

Supporting information

Facile access to [1,2]-oxazine derivatives *via* annulations of aminoxy-tethered 1,7-enynes

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1. Single X-ray crystal data of compound 4c:

Data for the compound KA648 was collected at room temperature on a Bruker D8 QUEST instrument with an I μ S Mo microsource ($\lambda = 0.7107 \text{ \AA}$) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [1]. The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL [2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H or $1.2U_{\text{eq}}(\text{C})$ for other H atoms].

Crystal structure determination of 4c

Crystal Data for $\text{C}_{27}\text{H}_{25}\text{NO}_5\text{S}$ ($M = 475.54 \text{ g/mol}$): monoclinic, space group $\text{P}2_1/\text{c}$ (no. 14), $a = 18.0027(3) \text{ \AA}$, $b = 17.5394(3) \text{ \AA}$, $c = 7.63400(10) \text{ \AA}$, $\beta = 91.6110(8)^\circ$, $V = 2409.53(7) \text{ \AA}^3$, $Z = 4$, $T = 294.15 \text{ K}$, $\mu(\text{MoK}\alpha) = 0.173 \text{ mm}^{-1}$, $D_{\text{calc}} = 1.311 \text{ g/cm}^3$, 27855 reflections measured ($4.526^\circ \leq 2\theta \leq 52.49^\circ$), 4856 unique ($R_{\text{int}} = 0.0650$, $R_{\text{sigma}} = 0.0533$) which were used in all calculations. The final R_1 was 0.0574 ($I > 2\sigma(I)$) and wR_2 was 0.1492 (all data). CCDC 2041259 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

1. Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015) Acta Crystallogr C71: 3-8.

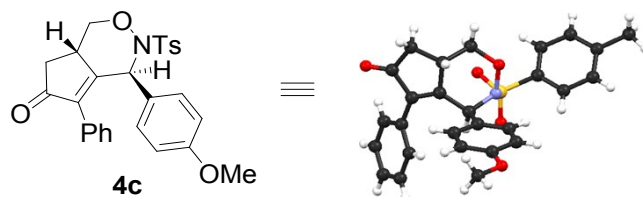
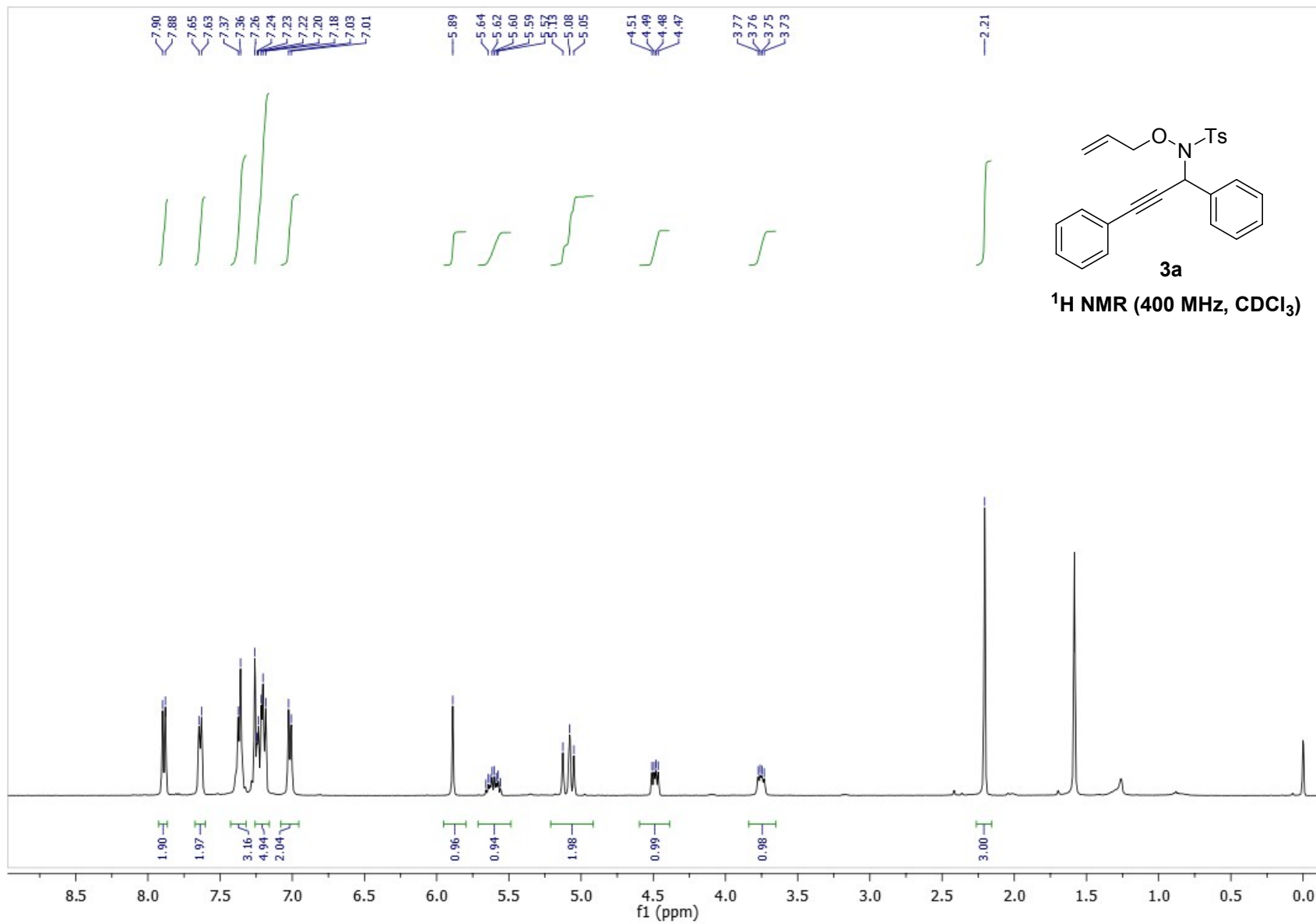
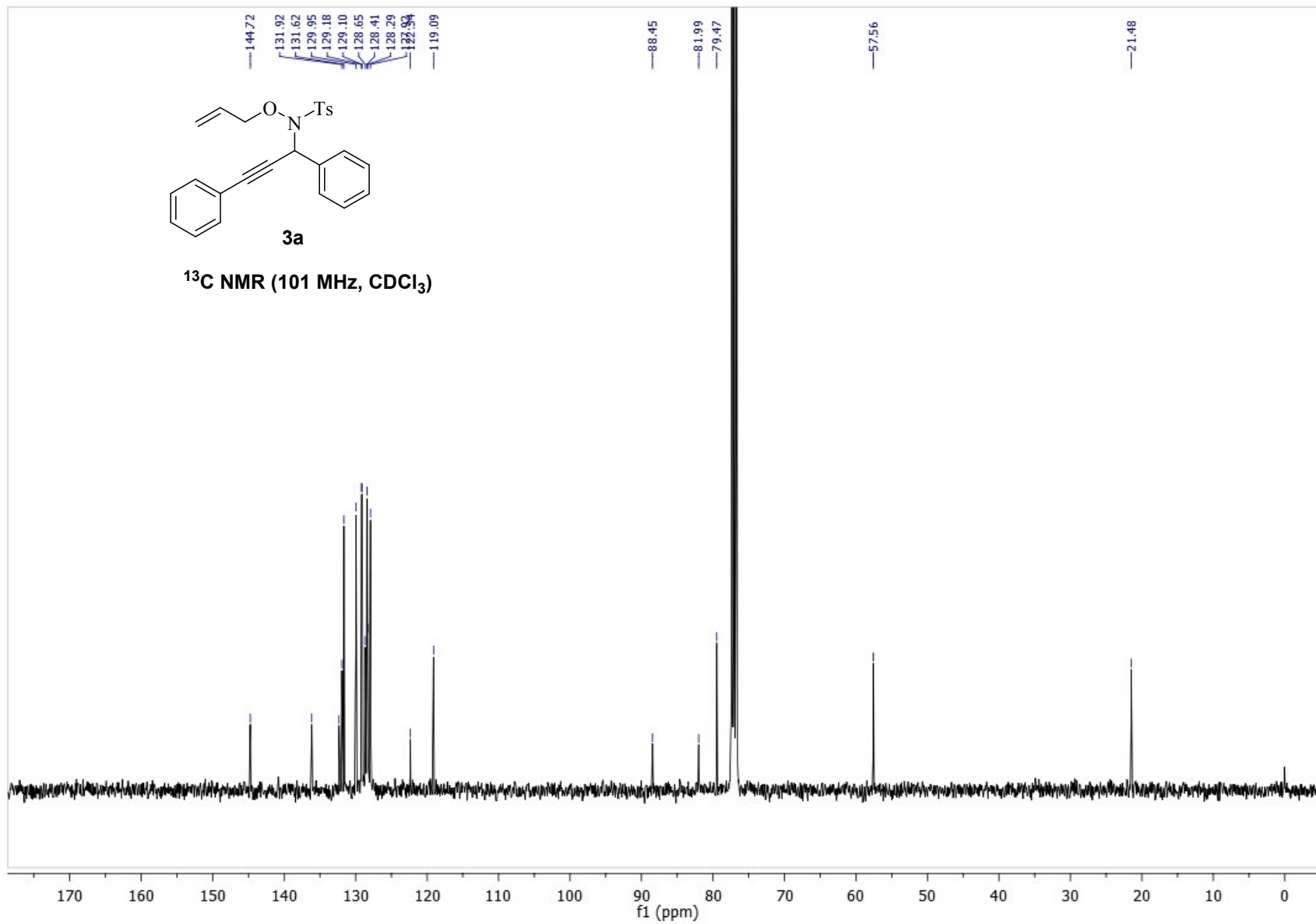
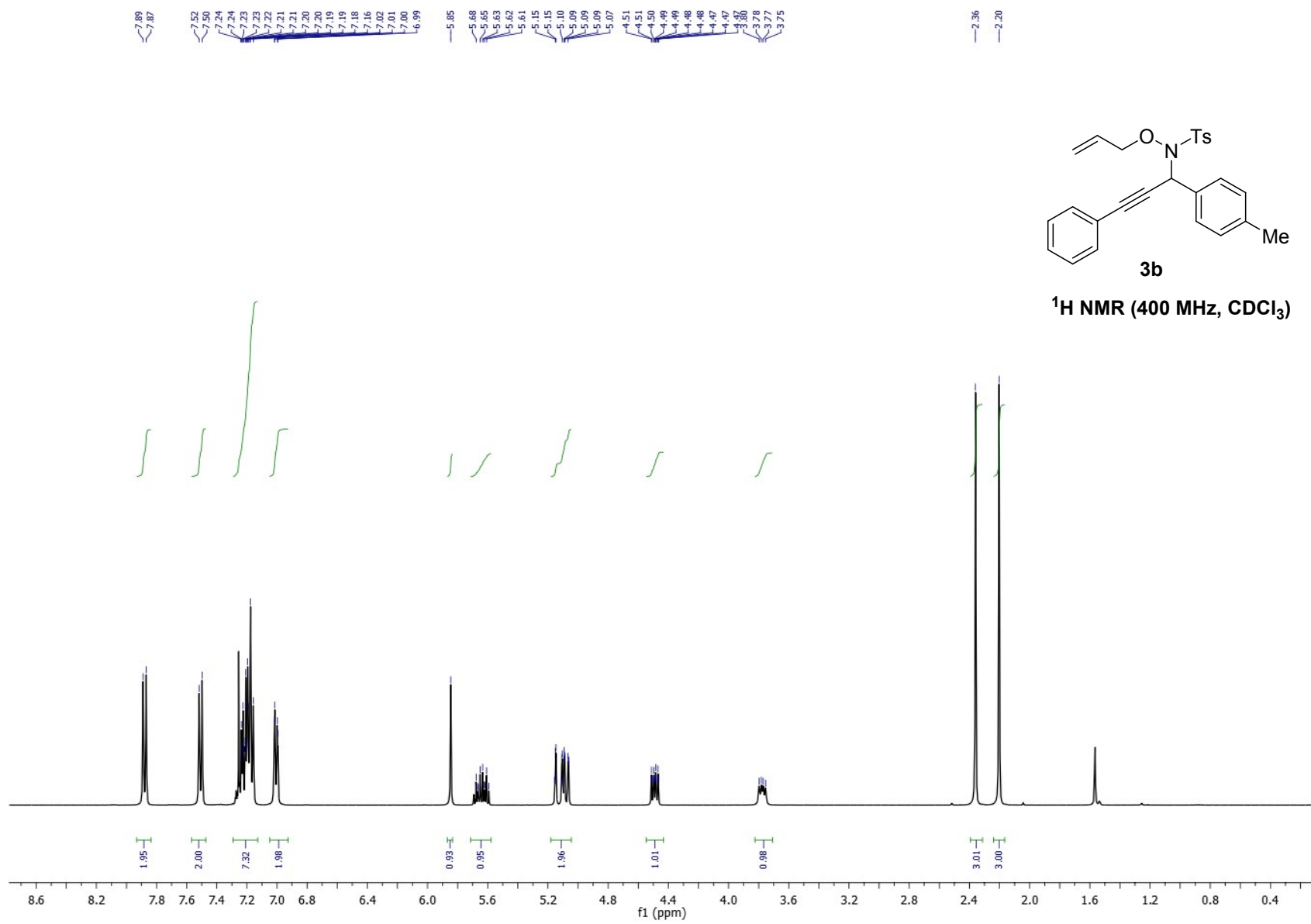


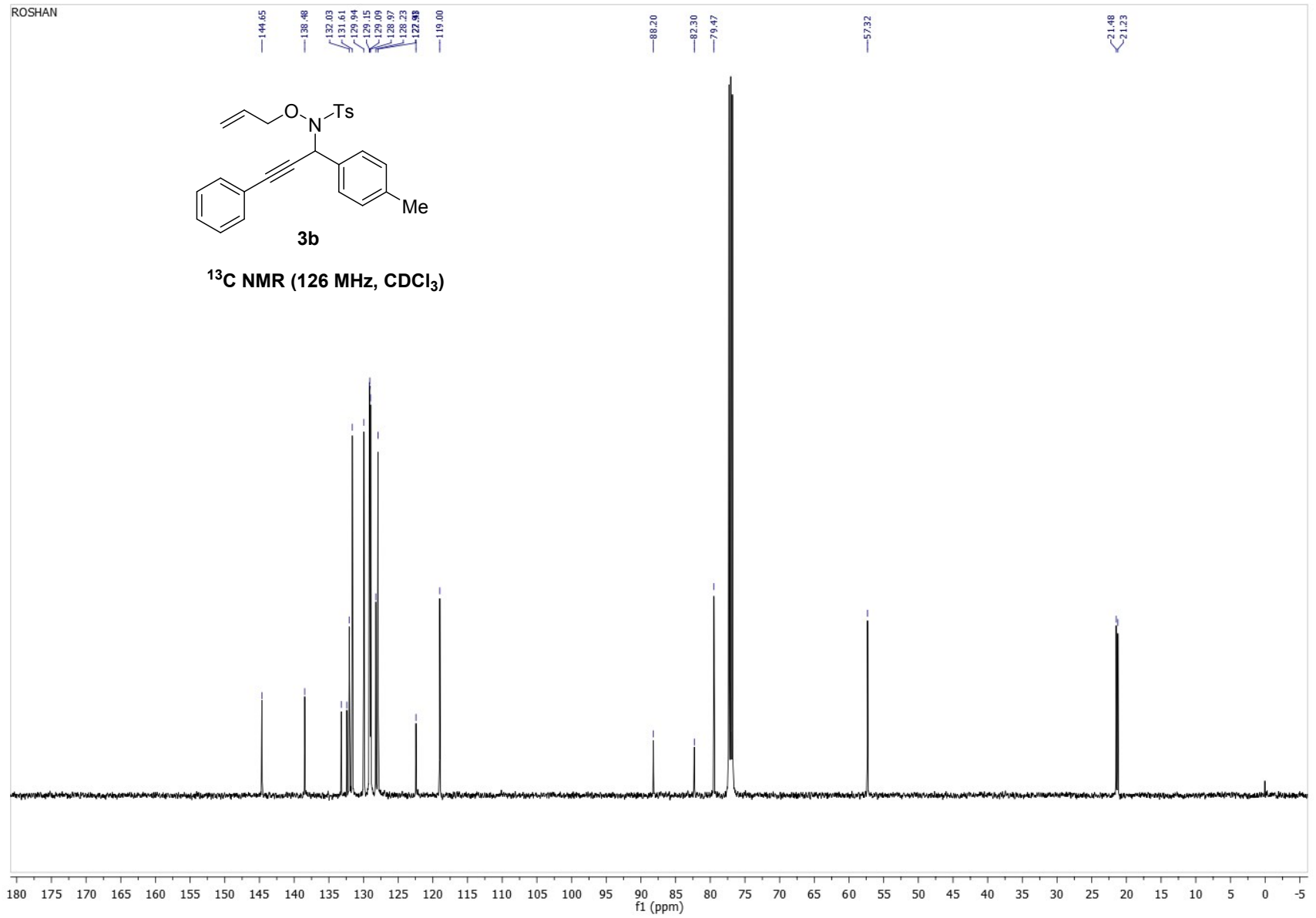
Figure S1. A view of **4c**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

^1H and ^{13}C NMR spectra of compounds

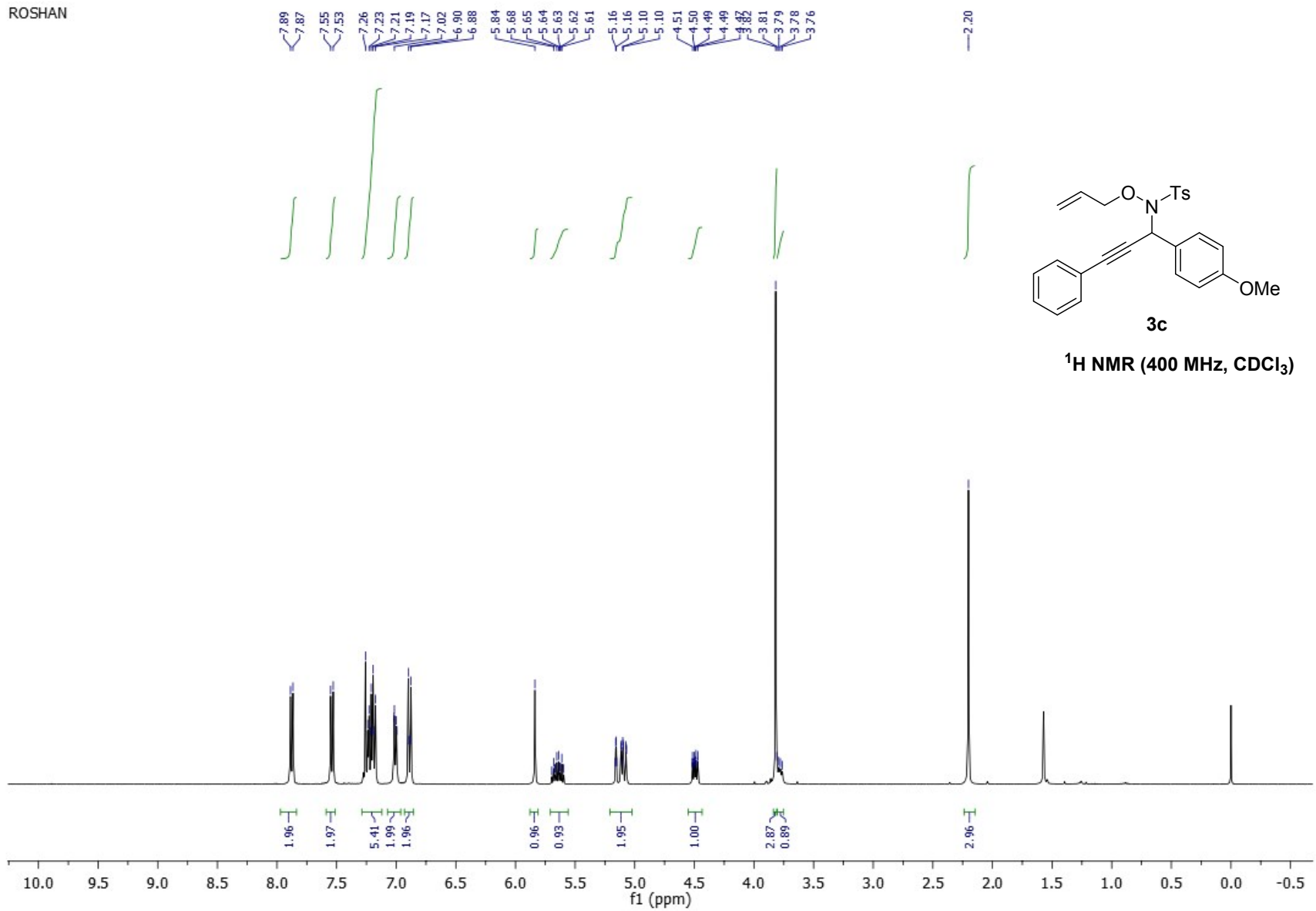


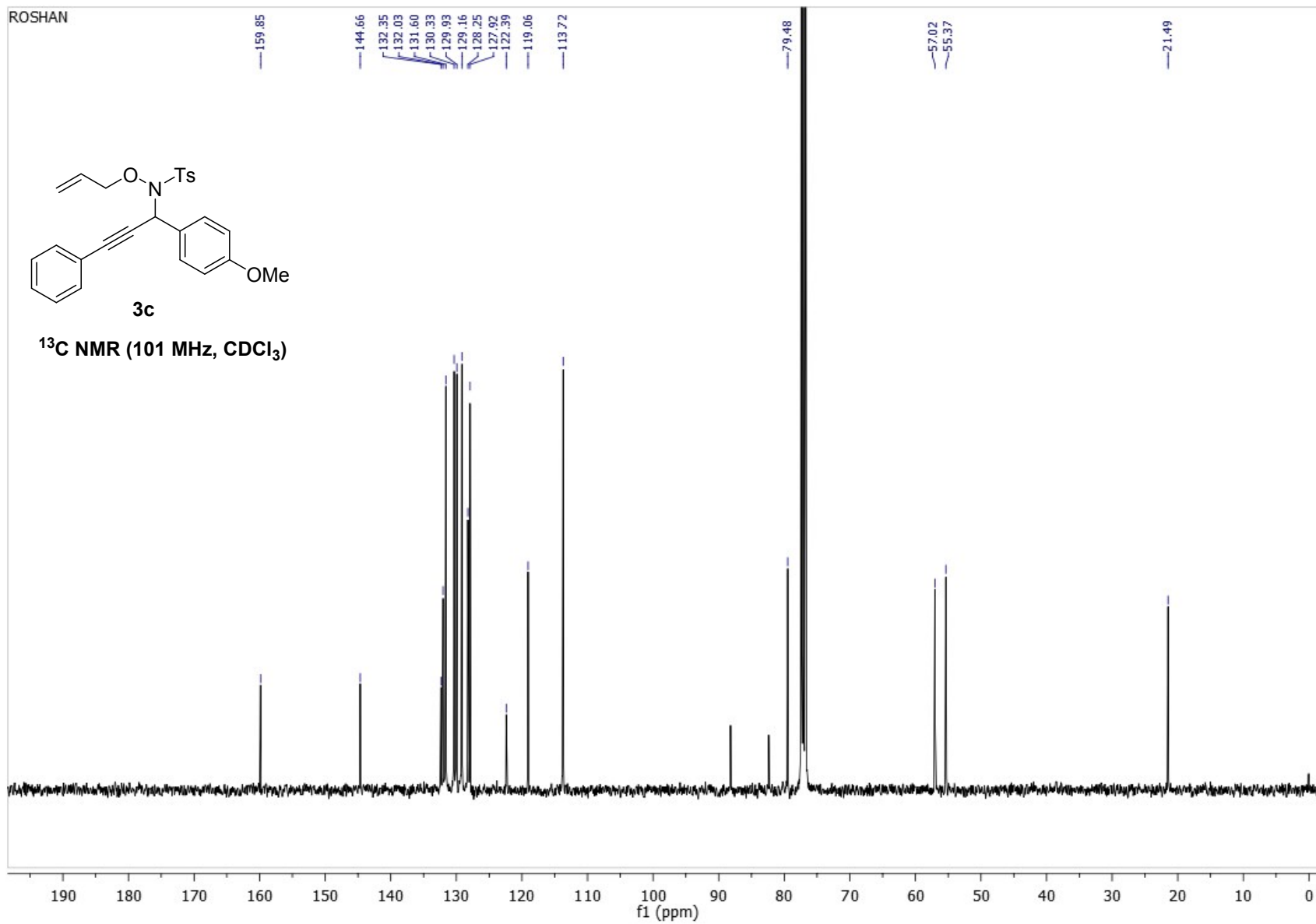


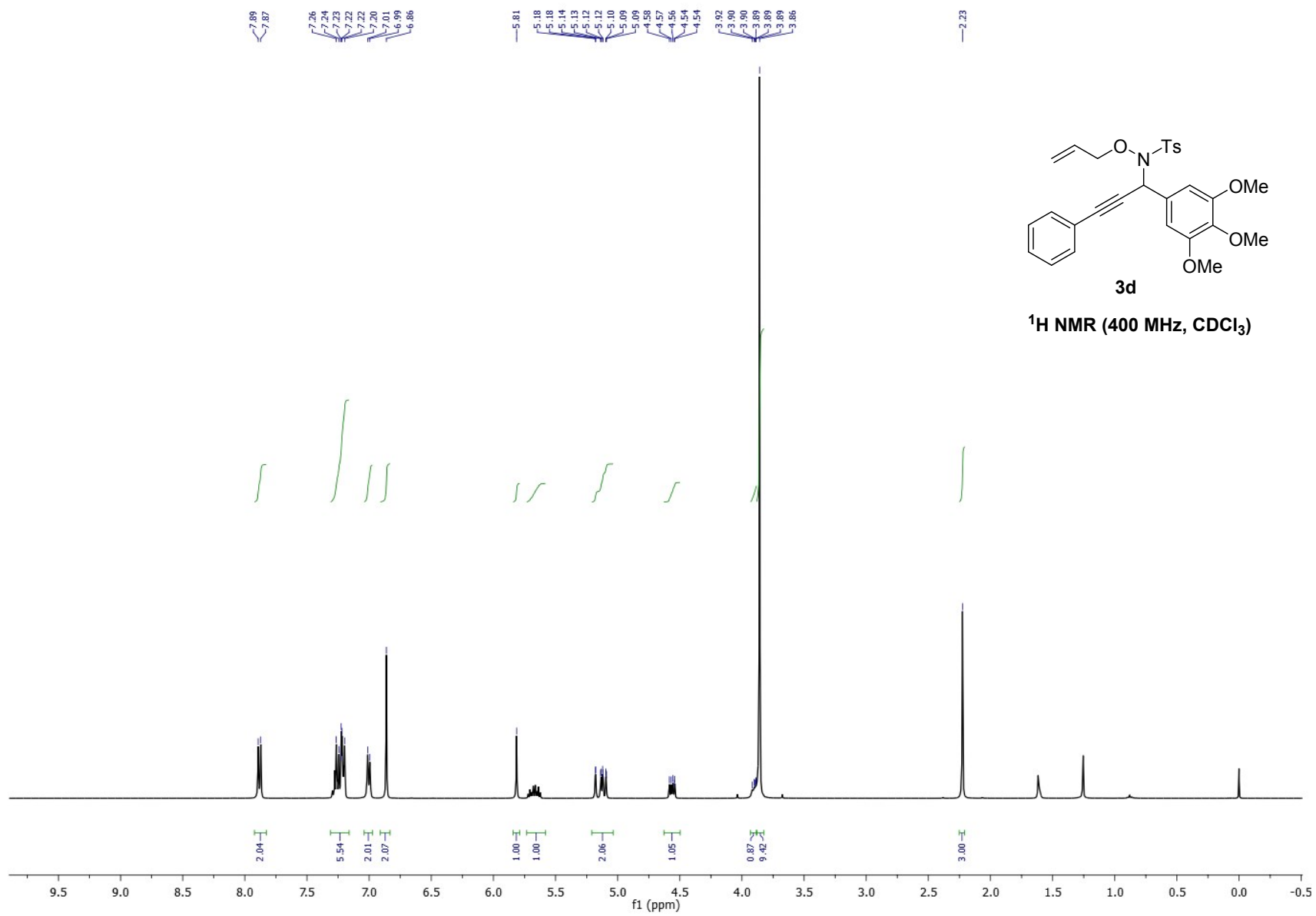




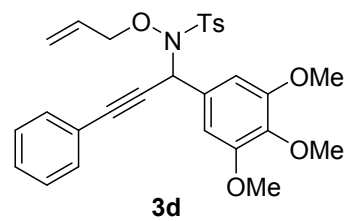
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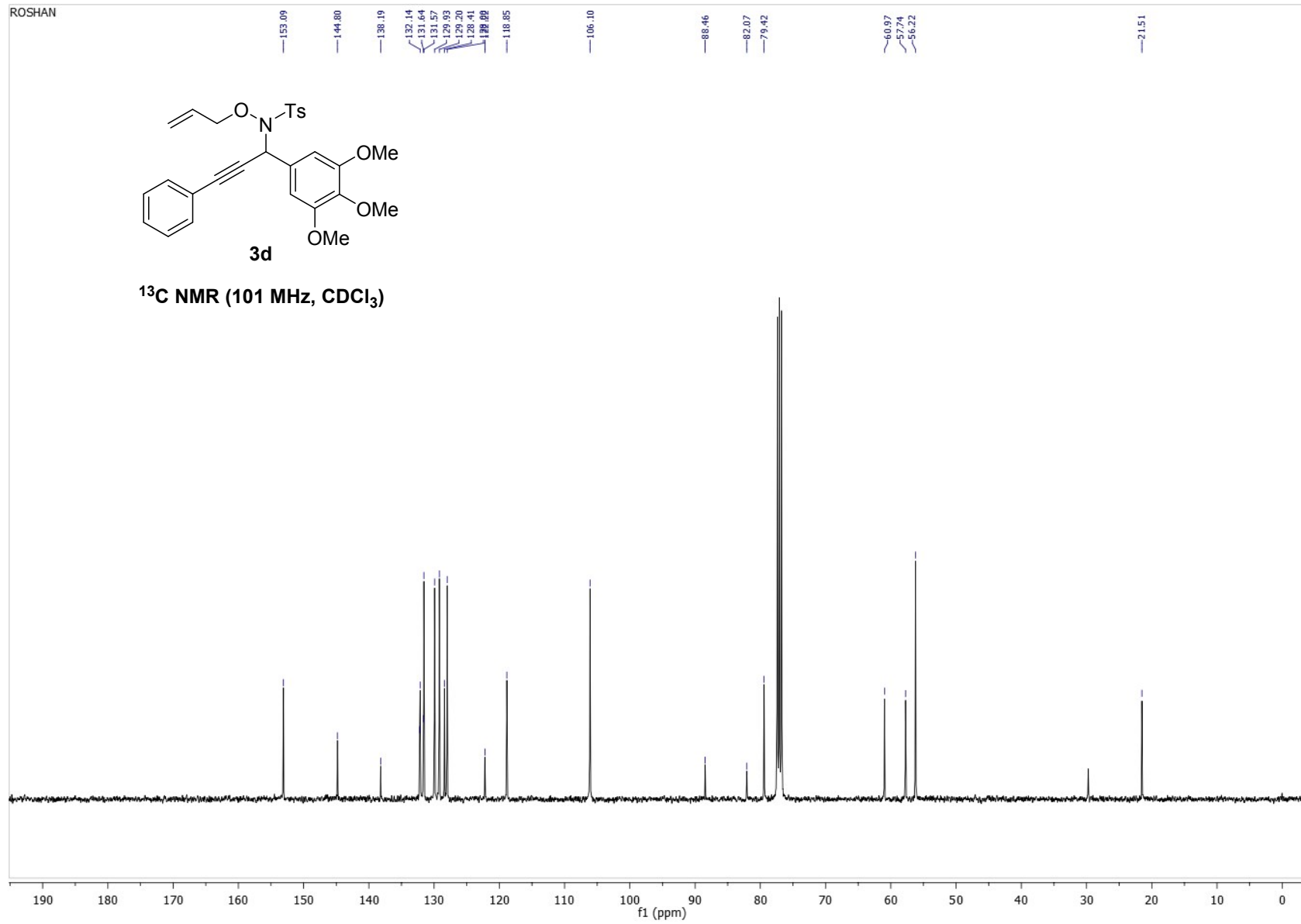


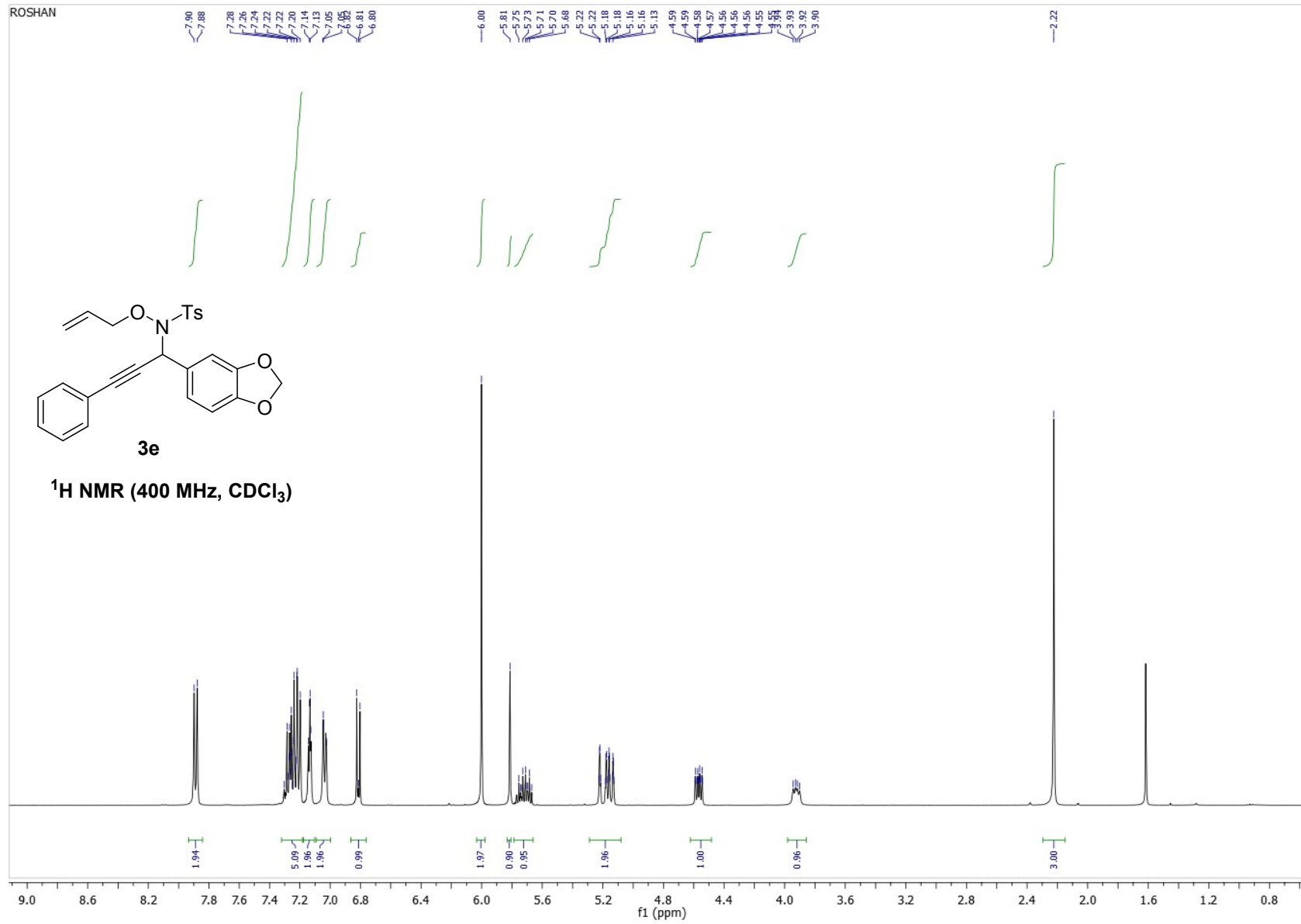


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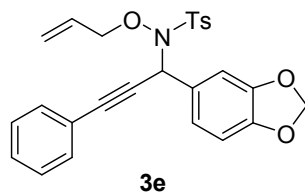


^{13}C NMR (101 MHz, CDCl_3)

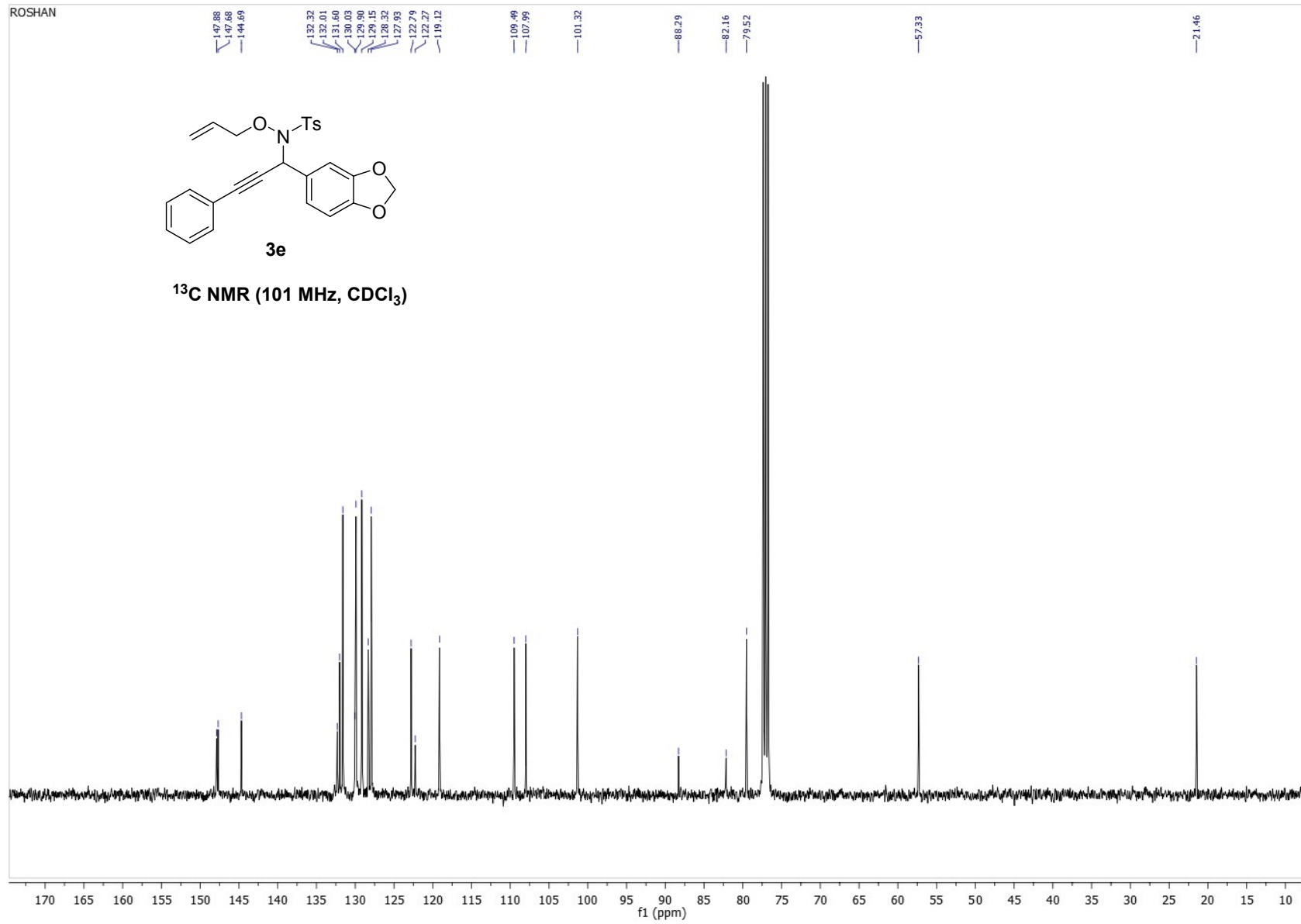


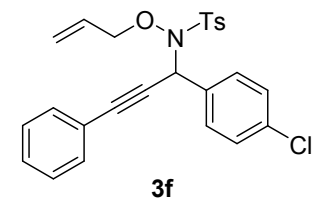
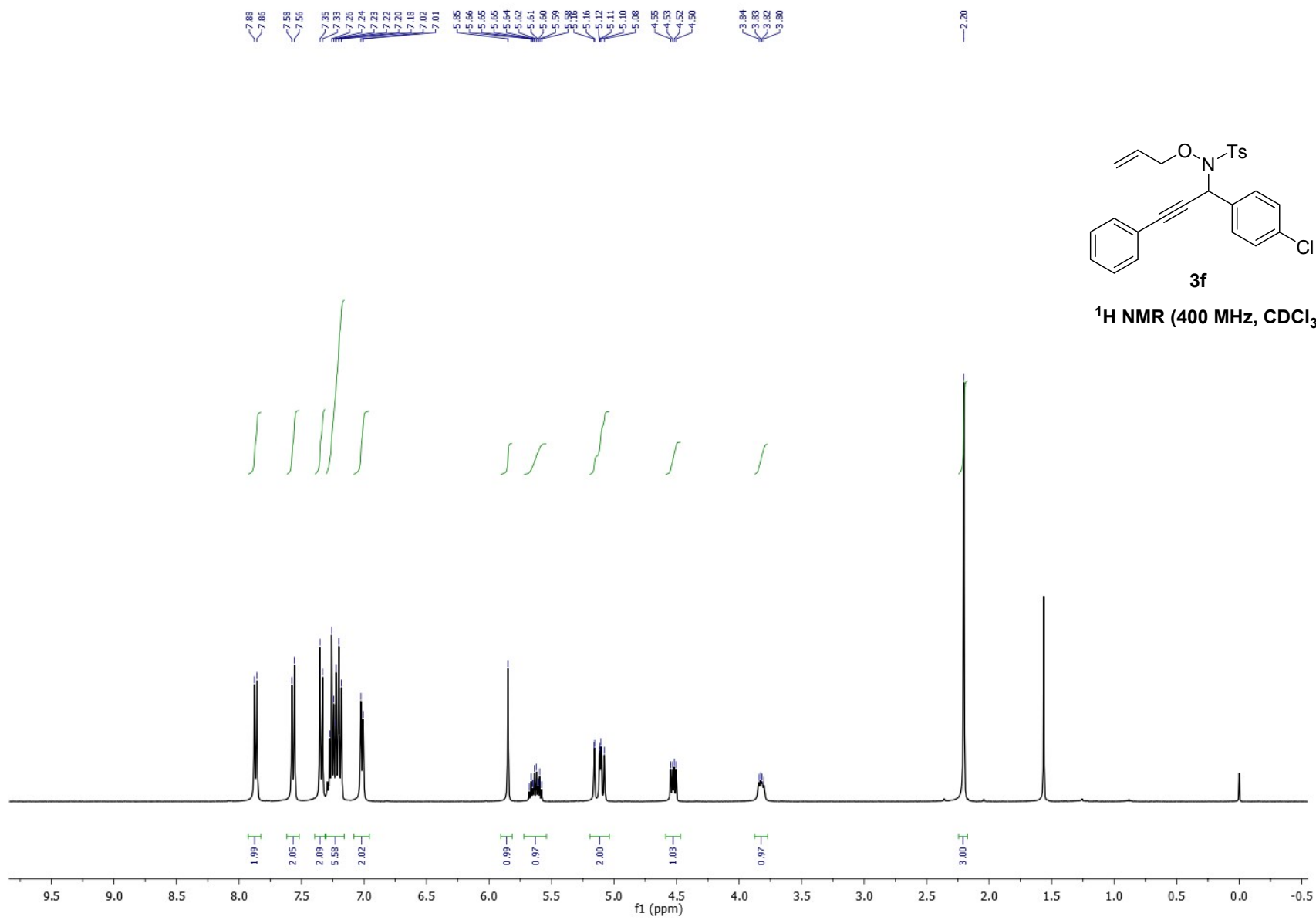


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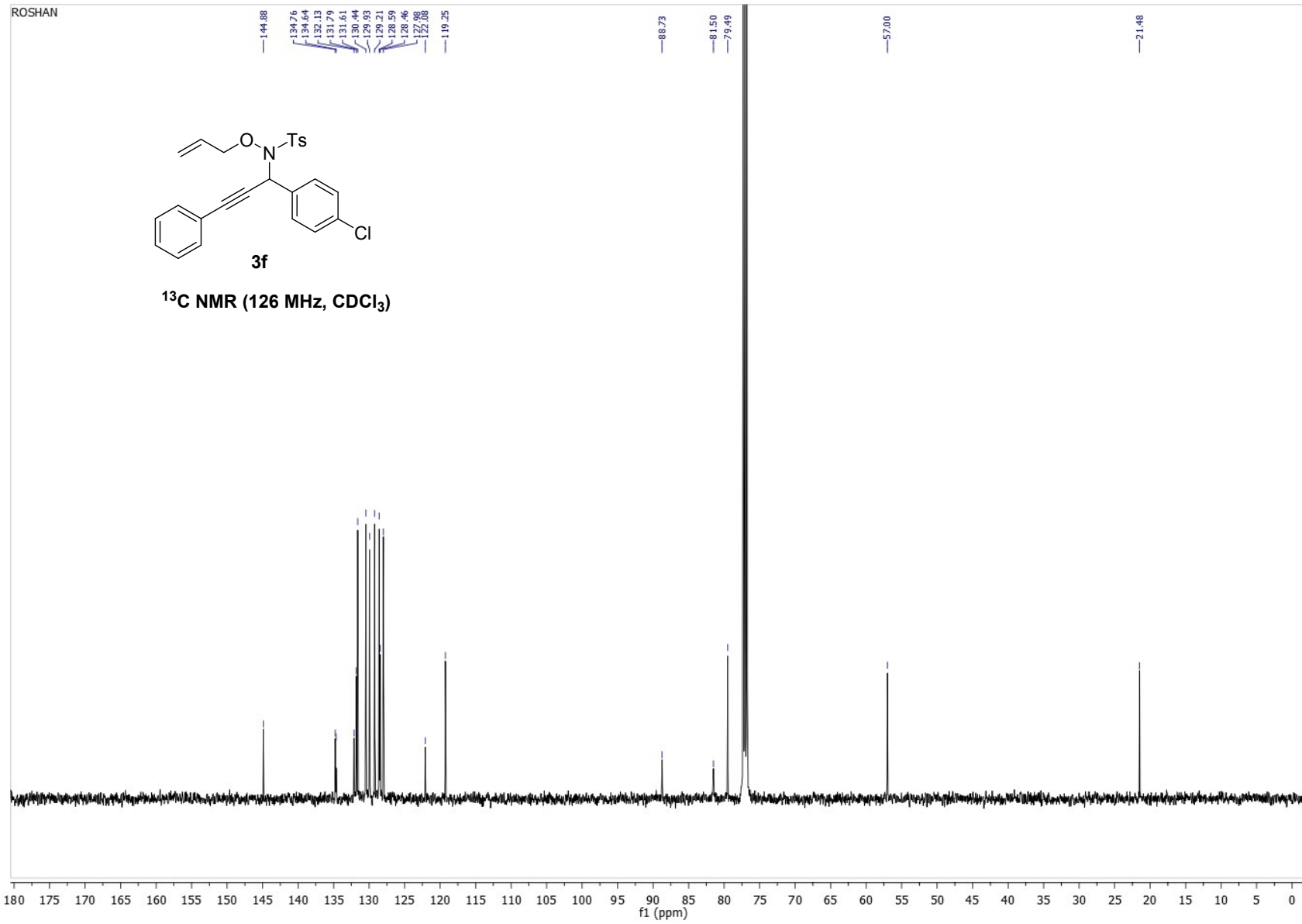


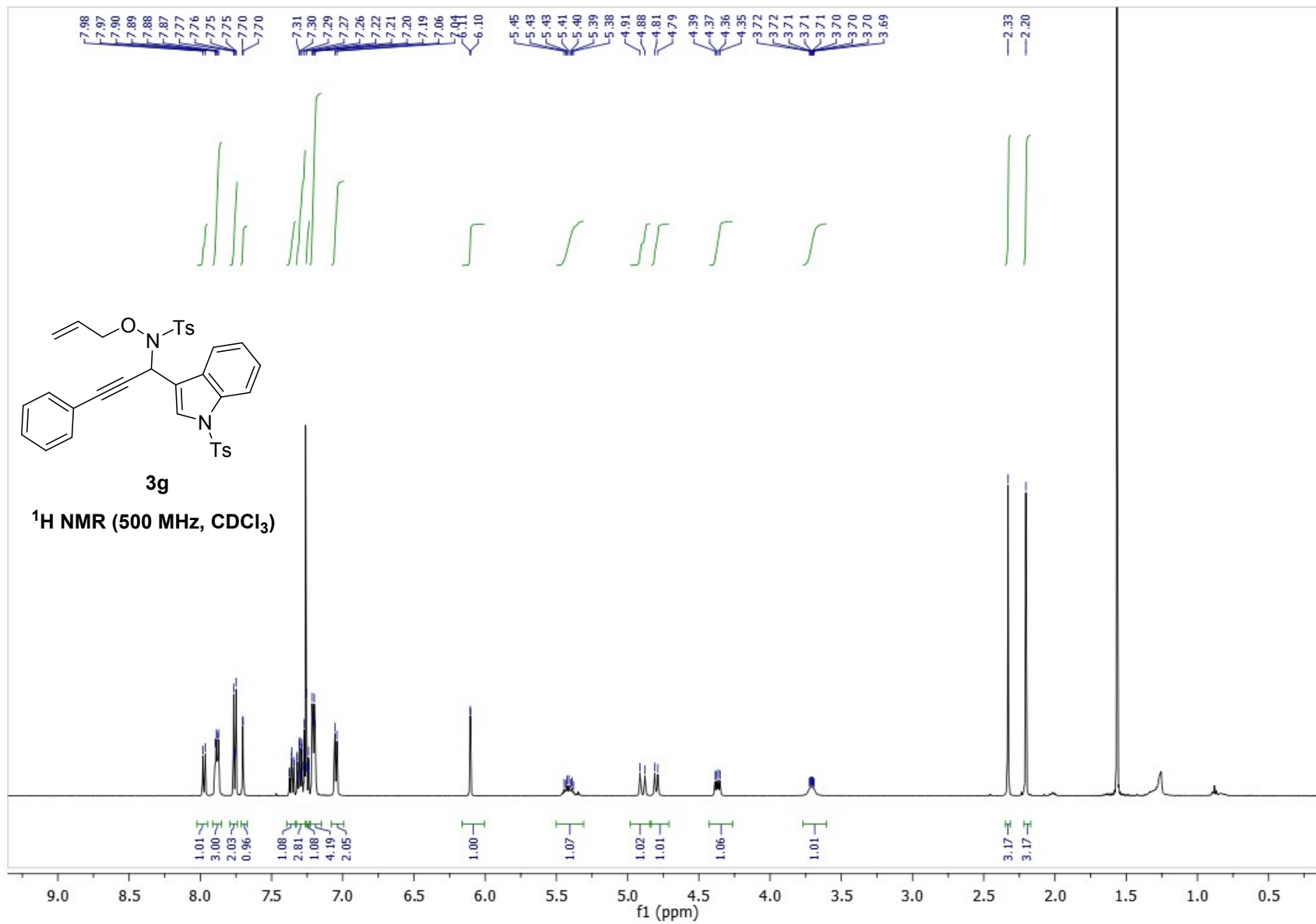
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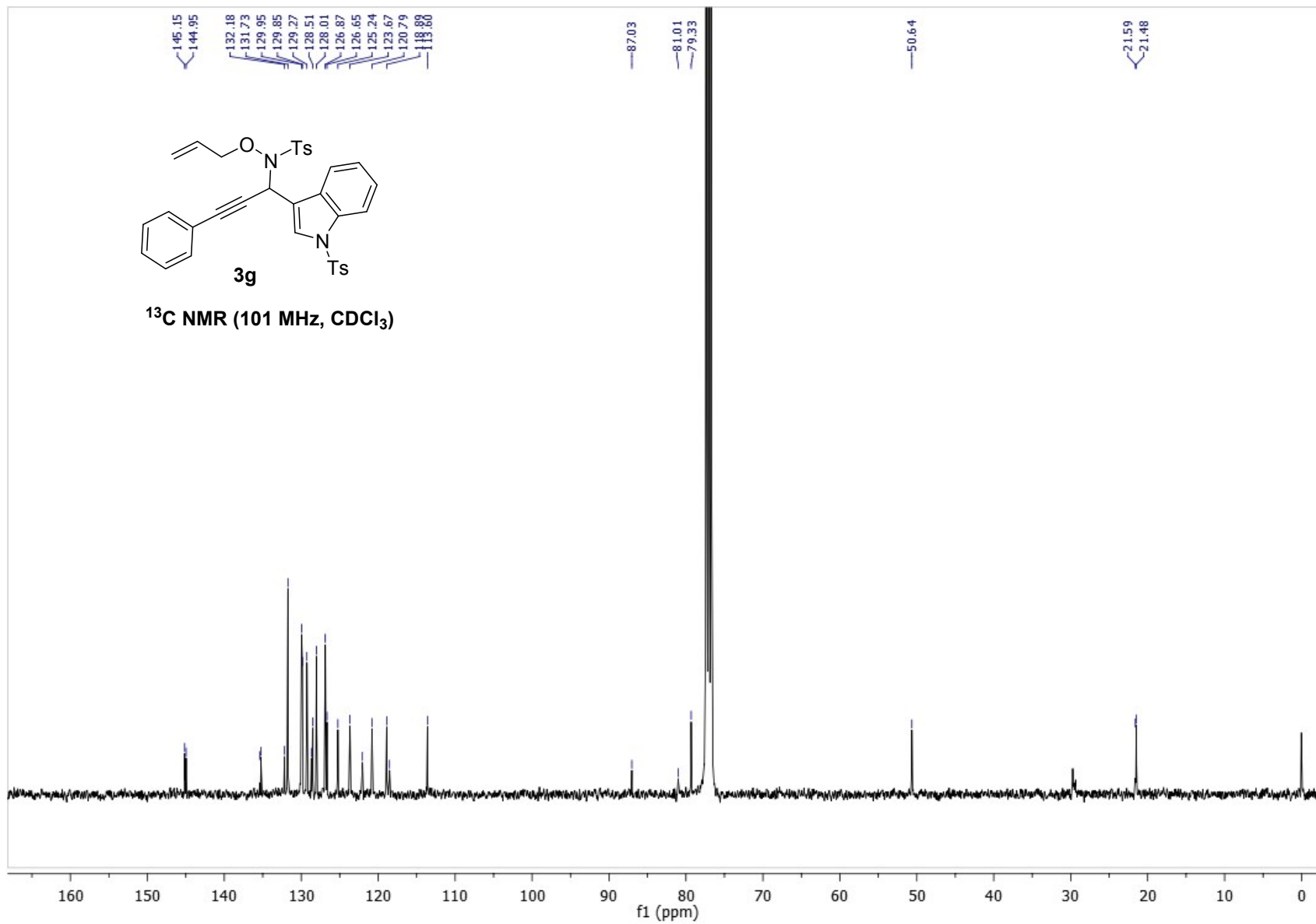


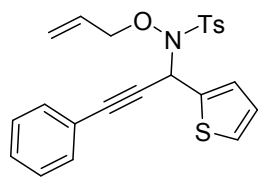


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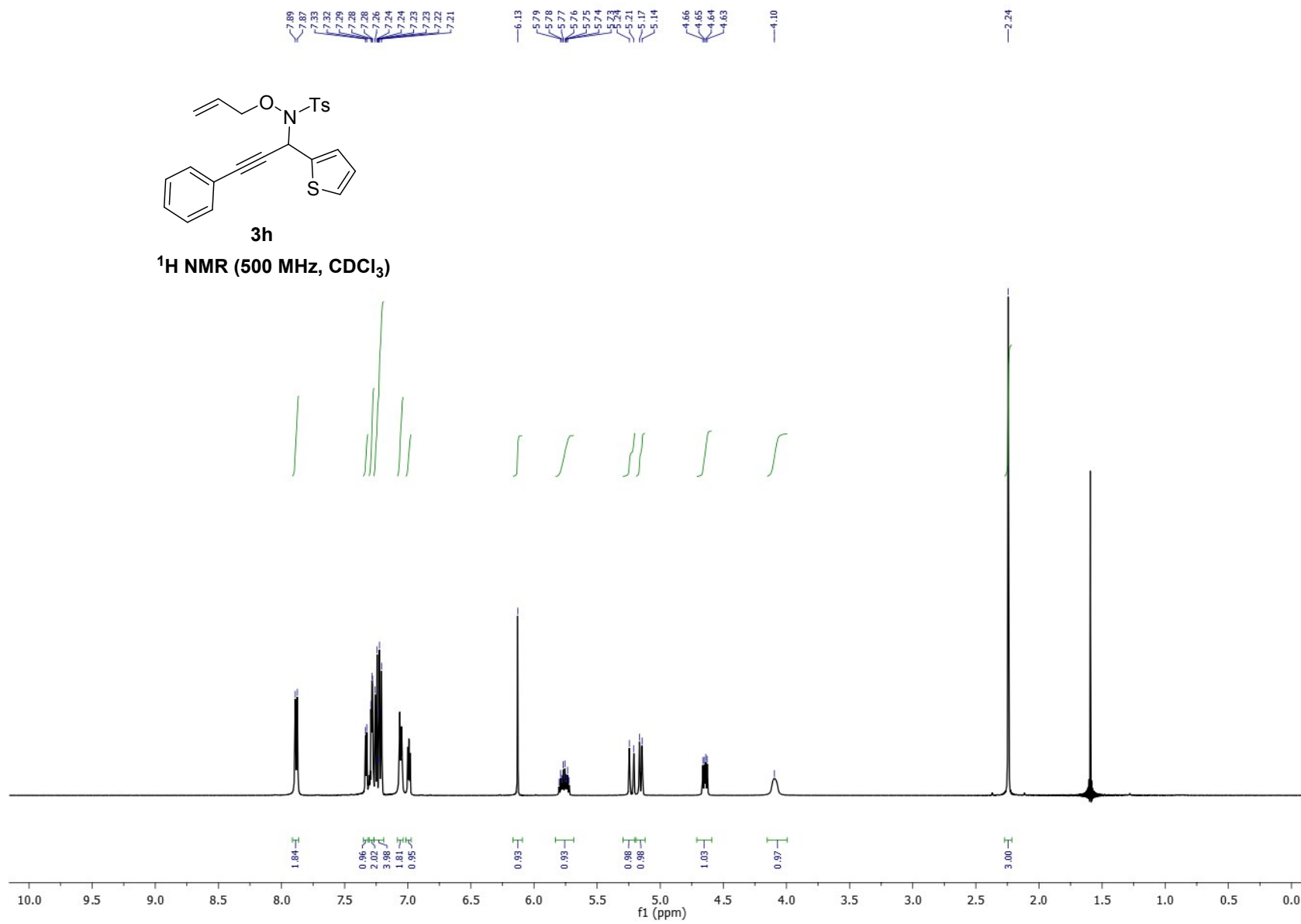


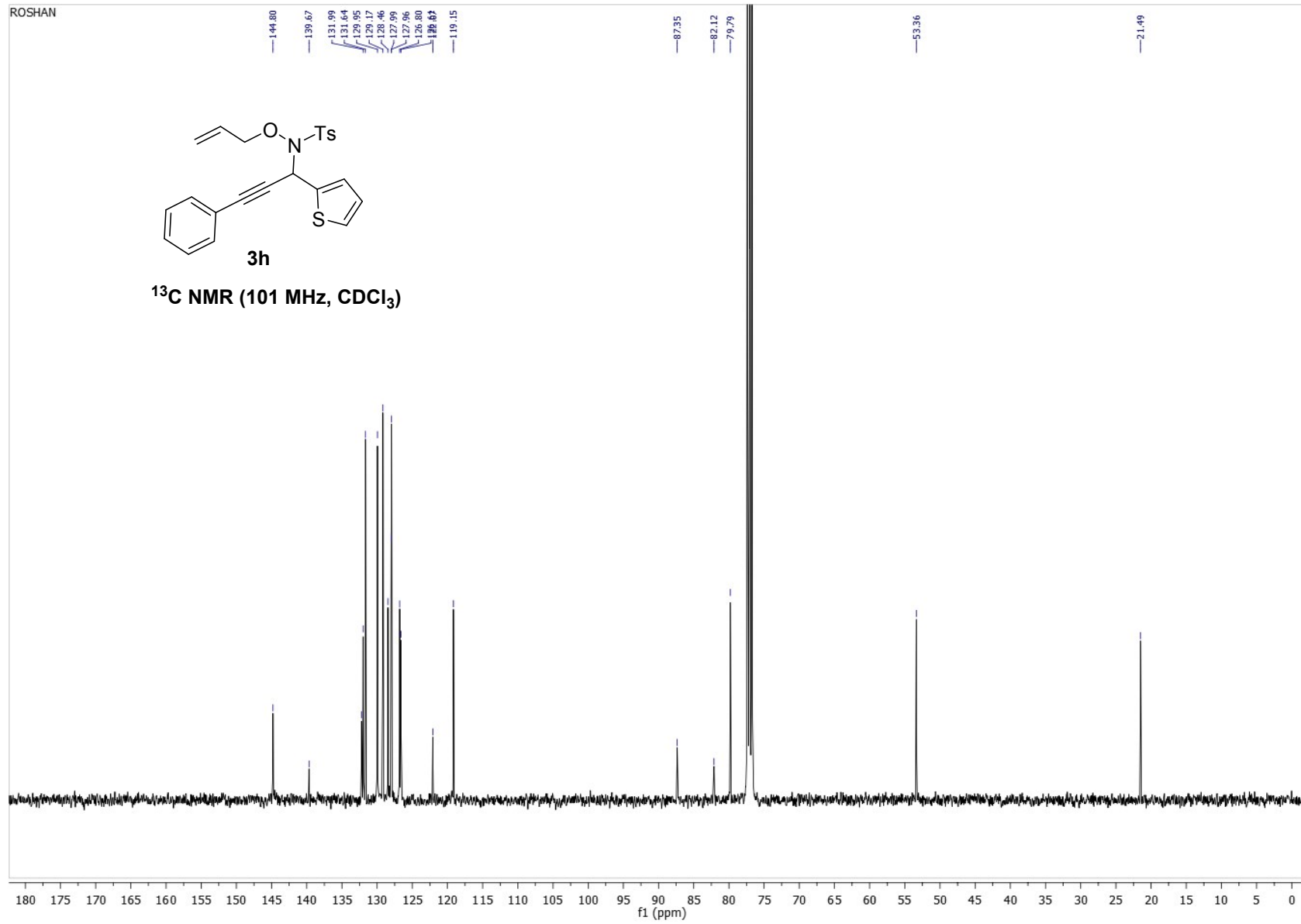


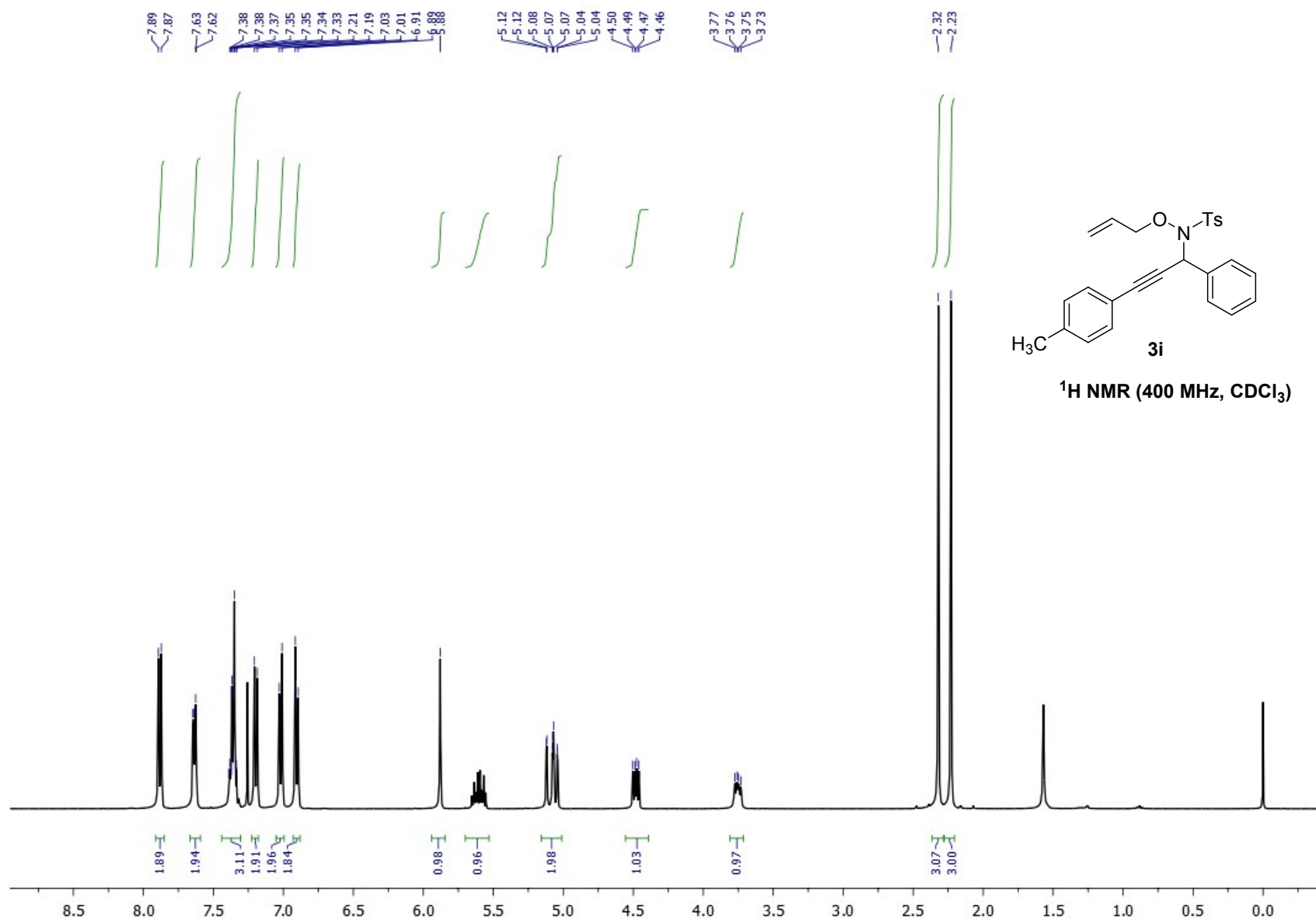


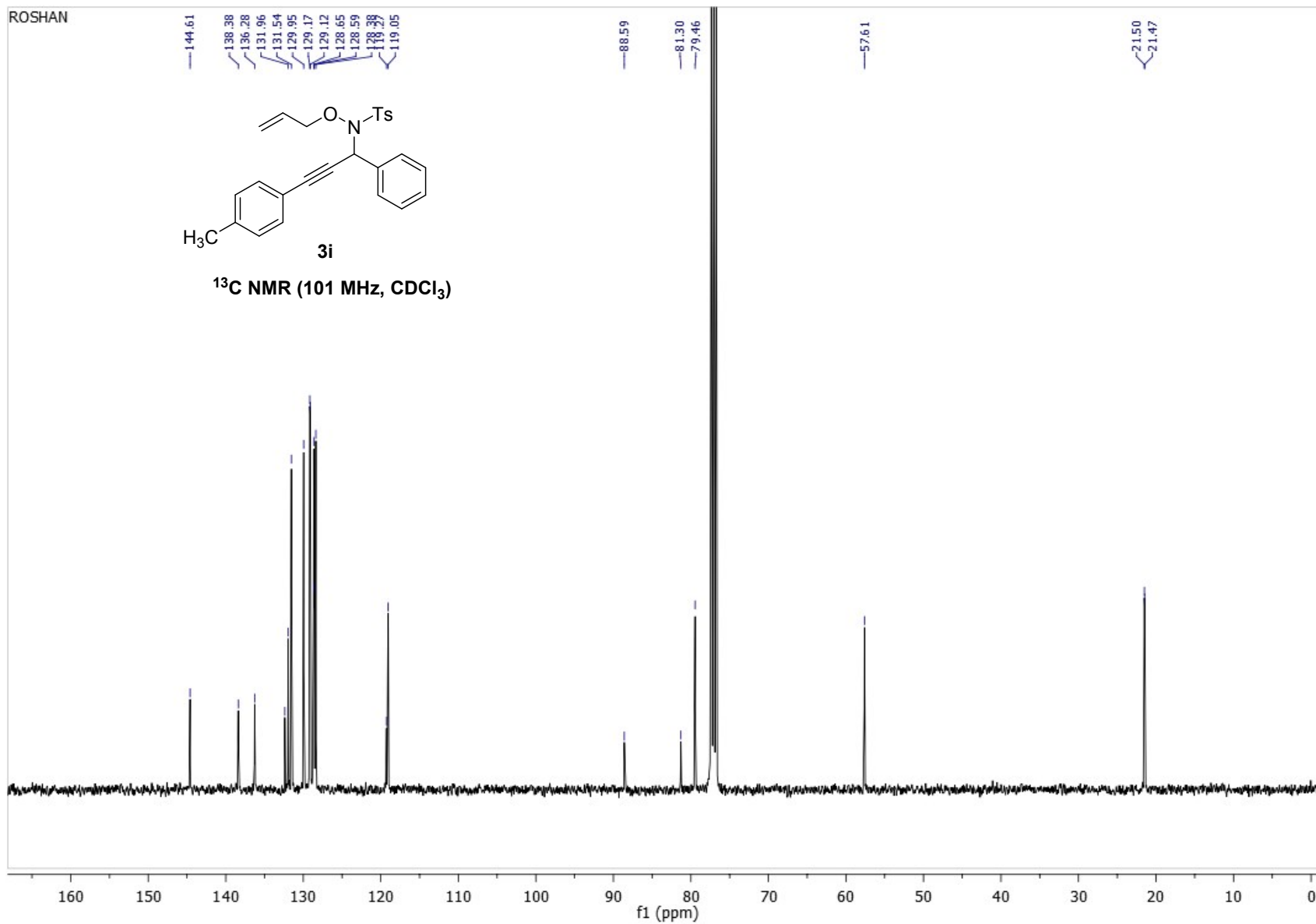
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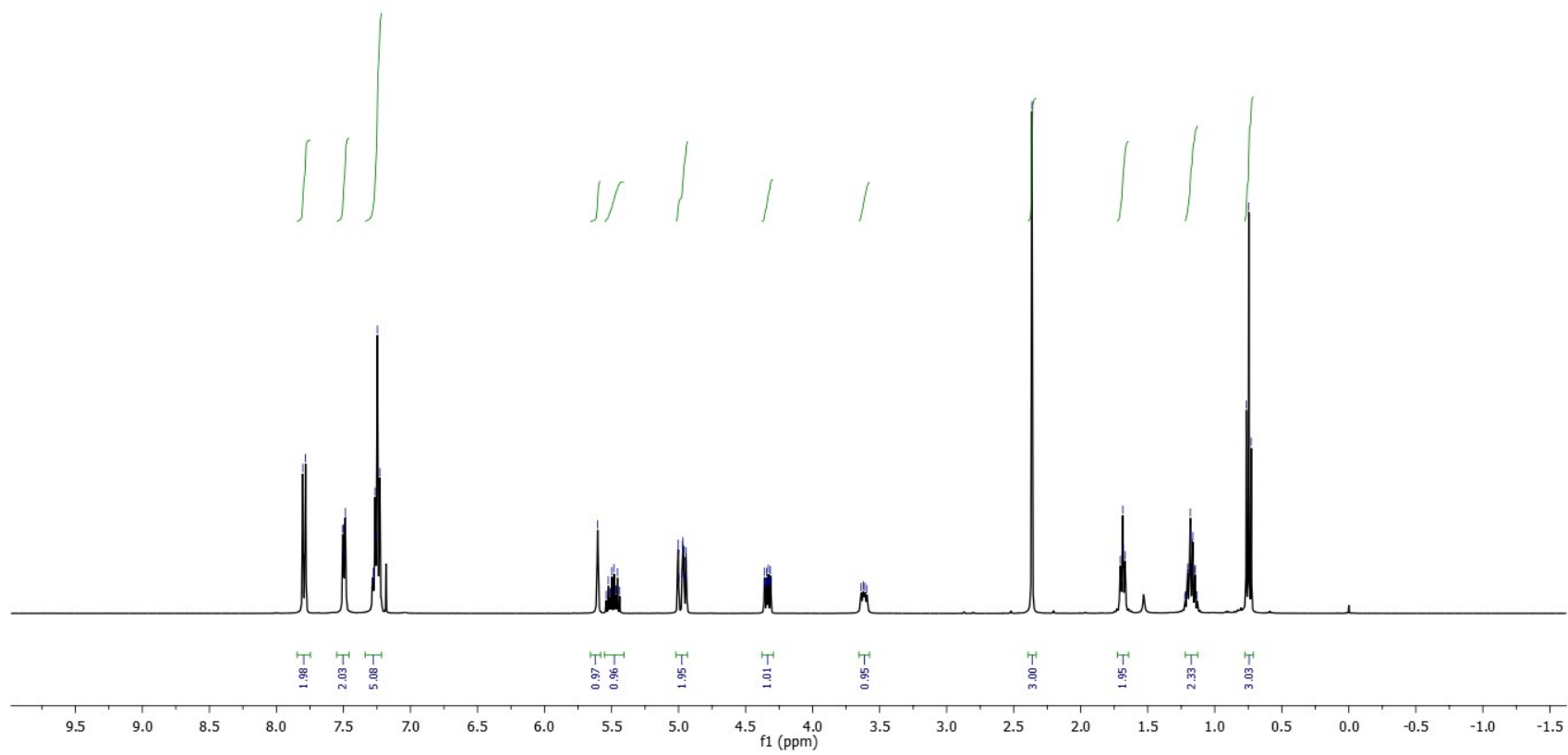
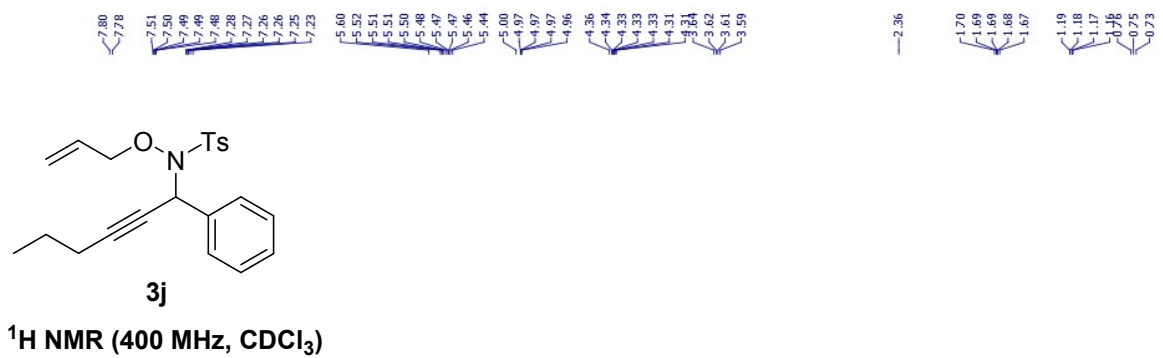
¹H NMR (500 MHz, CDCl₃)

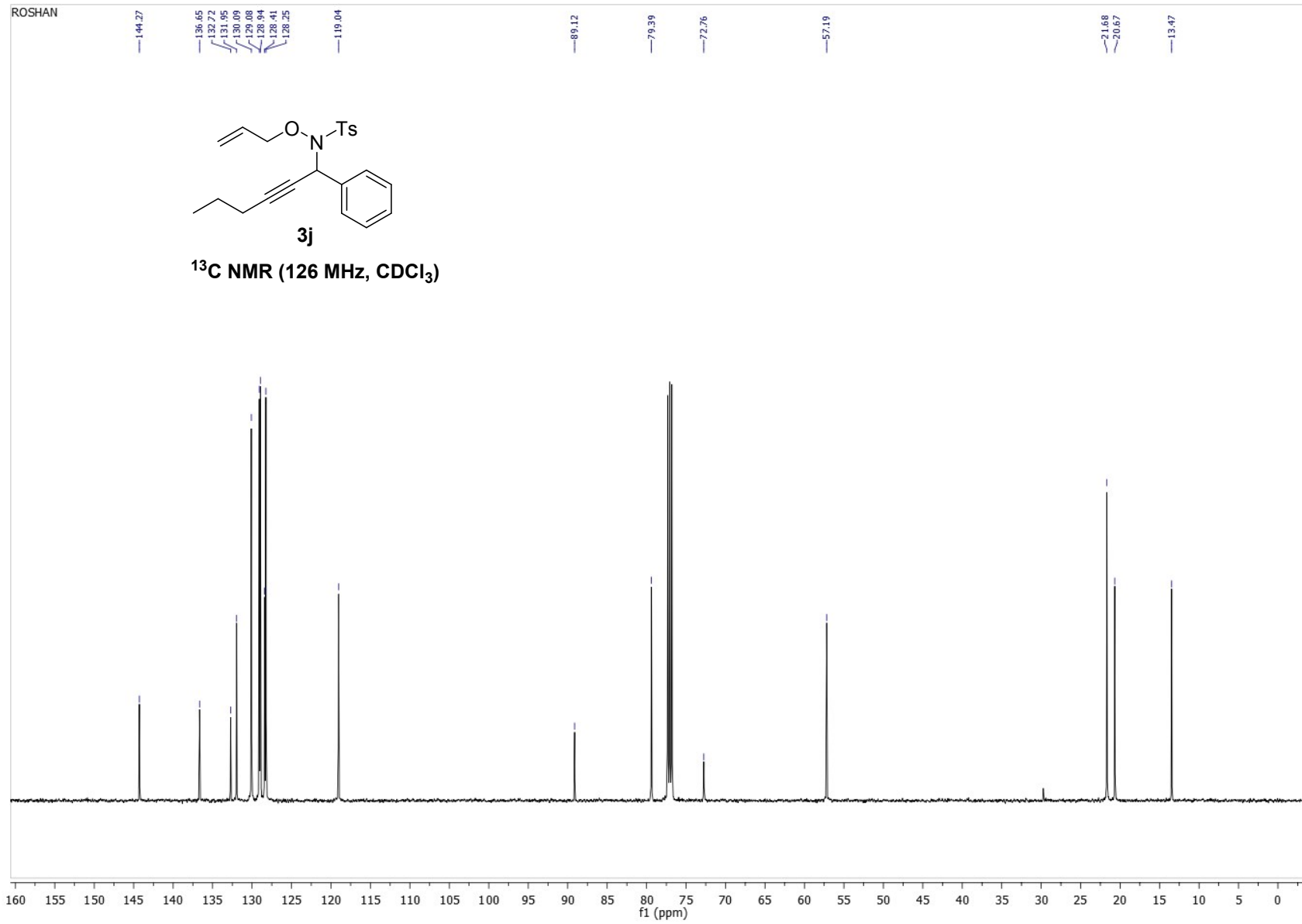


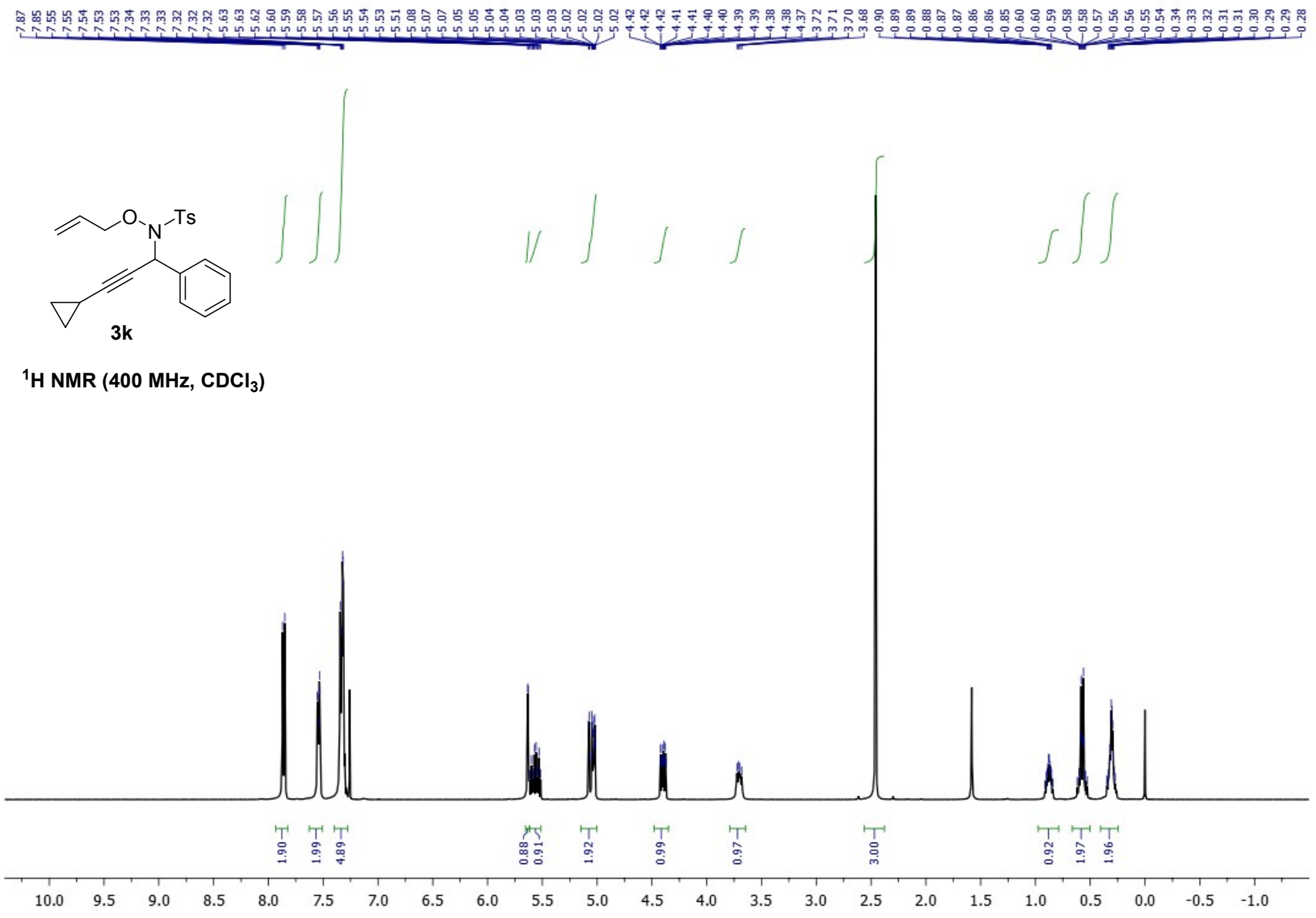


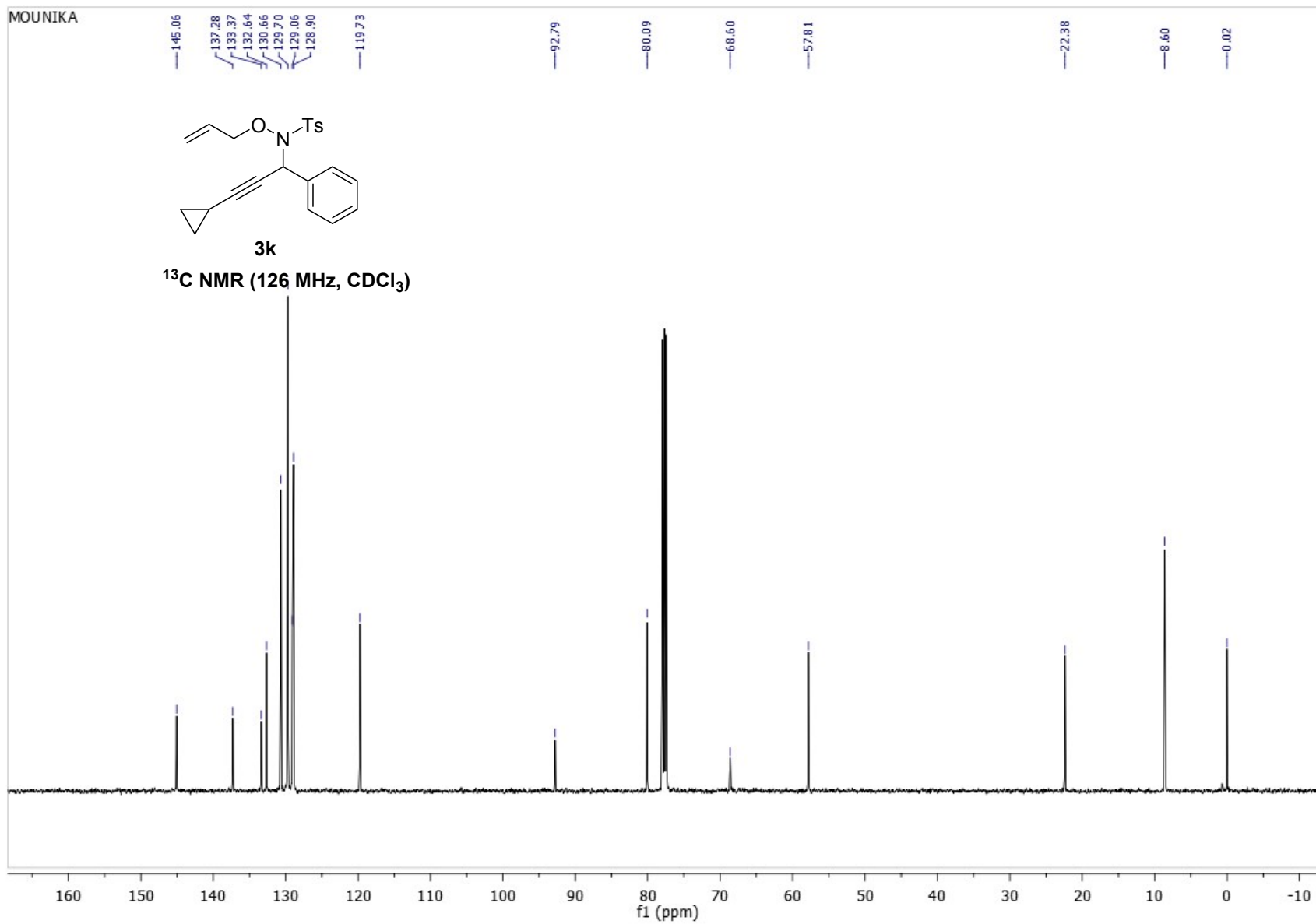


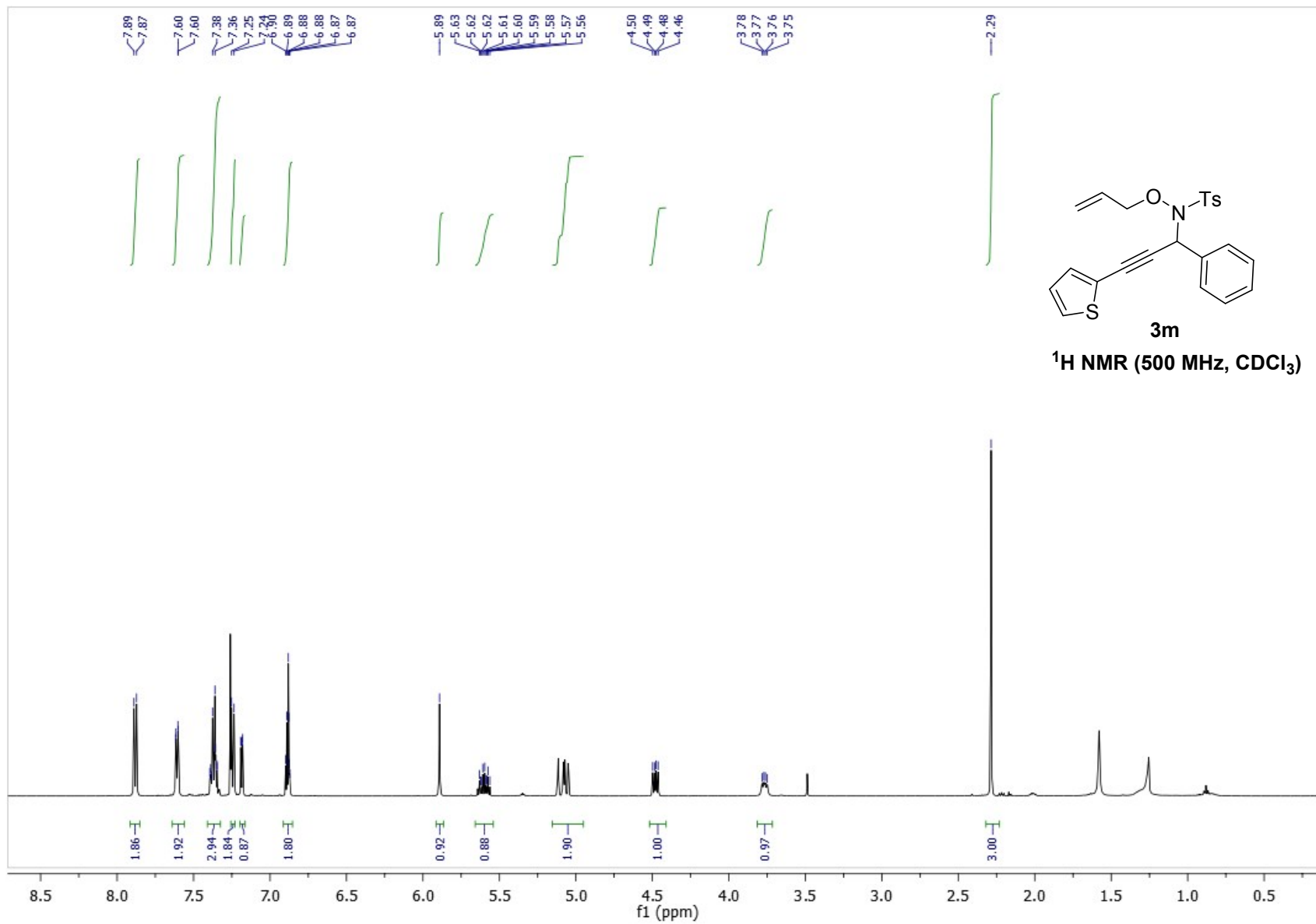


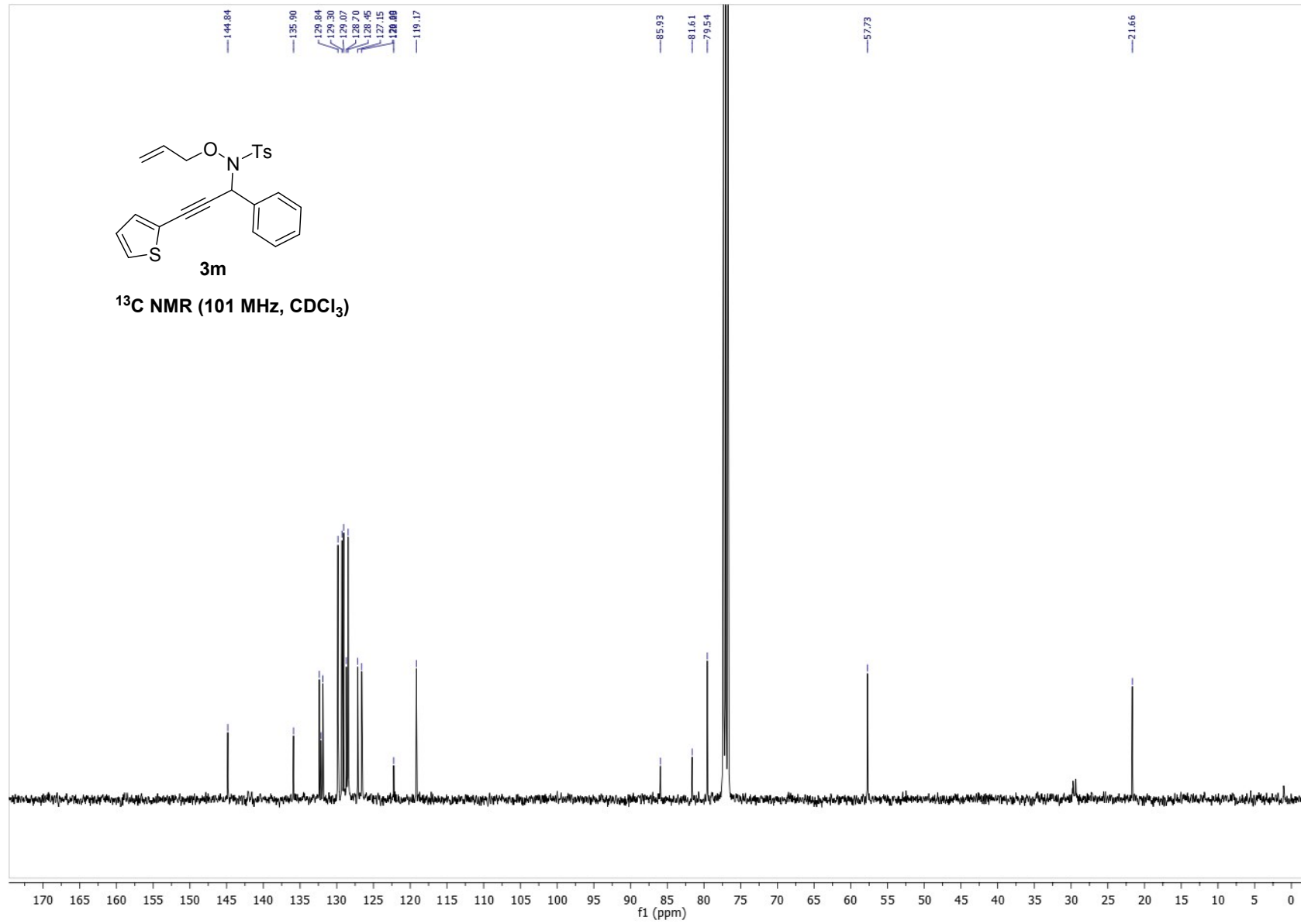


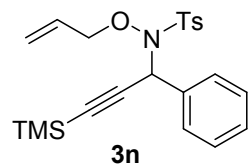




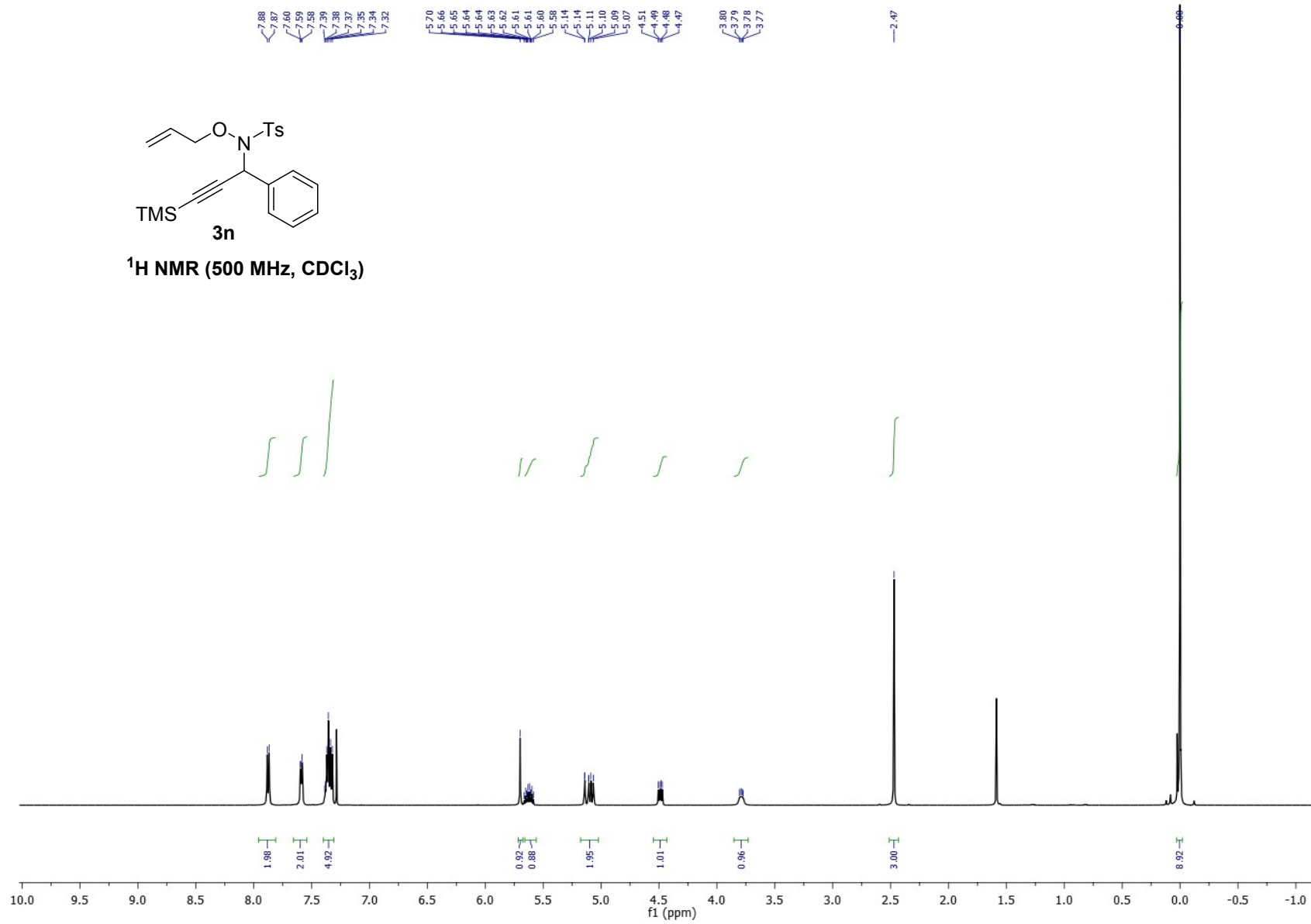


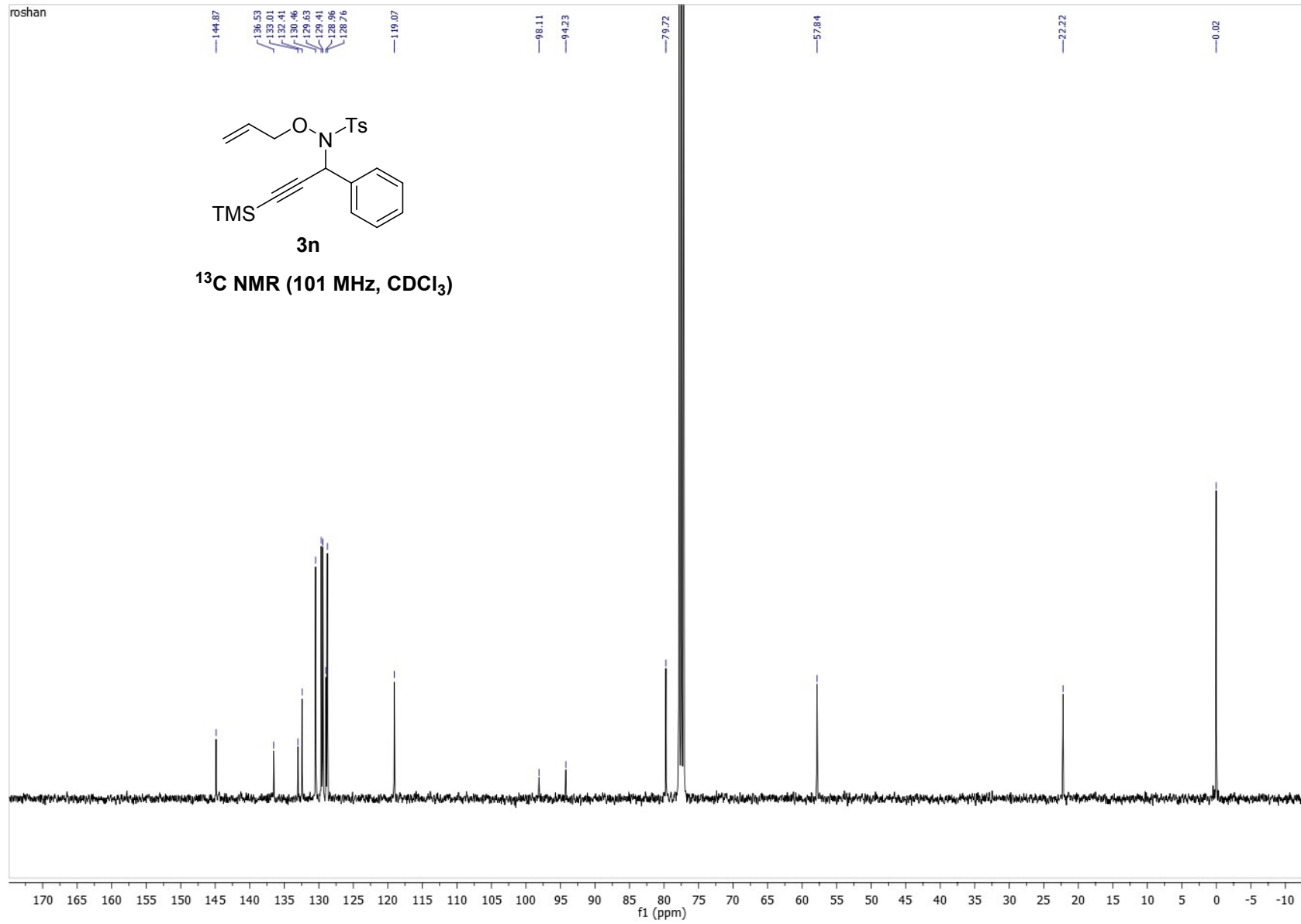


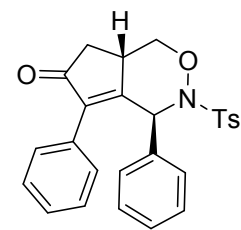
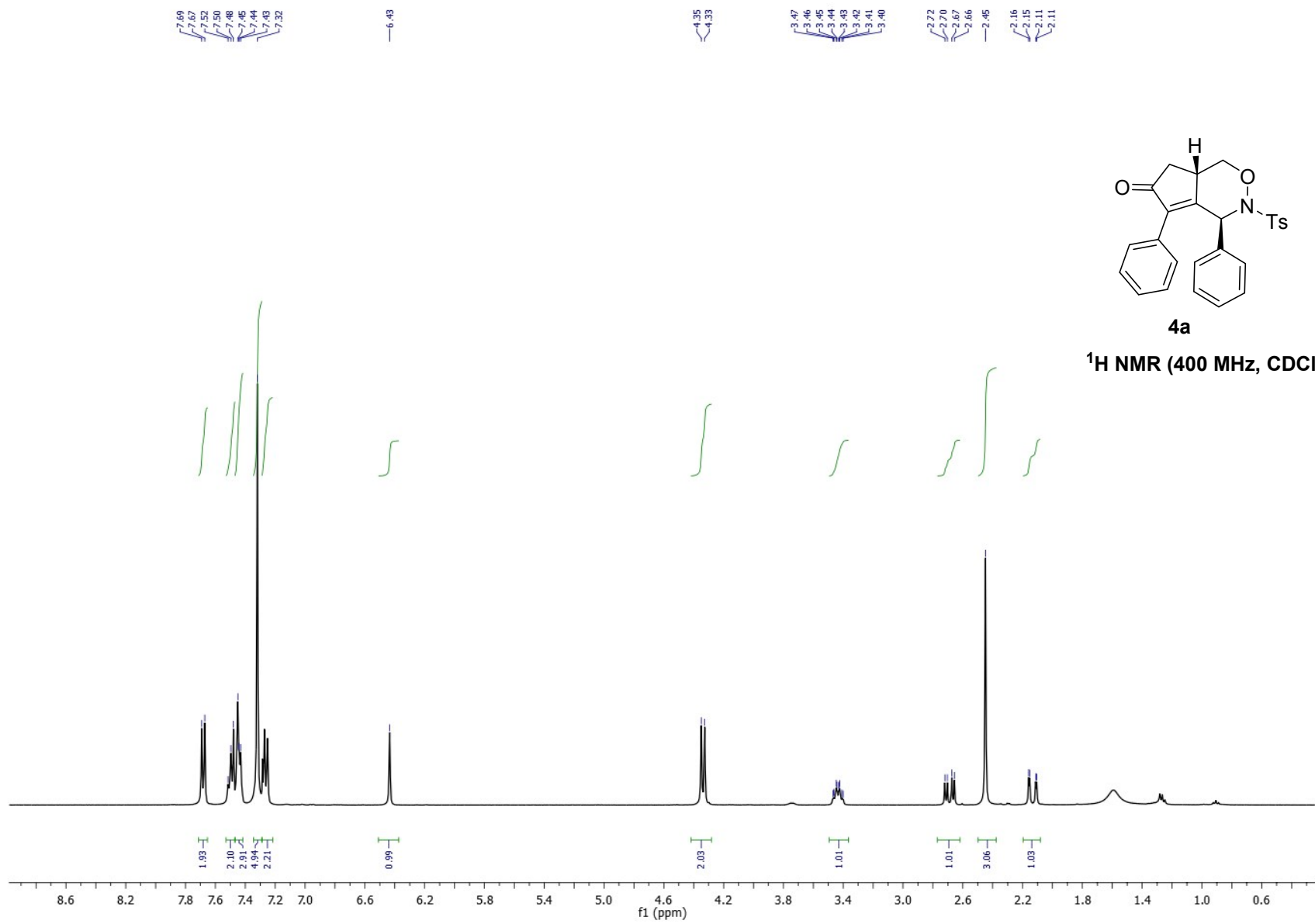




¹H NMR (500 MHz, CDCl₃)

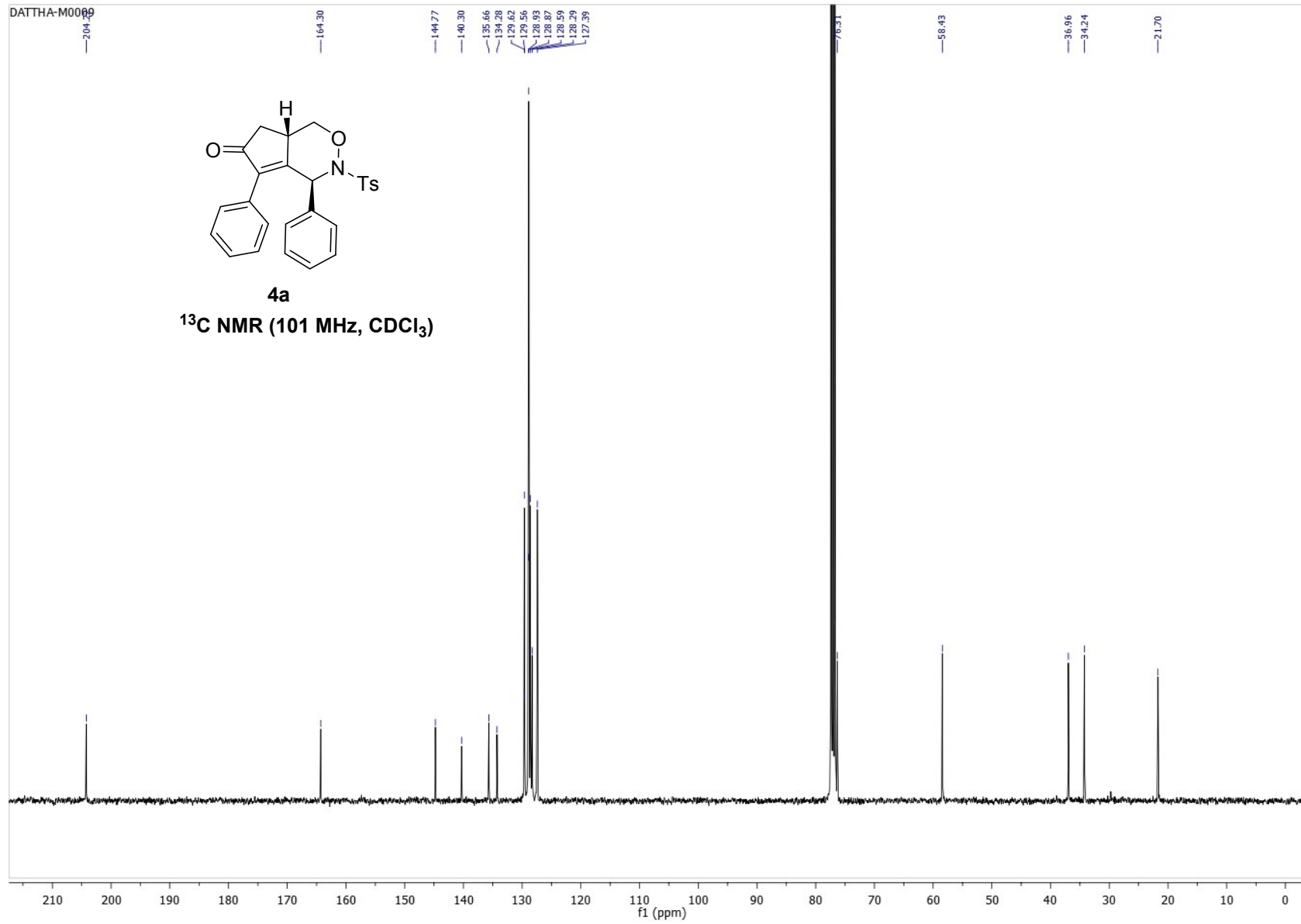


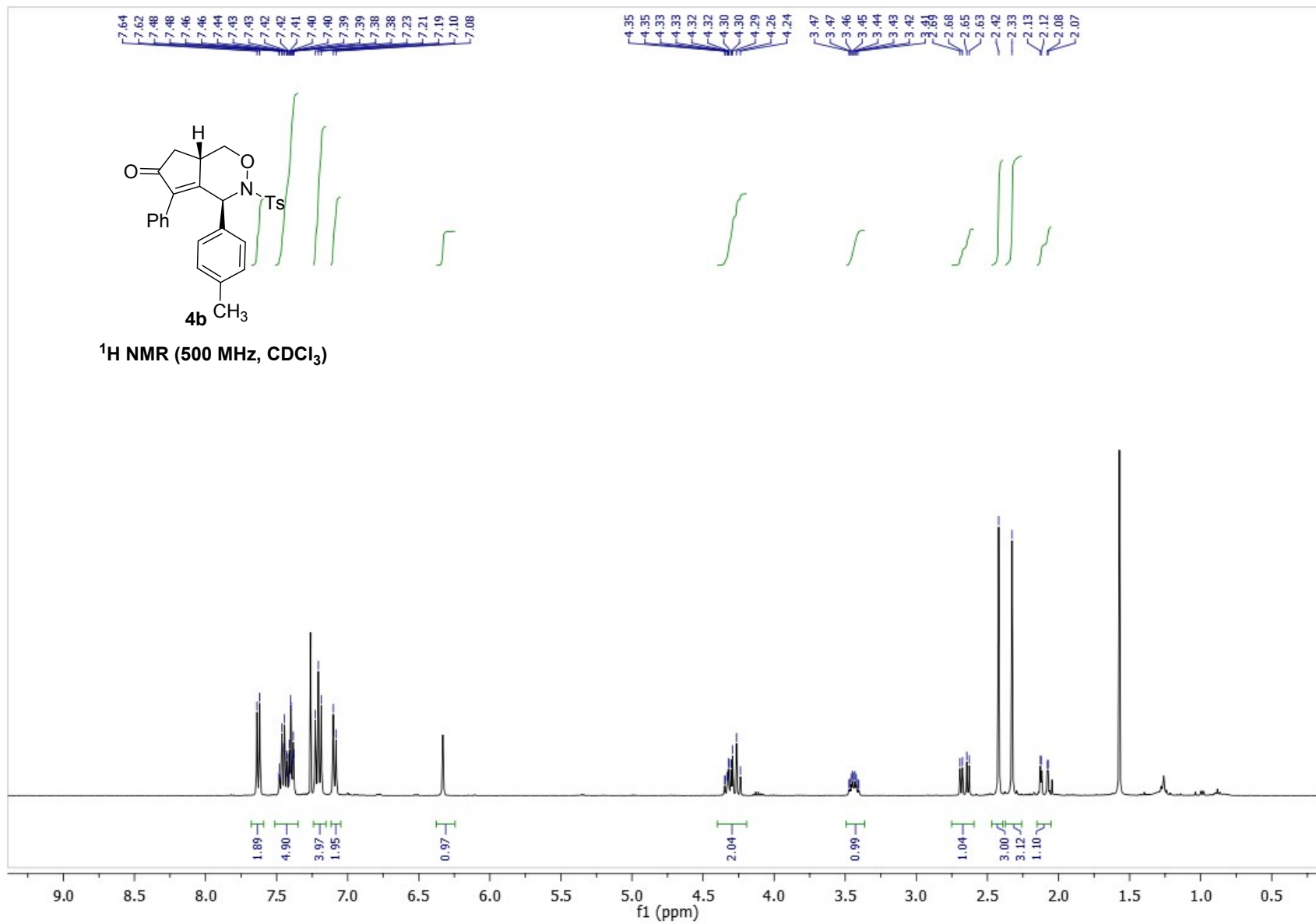


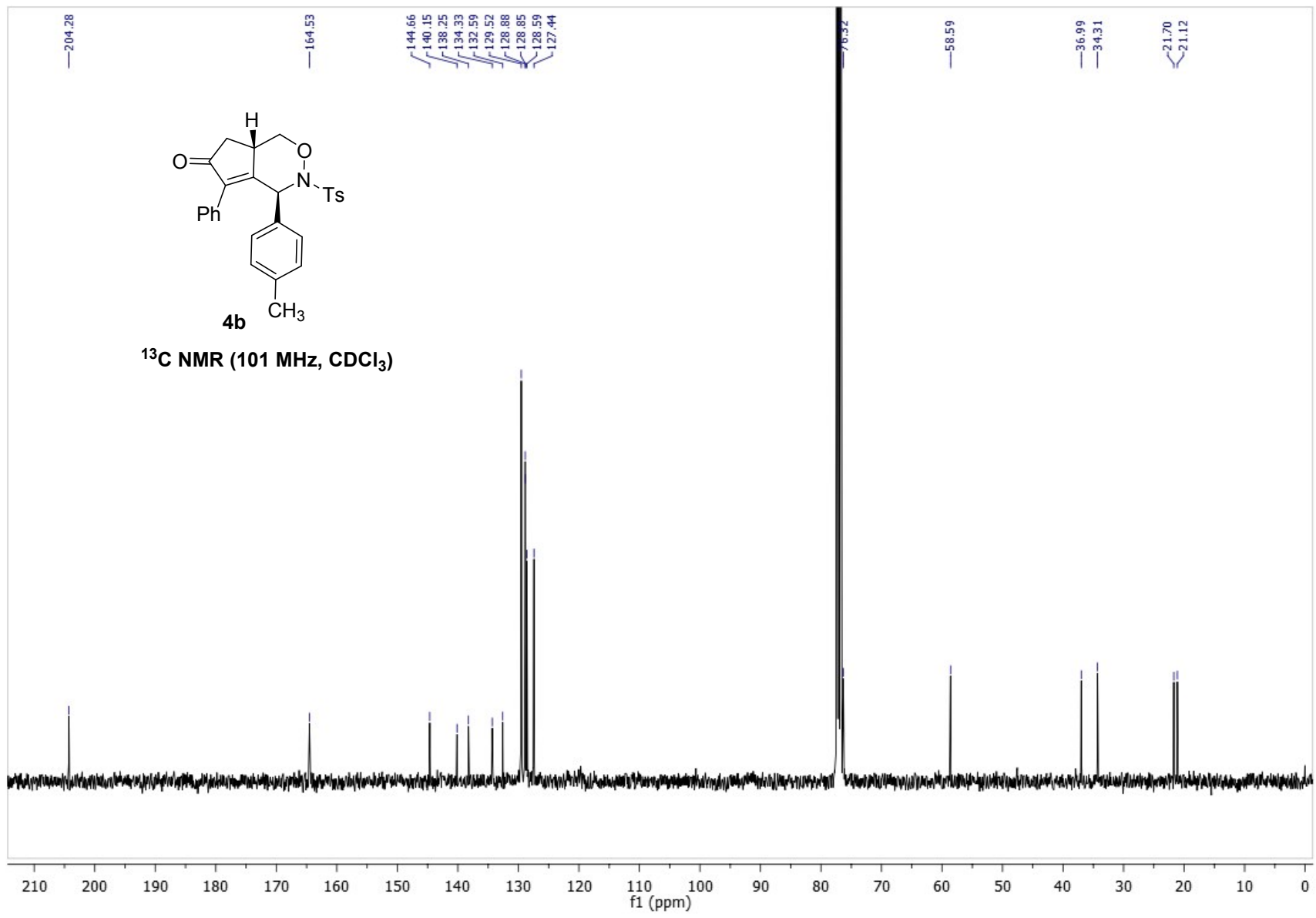


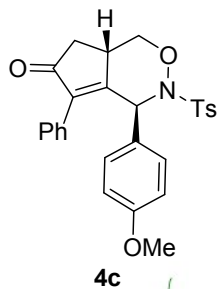
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^1H NMR (400 MHz, CDCl_3)

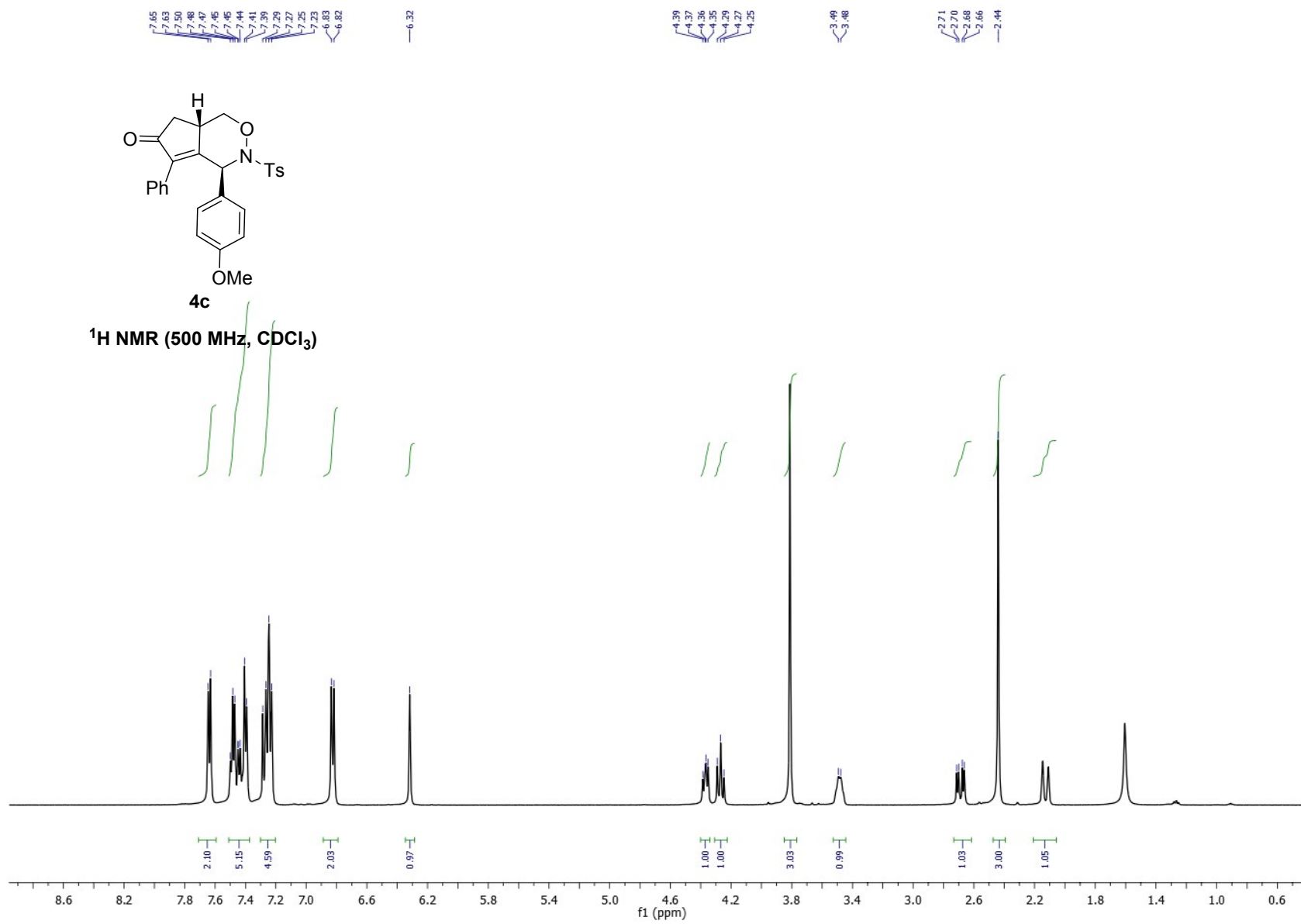


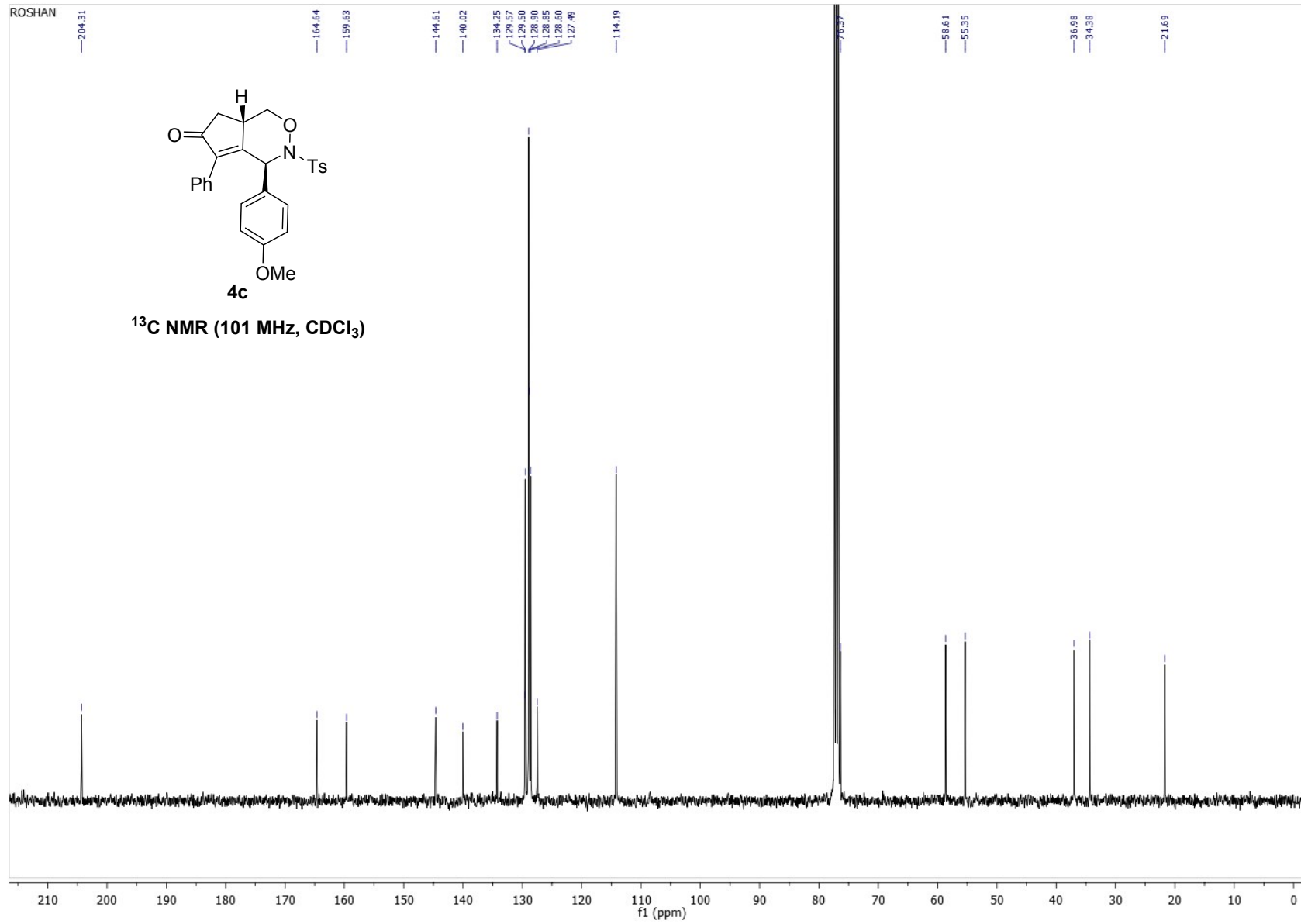


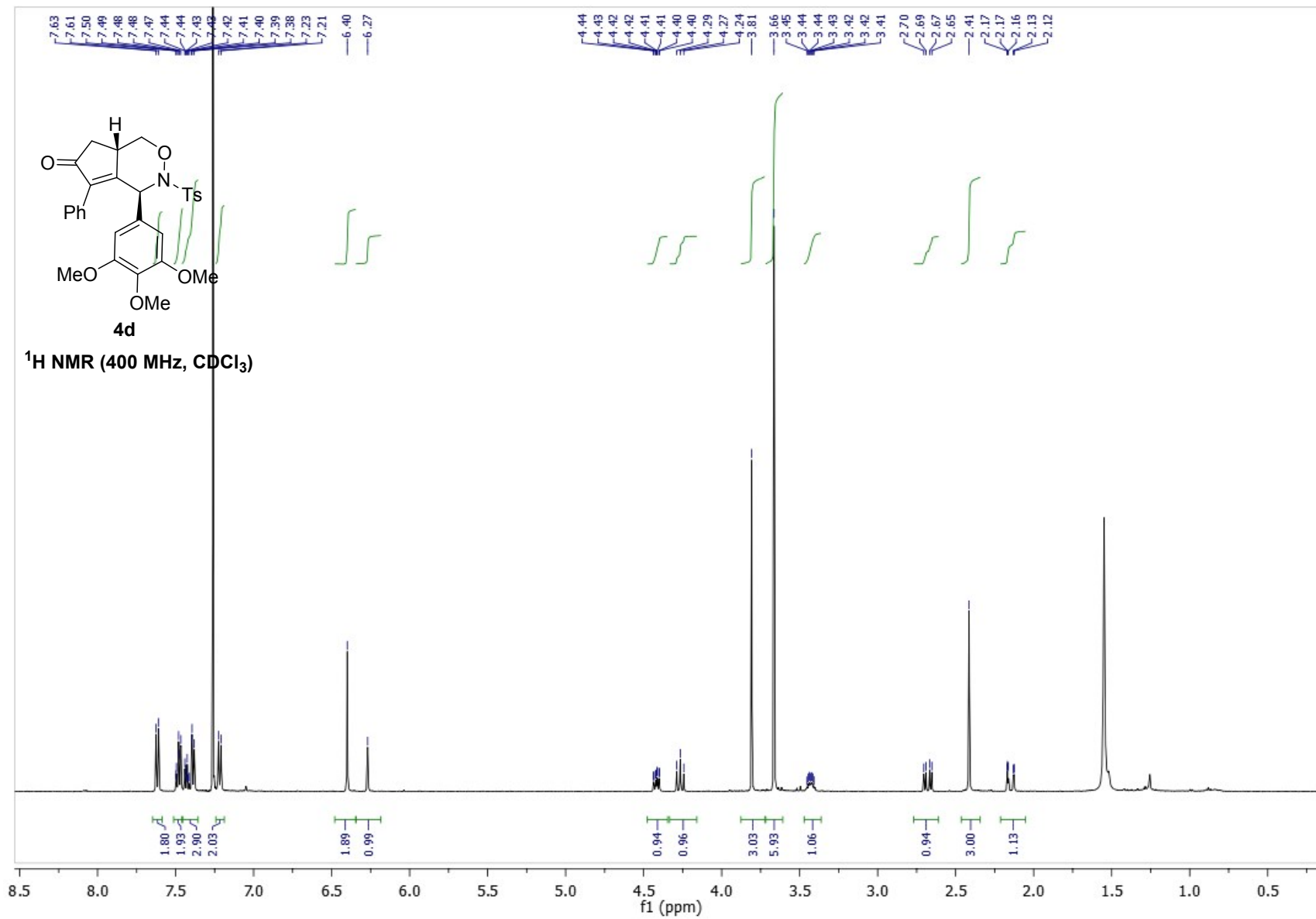


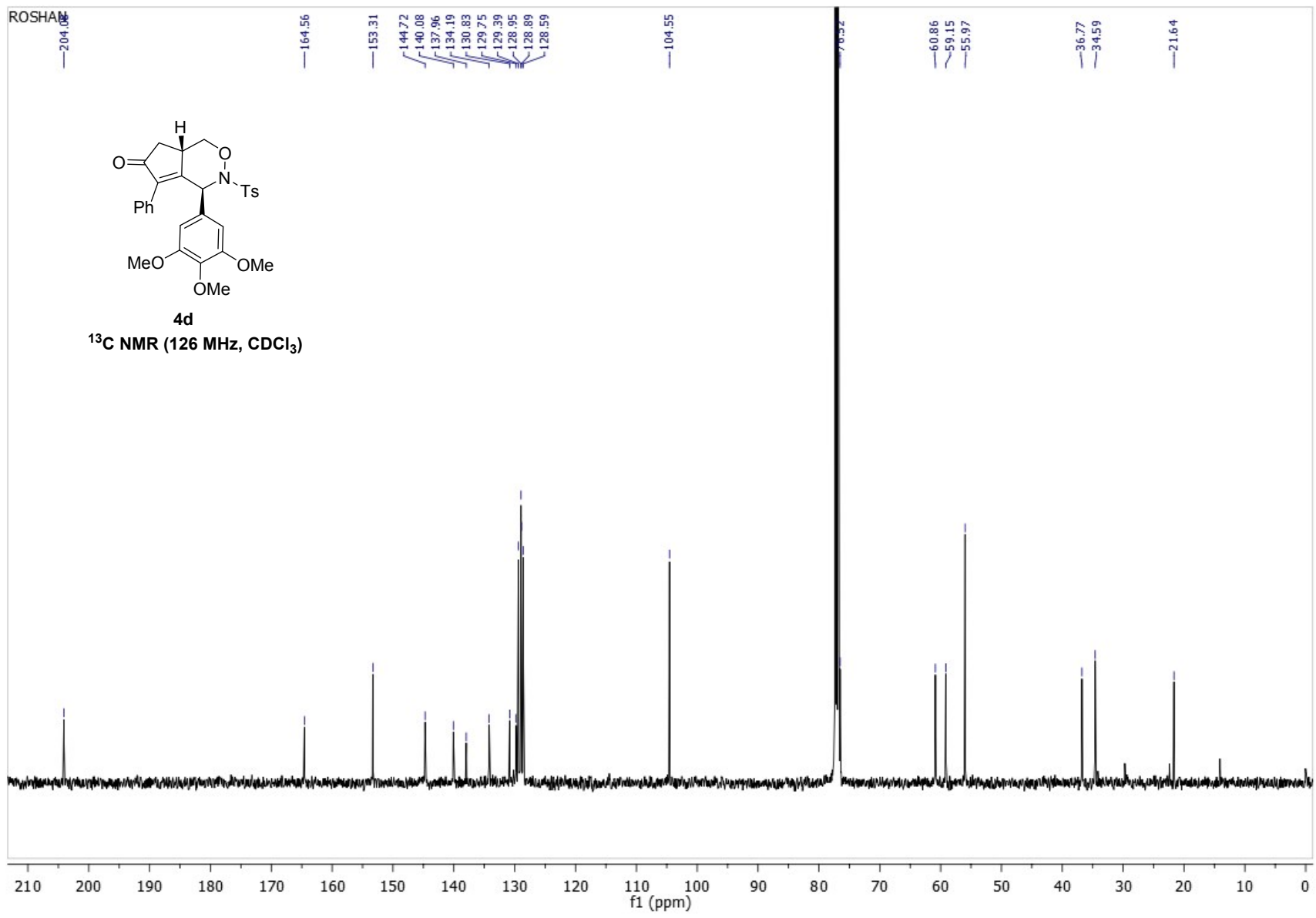


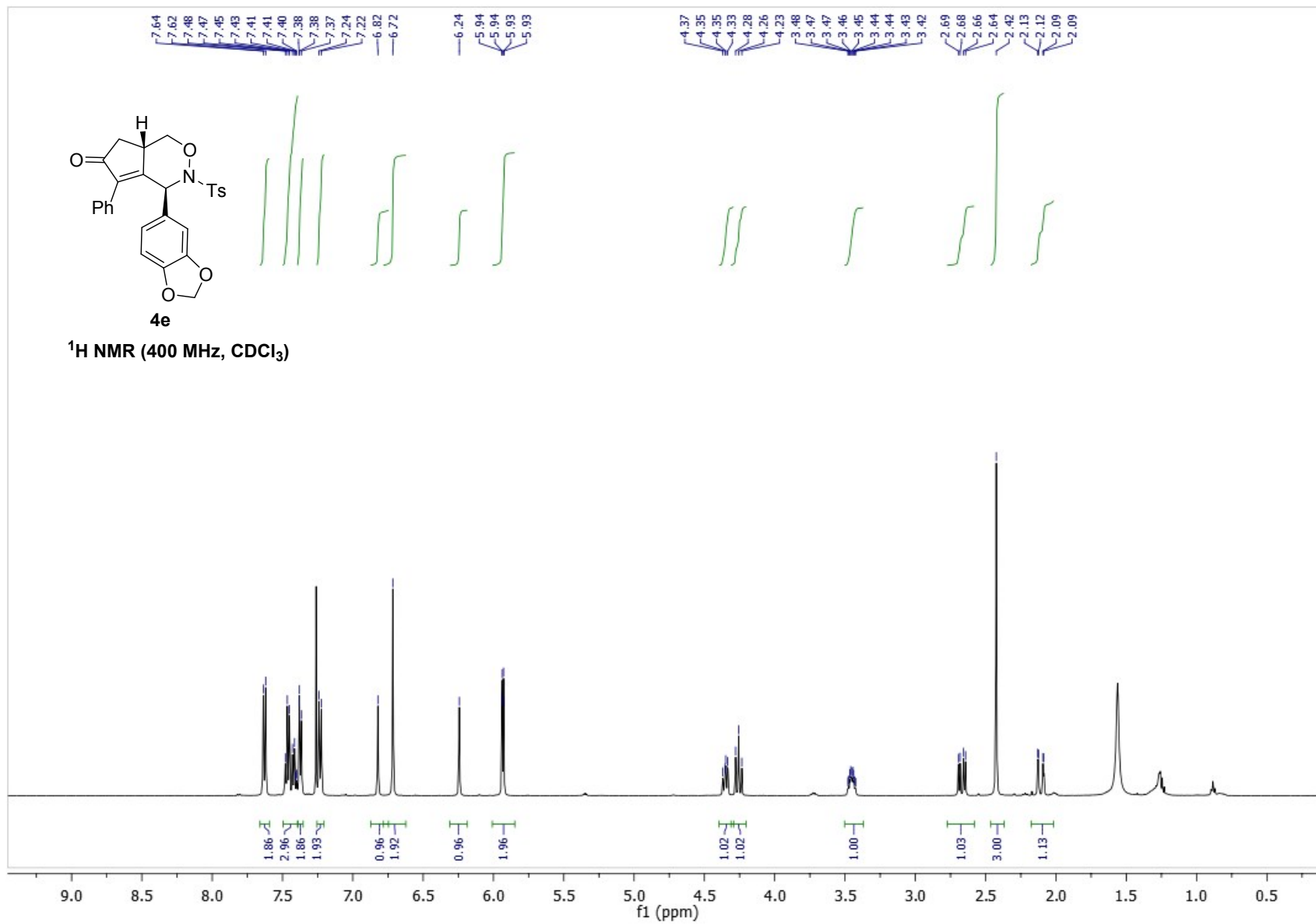
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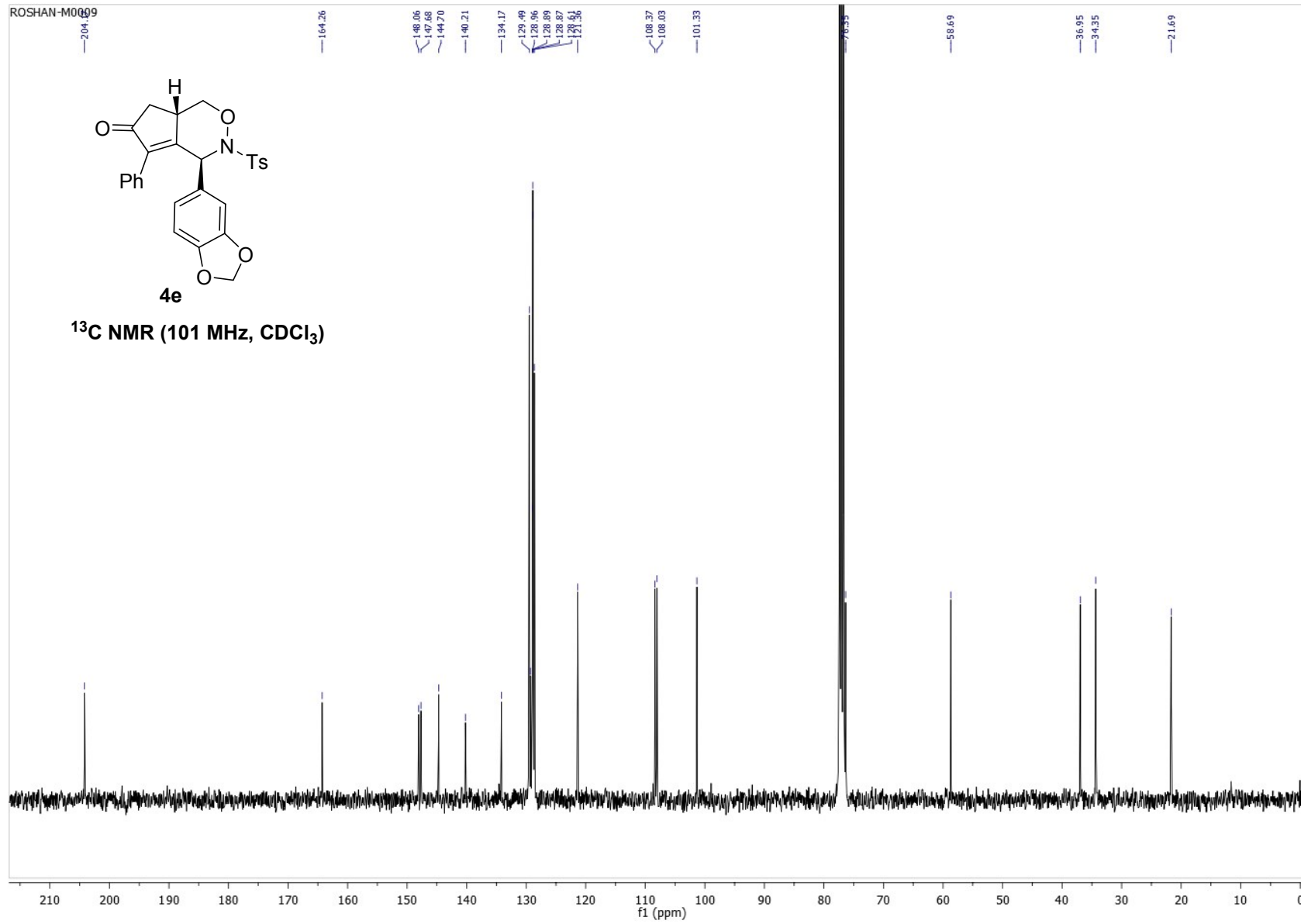


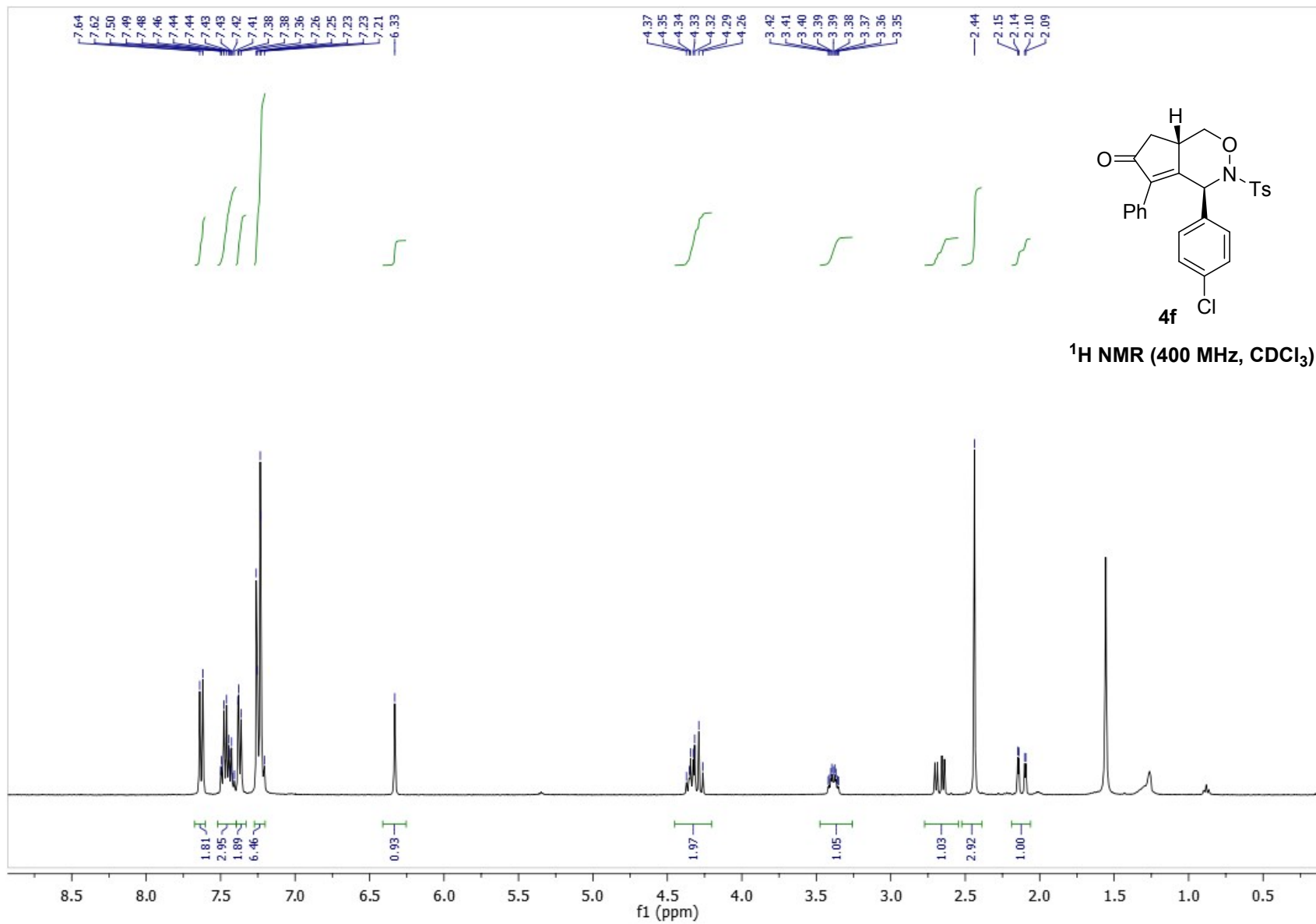


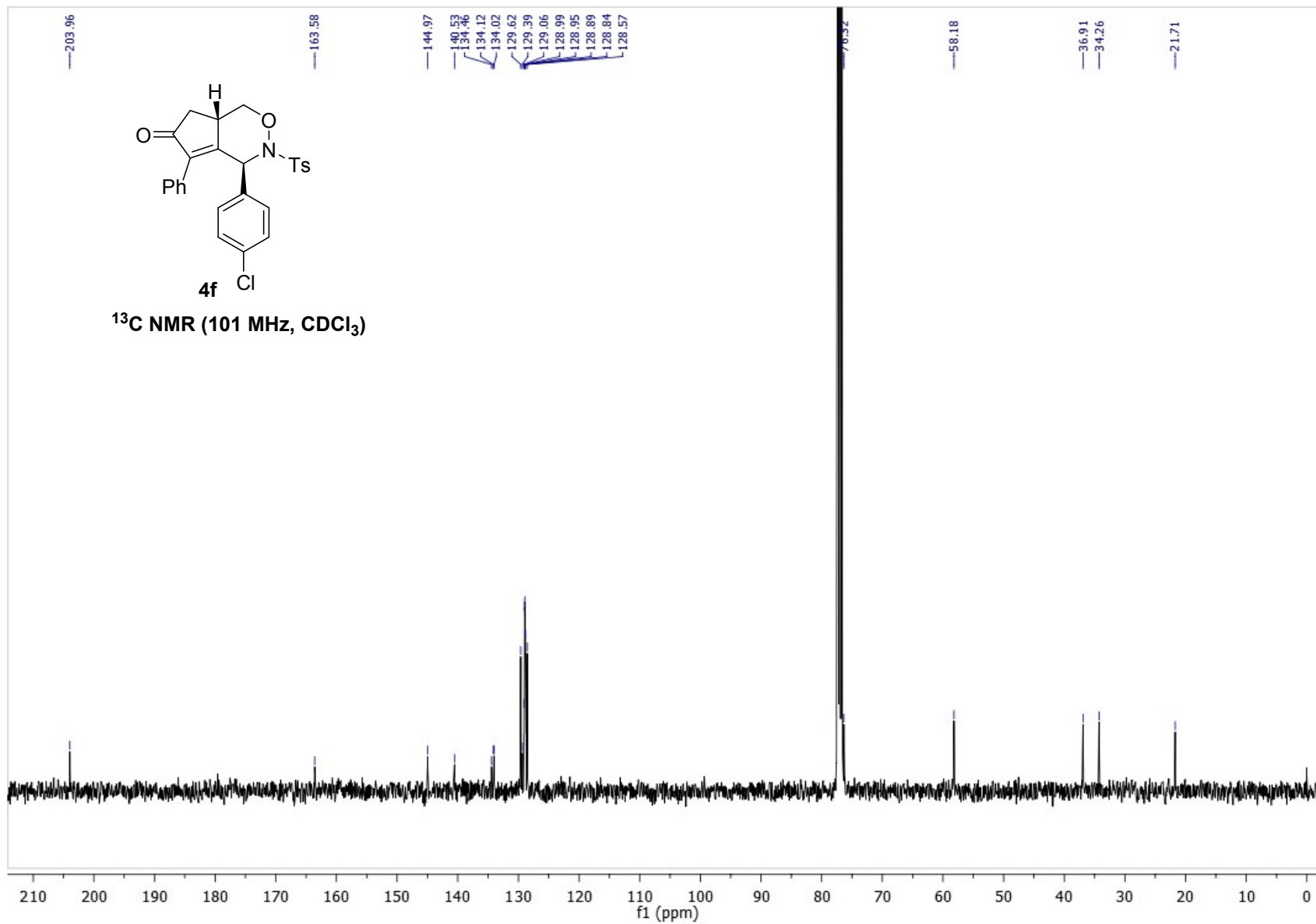


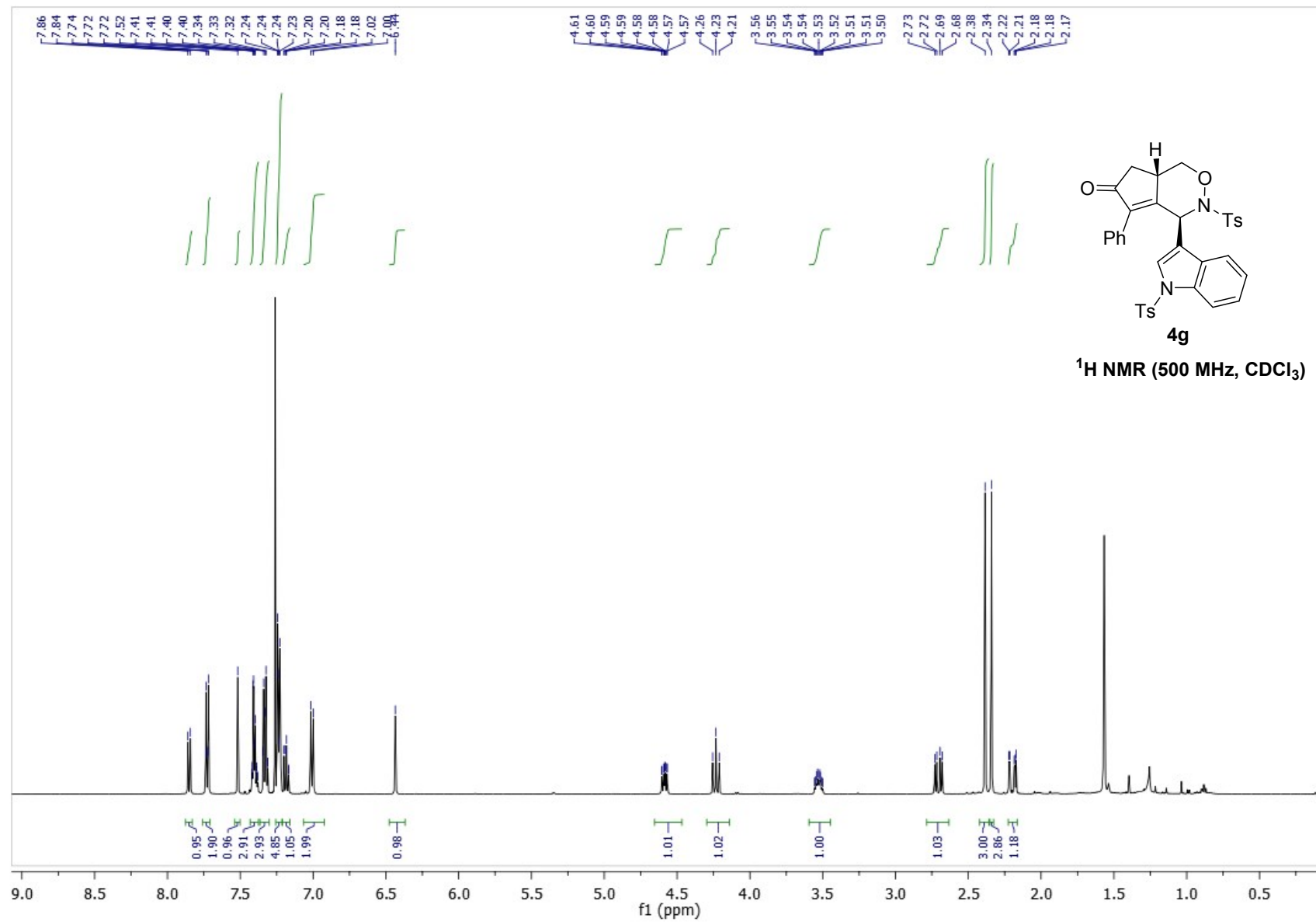


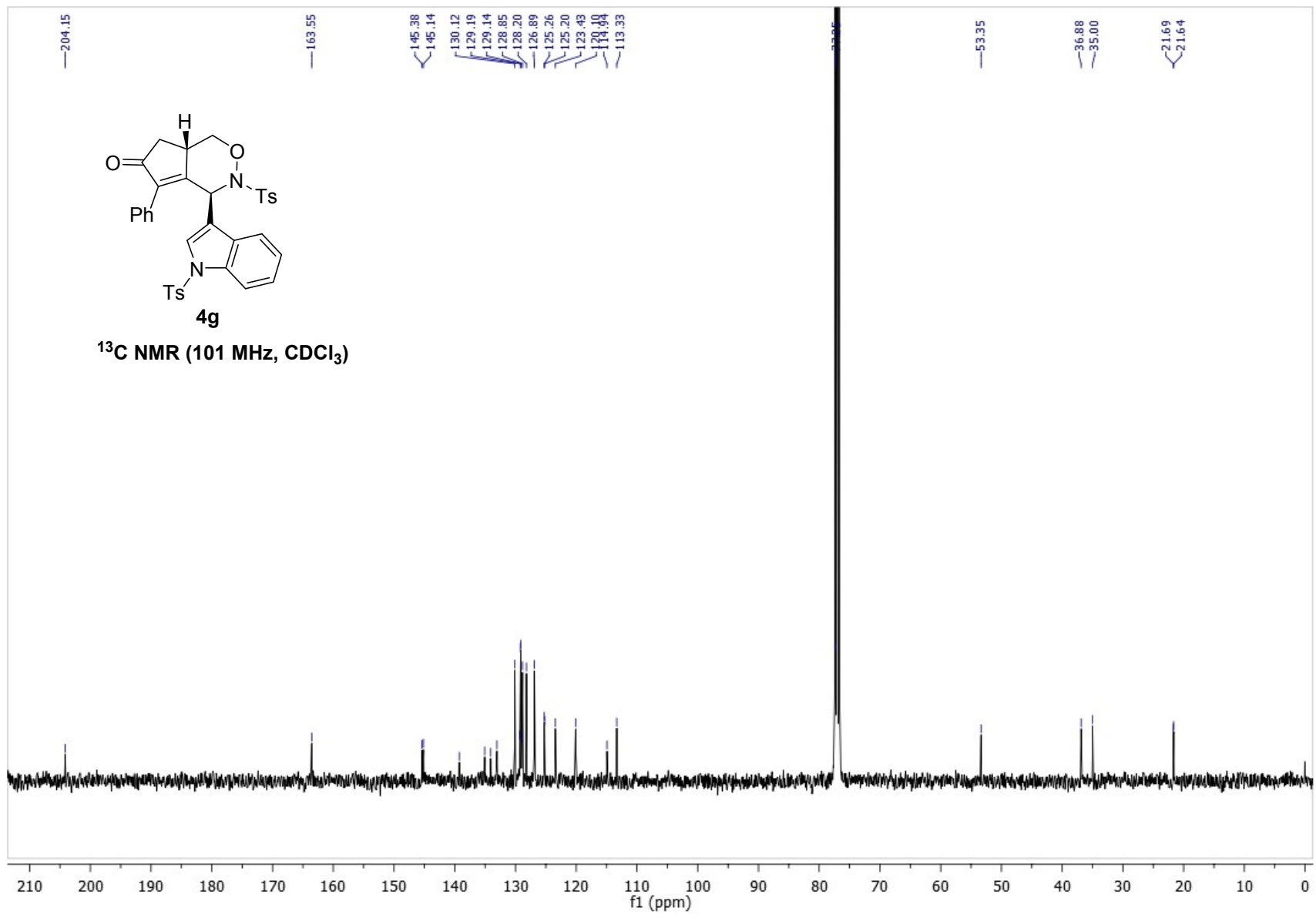


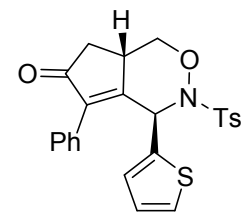
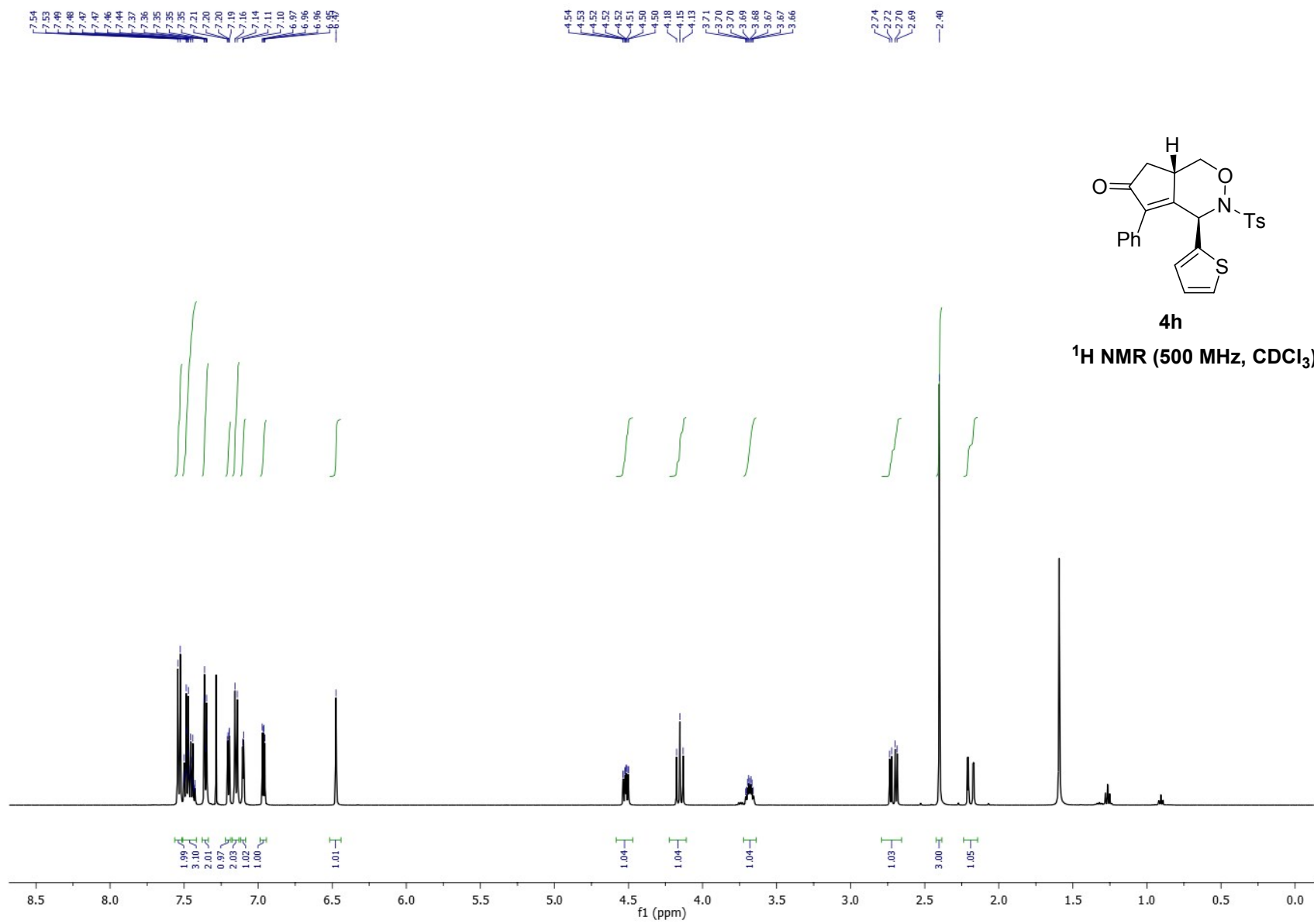






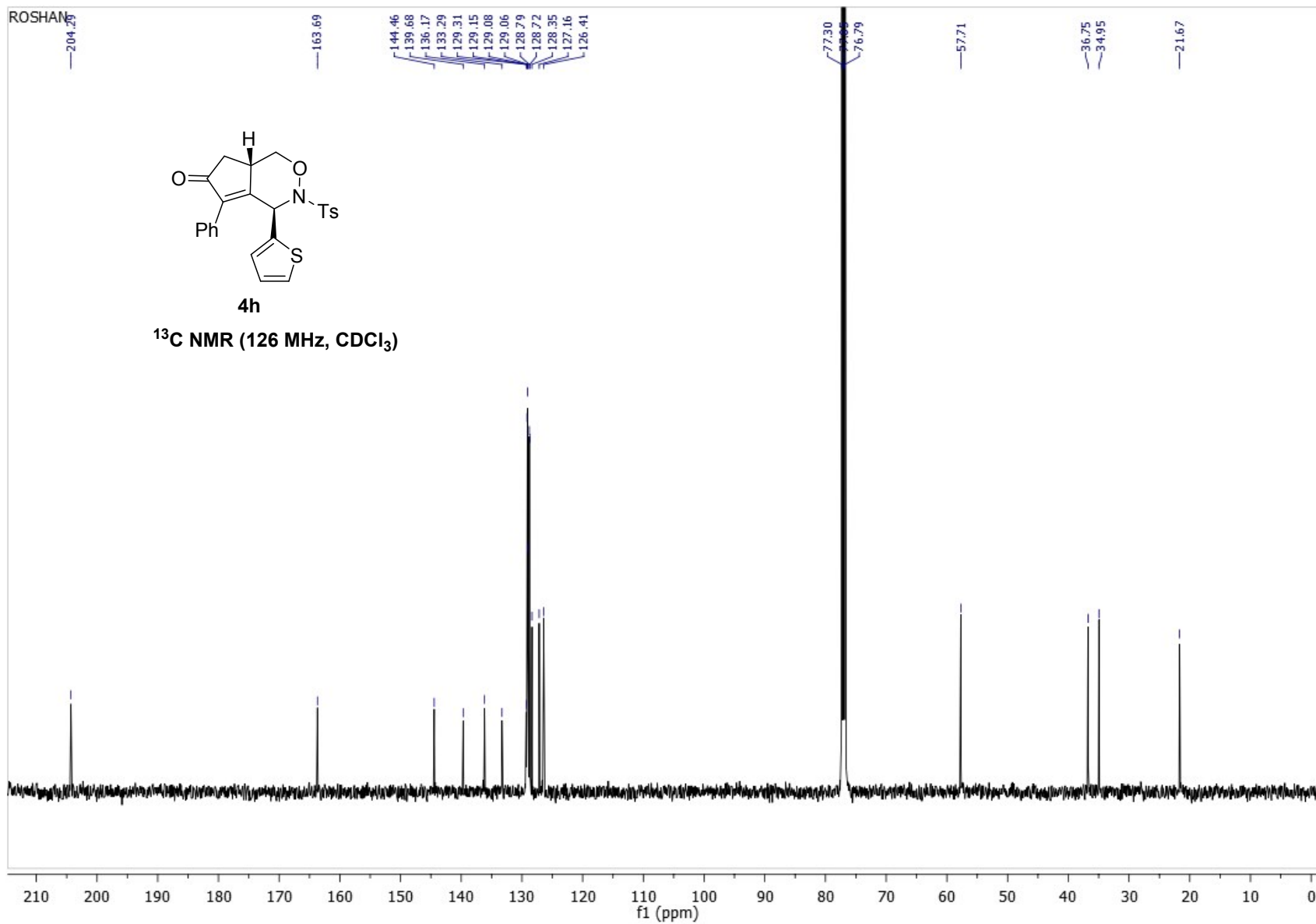


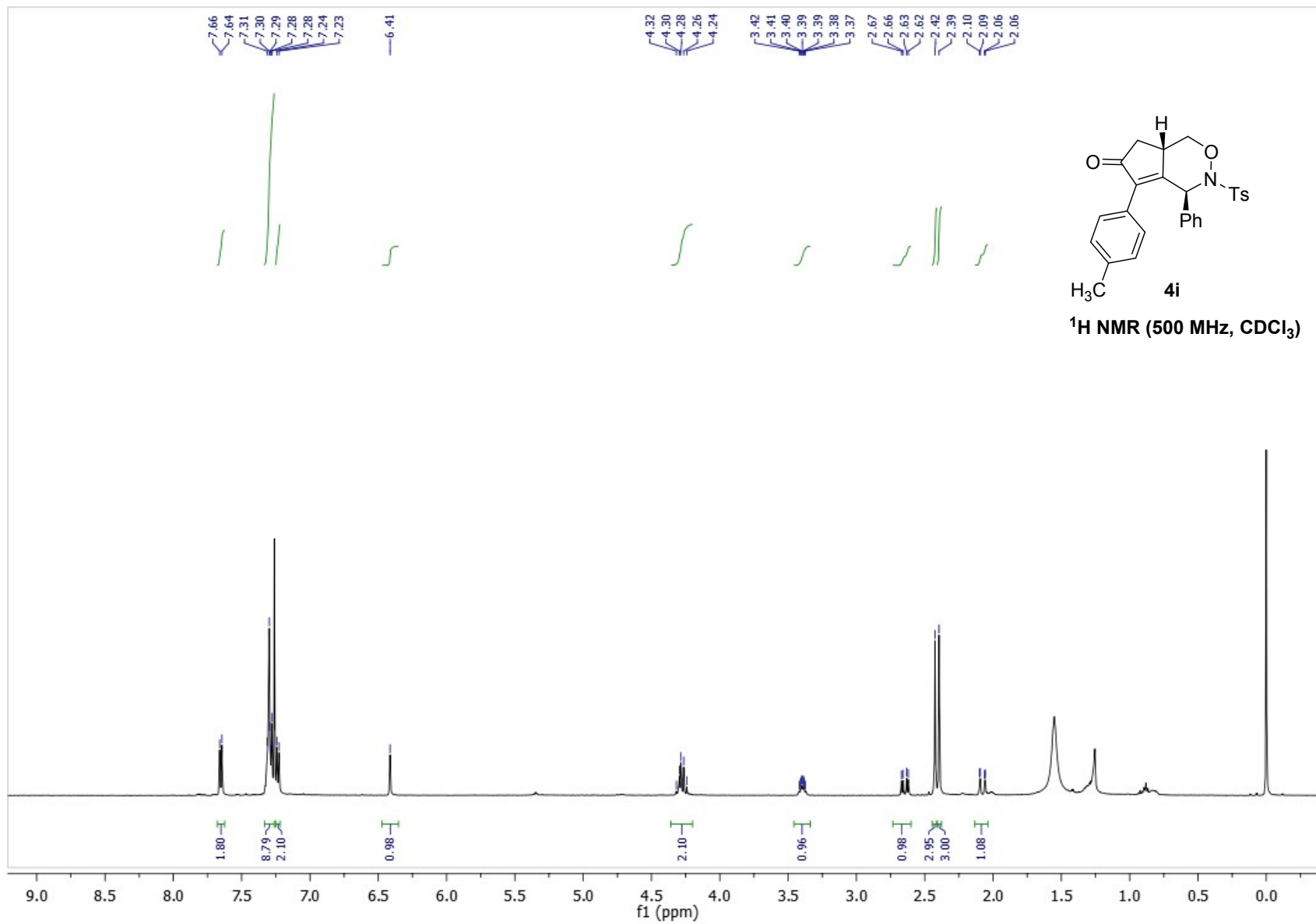




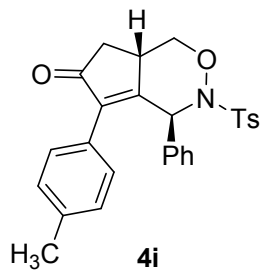
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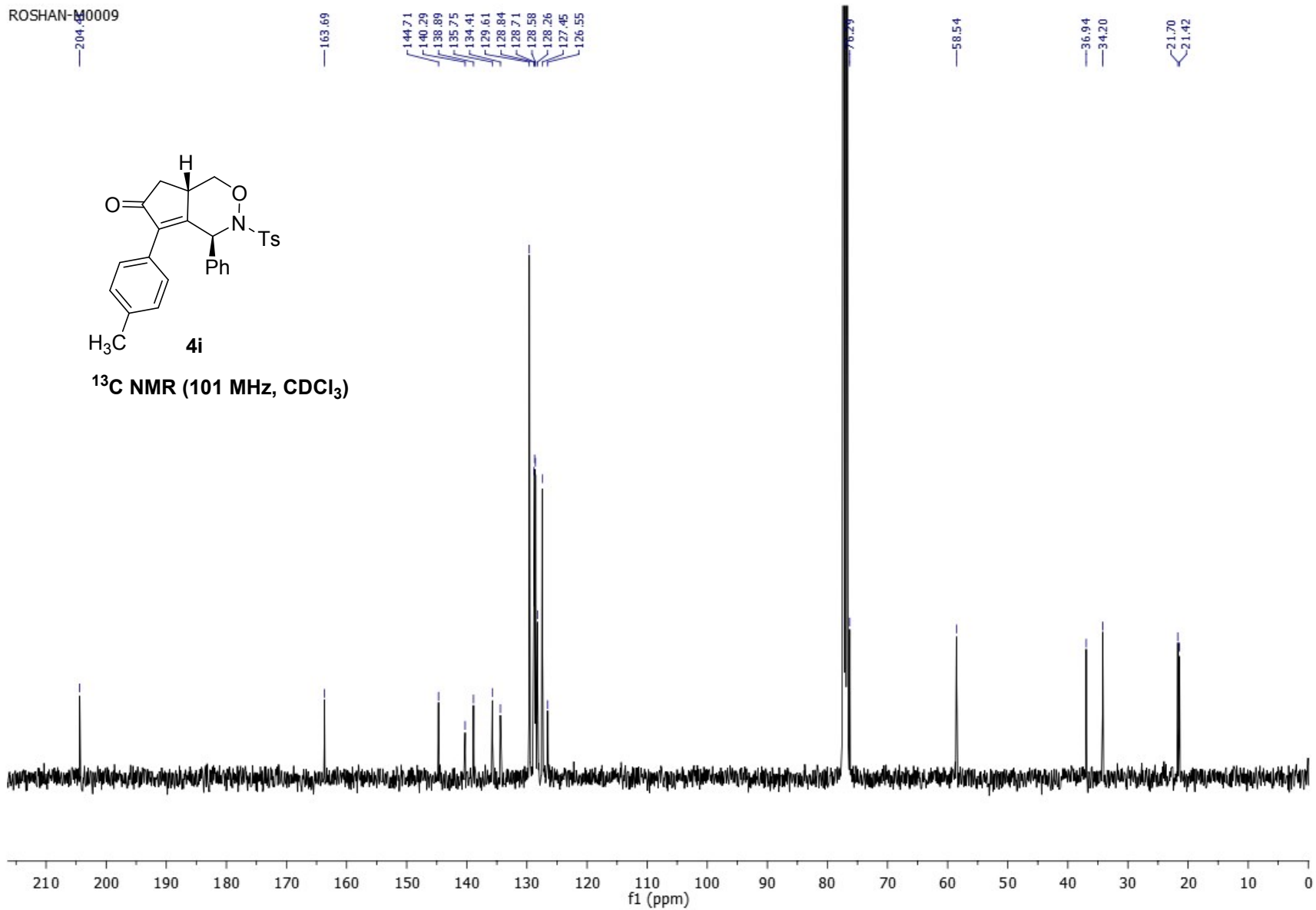


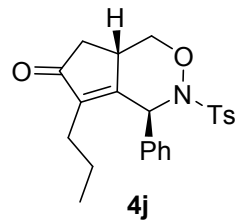


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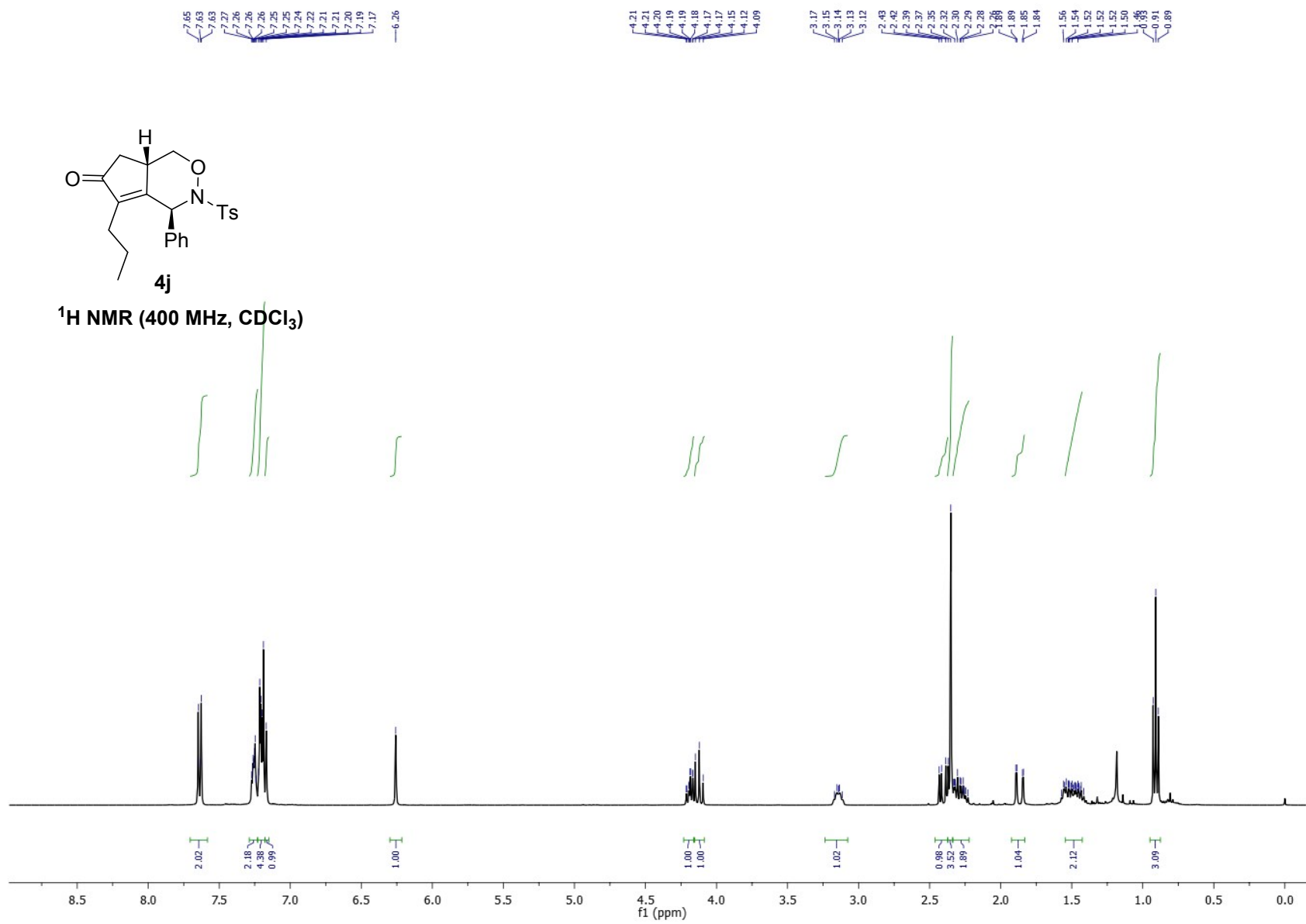


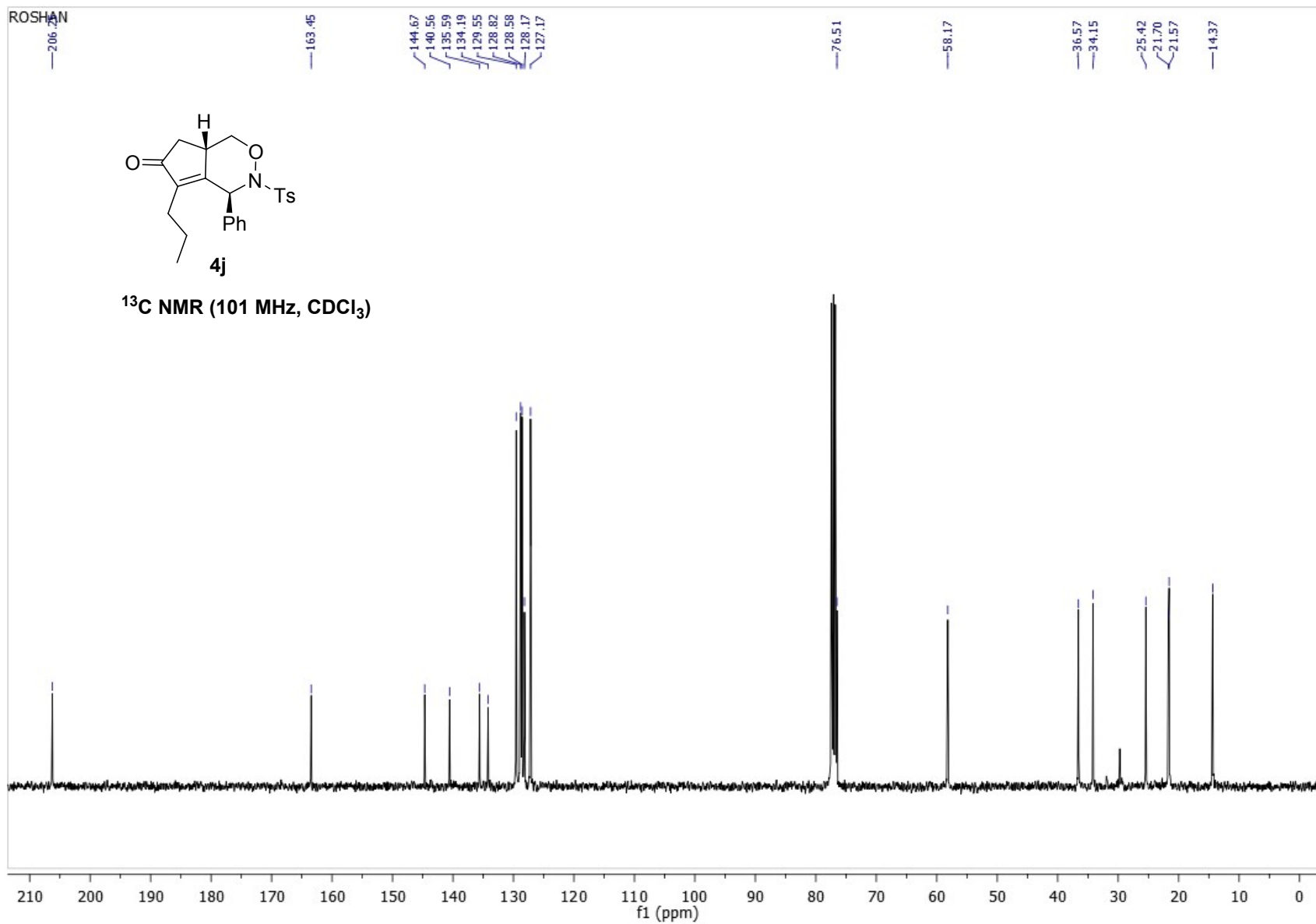
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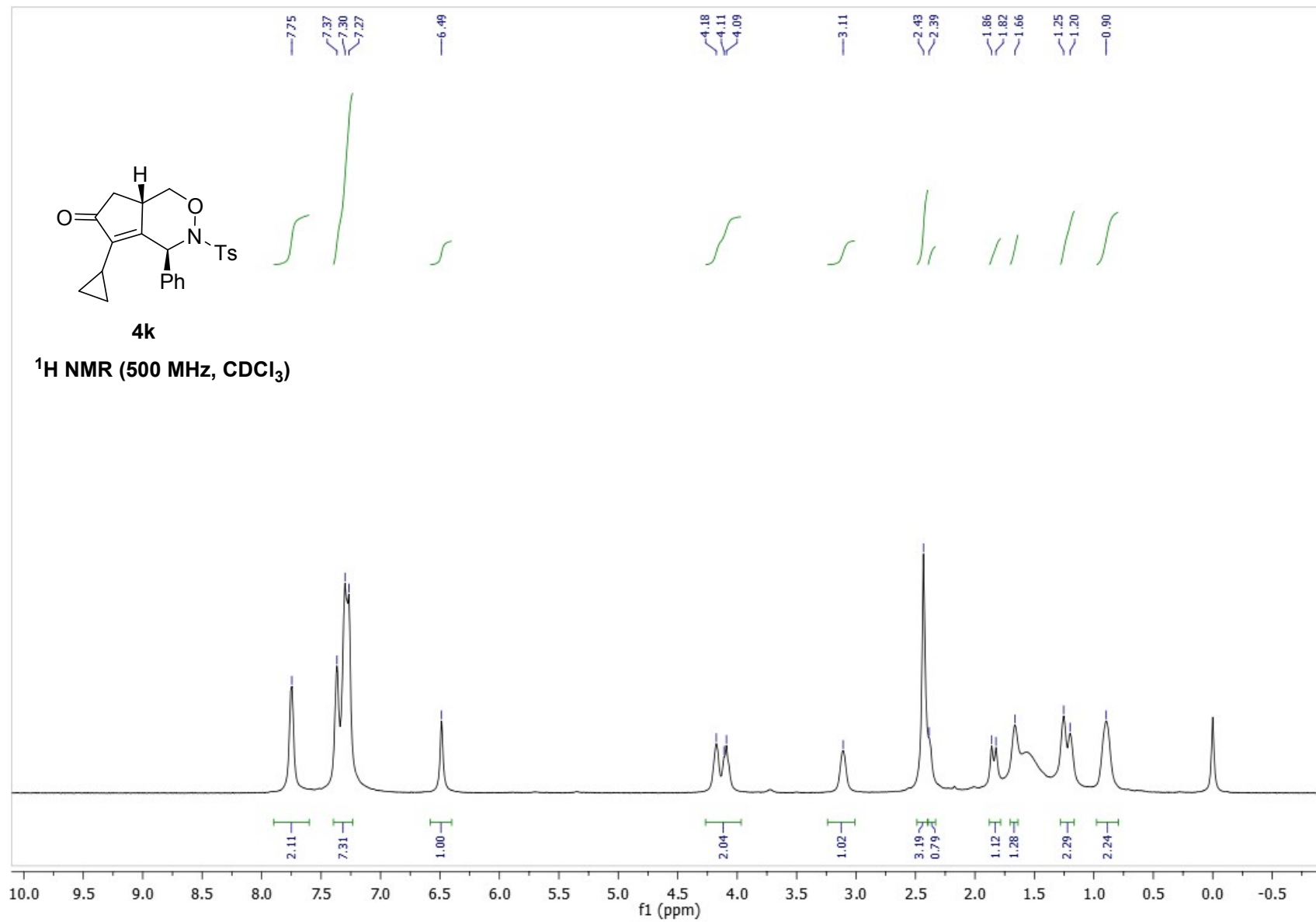


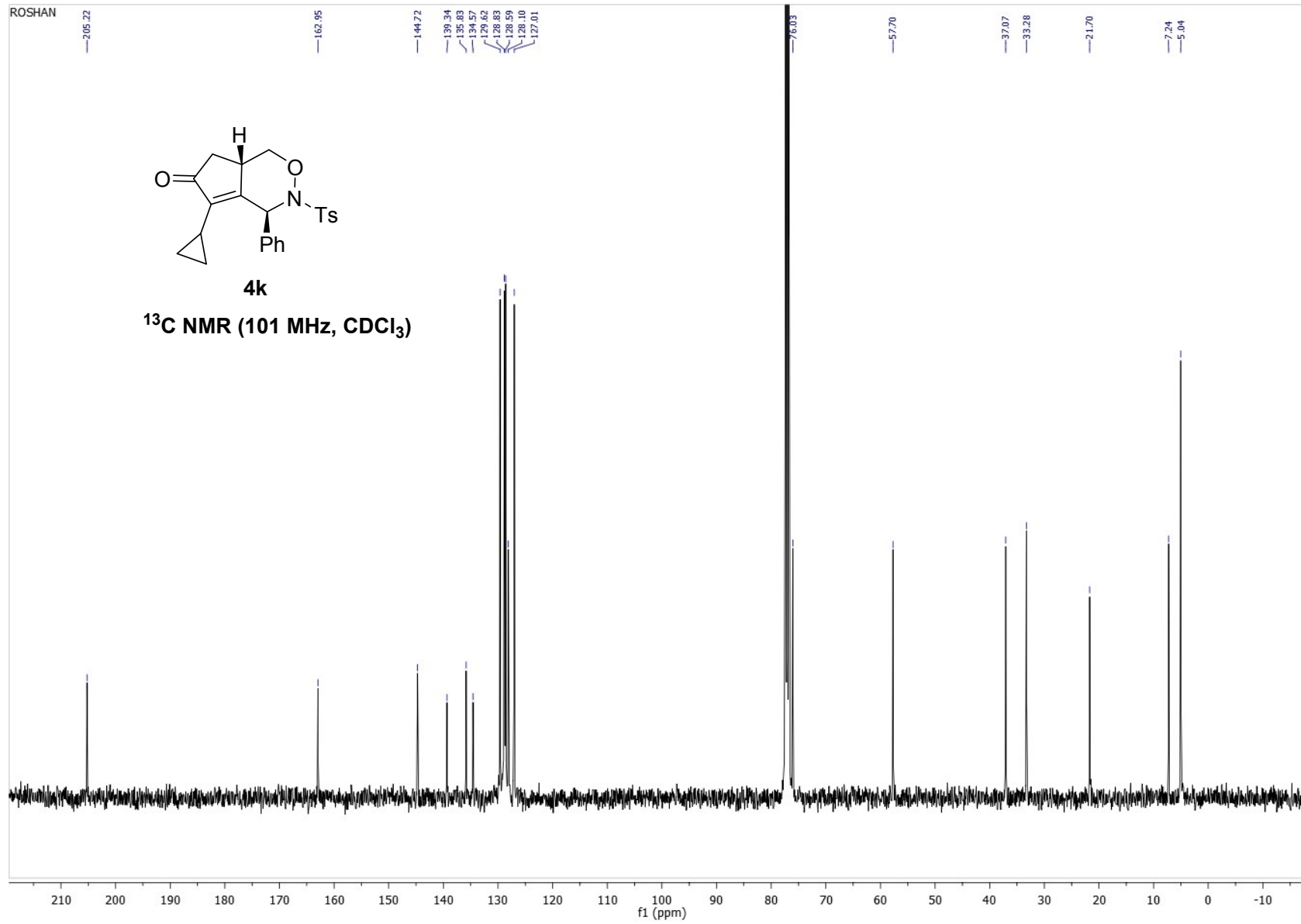


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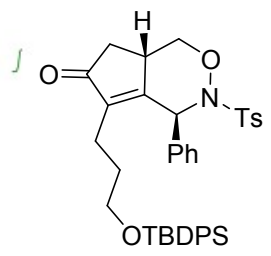


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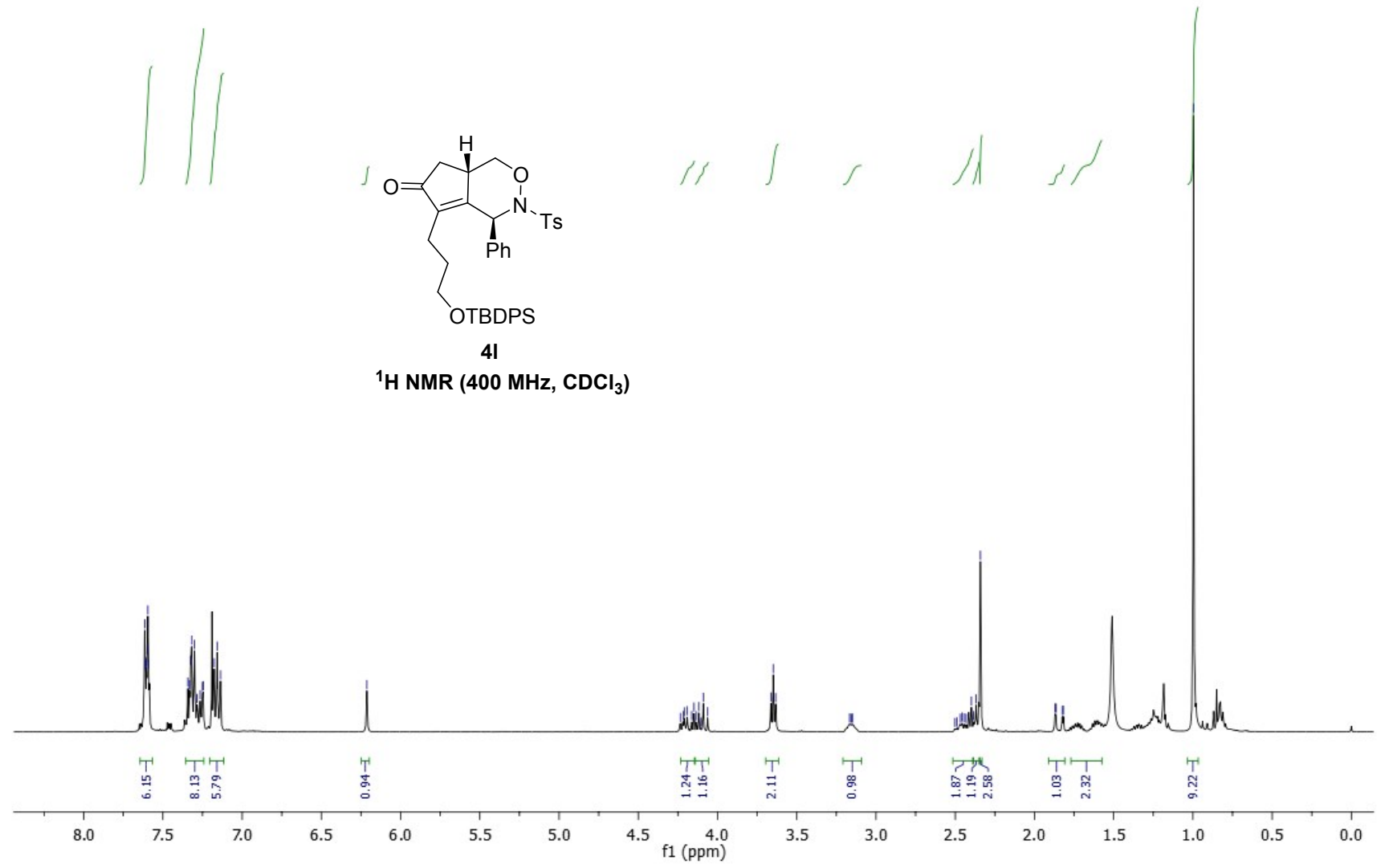
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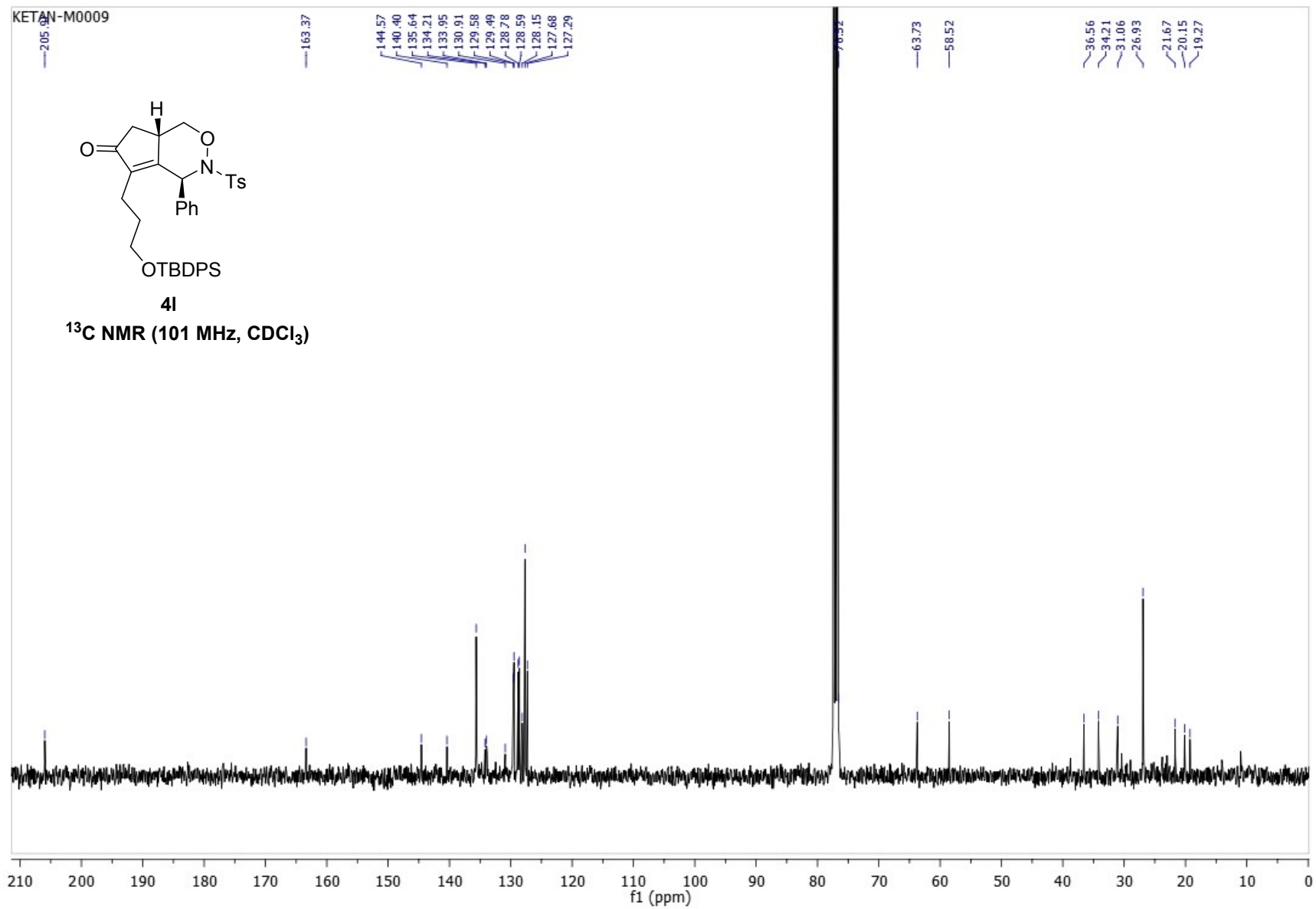
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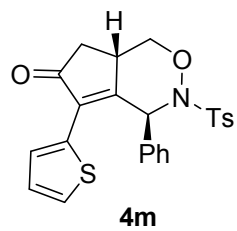
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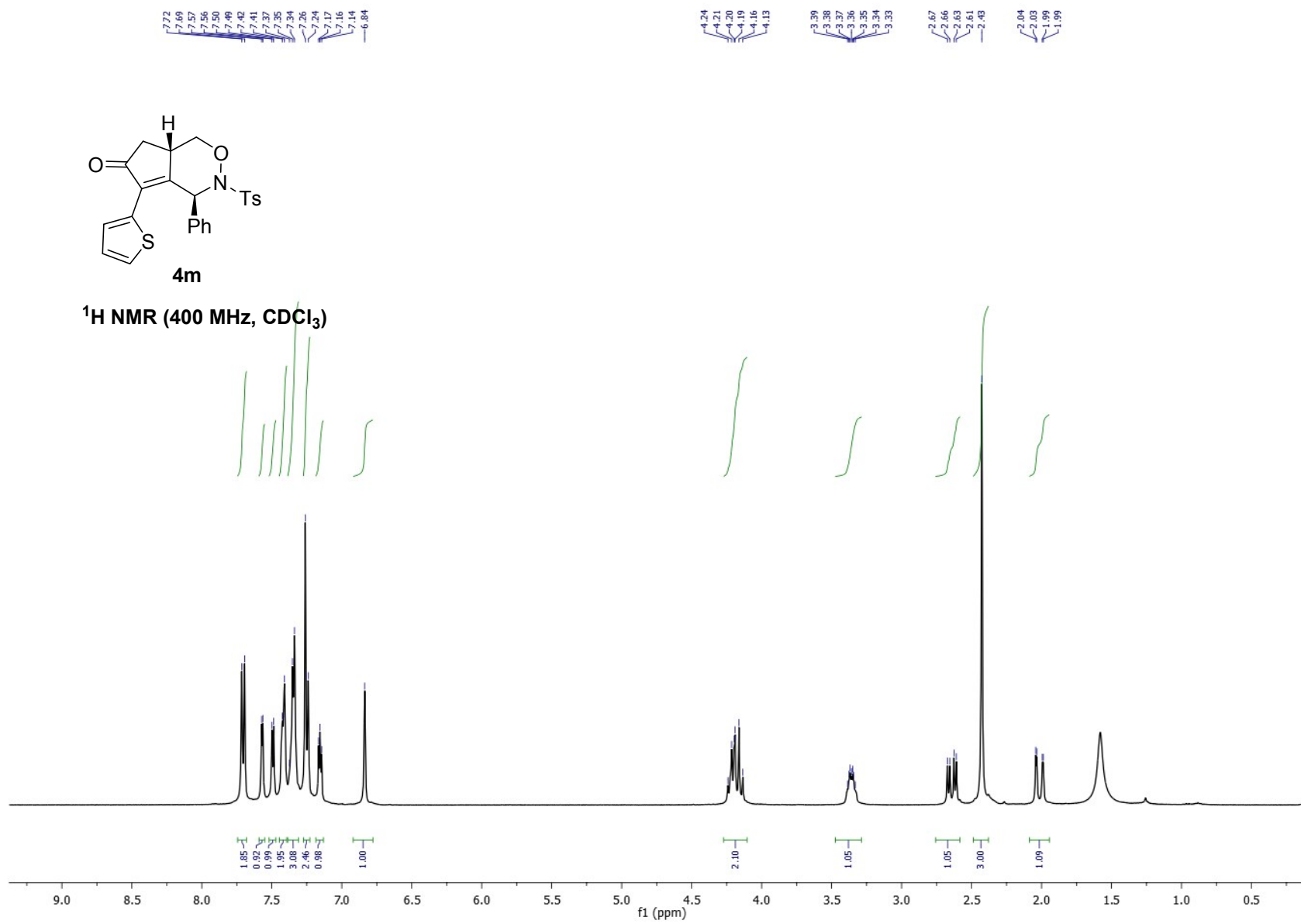
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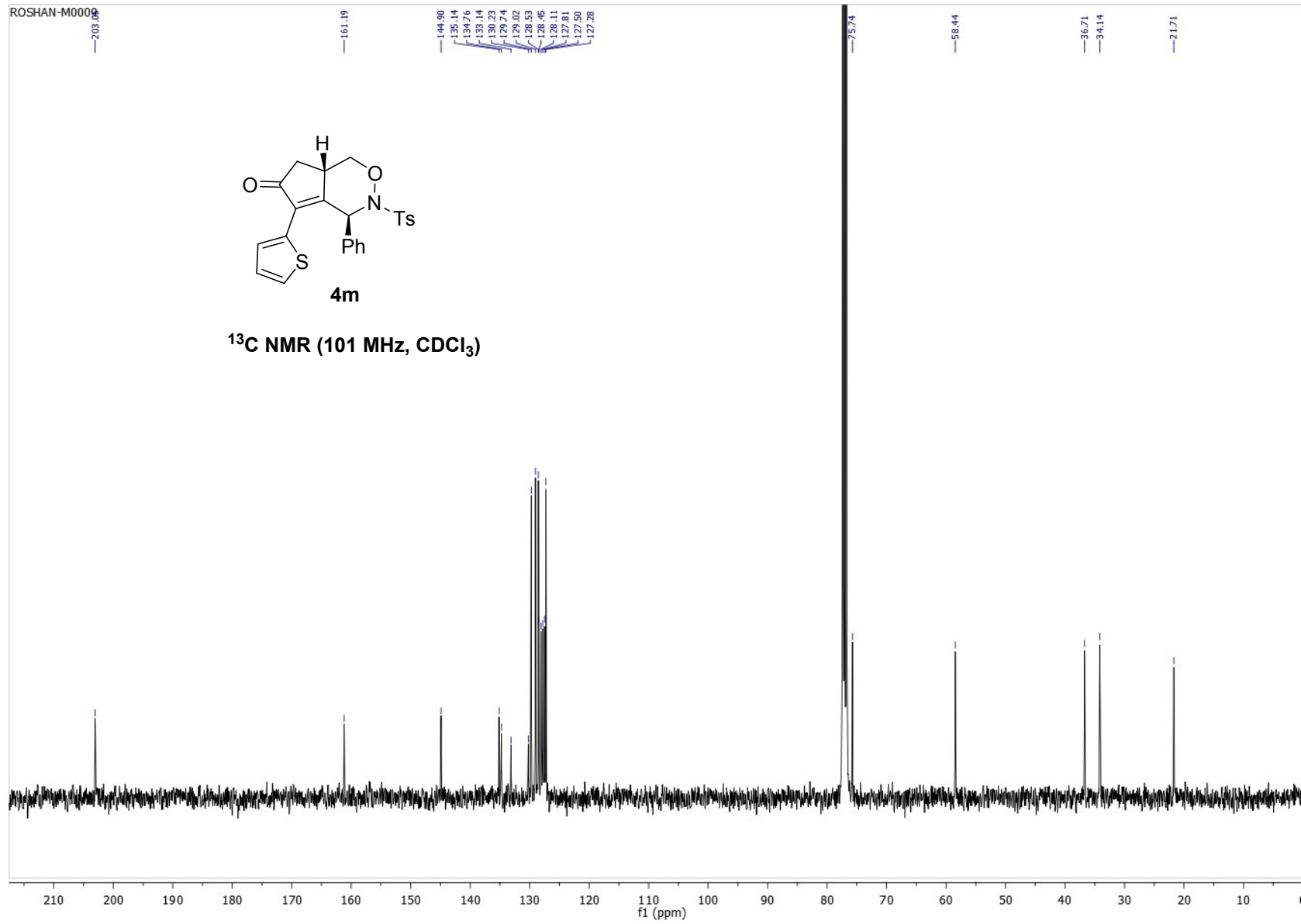






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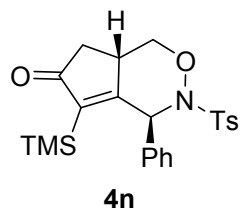




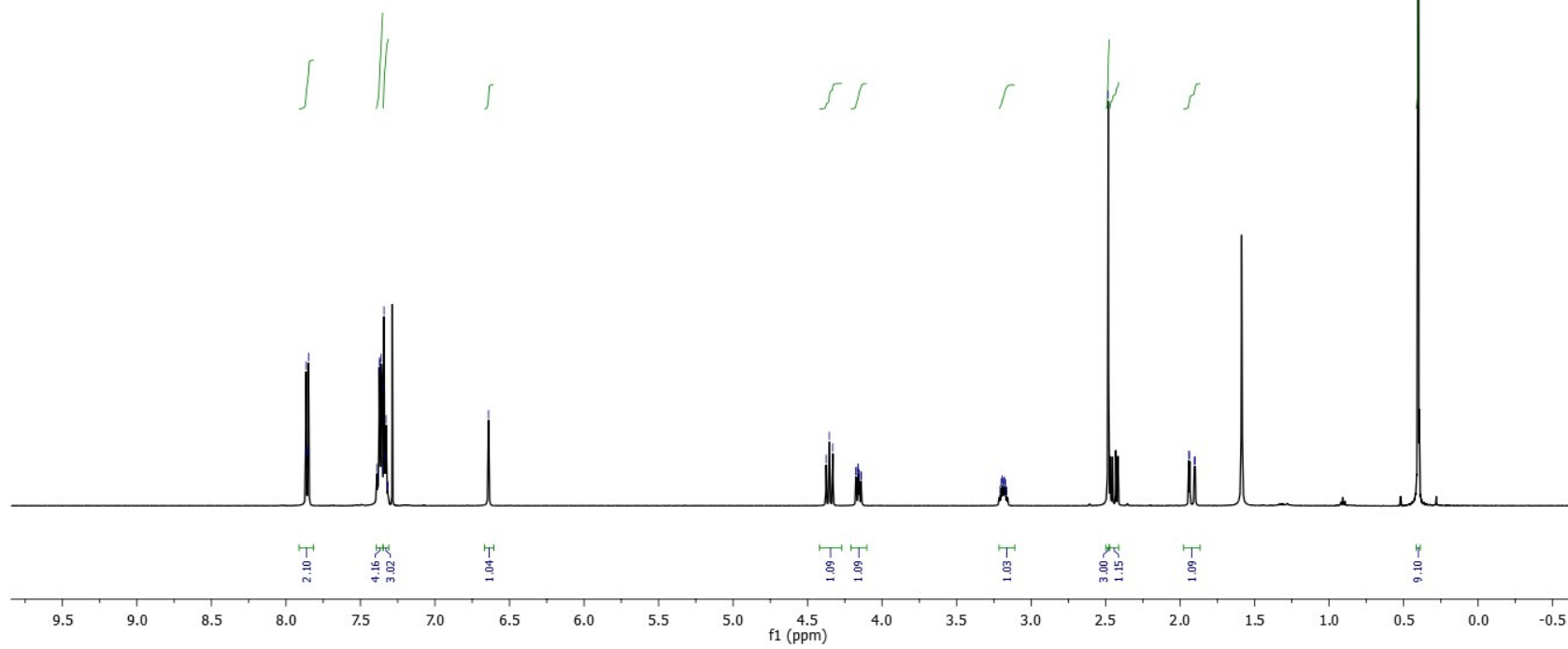
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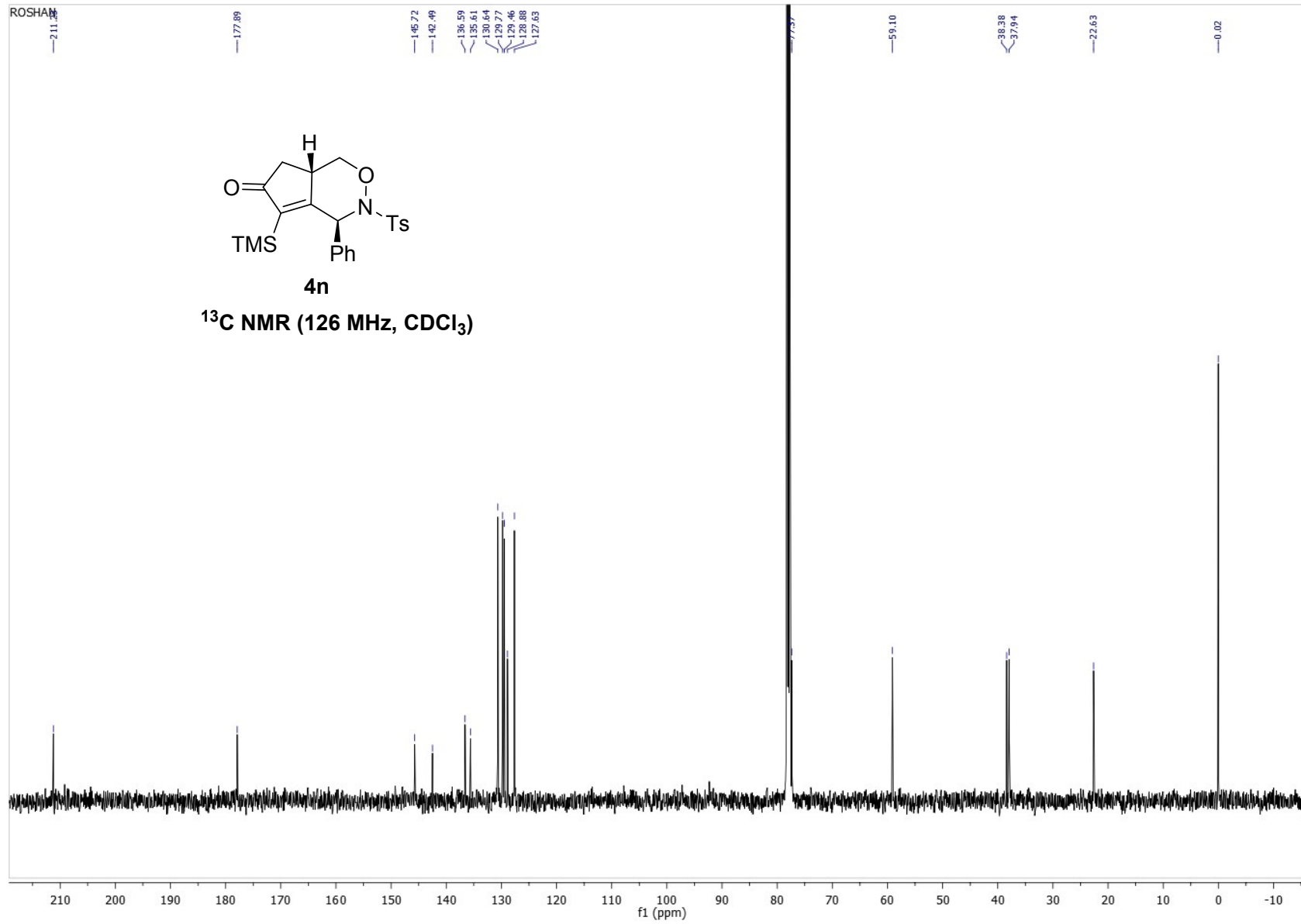
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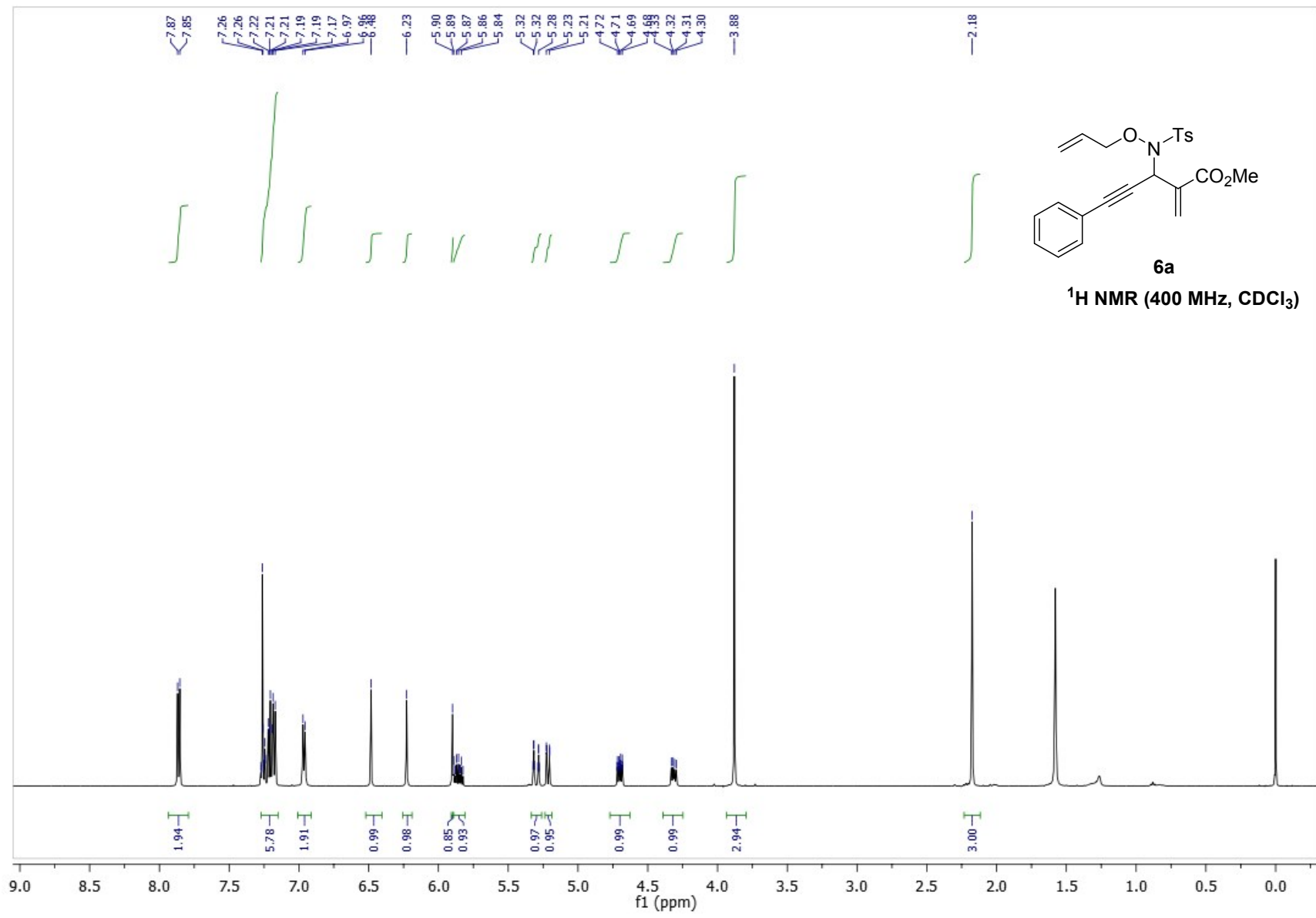
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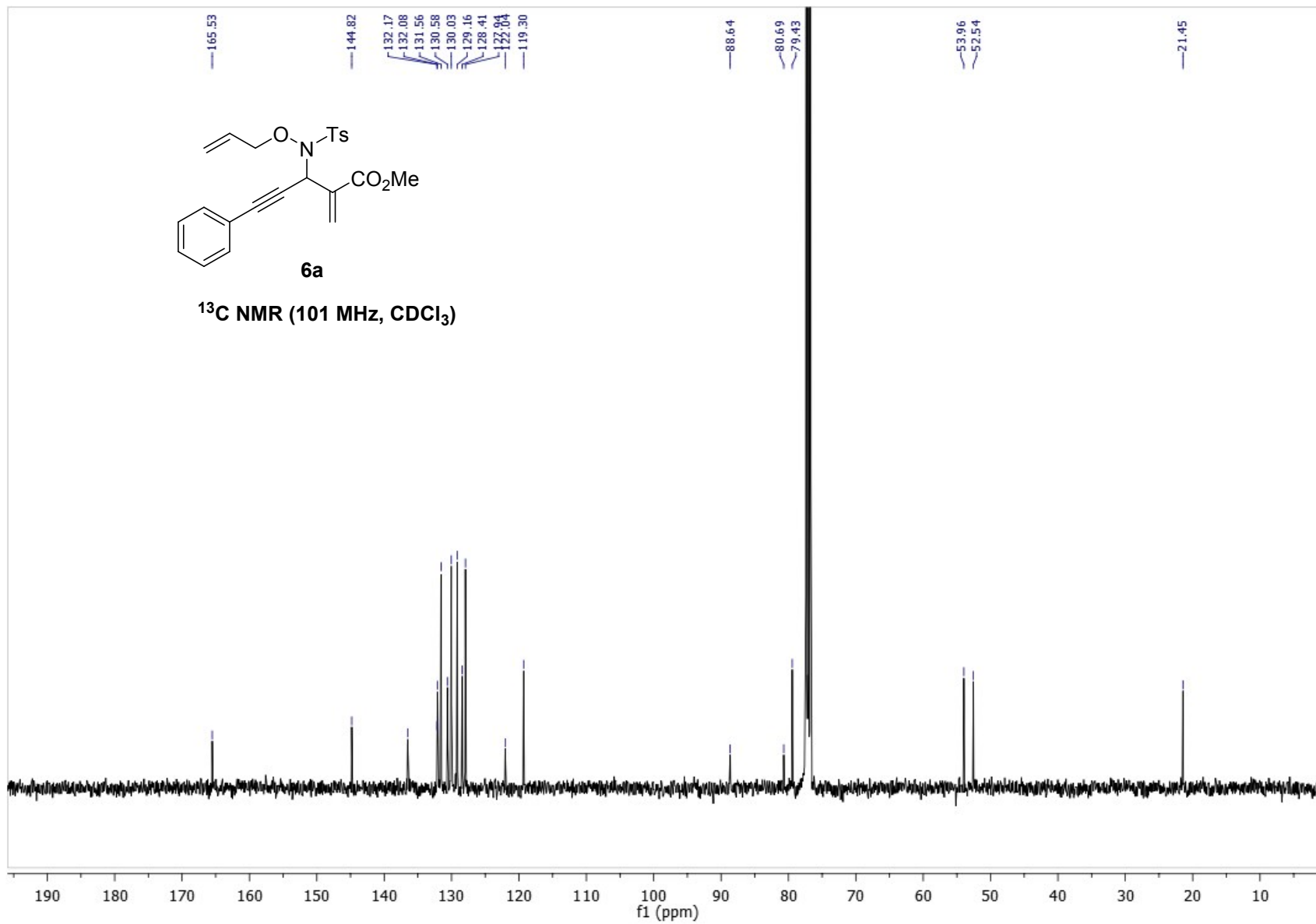


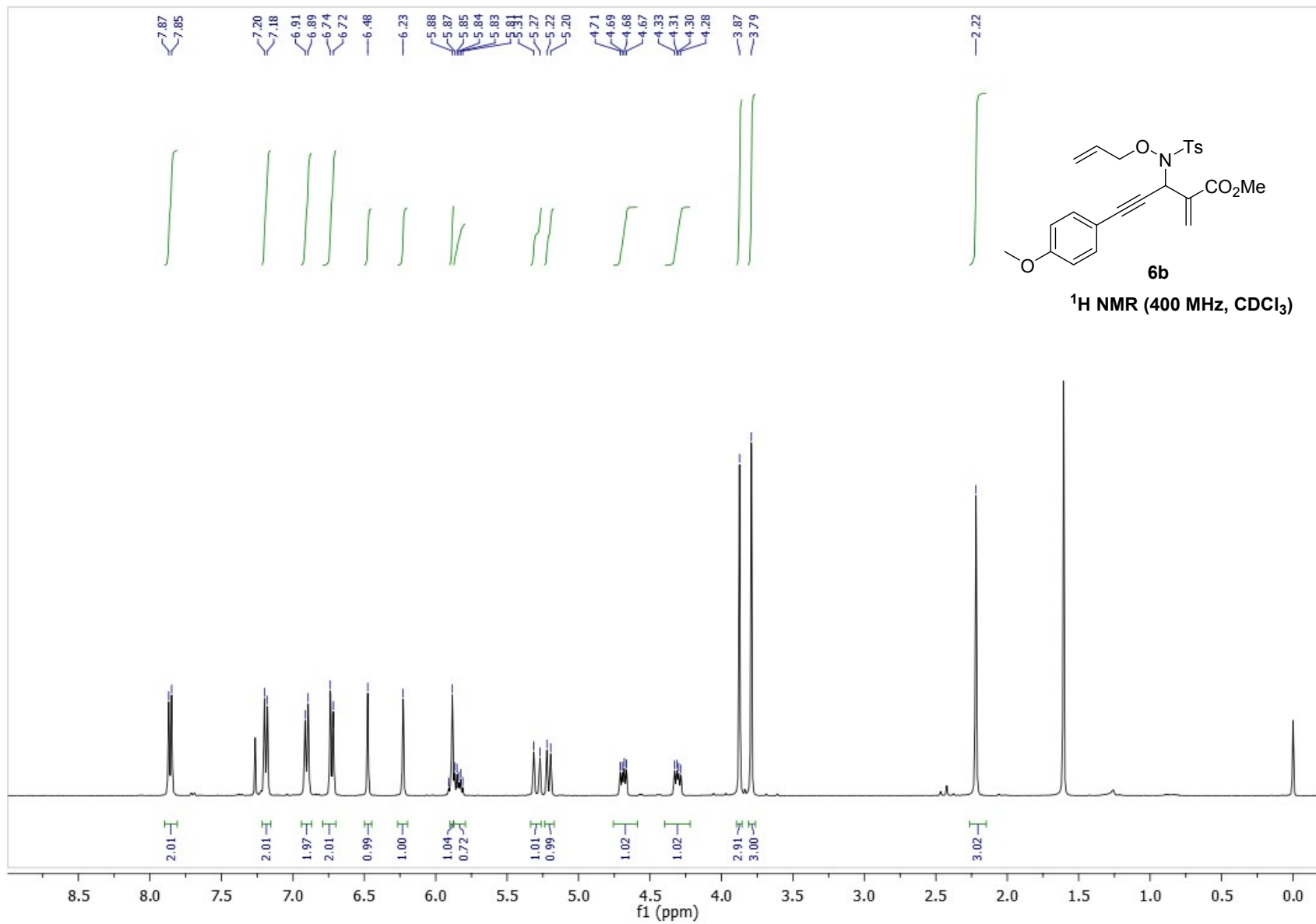
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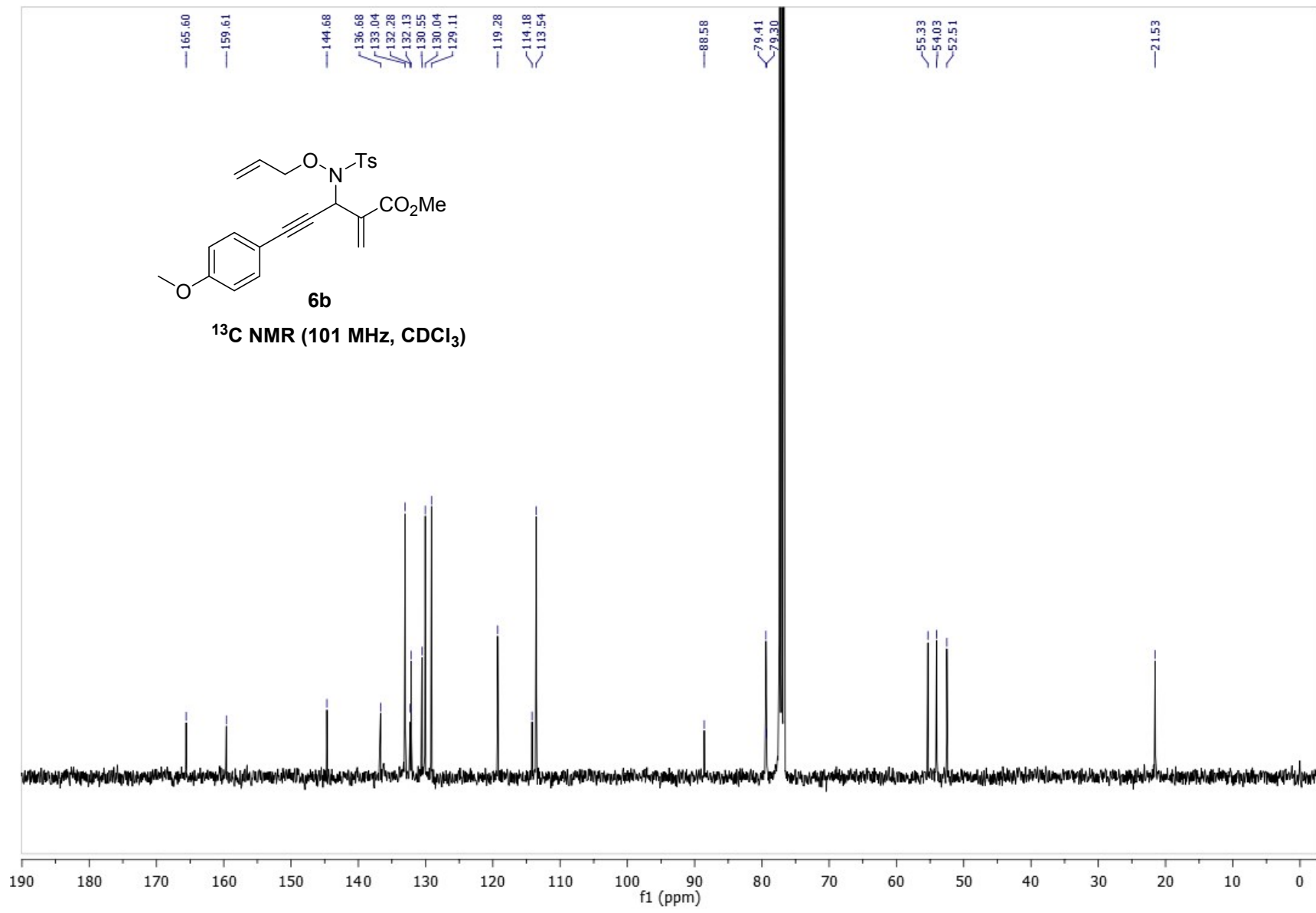


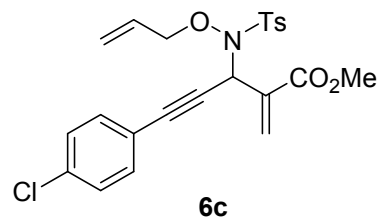




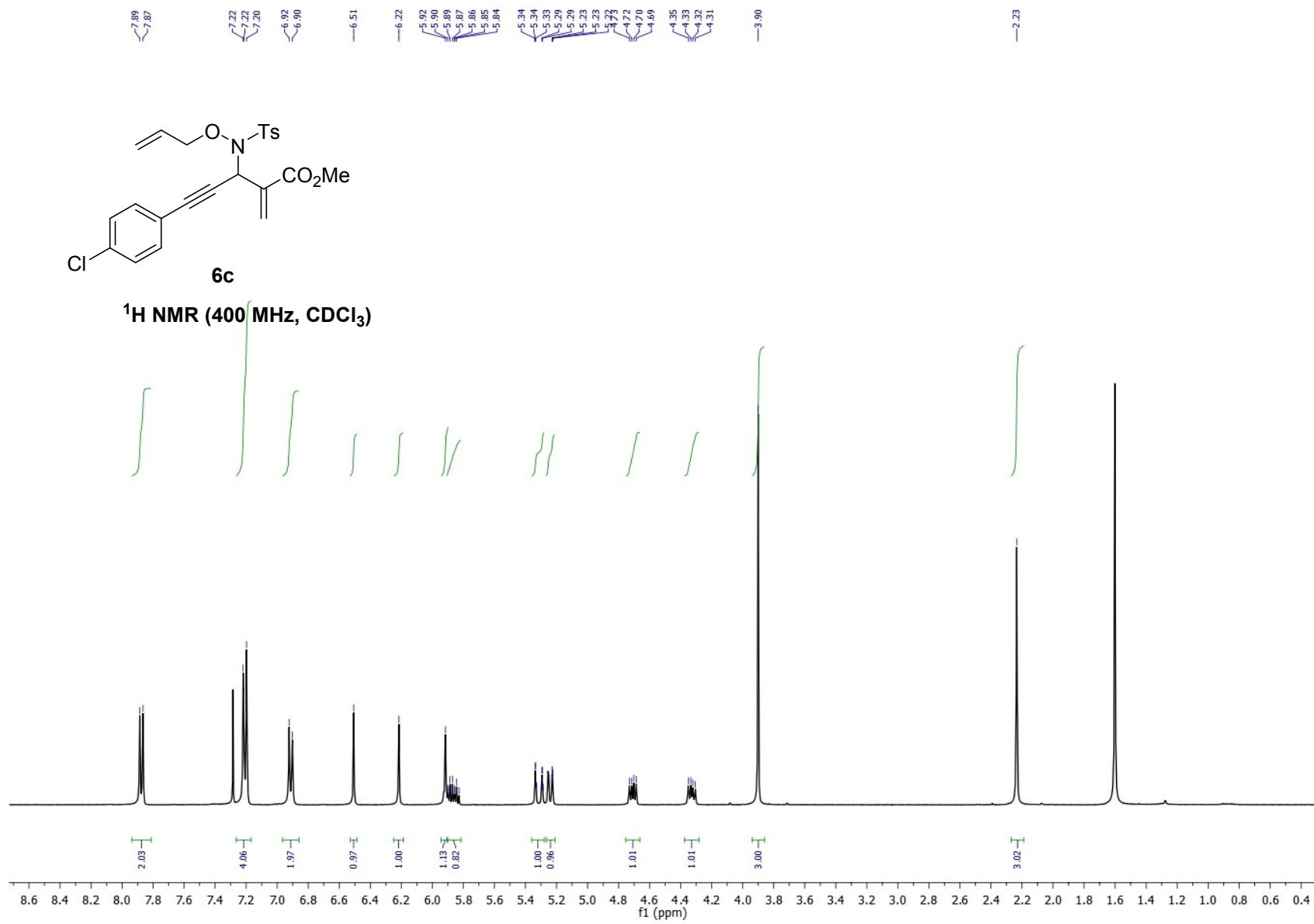




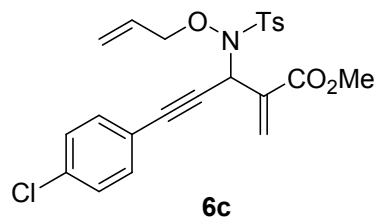




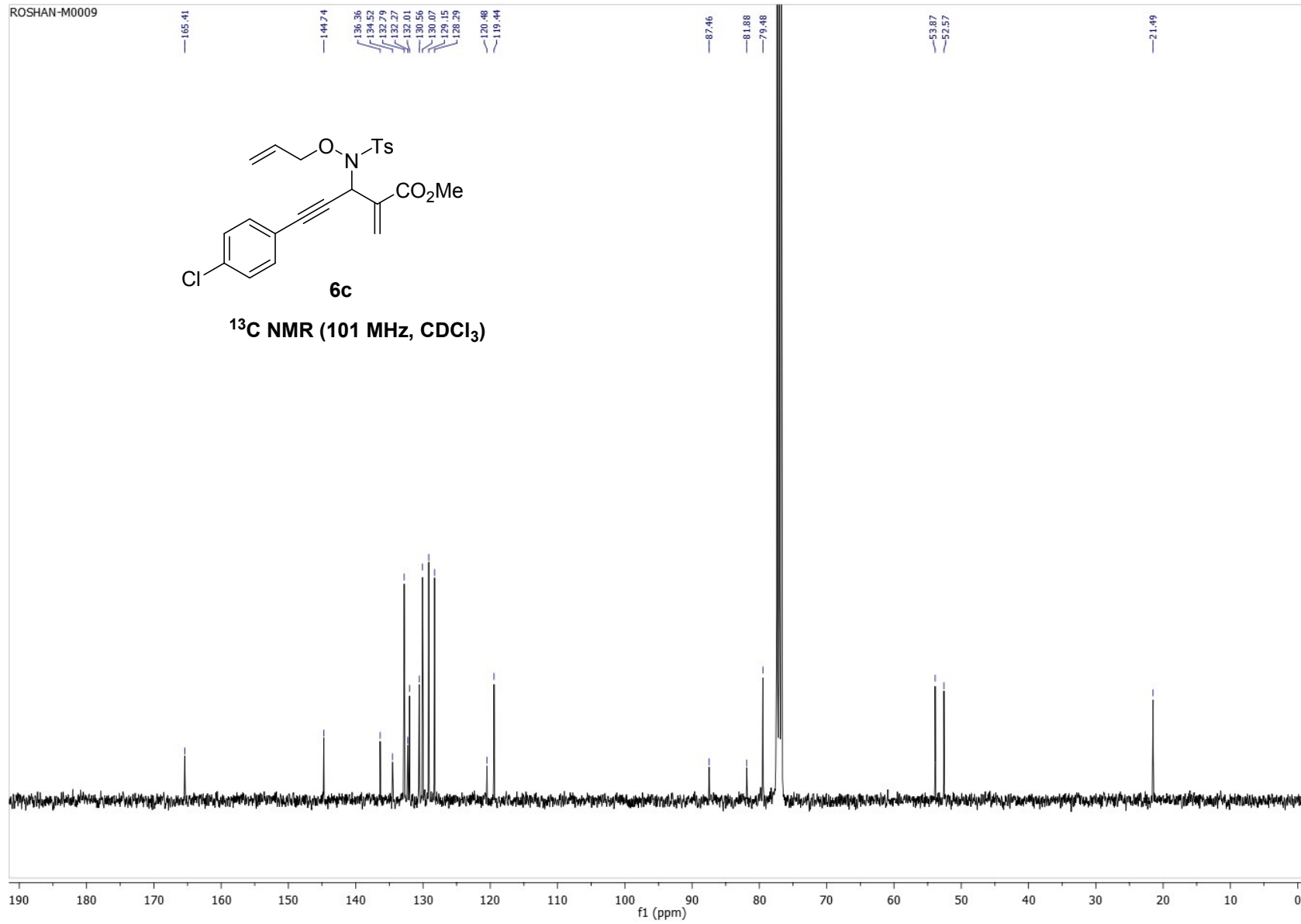
¹H NMR (400 MHz, CDCl₃)

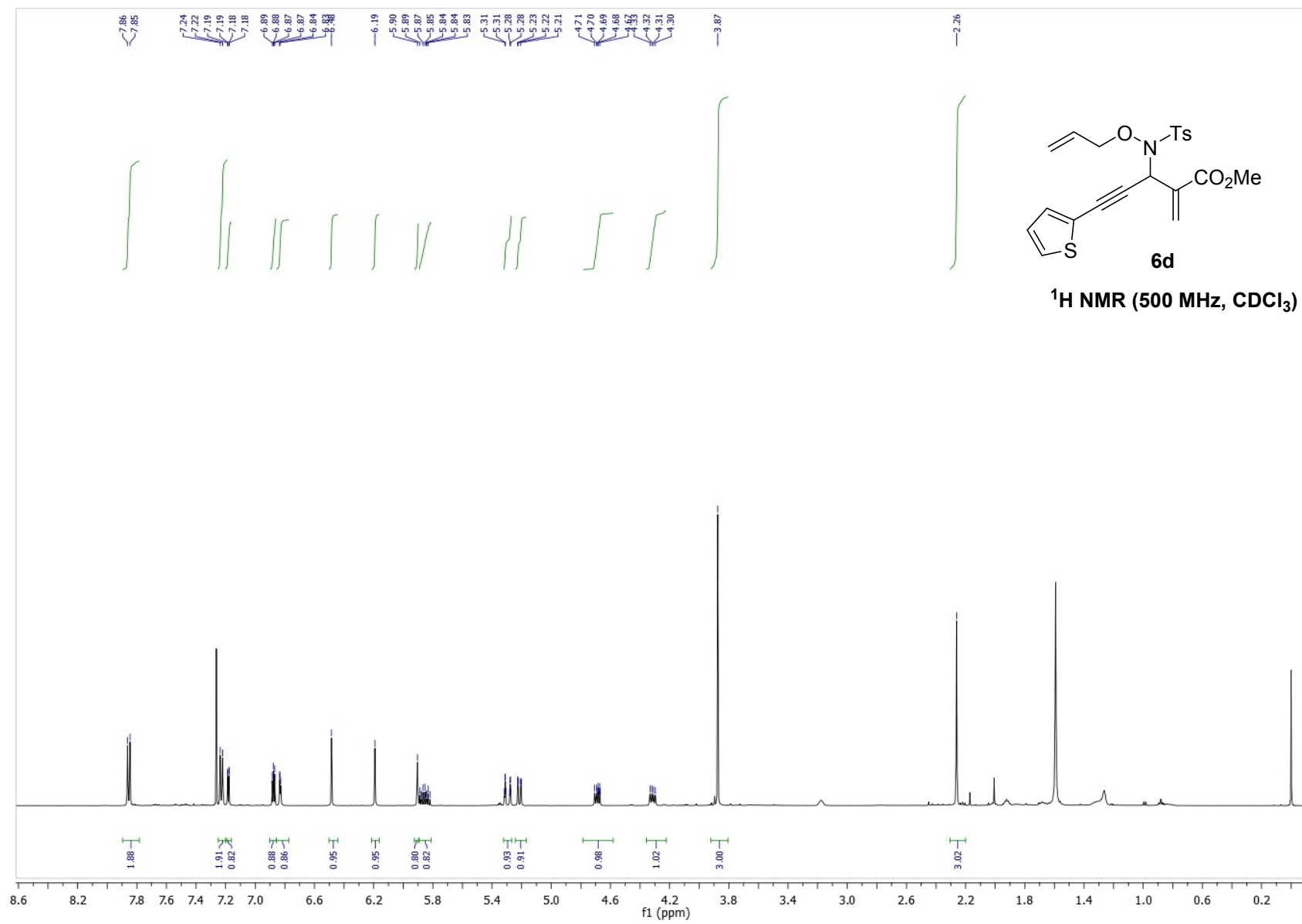


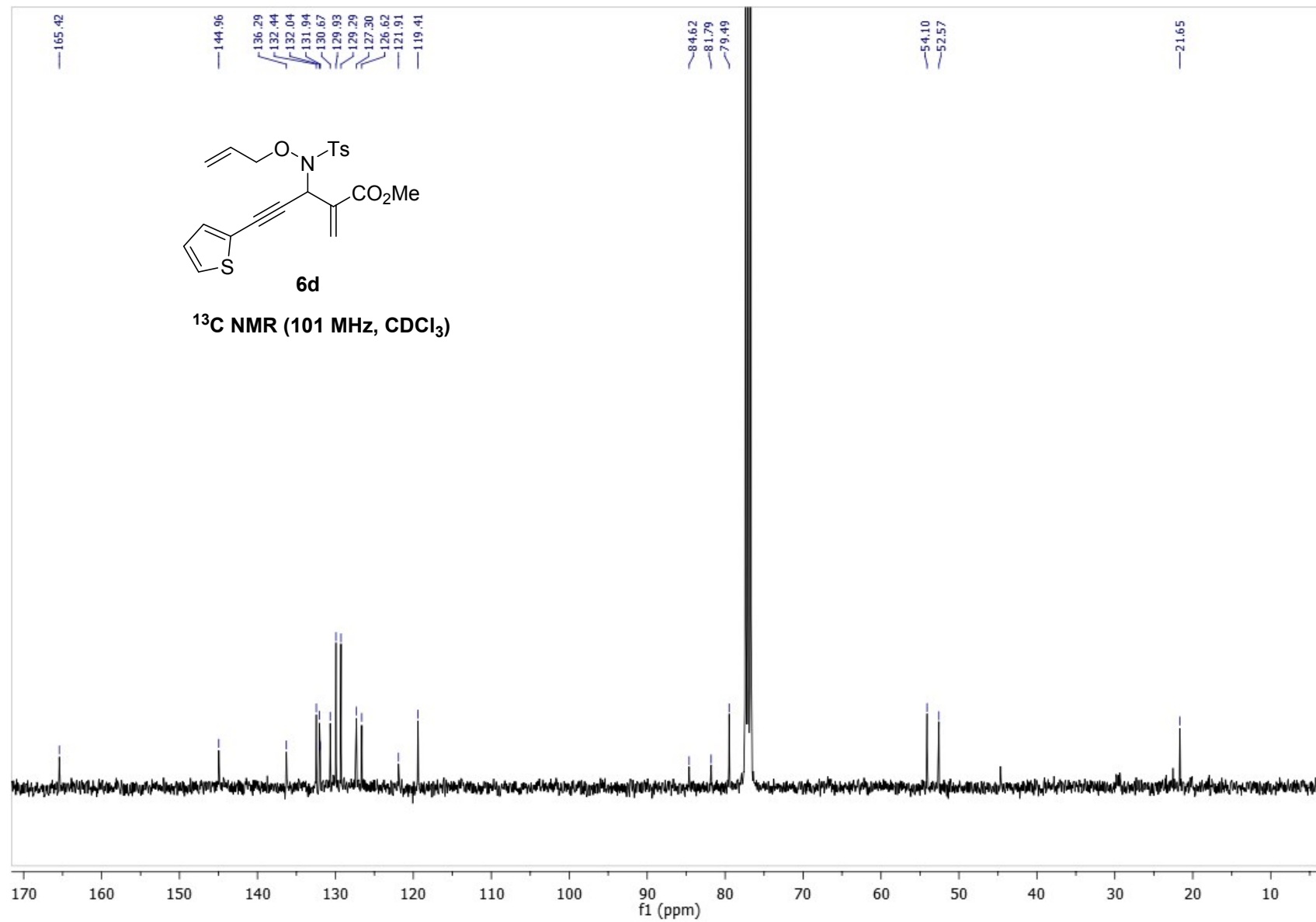
ROSHAN-M0009

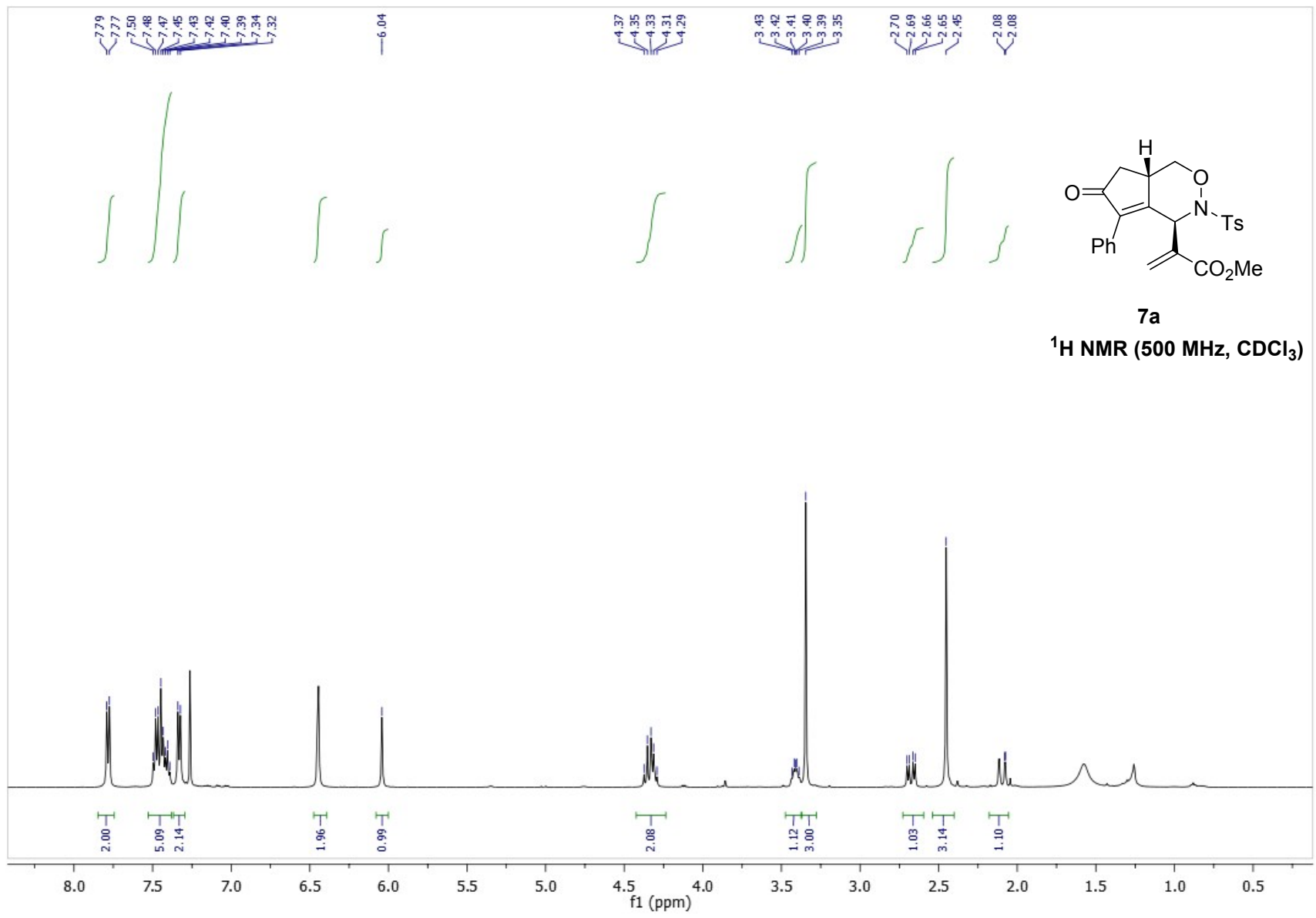


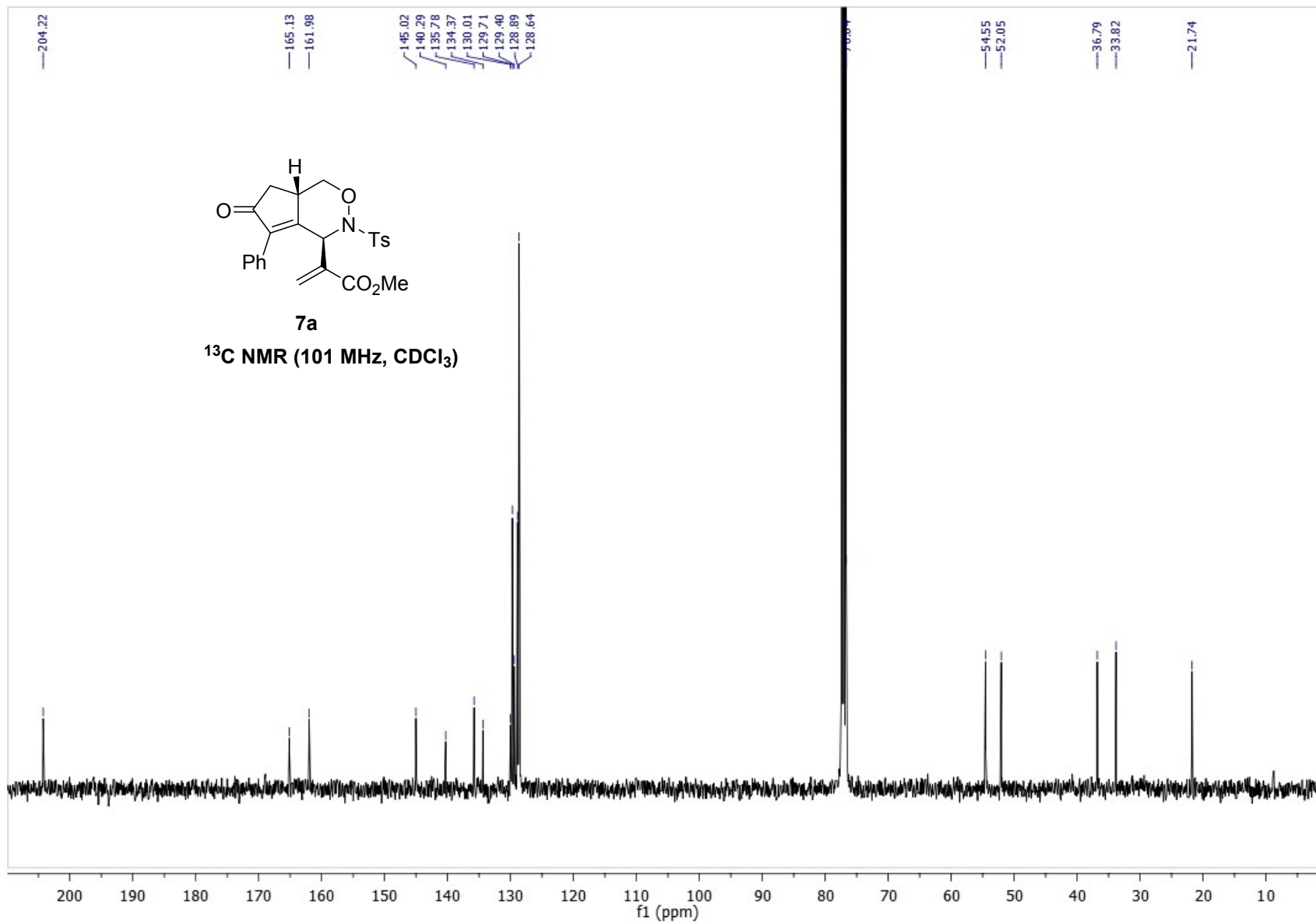
¹³C NMR (101 MHz, CDCl₃)





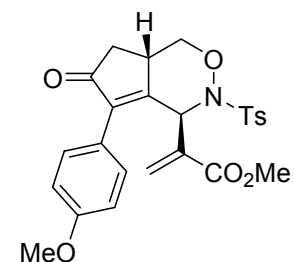




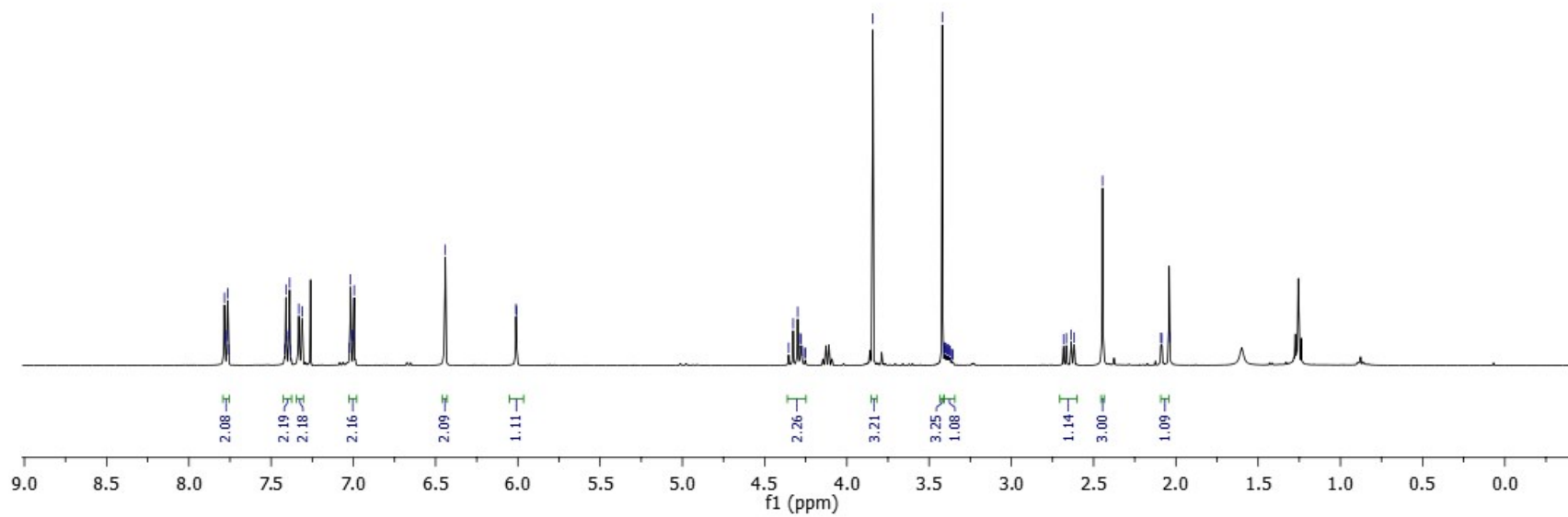


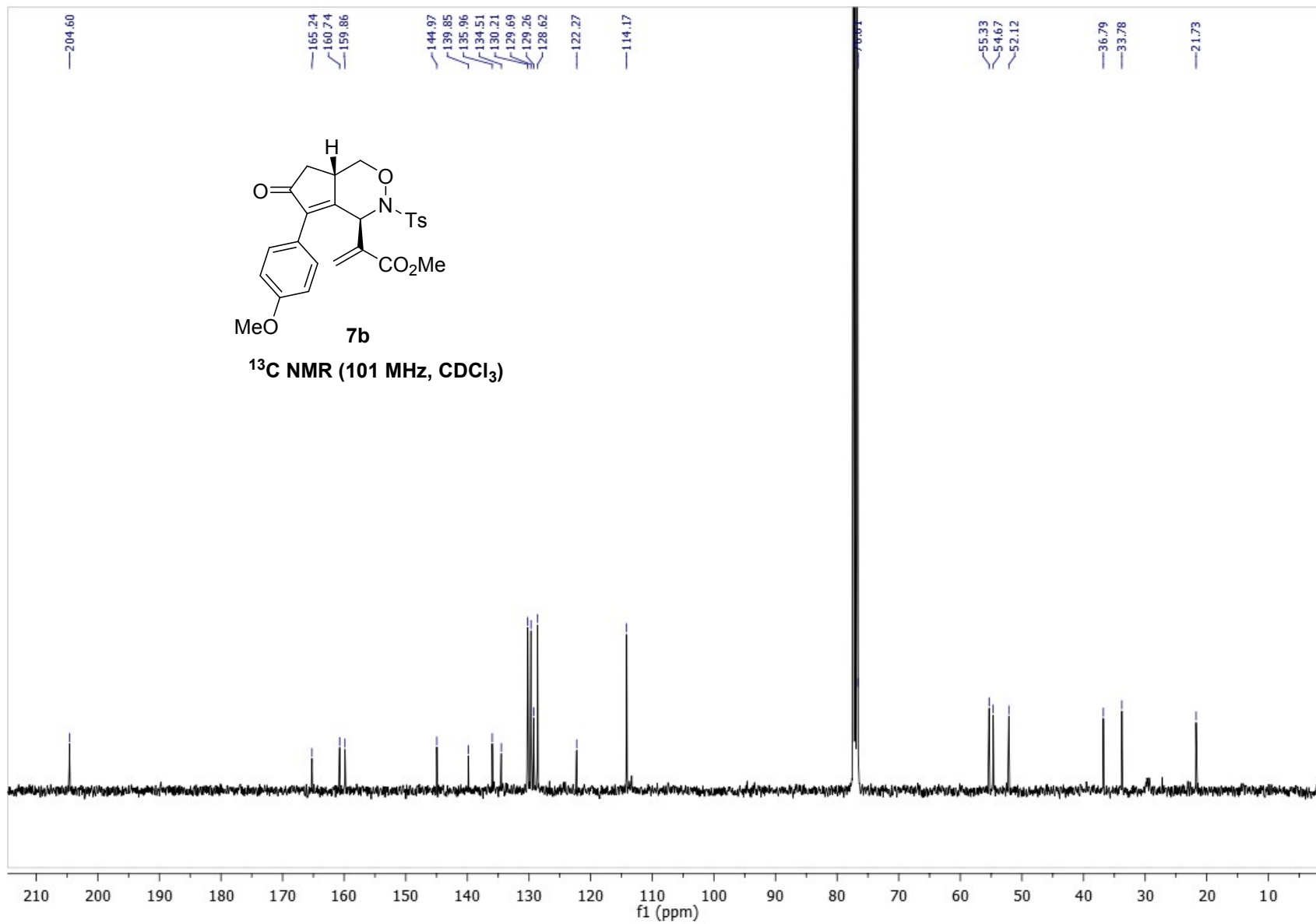
MAHENDER

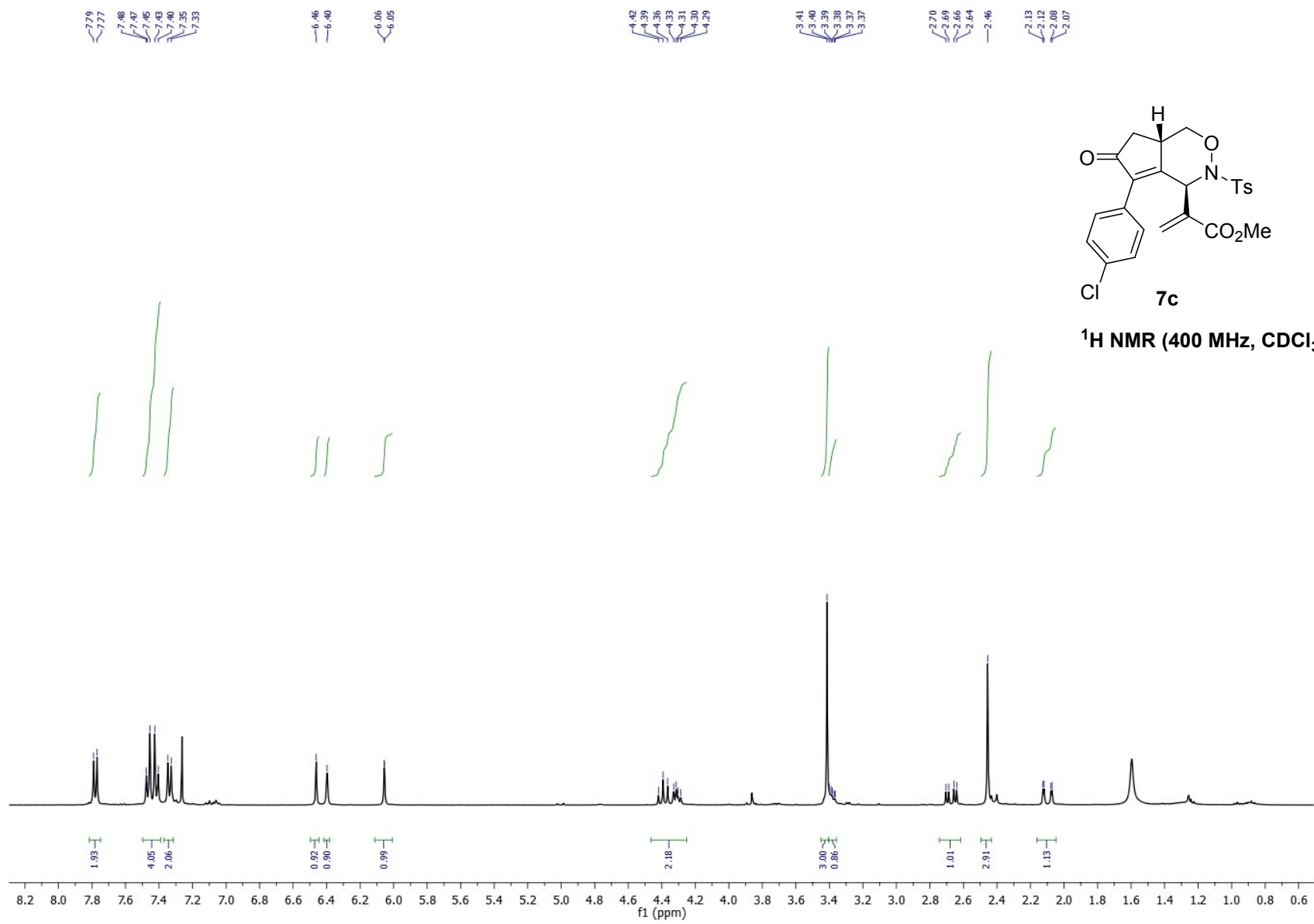
7.78
7.78
7.77
7.76
7.76
7.41
7.39
7.33
7.02
7.01
7.00
7.00
6.44
6.01
6.01
4.35
4.33
4.30
4.28
4.28
4.27
4.26
4.25
3.84
3.42
3.41
3.41
3.40
3.40
3.39
3.38
3.37
2.67
2.64
2.62
2.45
2.09
2.08
2.04

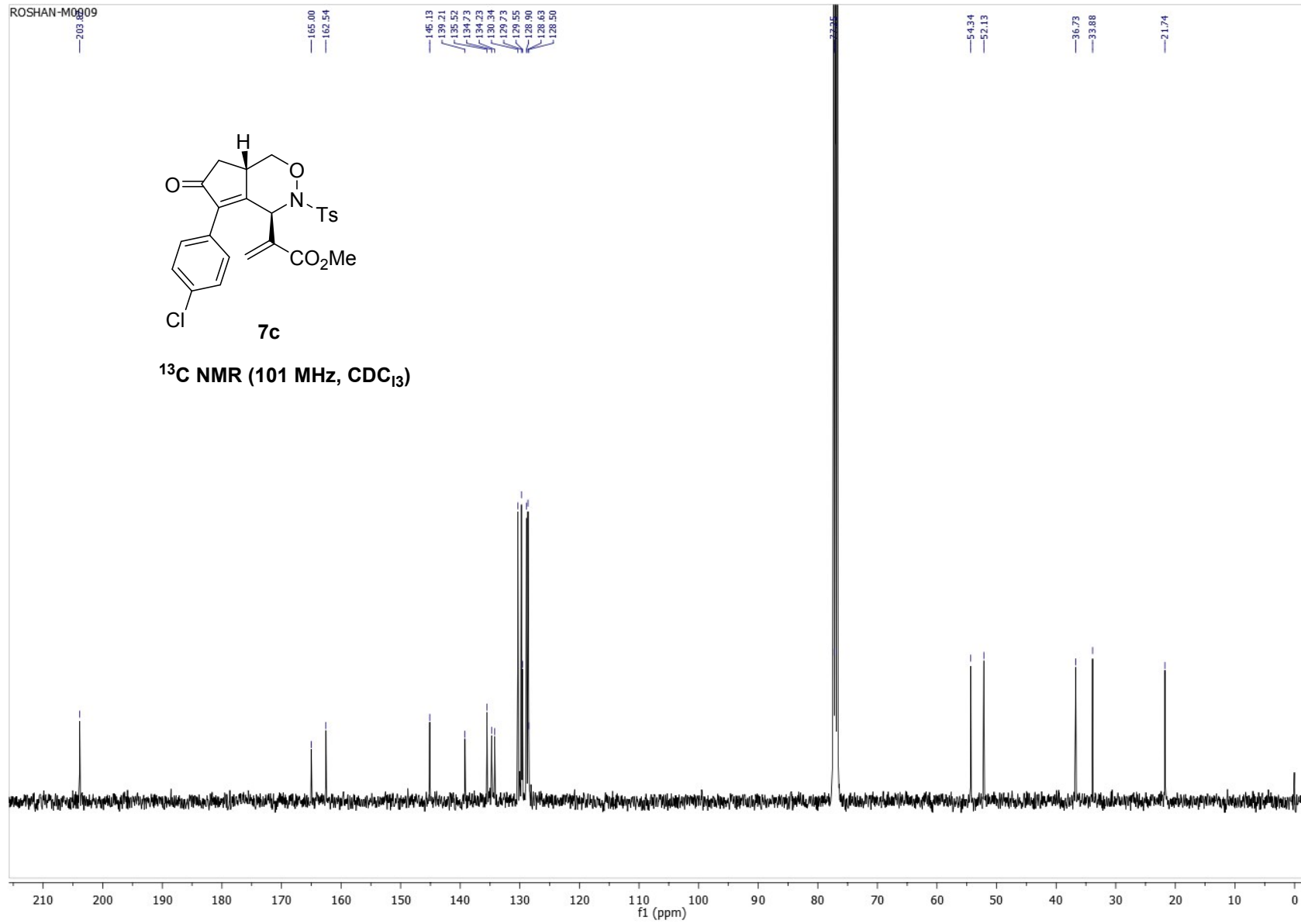


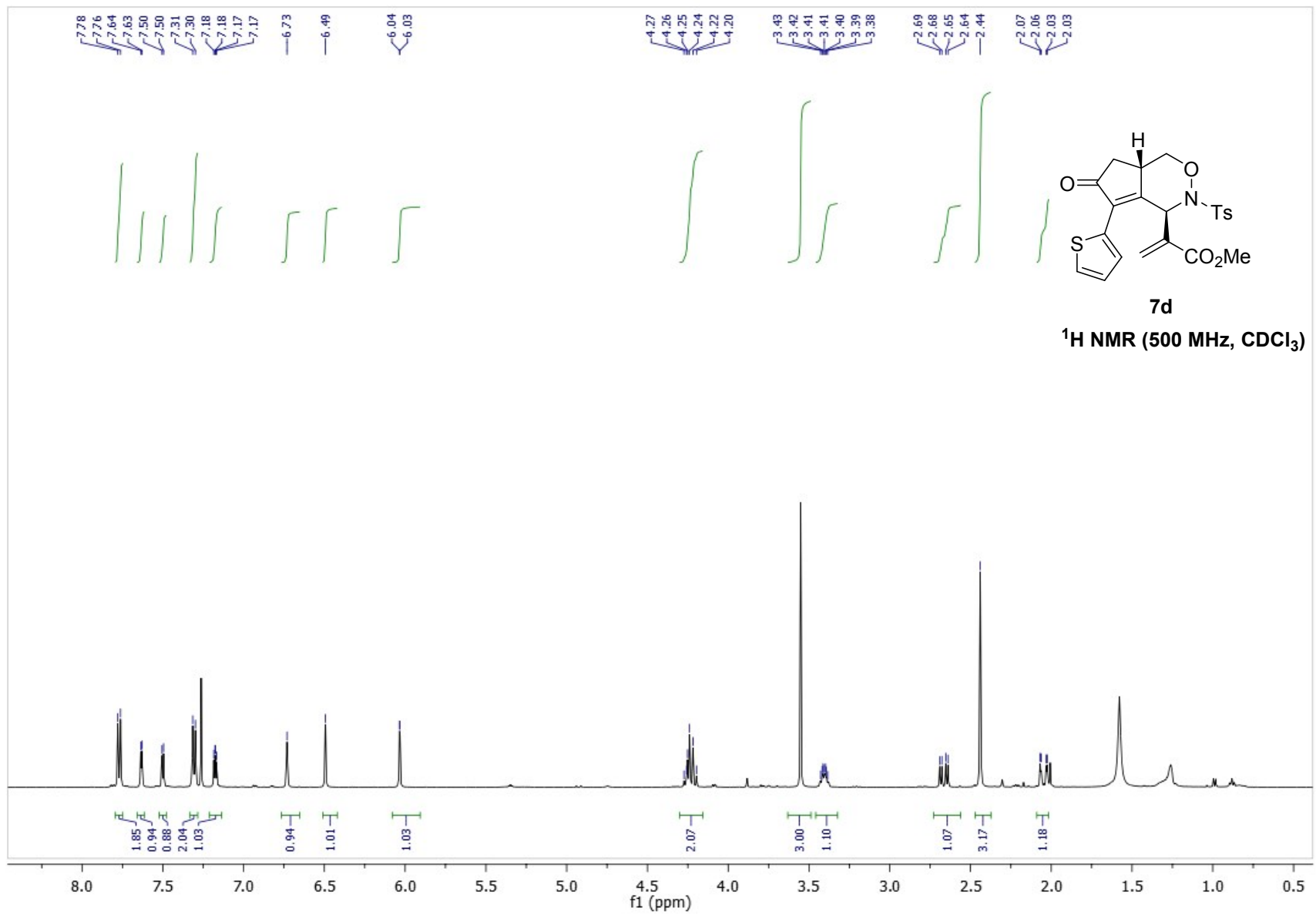
$^1\text{H NMR}$ (400 MHz, CDCl_3)

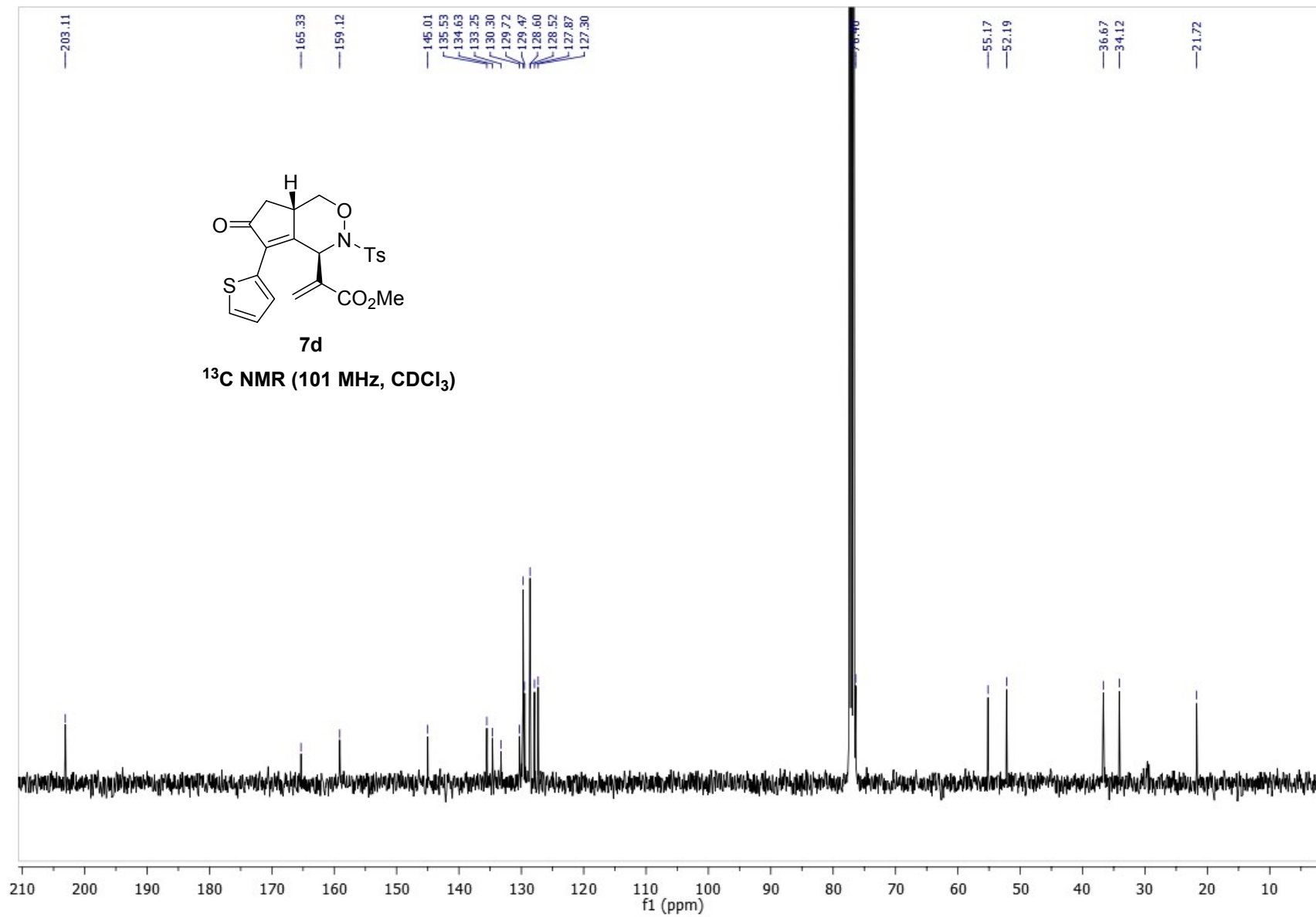


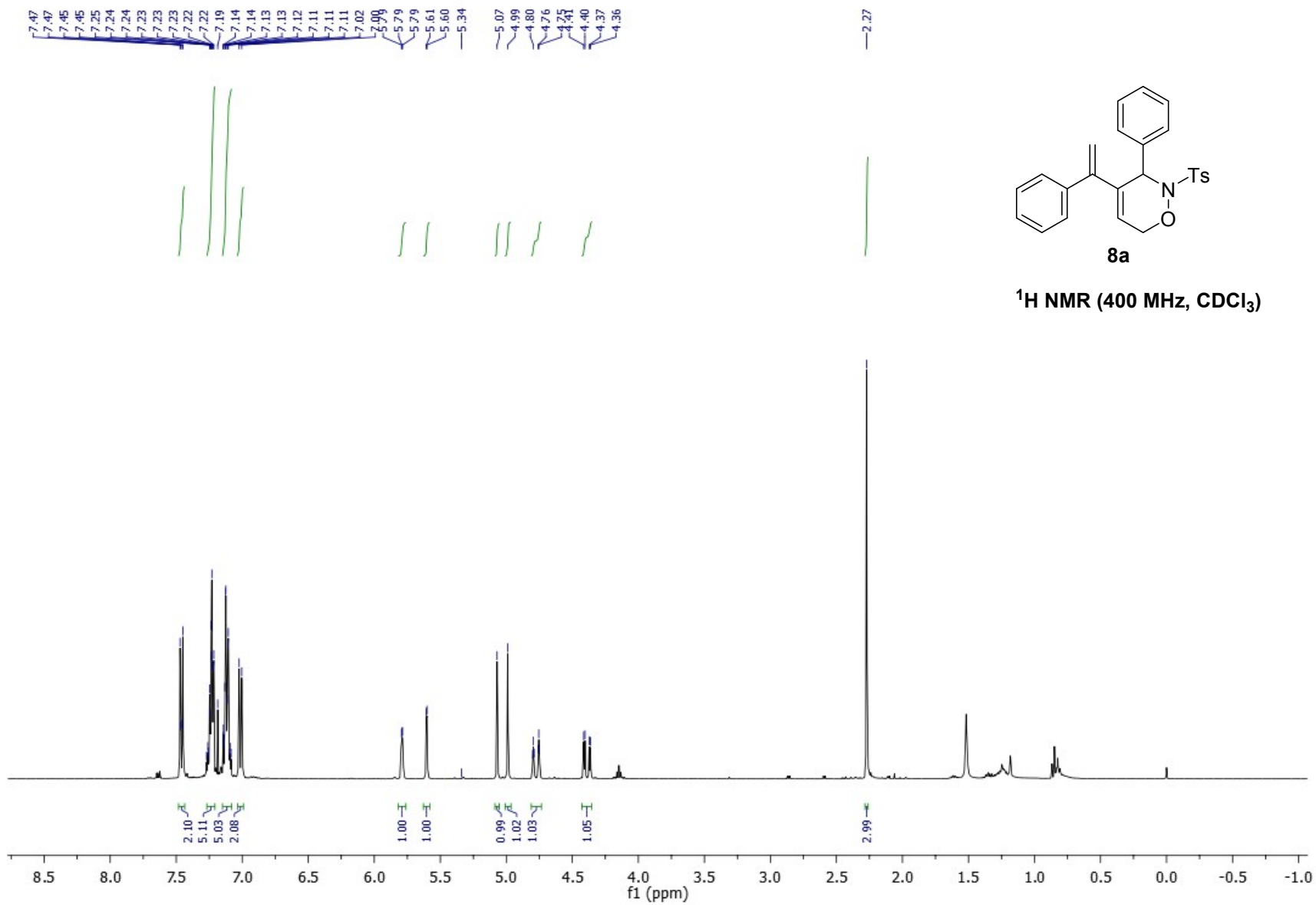










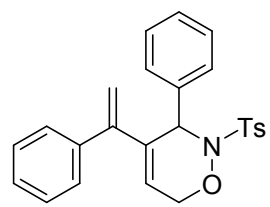


146.33
143.86
140.24
136.53
136.37
134.10
129.28
129.02
128.54
128.46
128.25
128.16
127.74
124.28
115.57

69.63

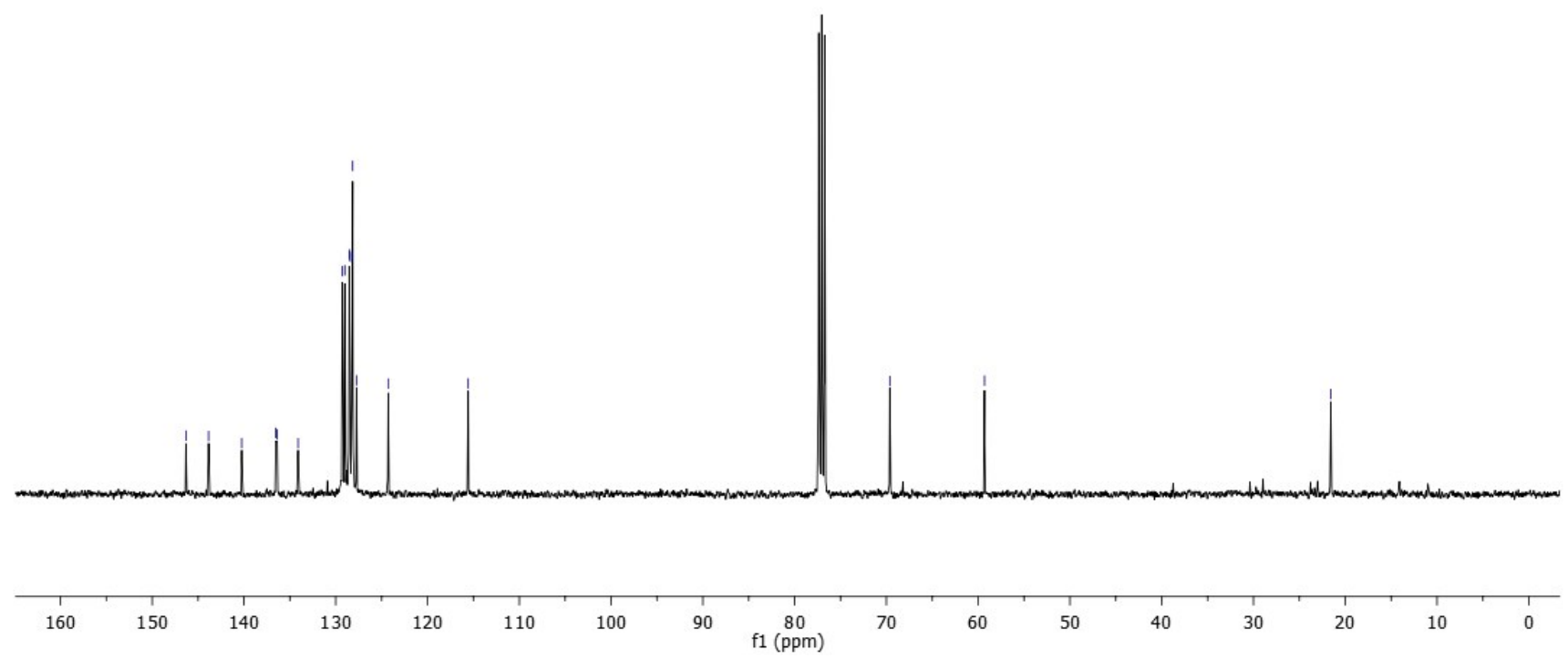
59.30

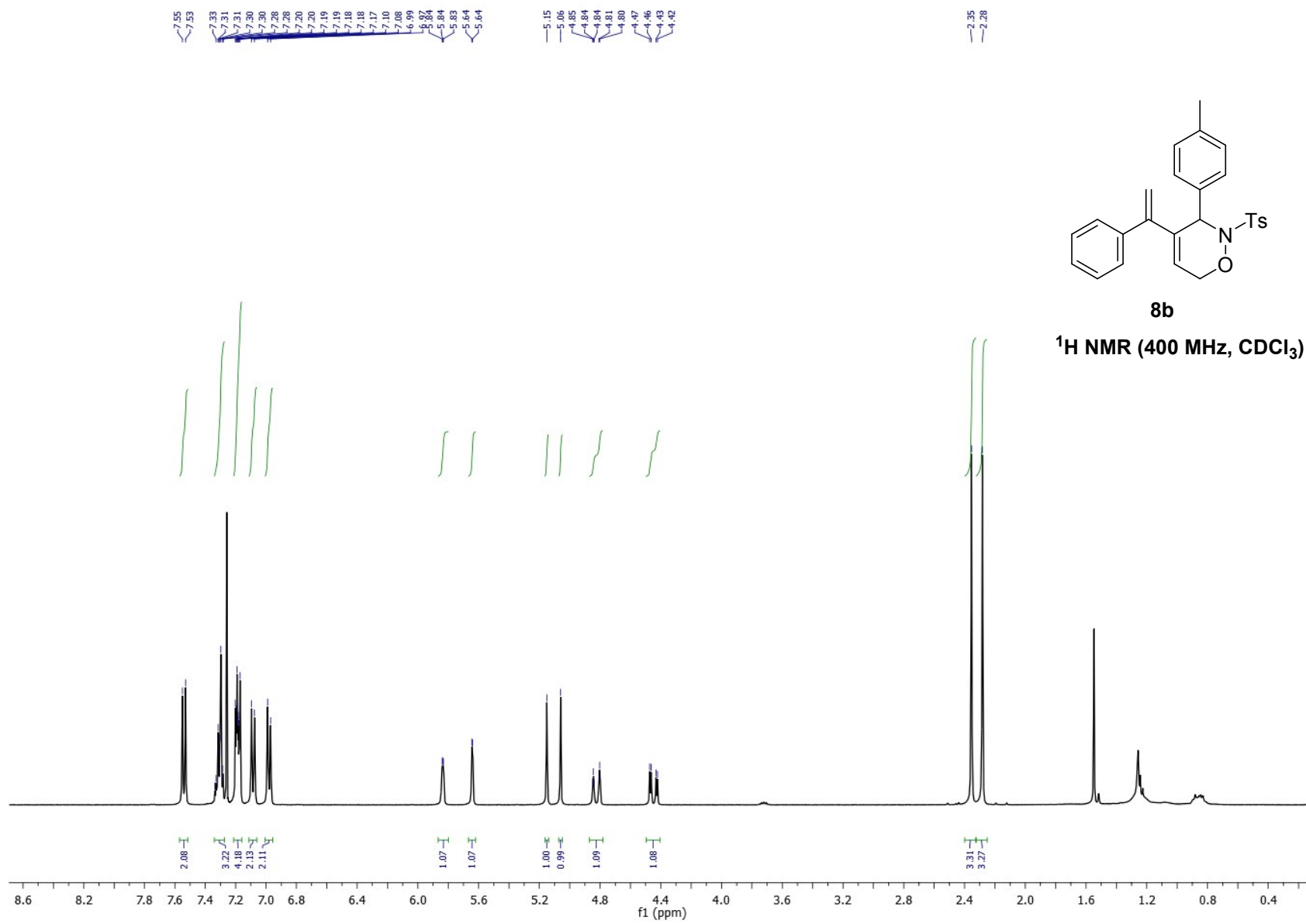
21.57



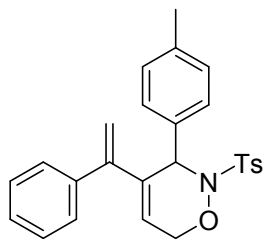
8a

¹³C NMR (101 MHz, CDCl₃)





146.34
143.75
140.34
137.99
136.61
134.22
133.37
129.15
128.93
128.83
128.57
128.49
128.22
127.70
124.22
115.49



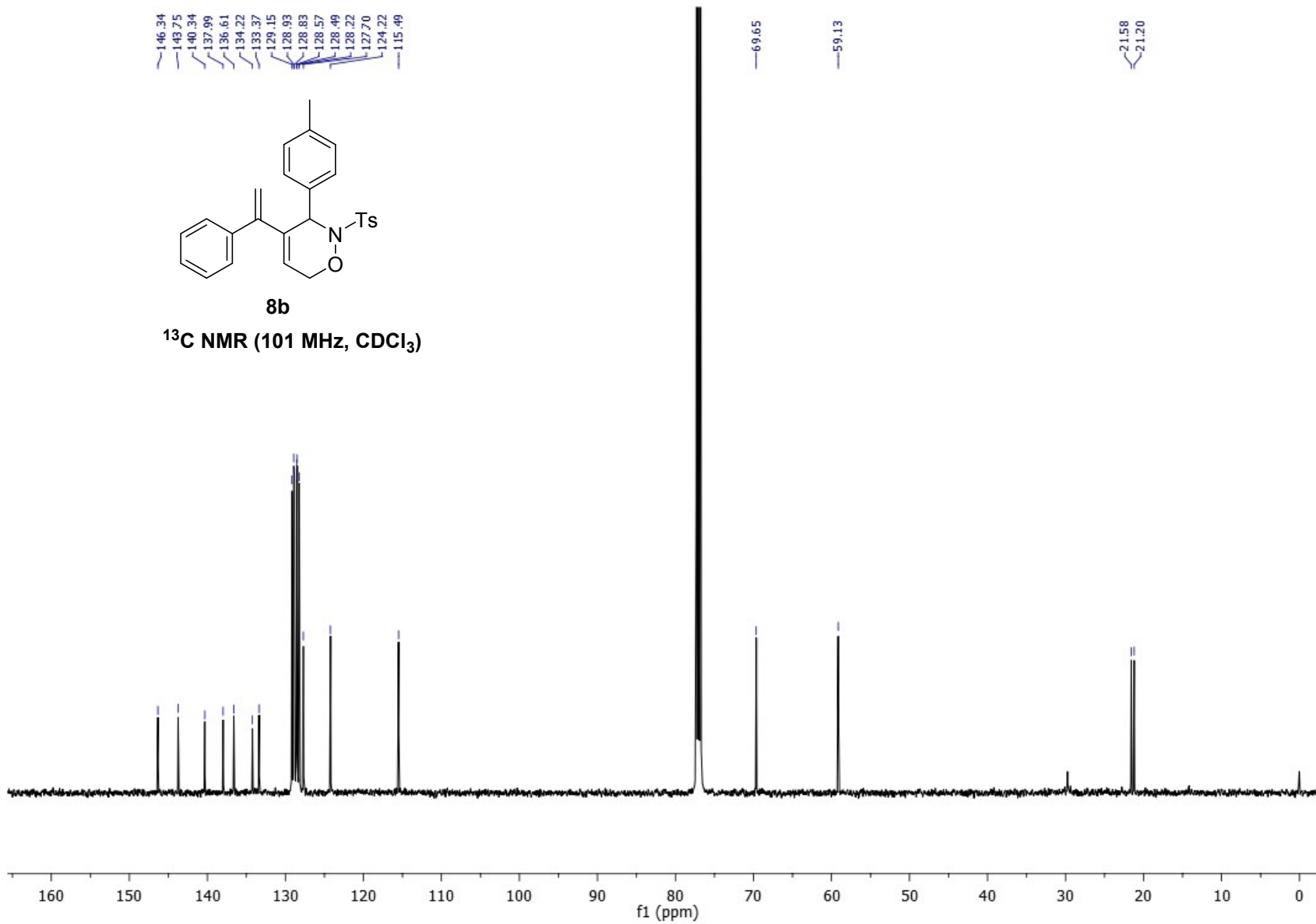
8b

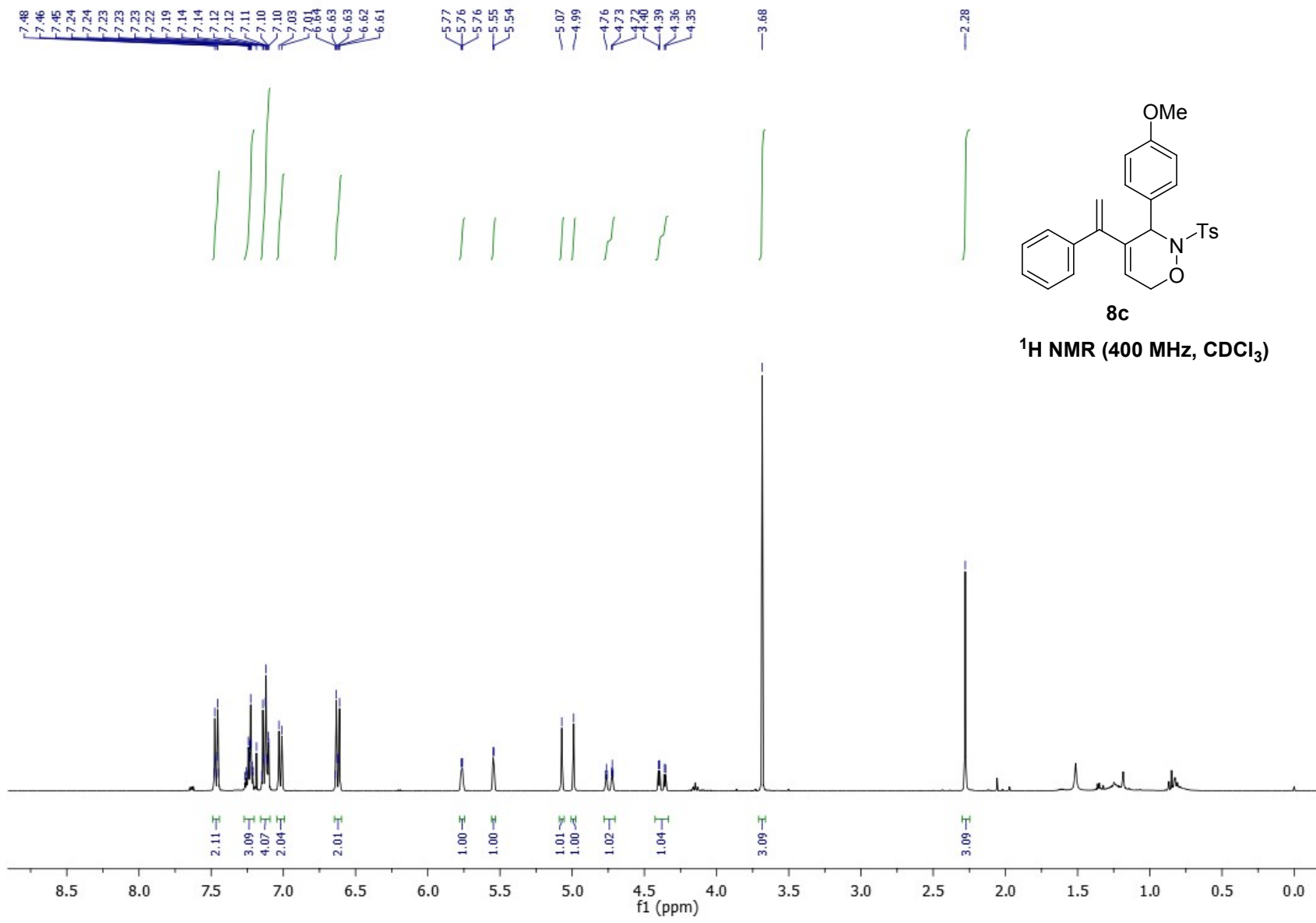
^{13}C NMR (101 MHz, CDCl_3)

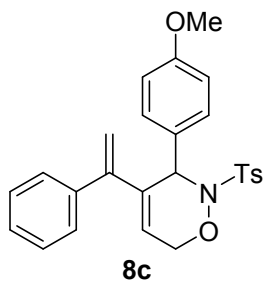
69.65

59.13

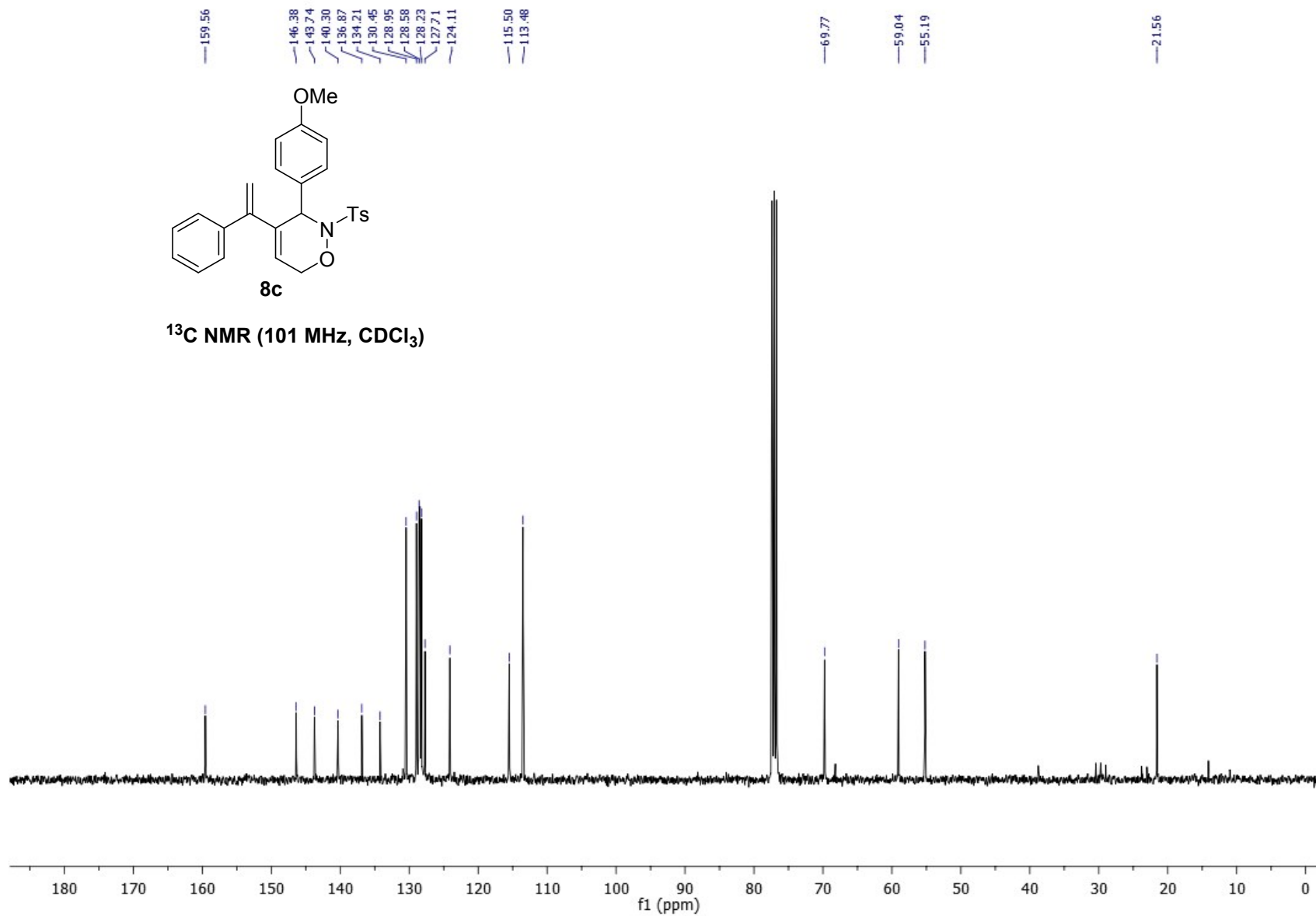
21.58
21.20

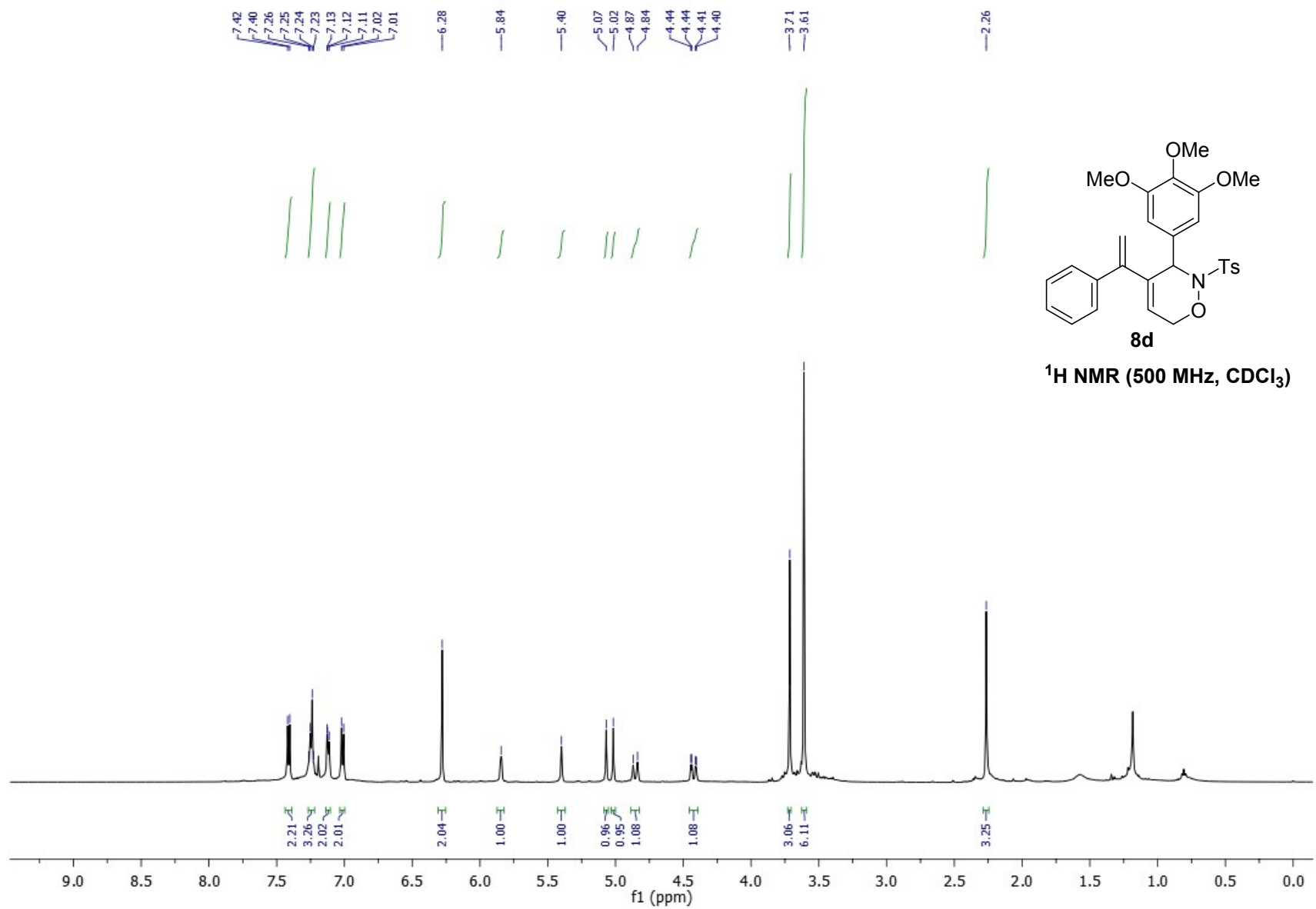


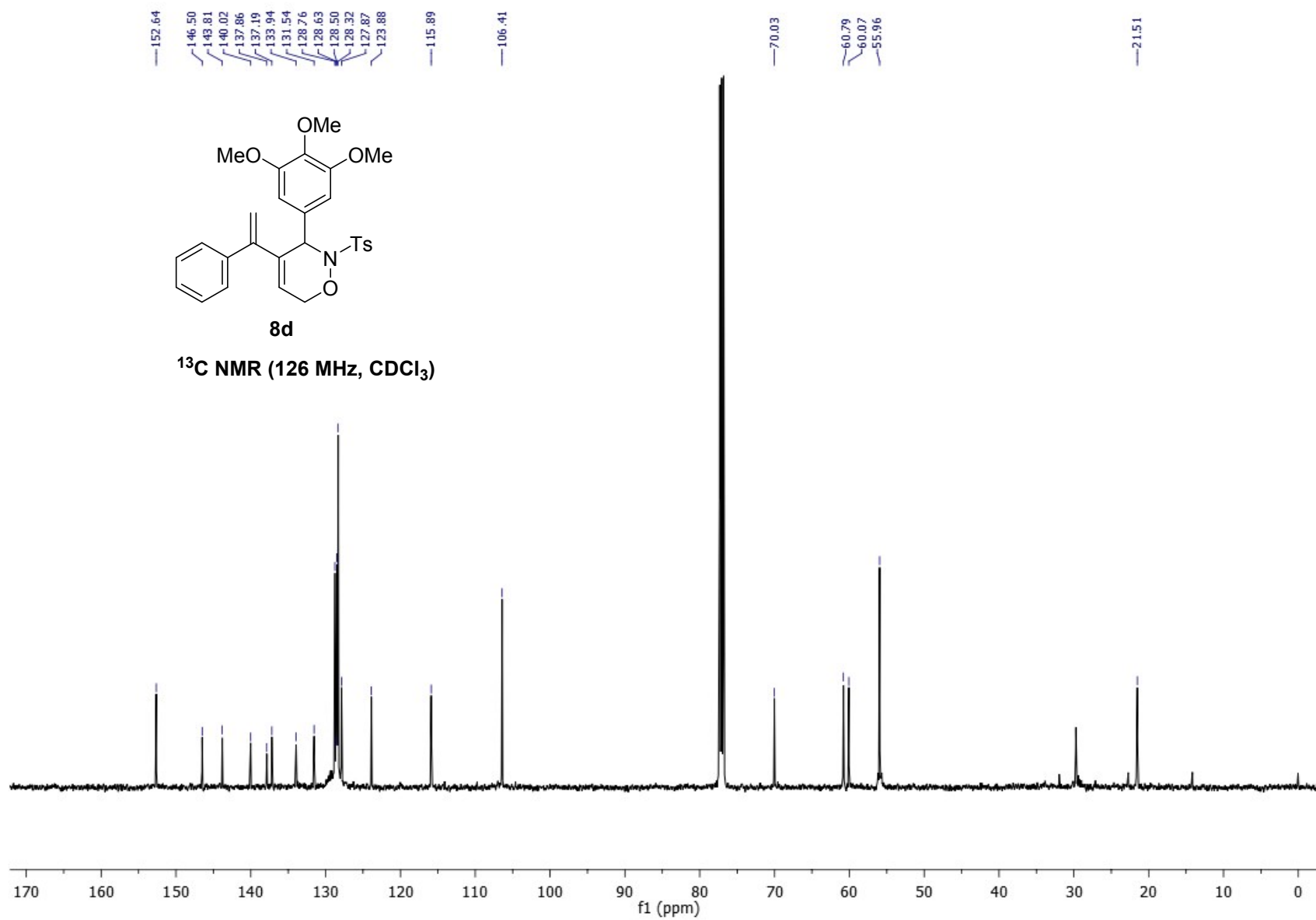


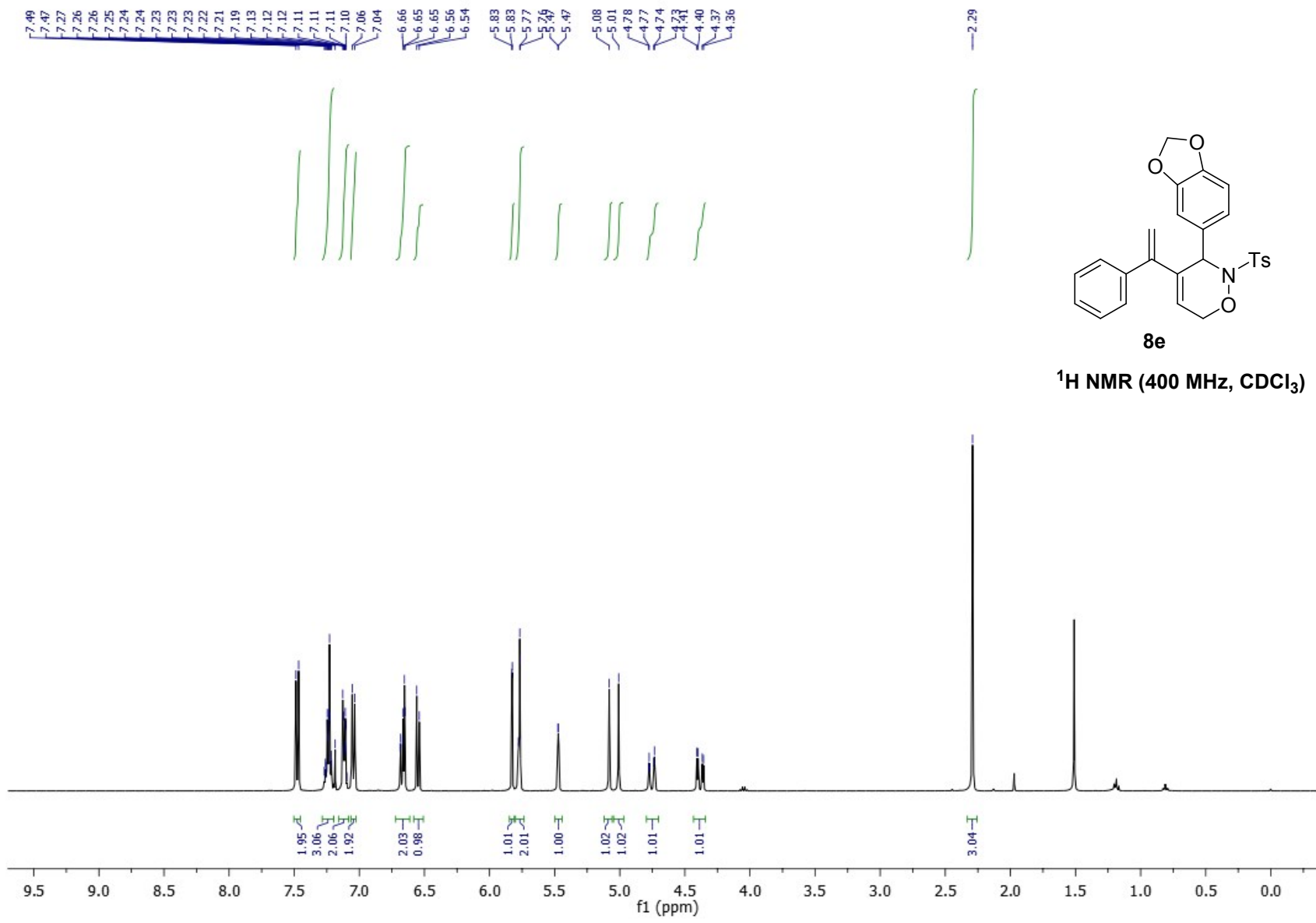


¹³C NMR (101 MHz, CDCl₃)

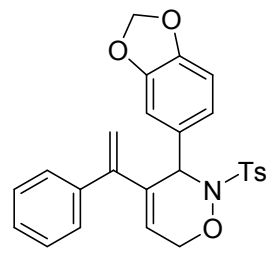






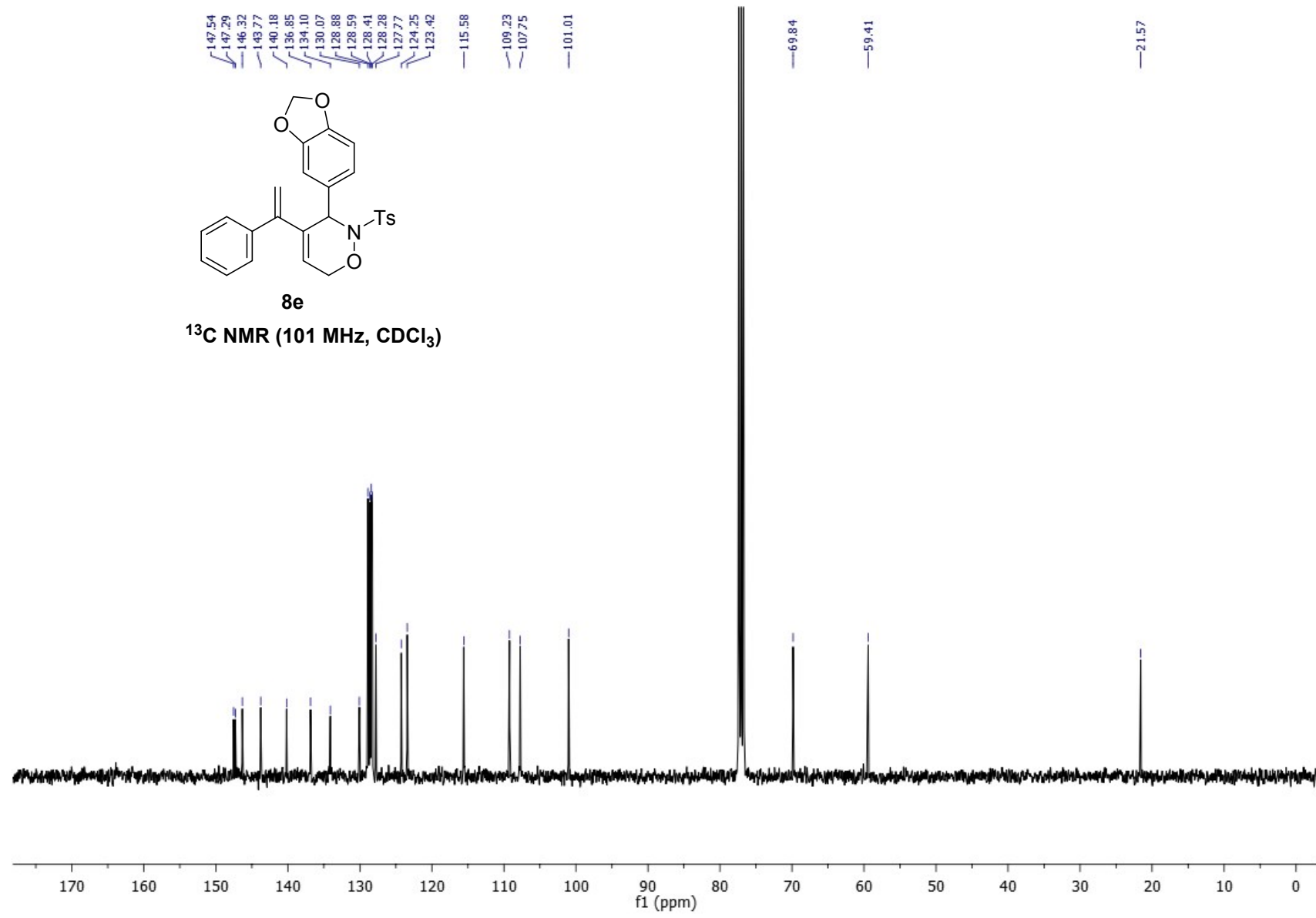


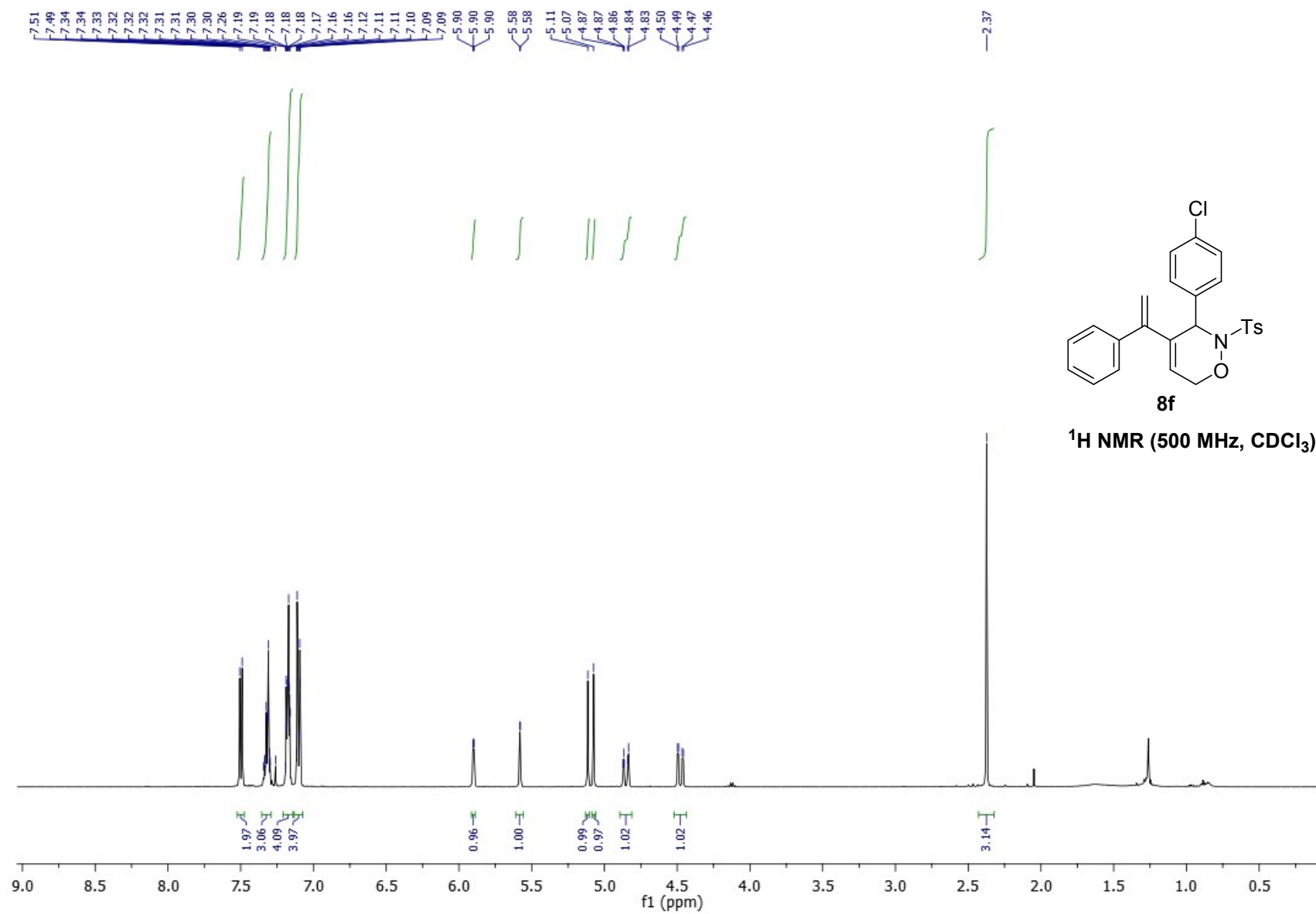
147.54
147.29
146.32
143.77
140.18
136.85
134.10
130.07
128.88
128.59
128.41
128.28
127.77
124.25
123.42
115.58
109.23
107.75
101.01
69.84
59.41
21.57

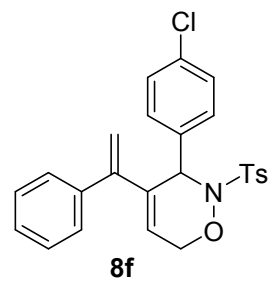


8e

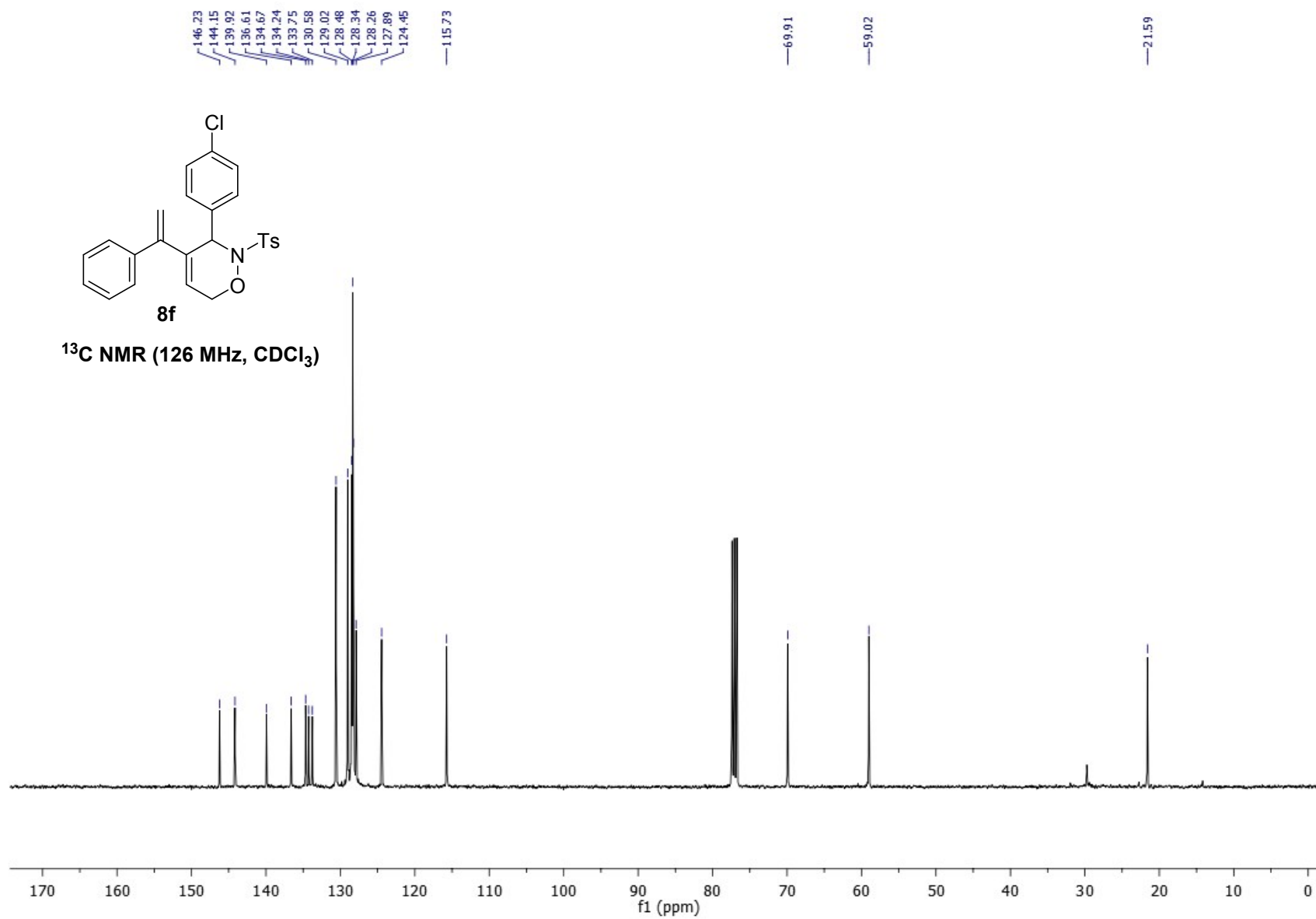
¹³C NMR (101 MHz, CDCl₃)

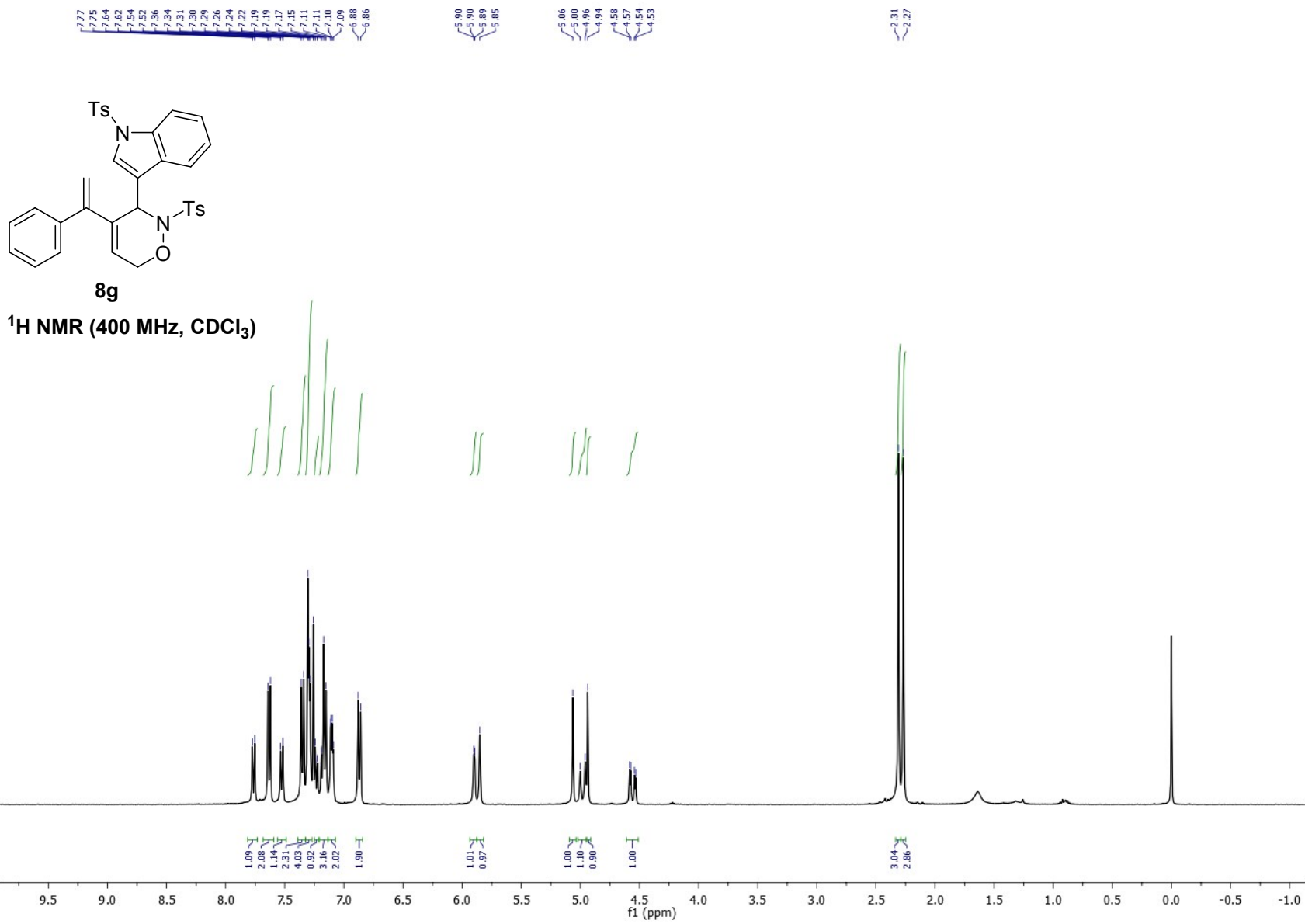


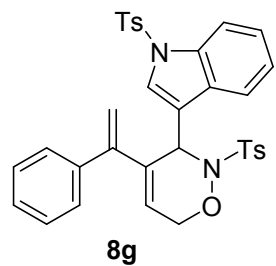




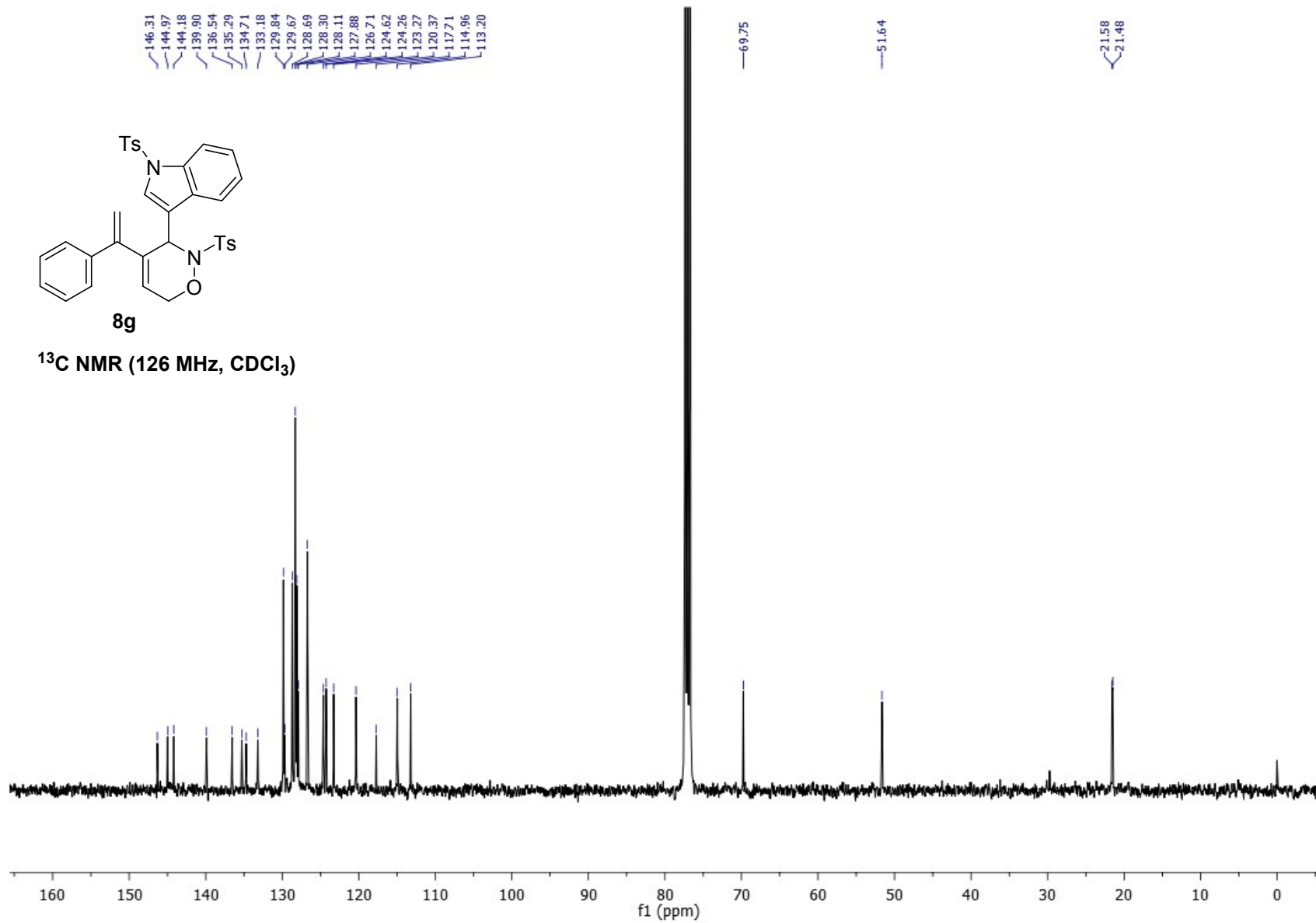
¹³C NMR (126 MHz, CDCl₃)

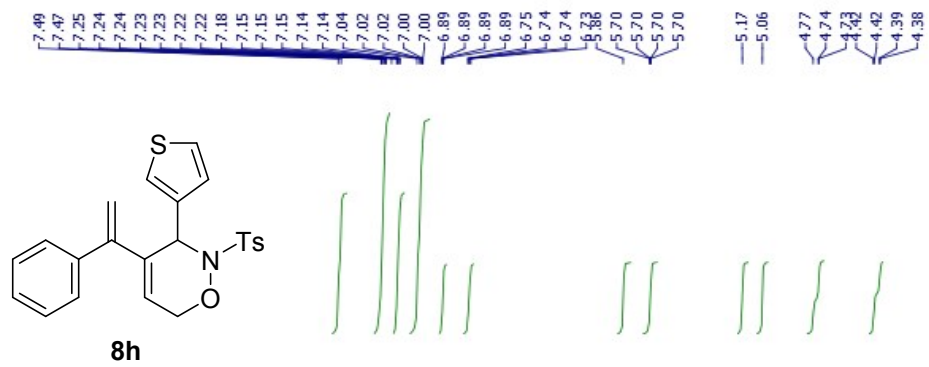




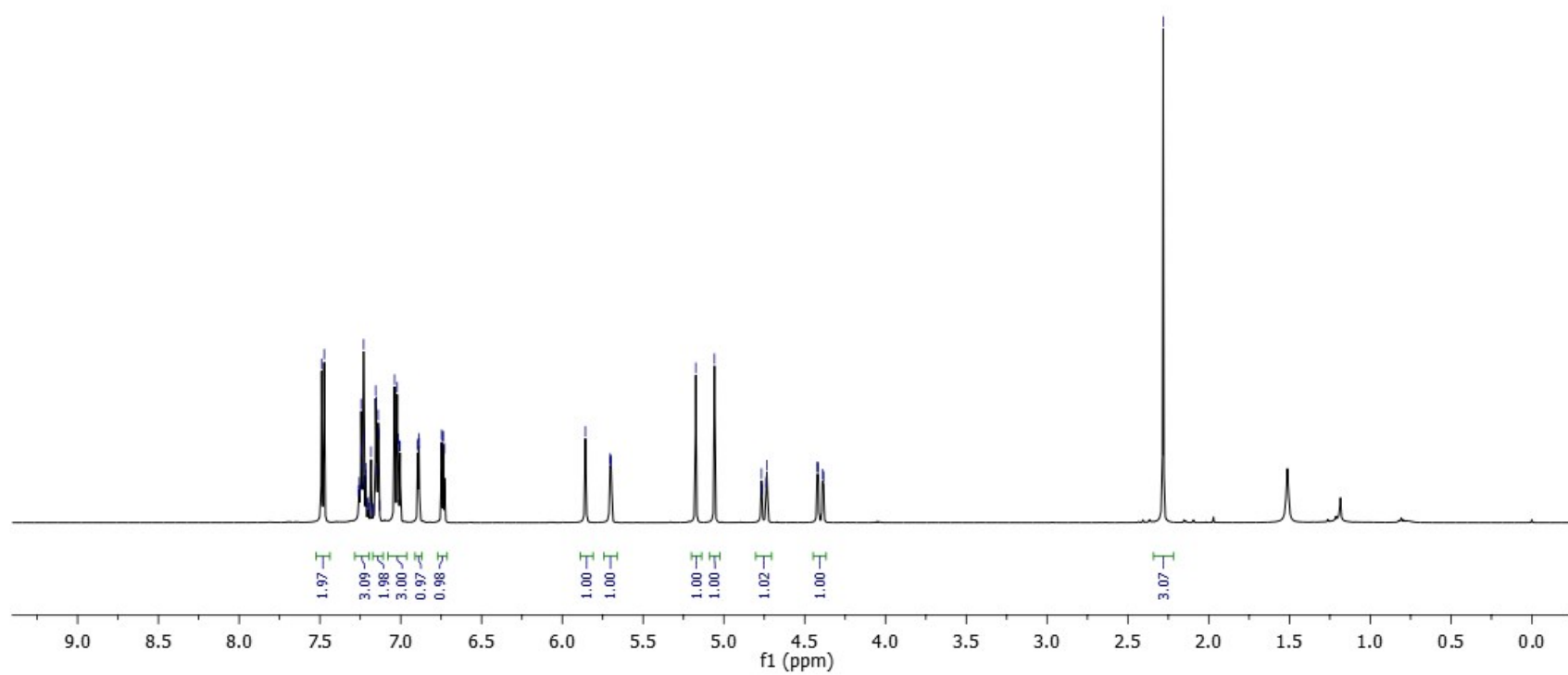


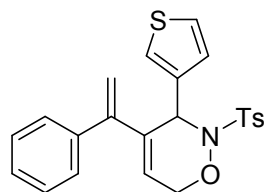
¹³C NMR (126 MHz, CDCl₃)





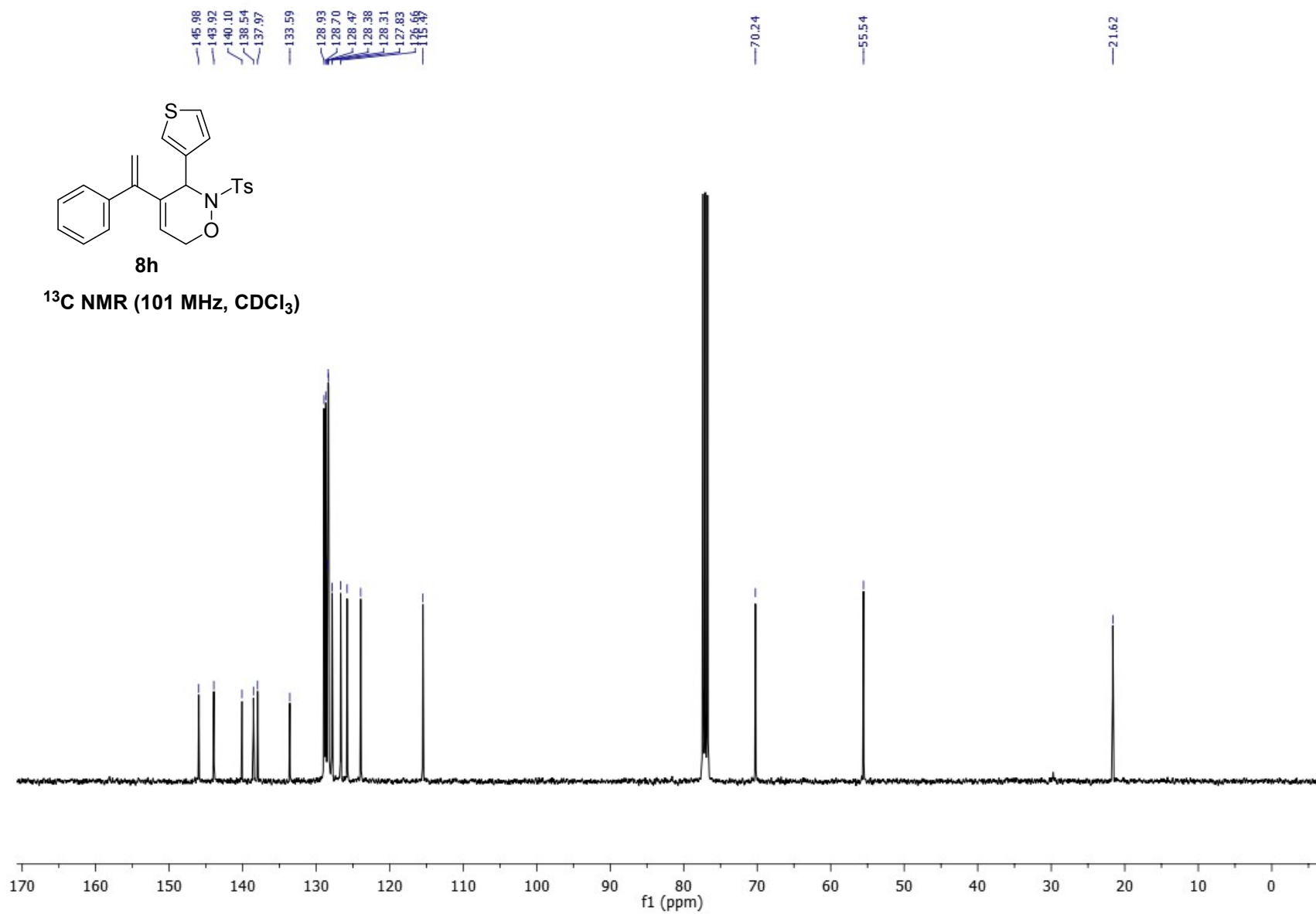
¹H NMR (500 MHz, CDCl₃)

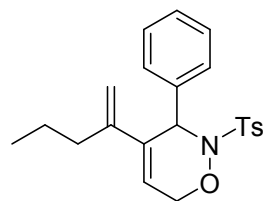




8h

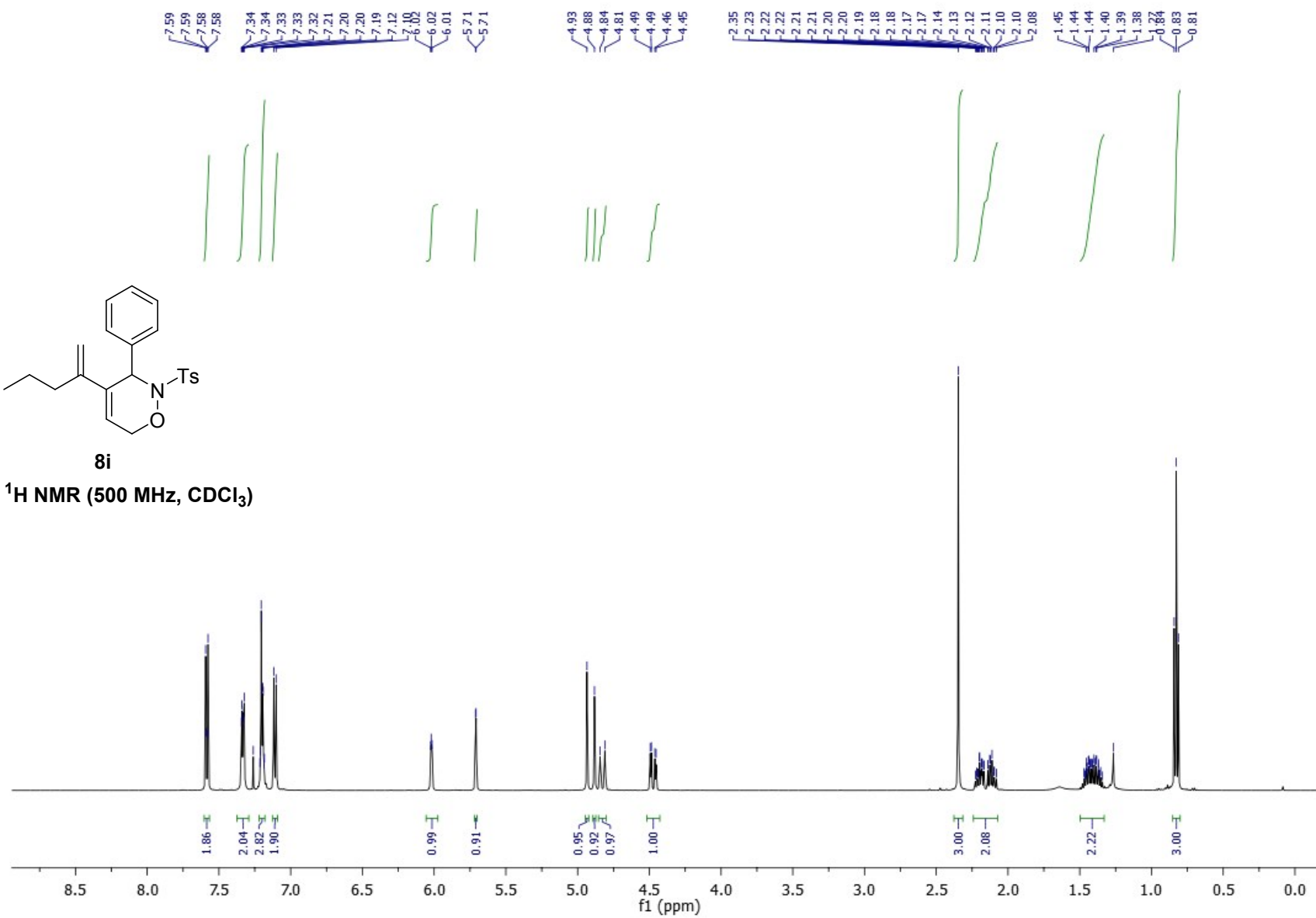
¹³C NMR (101 MHz, CDCl₃)

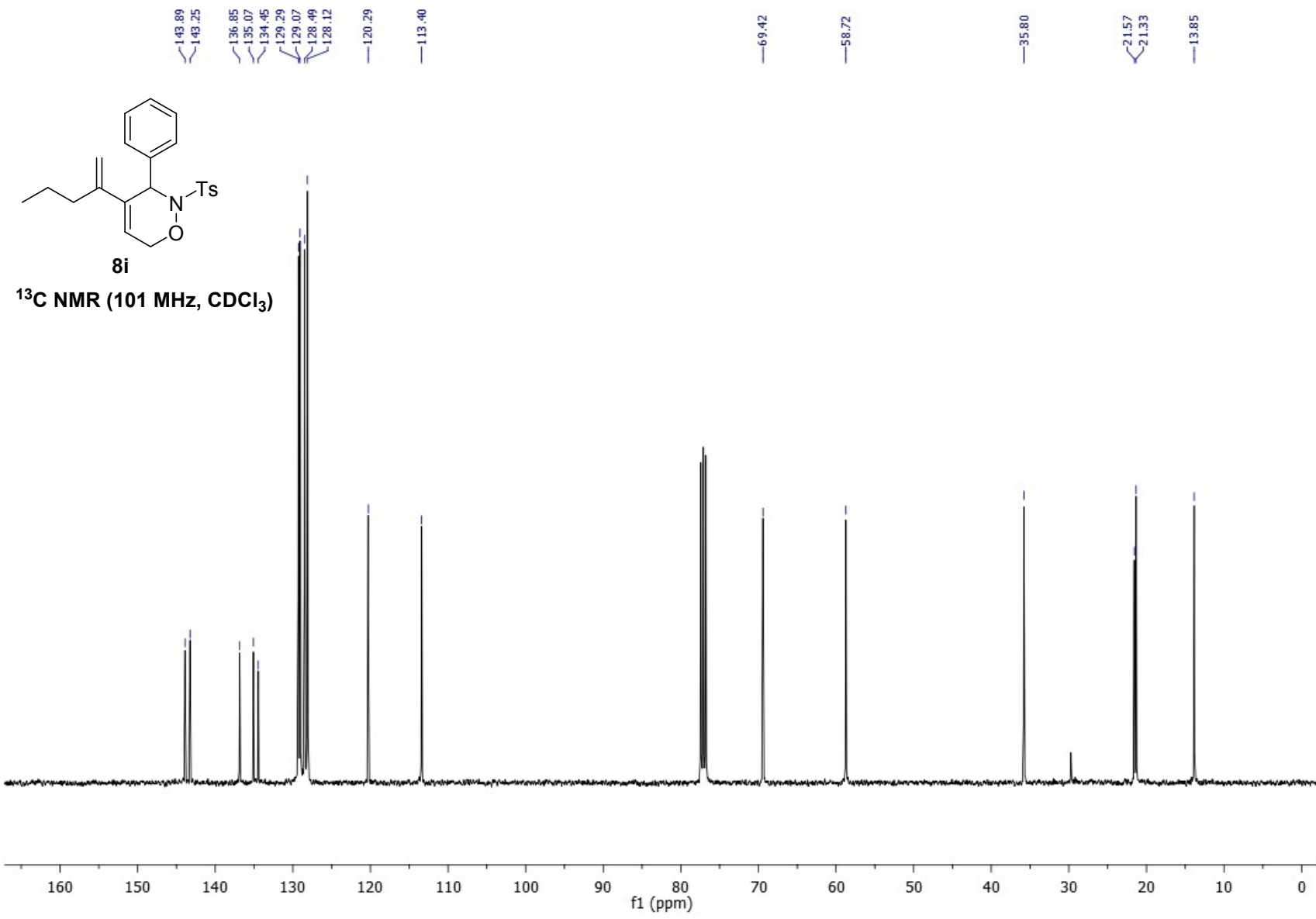


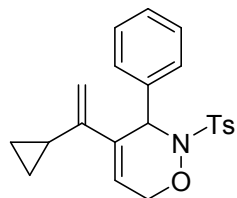


8i

¹H NMR (500 MHz, CDCl₃)

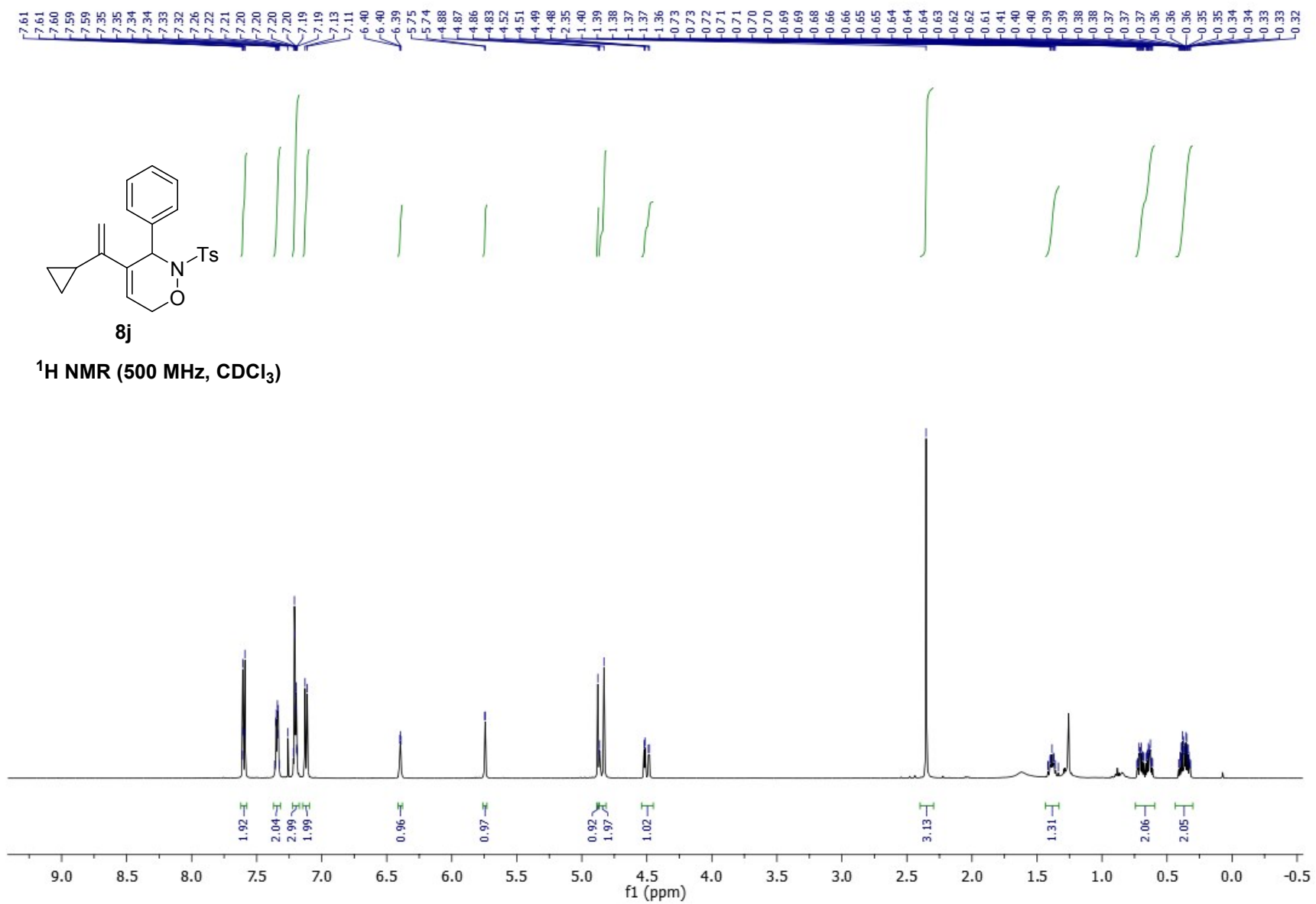


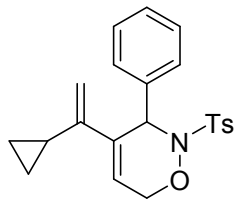




8j

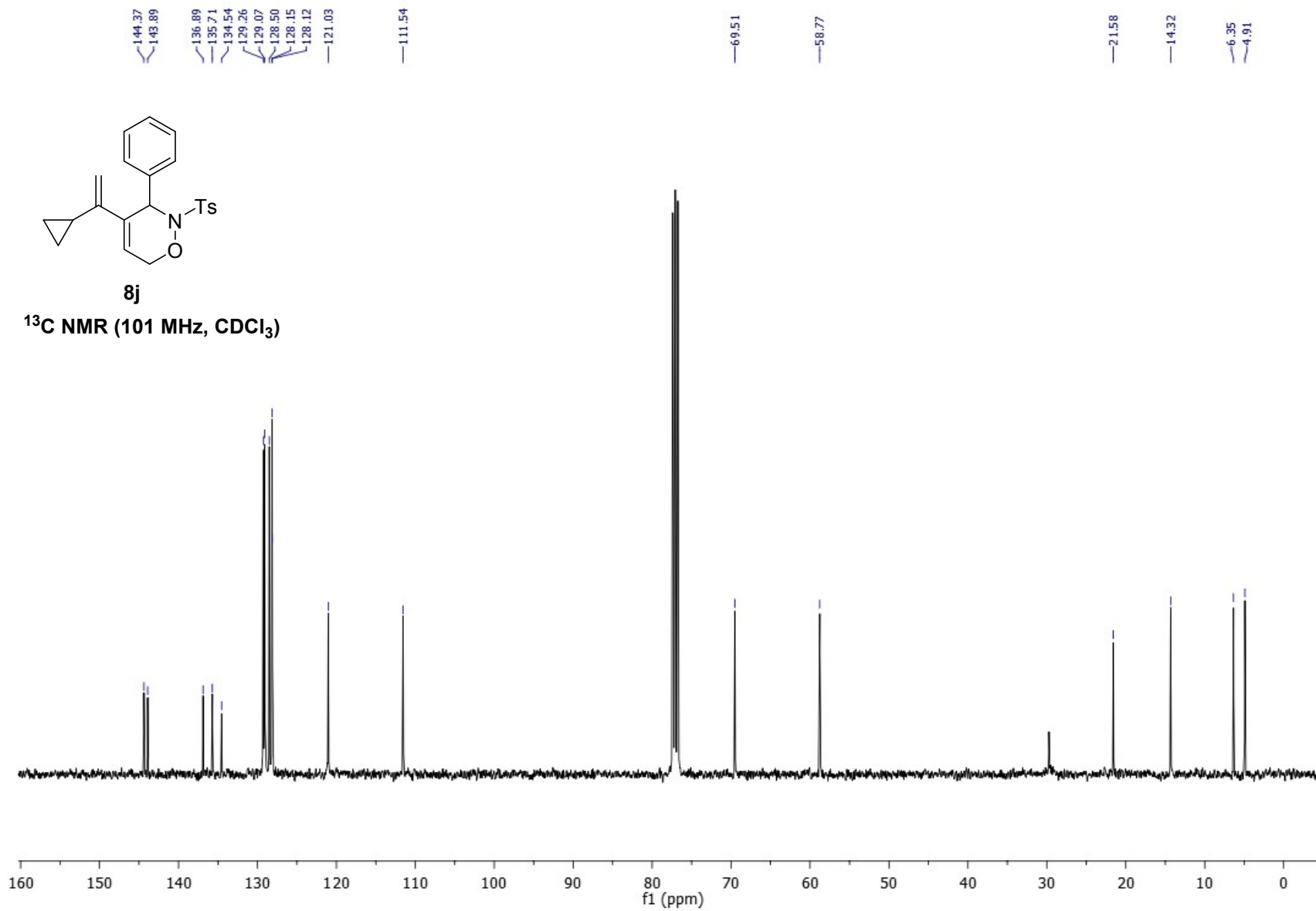
¹H NMR (500 MHz, CDCl₃)



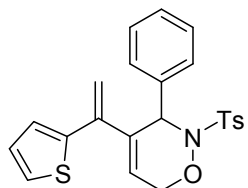


8j

¹³C NMR (101 MHz, CDCl₃)

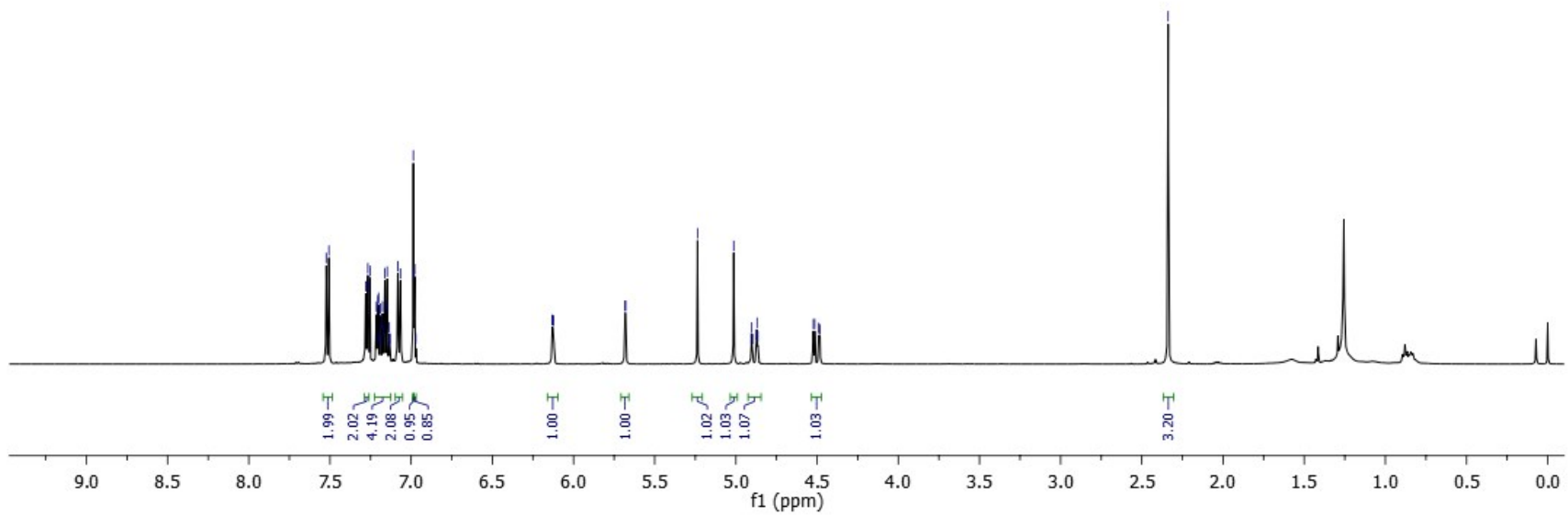


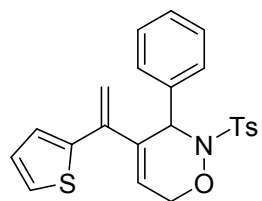
7.52
7.51
7.28
7.27
7.26
7.25
7.21
7.21
7.20
7.20
7.19
7.18
7.18
7.17
7.16
7.15
7.15
7.13
7.13
7.08
7.07
6.99
6.98
6.98
6.97
6.13
6.12
5.68
5.68
5.24
5.01
4.91
4.90
4.87
4.87
4.82
4.52
4.51
4.48
2.34



8k

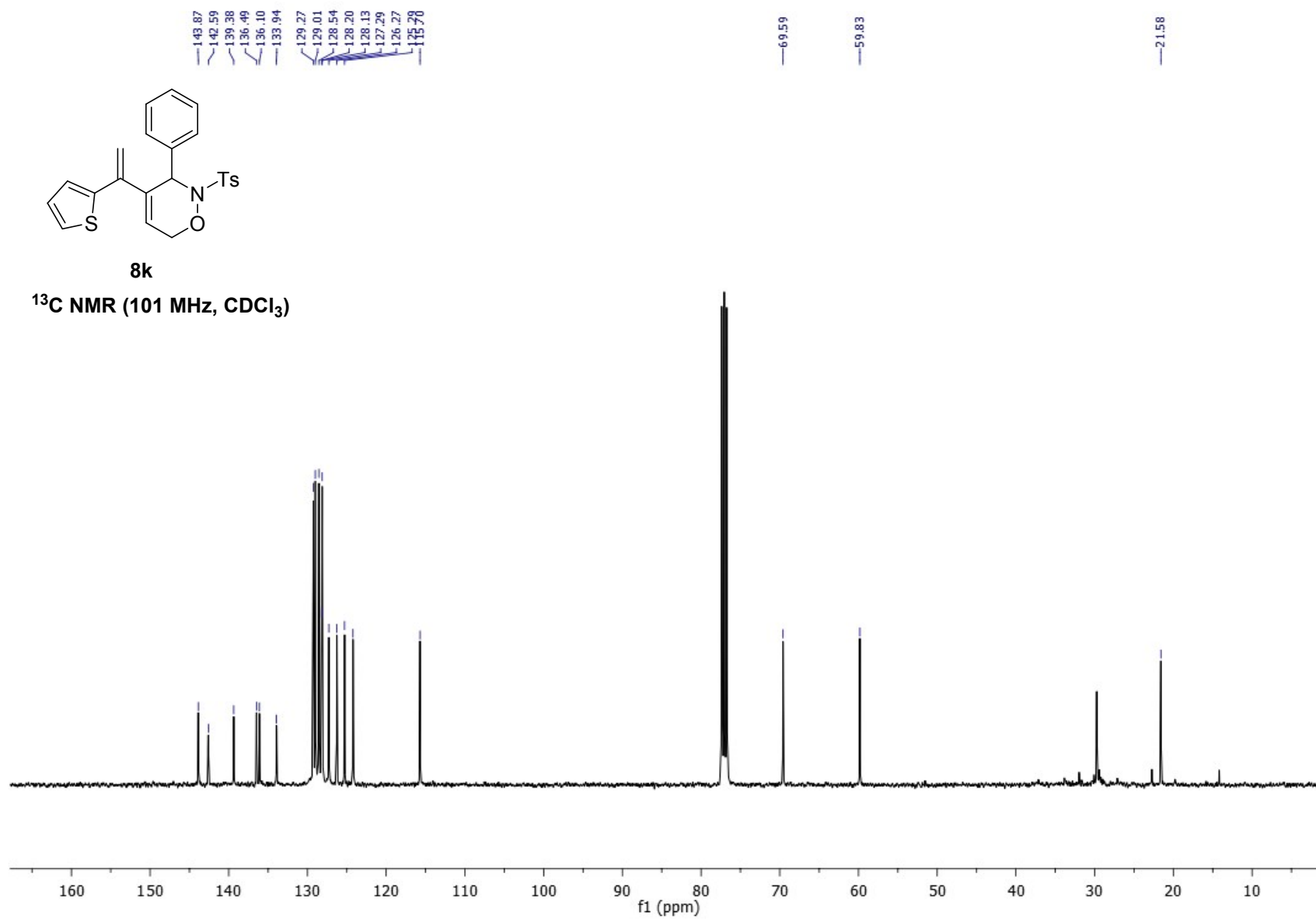
$^1\text{H NMR}$ (500 MHz, CDCl_3)

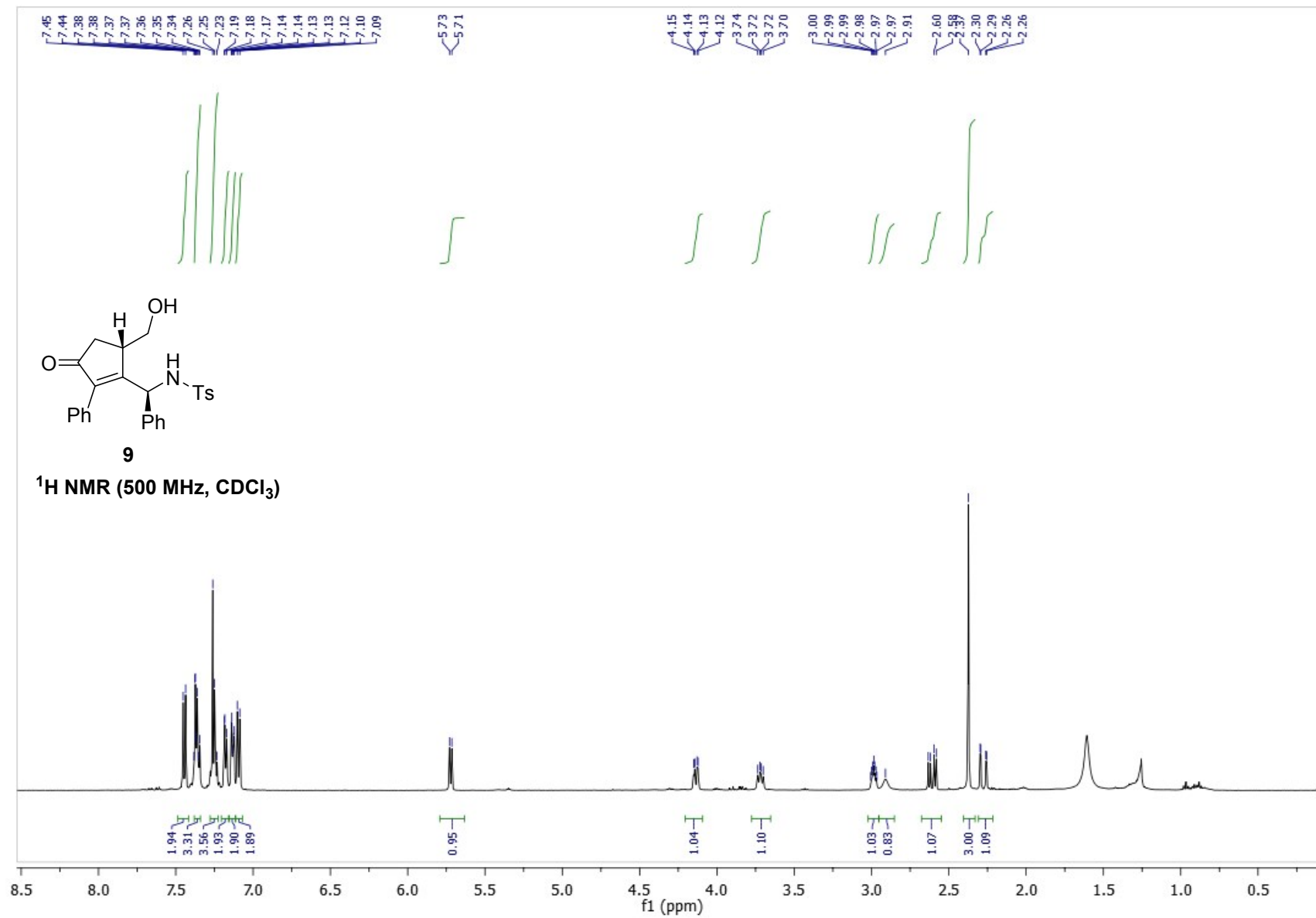


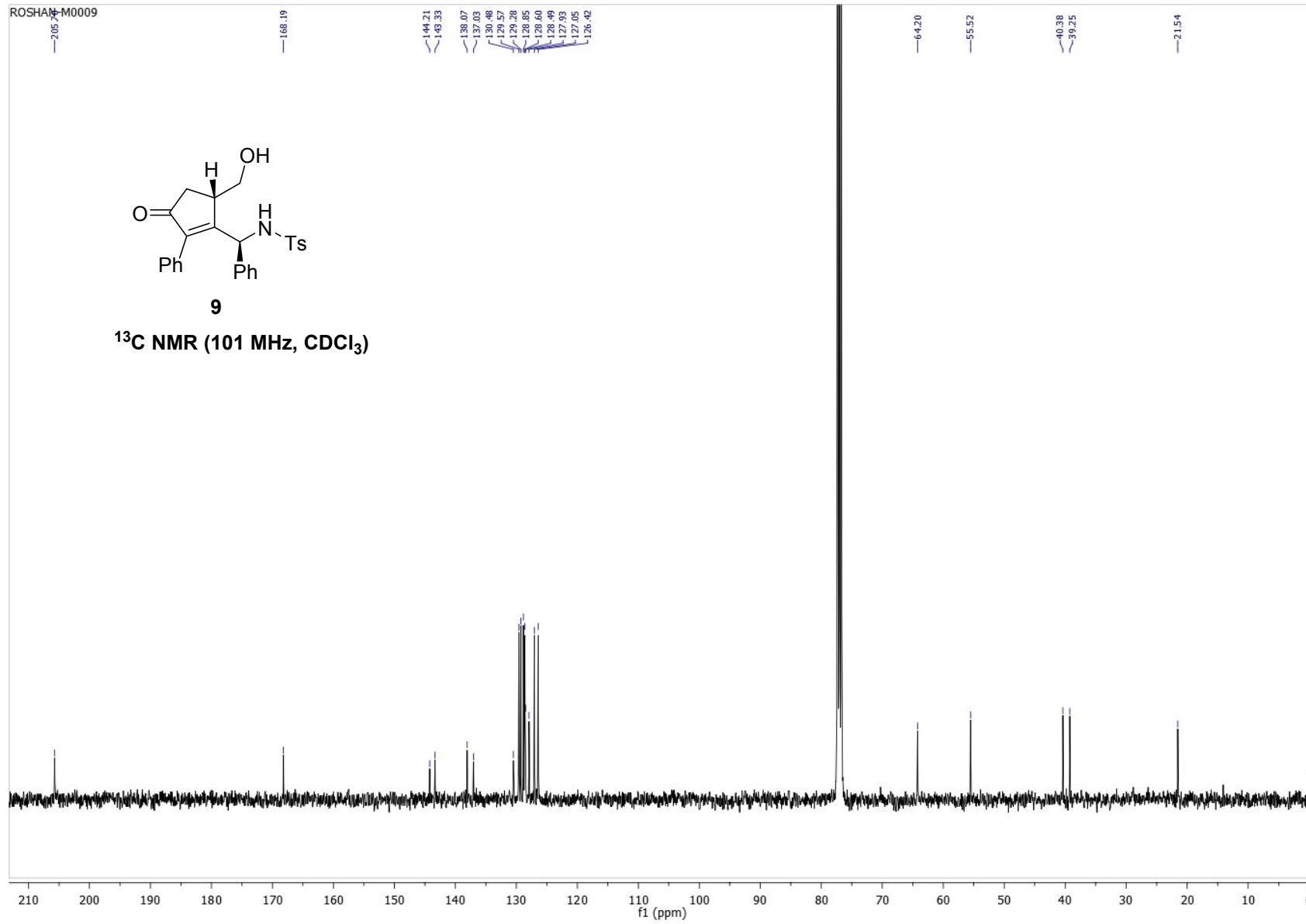


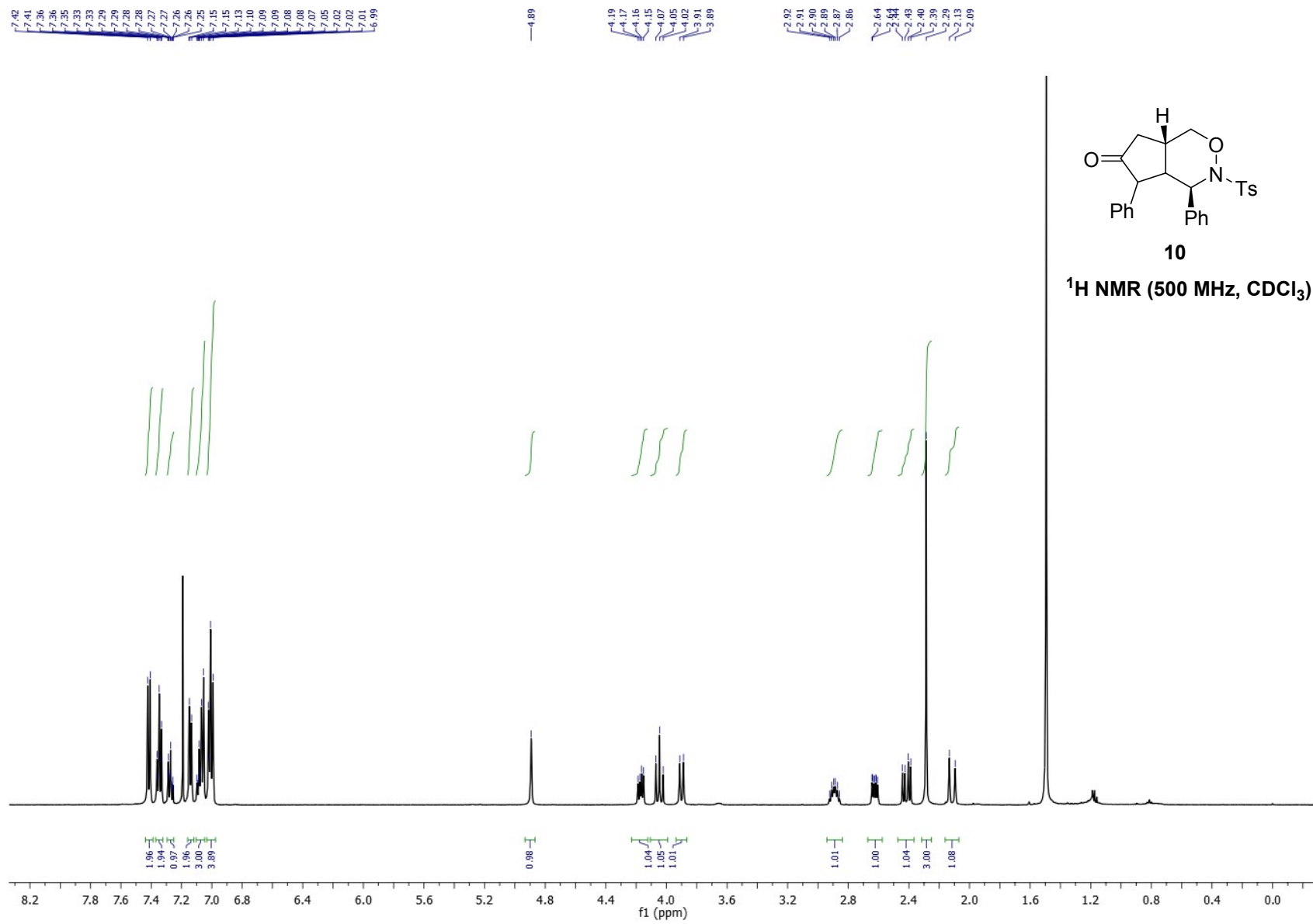
8k

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

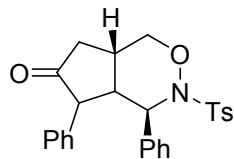








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10

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

