

Appendix

for the inaugural-dissertation with the title

Investigation of Structure-Reactivity Relationships of Arylpalladium Complexes in Transmetalations with Arylzinc Reagents

and

Palladium-Catalyzed Directed Halogenations of Bipyridine *N*-Oxides

and

**Mechanistic Investigations of the Direct Arylation of Pyridine *N*-Oxides with
Bromoarenes**

to obtain the academic degree

Doctor rerum naturalium (Dr. rer. nat.)

submitted to the Department of Biology, Chemistry and Pharmacy

of Freie Universität Berlin

by

SINA PATRICIA ZUCKER

2016

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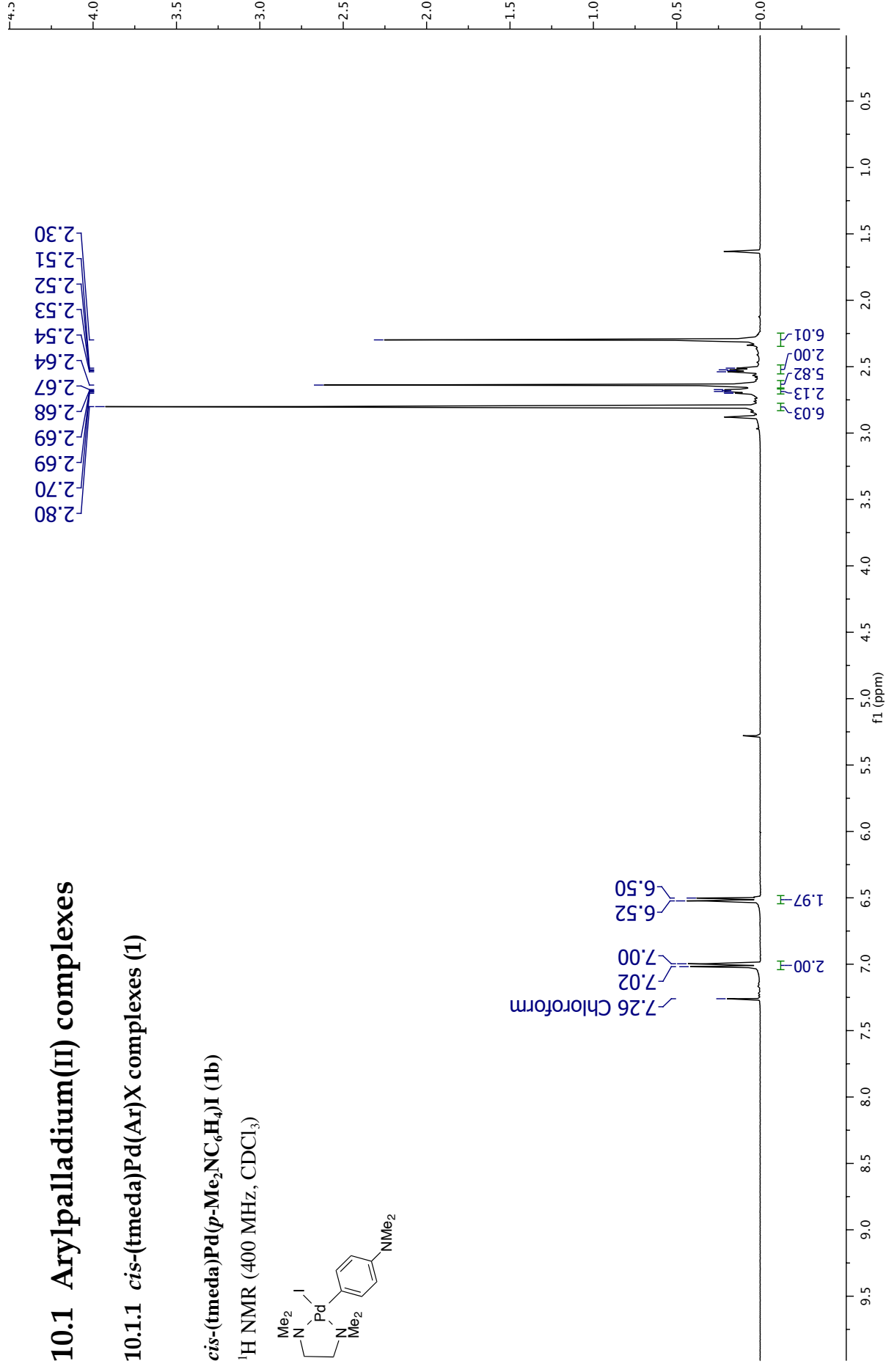
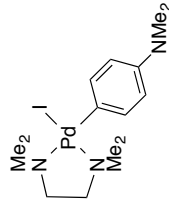
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10.1 Arylpalladium(II) complexes

10.1.1 *cis*-(*tmeda*)Pd(Ar)X complexes (1)

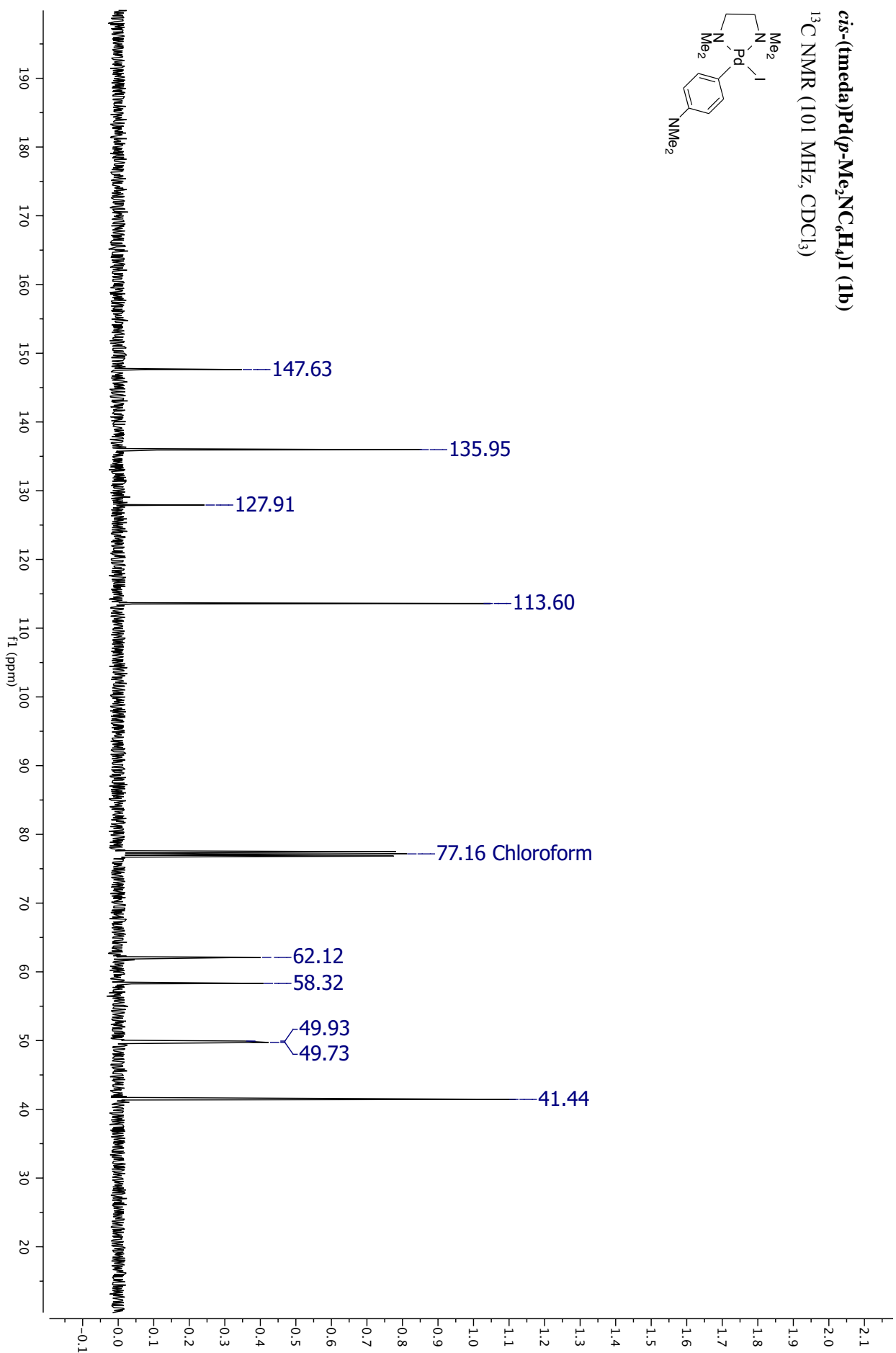
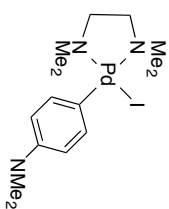
cis-(*tmeda*)Pd(*p*-Me₂NC₆H₄)I (1b)

¹H NMR (400 MHz, CDCl₃)



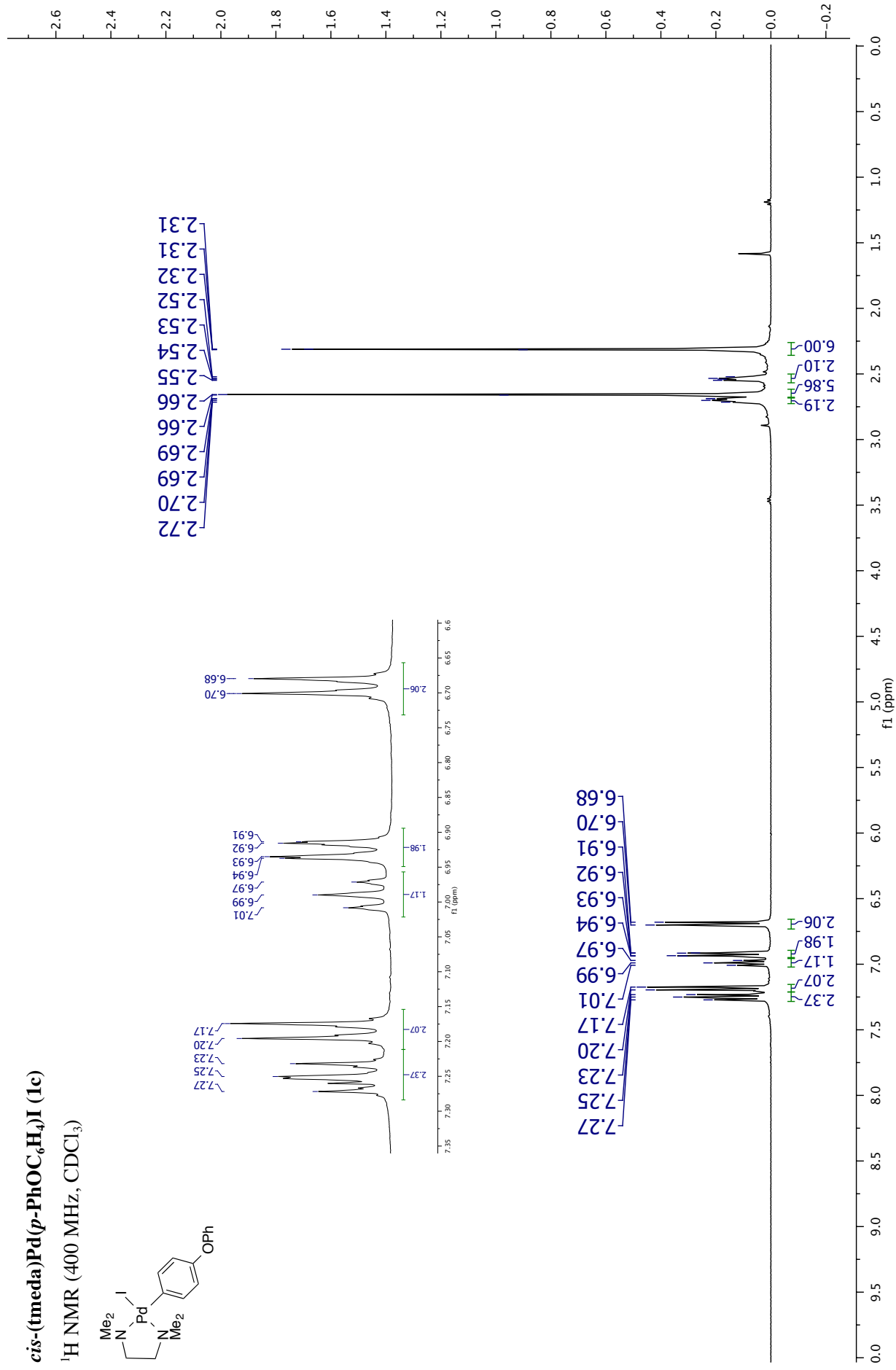
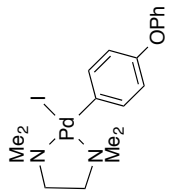
cis-(Imeda)Pd(*p*-Me₂NC₆H₄)I (**1b**)

¹³C NMR (101 MHz, CDCl₃)



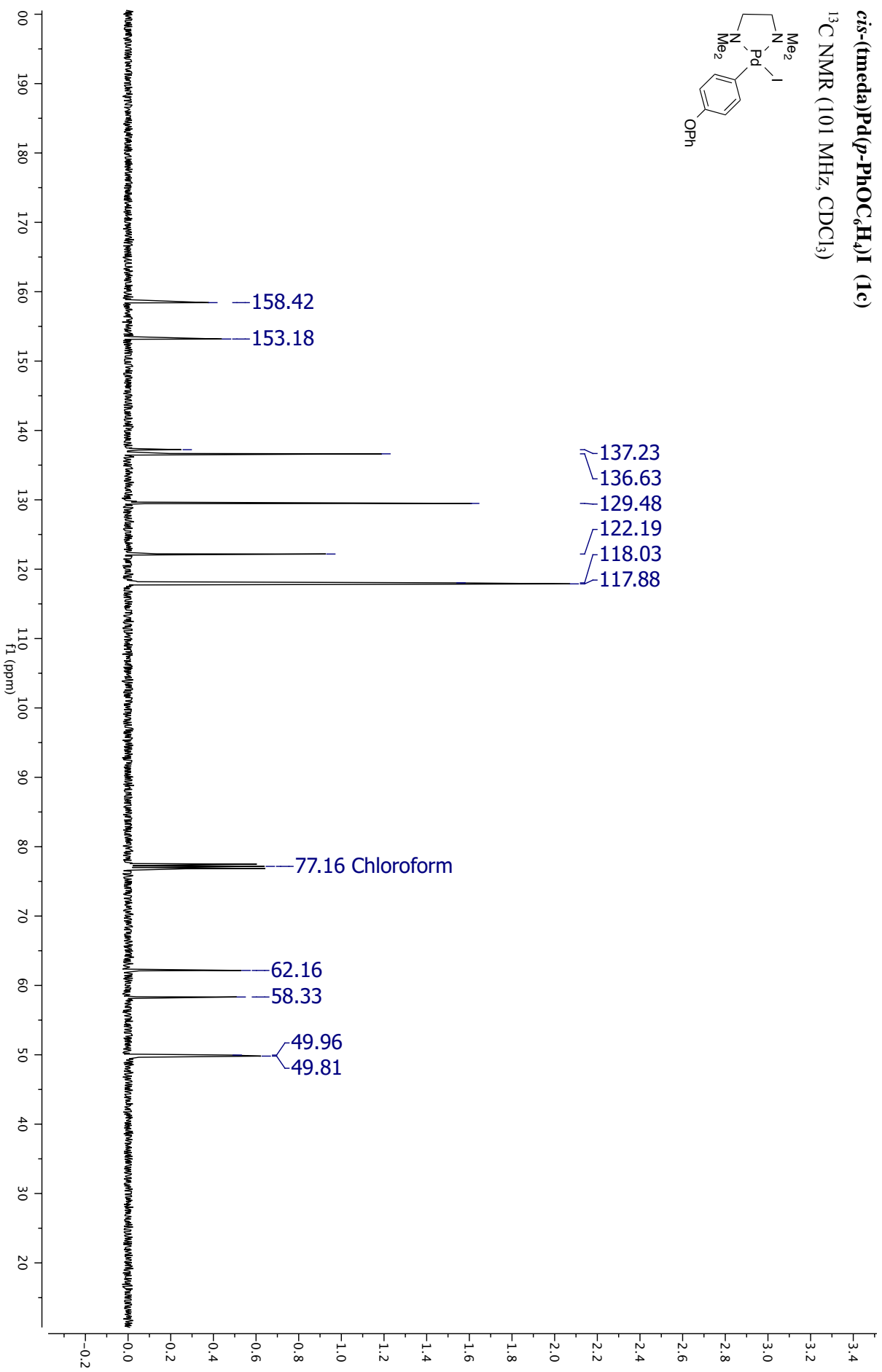
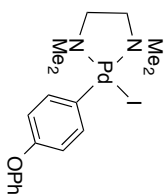
***cis*-(*tmeda*)Pd(*p*-PhOC₆H₄)I (**1c**)**

¹H NMR (400 MHz, CDCl₃)



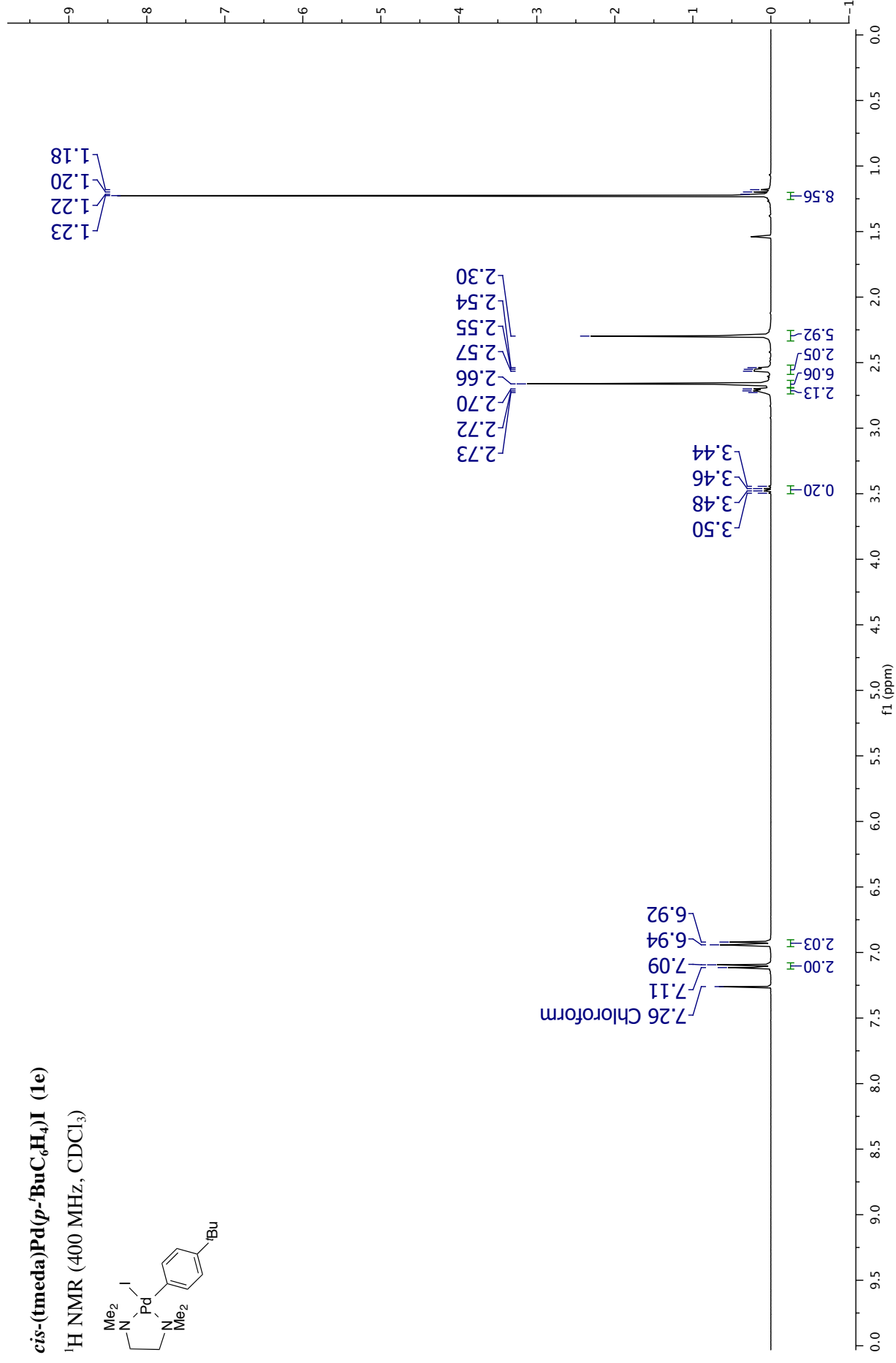
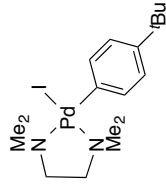
cis-(Imeda)Pd(*p*-PhOC₆H₄)I (**1c**)

¹³C NMR (101 MHz, CDCl₃)



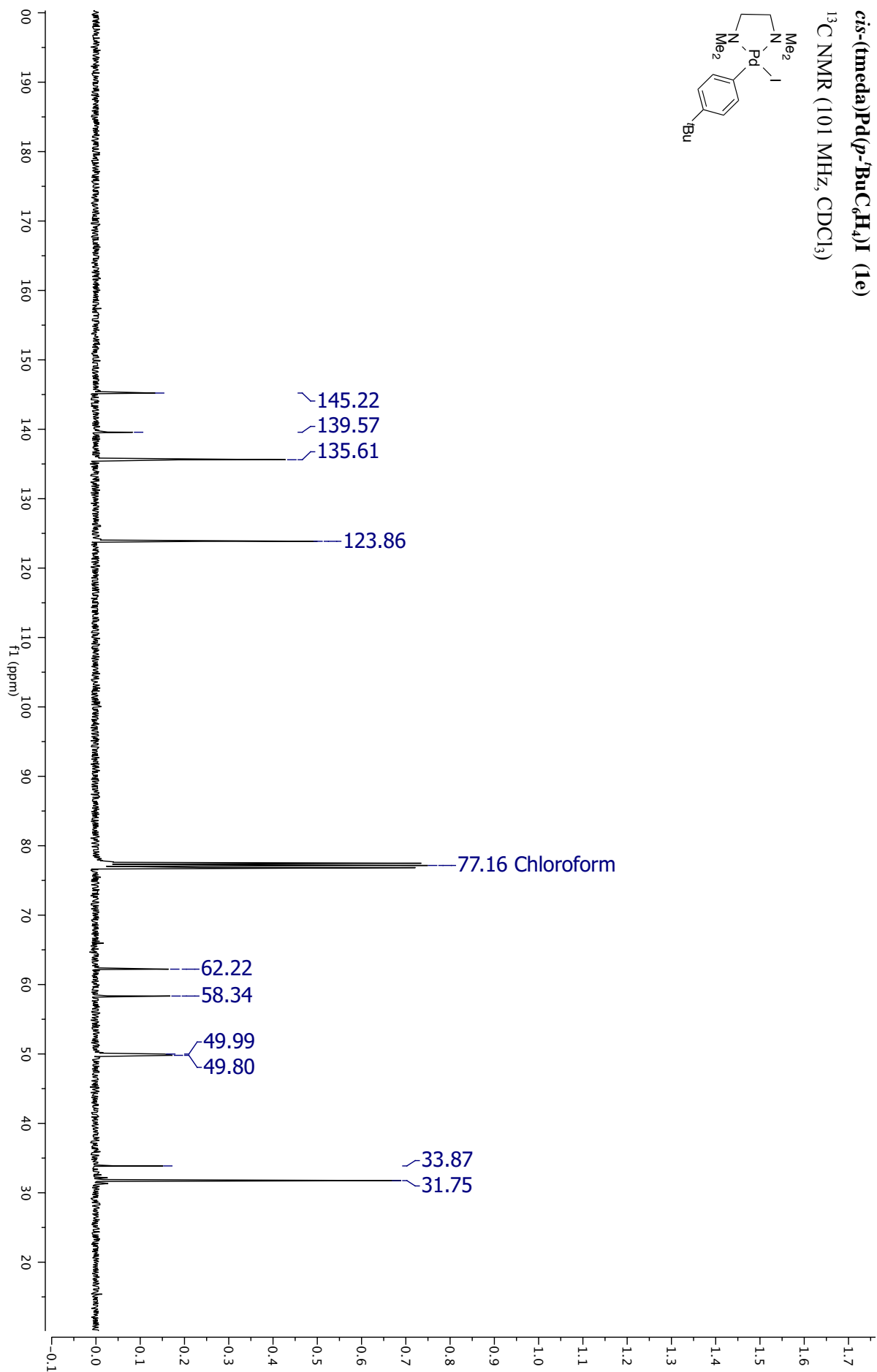
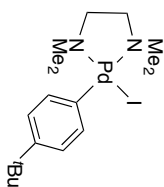
***cis*-(tmeda)Pd(*p*-BuC₆H₄)I (1e)**

¹H NMR (400 MHz, CDCl₃)



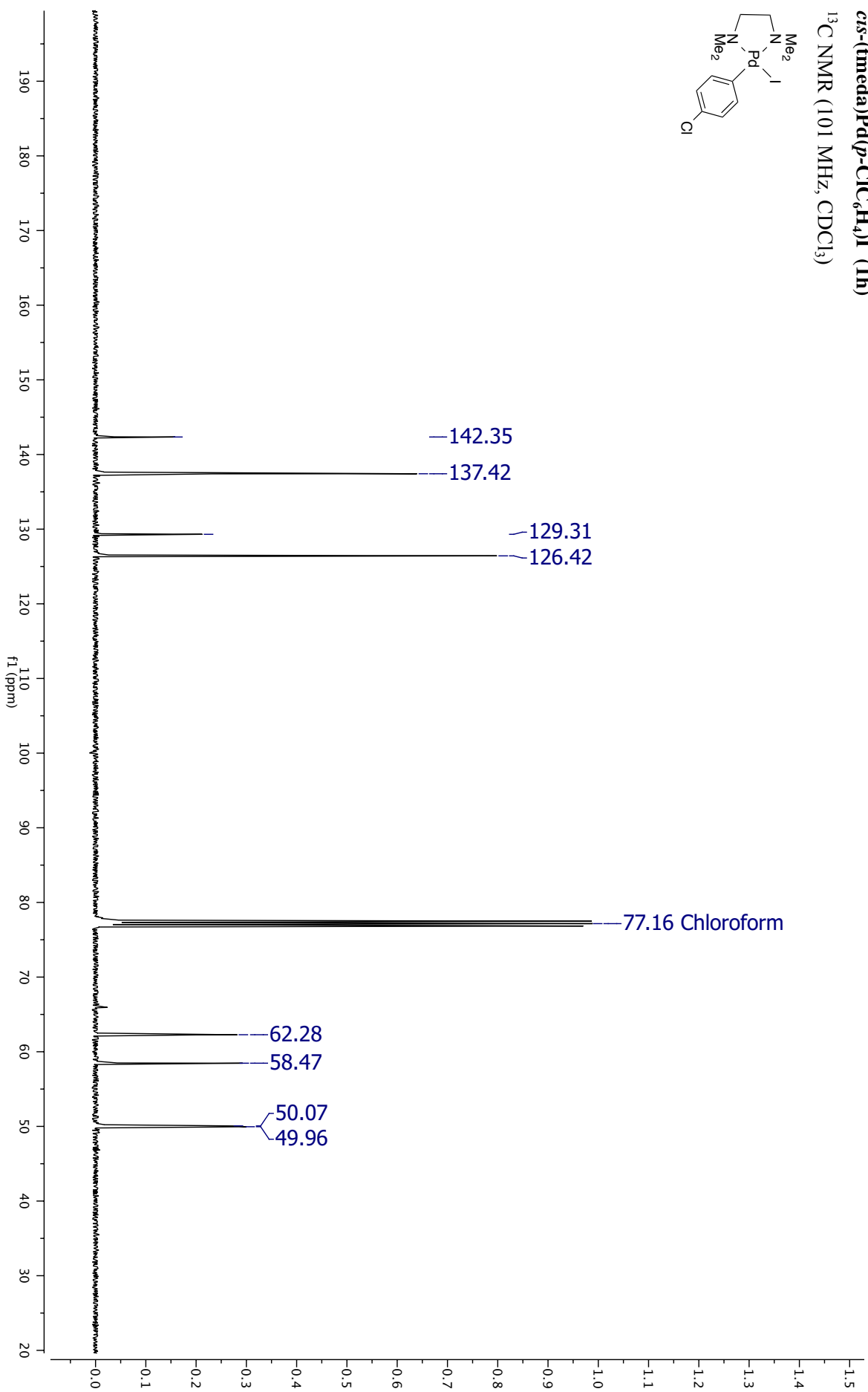
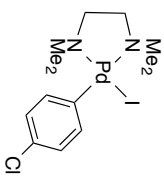
cis-(Imeda)Pd(*p*-¹BuC₆H₄)I (**1e**)

¹³C NMR (101 MHz, CDCl₃)



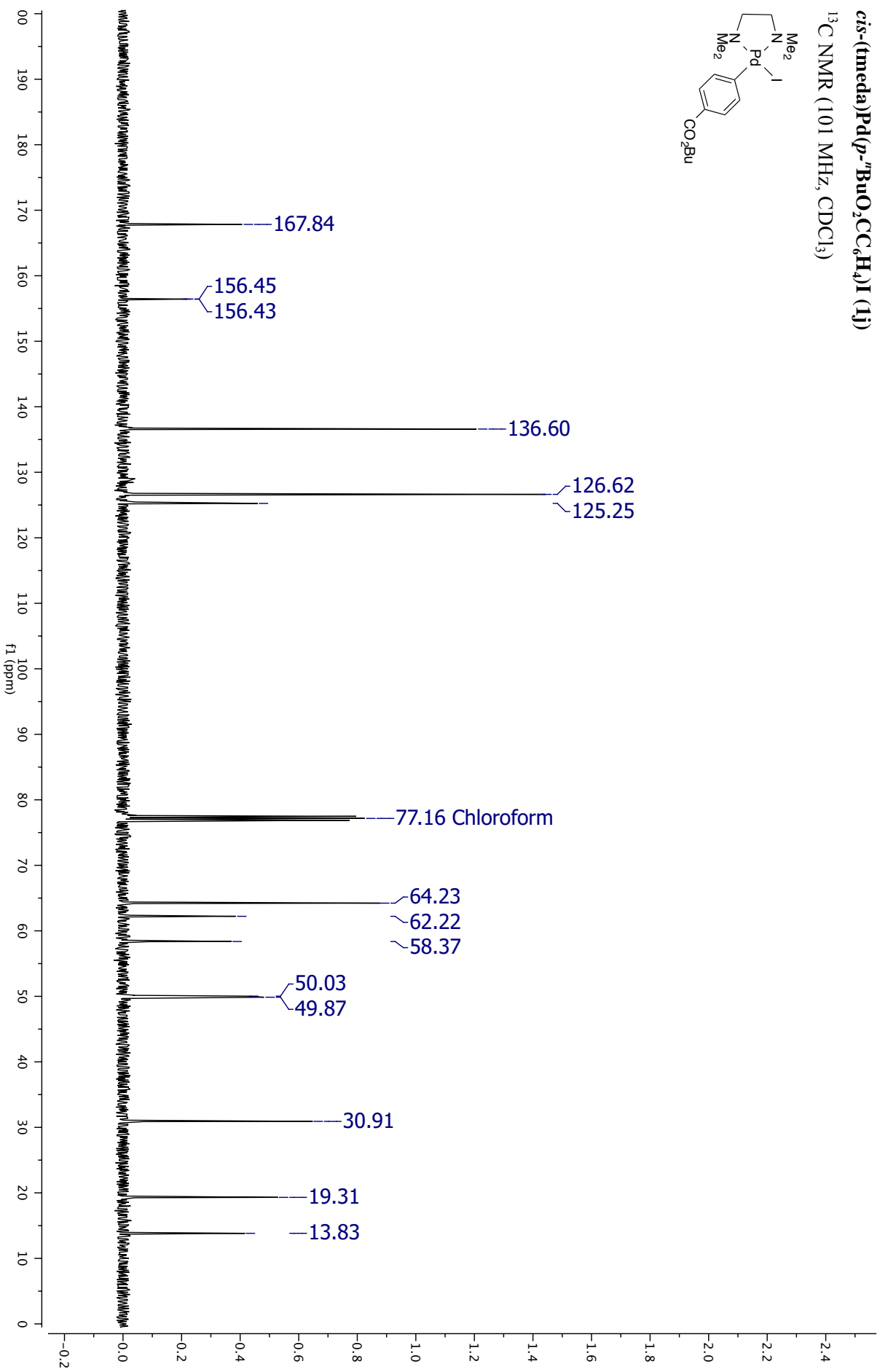
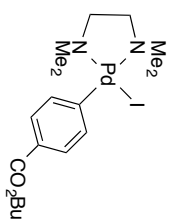
cis-(Imeda)Pd(*p*-ClC₆H₄)I (1h)

¹³C NMR (101 MHz, CDCl₃)



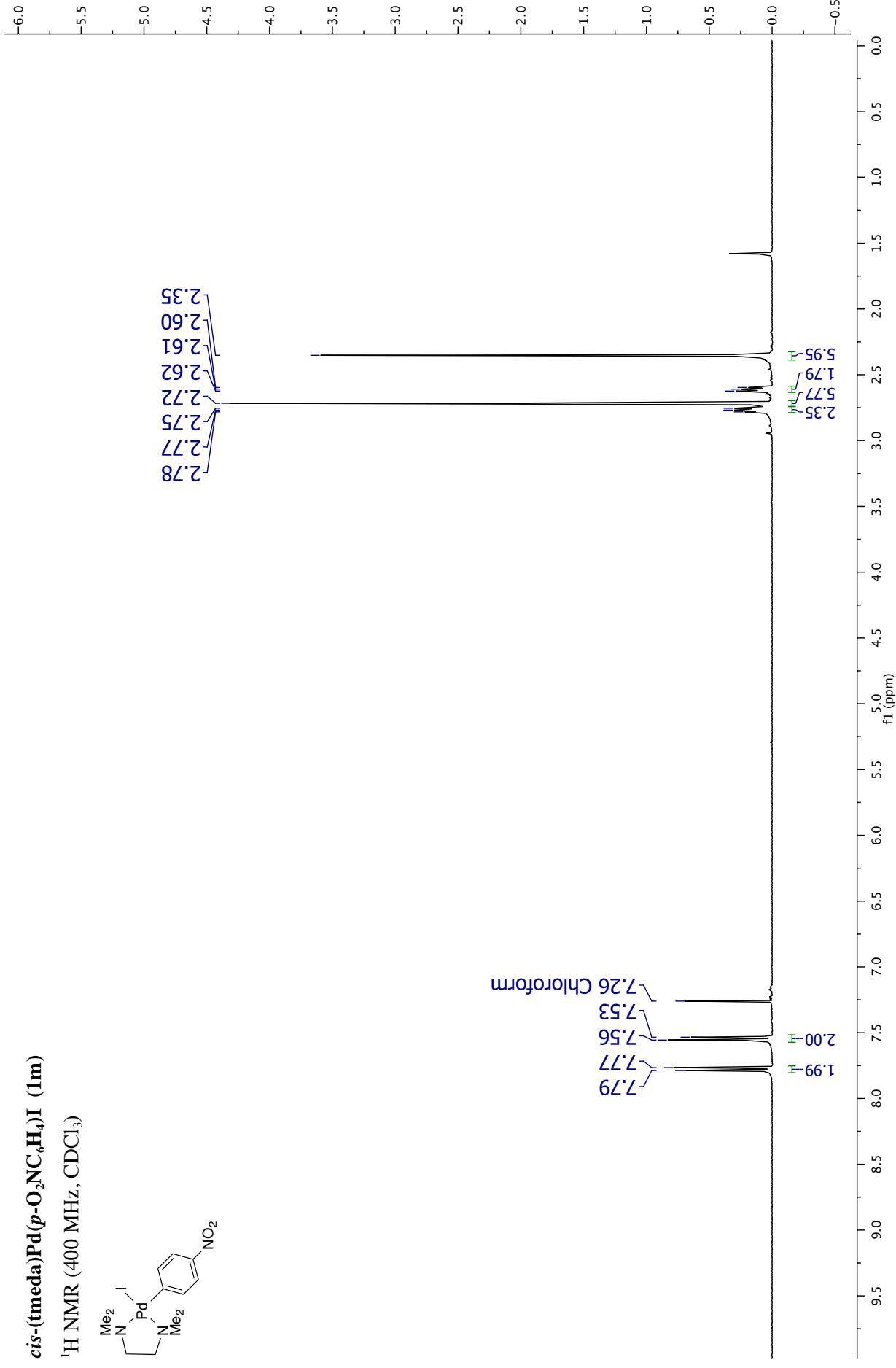
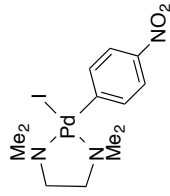
cis-(Imeda)Pd(*p*-^tBuO₂CC₆H₄)I (**1f**)

¹³C NMR (101 MHz, CDCl₃)



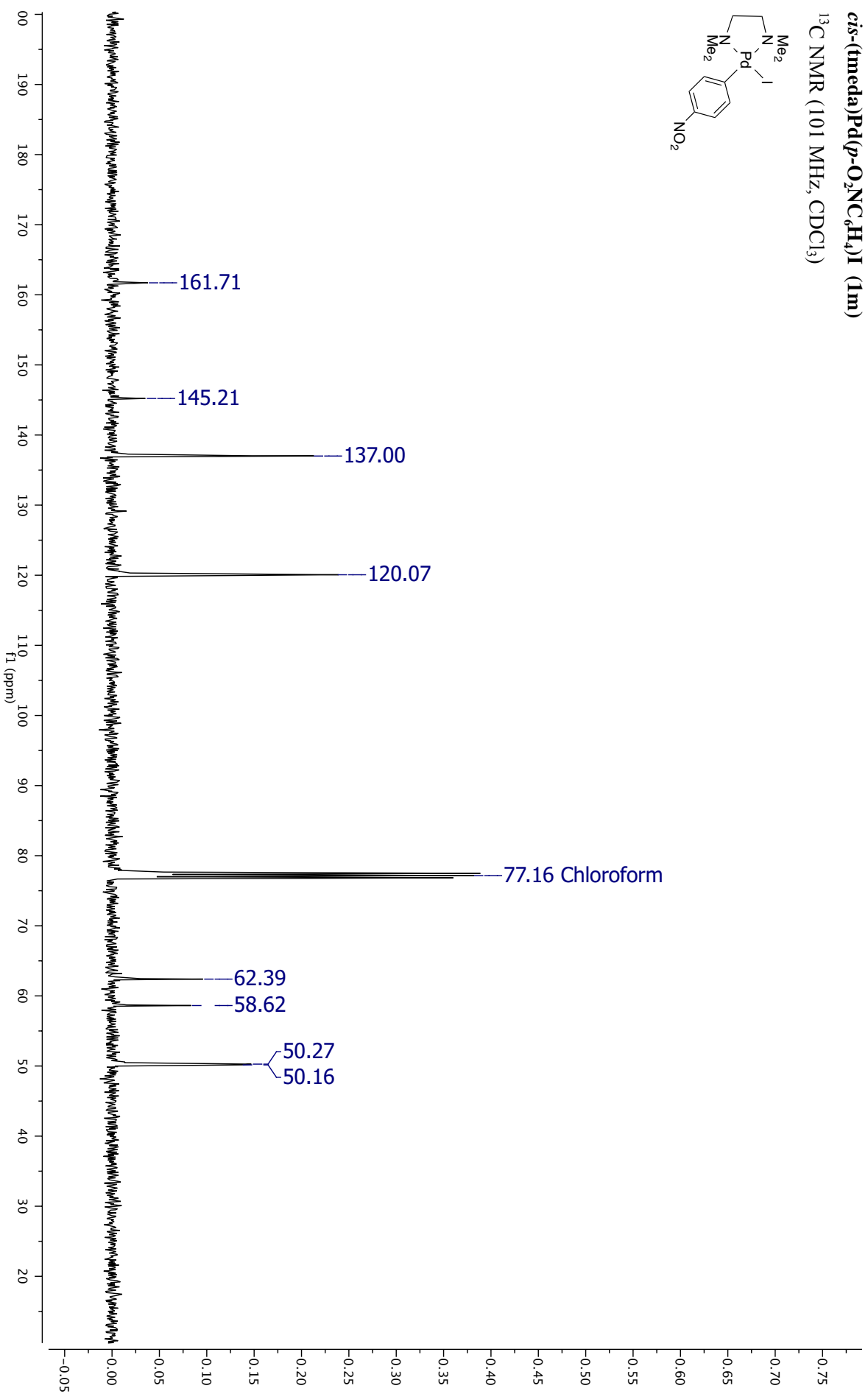
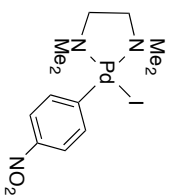
***cis*-(tmeda)Pd(*p*-O₂NC₆H₄)I (1m)**

¹H NMR (400 MHz, CDCl₃)



cis-(Imeda)Pd(*p*-O₂NC₆H₄)I (1m)

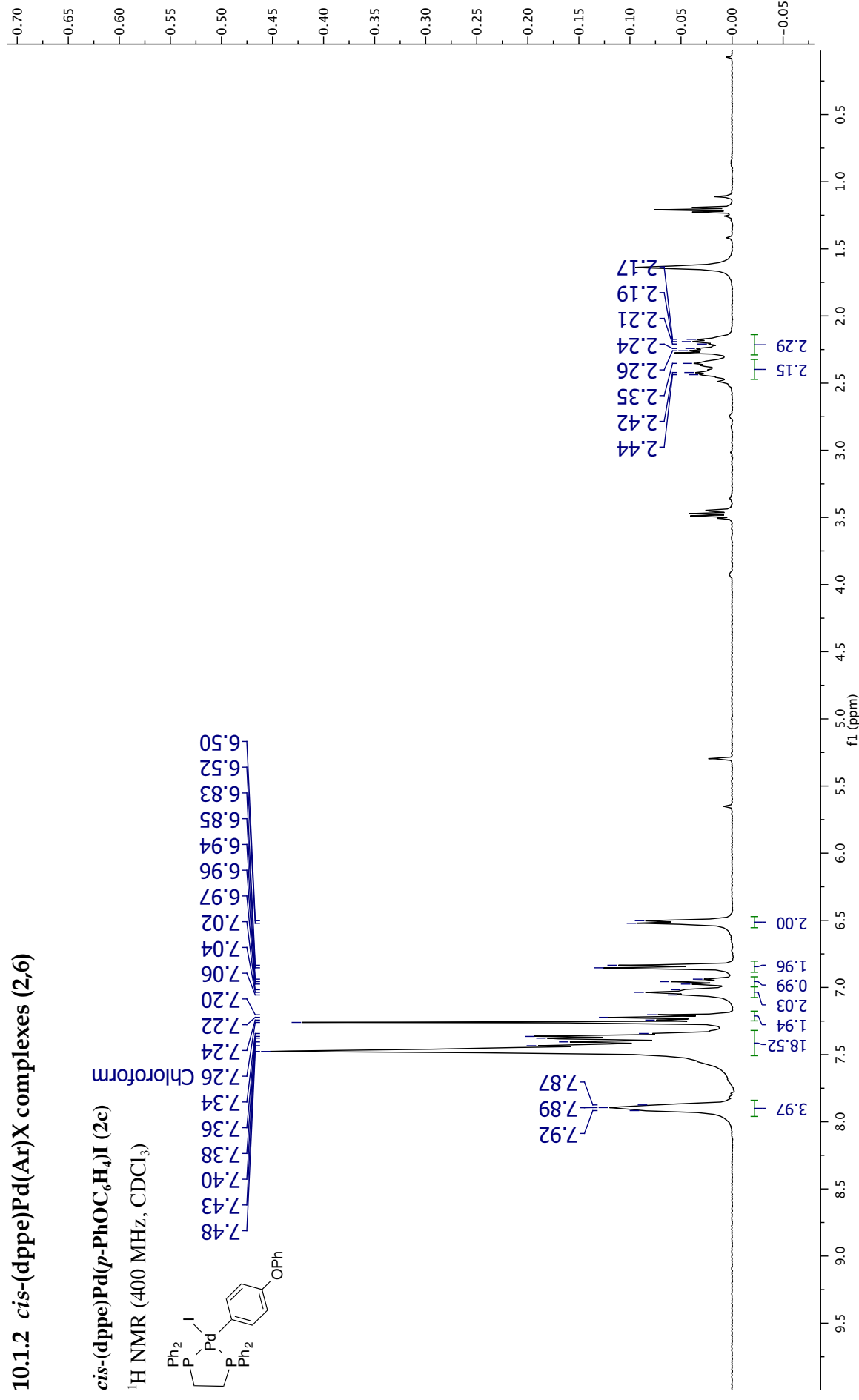
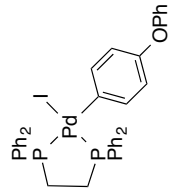
¹³C NMR (101 MHz, CDCl₃)



10.1.2 *cis*-(dppe)Pd(Ar)X complexes (2,6)

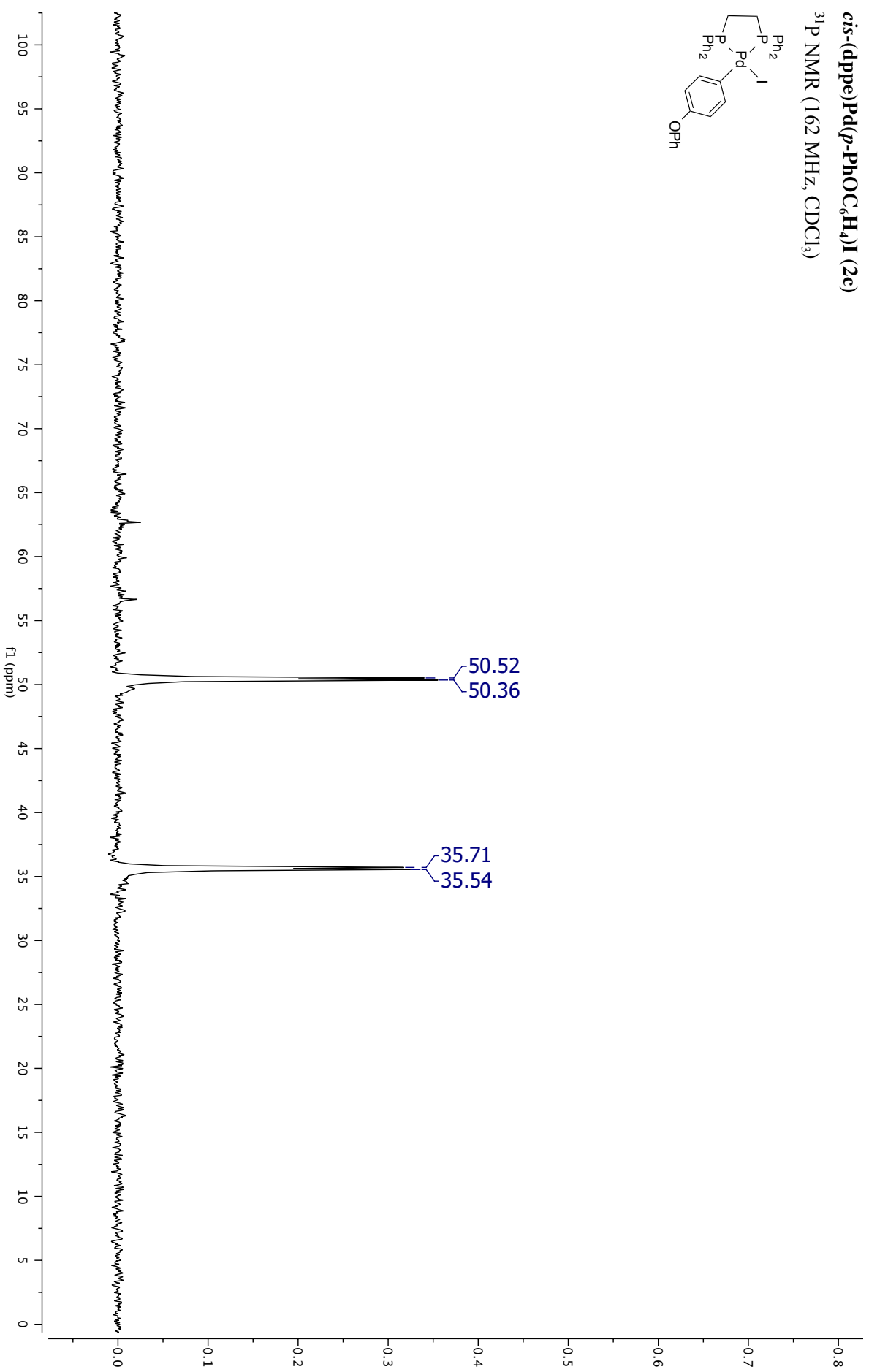
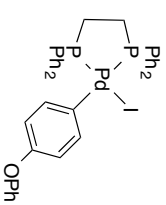
cis-(dppe)Pd(*p*-PhOC₆H₄)I (2c)

¹H NMR (400 MHz, CDCl₃)



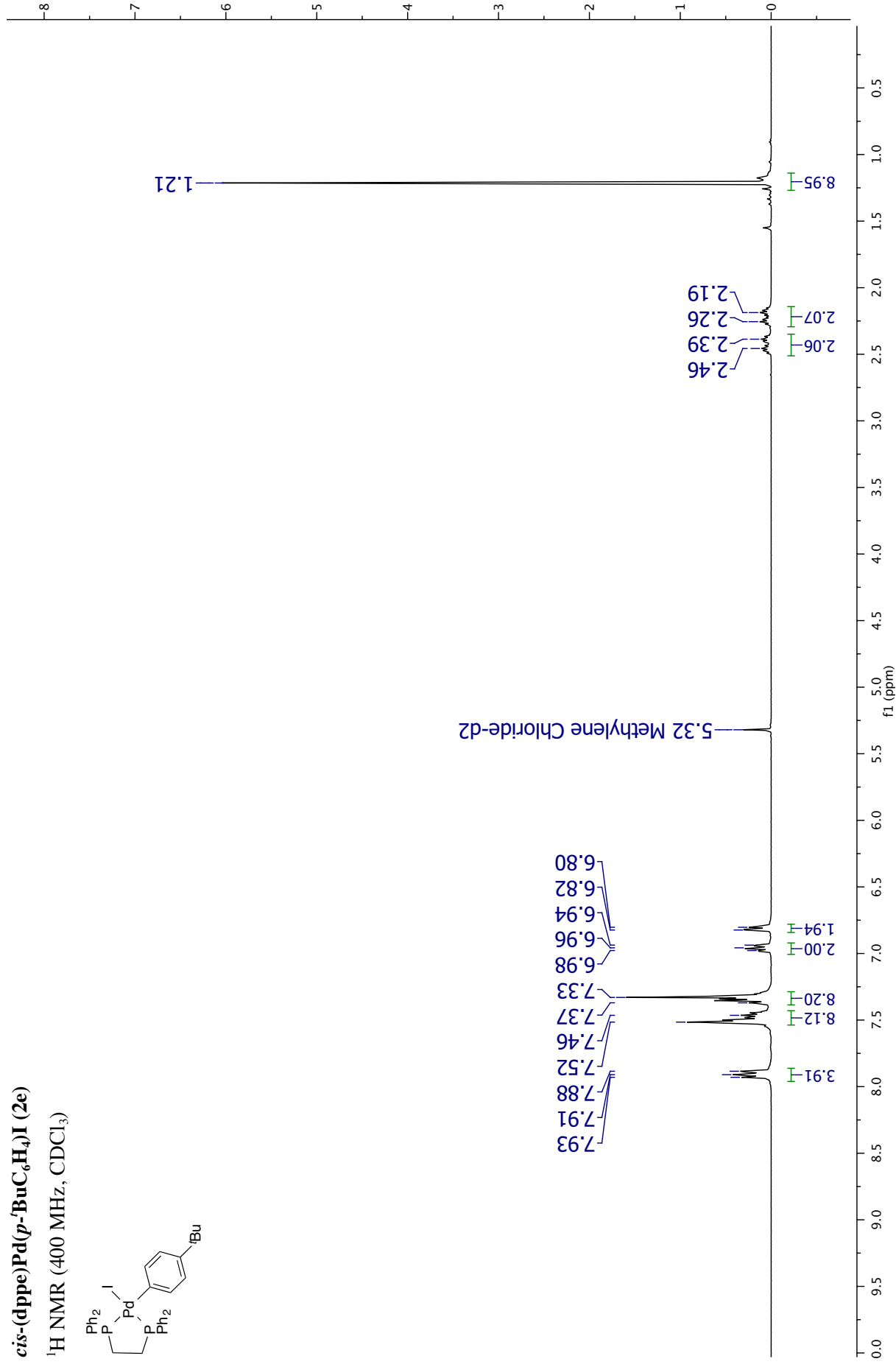
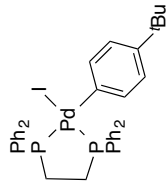
cis-(**dpppe**)Pd(*p*-PhOC₆H₄)I (**2c**)

³¹P NMR (162 MHz, CDCl₃)



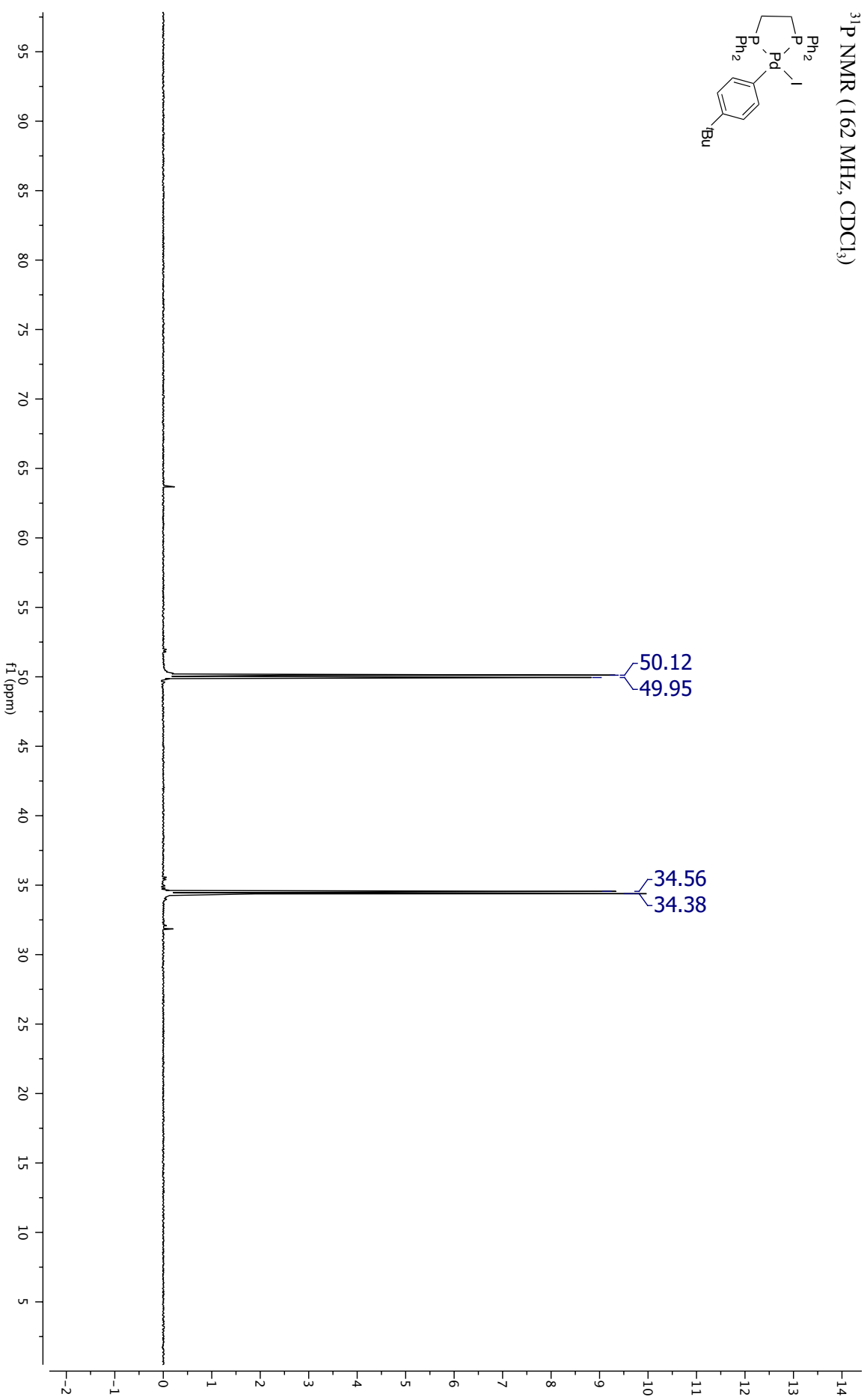
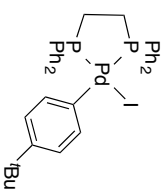
***cis*-(dpppe)Pd(*p*-^tBuC₆H₄)I (**2e**)**

¹H NMR (400 MHz, CDCl₃)



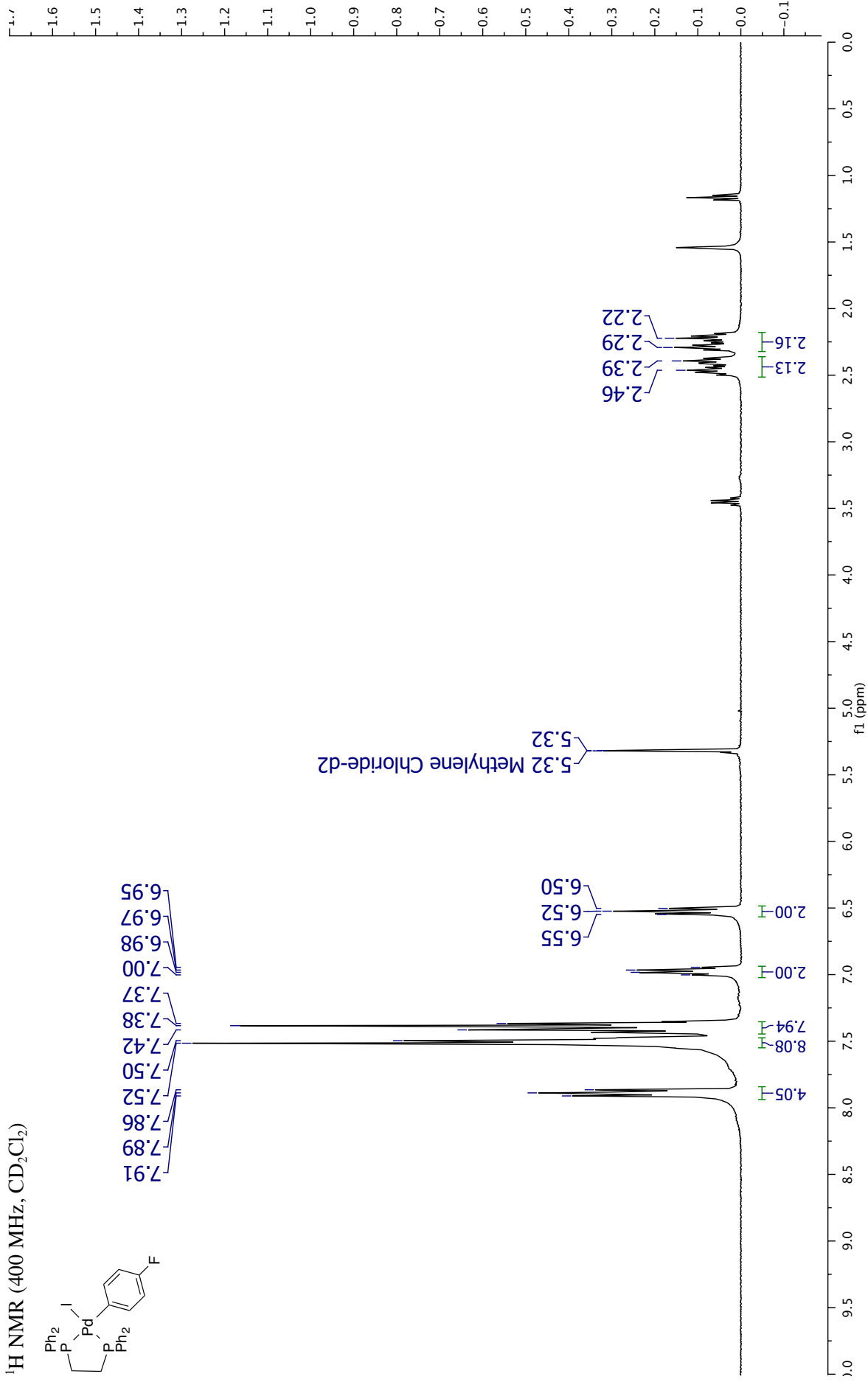
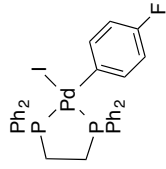
cis-(dpppe)Pd(*p*-^tBuC₆H₄)I (**2e**)

³¹P NMR (162 MHz, CDCl₃)



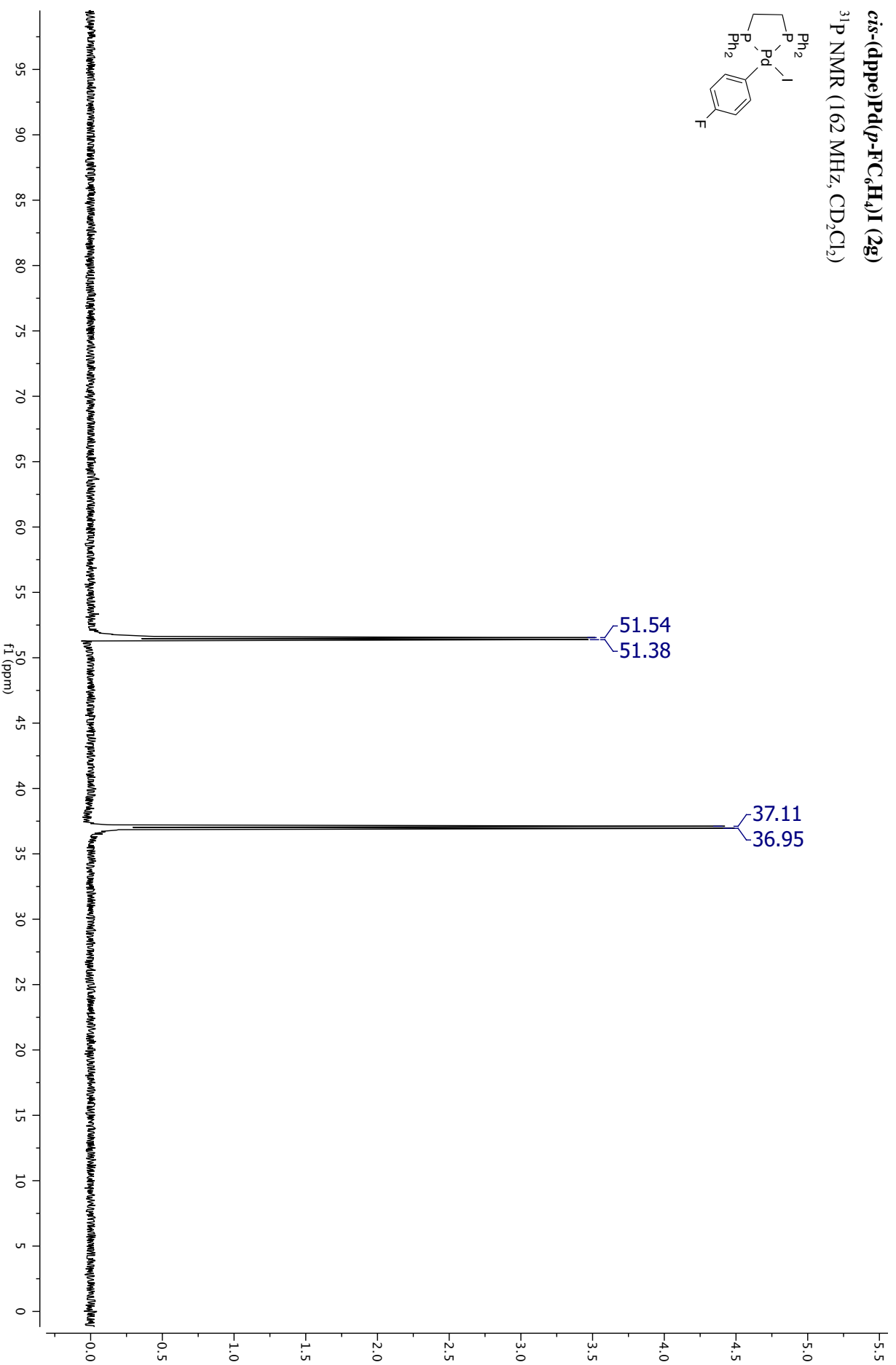
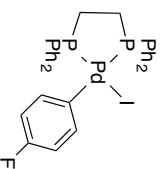
***cis*-(dppf)Pd(*p*-FC₆H₄)I (2g)**

¹H NMR (400 MHz, CD₂Cl₂)



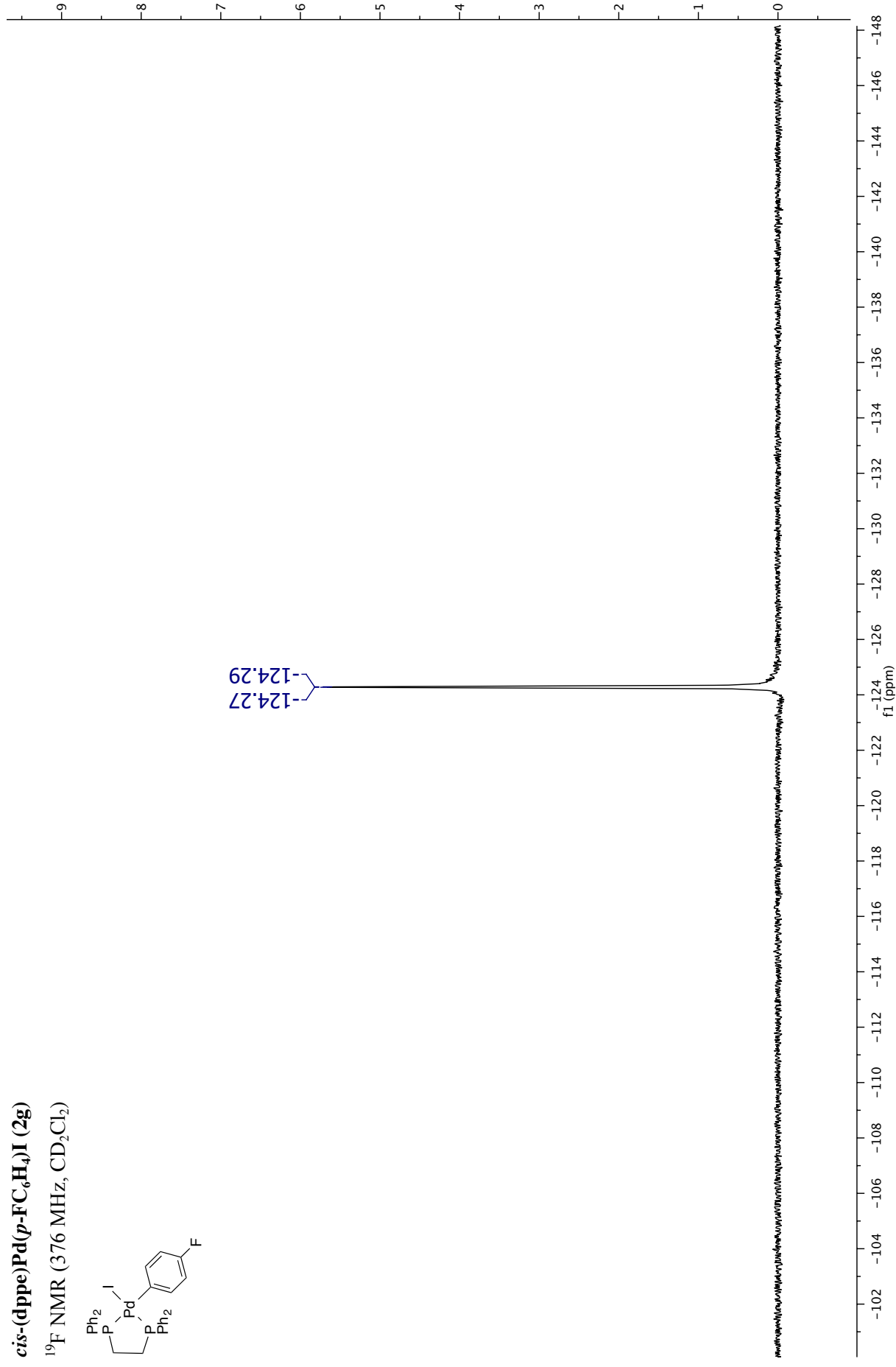
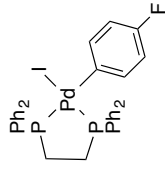
***cis*-(dippe)Pd(*p*-FC₆H₄)I (**2g**)**

³¹P NMR (162 MHz, CD₂Cl₂)



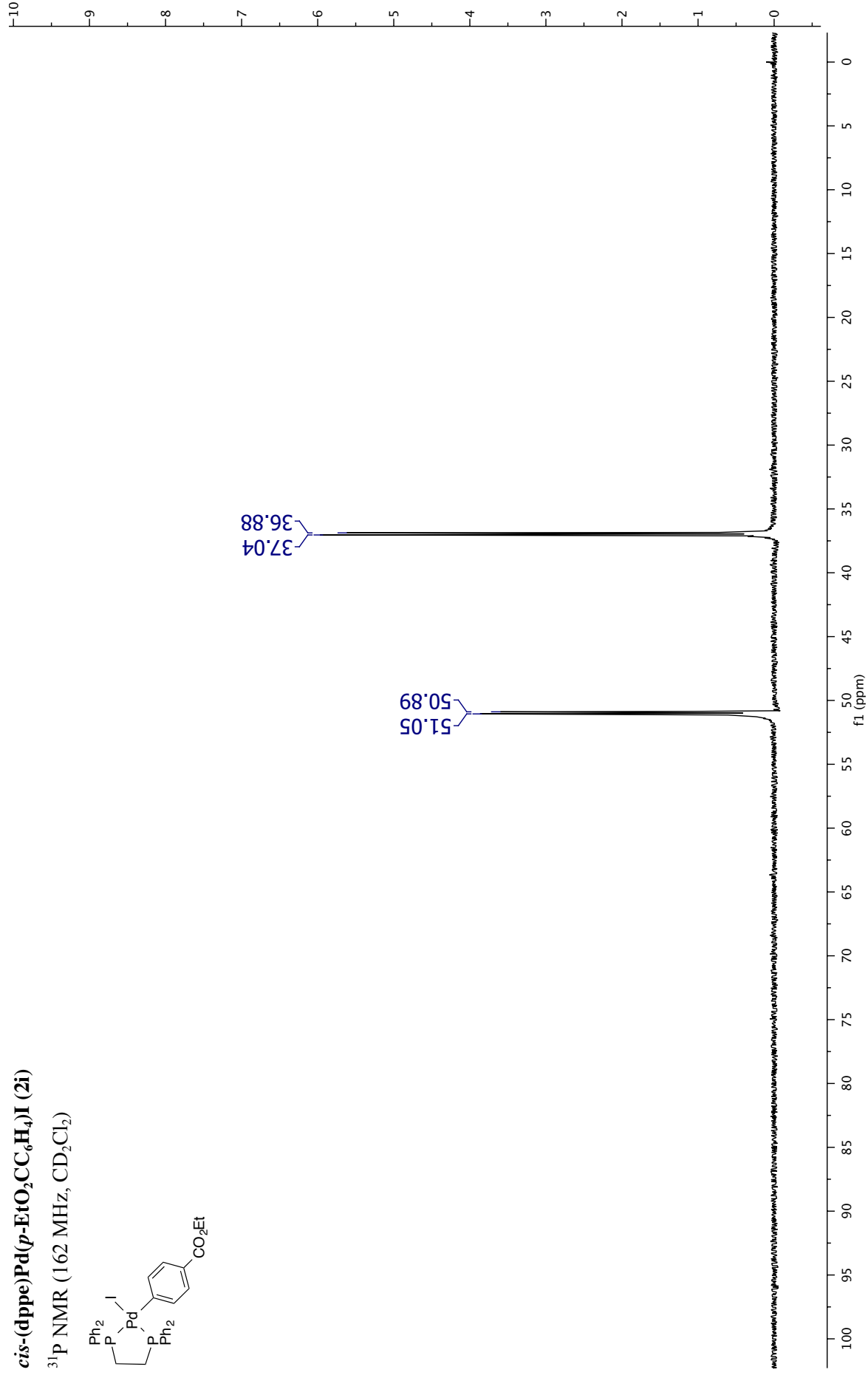
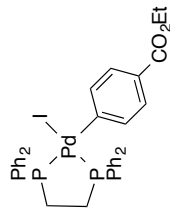
***cis*-(dppf)Pd(*p*-FC₆H₄)I (2g)**

¹⁹F NMR (376 MHz, CD₂Cl₂)



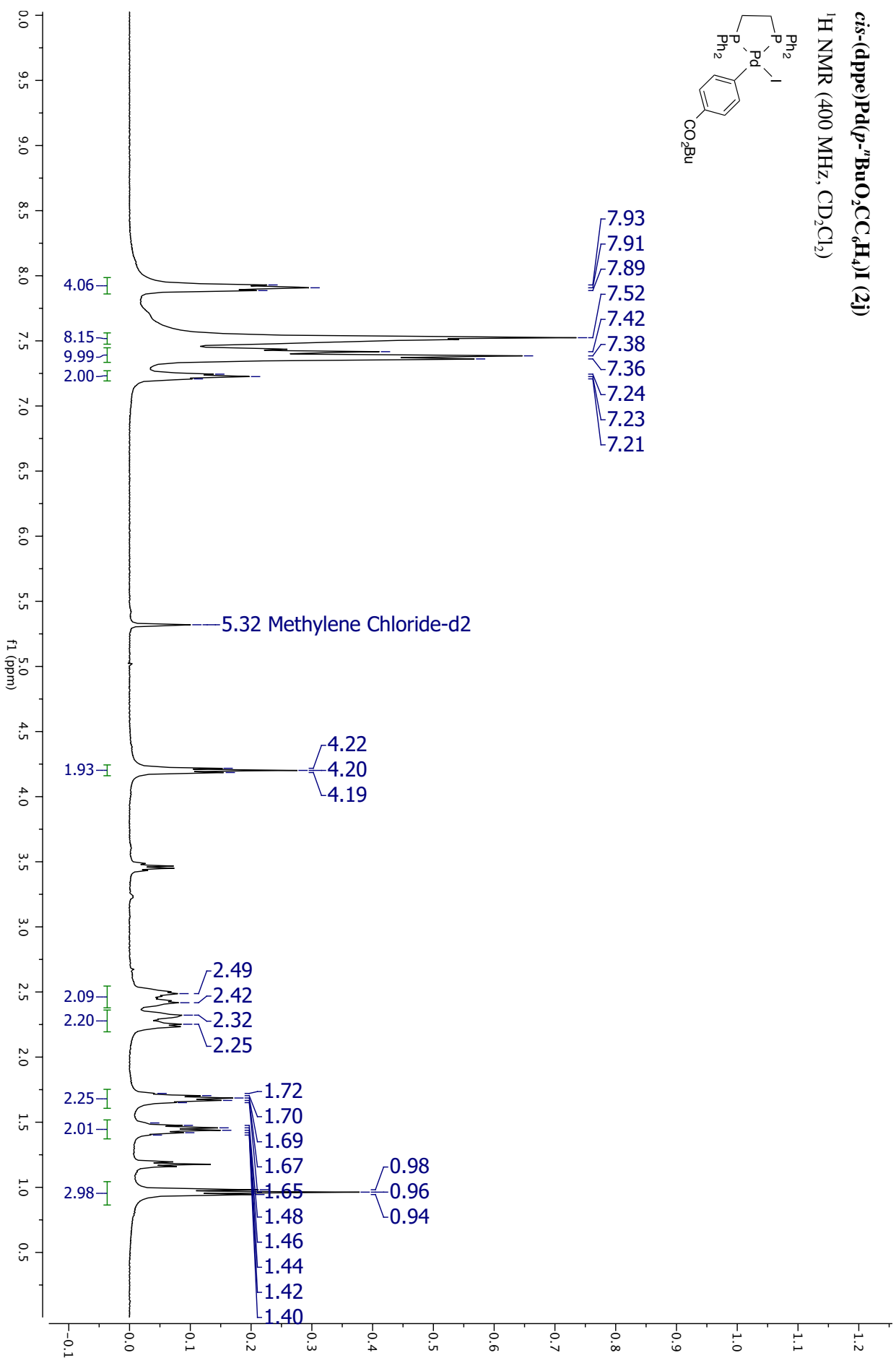
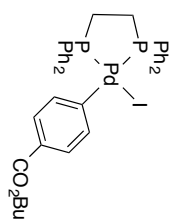
***cis*-(dpppe)Pd(*p*-EtO₂CC₆H₄)I (2i)**

³¹P NMR (162 MHz, CD₂Cl₂)



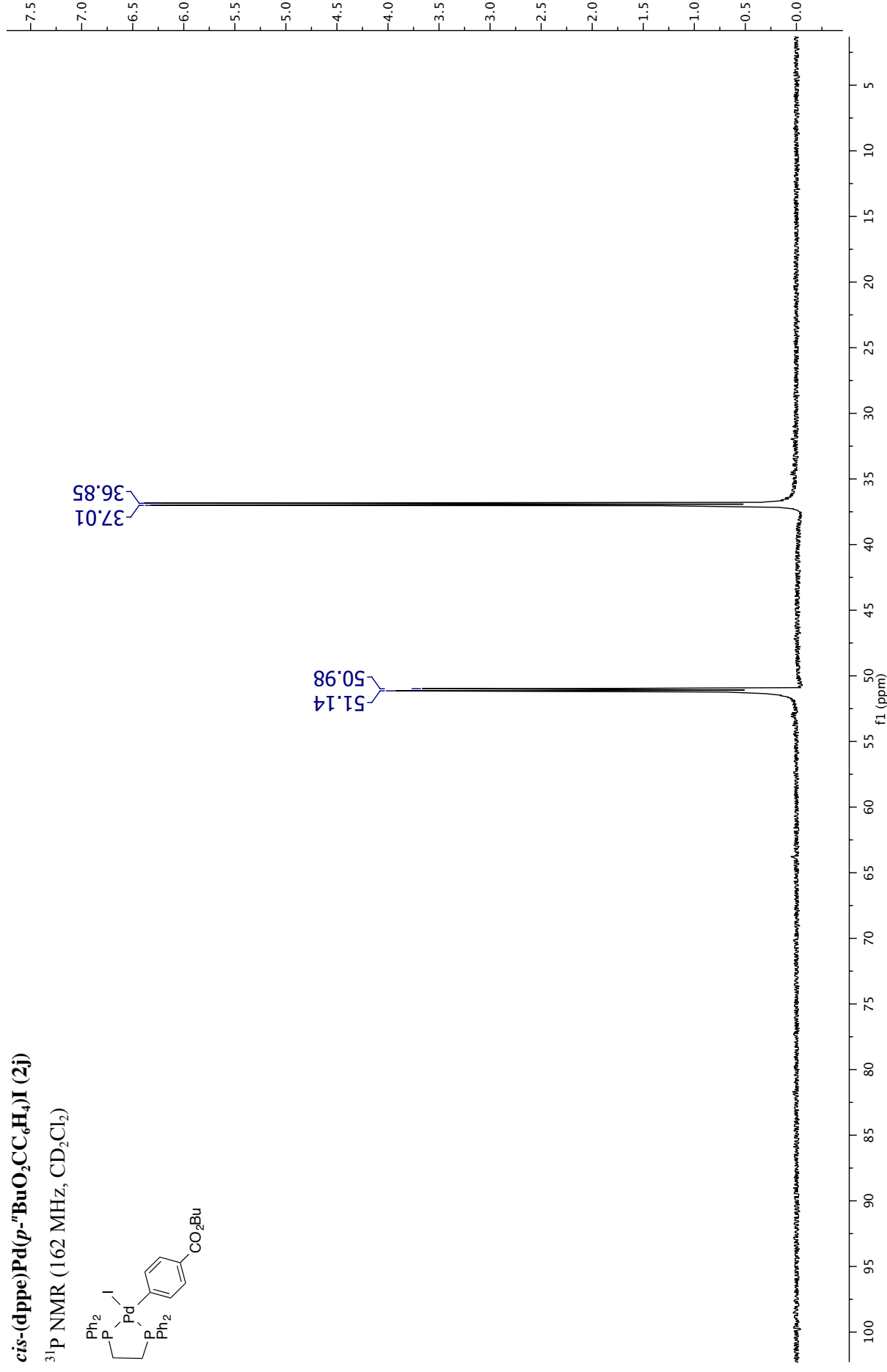
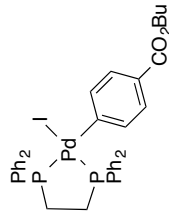
cis-(dippe)Pd(*p*-^tBuO₂CC₆H₄)I (2f)

¹H NMR (400 MHz, CD₂Cl₂)



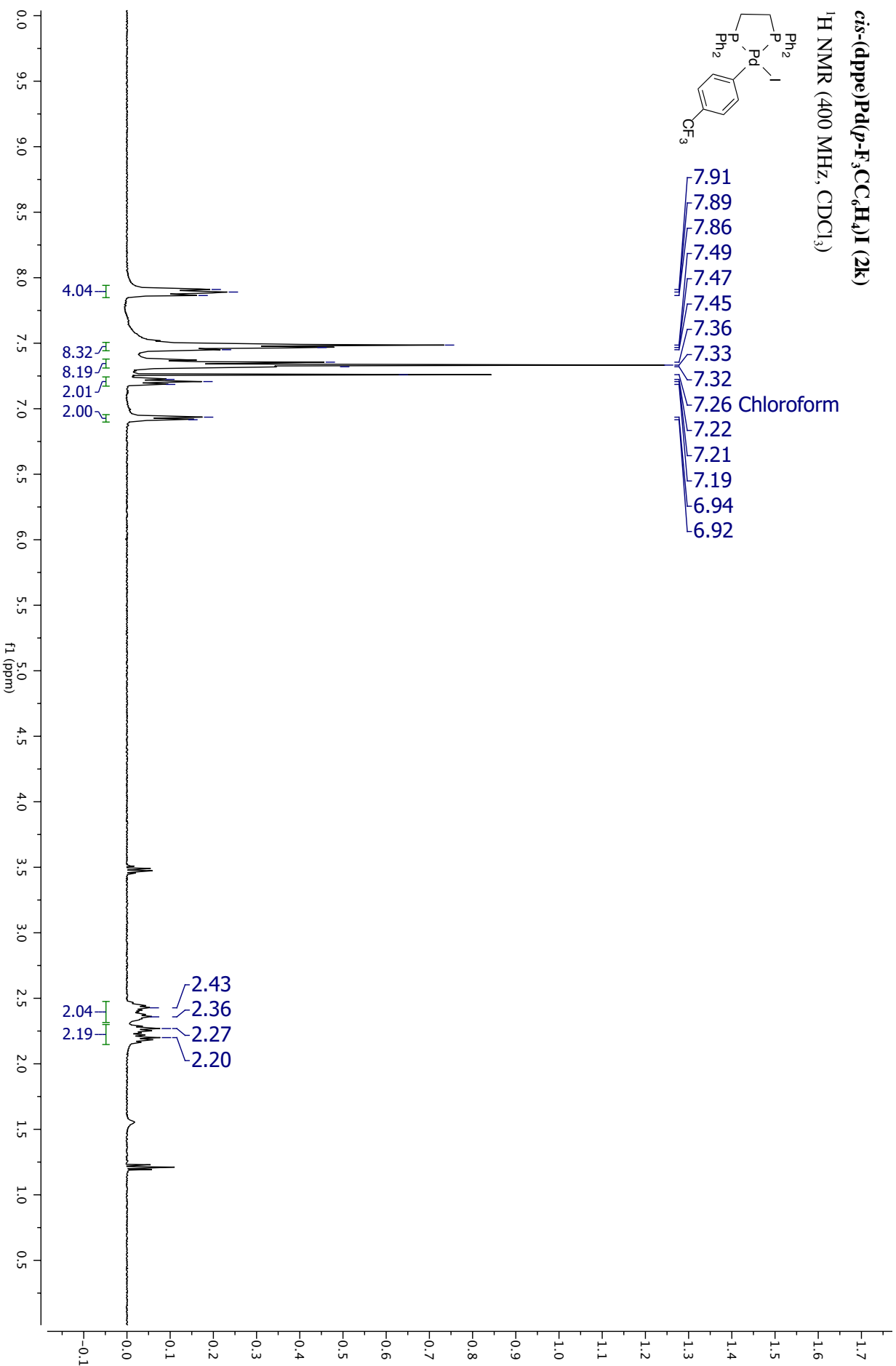
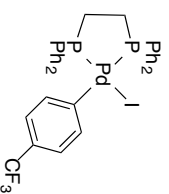
***cis*-(dppf)Pd(*p*-^tBuO₂CC₆H₄)I (2j)**

³¹P NMR (162 MHz, CD₂Cl₂)



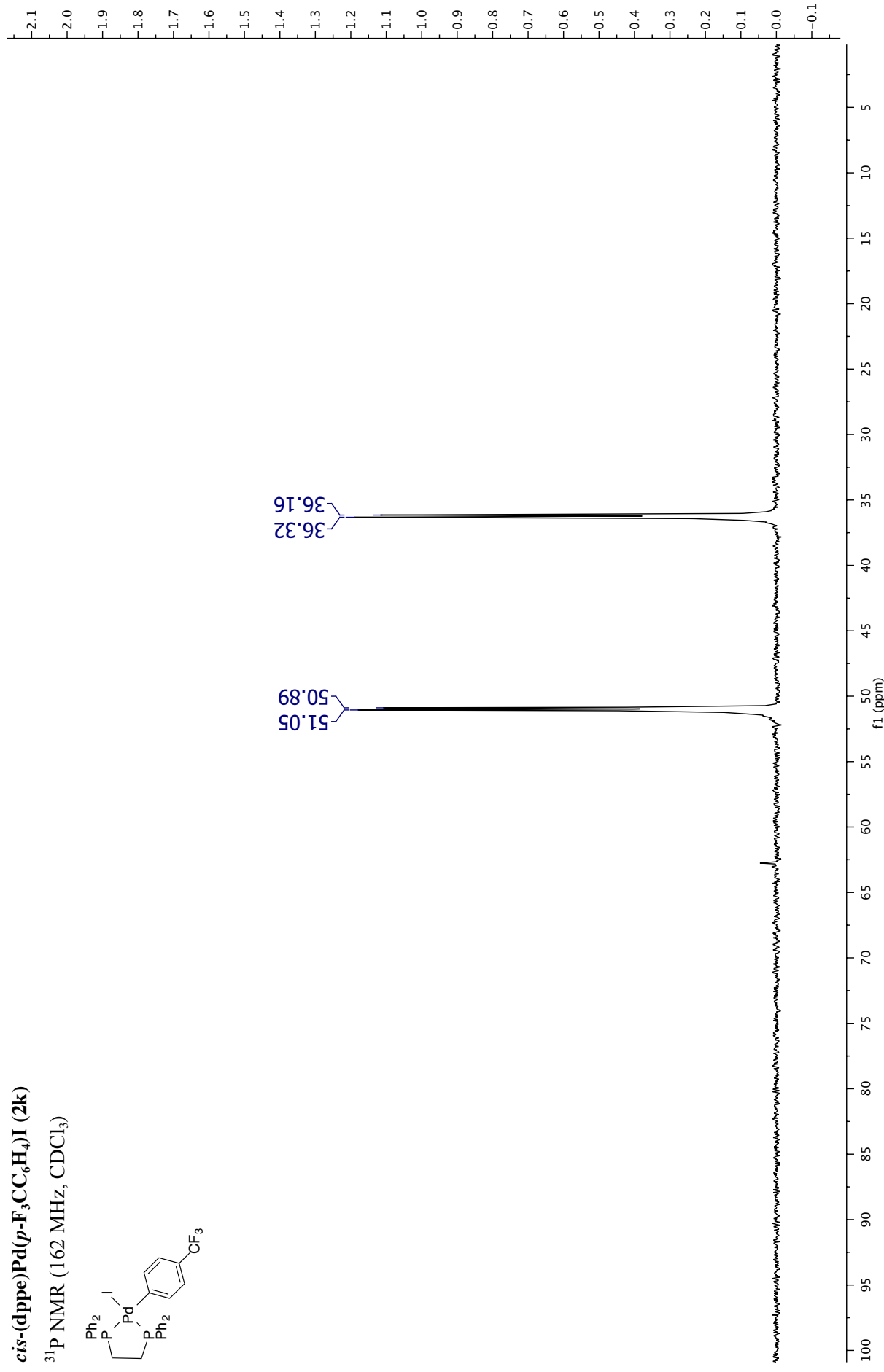
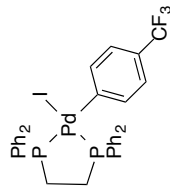
cis-(dpppe)Pd(*p*-F₃CC₆H₄)I (**2k**)

¹H NMR (400 MHz, CDCl₃)



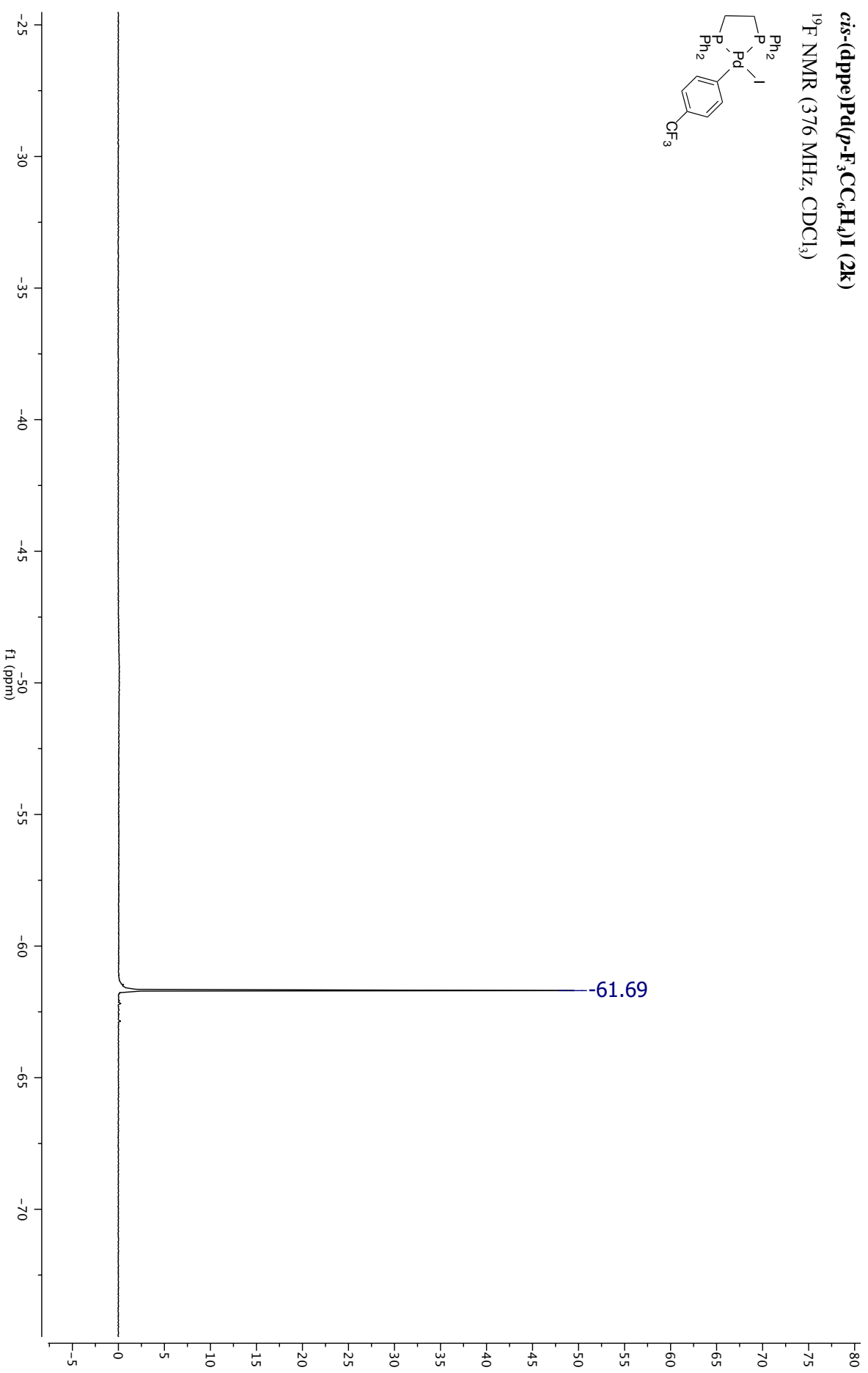
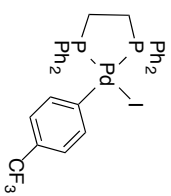
***cis*-(dppf)Pd(*p*-F₃CC₆H₄)I (2k)**

³¹P NMR (162 MHz, CDCl₃)



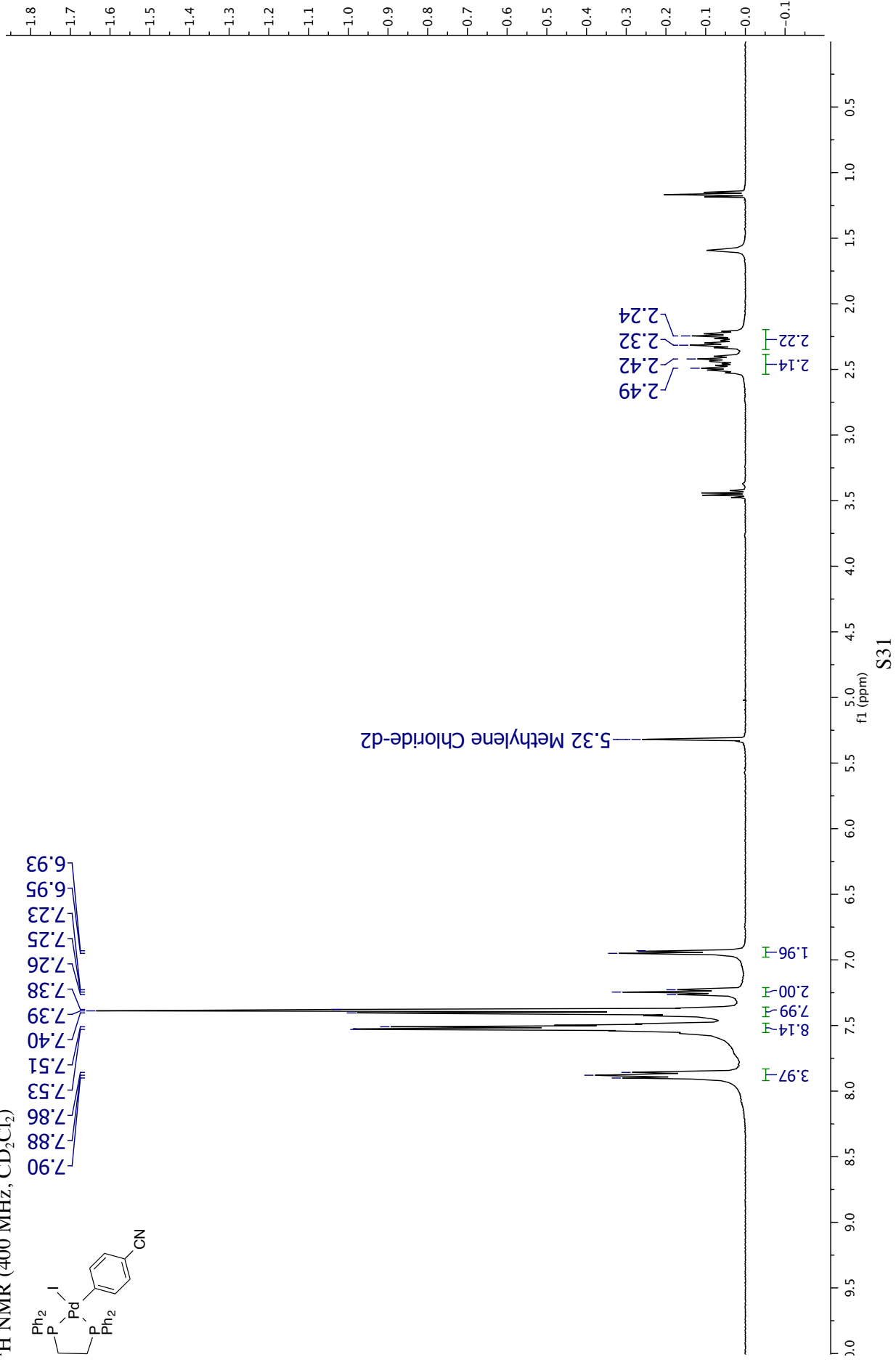
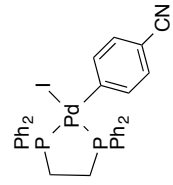
***cis*-(dpppe)Pd(*p*-F₃CC₆H₄)I (2k)**

¹⁹F NMR (376 MHz, CDCl₃)



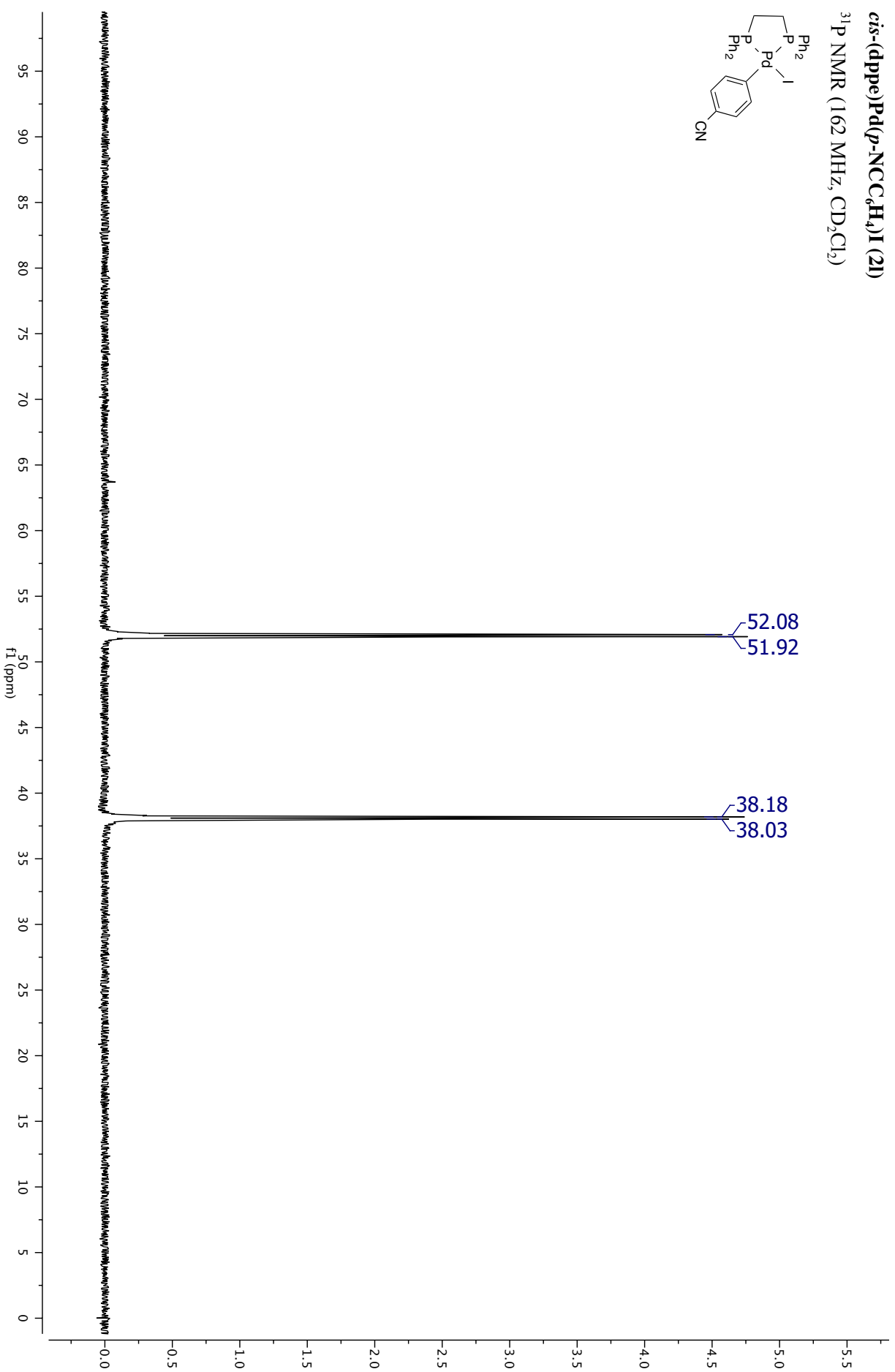
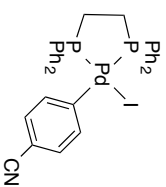
***cis*-(dippe)Pd(*p*-NC₆H₄)I (2I)**

¹H NMR (400 MHz, CD₂Cl₂)



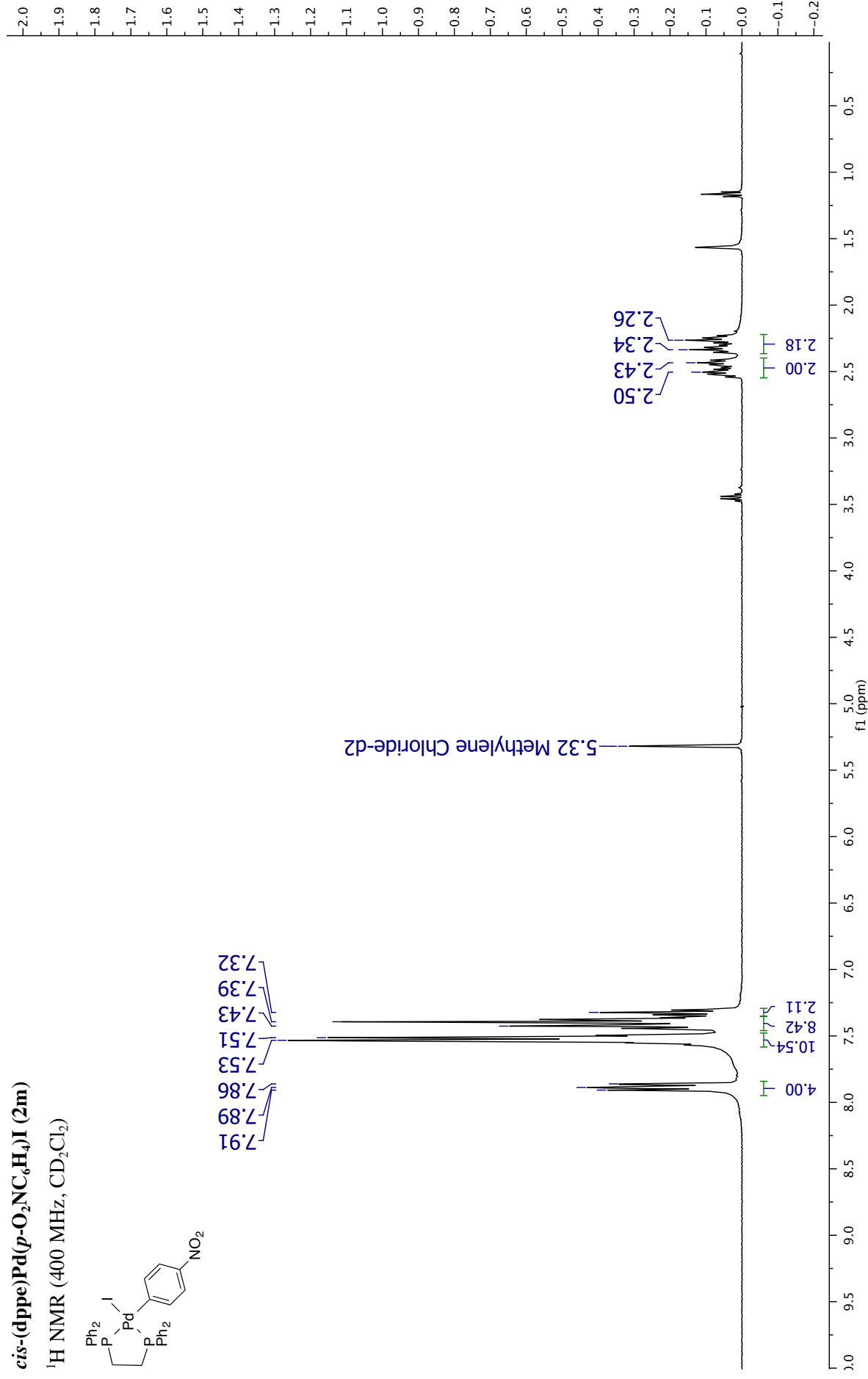
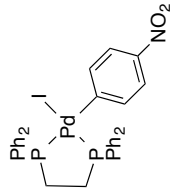
cis-(dpppe)Pd(*p*-NCC₆H₄)I (**21**)

³¹P NMR (162 MHz, CD₂Cl₂)



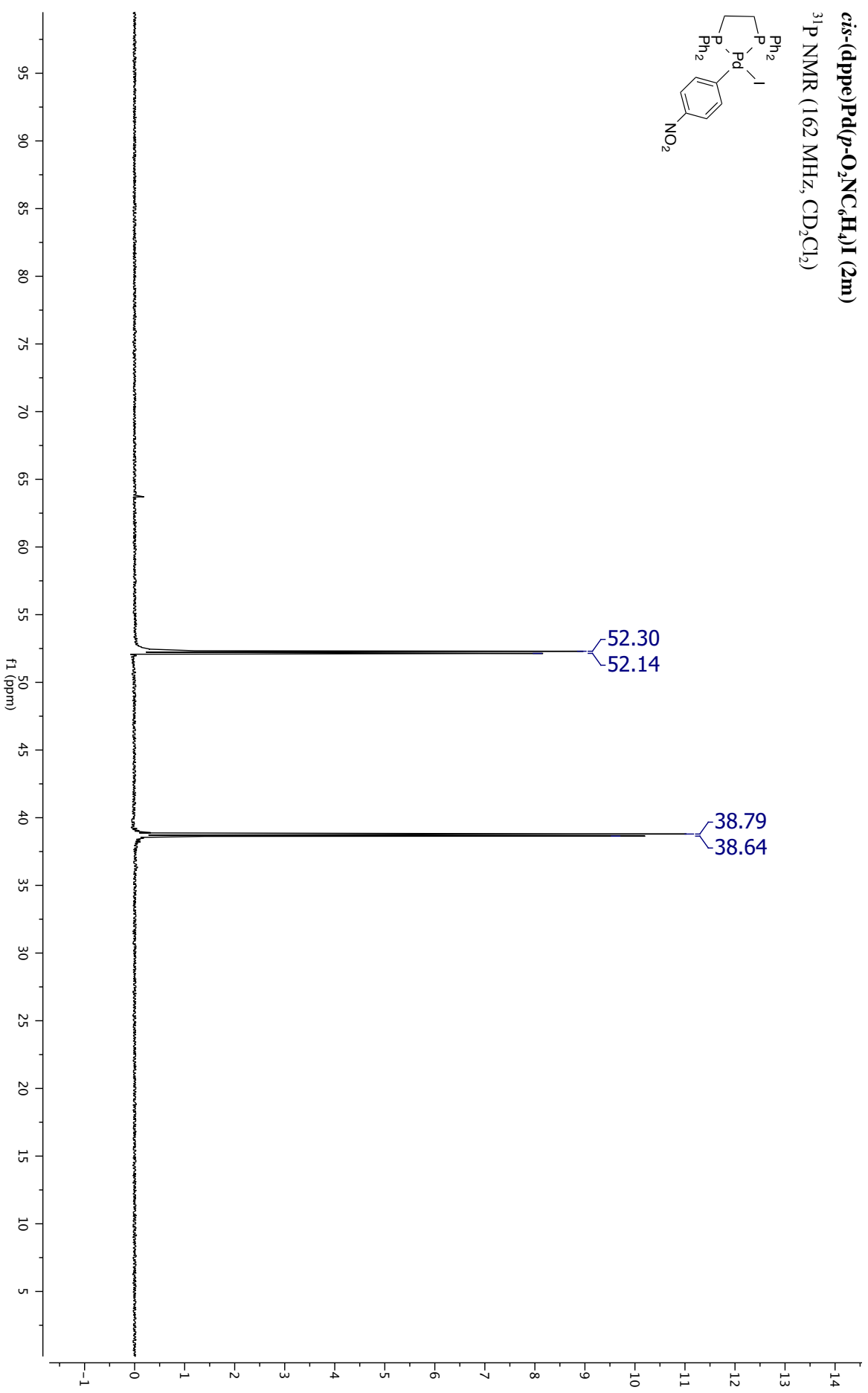
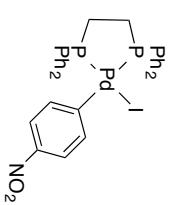
***cis*-(dpppe)Pd(*p*-O₂NC₆H₄)I (2m)**

¹H NMR (400 MHz, CD₂Cl₂)



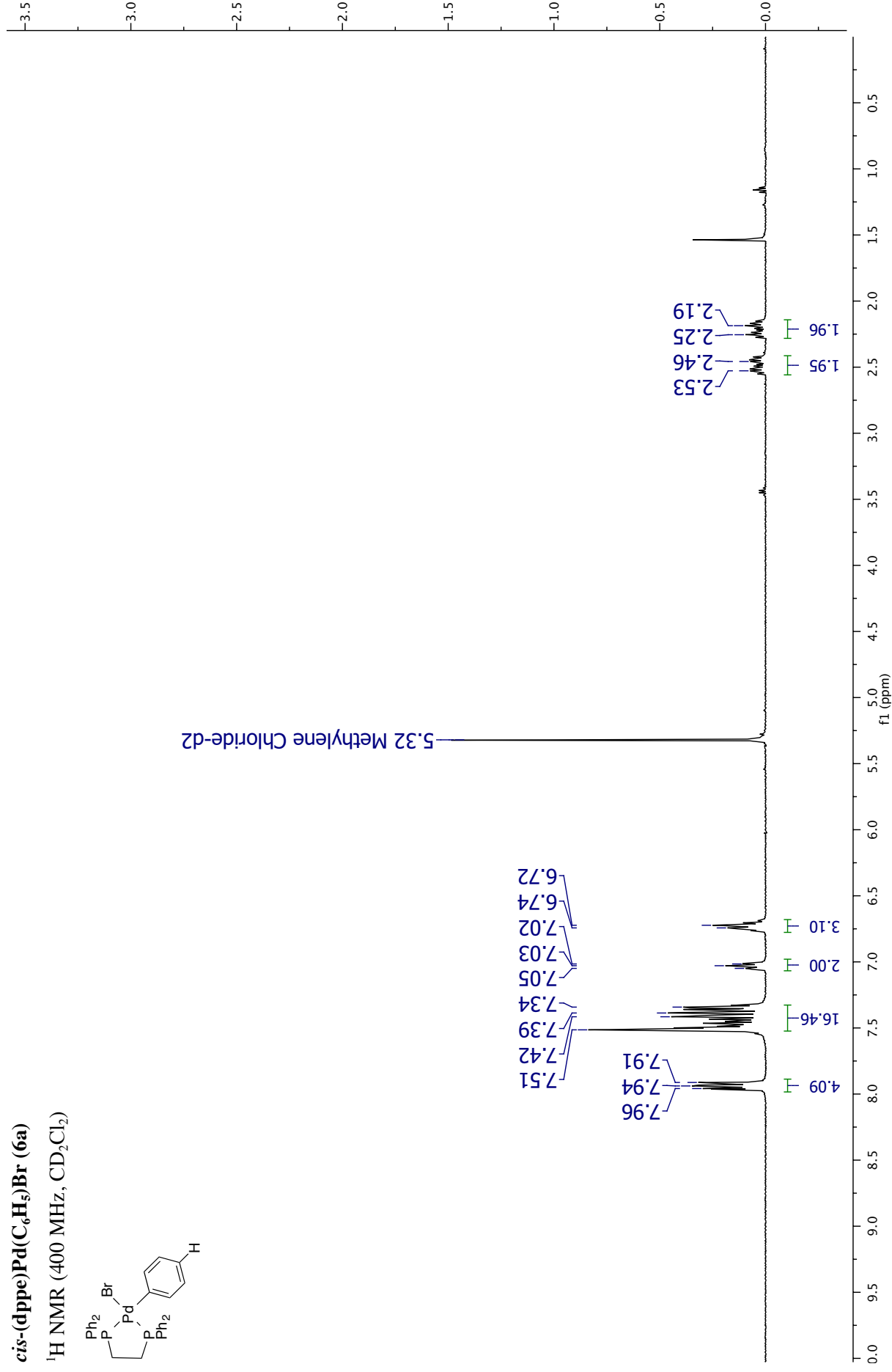
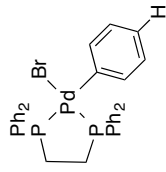
cis-(dippe)Pd(*p*-O₂NC₆H₄)I (2m)

³¹P NMR (162 MHz, CD₂Cl₂)



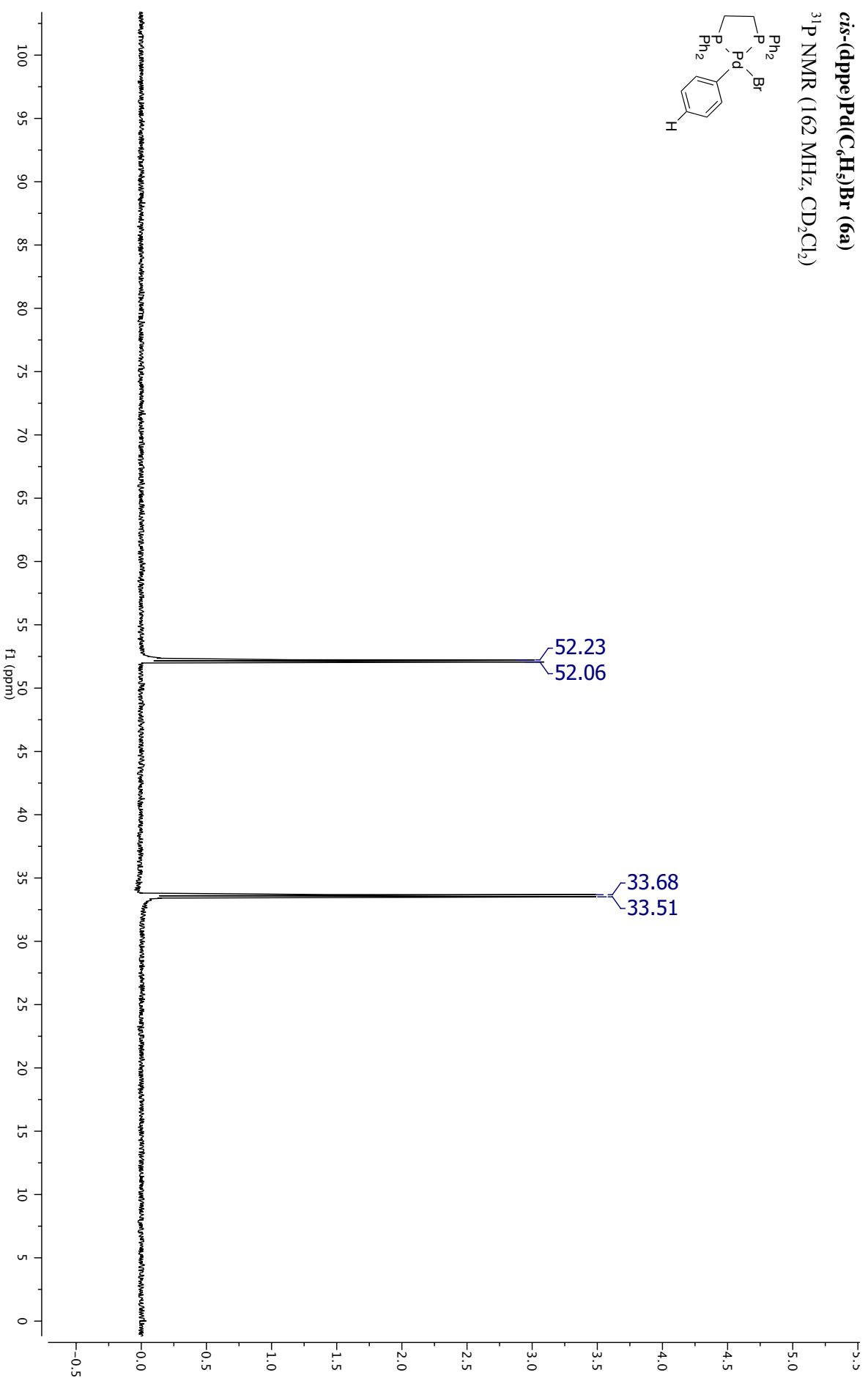
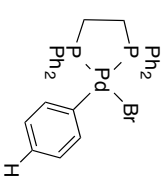
***cis*-(dippe)Pd(C₆H₅)Br (6a)**

¹H NMR (400 MHz, CD₂Cl₂)



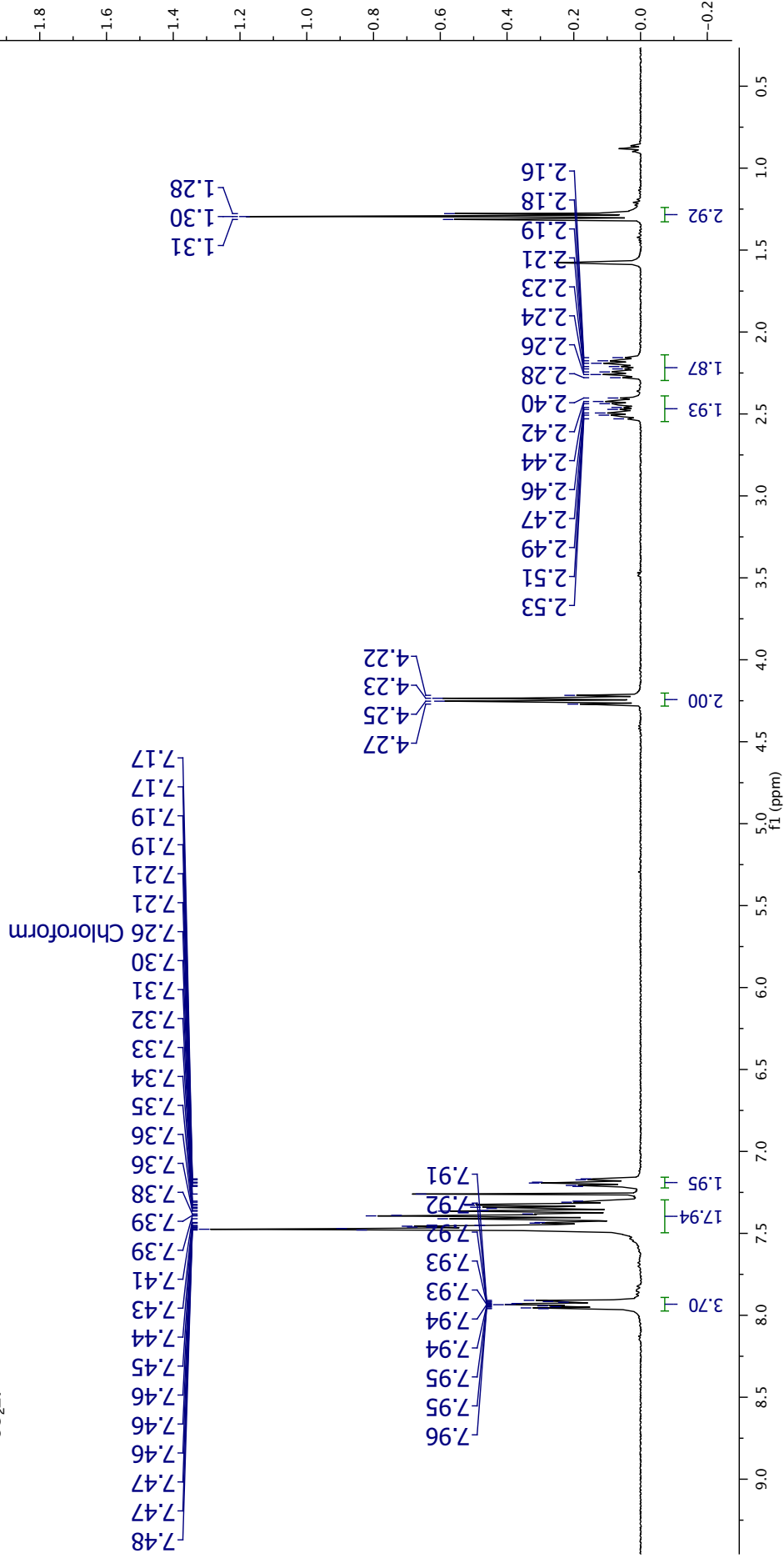
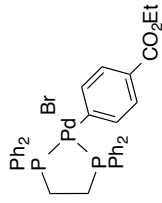
cis-(dippe)Pd(C₆H₅)Br (**6a**)

³¹P NMR (162 MHz, CD₂Cl₂)



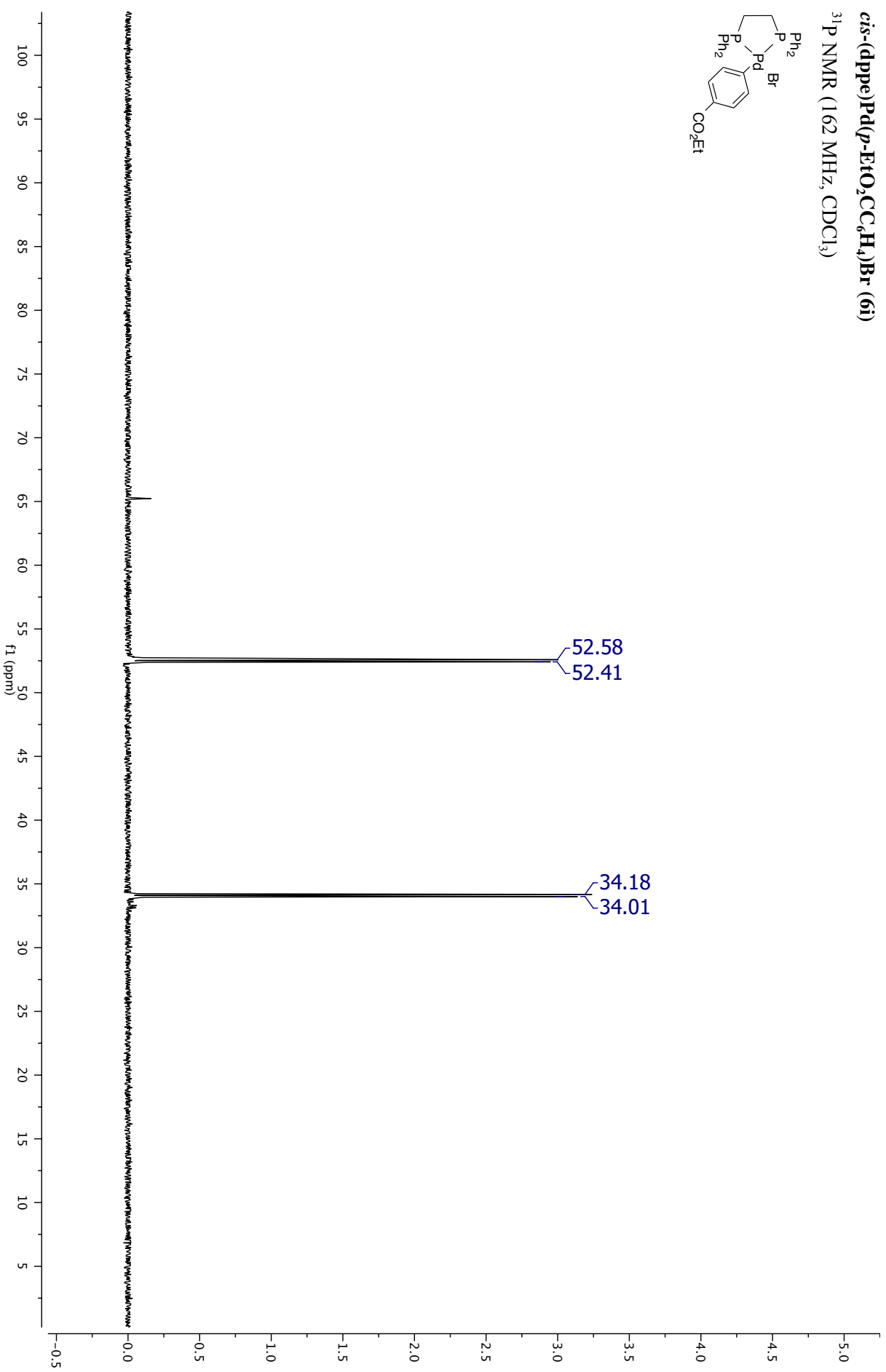
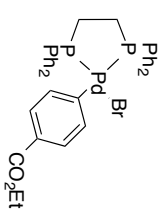
***cis*-(dppf)Pd(*p*-EtO₂CC₆H₄)Br (6i)**

¹H NMR (400 MHz, CDCl₃)



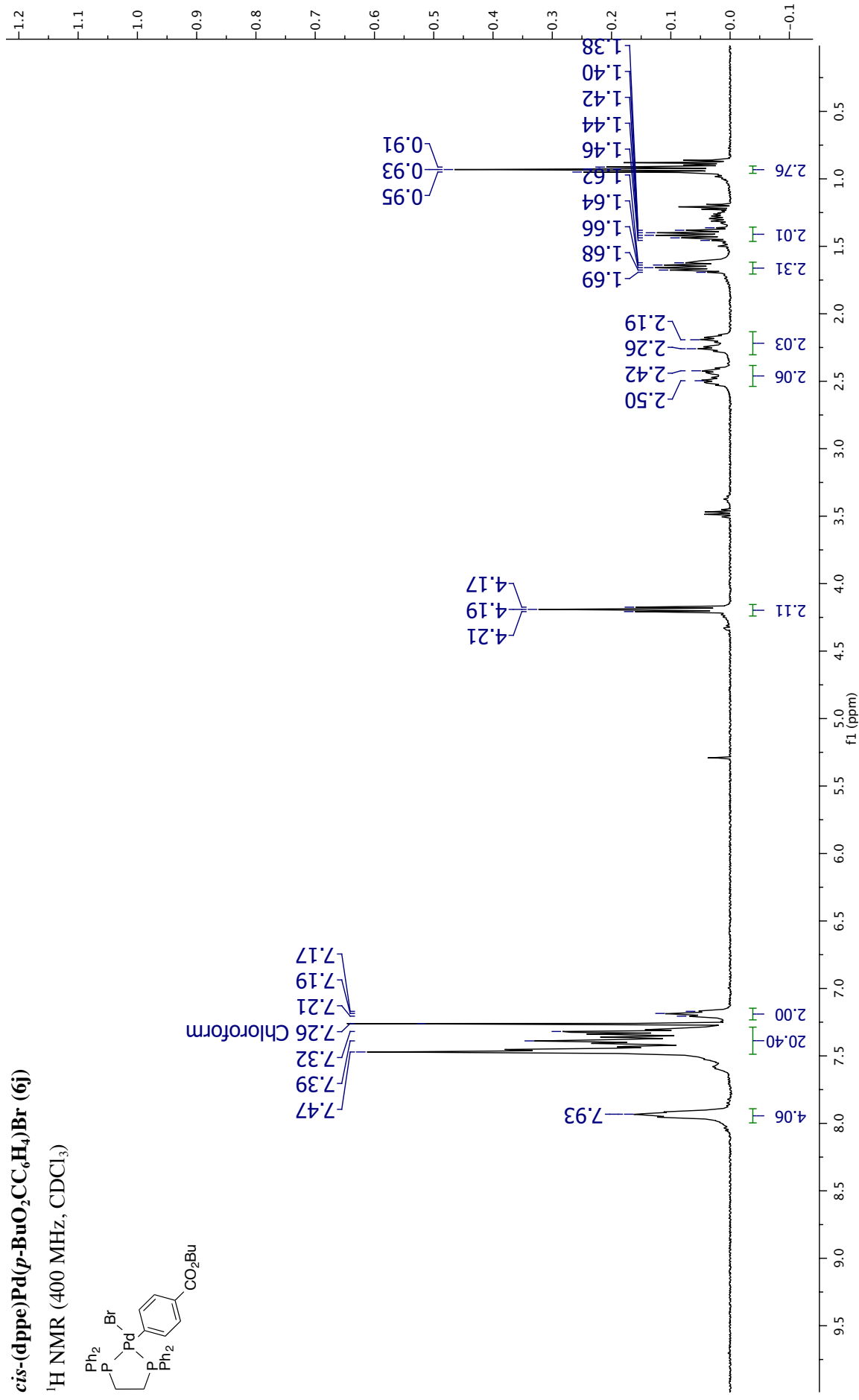
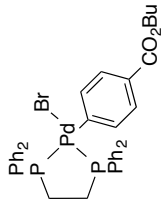
cis-(dpppe)Pd(*p*-EtO₂CC₆H₄)Br (**6i**)

³¹P NMR (162 MHz, CDCl₃)



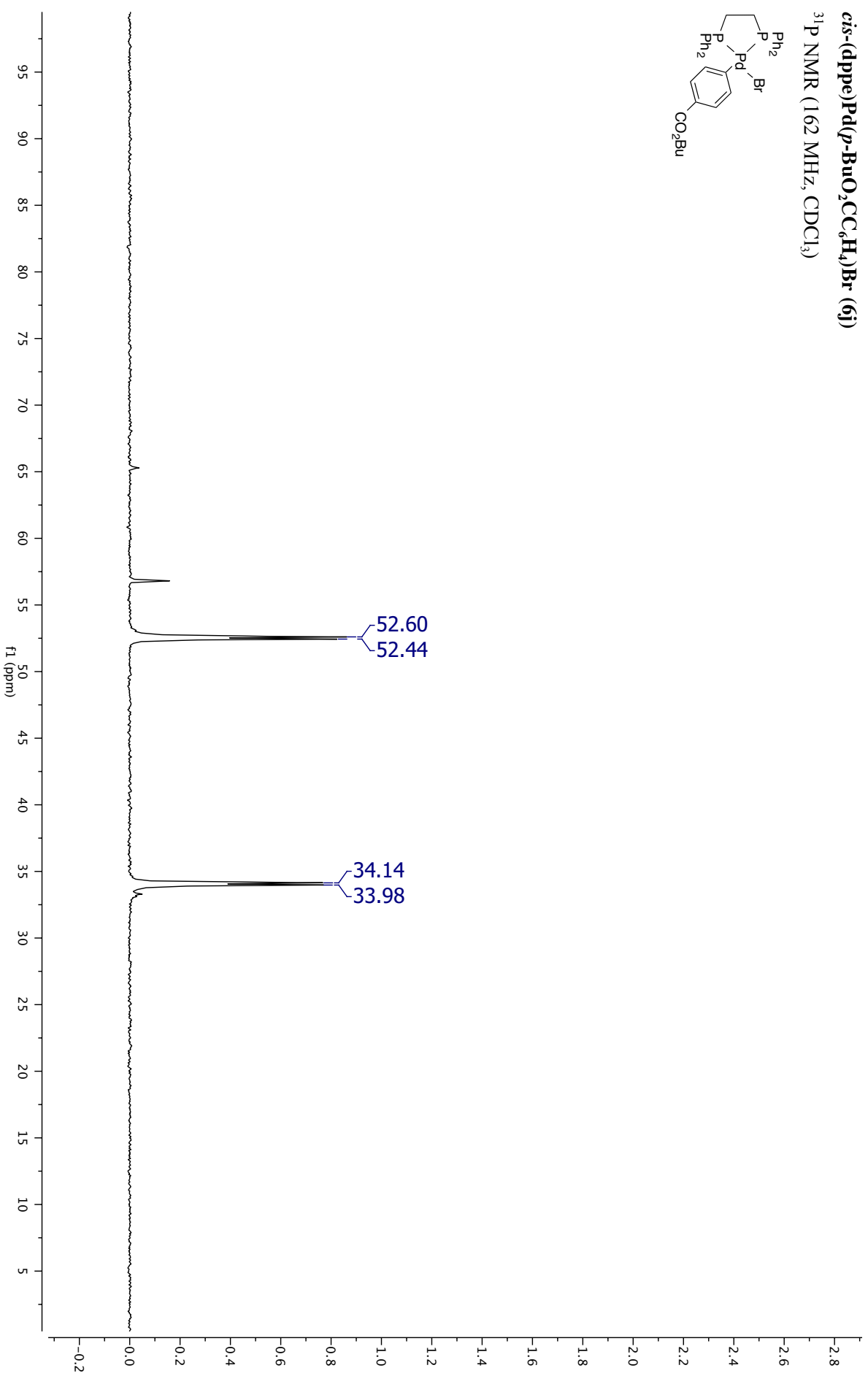
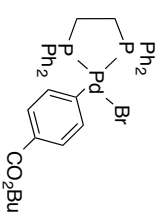
***cis*-(dpppe)Pd(*p*-BuO₂C₆H₄)Br (6j)**

¹H NMR (400 MHz, CDCl₃)



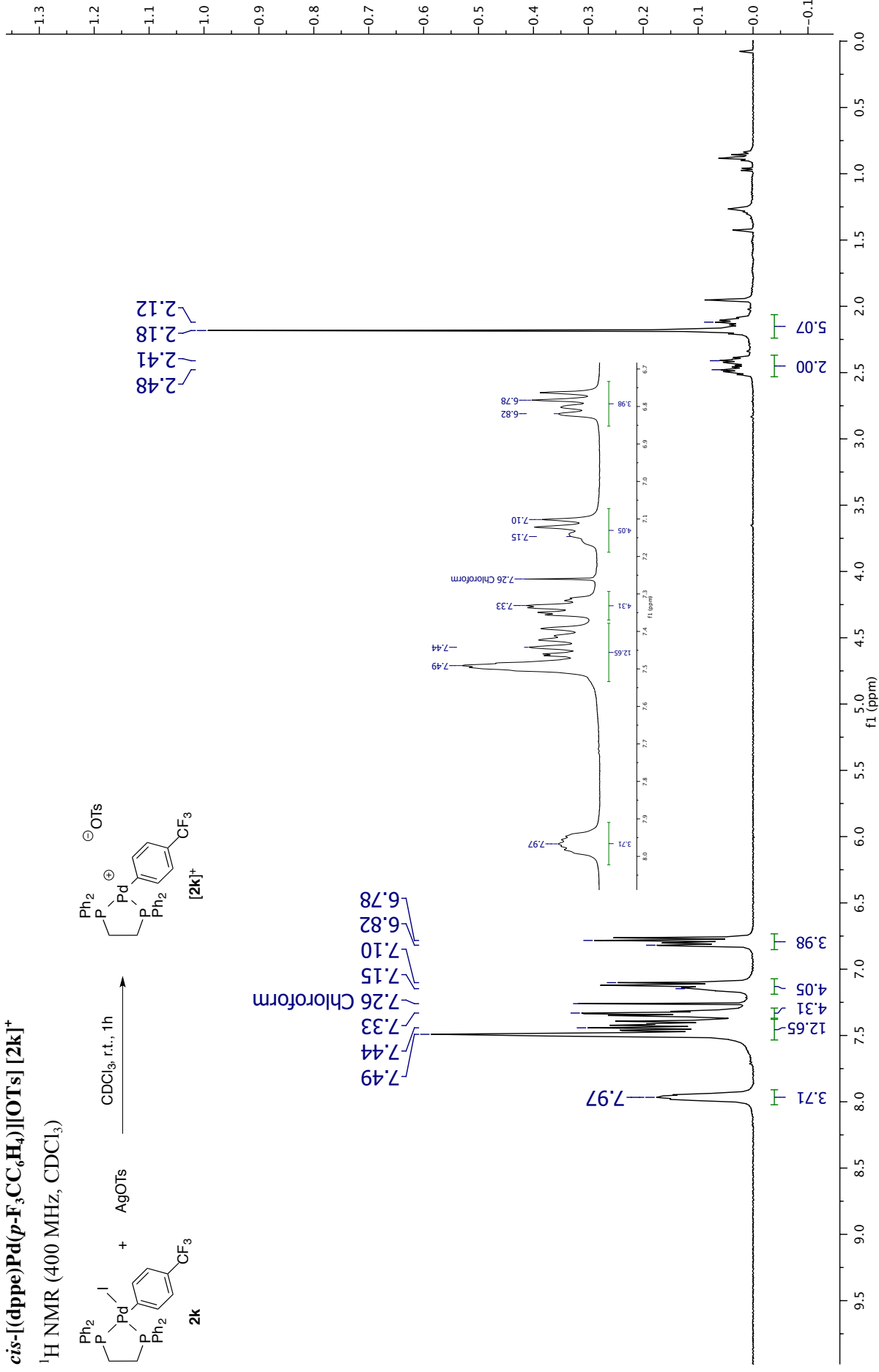
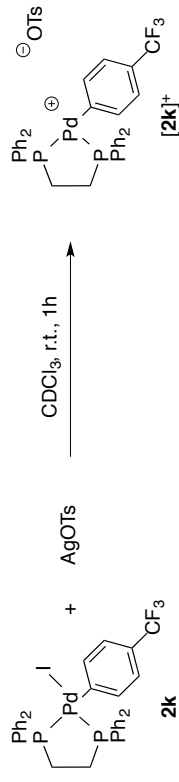
***cis*-(dippe)Pd(*p*-BuO₂CC₆H₄)Br (6j)**

³¹P NMR (162 MHz, CDCl₃)



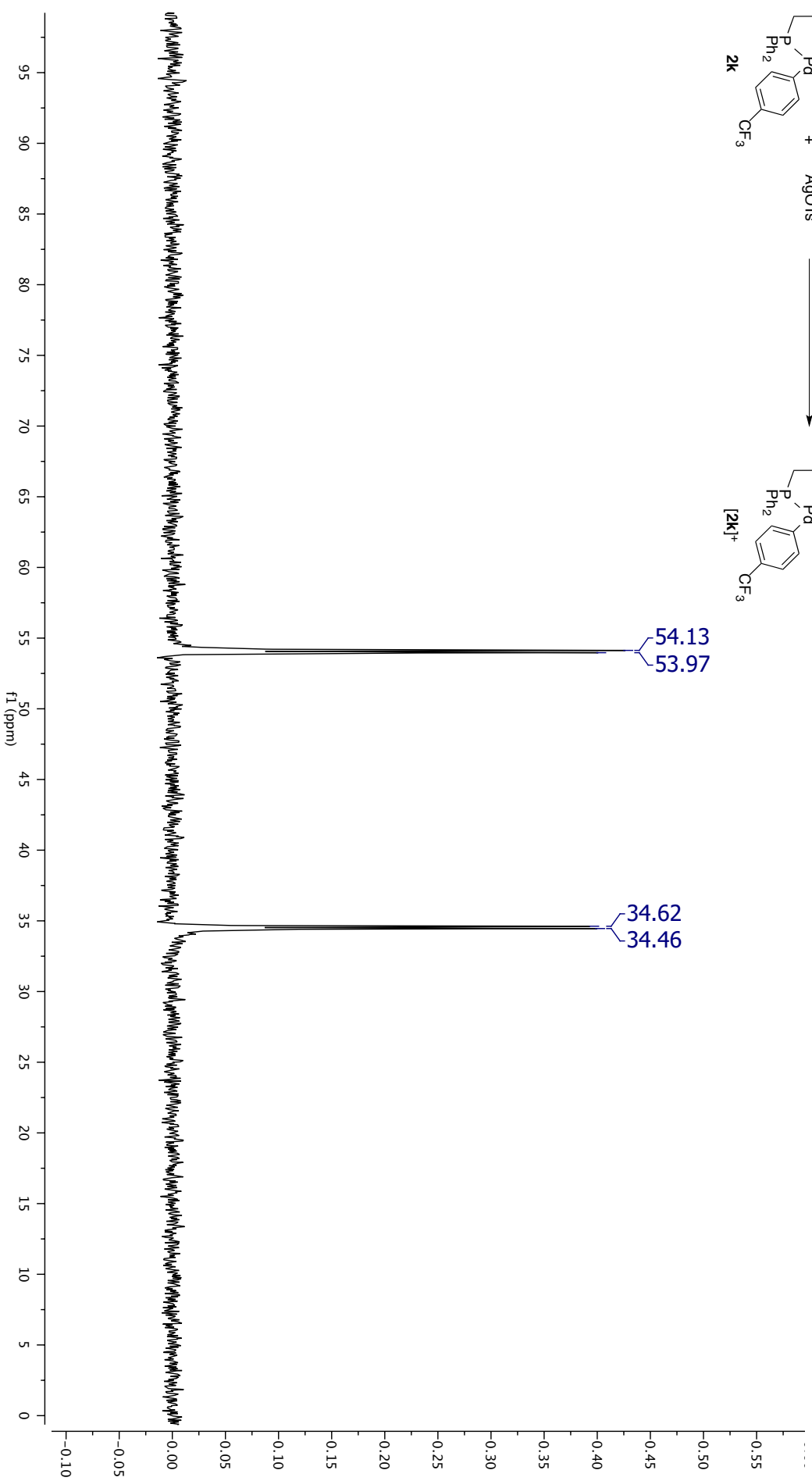
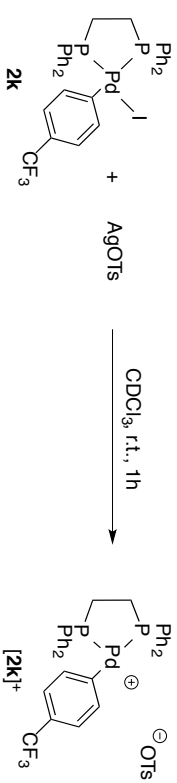
cis-[(dippe)Pd(*p*-F₃CC₆H₄)]OTs] [2k]⁺

¹H NMR (400 MHz, CDCl₃)



cis-[(dpppe)Pd(*p*-F₃CC₆H₄)][OTs]⁺ [2k]⁺

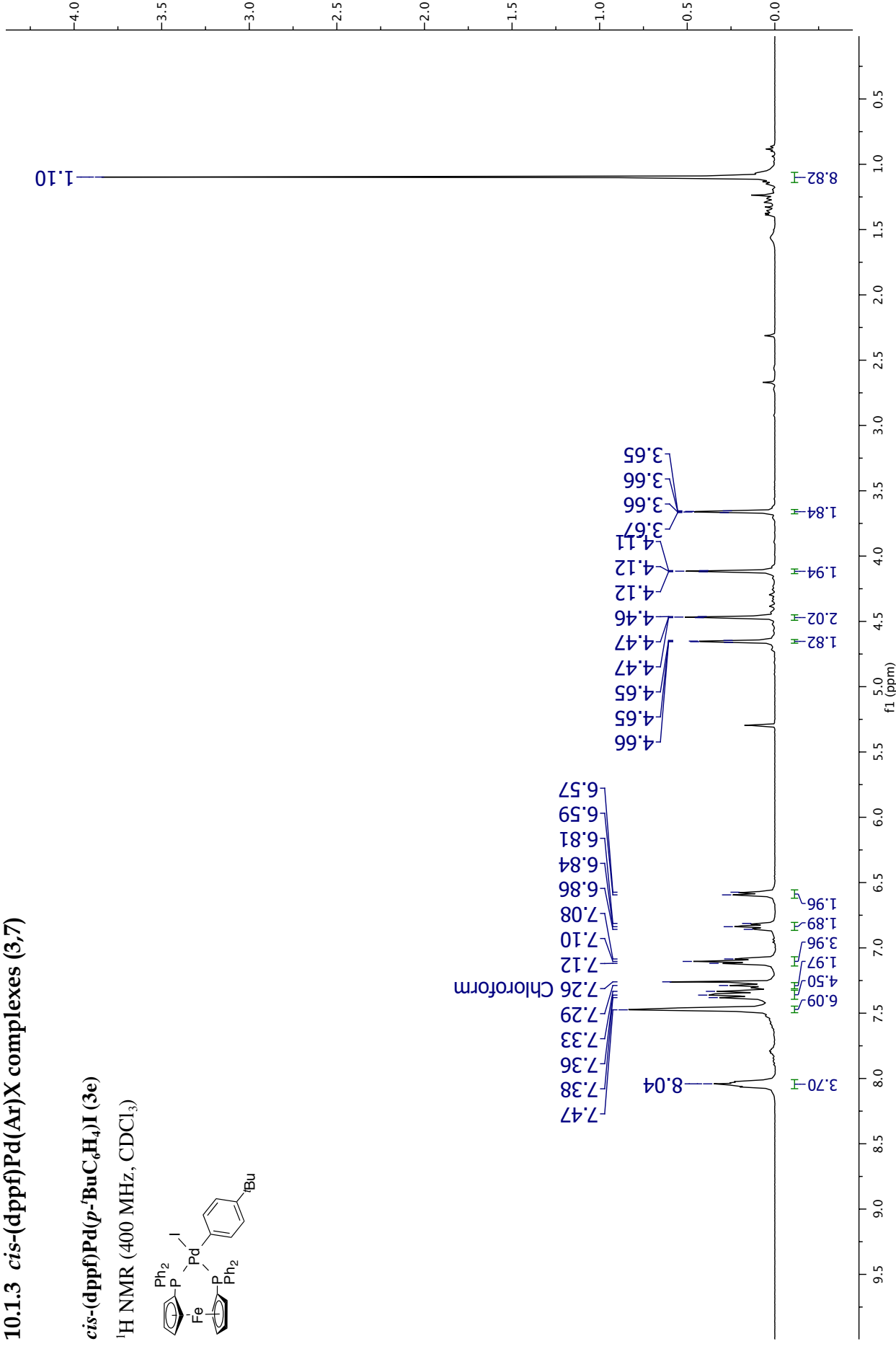
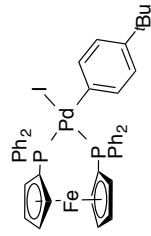
³¹P NMR (162 MHz, CDCl₃)



10.1.3 *cis*-(dpppf)Pd(Ar)X complexes (3,7)

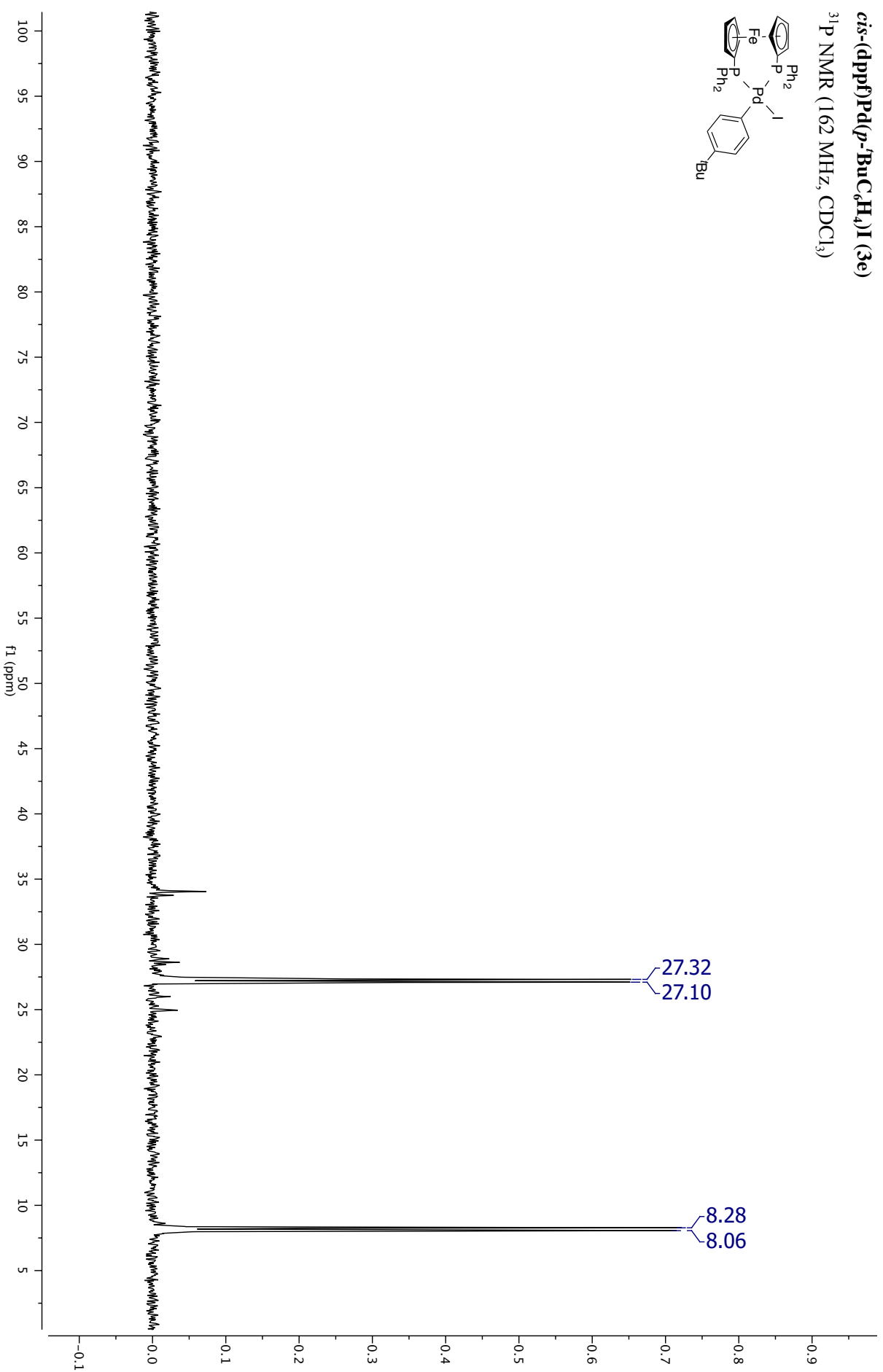
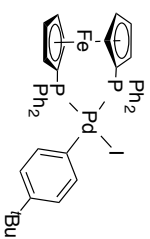
cis-(dpppf)Pd(*p*-BuC₆H₄)I (3e)

¹H NMR (400 MHz, CDCl₃)



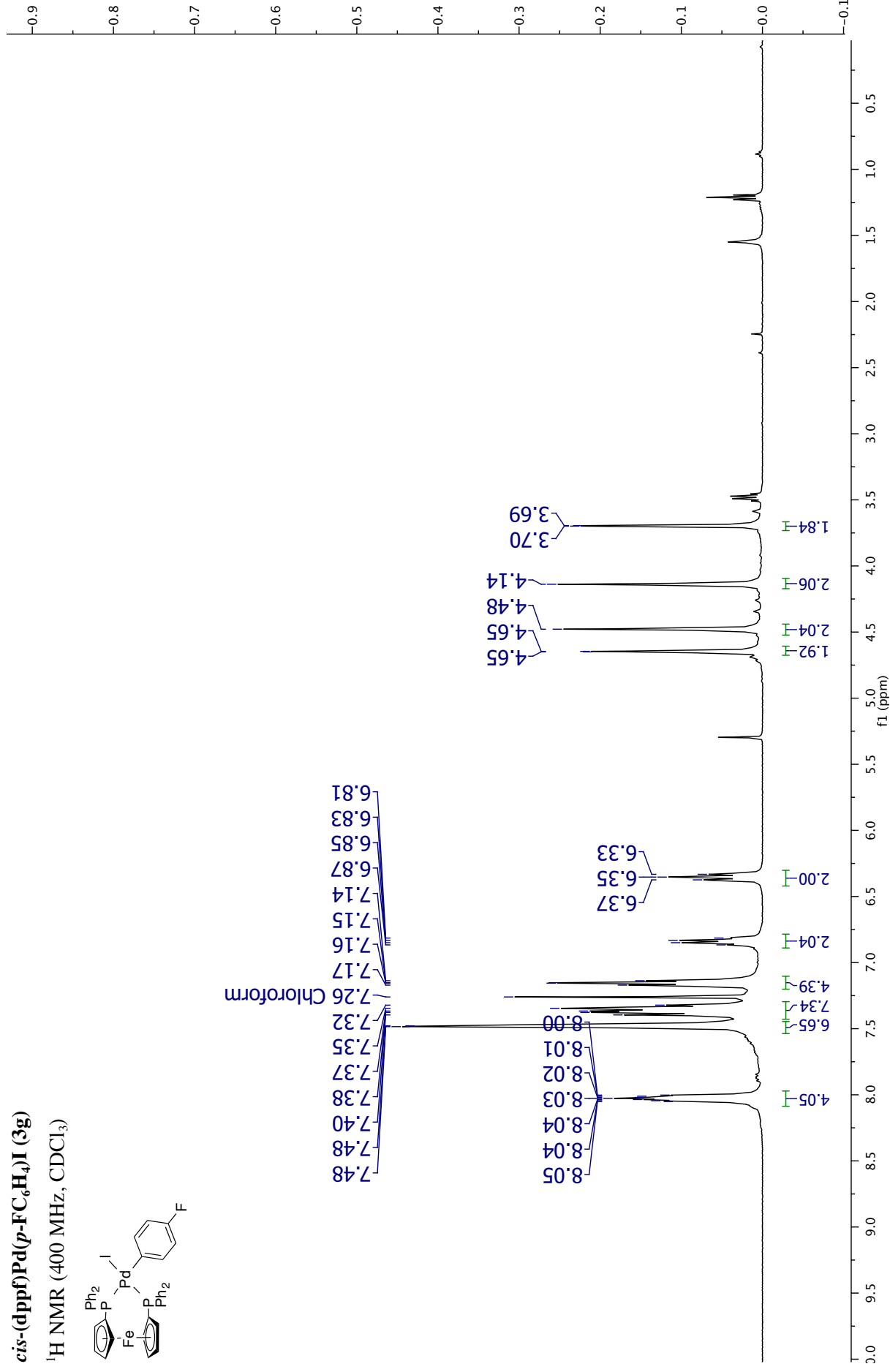
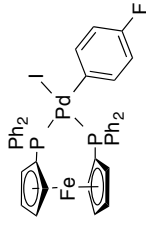
cis-(dppf)Pd(*p*-^tBuC₆H₄)I (**3e**)

³¹P NMR (162 MHz, CDCl₃)



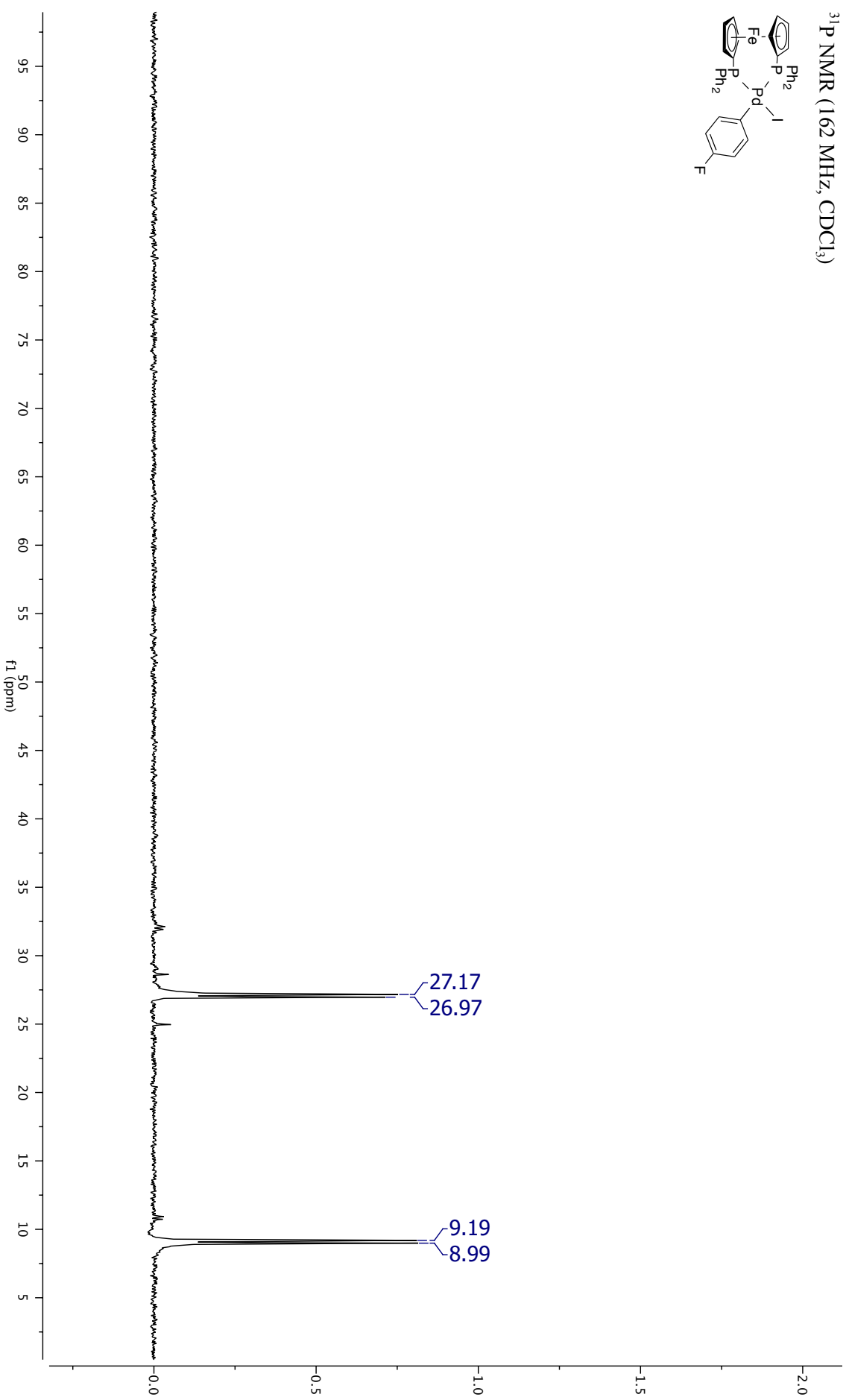
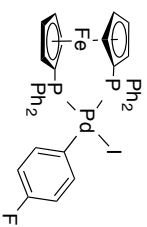
***cis*-(dppf)Pd(*p*-FC₆H₄)I (3g)**

¹H NMR (400 MHz, CDCl₃)



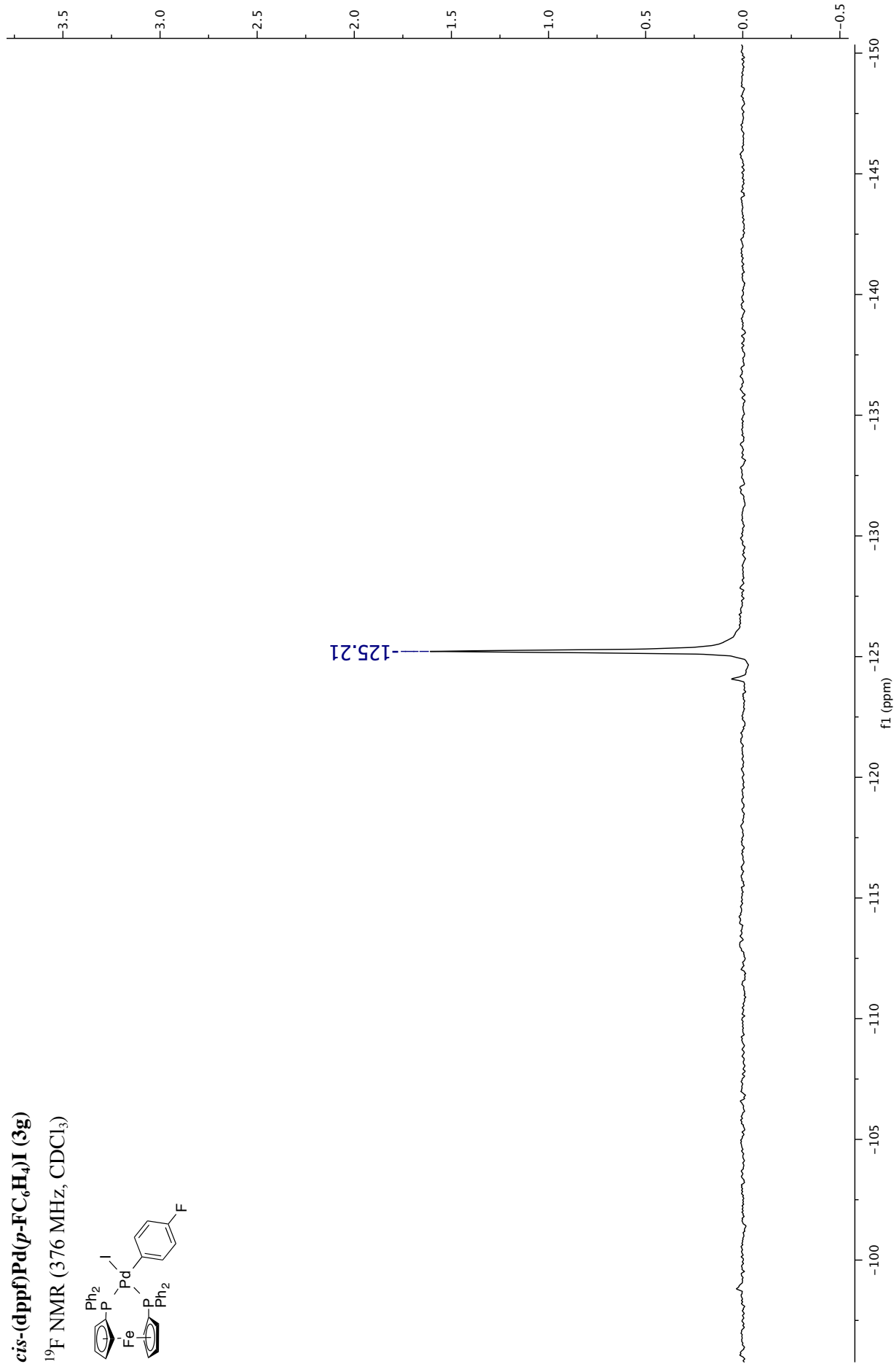
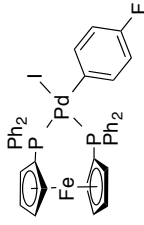
***cis*-(dppf)Pd(*p*-FC₆H₄)I (**3g**)**

³¹P NMR (162 MHz, CDCl₃)



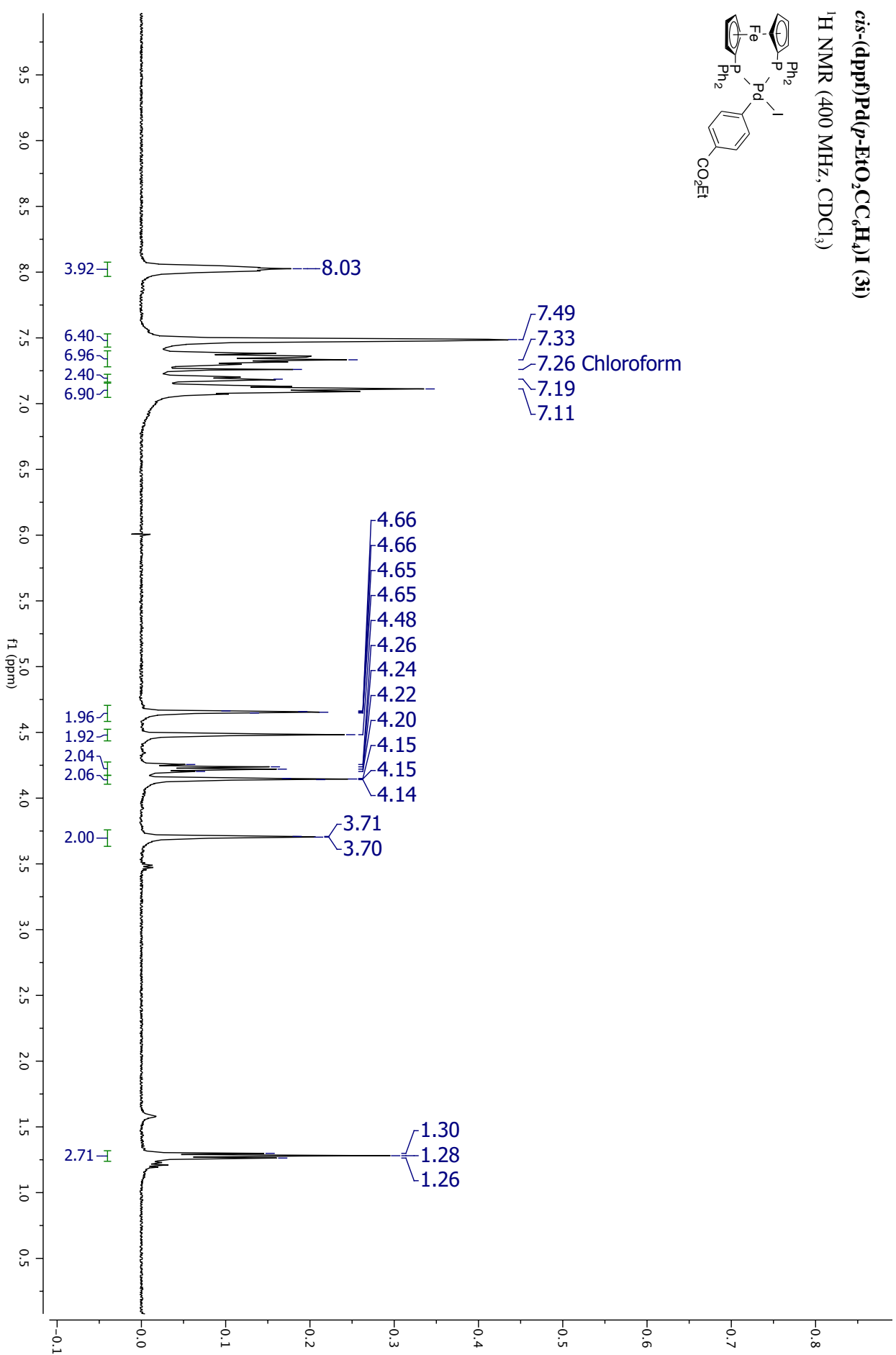
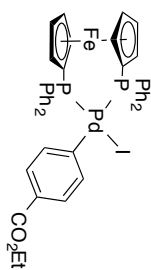
***cis*-(dppf)Pd(*p*-FC₆H₄)I (3g)**

¹⁹F NMR (376 MHz, CDCl₃)



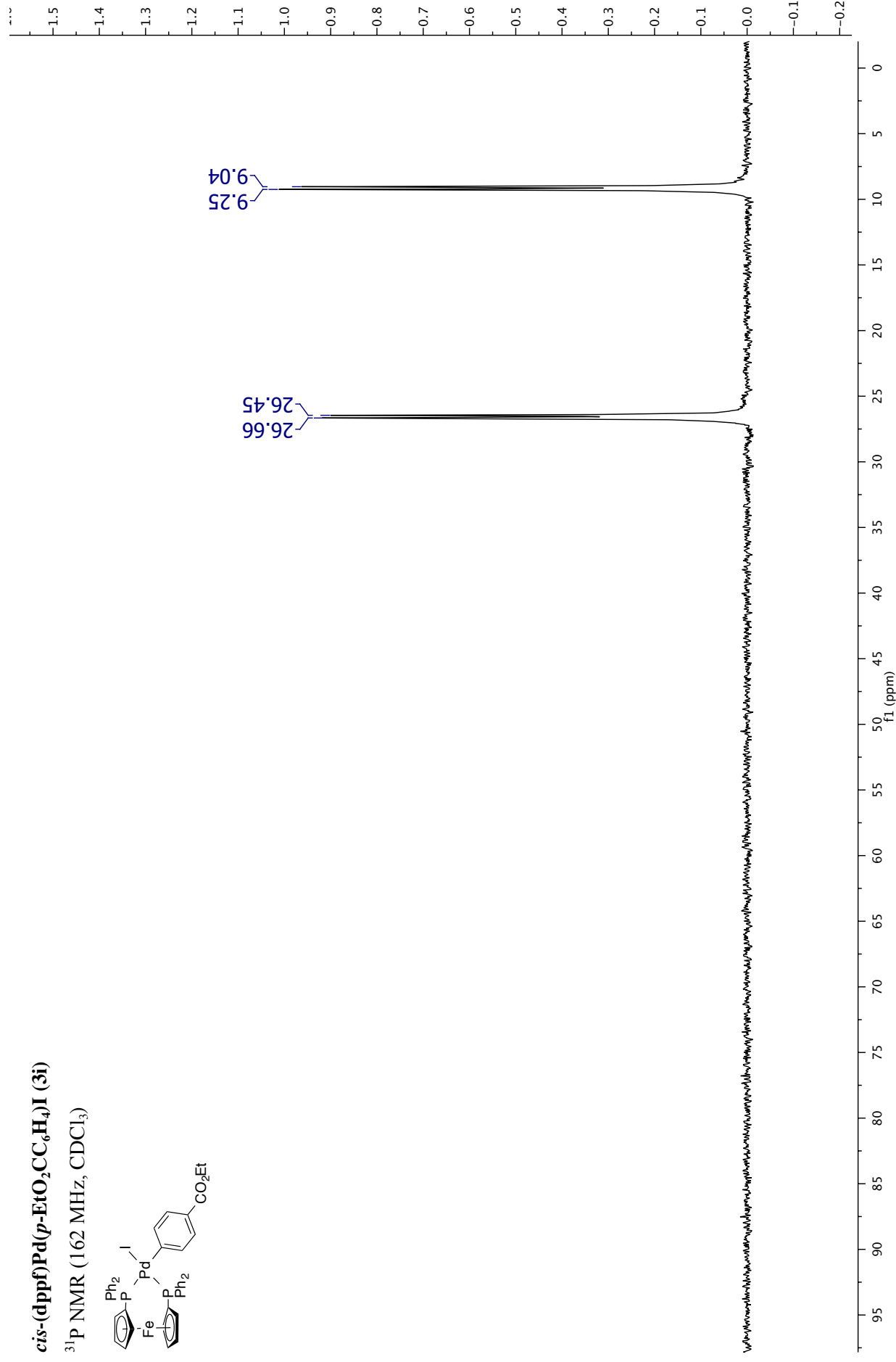
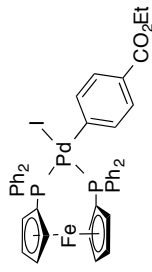
cis-(dppf)Pd(*p*-EtO₂CC₆H₄)I (3i)

¹H NMR (400 MHz, CDCl₃)



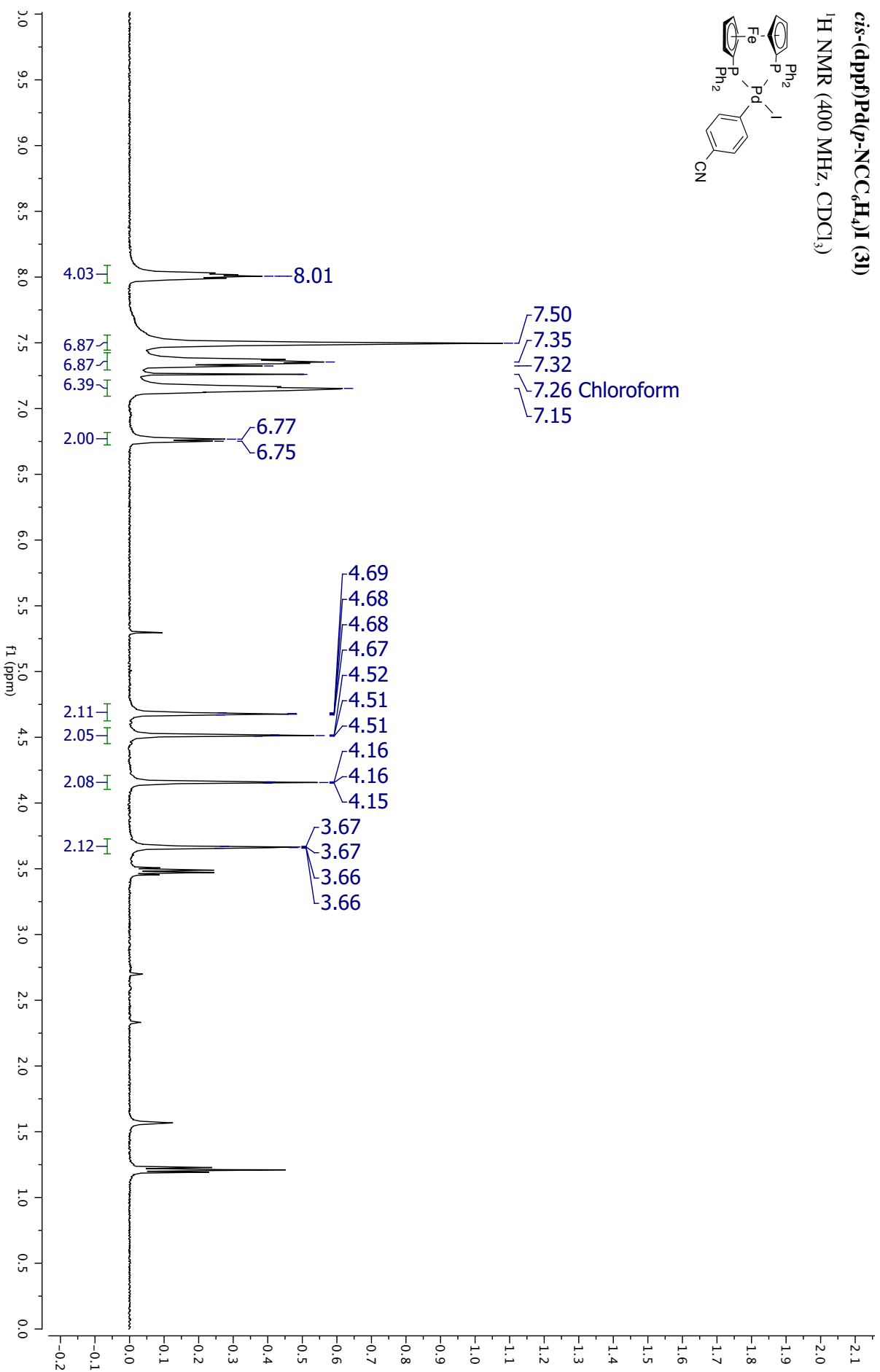
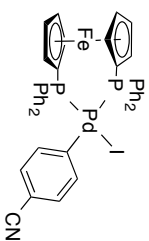
***cis*-(dppf)Pd(*p*-EtO₂CC₆H₄)I (3i)**

³¹P NMR (162 MHz, CDCl₃)



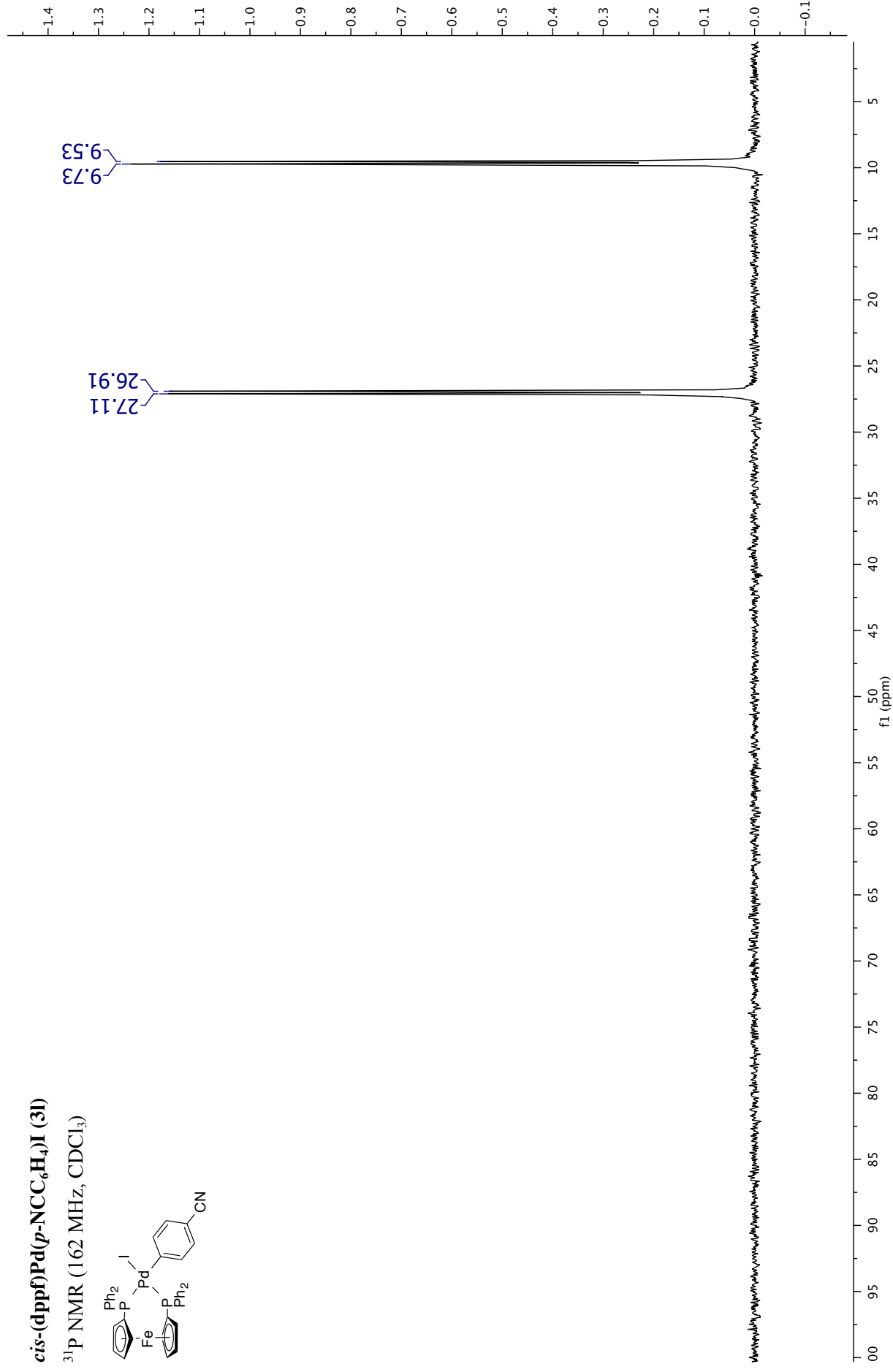
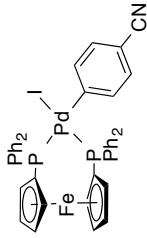
cis-(dppf)Pd(*p*-NCC₆H₄)I (**3I**)

¹H NMR (400 MHz, CDCl₃)



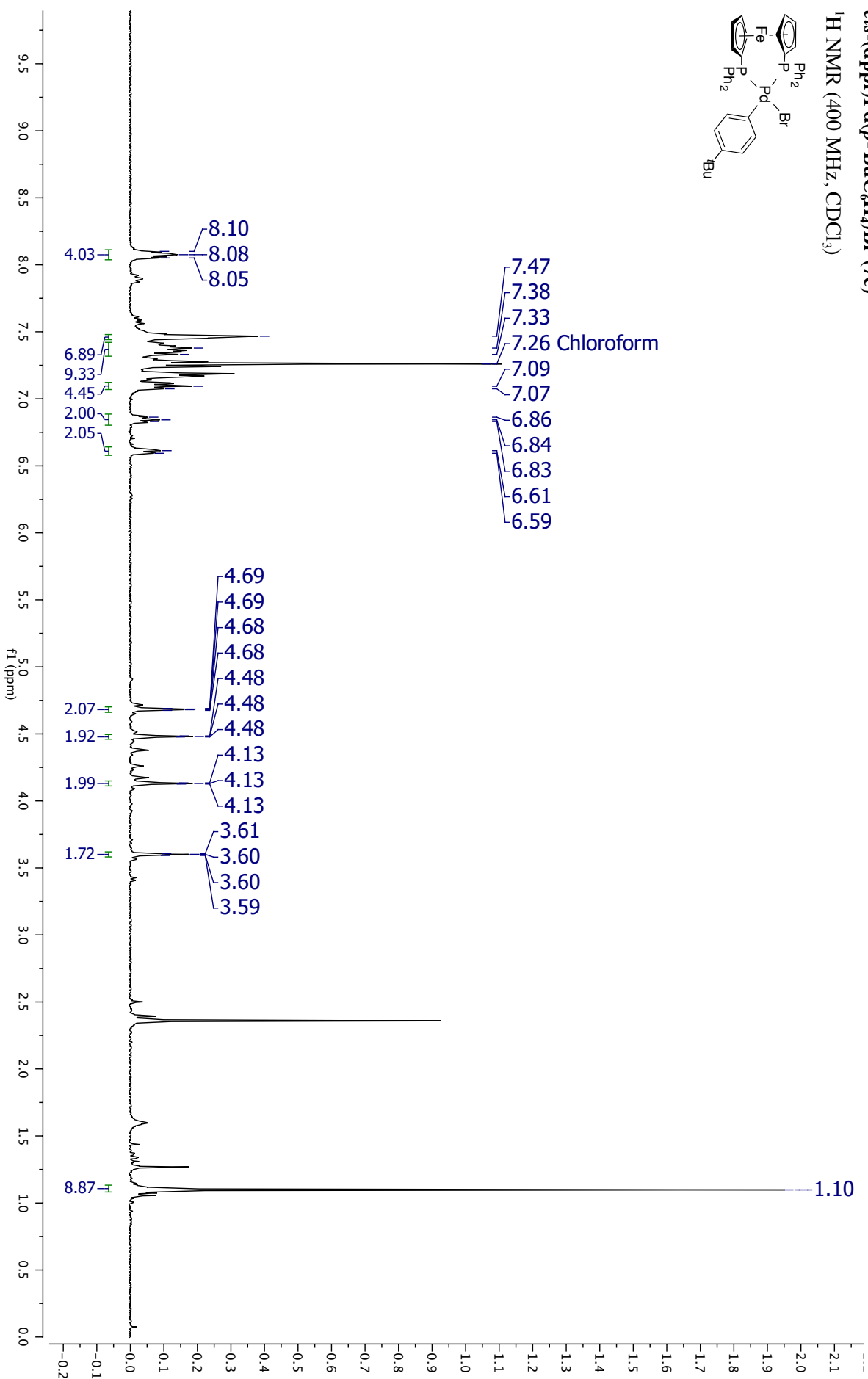
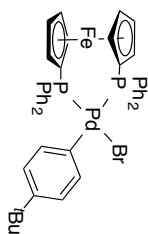
***cis*-(dppf)Pd(*p*-NCC₆H₄)I (31)**

³¹P NMR (162 MHz, CDCl₃)



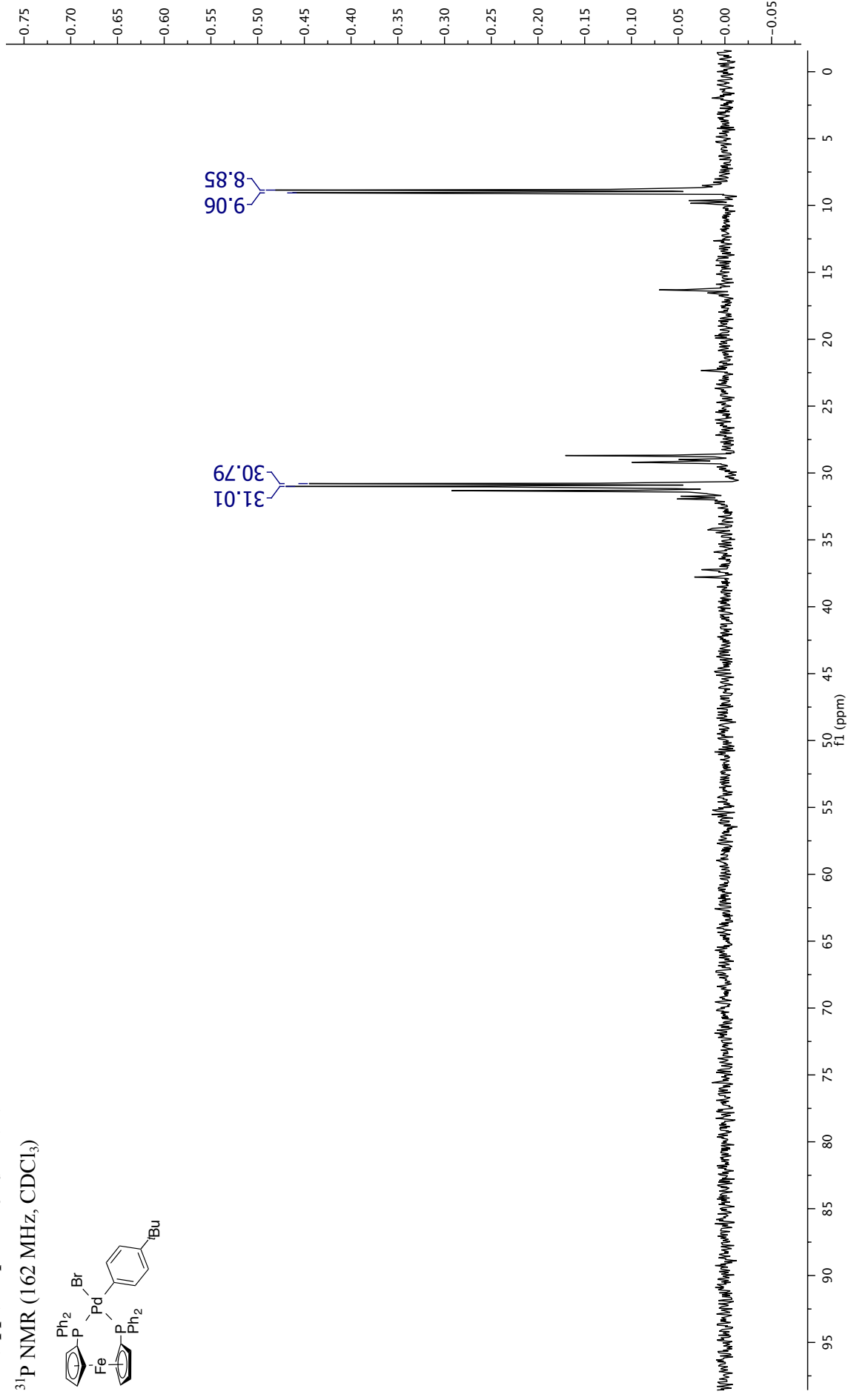
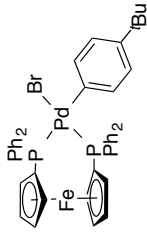
cis-(dppf)Pd(*p*-¹BuC₆H₄)Br (**7e**)

¹H NMR (400 MHz, CDCl₃)



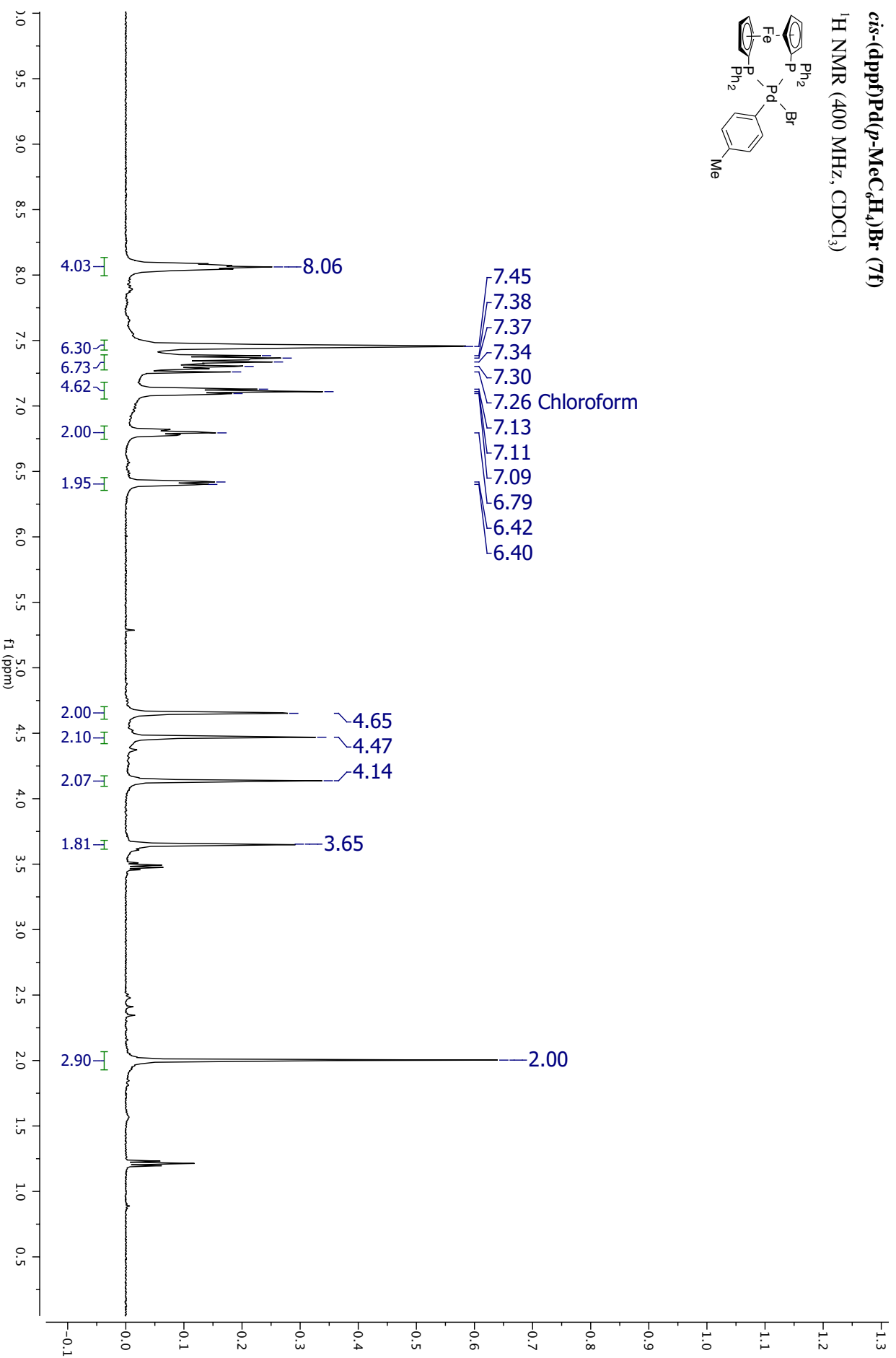
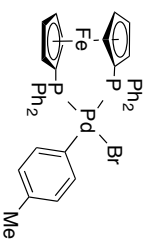
***cis*-(dppf)Pd(*p*-BuC₆H₄)Br (7e)**

³¹P NMR (162 MHz, CDCl₃)



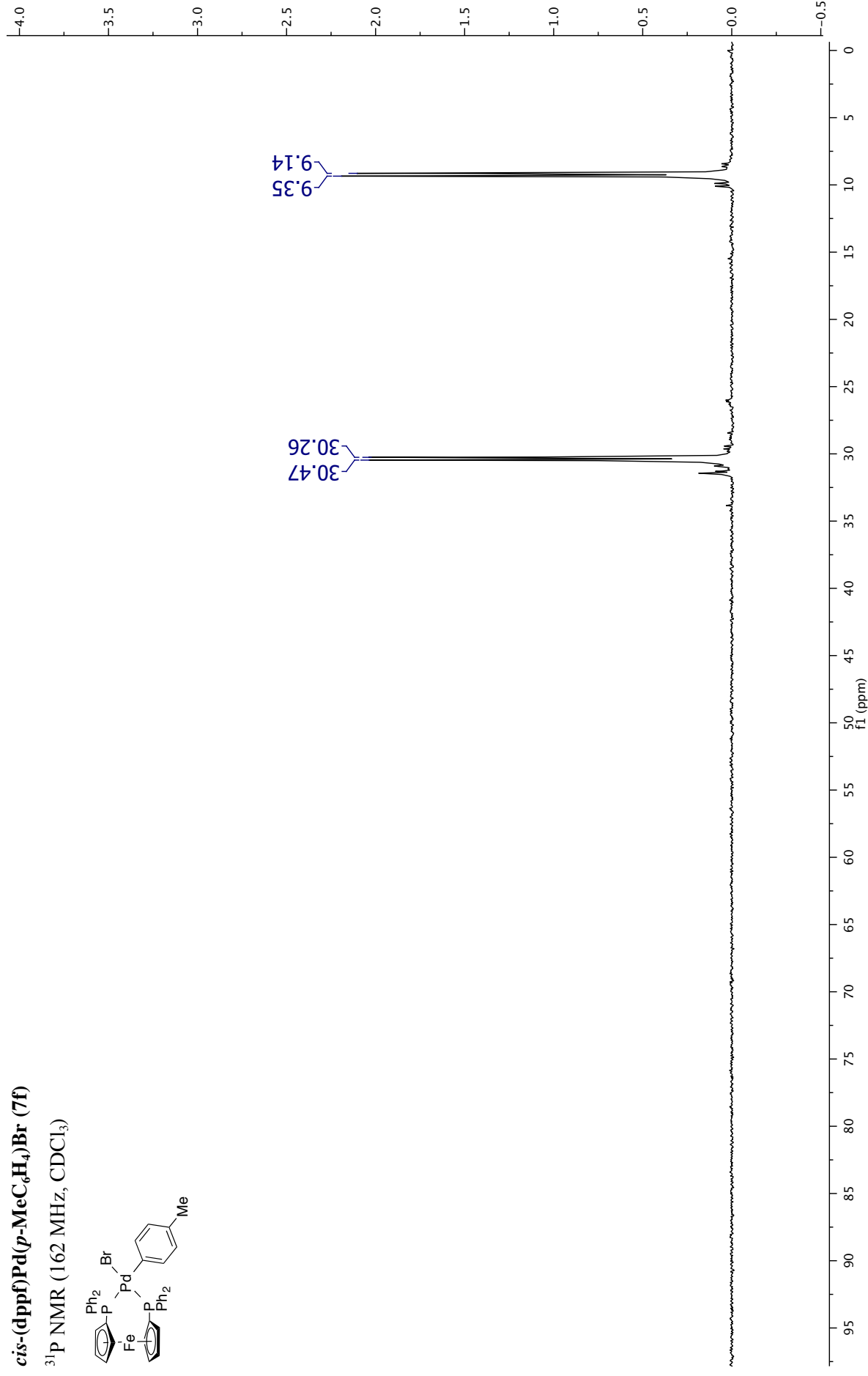
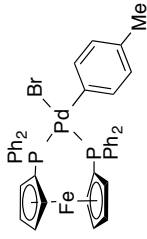
cis-(dppf)Pd(*p*-MeC₆H₄)Br (**7f**)

¹H NMR (400 MHz, CDCl₃)



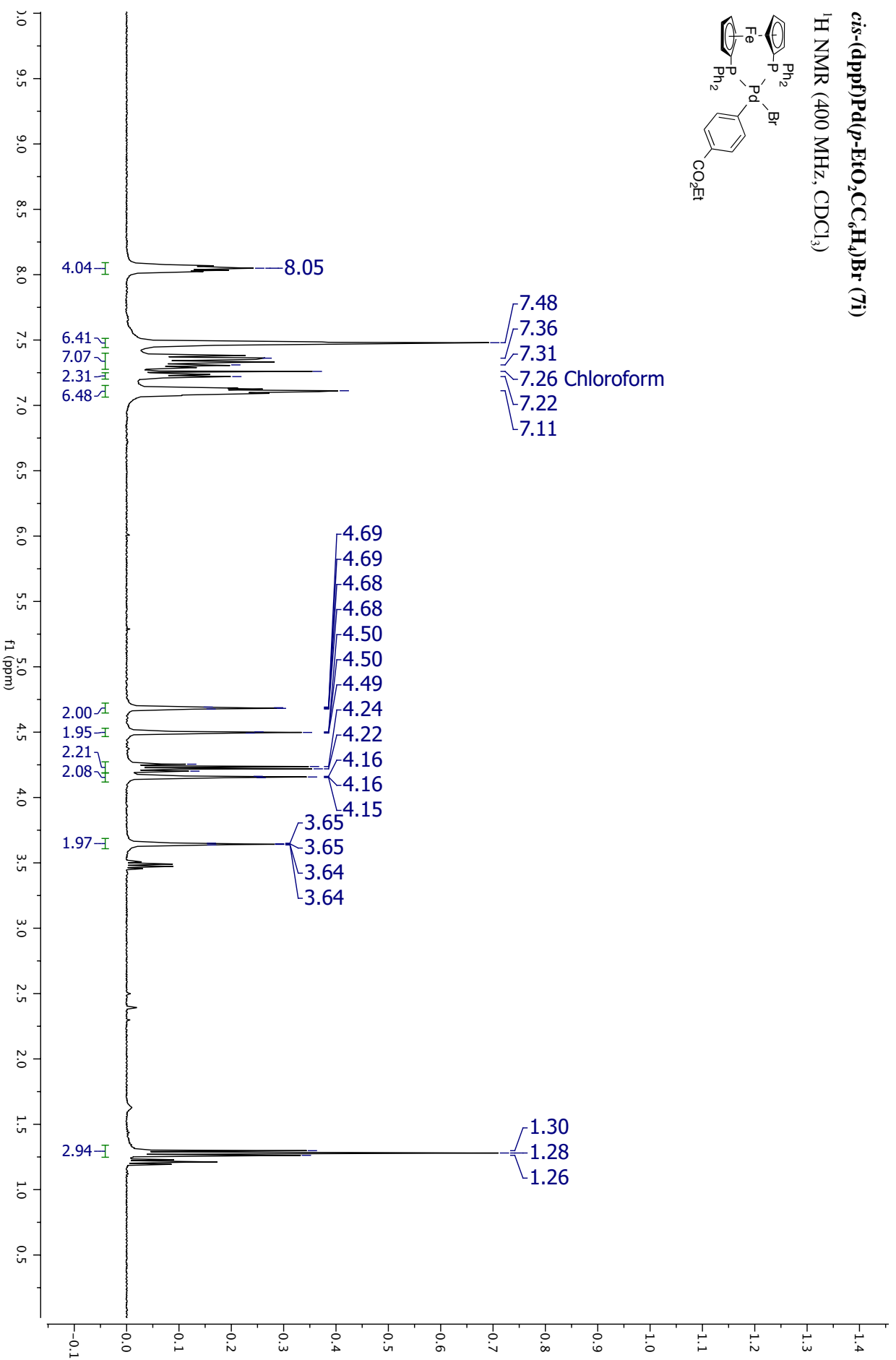
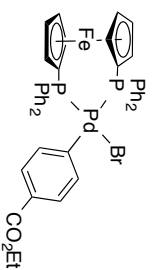
***cis*-(dppf)Pd(*p*-MeC₆H₄)Br (7f)**

³¹P NMR (162 MHz, CDCl₃)



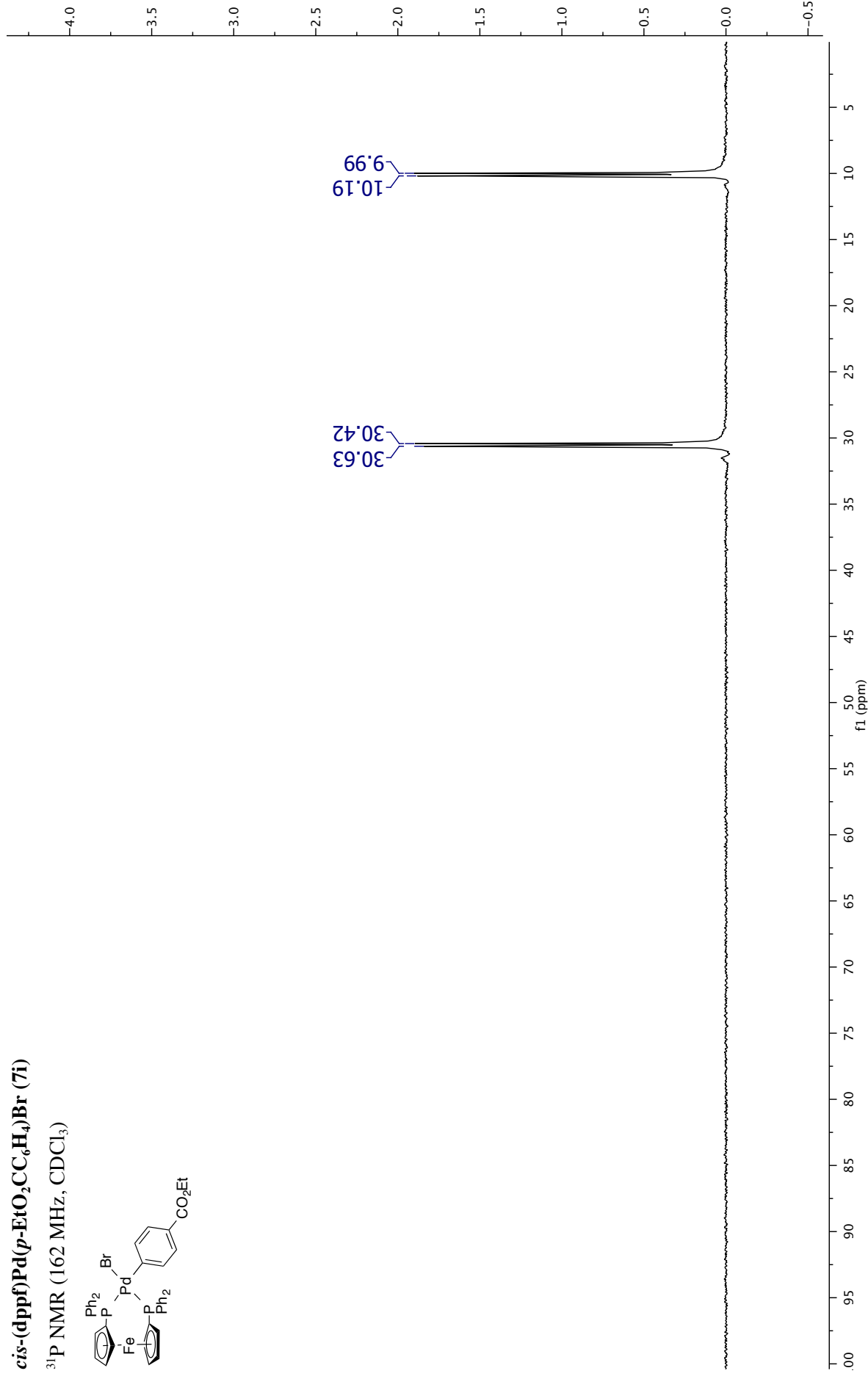
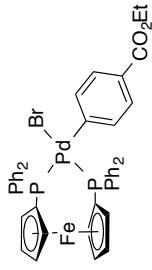
cis-(dppf)Pd(*p*-EtO₂CC₆H₄)Br (7i)

¹H NMR (400 MHz, CDCl₃)



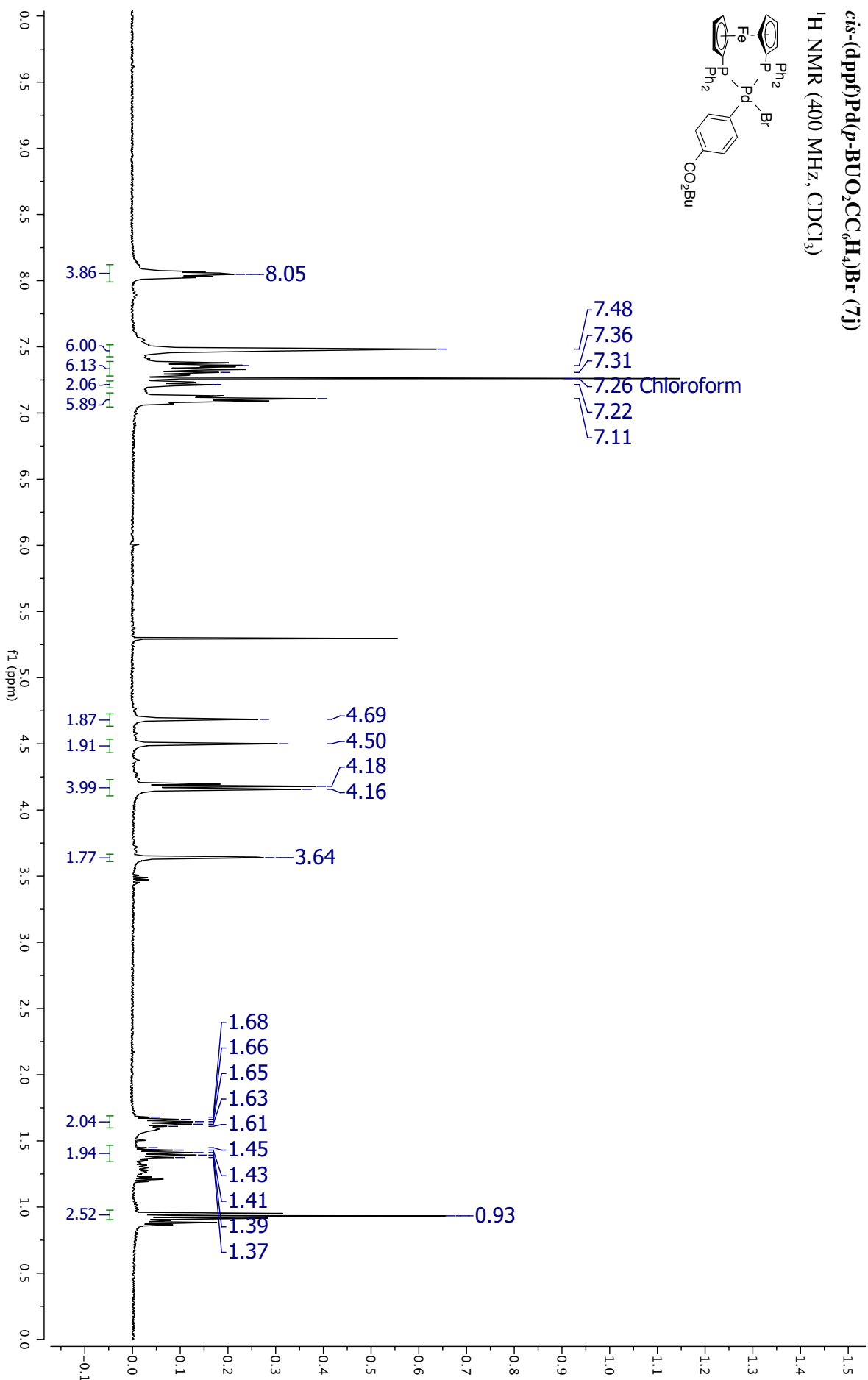
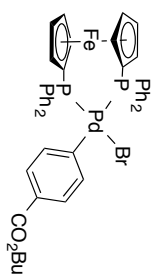
***cis*-(dppf)Pd(*p*-EtO₂CC₆H₄)Br (7i)**

³¹P NMR (162 MHz, CDCl₃)



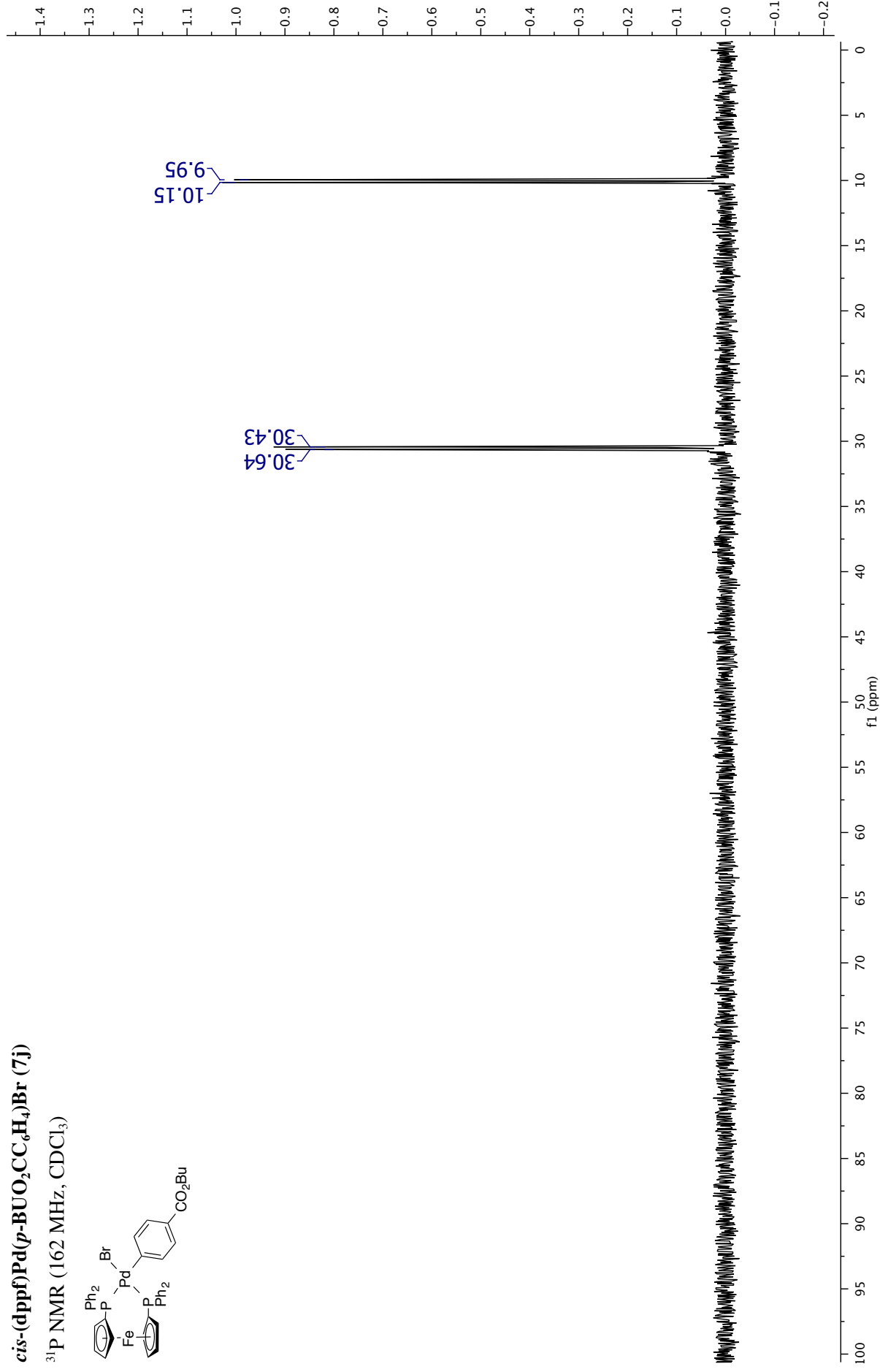
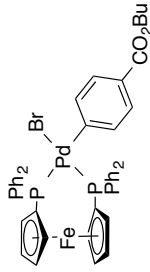
cis-(dppf)Pd(*p*-BU₂CC₆H₄)Br (**7j**)

¹H NMR (400 MHz, CDCl₃)



***cis*-(dppf)Pd(*p*-BUO₂CC₆H₄)Br (7j)**

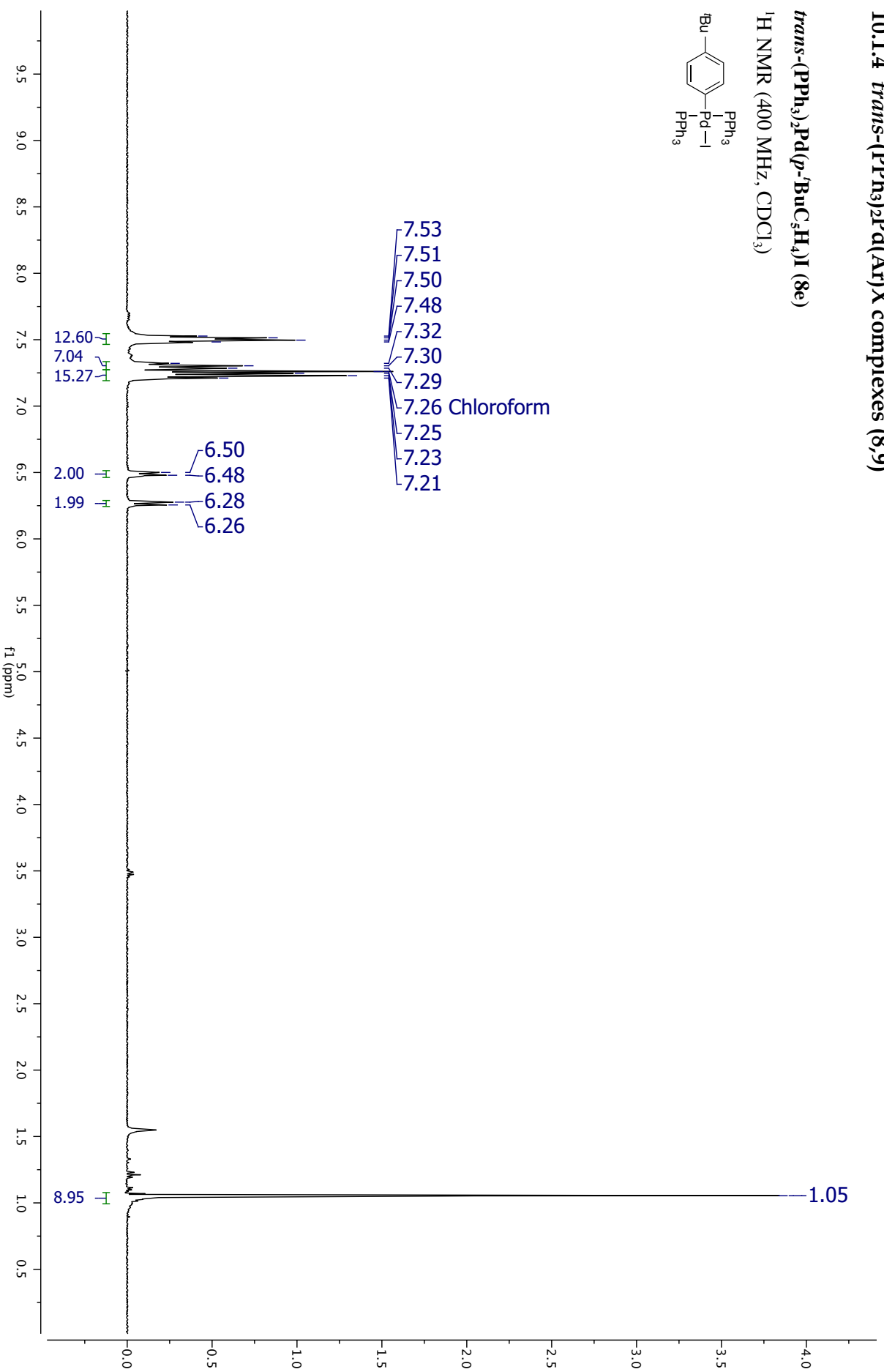
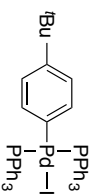
³¹P NMR (162 MHz, CDCl₃)



10.1.4 *trans*-(PPh₃)₂Pd(Ar)X complexes (8,9)

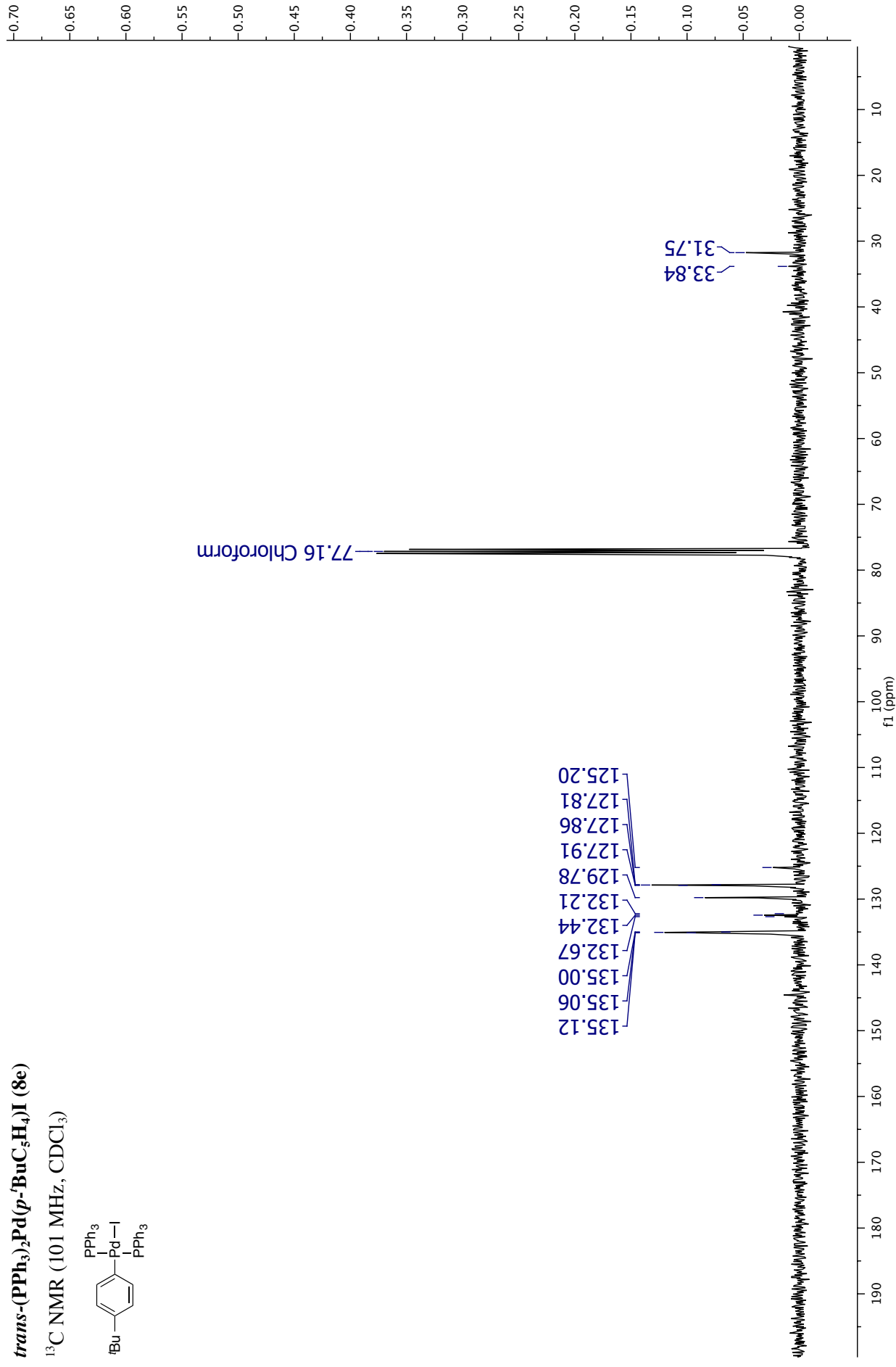
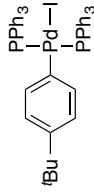
trans-(PPh₃)₂Pd(*p*-¹BuC₆H₄)I (8e)

¹H NMR (400 MHz, CDCl₃)



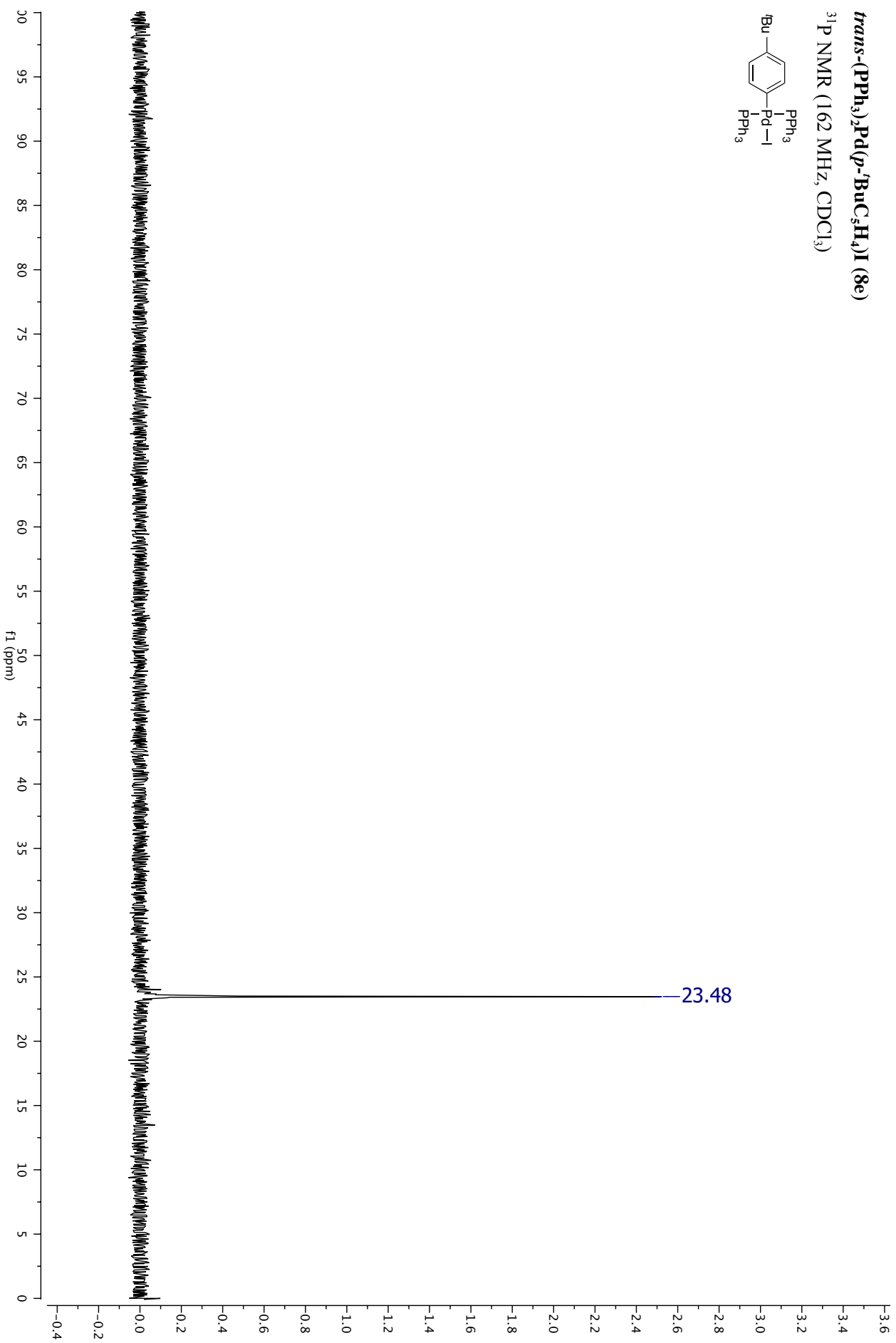
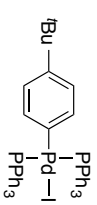
***trans*-(PPh₃)₂Pd(*p*-BuC₅H₄)I (8e)**

¹³C NMR (101 MHz, CDCl₃)



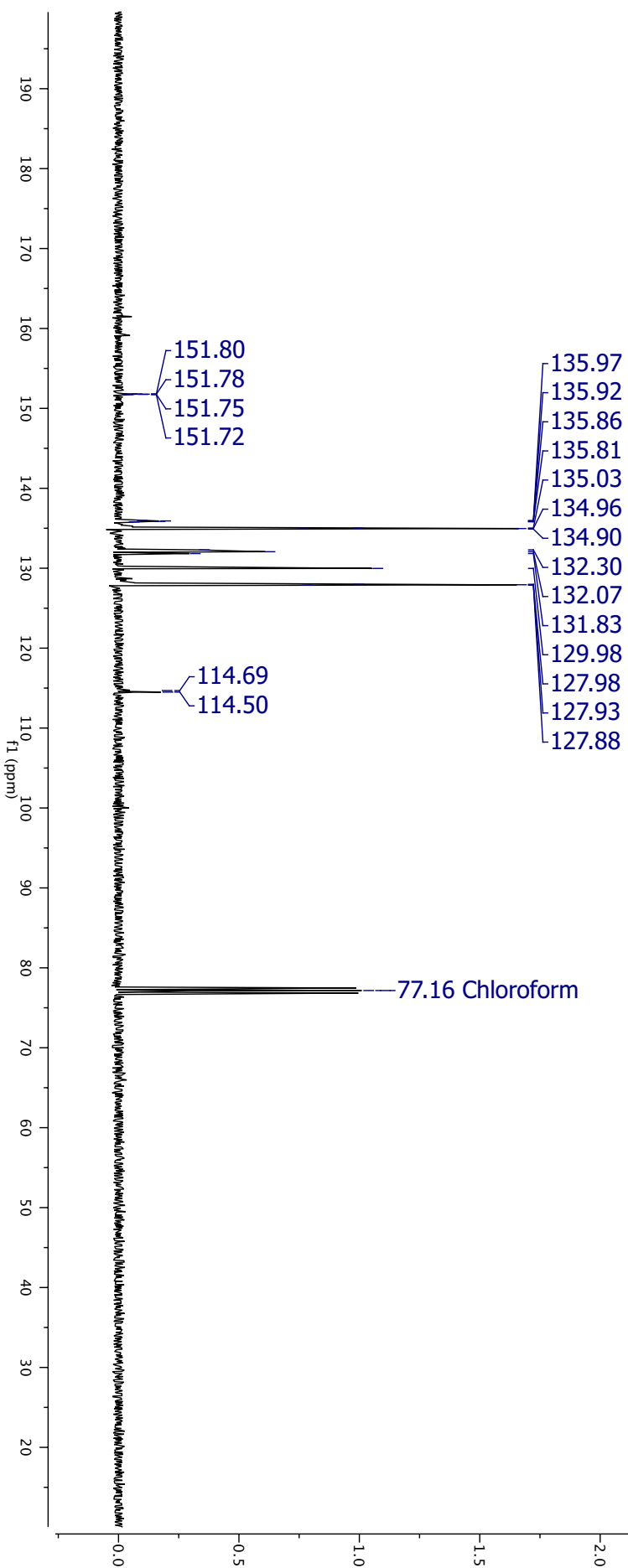
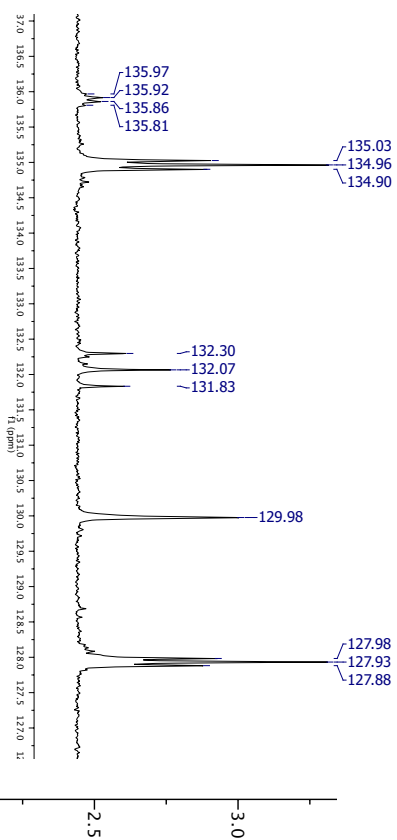
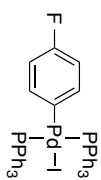
trans-(PPh₃)₂Pd(*p*-tBuC₆H₄)I (8e)

³¹P NMR (162 MHz, CDCl₃)



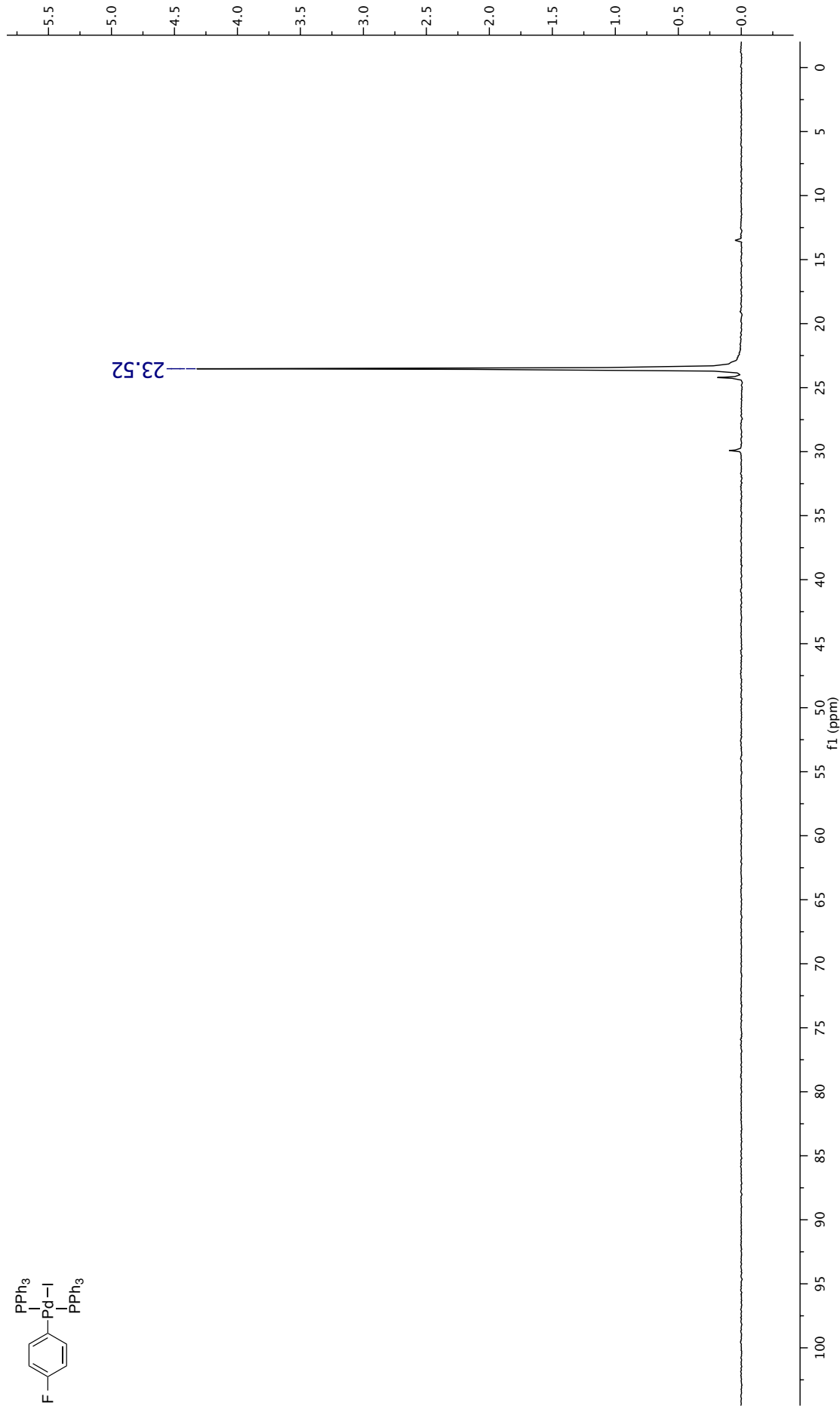
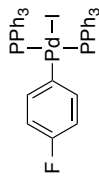
***trans*-(PPh₃)₂Pd(*p*-FC₆H₄)I (8g)**

¹³C NMR (101 MHz, CDCl₃)



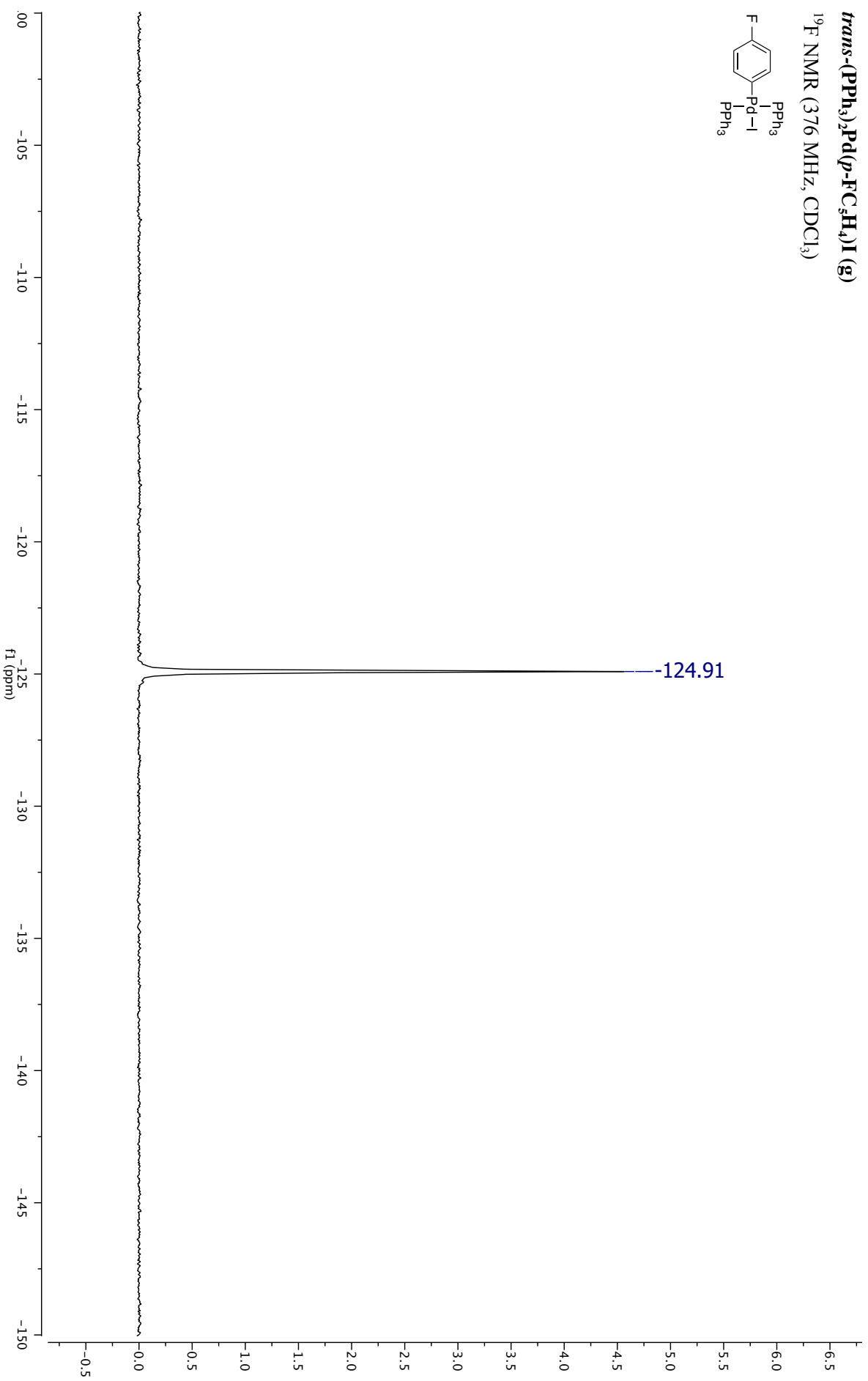
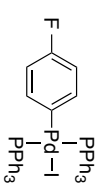
***trans*-(PPh₃)₂Pd(*p*-FC₆H₄)I (8g)**

³¹P NMR (162 MHz, CDCl₃)



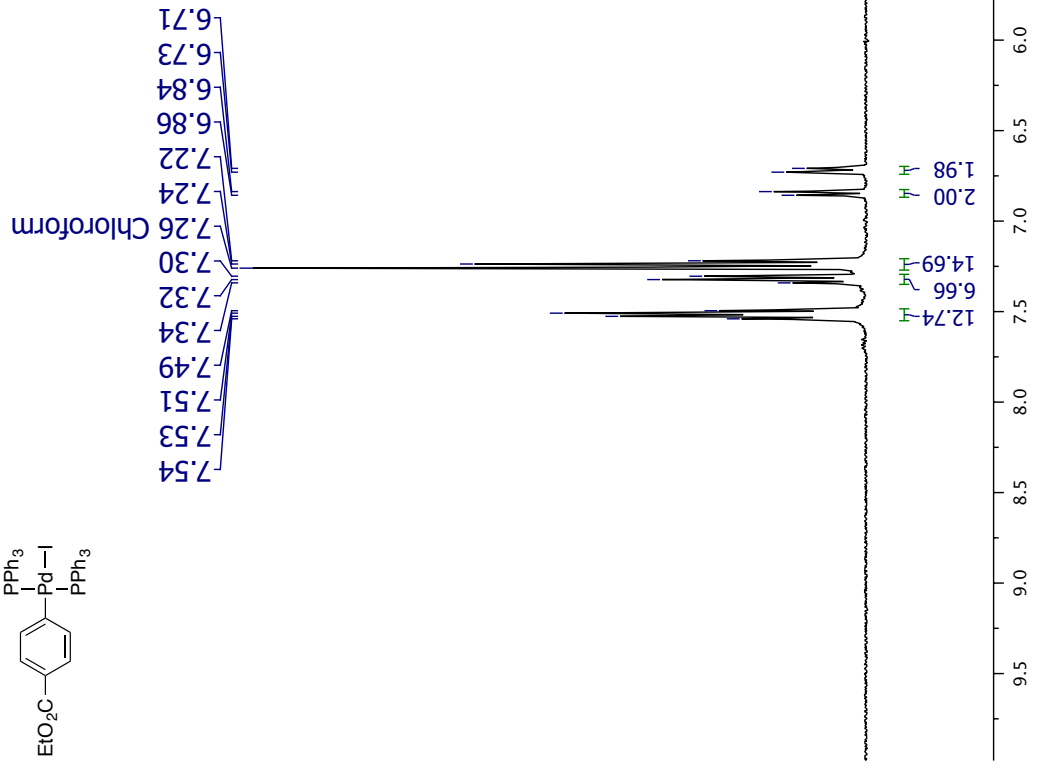
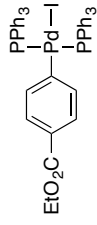
***trans*-(PPh₃)₂Pd(*p*-FC₆H₄)I (g)**

¹⁹F NMR (376 MHz, CDCl₃)



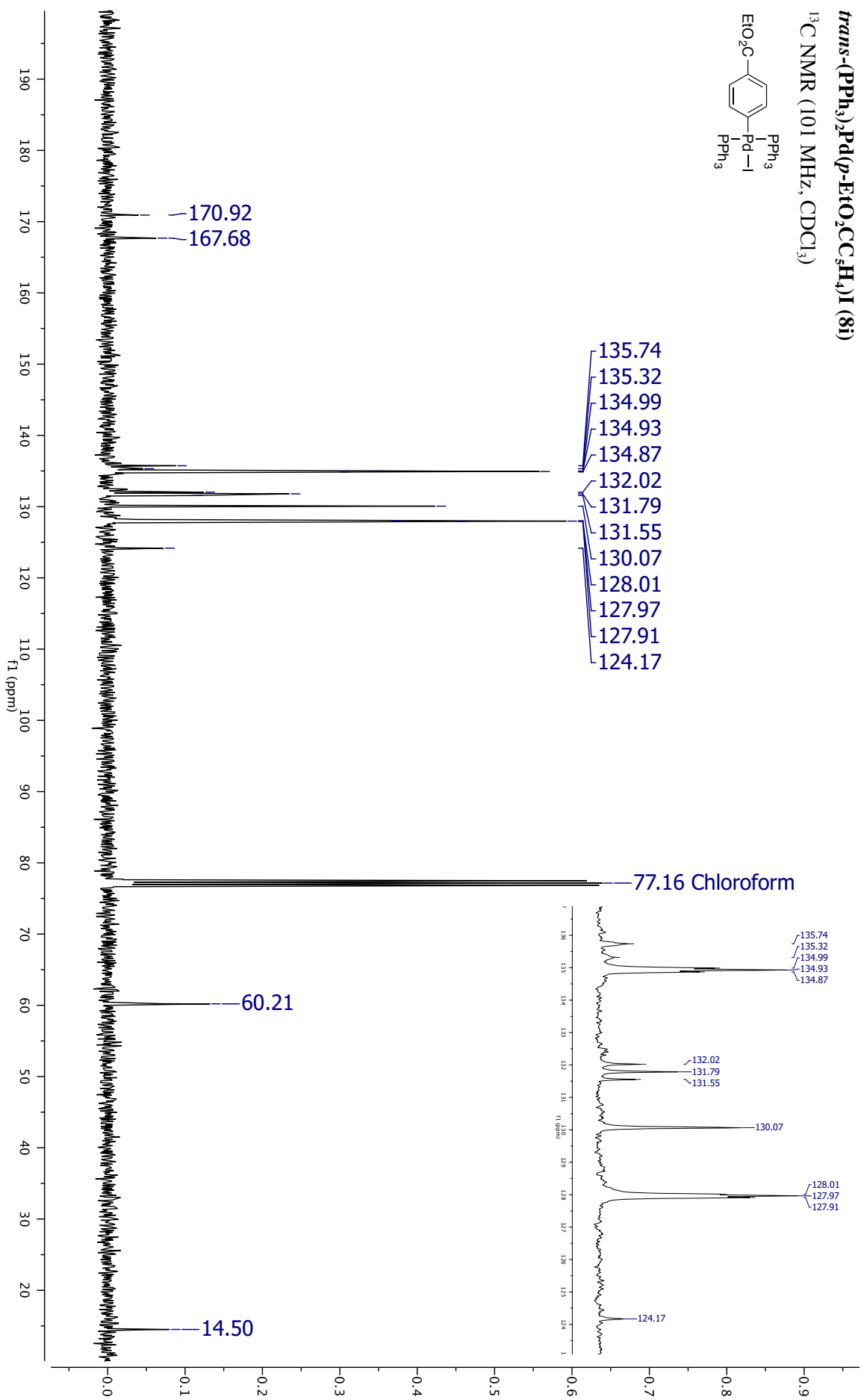
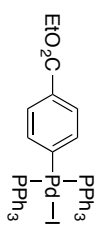
***trans*-(PPh₃)₂Pd(*p*-EtO₂CC₃H₄)I (8i)**

¹H NMR (400 MHz, CDCl₃)



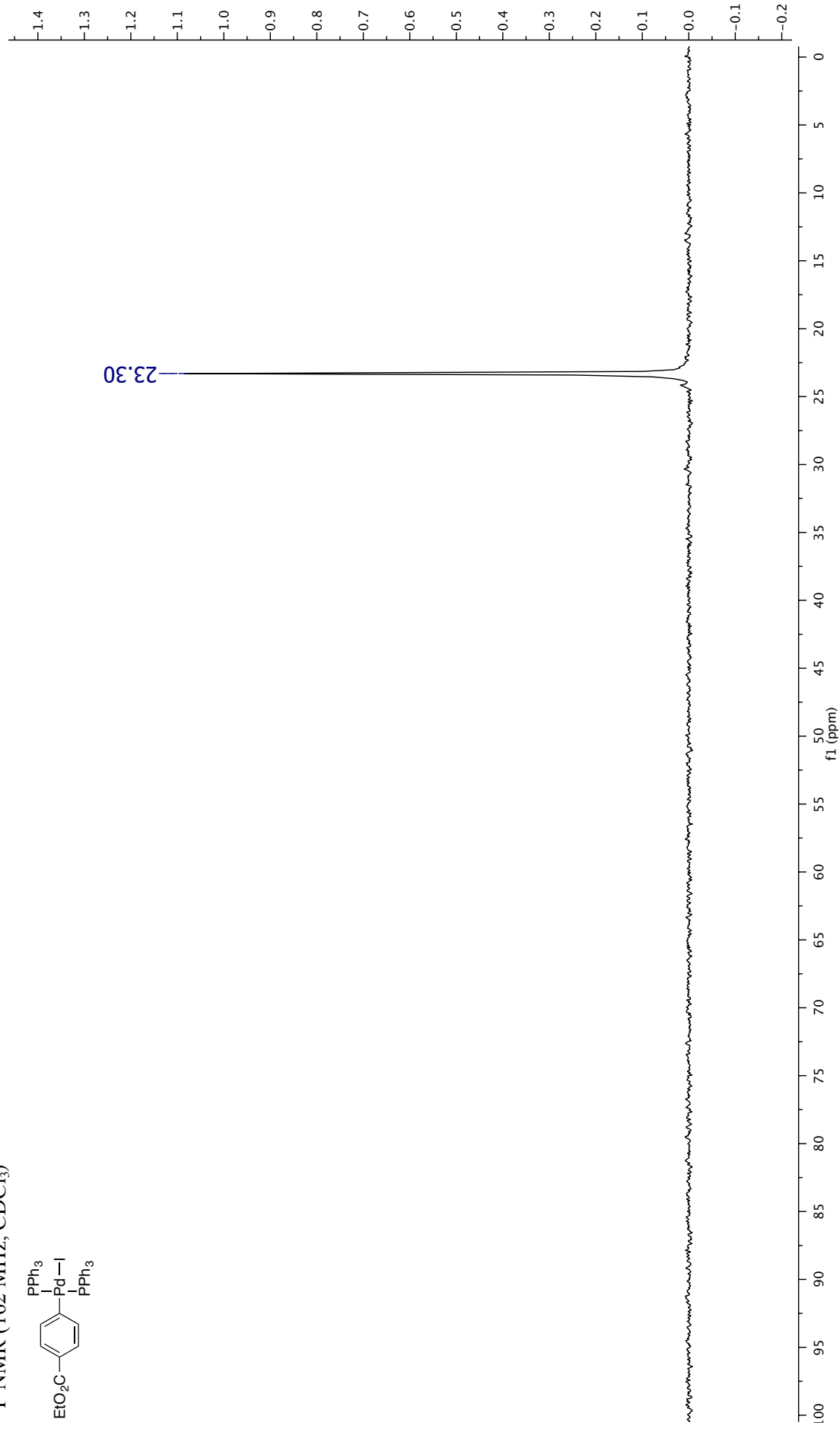
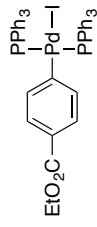
***trans*-(PPh₃)₂Pd(*p*-EtO₂CC₆H₄)I (81)**

¹³C NMR (101 MHz, CDCl₃)



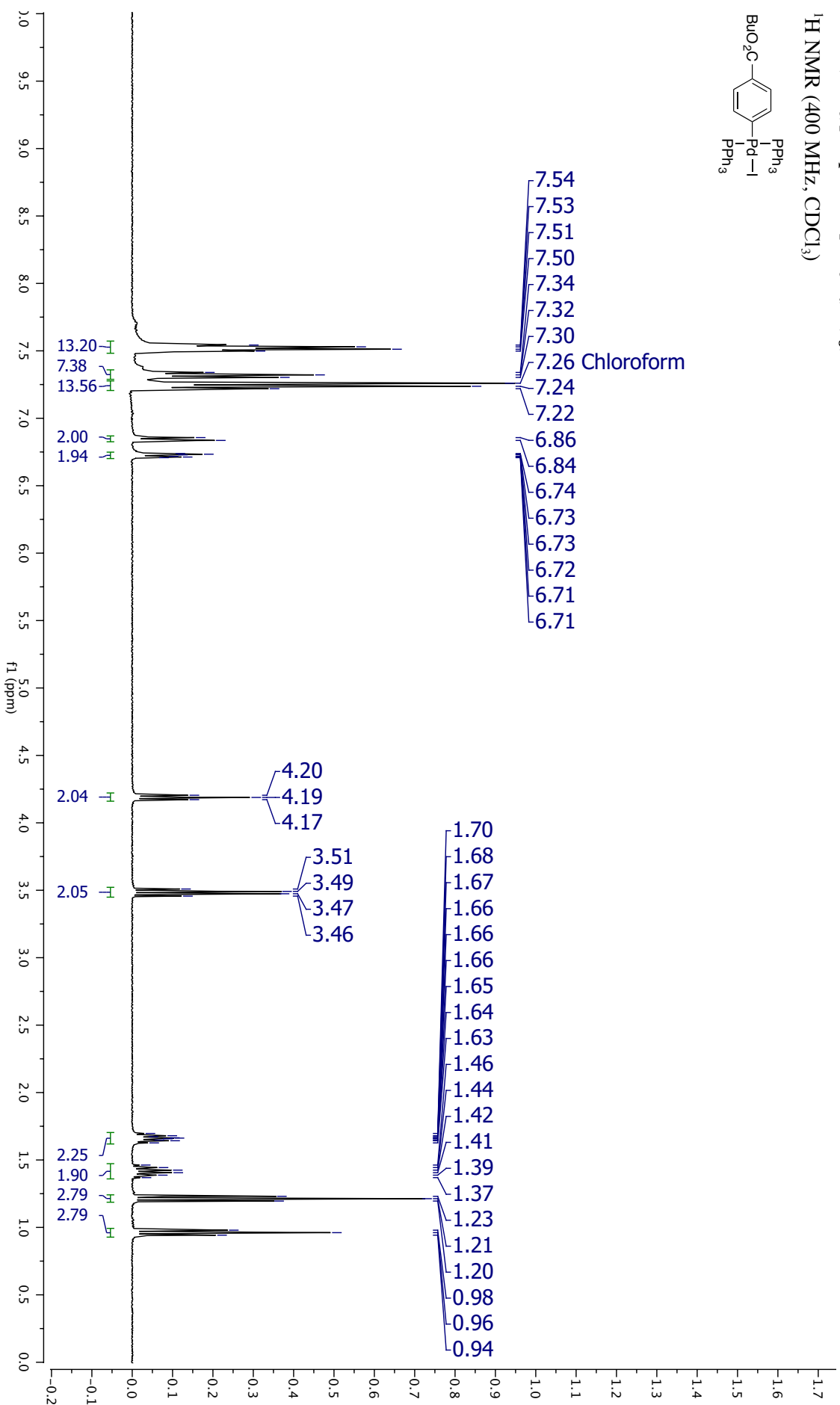
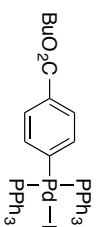
***trans*-(PPh₃)₂Pd(*p*-EtO₂CC₃H₄)I (8i)**

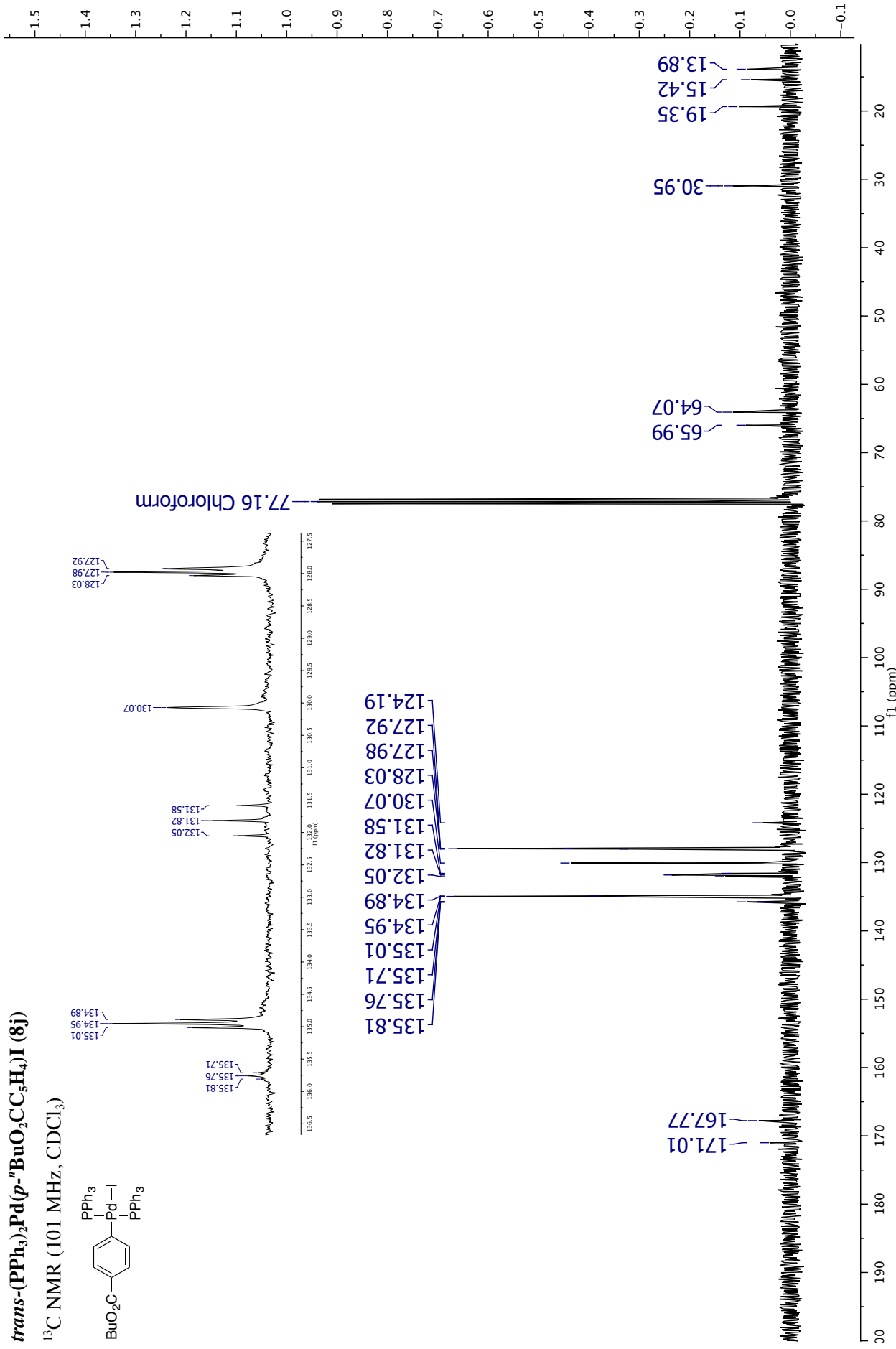
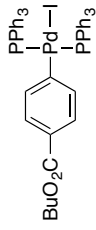
³¹P NMR (162 MHz, CDCl₃)



trans-(PPh₃)₂Pd(*p*-BuO₂C₆H₄)I (**8j**)

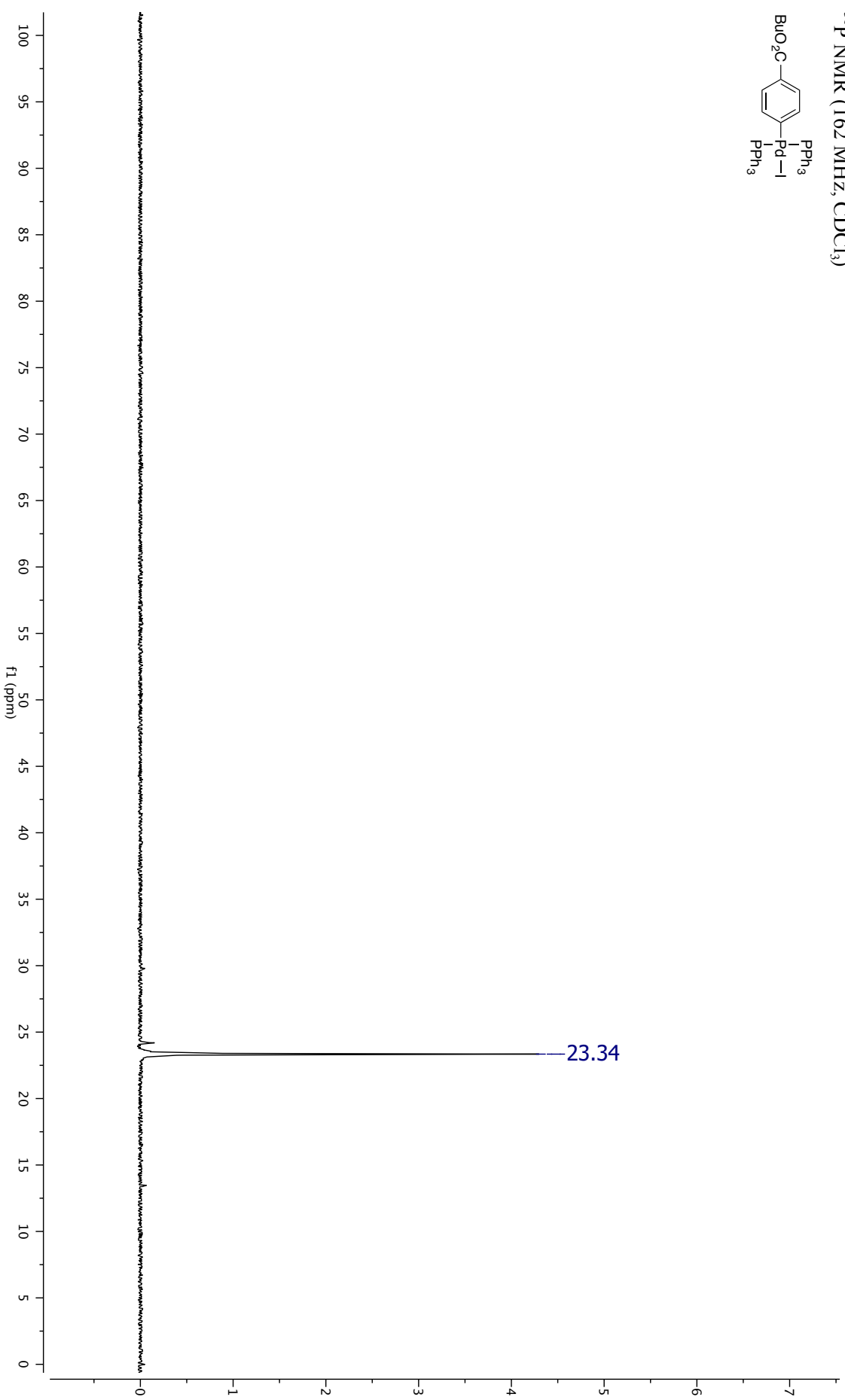
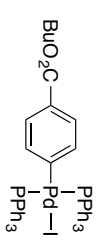
¹H NMR (400 MHz, CDCl₃)



***trans*-(PPh₃)₂Pd(*p*-BuO₂C₅H₄)I (8j)**¹³C NMR (101 MHz, CDCl₃)

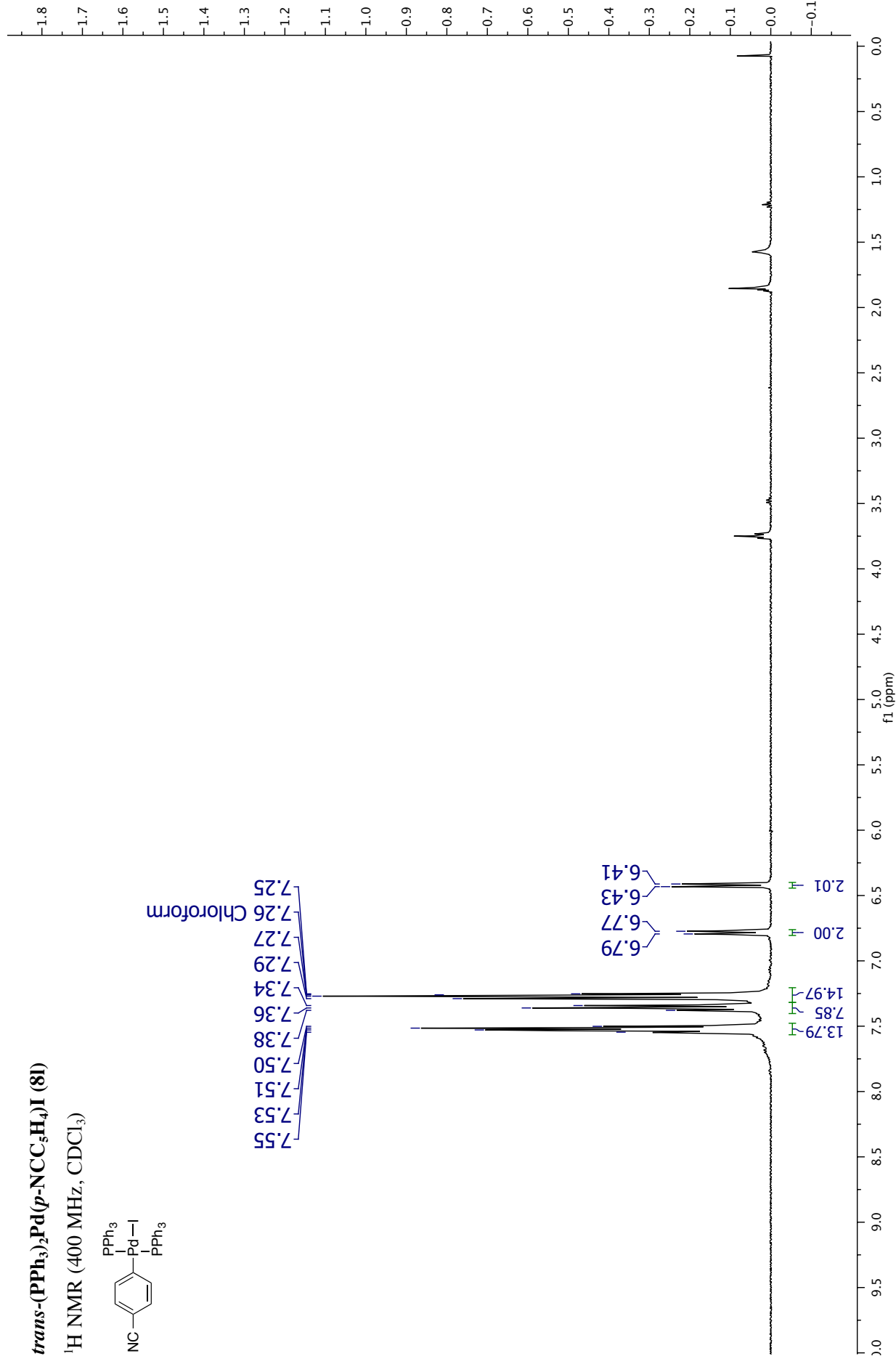
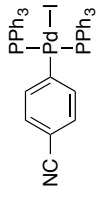
trans-(PPh₃)₂Pd(*p*-BuO₂C₆H₄)I (**8j**)

³¹P NMR (162 MHz, CDCl₃)



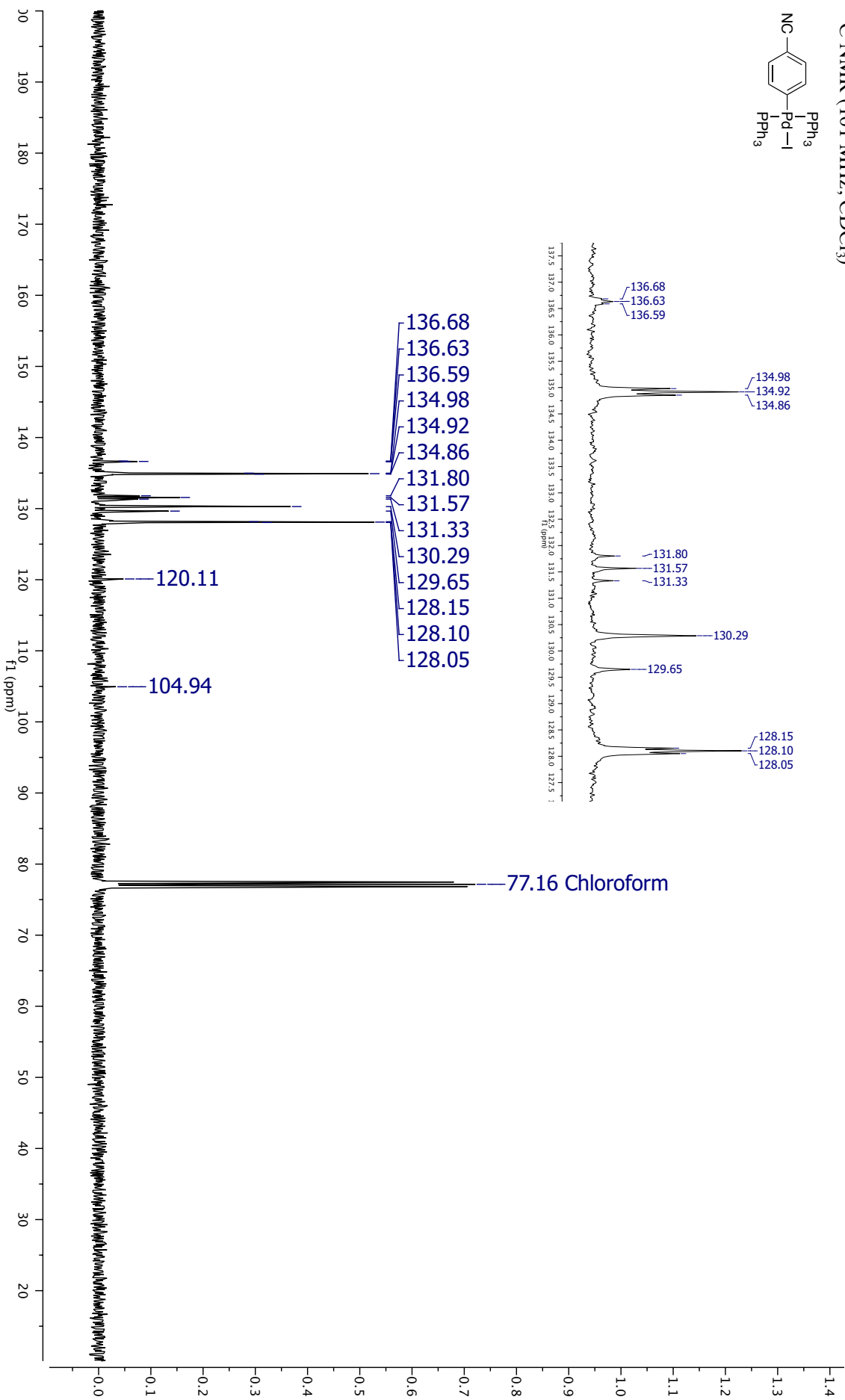
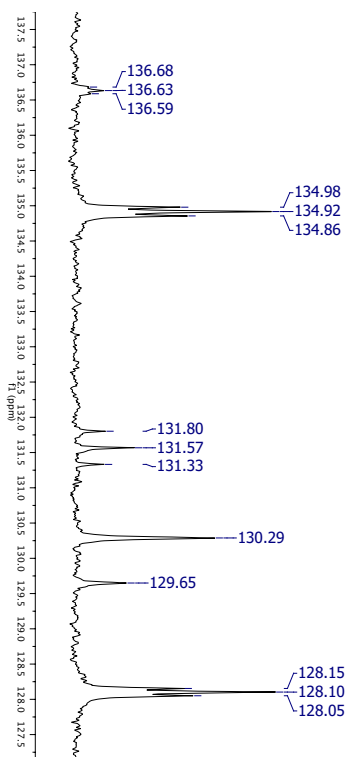
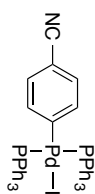
***trans*-(PPh₃)₂Pd(*p*-NCC₃H₄)I (81)**

¹H NMR (400 MHz, CDCl₃)



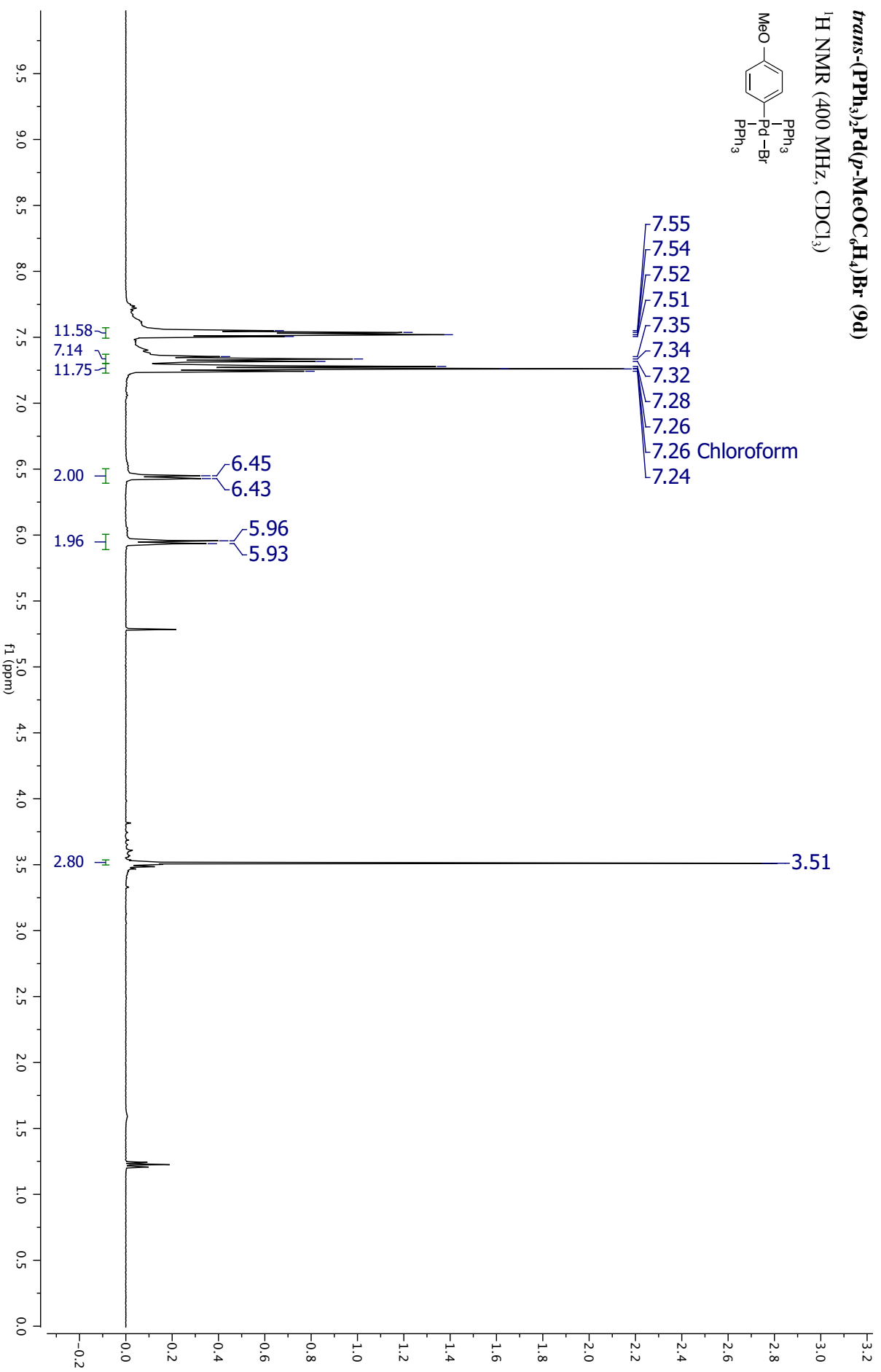
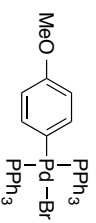
trans-(PPh₃)₂Pd(*p*-NCC₆H₄)I (**81**)

¹³C NMR (101 MHz, CDCl₃)



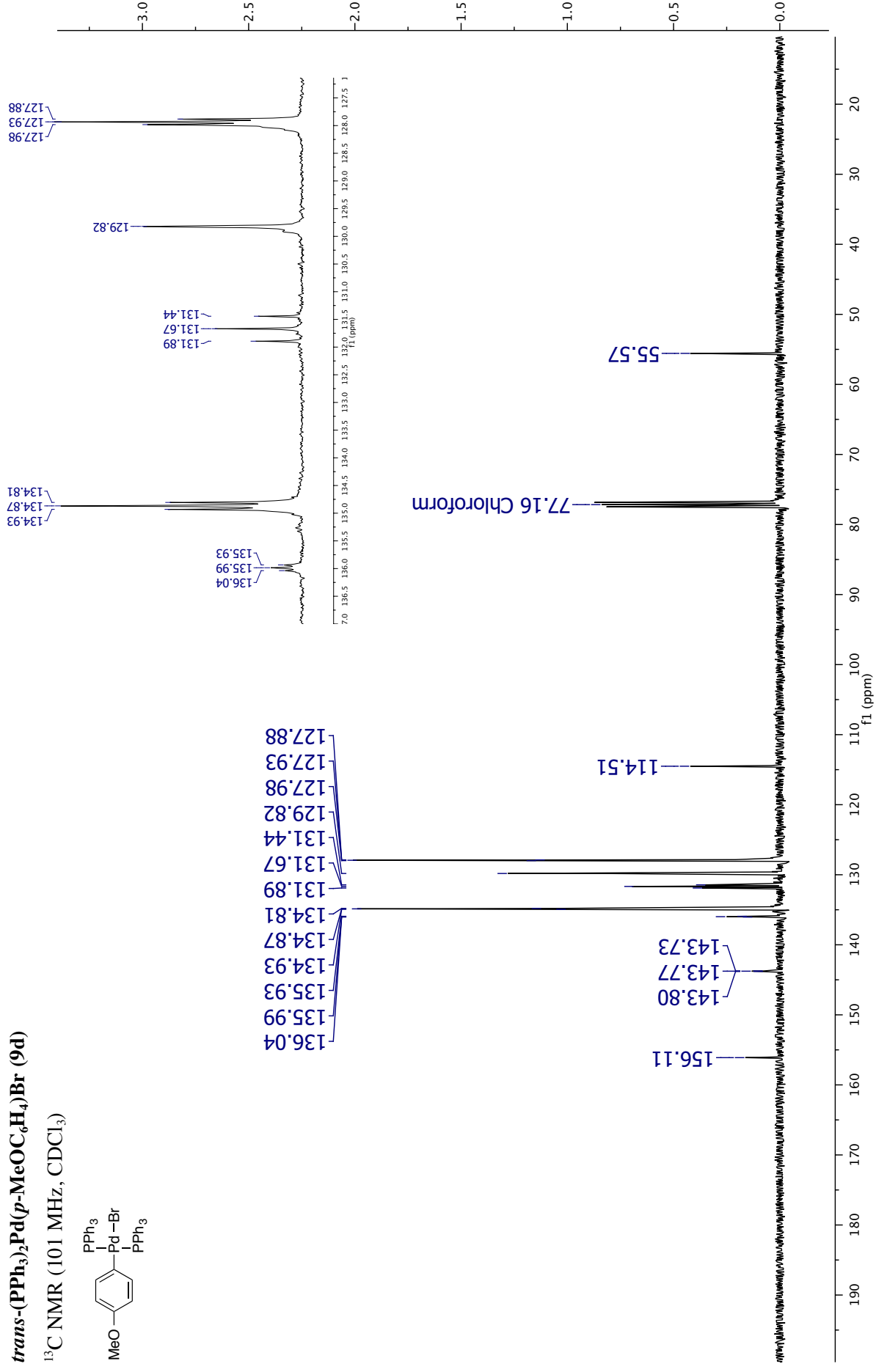
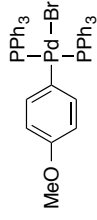
trans-(PPh₃)₂Pd(*p*-MeOC₆H₄)Br (9d)

¹H NMR (400 MHz, CDCl₃)



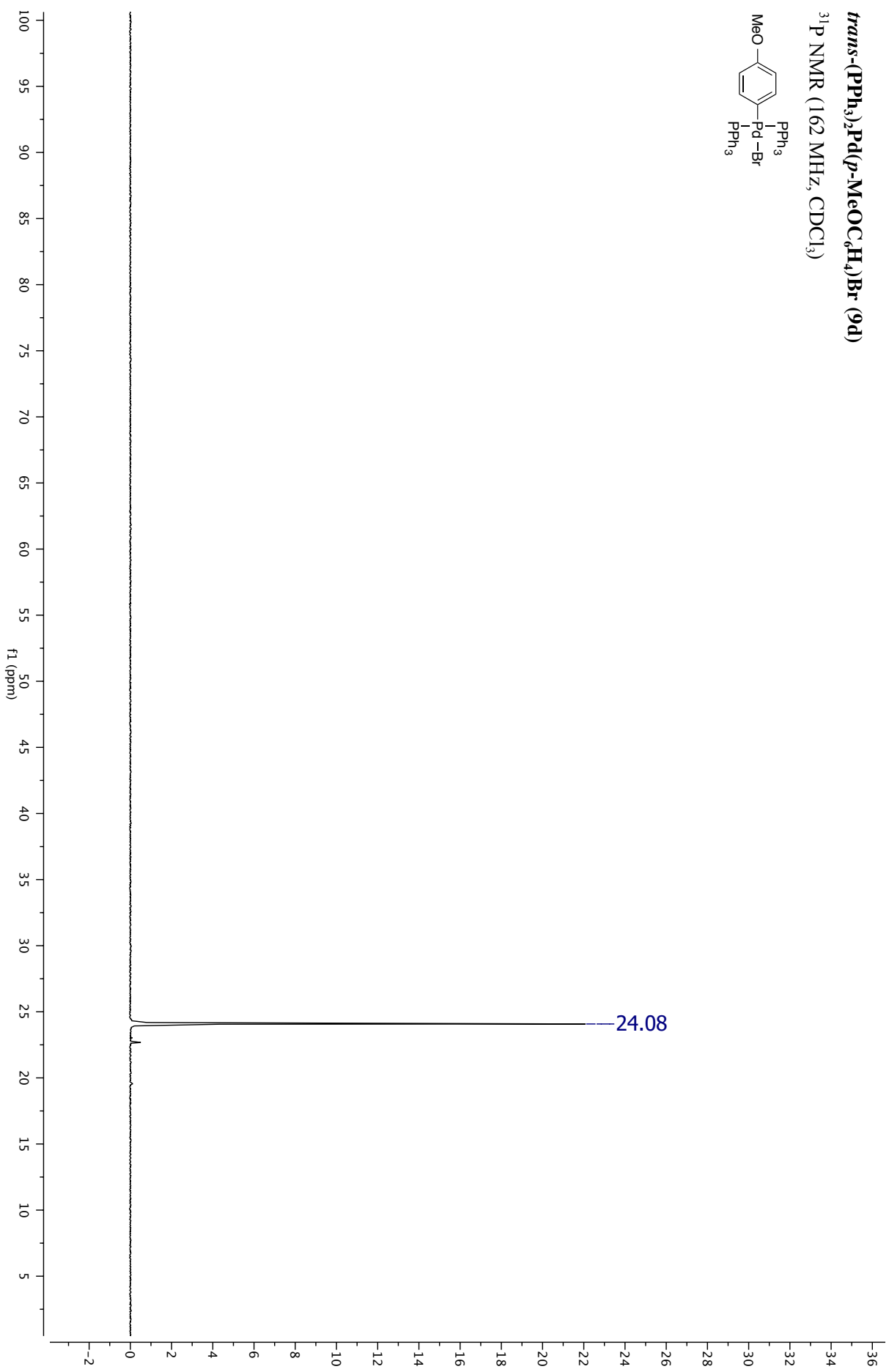
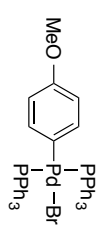
***trans*-(PPh₃)₂Pd(*p*-MeOC₆H₄)Br (9d)**

¹³C NMR (101 MHz, CDCl₃)



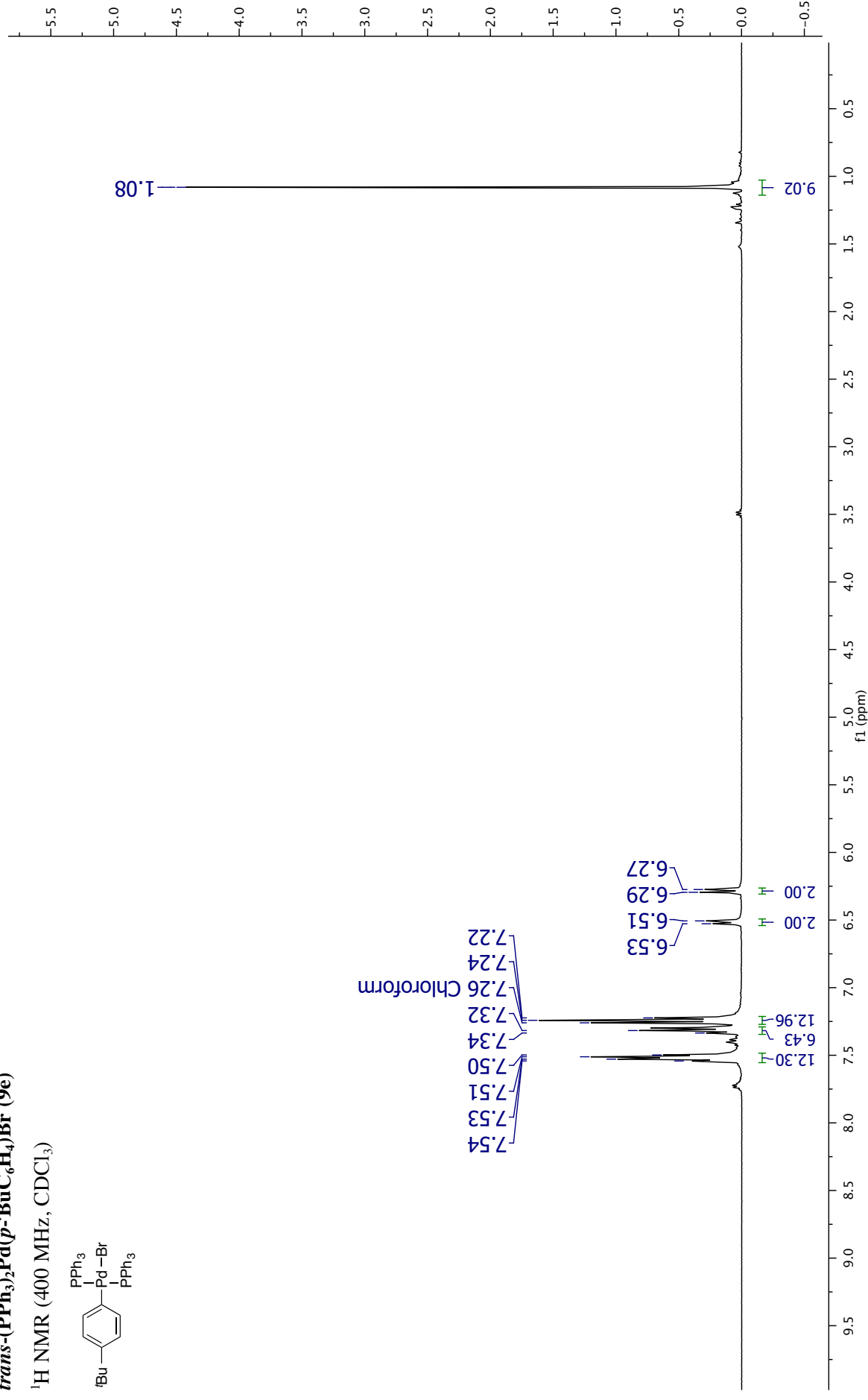
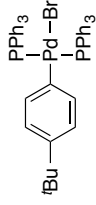
trans-(PPh₃)₂Pd(*p*-MeOC₆H₄)Br (**9d**)

³¹P NMR (162 MHz, CDCl₃)



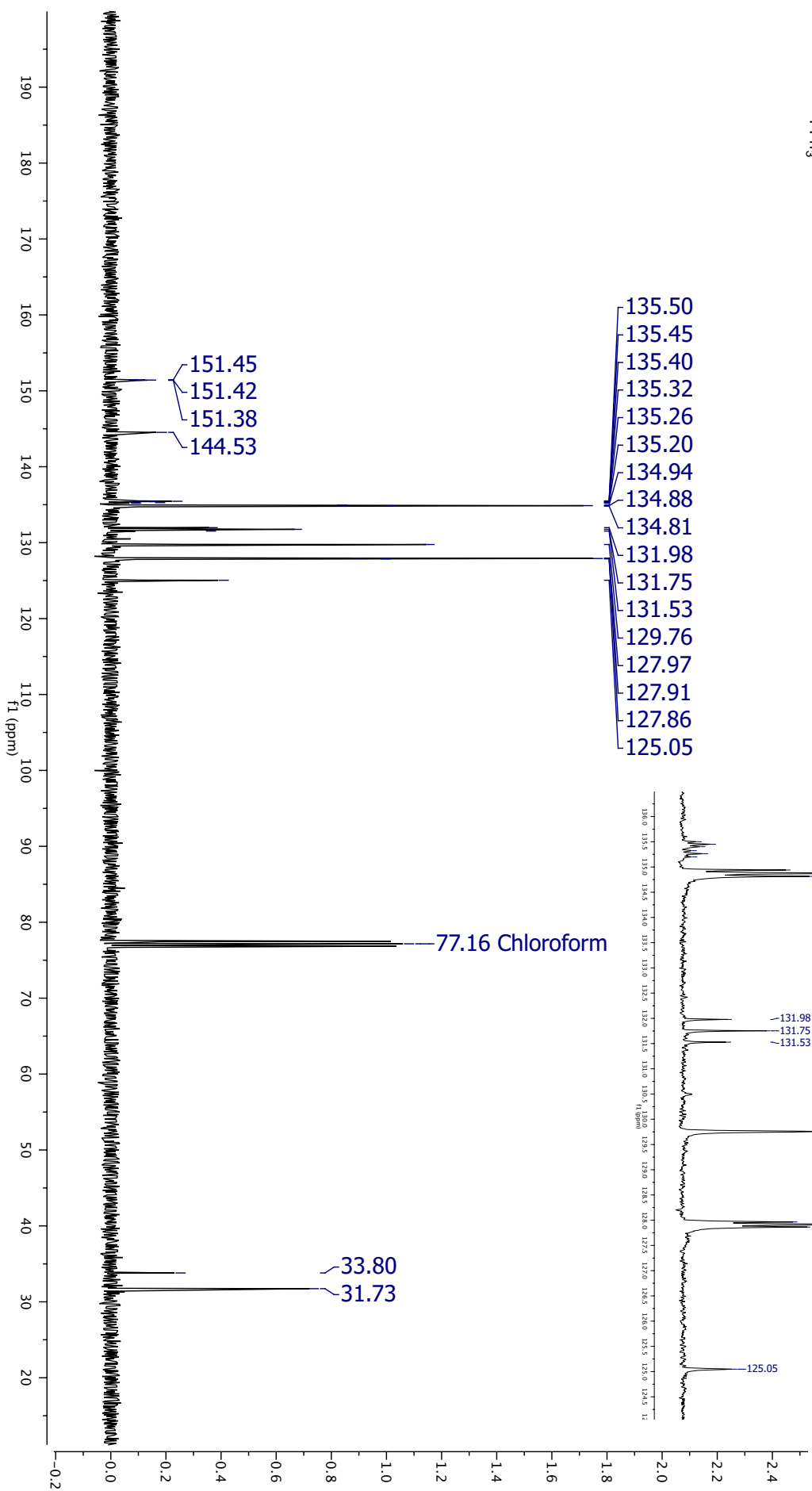
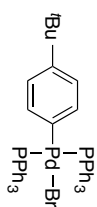
***trans*-(PPh₃)₂Pd(*p*-BuC₆H₄)Br (9e)**

¹H NMR (400 MHz, CDCl₃)



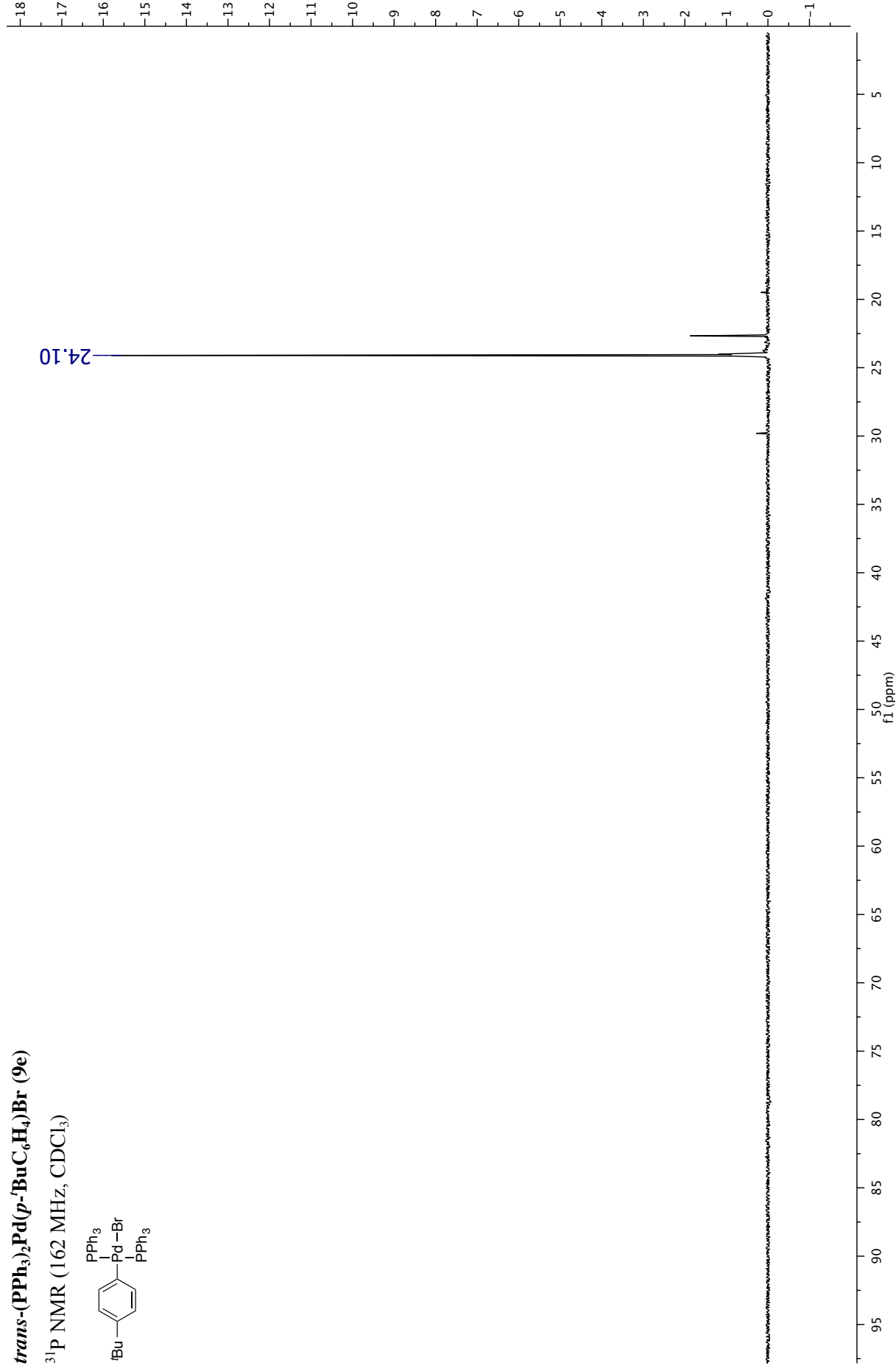
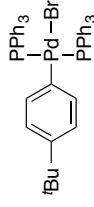
***trans*-(PPh₃)₂Pd(*p*-BuC₆H₄)Br (9c)**

¹³C NMR (101 MHz, CDCl₃)



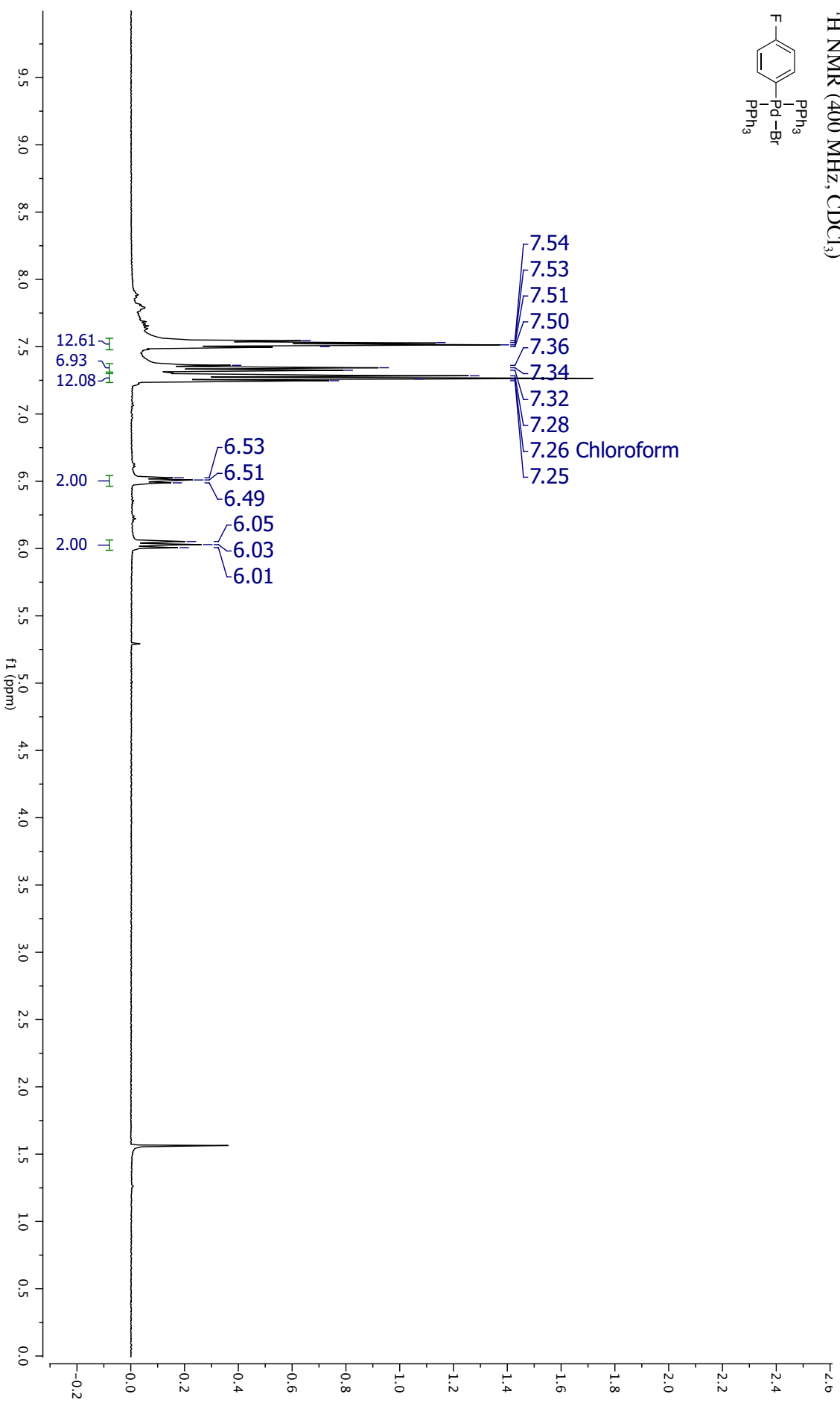
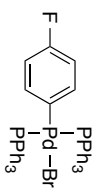
***trans*-(PPh₃)₂Pd(*p*-BuC₆H₄)Br (9e)**

³¹P NMR (162 MHz, CDCl₃)



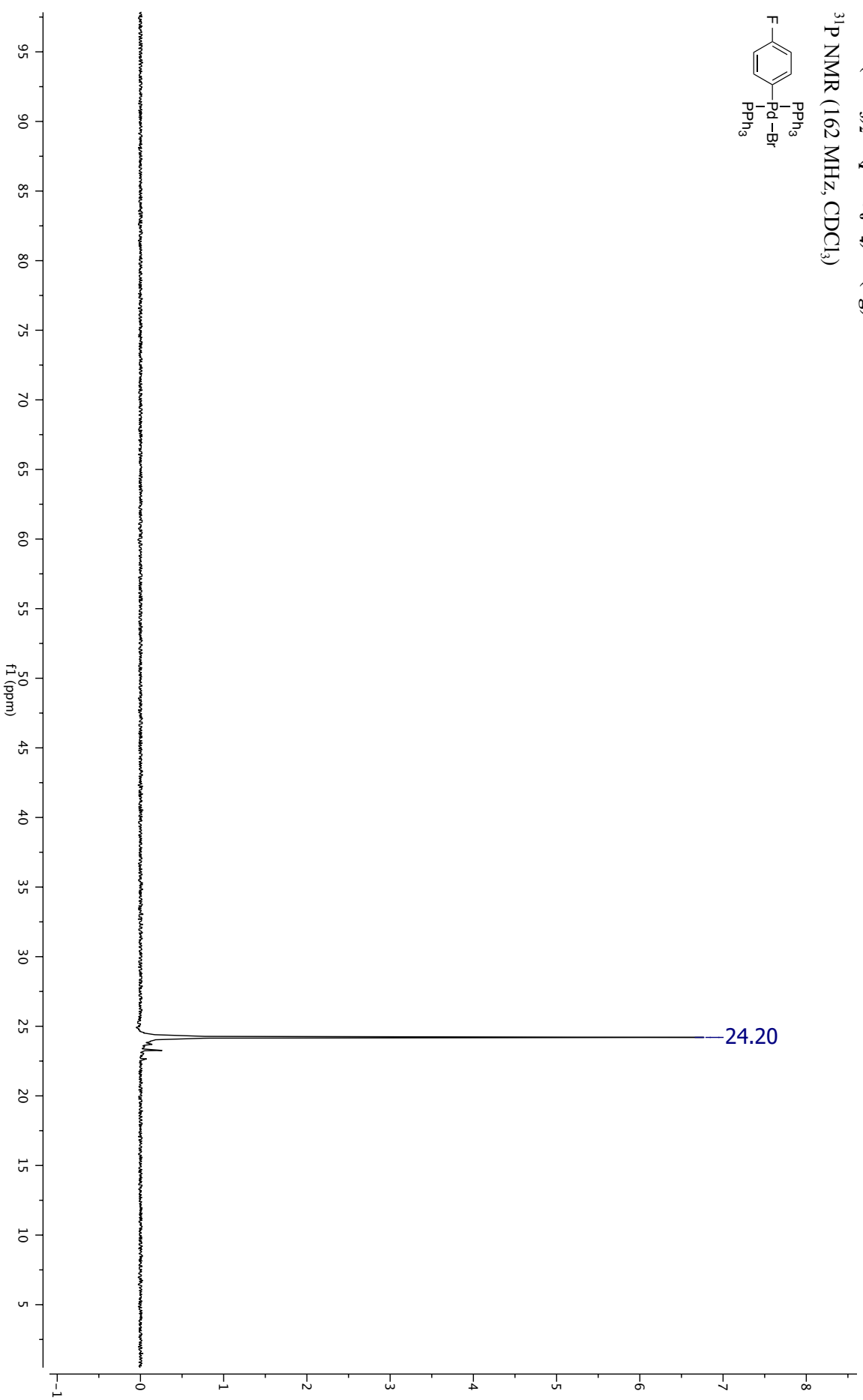
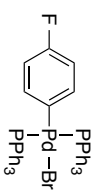
trans-(PPh₃)₂Pd(*p*-FC₆H₄)Br (9g)

¹H NMR (400 MHz, CDCl₃)



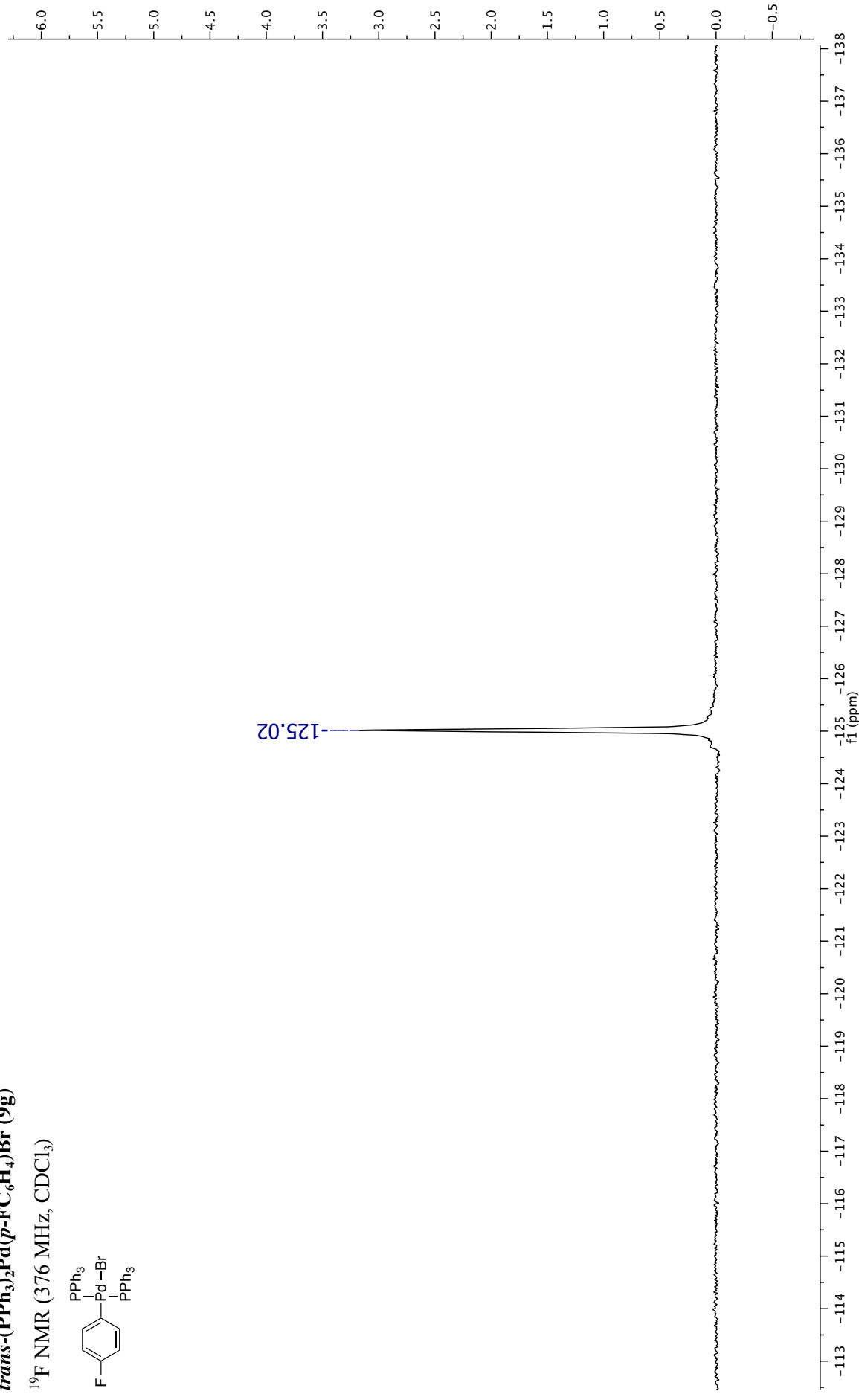
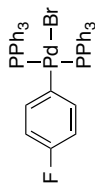
***trans*-(PPh₃)₂Pd(*p*-FC₆H₄)Br (9g)**

³¹P NMR (162 MHz, CDCl₃)



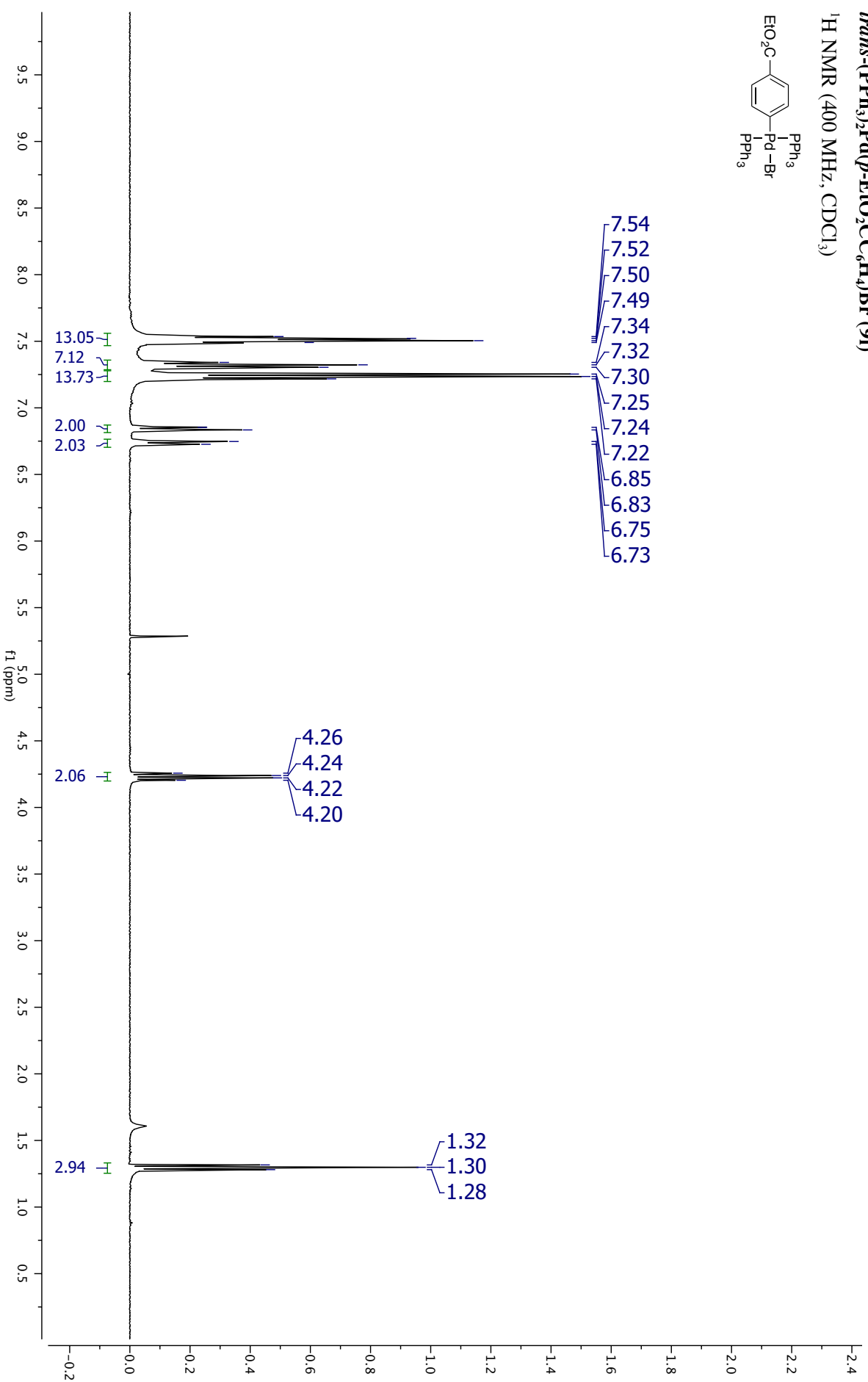
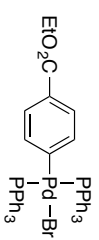
***trans*-(PPh₃)₂Pd(*p*-FC₆H₄)Br (9g)**

¹⁹F NMR (376 MHz, CDCl₃)



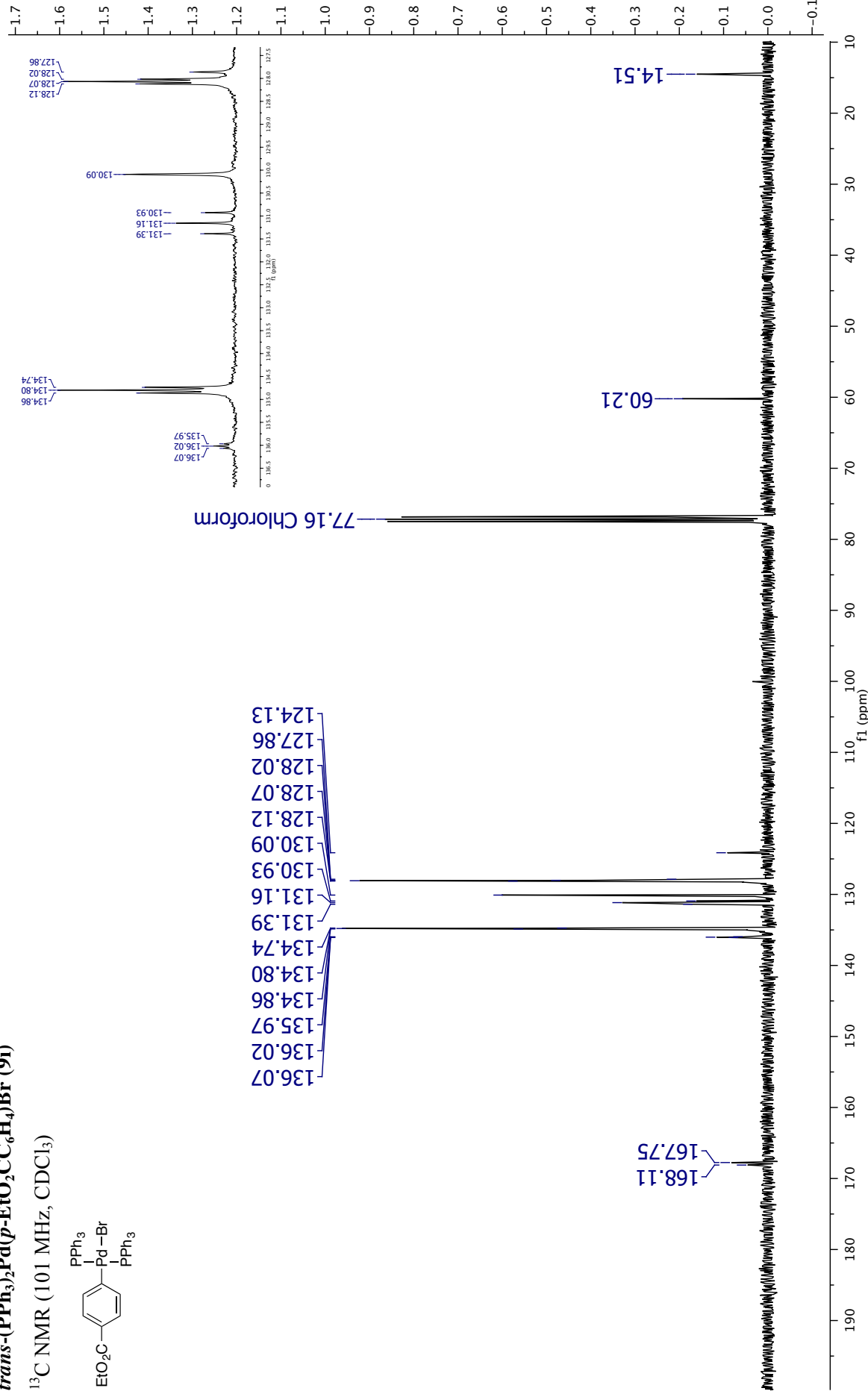
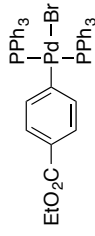
trans-(PPh₃)₂Pd(*p*-EtO₂CC₆H₄)Br (9i)

¹H NMR (400 MHz, CDCl₃)



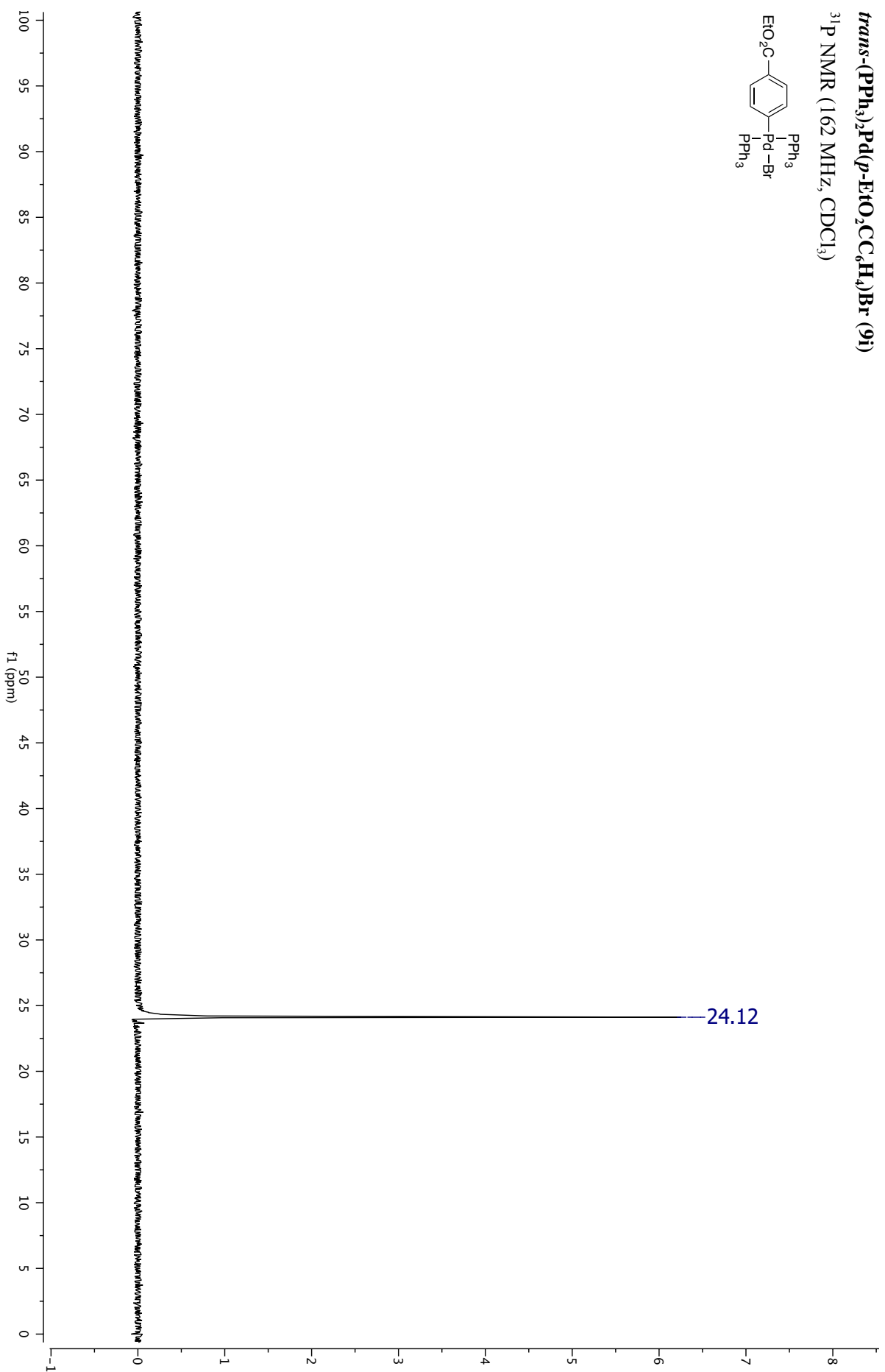
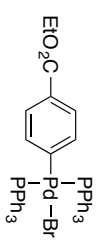
***trans*-(PPh₃)₂Pd(*p*-EtO₂CC₆H₄)Br (9i)**

¹³C NMR (101 MHz, CDCl₃)



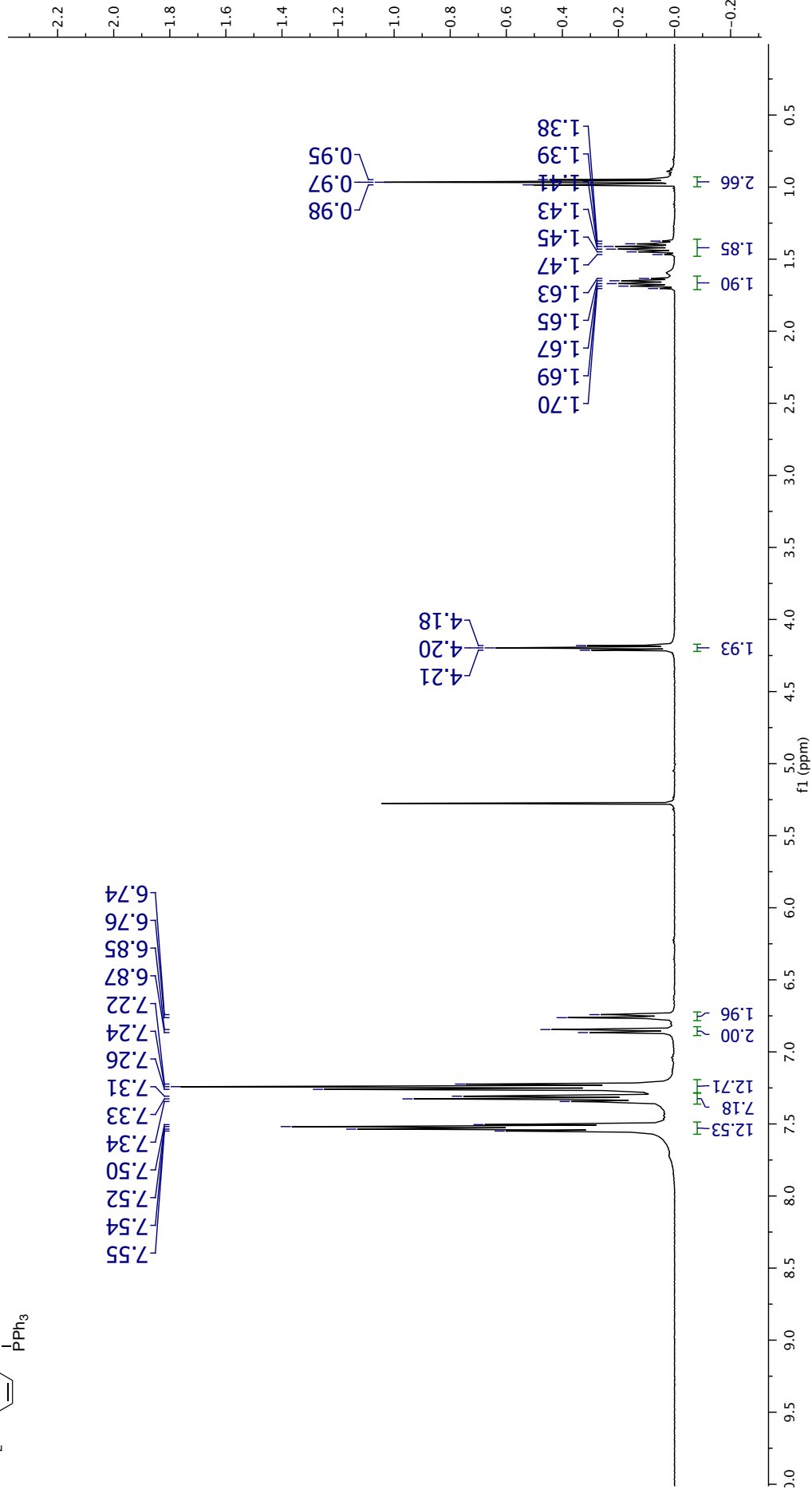
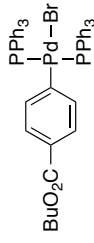
trans-(PPh₃)₂Pd(*p*-EtO₂CC₆H₄)Br (9i)

³¹P NMR (162 MHz, CDCl₃)



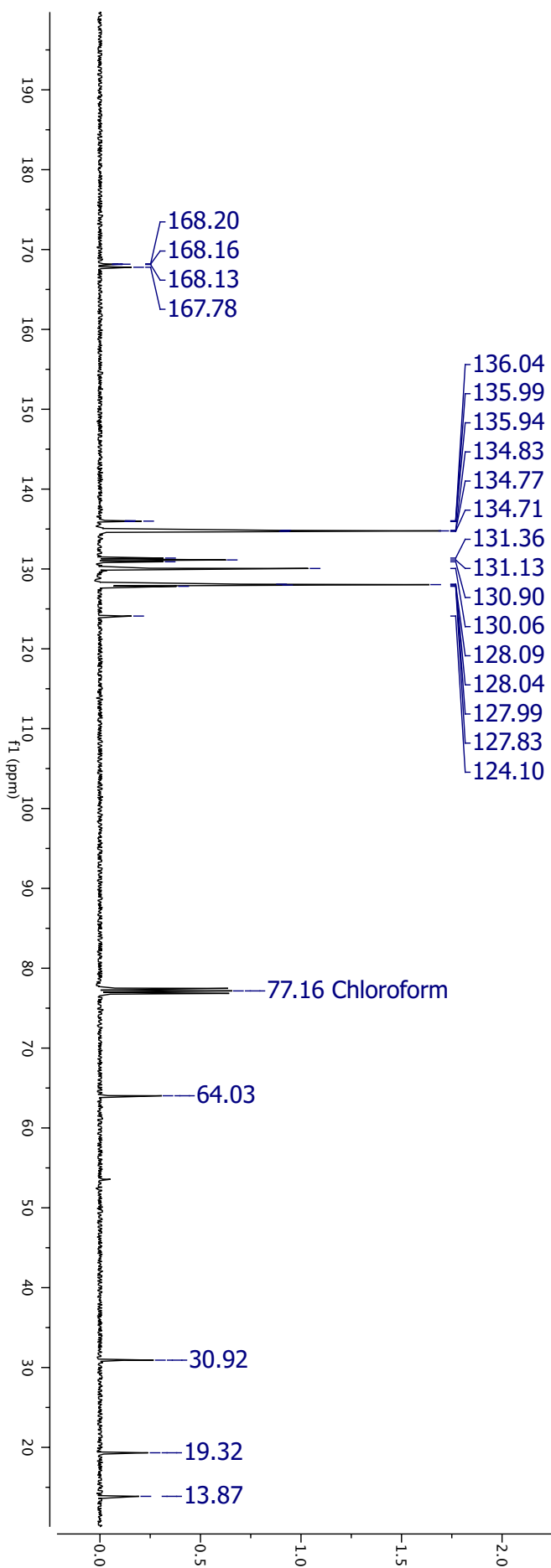
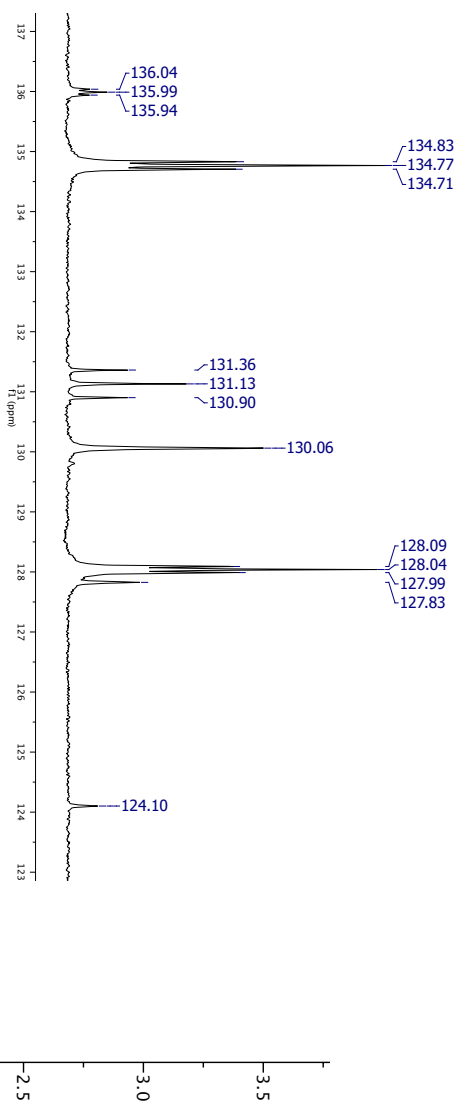
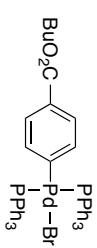
***trans*-(PPh₃)₂Pd(*p*-BuO₂CC₆H₄)Br (9j)**

¹H NMR (400 MHz, CDCl₃)



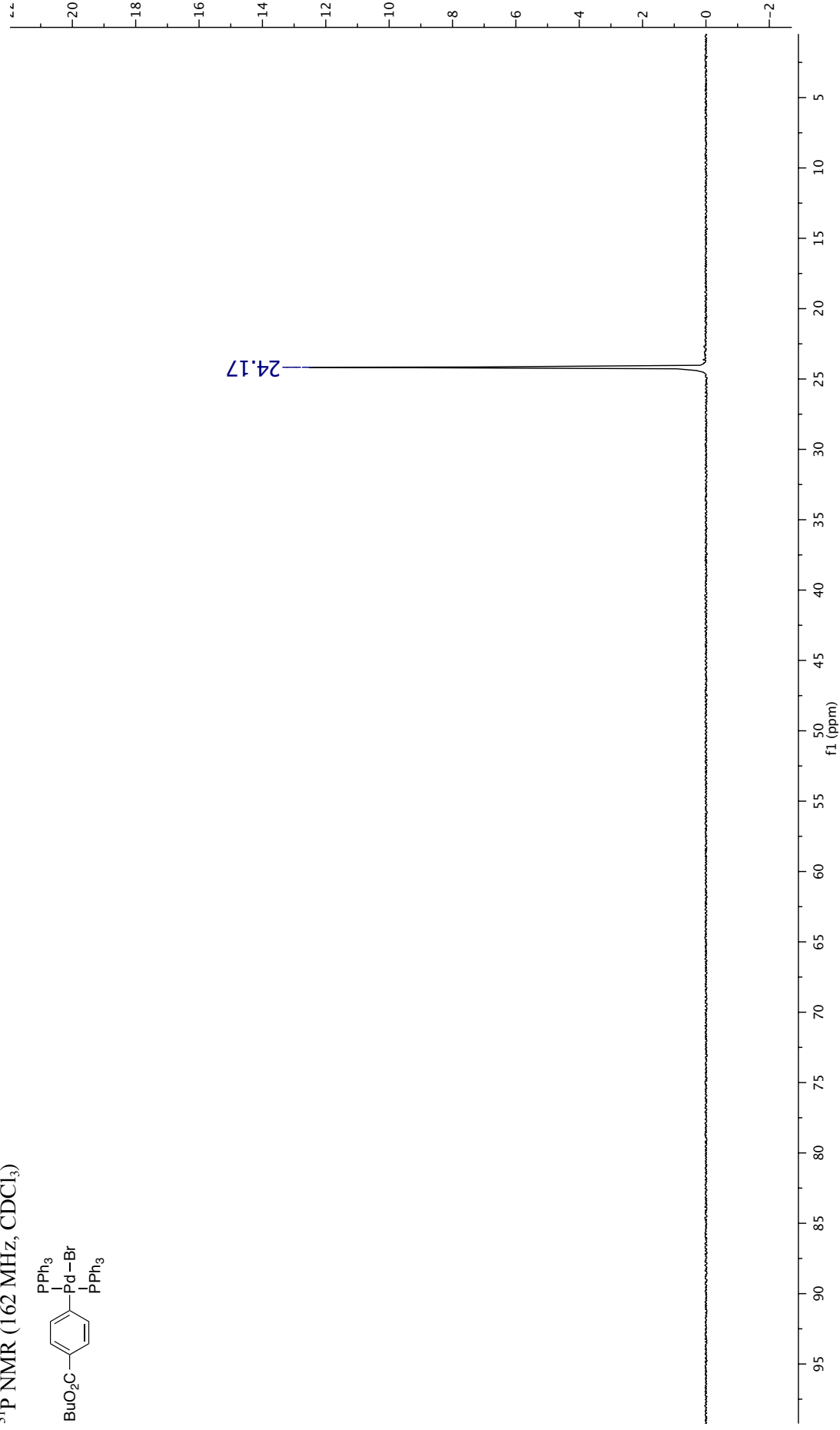
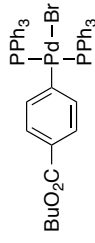
trans-(PPh₃)₂Pd(*p*-BuO₂CC₆H₄)Br (9j)

¹³C NMR (101 MHz, CDCl₃)



***trans*-(PPh₃)₂Pd(*p*-^tBuO₂CC₆H₄)Br (9j)**

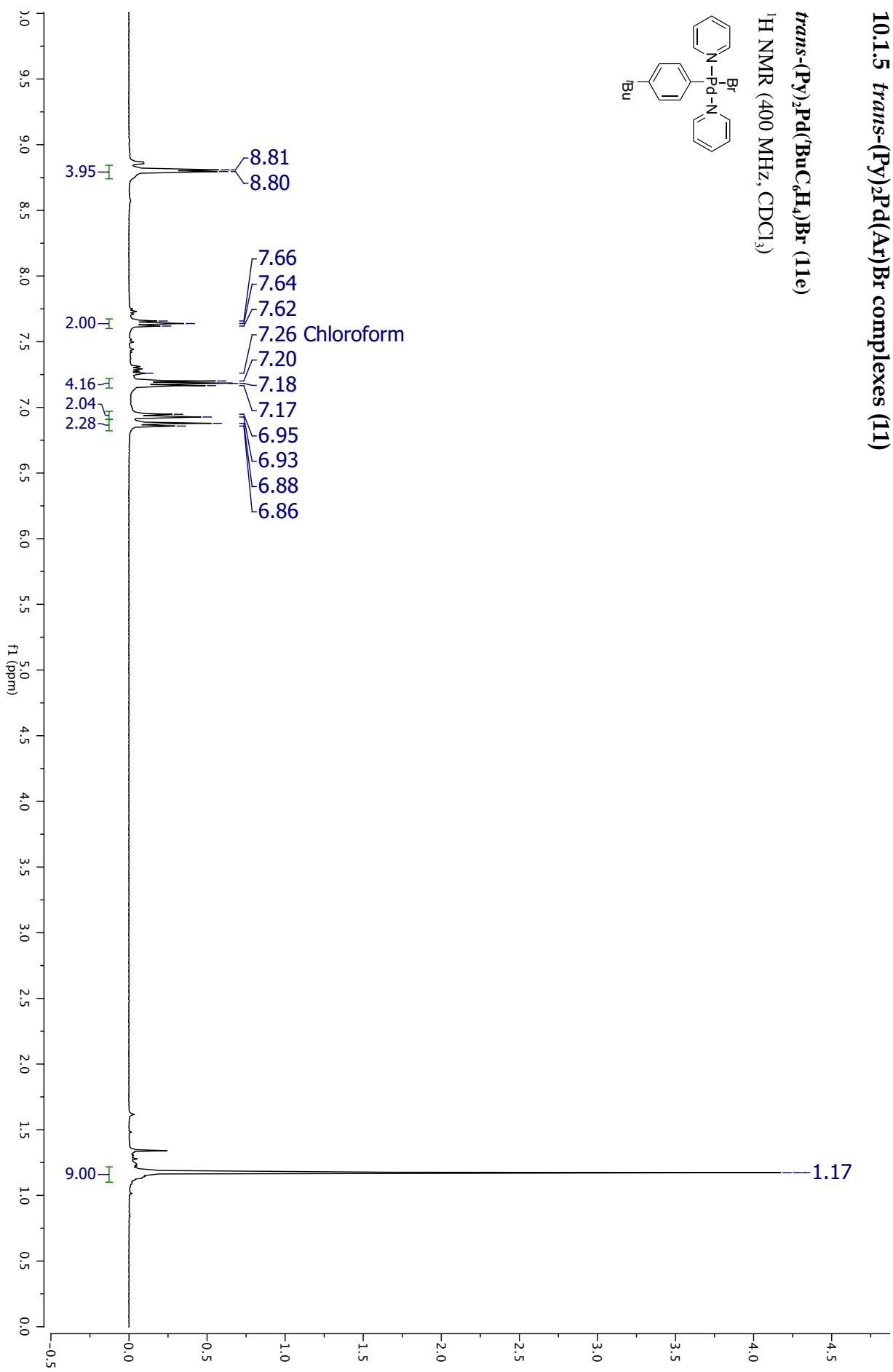
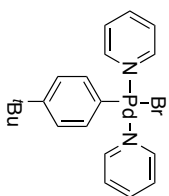
³¹P NMR (162 MHz, CDCl₃)



10.1.5 *trans*-(Py)₂Pd(Ar)Br complexes (11)

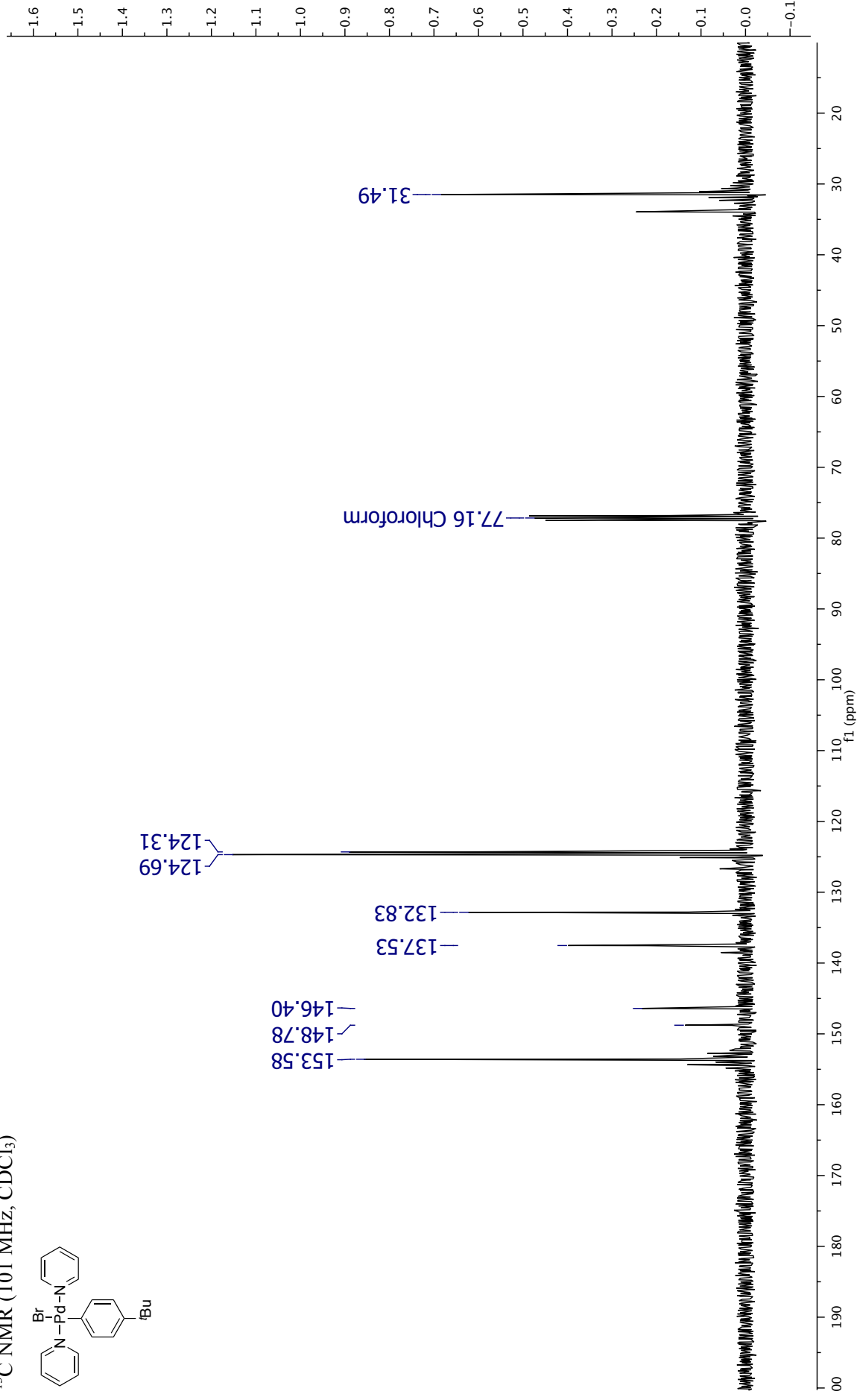
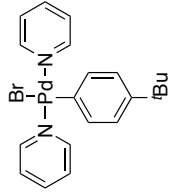
trans-(Py)₂Pd(^tBuC₆H₄)Br (11e)

¹H NMR (400 MHz, CDCl₃)



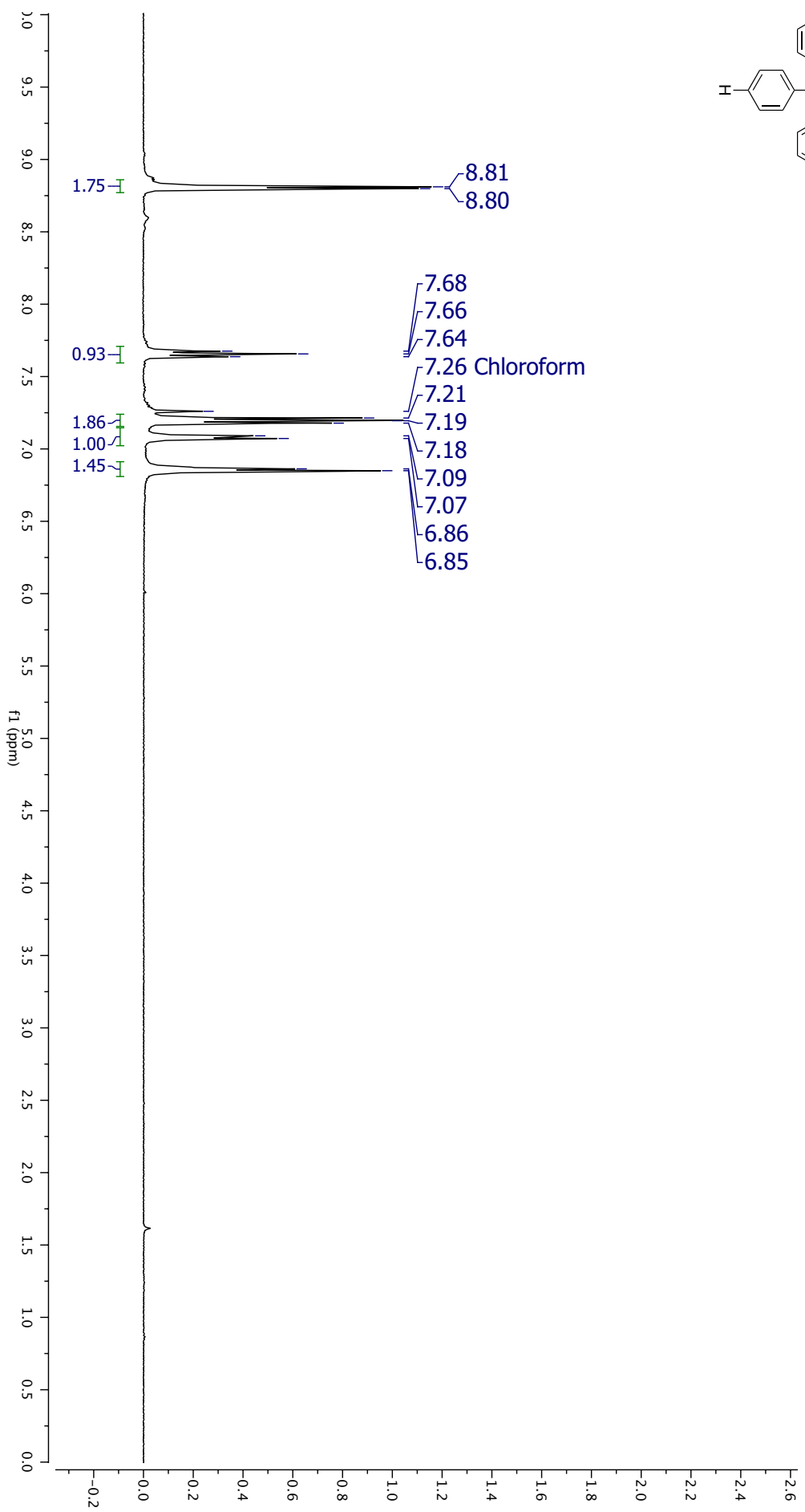
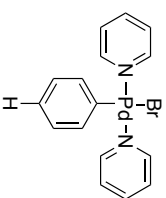
***trans*-(Py)₂Pd(^tBuC₆H₄)Br (11e)**

¹³C NMR (101 MHz, CDCl₃)



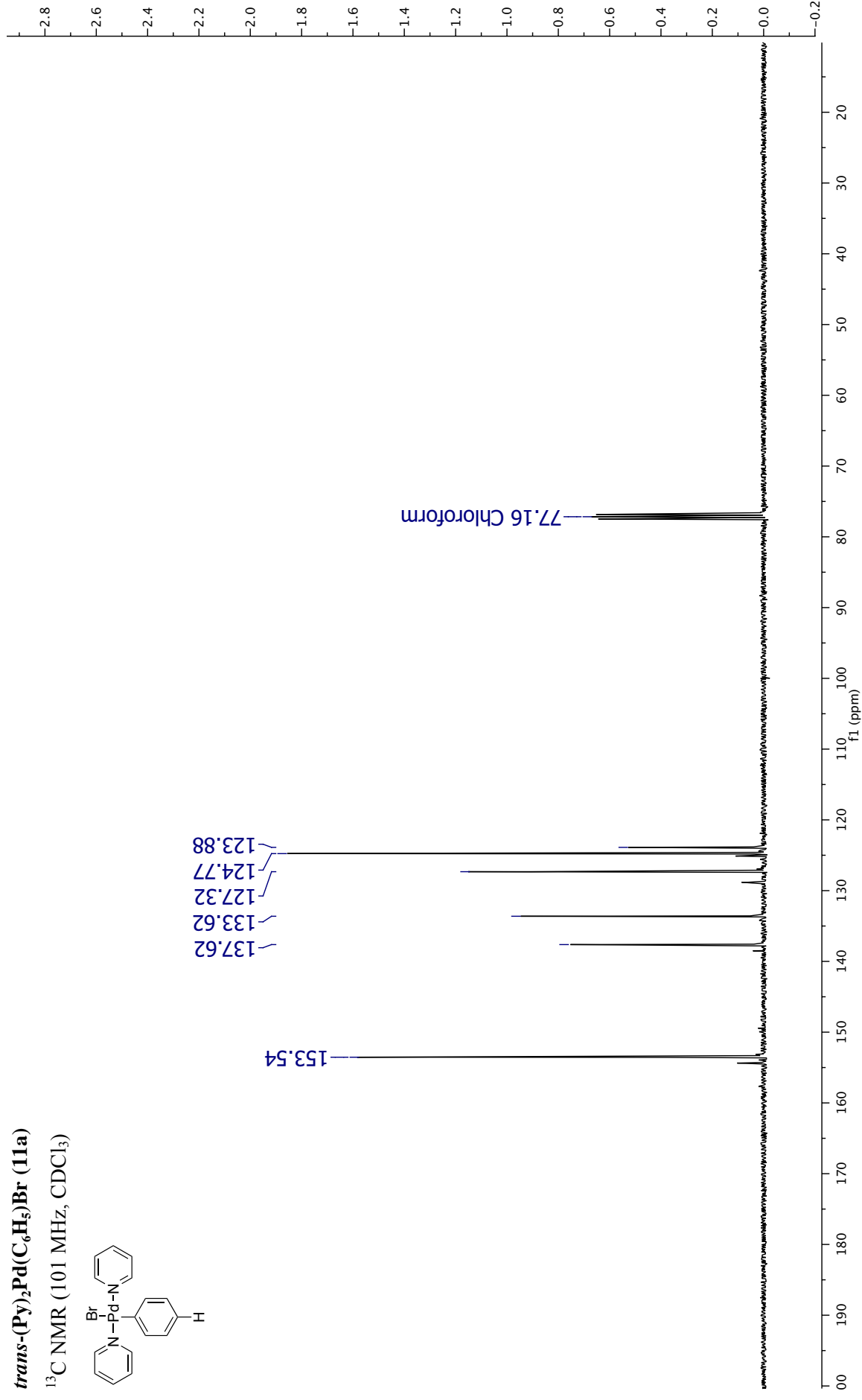
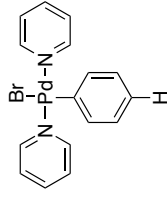
trans-(Py)₂Pd(C₆H₅)Br (11a)

¹H NMR (400 MHz, CDCl₃)



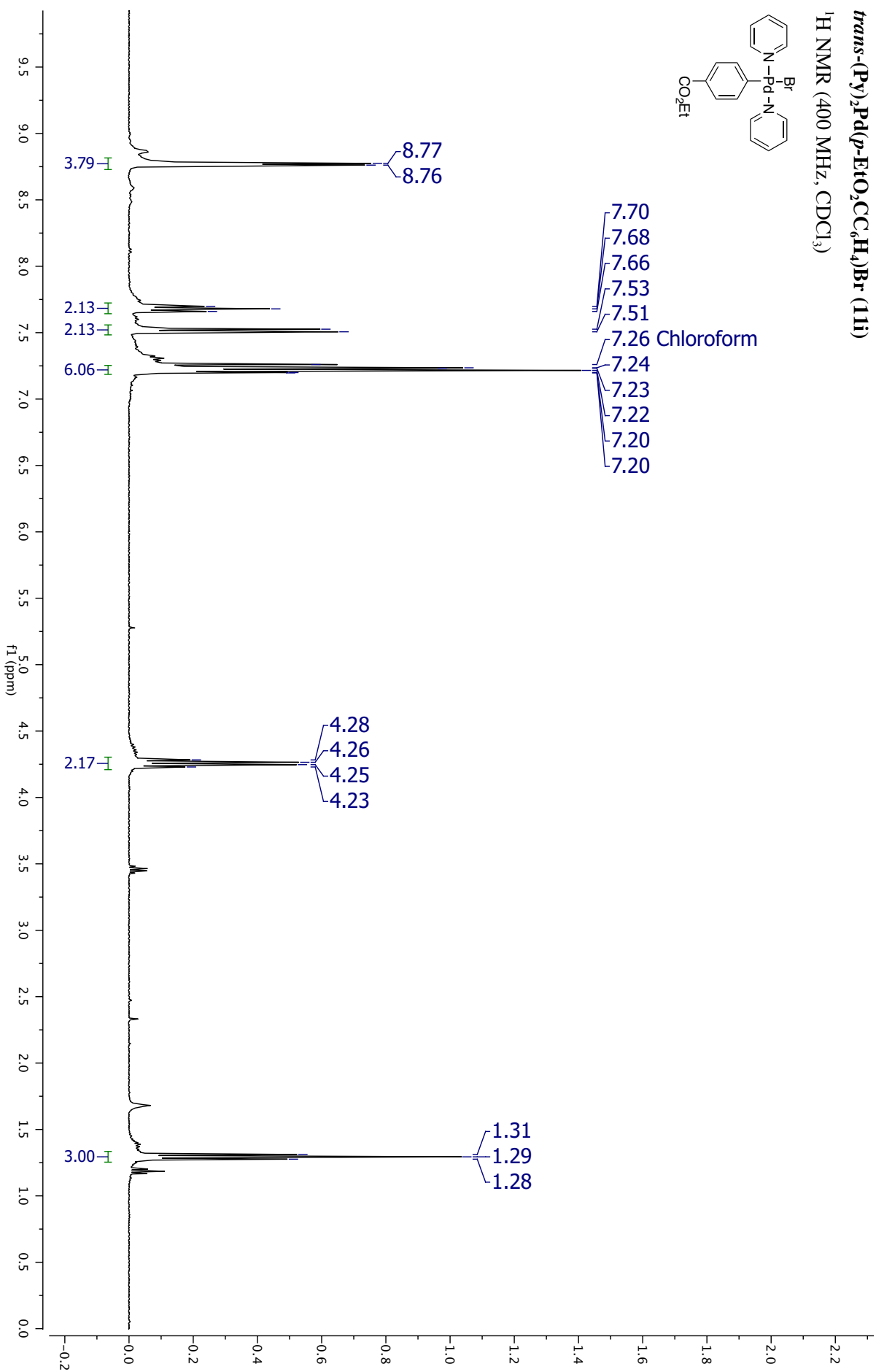
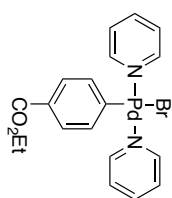
***trans*-(Py)₂Pd(C₆H₅)Br (11a)**

¹³C NMR (101 MHz, CDCl₃)



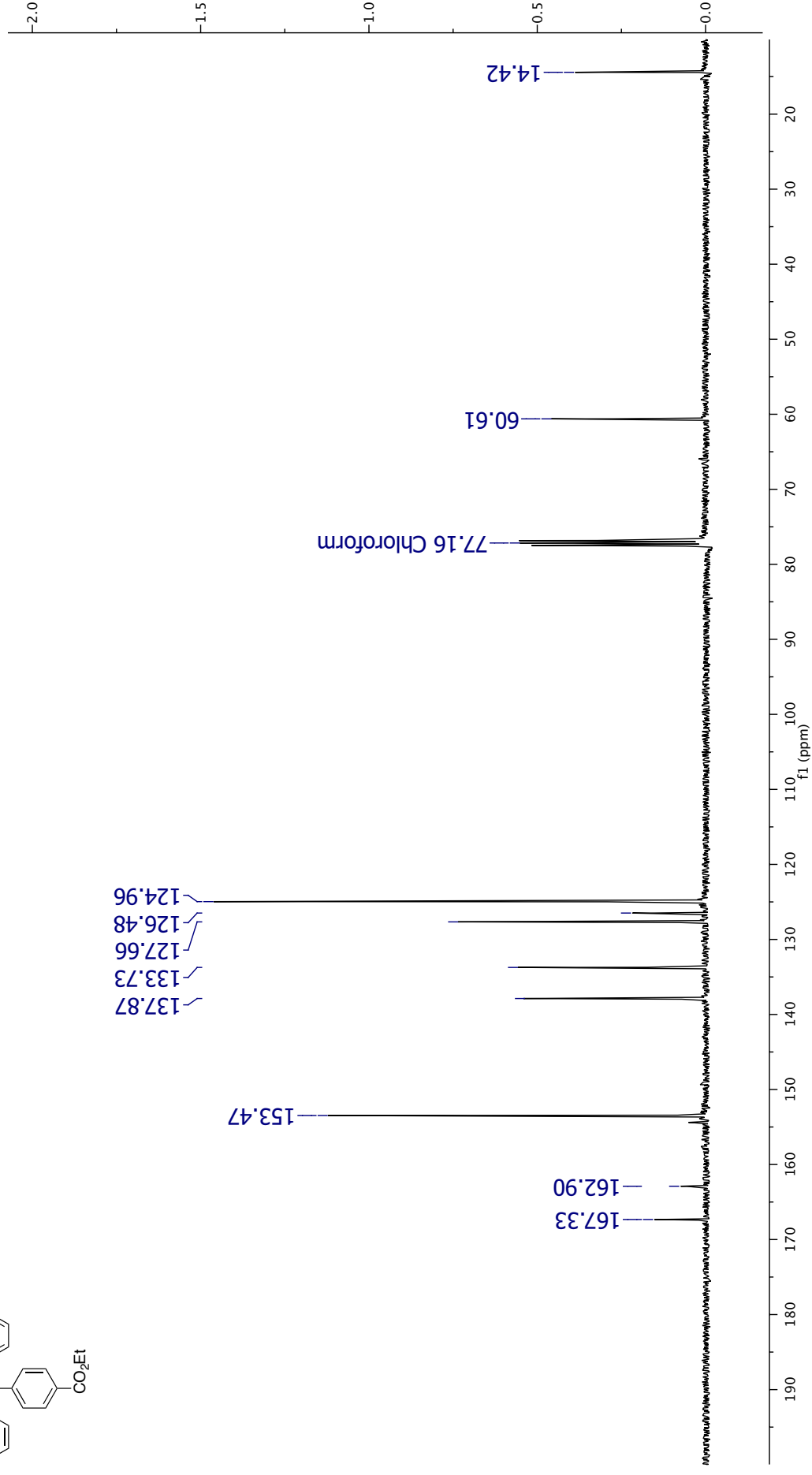
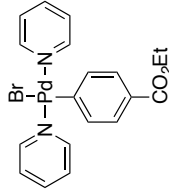
trans-(Py)₂Pd(*p*-EtO₂CC₆H₄)Br (11i)

¹H NMR (400 MHz, CDCl₃)



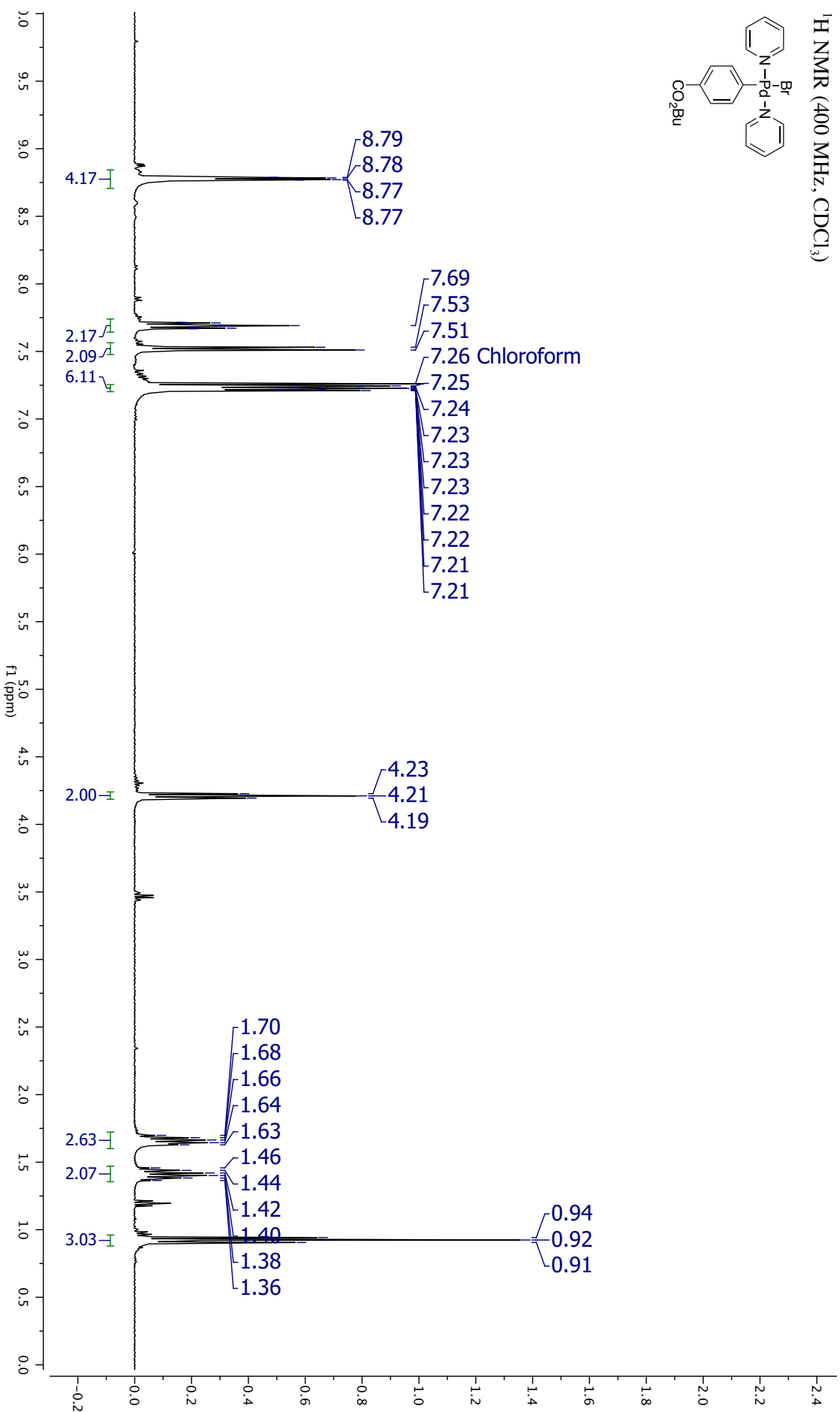
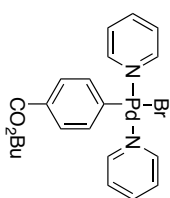
***trans*-(Py)₂Pd(*p*-EtO₂CC₆H₄)Br (11i)**

¹³C NMR (101 MHz, CDCl₃)



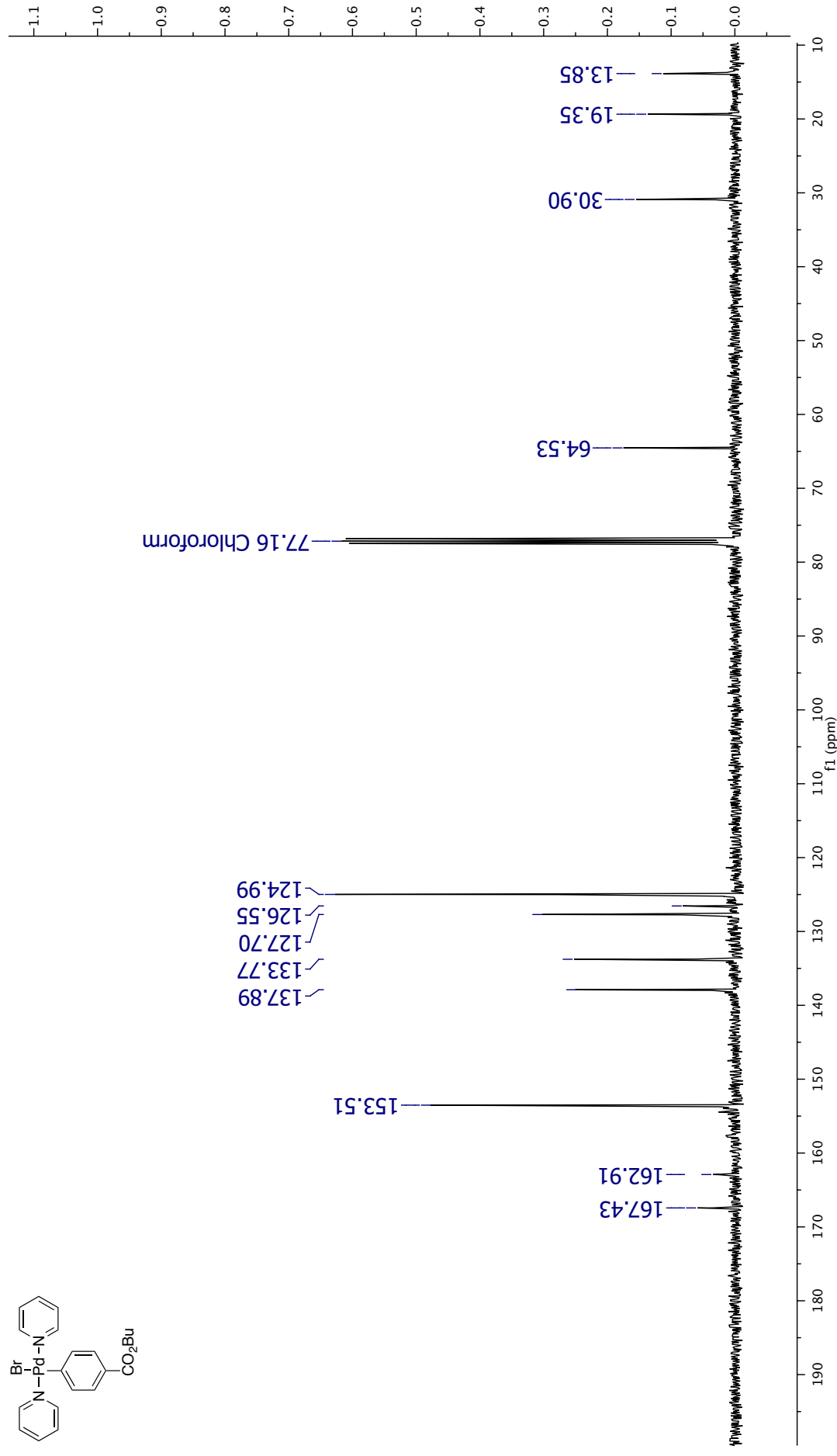
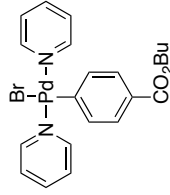
trans-(Py)₂Pd(*p*-^tBuO₂C₆H₄)Br (11j)

¹H NMR (400 MHz, CDCl₃)



***trans*-(Py)₂Pd(*p*-^tBuO₂CC₆H₄)Br (11j)**

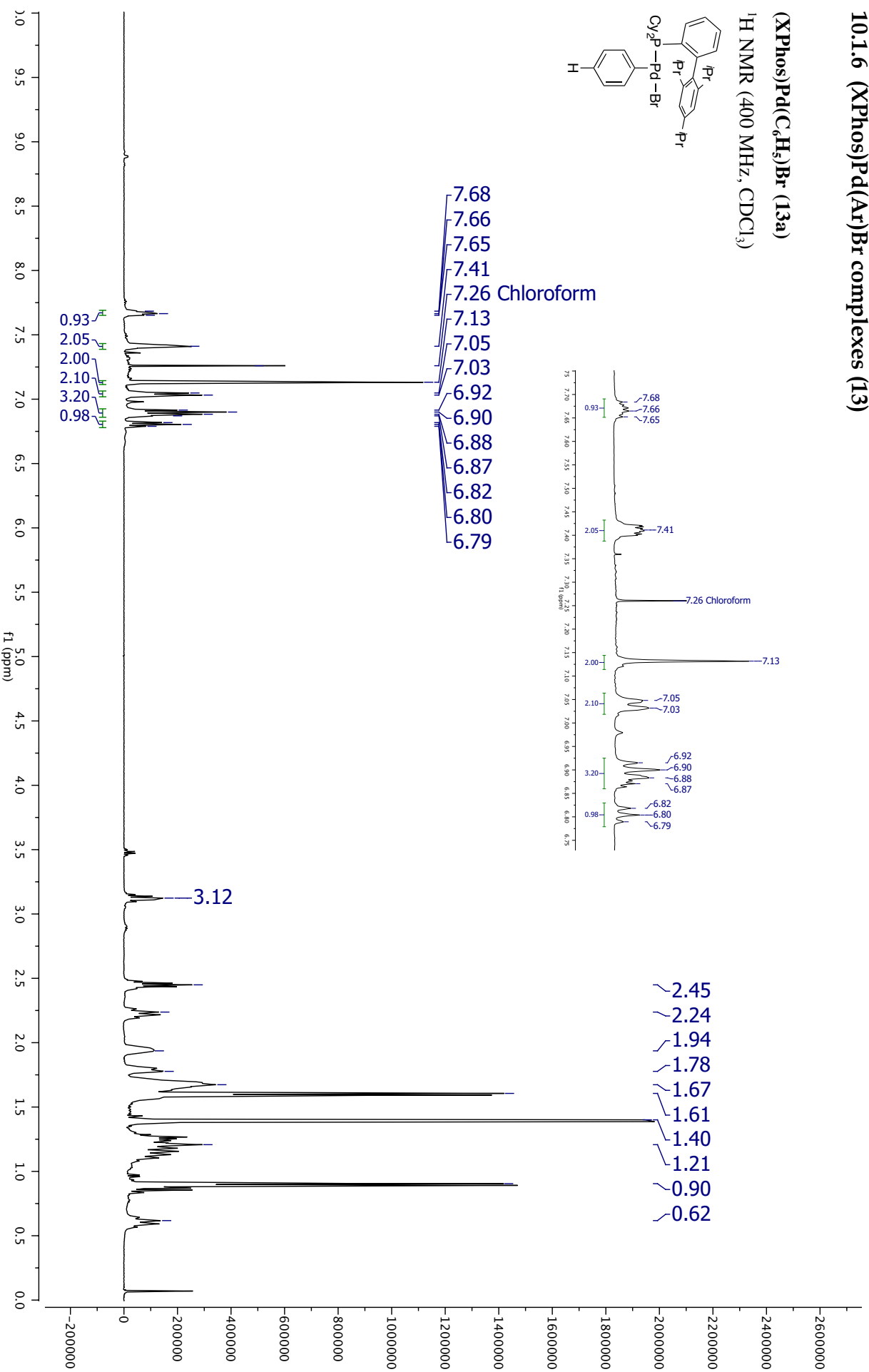
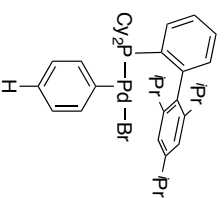
¹³C NMR (101 MHz, CDCl₃)



10.1.6 (XPhos)Pd(Ar)Br complexes (13)

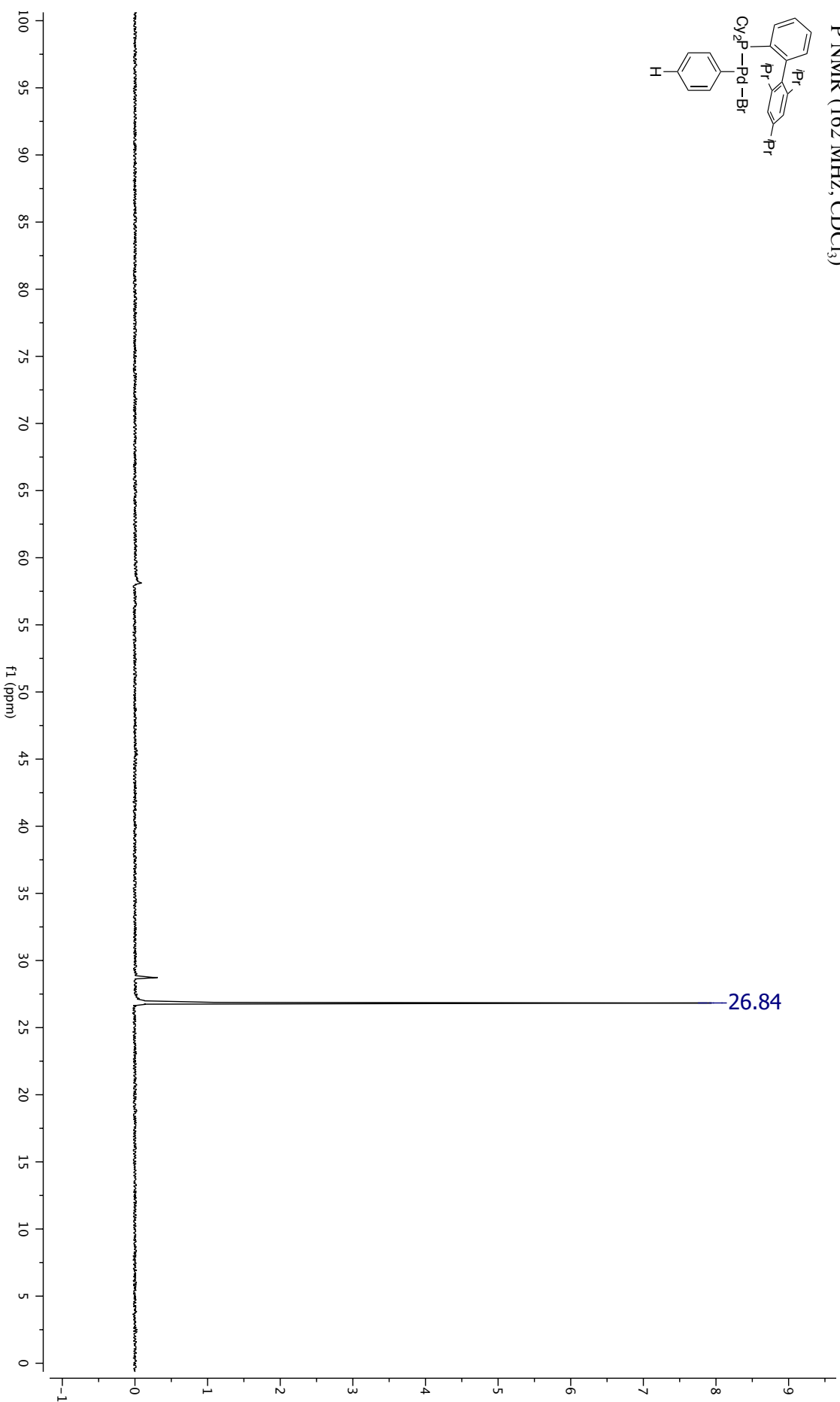
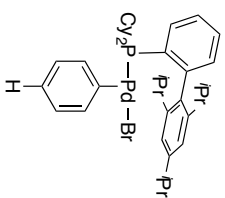
(XPhos)Pd(C₆H₅)Br (13a)

¹H NMR (400 MHz, CDCl₃)



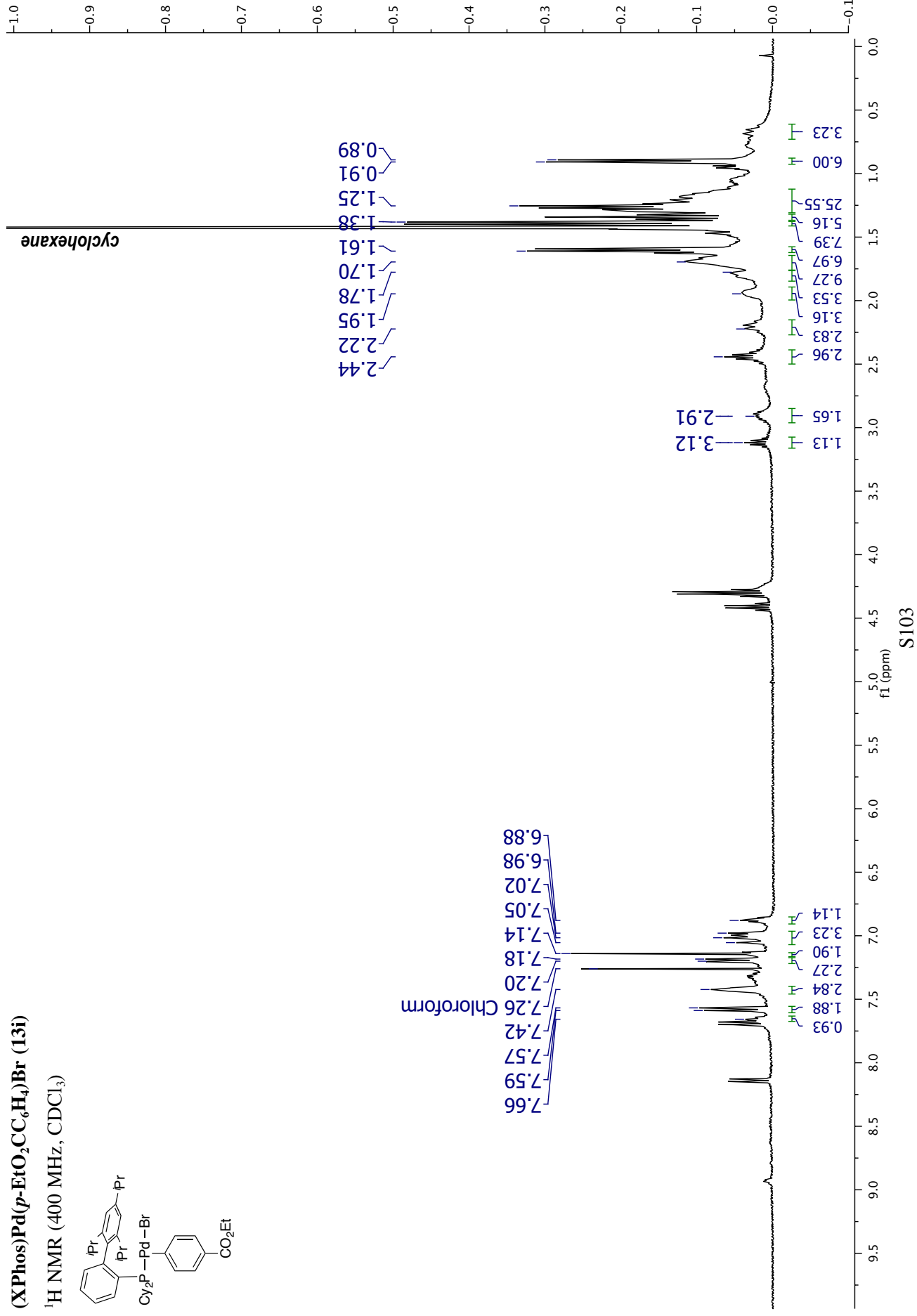
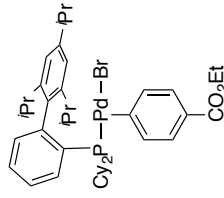
(XPhos)Pd(C₆H₅)Br (13a)

³¹P NMR (162 MHz, CDCl₃)



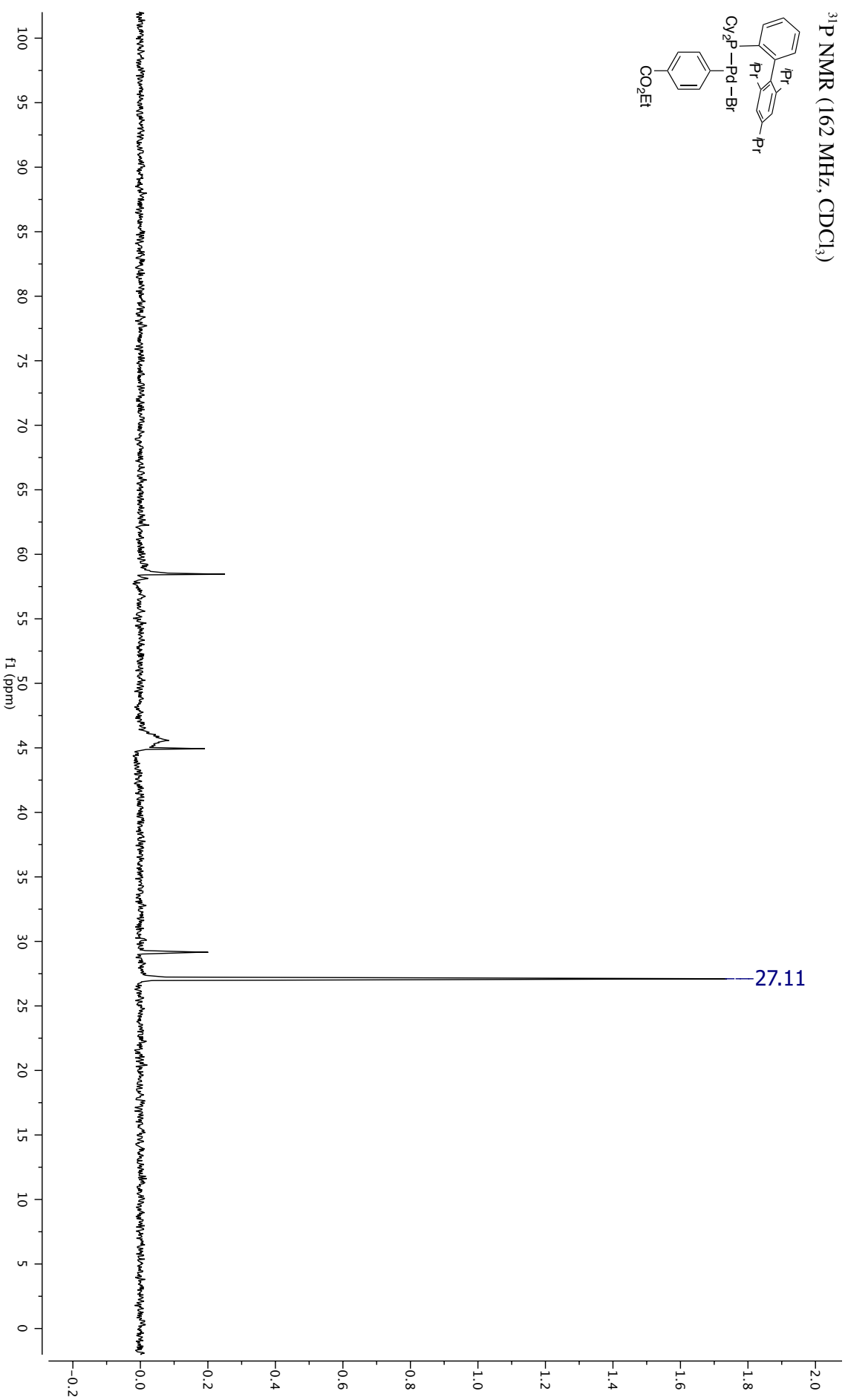
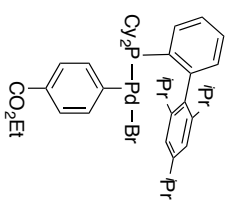
(XPhos)Pd(*p*-EtO₂CC₆H₄)Br (13i)

¹H NMR (400 MHz, CDCl₃)



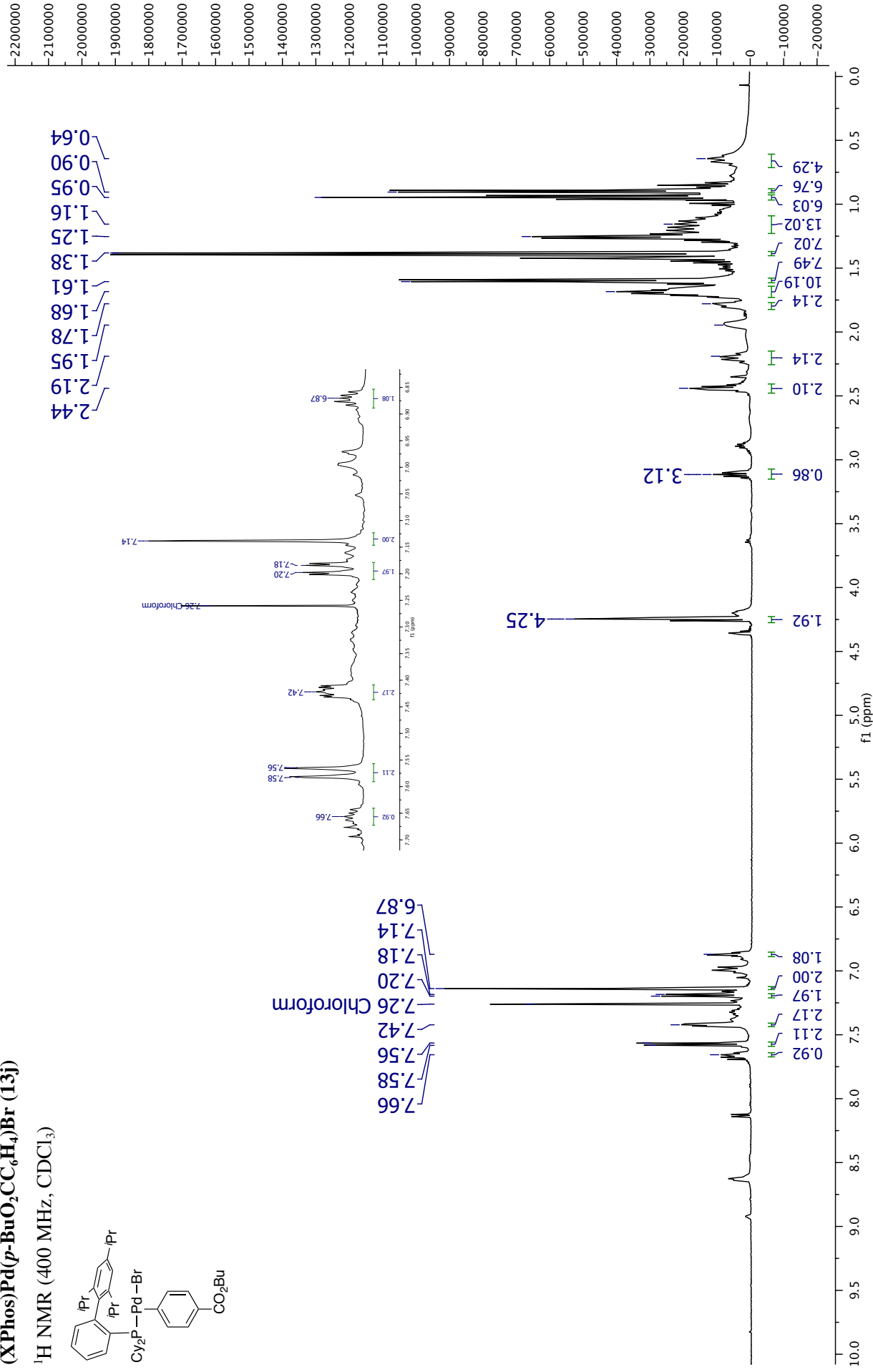
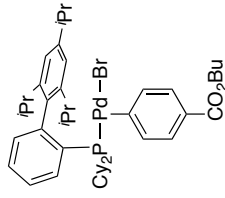
(XPhos)Pd(*p*-EtO₂CC₆H₄)Br (13i)

³¹P NMR (162 MHz, CDCl₃)



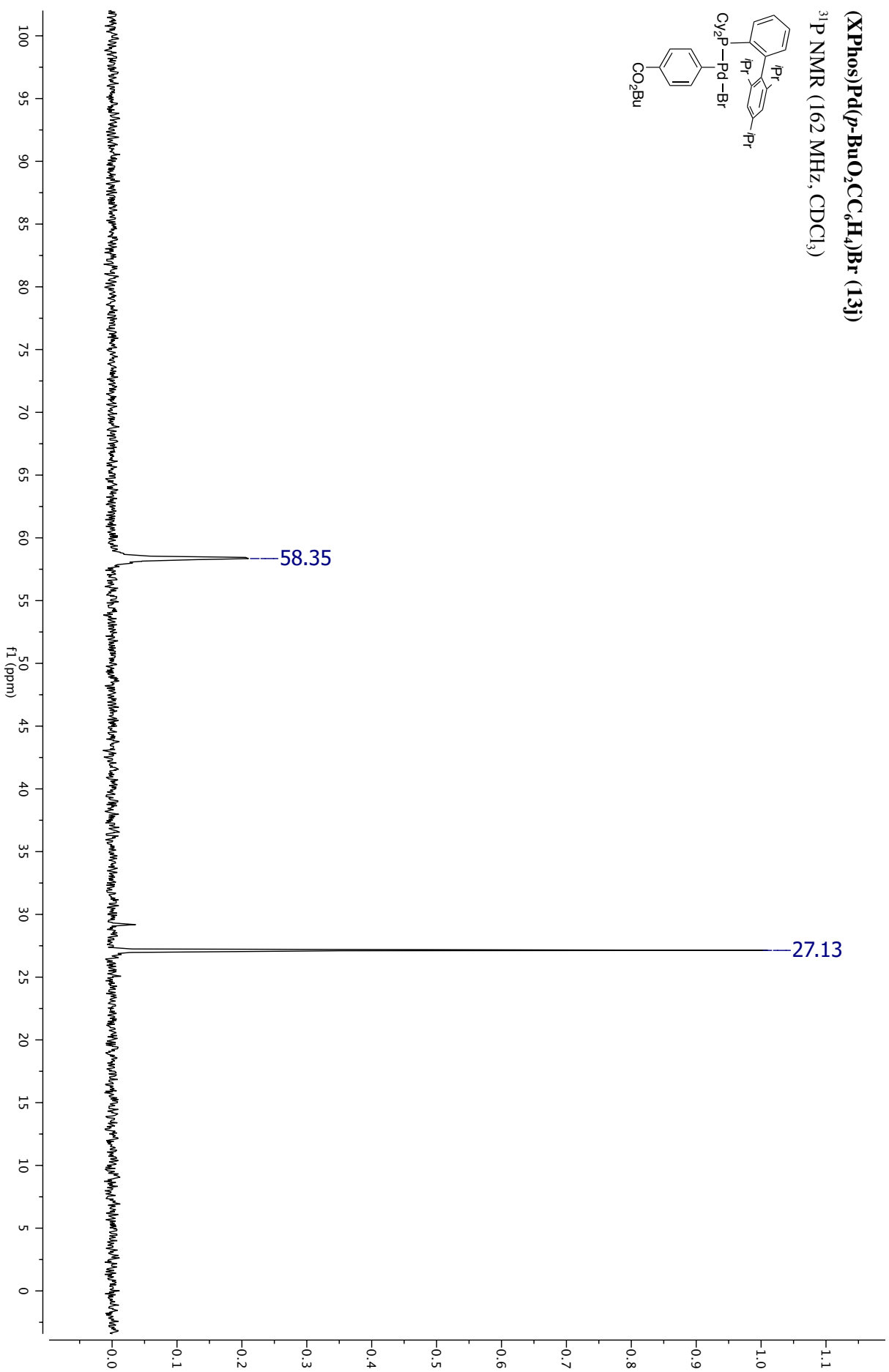
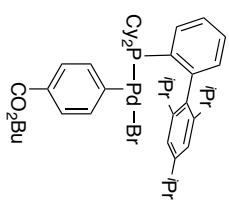
(XPhos)Pd(*p*-BuO₂CC₆H₄)Br (13j)

¹H NMR (400 MHz, CDCl₃)



(XPhos)Pd(*p*-BuO₂CC₆H₄)Br (13f)

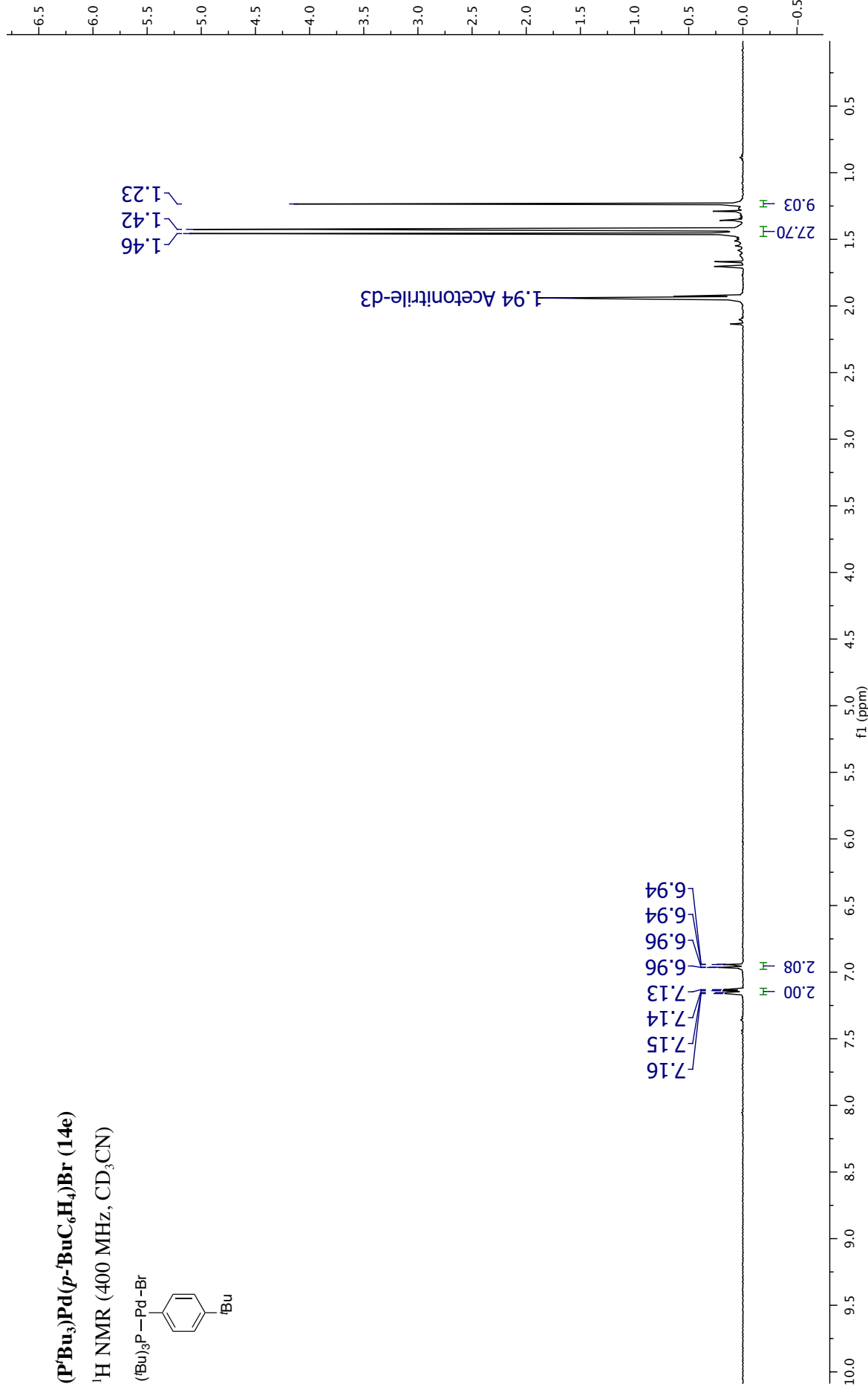
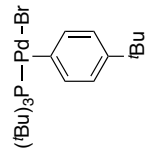
³¹P NMR (162 MHz, CDCl₃)



10.1.7 (P^tBu₃)Pd(Ar)Br complexes (14)

(P^tBu₃)Pd(*p*-^tBuC₆H₄)Br (14e)

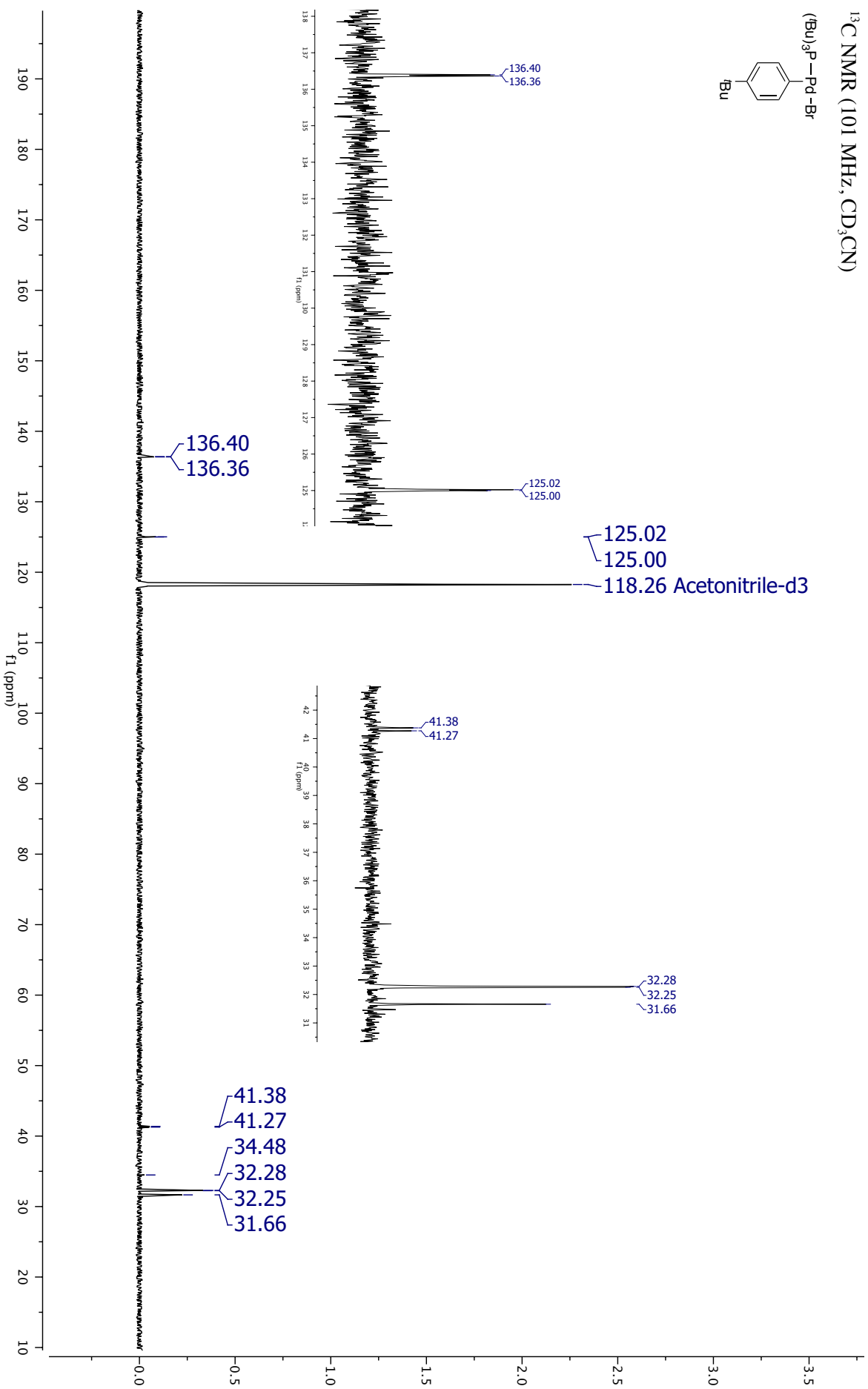
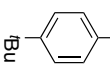
¹H NMR (400 MHz, CD₃CN)



(*P*Bu₃)₂Pd(*p*-BuC₆H₄)Br (14e)

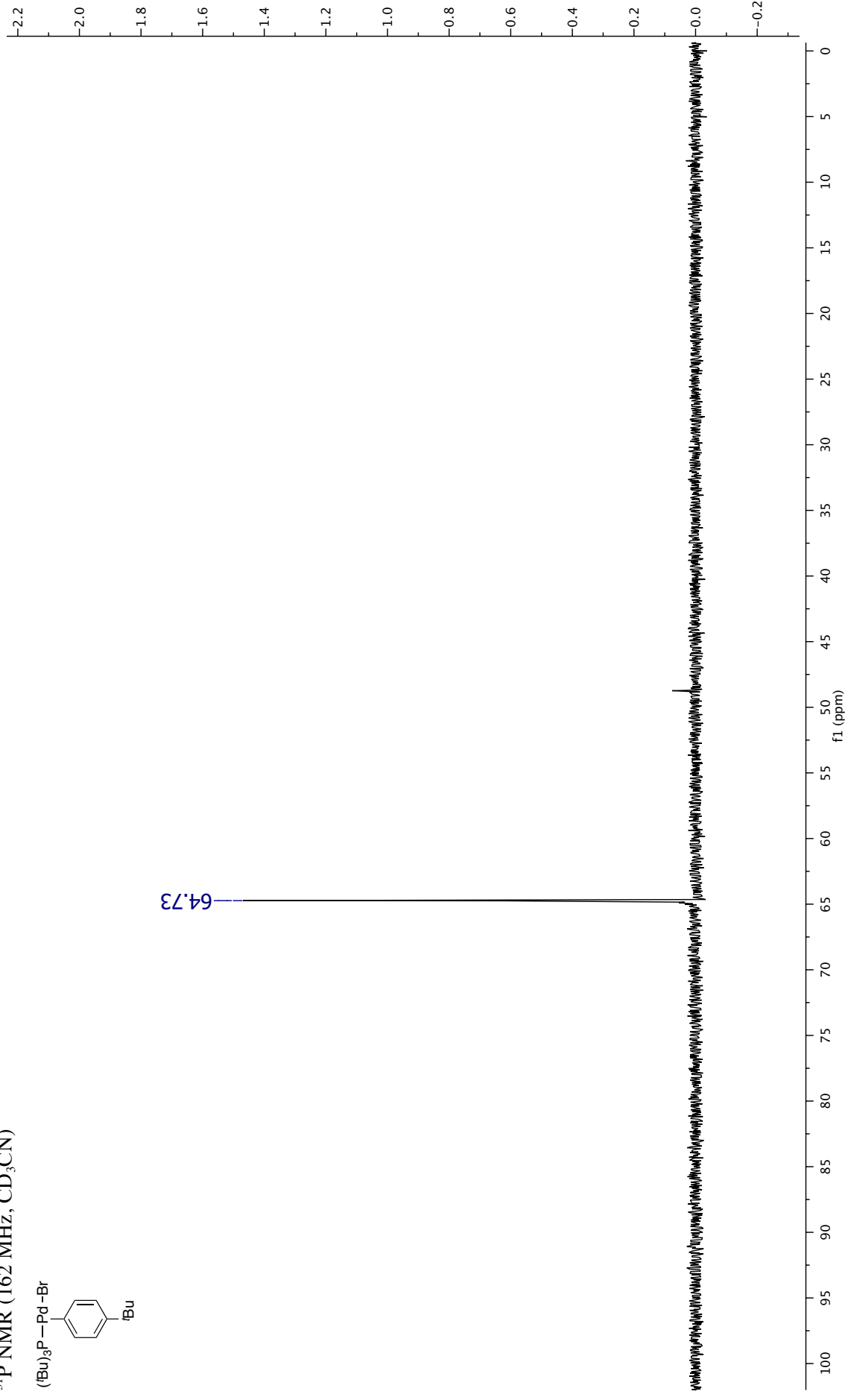
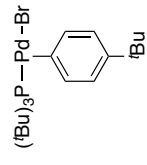
¹³C NMR (101 MHz, CD₃CN)

(Bu)₃P—Pd—Br



(P^tBu₃)₂Pd(*p*-tBuC₆H₄)Br (14e)

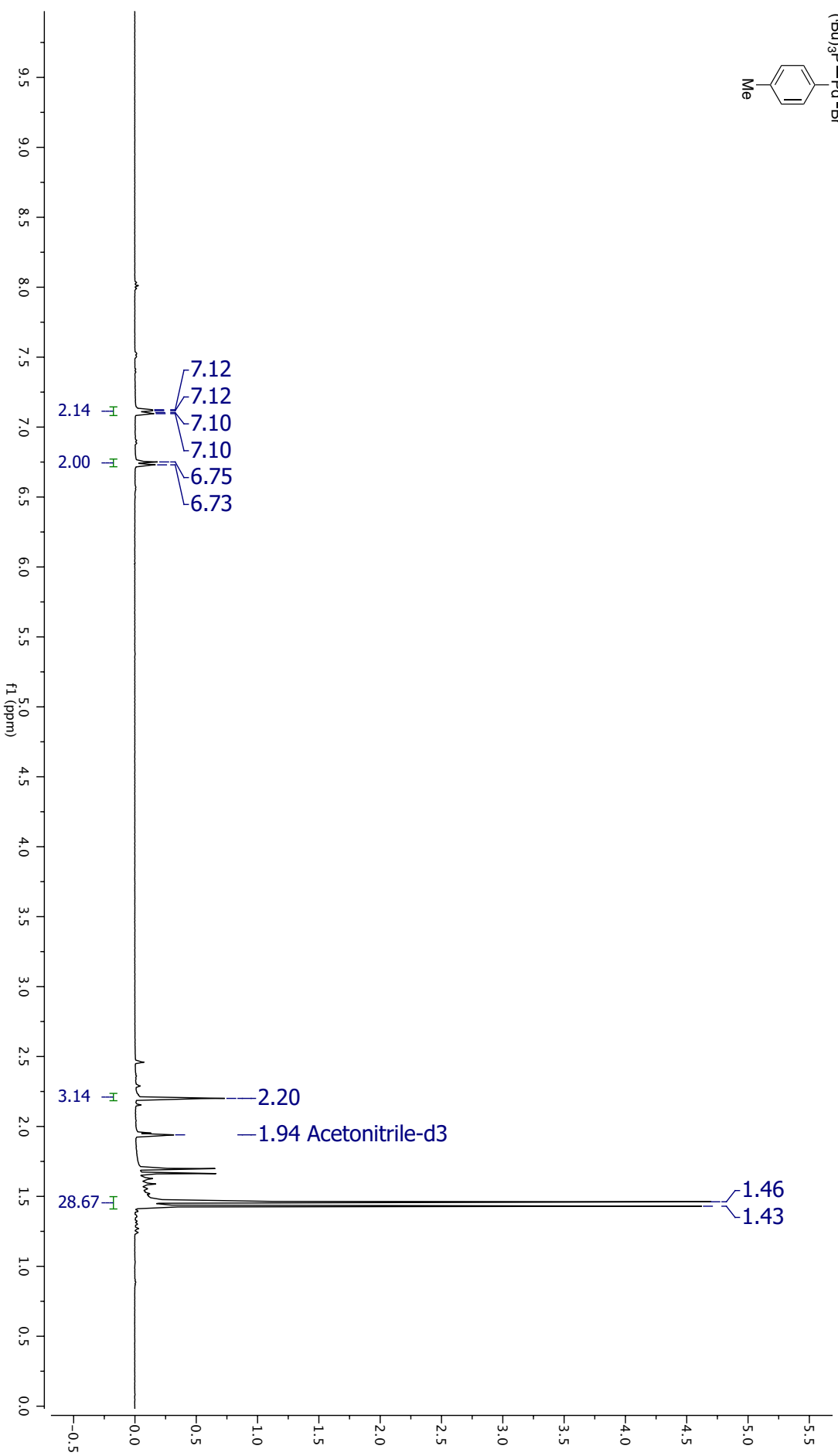
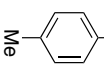
³¹P NMR (162 MHz, CD₃CN)



(^tBu)₃Pd(*p*-MeC₆H₄)Br (14f)

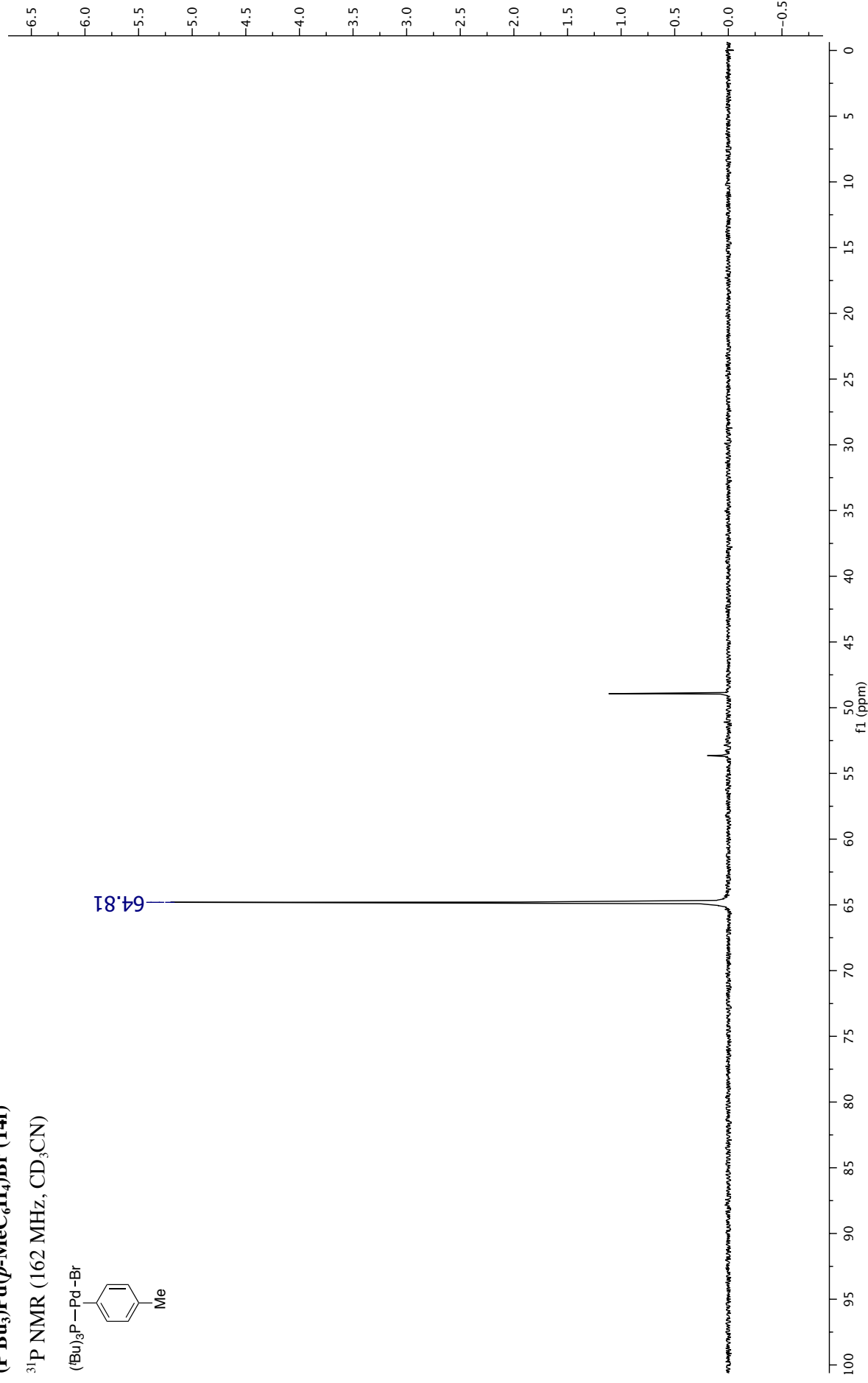
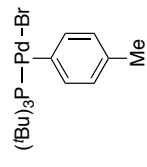
¹H NMR (400 MHz, CD₃CN)

(^tBu)₃P—Pd—Br



(P^tBu₃)Pd(*p*-MeC₆H₄)Br (14f)

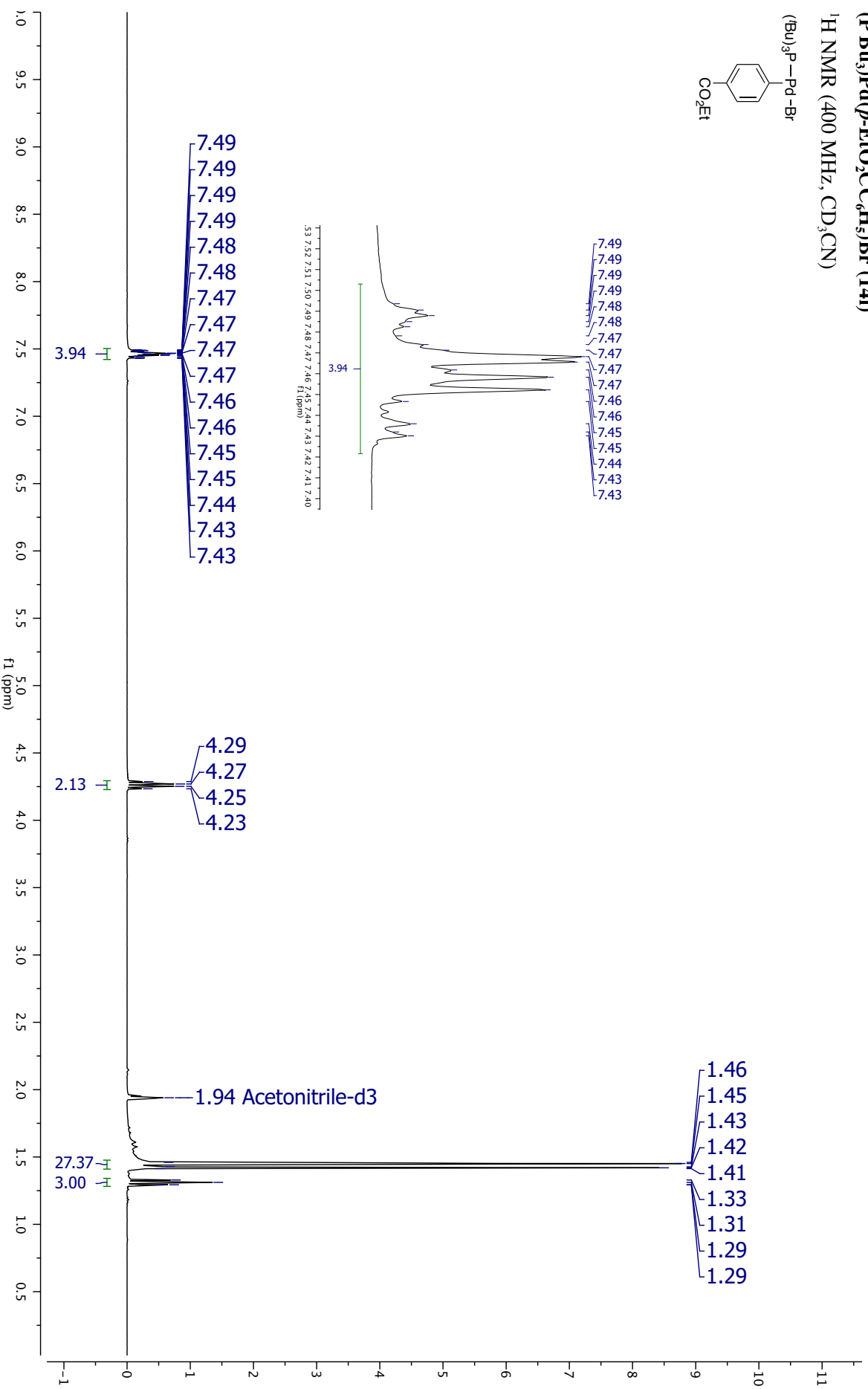
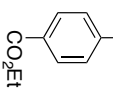
³¹P NMR (162 MHz, CD₃CN)



(P^tBu₃)₂Pd(*p*-EtO₂CC₆H₅)Br (14i)

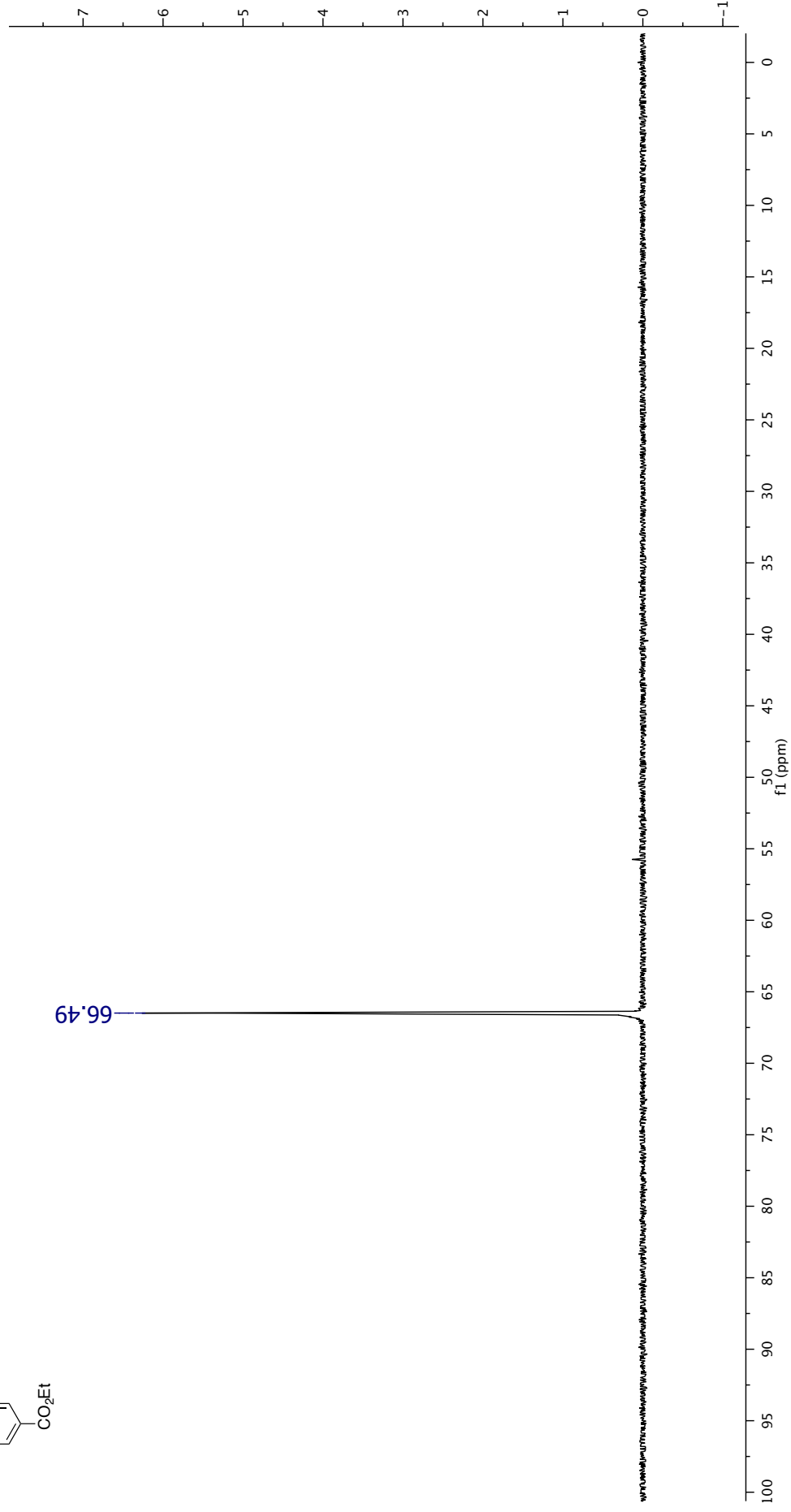
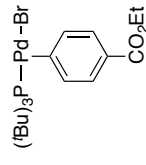
¹H NMR (400 MHz, CD₃CN)

(Bu)₃P-Pd-Br



(P^tBu₃)Pd(*p*-EtO₂CC₆H₅)Br (14i)

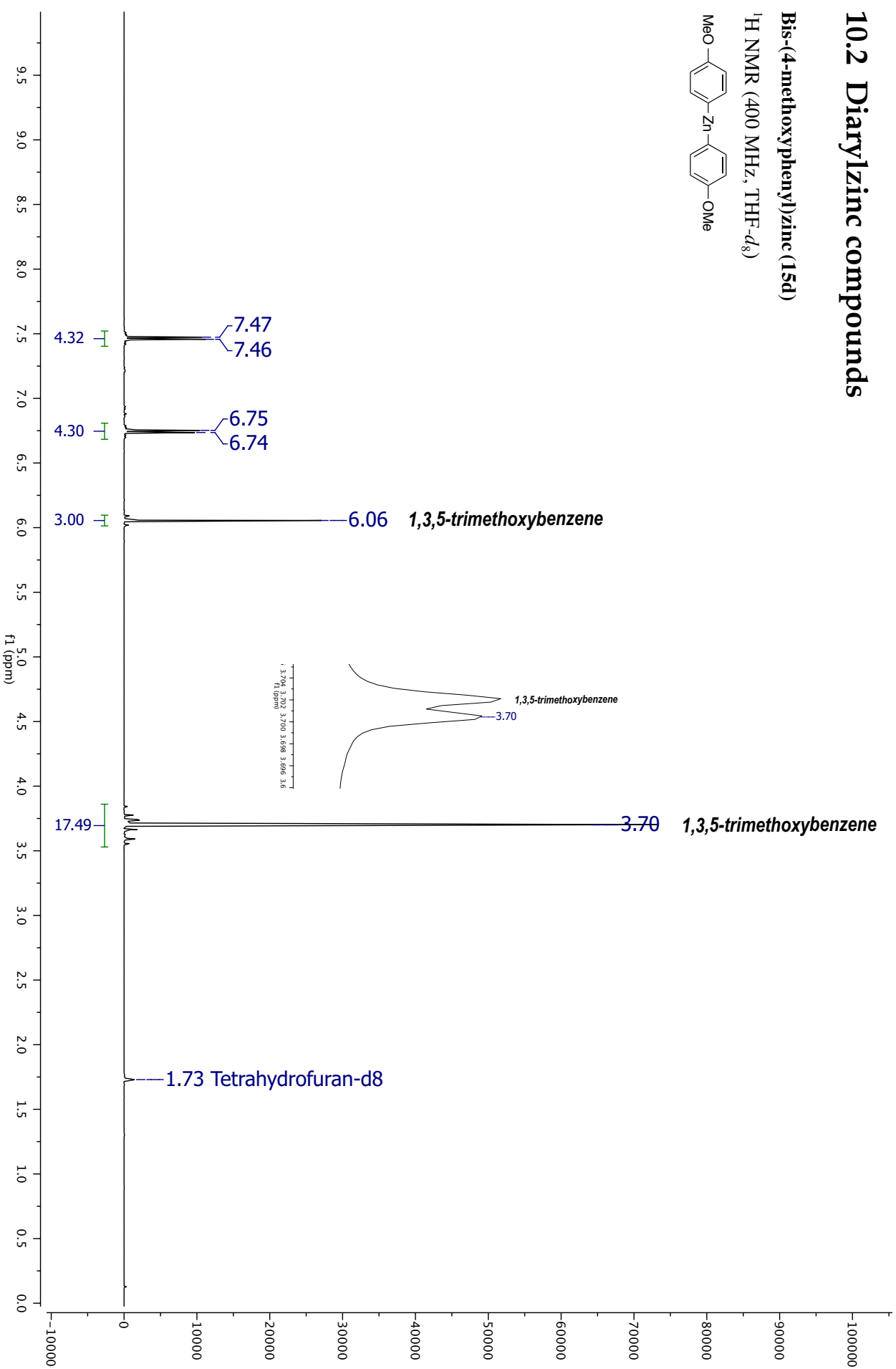
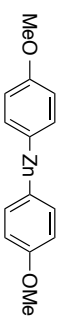
³¹P NMR (162 MHz, CD₃CN)



10.2 Diarylzinc compounds

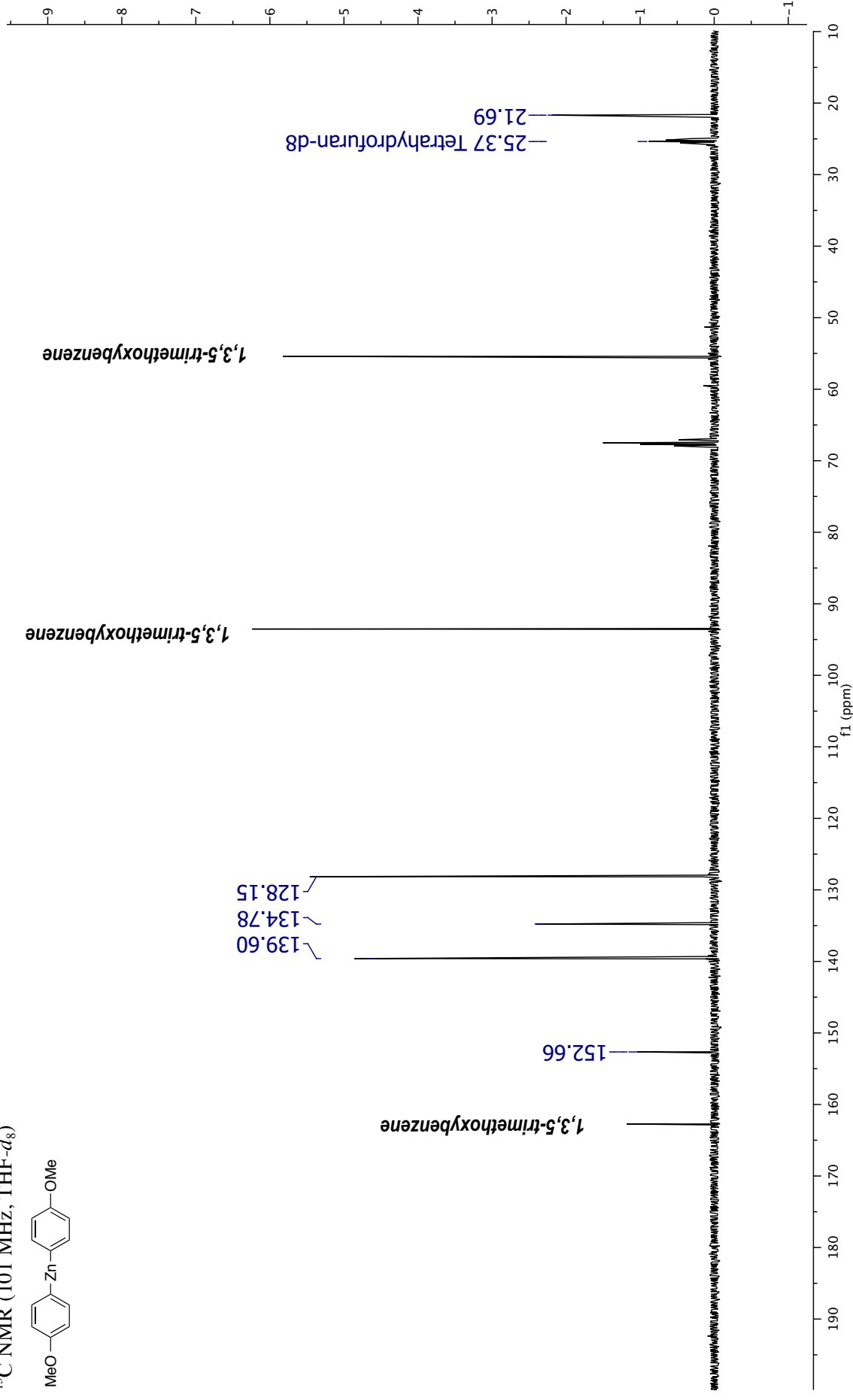
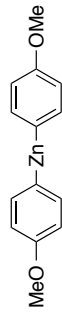
Bis-(4-methoxyphenyl)zinc (15d)

¹H NMR (400 MHz, THF-*d*₈)



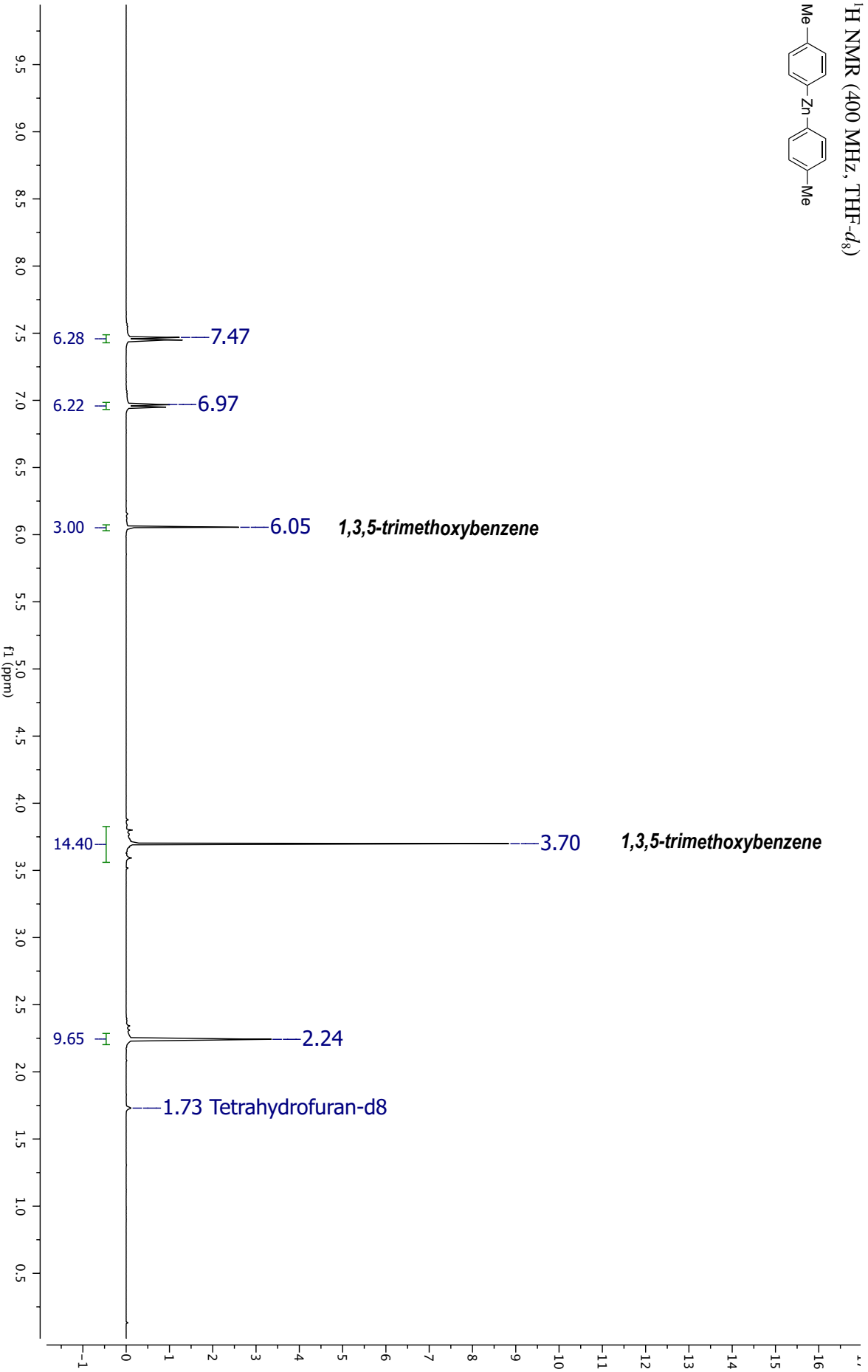
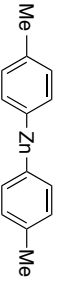
Bis-(4-methoxyphenyl)zinc (15d)

^{13}C NMR (101 MHz, THF- d_8)



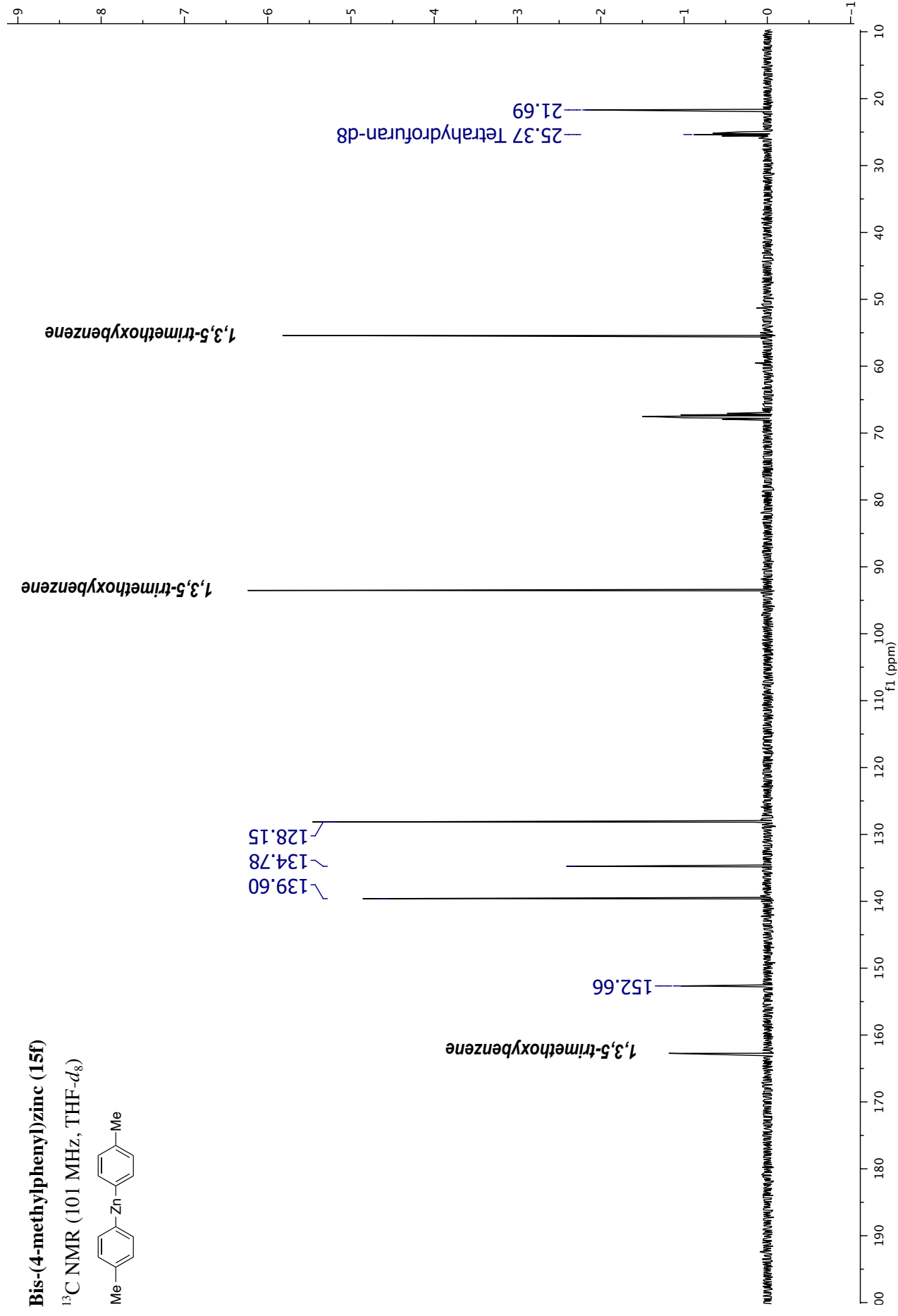
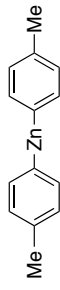
Bis-(4-methylphenyl)zinc (15f)

¹H NMR (400 MHz, THF-d₈)



Bis-(4-methylphenyl)zinc (15f)

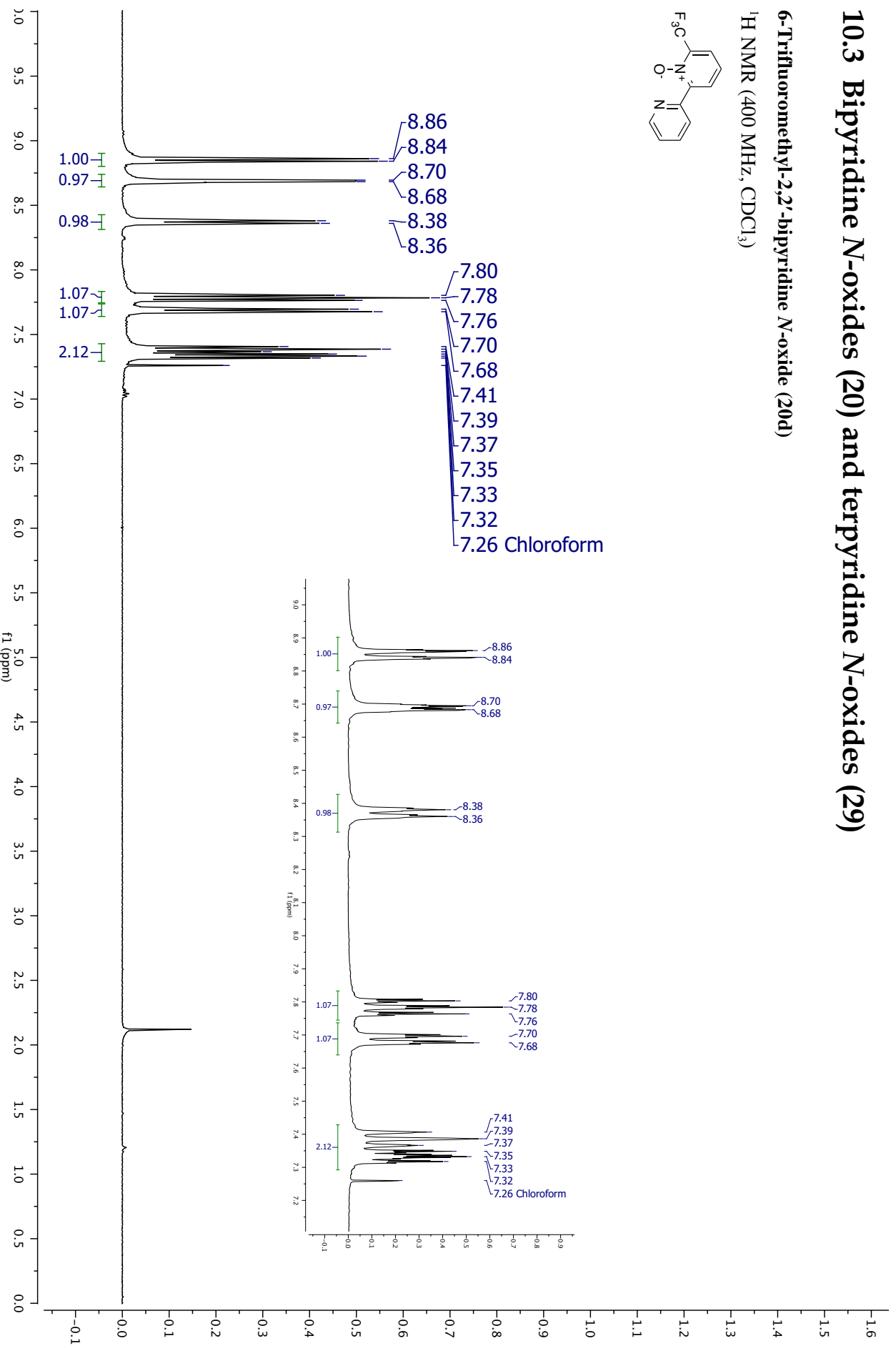
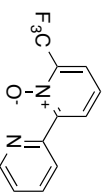
^{13}C NMR (101 MHz, THF- d_8)



10.3 Bipyridine N-oxides (20) and terpyridine N-oxides (29)

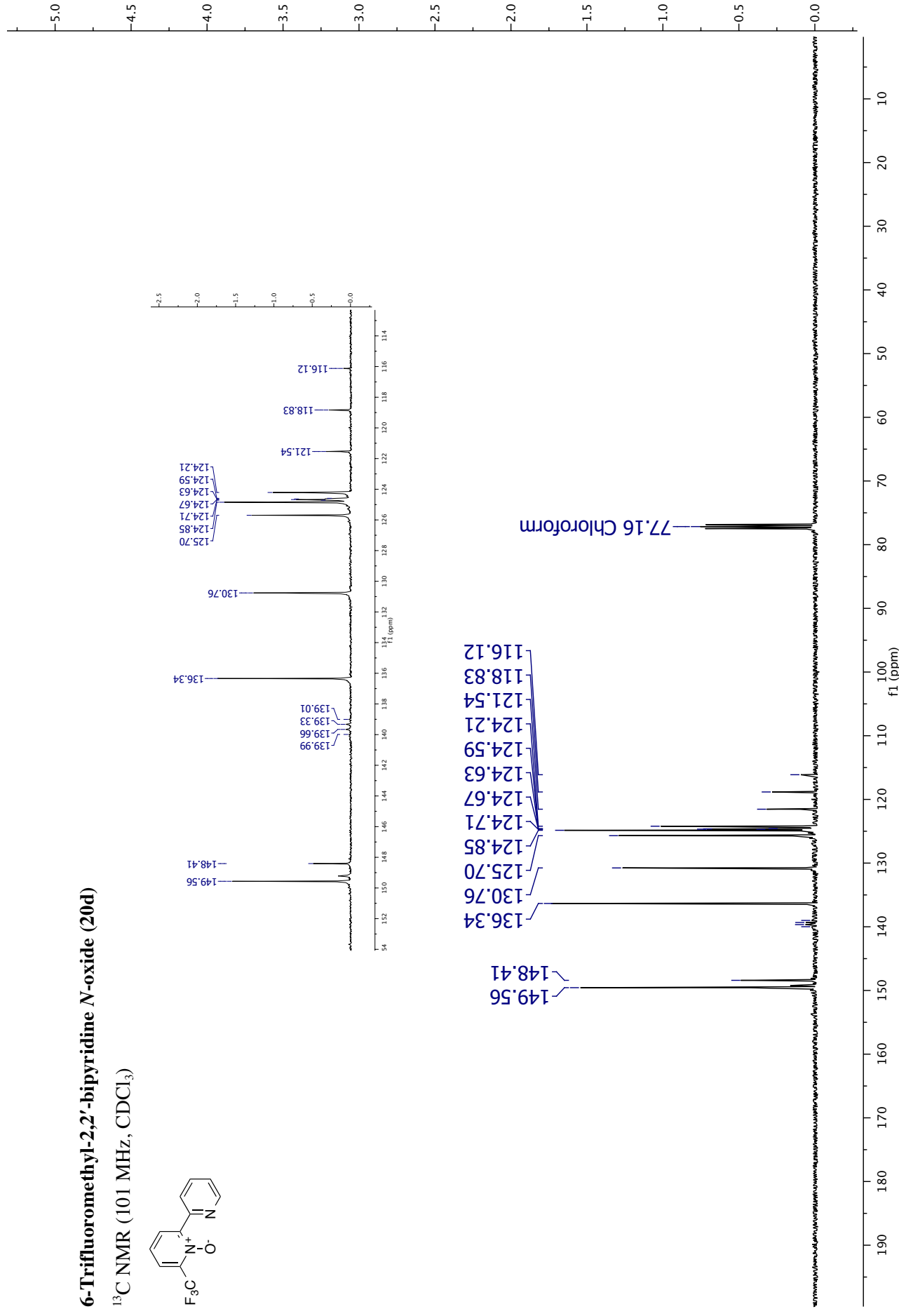
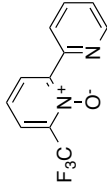
6-Trifluoromethyl-2,2'-bipyridine N-oxide (20d)

¹H NMR (400 MHz, CDCl₃)



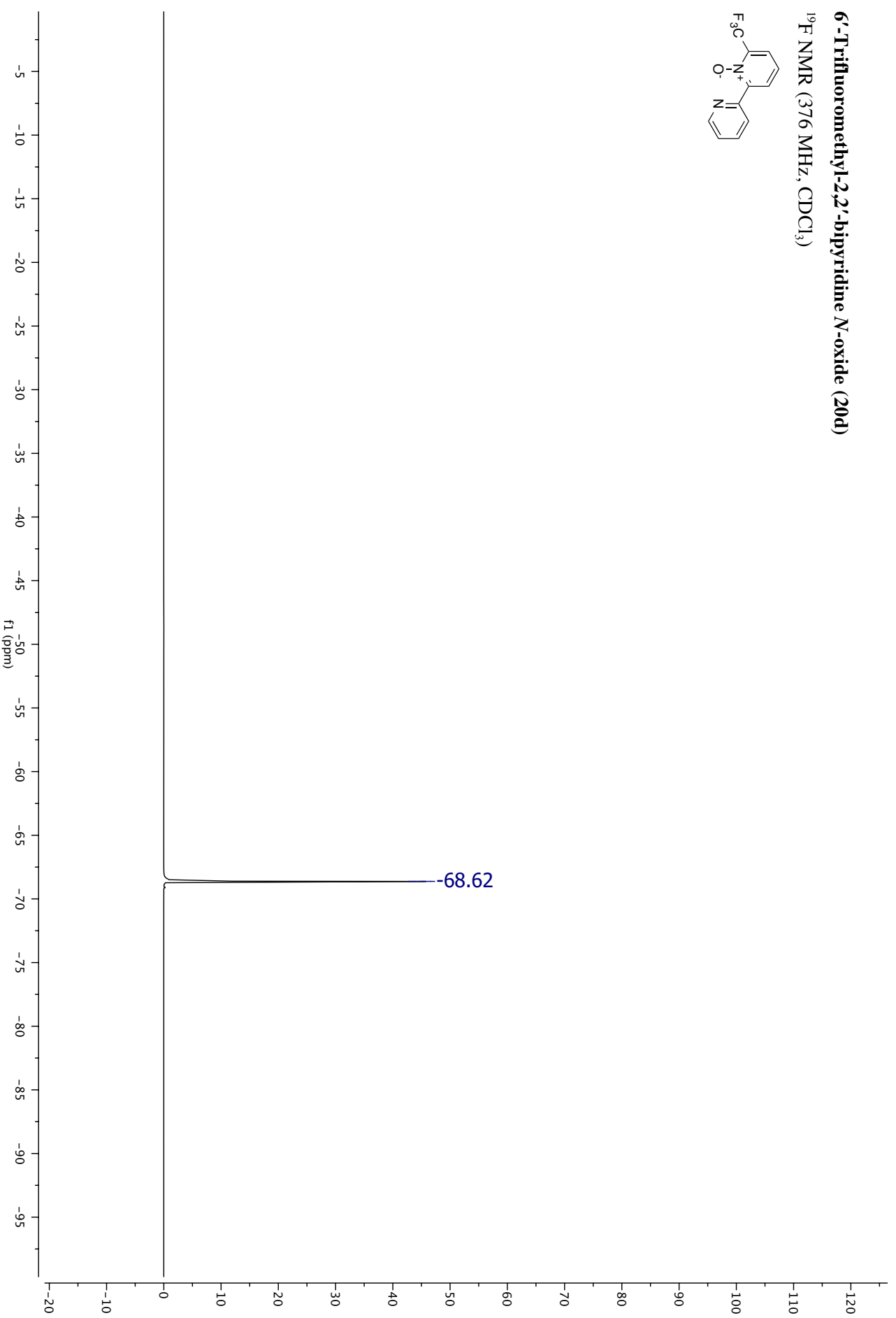
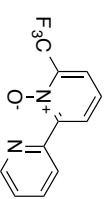
6-Trifluoromethyl-2,2'-bipyridine N-oxide (20d)

^{13}C NMR (101 MHz, CDCl_3)



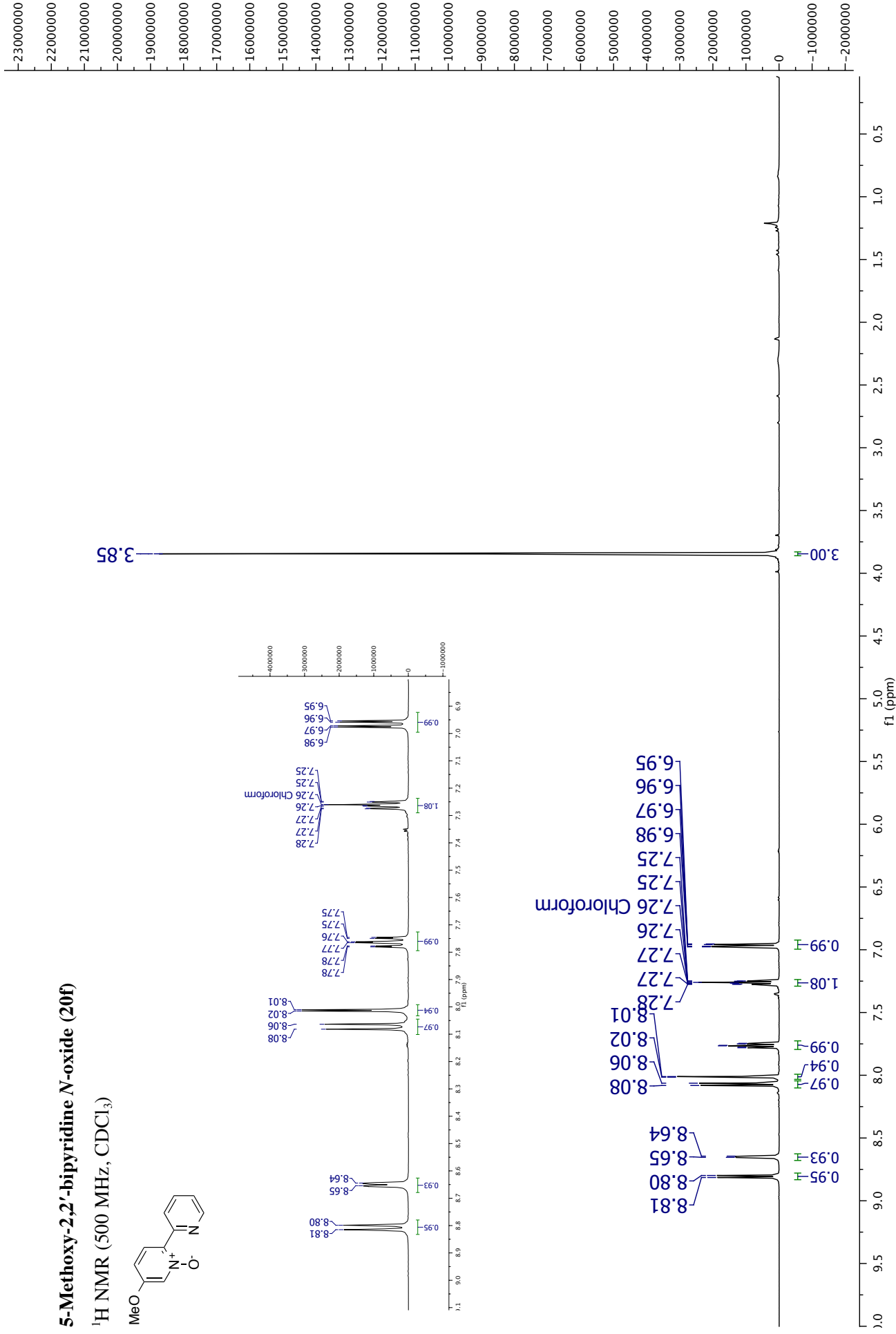
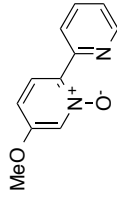
6'-Trifluoromethyl-2,2'-bipyridine N-oxide (20d)

¹⁹F NMR (376 MHz, CDCl₃)



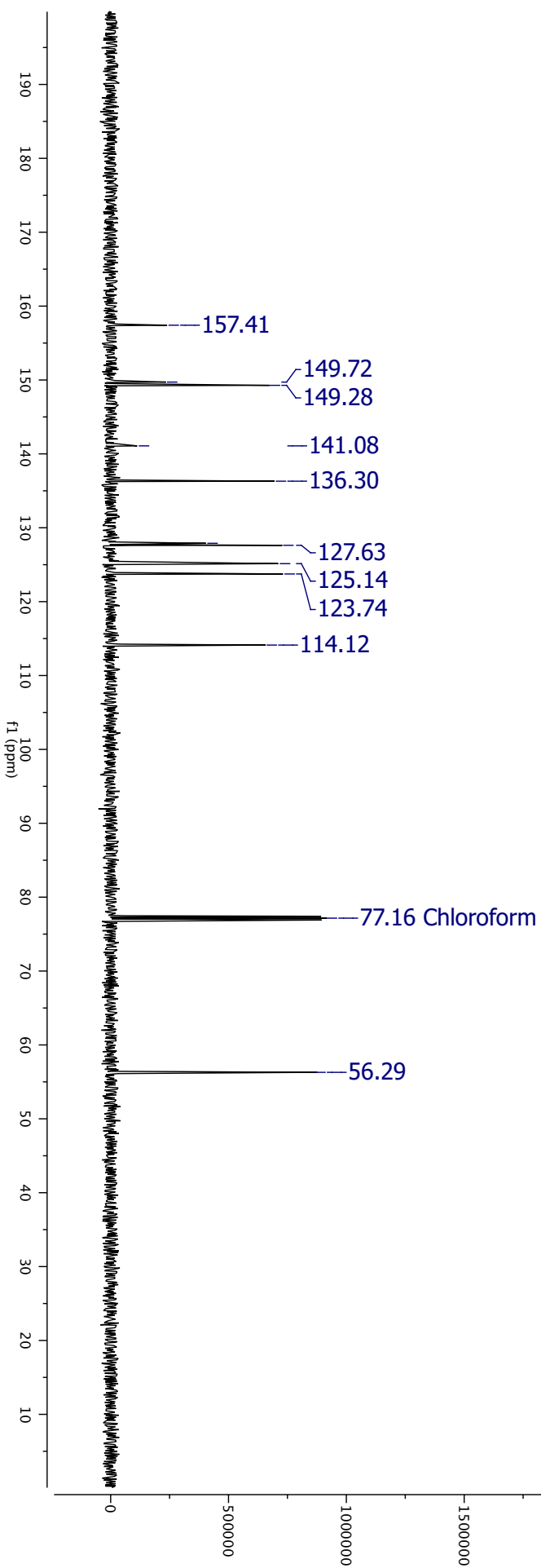
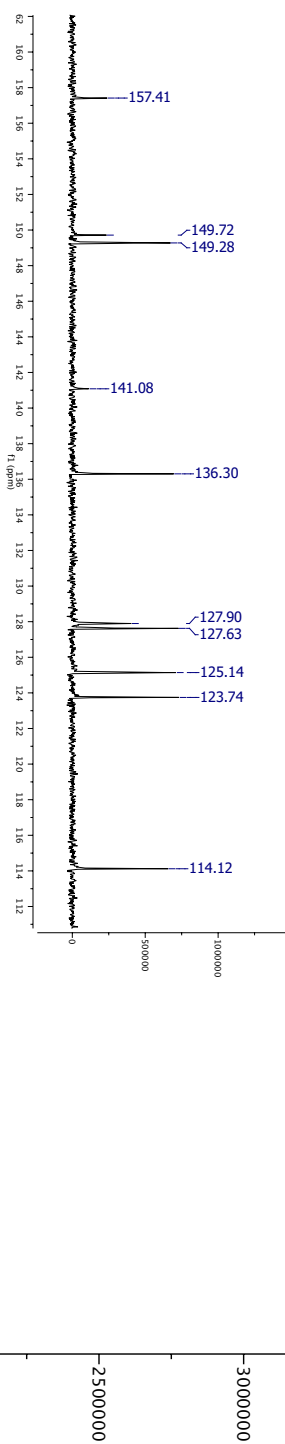
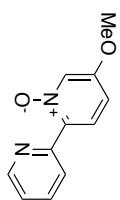
5-Methoxy-2,2'-bipyridine N-oxide (20f)

¹H NMR (500 MHz, CDCl₃)



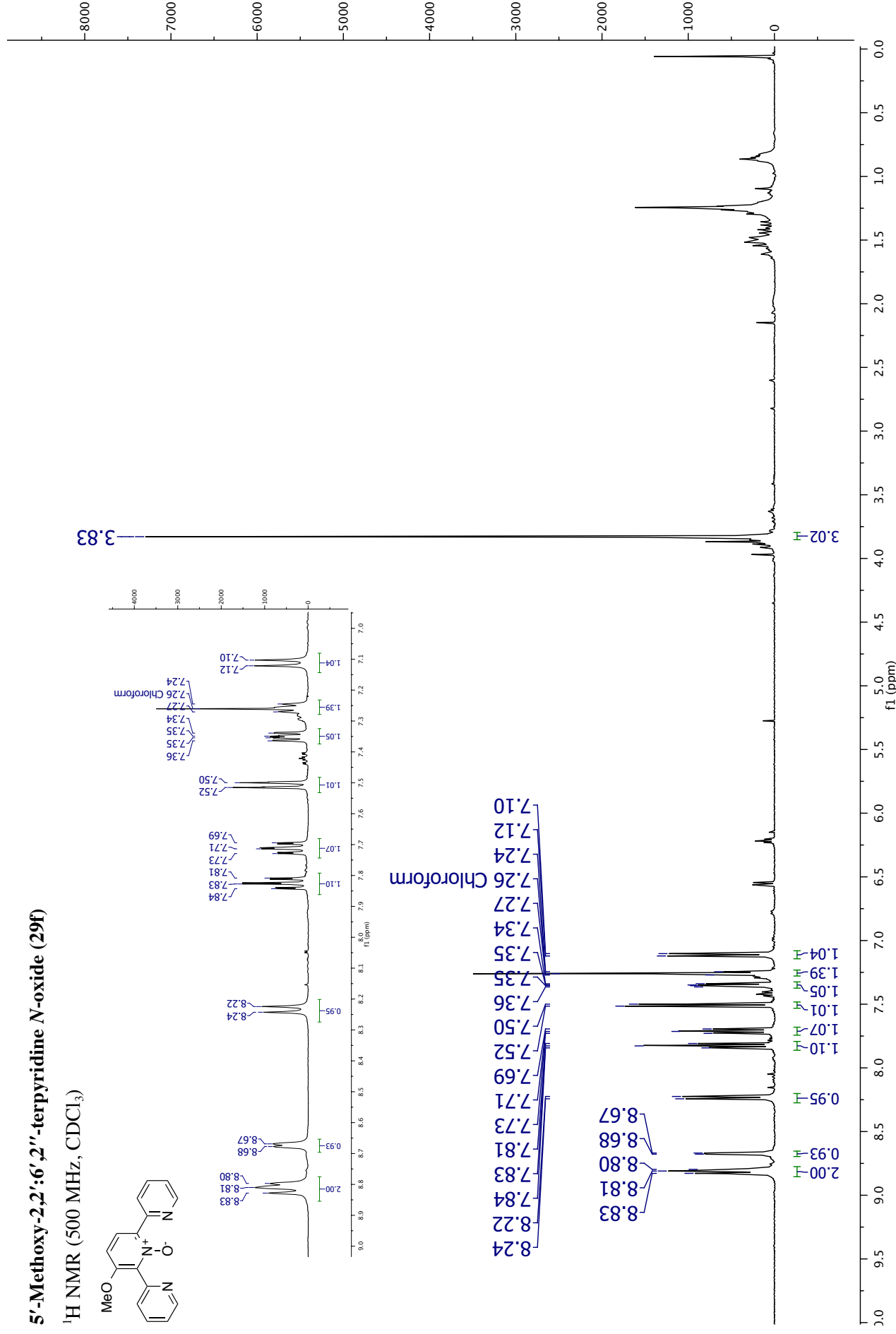
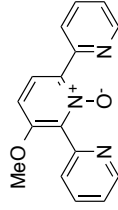
5-Methoxy-2,2'-bipyridine N-oxide (20f)

¹³C NMR (126 MHz, CDCl₃)



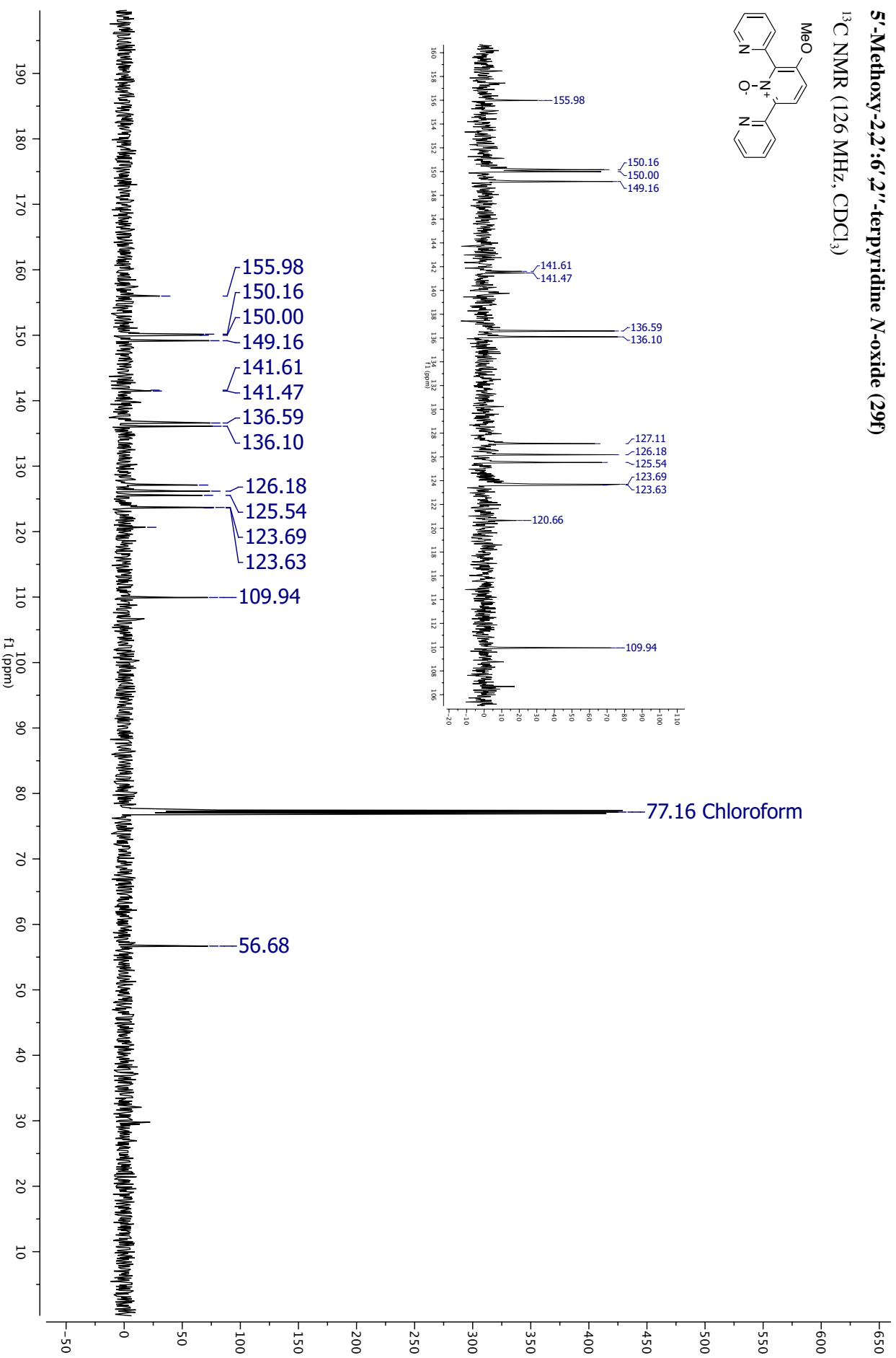
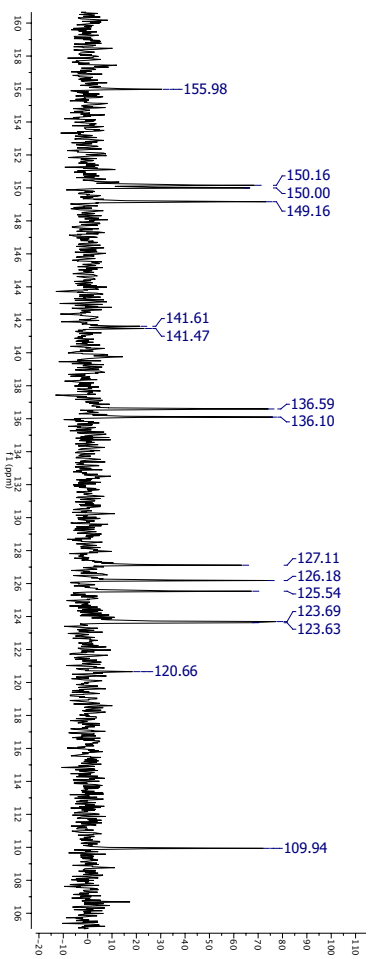
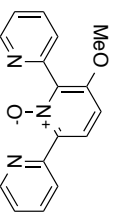
5'-Methoxy-2,2':6',2''-terpyridine N-oxide (29f)

¹H NMR (500 MHz, CDCl₃)



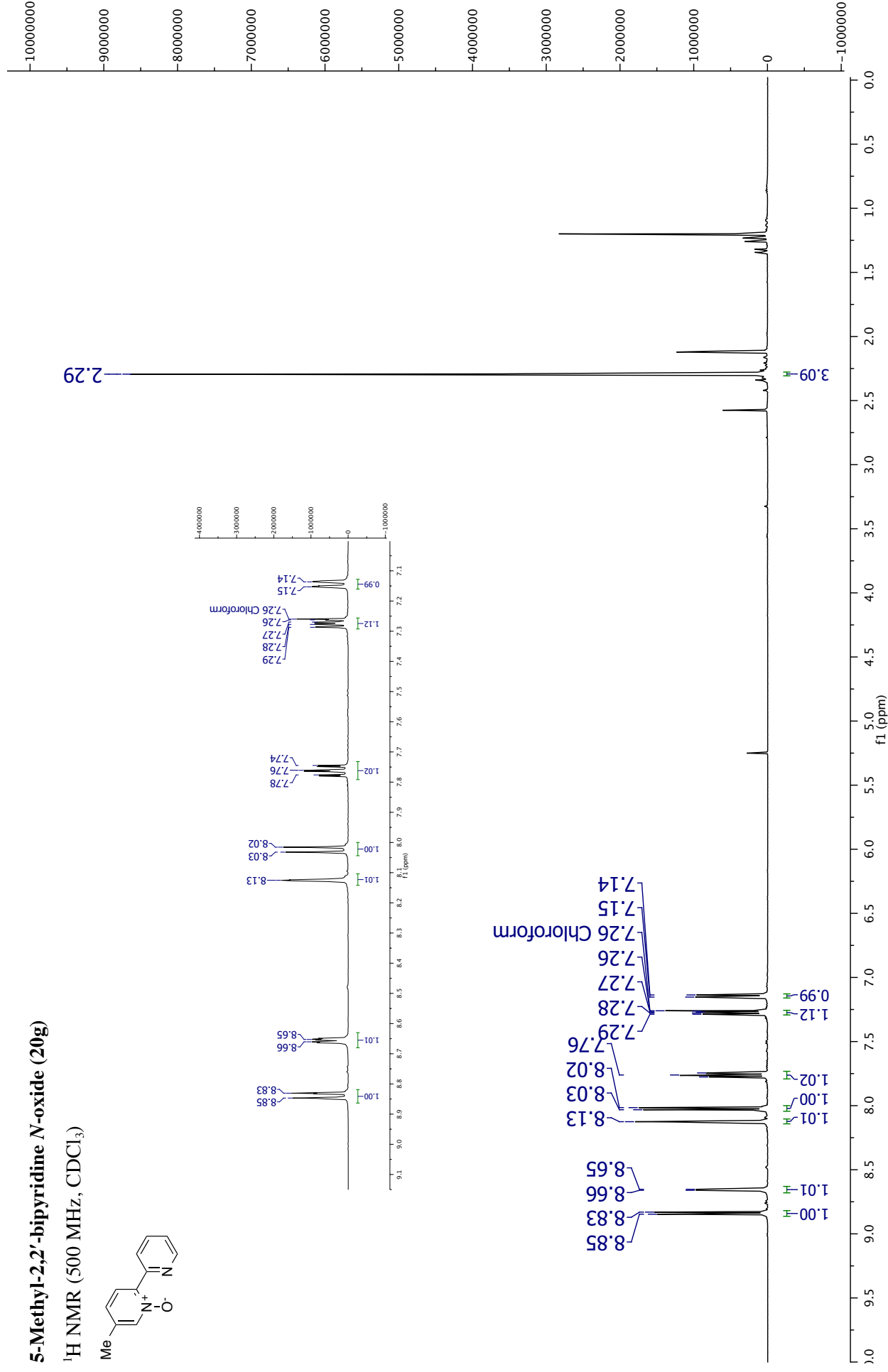
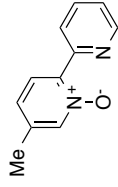
5'-Methoxy-2,2':6'-terpyridine N-oxide (29f)

¹³C NMR (126 MHz, CDCl₃)



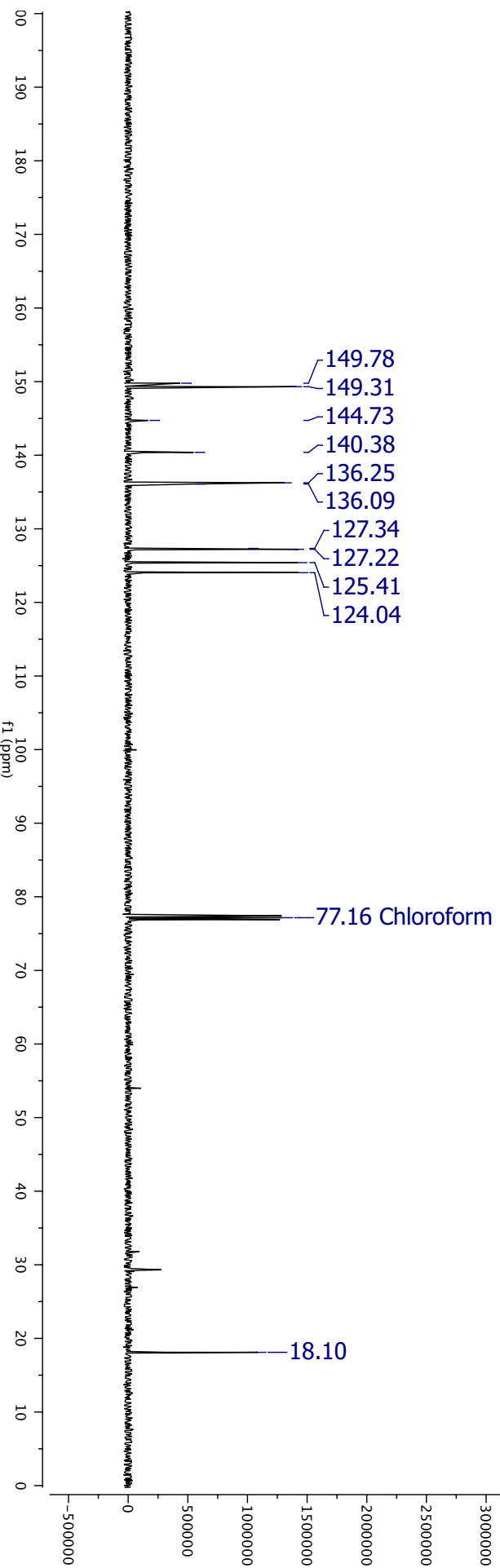
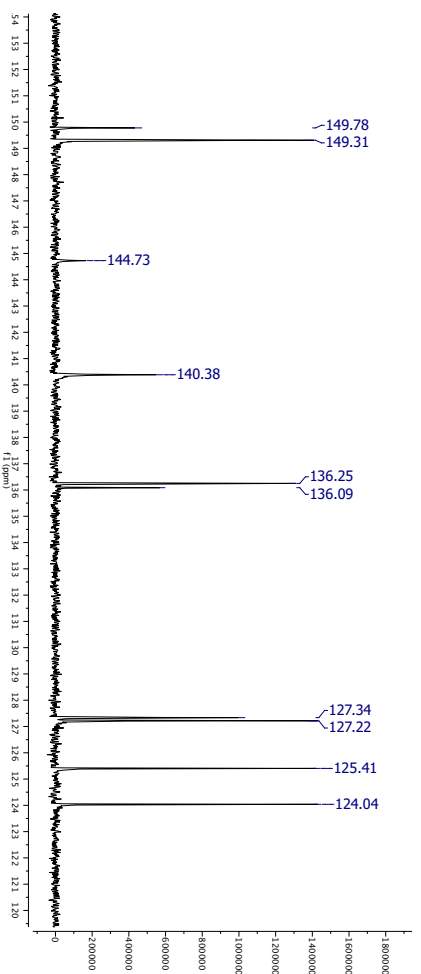
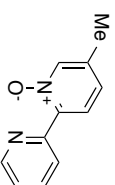
5-Methyl-2,2'-bipyridine N-oxide (20g)

¹H NMR (500 MHz, CDCl₃)



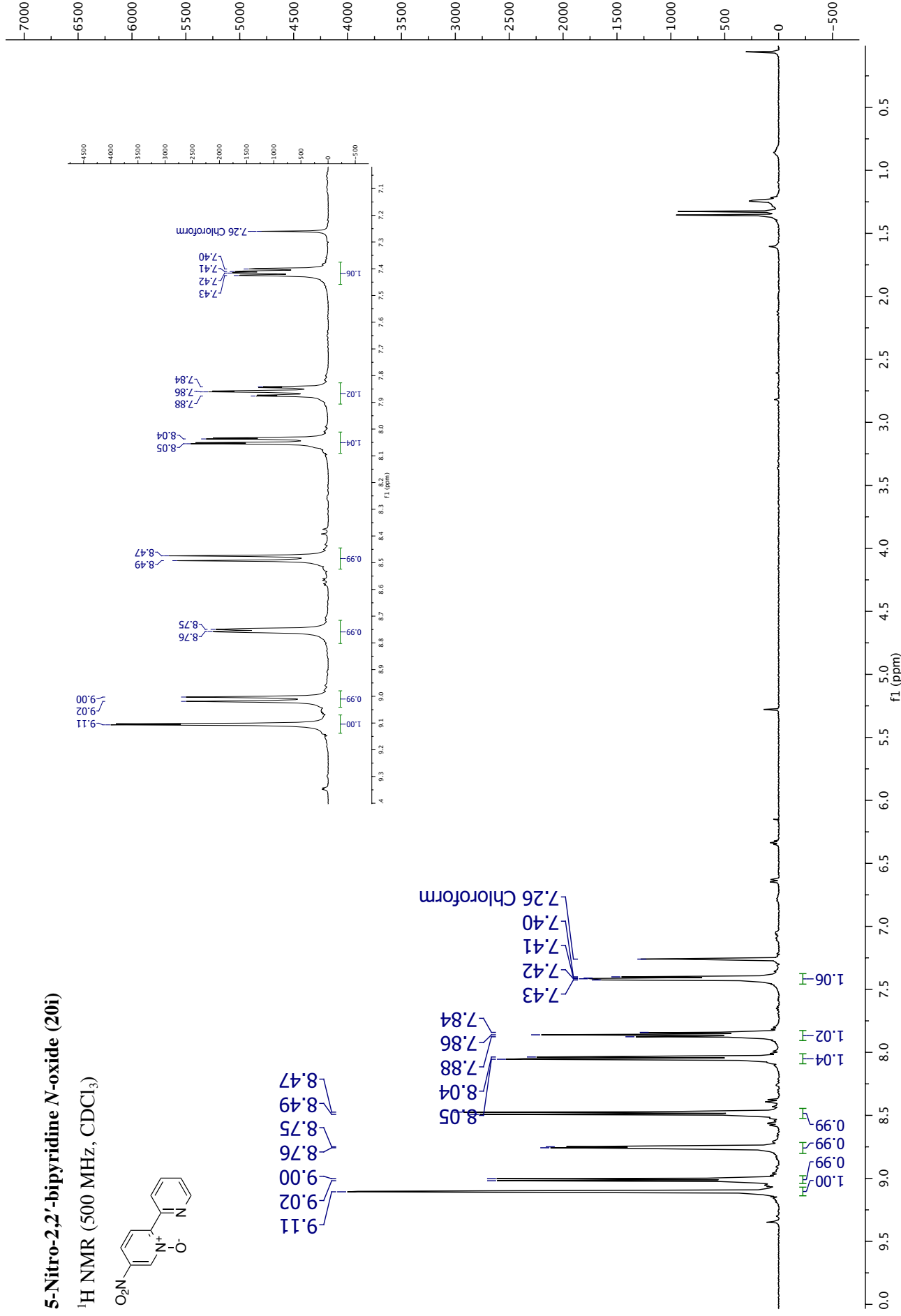
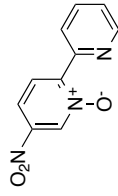
5-Methyl-2,2'-bipyridine N-oxide (20g)

^{13}C NMR (126 MHz, CDCl_3)



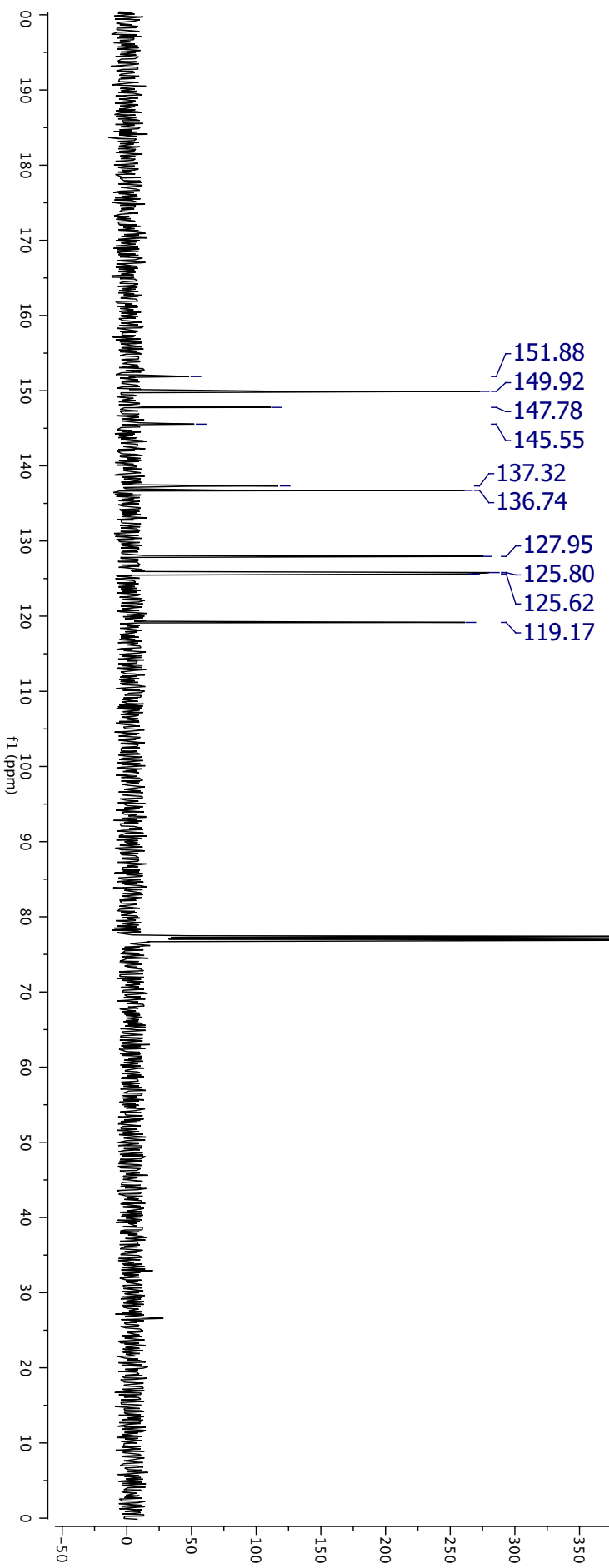
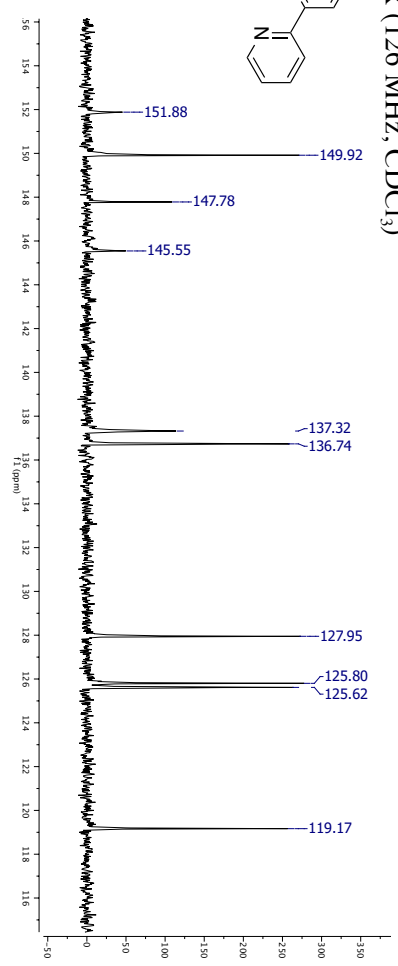
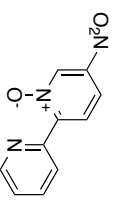
5-Nitro-2,2'-bipyridine N-oxide (20i)

¹H NMR (500 MHz, CDCl₃)



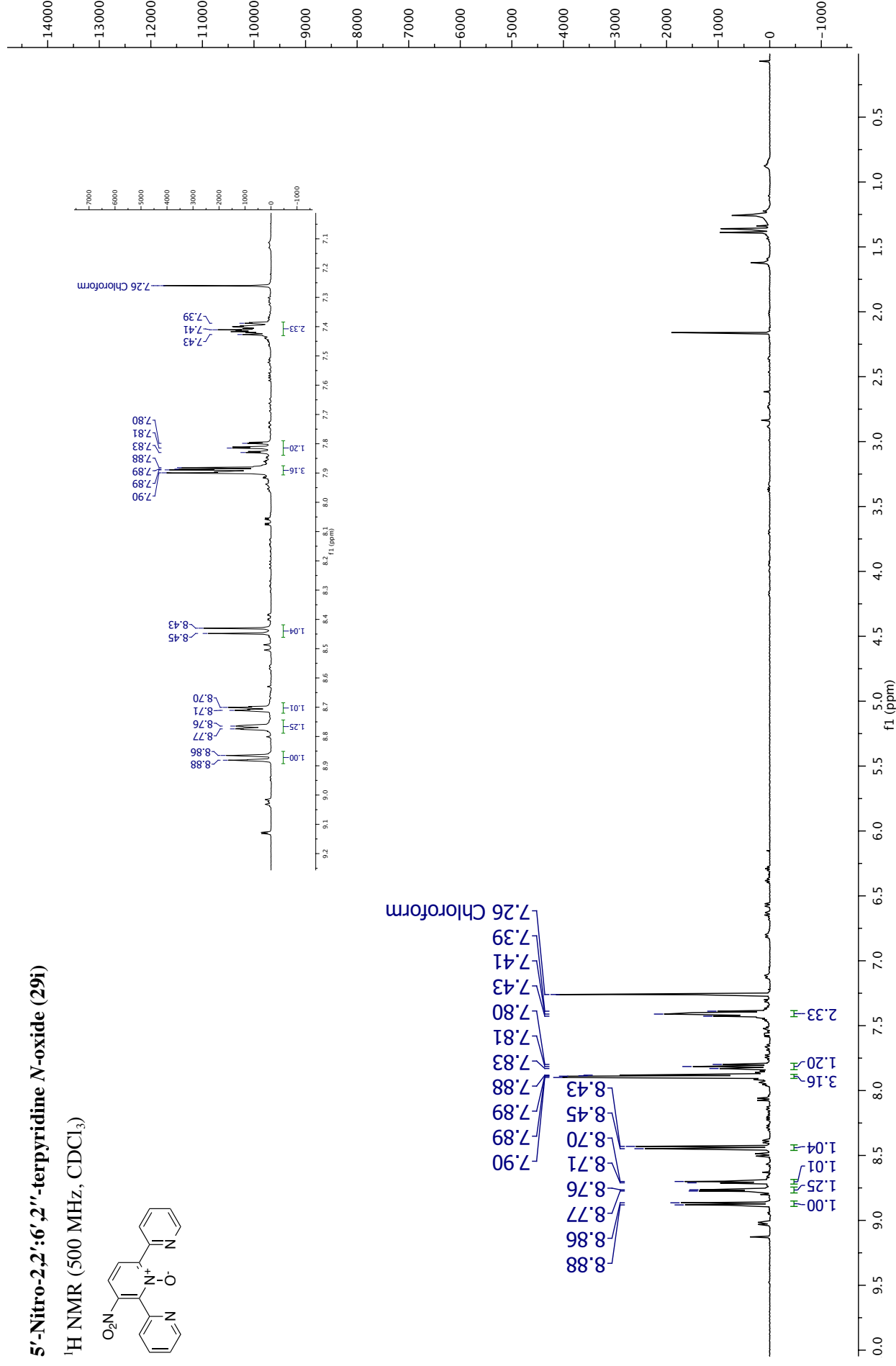
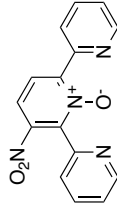
5-Nitro-2,2'-bipyridine N-oxide (20i)

¹³C NMR (126 MHz, CDCl₃)



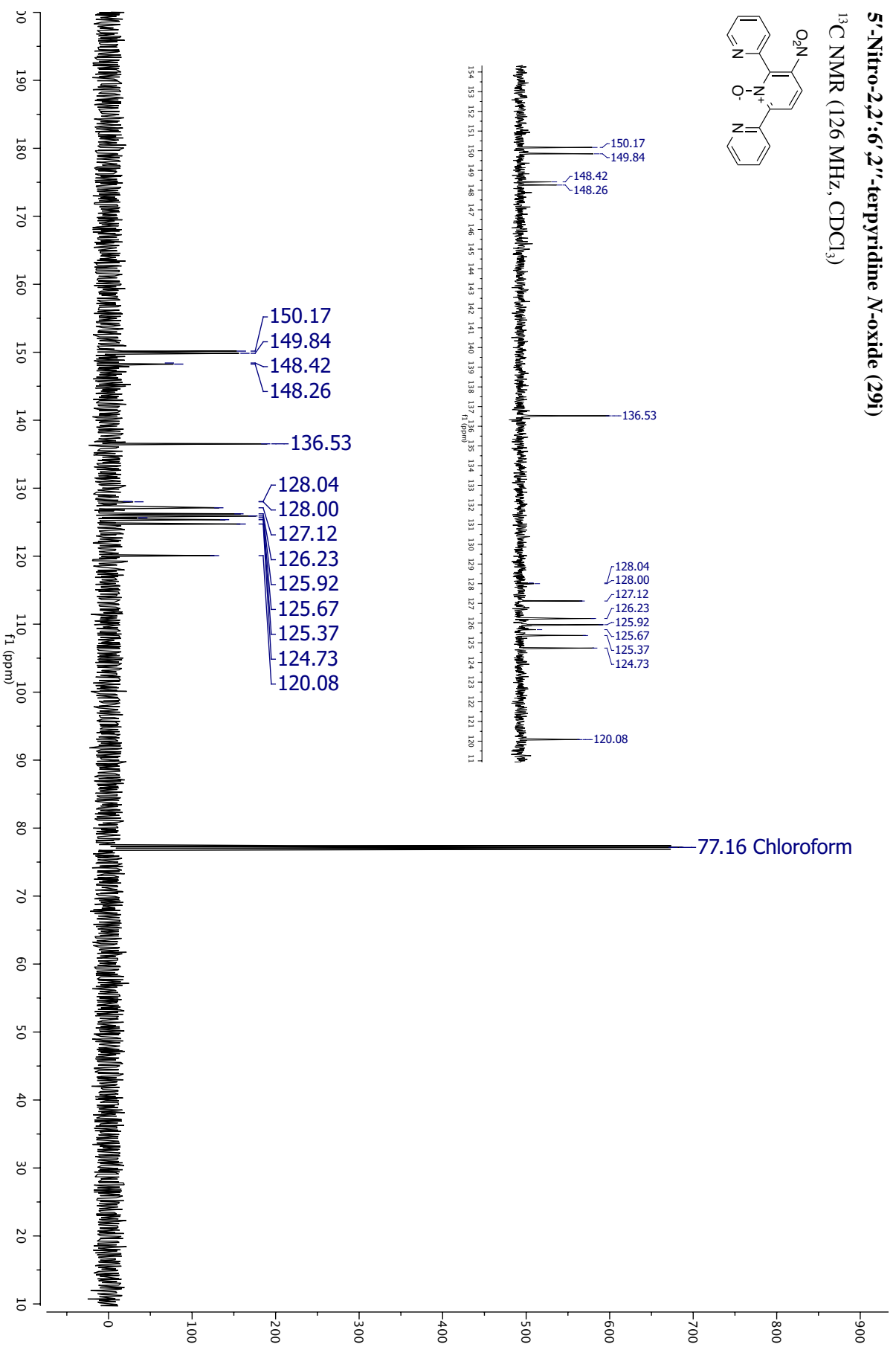
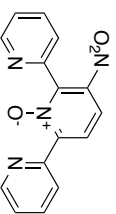
5'-Nitro-2,2':6',2''-terpyridine N-oxide (29j)

¹H NMR (500 MHz, CDCl₃)



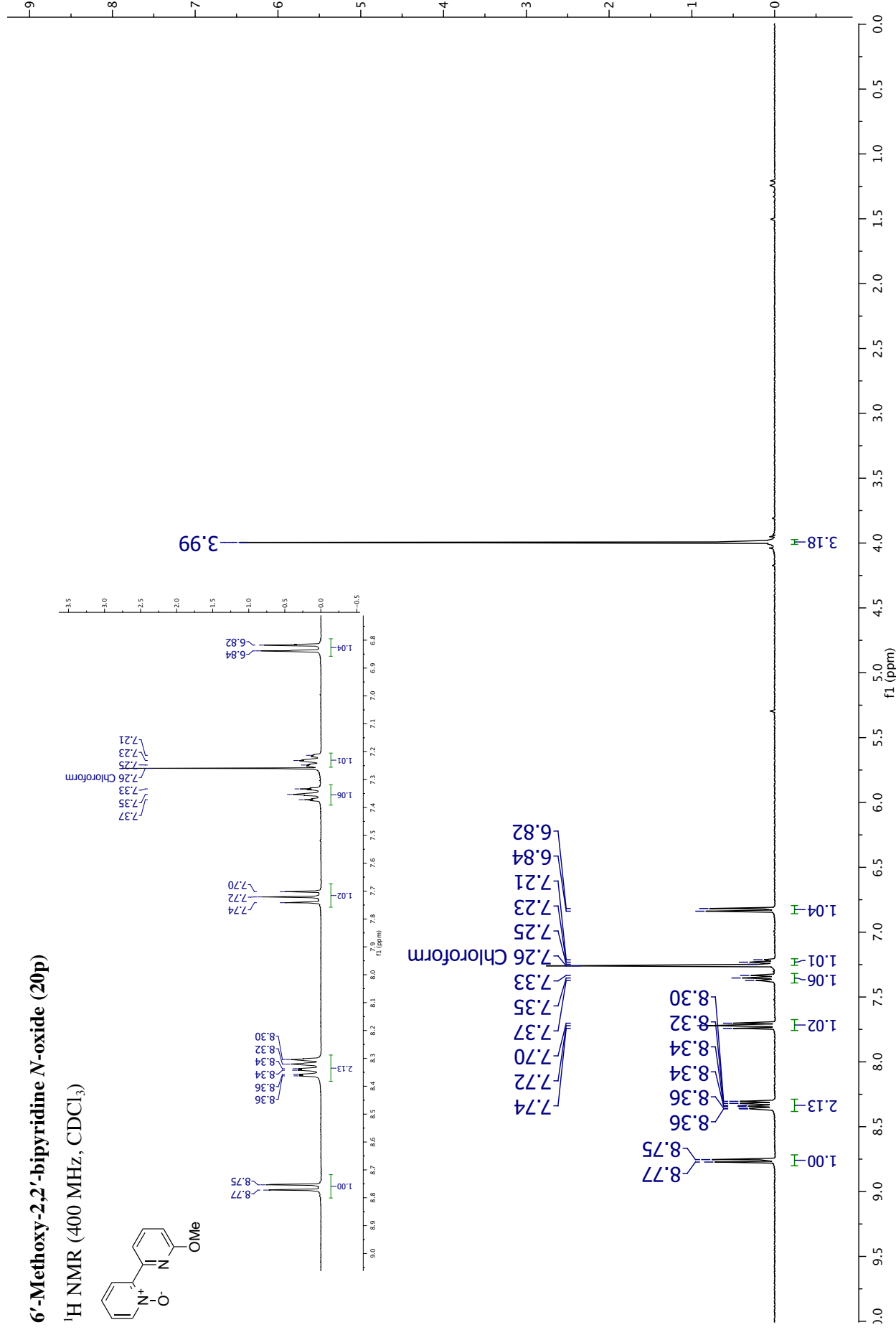
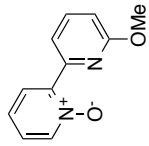
5'-Nitro-2,2':6',2''-terpyridine N-oxide (29f)

¹³C NMR (126 MHz, CDCl₃)



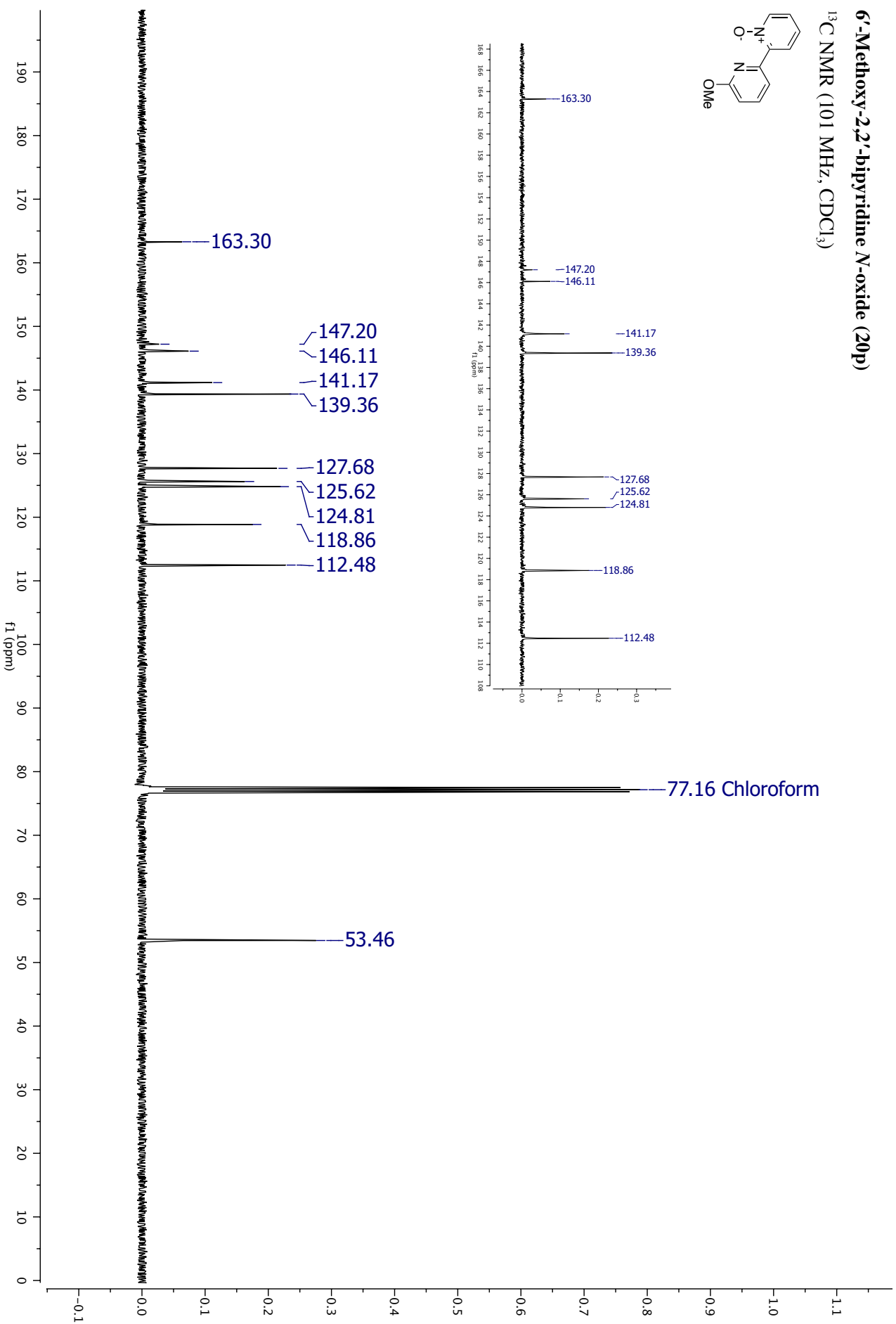
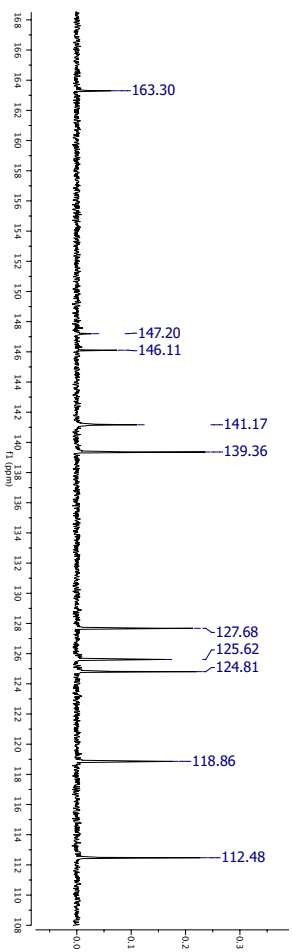
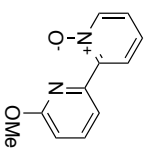
6'-Methoxy-2,2'-bipyridine N-oxide (20p)

¹H NMR (400 MHz, CDCl₃)



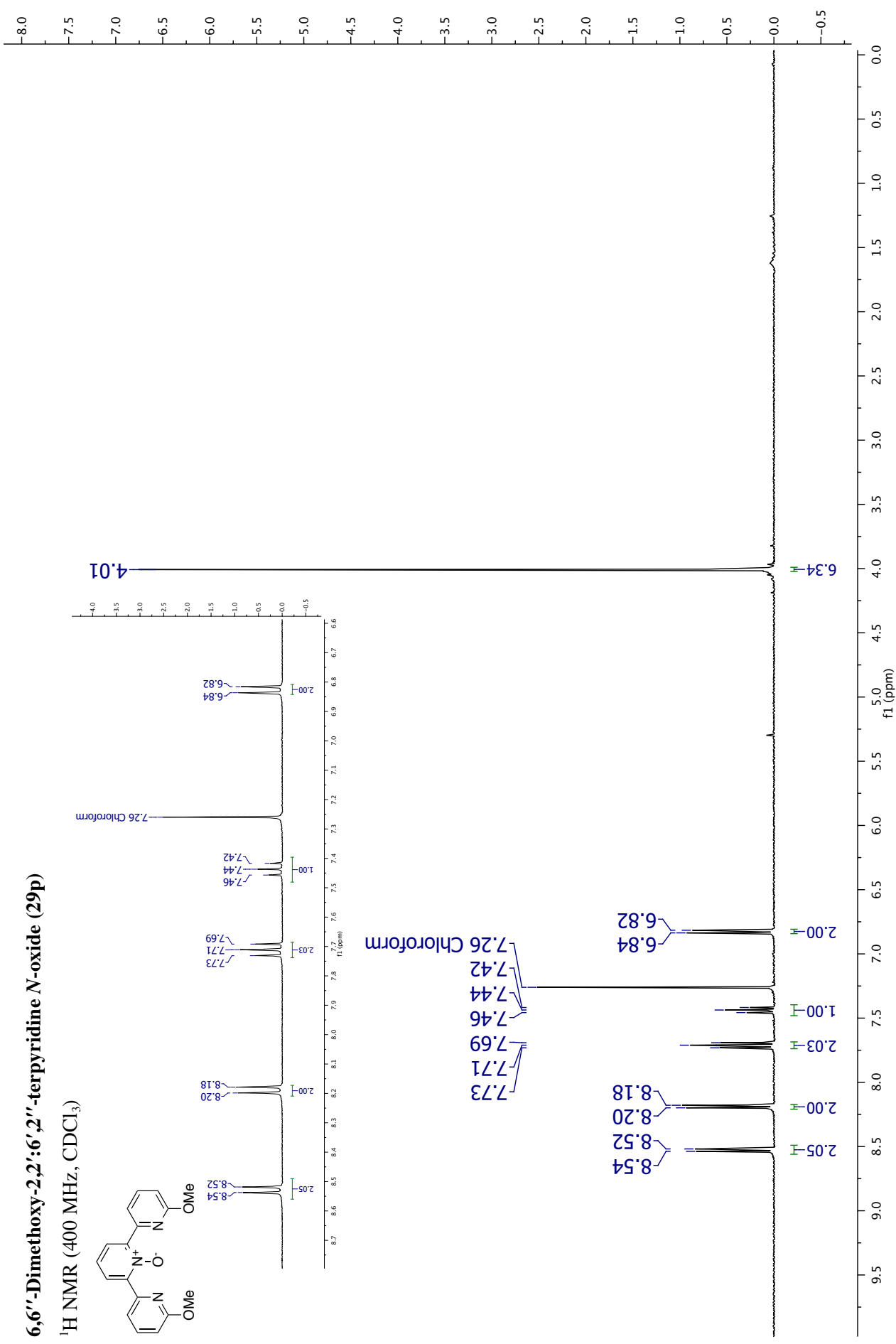
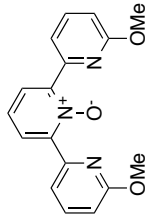
6'-Methoxy-2,2'-bipyridine N-oxide (20p)

¹³C NMR (101 MHz, CDCl₃)



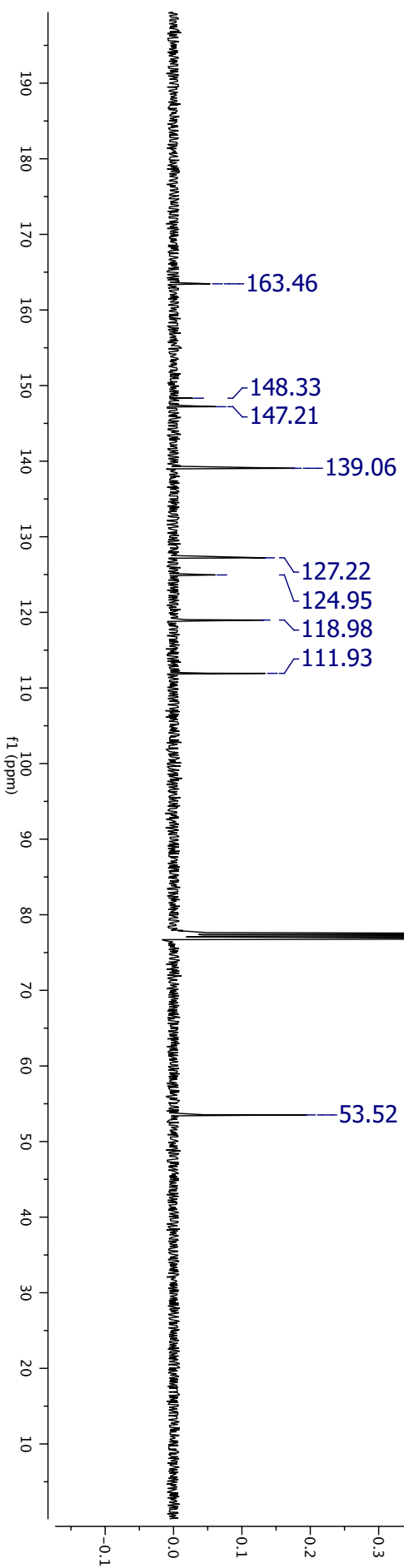
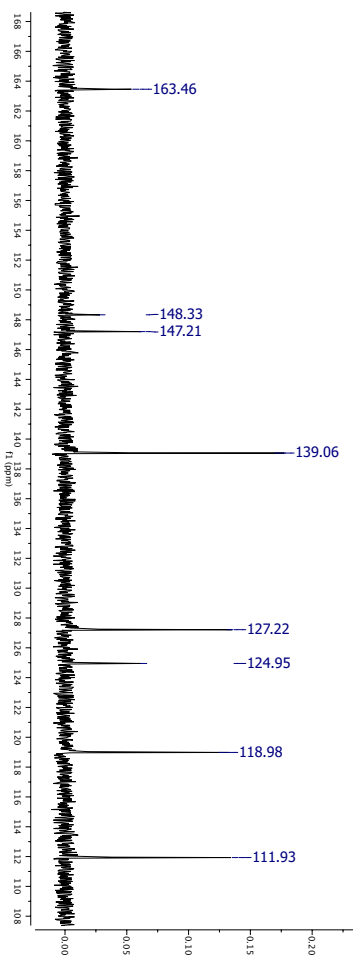
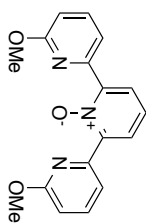
6,6''-Dimethoxy-2,2':6',2''-terpyridine N-oxide (29p)

¹H NMR (400 MHz, CDCl₃)



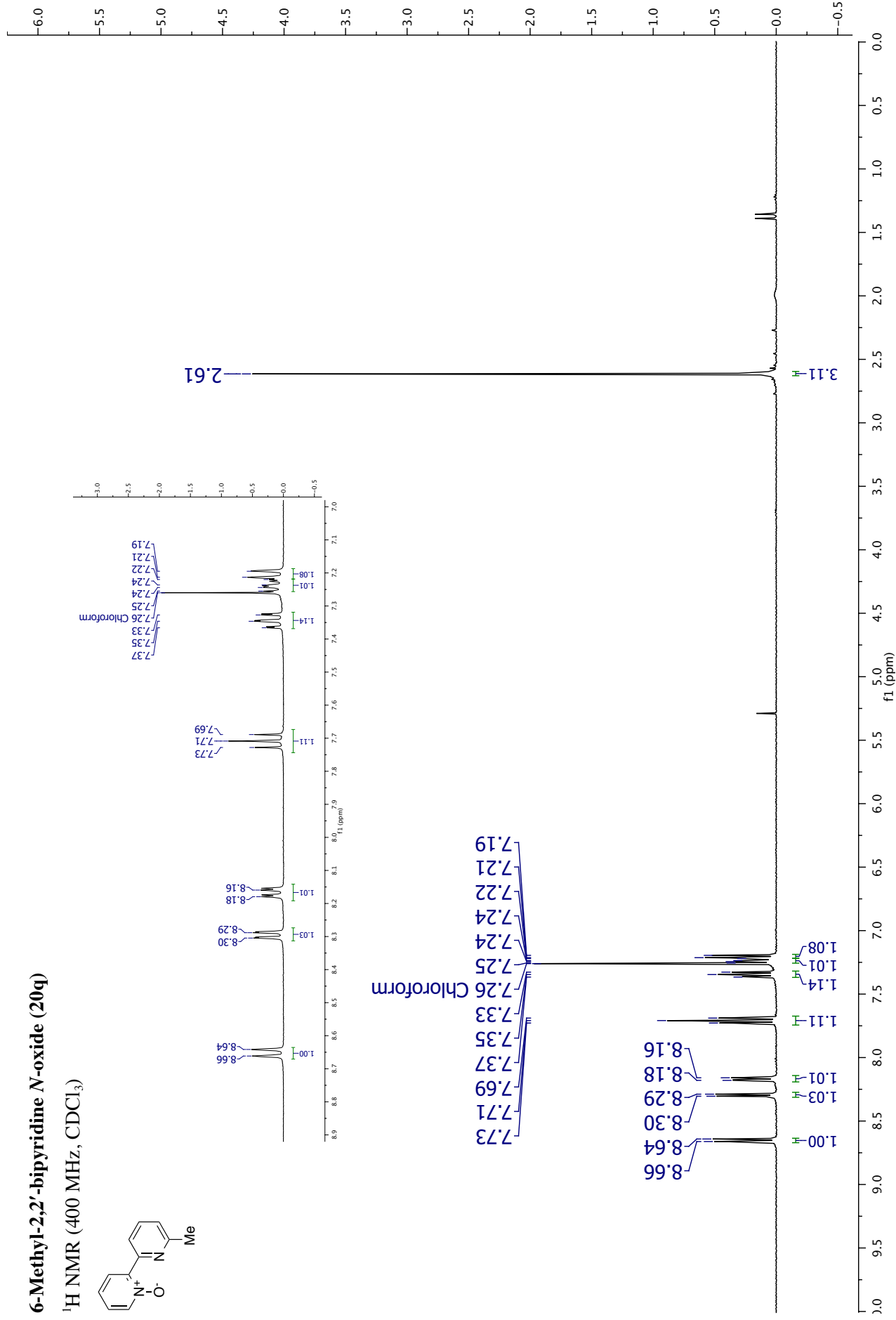
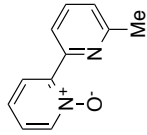
6,6'-Dimethoxy-2,2':6,2''-terpyridine N-oxide (29p)

¹³C NMR (101 MHz, CDCl₃)



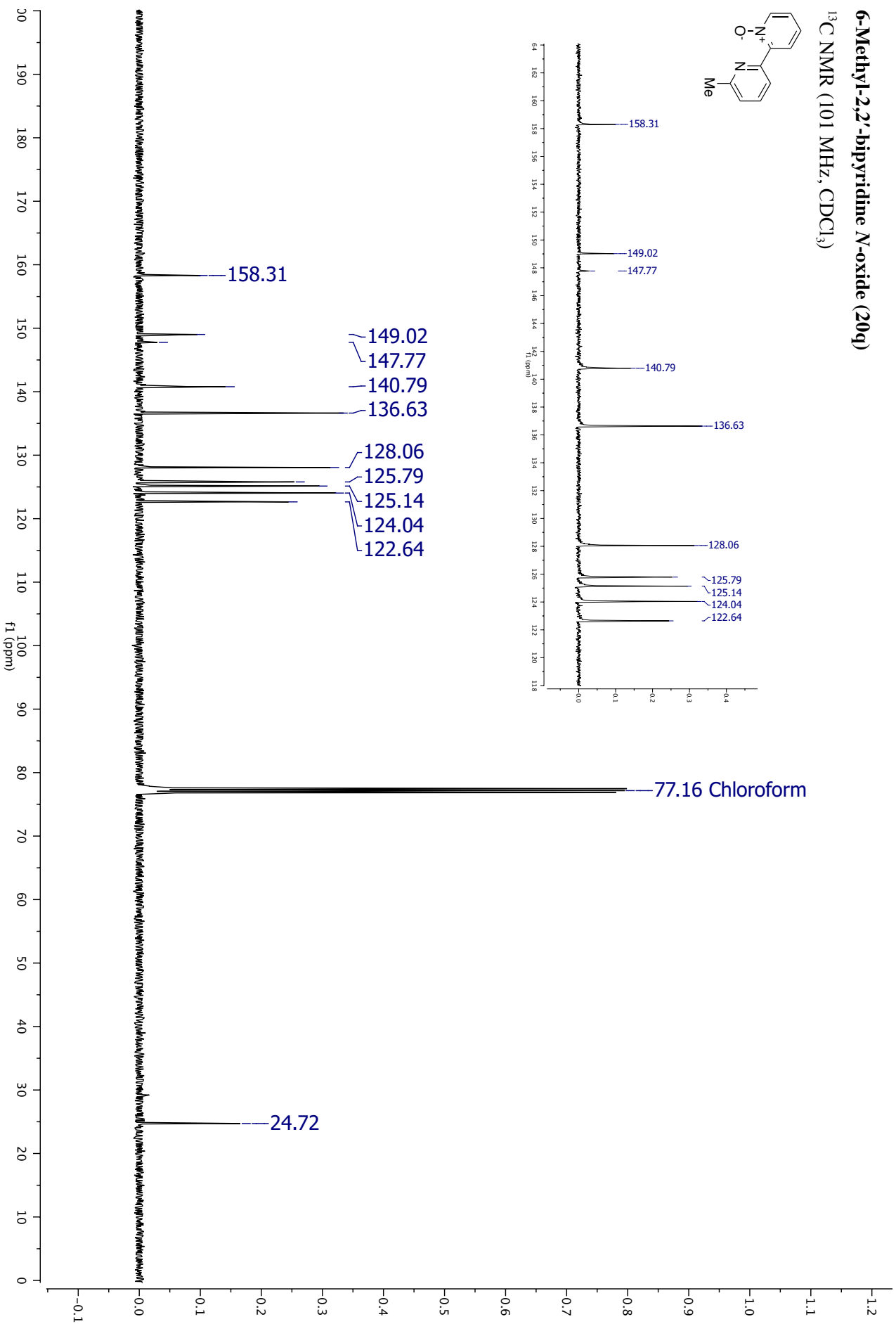
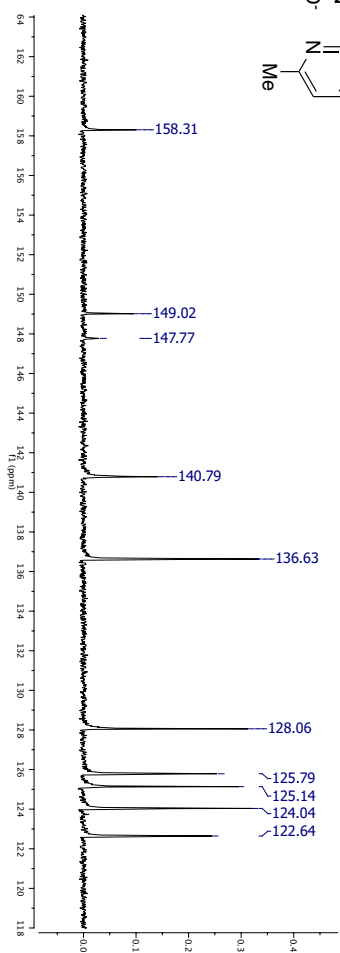
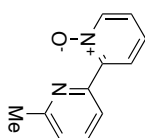
6-Methyl-2,2'-bipyridine N-oxide (20q)

¹H NMR (400 MHz, CDCl₃)



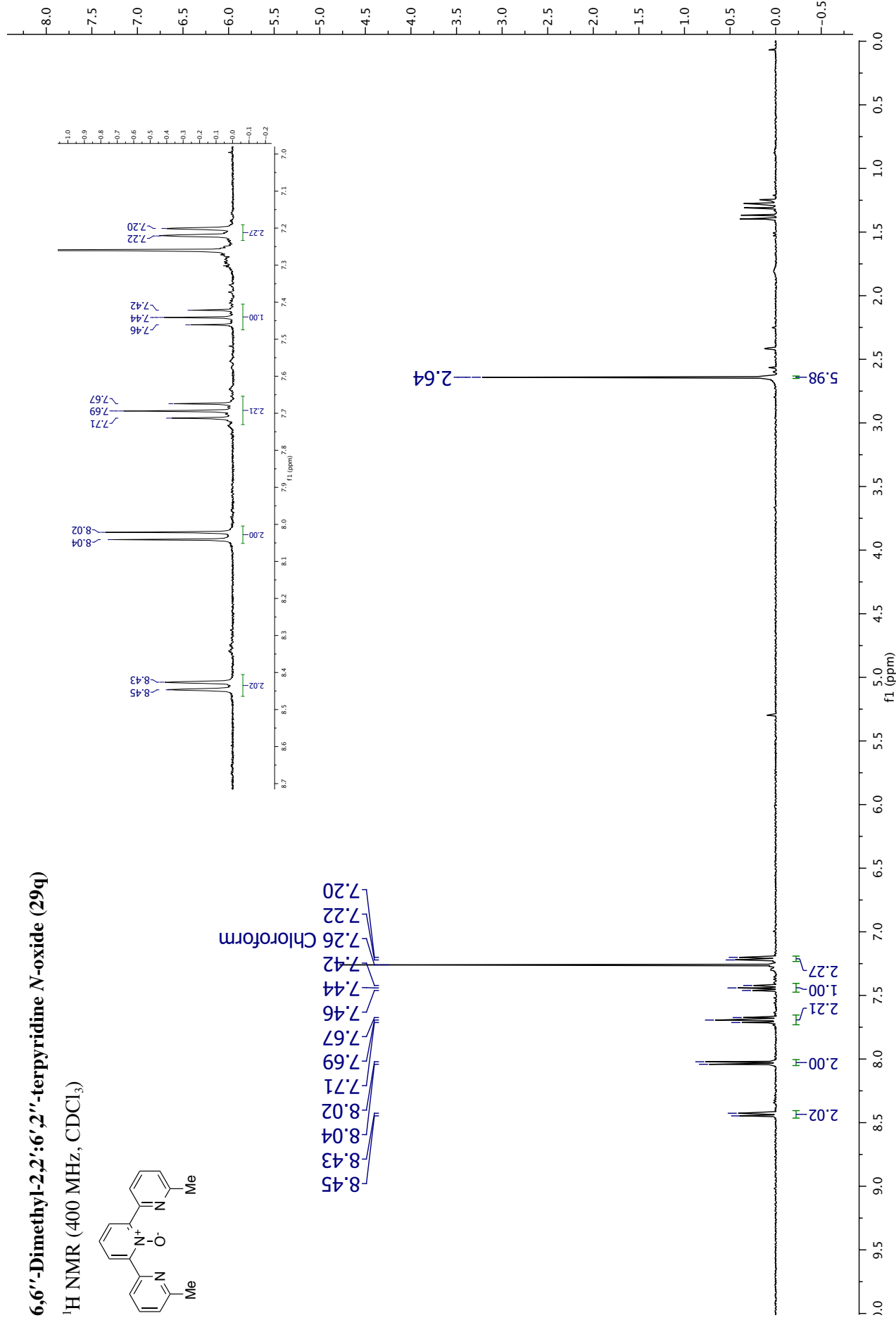
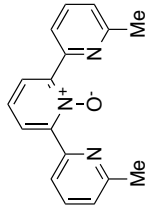
6-Methyl-2,2'-bipyridine N-oxide (20g)

¹³C NMR (101 MHz, CDCl₃)



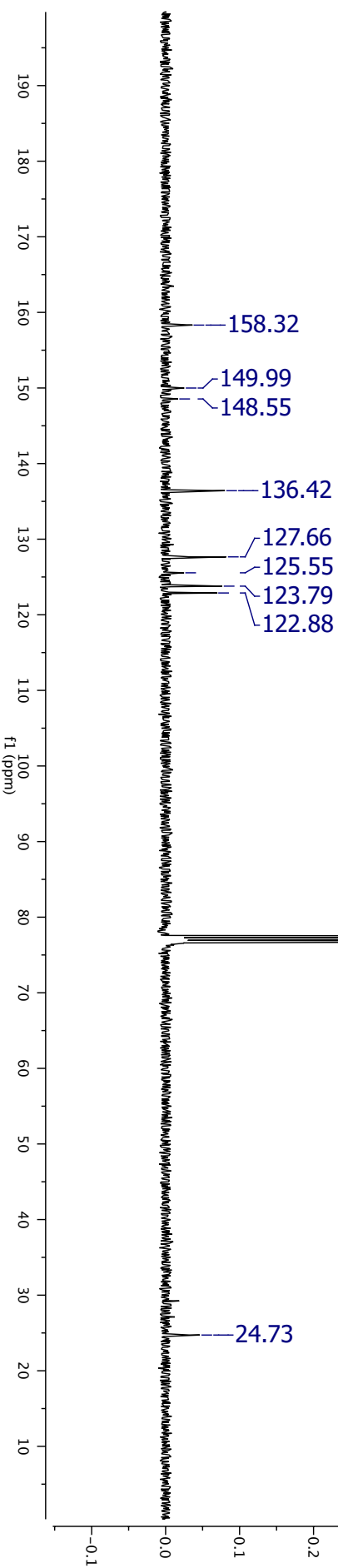
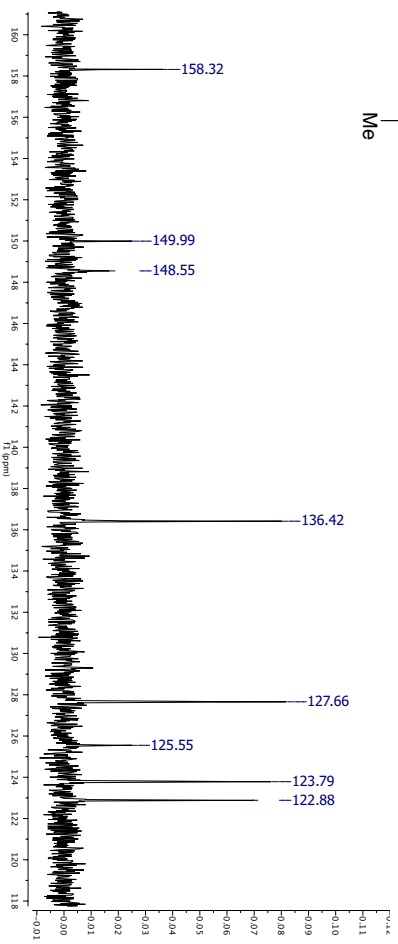
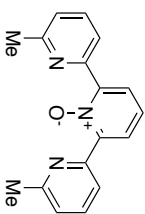
6,6''-Dimethyl-2,2':6',2''-terpyridine N-oxide (29q)

¹H NMR (400 MHz, CDCl₃)



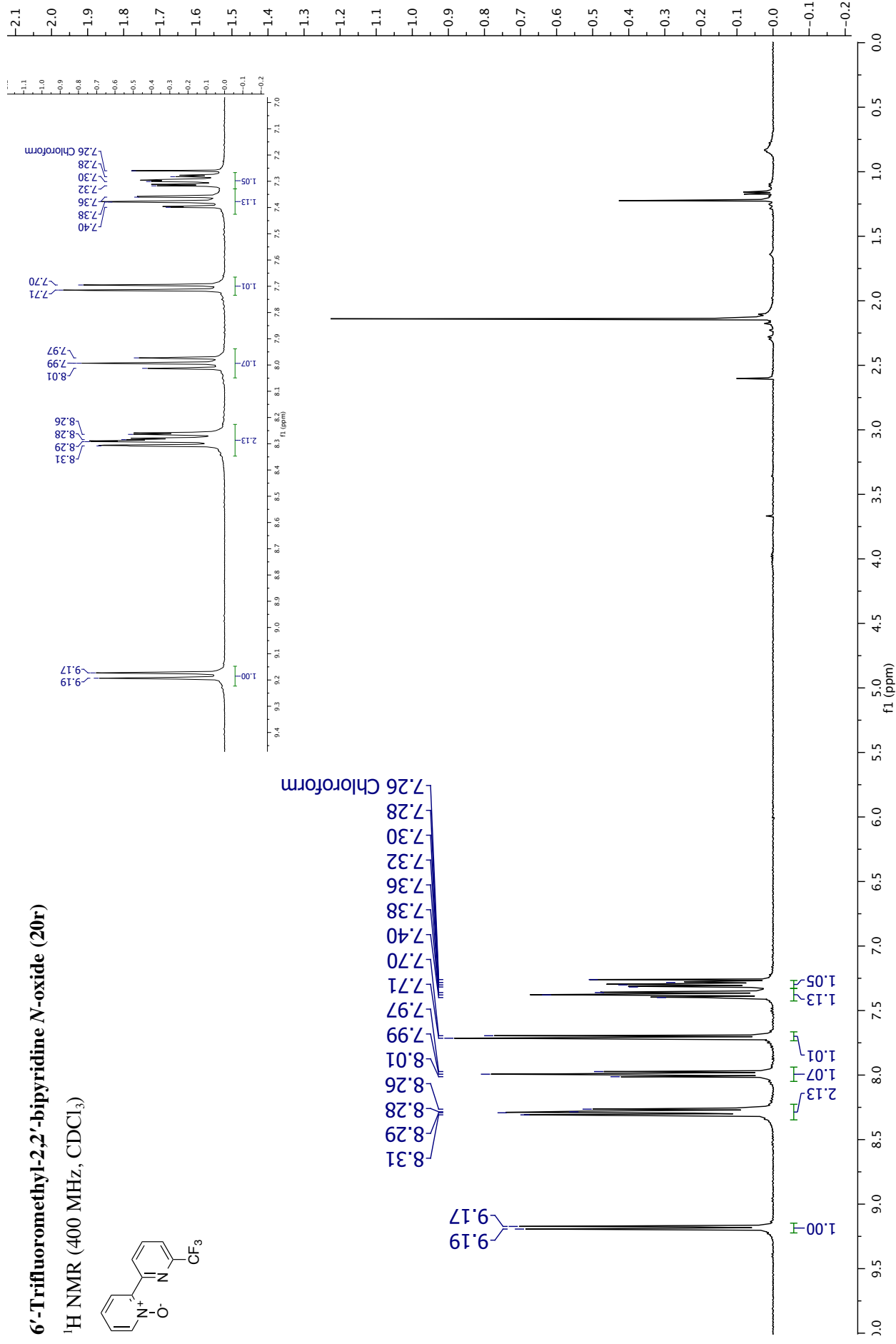
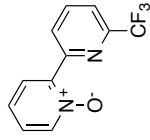
6,6'-Dimethyl-2,2':6',2''-terpyridine N-oxide (29q)

¹H NMR (400 MHz, CDCl₃)



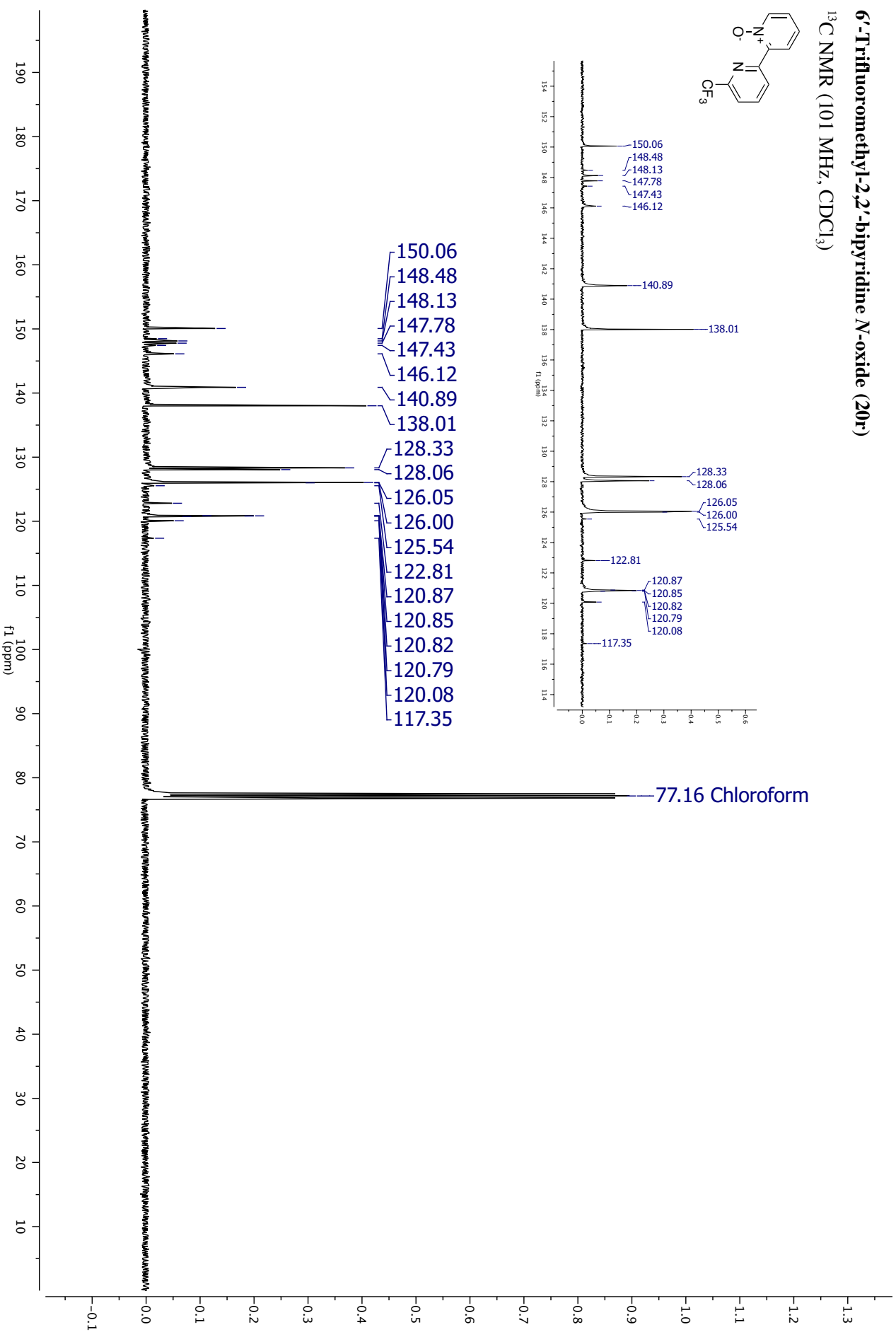
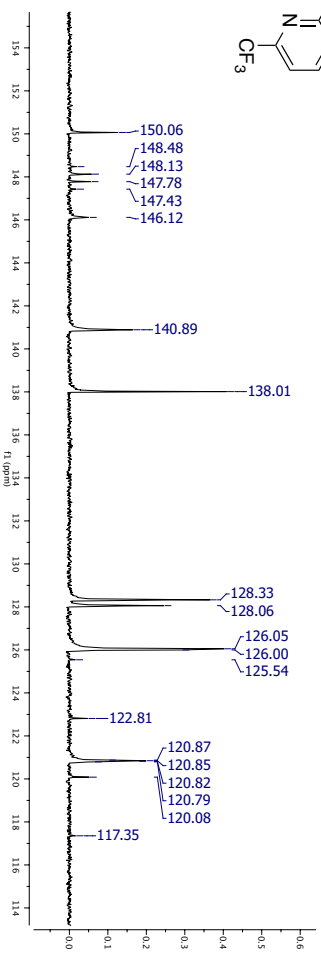
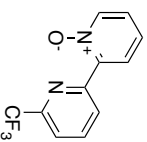
6'-Trifluoromethyl-2,2'-bipyridine N-oxide (20r)

¹H NMR (400 MHz, CDCl₃)



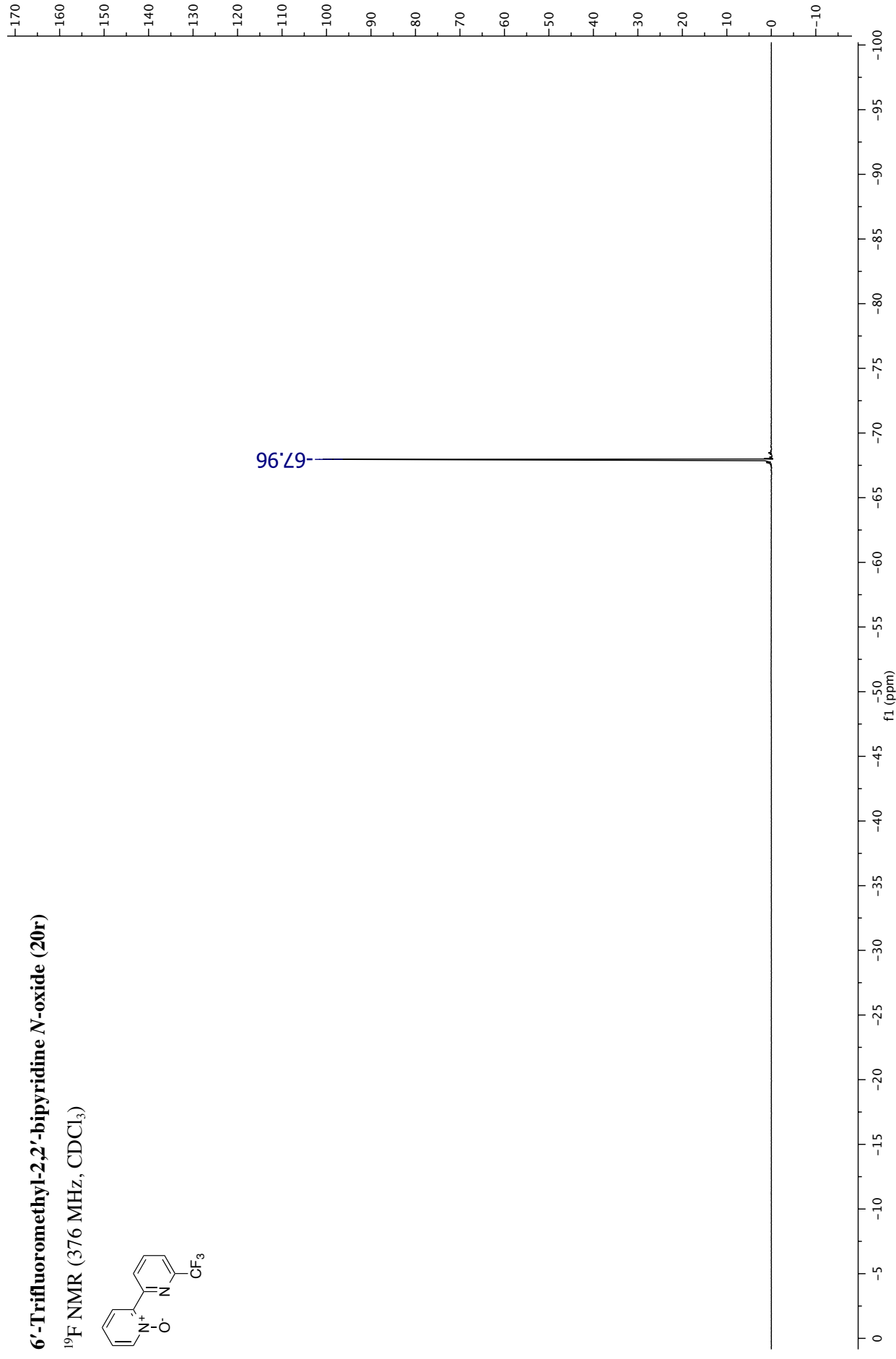
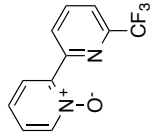
6'-Trifluoromethyl-2,2'-bipyridine N-oxide (20r)

¹³C NMR (101 MHz, CDCl₃)



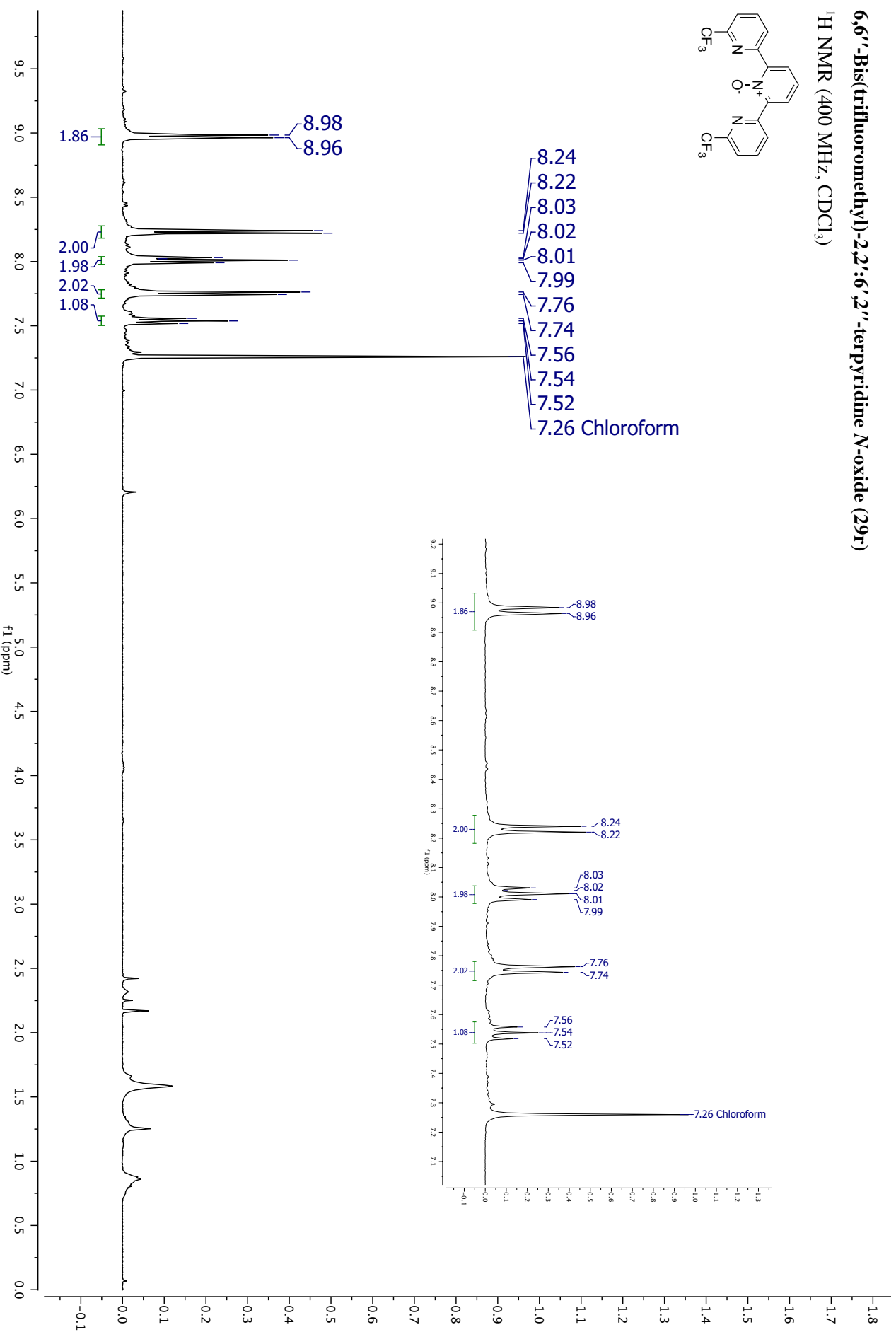
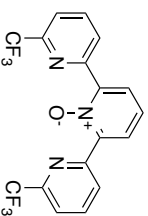
6'-Trifluoromethyl-2,2'-bipyridine N-oxide (20r)

¹⁹F NMR (376 MHz, CDCl₃)



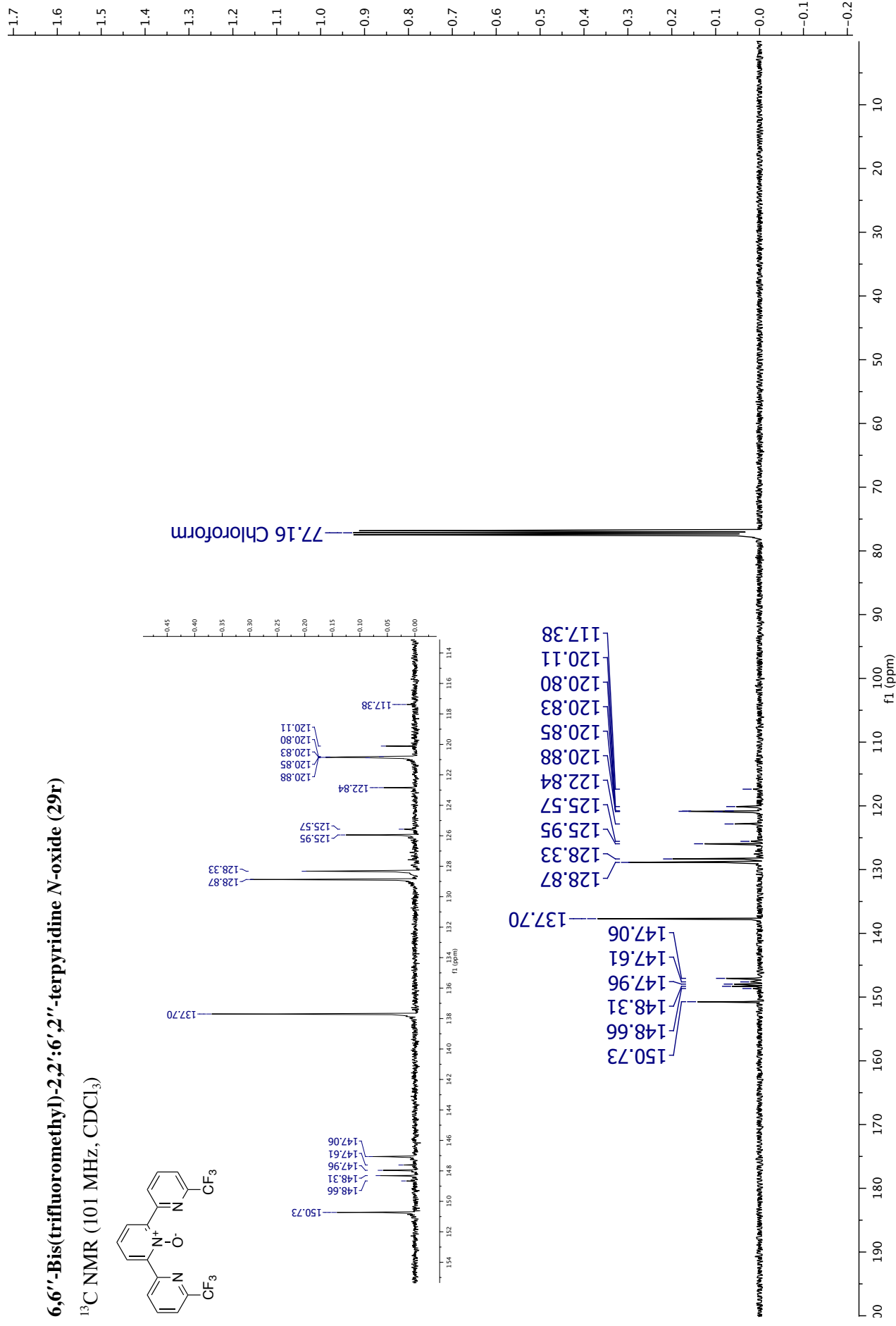
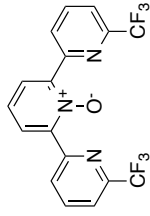
6,6'-Bis(trifluoromethyl)-2,2':6',2''-terpyridine N-oxide (29r)

¹H NMR (400 MHz, CDCl₃)



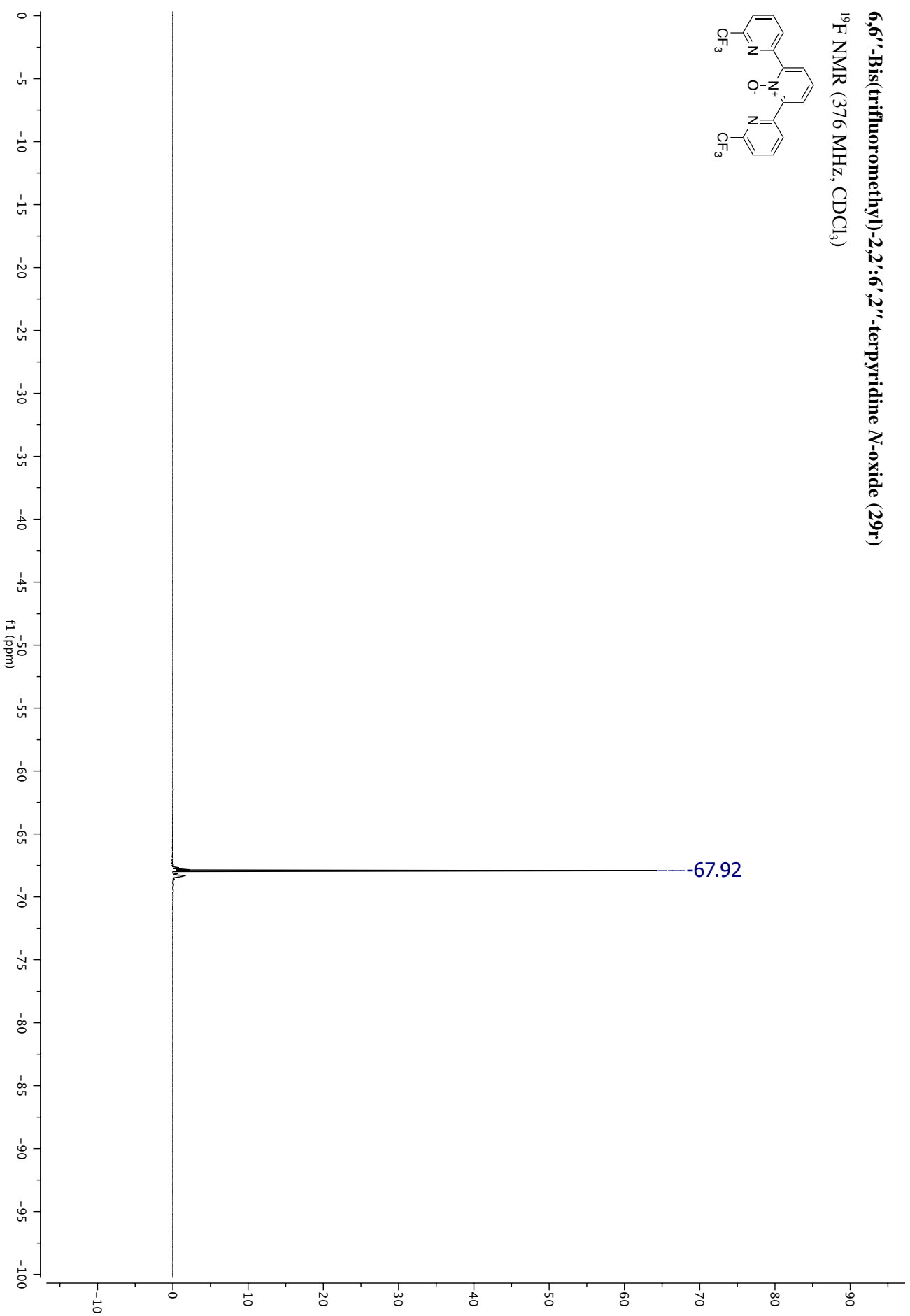
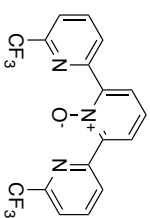
6,6''-Bis(trifluoromethyl)-2,2':6',2''-terpyridine N-oxide (29r)

¹³C NMR (101 MHz, CDCl₃)



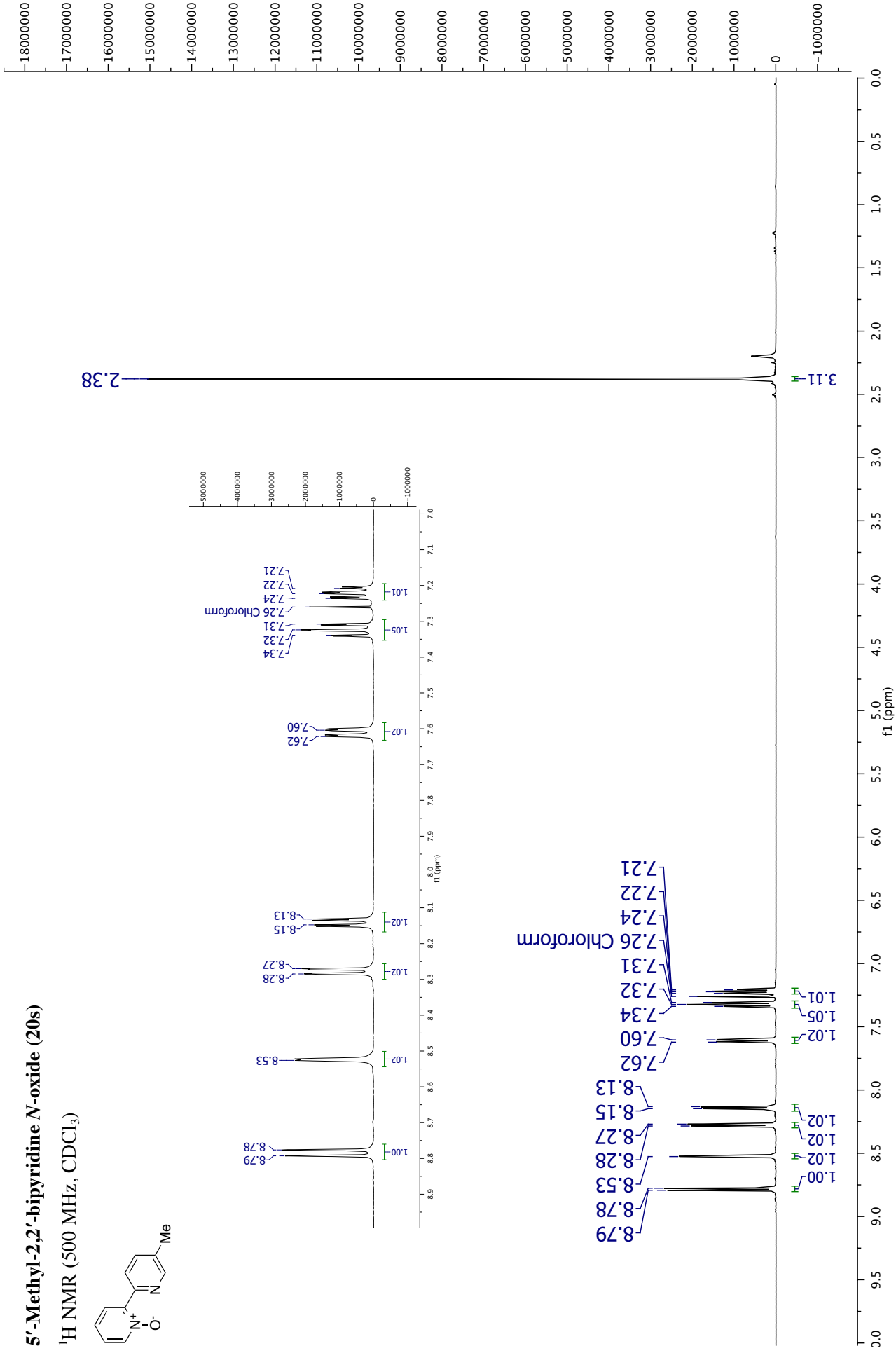
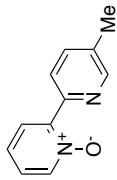
6,6'-Bis(trifluoromethyl)-2,2':6,2''-terpyridine N-oxide (29r)

¹⁹F NMR (376 MHz, CDCl₃)



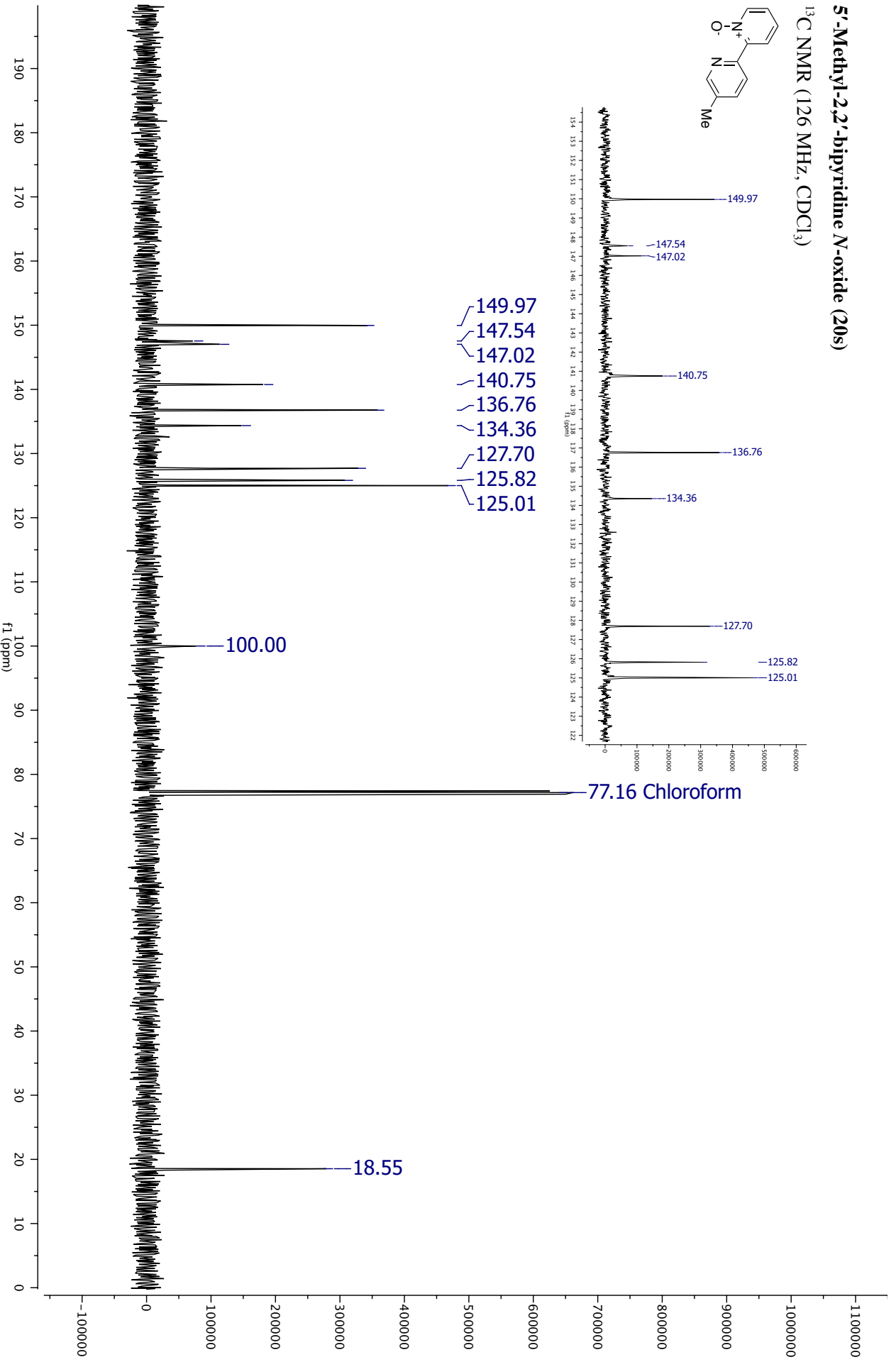
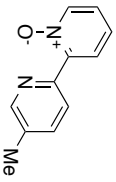
5'-Methyl-2,2'-bipyridine N-oxide (20s)

¹H NMR (500 MHz, CDCl₃)



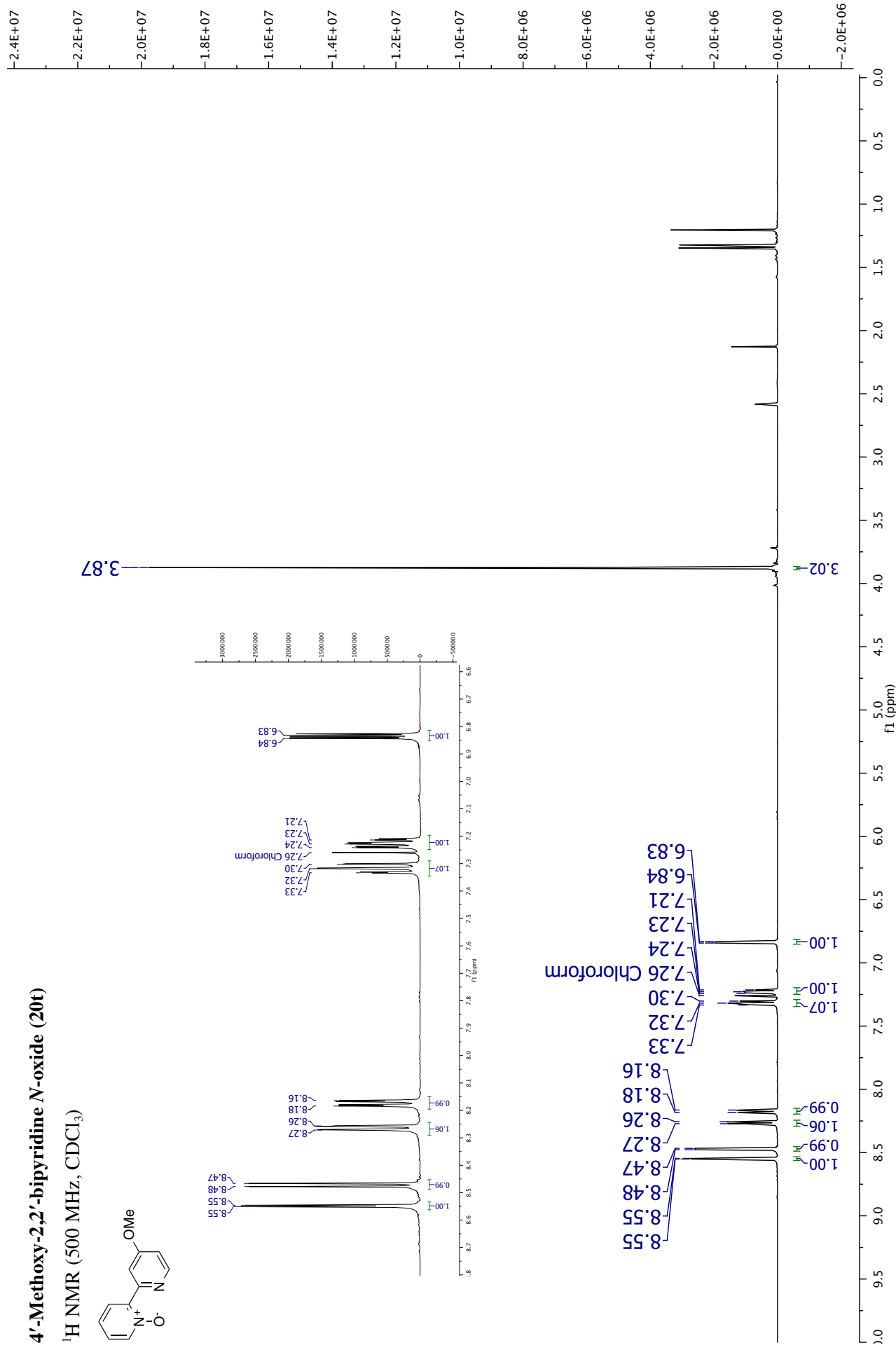
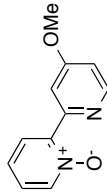
5'-Methyl-2,2'-bipyridine N-oxide (20s)

¹³C NMR (126 MHz, CDCl₃)



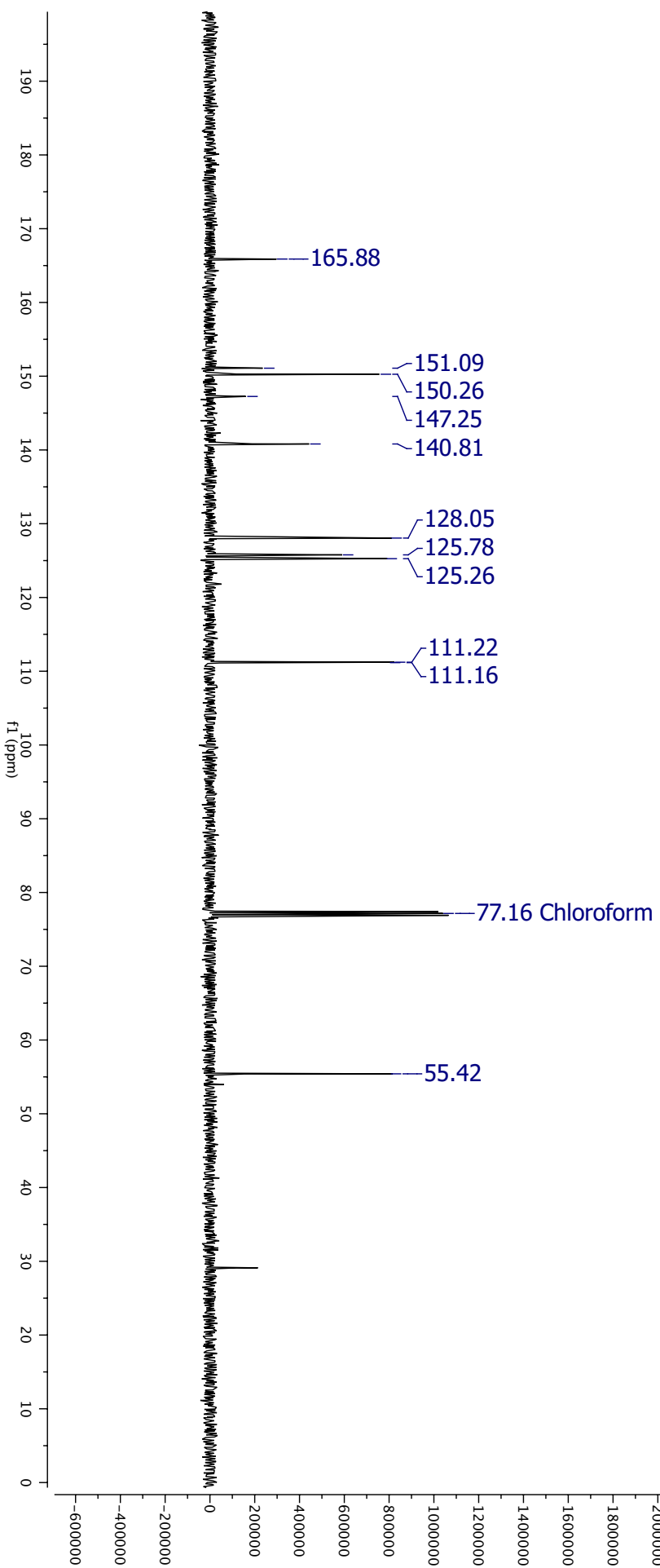
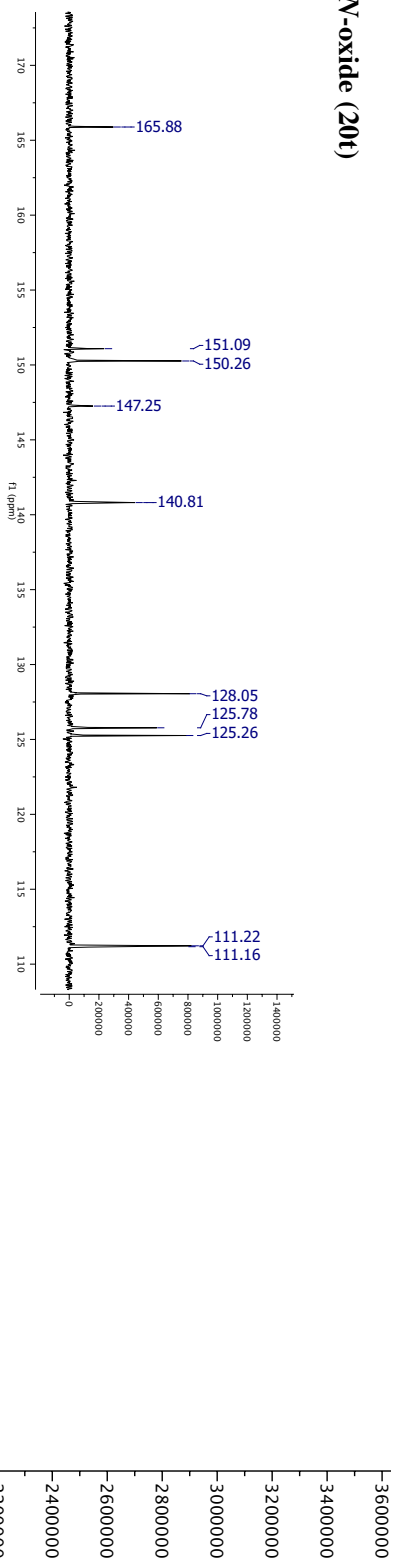
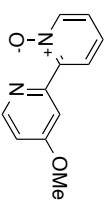
4'-Methoxy-2,2'-bipyridine N-oxide (20t)

¹H NMR (500 MHz, CDCl₃)



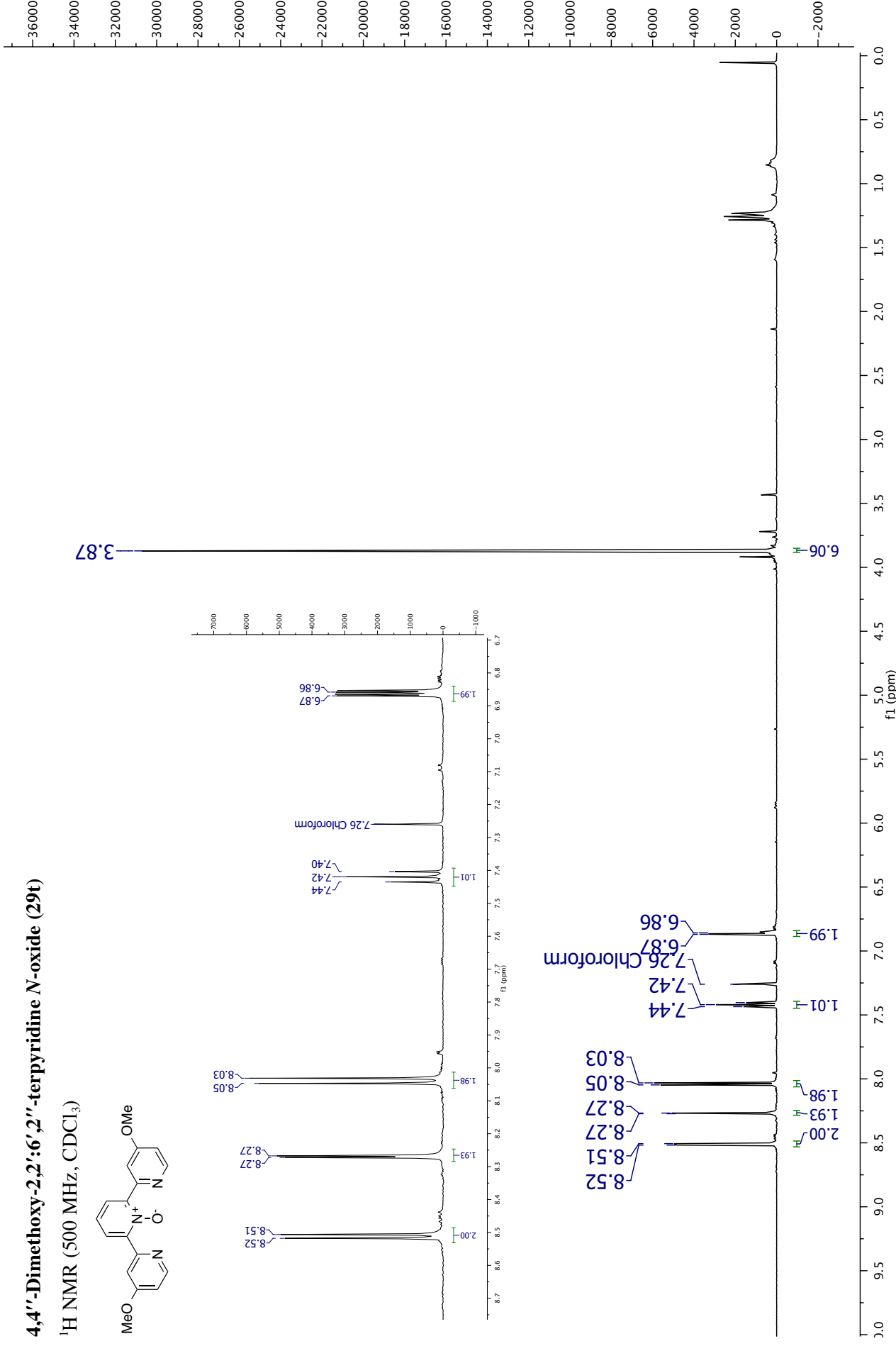
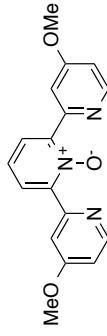
4'-Methoxy-2,2'-bipyridine N-oxide (20f)

¹³C NMR (126 MHz, CDCl₃)



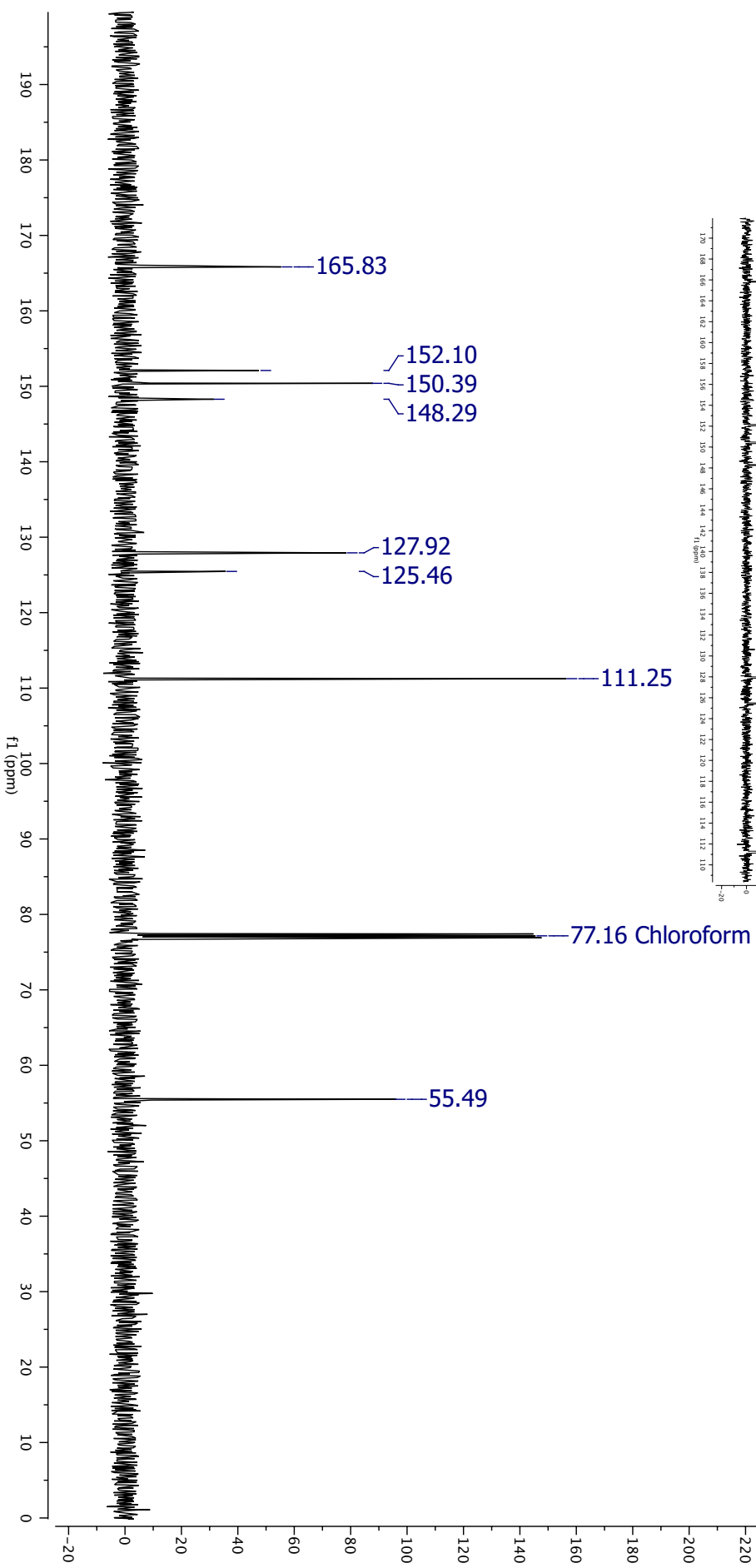
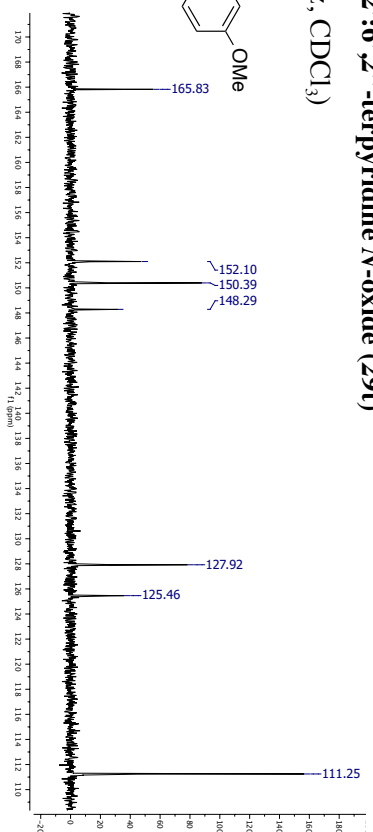
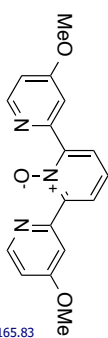
4,4''-Dimethoxy-2,2':6',2''-terpyridine N-oxide (29t)

¹H NMR (500 MHz, CDCl₃)



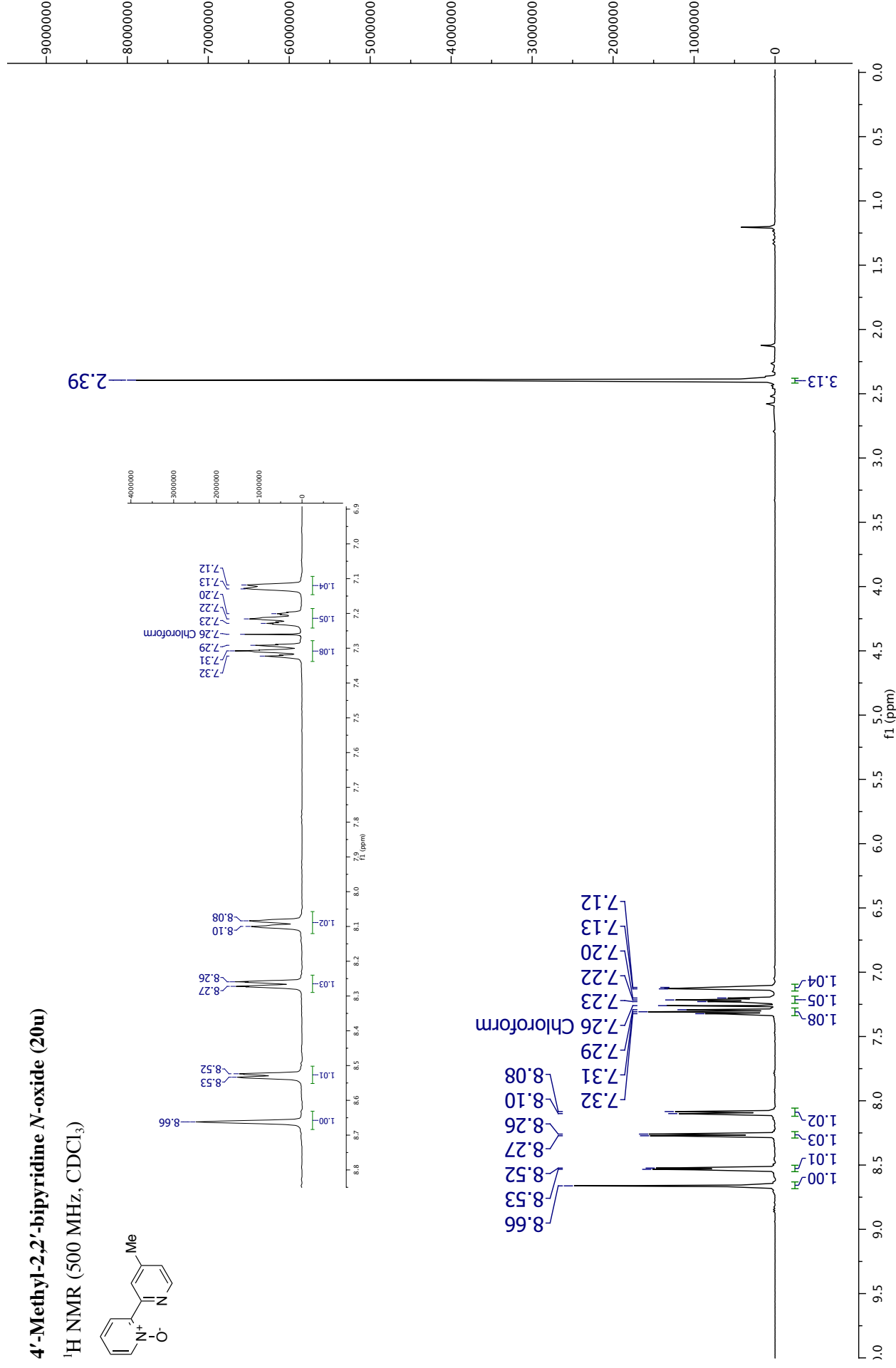
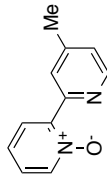
4,4'-Dimethoxy-2,2':6,6'-terpyridine N-oxide (29f)

¹³C NMR (126 MHz, CDCl₃)



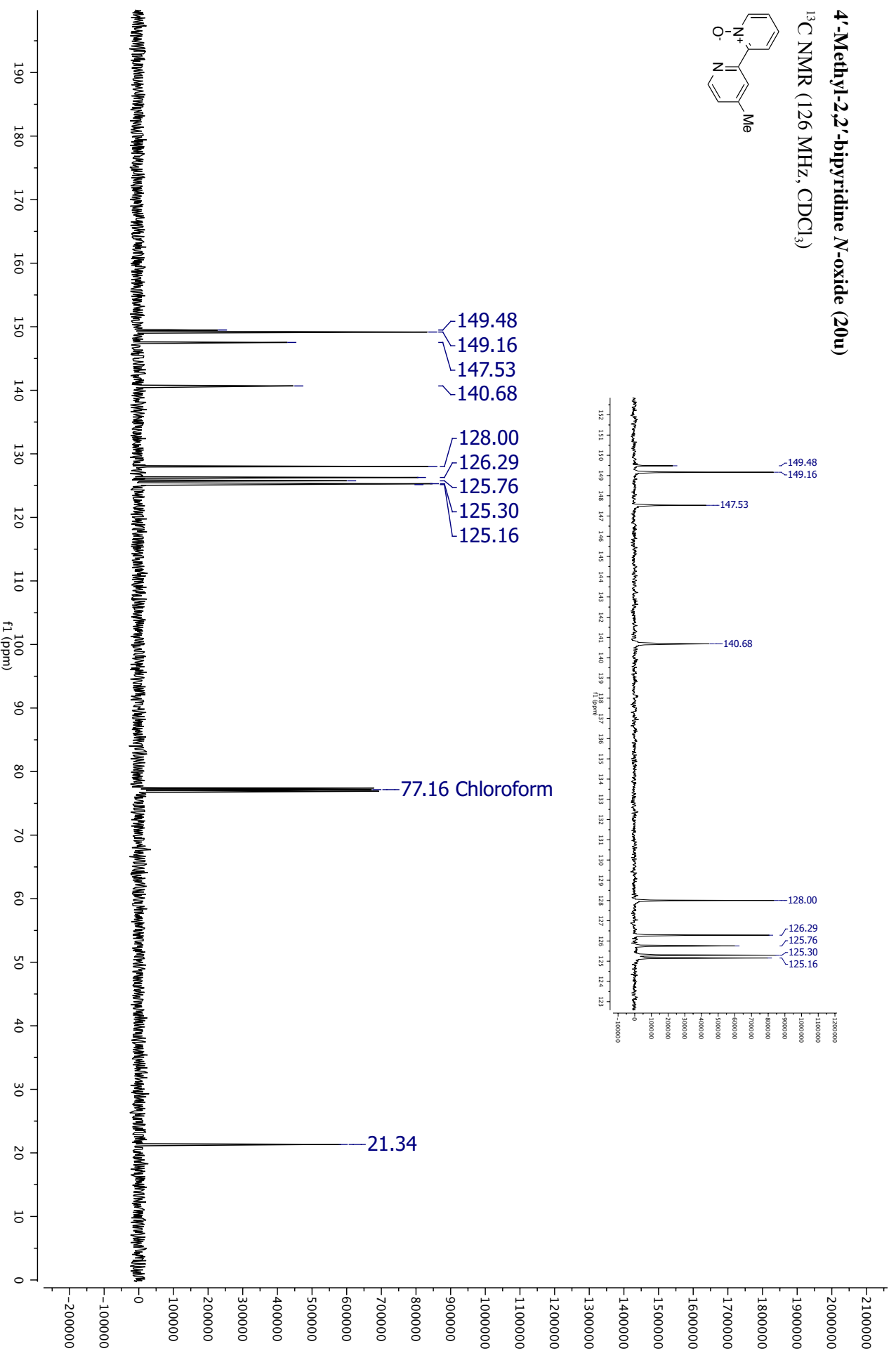
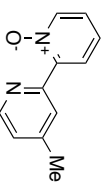
4'-Methyl-2,2'-bipyridine N-oxide (20u)

¹H NMR (500 MHz, CDCl₃)



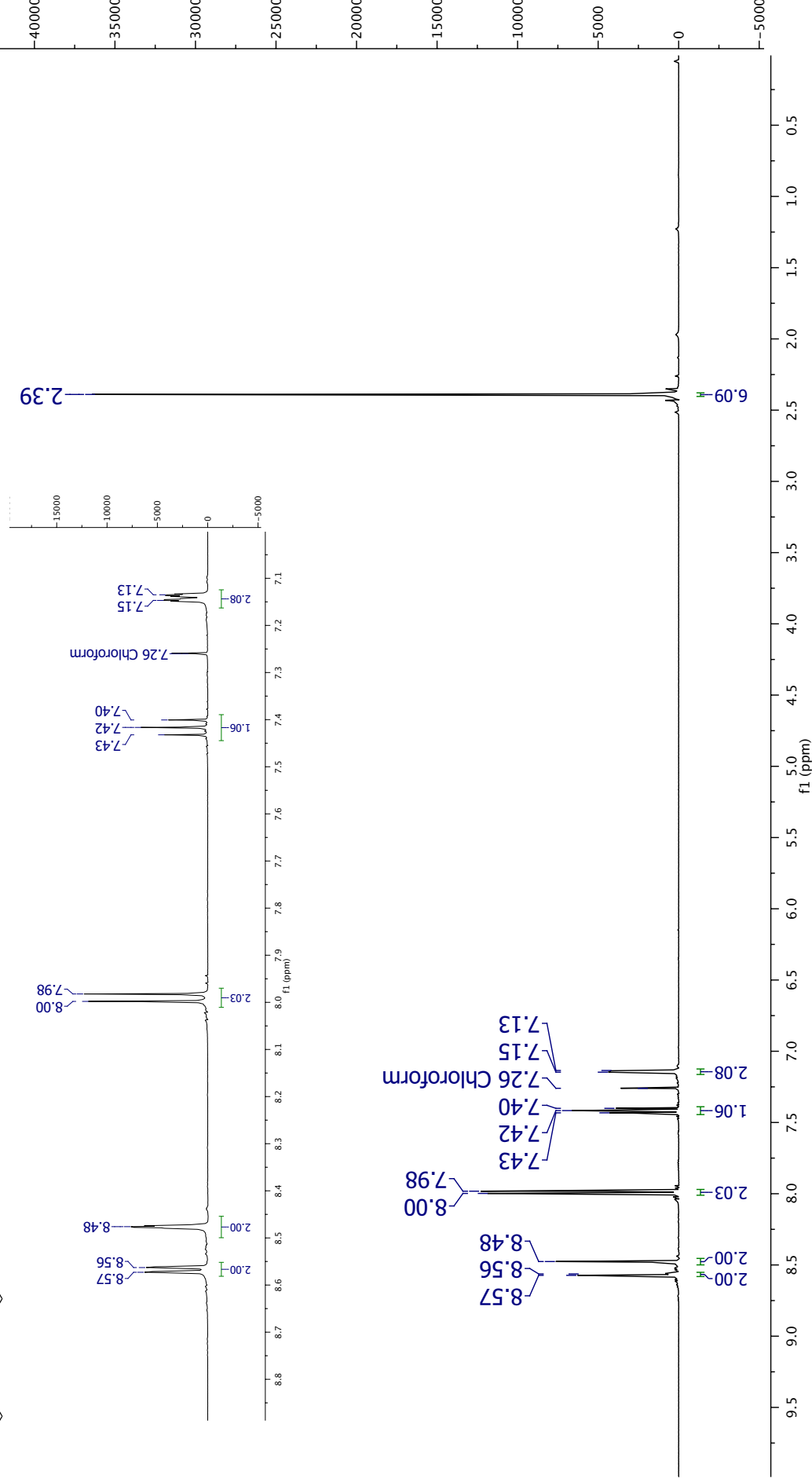
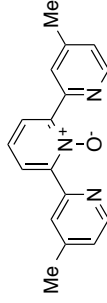
4'-Methyl-2,2'-bipyridine N-oxide (20u)

¹³C NMR (126 MHz, CDCl₃)



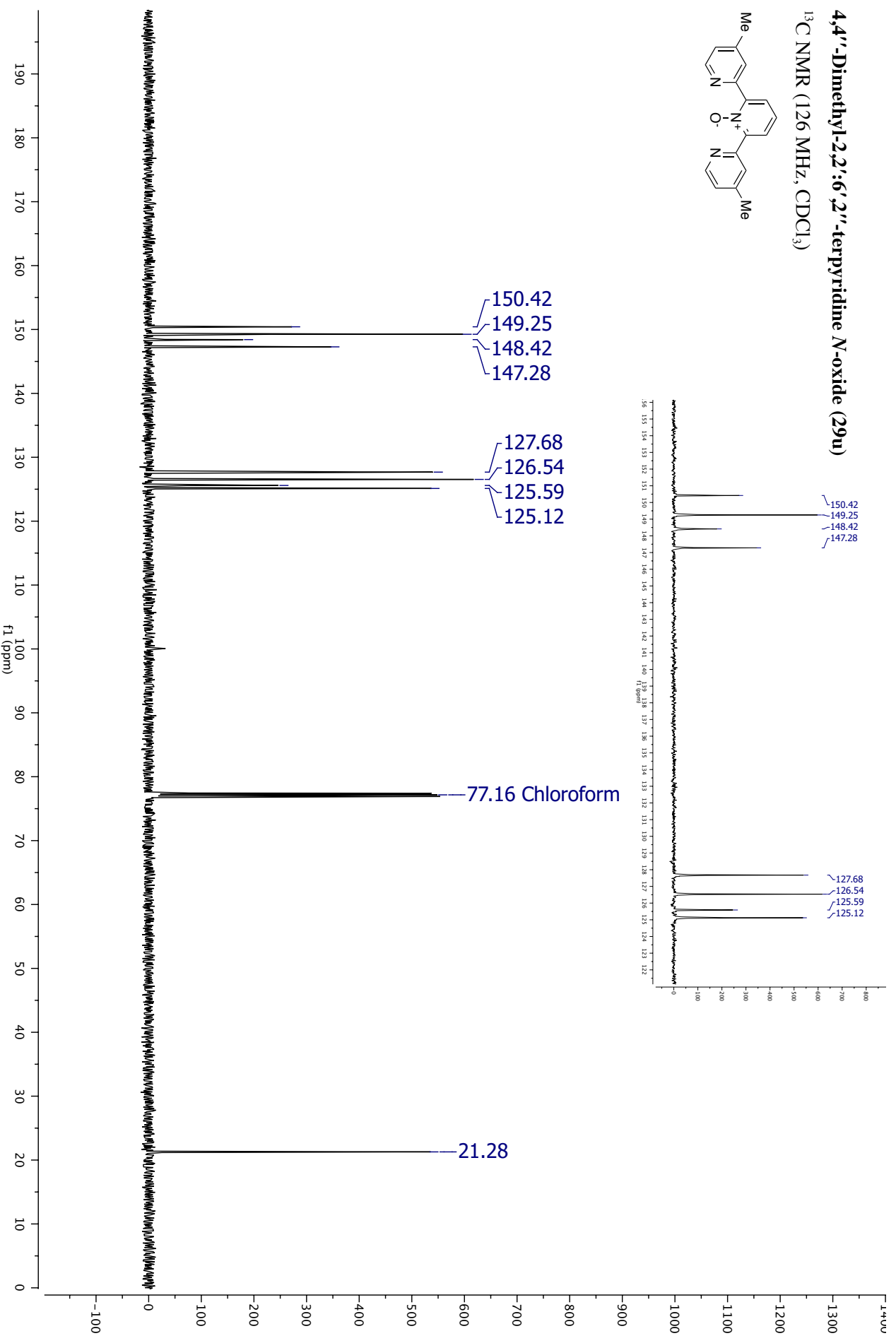
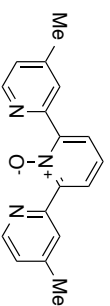
4,4''-Dimethyl-2,2':6,2''-terpyridine N-oxide (29u)

¹H NMR (500 MHz, CDCl₃)



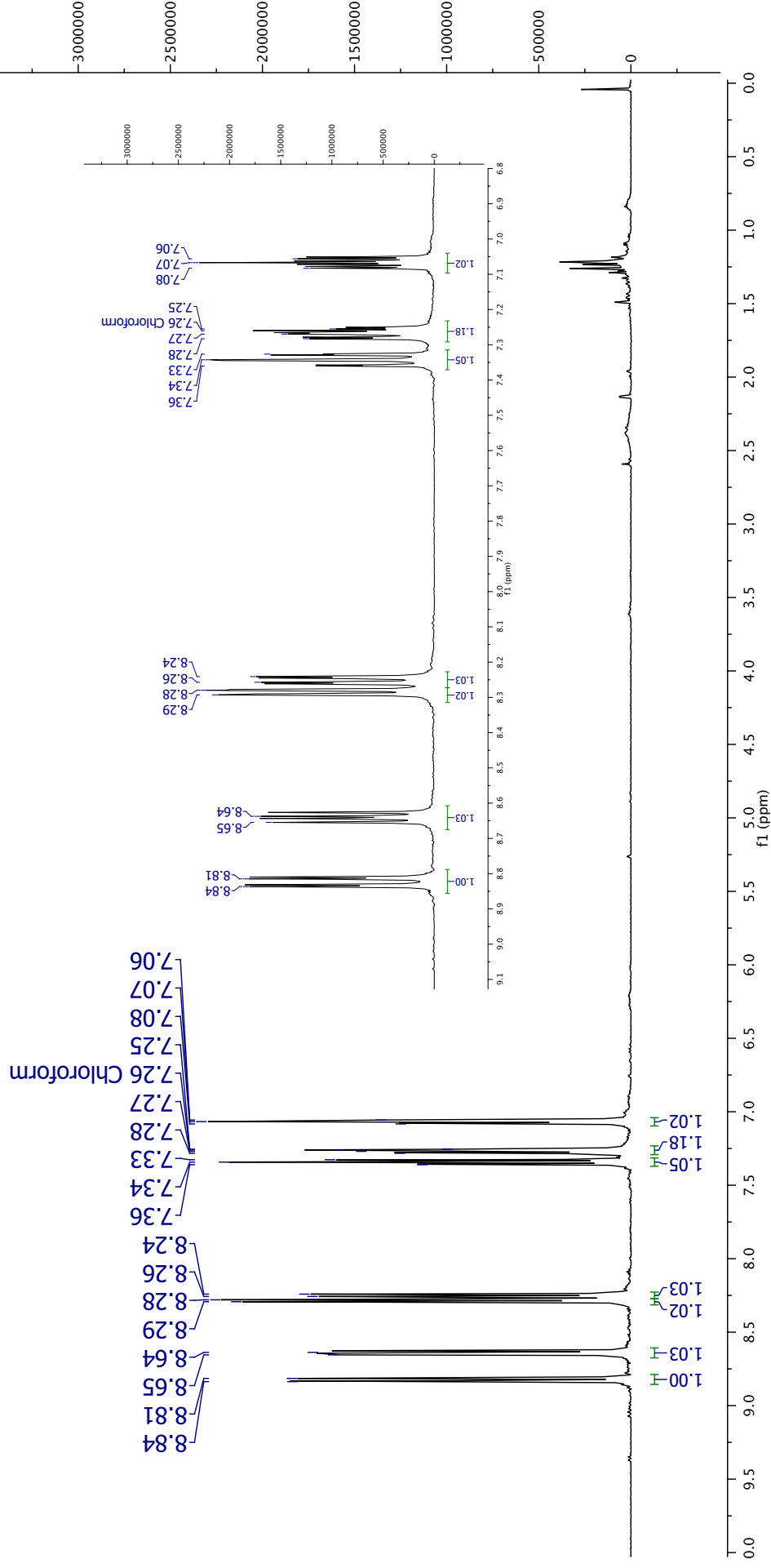
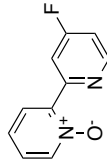
4,4'-Dimethyl-2,2':6',2''-terpyridine N-oxide (29u)

¹³C NMR (126 MHz, CDCl₃)



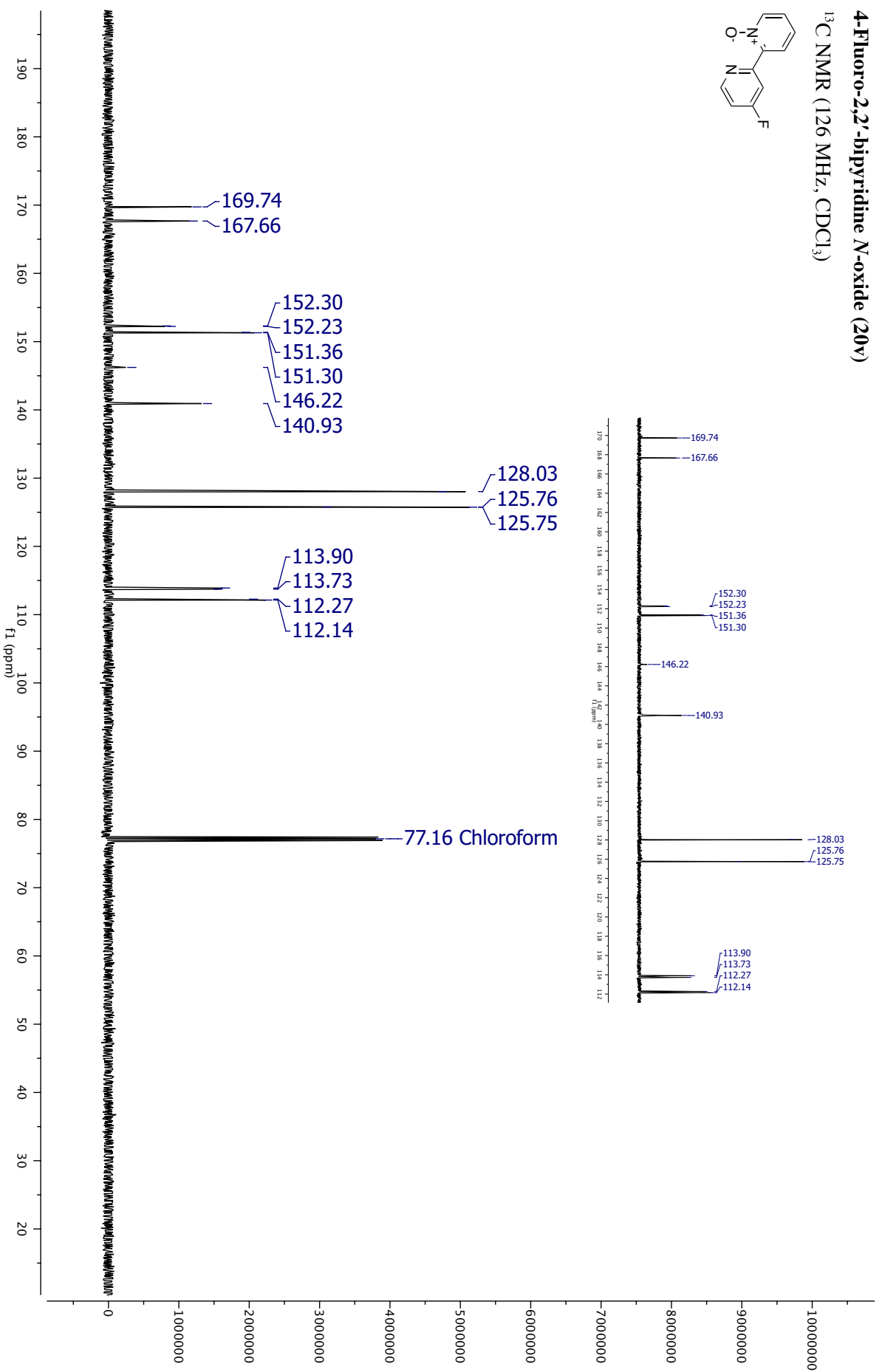
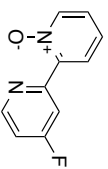
4-Fluoro-2,2'-bipyridine N-oxide (20v)

¹H NMR (500 MHz, CDCl₃)



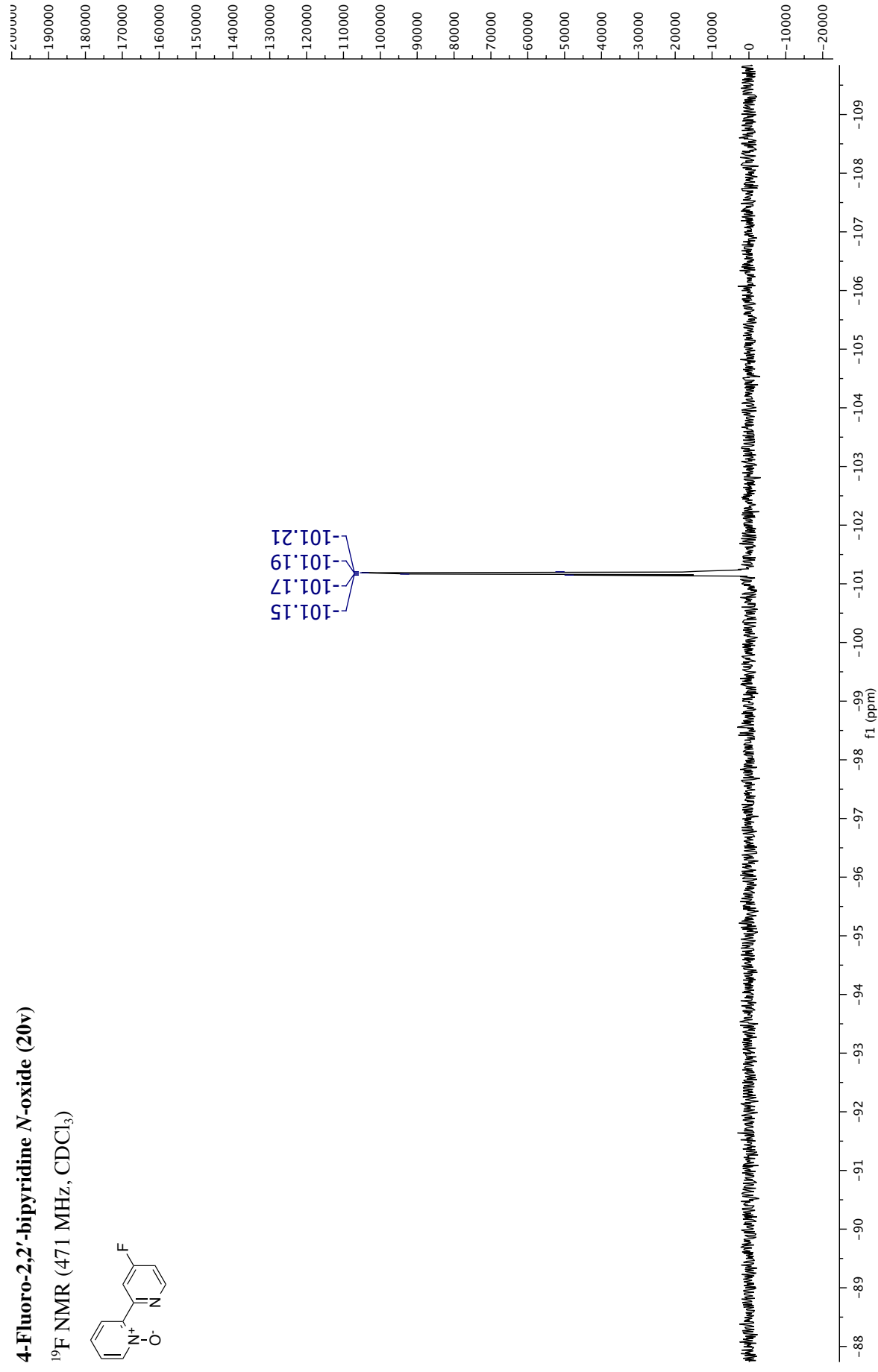
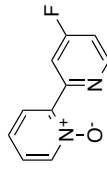
4-Fluoro-2,2'-bipyridine N-oxide (20v)

¹³C NMR (126 MHz, CDCl₃)



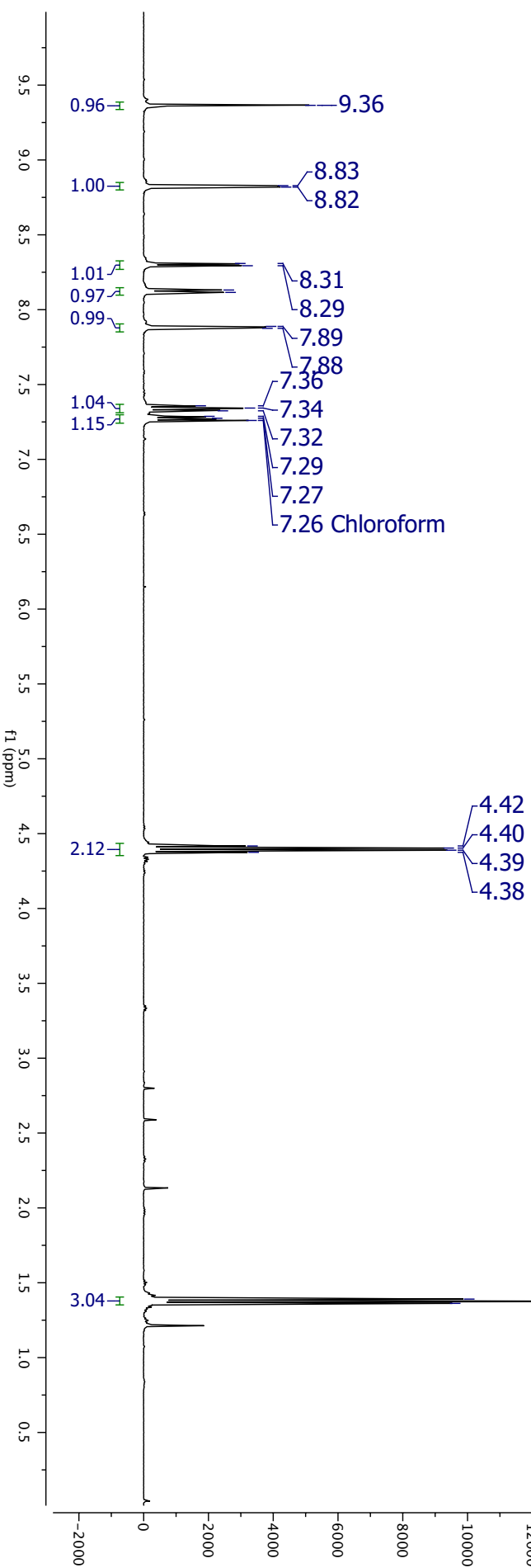
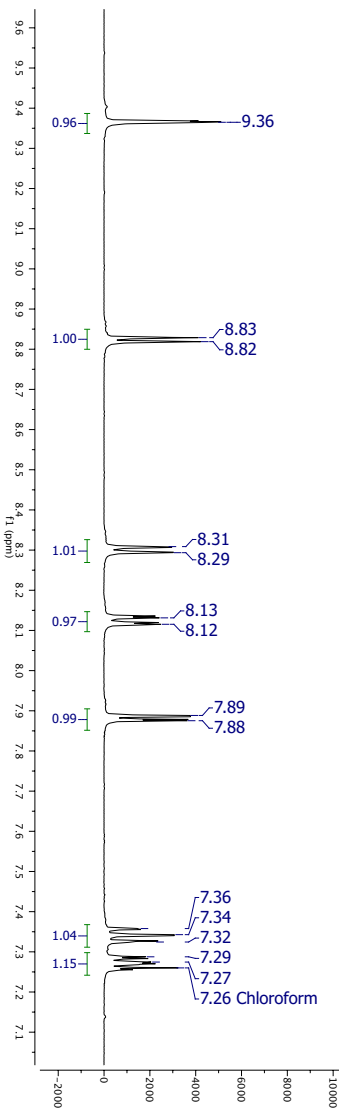
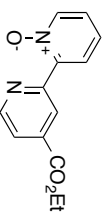
4-Fluoro-2,2'-bipyridine N-oxide (20v)

¹⁹F NMR (471 MHz, CDCl₃)



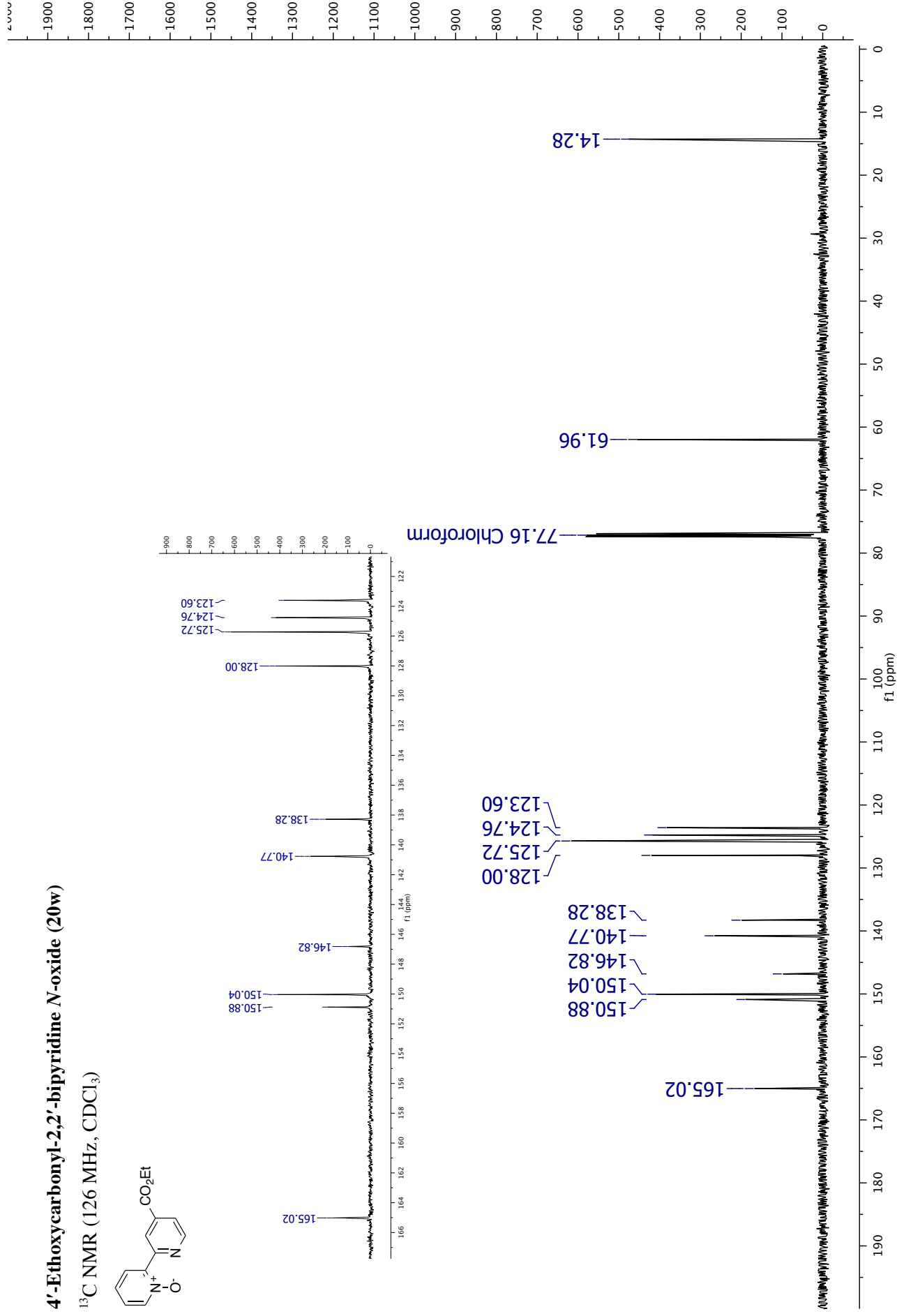
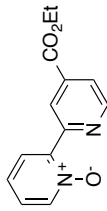
4'-(Ethoxycarbonyl)-2,2'-bipyridine N-oxide (20w)

¹H NMR (500 MHz, CDCl₃)



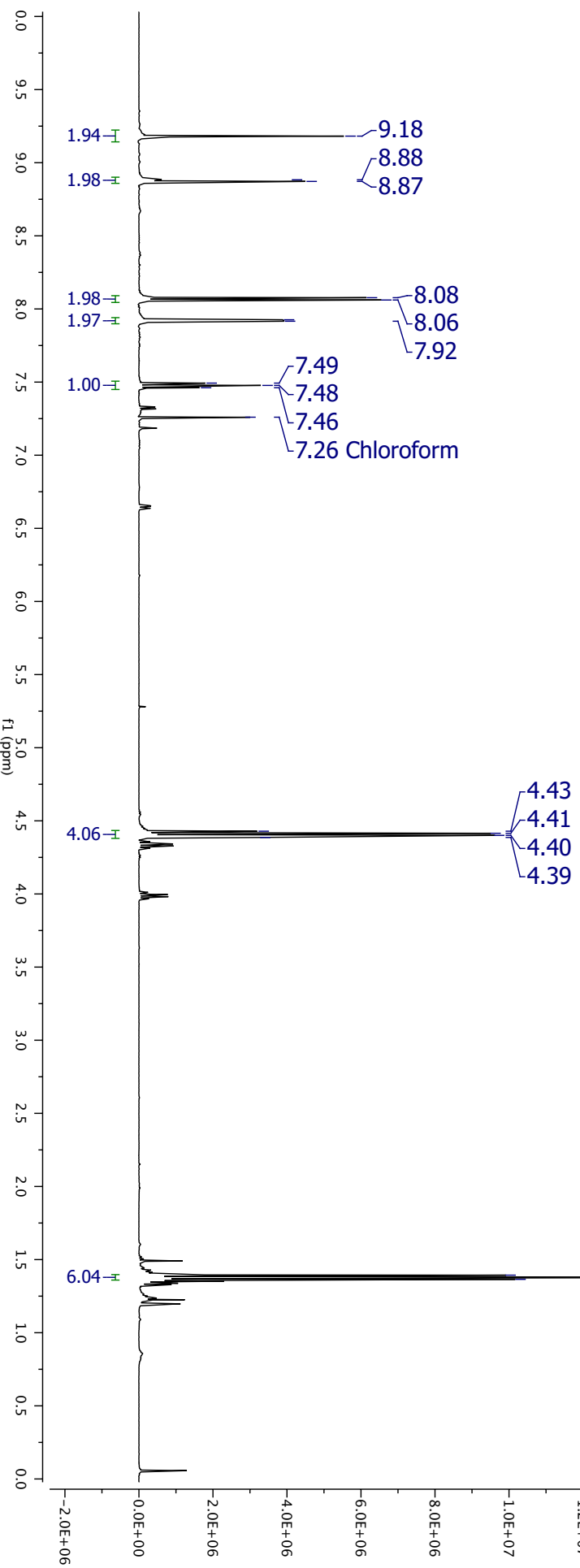
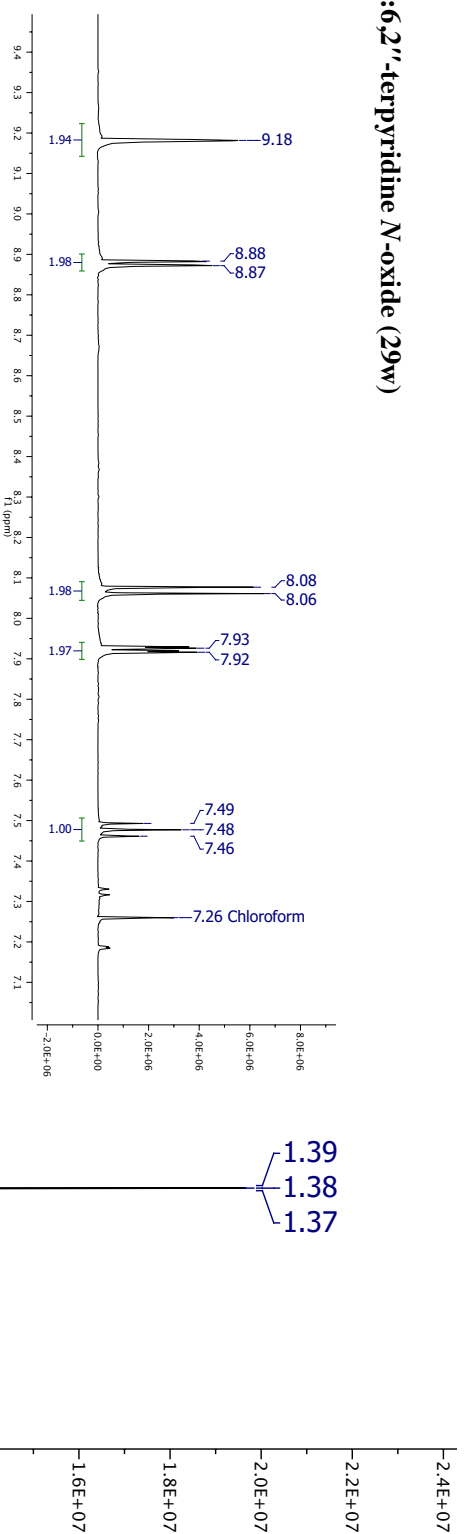
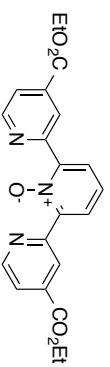
4'-Ethoxycarbonyl-2,2'-bipyridine N-oxide (20w)

¹³C NMR (126 MHz, CDCl₃)



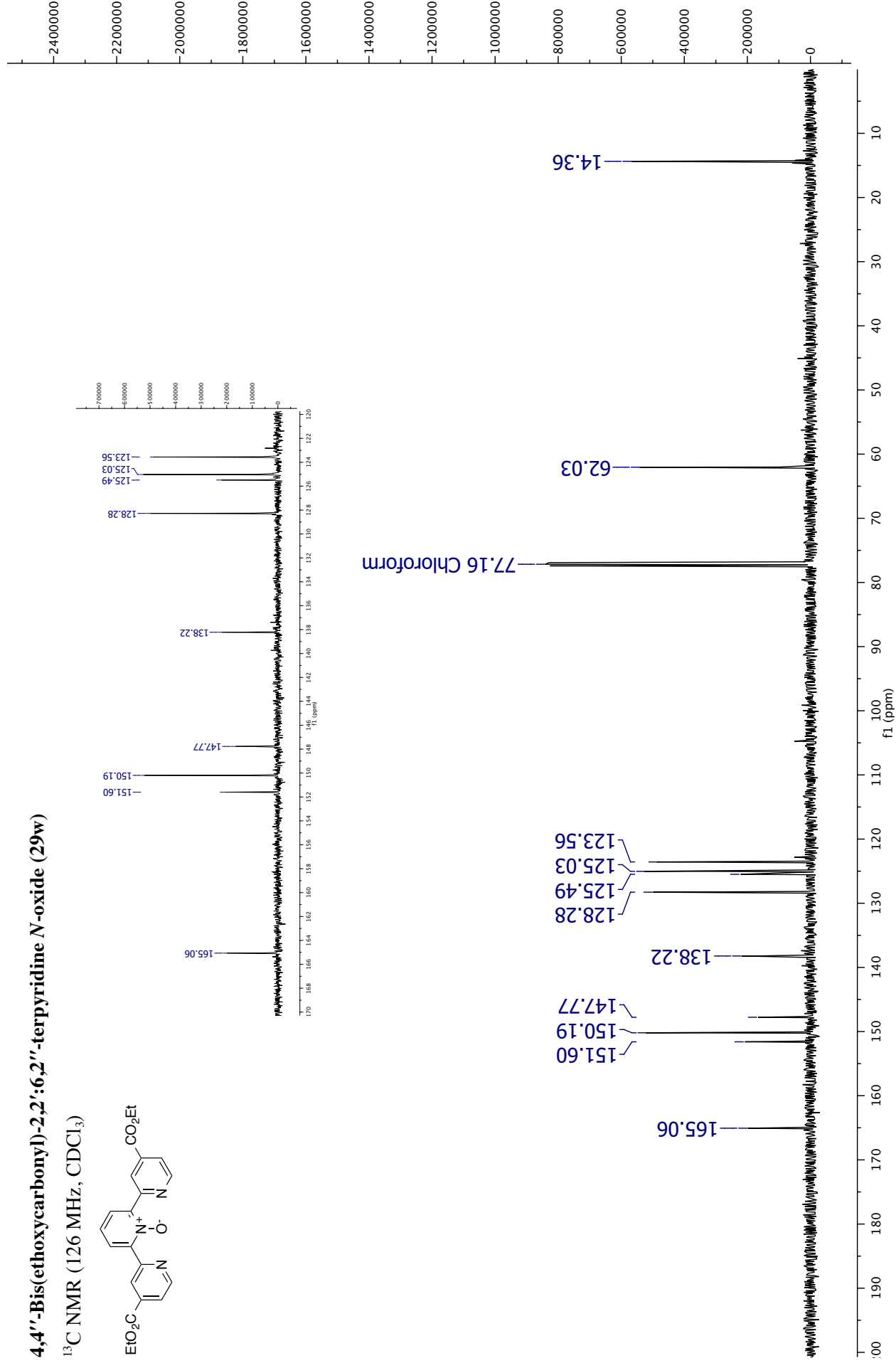
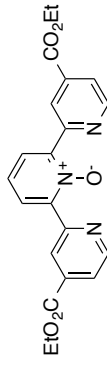
4,4'-Bis(ethoxycarbonyl)-2,2':6,2''-terpyridine N-oxide (29w)

¹H NMR (500 MHz, CDCl₃)



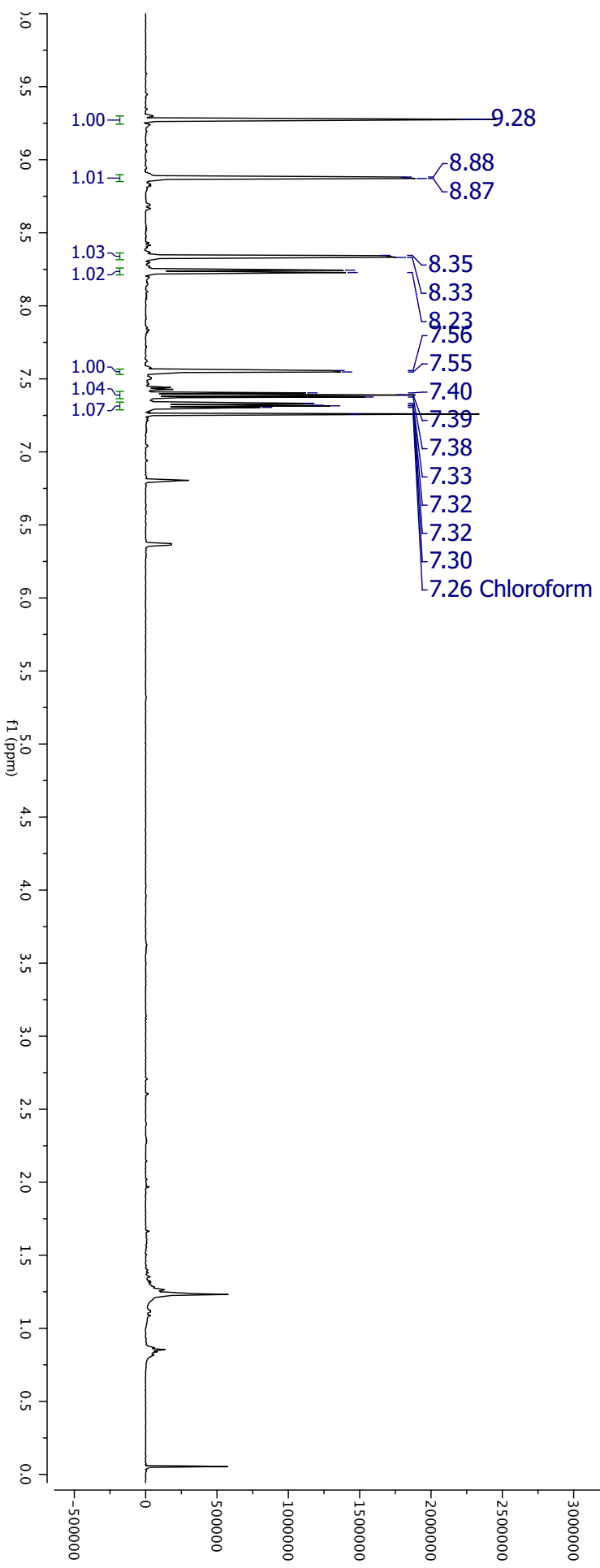
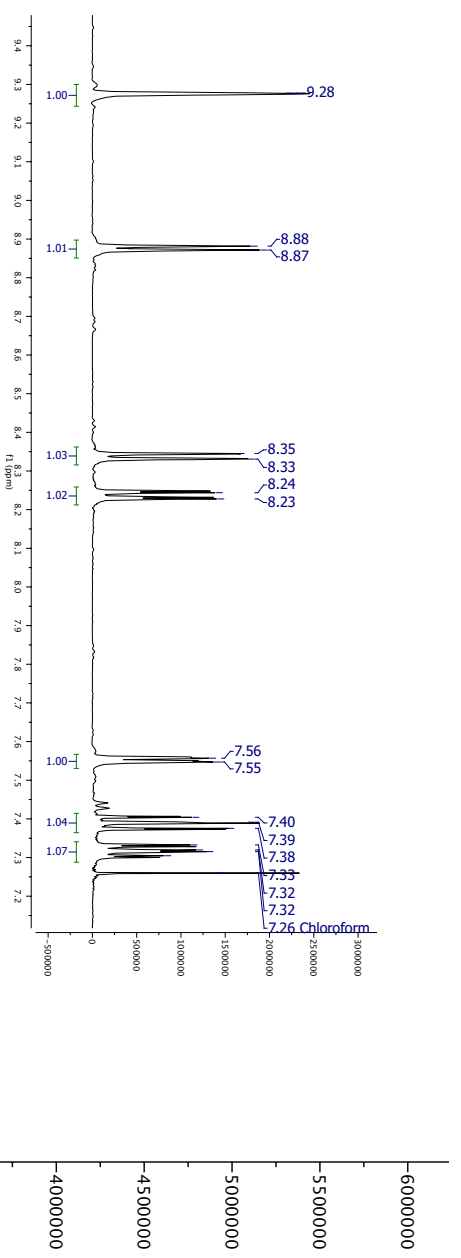
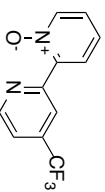
4,4''-Bis(ethoxycarbonyl)-2,2':6,2''-terpyridine N-oxide (29w)

¹³C NMR (126 MHz, CDCl₃)



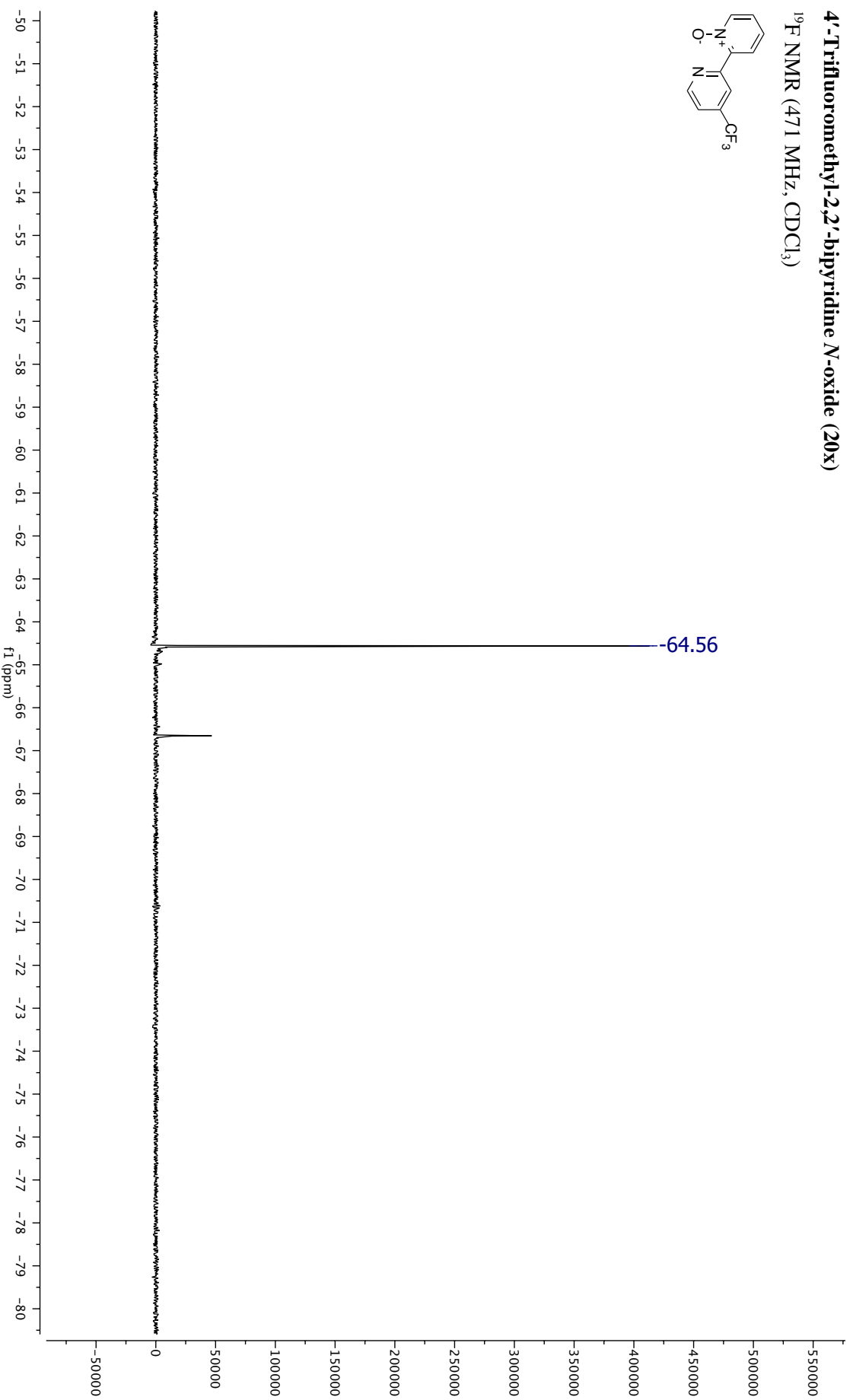
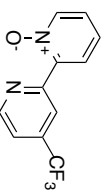
4'-Trifluoromethyl-2,2'-bipyridine N-oxide (20x)

¹H NMR (500 MHz, CDCl₃)



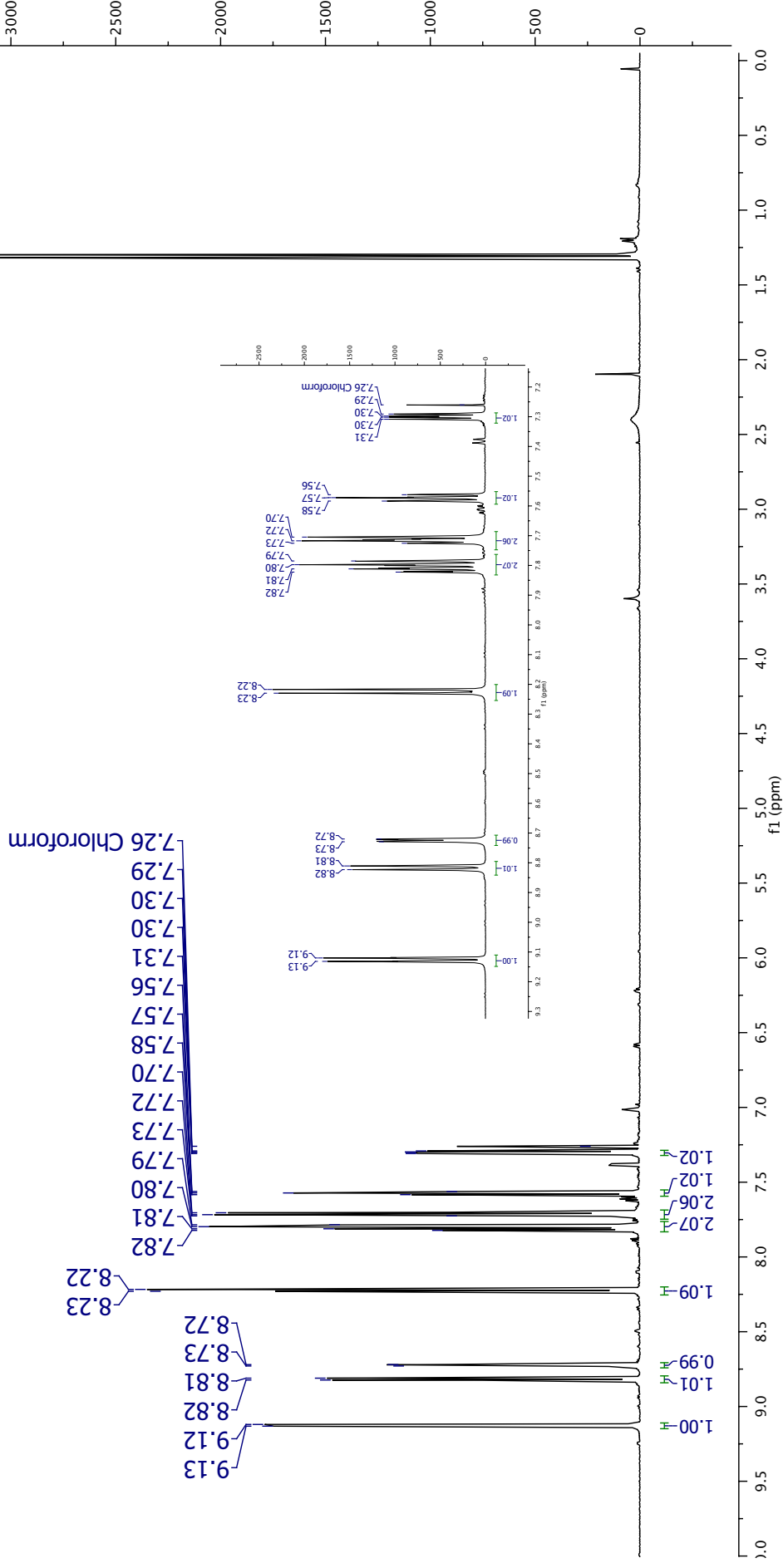
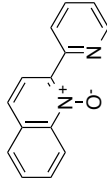
4'-Trifluoromethyl-2,2'-bipyridine N-oxide (20x)

¹⁹F NMR (471 MHz, CDCl₃)



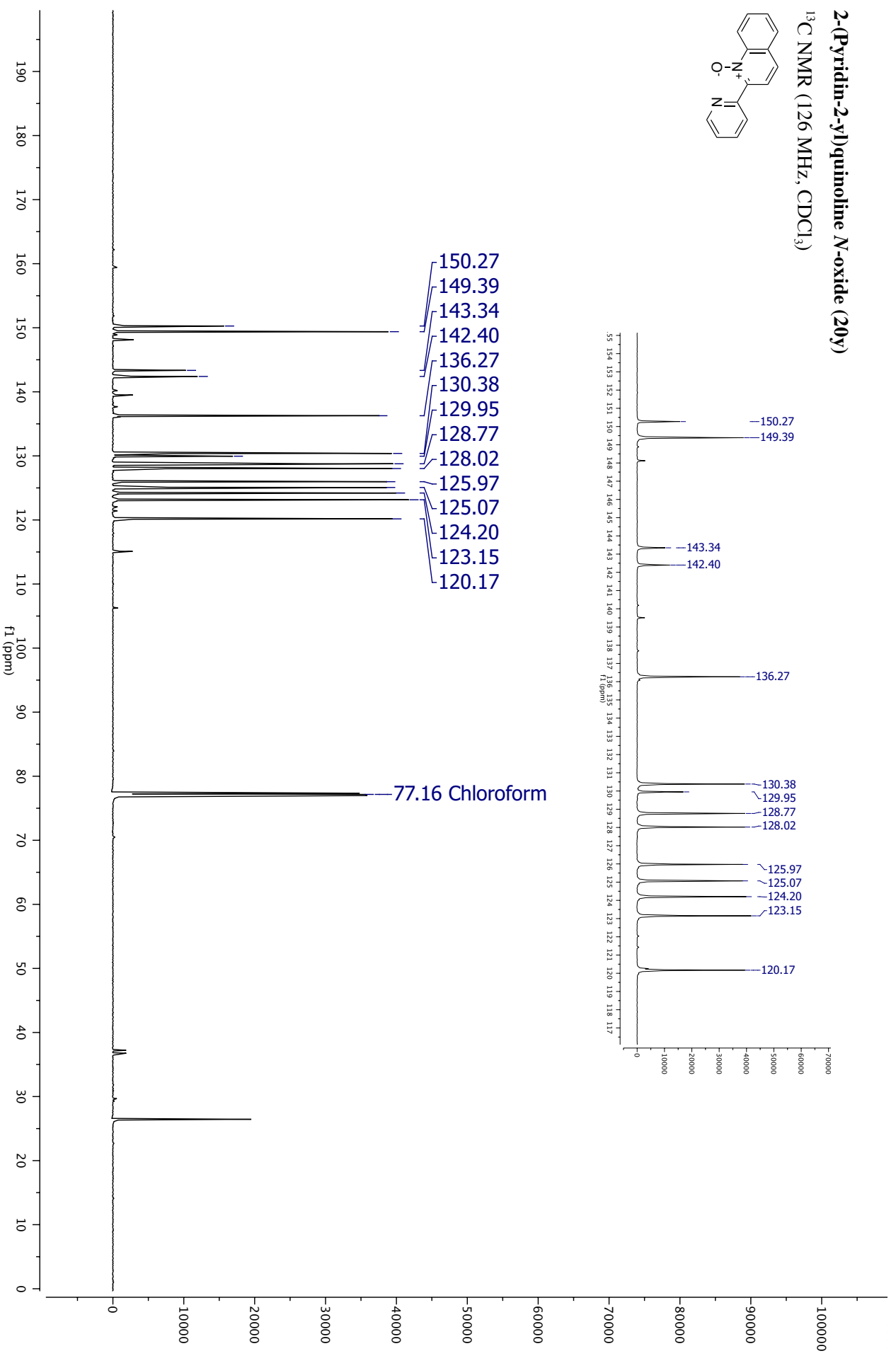
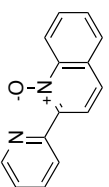
2-(Pyridin-2-yl)quinoline N-oxide (20y)

¹H NMR (500 MHz, CDCl₃)



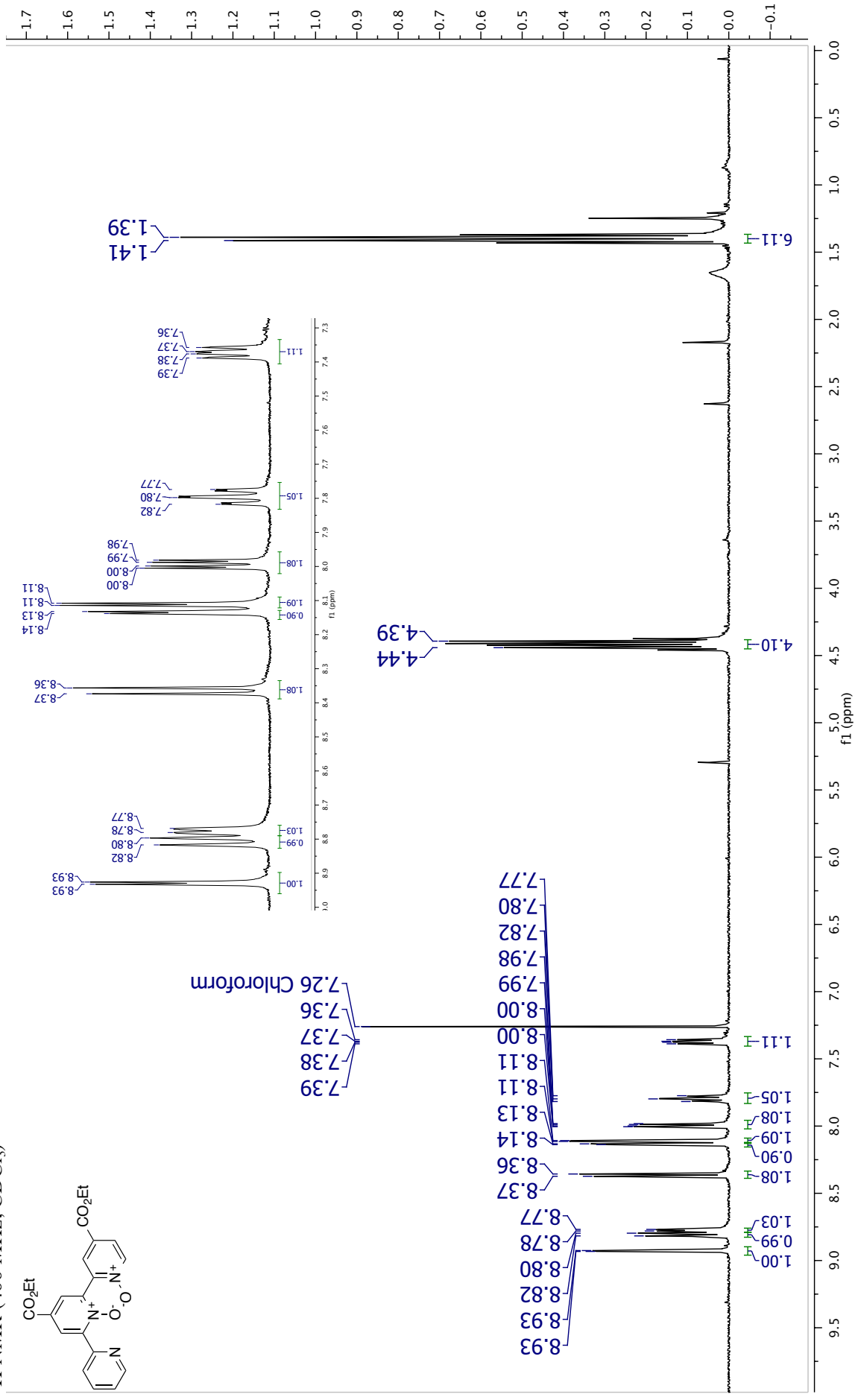
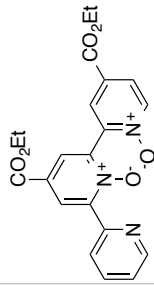
2-(Pyridin-2-yl)quinoline N-oxide (20y)

¹³C NMR (126 MHz, CDCl₃)



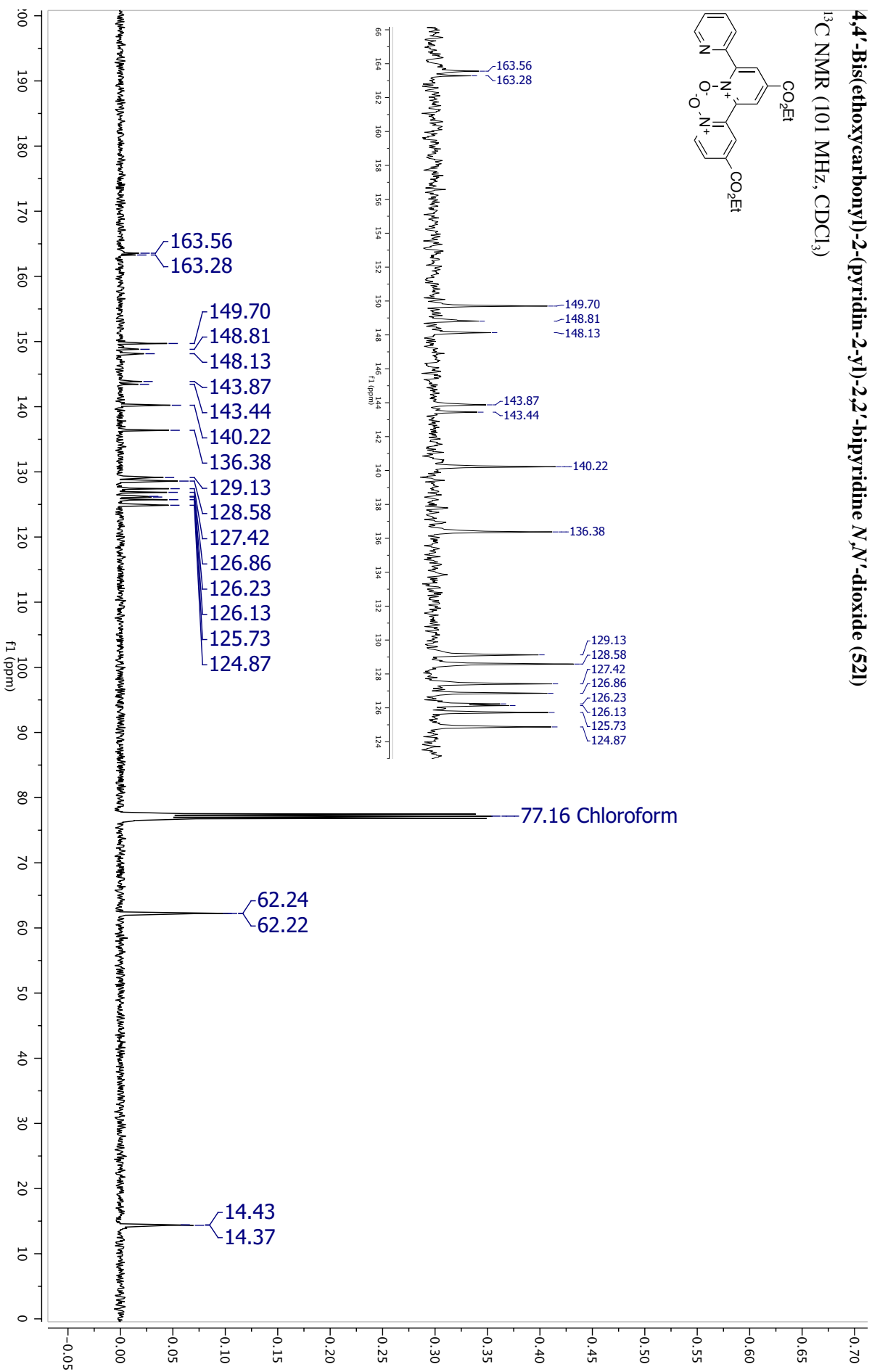
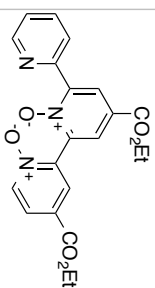
4,4'-Bis(ethoxycarbonyl)-2-(pyridin-2-yl)-2,2'-bipyridine N,N'-dioxide (52I)

¹H NMR (400 MHz, CDCl₃)



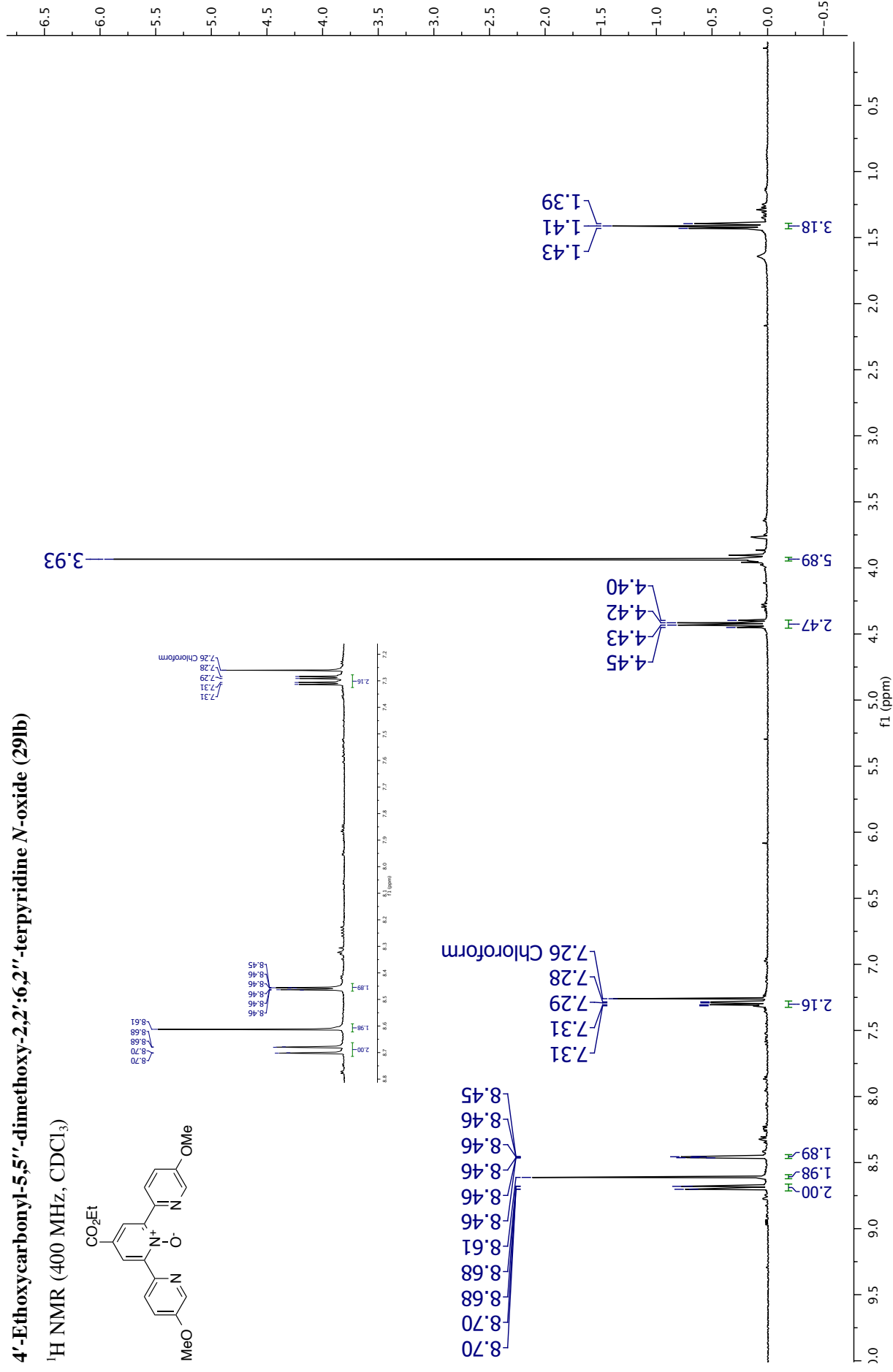
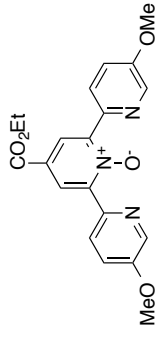
4,4'-Bis(ethoxycarbonyl)-2-(pyridin-2-yl)-2,2'-bipyridine *N,N'*-dioxide (521)

¹³C NMR (101 MHz, CDCl₃)



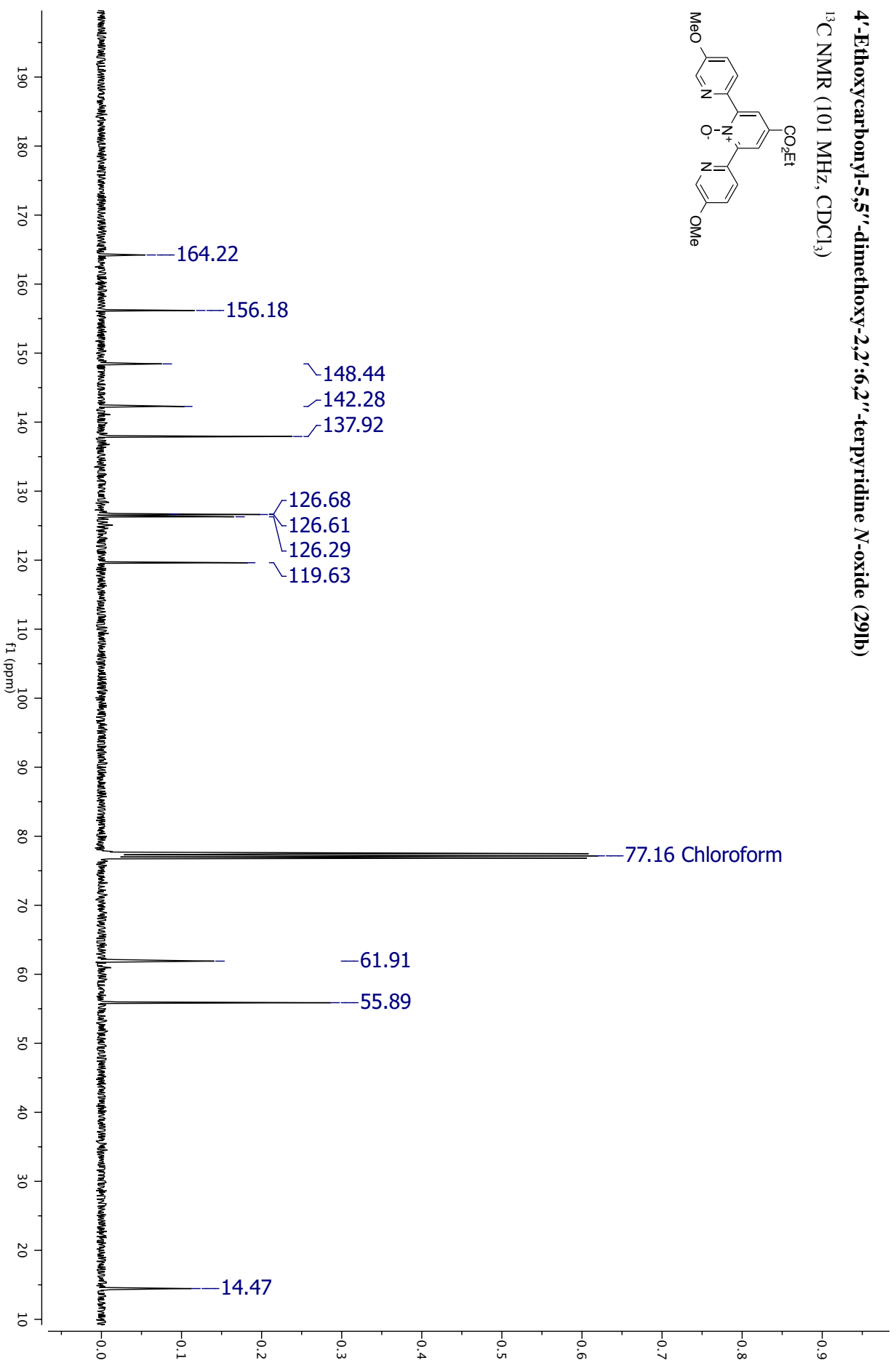
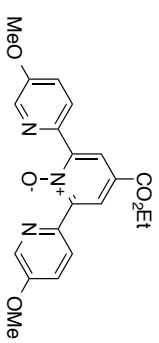
4'-Ethoxycarbonyl-5,5'-dimethoxy-2,2':6,2''-terpyridine N-oxide (29Ib)

¹H NMR (400 MHz, CDCl₃)



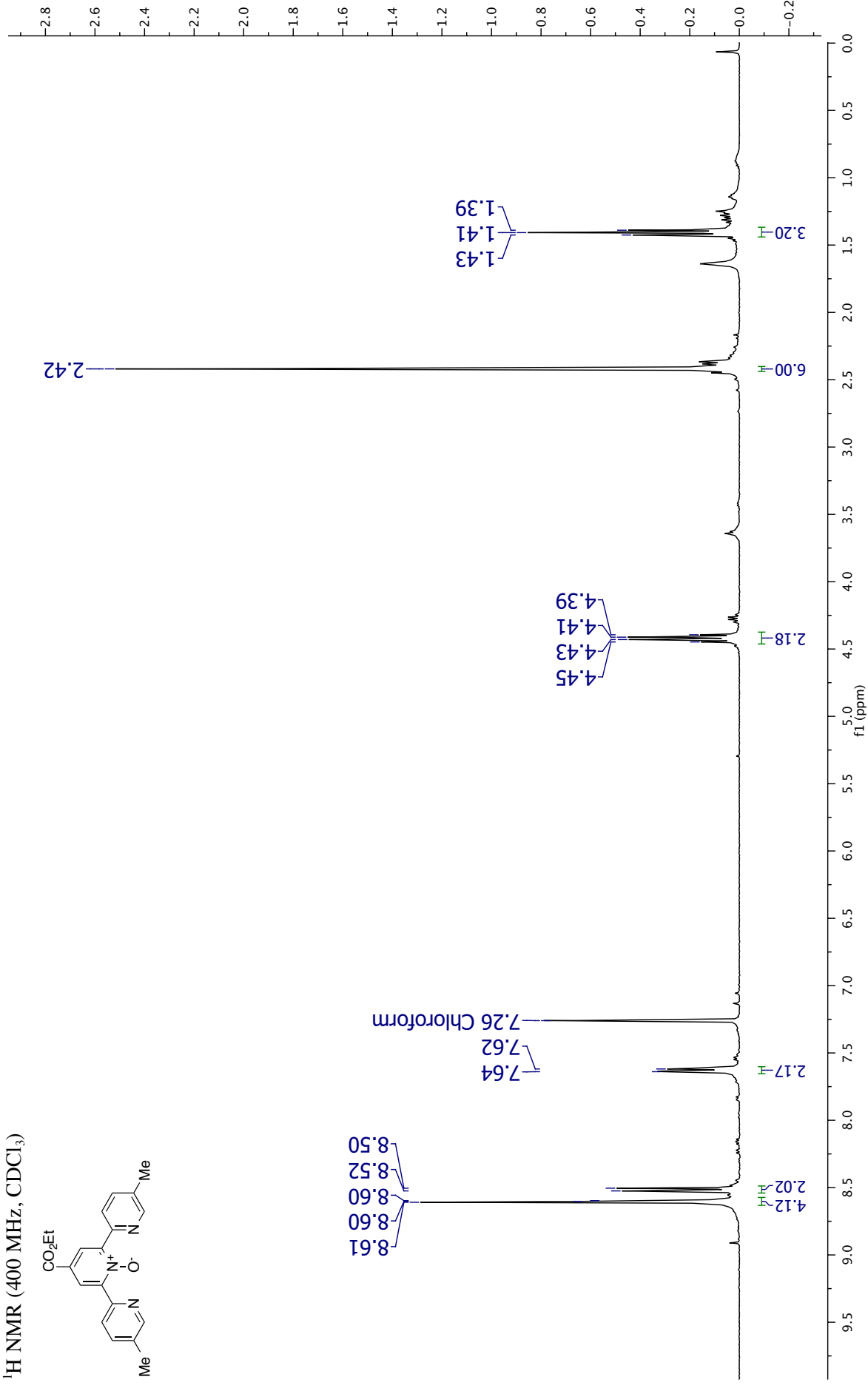
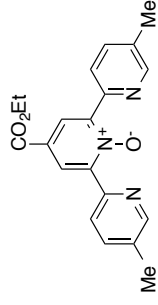
4'-Ethoxycarbonyl-5,5'-dimethoxy-2,2':6,2''-terpyridine N-oxide (291b)

¹³C NMR (101 MHz, CDCl₃)



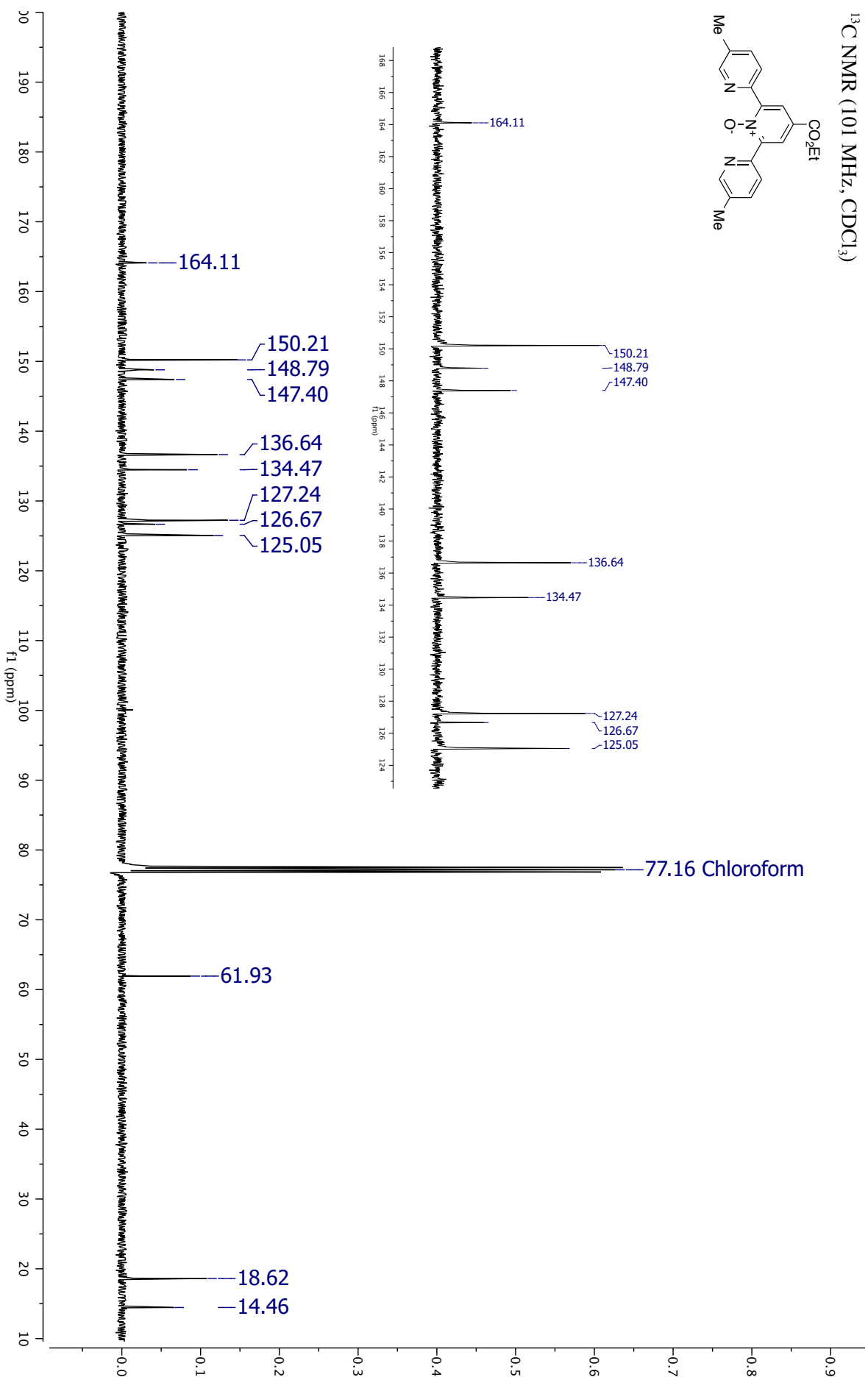
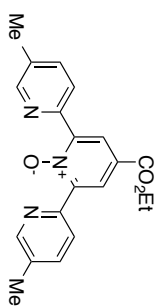
4'-Ethoxycarbonyl-5,5'-dimethyl-2,2':6,2''-terpyridine N-oxide (291c)

¹H NMR (400 MHz, CDCl₃)



4'-Ethoxycarbonyl-5,5'-dimethyl-2,2':6,2''-terpyridine N-oxide (291c)

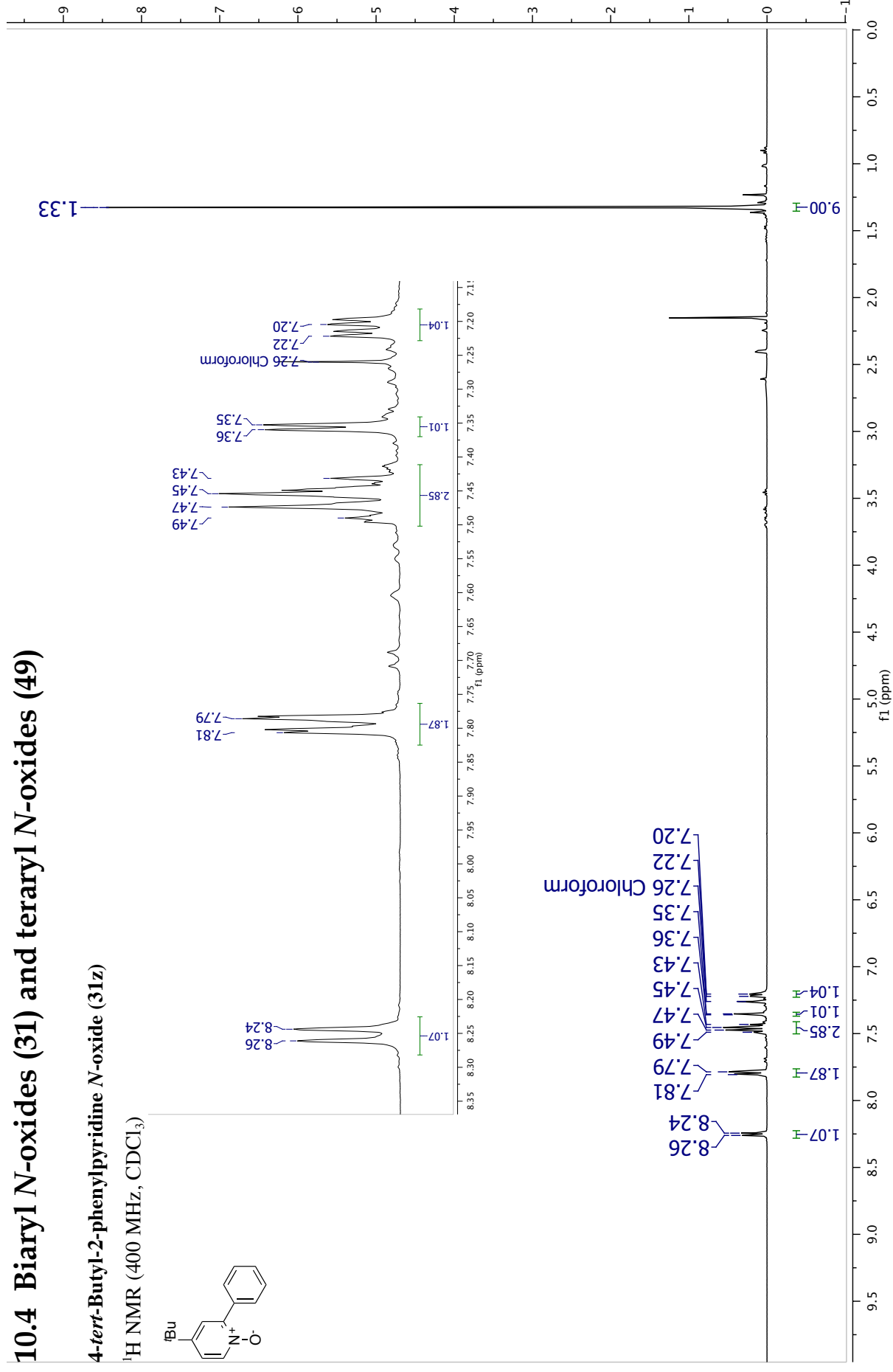
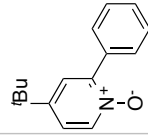
¹³C NMR (101 MHz, CDCl₃)



10.4 Biaryl N-oxides (31) and teraryl N-oxides (49)

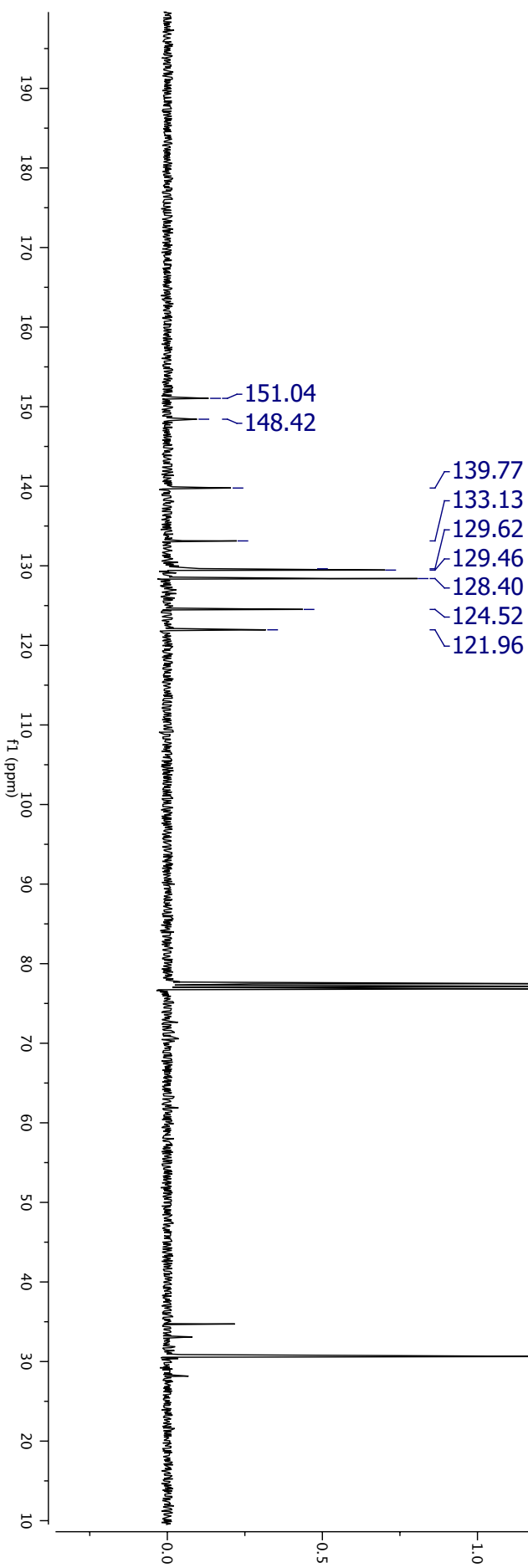
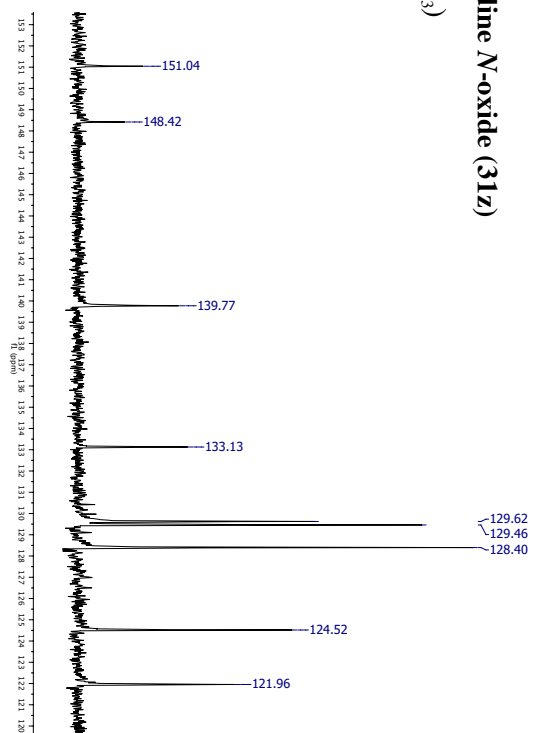
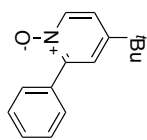
4-*tert*-Butyl-2-phenylpyridine N-oxide (31z)

¹H NMR (400 MHz, CDCl₃)



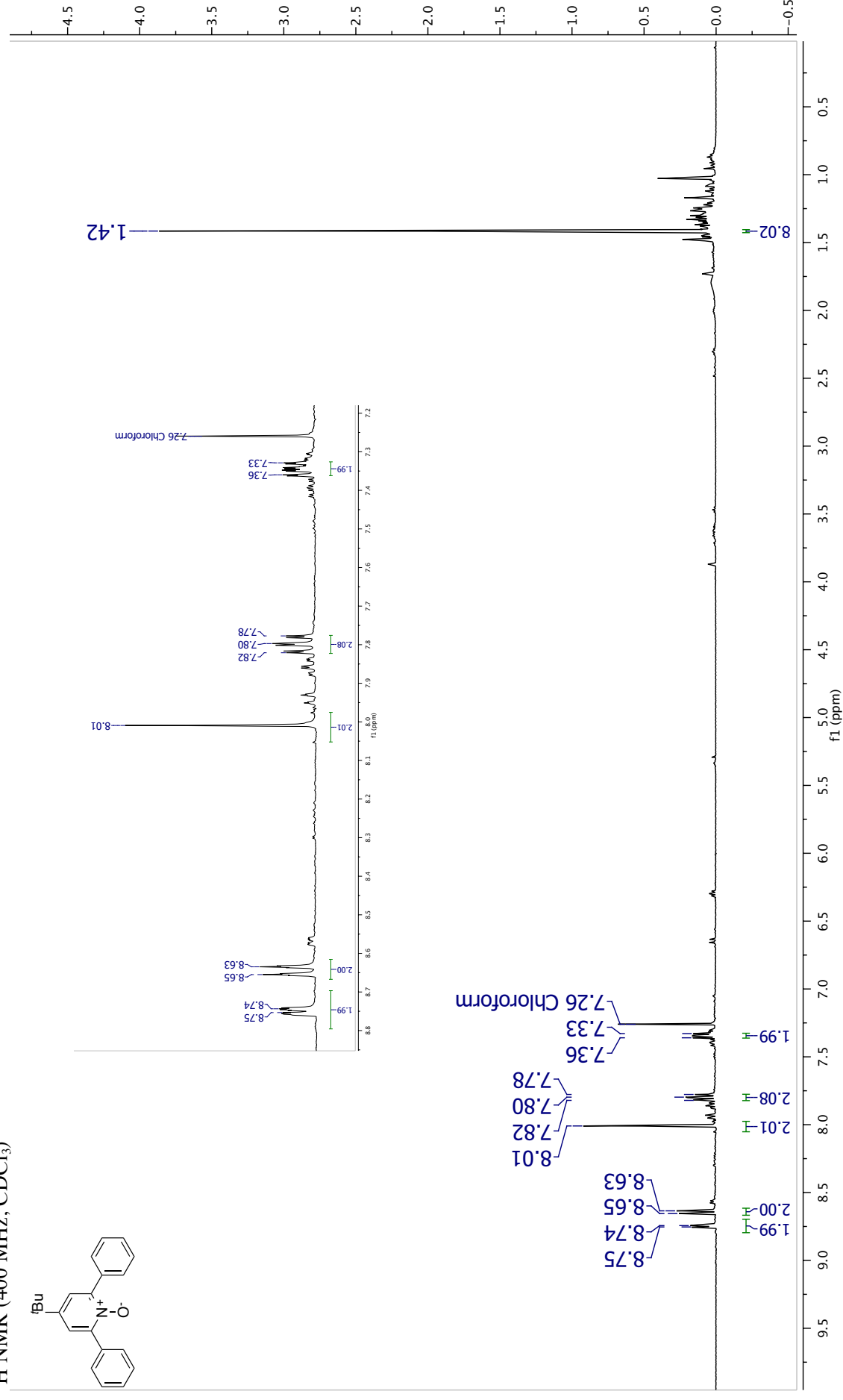
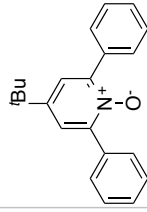
4-*tert*-Butyl-2-phenylpyridine N-oxide (31z)

^{13}C NMR (101 MHz, CDCl_3)



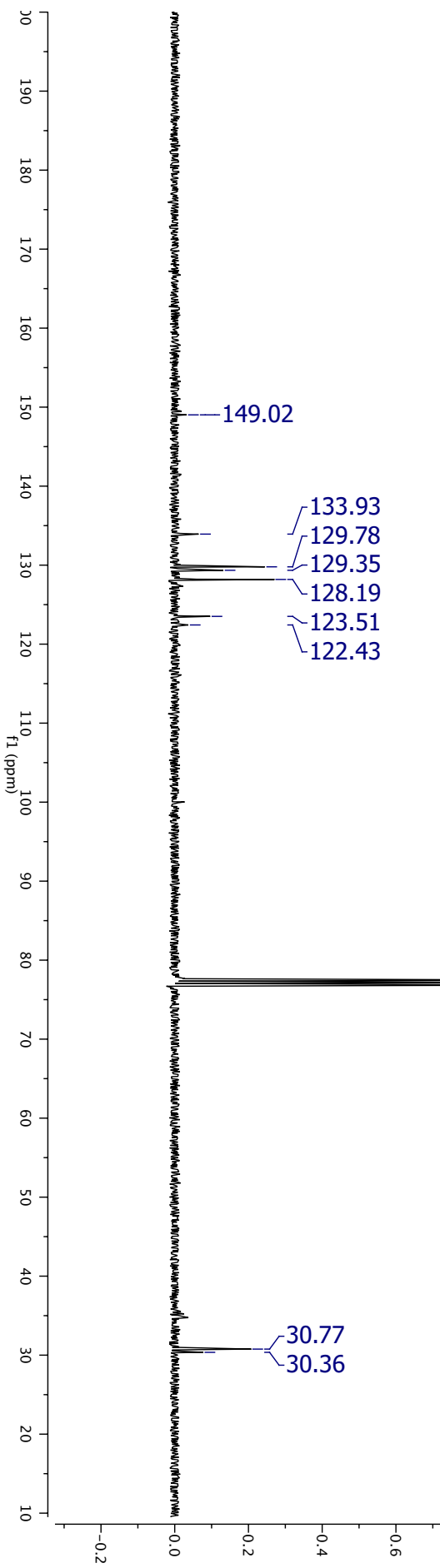
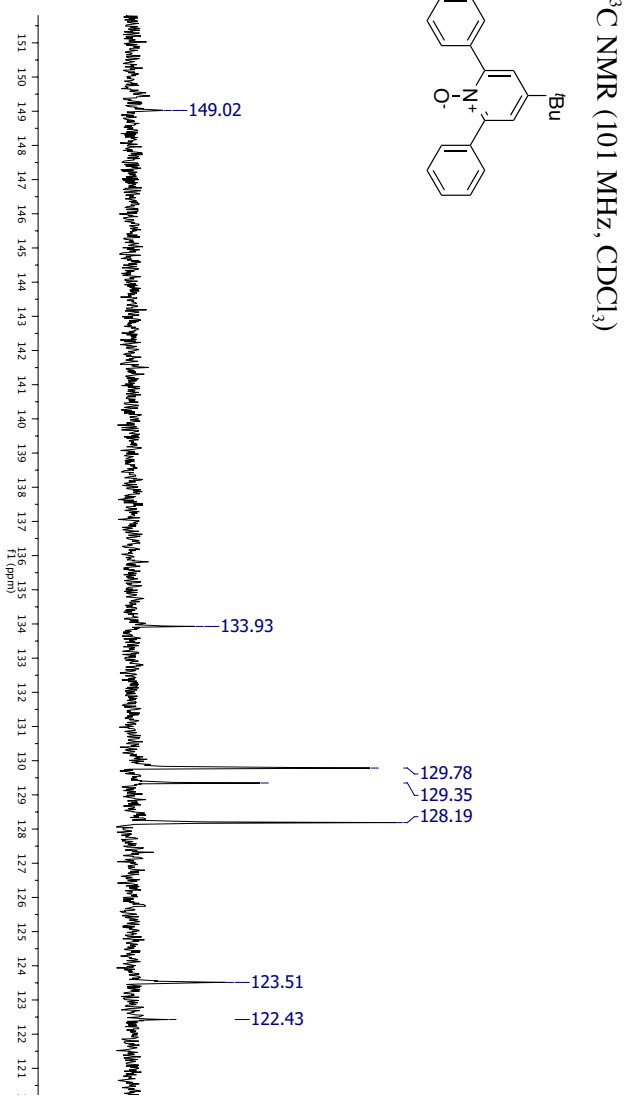
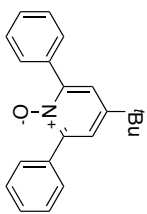
4-*tert*-Butyl-2,6-phenylpyridine N-oxide (49z)

¹H NMR (400 MHz, CDCl₃)



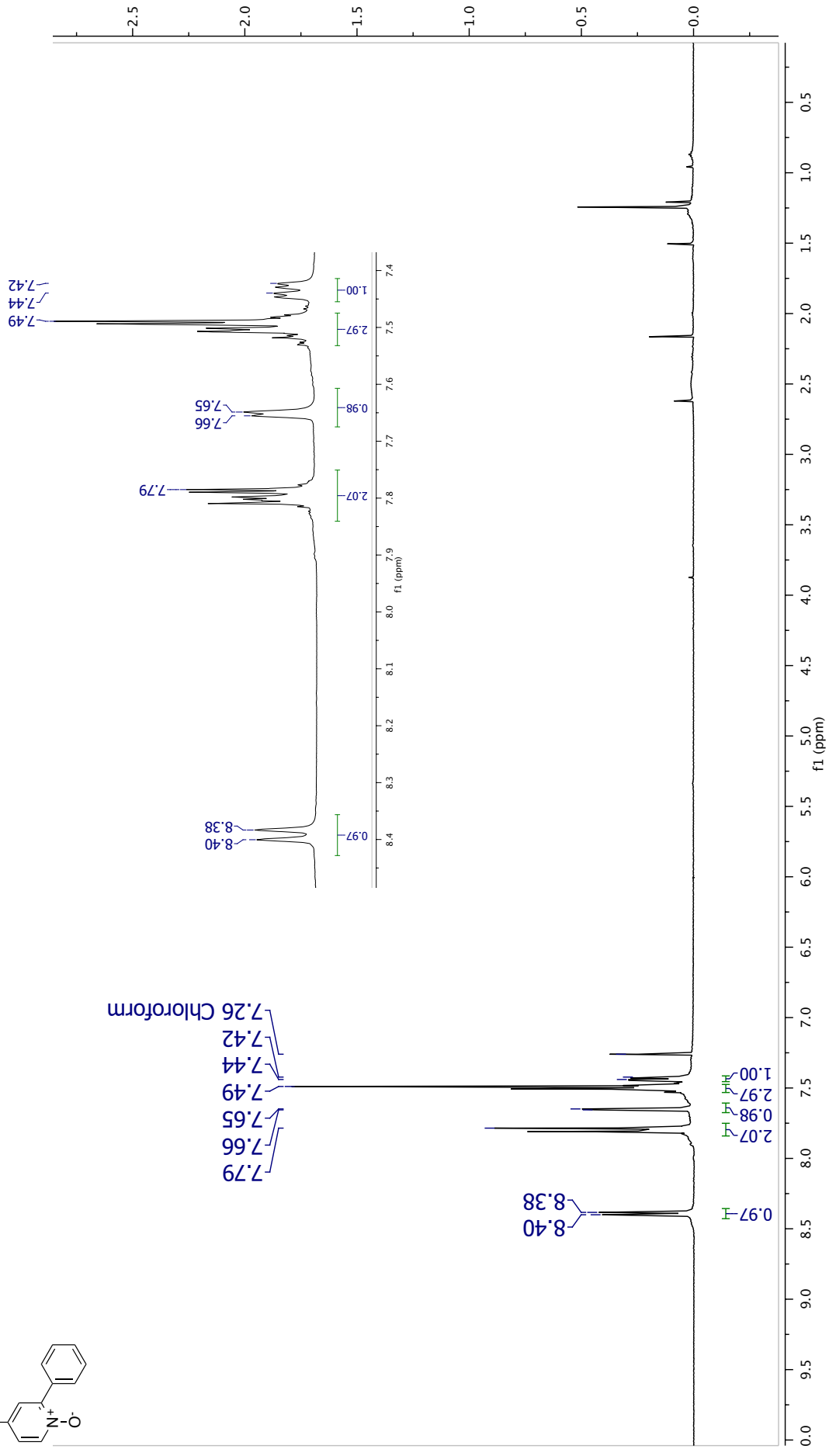
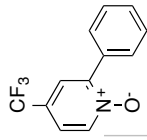
4-*tert*-Butyl-2,6-phenylpyridine N-oxide (49z)

¹³C NMR (101 MHz, CDCl₃)



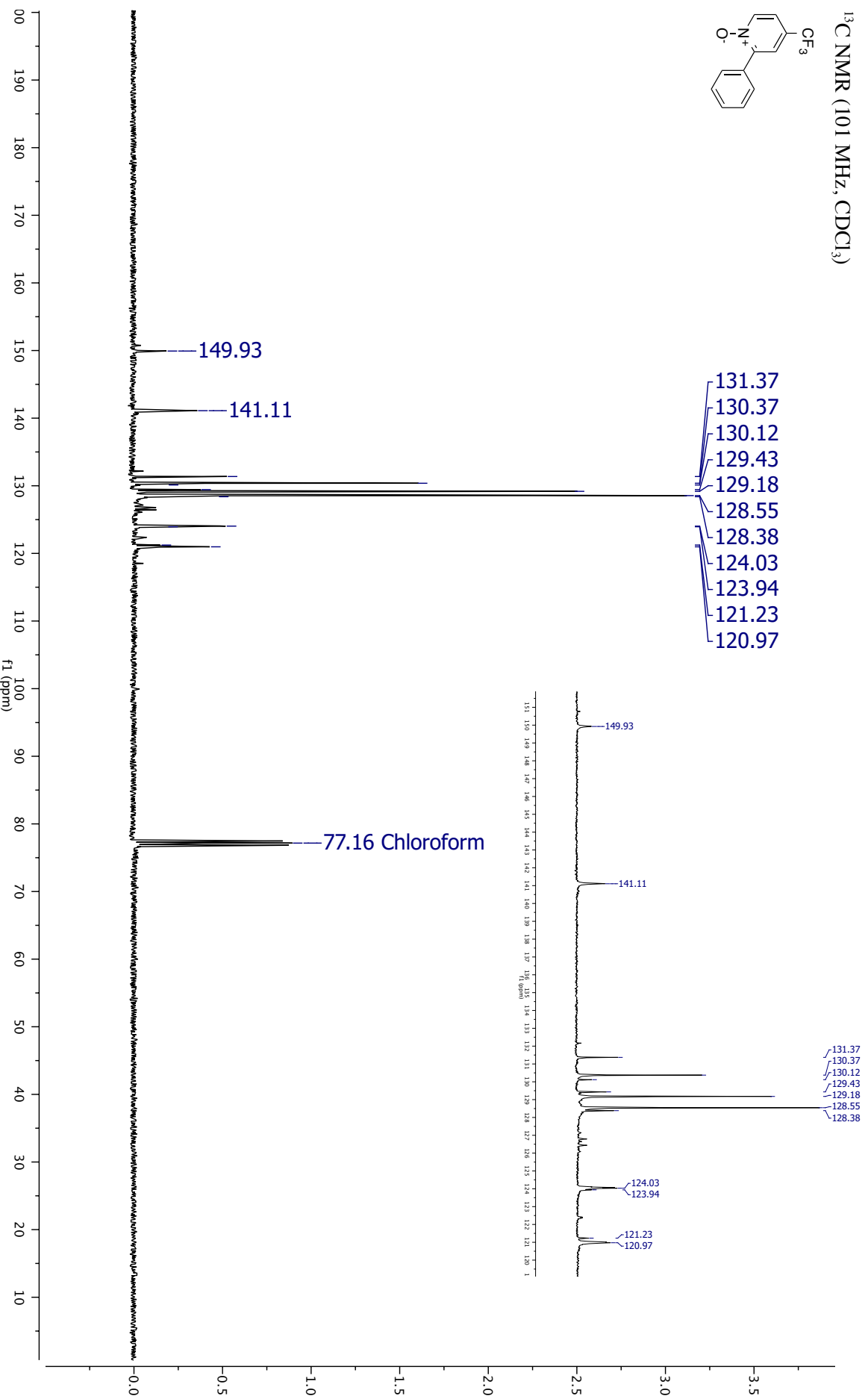
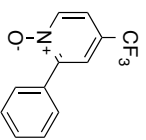
4-(Trifluoromethyl)-2-phenylpyridine N-oxide (31m)

¹H NMR (400 MHz, CDCl₃)



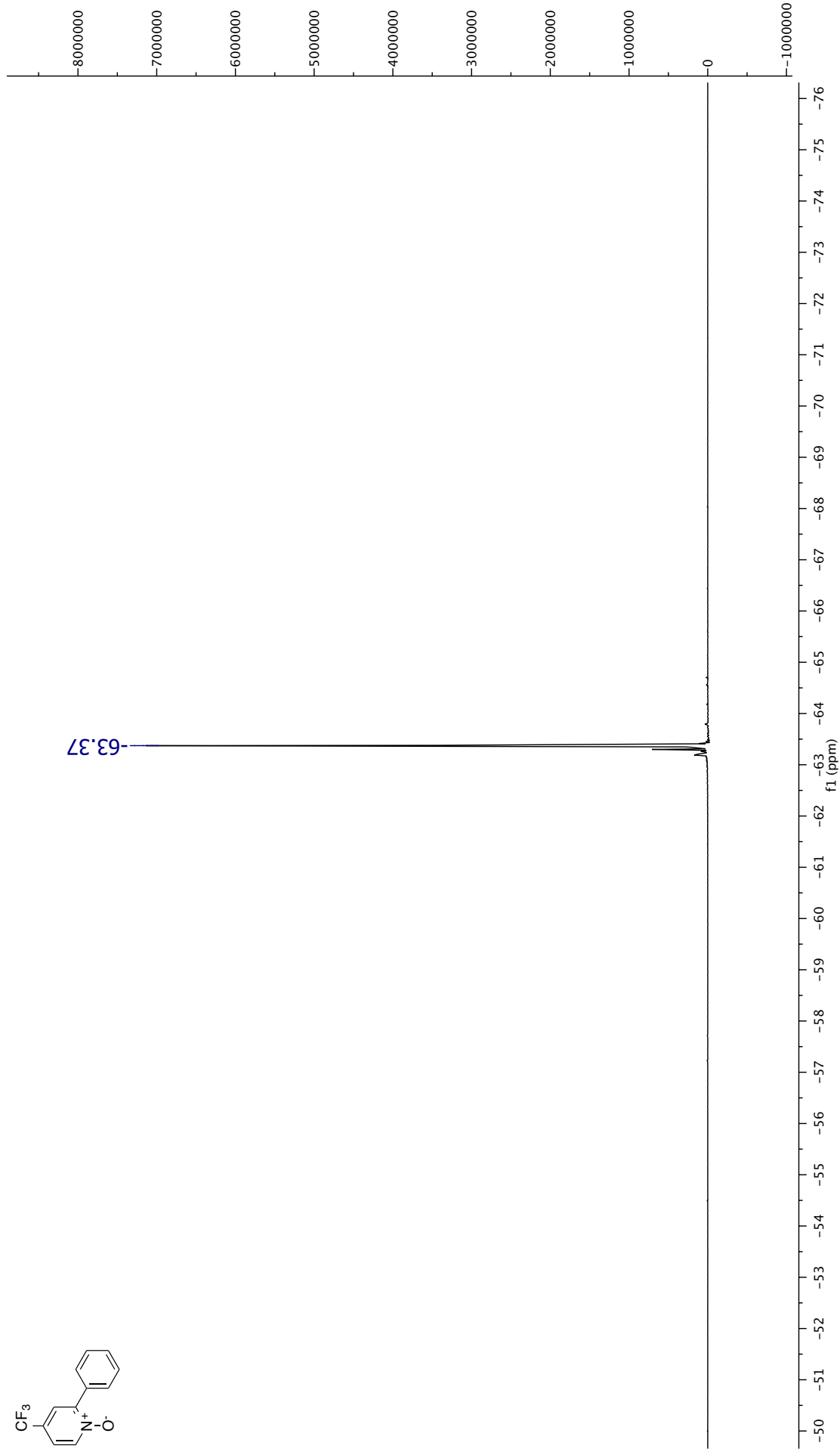
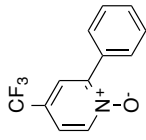
4-(Trifluoromethyl)-2-phenylpyridine N-oxide (3Im)

¹³C NMR (101 MHz, CDCl₃)



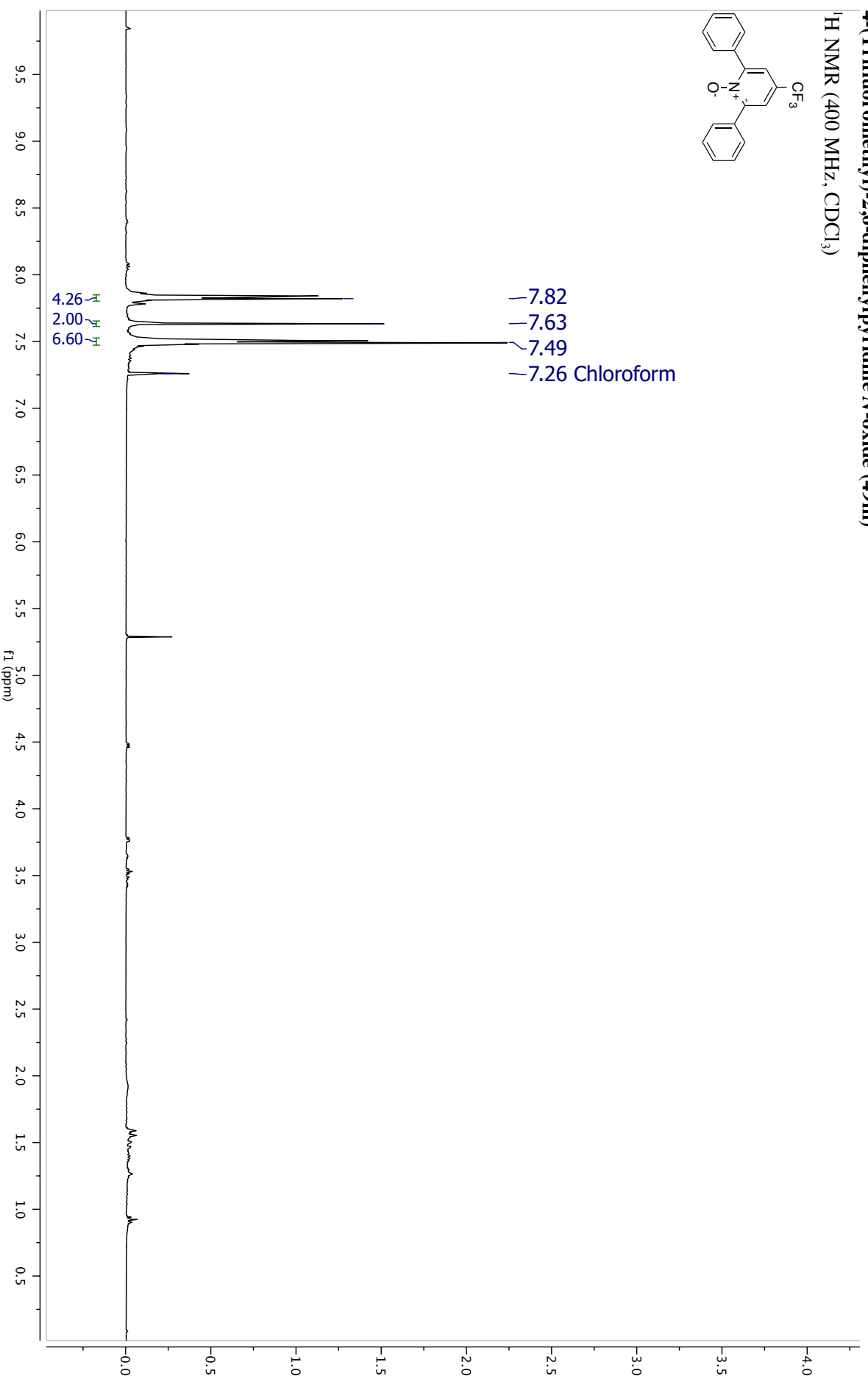
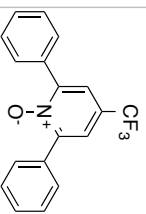
4-(Trifluoromethyl)-2-phenylpyridine N-oxide (31m)

¹⁹F NMR (471 MHz, CDCl₃)



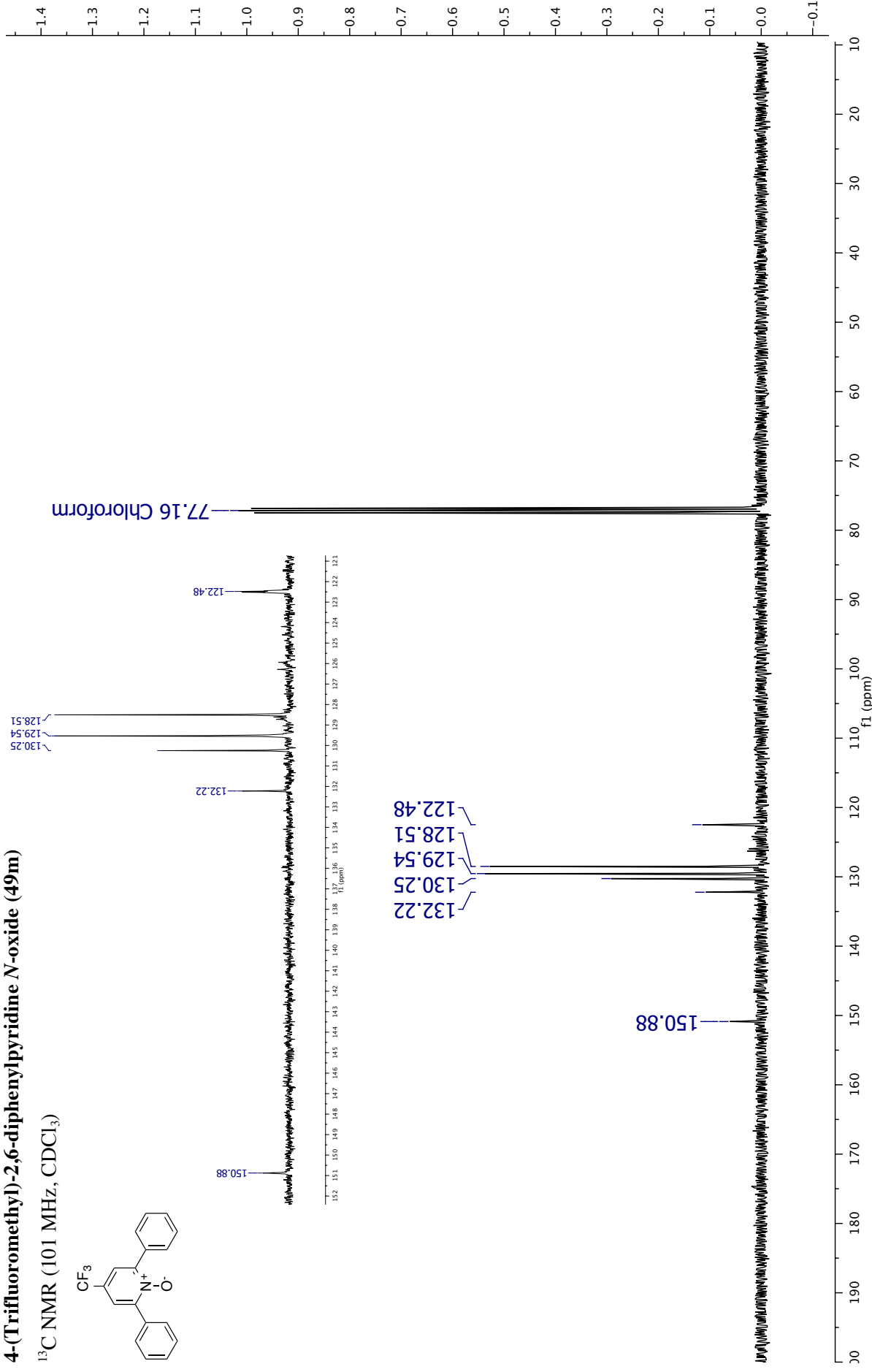
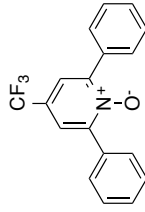
4-(Trifluoromethyl)-2,6-diphenylpyridine N-oxide (49m)

¹H NMR (400 MHz, CDCl₃)



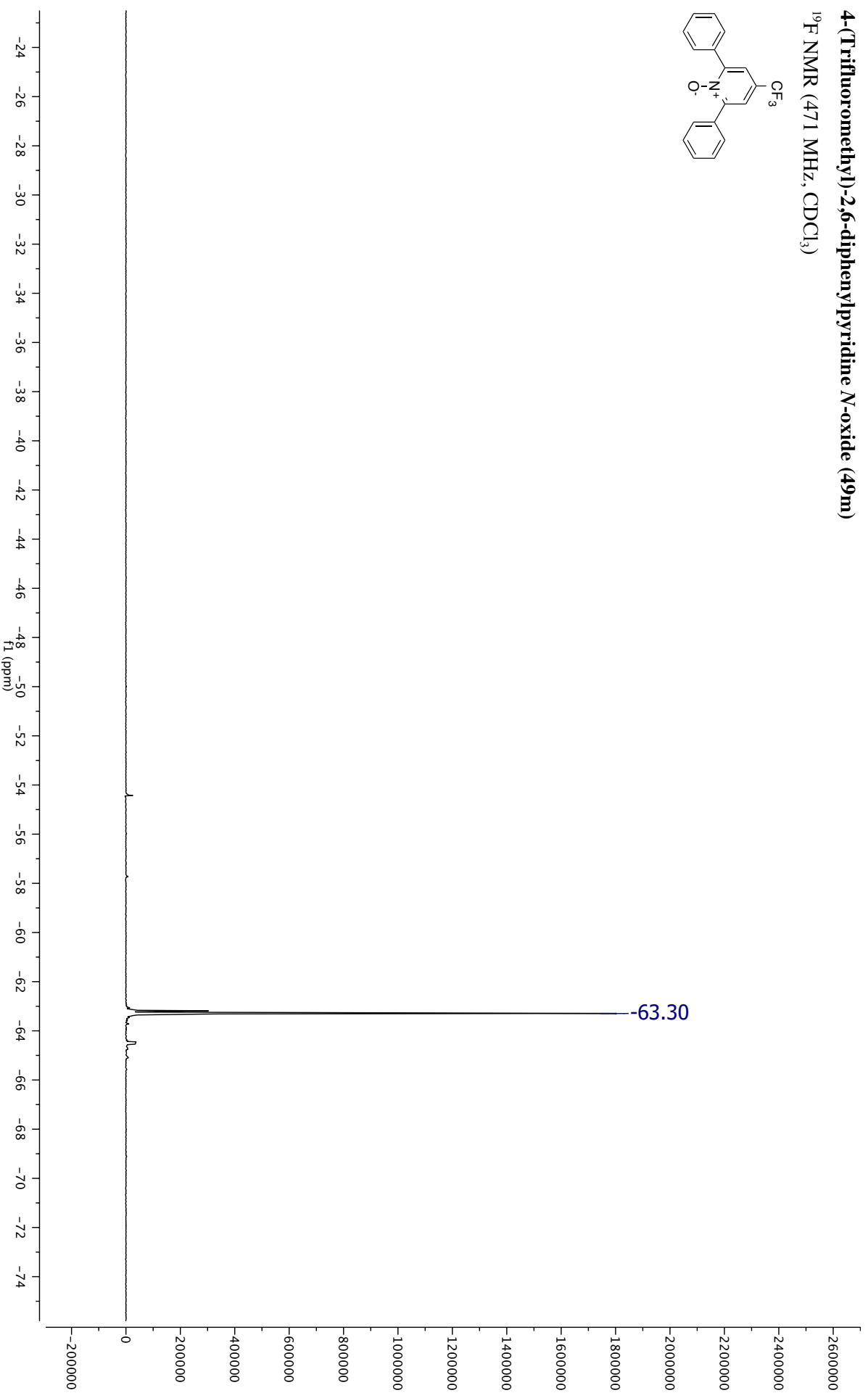
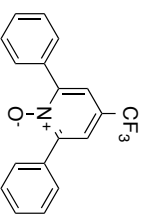
4-(Trifluoromethyl)-2,6-diphenylpyridine N-oxide (49m)

¹³C NMR (101 MHz, CDCl₃)



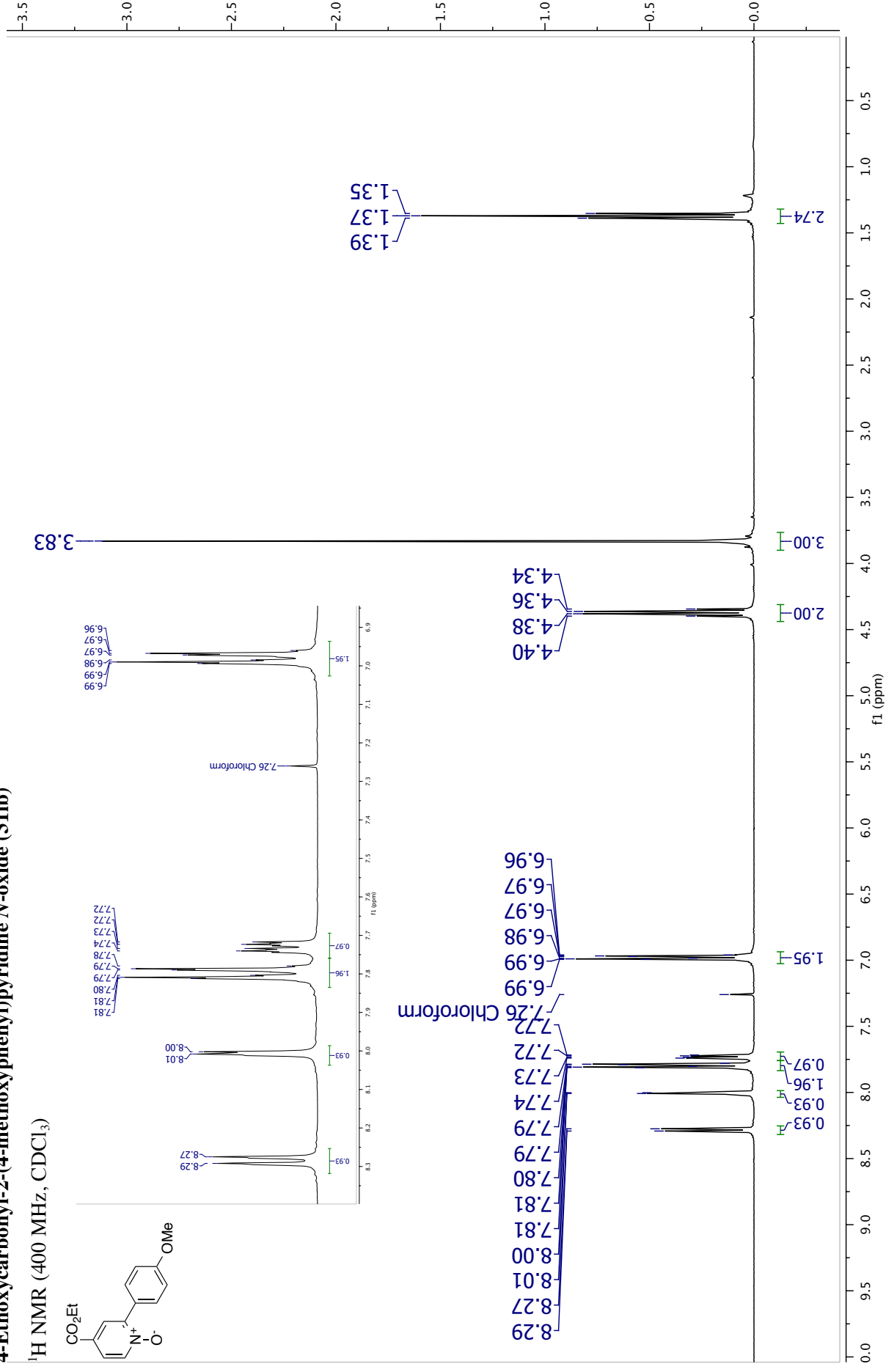
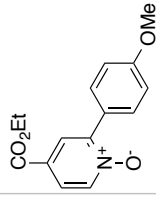
4-(Trifluoromethyl)-2,6-diphenylpyridine N-oxide (49m)

¹⁹F NMR (471 MHz, CDCl₃)



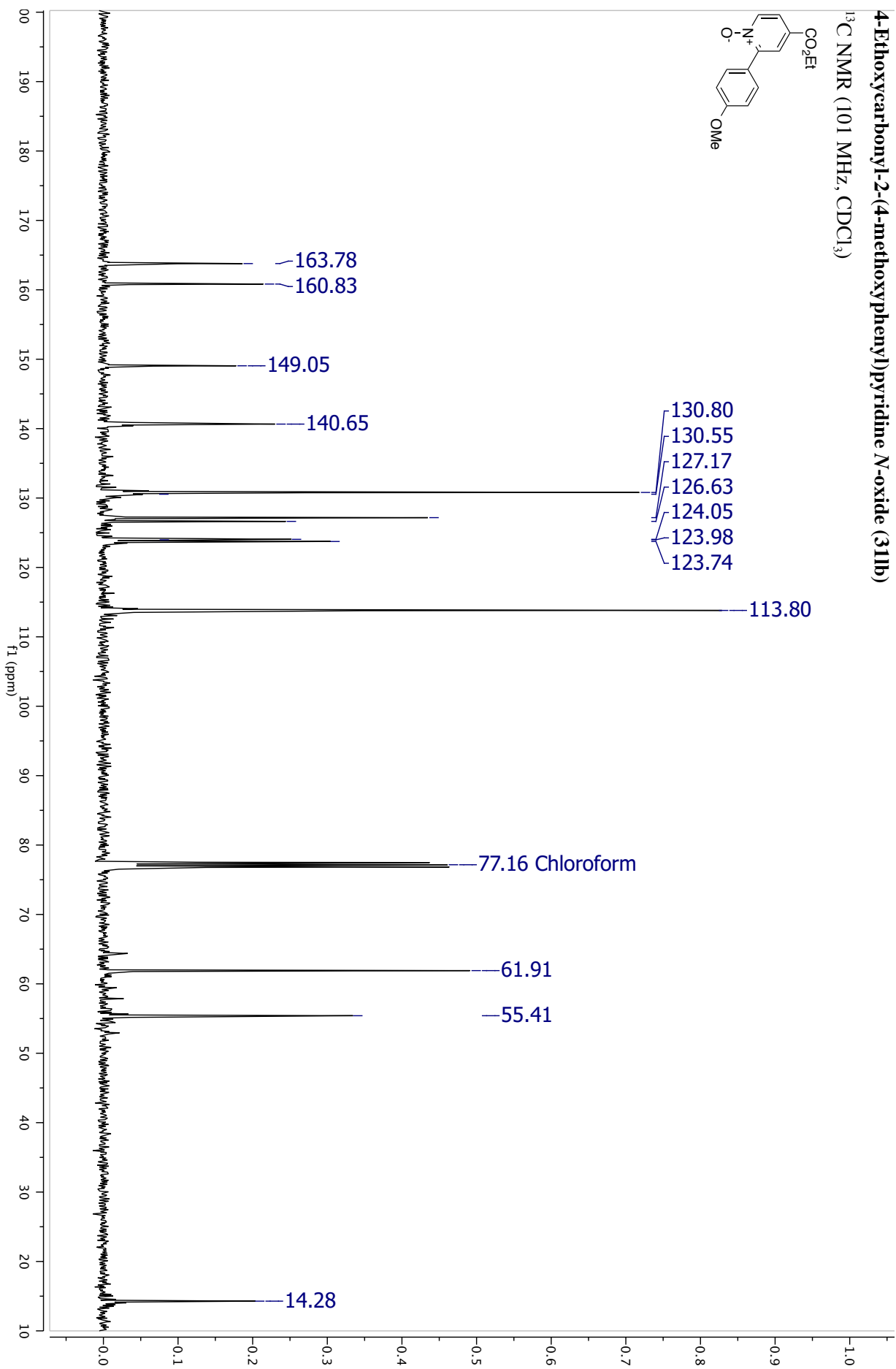
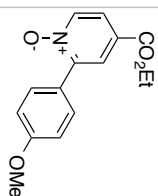
4-Ethoxycarbonyl-2-(4-methoxyphenyl)pyridine N-oxide (311b)

¹H NMR (400 MHz, CDCl₃)



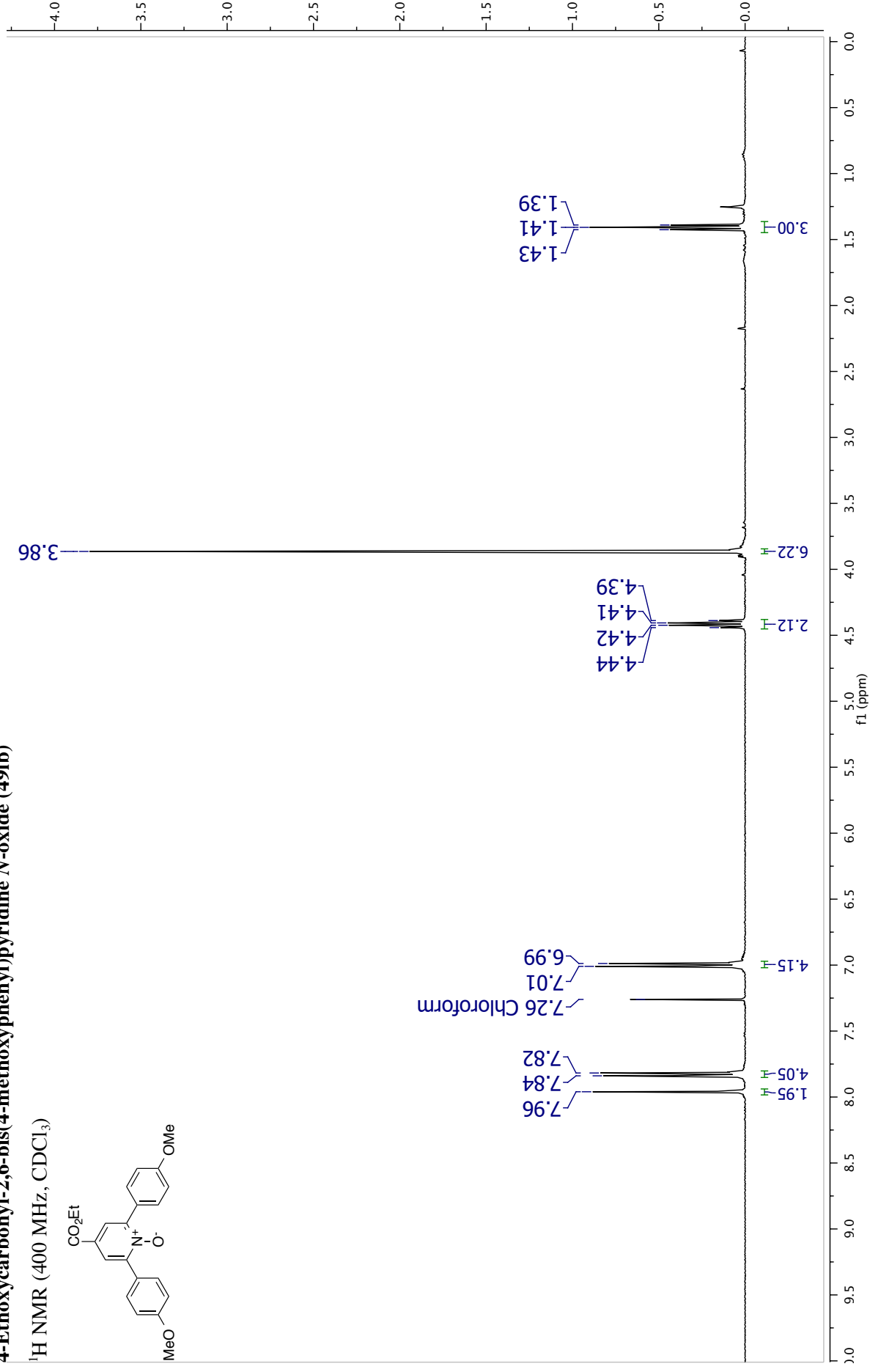
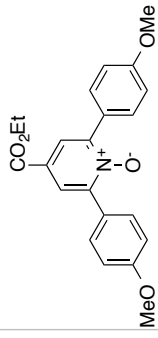
4-Ethoxycarbonyl-2-(4-methoxyphenyl)pyridine N-oxide (311b)

¹³C NMR (101 MHz, CDCl₃)



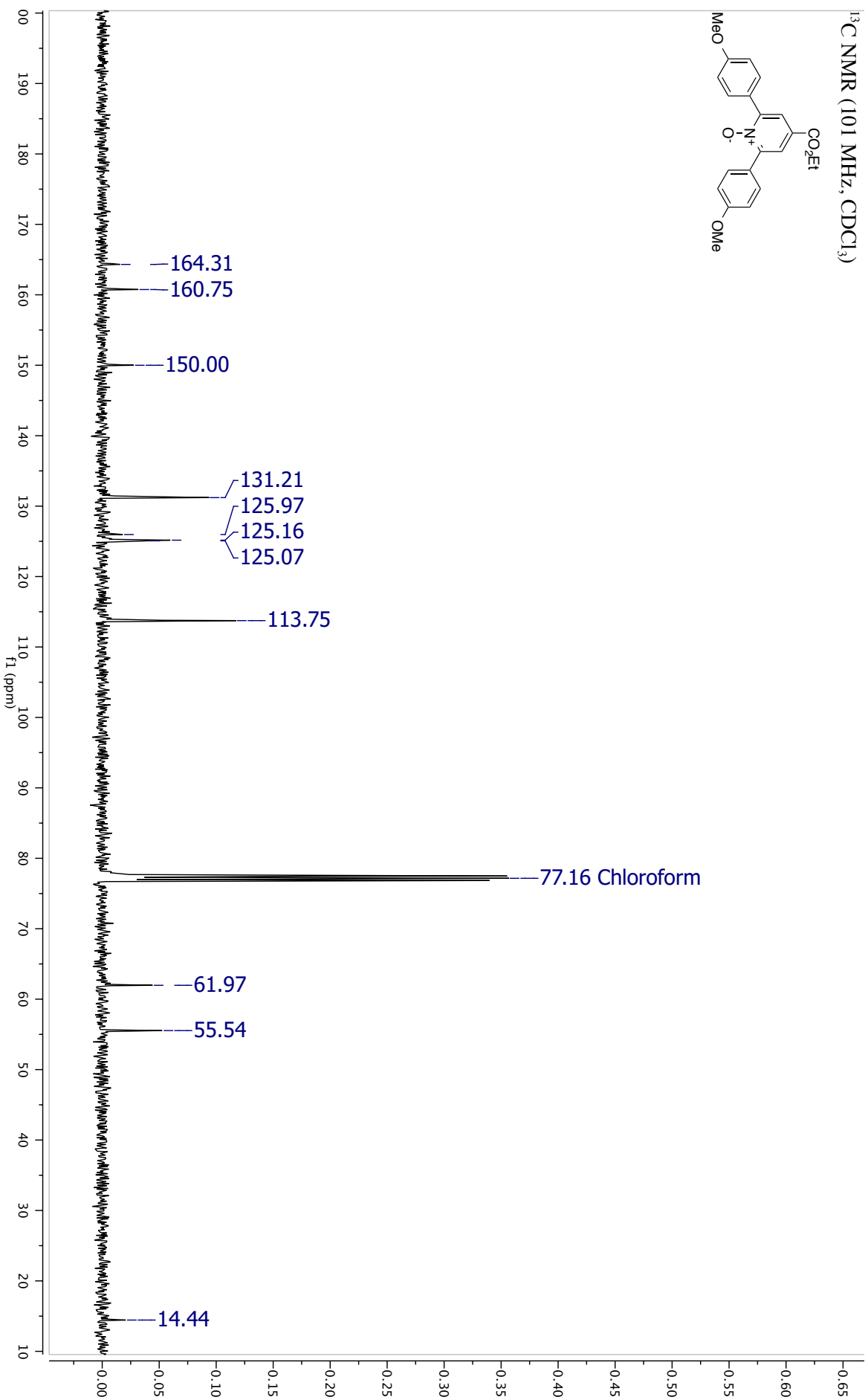
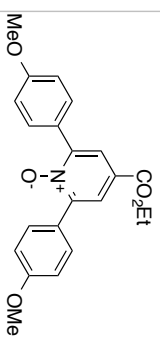
4-Ethoxycarbonyl-2,6-bis(4-methoxyphenyl)pyridine N-oxide (491b)

¹H NMR (400 MHz, CDCl₃)



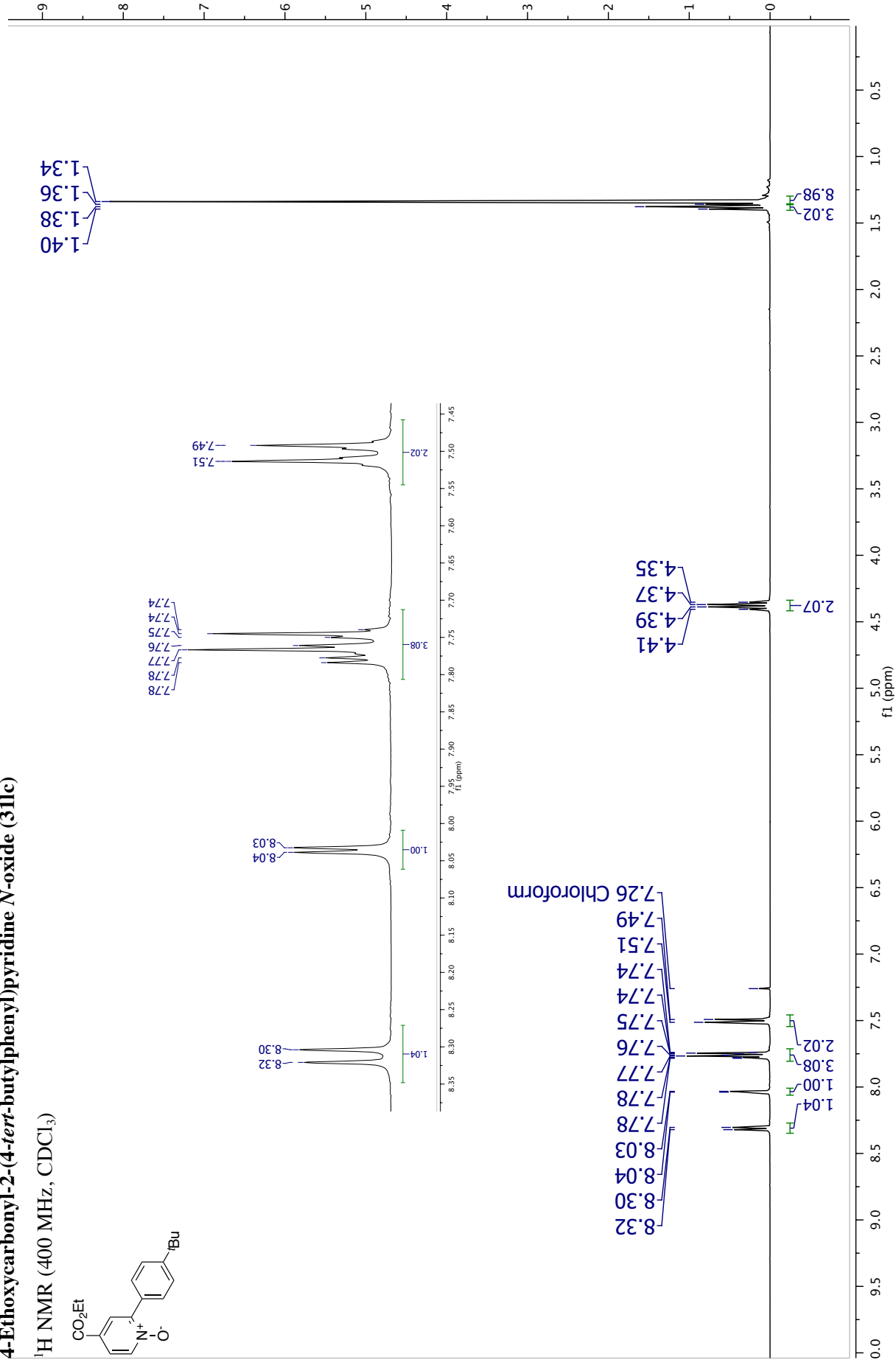
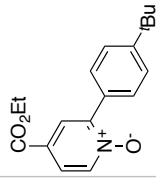
4-Ethoxycarbonyl-2,6-bis(4-methoxyphenyl)pyridine N-oxide (491b)

¹³C NMR (101 MHz, CDCl₃)



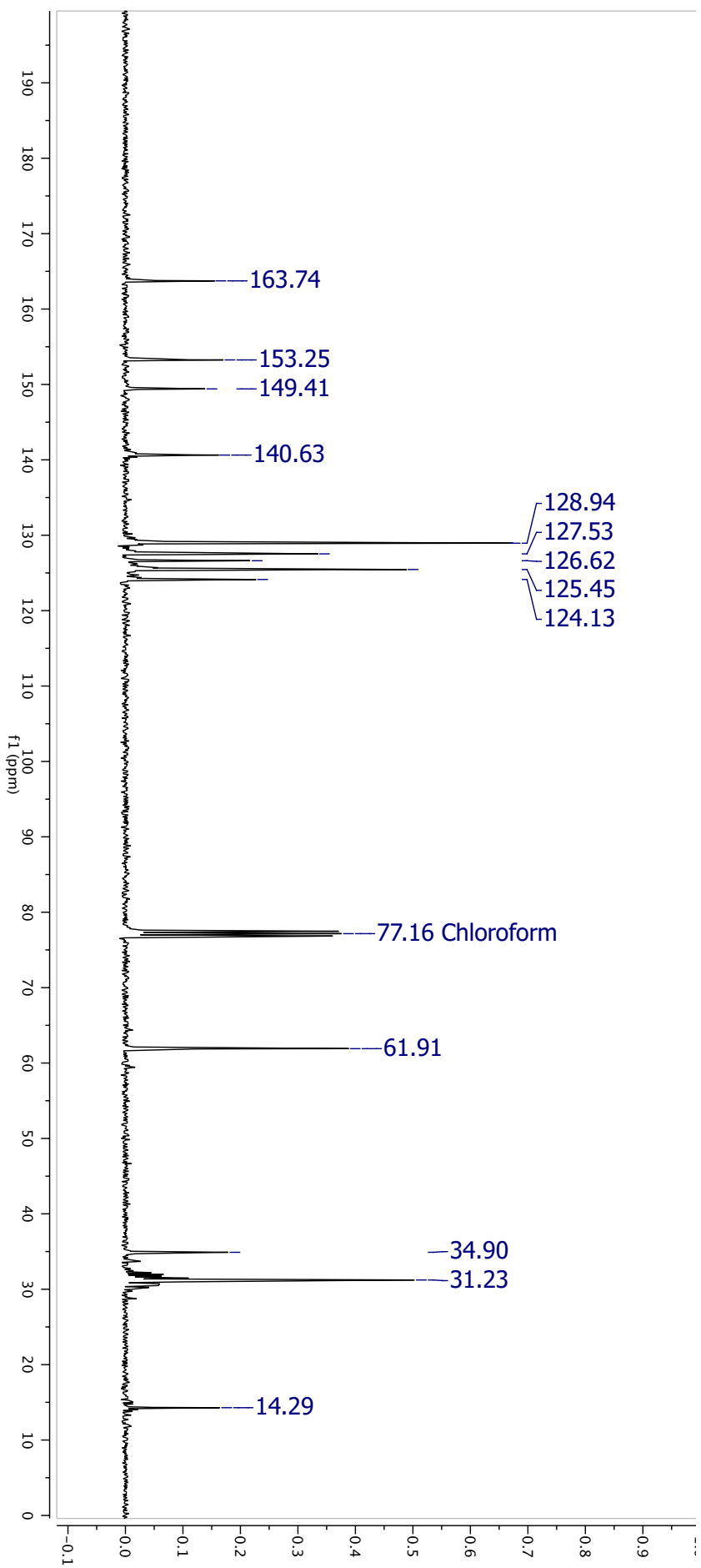
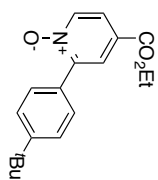
4-Ethoxycarbonyl-2-(4-*tert*-butylphenyl)pyridine *N*-oxide (311c)

¹H NMR (400 MHz, CDCl₃)



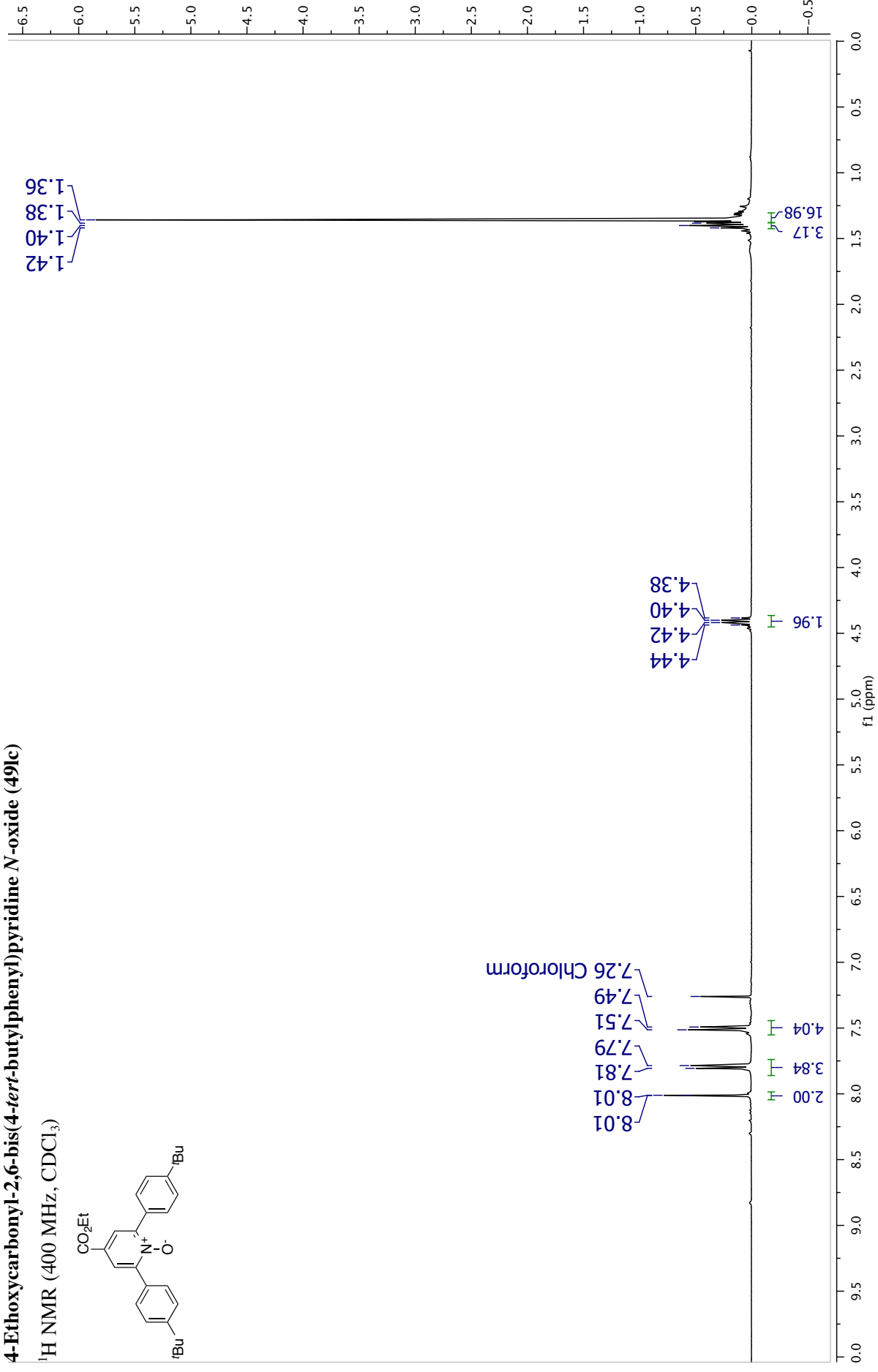
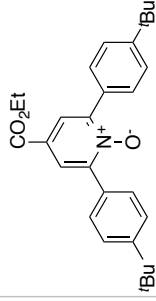
4-Ethoxycarbonyl-2-(4-*tert*-butylphenyl)pyridine N-oxide (311c)

¹³C NMR (101 MHz, CDCl₃)



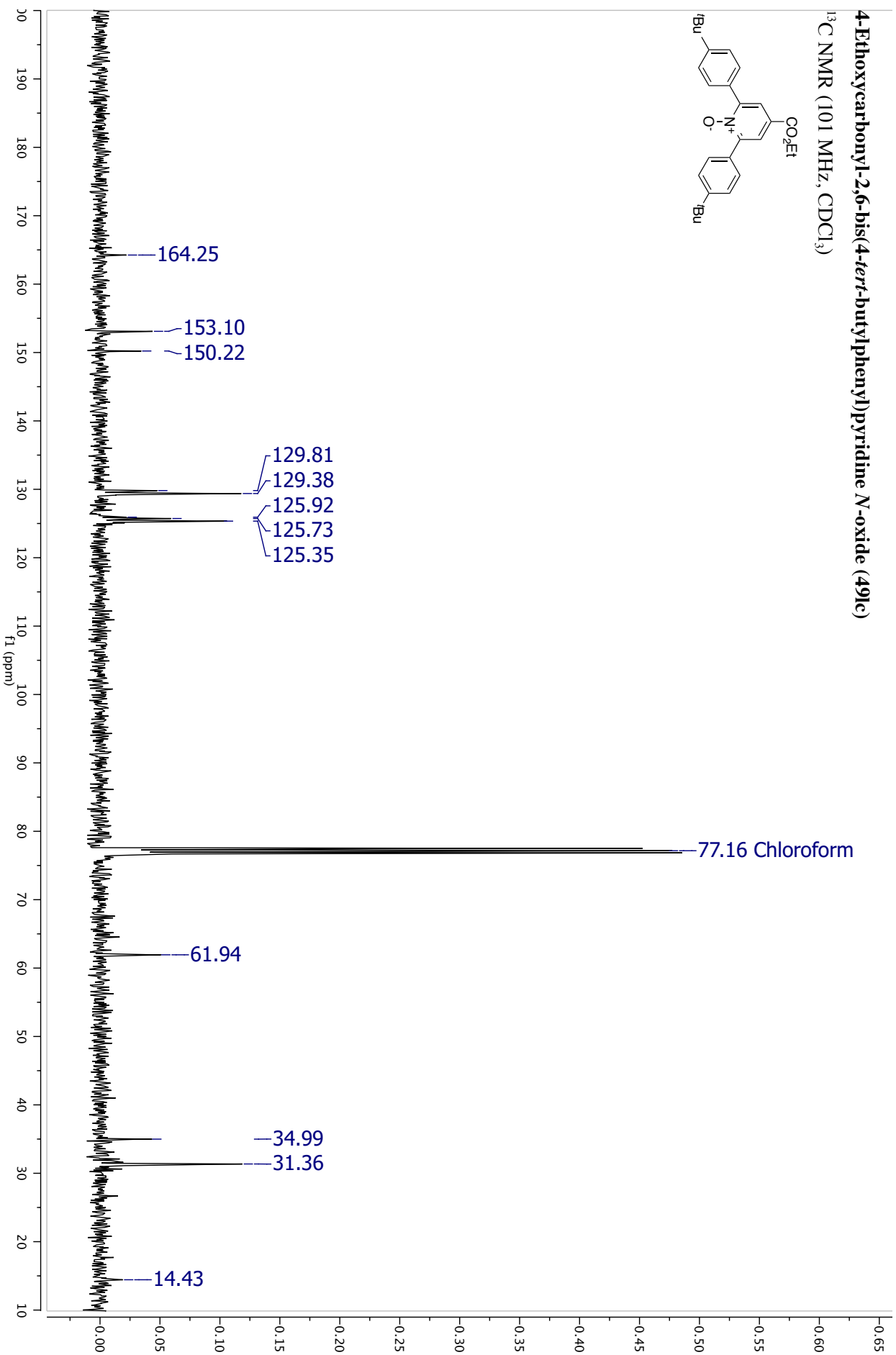
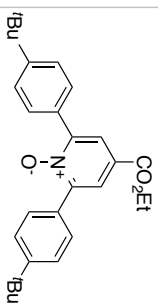
4-Ethoxycarbonyl-2,6-bis(4-*tert*-butylphenyl)pyridine N-oxide (49Ic)

¹H NMR (400 MHz, CDCl₃)



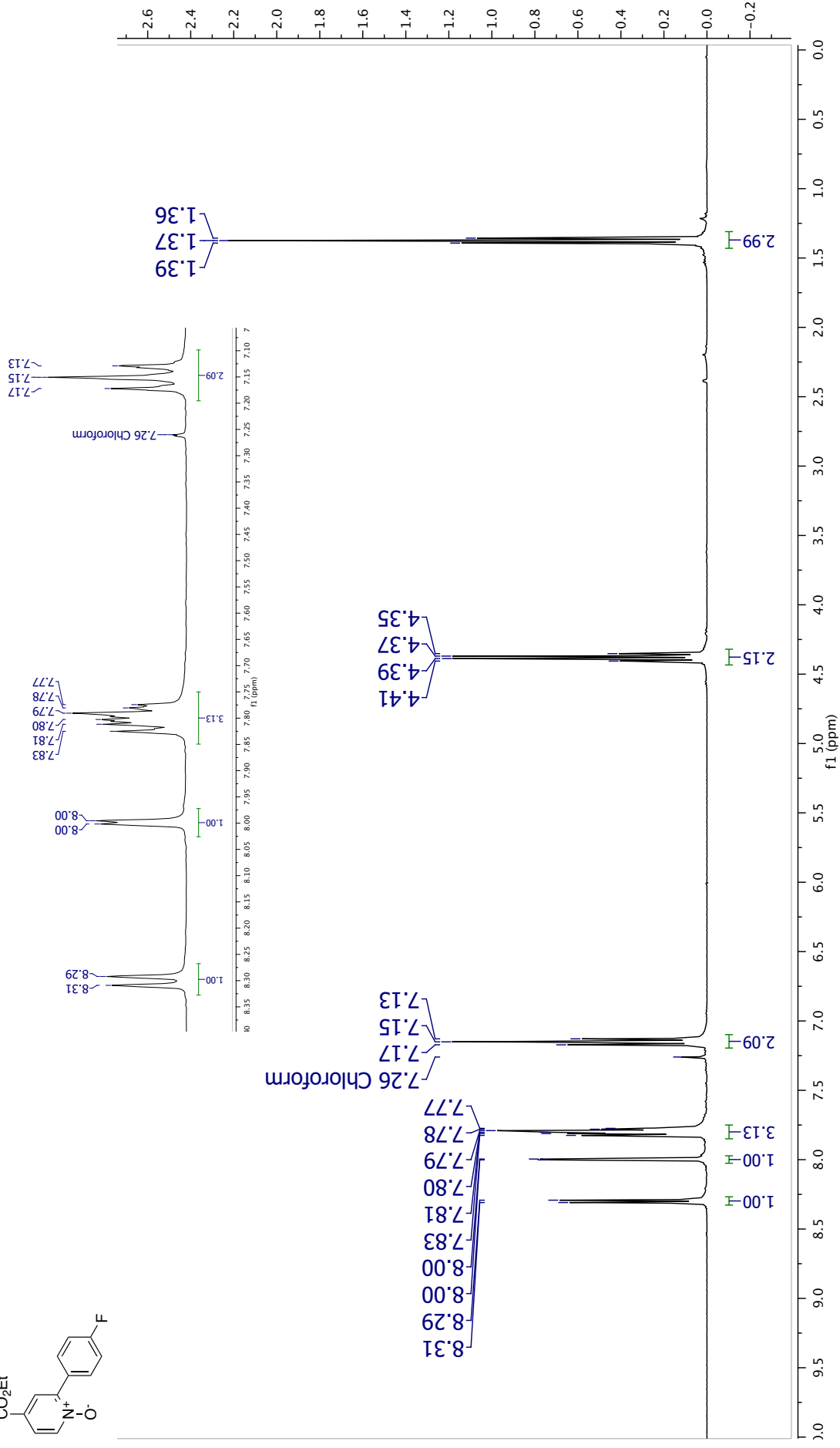
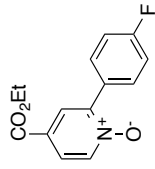
4-Ethoxycarbonyl-2,6-bis(4-*tert*-butylphenyl)pyridine N-oxide (49lc)

¹³C NMR (101 MHz, CDCl₃)



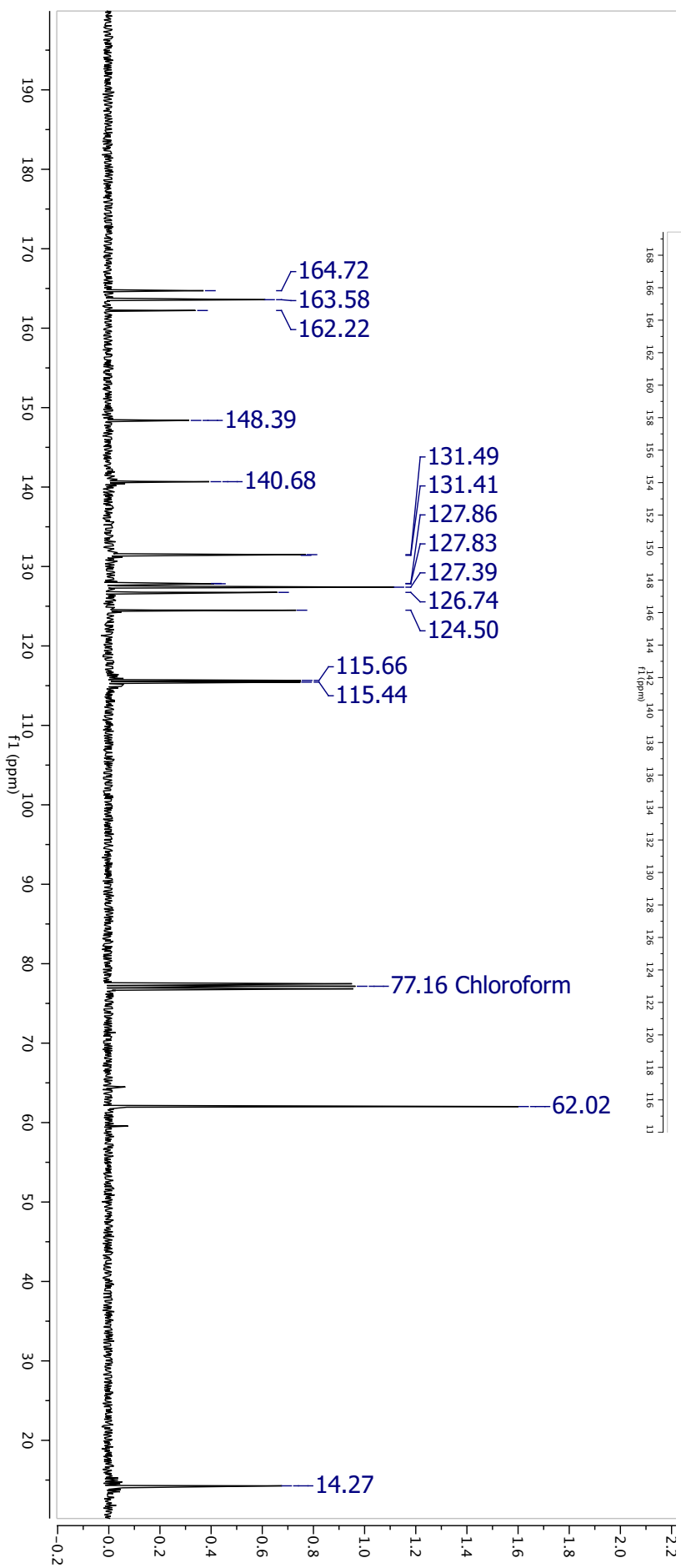
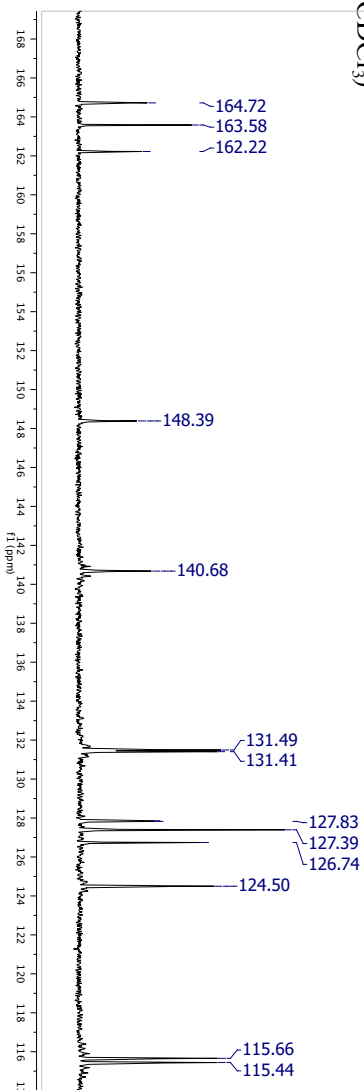
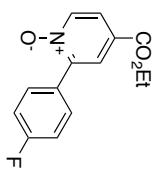
4-Ethoxycarbonyl-2-(4-fluorophenyl)pyridine N-oxide (311d)

¹H NMR (400 MHz, CDCl₃)



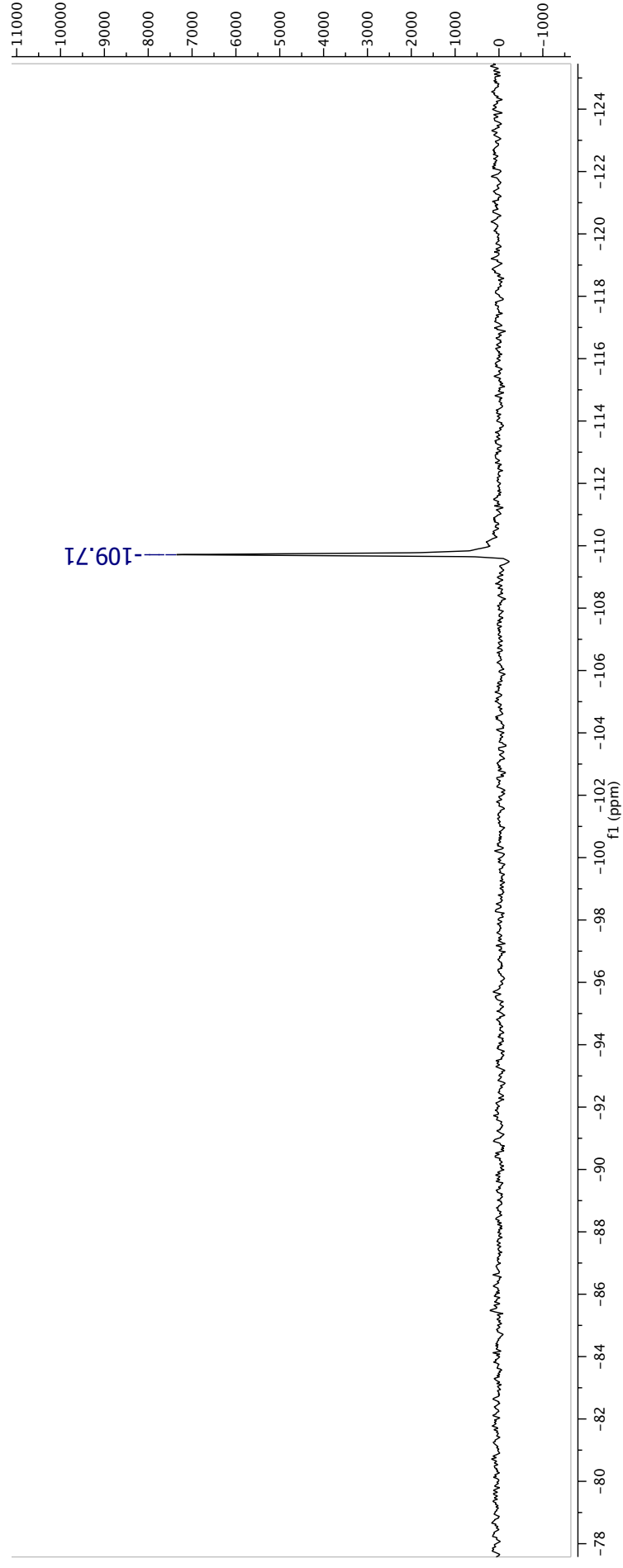
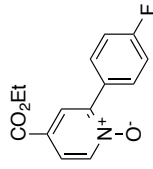
4-Ethoxycarbonyl-2-(4-fluorophenyl)pyridine N-oxide (311d)

¹³C NMR (101 MHz, CDCl₃)



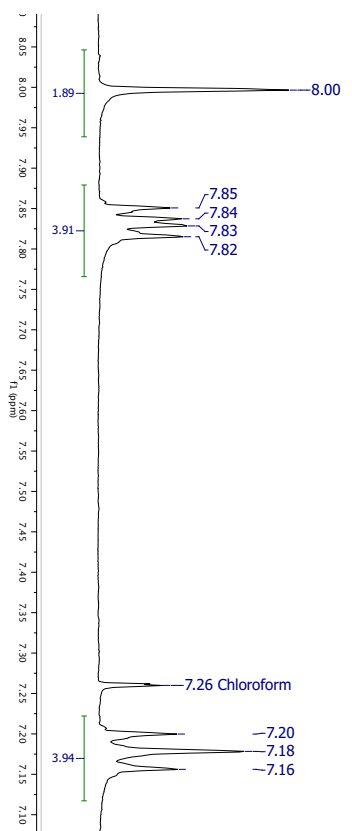
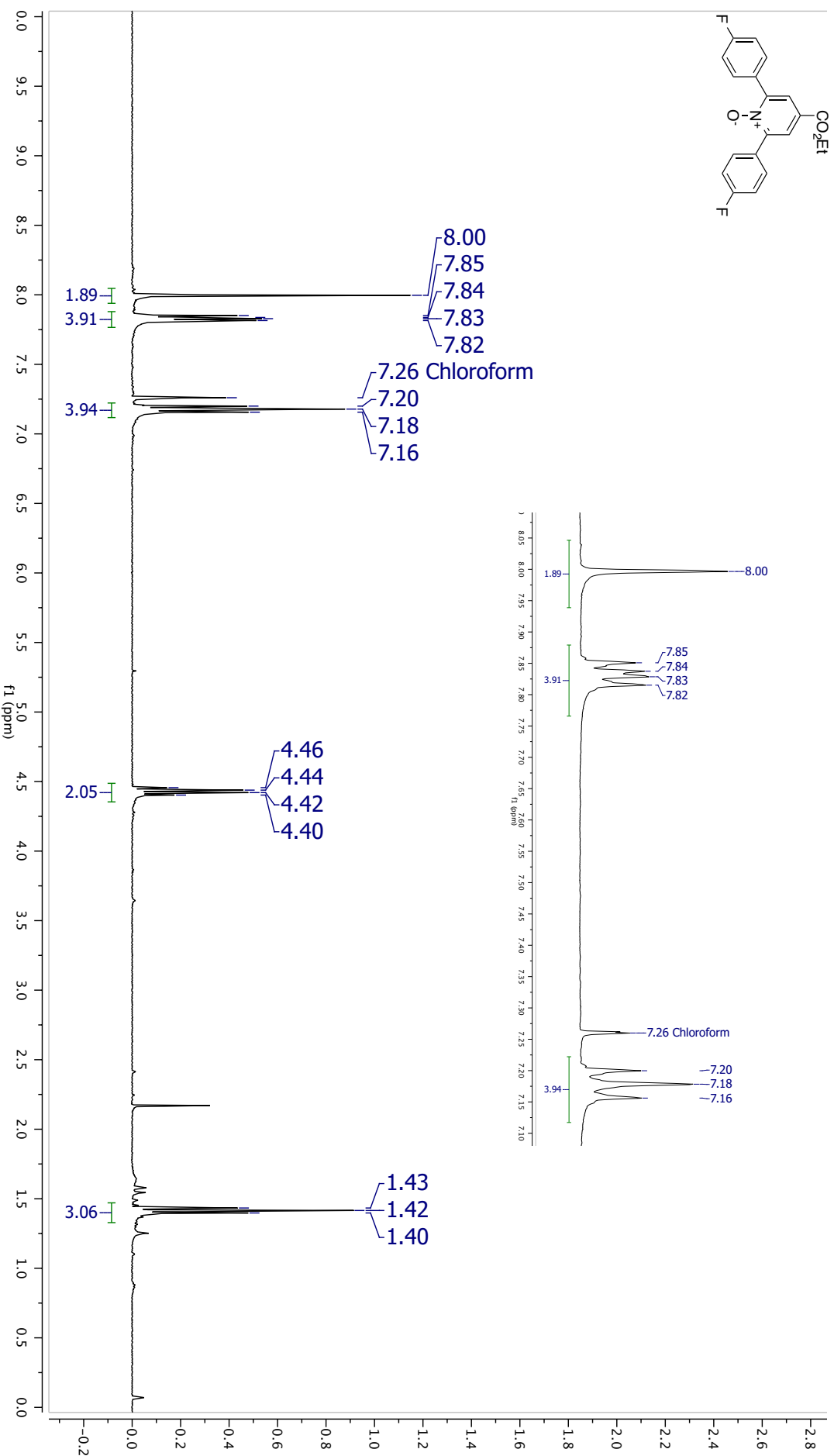
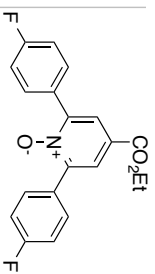
4-Ethoxycarbonyl-2-(4-fluorophenyl)pyridine N-oxide (311d)

¹⁹F NMR (471 MHz, CDCl₃)



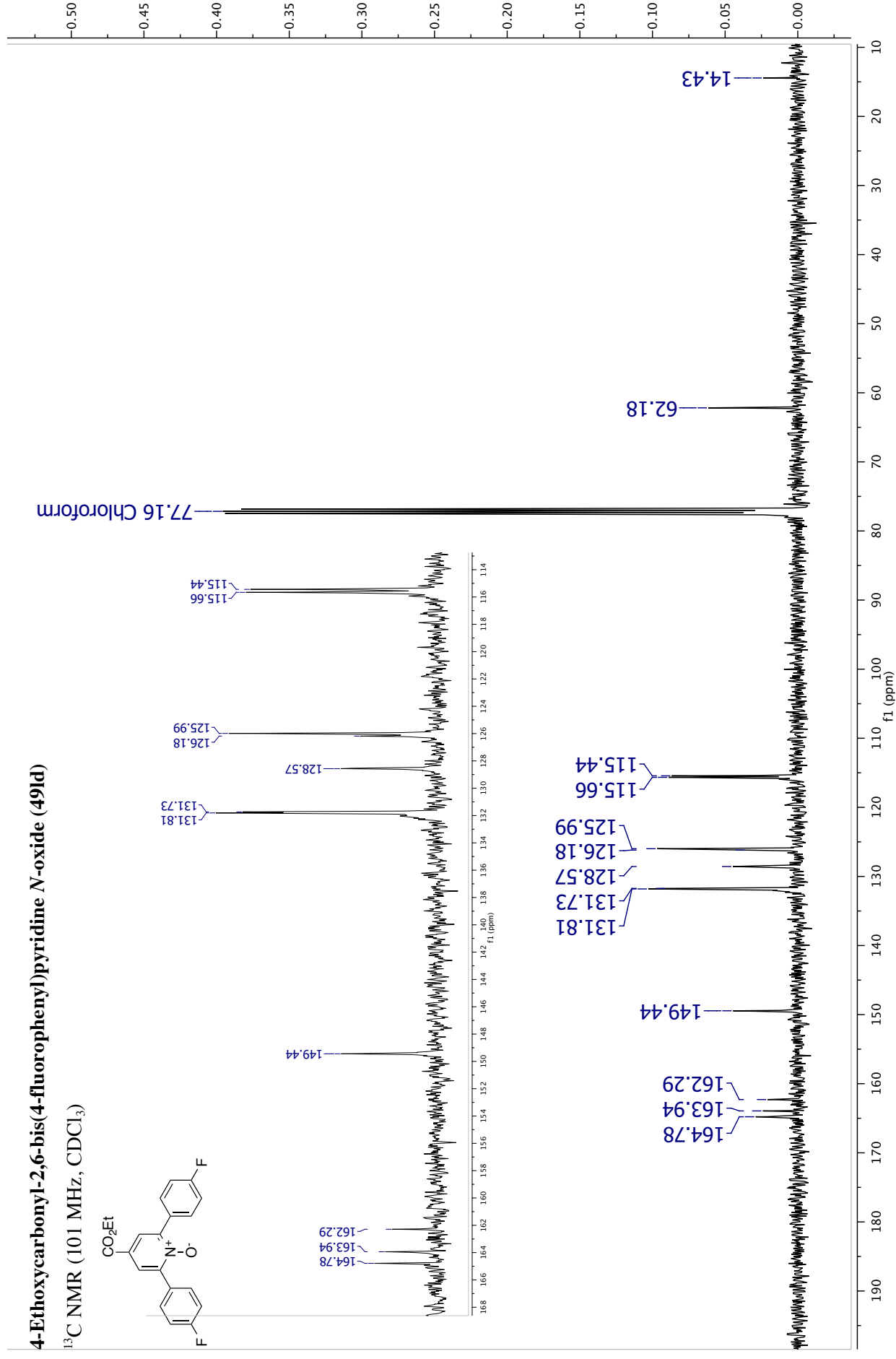
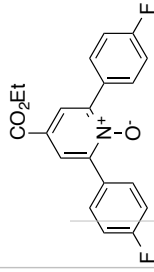
4-Ethoxycarbonyl-2,6-bis(4-fluorophenyl)pyridine N-oxide (491d)

¹H NMR (400 MHz, CDCl₃)



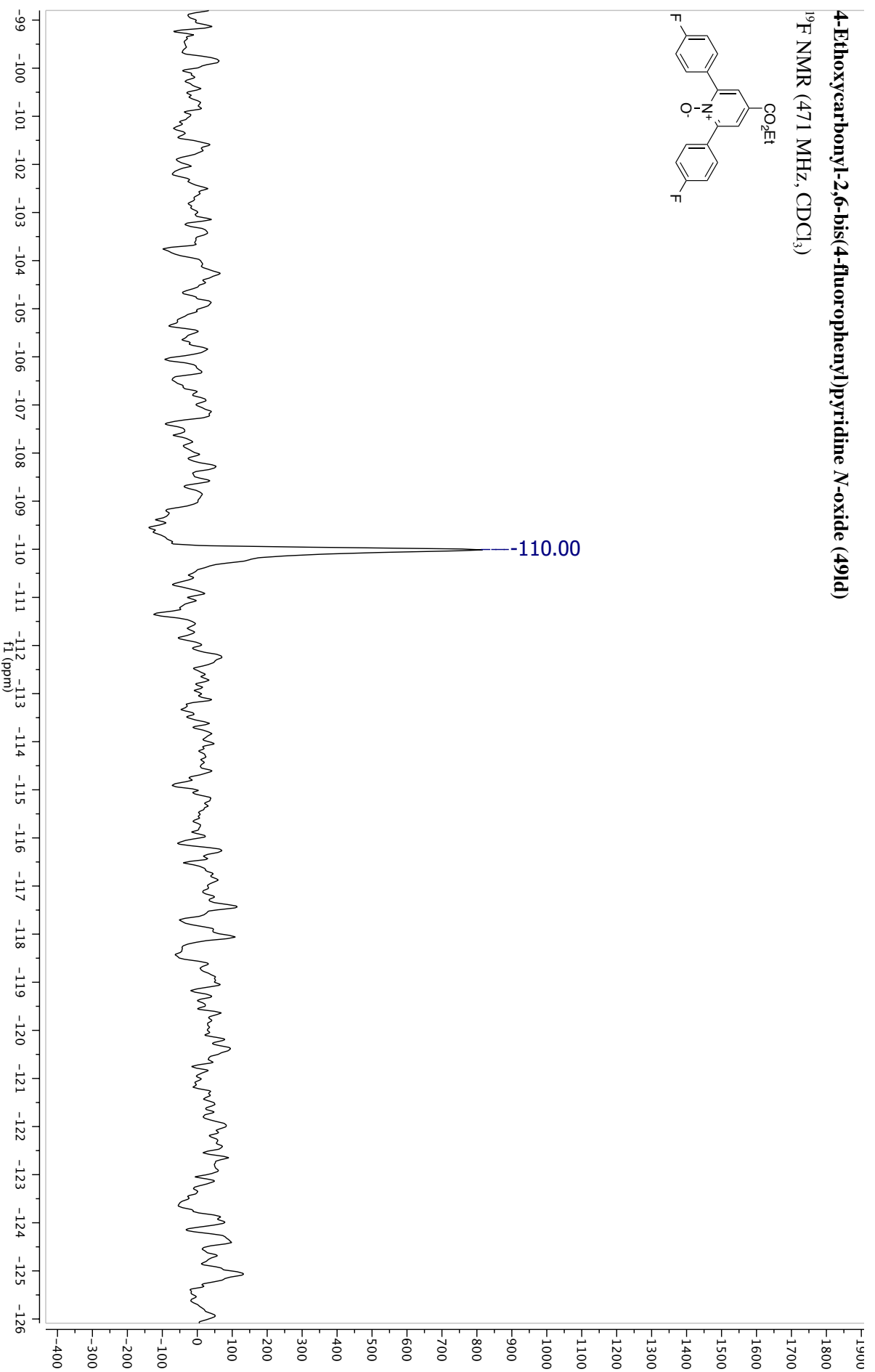
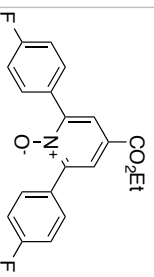
4-Ethoxycarbonyl-2,6-bis(4-fluorophenyl)pyridine N-oxide (49Id)

¹³C NMR (101 MHz, CDCl₃)



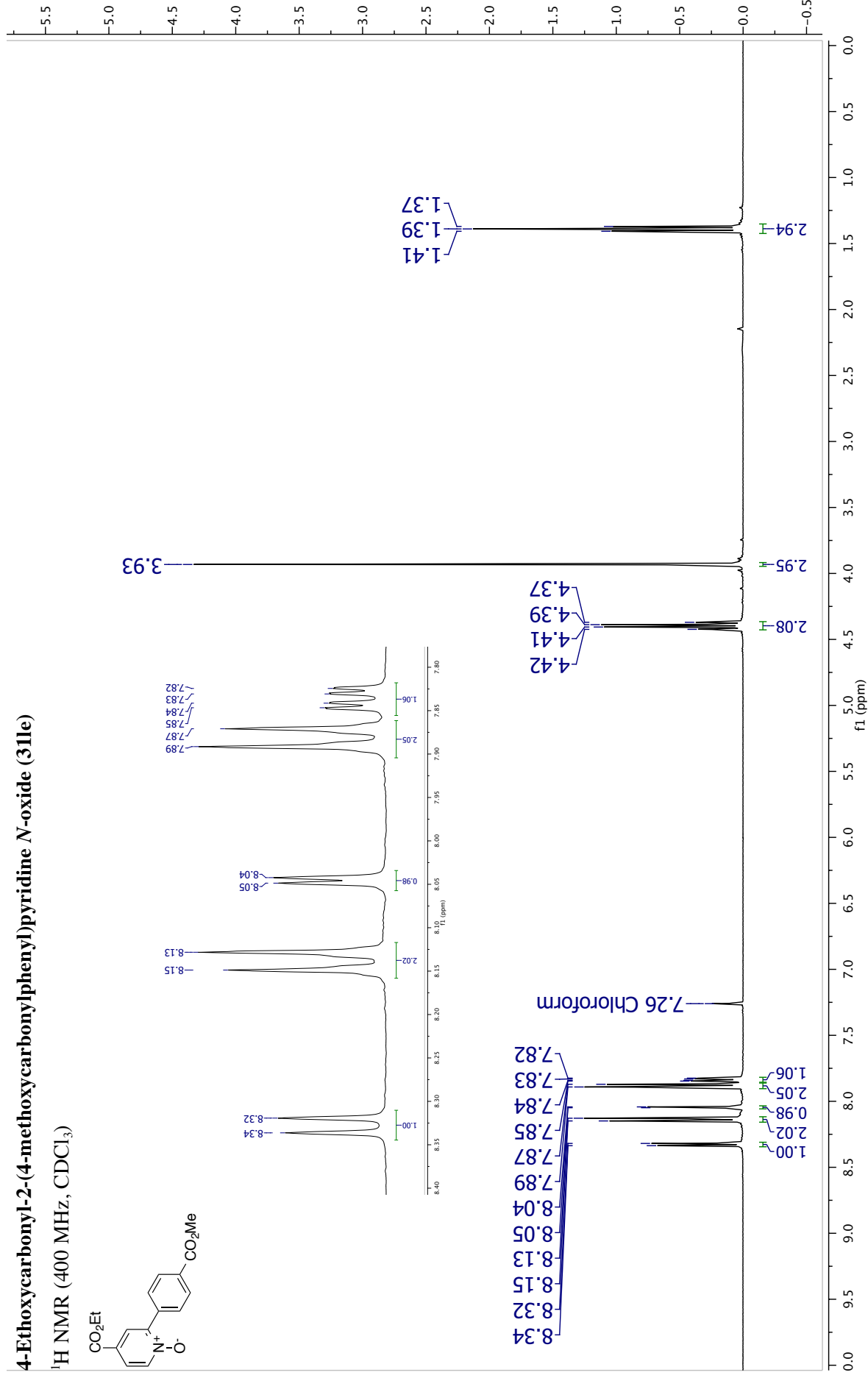
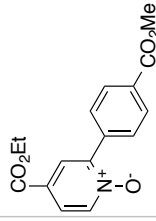
4-Ethoxycarbonyl-2,6-bis(4-fluorophenyl)pyridine N-oxide (491d)

¹⁹F NMR (471 MHz, CDCl₃)



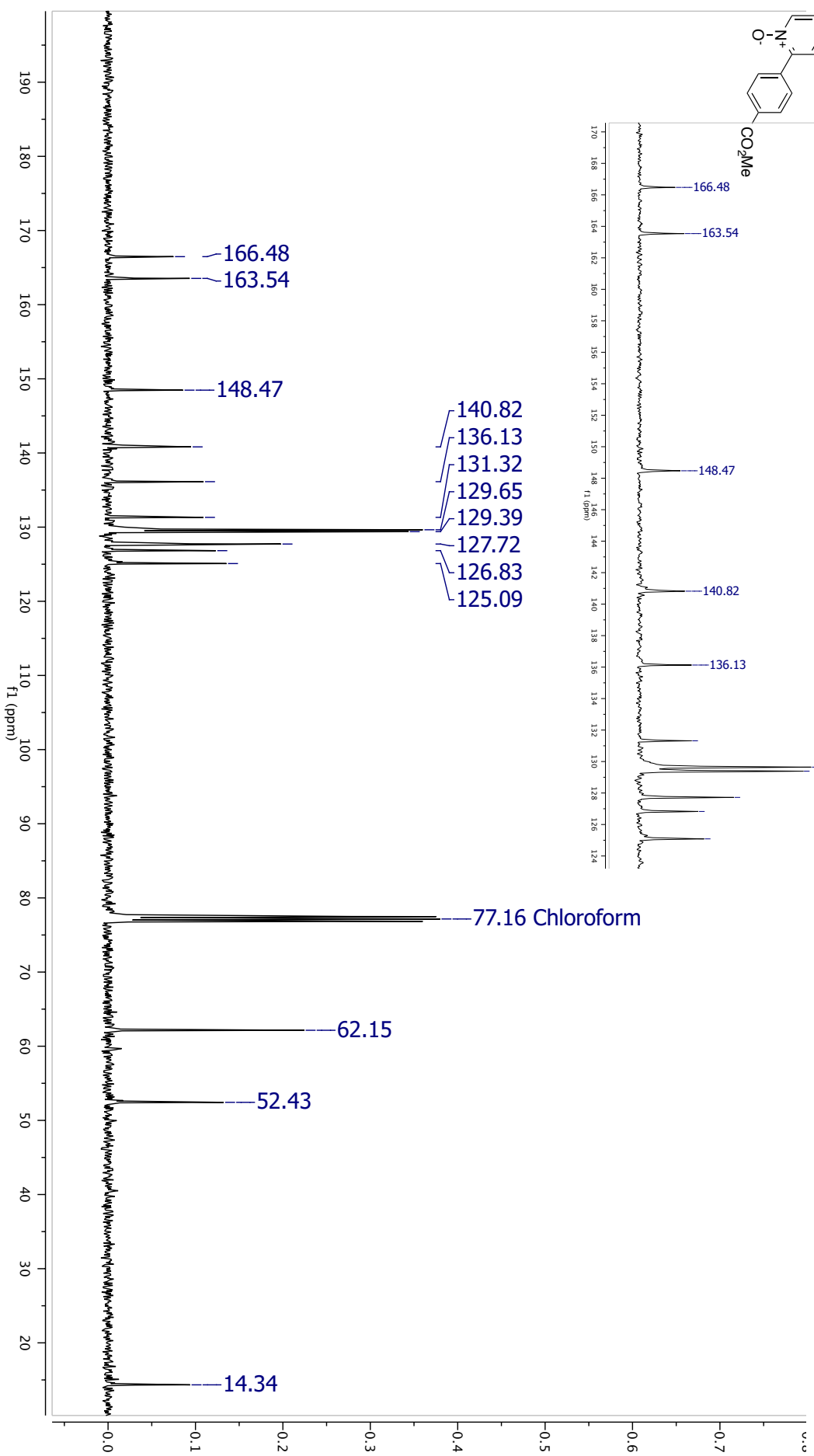
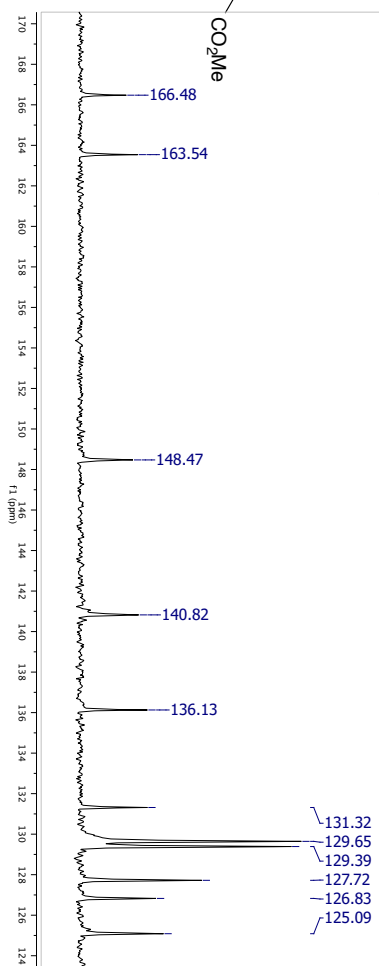
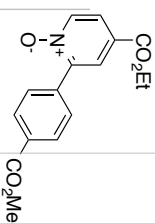
4-Ethoxycarbonyl-2-(4-methoxycarbonylphenyl)pyridine N-oxide (31le)

¹H NMR (400 MHz, CDCl₃)



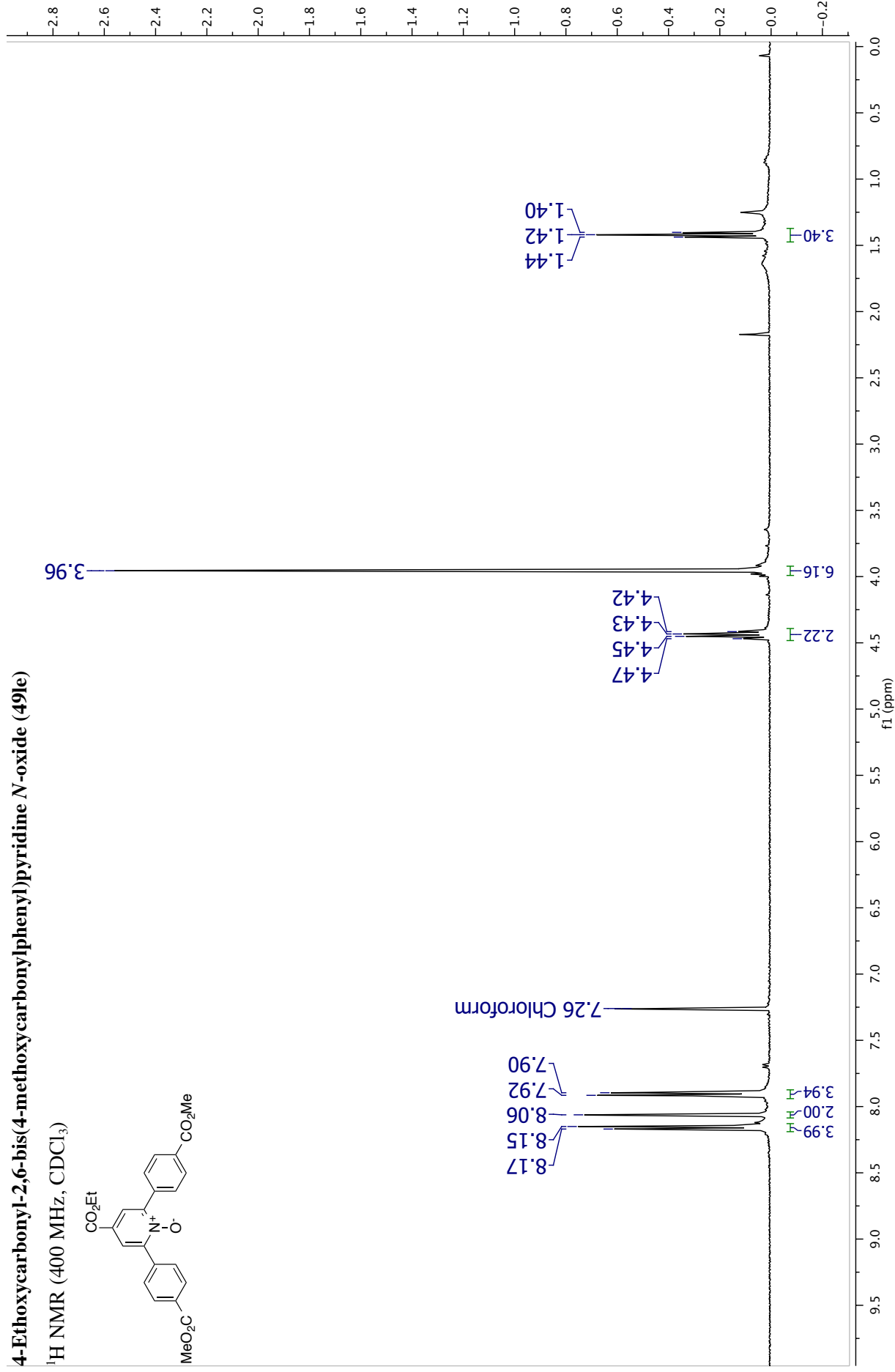
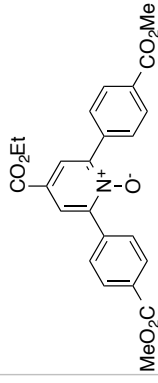
4-Ethoxycarbonyl-2-(4-methoxycarbonylphenyl)pyridine N-oxide (311e)

¹³C NMR (101 MHz, CDCl₃)



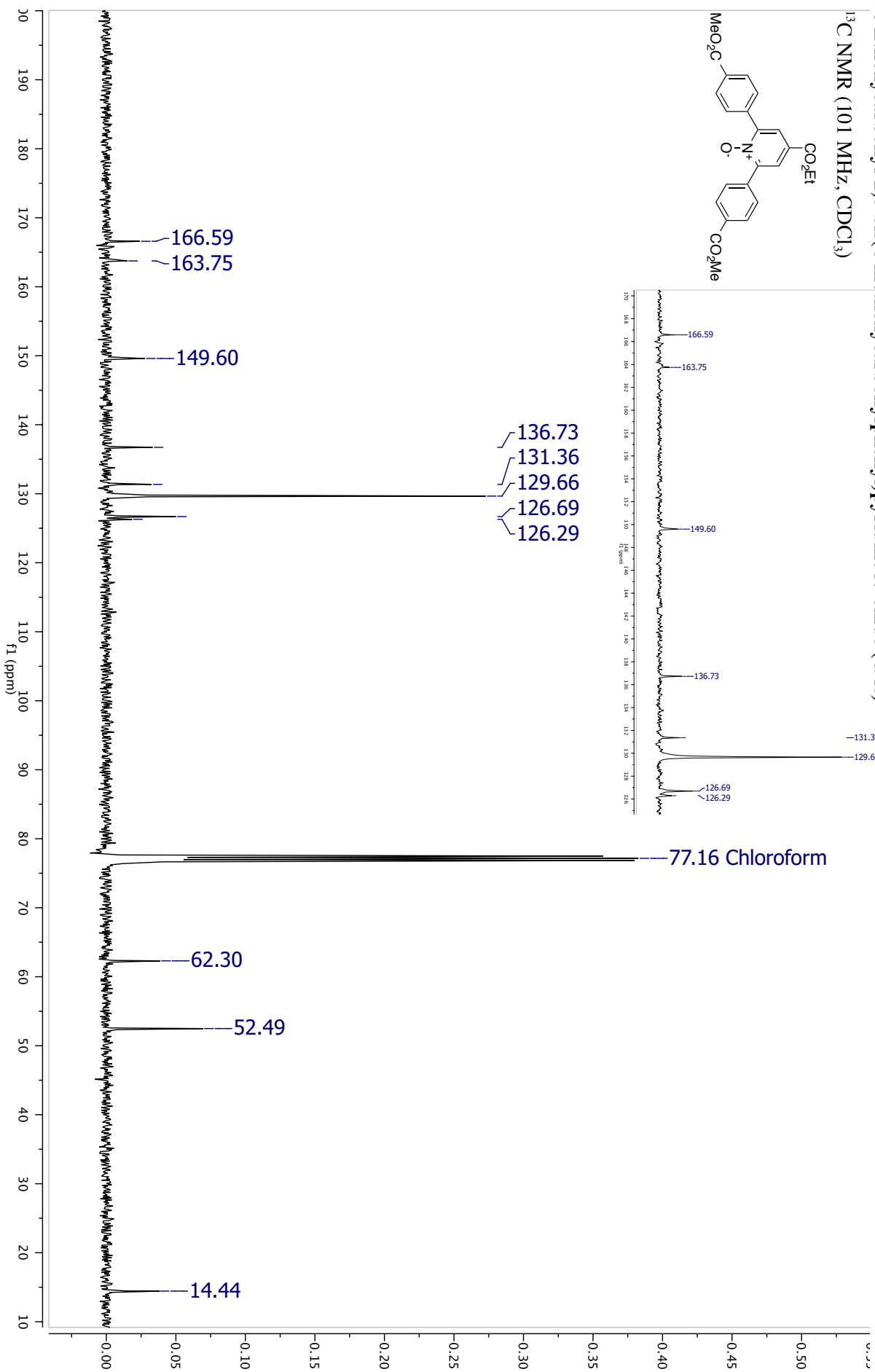
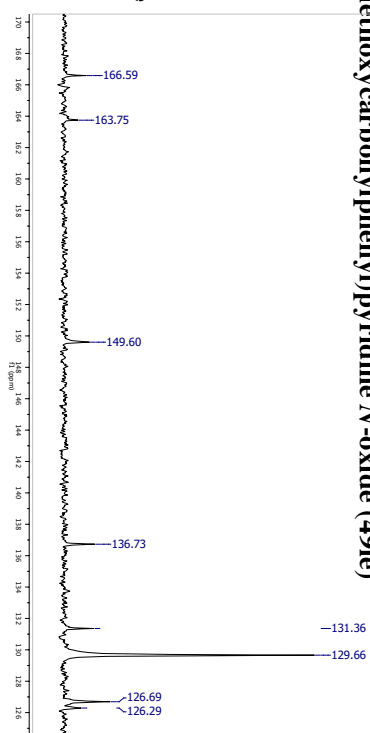
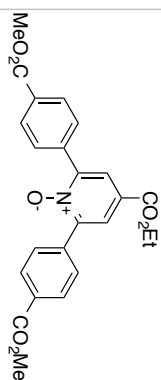
4-Ethoxycarbonyl-2,6-bis(4-methoxycarbonylphenyl)pyridine N-oxide (49le)

¹H NMR (400 MHz, CDCl₃)



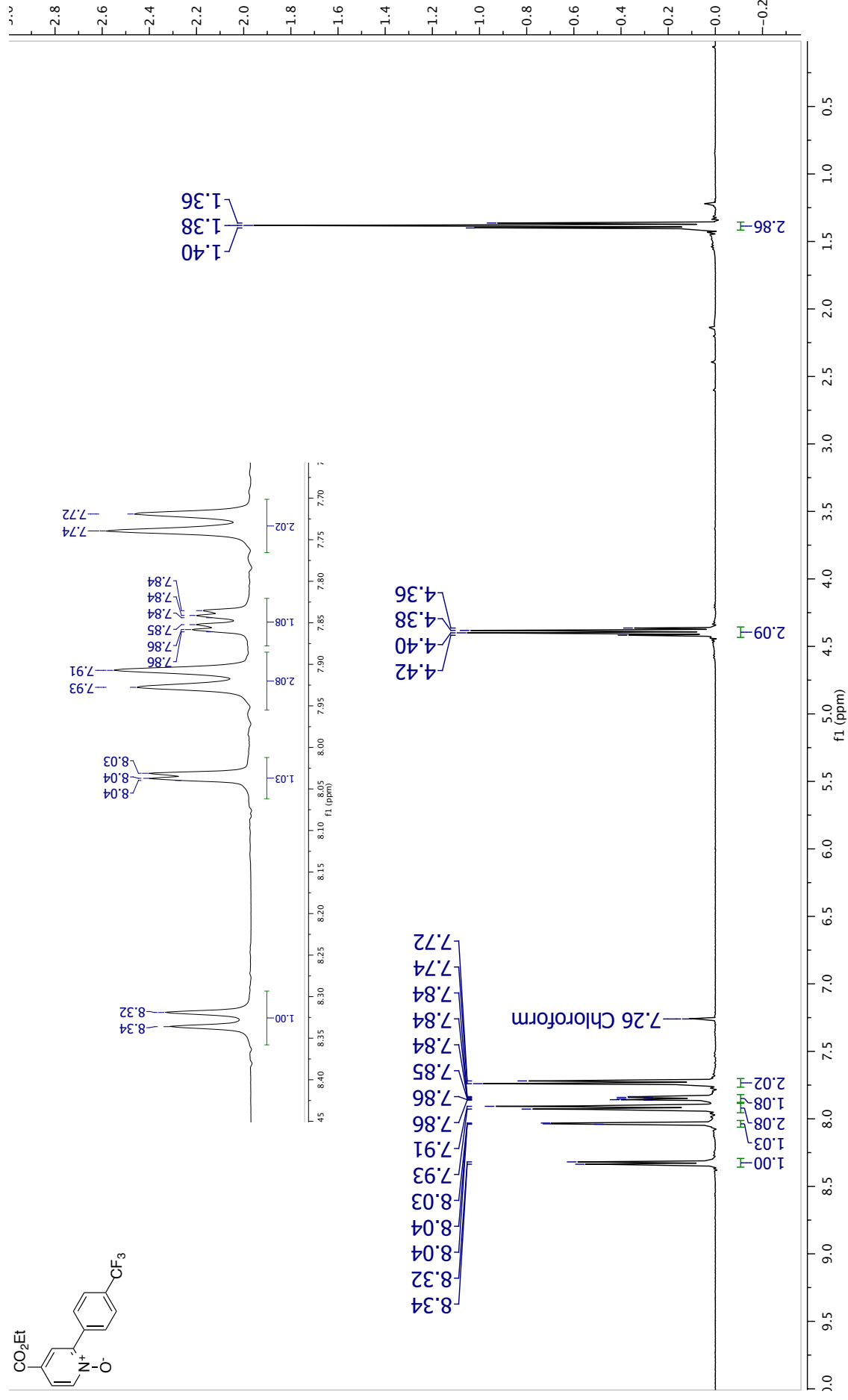
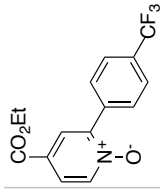
4-Ethoxycarbonyl-2,6-bis(4-methoxycarbonylphenyl)pyridine N-oxide (49le)

¹³C NMR (101 MHz, CDCl₃)



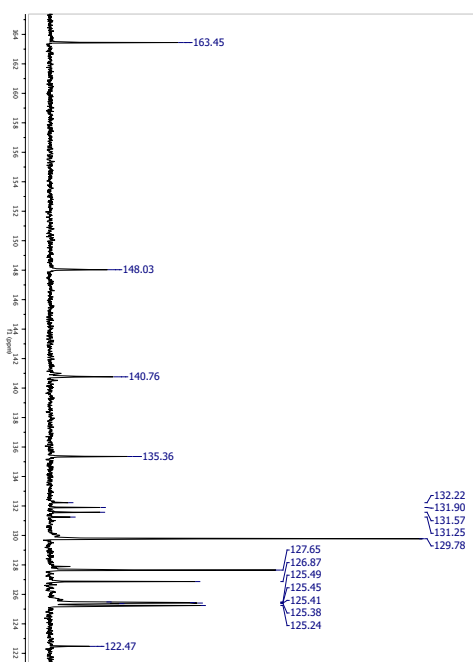
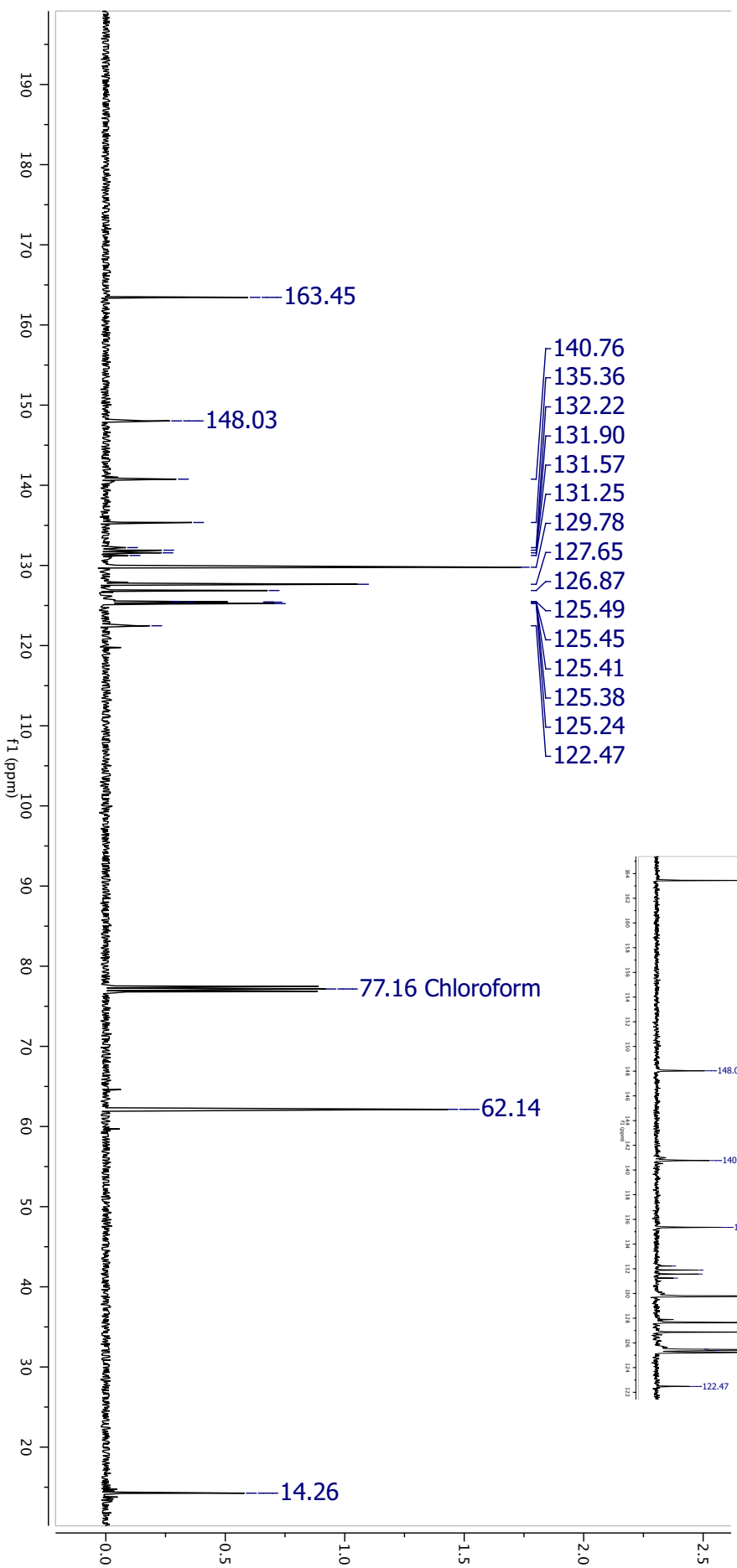
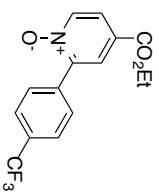
4-Ethoxycarbonyl-2-(4-trifluoromethylphenyl)pyridine N-oxide (31If)

¹H NMR (400 MHz, CDCl₃)



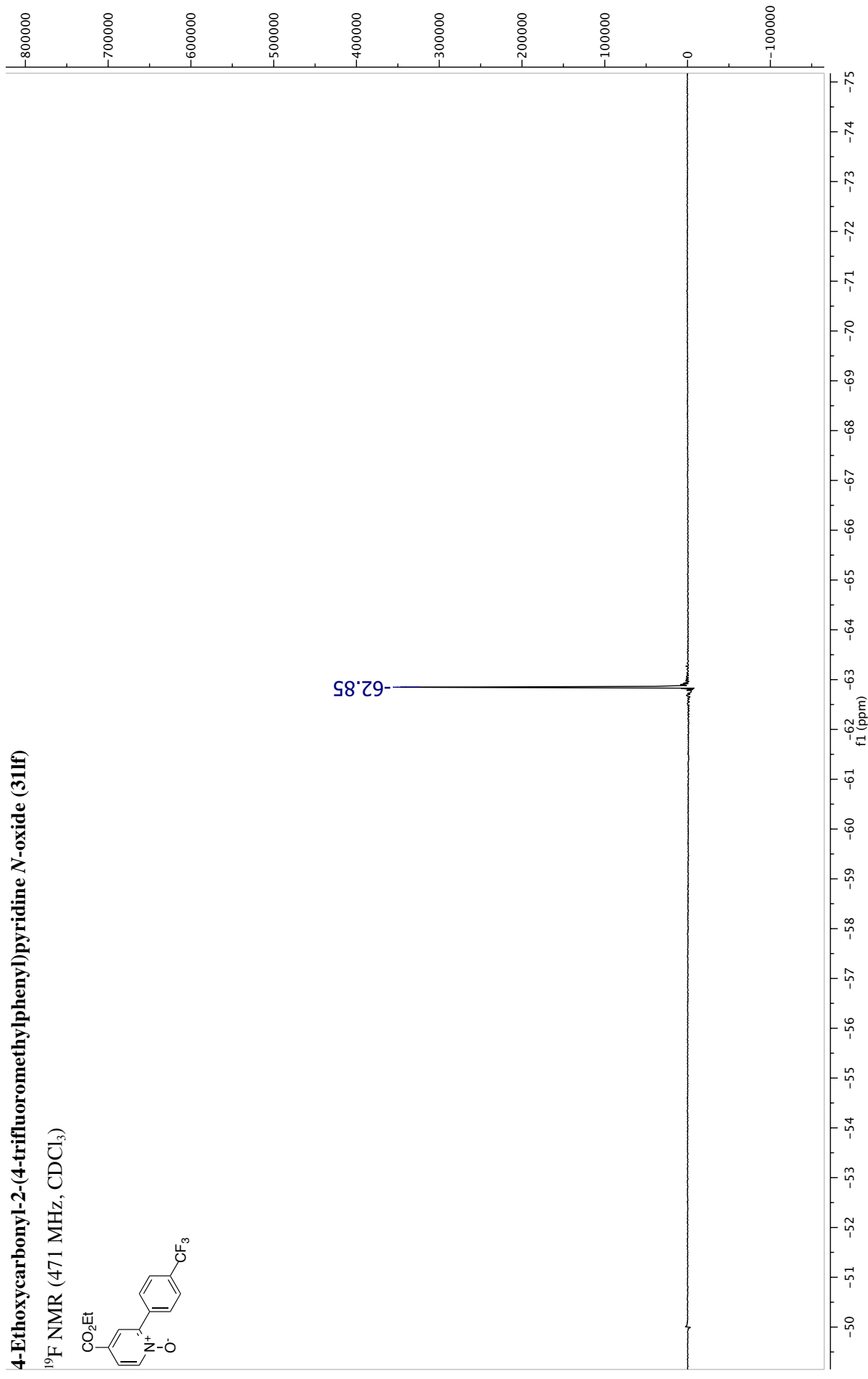
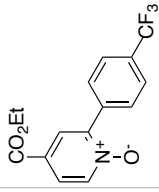
4-Ethoxycarbonyl-2-(4-trifluoromethylphenyl)pyridine N-oxide (311f)

¹³C NMR (101 MHz, CDCl₃)



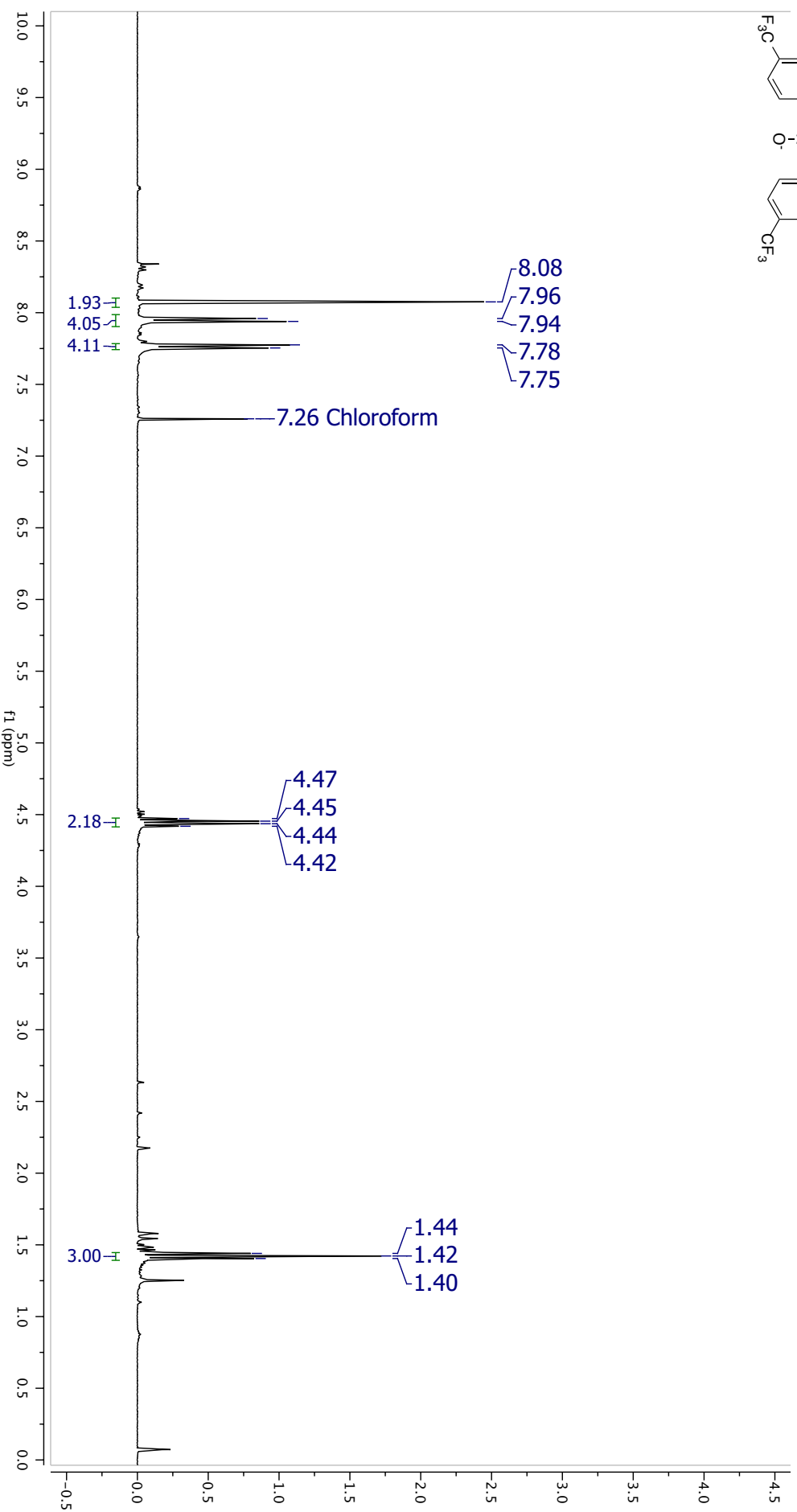
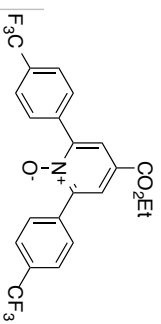
4-Ethoxycarbonyl-2-(4-trifluoromethylphenyl)pyridine N-oxide (311f)

¹⁹F NMR (471 MHz, CDCl₃)



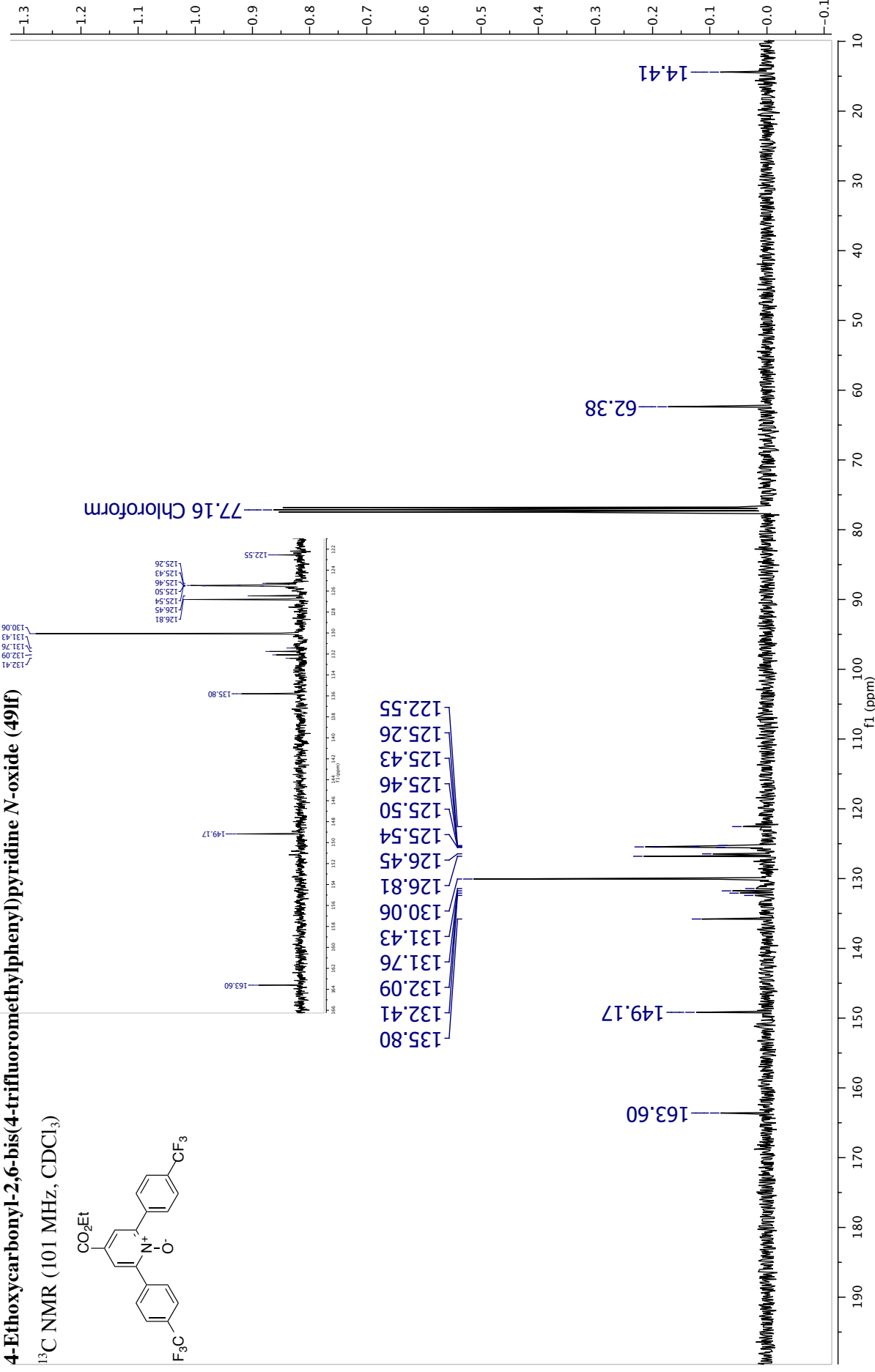
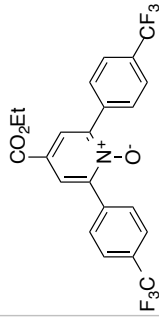
4-Ethoxycarbonyl-2,6-bis(4-trifluoromethylphenyl)pyridine N-oxide (49If)

¹H NMR (400 MHz, CDCl₃)



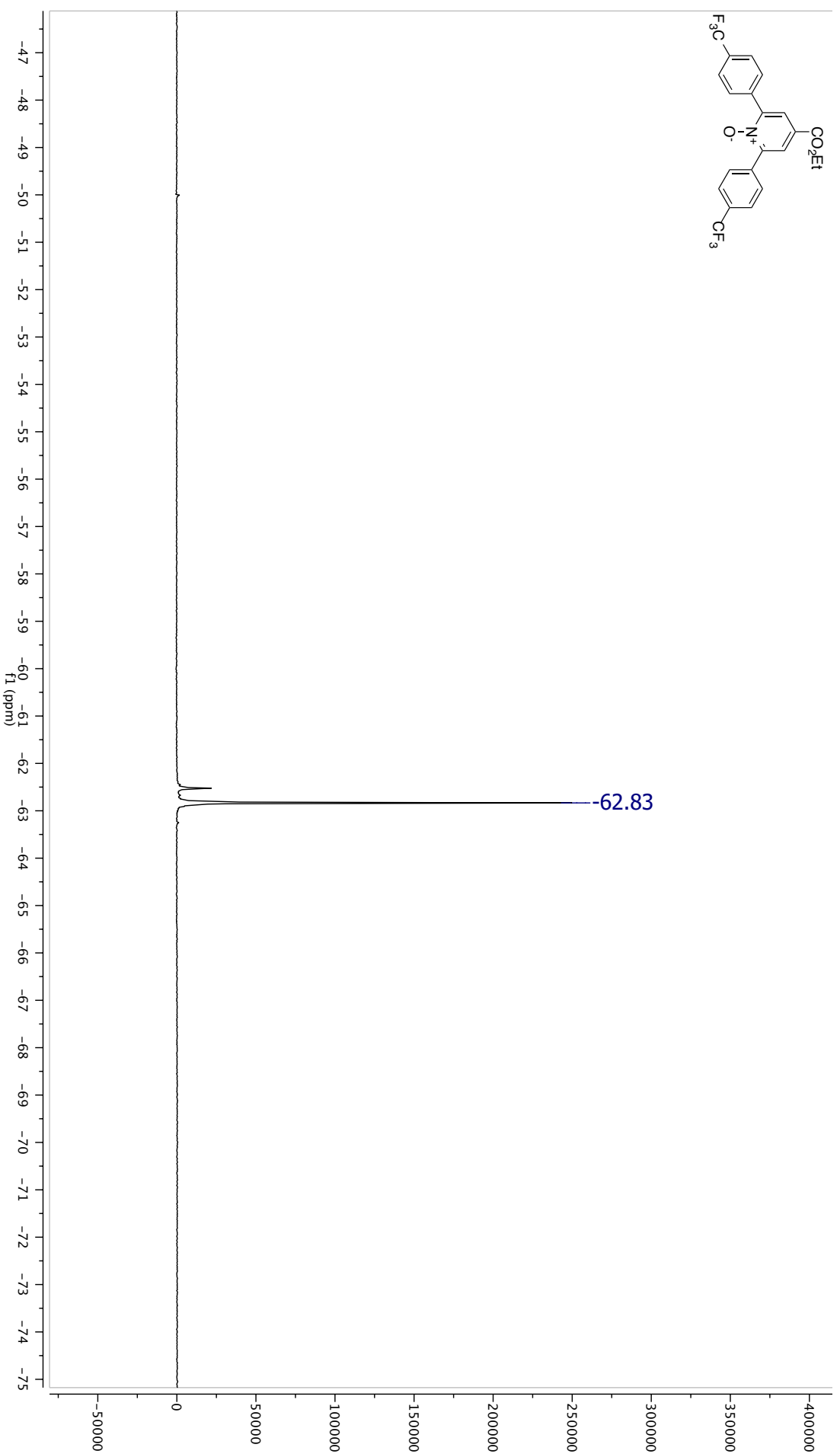
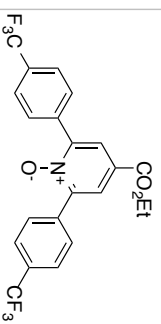
4-Ethoxycarbonyl-2,6-bis(4-trifluoromethylphenyl)pyridine N-oxide (49If)

¹³C NMR (101 MHz, CDCl₃)



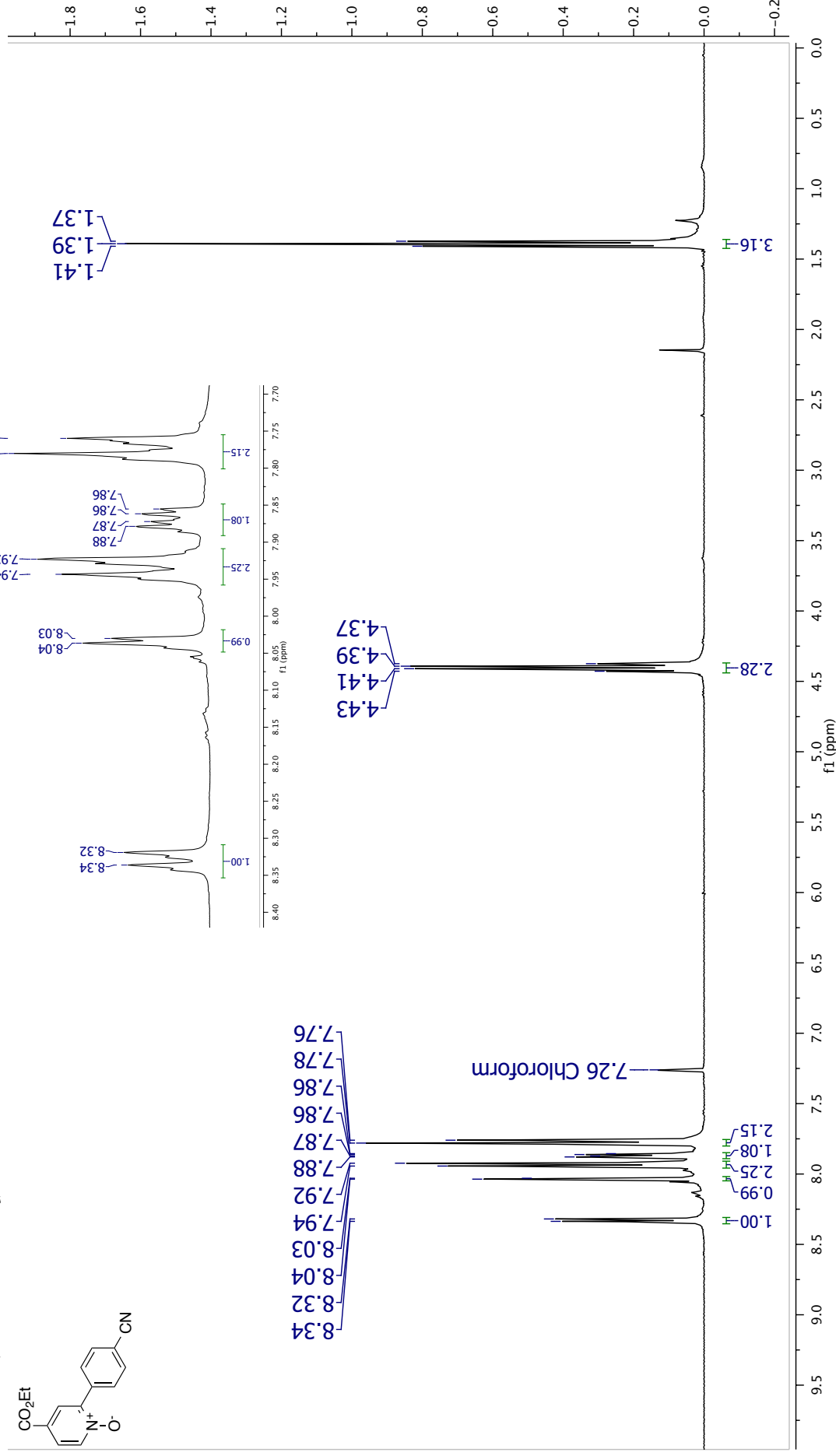
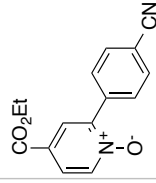
4-Ethoxycarbonyl-2,6-bis(4-trifluoromethylphenyl)pyridine N-oxide (49If)

¹⁹F NMR (471 MHz, CDCl₃)



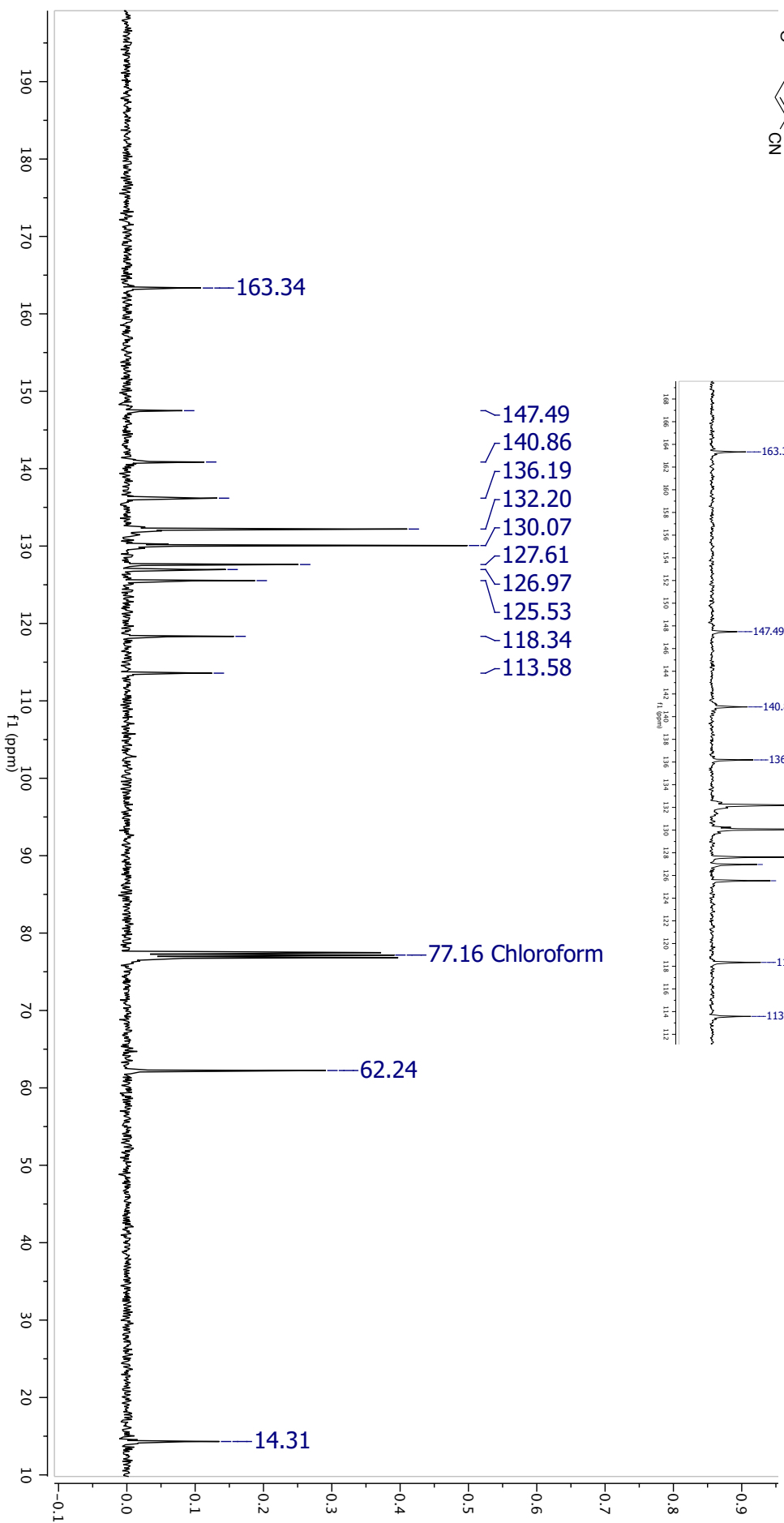
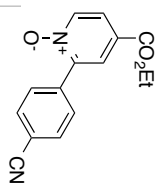
4-Ethoxycarbonyl-2-(4-cyanophenyl)pyridine N-oxide (31lg)

¹H NMR (400 MHz, CDCl₃)



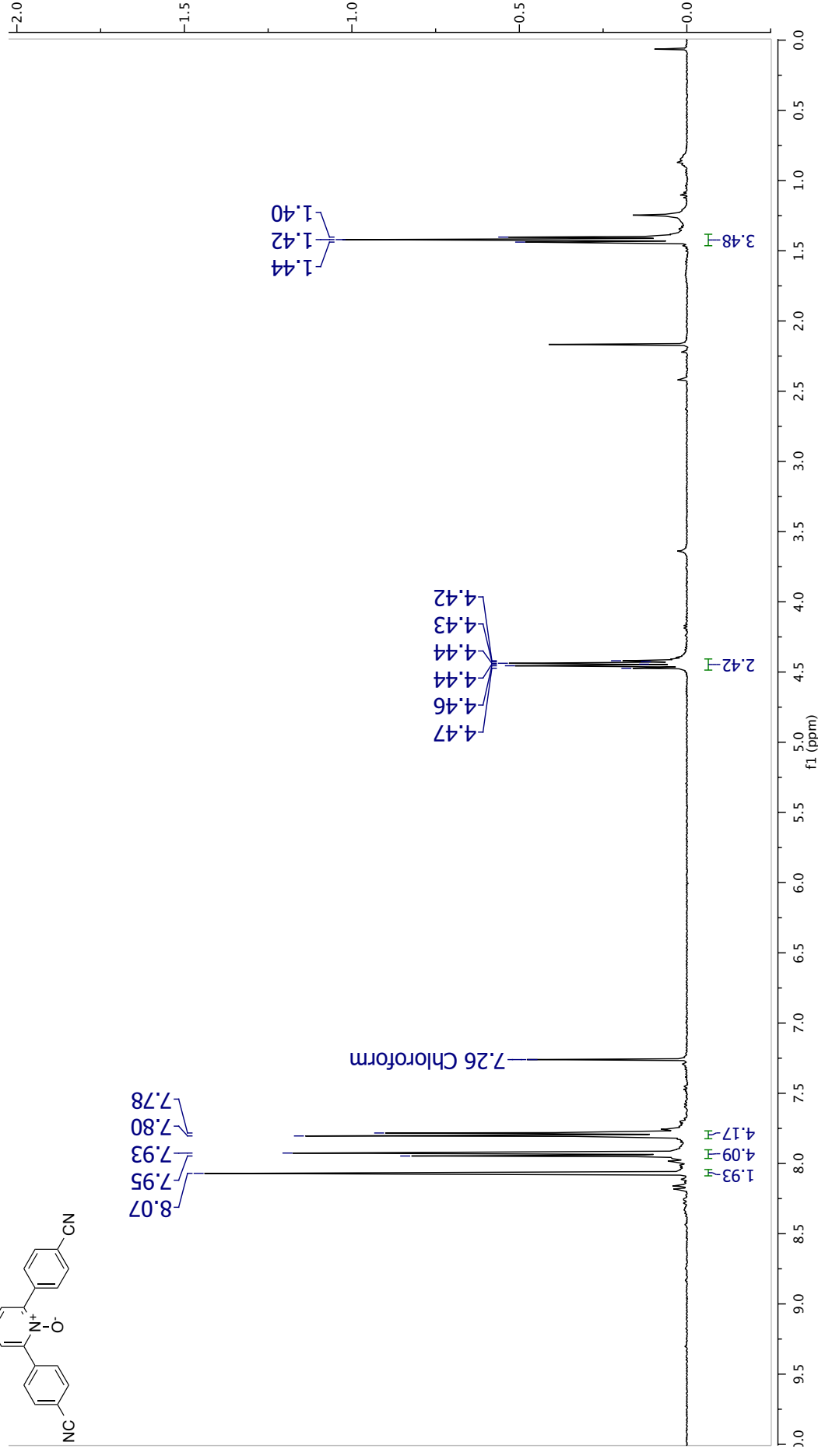
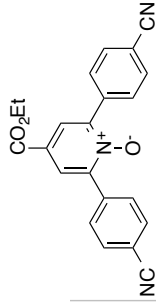
4-Ethoxycarbonyl-2-(4-cyanophenyl)pyridine N-oxide (31lg)

¹³C NMR (101 MHz, CDCl₃)



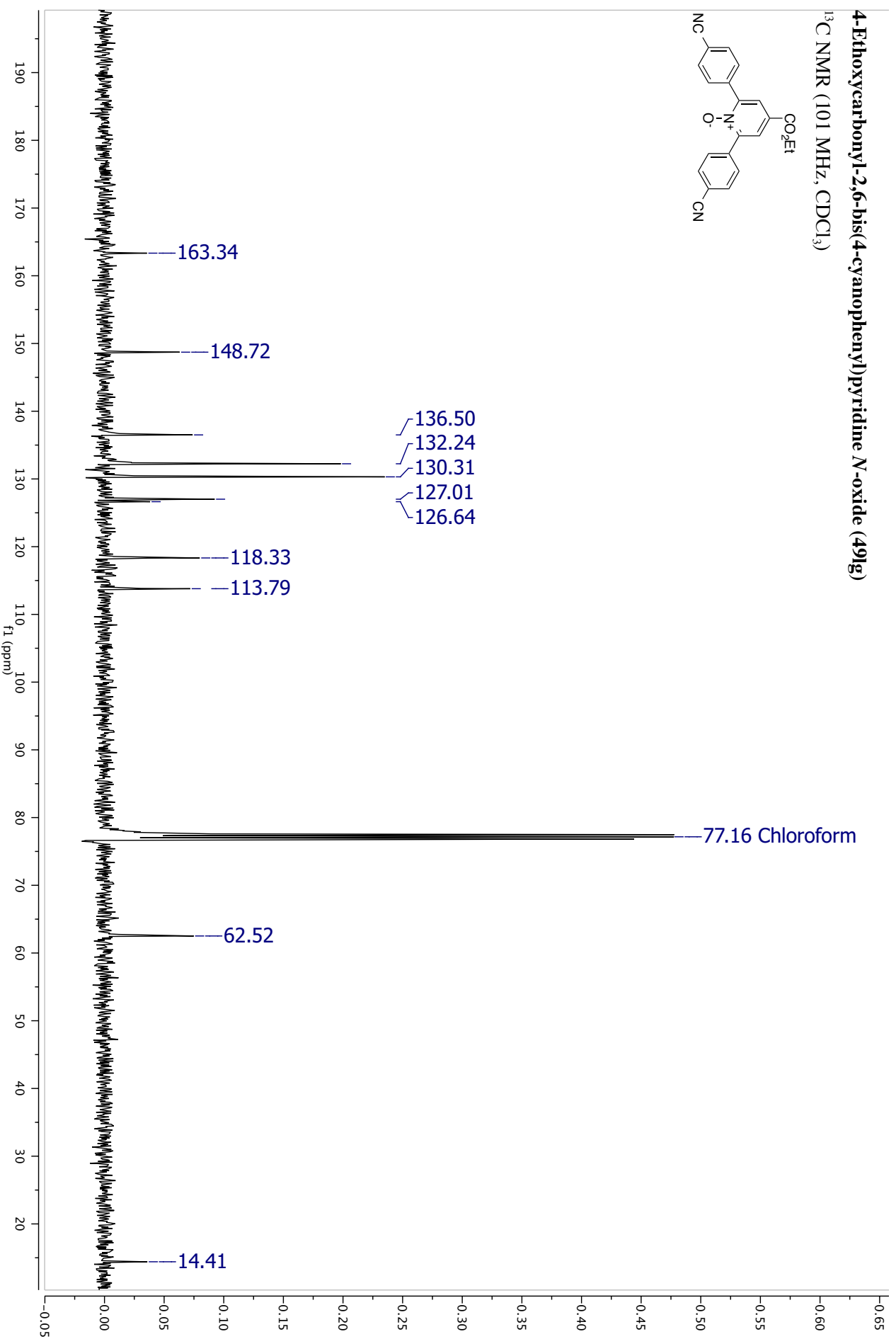
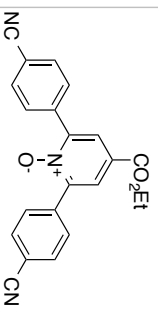
4-Ethoxycarbonyl-2,6-bis(4-cyanophenyl)pyridine N-oxide (49lg)

¹H NMR (400 MHz, CDCl₃)



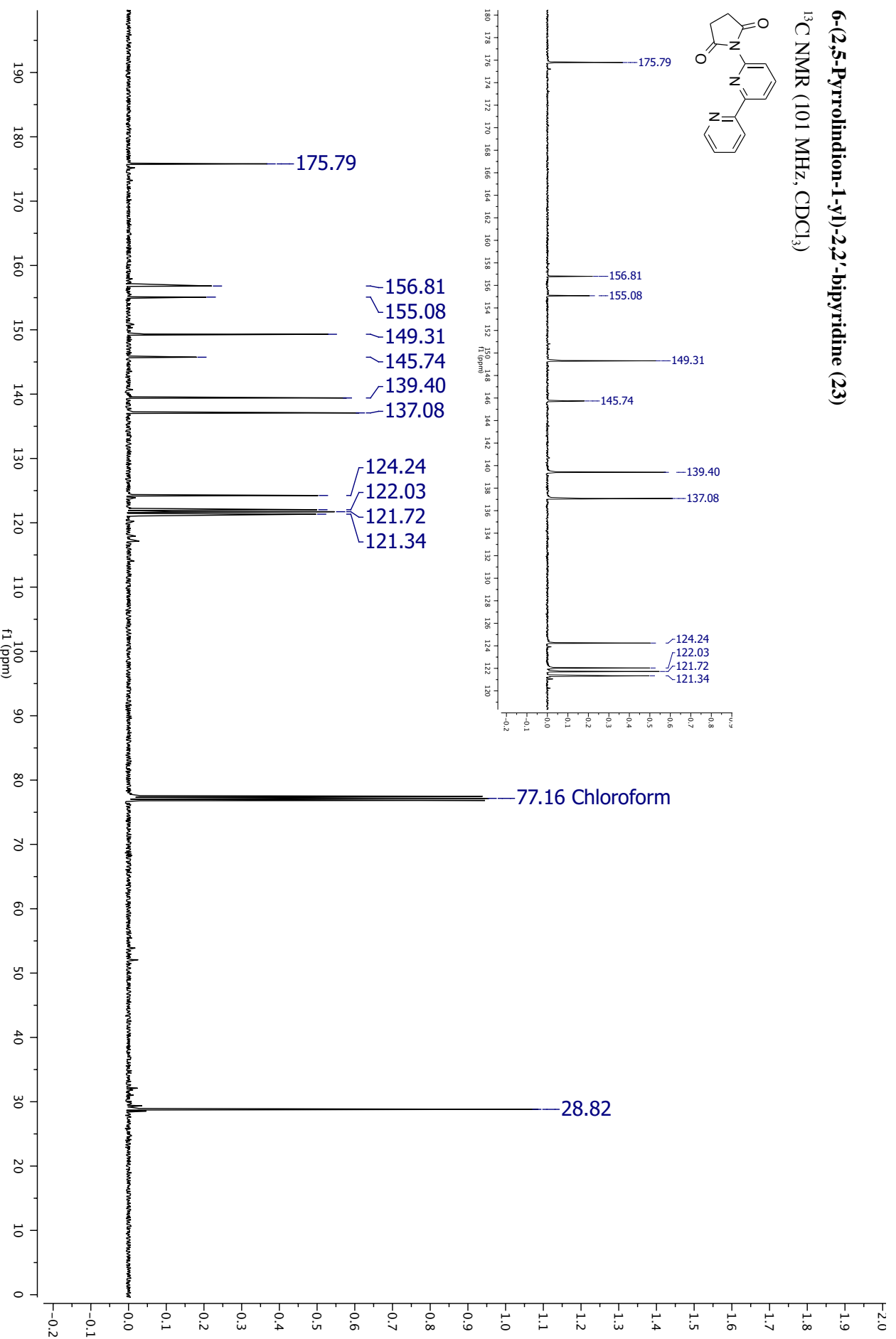
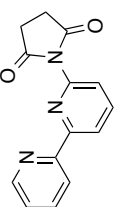
4-Ethoxycarbonyl-2,6-bis(4-cyanophenyl)pyridine N-oxide (491g)

¹³C NMR (101 MHz, CDCl₃)



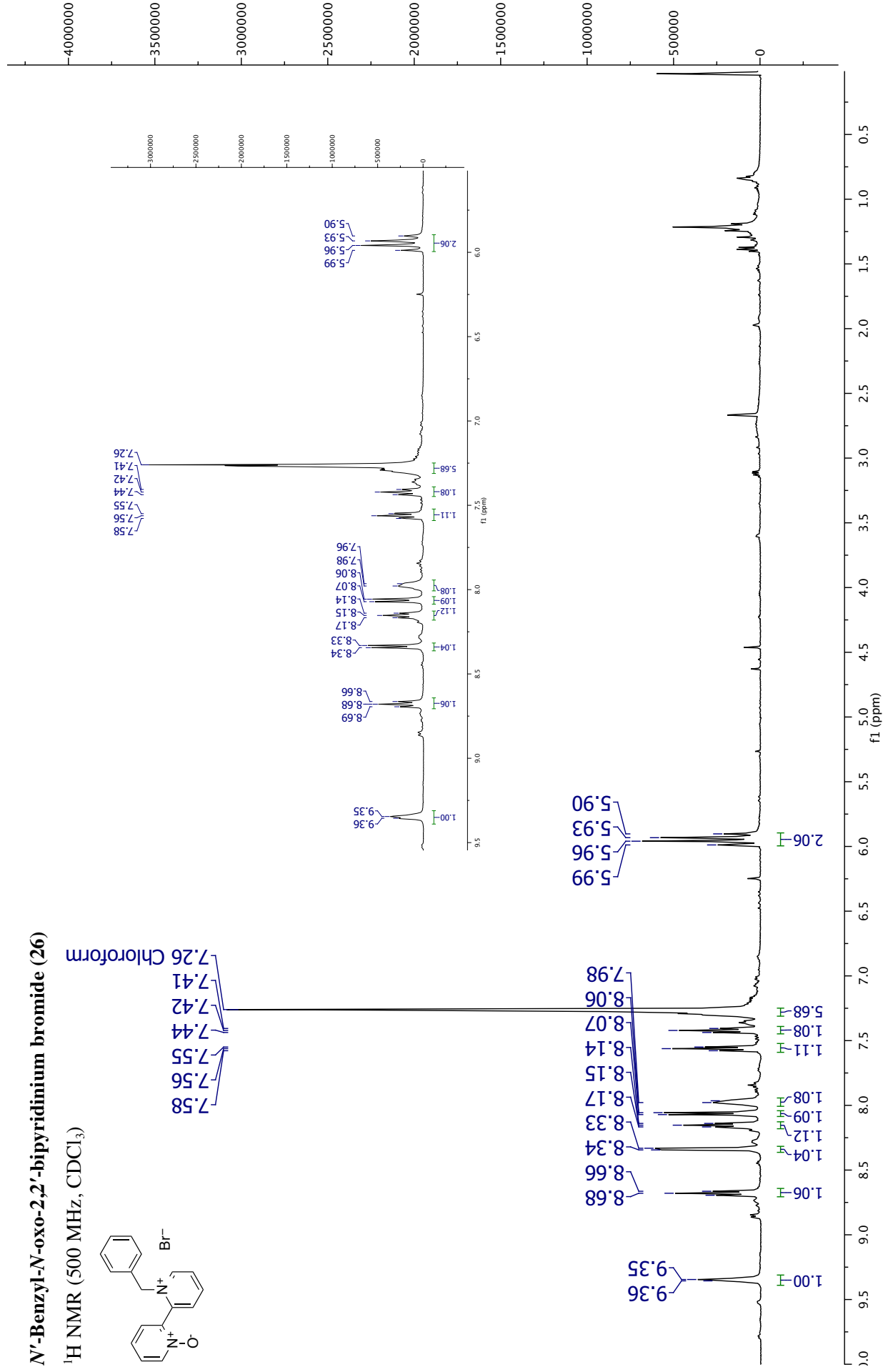
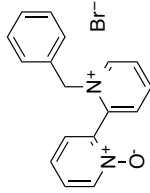
6-(2,5-Pyrrolidion-1-yl)-2,2'-bipyridine (23)

¹³C NMR (101 MHz, CDCl₃)



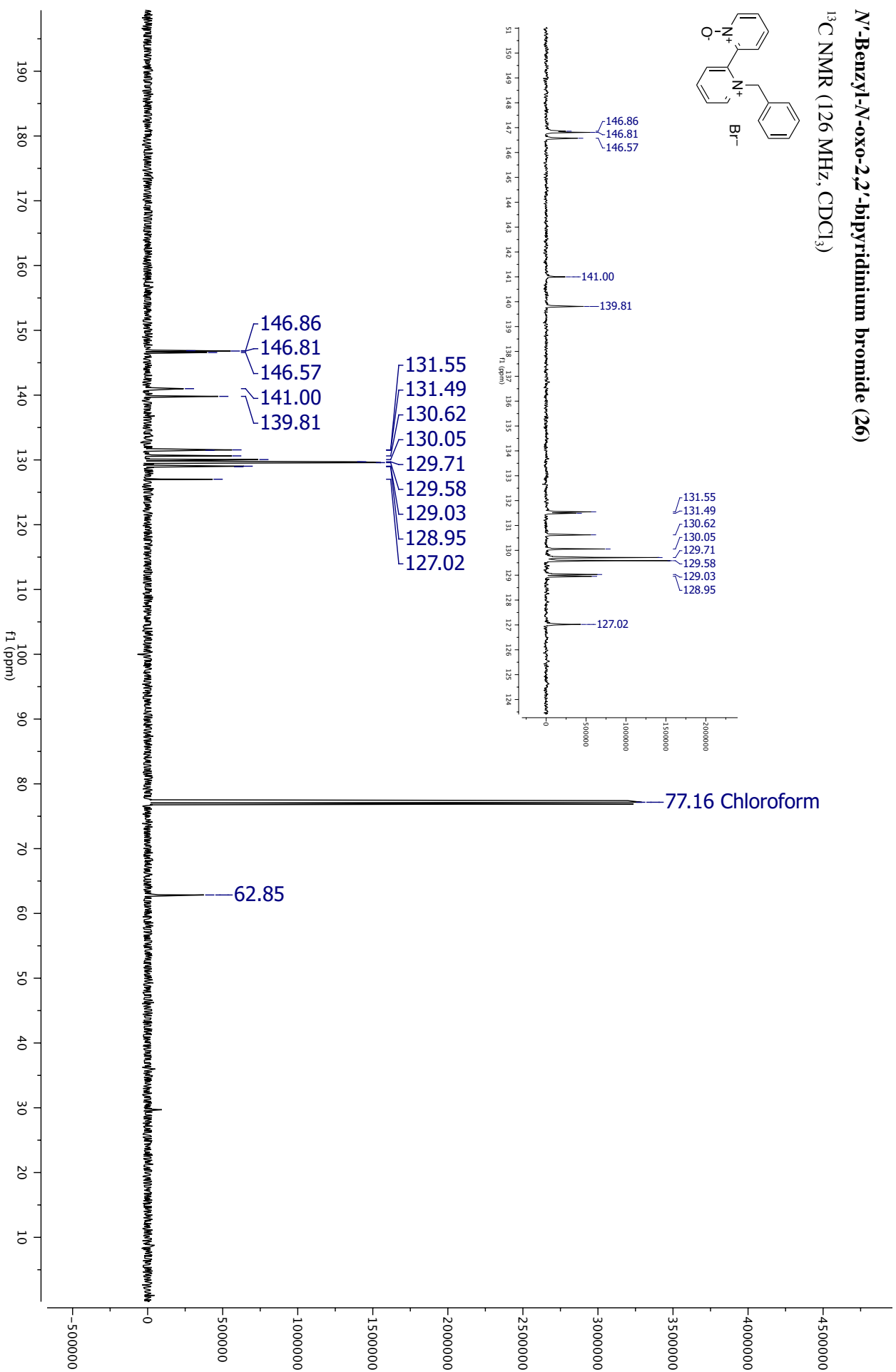
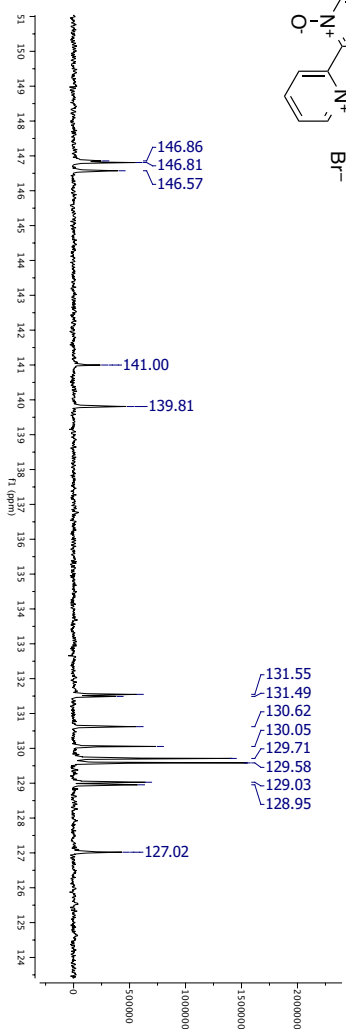
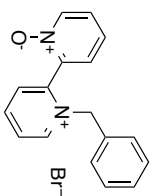
N'-Benzyl-N-oxo-2,2'-bipyridinium bromide (26)

¹H NMR (500 MHz, CDCl₃)



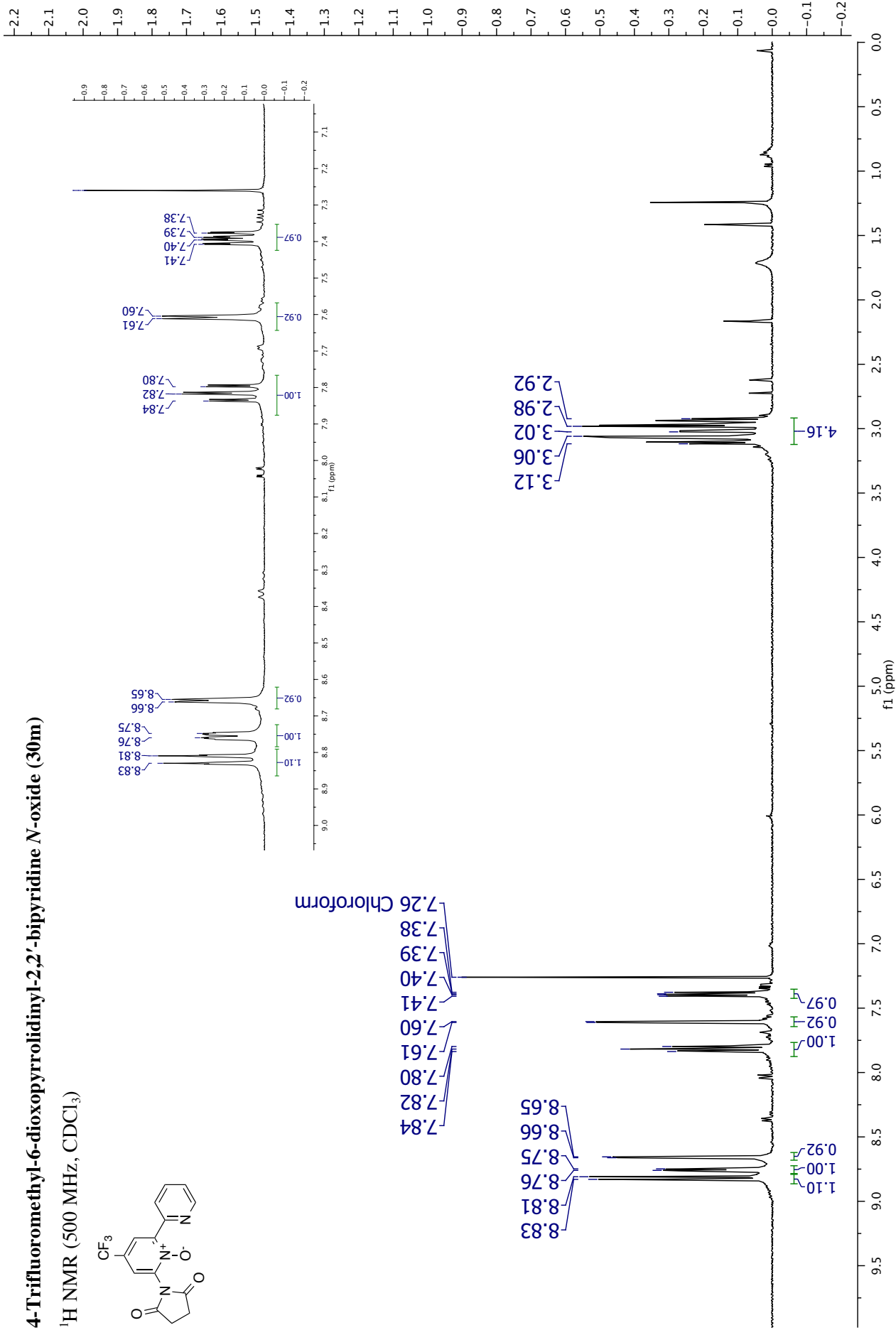
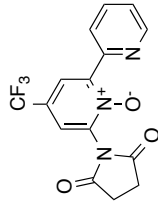
***N'*-Benzyl-*N*-oxo-2,2'-bipyridinium bromide (26)**

¹³C NMR (126 MHz, CDCl₃)



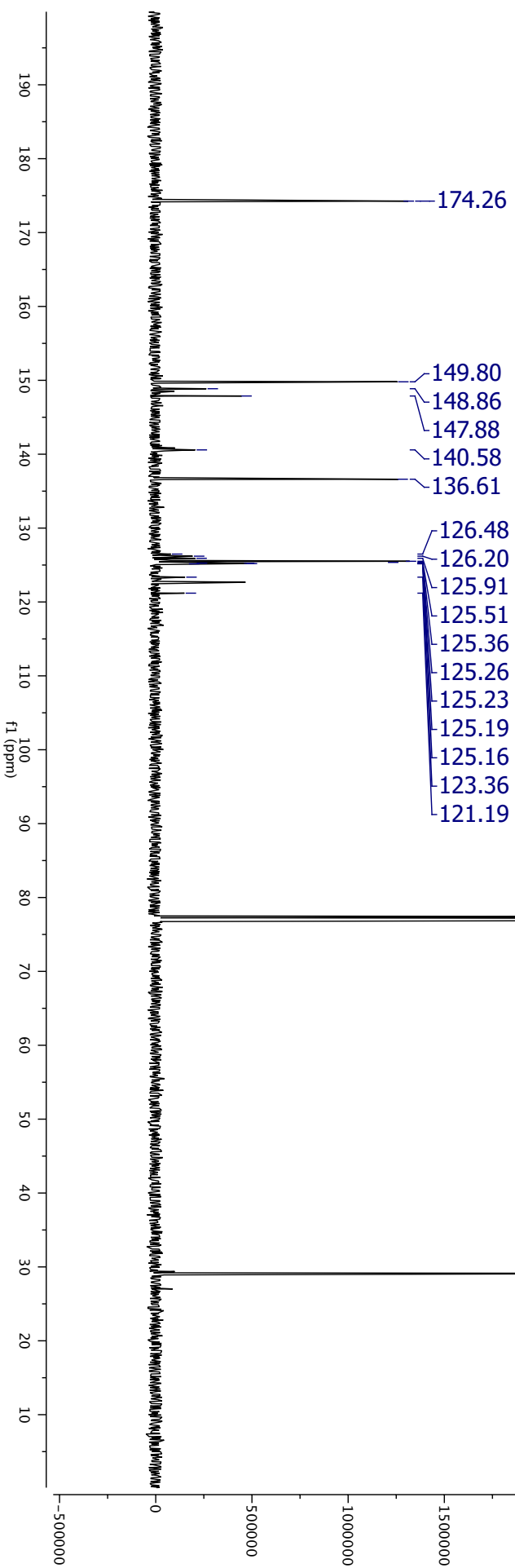
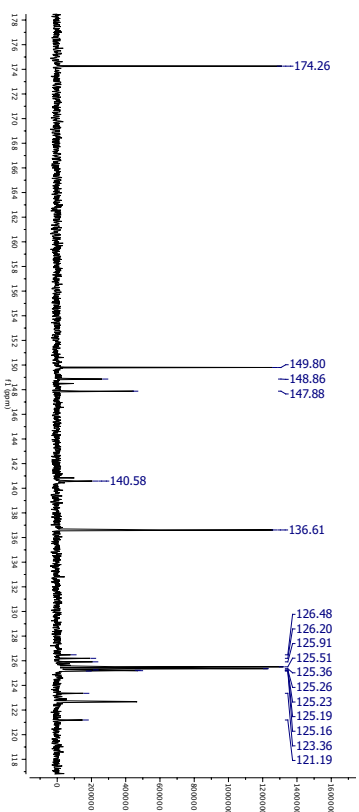
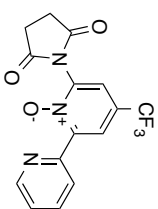
4-Trifluoromethyl-6-dioxopyrrolidinyl-2,2'-bipyridine N-oxide (30m)

¹H NMR (500 MHz, CDCl₃)



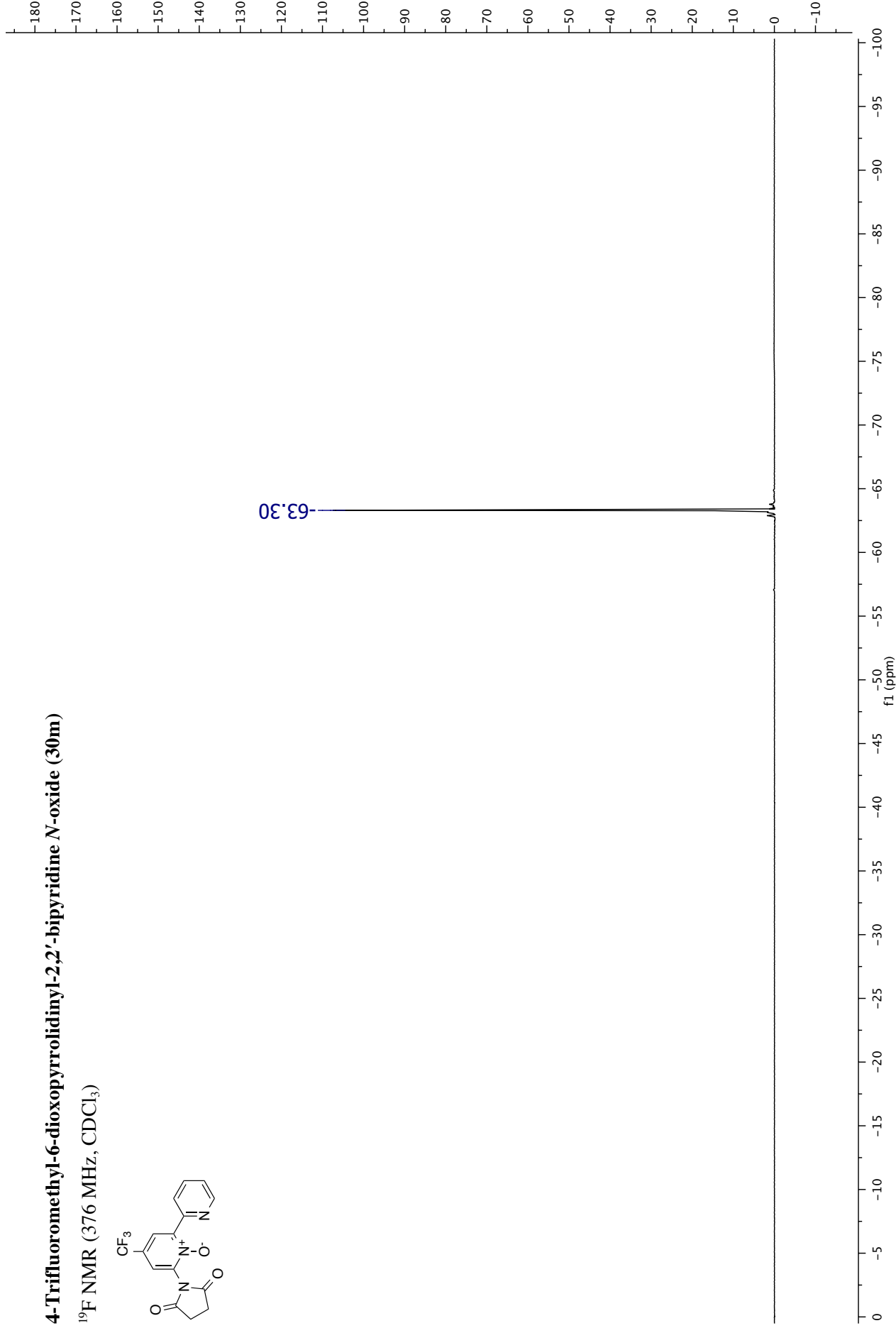
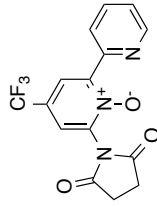
4-Trifluoromethyl-6-dioxopyrrolidinyl-2,2'-bipyridine N-oxide (30m)

¹³C NMR (126 MHz, CDCl₃)

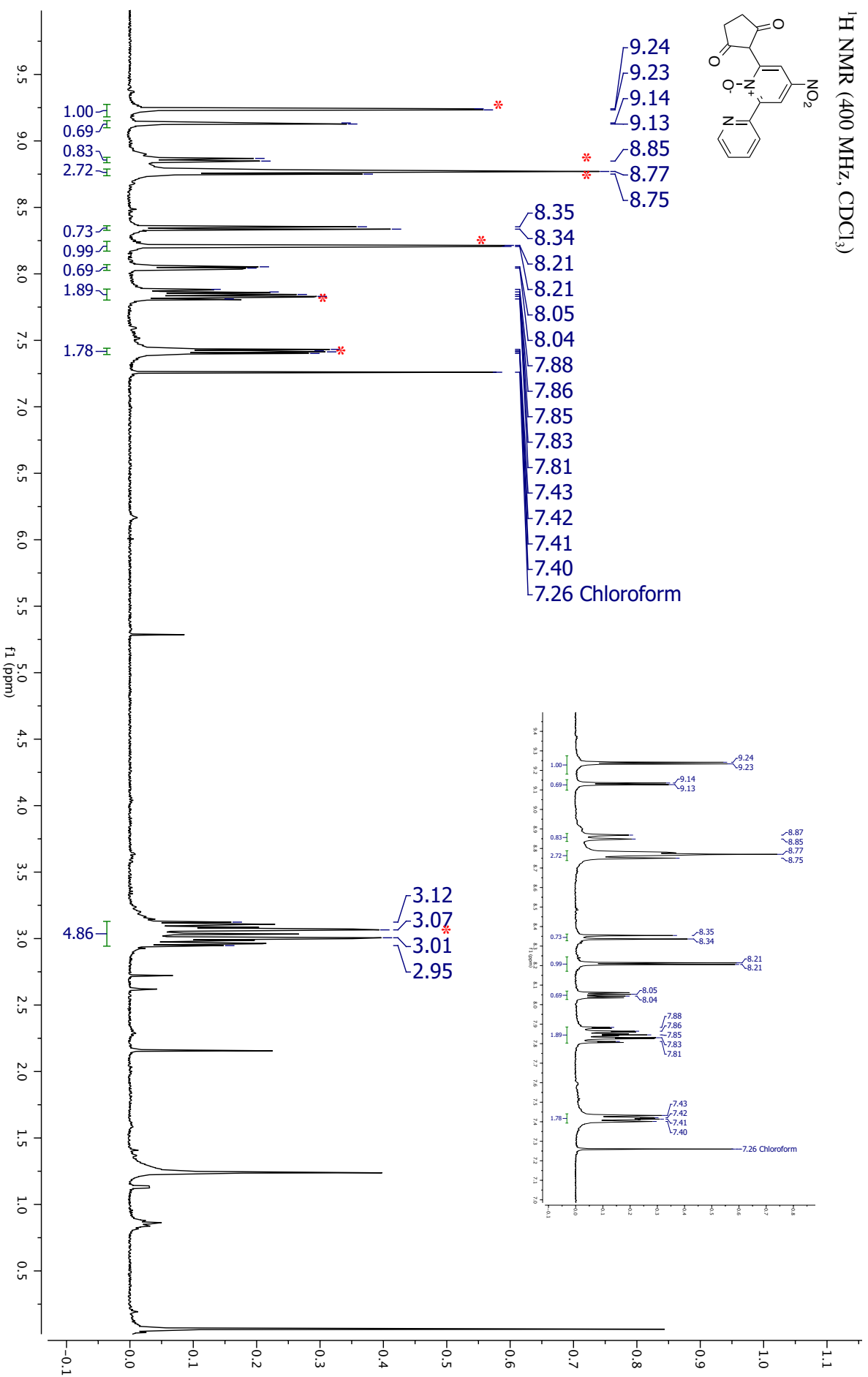
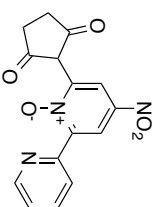


4-Trifluoromethyl-6-dioxopyrrolidinyl-2,2'-bipyridine N-oxide (30m)

¹⁹F NMR (376 MHz, CDCl₃)

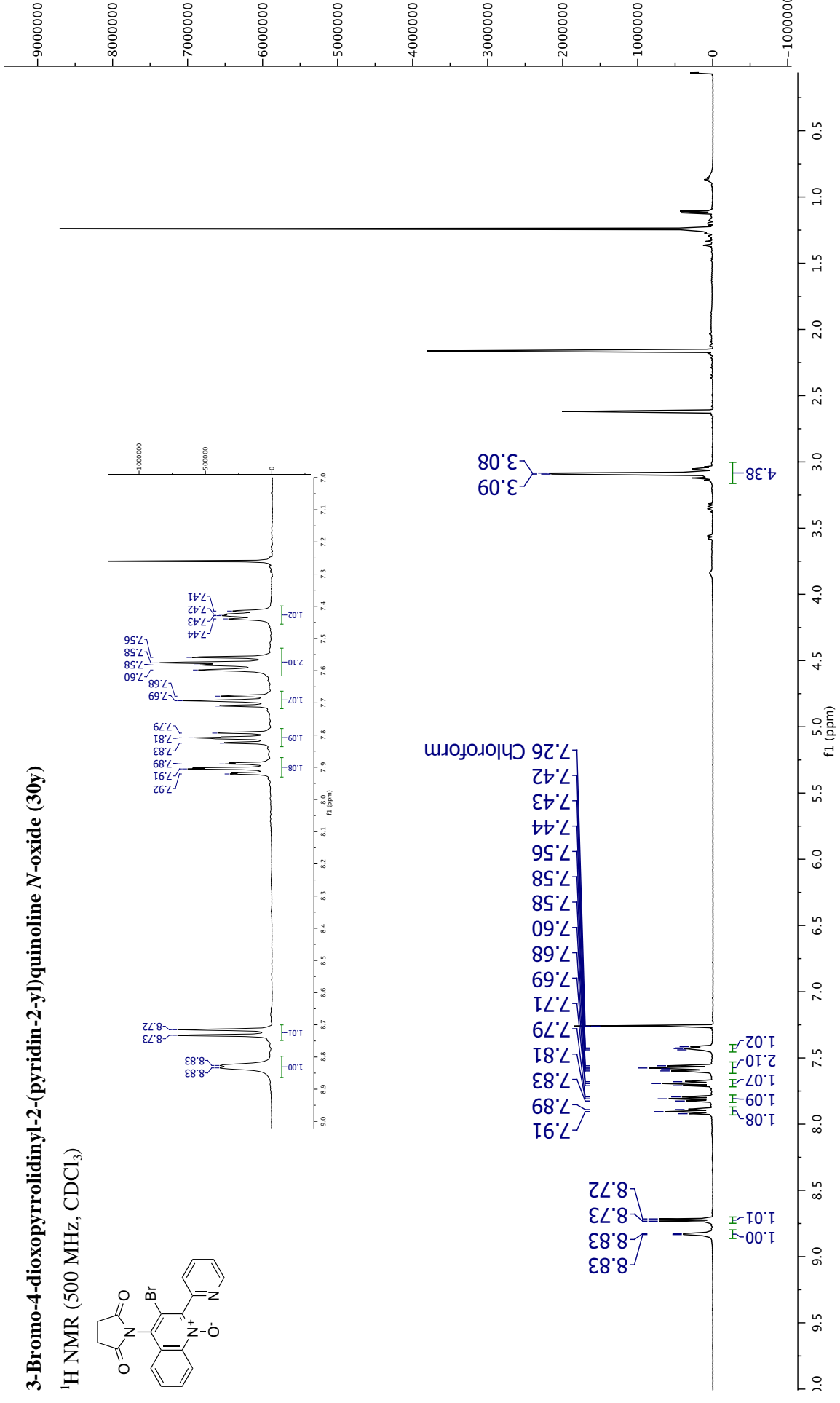
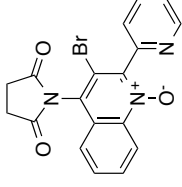


Mixture of 4-nitro-6-dioxopyrrolidinyl-2,2'-bipyridine *N*-oxide (30o, *) and 4-nitro-2,2'-bipyridine *N*-oxide (20o)



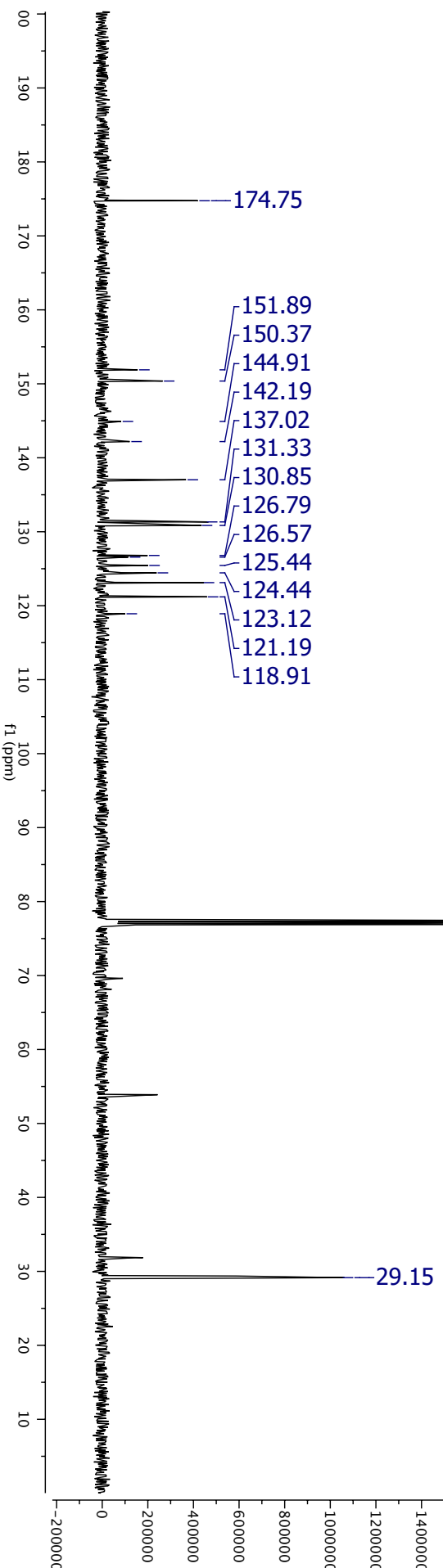
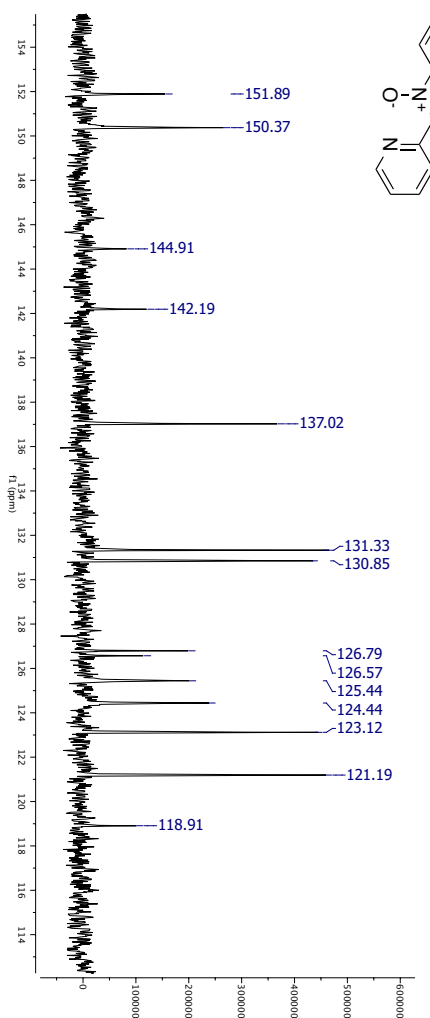
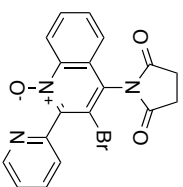
3-Bromo-4-dioxopyrrolidinyl-2-(pyridin-2-yl)quinoline N-oxide (30y)

¹H NMR (500 MHz, CDCl₃)



3-Bromo-4-dioxopyrrolidinyl-2-(pyridin-2-yl)quinoline N-oxide (30y)

¹³C NMR (126 MHz, CDCl₃)

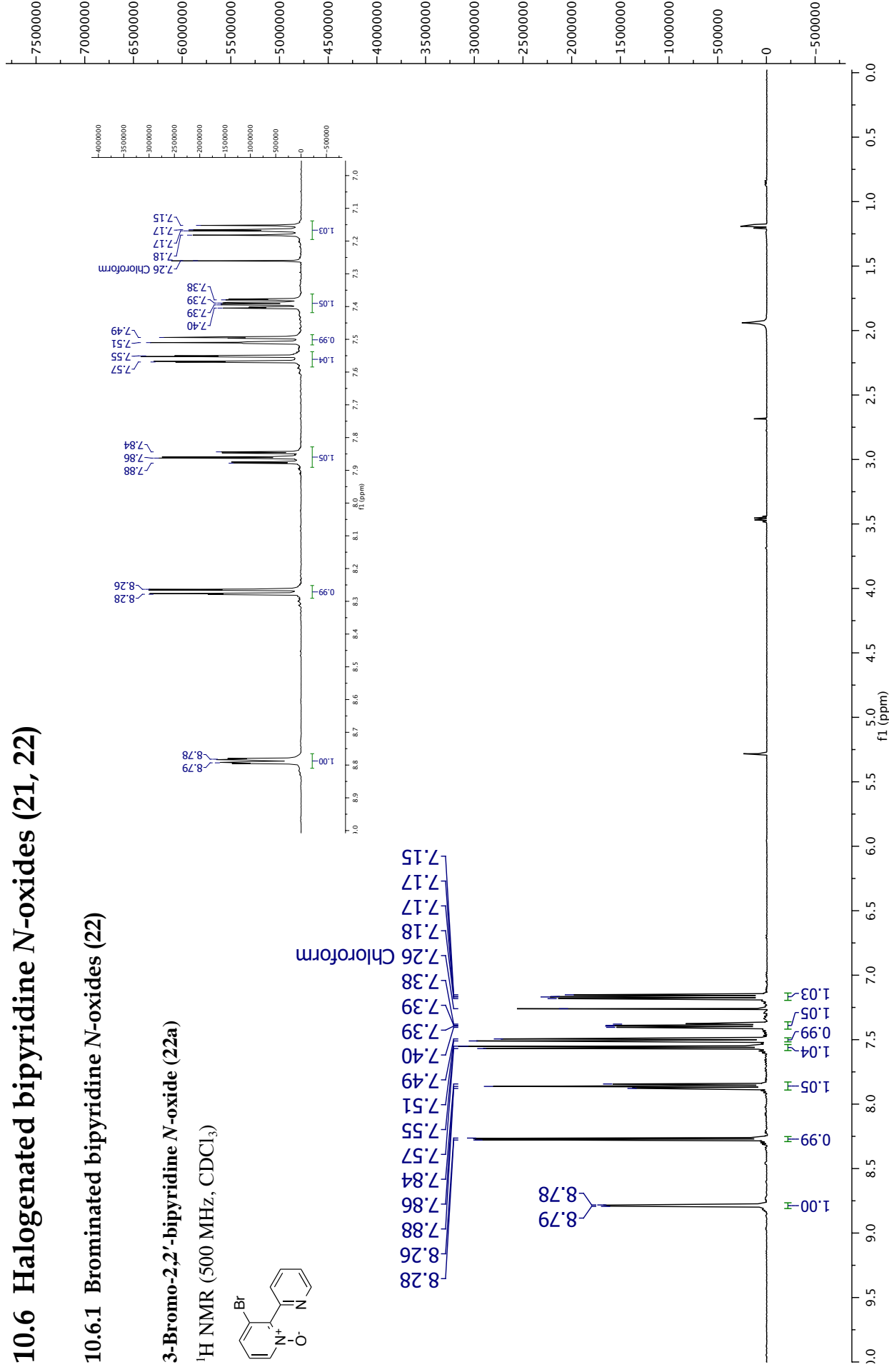
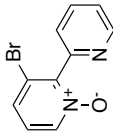


10.6 Halogenated bipyridine N-oxides (21, 22)

10.6.1 Brominated bipyridine N-oxides (22)

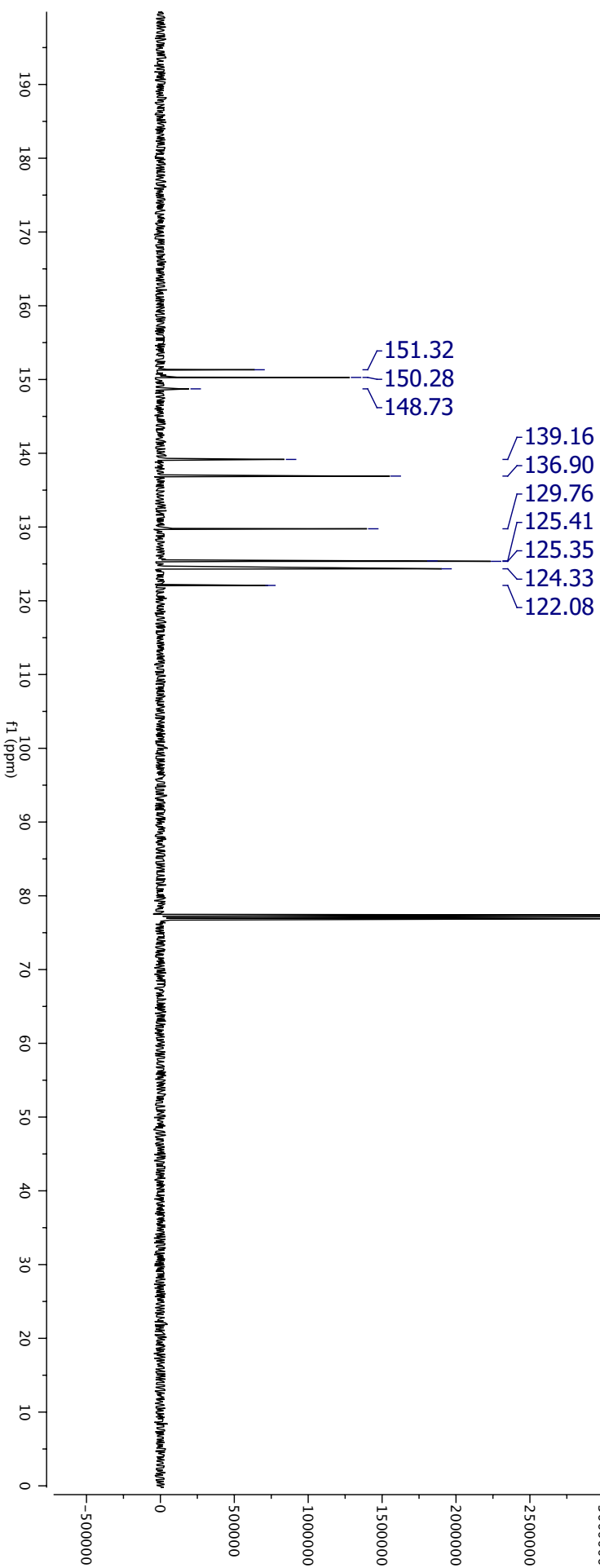
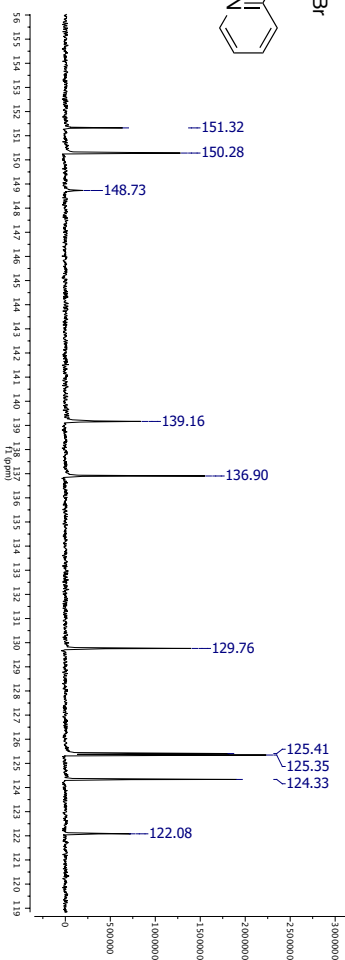
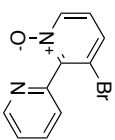
3-Bromo-2,2'-bipyridine N-oxide (22a)

¹H NMR (500 MHz, CDCl₃)



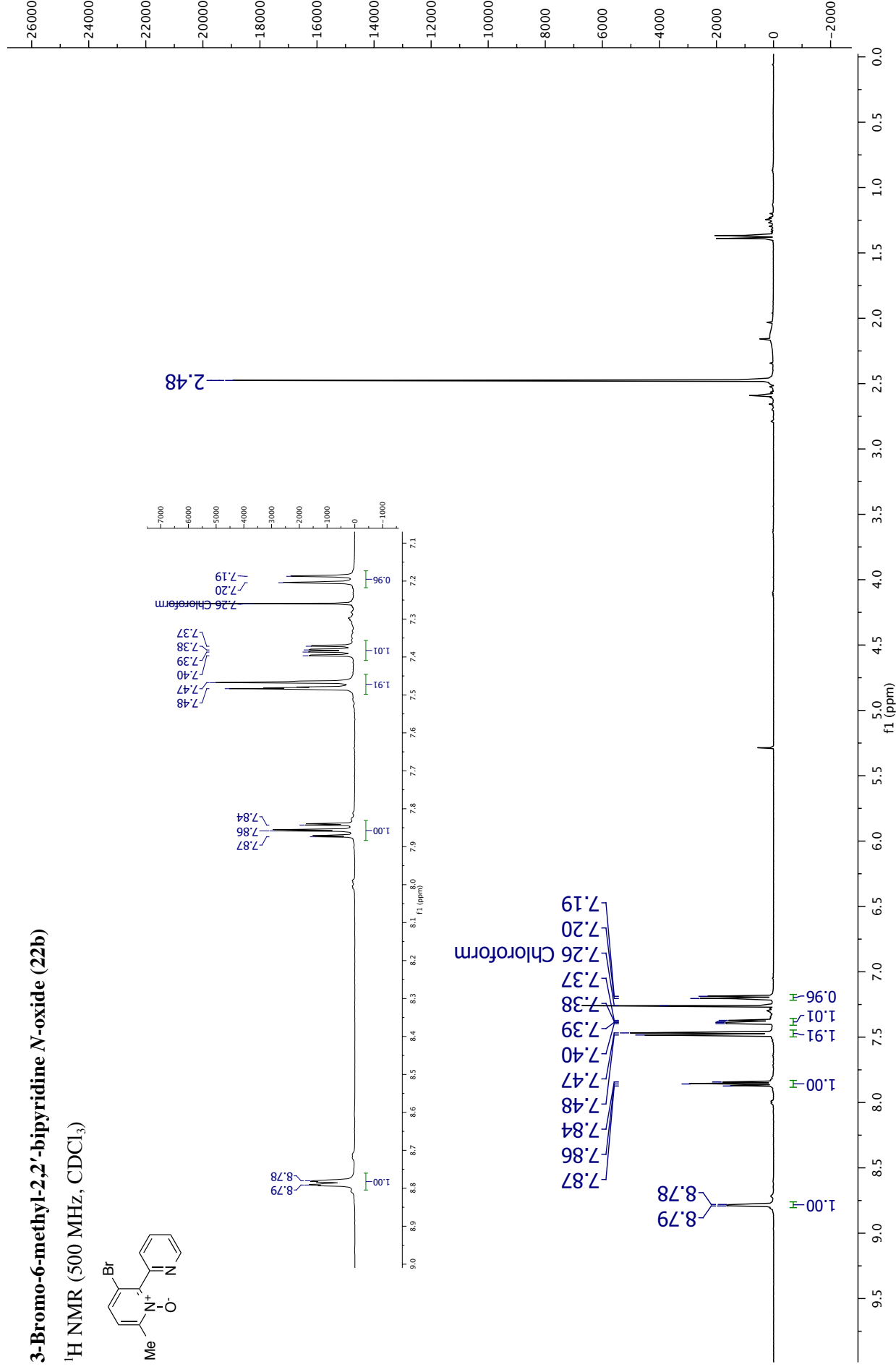
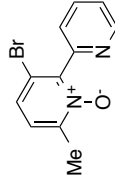
3-Bromo-2,2'-bipyridine N-oxide (22a)

^{13}C NMR (126 MHz, CDCl_3)



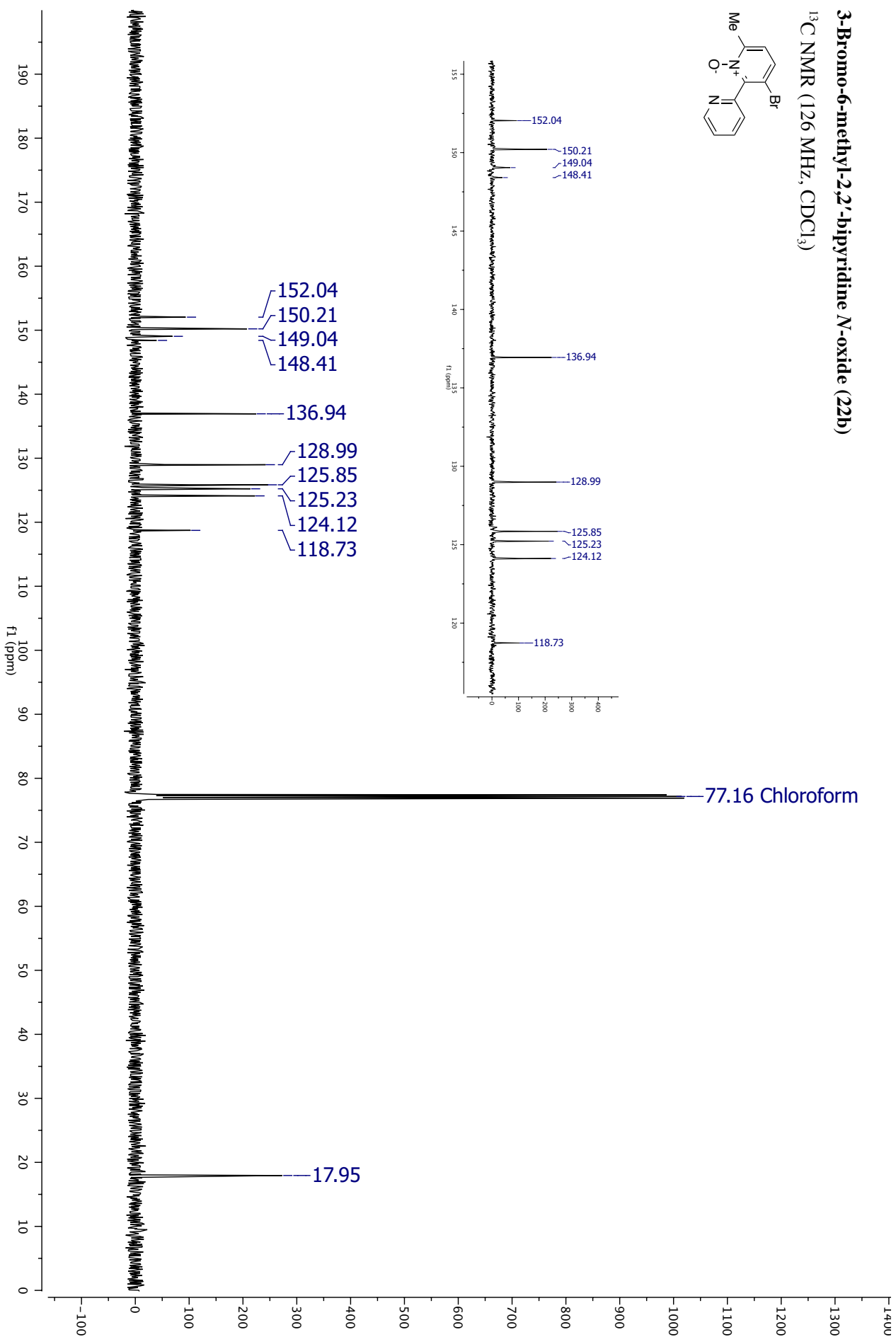
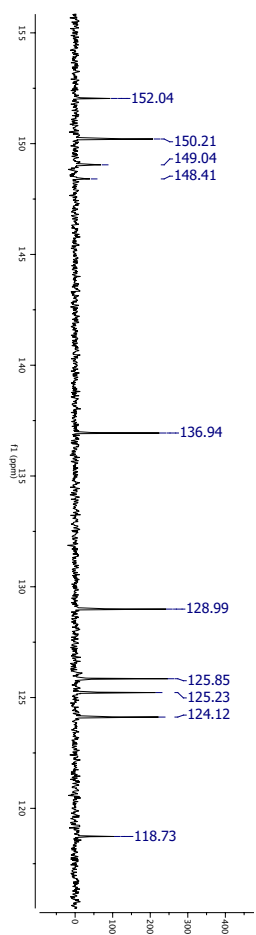
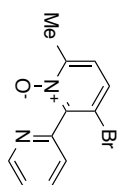
3-Bromo-6-methyl-2,2'-bipyridine N-oxide (22b)

¹H NMR (500 MHz, CDCl₃)



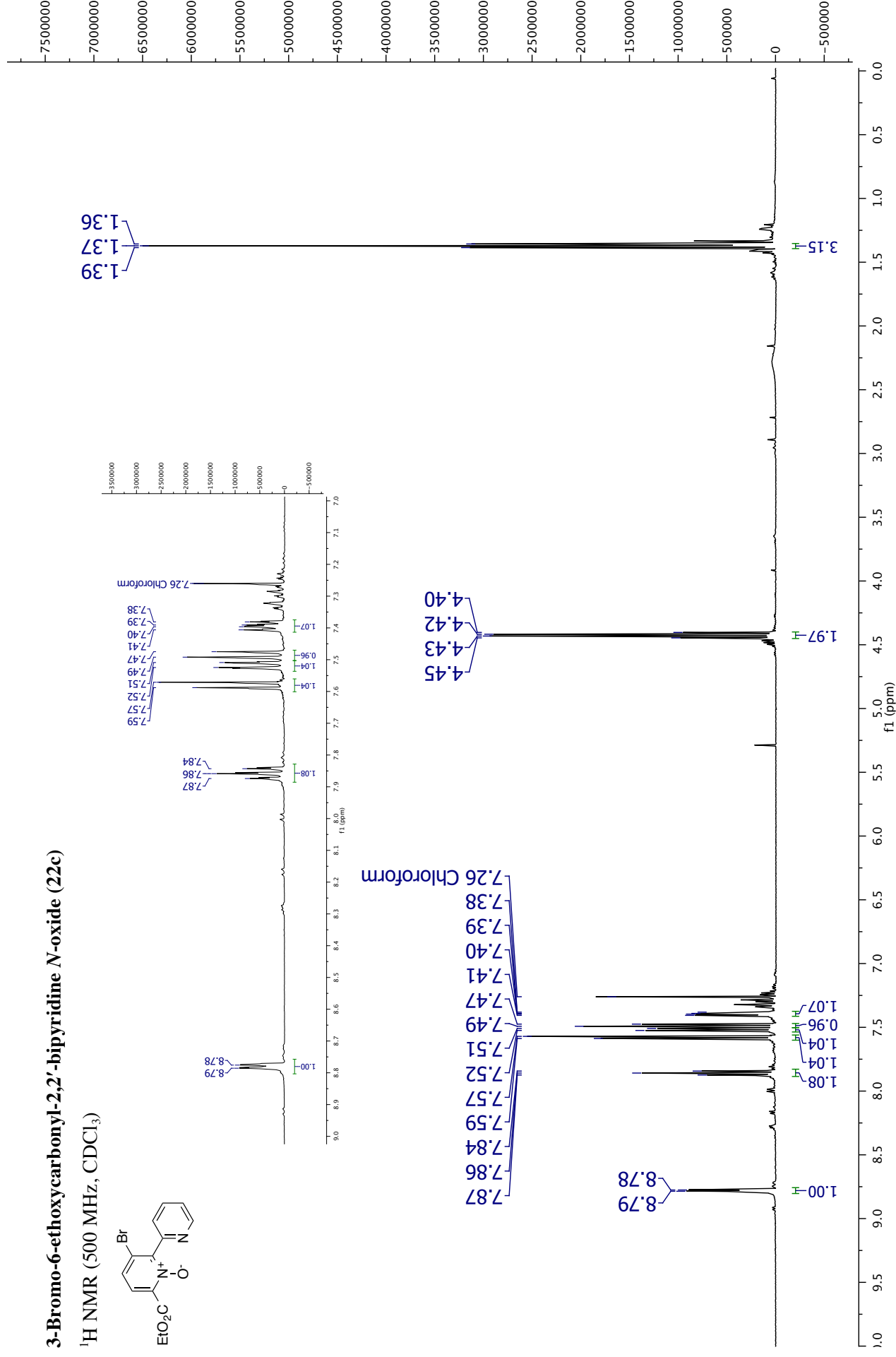
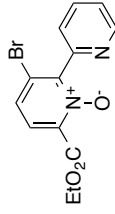
3-Bromo-6-methyl-2,2'-bipyridine N-oxide (22b)

^{13}C NMR (126 MHz, CDCl_3)



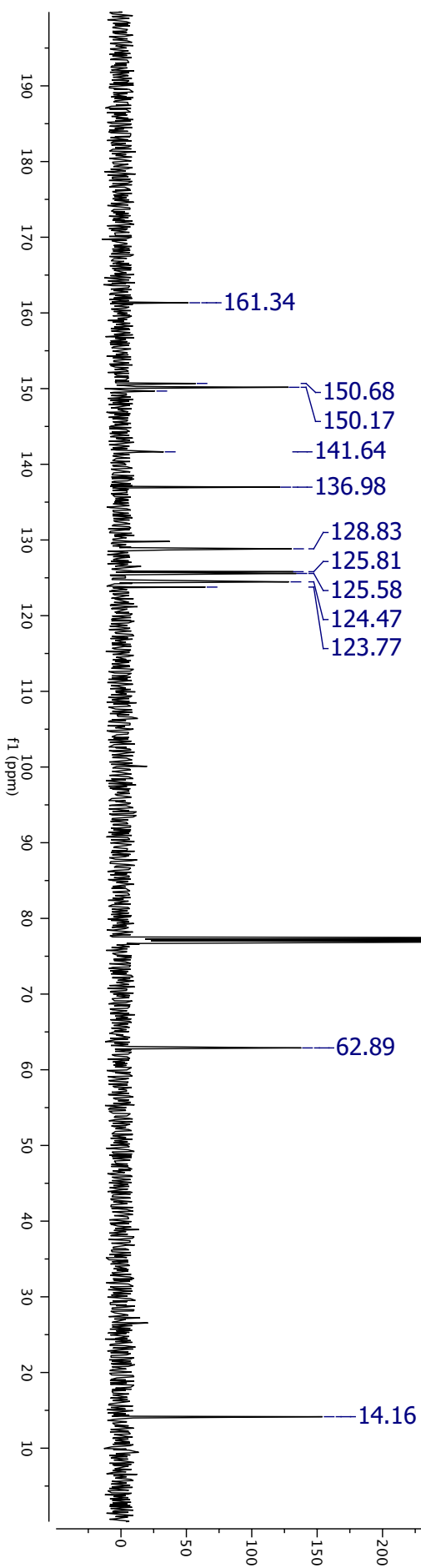
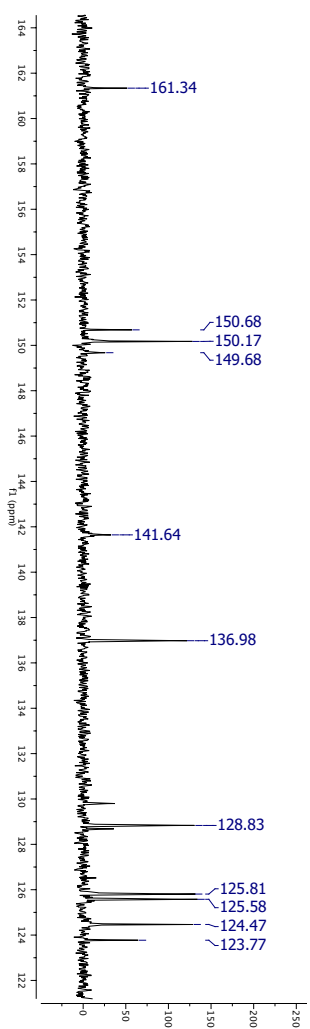
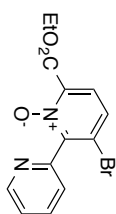
3-Bromo-6-ethoxycarbonyl-2,2'-bipyridine N-oxide (22c)

¹H NMR (500 MHz, CDCl₃)



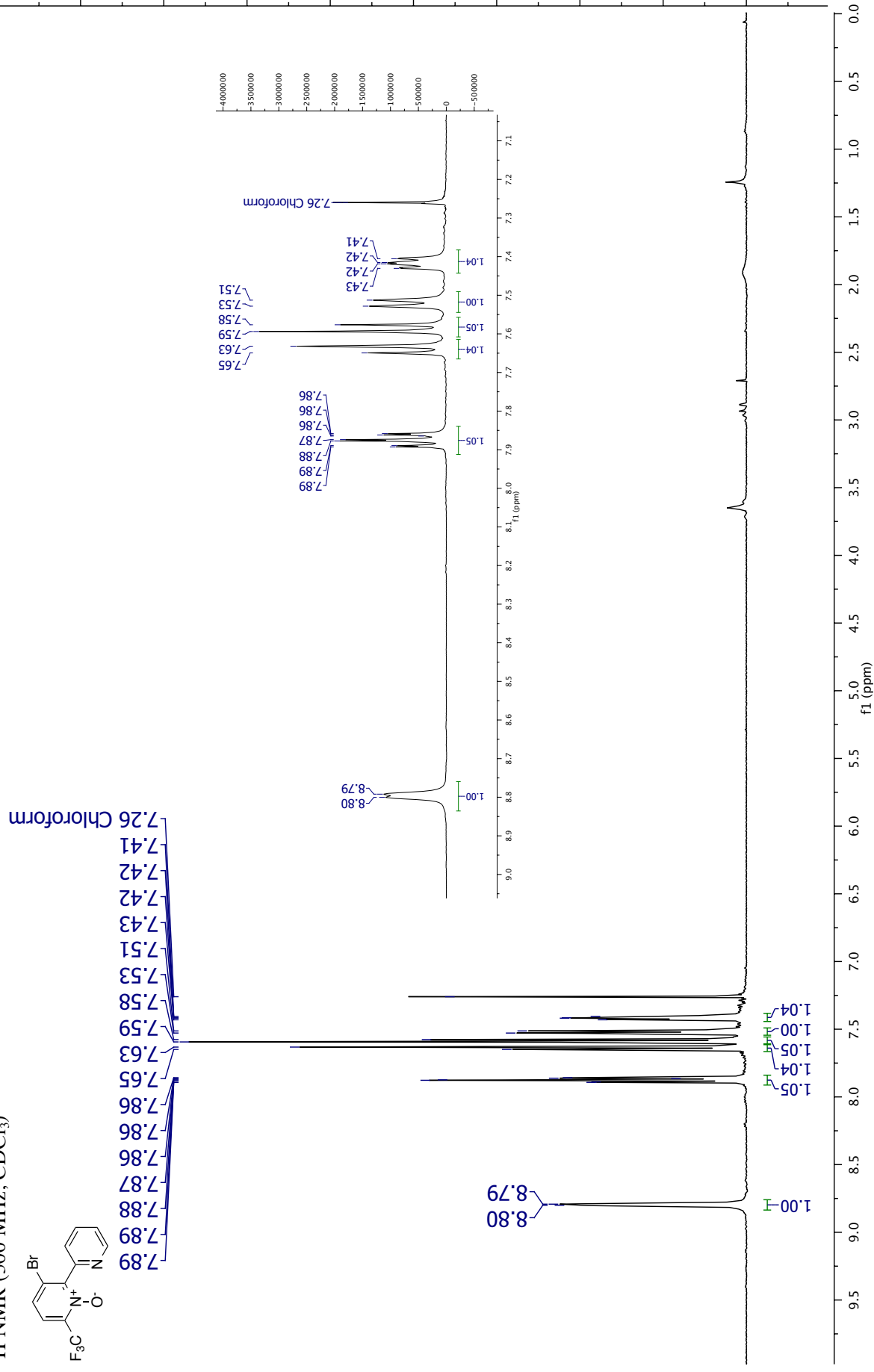
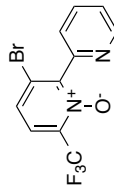
3-Bromo-6-ethoxycarbonyl-2,2'-bipyridine N-oxide (22c)

¹³C NMR (126 MHz, CDCl₃)



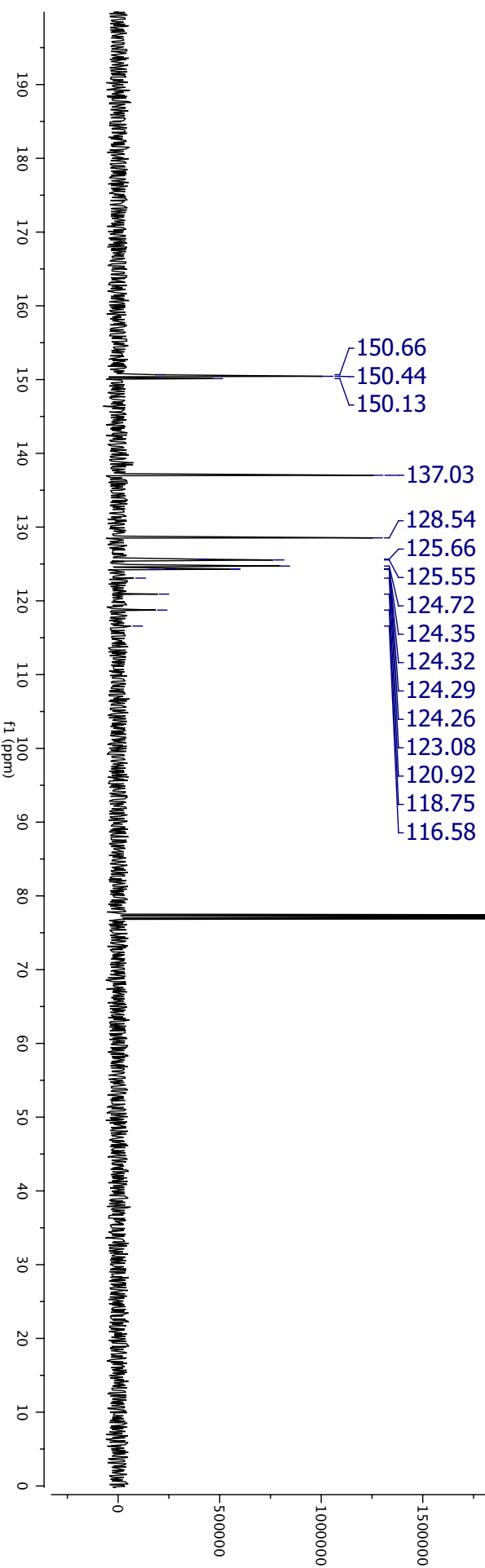
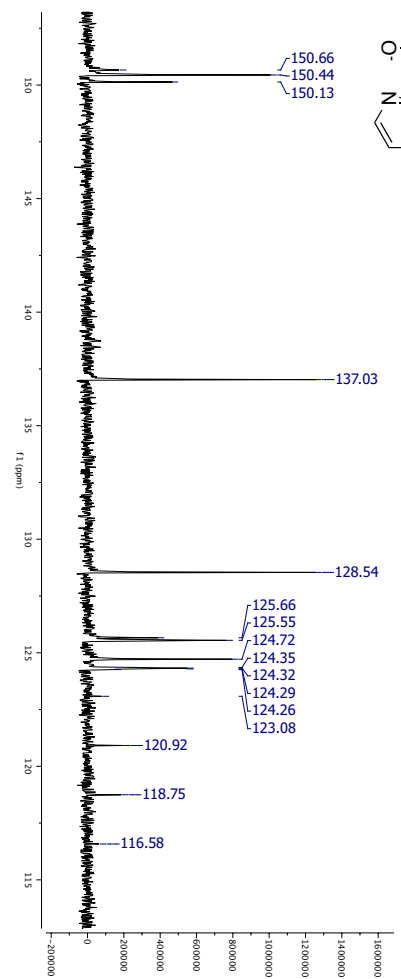
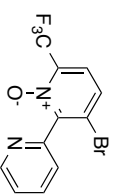
3-Bromo-6-trifluoromethyl-2,2'-bipyridine N-oxide (22d)

¹H NMR (500 MHz, CDCl₃)



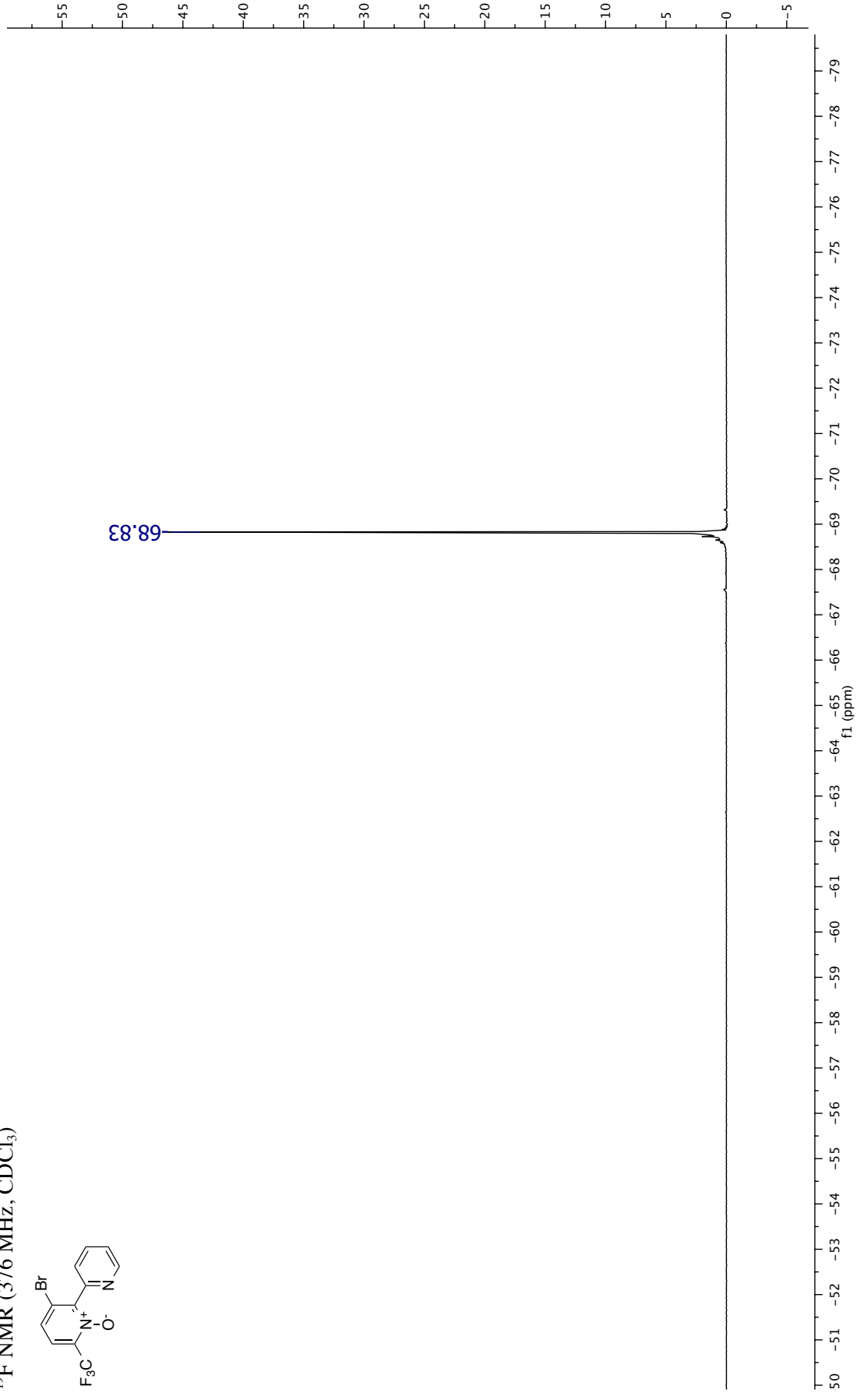
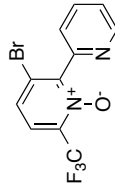
3-Bromo-6-(trifluoromethyl)-2,2'-bipyridine N-oxide (22d)

¹³C NMR (126 MHz, CDCl₃)



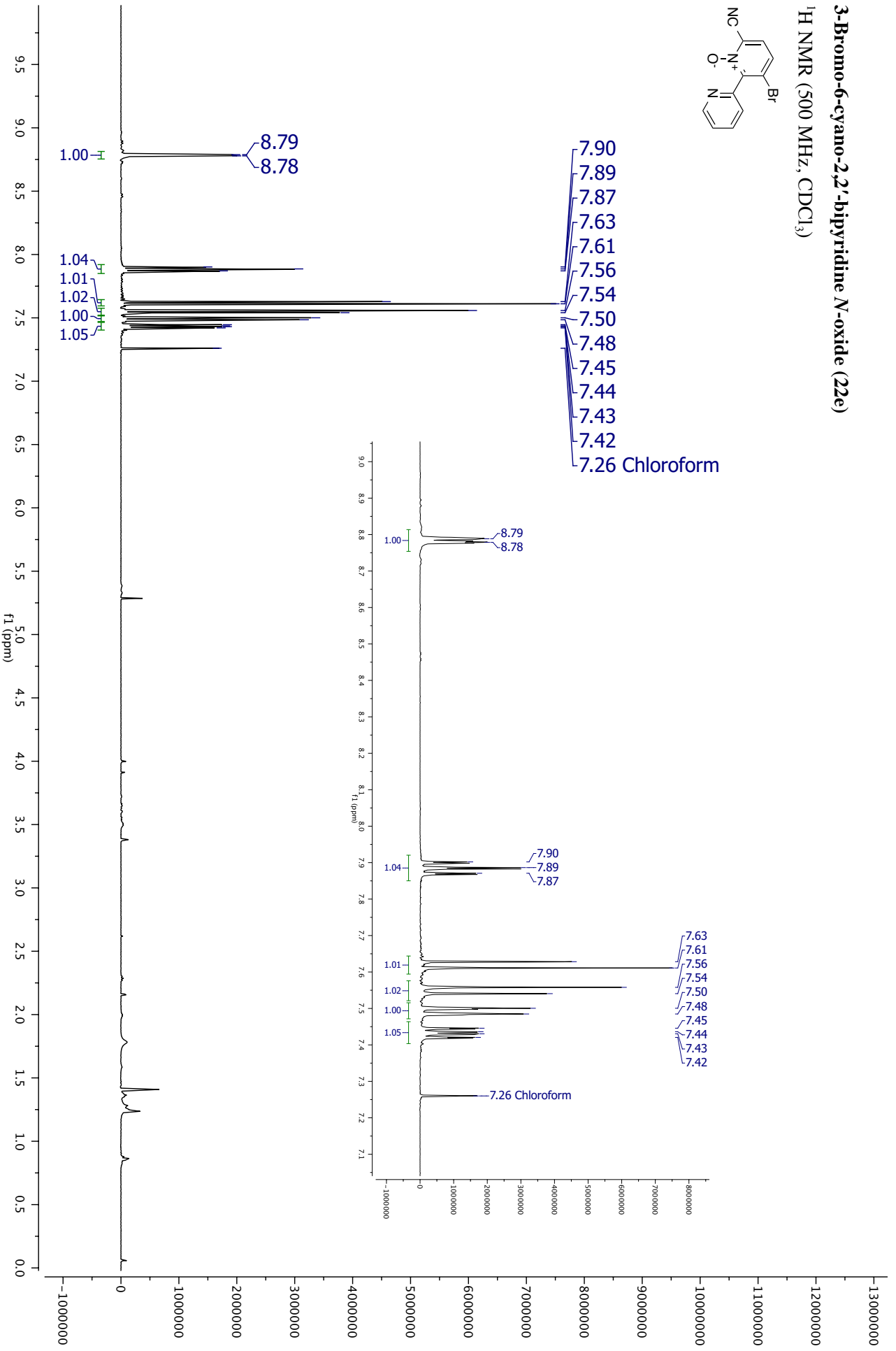
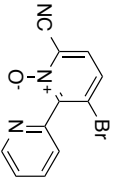
3-Bromo-6-trifluoromethyl-2,2'-bipyridine N-oxide (22d)

^{19}F NMR (376 MHz, CDCl_3)



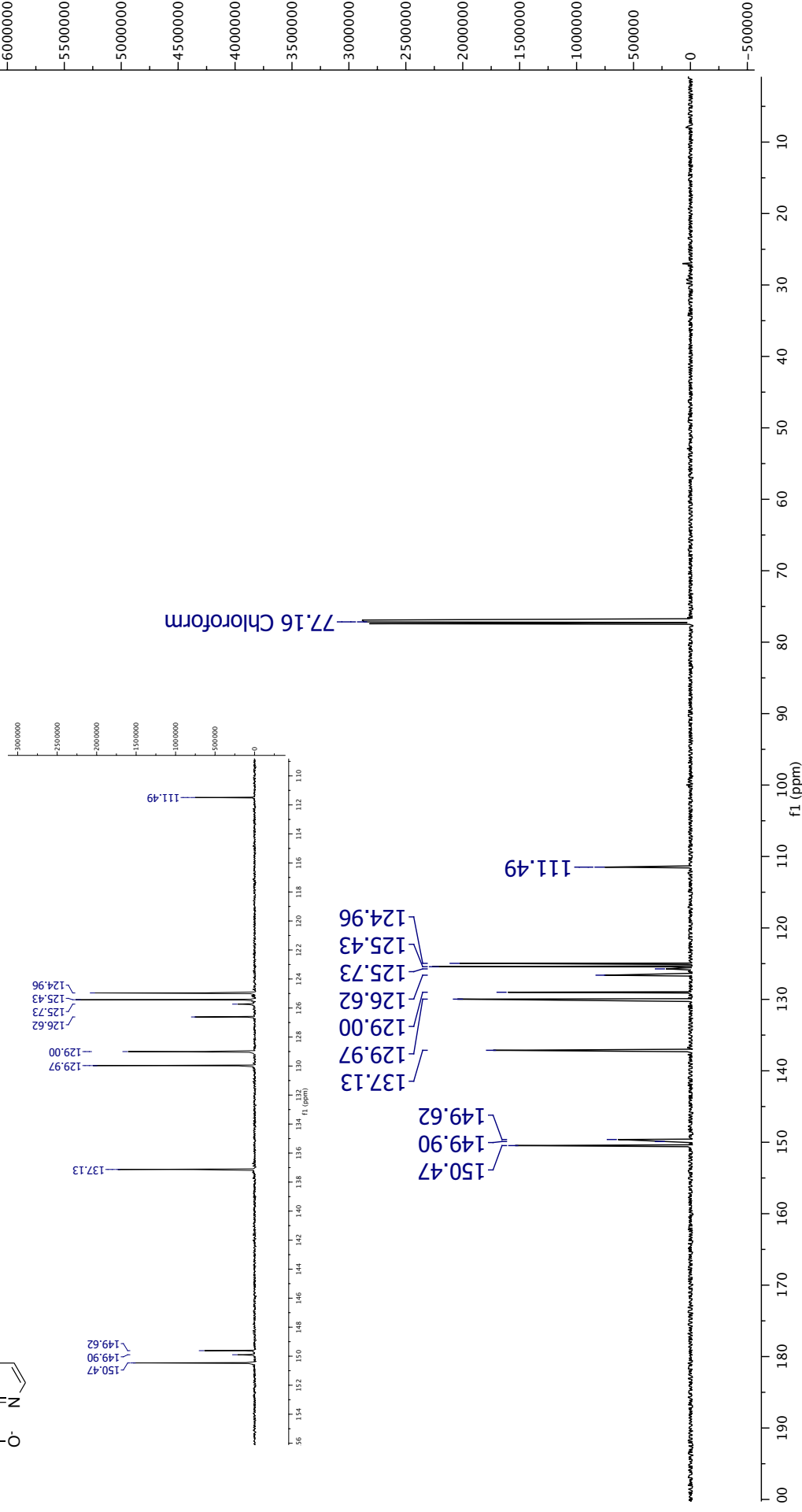
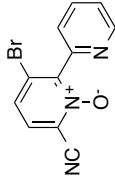
3-Bromo-6-cyano-2,2'-bipyridine N-oxide (22e)

¹H NMR (500 MHz, CDCl₃)



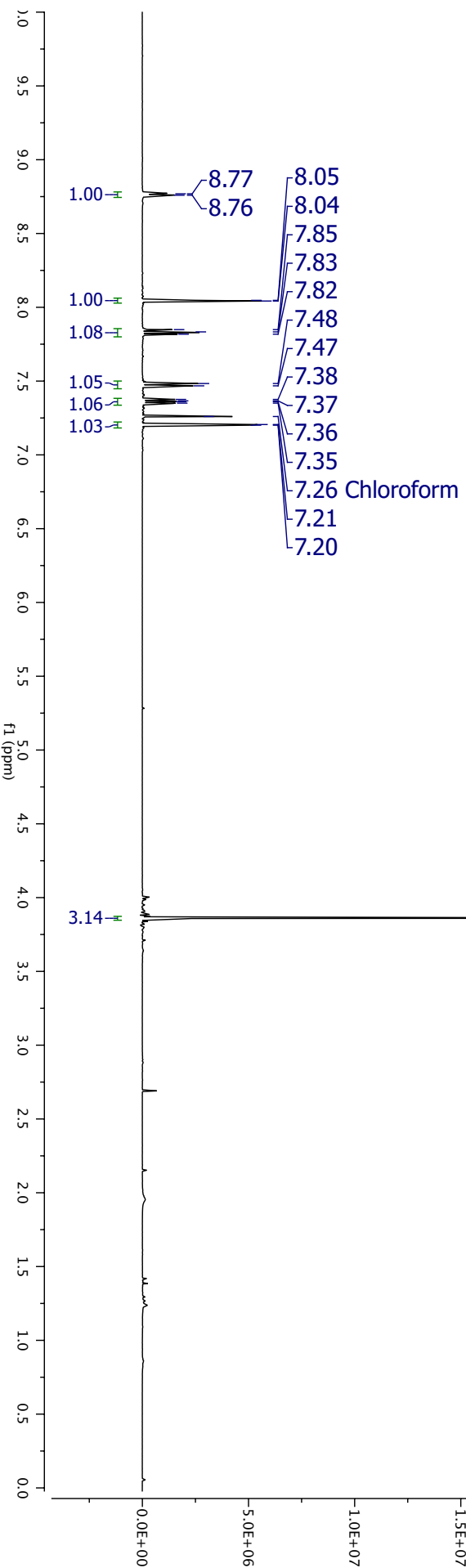
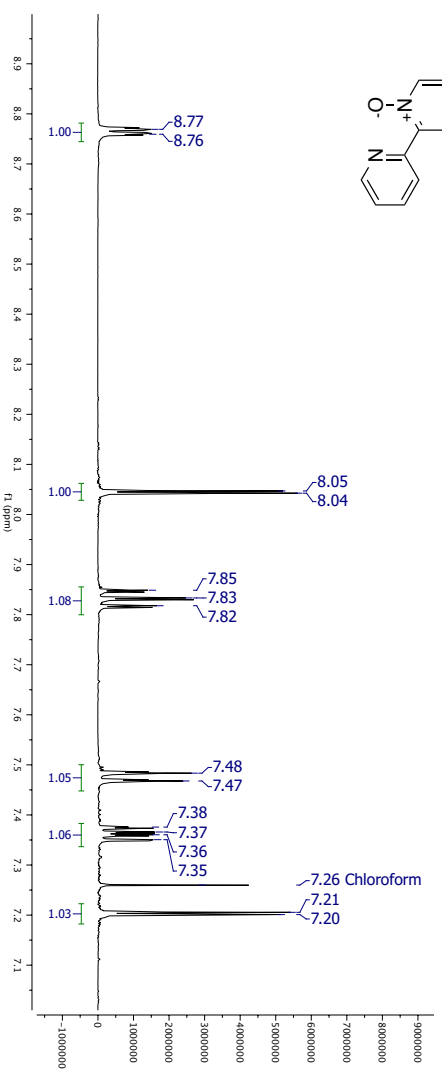
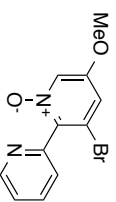
3-Bromo-6-cyano-2,2'-bipyridine N-oxide (22e)

^{13}C NMR (126 MHz, CDCl_3)



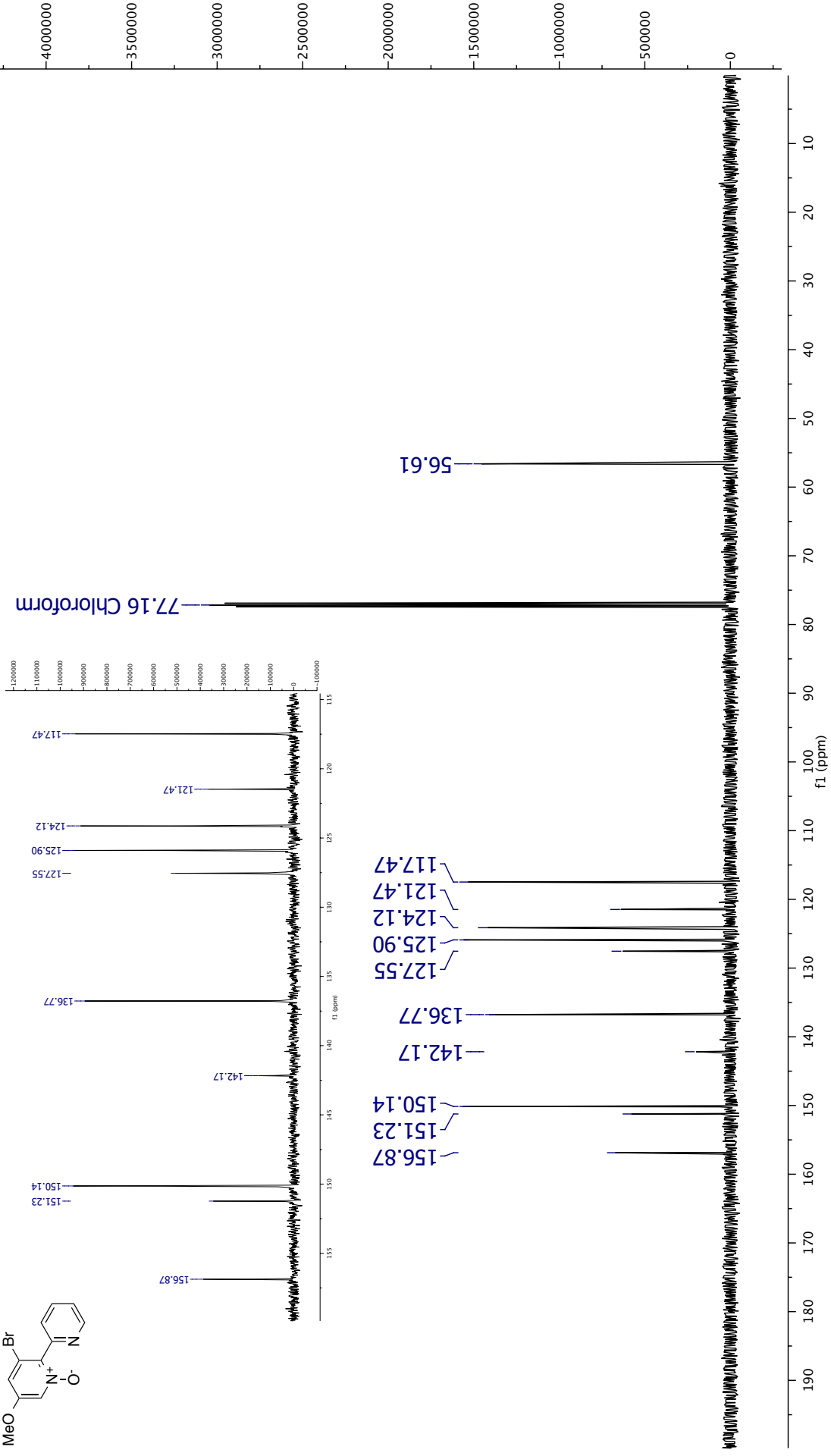
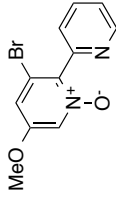
3-Bromo-5-methoxy-2,2'-bipyridine N-oxide (22f)

¹H NMR (500 MHz, CDCl₃)



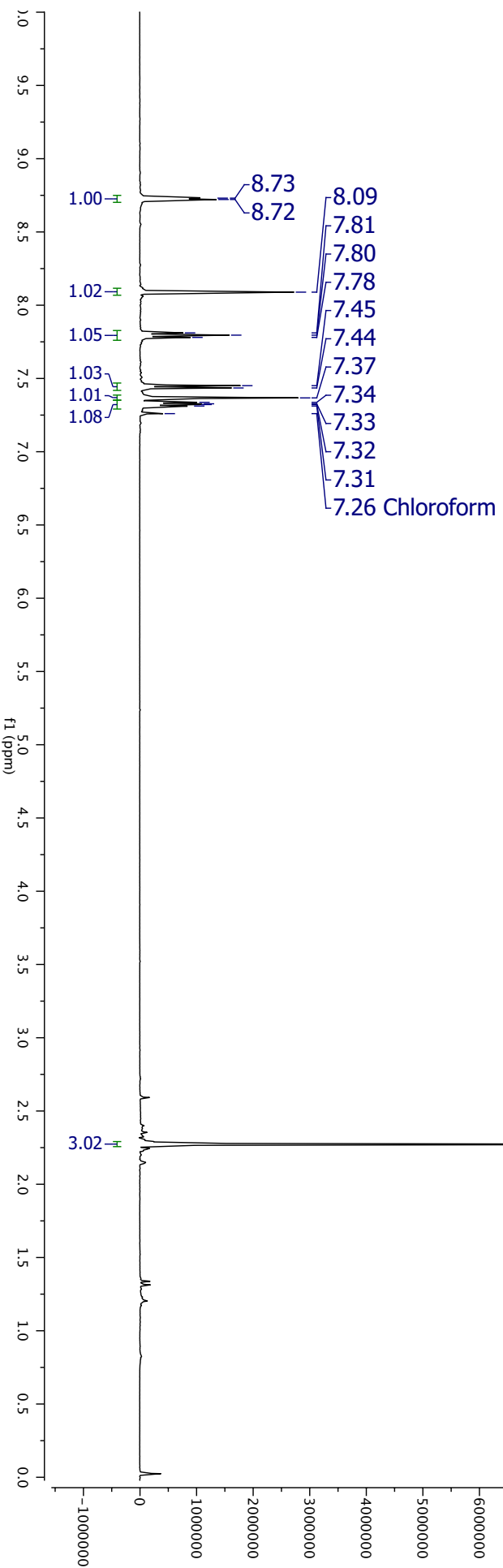
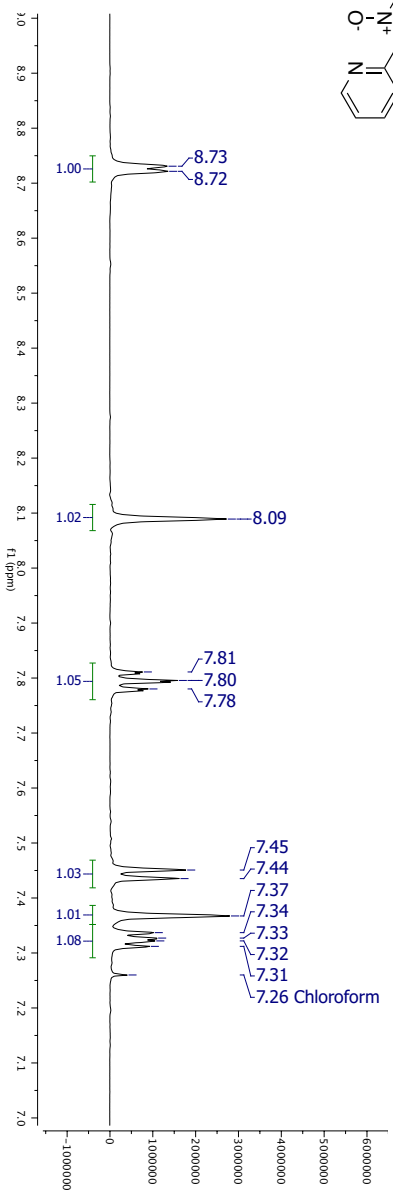
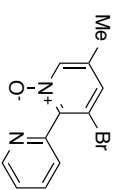
3-Bromo-5-methoxy-2,2'-bipyridine *N*-oxide (22f)

¹³C NMR (126 MHz, CDCl₃)



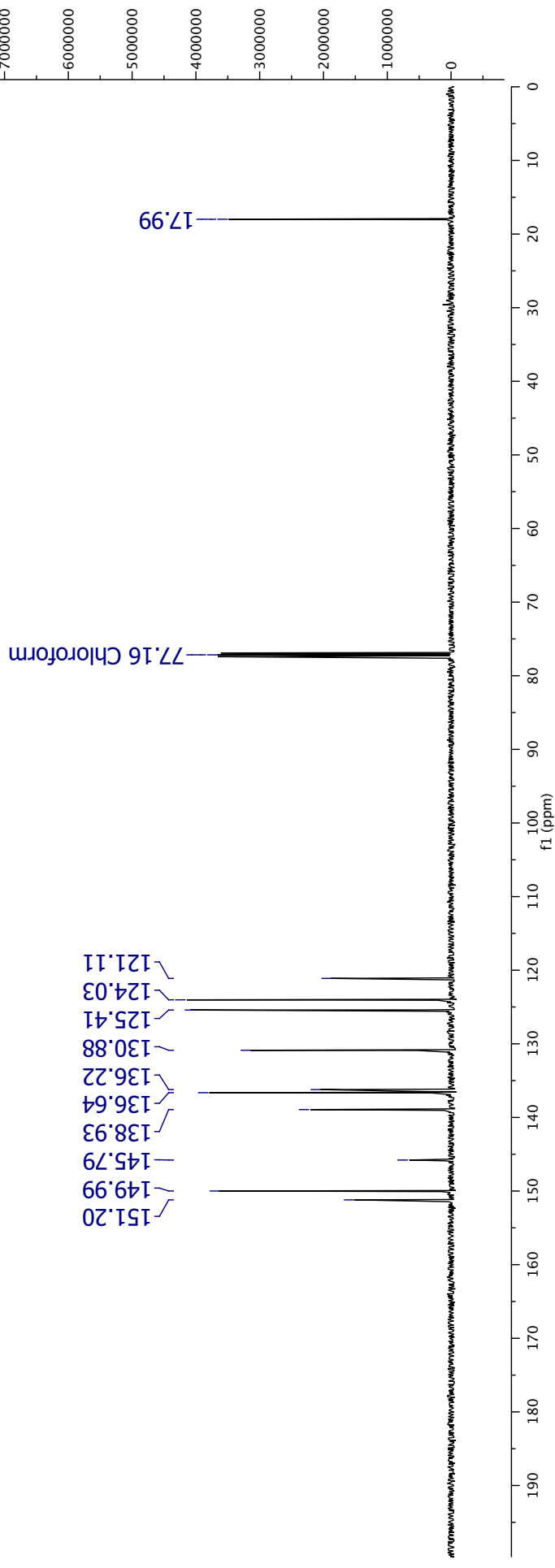
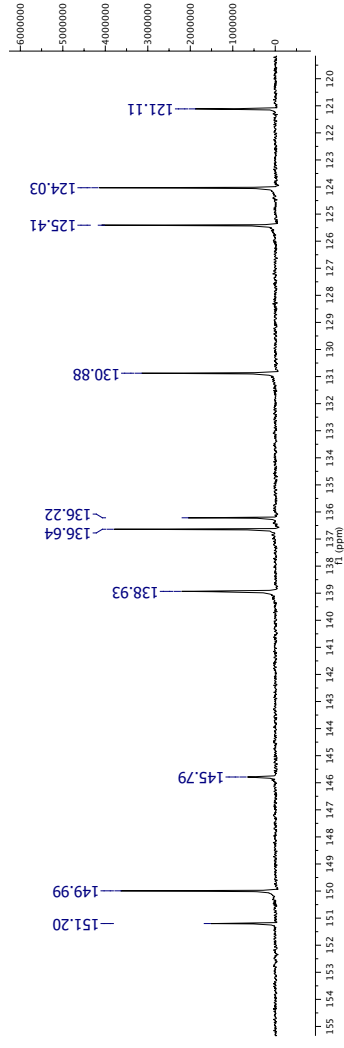
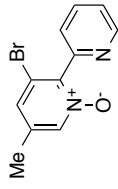
3-Bromo-5-methyl-2,2'-bipyridine N-oxide (22g)

¹H NMR (400 MHz, CDCl₃)



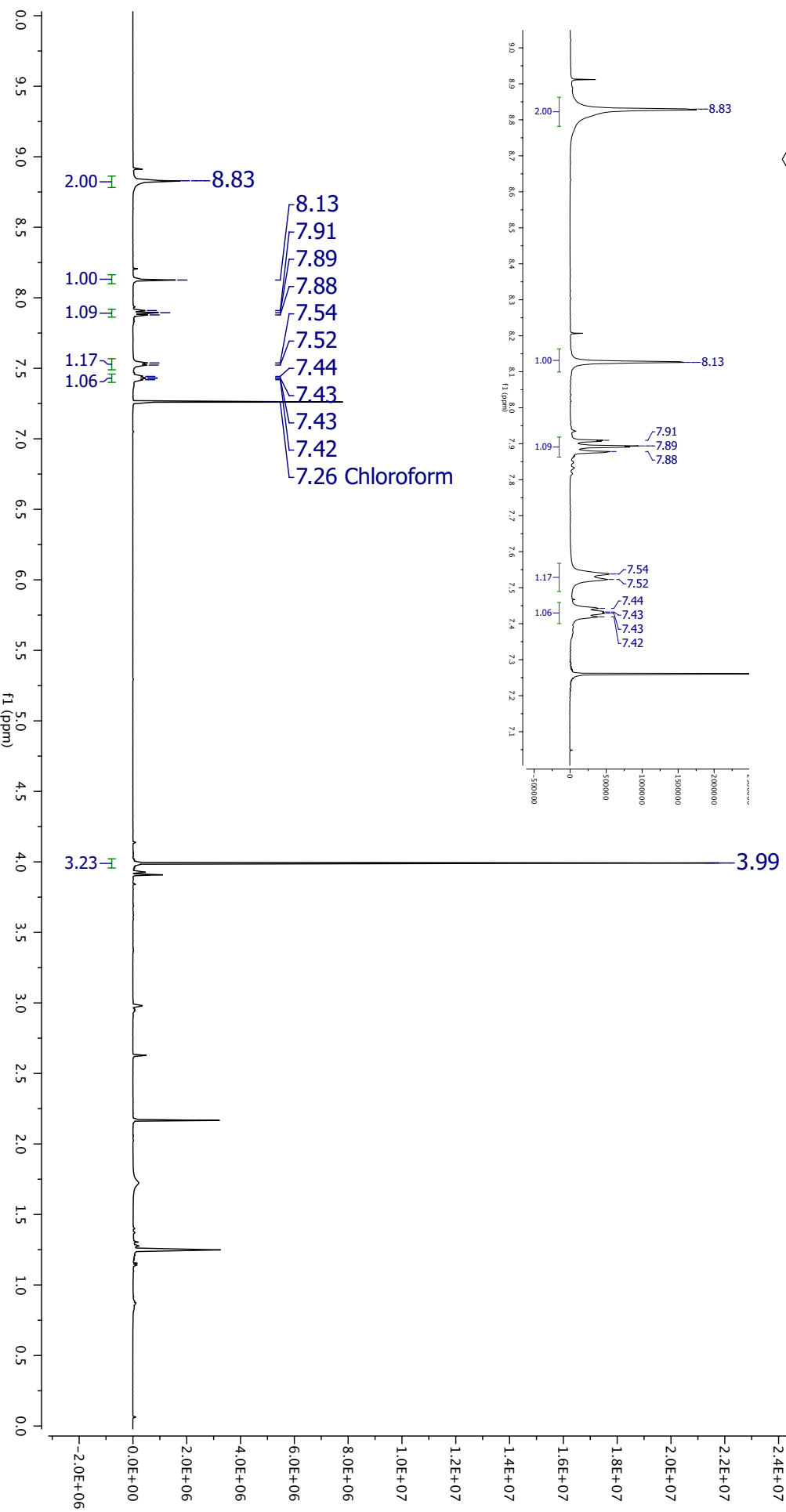
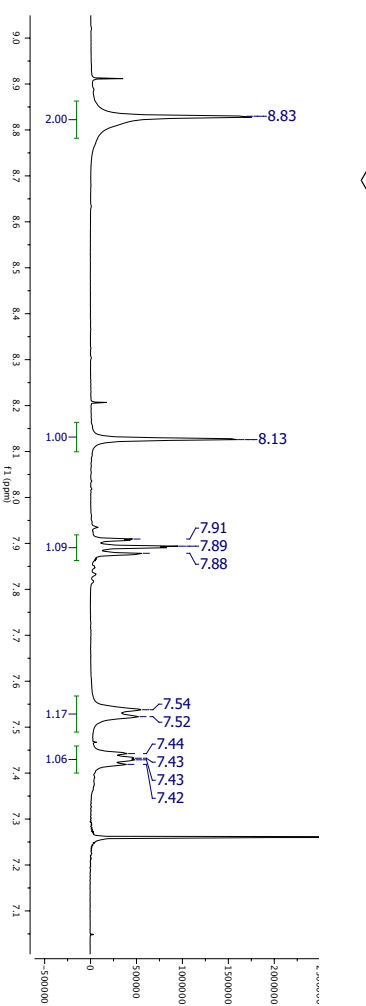
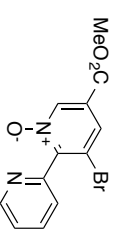
3-Bromo-5-methyl-2,2'-bipyridine N-oxide (22g)

^{13}C NMR (126 MHz, CDCl_3)



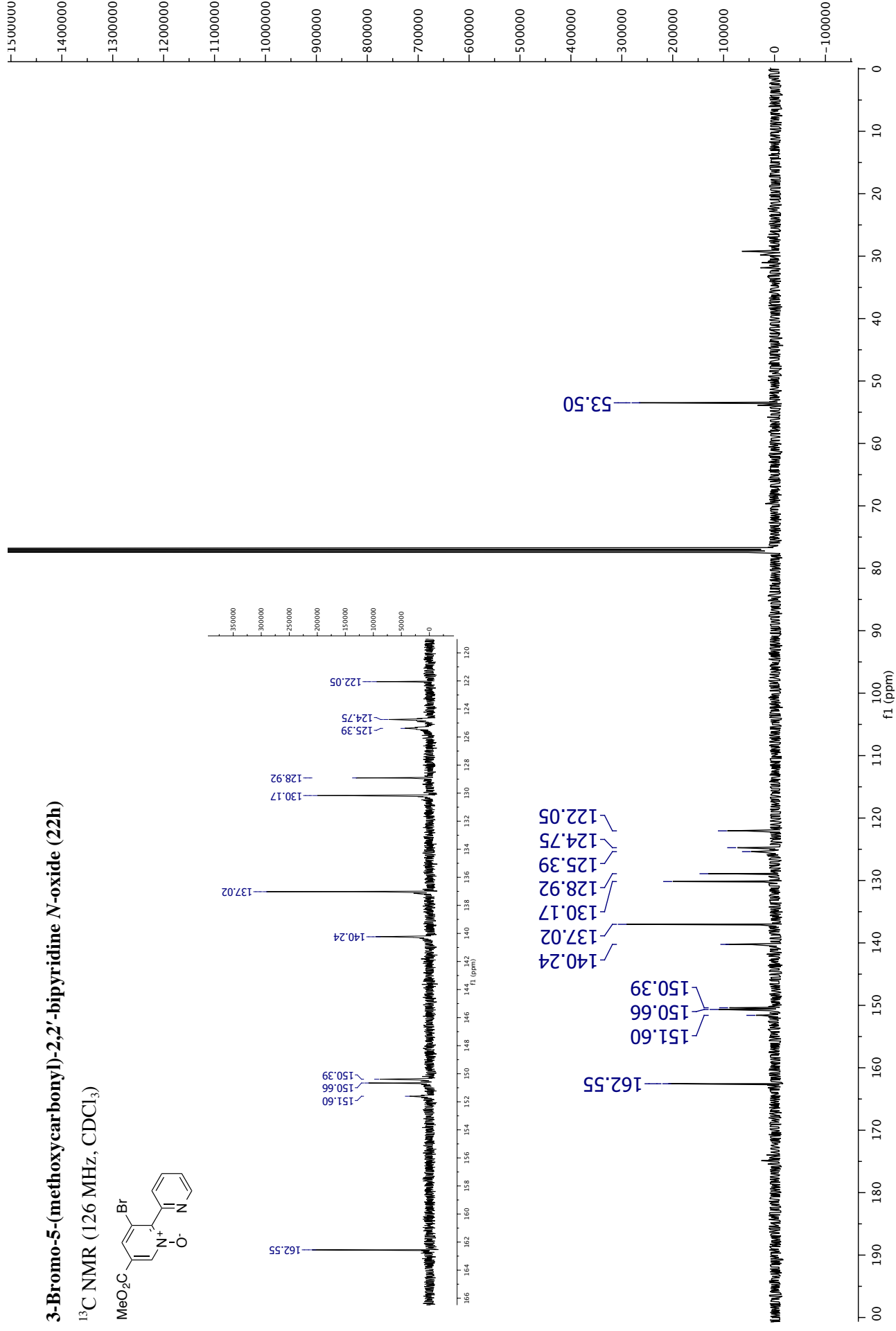
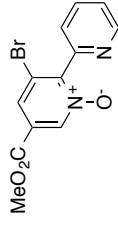
3-Bromo-5-methoxycarbonyl-2,2'-bipyridine N-oxide (22h)

¹H NMR (500 MHz, CDCl₃)



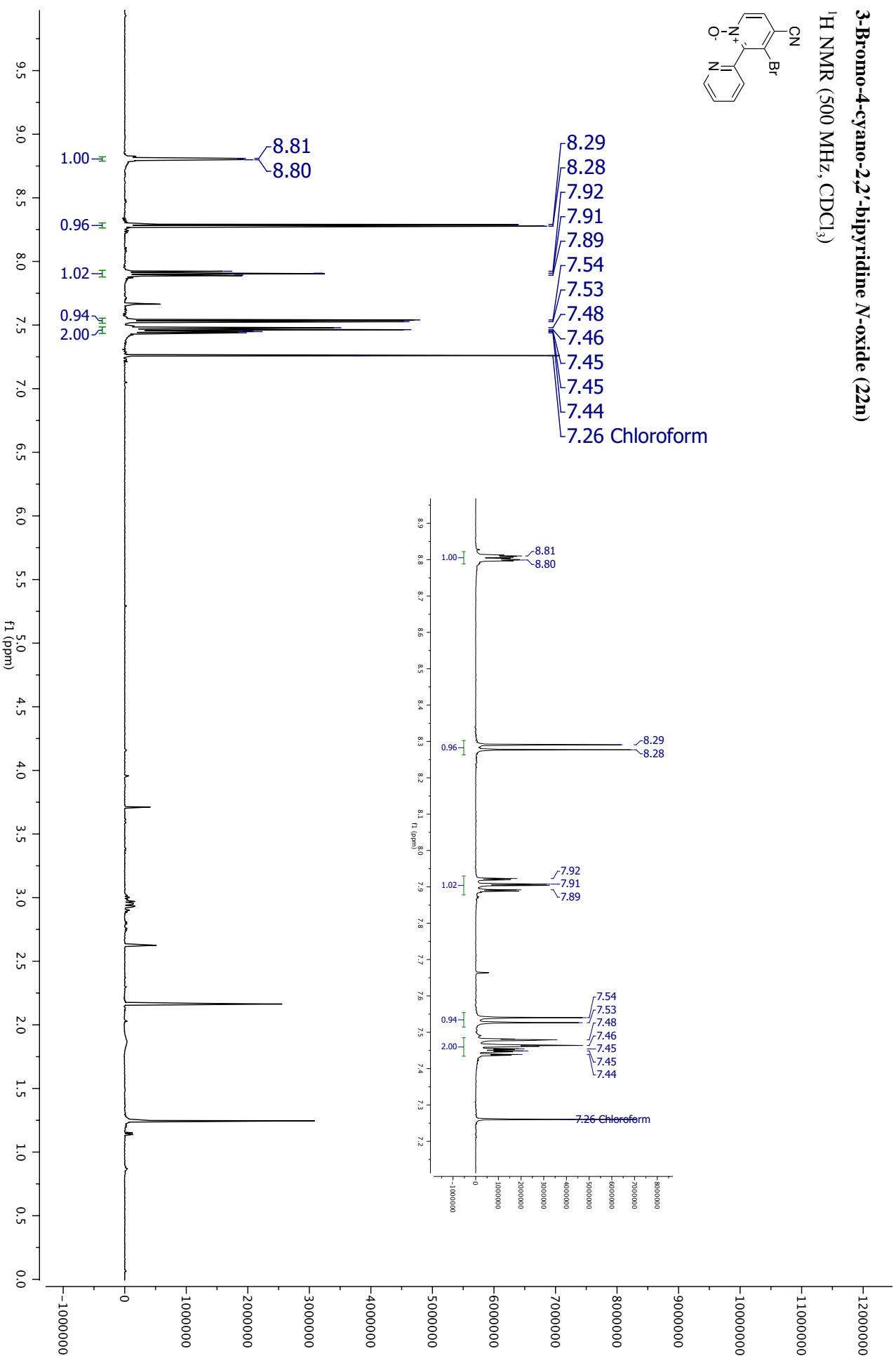
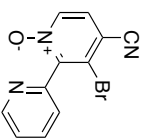
3-Bromo-5-(methoxycarbonyl)-2,2'-bipyridine N-oxide (22h)

^{13}C NMR (126 MHz, CDCl_3)



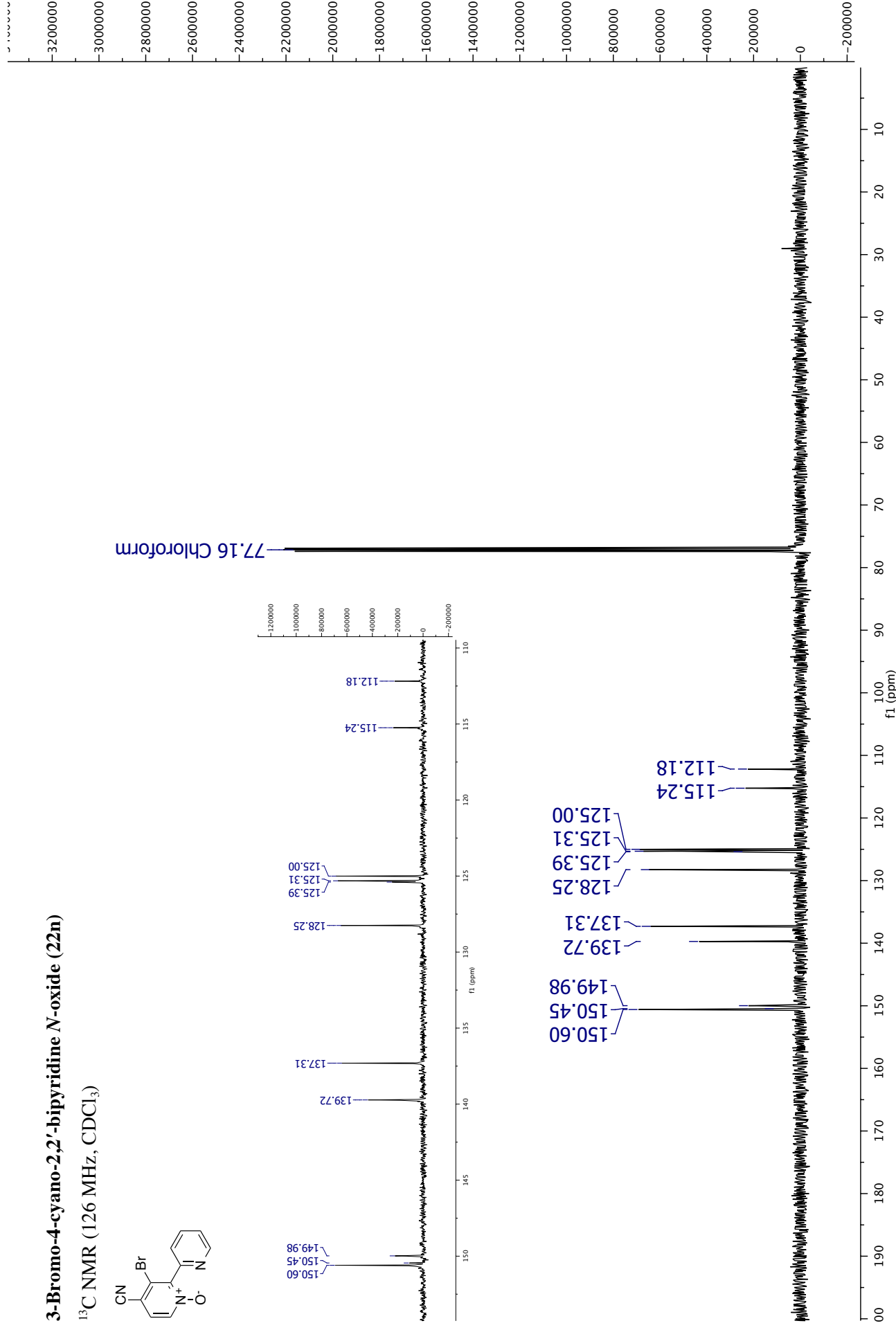
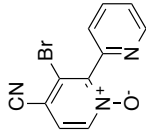
3-Bromo-4-cyano-2,2'-bipyridine N-oxide (22n)

¹H NMR (500 MHz, CDCl₃)



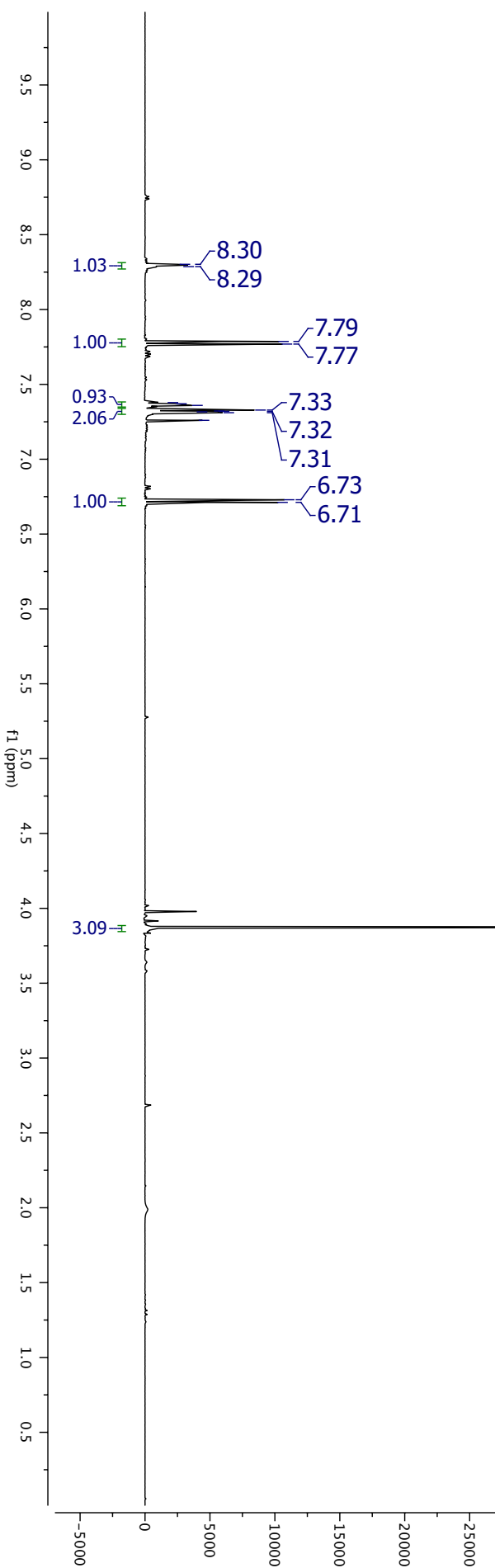
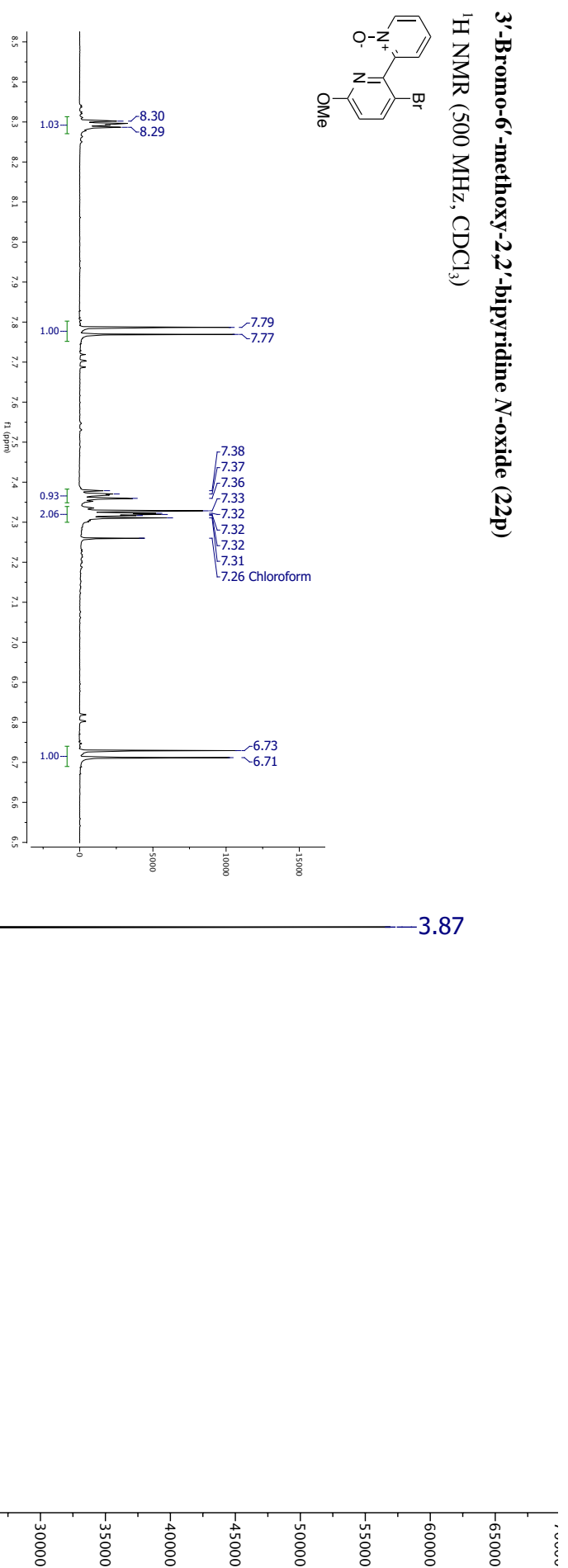
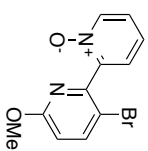
3-Bromo-4-cyano-2,2'-bipyridine N-oxide (22n)

^{13}C NMR (126 MHz, CDCl_3)



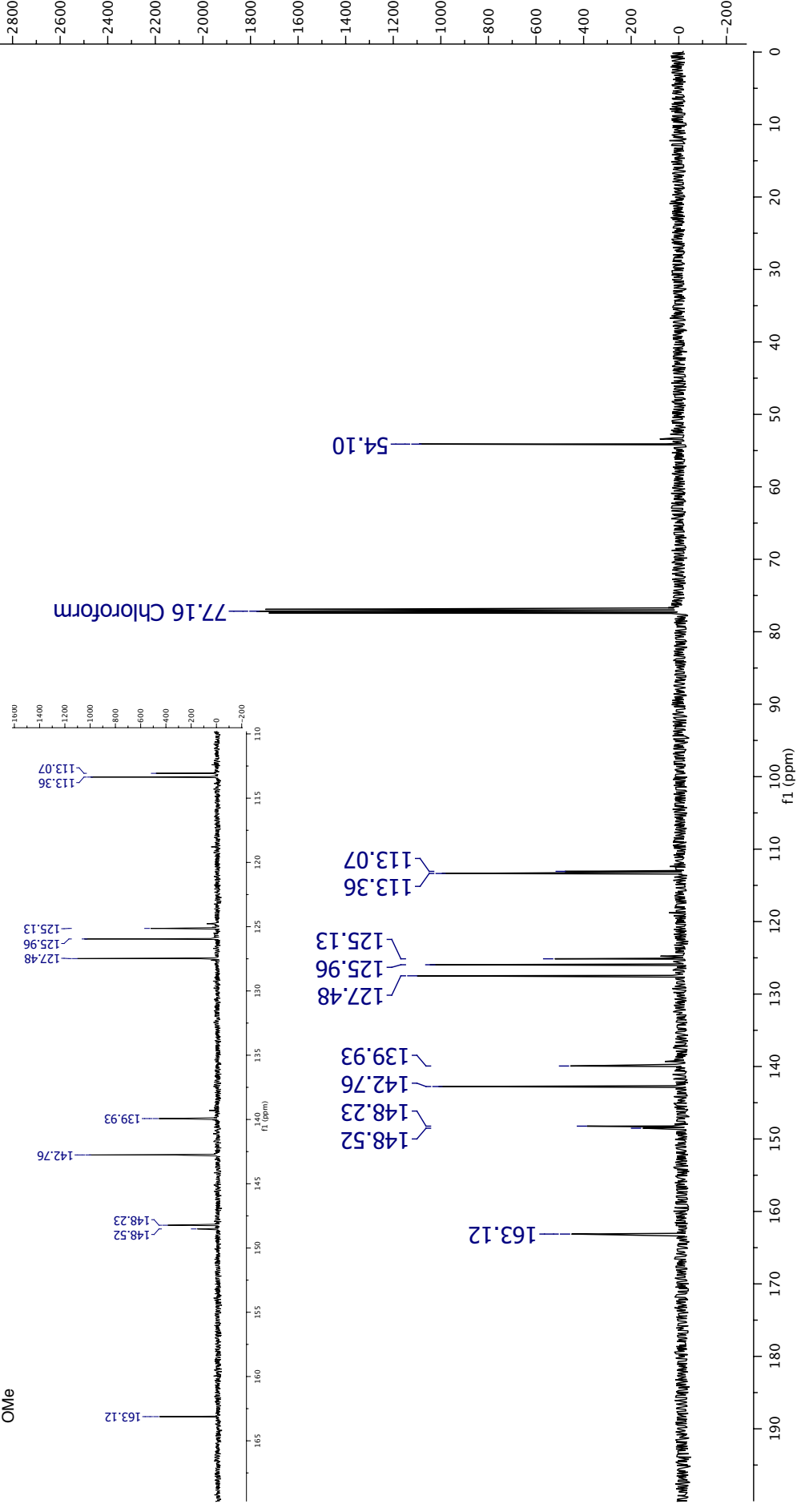
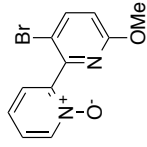
3'-Bromo-6'-methoxy-2,2'-bipyridine N-oxide (22p)

¹H NMR (500 MHz, CDCl₃)



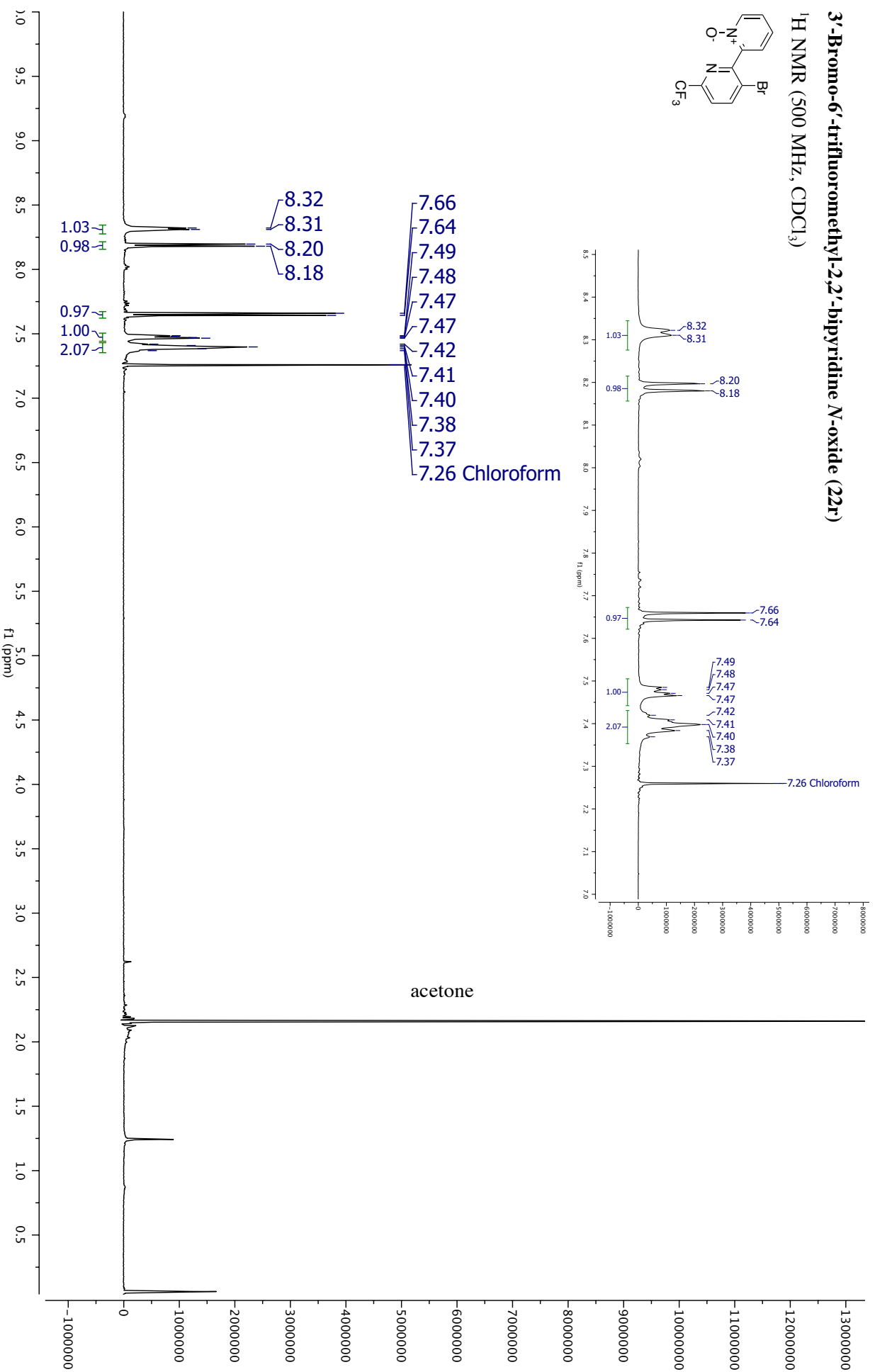
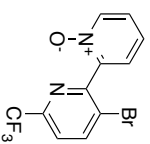
3'-Bromo-6'-methoxy-2,2'-bipyridine N-oxide (22p)

¹³C NMR (126 MHz, CDCl₃)



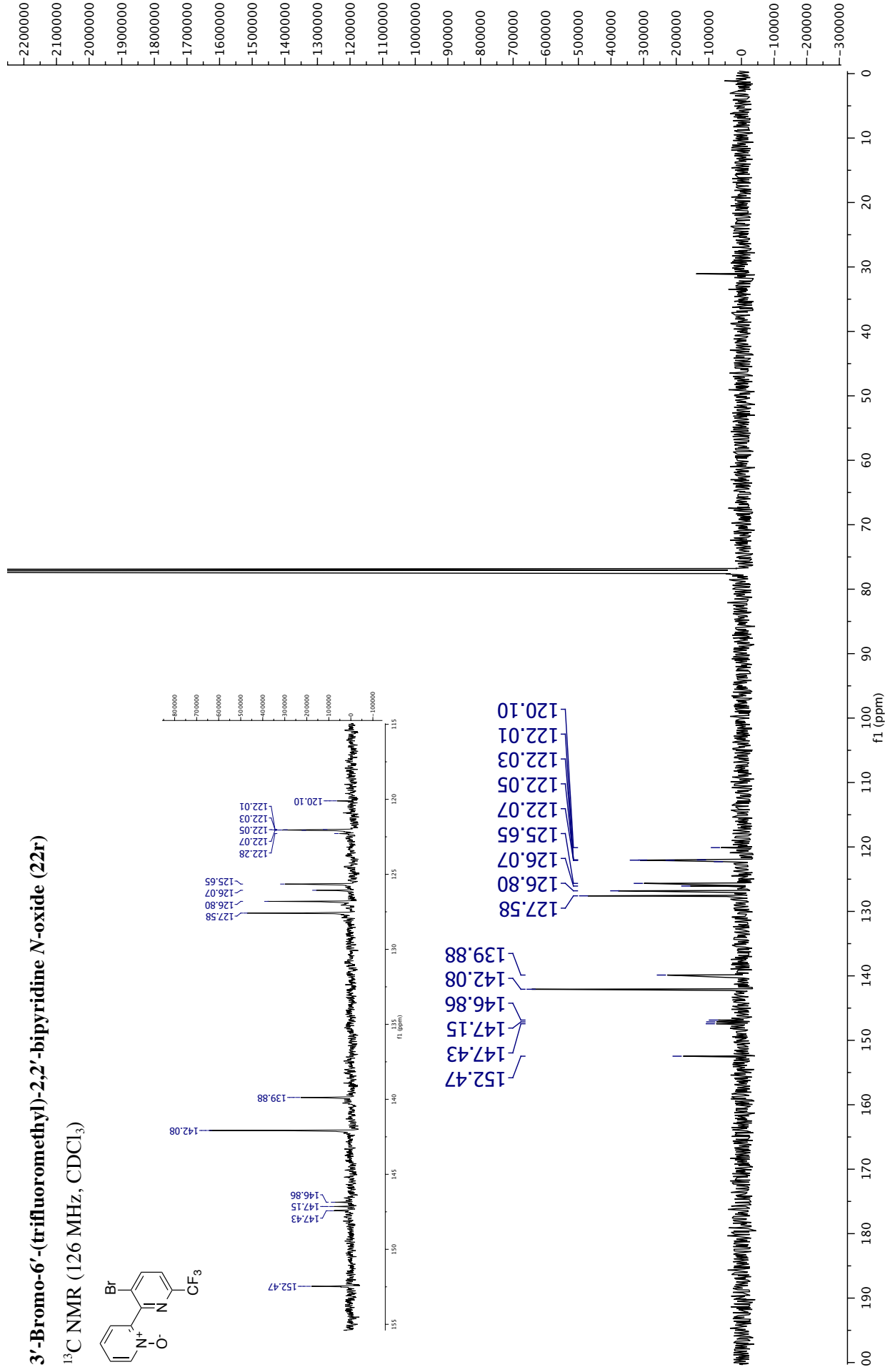
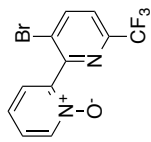
3'-Bromo-6'-trifluoromethyl-2,2'-bipyridine N-oxide (22r)

¹H NMR (500 MHz, CDCl₃)



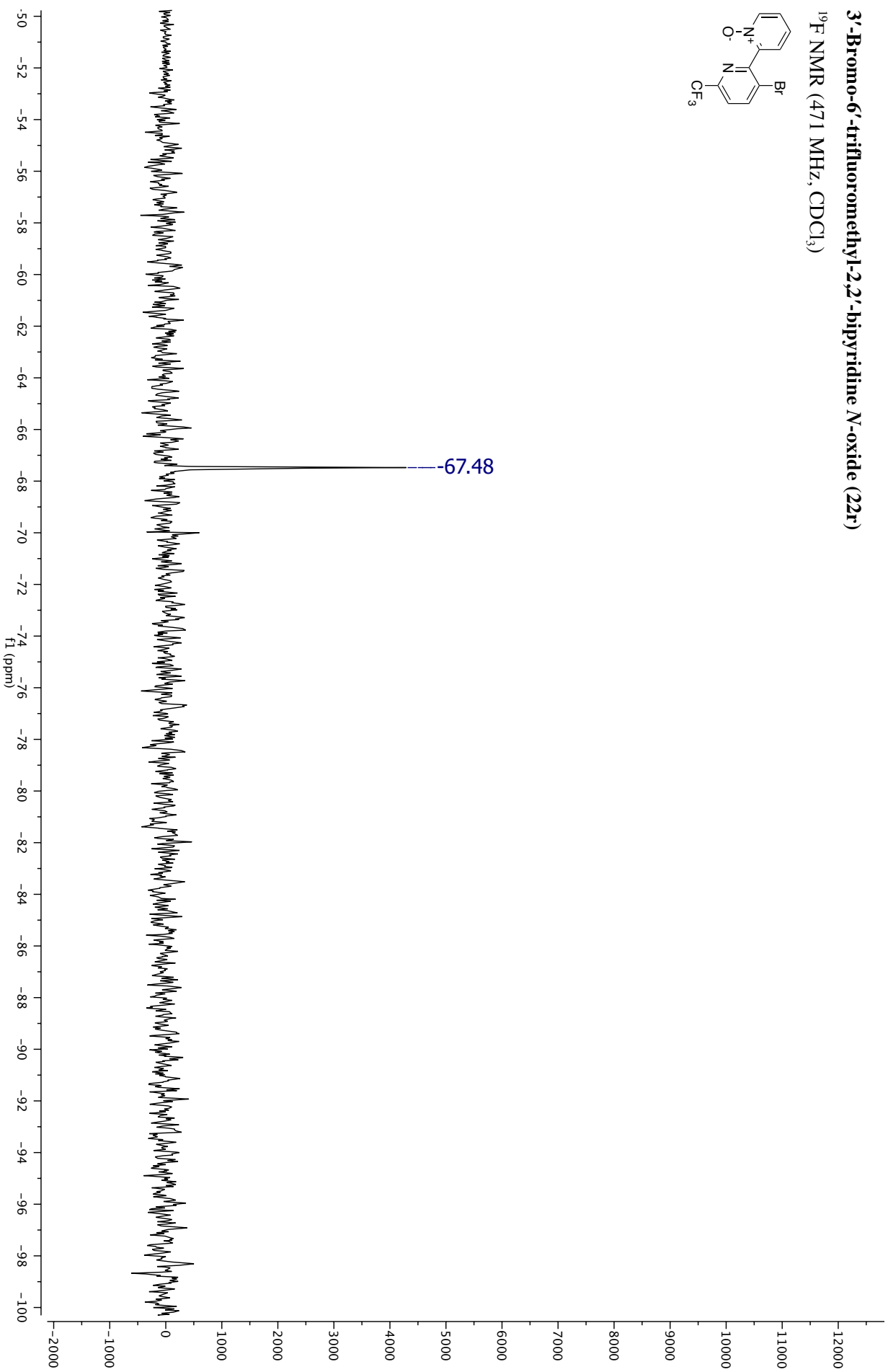
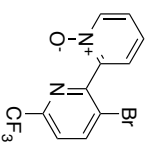
3'-Bromo-6'-(trifluoromethyl)-2,2'-bipyridine N-oxide (22r)

¹³C NMR (126 MHz, CDCl₃)



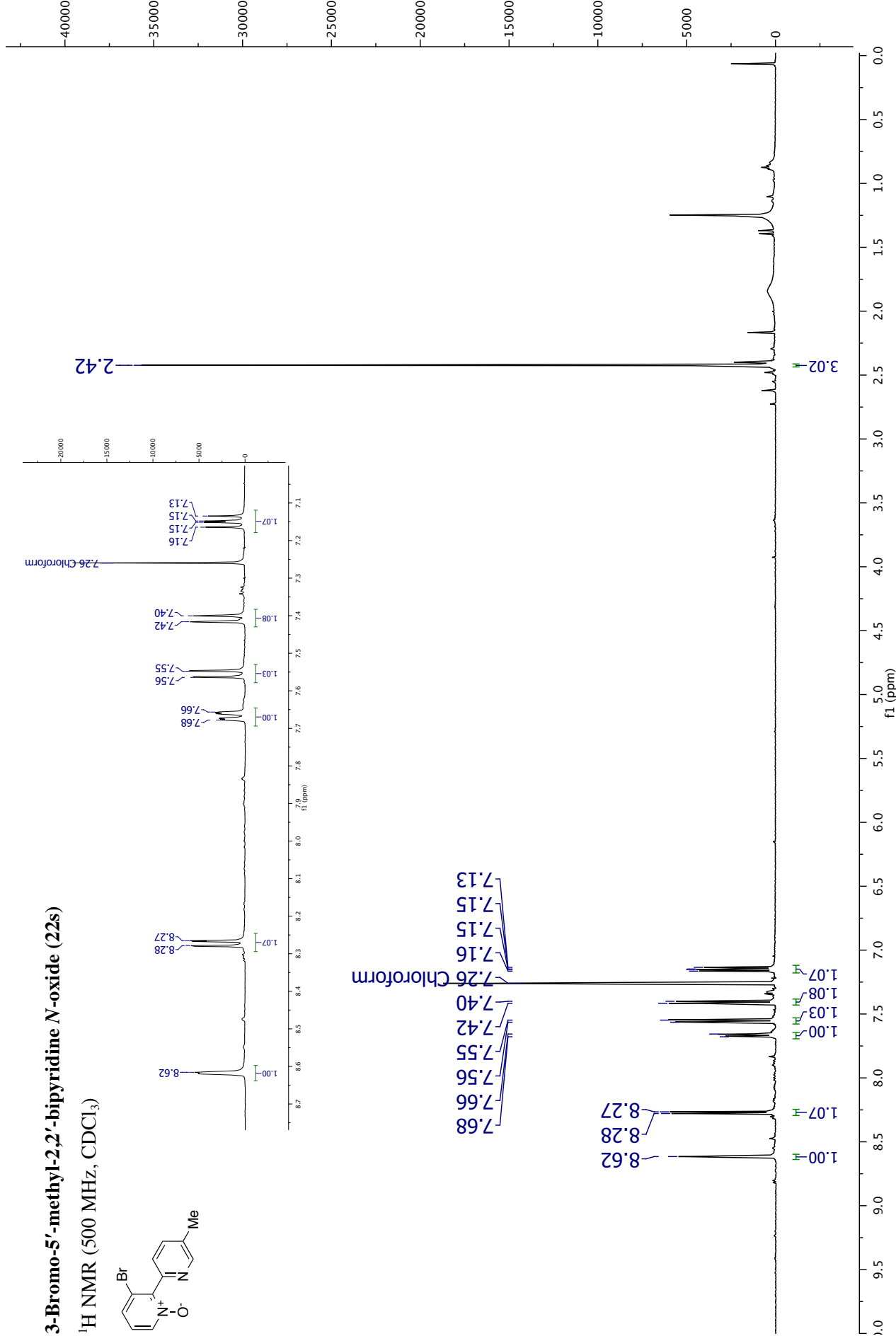
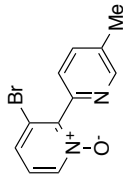
3'-Bromo-6'-trifluoromethyl-2,2'-bipyridine N-oxide (22r)

¹⁹F NMR (471 MHz, CDCl₃)



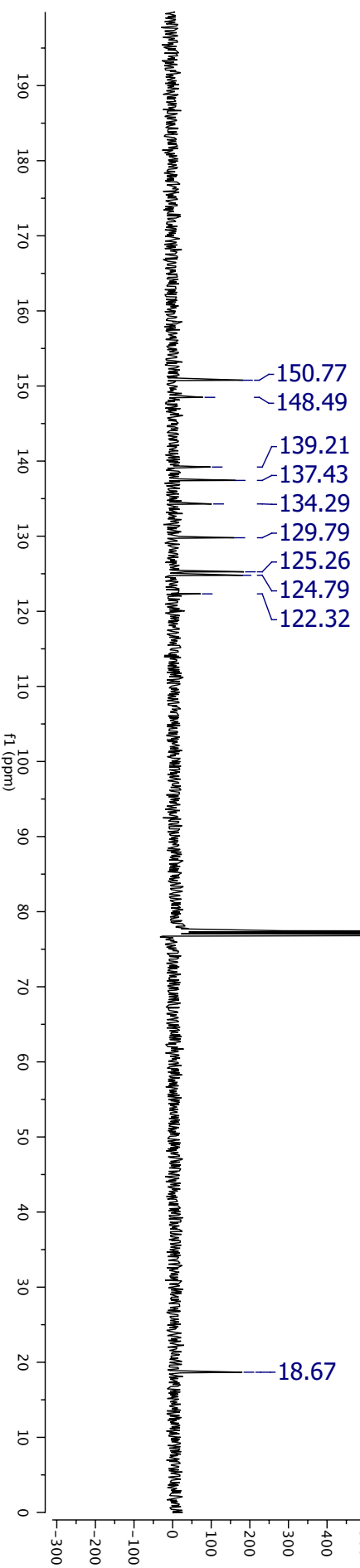
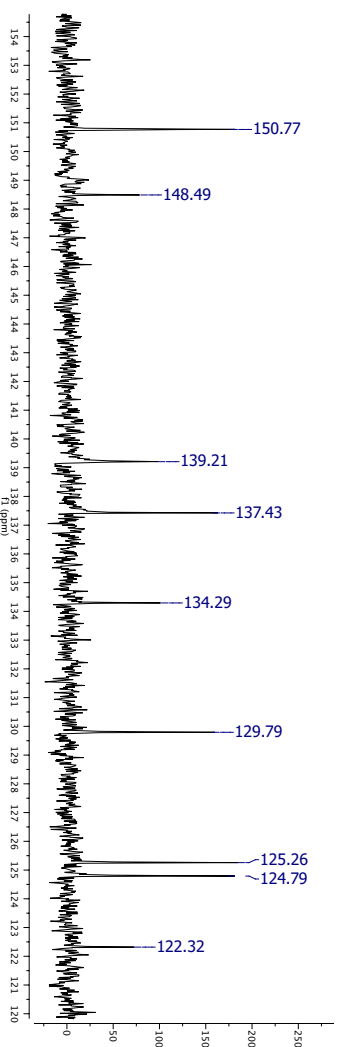
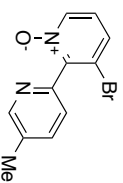
3-Bromo-5'-methyl-2,2'-bipyridine N-oxide (22s)

¹H NMR (500 MHz, CDCl₃)



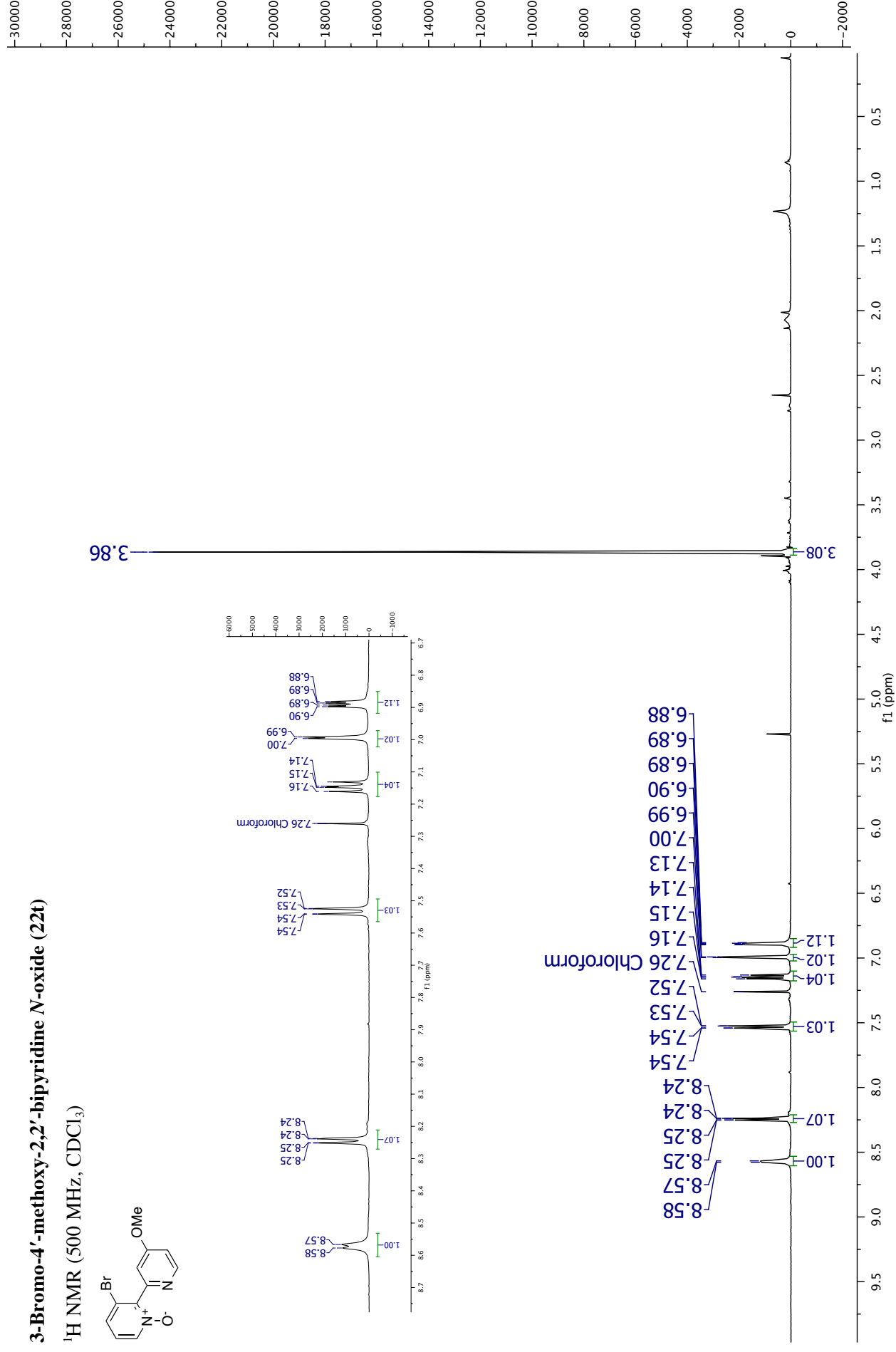
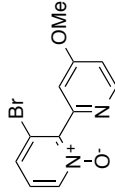
3-Bromo-5'-methyl-2,2'-bipyridine N-oxide (22s)

¹³C NMR (126 MHz, CDCl₃)



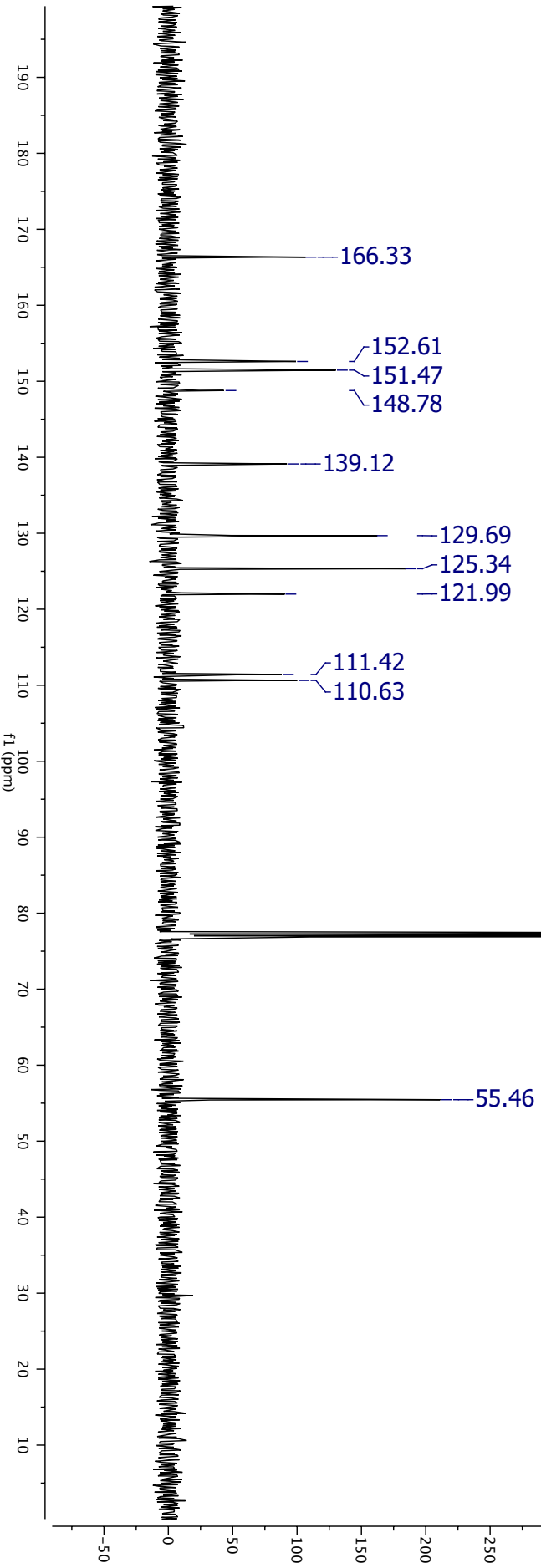
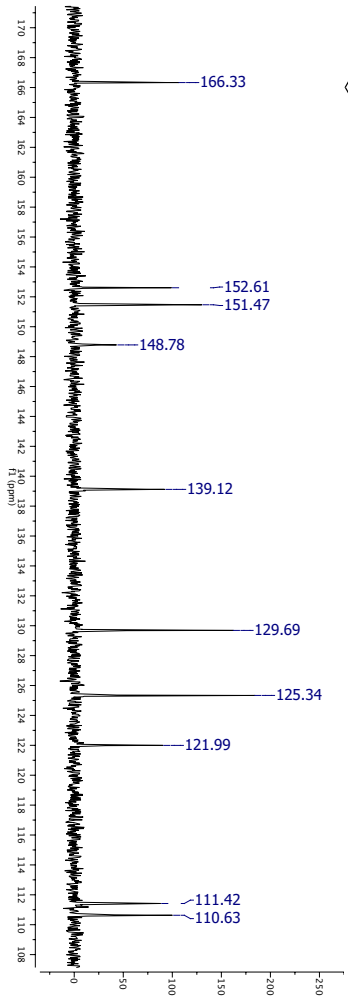
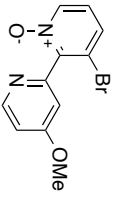
3-Bromo-4'-methoxy-2,2'-bipyridine N-oxide (22t)

¹H NMR (500 MHz, CDCl₃)



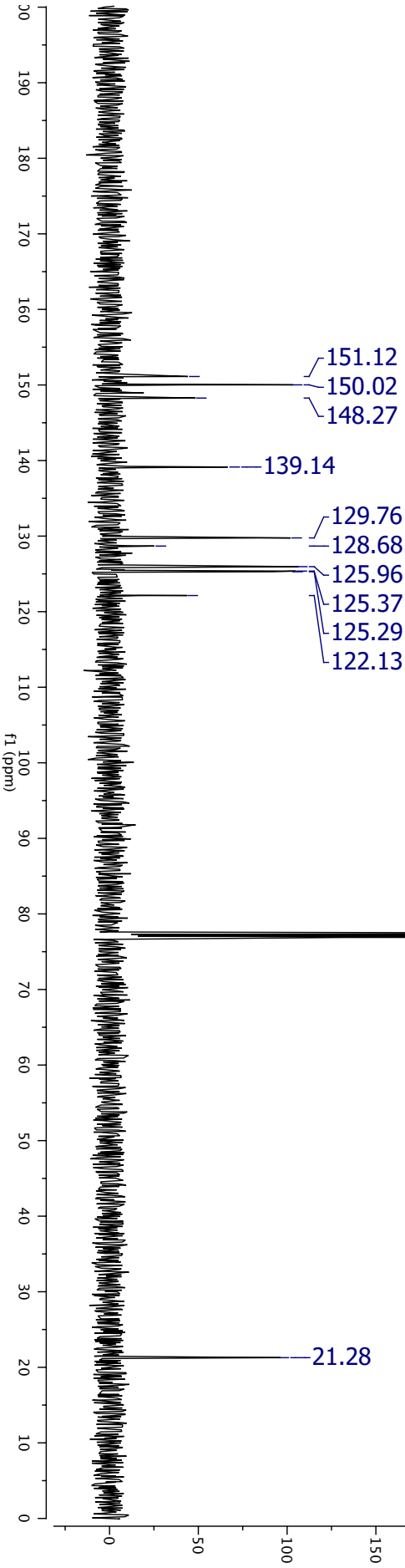
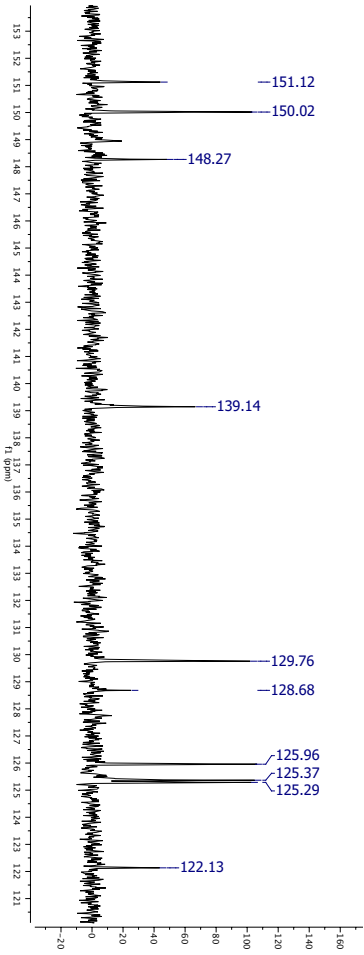
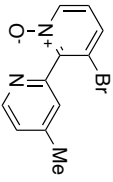
3-Bromo-4'-methoxy-2,2'-bipyridine N-oxide (22t)

¹³C NMR (126 MHz, CDCl₃)



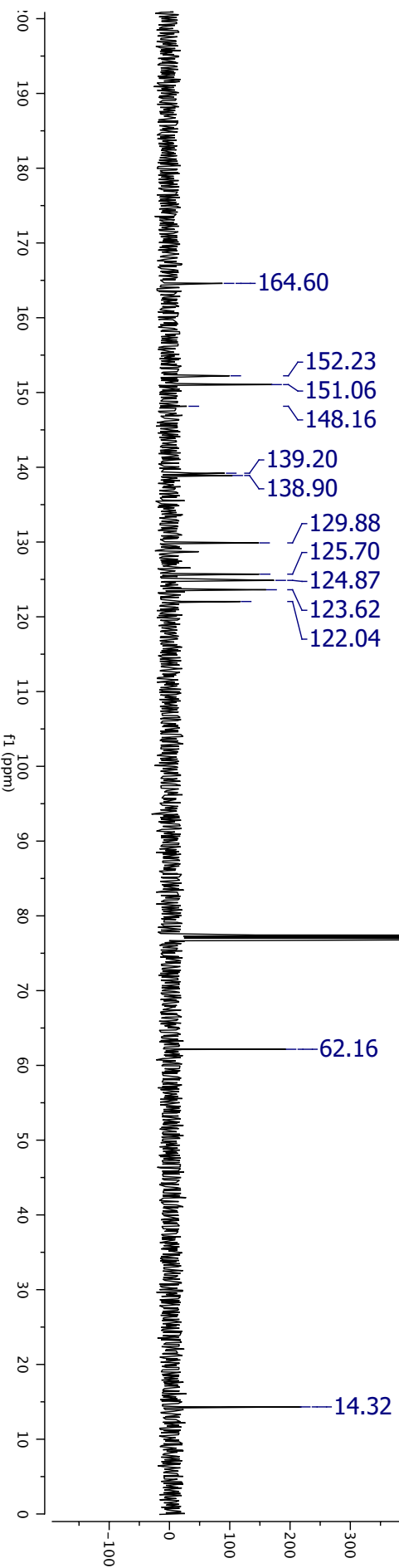
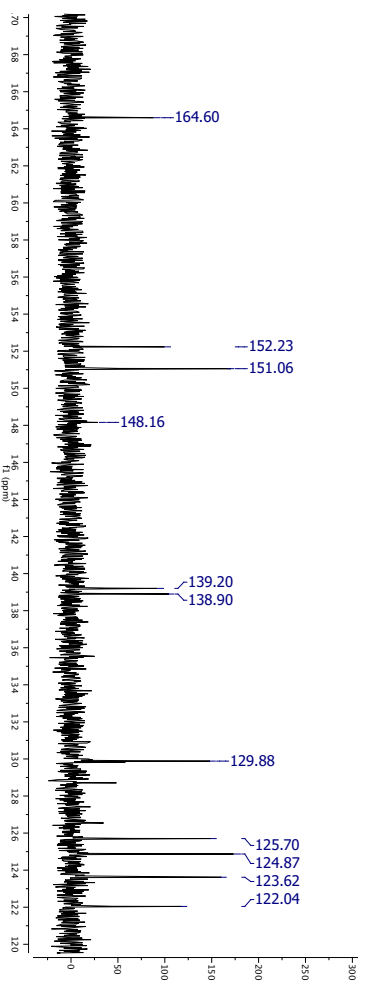
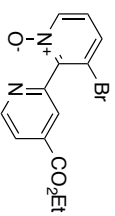
3-Bromo-4'-methyl-2,2'-bipyridine N-oxide (22u)

¹³C NMR (126 MHz, CDCl₃)



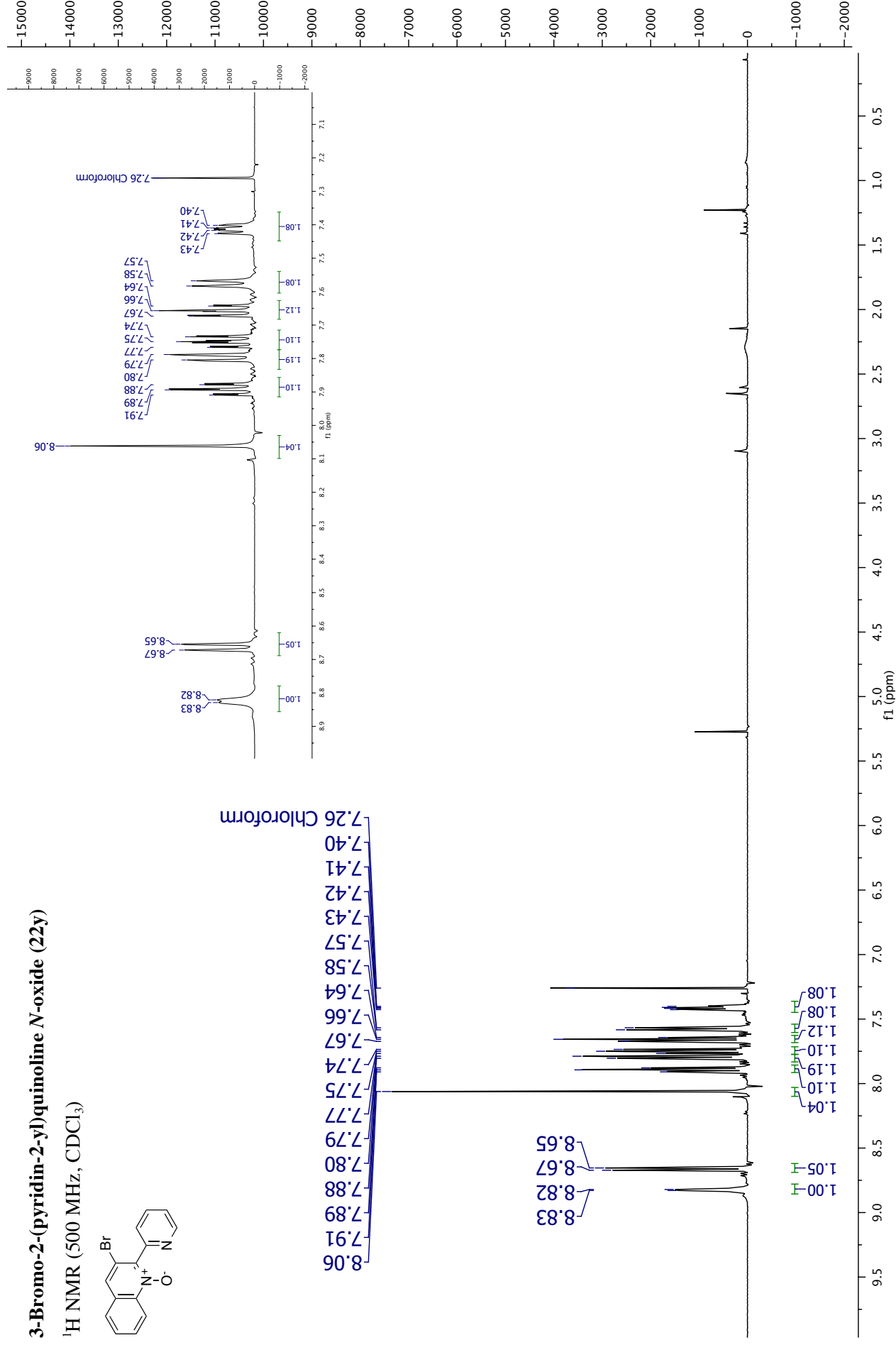
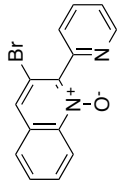
3-Bromo-4'-(ethoxycarbonyl)-2,2'-bipyridine N-oxide (22w)

¹³C NMR (126 MHz, CDCl₃)



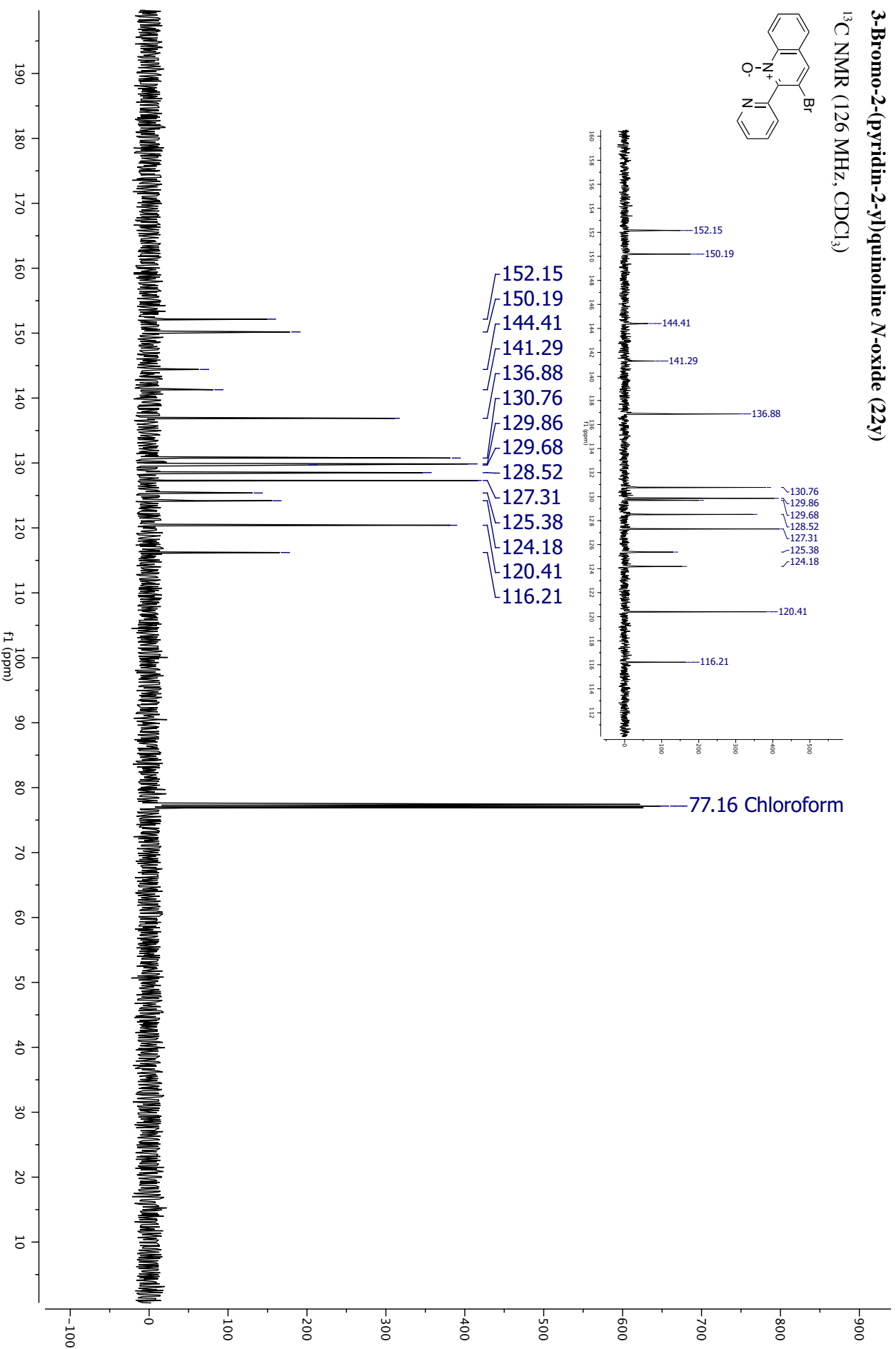
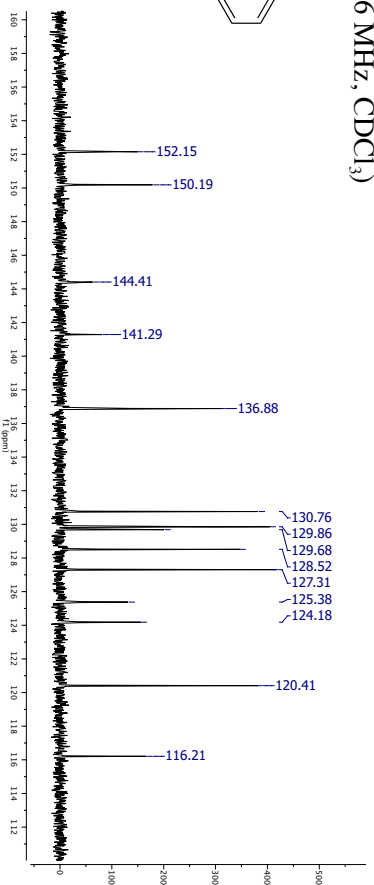
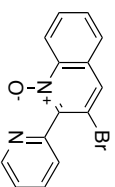
3-Bromo-2-(pyridin-2-yl)quinoline N-oxide (22y)

¹H NMR (500 MHz, CDCl₃)



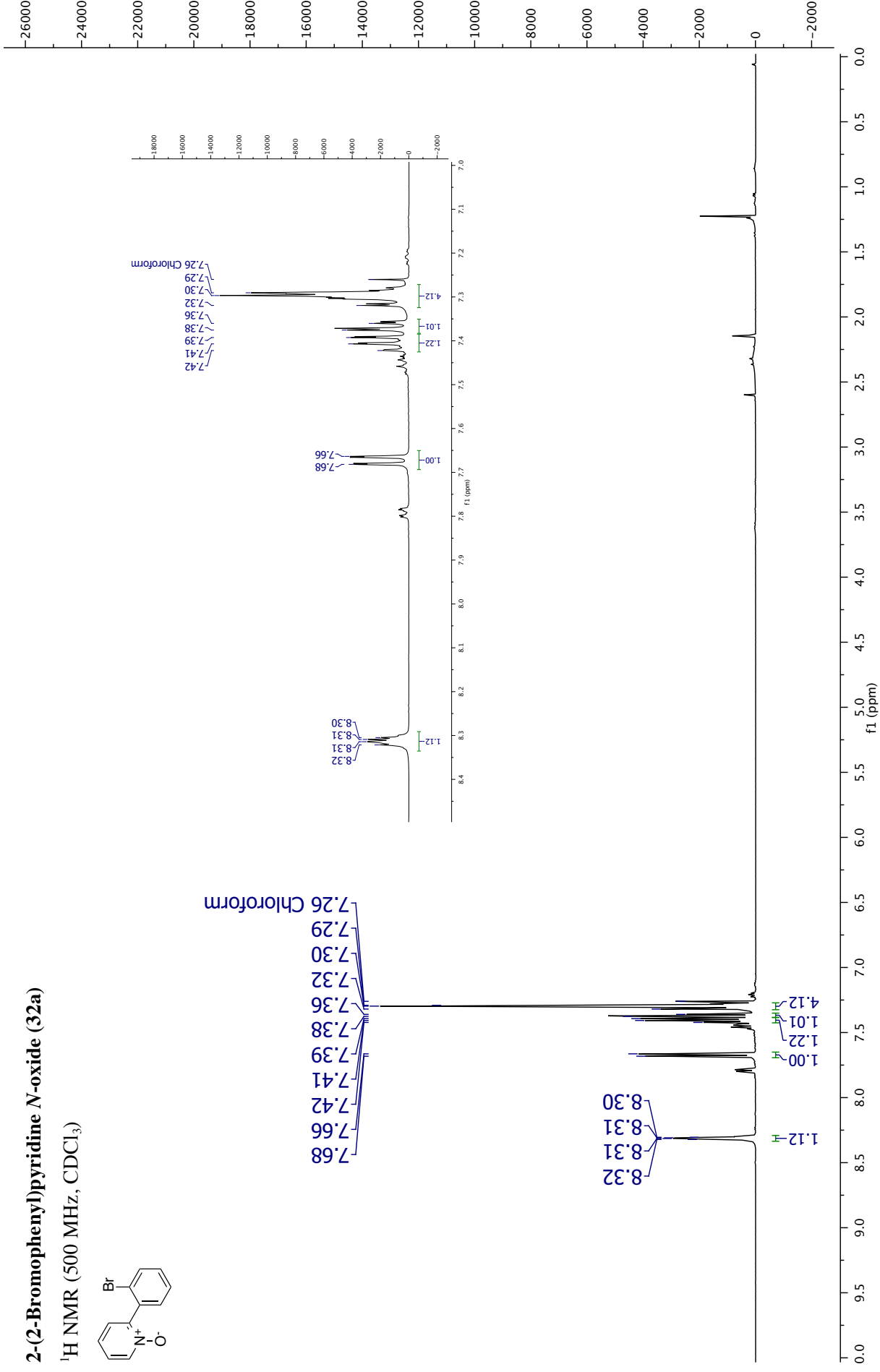
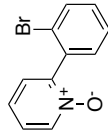
3-Bromo-2-(pyridin-2-yl)quinoline N-oxide (22y)

¹³C NMR (126 MHz, CDCl₃)



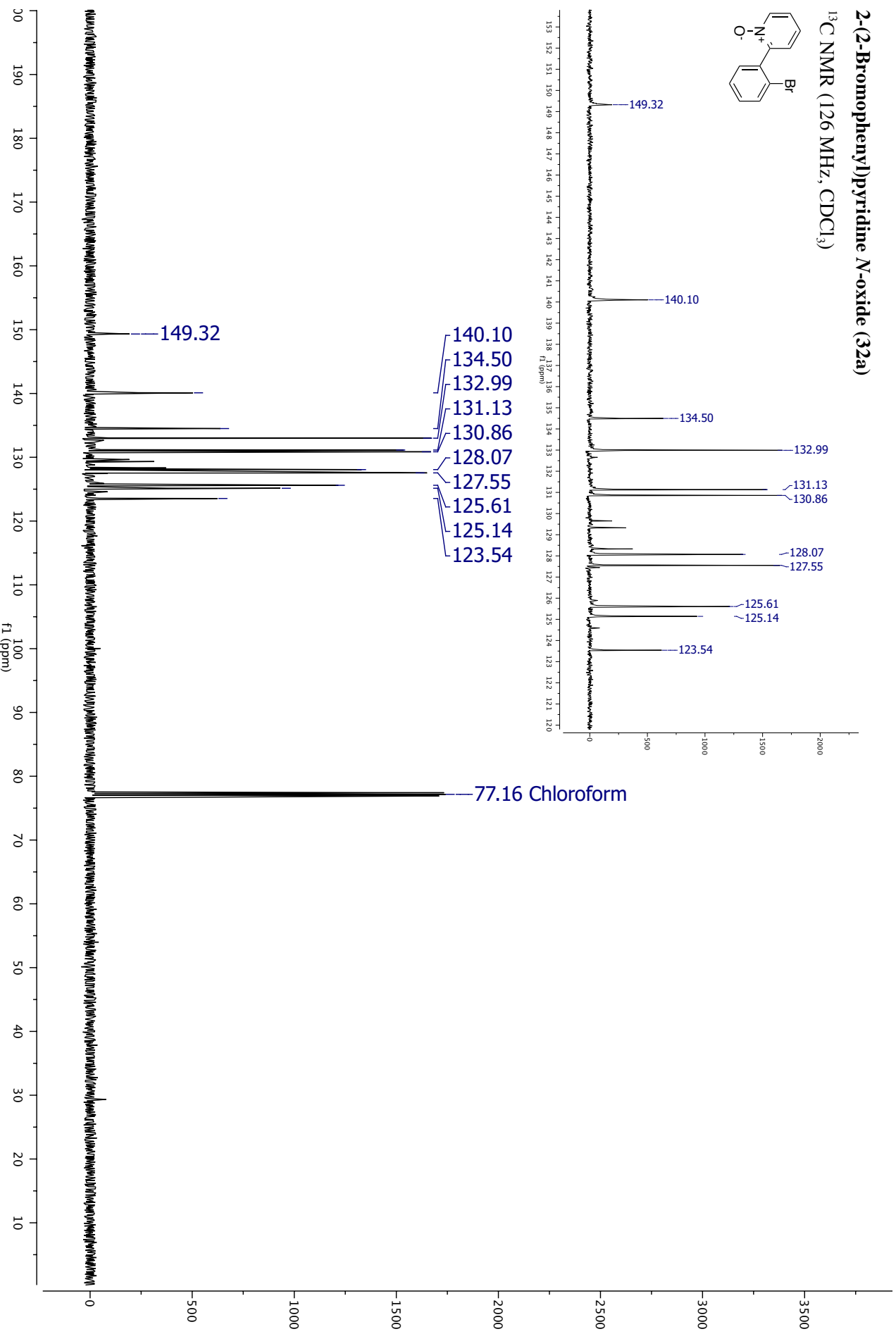
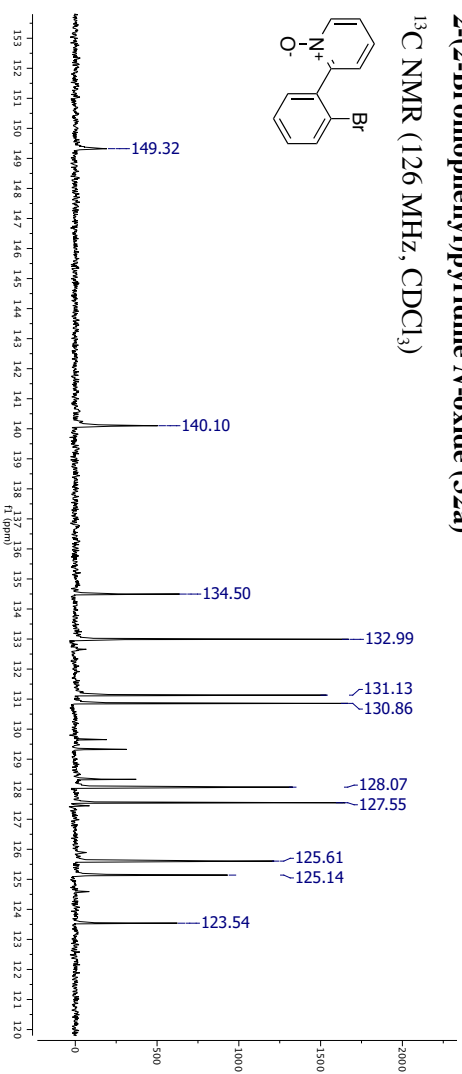
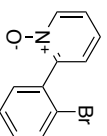
2-(2-Bromophenyl)pyridine N-oxide (32a)

¹H NMR (500 MHz, CDCl₃)



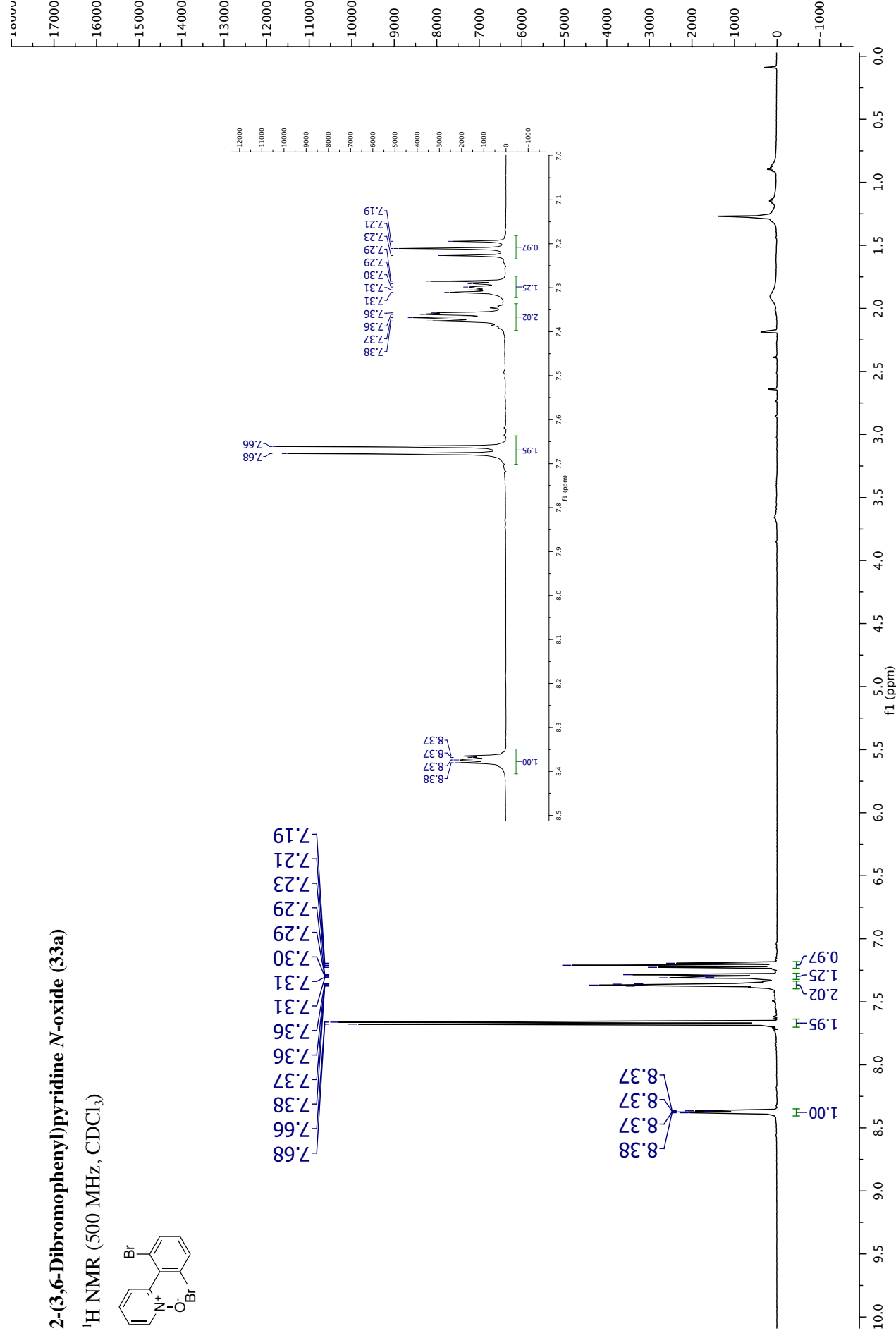
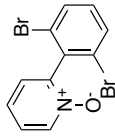
2-(2-Bromophenyl)pyridine N-oxide (32a)

¹³C NMR (126 MHz, CDCl₃)



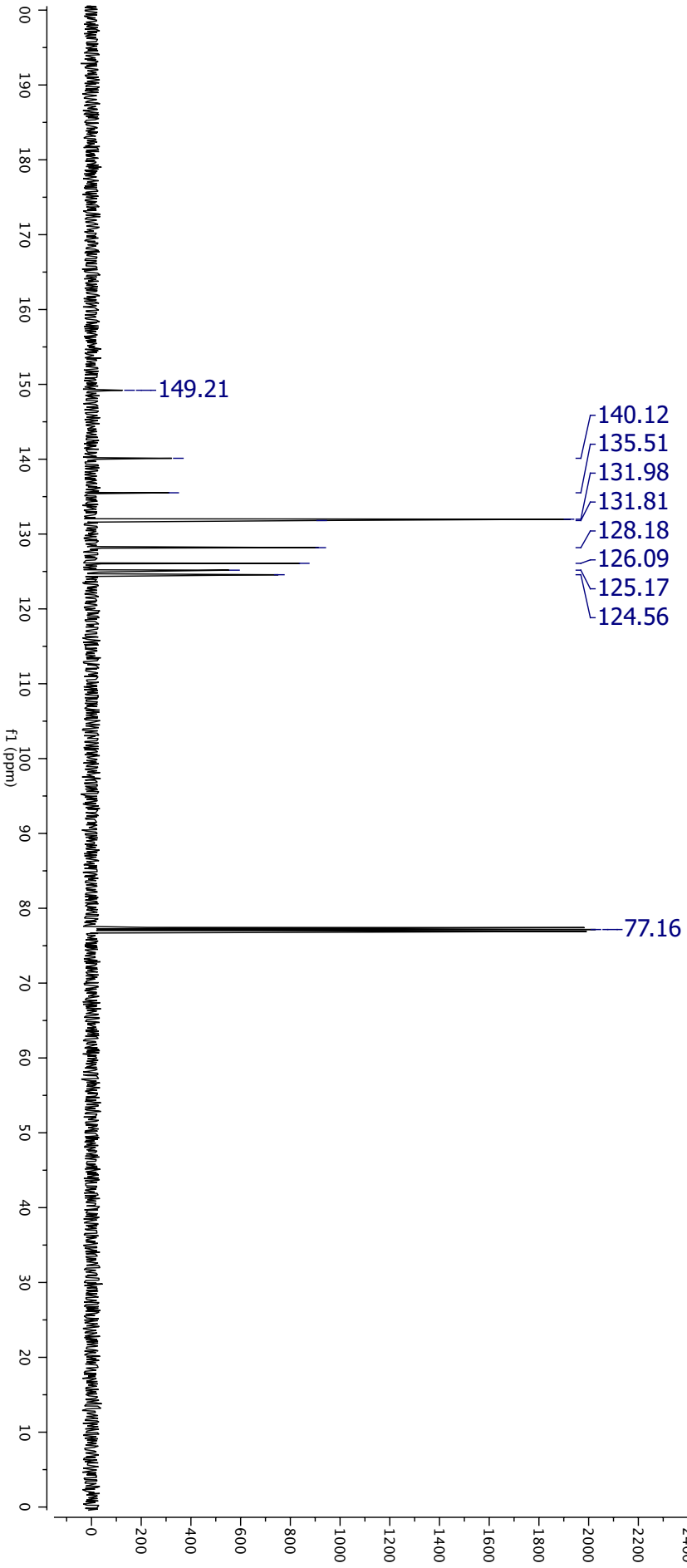
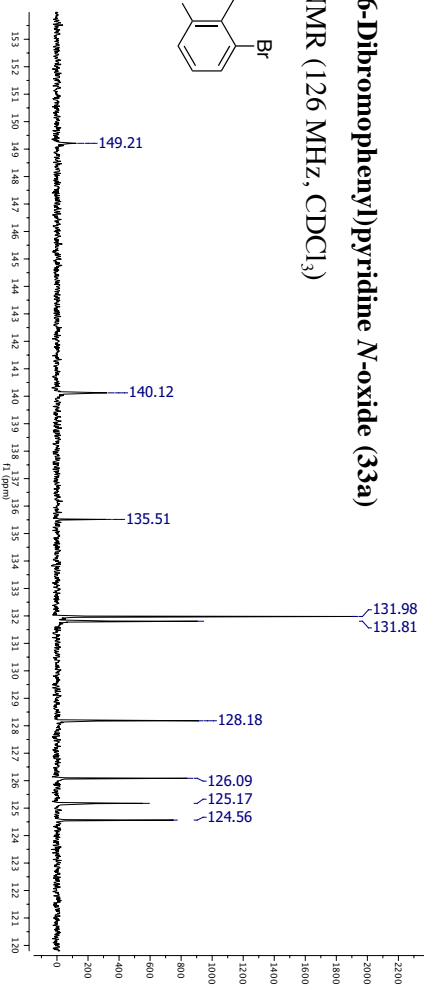
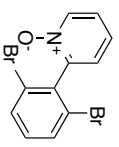
2-(3,6-Dibromophenyl)pyridine N-oxide (33a)

¹H NMR (500 MHz, CDCl₃)



2-(3,6-Dibromophenyl)pyridine N-oxide (33a)

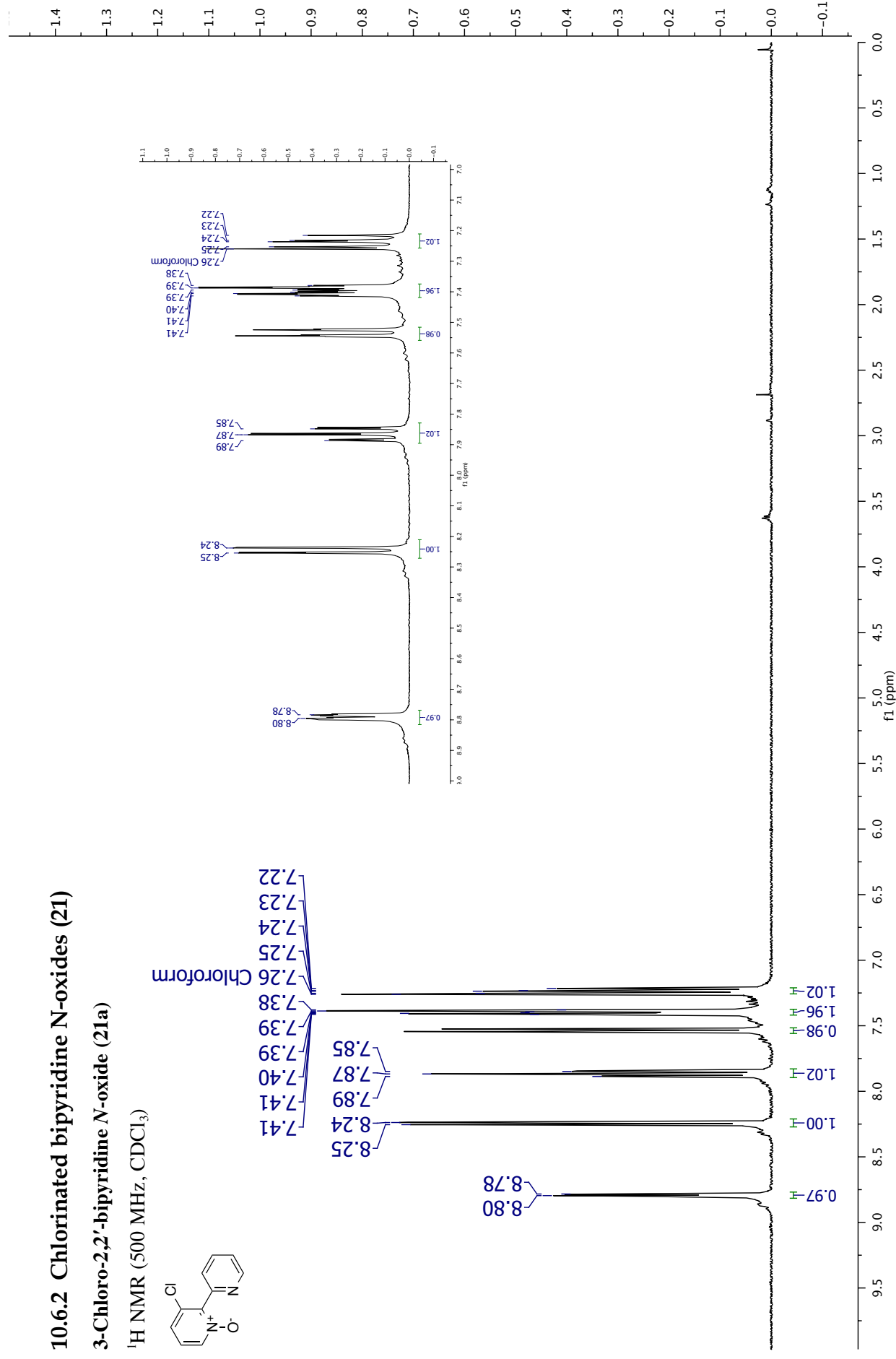
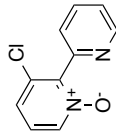
¹³C NMR (126 MHz, CDCl₃)



10.6.2 Chlorinated bipyridine N-oxides (21)

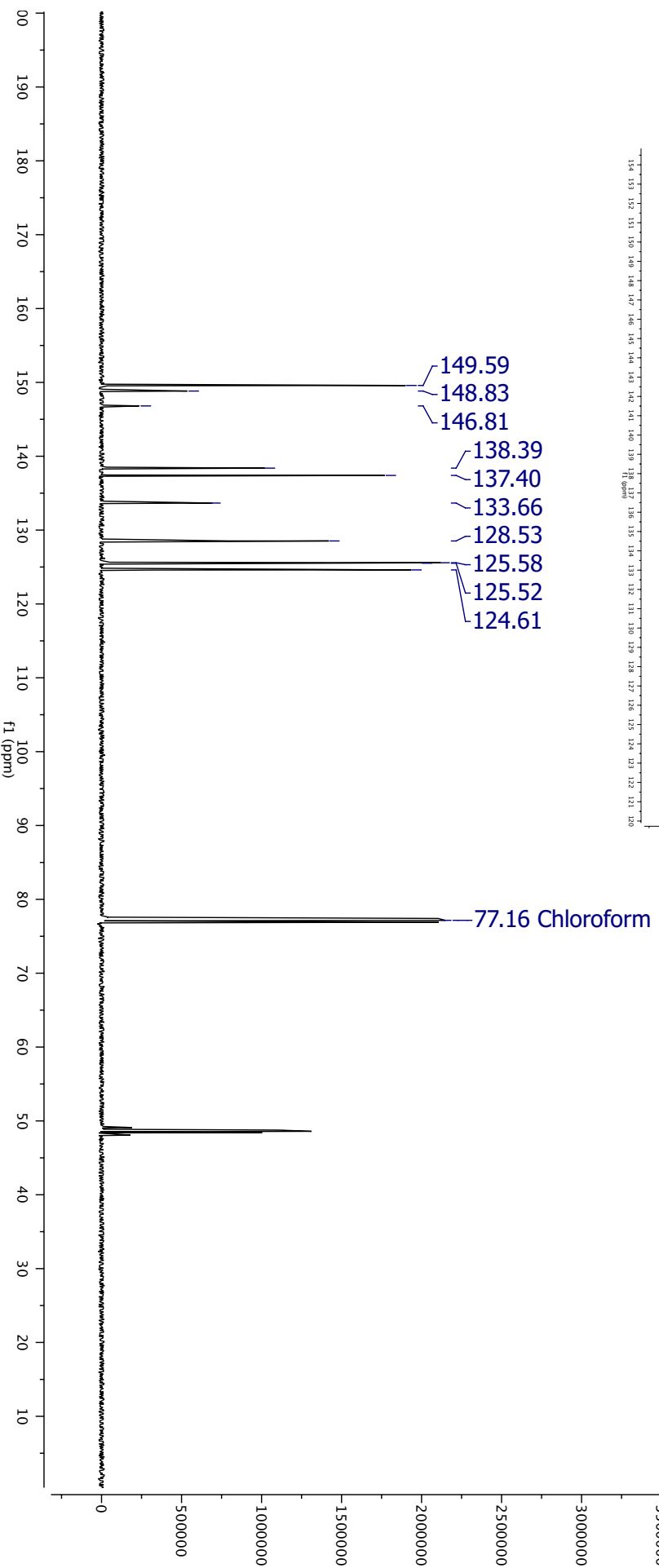
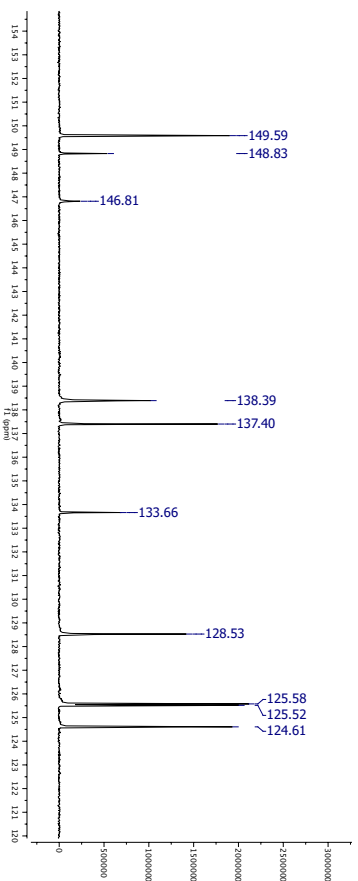
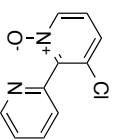
3-Chloro-2,2'-bipyridine N-oxide (21a)

¹H NMR (500 MHz, CDCl₃)



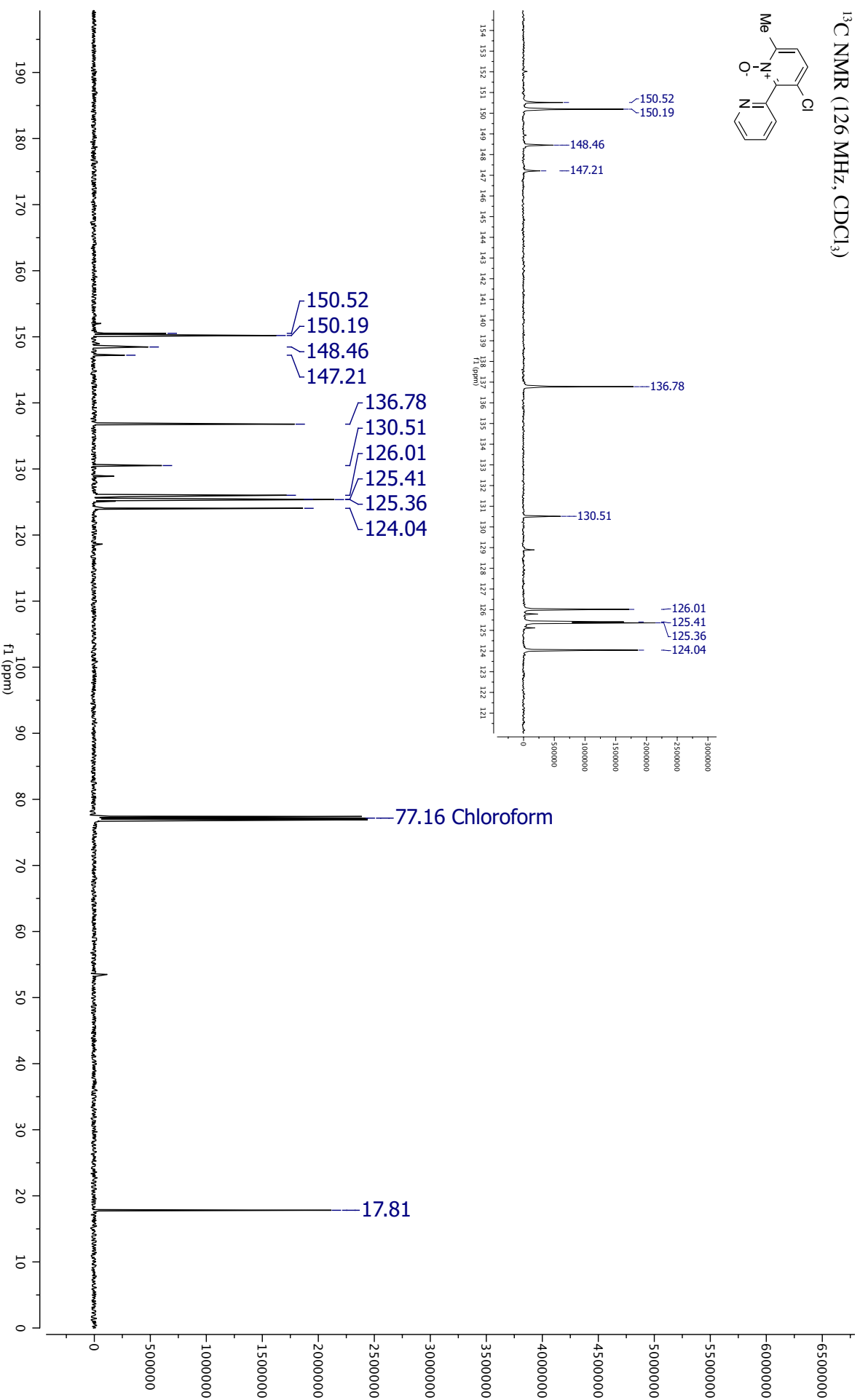
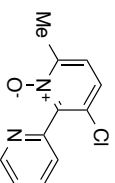
3-Chloro-2,2'-bipyridine N-oxide (21a)

^{13}C NMR (126 MHz, CDCl_3)



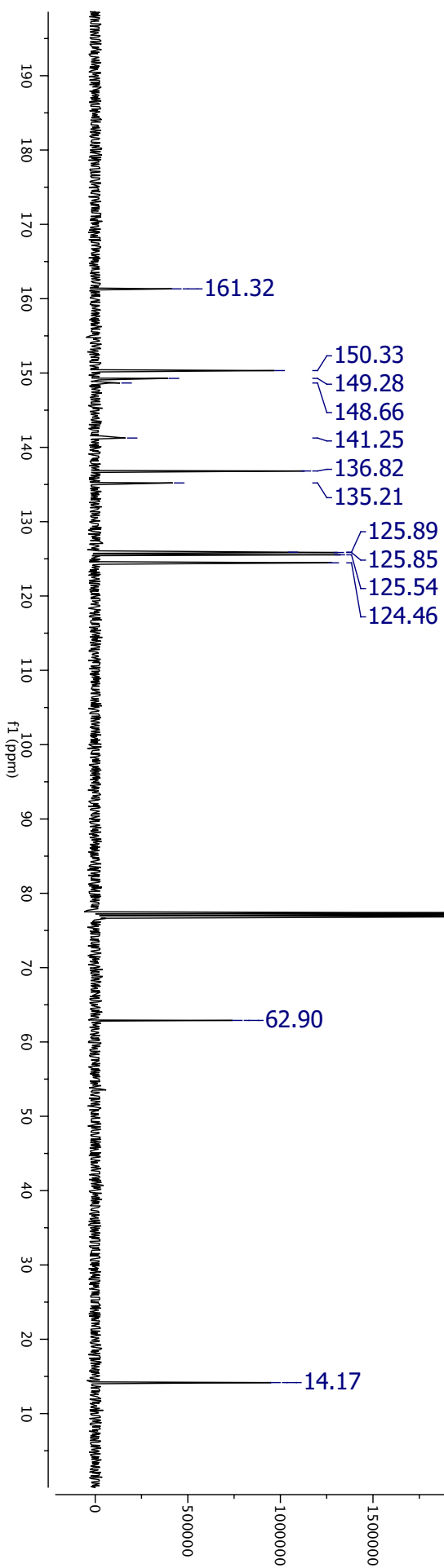
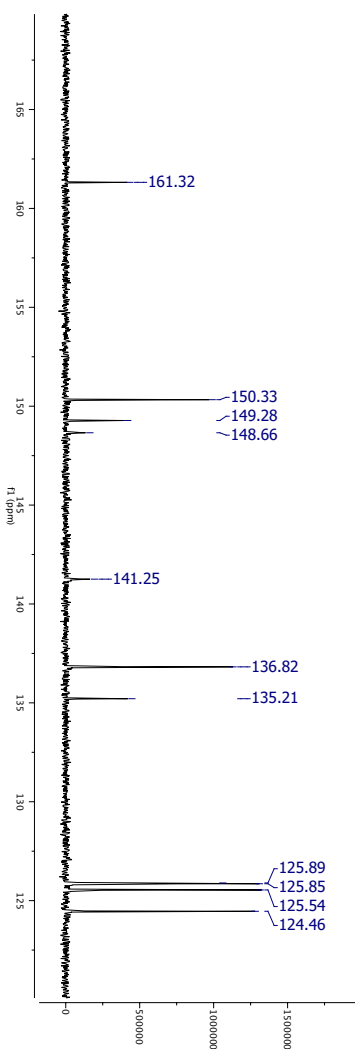
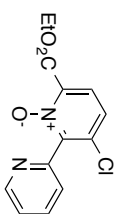
3-Chloro-6-methyl-2,2'-bipyridine N-oxide (21b)

^{13}C NMR (126 MHz, CDCl_3)



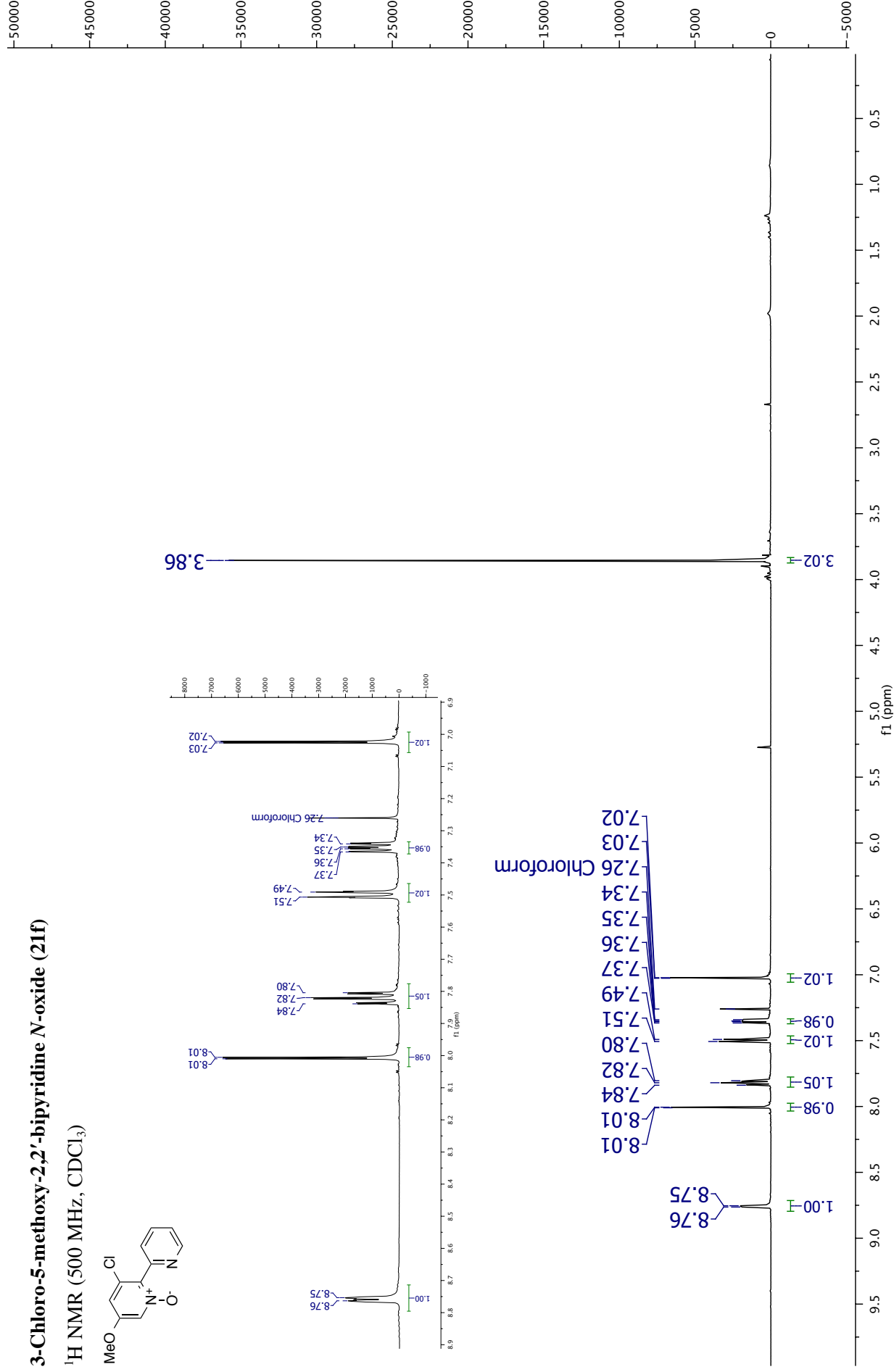
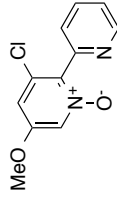
3-Chloro-6-(ethoxycarbonyl)-2,2'-bipyridine N-oxide (21c)

^{13}C NMR (126 MHz, CDCl_3)



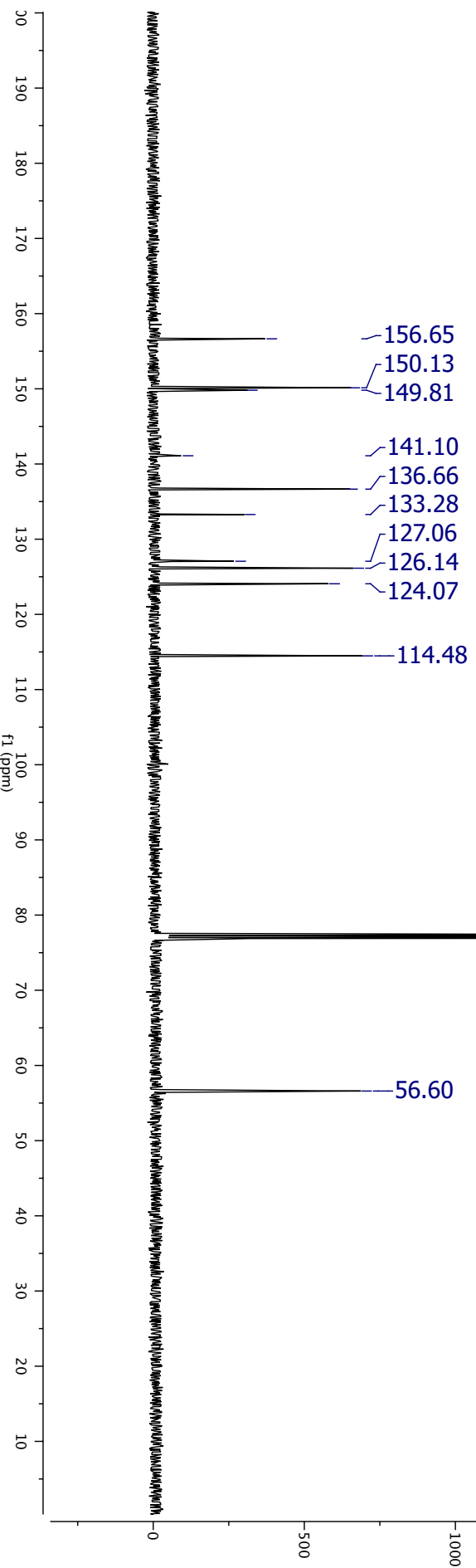
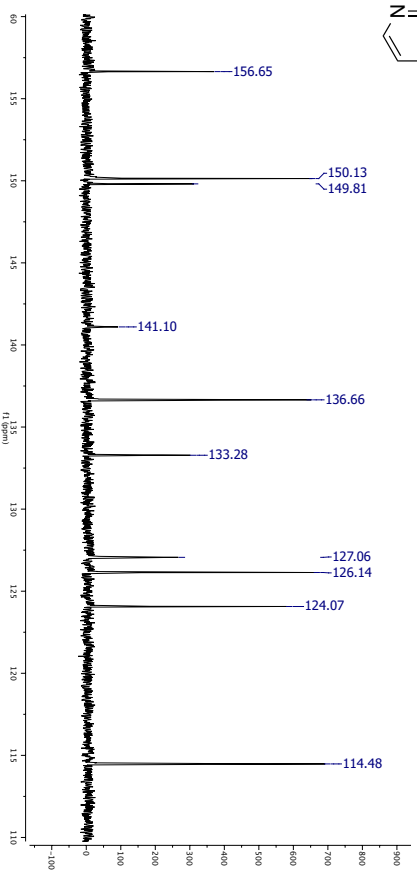
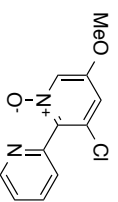
3-Chloro-5-methoxy-2,2'-bipyridine N-oxide (21f)

¹H NMR (500 MHz, CDCl₃)



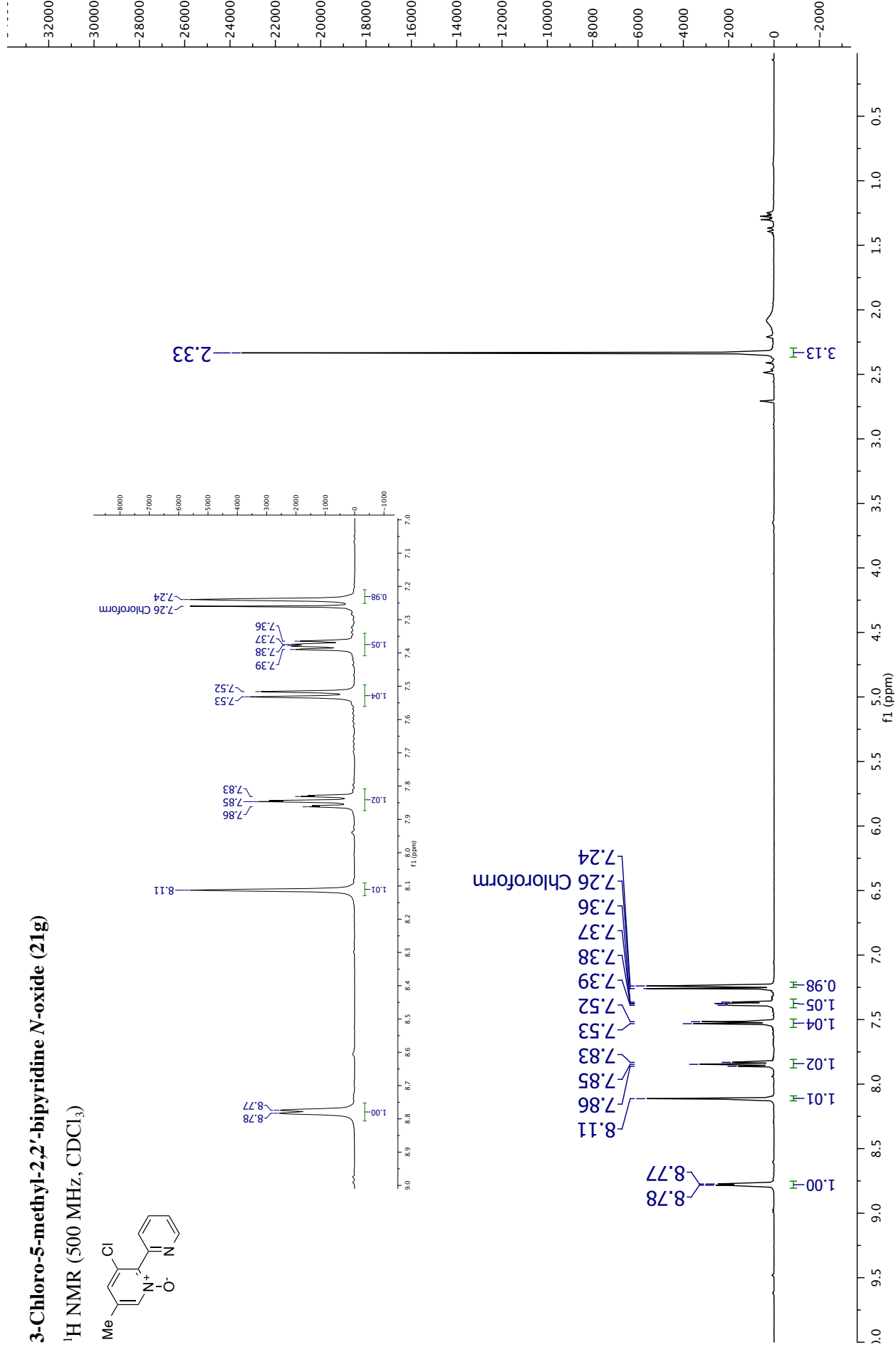
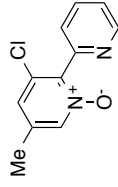
3-Chloro-5-methoxy-2,2'-bipyridine N-oxide (21f)

^{13}C NMR (126 MHz, CDCl_3)



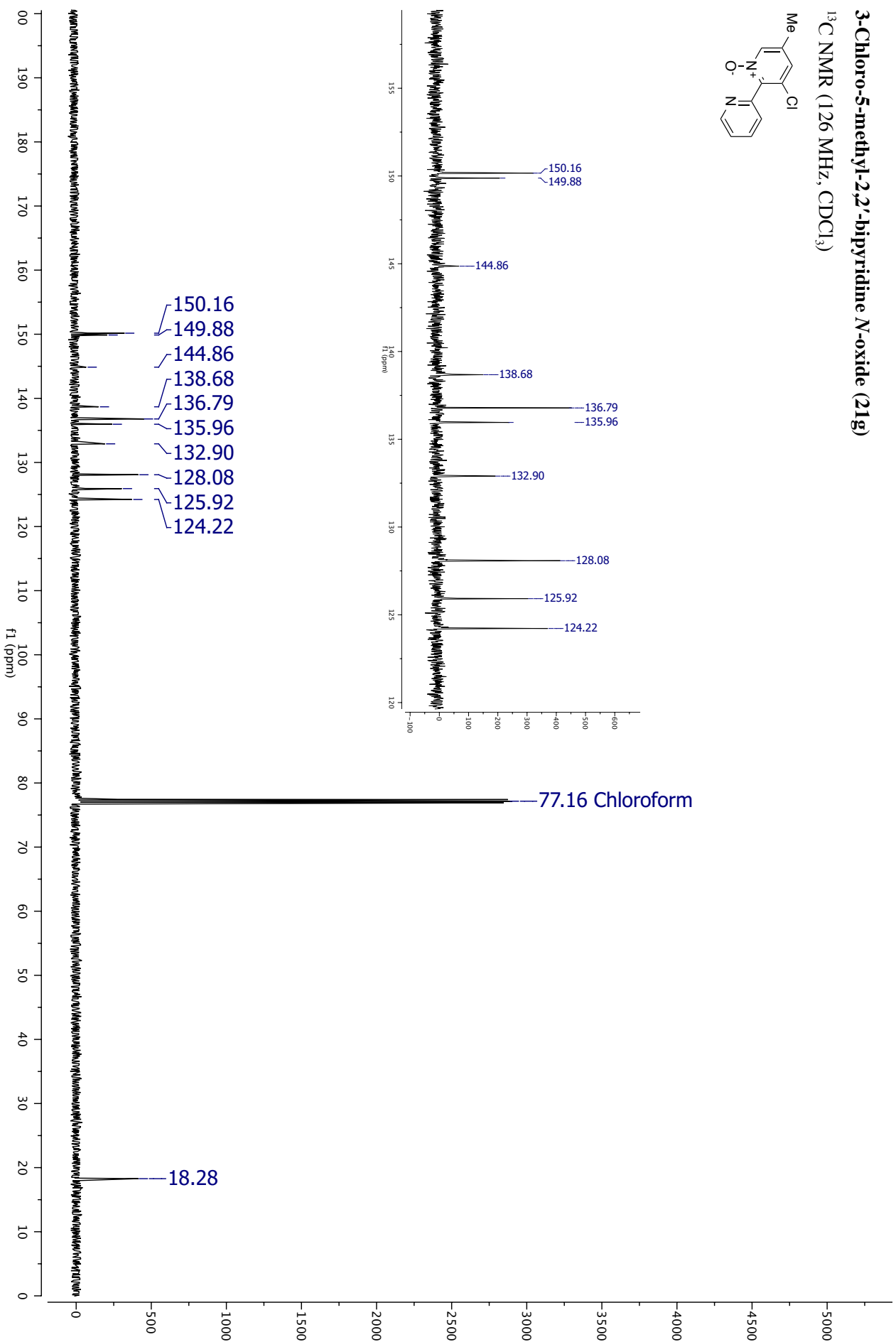
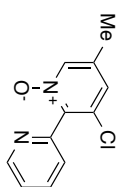
3-Chloro-5-methyl-2,2'-bipyridine N-oxide (21g)

¹H NMR (500 MHz, CDCl₃)



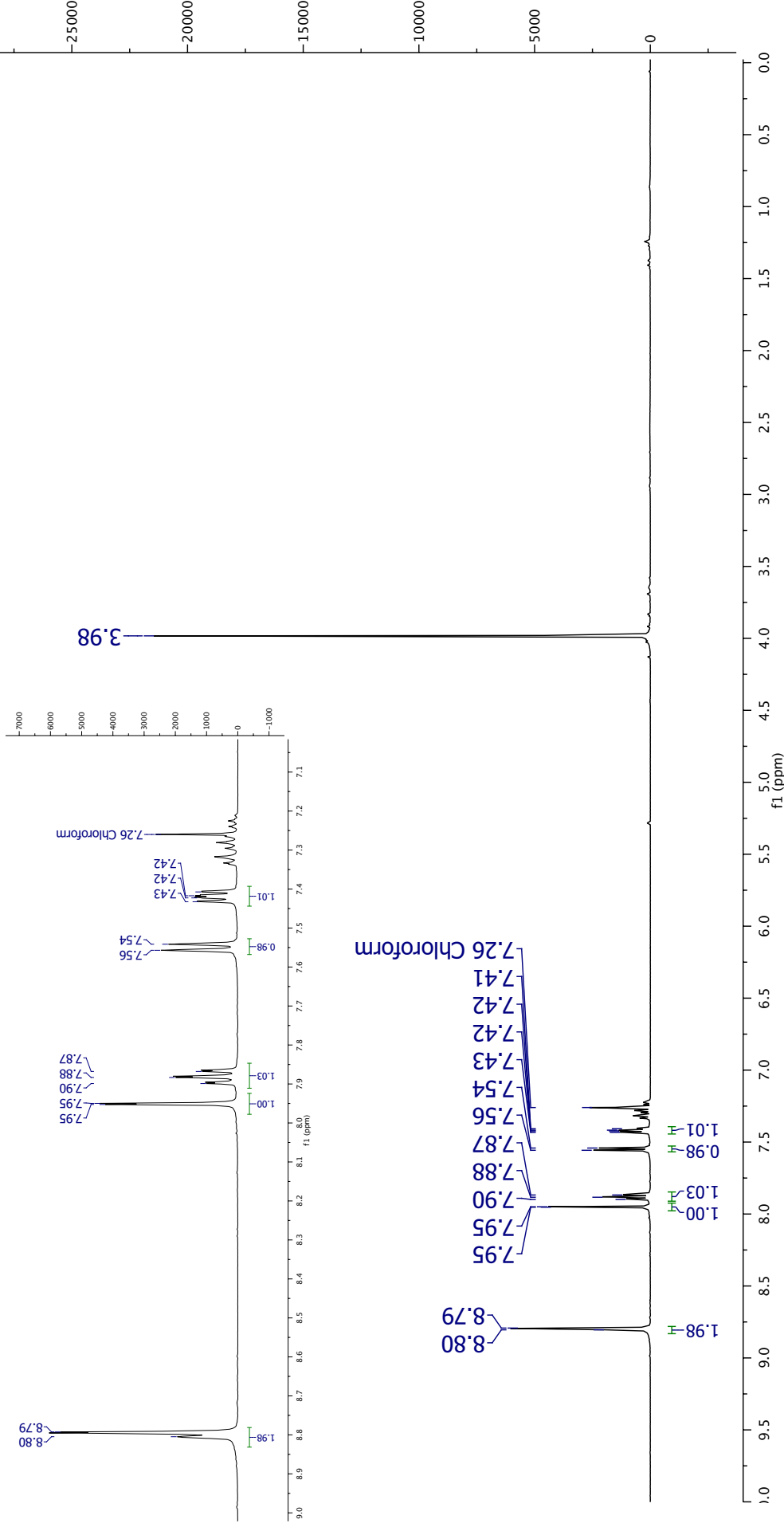
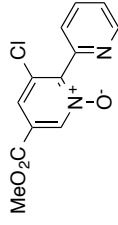
3-Chloro-5-methyl-2,2'-bipyridine N-oxide (21 g)

¹³C NMR (126 MHz, CDCl₃)



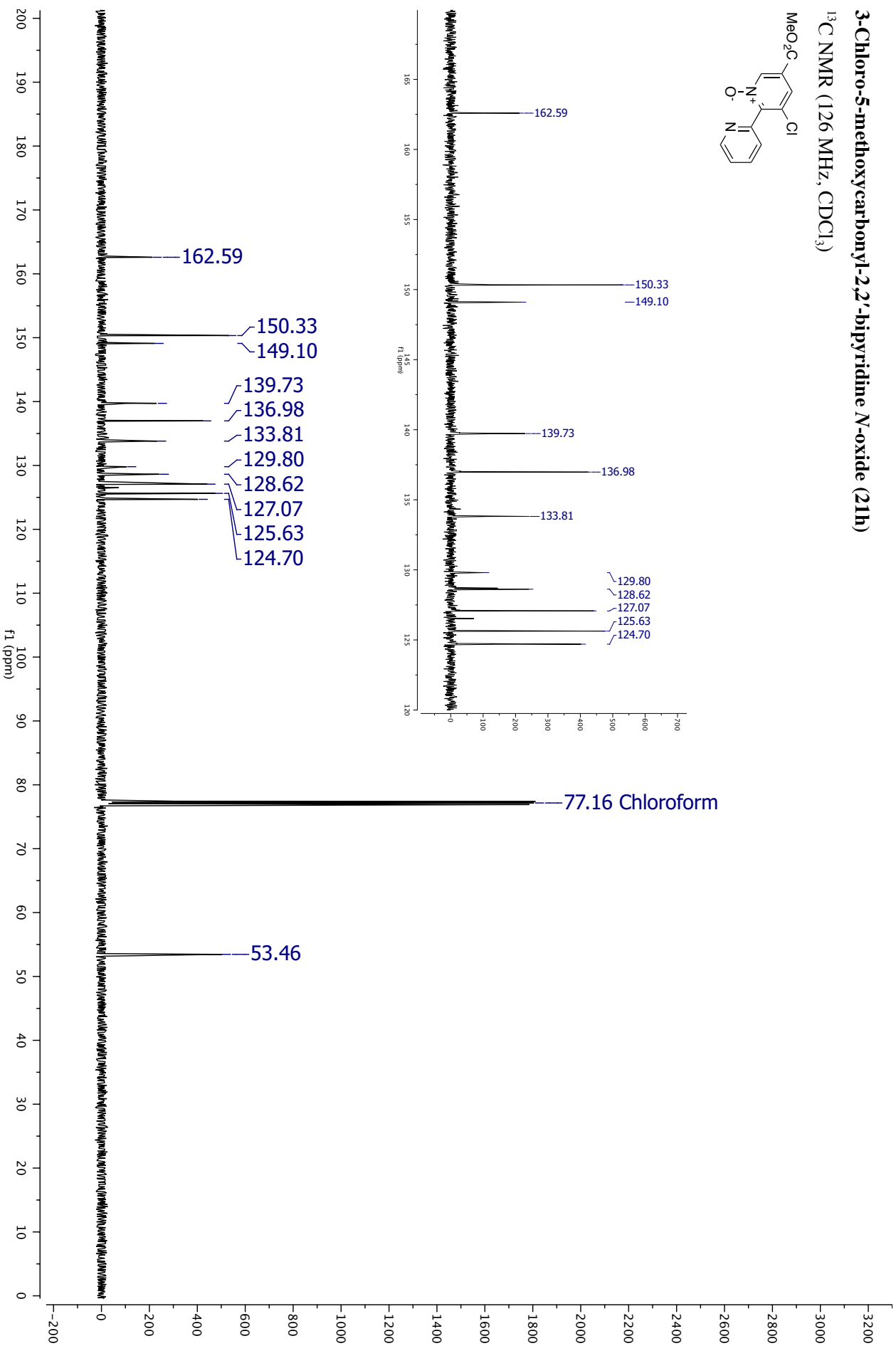
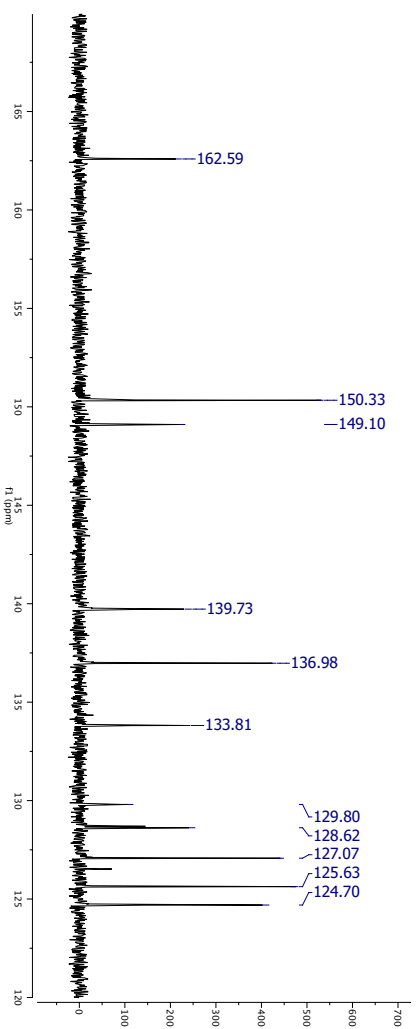
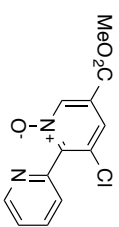
3-Chloro-5-methoxycarbonyl-2,2'-bipyridine N-oxide (21h)

¹H NMR (500 MHz, CDCl₃)



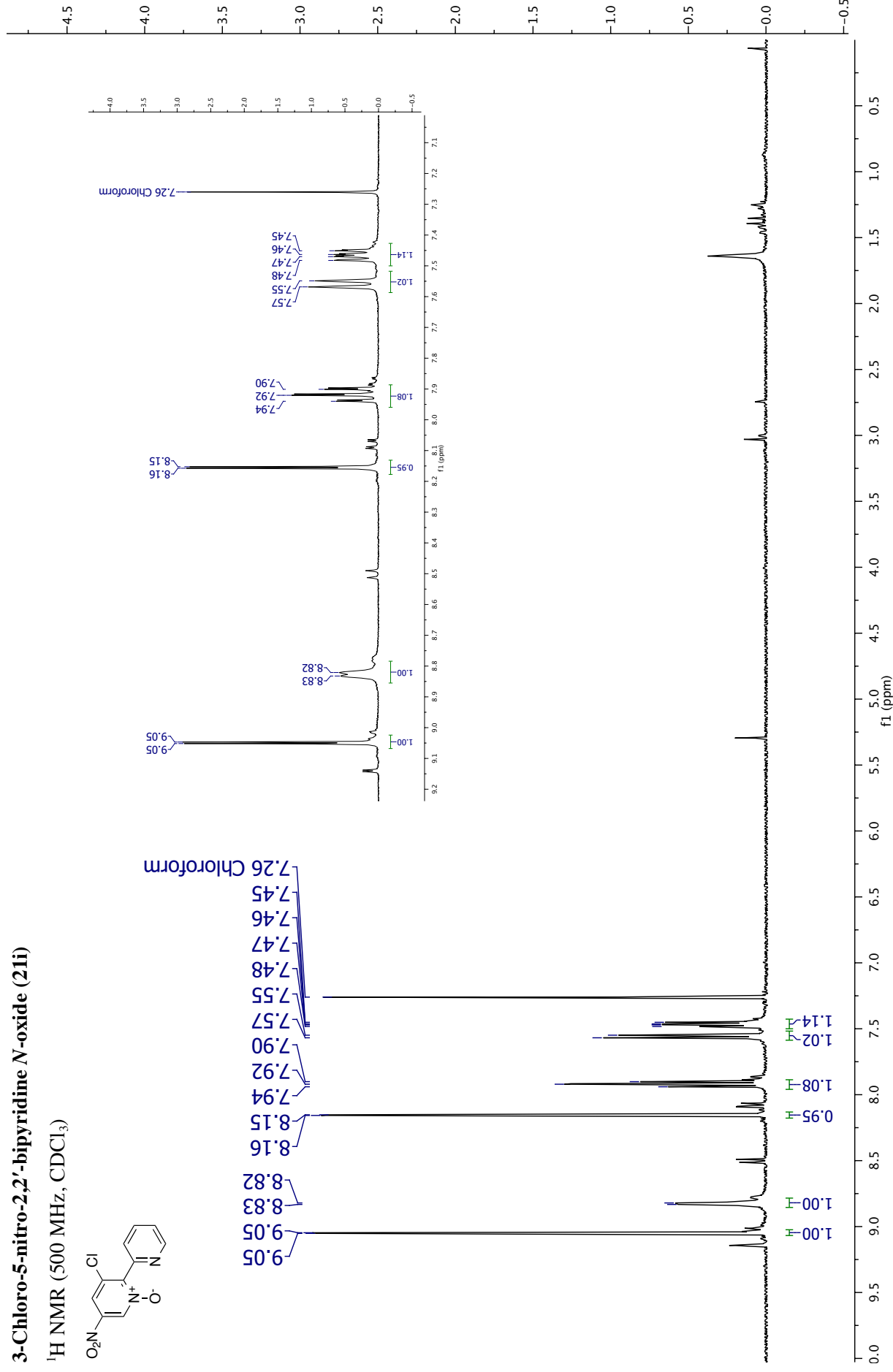
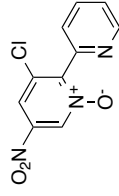
3-Chloro-5-methoxycarbonyl-2,2'-bipyridine N-oxide (21h)

^{13}C NMR (126 MHz, CDCl_3)



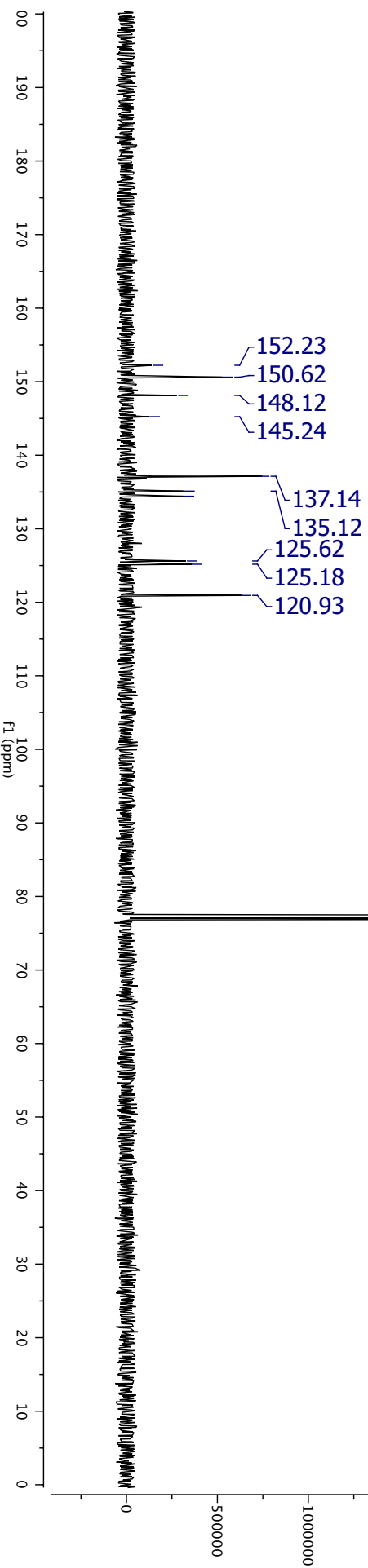
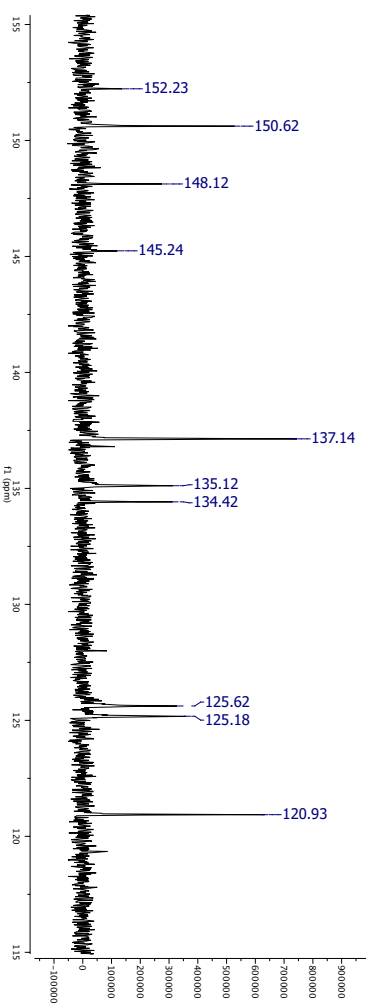
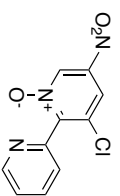
3-Chloro-5-nitro-2,2'-bipyridine N-oxide (21i)

¹H NMR (500 MHz, CDCl₃)



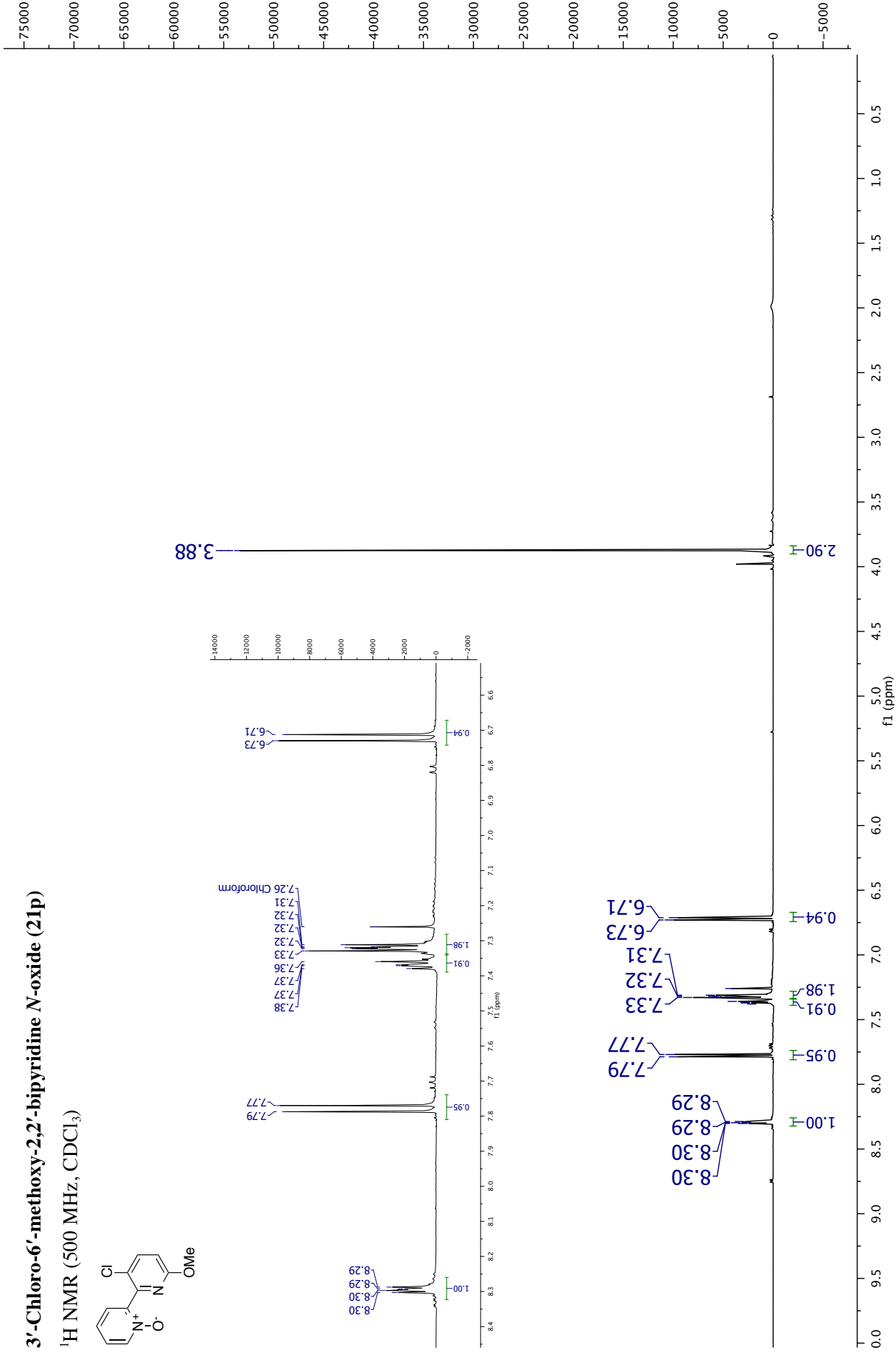
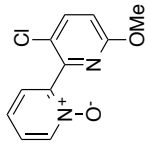
3-Chloro-5-nitro-2,2'-bipyridine N-oxide (21i)

¹³C NMR (126 MHz, CDCl₃)



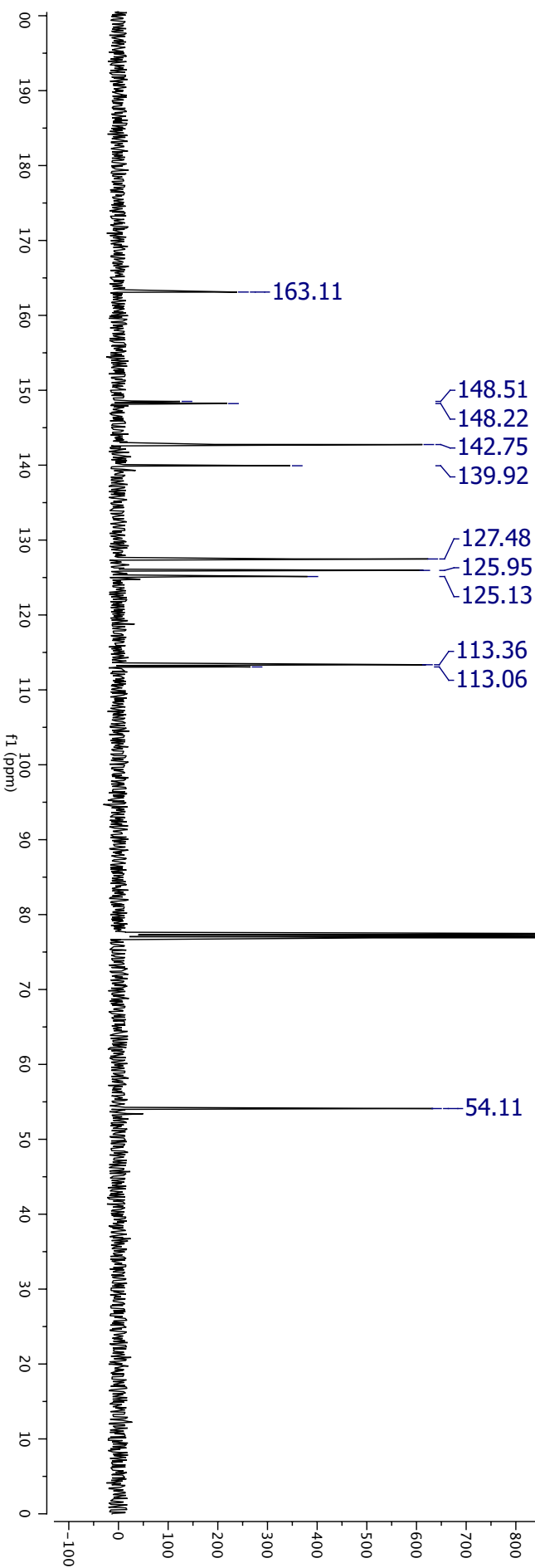
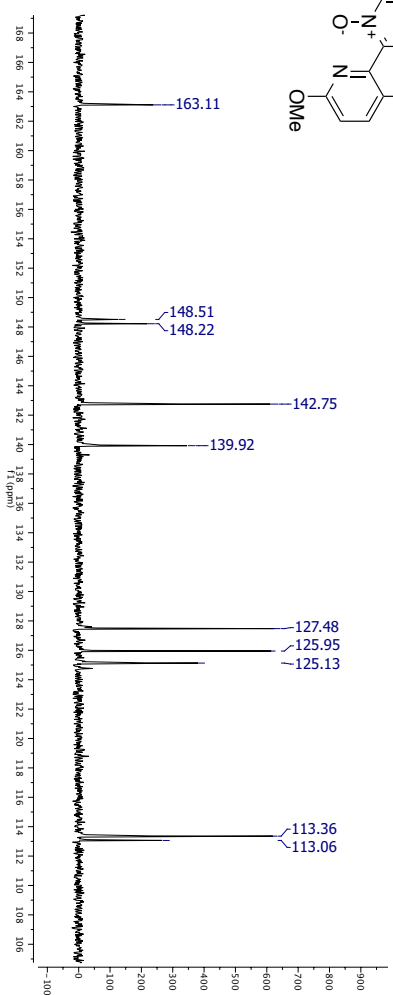
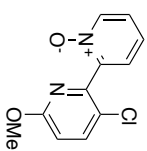
3'-Chloro-6'-methoxy-2,2'-bipyridine N-oxide (21p)

¹H NMR (500 MHz, CDCl₃)



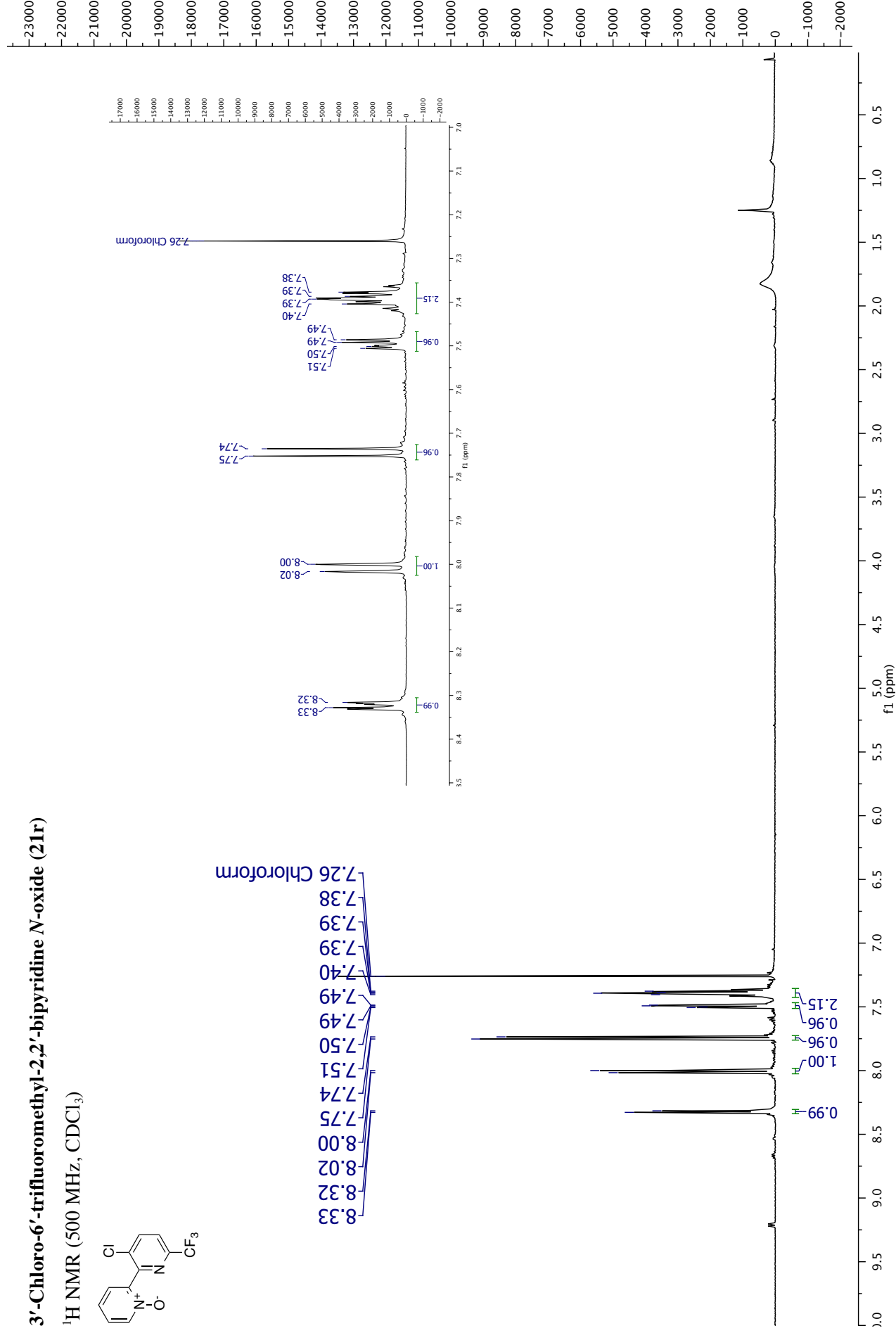
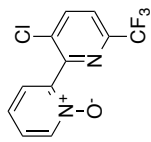
3'-Chloro-6'-methoxy-2,2'-bipyridine N-oxide (21p)

¹³C NMR (126 MHz, CDCl₃)



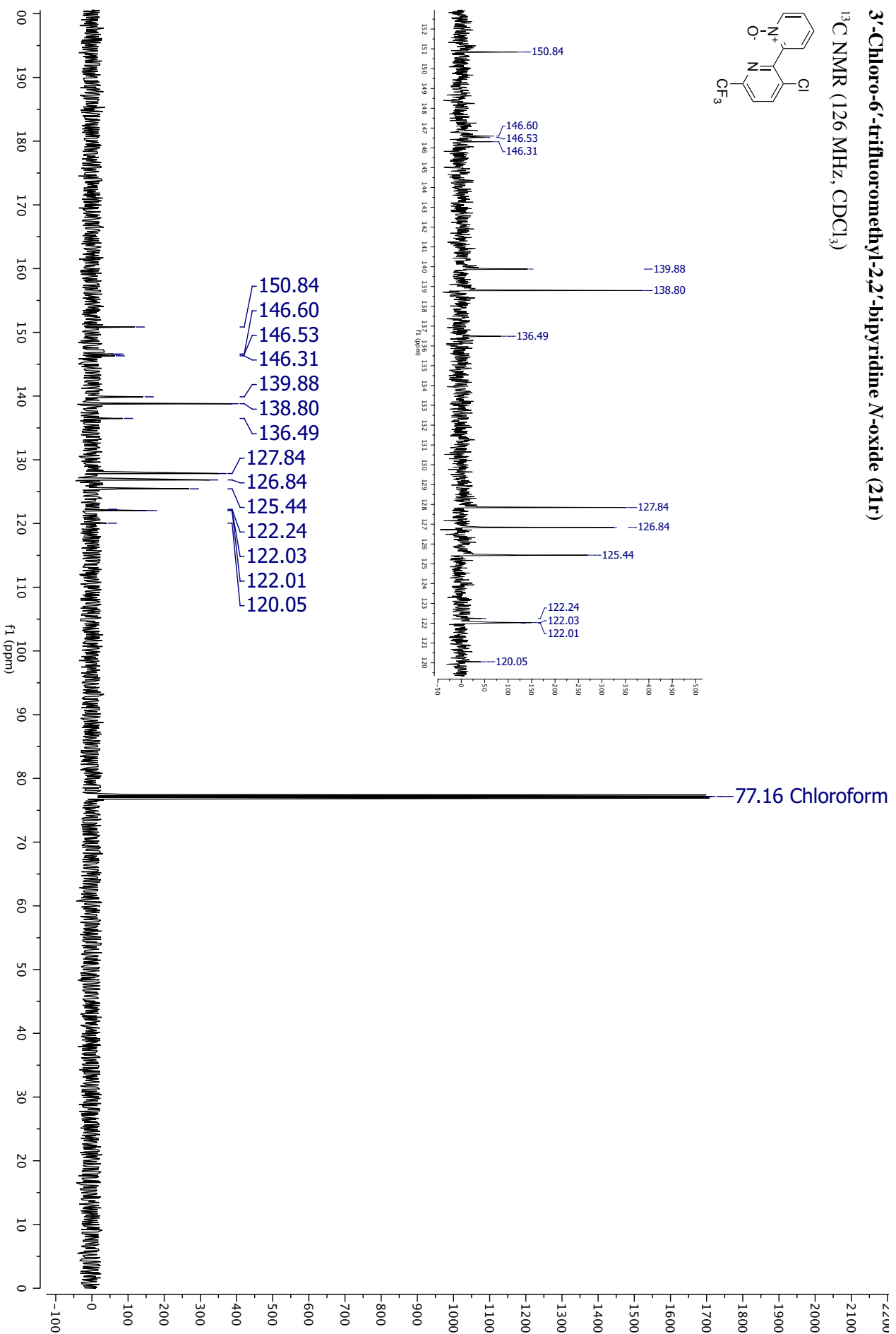
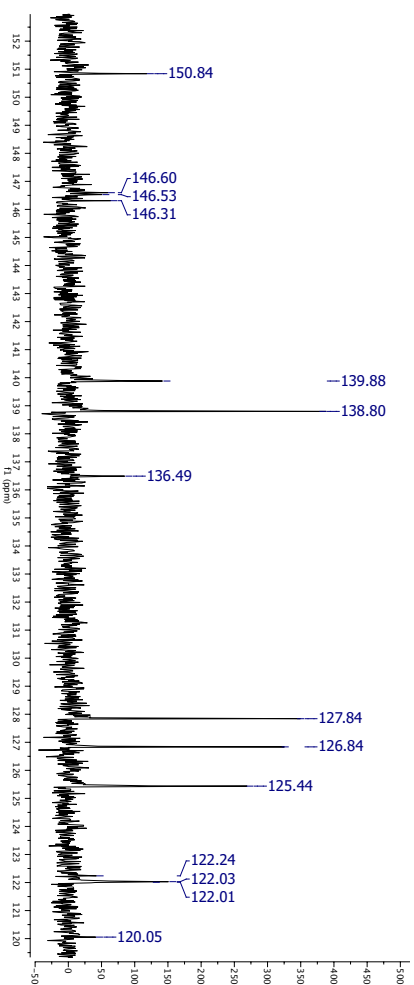
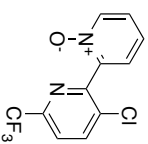
3'-Chloro-6'-trifluoromethyl-2,2'-bipyridine N-oxide (21r)

¹H NMR (500 MHz, CDCl₃)



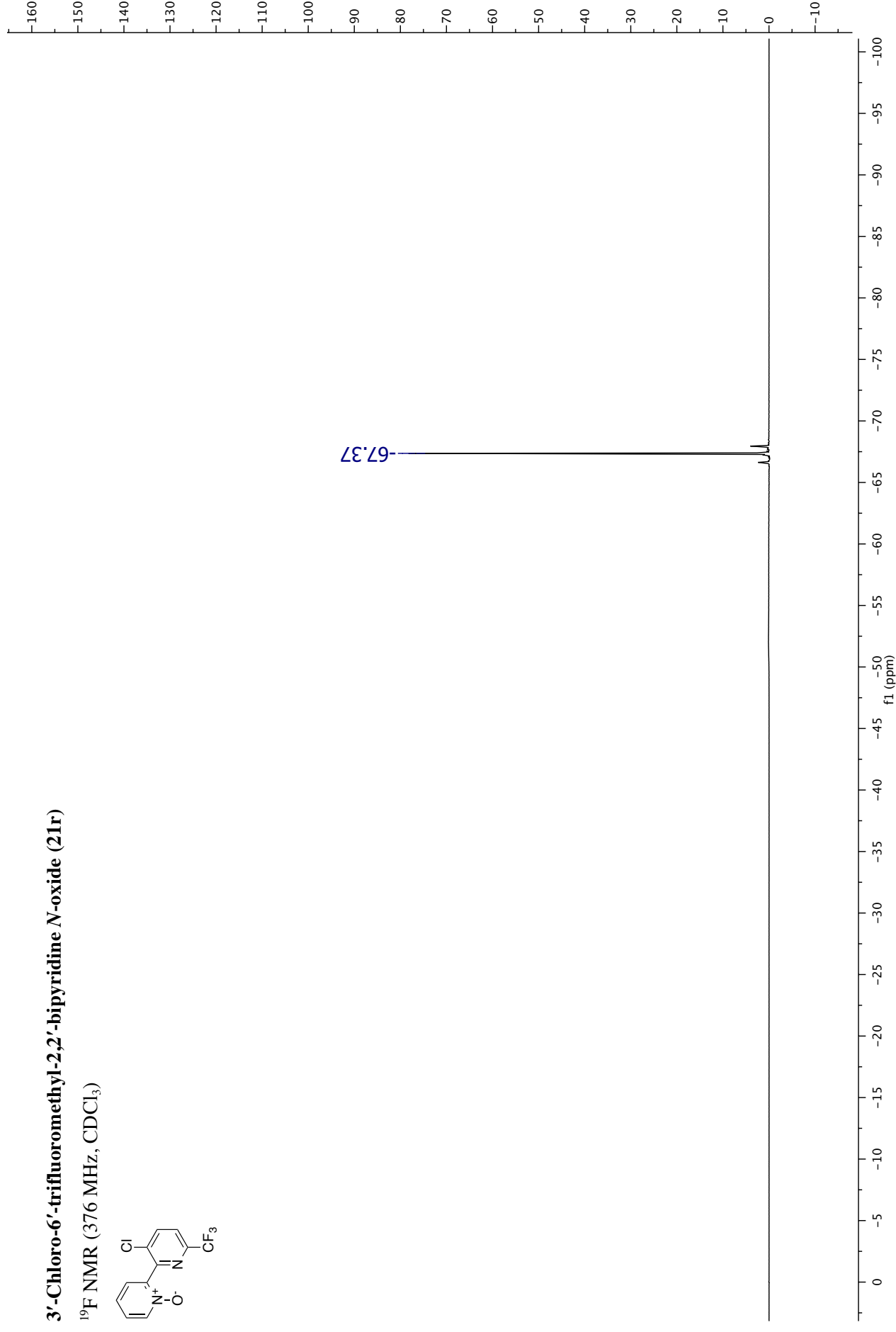
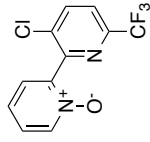
3'-Chloro-6'-trifluoromethyl-2,2'-bipyridine N-oxide (21r)

¹³C NMR (126 MHz, CDCl₃)



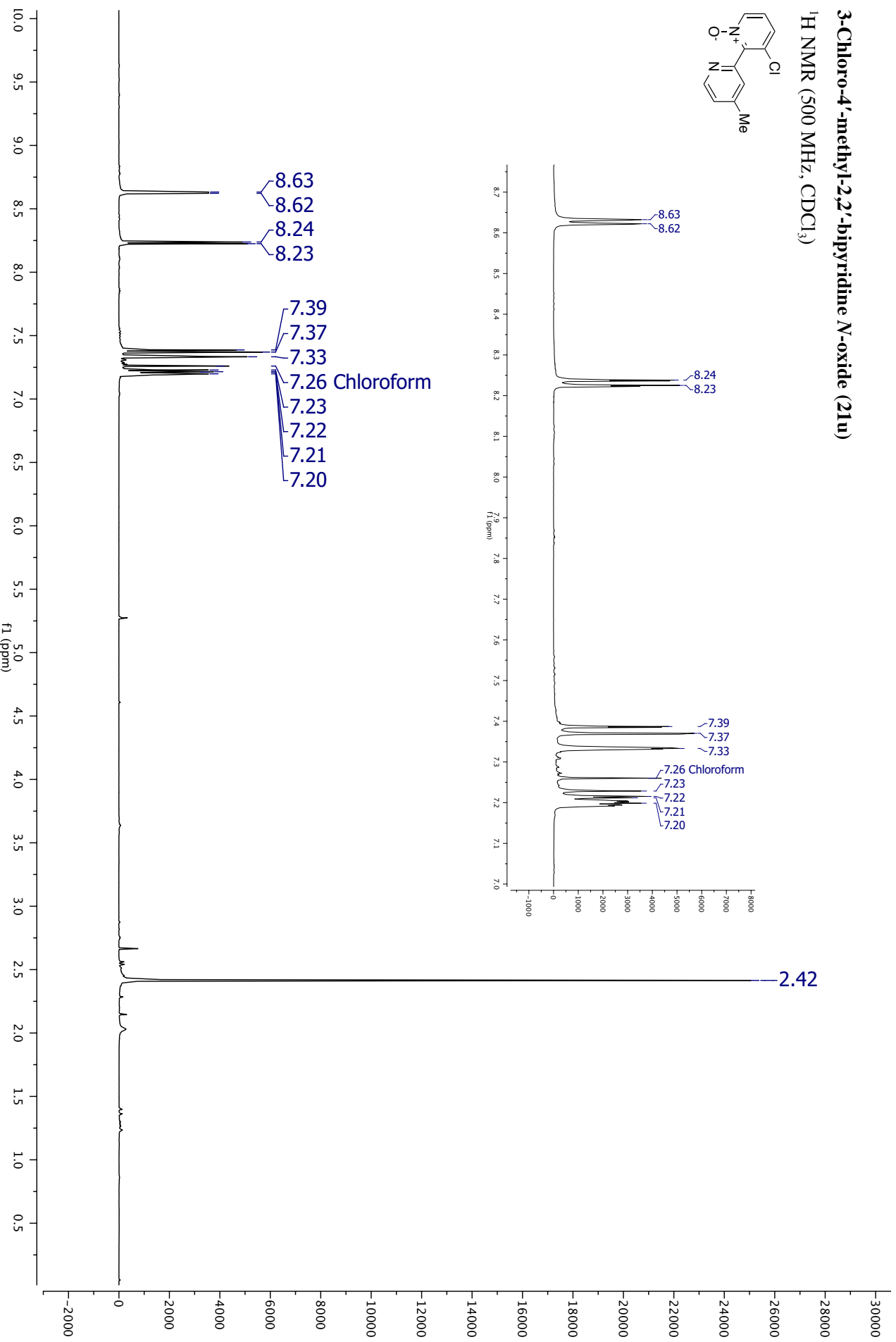
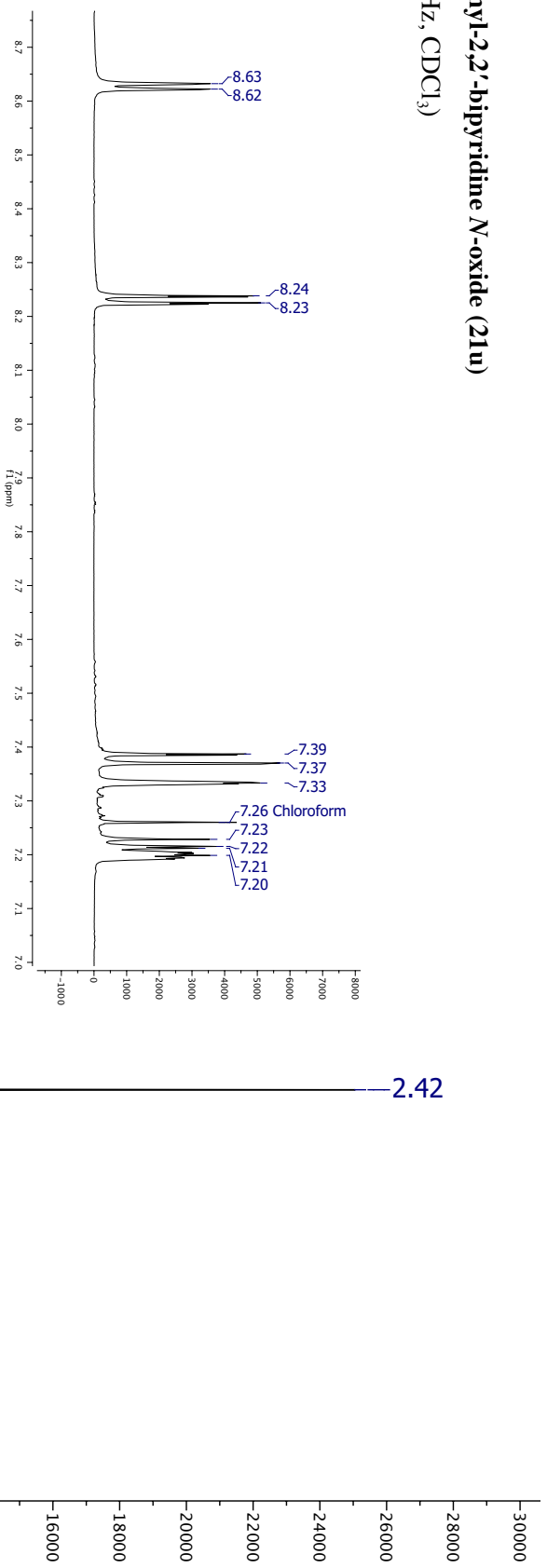
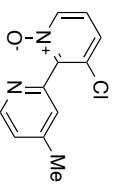
3'-Chloro-6'-trifluoromethyl-2,2'-bipyridine N-oxide (21r)

¹⁹F NMR (376 MHz, CDCl₃)



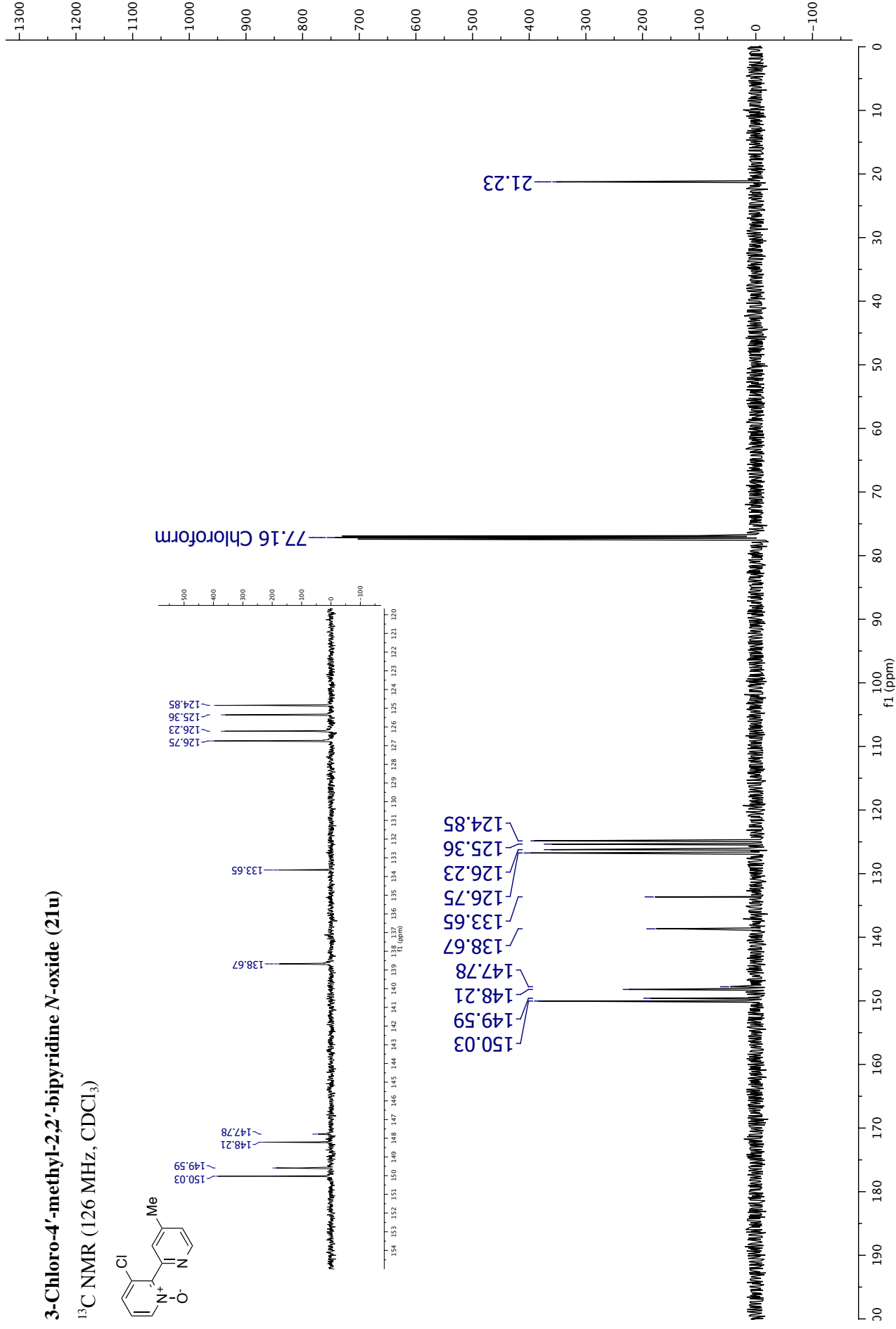
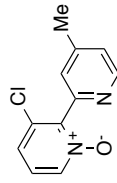
3-Chloro-4'-methyl-2,2'-bipyridine N-oxide (21u)

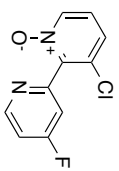
¹H NMR (500 MHz, CDCl₃)



3-Chloro-4'-methyl-2,2'-bipyridine N-oxide (21u)

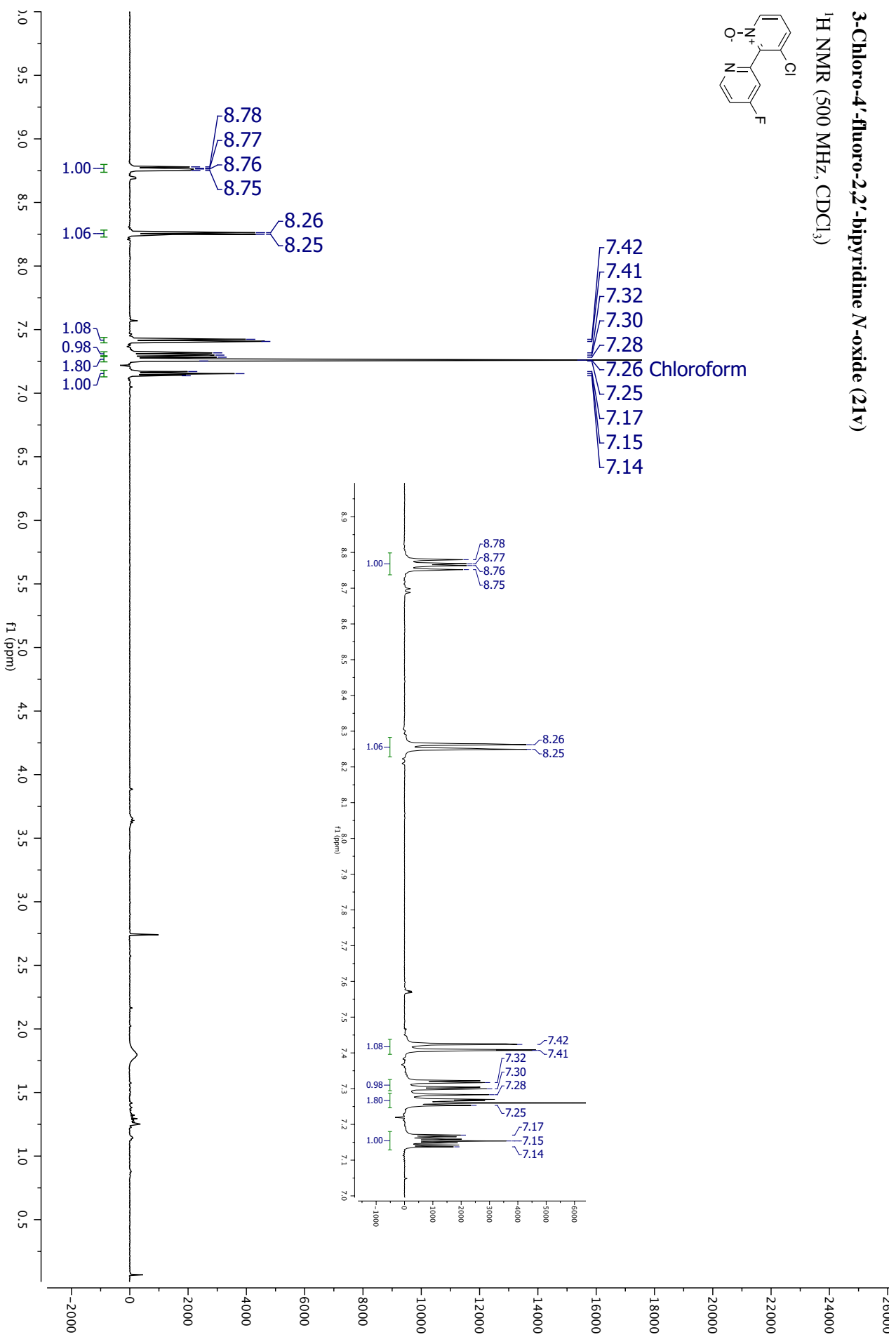
^{13}C NMR (126 MHz, CDCl_3)





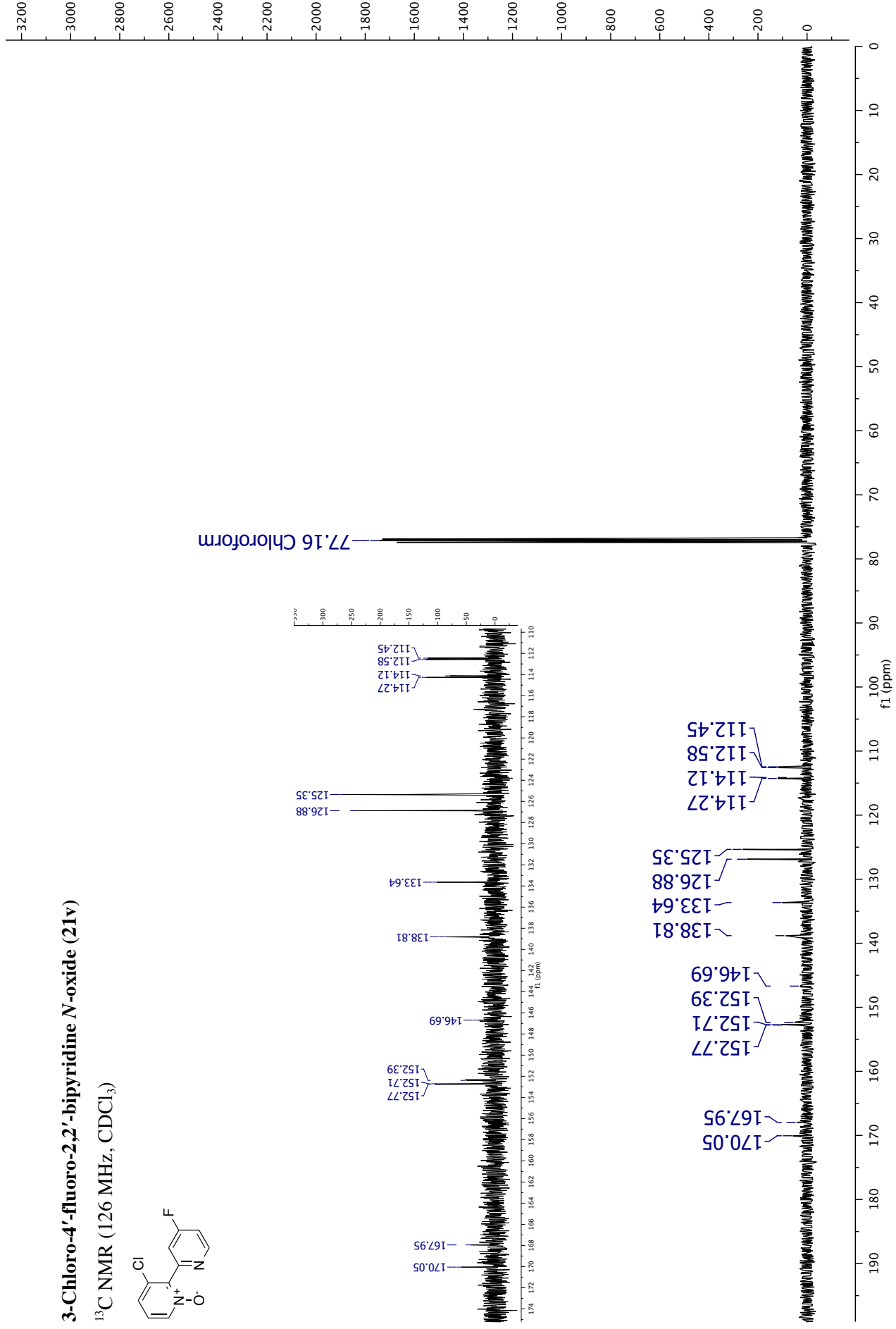
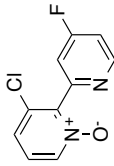
3-Chloro-4'-fluoro-2,2'-bipyridine N-oxide (21v)

¹H NMR (500 MHz, CDCl₃)



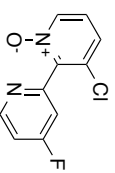
3-Chloro-4'-fluoro-2,2'-bipyridine N-oxide (21v)

¹³C NMR (126 MHz, CDCl₃)

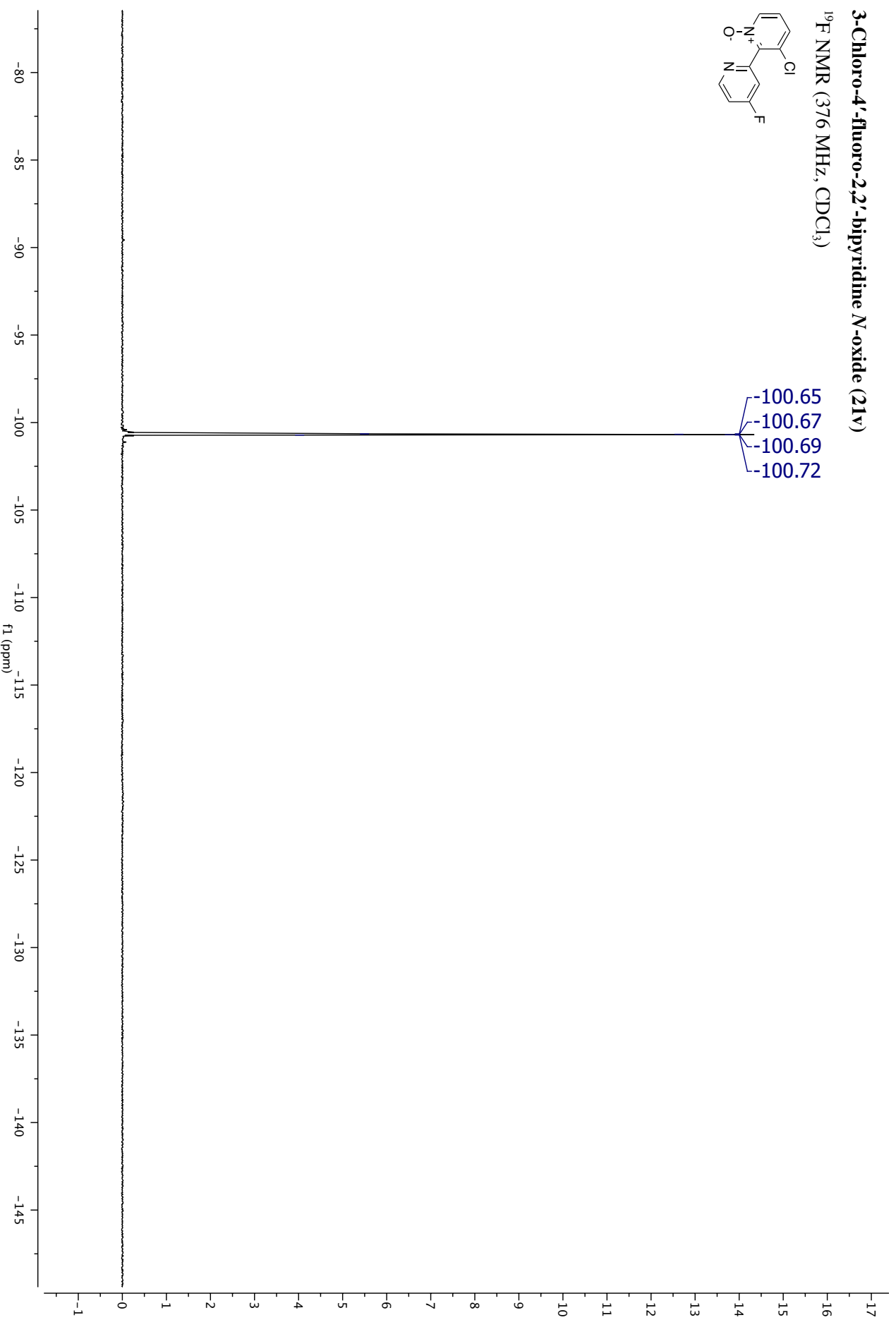


3-Chloro-4'-fluoro-2,2'-bipyridine N-oxide (21v)

¹⁹F NMR (376 MHz, CDCl₃)

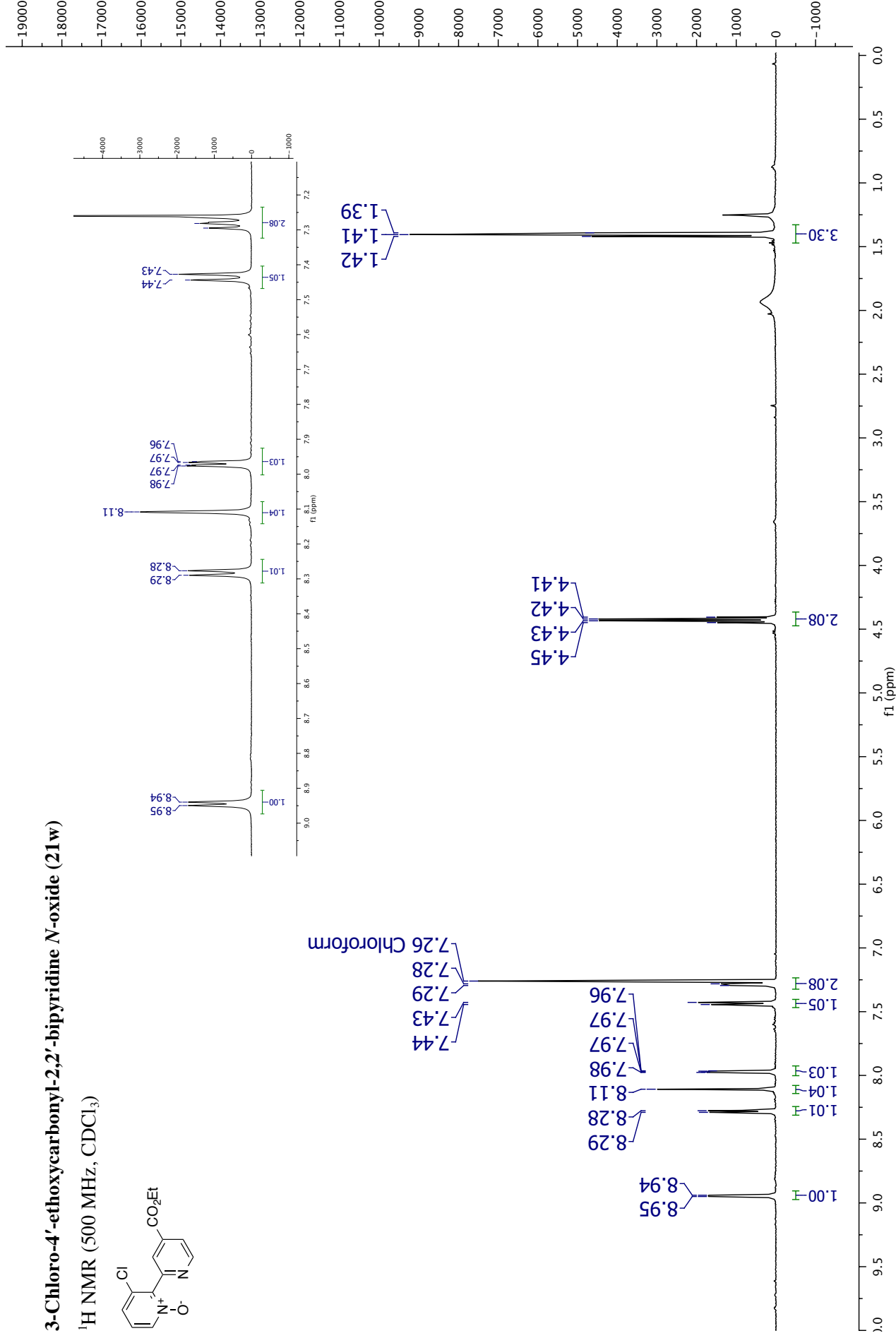
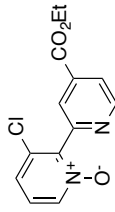


-100.65
-100.67
-100.69
-100.72



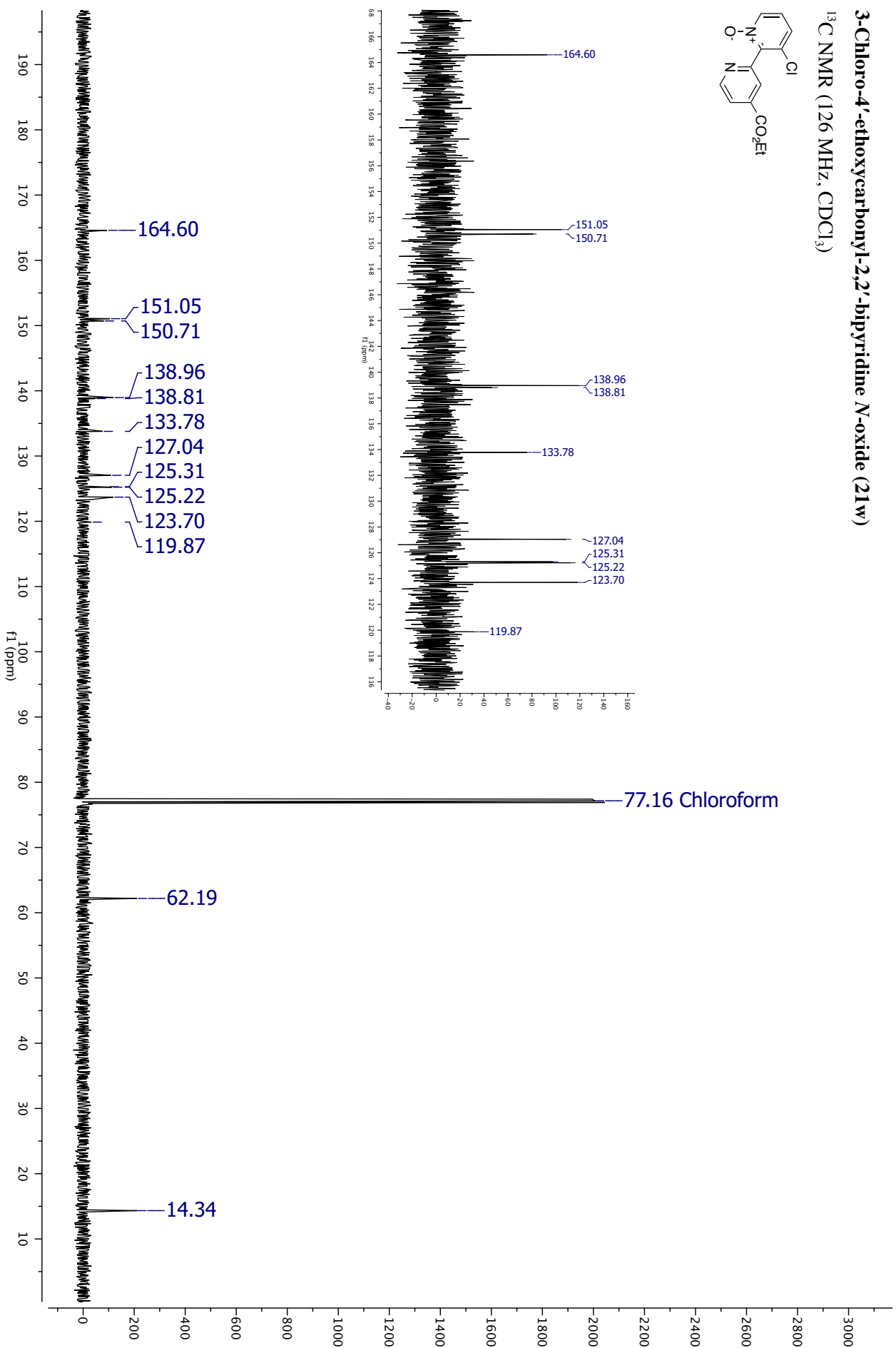
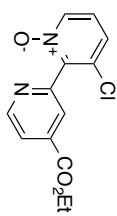
3-Chloro-4'-ethoxycarbonyl-2,2'-bipyridine N-oxide (21w)

¹H NMR (500 MHz, CDCl₃)



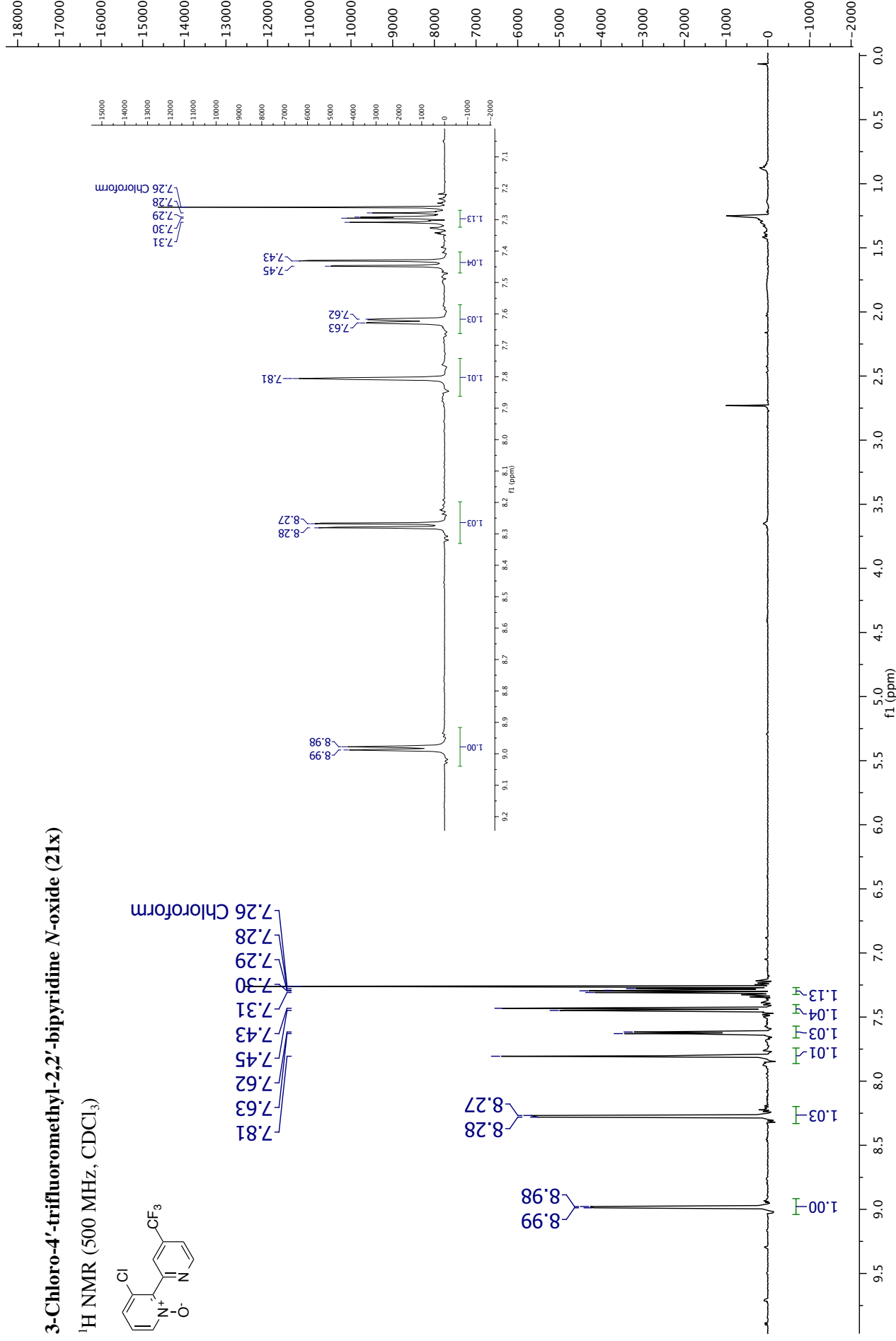
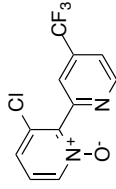
3-Chloro-4'-ethoxycarbonyl-2,2'-bipyridine N-oxide (21w)

¹³C NMR (126 MHz, CDCl₃)



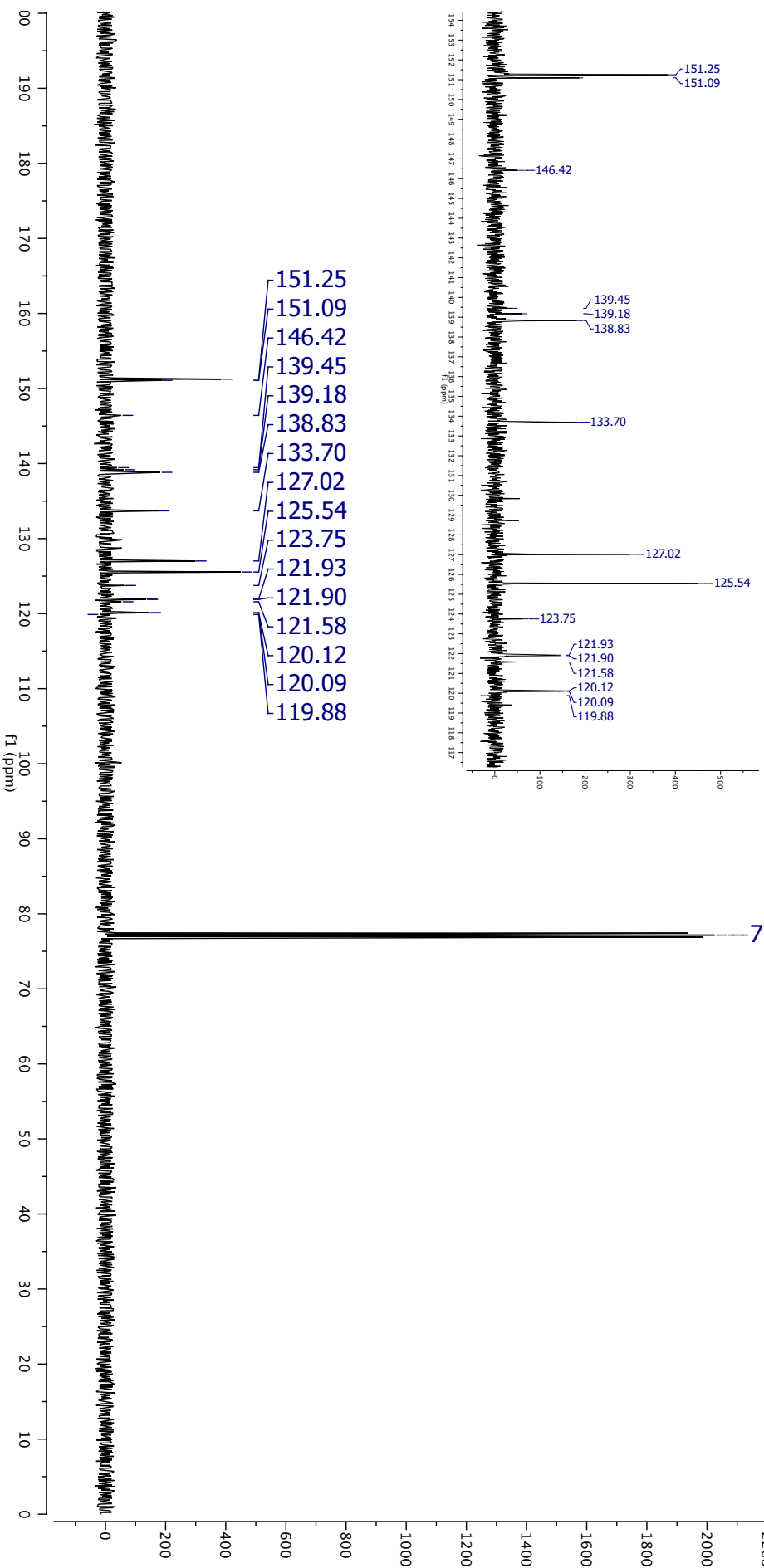
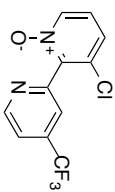
3-Chloro-4'-trifluoromethyl-2,2'-bipyridine N-oxide (21x)

¹H NMR (500 MHz, CDCl₃)



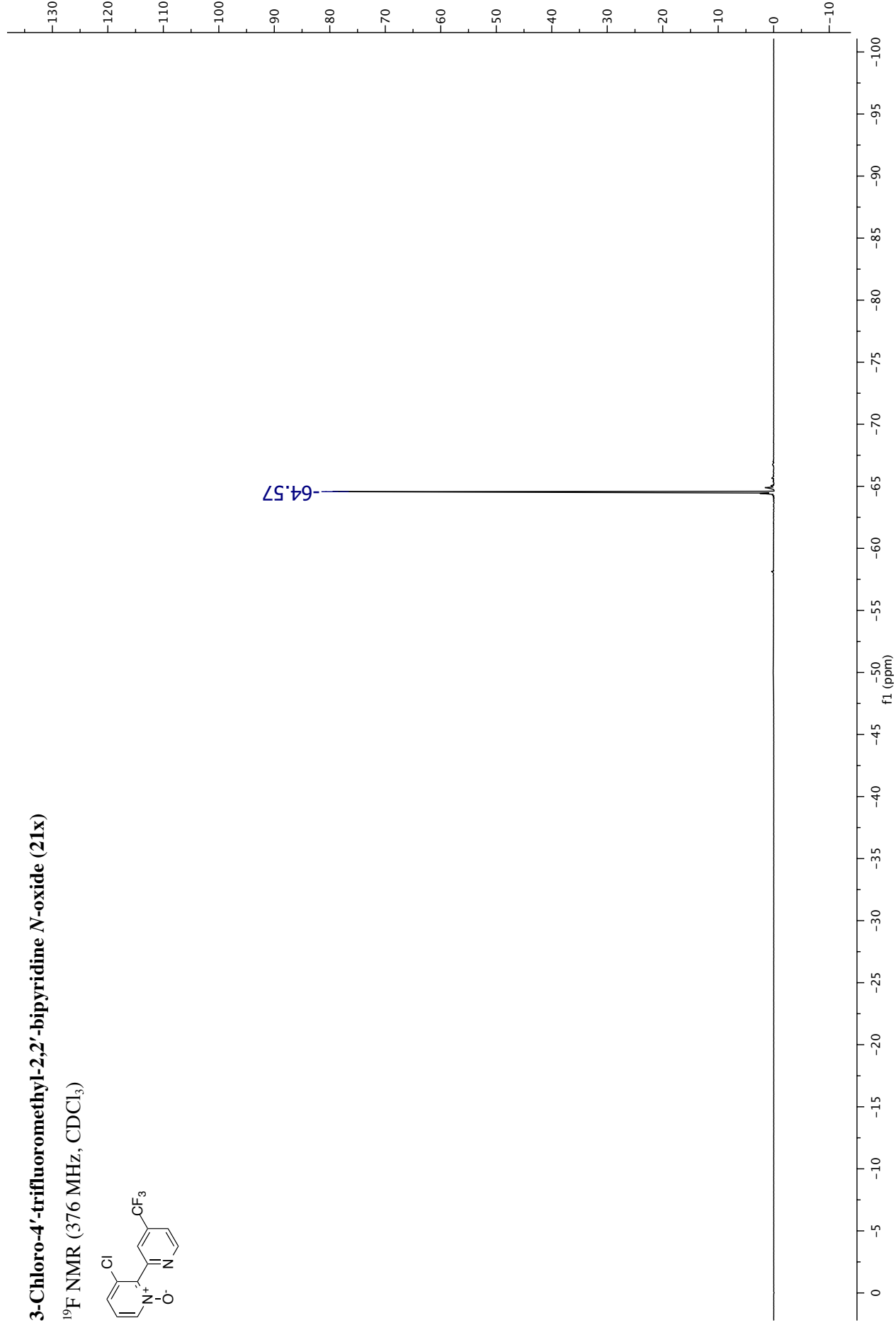
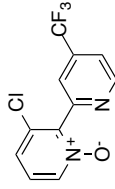
3-Chloro-4'-trifluoromethyl-2,2'-bipyridine N-oxide (21x)

¹³C NMR (126 MHz, CDCl₃)



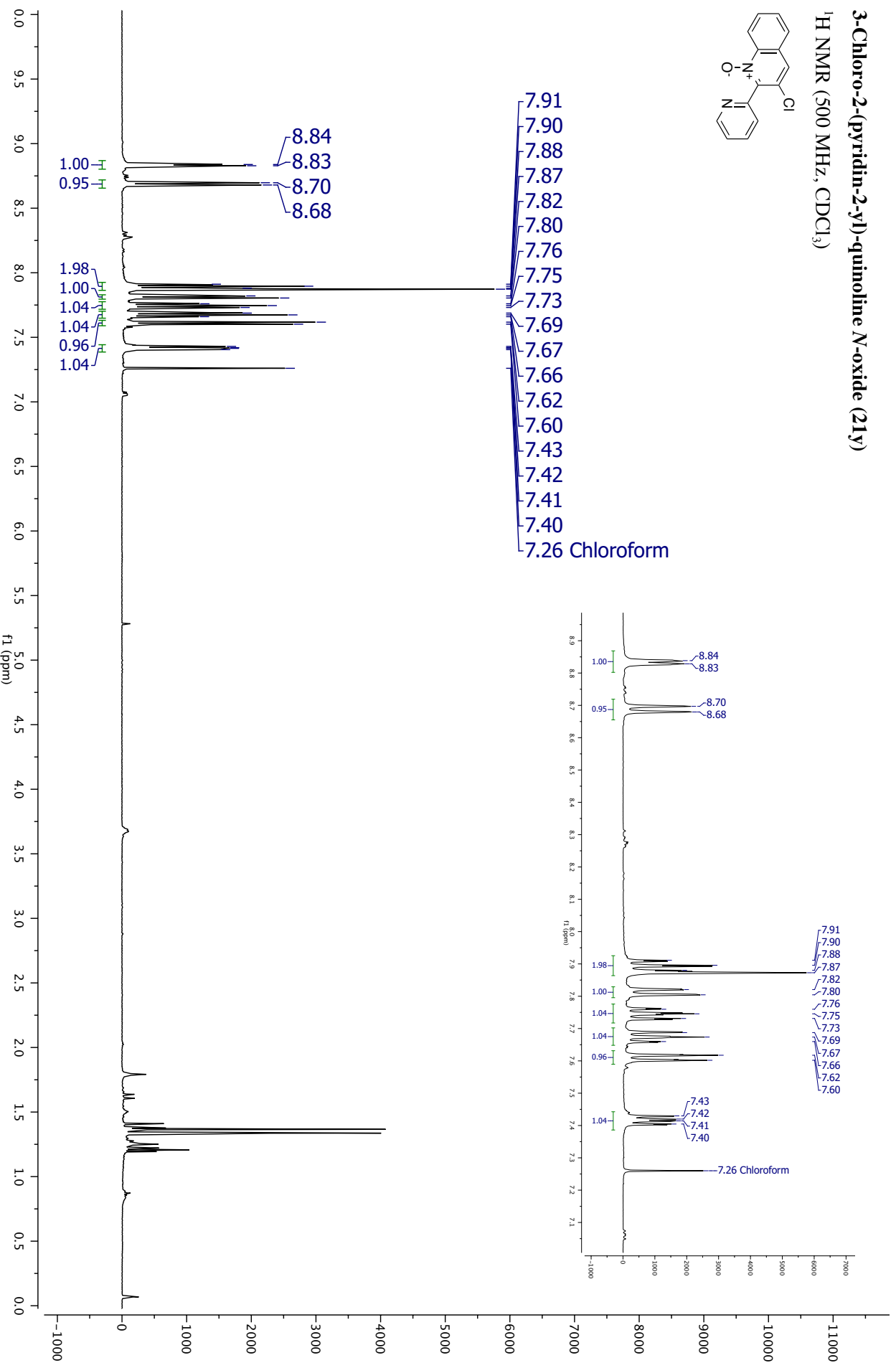
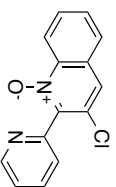
3-Chloro-4'-trifluoromethyl-2,2'-bipyridine N-oxide (21x)

^{19}F NMR (376 MHz, CDCl_3)



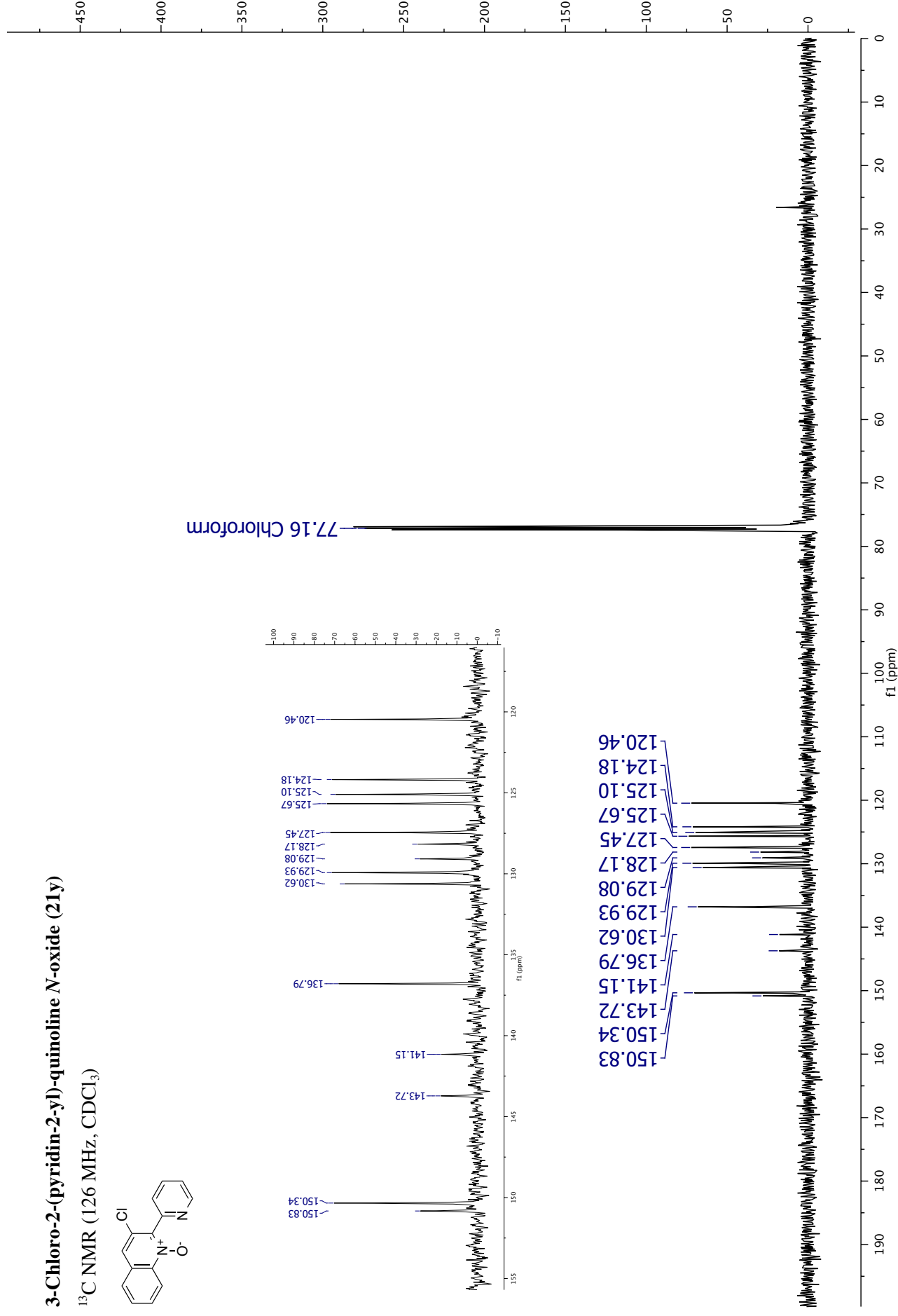
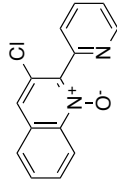
3-Chloro-2-(pyridin-2-yl)-quinoline N-oxide (21y)

¹H NMR (500 MHz, CDCl₃)



3-Chloro-2-(pyridin-2-yl)-quinoline N-oxide (21y)

¹³C NMR (126 MHz, CDCl₃)

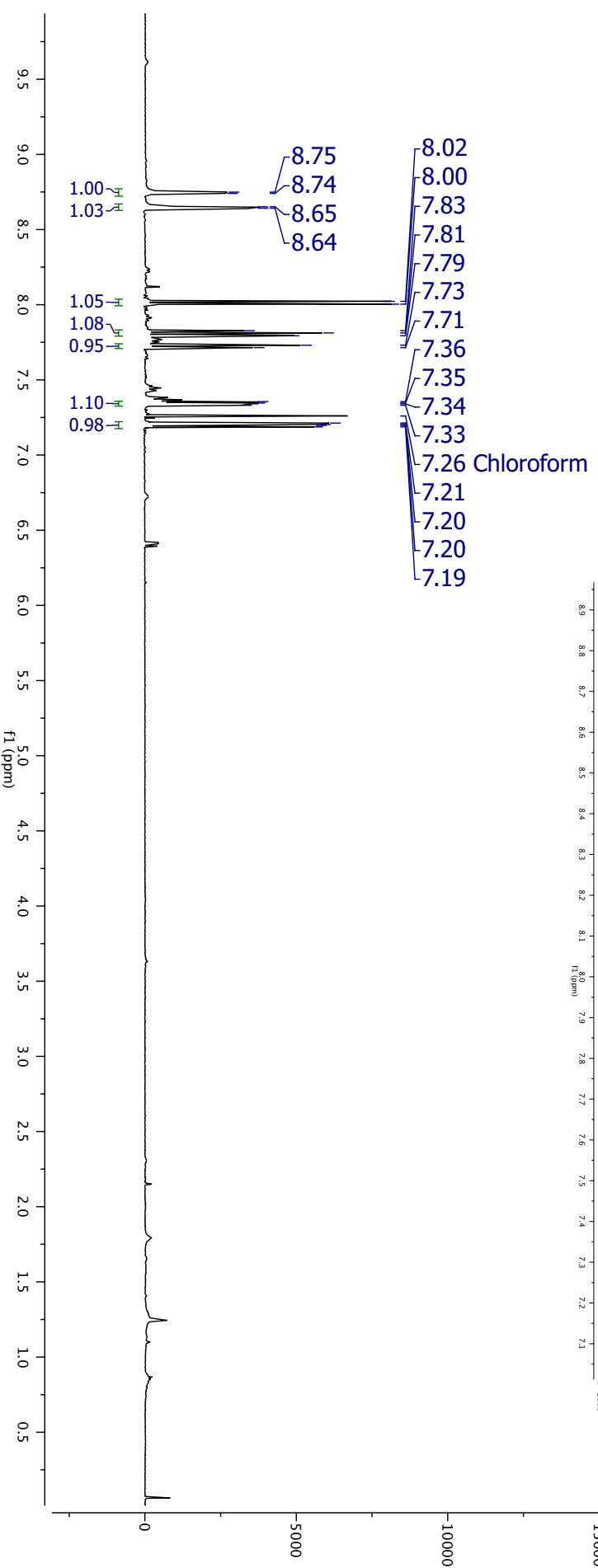
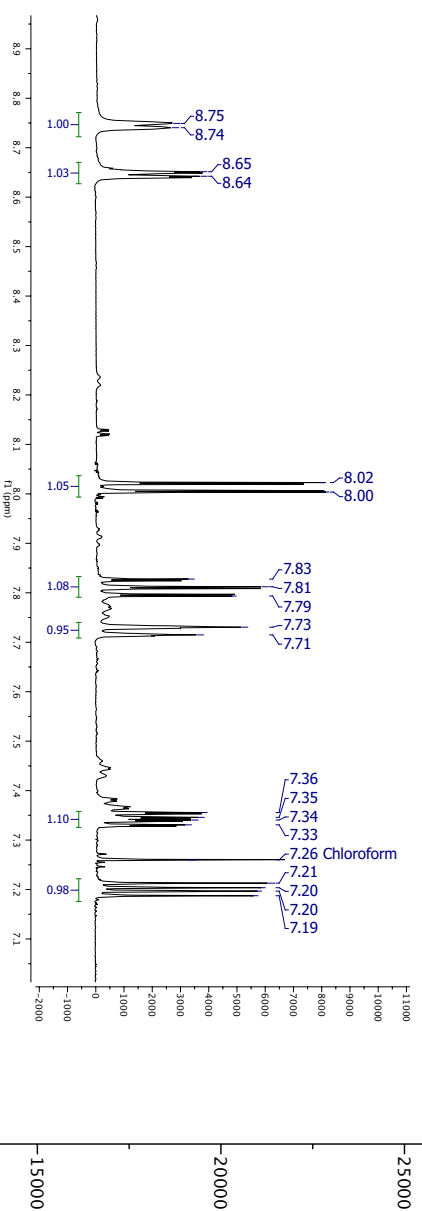
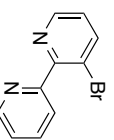


10.7 3-Halobipyridines (25, 34)

10.7.1 3-Bromobipyridines (25)

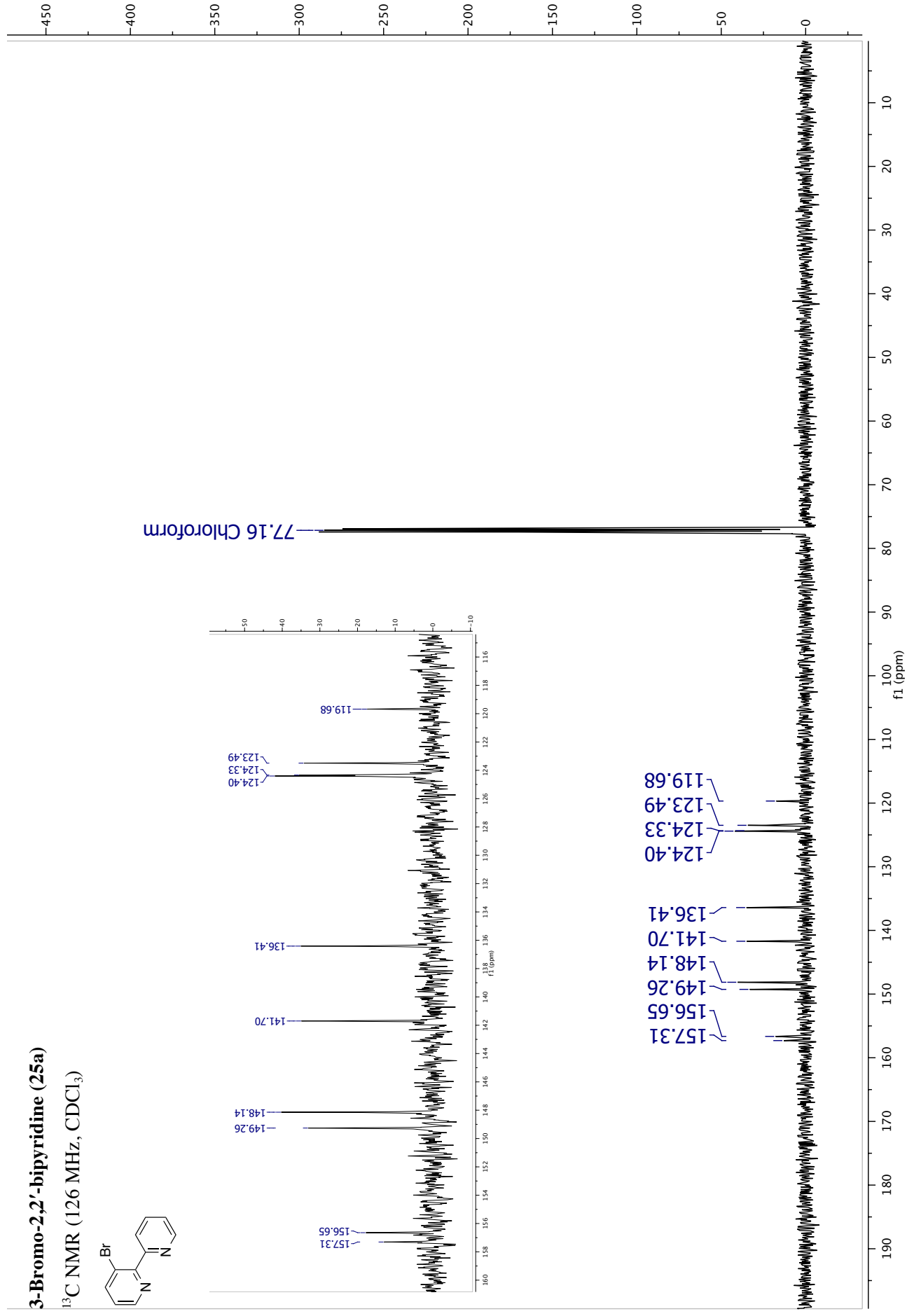
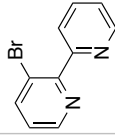
3-Bromo-2,2'-bipyridine (25a)

¹H NMR (500 MHz, CDCl₃)



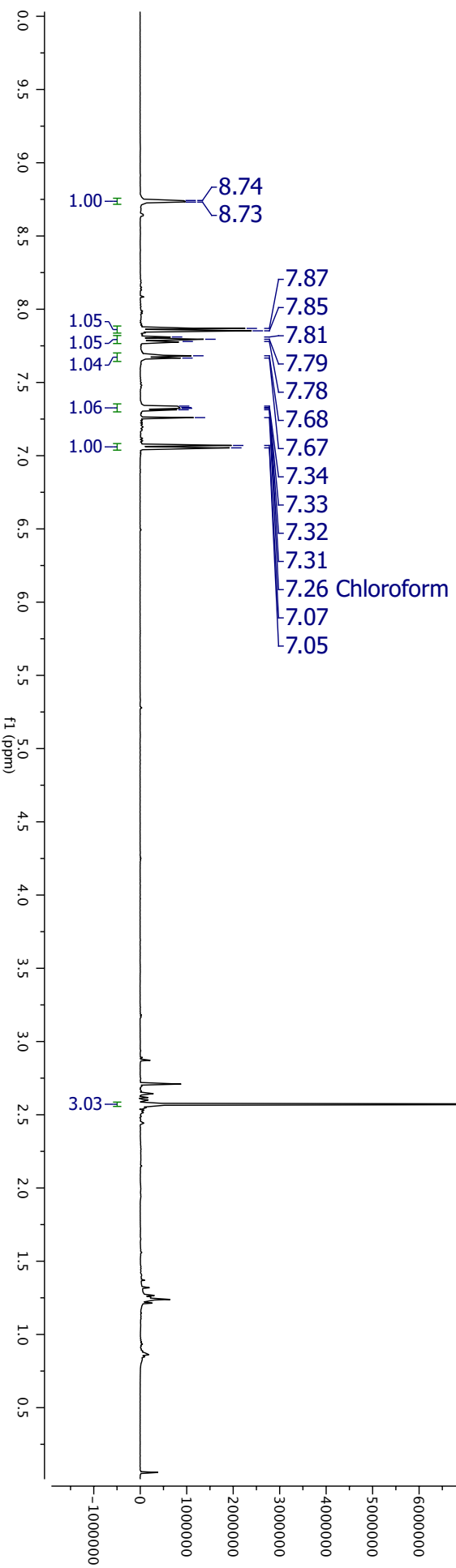
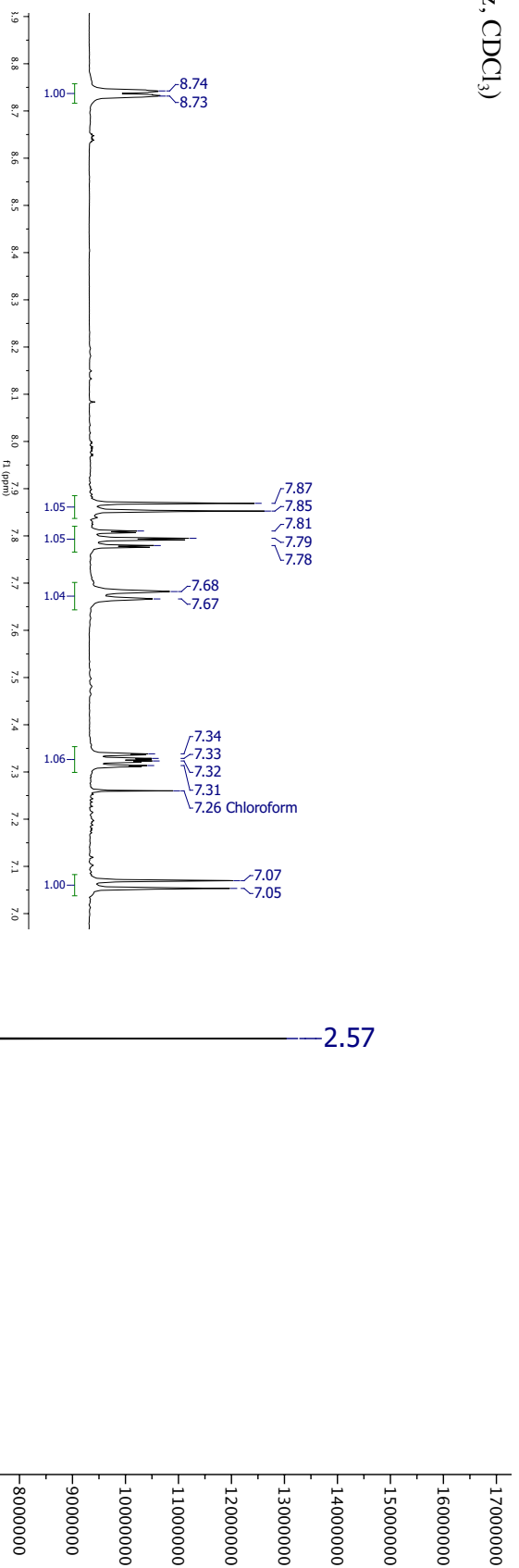
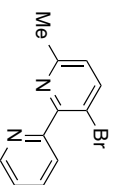
3-Bromo-2,2'-bipyridine (25a)

^{13}C NMR (126 MHz, CDCl_3)



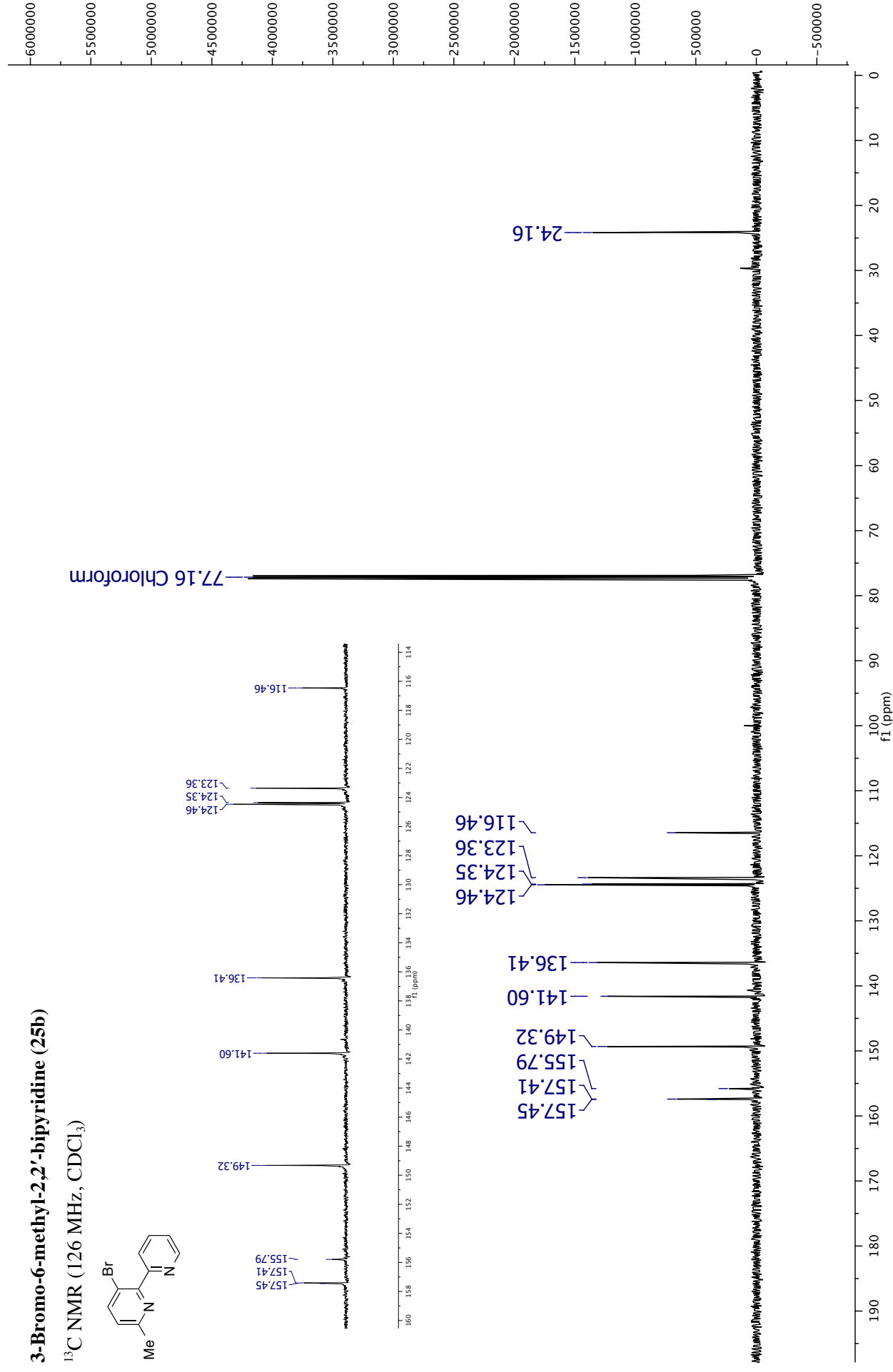
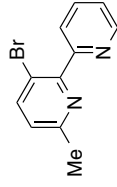
3-Bromo-6-methyl-2,2'-bipyridine (25b)

¹H NMR (500 MHz, CDCl₃)



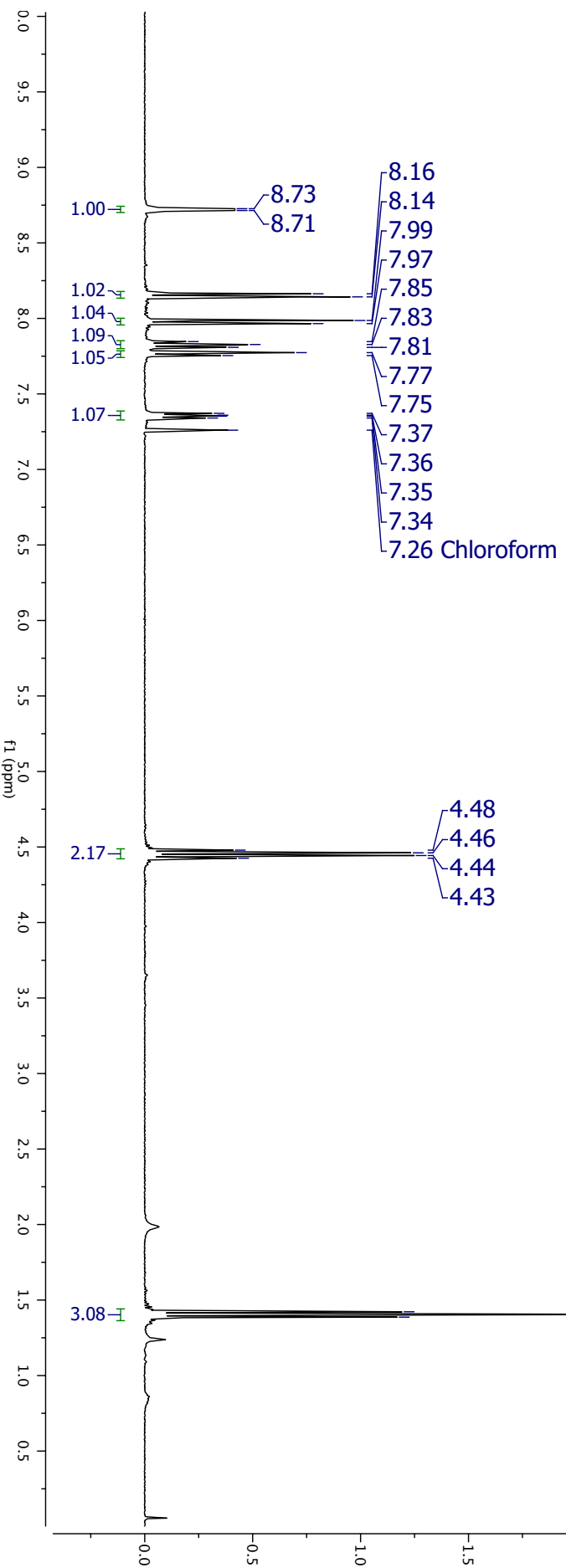
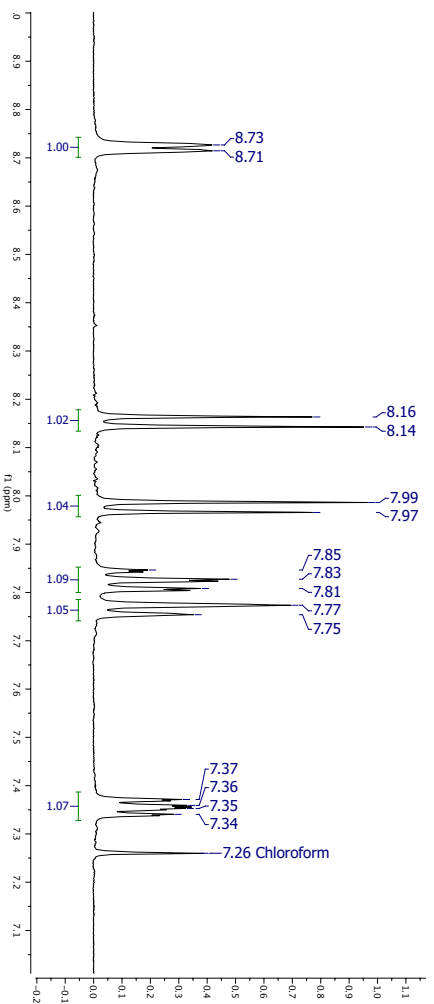
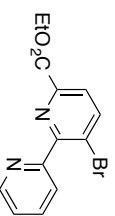
3-Bromo-6-methyl-2,2'-bipyridine (25b)

^{13}C NMR (126 MHz, CDCl_3)



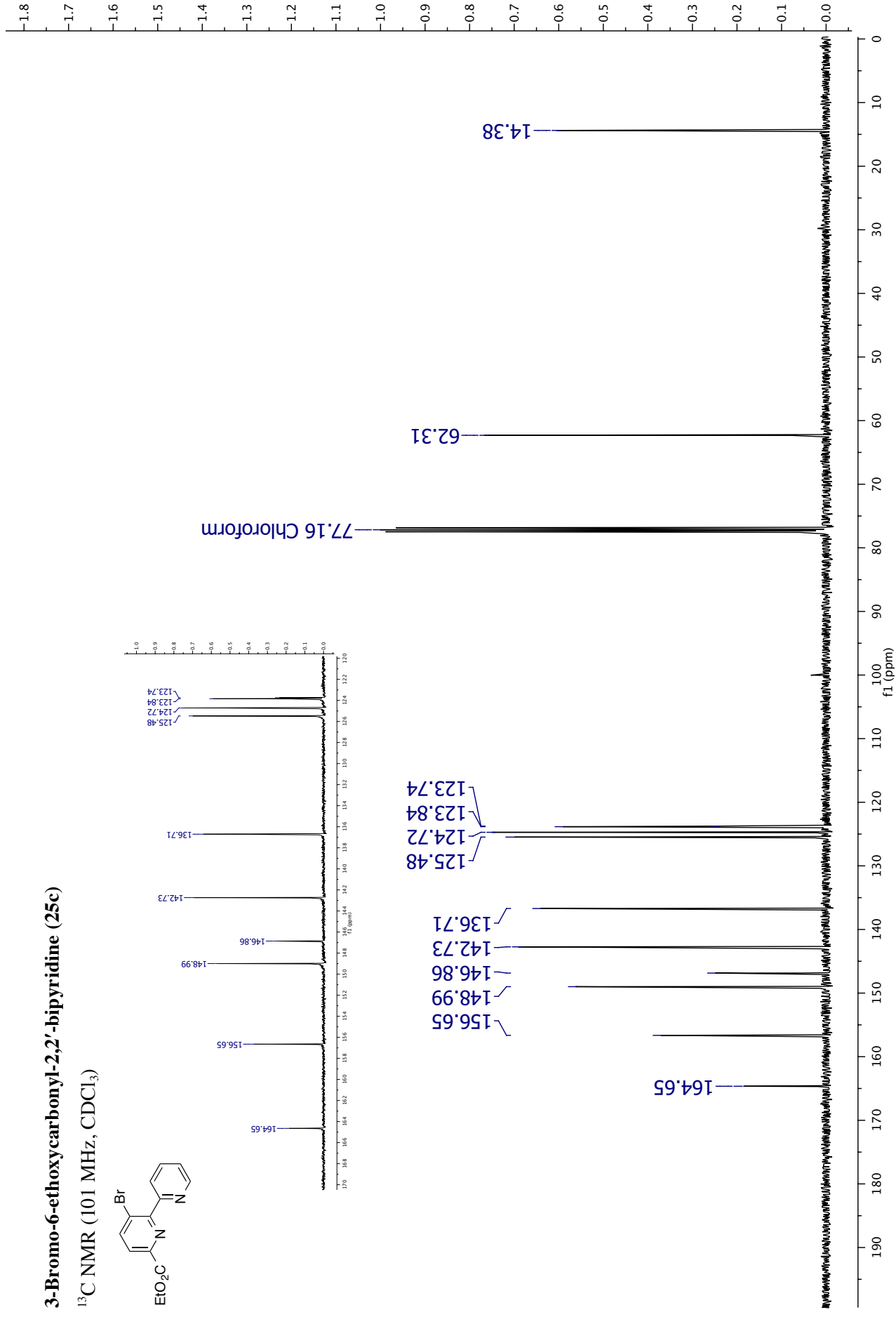
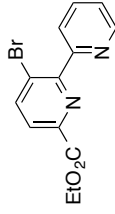
3-Bromo-6-ethoxycarbonyl-2,2'-bipyridine (25c)

¹H NMR (400 MHz, CDCl₃)



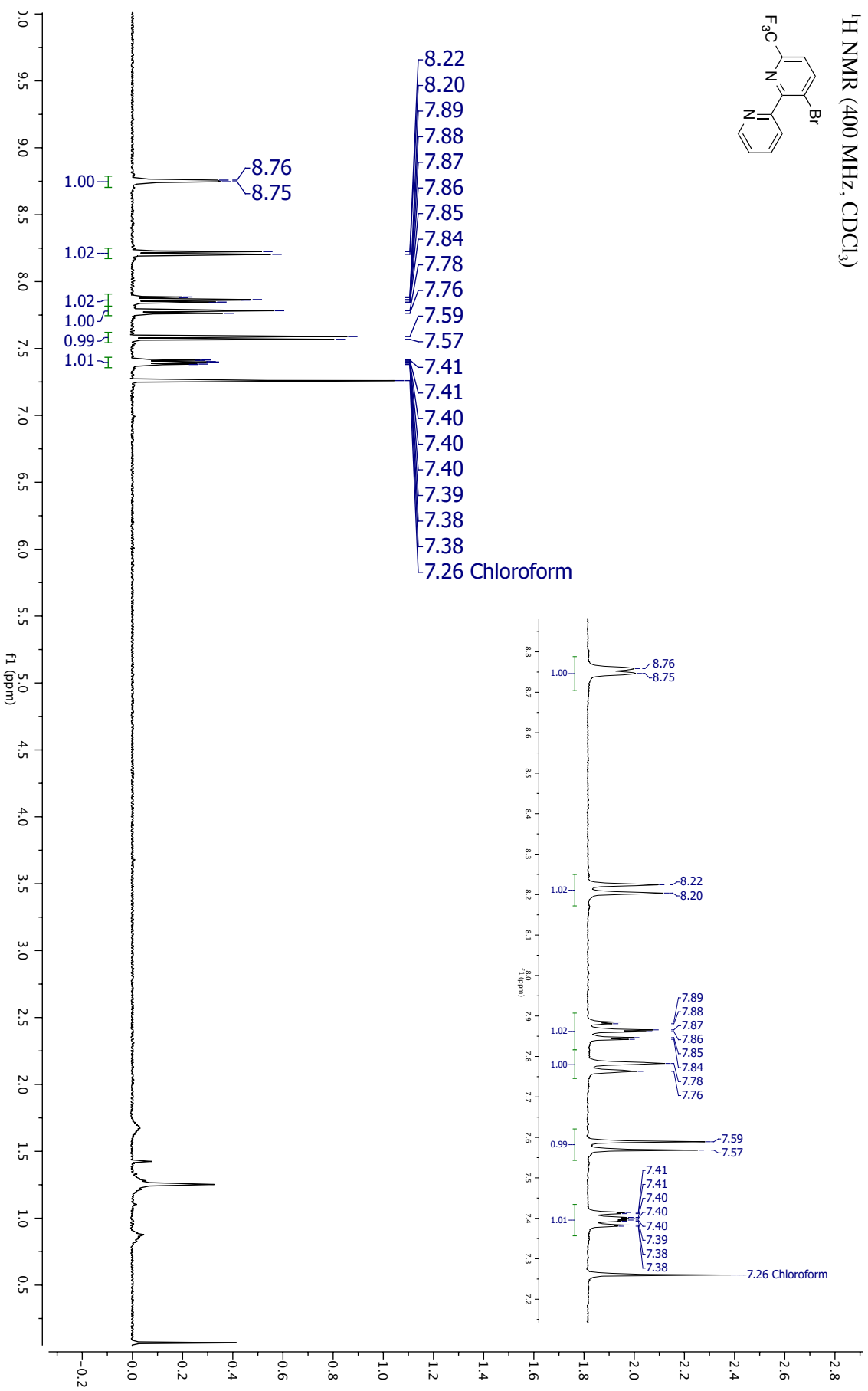
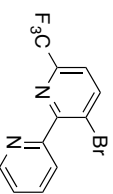
3-Bromo-6-ethoxycarbonyl-2,2'-bipyridine (25c)

^{13}C NMR (101 MHz, CDCl_3)



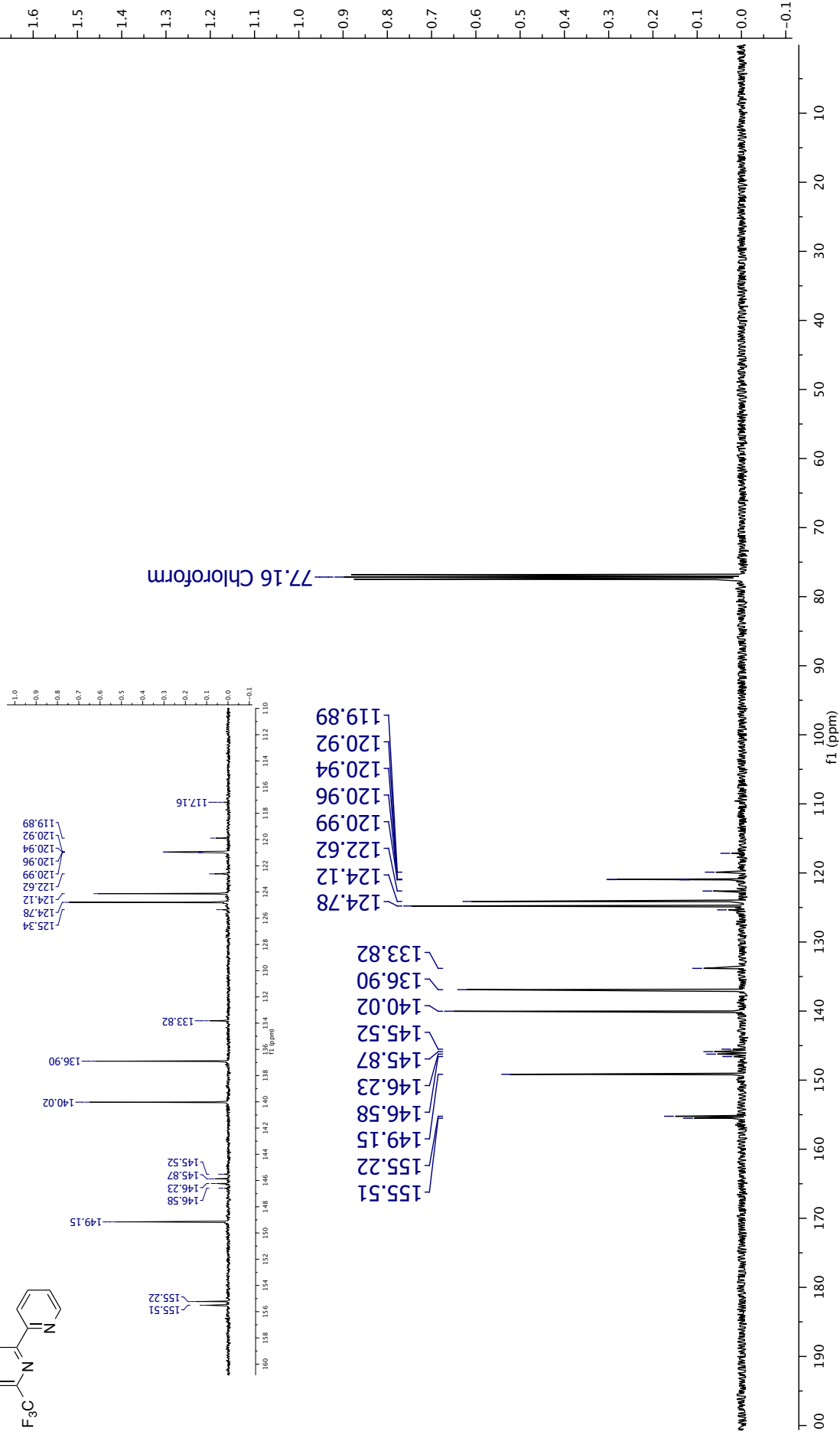
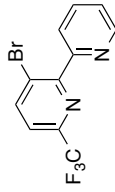
3-Bromo-6-(trifluoromethyl)-2,2'-bipyridine (25d)

¹H NMR (400 MHz, CDCl₃)



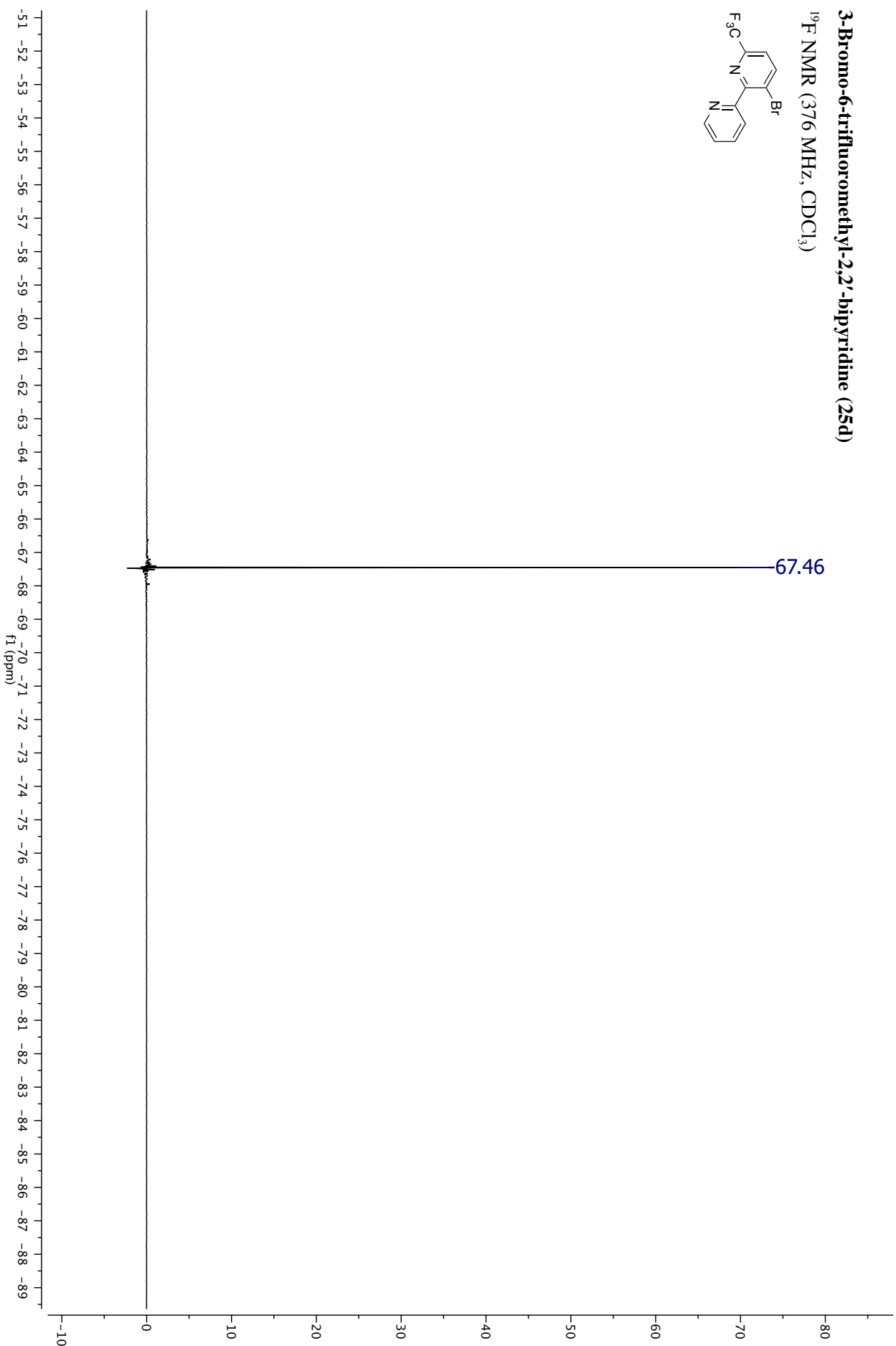
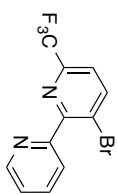
3-Bromo-6-trifluoromethyl-2,2'-bipyridine (25d)

^{13}C NMR (126 MHz, CDCl_3)



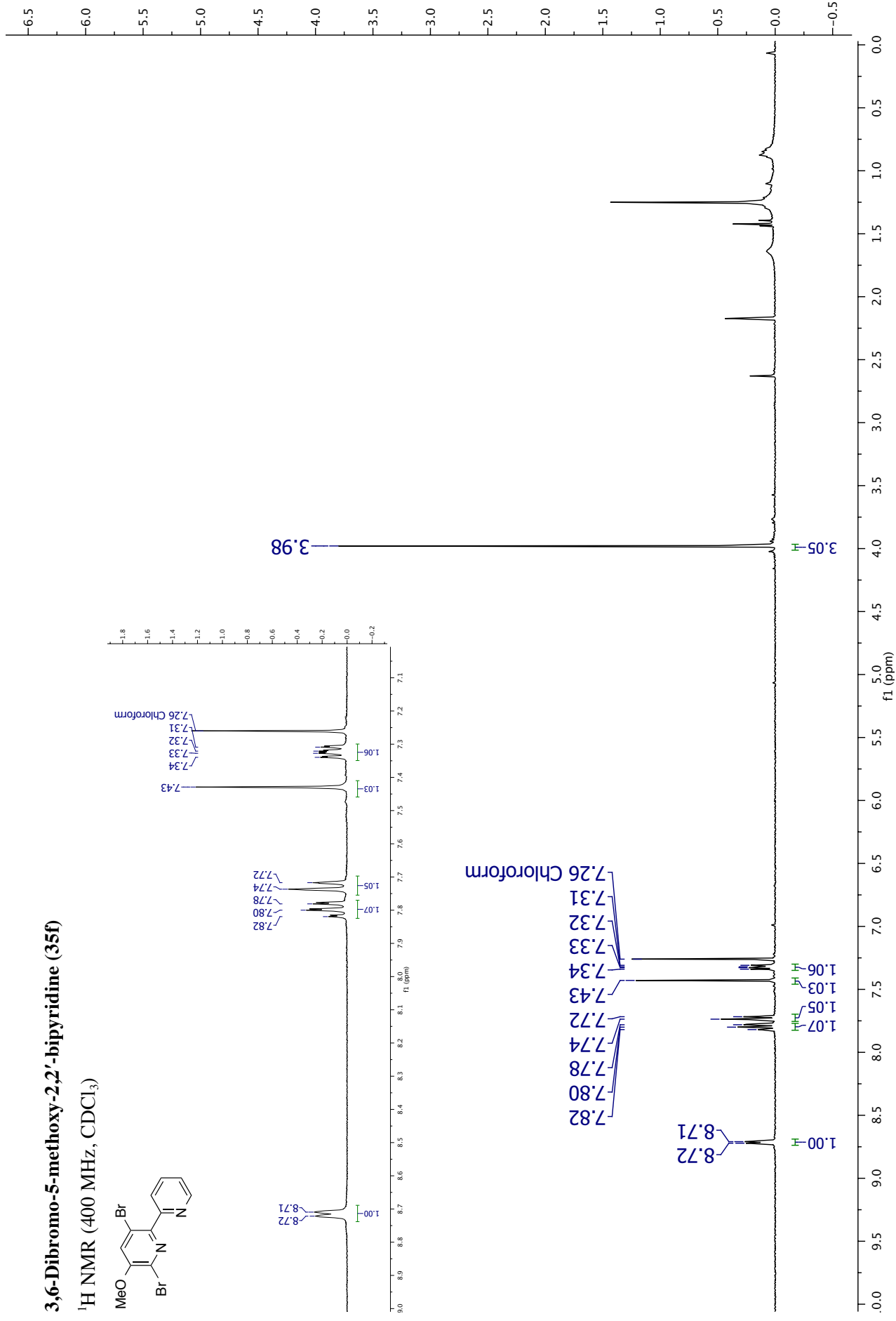
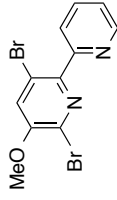
3-Bromo-6-trifluoromethyl-2,2'-bipyridine (25d)

¹⁹F NMR (376 MHz, CDCl₃)



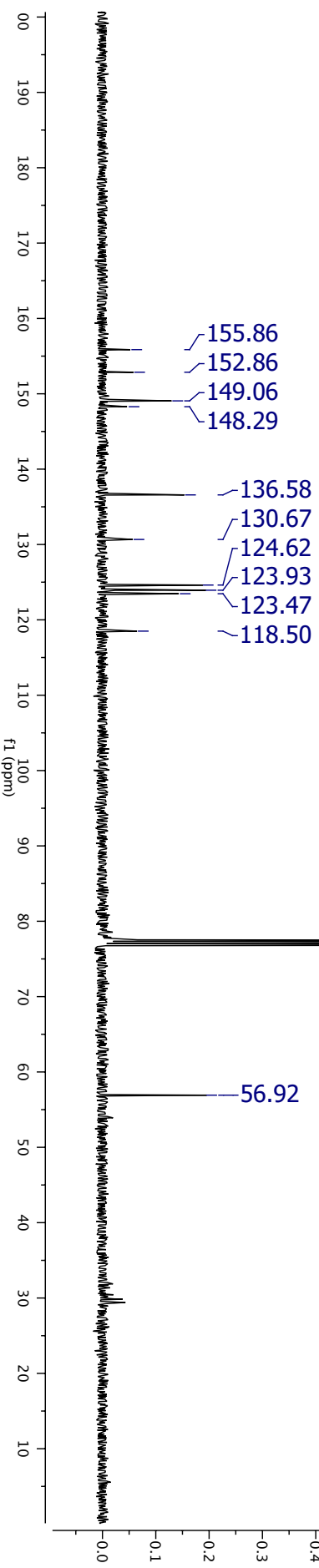
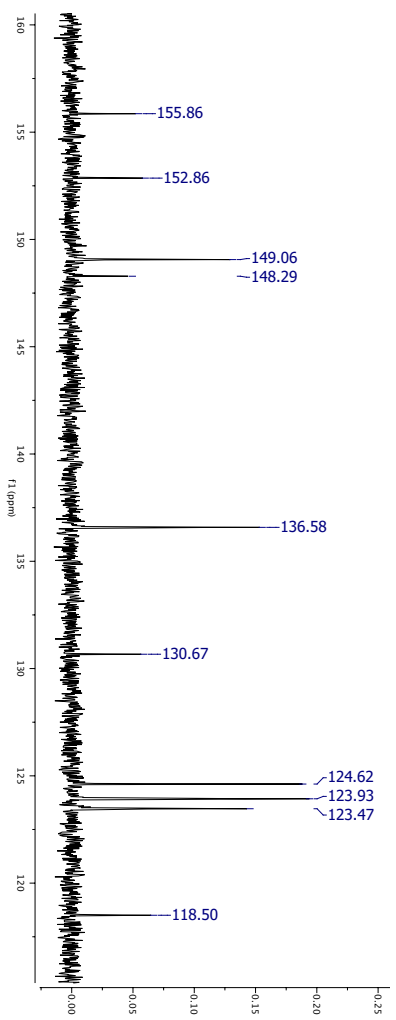
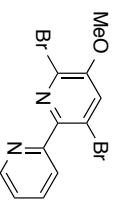
3,6-Dibromo-5-methoxy-2,2'-bipyridine (35f)

¹H NMR (400 MHz, CDCl₃)



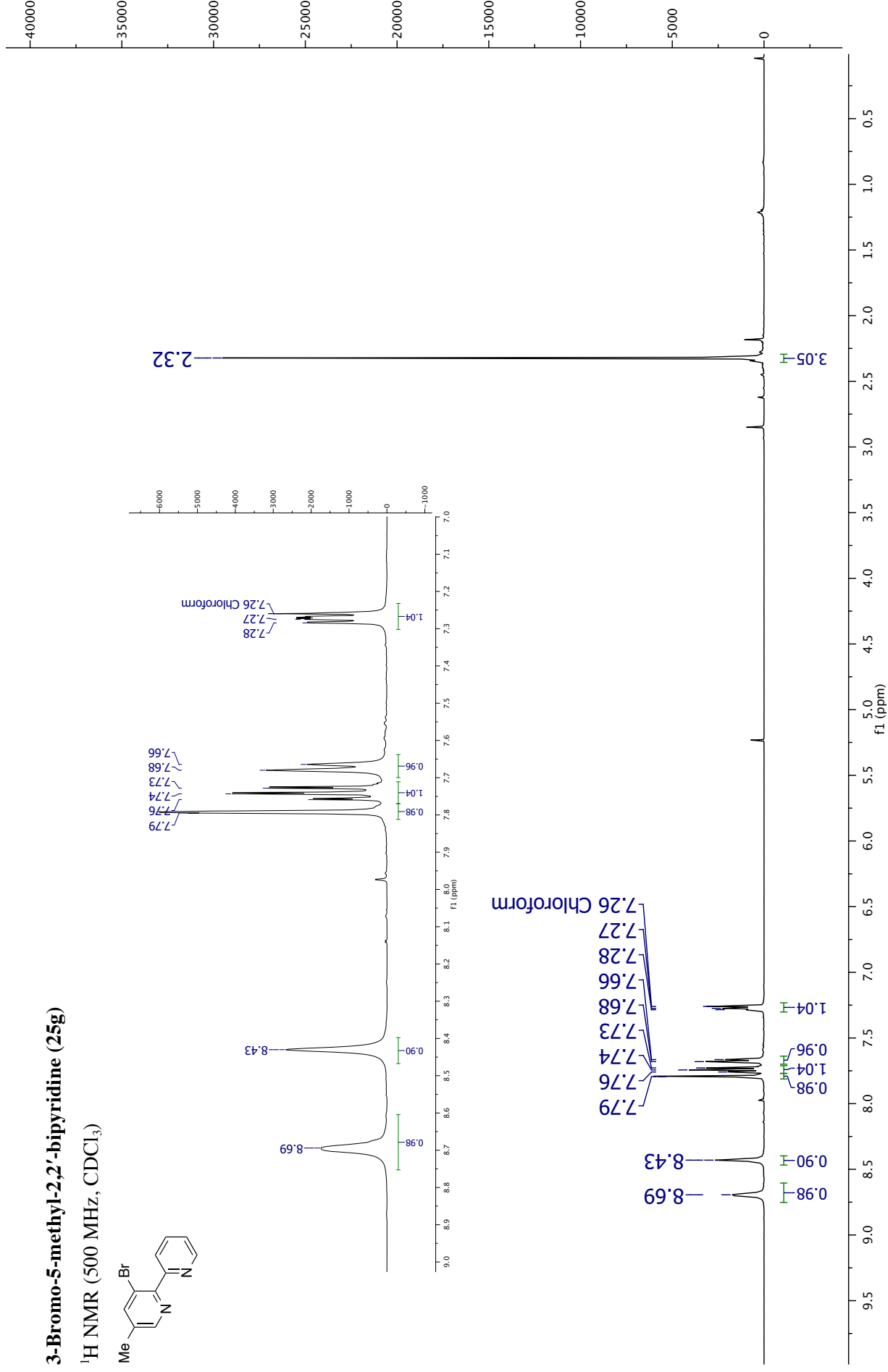
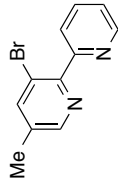
3,6-Dibromo-5-methoxy-2,2'-bipyridine (35f)

¹³C NMR (101 MHz, CDCl₃)



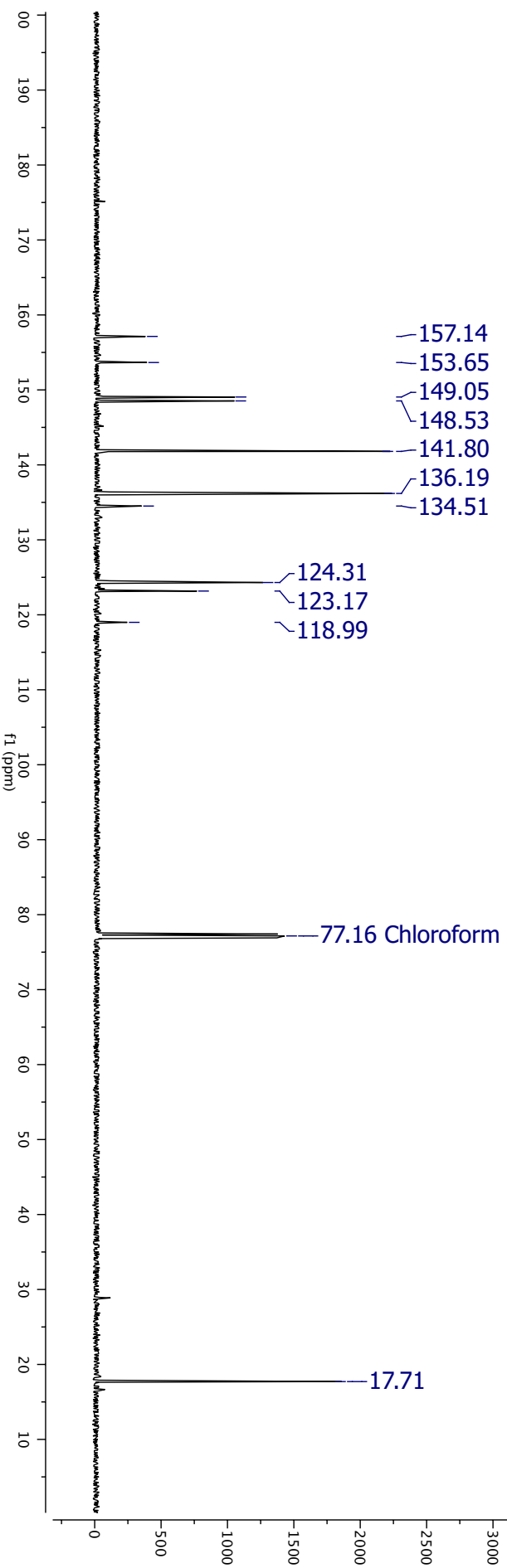
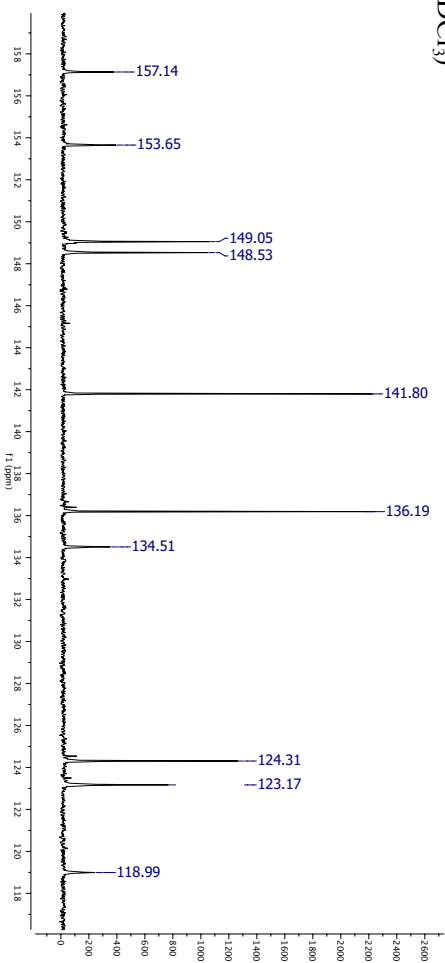
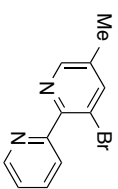
3-Bromo-5-methyl-2,2'-bipyridine (25g)

¹H NMR (500 MHz, CDCl₃)



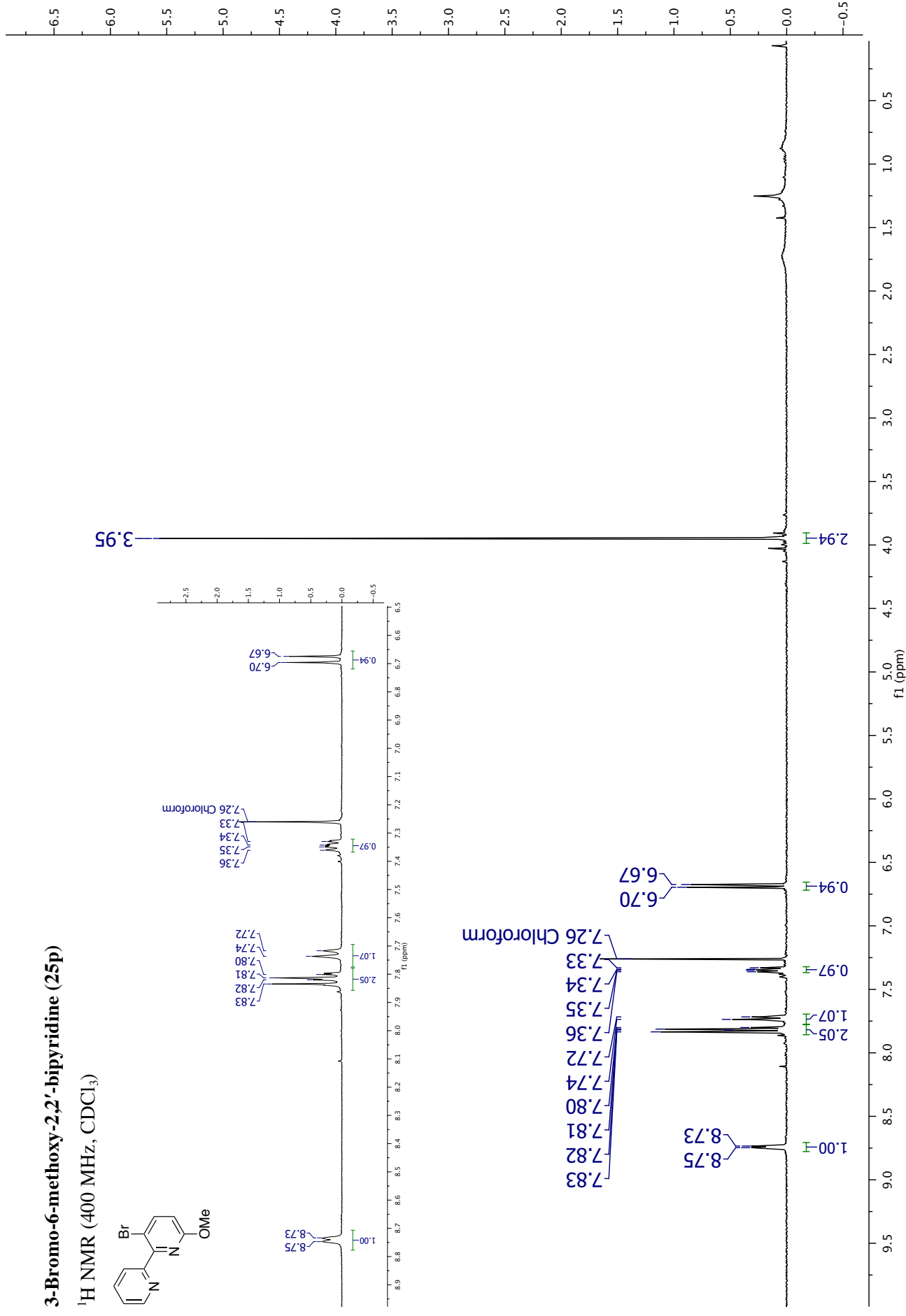
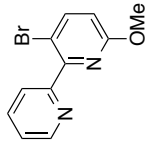
3-Bromo-5-methyl-2,2'-bipyridine (25g)

^{13}C NMR (126 MHz, CDCl_3)



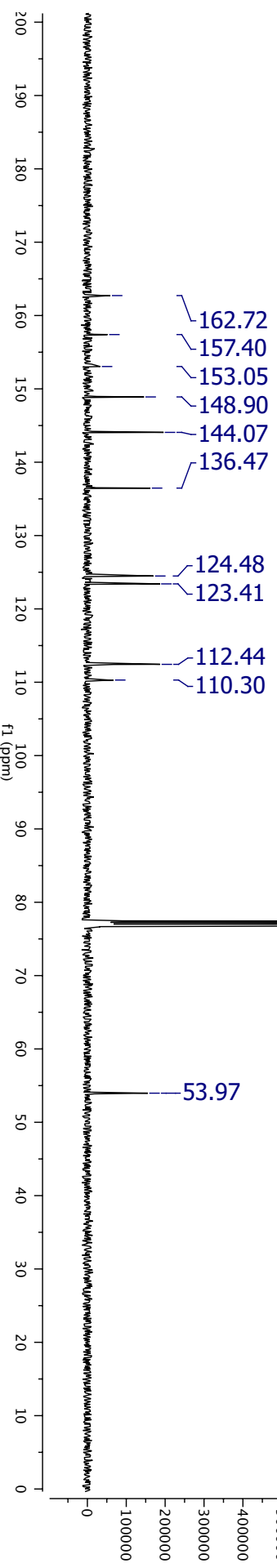
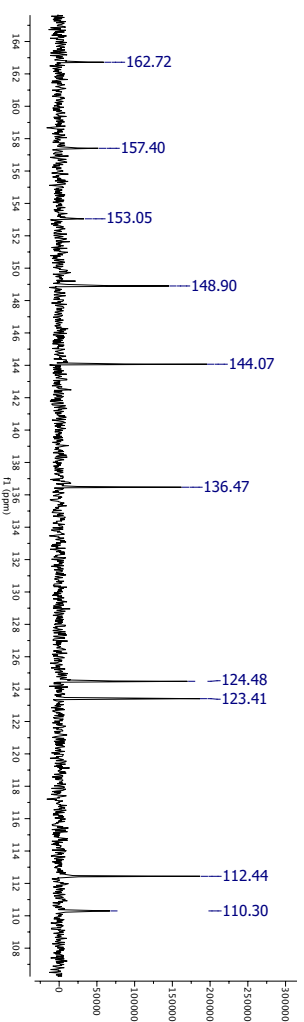
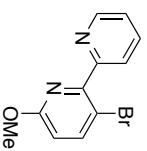
3-Bromo-6-methoxy-2,2'-bipyridine (25p)

¹H NMR (400 MHz, CDCl₃)



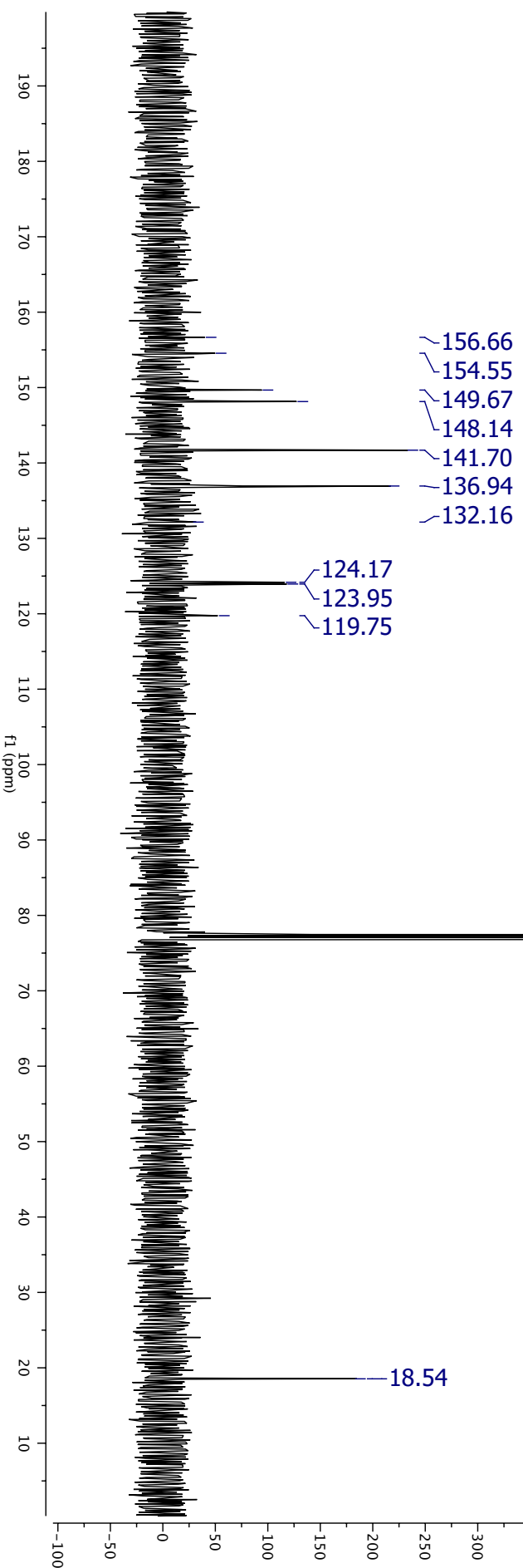
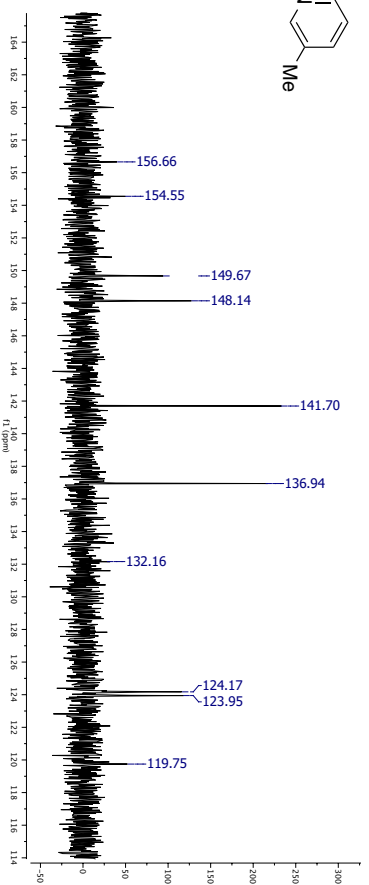
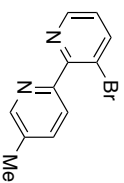
3-Bromo-6-methoxy-2,2'-bipyridine (25p)

^{13}C NMR (126 MHz, CDCl_3)



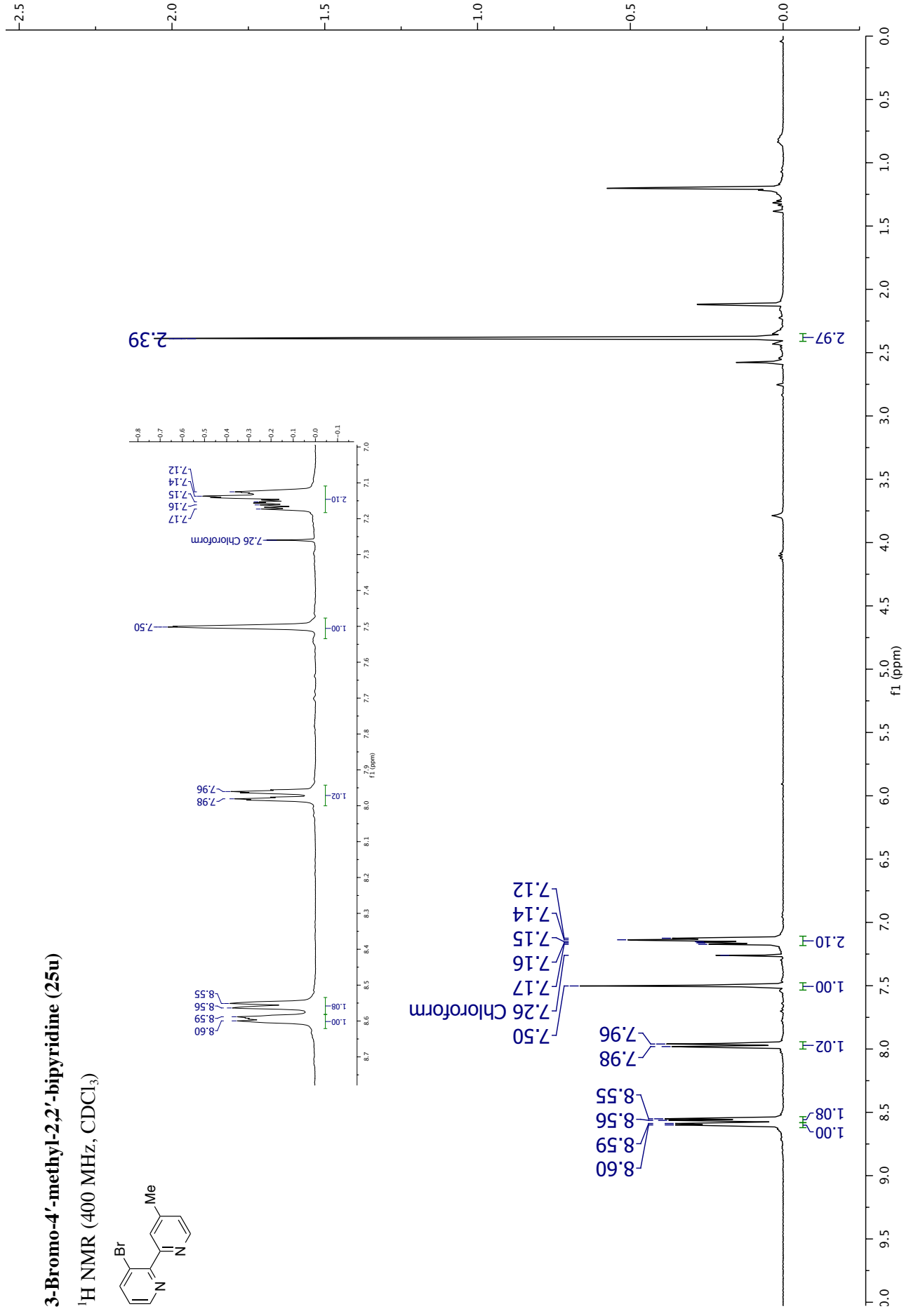
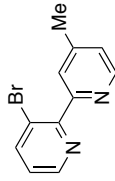
3-Bromo-5'-methyl-2,2'-bipyridine (25s)

¹³C NMR (126 MHz, CDCl₃)



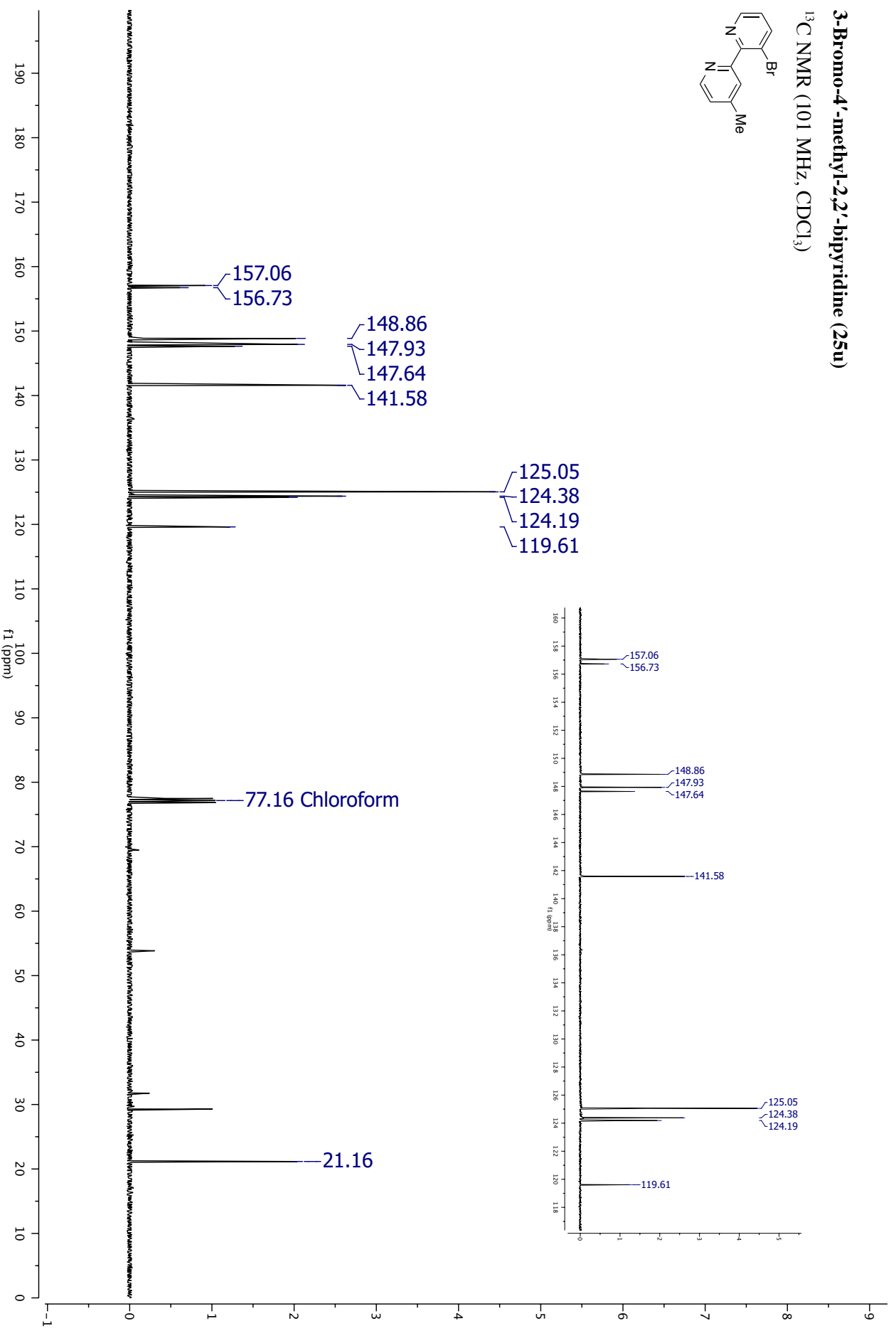
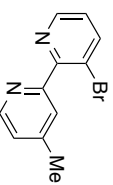
3-Bromo-4'-methyl-2,2'-bipyridine (25u)

¹H NMR (400 MHz, CDCl₃)



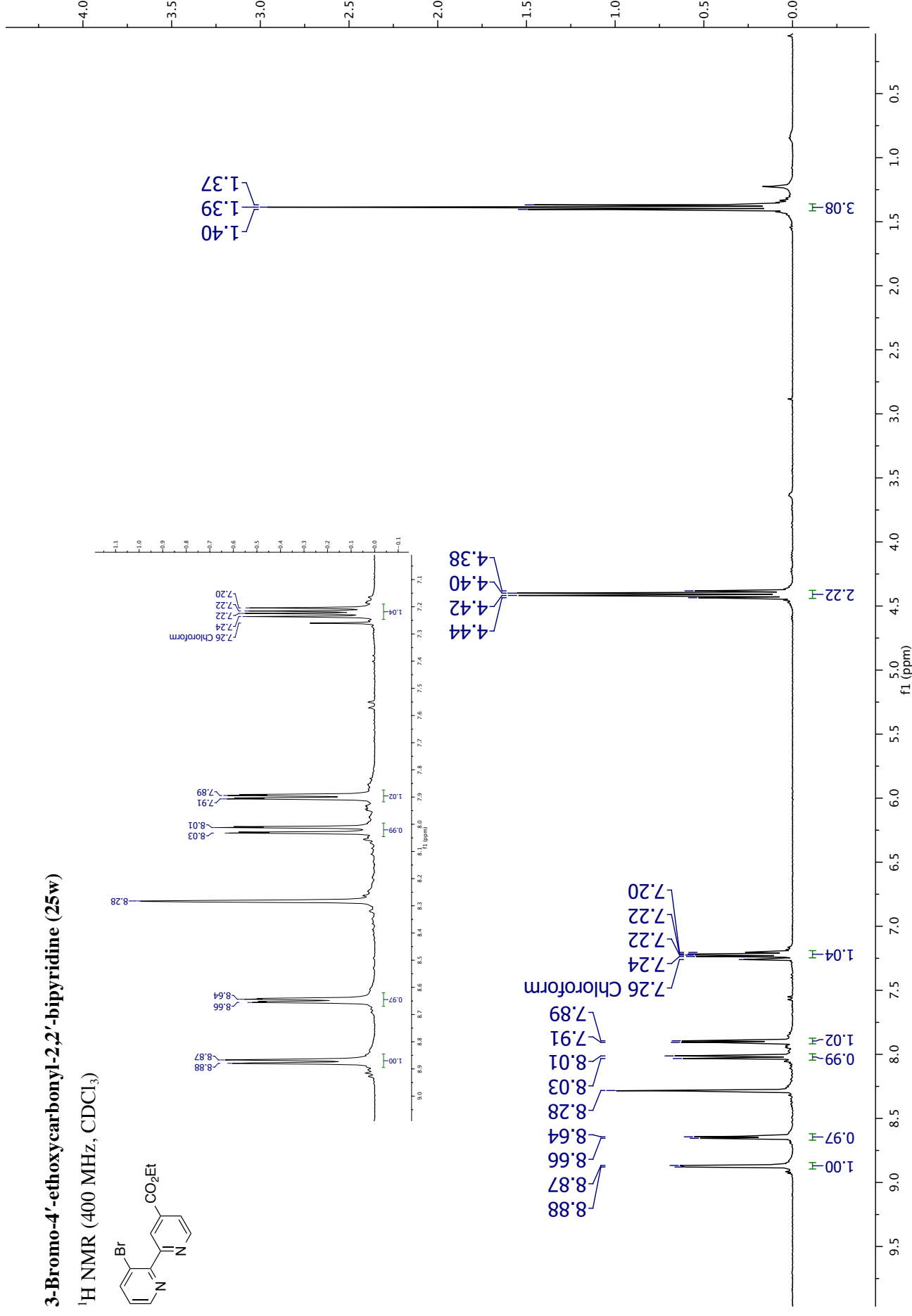
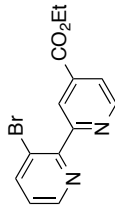
3-Bromo-4'-methyl-2,2'-bipyridine (25u)

^{13}C NMR (101 MHz, CDCl_3)



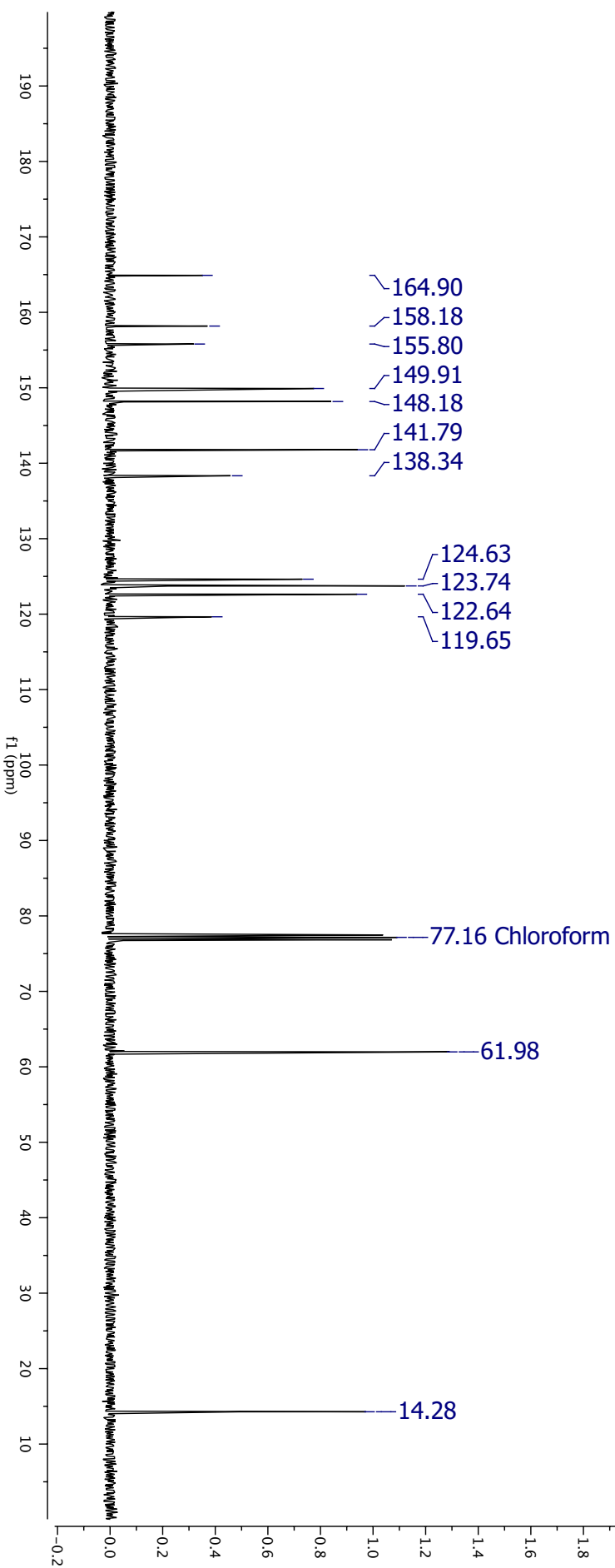
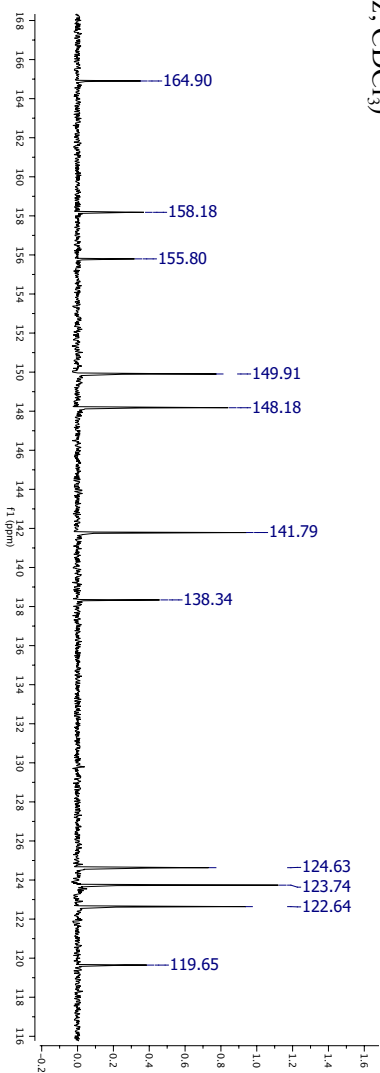
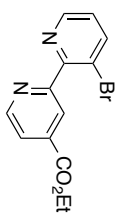
3-Bromo-4'-ethoxycarbonyl-2,2'-bipyridine (25w)

¹H NMR (400 MHz, CDCl₃)



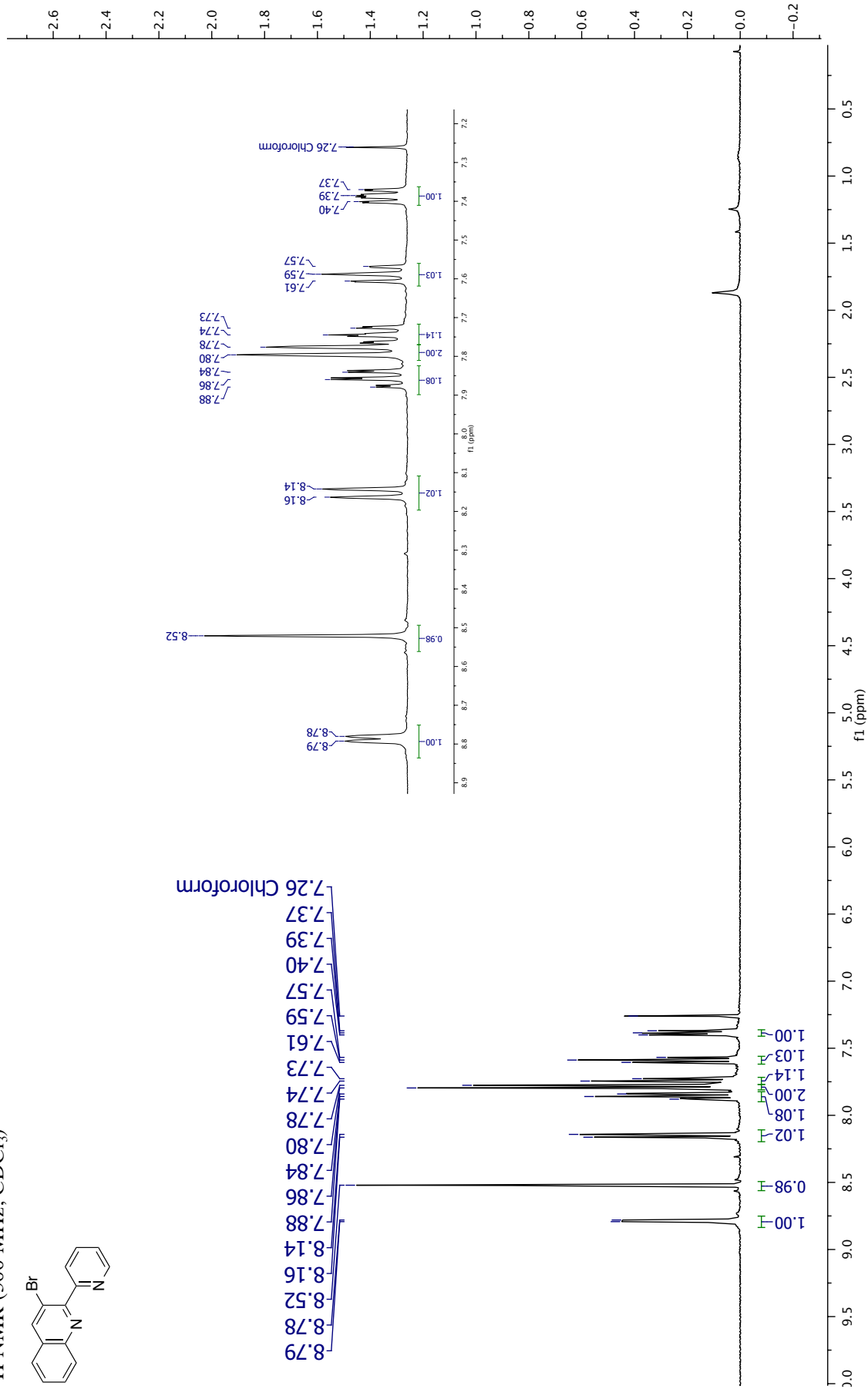
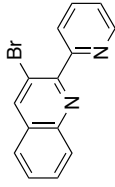
3-Bromo-4'-ethoxycarbonyl-2,2'-bipyridine (25w)

¹³C NMR (101 MHz, CDCl₃)



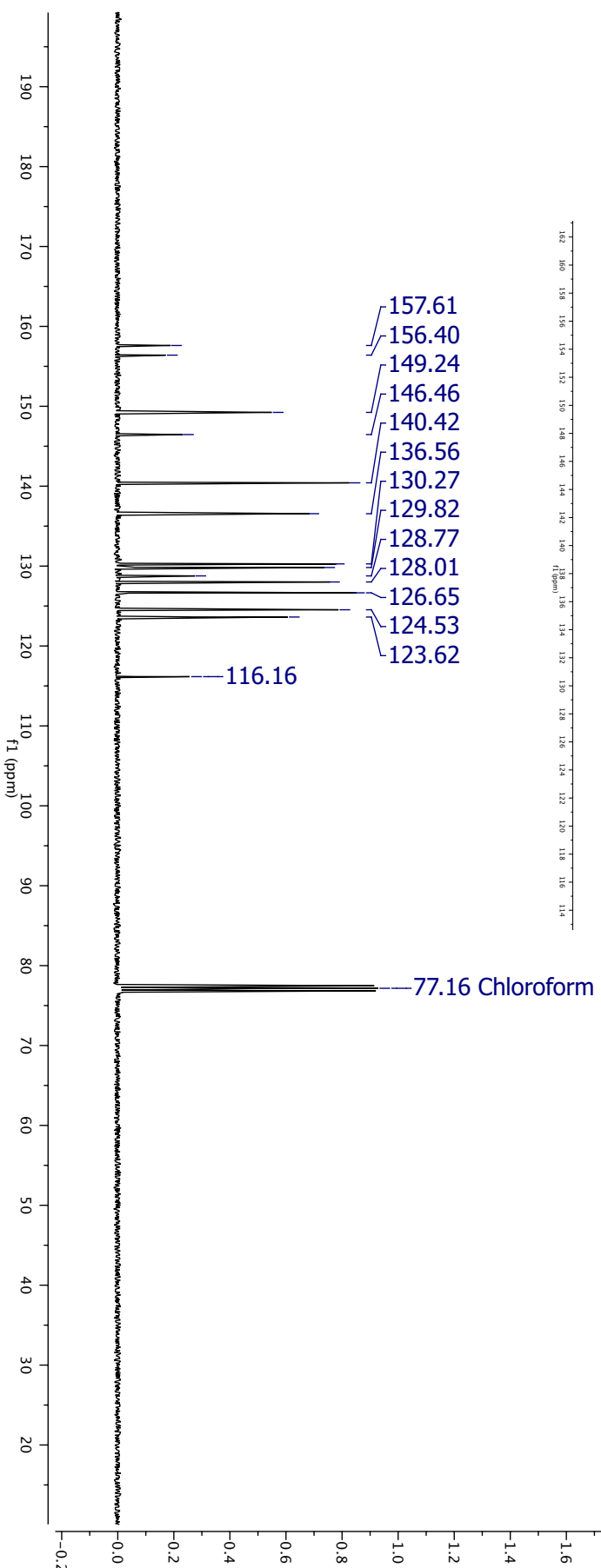
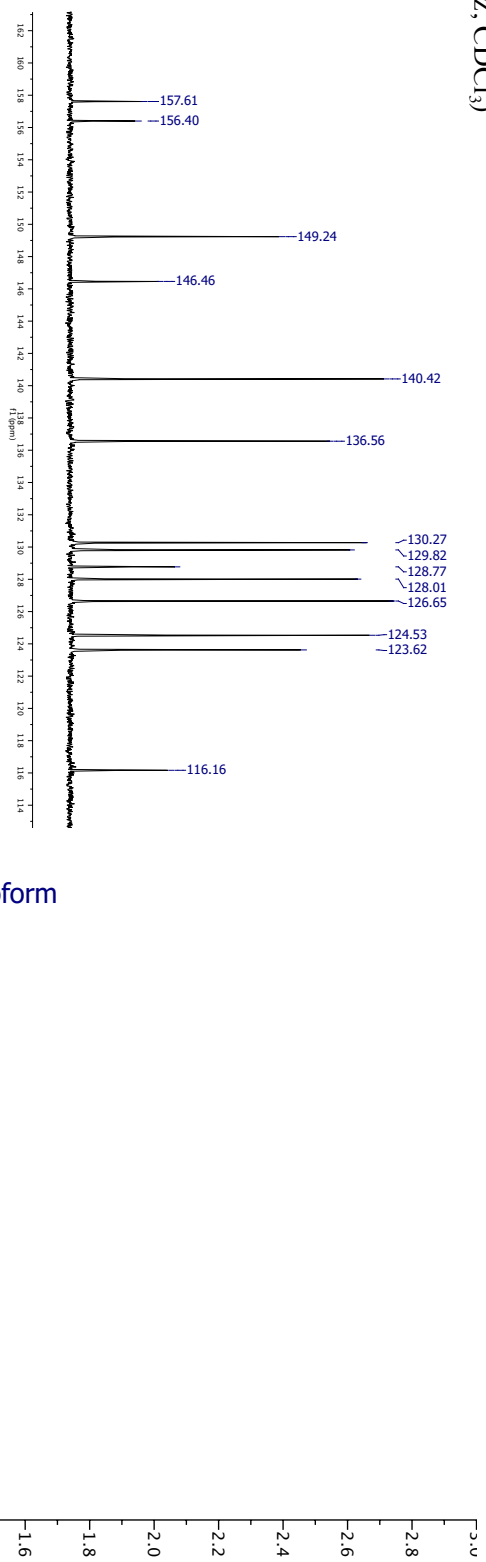
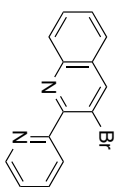
3-Bromo-2-(pyridin-2-yl)quinoline (25y)

¹H NMR (500 MHz, CDCl₃)



3-Bromo-2-(pyridin-2-yl)quinoline (25y)

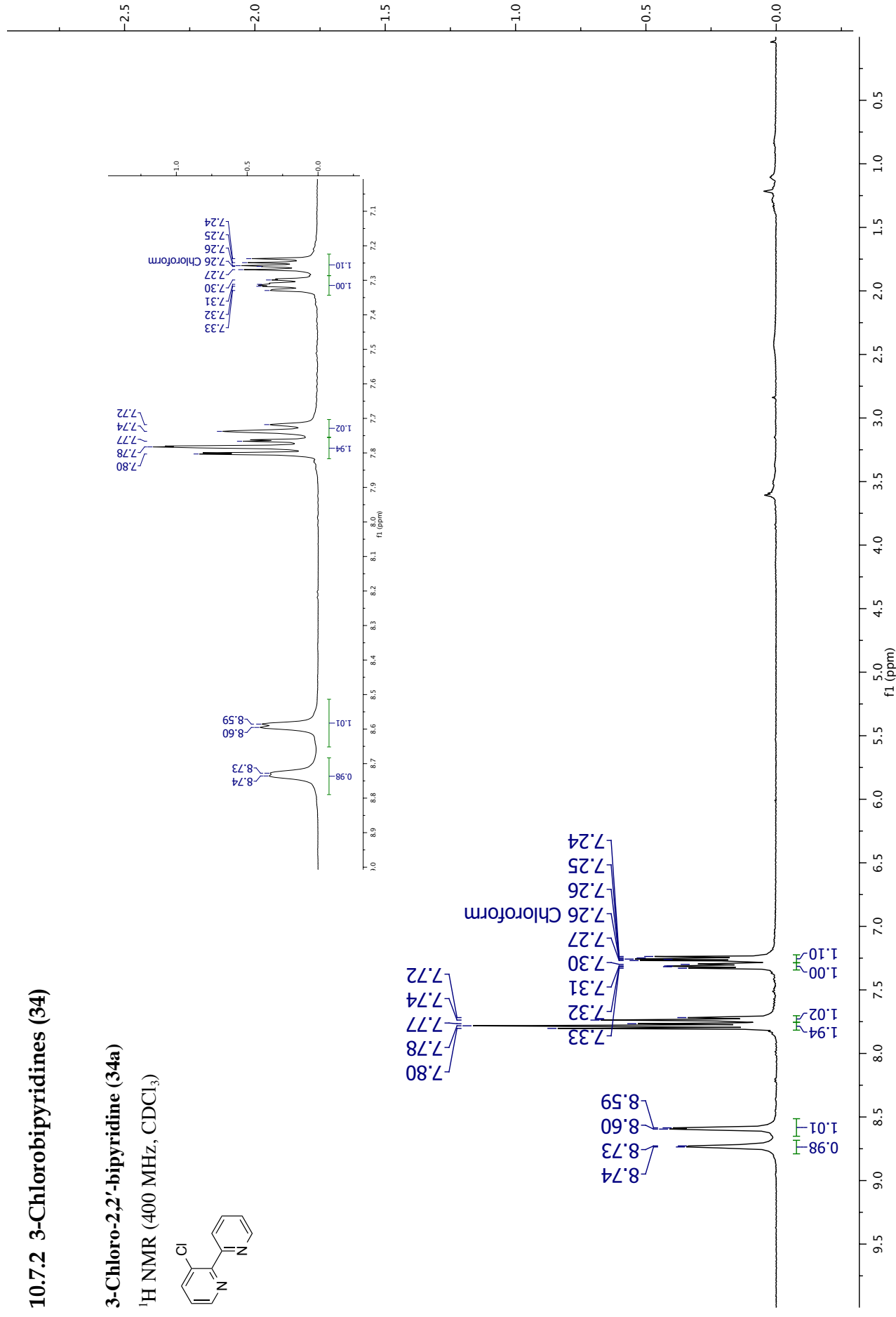
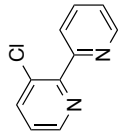
^{13}C NMR (126 MHz, CDCl_3)



10.7.2 3-Chlorobipyridines (34)

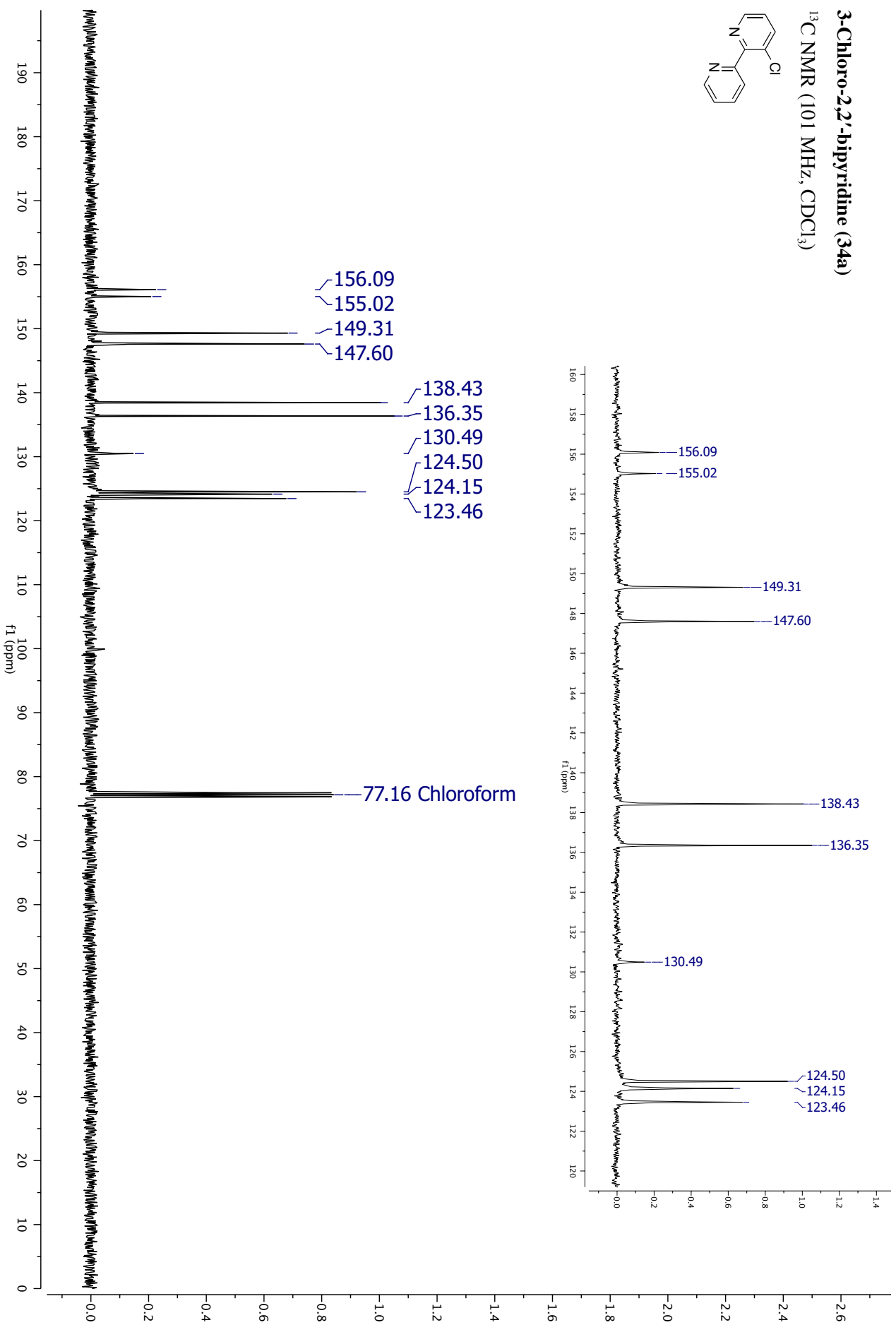
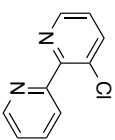
3-Chloro-2,2'-bipyridine (34a)

¹H NMR (400 MHz, CDCl₃)



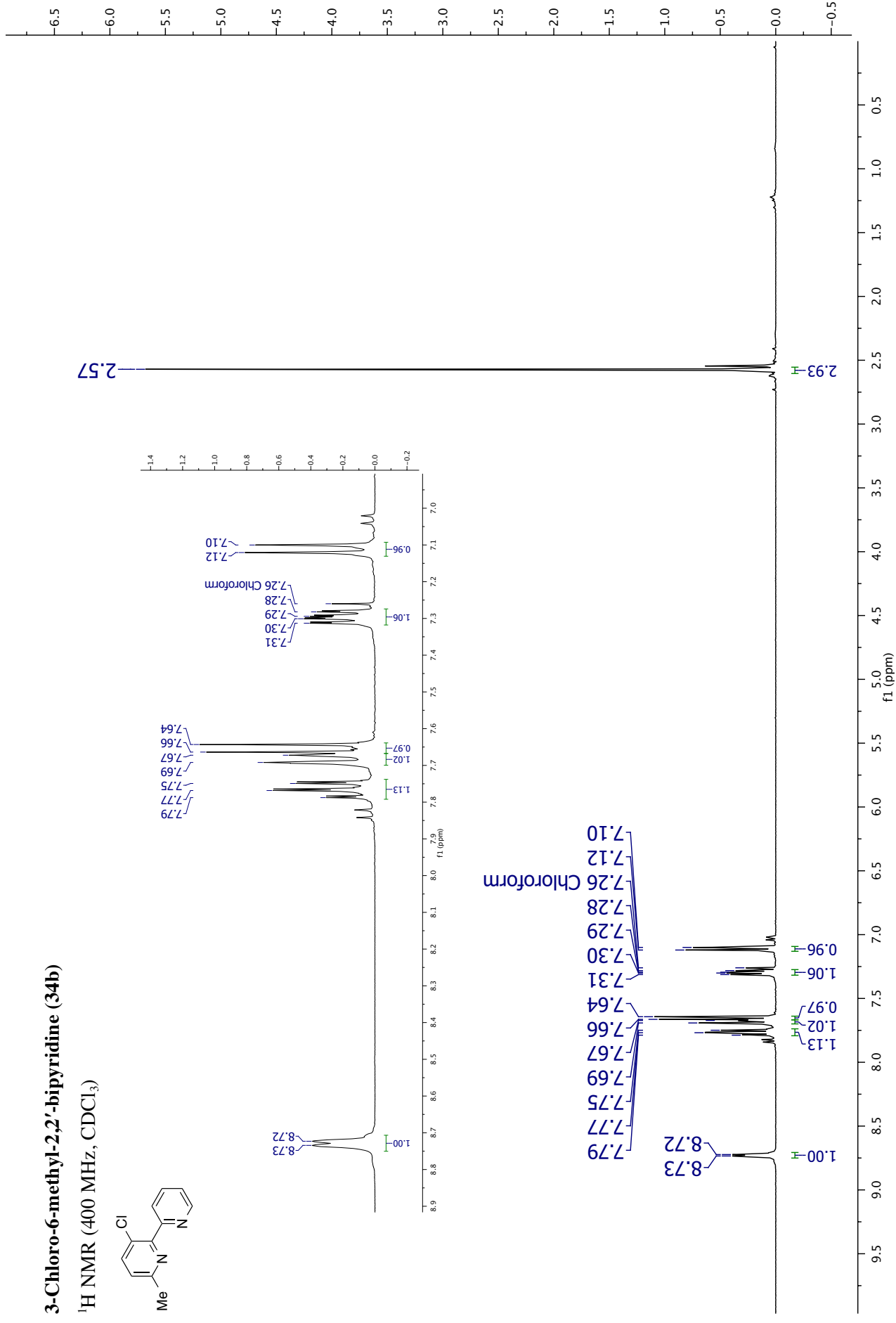
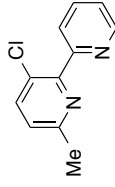
3-Chloro-2,2'-bipyridine (34a)

^{13}C NMR (101 MHz, CDCl_3)



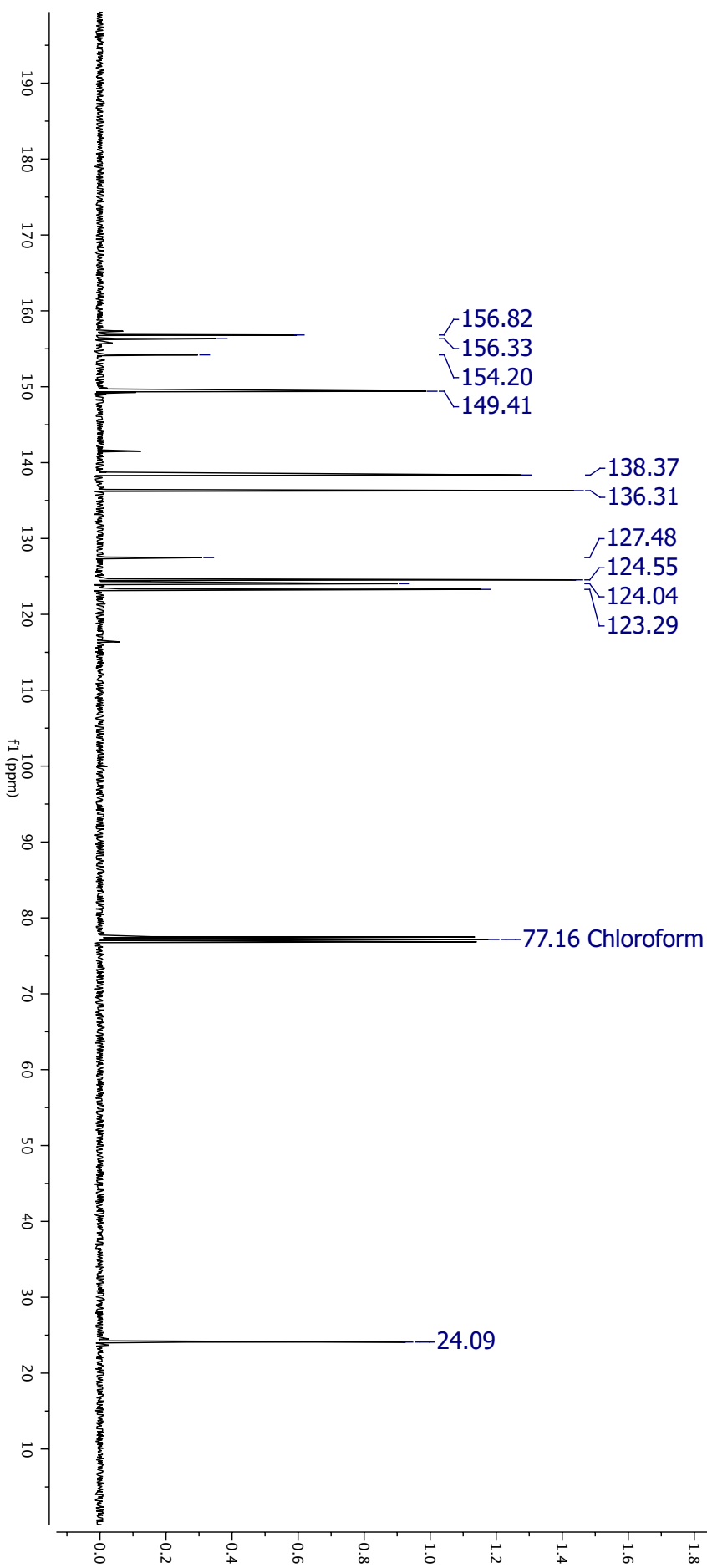
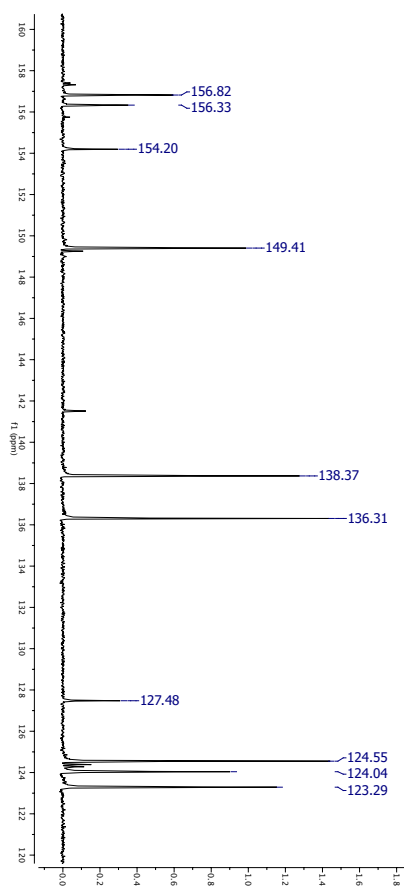
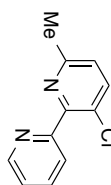
3-Chloro-6-methyl-2,2'-bipyridine (34b)

¹H NMR (400 MHz, CDCl₃)



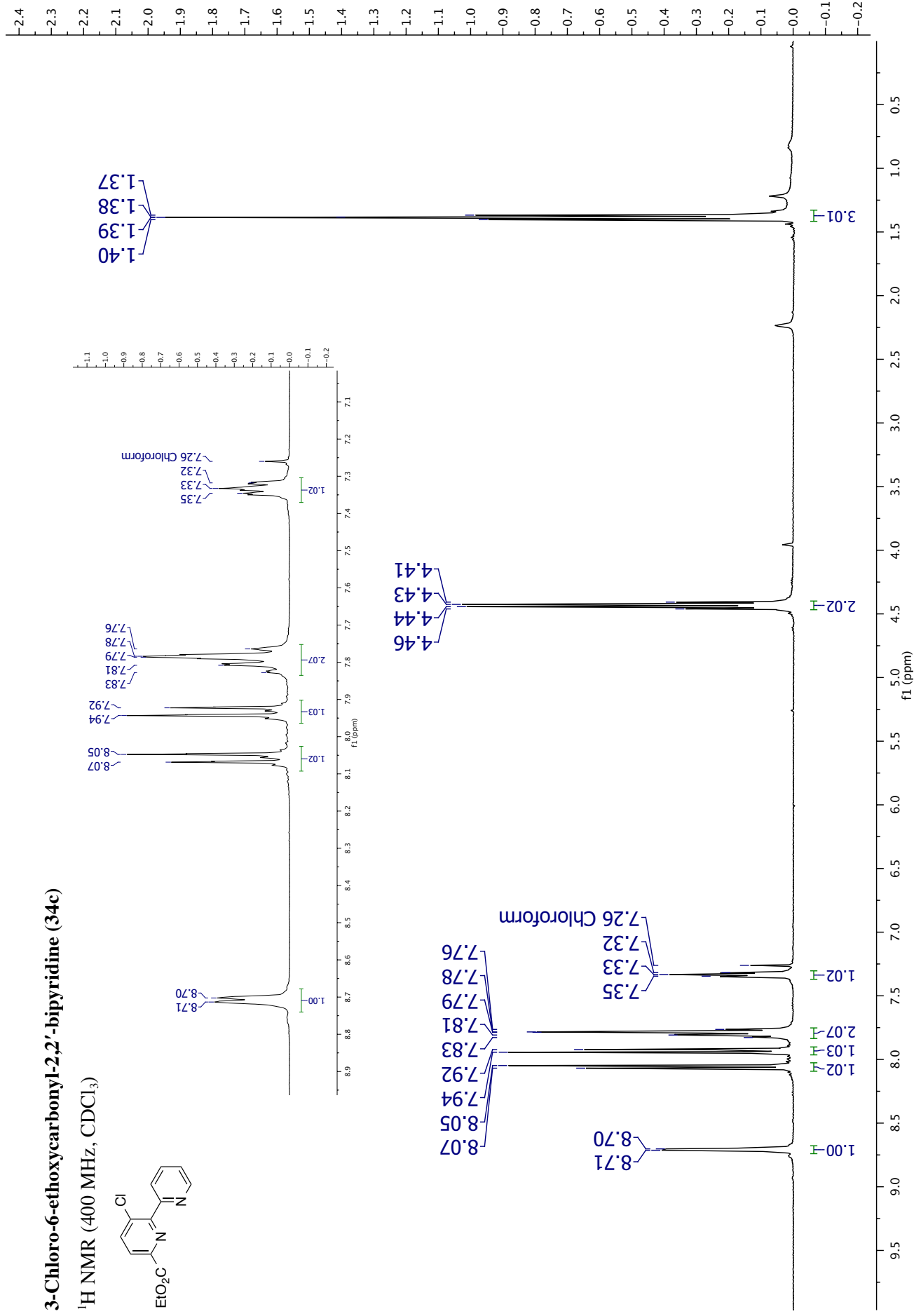
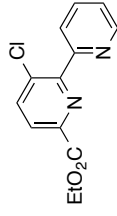
3-Chloro-6-methyl-2,2'-bipyridine (34b)

¹³C NMR (101 MHz, CDCl₃)



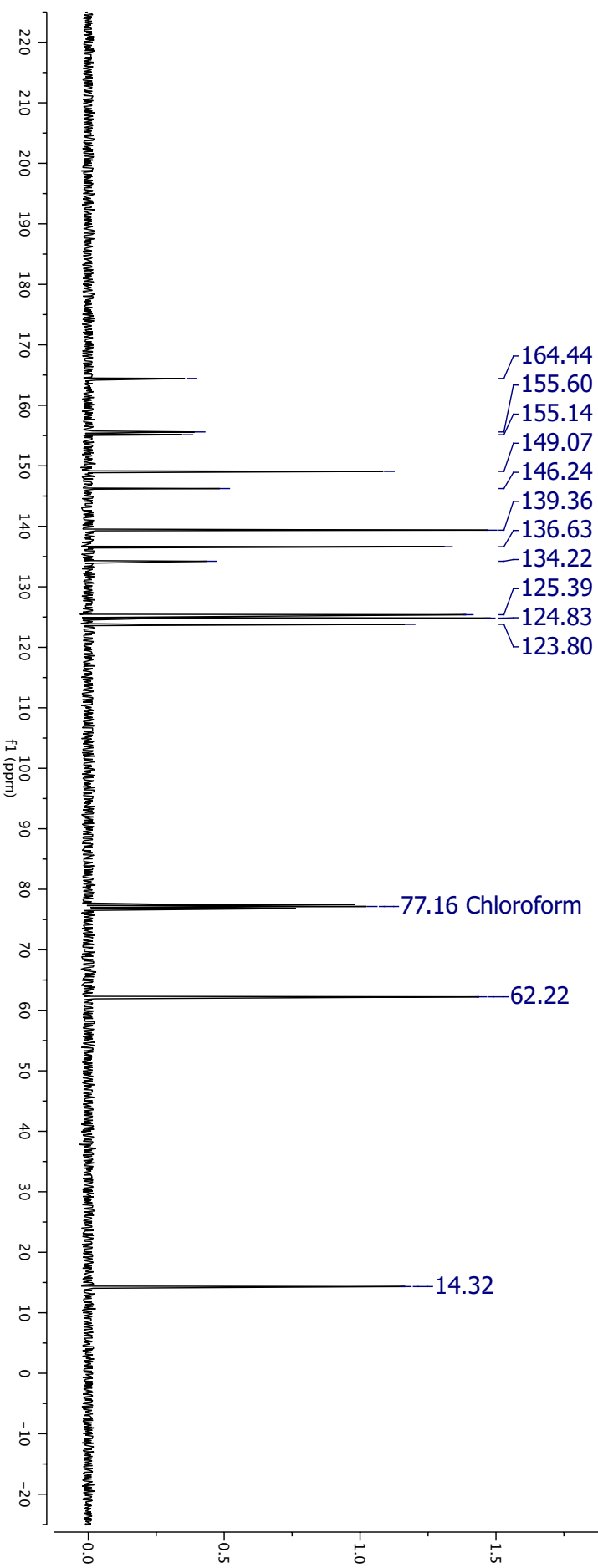
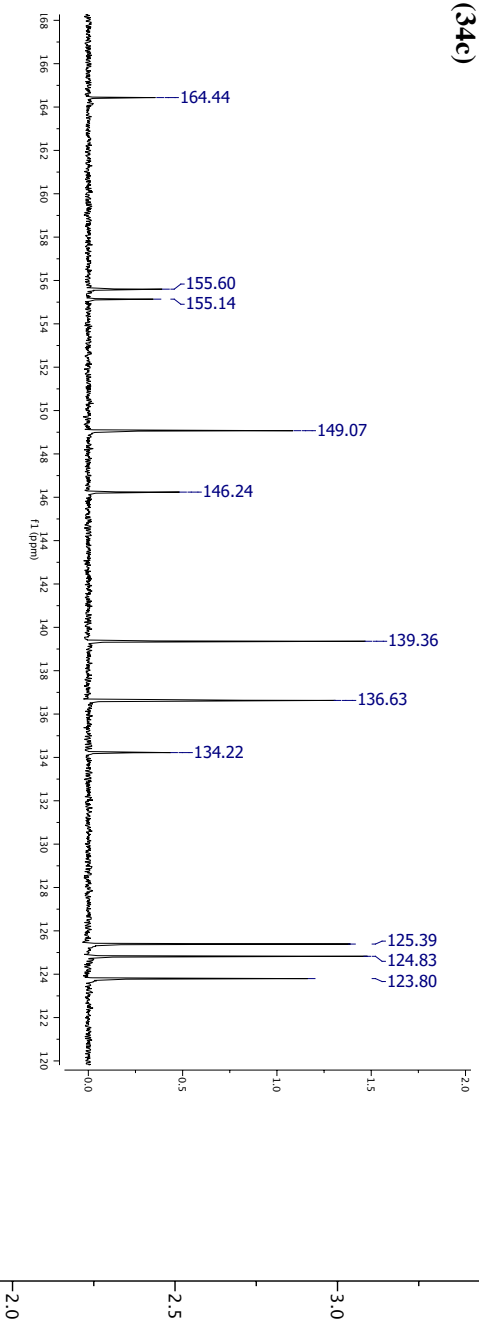
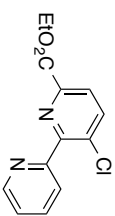
3-Chloro-6-ethoxycarbonyl-2,2'-bipyridine (34c)

¹H NMR (400 MHz, CDCl₃)



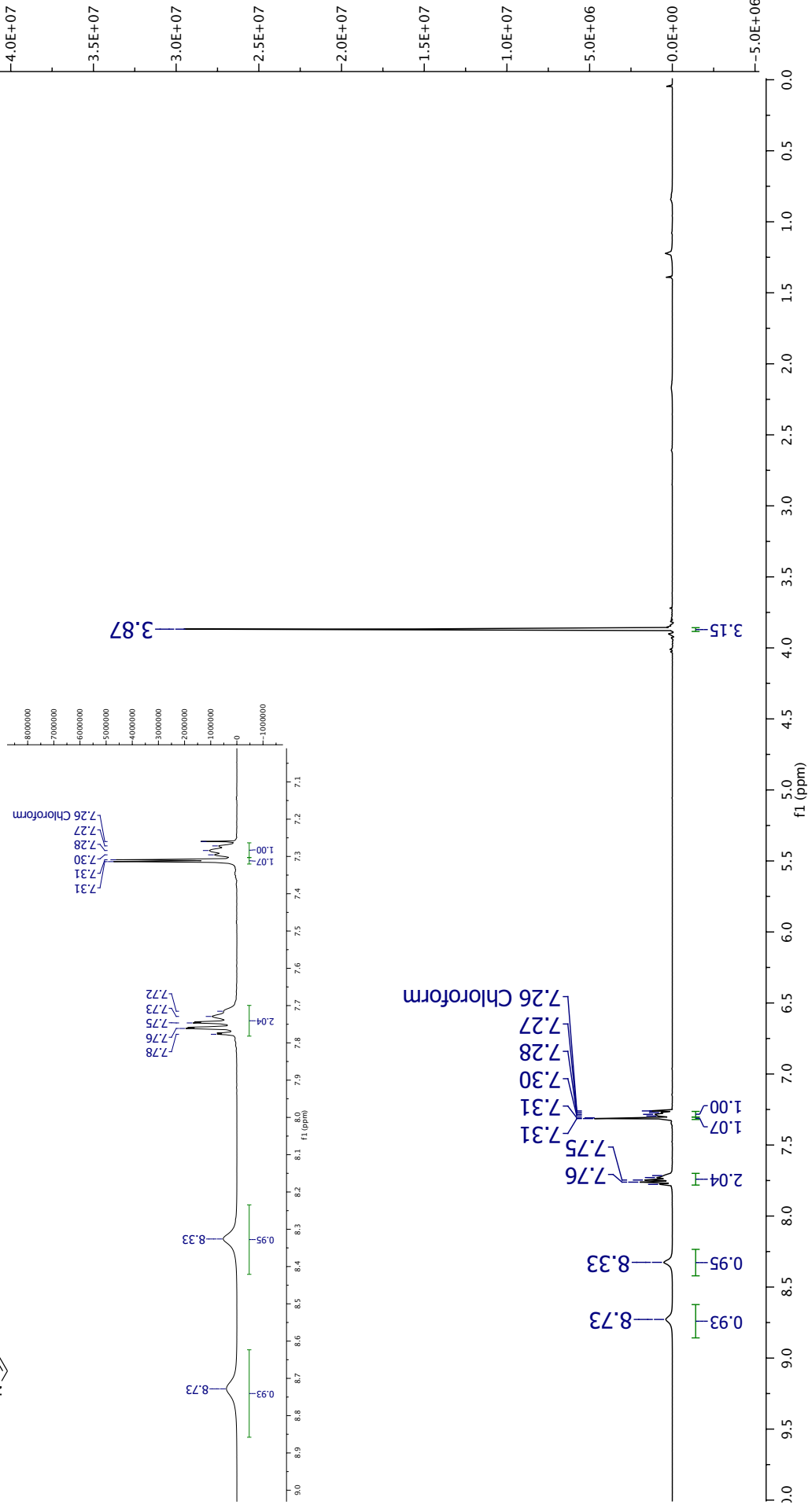
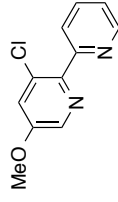
3-Chloro-6-ethoxycarbonyl-2,2'-bipyridine (34c)

¹³C NMR (101 MHz, CDCl₃)



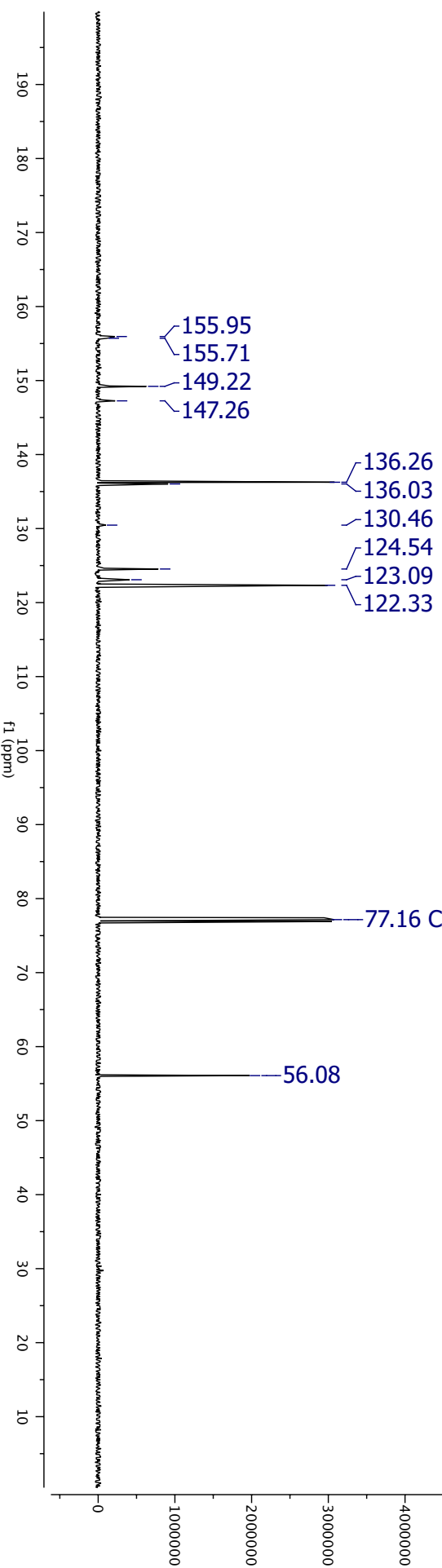
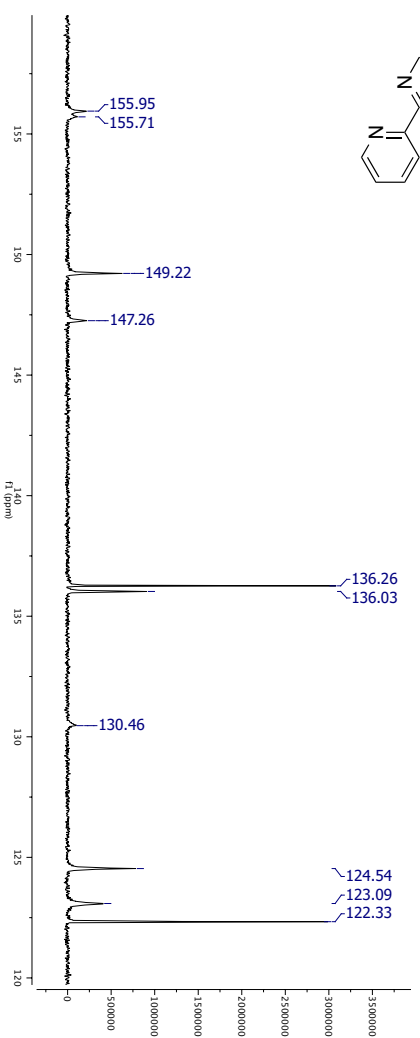
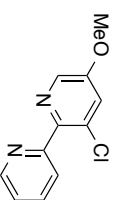
3-Chloro-5-methoxy-2,2'-bipyridine (34f)

¹H NMR (500 MHz, CDCl₃)



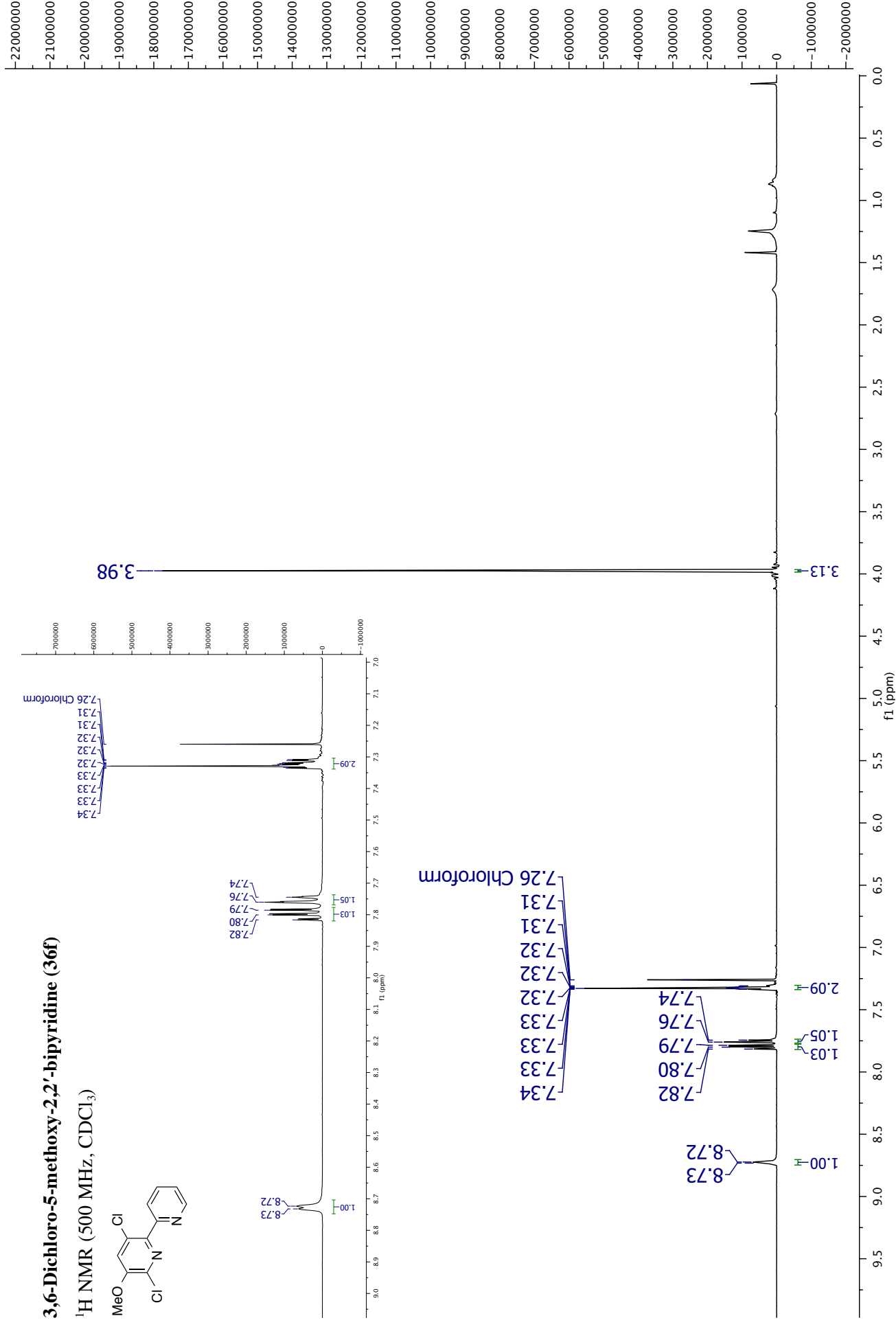
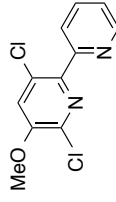
3-Chloro-5-methoxy-2,2'-bipyridine (34f)

^{13}C NMR (126 MHz, CDCl_3)



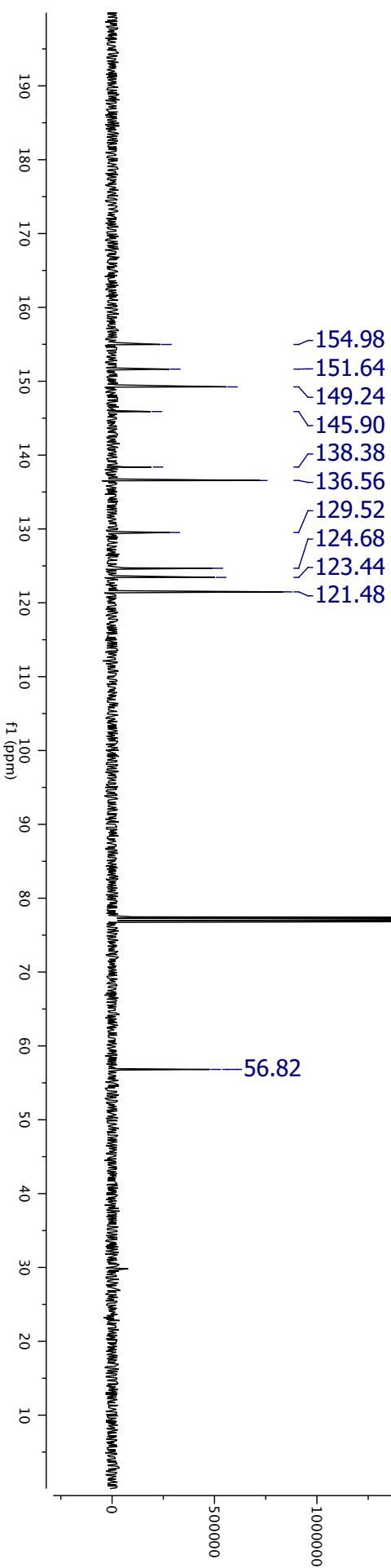
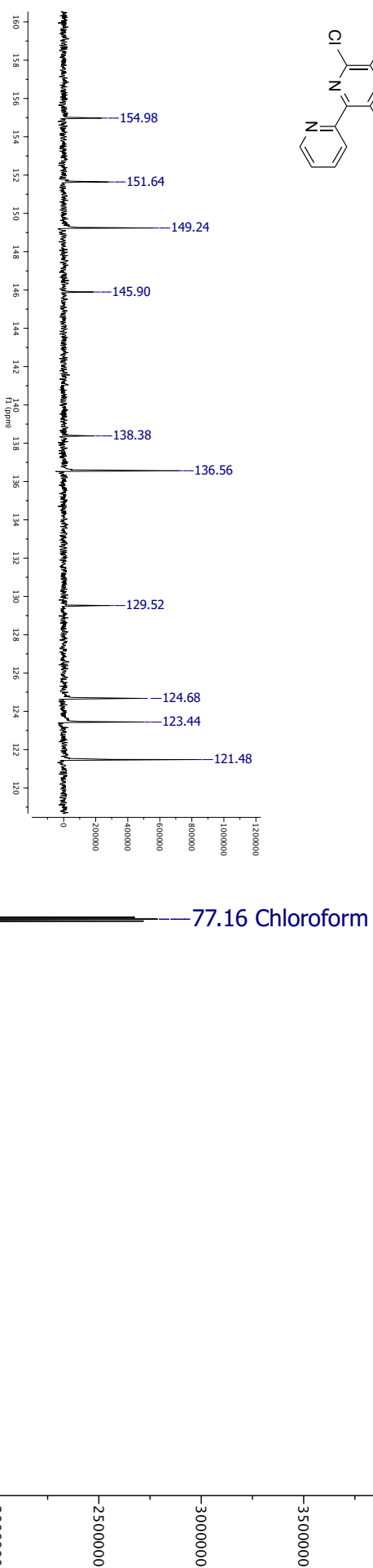
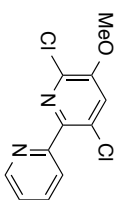
3,6-Dichloro-5-methoxy-2,2'-bipyridine (36f)

¹H NMR (500 MHz, CDCl₃)



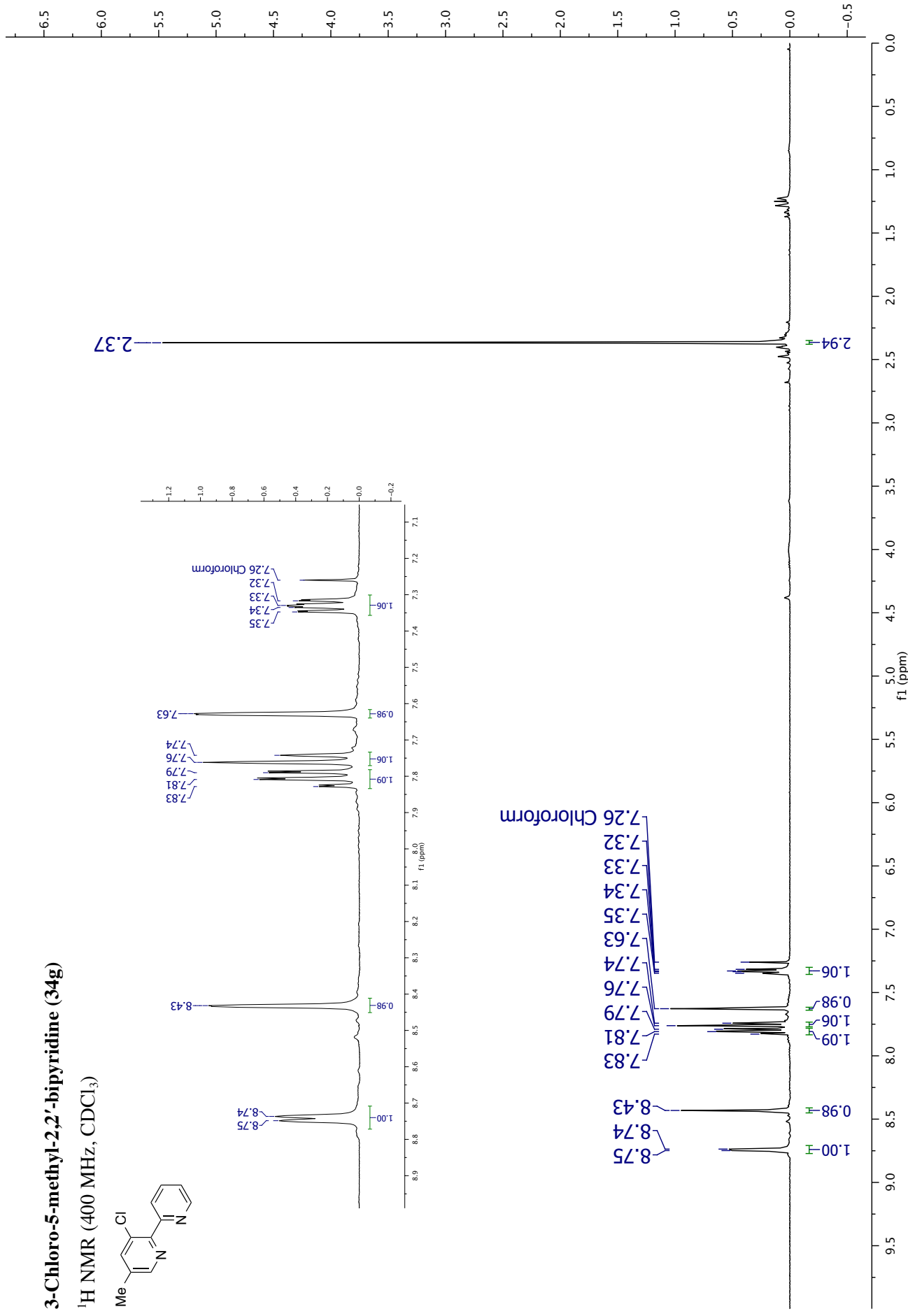
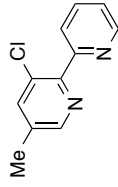
3,6-Dichloro-5-methoxy-2,2'-bipyridine (36f)

¹³C NMR (126 MHz, CDCl₃)



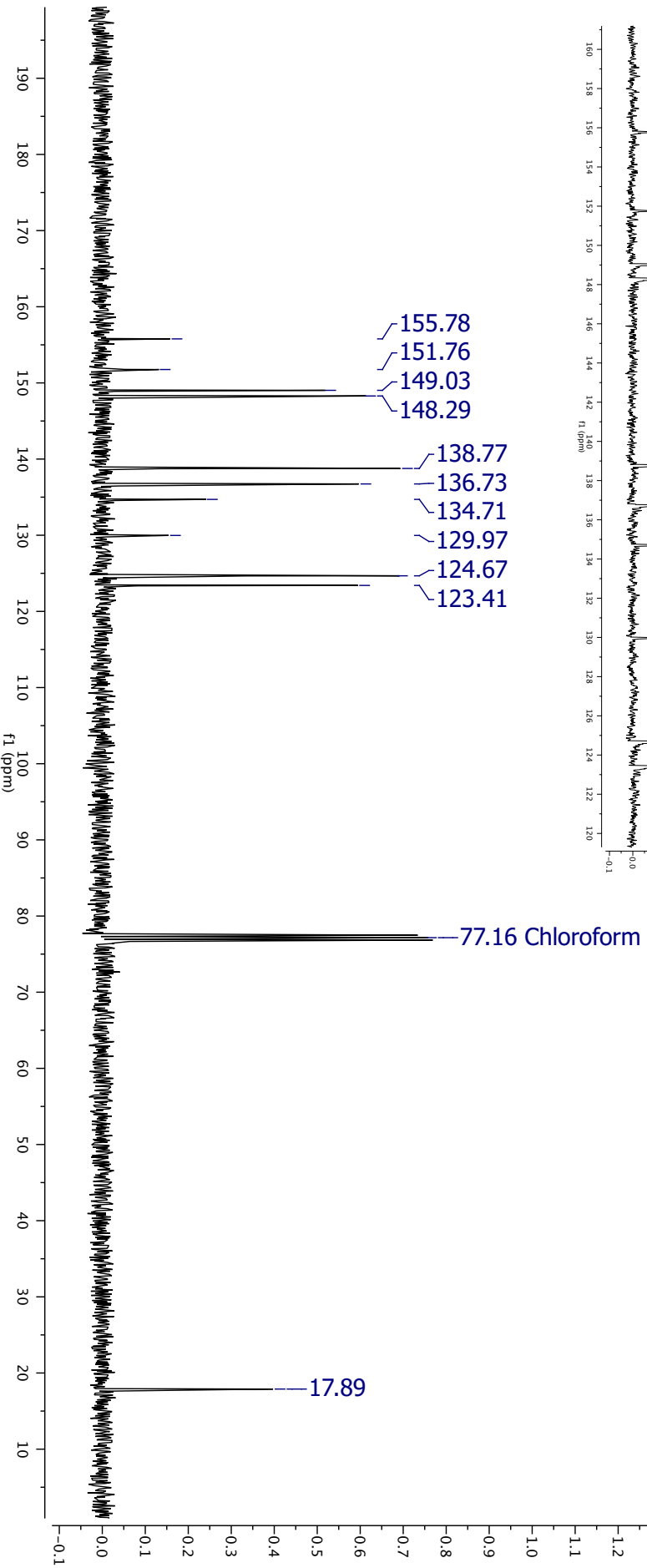
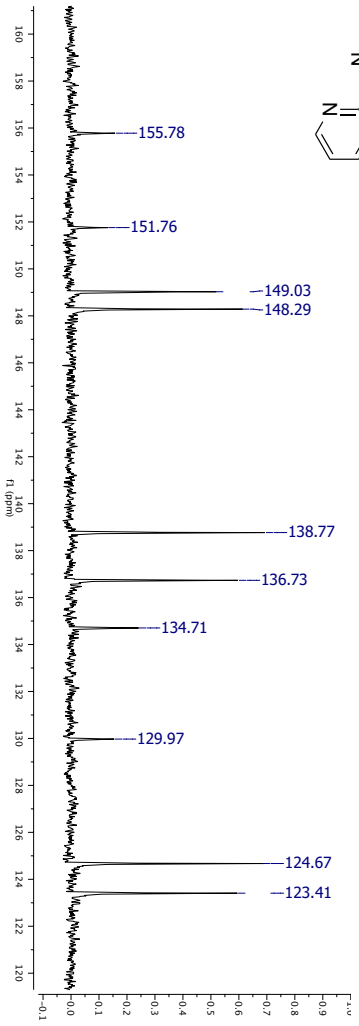
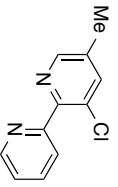
3-Chloro-5-methyl-2,2'-bipyridine (34g)

¹H NMR (400 MHz, CDCl₃)



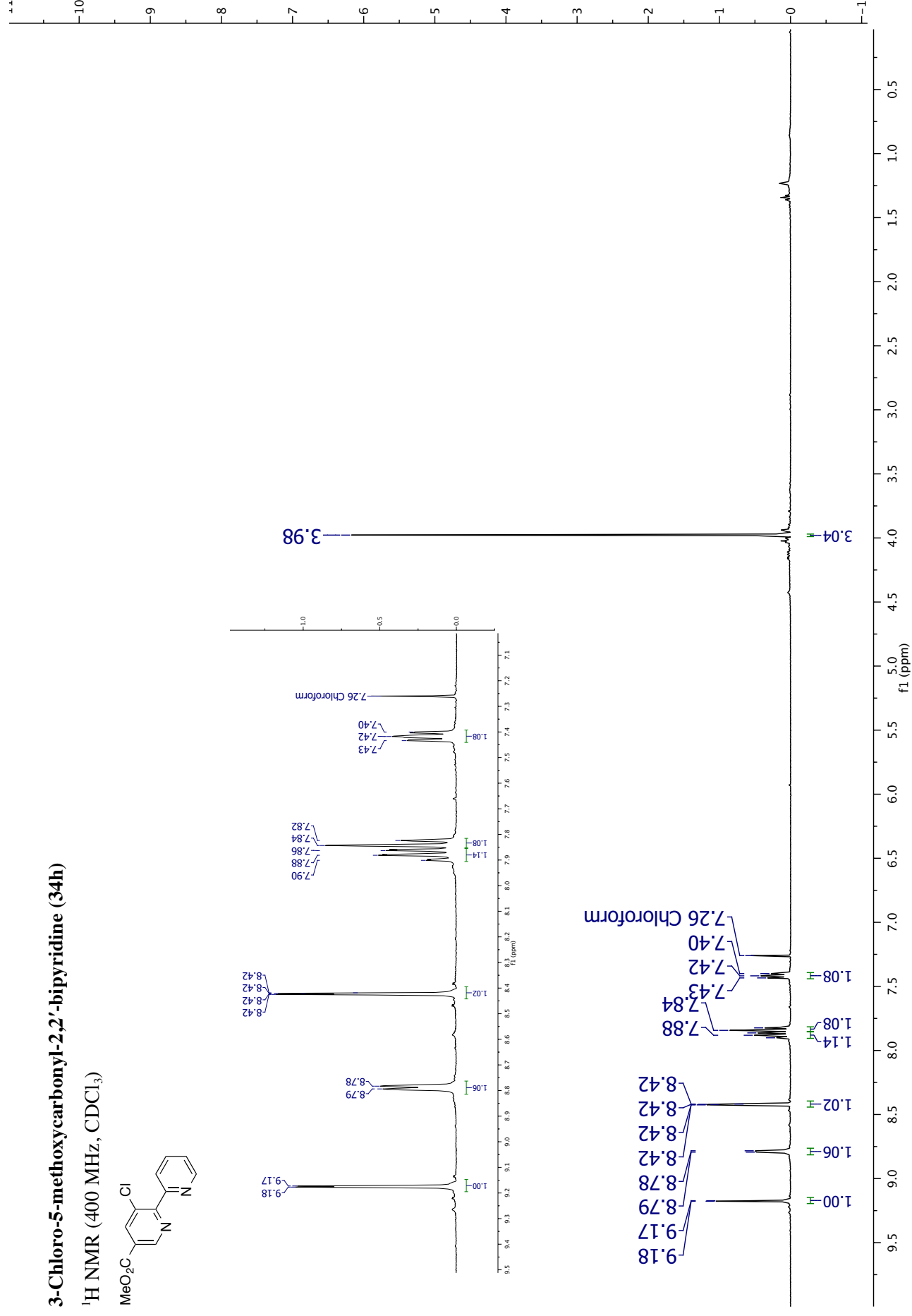
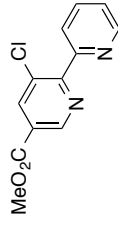
3-Chloro-5-methyl-2,2'-bipyridine (34g)

¹³C NMR (101 MHz, CDCl₃)



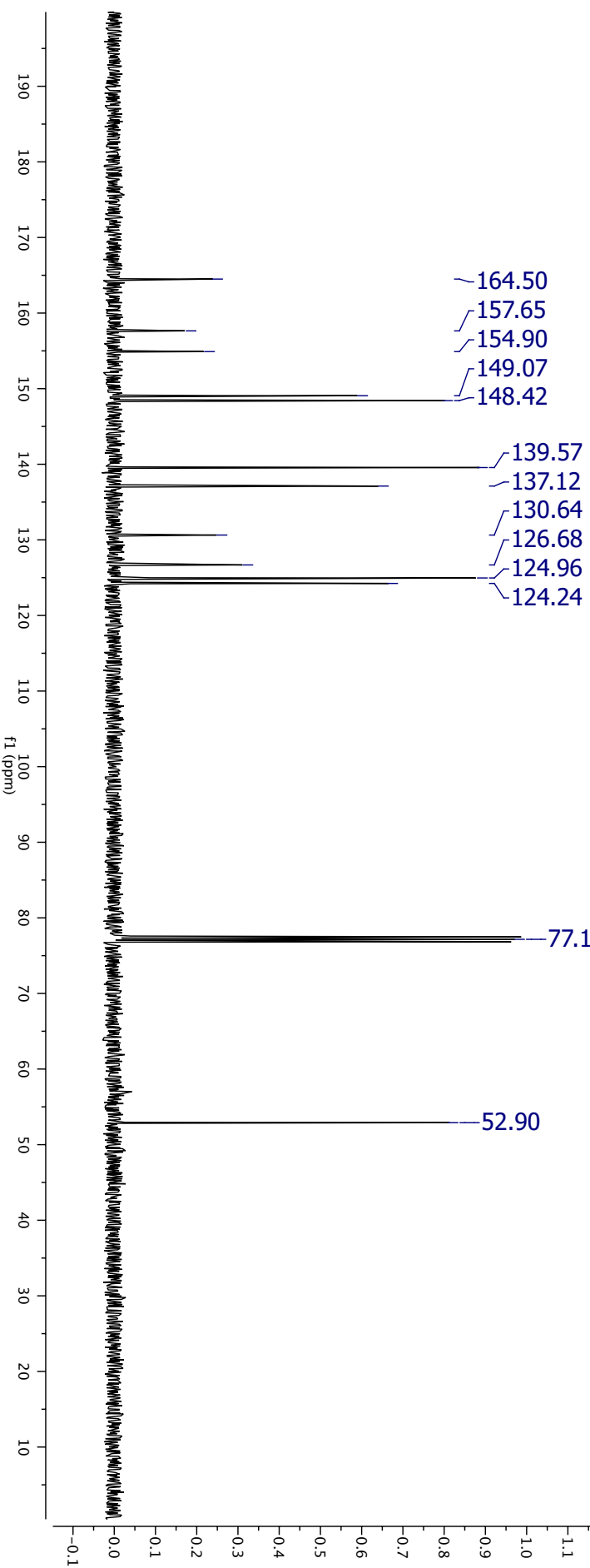
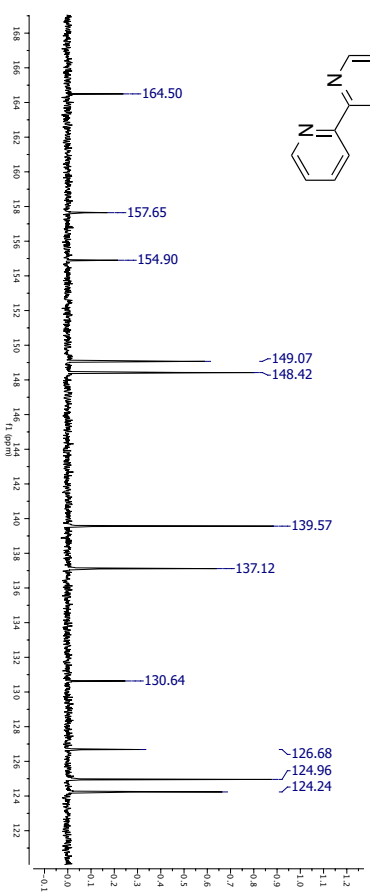
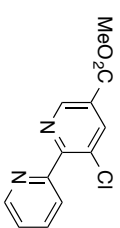
3-Chloro-5-methoxycarbonyl-2,2'-bipyridine (34h)

¹H NMR (400 MHz, CDCl₃)



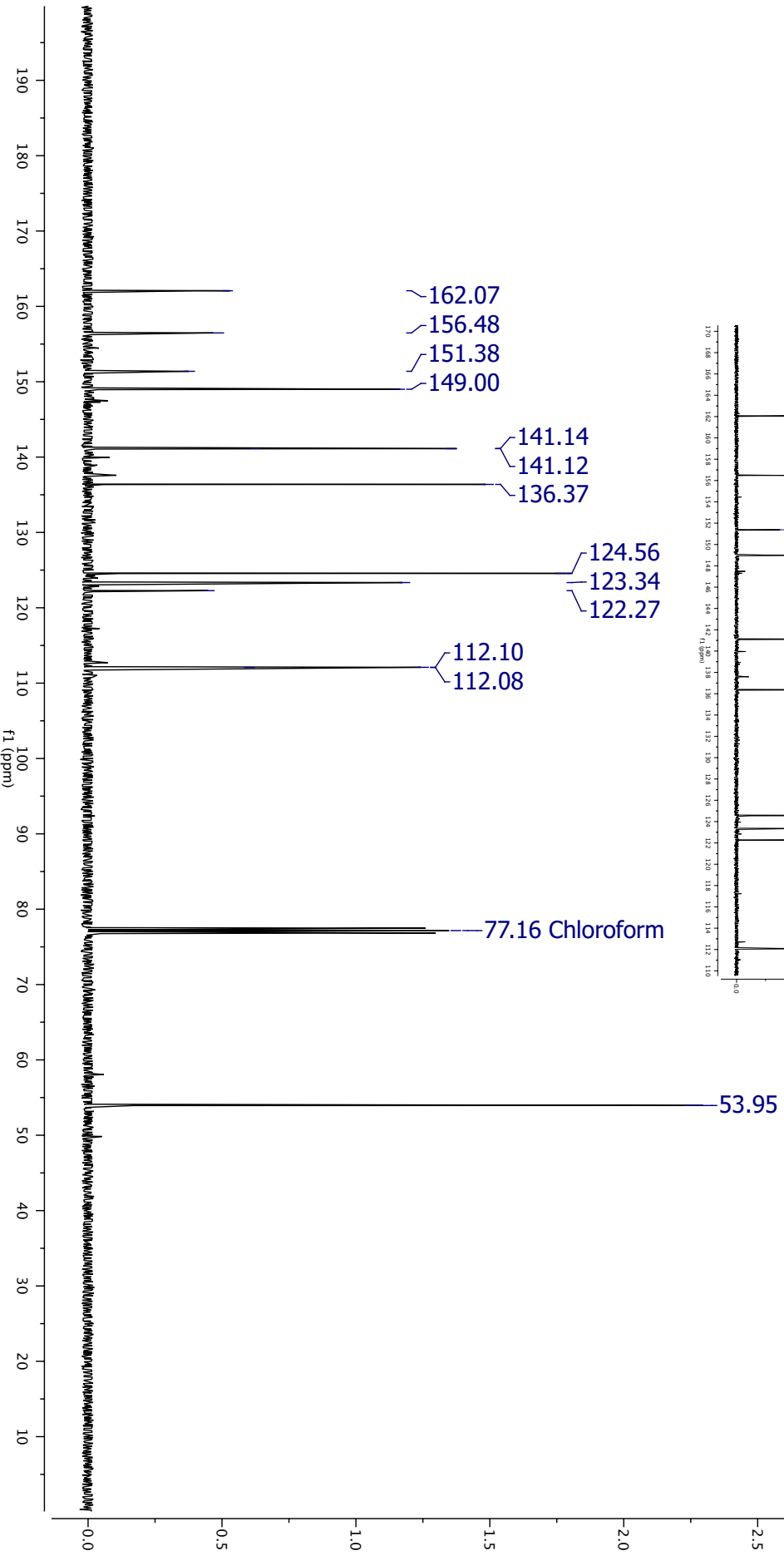
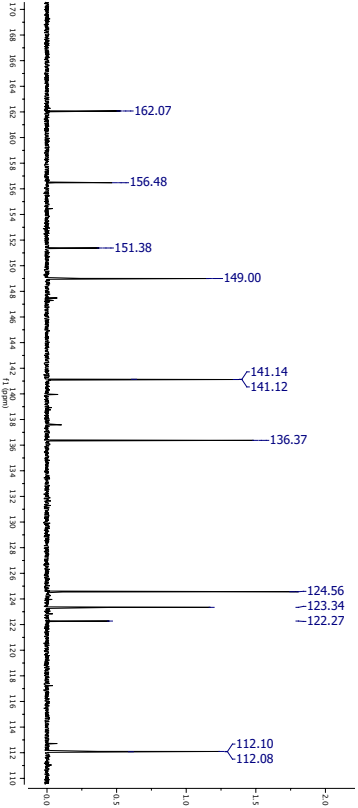
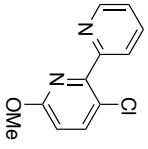
3-Chloro-5-methoxycarbonyl-2,2'-bipyridine (34h)

^{13}C NMR (101 MHz, CDCl_3)



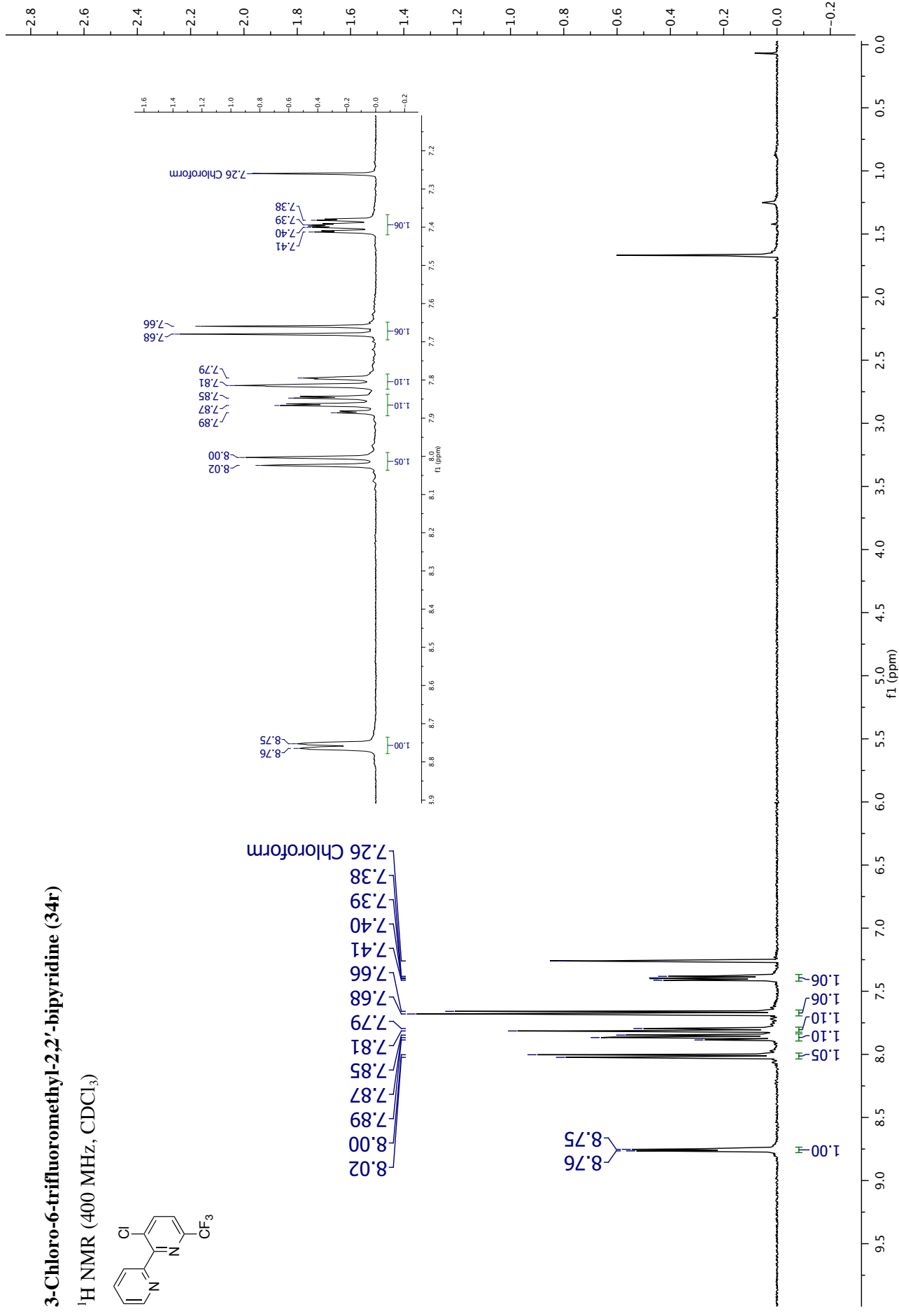
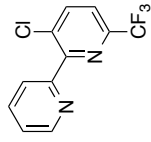
3-Chloro-6-methoxy-2,2'-bipyridine (34p)

¹³C NMR (101 MHz, CDCl₃)



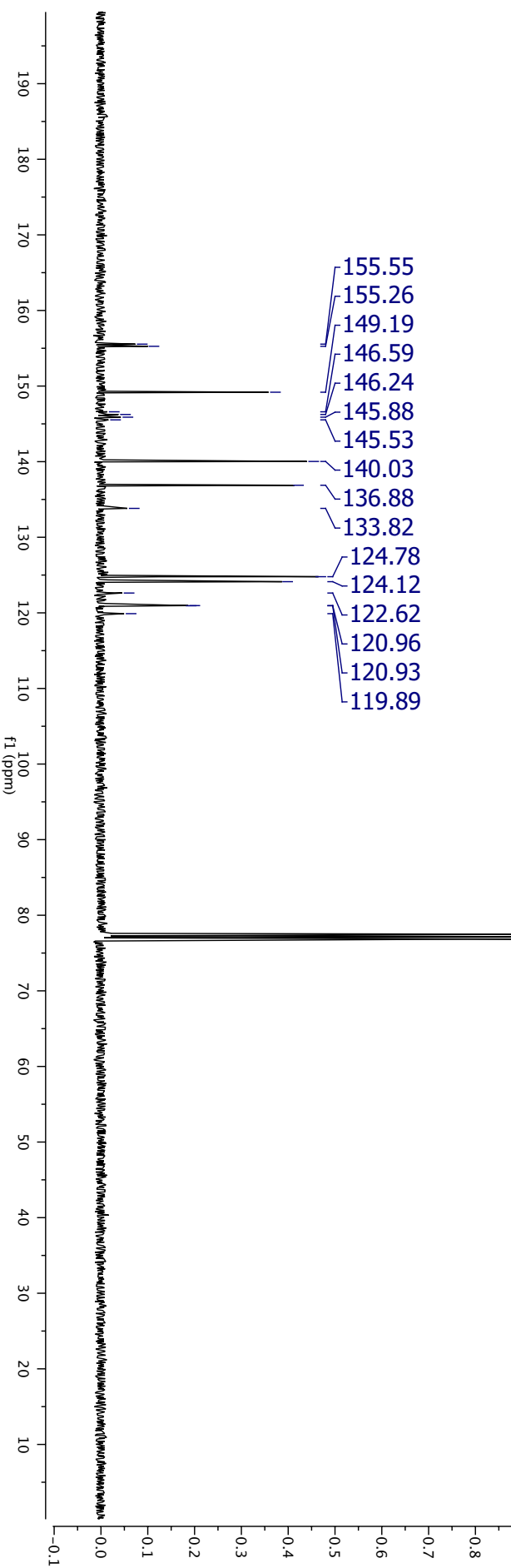
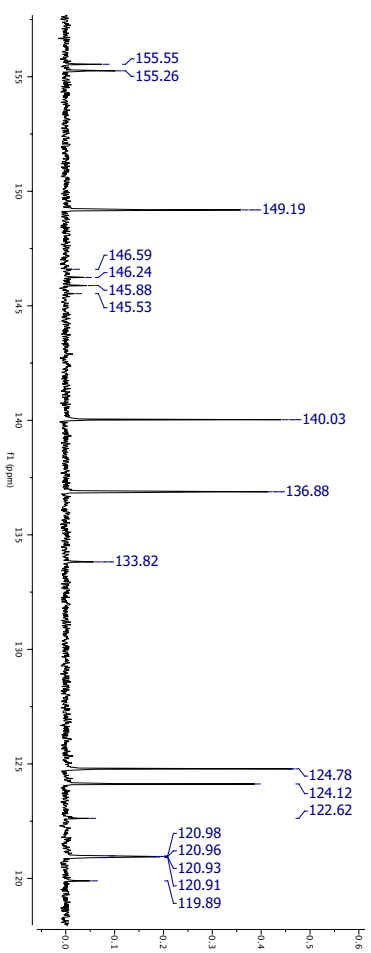
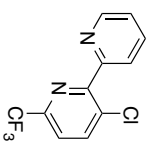
3-Chloro-6-trifluoromethyl-2,2'-bipyridine (34r)

¹H NMR (400 MHz, CDCl₃)



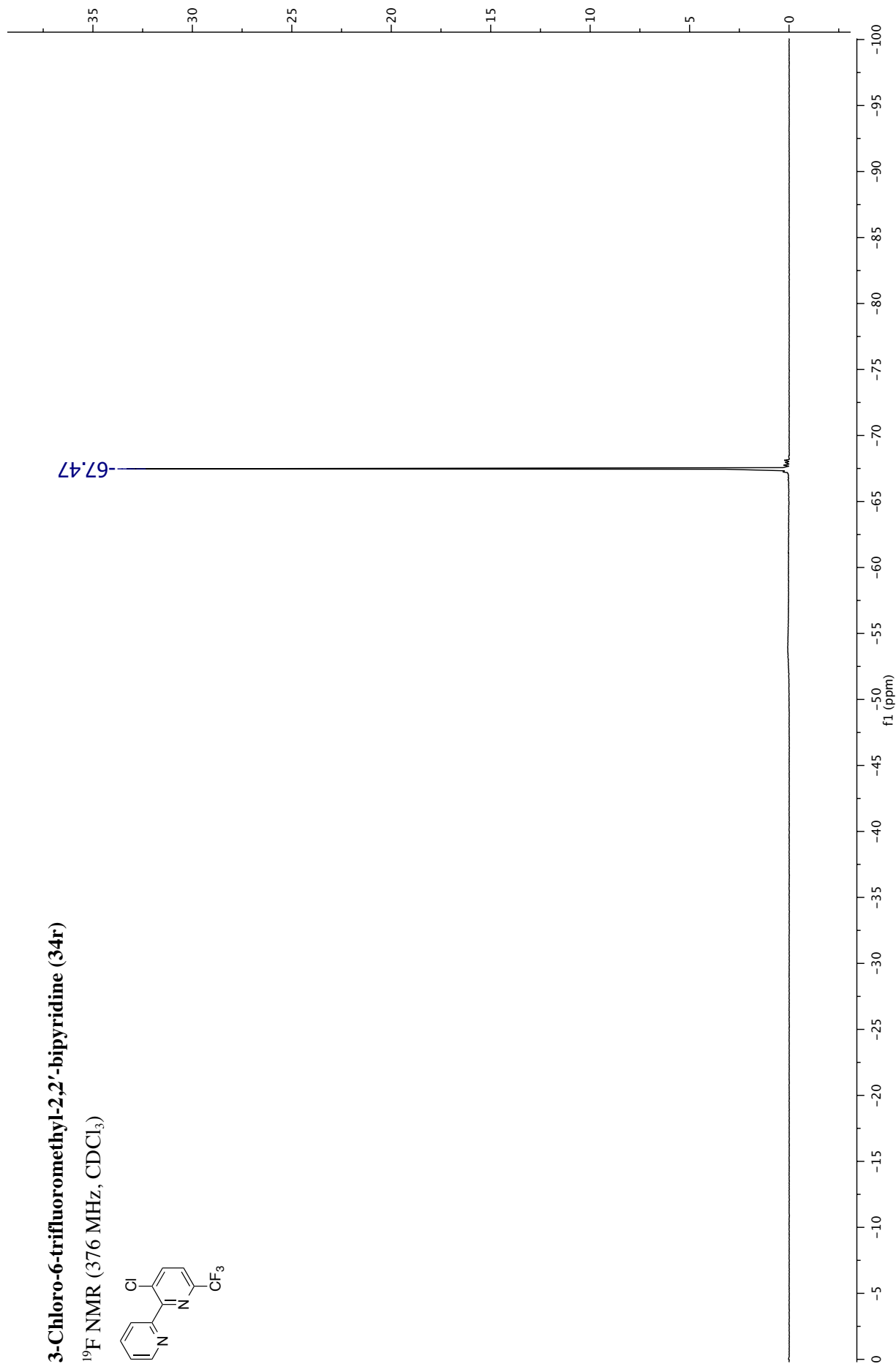
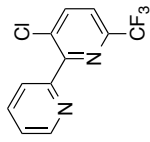
3-Chloro-6-(trifluoromethyl)-2,2'-bipyridine (34r)

¹³C NMR (101 MHz, CDCl₃)



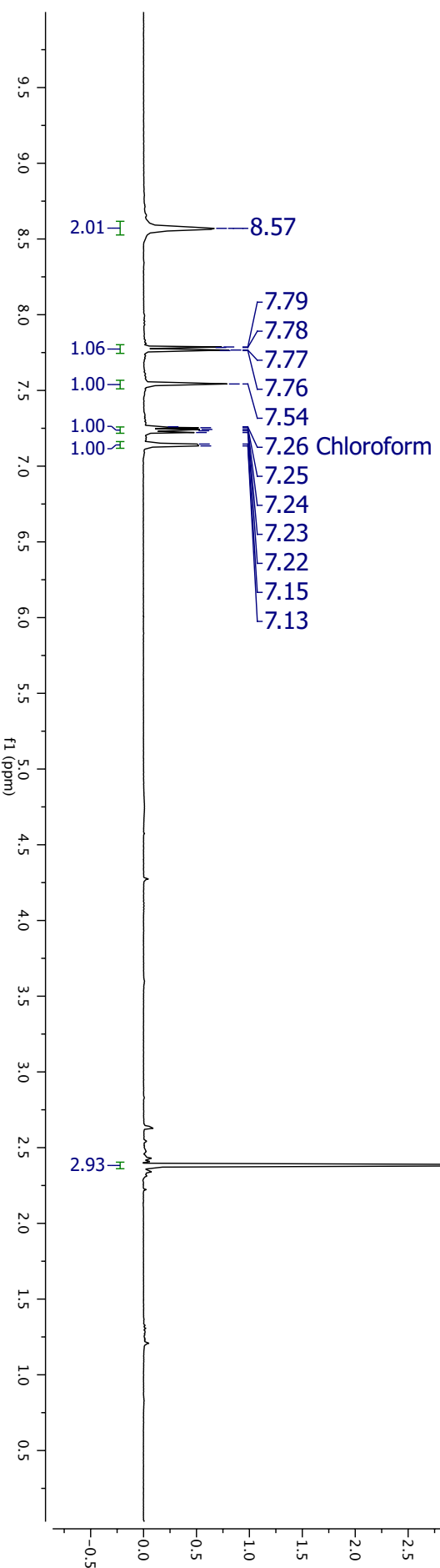
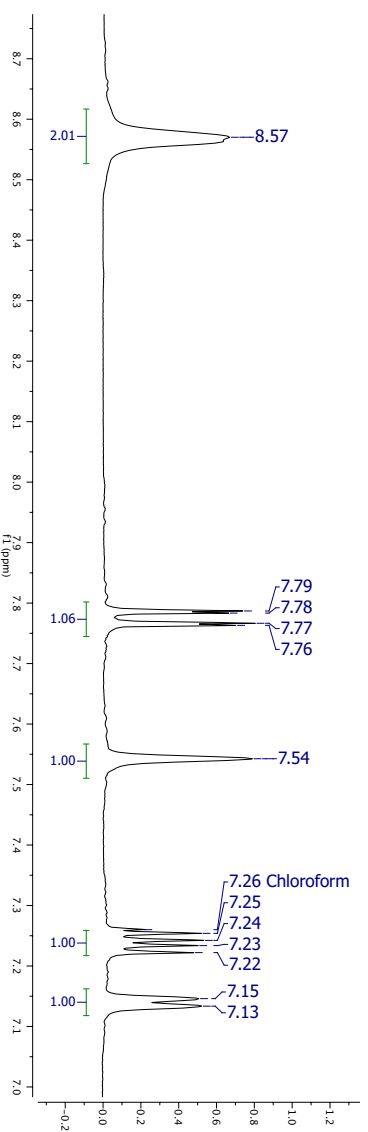
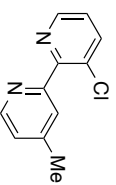
3-Chloro-6-trifluoromethyl-2,2'-bipyridine (34r)

¹⁹F NMR (376 MHz, CDCl₃)



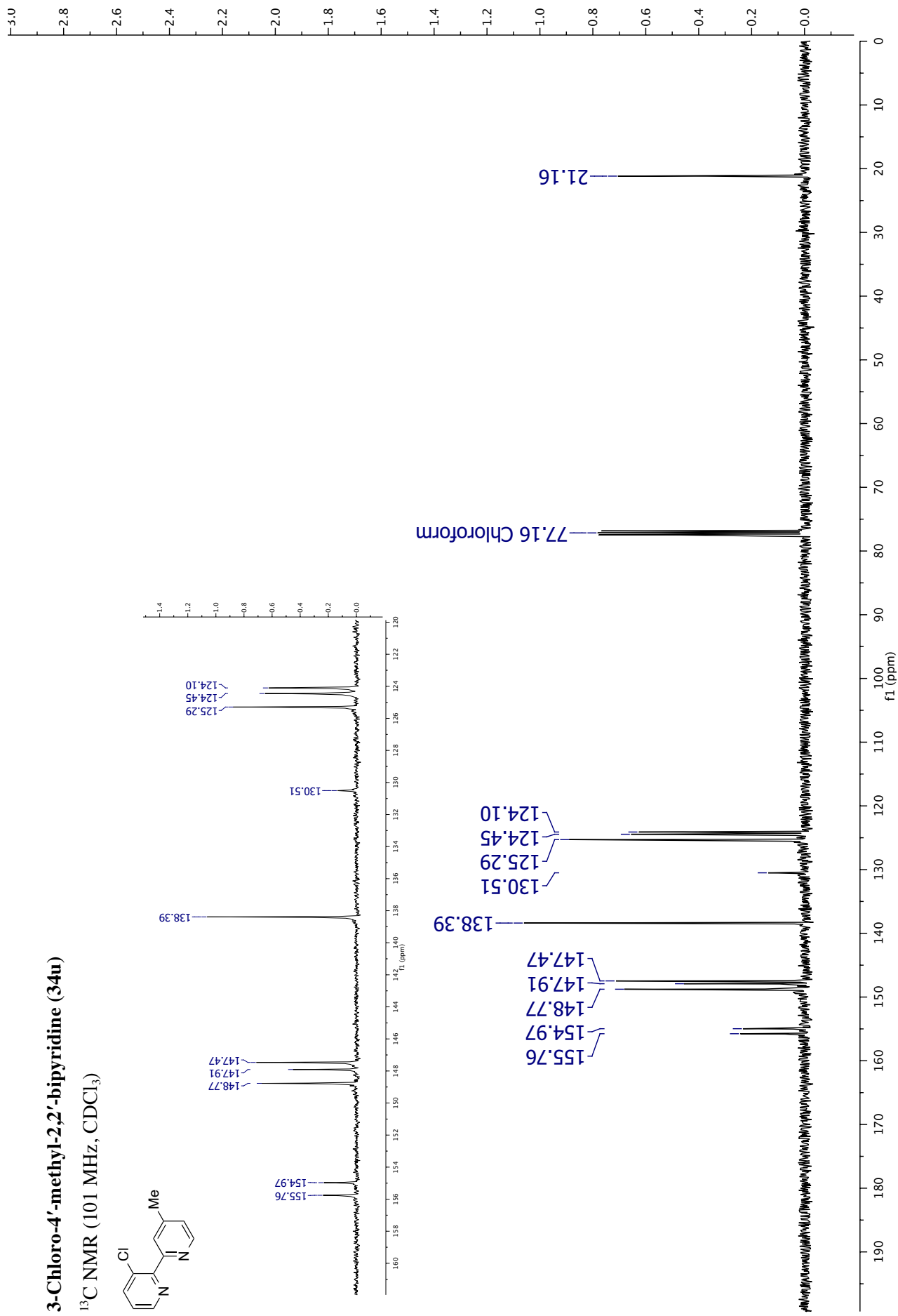
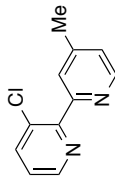
3-Chloro-4'-methyl-2,2'-bipyridine (34u)

¹H NMR (400 MHz, CDCl₃)



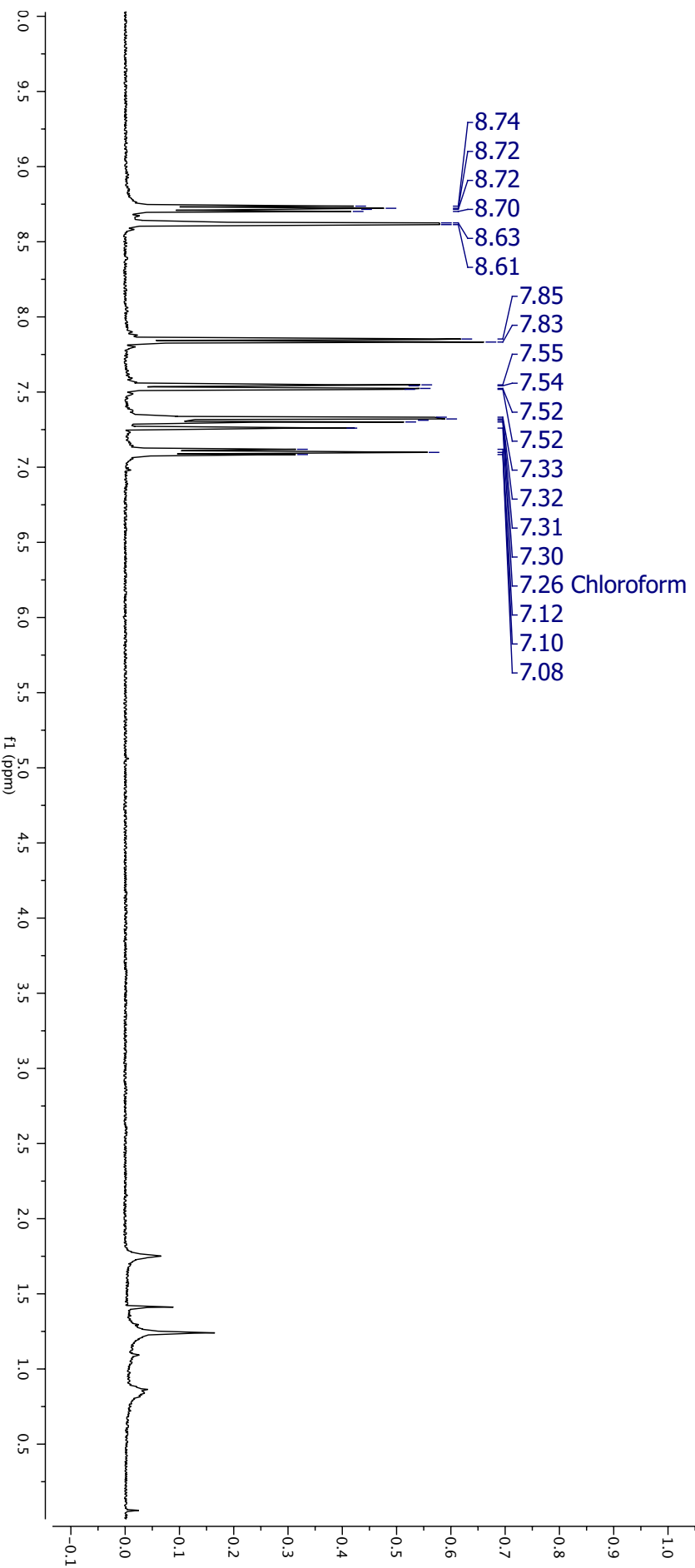
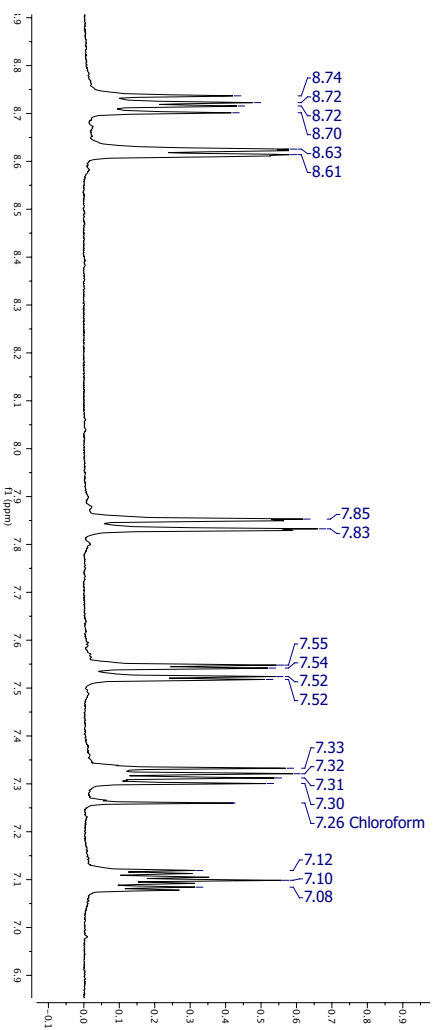
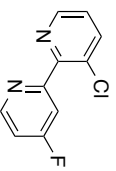
3-Chloro-4'-methyl-2,2'-bipyridine (34u)

^{13}C NMR (101 MHz, CDCl_3)



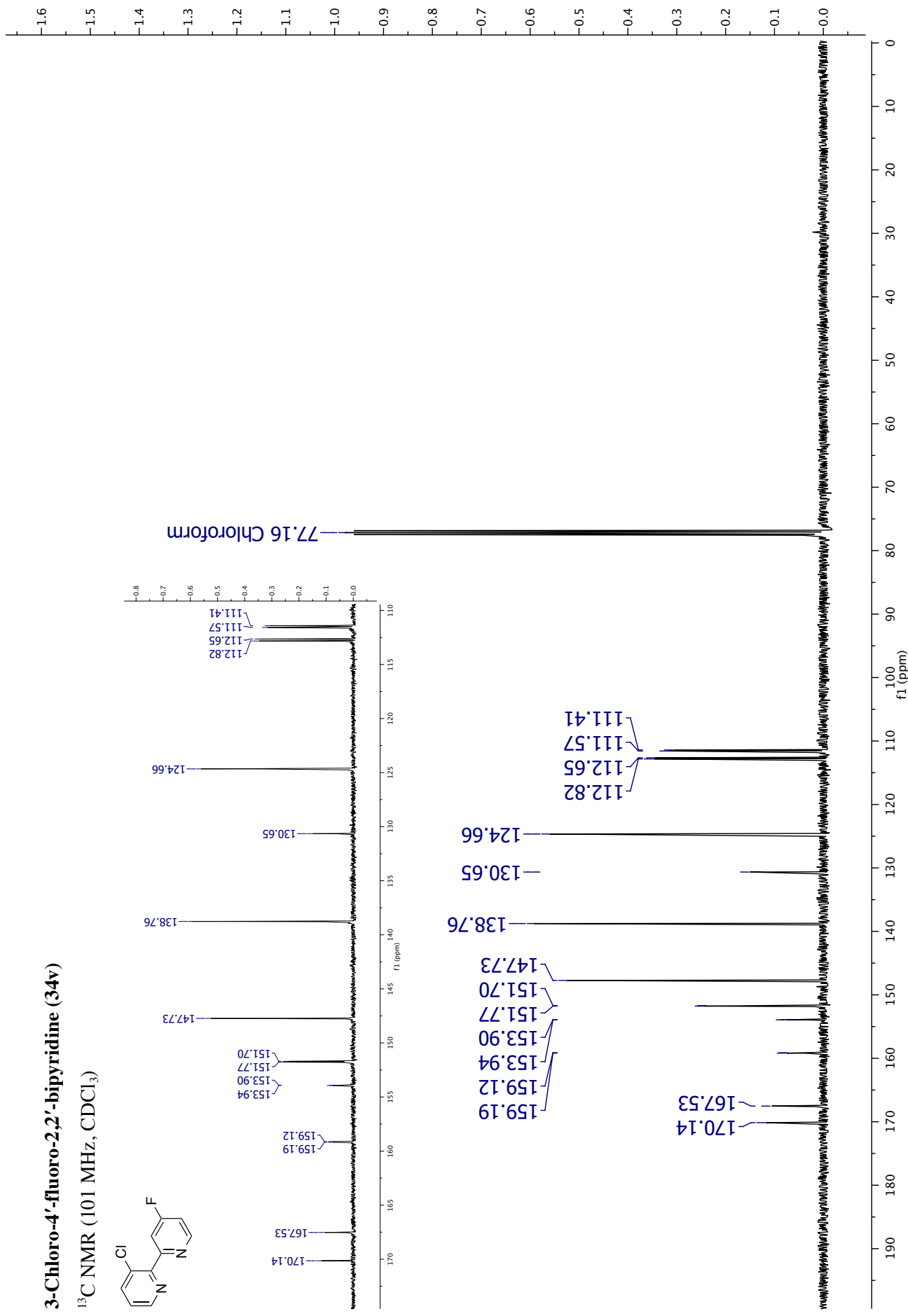
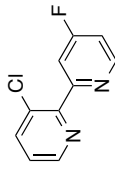
3-Chloro-4'-fluoro-2,2'-bipyridine (34v)

¹H NMR (400 MHz, CDCl₃)



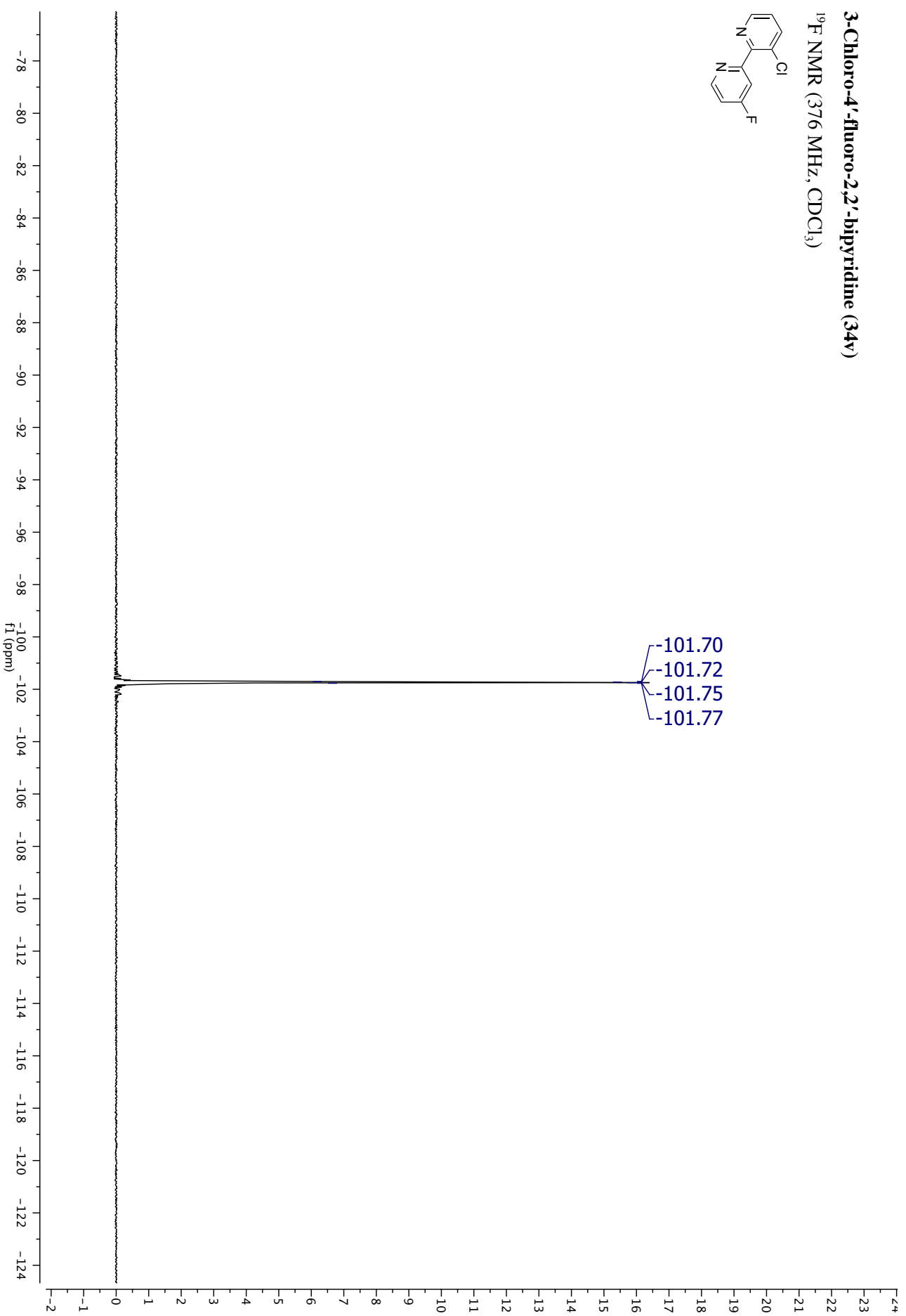
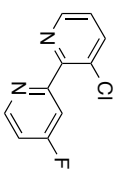
3-Chloro-4'-fluoro-2,2'-bipyridine (34v)

^{13}C NMR (101 MHz, CDCl_3)



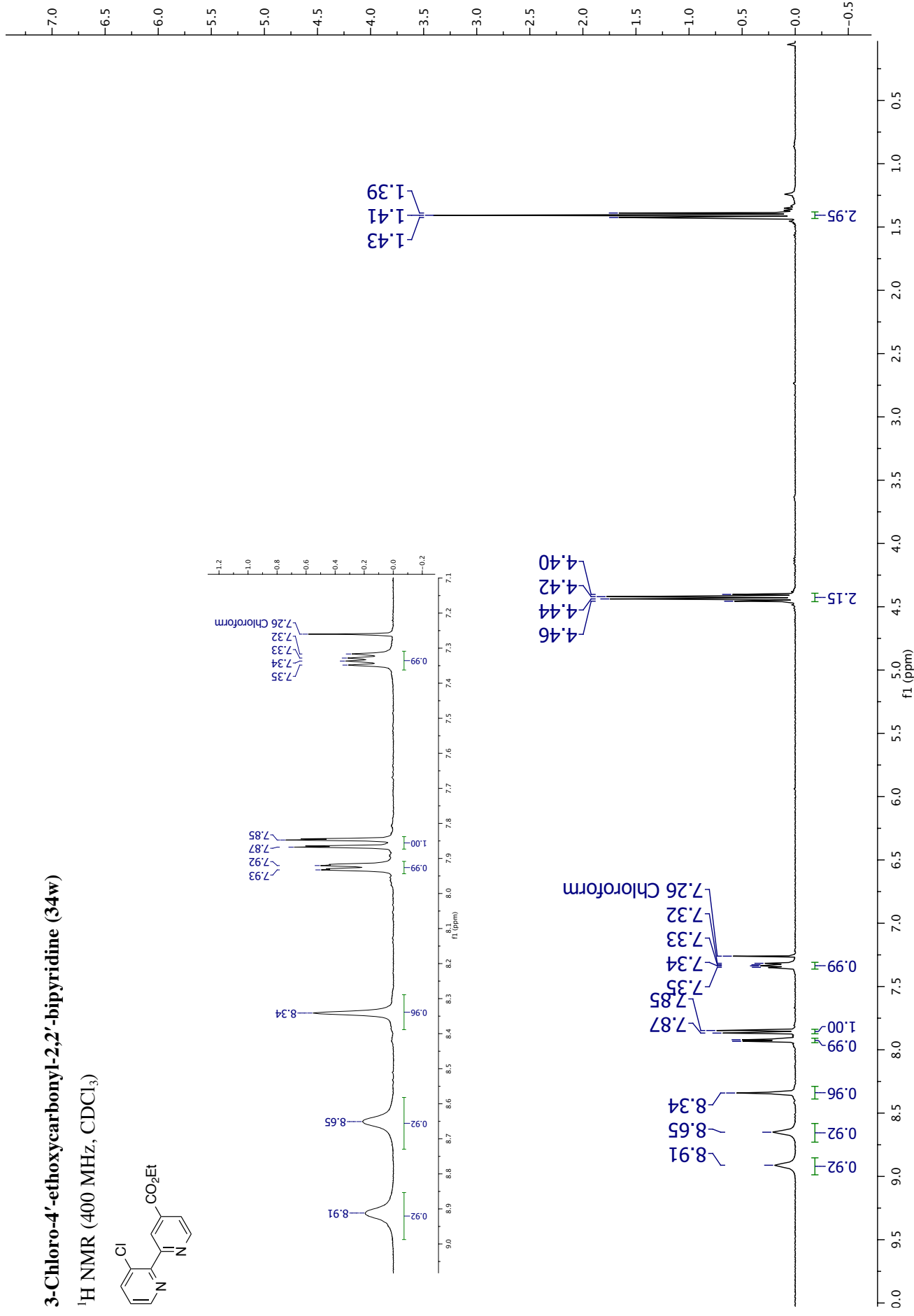
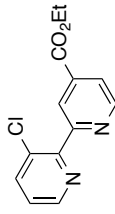
3-Chloro-4'-fluoro-2,2'-bipyridine (34v)

¹⁹F NMR (376 MHz, CDCl₃)



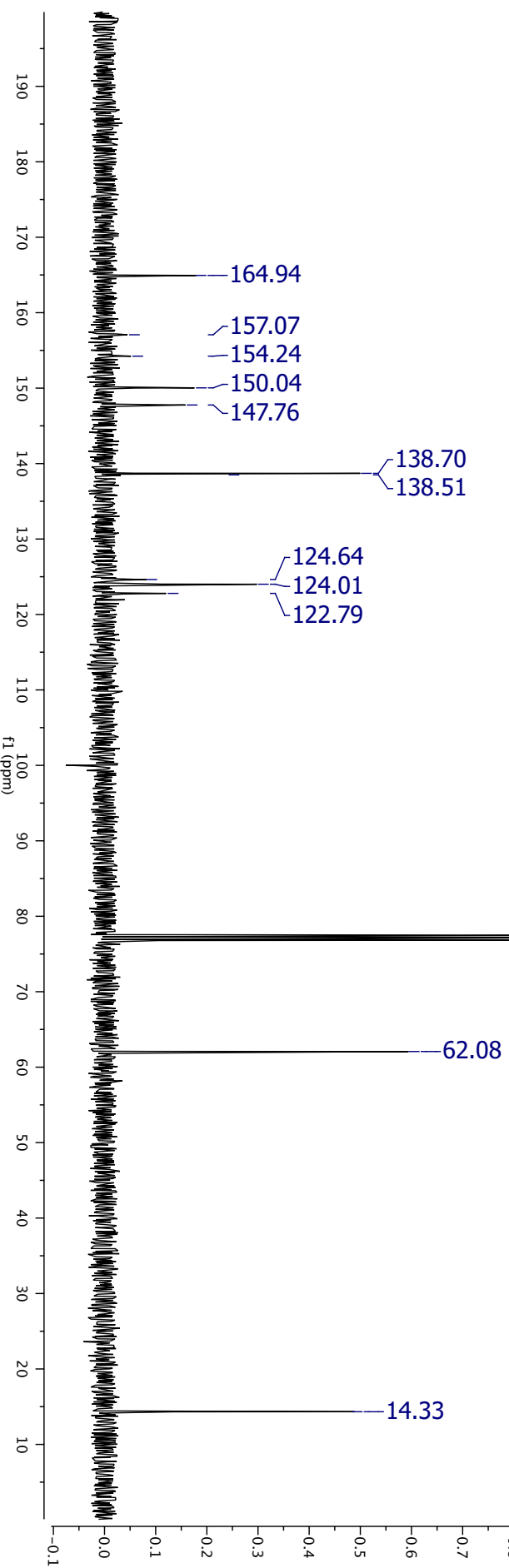
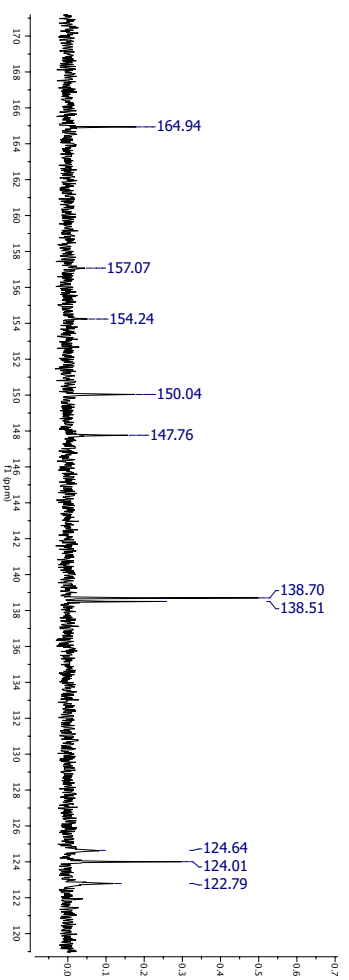
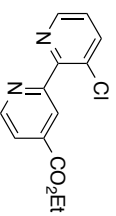
3-Chloro-4'-ethoxycarbonyl-2,2'-bipyridine (34w)

¹H NMR (400 MHz, CDCl₃)



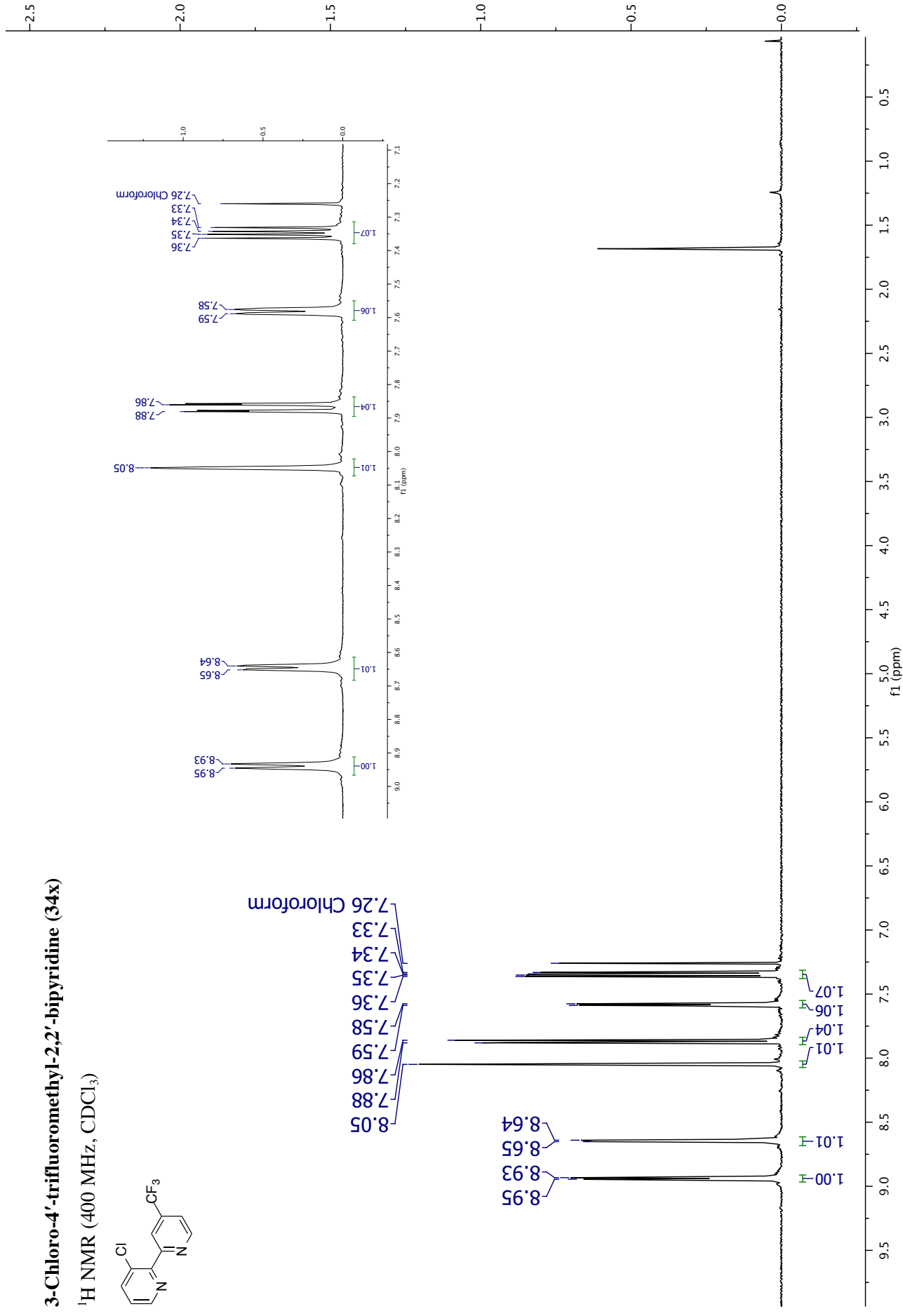
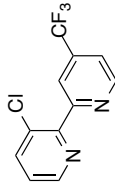
3-Chloro-4'-ethoxycarbonyl-2,2'-bipyridine (34w)

¹³C NMR (101 MHz, CDCl₃)



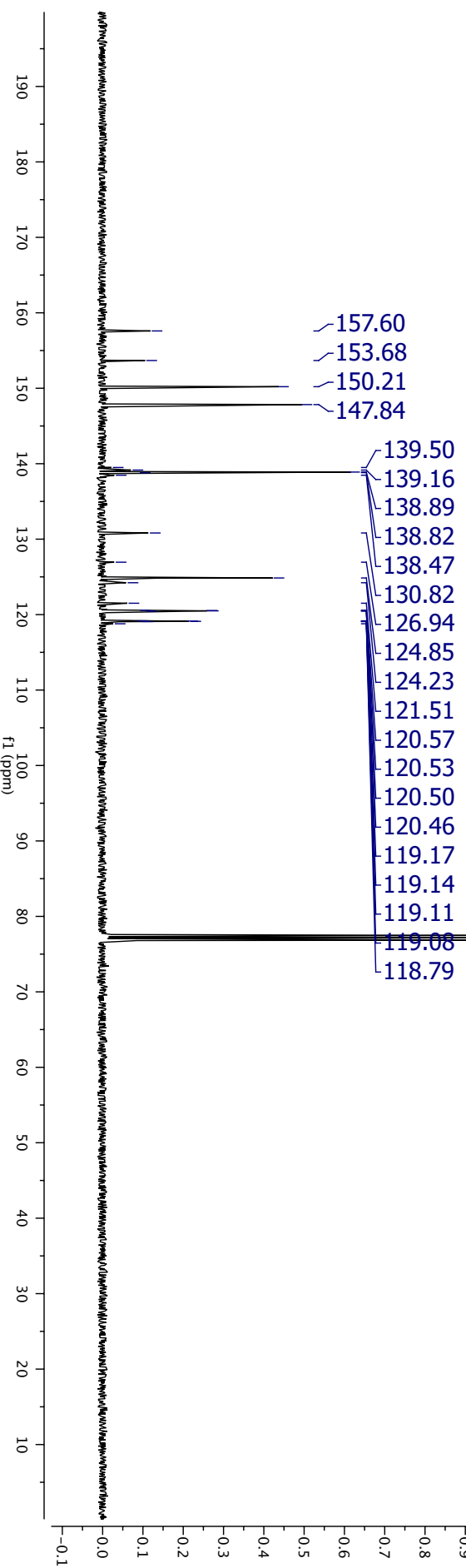
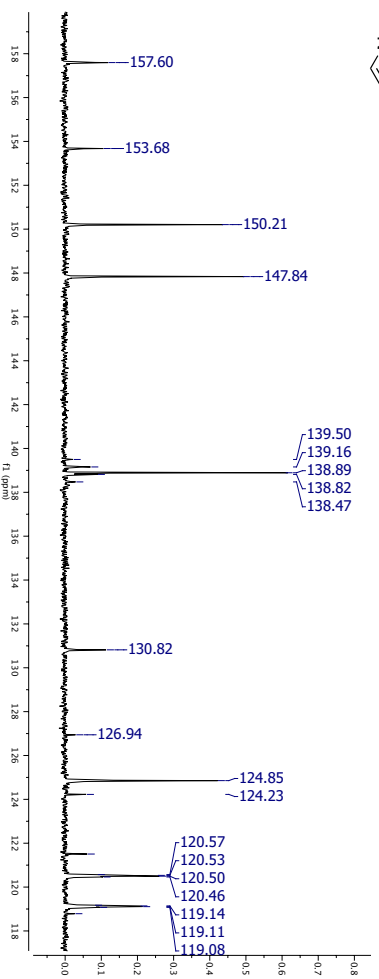
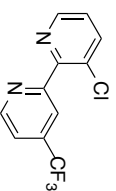
3-Chloro-4'-trifluoromethyl-2,2'-bipyridine (34x)

¹H NMR (400 MHz, CDCl₃)



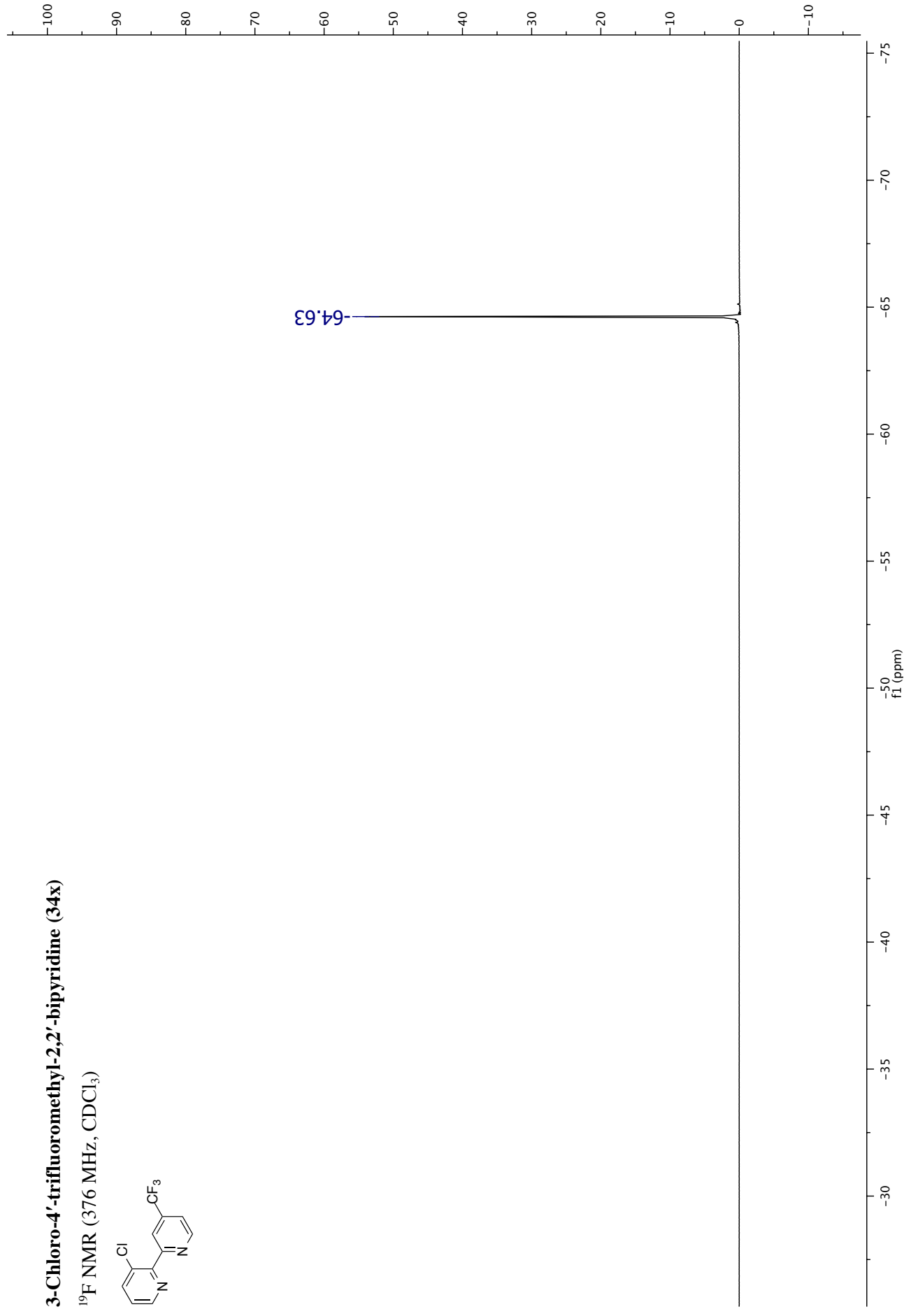
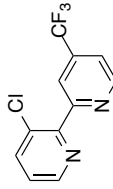
3-Chloro-4'-trifluoromethyl-2,2'-bipyridine (34x)

^{13}C NMR (101 MHz, CDCl_3)



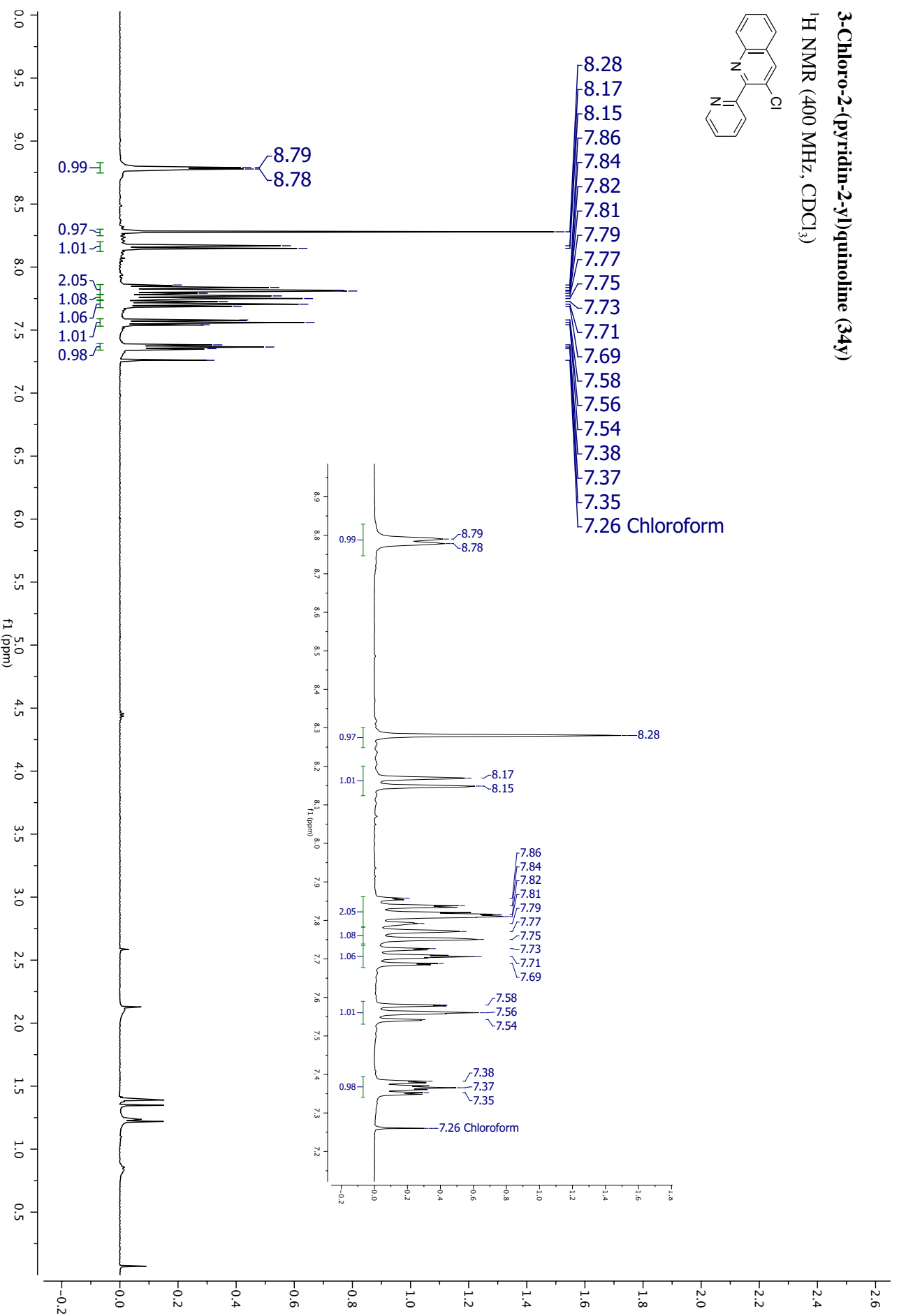
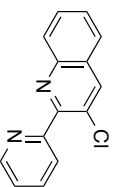
3-Chloro-4'-trifluoromethyl-2,2'-bipyridine (34x)

¹⁹F NMR (376 MHz, CDCl₃)



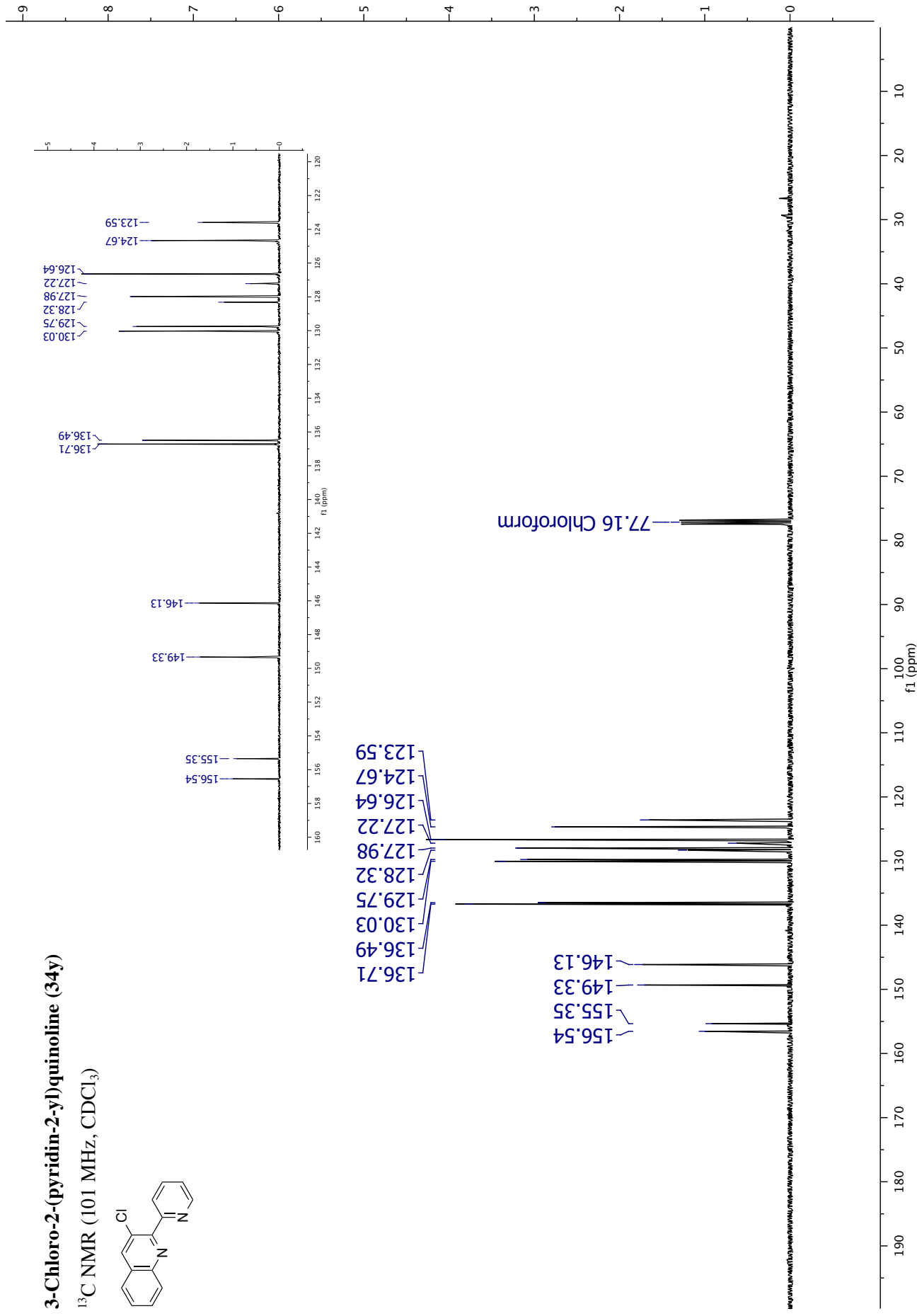
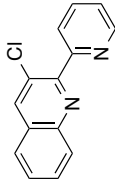
3-Chloro-2-(pyridin-2-yl)quinoline (34y)

¹H NMR (400 MHz, CDCl₃)



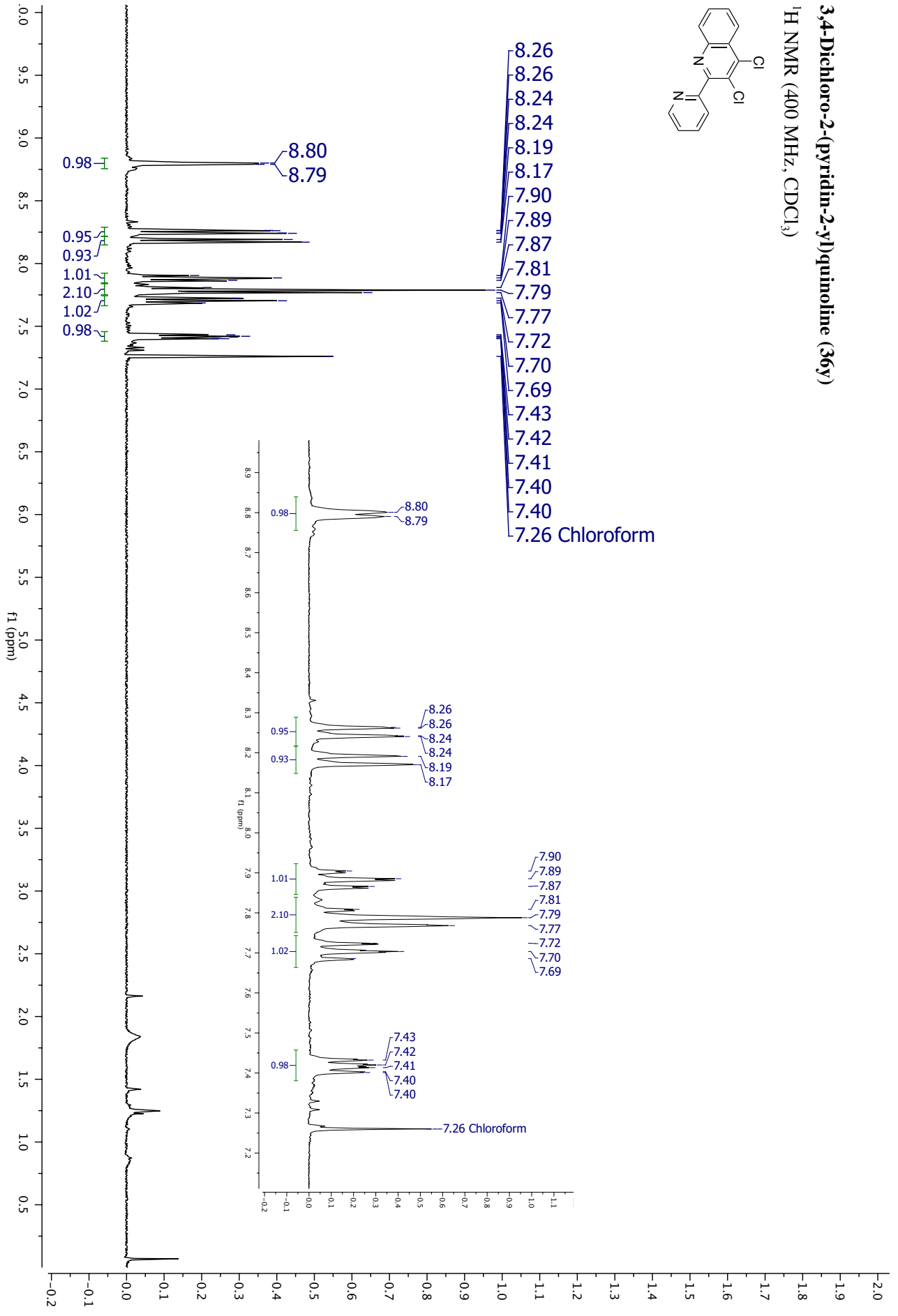
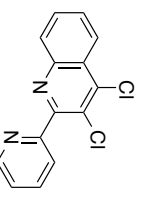
3-Chloro-2-(pyridin-2-yl)quinoline (34y)

^{13}C NMR (101 MHz, CDCl_3)



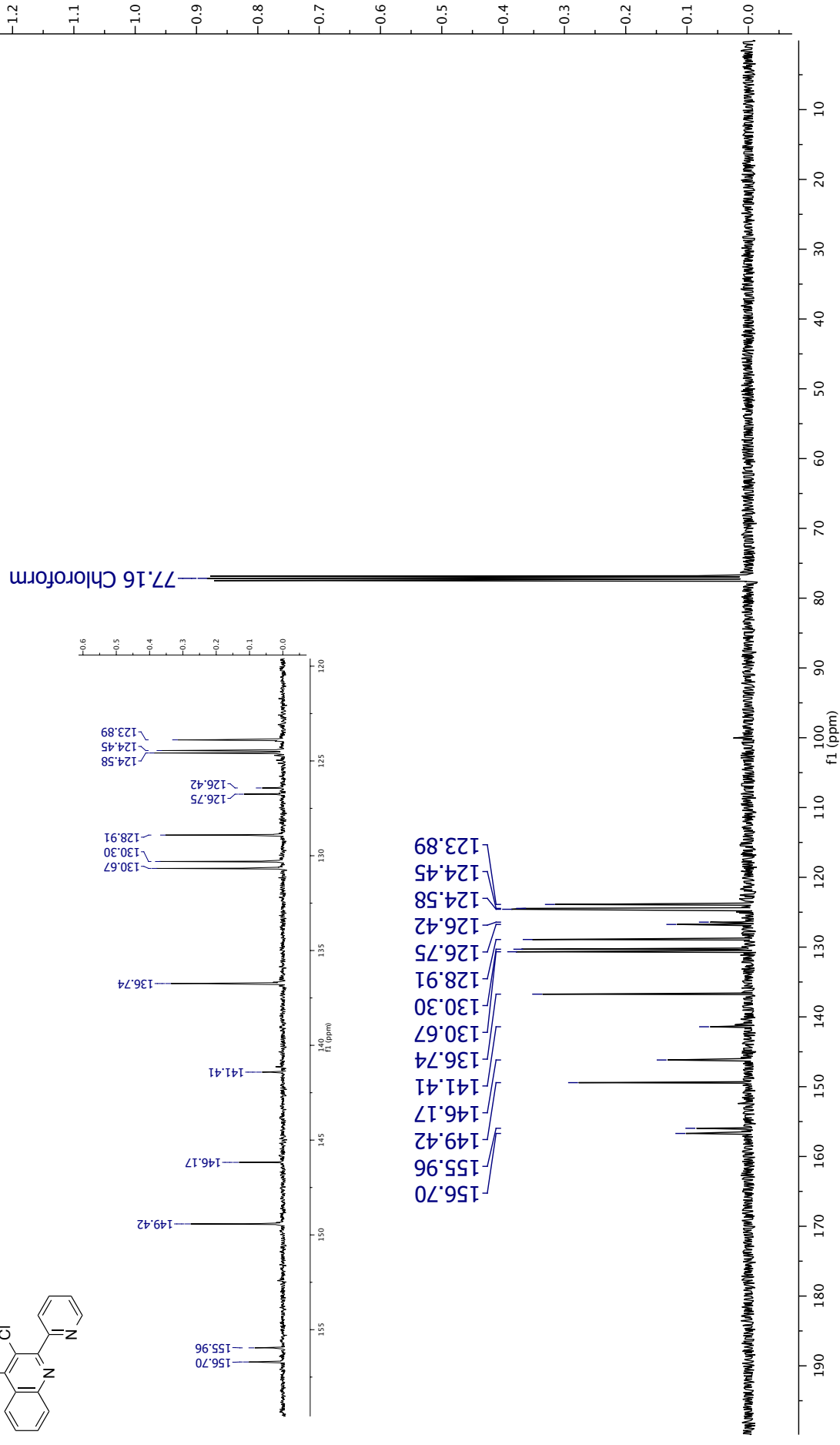
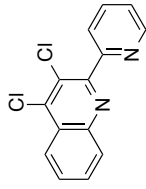
3,4-Dichloro-2-(pyridin-2-yl)quinoline (36y)

¹H NMR (400 MHz, CDCl₃)



3,4-Dichloro-2-(pyridin-2-yl)quinoline (36y)

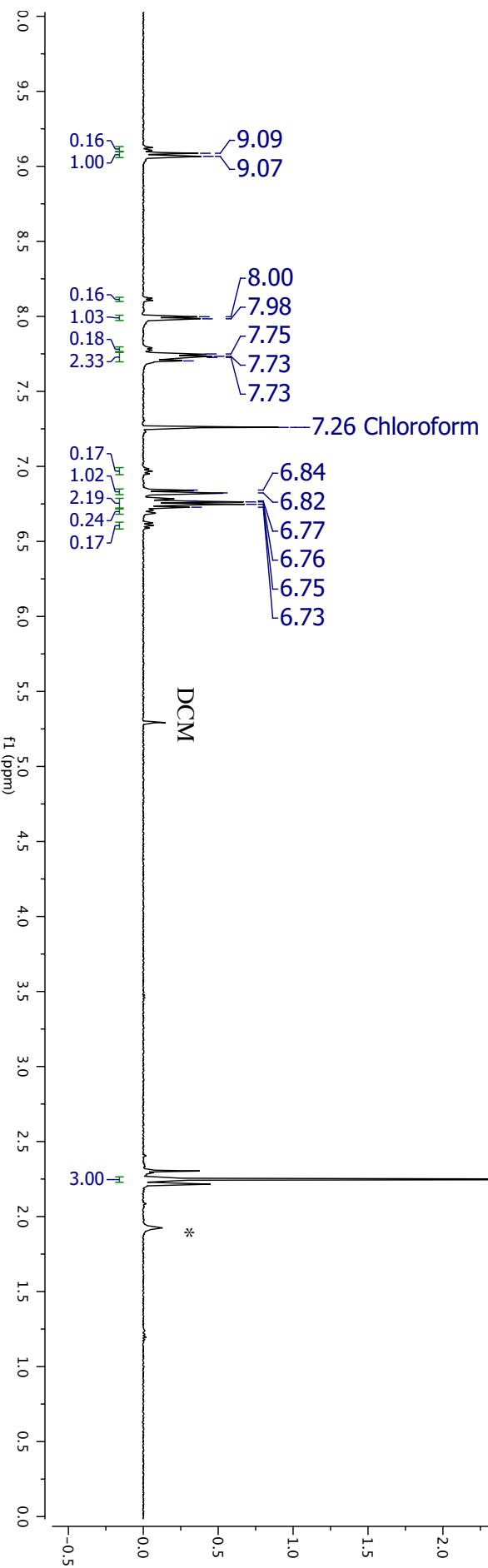
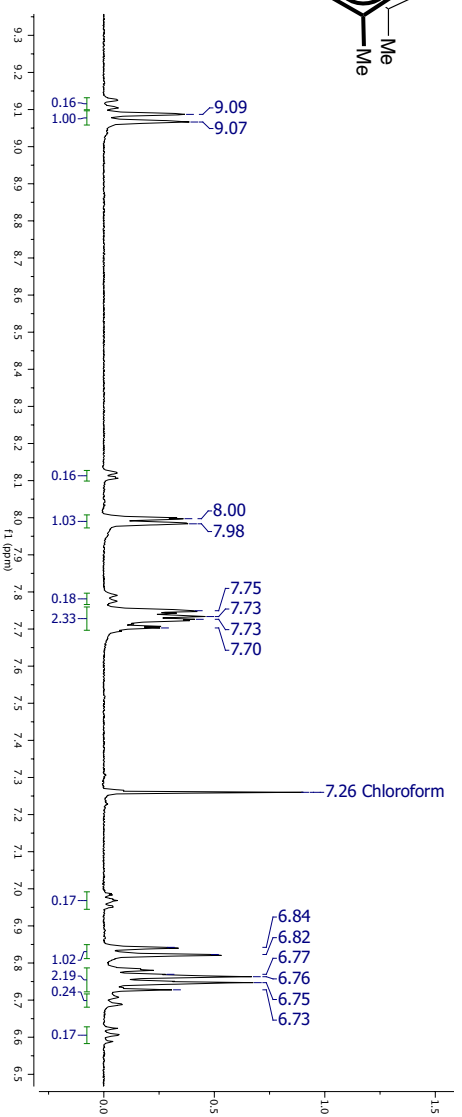
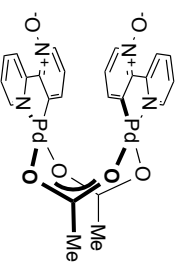
^{13}C NMR (101 MHz, CDCl_3)



10.8 Palladium intermediates of 3-halogenations

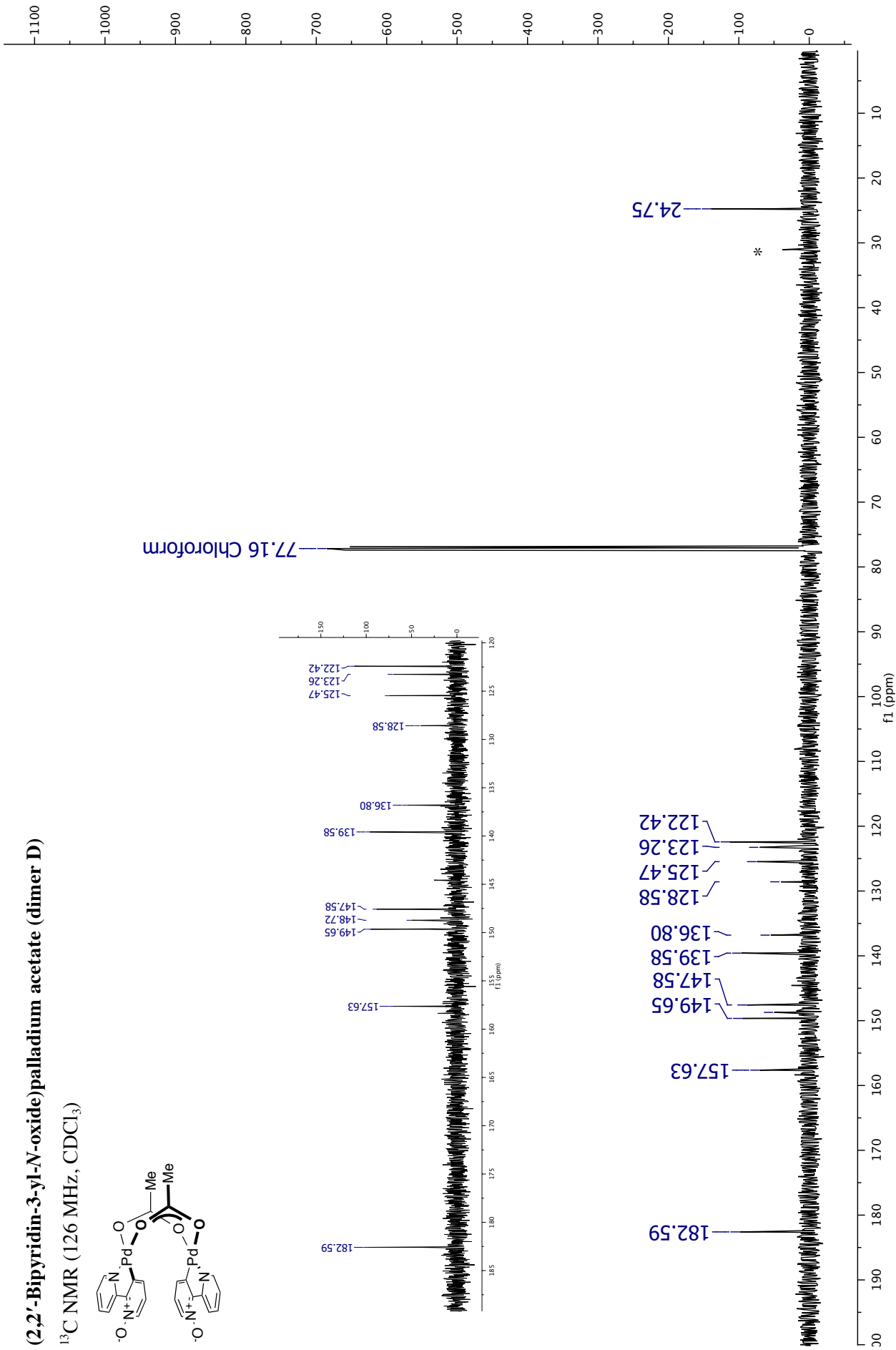
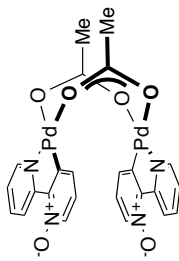
(2,2'-Bipyridin-3-yl-N-oxide)palladium acetate (dimer D)

¹H NMR (400 MHz, CDCl₃)



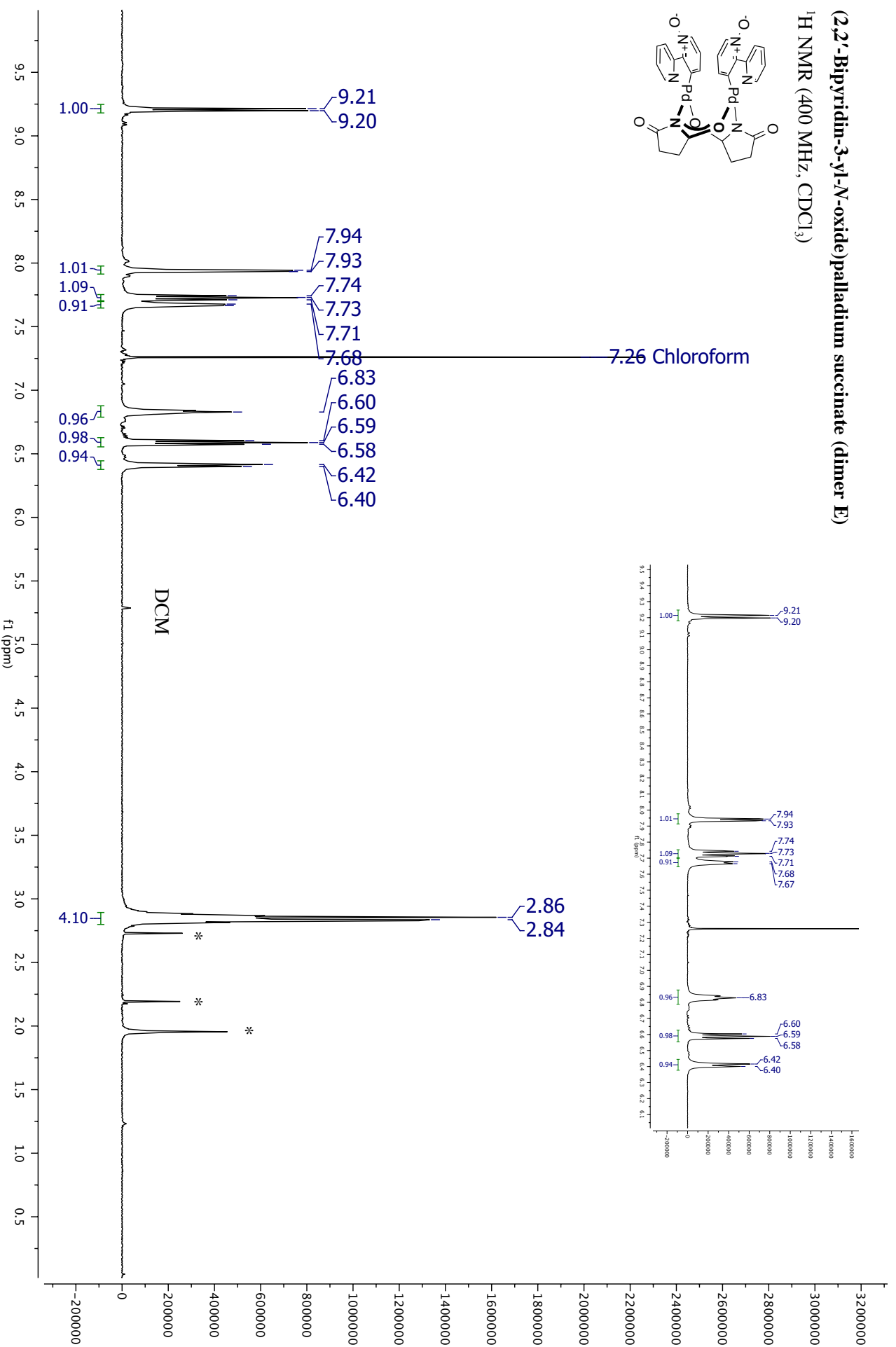
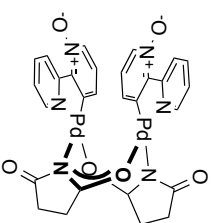
(2,2'-Bipyridin-3-yl-N-oxide)palladium acetate (dimer D)

^{13}C NMR (126 MHz, CDCl_3)



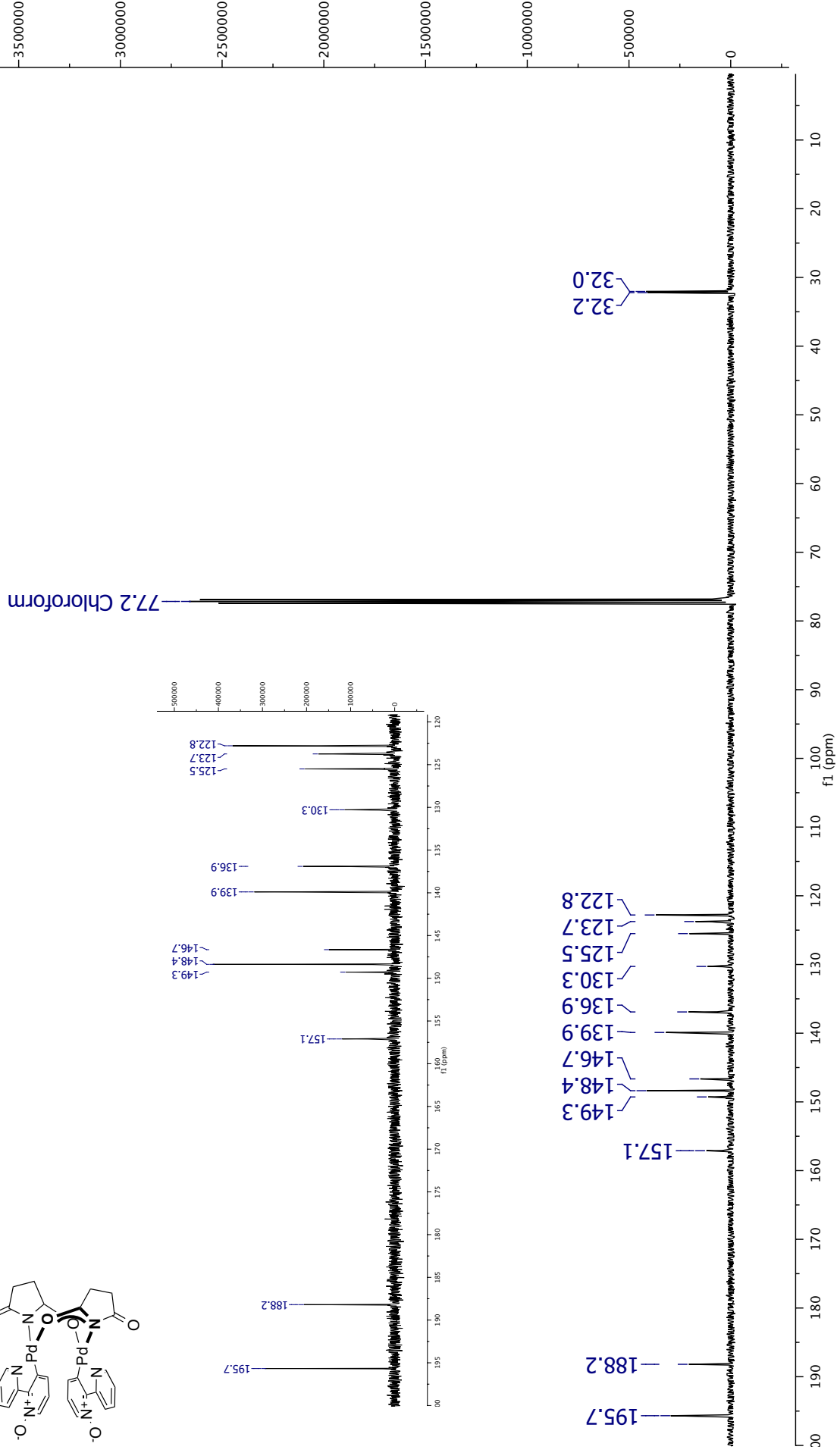
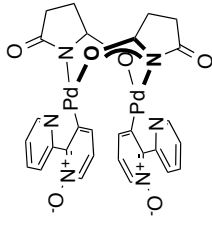
(2,2'-Bipyridin-3-yl-N-oxide)palladium succinate (dimer E)

¹H NMR (400 MHz, CDCl₃)



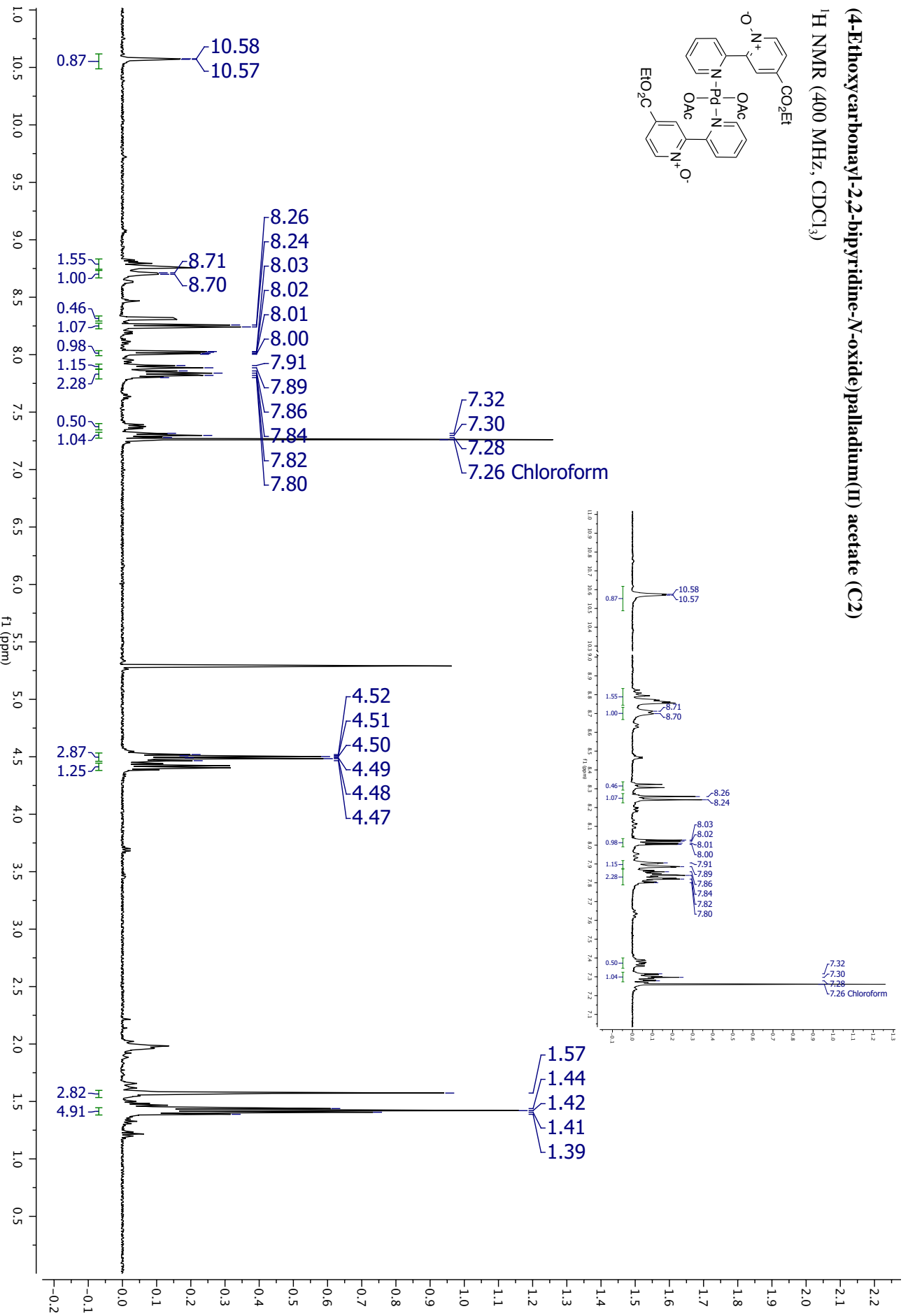
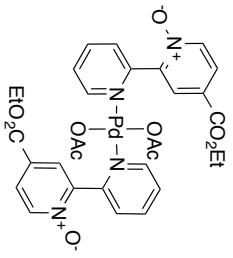
(2,2'-Bipyridin-3-yl-N-oxide)palladium succinate (dimer E)

^{13}C NMR (126 MHz, CDCl_3)

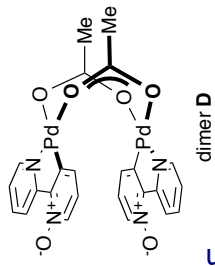
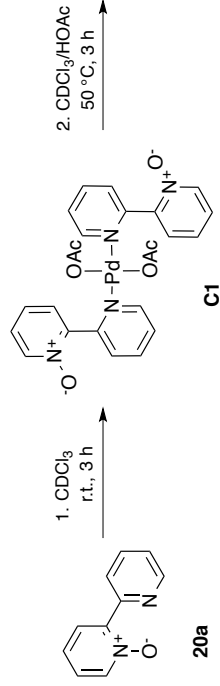


(4-Ethoxycarbonyl-2,2-bipyridine-N-oxide)palladium(II) acetate (C2)

¹H NMR (400 MHz, CDCl₃)



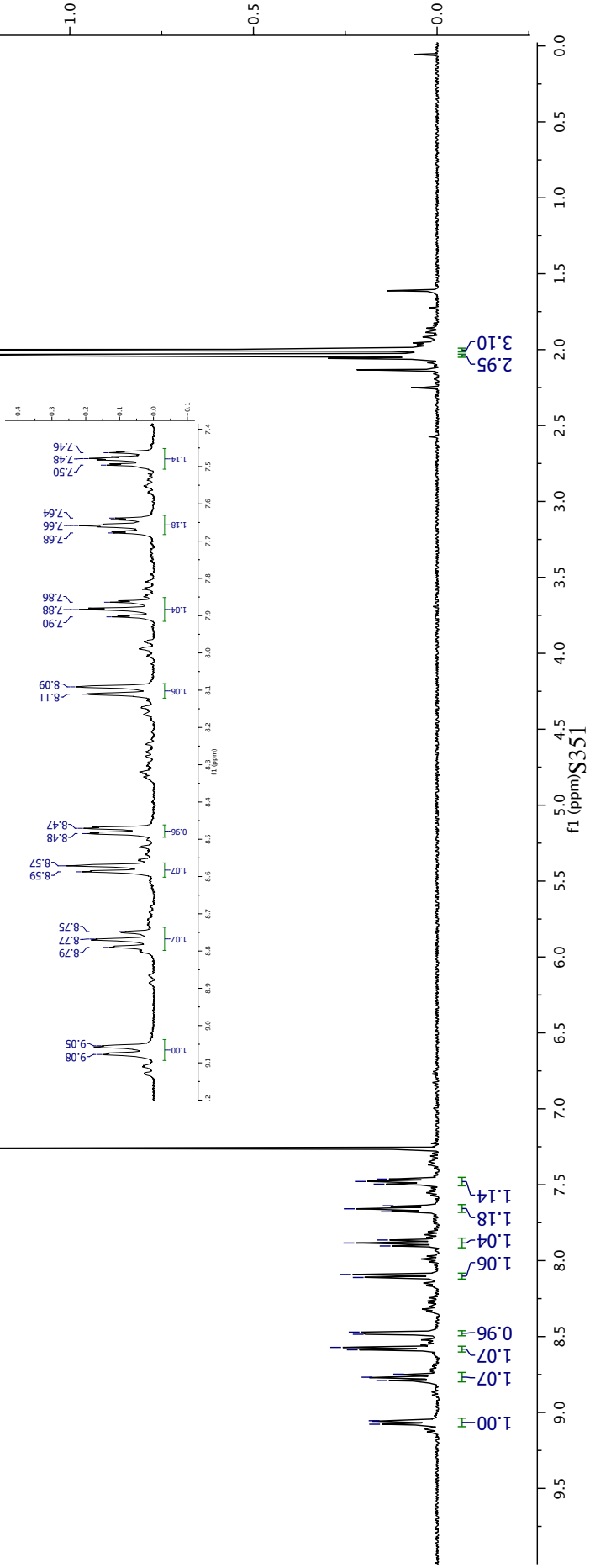
¹H NMR (400 MHz, CDCl₃), spectrum of the first step



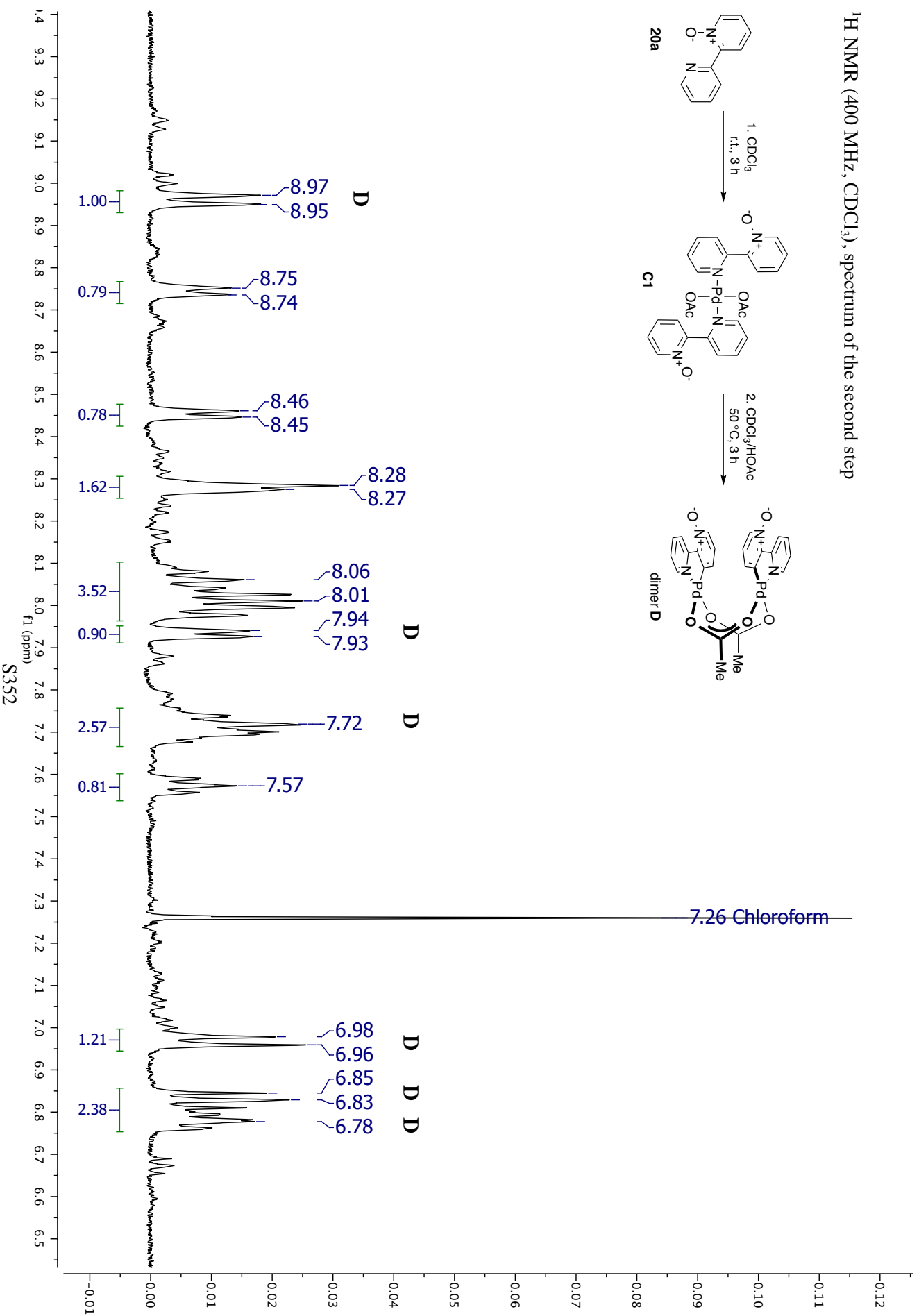
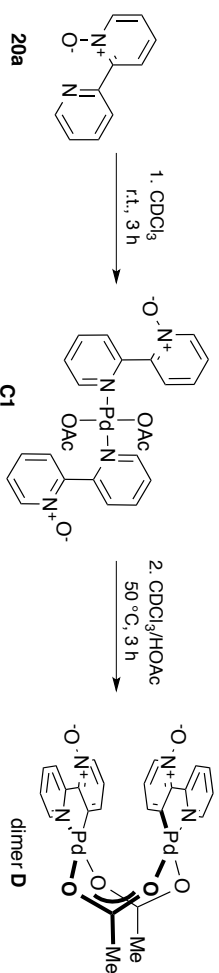
Chloroform

9.08, 9.05, 8.79, 8.77, 8.75, 8.59, 8.57, 8.48, 8.47, 8.11, 8.09, 7.90, 7.88, 7.86, 7.68, 7.66, 7.64, 7.50, 7.48, 7.46, 7.26

2.04, 2.00

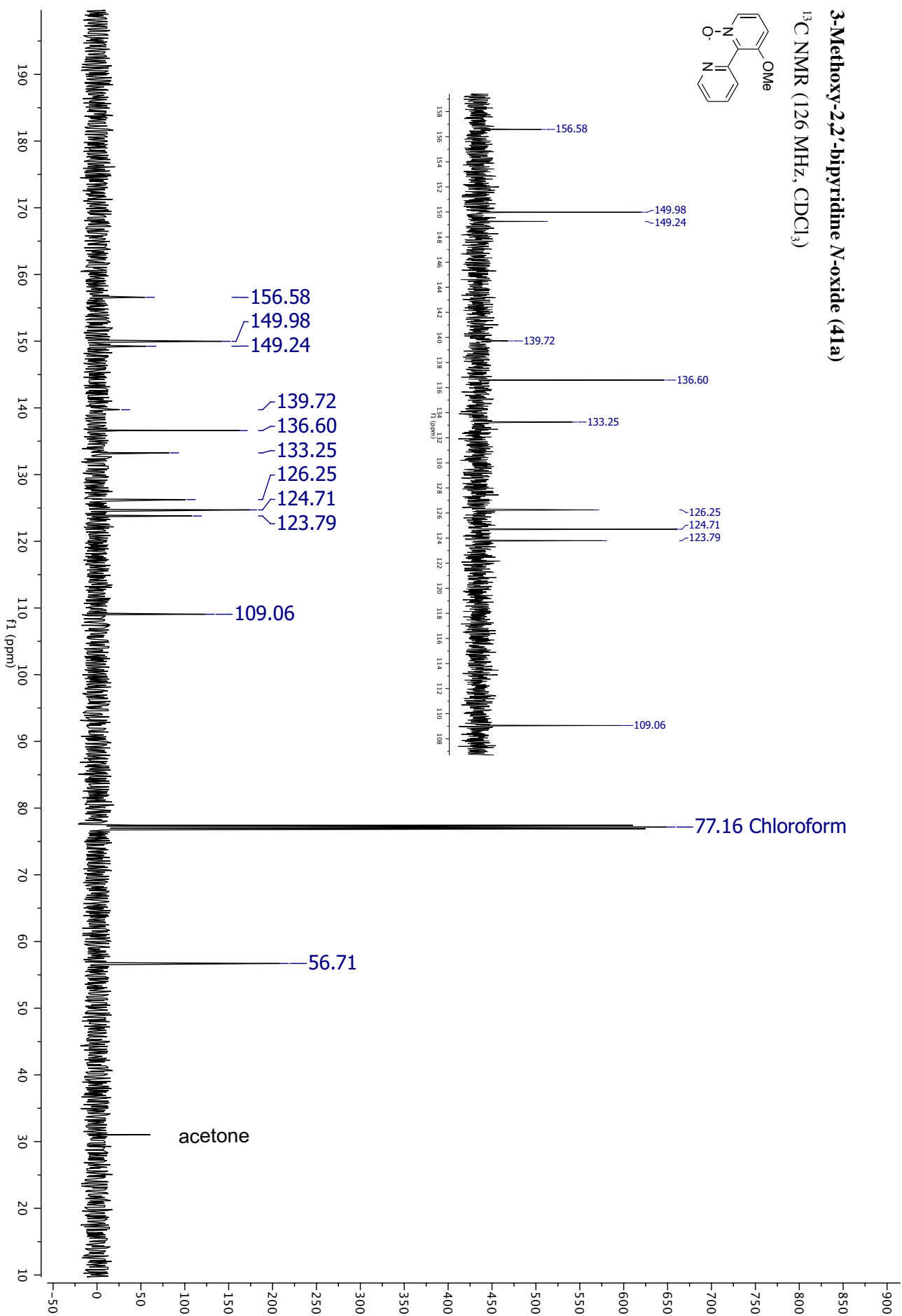
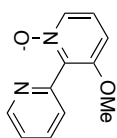


¹H NMR (400 MHz, CDCl₃), spectrum of the second step



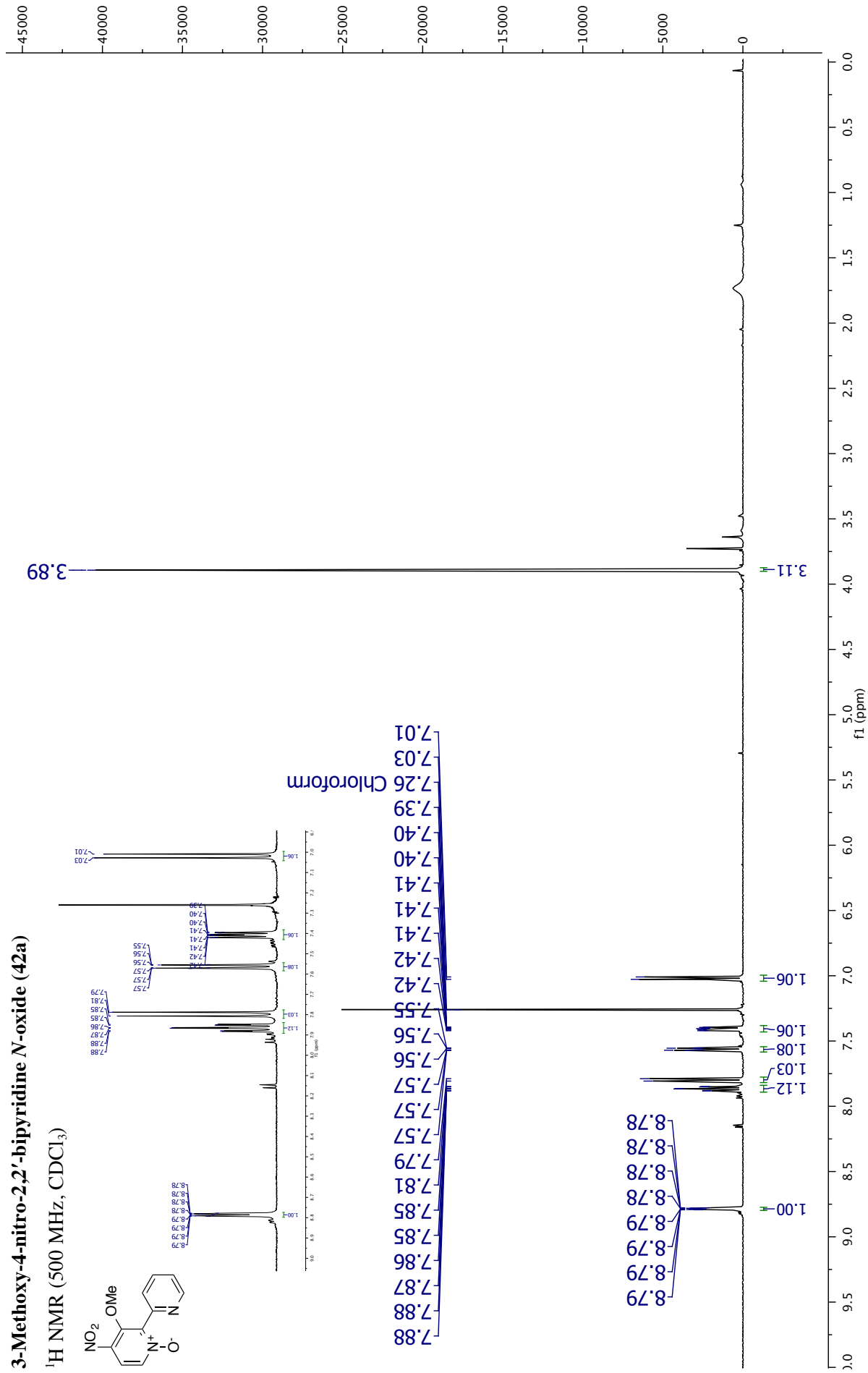
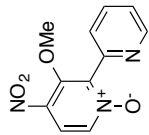
3-Methoxy-2,2'-bipyridine N-oxide (41a)

¹³C NMR (126 MHz, CDCl₃)



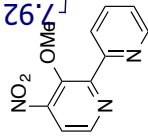
3-Methoxy-4-nitro-2,2'-bipyridine N-oxide (42a)

¹H NMR (500 MHz, CDCl₃)



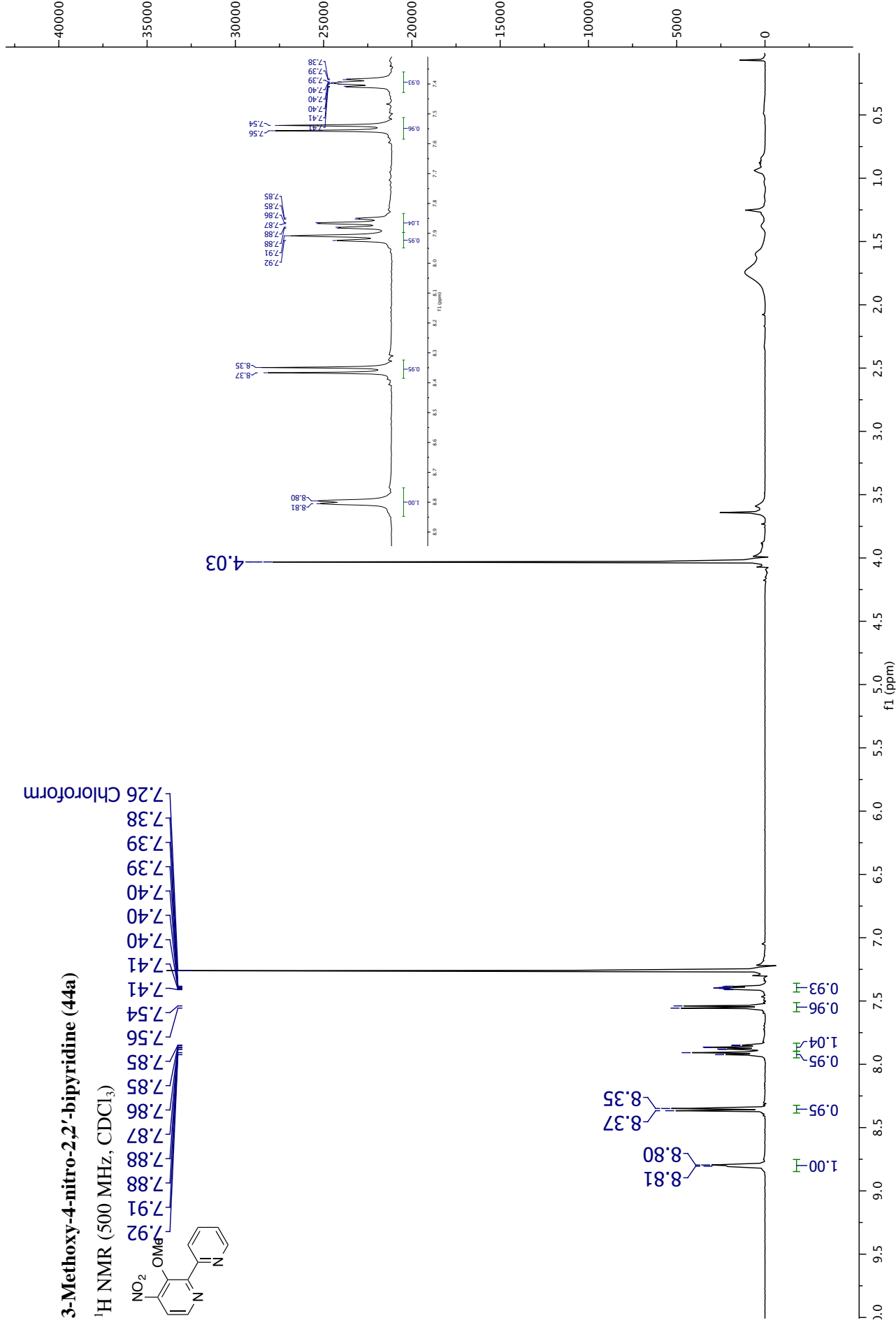
3-Methoxy-4-nitro-2,2'-bipyridine (44a)

¹H NMR (500 MHz, CDCl₃)



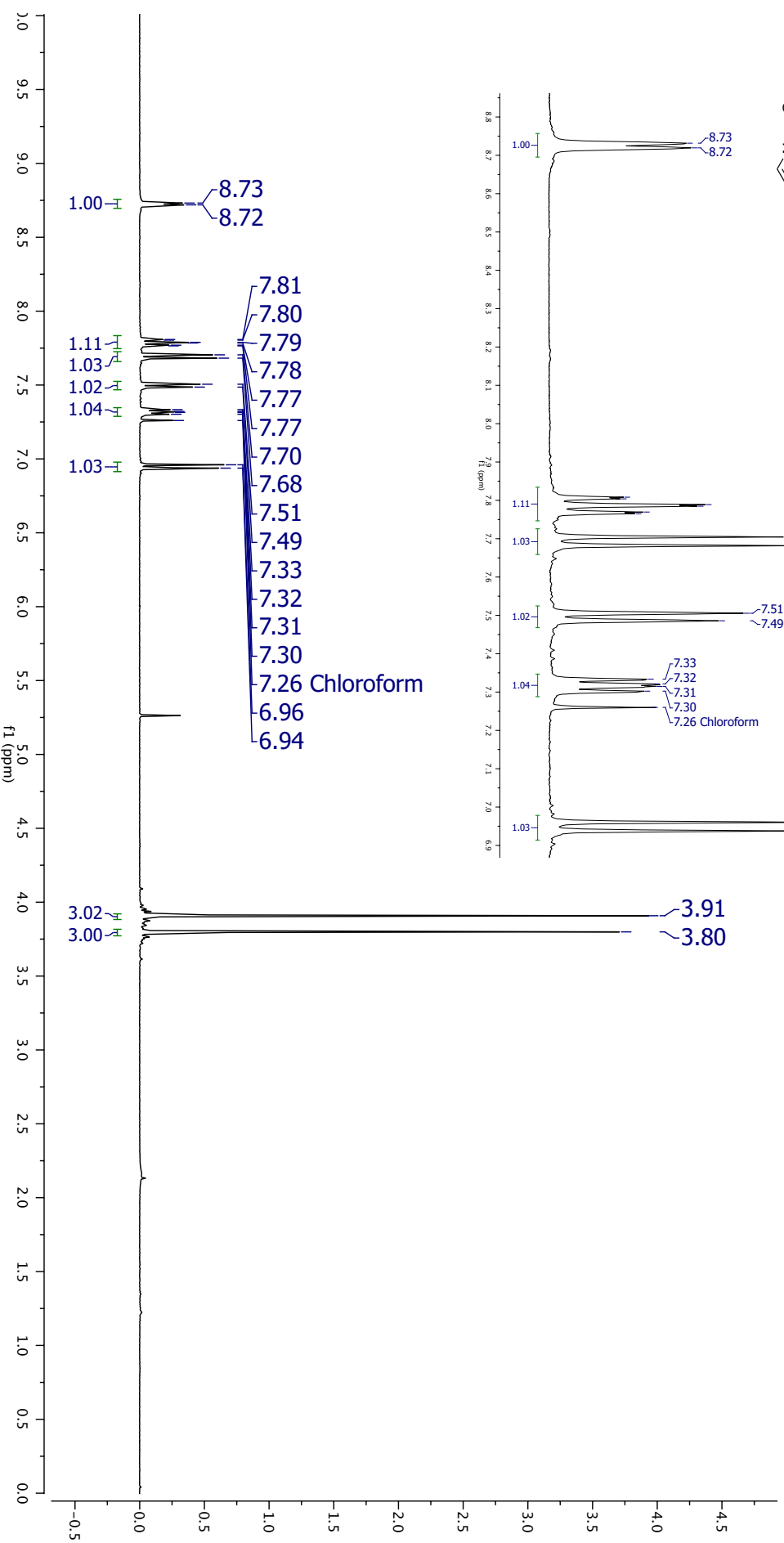
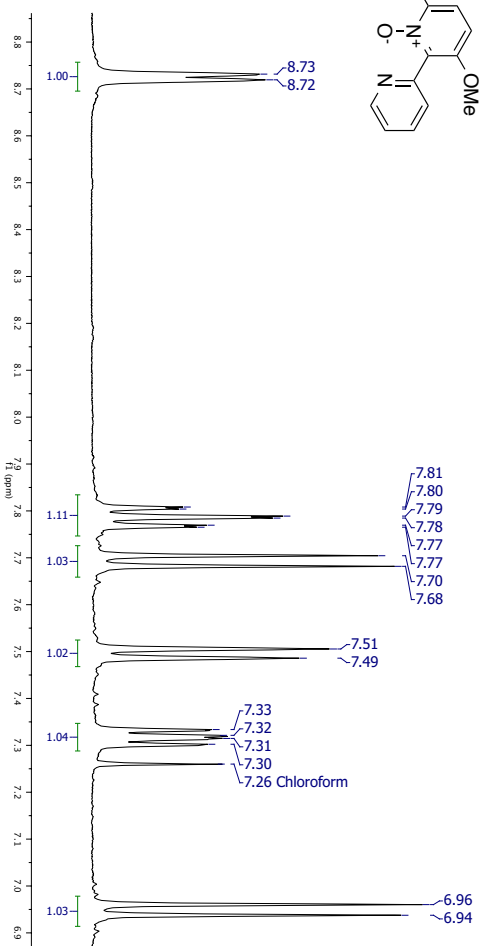
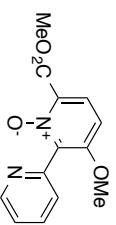
7.92
7.91
7.88
7.88
7.87
7.86
7.85
7.85
7.85
7.56
7.54
7.41
7.41
7.40
7.40
7.40
7.39
7.39
7.38
7.26 Chloroform

4.03



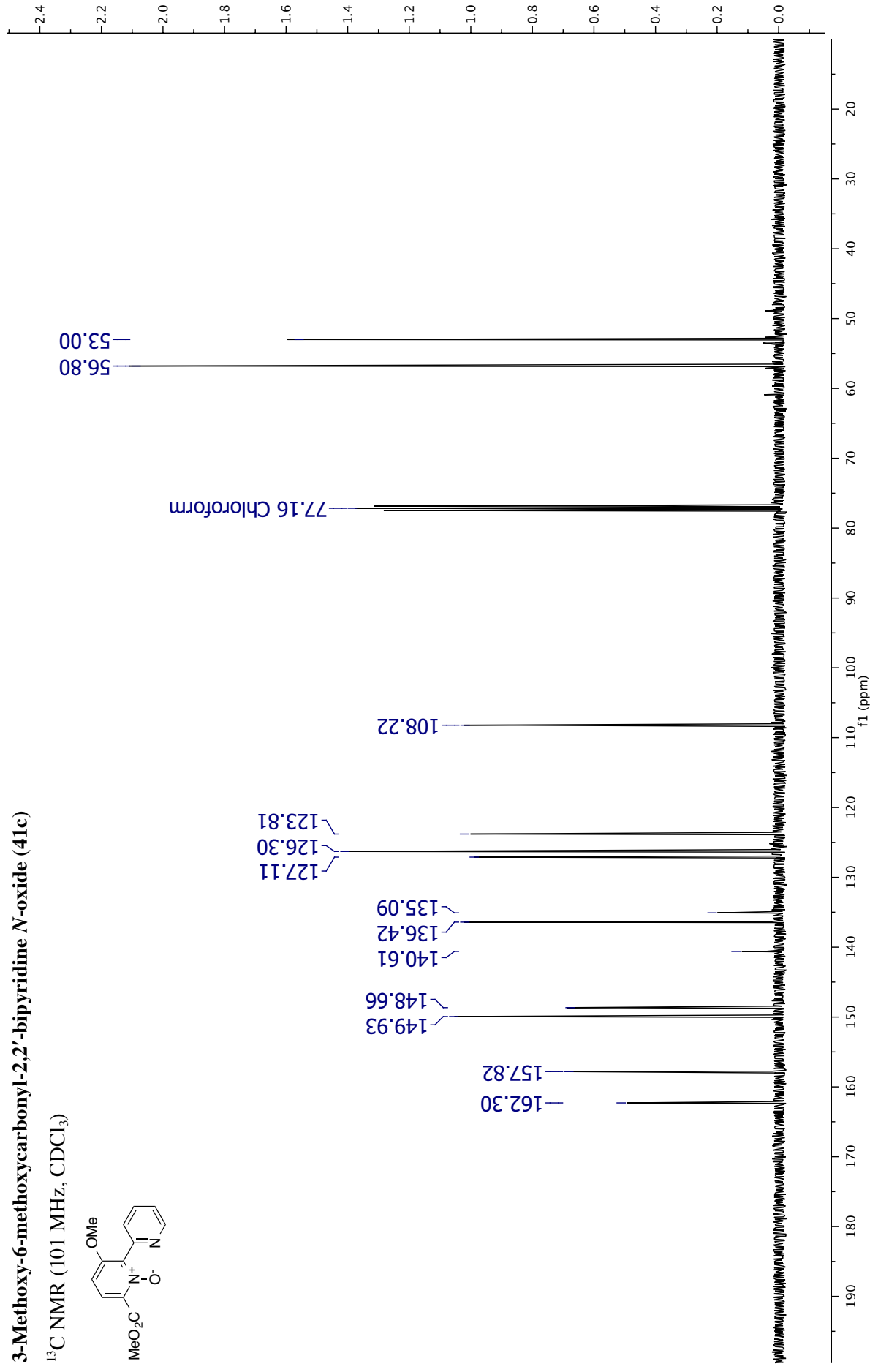
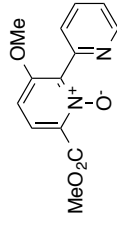
3-Methoxy-6-methoxycarbonyl-2,2'-bipyridine N-oxide (41c)

¹H NMR (400 MHz, CDCl₃)



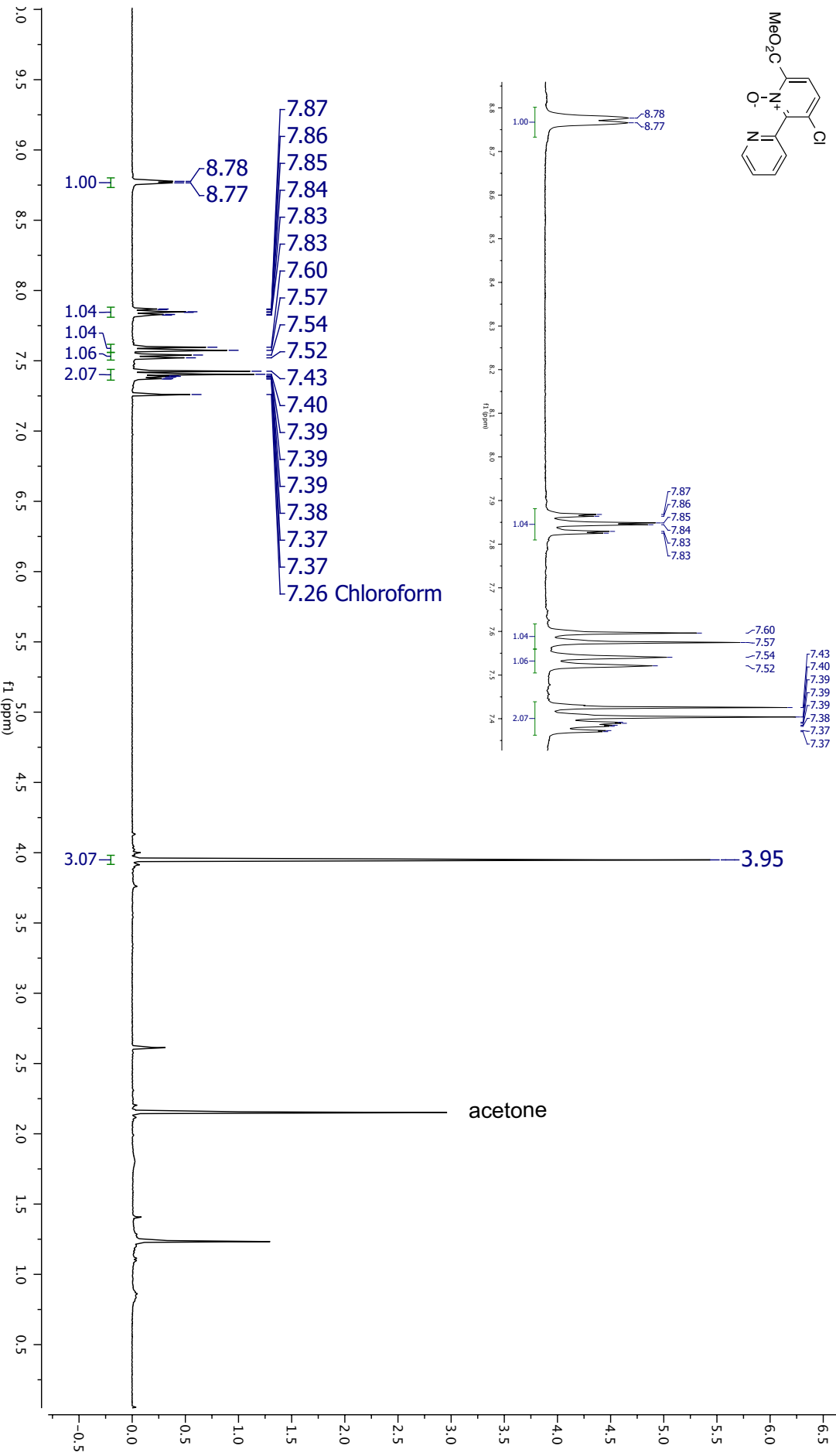
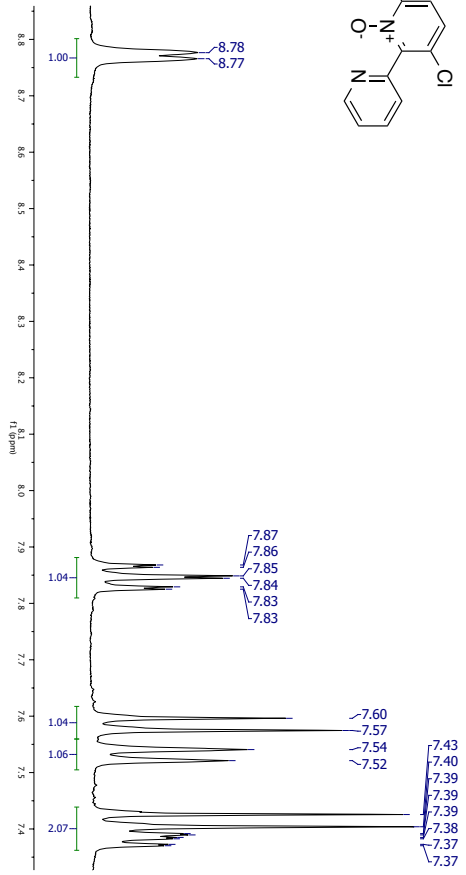
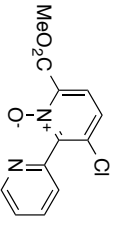
3-Methoxy-6-methoxycarbonyl-2,2'-bipyridine N-oxide (41c)

¹³C NMR (101 MHz, CDCl₃)



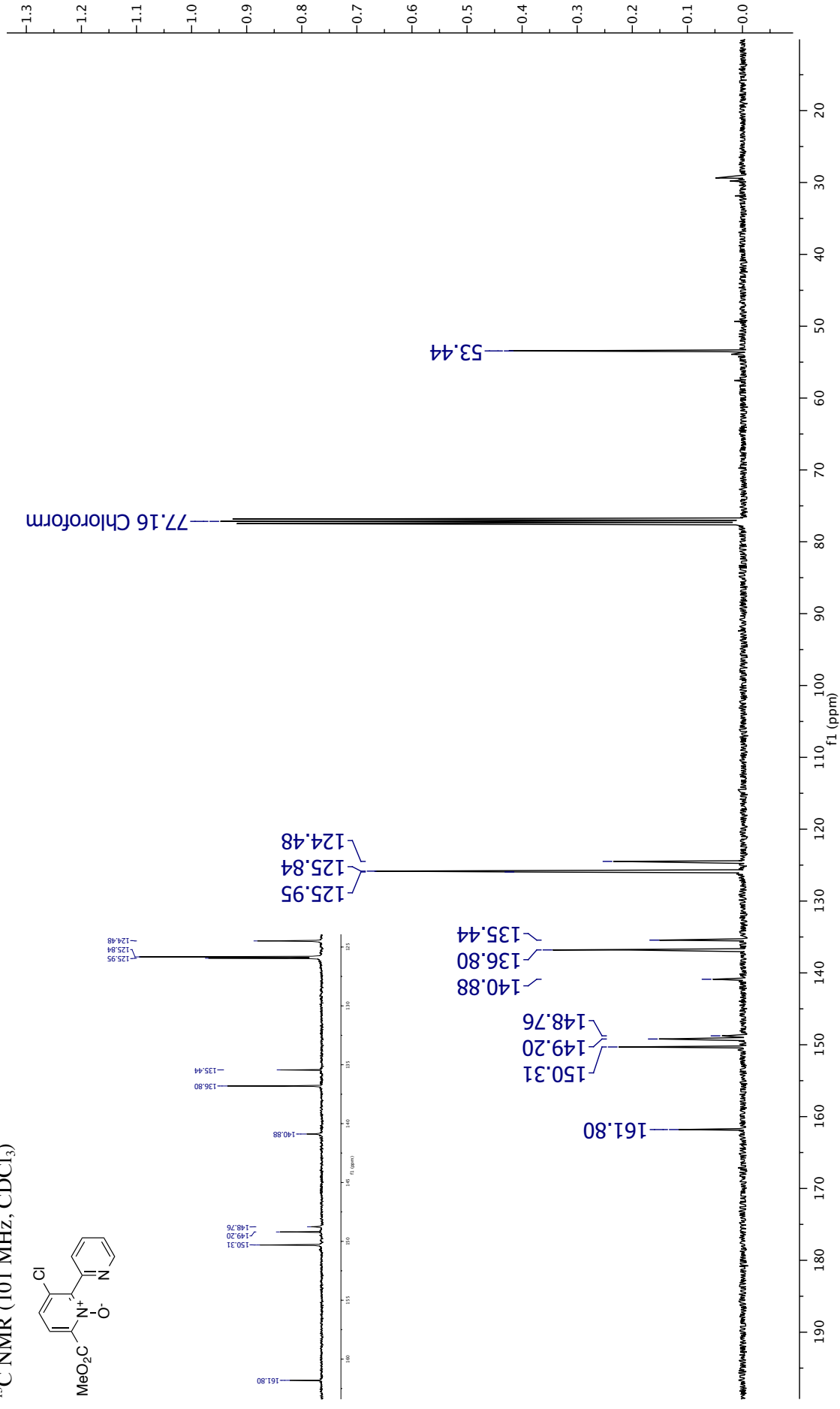
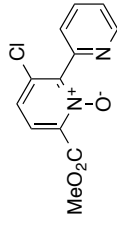
3-Chloro-6-methoxycarbonyl-2,2'-bipyridine N-oxide

¹H NMR (400 MHz, CDCl₃)



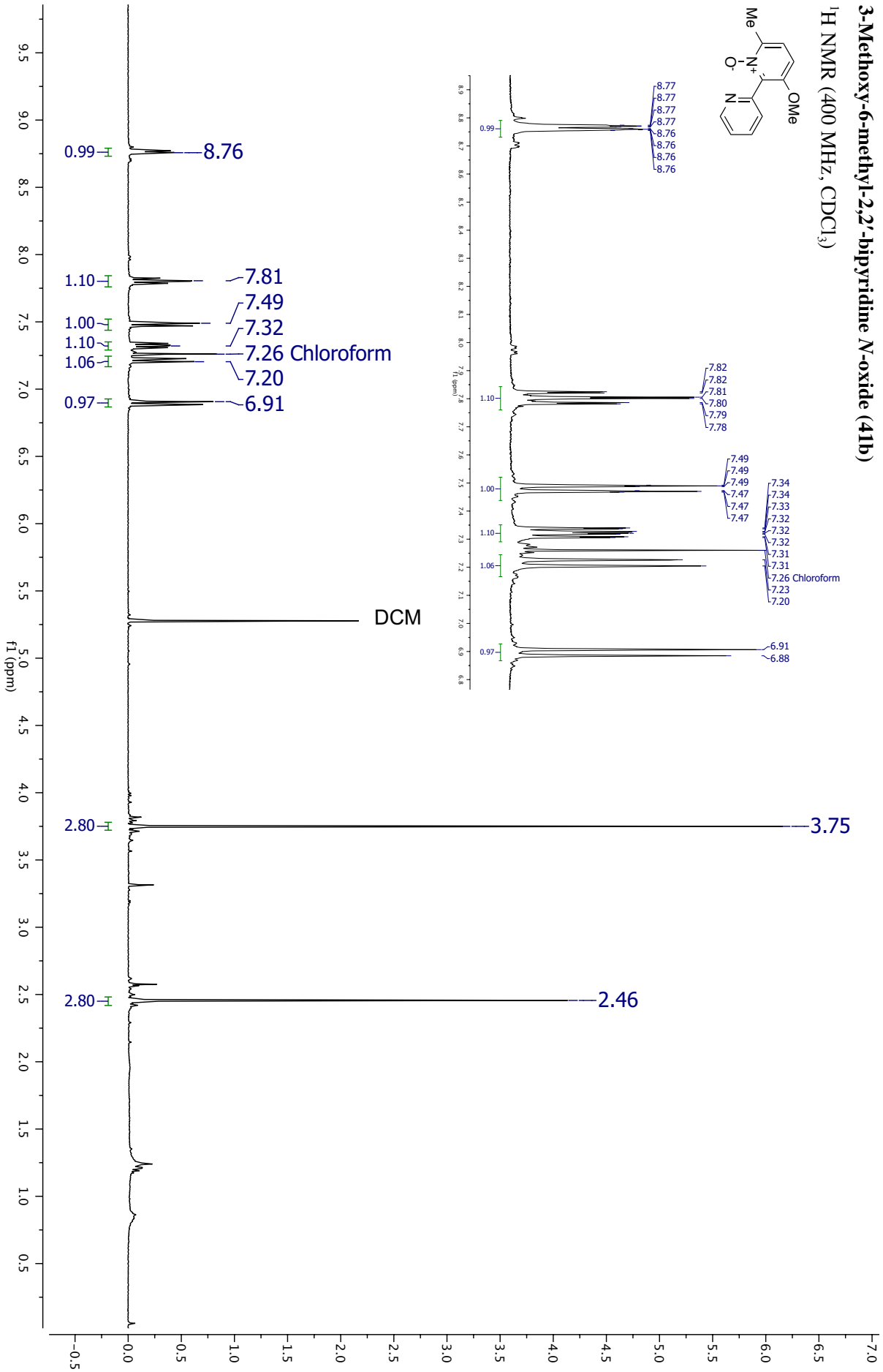
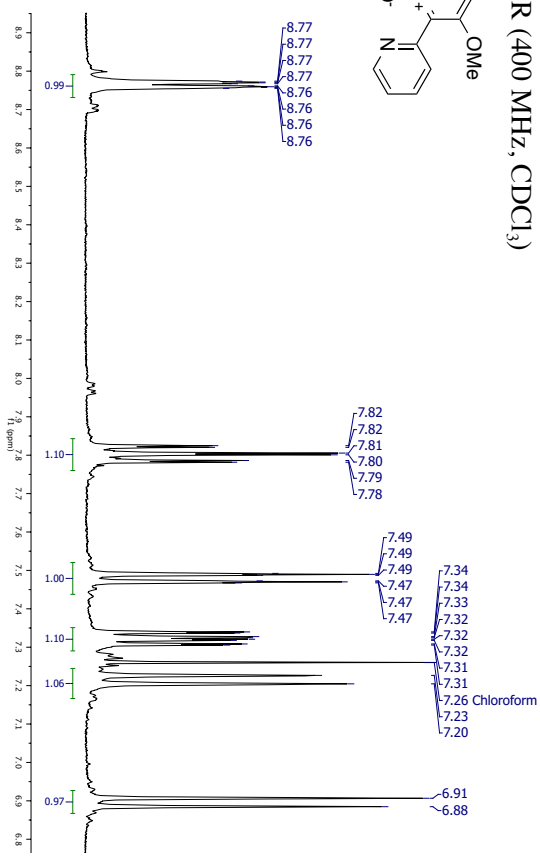
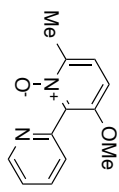
3-Chloro-6-methoxycarbonyl-2,2'-bipyridine *N*-oxide

^{13}C NMR (101 MHz, CDCl_3)



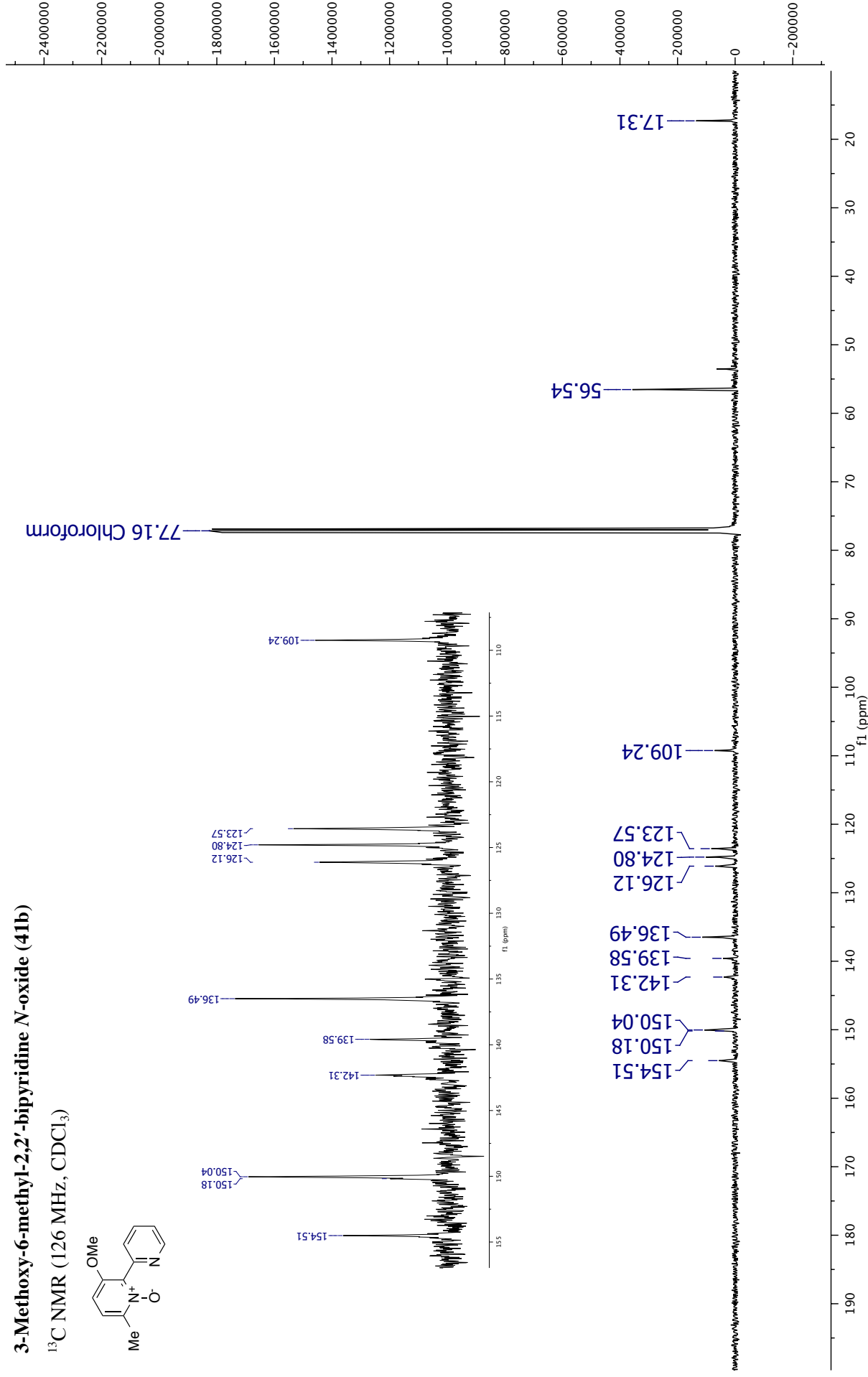
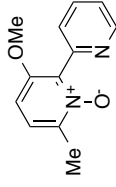
3-Methoxy-6-methyl-2,2'-bipyridine N-oxide (41b)

¹H NMR (400 MHz, CDCl₃)



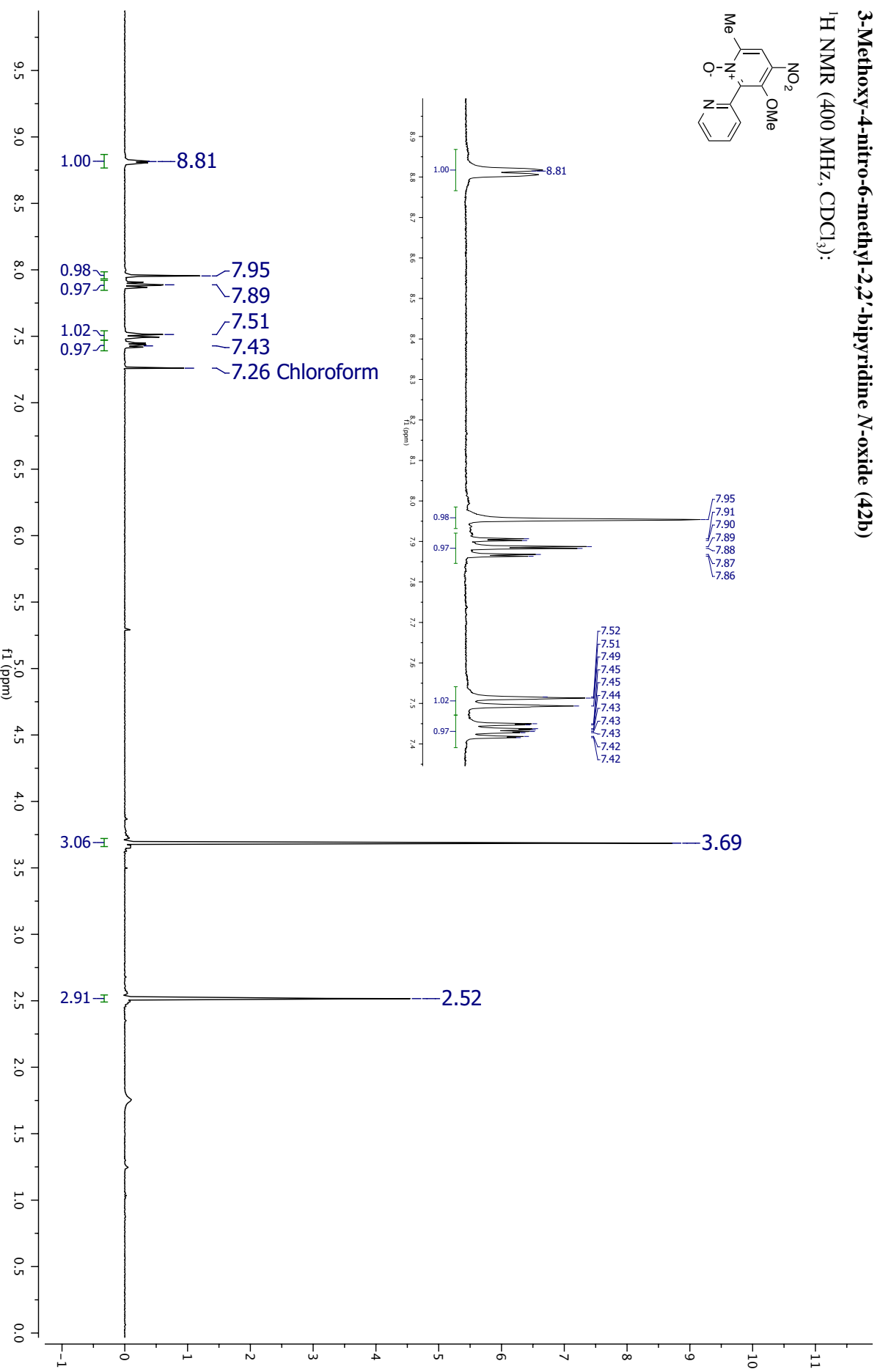
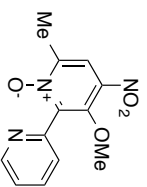
3-Methoxy-6-methyl-2,2'-bipyridine N-oxide (41b)

¹³C NMR (126 MHz, CDCl₃)



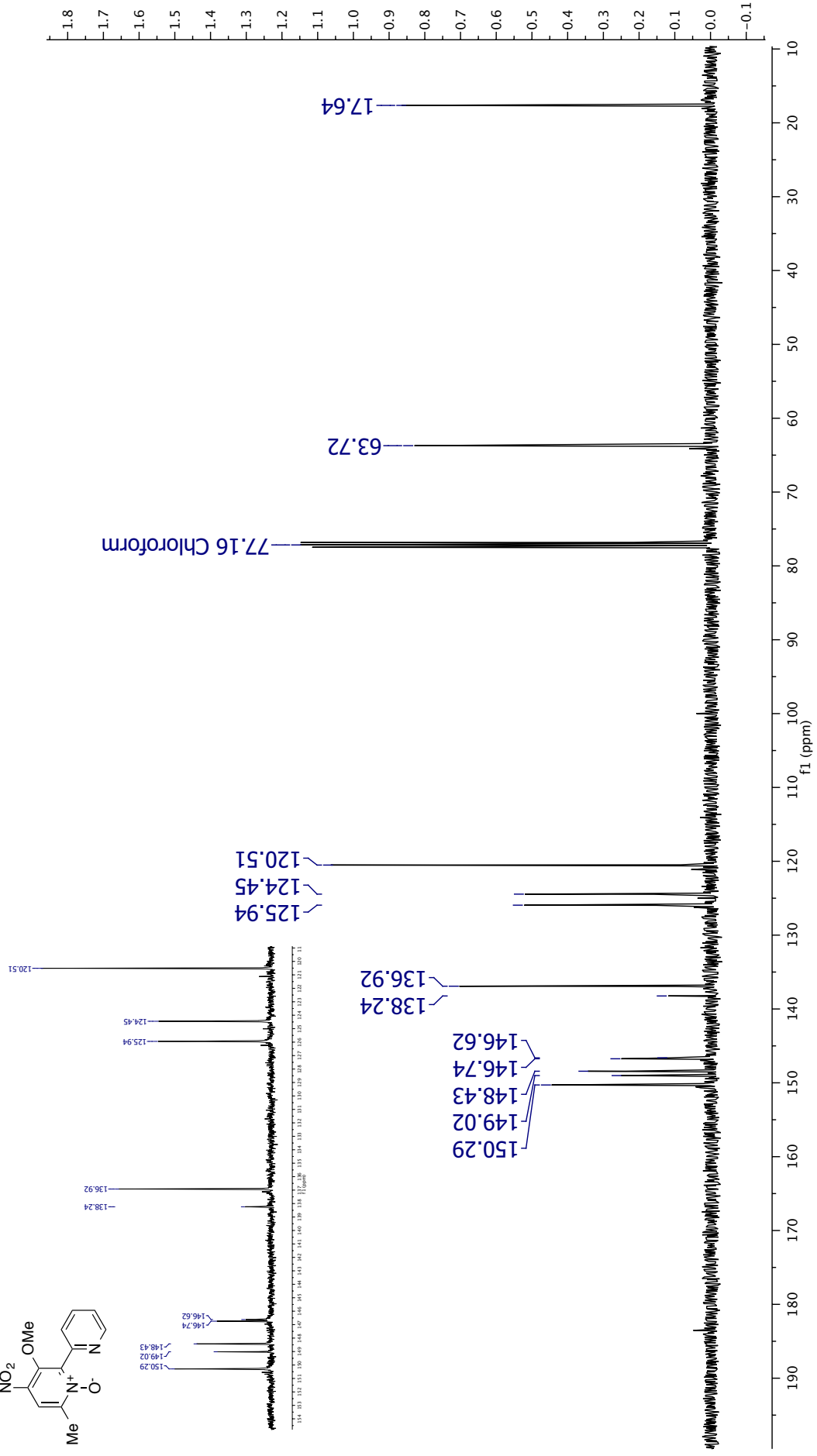
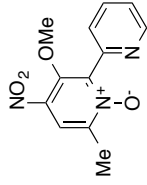
3-Methoxy-4-nitro-6-methyl-2,2'-bipyridine N-oxide (42b)

¹H NMR (400 MHz, CDCl₃):



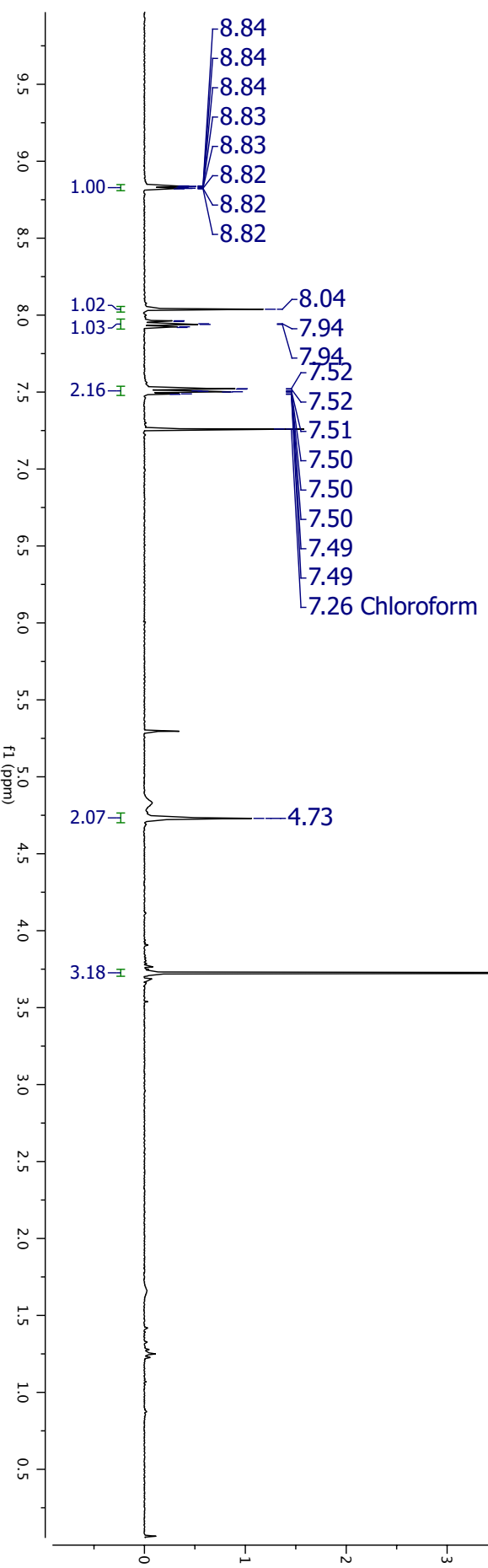
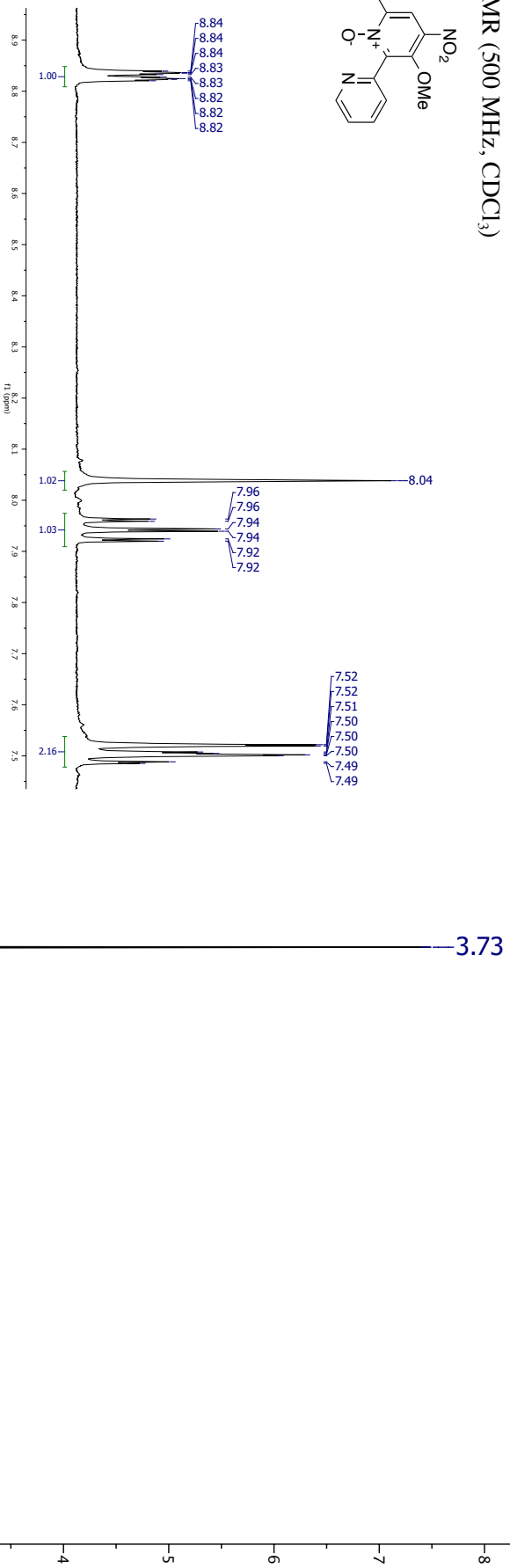
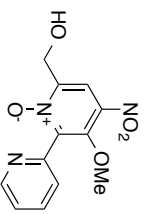
3-Methoxy-4-nitro-6-methyl-2,2'-bipyridine N-oxide (42b)

¹³C NMR (126 MHz, CDCl₃)



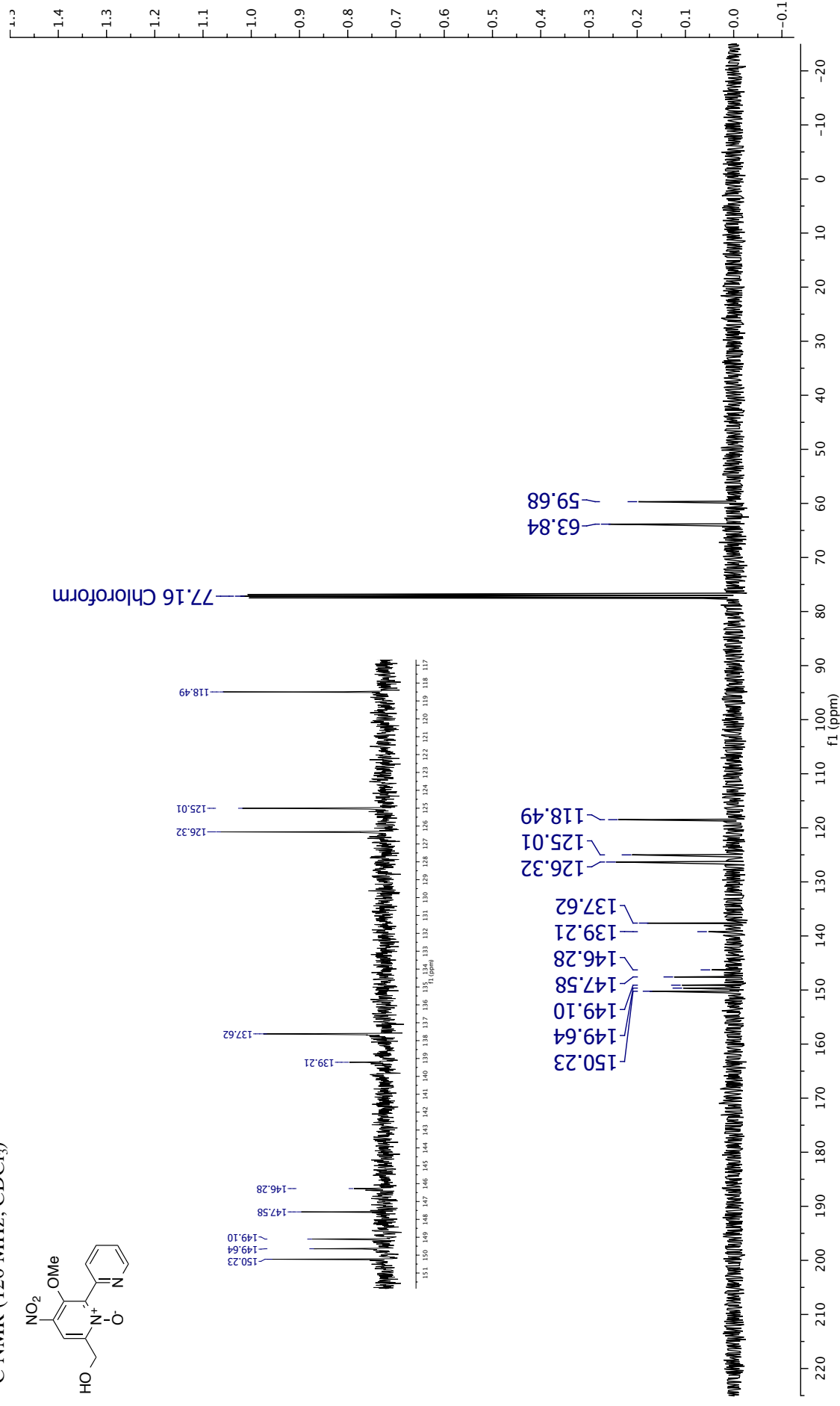
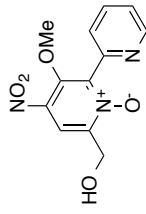
3-Methoxy-4-nitro-6-hydroxymethyl-2,2'-bipyridine N-oxide (45)

¹H NMR (500 MHz, CDCl₃)



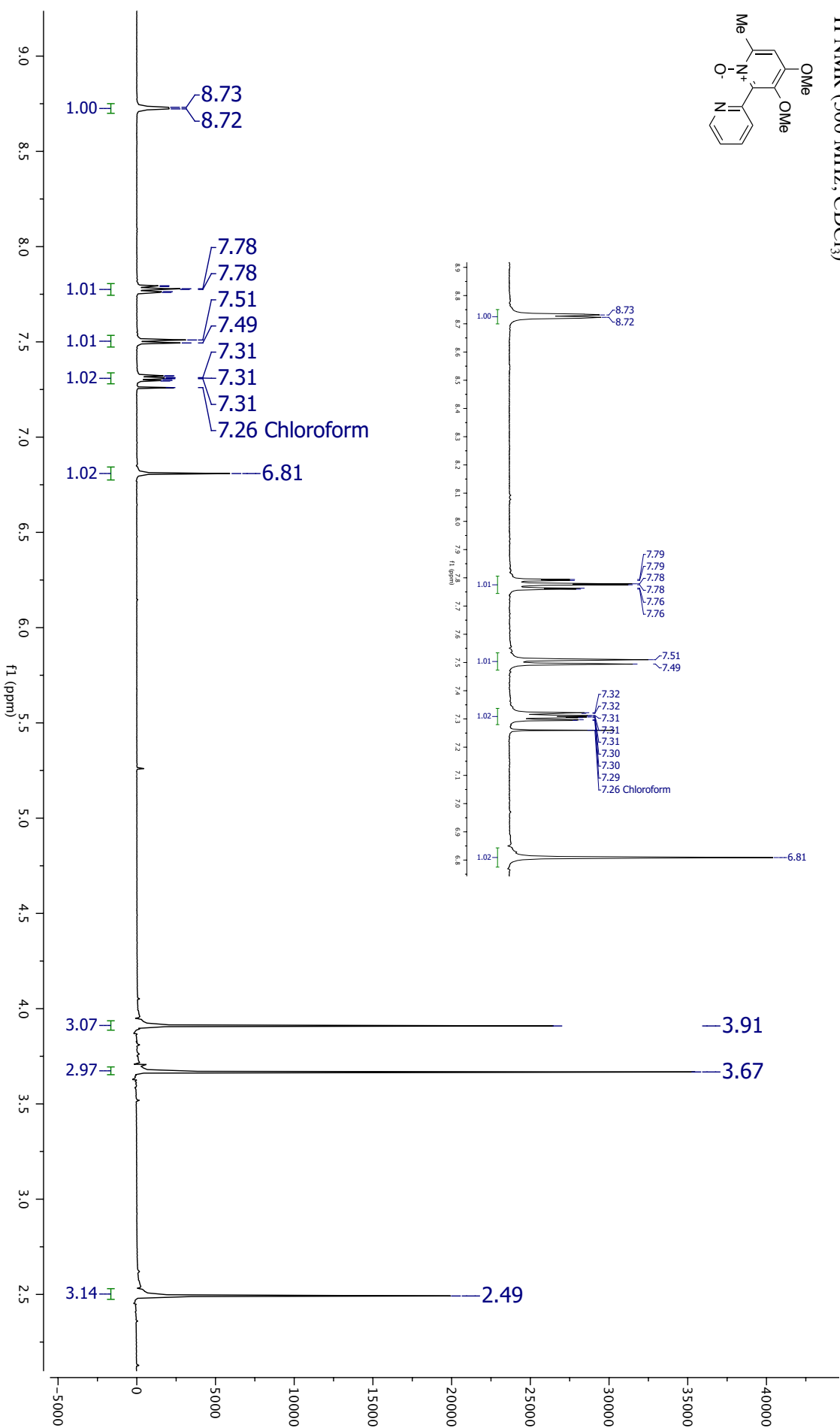
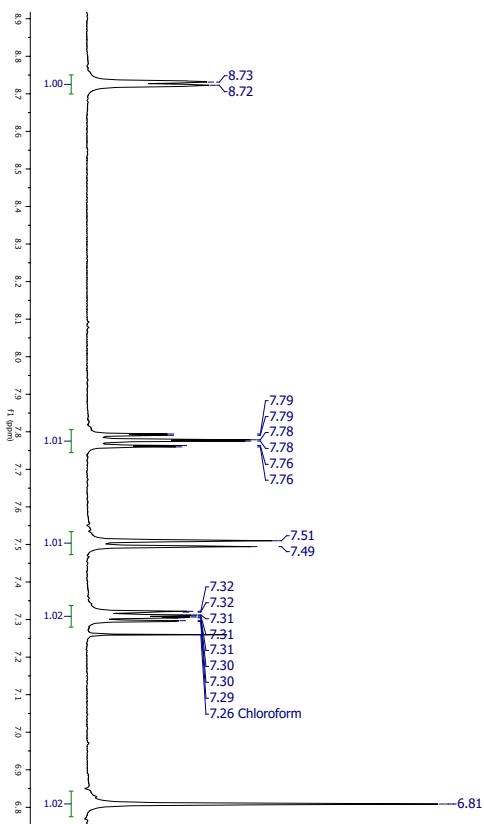
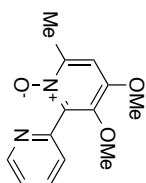
3-Methoxy-4-nitro-6-hydroxymethyl-2,2'-bipyridine N-oxide (45)

^{13}C NMR (126 MHz, CDCl_3)



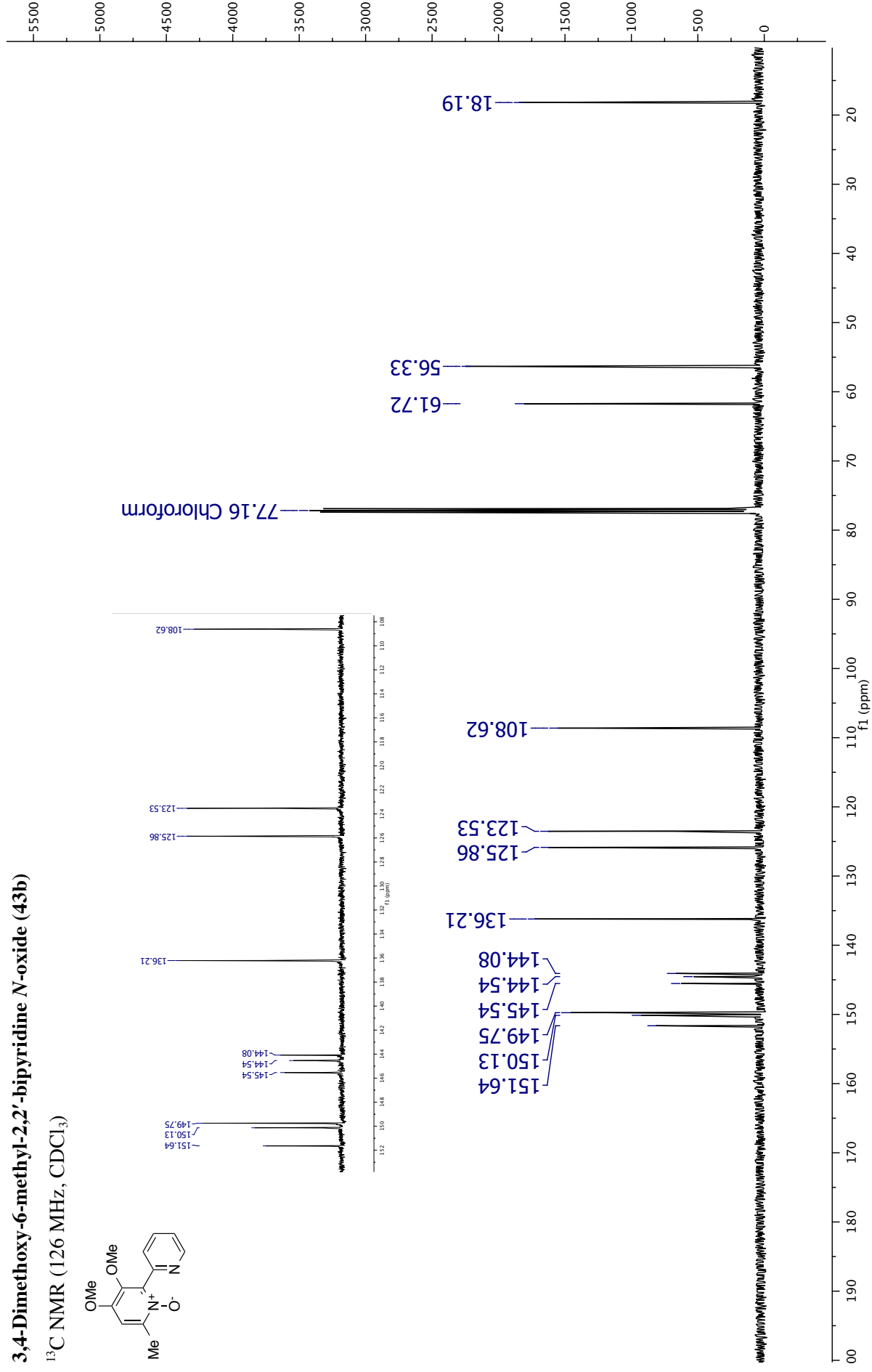
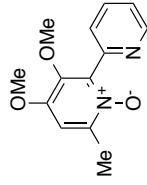
3,4-Dimethoxy-6-methyl-2,2'-bipyridine N-oxide (43b)

¹H NMR (500 MHz, CDCl₃)



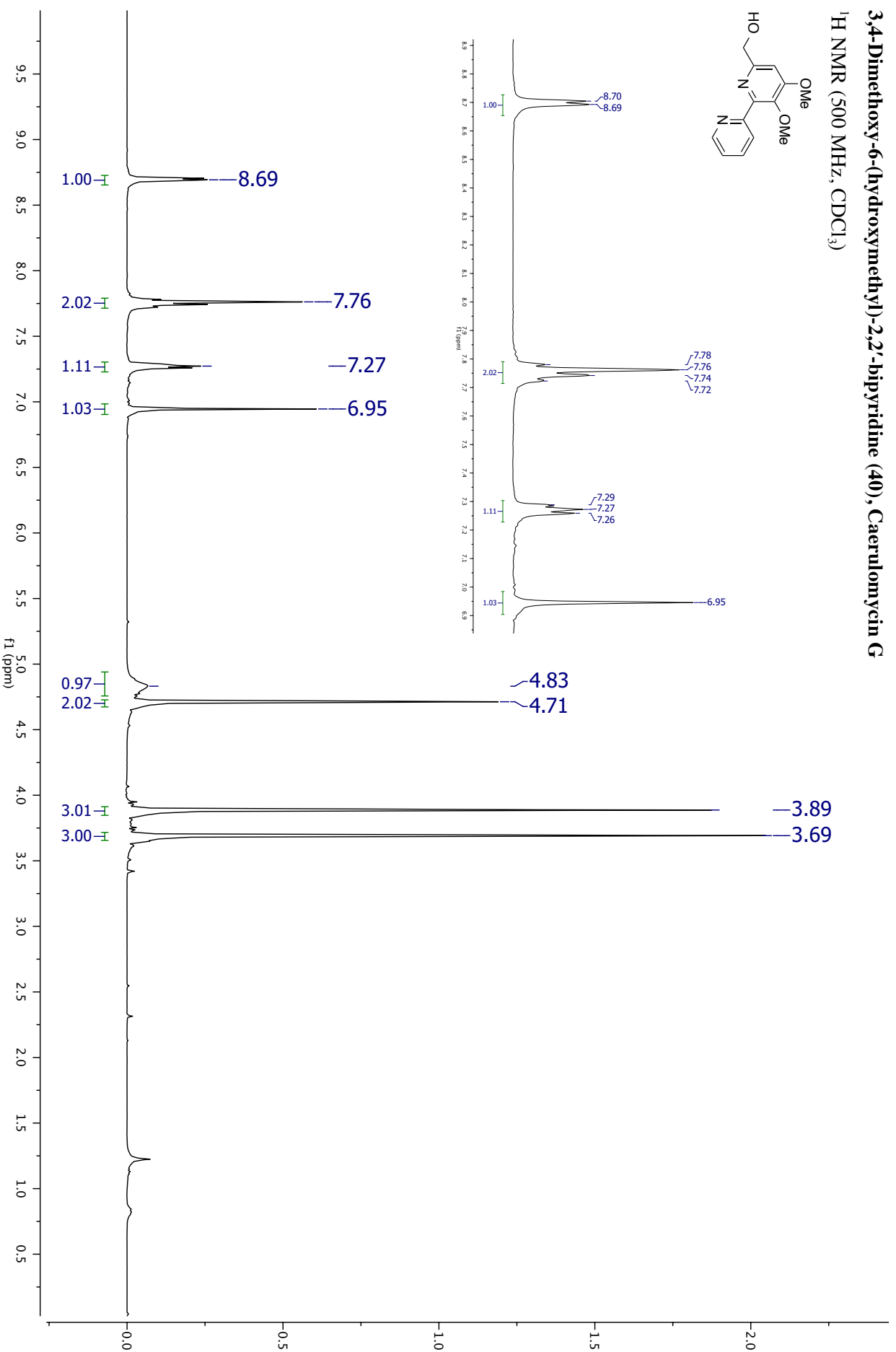
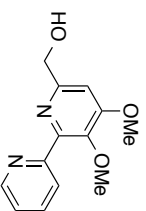
3,4-Dimethoxy-6-methyl-2,2'-bipyridine N-oxide (43b)

^{13}C NMR (126 MHz, CDCl_3)



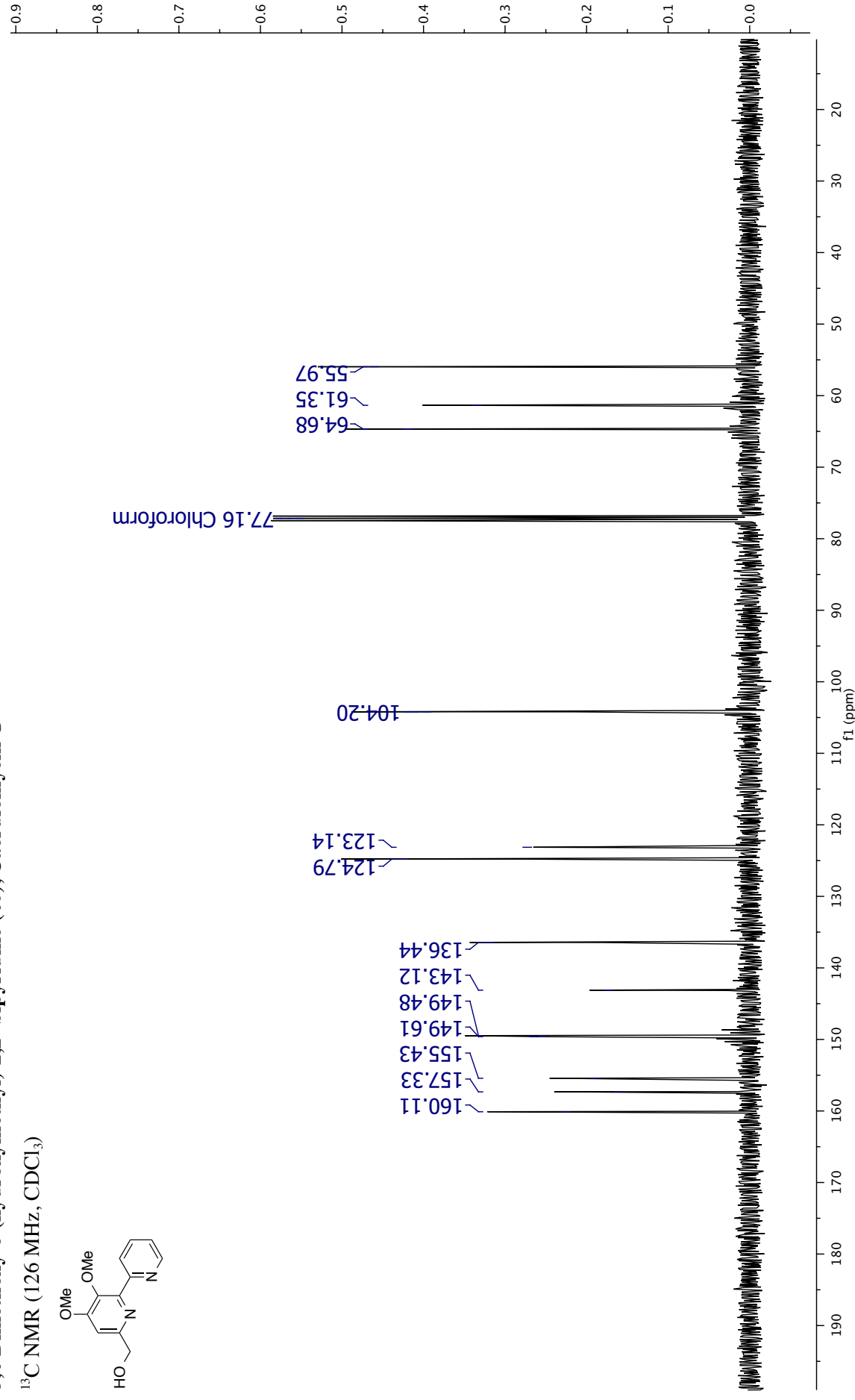
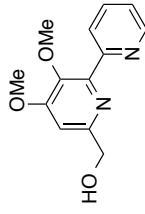
3,4-Dimethoxy-6-(hydroxymethyl)-2,2'-bipyridine (40), Caerulomycin G

¹H NMR (500 MHz, CDCl₃)



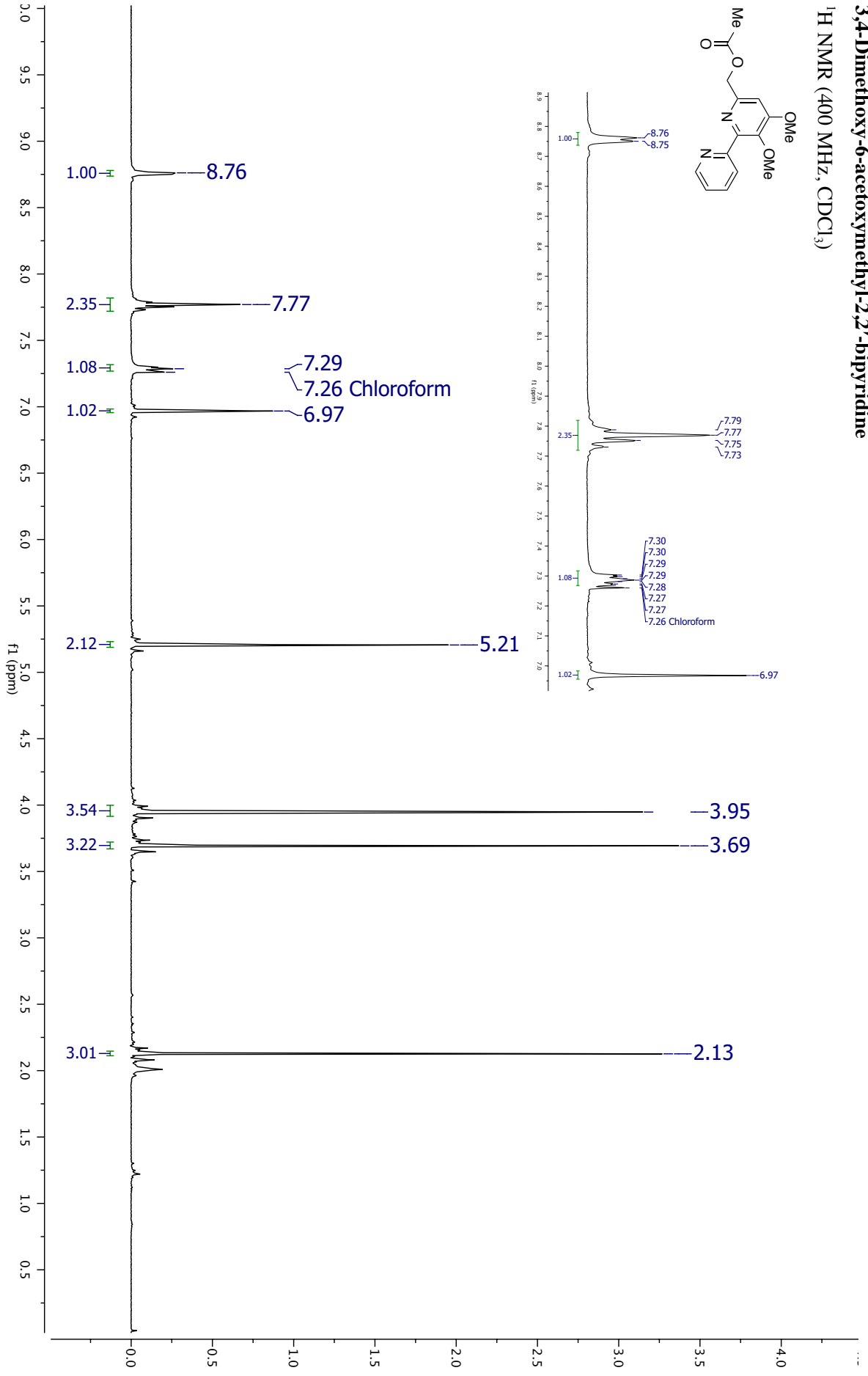
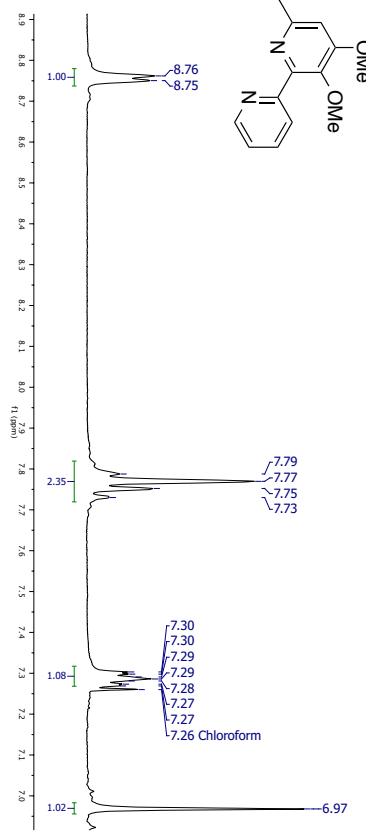
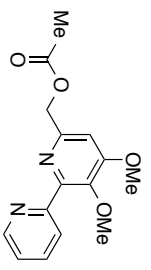
3,4-Dimethoxy-6-(hydroxymethyl)-2,2'-bipyridine (40), Caerulomycin G

¹³C NMR (126 MHz, CDCl₃)



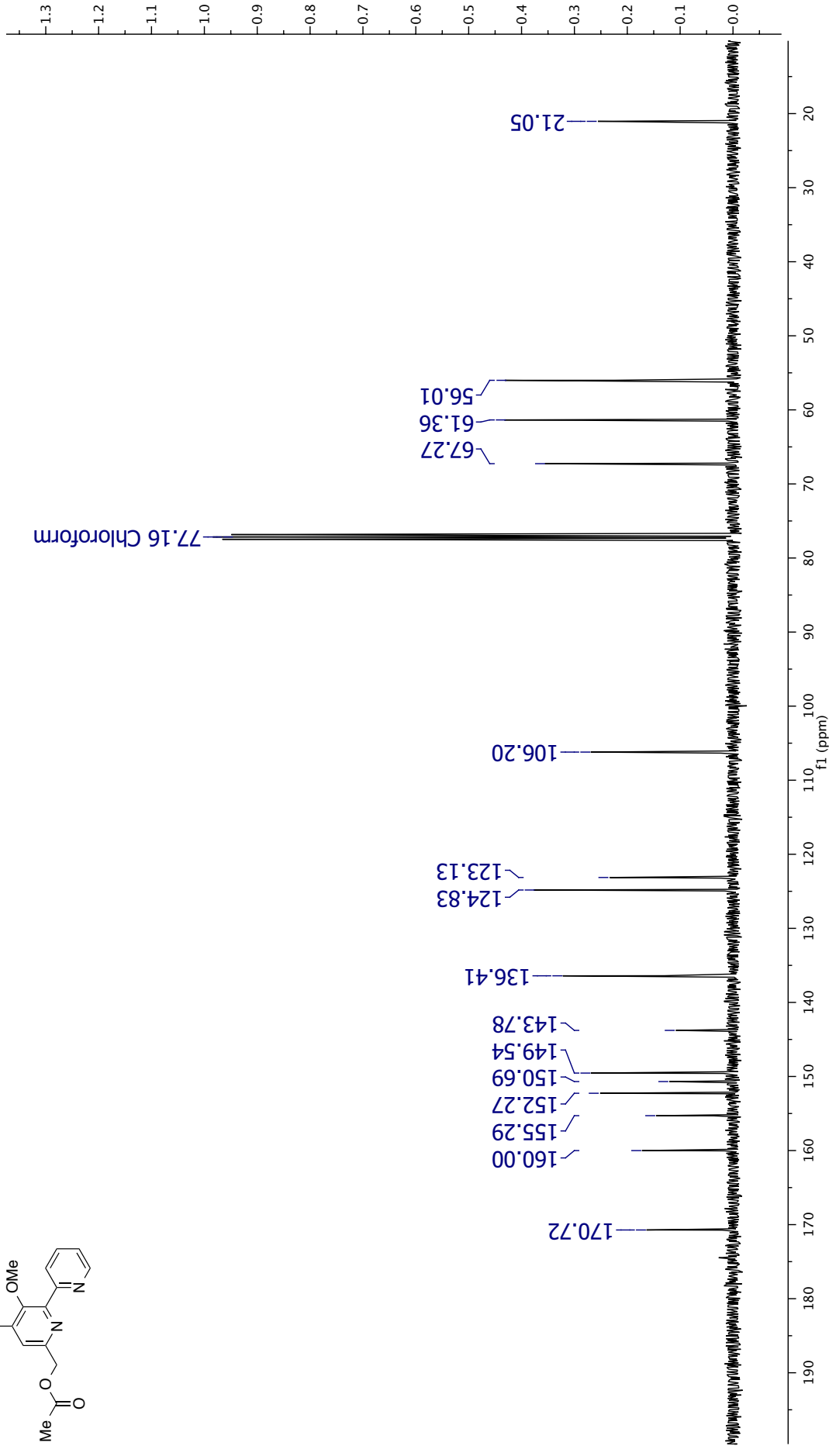
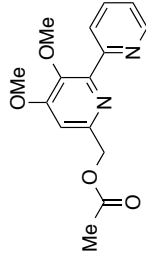
3,4-Dimethoxy-6-acetoxymethyl-2,2'-bipyridine

¹H NMR (400 MHz, CDCl₃)



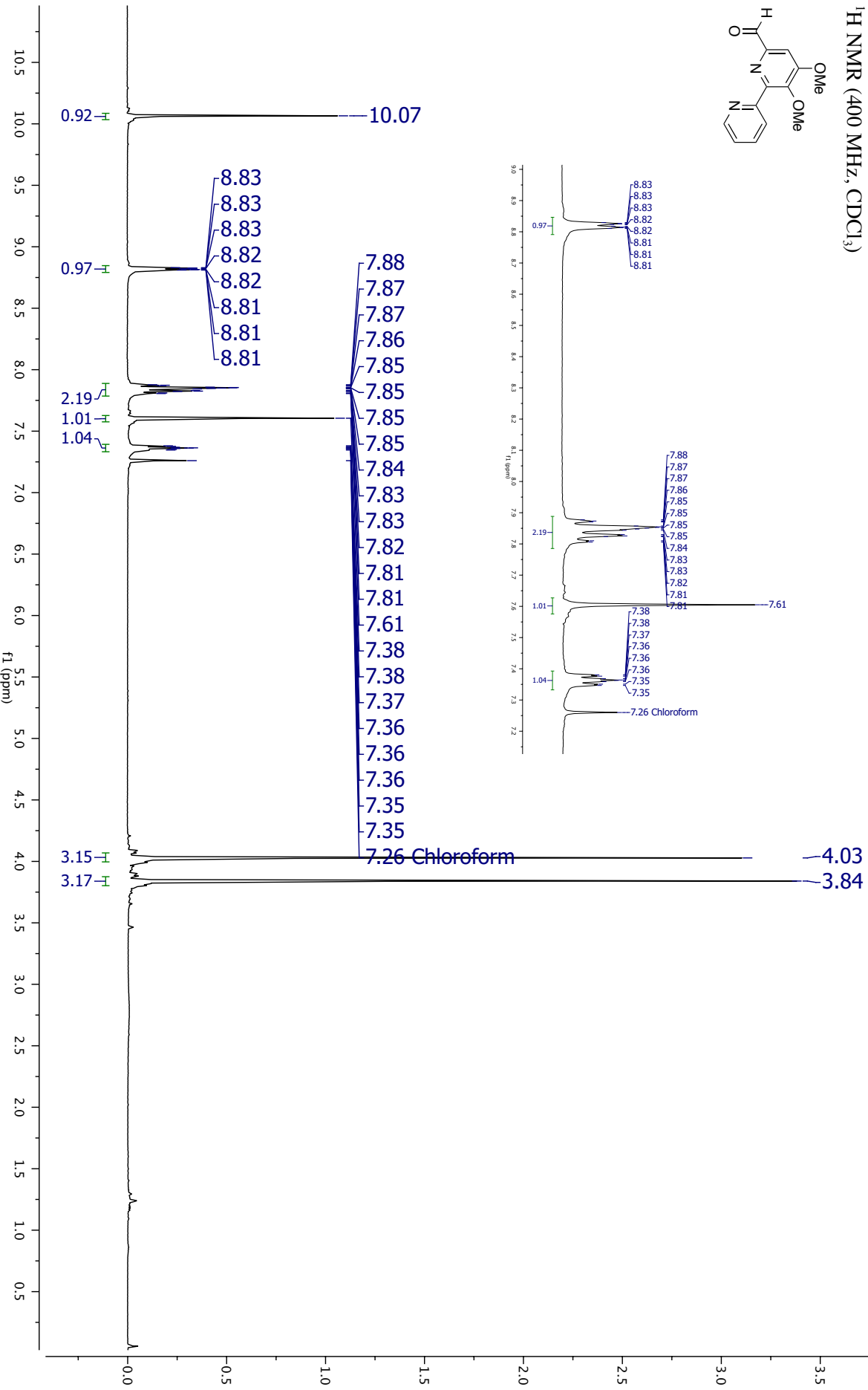
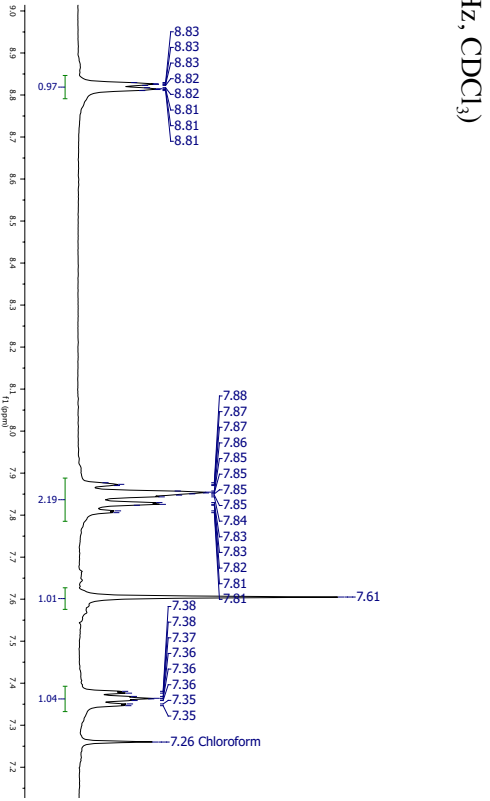
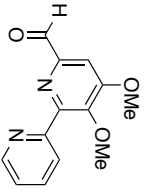
3,4-Dimethoxy-6-acetoxymethyl-2,2'-bipyridine

¹³C NMR (101 MHz, CDCl₃)



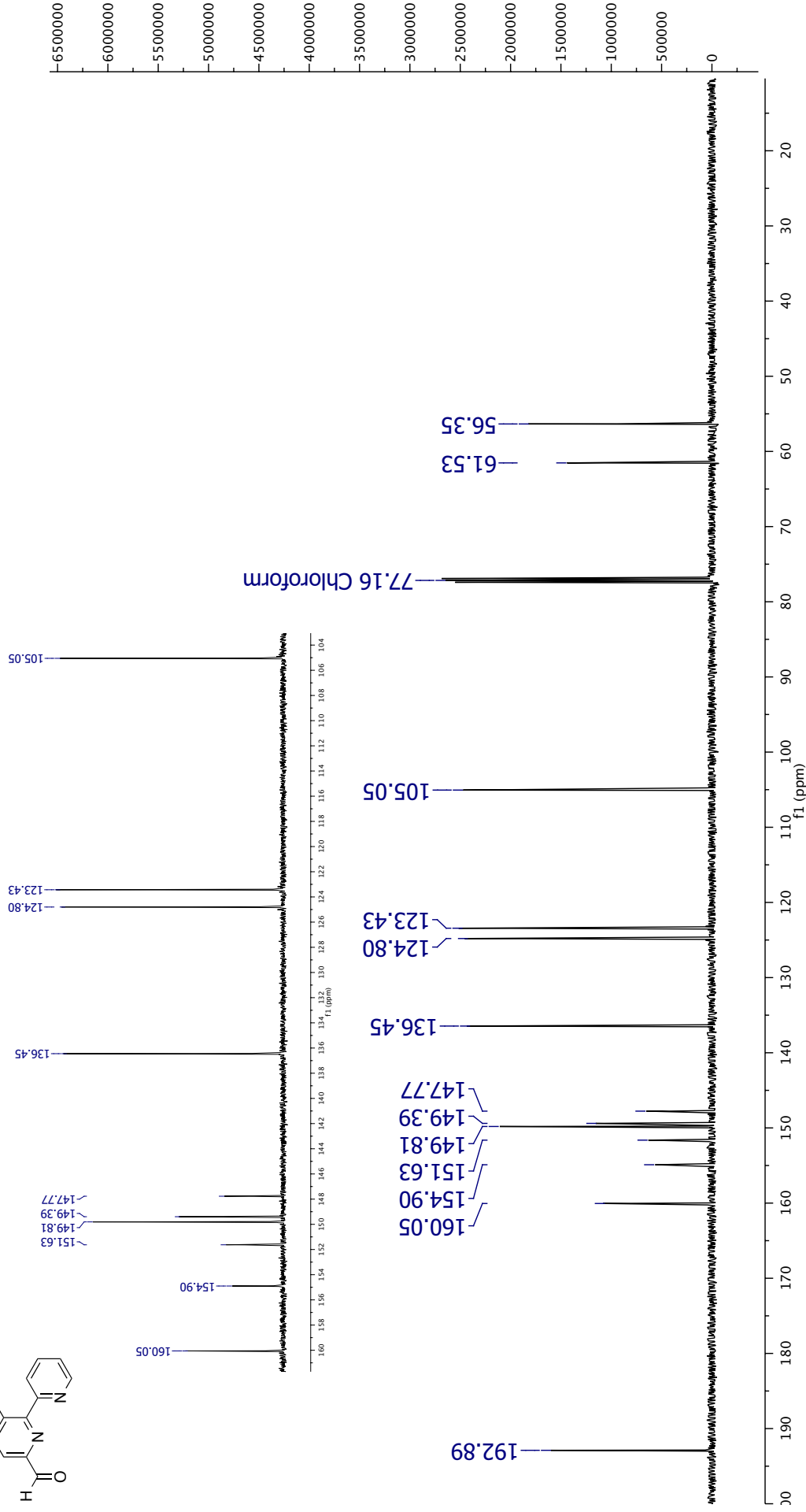
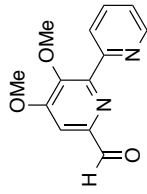
3,4-Dimethoxy-2,2'-bipyridine-6-carboxaldehyde (46)

¹H NMR (400 MHz, CDCl₃)



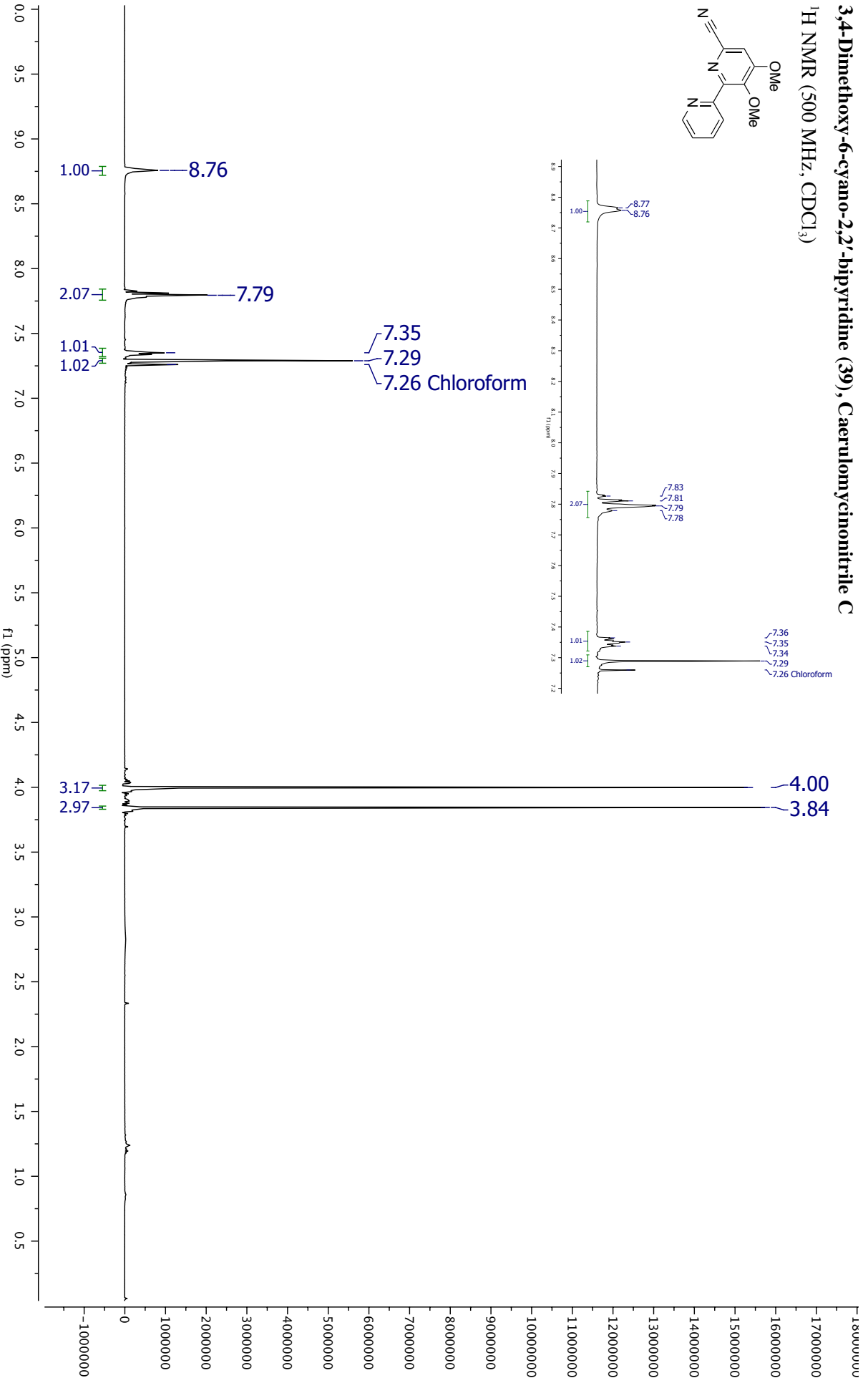
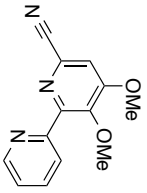
3,4-Dimethoxy-2,2'-bipyridine-6-carboxaldehyde (46)

^{13}C NMR (126 MHz, CDCl_3)



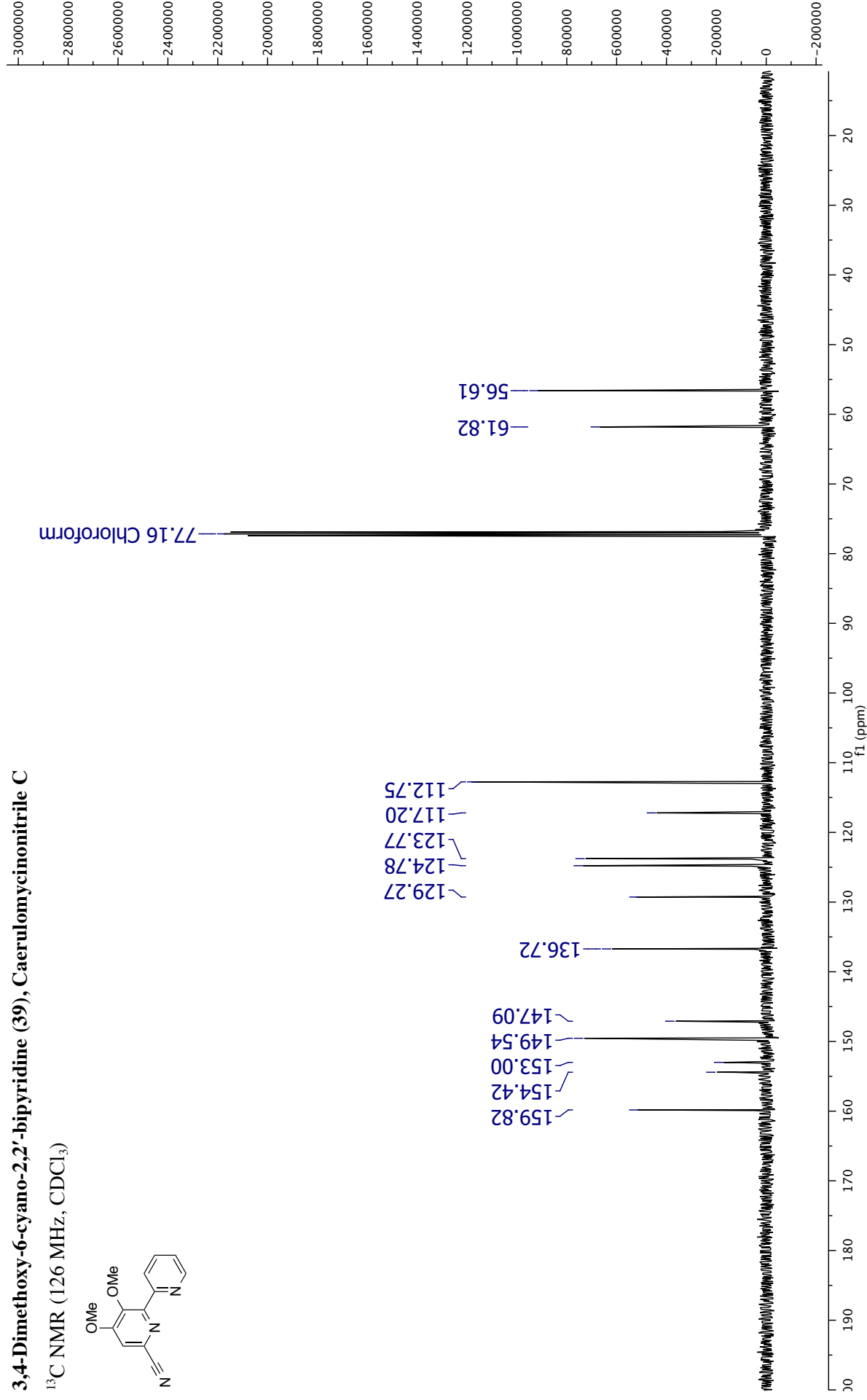
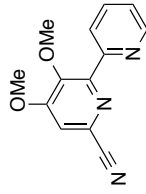
3,4-Dimethoxy-6-cyano-2,2'-bipyridine (39), Caerulomycin nitrile C

¹H NMR (500 MHz, CDCl₃)



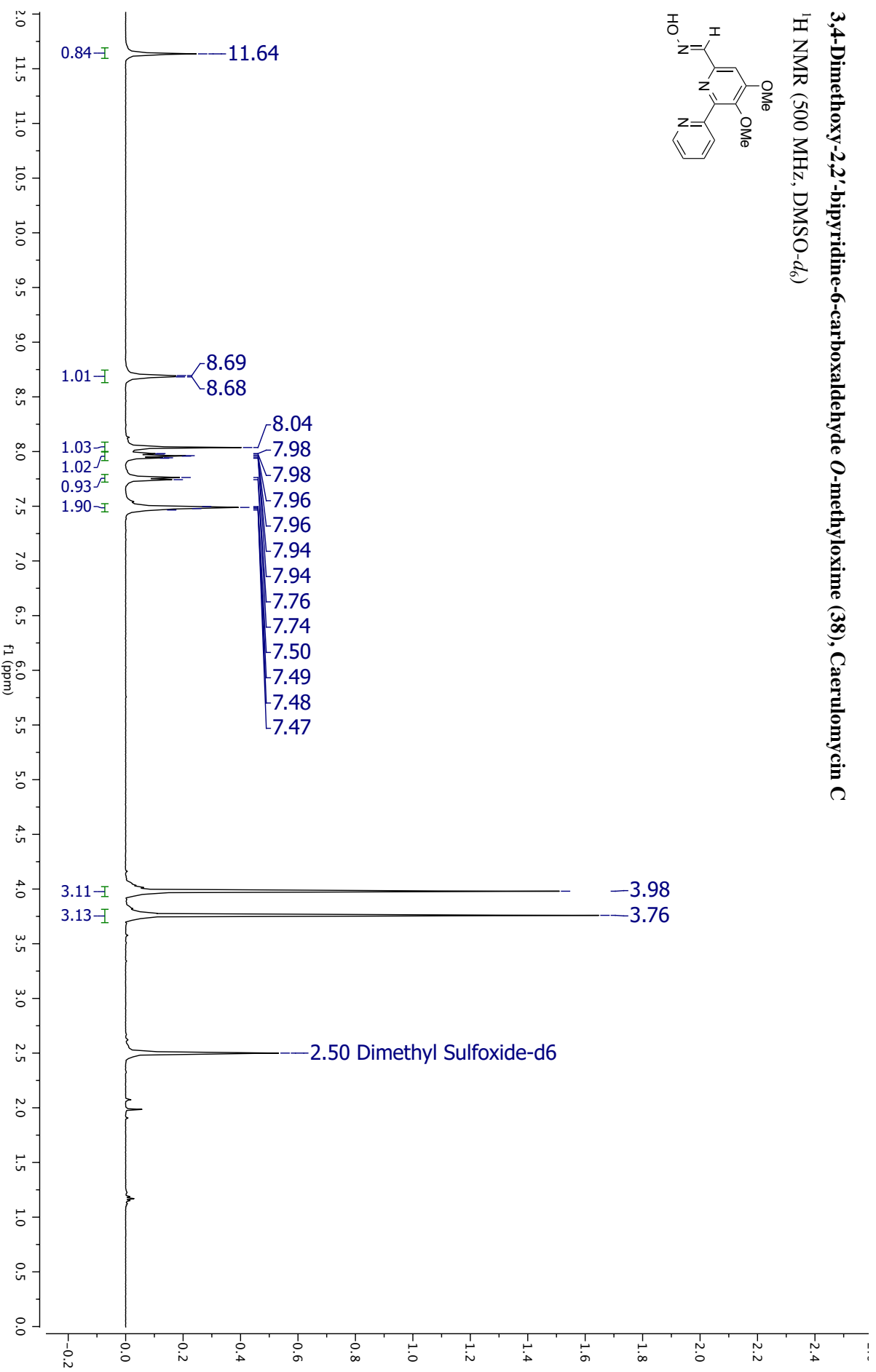
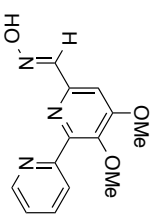
3,4-Dimethoxy-6-cyano-2,2'-bipyridine (39), Caerulomycinonitrile C

^{13}C NMR (126 MHz, CDCl_3)



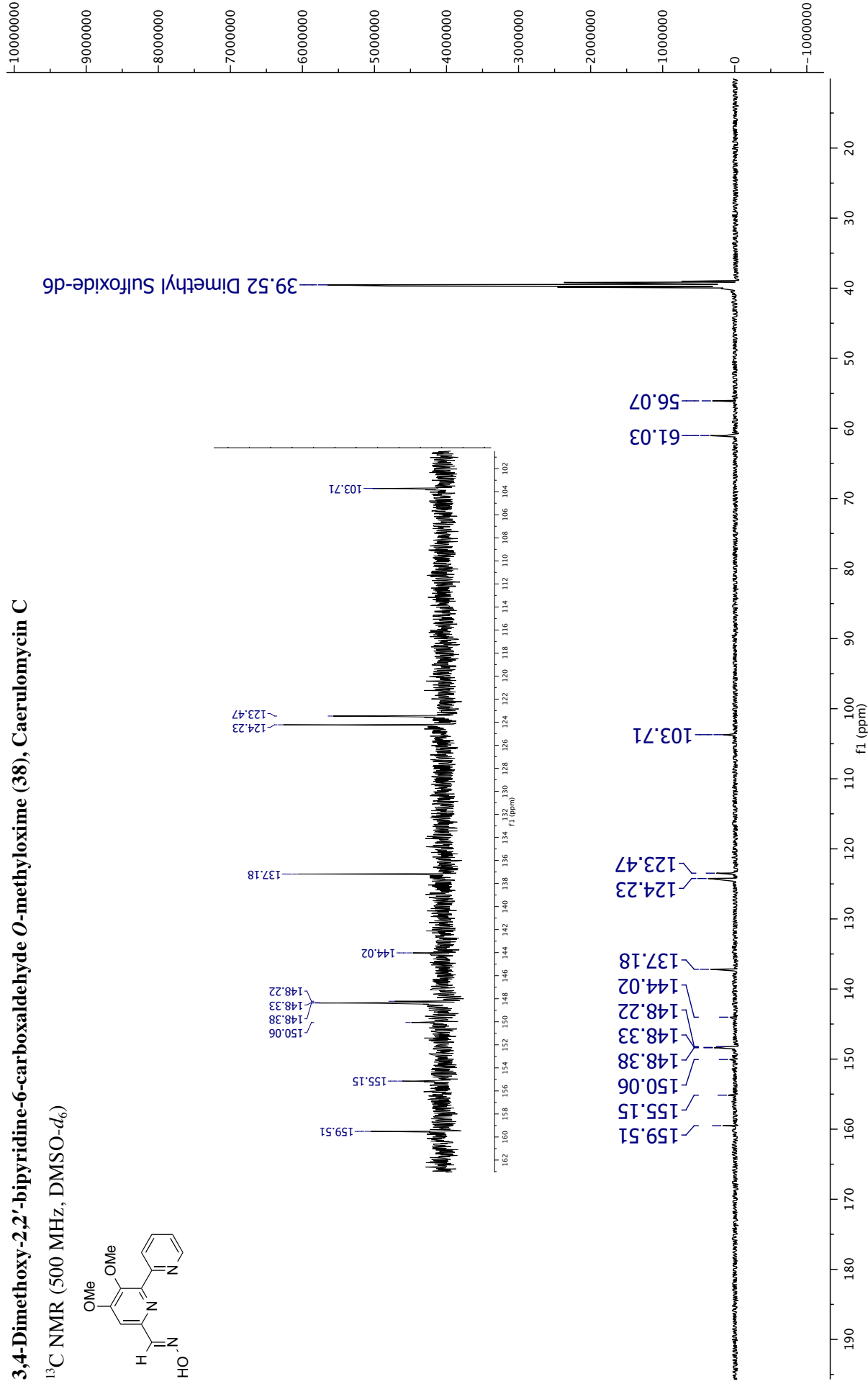
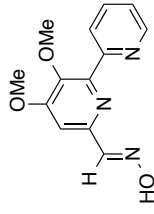
3,4-Dimethoxy-2,2'-bipyridine-6-carboxaldehyde *O*-methylloxime (38), Caerulomycin C

¹H NMR (500 MHz, DMSO-*d*₆)



3,4-Dimethoxy-2,2'-bipyridine-6-carboxaldehyde *O*-methylxime (38), Caerulomycin C

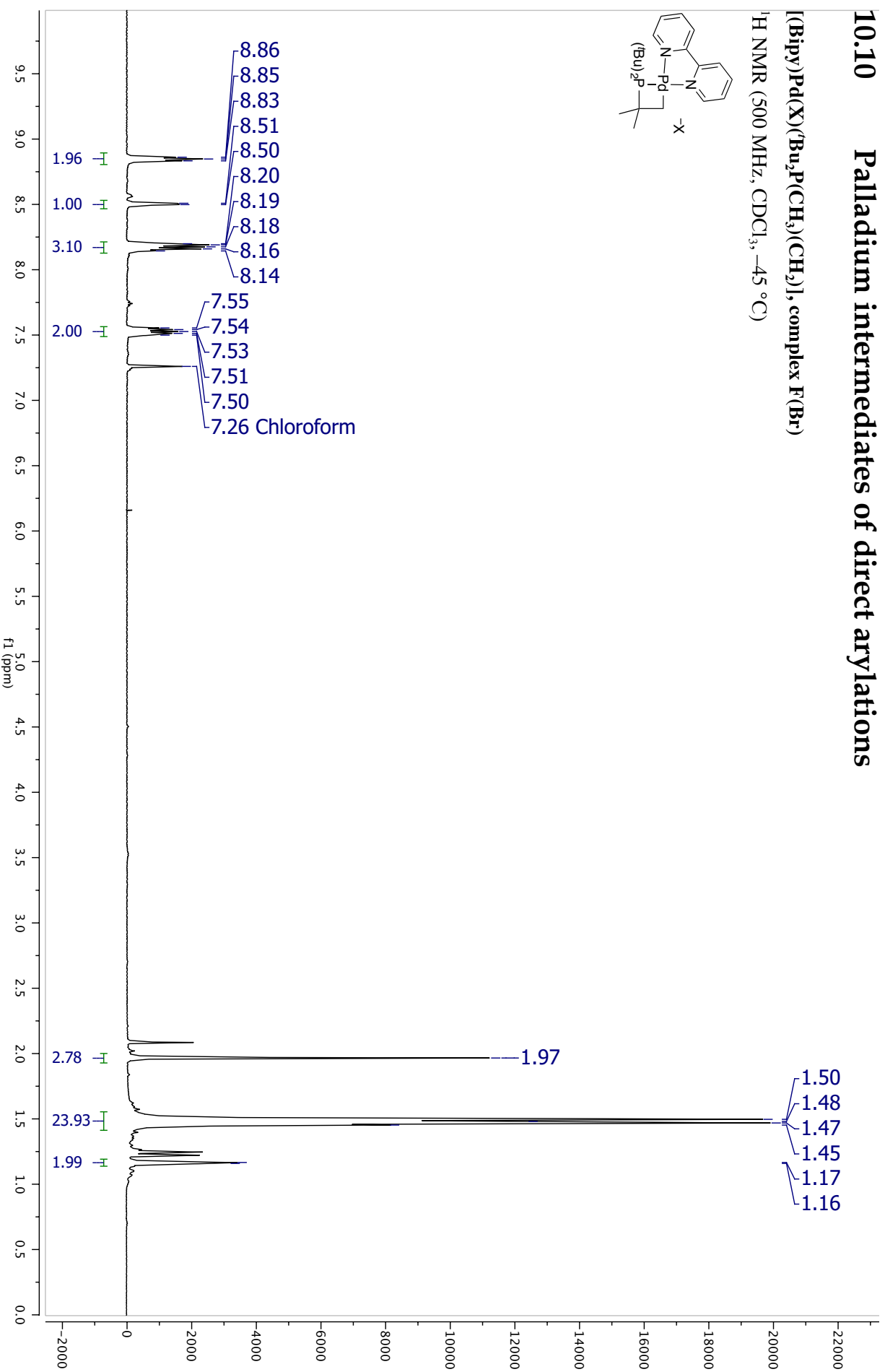
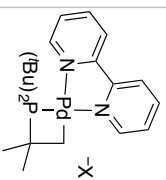
^{13}C NMR (500 MHz, $\text{DMSO-}d_6$)



10.10 Palladium intermediates of direct arylations

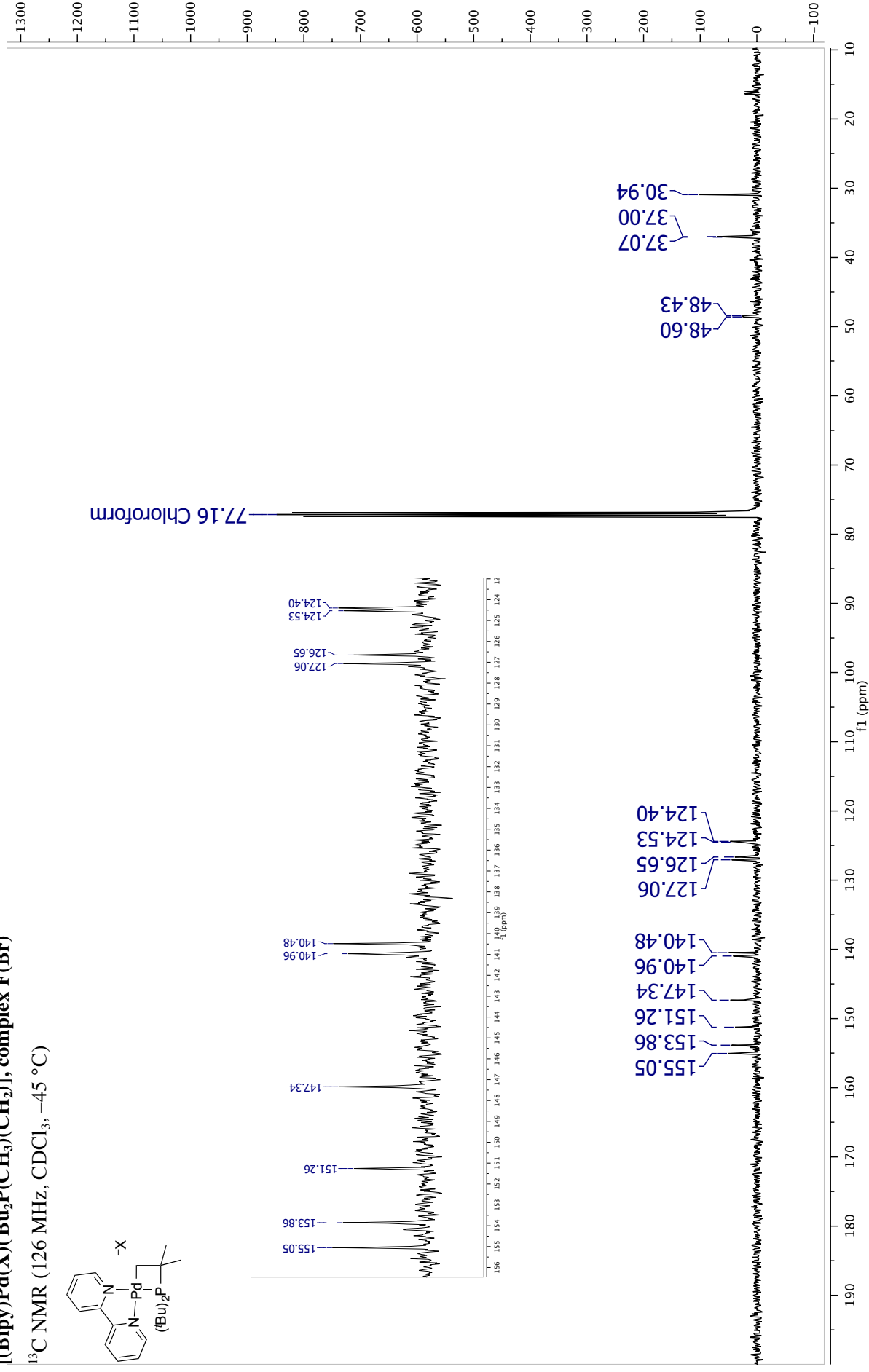
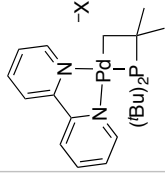
[Bipy]Pd(X)(^tBu₂P(CH₃)(CH₂)], complex F(Br)

¹H NMR (500 MHz, CDCl₃, -45 °C)



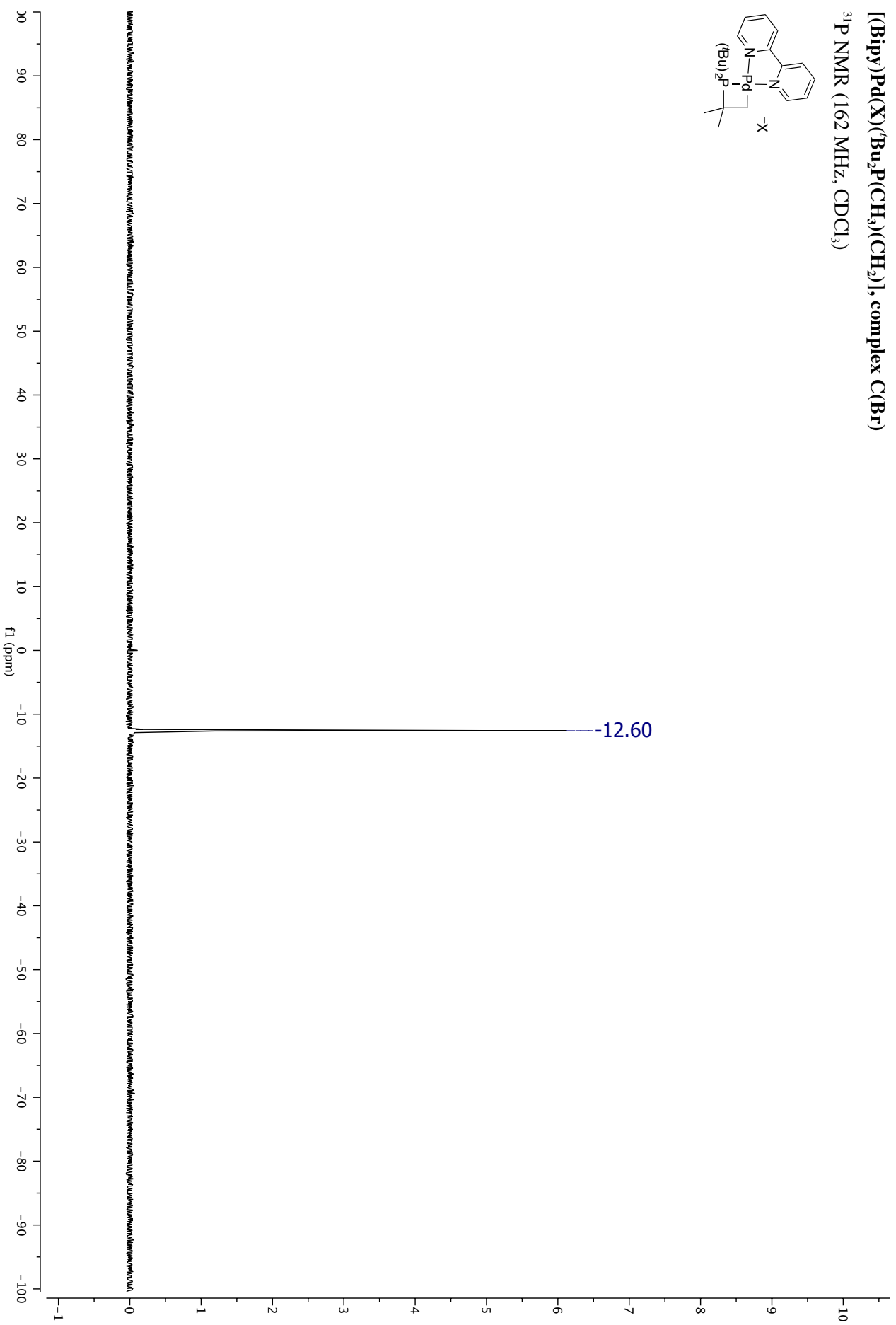
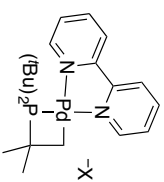
[(Bipy)Pd(X)(*t*-Bu₂P(CH₃)₂(CH₂)₂), complex F(Br)]

¹³C NMR (126 MHz, CDCl₃, -45 °C)



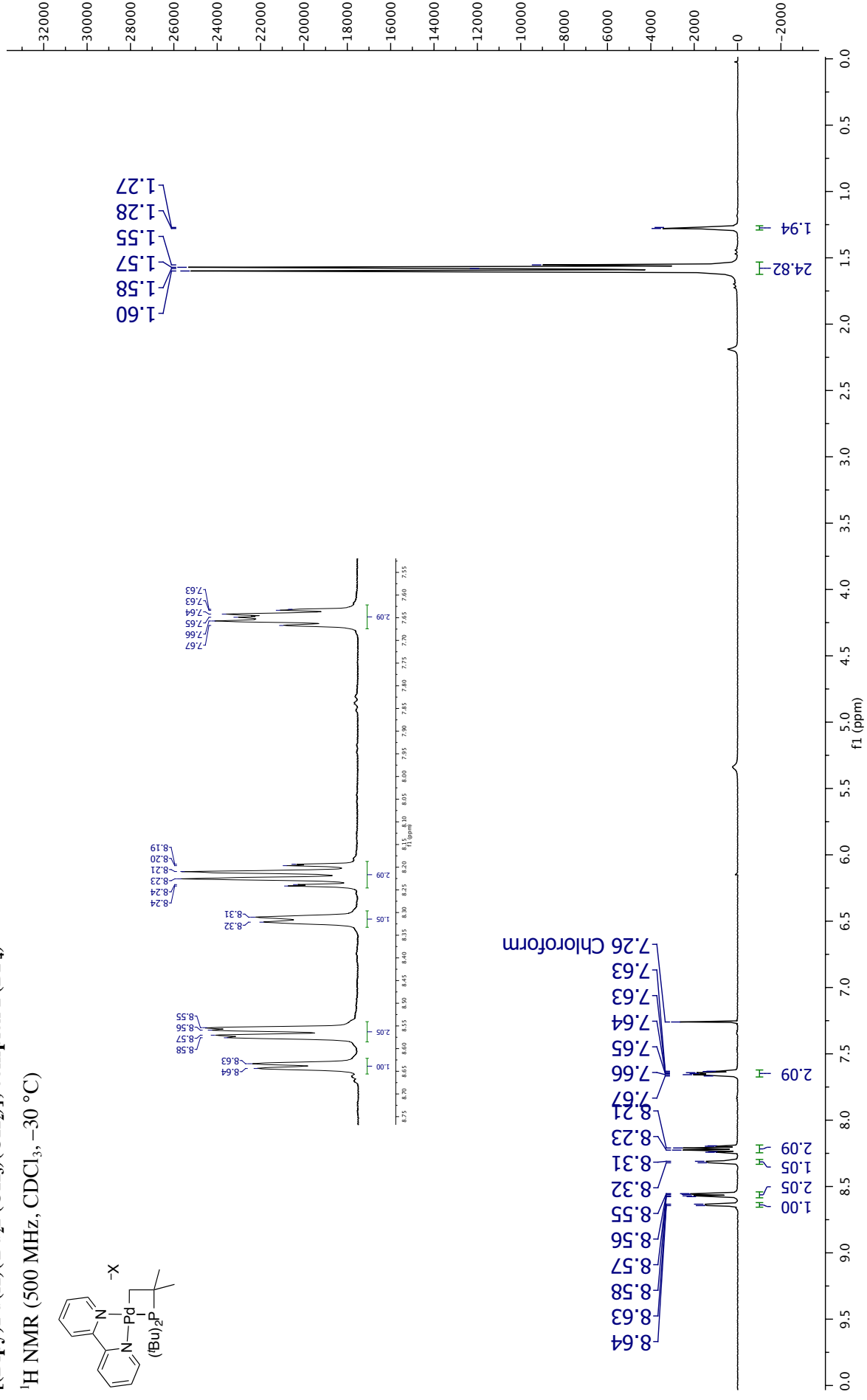
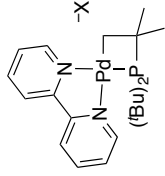
[Bipy)Pd(X)(^tBu₂P(CH₃)(CH₂)]₂, complex C(Br)

³¹P NMR (162 MHz, CDCl₃)



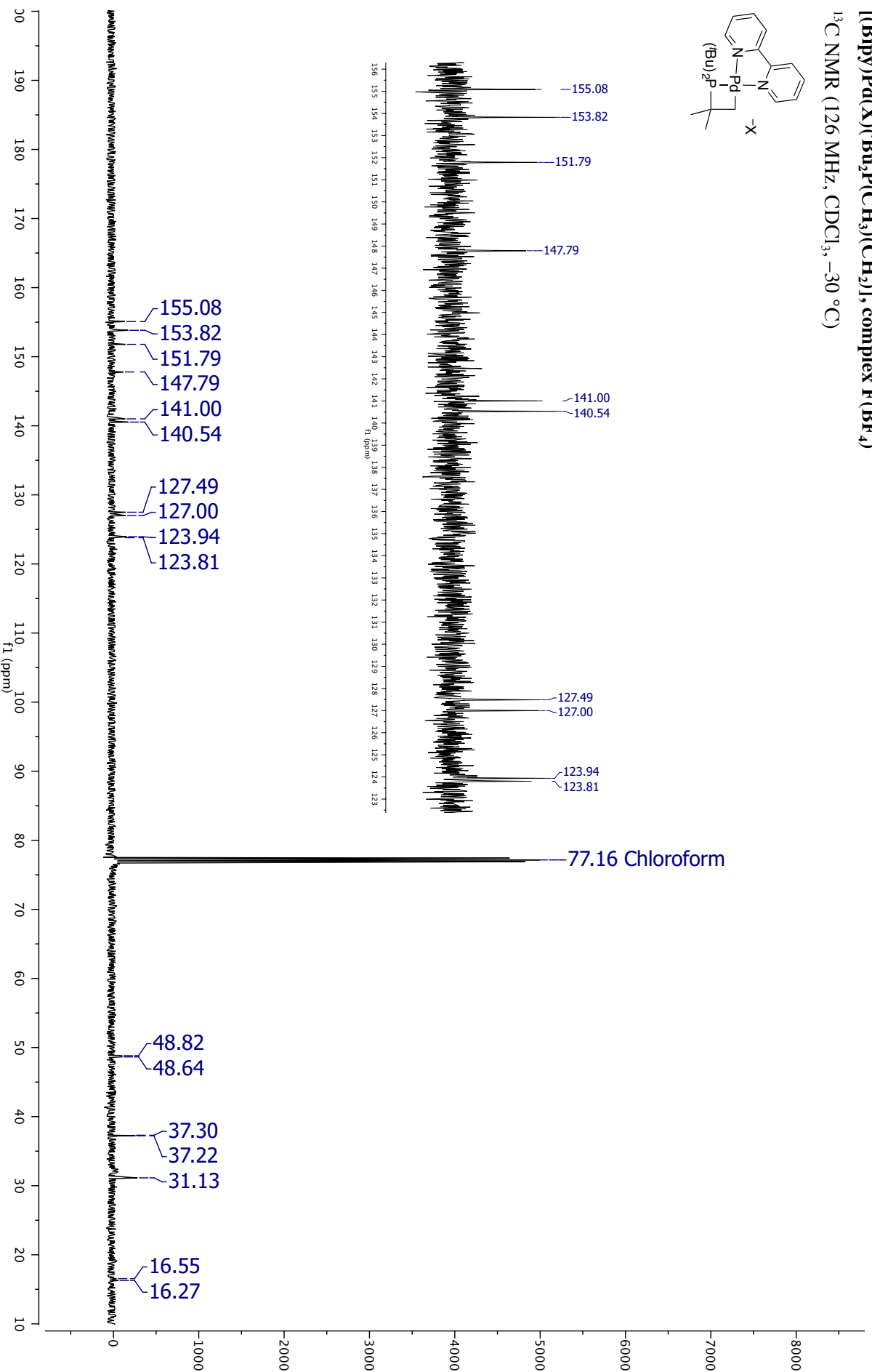
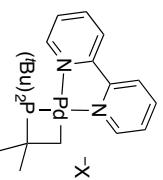
[(Bipy)Pd(X)(*t*Bu₂P(CH₃)₂(CH₂)₂), complex F(BF₄)]

¹H NMR (500 MHz, CDCl₃, -30 °C)



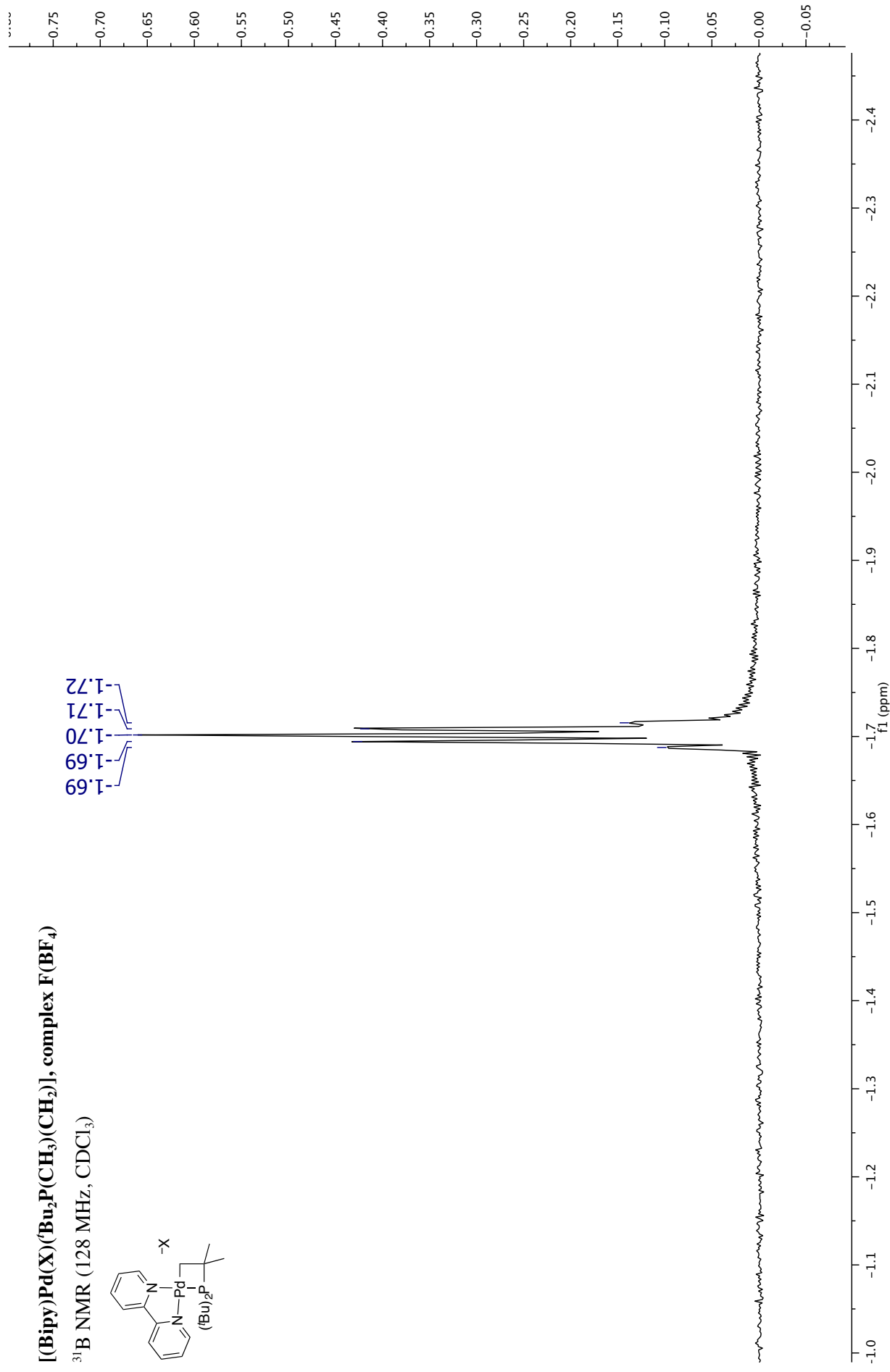
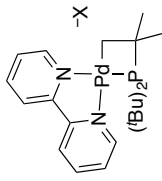
[Bipy)Pd(X)(^tBu₂P(CH₃))(CH₂], complex F(BF₄)

¹³C NMR (126 MHz, CDCl₃, -30 °C)



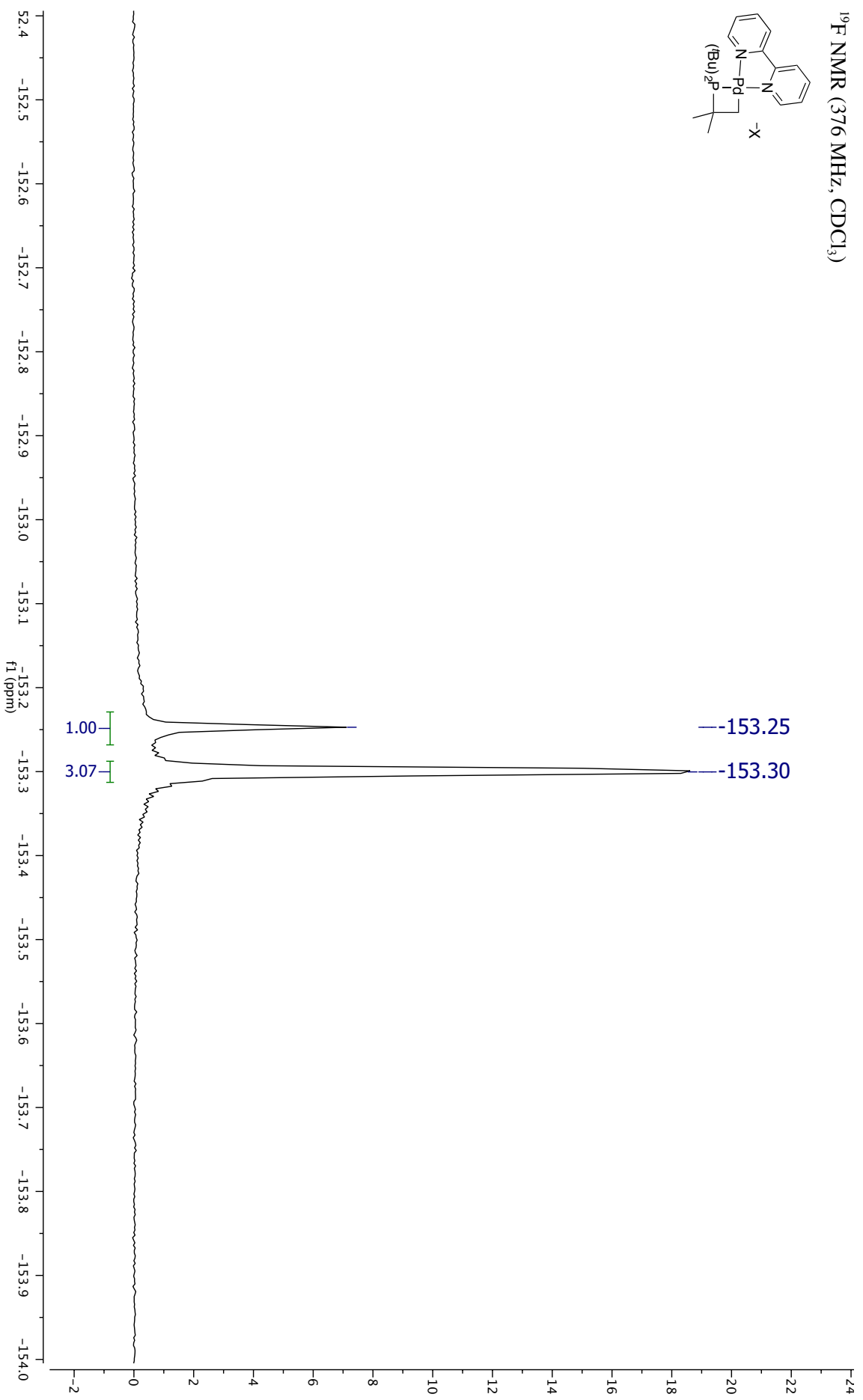
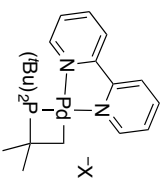
[(Bipy)Pd(X)(^tBu₂P(CH₃)(CH₂)₂), complex F(BF₄)

³¹B NMR (128 MHz, CDCl₃)



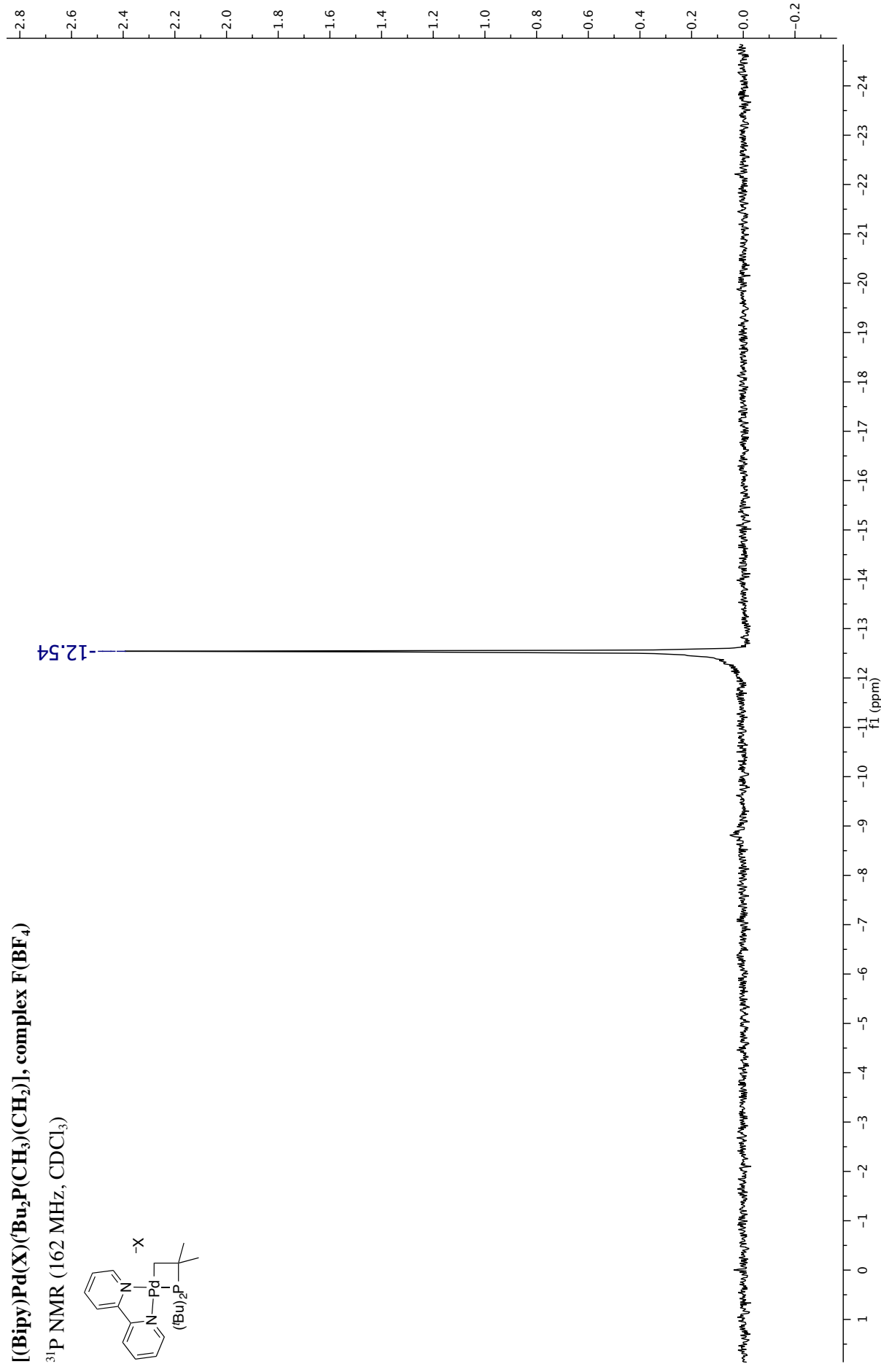
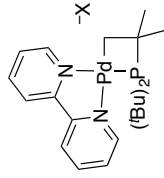
[Bipy)Pd(X)(^tBu₂P(CH₃)(CH₂)](BF₄)

¹⁹F NMR (376 MHz, CDCl₃)

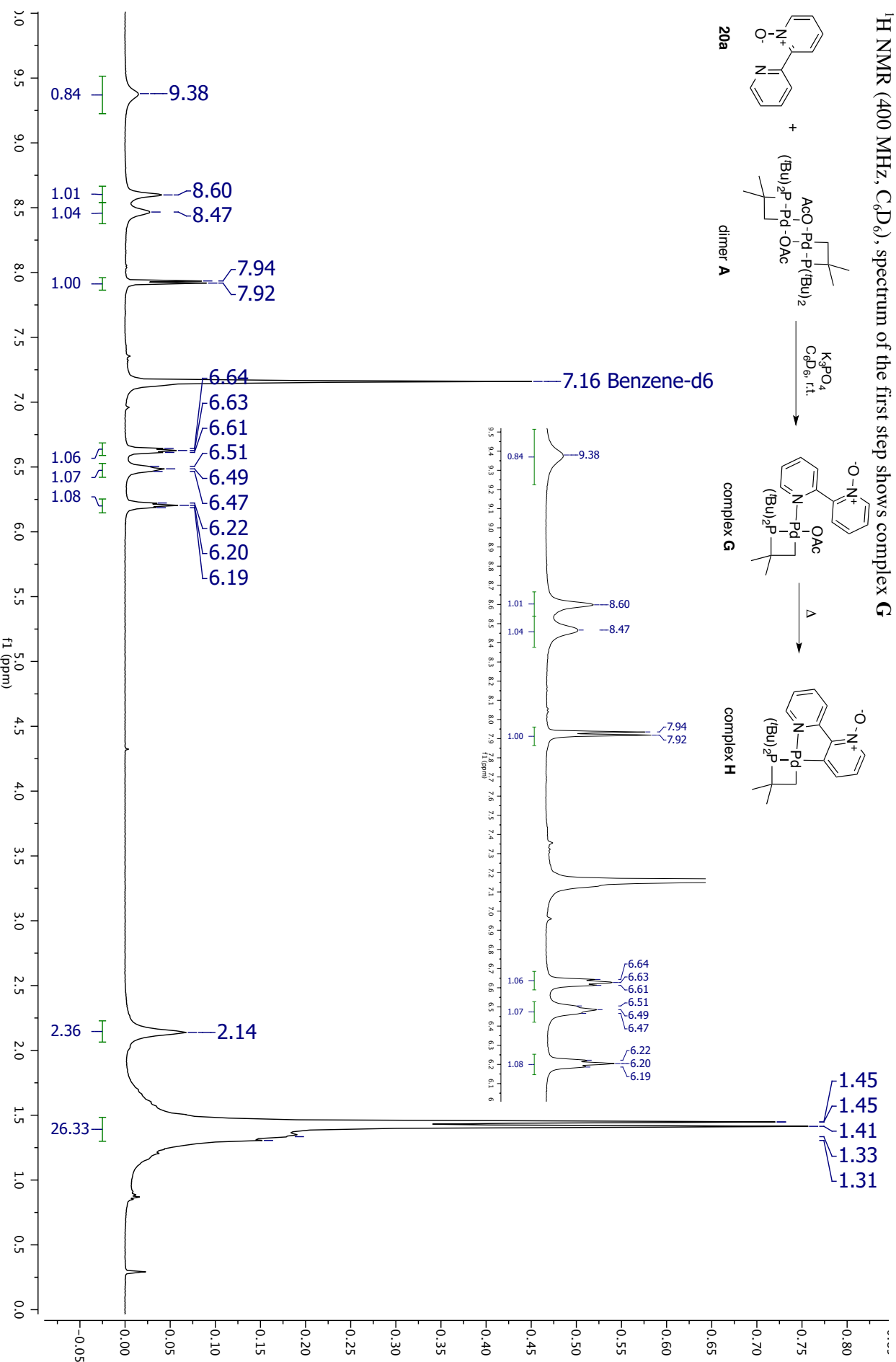
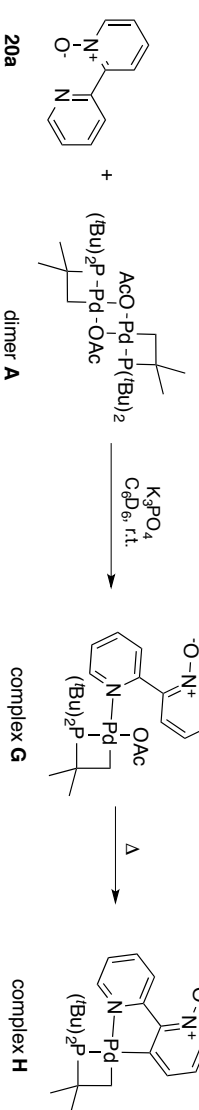


[(Bipy)Pd(X)(*t*-Bu₂P(CH₃)₂(CH₂)₂), complex F(BF₄)

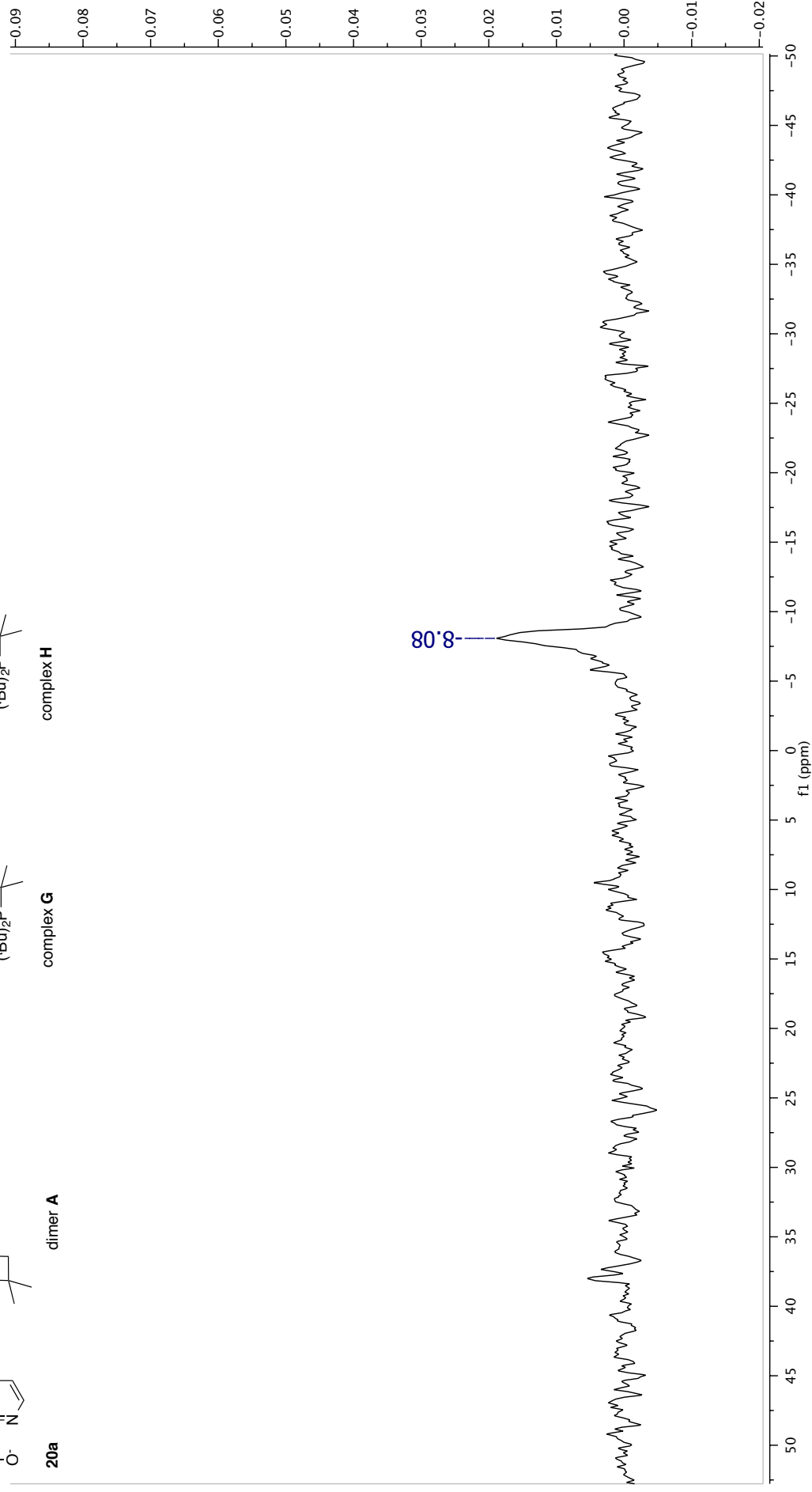
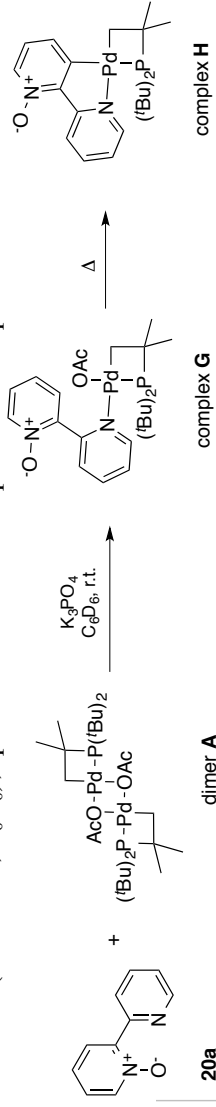
³¹P NMR (162 MHz, CDCl₃)



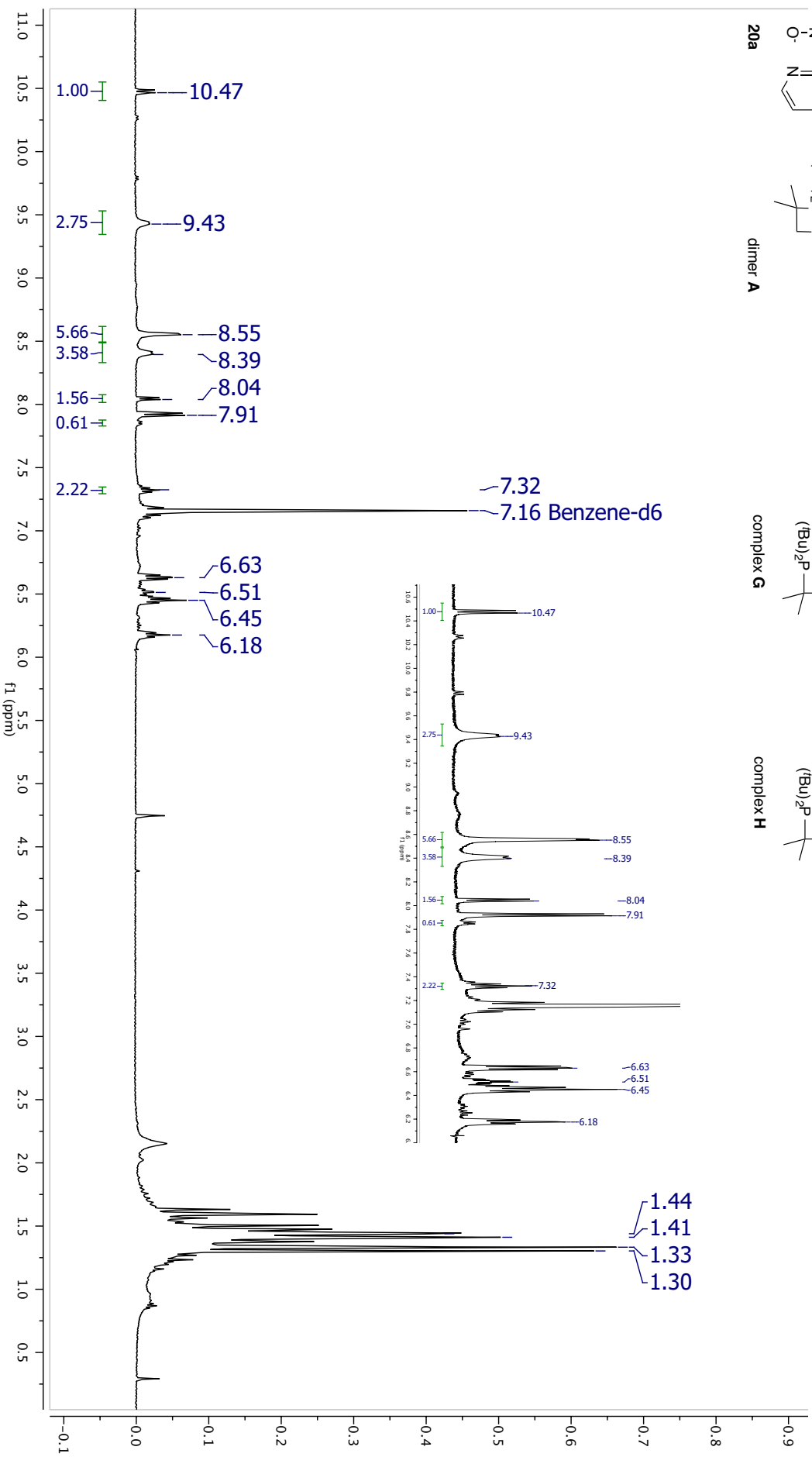
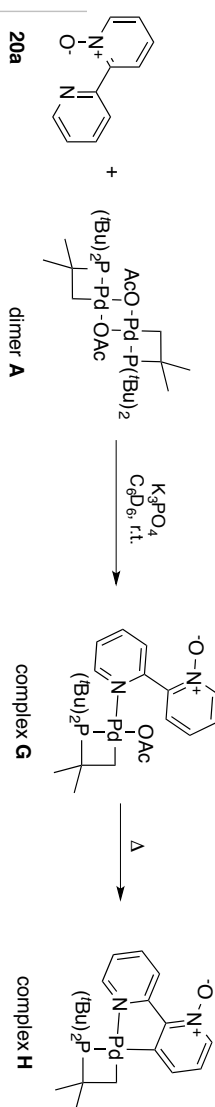
¹H NMR (400 MHz, C₆D₆), spectrum of the first step shows complex **G**



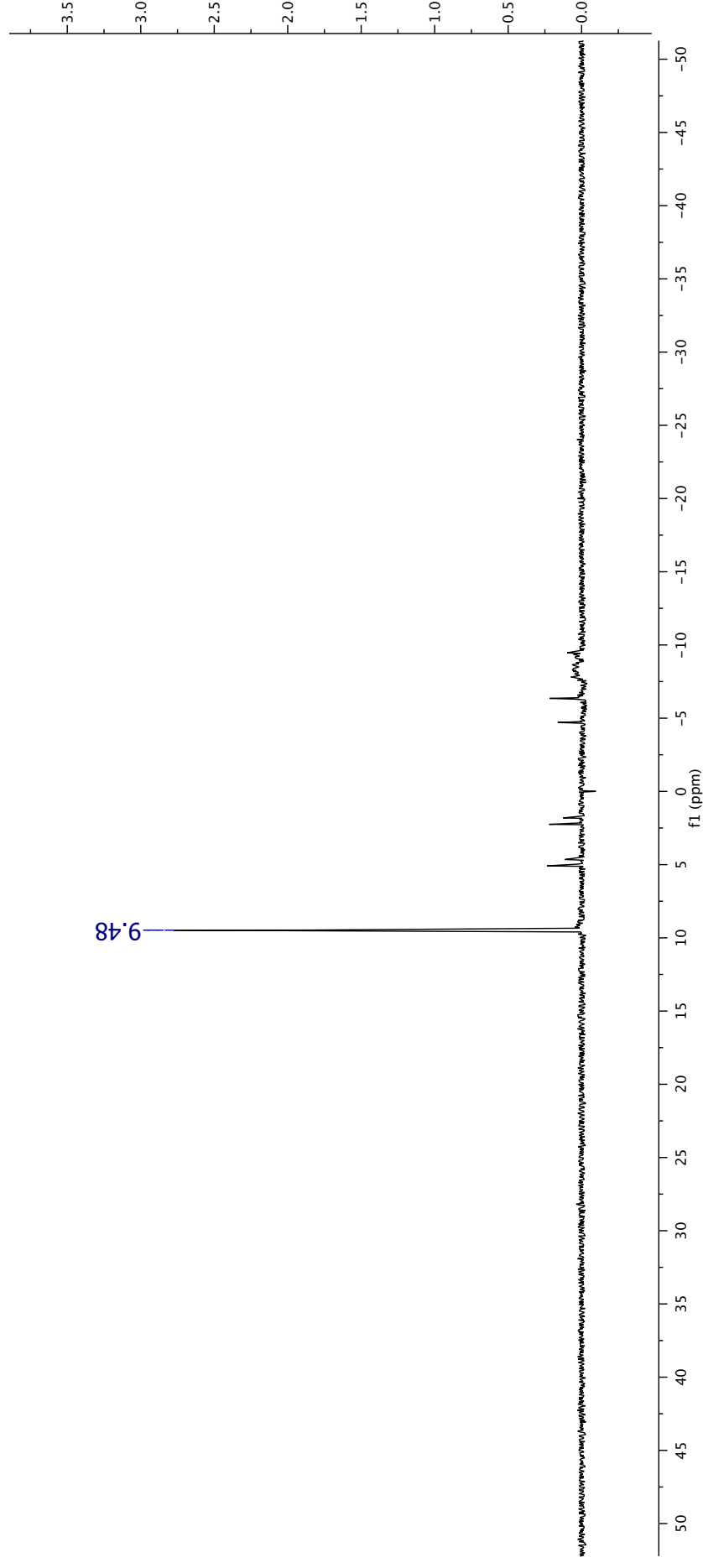
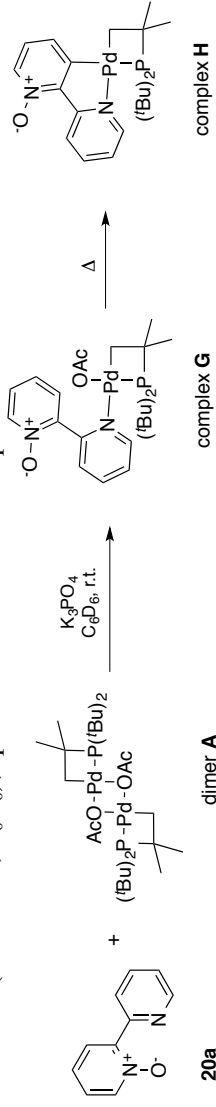
^{31}P NMR (162 MHz, C_6D_6), spectrum of the first step shows complex **G**



¹H NMR (400 MHz, C₆D₆), spectrum of the second step



^{31}P NMR (162 MHz, C_6D_6), spectrum of the second step



10.11 Atomic coordinates and displacement parameters of crystal structures

cis-(dppe)Pd(*p*-^tBuC₆H₄)I (2e)

[SZAC4117]

	x	y	z	U	
C1	0.18072(18)	0.68959(13)	0.52394(14)	0.0191(5)	Uani
H1A	0.1409	0.642	0.4894	0.023	Uiso
H1B	0.1295	0.736	0.5092	0.023	Uiso
C2	0.27867(19)	0.70924(13)	0.49903(14)	0.0187(5)	Uani
H2A	0.2527	0.7283	0.436	0.022	Uiso
H2B	0.3239	0.6602	0.5048	0.022	Uiso
C3	0.47564(17)	0.80655(13)	0.54310(13)	0.0163(4)	Uani
C4	0.5303(2)	0.74225(14)	0.52241(16)	0.0255(5)	Uani
H4	0.5031	0.6888	0.5207	0.031	Uiso
C5	0.6228(2)	0.75486(16)	0.50439(18)	0.0331(6)	Uani
H5	0.659	0.7102	0.4907	0.04	Uiso
C6	0.6632(2)	0.83217(17)	0.50620(17)	0.0320(6)	Uani
H6	0.7262	0.841	0.4925	0.038	Uiso
C7	0.6112(2)	0.89695(16)	0.52811(17)	0.0301(6)	Uani
H7	0.6395	0.9501	0.5306	0.036	Uiso
C8	0.51797(18)	0.88427(14)	0.54638(15)	0.0223(5)	Uani
H8	0.4828	0.9289	0.5612	0.027	Uiso
C9	0.27283(16)	0.87688(12)	0.53943(13)	0.0136(4)	Uani
C10	0.24541(18)	0.92090(13)	0.60121(14)	0.0194(5)	Uani
H10	0.2757	0.9063	0.6629	0.023	Uiso
C11	0.17382(19)	0.98624(14)	0.57319(15)	0.0239(5)	Uani
H11	0.1562	1.0166	0.6159	0.029	Uiso
C12	0.12846(17)	1.00695(14)	0.48354(15)	0.0220(5)	Uani
H12	0.0795	1.0515	0.4645	0.026	Uiso
C13	0.15410(18)	0.96279(14)	0.42087(15)	0.0215(5)	Uani
H13	0.1221	0.9768	0.359	0.026	Uiso
C14	0.22624(17)	0.89839(13)	0.44855(14)	0.0175(4)	Uani
H14	0.2442	0.8686	0.4057	0.021	Uiso
C15	0.25091(17)	0.55888(12)	0.65073(13)	0.0153(4)	Uani
C16	0.34980(18)	0.52599(13)	0.70704(15)	0.0191(5)	Uani
H16	0.4078	0.5605	0.7425	0.023	Uiso
C17	0.36460(19)	0.44223(14)	0.71178(16)	0.0237(5)	Uani
H17	0.4323	0.42	0.7512	0.028	Uiso
C18	0.2816(2)	0.39164(14)	0.65958(16)	0.0255(5)	Uani
H18	0.2921	0.3347	0.6632	0.031	Uiso
C19	0.1828(2)	0.42390(14)	0.60186(16)	0.0244(5)	Uani
H19	0.126	0.3891	0.5652	0.029	Uiso

C20	0.16703(19)	0.50713(13)	0.59765(15)	0.0205(5)	Uani
H20	0.099	0.5291	0.5585	0.025	Uiso
C21	0.11473(17)	0.68415(13)	0.67753(14)	0.0172(4)	Uani
C22	0.04381(19)	0.74971(14)	0.64281(16)	0.0251(5)	Uani
H22	0.0526	0.7836	0.5984	0.03	Uiso
C23	-0.0392(2)	0.76499(15)	0.67333(19)	0.0322(6)	Uani
H23	-0.0882	0.8087	0.6487	0.039	Uiso
C24	-0.0512(2)	0.71721(16)	0.73916(19)	0.0319(6)	Uani
H24	-0.1075	0.7286	0.7604	0.038	Uiso
C25	0.0192(2)	0.65248(16)	0.77417(17)	0.0297(5)	Uani
H25	0.0109	0.6193	0.8192	0.036	Uiso
C26	0.10193(18)	0.63626(14)	0.74336(15)	0.0229(5)	Uani
H26	0.1501	0.592	0.7676	0.028	Uiso
C27	0.52066(17)	0.82480(12)	0.75998(12)	0.0132(4)	Uani
C28	0.61962(17)	0.80221(12)	0.75490(13)	0.0159(4)	Uani
H28	0.6258	0.7504	0.7318	0.019	Uiso
C29	0.70968(17)	0.85393(13)	0.78290(13)	0.0155(4)	Uani
H29	0.7761	0.8366	0.7785	0.019	Uiso
C30	0.70450(16)	0.93055(12)	0.81719(13)	0.0138(4)	Uani
C31	0.60486(17)	0.95296(13)	0.82209(14)	0.0163(4)	Uani
H31	0.5983	1.0047	0.8453	0.02	Uiso
C32	0.51509(17)	0.90094(13)	0.79364(13)	0.0163(4)	Uani
H32	0.4484	0.9181	0.7974	0.02	Uiso
C33	0.80083(17)	0.99022(13)	0.84577(14)	0.0171(4)	Uani
C34	0.8291(2)	1.01860(16)	0.94297(16)	0.0315(6)	Uani
H34A	0.8908	1.0566	0.9601	0.047	Uiso
H34B	0.8494	0.9718	0.9834	0.047	Uiso
H34C	0.7653	1.0455	0.9474	0.047	Uiso
C35	0.7681(2)	1.06391(15)	0.78304(18)	0.0287(5)	Uani
H35A	0.7445	1.0458	0.7205	0.043	Uiso
H35B	0.8312	1.1002	0.7972	0.043	Uiso
H35C	0.7079	1.0927	0.7914	0.043	Uiso
C36	0.90344(18)	0.95327(15)	0.83913(17)	0.0269(5)	Uani
H36A	0.8878	0.9377	0.7767	0.04	Uiso
H36B	0.9254	0.9053	0.8777	0.04	Uiso
H36C	0.963	0.9931	0.8586	0.04	Uiso
P1	0.23090(4)	0.66803(3)	0.64494(3)	0.01399(11)	Uani
P2	0.36013(4)	0.78821(3)	0.57494(3)	0.01271(11)	Uani
Pd1	0.38627(2)	0.74868(2)	0.71411(2)	0.01132(5)	Uani
II	0.41151(2)	0.70272(2)	0.87858(2)	0.01501(4)	Uani

***cis*-(dppe)Pd(*p*-FC₆H₄)I (2g)**

[AC4119B1]

	x	y	z	U	
C1	0.1156(4)	0.7873(3)	0.73101(19)	0.0195(9)	Uani
H1A	0.1416	0.8592	0.7329	0.023	Uiso
H1B	0.0606	0.773	0.6929	0.023	Uiso
C2	0.0223(4)	0.7582(3)	0.78430(18)	0.0170(8)	Uani
H2A	-0.0198	0.6899	0.7785	0.02	Uiso
H2B	-0.0565	0.8035	0.7871	0.02	Uiso
C3	0.1786(4)	0.8975(3)	0.86620(18)	0.0147(8)	Uani
C4	0.3059(4)	0.9402(3)	0.84465(19)	0.0187(9)	Uani
H4	0.3697	0.9003	0.8246	0.022	Uiso
C5	0.3392(5)	1.0407(3)	0.8525(2)	0.0252(10)	Uani
H5	0.4257	1.0693	0.8377	0.03	Uiso
C6	0.2477(5)	1.0995(3)	0.8818(2)	0.0258(10)	Uani
H6	0.2707	1.1684	0.8868	0.031	Uiso
C7	0.1216(5)	1.0573(3)	0.9040(2)	0.0284(11)	Uani
H7	0.0589	1.0974	0.9245	0.034	Uiso
C8	0.0874(5)	0.9568(3)	0.8961(2)	0.0225(9)	Uani
H8	0.0012	0.9284	0.9113	0.027	Uiso
C9	0.0173(4)	0.7309(3)	0.91363(18)	0.0132(8)	Uani
C10	-0.1251(4)	0.6977(3)	0.90174(19)	0.0145(8)	Uani
H10	-0.1617	0.6928	0.8615	0.017	Uiso
C11	-0.2131(4)	0.6720(3)	0.94866(19)	0.0152(8)	Uani
H11	-0.3098	0.6498	0.9402	0.018	Uiso
C12	-0.1615(4)	0.6783(3)	1.00743(19)	0.0184(9)	Uani
H12	-0.2222	0.6598	1.0392	0.022	Uiso
C13	-0.0202(4)	0.7119(3)	1.02014(19)	0.0171(8)	Uani
H13	0.0151	0.7169	1.0606	0.02	Uiso
C14	0.0690(4)	0.7382(3)	0.97354(19)	0.0167(8)	Uani
H14	0.1652	0.7611	0.9823	0.02	Uiso
C15	0.4124(4)	0.8012(3)	0.69780(18)	0.0169(8)	Uani
C16	0.5547(5)	0.7733(3)	0.6989(2)	0.0220(9)	Uani
H16	0.5777	0.7116	0.7157	0.026	Uiso
C17	0.6615(5)	0.8352(4)	0.6756(2)	0.0287(11)	Uani
H17	0.7573	0.8157	0.6766	0.034	Uiso
C18	0.6297(6)	0.9246(4)	0.6510(2)	0.0349(13)	Uani
H18	0.7036	0.9673	0.6358	0.042	Uiso
C19	0.4914(6)	0.9517(4)	0.6484(2)	0.0361(13)	Uani
H19	0.4696	1.013	0.6308	0.043	Uiso
C20	0.3816(6)	0.8906(3)	0.6714(2)	0.0280(11)	Uani
H20	0.2858	0.9101	0.669	0.034	Uiso
C21	0.2509(4)	0.6165(3)	0.67821(18)	0.0145(8)	Uani
C22	0.2237(4)	0.5216(3)	0.6986(2)	0.0190(9)	Uani
H22	0.2175	0.5102	0.7405	0.023	Uiso
C23	0.2053(4)	0.4419(3)	0.6582(2)	0.0217(9)	Uani

H23	0.1849	0.3769	0.6724	0.026	Uiso
C24	0.2169(4)	0.4584(3)	0.5974(2)	0.0228(10)	Uani
H24	0.2073	0.4042	0.57	0.027	Uiso
C25	0.2423(5)	0.5533(3)	0.5763(2)	0.0229(10)	Uani
H25	0.2483	0.5644	0.5344	0.027	Uiso
C26	0.2591(4)	0.6330(3)	0.61669(19)	0.0190(9)	Uani
H26	0.276	0.6983	0.6023	0.023	Uiso
C27	0.3765(4)	0.6810(3)	0.92403(18)	0.0136(8)	Uani
C28	0.4368(4)	0.7681(3)	0.94983(18)	0.0153(8)	Uani
H28	0.446	0.8258	0.926	0.018	Uiso
C29	0.4845(4)	0.7729(3)	1.01031(19)	0.0167(8)	Uani
H29	0.5261	0.8325	1.0277	0.02	Uiso
C30	0.4686(4)	0.6884(3)	1.04320(18)	0.0177(9)	Uani
C31	0.4070(4)	0.6007(3)	1.02055(19)	0.0179(9)	Uani
H31	0.3955	0.5438	1.045	0.021	Uiso
C32	0.3619(4)	0.5988(3)	0.96008(18)	0.0170(8)	Uani
H32	0.3198	0.539	0.9432	0.02	Uiso
C33	0.4280(4)	0.7698(3)	0.23458(18)	0.0155(8)	Uani
H33A	0.4556	0.7448	0.195	0.019	Uiso
H33B	0.4929	0.8277	0.2458	0.019	Uiso
C34	0.4427(4)	0.6893(3)	0.28138(19)	0.0176(9)	Uani
H34A	0.5453	0.6823	0.2914	0.021	Uiso
H34B	0.4029	0.6255	0.2642	0.021	Uiso
C35	0.3031(4)	0.5906(3)	0.37475(18)	0.0145(8)	Uani
C36	0.1816(4)	0.5408(3)	0.3494(2)	0.0206(9)	Uani
H36	0.1194	0.5745	0.3231	0.025	Uiso
C37	0.1509(5)	0.4419(3)	0.3624(2)	0.0268(10)	Uani
H37	0.0669	0.4083	0.3456	0.032	Uiso
C38	0.2432(5)	0.3921(3)	0.3999(2)	0.0243(10)	Uani
H38	0.2225	0.3243	0.4084	0.029	Uiso
C39	0.3654(5)	0.4407(3)	0.4248(2)	0.0239(10)	Uani
H39	0.4286	0.4062	0.4503	0.029	Uiso
C40	0.3949(4)	0.5400(3)	0.4124(2)	0.0195(9)	Uani
H40	0.4782	0.5737	0.4297	0.023	Uiso
C41	0.4828(4)	0.7645(3)	0.40627(18)	0.0144(8)	Uani
C42	0.6207(4)	0.7997(3)	0.3914(2)	0.0173(9)	Uani
H42	0.6483	0.7983	0.3508	0.021	Uiso
C43	0.7162(4)	0.8365(3)	0.4357(2)	0.0221(9)	Uani
H43	0.8093	0.8603	0.4254	0.027	Uiso
C44	0.6780(4)	0.8390(3)	0.4948(2)	0.0221(9)	Uani
H44	0.7448	0.8642	0.5249	0.026	Uiso
C45	0.5419(4)	0.8046(3)	0.5104(2)	0.0199(9)	Uani
H45	0.5155	0.8062	0.5511	0.024	Uiso
C46	0.4453(4)	0.7679(3)	0.46626(18)	0.0164(8)	Uani
H46	0.3522	0.7447	0.4769	0.02	Uiso
C47	0.1335(4)	0.7072(3)	0.19259(18)	0.0144(8)	Uani
C48	-0.0154(5)	0.7072(3)	0.19709(19)	0.0195(9)	Uani
H48	-0.0565	0.7604	0.2169	0.023	Uiso

C49	-0.1032(5)	0.6298(3)	0.1727(2)	0.0244(10)	Uani
H49	-0.204	0.6307	0.1752	0.029	Uiso
C50	-0.0431(5)	0.5510(3)	0.1445(2)	0.0247(10)	Uani
H50	-0.1026	0.4972	0.1287	0.03	Uiso
C51	0.1038(5)	0.5511(3)	0.1397(2)	0.0255(10)	Uani
H51	0.1445	0.4979	0.1197	0.031	Uiso
C52	0.1919(5)	0.6283(3)	0.16376(19)	0.0188(9)	Uani
H52	0.2925	0.6273	0.1605	0.023	Uiso
C53	0.2537(4)	0.9060(3)	0.17444(18)	0.0139(8)	Uani
C54	0.2765(4)	1.0037(3)	0.19372(19)	0.0187(9)	Uani
H54	0.2783	1.0191	0.2354	0.022	Uiso
C55	0.2969(4)	1.0791(3)	0.1522(2)	0.0196(9)	Uani
H55	0.3155	1.1455	0.1656	0.024	Uiso
C56	0.2900(4)	1.0569(3)	0.0913(2)	0.0181(9)	Uani
H56	0.3006	1.1086	0.063	0.022	Uiso
C57	0.2680(4)	0.9599(3)	0.07156(19)	0.0190(9)	Uani
H57	0.2651	0.9451	0.0298	0.023	Uiso
C58	0.2501(4)	0.8839(3)	0.11306(19)	0.0160(8)	Uani
H58	0.2354	0.8172	0.0996	0.019	Uiso
C59	0.1175(4)	0.8110(3)	0.41773(19)	0.0166(8)	Uani
C60	0.0582(4)	0.7248(3)	0.44138(18)	0.0165(8)	Uani
H60	0.0445	0.6675	0.4165	0.02	Uiso
C61	0.0180(4)	0.7200(3)	0.50107(19)	0.0188(9)	Uani
H61	-0.0235	0.6607	0.5171	0.023	Uiso
C62	0.0404(4)	0.8039(3)	0.53576(18)	0.0185(9)	Uani
C63	0.0999(5)	0.8912(3)	0.5145(2)	0.0220(9)	Uani
H63	0.1147	0.948	0.5397	0.026	Uiso
C64	0.1380(5)	0.8937(3)	0.45464(19)	0.0195(9)	Uani
H64	0.179	0.9533	0.4388	0.023	Uiso
F1	0.5195(3)	0.6914(2)	1.10202(11)	0.0245(6)	Uani
F2	-0.0010(3)	0.8008(2)	0.59417(11)	0.0284(6)	Uani
P1	0.27989(11)	0.71798(8)	0.73255(5)	0.0131(2)	Uani
P2	0.13561(10)	0.76622(7)	0.85355(5)	0.0120(2)	Uani
P65	0.24209(11)	0.80707(8)	0.22953(5)	0.0133(2)	Uani
P66	0.35006(10)	0.71628(7)	0.35055(5)	0.0122(2)	Uani
Pd1	0.32903(3)	0.68306(2)	0.83356(2)	0.01108(7)	Uani
Pd2	0.17267(3)	0.81747(2)	0.32849(2)	0.01130(7)	Uani
I1	0.53817(3)	0.56495(2)	0.81451(2)	0.01920(7)	Uani
I2	-0.03353(3)	0.93922(2)	0.30542(2)	0.02128(7)	Uani

cis-(dppf)Pd(*p*-FC₆H₄)I (3g)

[SZ4028]

	x	y	z	U	
C1	0.3913(2)	0.22304(15)	0.50487(18)	0.0117(5)	Uani
C2	0.2942(2)	0.26208(16)	0.48628(18)	0.0123(6)	Uani
H2	0.2805	0.3153	0.5066	0.015	Uiso
C3	0.2214(2)	0.21158(16)	0.43408(18)	0.0148(6)	Uani
H3	0.1469	0.2227	0.413	0.018	Uiso
C4	0.2711(2)	0.14165(17)	0.41974(18)	0.0163(6)	Uani
H4	0.2378	0.0952	0.3869	0.02	Uiso
C5	0.3759(2)	0.14851(16)	0.46219(18)	0.0142(6)	Uani
H5	0.4293	0.1079	0.4636	0.017	Uiso
C6	0.3016(2)	0.18965(16)	0.69229(18)	0.0124(6)	Uani
C7	0.3544(2)	0.11904(16)	0.68047(19)	0.0172(6)	Uani
H7	0.4291	0.109	0.7022	0.021	Uiso
C8	0.2811(3)	0.06573(17)	0.6336(2)	0.0217(7)	Uani
H8	0.2962	0.0122	0.615	0.026	Uiso
C9	0.1848(2)	0.10180(17)	0.6143(2)	0.0207(7)	Uani
H9	0.1199	0.0783	0.5801	0.025	Uiso
C10	0.1959(2)	0.17780(17)	0.65010(18)	0.0160(6)	Uani
H10	0.14	0.2168	0.6461	0.019	Uiso
C11	0.3971(2)	0.25392(16)	0.86310(18)	0.0123(6)	Uani
C12	0.4579(2)	0.18838(17)	0.8877(2)	0.0172(6)	Uani
H12	0.4766	0.1573	0.8413	0.021	Uiso
C13	0.4910(2)	0.16837(18)	0.9788(2)	0.0222(7)	Uani
H13	0.5316	0.1236	0.9947	0.027	Uiso
C14	0.4645(2)	0.21418(19)	1.0466(2)	0.0224(7)	Uani
H14	0.4862	0.2002	1.109	0.027	Uiso
C15	0.4069(2)	0.27978(18)	1.0240(2)	0.0203(7)	Uani
H15	0.39	0.3113	1.0709	0.024	Uiso
C16	0.3731(2)	0.30017(17)	0.93252(19)	0.0157(6)	Uani
H16	0.3337	0.3457	0.9174	0.019	Uiso
C17	0.2476(2)	0.34173(16)	0.73344(18)	0.0126(6)	Uani
C18	0.2407(2)	0.40630(16)	0.67695(19)	0.0145(6)	Uani
H18	0.2944	0.4173	0.6456	0.017	Uiso
C19	0.1560(2)	0.45478(16)	0.6660(2)	0.0179(6)	Uani
H19	0.1512	0.4982	0.6266	0.022	Uiso
C20	0.0788(2)	0.43934(17)	0.7130(2)	0.0194(6)	Uani
H20	0.0214	0.4727	0.7065	0.023	Uiso
C21	0.0849(2)	0.37510(17)	0.7699(2)	0.0172(6)	Uani
H21	0.0317	0.3647	0.8021	0.021	Uiso
C22	0.1688(2)	0.32628(16)	0.77934(18)	0.0141(6)	Uani
H22	0.1724	0.282	0.8174	0.017	Uiso
C23	0.5965(2)	0.18772(15)	0.60742(18)	0.0117(5)	Uani
C24	0.6312(2)	0.18042(16)	0.70142(19)	0.0144(6)	Uani
H24	0.6063	0.2145	0.7418	0.017	Uiso

C25	0.7017(2)	0.12382(17)	0.7369(2)	0.0201(6)	Uani
H25	0.7251	0.1195	0.8011	0.024	Uiso
C26	0.7380(2)	0.07362(17)	0.6786(2)	0.0217(7)	Uani
H26	0.7854	0.0344	0.7027	0.026	Uiso
C27	0.7046(2)	0.08097(17)	0.5845(2)	0.0204(7)	Uani
H27	0.7299	0.0469	0.5444	0.025	Uiso
C28	0.6347(2)	0.13754(16)	0.5490(2)	0.0166(6)	Uani
H28	0.6125	0.1423	0.4846	0.02	Uiso
C29	0.5579(2)	0.30790(15)	0.47202(18)	0.0110(5)	Uani
C30	0.4907(2)	0.33632(16)	0.39500(19)	0.0148(6)	Uani
H30	0.4194	0.3275	0.388	0.018	Uiso
C31	0.5277(2)	0.37737(17)	0.3287(2)	0.0188(6)	Uani
H31	0.4818	0.3962	0.2762	0.023	Uiso
C32	0.6318(2)	0.39074(16)	0.33926(19)	0.0168(6)	Uani
H32	0.6569	0.4209	0.2954	0.02	Uiso
C33	0.6987(2)	0.36059(16)	0.4129(2)	0.0165(6)	Uani
H33	0.7701	0.3685	0.4186	0.02	Uiso
C34	0.6625(2)	0.31859(15)	0.47909(19)	0.0128(6)	Uani
H34	0.7093	0.2971	0.5293	0.015	Uiso
C35	0.6143(2)	0.40227(16)	0.65459(18)	0.0140(4)	Uani
C36	0.7147(2)	0.37840(17)	0.68689(18)	0.0140(4)	Uani
H36	0.7281	0.3351	0.7264	0.017	Uiso
C37	0.7953(2)	0.41782(18)	0.6615(2)	0.0195(6)	Uani
H37	0.8641	0.4024	0.6838	0.023	Uiso
C38	0.7731(2)	0.47943(17)	0.6033(2)	0.0205(7)	Uani
C39	0.6748(2)	0.50496(17)	0.5710(2)	0.0182(6)	Uani
H39	0.6614	0.5482	0.5312	0.022	Uiso
C40	0.5956(2)	0.46484(16)	0.59895(19)	0.0152(6)	Uani
H40	0.5271	0.4817	0.5786	0.018	Uiso
F1	0.85164(14)	0.51813(11)	0.57646(14)	0.0324(5)	Uani
P1	0.50784(5)	0.26579(4)	0.56614(4)	0.00889(14)	Uani
P2	0.35896(5)	0.27894(4)	0.74189(5)	0.00934(14)	Uani
Fe1	0.28783(3)	0.16372(2)	0.55770(3)	0.01073(9)	Uani
Pd1	0.49409(2)	0.34205(2)	0.68804(2)	0.00797(5)	Uani
I1	0.50555(2)	0.44094(2)	0.82517(2)	0.01276(5)	Uani

***cis*-(dppf)Pd(*p*-FC₆H₄)Br (7g)**

[SZ4032]

	x	y	z	U	
C1	0.61538(19)	0.22132(15)	0.49737(16)	0.0119(5)	Uani
C2	0.71255(19)	0.26216(15)	0.51349(17)	0.0139(5)	Uani
H2	0.7242	0.3159	0.4917	0.017	Uiso
C3	0.7882(2)	0.21260(15)	0.56502(17)	0.0159(5)	Uani
H3	0.8632	0.2248	0.5842	0.019	Uiso
C4	0.7407(2)	0.14147(16)	0.58202(18)	0.0178(6)	Uani
H4	0.7765	0.0951	0.6151	0.021	Uiso
C5	0.6342(2)	0.14647(15)	0.54144(17)	0.0146(5)	Uani
H5	0.5818	0.1047	0.5421	0.018	Uiso
C6	0.6991(2)	0.18812(15)	0.30910(17)	0.0141(5)	Uani
C7	0.6449(2)	0.11750(15)	0.32115(17)	0.0177(6)	Uani
H7	0.5693	0.1087	0.3006	0.021	Uiso
C8	0.7183(2)	0.06188(16)	0.36642(19)	0.0234(6)	Uani
H8	0.7024	0.0079	0.3849	0.028	Uiso
C9	0.8166(2)	0.09717(17)	0.38460(19)	0.0229(6)	Uani
H9	0.882	0.0724	0.4178	0.027	Uiso
C10	0.8059(2)	0.17448(16)	0.34935(18)	0.0177(6)	Uani
H10	0.8629	0.2132	0.3526	0.021	Uiso
C11	0.60191(19)	0.25649(16)	0.13894(17)	0.0145(5)	Uani
C12	0.5469(2)	0.18750(17)	0.11179(19)	0.0199(6)	Uani
H12	0.5312	0.1532	0.1567	0.024	Uiso
C13	0.5152(2)	0.16906(18)	0.0198(2)	0.0265(7)	Uani
H13	0.4784	0.1221	0.0018	0.032	Uiso
C14	0.5373(2)	0.21914(19)	-0.0454(2)	0.0273(7)	Uani
H14	0.5167	0.2059	-0.1083	0.033	Uiso
C15	0.5887(2)	0.2881(2)	-0.02033(19)	0.0262(7)	Uani
H15	0.6024	0.3227	-0.0659	0.031	Uiso
C16	0.6209(2)	0.30735(17)	0.07222(18)	0.0192(6)	Uani
H16	0.6558	0.3552	0.0894	0.023	Uiso
C17	0.75166(19)	0.34333(15)	0.27080(17)	0.0129(5)	Uani
C18	0.7589(2)	0.40915(15)	0.32767(17)	0.0151(5)	Uani
H18	0.7054	0.4205	0.3586	0.018	Uiso
C19	0.8445(2)	0.45792(16)	0.33889(19)	0.0193(6)	Uani
H19	0.8497	0.5019	0.3784	0.023	Uiso
C20	0.9215(2)	0.44278(16)	0.2930(2)	0.0219(6)	Uani
H20	0.9794	0.4765	0.3004	0.026	Uiso
C21	0.9146(2)	0.37773(17)	0.23540(19)	0.0194(6)	Uani
H21	0.9676	0.3674	0.2035	0.023	Uiso
C22	0.8309(2)	0.32848(16)	0.22500(17)	0.0155(5)	Uani
H22	0.8269	0.284	0.1863	0.019	Uiso
C23	0.40723(19)	0.18344(15)	0.39568(17)	0.0130(5)	Uani
C24	0.3700(2)	0.17623(15)	0.30163(18)	0.0169(6)	Uani
H24	0.3938	0.2109	0.2612	0.02	Uiso

C25	0.2986(2)	0.11904(17)	0.26636(19)	0.0231(6)	Uani
H25	0.2737	0.1149	0.2021	0.028	Uiso
C26	0.2638(2)	0.06817(16)	0.3245(2)	0.0242(6)	Uani
H26	0.2154	0.0287	0.3003	0.029	Uiso
C27	0.2996(2)	0.07469(17)	0.4185(2)	0.0244(6)	Uani
H27	0.2756	0.0397	0.4586	0.029	Uiso
C28	0.3706(2)	0.13241(16)	0.45406(19)	0.0193(6)	Uani
H28	0.3943	0.1371	0.5184	0.023	Uiso
C29	0.4475(2)	0.30541(15)	0.53124(17)	0.0131(5)	Uani
C30	0.5159(2)	0.33621(15)	0.60672(18)	0.0167(5)	Uani
H30	0.5877	0.3282	0.6132	0.02	Uiso
C31	0.4799(2)	0.37845(16)	0.67227(18)	0.0203(6)	Uani
H31	0.5268	0.3991	0.7238	0.024	Uiso
C32	0.3750(2)	0.39065(16)	0.66258(19)	0.0196(6)	Uani
H32	0.3504	0.4217	0.7059	0.024	Uiso
C33	0.3070(2)	0.35779(16)	0.59043(19)	0.0199(6)	Uani
H33	0.2352	0.3645	0.5854	0.024	Uiso
C34	0.3419(2)	0.31490(15)	0.52488(18)	0.0155(5)	Uani
H34	0.2942	0.2919	0.4755	0.019	Uiso
C35	0.38458(19)	0.40040(16)	0.34889(16)	0.0142(5)	Uani
C36	0.2836(2)	0.37534(16)	0.31629(18)	0.0174(6)	Uani
H36	0.2701	0.3312	0.2771	0.021	Uiso
C37	0.2029(2)	0.41499(17)	0.34119(19)	0.0211(6)	Uani
H37	0.1338	0.3992	0.3185	0.025	Uiso
C38	0.2253(2)	0.47758(17)	0.3994(2)	0.0222(6)	Uani
C39	0.3241(2)	0.50408(16)	0.43127(18)	0.0191(6)	Uani
H39	0.3376	0.5483	0.4703	0.023	Uiso
C40	0.4036(2)	0.46378(15)	0.40430(18)	0.0170(6)	Uani
H40	0.4724	0.4811	0.4252	0.02	Uiso
F1	0.14655(13)	0.51722(11)	0.42499(13)	0.0335(4)	Uani
P1	0.49583(5)	0.26313(4)	0.43674(4)	0.01046(13)	Uani
P2	0.64089(5)	0.27932(4)	0.26124(4)	0.01104(13)	Uani
Fe1	0.71729(3)	0.16175(2)	0.44329(2)	0.01261(8)	Uani
Br1	0.49578(2)	0.43672(2)	0.18966(2)	0.01612(7)	Uani
Pd1	0.50575(2)	0.34090(2)	0.31597(2)	0.00963(5)	Uani

***trans*-(PPh₃)₂Pd(*p*-MeC₆H₄)Br (9f)**

[SZ3020]

	x	y	z	U	
Pd01	0.25	0.252446(12)	0.5	0.01909(5)	Uani
Br02	0.25	0.055319(18)	0.5	0.03036(7)	Uani
P003	0.22223(3)	0.25495(3)	0.401493(17)	0.01904(9)	Uani
C1	0.25	0.41016(18)	0.5	0.0202(4)	Uani
C2	0.34397(13)	0.46426(12)	0.48142(7)	0.0217(3)	Uani
H2	0.4089	0.4276	0.4686	0.026	Uiso
C3	0.34417(14)	0.57240(13)	0.48140(7)	0.0244(3)	Uani
H3	0.4093	0.6088	0.4685	0.029	Uiso
C4	0.25	0.62729(18)	0.5	0.0253(4)	Uani
C5	0.25	0.7438(2)	0.5	0.0464(8)	Uani
H5A	0.2867	0.7691	0.5361	0.07	Uiso
H5B	0.1694	0.7691	0.4953	0.07	Uiso
H5C	0.2939	0.7691	0.4685	0.07	Uiso
C1A	0.22957(13)	0.38109(12)	0.36681(7)	0.0209(3)	Uani
C2A	0.32488(14)	0.41165(14)	0.33735(7)	0.0262(3)	Uani
H2A	0.384	0.3629	0.33	0.031	Uiso
C3A	0.33368(16)	0.51381(15)	0.31866(8)	0.0328(4)	Uani
H3A	0.3992	0.5344	0.2988	0.039	Uiso
C4A	0.24789(17)	0.58512(15)	0.32880(8)	0.0339(4)	Uani
H4A	0.255	0.6549	0.3166	0.041	Uiso
C5A	0.15106(16)	0.55458(13)	0.35695(8)	0.0301(4)	Uani
H5A1	0.0912	0.6032	0.3633	0.036	Uiso
C6A	0.14171(14)	0.45329(12)	0.37573(7)	0.0247(3)	Uani
H6A	0.0752	0.4327	0.3948	0.03	Uiso
C1B	0.33615(13)	0.18122(12)	0.36949(7)	0.0218(3)	Uani
C2B	0.44429(15)	0.17386(15)	0.39974(8)	0.0306(4)	Uani
H2B	0.4548	0.2031	0.4367	0.037	Uiso
C3B	0.53721(15)	0.12392(17)	0.37611(9)	0.0361(4)	Uani
H3B	0.6107	0.1191	0.397	0.043	Uiso
C4B	0.52258(15)	0.08149(14)	0.32241(8)	0.0319(4)	Uani
H4B	0.5862	0.048	0.3062	0.038	Uiso
C5B	0.41554(15)	0.08763(13)	0.29207(7)	0.0275(3)	Uani
H5B1	0.4056	0.0579	0.2552	0.033	Uiso
C6B	0.32194(15)	0.13736(12)	0.31544(7)	0.0240(3)	Uani
H6B	0.2485	0.1413	0.2945	0.029	Uiso
C1C	0.08114(13)	0.20716(12)	0.37271(7)	0.0214(3)	Uani
C2C	0.04297(14)	0.22860(13)	0.31666(8)	0.0253(3)	Uani
H2C	0.0925	0.2654	0.293	0.03	Uiso
C3C	-0.06654(15)	0.19683(14)	0.29494(9)	0.0302(4)	Uani
H3C	-0.0917	0.2111	0.2565	0.036	Uiso
C4C	-0.13919(15)	0.14401(13)	0.32990(10)	0.0338(4)	Uani
H4C	-0.2147	0.123	0.3154	0.041	Uiso
C5C	-0.10261(15)	0.12200(14)	0.38528(9)	0.0336(4)	Uani

H5C1	-0.1527	0.0852	0.4087	0.04	Uiso
C6C	0.00757(15)	0.15332(12)	0.40733(8)	0.0266(3)	Uani
H6C	0.0325	0.1381	0.4457	0.032	Uiso

***trans*-(PPh₃)₂Pd(*p*-FC₆H₄)Br (9g)**

[SZ3021]

	x	y	z	U	
Pd1	0.25648(2)	0.37696(2)	0.22262(2)	0.00803(9)	Uani
Br1	0.25918(3)	0.27265(3)	0.42036(3)	0.01318(11)	Uani
P2	0.22243(8)	0.55933(8)	0.24024(7)	0.0095(2)	Uani
P1	0.27651(8)	0.19083(8)	0.20955(7)	0.0099(2)	Uani
F005	0.2586(3)	0.6418(2)	-0.25730(17)	0.0342(7)	Uani
C4P	0.2575(4)	0.5826(3)	-0.1512(3)	0.0180(9)	Uani
C6P	0.1611(3)	0.4544(3)	0.0069(3)	0.0142(8)	Uani
H6P	0.0947	0.4076	0.0417	0.017	Uiso
C2P	0.3506(3)	0.5324(3)	0.0115(3)	0.0137(8)	Uani
H2P	0.4156	0.5397	0.0498	0.016	Uiso
C32	0.0113(3)	0.4636(3)	0.3468(3)	0.0128(8)	Uani
H32	0.0385	0.3906	0.3424	0.015	Uiso
C19	0.3351(3)	0.5855(3)	0.3189(3)	0.0117(8)	Uani
C8	0.0444(3)	0.1536(3)	0.2782(3)	0.0148(8)	Uani
H8	0.0362	0.2364	0.2358	0.018	Uiso
C1P	0.2551(3)	0.4613(3)	0.0656(3)	0.0116(8)	Uani
C13	0.4094(3)	0.1039(3)	0.2576(3)	0.0149(8)	Uani
C31	0.0793(3)	0.5674(3)	0.3013(3)	0.0103(8)	Uani
C24	0.3172(4)	0.6539(3)	0.3797(3)	0.0149(8)	Uani
H24	0.2406	0.6826	0.388	0.018	Uiso
C30	0.1401(3)	0.7136(3)	0.0496(3)	0.0153(8)	Uani
H30	0.0753	0.6603	0.0658	0.018	Uiso
C5P	0.1617(4)	0.5142(3)	-0.1017(3)	0.0175(9)	Uani
H5P	0.097	0.5077	-0.1407	0.021	Uiso
C2	0.3572(4)	0.2416(3)	0.0056(3)	0.0173(9)	Uani
H2	0.4256	0.2687	0.0269	0.021	Uiso
C25	0.2262(3)	0.6964(3)	0.1228(3)	0.0115(8)	Uani
C7	0.1542(3)	0.0987(3)	0.2853(3)	0.0115(8)	Uani
C1	0.2657(3)	0.1886(3)	0.0789(3)	0.0121(8)	Uani
C20	0.4488(3)	0.5438(3)	0.3077(3)	0.0153(8)	Uani
H20	0.4618	0.4959	0.2673	0.018	Uiso
C33	-0.0952(3)	0.4665(3)	0.3982(3)	0.0156(8)	Uani
H33	-0.1412	0.3958	0.4278	0.019	Uiso
C3P	0.3531(4)	0.5929(3)	-0.0970(3)	0.0168(8)	Uani
H3P	0.419	0.64	-0.1328	0.02	Uiso
C36	0.0356(3)	0.6751(3)	0.3061(3)	0.0143(8)	Uani

H36	0.0786	0.7472	0.2726	0.017	Uiso
C18	0.4824(4)	0.1295(4)	0.3236(3)	0.0217(9)	Uani
H18	0.4651	0.1959	0.3429	0.026	Uiso
C6	0.1679(4)	0.1463(3)	0.0469(3)	0.0175(9)	Uani
H6	0.1068	0.1075	0.0967	0.021	Uiso
C26	0.3185(4)	0.7775(3)	0.0988(3)	0.0167(8)	Uani
H26	0.3771	0.7677	0.1487	0.02	Uiso
C34	-0.1346(3)	0.5716(4)	0.4064(3)	0.0171(8)	Uani
H34	-0.2061	0.5726	0.4441	0.02	Uiso
C9	-0.0536(4)	0.0889(4)	0.3322(3)	0.0196(9)	Uani
H9	-0.1287	0.1267	0.3251	0.024	Uiso
C29	0.1483(4)	0.8078(3)	-0.0467(3)	0.0185(9)	Uani
H29	0.0897	0.818	-0.0965	0.022	Uiso
C22	0.5242(4)	0.6398(3)	0.4151(3)	0.0203(9)	Uani
H22	0.5885	0.6592	0.4474	0.024	Uiso
C21	0.5425(4)	0.5718(3)	0.3554(3)	0.0180(9)	Uani
H21	0.6194	0.5439	0.3467	0.022	Uiso
C35	-0.0694(4)	0.6765(3)	0.3592(3)	0.0162(8)	Uani
H35	-0.0975	0.7493	0.3636	0.019	Uiso
C12	0.1654(4)	-0.0223(3)	0.3489(3)	0.0163(8)	Uani
H12	0.2398	-0.0611	0.3541	0.02	Uiso
C23	0.4111(4)	0.6803(3)	0.4283(3)	0.0198(9)	Uani
H23	0.3984	0.7261	0.4706	0.024	Uiso
C11	0.0680(4)	-0.0864(4)	0.4047(3)	0.0215(9)	Uani
H11	0.0761	-0.1687	0.4487	0.026	Uiso
C14	0.4404(3)	0.0085(3)	0.2256(3)	0.0169(8)	Uani
H14	0.3931	-0.008	0.1775	0.02	Uiso
C28	0.2409(4)	0.8876(4)	-0.0713(3)	0.0215(9)	Uani
H28	0.2464	0.9518	-0.1379	0.026	Uiso
C10	-0.0412(4)	-0.0303(4)	0.3963(3)	0.0214(9)	Uani
H10	-0.1075	-0.0742	0.4348	0.026	Uiso
C15	0.5389(4)	-0.0609(4)	0.2639(3)	0.0232(10)	Uani
H15	0.5585	-0.1257	0.2429	0.028	Uiso
C3	0.3477(4)	0.2546(4)	-0.0976(3)	0.0224(9)	Uani
H3	0.4099	0.2906	-0.147	0.027	Uiso
C27	0.3255(4)	0.8730(4)	0.0020(3)	0.0236(10)	Uani
H27	0.3884	0.9283	-0.0137	0.028	Uiso
C4	0.2484(4)	0.2155(4)	-0.1296(3)	0.0244(10)	Uani
H4	0.2417	0.2265	-0.2011	0.029	Uiso
C5	0.1586(4)	0.1604(4)	-0.0574(3)	0.0248(10)	Uani
H5	0.0909	0.1323	-0.0789	0.03	Uiso
C17	0.5808(4)	0.0589(4)	0.3620(3)	0.0311(11)	Uani
H17	0.6295	0.076	0.4088	0.037	Uiso
C16	0.6086(4)	-0.0365(4)	0.3322(3)	0.0283(11)	Uani
H16	0.6758	-0.0849	0.3591	0.034	Uiso

trans-(py)₂Pd(*p*-Et₂OCC₆H₄)Br (11i)

[SZ4127a]

	x	y	z	U	
Pd1	0.83902(2)	1.00176(2)	0.54195(2)	0.01780(9)	Uani
Br1	0.94511(2)	1.24679(4)	0.51870(2)	0.02257(10)	Uani
O2	0.49202(19)	0.4403(3)	0.61308(19)	0.0410(7)	Uani
N1	0.87658(19)	0.9817(3)	0.66228(17)	0.0205(5)	Uani
N2	0.7894(2)	1.0201(3)	0.42533(18)	0.0234(6)	Uani
O1	0.5978(2)	0.2548(3)	0.5764(2)	0.0467(7)	Uani
C1	0.7547(2)	0.8103(4)	0.55628(19)	0.0225(6)	Uani
C2	0.6640(2)	0.8353(4)	0.5778(2)	0.0282(7)	Uani
H2	0.6424	0.9441	0.5875	0.034	Uiso
C5	0.7262(2)	0.5177(4)	0.5505(2)	0.0259(7)	Uani
H5	0.7478	0.4089	0.5407	0.031	Uiso
C4	0.6350(2)	0.5431(4)	0.5723(2)	0.0239(6)	Uani
C6	0.7860(2)	0.6506(4)	0.5428(2)	0.0234(6)	Uani
H6	0.8484	0.6322	0.5283	0.028	Uiso
C6P	0.7088(2)	1.0963(4)	0.4112(2)	0.0287(7)	Uani
H6P	0.6749	1.1373	0.4567	0.034	Uiso
C7	0.5745(2)	0.3970(4)	0.5855(2)	0.0289(7)	Uani
C3	0.6038(2)	0.7024(4)	0.5854(2)	0.0302(7)	Uani
H3	0.5413	0.7211	0.5996	0.036	Uiso
C1P	0.9464(2)	0.8870(4)	0.6884(2)	0.0266(7)	Uani
H1P	0.9788	0.8223	0.6494	0.032	Uiso
C10P	0.8366(3)	0.9596(5)	0.3612(2)	0.0295(7)	Uani
H10P	0.8931	0.9037	0.3711	0.035	Uiso
C3P	0.9284(3)	0.9753(4)	0.8276(2)	0.0273(7)	Uani
H3P	0.9464	0.9729	0.884	0.033	Uiso
C2P	0.9730(3)	0.8802(5)	0.7700(2)	0.0312(8)	Uani
H2P	1.0222	0.81	0.7866	0.037	Uiso
C5P	0.8325(3)	1.0726(5)	0.7184(2)	0.0312(8)	Uani
H5P	0.7822	1.1392	0.7008	0.037	Uiso
C4P	0.8572(3)	1.0736(5)	0.8011(2)	0.0346(8)	Uani
H4P	0.8252	1.1415	0.839	0.042	Uiso
C9P	0.8051(3)	0.9765(5)	0.2813(3)	0.0406(9)	Uani
H9P	0.84	0.9348	0.2366	0.049	Uiso
C7P	0.6735(3)	1.1168(5)	0.3322(3)	0.0397(9)	Uani
H7P	0.6168	1.1726	0.3235	0.048	Uiso
C8P	0.7220(3)	1.0550(6)	0.2671(2)	0.0433(10)	Uani
H8P	0.6988	1.066	0.2125	0.052	Uiso
C8	0.4304(3)	0.3072(6)	0.6362(3)	0.0468(11)	Uani
H8A	0.4109	0.2443	0.5868	0.056	Uiso
H8B	0.4618	0.2308	0.6748	0.056	Uiso
C9	0.3515(4)	0.3813(7)	0.6752(4)	0.0672(15)	Uani
H9A	0.3083	0.2947	0.6917	0.101	Uiso
H9B	0.3716	0.443	0.7241	0.101	Uiso
H9C	0.3209	0.4564	0.6364	0.101	Uiso

***N*-Methyl-2-aminobiphenylpalladium methanesulfonate, Buchwald pre-catalyst G4**

[SZ1028BA]

	x	y	z	U	
Pd1	0.084593(12)	0.45955(2)	0.374646(18)	0.01563(7)	Uani
C1	0.19822(17)	0.4696(3)	0.3699(2)	0.0188(5)	Uani
C2	0.22908(18)	0.5899(3)	0.3449(3)	0.0221(6)	Uani
H2	0.1957	0.6645	0.3368	0.027	Uiso
C3	0.30746(18)	0.6024(3)	0.3318(3)	0.0262(6)	Uani
H3	0.3279	0.685	0.3157	0.031	Uiso
C4	0.35618(18)	0.4922(3)	0.3424(3)	0.0264(6)	Uani
H4	0.4095	0.4992	0.3311	0.032	Uiso
C5	0.32732(18)	0.3744(3)	0.3691(3)	0.0266(6)	Uani
H5	0.3615	0.3008	0.3781	0.032	Uiso
C6	0.24827(16)	0.3595(3)	0.3836(3)	0.0197(5)	Uani
C7	0.21882(18)	0.2296(3)	0.4123(3)	0.0218(6)	Uani
C8	0.2694(2)	0.1416(3)	0.4866(3)	0.0279(6)	Uani
H8	0.3236	0.1646	0.5177	0.033	Uiso
C9	0.2417(2)	0.0212(3)	0.5154(3)	0.0320(7)	Uani
H9	0.2771	-0.0374	0.5654	0.038	Uiso
C10	0.1633(2)	-0.0138(3)	0.4721(3)	0.0300(7)	Uani
H10	0.1445	-0.0962	0.4921	0.036	Uiso
C11	0.1118(2)	0.0721(3)	0.3992(3)	0.0246(6)	Uani
H11	0.0576	0.0484	0.3691	0.03	Uiso
C12	0.13911(17)	0.1926(3)	0.3699(2)	0.0192(5)	Uani
C13	0.09298(18)	0.2839(3)	0.1647(3)	0.0215(6)	Uani
H13A	0.1478	0.3096	0.1623	0.032	Uiso
H13B	0.0554	0.3467	0.1184	0.032	Uiso
H13C	0.0821	0.1974	0.1284	0.032	Uiso
C14	-0.19028(17)	0.3877(3)	0.3402(3)	0.0261(6)	Uani
H14A	-0.1965	0.3896	0.2512	0.039	Uiso
H14B	-0.2055	0.4722	0.3687	0.039	Uiso
H14C	-0.2247	0.3198	0.3628	0.039	Uiso
C1L	0.3908(3)	0.5562(5)	0.6777(4)	0.0478(10)	Uani
H1L	0.3589	0.505	0.6155	0.057	Uiso
C2L	0.3914(4)	0.5283(5)	0.7955(6)	0.0722(18)	Uani
H2L	0.3585	0.4602	0.8144	0.087	Uiso
C3L	0.4367(5)	0.5935(9)	0.8843(5)	0.097(3)	Uani
H3L	0.4358	0.5729	0.9668	0.117	Uiso
C4L	0.4866(3)	0.6940(9)	0.8588(7)	0.107(3)	Uani
H4L	0.5217	0.7385	0.9227	0.128	Uiso
C5L	0.4830(3)	0.7269(6)	0.7341(7)	0.081(2)	Uani
H5L	0.5137	0.7967	0.7125	0.097	Uiso
C6L	0.4338(3)	0.6543(5)	0.6458(4)	0.0507(11)	Uani
H6L	0.4303	0.6737	0.5619	0.061	Uiso
N1	0.08334(14)	0.2809(2)	0.2940(2)	0.0176(4)	Uani
H1	0.0327	0.2469	0.2918	0.021	Uiso

O1	-0.04389(12)	0.45902(19)	0.36675(19)	0.0191(4)	Uani
O2	-0.06996(13)	0.2262(2)	0.3704(2)	0.0247(4)	Uani
O3	-0.08510(12)	0.35876(19)	0.54203(18)	0.0196(4)	Uani
S2	-0.09001(4)	0.35435(7)	0.40821(6)	0.01759(13)	Uani

3-Bromo-2,2'-bipyridine *N*-oxide (22a)

[FW46a]

	x	y	z	U	
Br01	0.59375(3)	0.83845(2)	0.88608(2)	0.01023(7)	Uani
C1	0.3670(3)	0.7789(2)	0.86205(16)	0.0090(5)	Uani
C2	0.3385(3)	0.6474(3)	0.81970(17)	0.0120(5)	Uani
H2	0.4303	0.5858	0.8047	0.014	Uiso
C3	0.1709(3)	0.6089(3)	0.79996(18)	0.0134(5)	Uani
H3	0.1468	0.5198	0.7704	0.016	Uiso
C4	0.0397(3)	0.6991(2)	0.82301(18)	0.0123(5)	Uani
H4	-0.0743	0.6719	0.8087	0.015	Uiso
C5	0.2354(3)	0.8701(2)	0.8848(2)	0.0092(5)	Uani
C6	0.2577(3)	1.0130(3)	0.92816(17)	0.0089(4)	Uani
C7	0.2458(3)	1.0372(3)	1.03587(18)	0.0144(5)	Uani
H7	0.2163	0.9638	1.083	0.017	Uiso
C8	0.2779(3)	1.1703(3)	1.07353(19)	0.0193(5)	Uani
H8	0.2712	1.1896	1.1471	0.023	Uiso
C9	0.3200(3)	1.2747(3)	1.0028(2)	0.0189(6)	Uani
H9	0.3443	1.3668	1.0264	0.023	Uiso
C10	0.3254(4)	1.2408(3)	0.8964(2)	0.0214(6)	Uani
H10	0.3516	1.3131	0.8475	0.026	Uiso
N1	0.0713(2)	0.8270(2)	0.86613(13)	0.0092(4)	Uani
N2	0.2963(3)	1.1130(2)	0.85781(15)	0.0162(5)	Uani
O002	-0.05428(19)	0.91034(18)	0.88955(15)	0.0145(3)	Uani

3-Bromo-5-methoxy-2,2'-bipyridine *N*-oxide (22f)

[FW2058]

	x	y	z	U	
C1	0.25350(19)	0.3558(2)	0.66300(19)	0.0116(4)	Uani
C2	0.3063(2)	0.2205(2)	0.7084(2)	0.0133(5)	Uani
H2	0.2907	0.1283	0.6651	0.016	Uiso
C3	0.3828(2)	0.2269(2)	0.8201(2)	0.0133(5)	Uani
C4	0.4073(2)	0.3634(2)	0.8796(2)	0.0130(4)	Uani
H4	0.4608	0.3665	0.9556	0.016	Uiso
C5	0.27346(18)	0.4919(2)	0.7225(2)	0.0112(4)	Uani
C6	0.20926(19)	0.6376(2)	0.68760(19)	0.0117(4)	Uani

C7	0.2385(2)	0.7250(2)	0.5927(2)	0.0132(5)	Uani
H7	0.301	0.694	0.5467	0.016	Uiso
C8	0.1738(2)	0.8599(3)	0.5660(2)	0.0158(5)	Uani
H8	0.1903	0.922	0.5005	0.019	Uiso
C9	0.0854(2)	0.9012(3)	0.6369(2)	0.0155(5)	Uani
H9	0.041	0.9934	0.6222	0.019	Uiso
C10	0.0628(2)	0.8059(3)	0.7294(2)	0.0172(5)	Uani
H10	0.0017	0.8354	0.7776	0.021	Uiso
C11	0.4026(2)	-0.0406(2)	0.8352(2)	0.0171(5)	Uani
H11A	0.3139	-0.0549	0.8395	0.026	Uiso
H11B	0.4512	-0.1172	0.8853	0.026	Uiso
H11C	0.4168	-0.0504	0.7505	0.026	Uiso
N3	0.35548(16)	0.49248(19)	0.83034(17)	0.0124(4)	Uani
N4	0.12175(17)	0.6742(2)	0.75548(18)	0.0155(4)	Uani
O1	0.44036(14)	0.10723(17)	0.87989(15)	0.0173(4)	Uani
O2	0.38386(15)	0.62031(16)	0.88527(15)	0.0167(4)	Uani
Br1	0.14499(2)	0.34998(3)	0.51253(2)	0.01605(8)	Uani

3-Bromo-4-cyano-2,2'-bipyridine *N*-oxide (22n)

[FW2049F4]

	x	y	z	U	
C1	0.3800(14)	0.5107(12)	0.309(3)	0.014(2)	Uani
C2	0.4056(15)	0.5874(13)	0.280(3)	0.016(3)	Uani
C3	0.4115(15)	0.6111(13)	0.104(3)	0.016(3)	Uani
H3	0.428	0.6628	0.0779	0.019	Uiso
C4	0.3933(19)	0.5586(13)	-0.022(3)	0.026(6)	Uani
H4	0.396	0.5746	-0.1381	0.031	Uiso
C5	0.3631(15)	0.4599(12)	0.173(3)	0.014(2)	Uani
C6	0.3360(15)	0.3768(12)	0.197(3)	0.014(2)	Uani
C7	0.2569(14)	0.3651(12)	0.253(3)	0.013(4)	Uani
H7	0.2181	0.4074	0.271	0.016	Uiso
C8	0.2333(15)	0.2910(15)	0.284(3)	0.024(5)	Uani
H8	0.1775	0.2829	0.3277	0.028	Uiso
C9	0.2829(15)	0.2278(13)	0.256(3)	0.021(5)	Uani
H9	0.2616	0.1767	0.2749	0.025	Uiso
C10	0.3664(16)	0.2401(13)	0.199(3)	0.023(5)	Uani
H10	0.4044	0.1972	0.1824	0.028	Uiso
C11	0.4257(15)	0.6424(13)	0.413(3)	0.016(4)	Uani
C12	0.1187(14)	0.4902(12)	0.804(3)	0.014(4)	Uani
C13	0.0931(15)	0.4126(12)	0.768(3)	0.016(3)	Uani
C14	0.0878(14)	0.3897(13)	0.592(3)	0.016(4)	Uani
H14	0.073	0.3376	0.5601	0.019	Uiso
C15	0.1039(15)	0.4426(13)	0.470(3)	0.016(3)	Uani
H15	0.0988	0.4266	0.3531	0.019	Uiso
C16	0.1333(15)	0.5410(12)	0.676(3)	0.016(3)	Uani

C17	0.1590(15)	0.6257(13)	0.709(3)	0.017(3)	Uani
C18	0.0963(15)	0.6795(12)	0.745(3)	0.017(3)	Uani
H18	0.0353	0.6648	0.7412	0.02	Uiso
C19	0.1216(14)	0.7564(13)	0.789(3)	0.020(4)	Uani
H19	0.0806	0.7946	0.8202	0.024	Uiso
C20	0.2123(14)	0.7716(12)	0.781(3)	0.015(4)	Uani
H20	0.234	0.8228	0.8057	0.017	Uiso
C21	0.2700(14)	0.7165(13)	0.741(3)	0.020(4)	Uani
H21	0.3307	0.731	0.738	0.024	Uiso
C22	0.0791(14)	0.3572(12)	0.895(3)	0.013(4)	Uani
N1	0.3710(13)	0.4834(11)	0.008(2)	0.016(3)	Uani
N2	0.3944(16)	0.3165(13)	0.167(3)	0.033(5)	Uani
N3	0.4422(14)	0.6905(12)	0.516(2)	0.023(4)	Uani
N4	0.1267(13)	0.5171(11)	0.507(2)	0.016(3)	Uani
N5	0.2470(13)	0.6407(11)	0.705(3)	0.020(4)	Uani
N6	0.0647(14)	0.3099(11)	0.995(3)	0.022(4)	Uani
O1	0.3532(13)	0.4369(10)	-0.1181(19)	0.028(4)	Uani
O2	0.1377(11)	0.5657(8)	0.3868(18)	0.018(3)	Uani
Br1	0.37070(14)	0.47900(12)	0.5357(2)	0.0159(6)	Uani
Br2	0.12876(14)	0.52301(12)	1.0359(2)	0.0157(6)	Uani

(4-Ethoxycarbonyl-2,2'-bipyridine-N-oxide)palladium(II) acetate (C2)

[SZ2027a]

	x	y	z	U	
Pd1	0.5	0.5	0	0.01738(8)	Uani
C1	0.7951(3)	0.6084(2)	-0.00952(16)	0.0273(6)	Uani
H1	0.73	0.6298	-0.0576	0.033	Uiso
C2	0.9528(4)	0.6416(3)	0.00948(18)	0.0326(6)	Uani
H2	0.9953	0.6845	-0.0253	0.039	Uiso
C3	1.0472(4)	0.6116(3)	0.07947(18)	0.0348(7)	Uani
H3	1.1556	0.634	0.0941	0.042	Uiso
C4	0.9804(3)	0.5478(3)	0.12835(17)	0.0305(6)	Uani
H4	1.0433	0.5262	0.177	0.037	Uiso
C5	0.8222(3)	0.5157(2)	0.10615(15)	0.0230(5)	Uani
C6	0.7472(3)	0.4505(2)	0.15826(14)	0.0219(5)	Uani
C7	0.6145(3)	0.4845(2)	0.18305(15)	0.0214(5)	Uani
H7	0.5641	0.5513	0.165	0.026	Uiso
C8	0.5545(3)	0.4212(2)	0.23435(15)	0.0257(5)	Uani
C9	0.6298(4)	0.3235(3)	0.25986(18)	0.0334(6)	Uani
H9	0.5914	0.2797	0.2956	0.04	Uiso
C10	0.7597(4)	0.2907(3)	0.23319(18)	0.0345(7)	Uani
H10	0.8101	0.2235	0.2503	0.041	Uiso
C11	0.4106(4)	0.4602(3)	0.25987(18)	0.0304(6)	Uani
C12	0.2388(6)	0.4212(4)	0.3425(4)	0.0852(19)	Uani
H12A	0.2677	0.4736	0.3856	0.102	Uiso

H12B	0.157	0.4556	0.3013	0.102	Uiso
C13	0.1785(7)	0.3308(4)	0.3669(5)	0.108(3)	Uani
H13A	0.0948	0.3507	0.3935	0.162	Uiso
H13B	0.2636	0.2913	0.4024	0.162	Uiso
H13C	0.1331	0.2844	0.3228	0.162	Uiso
C14	0.5898(3)	0.2831(2)	-0.02253(17)	0.0268(5)	Uani
C15	0.6429(5)	0.1694(3)	0.0056(2)	0.0461(9)	Uani
H15A	0.6129	0.1177	-0.037	0.069	Uiso
H15B	0.591	0.1488	0.047	0.069	Uiso
H15C	0.759	0.1685	0.025	0.069	Uiso
N1	0.7307(3)	0.54646(18)	0.03800(12)	0.0212(4)	Uani
N2	0.8176(3)	0.3530(2)	0.18255(13)	0.0287(5)	Uani
O1	0.9397(3)	0.3185(2)	0.15788(13)	0.0415(6)	Uani
O2	0.5584(2)	0.34537(15)	0.03002(11)	0.0273(4)	Uani
O3	0.5814(3)	0.30995(17)	-0.08893(13)	0.0356(5)	Uani
O4	0.3334(3)	0.5373(2)	0.23479(14)	0.0371(5)	Uani
O5	0.3783(4)	0.3963(2)	0.3137(2)	0.0792(12)	Uani

(2,2'-Bipyridin-3-yl-N-oxide)palladium acetate dimer (D)

[SZ4085]

	x	y	z	U	
C1	0.1220(3)	0.6494(5)	0.4690(3)	0.0219(10)	Uani
H1	0.1024	0.6626	0.4102	0.026	Uiso
C2	0.1565(3)	0.7601(5)	0.5187(3)	0.0289(11)	Uani
H2	0.1606	0.8486	0.4942	0.035	Uiso
C3	0.1851(4)	0.7421(5)	0.6042(3)	0.0321(12)	Uani
H3	0.2109	0.817	0.6388	0.039	Uiso
C4	0.1757(3)	0.6129(5)	0.6390(3)	0.0258(11)	Uani
H4	0.1929	0.5997	0.698	0.031	Uiso
C5	0.1410(3)	0.5032(5)	0.5874(3)	0.0200(10)	Uani
C6	0.1298(3)	0.3594(5)	0.6096(3)	0.0191(9)	Uani
C7	0.1033(3)	0.2664(5)	0.5432(3)	0.0179(9)	Uani
C8	0.0906(3)	0.1288(5)	0.5611(3)	0.0228(10)	Uani
H8	0.0744	0.0635	0.517	0.027	Uiso
C9	0.1019(3)	0.0873(5)	0.6449(3)	0.0286(11)	Uani
H9	0.0928	-0.0067	0.6581	0.034	Uiso
C10	0.1261(3)	0.1813(6)	0.7080(3)	0.0298(12)	Uani
H10	0.1321	0.1517	0.7647	0.036	Uiso
C11	0.3272(3)	0.1589(5)	0.5250(3)	0.0233(10)	Uani
H11	0.2979	0.0886	0.4884	0.028	Uiso
C12	0.3635(4)	0.1263(5)	0.6074(3)	0.0293(12)	Uani
H12	0.3592	0.0348	0.6274	0.035	Uiso
C13	0.4060(4)	0.2279(6)	0.6603(3)	0.0332(12)	Uani
H13	0.4309	0.2066	0.7173	0.04	Uiso
C14	0.4128(3)	0.3620(5)	0.6308(3)	0.0242(10)	Uani

H14	0.4426	0.4325	0.667	0.029	Uiso
C15	0.3750(3)	0.3906(5)	0.5471(3)	0.0182(9)	Uani
C16	0.3731(3)	0.5243(5)	0.5047(3)	0.0166(9)	Uani
C17	0.3242(3)	0.5273(4)	0.4219(3)	0.0145(8)	Uani
C18	0.3198(3)	0.6494(5)	0.3768(3)	0.0209(10)	Uani
H18	0.2877	0.6531	0.3202	0.025	Uiso
C19	0.3628(4)	0.7654(5)	0.4153(3)	0.0295(11)	Uani
H19	0.3594	0.8499	0.385	0.035	Uiso
C20	0.4103(4)	0.7605(5)	0.4966(3)	0.0307(12)	Uani
H20	0.4397	0.8415	0.522	0.037	Uiso
C21	0.1092(3)	0.4878(5)	0.2680(3)	0.0180(9)	Uani
C22	0.0729(3)	0.5823(5)	0.1955(3)	0.0280(11)	Uani
H22A	0.0447	0.5272	0.1466	0.042	Uiso
H22B	0.1245	0.6369	0.1816	0.042	Uiso
H22C	0.0258	0.6443	0.2112	0.042	Uiso
C23	0.1310(3)	0.1075(5)	0.3425(3)	0.0189(9)	Uani
C24	0.1140(3)	-0.0342(5)	0.3050(3)	0.0222(10)	Uani
H24A	0.0791	-0.0266	0.2473	0.033	Uiso
H24B	0.0778	-0.0887	0.3387	0.033	Uiso
H24C	0.1739	-0.0798	0.3047	0.033	Uiso
N1	0.1154(3)	0.5233(4)	0.5019(2)	0.0194(8)	Uani
N2	0.1420(3)	0.3164(4)	0.6919(2)	0.0254(9)	Uani
N3	0.3321(3)	0.2894(4)	0.4946(2)	0.0208(8)	Uani
N4	0.4160(3)	0.6407(4)	0.5417(3)	0.0263(9)	Uani
O1	0.1685(3)	0.4023(4)	0.7547(2)	0.0353(9)	Uani
O2	0.4608(3)	0.6369(5)	0.6212(3)	0.0549(12)	Uani
O3	0.0550(2)	0.4637(3)	0.31815(19)	0.0226(7)	Uani
O4	0.1914(2)	0.4408(3)	0.27377(19)	0.0226(7)	Uani
O5	0.2107(2)	0.1566(3)	0.3453(2)	0.0217(7)	Uani
O6	0.0634(2)	0.1660(3)	0.3695(2)	0.0239(7)	Uani
Pd1	0.08485(2)	0.35230(3)	0.43190(2)	0.01584(11)	Uani
Pd2	0.26357(2)	0.35260(3)	0.38285(2)	0.01448(11)	Uani

[(2,2'-Bipyridine)Pd(X)(^tBu₂P(CH₃)(CH₂)], complex F(BF₄)

[FW1006]

	x	y	z	U	
C11	0.5316(8)	0.2692(7)	0.4868(6)	0.050(2)	Uani
C12	0.4912(11)	0.1685(9)	0.5315(7)	0.067(3)	Uani
H12A	0.4432	0.1195	0.4992	0.1	Uiso
H12B	0.5616	0.13	0.5531	0.1	Uiso
H12C	0.4439	0.1938	0.5698	0.1	Uiso
C13	0.6061(10)	0.3408(8)	0.5422(6)	0.059(3)	Uani
H13A	0.6776	0.3013	0.5611	0.088	Uiso
H13B	0.6293	0.4074	0.5186	0.088	Uiso
H13C	0.5587	0.359	0.5821	0.088	Uiso

C14	0.4180(10)	0.3346(9)	0.4576(8)	0.072(3)	Uani
H14A	0.3695	0.2905	0.4224	0.107	Uiso
H14B	0.3714	0.3528	0.4979	0.107	Uiso
H14C	0.442	0.4013	0.4344	0.107	Uiso
C15	0.7192(9)	0.3269(7)	0.3764(5)	0.049(2)	Uani
C16	0.8257(9)	0.3454(9)	0.4351(6)	0.057(3)	Uani
H16A	0.7955	0.371	0.4798	0.086	Uiso
H16B	0.8686	0.2771	0.4444	0.086	Uiso
H16C	0.8797	0.3997	0.4179	0.086	Uiso
C17	0.6528(11)	0.4388(8)	0.3597(8)	0.079(4)	Uani
H17A	0.586	0.4278	0.323	0.118	Uiso
H17B	0.6231	0.4666	0.404	0.118	Uiso
H17C	0.7085	0.4911	0.342	0.118	Uiso
C18	0.7812(10)	0.2867(11)	0.3091(6)	0.072(3)	Uani
H18A	0.7208	0.2727	0.2689	0.108	Uiso
H18B	0.8363	0.3424	0.2949	0.108	Uiso
H18C	0.8253	0.2198	0.3215	0.108	Uiso
C19	0.5200(8)	0.1573(7)	0.3295(5)	0.045(2)	Uani
C20	0.4107(8)	0.0939(8)	0.3533(6)	0.055(2)	Uani
H20A	0.4359	0.0488	0.3953	0.083	Uiso
H20B	0.35	0.1453	0.366	0.083	Uiso
H20C	0.3777	0.0477	0.3136	0.083	Uiso
C21	0.4767(10)	0.2273(9)	0.2632(6)	0.063(3)	Uani
H21A	0.5438	0.268	0.2471	0.095	Uiso
H21B	0.4432	0.1802	0.224	0.095	Uiso
H21C	0.4155	0.2778	0.2765	0.095	Uiso
C22	0.6164(8)	0.0680(7)	0.3185(5)	0.046(2)	Uani
H22A	0.6655	0.0891	0.2794	0.055	Uiso
H22B	0.5779	-0.0024	0.3059	0.055	Uiso
B1	0.8620(12)	0.9609(11)	0.1505(6)	0.058(3)	Uani
F1	0.7652(14)	0.9984(17)	0.1713(5)	0.245(10)	Uani
F2	0.9608(15)	0.9974(14)	0.1830(5)	0.188(7)	Uani
F3	0.8653(8)	0.9666(9)	0.0750(4)	0.112(3)	Uani
F4	0.8841(16)	0.8644(11)	0.1700(9)	0.201(7)	Uani
C1	0.8458(8)	0.0950(10)	0.5810(5)	0.054(2)	Uani
H1	0.8183	0.1675	0.5759	0.065	Uiso
C2	0.9054(9)	0.0623(14)	0.6479(5)	0.081(5)	Uani
H2	0.9191	0.1128	0.6863	0.098	Uiso
C3	0.9444(12)	-0.0464(15)	0.6570(7)	0.093(5)	Uani
H3	0.9849	-0.0712	0.7009	0.111	Uiso
C4	0.9202(9)	-0.1143(12)	0.5983(7)	0.071(4)	Uani
H4	0.9424	-0.1882	0.6034	0.086	Uiso
C5	0.8641(7)	-0.0793(8)	0.5311(5)	0.046(2)	Uani
C6	0.8467(7)	-0.1486(7)	0.4664(6)	0.047(2)	Uani
C7	0.8850(9)	-0.2576(9)	0.4614(10)	0.090(5)	Uani
H7	0.9153	-0.2942	0.5041	0.108	Uiso
C8	0.8796(10)	-0.3113(9)	0.3971(9)	0.085(5)	Uani
H8	0.9049	-0.3846	0.3962	0.102	Uiso

C9	0.8363(10)	-0.2589(10)	0.3305(11)	0.110(7)	Uani
H9	0.8364	-0.2931	0.2848	0.132	Uiso
C10	0.7936(8)	-0.1524(8)	0.3389(6)	0.056(3)	Uani
H10	0.7595	-0.1164	0.2968	0.067	Uiso
N1	0.8259(6)	0.0255(6)	0.5226(4)	0.0417(17)	Uani
N2	0.7977(6)	-0.0982(6)	0.4017(4)	0.0426(17)	Uani
P1	0.61998(18)	0.21636(16)	0.40921(12)	0.0339(5)	Uani
Pd1	0.72126(5)	0.05711(5)	0.41730(3)	0.0326(2)	Uani

Complex G

[SZ2032b]

	x	y	z
PD1	0.26553	0.336102	0.771642
C16	0.126173	0.487508	0.655496
P1	0.320268	0.153533	0.812032
N2	0.209095	0.485747	0.6965
C10	0.243107	0.662991	0.618636
H10	0.284154	0.722085	0.607389
N1	0.015898	0.323563	0.626052
C17	0.160726	0.663452	0.575416
H17	0.145009	0.722032	0.534618
O2	0.035624	0.32202	0.549526
C1	0.222058	0.203964	0.68514
H1A	0.164561	0.172064	0.694241
H1B	0.218588	0.236427	0.629401
C2	0.295885	0.101996	0.700924
C9	0.266873	0.57435	0.680014
H9	0.32309	0.576519	0.709767
C14	-0.021814	0.321555	0.788785
H14	-0.034495	0.321996	0.84313
C3	0.247929	0.073963	0.882778
O1	0.318729	0.462161	0.867054
C6	0.47616	0.008661	0.83571
H6A	0.466649	-0.006471	0.777258
H6B	0.444887	-0.051803	0.863761
H6C	0.53829	0.003619	0.854848
C12	0.062201	0.399371	0.683715
C11	0.099453	0.572726	0.593949
H11	0.042583	0.570256	0.565543
C7	0.494983	0.234409	0.811507
H7A	0.488144	0.220801	0.752872
H7B	0.556543	0.229533	0.832923
H7C	0.472654	0.314479	0.822791
C15	-0.048463	0.247795	0.651019
H15	-0.079685	0.195708	0.61256

C13	0.044601	0.397154	0.764913
H13	0.077396	0.446596	0.804024
C8	0.442706	0.135026	0.853357
C5	0.248513	0.146573	0.962579
H5A	0.230837	0.229942	0.94988
H5B	0.307079	0.14593	0.992254
H5C	0.207994	0.109692	0.995987
C4	0.277142	-0.060894	0.90291
H4A	0.337458	-0.061698	0.928469
H4B	0.272246	-0.10805	0.852745
H4C	0.239769	-0.096236	0.939952
C18	0.457377	0.163877	0.944053
H18A	0.434897	0.244592	0.953301
H18B	0.519588	0.161199	0.963183
H18C	0.427034	0.104296	0.973695
C19	0.152229	0.073657	0.843674
H19A	0.133286	0.156663	0.83146
H19B	0.115836	0.037602	0.881304
H19C	0.146959	0.02651	0.793494
C20	-0.067793	0.24717	0.731516
H20	-0.112106	0.196067	0.746566
C21	0.369025	0.13327	0.650147
H21A	0.388395	0.216258	0.661755
H21B	0.347512	0.125615	0.592466
H21C	0.417762	0.077861	0.663871
C22	0.266203	-0.032564	0.683529
H22A	0.219471	-0.052553	0.715701
H22B	0.315425	-0.086807	0.698246
H22C	0.245278	-0.041899	0.625838
O3	0.191223	0.544571	0.938015
C24	0.371025	0.613798	0.956072
H24A	0.343382	0.677769	0.984385
H24B	0.410464	0.649842	0.921232
H24C	0.403826	0.56065	0.995803
C23	0.294457	0.533331	0.899063

Complex I

[SZ2081c]

	x	y	z	U	
Pd1	0.63181(4)	0.63804(4)	0.68089(3)	0.03134(15)	Uani
Br2	1.02801(7)	0.62203(5)	0.78307(4)	0.0475(2)	Uani
Pd3	0.88804(4)	0.61801(4)	0.65451(3)	0.03323(15)	Uani
Br4	0.56107(7)	0.79691(5)	0.66511(4)	0.0434(2)	Uani
Br3	0.38783(7)	0.59778(6)	0.75913(5)	0.0503(2)	Uani
Br1	1.12739(7)	0.65972(7)	0.56852(5)	0.0601(3)	Uani

C11	0.7329(6)	0.6584(5)	0.8552(4)	0.0403(17)	Uani
H11	0.8015	0.6699	0.8355	0.048	Uiso
N1	0.6270(5)	0.6417(4)	0.8036(3)	0.0357(13)	Uani
N2	0.9490(5)	0.7491(4)	0.6229(3)	0.0374(14)	Uani
N4	0.7115(4)	0.5109(4)	0.6999(3)	0.0318(13)	Uani
C16	0.8866(6)	0.8216(5)	0.6400(4)	0.0419(18)	Uani
H16	0.8201	0.8115	0.6624	0.05	Uiso
C4	0.5444(6)	0.6281(5)	0.5022(4)	0.0411(17)	Uani
C8	0.6402(8)	0.6414(6)	0.9641(4)	0.059(2)	Uani
H8	0.6446	0.6427	1.0185	0.071	Uiso
C14	1.0421(6)	0.7646(5)	0.5902(4)	0.0410(17)	Uani
C7	0.5296(7)	0.6217(6)	0.9135(5)	0.051(2)	Uani
C3	0.8763(6)	0.4164(5)	0.6888(4)	0.0386(17)	Uani
C5	0.7764(7)	0.6054(5)	0.4823(4)	0.049(2)	Uani
H5	0.8547	0.595	0.4764	0.059	Uiso
C2	0.8184(7)	0.3440(5)	0.7159(4)	0.0439(18)	Uani
H2	0.8525	0.2861	0.7185	0.053	Uiso
C9	0.7400(7)	0.6586(6)	0.9359(4)	0.052(2)	Uani
H9	0.8125	0.6703	0.9704	0.063	Uiso
C1	0.6584(6)	0.4398(5)	0.7301(4)	0.0368(16)	Uani
H1	0.5851	0.4485	0.7449	0.044	Uiso
C13	1.0803(7)	0.8511(6)	0.5736(4)	0.047(2)	Uani
C10	0.5310(6)	0.6236(5)	0.8337(4)	0.0407(17)	Uani
C15	0.9167(7)	0.9097(5)	0.6258(4)	0.0476(19)	Uani
H15	0.872	0.9586	0.6384	0.057	Uiso
C17	1.0151(7)	0.9239(5)	0.5923(4)	0.051(2)	Uani
H17	1.0376	0.983	0.5823	0.061	Uiso
C6	0.4188(8)	0.6018(8)	0.9436(6)	0.084(3)	Uani
H6A	0.4365	0.6042	1.0004	0.126	Uiso
H6B	0.3899	0.5421	0.9265	0.126	Uiso
H6C	0.3586	0.6464	0.9232	0.126	Uiso
C12	1.1873(8)	0.8670(6)	0.5364(6)	0.071(3)	Uani
H12A	1.1989	0.9313	0.5311	0.107	Uiso
H12B	1.1736	0.8388	0.4852	0.107	Uiso
H12C	1.2574	0.8409	0.5694	0.107	Uiso
N3	0.7543(5)	0.6164(4)	0.5545(3)	0.0340(13)	Uani
C21	0.8203(6)	0.5024(4)	0.6832(4)	0.0314(15)	Uani
C22	0.6417(6)	0.6269(5)	0.5674(4)	0.0351(16)	Uani
C20	0.7112(6)	0.3564(5)	0.7389(4)	0.0408(17)	Uani
H20	0.6752	0.3082	0.7603	0.049	Uiso
C23	0.4189(7)	0.6355(6)	0.5130(5)	0.056(2)	Uani
H23A	0.4184	0.6392	0.5685	0.085	Uiso
H23B	0.3745	0.5828	0.4908	0.085	Uiso
H23C	0.3827	0.6894	0.4868	0.085	Uiso
C25	0.6860(8)	0.6093(5)	0.4164(4)	0.055(2)	Uani
H25	0.702	0.6049	0.3658	0.066	Uiso
C19	0.9947(7)	0.4067(6)	0.6639(5)	0.053(2)	Uani
H19A	1.0187	0.4648	0.6468	0.079	Uiso

H19B	0.9868	0.3637	0.6212	0.079	Uiso
H19C	1.0541	0.3854	0.7079	0.079	Uiso
C24	0.5698(8)	0.6200(6)	0.4278(5)	0.056(2)	Uani
H24	0.507	0.6218	0.3838	0.067	Uiso

10.12 Cartesian Coordinates of calculated structures

10.12.1 Reactants and products

THF							
	x	y	z				
O	0	0	1.249114	H	0.494225	0.845491	-1.738203
C	0	-1.165518	0.421005	H	-1.172505	0.92731	-2.372257
C	0.319436	-0.691248	-0.986117	H	-2.210781	2.515131	0.752648
C	-0.319436	0.691248	-0.986117	H	-0.485277	2.935055	0.833568
C	0	1.165518	0.421005	H	-2.274952	-3.785064	-1.49009
H	0.992343	1.642488	0.458944	H	-1.721755	-2.934503	-2.938638
H	-0.728225	1.880798	0.819567	H	-3.965402	-2.026719	-1.718416
H	-0.992343	-1.642488	0.458944	H	-2.734867	-0.83291	-2.156592
H	0.728225	-1.880798	0.819567	H	-3.151805	-2.147179	0.573775
H	-0.06997	-1.358444	-1.758628	H	-2.853245	-0.424033	0.231864
H	1.403184	-0.608319	-1.125668	H	2.085734	-2.432708	0.513149
H	-1.403184	0.608319	-1.125668	H	4.391741	-2.541138	-0.320852
H	0.06997	1.358444	-1.758628	H	5.622754	-0.457625	-0.88545
				H	4.505441	1.74314	-0.600371
				H	2.196501	1.863545	0.229312

16a(thf) ₂				16d(thf) ₂			
	x	y	z		x	y	z
Zn	-0.019371	-0.143303	1.030789	Zn	-0.581934	-0.254465	1.077208
Cl	-1.494357	0.281591	2.846489	Cl	-2.135677	-0.069268	2.845186
O	-0.973566	1.288146	-0.34341	O	-1.658096	1.028831	-0.349401
O	-1.208464	-1.65229	0.047457	O	-1.417118	-1.926598	-0.060036
C	-0.309521	2.885358	-1.957368	O	5.4356	0.580245	-0.365922
C	-0.45116	1.398704	-1.692357	C	6.281756	-0.530329	-0.594466
C	-1.394495	3.479433	-1.065354	C	-1.382953	2.963898	-1.652357
C	-1.294536	2.606914	0.165829	C	-0.986613	1.508648	-1.539528
C	-0.695103	-2.36975	-1.102209	C	-2.813717	2.930884	-1.126967
C	-1.92039	-2.821655	-1.871083	C	-2.710268	1.956441	0.028135
C	-2.929657	-1.725008	-1.550634	C	-0.799779	-2.103933	-1.363129
C	-2.638323	-1.444664	-0.09359	C	-1.939812	-2.329315	-2.340488
C	2.597693	-1.499075	0.273484	C	-3.113442	-1.629022	-1.663325
C	3.908905	-1.573467	-0.199017	C	-2.861434	-1.941628	-0.206527
C	4.601313	-0.406734	-0.516015	C	2.241924	-1.121235	0.373117
C	3.972468	0.826254	-0.355749	C	3.592452	-0.973751	0.041746
C	2.660325	0.881166	0.116673	C	4.134709	0.309297	-0.052087
C	1.929193	-0.274692	0.4465	C	3.318976	1.420494	0.18579
H	-0.067573	-3.18814	-0.738854	C	1.980584	1.236447	0.513325
H	-0.06396	-1.685328	-1.686143	C	1.38678	-0.037733	0.620349
H	-2.379165	3.368483	-1.531688	H	7.26866	-0.122957	-0.813398
H	-1.241368	4.536908	-0.841536	H	6.346171	-1.179072	0.287973
H	0.678292	3.238638	-1.64183	H	5.942077	-1.131593	-1.447352
H	-0.430861	3.130143	-3.01441	H	-0.101508	-2.943117	-1.298168

H	-0.220414	-1.197715	-1.587576
H	-3.49029	2.542671	-1.896682
H	-3.187375	3.906934	-0.811509
H	-0.749693	3.581573	-1.005941
H	-1.300607	3.342703	-2.672856
H	0.084922	1.327592	-1.409168
H	-1.343995	0.923772	-2.400462
H	-3.619613	1.377574	0.214291
H	-2.415476	2.444284	0.964439
H	-2.147352	-3.399223	-2.444567
H	-1.71341	-1.935966	-3.334115
H	-4.085052	-1.989635	-2.007083
H	-3.068771	-0.546965	-1.827322
H	-3.22343	-2.940332	0.068079
H	-3.265177	-1.213642	0.502516
H	1.85701	-2.140701	0.436747
H	4.20523	-1.851621	-0.139719
H	3.757467	2.412491	0.109099
H	1.377089	2.12966	0.689703

19a(thf)₂

	x	y	z
I	2.321726	1.807616	0.002076
Zn	-0.077274	0.52695	-0.223067
O	0.331005	-1.248899	1.020519
O	0.184276	-0.825494	-1.921306
C	-0.423456	-2.307028	2.973547
C	-0.773682	-2.038562	1.528618
C	1.088884	-2.479063	2.889599
C	1.483115	-1.406311	1.893666
C	-0.937835	-1.740593	-2.060483
C	-0.335455	-3.096787	-2.371242
C	1.039683	-3.010475	-1.717241
C	1.4249	-1.576241	-2.003445
C	-2.928649	1.037164	-1.161158
C	-4.295466	1.287822	-1.031149
C	-4.864252	1.403039	0.235693
C	-4.057254	1.266681	1.363181
C	-2.692256	1.017129	1.2144
C	-2.083941	0.88925	-0.047388
H	-1.596076	-1.353954	-2.8432
H	-1.496609	-1.738335	-1.114878
H	1.334381	-3.473304	2.500144
H	1.597308	-2.357733	3.847926
H	-0.679929	-1.440551	3.59319
H	-0.941023	-3.180236	3.375266
H	-1.690912	-1.463427	1.369862

H	-0.832771	-2.970302	0.946457
H	2.347234	-1.664652	1.273322
H	1.678442	-0.439824	2.371796
H	-0.232734	-3.232985	-3.452583
H	-0.949069	-3.915117	-1.987719
H	1.757337	-3.725798	-2.123308
H	0.966177	-3.169746	-0.635785
H	1.831961	-1.454241	-3.014883
H	2.124883	-1.132746	-1.289034
H	-2.515118	0.954312	-2.167848
H	-4.918271	1.394663	-1.917238
H	-5.928427	1.598757	0.343329
H	-4.492264	1.357978	2.356442
H	-2.086042	0.914088	2.117439

16a(tmeda)

	x	y	z
Zn	0.200652	-0.524983	0.123822
Cl	1.326922	-2.606194	0.553573
N	1.394244	0.319702	-1.583295
N	1.447362	0.967705	1.283975
C	0.501202	1.155965	-2.395664
C	0.583034	1.678554	2.233545
C	2.552718	0.330235	2.011238
C	1.974892	-0.735971	-2.421586
C	2.462156	1.130212	-0.962787
C	1.954915	1.888566	0.248229
C	-2.366573	1.146226	-0.086383
C	-3.74207	1.377448	-0.143358
C	-4.629744	0.307403	-0.052549
C	-4.128754	-0.984051	0.096893
C	-2.749969	-1.194419	0.153396
C	-1.82075	-0.141923	0.063713
H	1.169814	-1.317414	-2.877079
H	2.600219	-0.31527	-3.222709
H	2.571561	-1.405658	-1.798943
H	0.062129	1.951296	-1.788931
H	1.038722	1.613005	-3.239621
H	-0.316727	0.544019	-2.782673
H	0.202077	0.970933	2.973654
H	1.125079	2.478298	2.759415
H	-0.269928	2.112628	1.705105
H	3.263458	0.444545	-0.66825
H	2.895103	1.830121	-1.693513
H	1.129505	2.551356	-0.035946
H	2.752079	2.53176	0.651407
H	-2.391224	-2.218169	0.271171

H	2.146855	-0.3701	2.743063
H	3.181474	-0.242998	1.328022
H	3.167982	1.080029	2.530691
H	-1.703756	2.012394	-0.164675
H	-4.122718	2.390566	-0.2593
H	-5.702688	0.479009	-0.097566
H	-4.813836	-1.826879	0.168391

[16al(thf)]⁻

	x	y	z
I	-1.647997	-1.629703	-0.507912
Zn	0.190701	-0.162361	0.828235
Cl	-0.565429	0.274496	2.939591
O	-0.457117	1.831688	-0.028217
C	2.944886	0.885529	0.473101
C	4.248009	0.947011	-0.007836
C	4.736599	-0.068503	-0.818562
C	3.910155	-1.136294	-1.141174
C	2.608049	-1.180629	-0.653756
C	2.082173	-0.176642	0.168553
C	-1.752372	2.361938	0.322162
C	-2.257213	3.056421	-0.924657
C	-1.627361	2.220009	-2.02958
C	-0.261529	1.922554	-1.454079
H	2.594316	1.696268	1.104217
H	4.883377	1.785017	0.249218
H	5.749853	-0.028369	-1.194757
H	4.280609	-1.933371	-1.773403
H	1.984232	-2.024385	-0.930028
H	-1.62504	3.019491	1.178774
H	-2.395291	1.529141	0.616767
H	-1.890923	4.081616	-0.967285
H	-3.34197	3.085018	-0.968512
H	-1.575307	2.730432	-2.986876
H	-2.181782	1.291037	-2.161574
H	0.45294	2.724522	-1.65376
H	0.168637	0.980365	-1.792855

[16al(tmeda)]⁻

	x	y	z
I	-2.174563	-1.290305	-0.886769
Zn	-0.236954	-0.213357	0.711171
Cl	-0.946827	-0.465991	2.983596
N	-0.877267	1.945822	0.57555
N	1.260451	1.526121	-1.513258
C	0.027568	2.648931	1.492234

C	2.690798	1.729353	-1.509262
C	0.847246	0.748171	-2.660373
C	-2.253362	2.052678	1.079493
C	-0.862684	2.543281	-0.779854
C	0.510139	2.756098	-1.378686
C	2.06921	-1.75391	-0.45946
C	3.399274	-2.12568	-0.629941
C	4.384839	-1.573349	0.177539
C	4.020494	-0.658949	1.156997
C	2.685502	-0.302805	1.315232
C	1.665049	-0.8259	0.509016
H	-2.315828	1.592243	2.06029
H	-2.560745	3.101356	1.143524
H	-2.922715	1.527535	0.402153
H	1.06123	2.475655	1.203243
H	-0.167128	3.726469	1.506564
H	-0.119095	2.246663	2.491011
H	3.192431	0.761993	-1.501556
H	3.049556	2.297228	-2.382502
H	2.988571	2.265294	-0.609492
H	-1.469144	1.892725	-1.412594
H	-1.369427	3.515368	-0.740781
H	1.081165	3.440478	-0.752319
H	0.378083	3.27479	-2.342325
H	2.439392	0.409544	2.097375
H	1.351033	-0.216785	-2.643428
H	-0.223868	0.558987	-2.628583
H	1.085158	1.247518	-3.613483
H	1.324941	-2.206216	-1.107928
H	3.667558	-2.848931	-1.390299
H	5.420908	-1.857213	0.050222
H	4.777722	-0.227049	1.799738

ZnClI(thf)₂

	x	y	z
I	2.243241	-1.082615	-0.45025
Zn	0.014429	-0.340352	0.805367
Cl	-0.789134	-0.235037	2.992928
O	-0.273659	1.656838	0.135031
O	-1.740823	-0.664363	-0.299585
C	0.605683	3.019653	-1.580902
C	-0.339475	1.869663	-1.303948
C	0.526555	3.826004	-0.289877
C	0.477239	2.736356	0.756619
C	-1.990703	-1.500925	-1.457814
C	-3.49562	-1.657622	-1.501373
C	-3.975009	-0.325078	-0.934378

C	-2.98353	-0.078047	0.18027
H	-0.390473	4.423507	-0.263939
H	1.374703	4.49801	-0.146512
H	1.622758	2.642142	-1.732842
H	0.317483	3.587011	-2.467657
H	-0.059615	0.93479	-1.800323
H	-1.380898	2.106976	-1.554879
H	-0.041603	3.003286	1.679445
H	1.479547	2.362863	1.005499
H	-1.435323	-2.432483	-1.327682
H	-1.604682	-0.979174	-2.343438
H	-3.81241	-2.482741	-0.855378
H	-3.861635	-1.856088	-2.510234
H	-5.003405	-0.354382	-0.570007
H	-3.905747	0.461722	-1.693401
H	-3.261402	-0.584948	1.111168
H	-2.781659	0.974457	0.397496

ZnClI(tmeda)

	x	y	z
I	-2.416695	-0.018169	-0.067768
Zn	0.236706	-0.030364	0.57022
Cl	1.279983	-0.229734	2.675516
N	1.340318	-1.402365	-0.783164
N	1.273309	1.538993	-0.556461
C	2.000715	-2.486464	-0.040509
C	0.369883	2.633809	-0.944685
C	2.351509	-0.524661	-1.420766
C	0.450213	-1.984205	-1.800116
C	1.774138	0.836667	-1.762604
C	2.387582	2.08281	0.23773
H	0.928026	0.728346	-2.451203
H	2.526076	1.453463	-2.274224
H	1.241738	-3.122238	0.418514
H	2.618407	-3.101881	-0.709166
H	2.62195	-2.065865	0.752775
H	-0.000648	3.131478	-0.046198
H	0.887427	3.373907	-1.569965
H	-0.483396	2.229182	-1.493344
H	3.187152	-0.418915	-0.72081
H	2.75279	-1.001024	-2.326733
H	-0.060839	-1.197346	-2.358481
H	1.016809	-2.612898	-2.500539
H	-0.313673	-2.589506	-1.307641
H	3.051462	1.282727	0.569328
H	2.963607	2.81441	-0.346277
H	1.987463	2.571346	1.128372

ZnCl₂(thf)₂

	x	y	z
Zn	0.15959	0.990889	0.193242
Cl	0.541217	0.798247	2.480321
Cl	0.333563	2.705998	-1.34254
O	-1.553067	-0.181278	-0.033767
O	1.18973	-0.650005	-0.661357
C	-2.466445	-0.60815	1.013419
C	-3.719839	-1.035217	0.279572
C	-3.165762	-1.543968	-1.047971
C	-2.075443	-0.538423	-1.340031
C	1.043891	-1.912016	0.057832
C	2.380339	-2.614511	-0.082549
C	3.354924	-1.451017	-0.227907
C	2.569289	-0.500042	-1.099988
H	-2.600931	0.22623	1.704725
H	-1.992792	-1.437545	1.552321
H	-4.377318	-0.175881	0.113337
H	-4.282378	-1.790041	0.831722
H	-3.913582	-1.586554	-1.841678
H	-2.739895	-2.54579	-0.92651
H	-2.46051	0.370079	-1.818021
H	-1.238536	-0.921119	-1.930859
H	0.203342	-2.454802	-0.383819
H	0.808025	-1.670381	1.101021
H	2.395841	-3.23749	-0.982584
H	2.596205	-3.255293	0.774132
H	4.307574	-1.737568	-0.677349
H	3.559081	-0.993593	0.746243
H	2.618953	-0.772663	-2.160617
H	2.838932	0.553905	-0.994886

2a

	x	y	z
I	1.512789	-1.655478	-2.41907
Pd	-0.068138	-0.288	-0.571824
P	-1.369783	0.801866	0.945727
P	1.779031	0.49067	0.761859
C	-2.468992	-0.332586	-2.463702
C	-3.652771	-0.850638	-2.997175
C	-4.198138	-2.026399	-2.486832
C	-3.553856	-2.684549	-1.440447
C	-2.375092	-2.164547	-0.906705
C	-1.817085	-0.988115	-1.416397
C	4.48905	0.615747	0.025013
C	5.605174	1.240963	-0.523394
C	5.528475	2.563068	-0.954295

C	4.325915	3.258237	-0.845264	H	-0.203913	0.295763	3.008652
C	3.206607	2.636201	-0.303391	H	-0.83005	1.945976	3.040534
C	3.281049	1.312813	0.153499	H	0.939201	2.667793	1.43024
C	3.273357	-0.612088	2.892308	H	1.714571	1.872382	2.800933
C	3.640486	-1.643716	3.749426				
C	3.088088	-2.914896	3.590452				
C	2.172403	-3.155773	2.569886	2f			
C	1.806442	-2.125465	1.707164		x	y	z
C	2.350378	-0.845379	1.862868	I	1.303857	-2.181082	-2.099325
C	-2.790809	3.219664	1.125321	Pd	-0.003275	-0.383676	-0.414212
C	-3.170056	4.479066	0.6751	P	-1.089707	1.083928	0.943833
C	-2.693161	4.957433	-0.545305	P	2.003675	0.485614	0.590306
C	-1.835783	4.176588	-1.316004	C	-5.887761	-2.244952	-2.104652
C	-1.456591	2.912913	-0.870032	C	-2.571603	-0.361709	-2.049165
C	-1.932593	2.425159	0.35195	C	-3.859477	-0.770881	-2.406028
C	-4.092383	0.174668	1.03836	C	-4.497543	-1.818172	-1.739537
C	-5.182492	-0.589832	1.440341	C	-3.79947	-2.454585	-0.705487
C	-5.022065	-1.588583	2.39819	C	-2.517458	-2.047918	-0.344476
C	-3.765438	-1.825836	2.951568	C	-1.882407	-0.997097	-1.015207
C	-2.67132	-1.066117	2.550241	C	4.611893	0.292592	-0.439183
C	-2.829329	-0.048801	1.600362	C	5.674663	0.715087	-1.232152
C	-0.318341	1.208539	2.412966	C	5.59033	1.911705	-1.938518
C	1.043192	1.709045	1.951414	C	4.431734	2.682561	-1.859652
H	-5.120837	-2.425959	-2.899646	C	3.365361	2.262636	-1.071836
H	-2.058387	0.587361	-2.877446	C	3.451465	1.07079	-0.338107
H	-4.148252	-0.329382	-3.813592	C	3.746935	-0.247761	2.68577
H	-3.972968	-3.601972	-1.031703	C	4.16317	-1.067962	3.728392
H	-1.897985	-2.678645	-0.072154	C	3.475734	-2.250041	4.003866
H	4.557138	-0.416616	0.359386	C	2.374818	-2.613445	3.232949
H	6.537501	0.690973	-0.61325	C	1.960938	-1.797804	2.182232
H	6.401439	3.04871	-1.380745	C	2.642309	-0.607843	1.901196
H	4.257002	4.287098	-1.186463	C	-2.307682	3.61306	0.68878
H	2.269897	3.186422	-0.242677	C	-2.566907	4.80465	0.019752
H	3.712076	0.37633	3.015944	C	-2.061498	5.010838	-1.263562
H	4.358771	-1.457512	4.54262	C	-1.299713	4.023087	-1.882155
H	3.376449	-3.71836	4.262374	C	-1.044823	2.825702	-1.218706
H	1.745922	-4.145978	2.440247	C	-1.544734	2.612392	0.070917
H	1.102136	-2.305047	0.894801	C	-3.837399	0.747035	1.319126
H	-3.171279	2.84564	2.073748	C	-4.951706	0.172757	1.921569
H	-3.838373	5.088471	1.276094	C	-4.800152	-0.640817	3.042037
H	-2.993245	5.940937	-0.895365	C	-3.528601	-0.881819	3.559113
H	-1.464152	4.547713	-2.266285	C	-2.41072	-0.312935	2.958209
H	-0.788732	2.291081	-1.465527	C	-2.557832	0.517313	1.839274
H	-4.21784	0.935902	0.272224	C	0.112925	1.661315	2.225345
H	-6.157234	-0.410406	0.996326	C	1.450472	1.966084	1.564217
H	-5.873658	-2.187241	2.707598	H	-5.930507	-3.306728	-2.370388
H	-3.633805	-2.608361	3.692863	H	-6.586249	-2.10549	-1.271289
H	-1.689527	-1.283487	2.966162	H	-6.272611	-1.675431	-2.954831

H	-2.114029	0.465061	-2.59103	C	-4.209364	-0.900029	-0.207917
H	-4.379557	-0.261069	-3.21659	C	-5.240903	-1.259476	-1.069572
H	-4.274166	-3.274666	-0.16678	C	-5.026953	-2.217498	-2.057666
H	-2.015454	-2.553928	0.480324	C	-3.773742	-2.814788	-2.182413
H	4.685863	-0.644546	0.106677	C	-2.7395	-2.456204	-1.323992
H	6.570553	0.104661	-1.297031	C	-2.949326	-1.502257	-0.317779
H	6.421363	2.240109	-2.555771	C	-3.162216	-1.044175	2.971934
H	4.355798	3.612479	-2.415775	C	-3.651314	-0.564568	4.182286
H	2.460623	2.866354	-1.034501	C	-3.249037	0.686147	4.651452
H	4.285913	0.673544	2.471842	C	-2.361916	1.458991	3.90745
H	5.023482	-0.785125	4.327873	C	-1.874265	0.982665	2.692162
H	3.80148	-2.888037	4.820485	C	-2.268199	-0.27252	2.216261
H	1.840226	-3.53496	3.444085	C	3.091566	-3.041422	-0.659184
H	1.105878	-2.080009	1.567802	C	3.326543	-3.988748	-1.651221
H	-2.705379	3.454698	1.689295	C	2.52096	-4.026726	-2.789124
H	-3.16234	5.574592	0.501528	C	1.484373	-3.109064	-2.940119
H	-2.265428	5.94348	-1.781758	C	1.253746	-2.154348	-1.952858
H	-0.90736	4.180325	-2.882358	C	2.048091	-2.118091	-0.799709
H	-0.455809	2.04185	-1.695466	C	4.05931	0.362079	0.544744
H	-3.958285	1.365677	0.433219	C	5.268684	0.779145	1.08686
H	-5.939173	0.353235	1.506377	C	5.638067	0.373934	2.368842
H	-5.670401	-1.093168	3.508667	C	4.793195	-0.452736	3.104799
H	-3.404964	-1.520926	4.428511	C	3.579821	-0.875926	2.565259
H	-1.421726	-0.534259	3.354799	C	3.202158	-0.472802	1.278453
H	0.229378	0.858462	2.962761	C	0.748916	-1.995896	1.742247
H	-0.291135	2.53408	2.749224	C	-0.616158	-2.394099	1.189214
H	1.350828	2.811915	0.87371	H	-0.927735	3.621518	0.184785
H	2.208328	2.237947	2.306356	H	-2.786755	5.039918	-0.584111
				H	-4.395721	4.193136	-2.282168
				H	-4.122535	1.887657	-3.182443
				H	-2.301073	0.448424	-2.383569
				H	4.420527	4.229963	-2.135464
				H	1.798966	0.908182	-2.871421
				H	3.669238	2.346884	-3.576458
				H	3.239424	4.678206	0.007245
				H	1.357486	3.256592	0.711708
				H	-4.379009	-0.139442	0.550378
				H	-6.213013	-0.784905	-0.970978
				H	-5.831933	-2.49524	-2.732003
				H	-3.598801	-3.559859	-2.953195
				H	-1.761099	-2.916134	-1.450416
				H	-3.483811	-2.017405	2.6049
				H	-4.346237	-1.166305	4.761114
				H	-3.631811	1.057833	5.597616
				H	-2.050242	2.434083	4.27049
				H	-1.184927	1.57942	2.094962
				H	3.720761	-3.015298	0.2287
				H	4.139003	-4.700663	-1.535829
cis-I-2aa							
	x	y	z				
Pd	0.008106	0.649923	-0.295842				
P	1.616329	-0.918893	0.51095				
P	-1.547745	-0.879784	0.656499				
C	-1.630342	3.221177	-0.546733				
C	-2.677616	4.033543	-0.984925				
C	-3.579944	3.562198	-1.937382				
C	-3.423294	2.273098	-2.441836				
C	-2.380101	1.462638	-1.9889				
C	-1.461439	1.915689	-1.029249				
C	2.094072	1.741988	-2.233873				
C	3.16226	2.548446	-2.634261				
C	3.584983	3.605342	-1.829281				
C	2.92139	3.854109	-0.629208				
C	1.852356	3.046056	-0.237656				
C	1.423765	1.966067	-1.021961				

H	2.706512	-4.769113	-3.560027	C	1.67116	-3.666431	-3.762751
H	0.859868	-3.129674	-3.828622	C	0.81082	-2.575406	-3.664193
H	0.455481	-1.419272	-2.06989	C	0.64252	-1.932871	-2.440242
H	3.7686	0.695176	-0.449573	C	1.320852	-2.386109	-1.300893
H	5.918508	1.430398	0.508565	C	3.642512	-1.041866	0.864359
H	6.580874	0.705109	2.794821	C	4.823075	-1.130668	1.592625
H	5.076812	-0.772323	4.103691	C	4.891273	-1.94656	2.721315
H	2.932344	-1.521778	3.152639	C	3.773956	-2.677801	3.115679
H	0.631174	-1.412197	2.663995	C	2.588007	-2.593321	2.389151
H	1.348549	-2.880947	1.983621	C	2.510629	-1.774558	1.256128
H	-0.487914	-3.036104	0.309221	C	-0.256977	-2.693592	1.072905
H	-1.194881	-2.963808	1.92384	C	-1.597606	-2.531909	0.365042

cis-I-2ad

	x	y	z				
Pd	-0.106609	0.533296	-0.059172	H	6.36294	2.99075	0.952914
P	0.983598	-1.560708	0.294284	H	7.217553	3.942196	-0.290283
P	-2.082945	-0.740252	0.331059	H	5.704597	4.559059	0.422273
O	5.566196	3.015673	-0.974937	H	-0.131319	3.410755	1.187344
C	6.236169	3.657911	0.089733	H	-1.415239	5.485395	0.859112
C	-0.882035	3.448754	0.397562	H	-3.107111	5.642859	-0.958404
C	-1.600665	4.63046	0.210848	H	-3.50618	3.67484	-2.430274
C	-2.548229	4.722295	-0.807592	H	-2.259697	1.586737	-2.080214
C	-2.768225	3.620088	-1.631096	H	1.910415	0.870105	-2.431465
C	-2.052205	2.437804	-1.430244	H	4.181077	1.802228	-2.717897
C	-1.095303	2.32219	-0.410143	H	4.121458	3.201295	1.34284
C	2.373952	1.392602	-1.594522	H	1.868597	2.299272	1.627965
C	3.657722	1.902287	-1.769815	H	-4.66275	0.66158	0.366978
C	4.302838	2.554303	-0.713993	H	-6.398286	0.993546	-1.355357
C	3.643873	2.697908	0.507499	H	-6.192349	-0.116503	-3.568423
C	2.351941	2.17993	0.657428	H	-4.228651	-1.561459	-4.044399
C	1.688685	1.509835	-0.374166	H	-2.480842	-1.881334	-2.343236
C	-4.569902	0.163373	-0.595121	H	-4.396431	-1.977188	1.692524
C	-5.546196	0.354337	-1.56839	H	-5.361384	-1.659793	3.946086
C	-5.430227	-0.266855	-2.80952	H	-4.376379	0.0078	5.498341
C	-4.328623	-1.077747	-3.076948	H	-2.4177	1.355791	4.79138
C	-3.347635	-1.265748	-2.108407	H	-1.44274	1.034822	2.520145
C	-3.464024	-0.657452	-0.850255	H	2.726571	-3.83347	-0.533946
C	-3.954314	-1.252927	2.374276	H	3.037366	-4.961804	-2.715335
C	-4.501535	-1.07142	3.639159	H	1.810822	-4.163373	-4.71855
C	-3.947416	-0.133303	4.510404	H	0.2785	-2.217119	-4.540899
C	-2.84807	0.62369	4.114403	H	-0.008052	-1.059689	-2.35714
C	-2.299455	0.445203	2.845432	H	3.592825	-0.393553	-0.008286
C	-2.847135	-0.49552	1.967011	H	5.688778	-0.552335	1.280241
C	2.185814	-3.481542	-1.410645	H	5.812755	-2.010694	3.293084
C	2.361002	-4.115236	-2.637234	H	3.821788	-3.317958	3.991977
				H	1.726941	-3.173096	2.710182
				H	-0.347877	-2.401767	2.126875
				H	0.082126	-3.735292	1.044453
				H	-1.516244	-2.876977	-0.672628
				H	-2.377357	-3.132986	0.844548

<i>cis-I-2fa</i>							
	x	y	z				
Pd	-0.033533	0.612533	-0.129741	H	-2.141818	5.32007	0.450091
P	1.313644	-1.251508	0.508429	H	-3.804174	5.091093	-1.386834
P	-1.836772	-0.846546	0.421293	H	-3.830969	3.013754	-2.759051
C	-1.257987	3.385569	0.099237	H	-2.254846	1.191283	-2.289027
C	-2.16469	4.415682	-0.155537	H	1.922626	0.896713	-2.553946
C	-3.096277	4.290768	-1.185069	H	4.067566	2.021819	-2.970416
C	-3.107667	3.128179	-1.952887	H	3.823494	3.940683	0.855097
C	-2.203854	2.097783	-1.684306	H	1.673483	2.837065	1.281973
C	-1.262703	2.198691	-0.648129	H	-4.586774	0.149972	0.125678
C	5.43603	3.719446	-1.330897	H	-6.240455	-0.052932	-1.695727
C	2.314764	1.575142	-1.795851	H	-5.74224	-1.453353	-3.686201
C	3.539542	2.20398	-2.033928	H	-3.56798	-2.645949	-3.840781
C	4.111948	3.058196	-1.087476	H	-1.904474	-2.432451	-2.043018
C	3.40337	3.276139	0.099415	H	-4.017564	-2.190778	1.890588
C	2.180347	2.649051	0.334354	H	-5.168293	-1.657221	4.012427
C	1.613262	1.769332	-0.598495	H	-4.551599	0.383582	5.283335
C	-4.364802	-0.472376	-0.73791	H	-2.777202	1.890282	4.426459
C	-5.295074	-0.583429	-1.767235	H	-1.618969	1.355654	2.285947
C	-5.015056	-1.366929	-2.884075	H	3.289926	-3.43551	0.065389
C	-3.795678	-2.036326	-2.971123	H	3.771029	-4.848519	-1.908599
C	-2.861093	-1.92169	-1.947268	H	2.524295	-4.501154	-4.024942
C	-3.140186	-1.148737	-0.811286	H	0.793208	-2.72566	-4.168561
C	-3.736645	-1.300356	2.450406	H	0.329698	-1.283836	-2.191636
C	-4.388624	-0.998856	3.639952	H	3.74381	0.152622	-0.060628
C	-4.041276	0.148836	4.353363	H	5.852623	0.484739	1.170553
C	-3.045502	0.994953	3.873241	H	6.175469	-0.564481	3.404948
C	-2.392306	0.696294	2.67874	H	4.368469	-1.953582	4.386628
C	-2.731627	-0.454863	1.960042	H	2.260437	-2.299268	3.16275
C	2.738858	-3.28184	-0.860779	H	0.078346	-1.934673	2.470897
C	3.010277	-4.075543	-1.971037	H	0.693652	-3.364637	1.626529
C	2.308464	-3.880507	-3.160023	H	-0.973295	-3.028371	-0.198713
C	1.337048	-2.885465	-3.241641	H	-1.819681	-3.132598	1.343953
C	1.071048	-2.08325	-2.134288				
C	1.763879	-2.279342	-0.932845				
C	3.882263	-0.319894	0.910084				
C	5.069553	-0.130914	1.60627				
C	5.24833	-0.716286	2.85934				
C	4.233893	-1.493667	3.411781				
C	3.041213	-1.687802	2.717768				
C	2.854752	-1.103854	1.458861				
C	0.221778	-2.386239	1.481111				
C	-1.117857	-2.524092	0.764257				
H	5.346184	4.810728	-1.378292				
H	6.152108	3.502473	-0.529973				
H	5.882694	3.387192	-2.272136				
H	-0.529601	3.5148	0.900677				

<i>cis-I-2fd</i>			
	x	y	z
Pd	-0.055536	0.376856	-0.035149
P	1.294899	-1.565069	0.25476
P	-1.832413	-1.12317	0.454699
O	5.181959	3.691551	-0.876538
C	5.824585	4.266856	0.241941
C	-1.335805	3.127896	0.43503
C	-4.116724	5.244111	-1.084682
C	-2.241367	4.164996	0.216902
C	-3.148075	4.12347	-0.849363
C	-3.112578	3.003574	-1.682533
C	-2.213945	1.959204	-1.45348
C	-1.305903	1.991139	-0.386454

C	2.19775	1.743385	-1.591119	H	-6.152722	-1.048685	-3.258374
C	3.39464	2.438742	-1.742649	H	-4.083451	-2.318556	-3.783255
C	3.994011	3.051358	-0.637498	H	-2.237178	-2.41138	-2.160928
C	3.370346	2.97757	0.608626	H	-3.831378	-2.631499	2.027535
C	2.167057	2.274019	0.734548	H	-4.775409	-2.282682	4.284577
C	1.558873	1.628286	-0.345954	H	-4.057919	-0.336416	5.647209
C	-4.43176	-0.512555	-0.377605	H	-2.382152	1.256836	4.748657
C	-5.4659	-0.450301	-1.306382	H	-1.424416	0.904278	2.477197
C	-5.346361	-1.100044	-2.532449	H	3.182584	-3.670762	-0.669054
C	-4.185201	-1.812173	-2.827527	H	3.453985	-4.805193	-2.85368
C	-3.146924	-1.871563	-1.903343	H	2.018191	-4.170195	-4.774621
C	-3.263543	-1.231402	-0.661173	H	0.310963	-2.386115	-4.510362
C	-3.502555	-1.784154	2.626639	H	0.060185	-1.223004	-2.324636
C	-4.039482	-1.586037	3.89362	H	3.67632	-0.066997	-0.257765
C	-3.635521	-0.491501	4.658506	H	5.896472	0.034429	0.80848
C	-2.694679	0.402703	4.155059	H	6.410356	-1.410751	2.768232
C	-2.154649	0.206061	2.88529	H	4.683789	-2.965847	3.639215
C	-2.554721	-0.888874	2.111457	H	2.465932	-3.084327	2.575673
C	2.551541	-3.390705	-1.510558	H	0.206468	-2.525405	2.191416
C	2.703647	-4.028284	-2.738042	H	0.719134	-3.815647	1.09273
C	1.895995	-3.671558	-3.817308	H	-1.083405	-3.216839	-0.509141
C	0.937827	-2.67116	-3.670138	H	-1.806393	-3.511822	1.071557
C	0.791702	-2.024381	-2.445404				
C	1.592043	-2.383209	-1.353086				
C	3.897833	-0.711996	0.590464				
C	5.148019	-0.65296	1.19438				
C	5.434534	-1.461421	2.293477				
C	4.465207	-2.332392	2.784235				
C	3.210414	-2.397505	2.181384				
C	2.915375	-1.589015	1.077061				
C	0.258622	-2.822082	1.136448				
C	-1.137868	-2.842284	0.520498				
H	-4.775908	5.402297	-0.223398				
H	-3.603637	6.196745	-1.259354				
H	-4.751546	5.049271	-1.953551				
H	6.05588	3.51505	1.008662				
H	6.754169	4.701352	-0.125801				
H	5.21593	5.05567	0.702967				
H	-0.632634	3.213443	1.264741				
H	-2.241881	5.029868	0.881214				
H	-3.809108	2.941343	-2.519687				
H	-2.245849	1.094598	-2.118753				
H	1.769275	1.261553	-2.470132				
H	3.886735	2.513623	-2.709666				
H	3.81082	3.450874	1.481351				
H	1.712012	2.220644	1.724731				
H	-4.52637	0.008627	0.572304				
H	-6.364916	0.11256	-1.071907				

C	3.017458	-2.706239	-2.842094	H	4.658147	0.071145	0.283261
C	2.115327	-3.790203	-2.261199	H	6.432403	1.27063	-0.940523
C	0.788897	-3.072005	-2.103373	H	5.939397	3.432359	-2.058032
C	-2.407059	-0.570289	-2.454004	H	3.646153	4.380361	-1.955304
C	-3.529226	-1.166078	-3.036151	H	1.859218	3.181472	-0.761742
C	-4.062453	-2.333352	-2.495511	H	3.740377	0.882897	2.860267
C	-3.47042	-2.909413	-1.37278	H	4.733709	-0.795832	4.376469
C	-2.352976	-2.313518	-0.788433	H	4.131979	-3.191486	4.151052
C	-1.808421	-1.147862	-1.333165	H	2.520198	-3.9099	2.406112
C	4.431247	1.015726	-0.205649	H	1.506102	-2.222759	0.886093
C	5.432697	1.692599	-0.895975	H	-3.250306	2.835132	1.81704
C	5.156055	2.904915	-1.52241	H	-3.962253	5.01838	0.906229
C	3.869259	3.437473	-1.464769	H	-3.124735	5.779503	-1.302174
C	2.863141	2.76138	-0.783424	H	-1.563166	4.352971	-2.597764
C	3.138224	1.549499	-0.133083	H	-0.839353	2.157254	-1.686217
C	3.462532	-0.164914	2.764506	H	-4.238933	0.814032	0.107512
C	4.027397	-1.109833	3.61382	H	-6.164236	-0.510527	0.90167
C	3.688669	-2.456886	3.485435	H	-5.876138	-2.151801	2.741948
C	2.784069	-2.861299	2.507364	H	-3.64965	-2.447799	3.799136
C	2.216086	-1.916649	1.655588	H	-1.719289	-1.136382	3.01362
C	2.551333	-0.562316	1.776418	H	-0.197563	0.429065	2.899937
C	-2.873057	3.169325	0.852914	H	-0.908705	2.044199	2.872019
C	-3.277756	4.395214	0.338939	H	0.810473	2.787848	1.206338
C	-2.805587	4.821771	-0.902065	H	1.626854	2.10972	2.613417
C	-1.929303	4.021718	-1.630811				
C	-1.523487	2.790544	-1.121912				
C	-1.992895	2.357467	0.123463				
C	-4.111533	0.113654	0.929378				
C	-5.193488	-0.63923	1.370632				
C	-5.030537	-1.560973	2.402842				
C	-3.781386	-1.7285	2.99654				
C	-2.694427	-0.978254	2.558941				
C	-2.8551	-0.04378	1.528431				
C	-0.363207	1.310013	2.26976				
C	0.966204	1.864249	1.775912				
H	3.015325	-1.461634	-1.066301				
H	2.728753	-0.529548	-2.559908				
H	4.081288	-2.909822	-2.706804				
H	2.826298	-2.572624	-3.911698				
H	2.495435	-4.112386	-1.284976				
H	2.031622	-4.673657	-2.896429				
H	0.206528	-3.391736	-1.233729				
H	0.152125	-3.148469	-2.991604				
H	-4.940771	-2.790051	-2.943522				
H	-2.010756	0.348112	-2.883704				
H	-3.98867	-0.709541	-3.909763				
H	-3.885935	-3.816906	-0.940525				
H	-1.919218	-2.758511	0.107327				
				[2f(thf)] ⁺			
					x	y	z
				Pd	-0.024216	-0.397779	-0.35292
				P	-1.124546	1.269783	0.678869
				P	2.004571	0.714278	0.34183
				O	0.940969	-2.166534	-1.363815
				C	2.375666	-2.23211	-1.522189
				C	2.645378	-3.670293	-1.89517
				C	1.646142	-4.400882	-1.004015
				C	0.42838	-3.494977	-1.044752
				C	-5.360802	-3.396554	-2.089267
				C	-2.306871	-1.115256	-2.156202
				C	-3.434022	-1.835451	-2.559363
				C	-4.144171	-2.634042	-1.659158
				C	-3.693547	-2.690536	-0.334733
				C	-2.573217	-1.970782	0.07484
				C	-1.859616	-1.189659	-0.837037
				C	4.607687	0.457532	-0.7203
				C	5.572945	0.669614	-1.700975
				C	5.296695	1.491026	-2.790802
				C	4.047407	2.099772	-2.903027

				[2a-16a(tmeda)]			
				x	y	z	
C	6.19184	1.452714	0.18955	I	-0.43132	1.052537	-2.769883
C	5.093535	0.870448	0.813786	Pd	0.982296	0.124352	-0.499193
C	3.876488	0.757616	0.128273	Zn	-1.868904	-1.156013	-1.223753
C	0.500395	1.669579	2.412508	Cl	-2.391938	-2.913253	-2.789168
C	1.994603	1.472835	2.195516	P	0.492846	2.058308	0.909202
C	2.65332	-4.041709	-2.345186	P	2.499097	-0.44304	1.128009
C	2.83006	-2.819616	-2.991891	N	-6.518515	-0.373633	1.243007
C	2.264379	-1.656522	-2.465863	N	-3.852921	-0.060149	-1.293099
C	1.523535	-1.703304	-1.282158	C	-3.713173	1.294261	-0.749693
C	1.362022	-2.930014	-0.630838	C	-6.424133	-1.649876	1.926989
C	1.911566	-4.09588	-1.168116	C	-5.783041	0.65294	1.954155
H	-4.08066	-0.767278	2.348874	C	-1.88089	-2.456549	3.500321
H	-4.311074	-2.34225	1.541022	C	-1.875966	-1.107514	3.153384
H	-6.190628	0.067696	1.446048	C	-1.759307	-0.739032	1.810872
H	-6.621559	-1.621972	1.777247	C	-1.762783	-3.4172	2.497063
H	-6.913074	-0.745558	-0.771766	C	-1.647269	-3.028364	1.161179
H	-6.066666	-2.280617	-0.518394	C	-4.678801	-0.922576	-0.41179
H	-4.820467	0.458263	-1.035592	C	-6.131253	-0.47379	-0.163026
H	-4.321358	-1.134662	-1.666875	C	-4.399264	-0.002175	-2.652887
H	0.944488	2.561349	-1.717239	C	-1.647036	-1.676809	0.770303
H	1.856057	4.707445	-2.58569	C	2.416502	3.4172	-0.613134
H	1.669905	6.771846	-1.21848	C	3.341999	4.430734	-0.856651
H	0.571973	6.691731	1.005408	C	3.504744	5.460331	0.065879
H	-0.329912	4.560997	1.869196	C	2.734202	5.485576	1.228528
H	-2.394387	3.07758	-0.792093	C	1.810688	4.475967	1.472823
H	-4.798798	3.490556	-0.411091	C	1.652622	3.425488	0.558508
H	-5.863135	2.781413	1.721538	C	-1.575532	3.789144	0.219878
H	-4.505567	1.639916	3.457637	C	-2.81433	4.402529	0.377239
H	-2.113234	1.192799	3.072382	C	-3.579185	4.157274	1.516793
H	4.334222	-1.988548	0.450203	C	-3.091508	3.311438	2.509537
H	4.957589	-4.008482	1.729516	C	-1.848084	2.702373	2.359961
H	3.879147	-4.483659	3.915158	C	-1.081779	2.925105	1.208241
H	2.173927	-2.922317	4.820498	C	2.891006	-3.192171	1.414749
H	1.539725	-0.907624	3.547103	C	2.715467	-4.424205	2.034036
H	2.832915	1.134226	-1.713172	C	1.969531	-4.517747	3.207915
H	4.793374	2.182907	-2.823319	C	1.39242	-3.376682	3.75744
H	6.944601	2.38528	-1.598834	C	1.557187	-2.141857	3.137584
H	7.132799	1.537904	0.725141	C	2.319122	-2.037353	1.968804
H	5.180936	0.501695	1.833844	C	4.573005	0.450848	-0.486729
H	0.05985	0.798946	2.911236	C	5.90328	0.629781	-0.851437
H	0.30977	2.554232	3.030169	C	6.912645	-0.000692	-0.127113
H	2.515973	1.25711	3.134038	C	6.590211	-0.801482	0.966829
H	2.437643	2.388065	1.785963	C	5.260566	-0.976237	1.339199
H	3.092735	-4.946263	-2.757359	C	4.240768	-0.352372	0.609765
H	3.407945	-2.767766	-3.912099	C	1.027436	1.478553	2.579742
H	2.400683	-0.714121	-2.993556	C	2.403021	0.837546	2.46917
H	0.817919	-2.982848	0.313634				
H	1.768042	-5.043447	-0.653629				

C	3.066117	5.231442	-0.046433	H	1.514411	5.570446	-1.504188
C	1.82872	4.988569	-0.64277	H	-1.874581	2.522496	-1.737324
C	0.998776	3.99192	-0.143028	H	-2.915869	4.488983	-2.847915
C	1.391538	3.232664	0.968809	H	-5.072663	5.38567	-2.009941
C	-2.817695	2.927178	-1.372564	H	-6.18486	4.324586	-0.061381
C	-3.404141	4.027392	-1.994713	H	-5.151532	2.371866	1.044642
C	-4.613945	4.529923	-1.523127	H	-2.812515	-1.271109	2.458769
C	-5.240222	3.934522	-0.428298	H	-4.404676	-3.138232	2.667043
C	-4.655495	2.839084	0.195957	H	-6.351793	-3.298413	1.132899
C	-3.438326	2.325073	-0.273131	H	-6.698412	-1.564847	-0.610959
C	-3.681228	-1.310984	1.805119	H	-5.108156	0.31433	-0.825079
C	-4.571677	-2.373815	1.913931	H	-1.477315	3.513744	1.474544
C	-5.661337	-2.464078	1.049914	H	-0.987142	3.170128	3.133876
C	-5.857289	-1.491112	0.072256	H	-3.257057	2.147522	2.648288
C	-4.967519	-0.428426	-0.043457	H	-2.064471	0.881254	2.964182
C	-3.879816	-0.323796	0.831352	H	-3.775151	-2.185163	-4.606102
C	-1.205858	2.706694	2.167054	H	-3.595559	-3.263918	-2.366691
C	-2.334633	1.690552	2.274992	H	-2.244294	-2.235046	-0.599426
C	-3.165004	-1.736329	-3.826637	H	-1.181167	0.965086	-3.286035
C	-3.062566	-2.339111	-2.577229	H	-2.571429	-0.050803	-5.032658
C	-2.283109	-1.756186	-1.577304				
C	-1.56603	-0.576399	-1.811097				
C	-1.696153	0.030782	-3.069017				
C	-2.487227	-0.542257	-4.065879				
H	5.729335	2.969239	-1.615619	I	0.24338	-2.984792	1.850811
H	6.420721	1.329881	-1.762201	Pd	-0.284816	0.504046	-0.34218
H	6.736051	2.547749	-3.026345	Zn	0.771901	-1.937802	-0.711712
H	0.043718	3.787249	-0.627574	Cl	0.475117	-3.454993	-2.536263
H	4.581209	1.398179	-0.401307	P	0.845443	2.281332	0.840734
H	2.584957	0.488122	0.622799	P	-2.16771	1.27019	0.85962
H	2.790115	0.978446	-4.291186	O	2.901331	-2.505188	-0.519343
H	0.760296	0.041518	-3.249354	C	1.31028	-0.005135	-2.98287
H	3.597803	-1.536466	-2.049155	C	2.342181	0.314802	-3.869079
H	3.76288	-3.306717	-2.015237	C	3.574664	0.743151	-3.384156
H	5.450281	-1.213496	-0.576698	C	3.775548	0.824545	-2.006202
H	5.99825	-2.742858	-1.280296	C	2.73924	0.50913	-1.133397
H	5.640857	-2.631508	1.409276	C	3.678641	-2.65012	-1.740135
H	4.947827	-4.0175	0.54791	C	5.128984	-2.483569	-1.321262
H	3.526621	-1.41747	1.309362	C	5.103578	-2.889752	0.147703
H	2.941492	-3.077422	1.60775	C	3.786711	-2.300017	0.5985
H	1.224158	-0.819491	2.043537	C	1.466563	0.107592	-1.590802
H	2.229924	-1.886943	4.0324	C	2.061561	0.418376	2.496067
H	2.633162	-0.553195	6.091988	C	2.736259	-0.020909	3.632317
H	2.020393	1.851204	6.148871	C	3.119273	0.893239	4.609424
H	1.022198	2.925927	4.164847	C	2.823856	2.247688	4.453199
H	2.967684	2.877755	2.399747	C	2.147368	2.688501	3.320647
H	4.434196	4.652921	1.512687	C	1.765054	1.775441	2.326705
H	3.717351	6.005246	-0.442616	C	3.17963	3.819031	0.323843

[I-2fa-ZnClI(thf)]

	x	y	z
I	0.24338	-2.984792	1.850811
Pd	-0.284816	0.504046	-0.34218
Zn	0.771901	-1.937802	-0.711712
Cl	0.475117	-3.454993	-2.536263
P	0.845443	2.281332	0.840734
P	-2.16771	1.27019	0.85962
O	2.901331	-2.505188	-0.519343
C	1.31028	-0.005135	-2.98287
C	2.342181	0.314802	-3.869079
C	3.574664	0.743151	-3.384156
C	3.775548	0.824545	-2.006202
C	2.73924	0.50913	-1.133397
C	3.678641	-2.65012	-1.740135
C	5.128984	-2.483569	-1.321262
C	5.103578	-2.889752	0.147703
C	3.786711	-2.300017	0.5985
C	1.466563	0.107592	-1.590802
C	2.061561	0.418376	2.496067
C	2.736259	-0.020909	3.632317
C	3.119273	0.893239	4.609424
C	2.823856	2.247688	4.453199
C	2.147368	2.688501	3.320647
C	1.765054	1.775441	2.326705
C	3.17963	3.819031	0.323843

C	1.048488	0.90673	-1.384953	H	2.342775	1.834328	4.022197
C	0.797722	2.132486	2.560628	H	1.669029	3.805992	5.383024
C	1.502888	2.45279	3.717671	H	-0.2714	5.185319	4.684684
C	1.121184	3.5527	4.480046	H	-1.524739	4.623078	2.63536
C	0.02939	4.328639	4.088944	H	0.178194	5.102394	0.720597
C	-0.67876	4.007873	2.935518	H	0.384169	6.875063	-0.983636
C	-0.294562	2.906306	2.156421	H	-0.706515	6.614491	-3.198385
C	-0.318555	4.98648	-0.239336	H	-2.021397	4.565577	-3.69463
C	-0.197037	5.984301	-1.204054	H	-2.800414	0.465823	-2.204906
C	-0.808889	5.838267	-2.445807	H	-4.580592	0.794634	-3.906308
C	-1.547242	4.688595	-2.725321	H	-6.95152	0.35315	-3.315829
C	-1.66833	3.690058	-1.765891	H	-7.53965	-0.397237	-1.025123
C	-1.06344	3.834729	-0.508633	H	-5.772072	-0.711735	0.672386
C	-3.843793	0.283366	-1.951792	H	-2.062972	-1.207928	3.235915
C	-4.842774	0.465754	-2.905008	H	-2.276145	-3.380478	4.37503
C	-6.171577	0.218078	-2.572384	H	-3.437384	-5.270123	3.25671
C	-6.503204	-0.20376	-1.285074	H	-4.384183	-4.967256	0.980949
C	-5.50795	-0.378806	-0.329534	H	-4.166821	-2.796045	-0.174221
C	-4.166088	-0.140153	-0.658335	H	-3.565049	2.566603	0.255348
C	-2.597225	-2.019455	2.746723	H	-3.175428	3.230013	1.840413
C	-2.70761	-3.249194	3.387165	H	-4.35284	0.985624	2.051493
C	-3.356572	-4.309216	2.75703	H	-2.712946	0.905113	2.703832
C	-3.890564	-4.139553	1.481469	H	-1.287235	-5.264351	-2.653958
C	-3.778169	-2.913751	0.834644	H	-0.709783	-5.006681	-0.243941
C	-3.143125	-1.839397	1.469199	H	-0.452905	-2.777462	0.738292
C	-2.960669	2.403094	1.15657	H	-1.293118	-1.000629	-3.100165
C	-3.292902	1.057186	1.785757	H	-1.597192	-3.234888	-4.058901
C	-1.15717	-4.275589	-2.222283				
C	-0.832695	-4.130988	-0.877712				
C	-0.674053	-2.859992	-0.324735				
C	-0.800343	-1.708122	-1.109902				
C	-1.147999	-1.868689	-2.459909				
C	-1.325733	-3.138402	-3.009952				
H	-2.229369	2.784216	-1.996811				
H	2.639689	3.935865	-1.618971				
H	1.614468	2.449437	0.030069				
H	1.782477	1.09052	-4.727927				
H	2.721914	3.28235	-4.021735				
H	0.742626	-0.403306	-3.07244				
H	3.844391	0.675986	-1.883991				
H	5.112442	-0.412448	-1.270313				
H	4.860239	2.604416	-0.900013				
H	6.341353	1.665889	-1.143524				
H	5.728748	2.449913	1.383349				
H	6.199934	0.758391	1.143754				
H	3.361004	1.894477	1.243351				
H	3.977526	0.478916	2.139108				
H	1.086419	1.260048	1.974709				