

## A Convenient Access to N-Phosphonio-Substituted NHC Metal Complexes

[M = Ag(I), Rh(I), Pd(II)]

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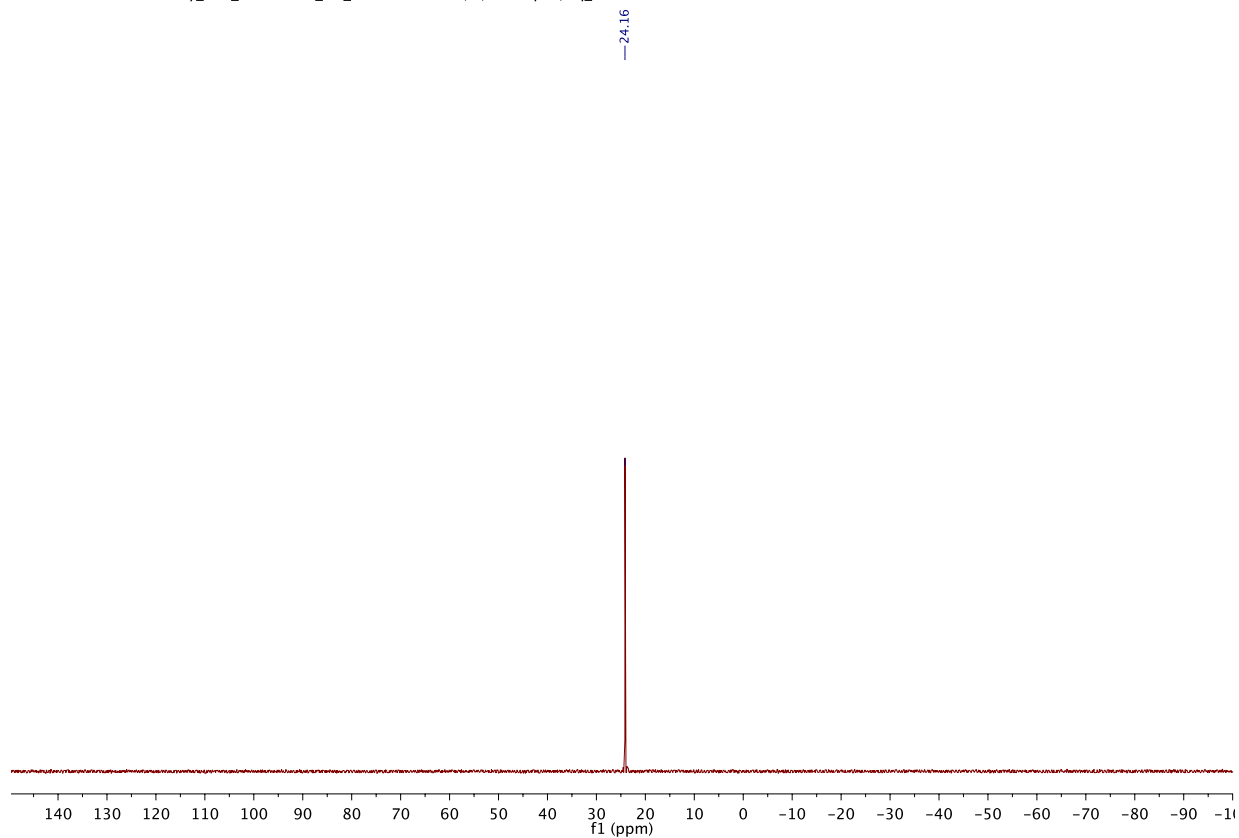
### SUPPORTING INFORMATION

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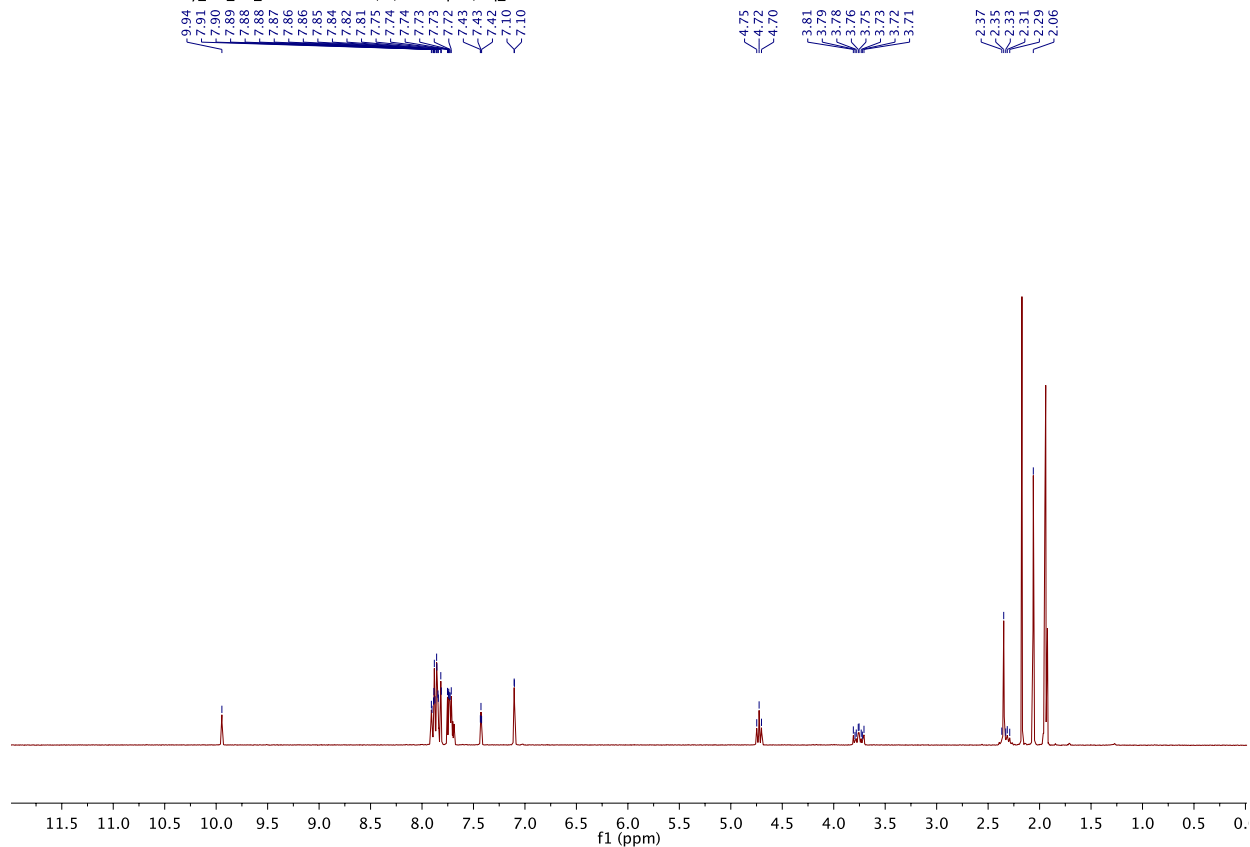
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[1]\text{Br}_2$ (in $\text{CD}_3\text{CN}$ )

ibeH0099 — IB2 2 — Day\_P31\_DECOUPLE\_H1\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 23 —



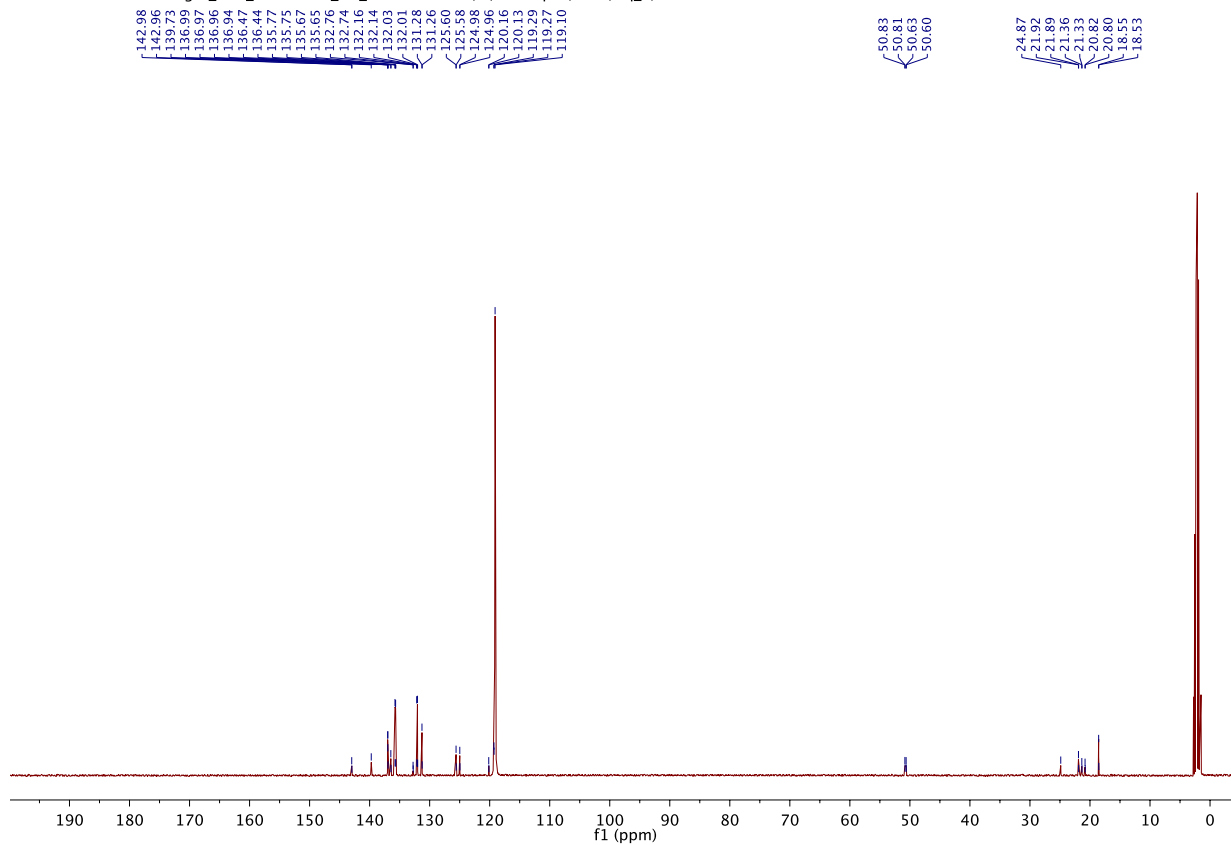
# $^1\text{H}$ NMR spectrum of $[1]\text{Br}_2$ (in $\text{CD}_3\text{CN}$ )

ibeH0099 — IB2 2 — Day\_H1\_int\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 23 —



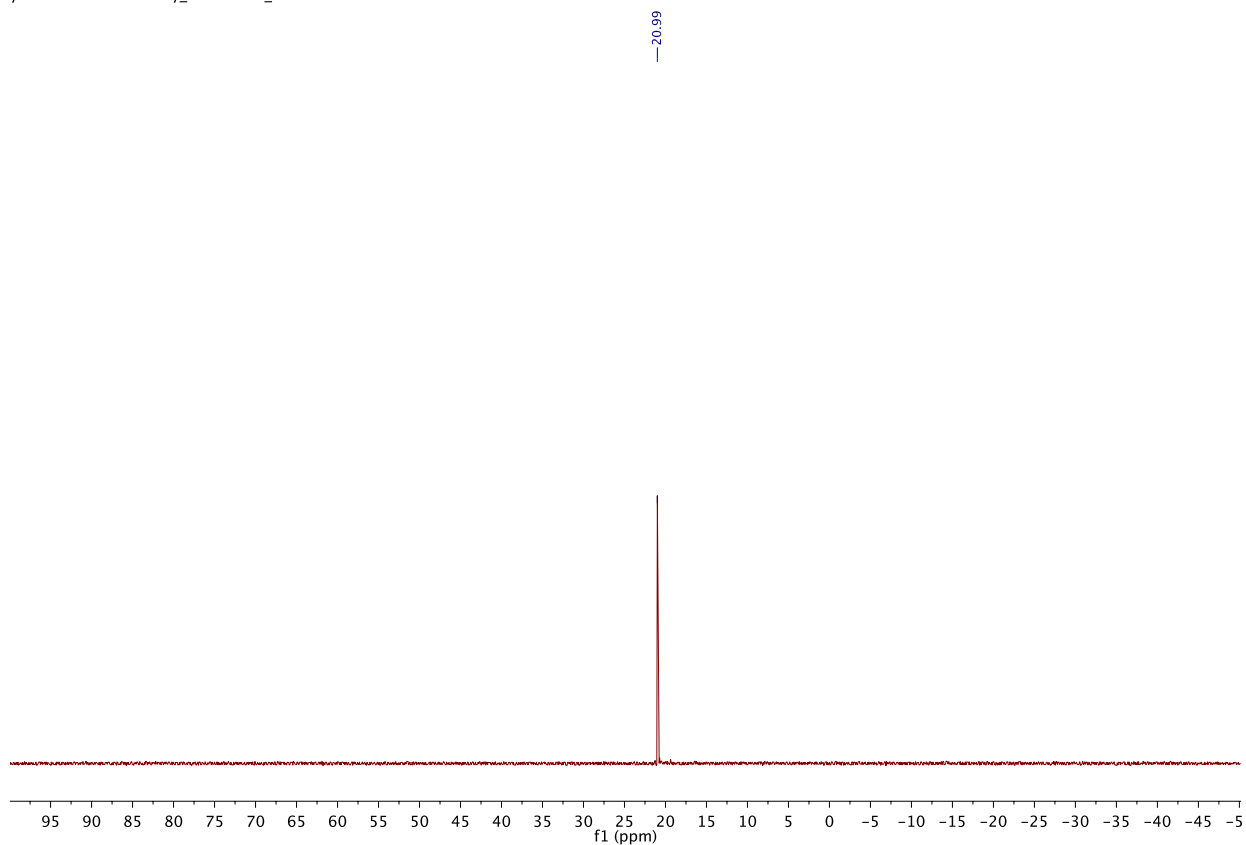
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [1]Br<sub>2</sub> (in CD<sub>3</sub>CN)

ibeG0024 — IB 12 — Night\_C13\_DECOUPLE\_H1\_LONG CD3CN /x/av400pas/data/eq\_a/nmr i.benaissa 24 —



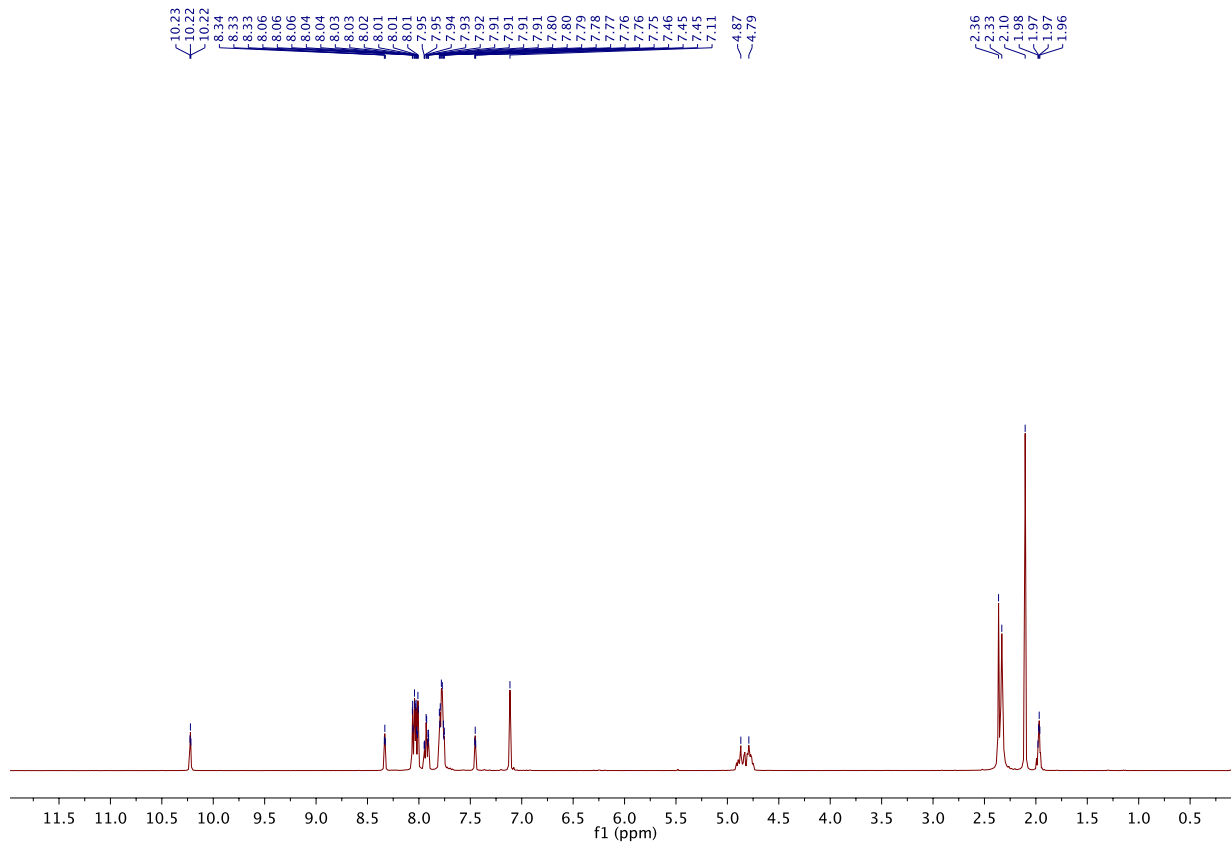
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [1']Br<sub>2</sub> (in CD<sub>3</sub>CN)

ycaL0007.1.fid — P31y\_DECOUPLE\_H1



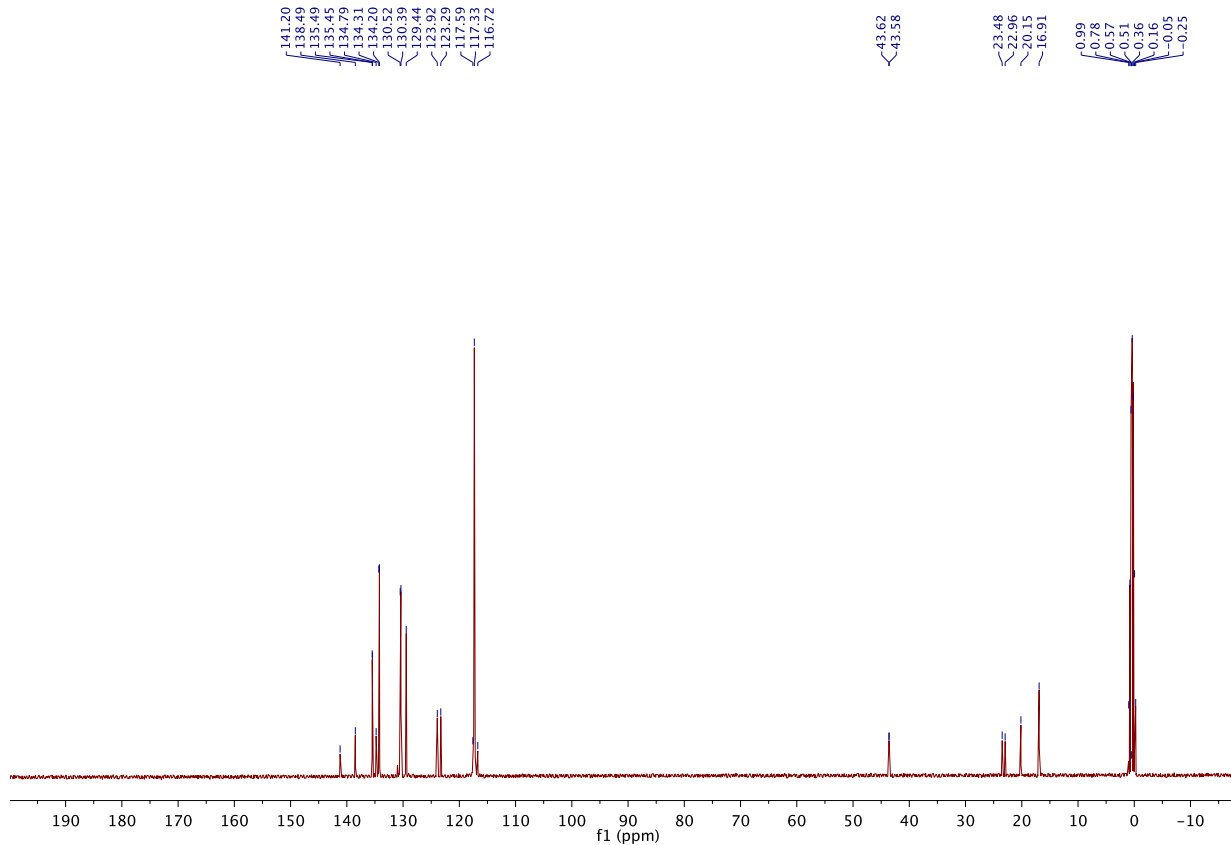
# $^1\text{H}$ NMR spectrum of $[1']\text{Br}_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0007.2.fid — H1\_NO\_INT



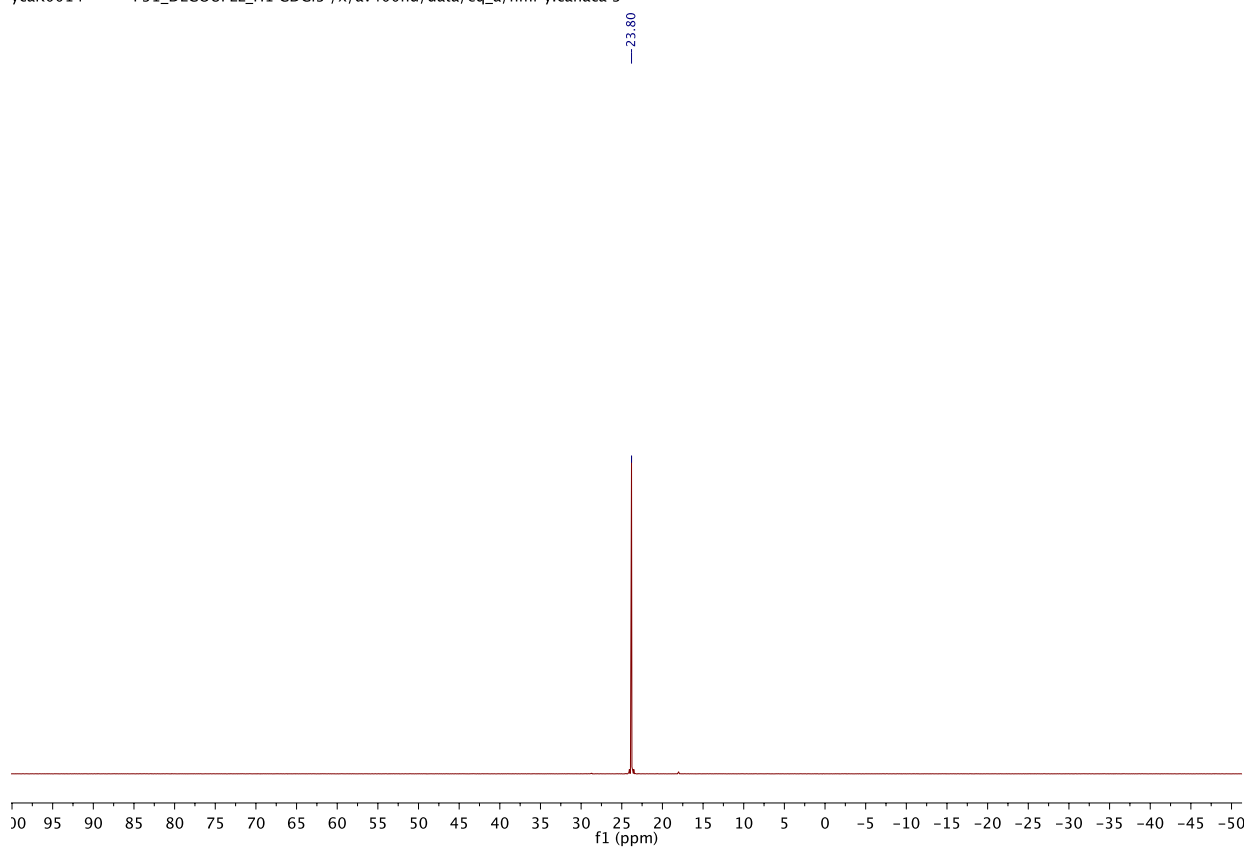
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[1']\text{Br}_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0007.3.fid — C13\_DECOUPLE\_H1



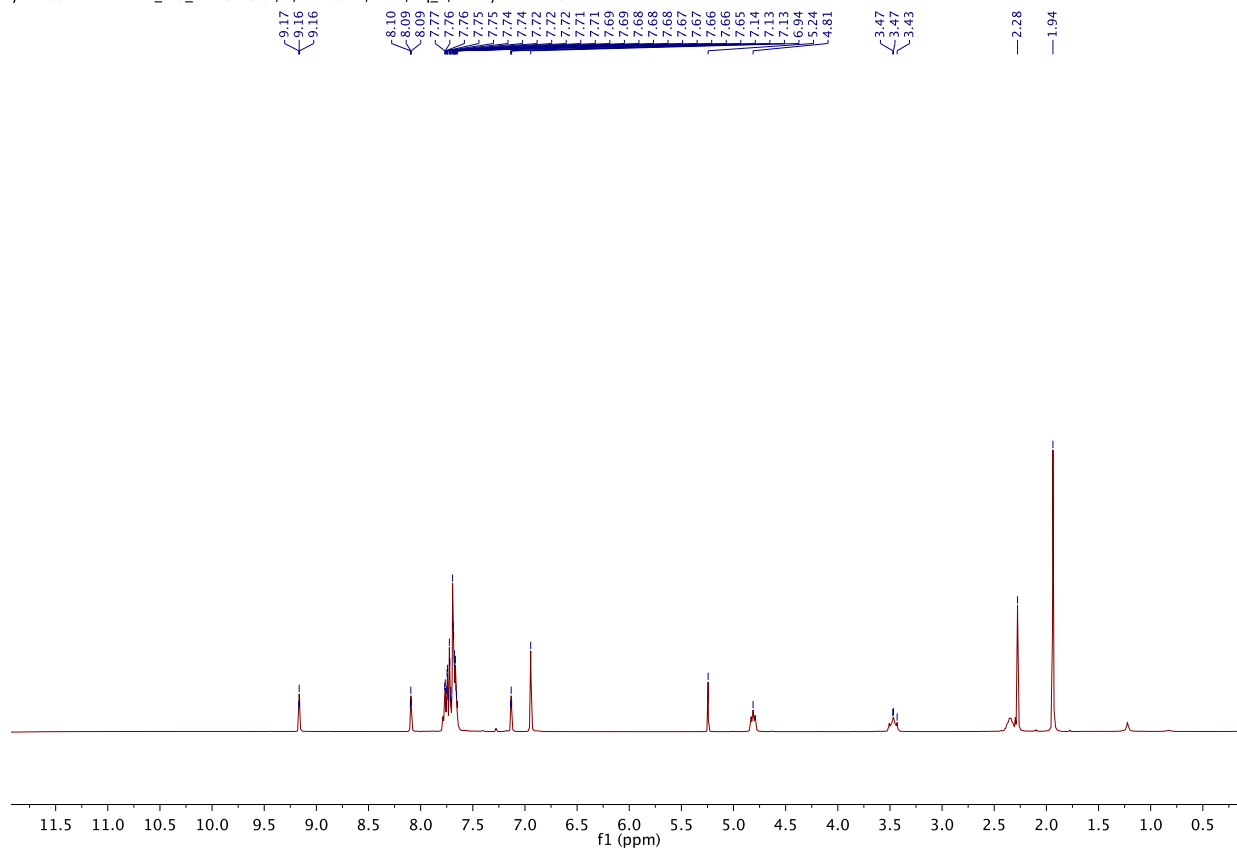
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\mathbf{1}](\text{OTf})_2$ (in $\text{CDCl}_3$ )

ycaK0014 — — P31\_DECOUPLE\_H1 CDCI3 /x/av400hd/data/eq\_a/nmr y.canaca 3 —



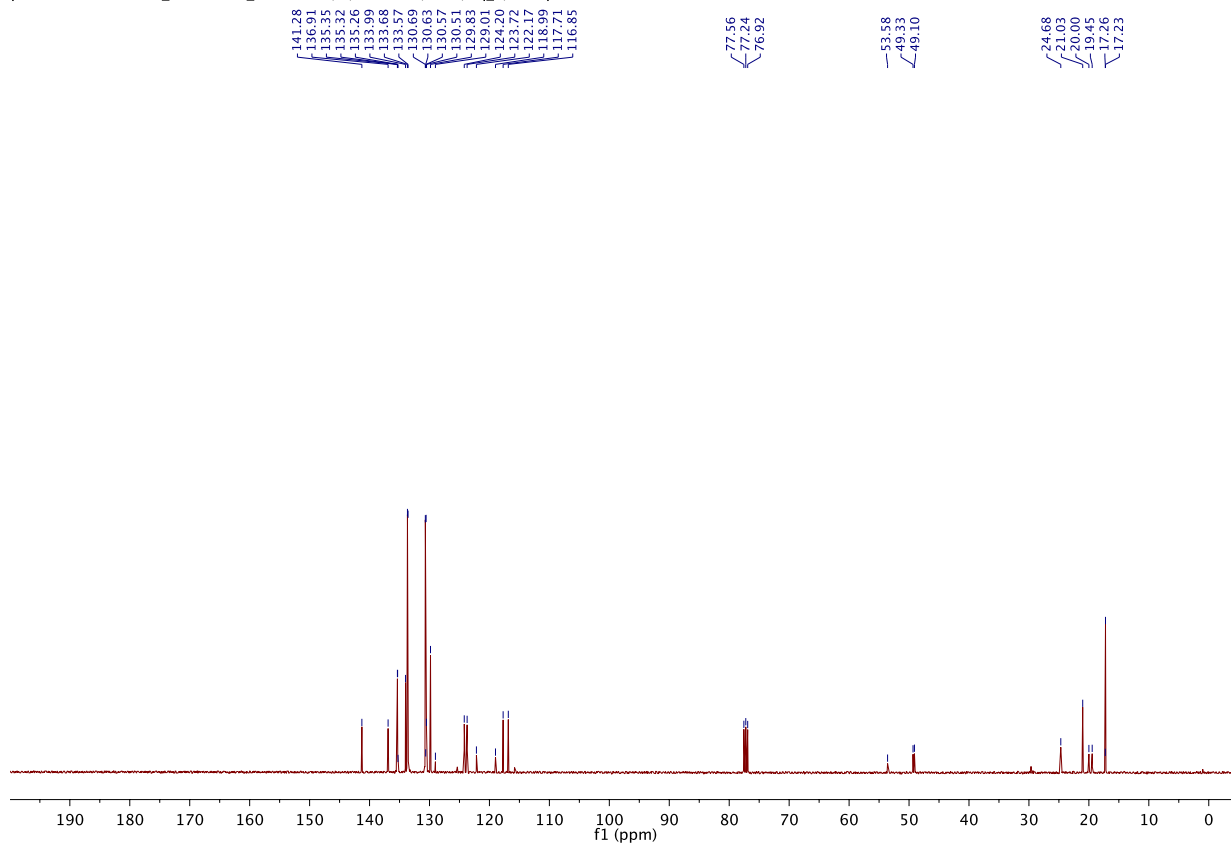
# $^1\text{H}$ NMR spectrum of $[\mathbf{1}](\text{OTf})_2$ (in $\text{CDCl}_3$ )

ycaK0014 — — H1\_NO\_INT CDCI3 /x/av400hd/data/eq\_a/nmr y.canaca 3 —



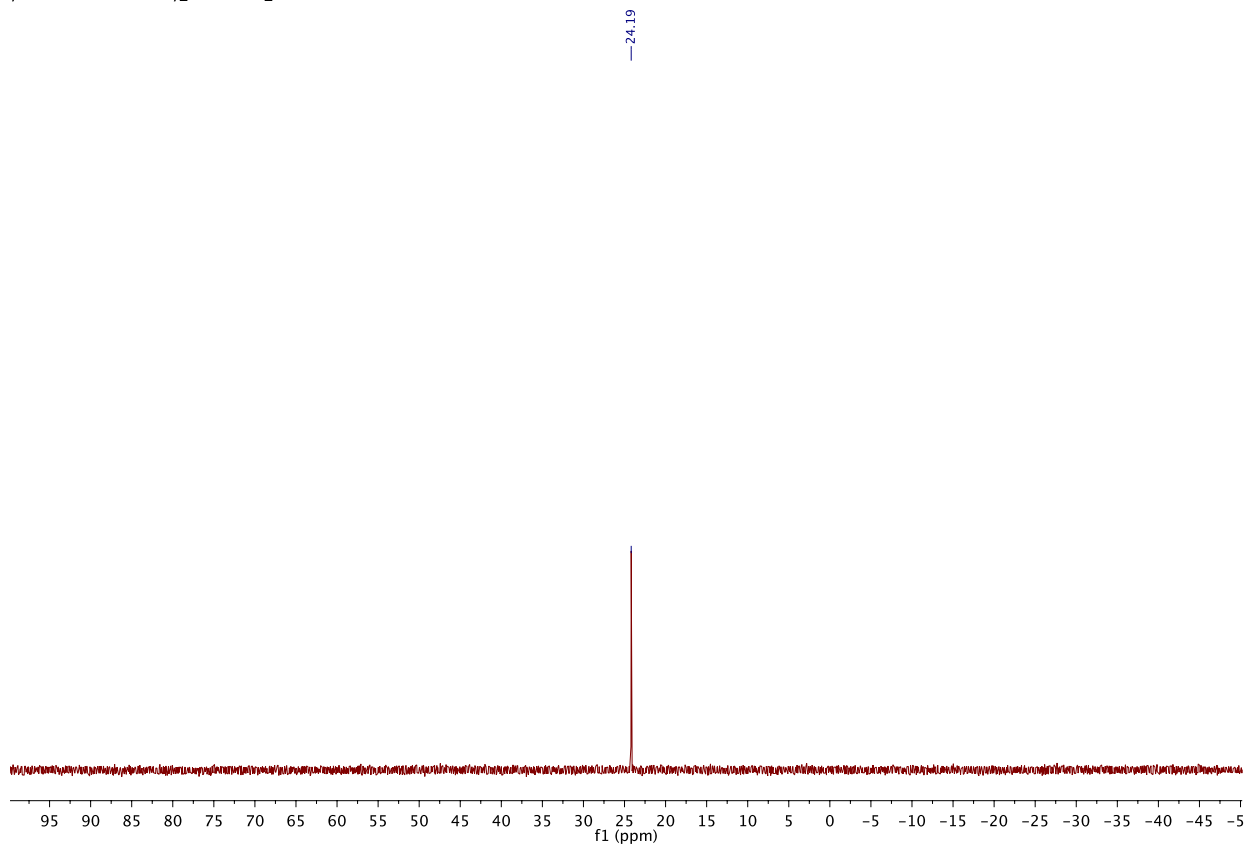
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [1](OTf)<sub>2</sub> (in CDCl<sub>3</sub>)

ycaK0014 — — C13\_DECOUPLE\_H1 CDCl3 /x/av400hd/data/eq\_a/nmr y.canaca 3 —



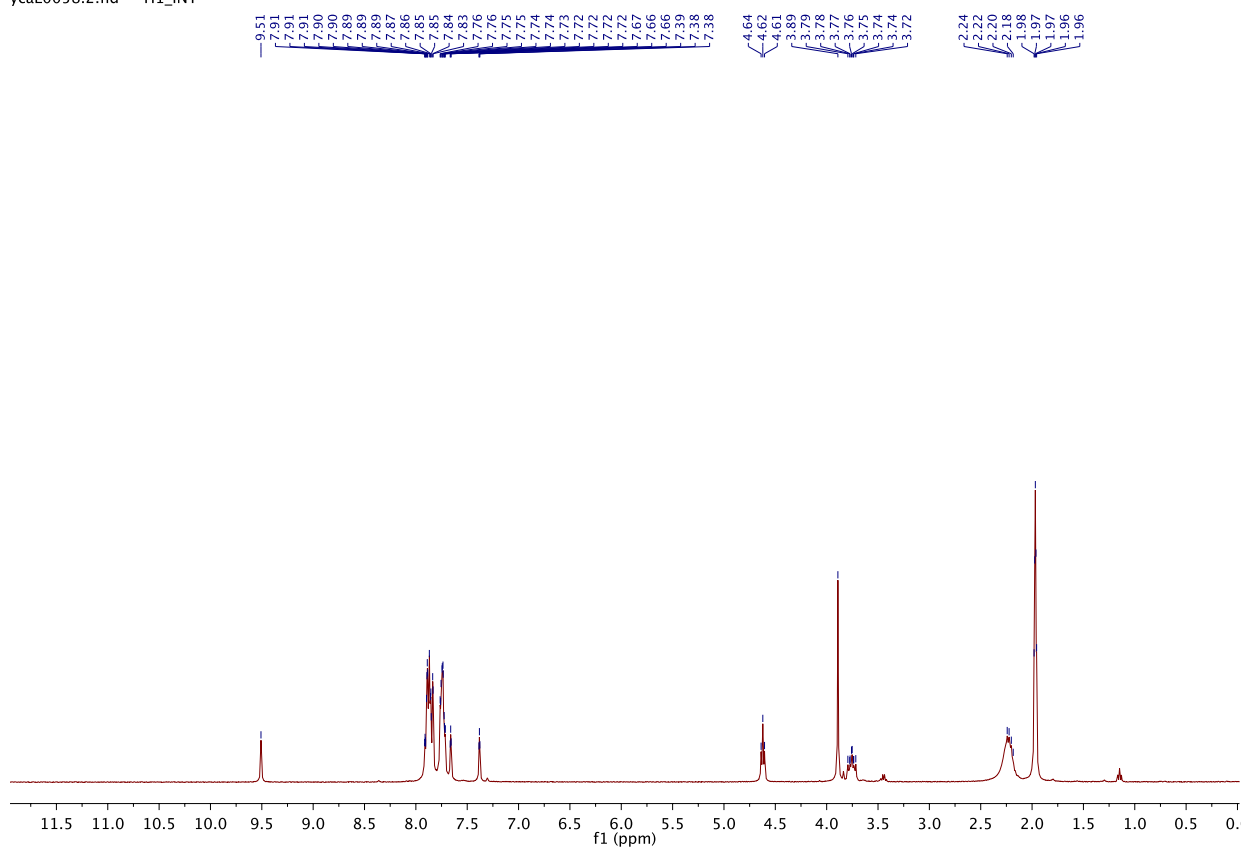
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [2]Br<sub>2</sub> (in CD<sub>3</sub>CN)

ycaL0058.1.fid — P31y\_DECOUPLE\_H1



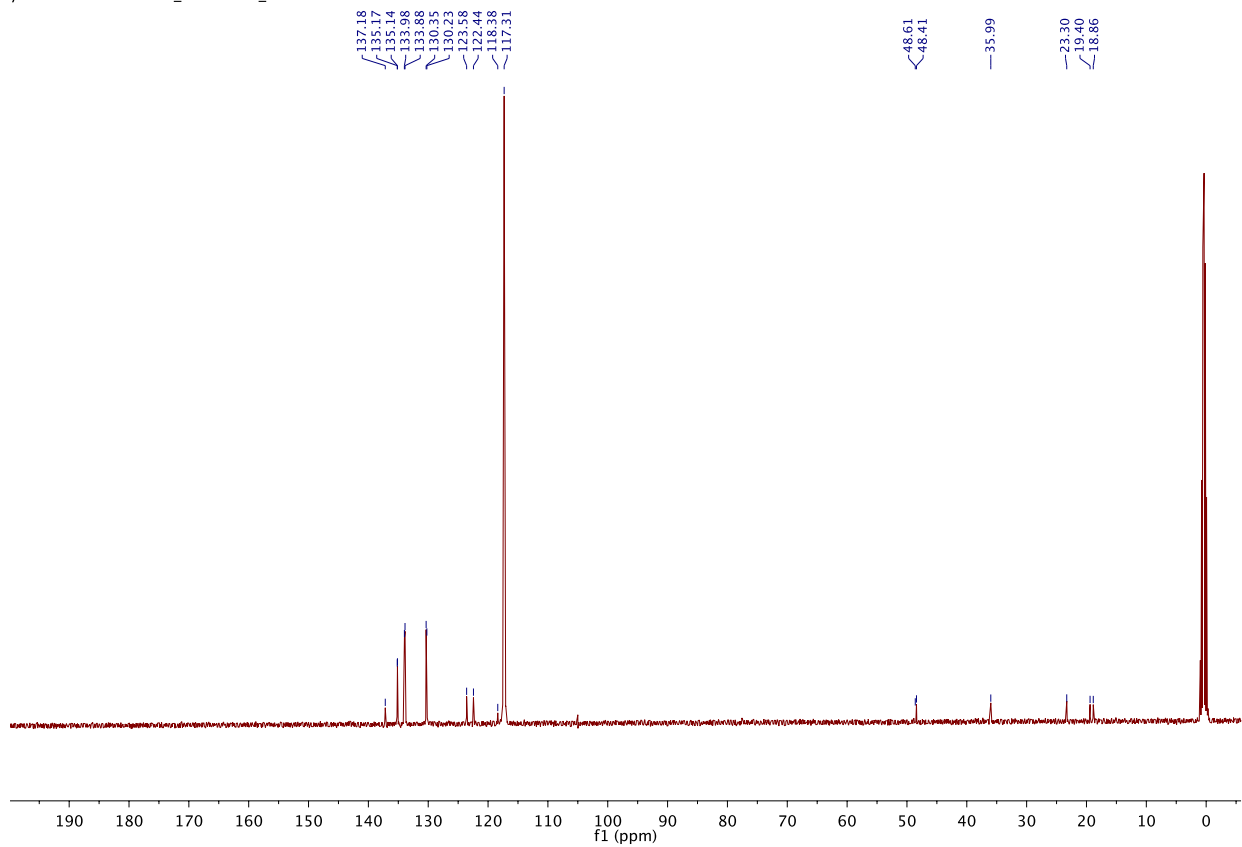
# $^1\text{H}$ NMR spectrum of [2]Br<sub>2</sub> (in CD<sub>3</sub>CN)

ycaL0058.2.fid — H1\_INT



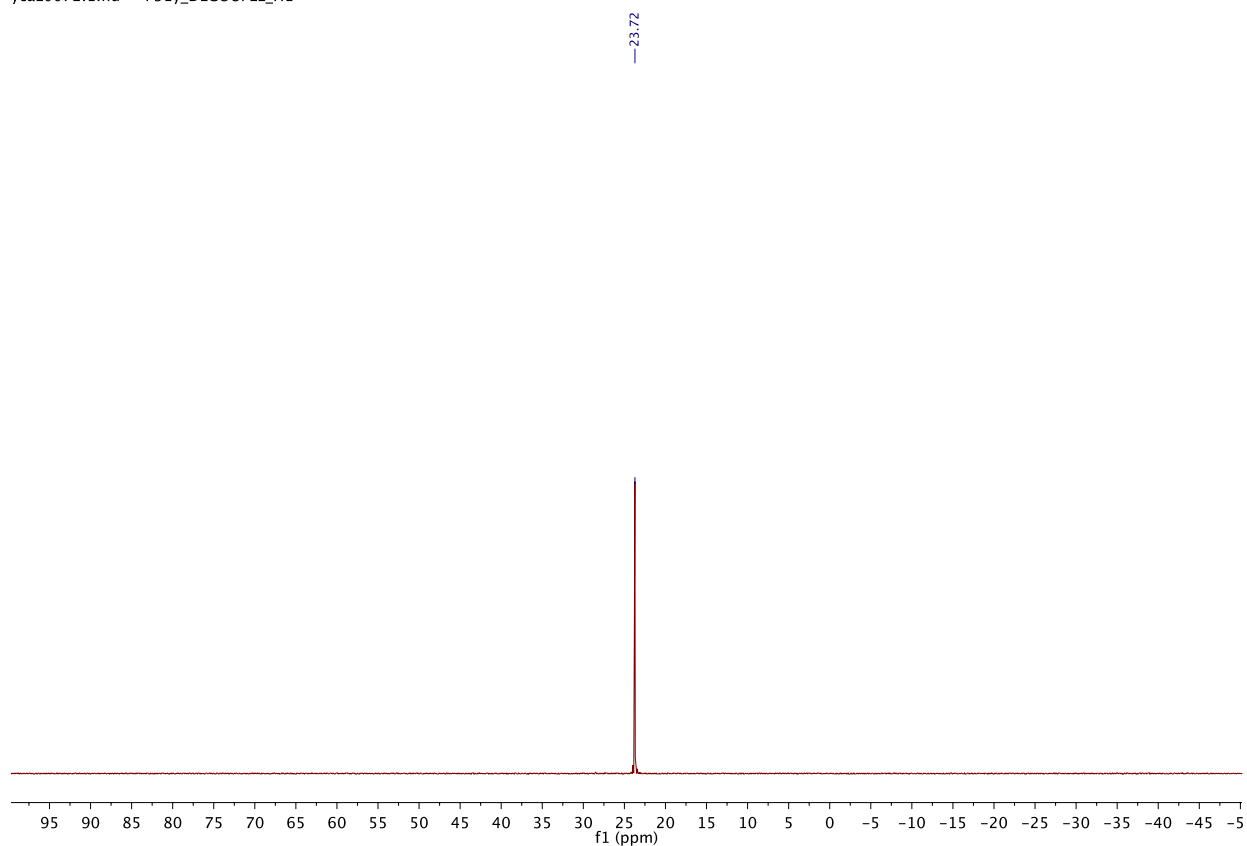
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [2]Br<sub>2</sub> (in CD<sub>3</sub>CN)

ycaL0058.3.fid — C13\_DECOUPLE\_H1



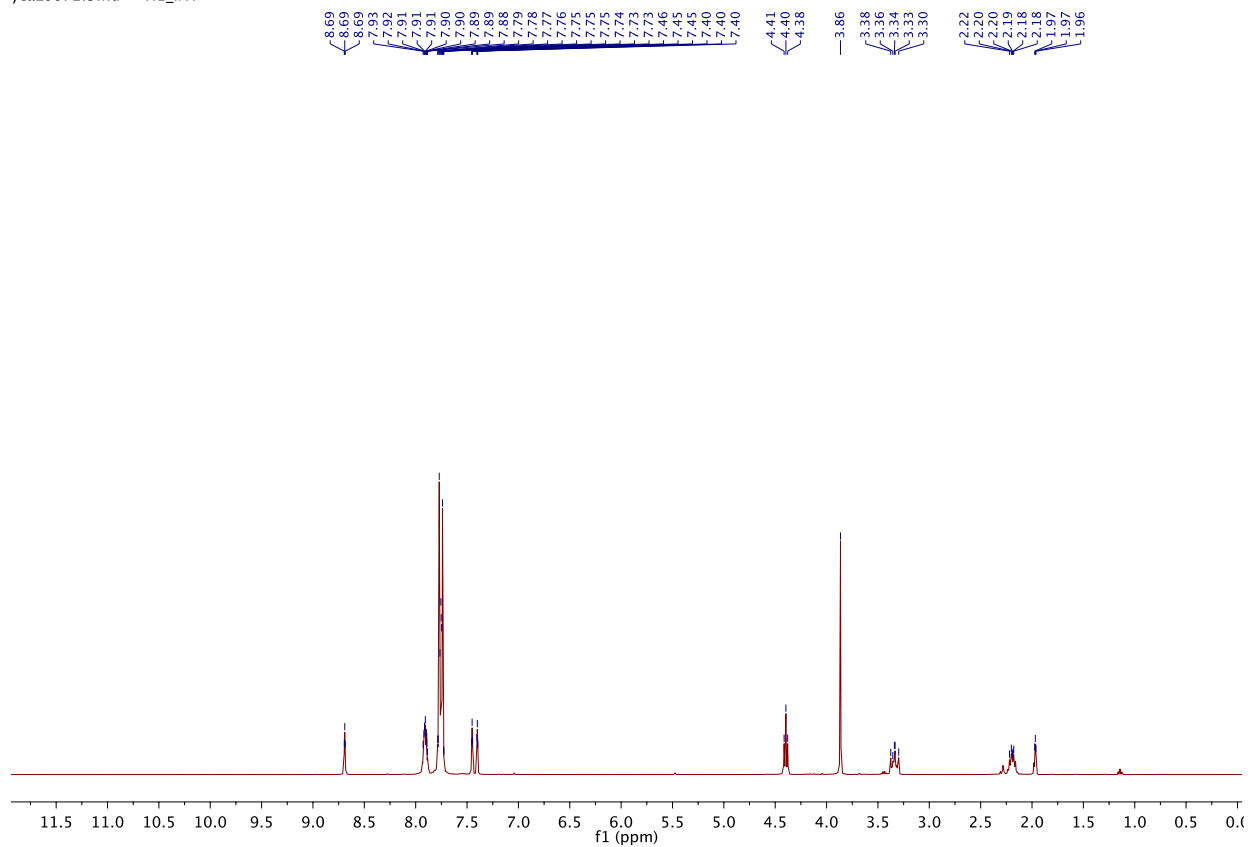
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[2](\text{OTf})_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0072.1.fid — P31y\_DECOUPLE\_H1



# $^1\text{H}$ NMR spectrum of $[2](\text{OTf})_2$ (in $\text{CD}_3\text{CN}$ )

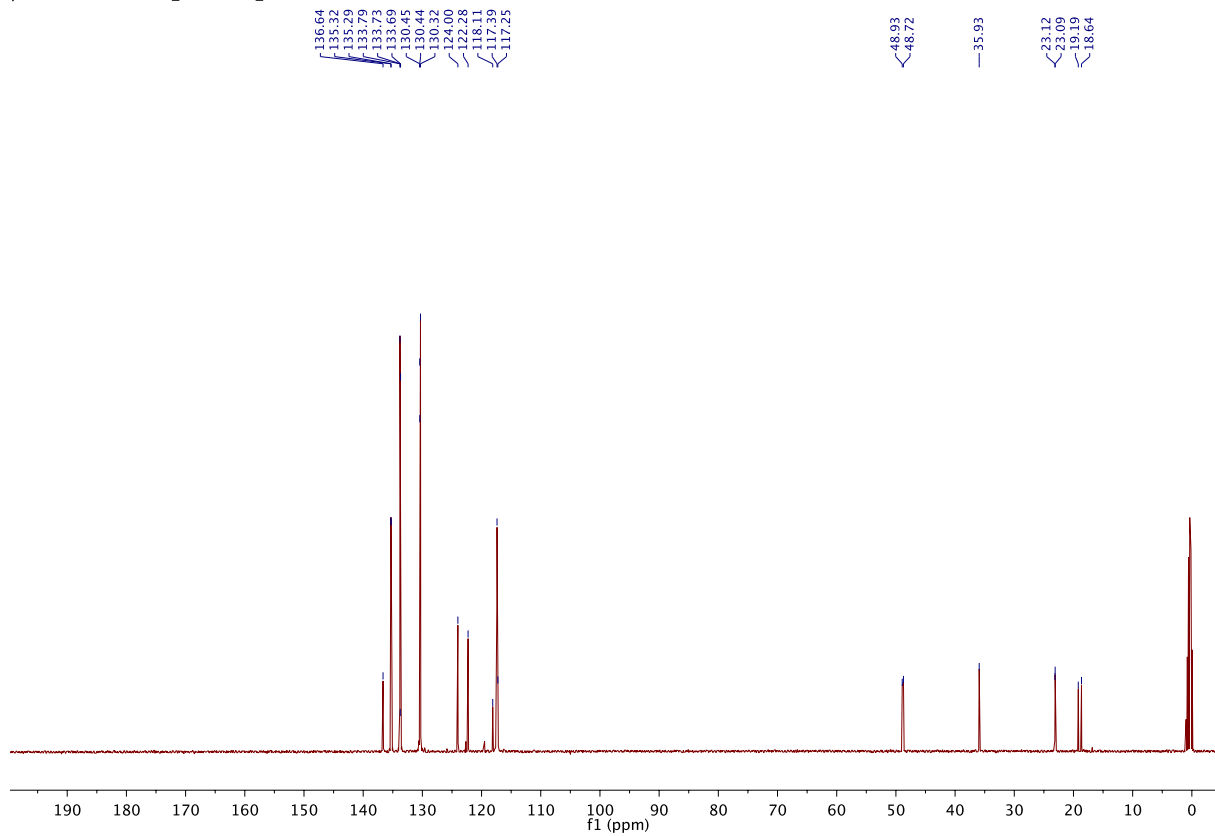
ycaL0072.5.fid — H1\_INT





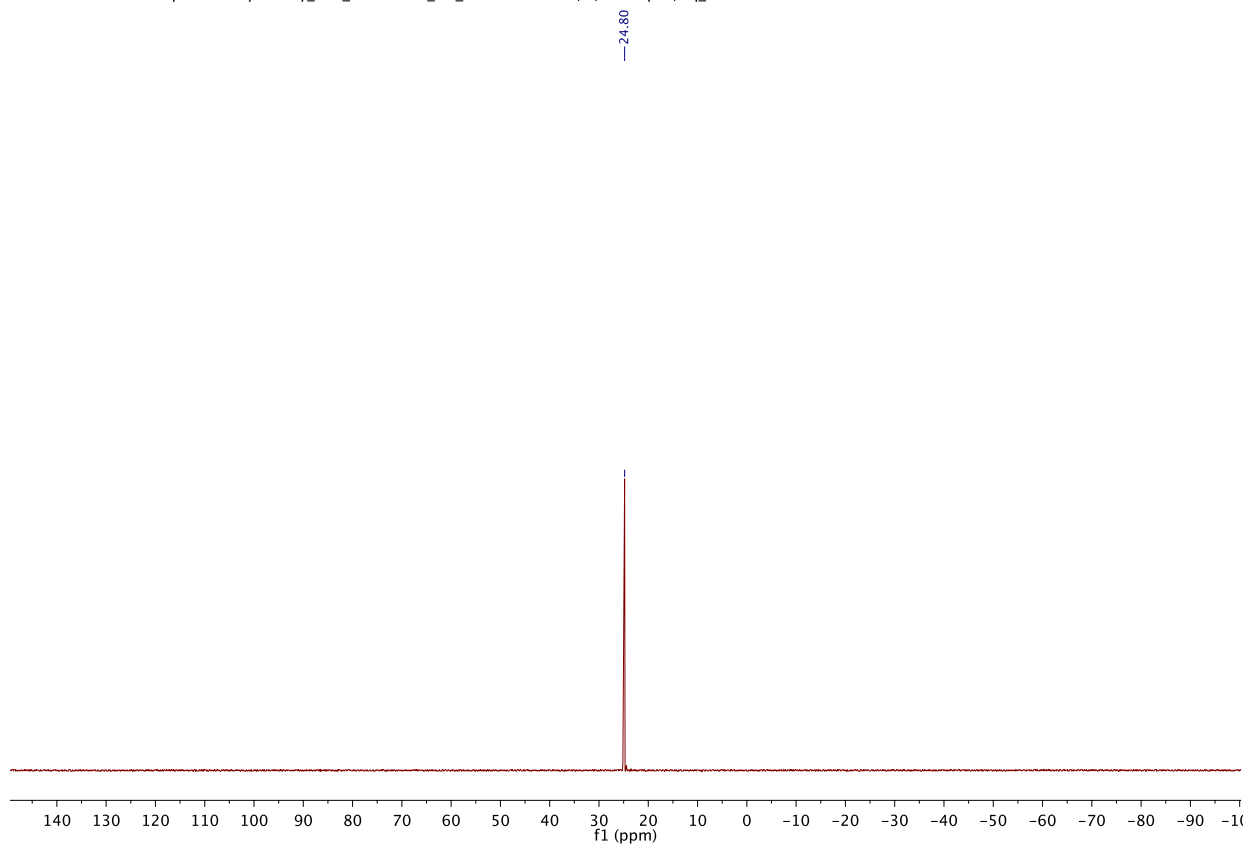
### $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[2](\text{OTf})_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0072.2.fid — C13\_DECOUPLE\_H1



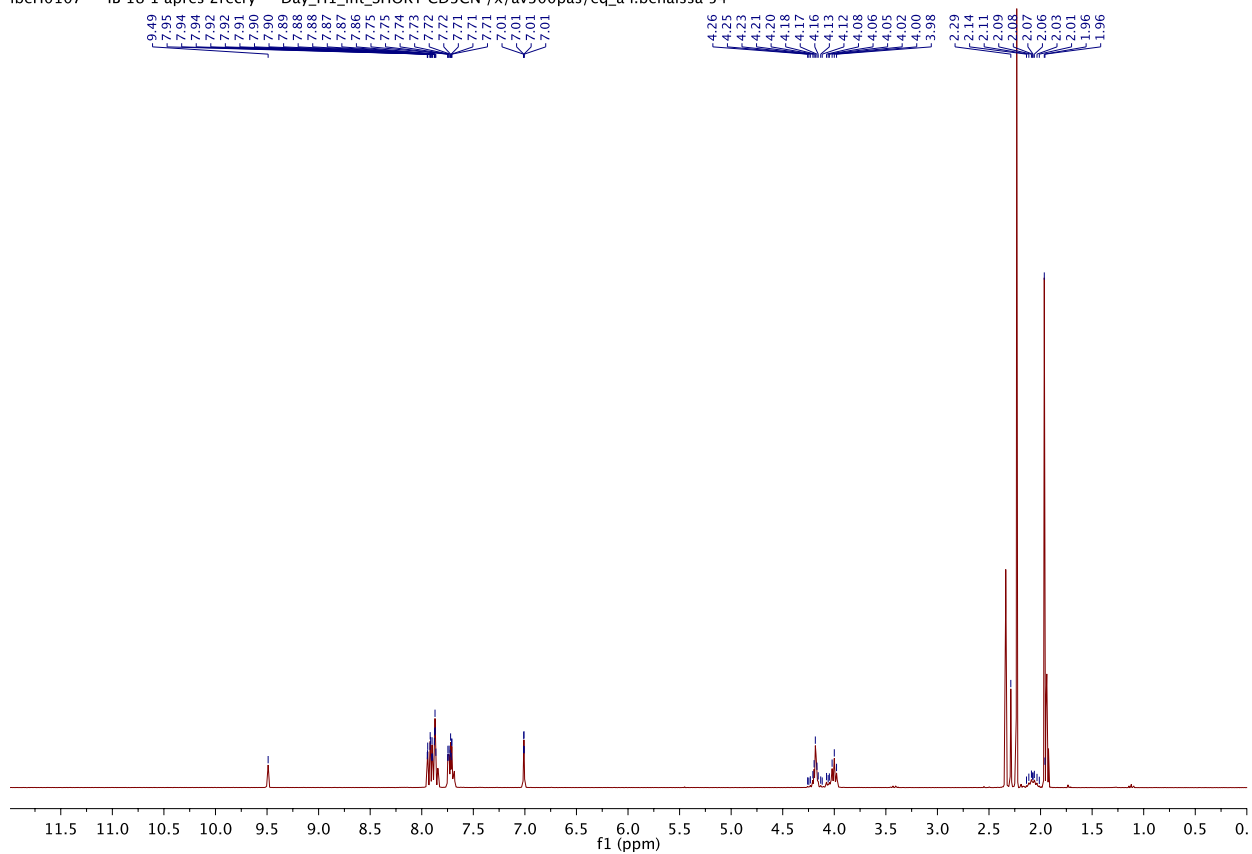
### $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[3]\text{Br}_2$ (in $\text{CD}_3\text{CN}$ )

ibeH0107 — IB 18 1 apres 2recry — Day\_P31\_DECOUPLE\_H1\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 54 —



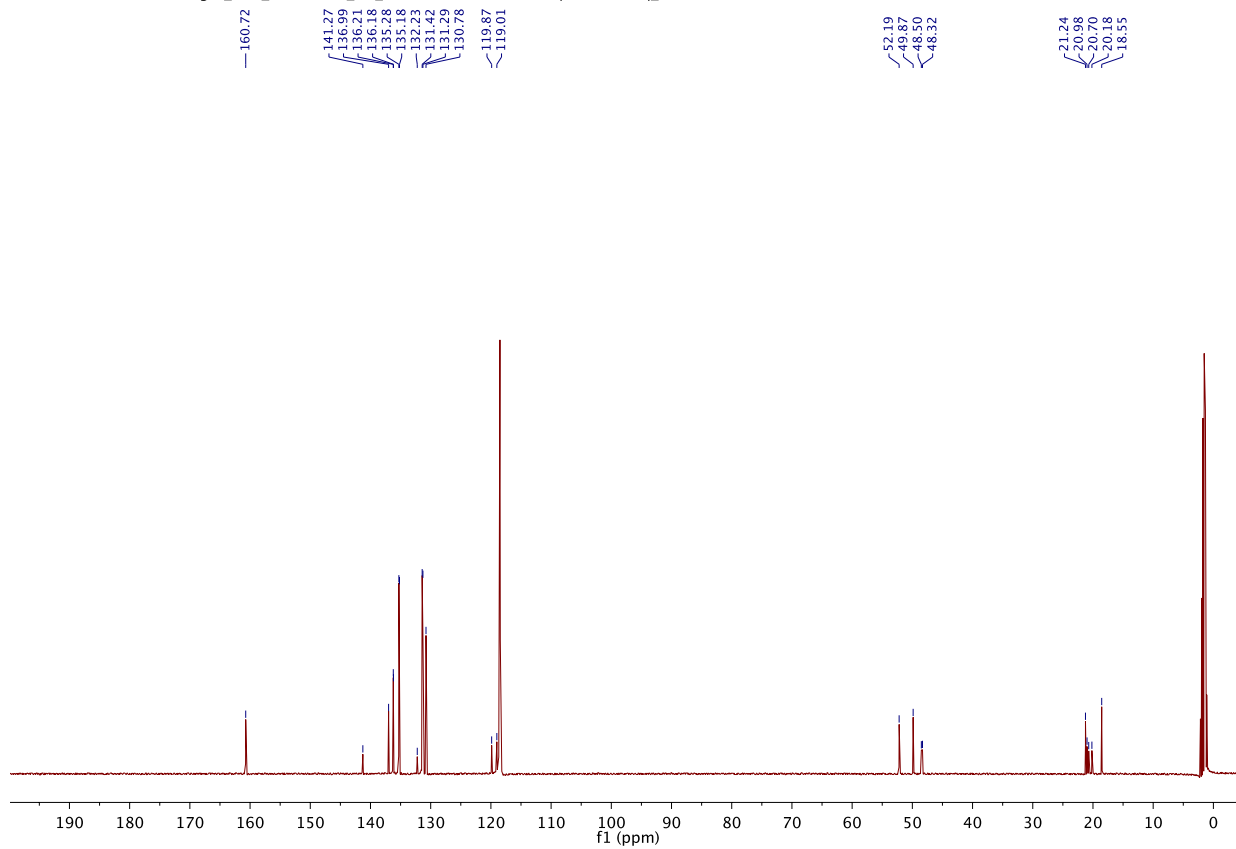
# $^1\text{H}$ NMR spectrum of [3]Br<sub>2</sub> (in CD<sub>3</sub>CN)

ibeH0107 — IB 18 1 apres 2recry — Day\_H1\_int\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 54 —



# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [3]Br<sub>2</sub> (in CD<sub>3</sub>CN)

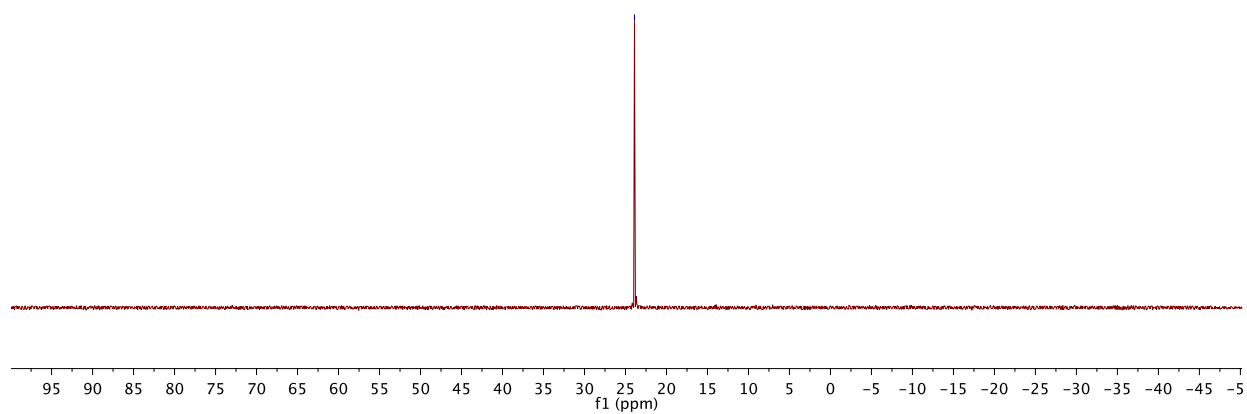
ibeG0039 — IB 18 1 — Night\_C13\_DECOUPLE\_H1\_LONG CD3CN /x/av400pas/data/eq\_a/nmr i.benaissa 6 —



# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\mathbf{3}](\text{OTf})_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0068.1.fid — P31y\_DECOUPLE\_H1

—23.91

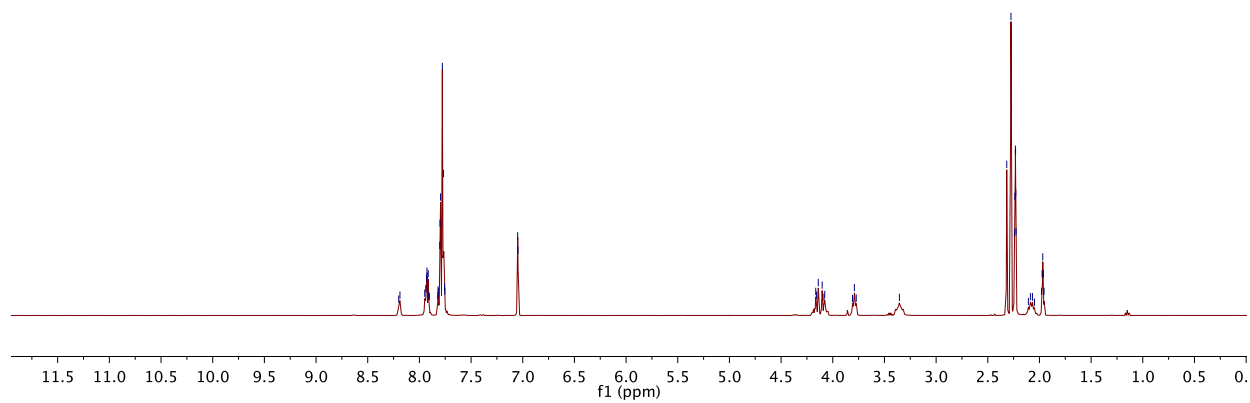


# $^1\text{H}$ NMR spectrum of $[\mathbf{3}](\text{OTf})_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0068.2.fid — H1\_INT

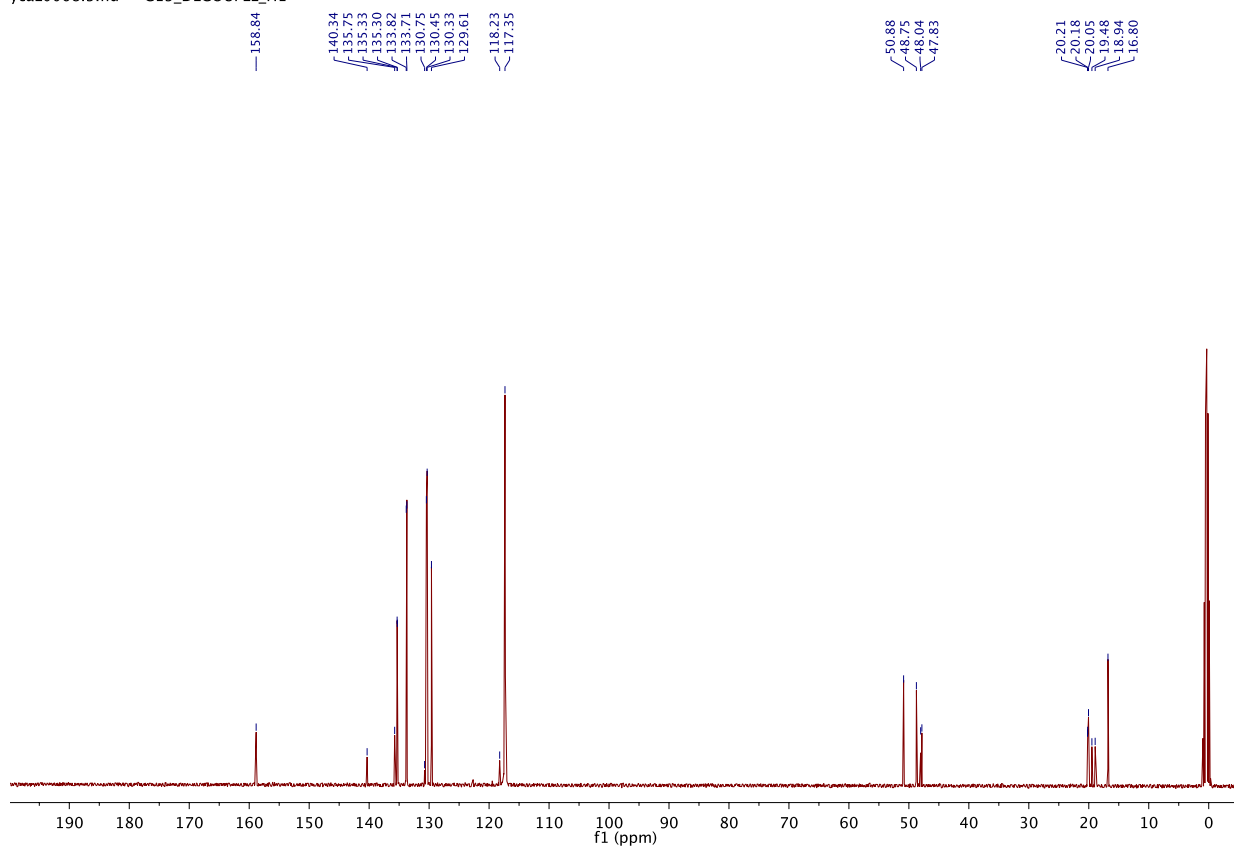
8.20  
7.95  
7.94  
7.93  
7.93  
7.91  
7.90  
7.82  
7.82  
7.80  
7.80  
7.78  
7.77  
7.76  
7.75  
7.05

4.16  
4.16  
4.14  
4.10  
4.09  
4.08  
3.81  
3.79  
3.77  
3.76  
3.32  
2.28  
2.24  
2.24  
2.23  
2.23  
2.23  
2.23  
2.11  
2.09  
2.07  
2.07  
2.05  
1.98  
1.97  
1.96  
1.96



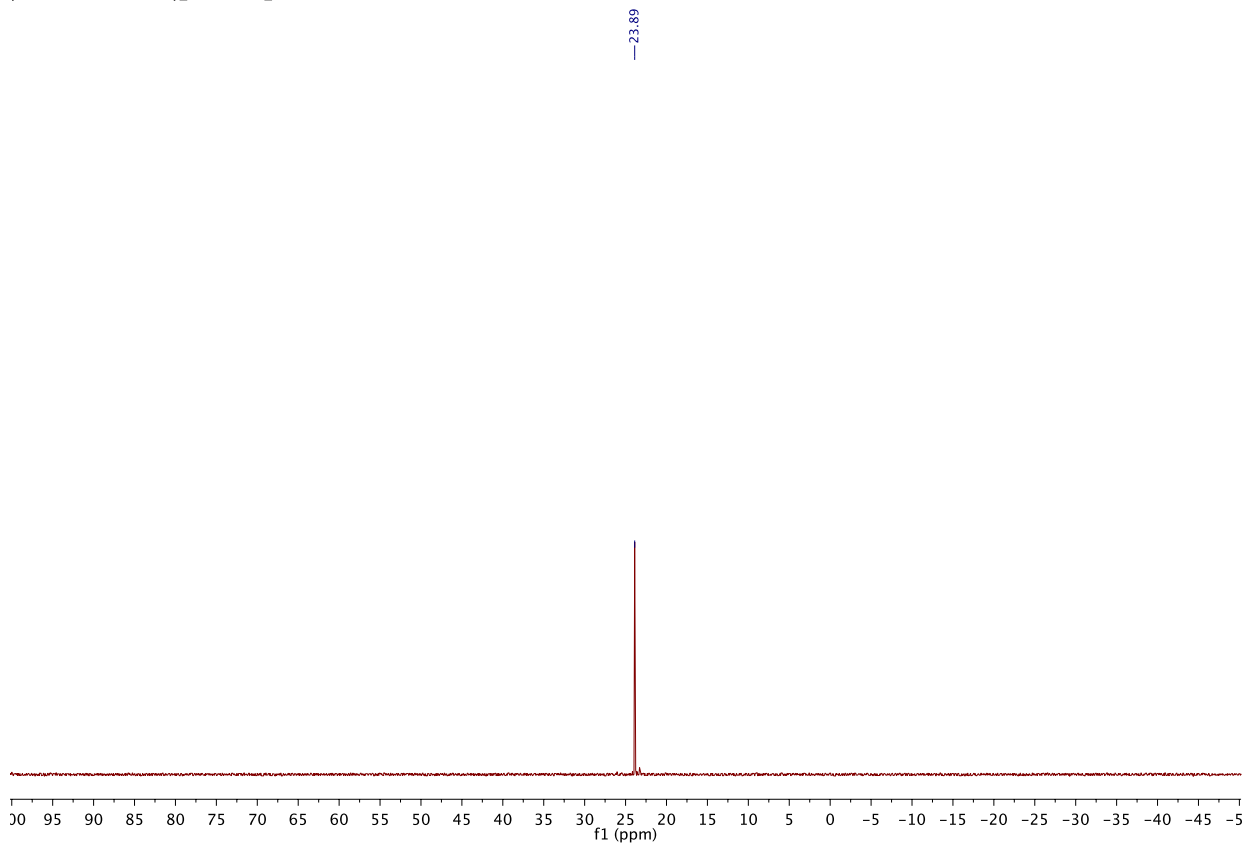
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\mathbf{3}](\text{OTf})_2$ (in $\text{CD}_3\text{CN}$ )

ycaL0068.3.fid — C13\_DECOUPLE\_H1



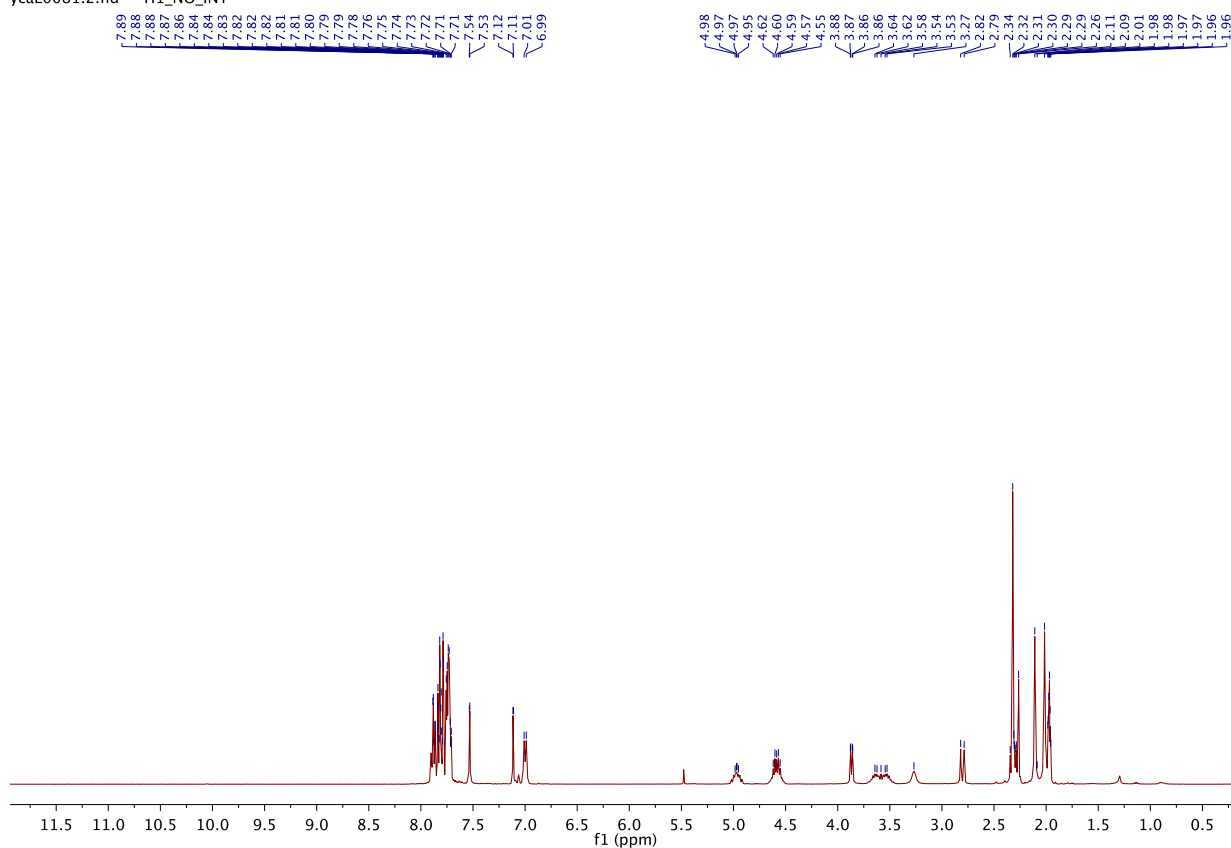
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\mathbf{5}]\text{Br}$ (in $\text{CD}_3\text{CN}$ )

ycaL0081.1.fid — P31y\_DECOUPLE\_H1



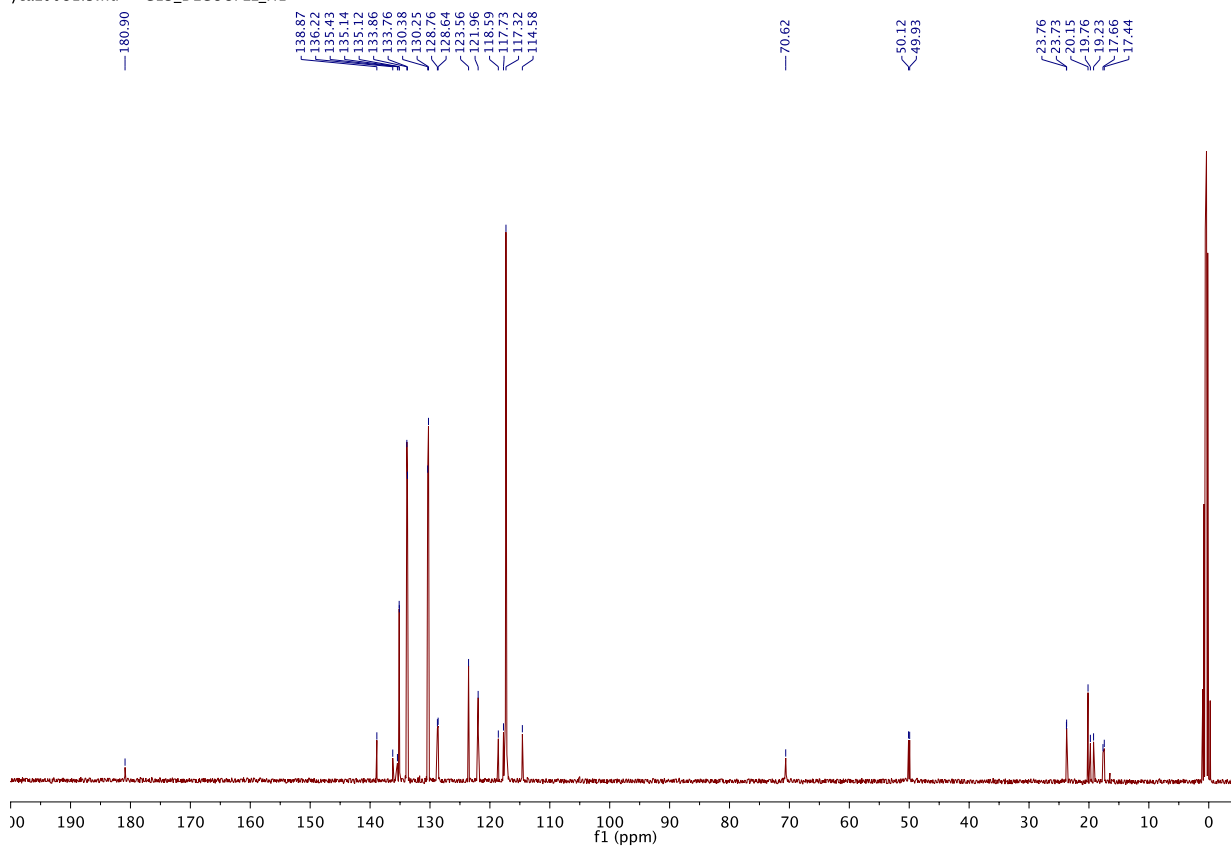
# $^1\text{H}$ NMR spectrum of [5]Br (in $\text{CD}_3\text{CN}$ )

ycaL0081.2.fid — H1\_NO\_INT



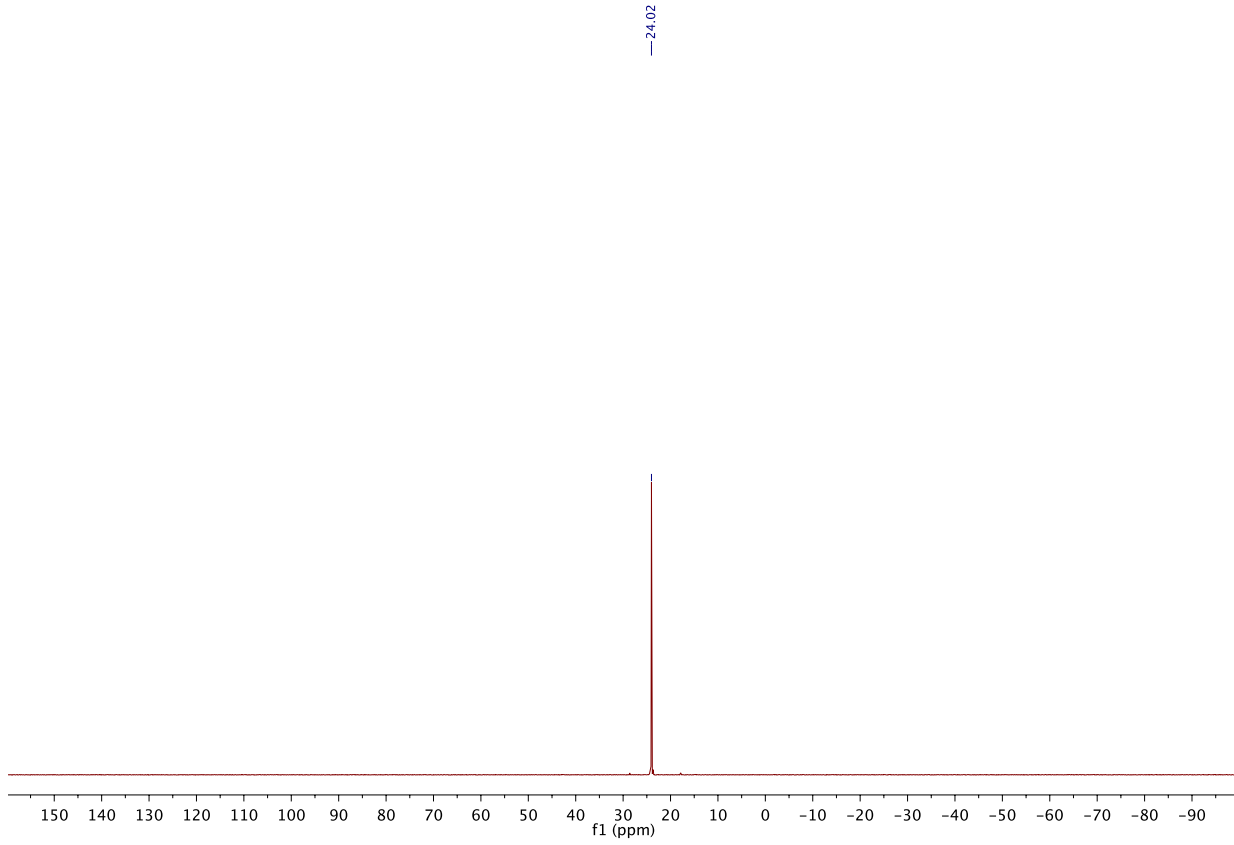
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [5]Br (in $\text{CD}_3\text{CN}$ )

ycaL0081.3.fid — C13\_DECOUPLE\_H1



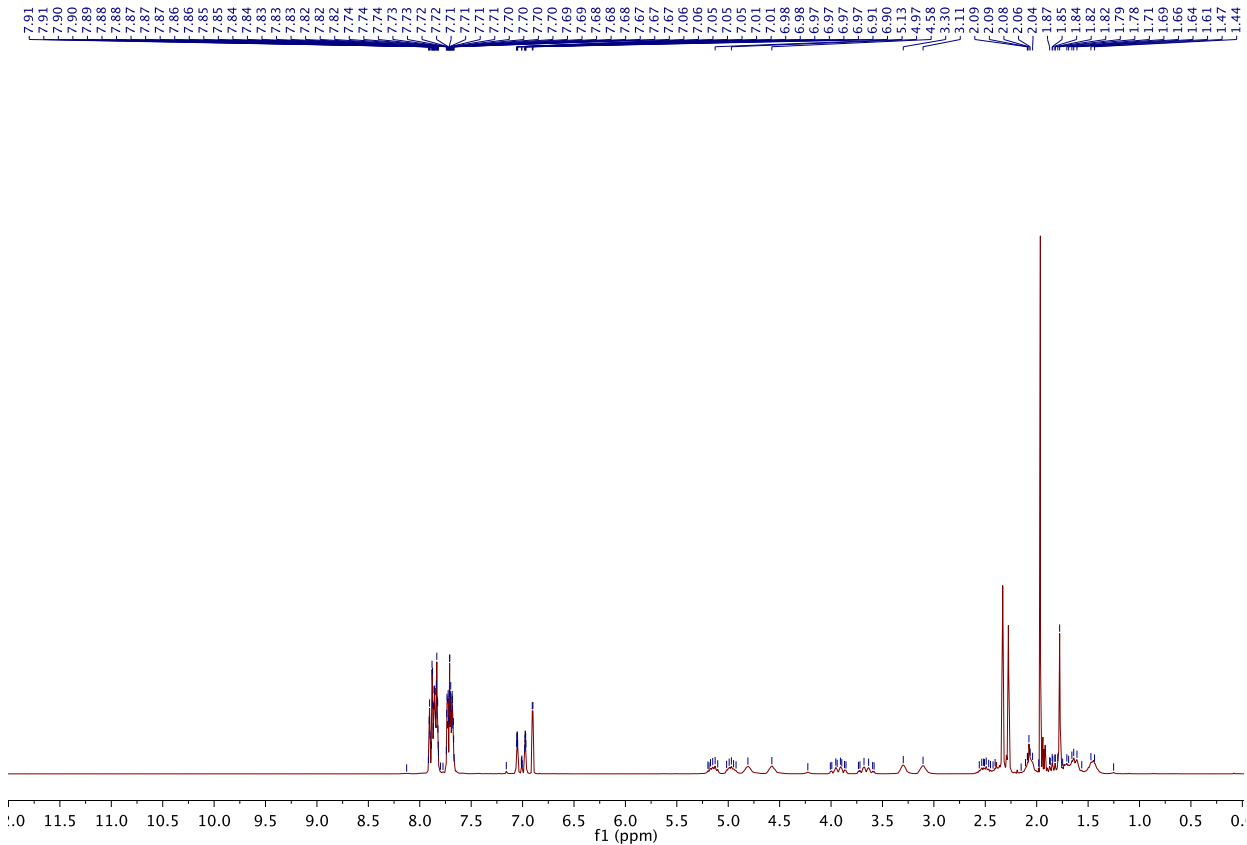
### $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [6]Br (in $\text{CD}_3\text{CN}$ )

ibeH0137 — ib 26 K2CO3 — Day\_P31\_DECOUPLE\_H1\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 6 —



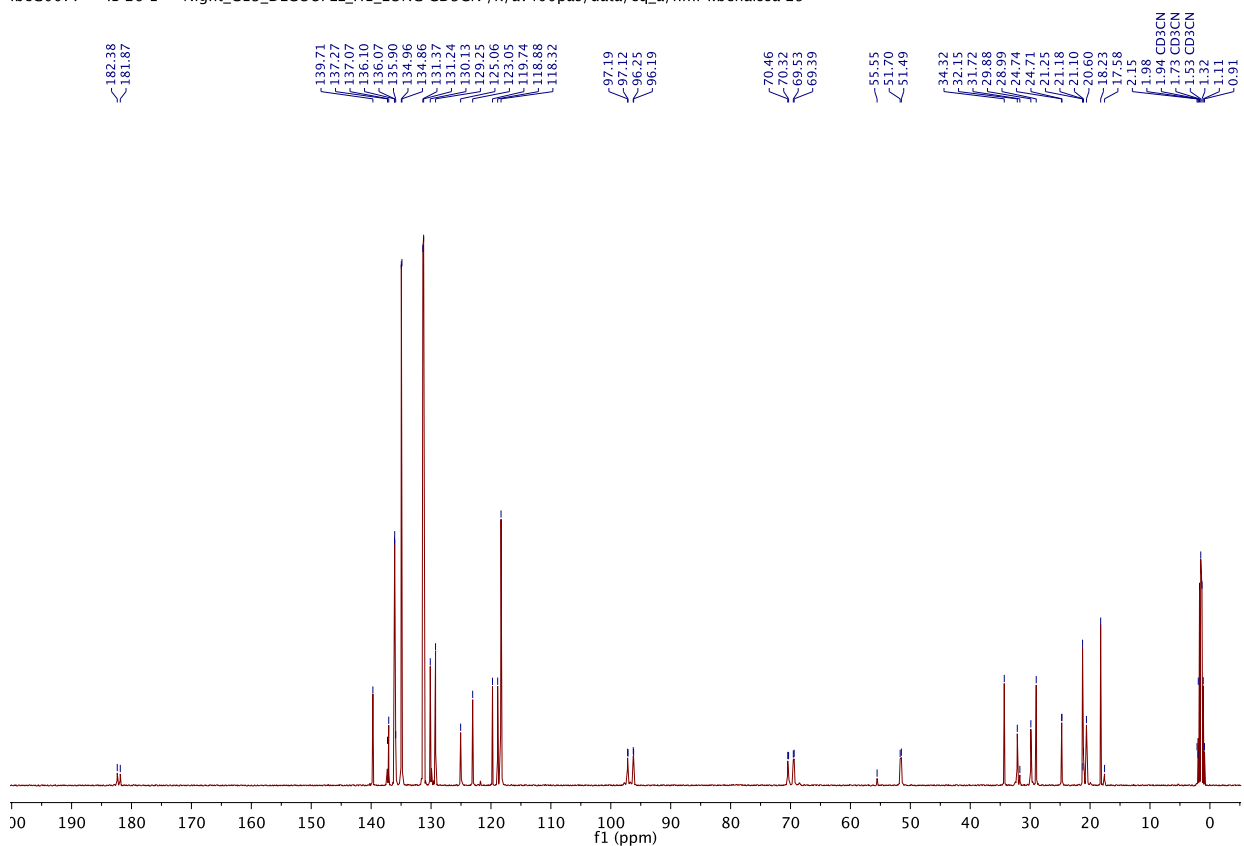
### $^1\text{H}$ NMR spectrum of [6]Br (in $\text{CD}_3\text{CN}$ )

ibeH0137 — ib 26 K2CO3 — Day\_H1\_int\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 6 —



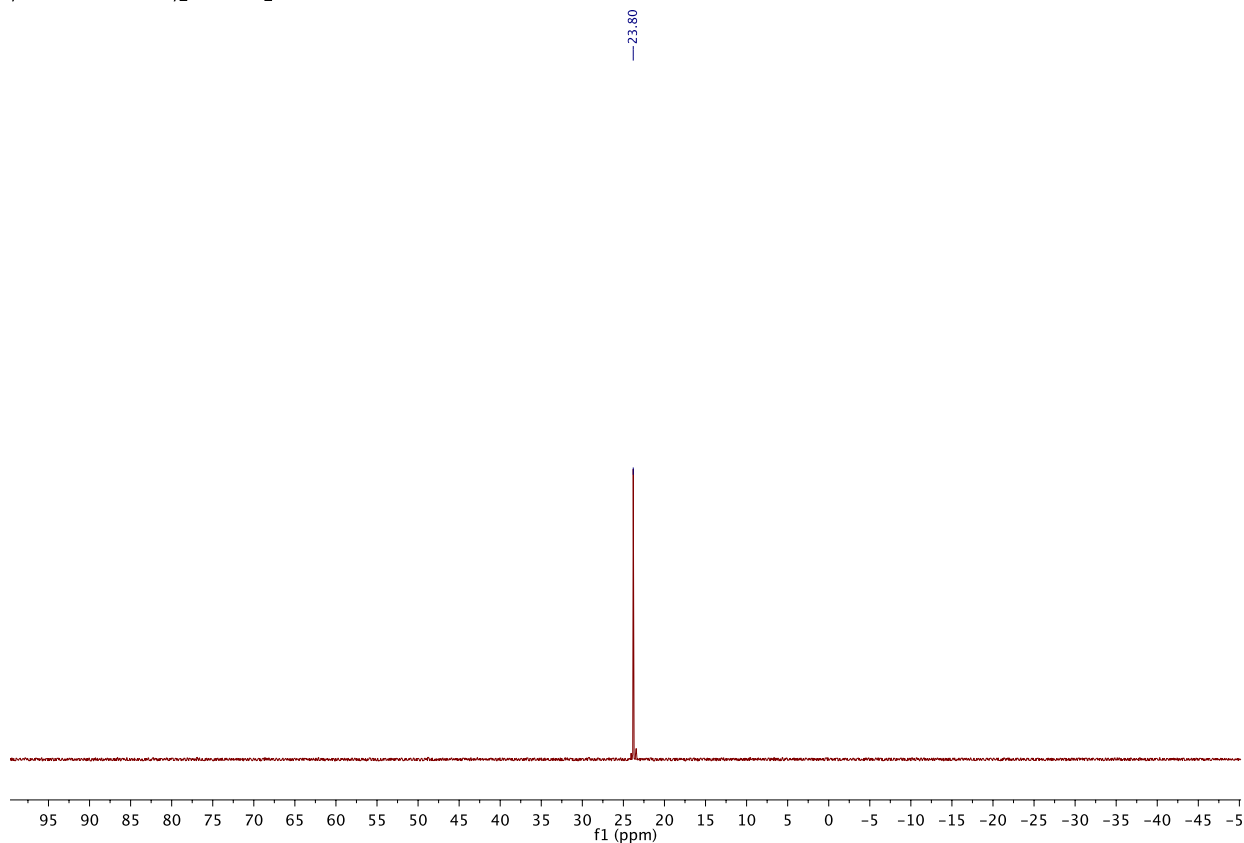
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [6]Br (in $\text{CD}_3\text{CN}$ )

ibeG0077 — IB 26 1 — Night\_C13\_DECOUPLE\_H1\_LONG CD3CN /x/av400pas/data/eq\_a/nmr i.benaissa 29 —



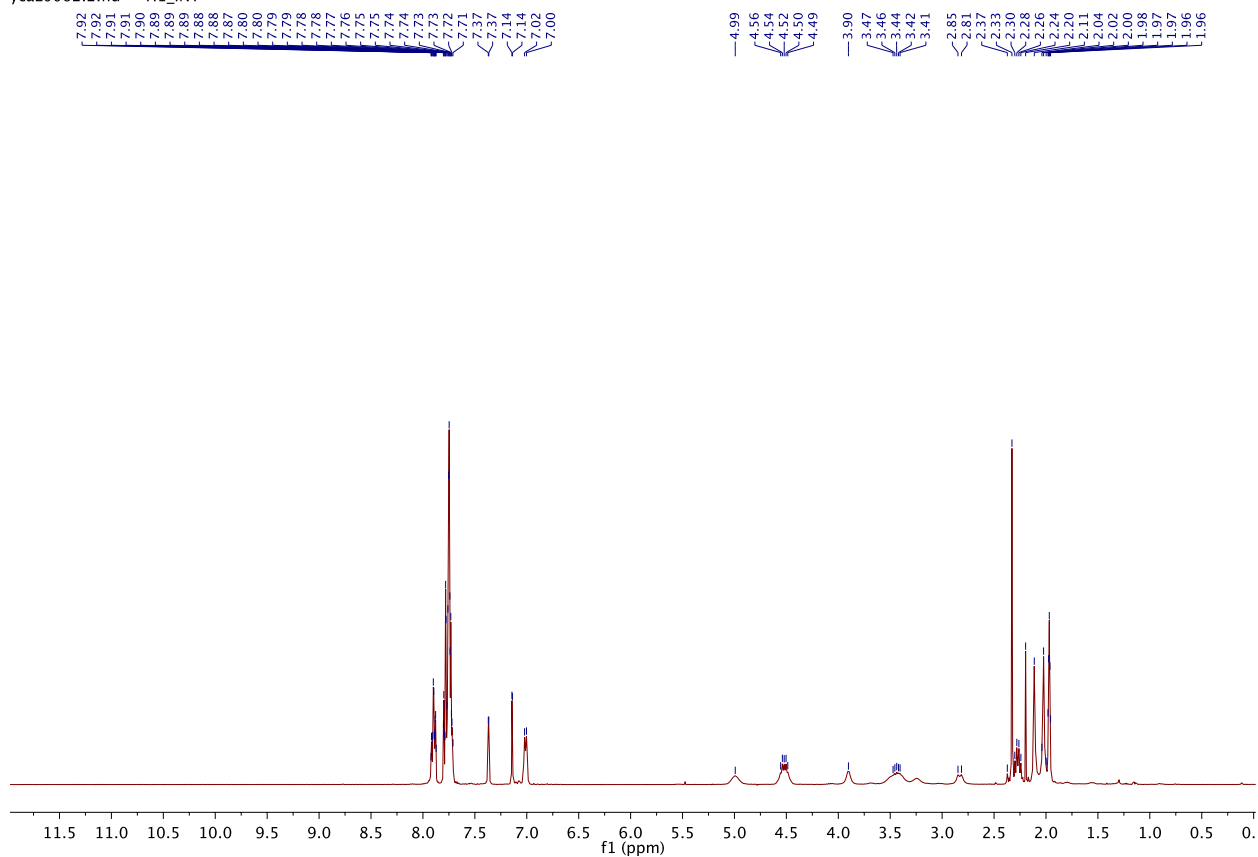
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [6](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0062.1.fid — P31y\_DECOUPLE\_H1



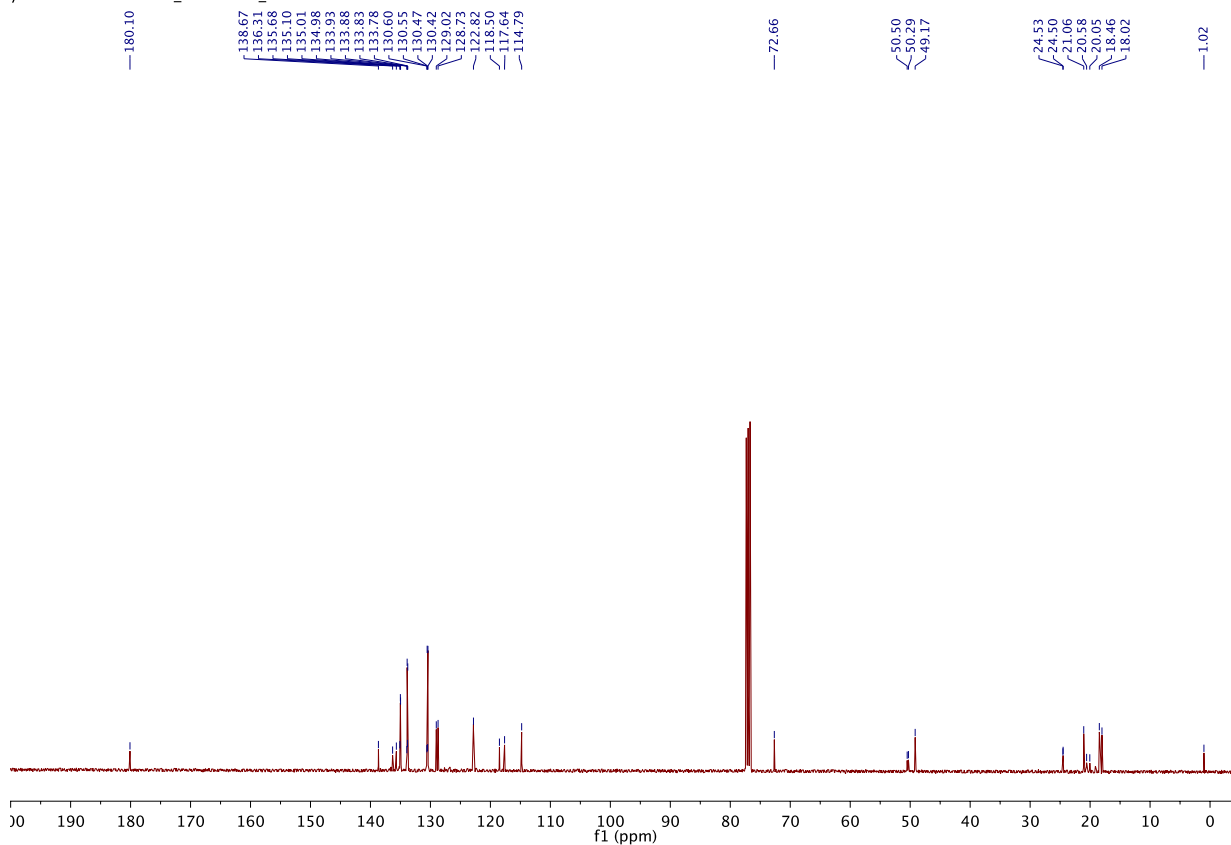
# $^1\text{H}$ NMR spectrum of [6](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0062.2.fid — H1\_INT



# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [6](OTf) (in $\text{CDCl}_3$ )

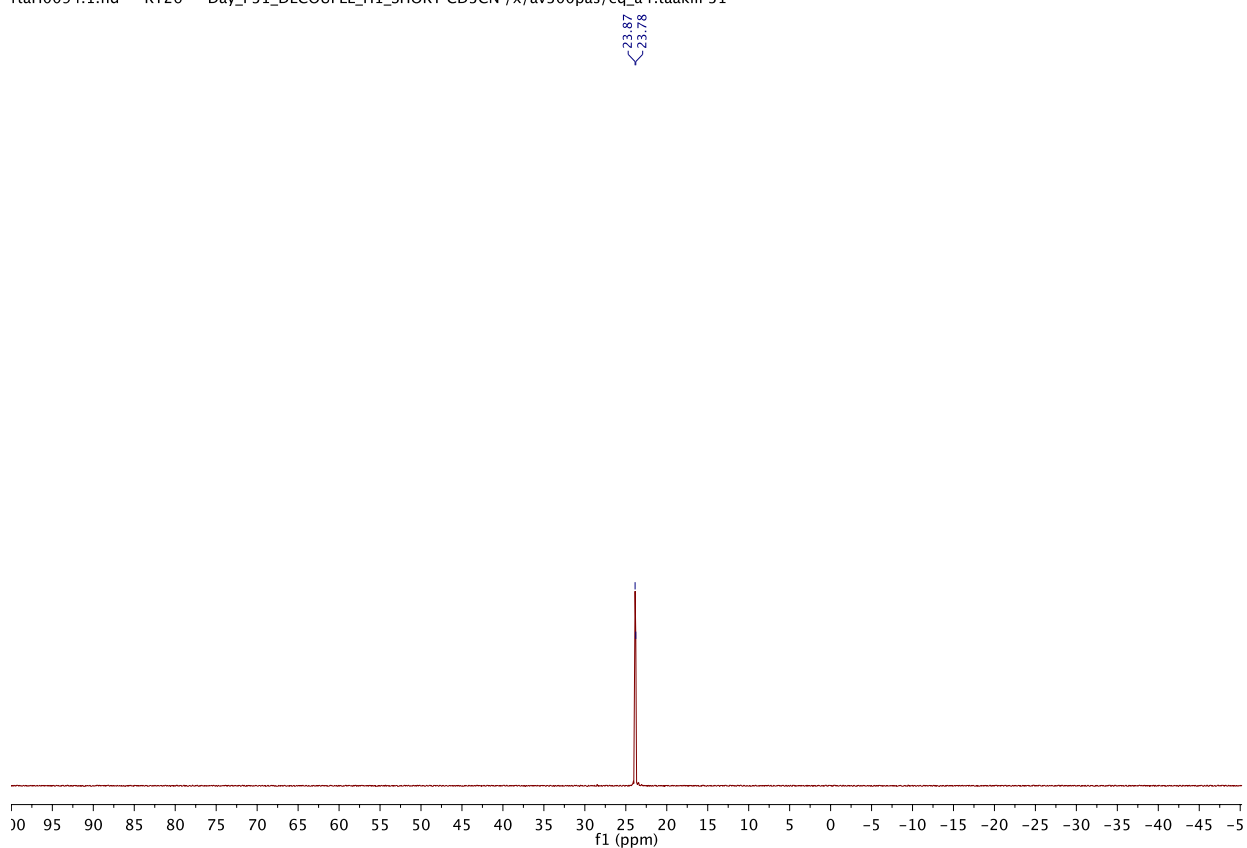
ycaL0057.3.fid — C13\_DECOUPLE\_H1





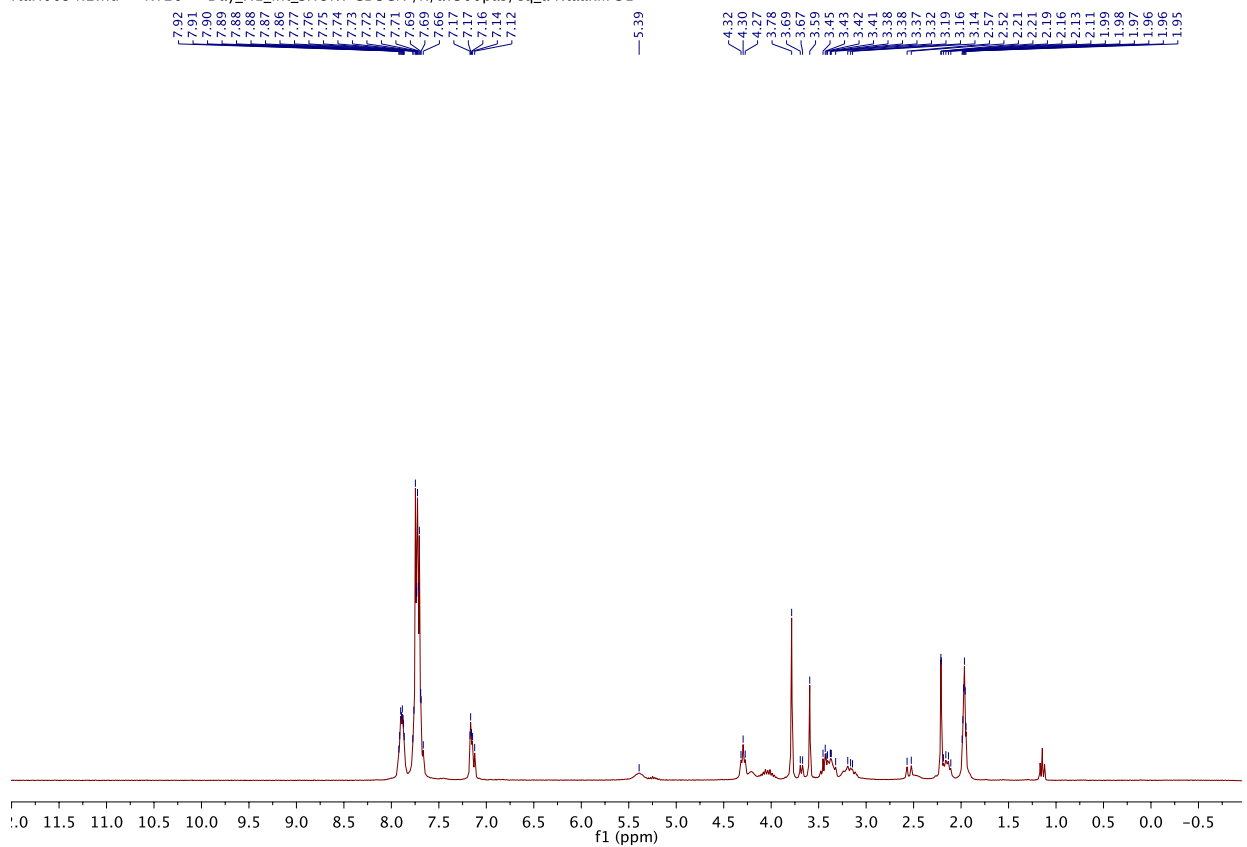
### $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [7a,b](OTf) (in $\text{CD}_3\text{CN}$ )

rtaH0094.1.fid — RT26 — Day\_P31\_DECOUPLE\_H1\_SHORT CD3CN /x/av300pas/eq\_a r.taakili 31



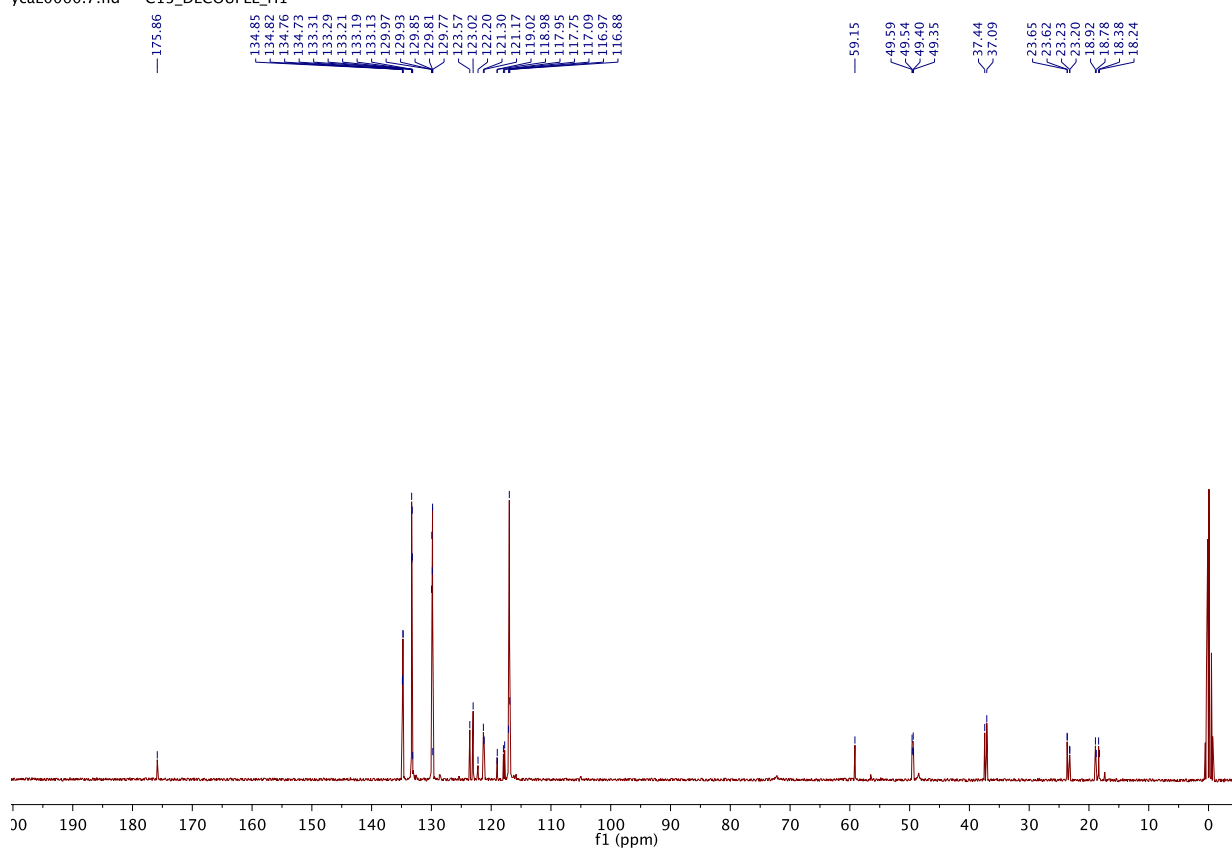
### $^1\text{H}$ NMR spectrum of [7a,b](OTf) (in $\text{CD}_3\text{CN}$ )

rtaH0094.2.fid — RT26 — Day\_H1\_int\_SHORT CD3CN /x/av300pas/eq\_a r.taakili 31



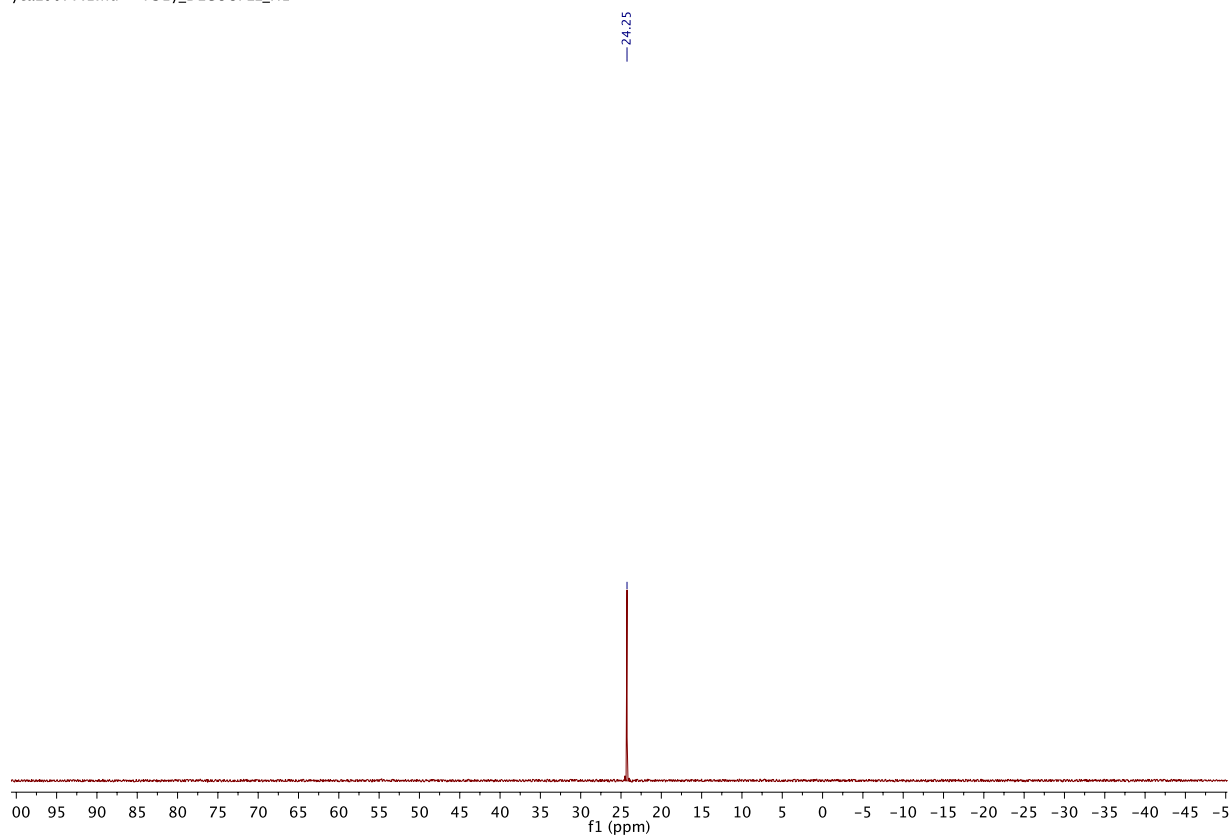
### $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [7a,b](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0060.7.fid — C13\_DECOUPLE\_H1



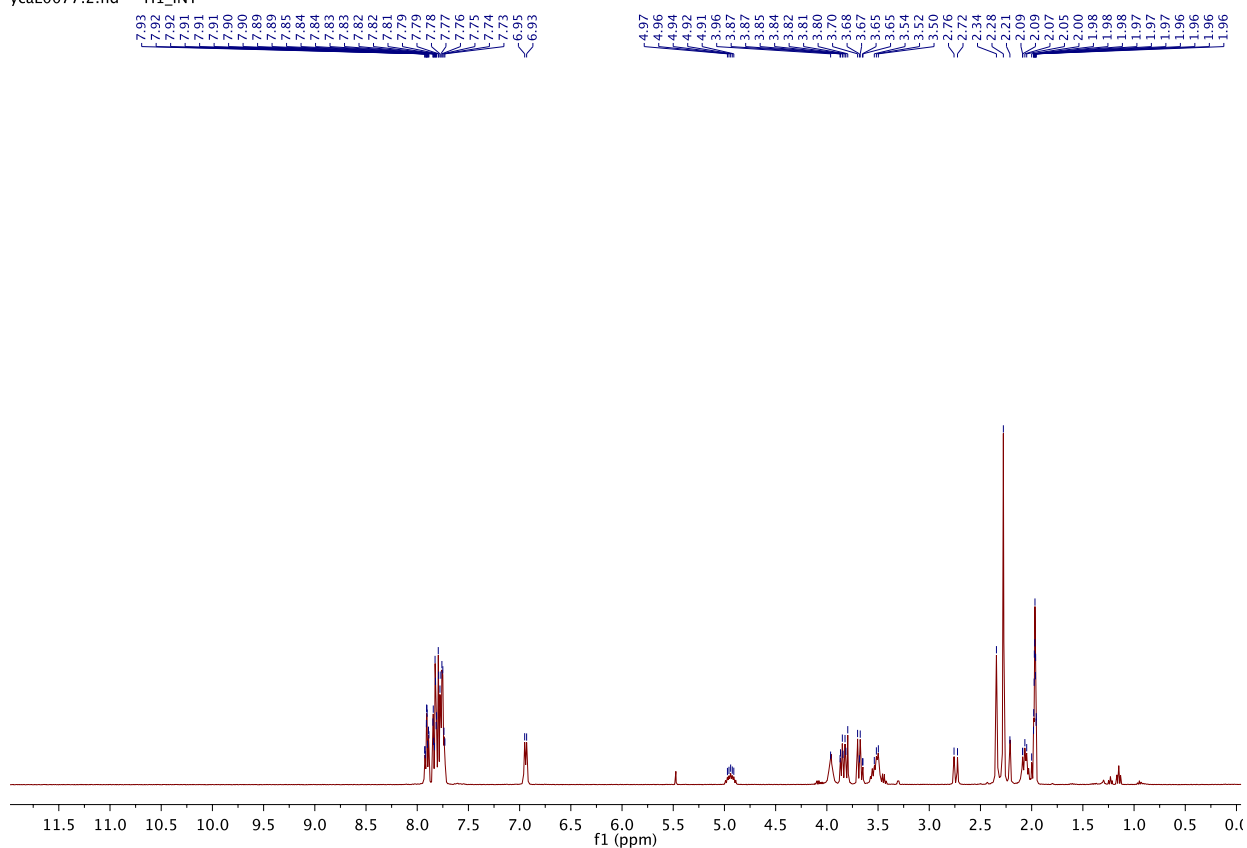
### $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [8](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0077.1.fid — P31y\_DECOUPLE\_H1



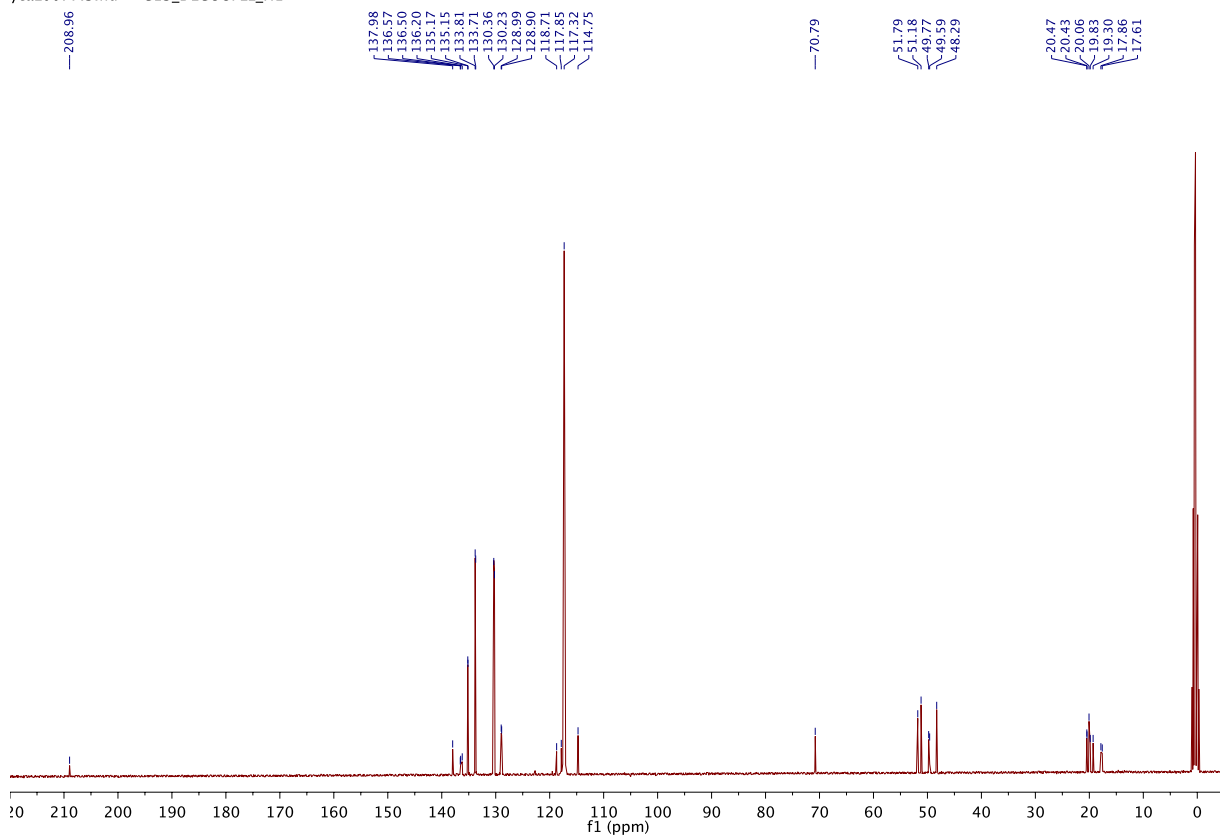
# $^1\text{H}$ NMR spectrum of [8](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0077.2.fid — H1\_INT



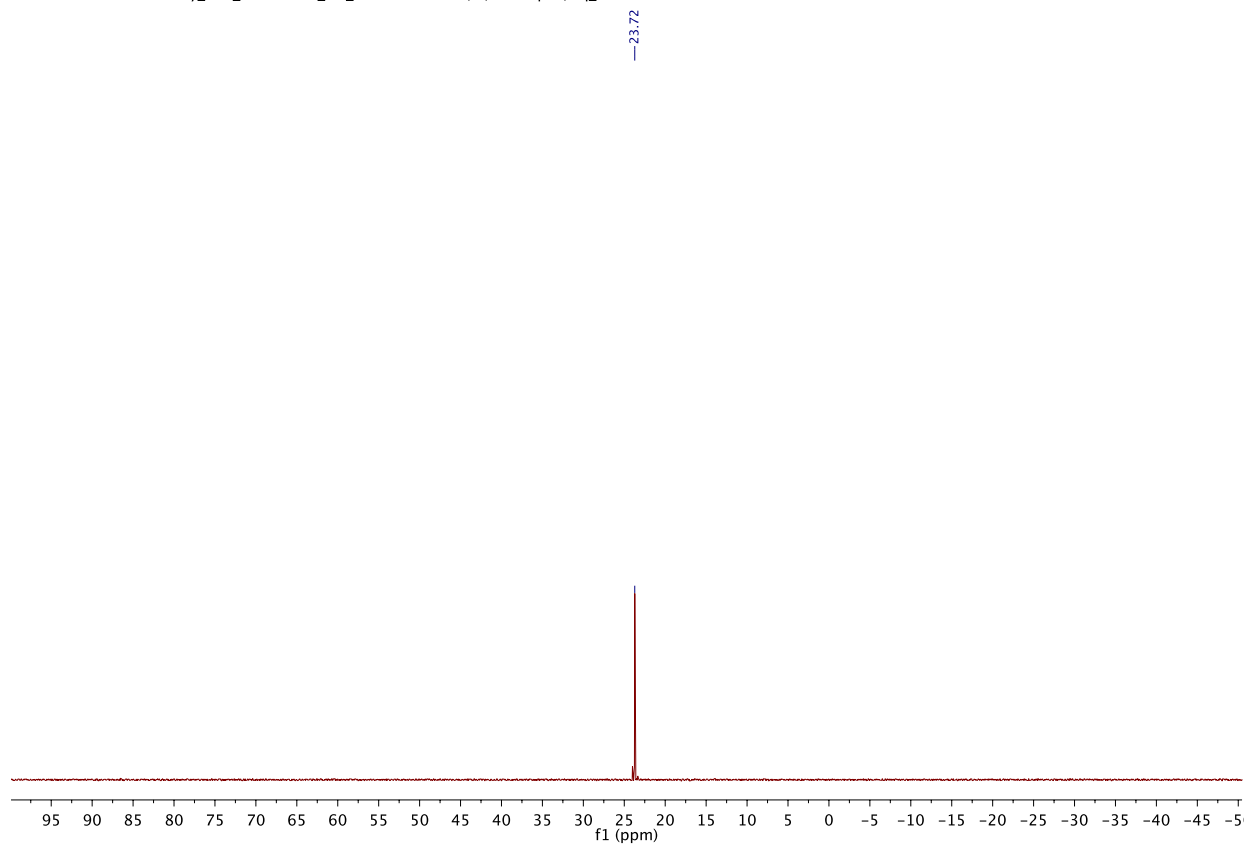
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [8](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0077.3.fid — C13\_DECOUPLE\_H1



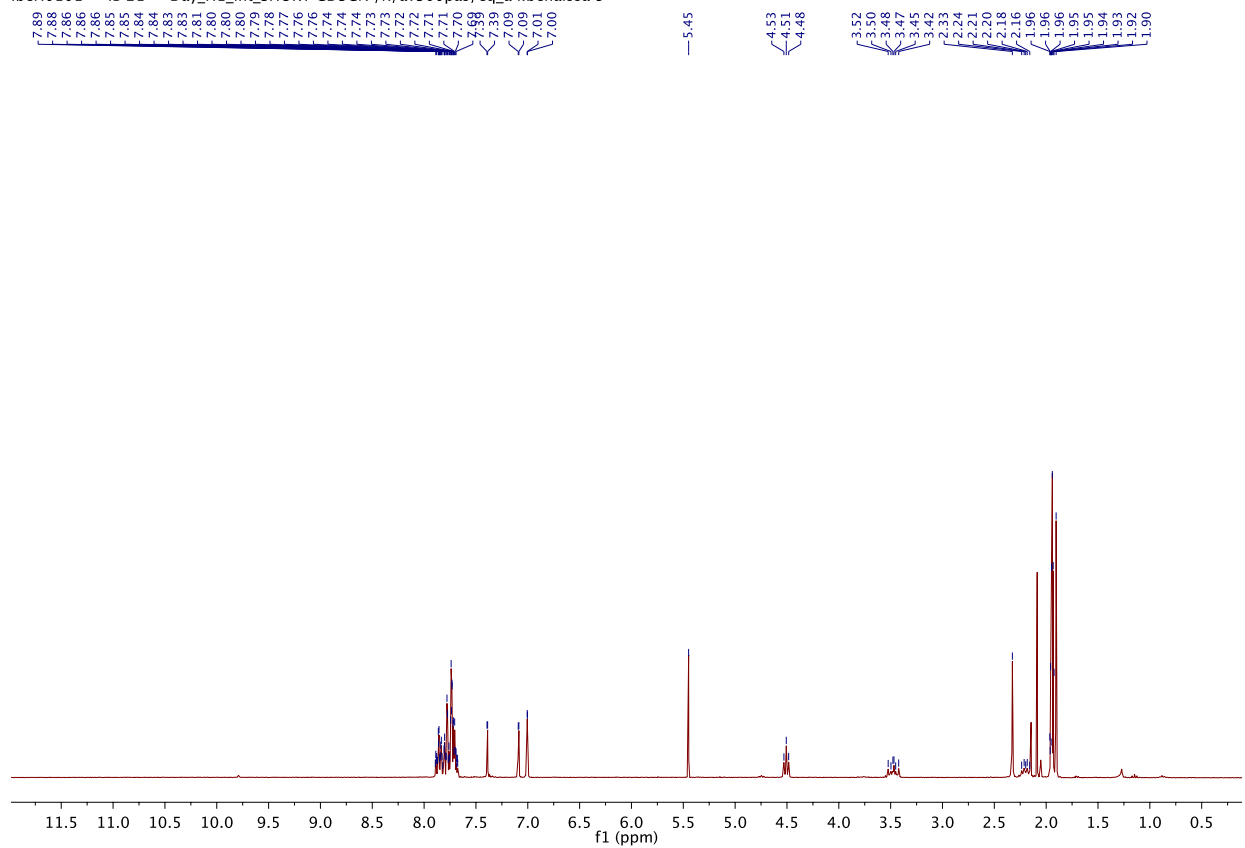
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [9] (in $\text{CD}_3\text{CN}$ )

ibeH0101 — IB 21 — Day\_P31\_DECOUPLE\_H1\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 5 —



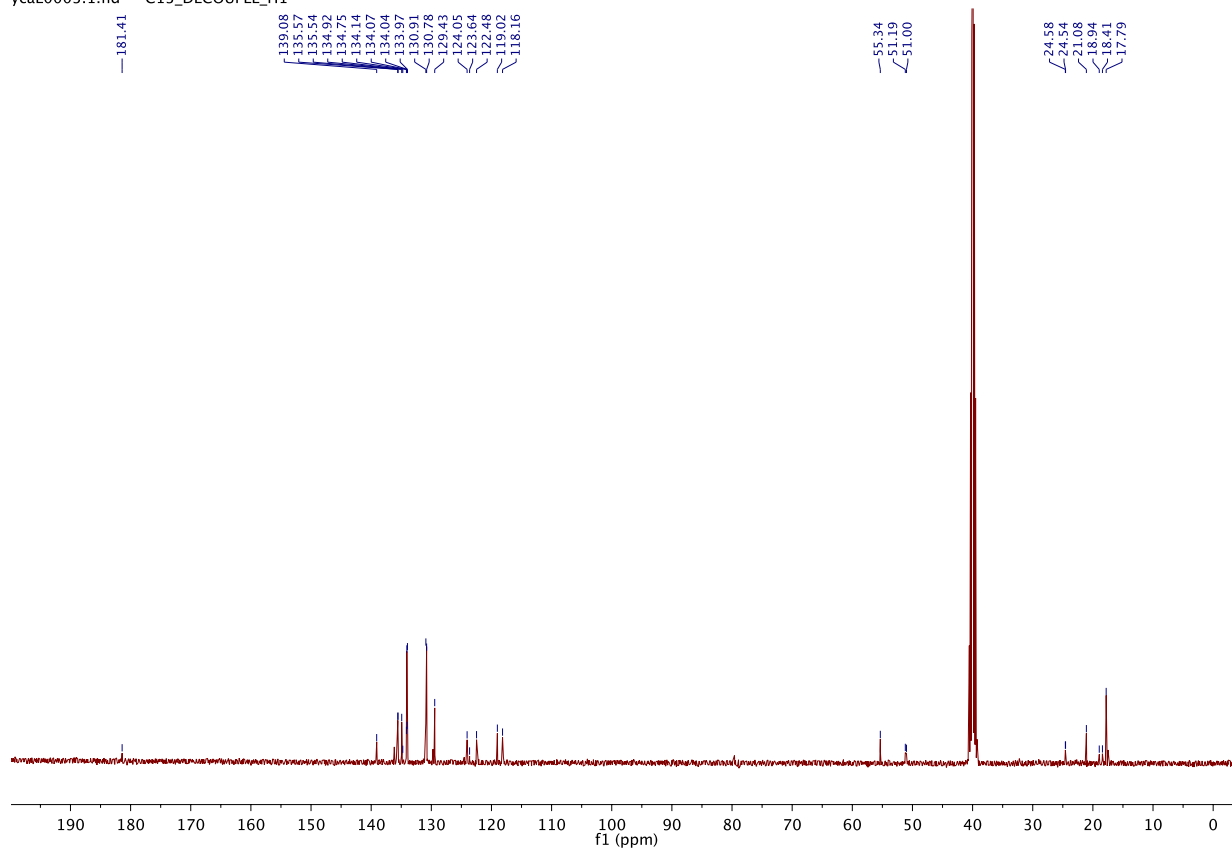
# $^1\text{H}$ NMR spectrum of [9] (in $\text{CD}_3\text{CN}$ )

ibeH0101 — IB 21 — Day\_H1\_int\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 5 —



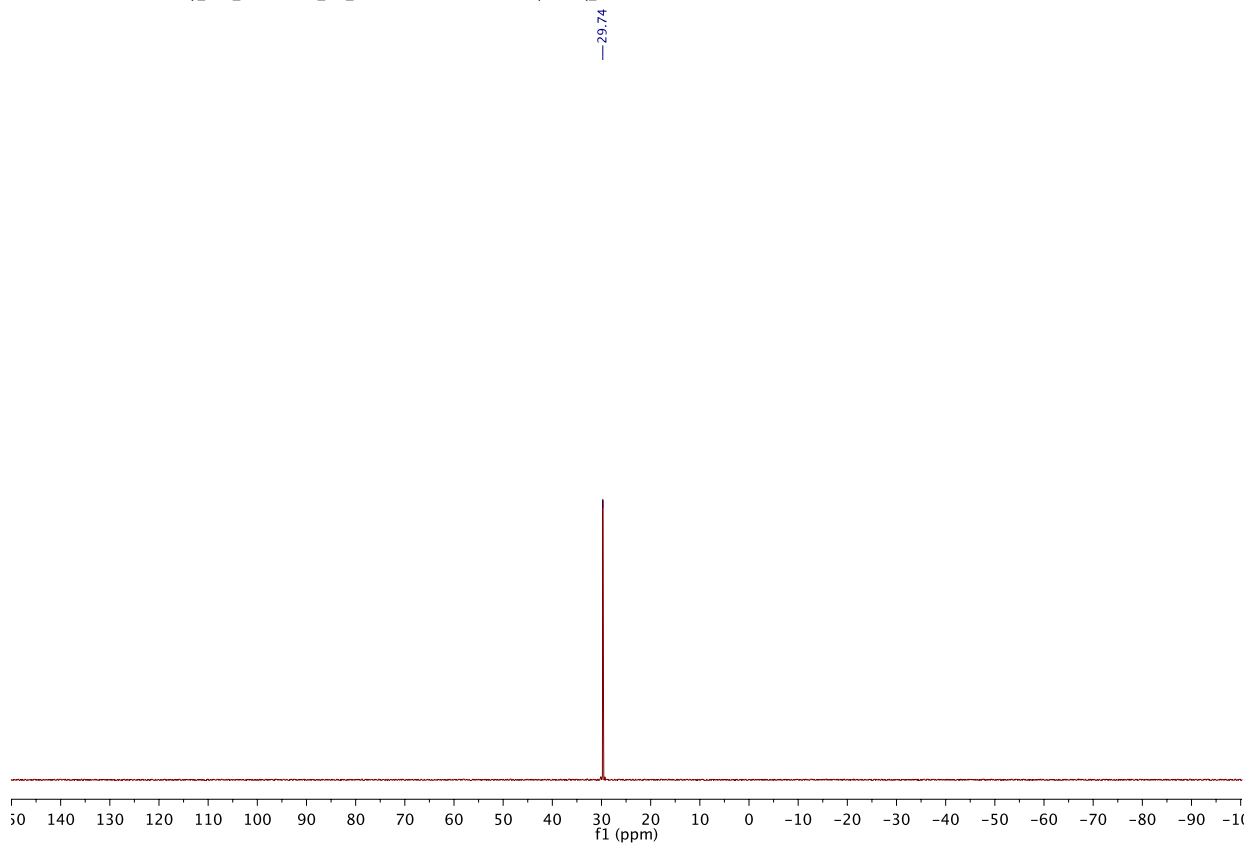
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [9] (in DMSO)

ycaL0003.1.fid — C13\_DECOUPLE\_H1



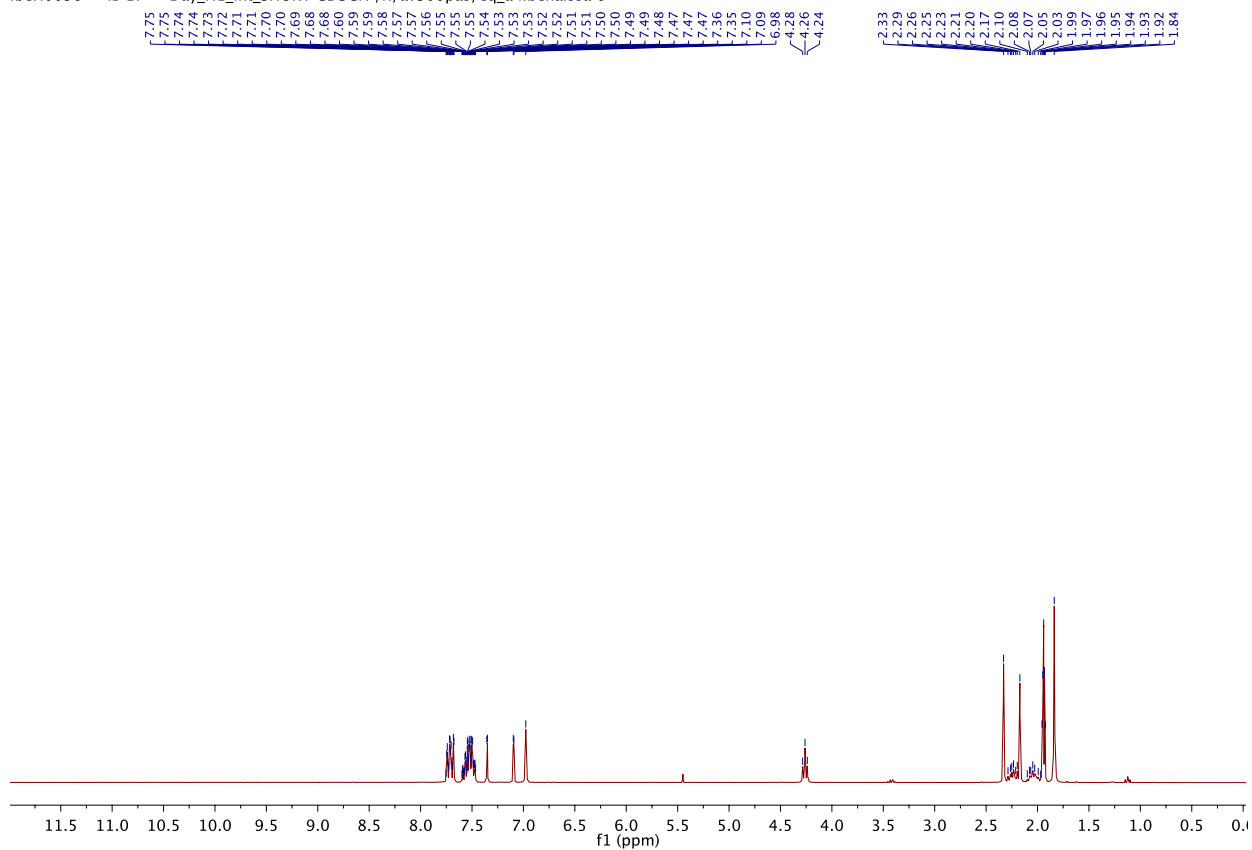
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [10] (in $\text{CD}_3\text{CN}$ )

ibeH0096 — IB 17 — Day\_P31\_DECOUPLE\_H1\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 6 —



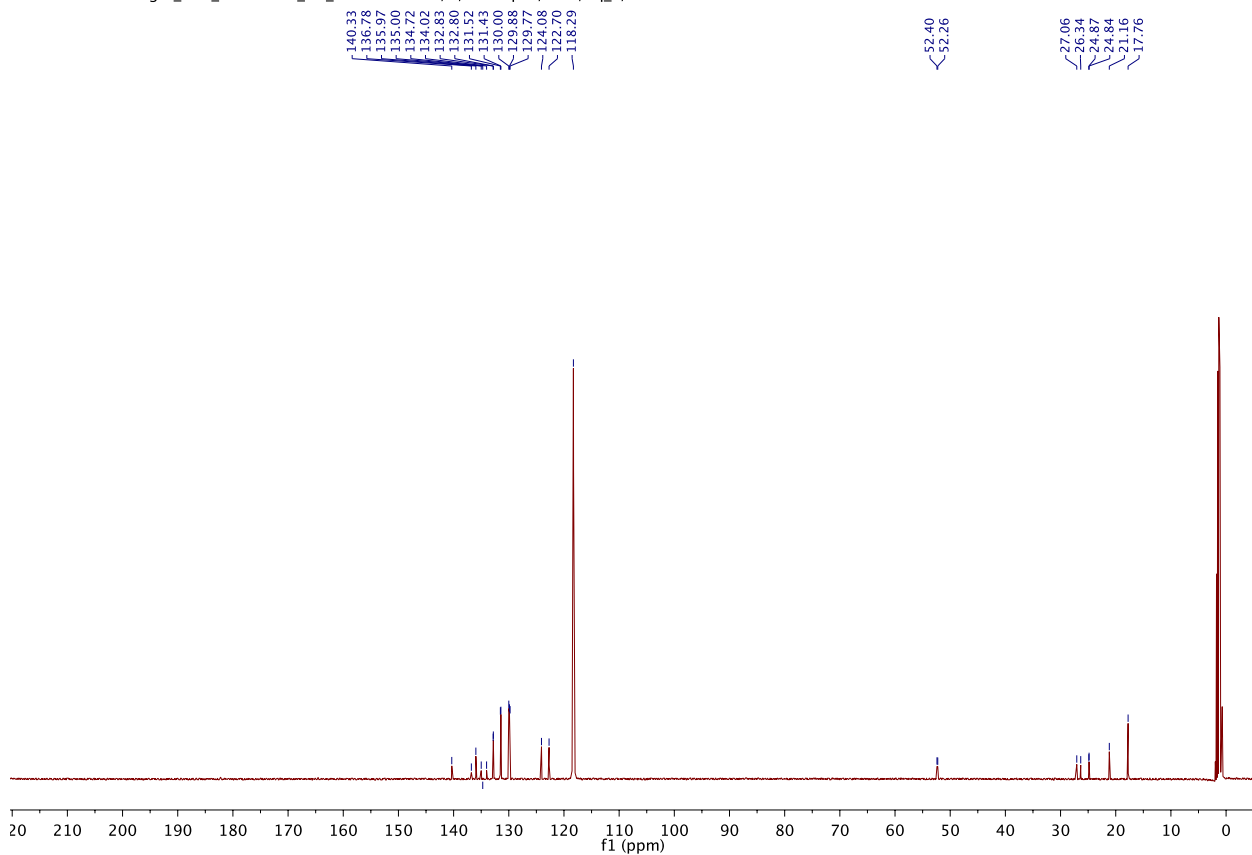
# $^1\text{H}$ NMR spectrum of [10] (in $\text{CD}_3\text{CN}$ )

ibeH0096 — IB 17 — Day\_H1\_int\_SHORT CD3CN /x/av300pas/eq\_a i.benaissa 6 —



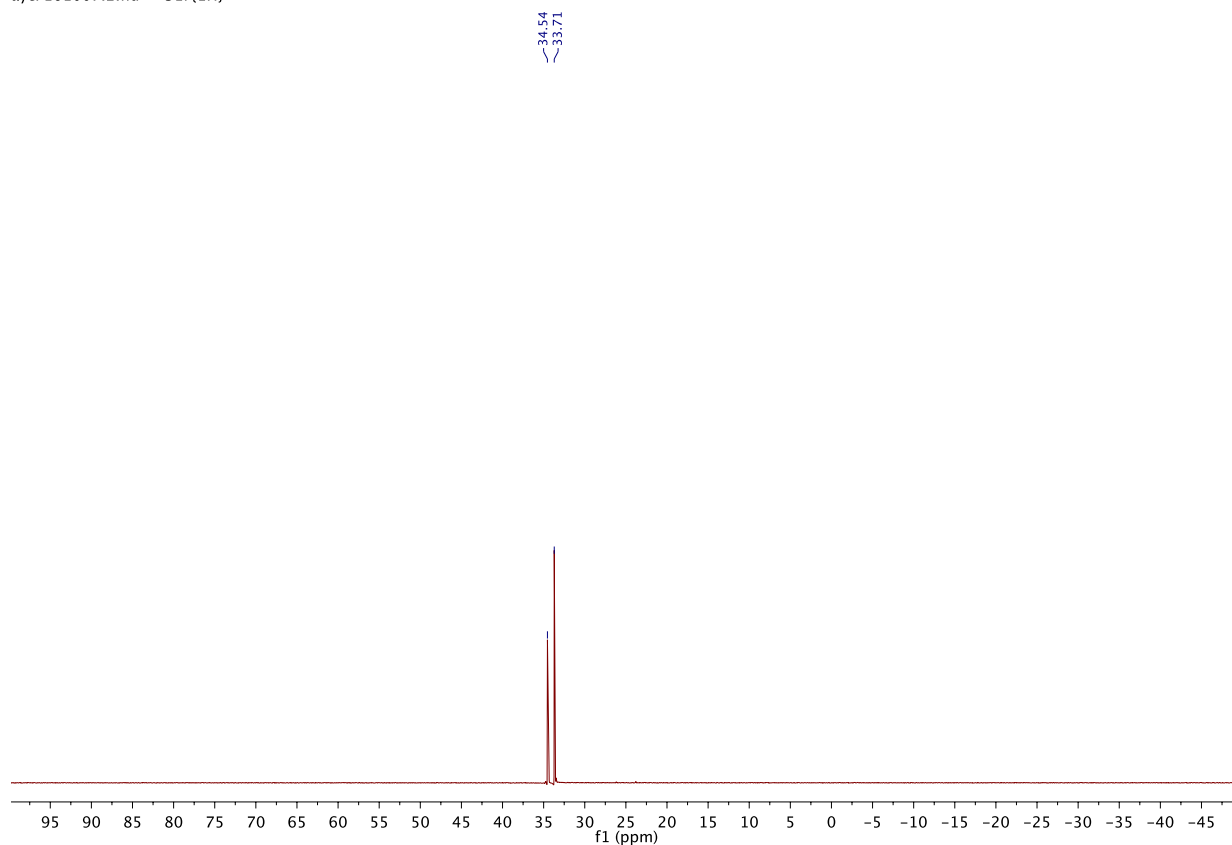
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [10] (in $\text{CD}_3\text{CN}$ )

ibeG0036 — Night\_C13\_DECOUPLE\_H1\_LONG CD3CN /x/av400pas/data/eq\_a/nmr i.benaissa 13 —



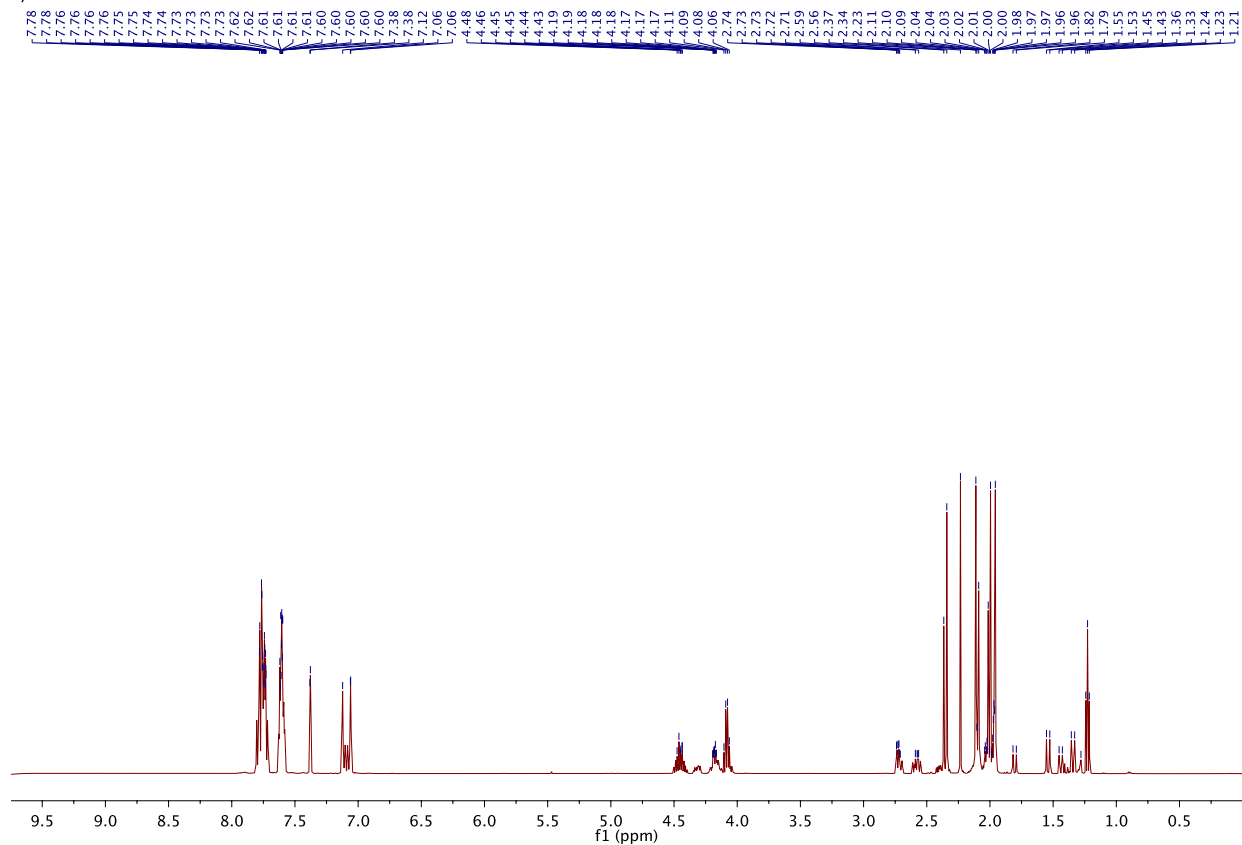
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [11a,b](OTf) (in $\text{CD}_3\text{CN}$ )

aycF161007.2.fid — 31P{1H}



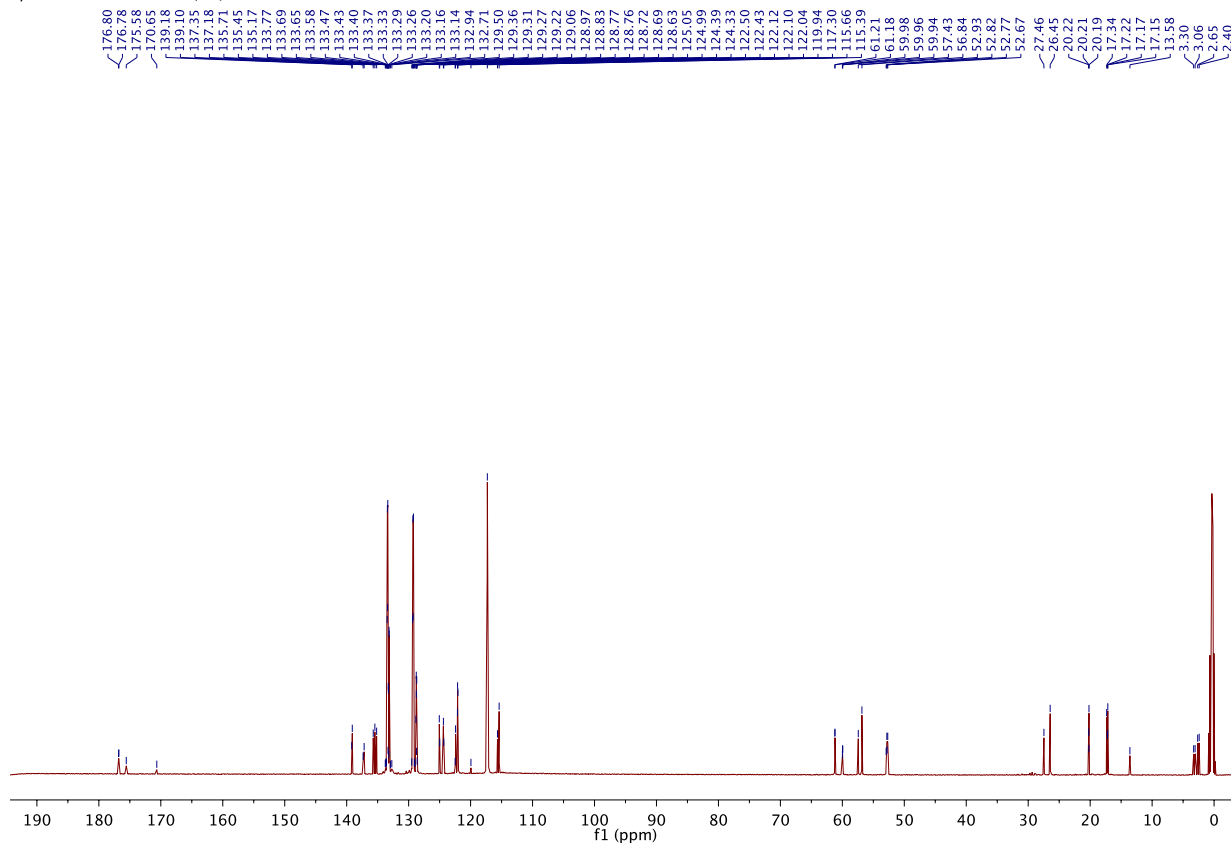
# $^1\text{H}$ NMR spectrum of [11a,b](OTf) (in $\text{CD}_3\text{CN}$ )

aycF161007.1.fid — 1H



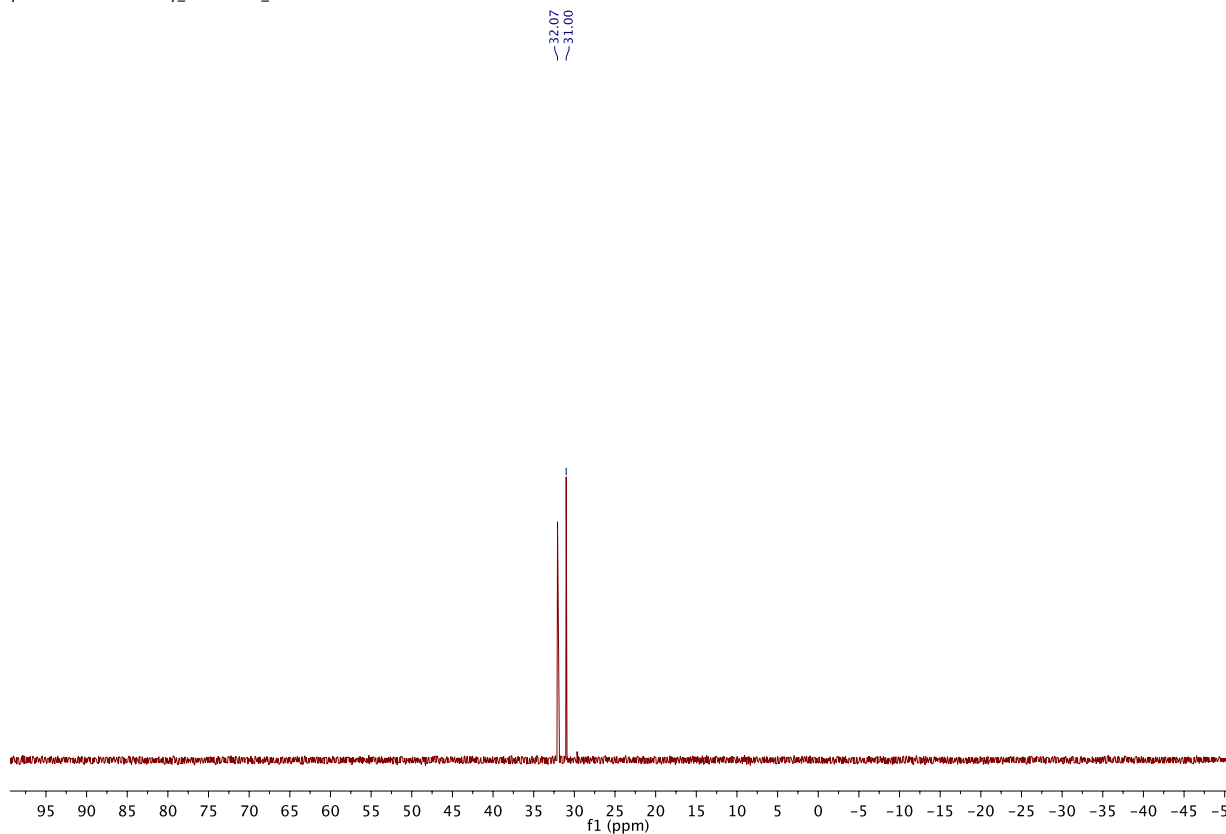
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [11a,b](OTf) (in $\text{CD}_3\text{CN}$ )

aycF161007.8.fid —  $^{13}\text{C}\{^1\text{H}\}$



# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [12a,b](OTf) (in $\text{CD}_3\text{CN}$ )

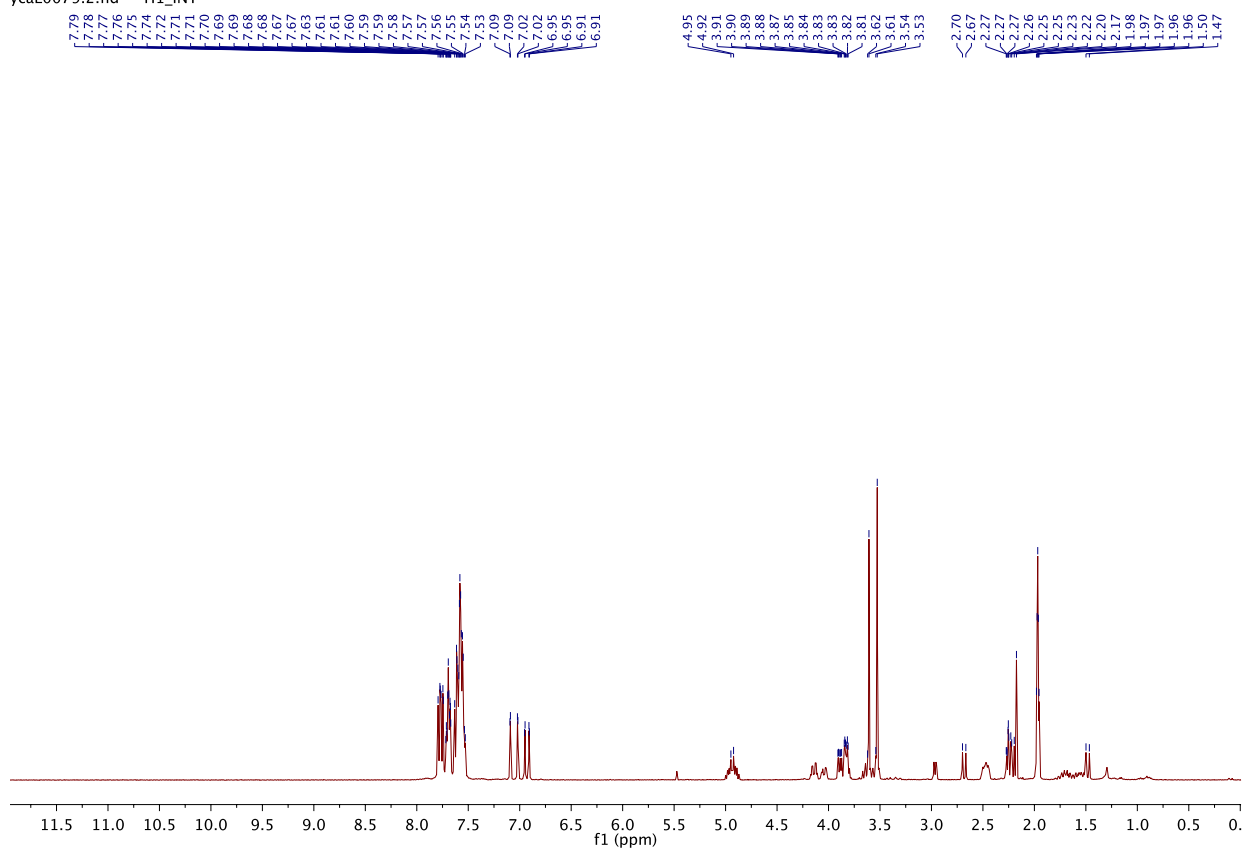
ycaL0079.1.fid —  $^{31}\text{P}\{^1\text{H}\}$  DECOUPLE\_H1





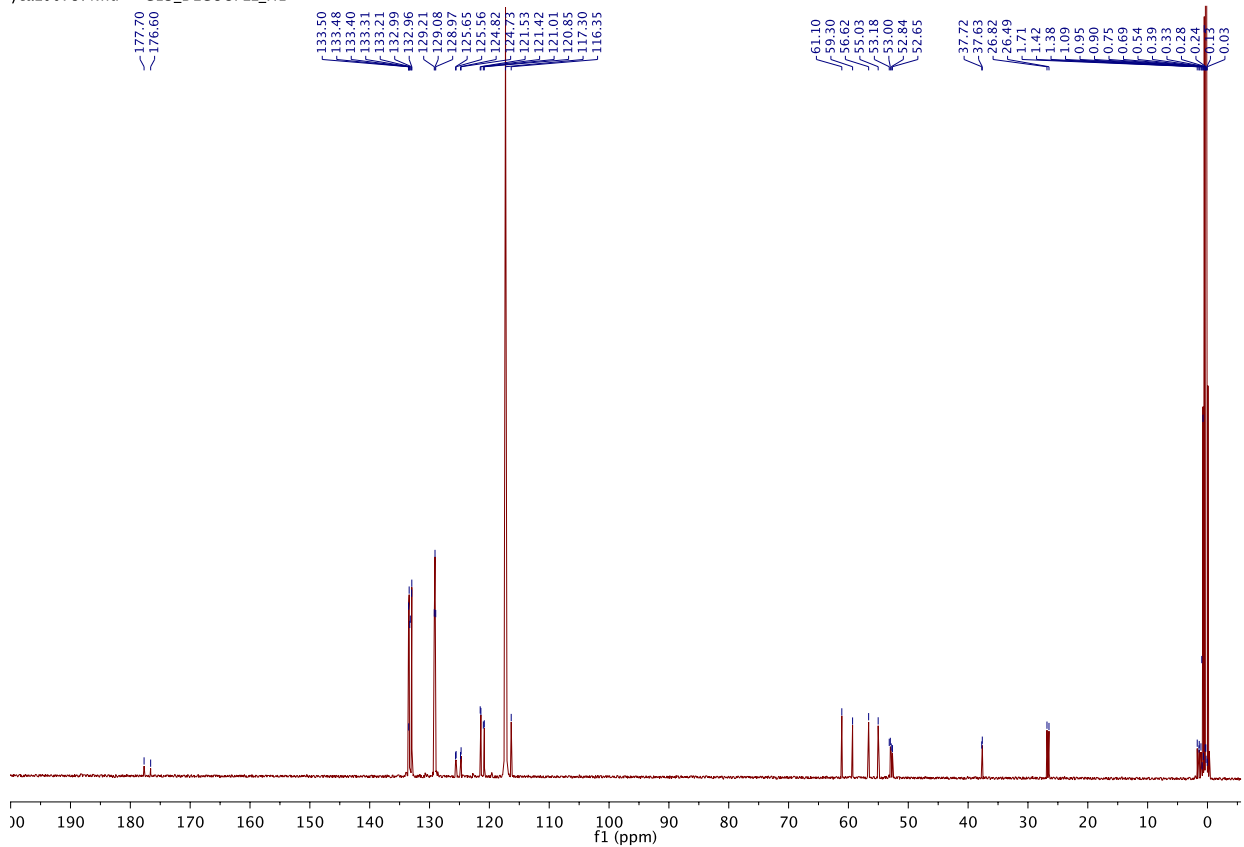
# $^1\text{H}$ NMR spectrum of [12a,b](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0079.2.fid — H1\_INT



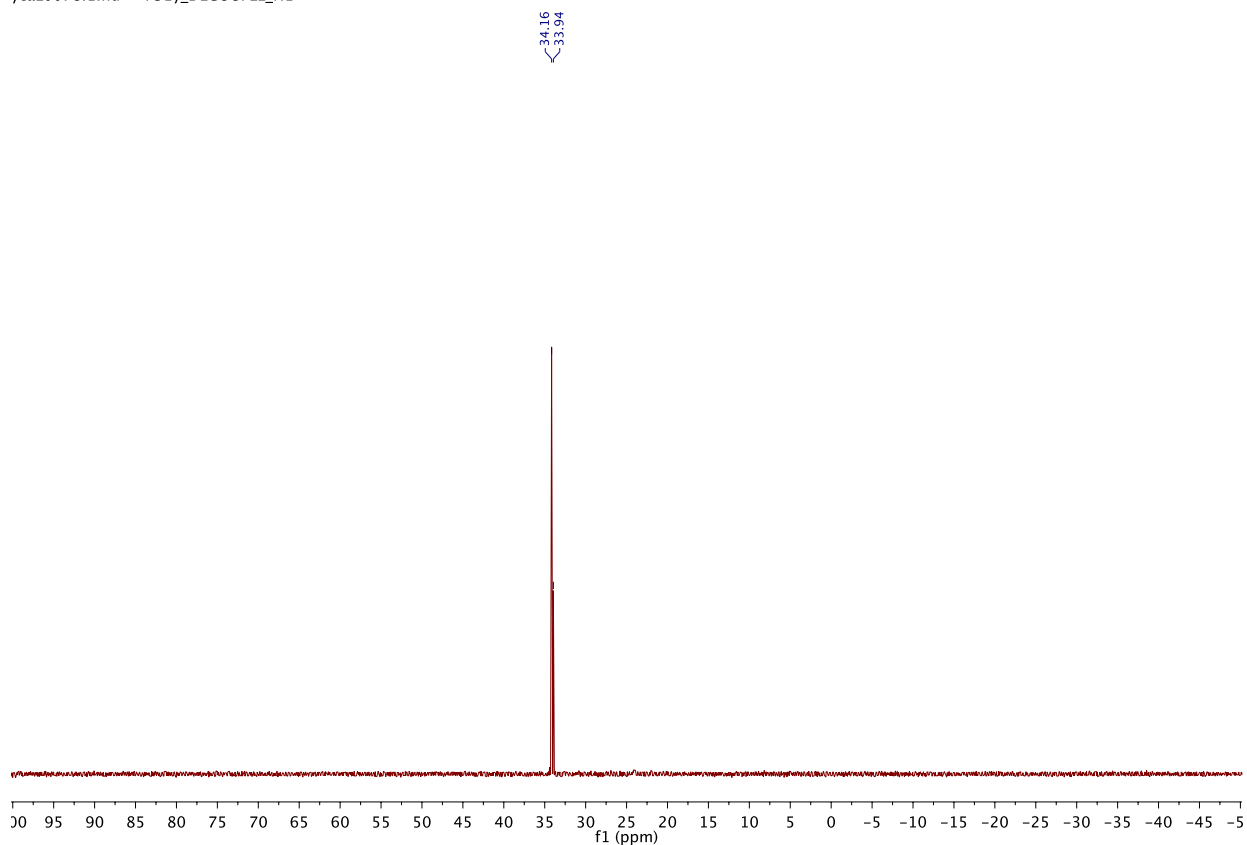
# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [12a,b](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0079.4.fid — C13\_DECOUPLE\_H1



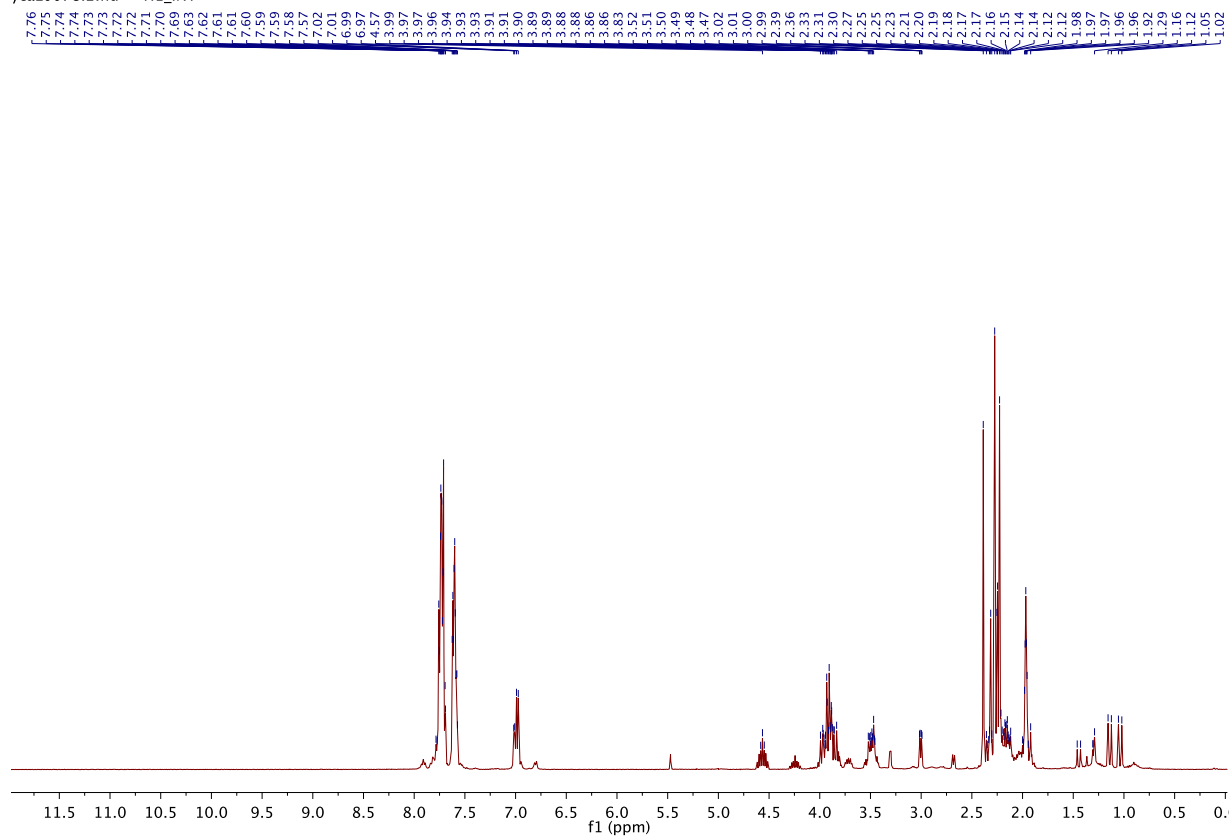
# $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [13a,b](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0078.1.fid — P31y\_DECOUPLE\_H1



# $^1\text{H}$ NMR spectrum of [13a,b](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0078.2.fid — H1\_INT



# $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of [13a,b](OTf) (in $\text{CD}_3\text{CN}$ )

ycaL0078.3.fid — C13\_DECOUPLE\_H1

