

Supporting information for

# Phosphinophosphonates and their tris-pivaloyloxymethyl prodrugs reveal a negatively cooperative butyrophilin activation mechanism

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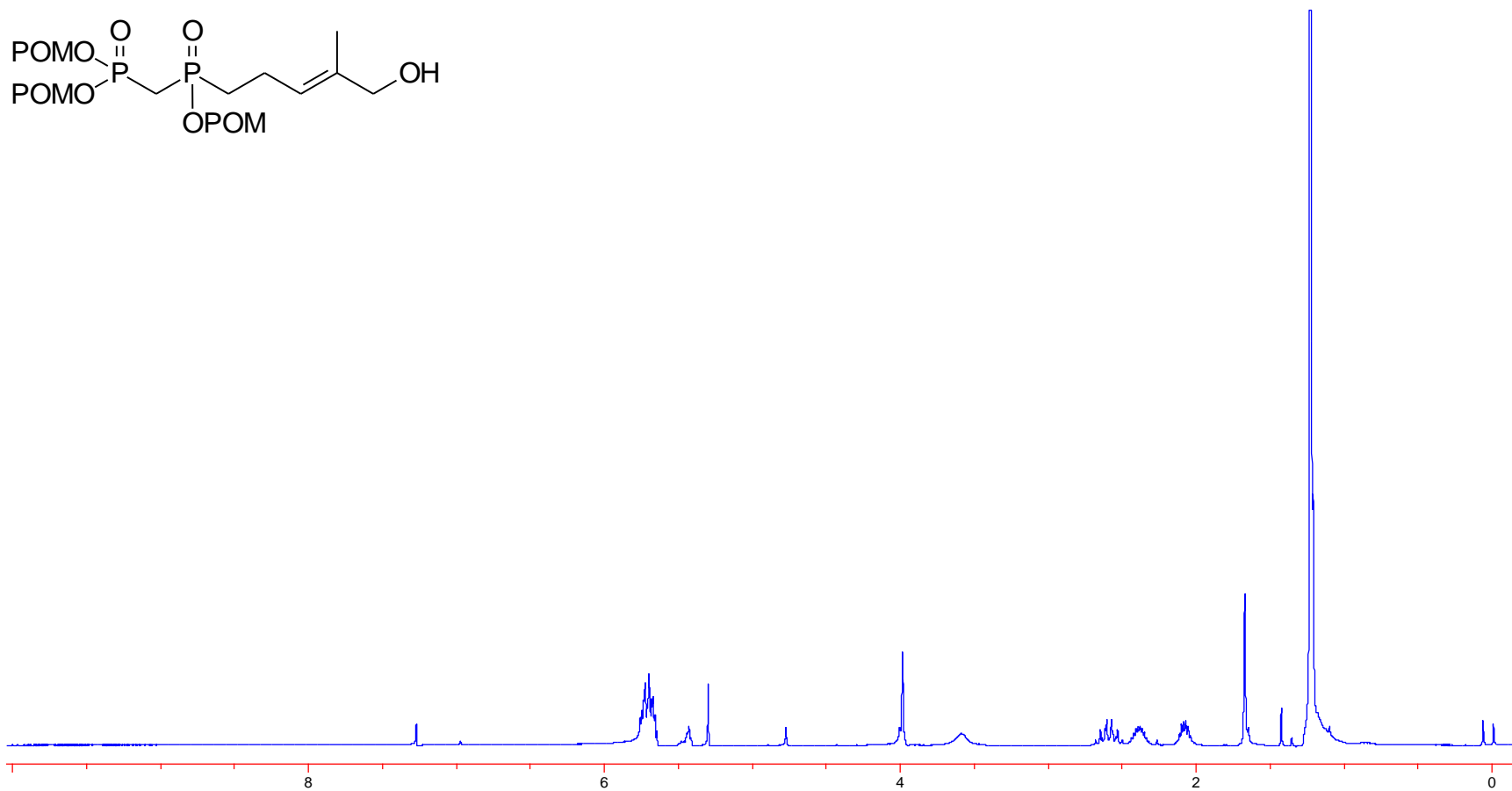
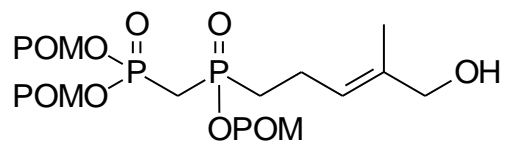
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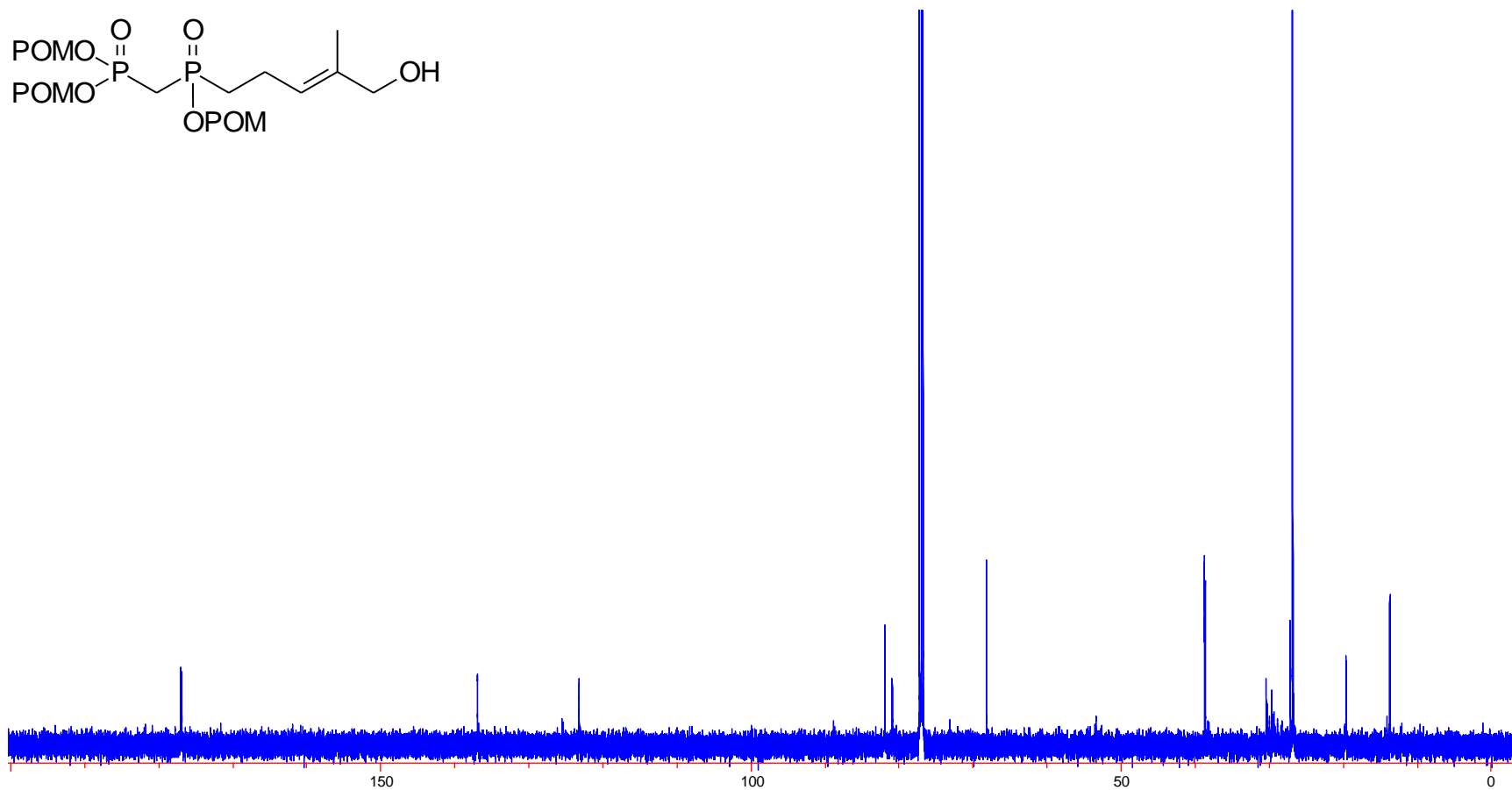
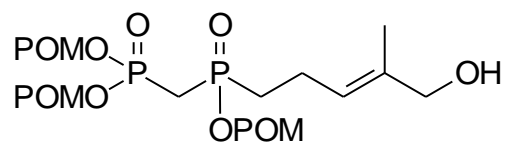
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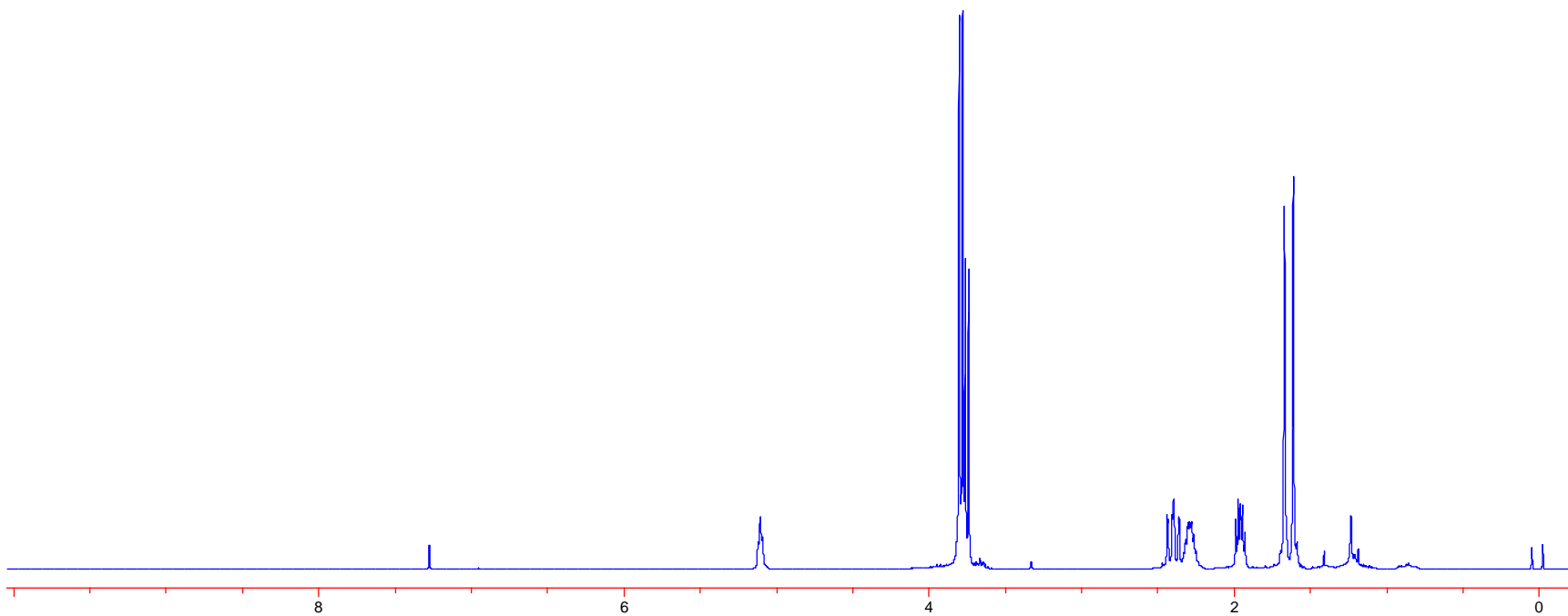
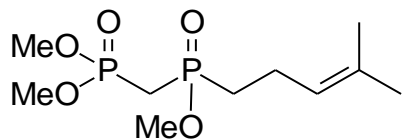
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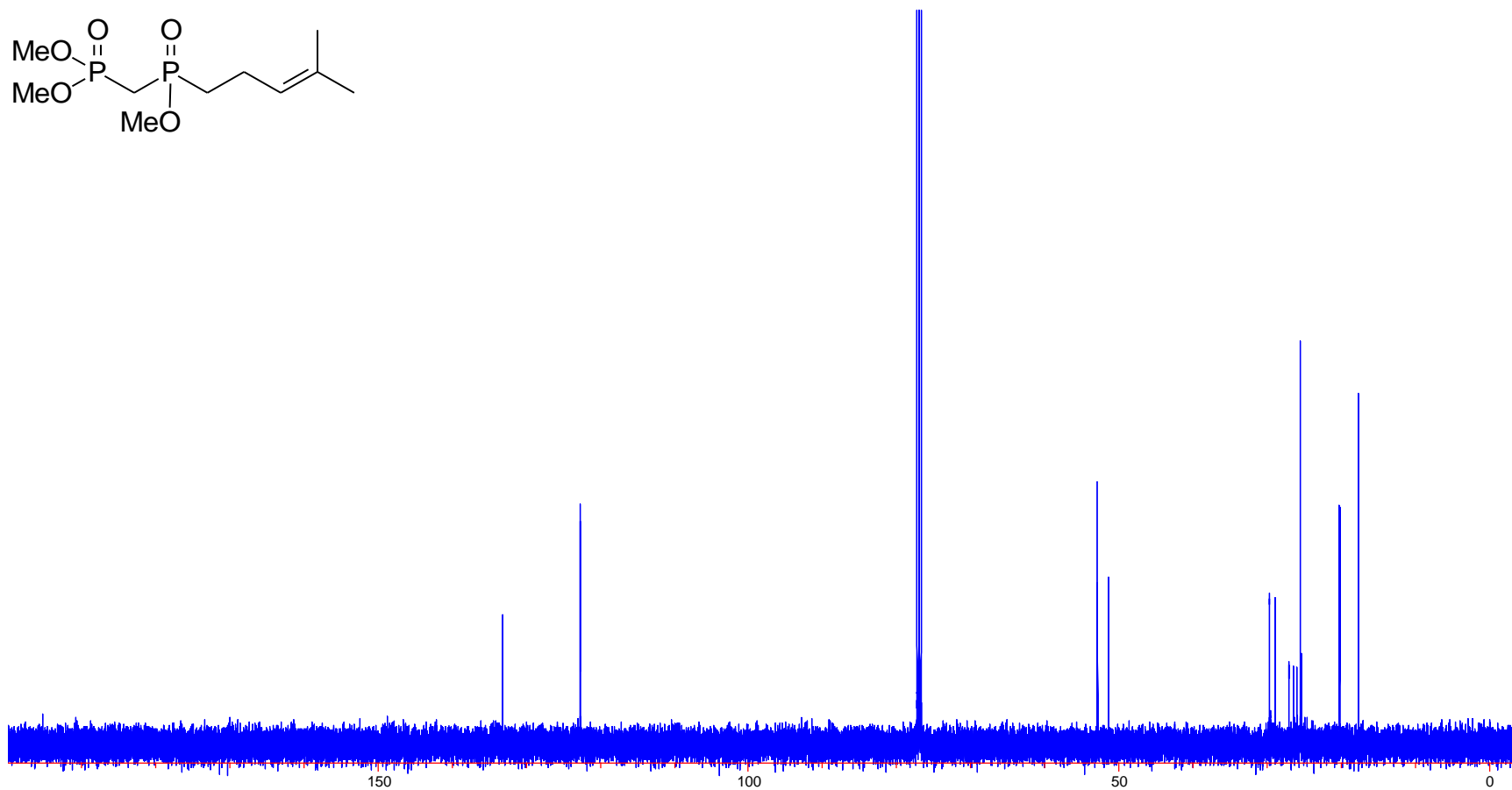
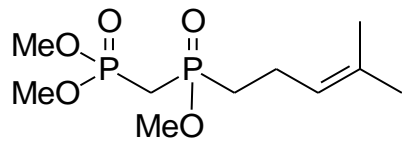
<sup>1</sup>H NMR spectrum of compound **4** (300 MHz).



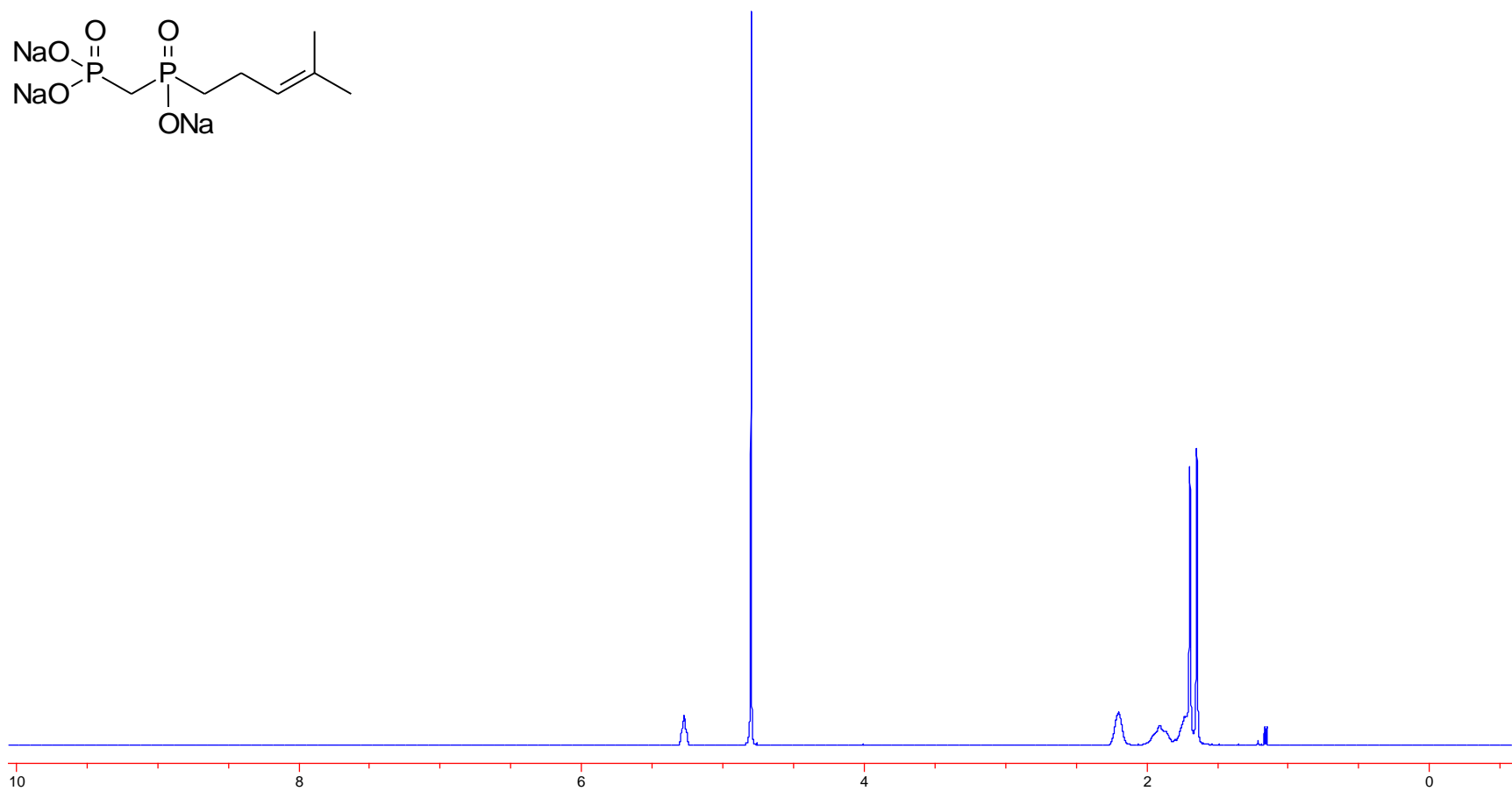
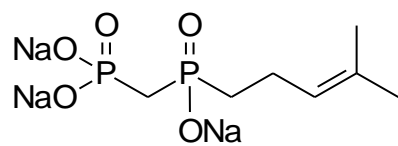
<sup>13</sup>C NMR spectrum of compound 4 (75 MHz).



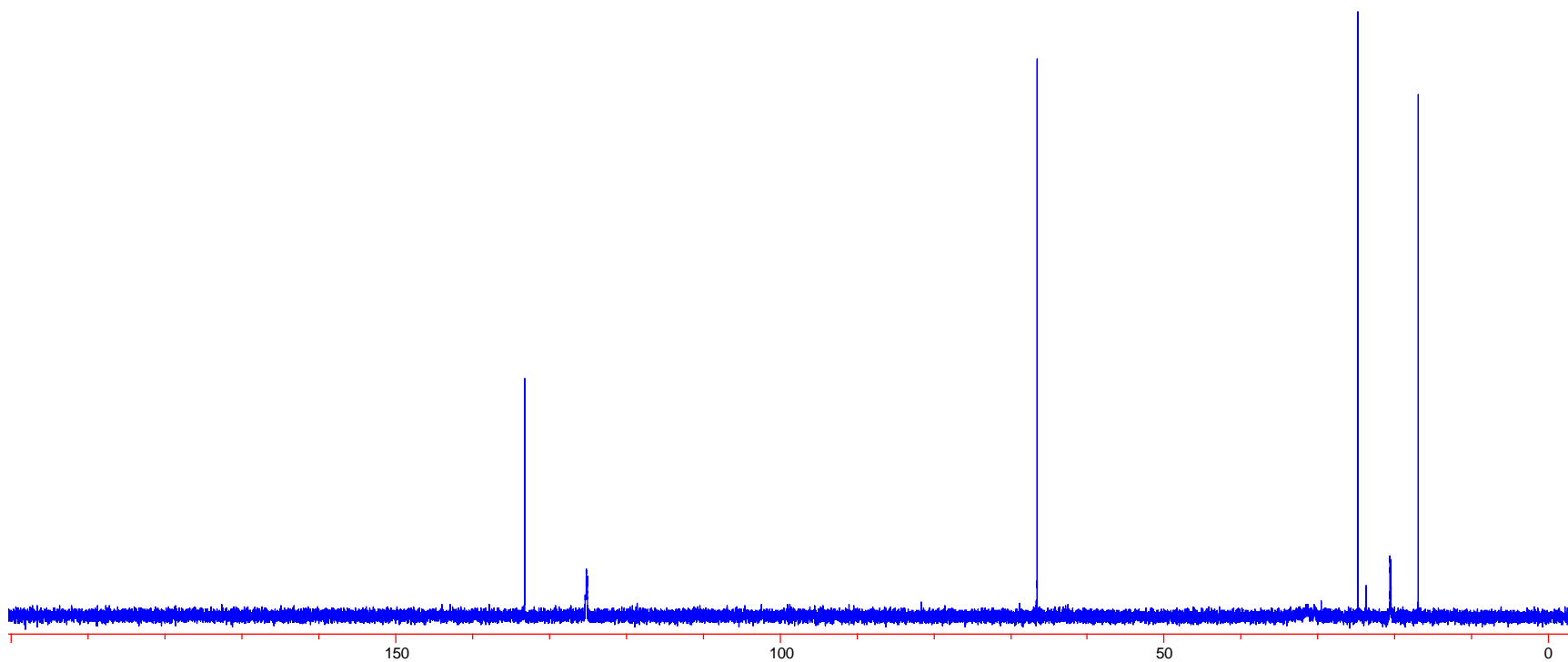
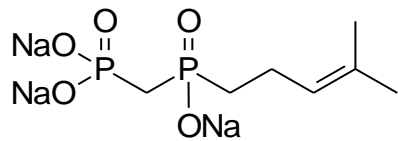
$^1\text{H}$  NMR spectrum of compound 7 (300 MHz).



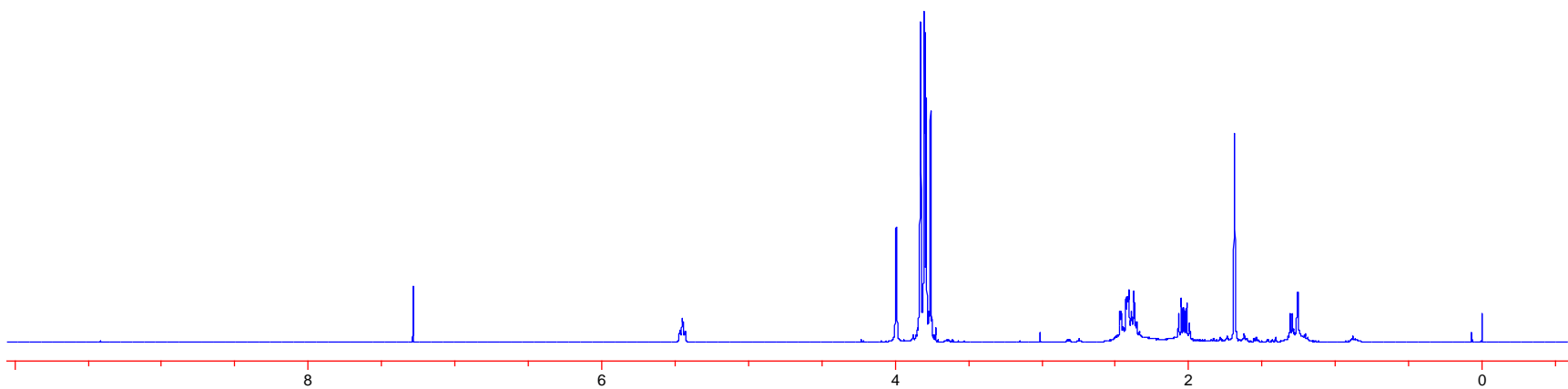
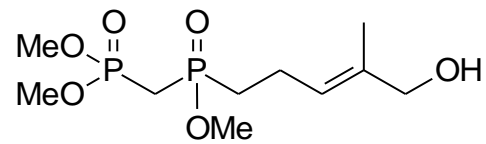
<sup>13</sup>C NMR spectrum of compound 7 (75 MHz).



$^1\text{H}$  NMR spectrum of compound **8** (400 MHz).

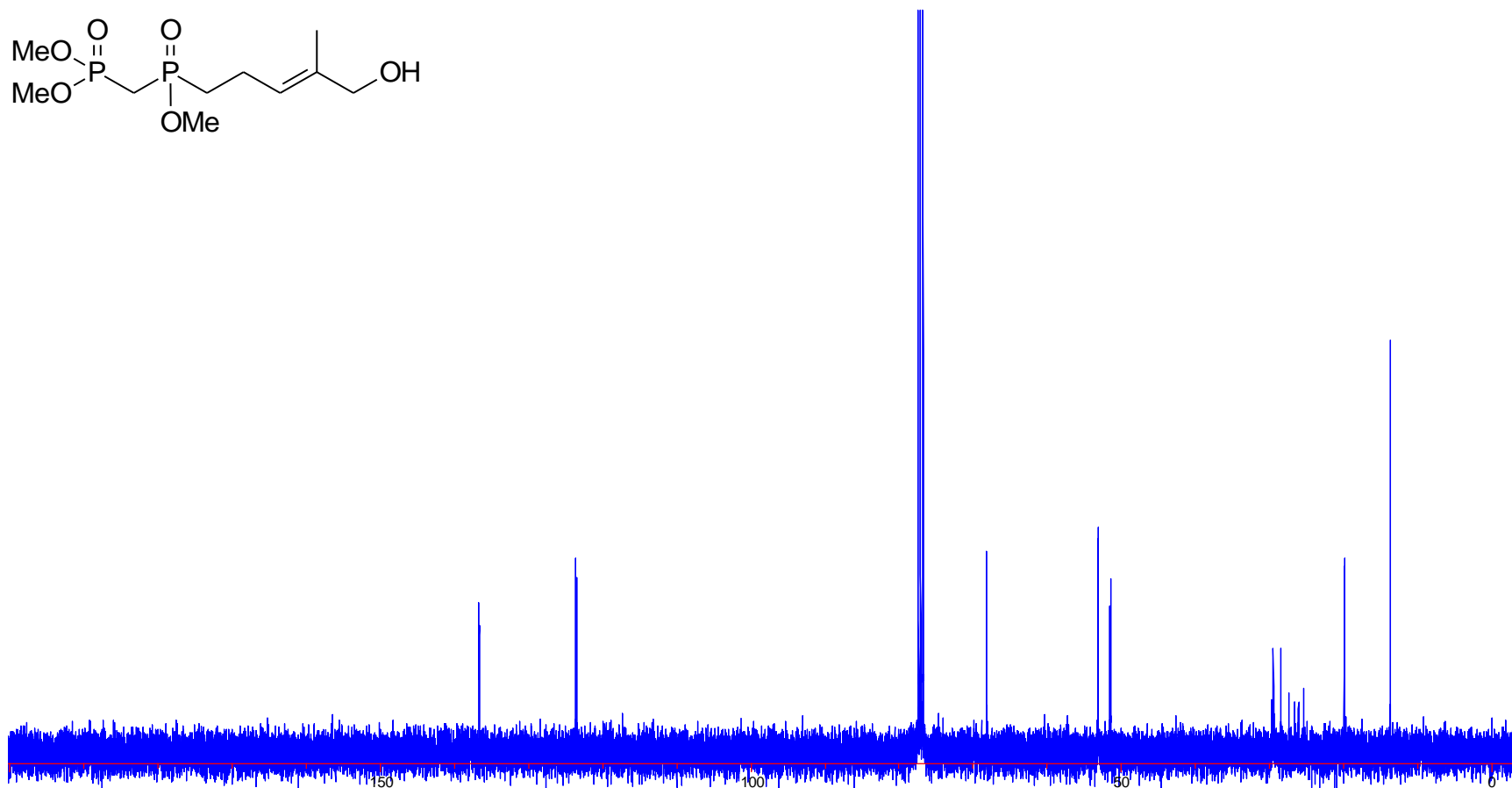
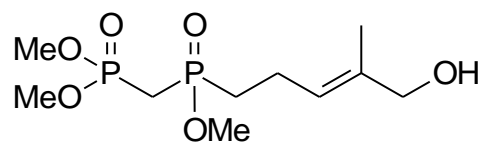


<sup>13</sup>C NMR spectrum of compound **8** (100 MHz).



<sup>1</sup>H NMR spectrum for compound **9** (400 MHz).





$^{13}\text{C}$  NMR spectrum for compound **9** (100 MHz).

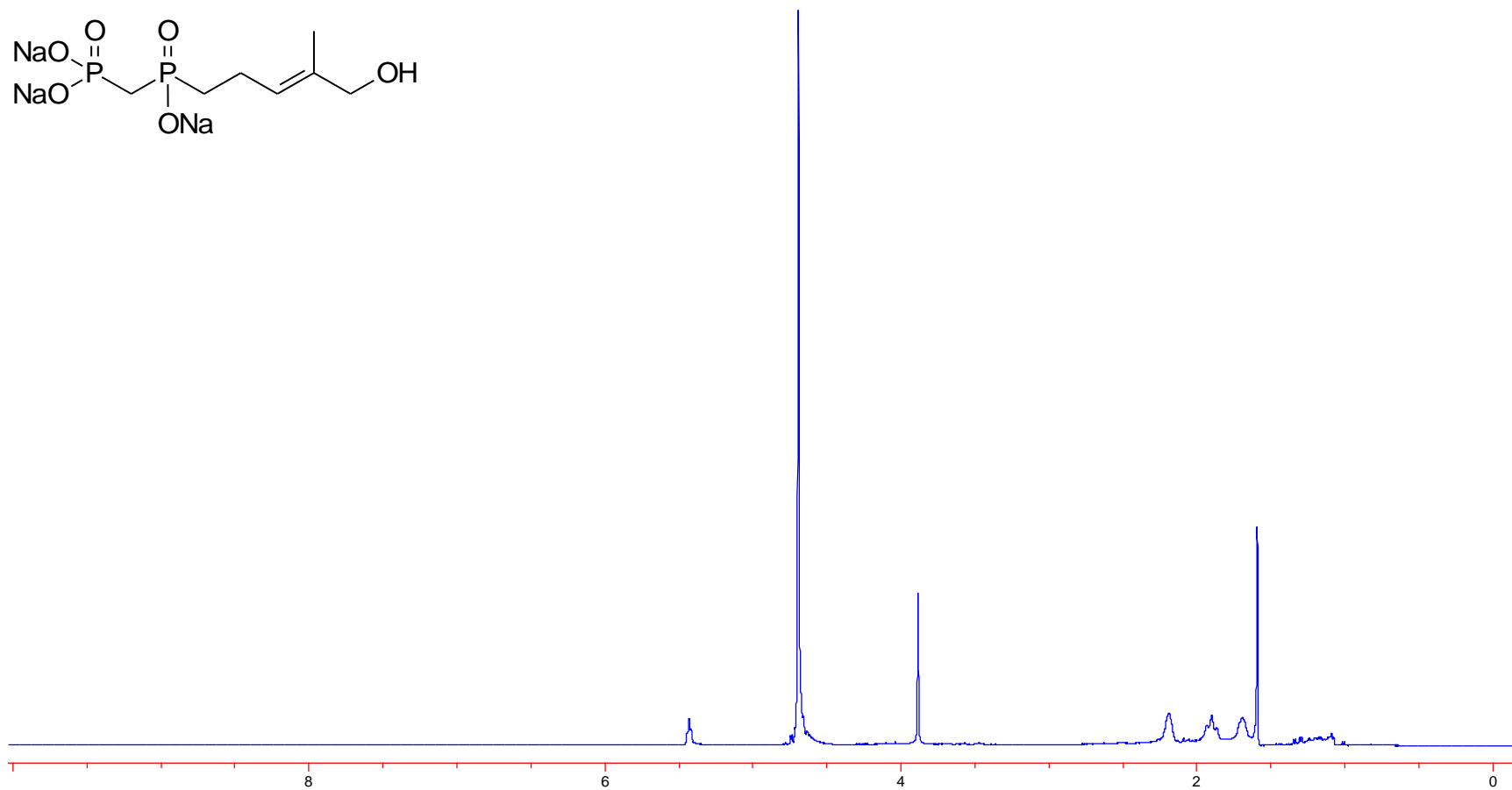
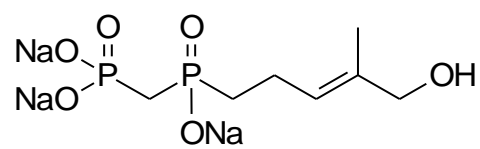
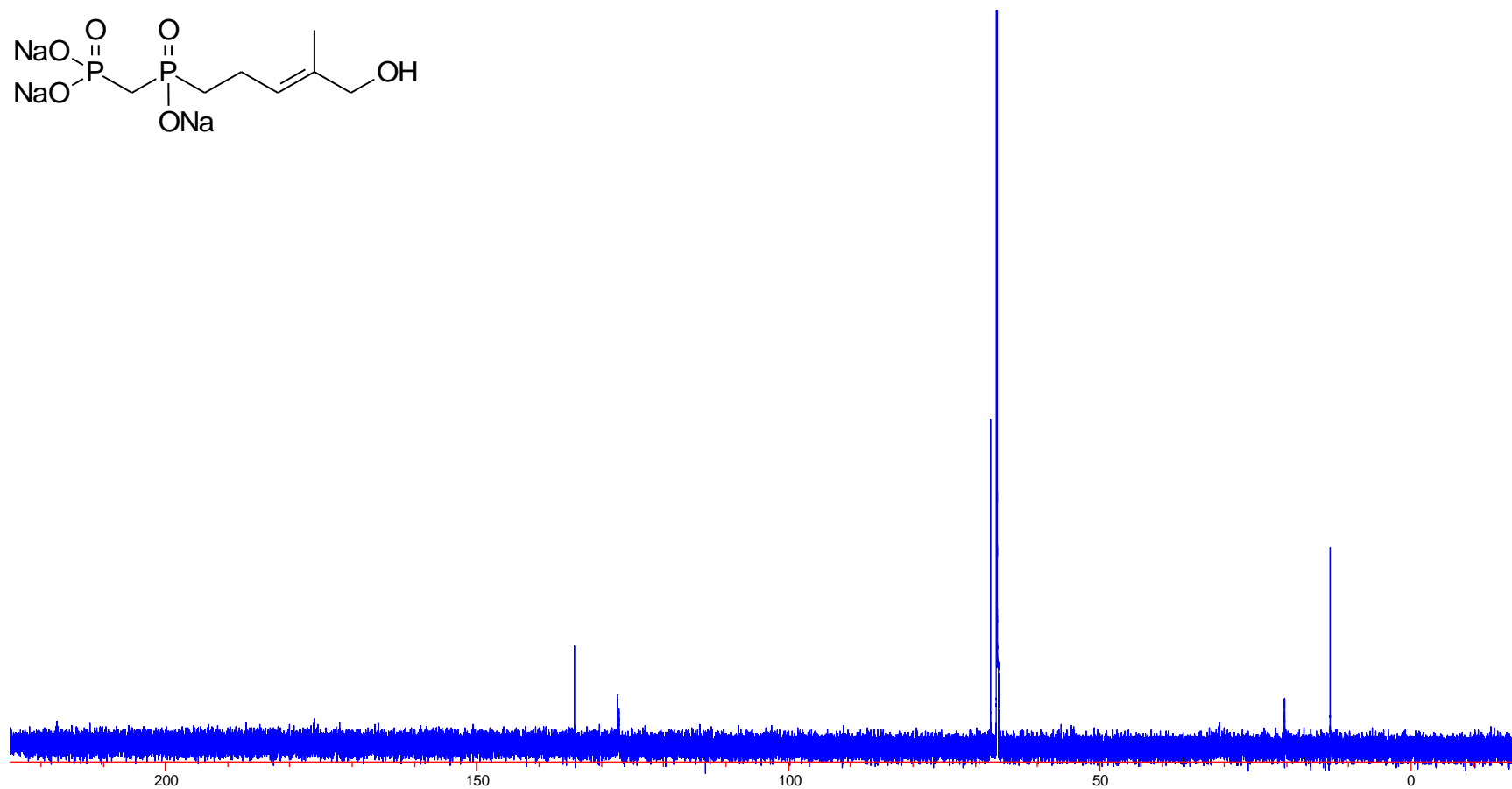
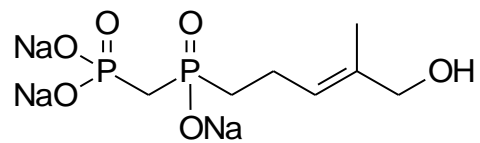
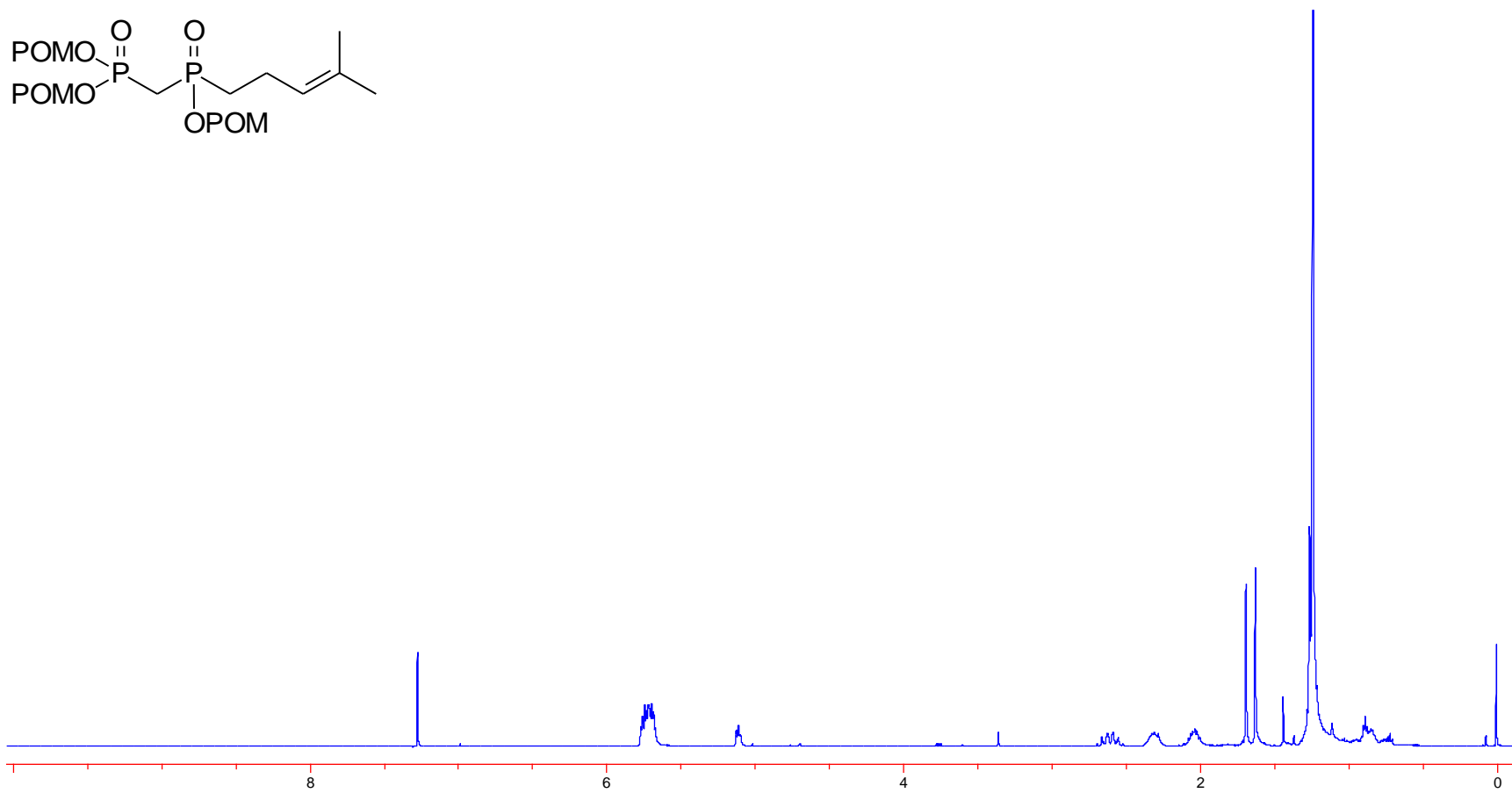
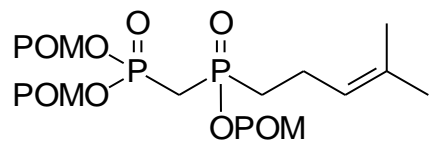


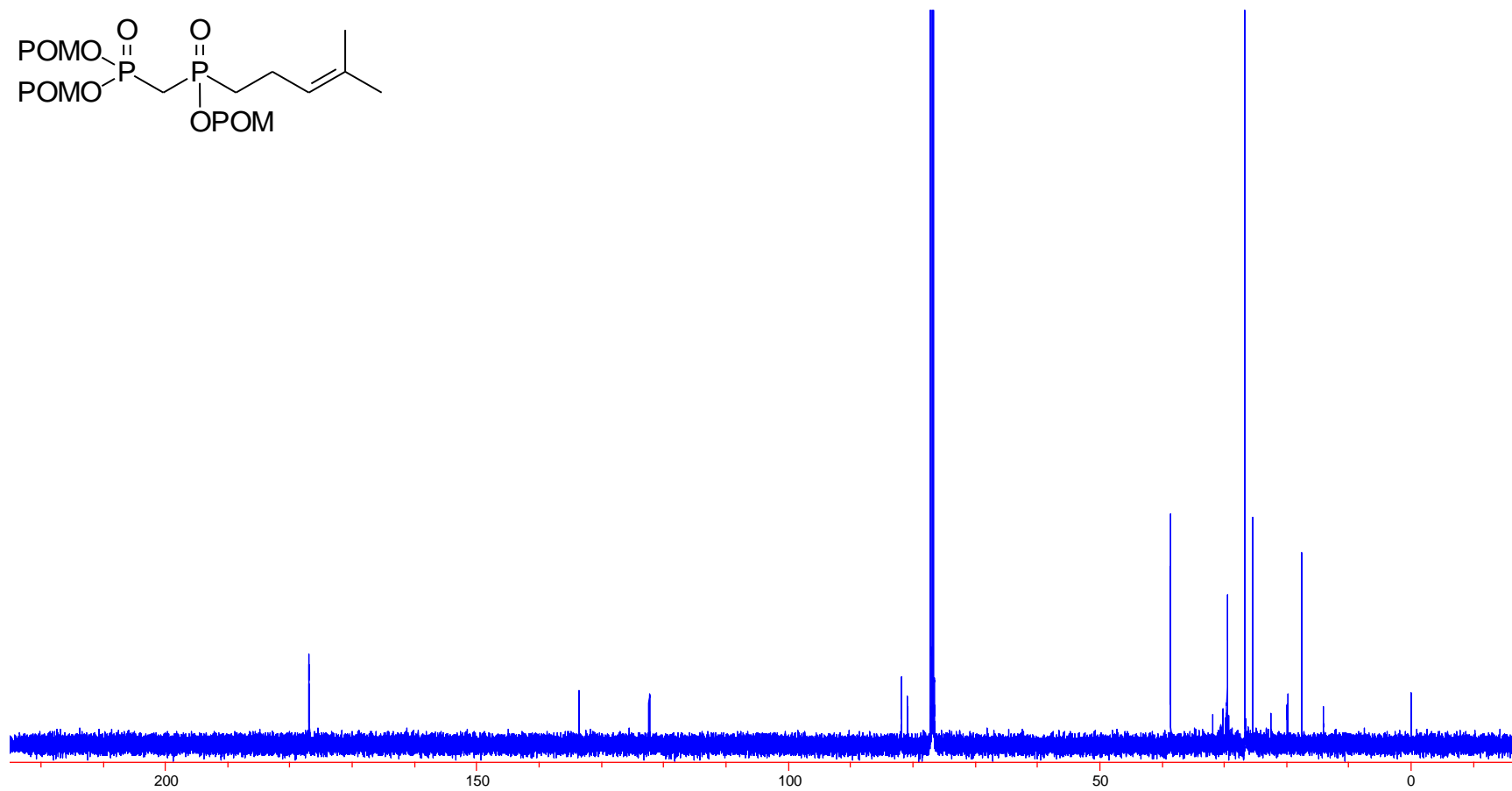
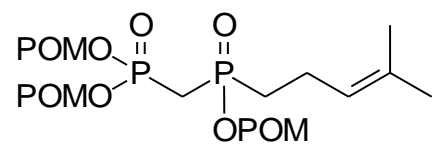
Figure A- 1.  $^1\text{H}$  NMR spectrum of compound **10** (400 MHz).



$^{13}\text{C}$  NMR spectrum of compound **10** (125 MHz).



<sup>1</sup>H NMR spectrum of compound **11** (300 MHz).



$^{13}\text{C}$  NMR spectrum of compound **11** (75 MHz).