

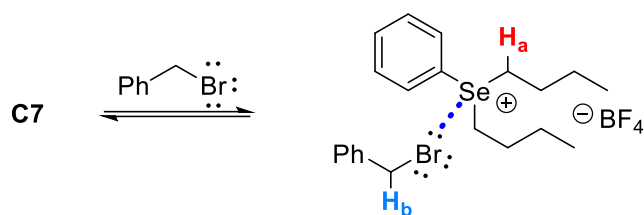
Supporting Information for:

**Selenonium Salt as a Catalyst for Nucleophilic Substitution
Reactions in Water: Synthesis of Thiocyanites and Selenocyanates**

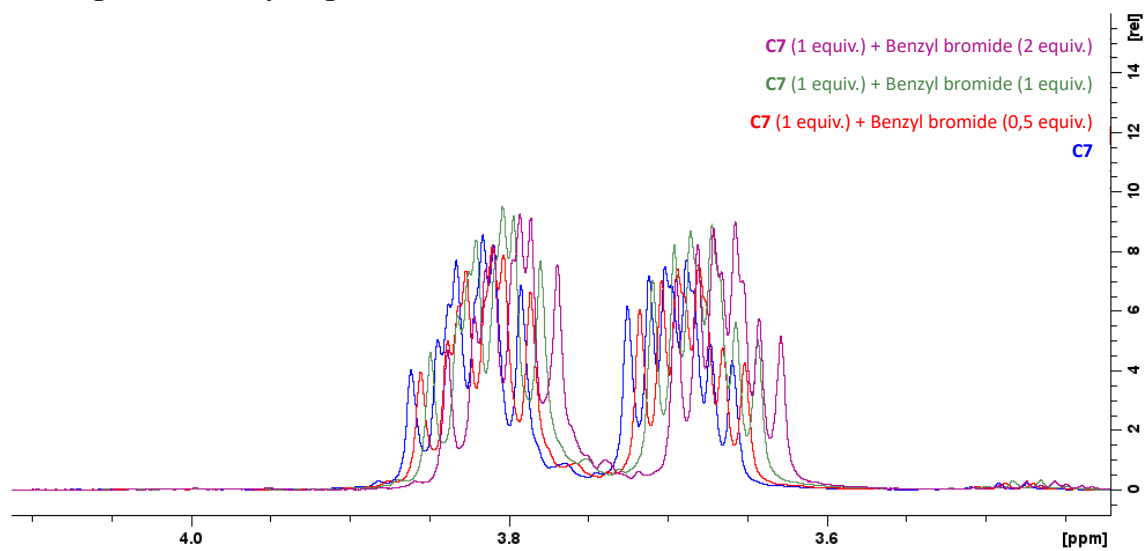
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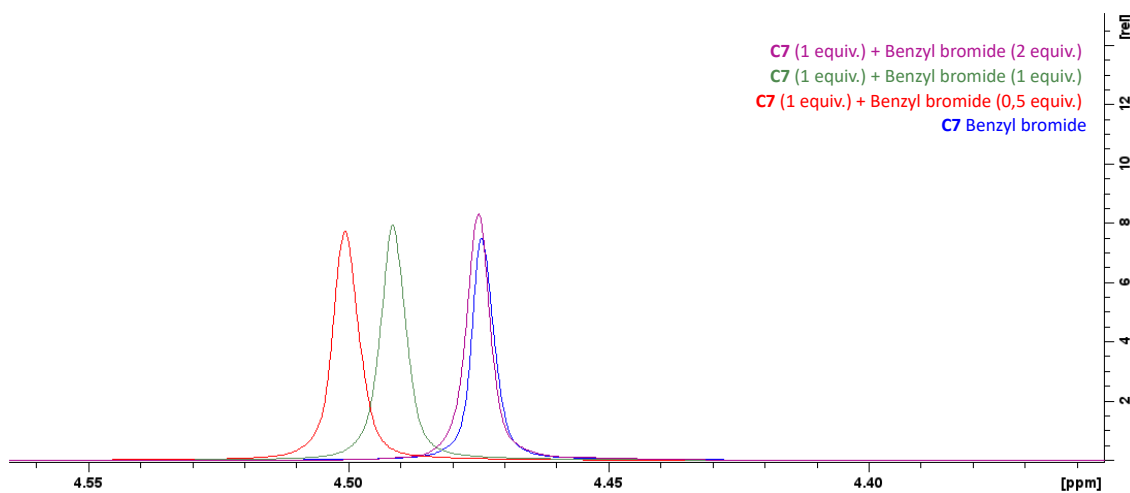
^1H NMR of catalyst **C7** and varying amounts of benzyl bromide.



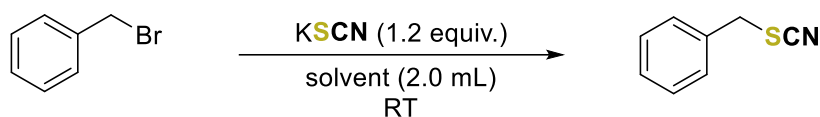
The signal shift of hydrogen H_a :



The signal shift of hydrogen H_b :



Optimization of the reaction conditions for the synthesis of thiocyanates without a catalyst:

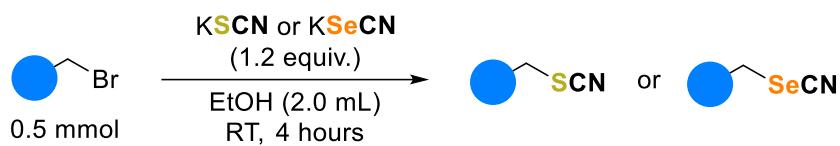


Entry	Solvent	Time	Isolated Yield (%)
1	Dimethyl carbonate	10 min	8
2	Anisole	10 min	3
3	Ethylene glycol	10 min	2
4	1-Butanol	10 min	6
5	Ethyl acetate	10 min	1
6	EtOH ^[a]	10 min	26
7	EtOH ^[a]	4 h	83
8	EtOH ^[a]	2 h	74

^[a] 95% EtOH grade (used as received).

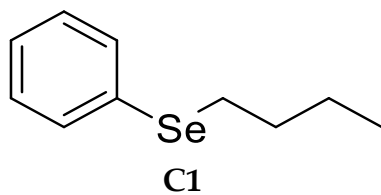
Experimental procedure: a test tube was charged with the corresponding solvent (2.0 mL) and benzyl bromide (85.5 mg, 0.5 mmol). The mixture was stirred until became homogeneous and then KSCN (58.3 mg, 0.6 mmol) was added. The reaction mixture was stirred at 25 ± 2 °C (water bath) at a constant rate of 360 rpm during the period indicated on the table above. Afterwards, the mixture was extracted with AcOEt (3 x 10.0 mL) and the combined organic phases washed with water (3 x 10.0 mL), brine (3 x 10.0 mL), dried over MgSO_4 and evaporated under reduced pressure. Purification was performed by silica gel chromatography column with a mixture of hexanes/AcOEt = 9/1.

Substrate scope for the preparation of thio- and selenocyanates in uncatalyzed using hydrated EtOH as solvent.

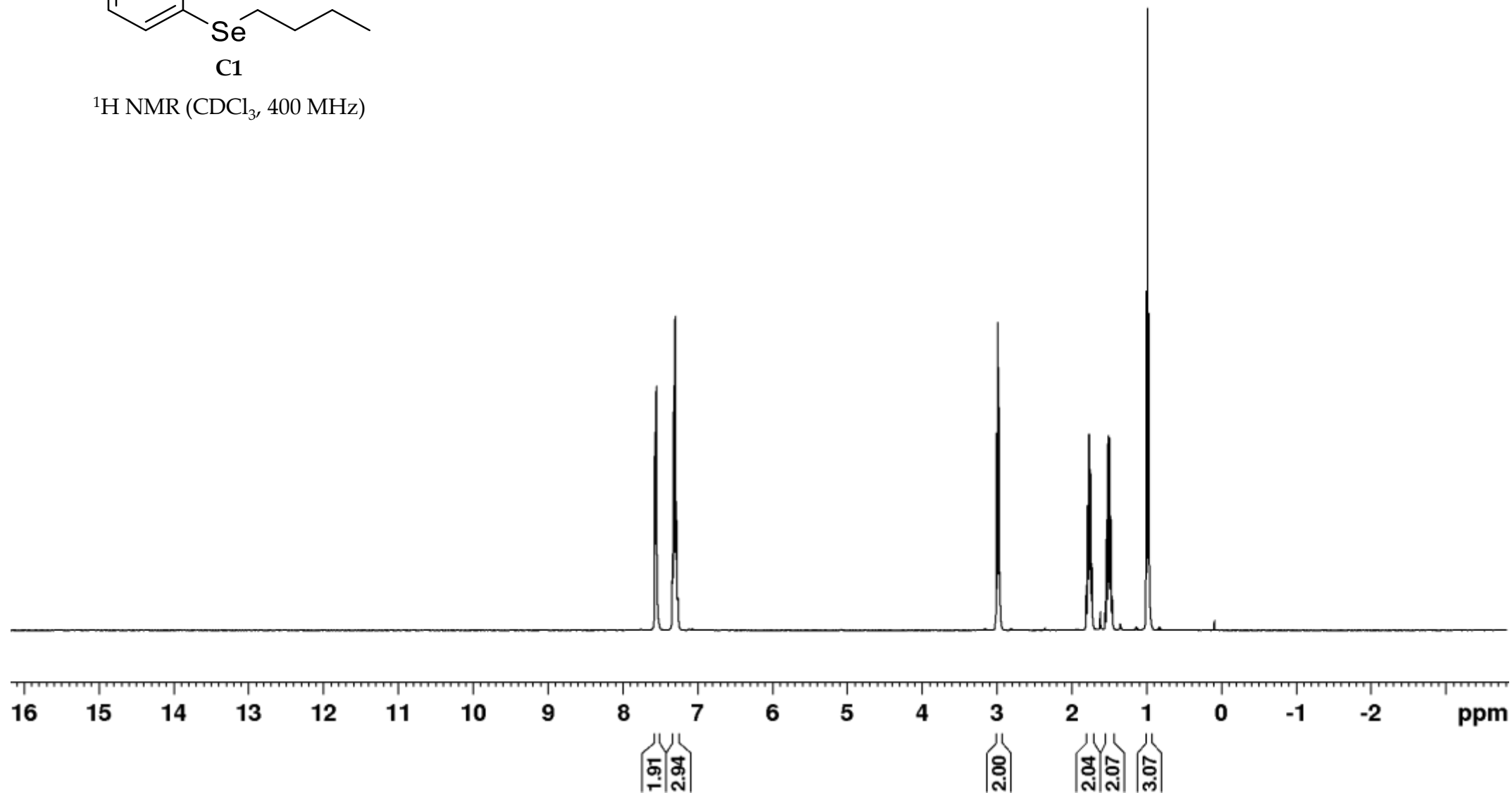


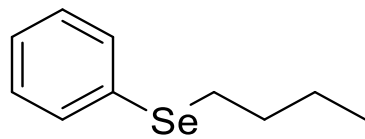
Entry	Product	Yield (%) ^[a]	Product	Yield (%) ^[a]
1	 1a	83	 1b	75
2	 2a	79		
3	 3a	65		
4	 4a	35		
5	 6a	81	 6b	86
6	 7a	49		
7	 8a	81		
8	 9a	47	 9b	47
9	 10a	78	 10b	69
10	 13a	82	 13b	78

^[a] Yields for pure and isolated products.



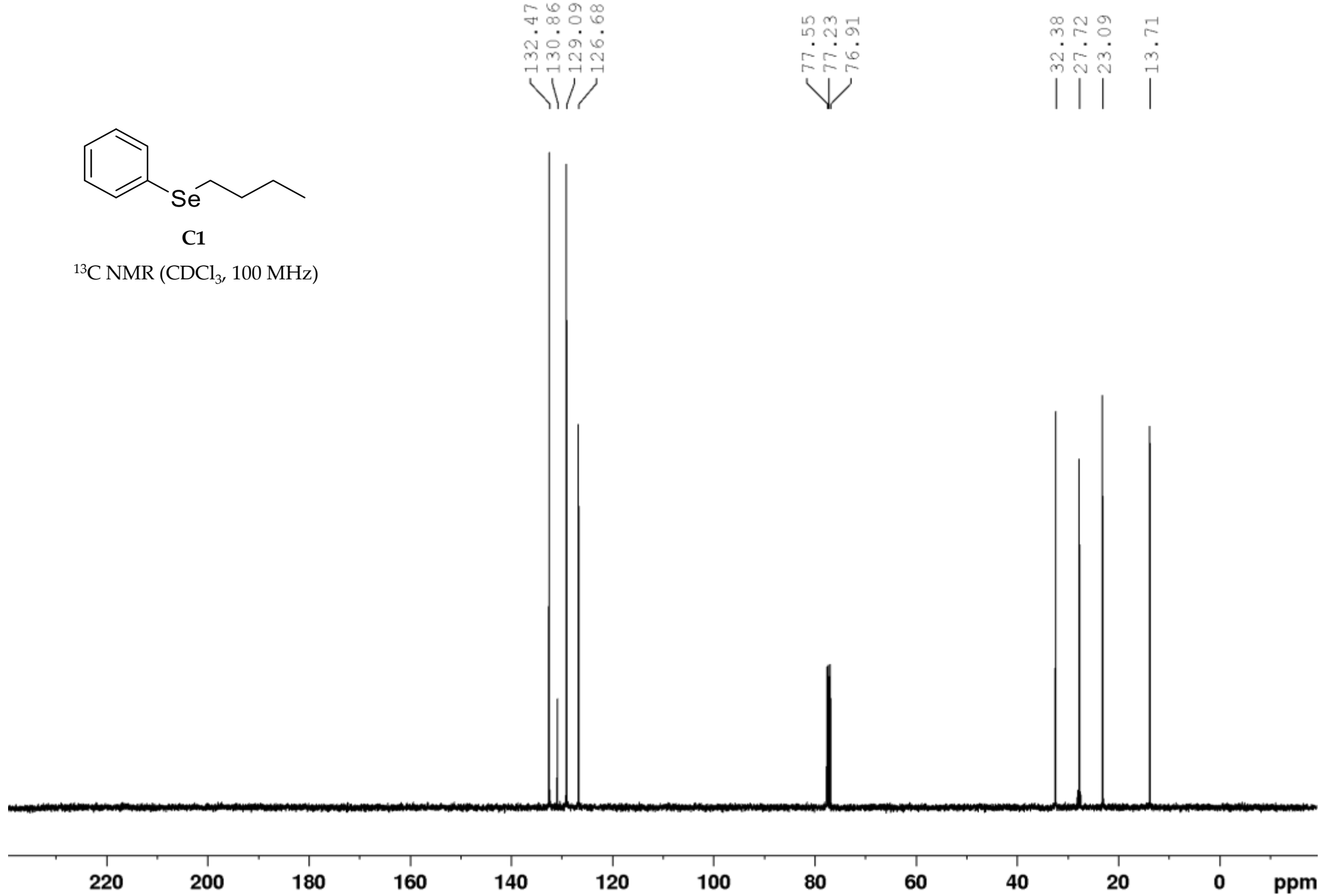
^1H NMR (CDCl_3 , 400 MHz)

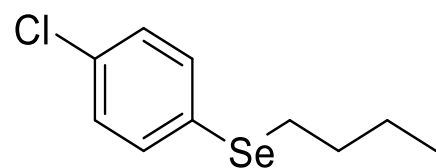




C1

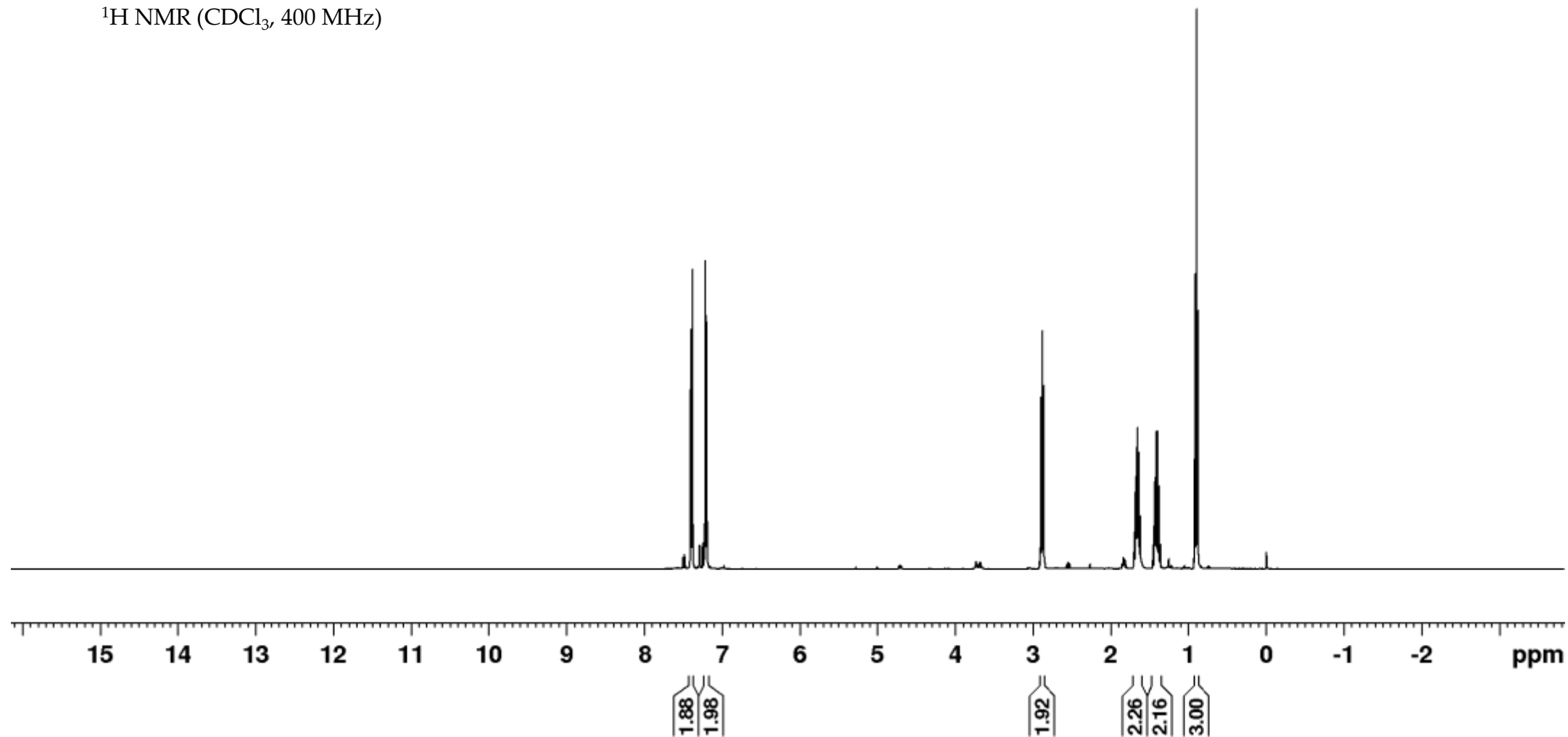
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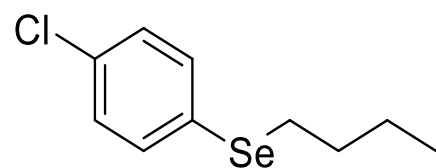




C2

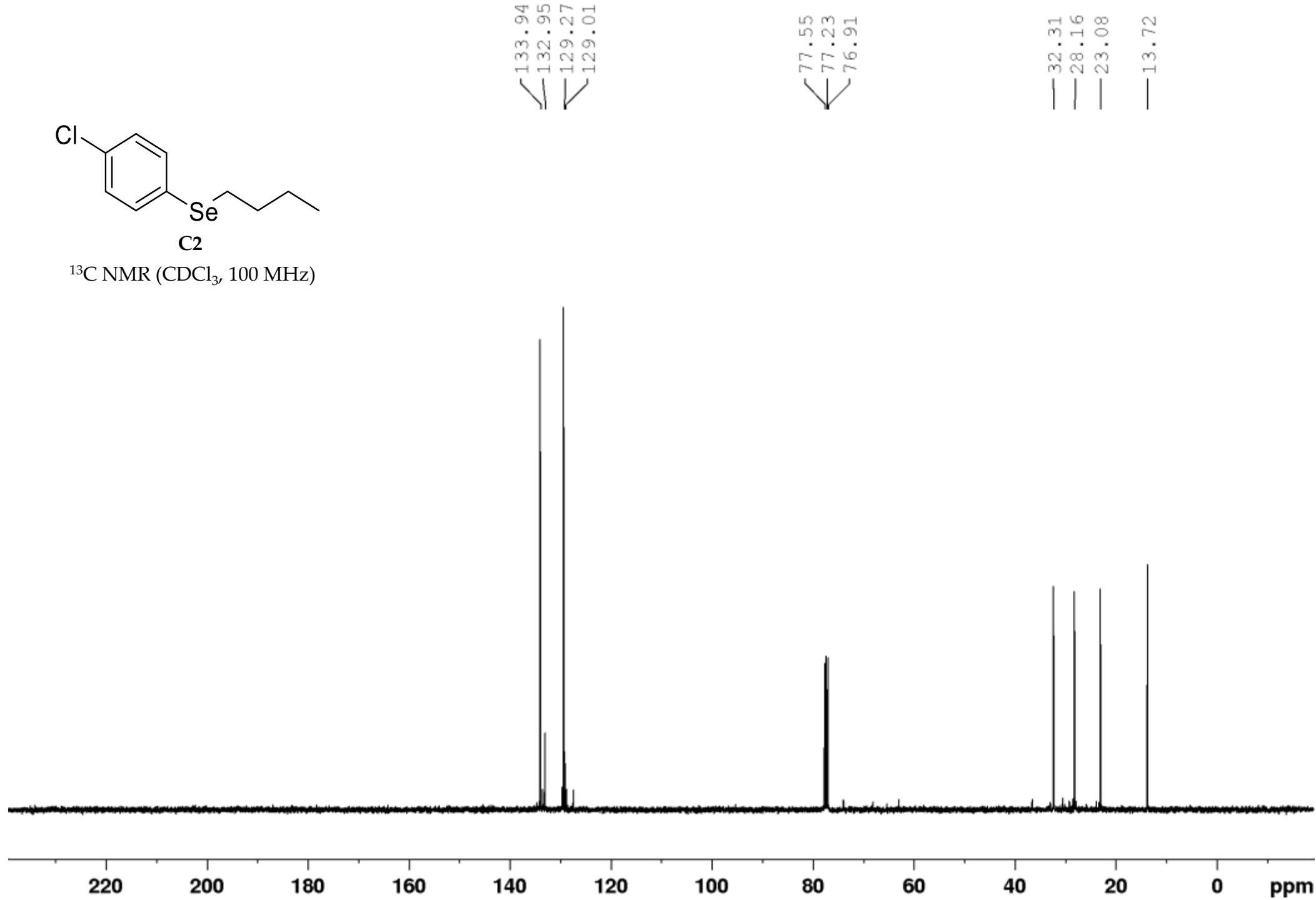
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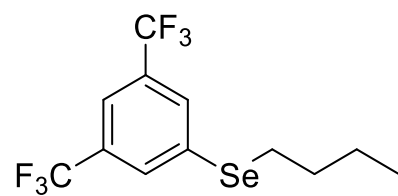




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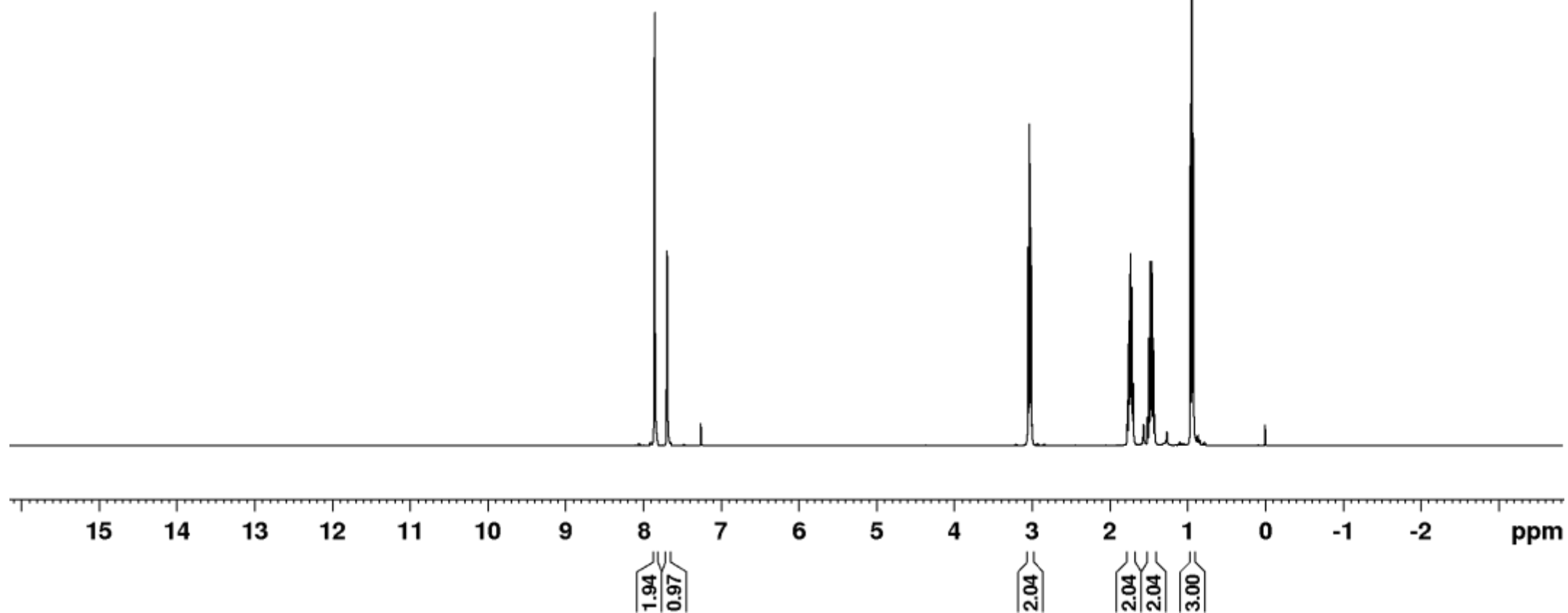
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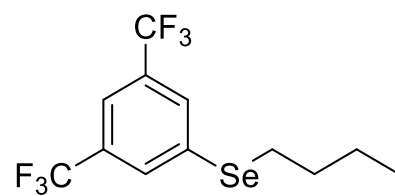




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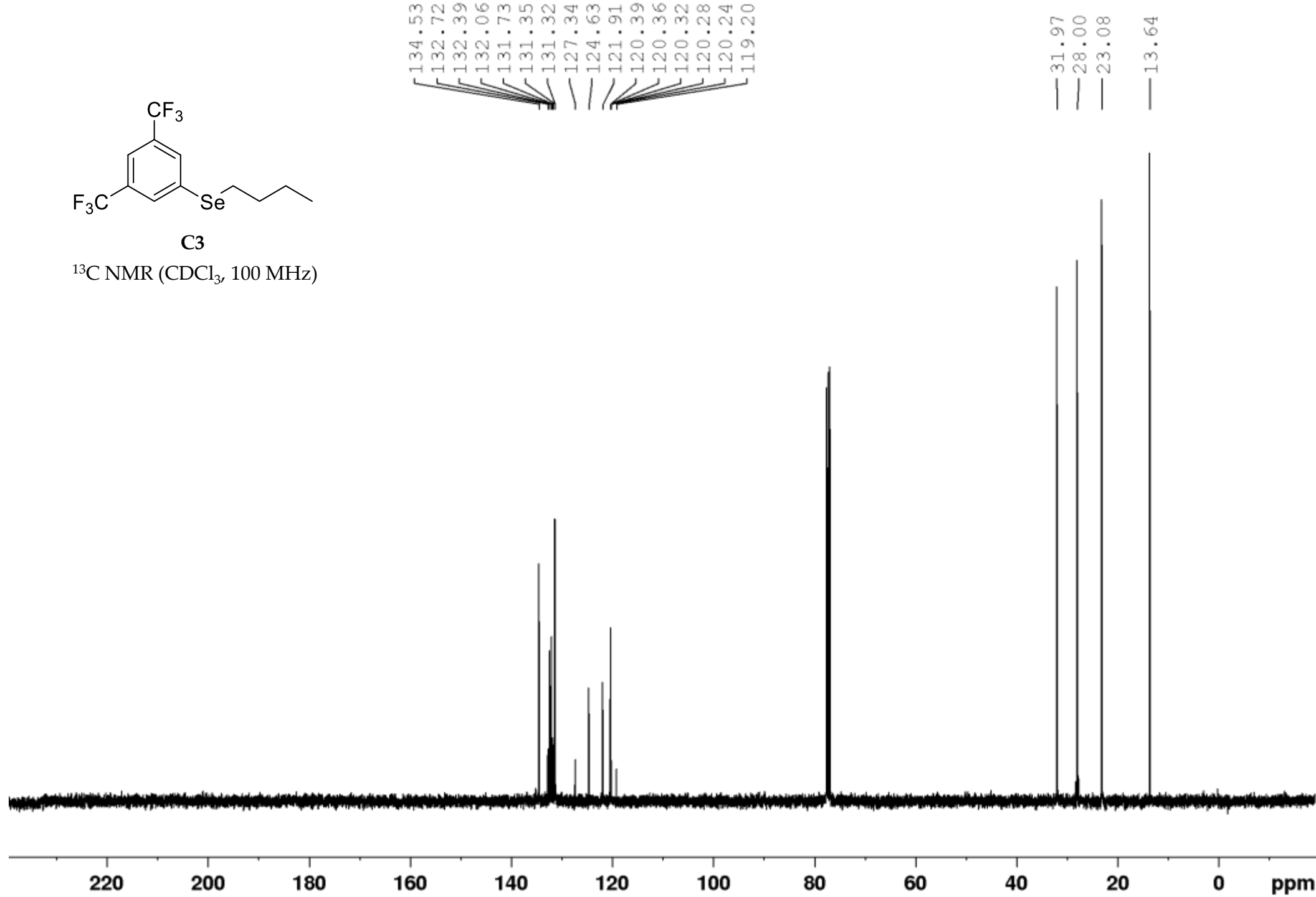
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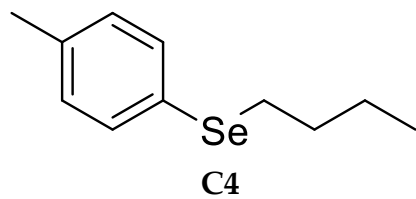




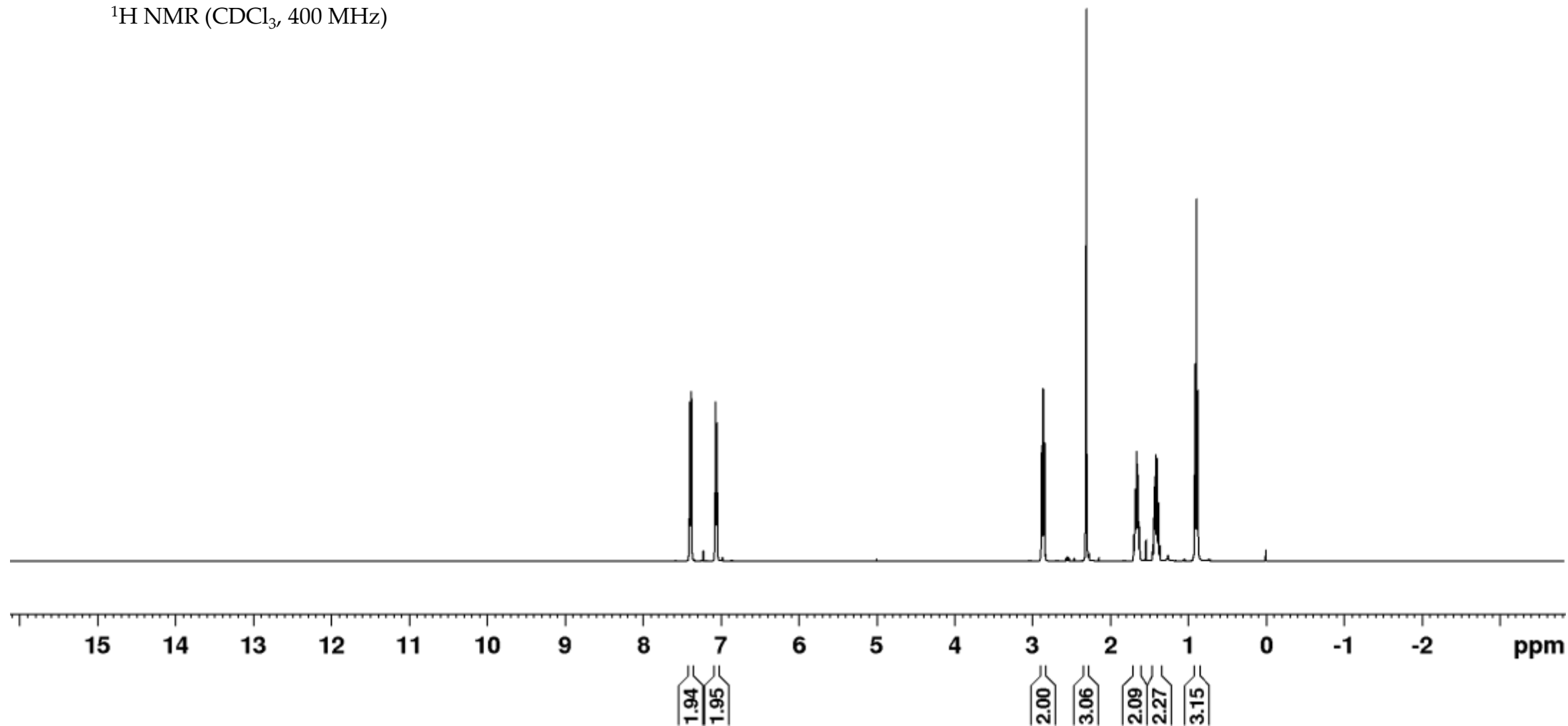
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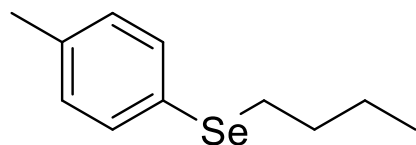
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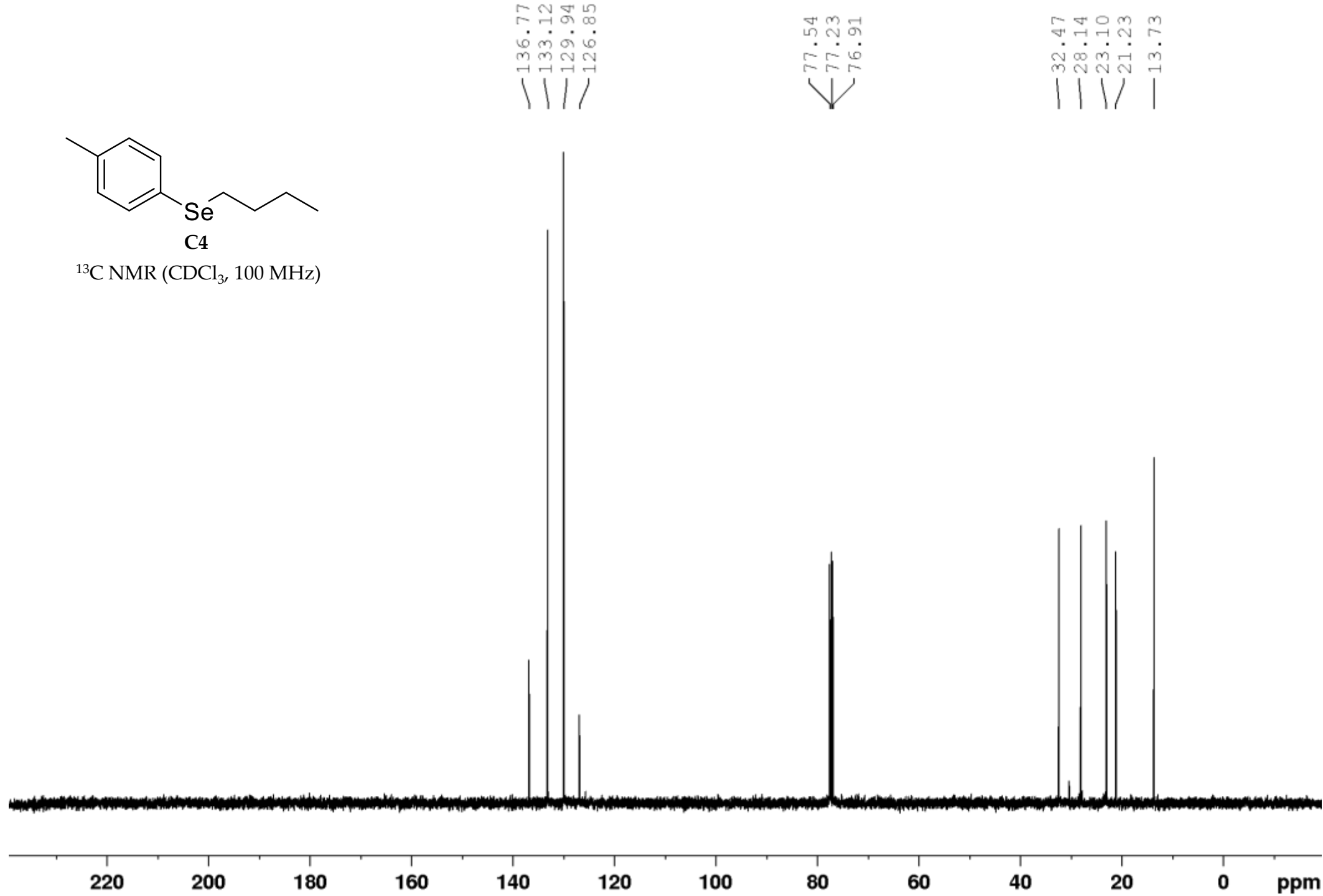
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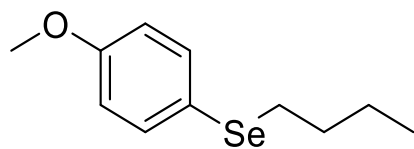




C4

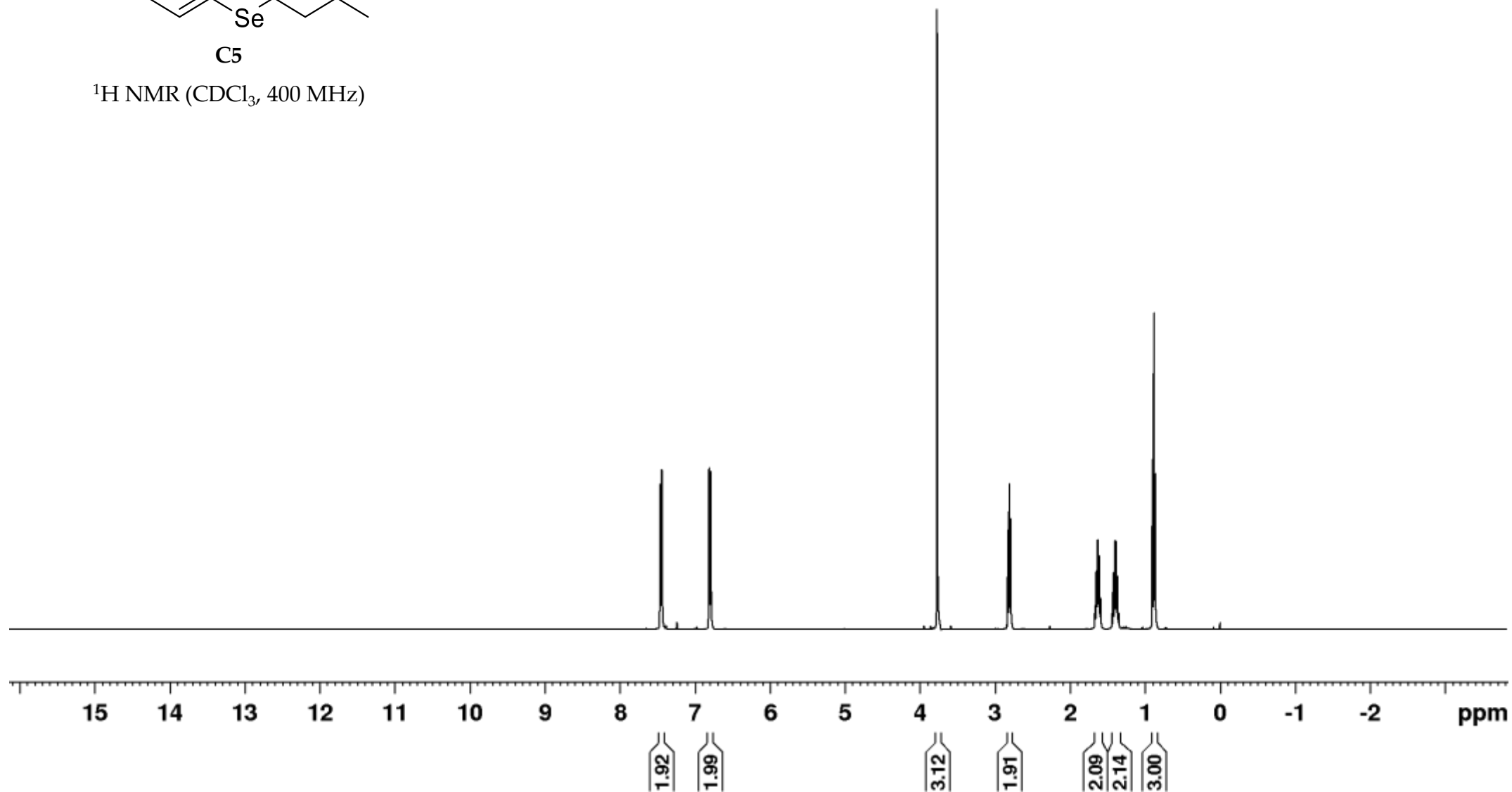
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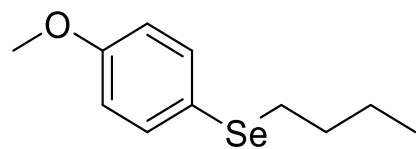




C5

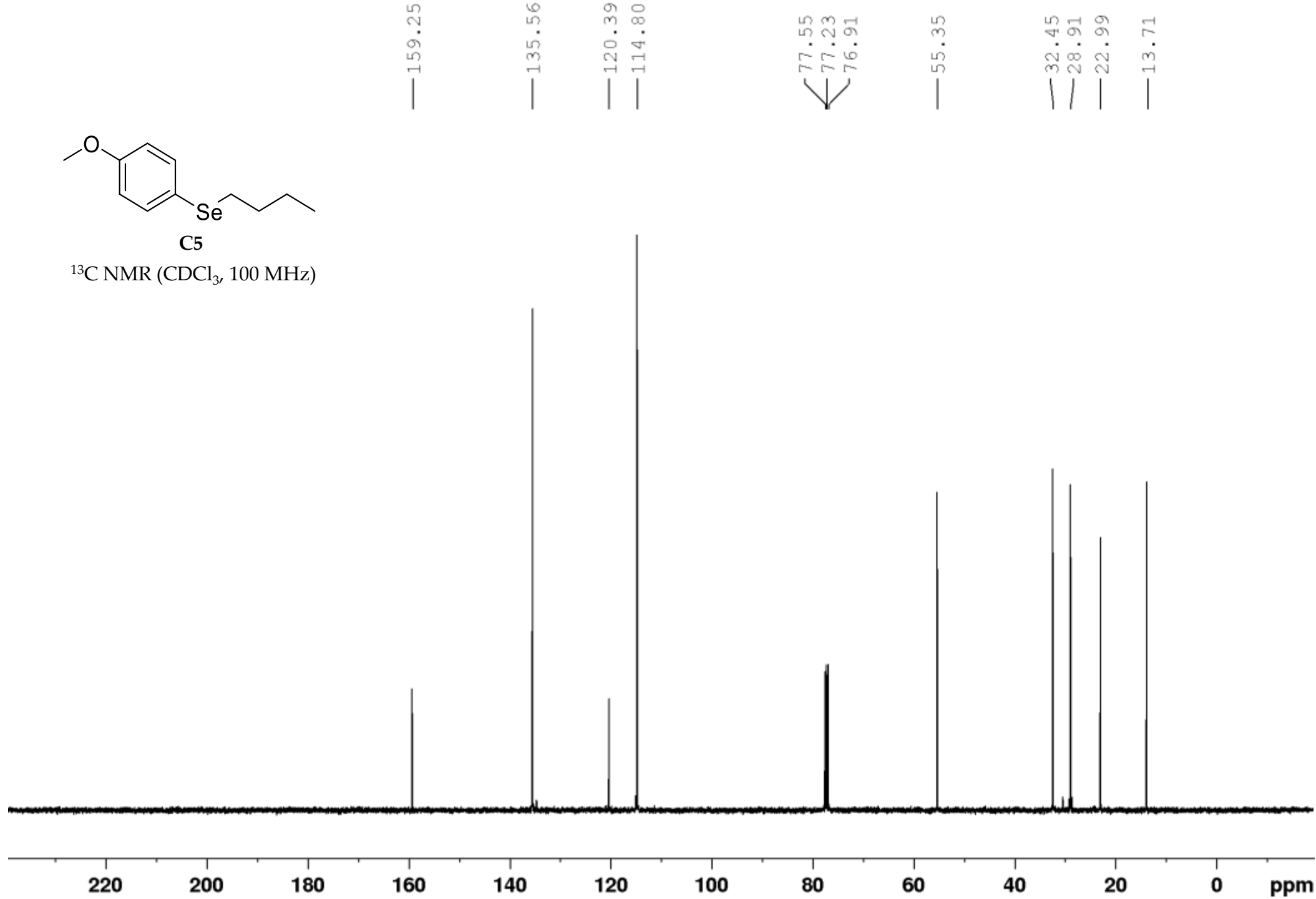
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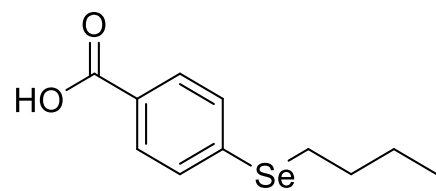




C5

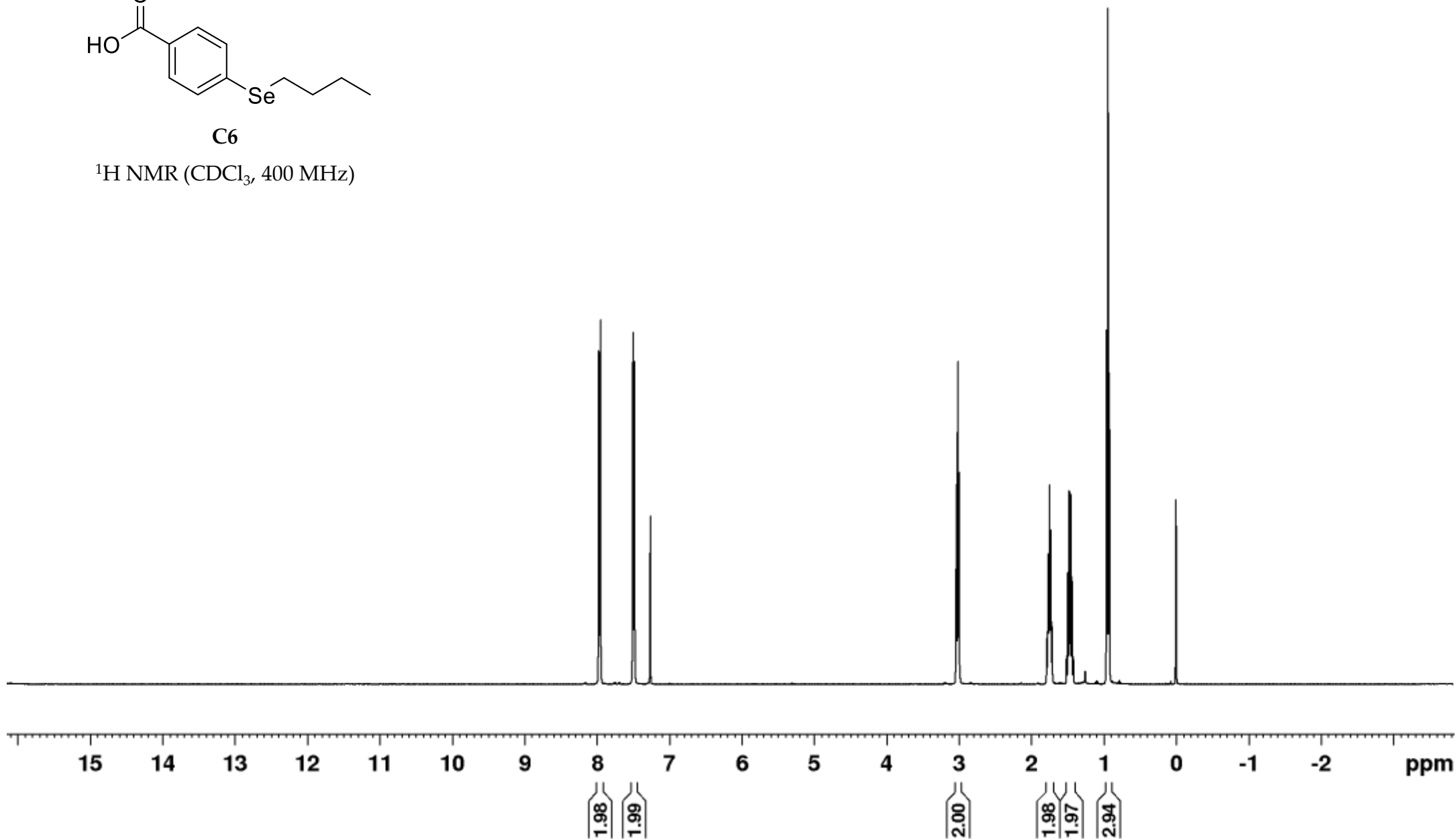
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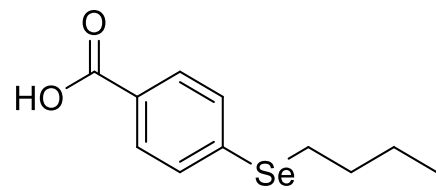




C6

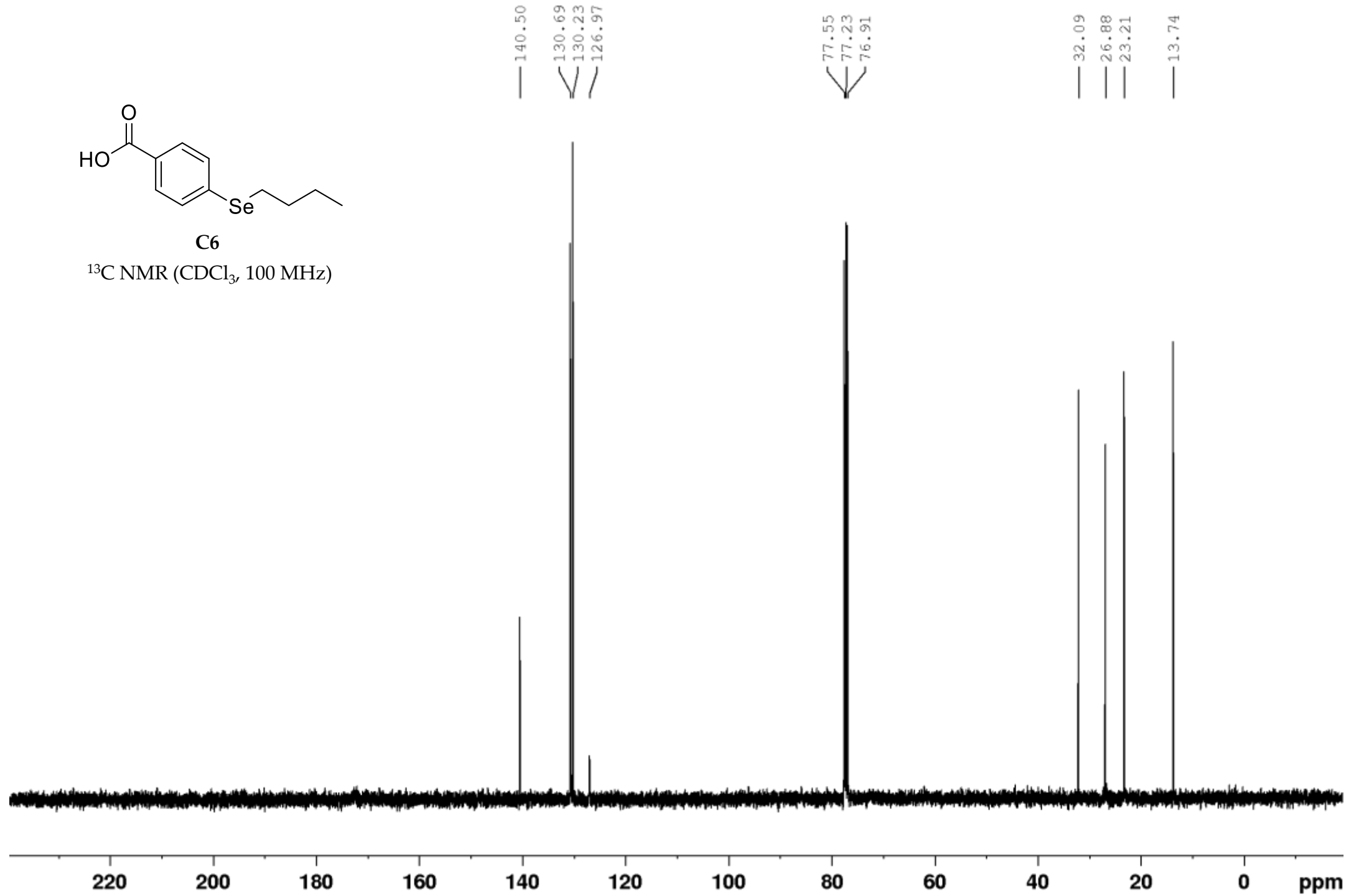
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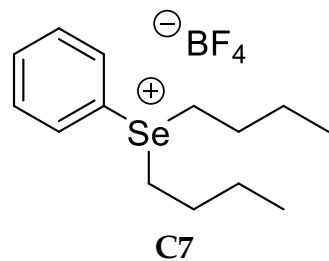




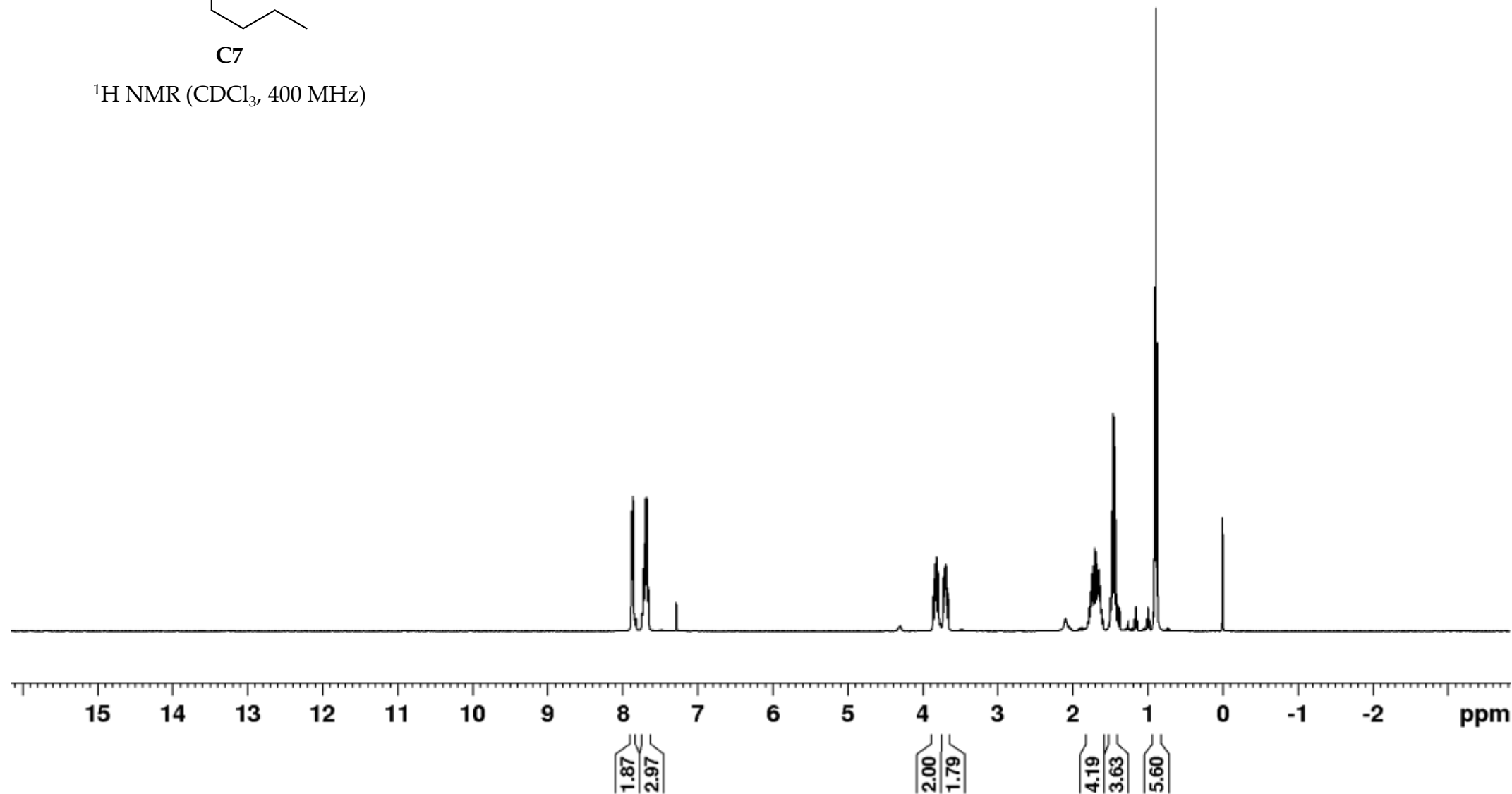
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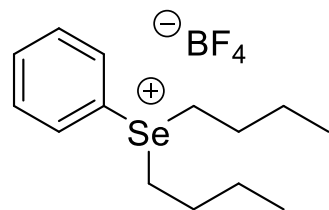
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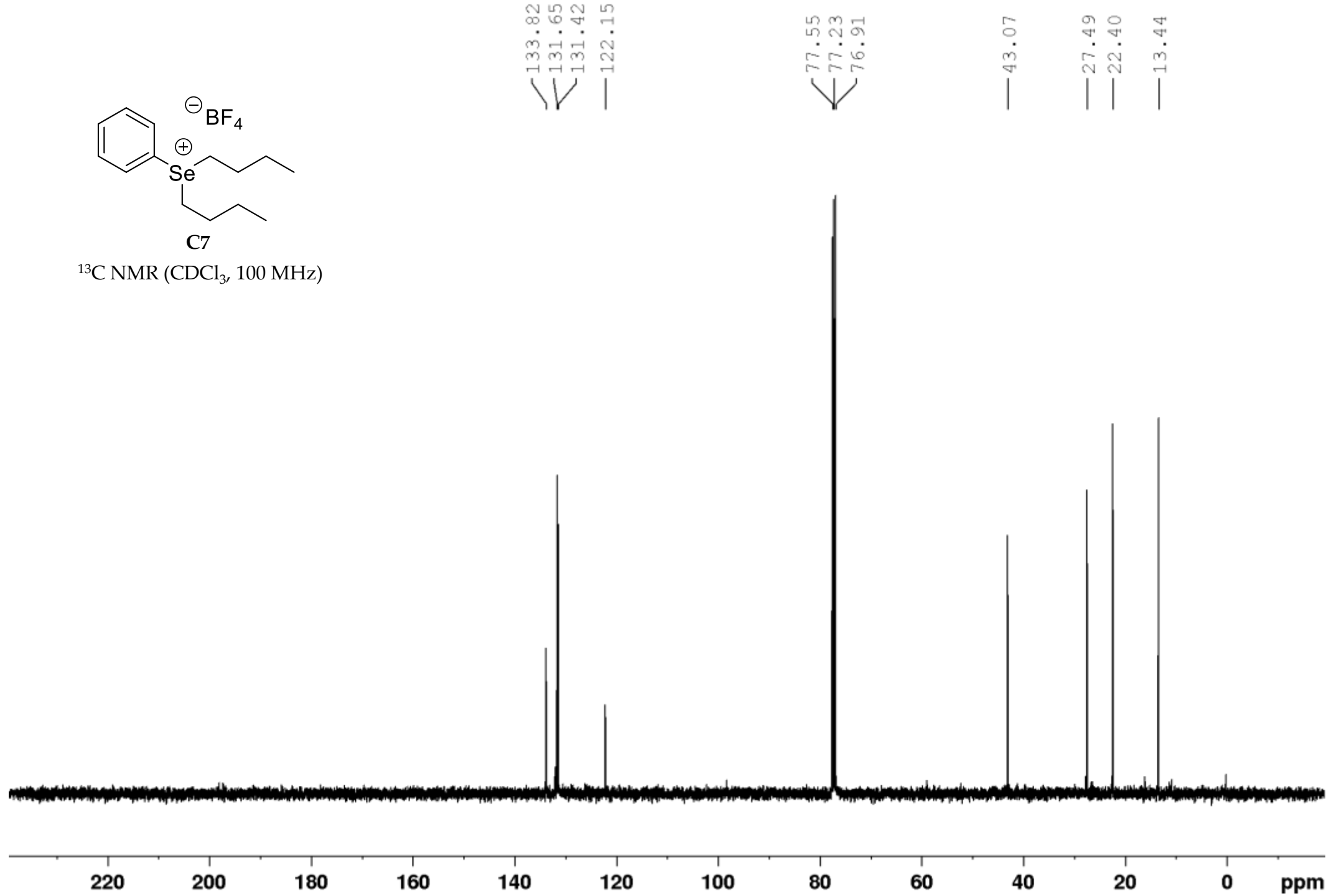
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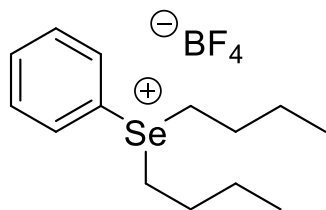




C7

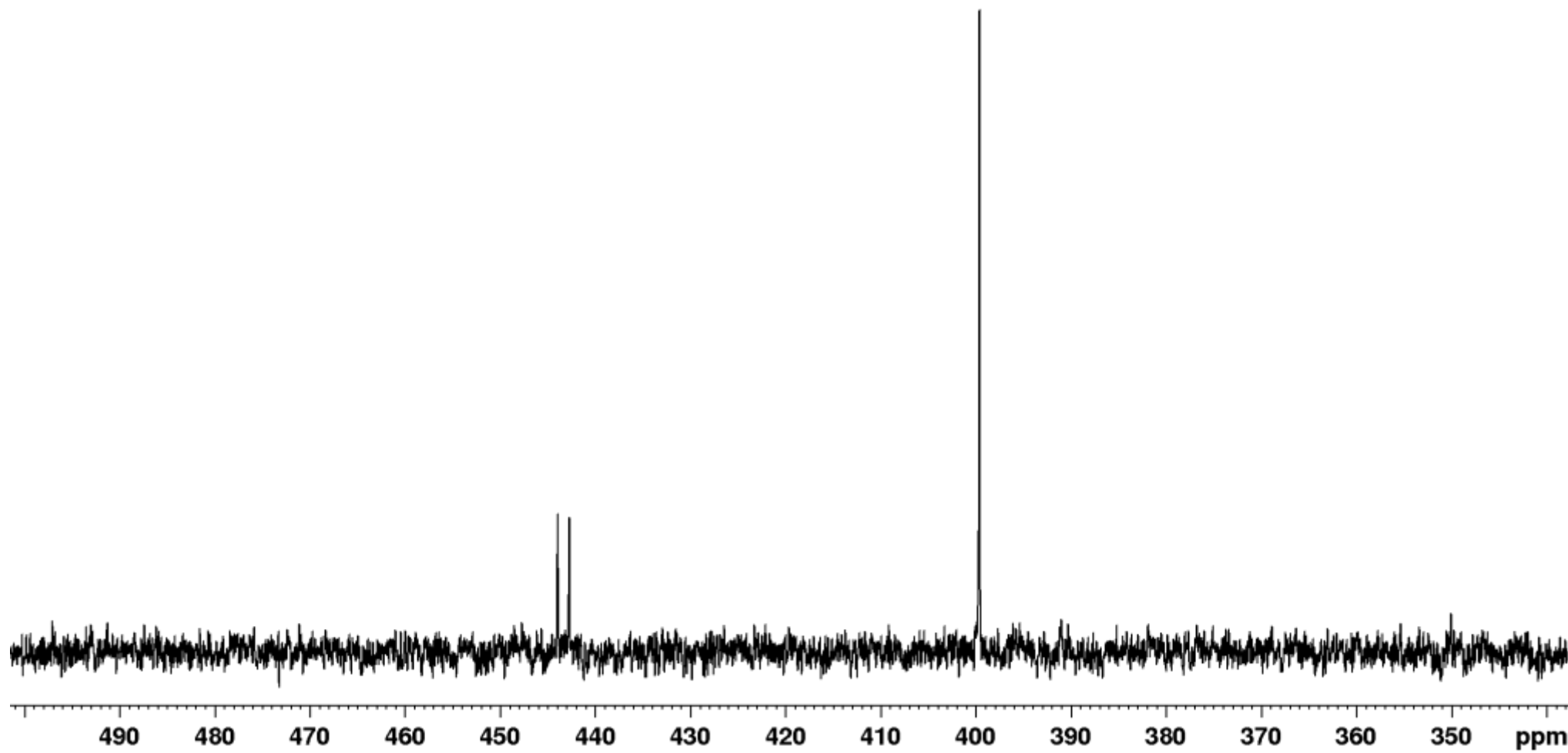
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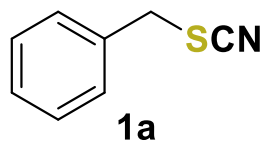




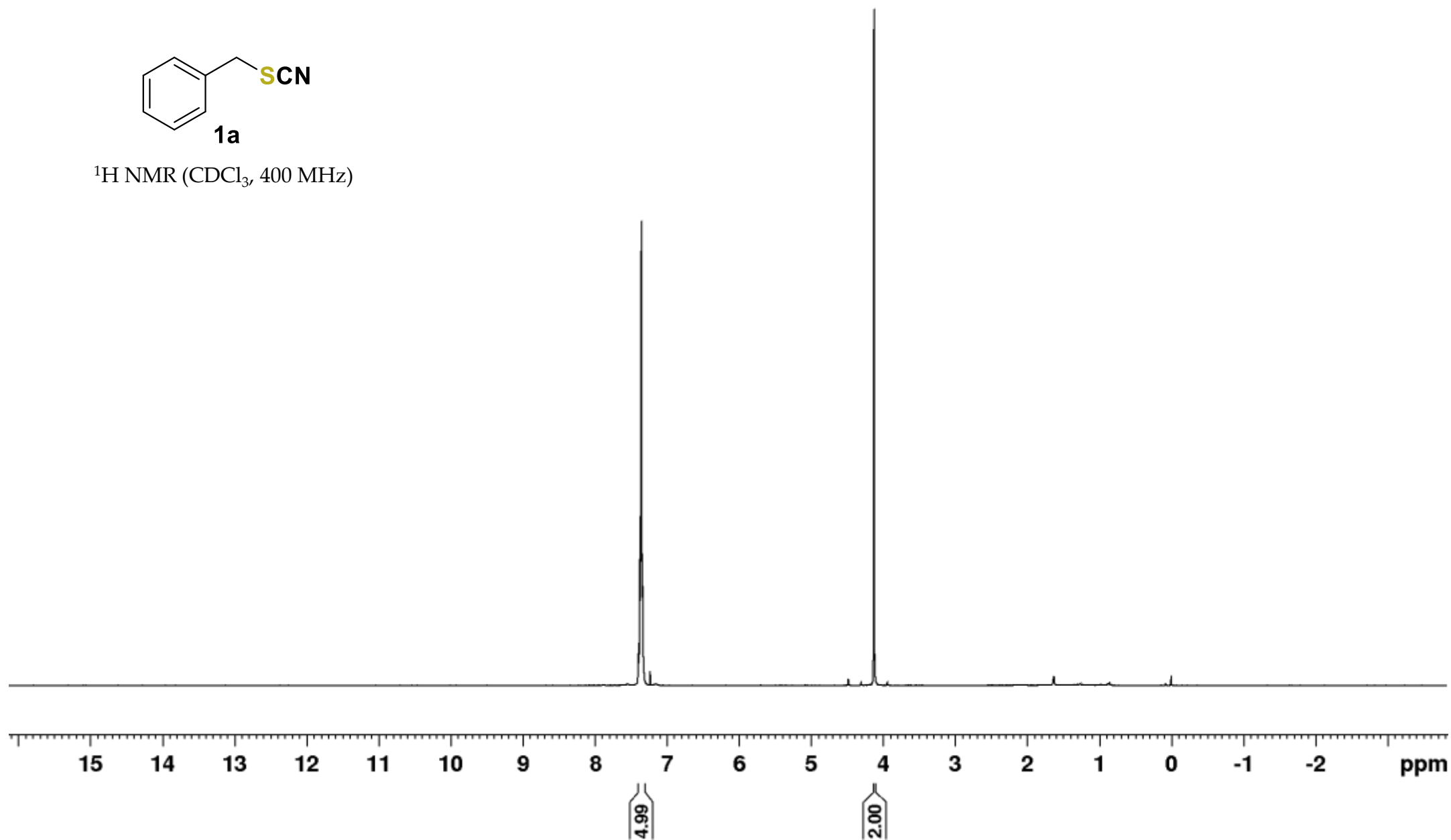
C7

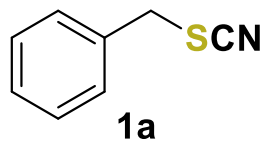
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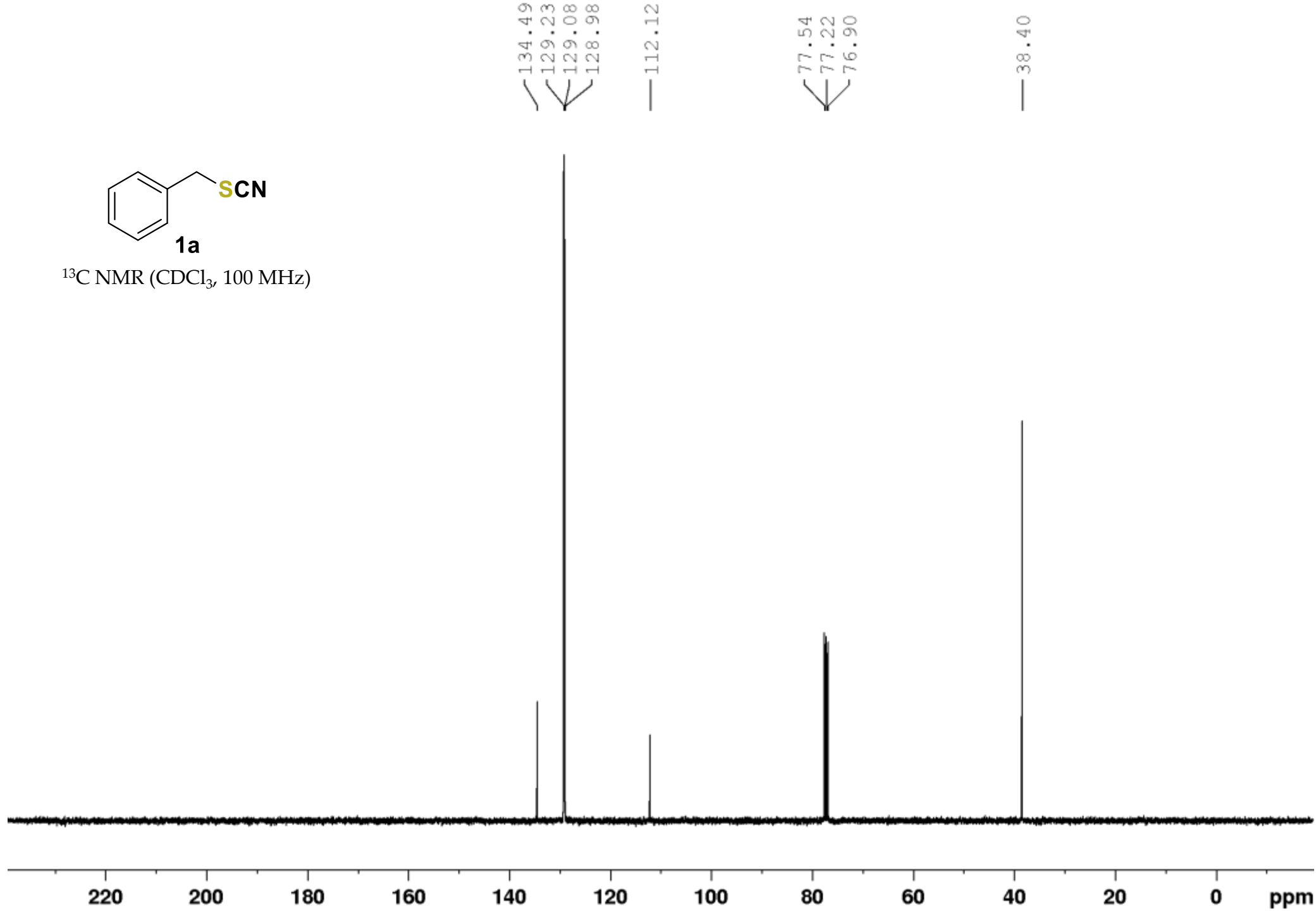


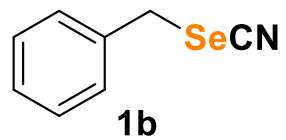
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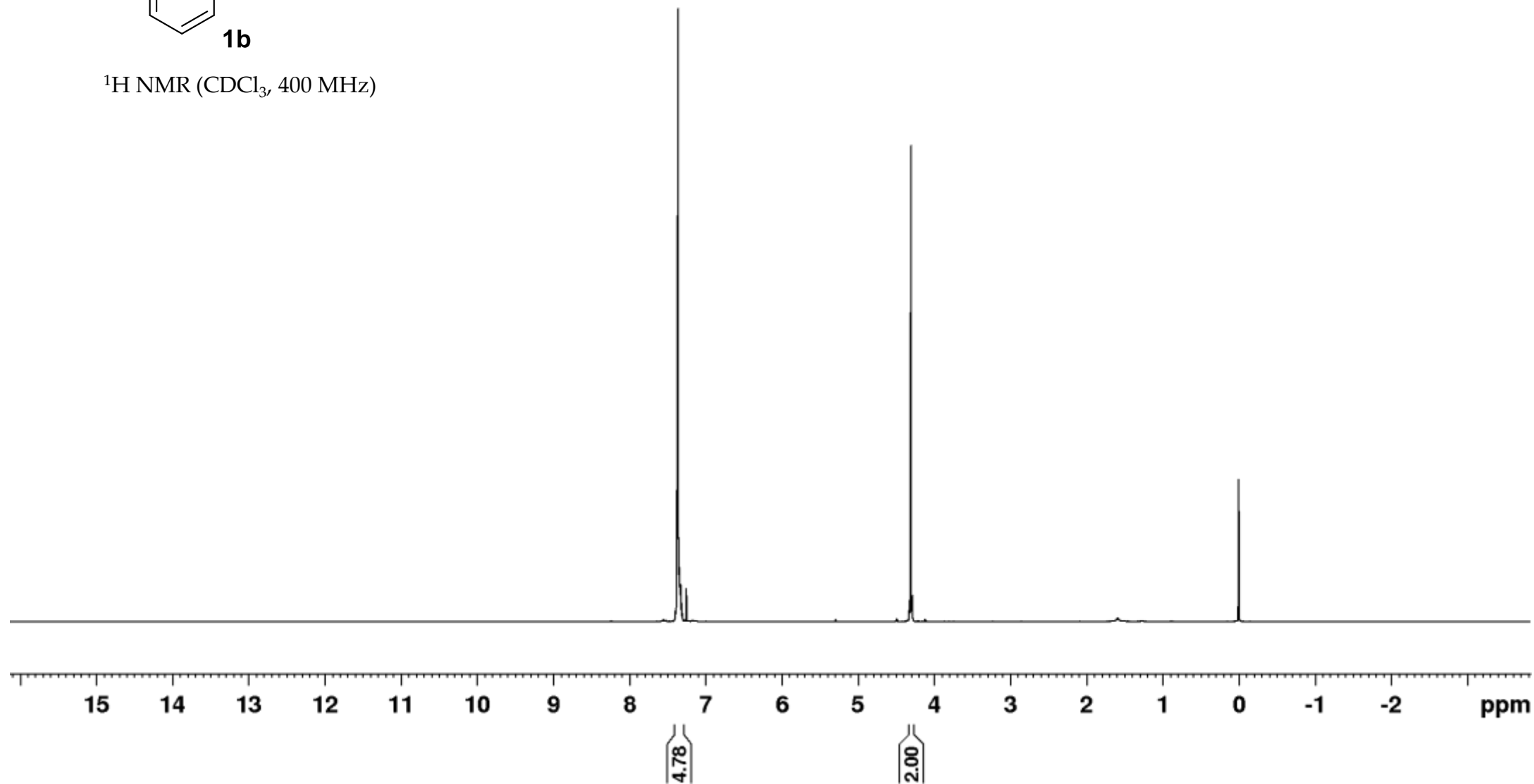


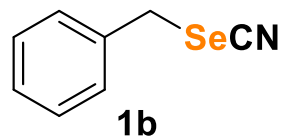
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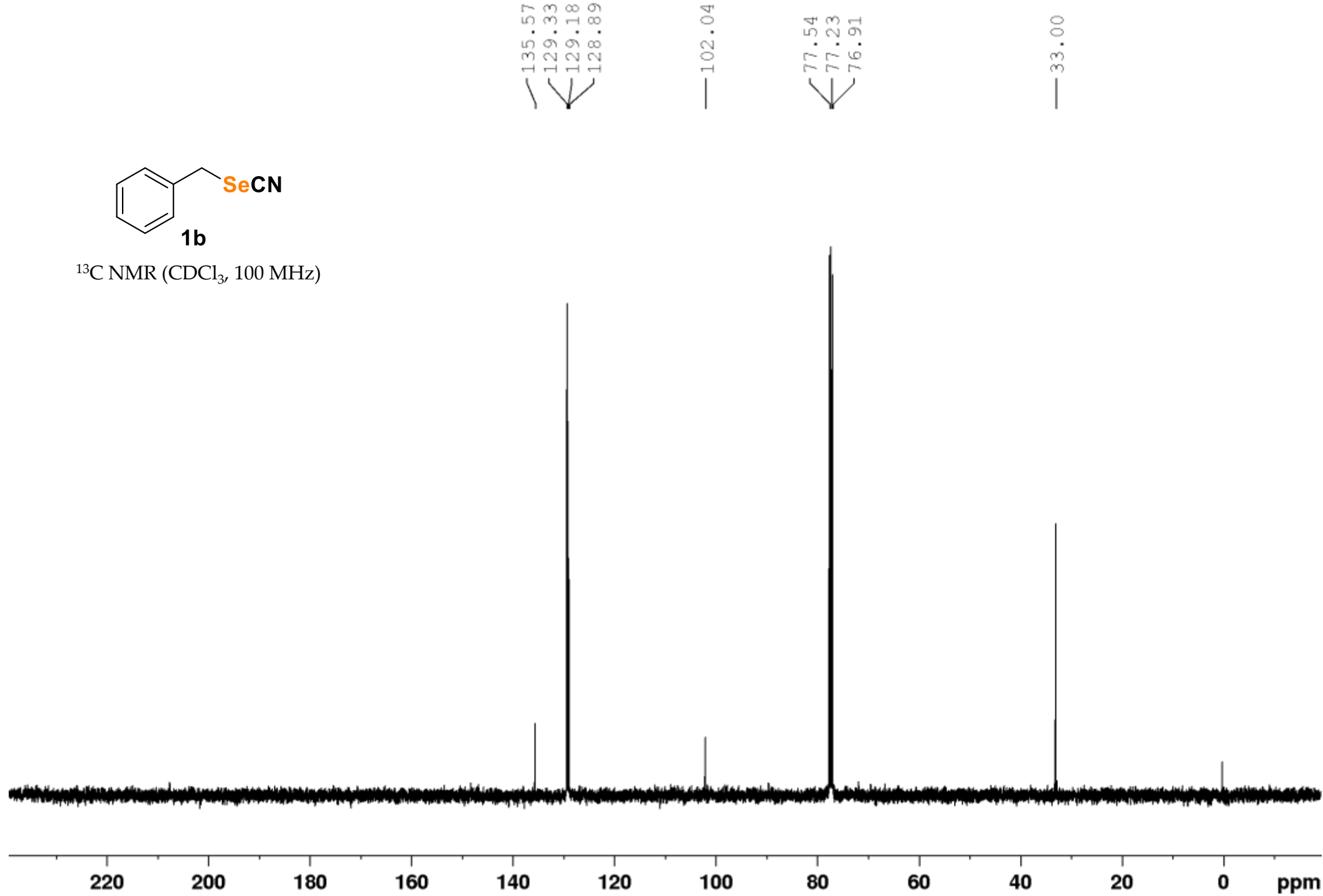


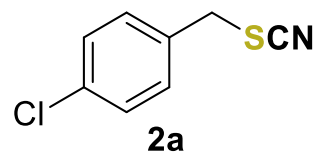
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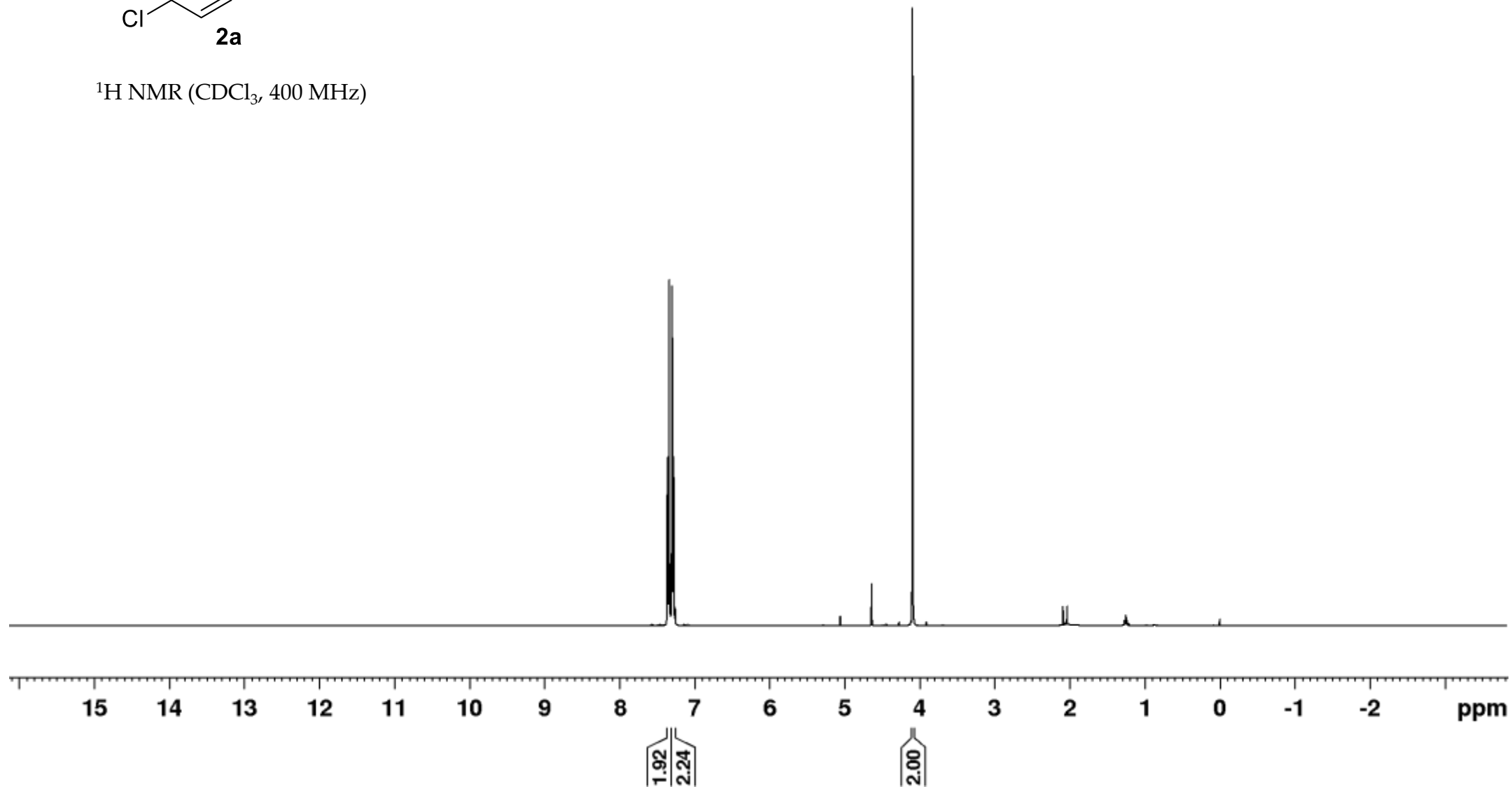


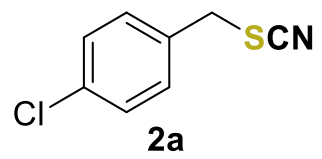
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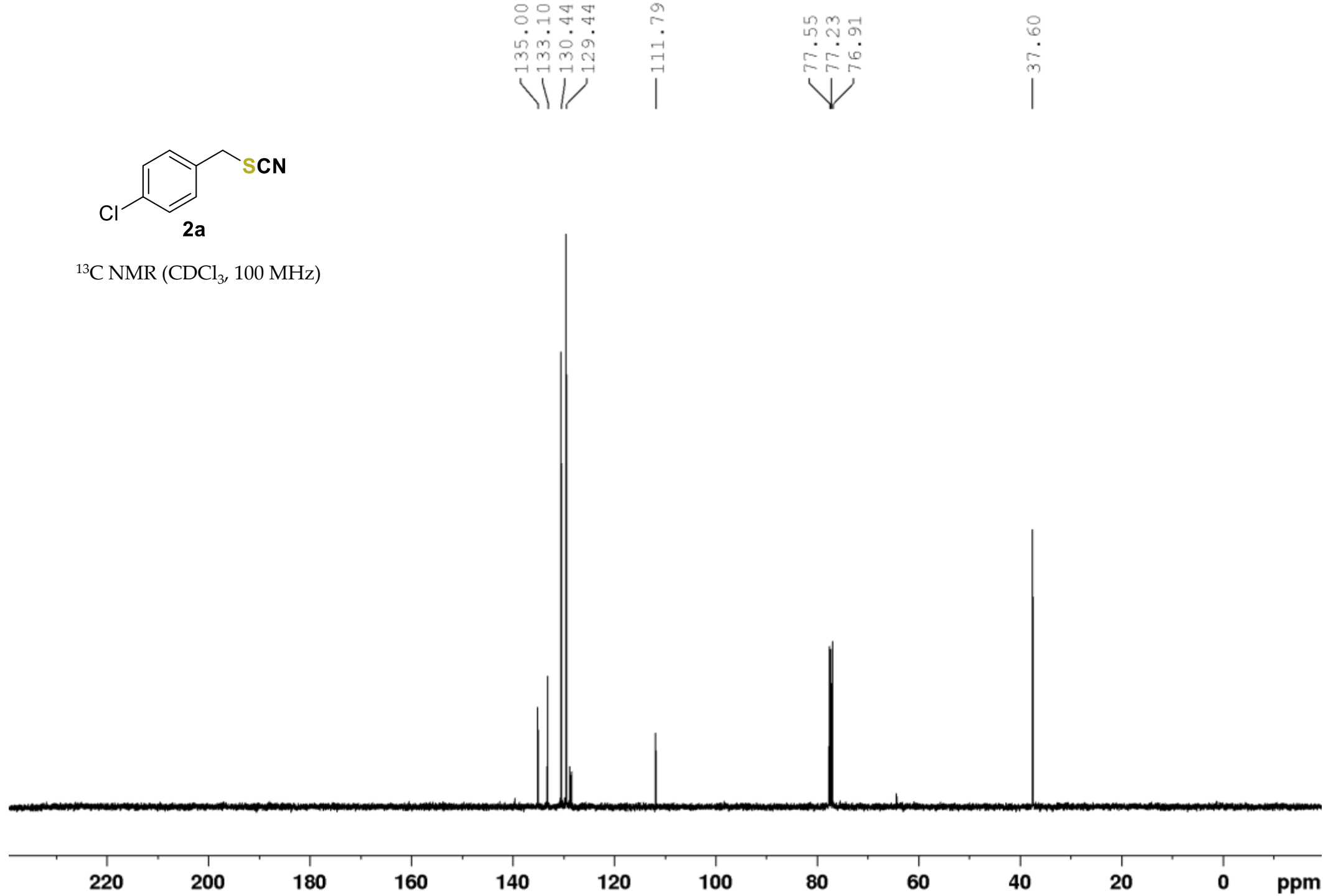


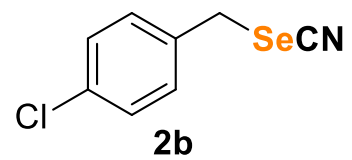
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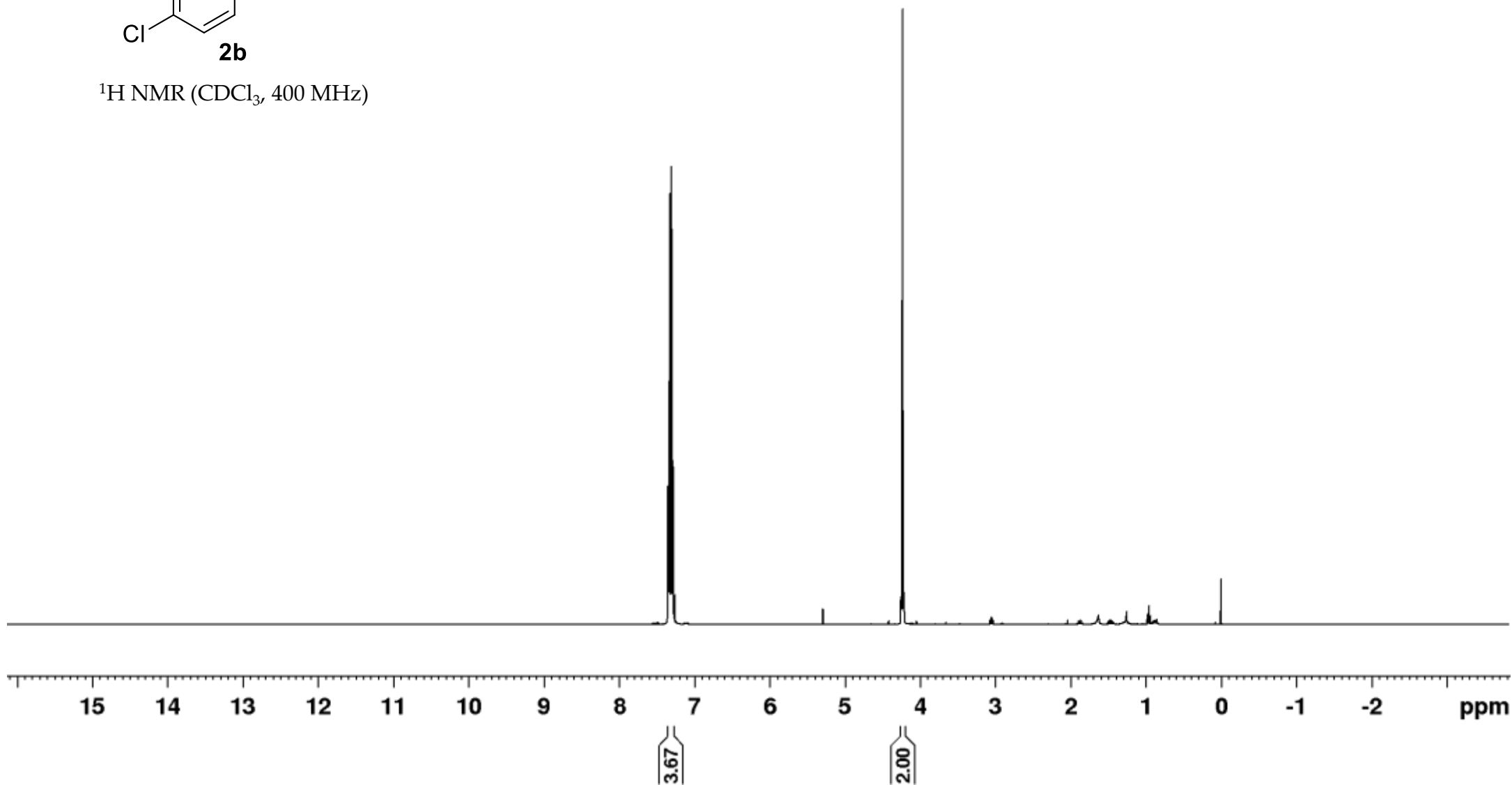


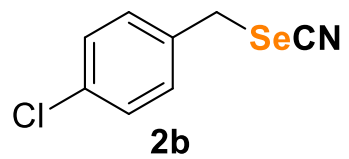
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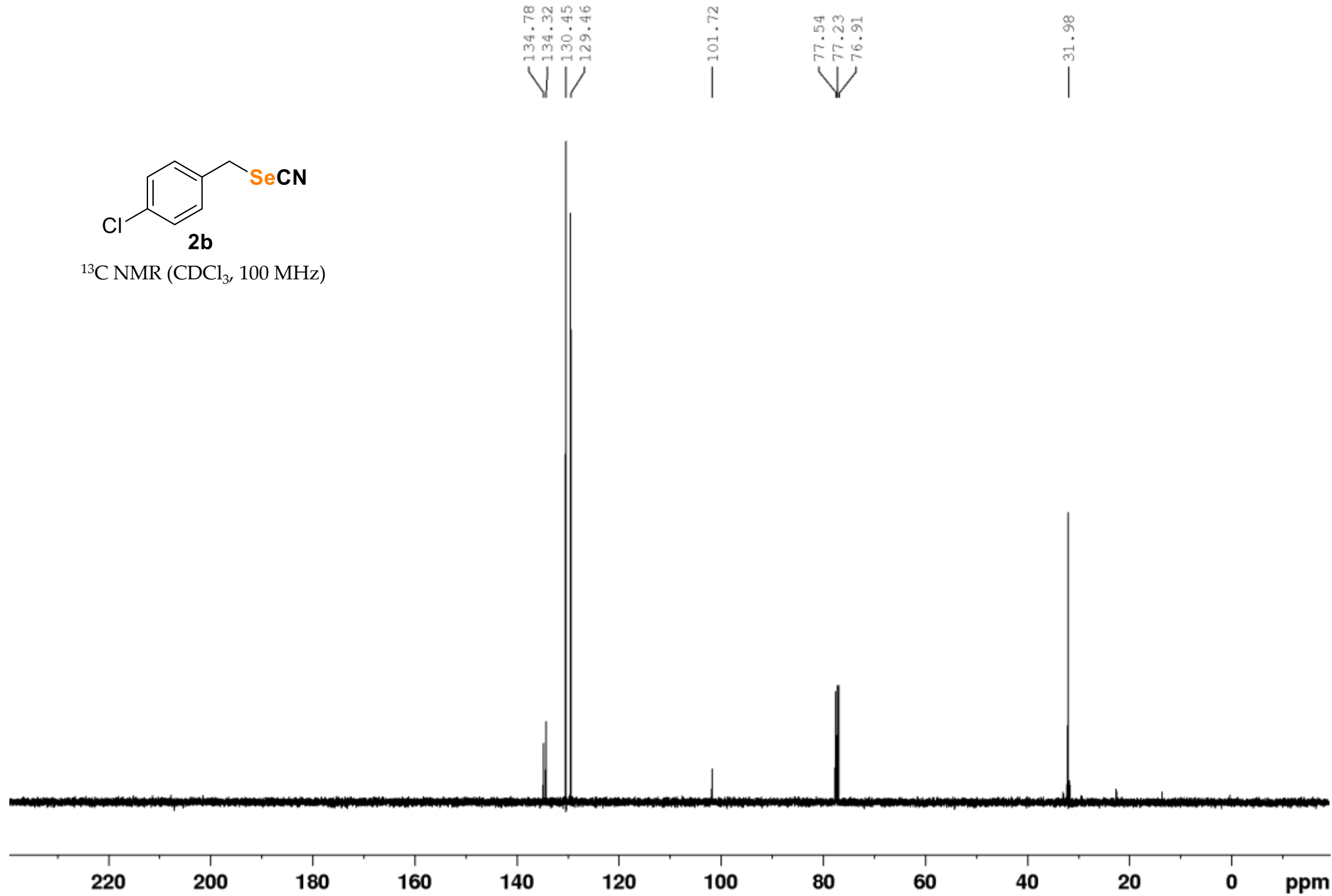


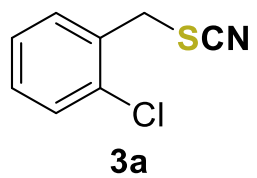
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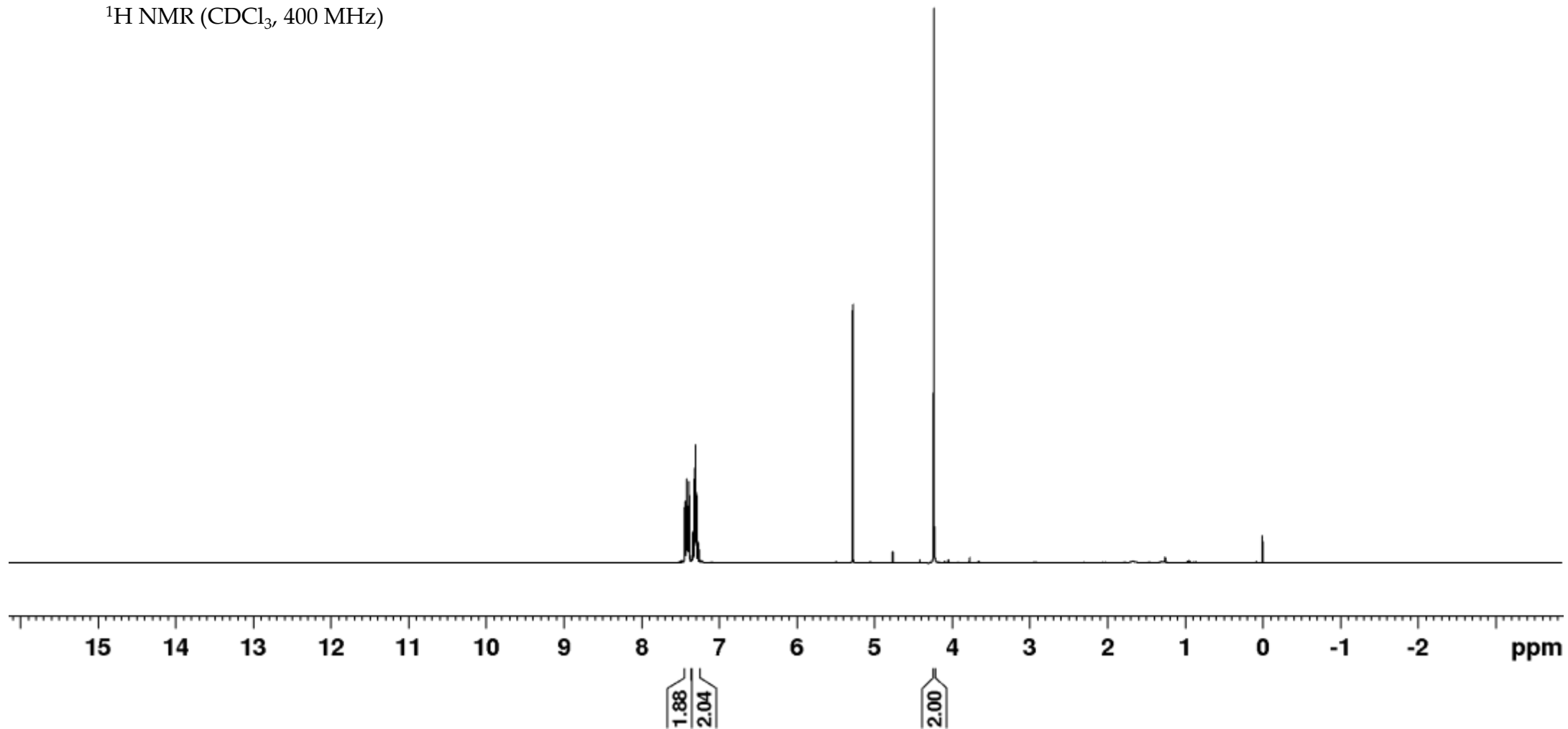


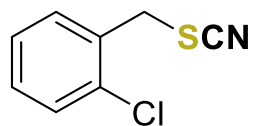
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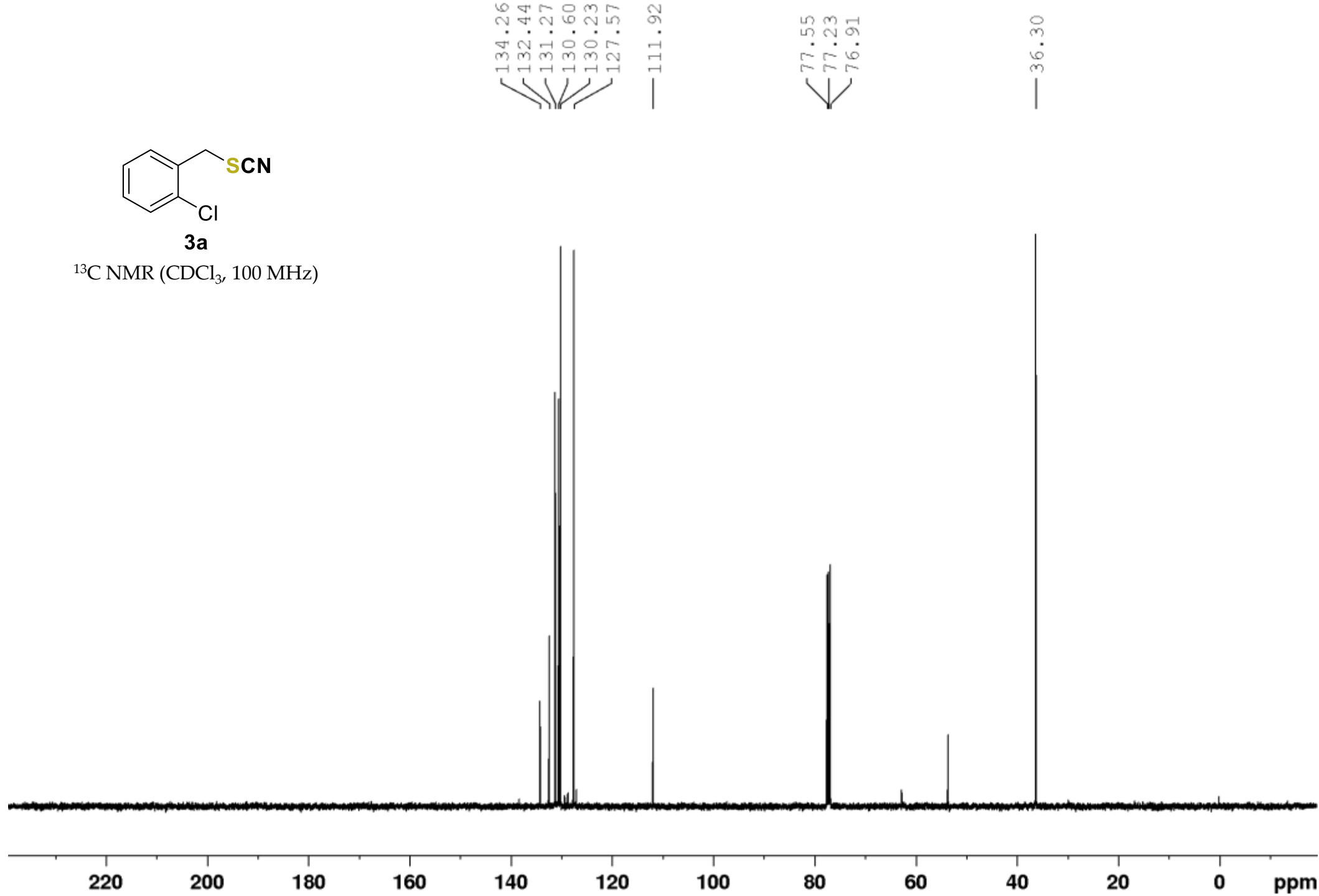
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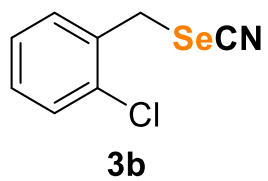




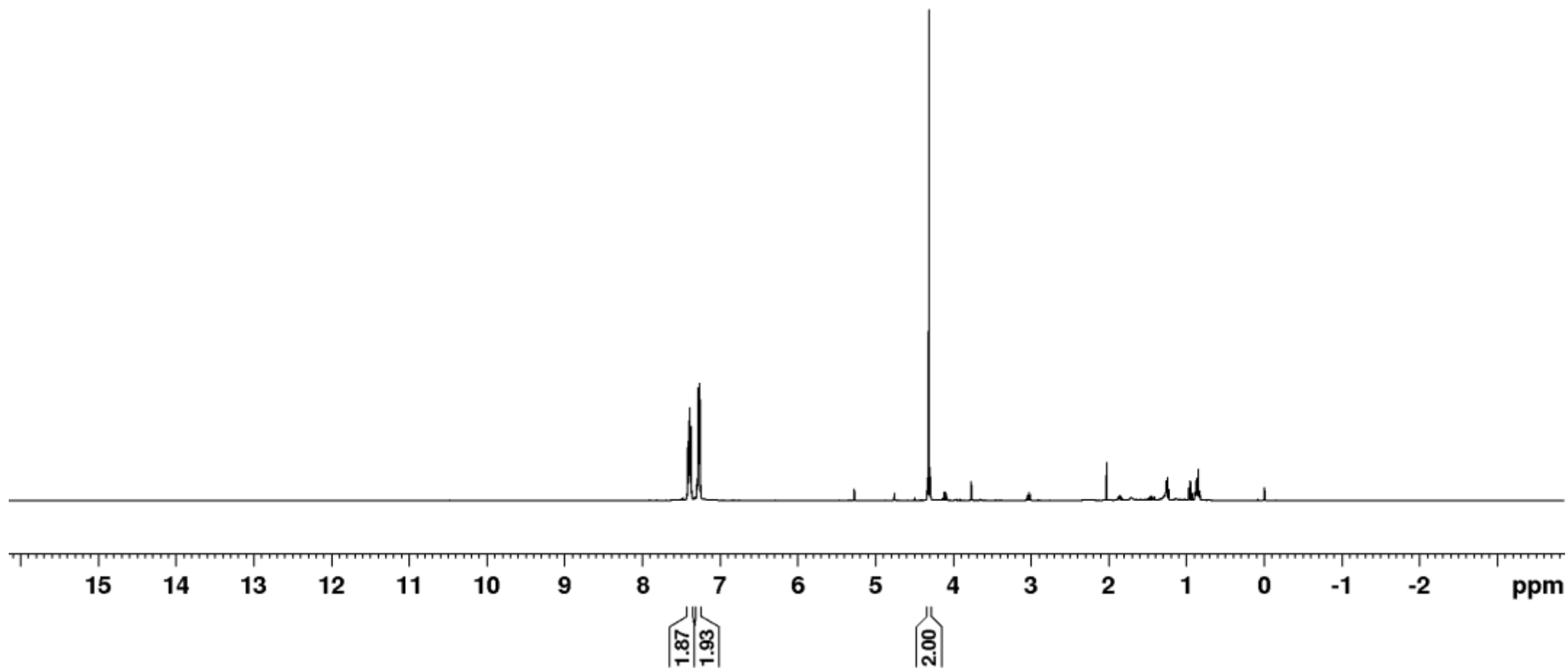
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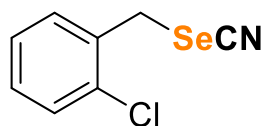
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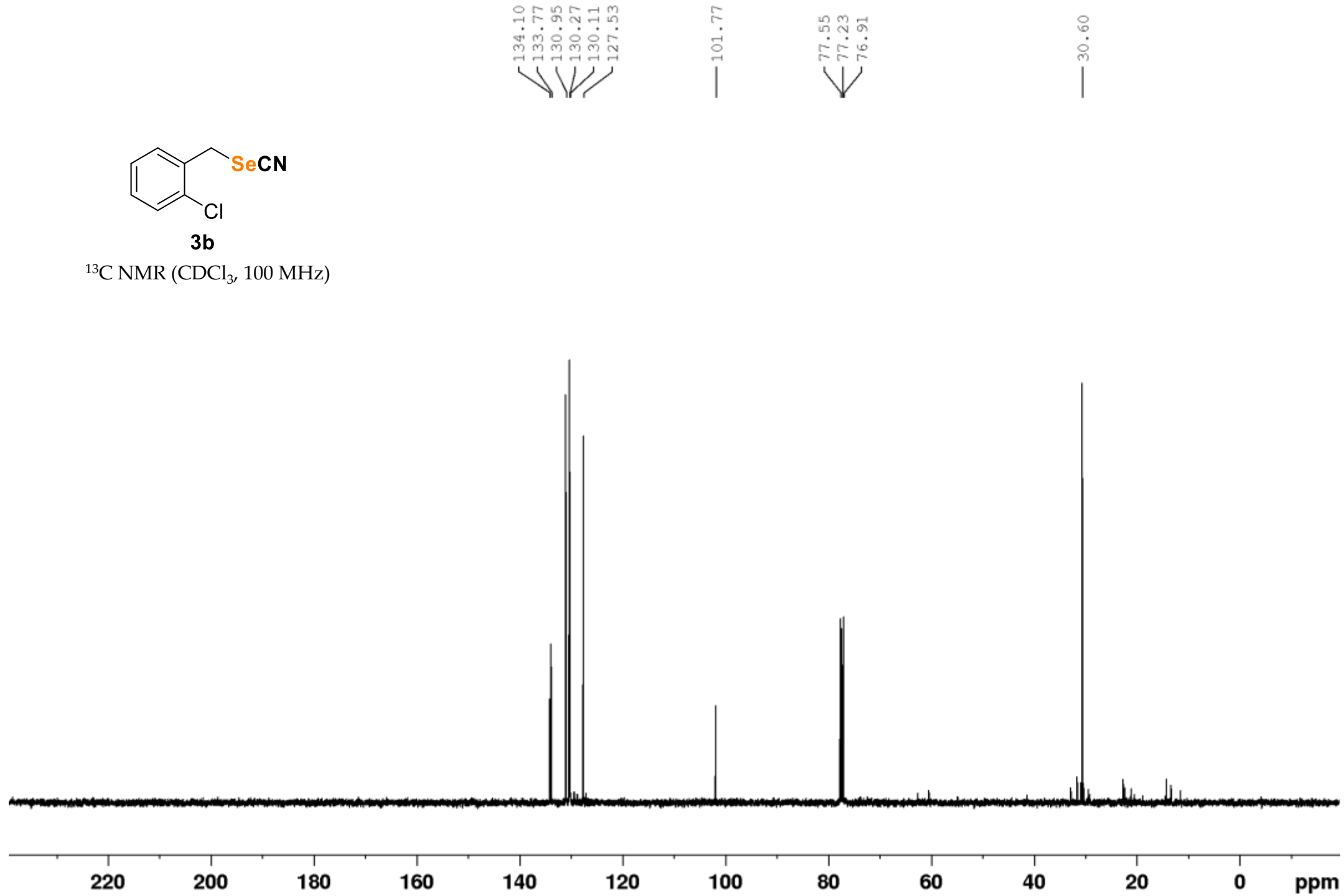
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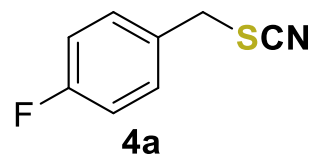




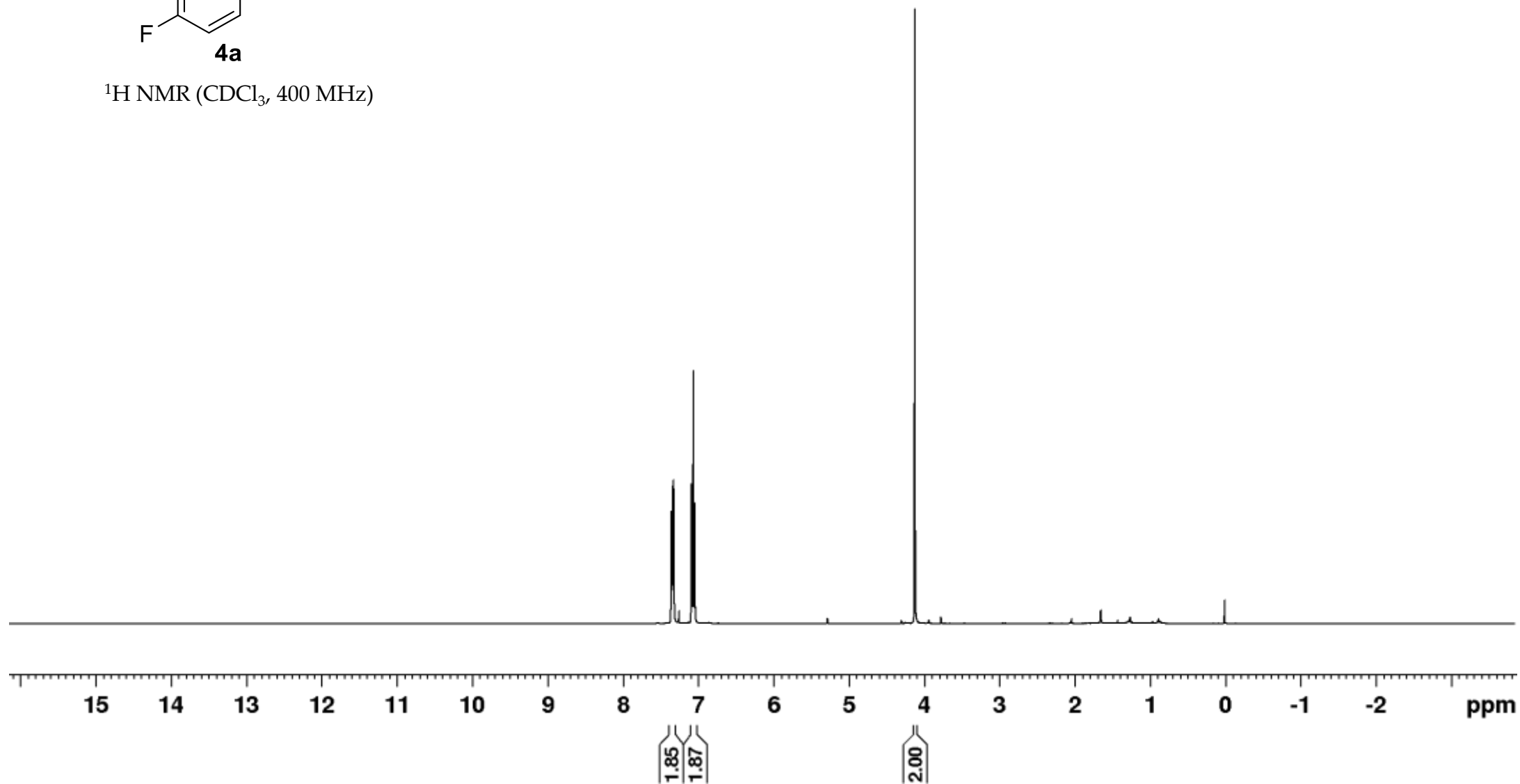
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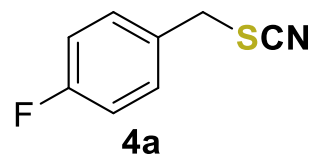
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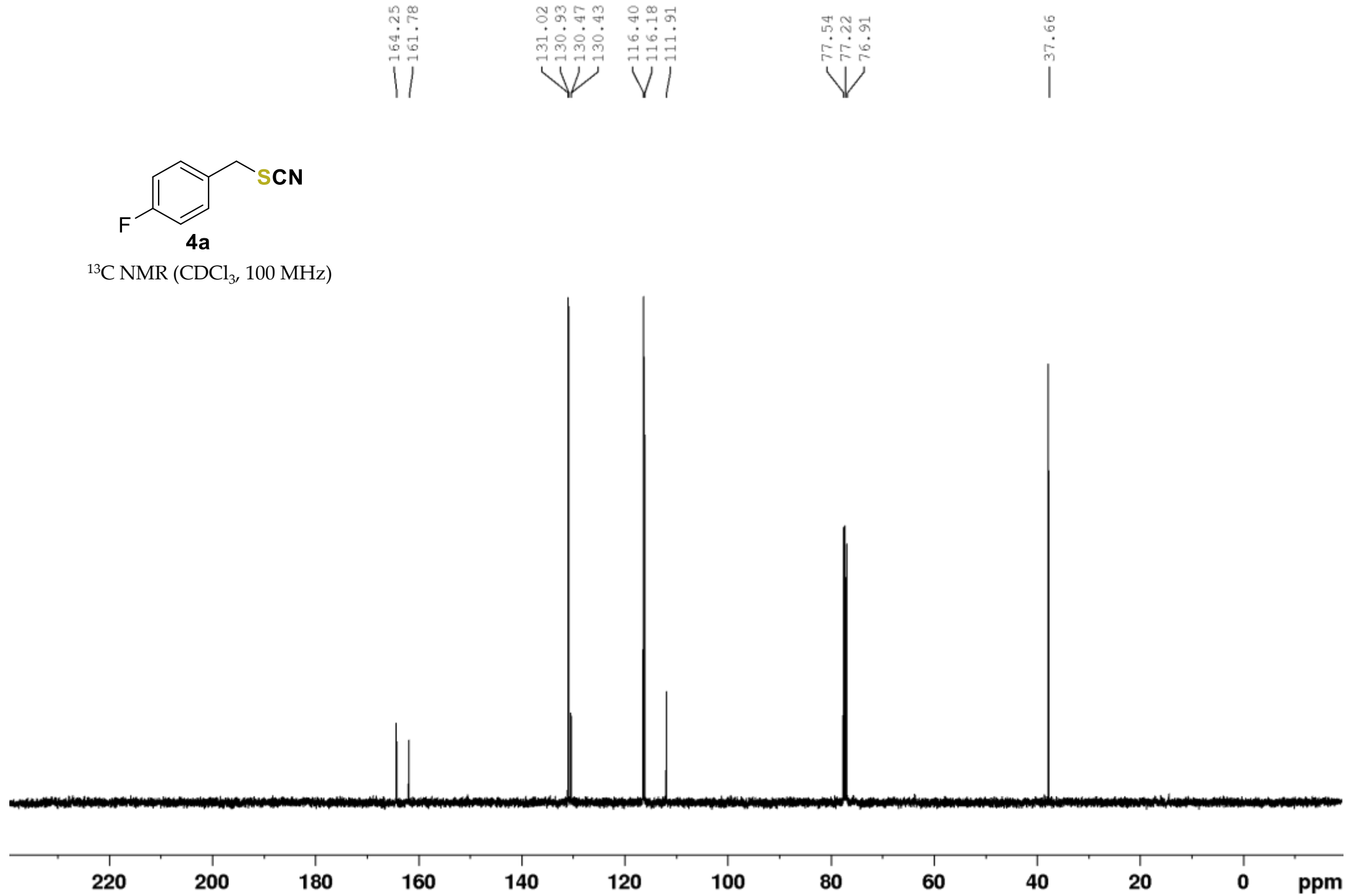


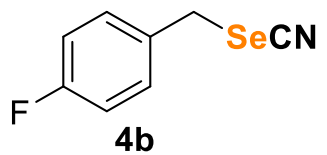
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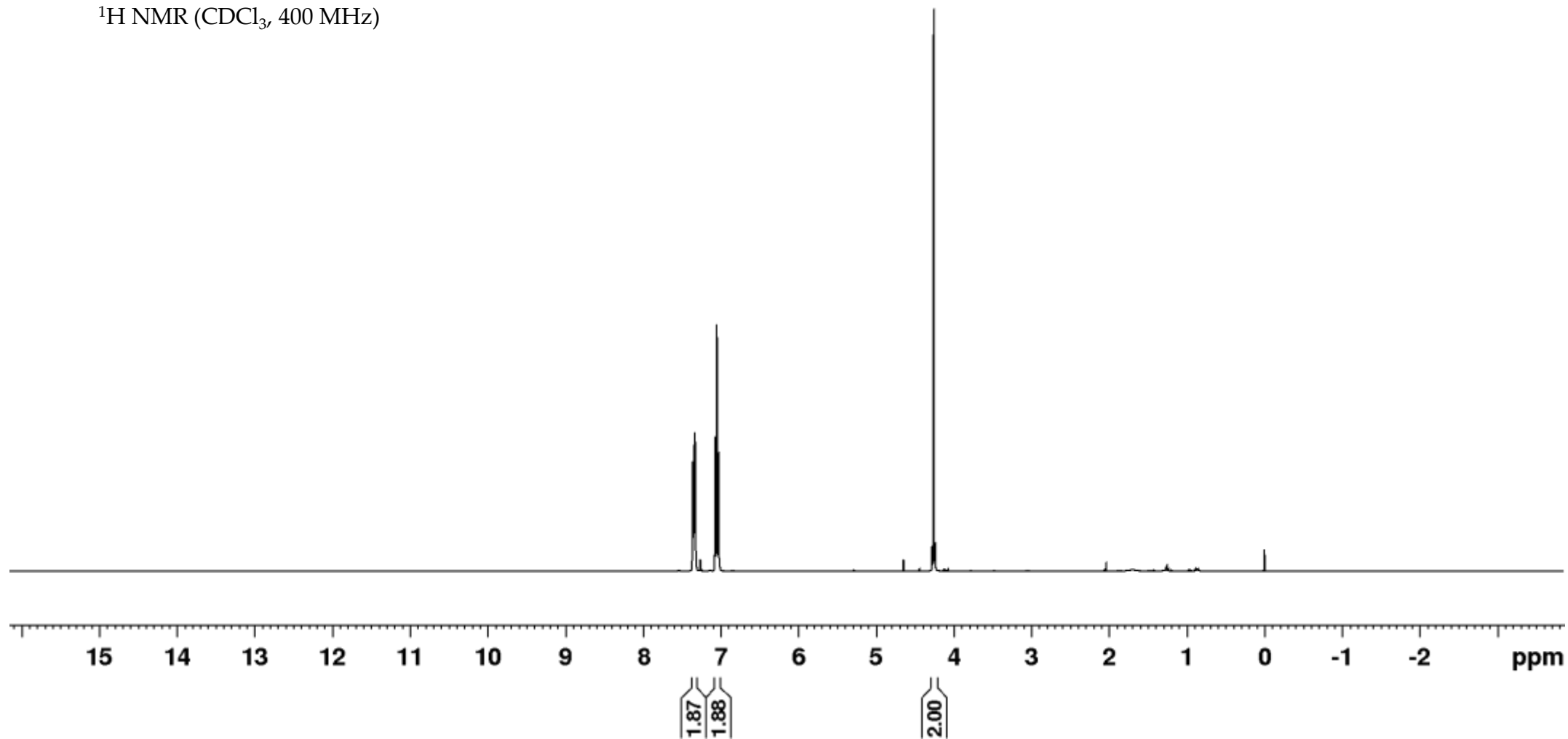


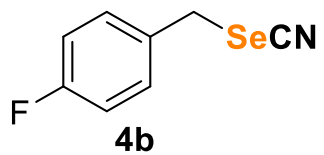
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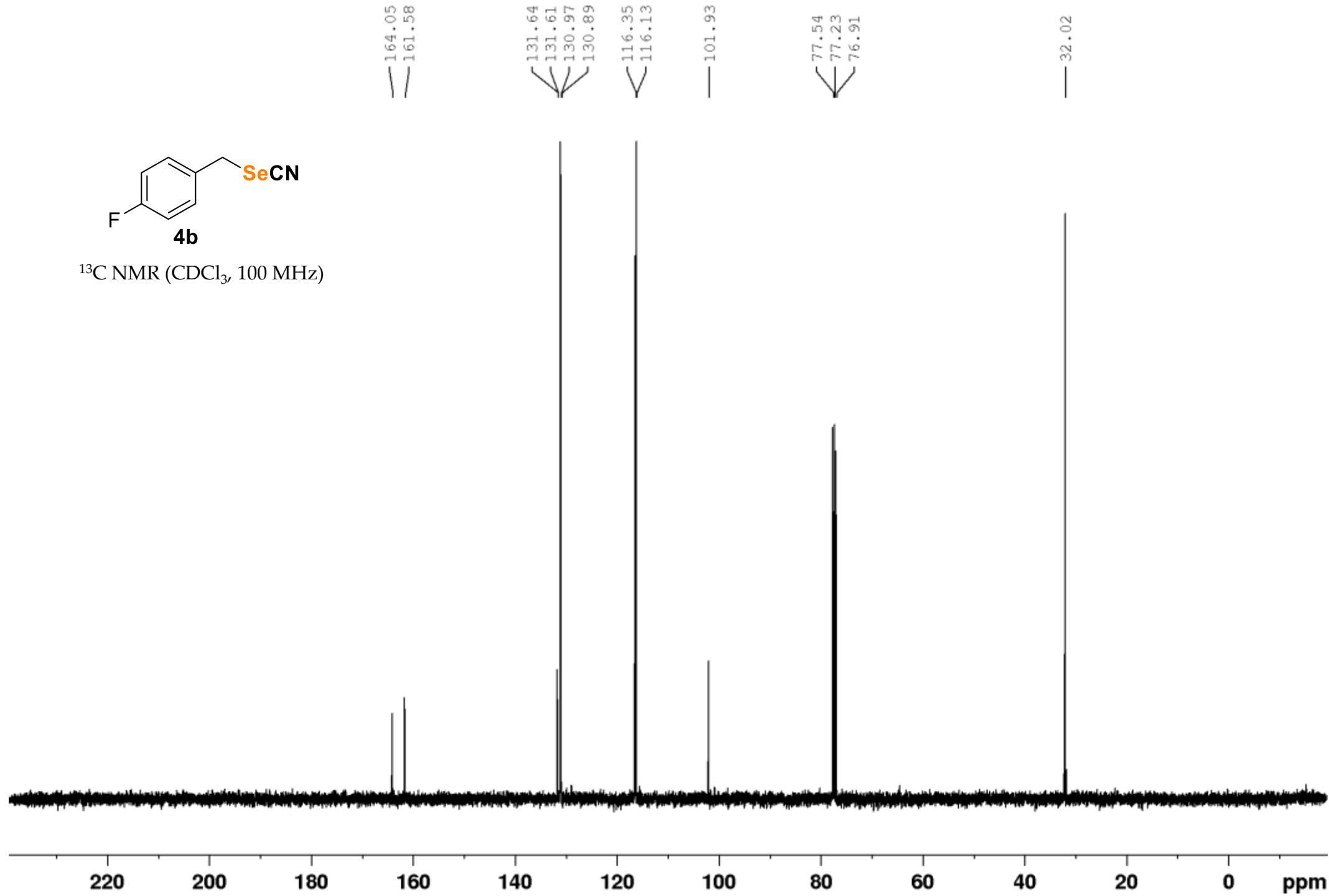


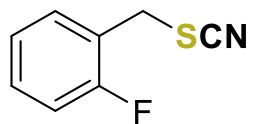
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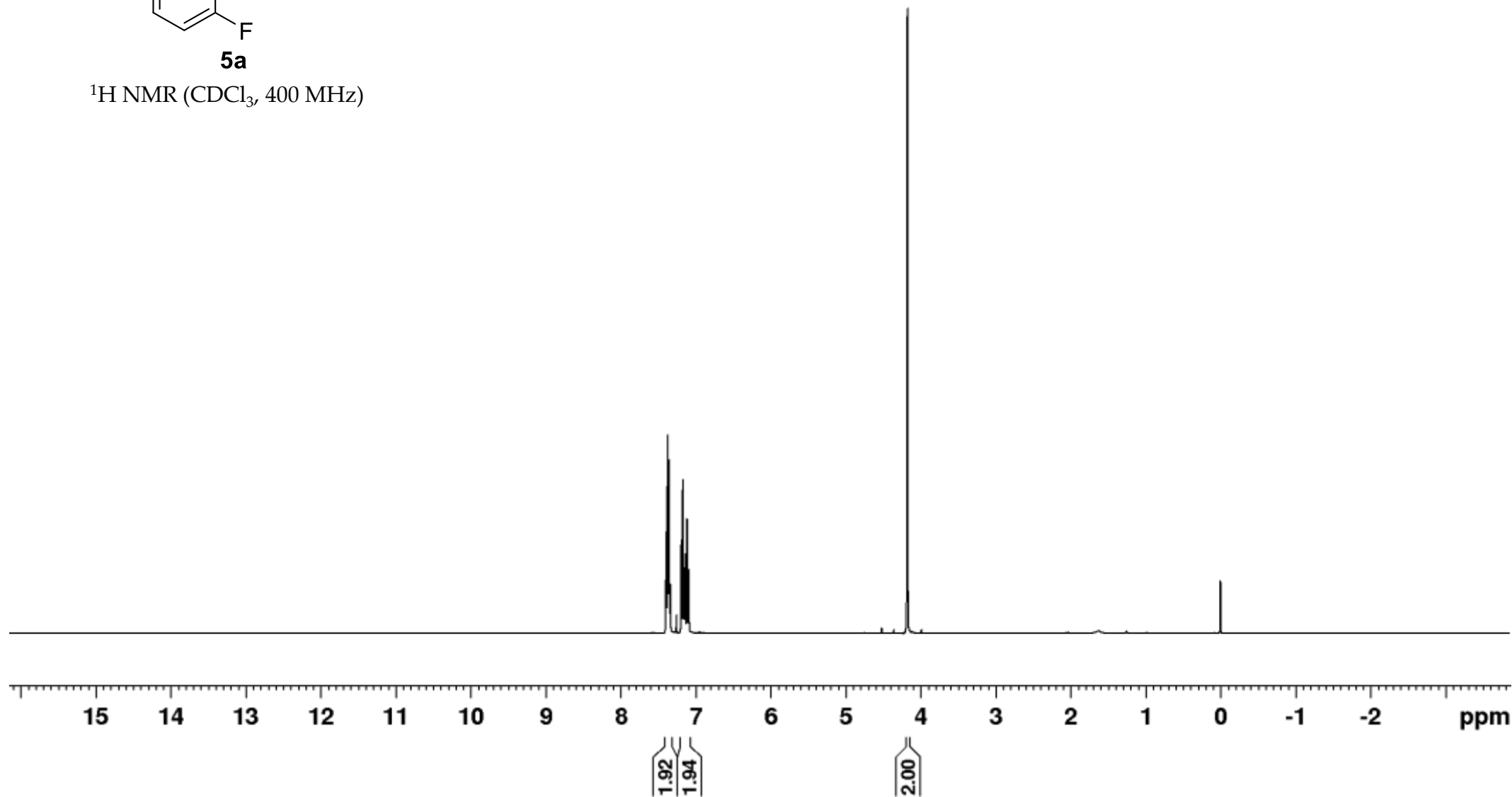
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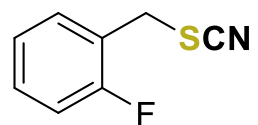




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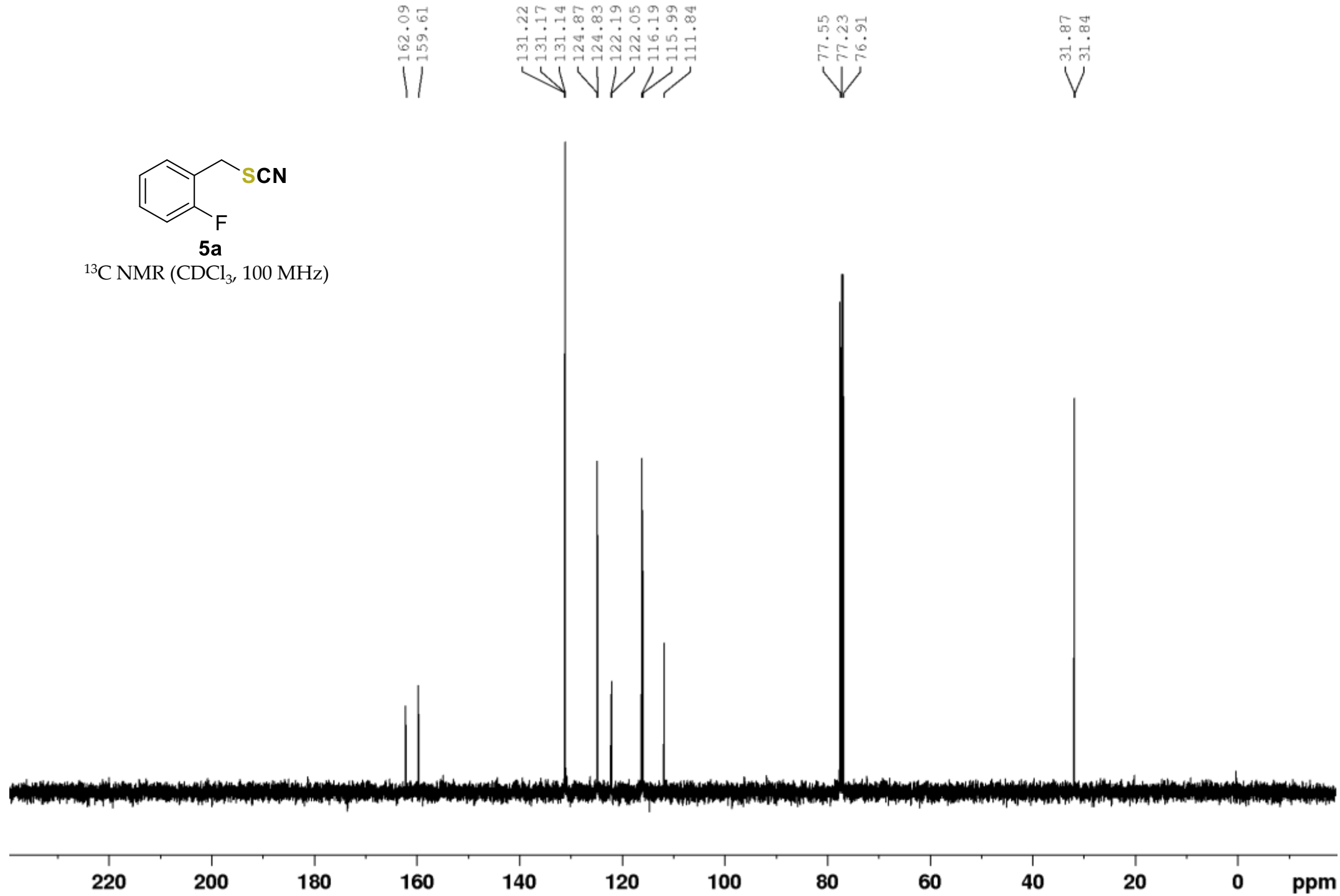
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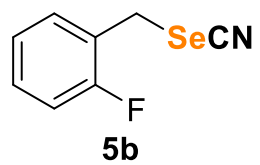




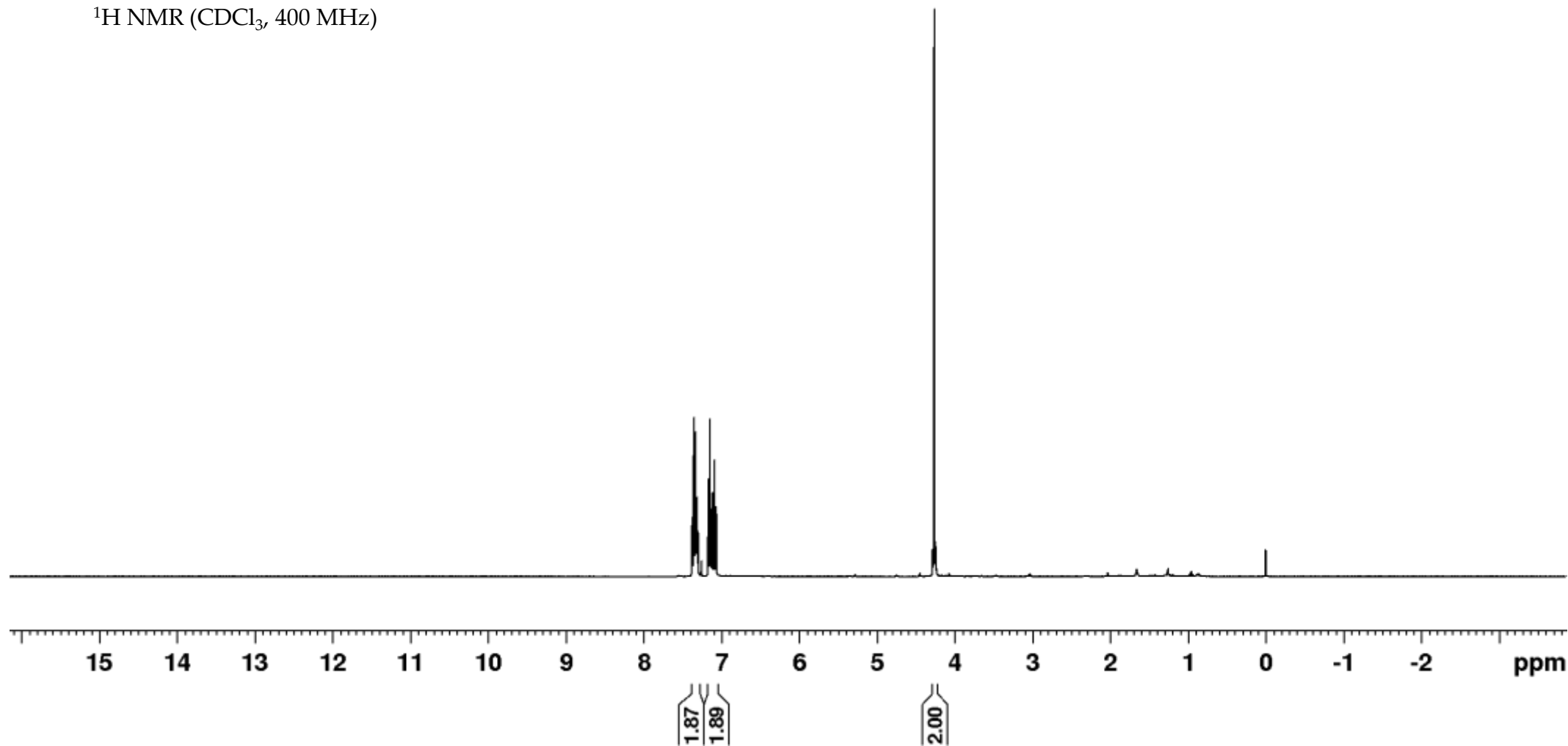
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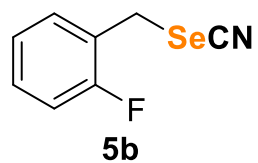
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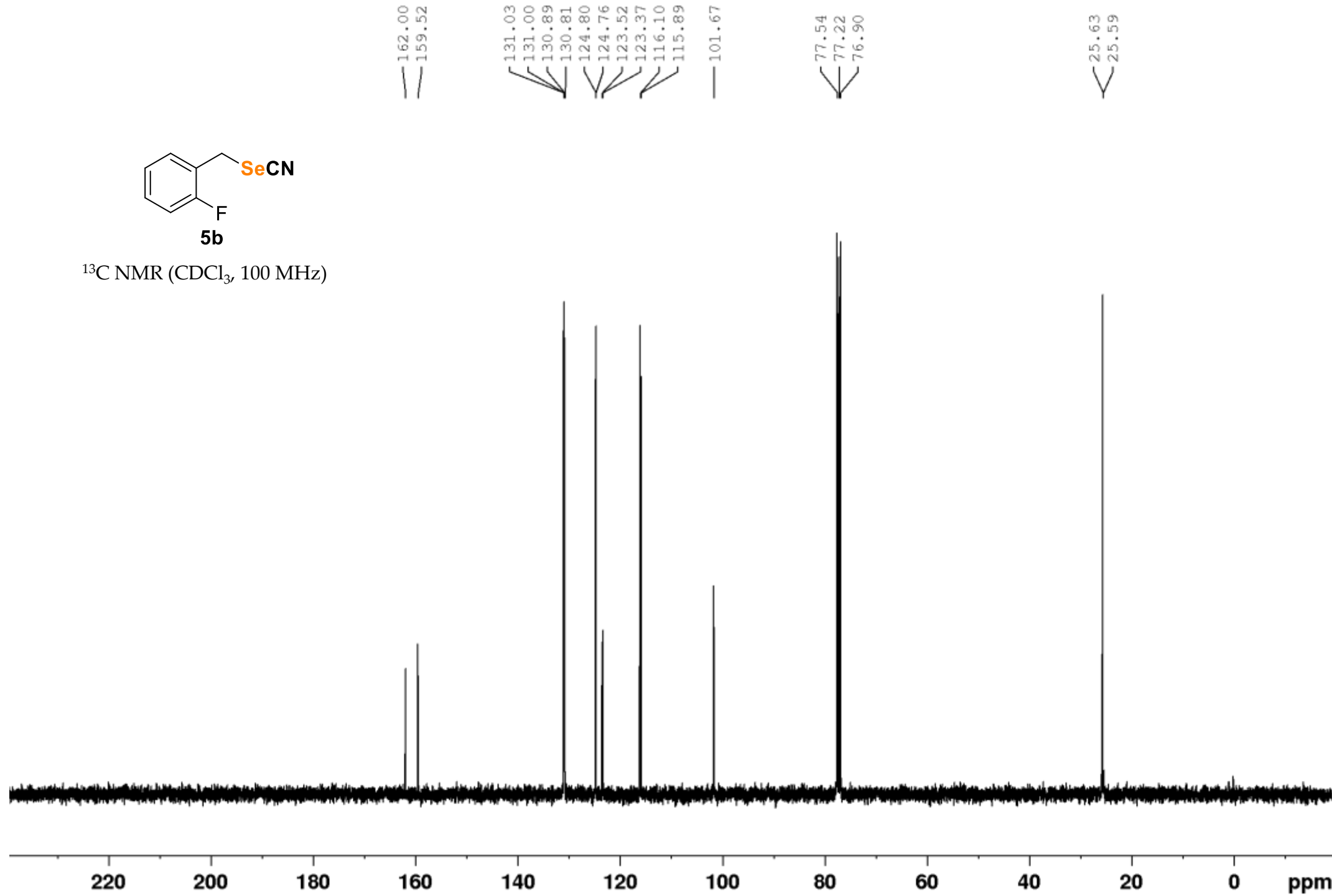


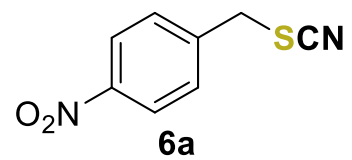
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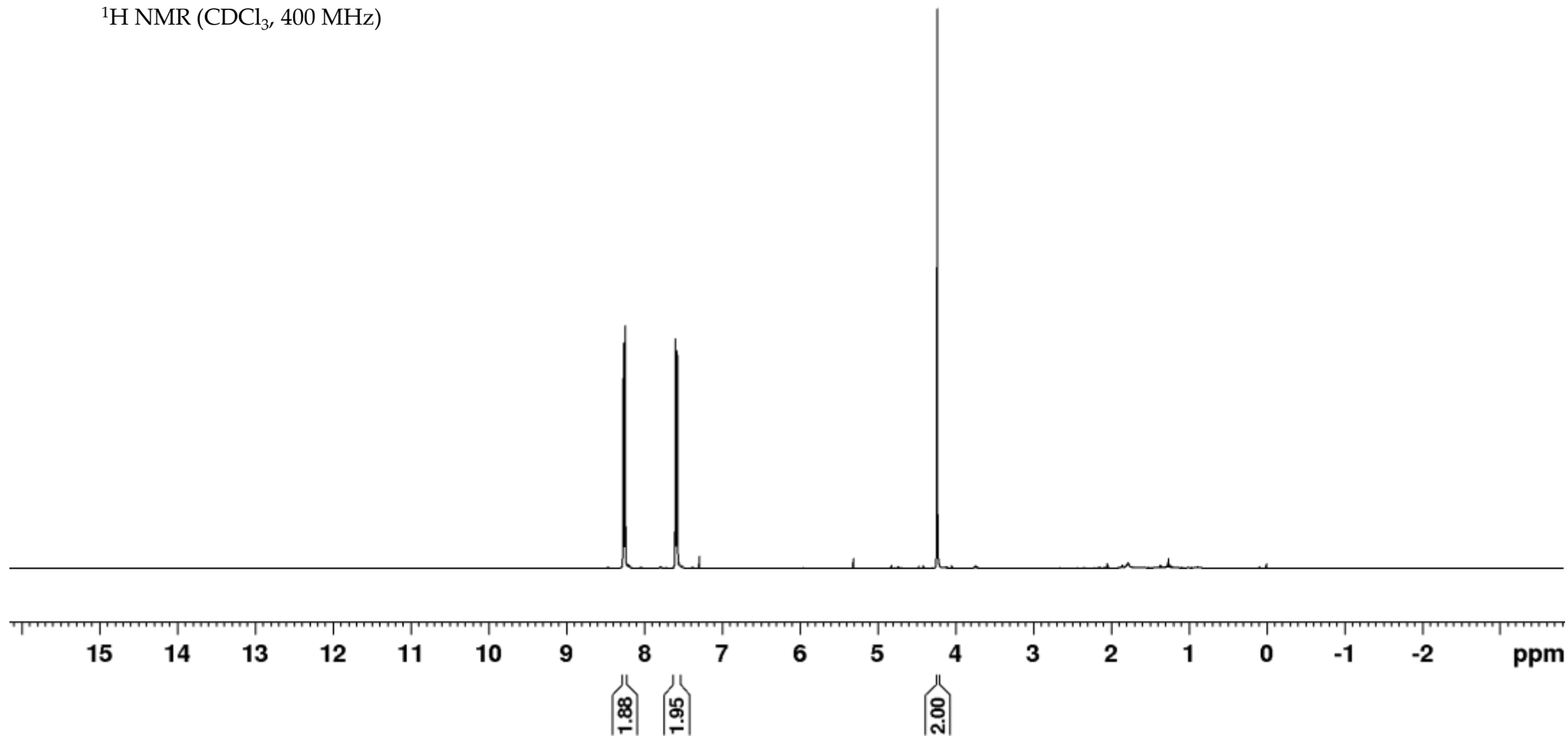


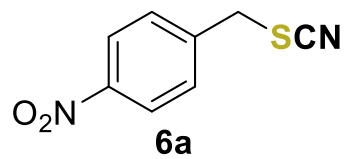
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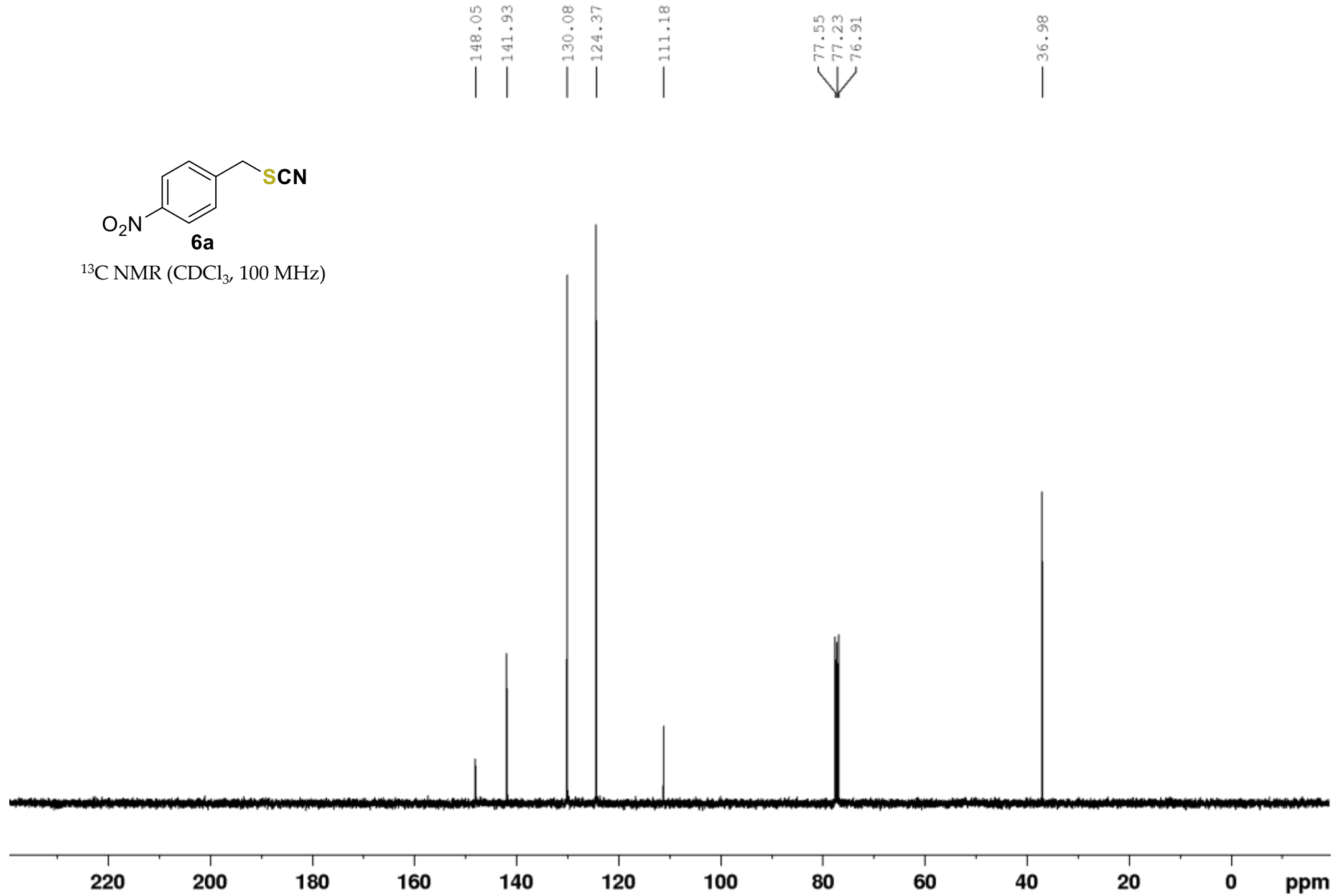


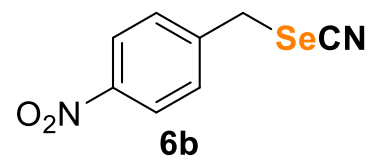
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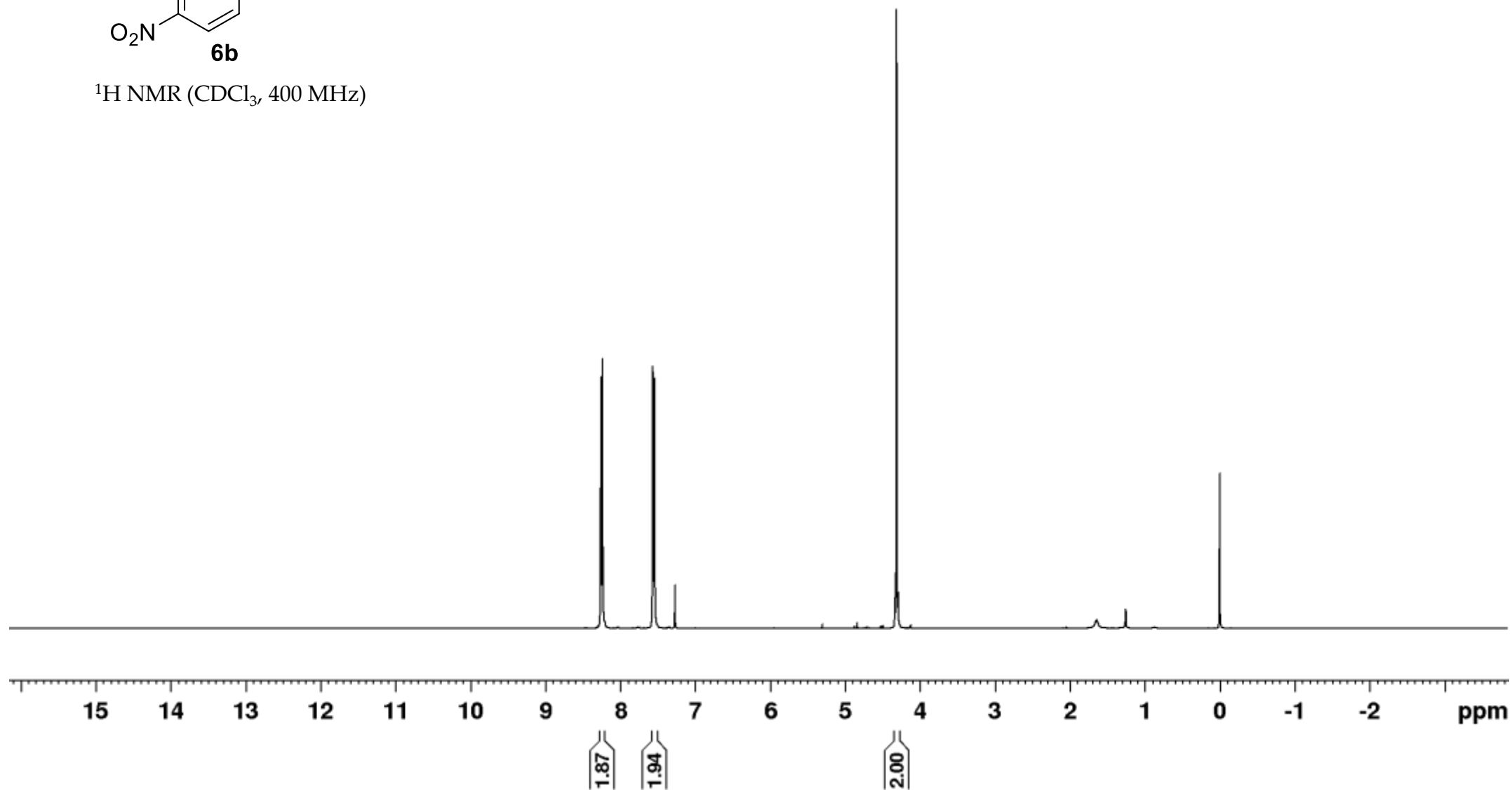


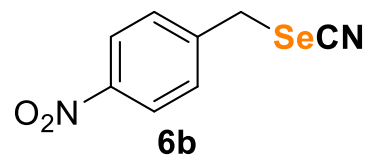
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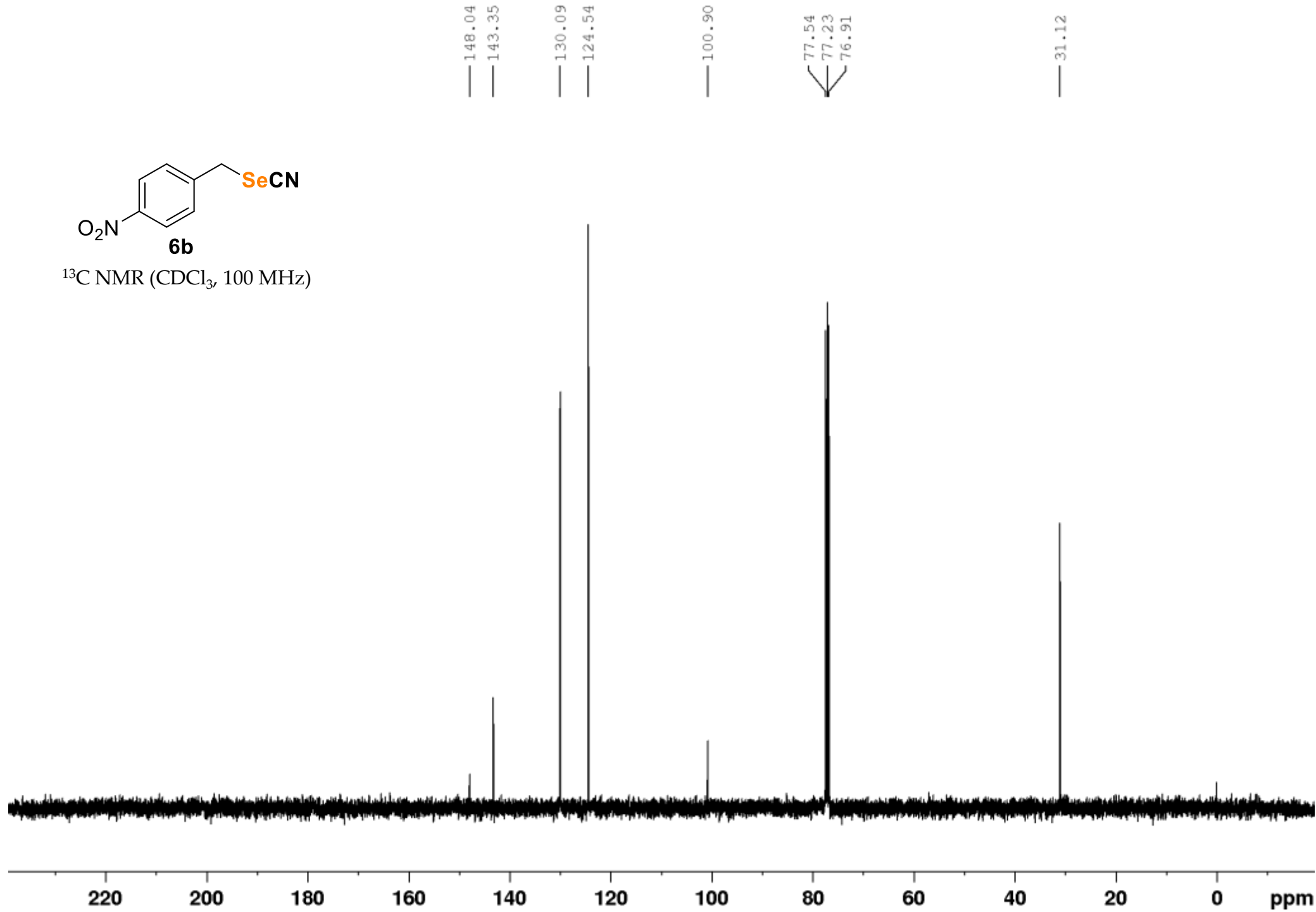


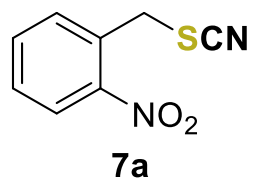
^1H NMR (CDCl_3 , 400 MHz)



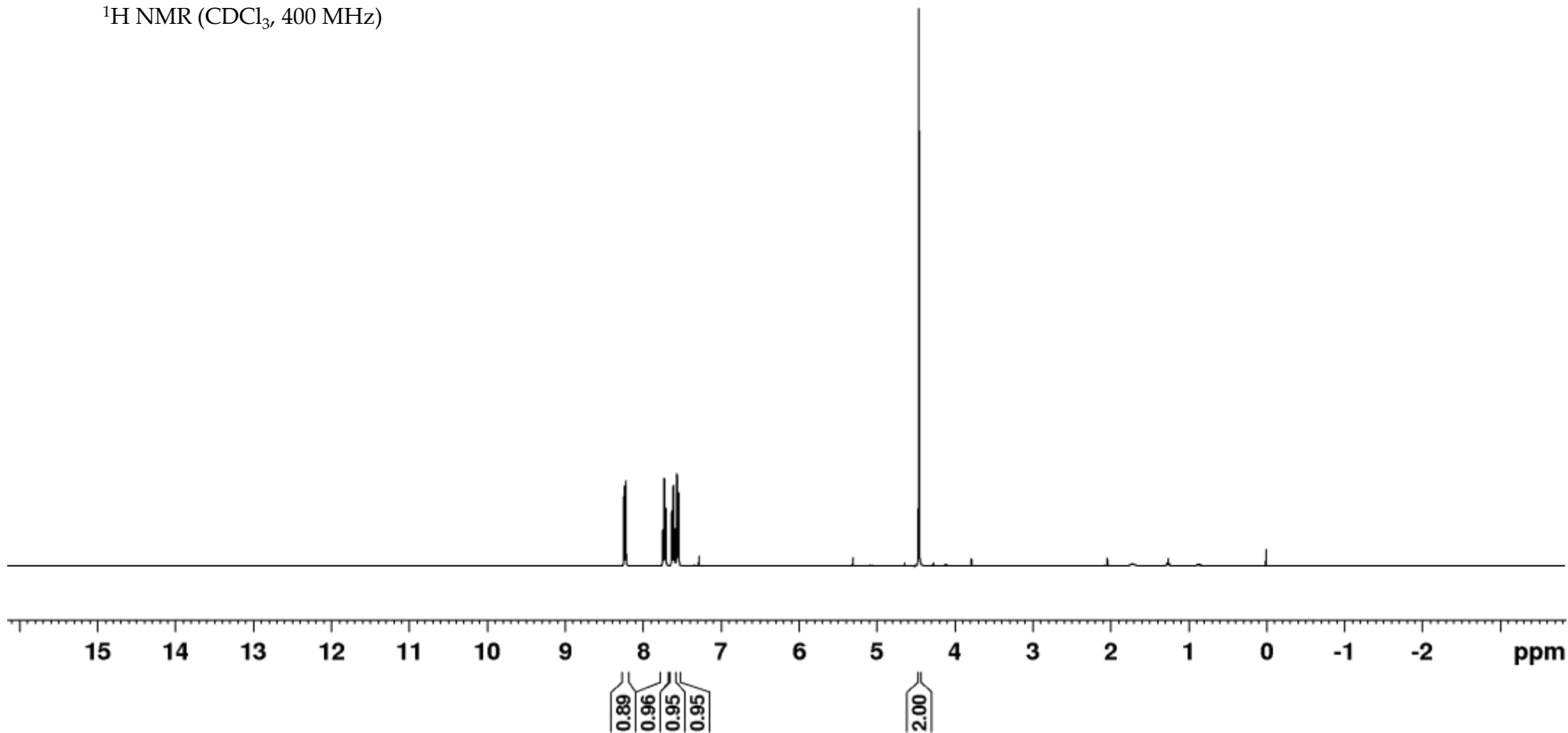


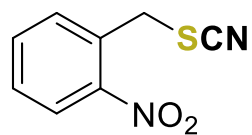
^{13}C NMR (CDCl_3 , 100 MHz)





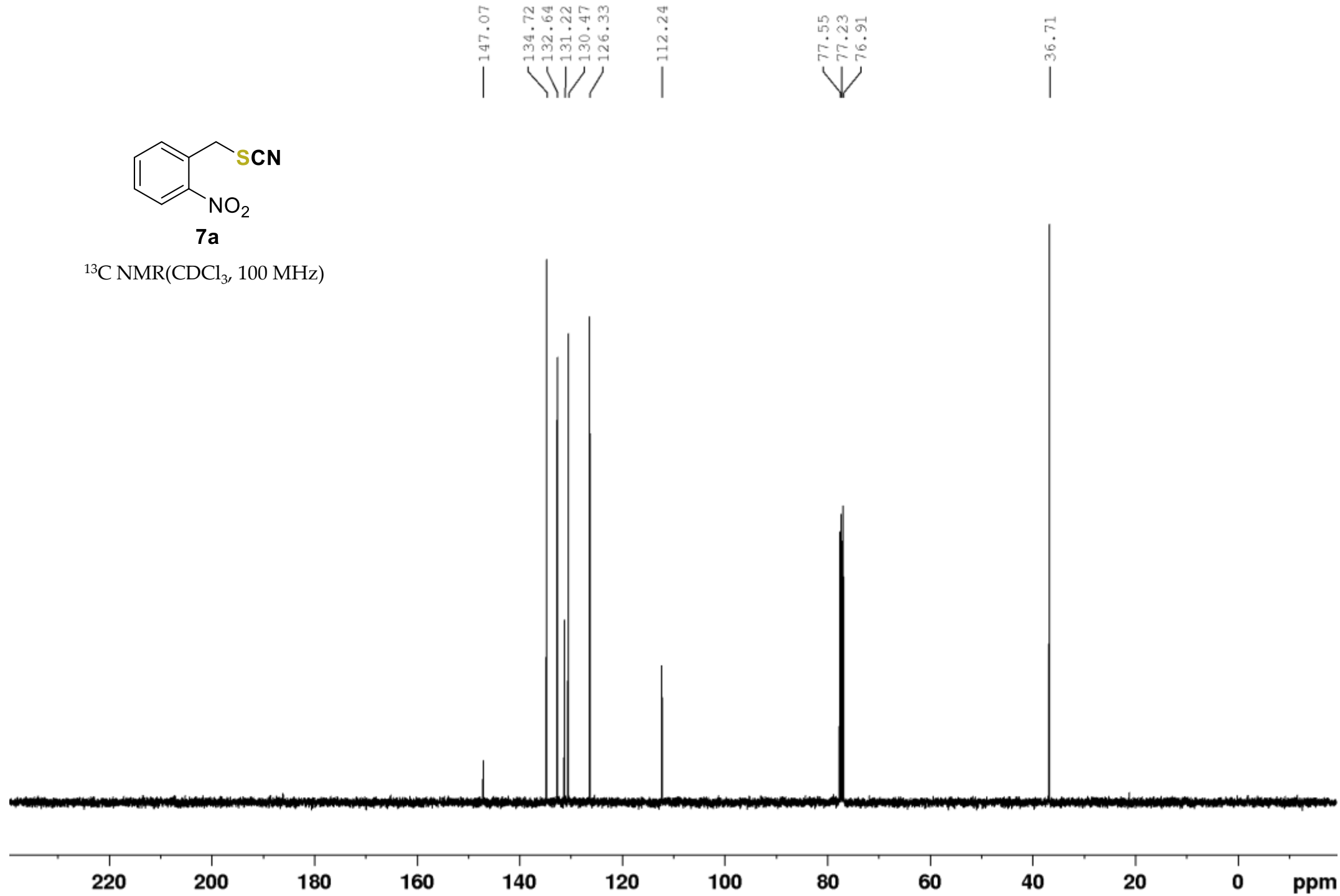
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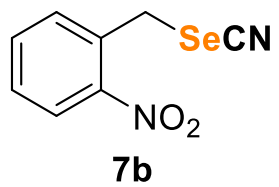




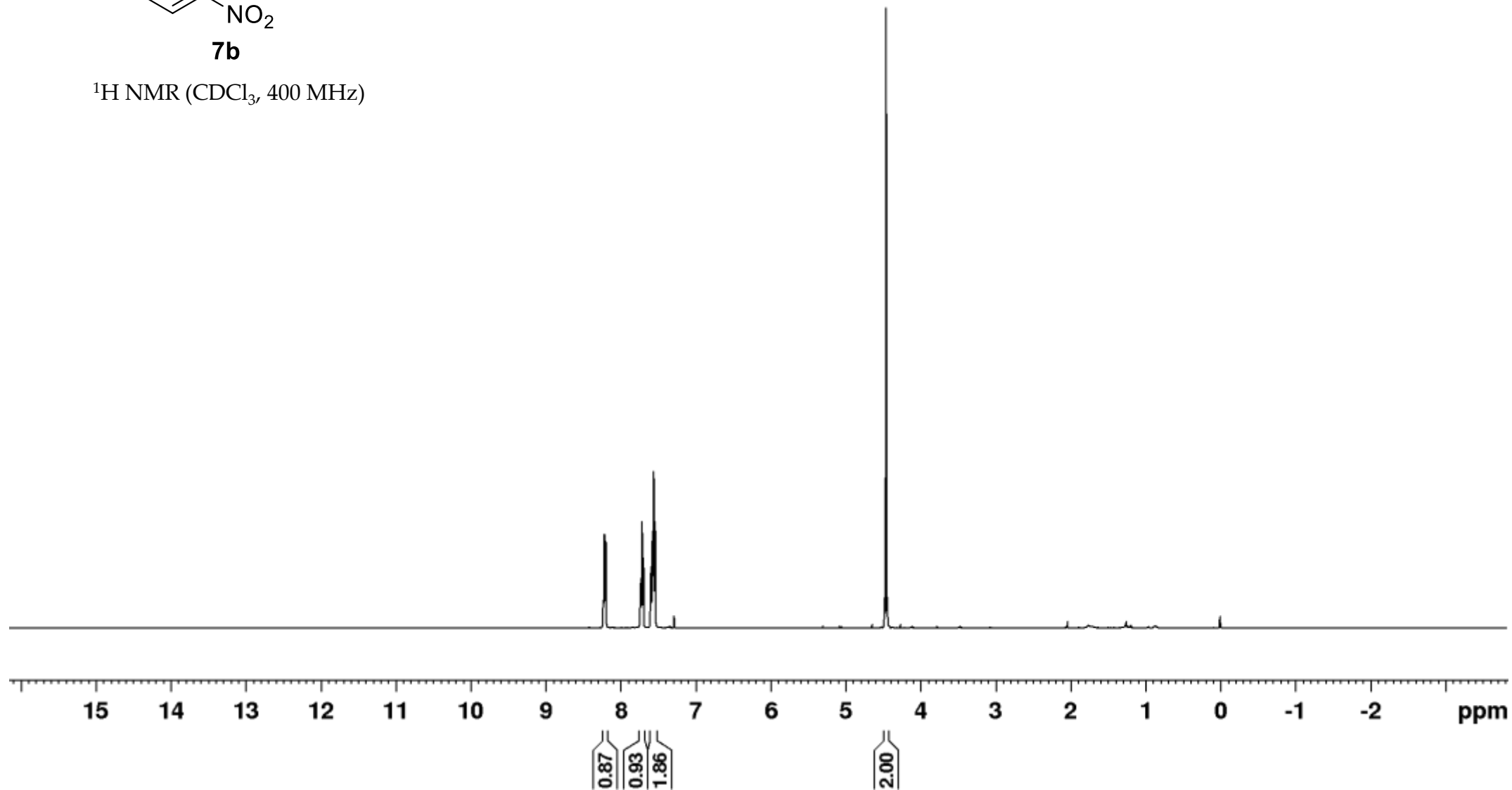
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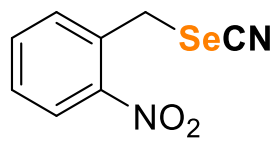
^{13}C NMR(CDCl_3 , 100 MHz)





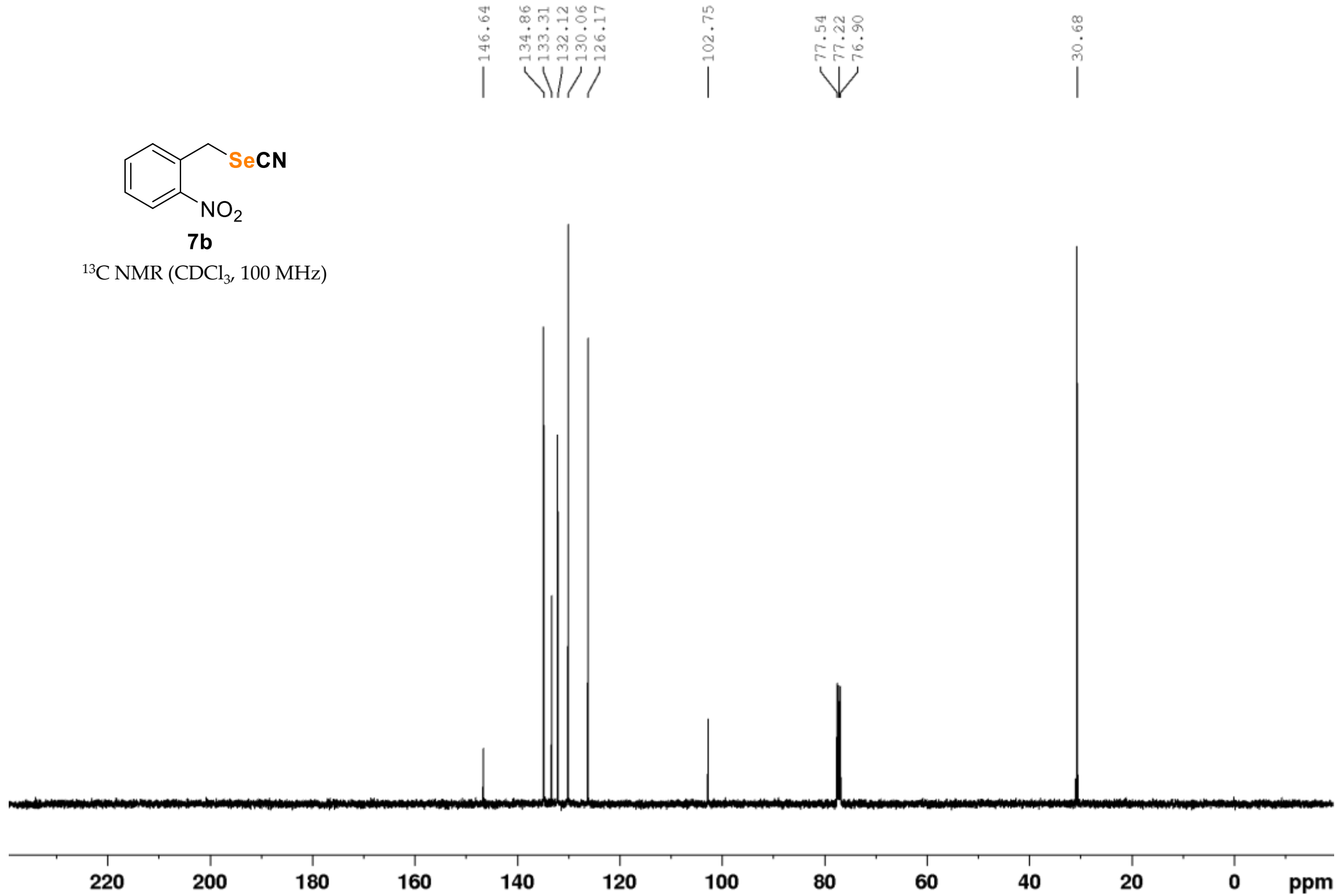
^1H NMR (CDCl_3 , 400 MHz)

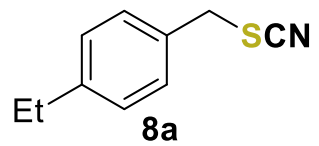




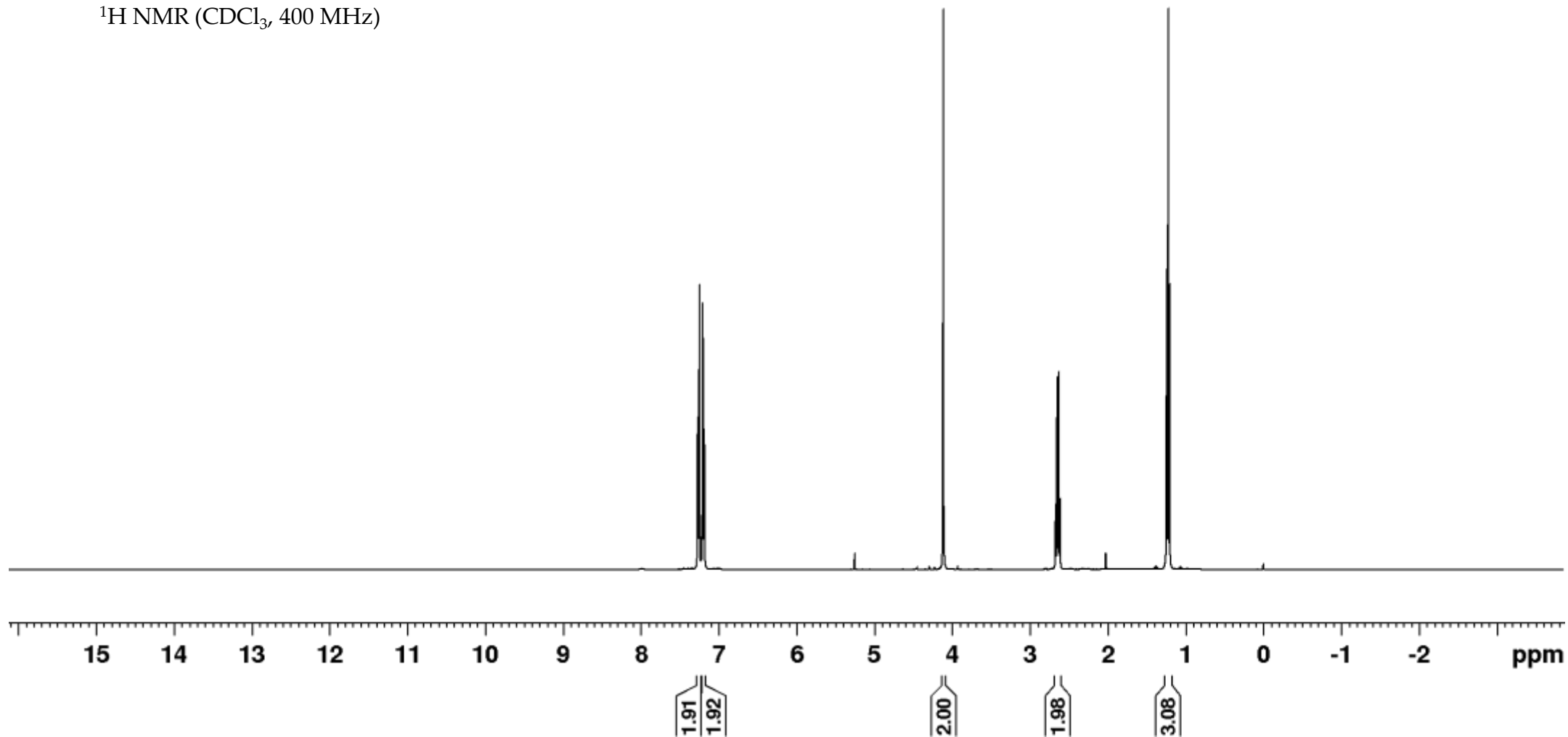
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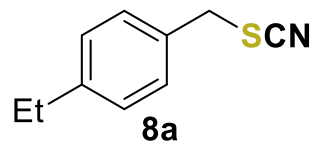
^{13}C NMR (CDCl_3 , 100 MHz)



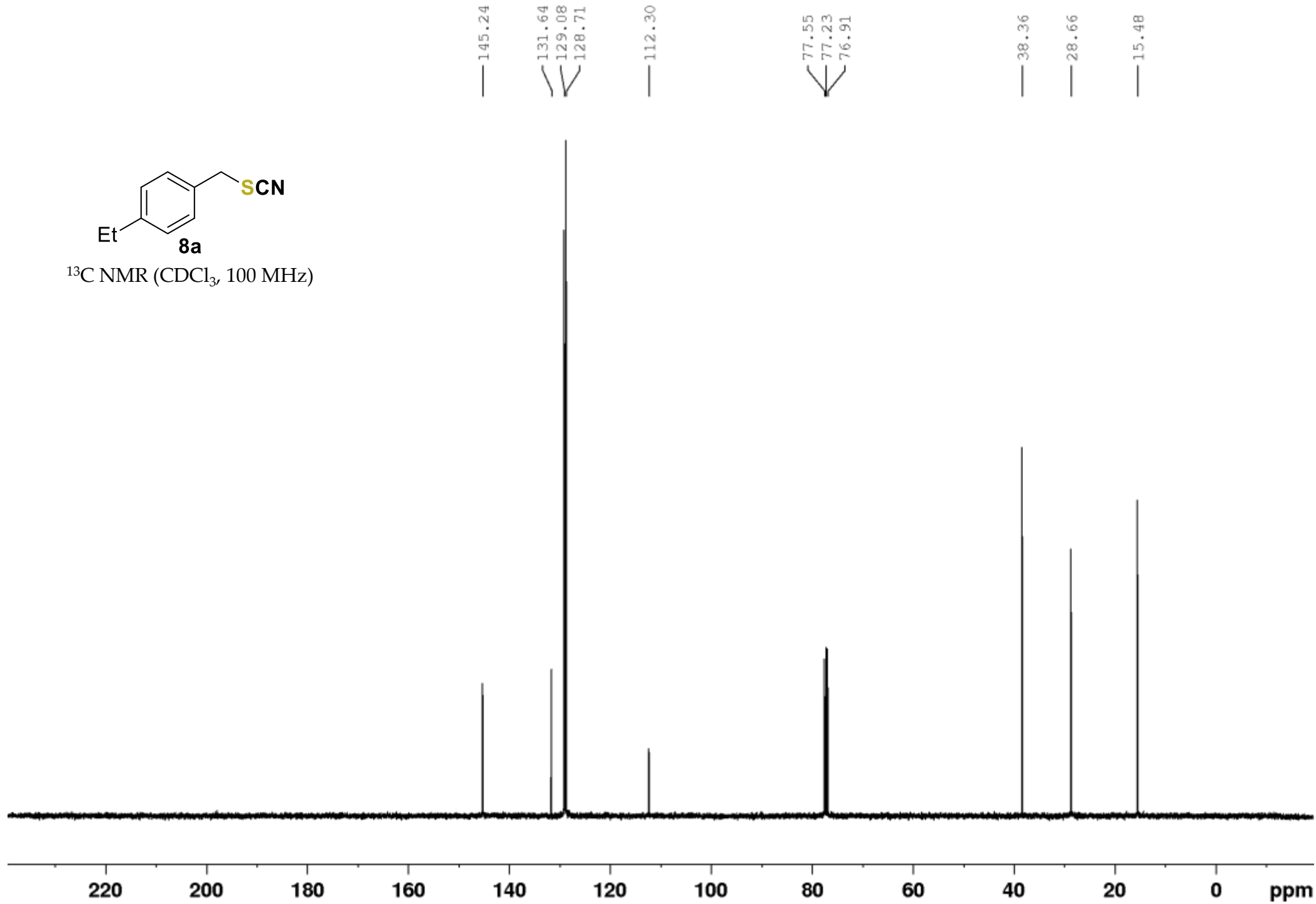


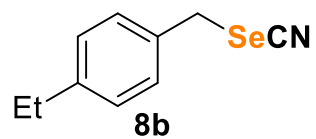
^1H NMR (CDCl_3 , 400 MHz)



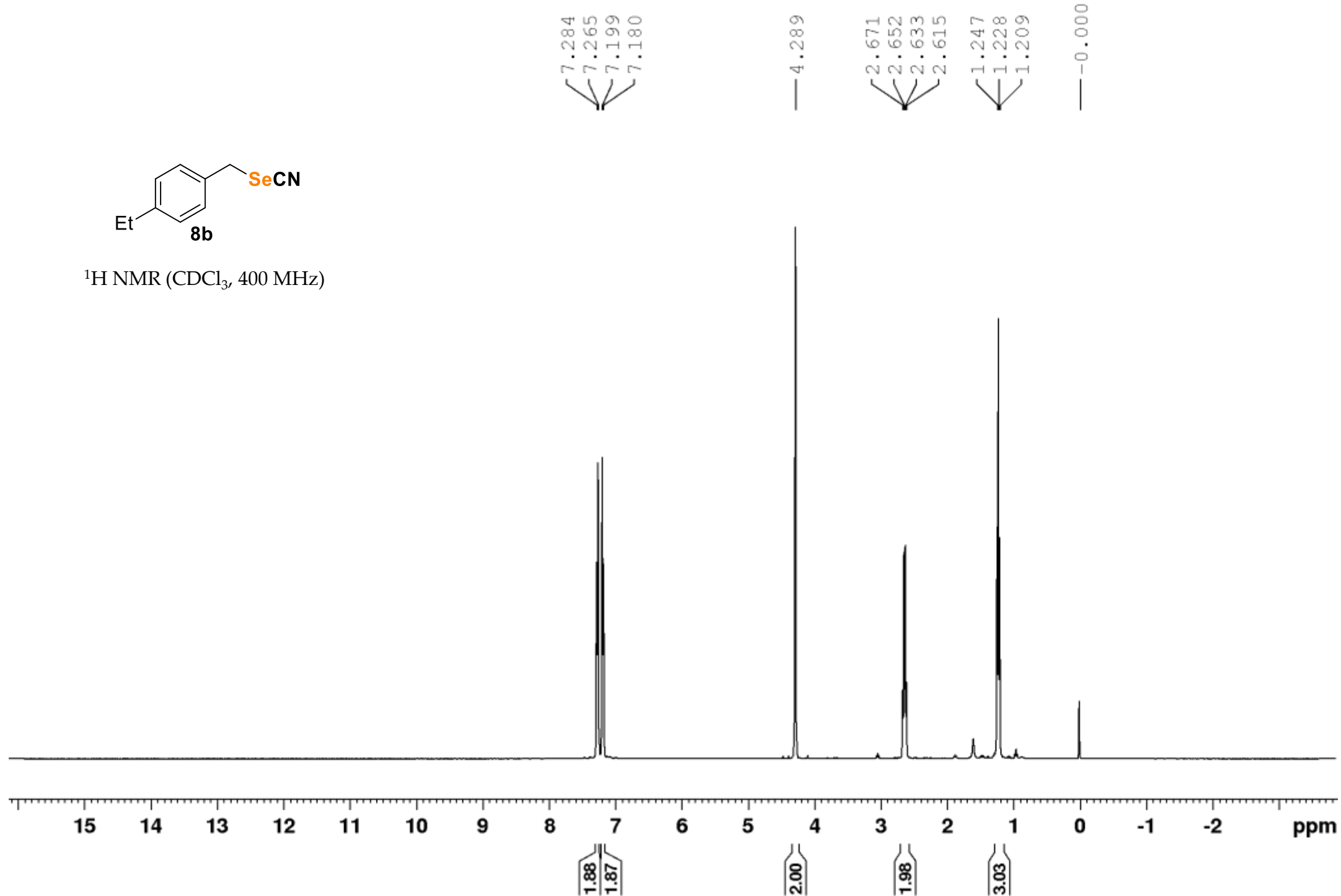


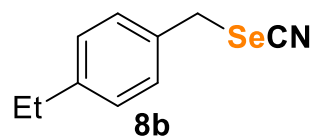
^{13}C NMR (CDCl_3 , 100 MHz)



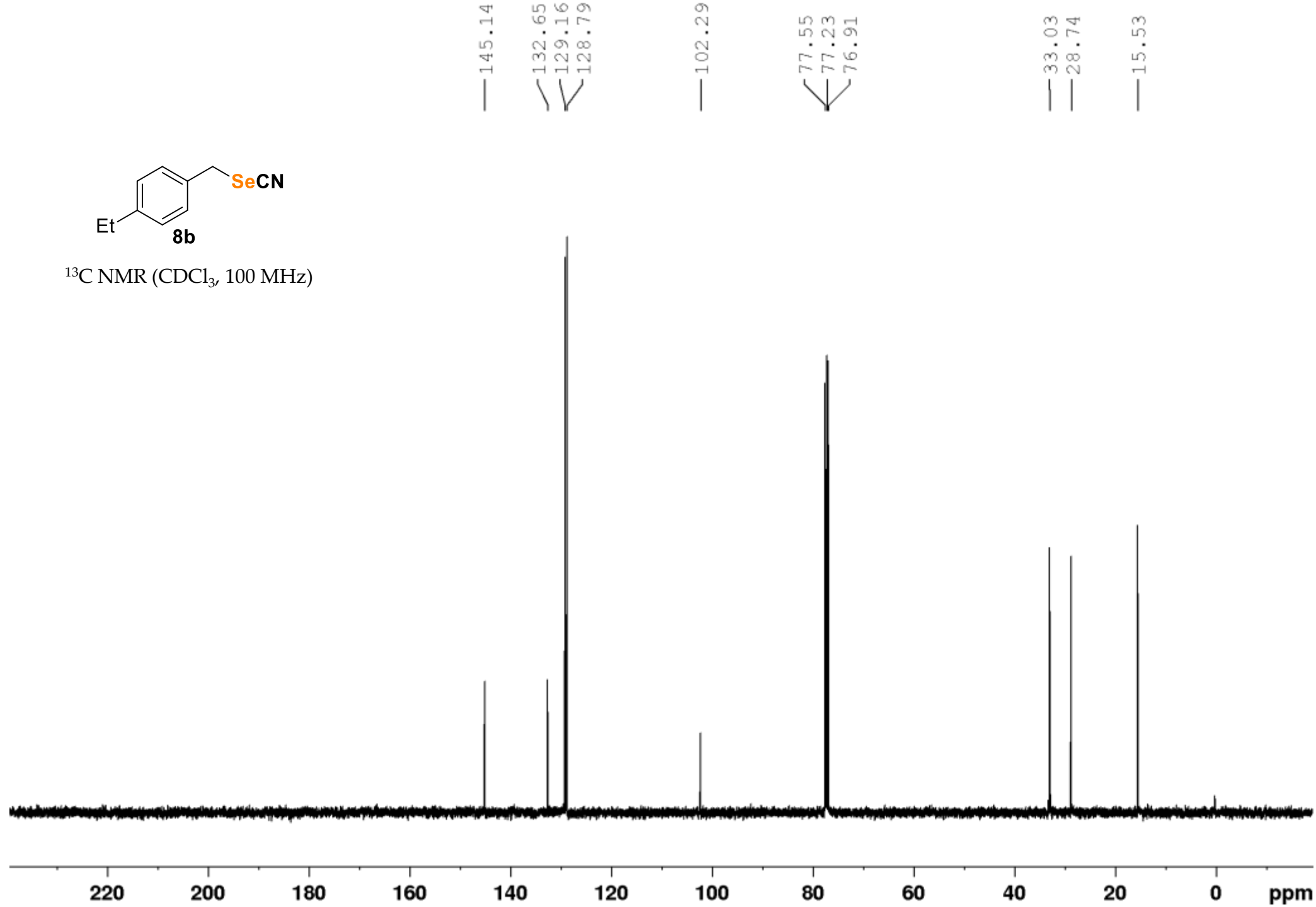


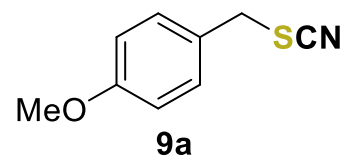
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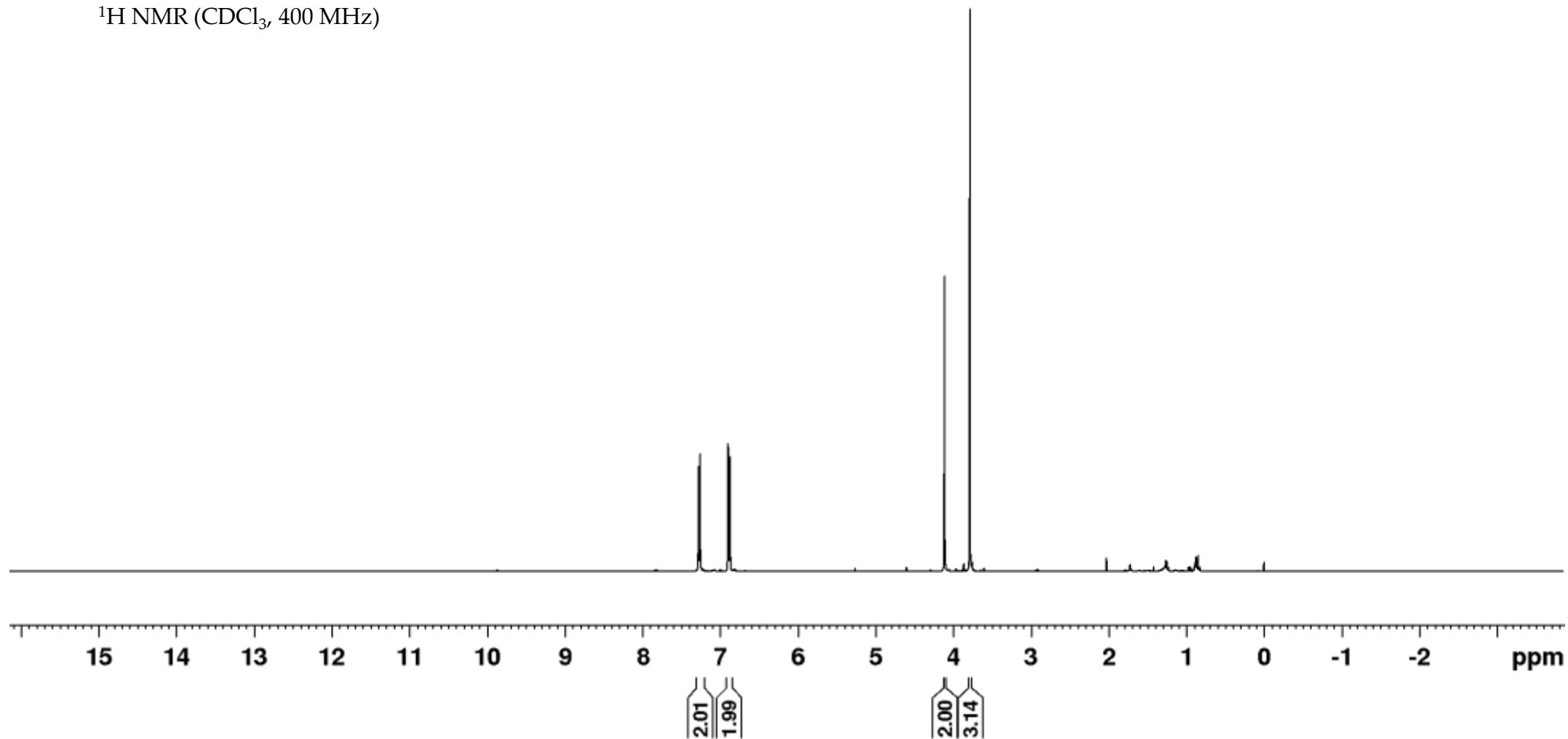


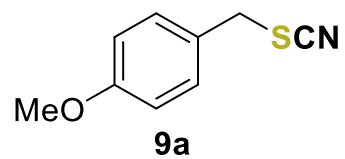
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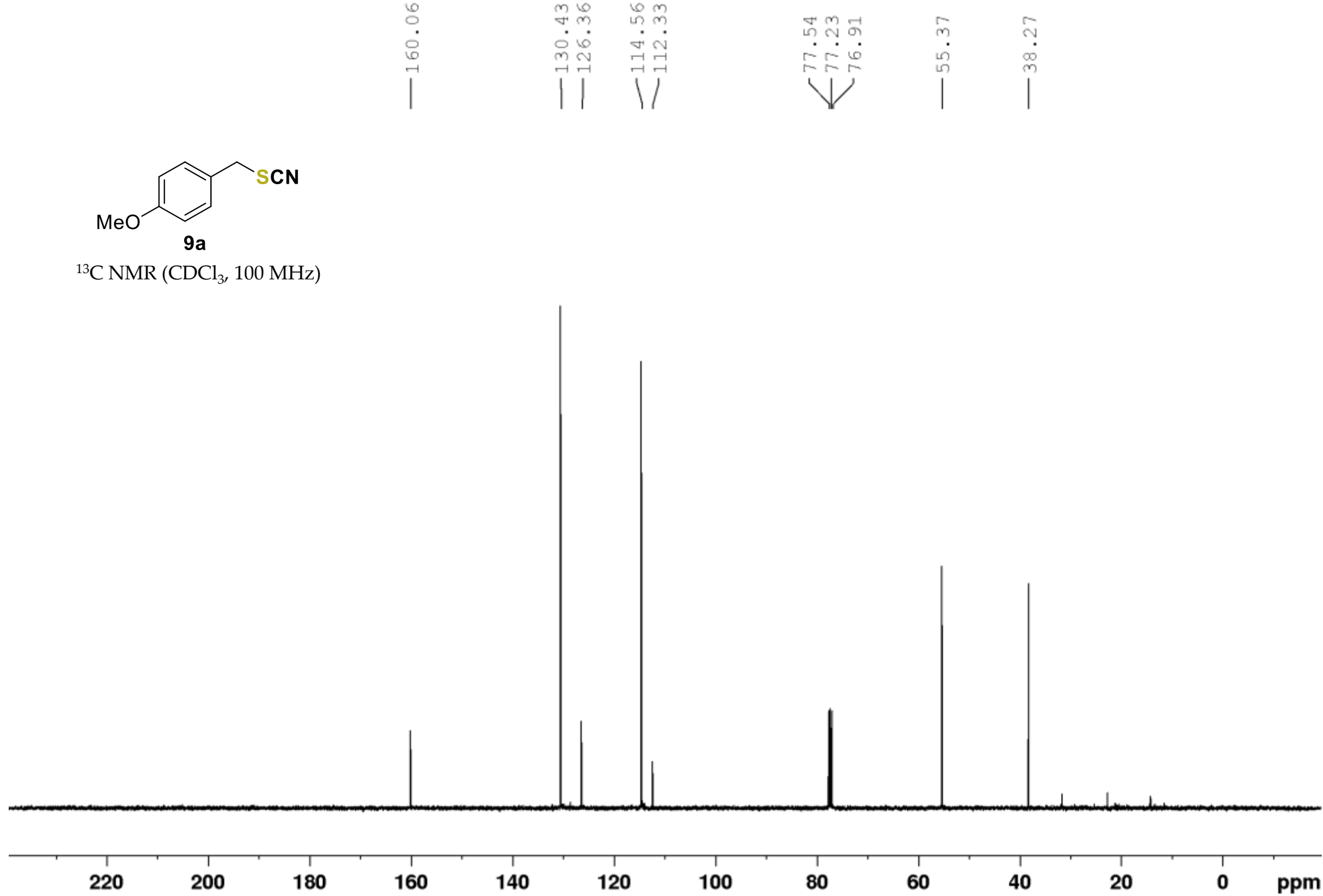


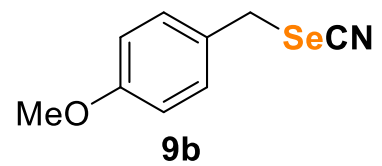
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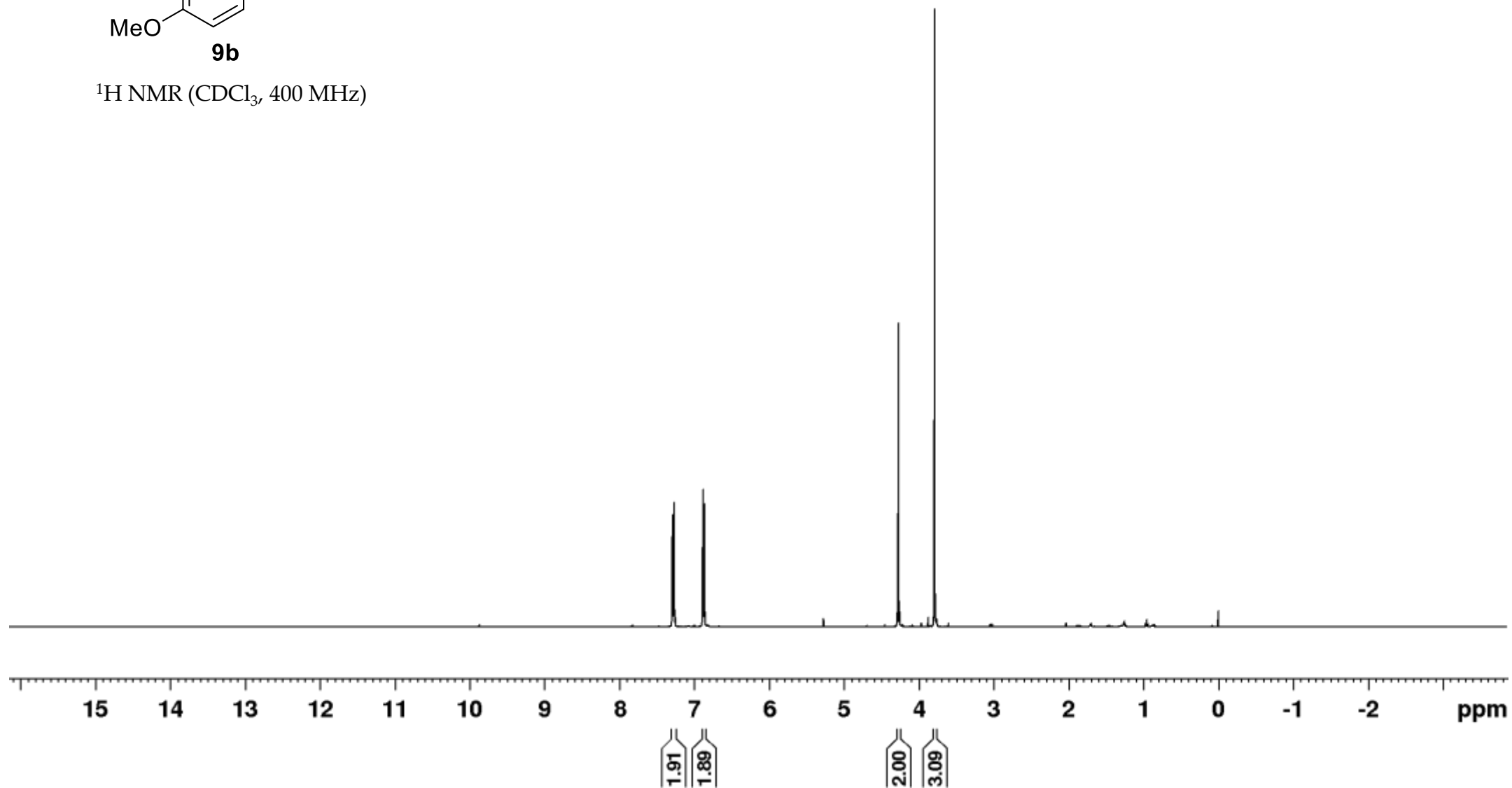


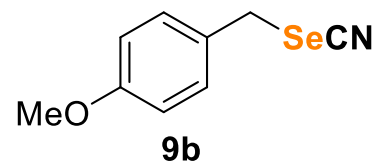
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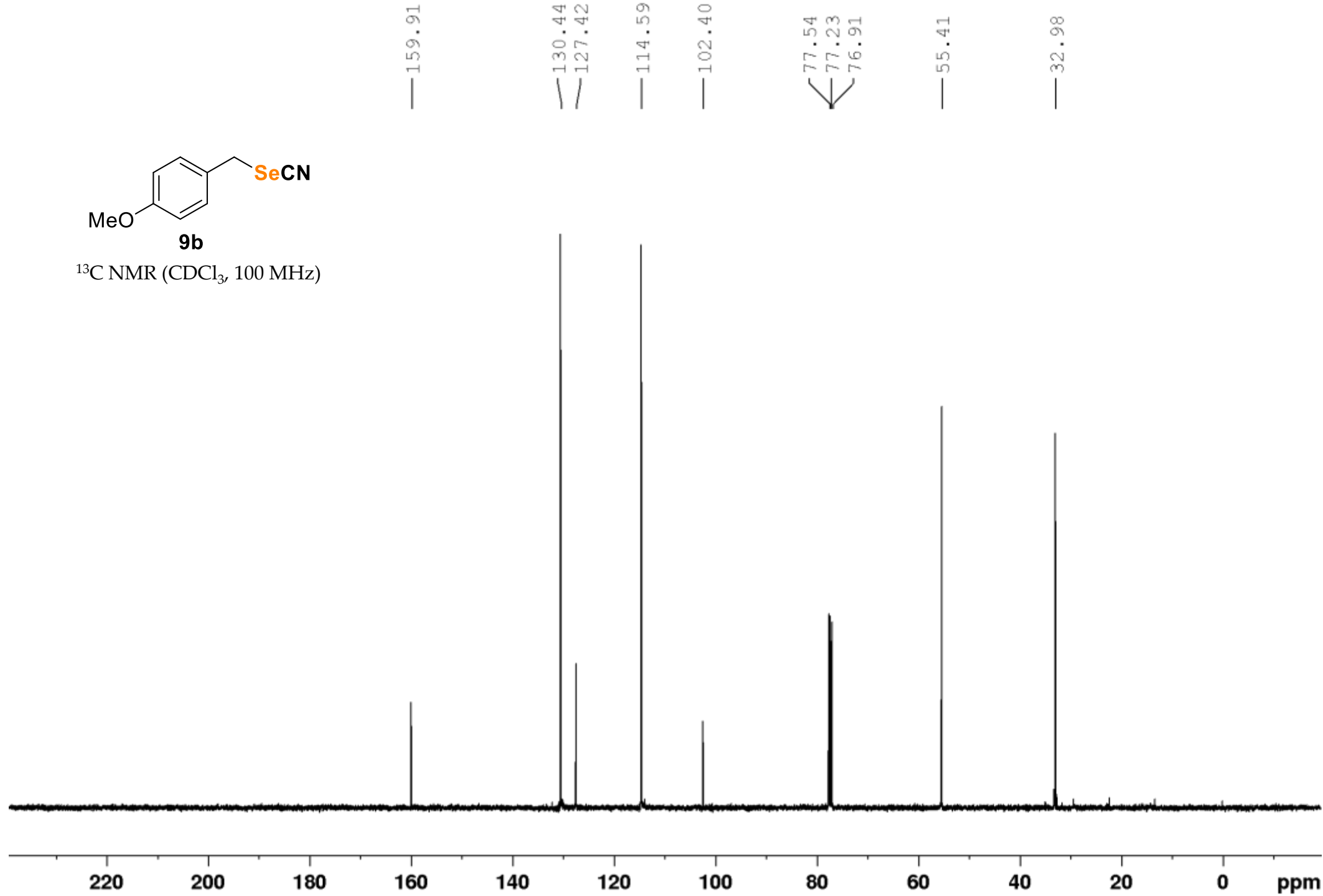


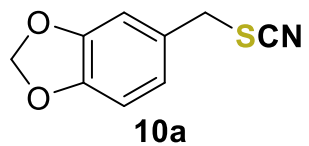
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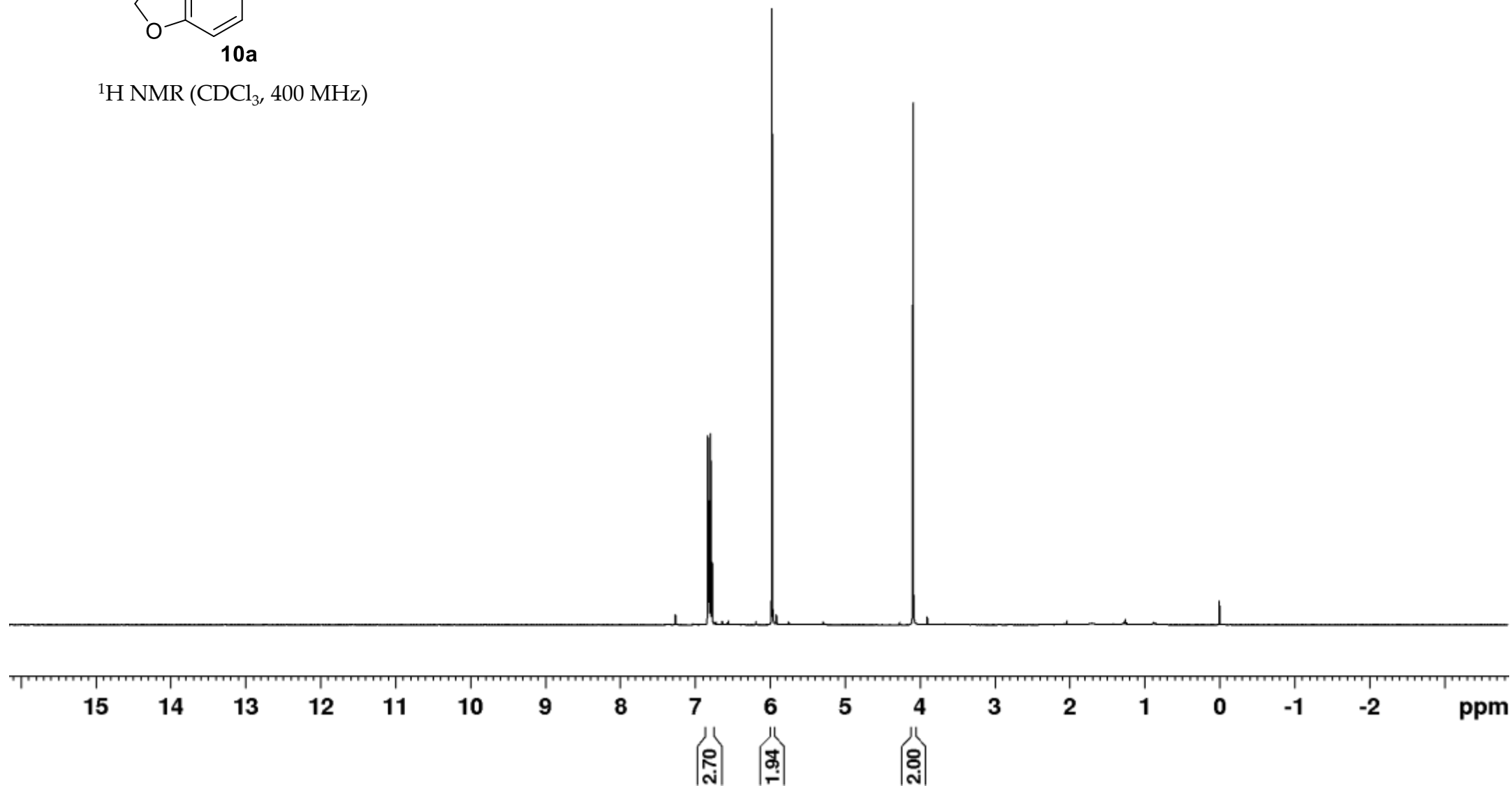


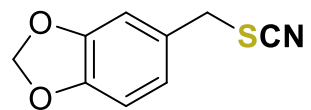
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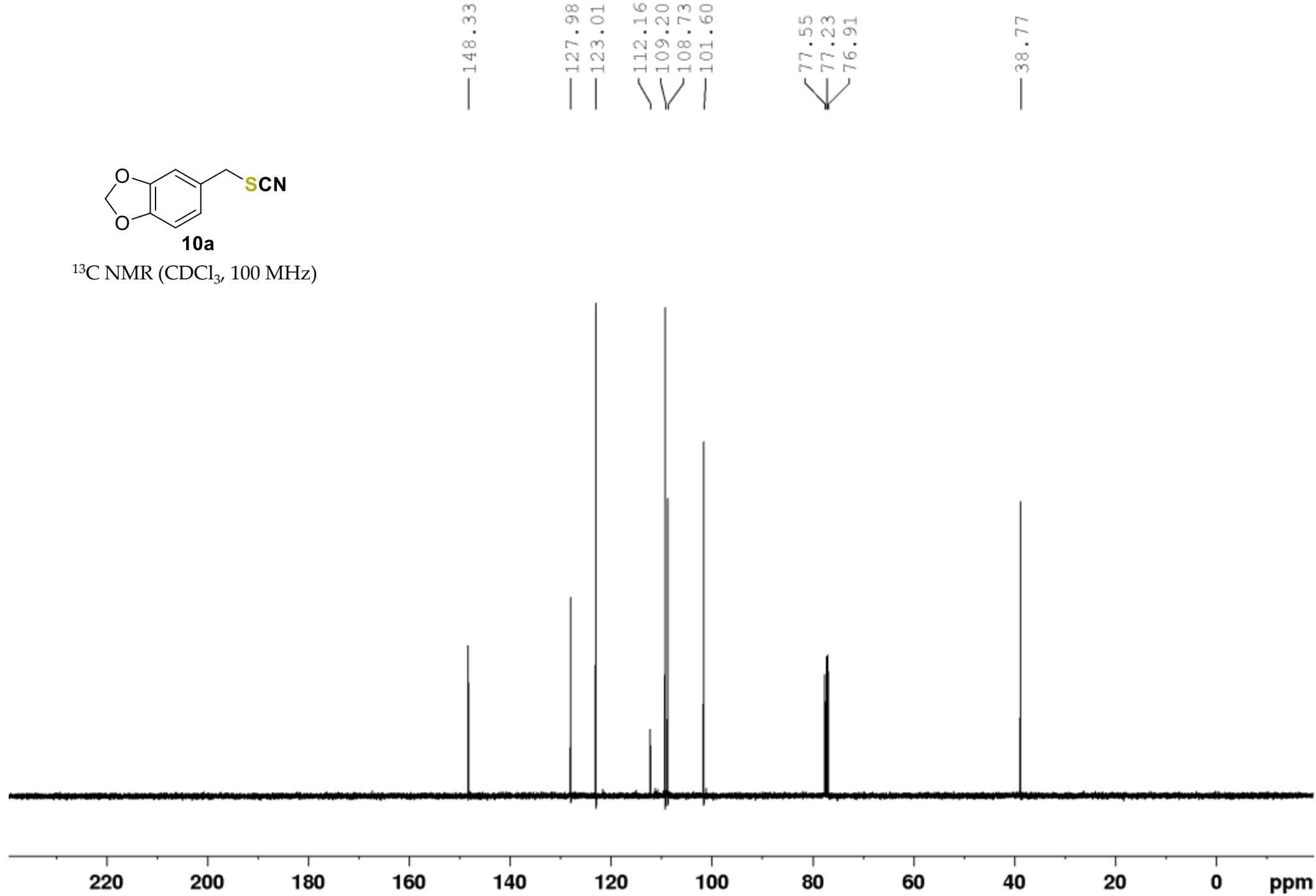
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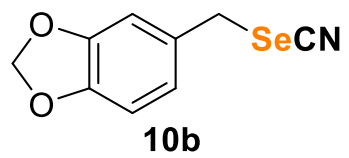




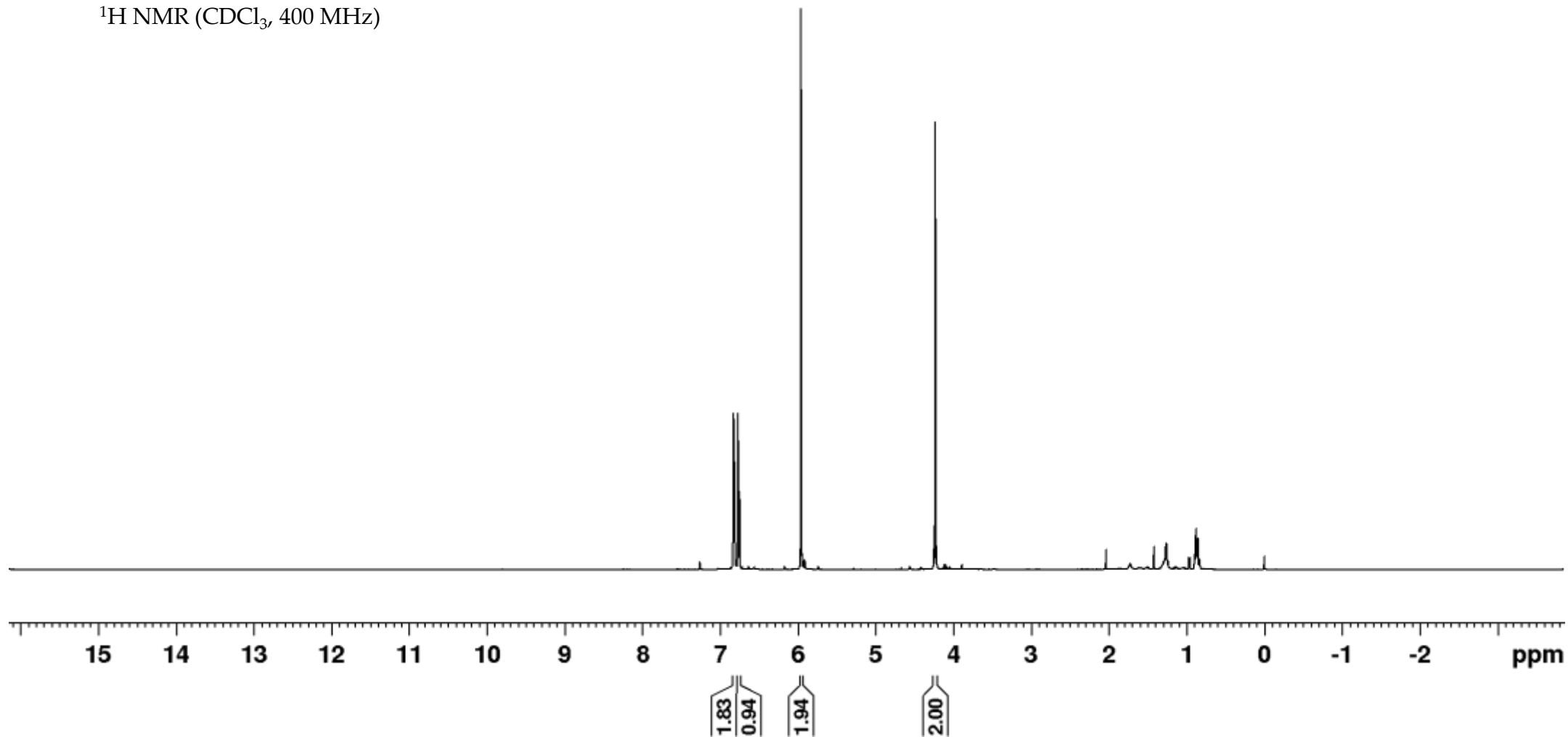
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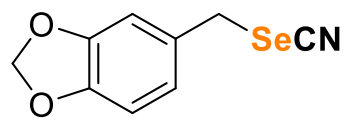
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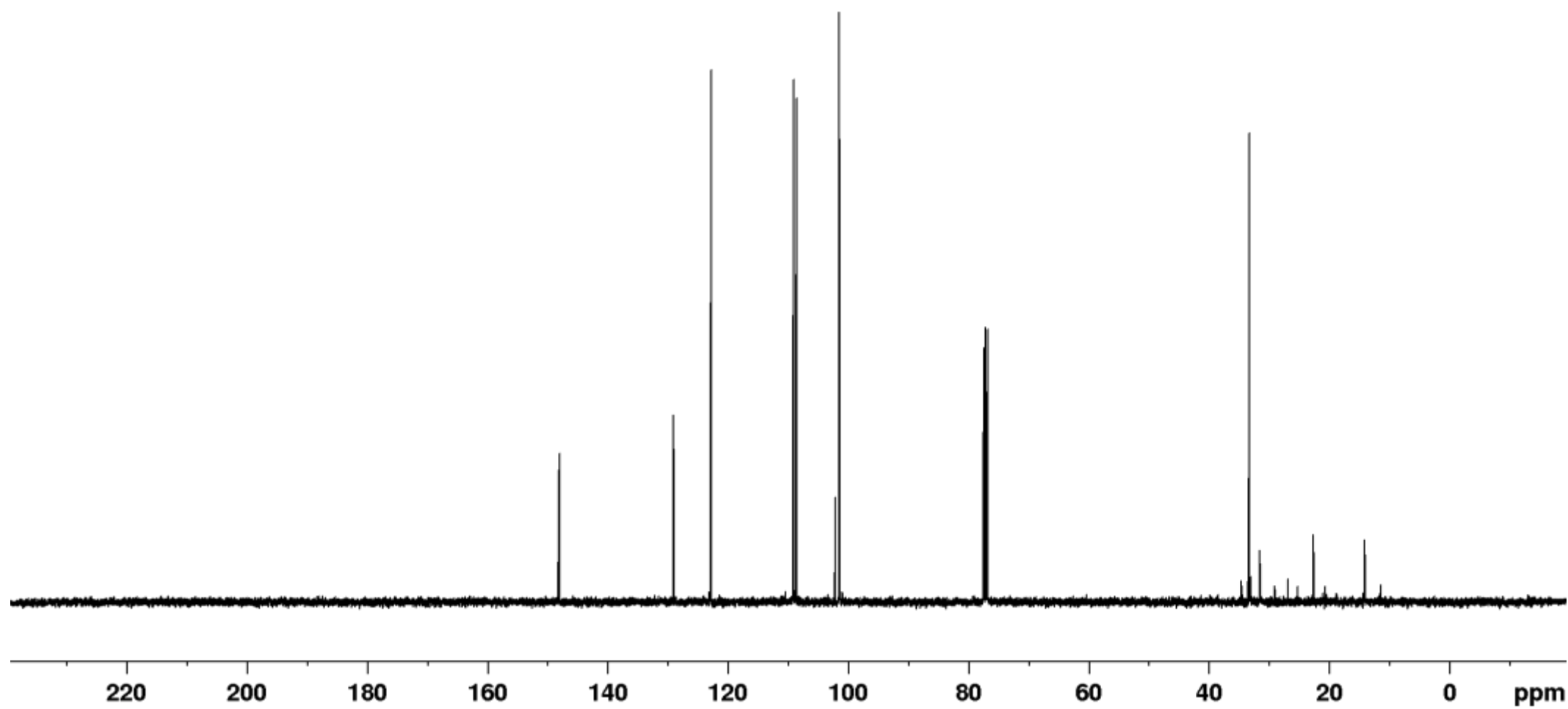
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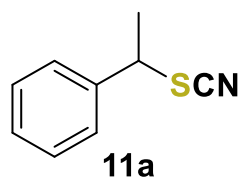




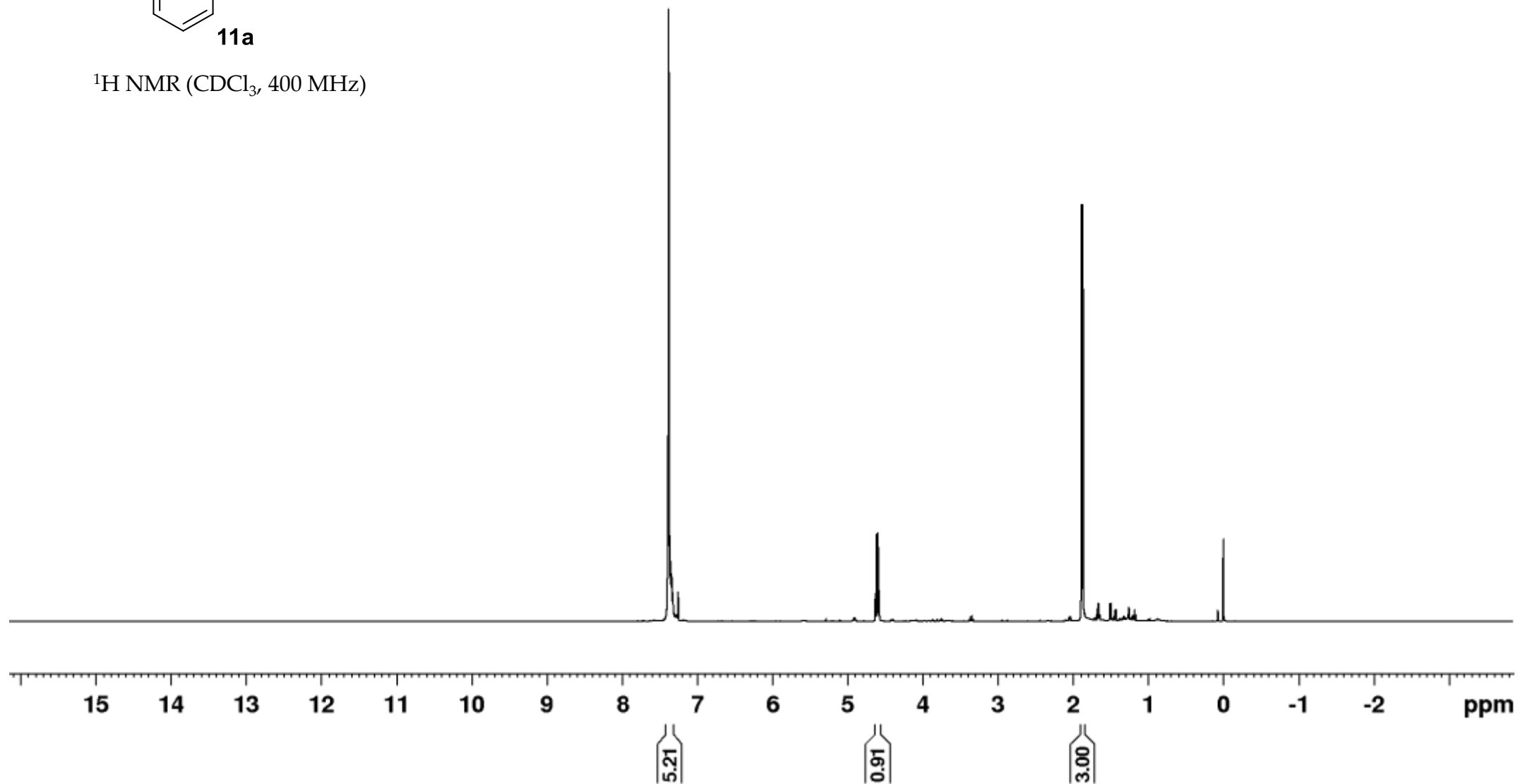
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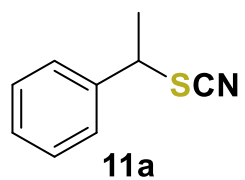
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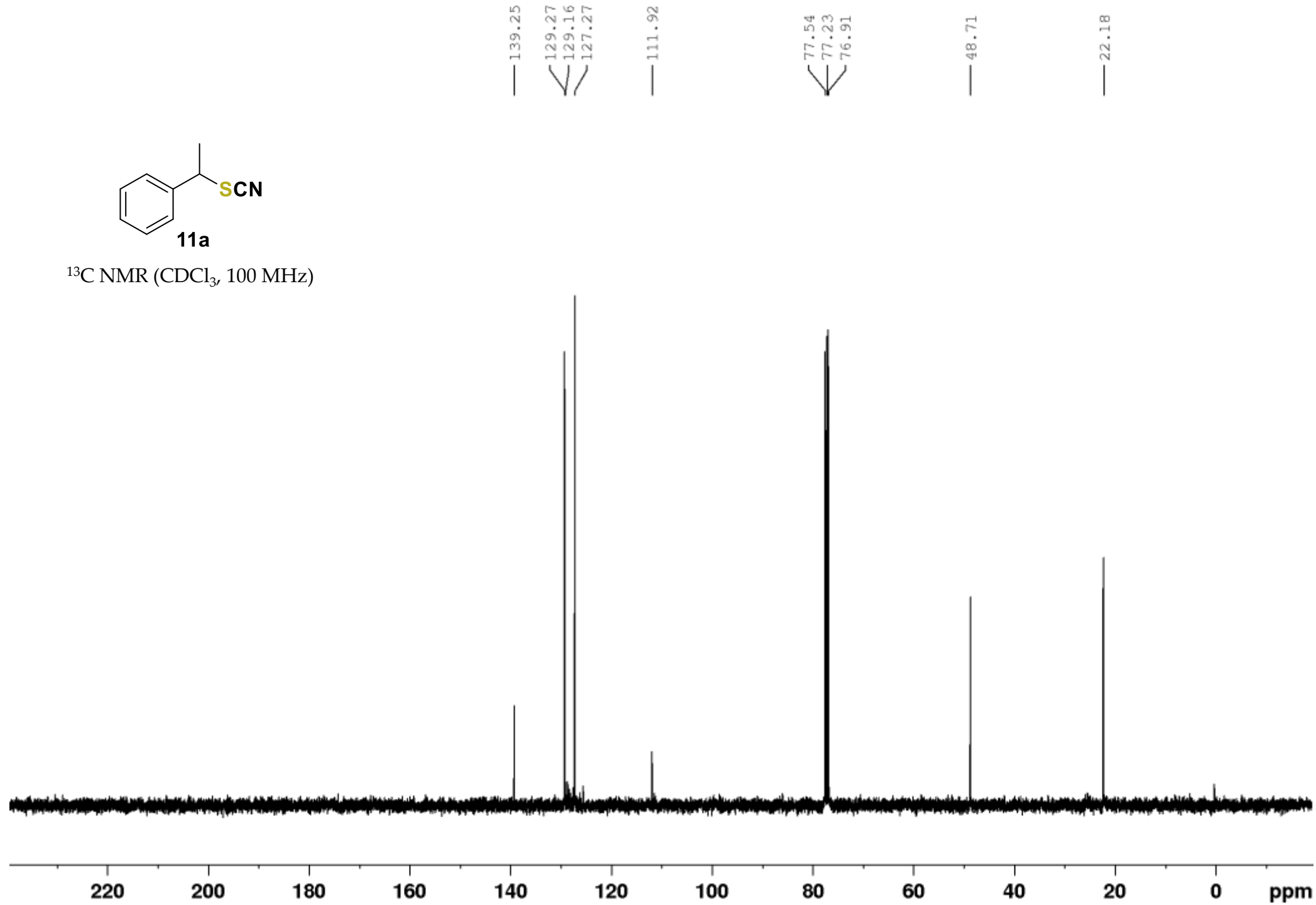


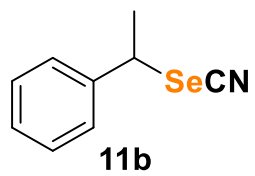
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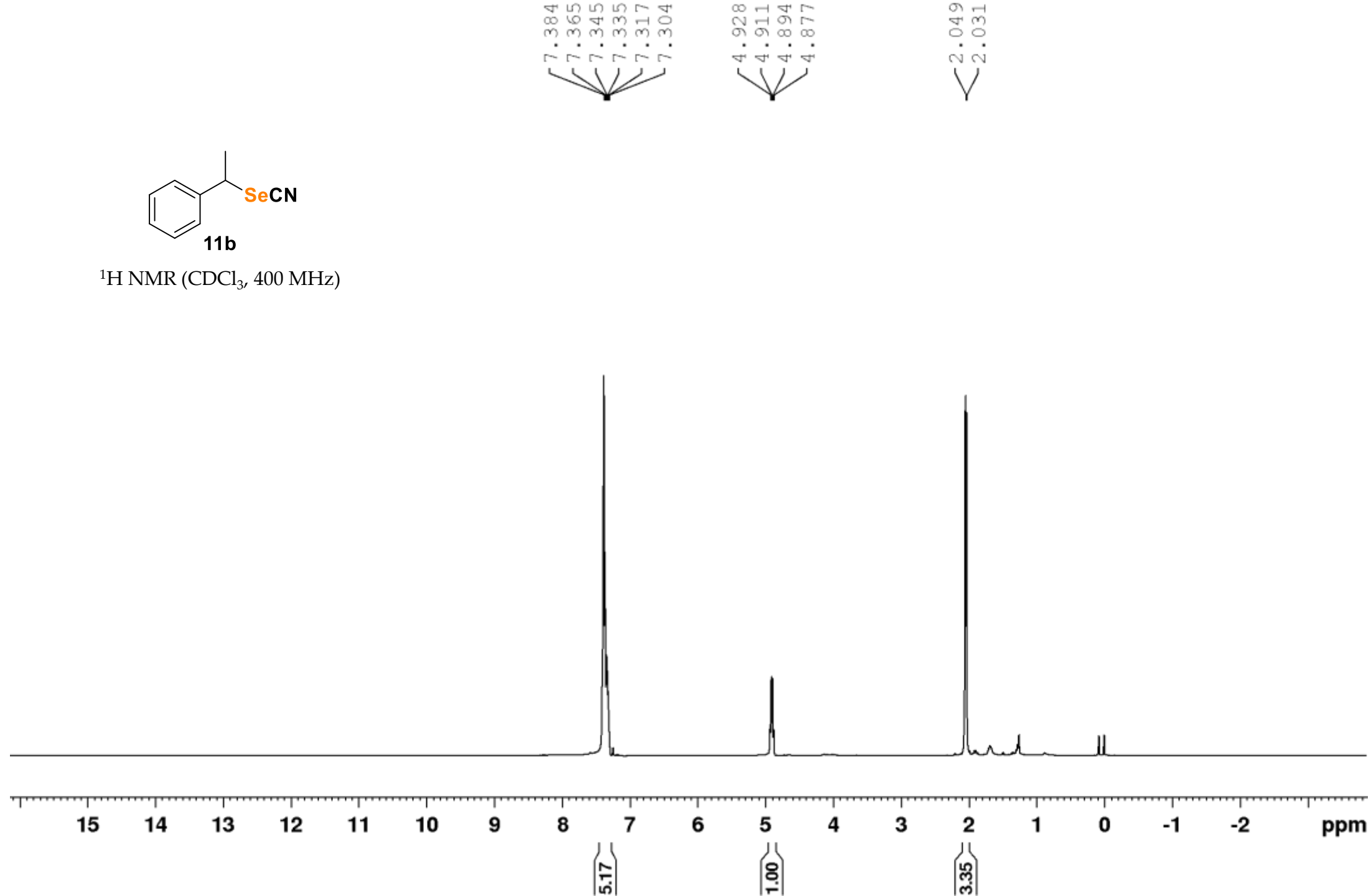


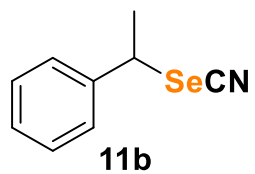
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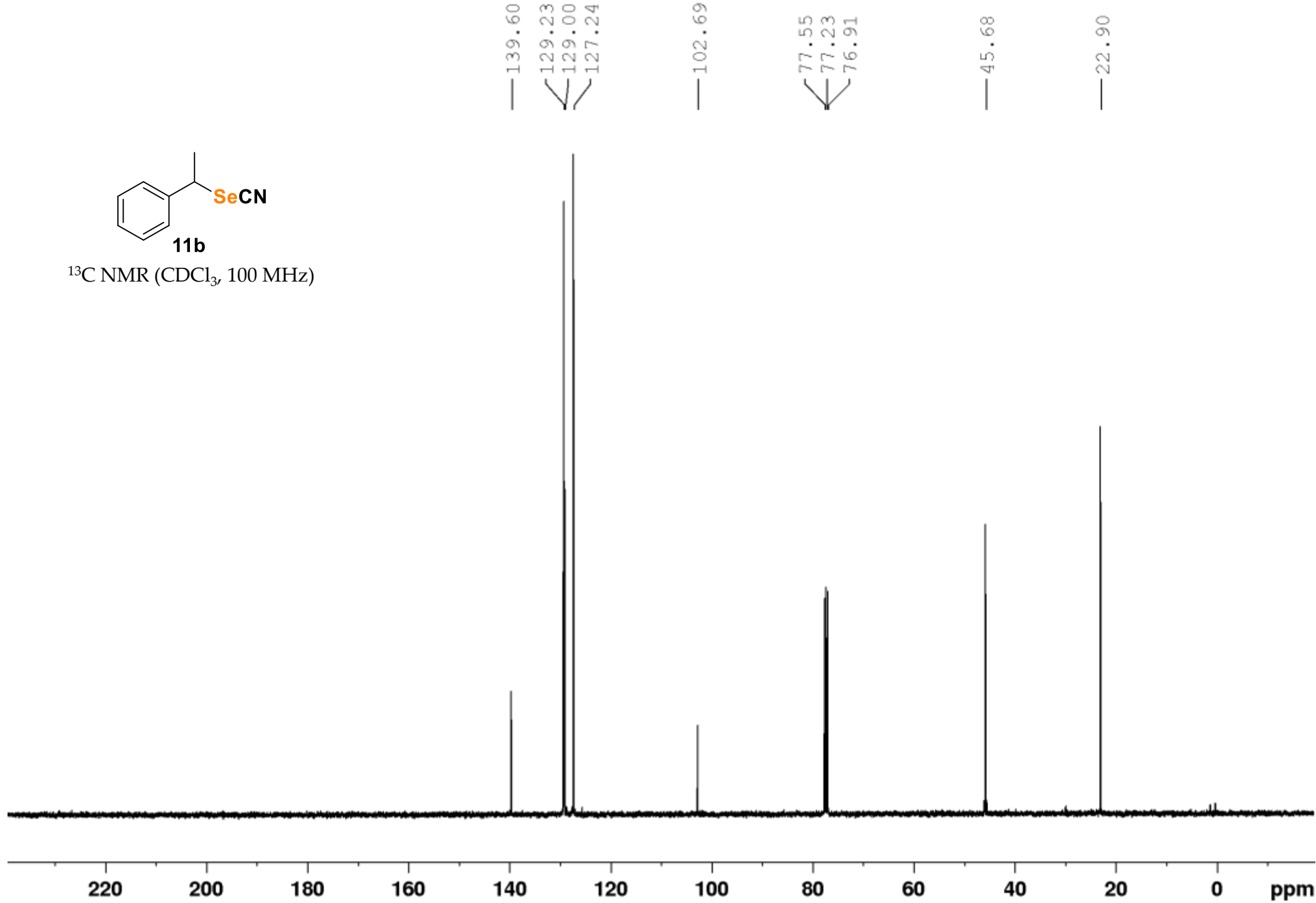


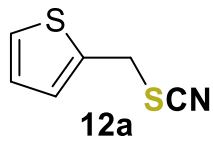
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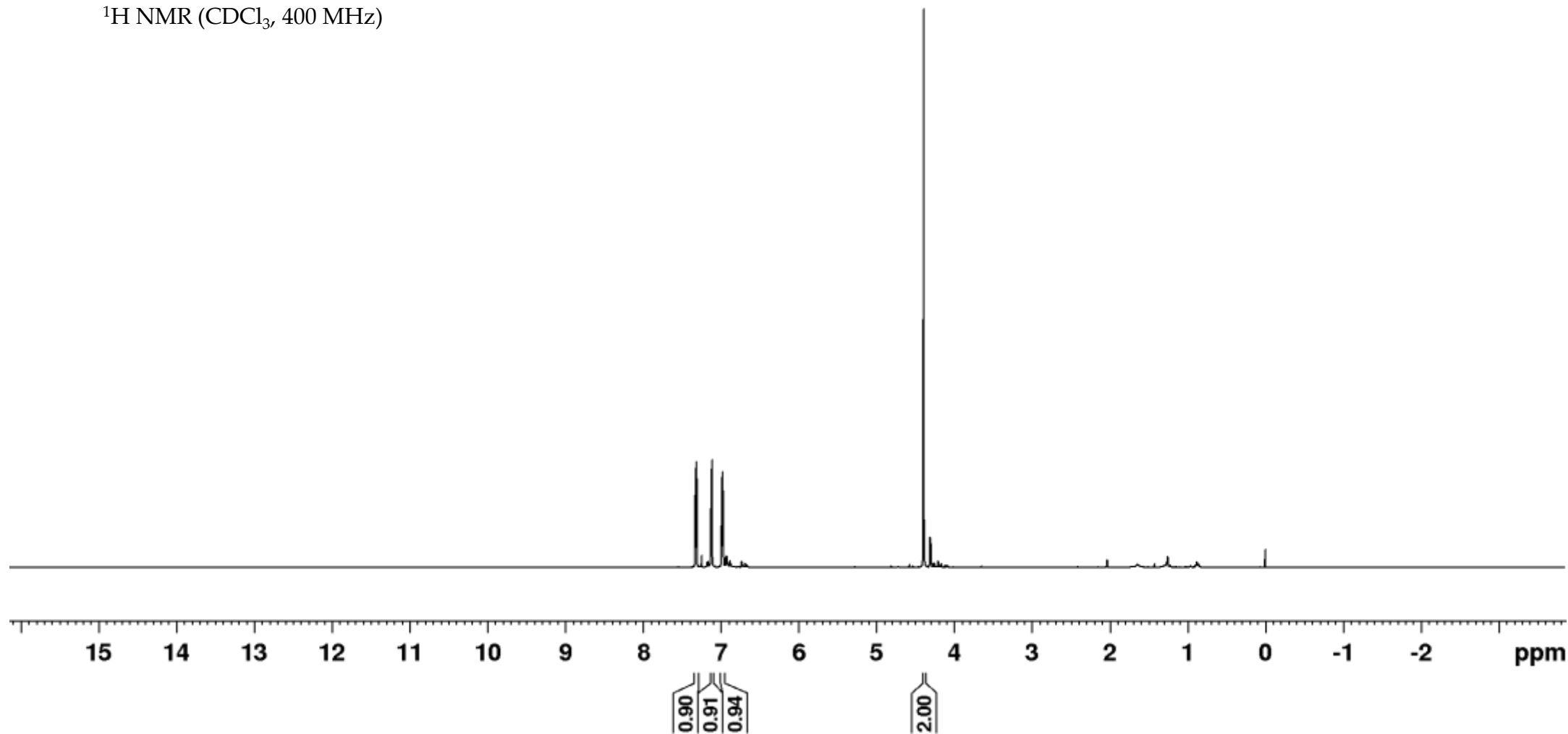


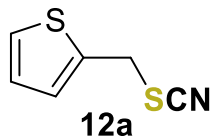
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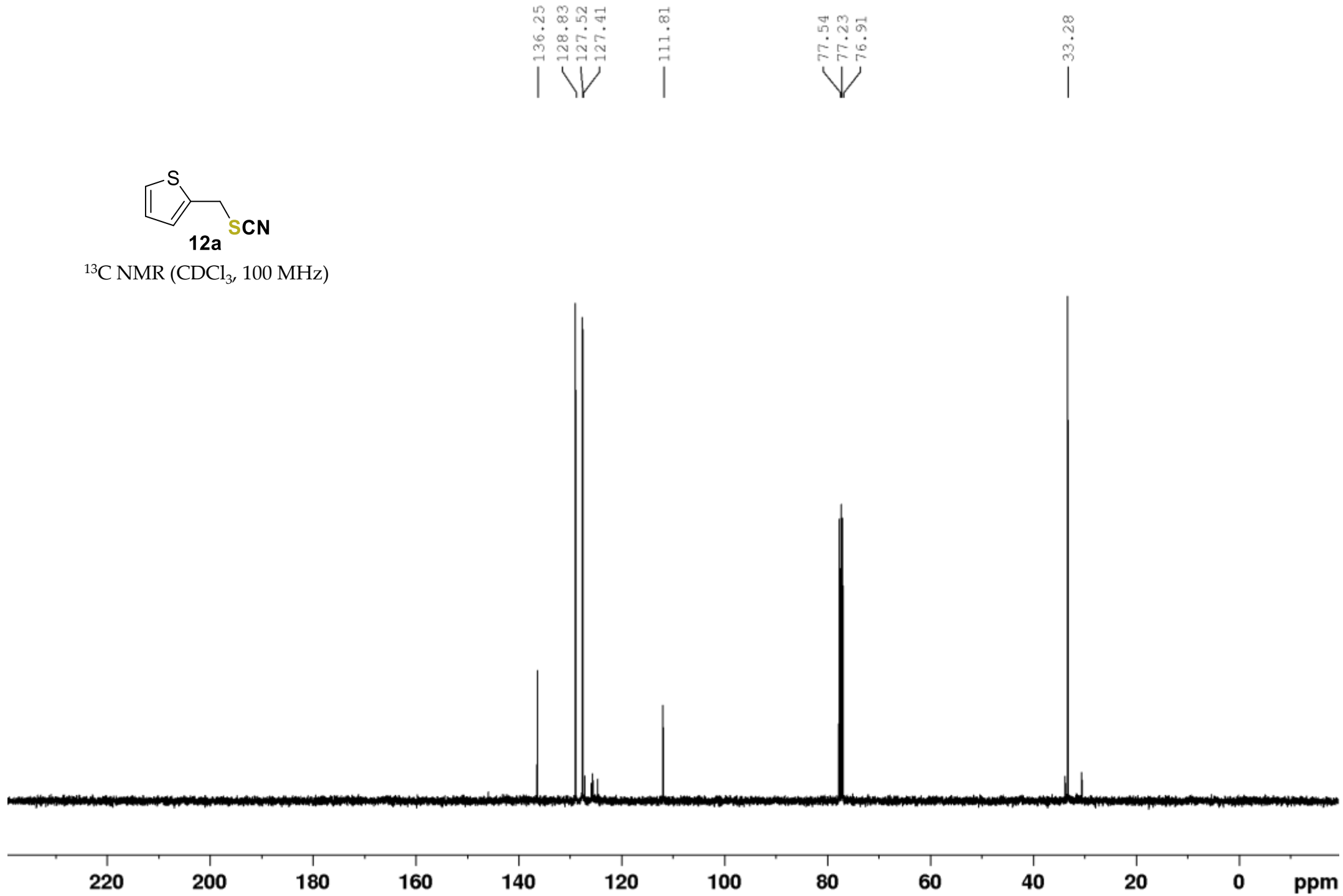


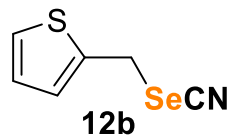
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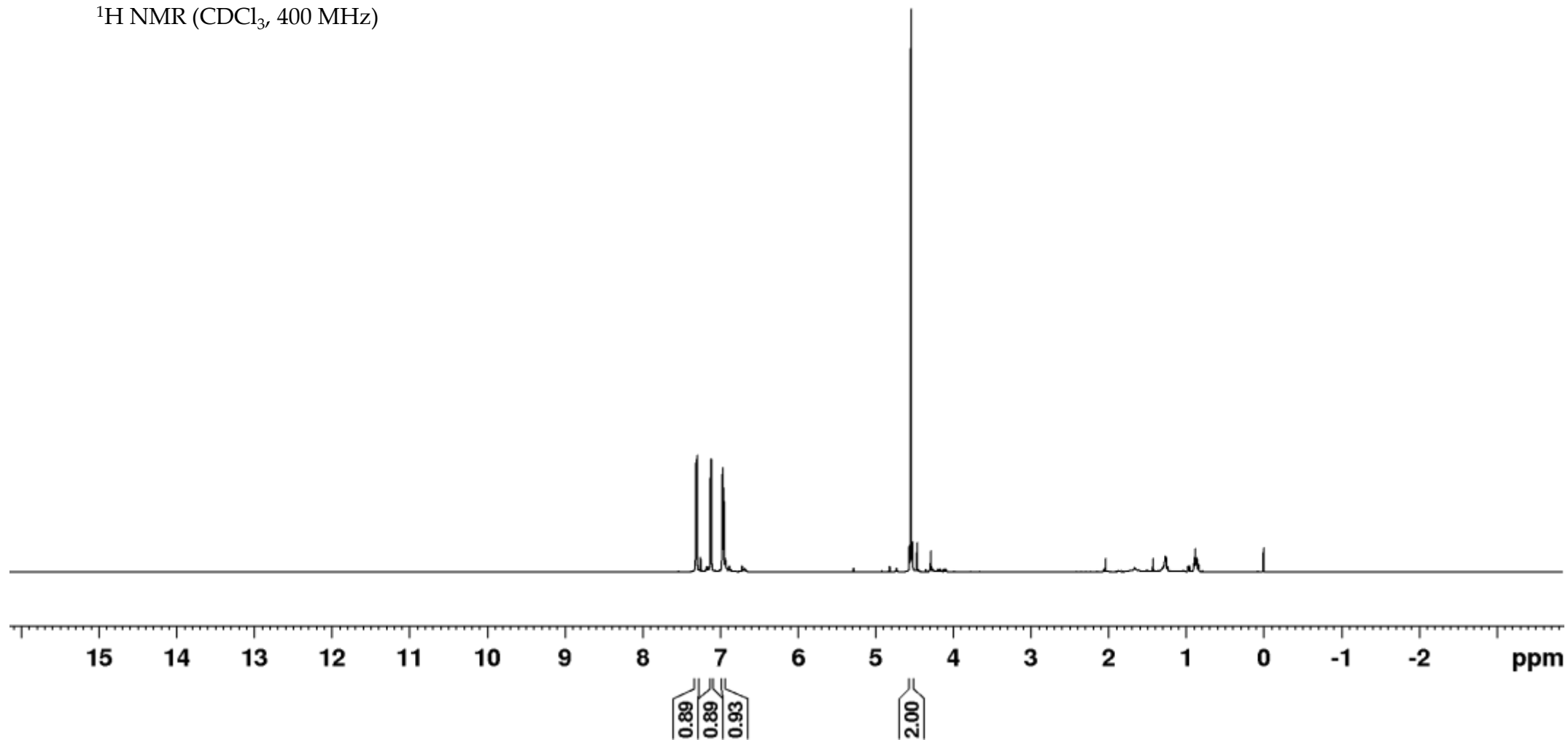


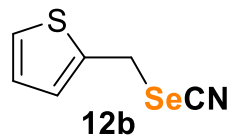
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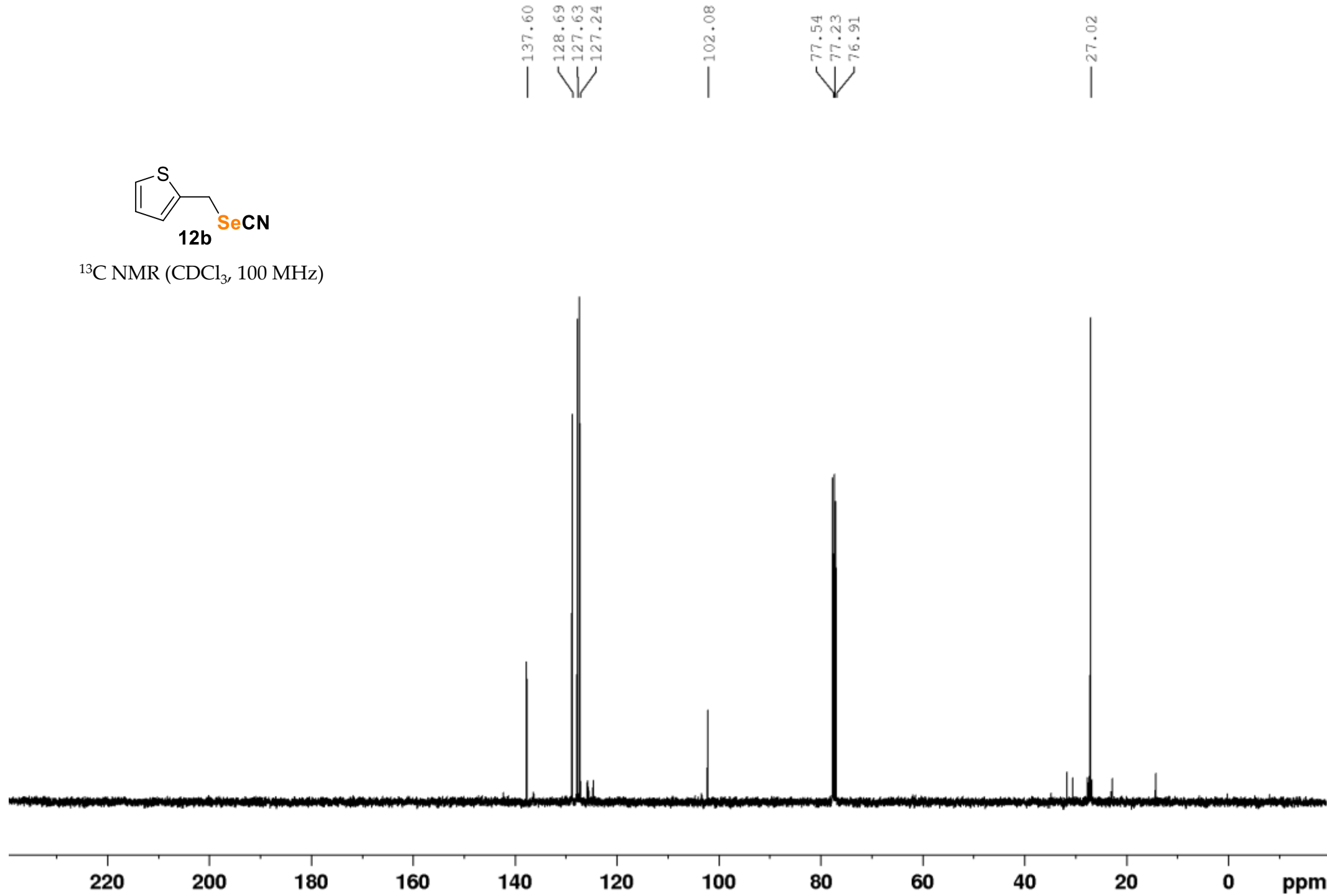


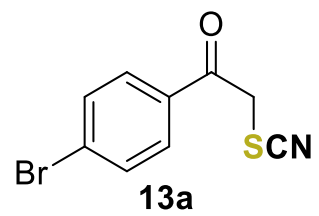
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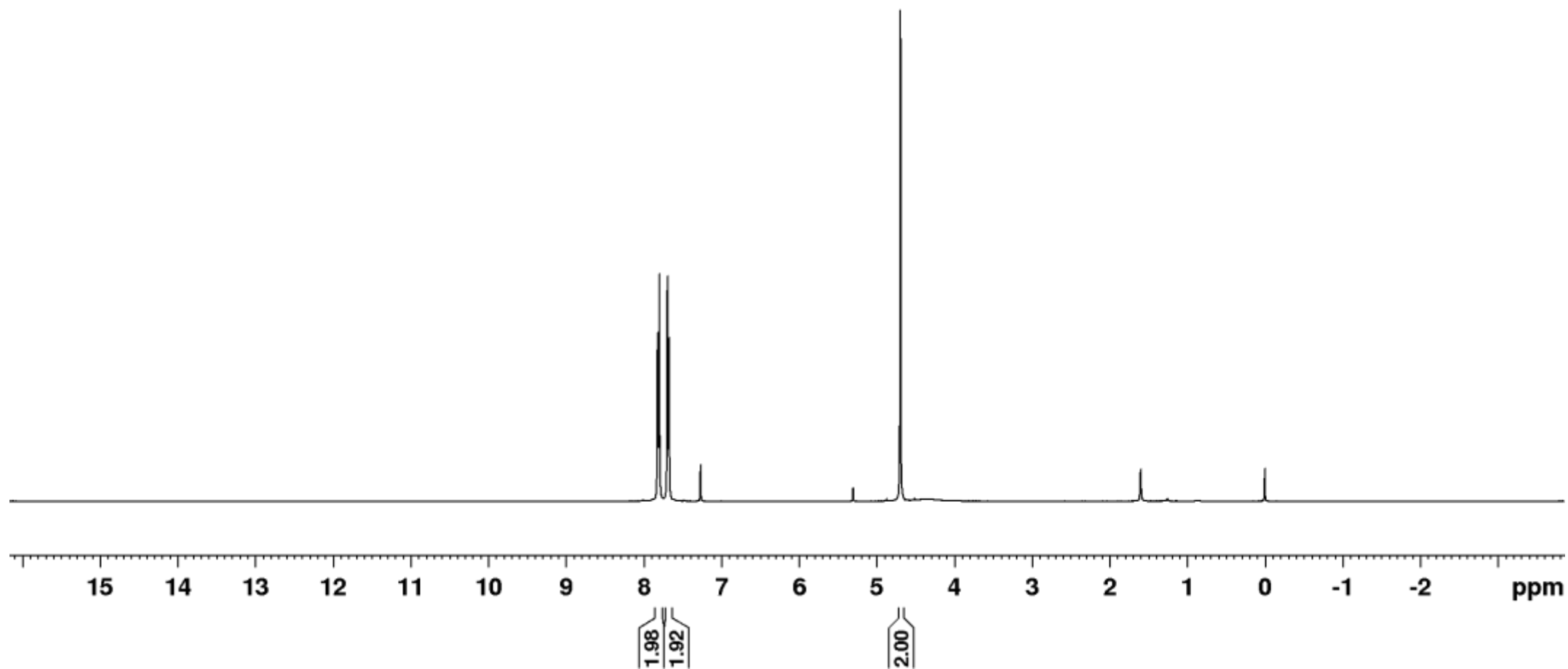


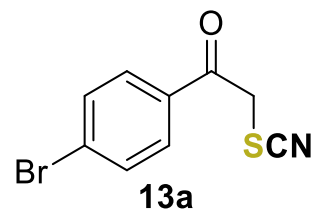
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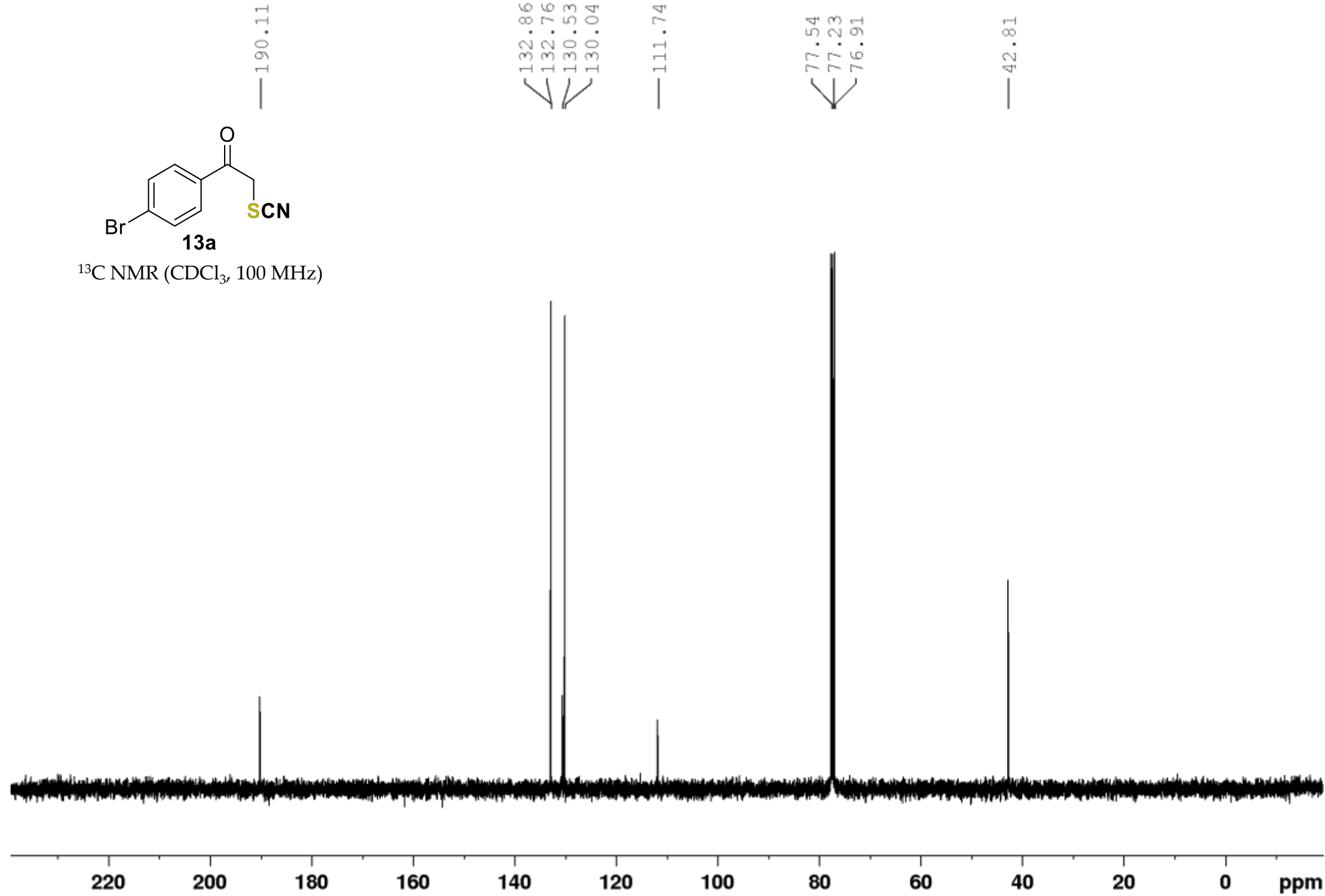


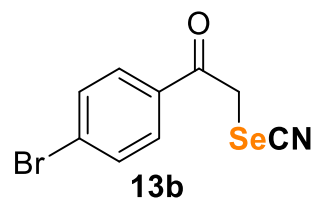
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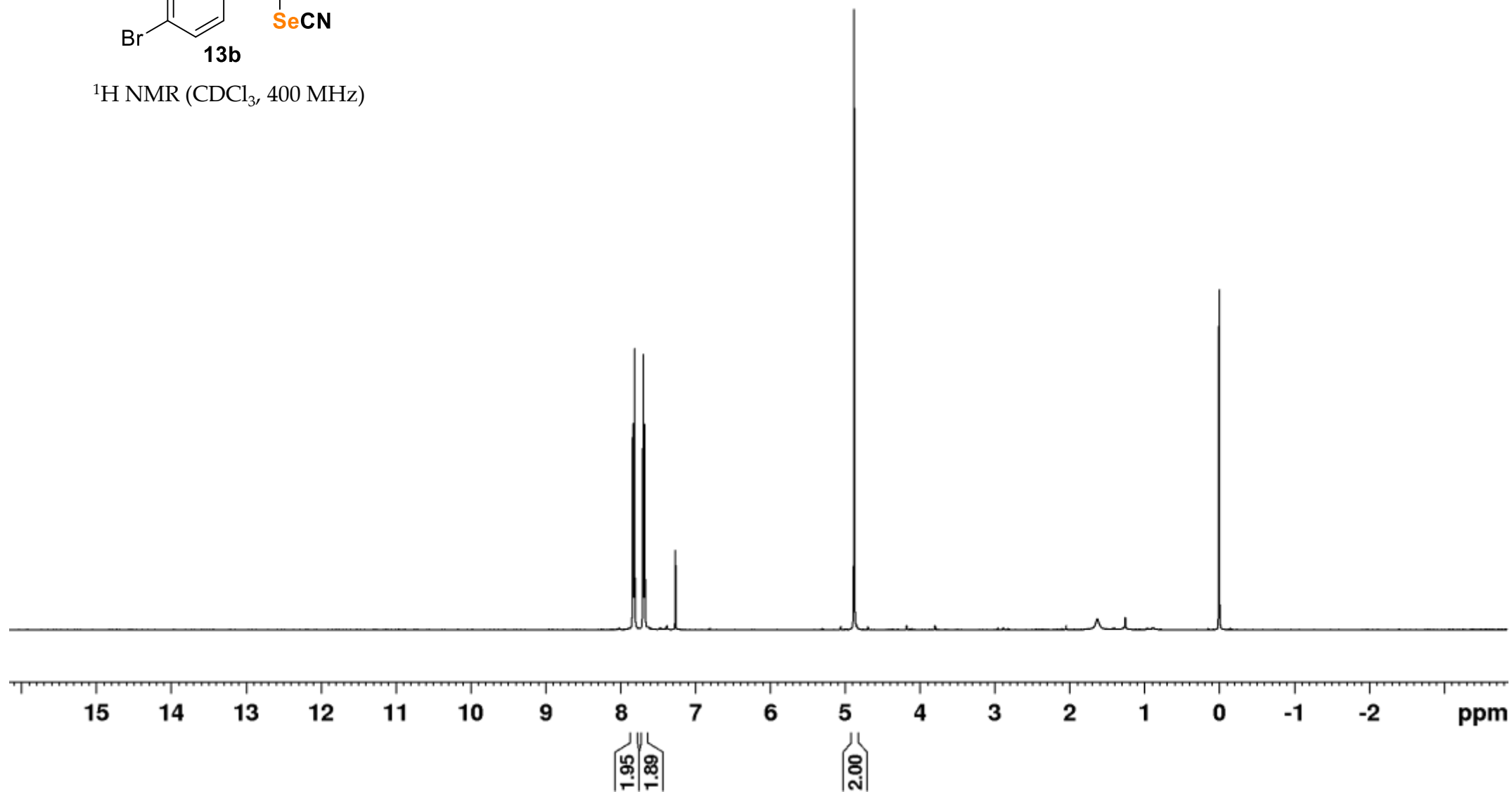


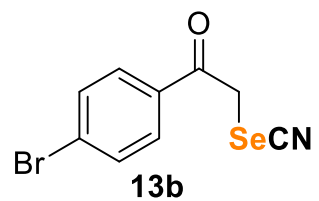
^{13}C NMR (CDCl_3 , 100 MHz)





^1H NMR (CDCl_3 , 400 MHz)





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

