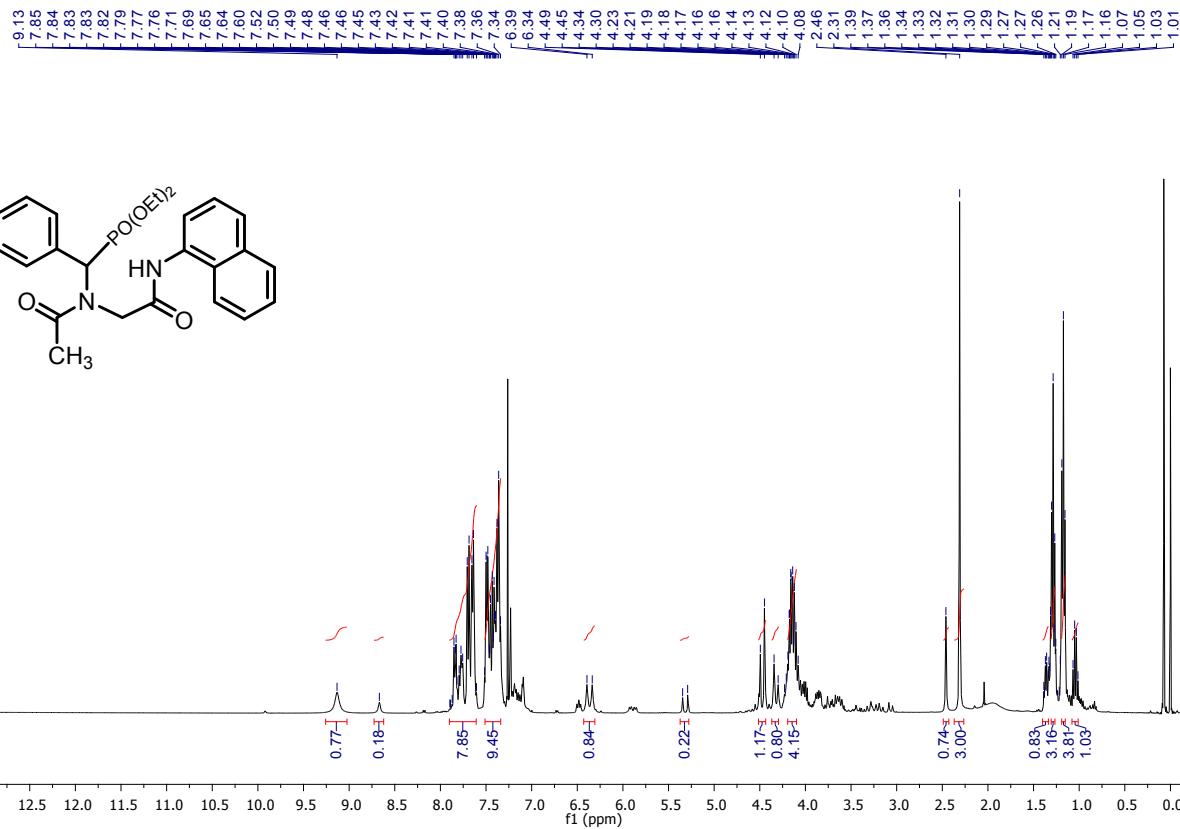


FIGURE 15: 400 MHz <sup>1</sup>H NMR spectrum in CDCl<sub>3</sub> of **4**.

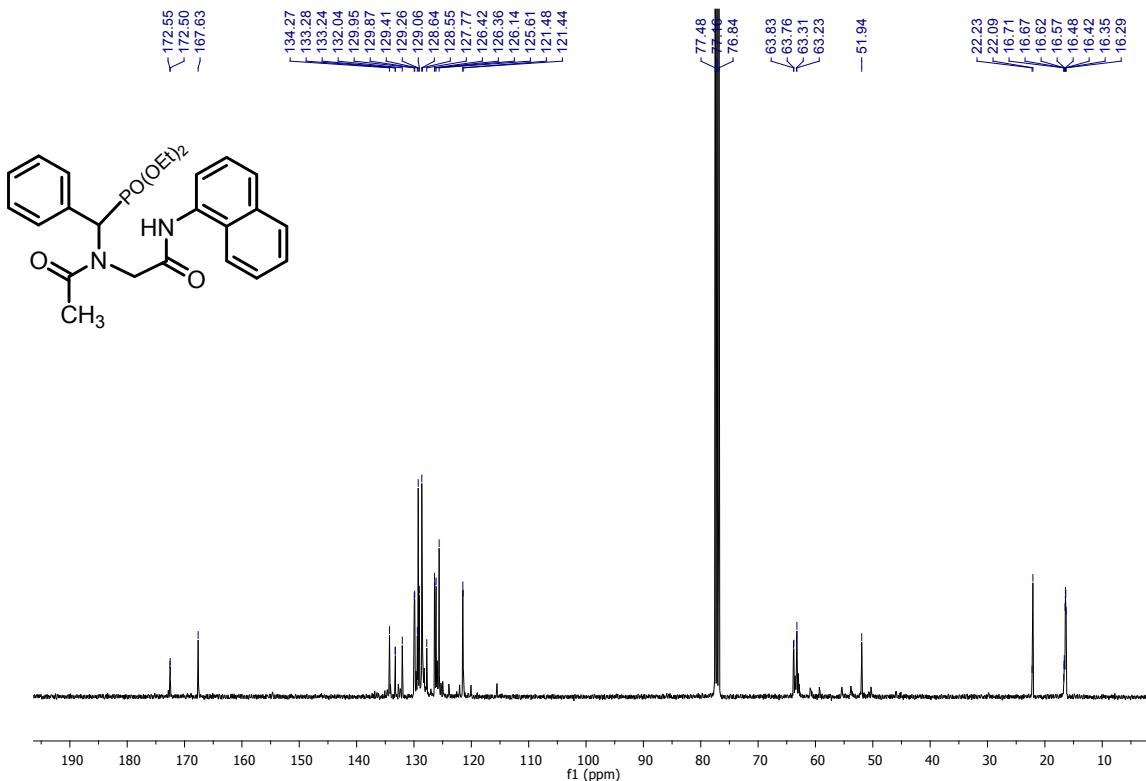


FIGURE 16: 100 MHz <sup>13</sup>C NMR spectrum in CDCl<sub>3</sub> of **4**.

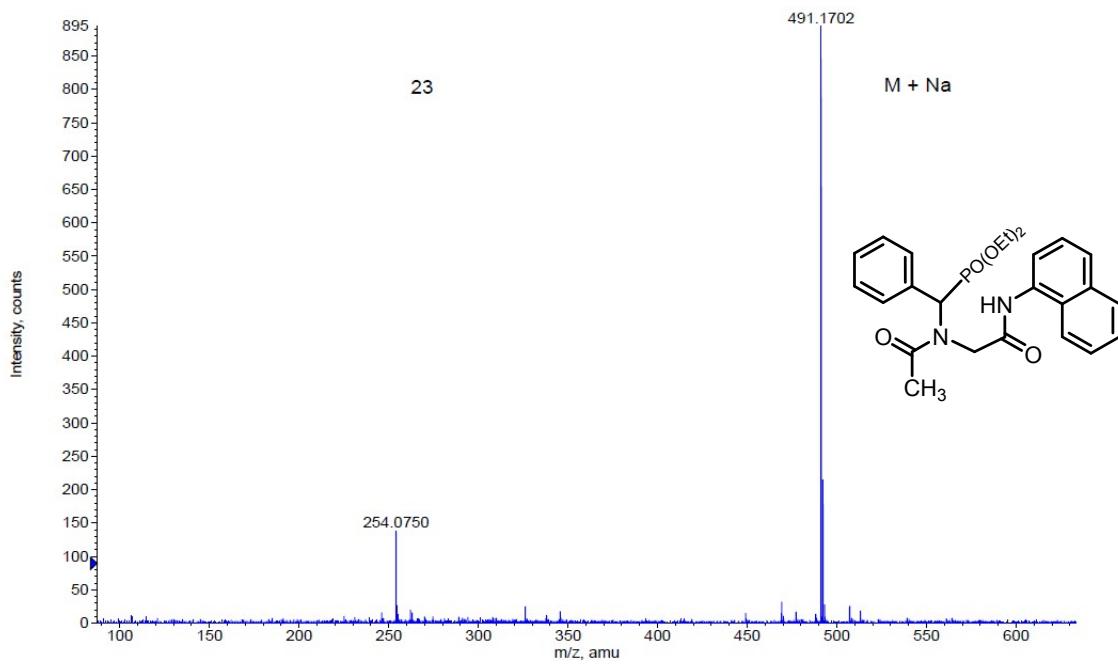


FIGURE 17- HRMS (ESI-FT-ICR)  $m/z$  spectrum of 4.

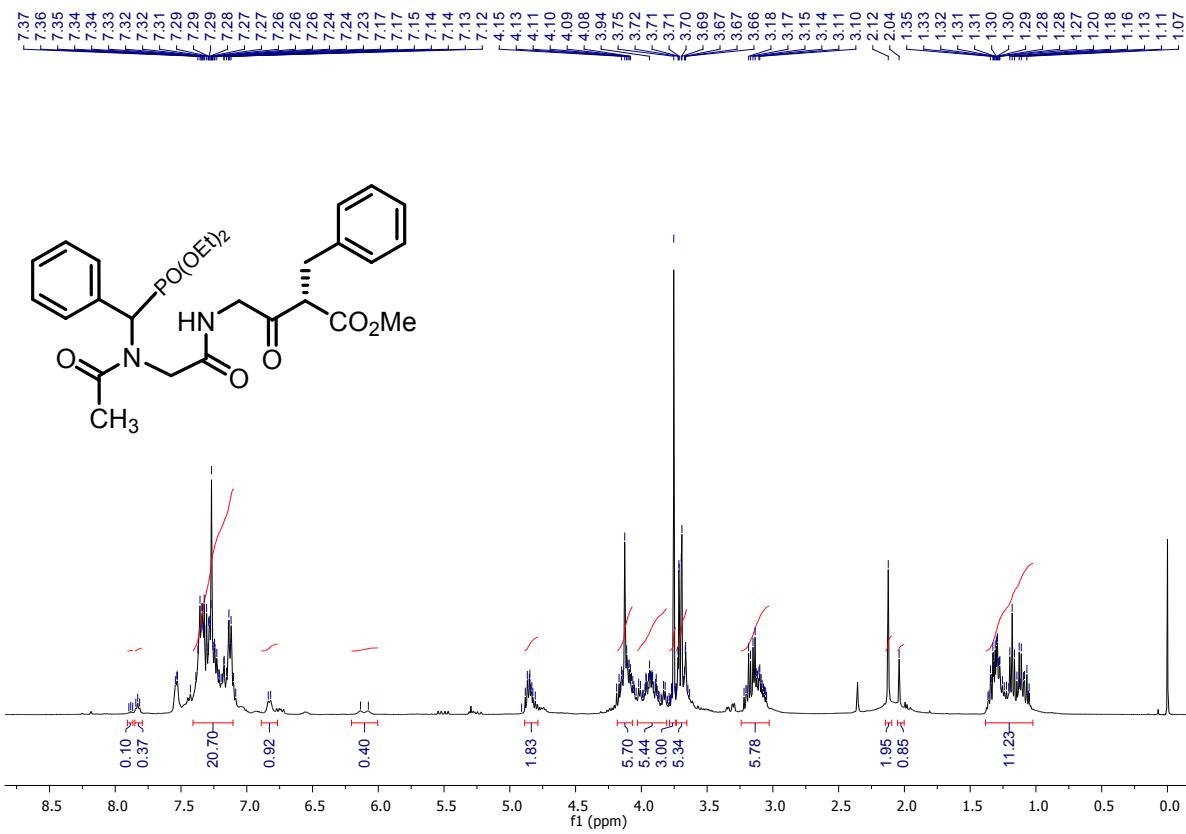


FIGURE 18: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of 5.

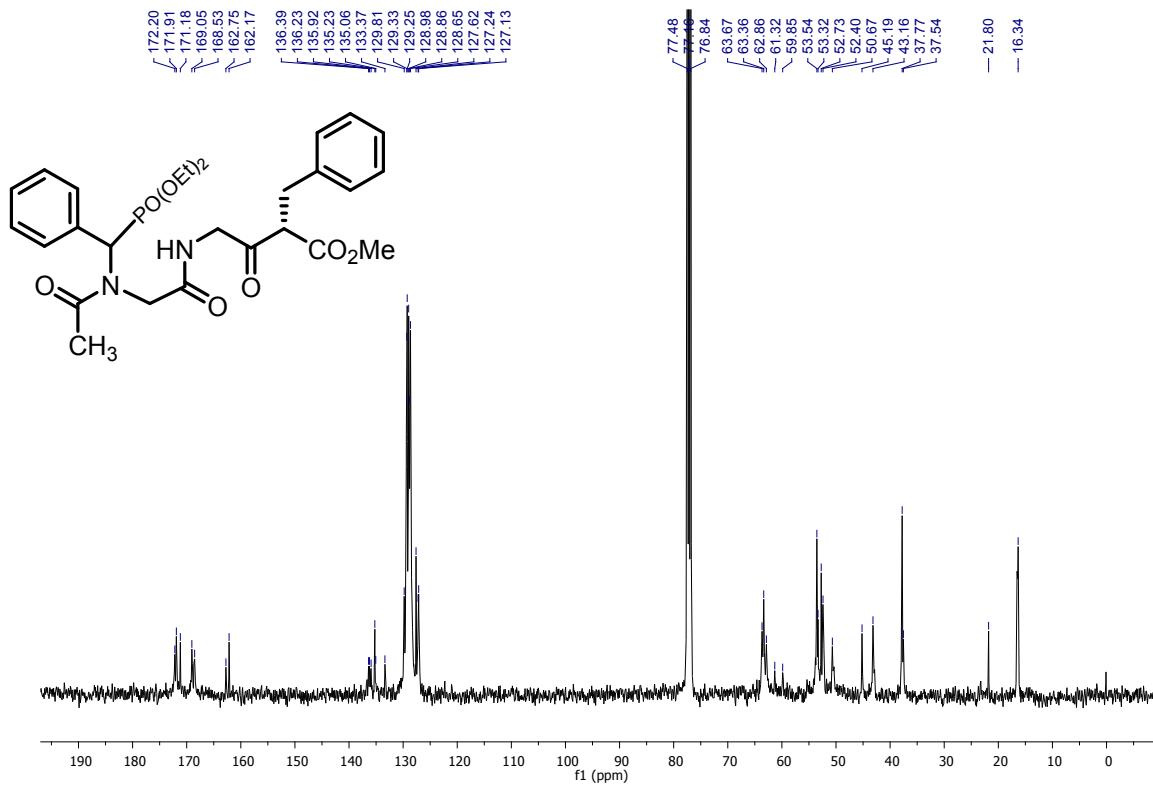


FIGURE 19: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **5**.

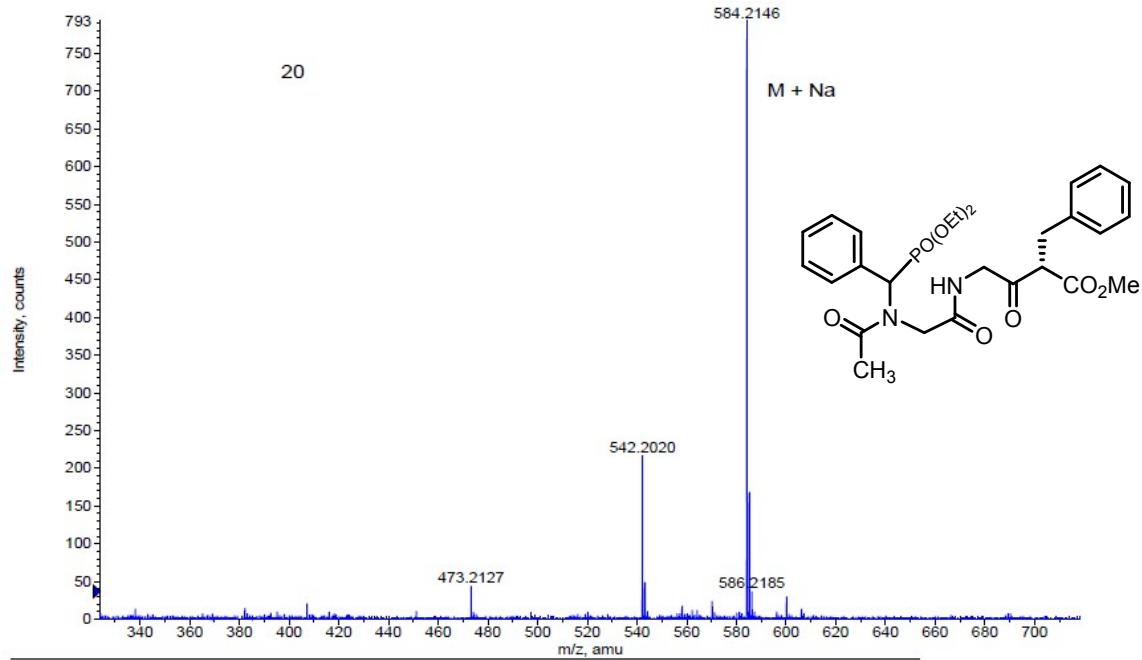


FIGURE 20- HRMS (ESI-FT-ICR)  $m/z$  spectrum of **5**.

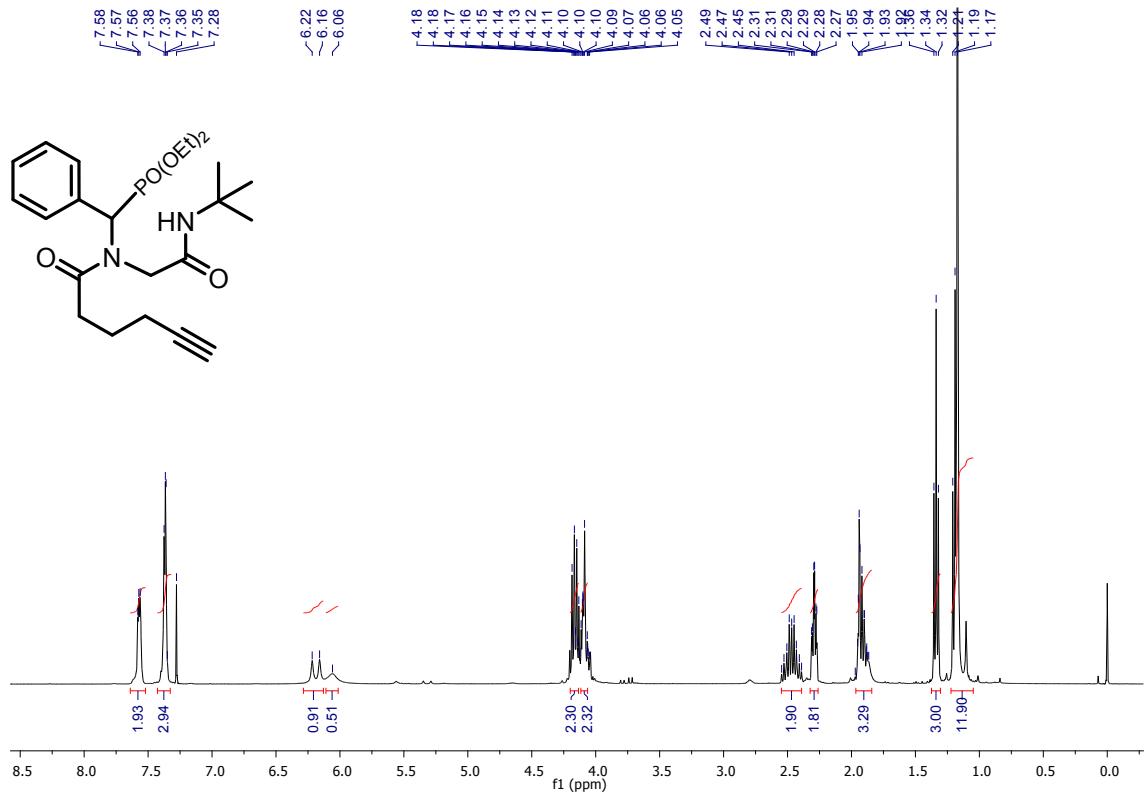


FIGURE 21: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **6**.

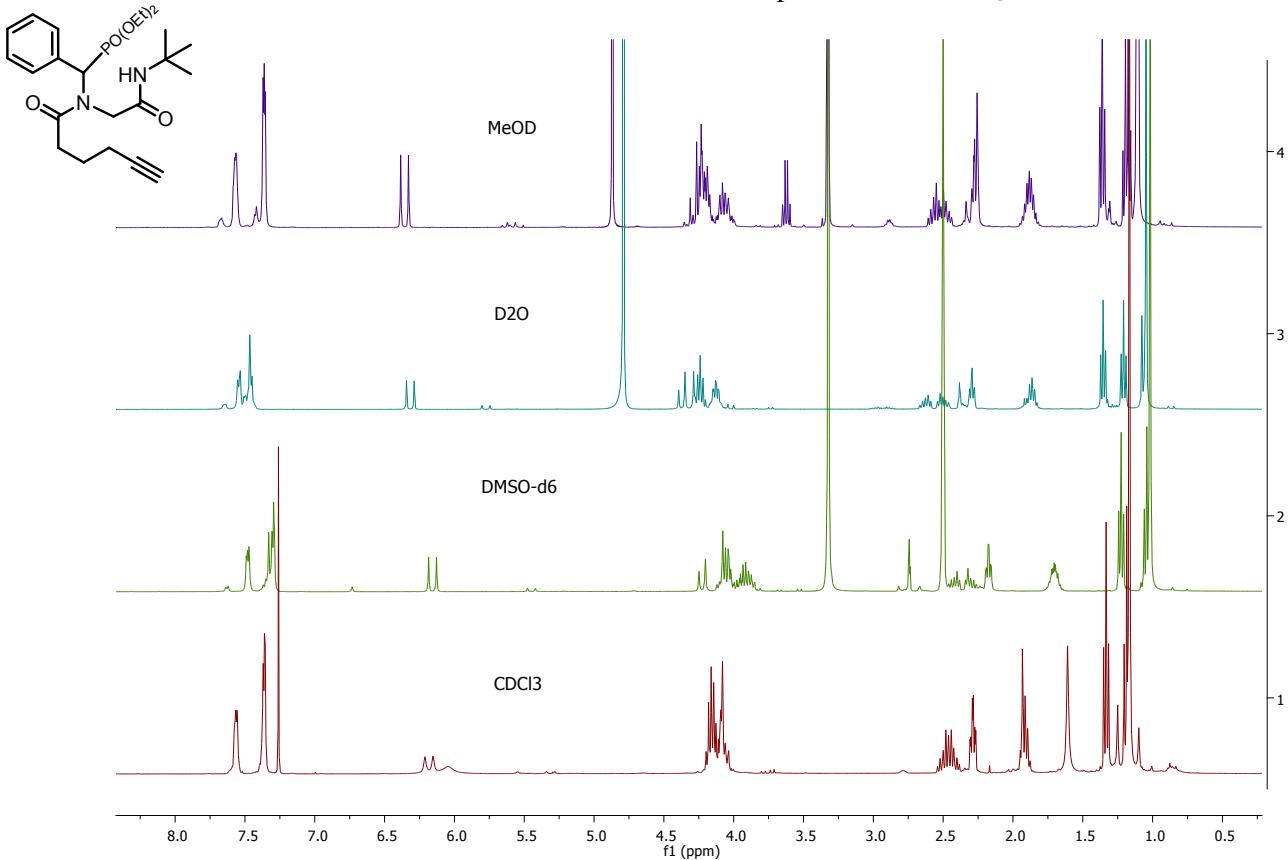


FIGURE 22: 400 MHz  $^1\text{H}$  NMR spectra of **6** in different deuterated solvents at 15 mM.

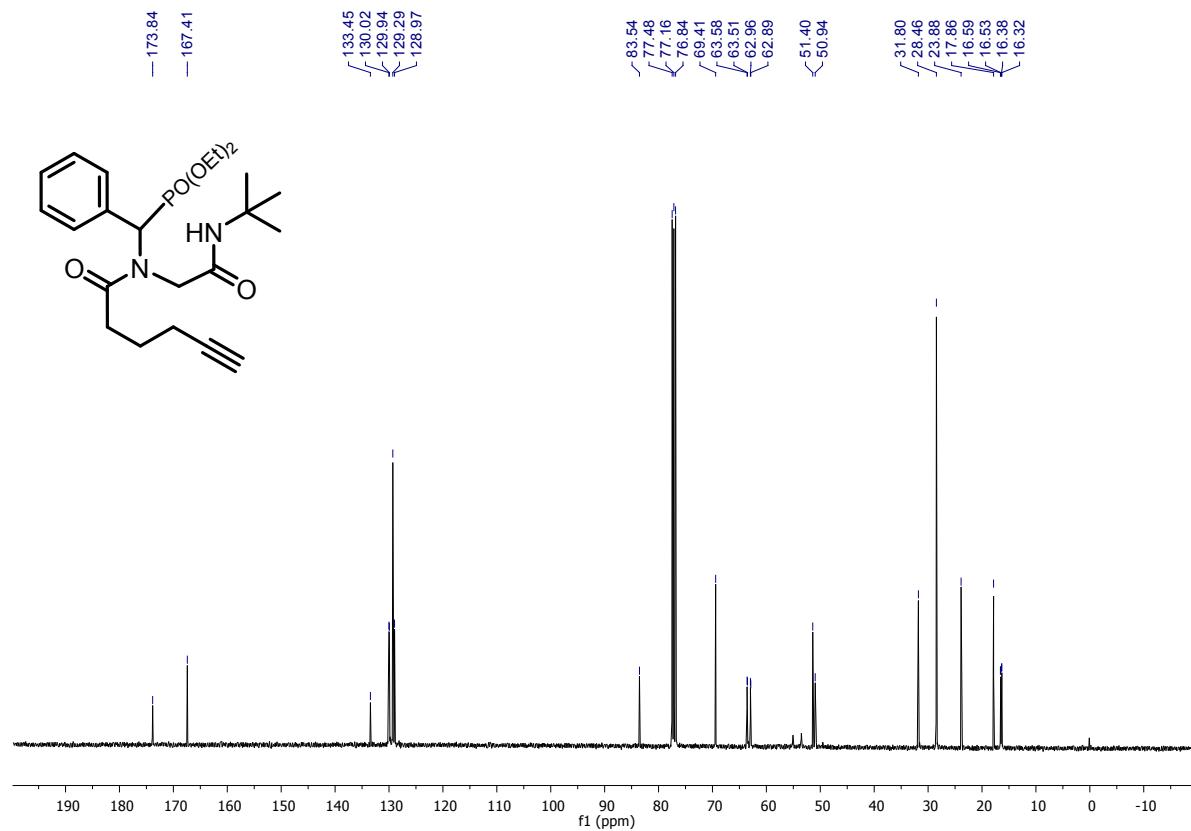


FIGURE 23: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **6**.

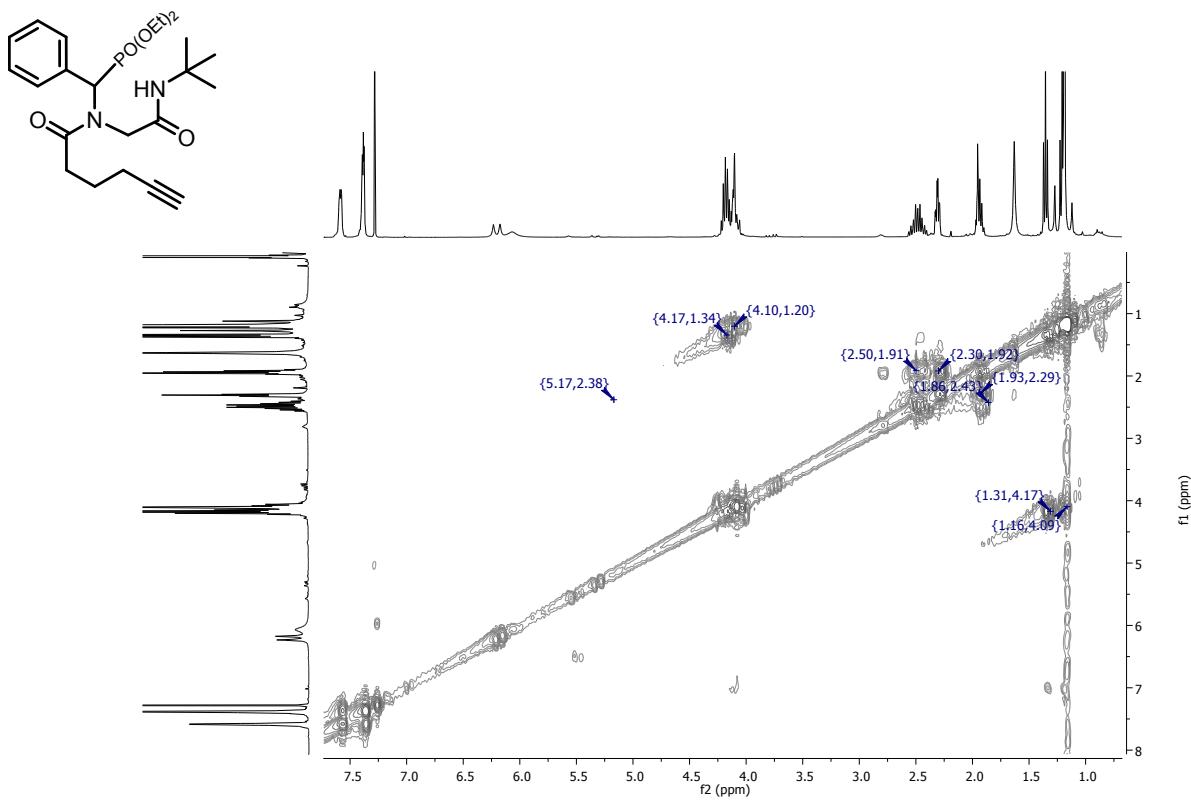


FIGURE 24: 400 MHz COSY spectrum in  $\text{CDCl}_3$  of **6**.

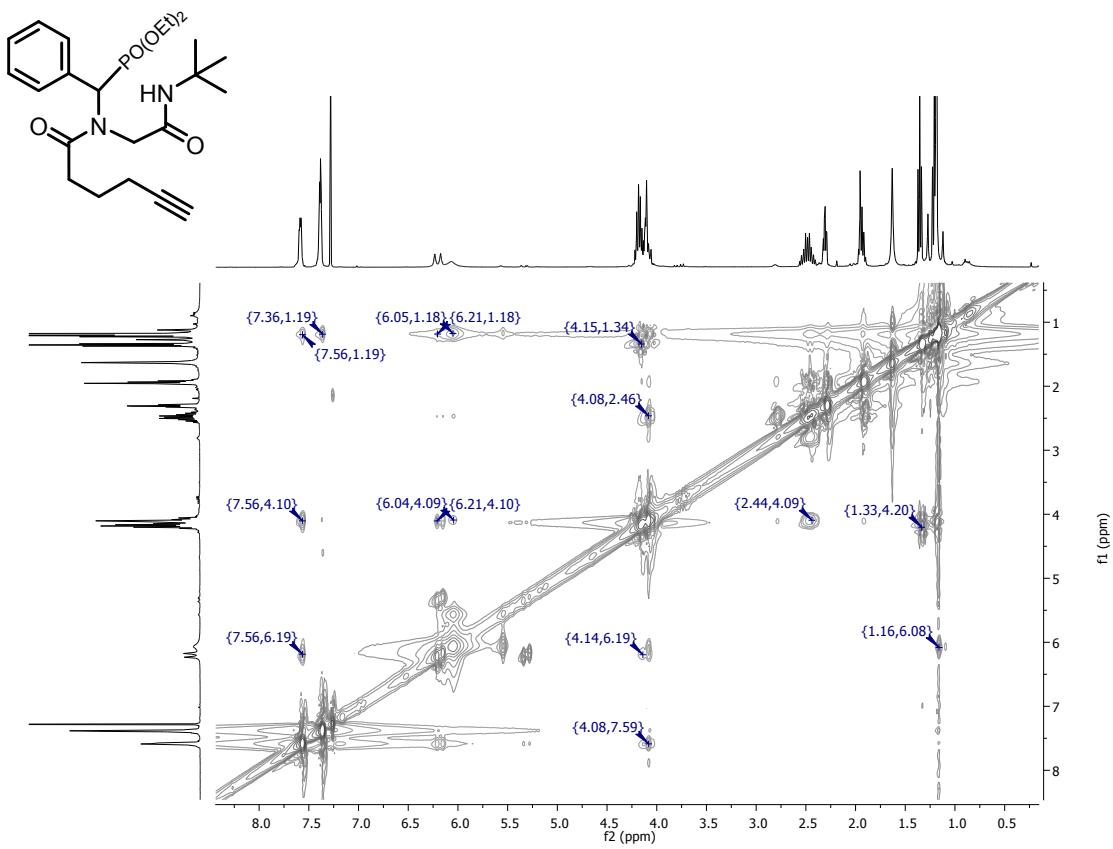


FIGURE 25: 400 MHz NOESY spectrum in  $\text{CDCl}_3$  of **6**.

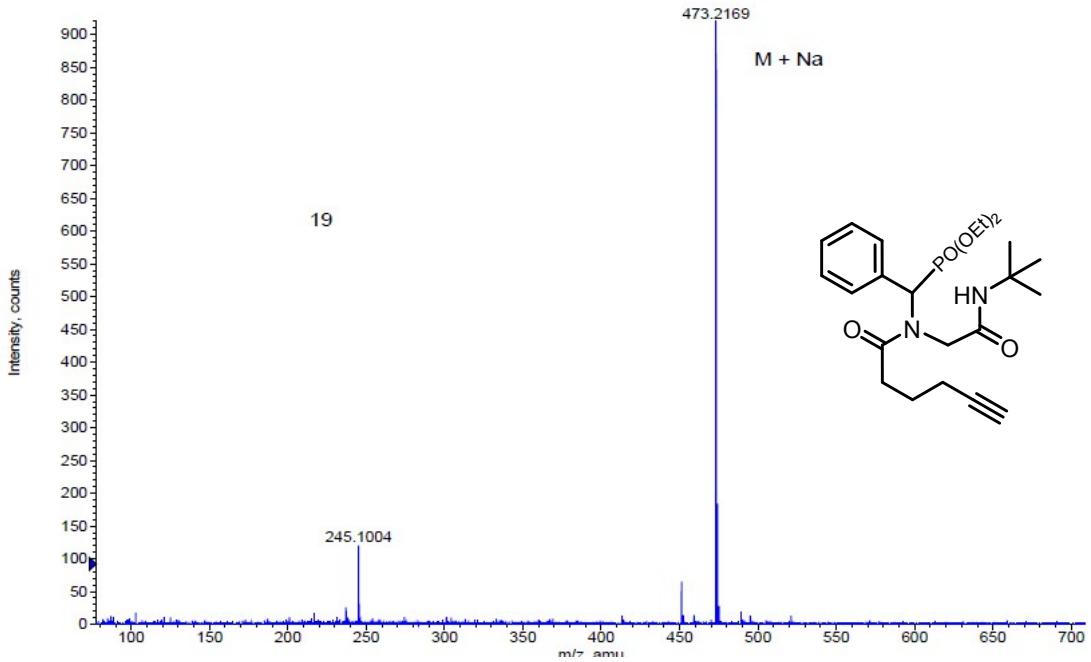


FIGURE 26- HRMS (ESI-FT-ICR) m/z spectrum of **6**.

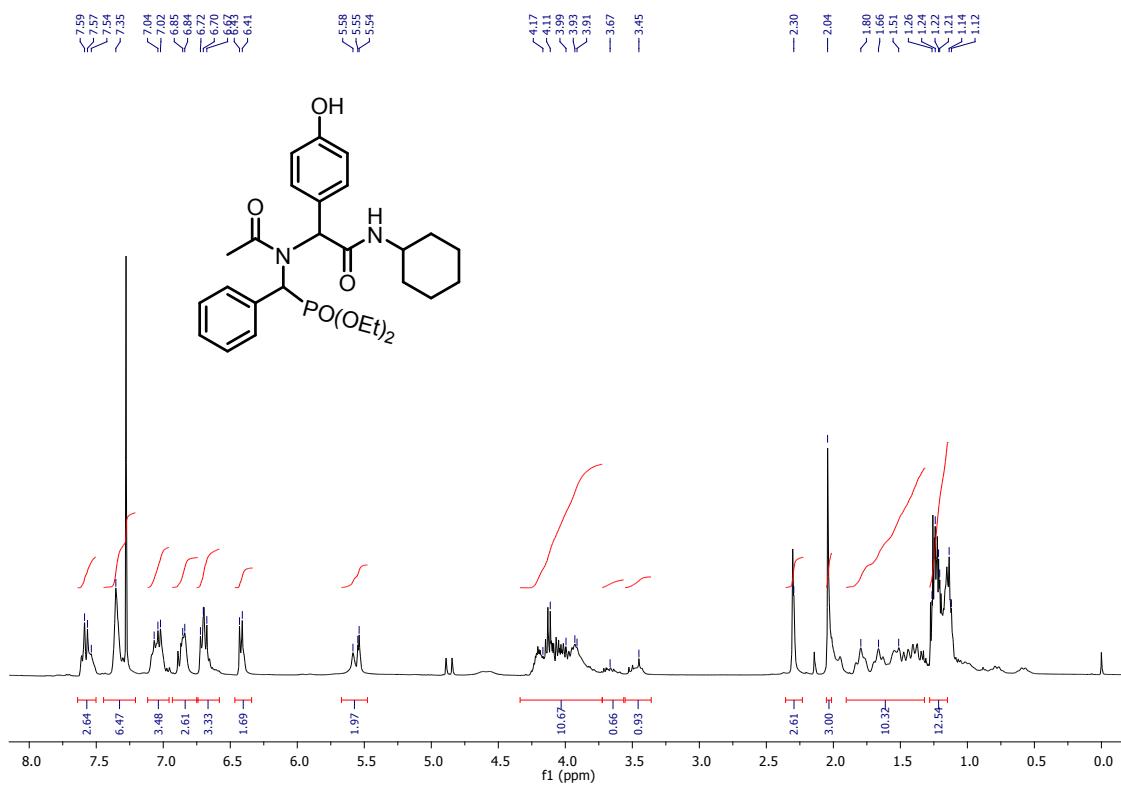


FIGURE 27: 400 MHz <sup>1</sup>H NMR spectrum in CDCl<sub>3</sub> of 7.

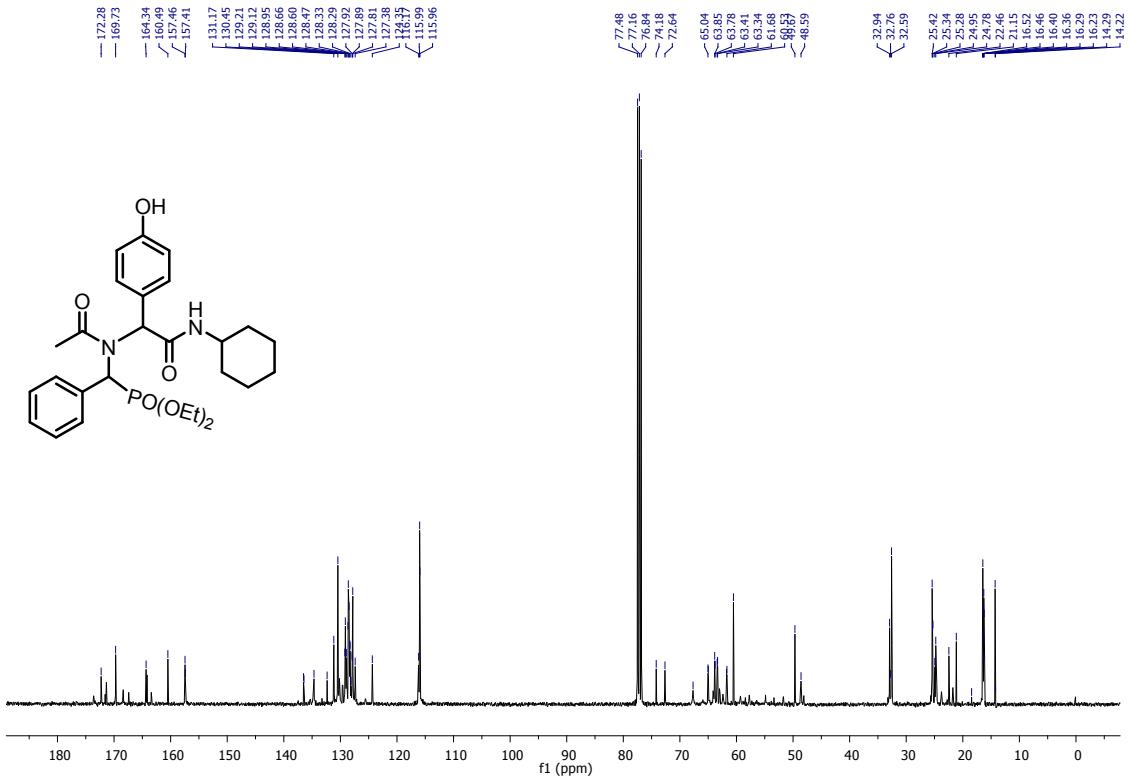


FIGURE 28: 100 MHz <sup>13</sup>C NMR spectrum in CDCl<sub>3</sub> of 7.

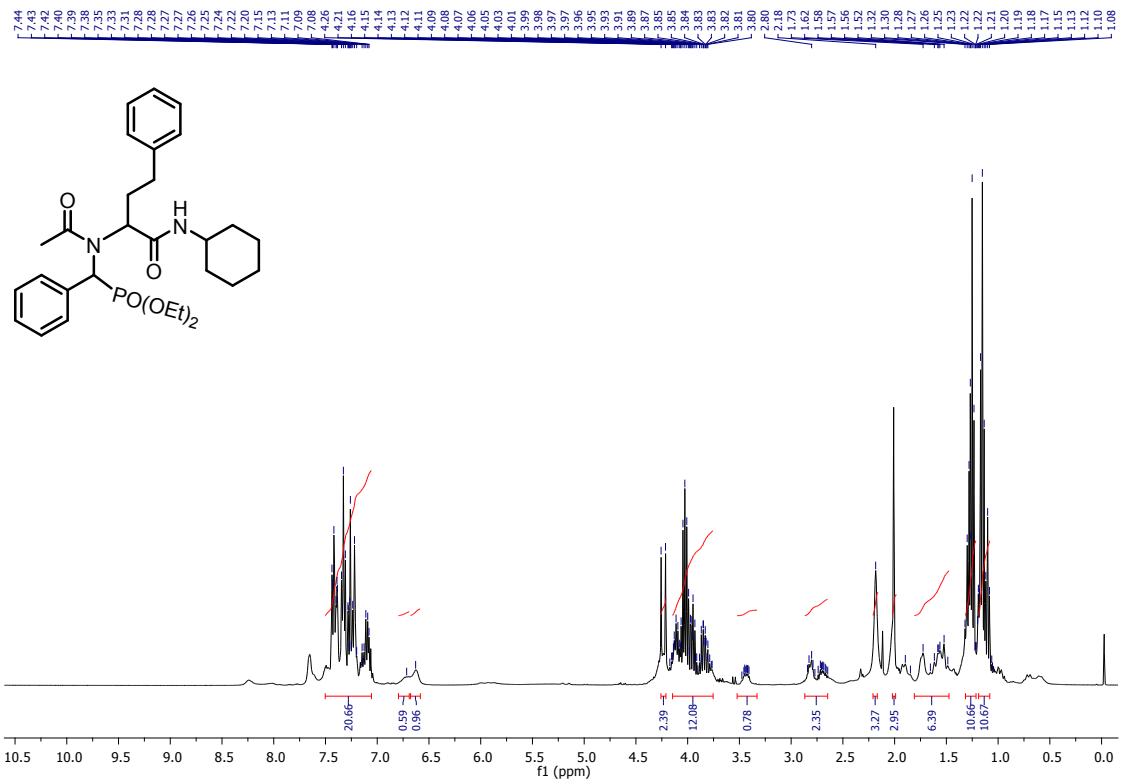


FIGURE 29: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **8**.

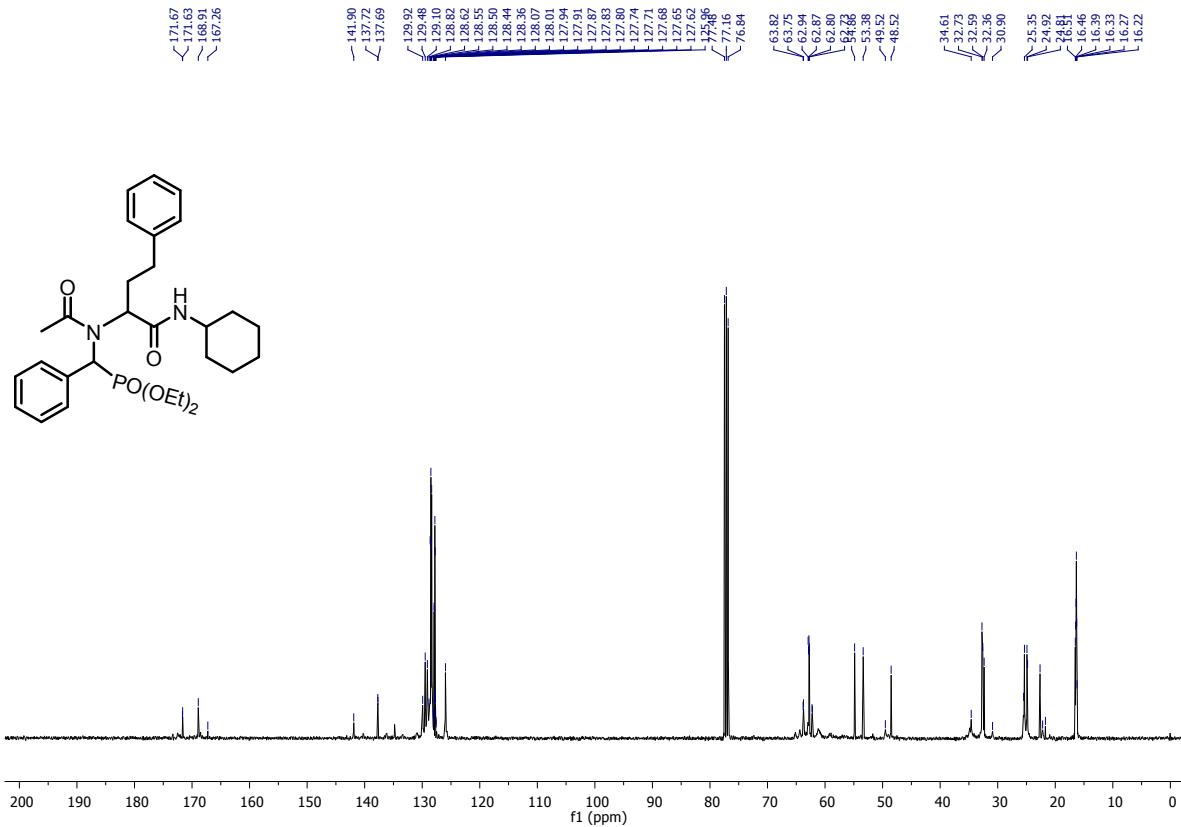


FIGURE 30: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **8**.

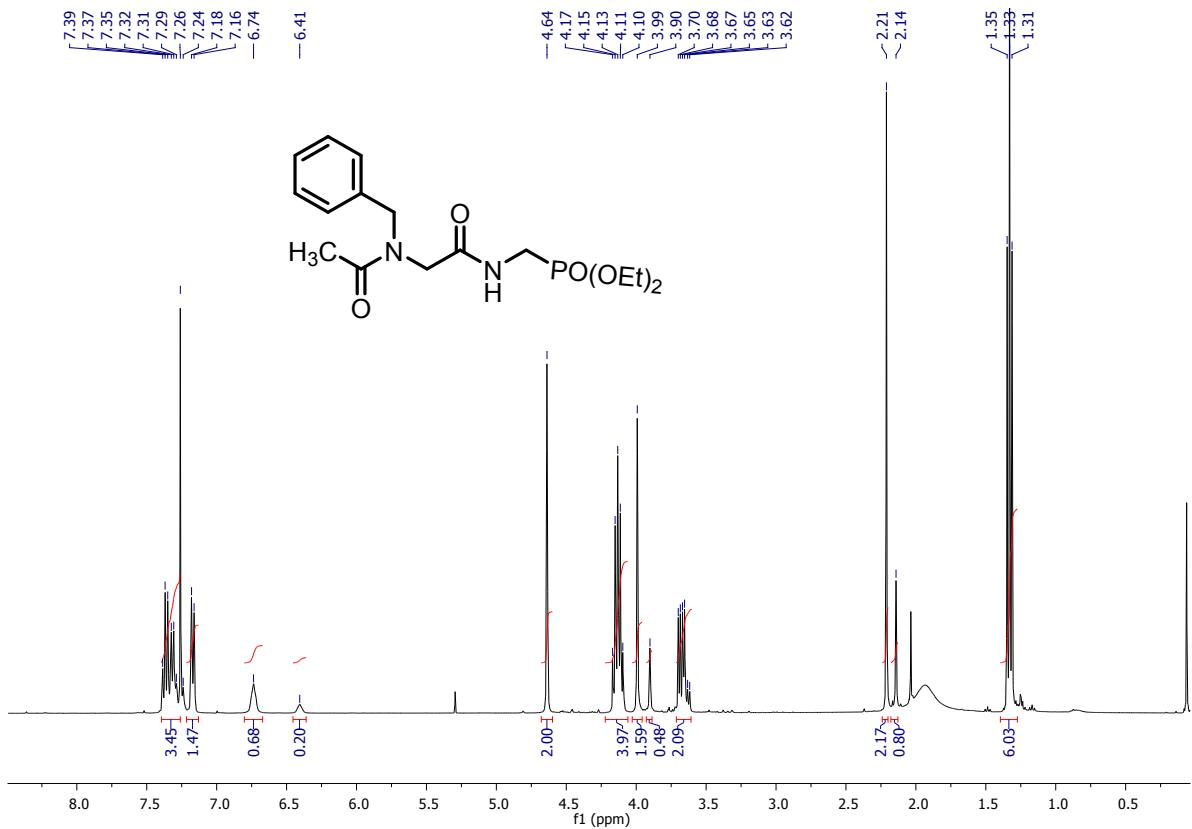


FIGURE 31: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **9**.

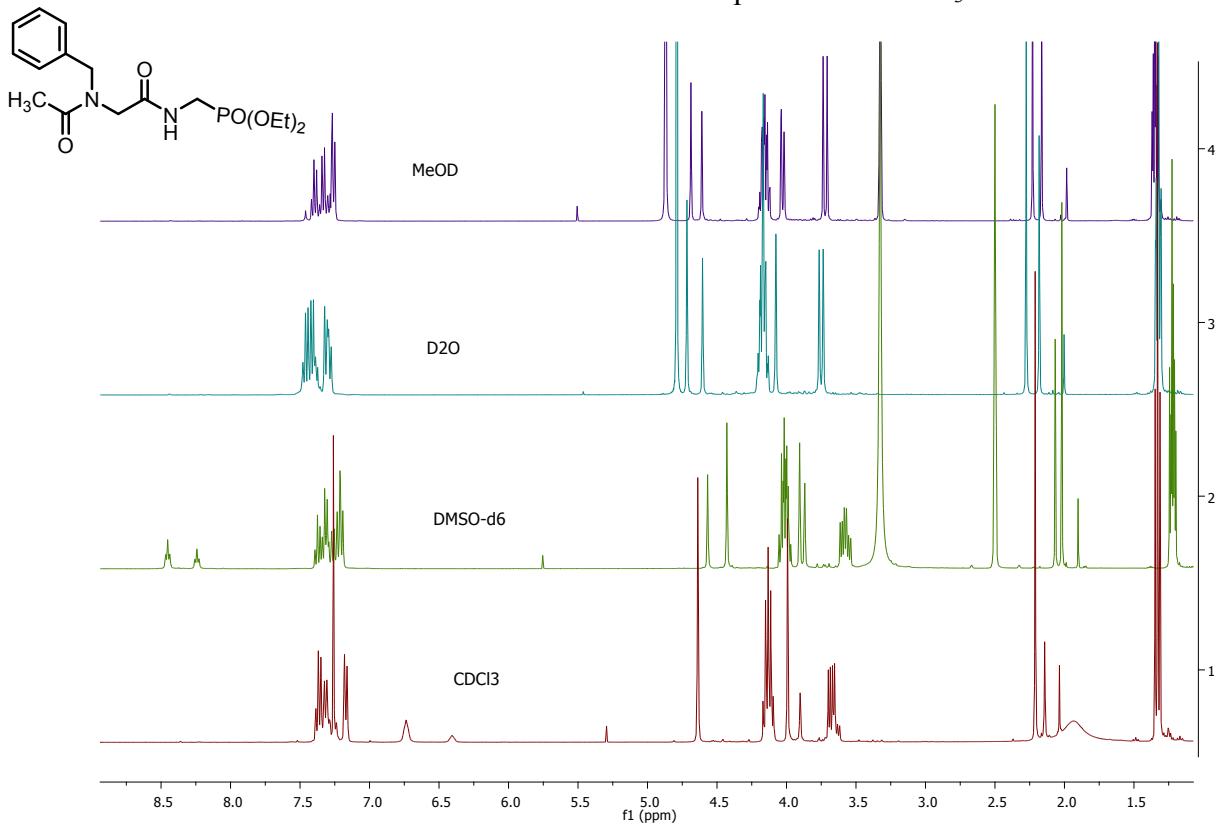


FIGURE 32: 400 MHz  $^1\text{H}$  NMR spectrum of **9** in different deuterated solvents at 15 mM.

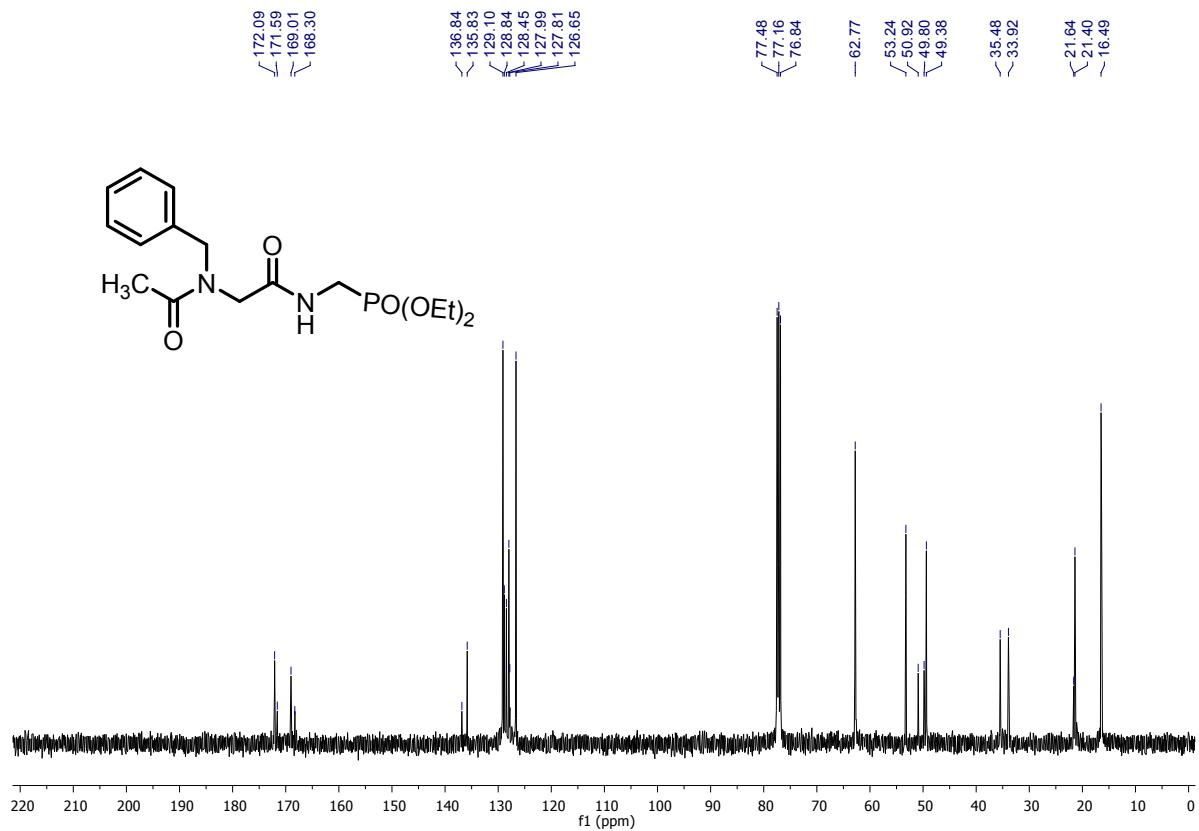


FIGURE 33: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **9**.

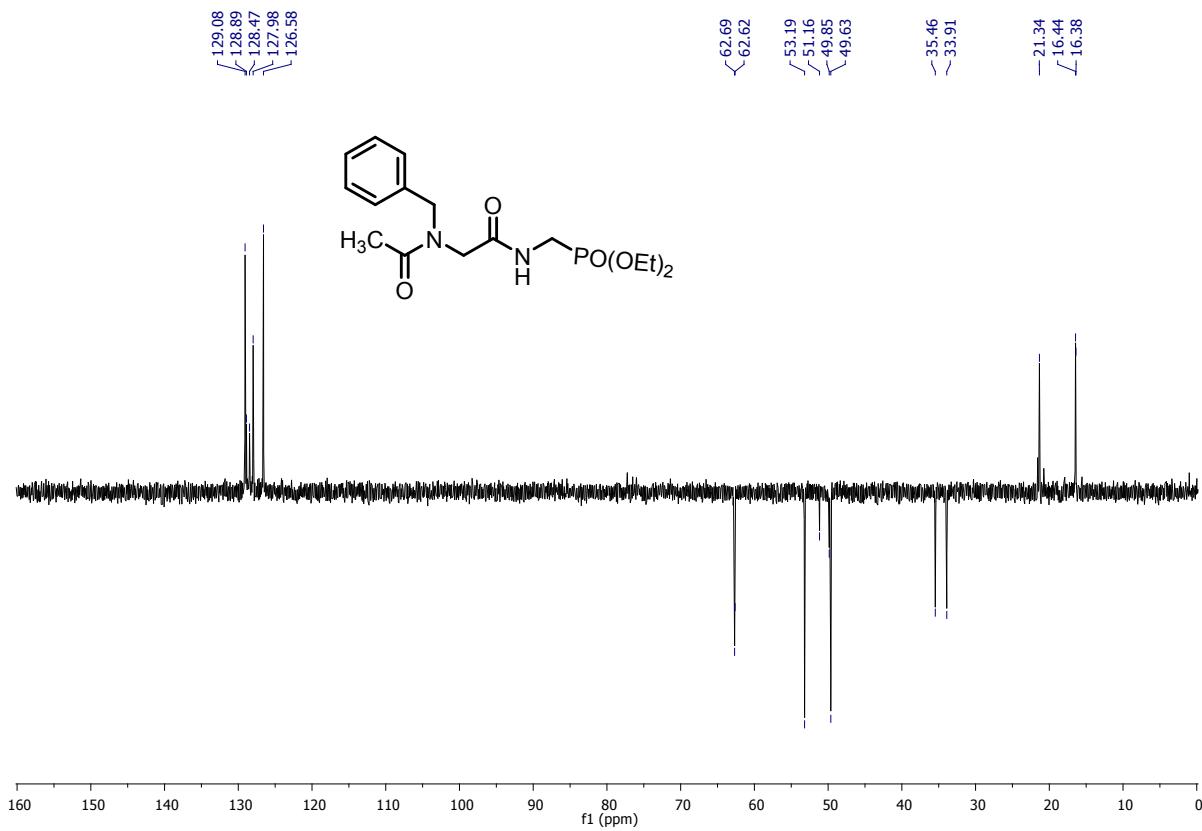


FIGURE 34: DEPT-135° spectrum in  $\text{CDCl}_3$  of **9**.

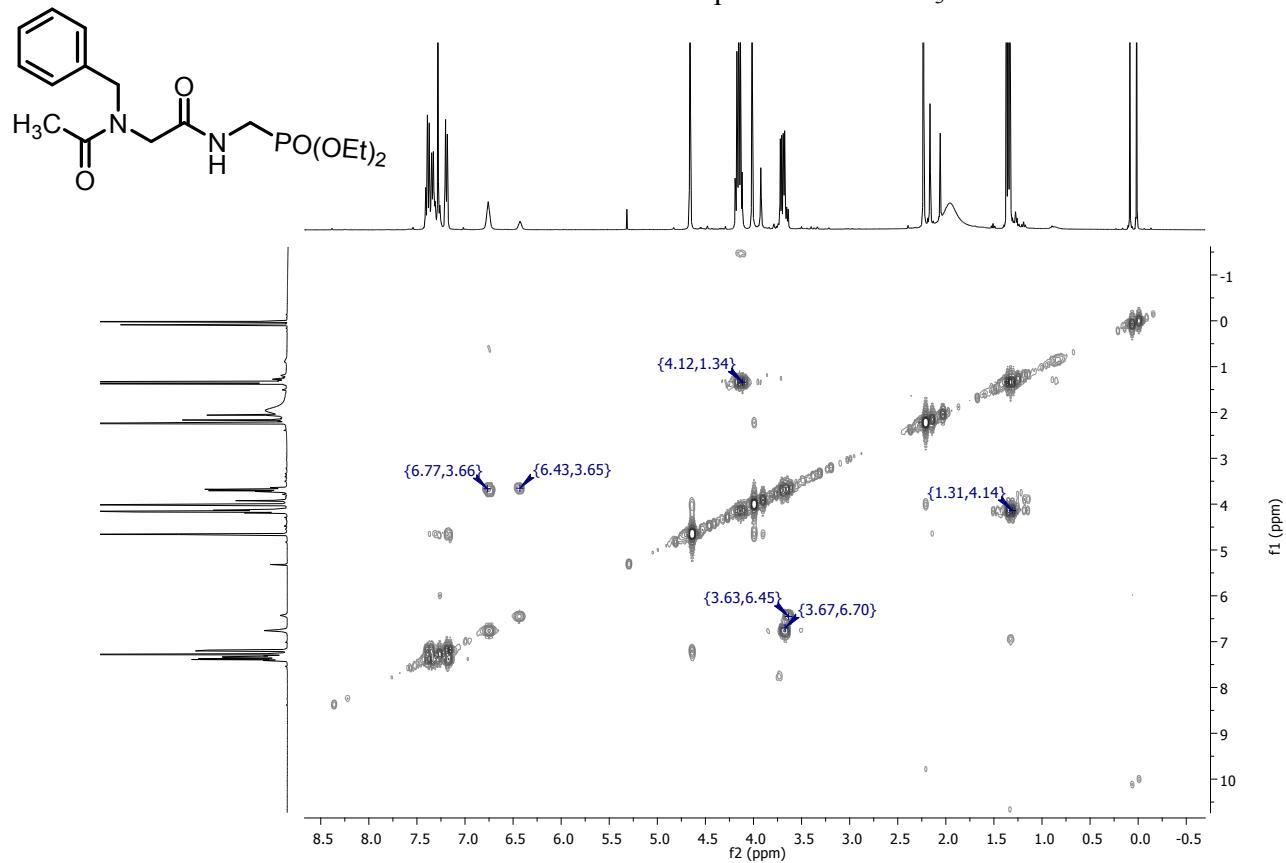


FIGURE 35: COSY spectrum in  $\text{CDCl}_3$  of **9**.

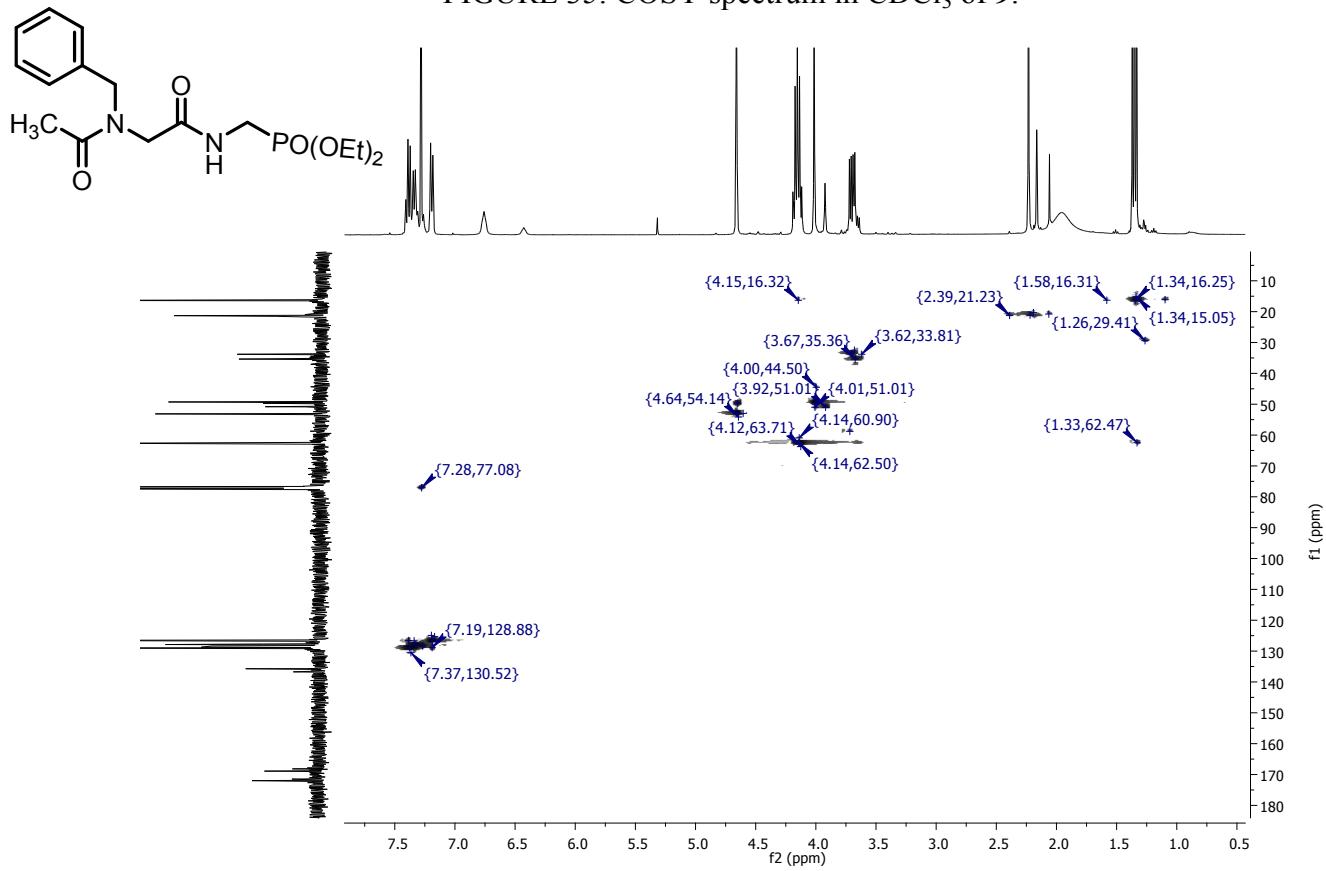


FIGURE 36: HSQC spectrum in  $\text{CDCl}_3$  of **9**.

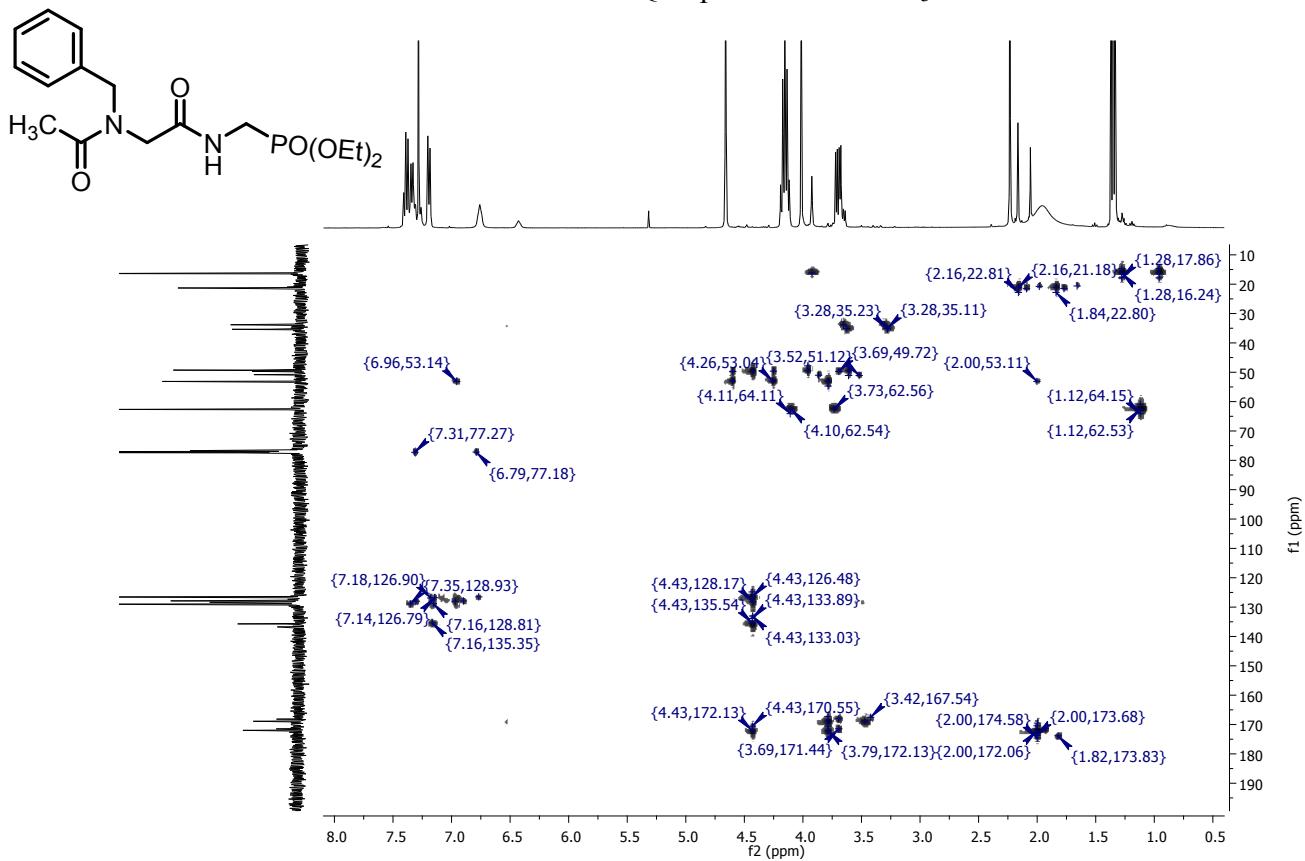


FIGURE 37: HMBC spectrum in  $\text{CDCl}_3$  of **9**.

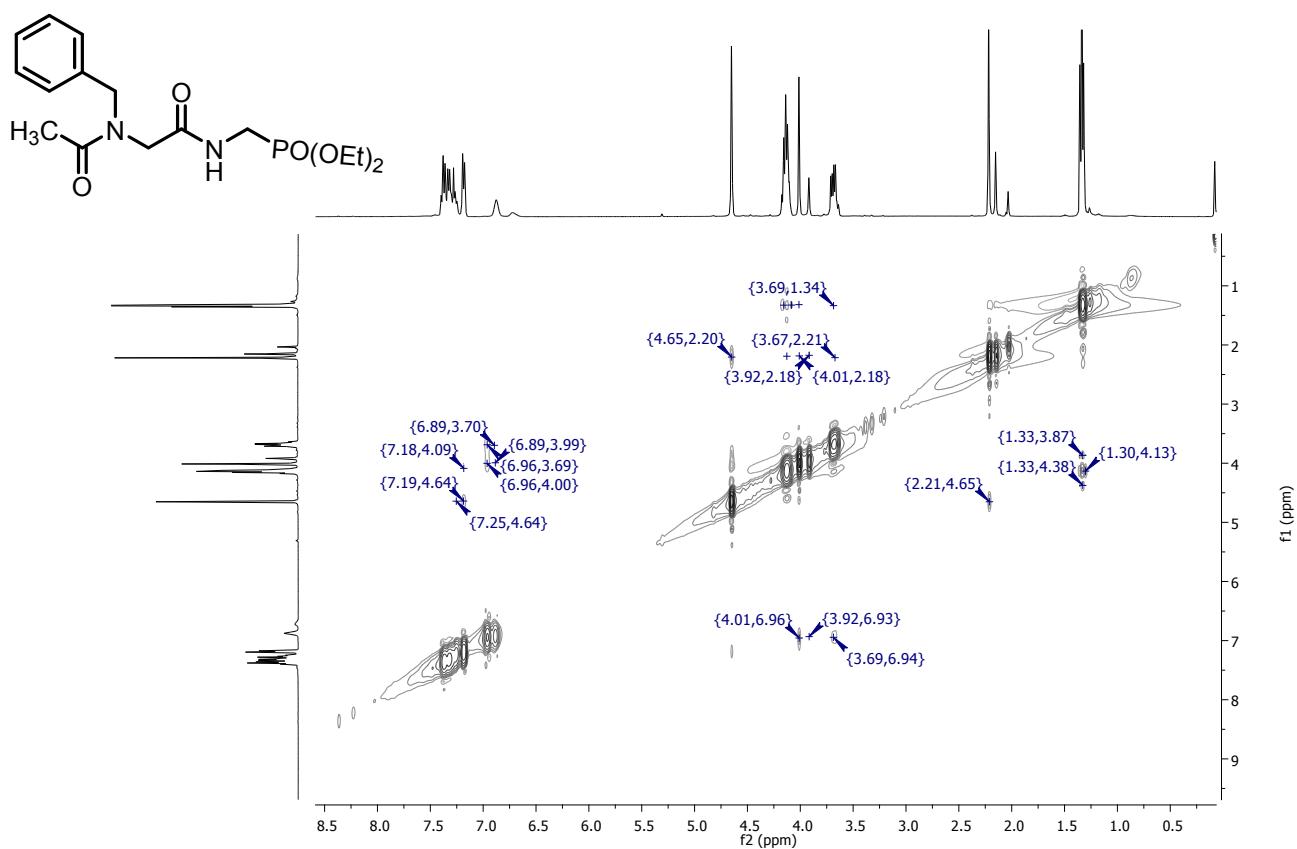


FIGURE 38: NOESY spectrum in  $\text{CDCl}_3$  of **9**.

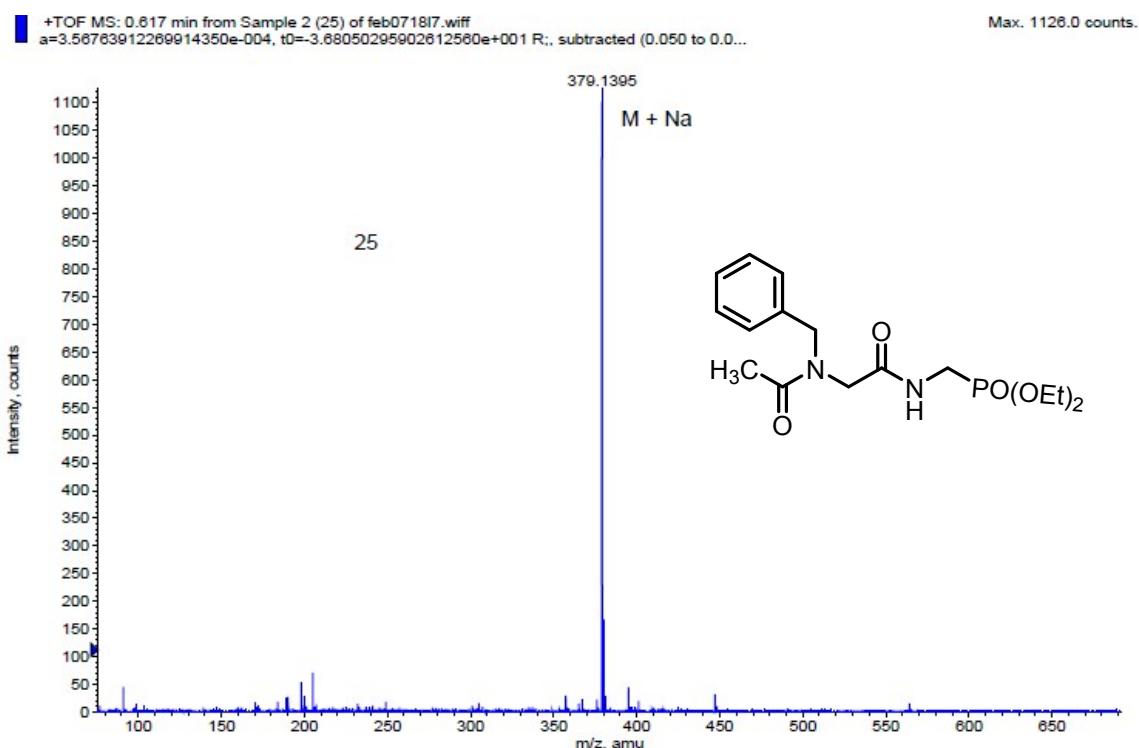


FIGURE 39- HRMS (ESI-FT-ICR)  $m/z$  spectrum of **9**.

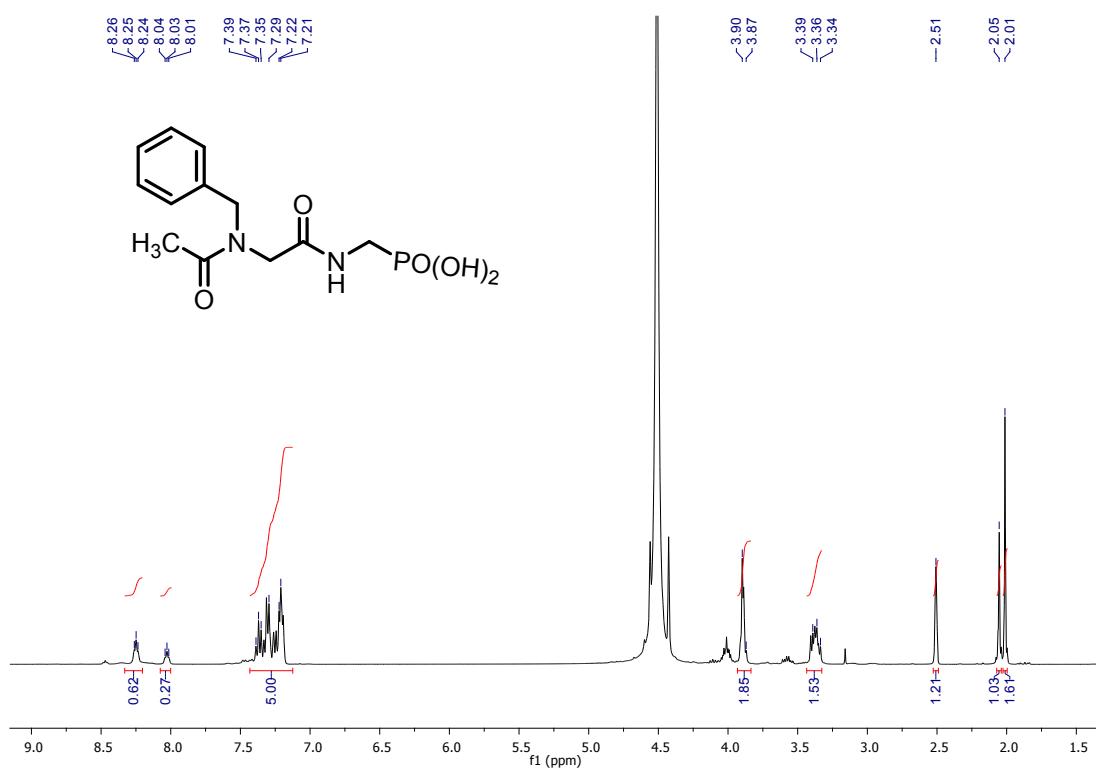


FIGURE 40: 400 MHz  $^1\text{H}$  NMR spectrum in DMSO-d<sub>6</sub> of **10**.

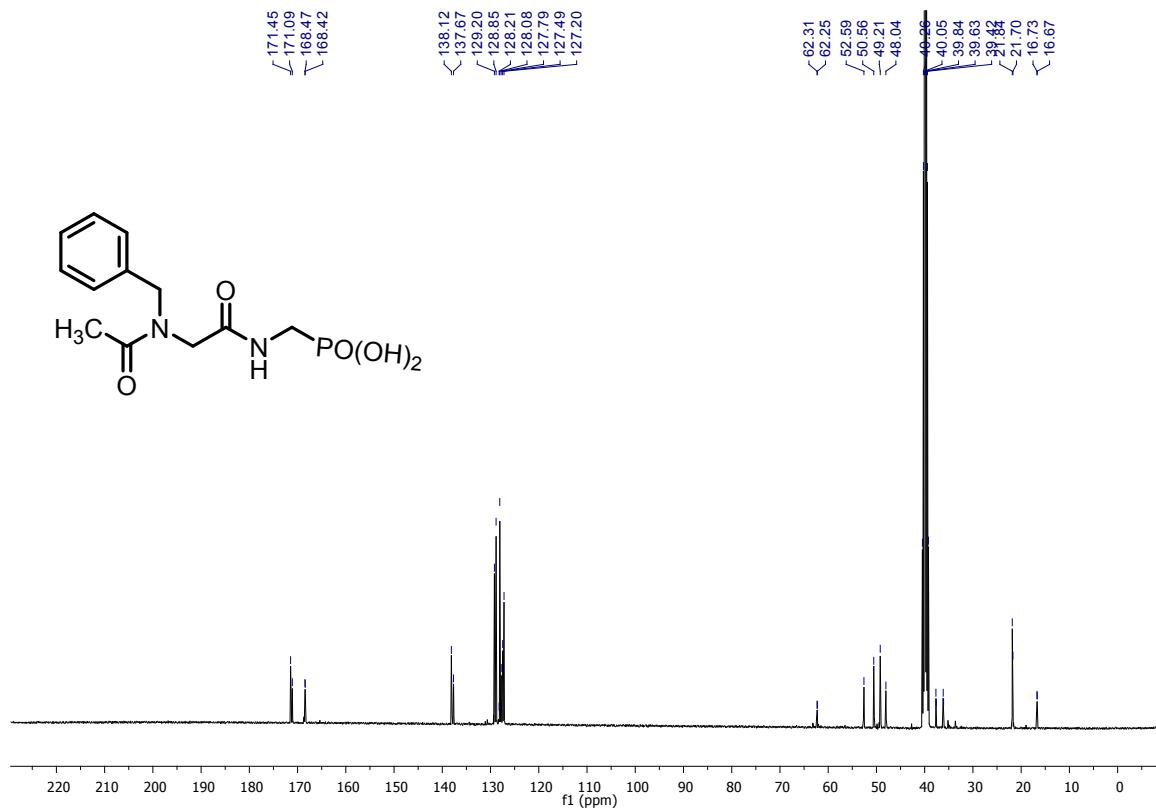


FIGURE 41: 100 MHz  $^{13}\text{C}$  NMR spectrum in DMSO-d<sub>6</sub> of **10**.

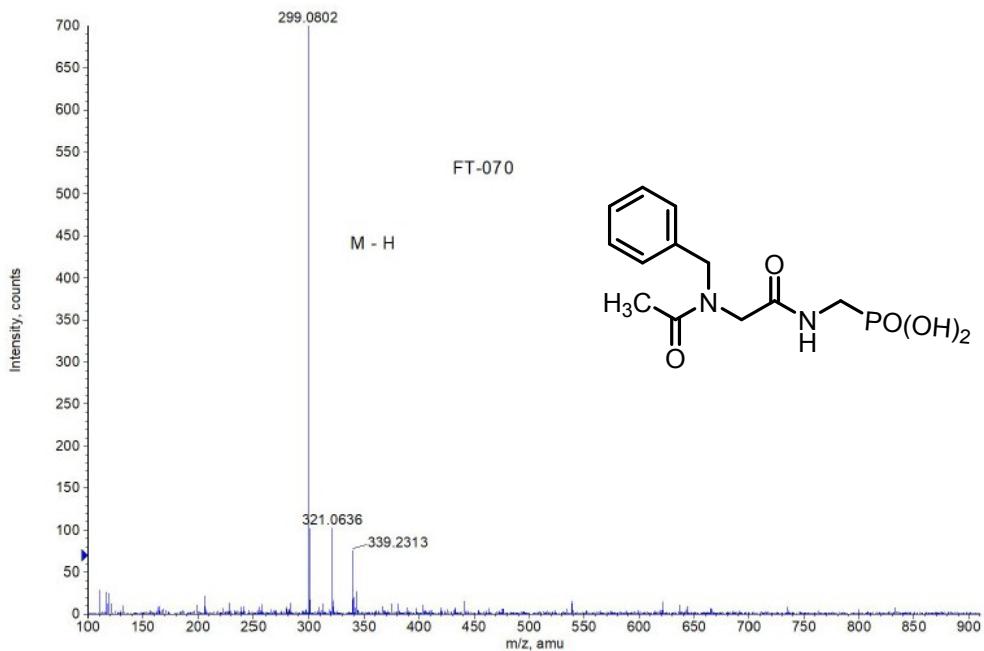


FIGURE 42: HRMS (ESI-FT-ICR) m/z spectrum of **10**.

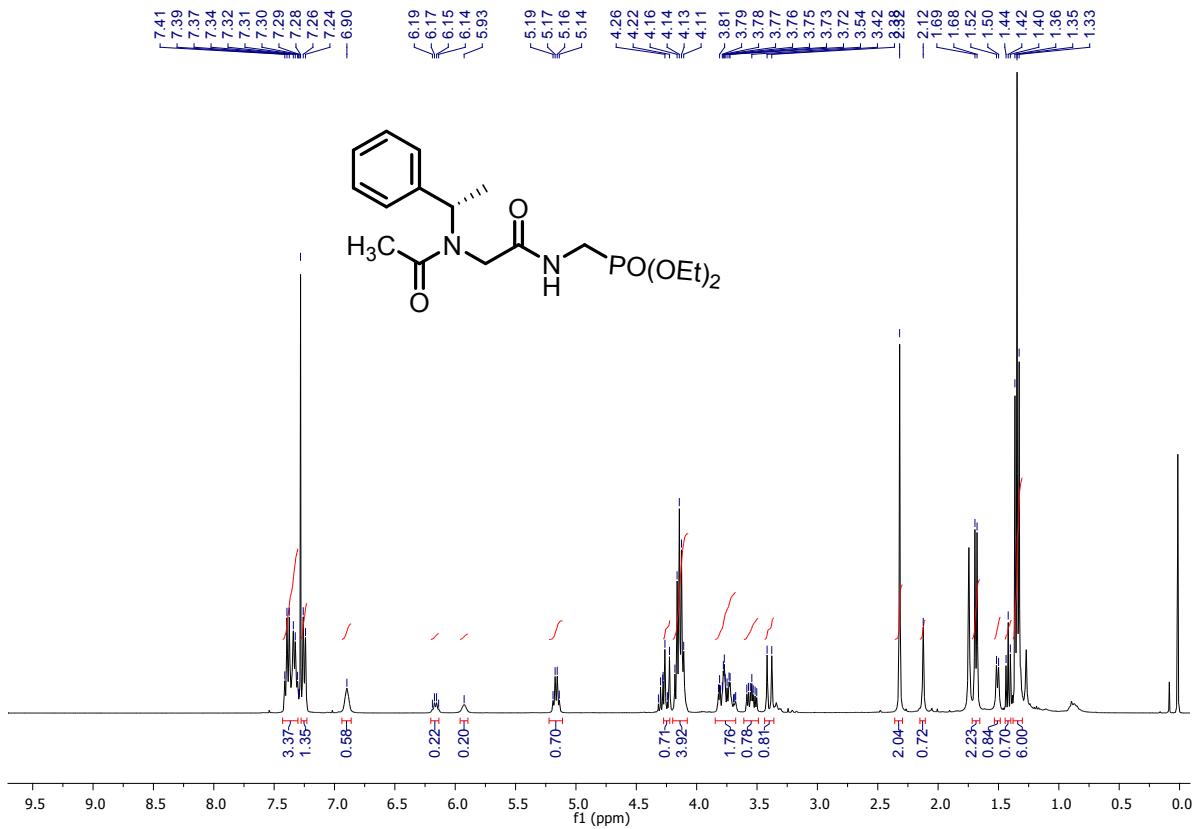


FIGURE 43: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **11**.

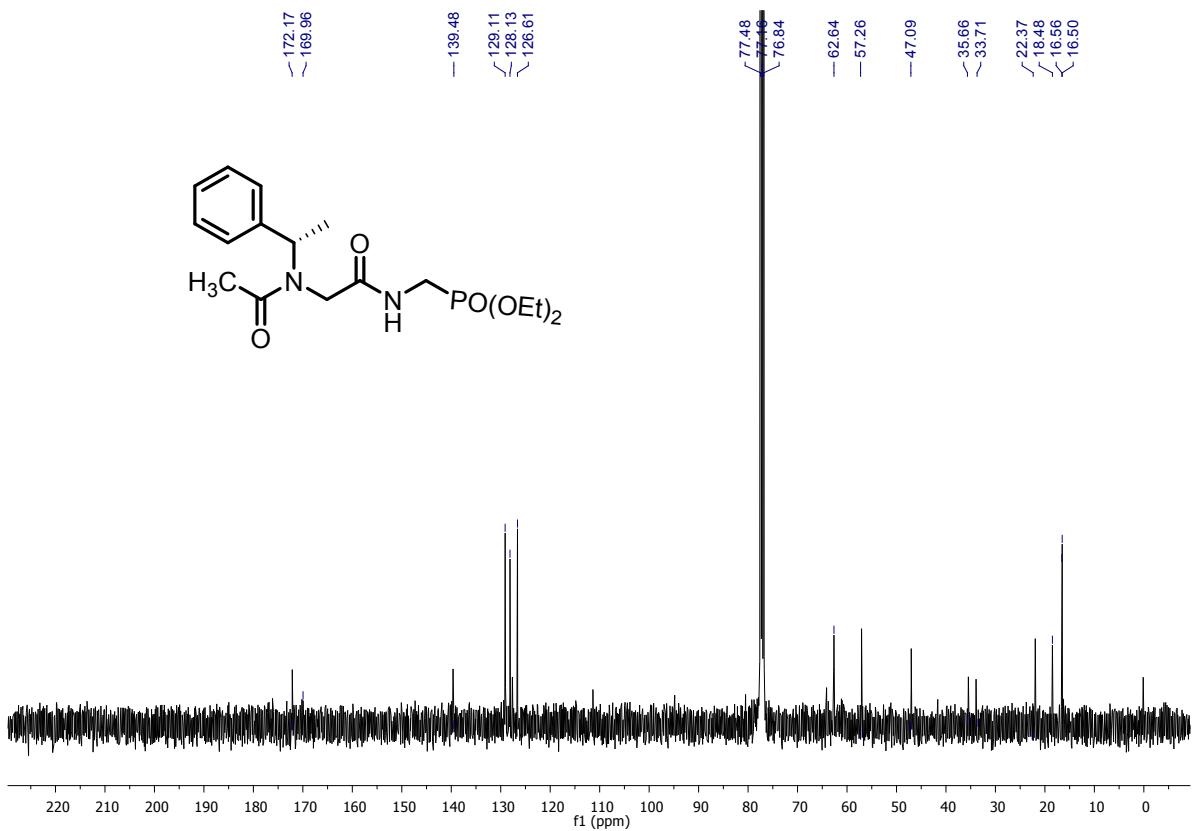


FIGURE 44: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **11**.

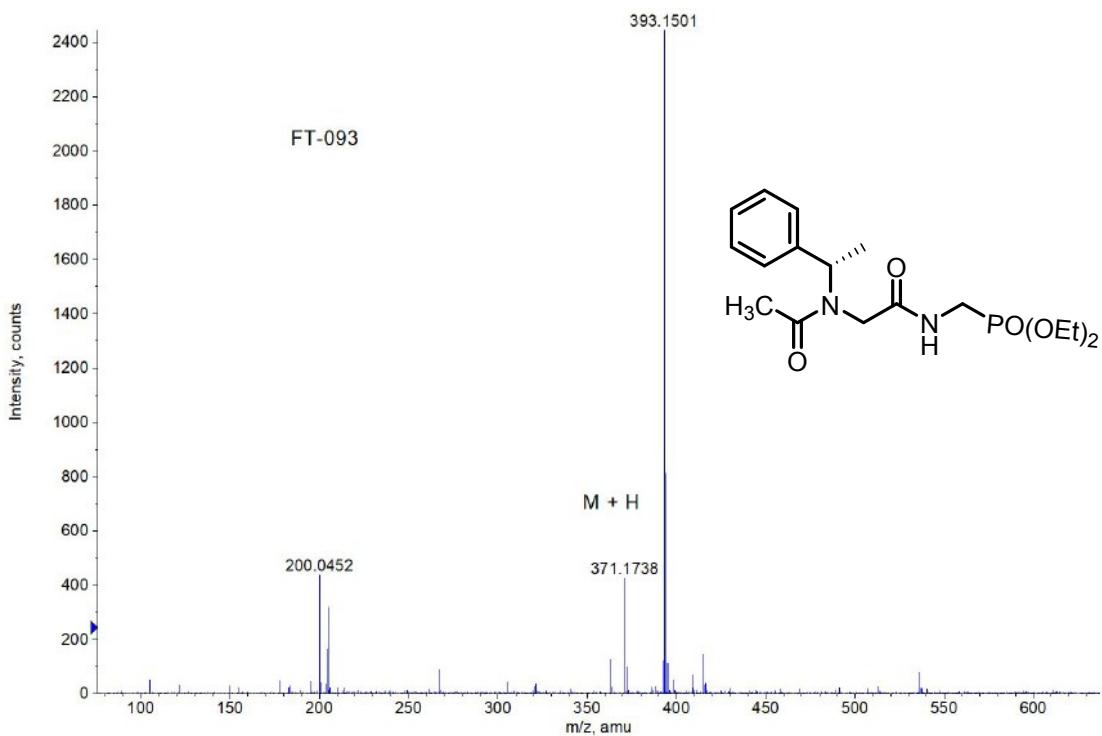


FIGURE 45: HRMS (ESI-FT-ICR)  $m/z$  spectrum of **11**.

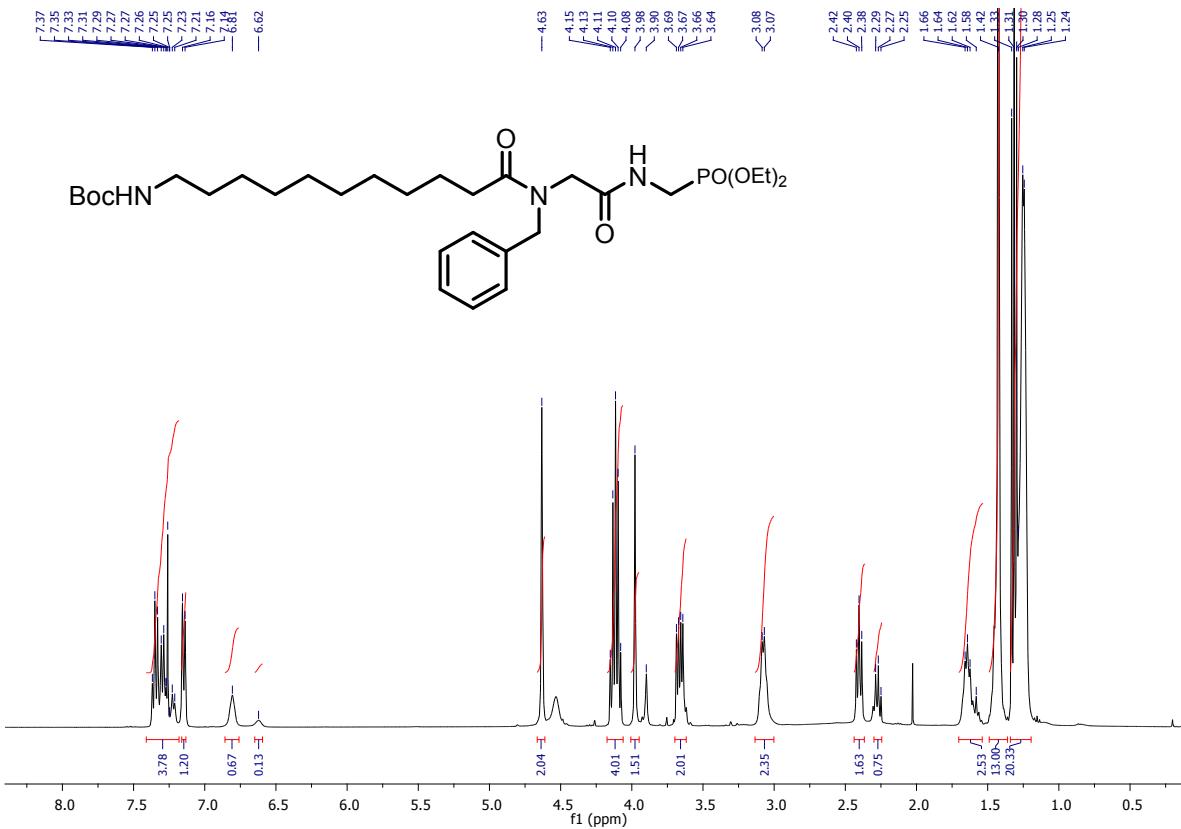


FIGURE 46: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **12**.

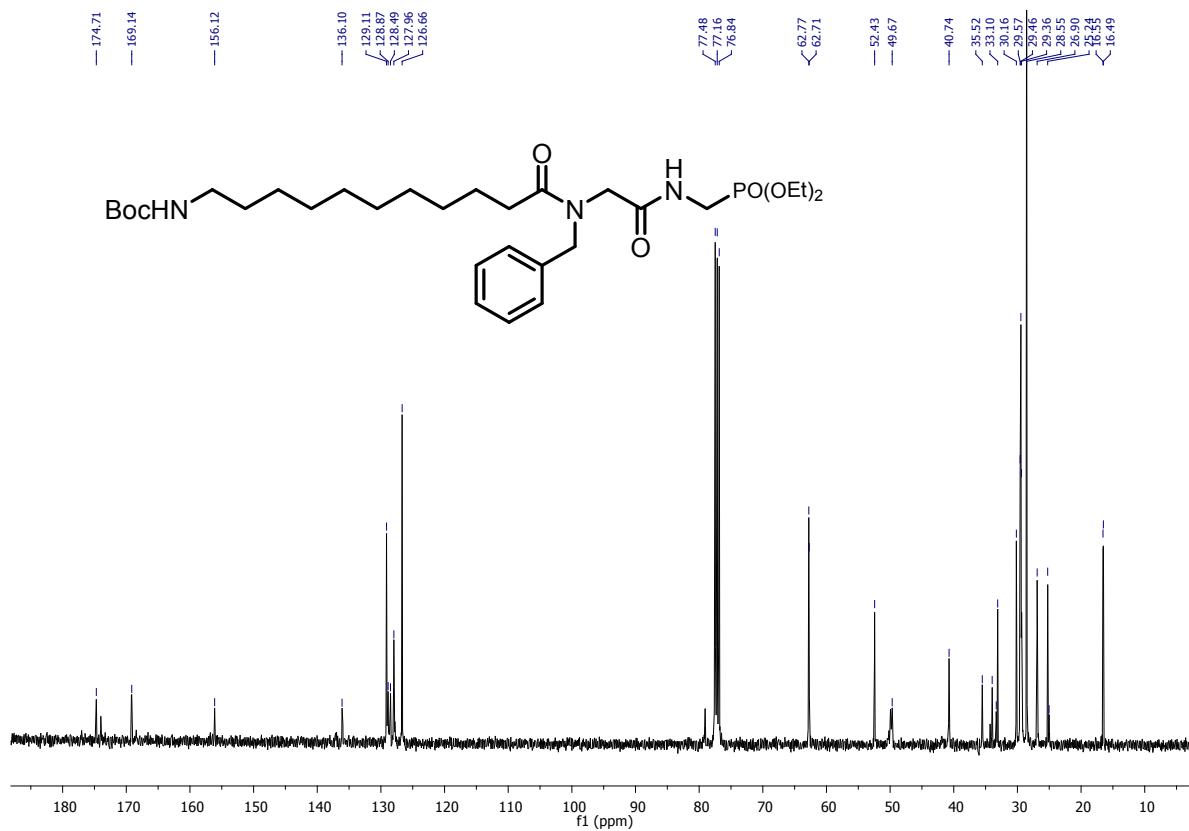


FIGURE 47: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **12**.

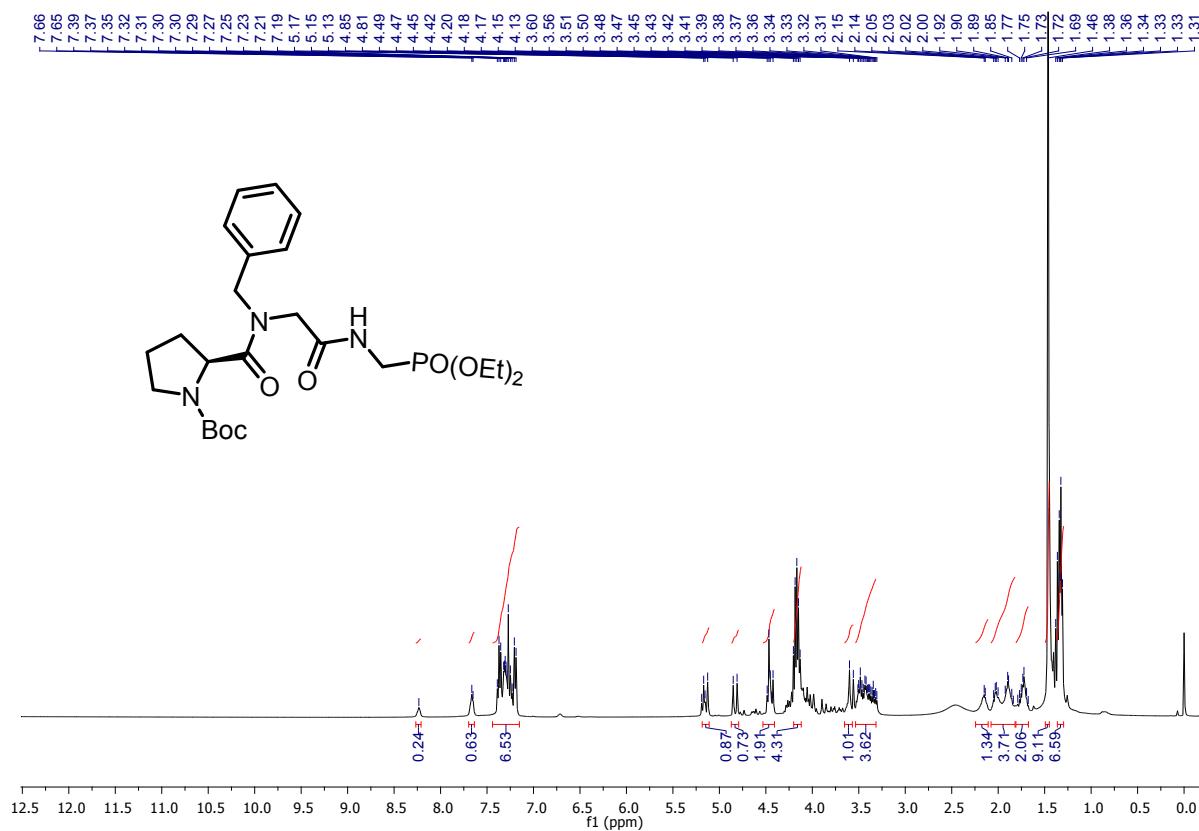


FIGURE 48: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **13**.

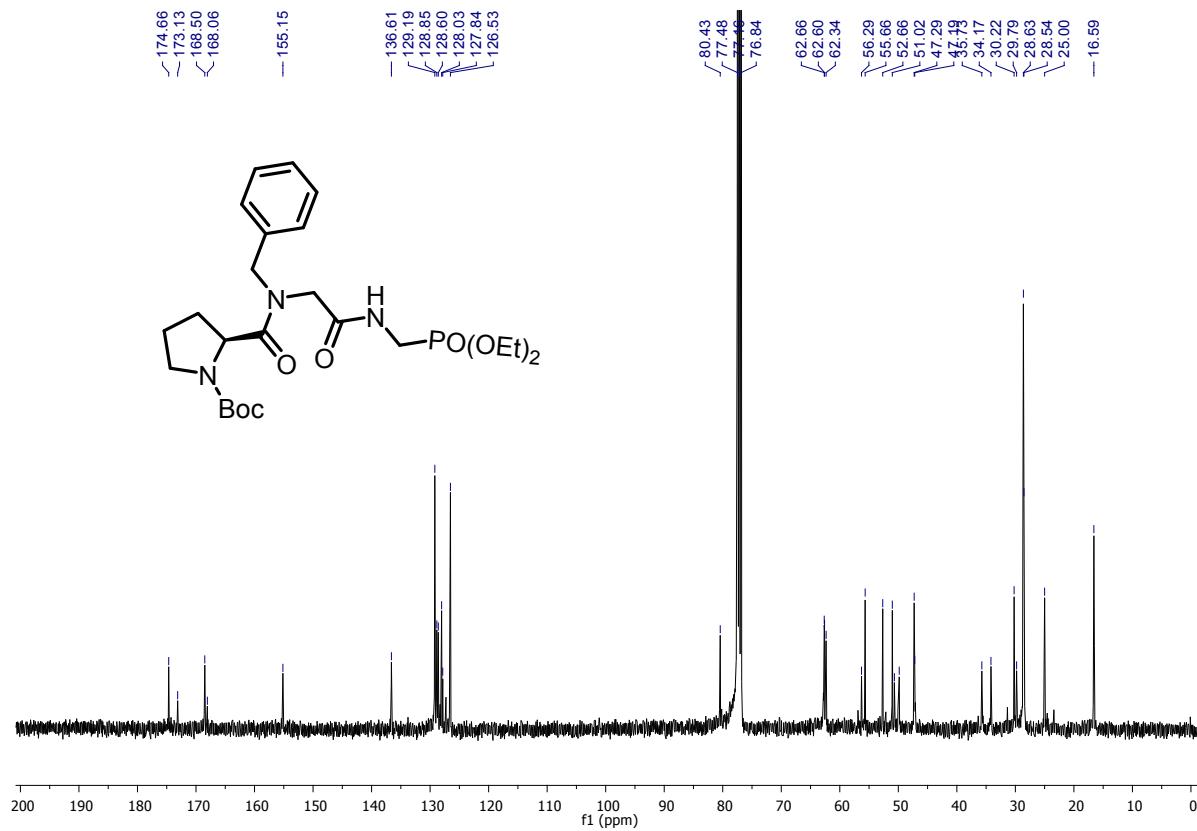


FIGURE 49: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **13**.

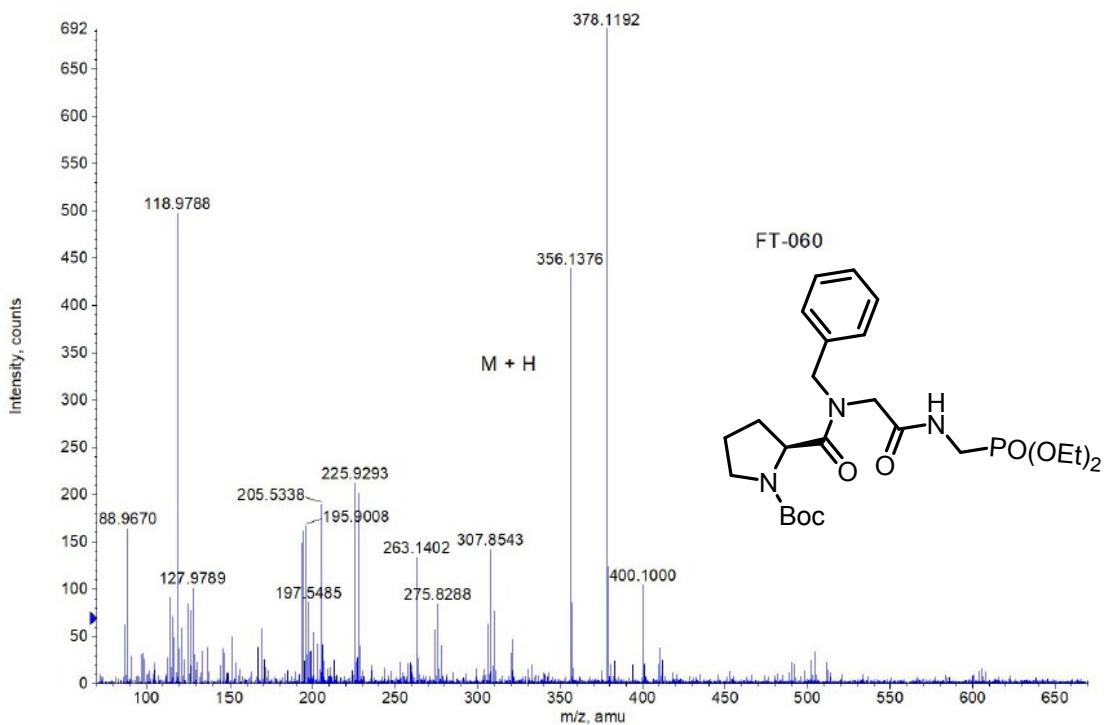


FIGURE 50: HRMS (ESI-FT-ICR)  $m/z$  spectrum of **13**.

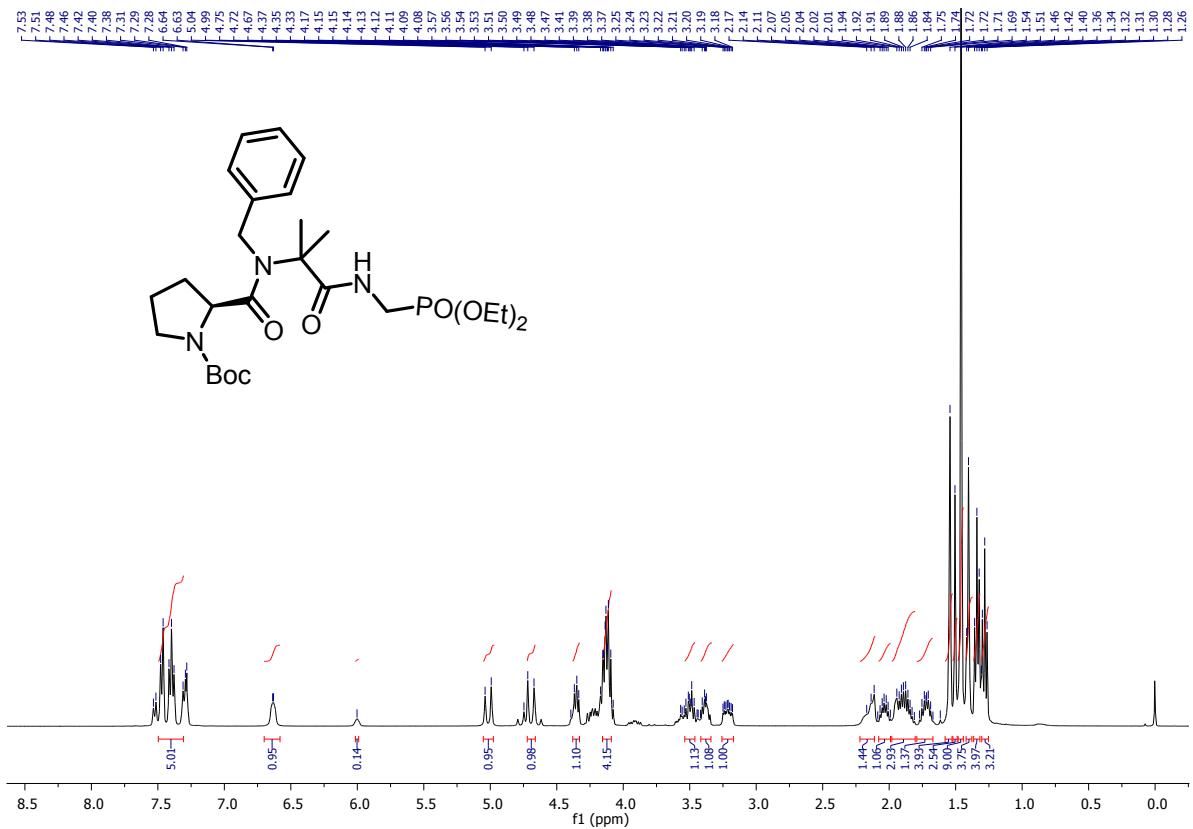


FIGURE 51: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **14**.

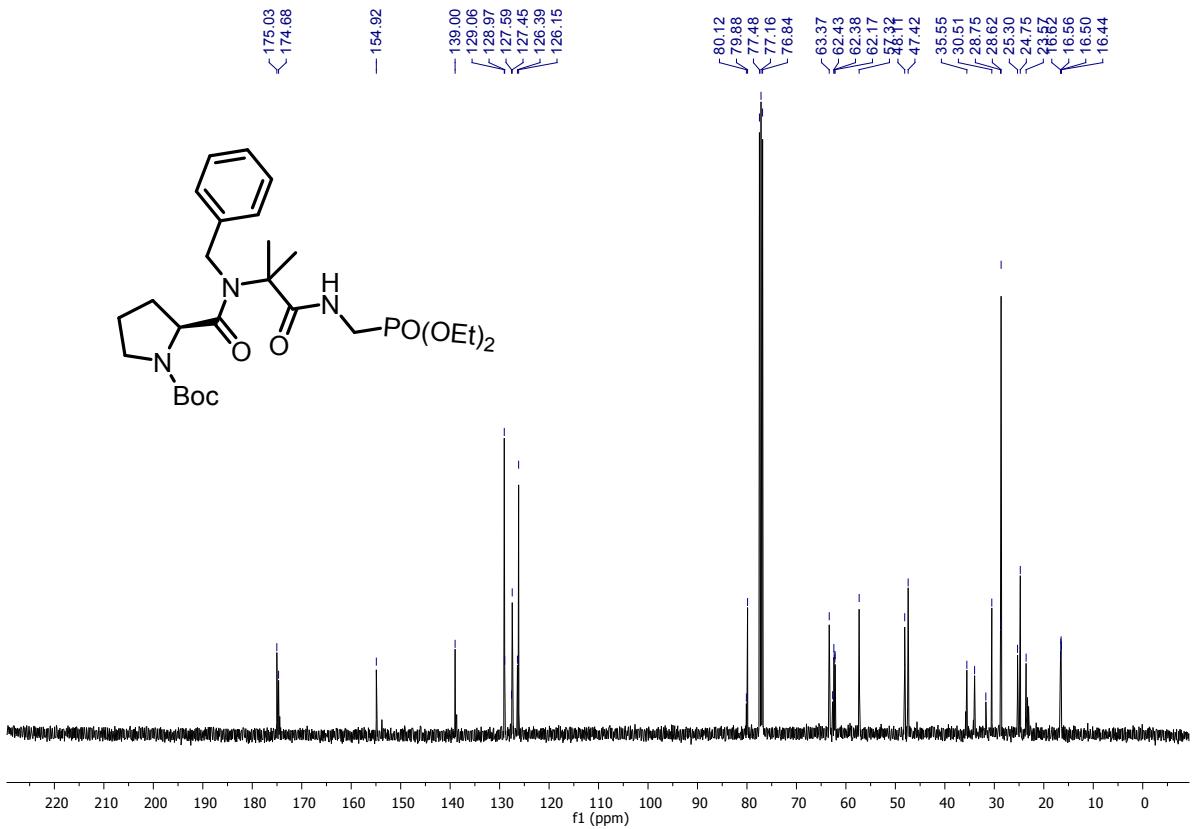


FIGURE 52: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **14**.

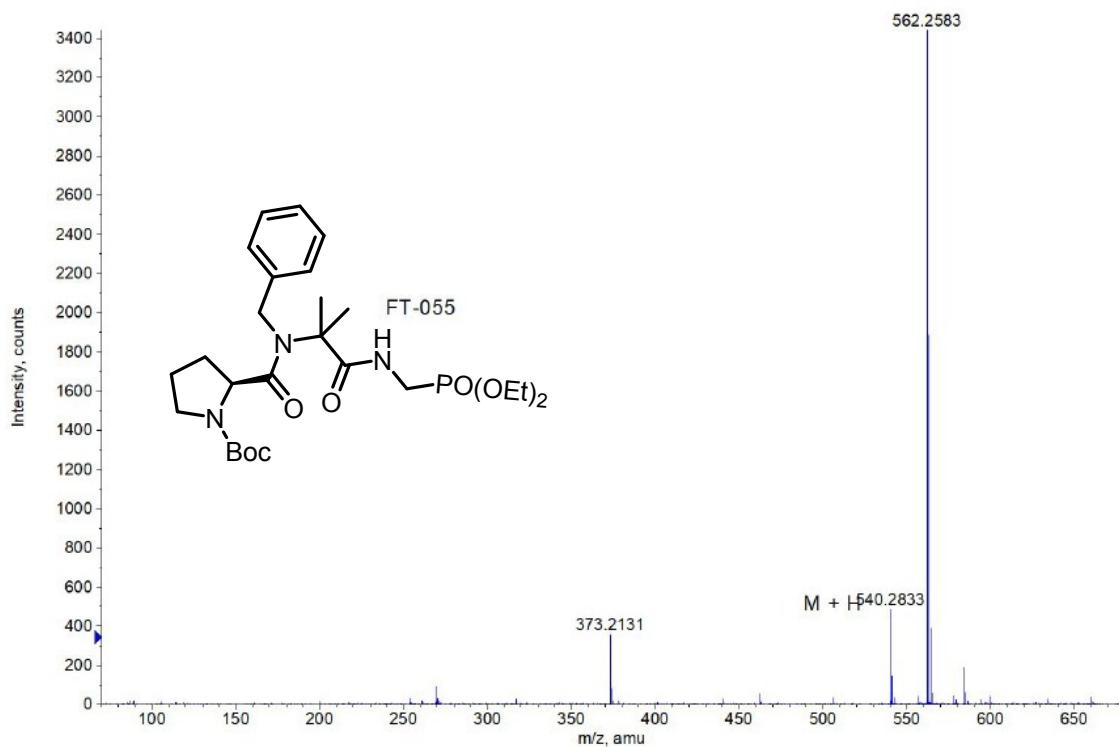


FIGURE 53: HRMS (ESI-FT-ICR)  $m/z$  spectrum of **14**.

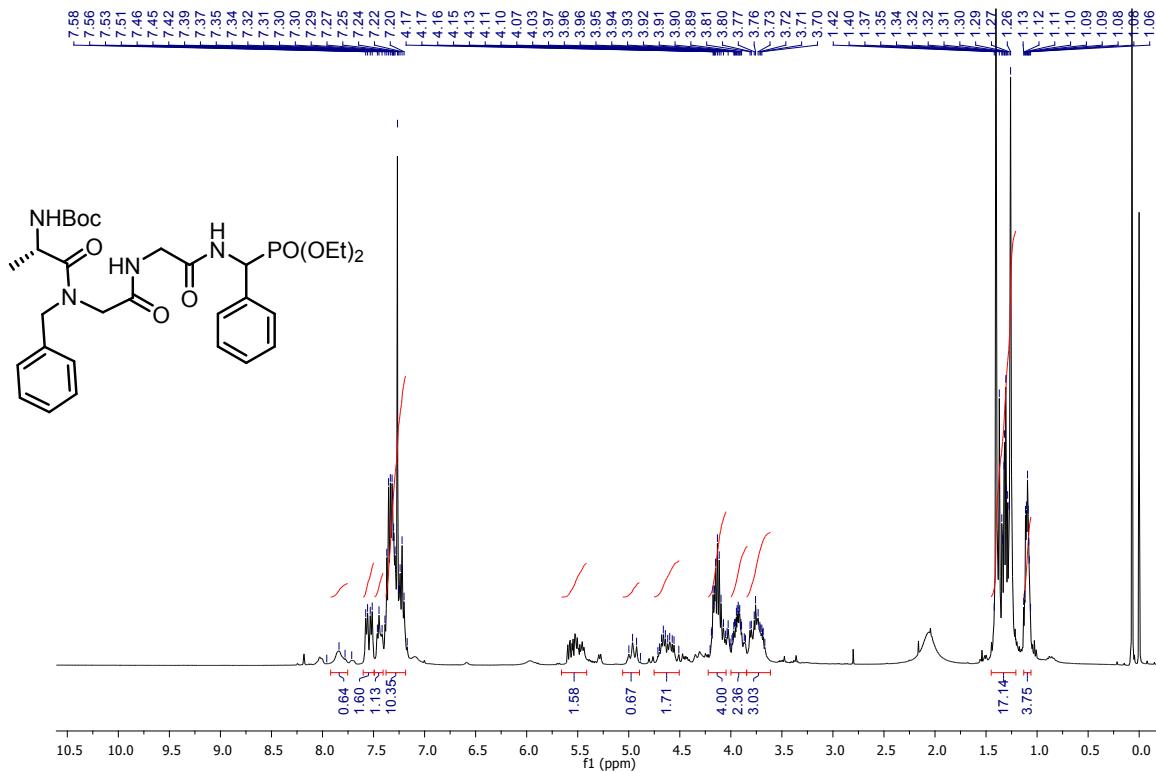


FIGURE 54: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **15**.

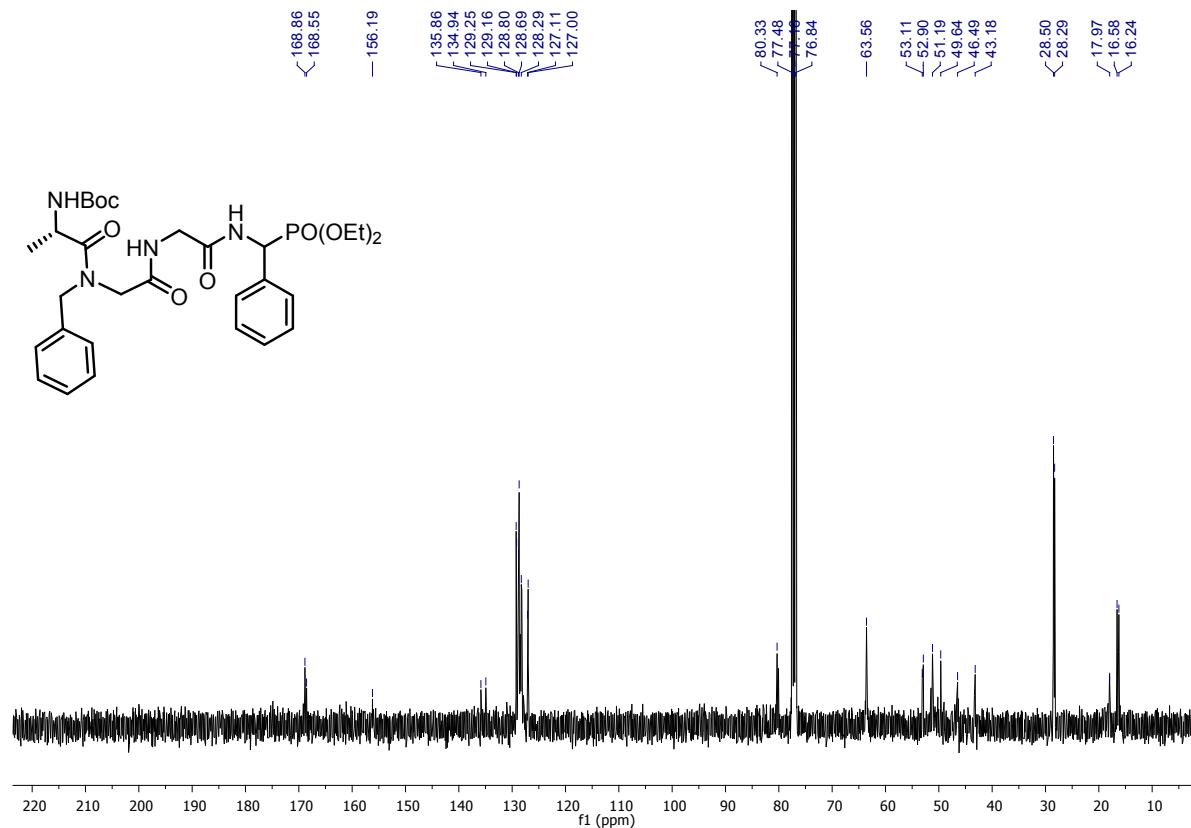


FIGURE 55: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **15**.

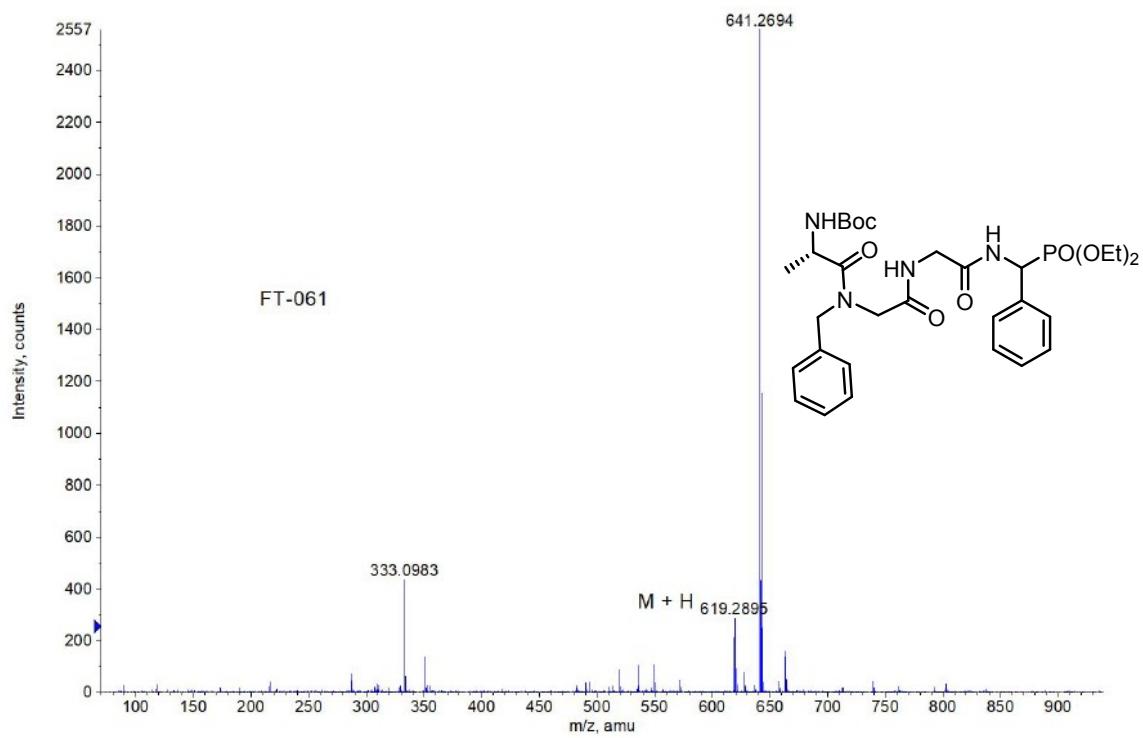


FIGURE 56: HRMS (ESI-FT-ICR)  $m/z$  spectrum of **15**.

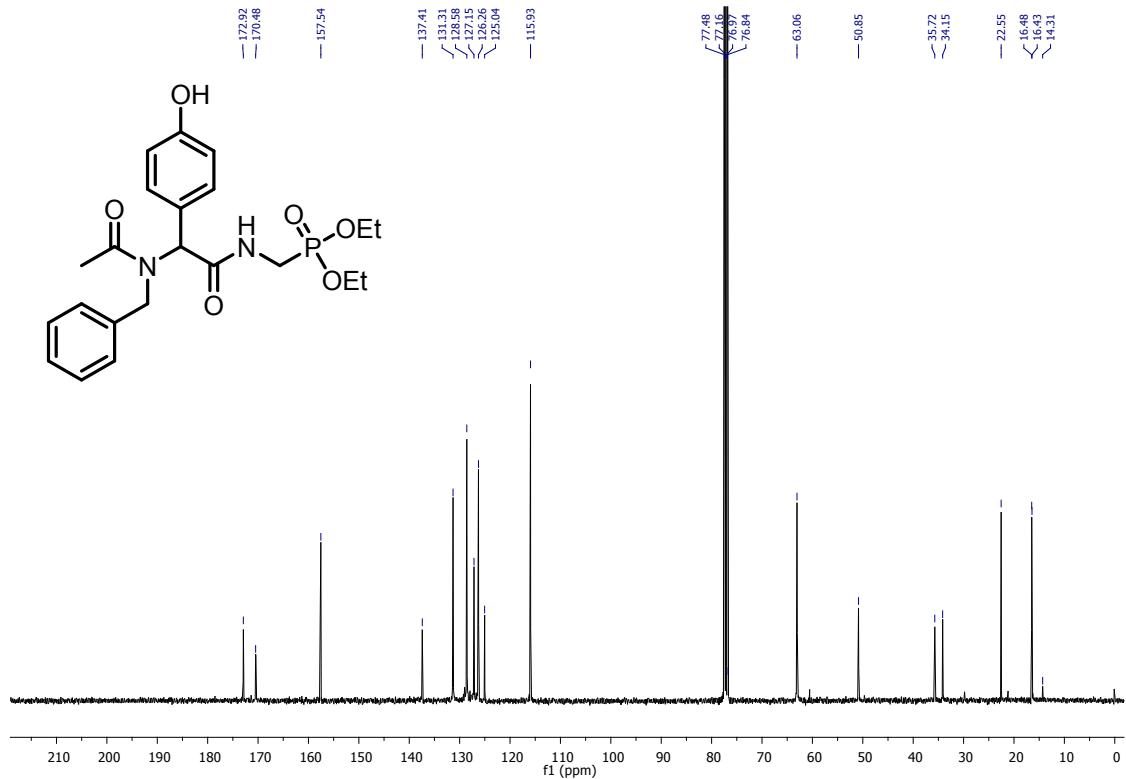
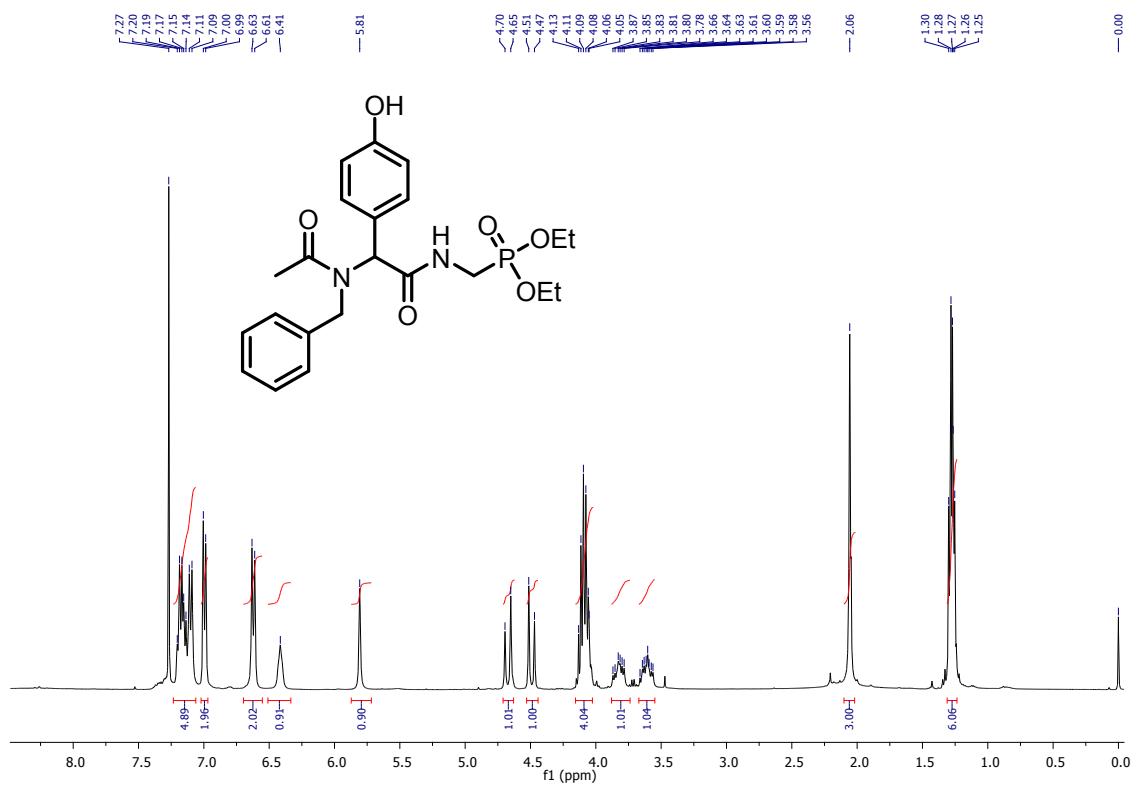


FIGURE 58: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **16**.

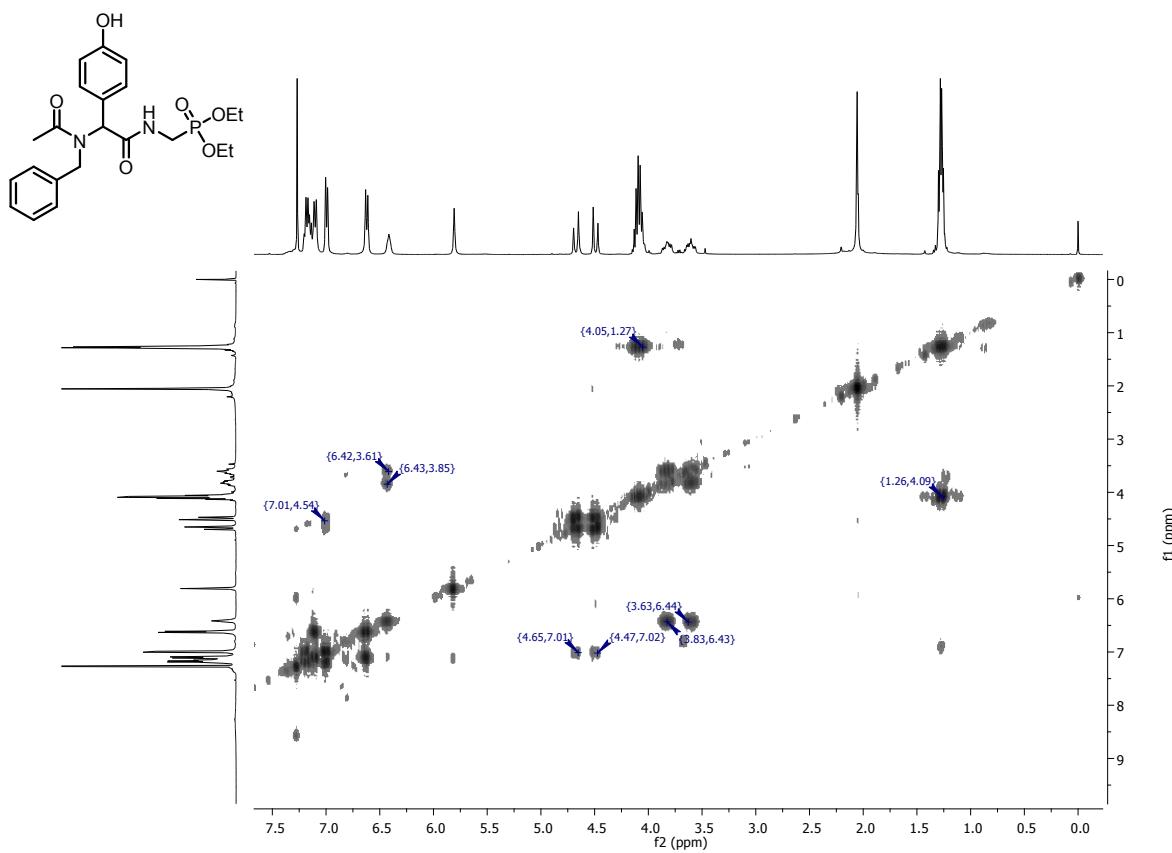


FIGURE 59: COSY spectrum in  $\text{CDCl}_3$  of **16**.

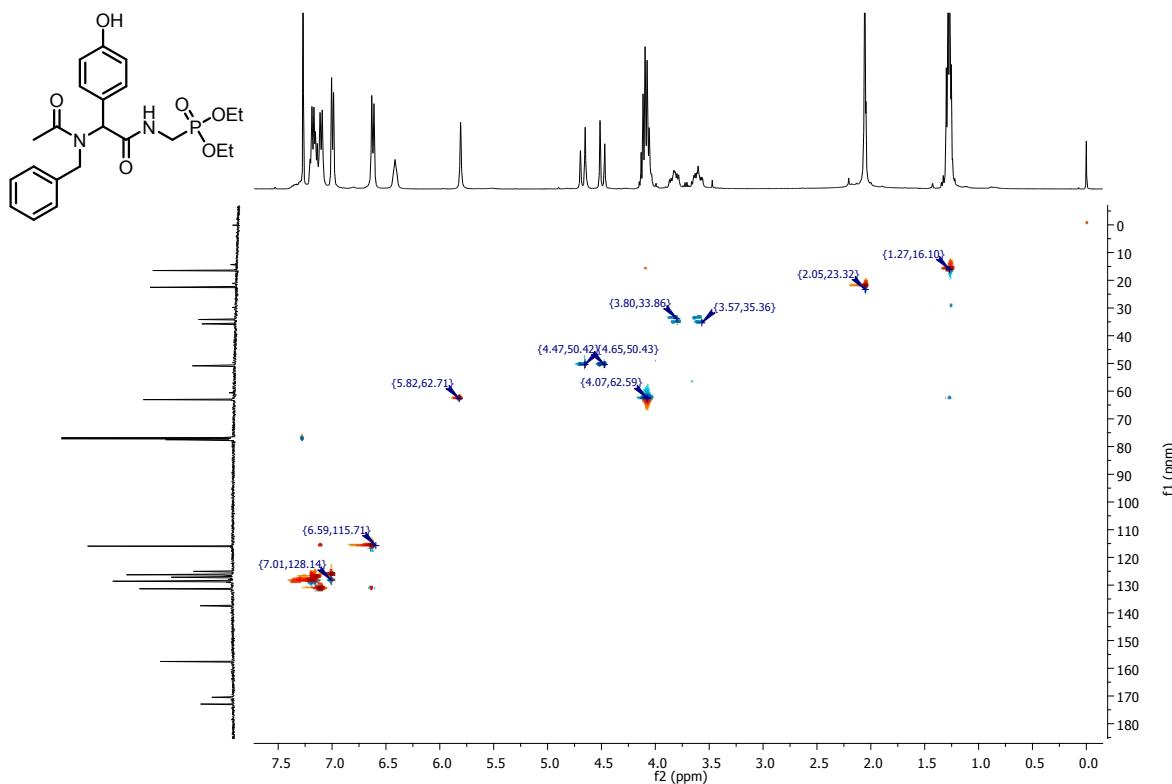


FIGURE 60: Multiplicity-edited HSQC spectrum of **16**. (In the 2D spectrum shown above the red peaks denote  $\text{CH}_3$  or  $\text{CH}$  signals, while the blue signal denote  $\text{CH}_2$  signals)

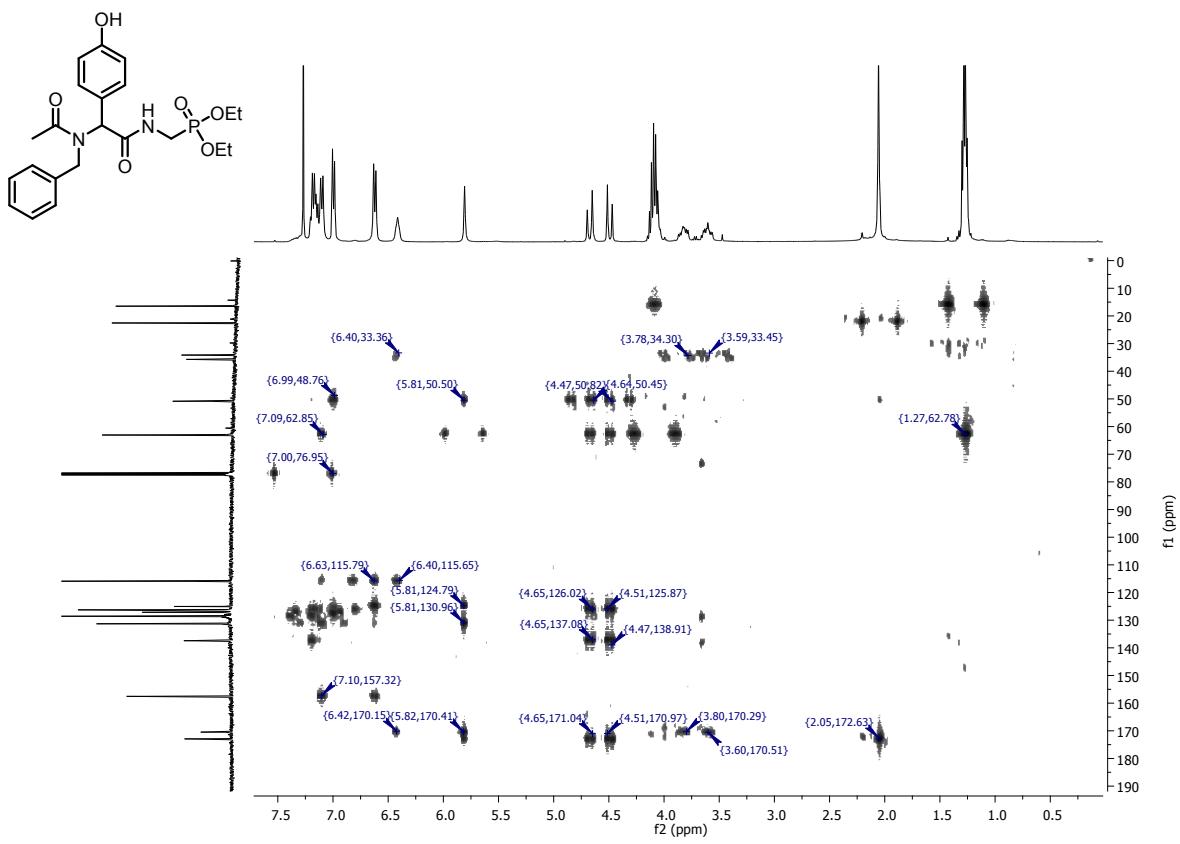


FIGURE 61: HMBC spectrum in  $\text{CDCl}_3$  of **16**.

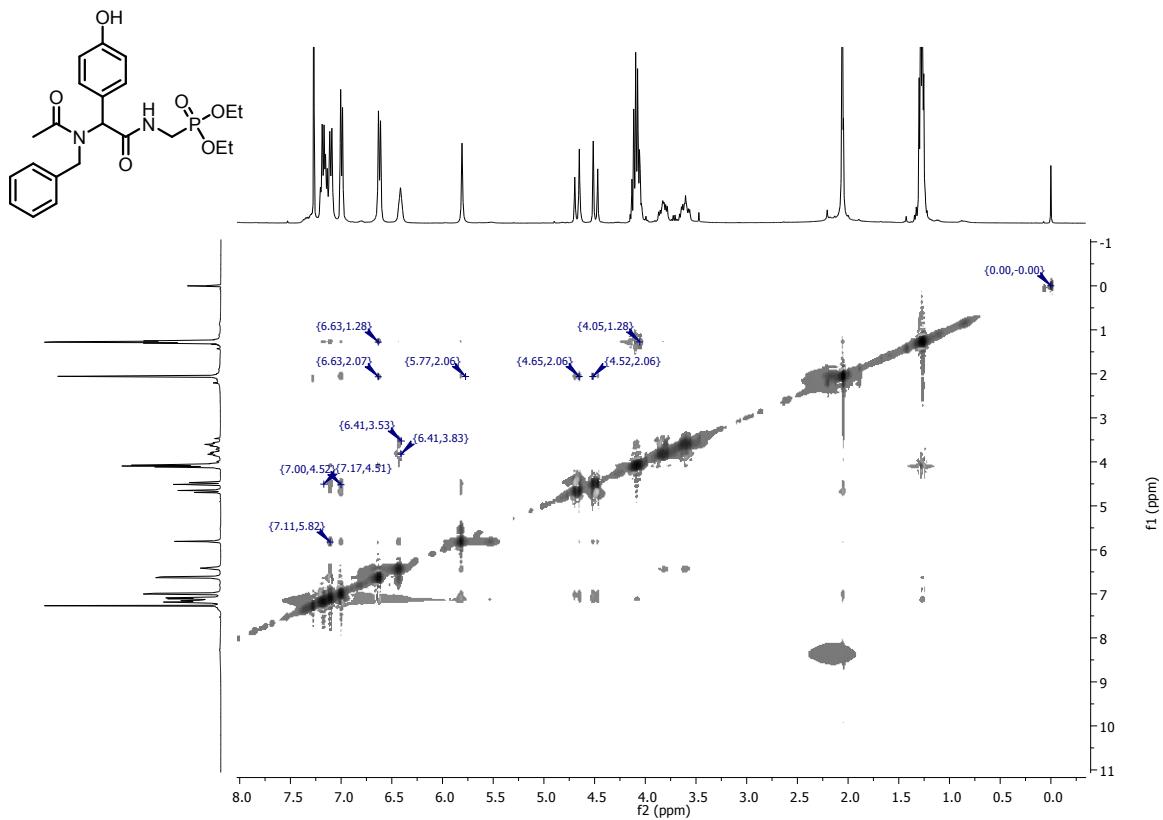


FIGURE 62: NOESY spectrum in  $\text{CDCl}_3$  of **16**.

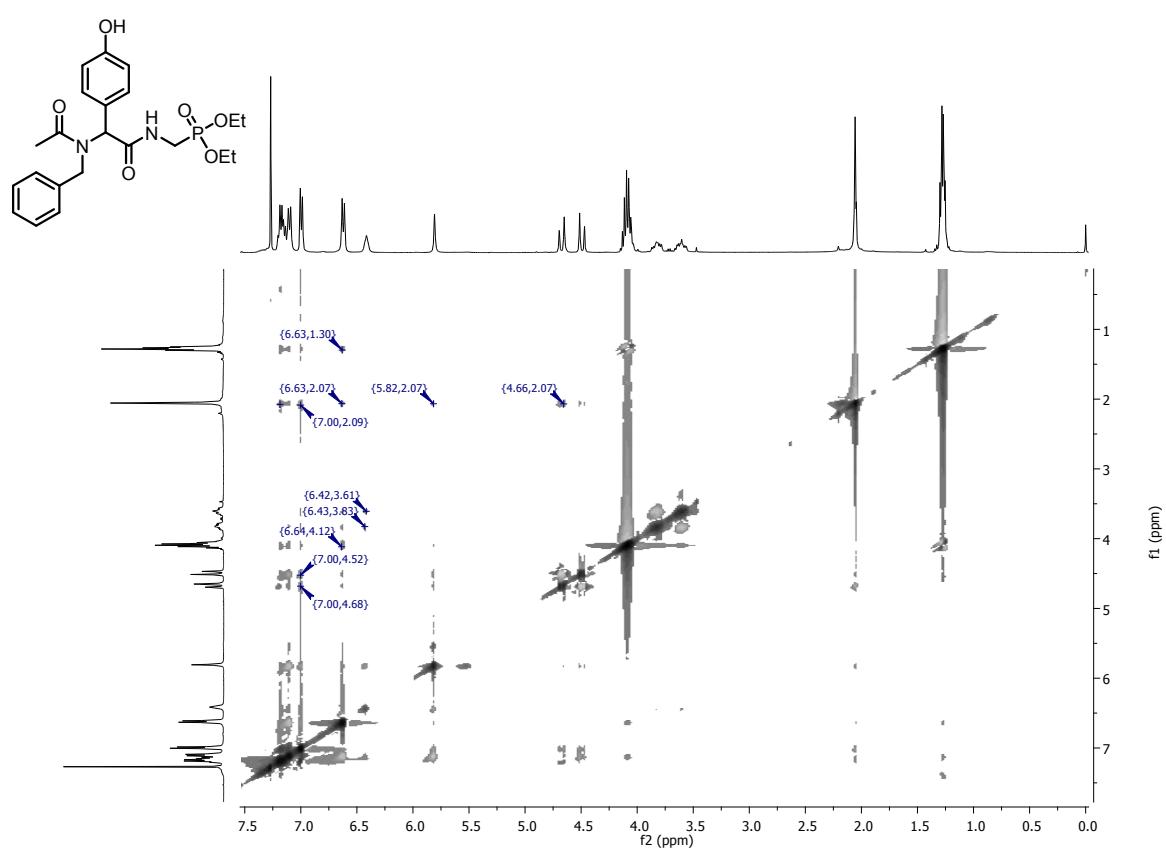


FIGURE 63: ROESY spectrum in  $\text{CDCl}_3$  of **16**.

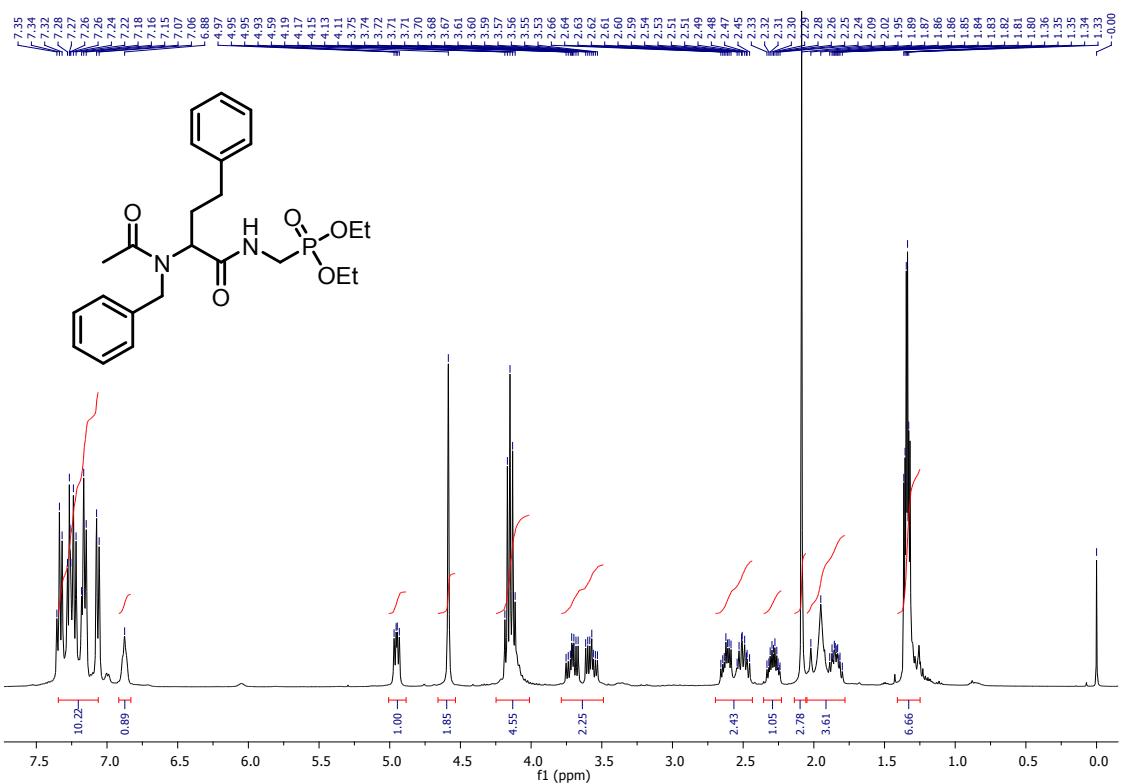


FIGURE 64: 400 MHz  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  of **17**.

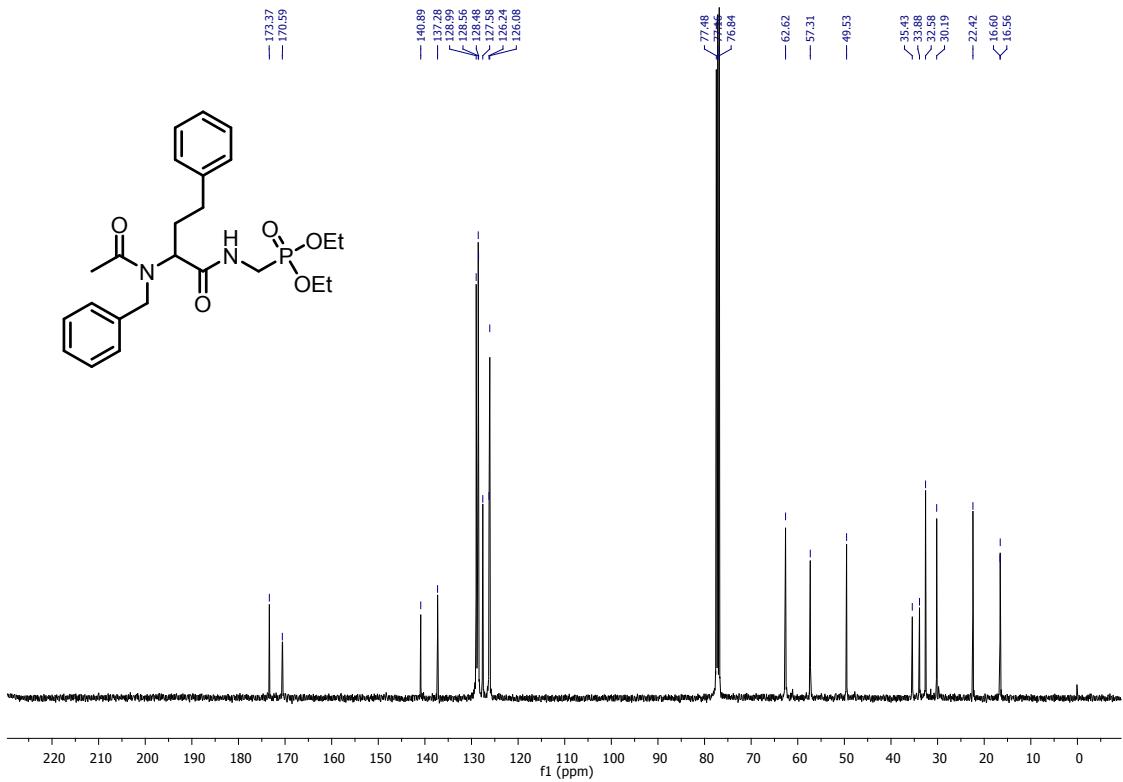


FIGURE 65: 100 MHz  $^{13}\text{C}$  NMR spectrum in  $\text{CDCl}_3$  of **17**.