

Synthesis of four enantiomers of (1-amino-3-hydroxypropane-1,3-diyl)diphosphonic acid as diphosphonate analogues of 4-hydroxyglutamic acid

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NMR spectra for compounds (1*R*,3*S*)-**6** and (1*R*,3*R*)-**6**, (1*R*,3*S*)-**11**, (1*R*,3*R*)-**11**, (1*R*,3*S*)-**12**, (1*R*,3*S*)-**12**, (1*R*,3*R*)-**4**, (1*R*,3*S*)-**4**, **14**, **15**, (1*R*,3*R*)-**6** [*anti*-**6**], (1*R*,3*R*,1'*S*)-**16**, (1*S*,3*S*,1'*S*)-**16**, (1*S*,3*R*,1'*S*)-**16**.

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Figure S1: ³¹P NMR Spectrum for (1*R*,3*S*)-**6** and (1*R*,3*R*)-**6** in CDCl₃

Figure S2: ¹H NMR Spectrum for (1*R*,3*S*)-**11** in CDCl₃

Figure S3: ¹³C NMR Spectrum for (1*R*,3*S*)-**11** in CDCl₃

Figure S4: ³¹P NMR Spectrum for (1*R*,3*S*)-**11** in CDCl₃

Figure S5: ¹H NMR Spectrum for (1*R*,3*R*)-**11** in CDCl₃

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Figure S7: ³¹P NMR Spectrum for (1*R*,3*R*)-**11** in CDCl₃

Figure S8: ¹H NMR Spectrum for (1*R*,3*S*)-**12** in CDCl₃

Figure S9: ¹³C NMR Spectrum for (1*R*,3*S*)-**12** in CDCl₃

Figure S10: ³¹P NMR Spectrum for (1*R*,3*S*)-**12** in CDCl₃

Figure S11: ¹H NMR Spectrum for (1*R*,3*R*)-**12** in CDCl₃

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Figure S13: ³¹P NMR Spectrum for (1*R*,3*R*)-**12** in CDCl₃

Figure S14: ¹H NMR Spectrum for (1*R*,3*R*)-**4** in D₂O

Figure S15: ^{13}C NMR Spectrum for (1*R*,3*R*)-**4** in D_2O

Figure S16: ^{31}P NMR Spectrum for (1*R*,3*R*)-**4** in D_2O

Figure S17: ^1H NMR Spectrum for (1*R*,3*S*)-**4** in D_2O

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Figure S19: ^{31}P NMR Spectrum for (1*R*,3*S*)-**4** in D_2O

Figure S20: ^1H NMR Spectrum for *trans*-**14** in CDCl_3

Figure S21: ^{13}C NMR Spectrum for *trans*-**14** in CDCl_3

Figure S22: ^{31}P NMR Spectrum for *trans*-**14** in CDCl_3

Figure S23: ^1H NMR Spectrum for *trans*-**15** in CDCl_3

Figure S24: ^{13}C NMR Spectrum for *trans*-**15** in CDCl_3

Figure S25: ^{31}P NMR Spectrum for *trans*-**15** in CDCl_3

Figure S26: ^1H NMR Spectrum for (1*R*,3*R*)-**6** [*anti*-**6**] in CDCl_3

Figure S27: ^{13}C NMR Spectrum for (1*R*,3*R*)-**6** [*anti*-**6**] in CDCl_3

Figure S28: ^{31}P NMR Spectrum for (1*R*,3*R*)-**6** [*anti*-**6**] in CDCl_3

Figure S29: ^1H NMR Spectrum for (1*R*,3*R*)-**6** [*anti*-**6**] in C_6D_6

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Figure S32: ^1H NMR Spectrum for (1*R*,3*R*,1'*S*)-**16** in C_6D_6

Figure S33: ^{31}P NMR Spectrum for (1*R*,3*R*,1'*S*)-**16** in C_6D_6

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Figure S35: ^1H NMR Spectrum for (1*S*,3*S*,1'*S*)-**16** in C_6D_6

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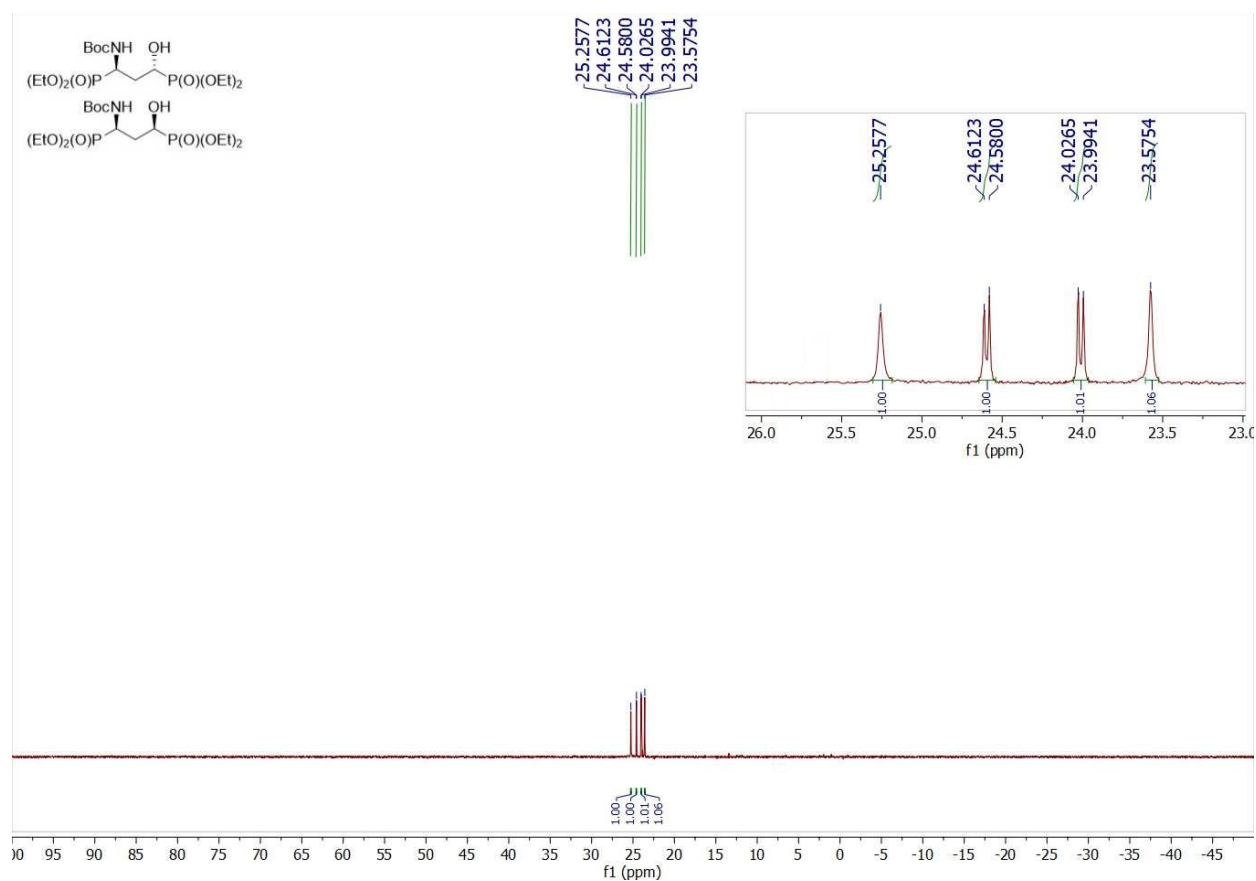


Figure S1: ³¹P NMR Spectrum for (1R,3S)-6 and (1R,3R)-6 in CDCl₃

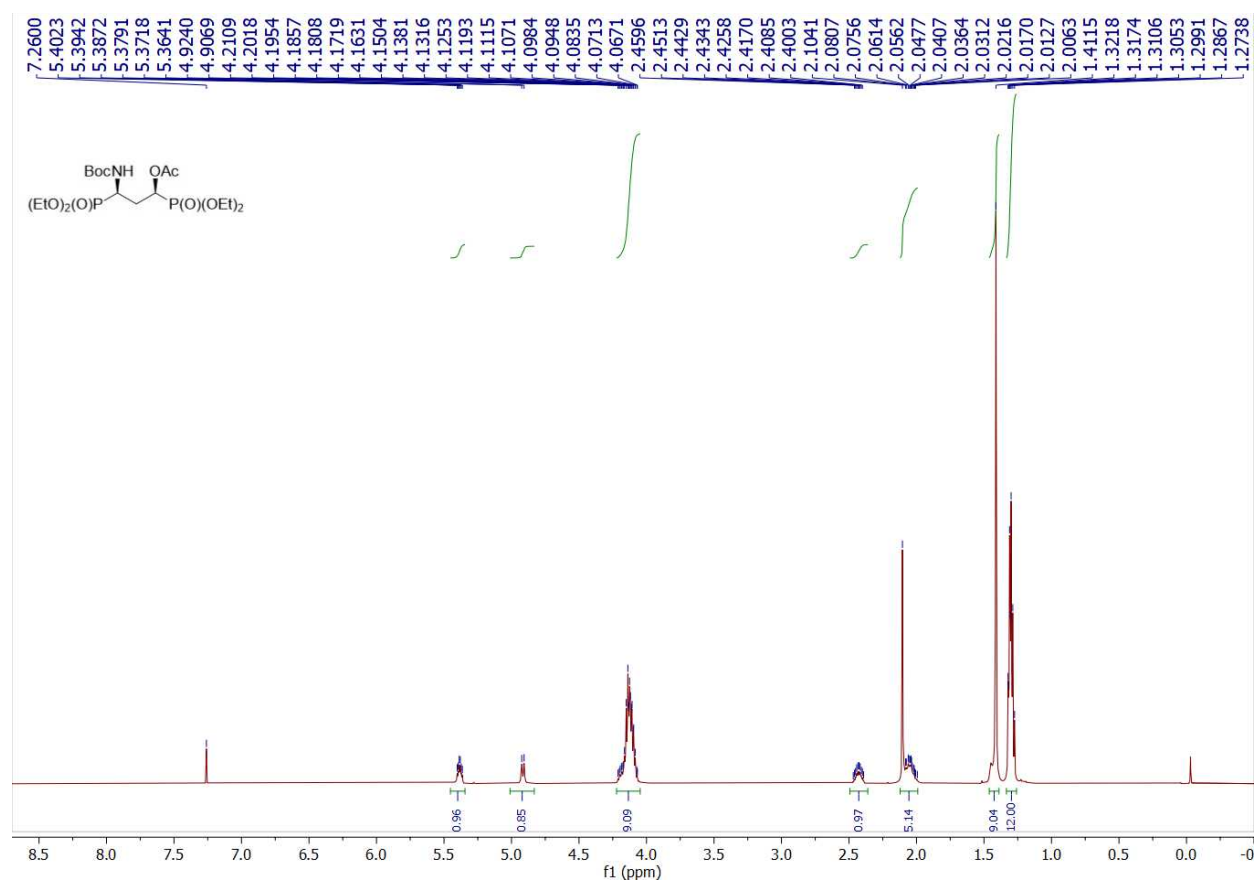


Figure S2: ¹H NMR Spectrum for (1R,3S)-11 in CDCl₃

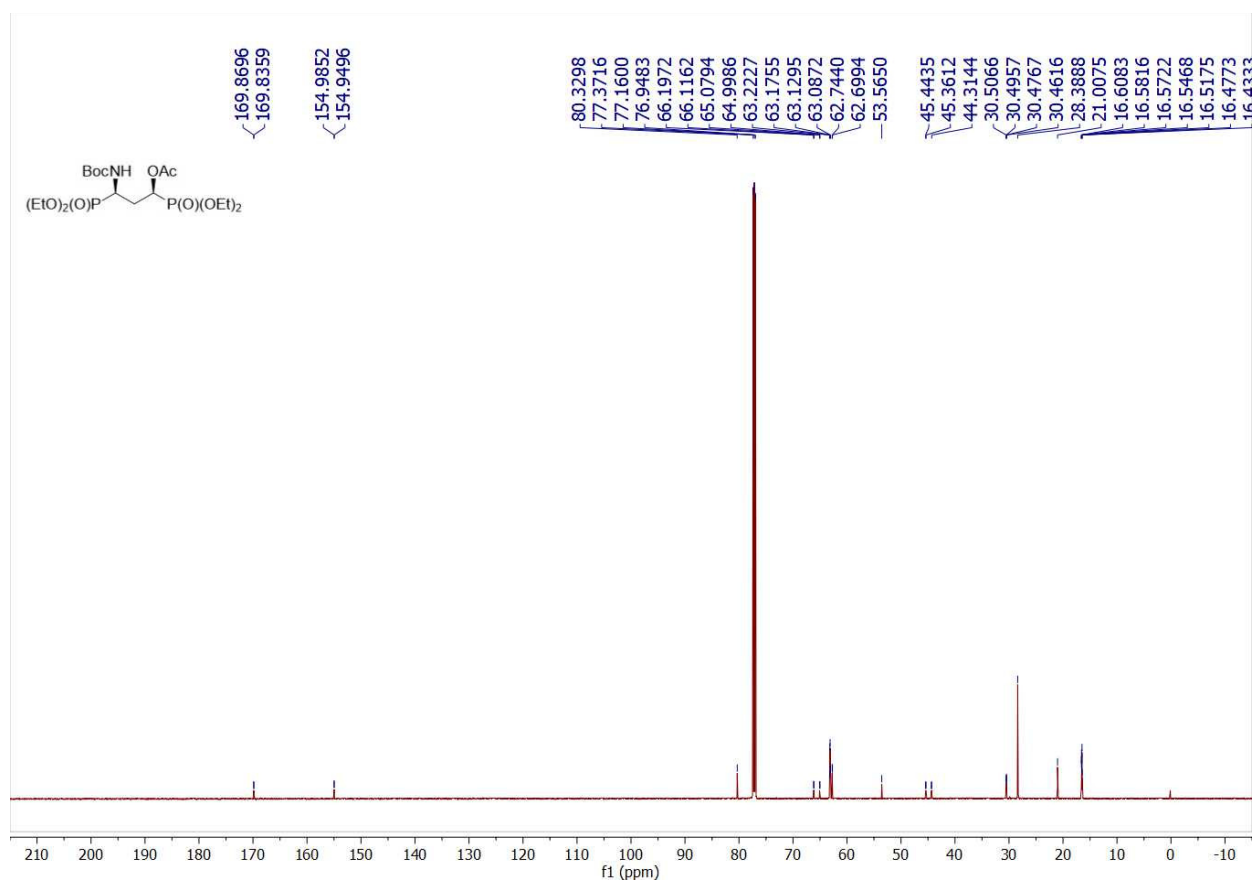


Figure S3: ¹³C NMR Spectrum for (1R,3S)-**11** in CDCl₃

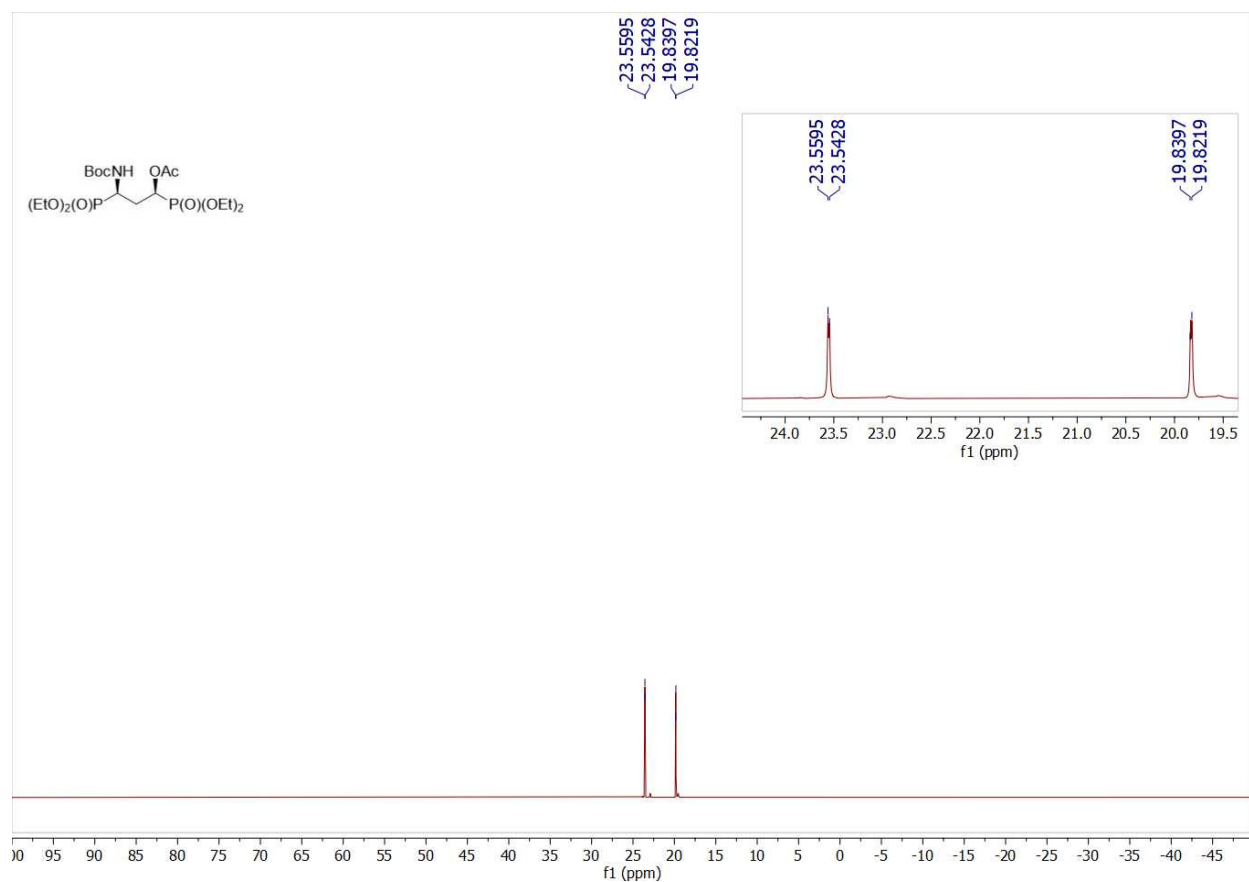


Figure S4: ³¹P NMR Spectrum for (1R,3S)-**11** in CDCl₃

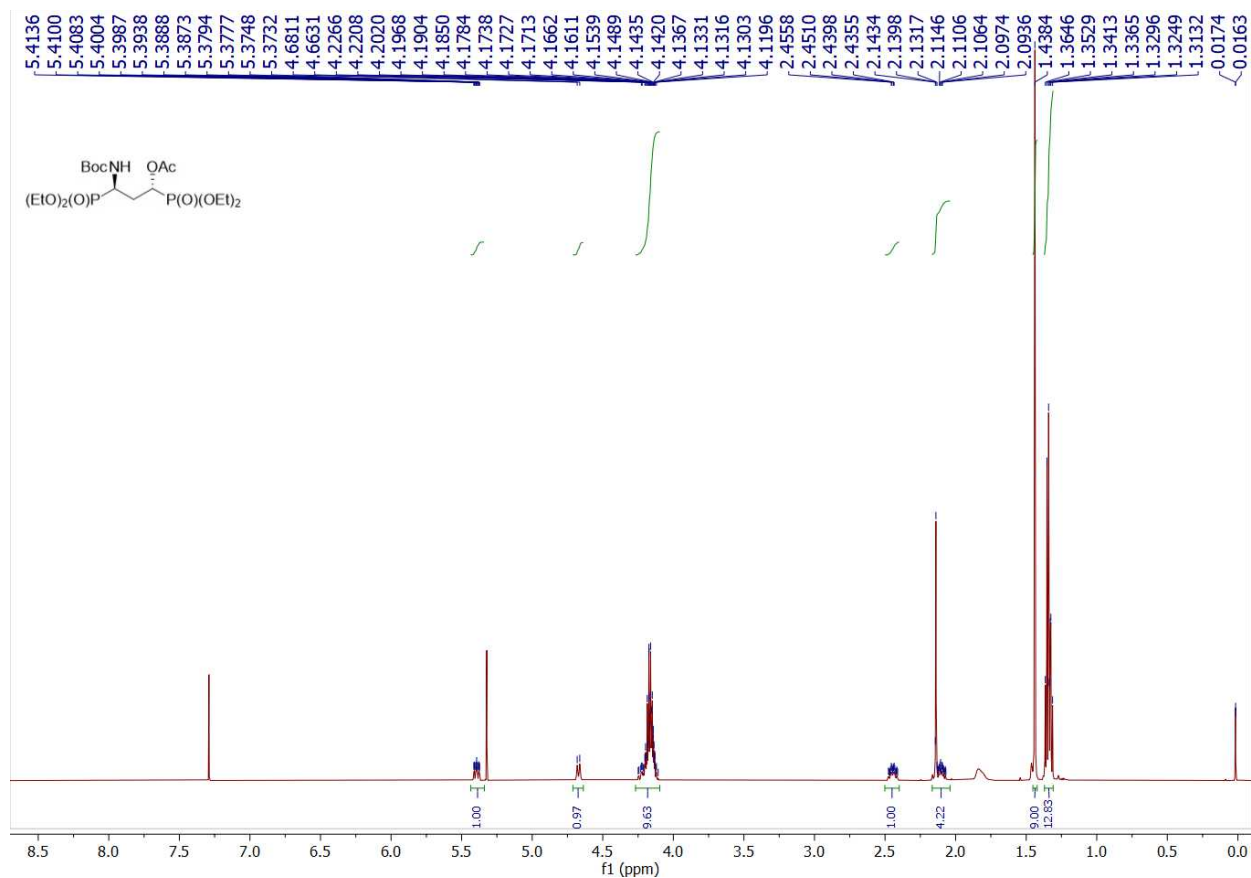


Figure S5: ¹H NMR Spectrum for (1R,3R)-11 in CDCl₃

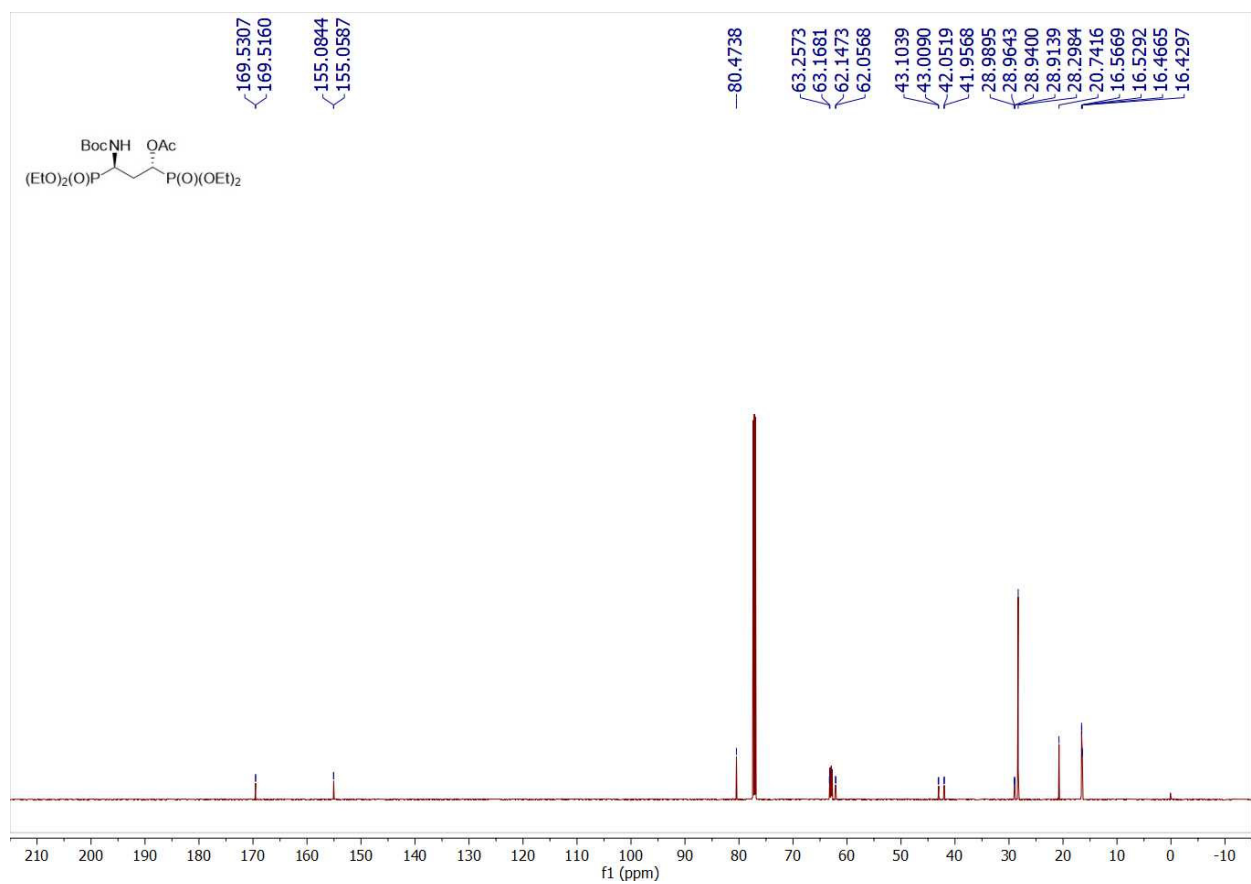


Figure S6: ¹³C NMR Spectrum for (1R,3R)-11 in CDCl₃

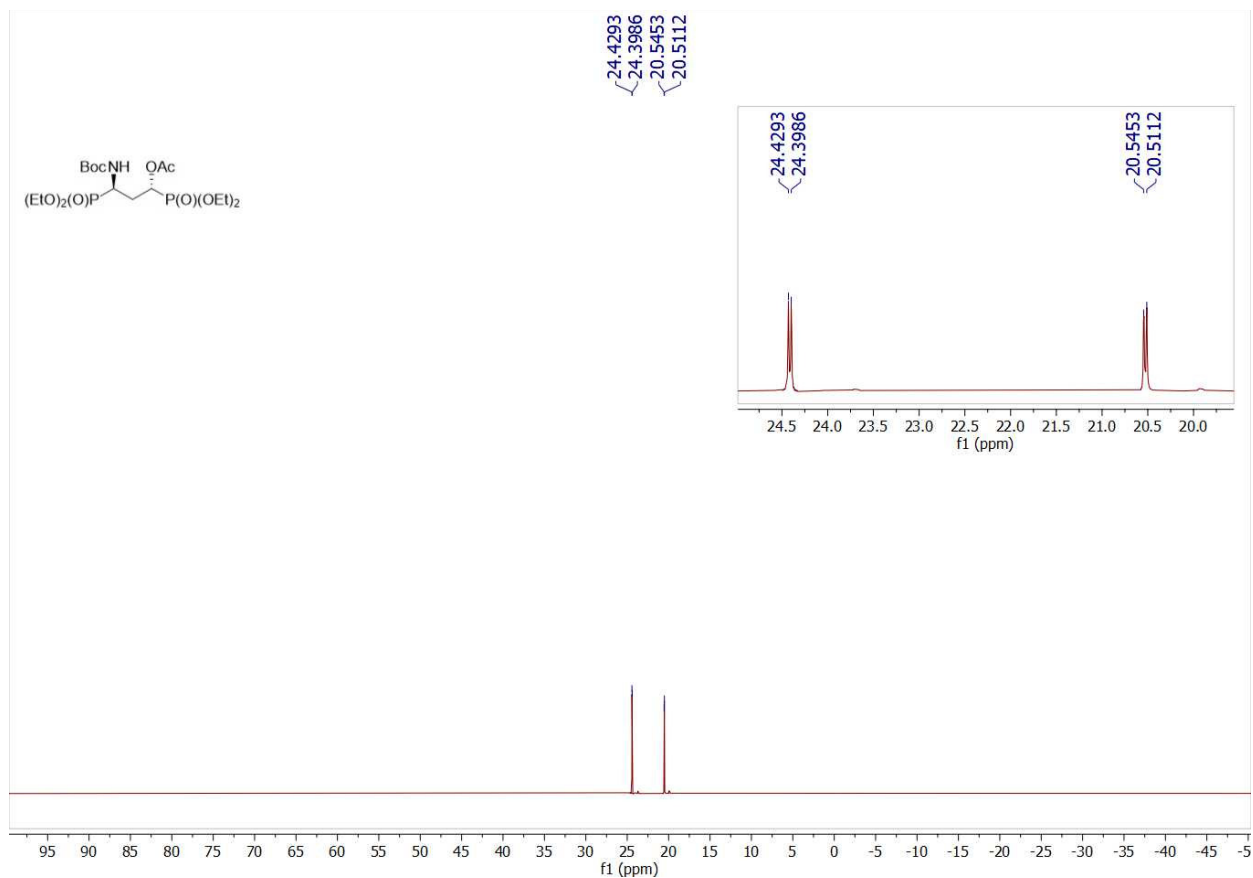


Figure S7: ³¹P NMR Spectrum for (1R,3R)-11 in CDCl₃

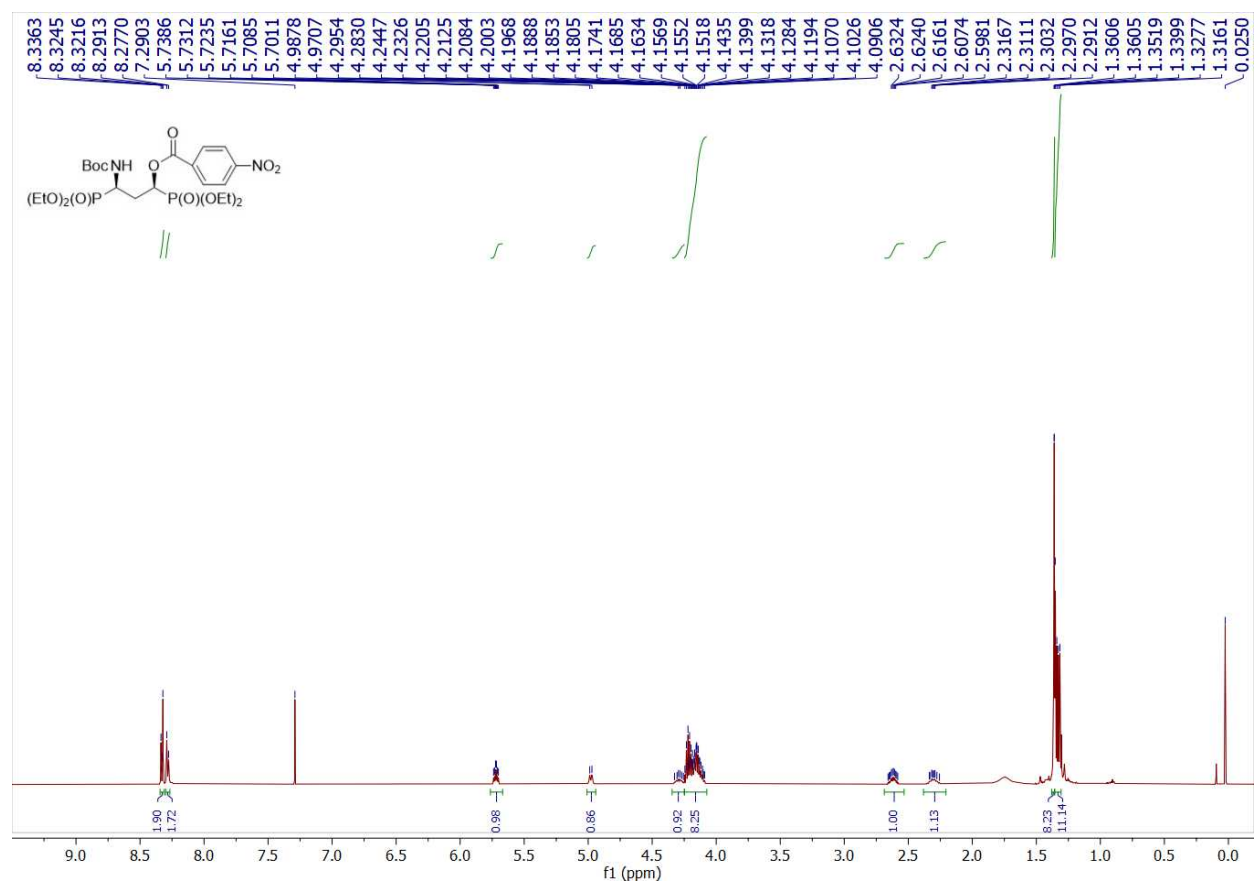


Figure S8: ¹H NMR Spectrum for (1R,3S)-12 in CDCl₃

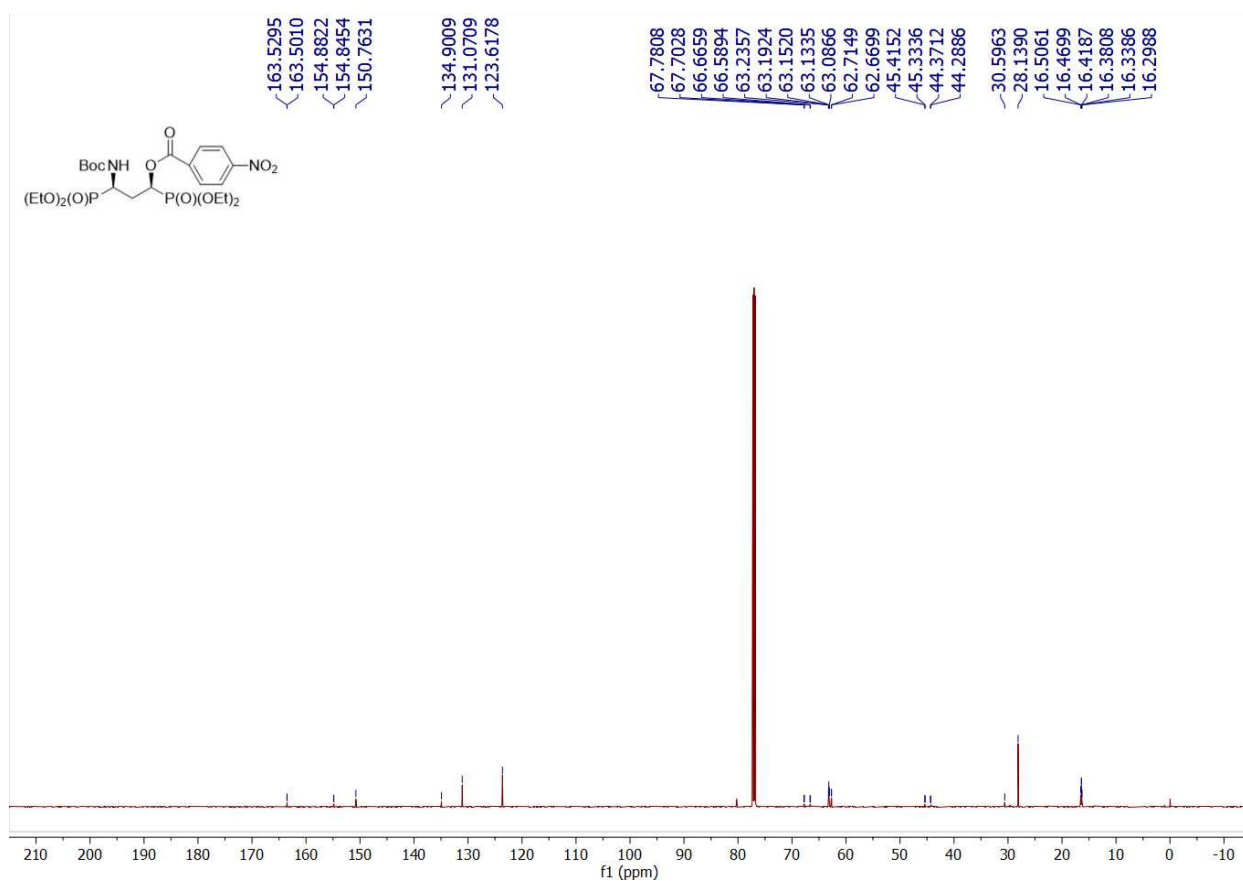


Figure S9: ¹³C NMR Spectrum for (1R,3S)-12 in CDCl₃

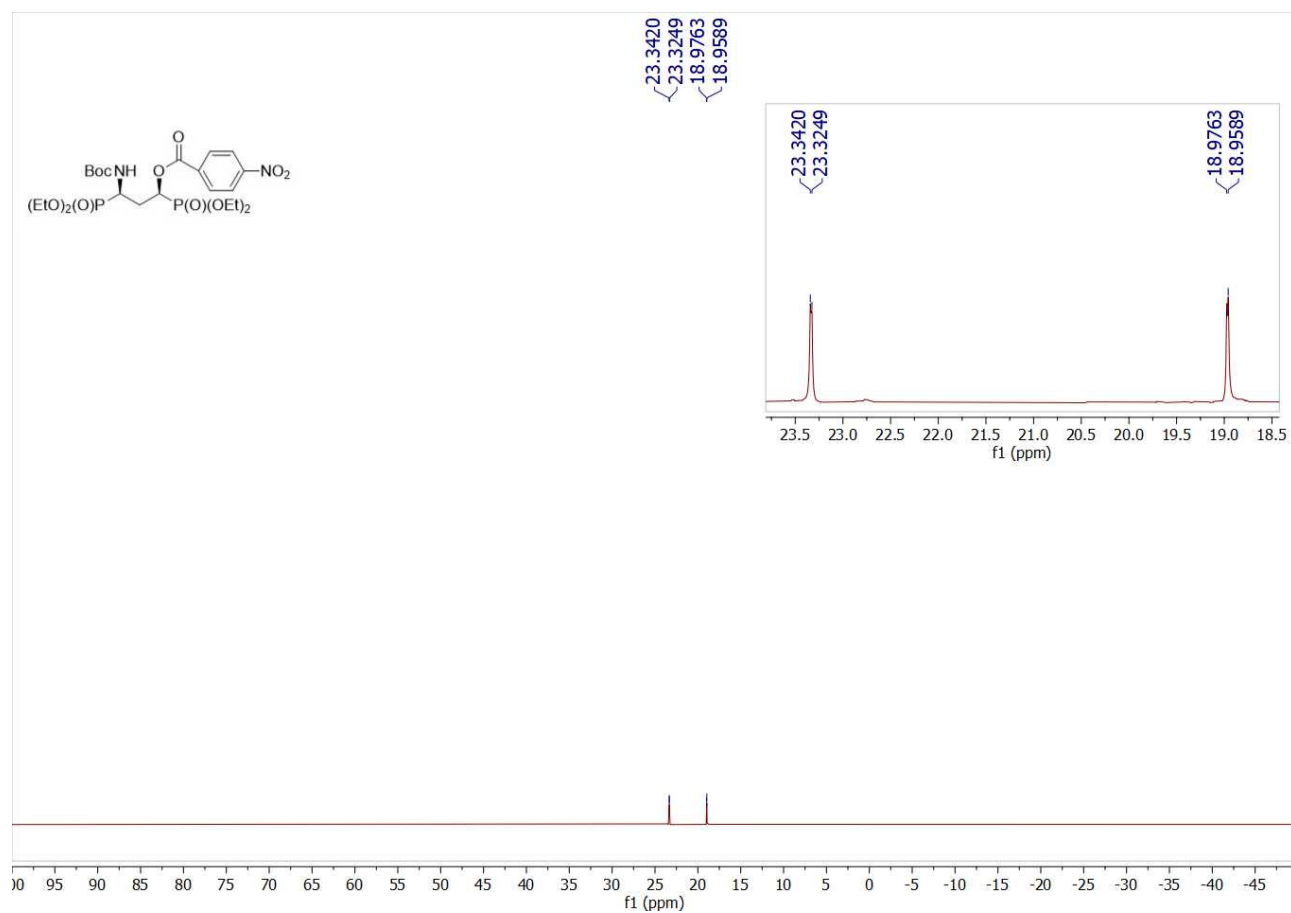


Figure S10: ³¹P NMR Spectrum for (1R,3S)-12 in CDCl₃

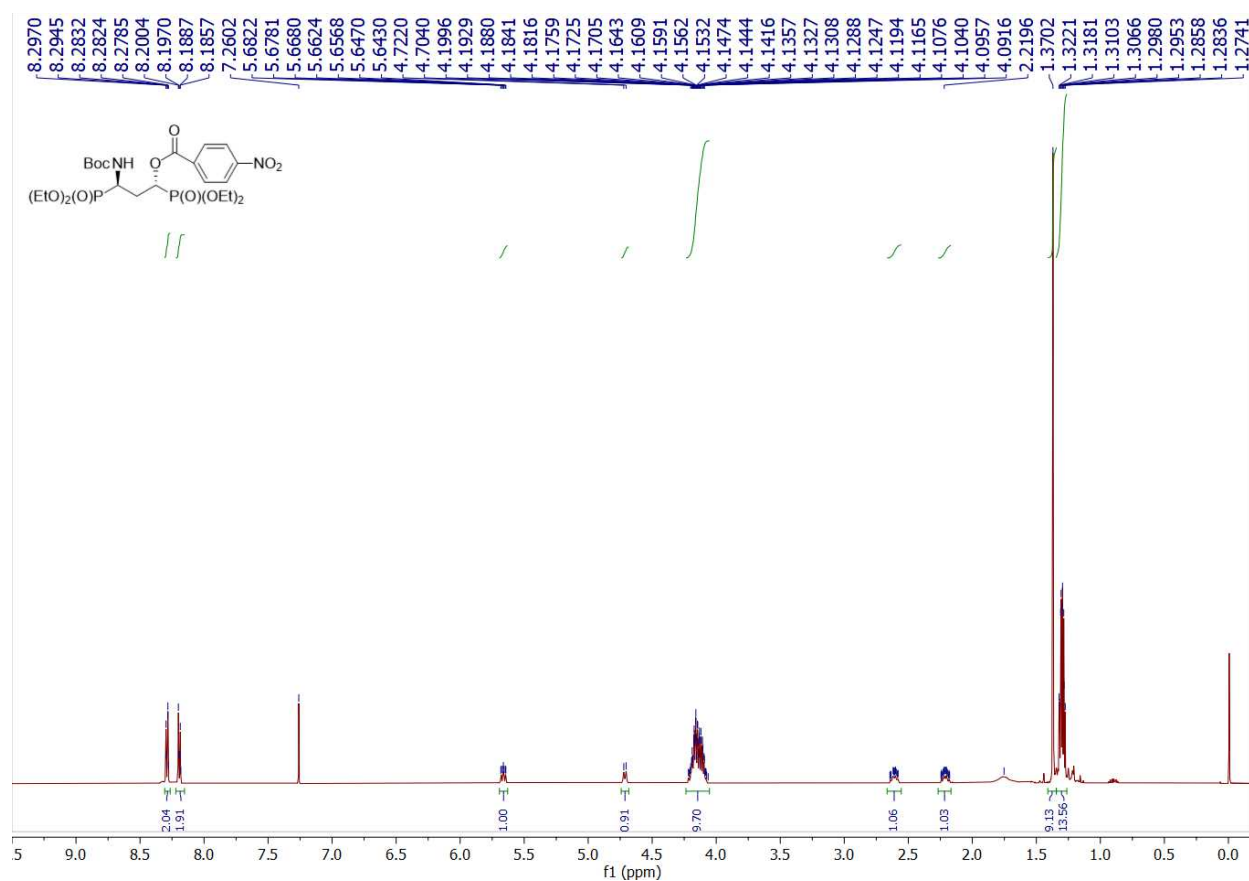


Figure S11: ¹H NMR Spectrum for (1R,3R)-12 in CDCl₃

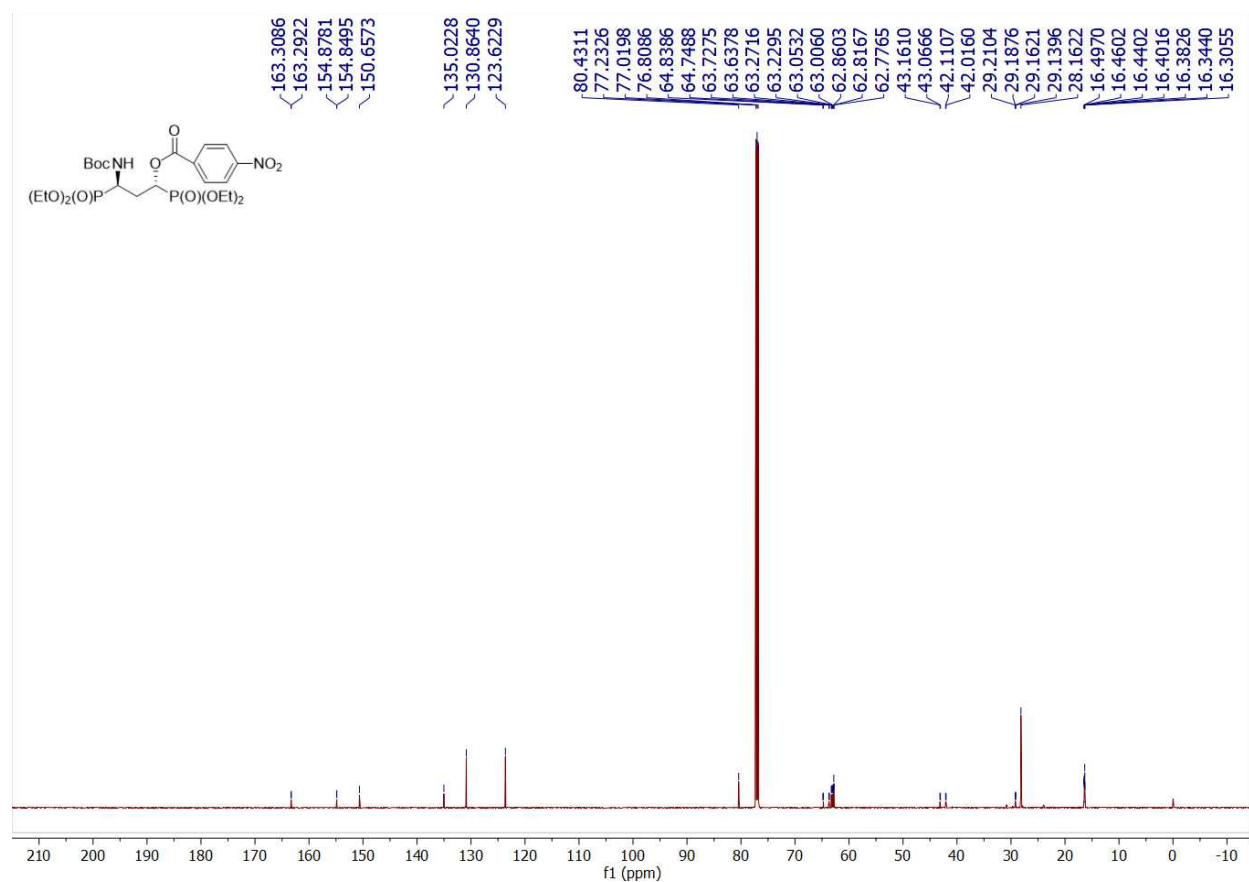


Figure S12: ¹³C NMR Spectrum for (1R,3R)-12 in CDCl₃

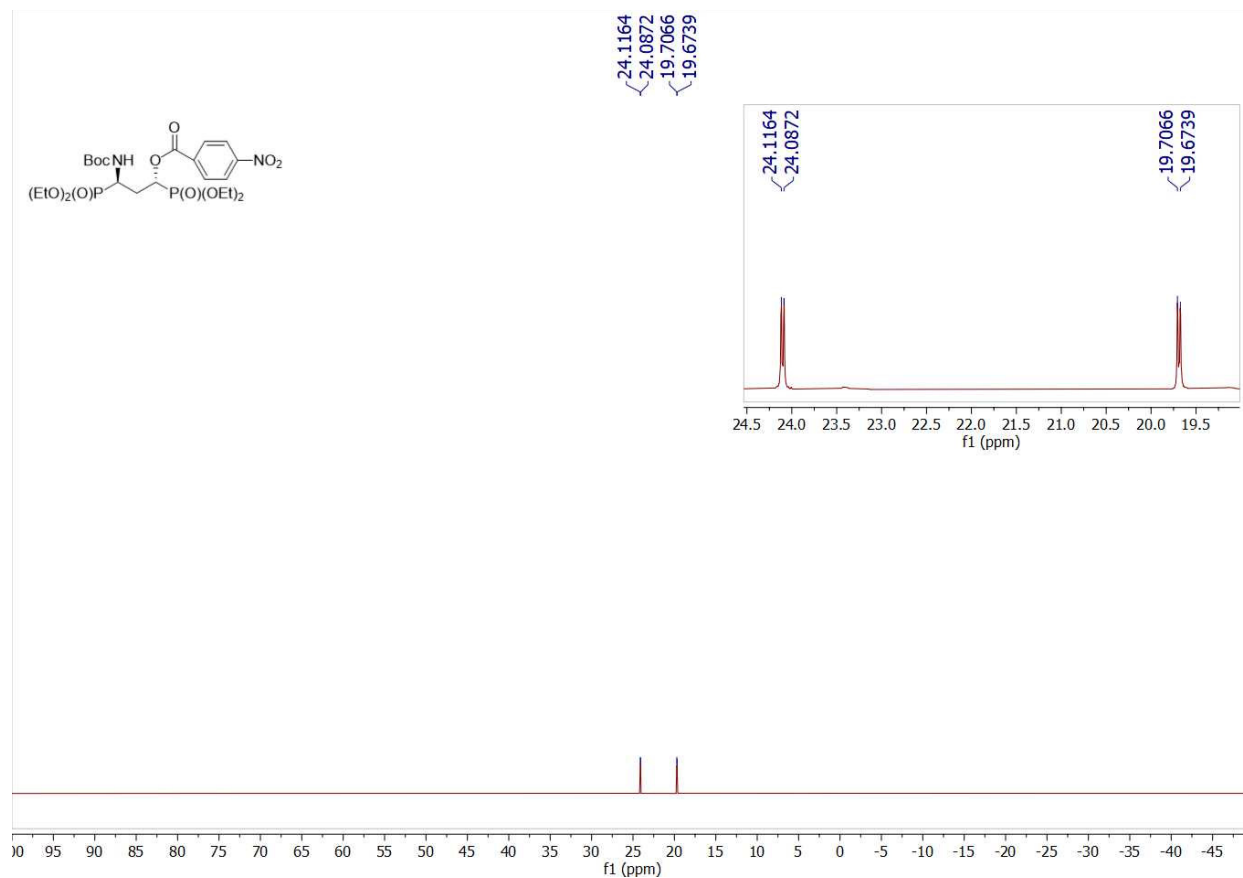


Figure S13: ³¹P NMR Spectrum for (1R,3R)-12 in CDCl₃

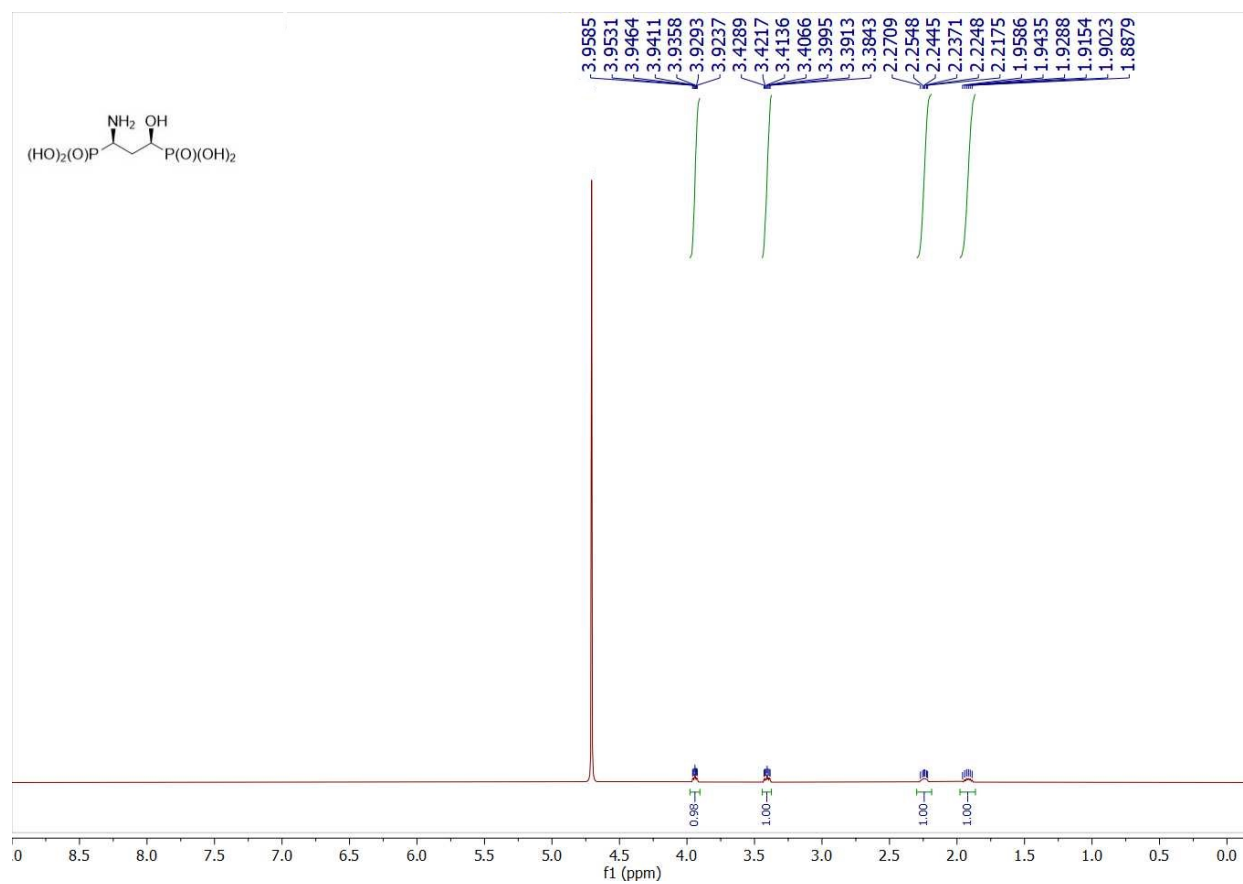


Figure S14: ¹H NMR Spectrum for (1R,3R)-4 in D₂O

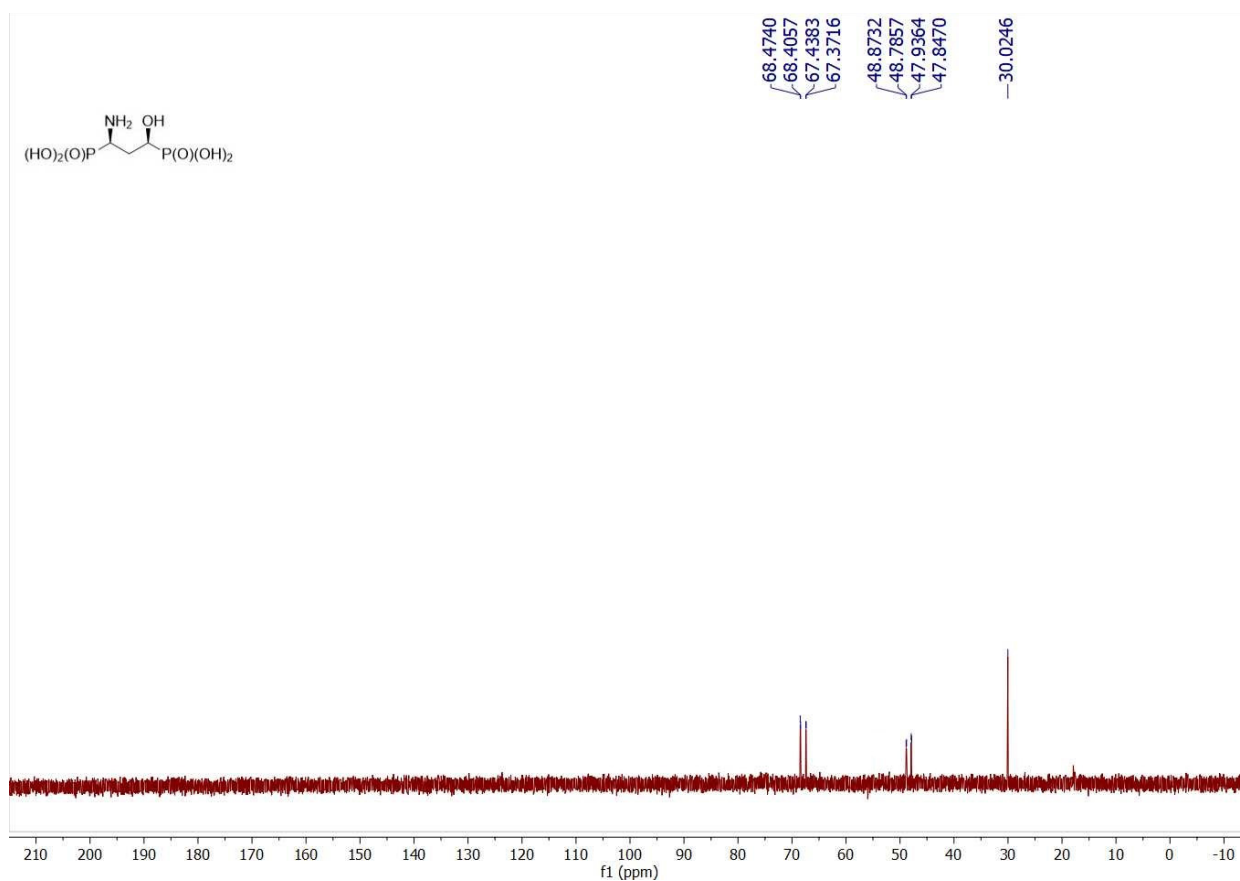


Figure S15: ¹³C NMR Spectrum for (1R,3R)-4 in D₂O

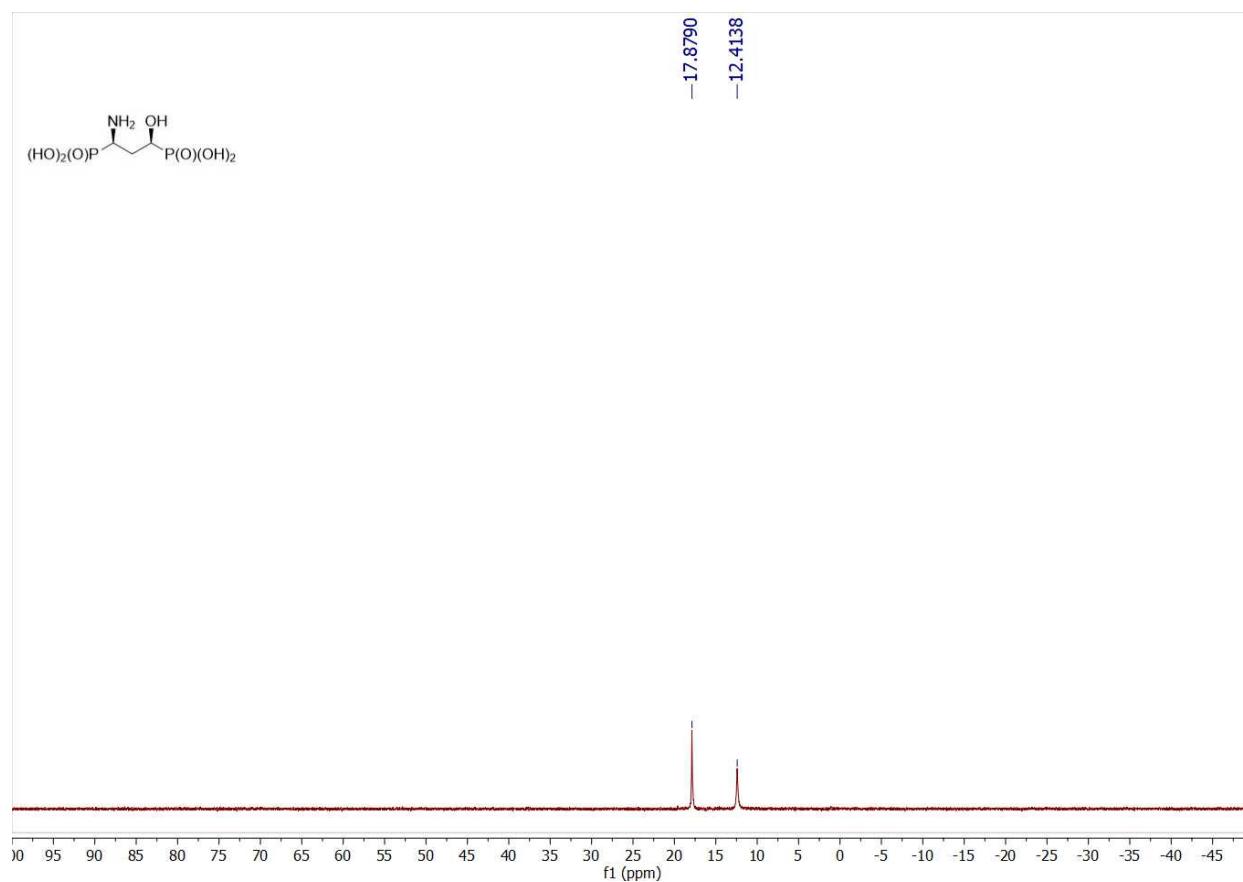


Figure S16: ³¹P NMR Spectrum for (1R,3R)-4 in D₂O

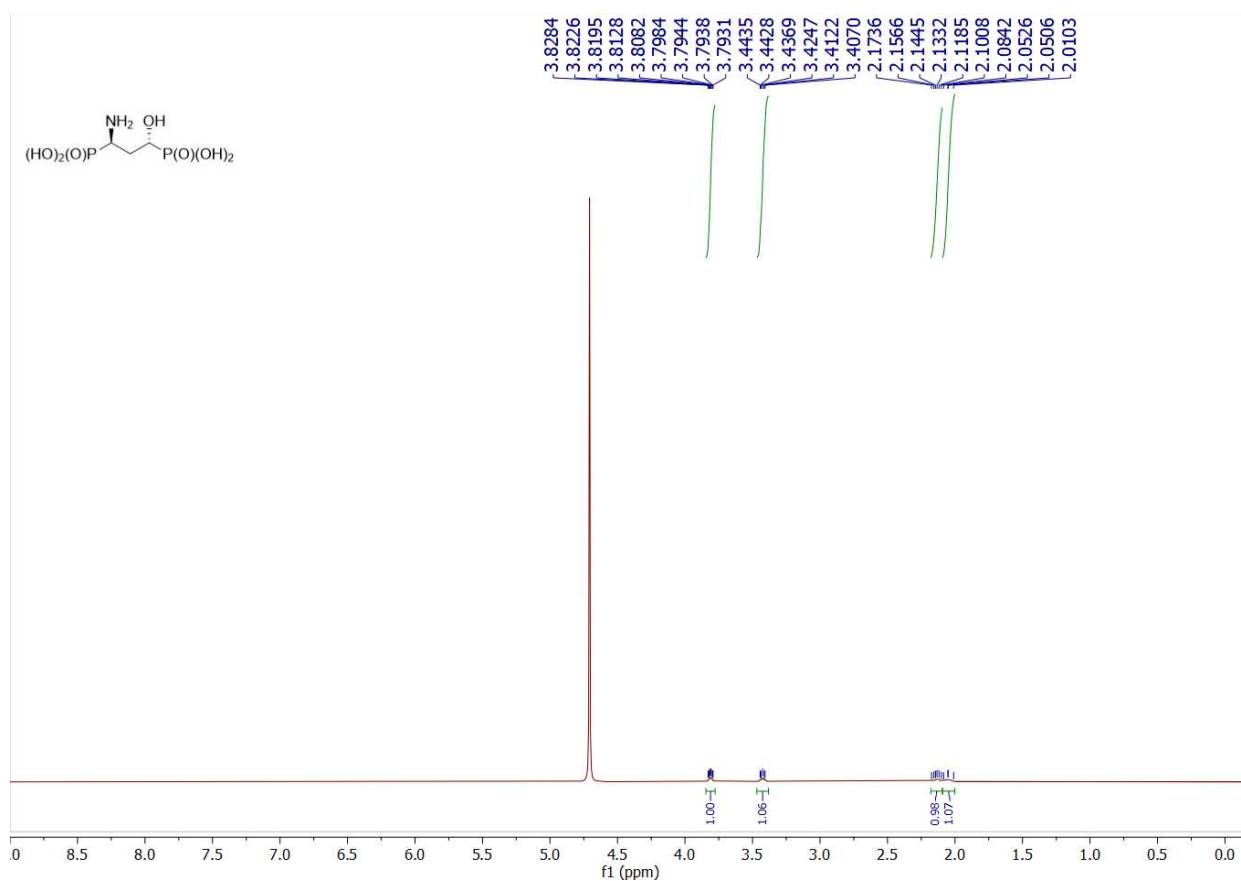


Figure S17: ¹H NMR Spectrum for (1R,3S)-4 in D₂O

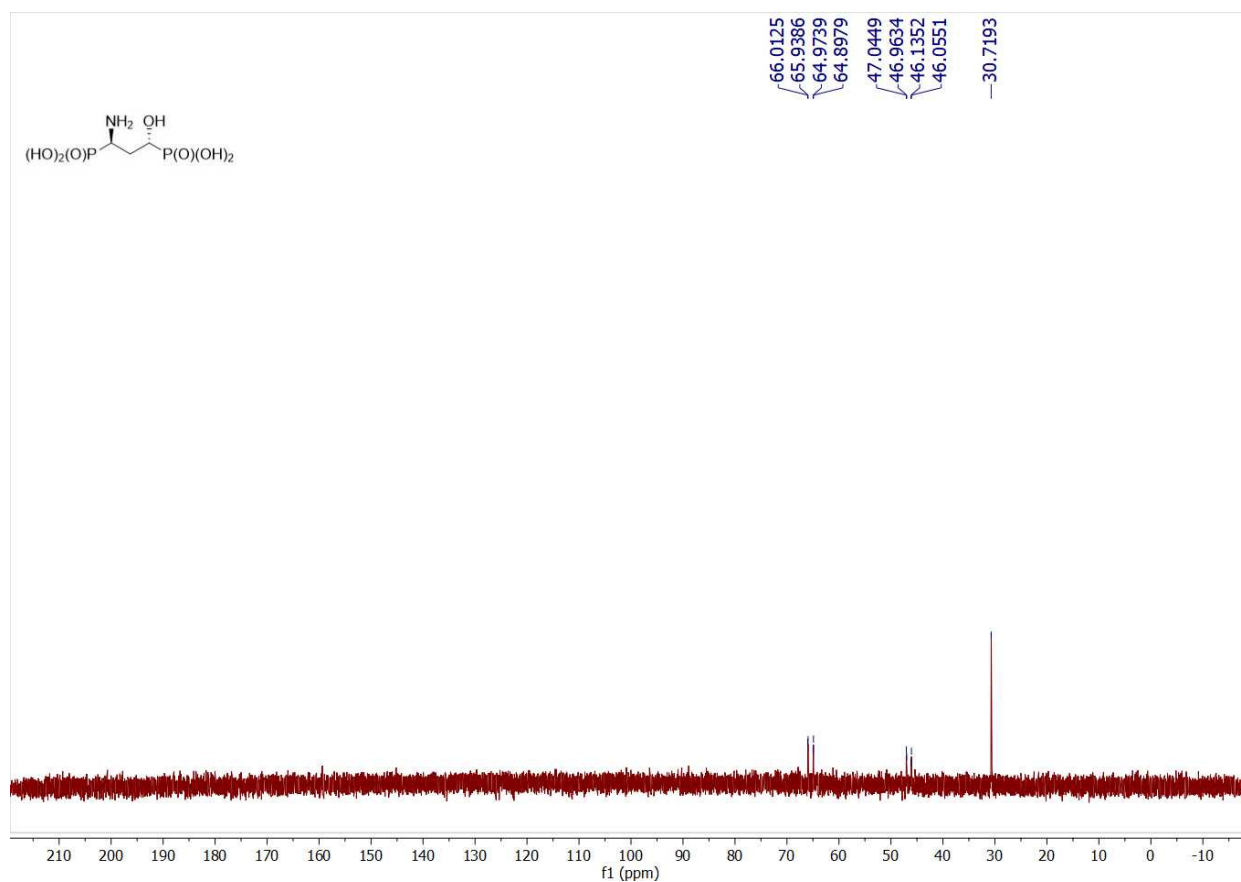


Figure S18: ¹³C NMR Spectrum for (1R,3S)-4 in D₂O

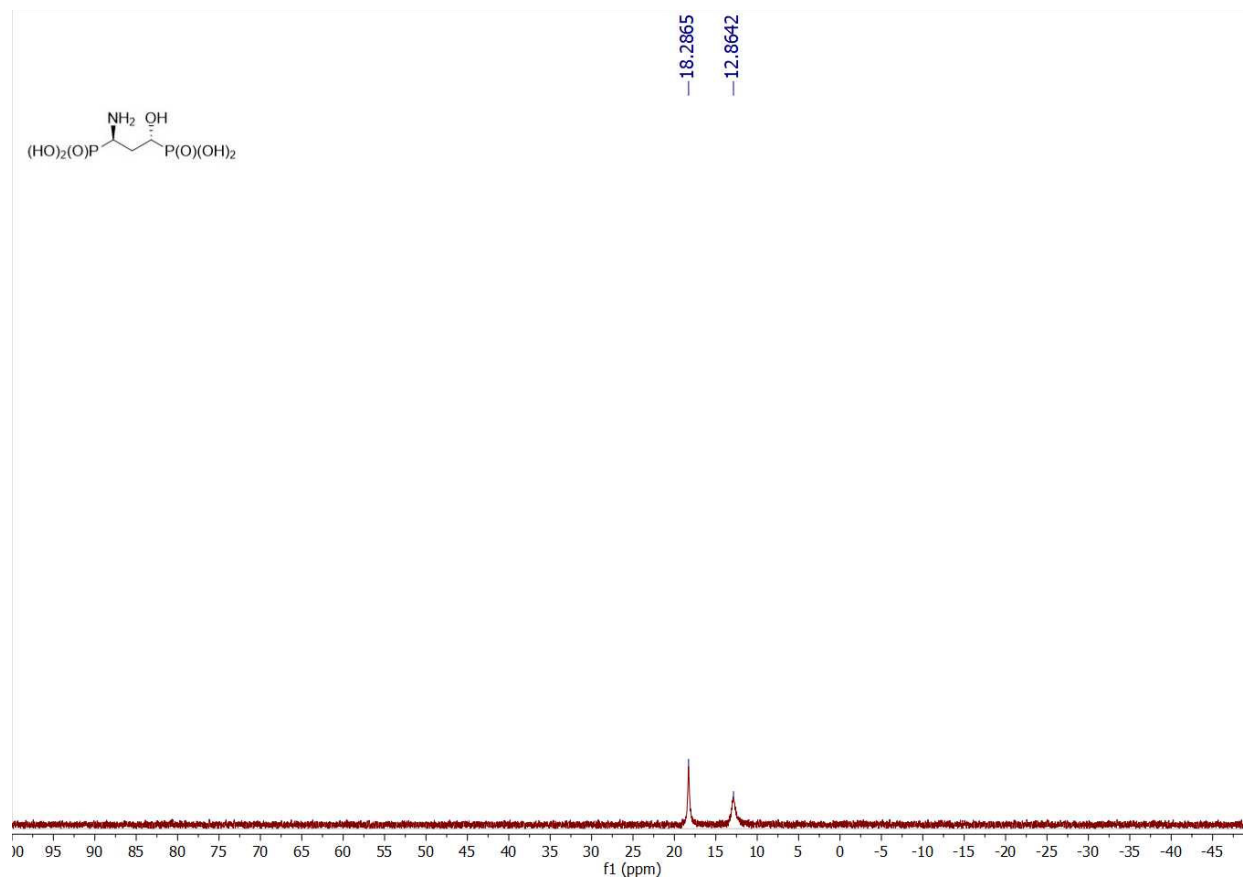


Figure S19: ³¹P NMR Spectrum for (1R,3S)-4 in D₂O

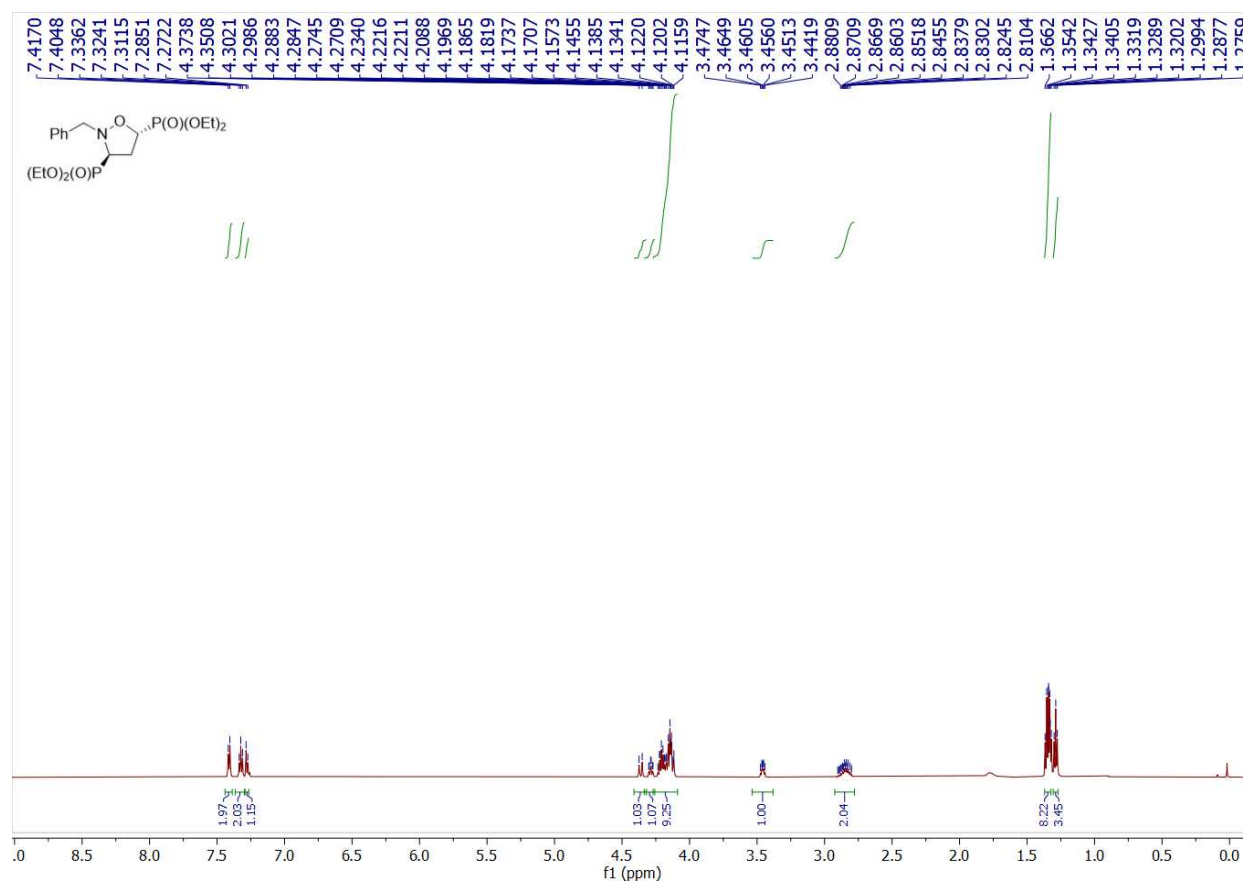


Figure S20: ¹H NMR Spectrum for *trans*-14 in CDCl₃

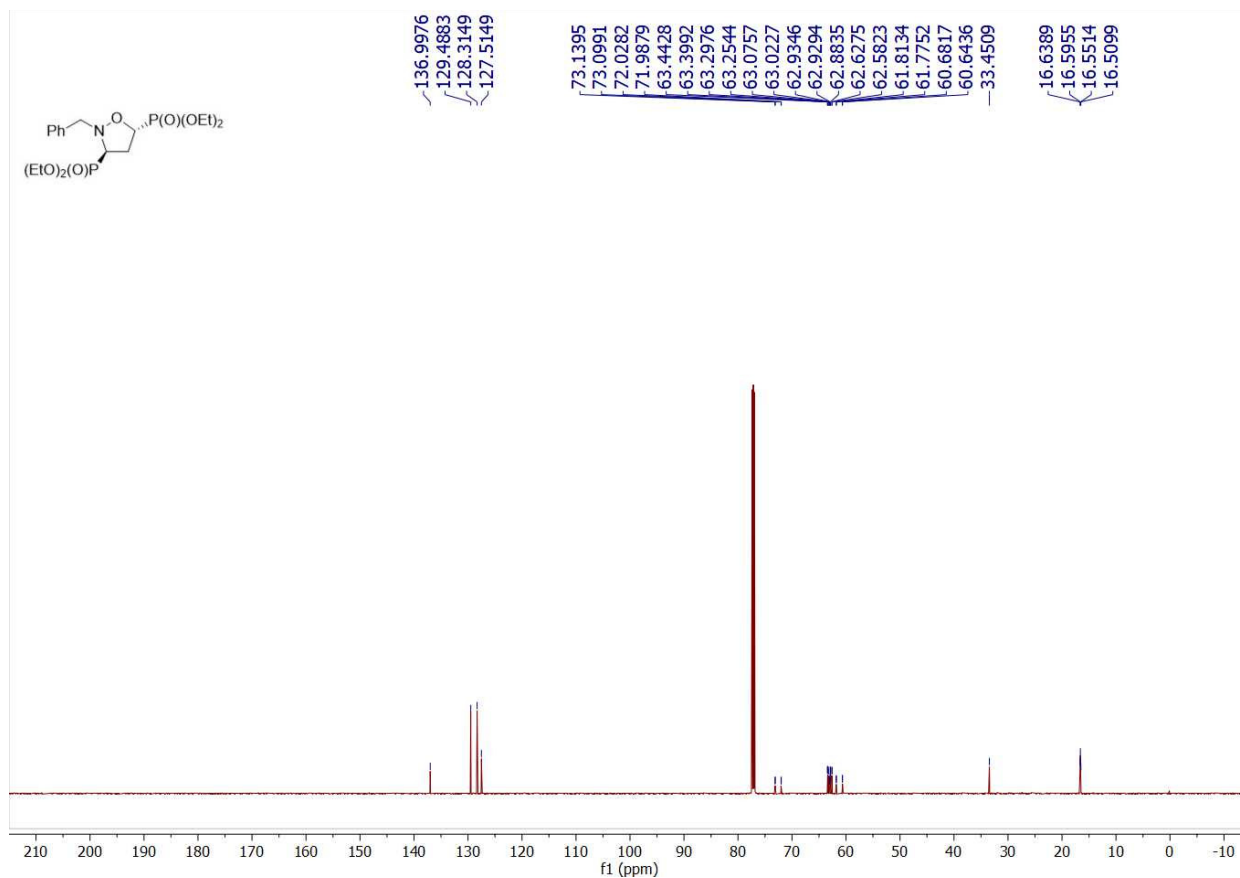


Figure S21: ¹³C NMR Spectrum for *trans*-14 in CDCl₃

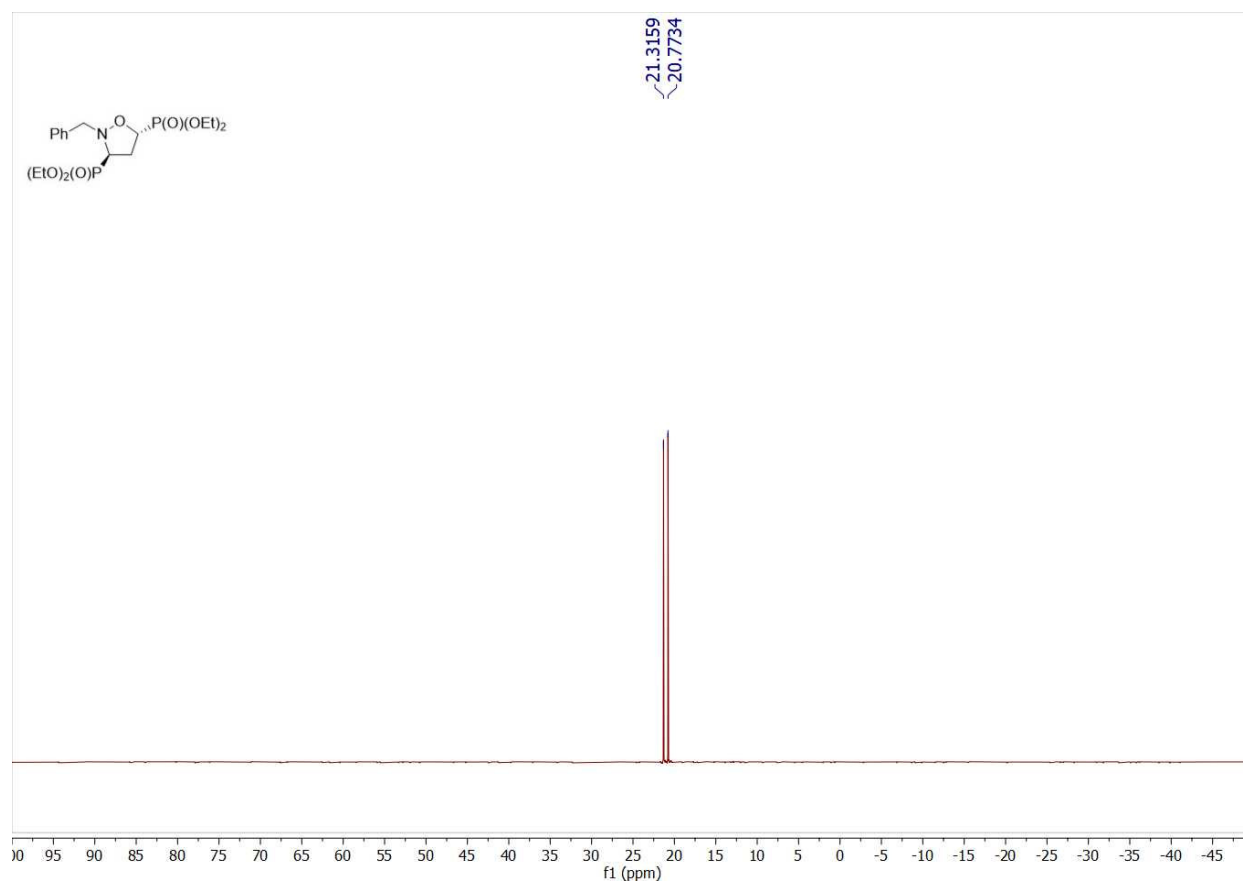


Figure S22: ³¹P NMR Spectrum for *trans*-14 in CDCl₃

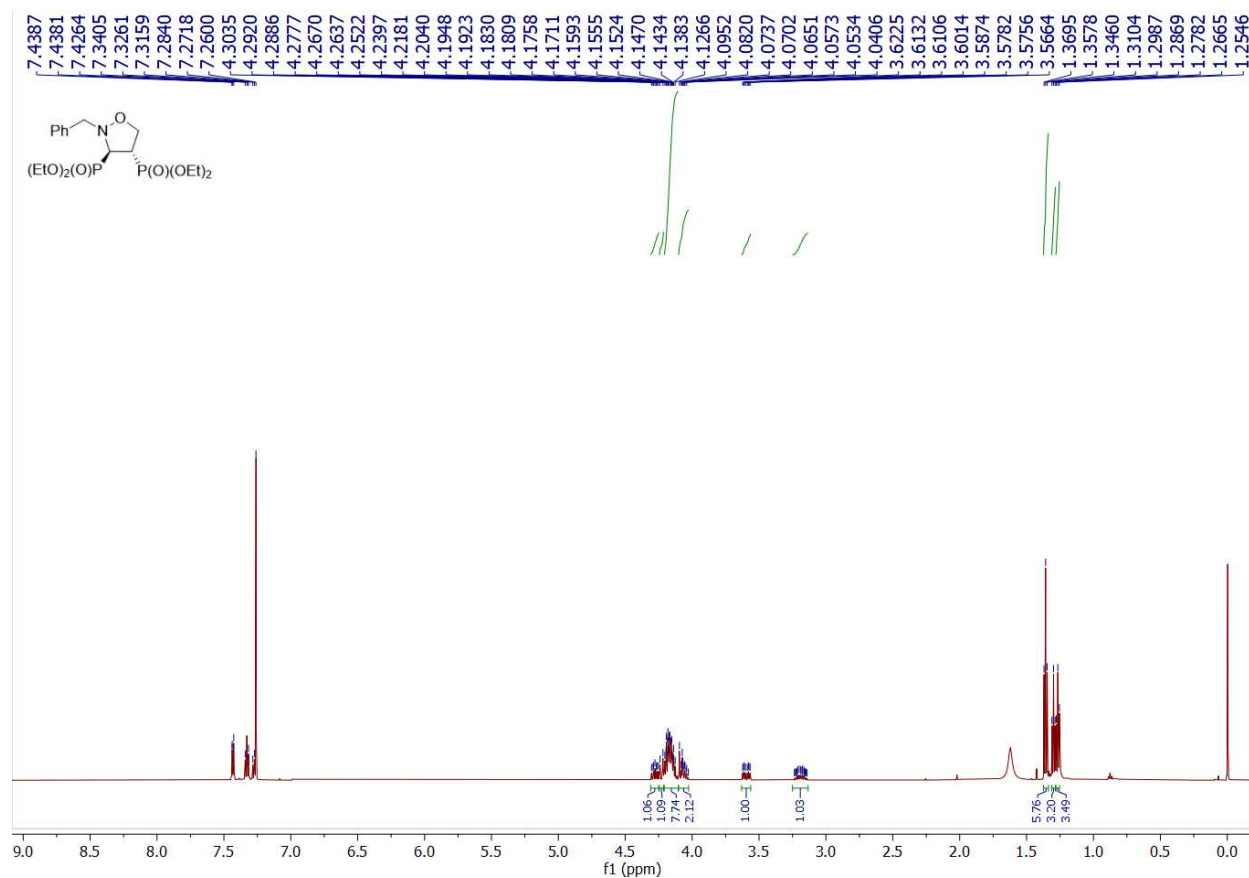


Figure S23: ¹H NMR Spectrum for *trans*-15 in CDCl₃

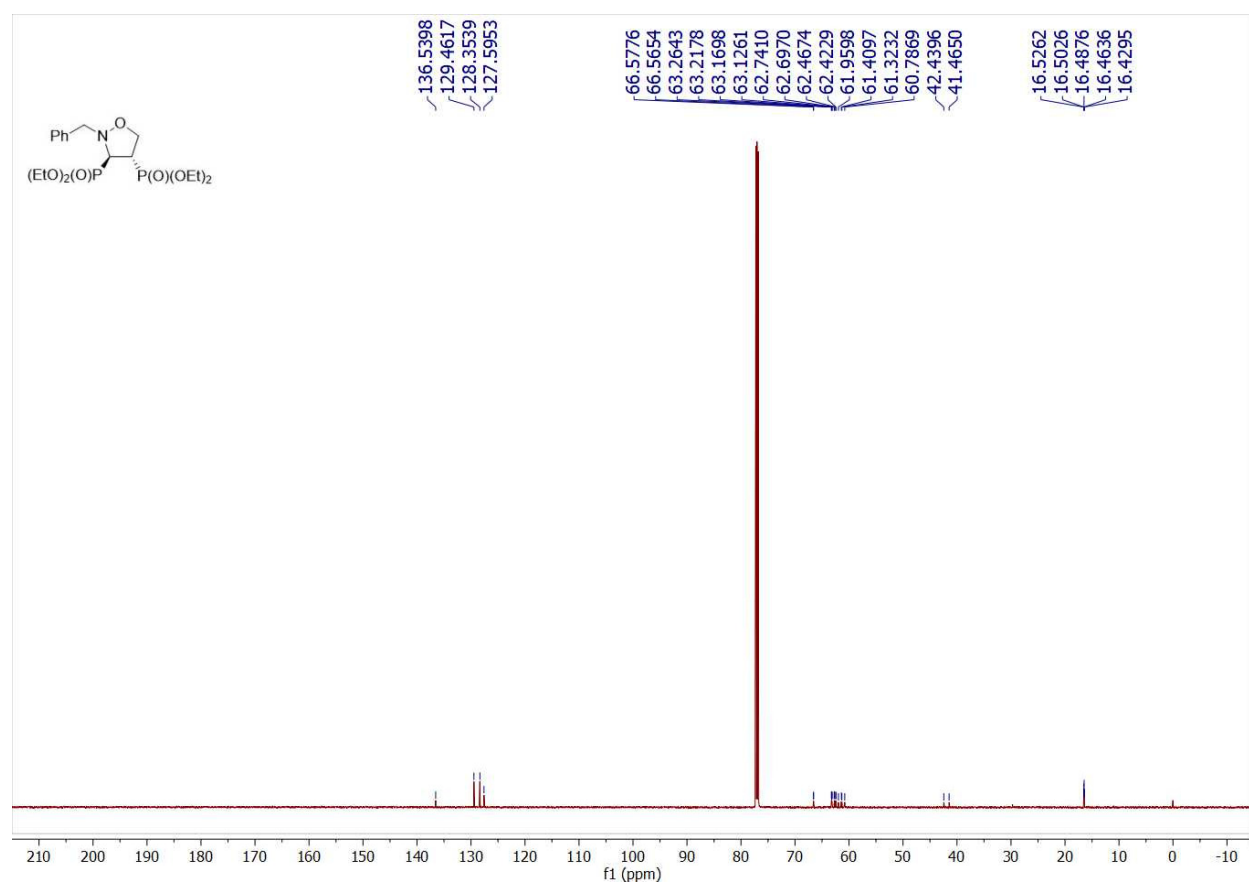


Figure S24: ¹³C NMR Spectrum for *trans*-15 in CDCl₃

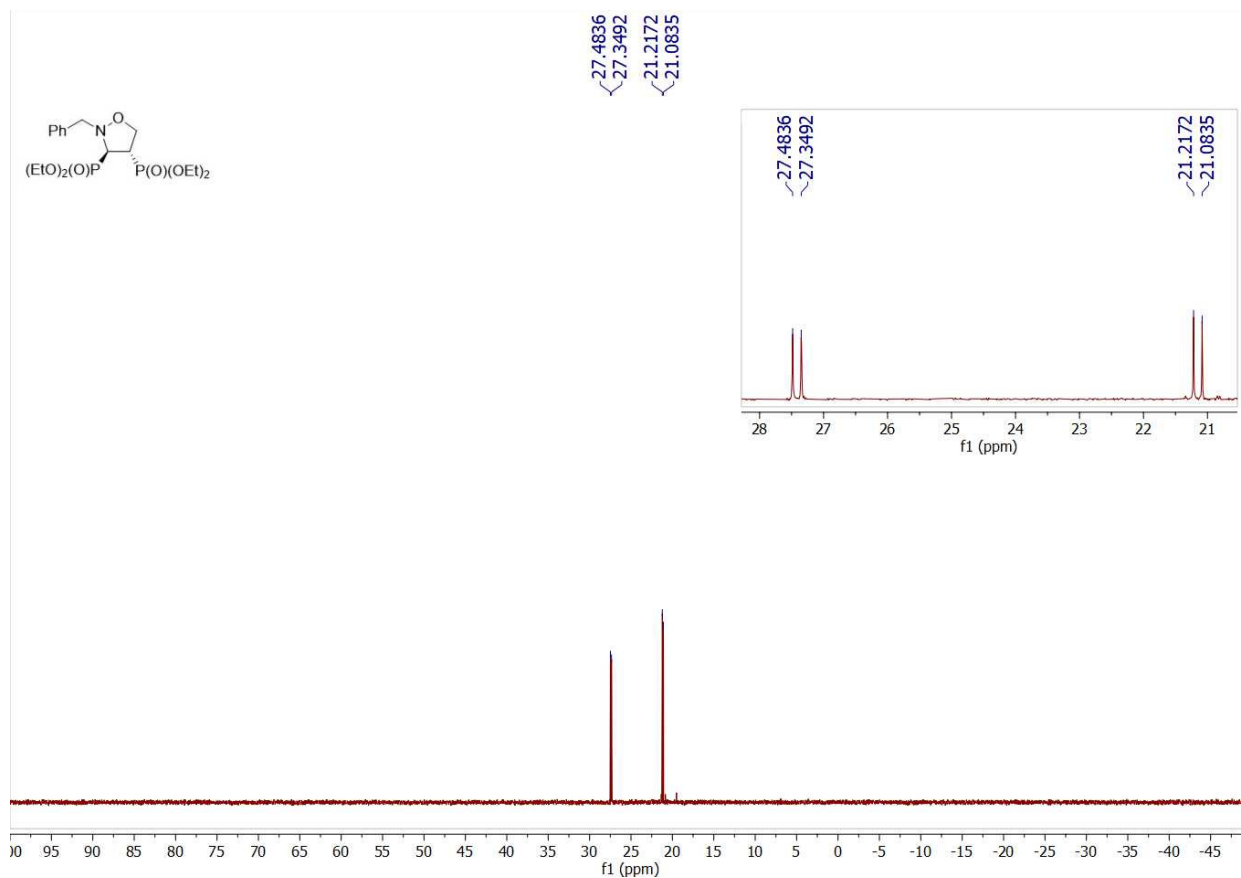


Figure S25: ³¹P NMR Spectrum for *trans*-15 in CDCl₃

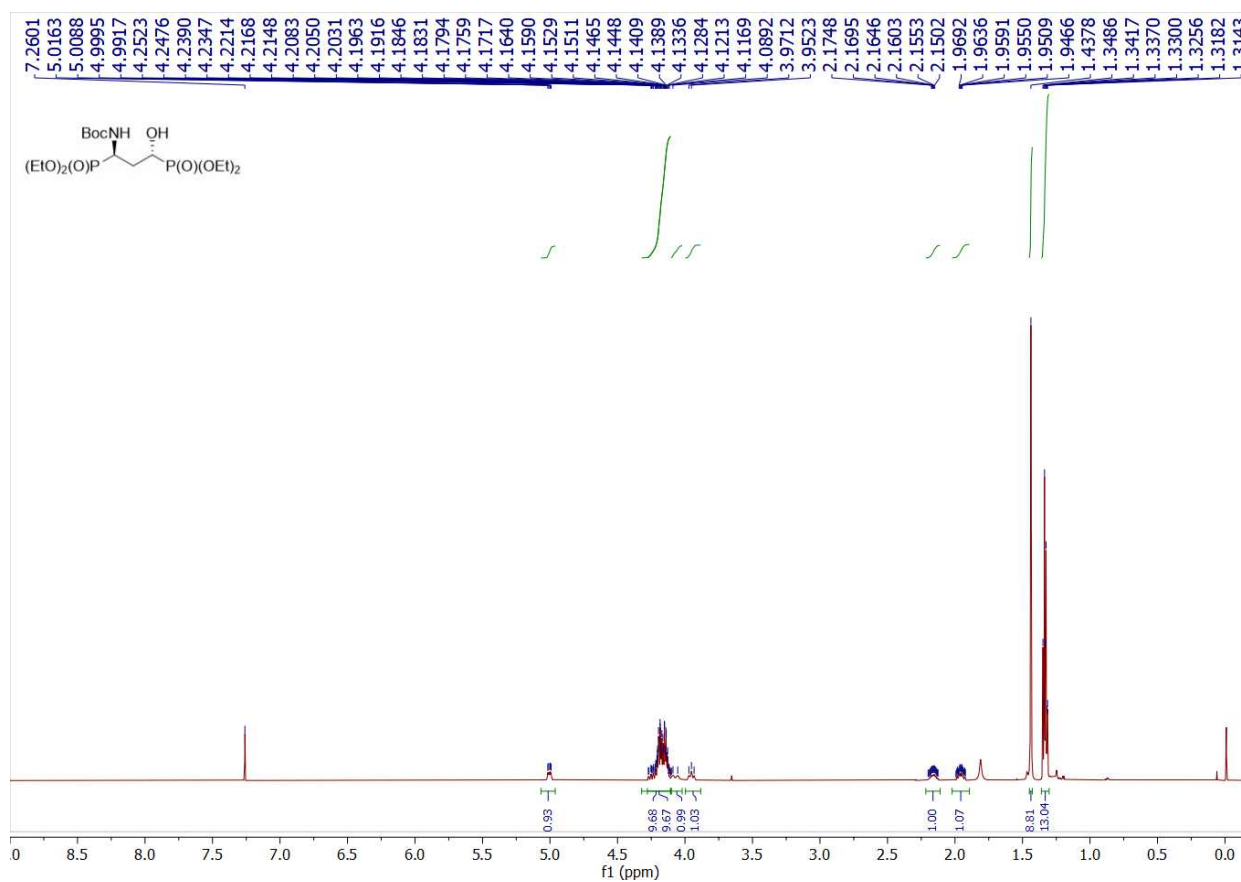


Figure S26: ¹H NMR Spectrum for (1*R*/*S*,3*R*/*S*)-6 [*anti*-6] in CDCl₃

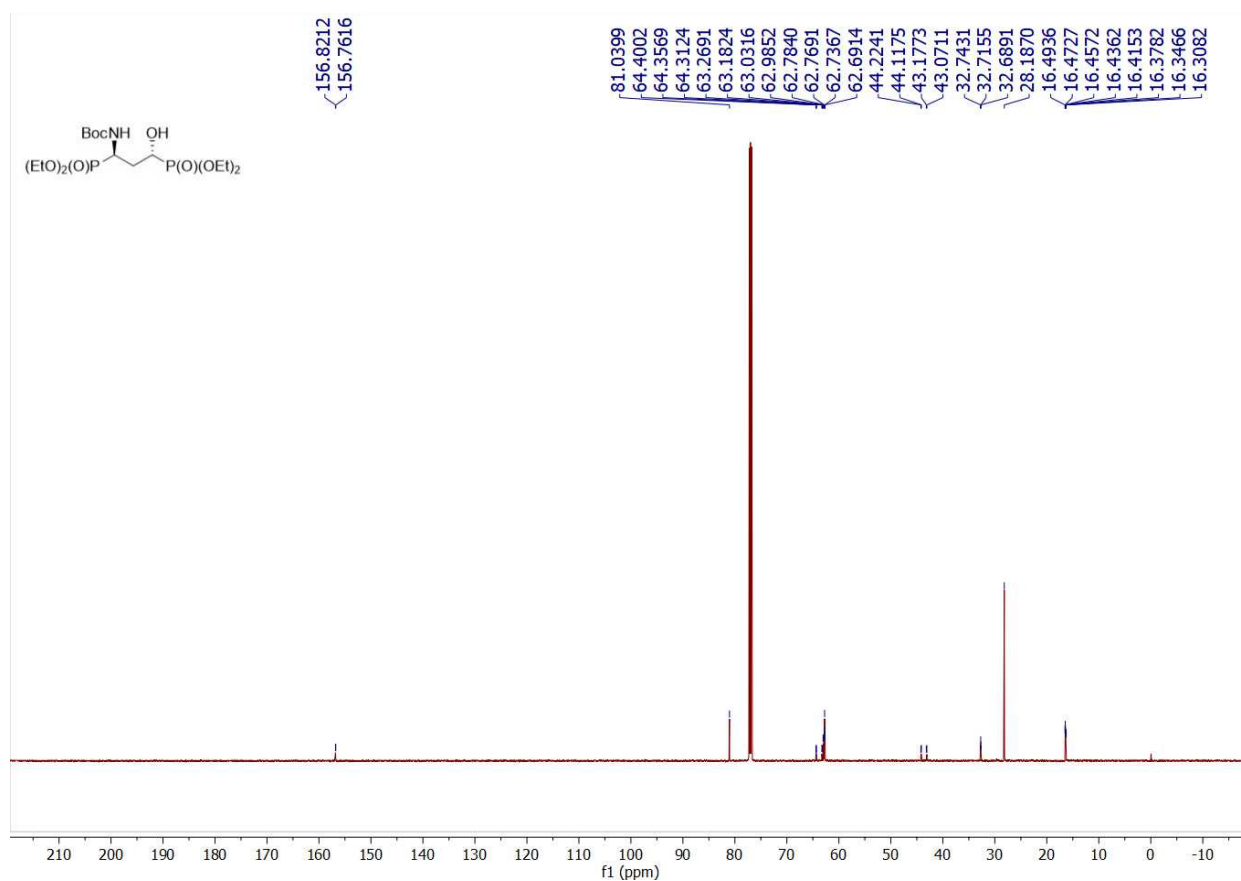


Figure S27: ¹³C NMR Spectrum for (1R/S,3R/S)-6 [*anti*-6] in CDCl₃

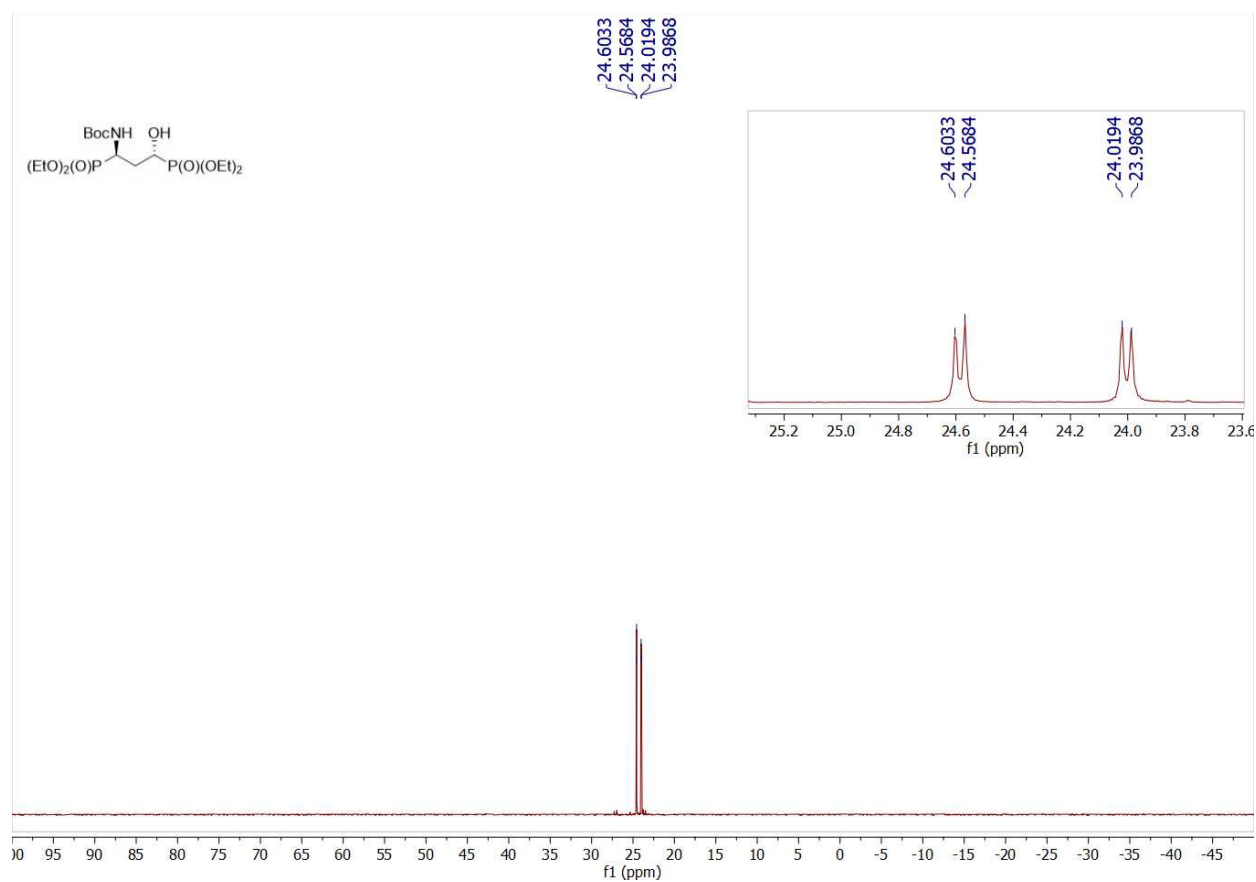


Figure S28: ³¹P NMR Spectrum for (1R/S,3R/S)-6 [*anti*-6] in CDCl₃

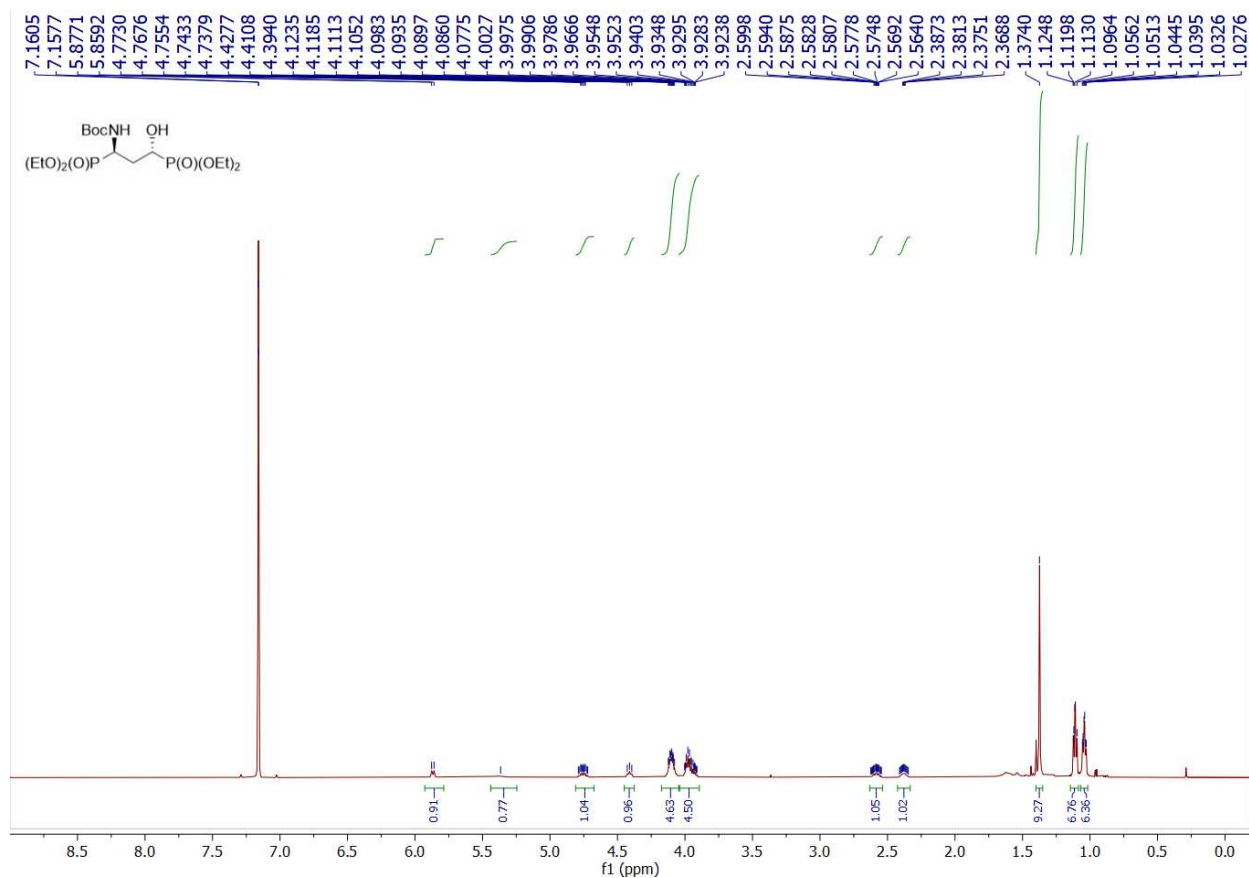


Figure S29: ¹H NMR Spectrum for (1R/S,3R/S)-6 [*anti*-6] in C₆D₆

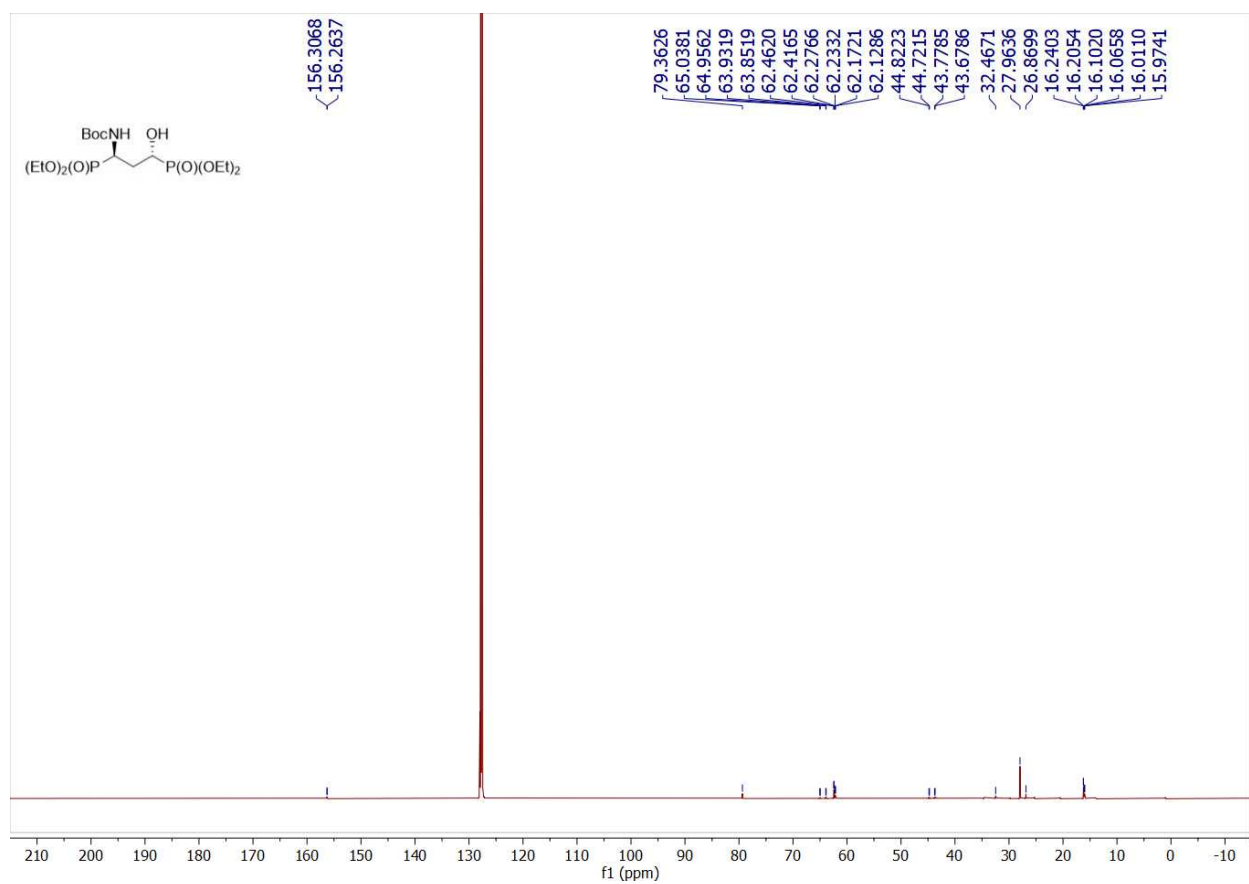


Figure S30: ¹³C NMR Spectrum for (1R/S,3R/S)-6 [*anti*-6] in C₆D₆

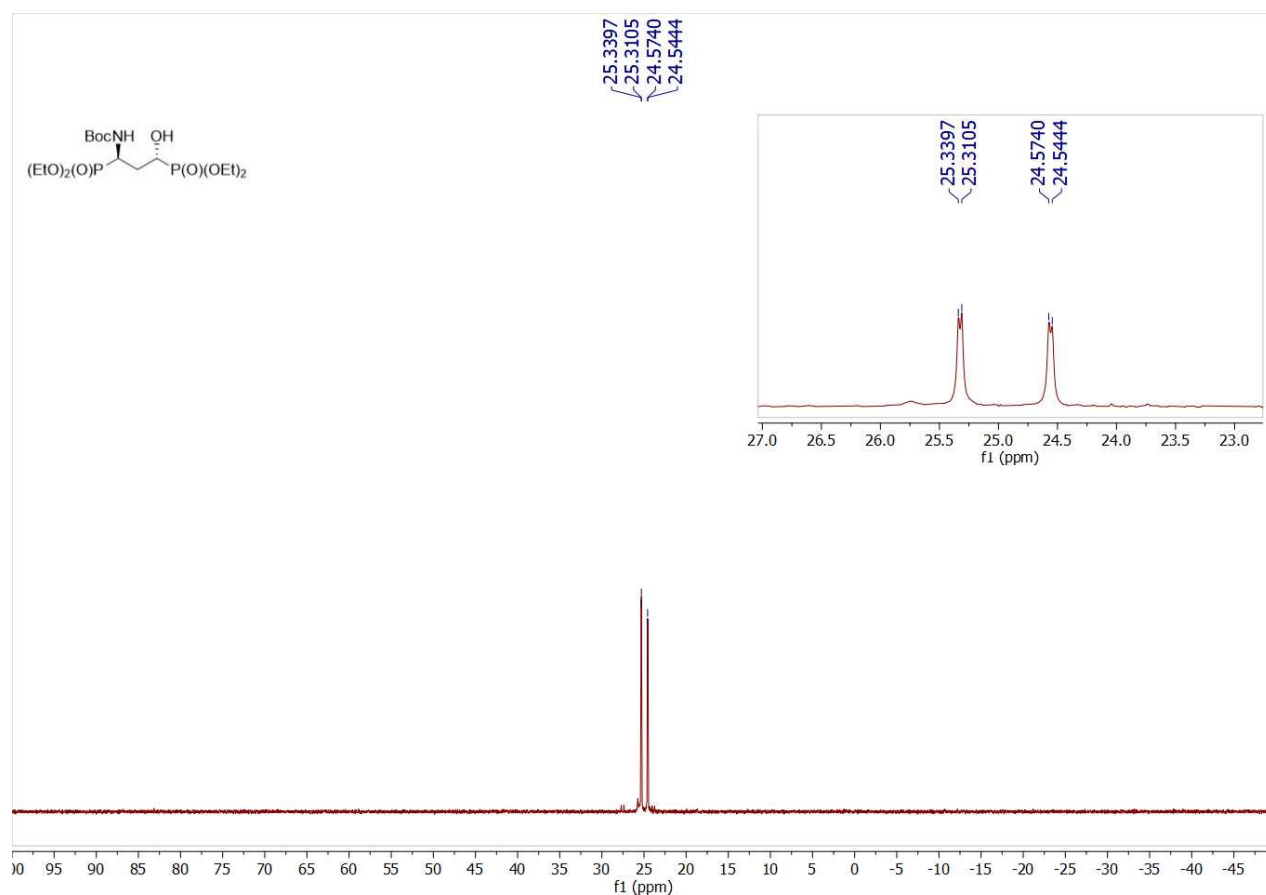


Figure S31: ³¹P NMR Spectrum for (1R/S,3R/S)-6 [*anti*-6] in C₆D₆

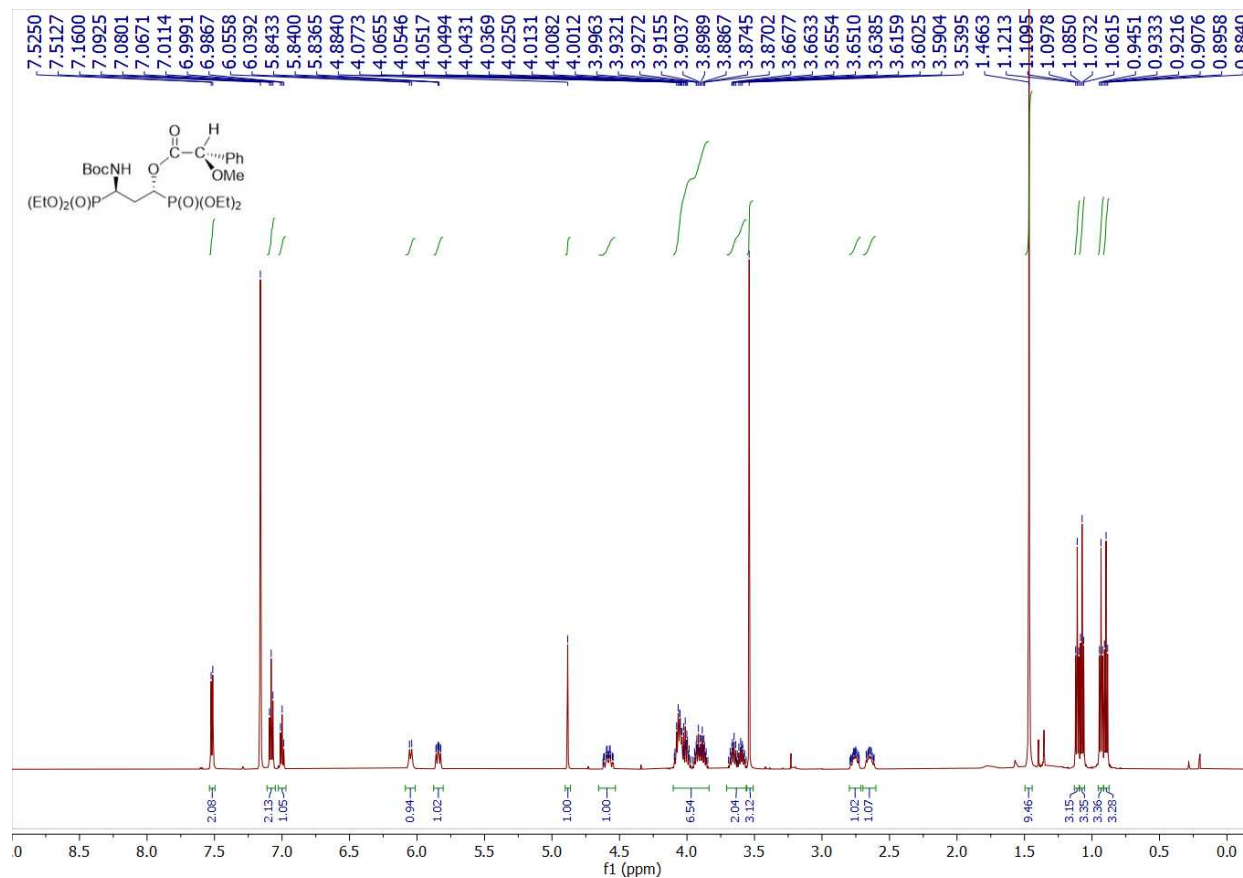


Figure S32: ¹H NMR Spectrum for (1R,3R,1'S)-16 in C₆D₆

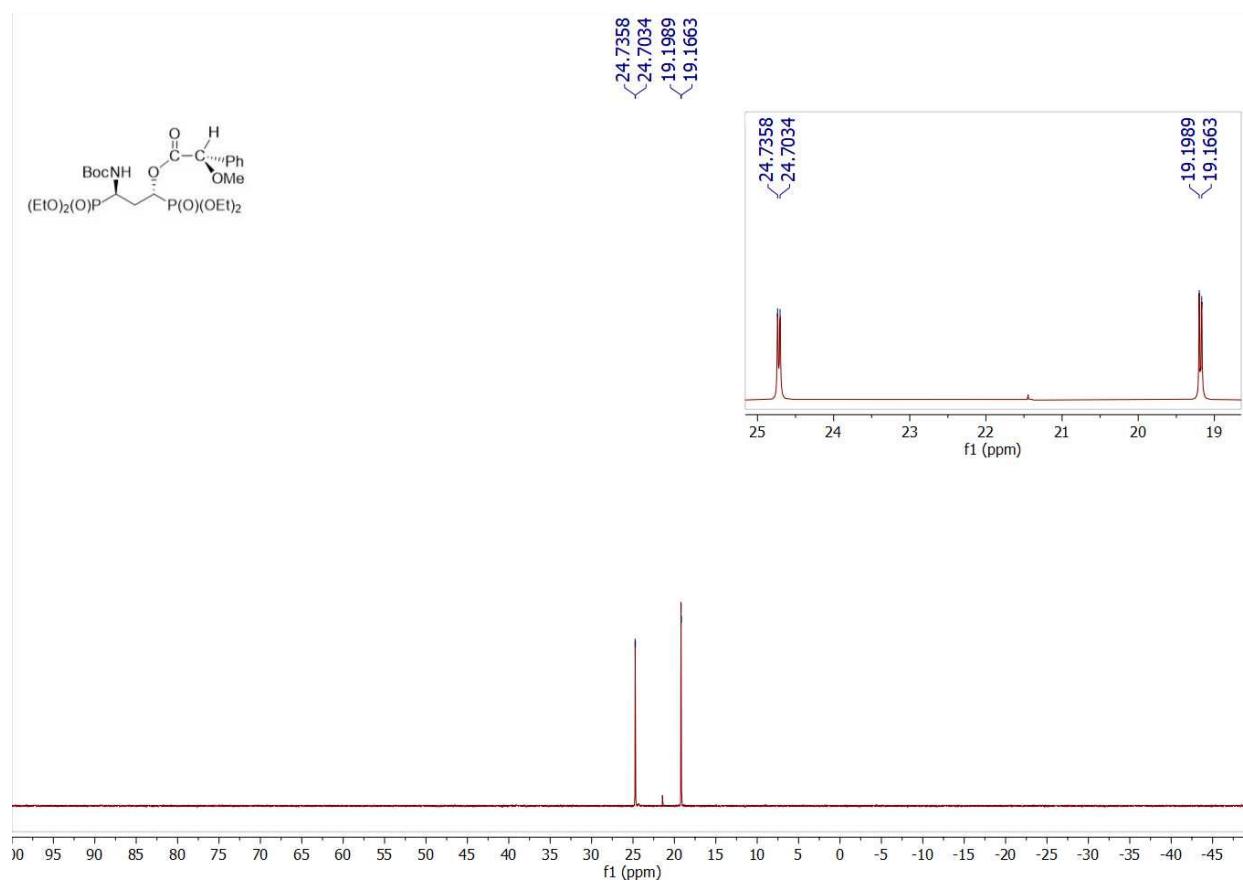


Figure S33: ³¹P NMR Spectrum for (1R,3R,1'S)-16 in C₆D₆

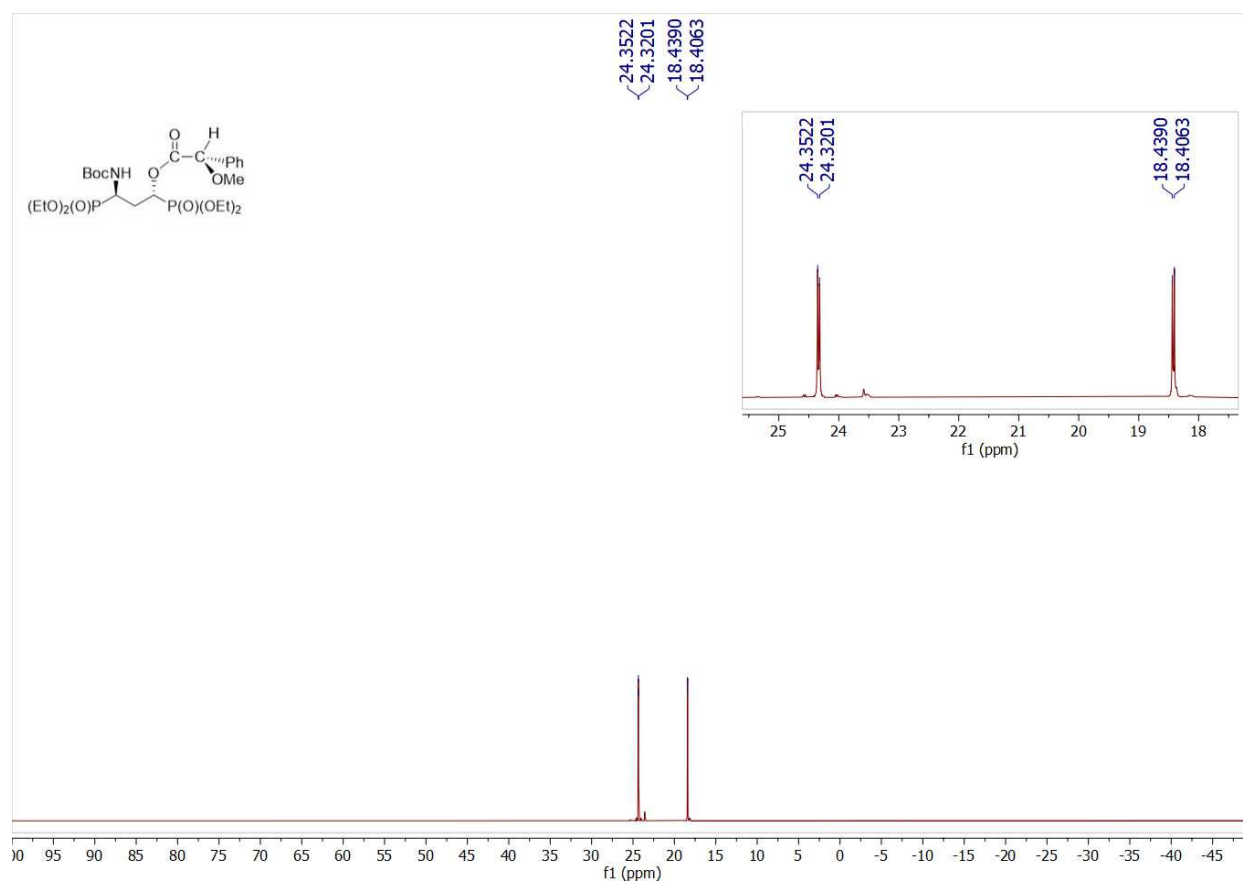


Figure S34: ³¹P NMR Spectrum for (1R,3R,1'S)-16 in CDCl₃

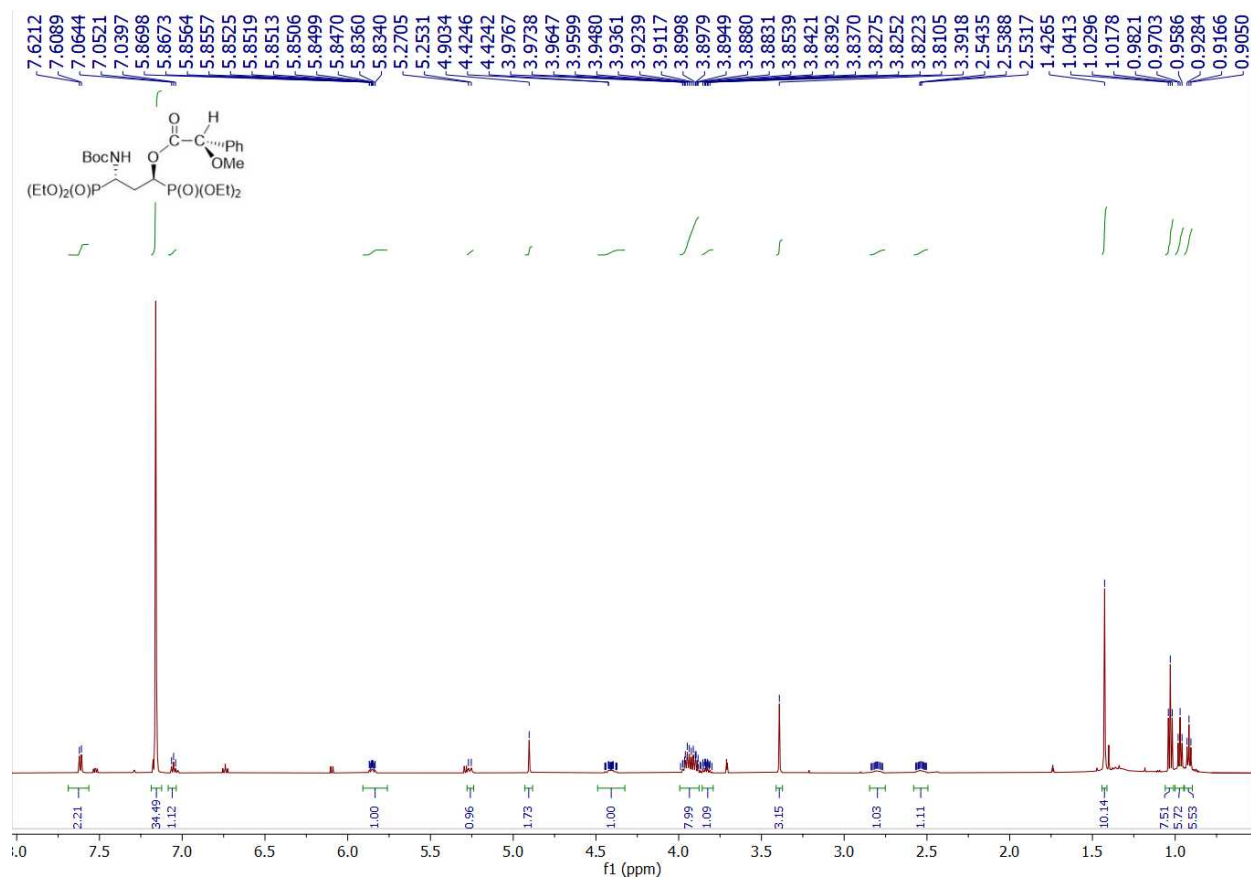


Figure S35: ¹H NMR Spectrum for (1S,3S,1'S)-16 in C₆D₆

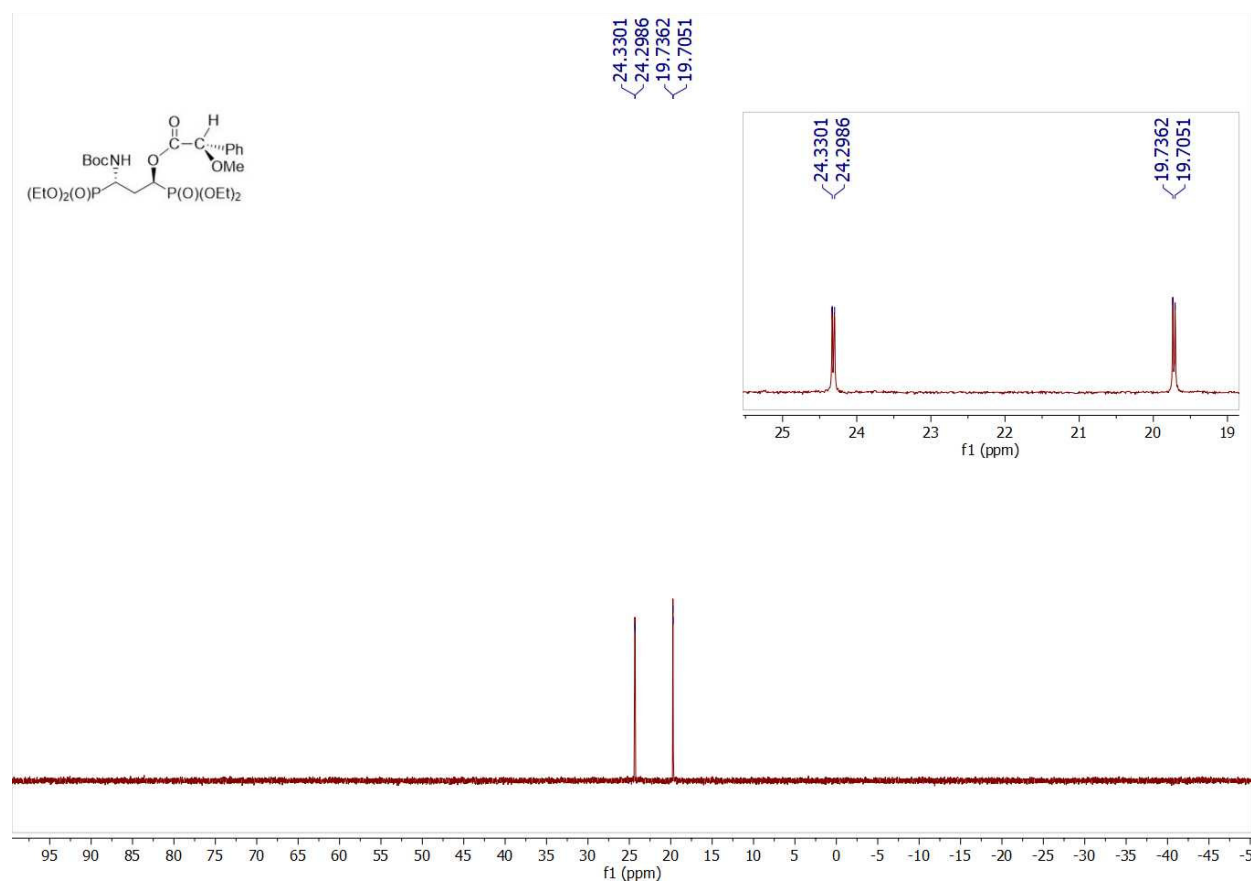


Figure S36: ³¹P NMR Spectrum for (1S,3S,1'S)-16 in C₆D₆

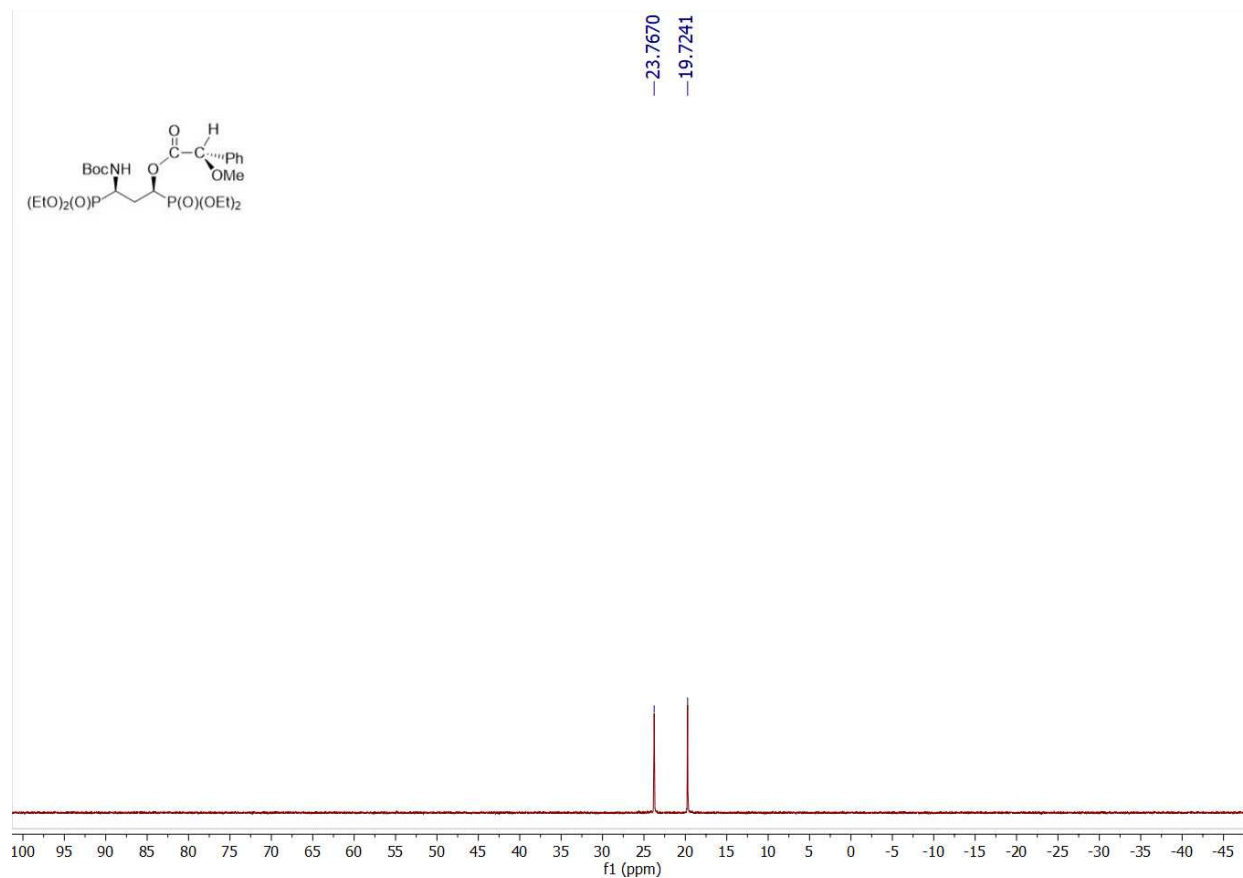


Figure S39: ³¹P NMR Spectrum for (1*R*,3*S*,1'*S*)-**16** in C₆D₆

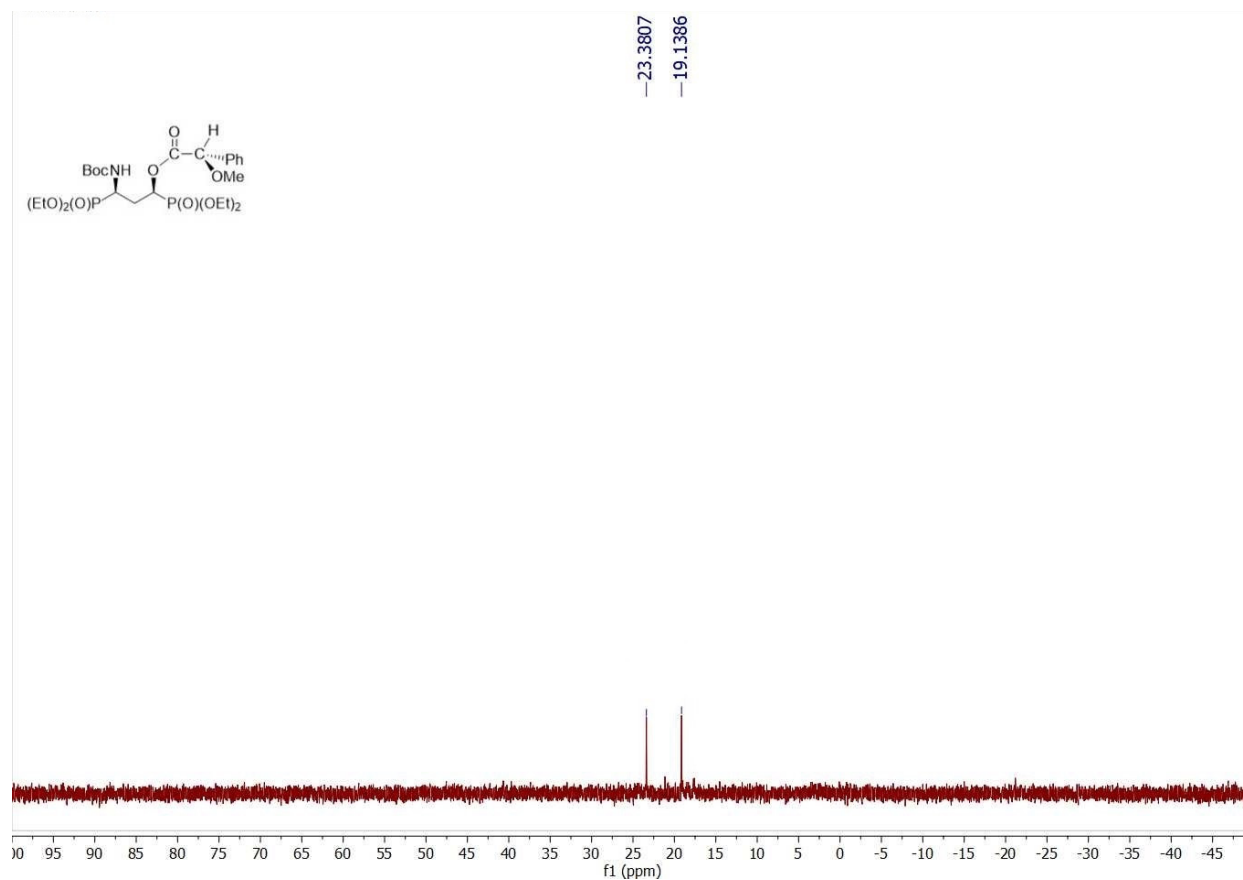


Figure S40: ³¹P NMR Spectrum for (1*R*,3*S*,1'*S*)-**16** in CDCl₃

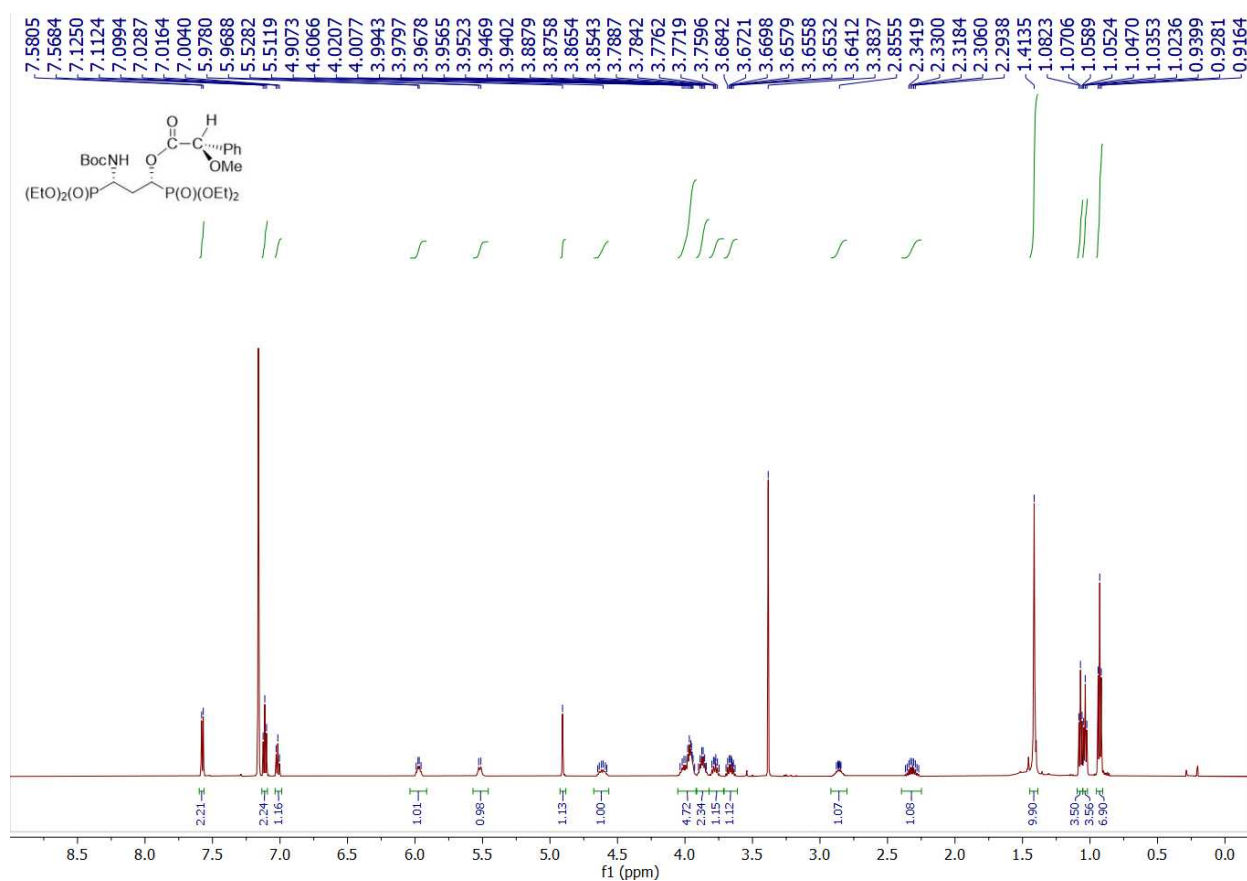


Figure S41: ¹H NMR Spectrum for (1*S*,3*R*,1'*S*)-16 in C₆D₆

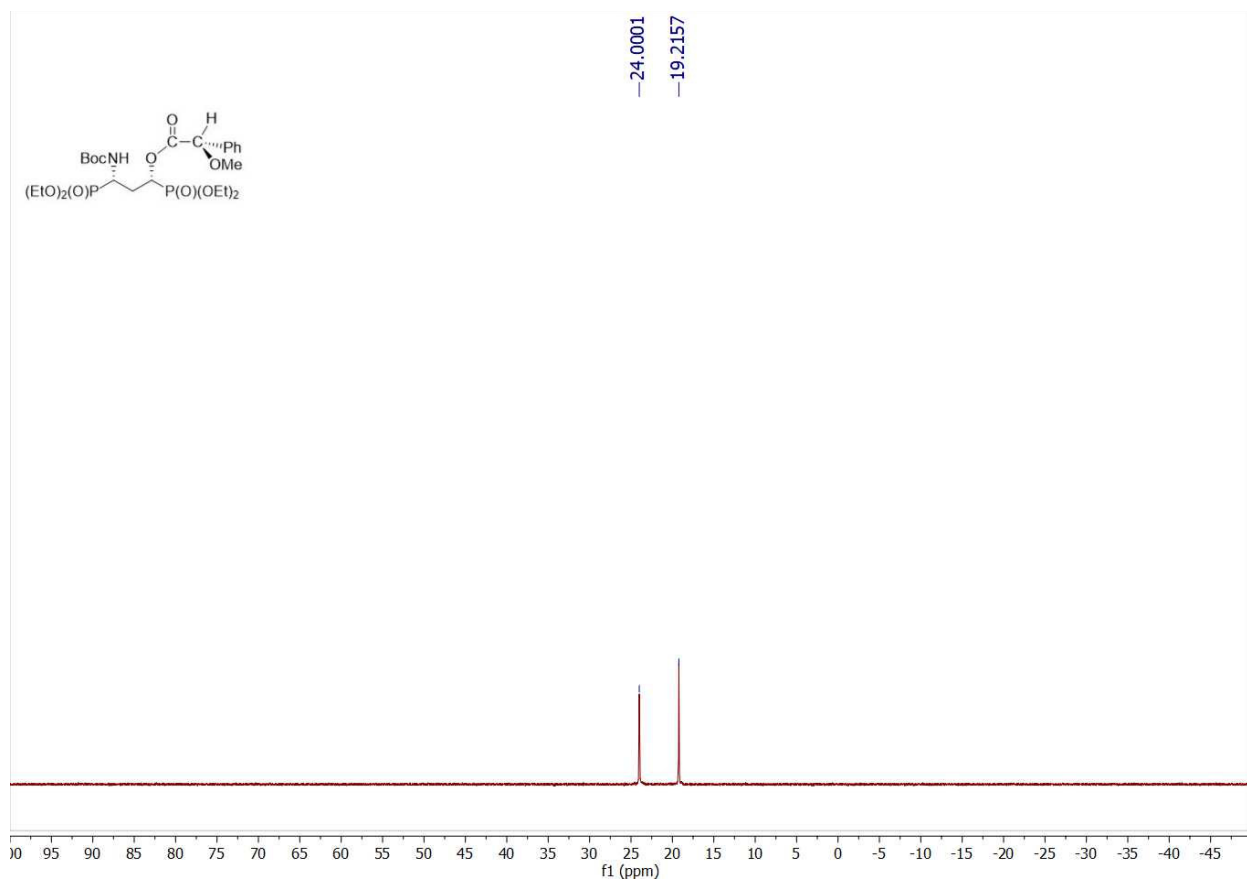


Figure S42: ³¹P NMR Spectrum for (1*S*,3*R*,1'*S*)-16 in C₆D₆

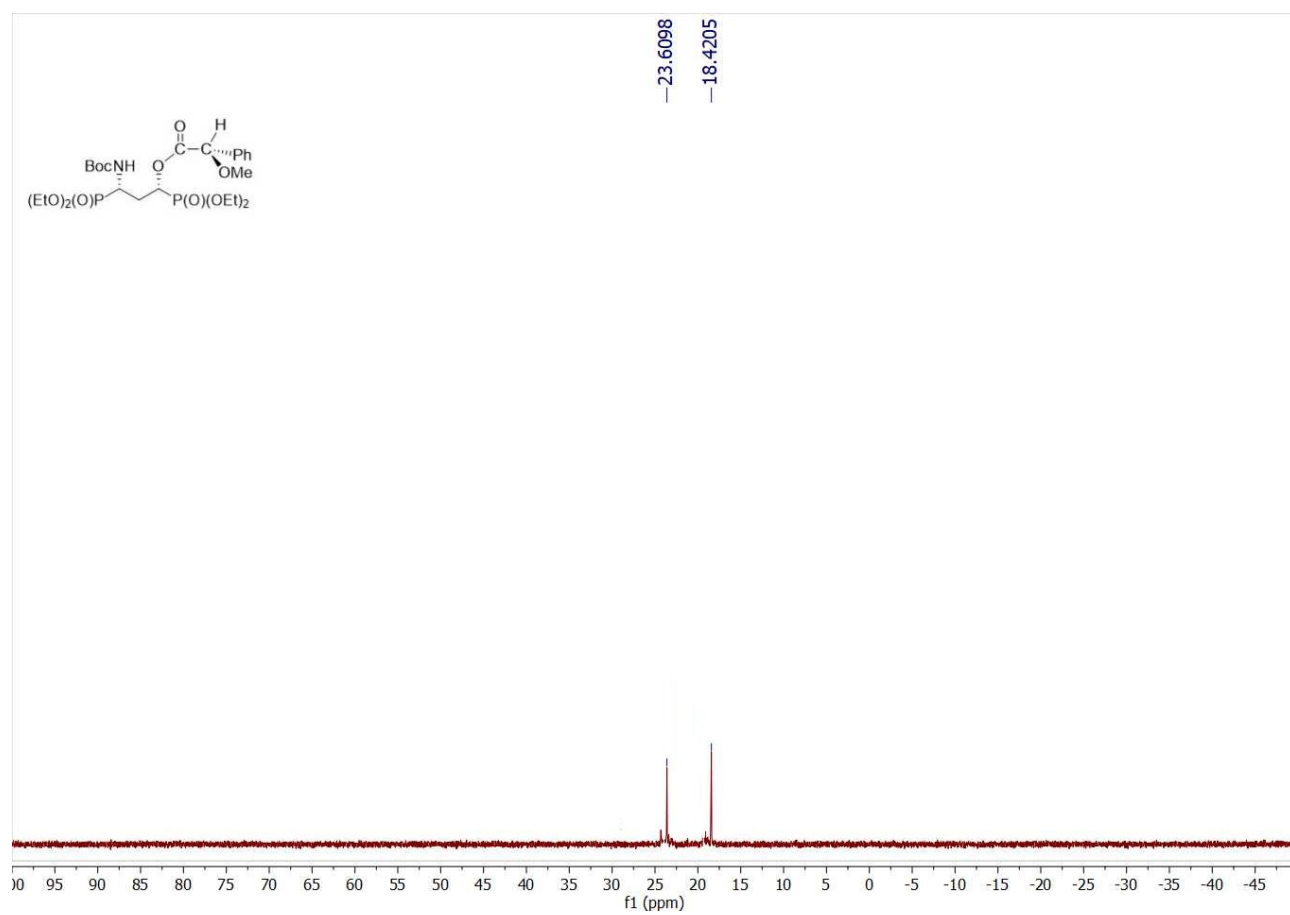


Figure S43: ³¹P NMR Spectrum for (1*S*,3*R*,1'*S*)-**16** in CDCl₃

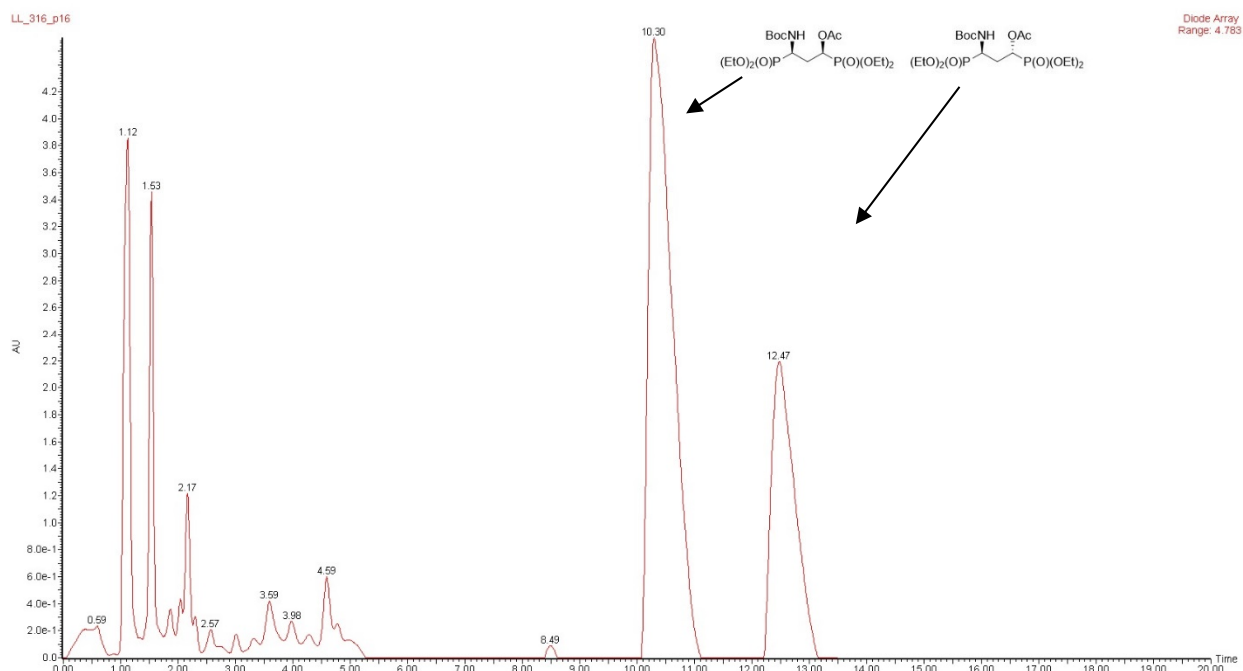


Figure S44: Separation of (1R,3S)-11 and (1R,3R)-11 by preparative HPLC

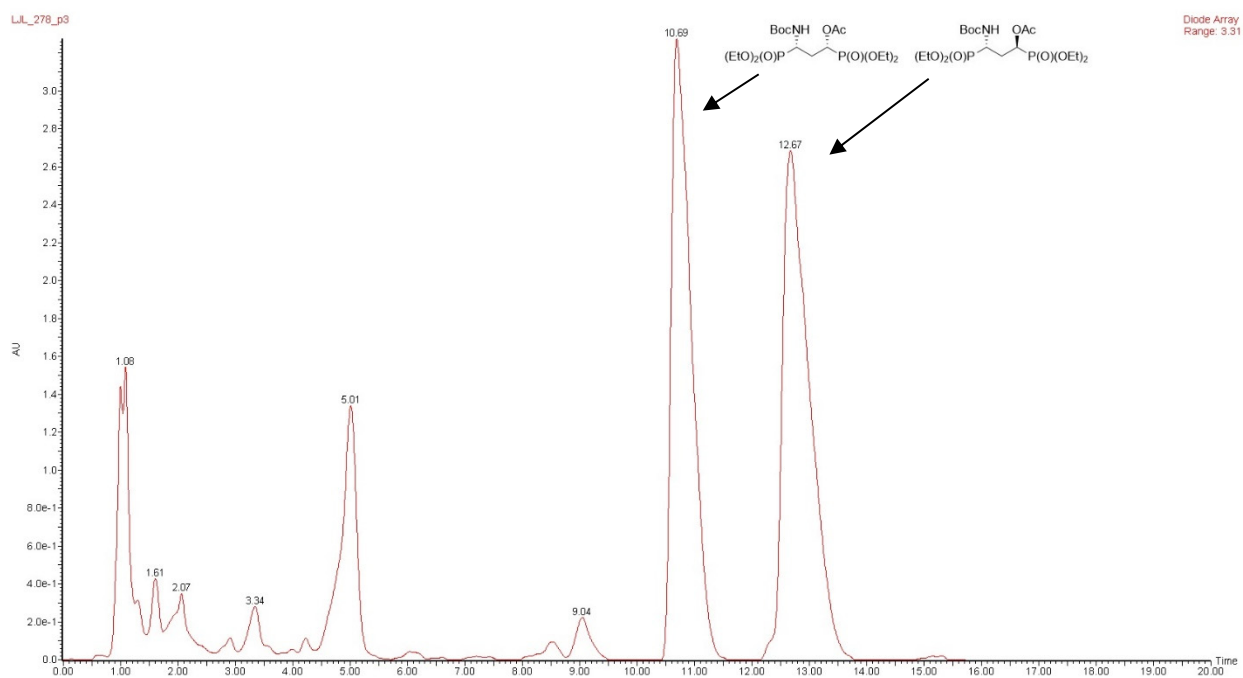


Figure S45: Separation of (1S,3R)-11 and (1S,3S)-11 by preparative HPLC

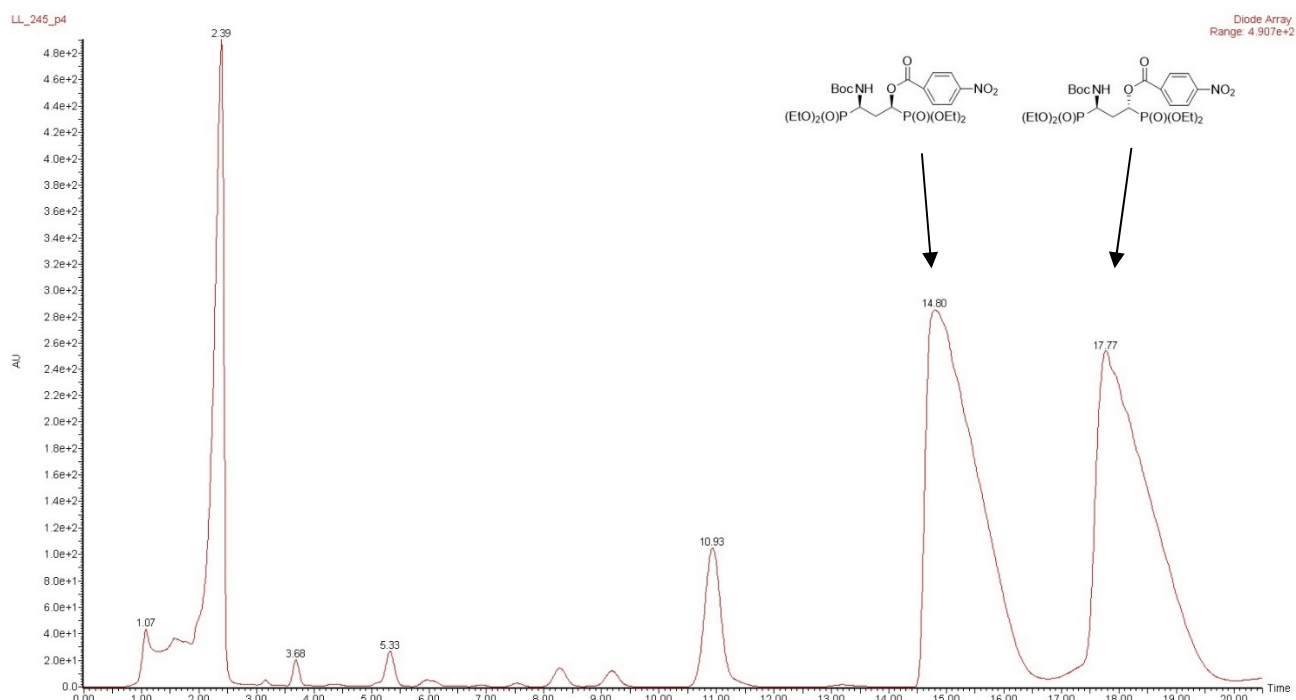


Figure S46: Separation of (1*R*,3*S*)-**12** and (1*R*,3*R*)-**12** by preparative HPLC

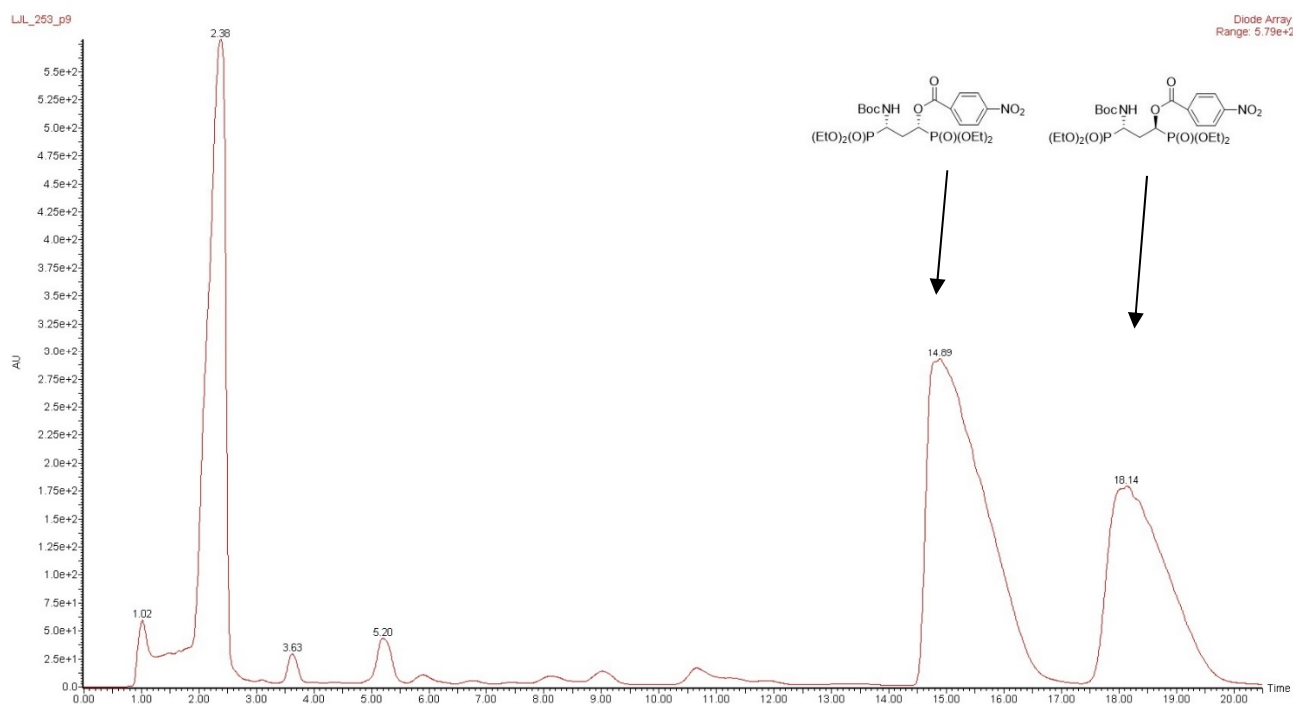


Figure S47: Separation of (1*S*,3*R*)-**12** and (1*S*,3*S*)-**12** by preparative HPLC

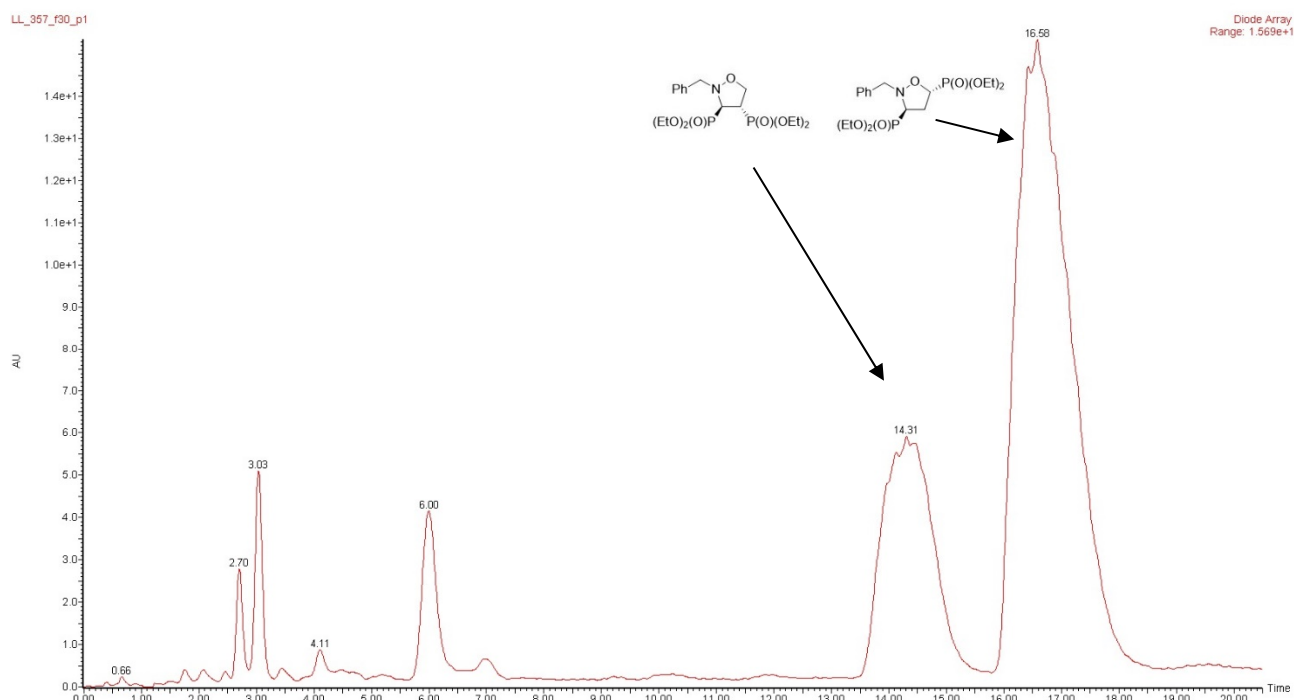


Figure S48: Separation of *trans*-**14** and *trans*-**15** by preparative HPLC

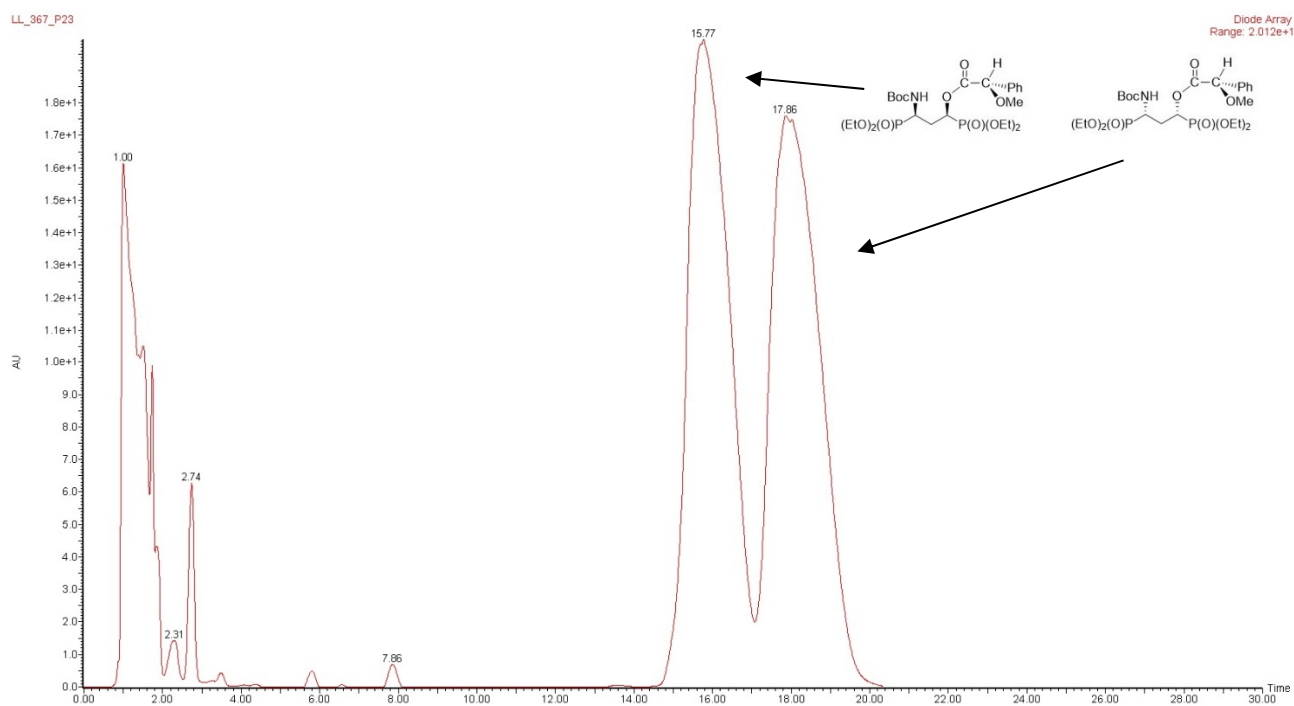


Figure S49: Separation of (1*R*,3*R*,1'*S*)-**16** and (1*R*,3*S*,1'*S*)-**16** by preparative HPLC

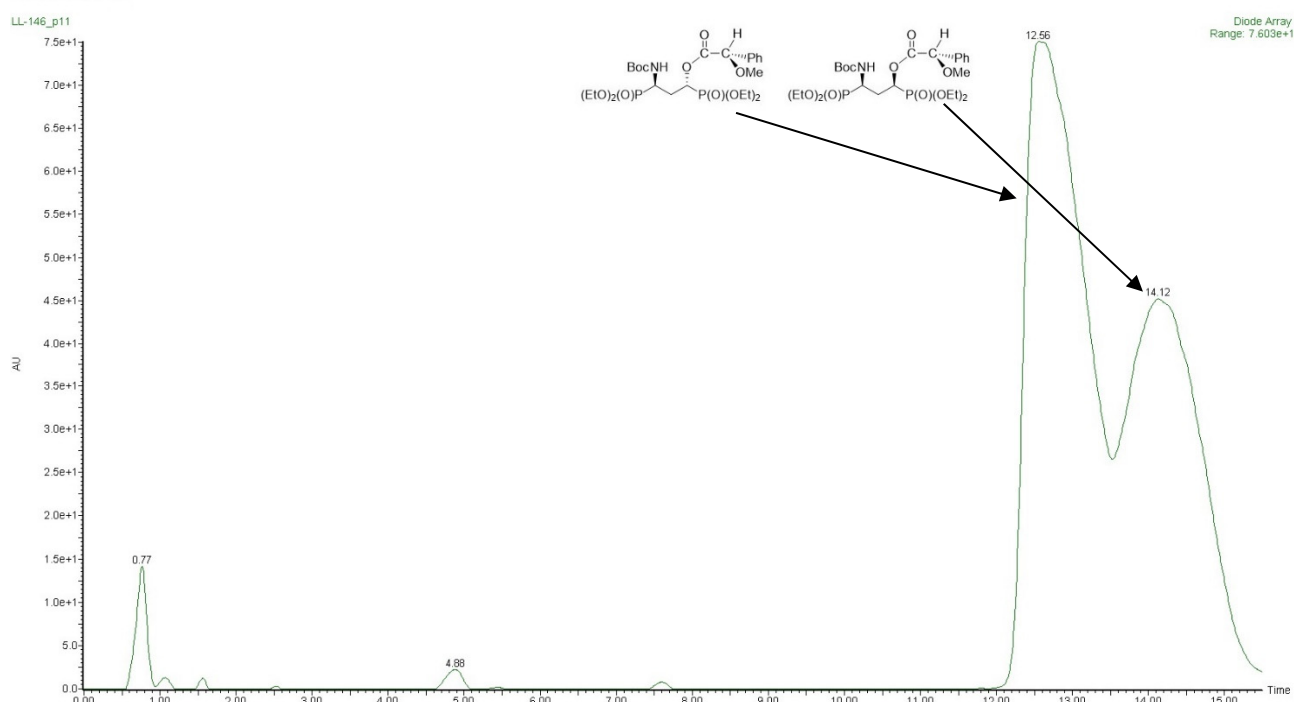


Figure S50: Separation of (1R,3R,1'S)-16 and (1R,3S,1'S)-16 by preparative HPLC

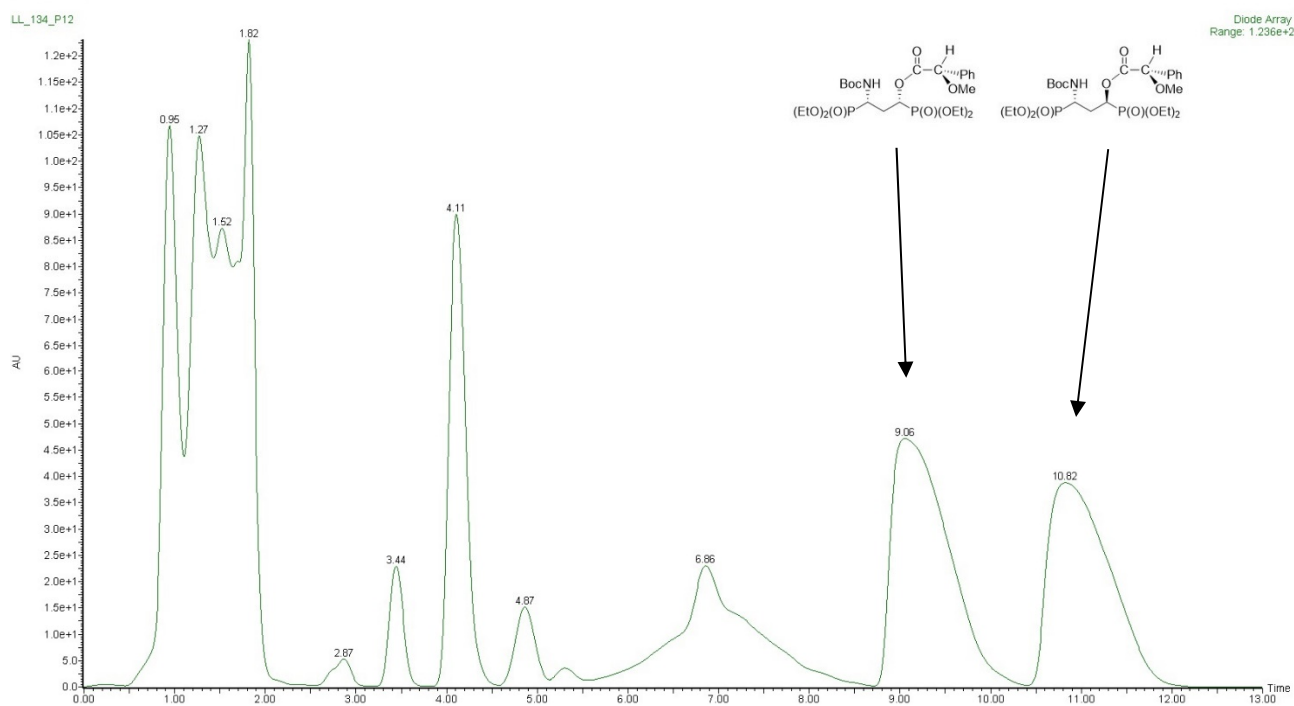


Figure S51: Separation of (1S,3R,1'S)-16 and (1S,3S,1'S)-16 by preparative HPLC