Electronic Supplementary Material (ESI) for Chemical Communications

Highly Active Catalysts of Bisphosphine Oxides for Asymmetric Heck Reaction

Jian Hu, Yunpeng Lu, Yongxin Li and Jianrong (Steve) Zhou*

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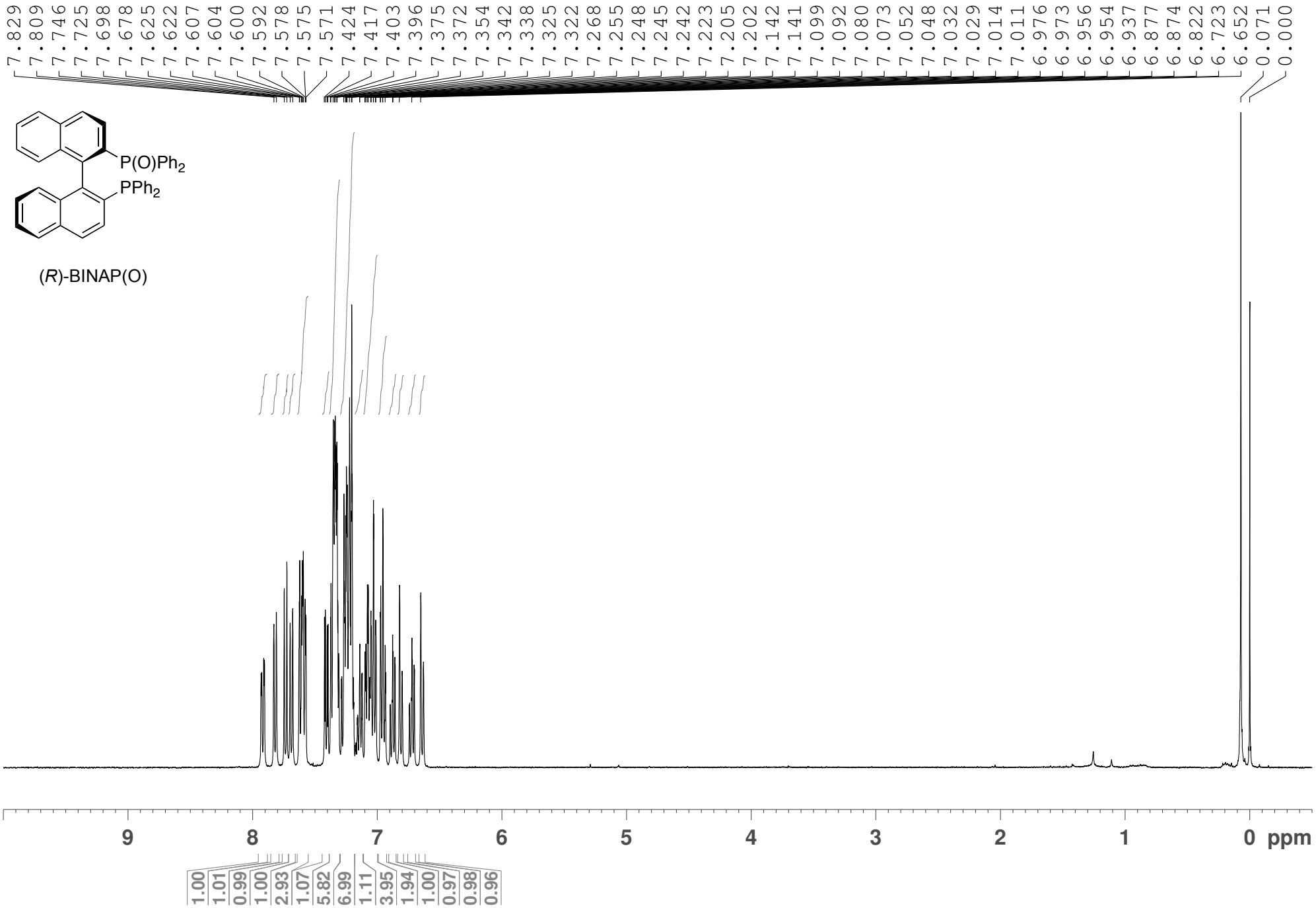
E-mail: jrzhou@ntu.edu.sg

Supporting Information: NMR Spectra

^{1}H NMR (400 MHz, $CDCl_3$)



(*R*)-BINAP(O)

$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)

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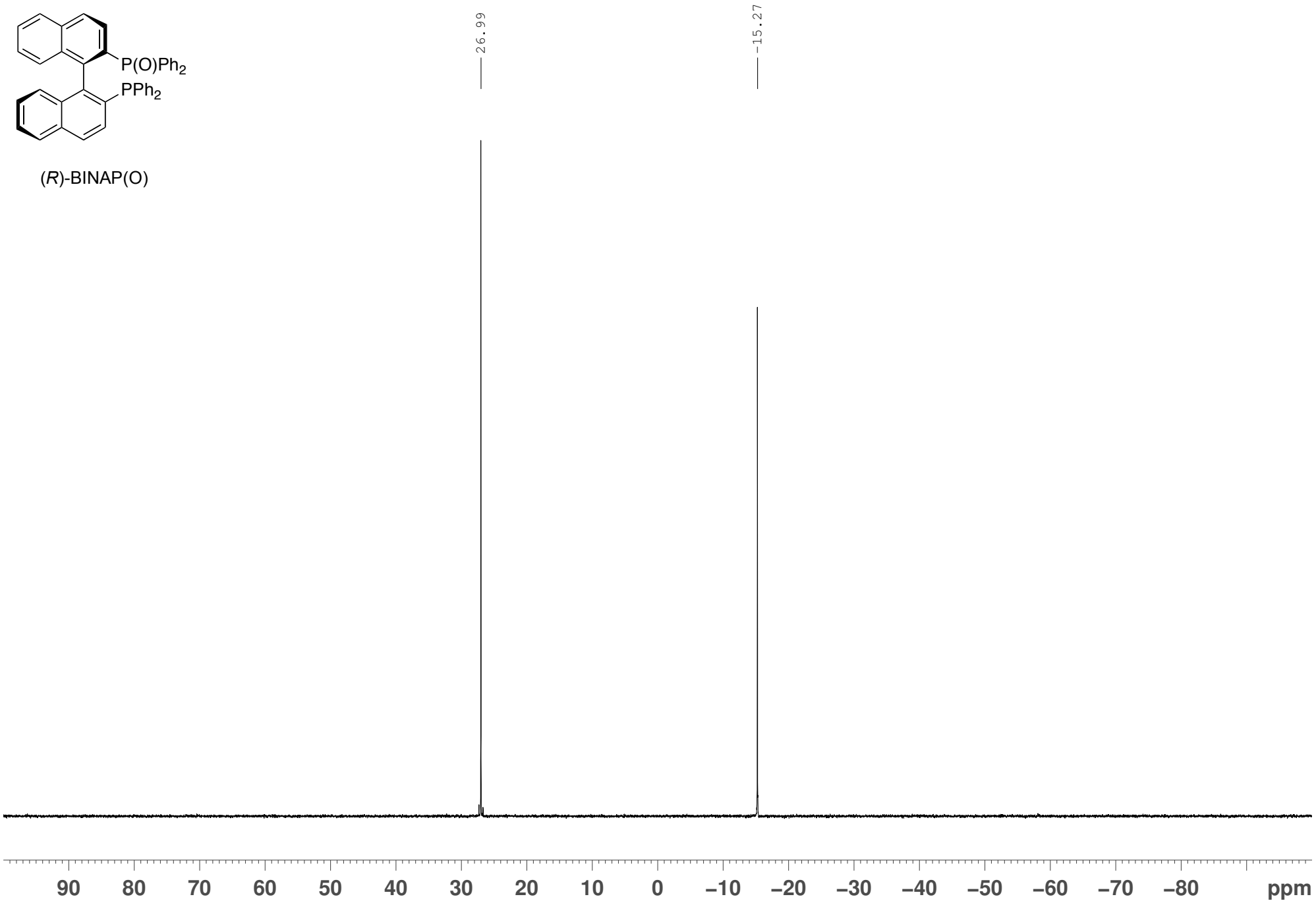
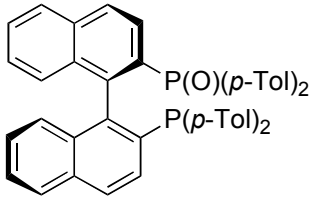
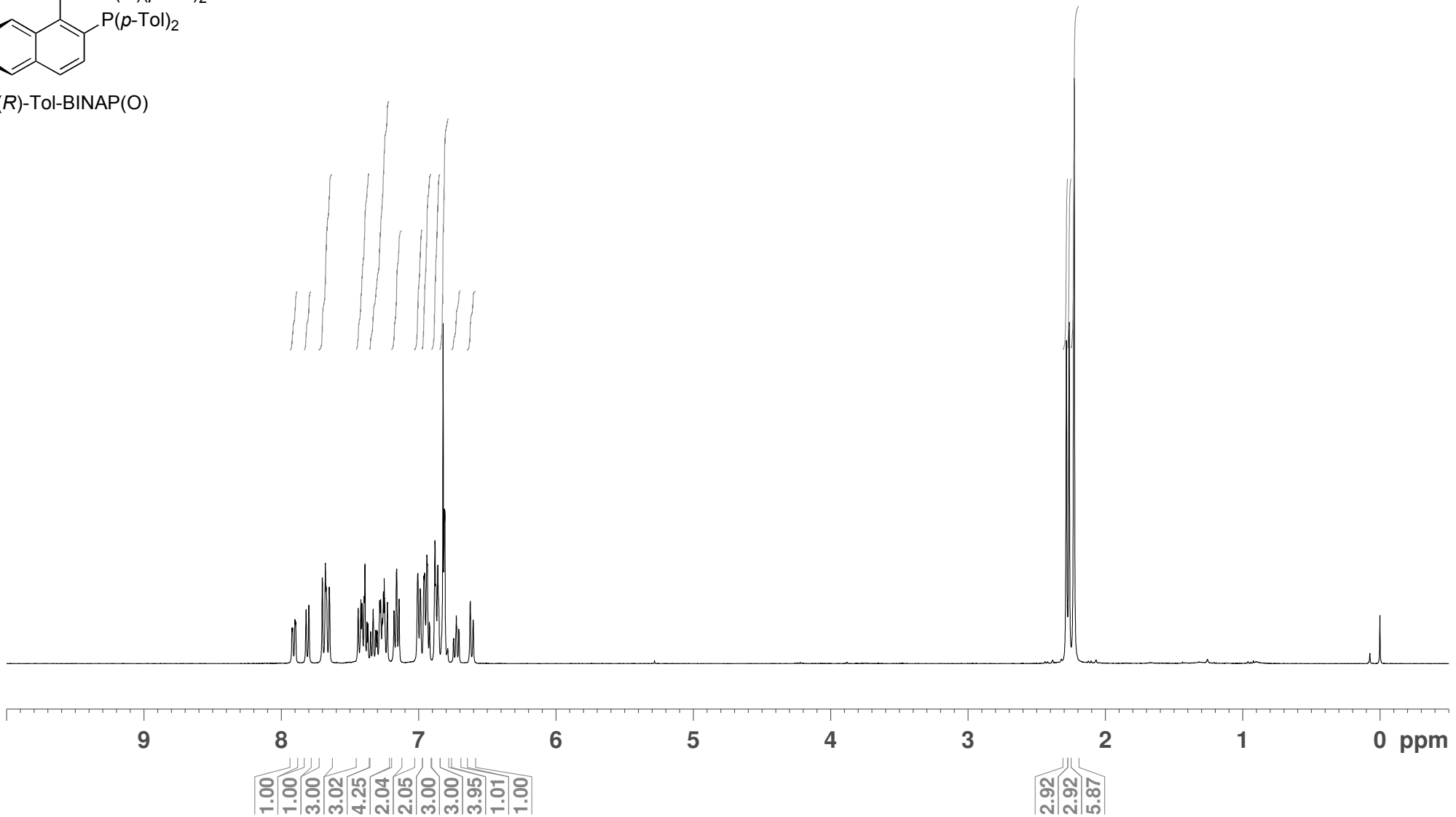


^{1}H NMR (400 MHz, $CDCl_3$)



(*R*)-Tol-BINAP(O)



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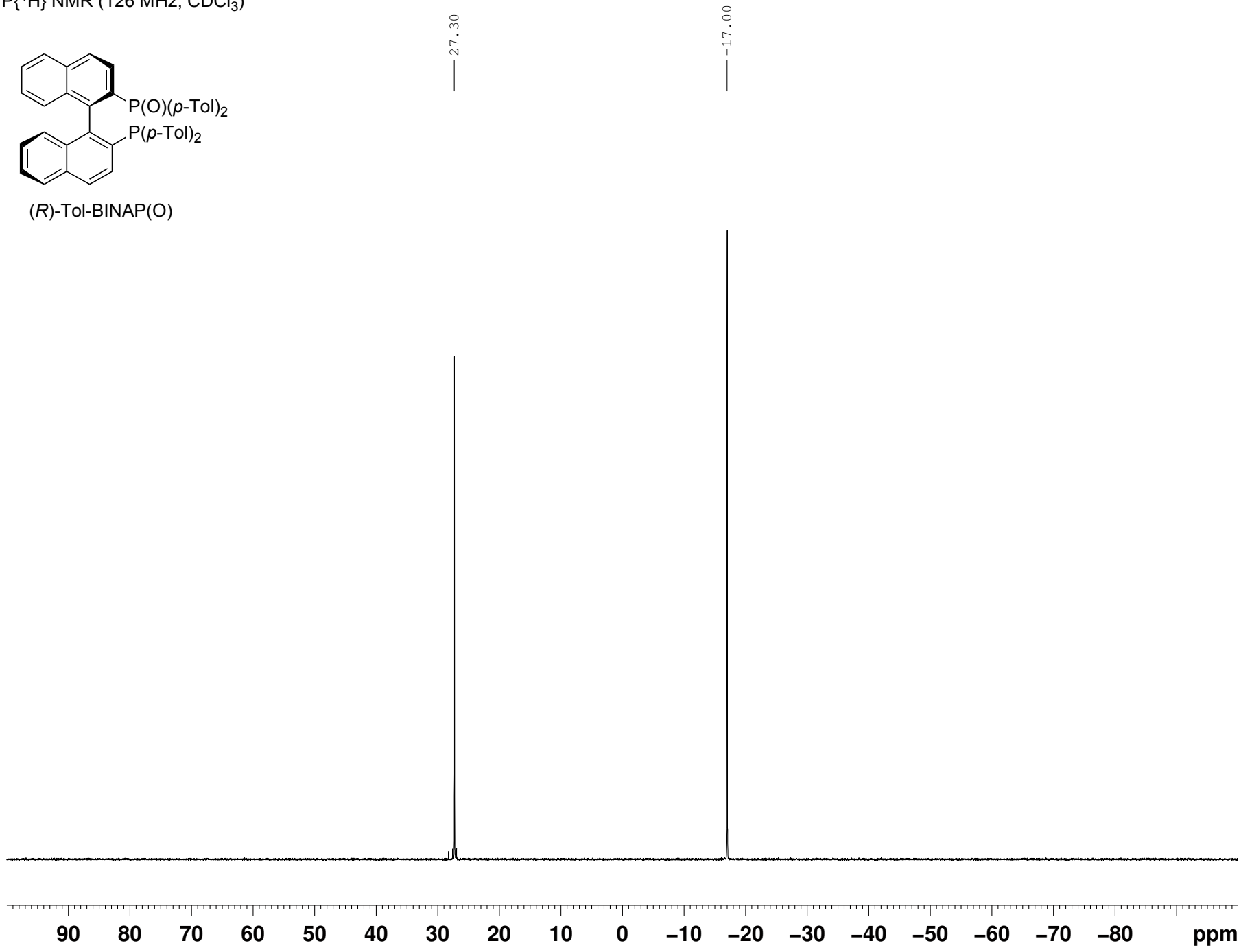
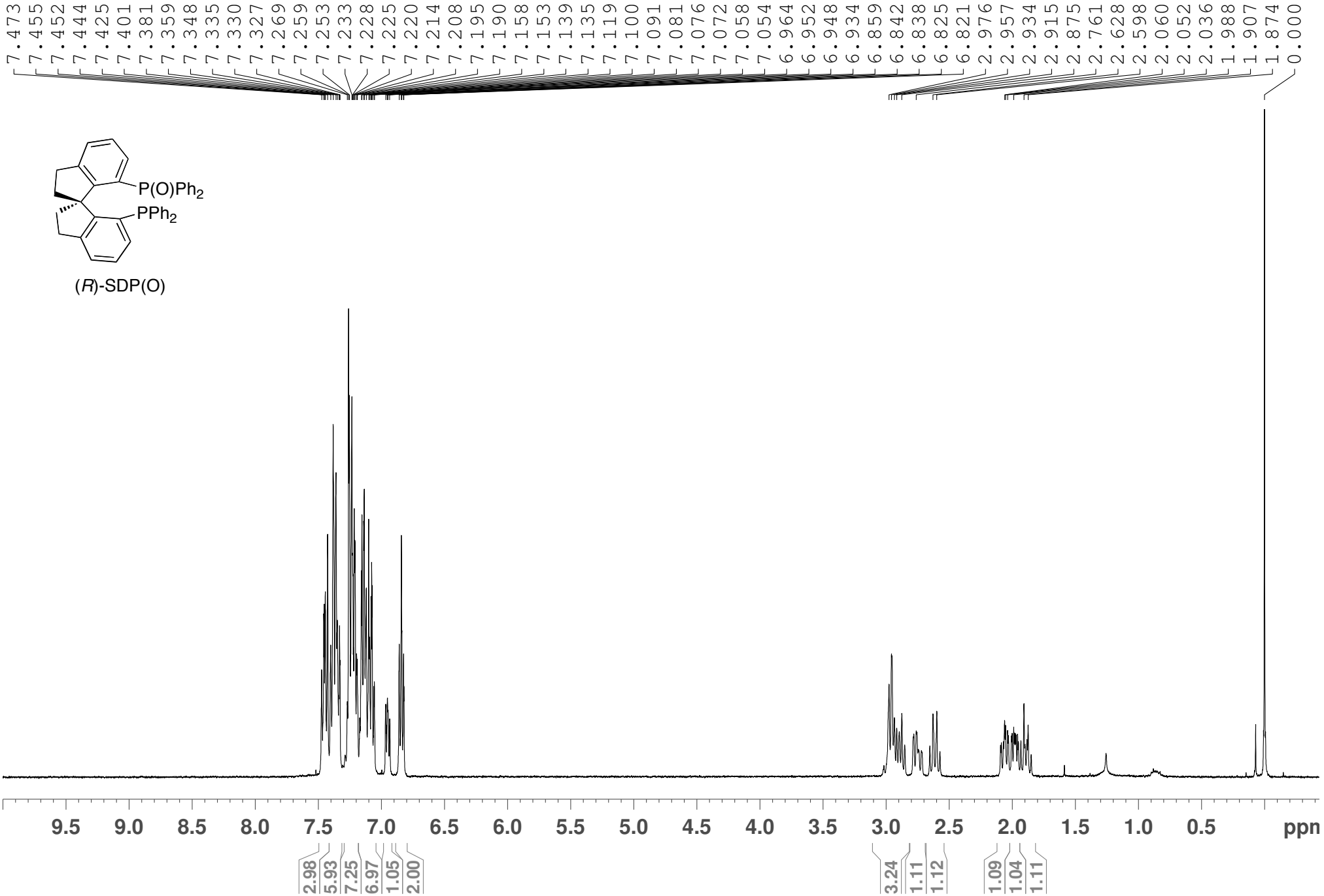
(*R*)-Tol-BINAP(O)



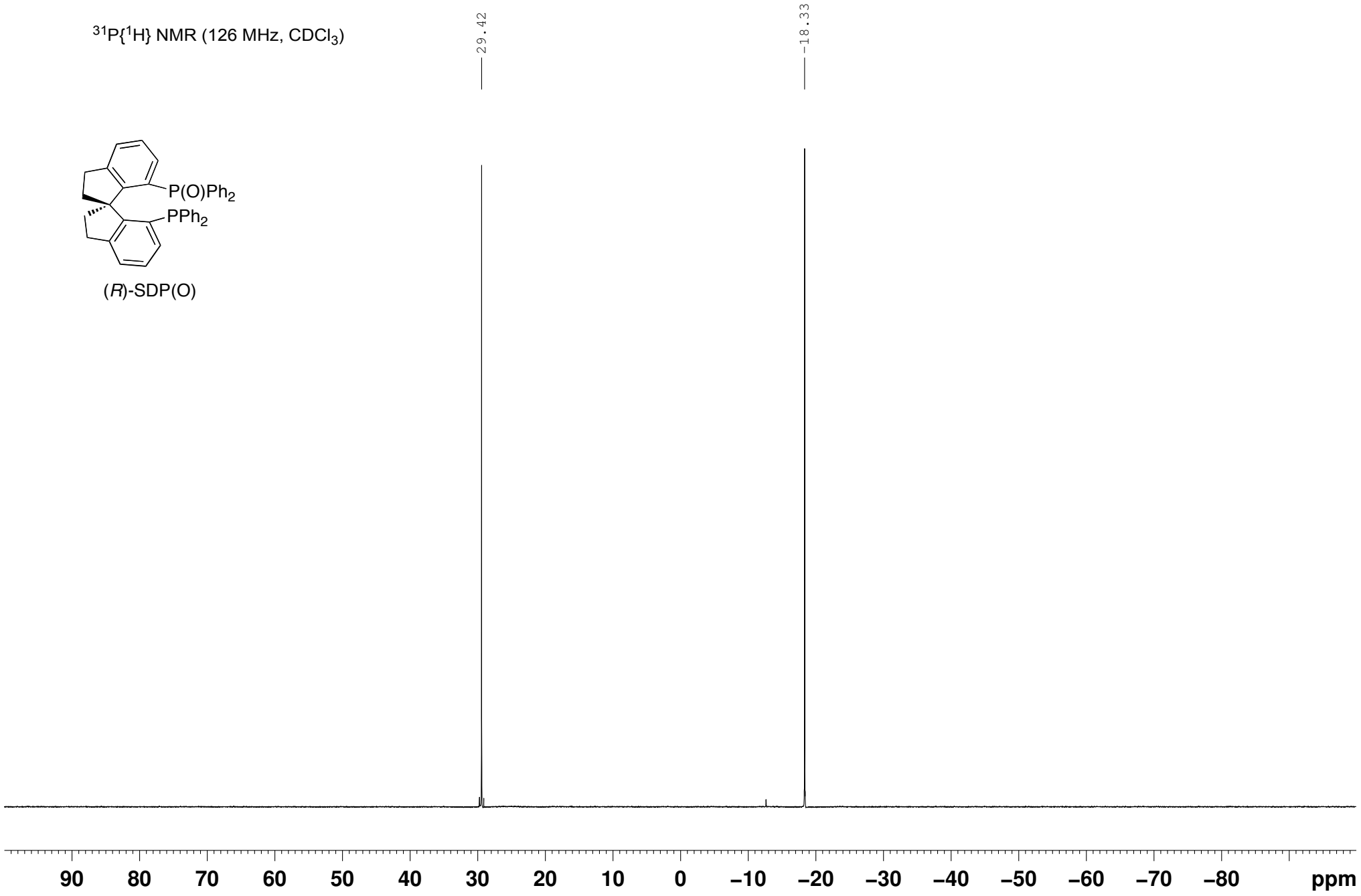
^{1}H NMR (400 MHz, $CDCl_3$)



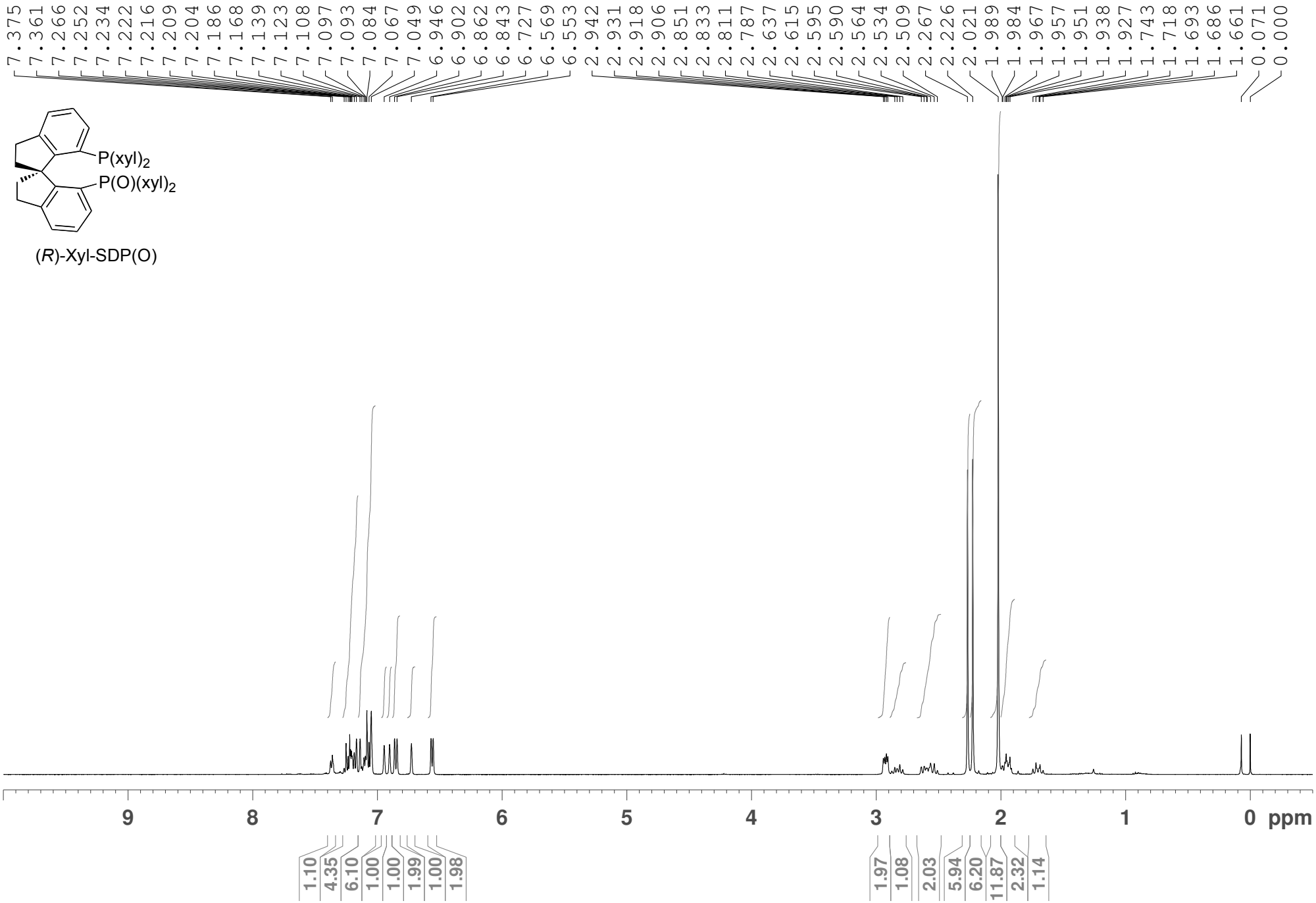
(*R*)-SDP(O)

$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)

(*R*)-SDP(O)



^{1}H NMR (400 MHz, $CDCl_3$)



(*R*)-Xyl-SDP(O)

$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)

(R)-Xyl-SDPO 31P

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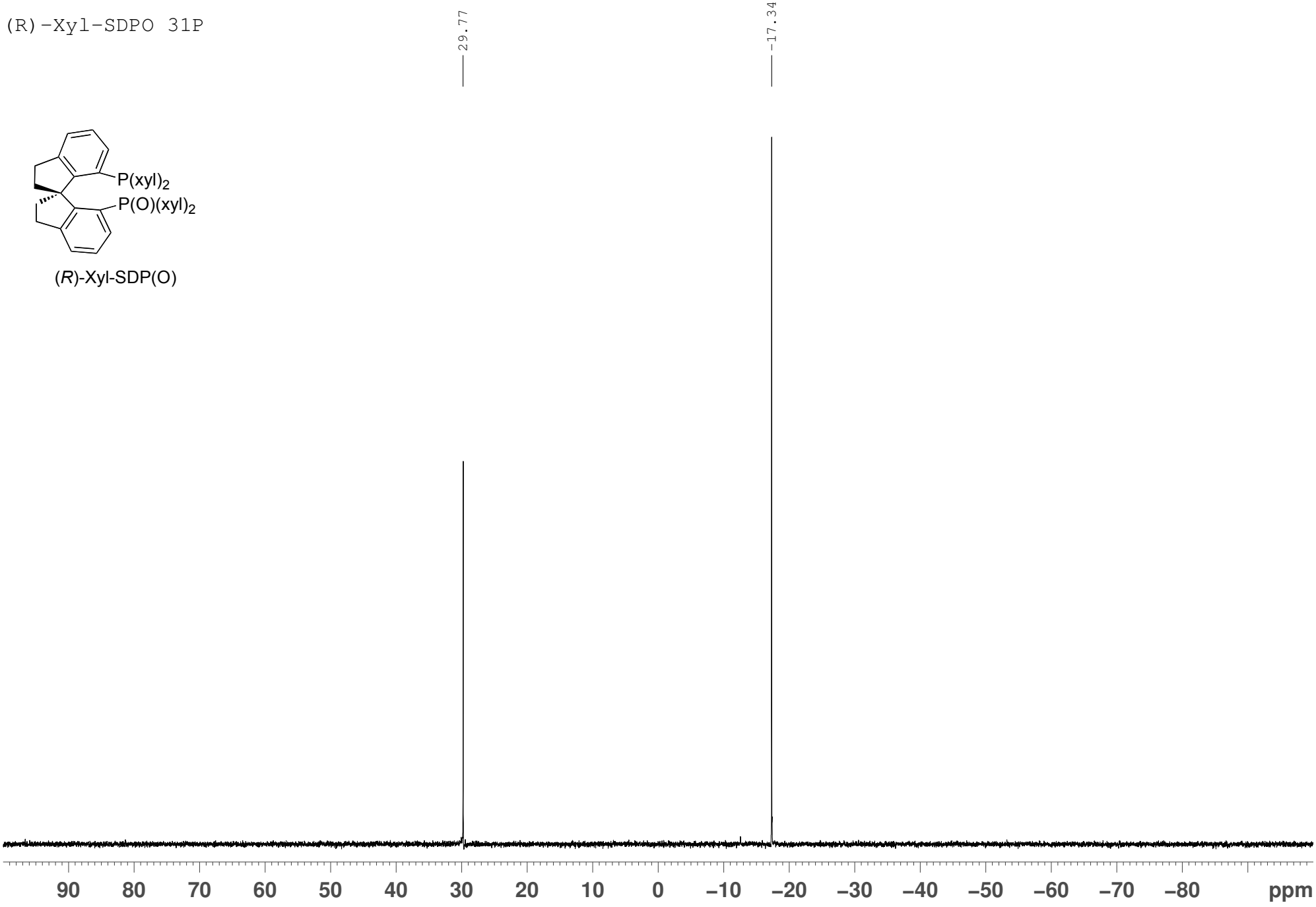
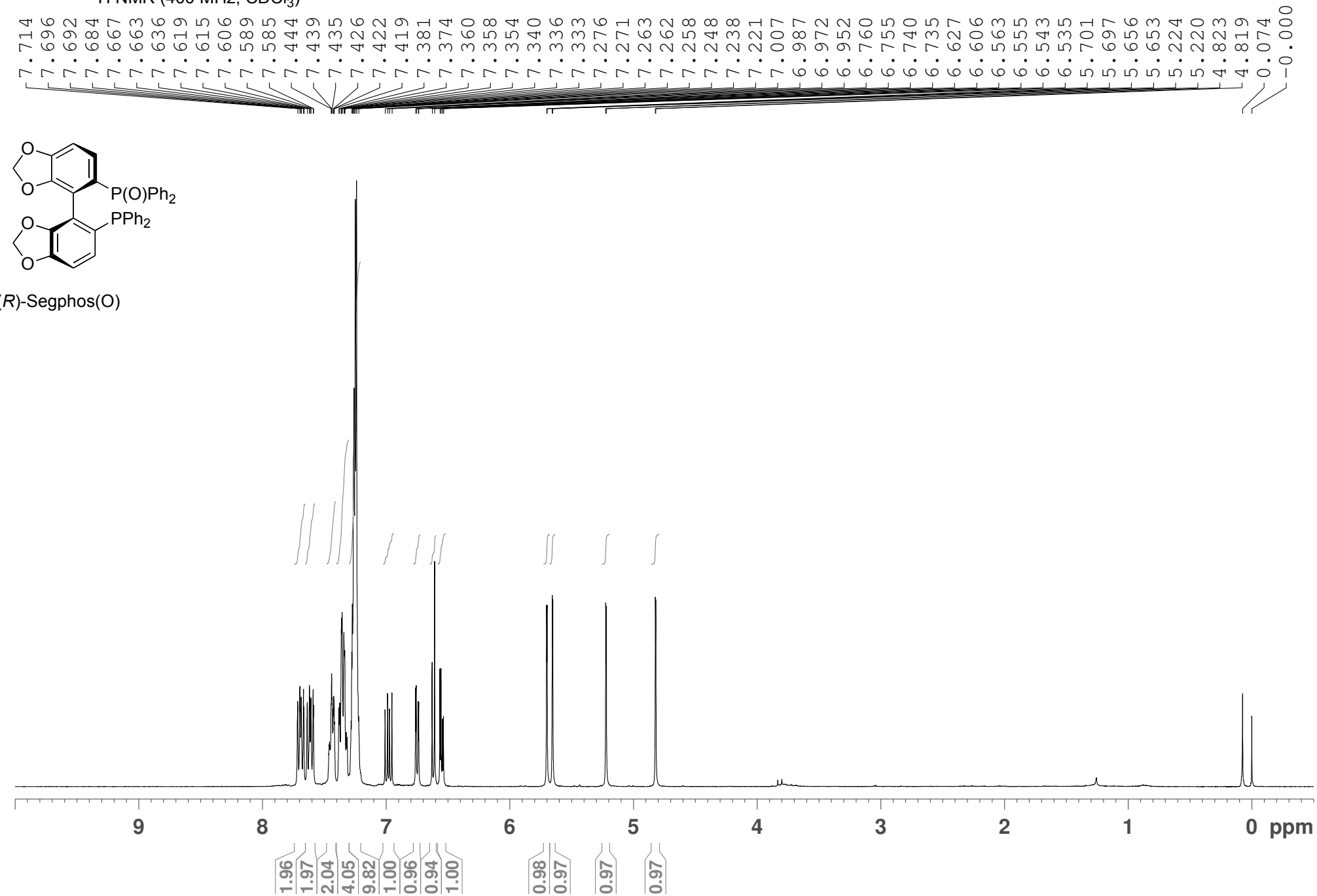
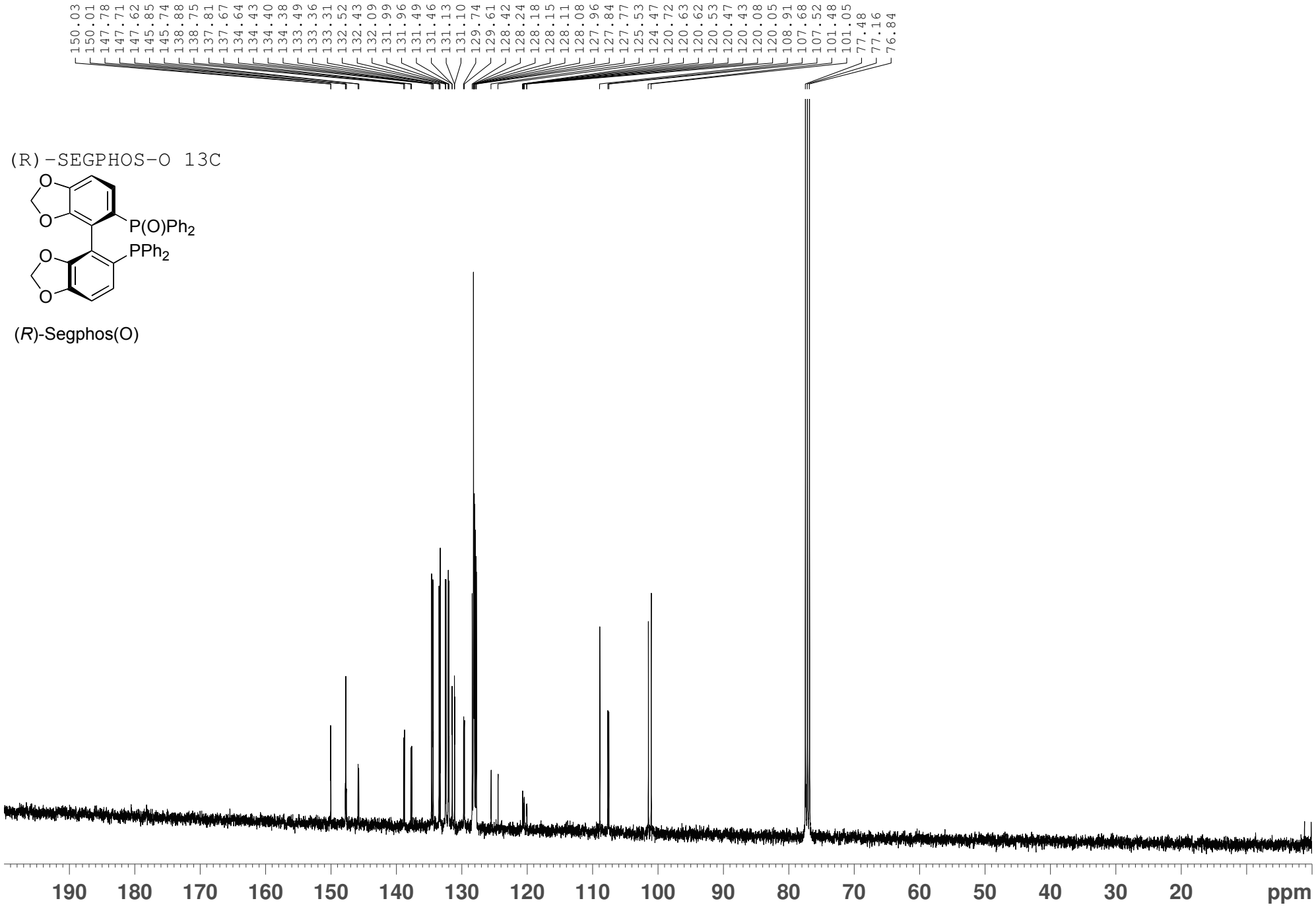


^{1}H NMR (400 MHz, $CDCl_3$)



(*R*)-Segphos(O)

^{13}C NMR (100 MHz, $CDCl_3$)



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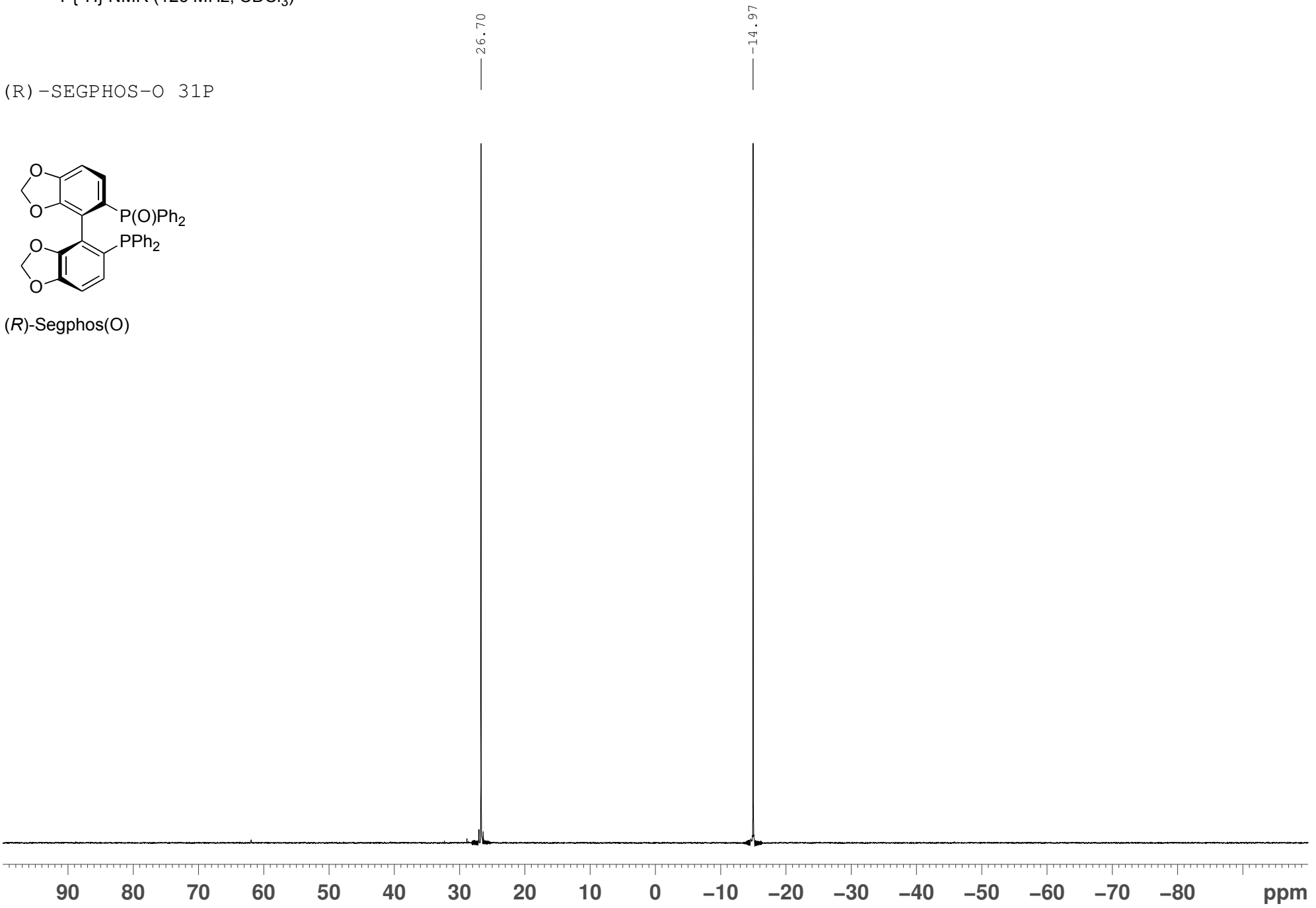
$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)



(*R*)-Segphos(O)

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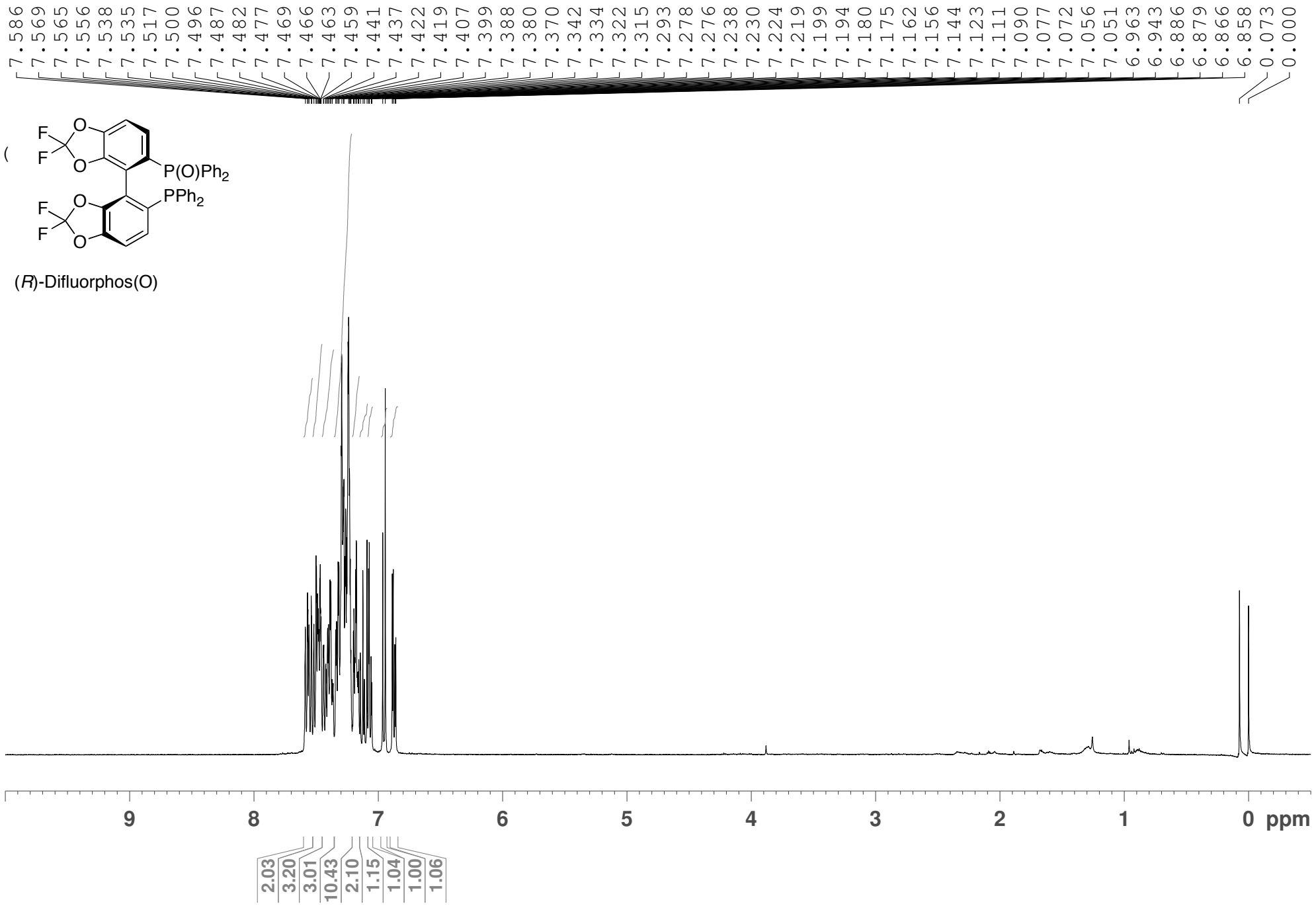
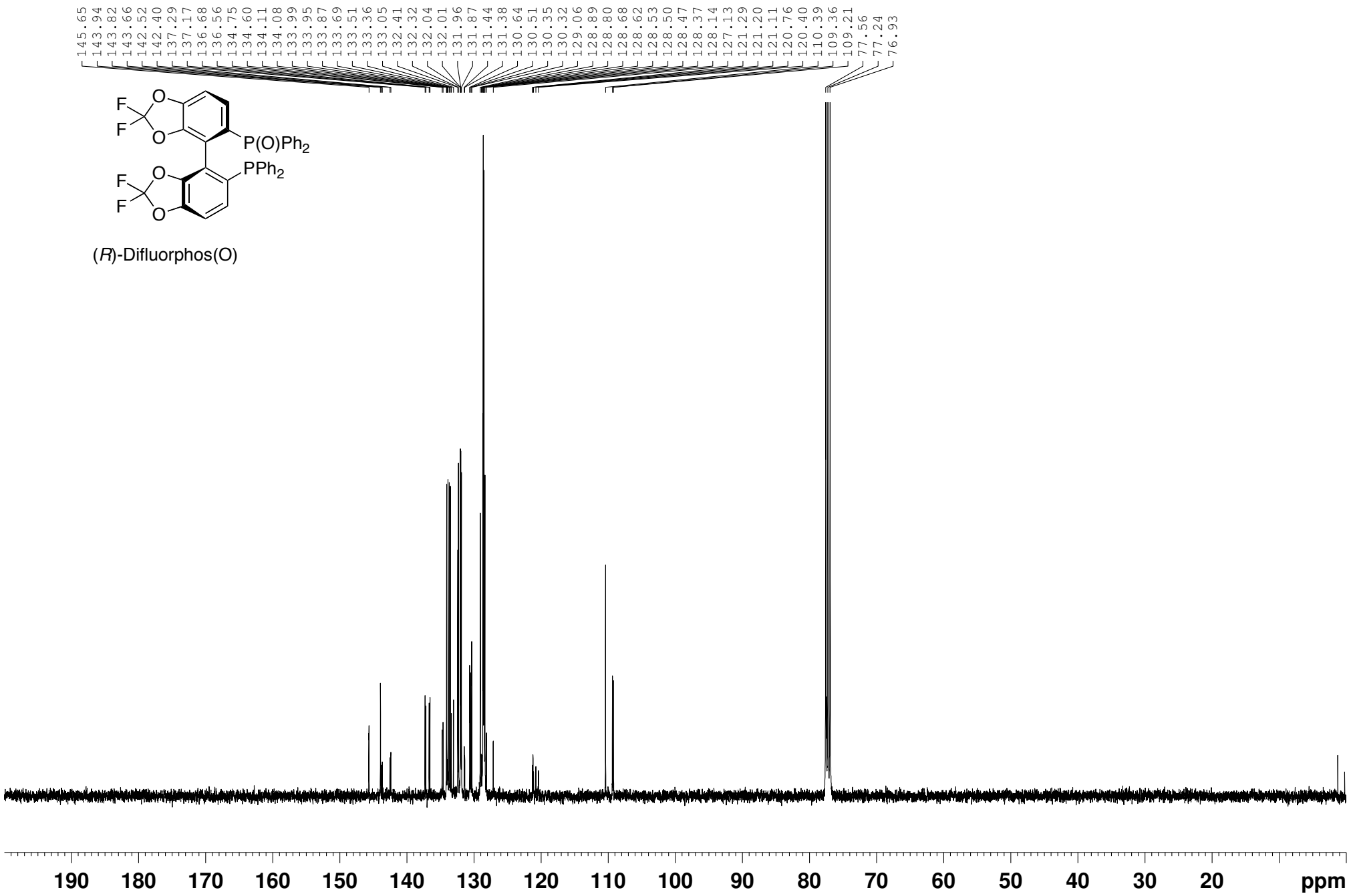


(*R*)-Difluorphos(O)

^{13}C NMR (100 MHz, $CDCl_3$)



(*R*)-Difluorphos(O)

$^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$)

(R)-DIFLUOROPHOS-O 19F

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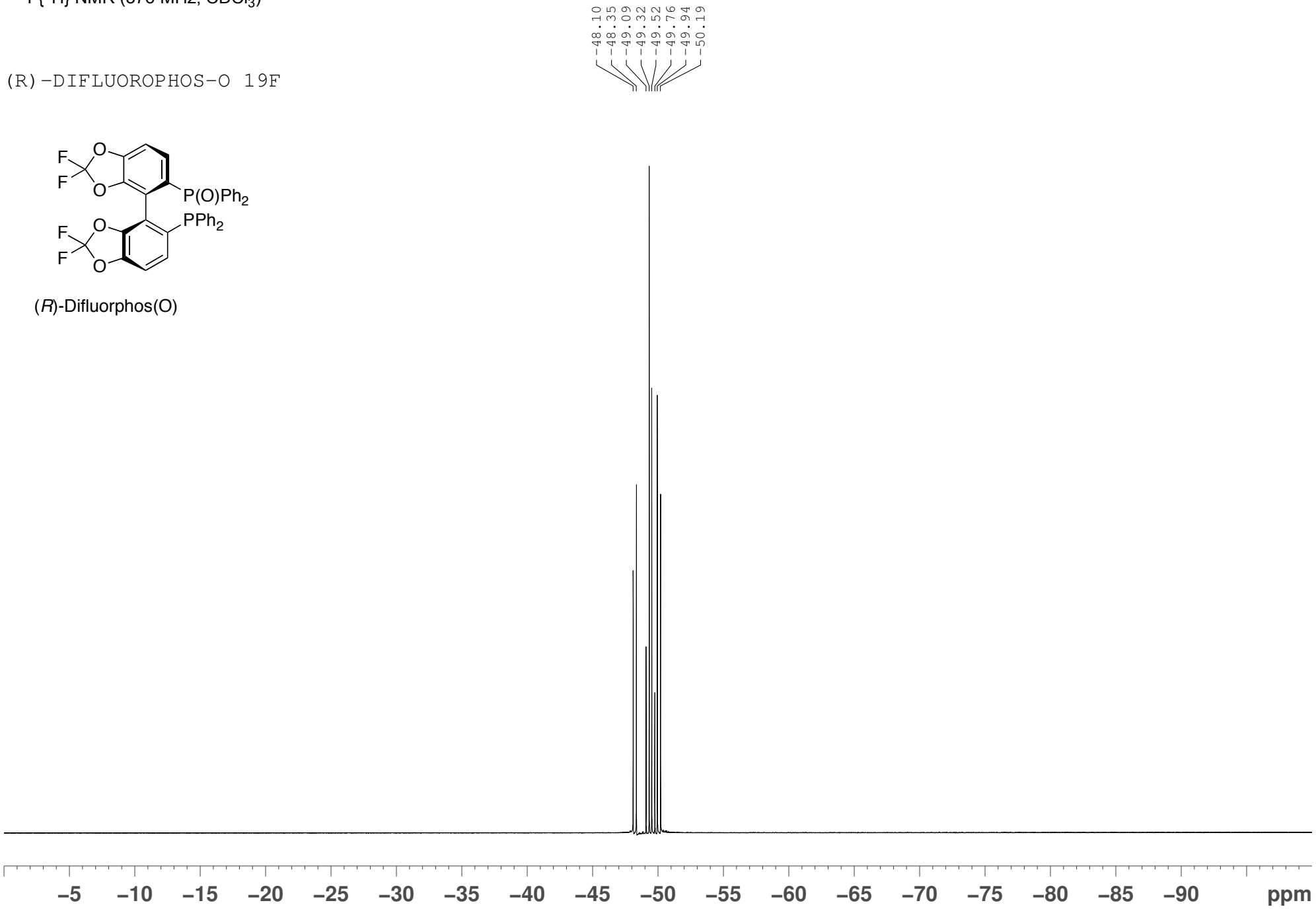

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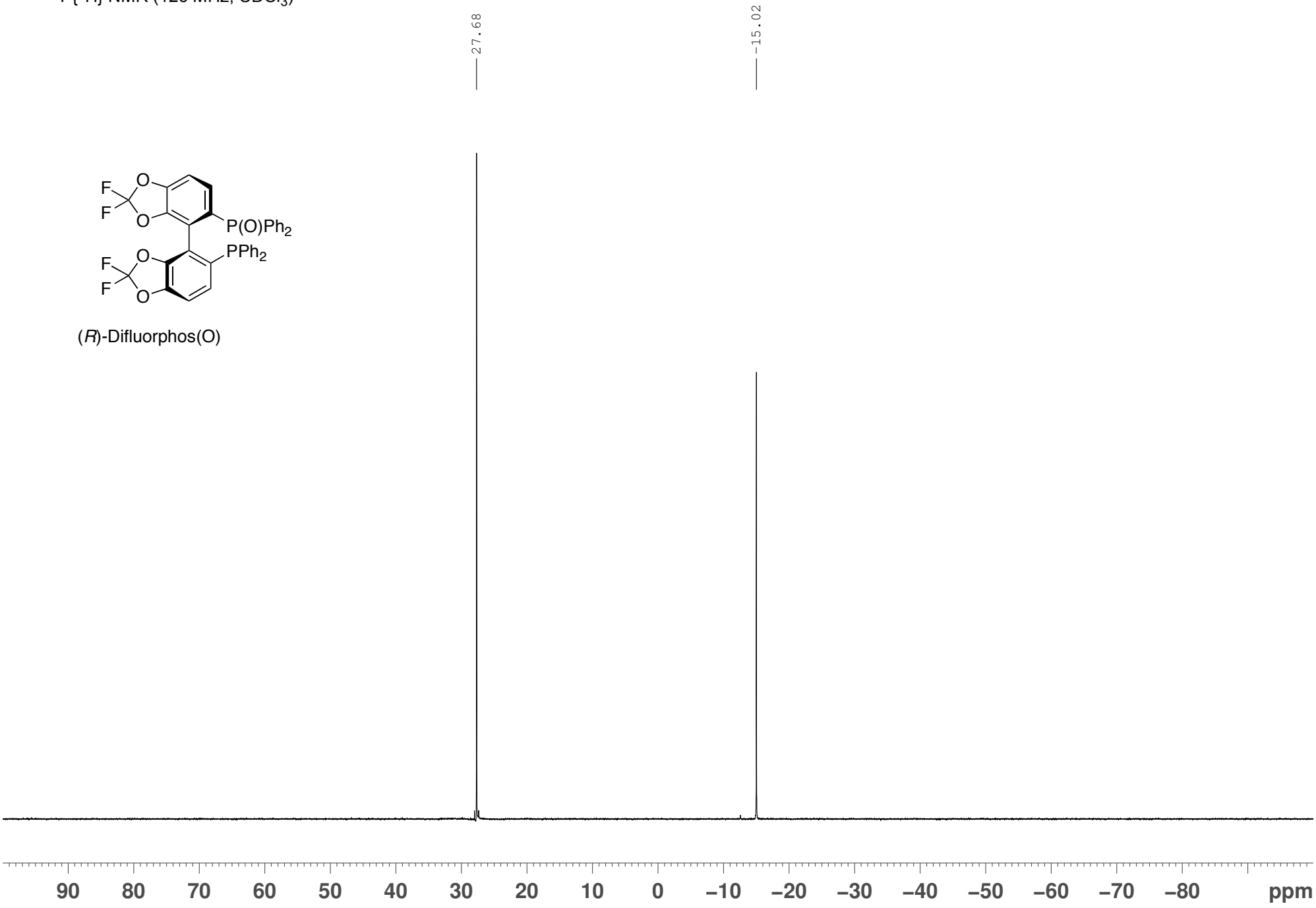
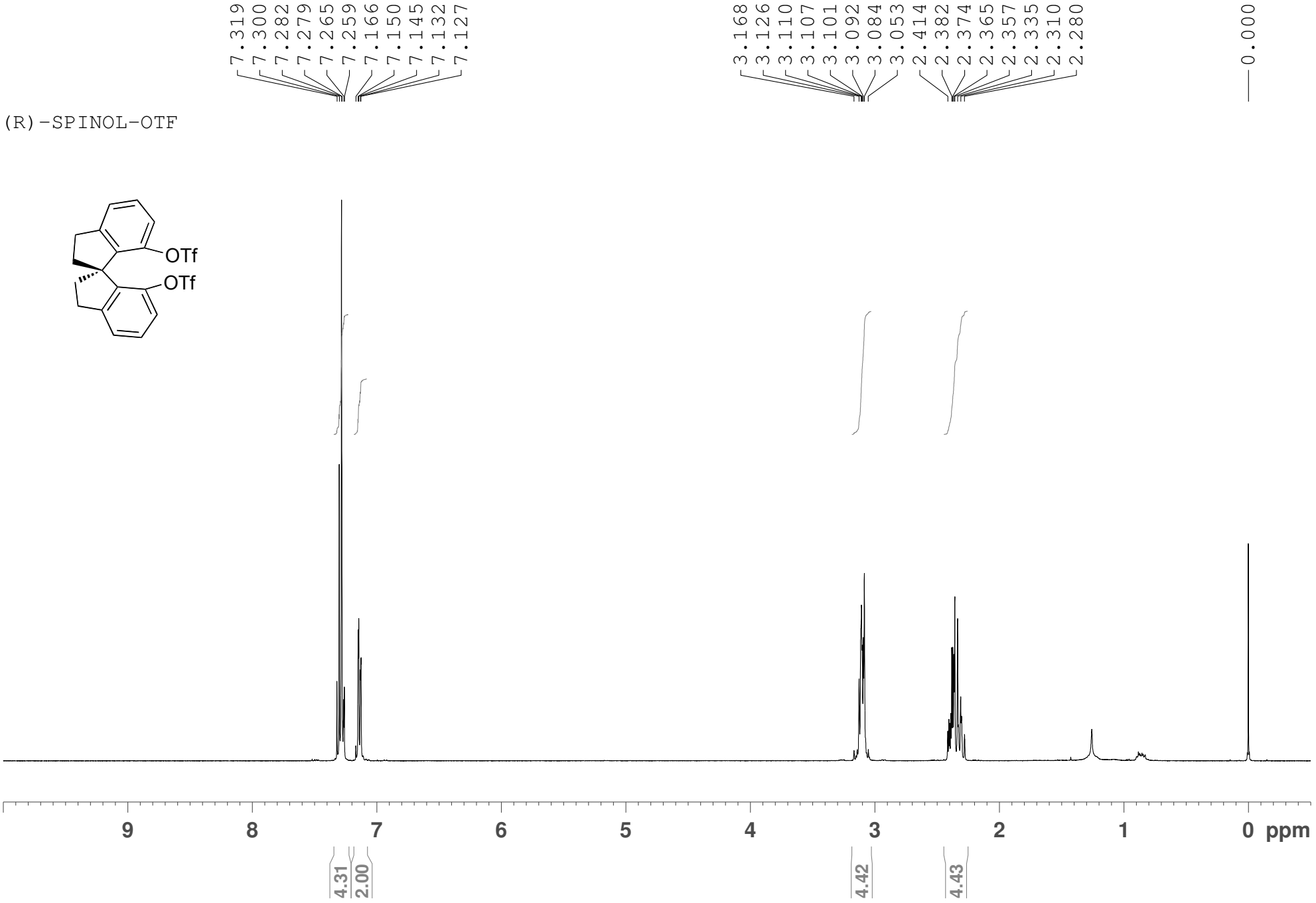
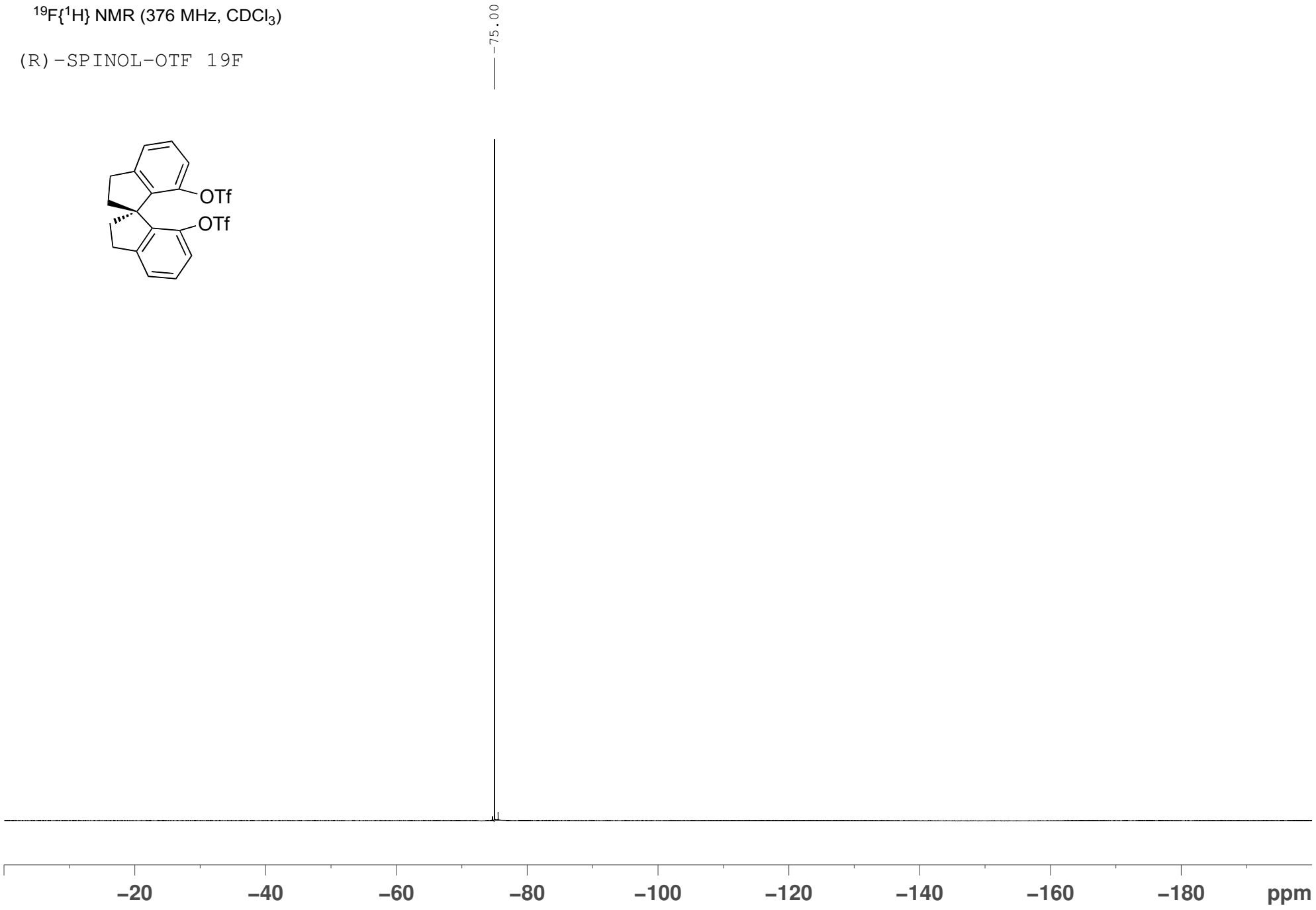


^{1}H NMR (400 MHz, $CDCl_3$)

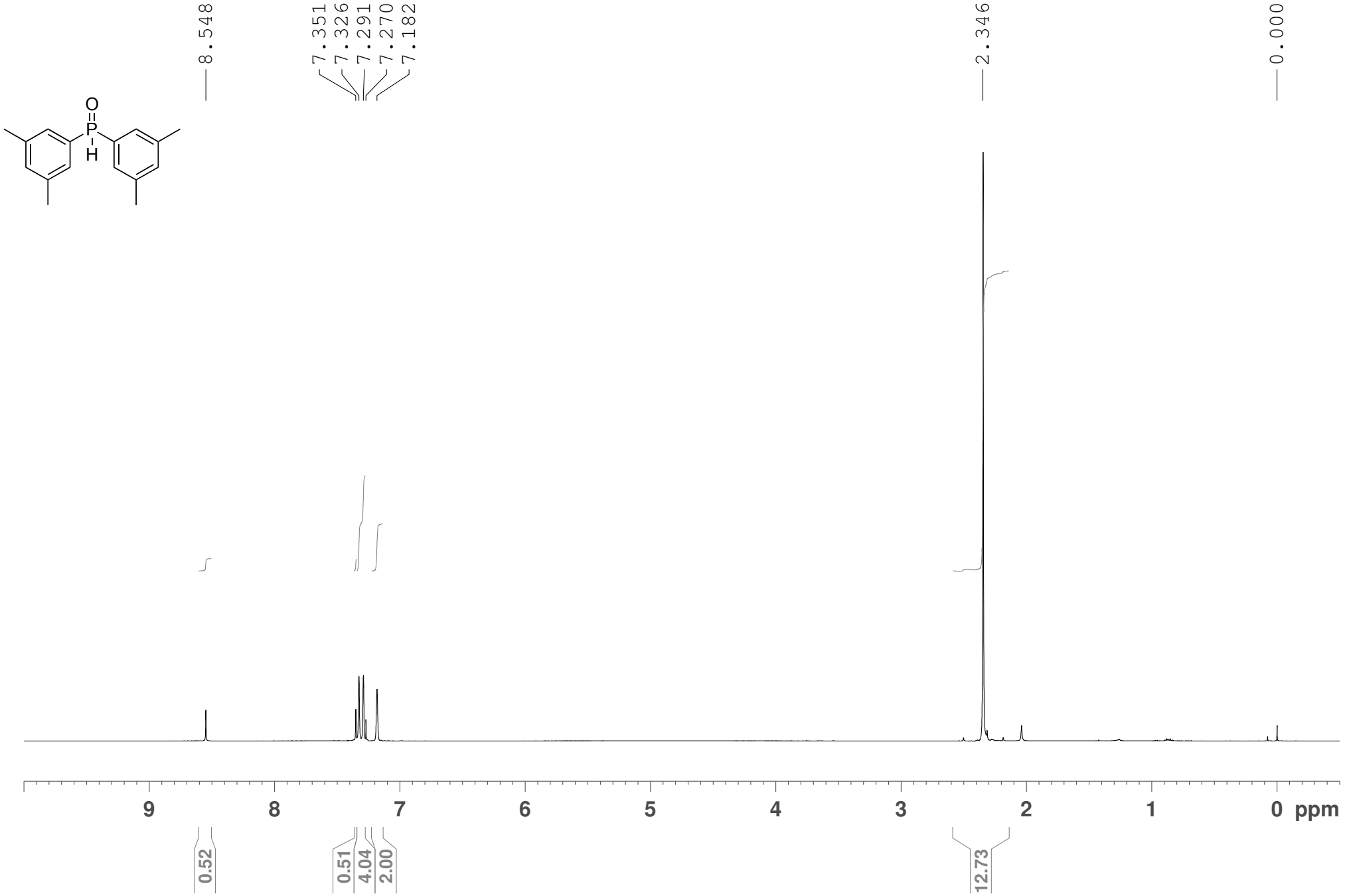


$^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$)

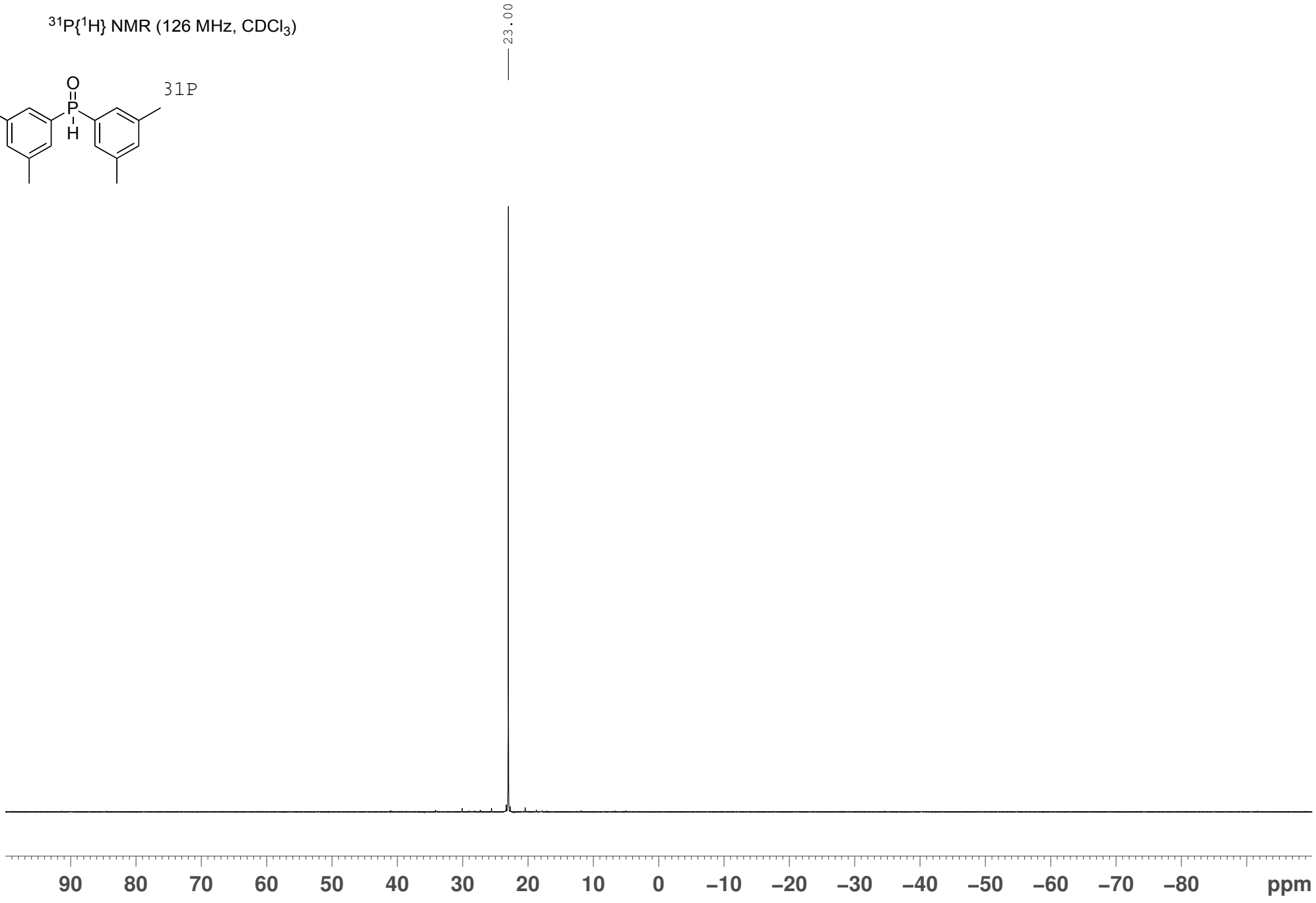
(R)-SPINOL-OTF 19F



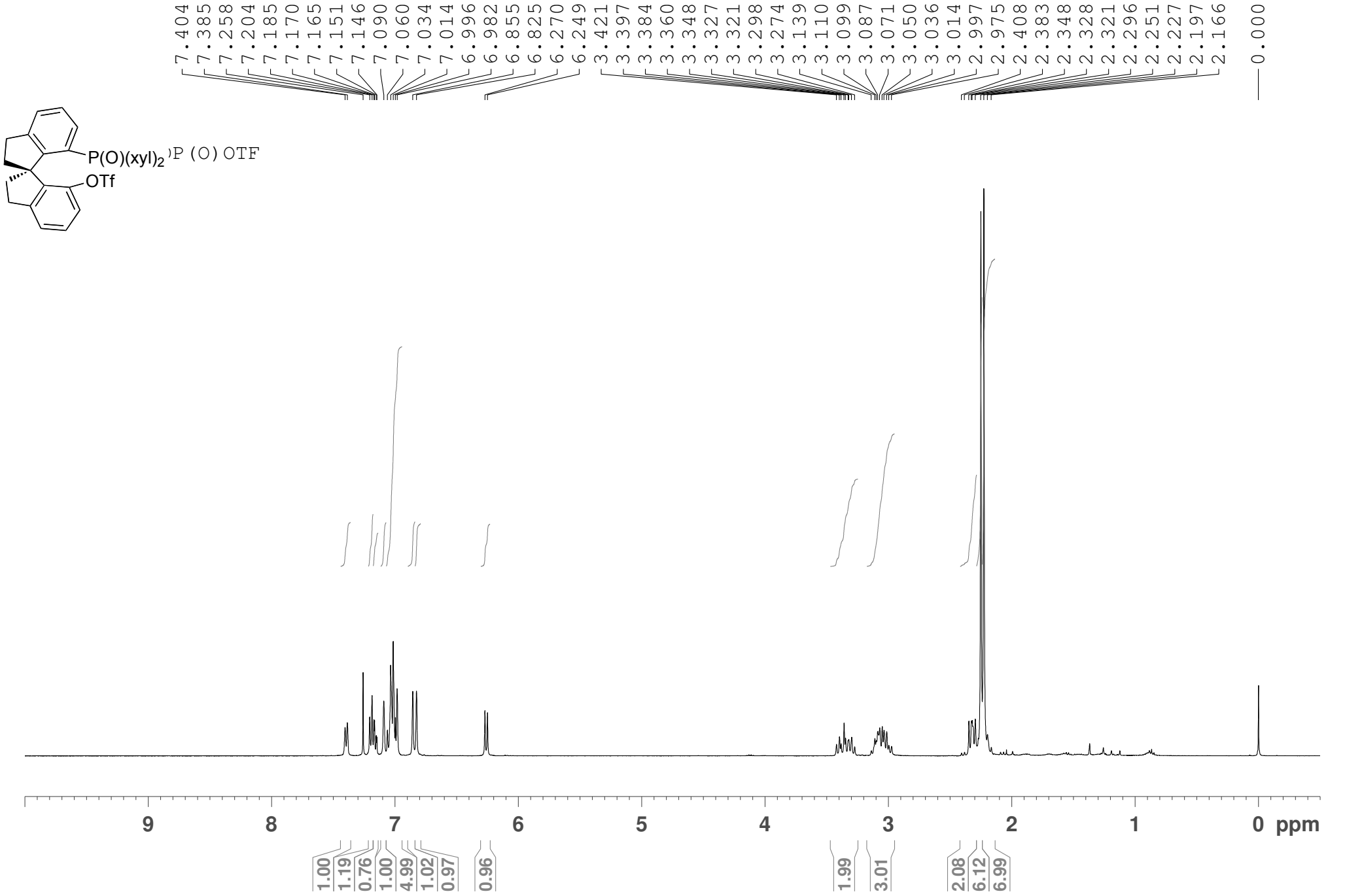
^{1}H NMR (400 MHz, $CDCl_3$)



$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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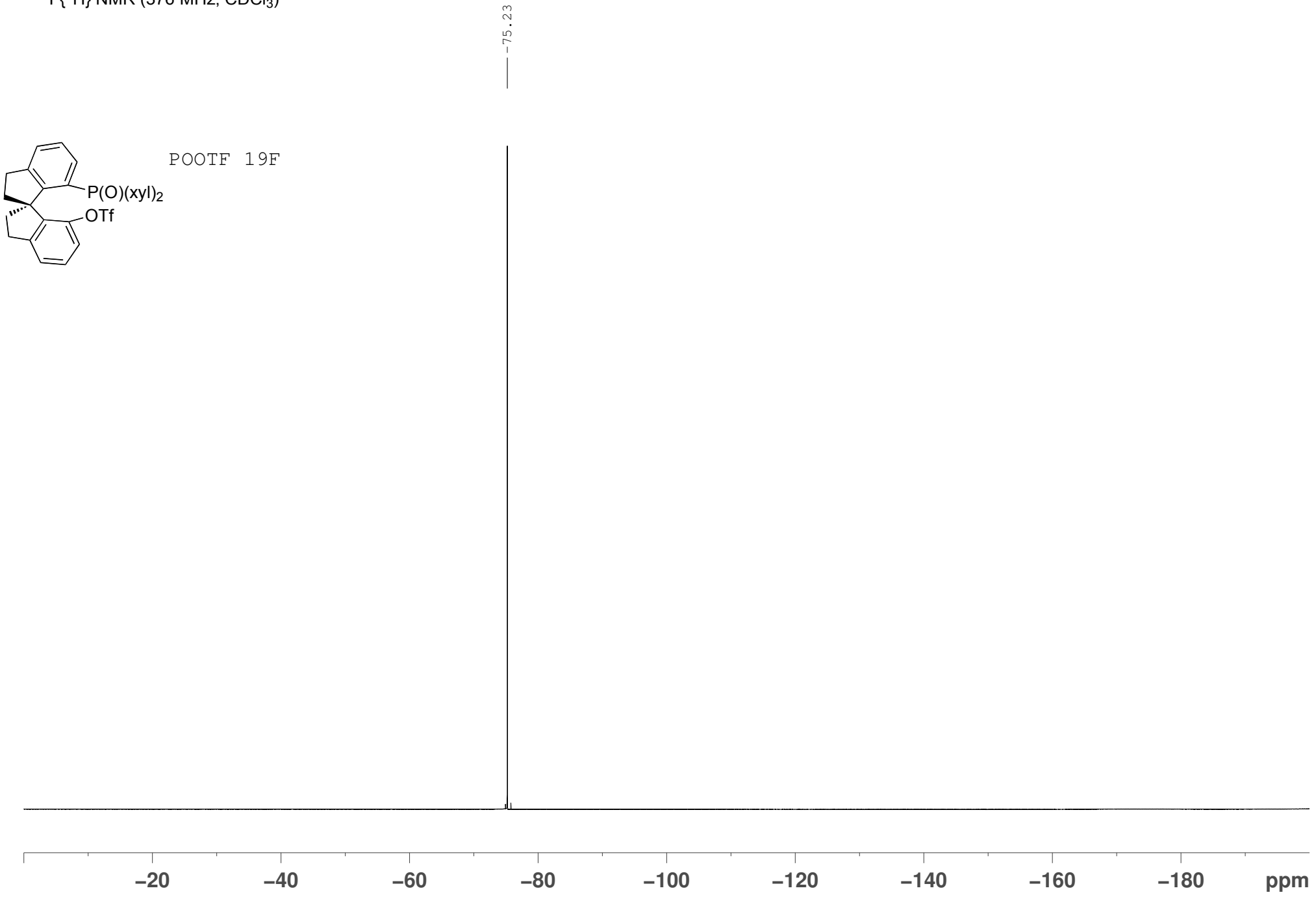
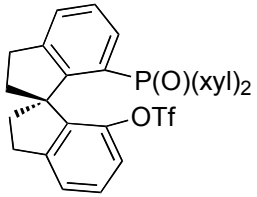
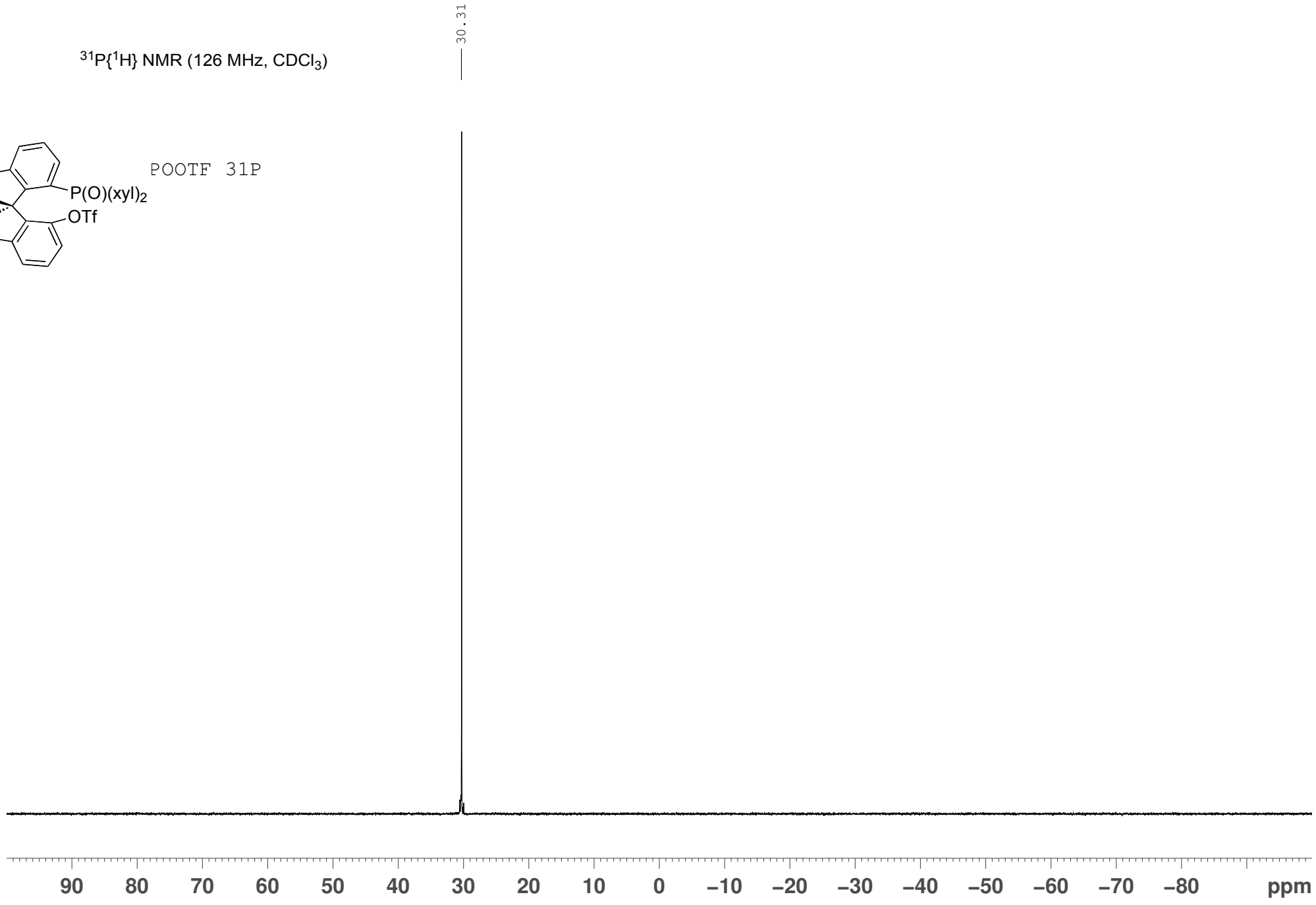


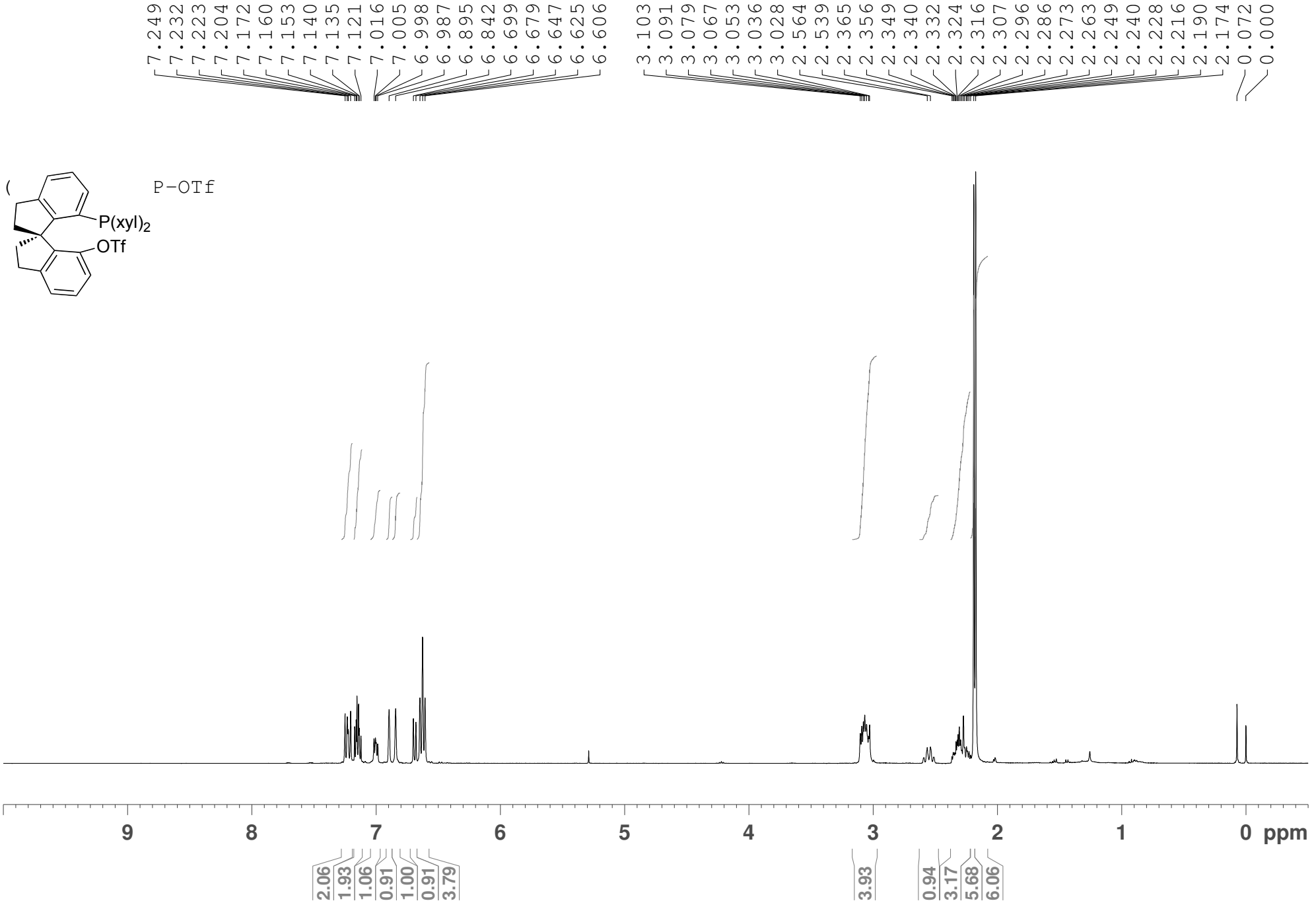
$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)



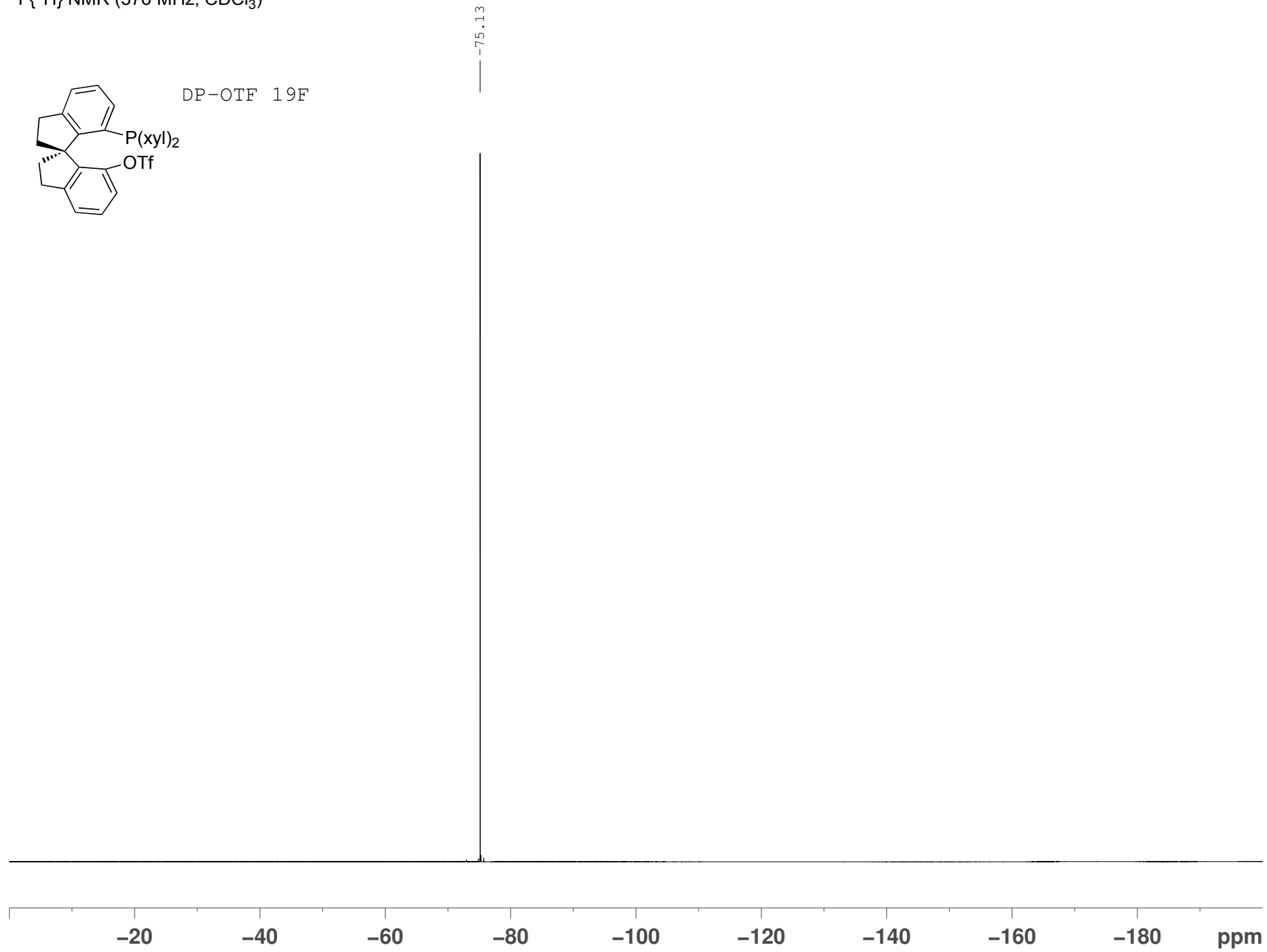
POOTF 31P



^{1}H NMR (400 MHz, $CDCl_3$)

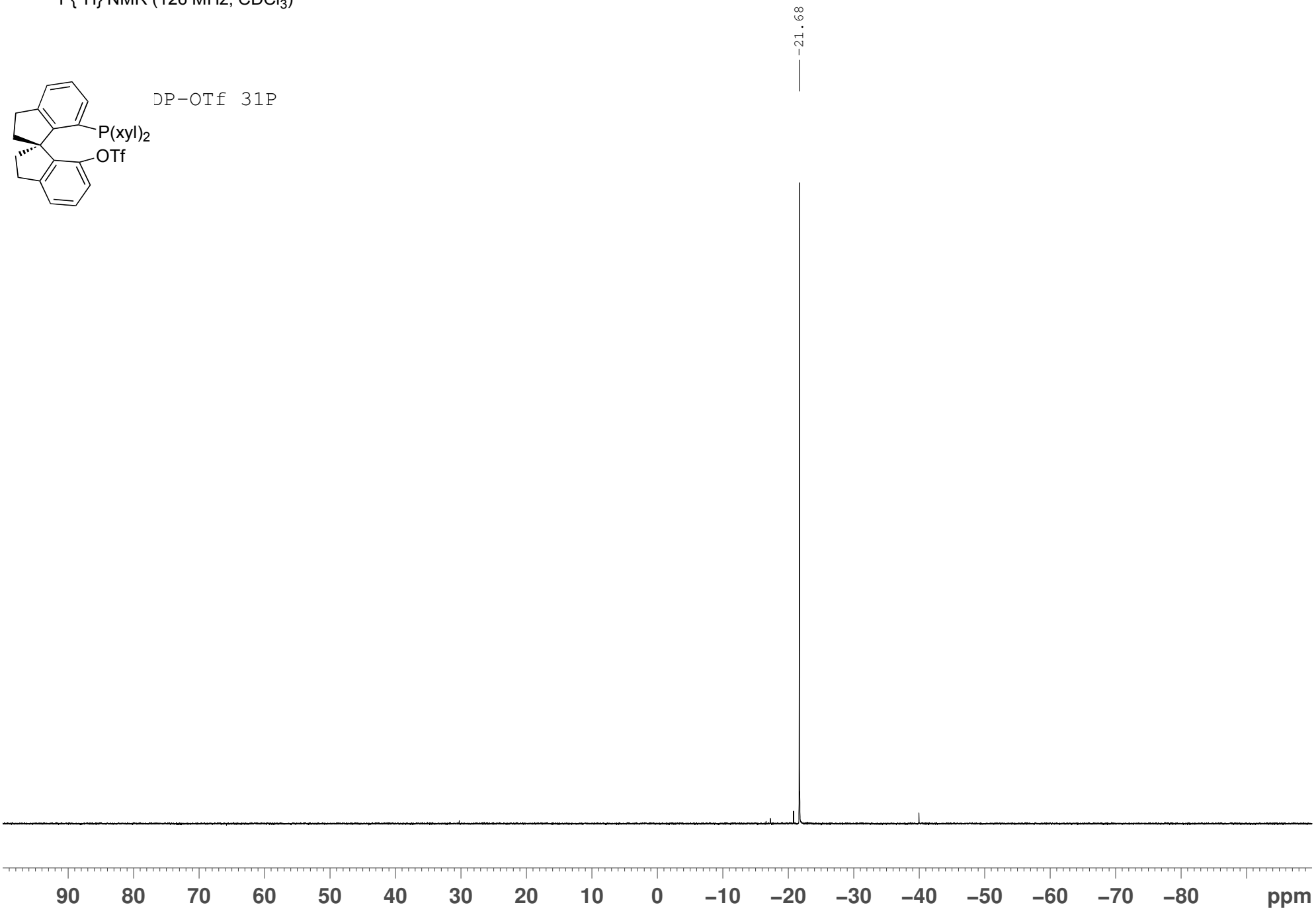


$^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$)

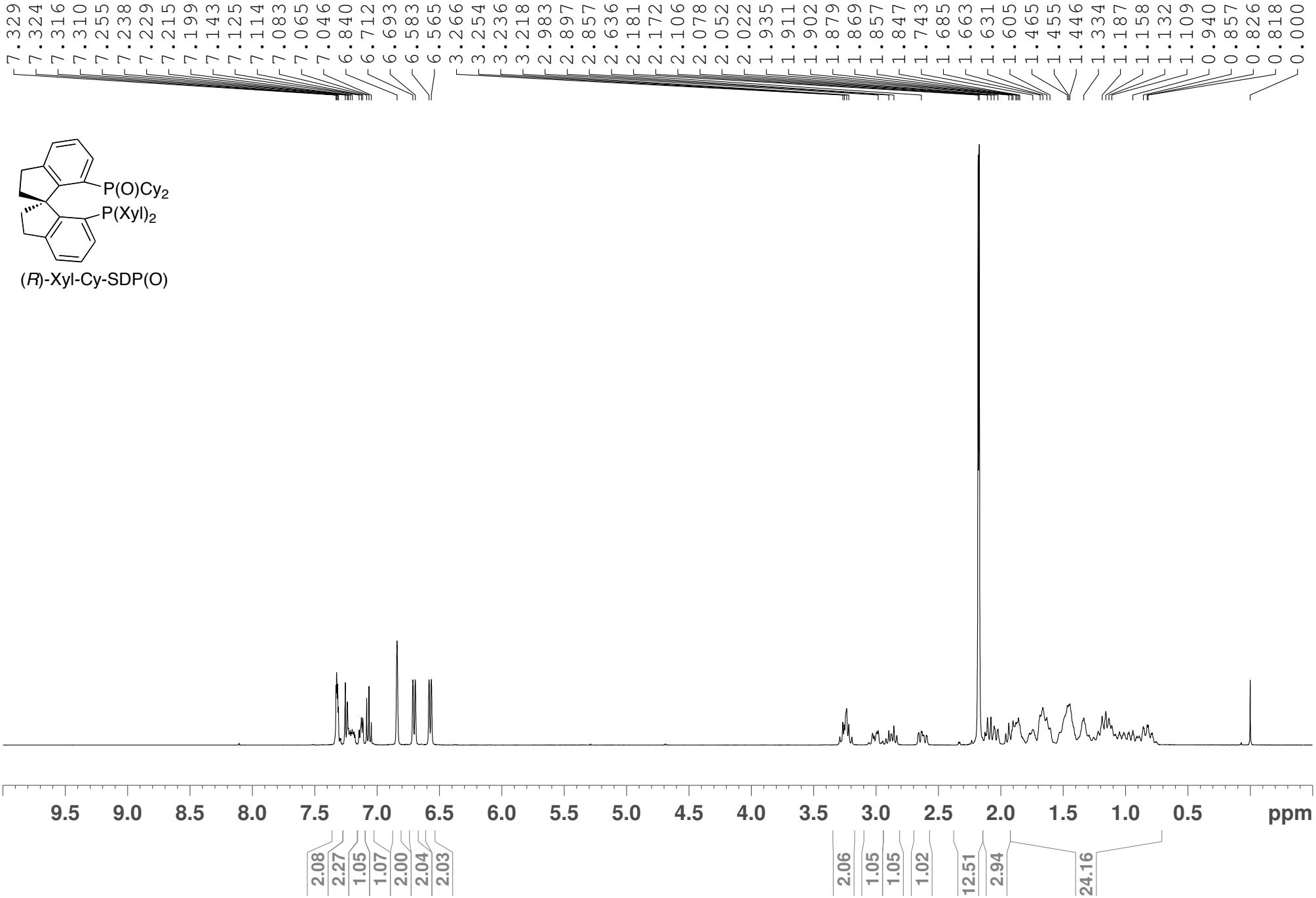


$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)

DP-OTf 31P



^{1}H NMR (400 MHz, $CDCl_3$)



(*R*)-Xyl-Cy-SDP(O)

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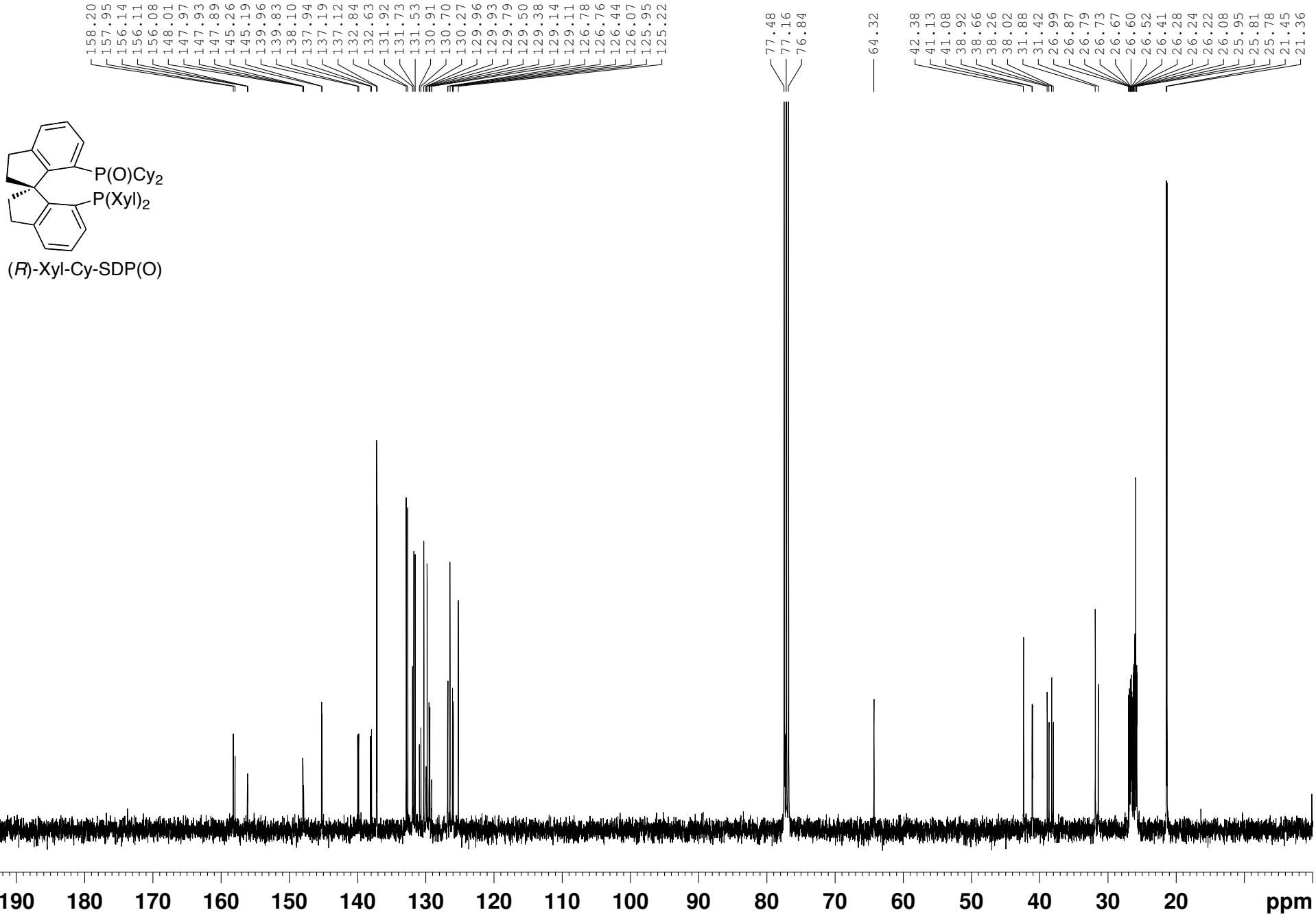

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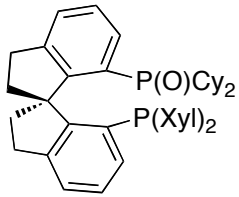

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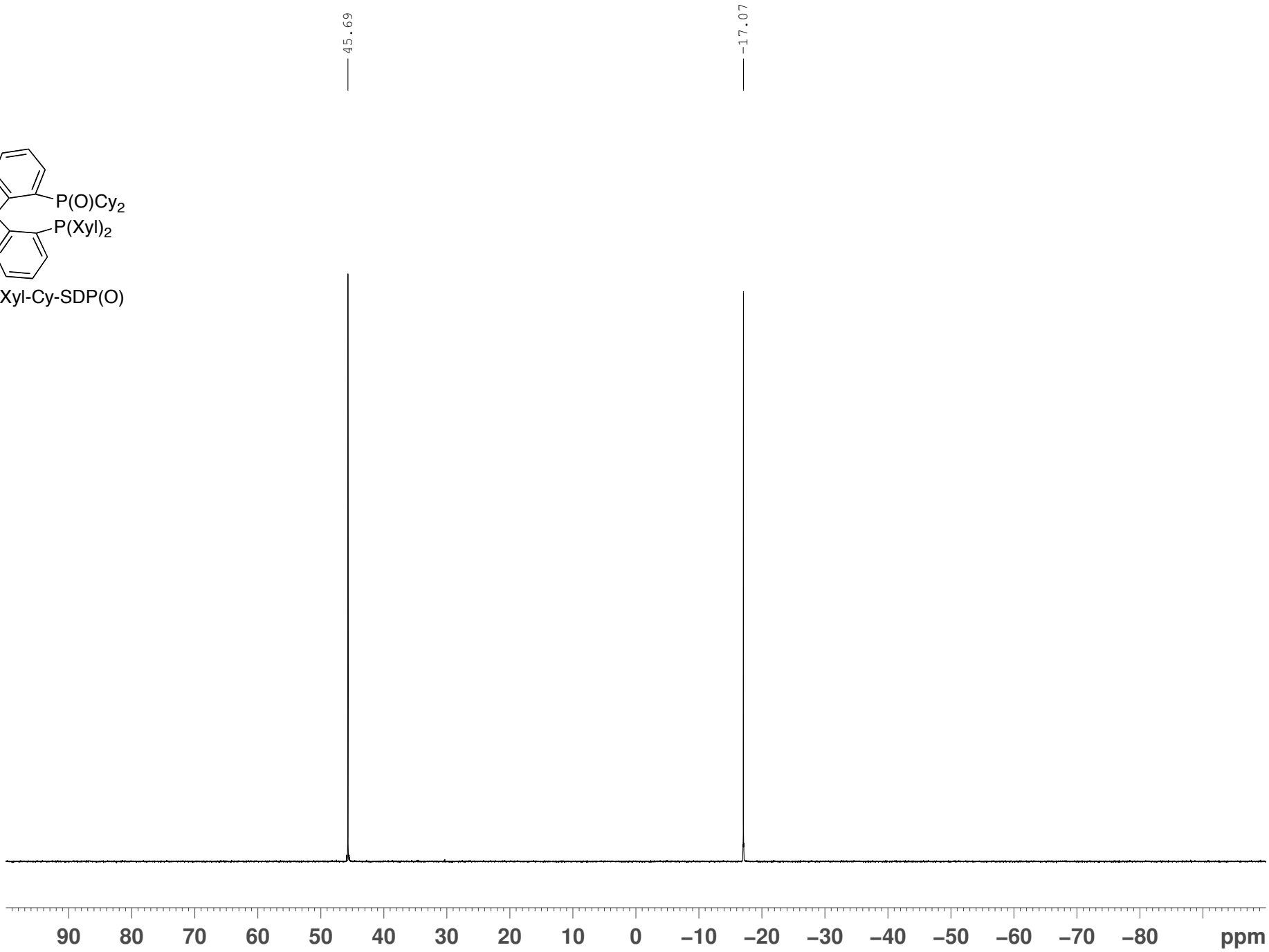

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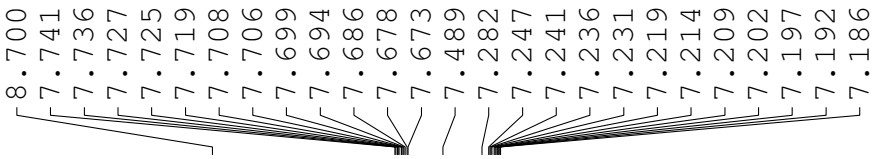
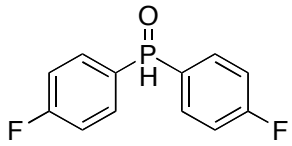
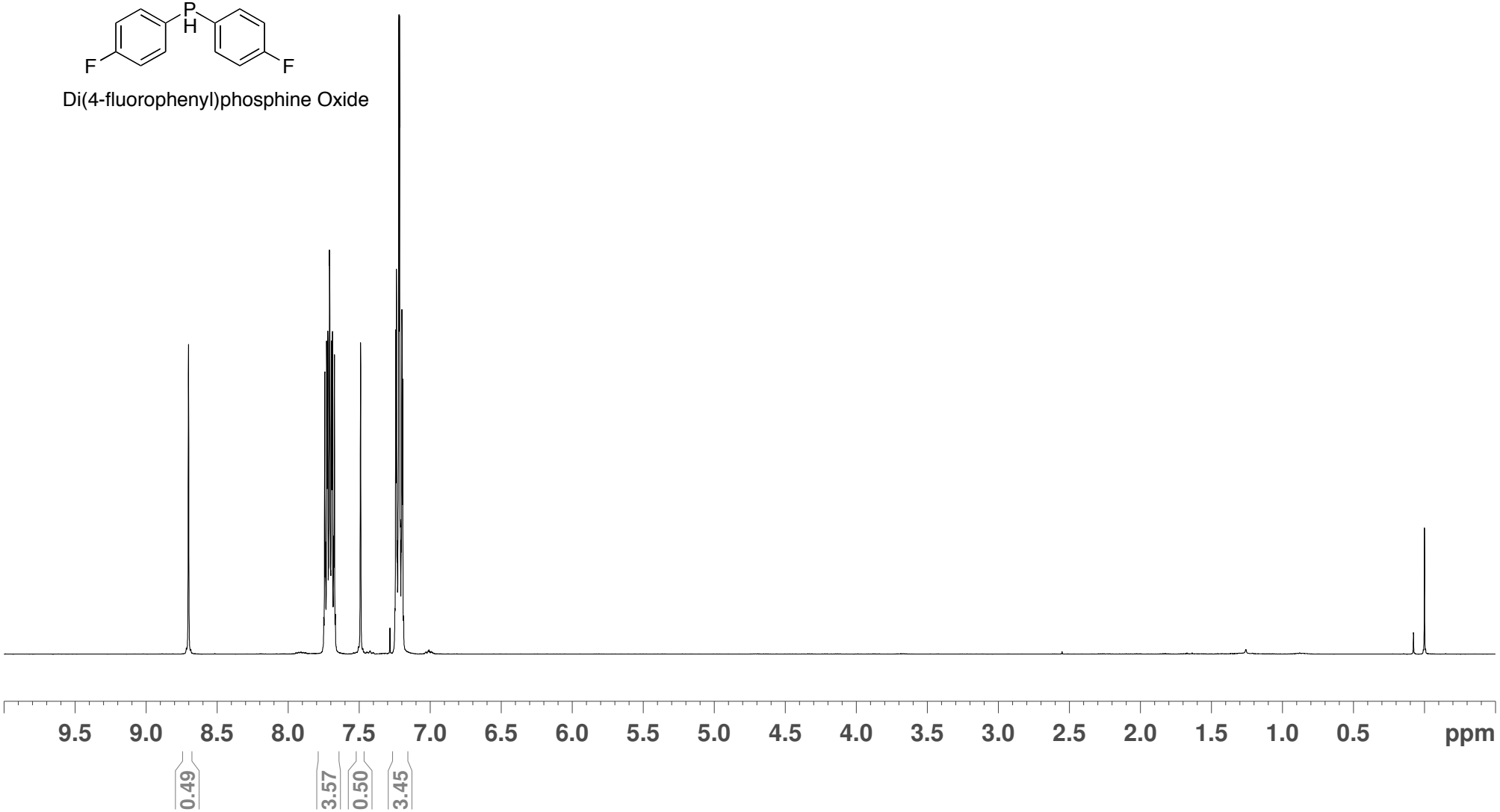




Di(4-fluorophenyl)phosphine Oxide



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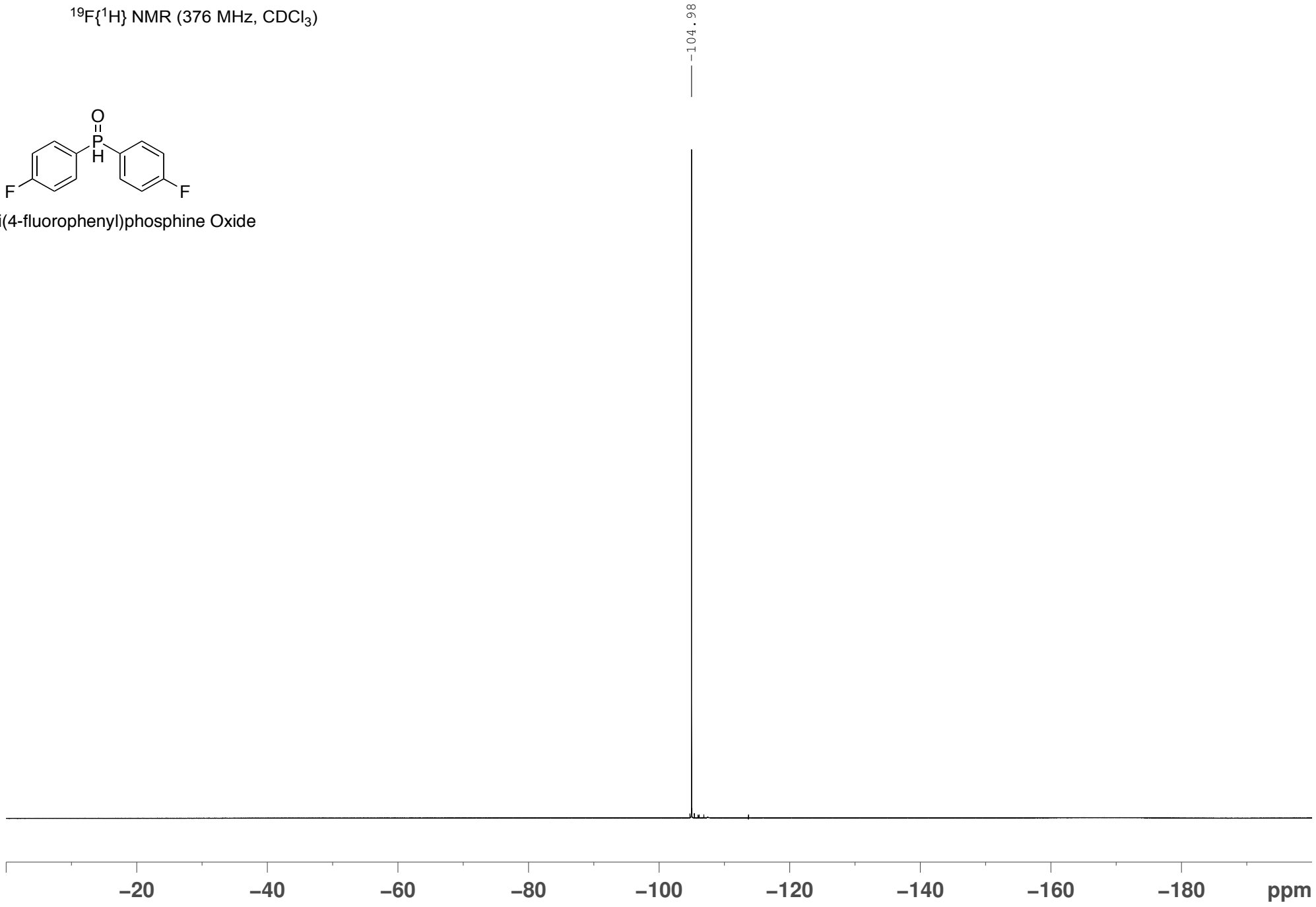

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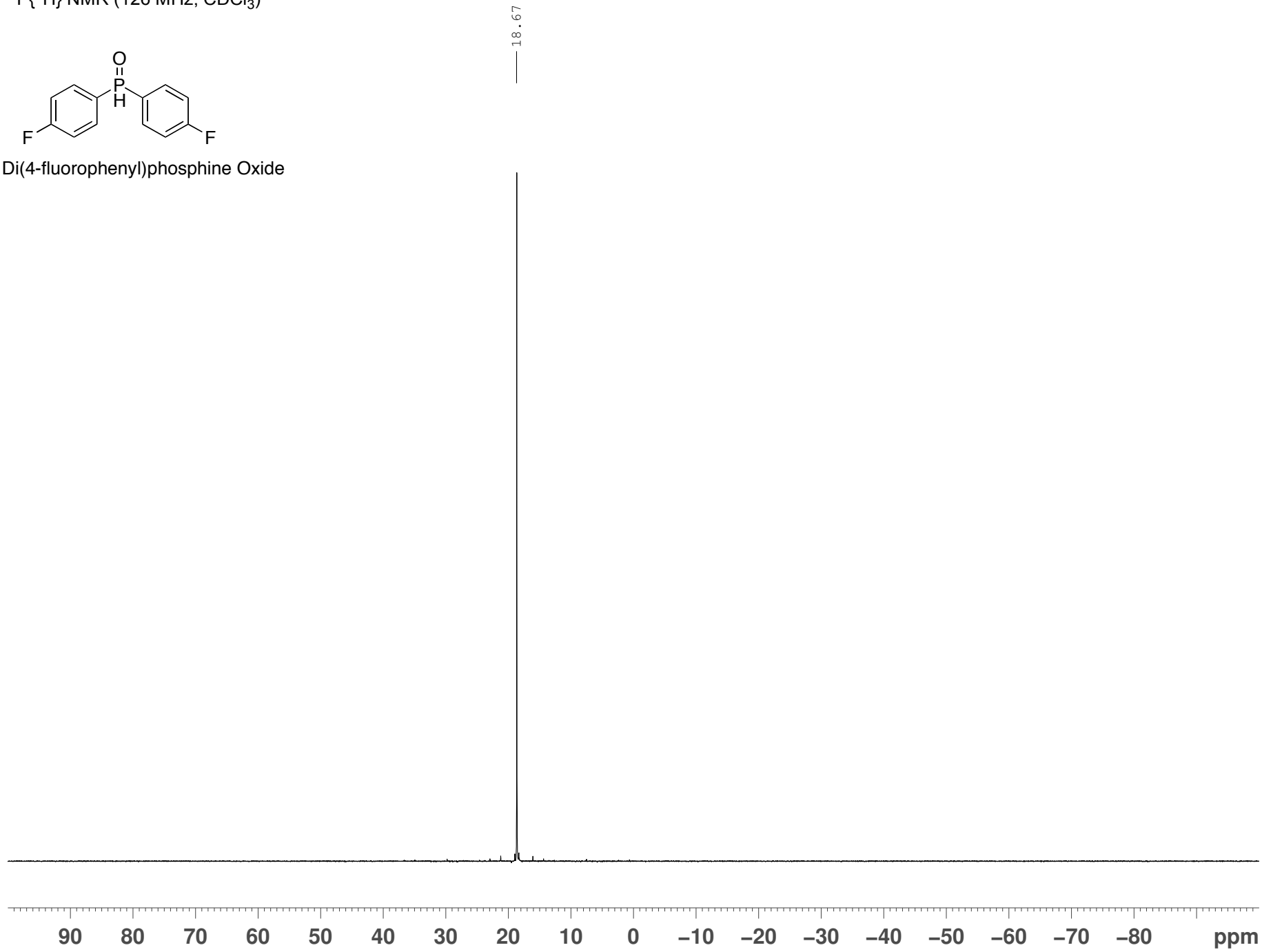
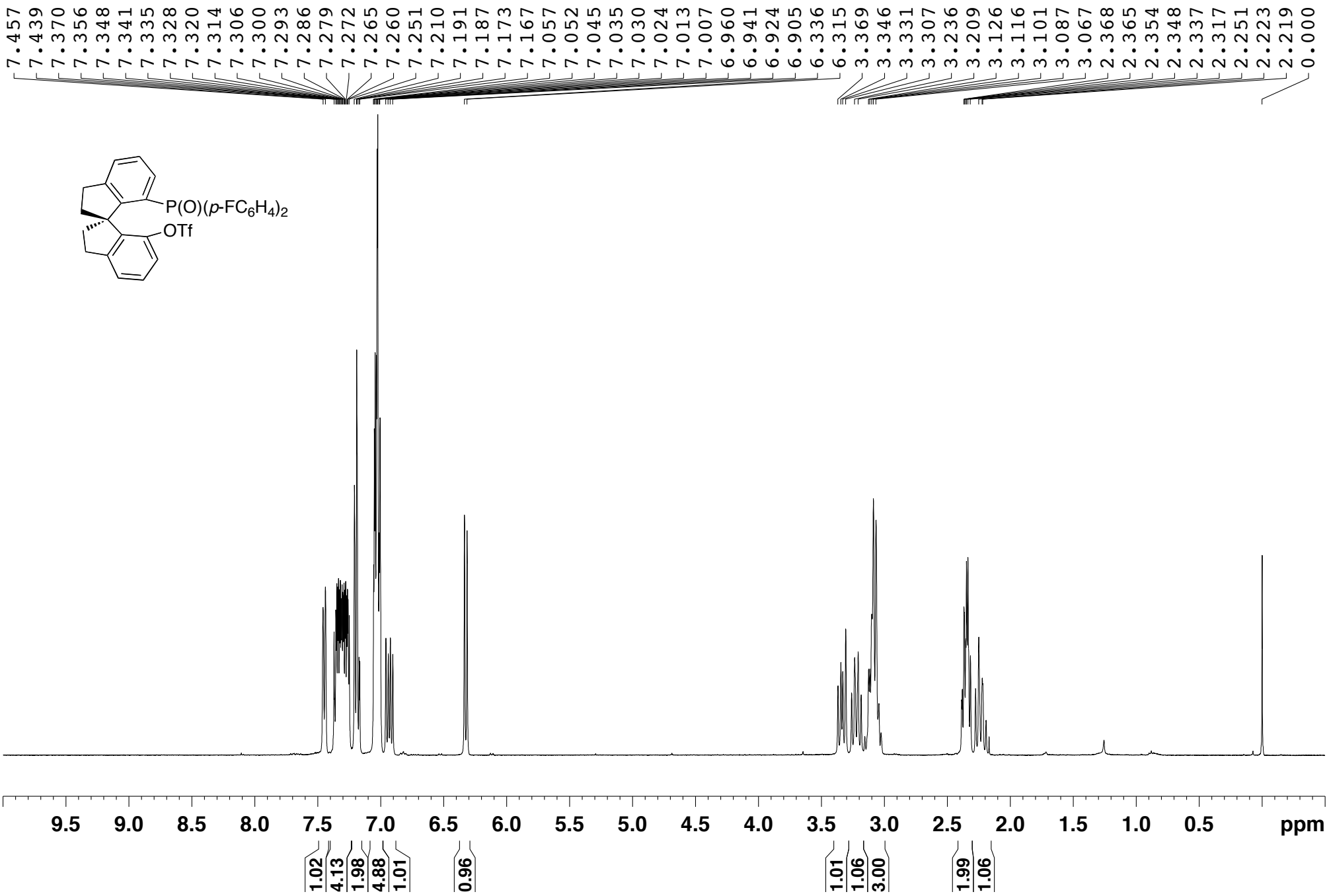


^{1}H NMR (400 MHz, $CDCl_3$)



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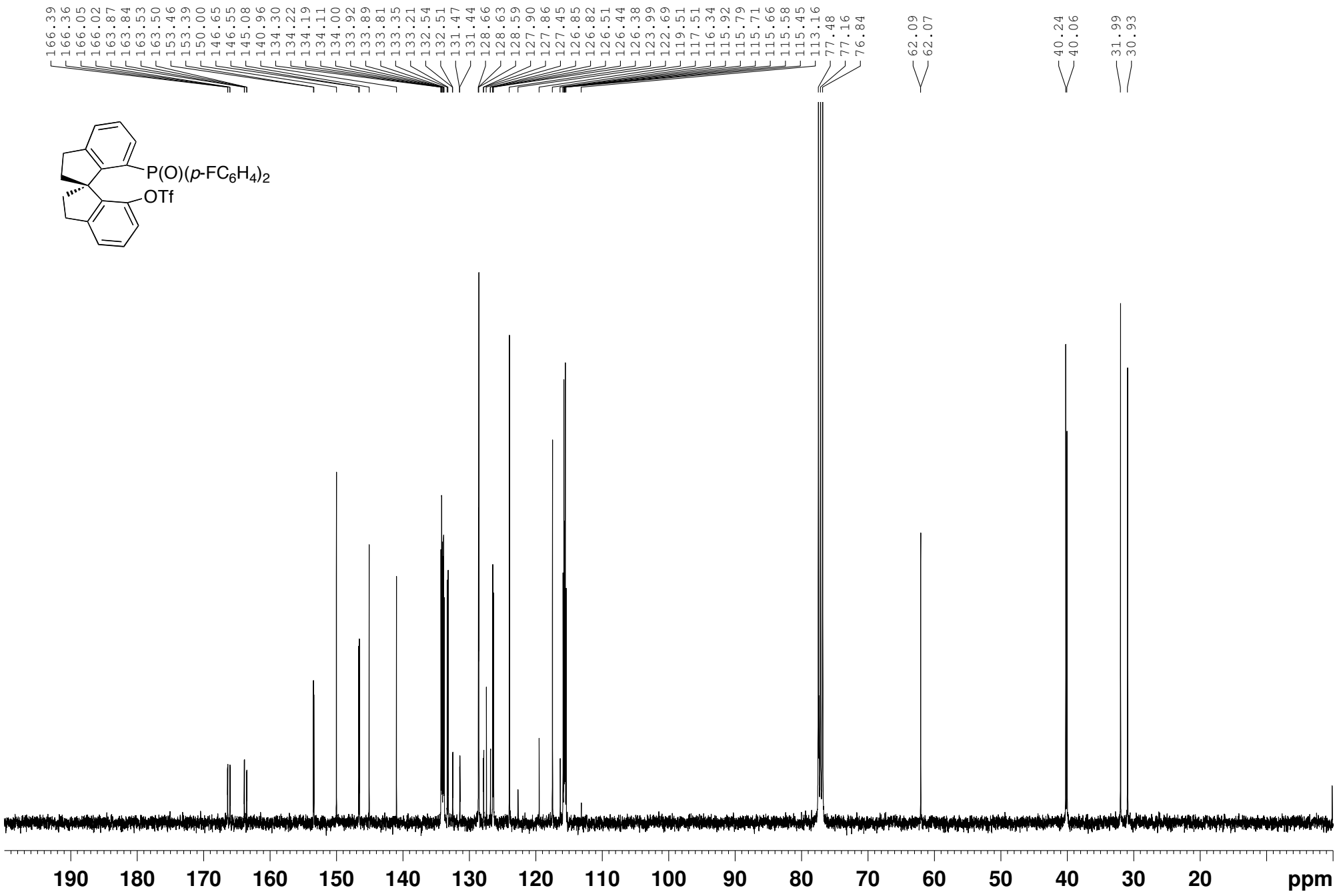

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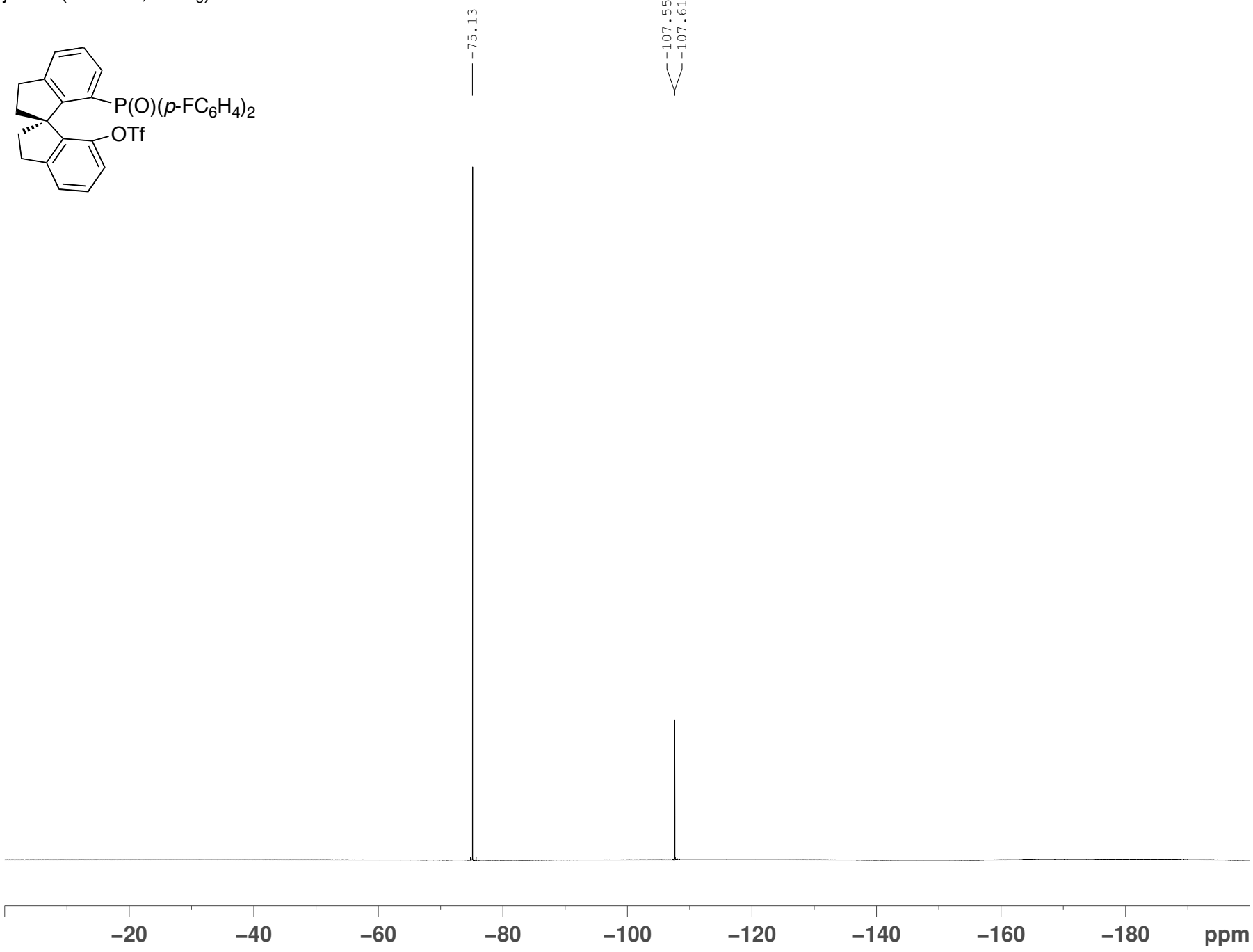
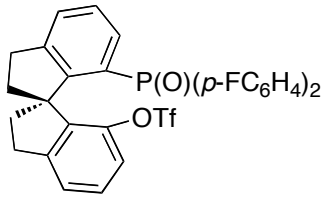


$^{31}P\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)

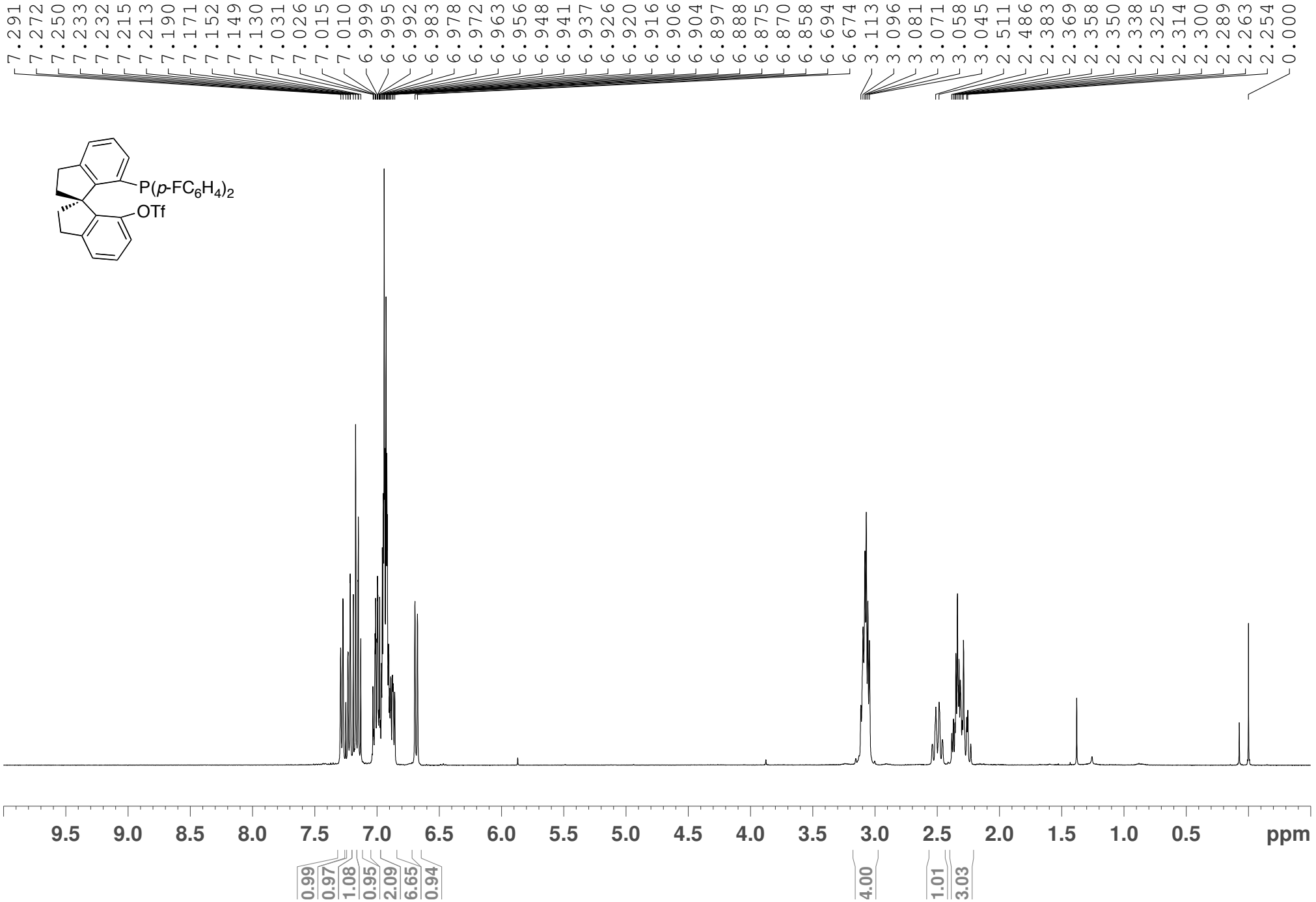


31P

29.20

90 80 70 60 50 40 30 20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 ppm

^{1}H NMR (400 MHz, $CDCl_3$)



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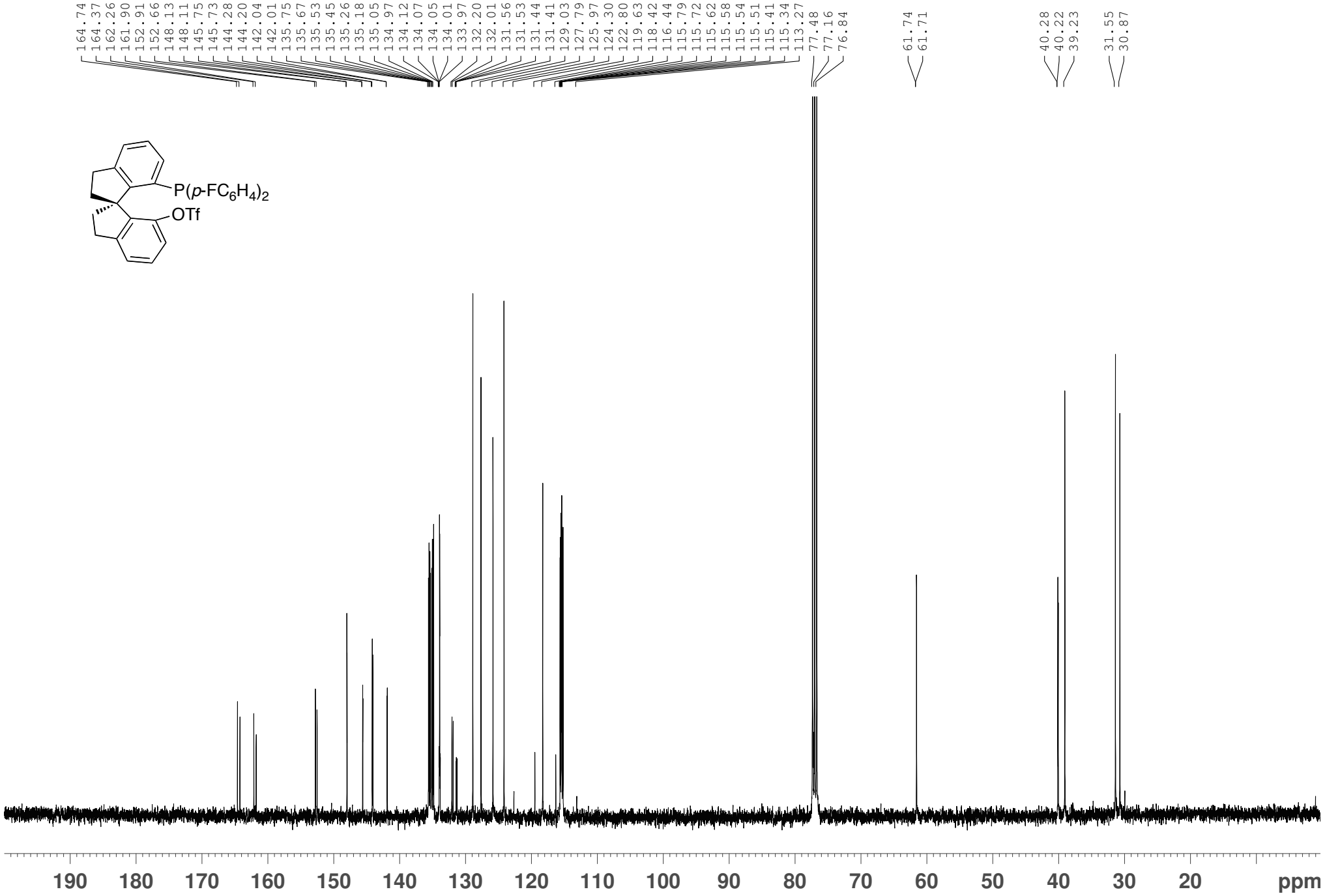

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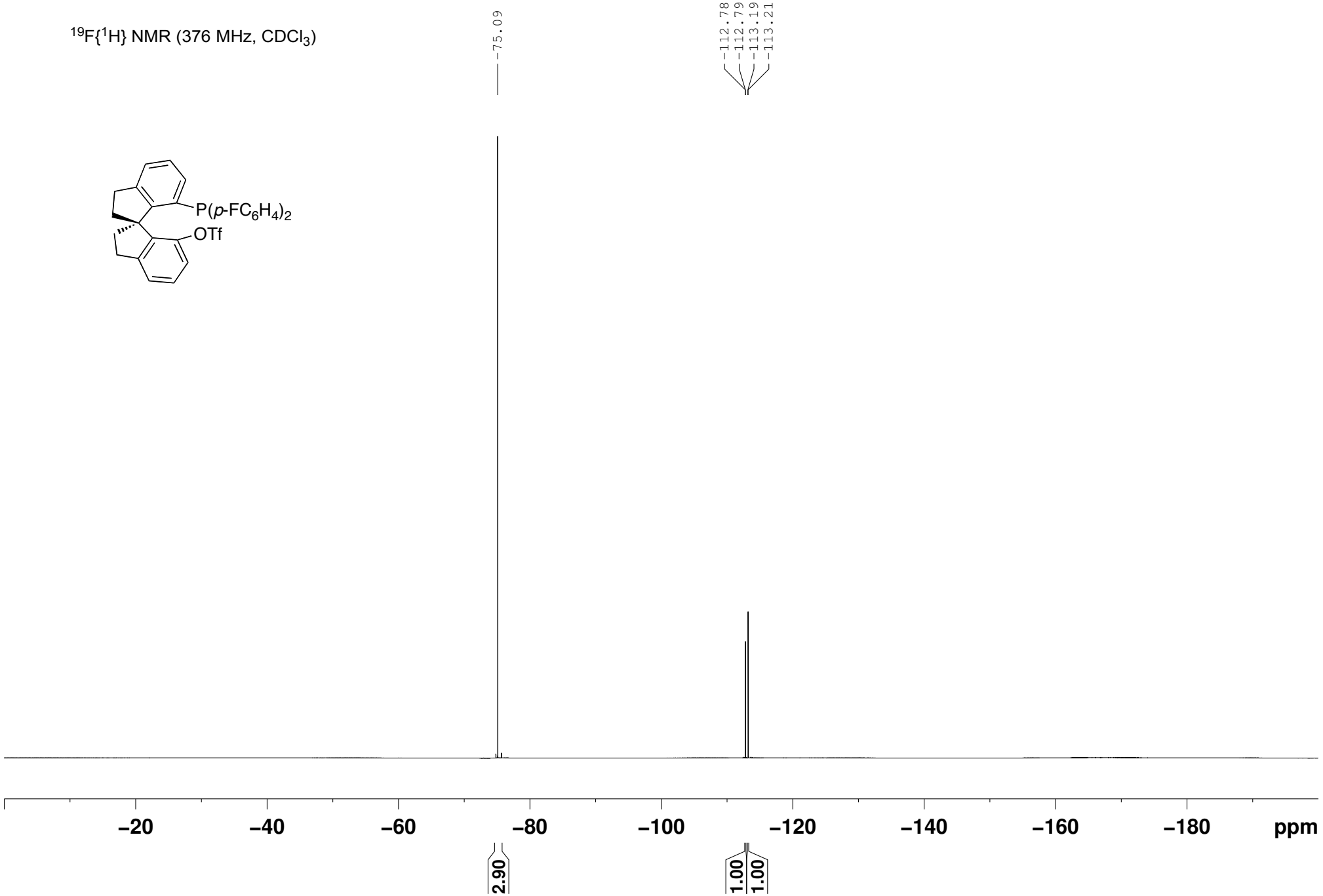

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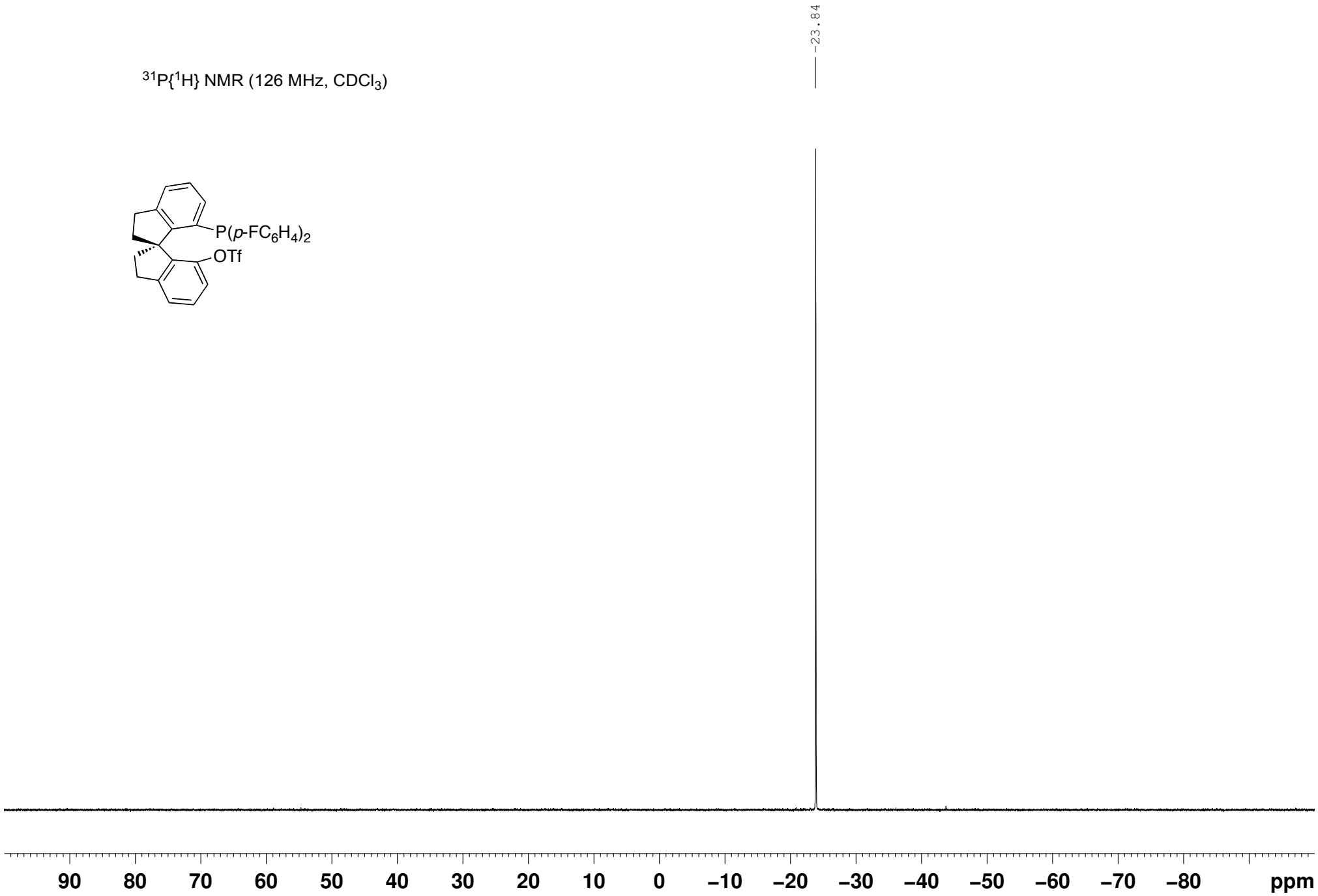
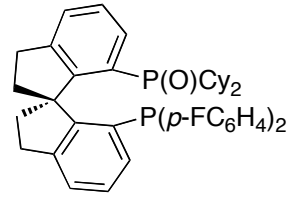
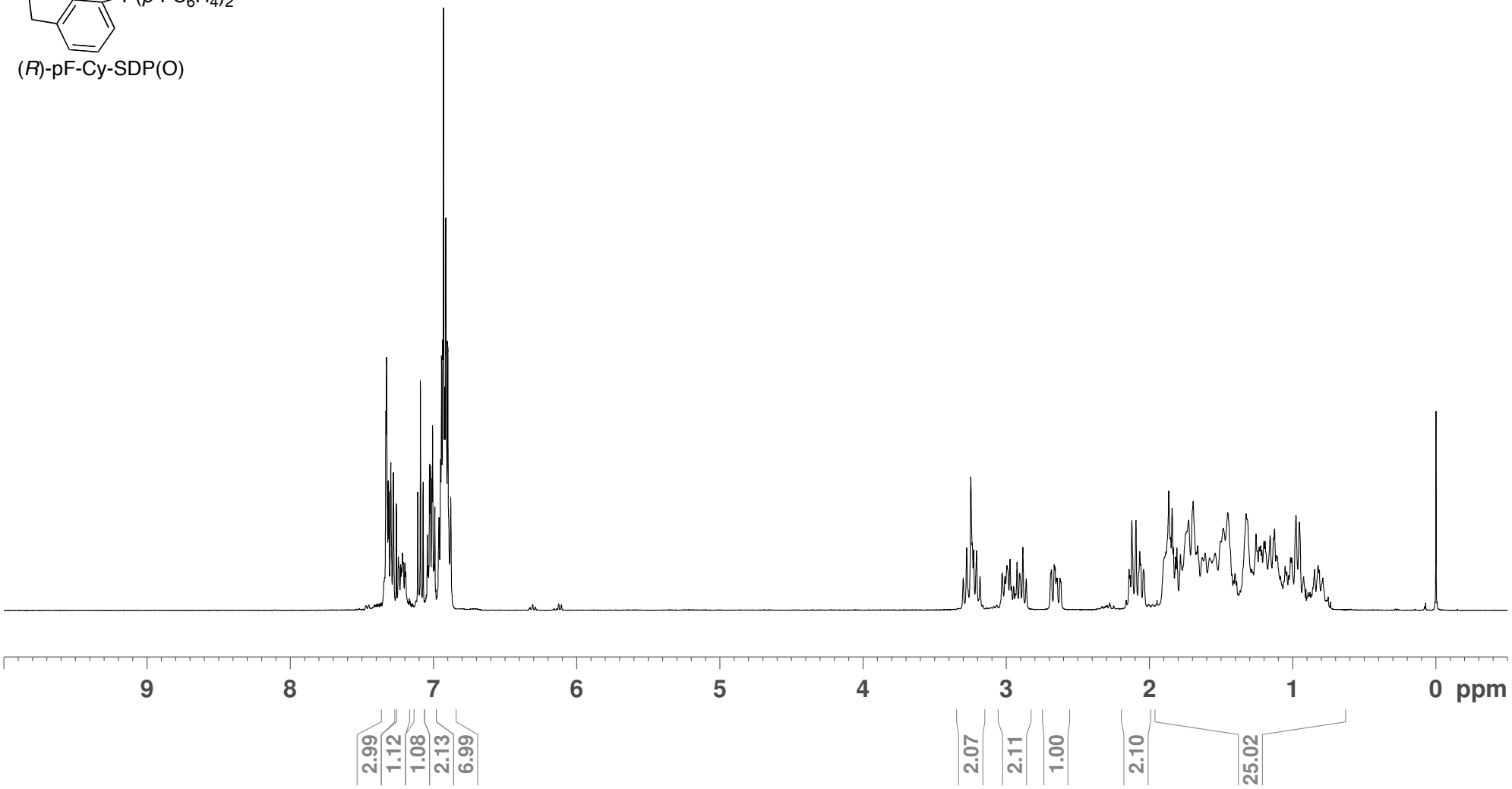


^{1}H NMR (400 MHz, $CDCl_3$)

7.333 7.328 7.317 7.312 7.299 7.281 7.260 7.111 7.092 7.073 7.044 7.028 7.022 7.013 7.007 6.991 6.962 6.951 6.945 6.936 6.931 6.924 6.923 6.915 6.911 6.902 6.901 6.880 3.277 3.248 3.238 3.229 2.885 2.124 2.095 1.866 1.854 1.843 1.834 1.809 1.727 1.696 1.664 1.504 1.485 1.454 1.326 1.257 1.234 1.225 1.202 1.194 1.158 1.135 1.128 0.978 0.954 0.000



(*R*)-pF-Cy-SDP(O)



^{13}C NMR (100 MHz, $CDCl_3$)

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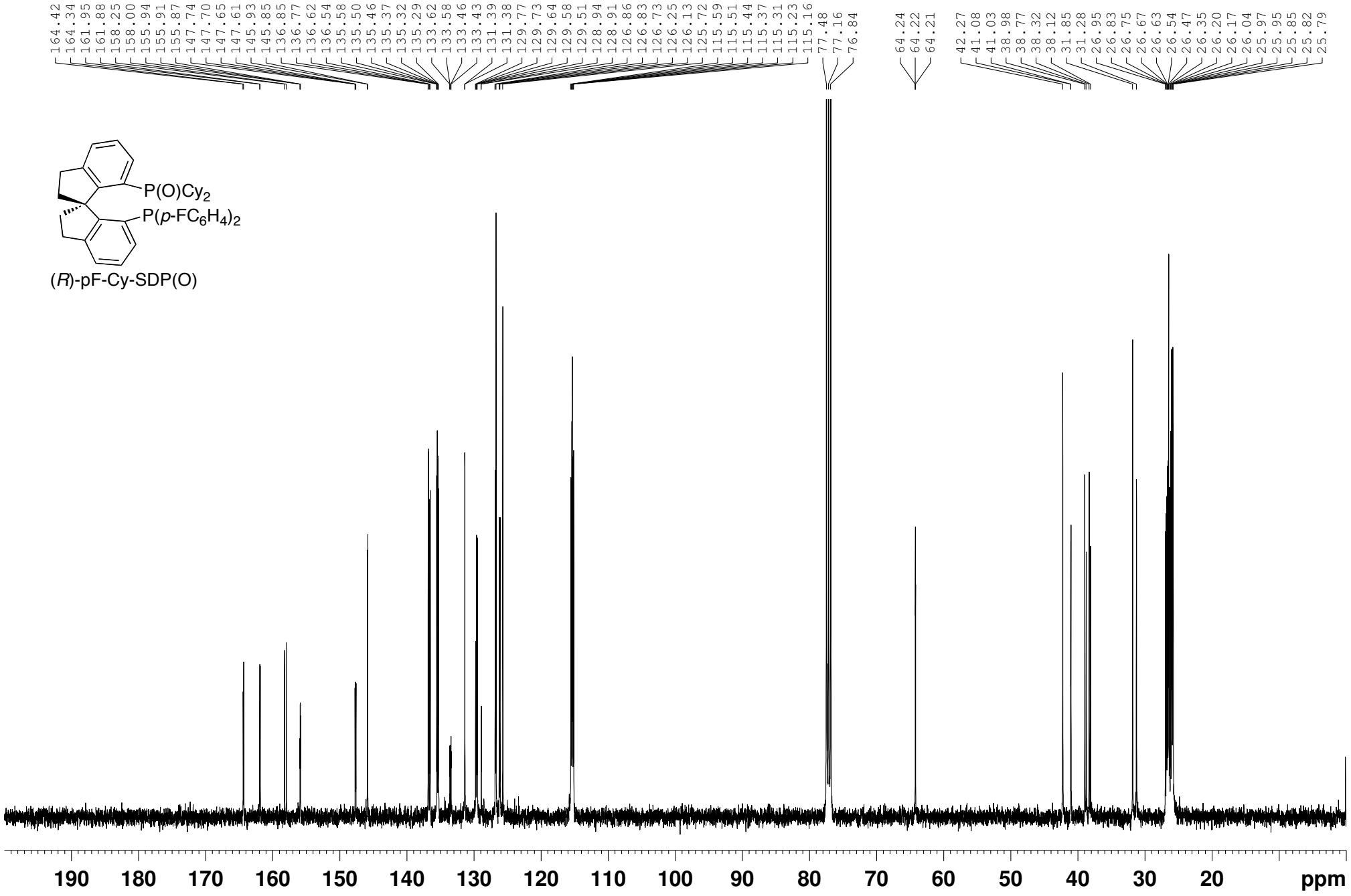

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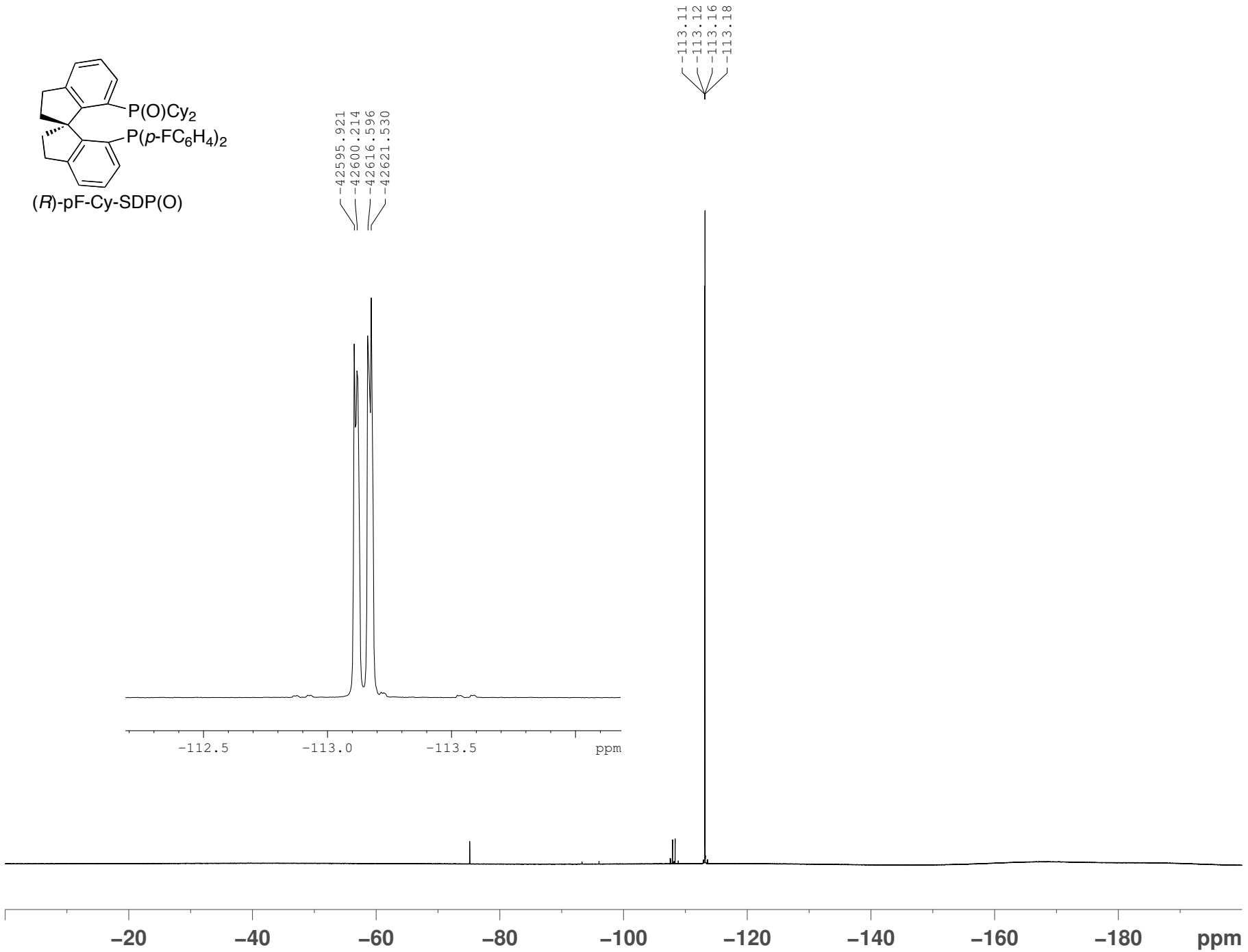

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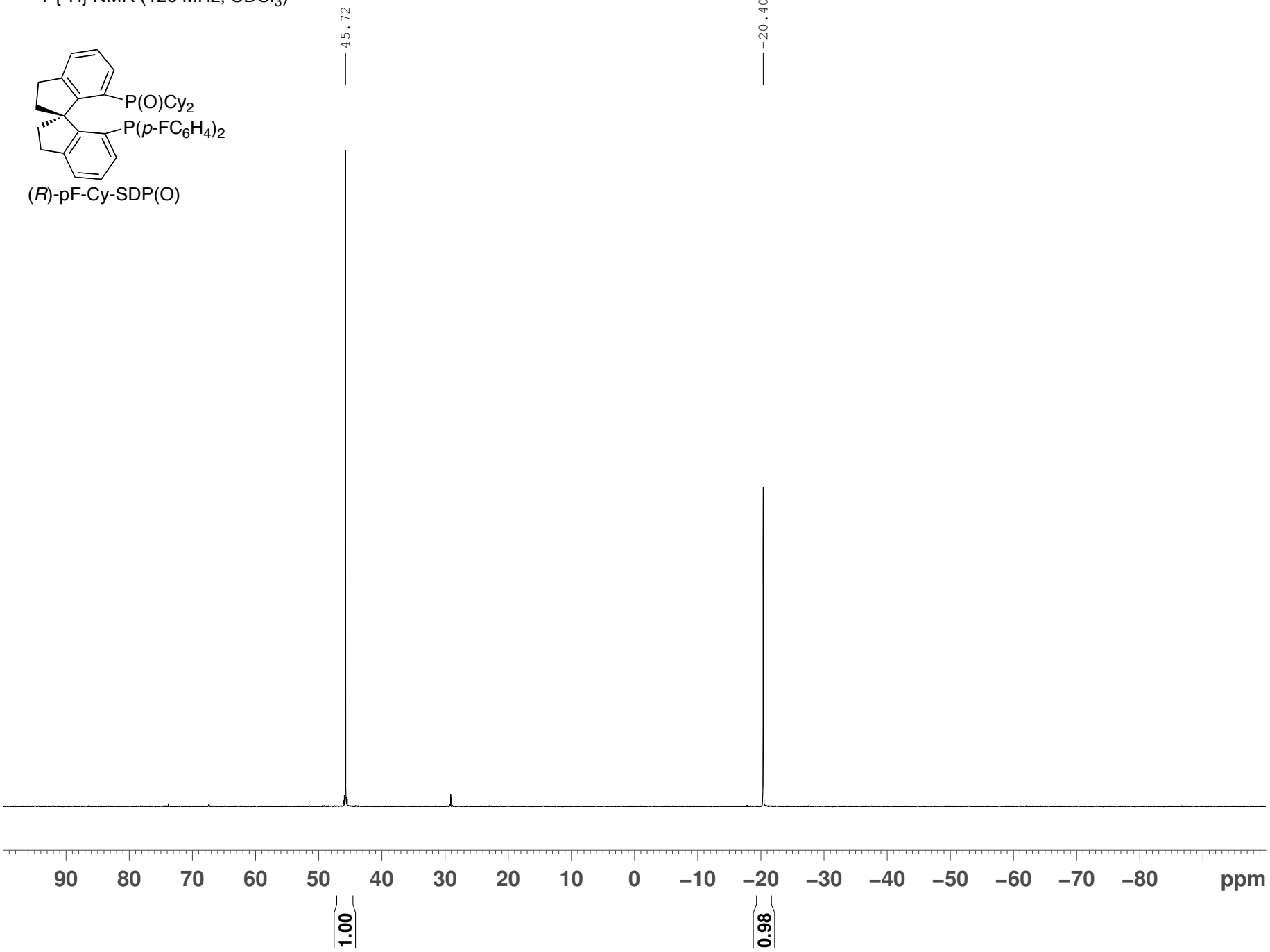
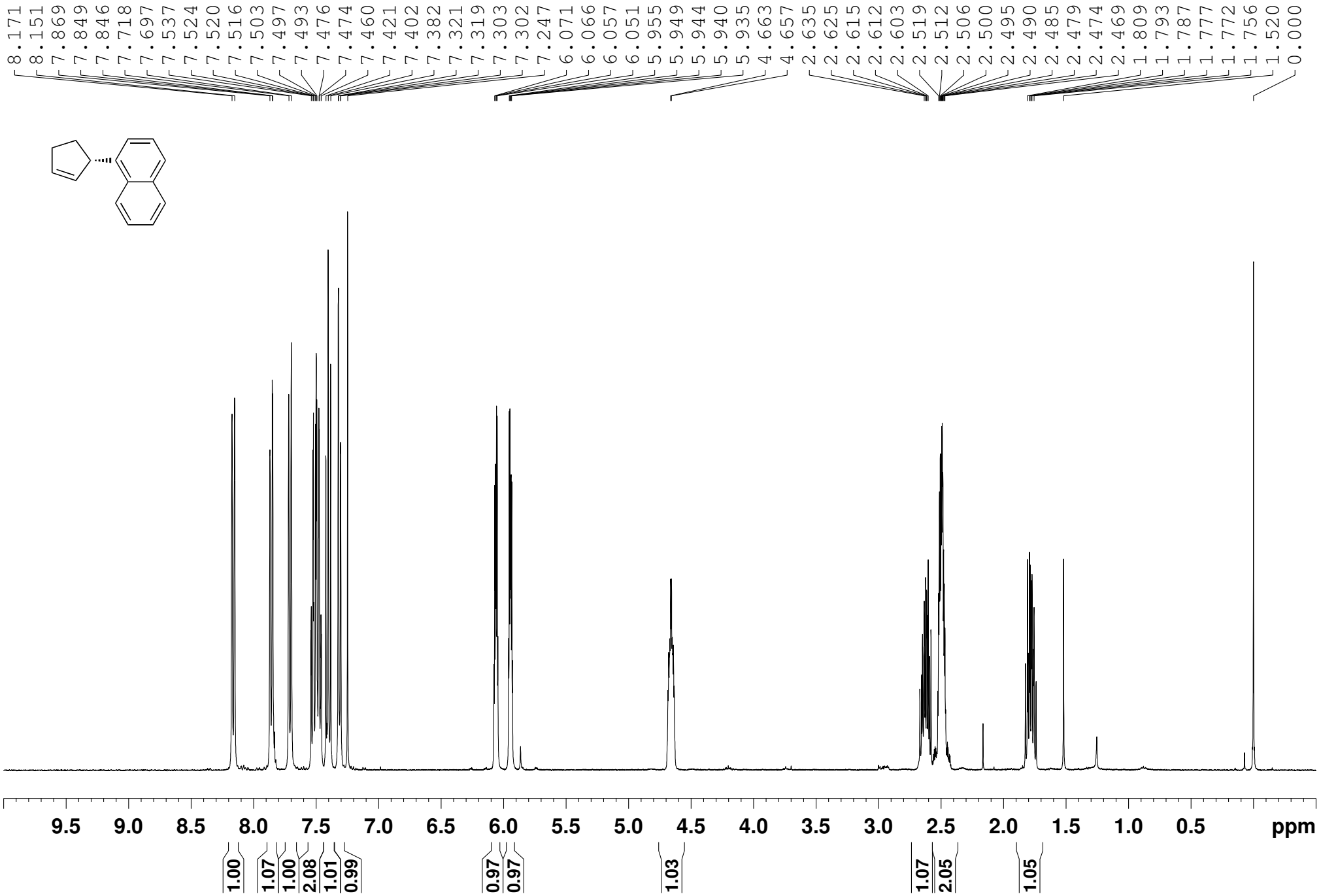
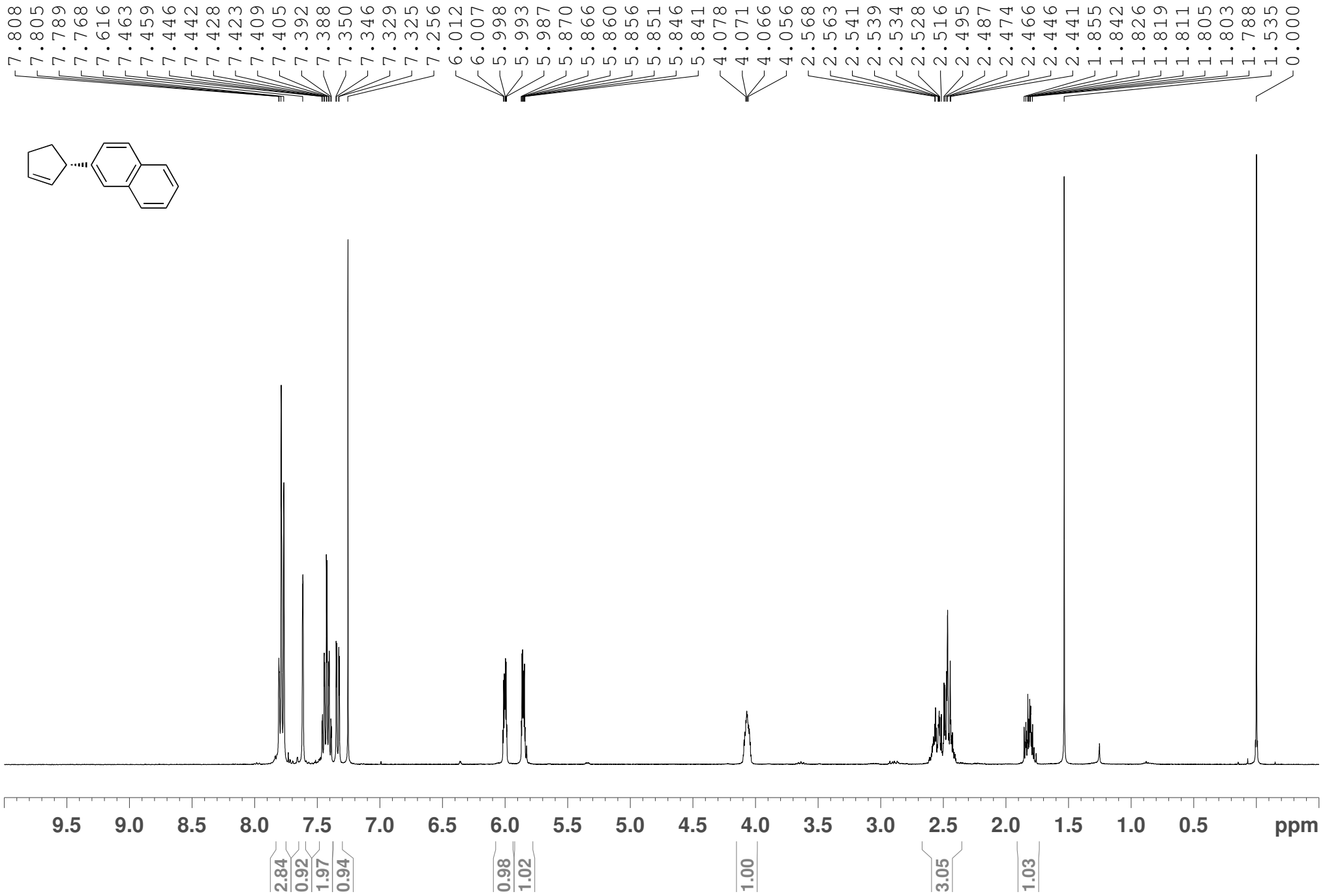


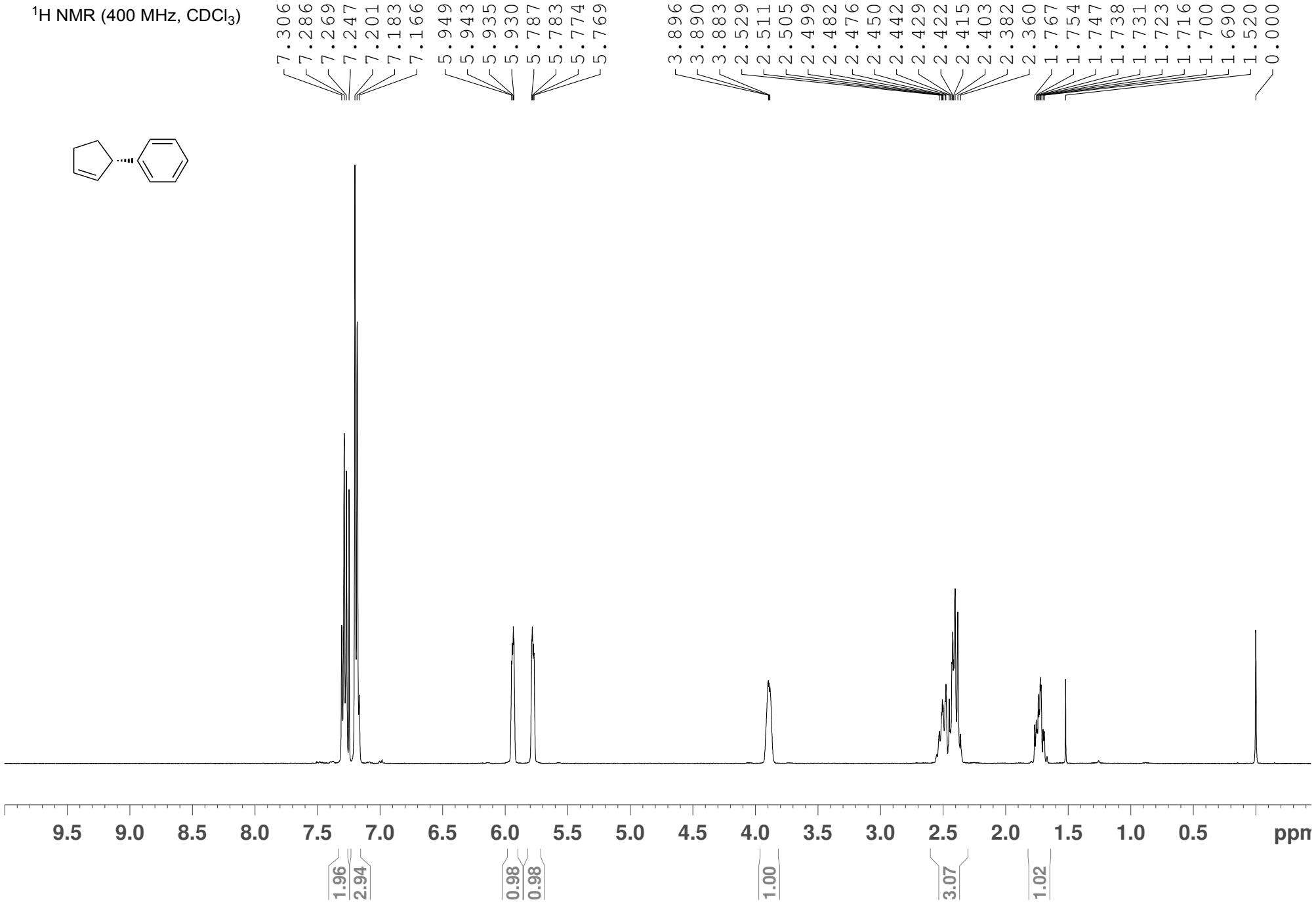
^{1}H NMR (400 MHz, $CDCl_3$)



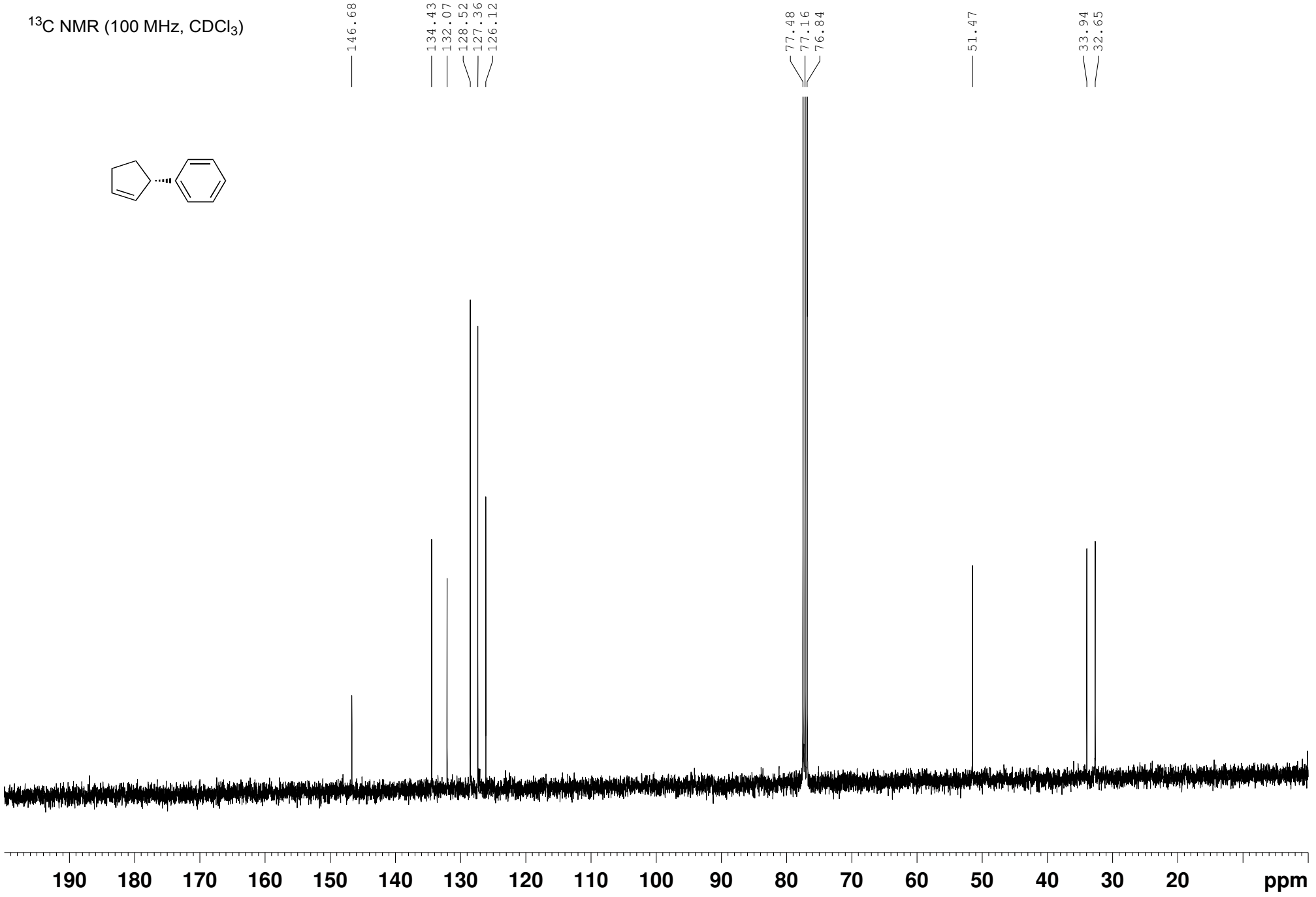
^{1}H NMR (400 MHz, $CDCl_3$)



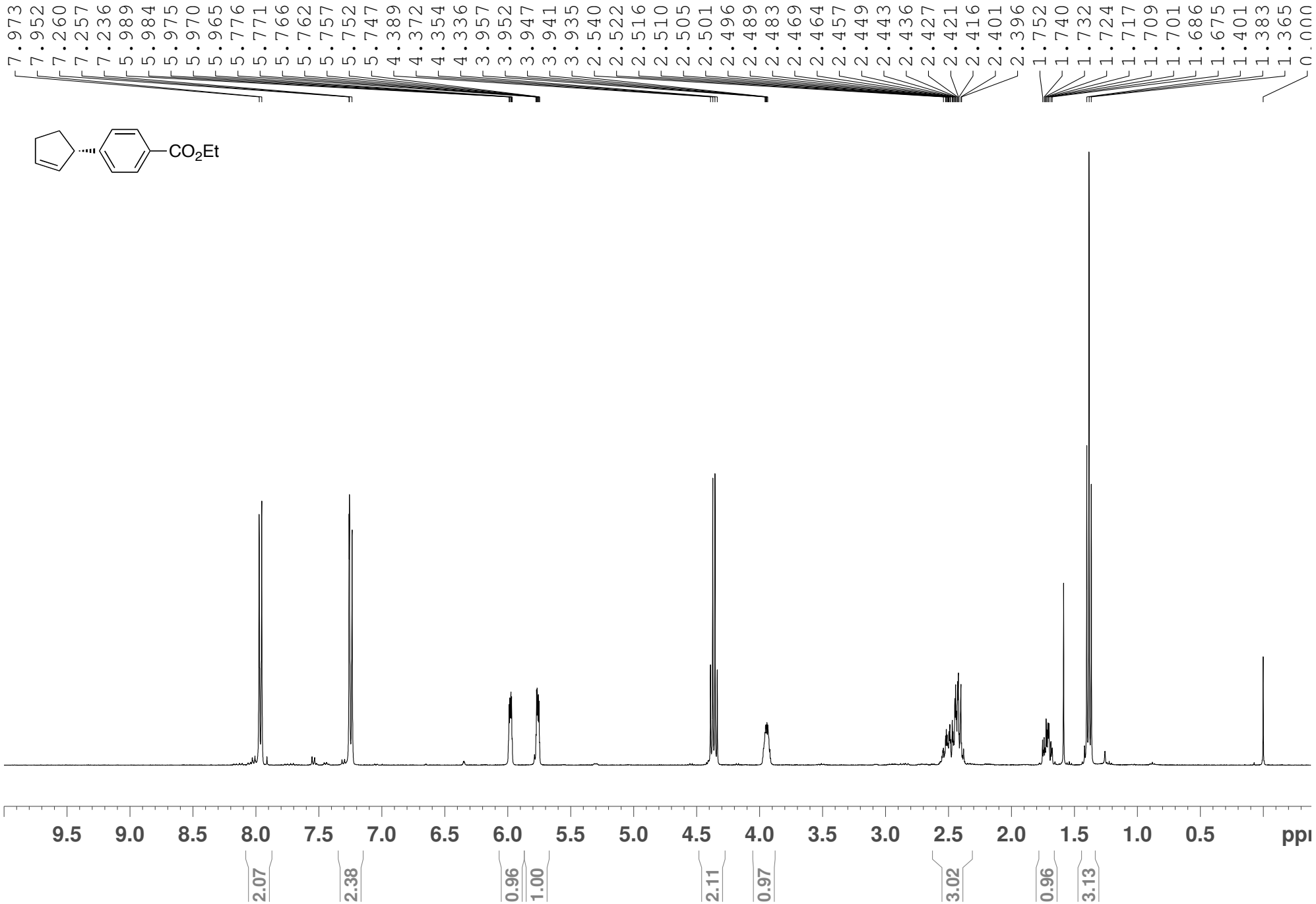
^{1}H NMR (400 MHz, $CDCl_3$)



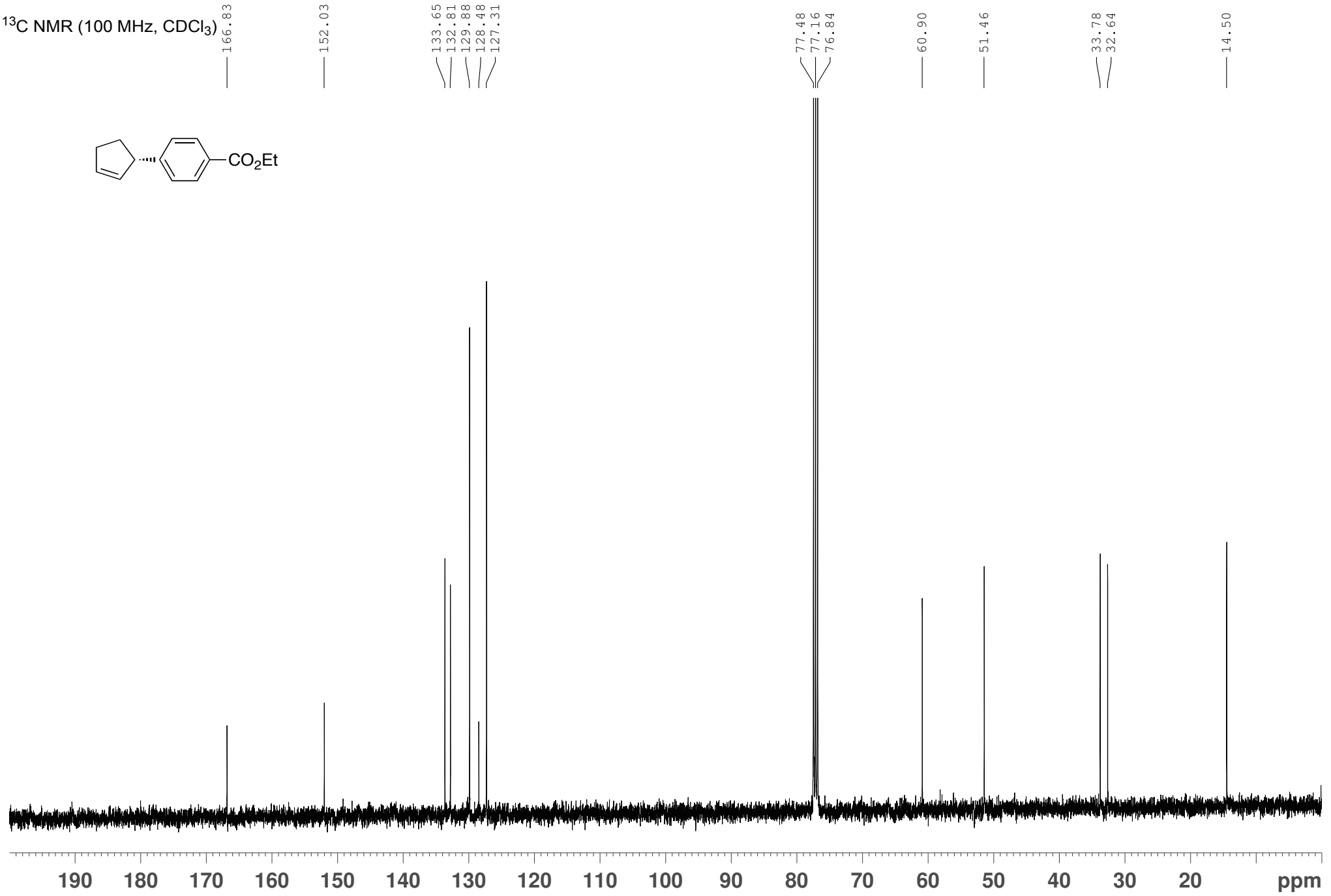
^{13}C NMR (100 MHz, $CDCl_3$)



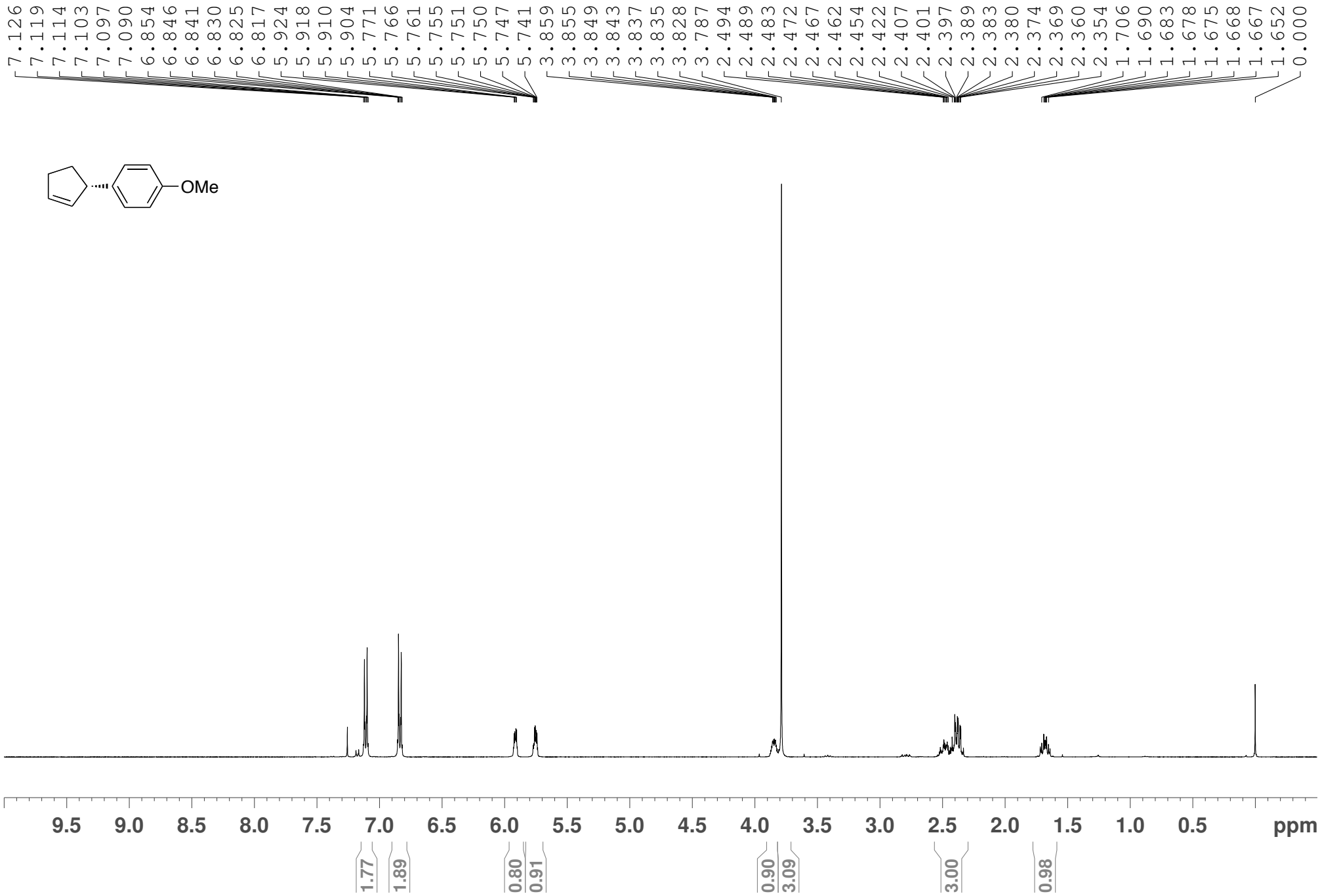
^{1}H NMR (400 MHz, $CDCl_3$)



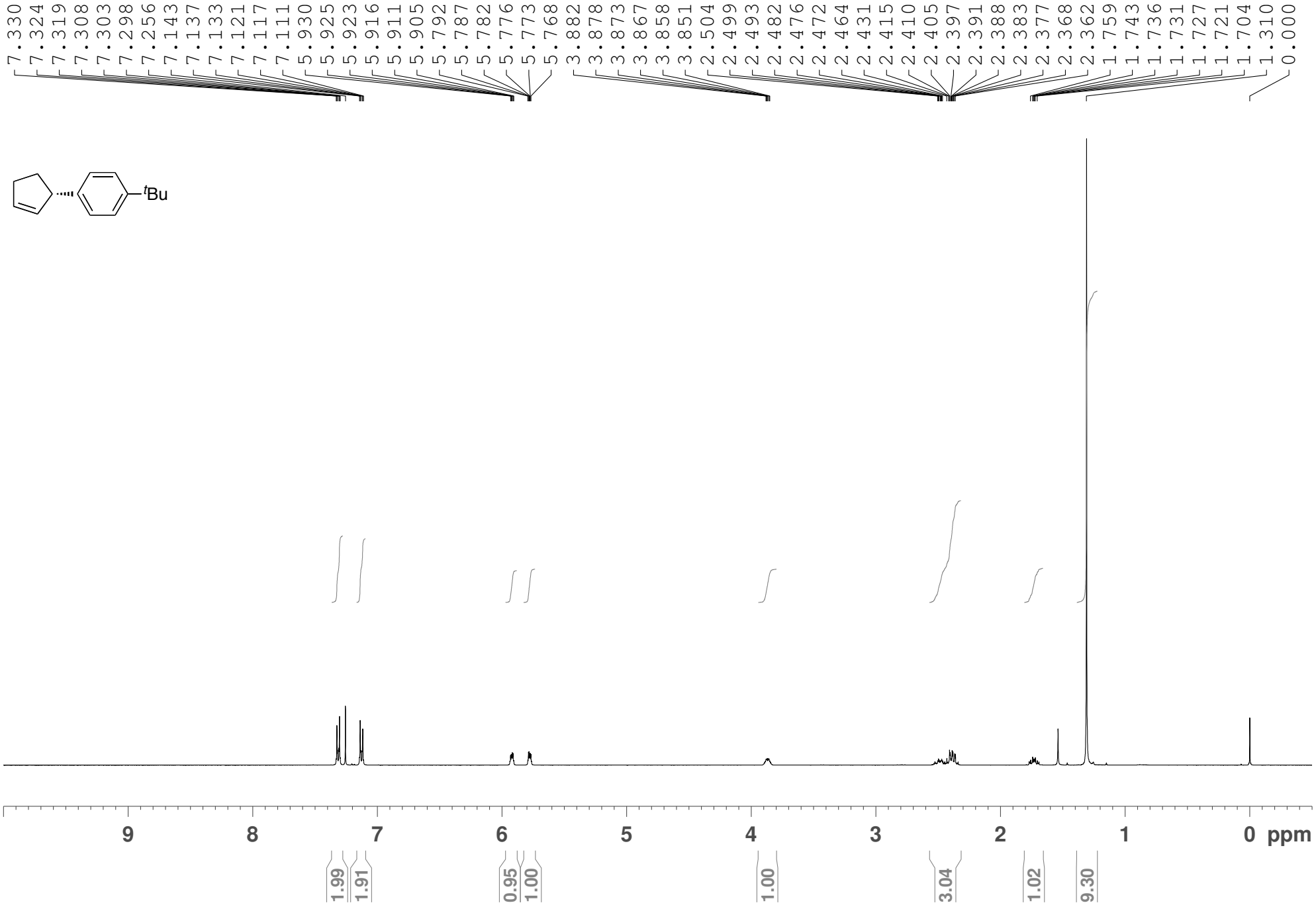
^{13}C NMR (100 MHz, $CDCl_3$)



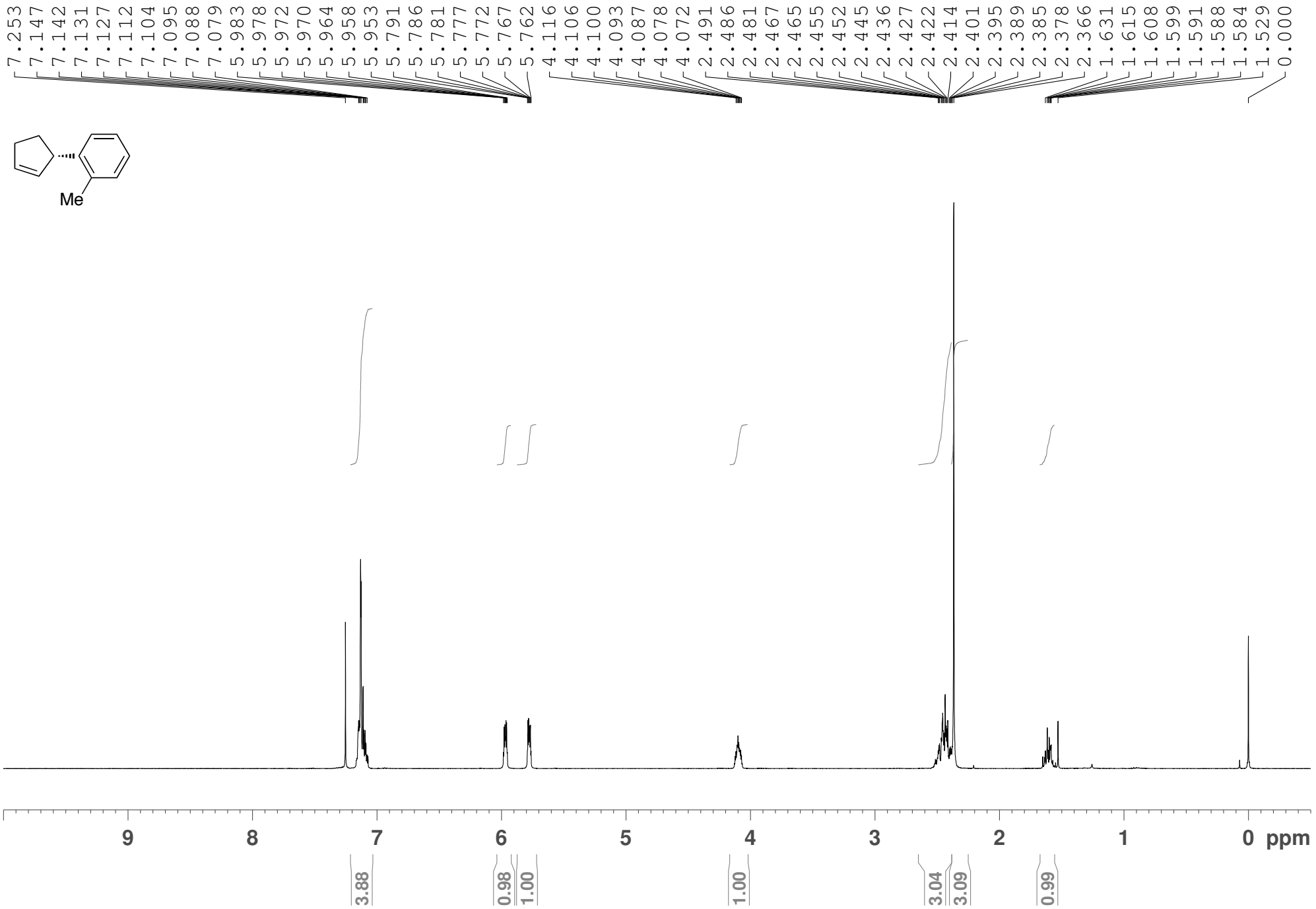
^{1}H NMR (400 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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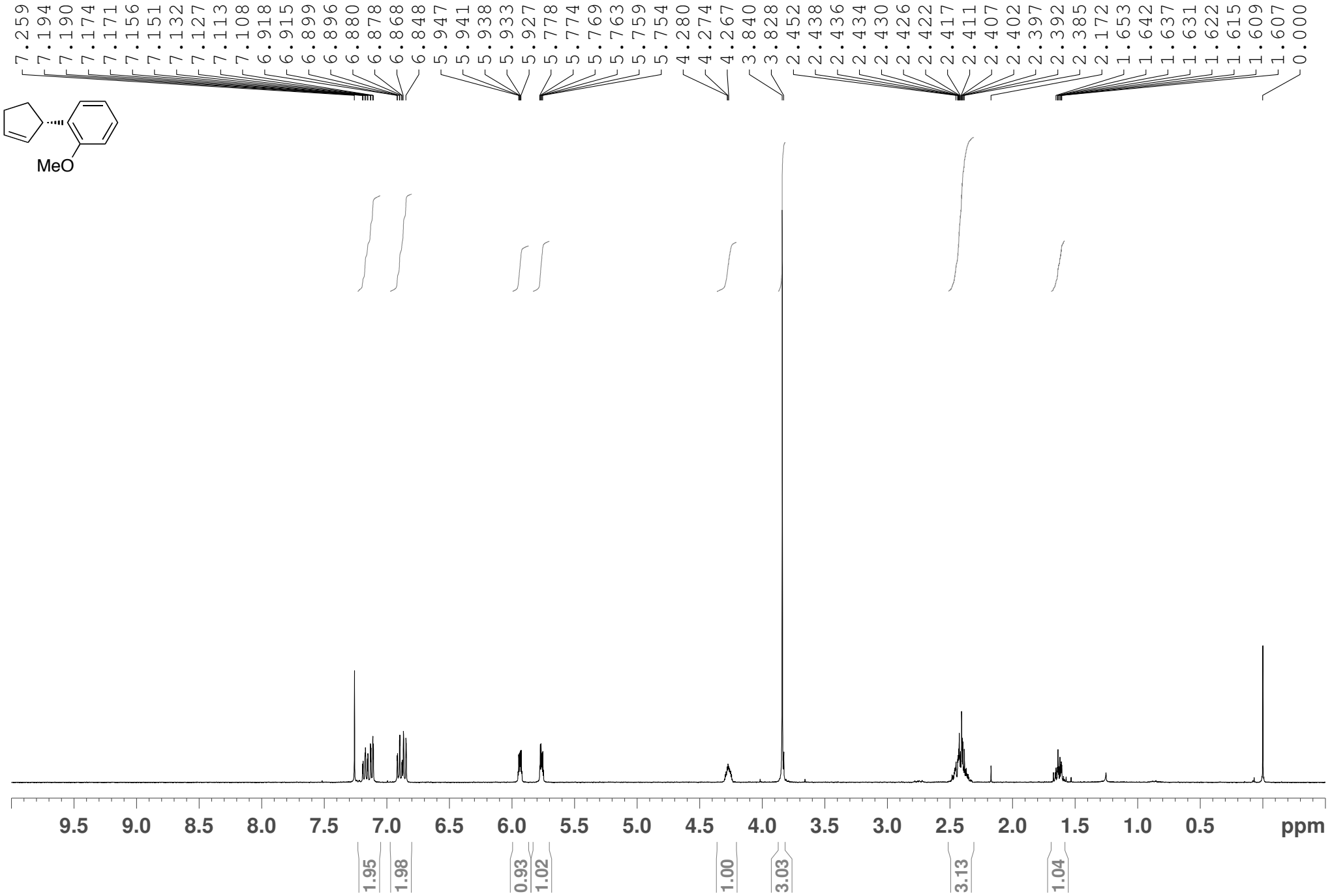

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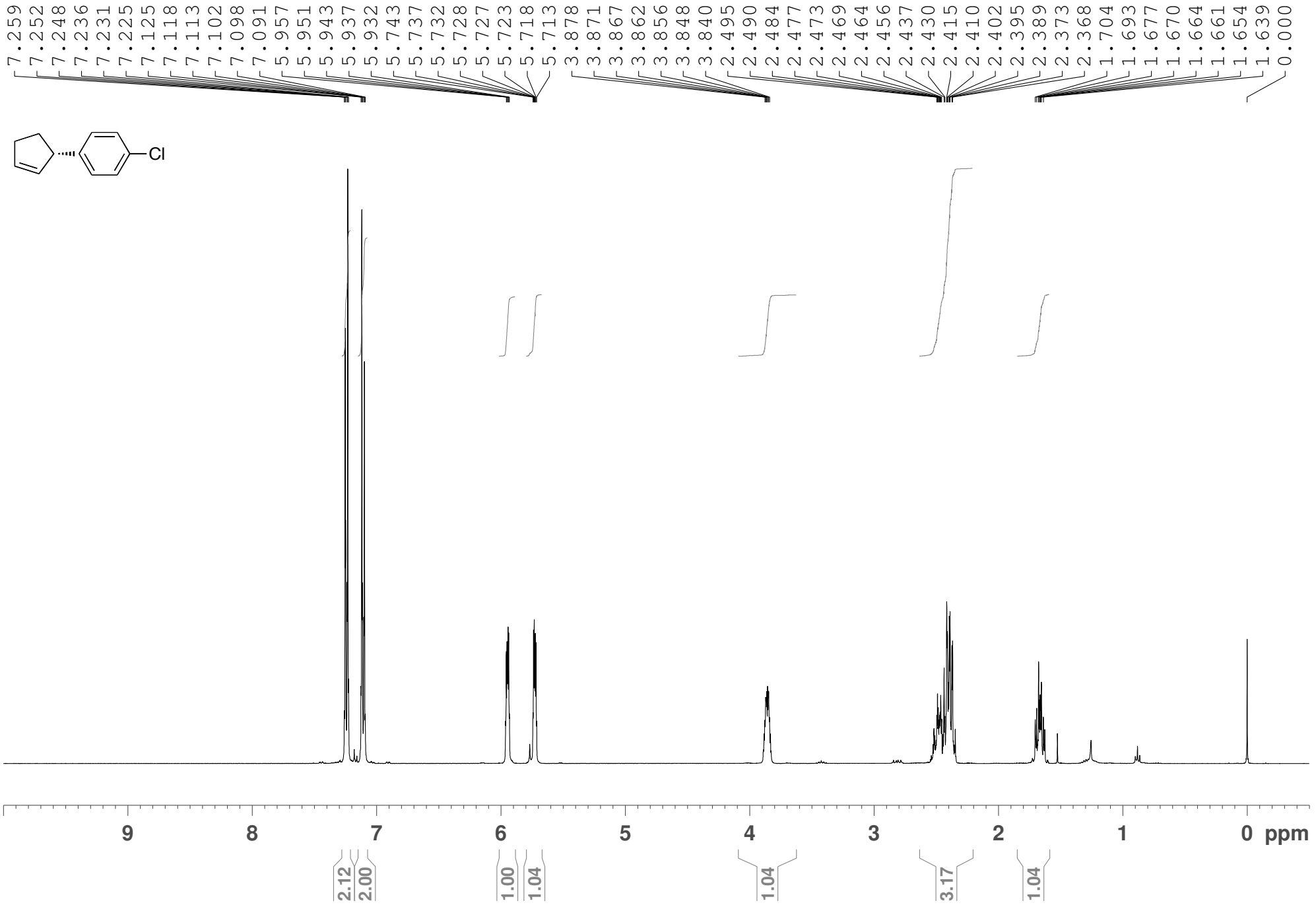
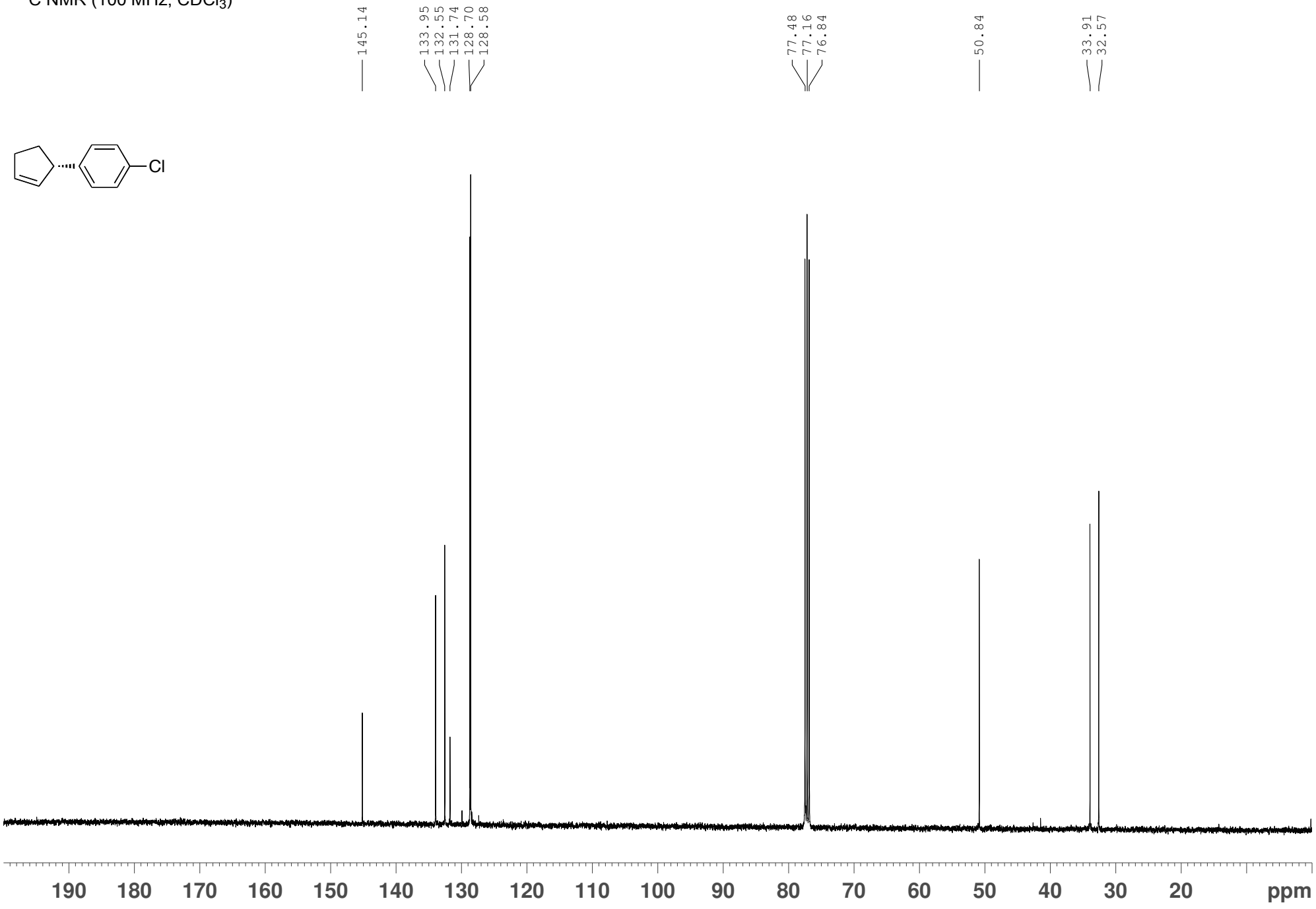


^{13}C NMR (100 MHz, $CDCl_3$)



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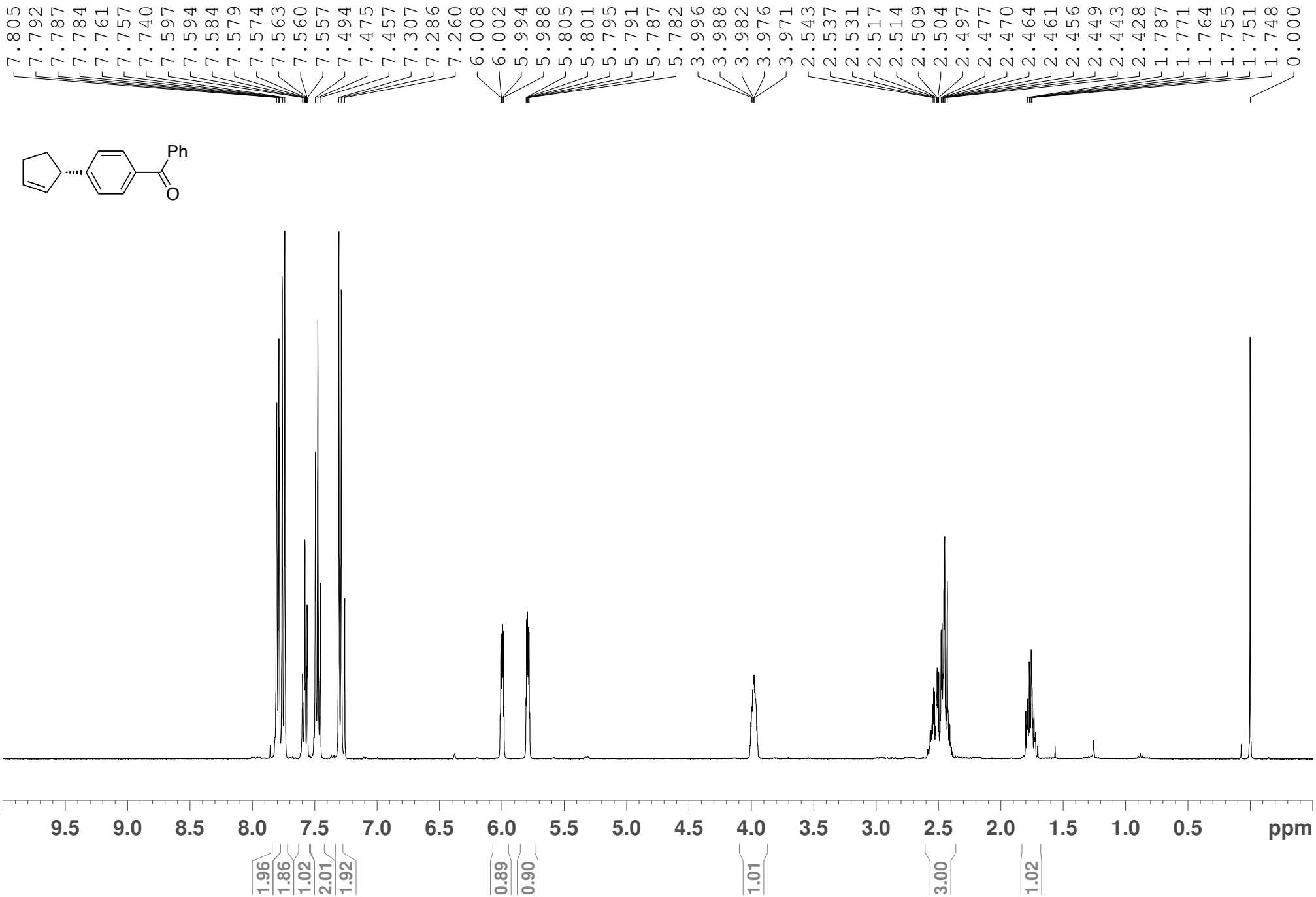

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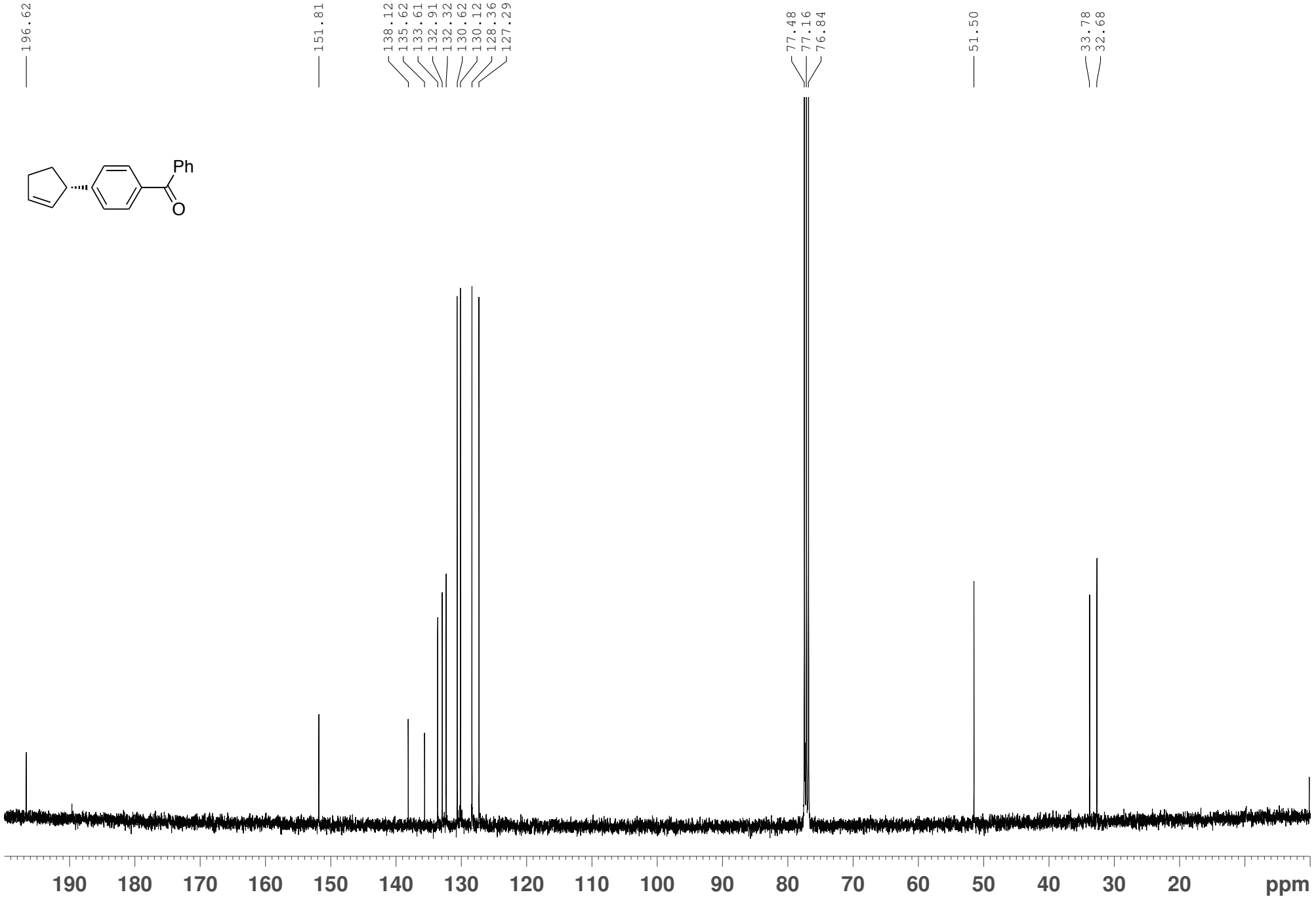

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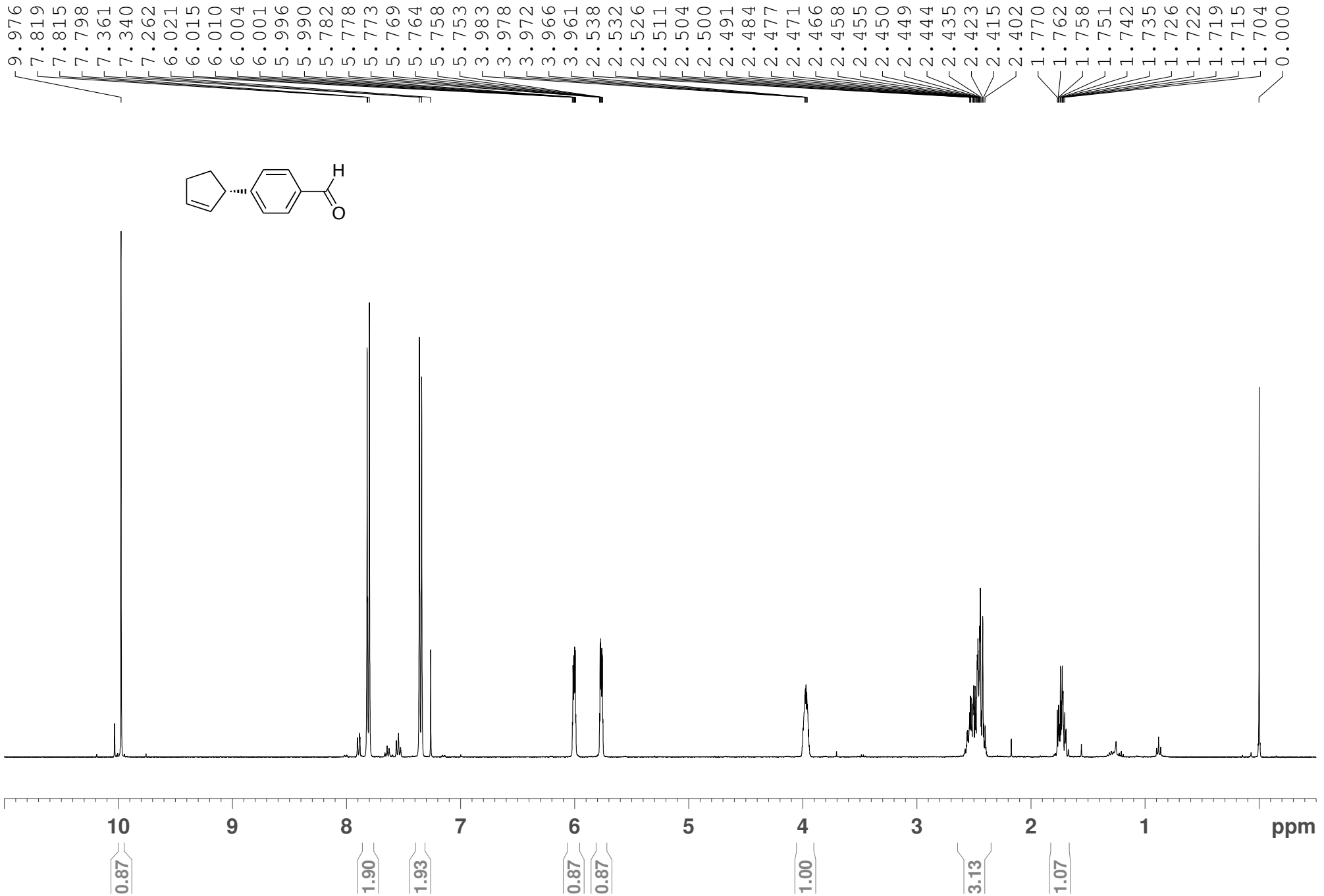
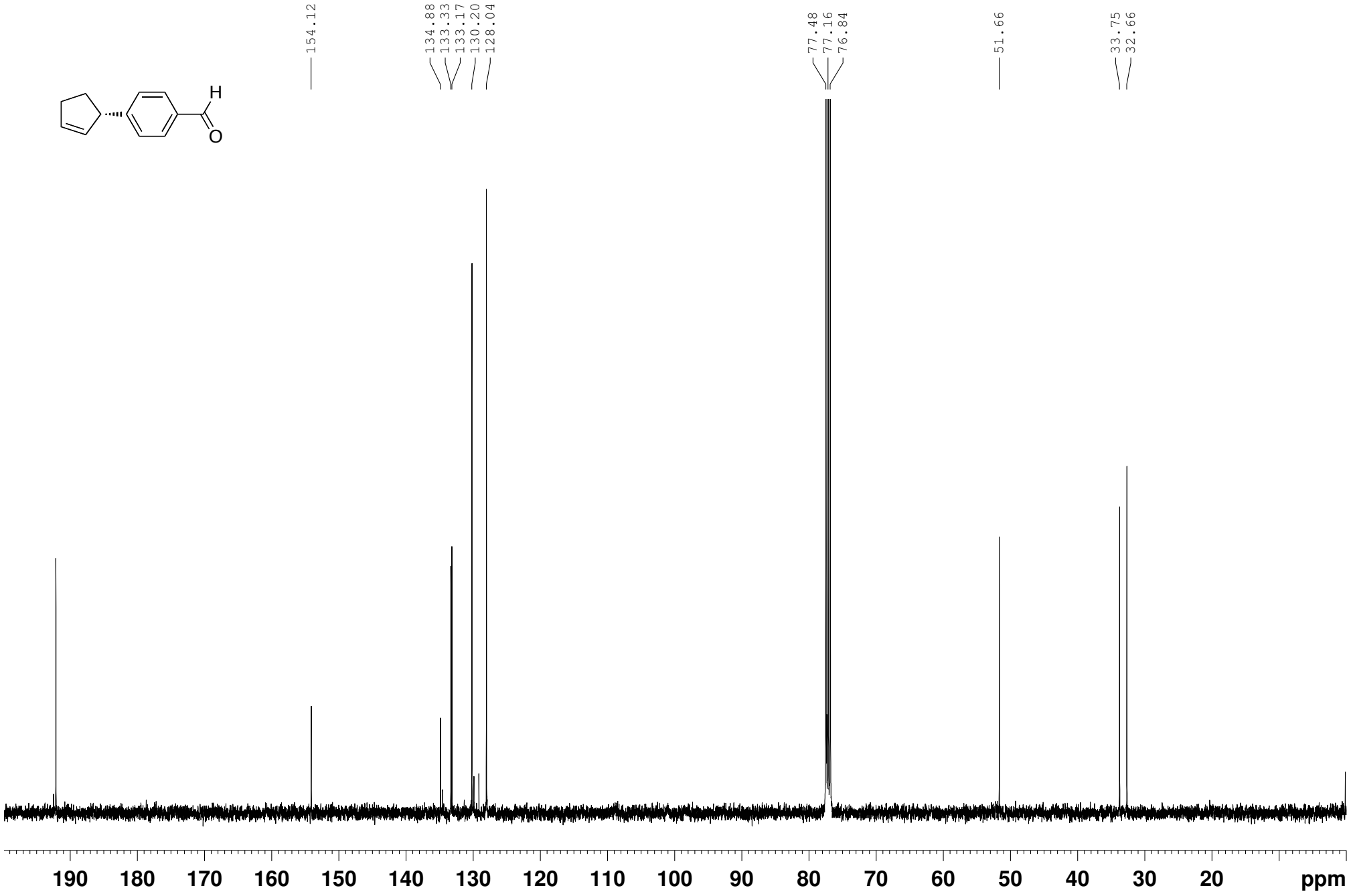


^{13}C NMR (100 MHz, $CDCl_3$)



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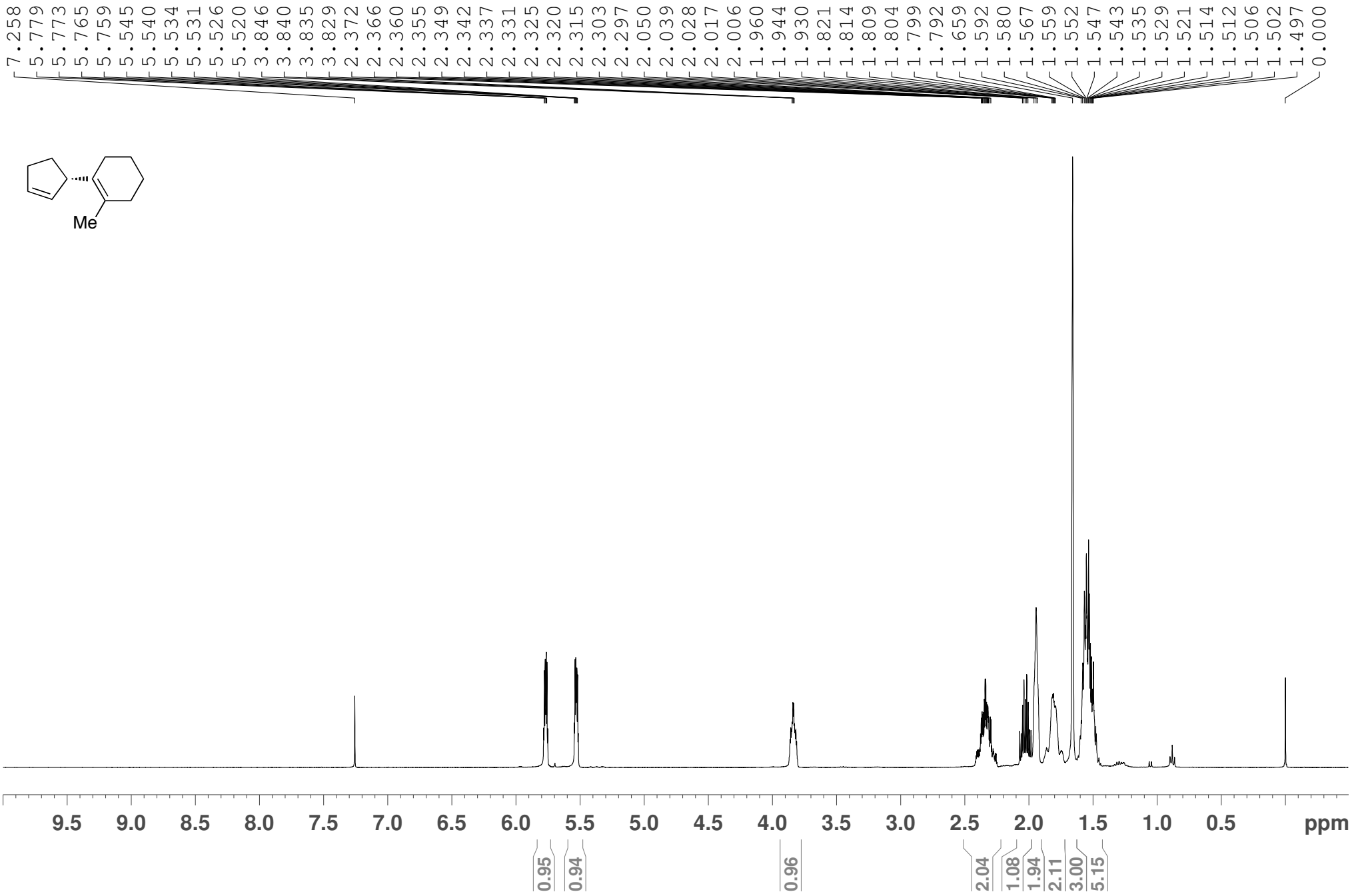

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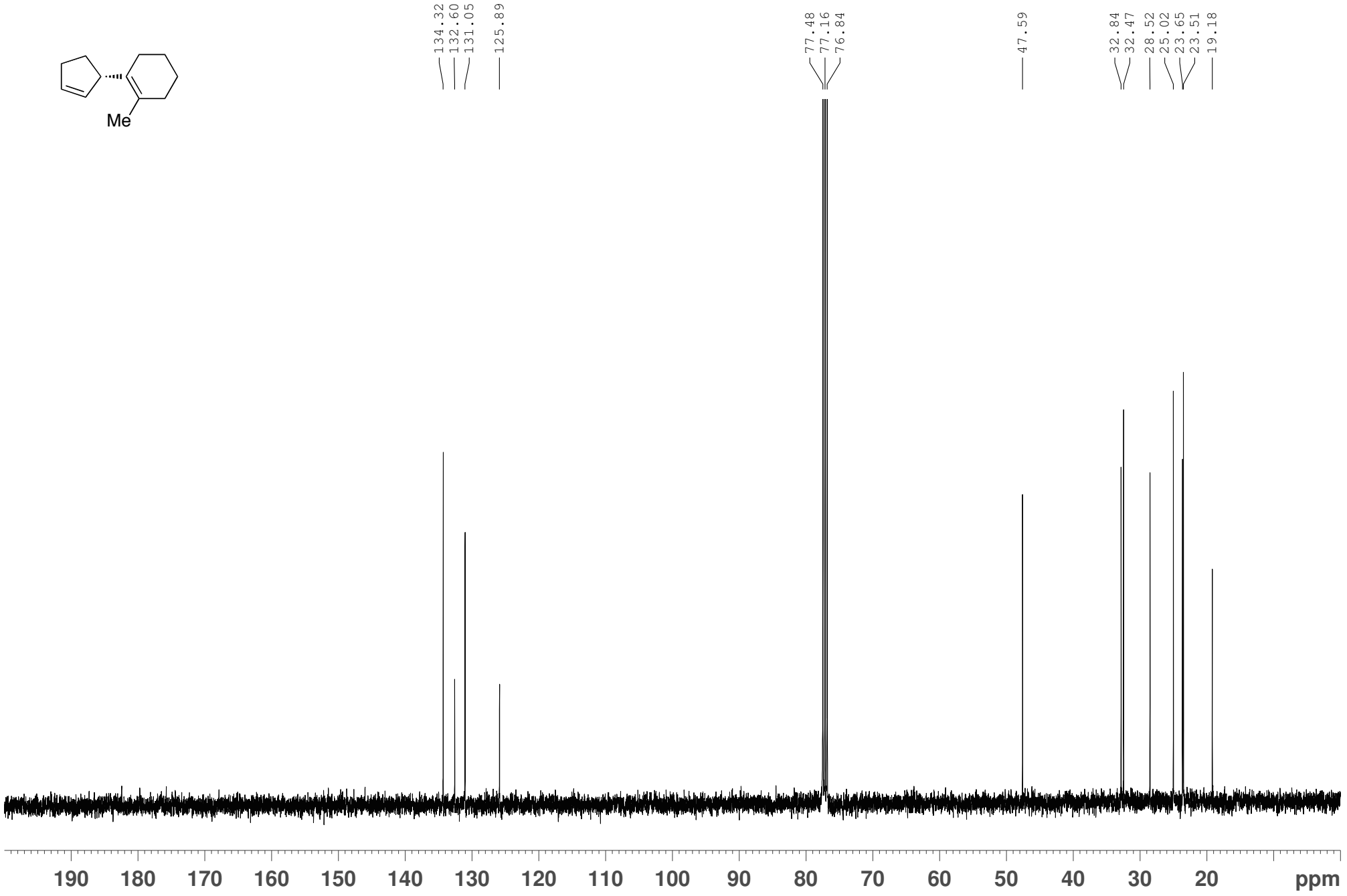

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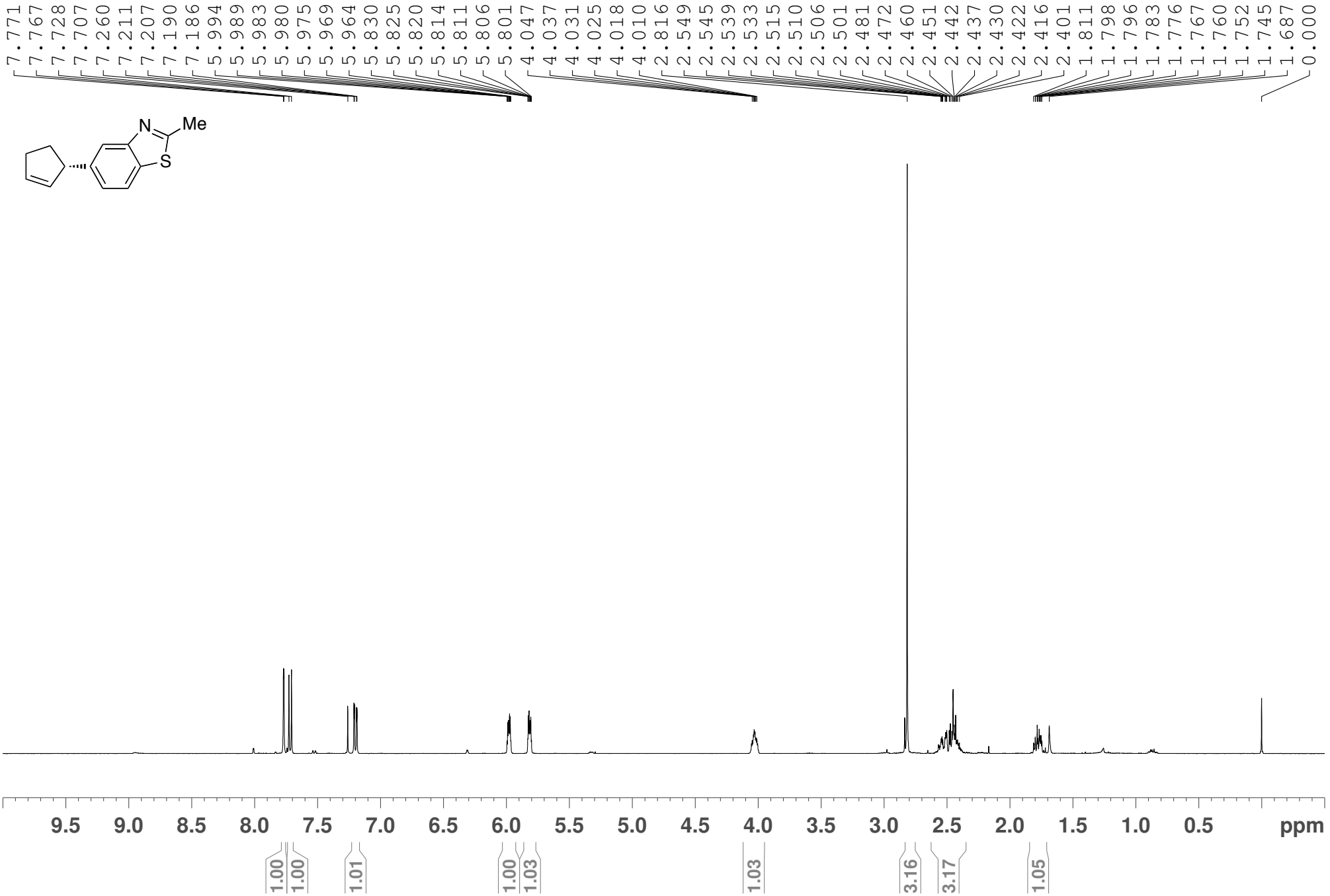

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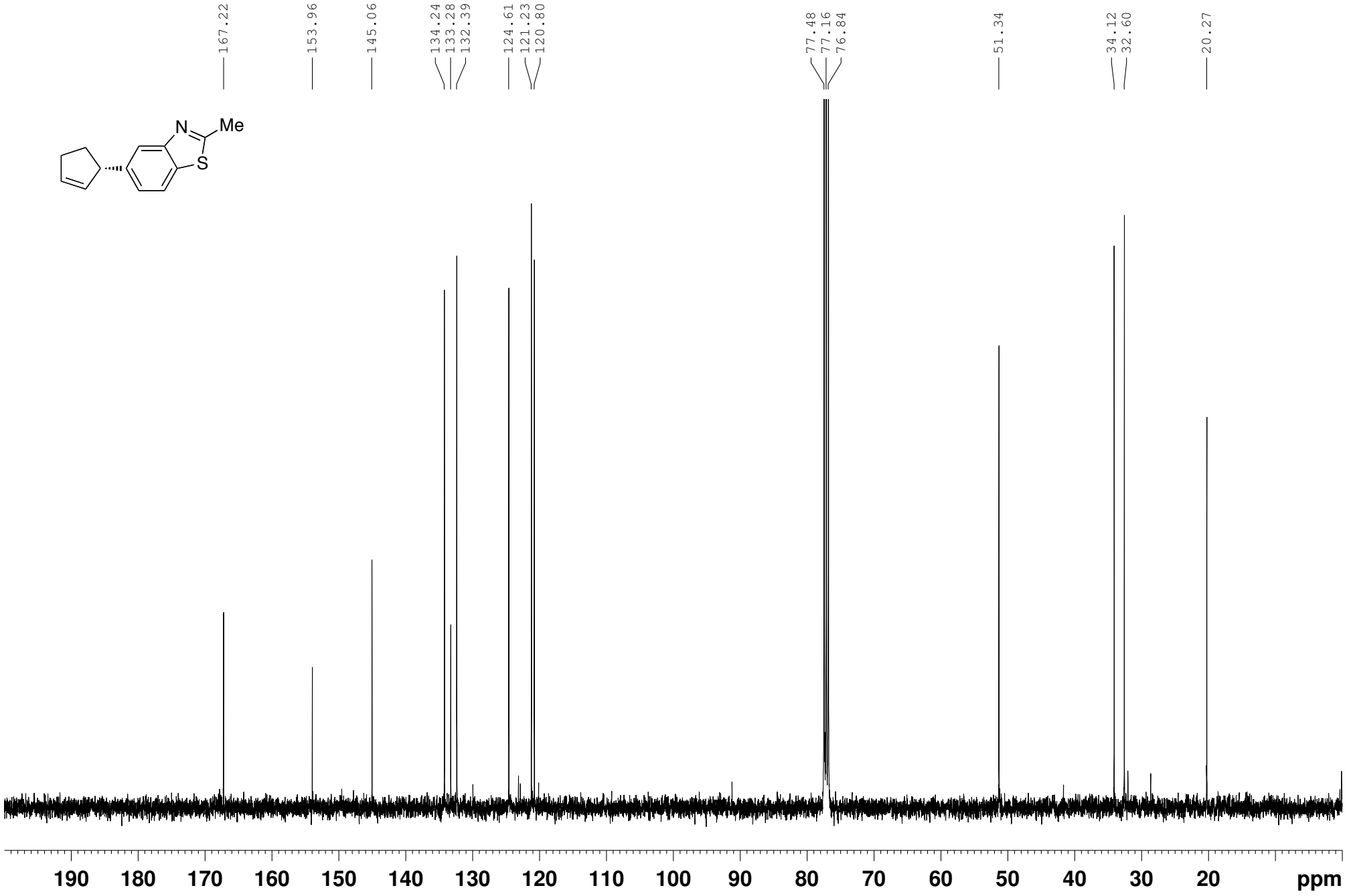

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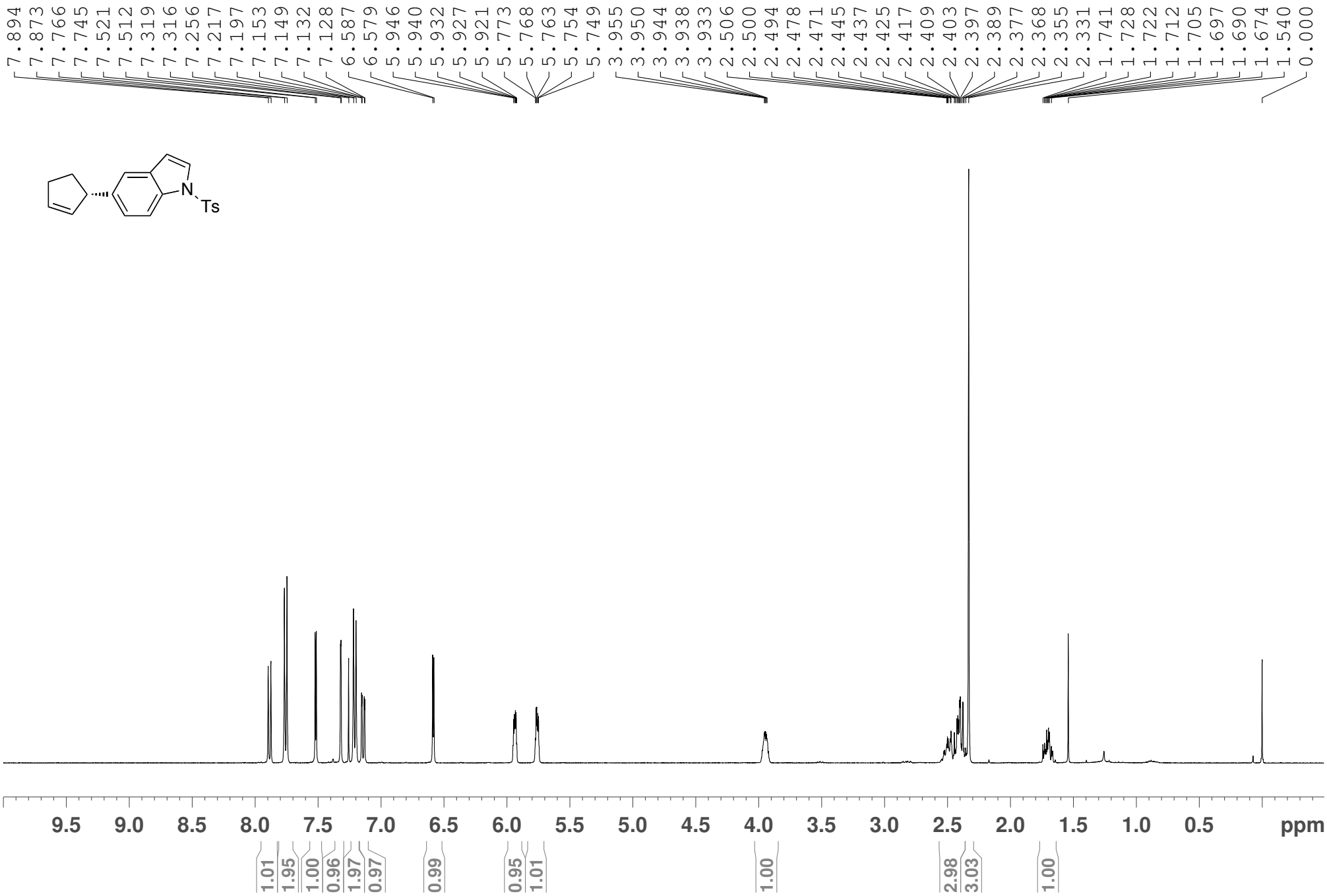

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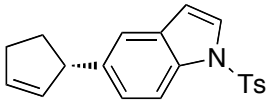
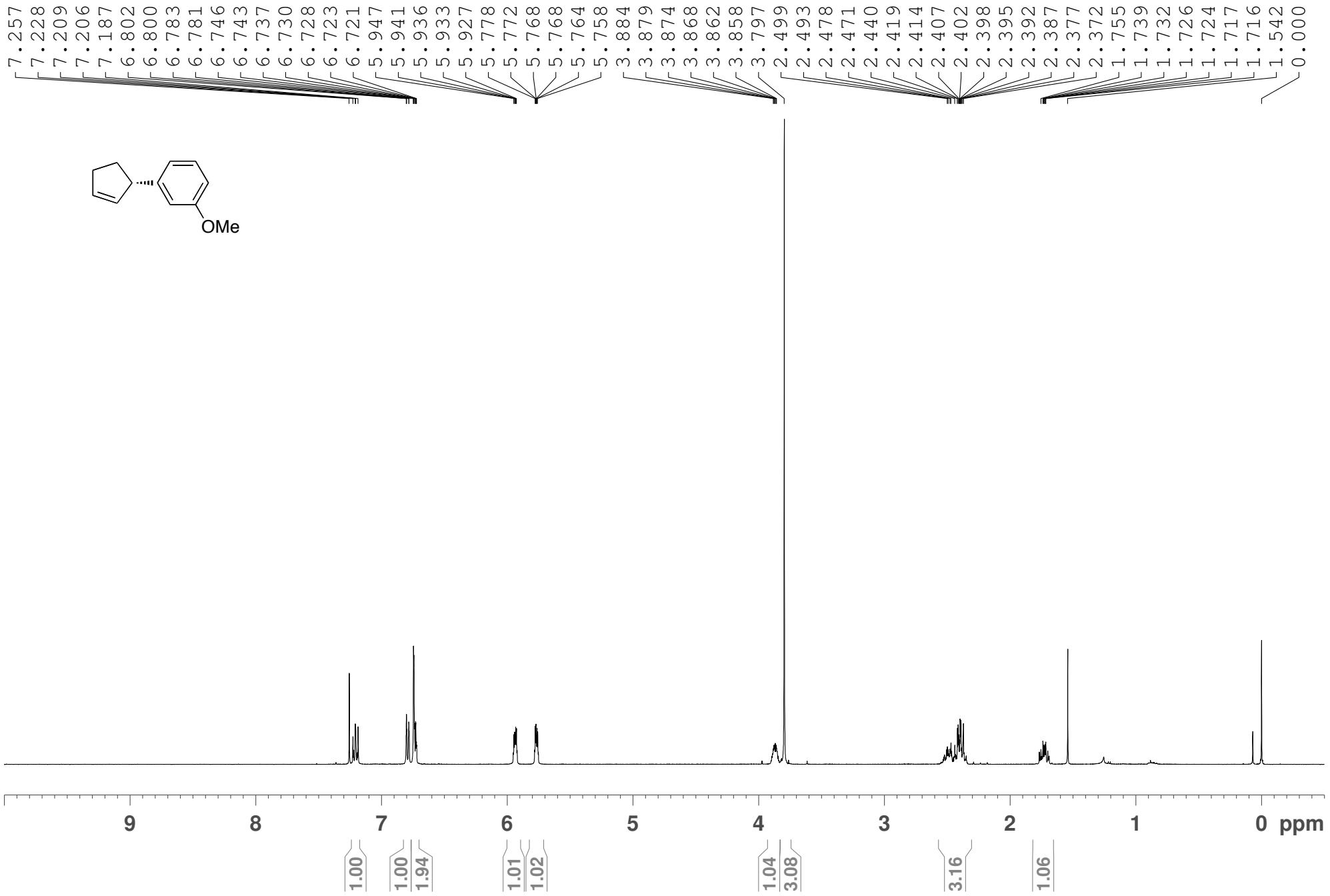


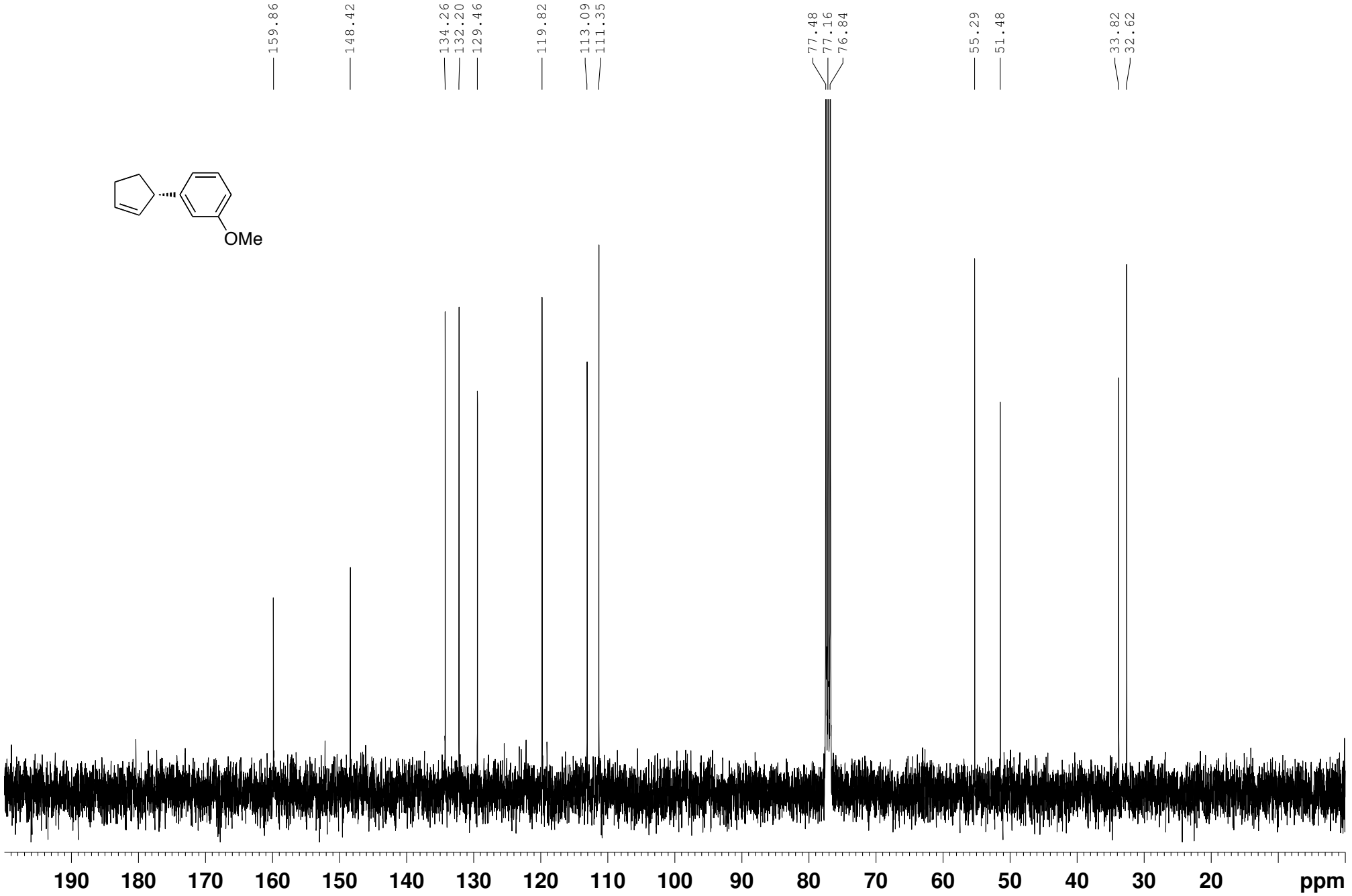
144.93
141.88
135.61
134.56
133.59
132.06
131.11
129.98
126.98
126.56
124.45
119.54
113.53
109.10
77.48
77.16
76.84
51.30
34.17
32.62
21.69

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

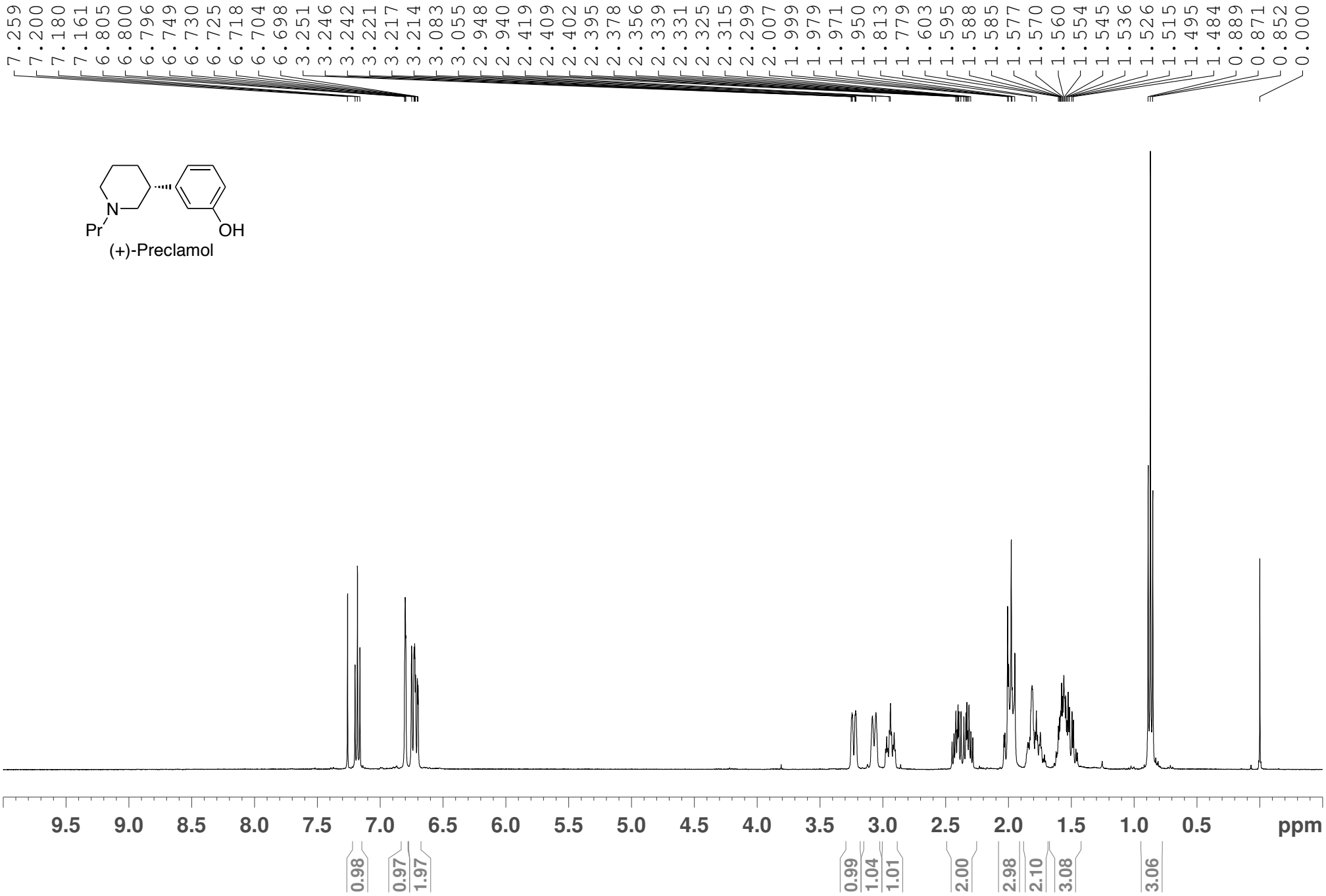
^{1}H NMR (400 MHz, $CDCl_3$)



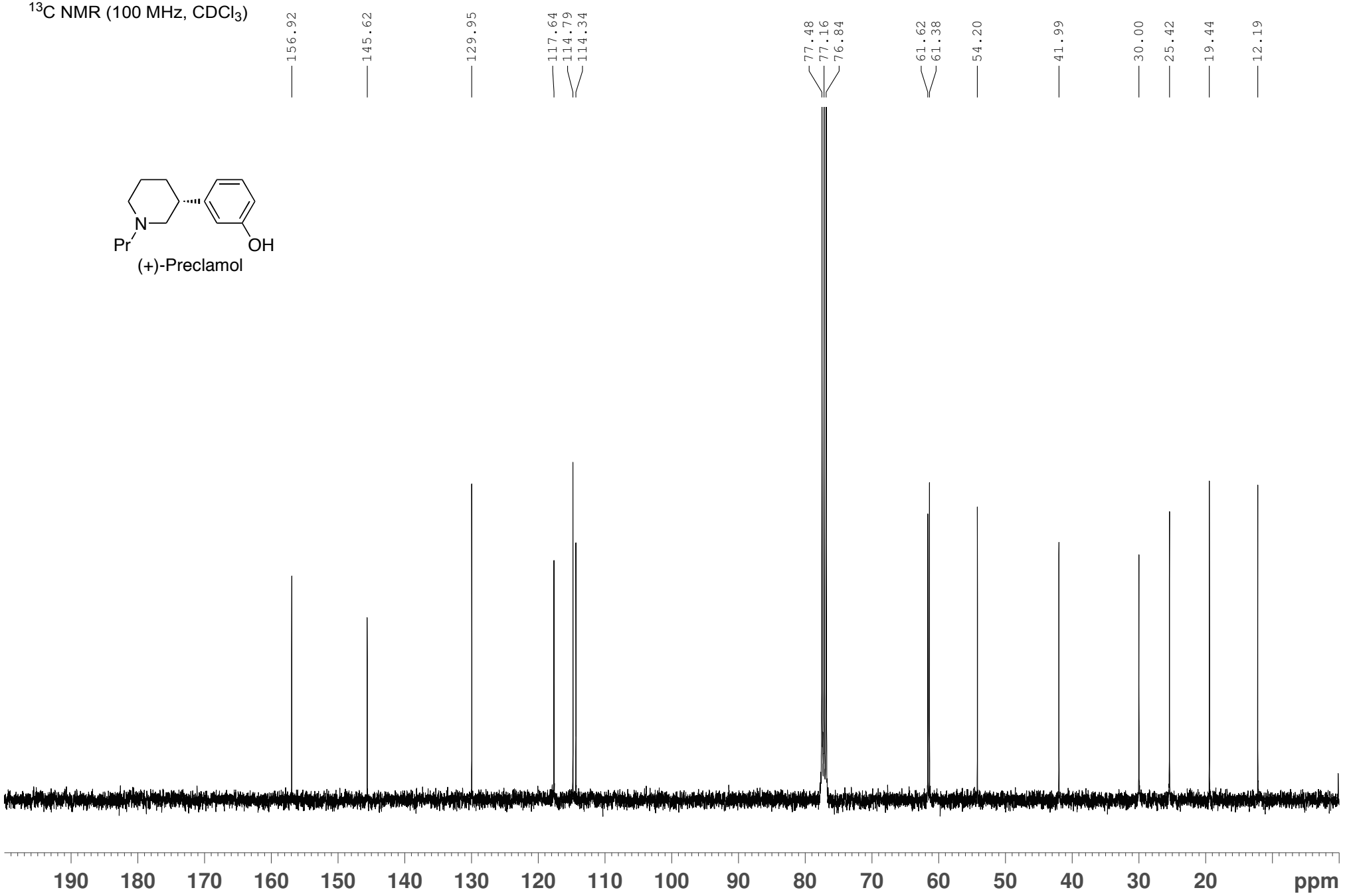
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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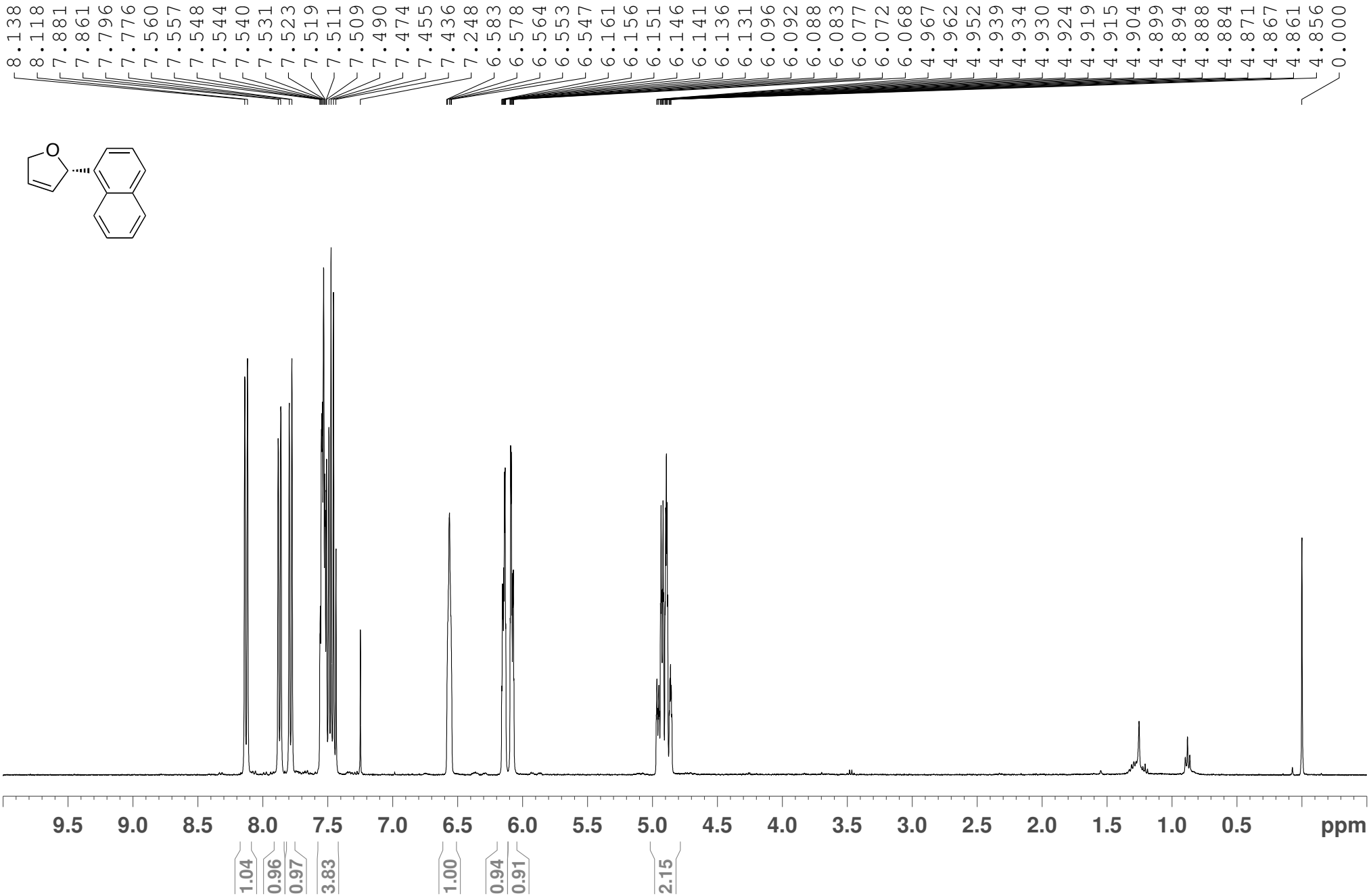
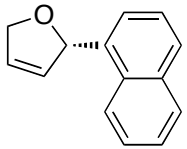


hj5031(17) rxn 1. in CDCl3 1-naph dihydrofuran 13C

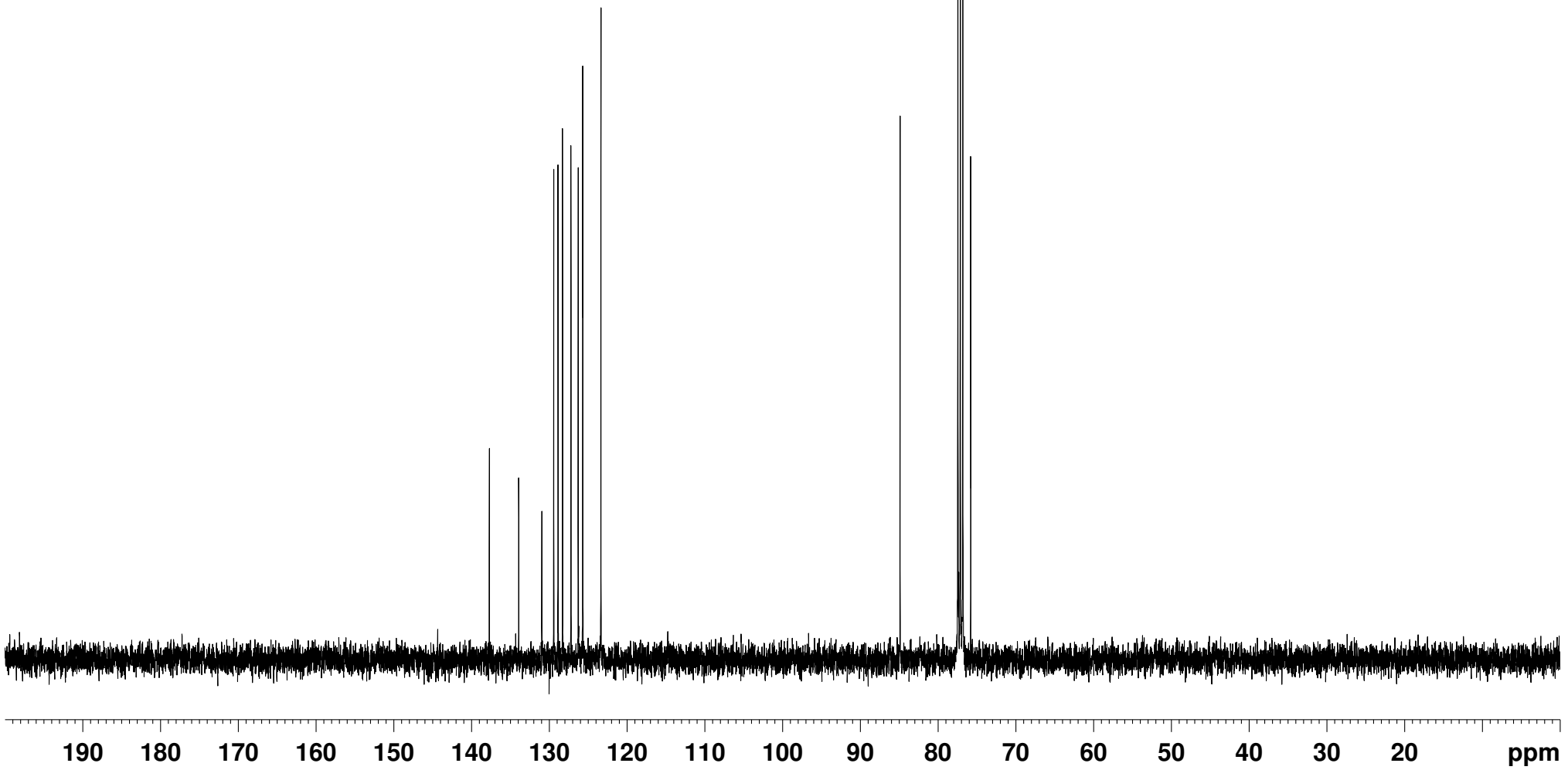
^{13}C NMR (100 MHz, $CDCl_3$)



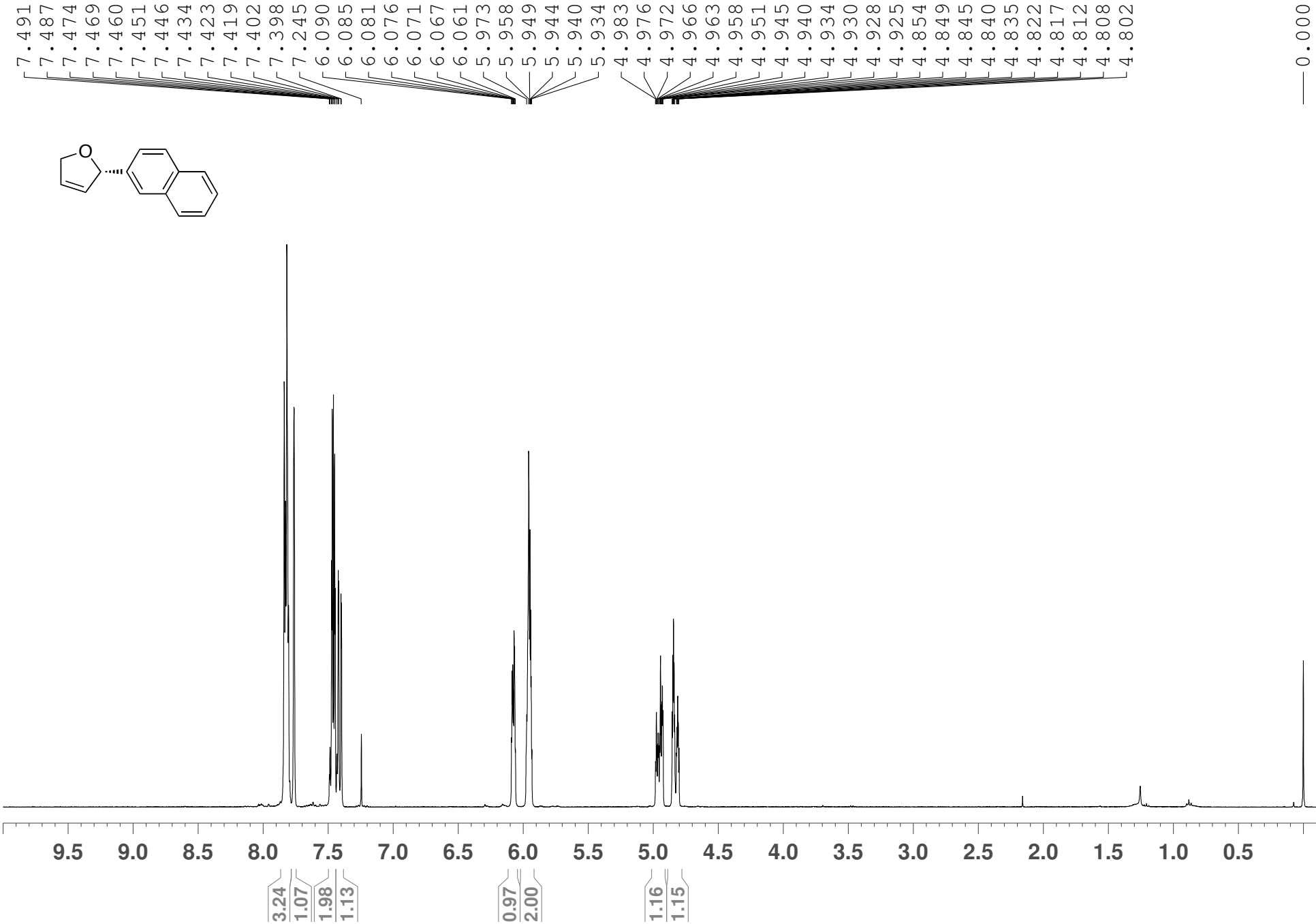
137.73
133.95
130.98
129.45
128.90
128.32
127.24
126.30
125.73
125.71
123.38

84.91

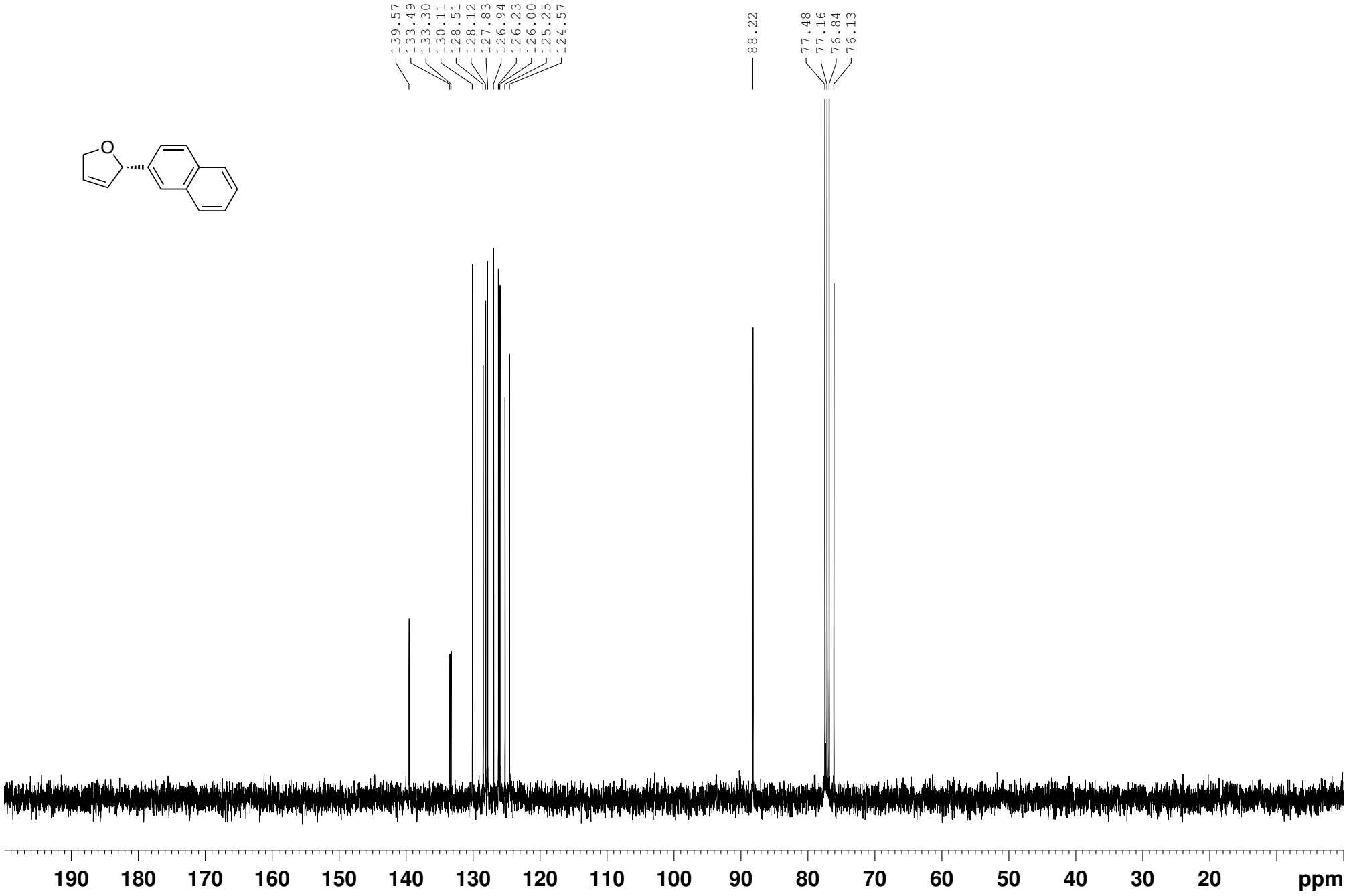
77.48
77.16
76.84
75.83



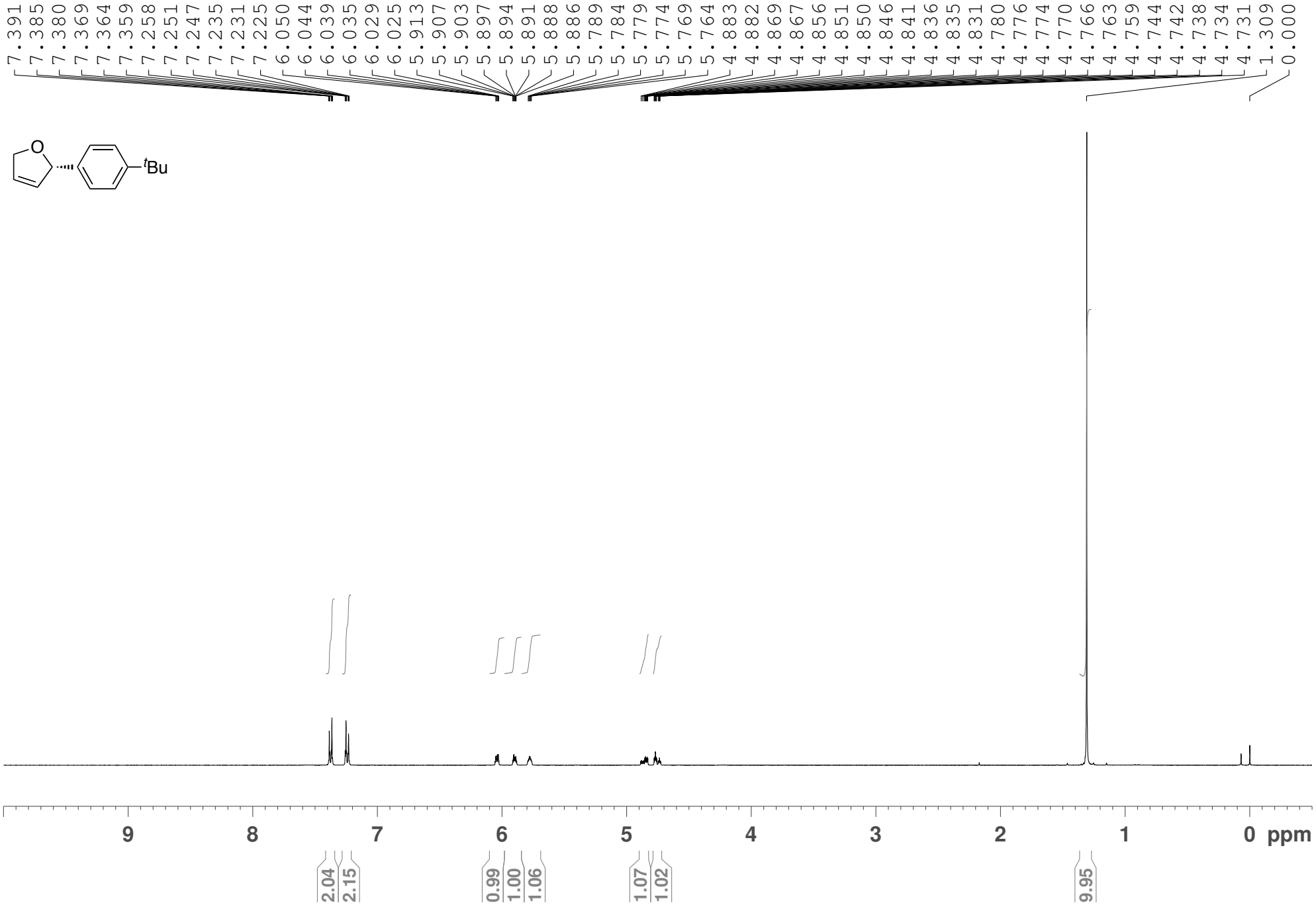
^{1}H NMR (400 MHz, $CDCl_3$)



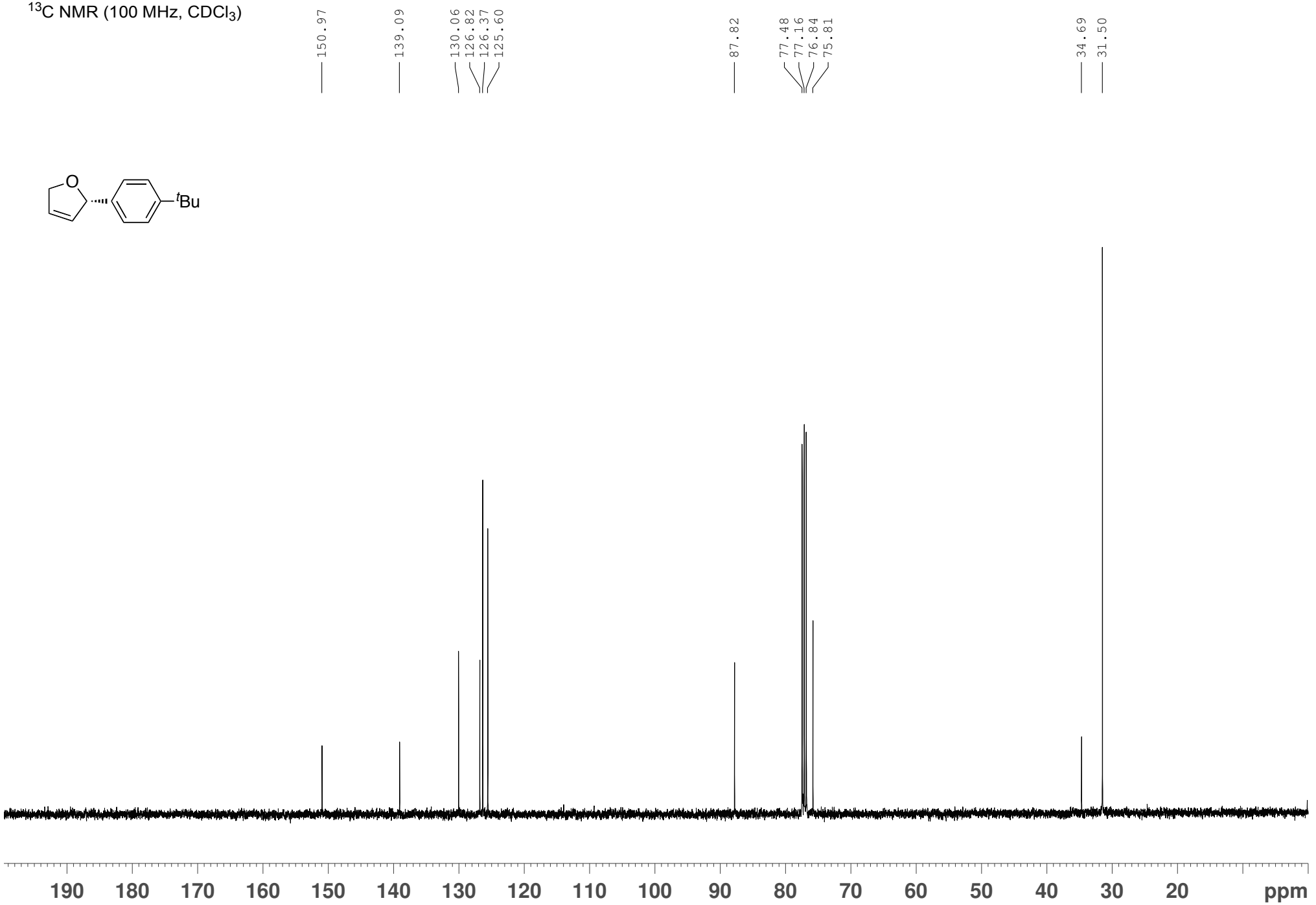
^{13}C NMR (100 MHz, $CDCl_3$)



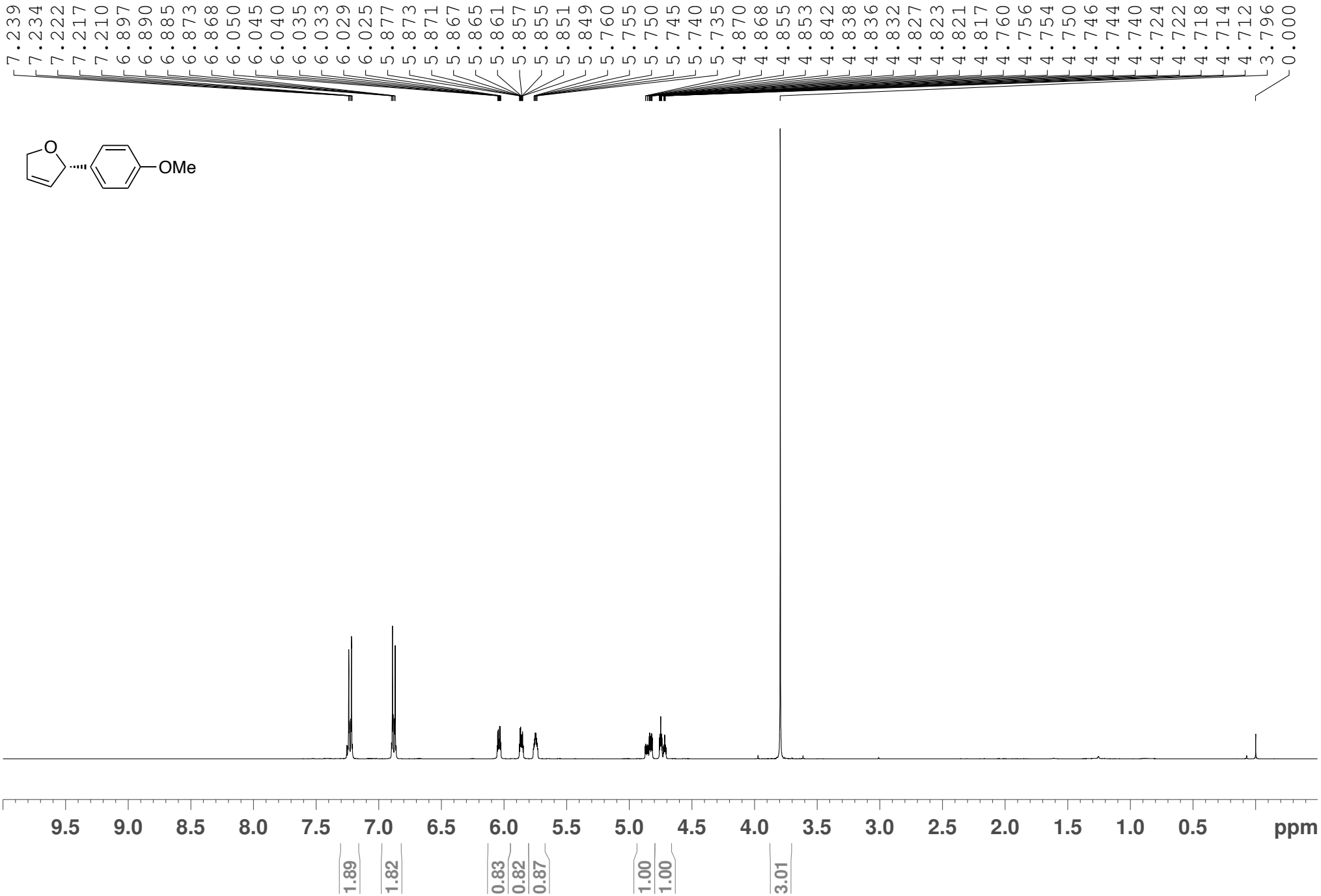
^{1}H NMR (400 MHz, $CDCl_3$)



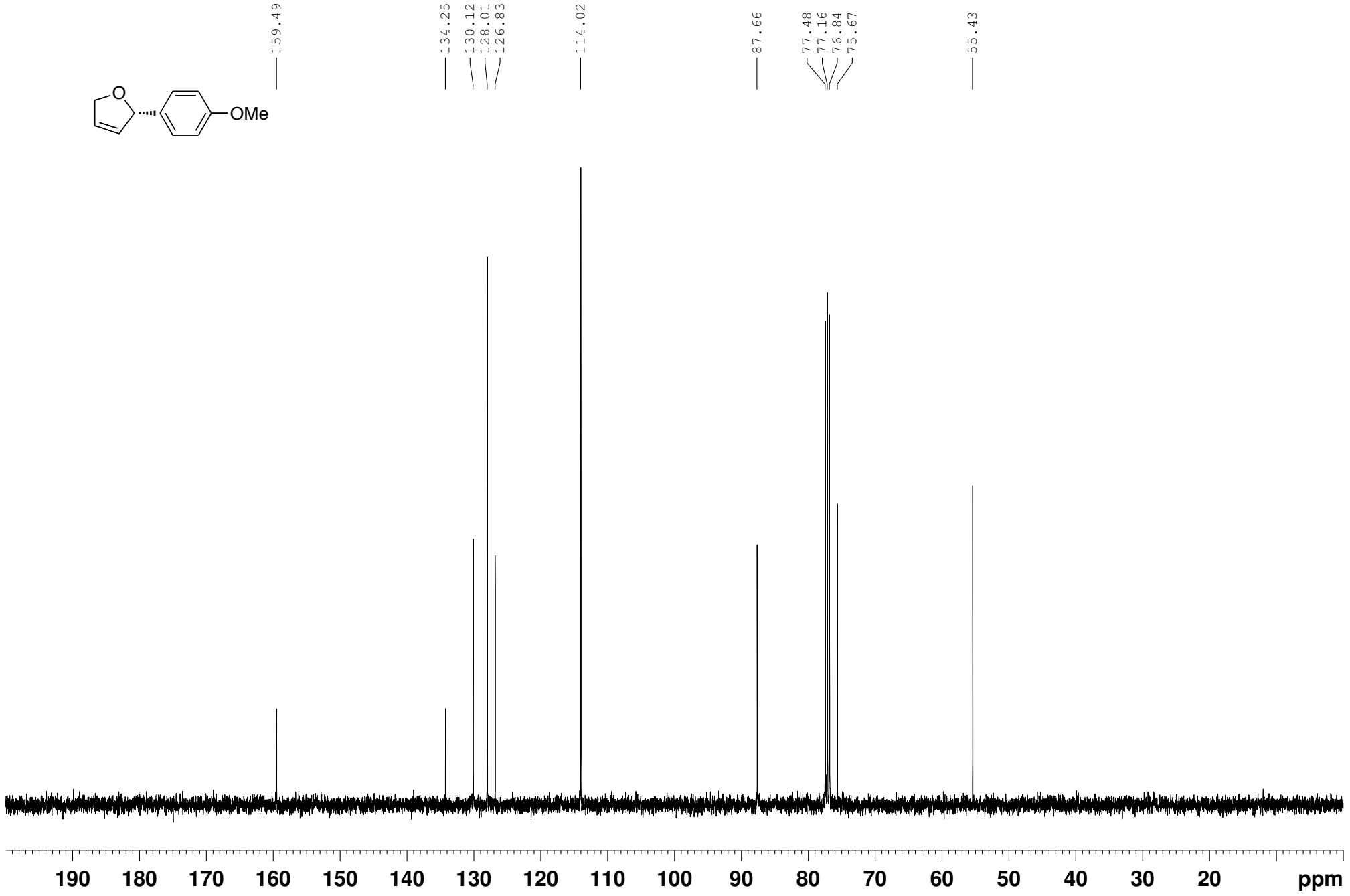
^{13}C NMR (100 MHz, $CDCl_3$)



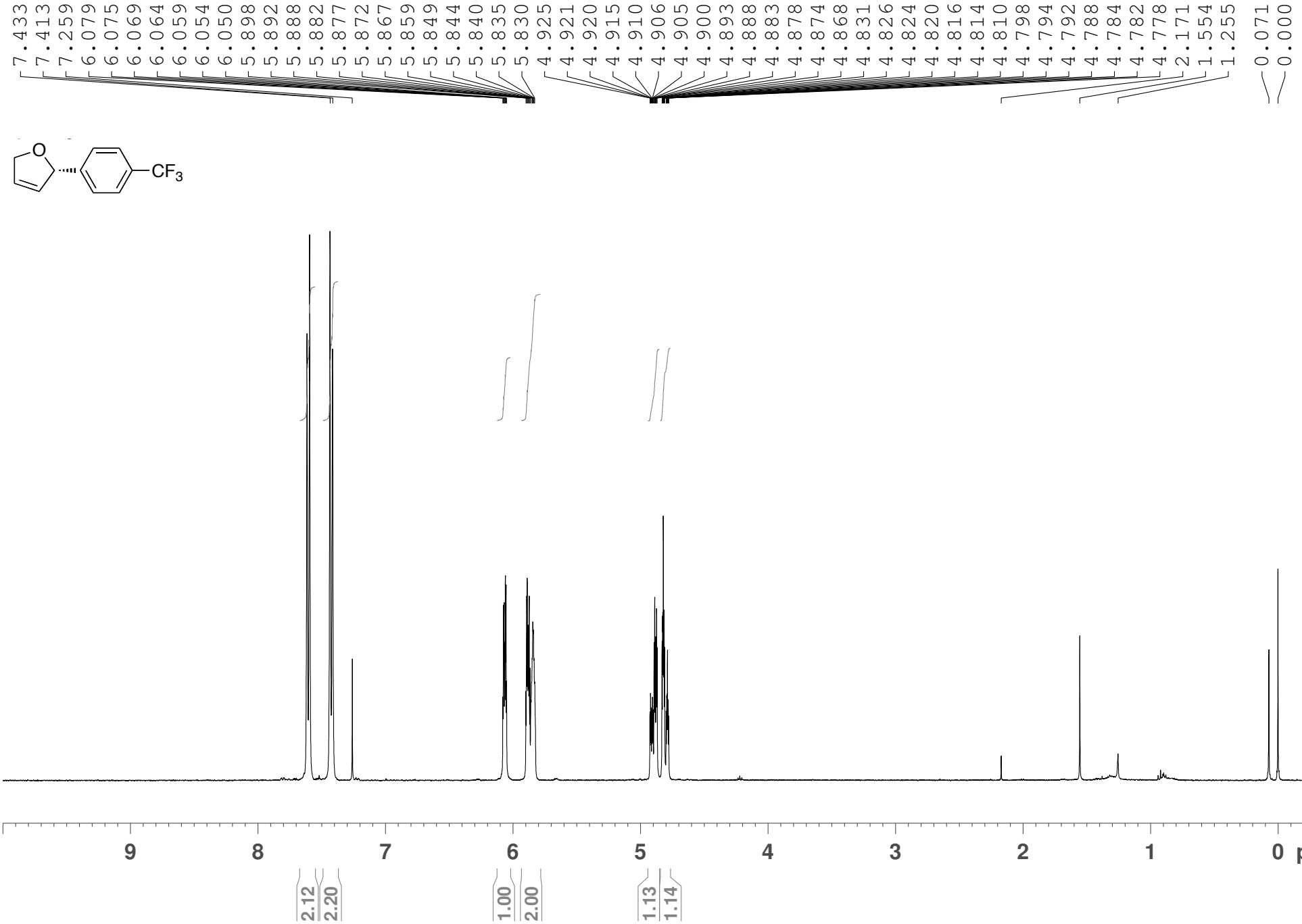
^{1}H NMR (400 MHz, $CDCl_3$)



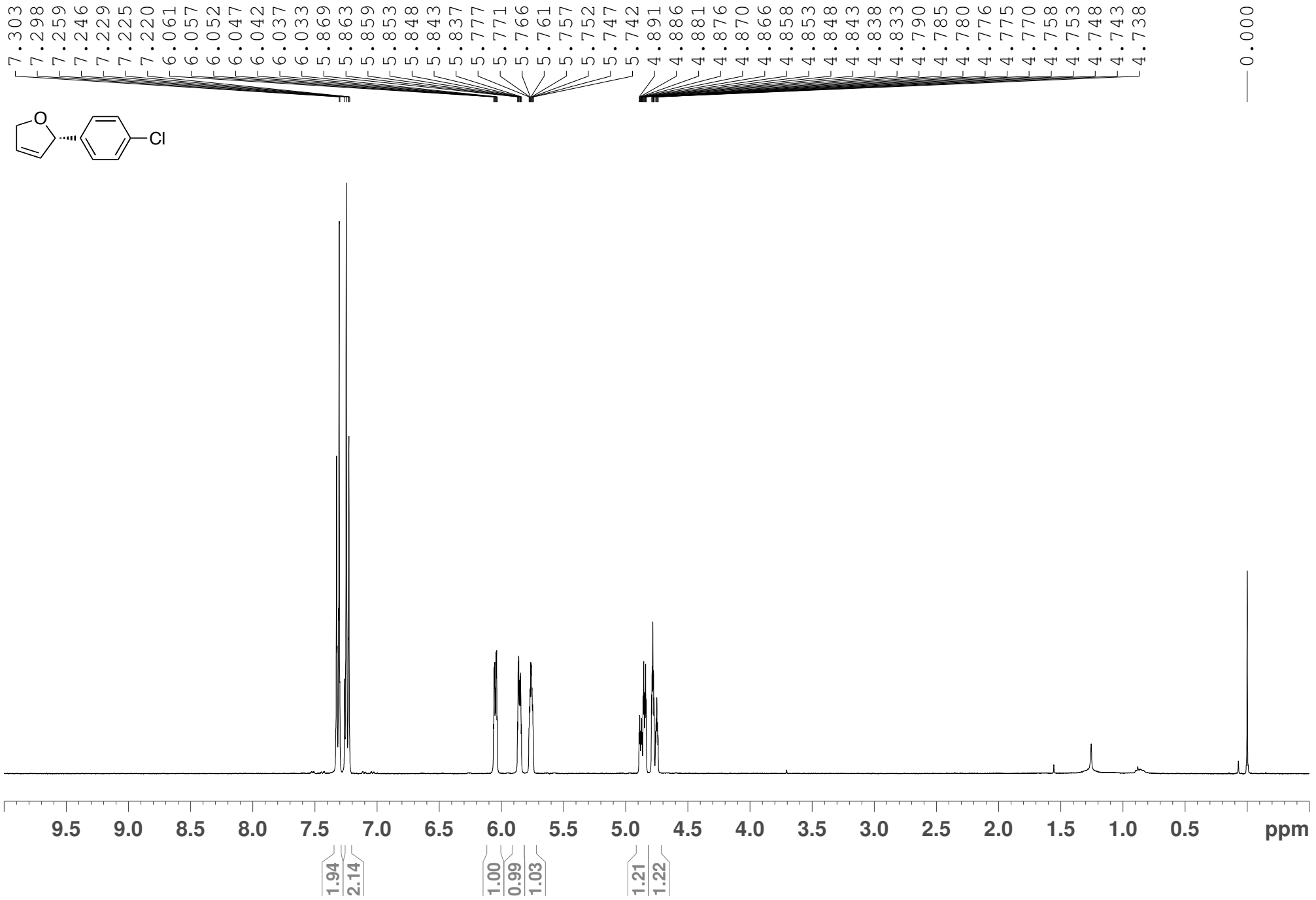
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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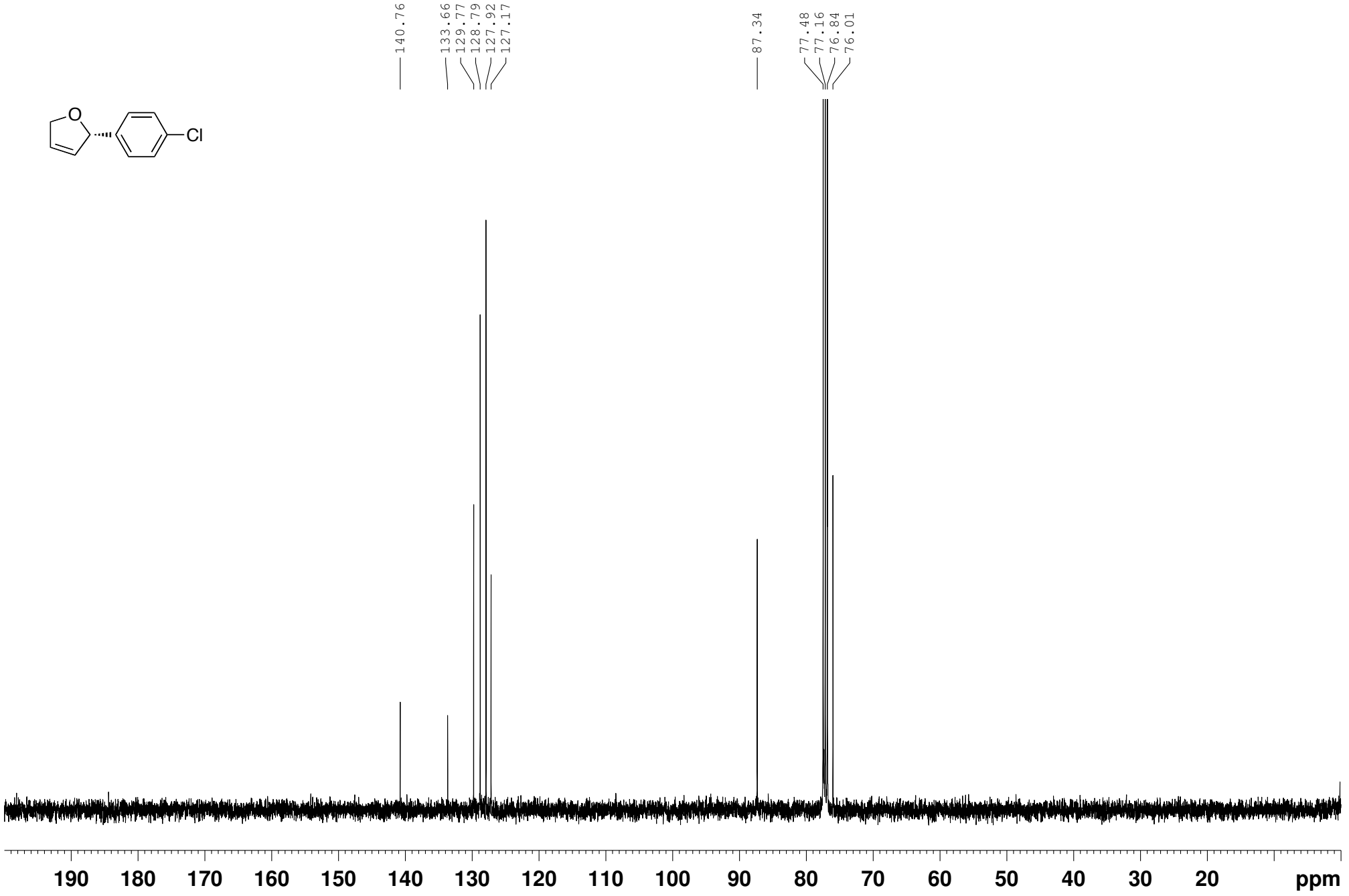
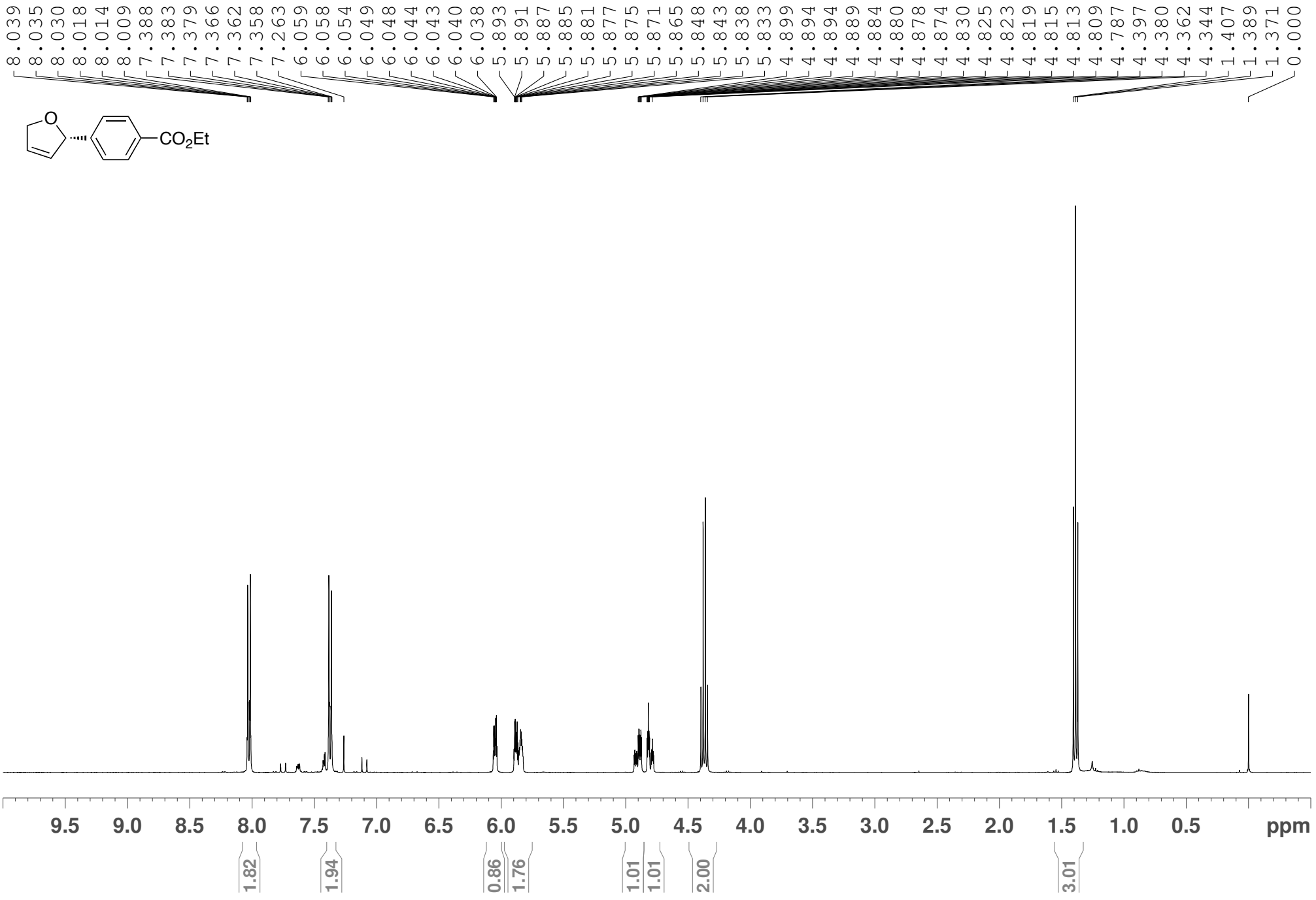
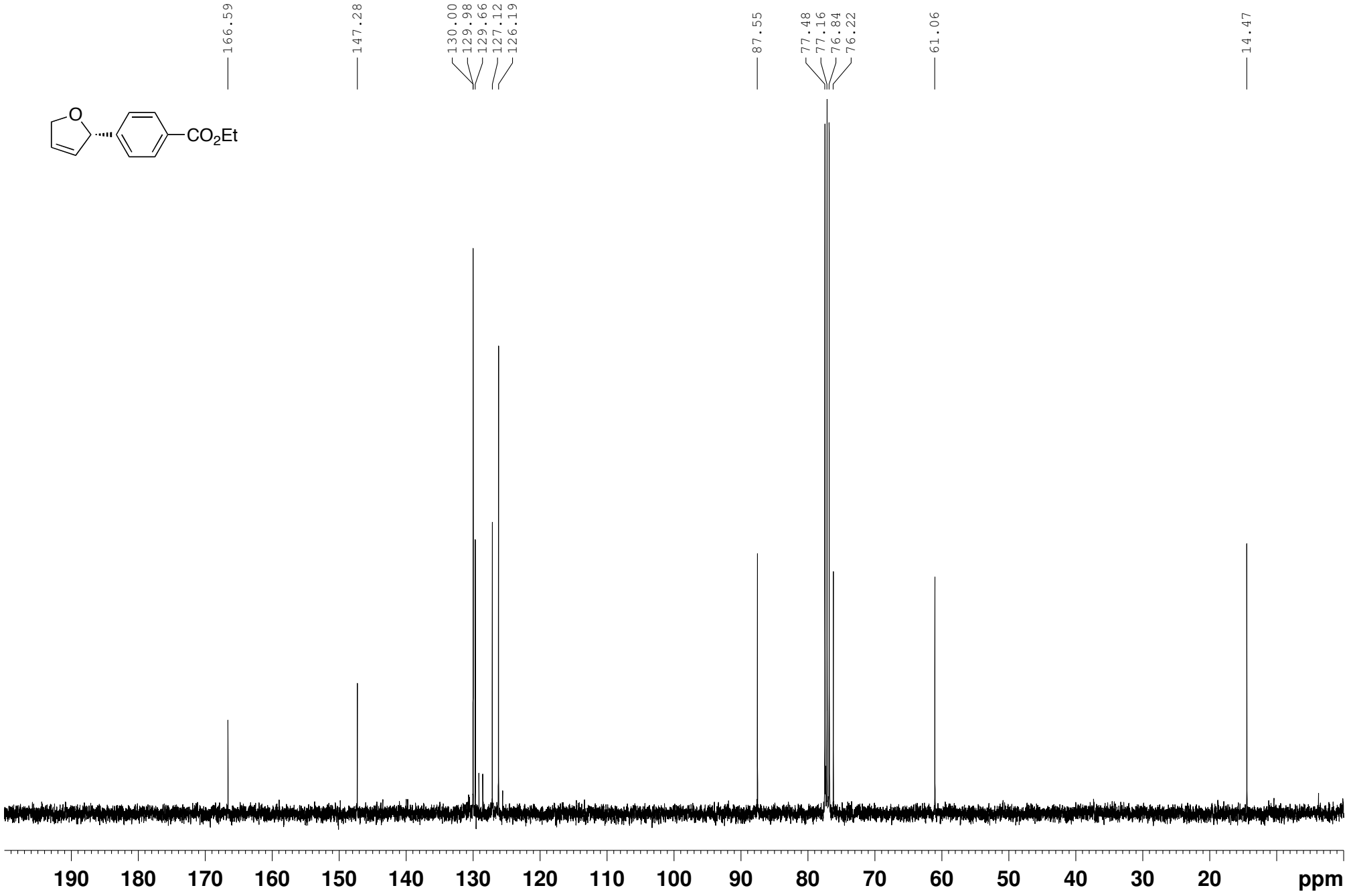


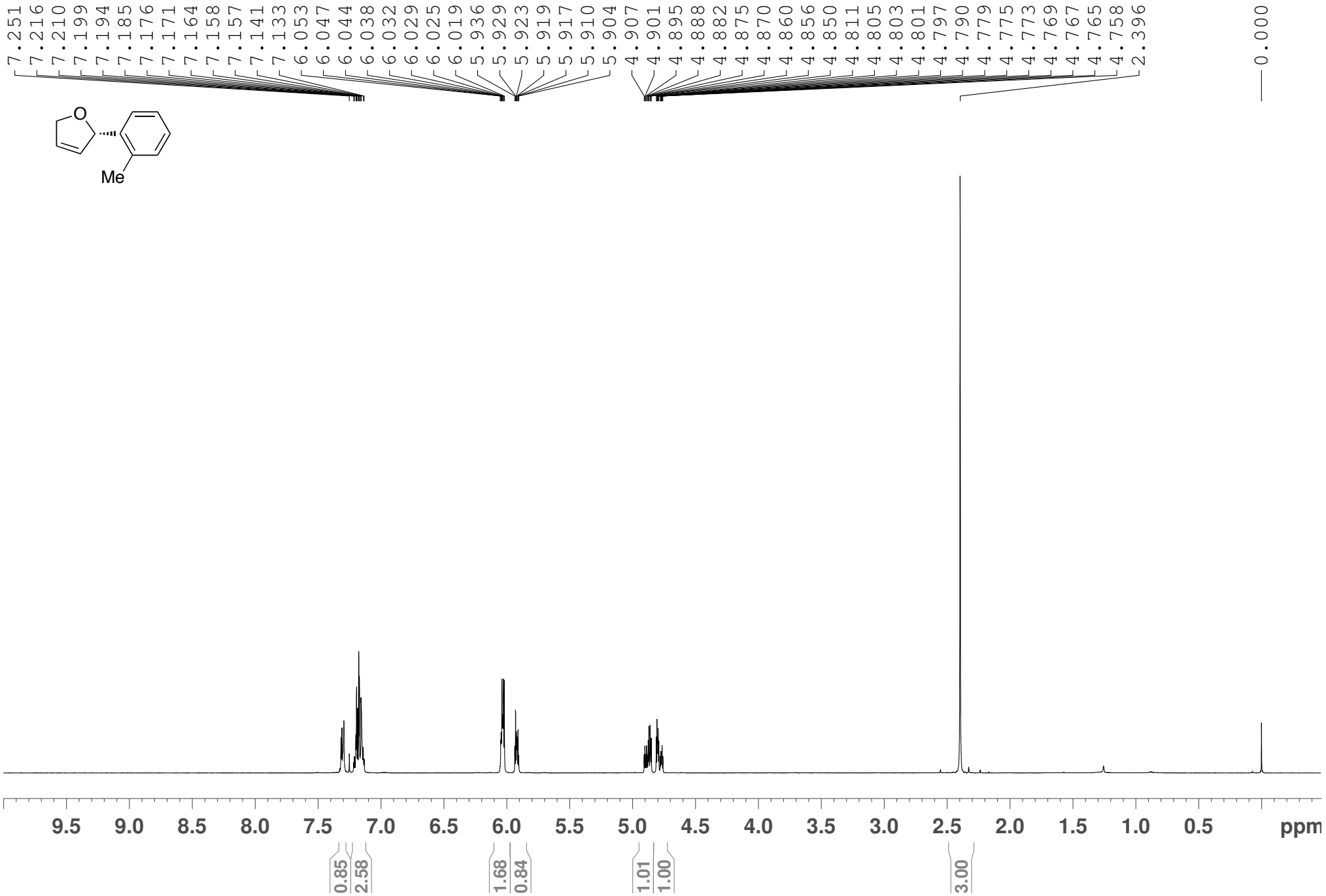
^{1}H NMR (400 MHz, $CDCl_3$)



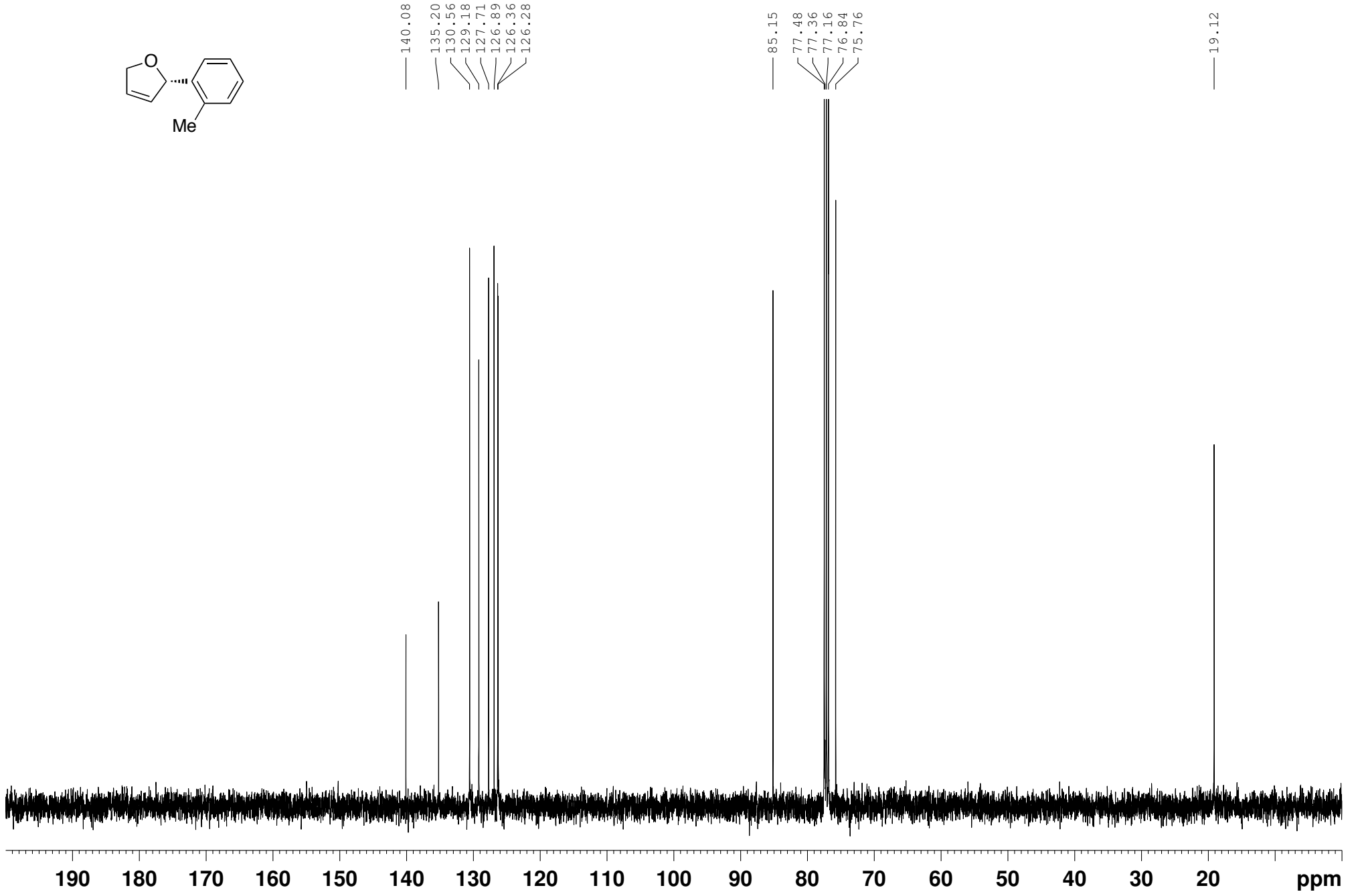
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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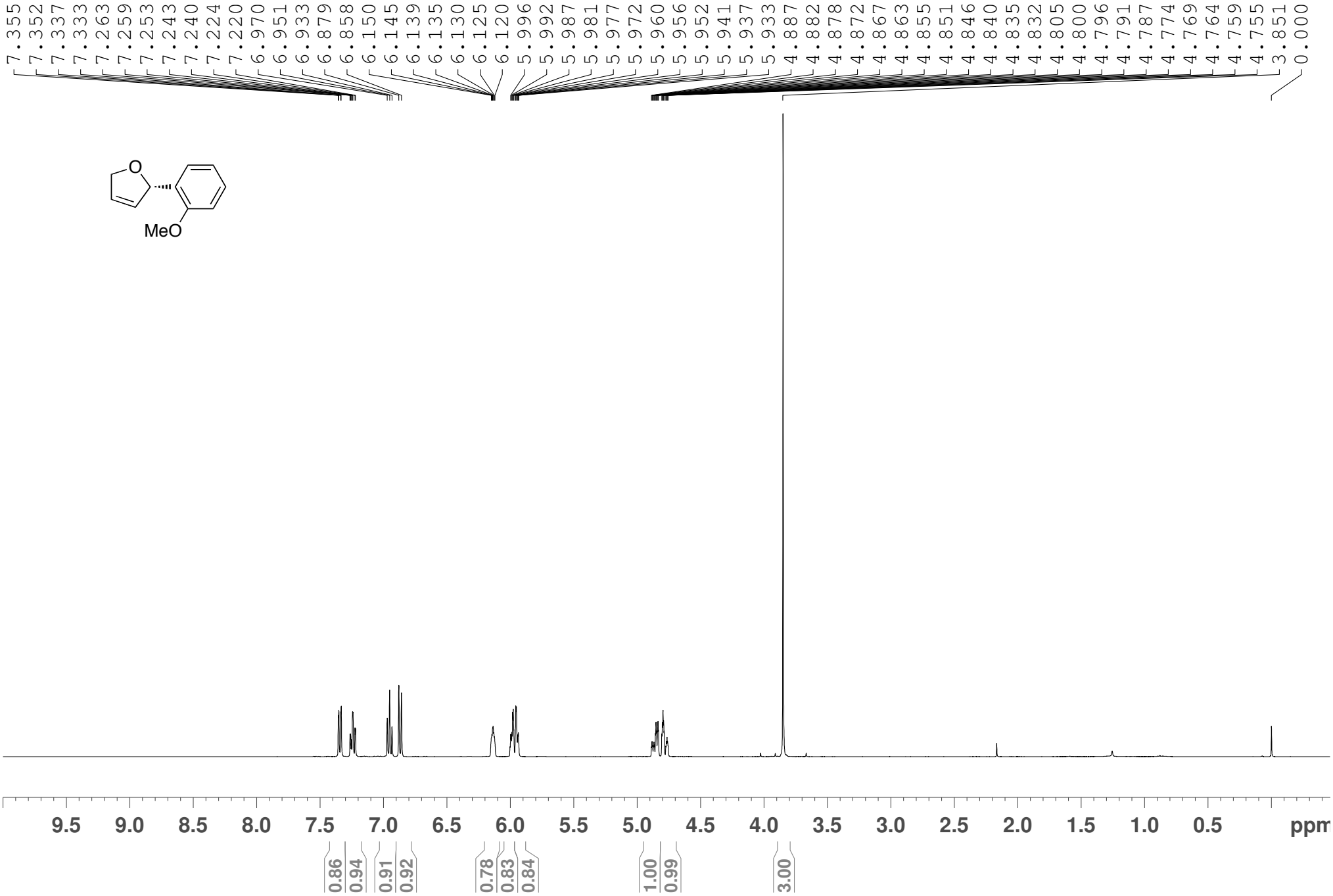
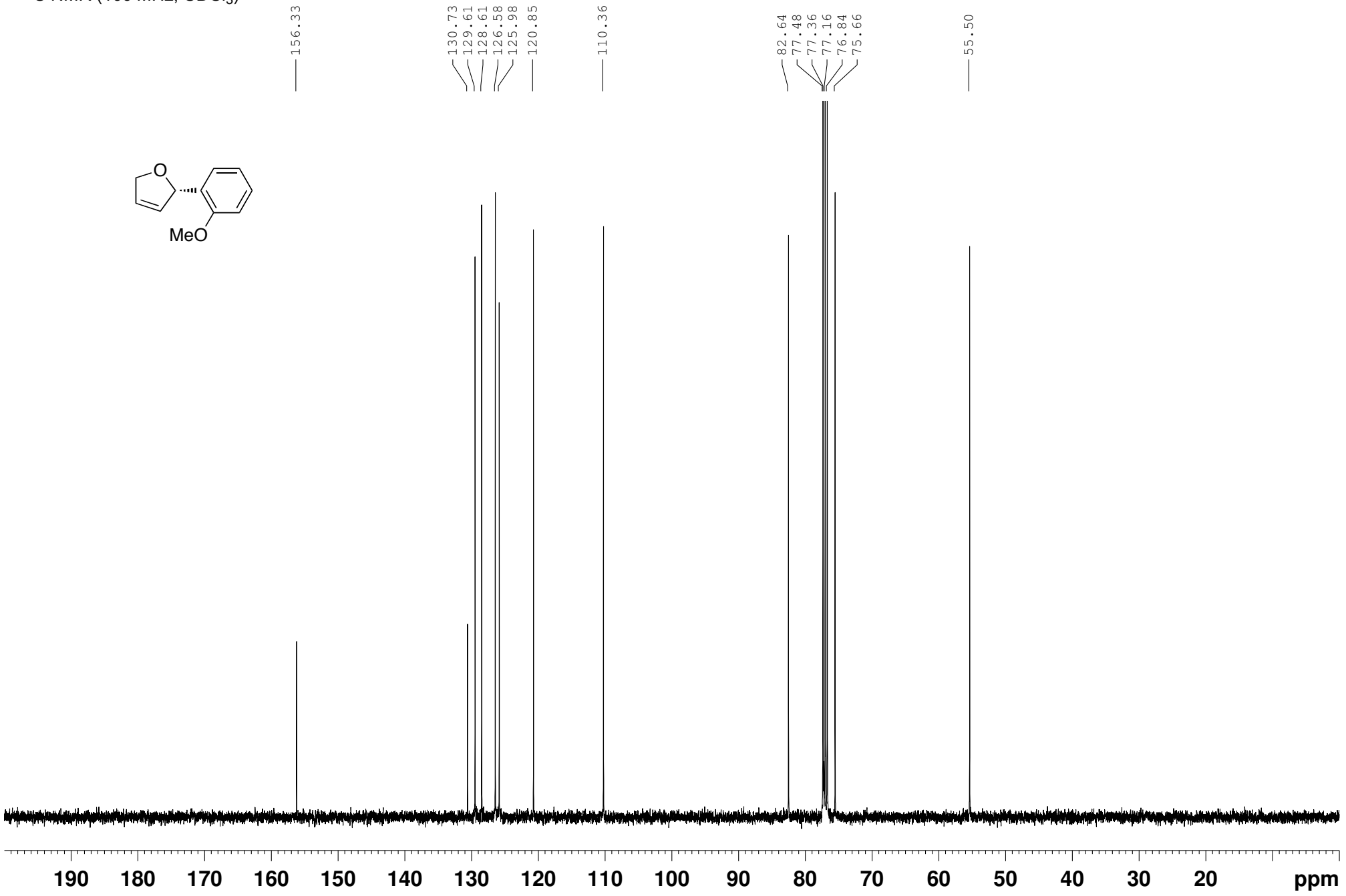
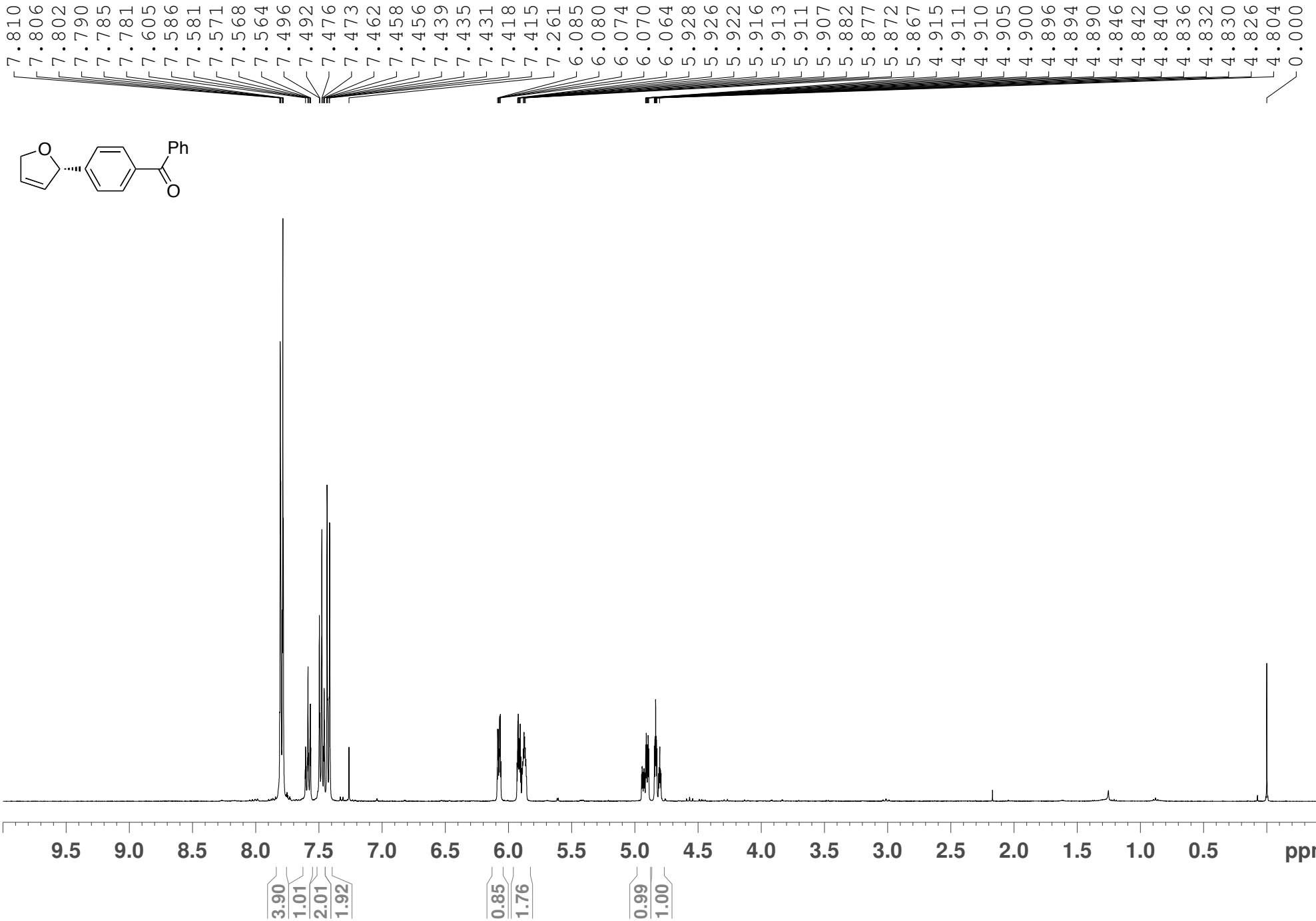


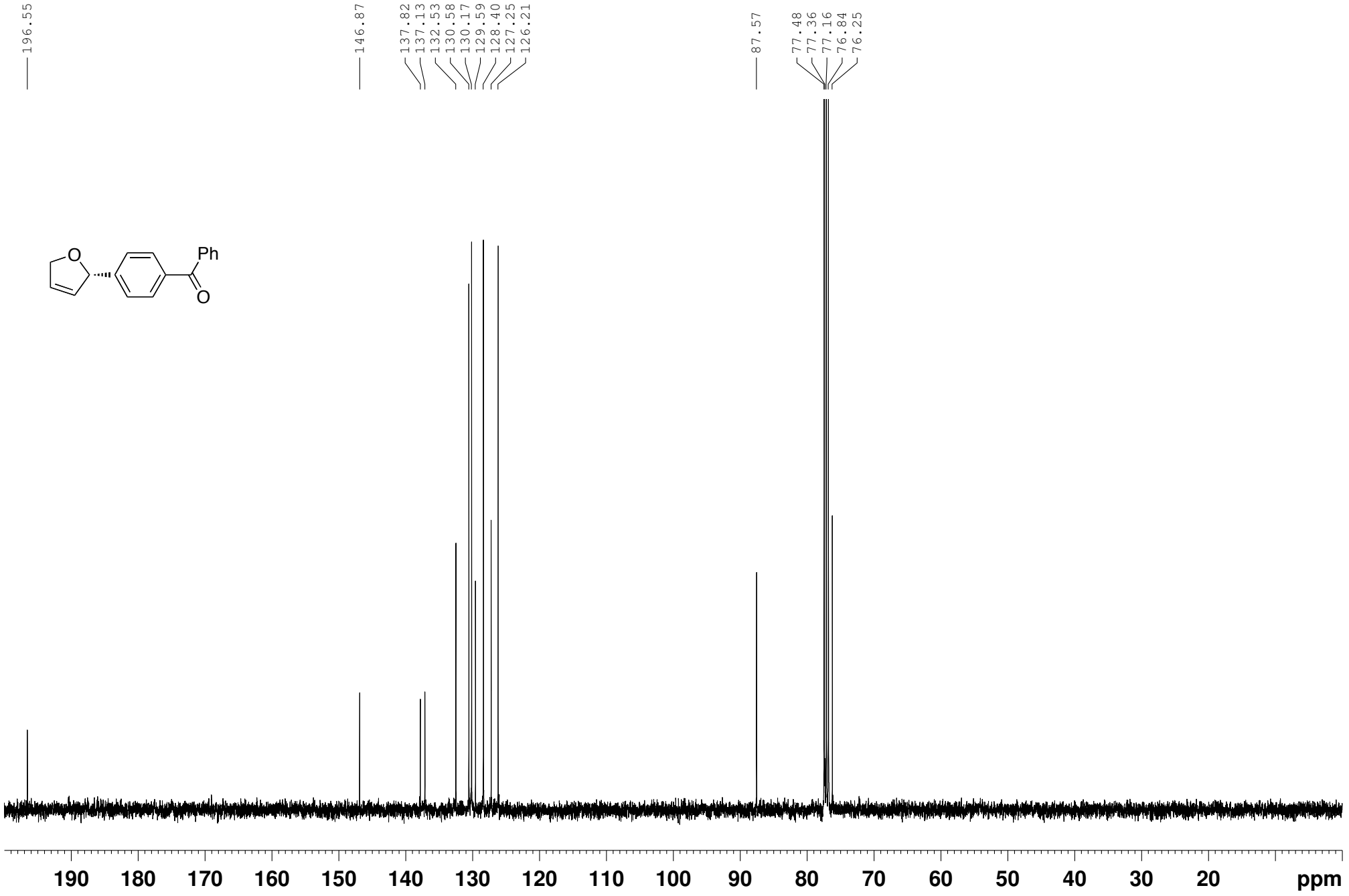
^{13}C NMR (100 MHz, $CDCl_3$)



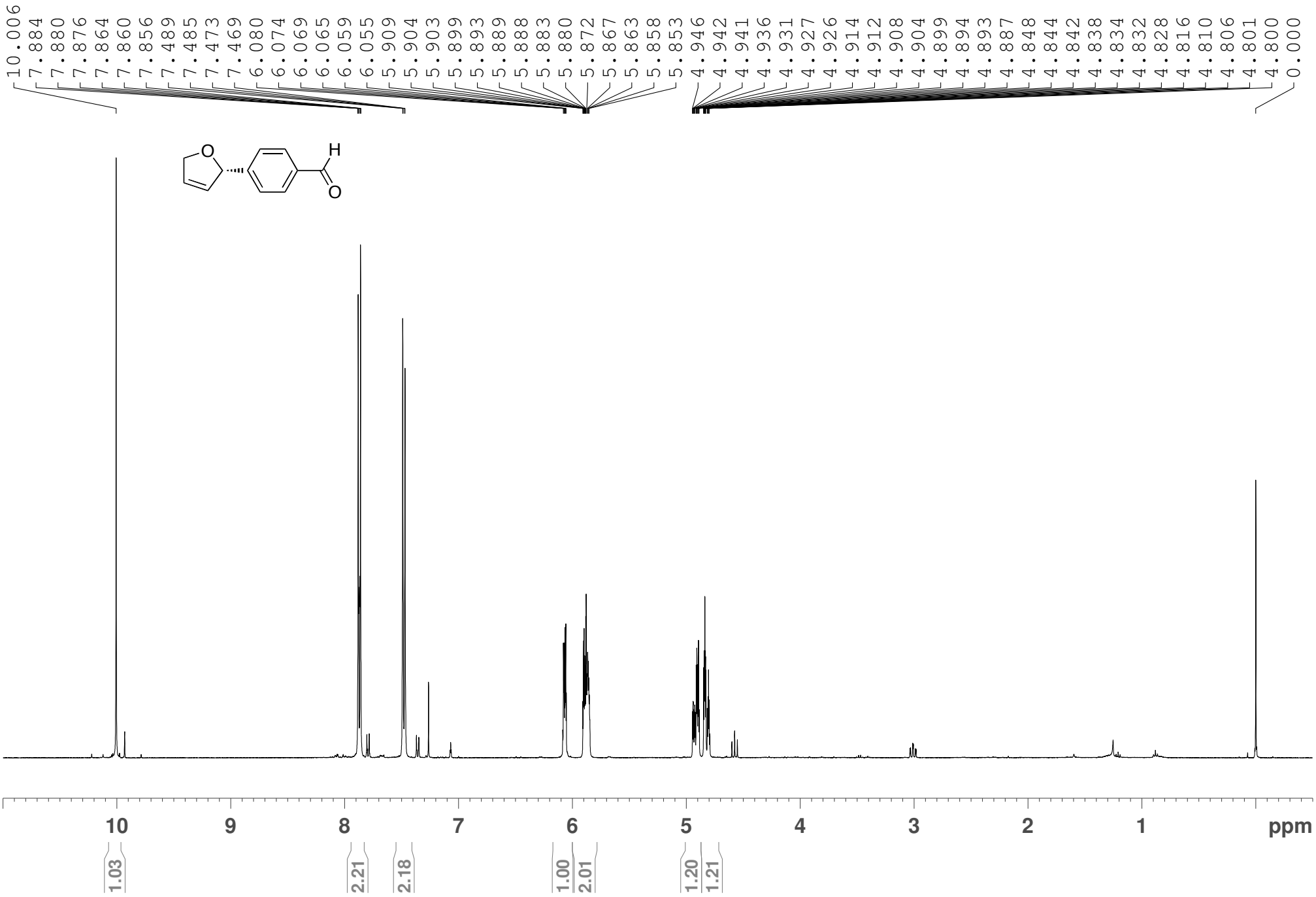
^{1}H NMR (400 MHz, $CDCl_3$)

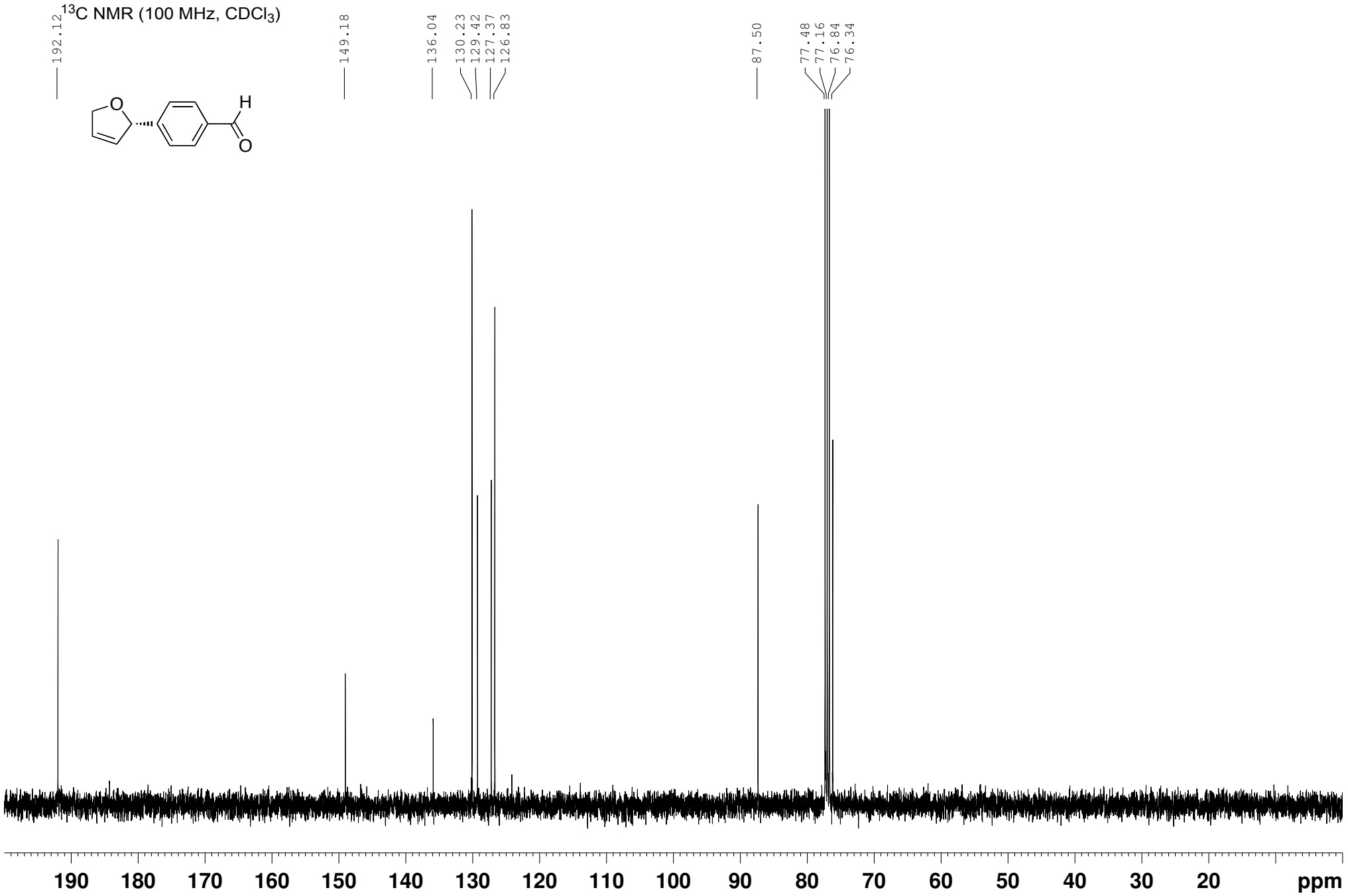


^{13}C NMR (100 MHz, $CDCl_3$)

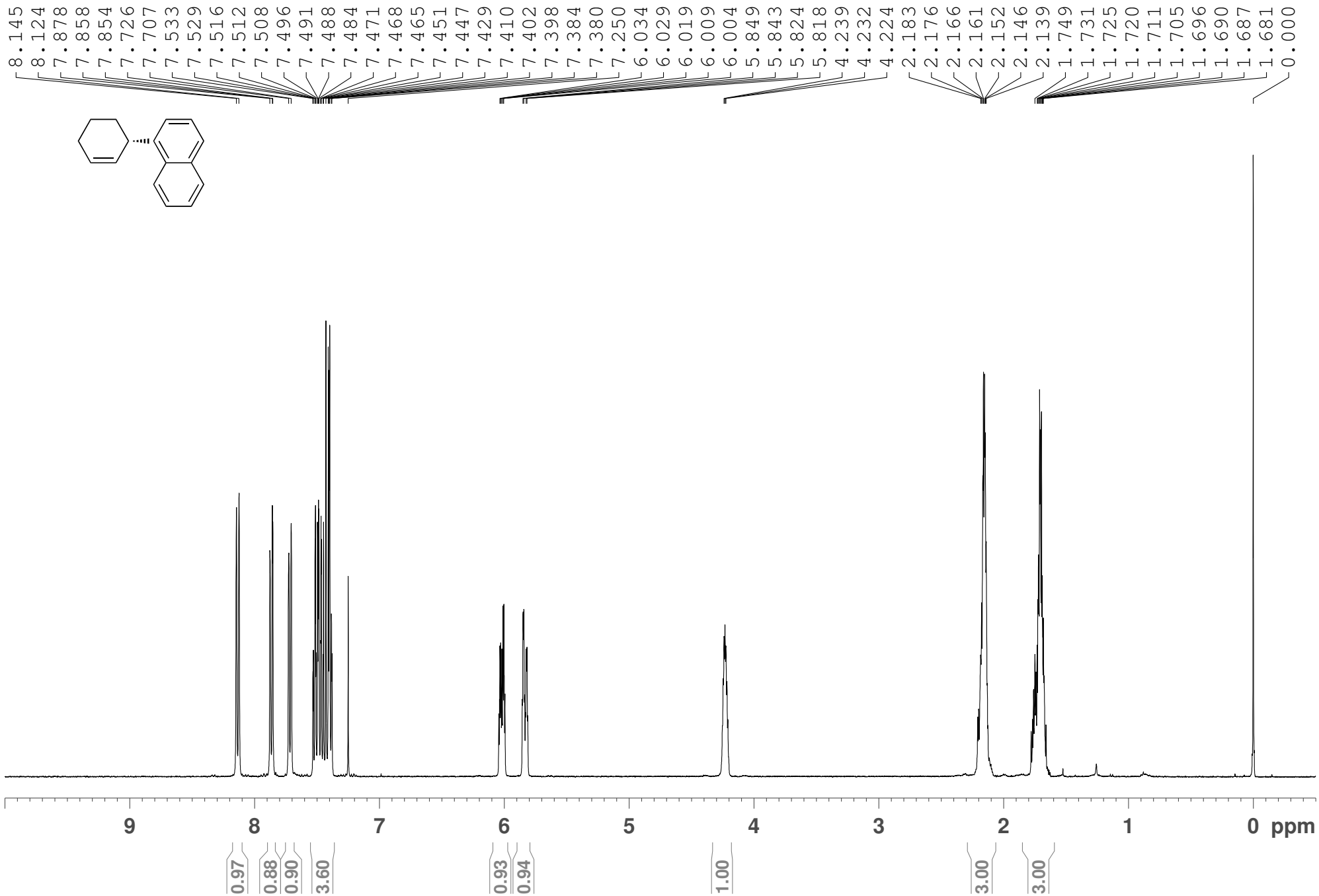


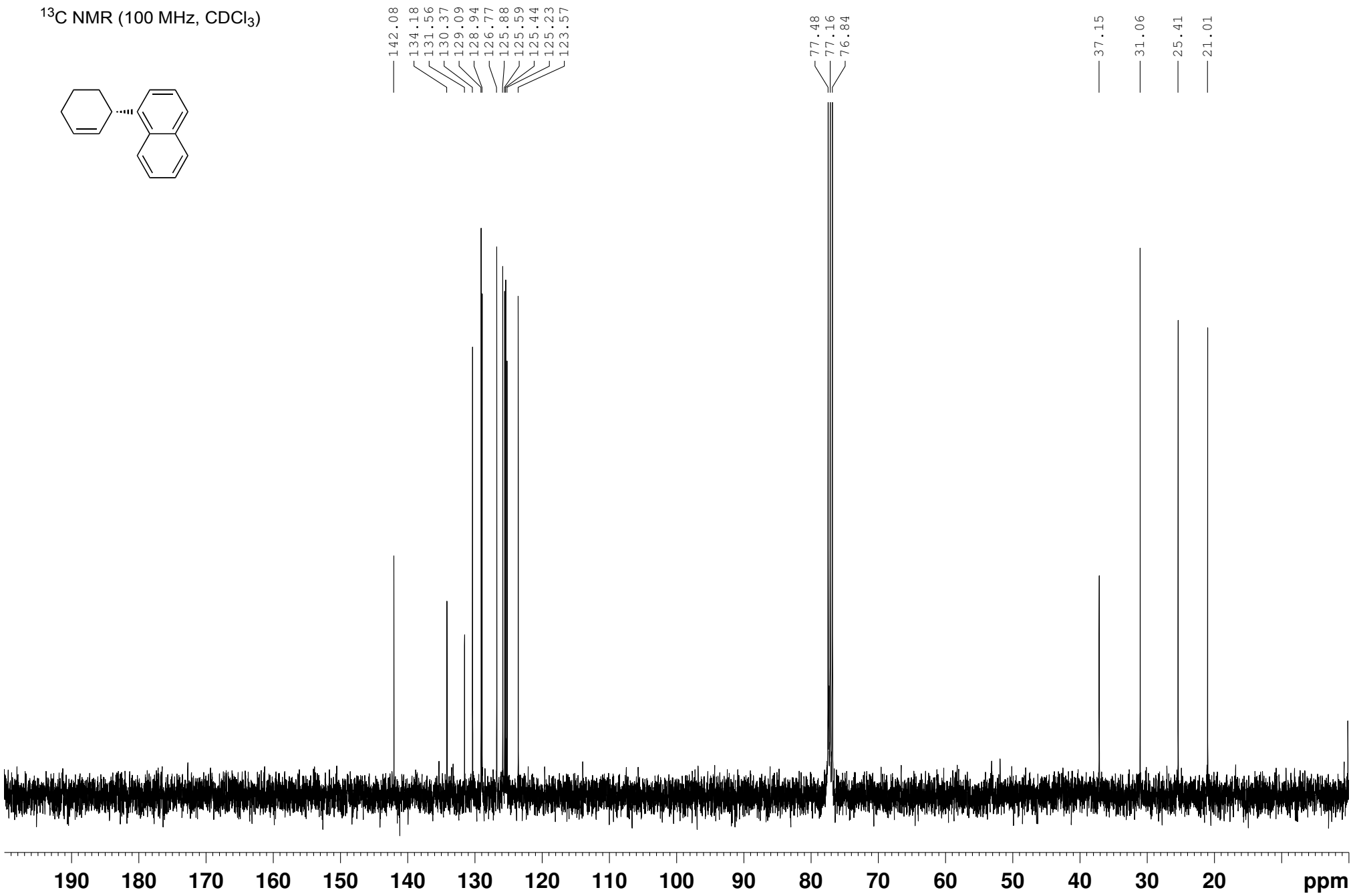
^{1}H NMR (400 MHz, $CDCl_3$)



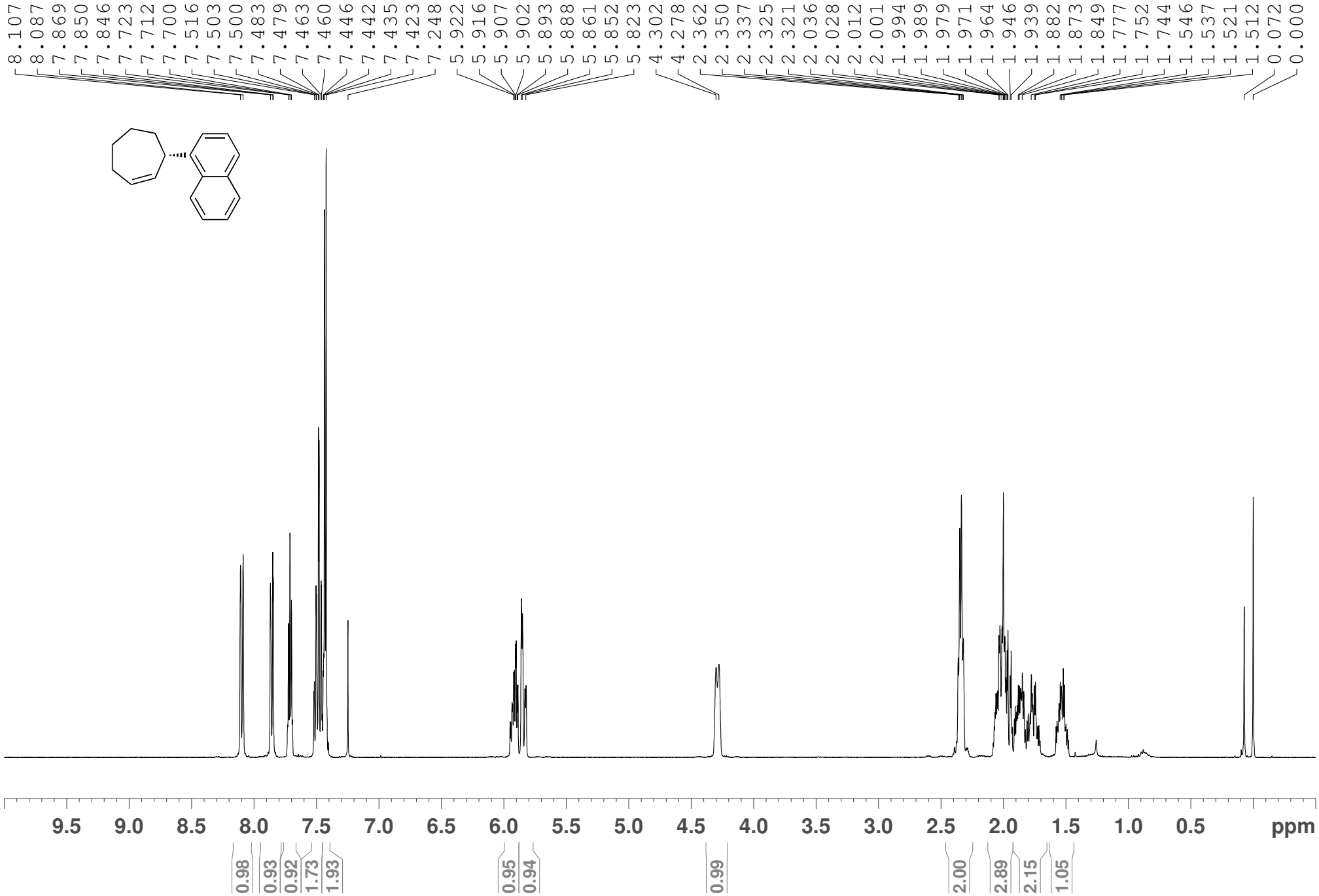


^{1}H NMR (400 MHz, $CDCl_3$)

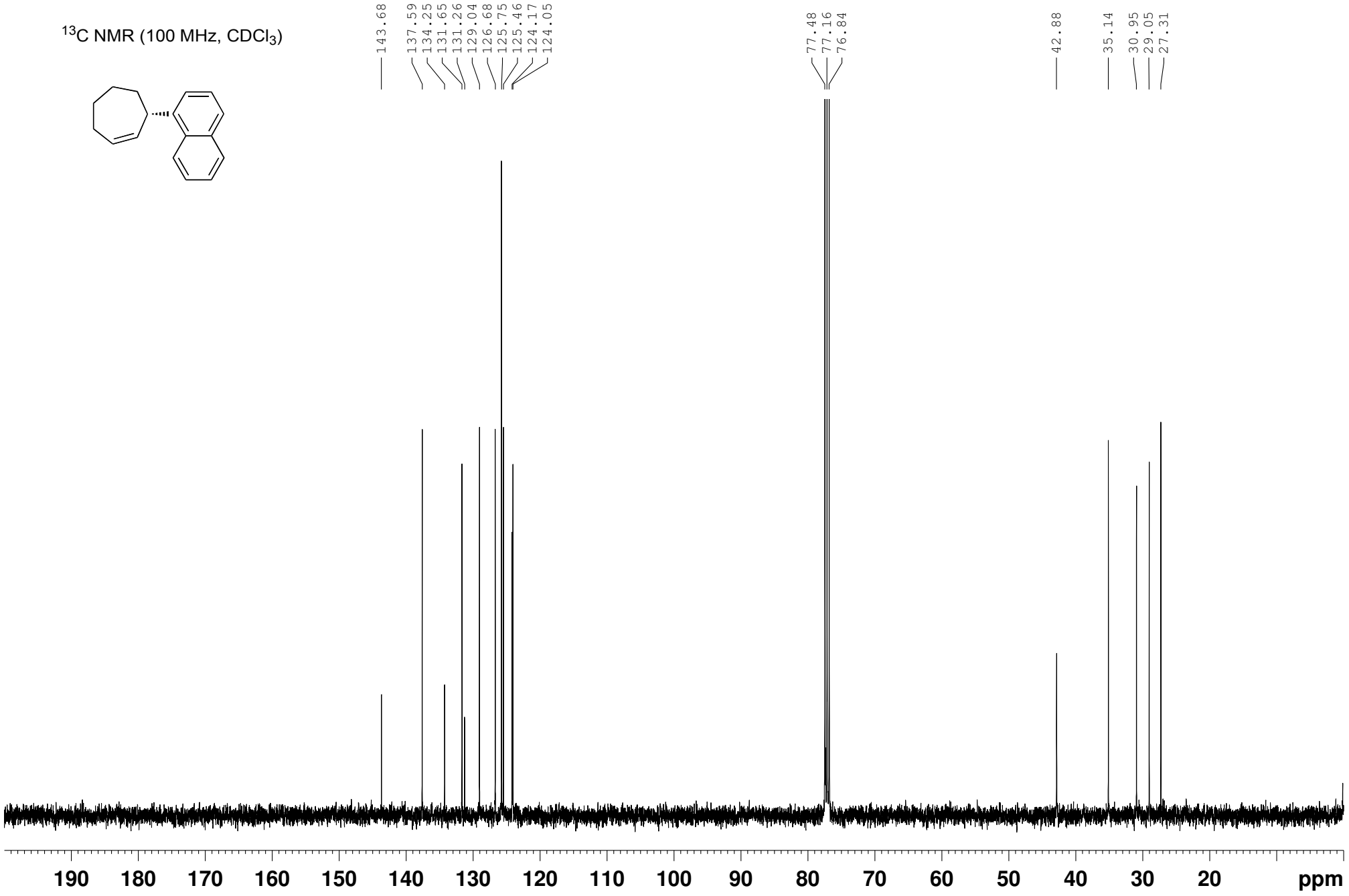




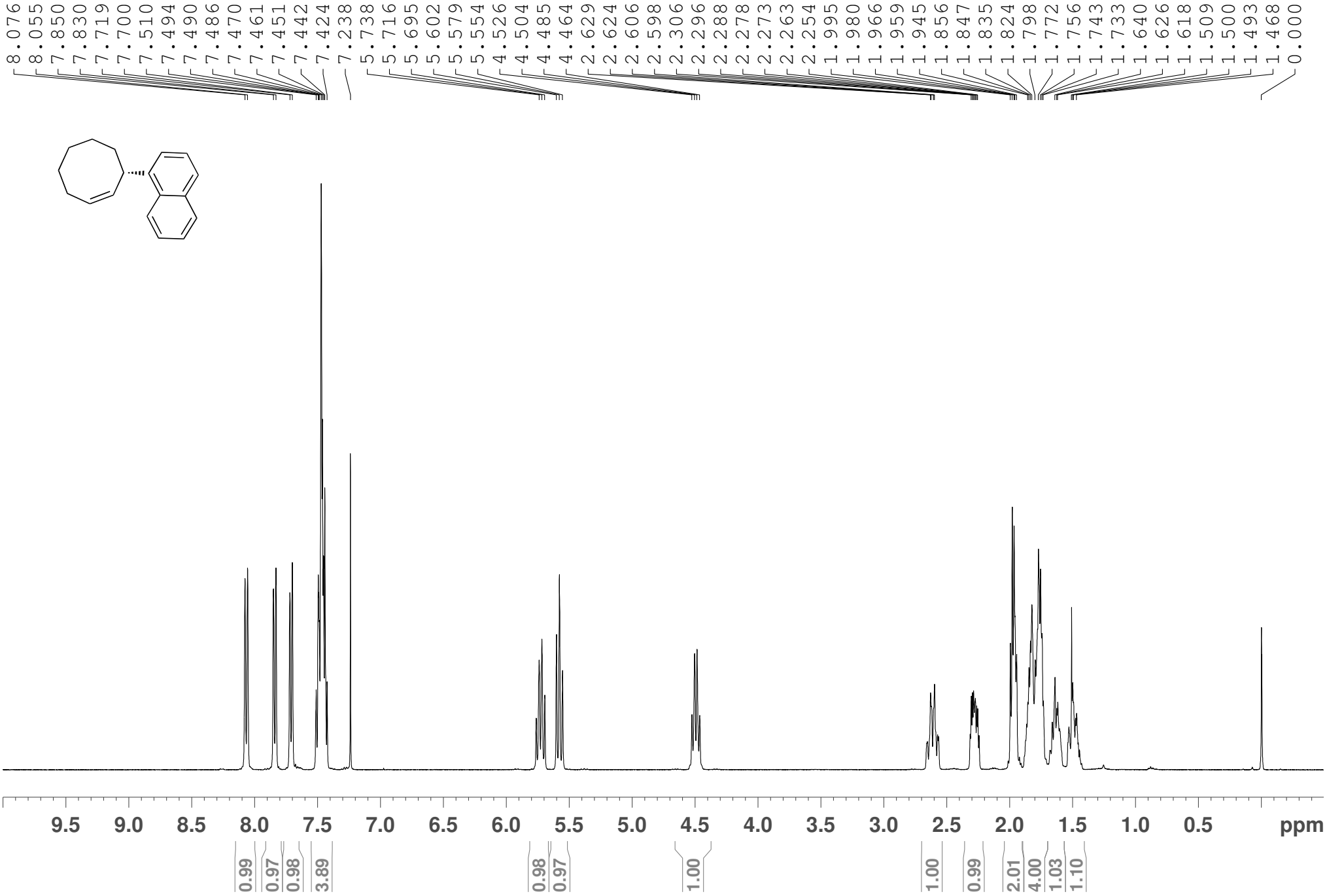
^{1}H NMR (400 MHz, $CDCl_3$)



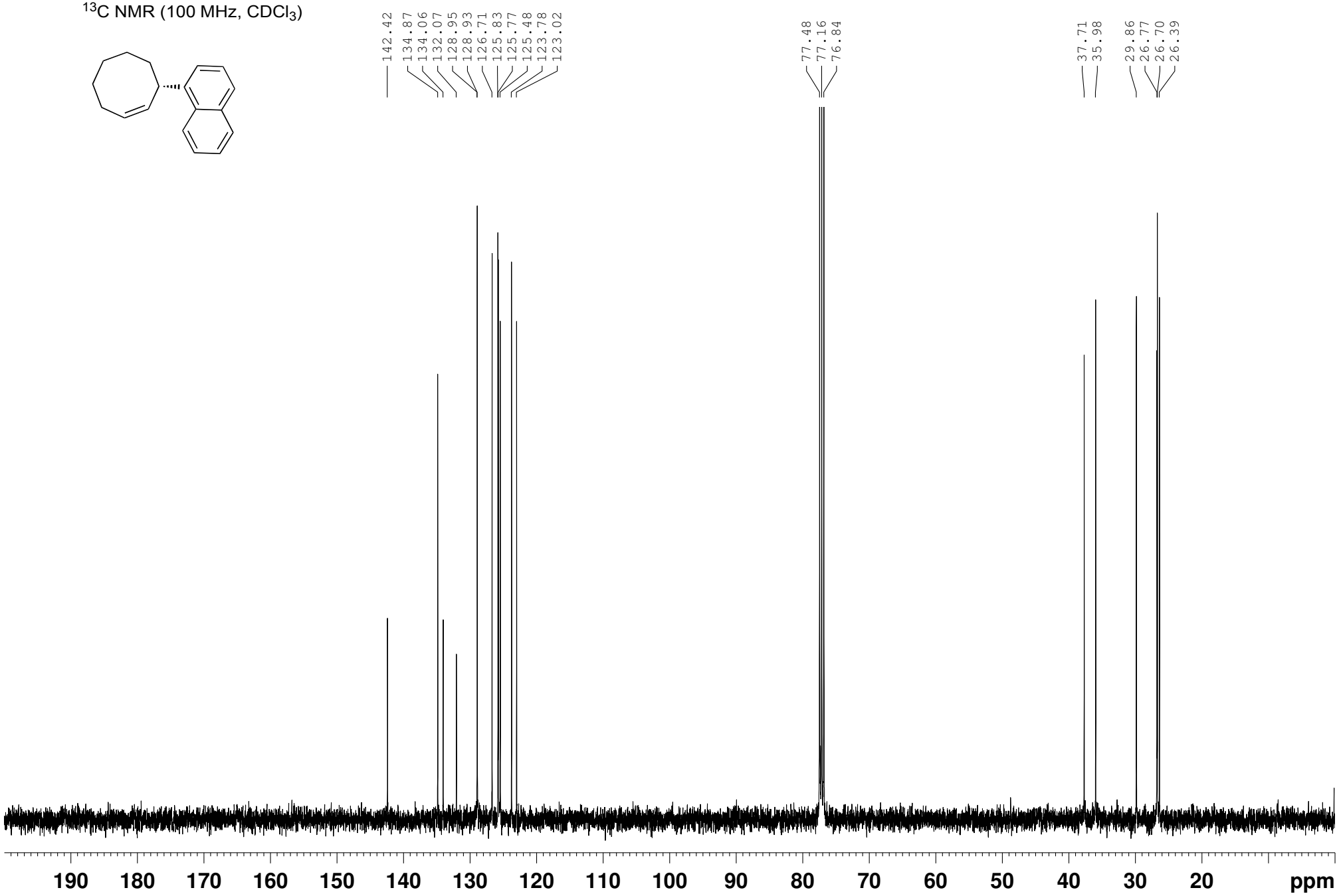
^{13}C NMR (100 MHz, $CDCl_3$)



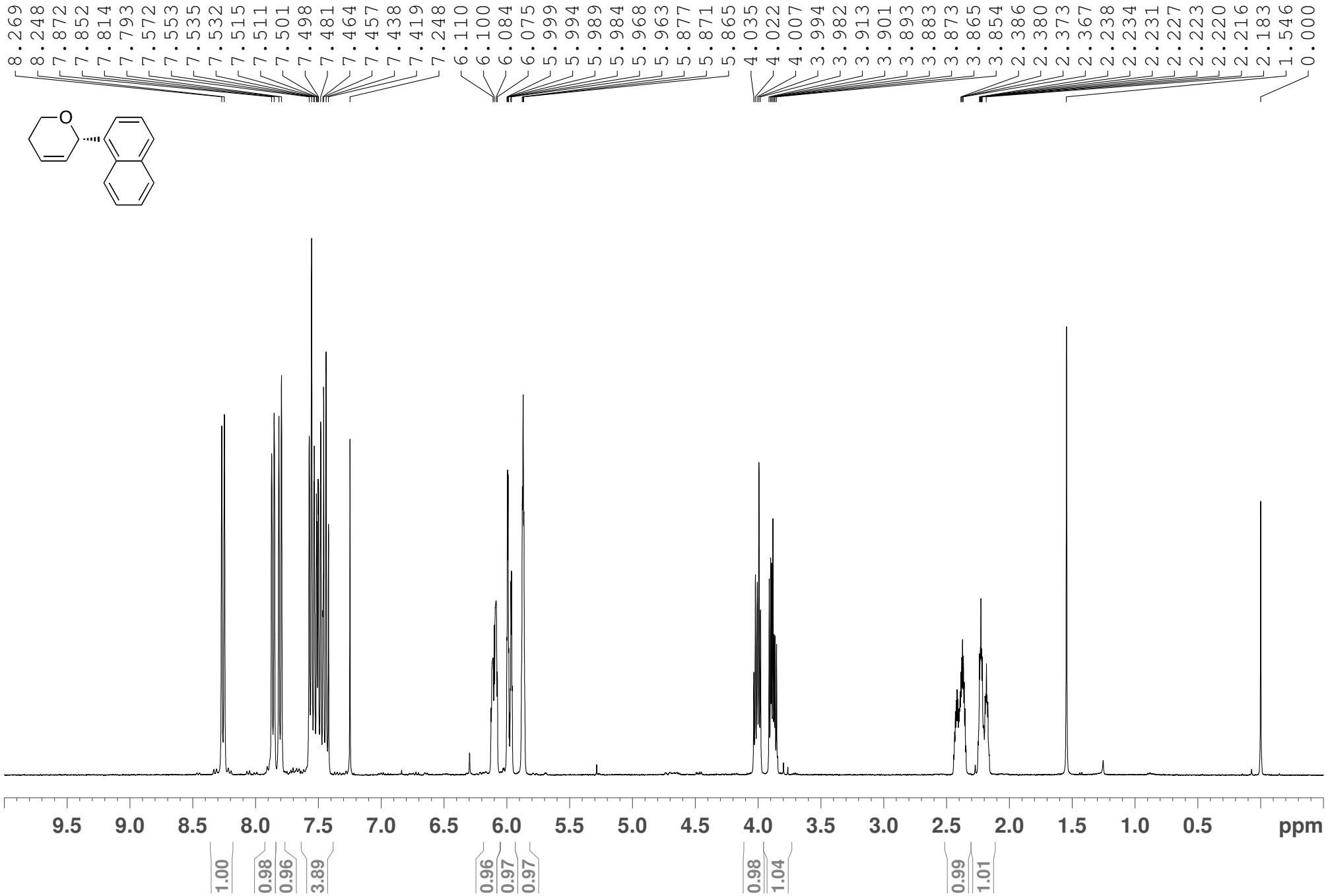
^{1}H NMR (400 MHz, $CDCl_3$)



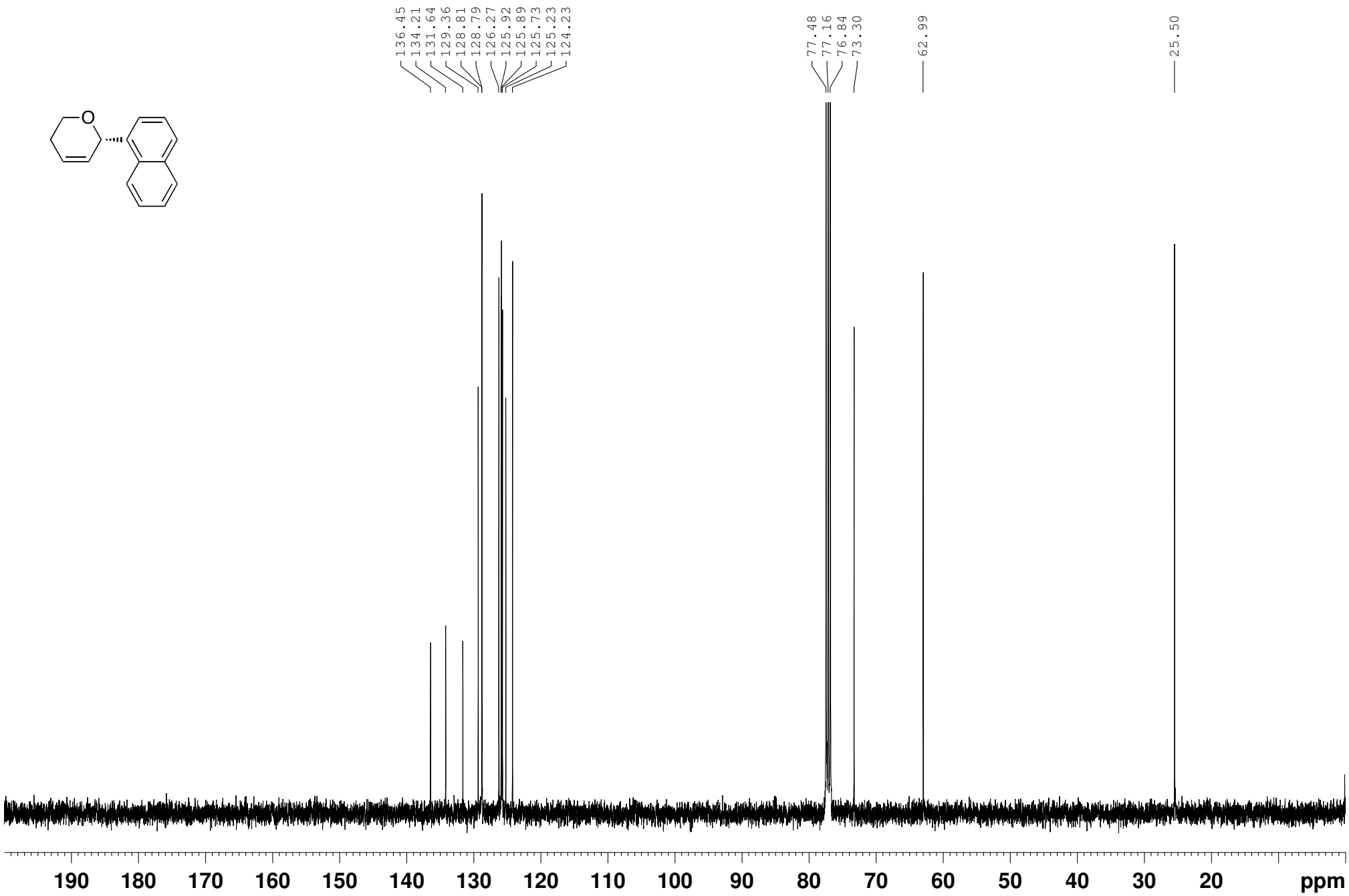
^{13}C NMR (100 MHz, $CDCl_3$)



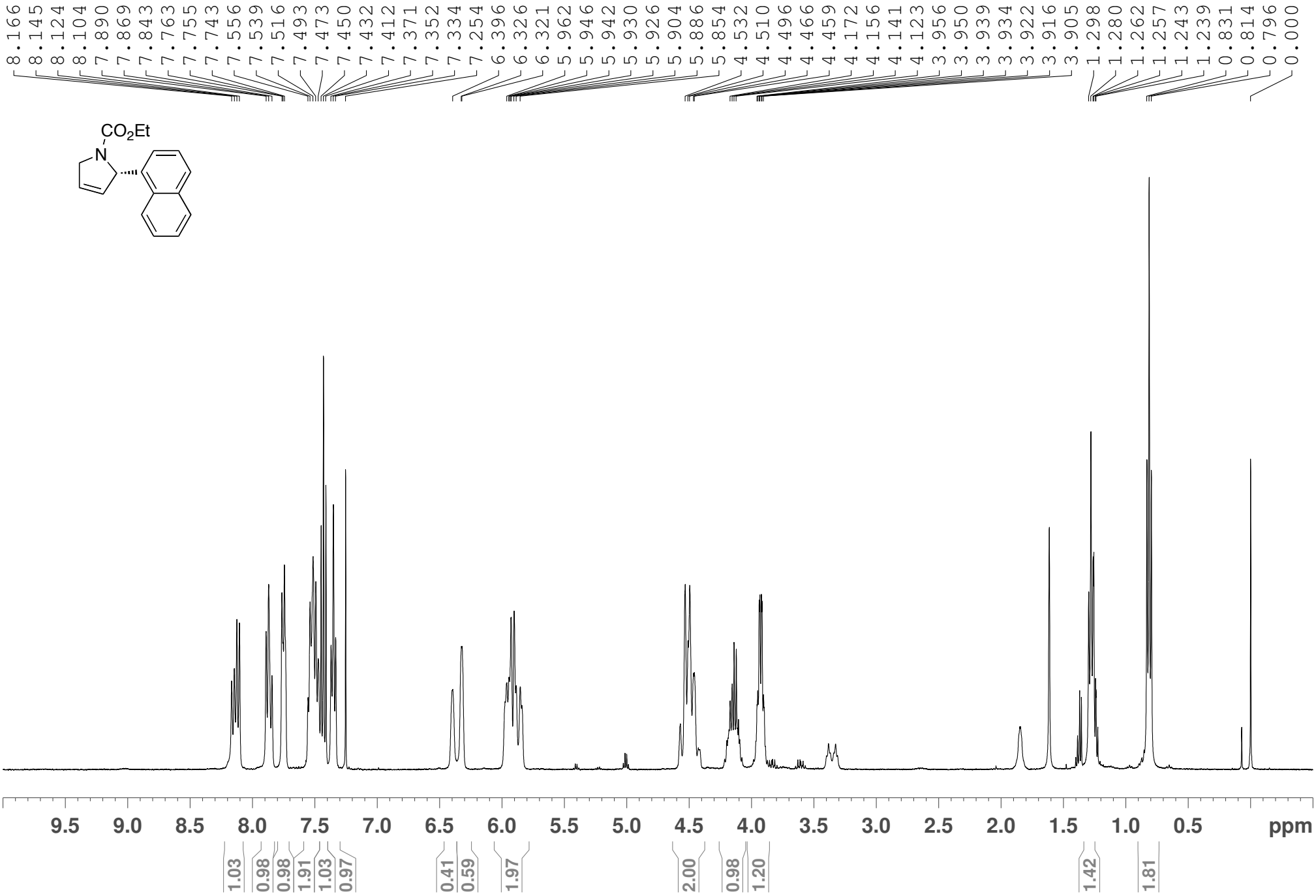
^{1}H NMR (400 MHz, $CDCl_3$)



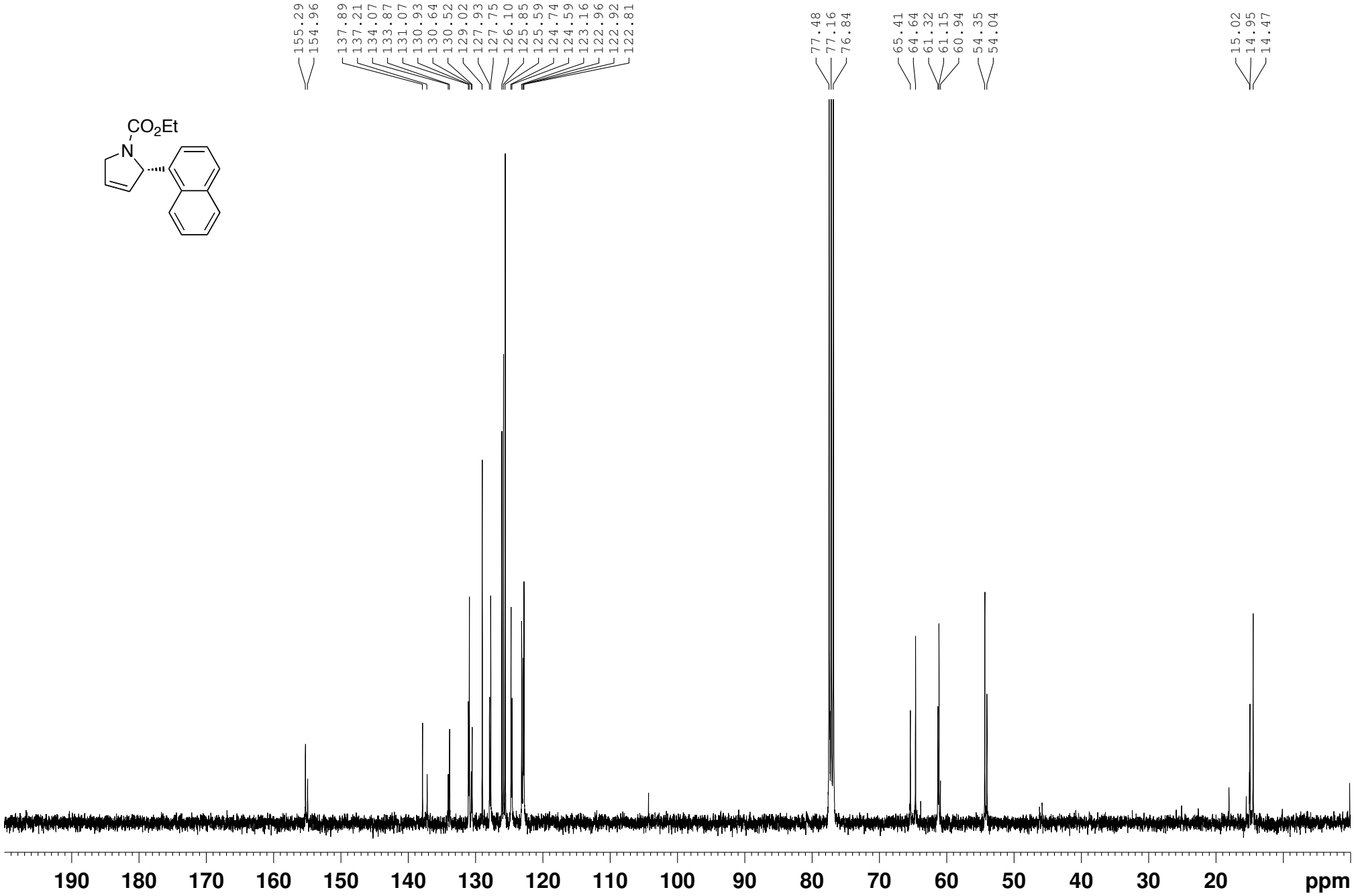
^{13}C NMR (100 MHz, $CDCl_3$)



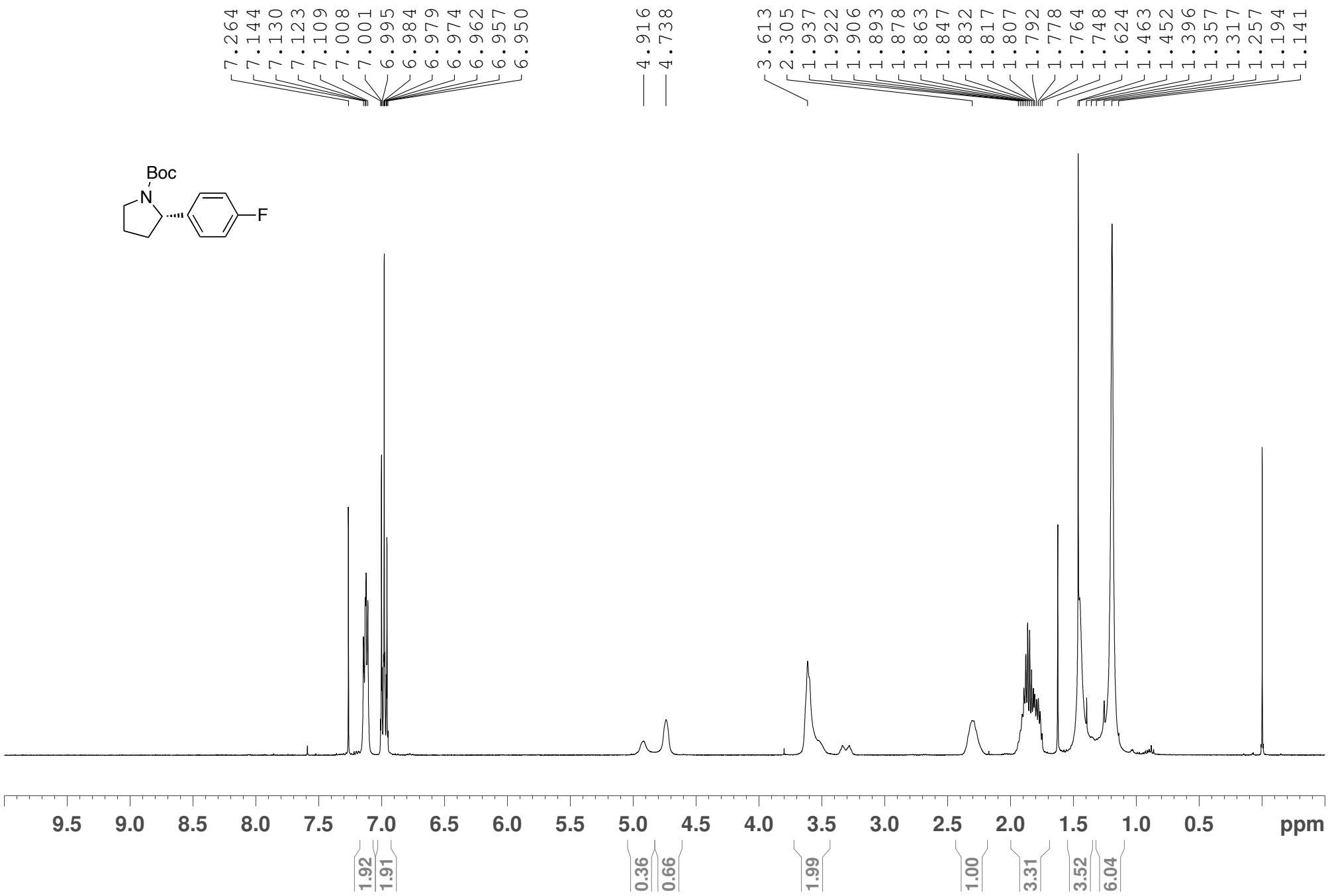
^{1}H NMR (400 MHz, $CDCl_3$)



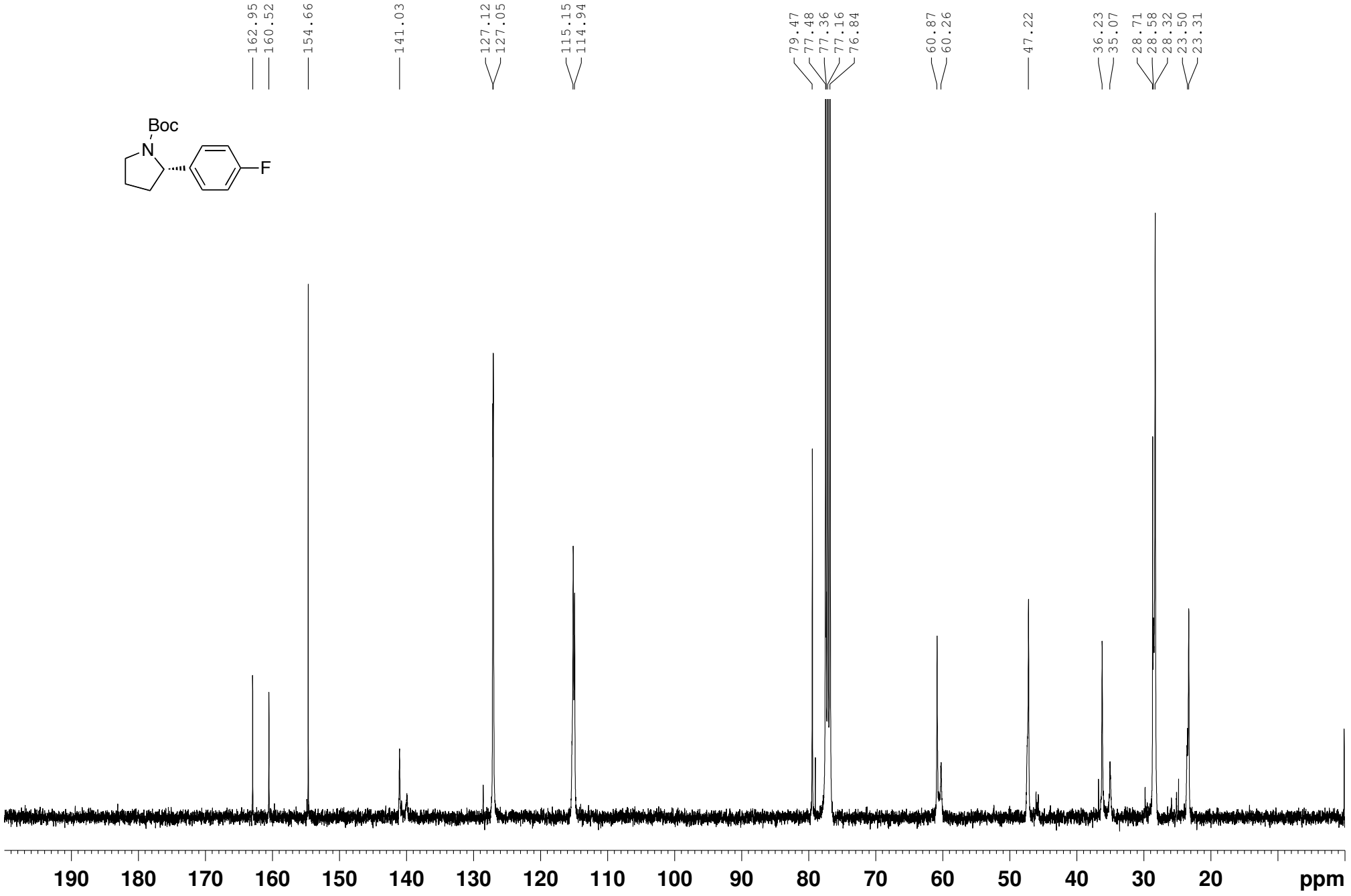
^{13}C NMR (100 MHz, $CDCl_3$)

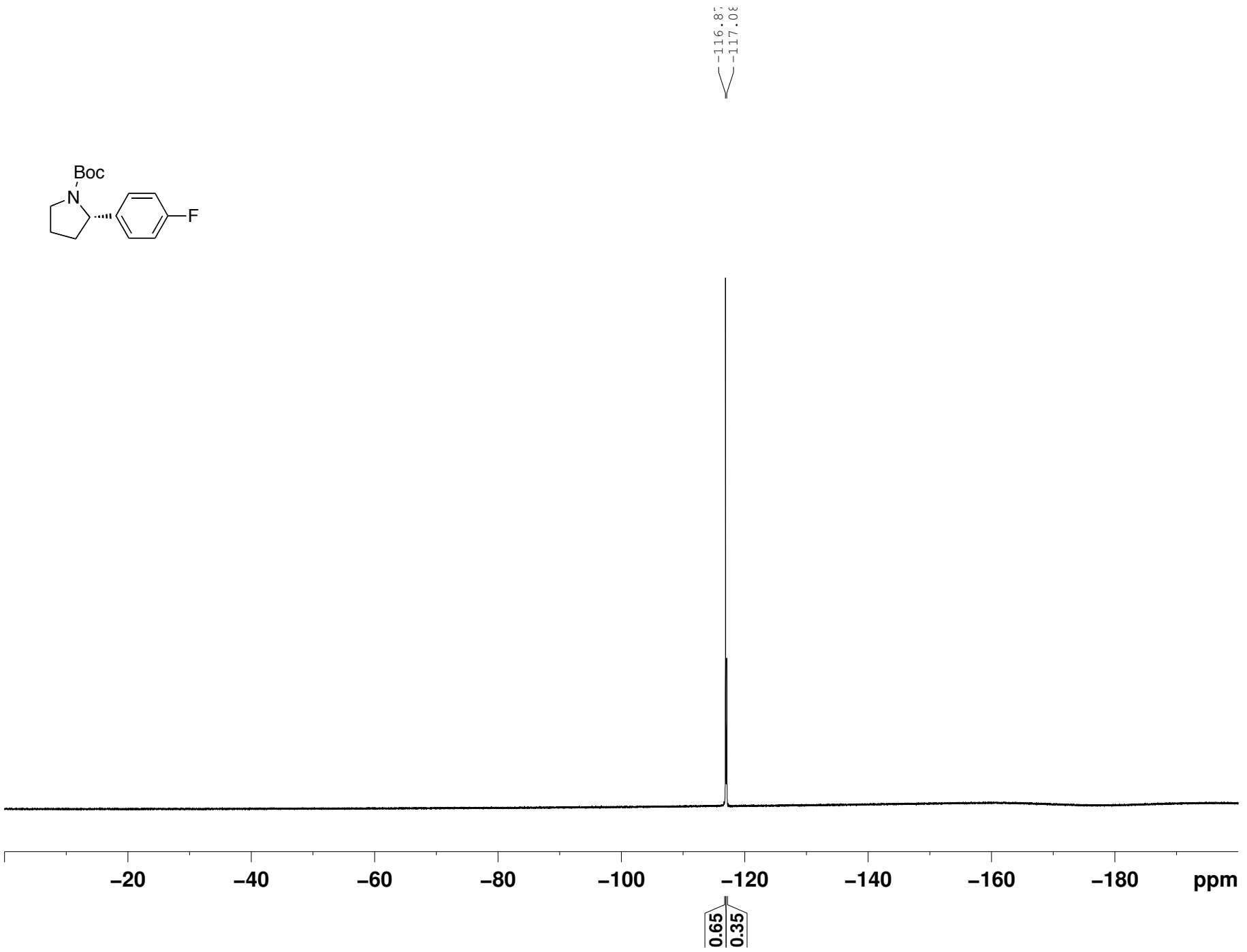


^{1}H NMR (400 MHz, $CDCl_3$)

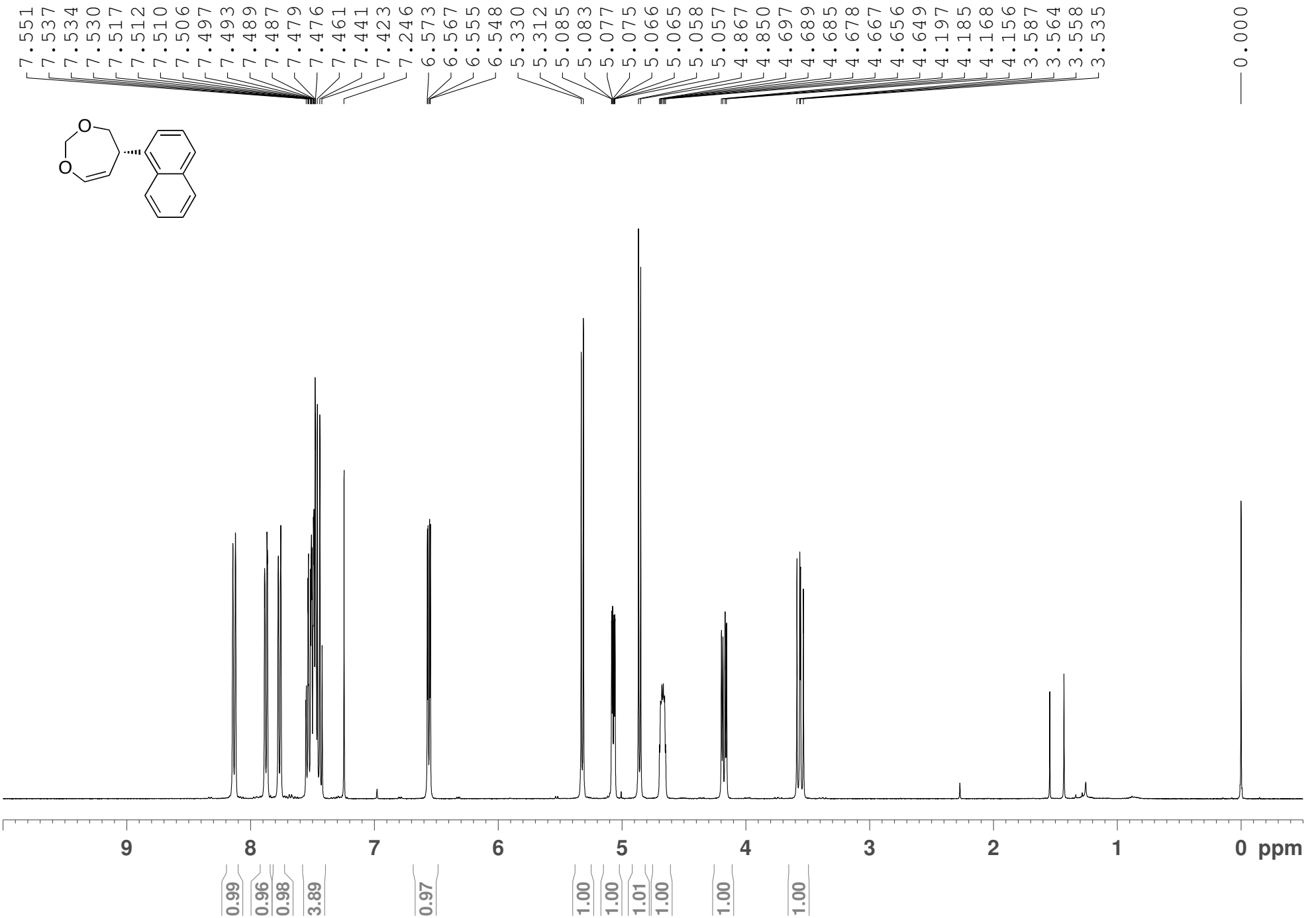


^{13}C NMR (100 MHz, $CDCl_3$)

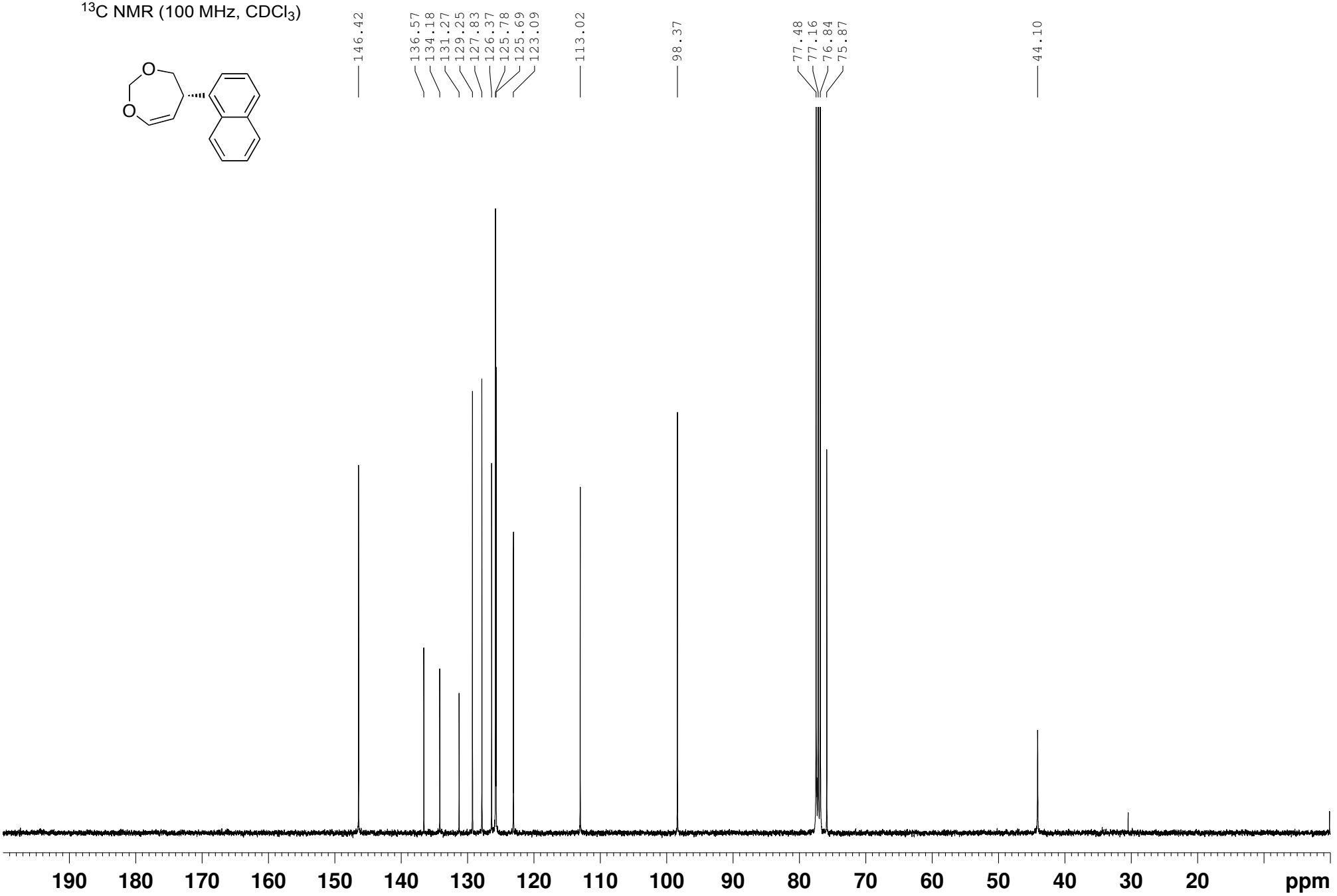




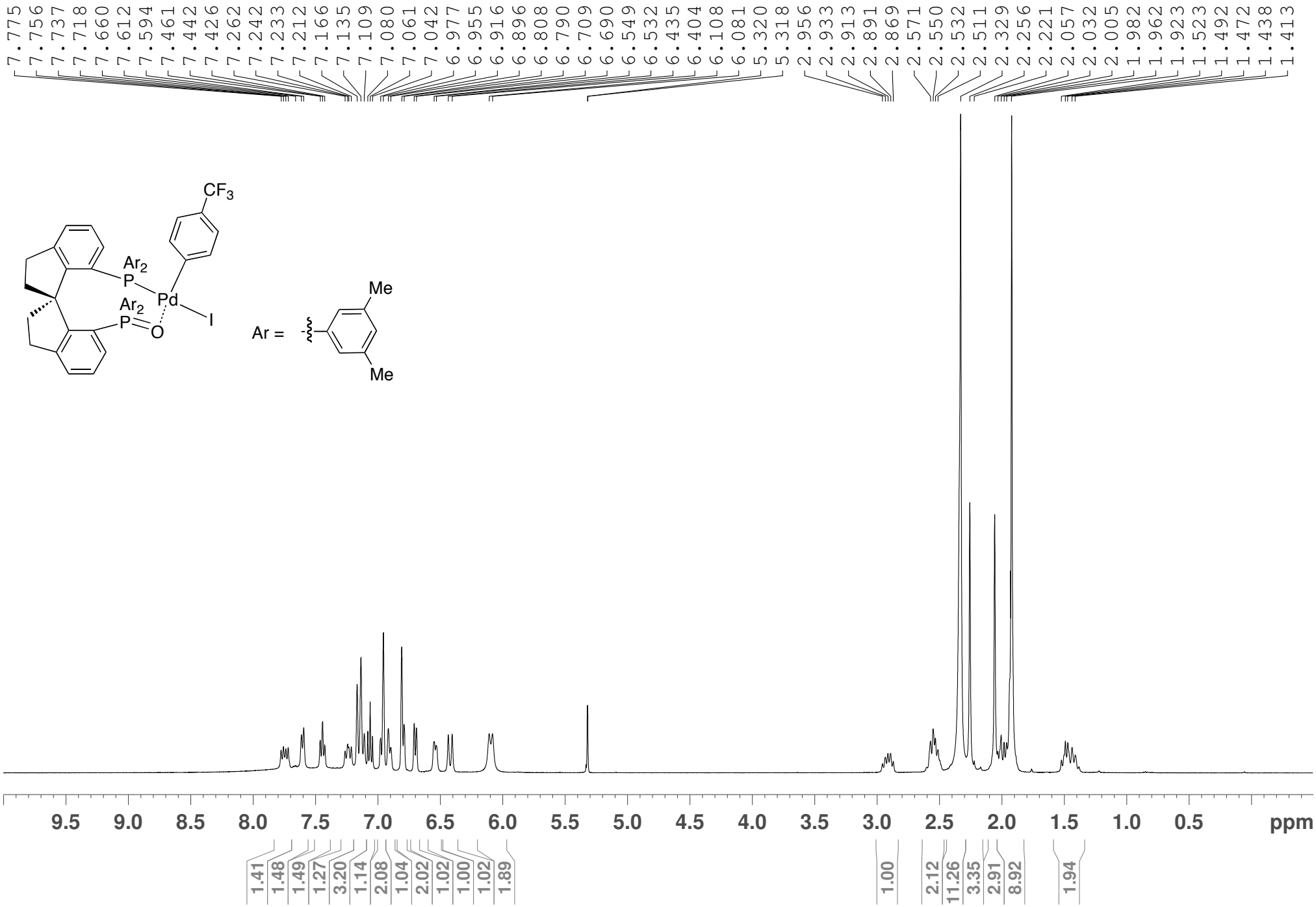
^{1}H NMR (400 MHz, $CDCl_3$)



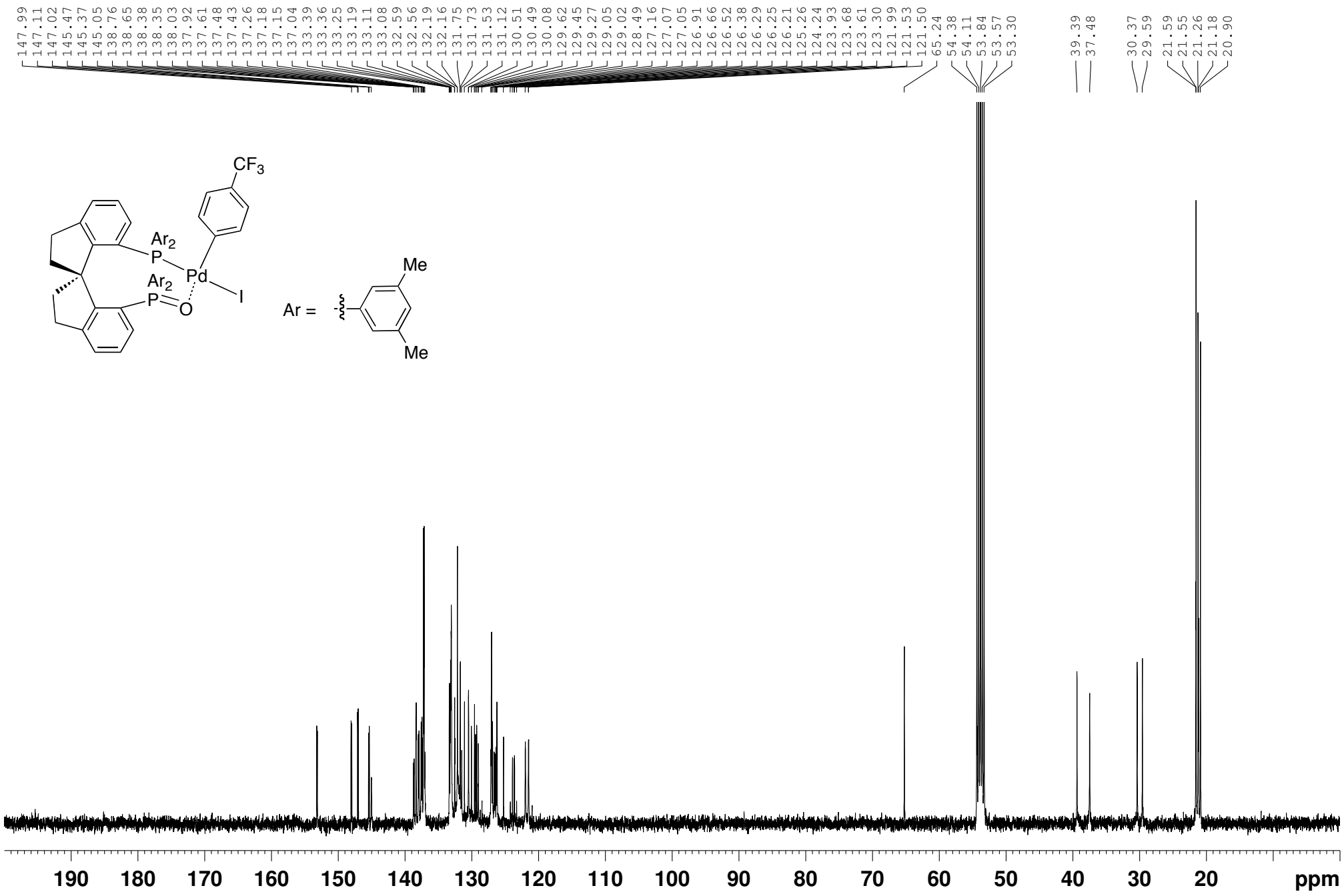
^{13}C NMR (100 MHz, $CDCl_3$)



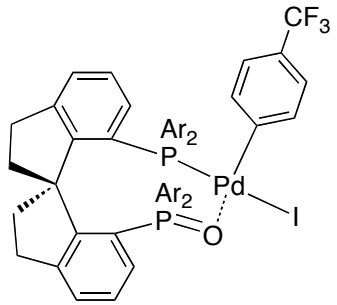
^{1}H NMR (400 MHz, CD_2Cl_2)



^{13}C NMR (100 MHz, CD_2Cl_2)



$^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2)



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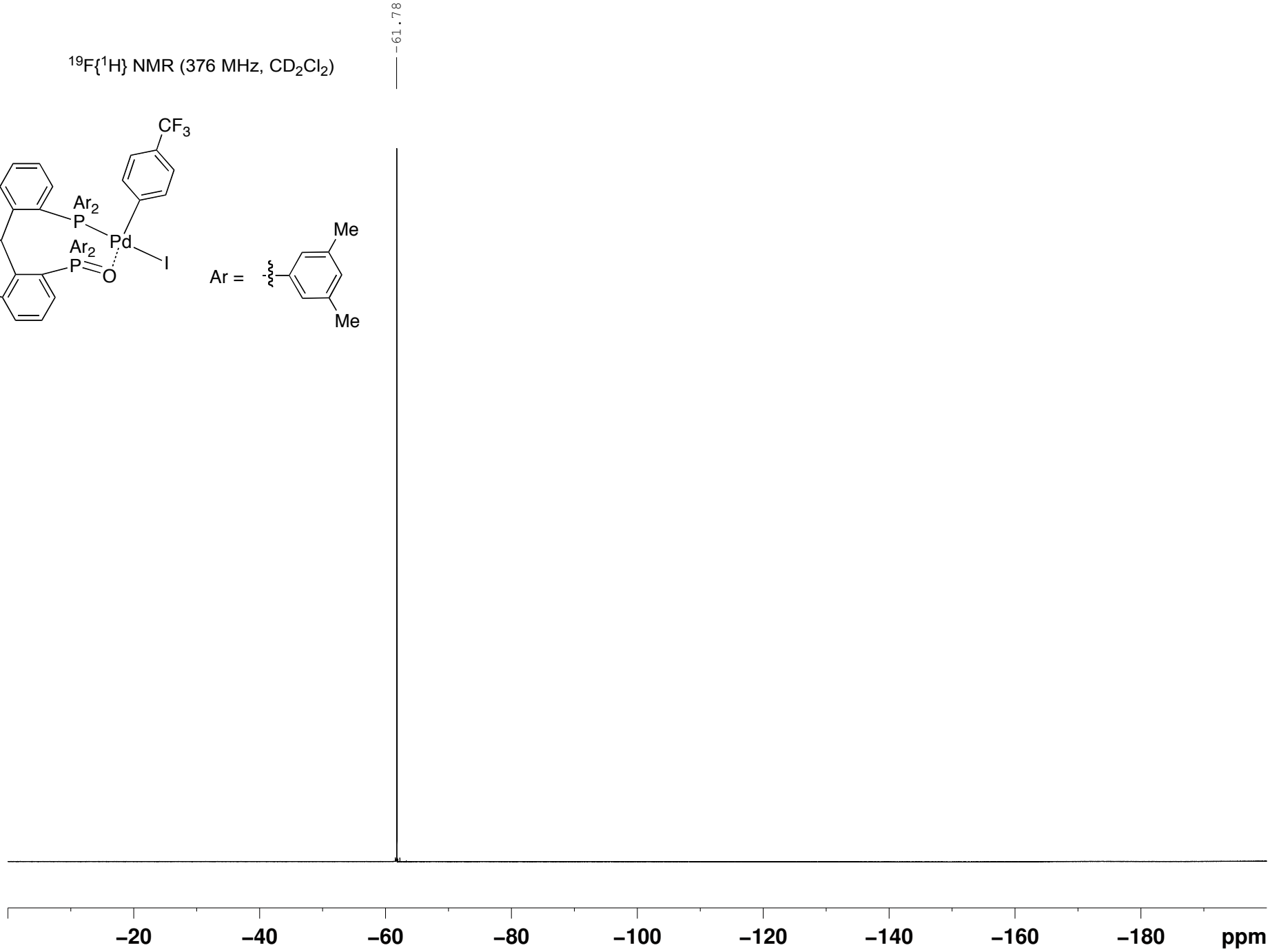
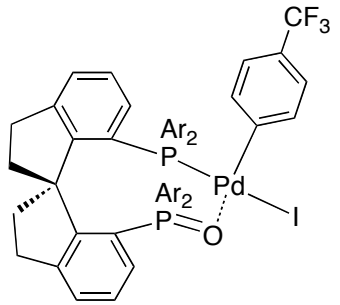


$^{31}P\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2)



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