

Highly tunable chiral Clickphine P,N ligands for Ir-catalyzed asymmetric hydrogenation

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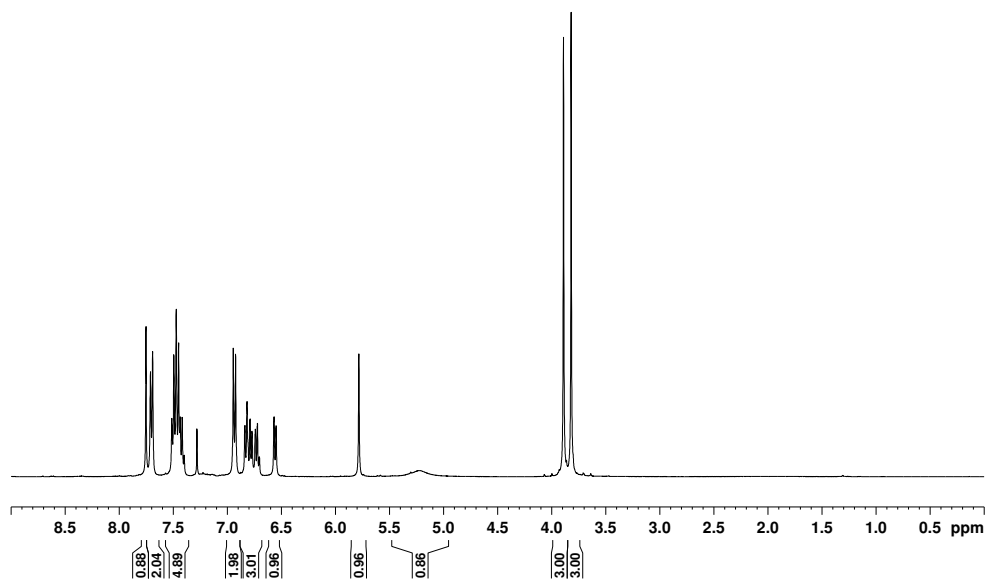
Supplementary Material

I NMR spectra of new compounds

S-2

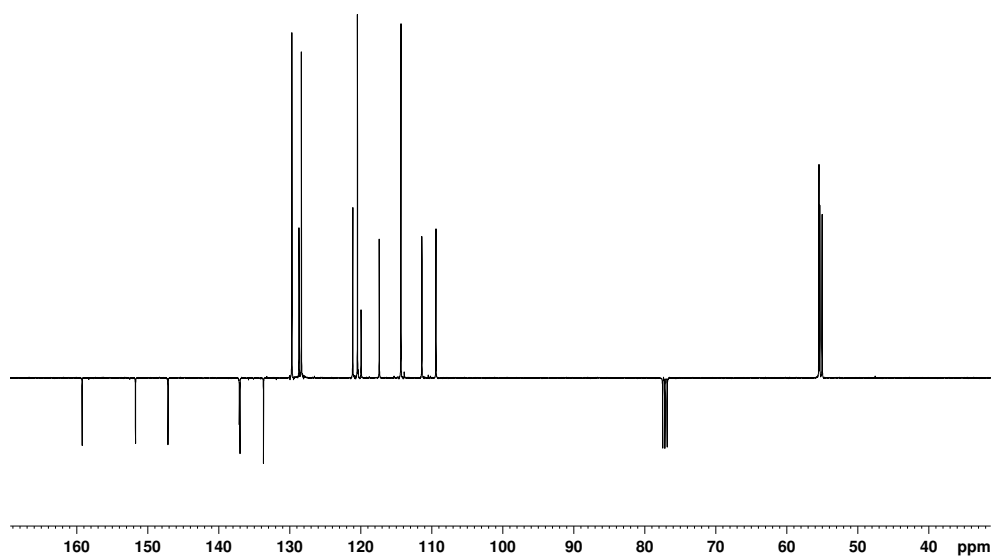
I NMR spectra of new compounds

RD516 in CDCl₃ 1H



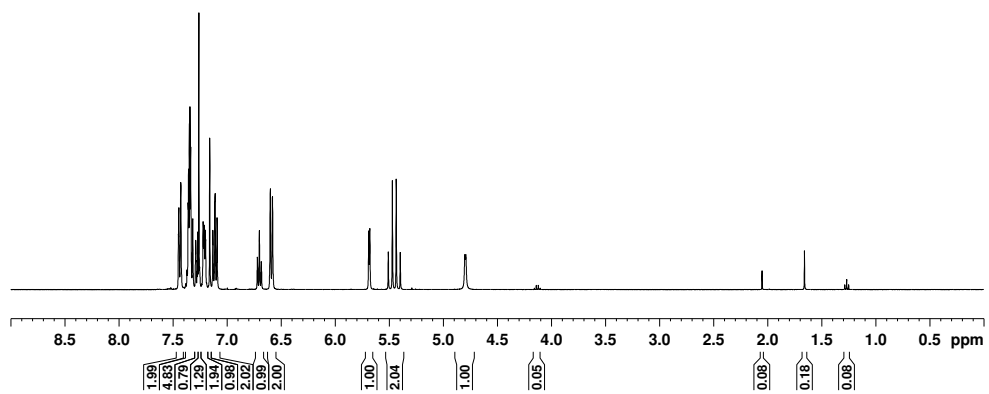
(R)-2b ¹H NMR (400 MHz; CDCl₃).

RD516 in CDCl₃ 13C



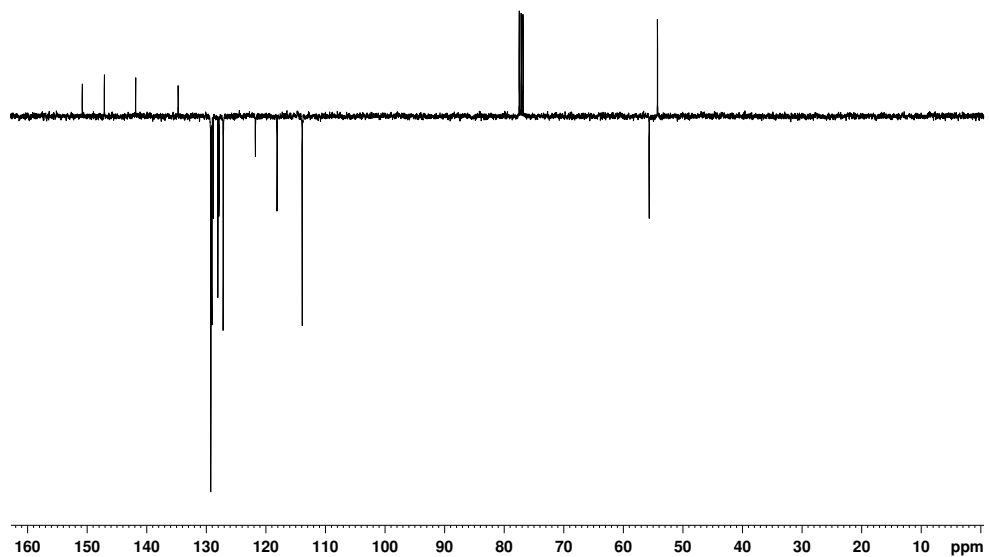
(R)-2b ¹³C {¹H} NMR (101 MHz; CDCl₃).

RD425 crystals in CDCl₃ 1H

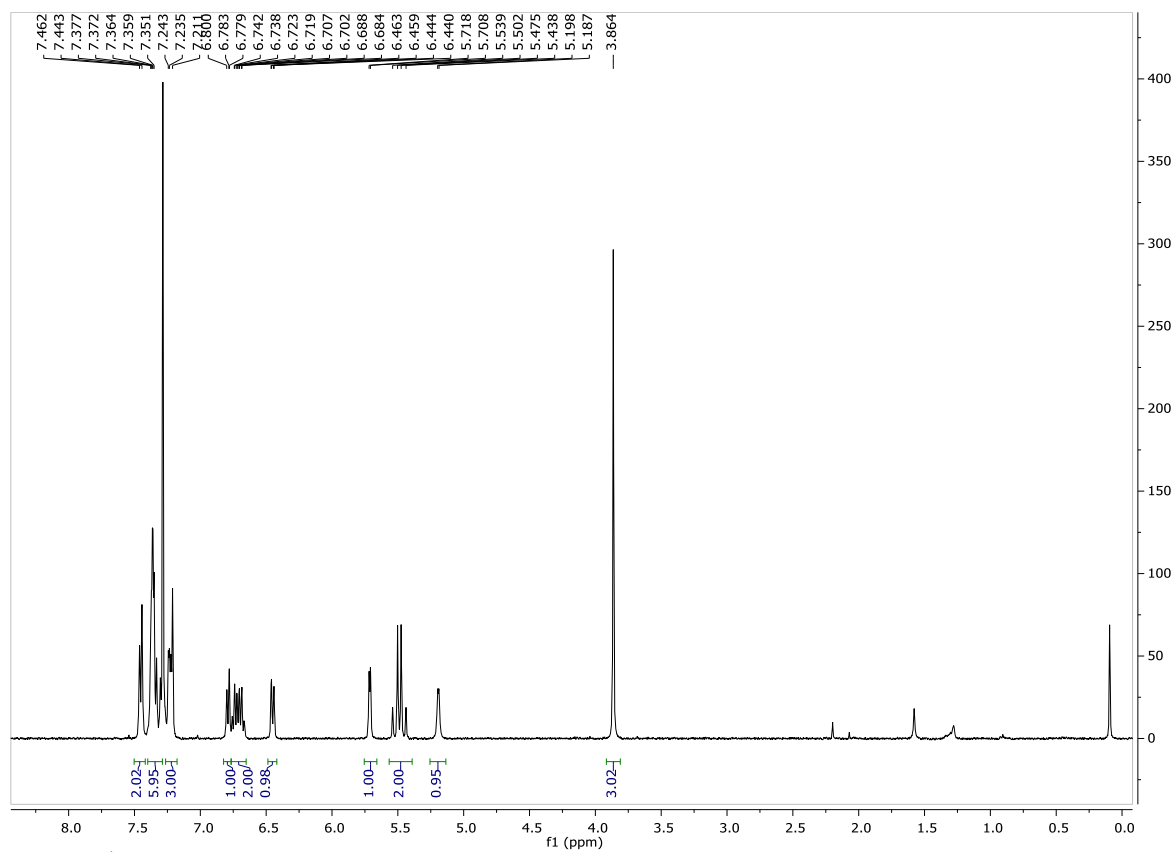


(*S*)-**2c** ¹H NMR (400 MHz; CDCl₃).

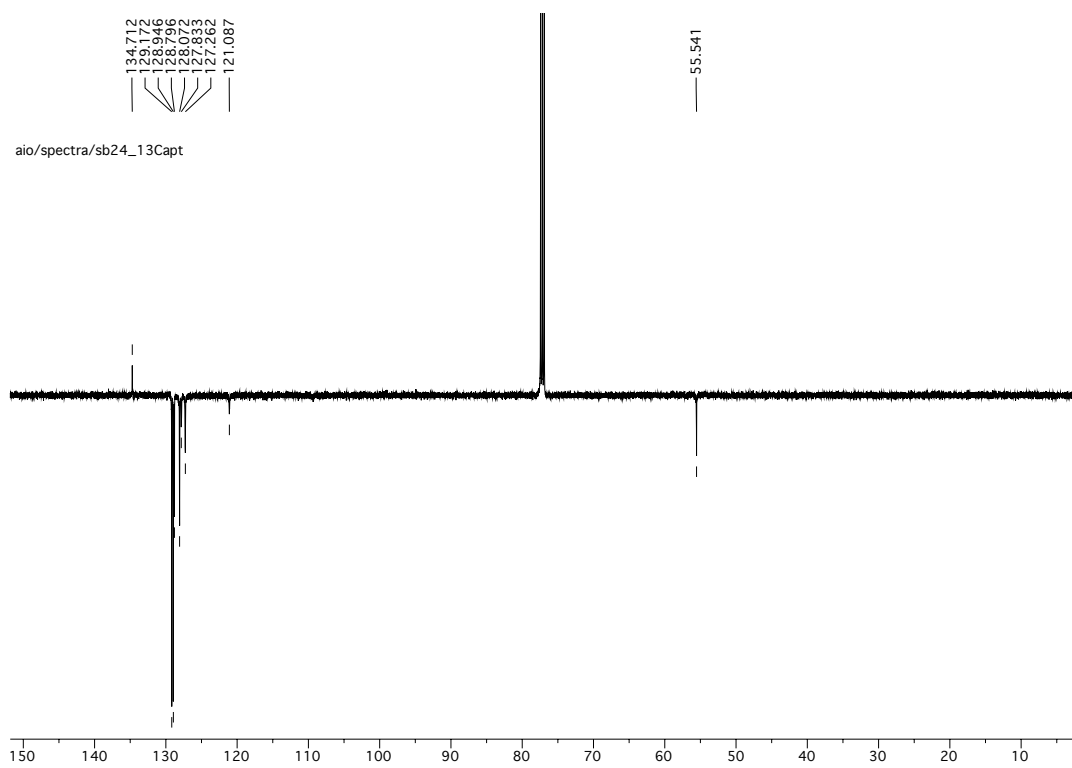
RD425 cryst in CDCl₃ 13C



(*S*)-**2c** ¹³C{¹H} NMR (101 MHz; CDCl₃).

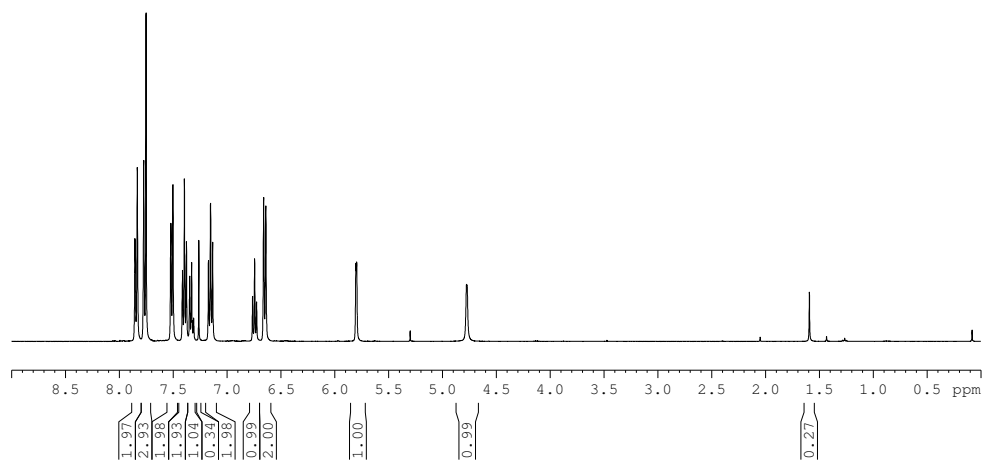


(R)-2d ^1H NMR (400 MHz; CDCl_3).



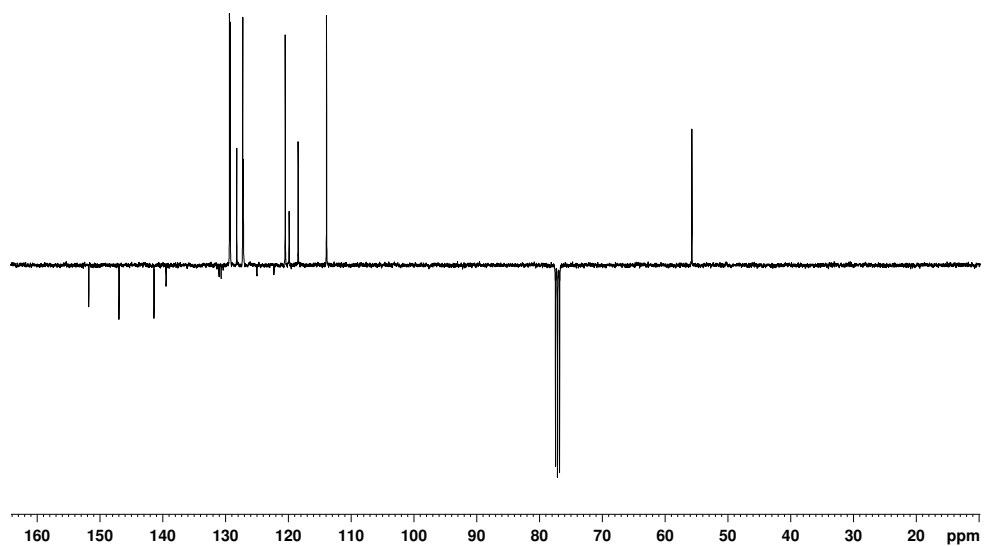
(R)-2d $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).

RD437A cr in CDCl₃ 1H

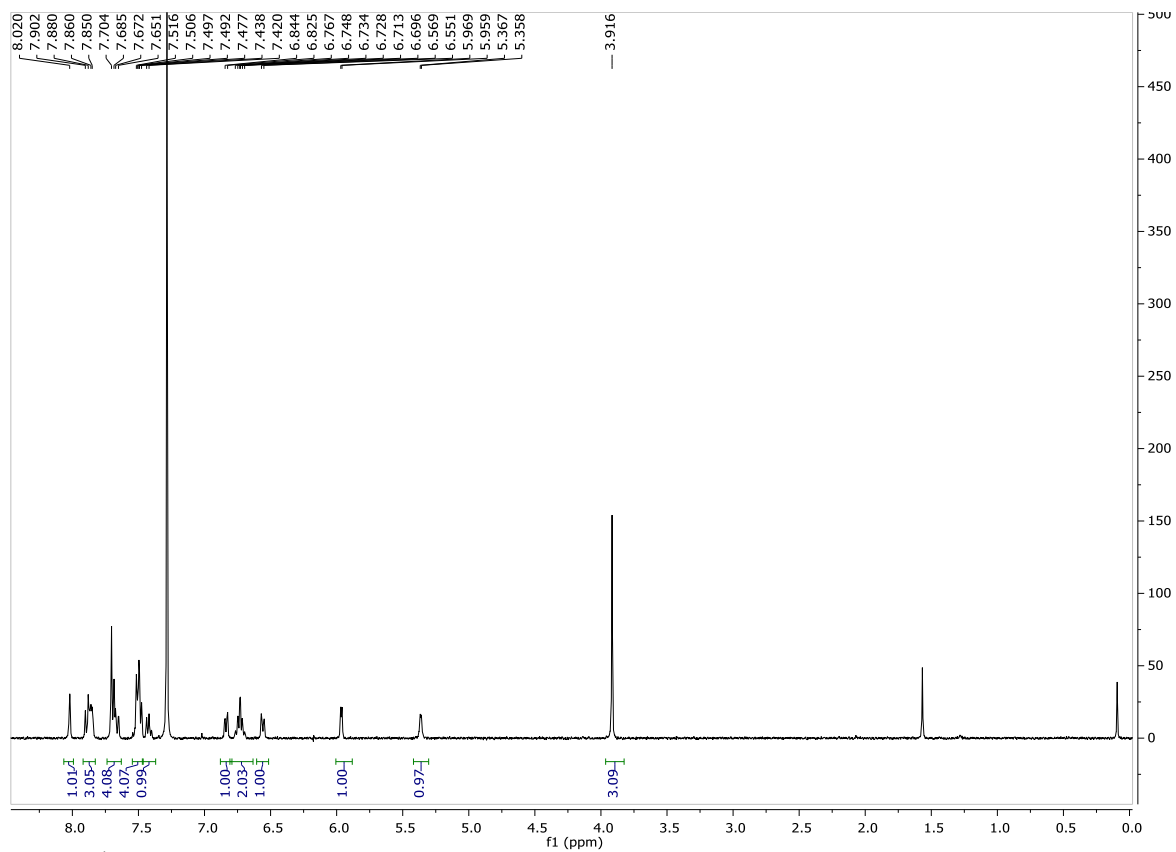


(S)-2e ¹H NMR (400 MHz; CDCl₃).

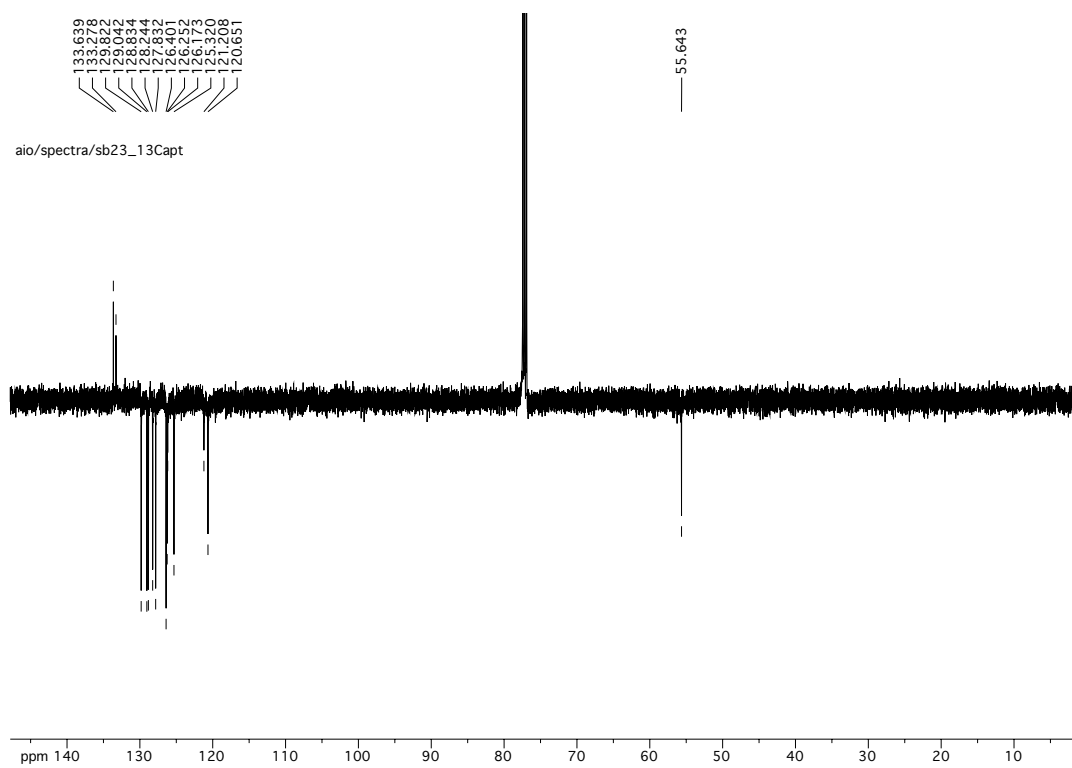
RD437A cryst in CDCl₃ 13C



(S)-2e ¹³C{¹H} NMR (101 MHz; CDCl₃).

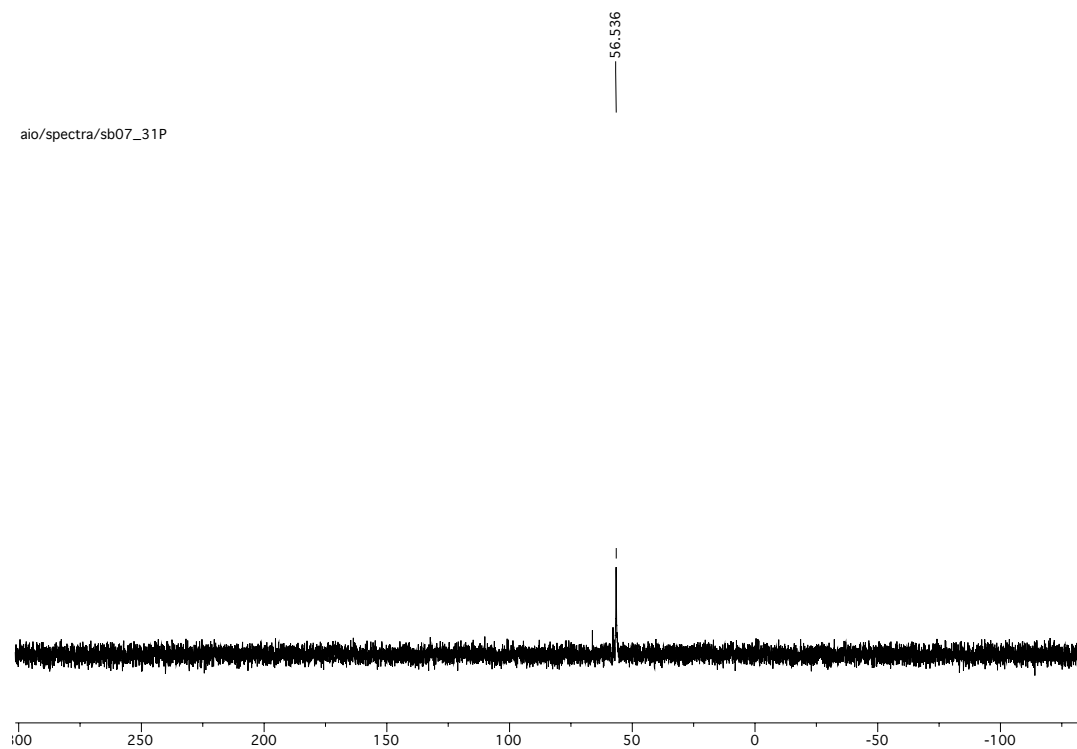


(*R*)-2f ^1H NMR (400 MHz; CDCl_3).

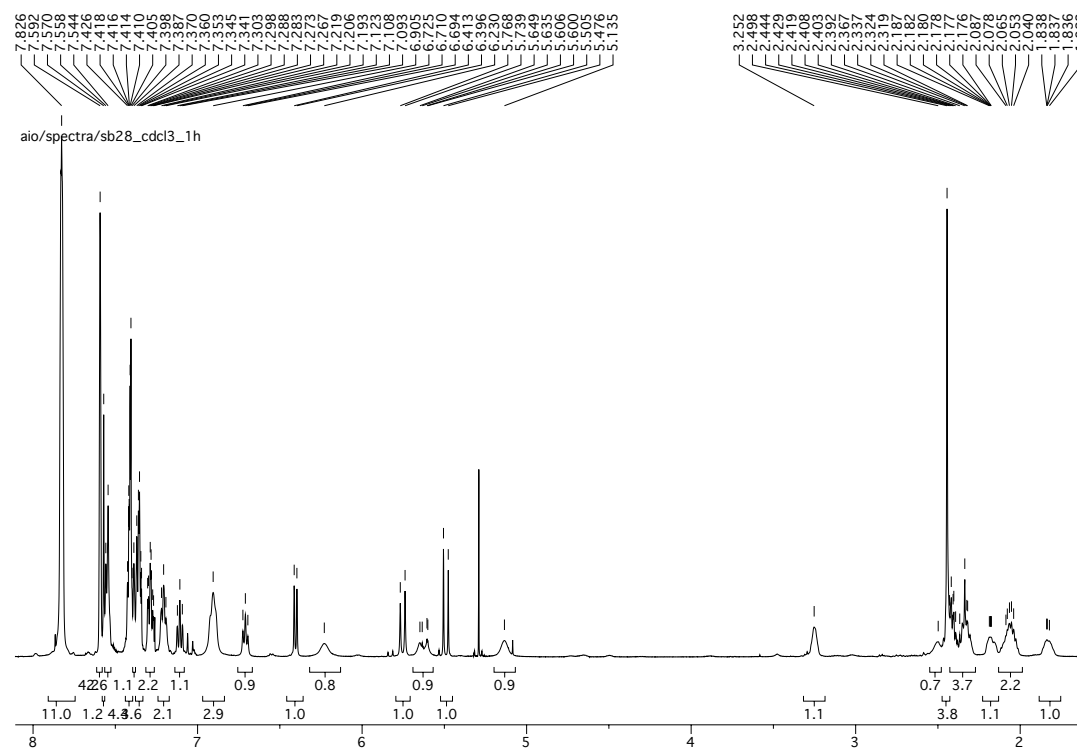


(*R*)-2f $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).

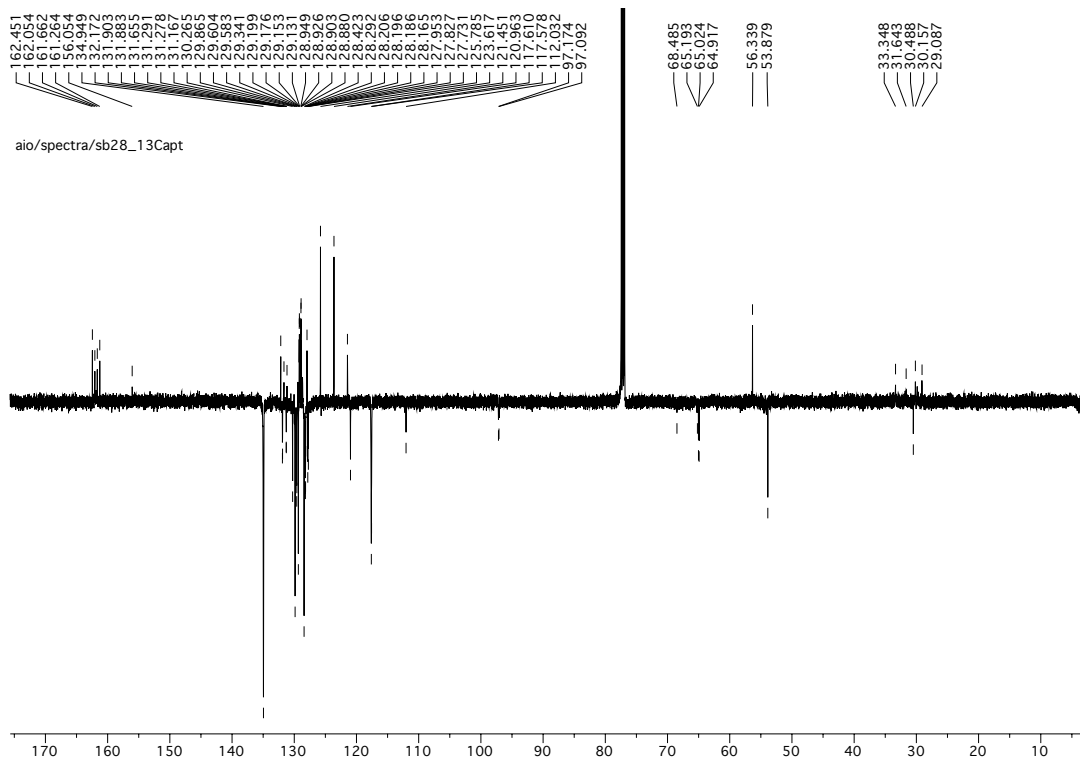
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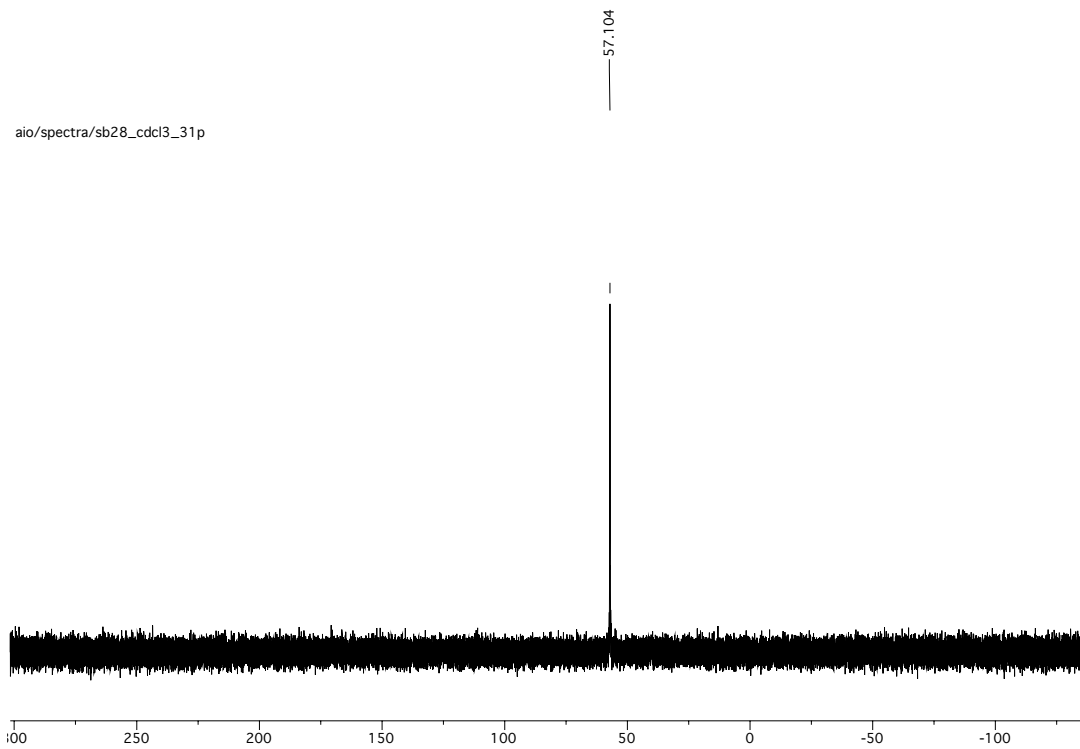
(R)-4b $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz; CDCl_3).



(R)-4c ^1H NMR (500 MHz; CDCl_3).

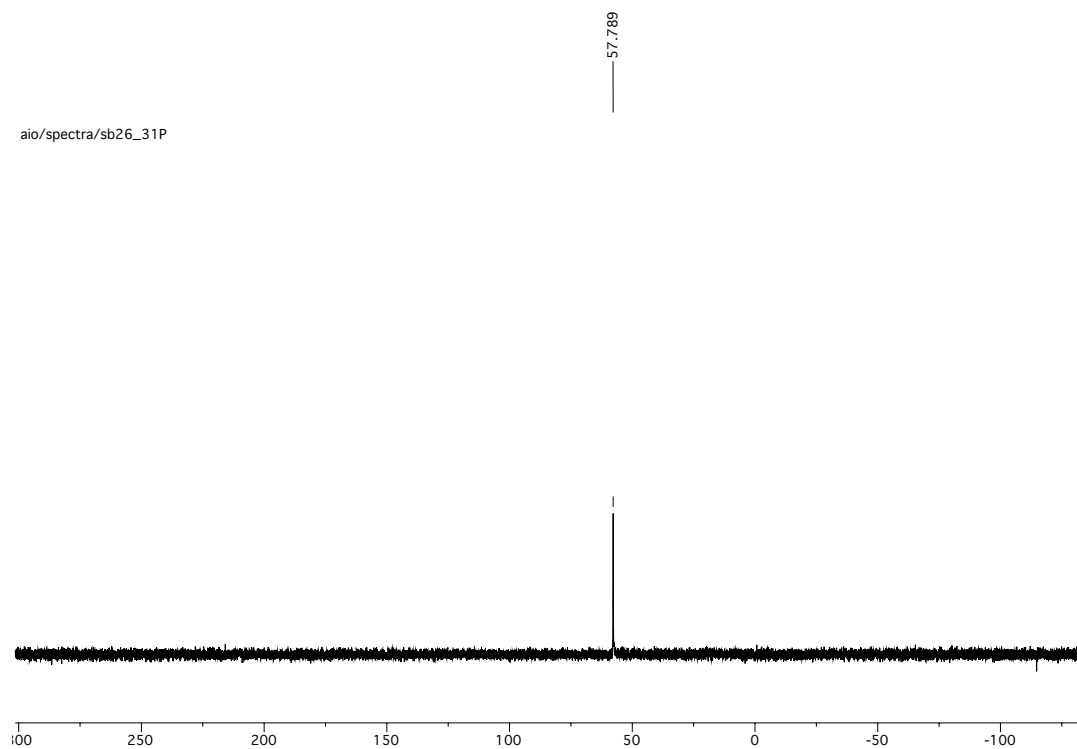


(R)-4c $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).

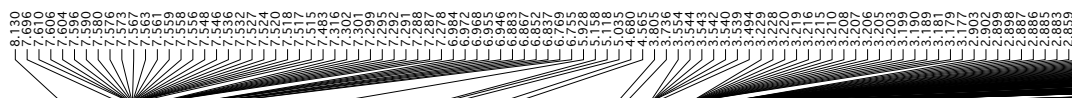


(R)-4c $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz; CDCl_3).

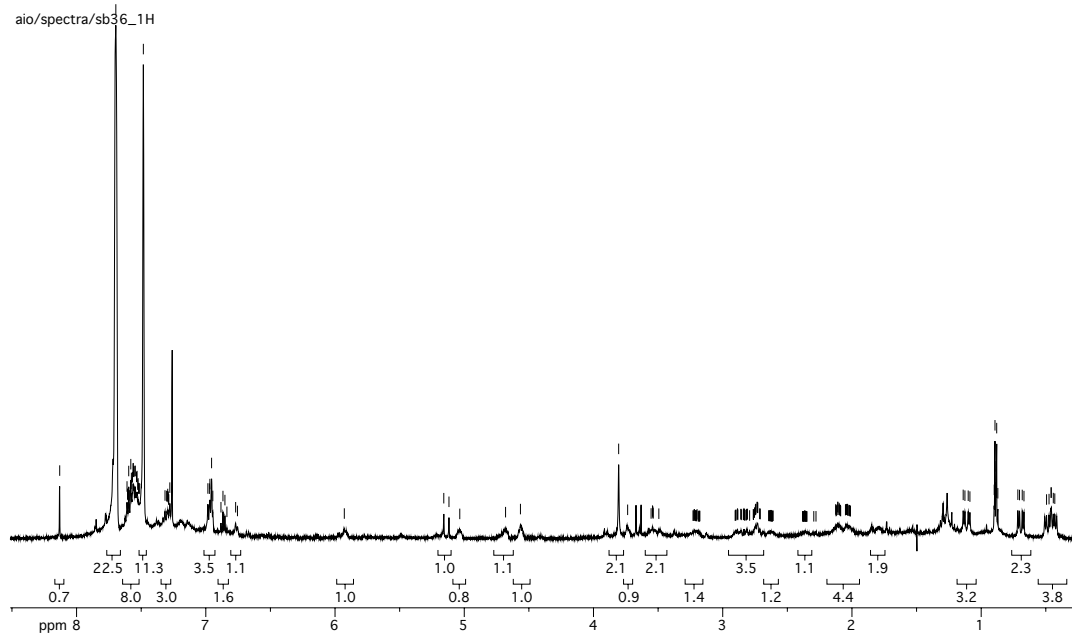
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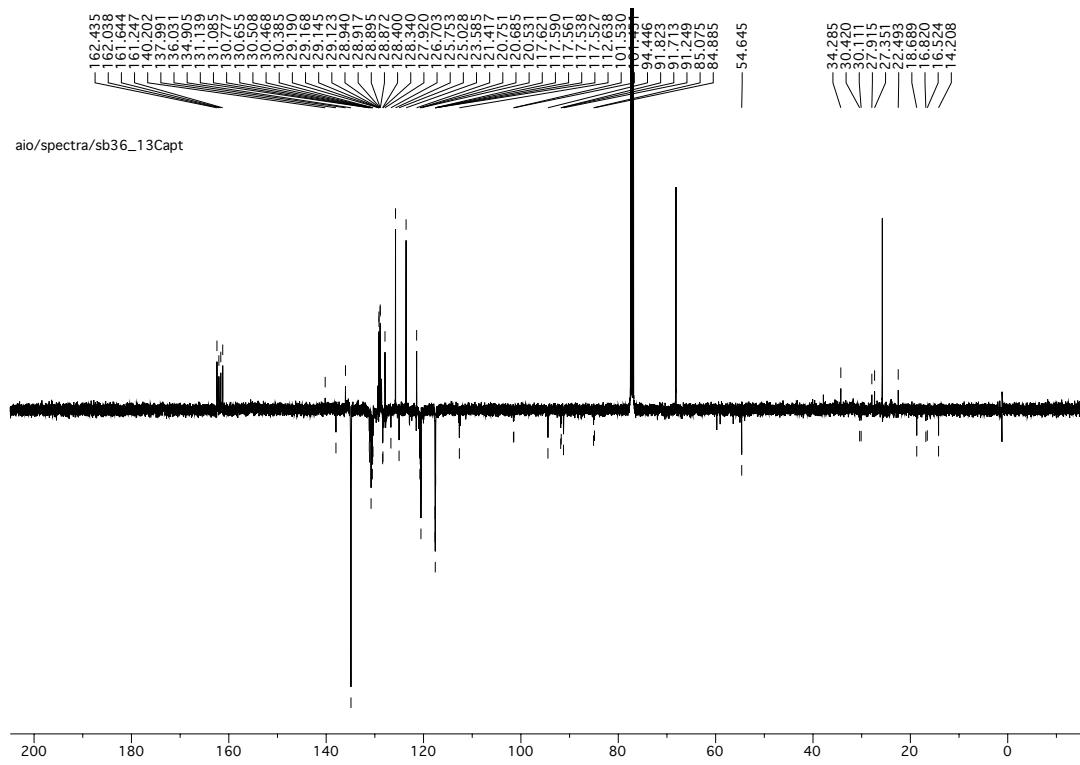
(R)-4d ^{31}P { ^1H } NMR (202 MHz; CDCl_3).



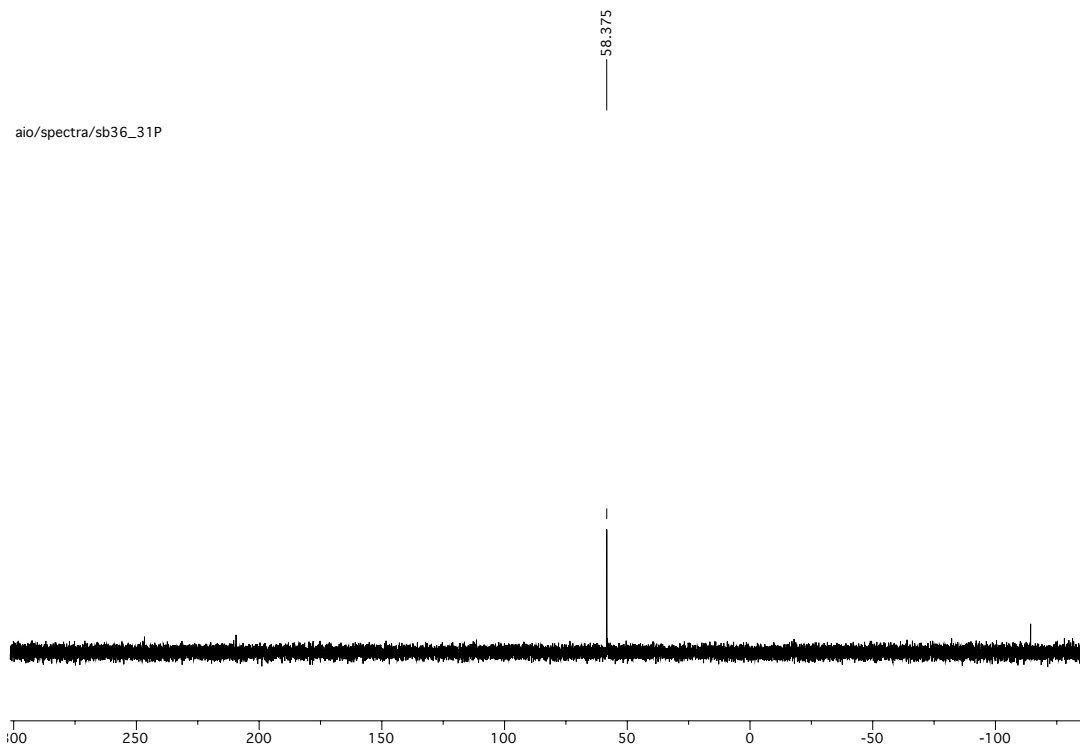
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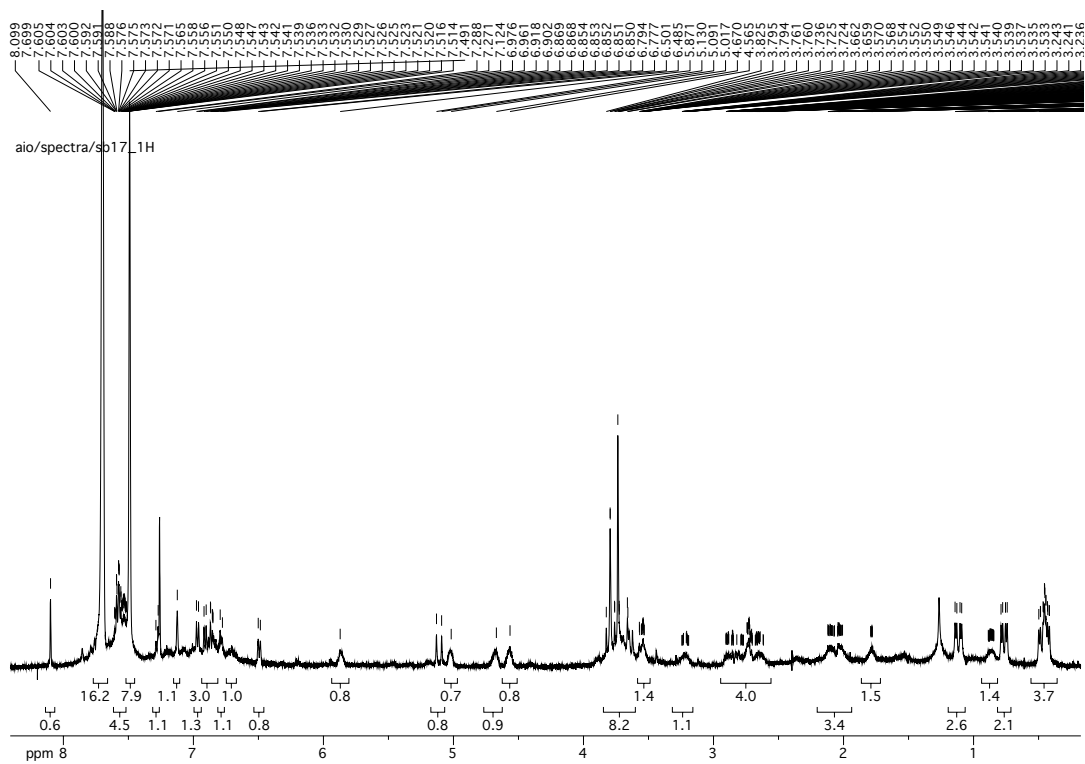
(R)-4e ^1H NMR (500 MHz; CDCl_3).



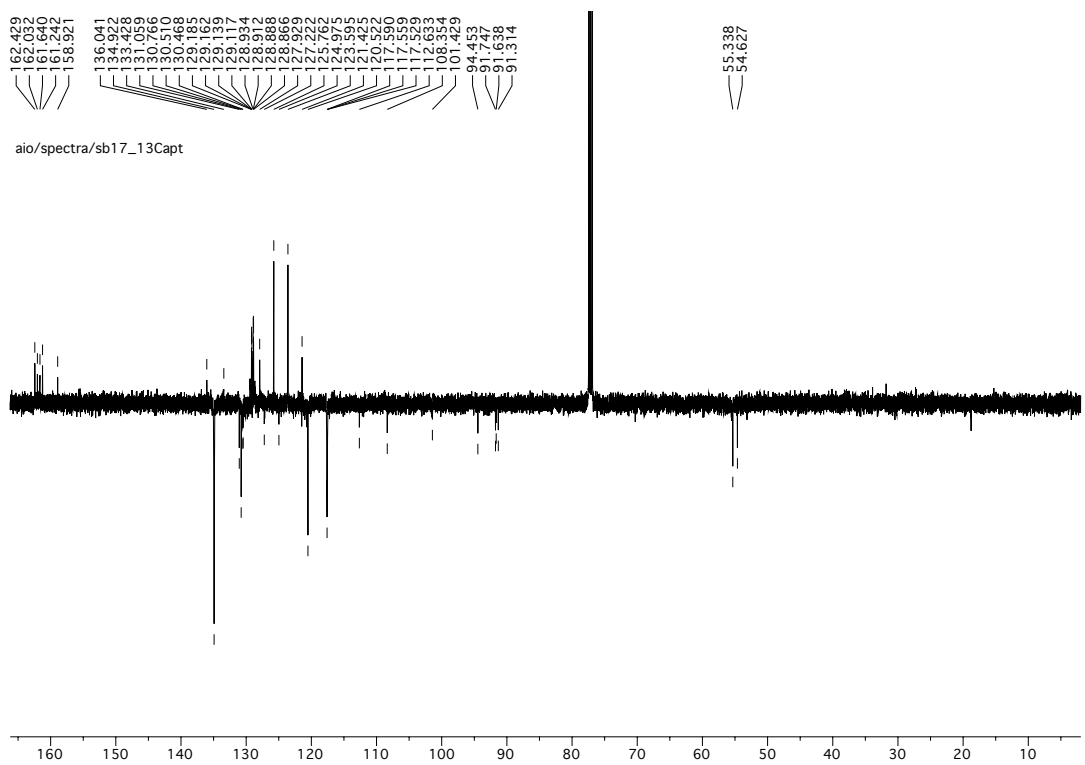
(*R*)-4e $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).



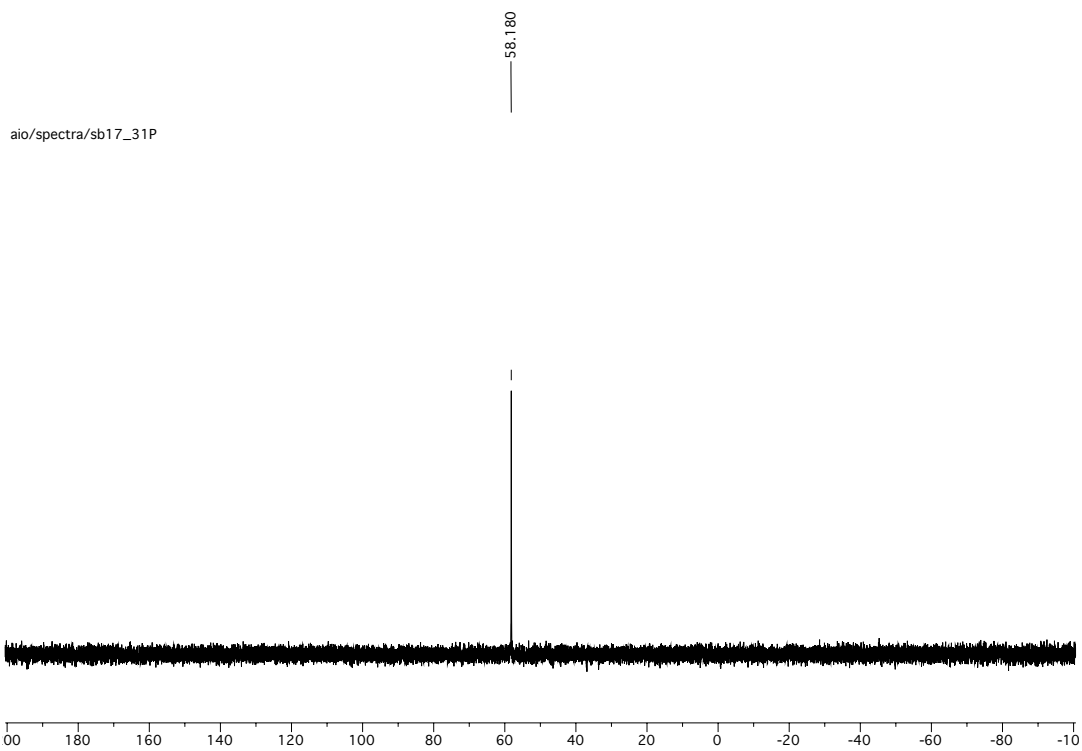
(*R*)-4e $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz; CDCl_3).



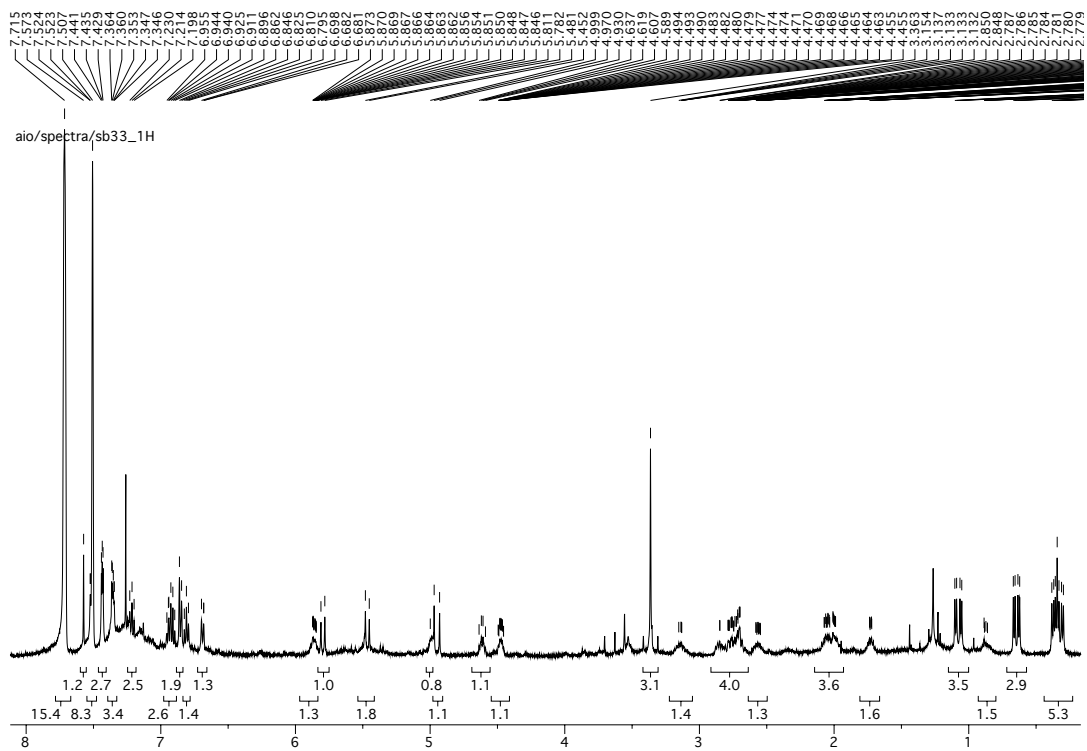
(R)-4f ^1H NMR (500 MHz; CDCl_3).



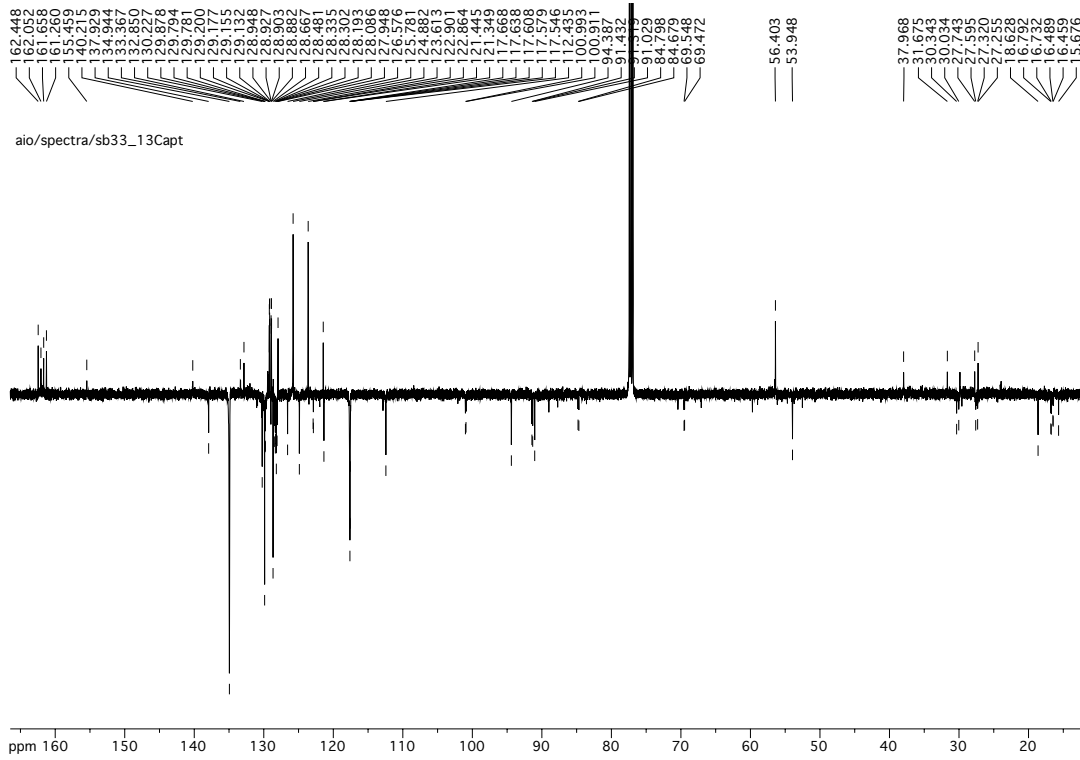
(R)-4f $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).



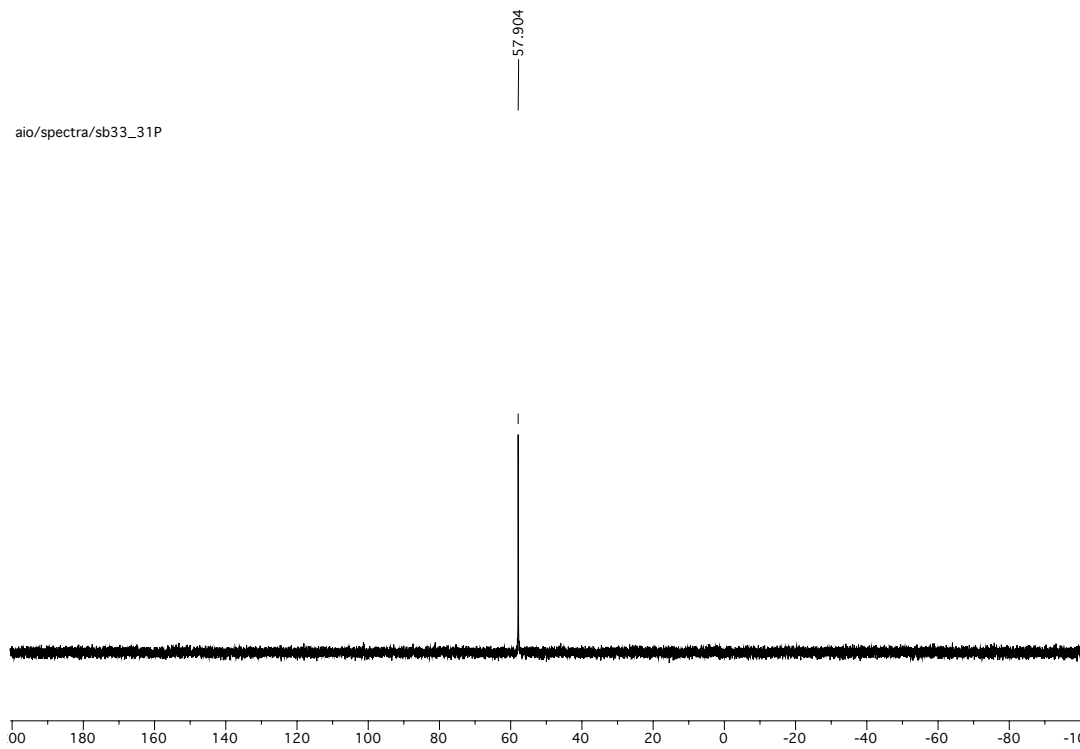
(R)-4f $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz; CDCl_3).



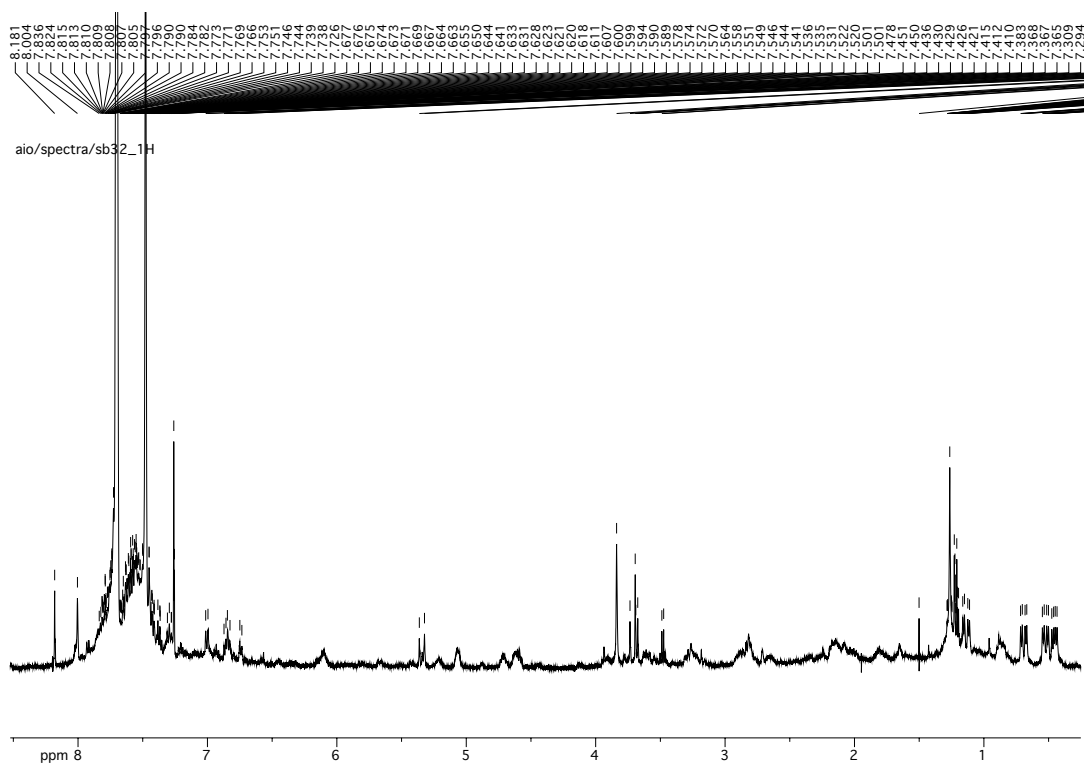
(R)-4g ^1H NMR (500 MHz; CDCl_3).



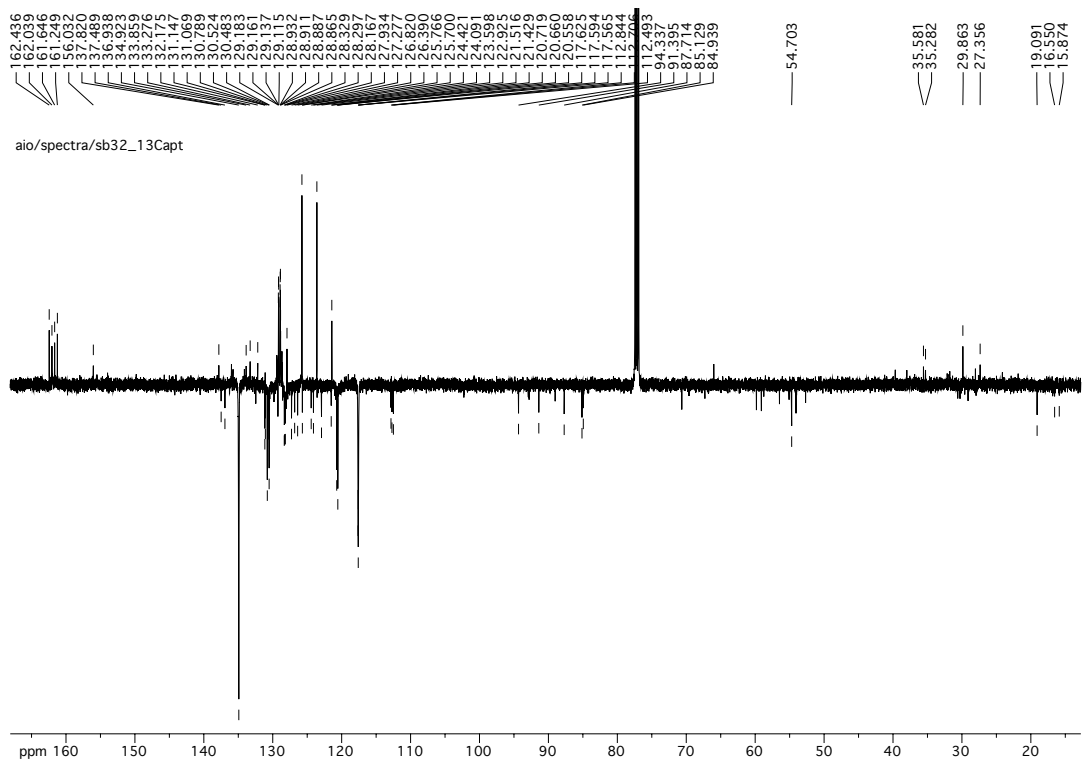
(R)-4g $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).



(R)-4g $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz; CDCl_3).

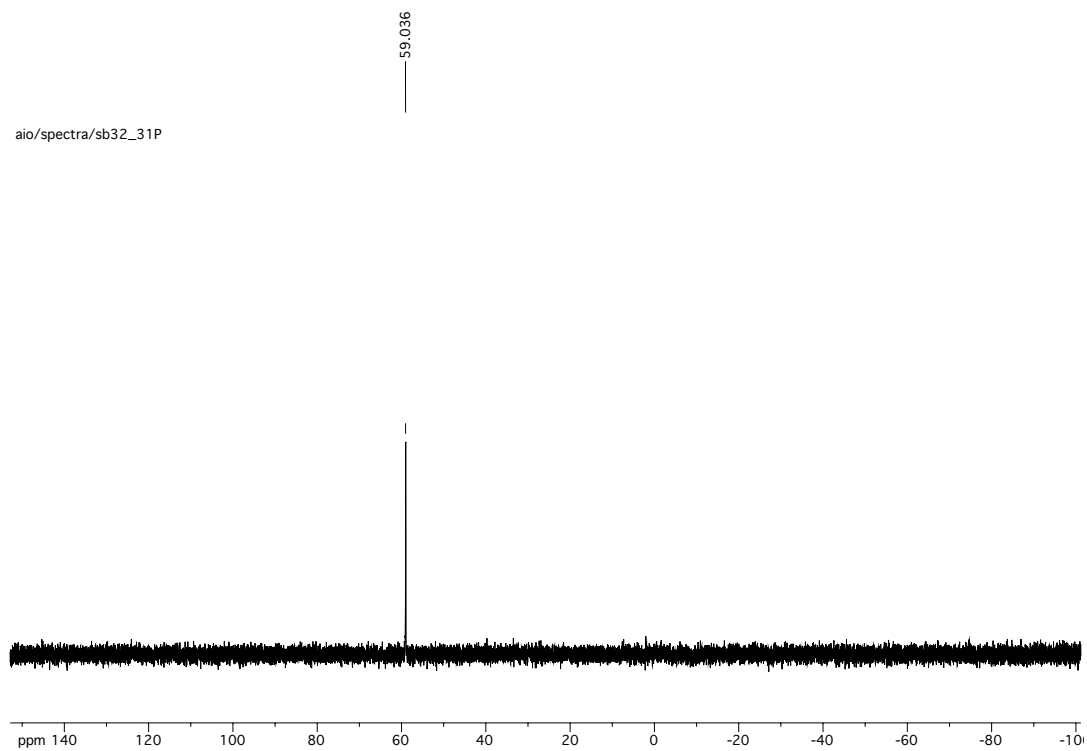


(R)-4h ^1H NMR (500 MHz; CDCl_3).



(R)-4h $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz; CDCl_3).

aio/spectra/sb32_31P



(R)-4h $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz; CDCl_3).