

One-pot synthesis of benzoxazoles via the metal-free *ortho*-C-H functionalization of phenols with nitroalkanes

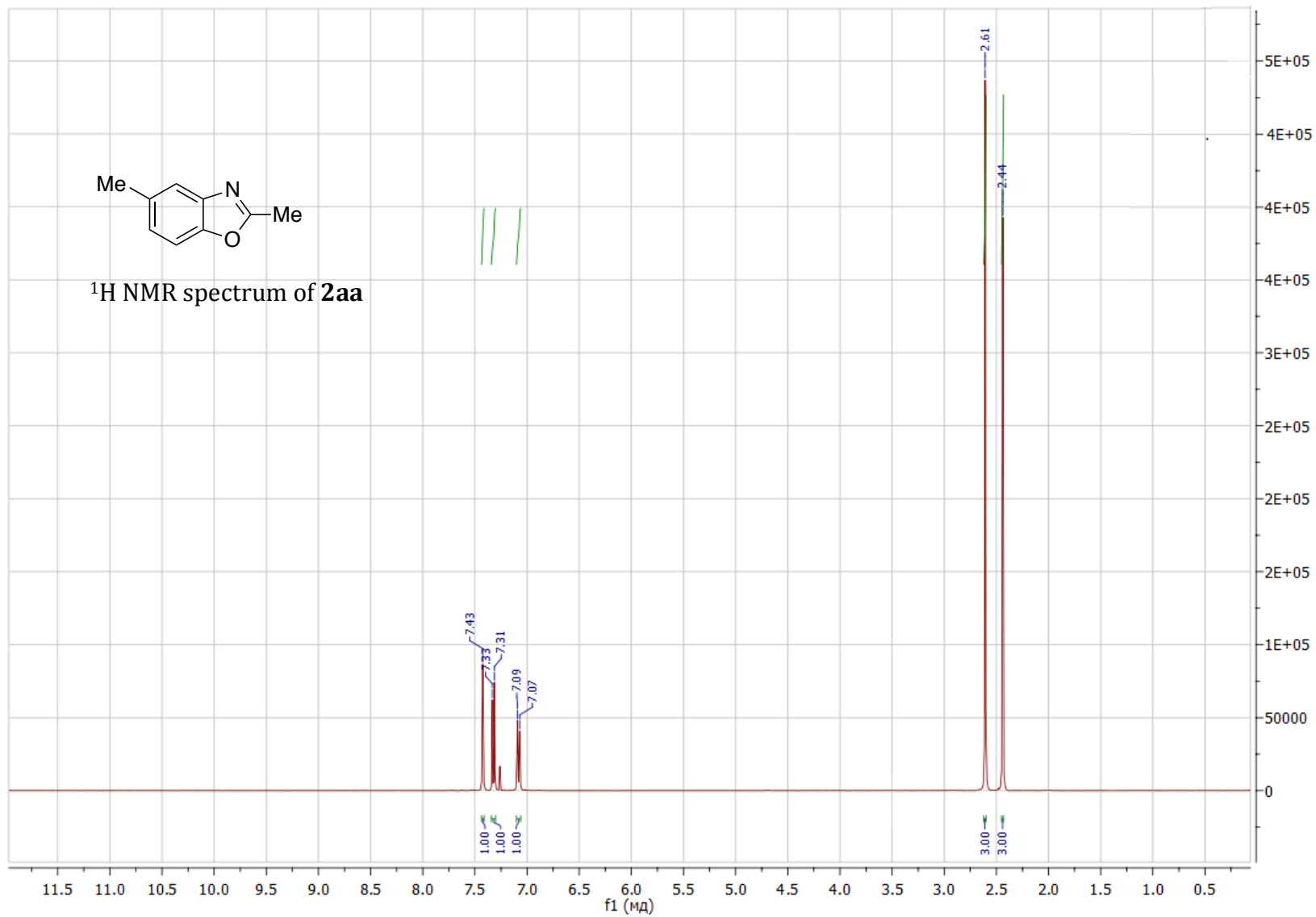
Nicolai A. Aksenov, Alexander V. Aksenov,* Oleg N. Nadein, Dmitrii A. Aksenov, Alexander N. Smirnov, and Michael Rubin*

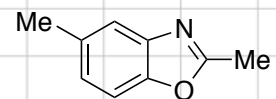
Supporting Information

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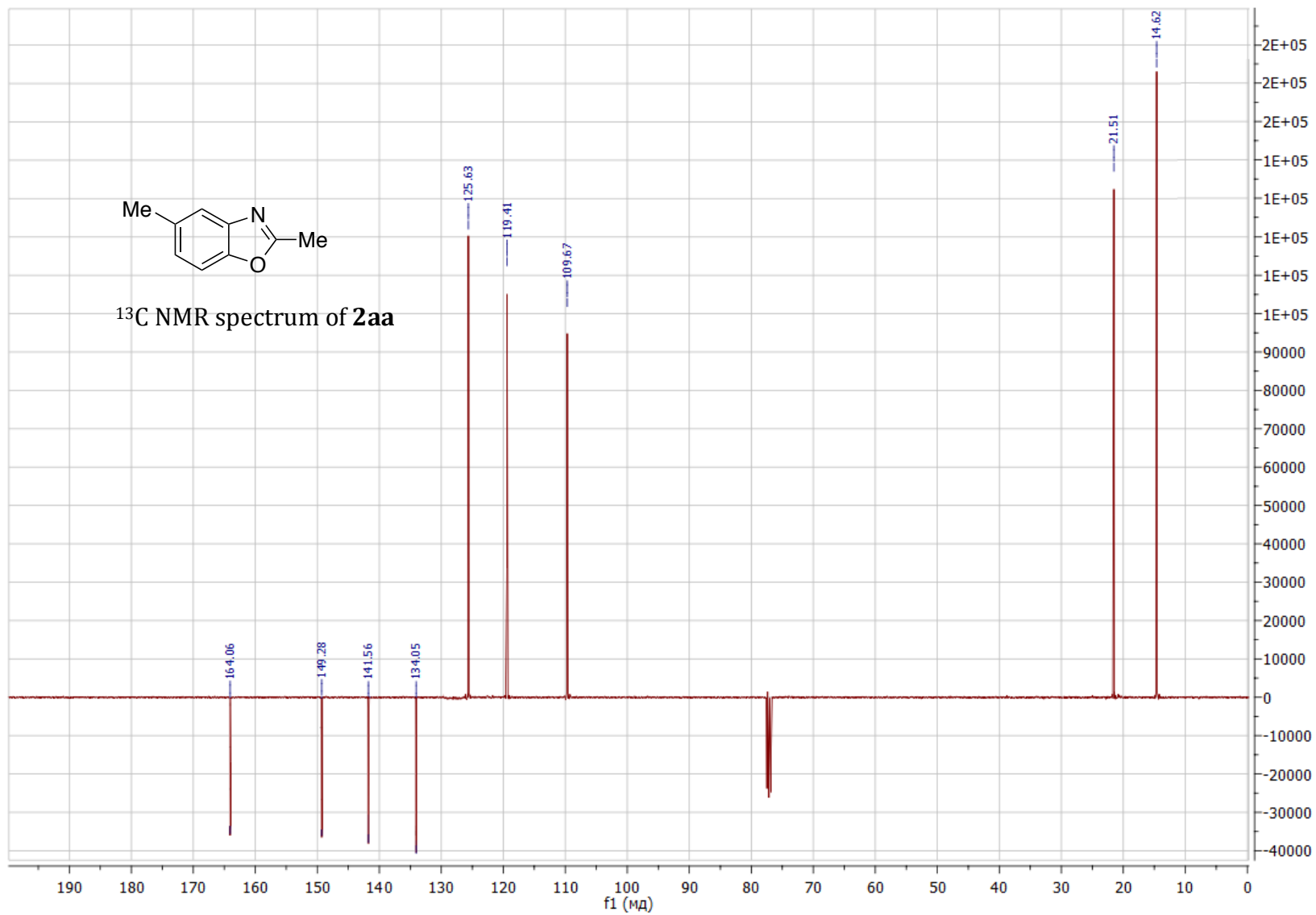
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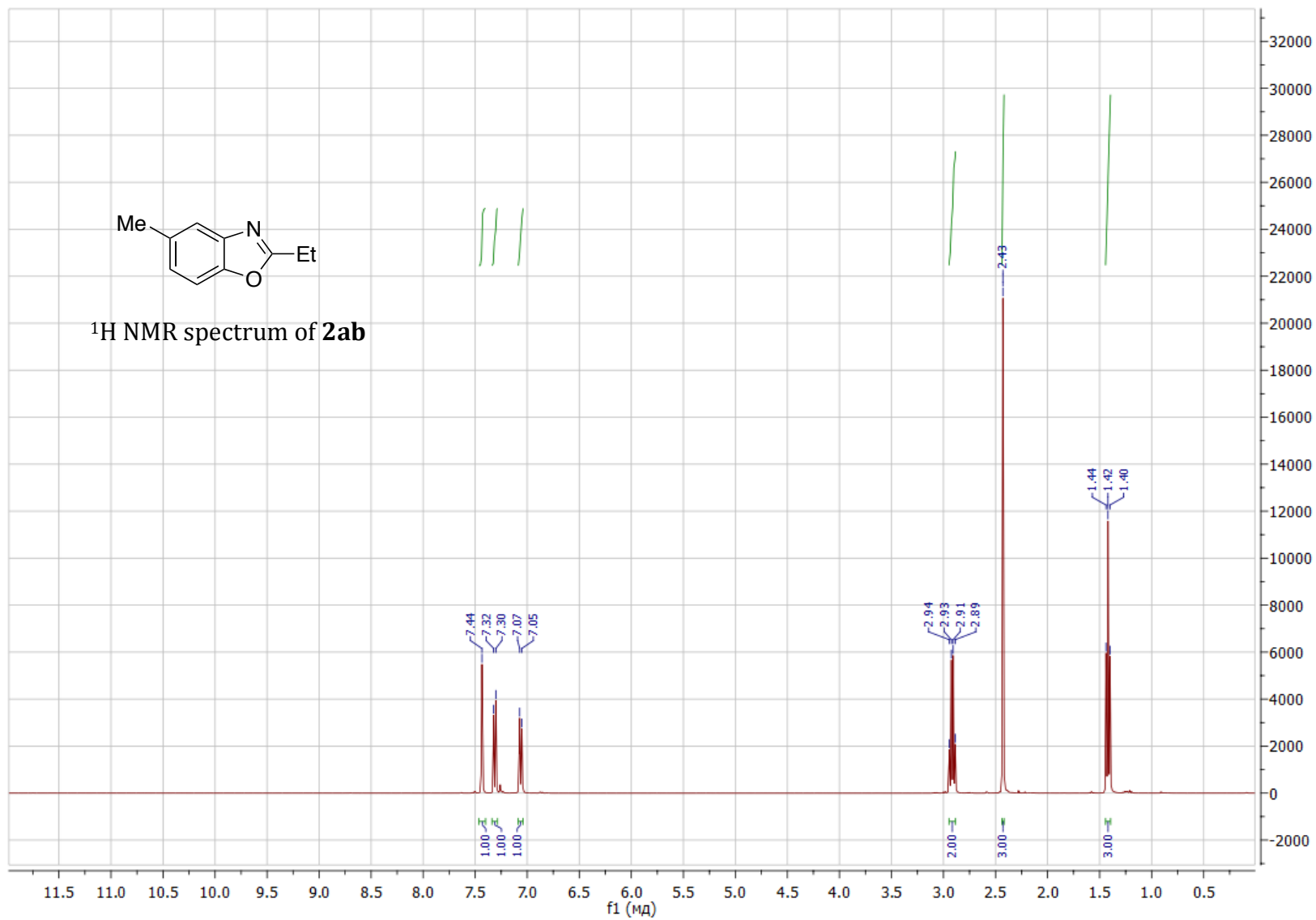
¹H and ¹³C NMR Spectral Charts

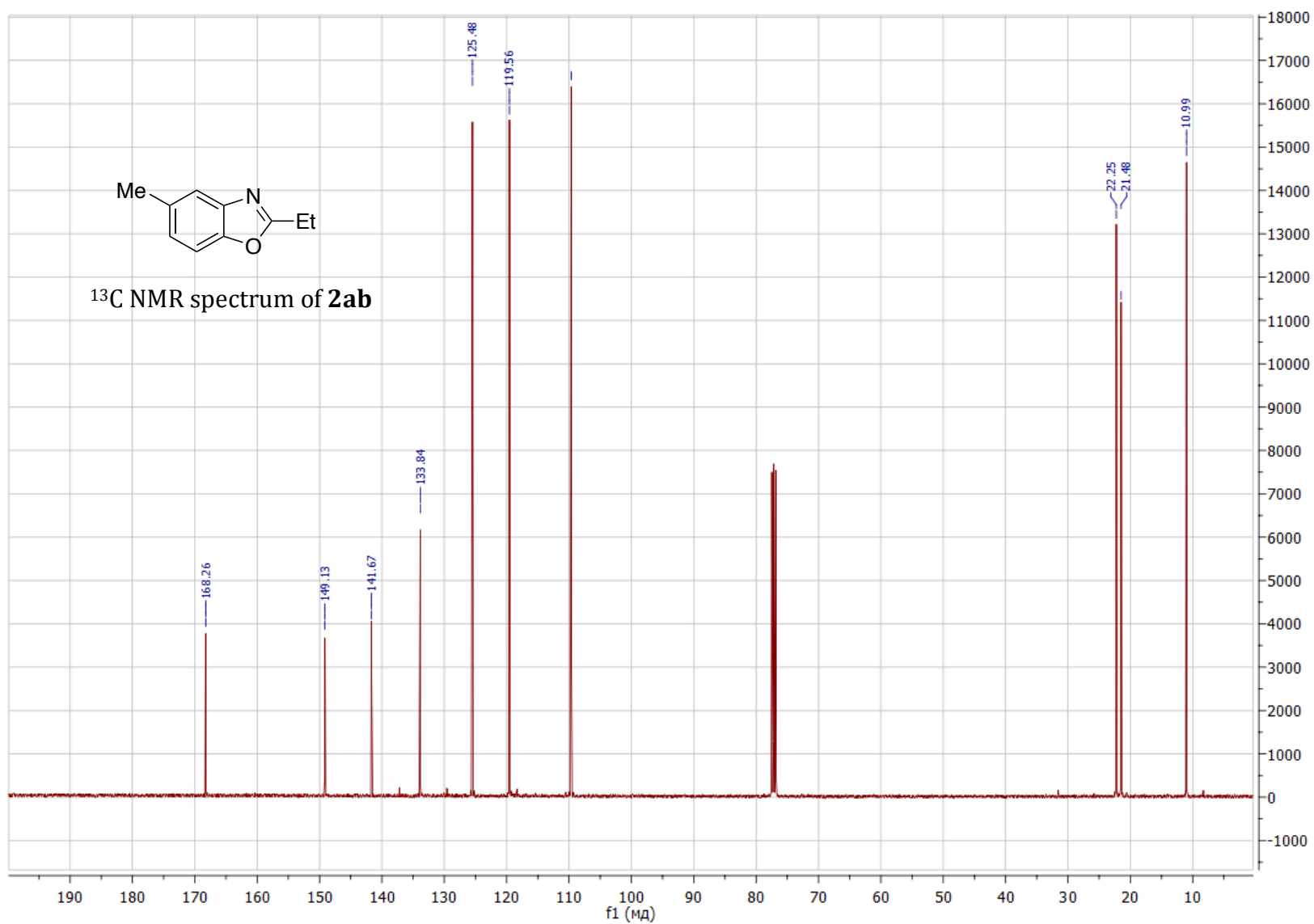


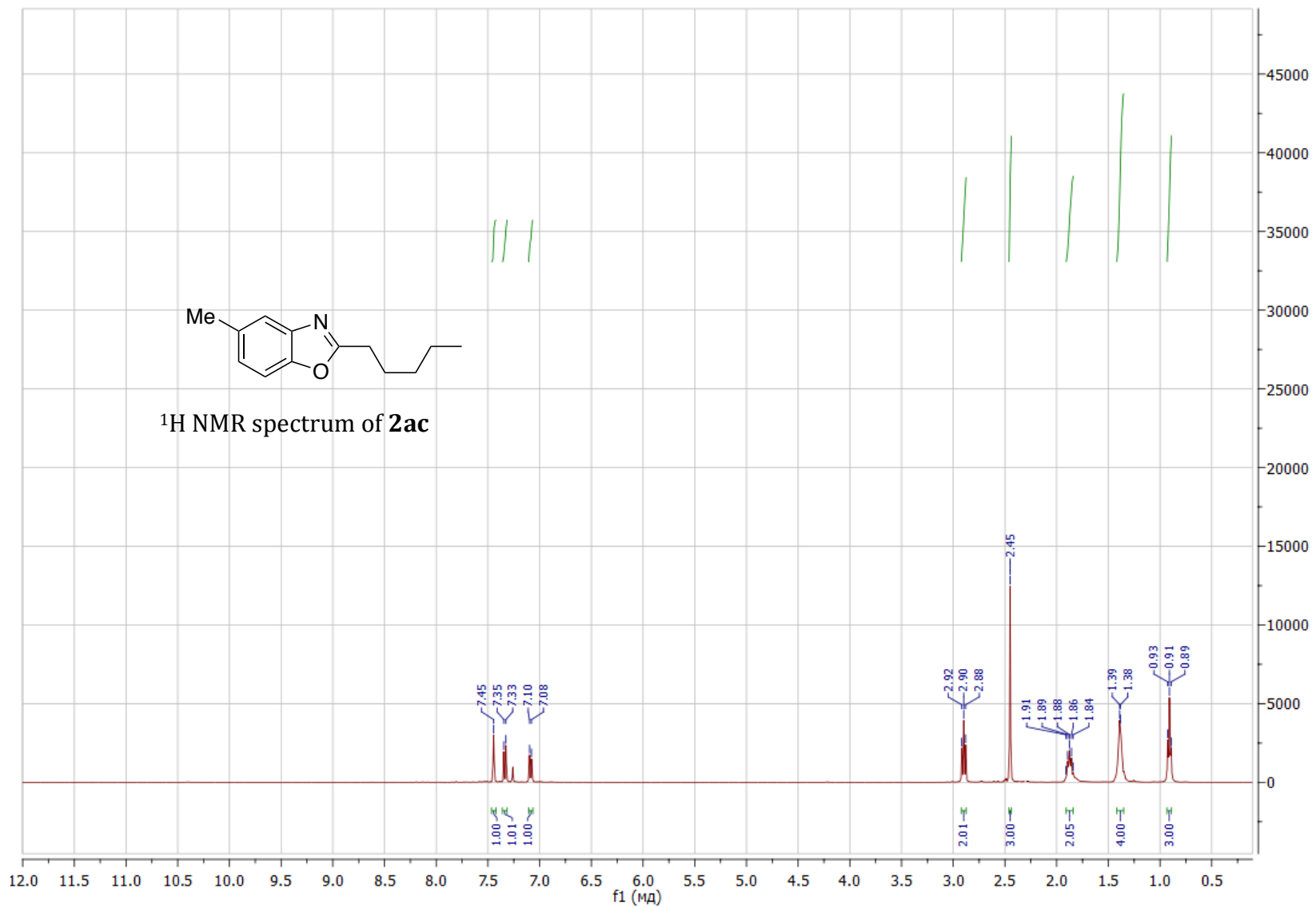


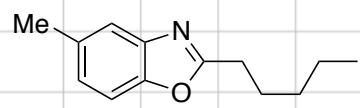
¹³C NMR spectrum of **2aa**



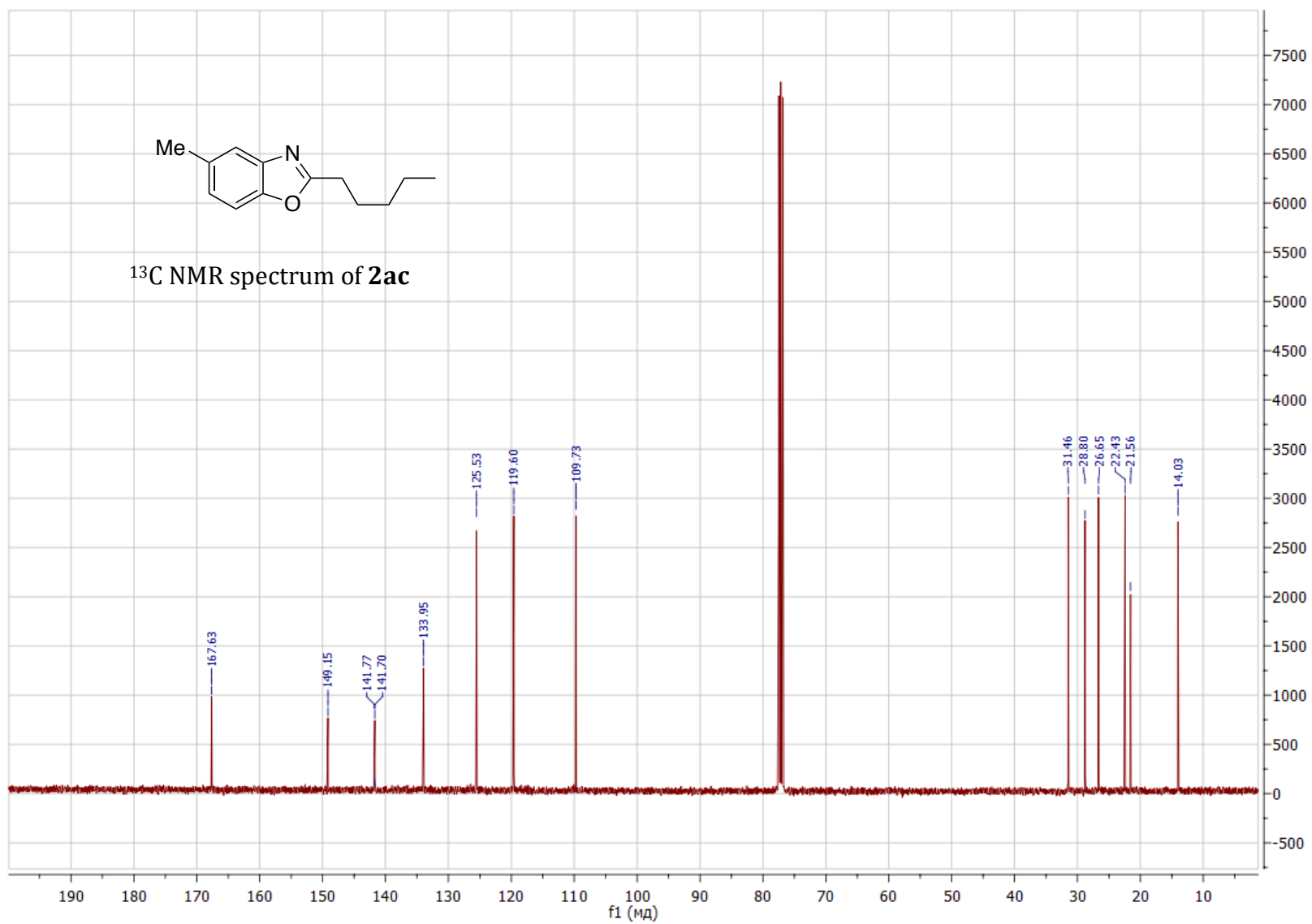


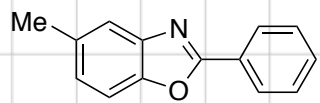




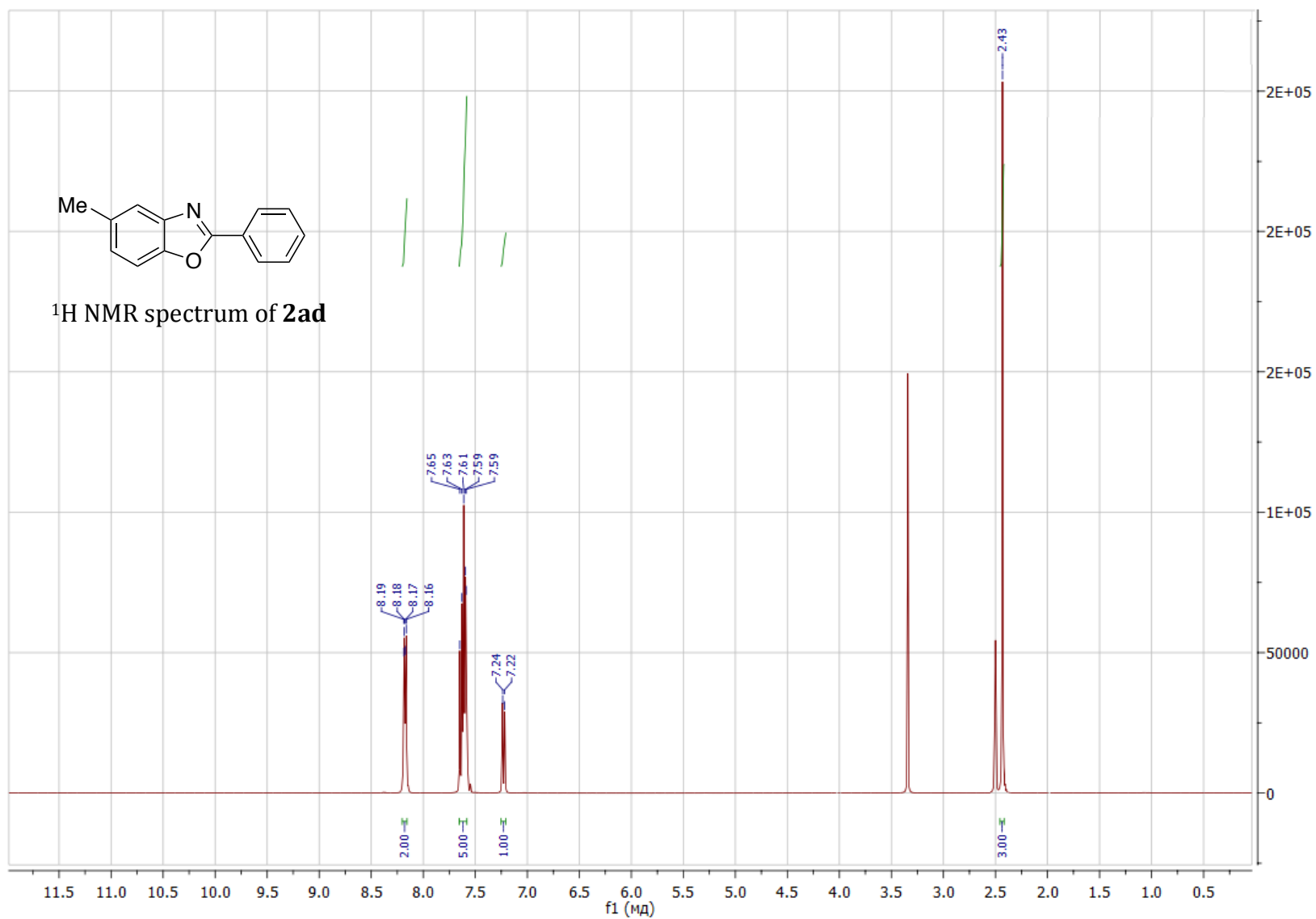


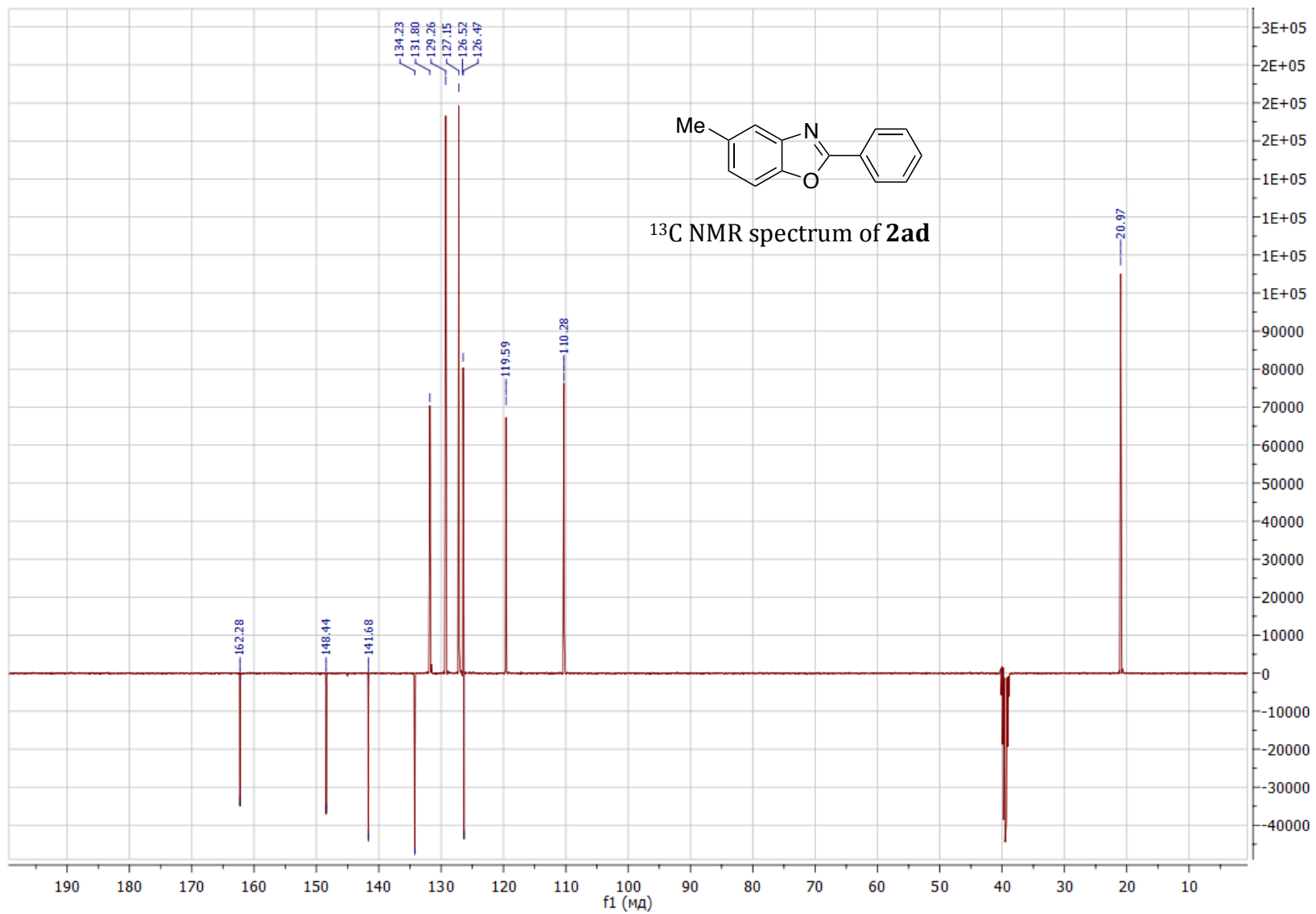
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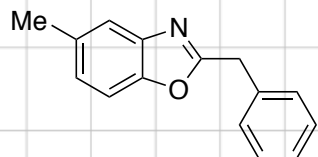




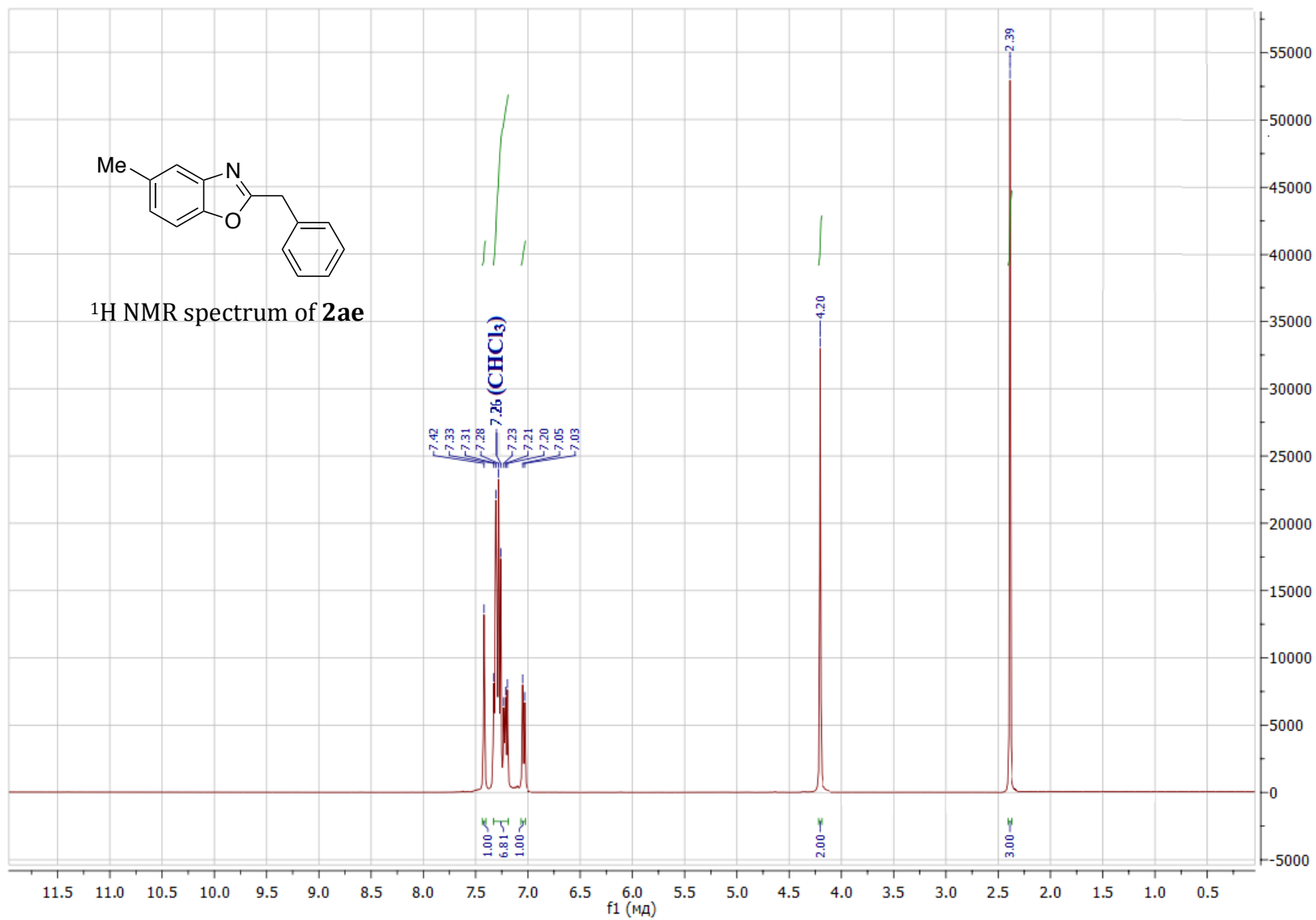
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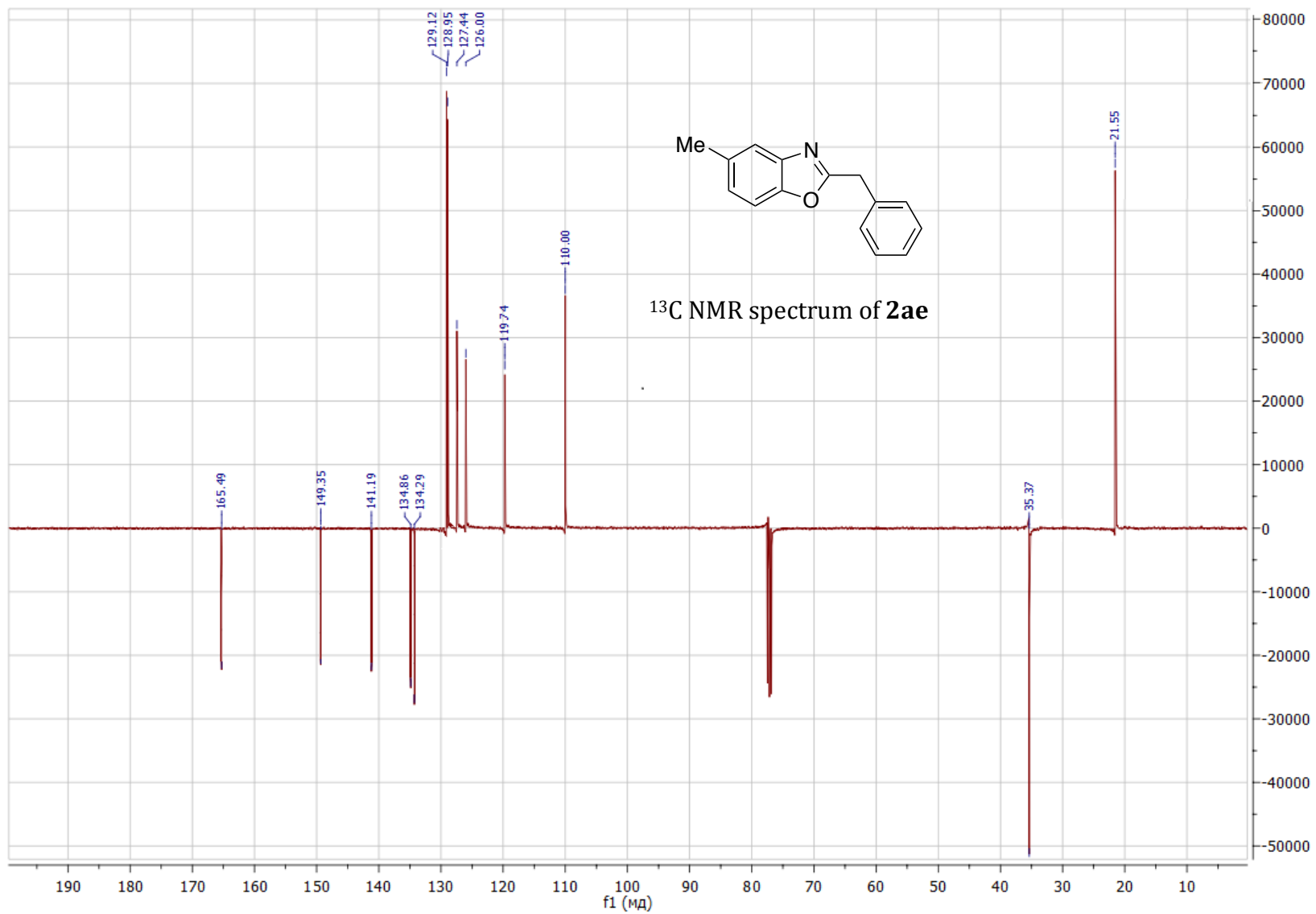


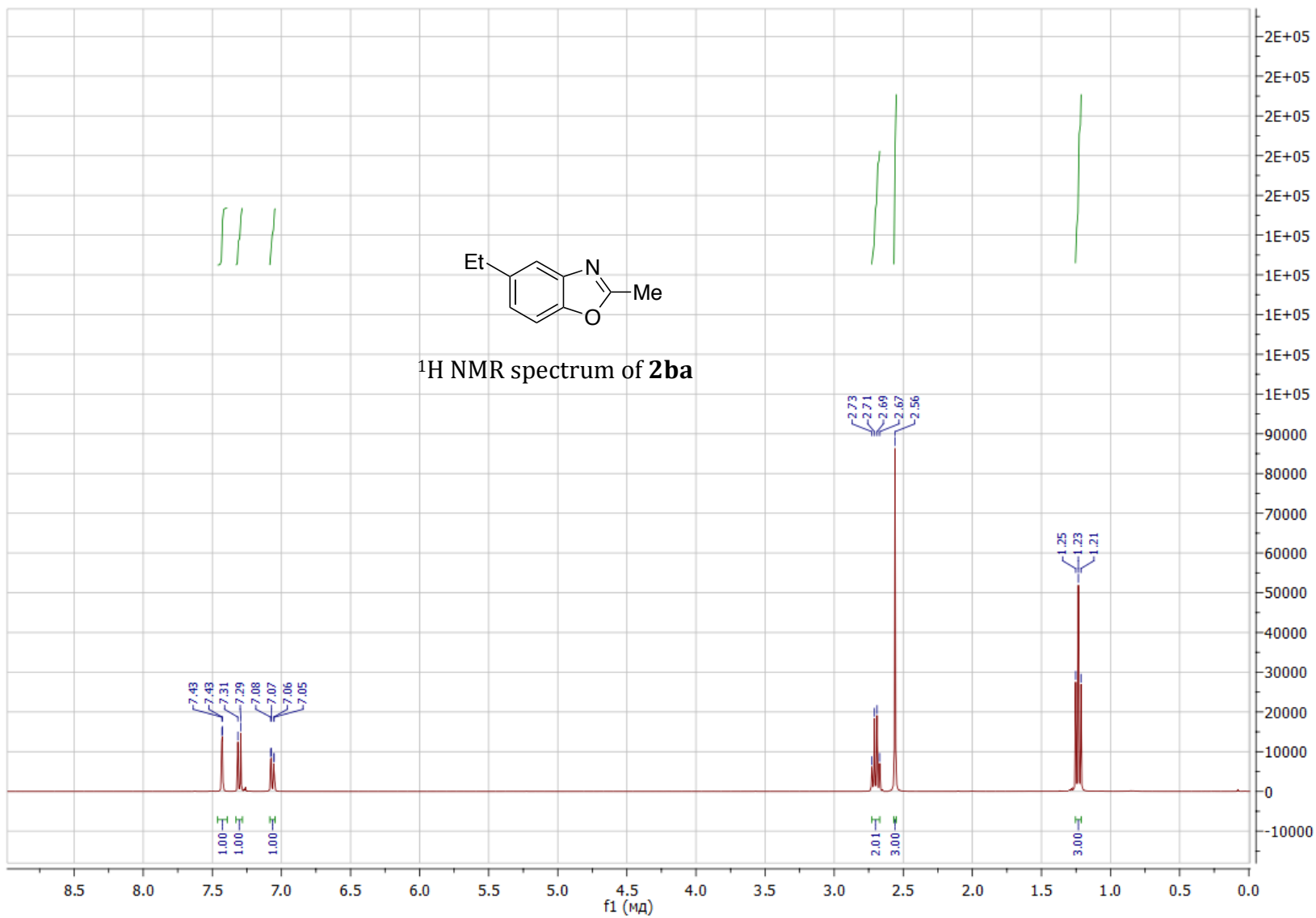


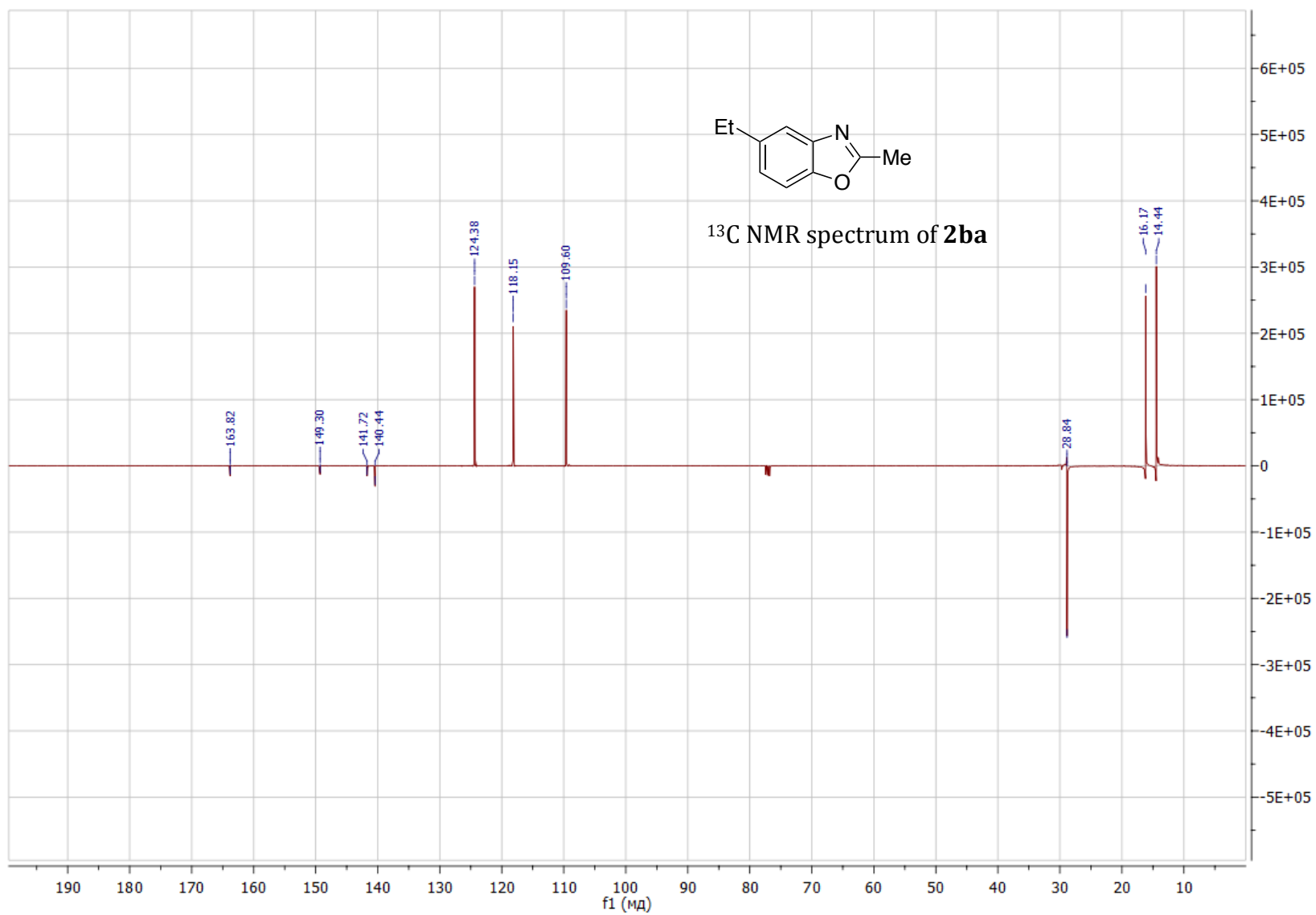


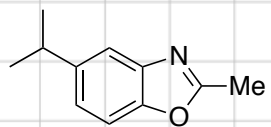
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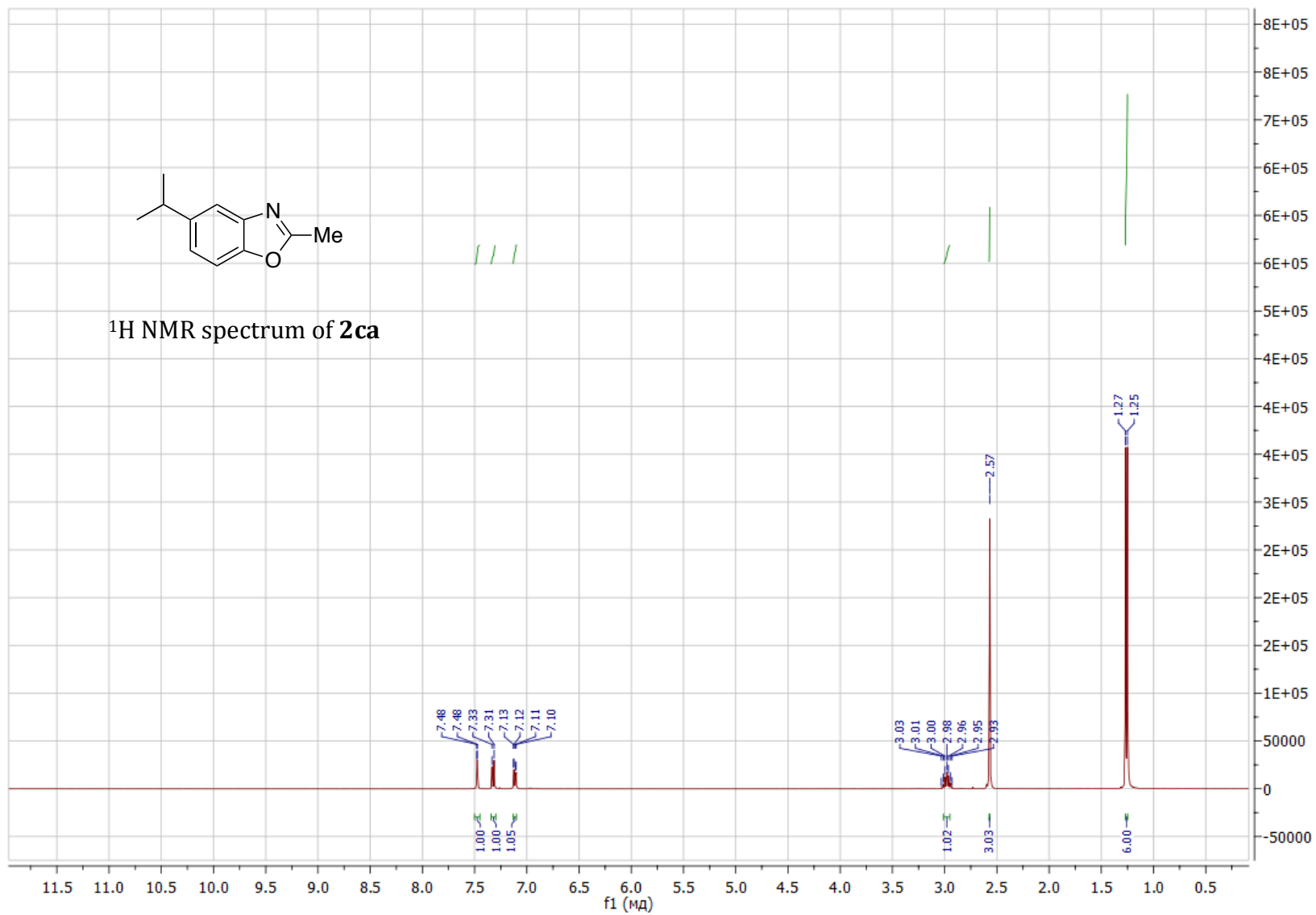


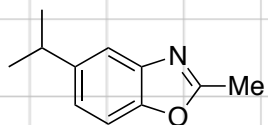




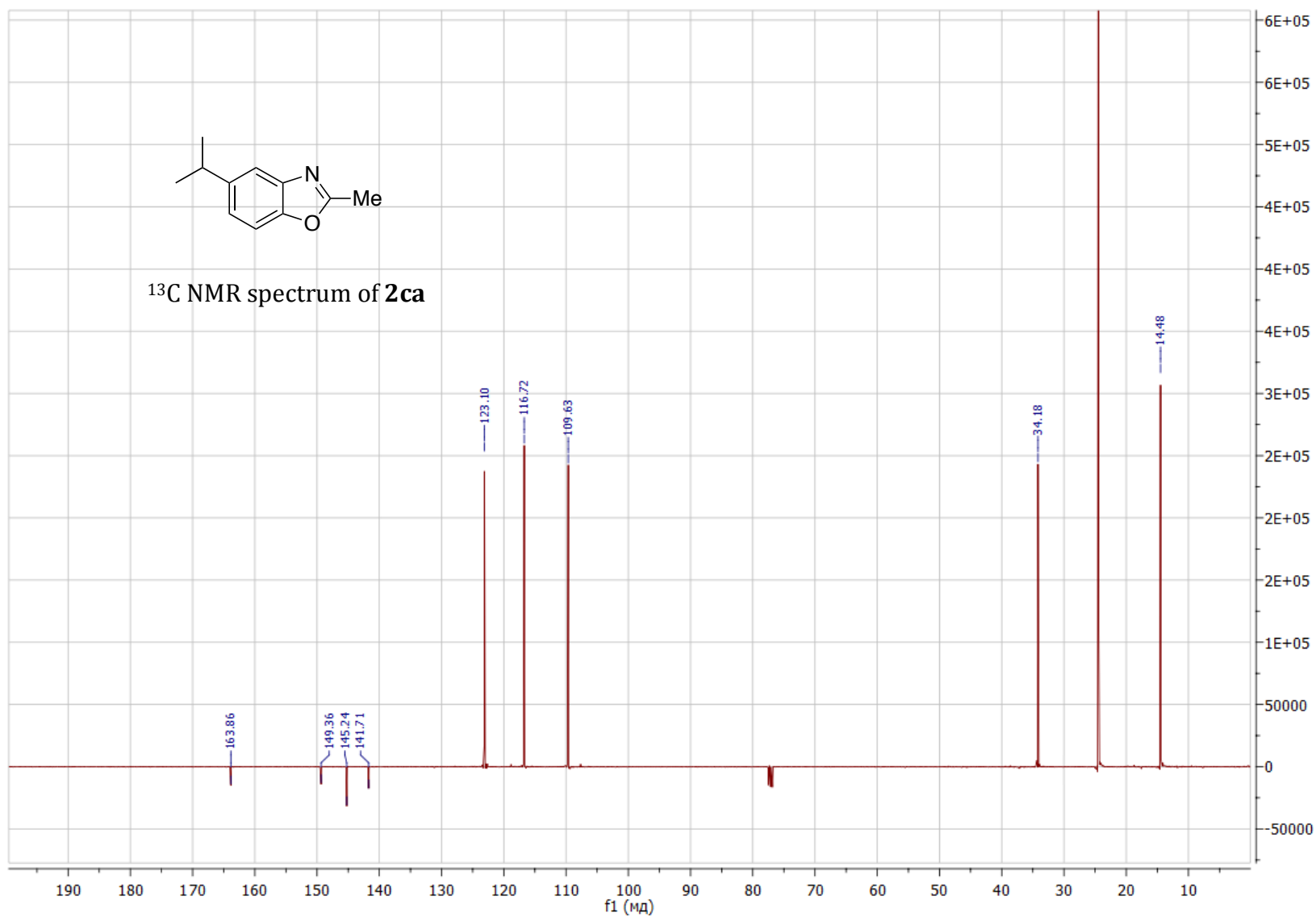


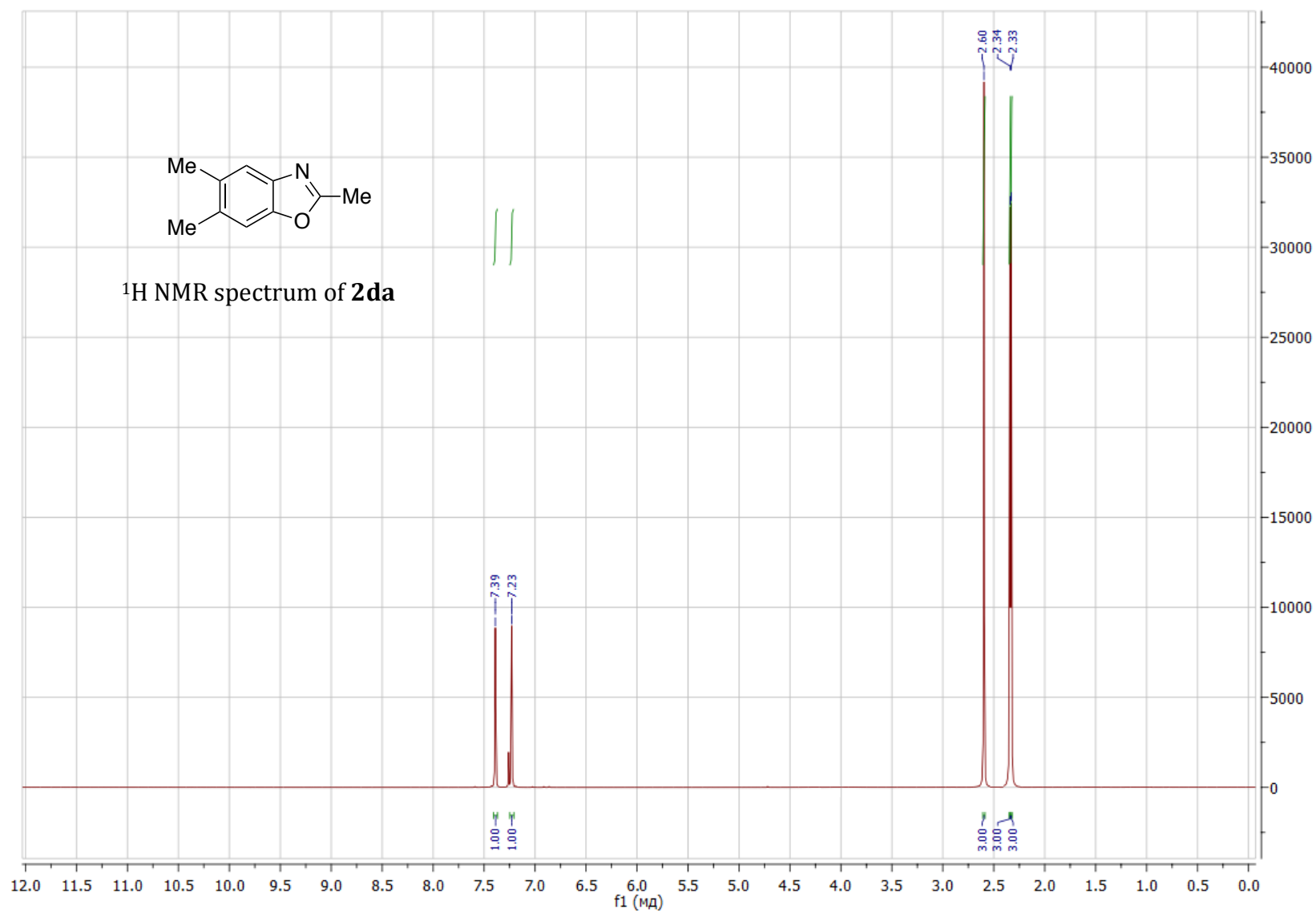
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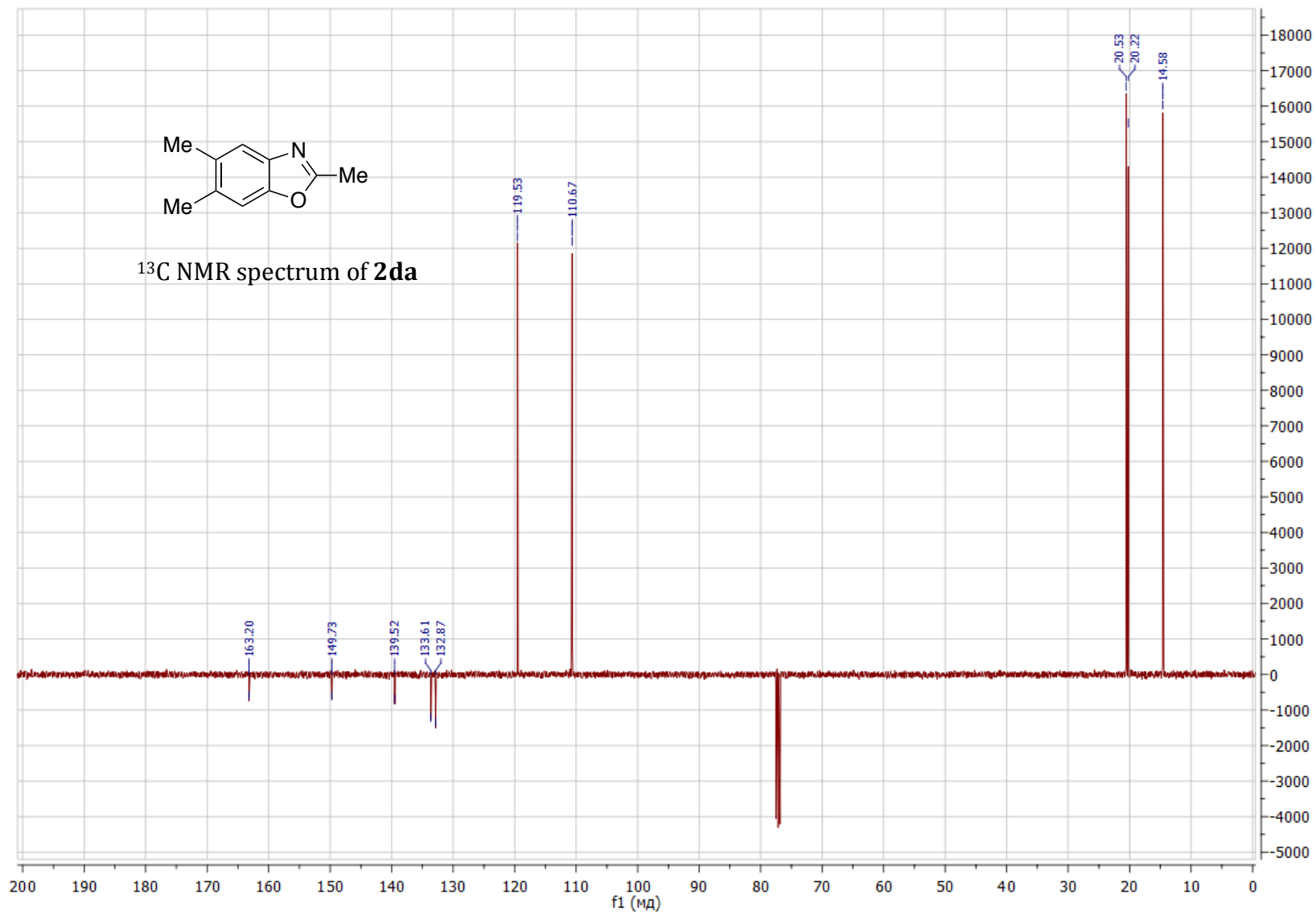


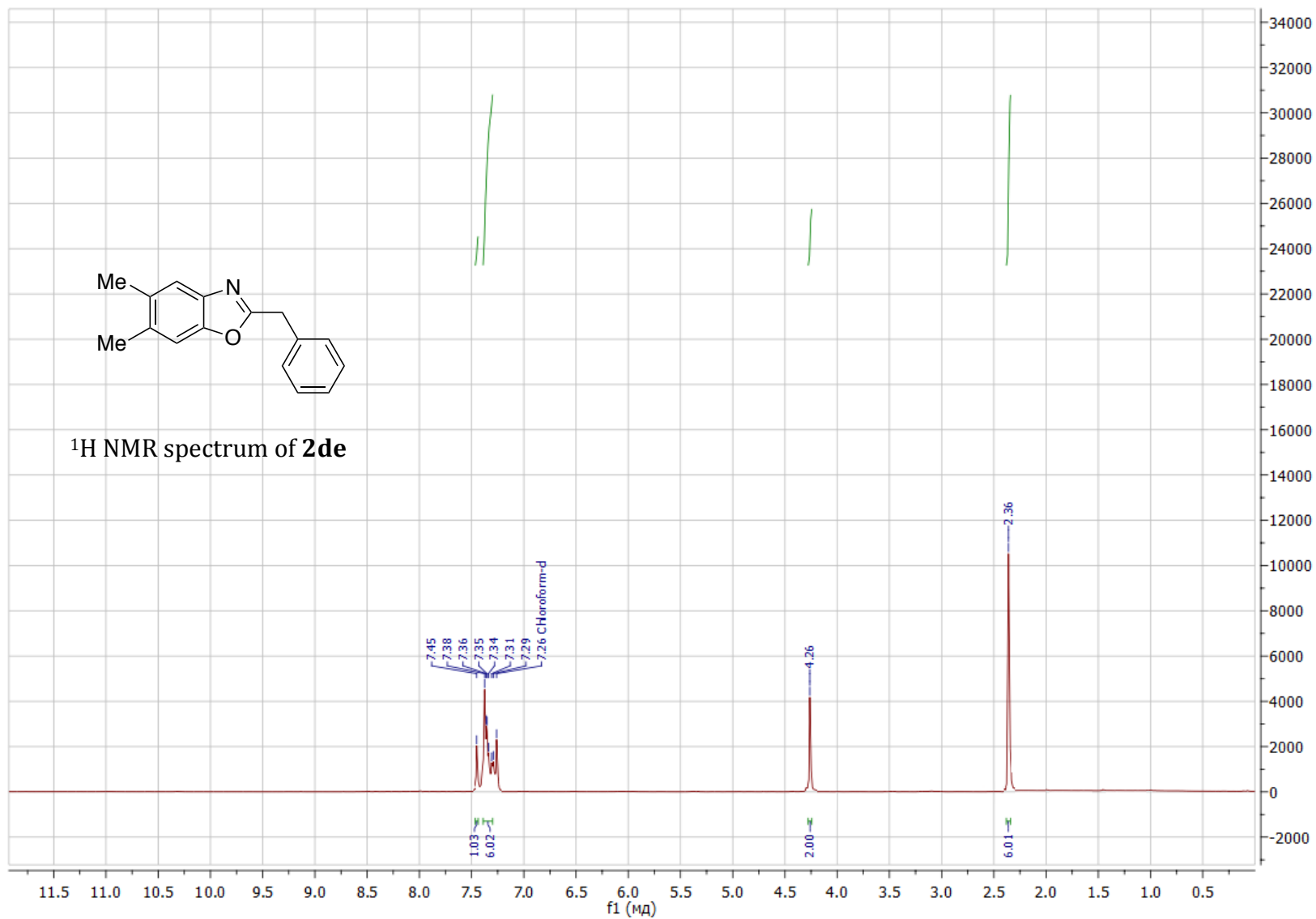


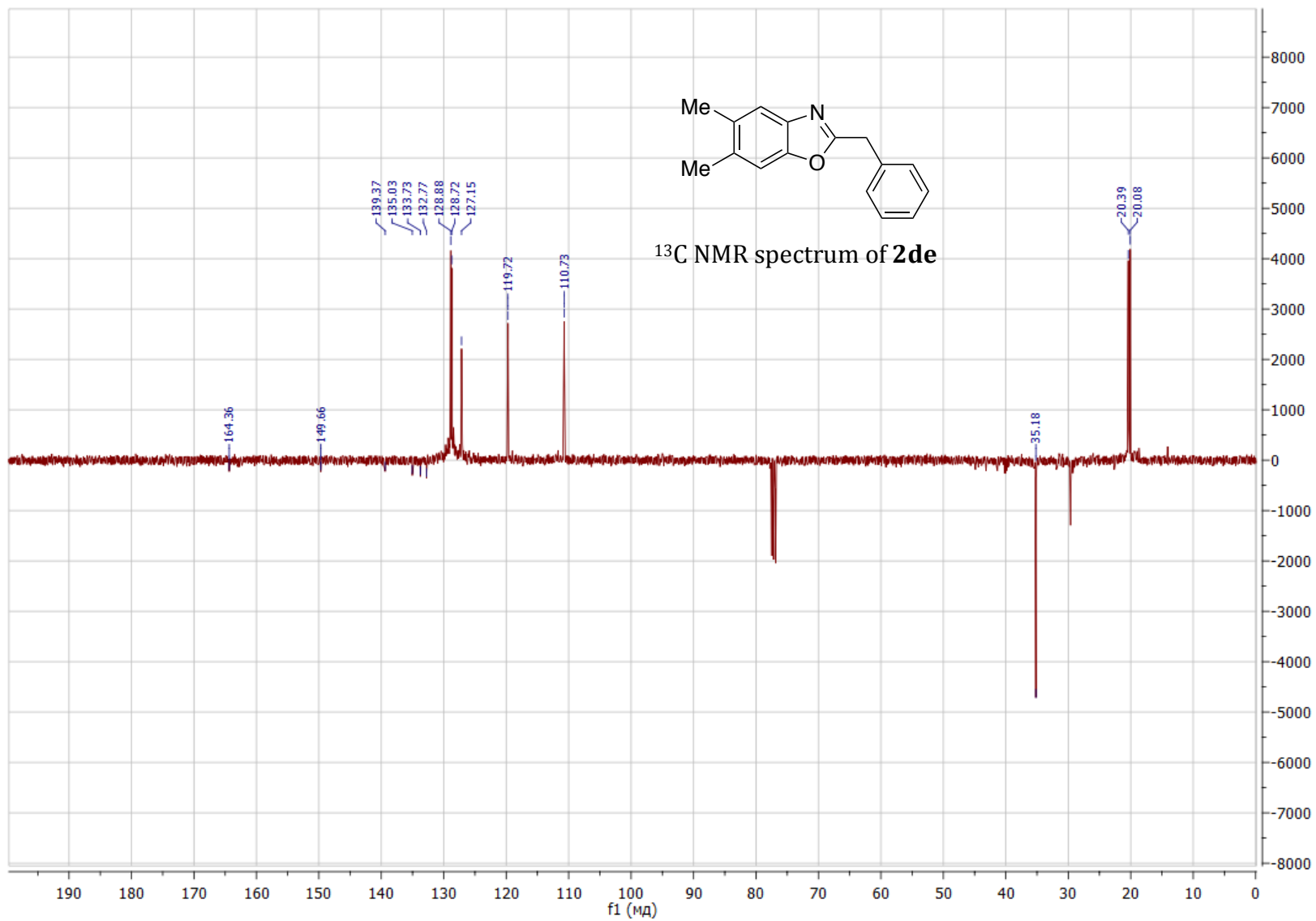
^{13}C NMR spectrum of **2ca**

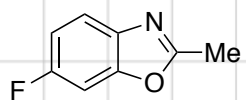




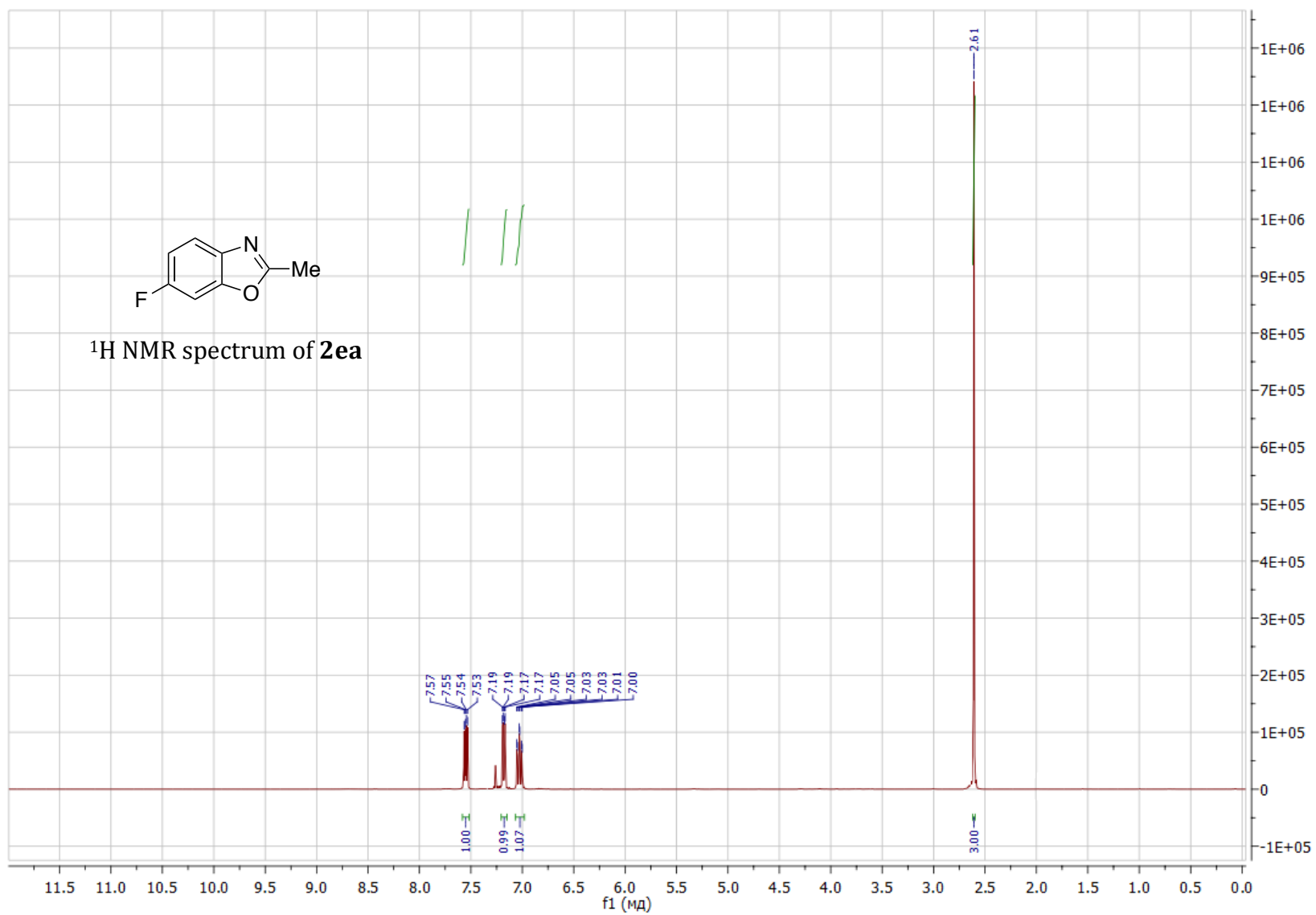


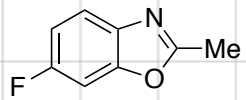




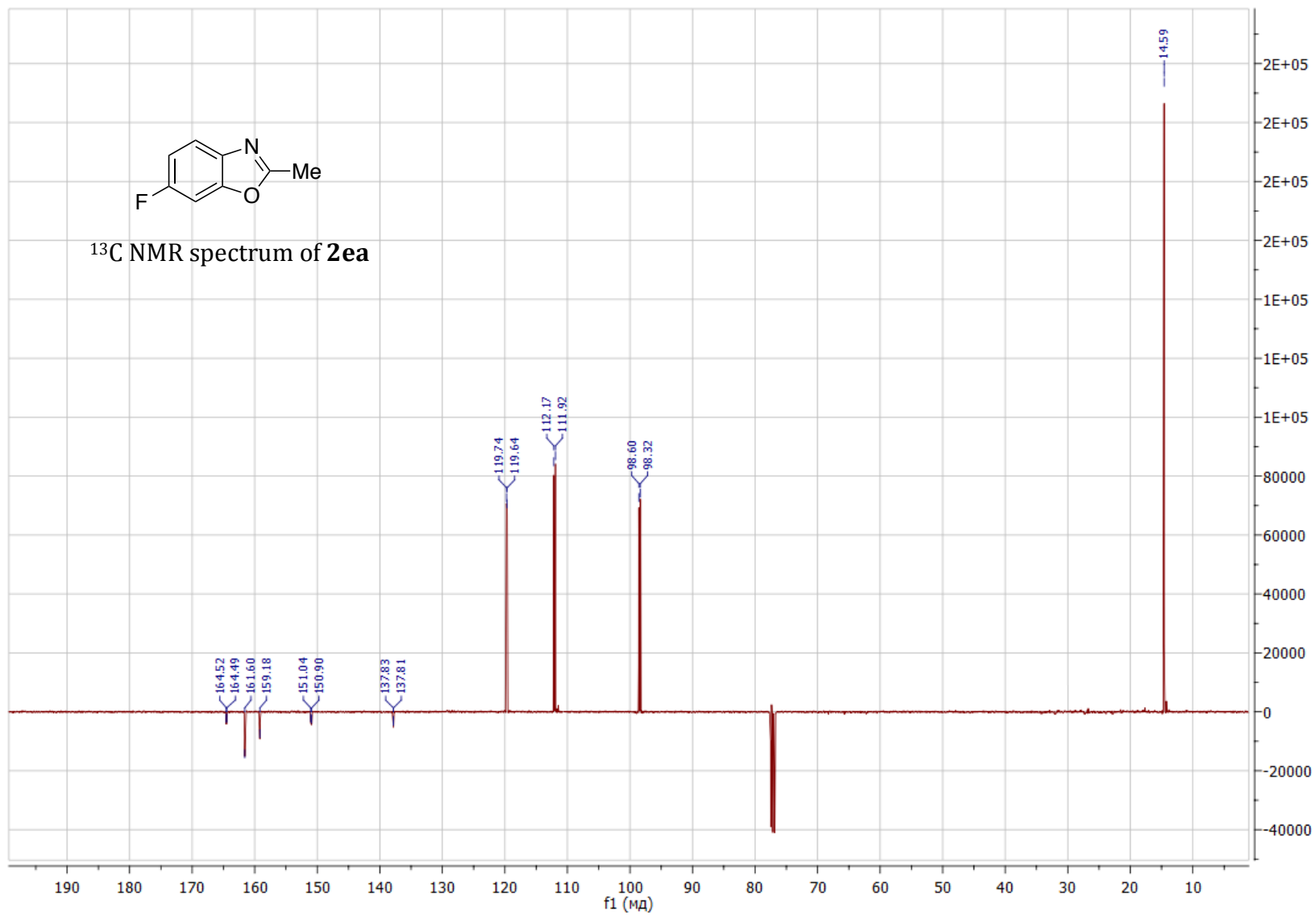


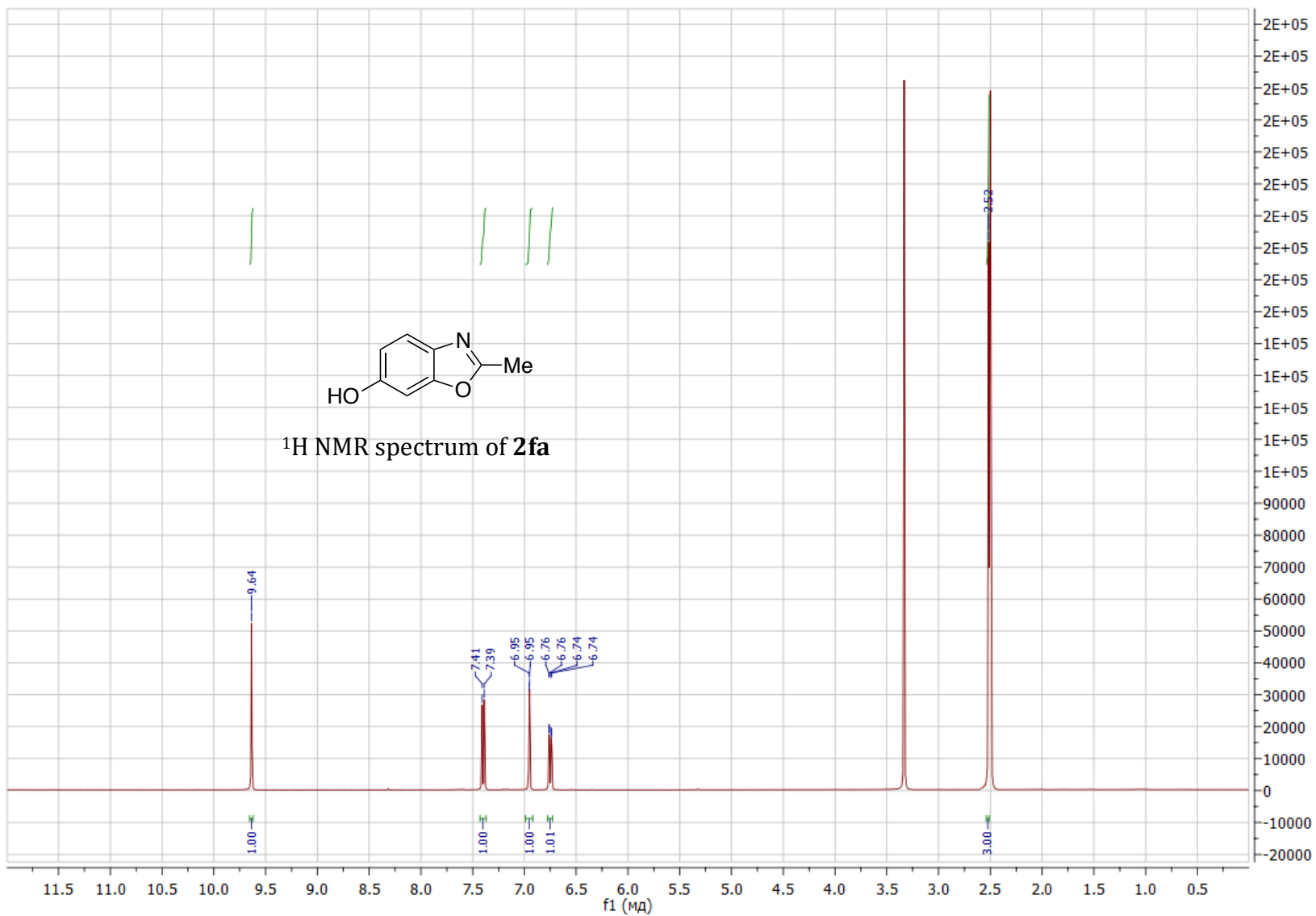
^1H NMR spectrum of **2ea**

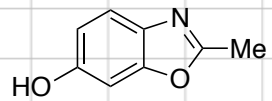




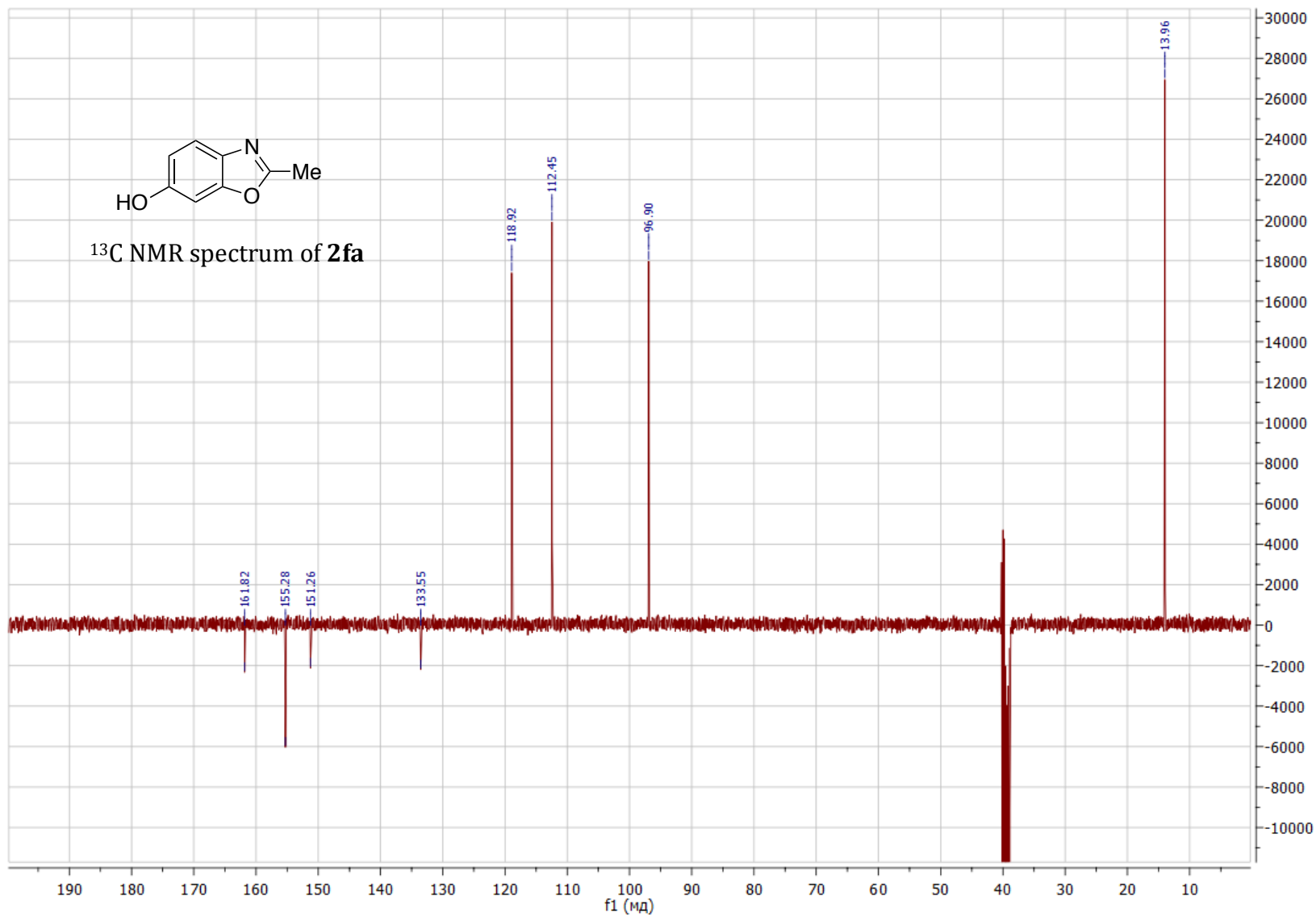
¹³C NMR spectrum of **2ea**

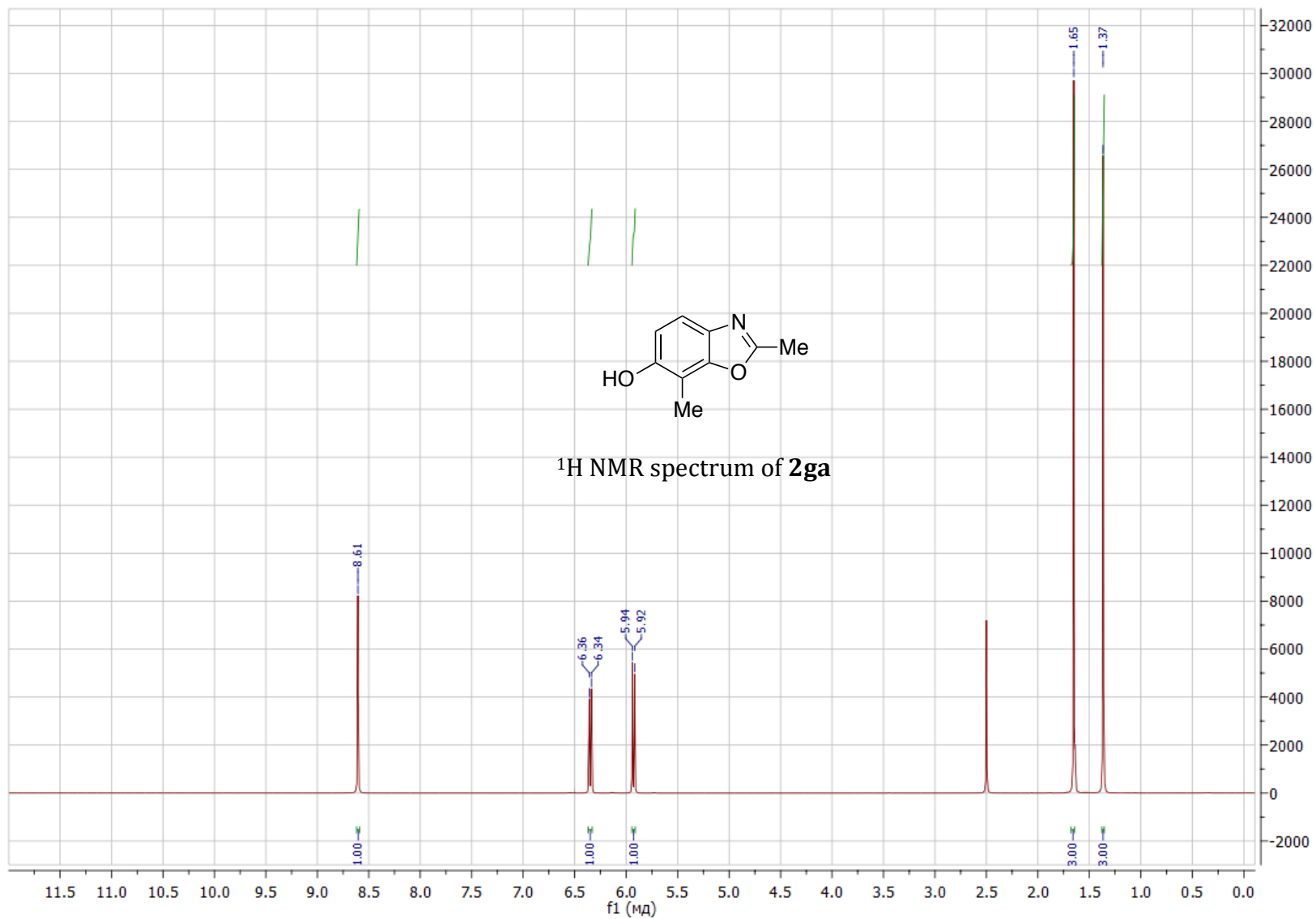


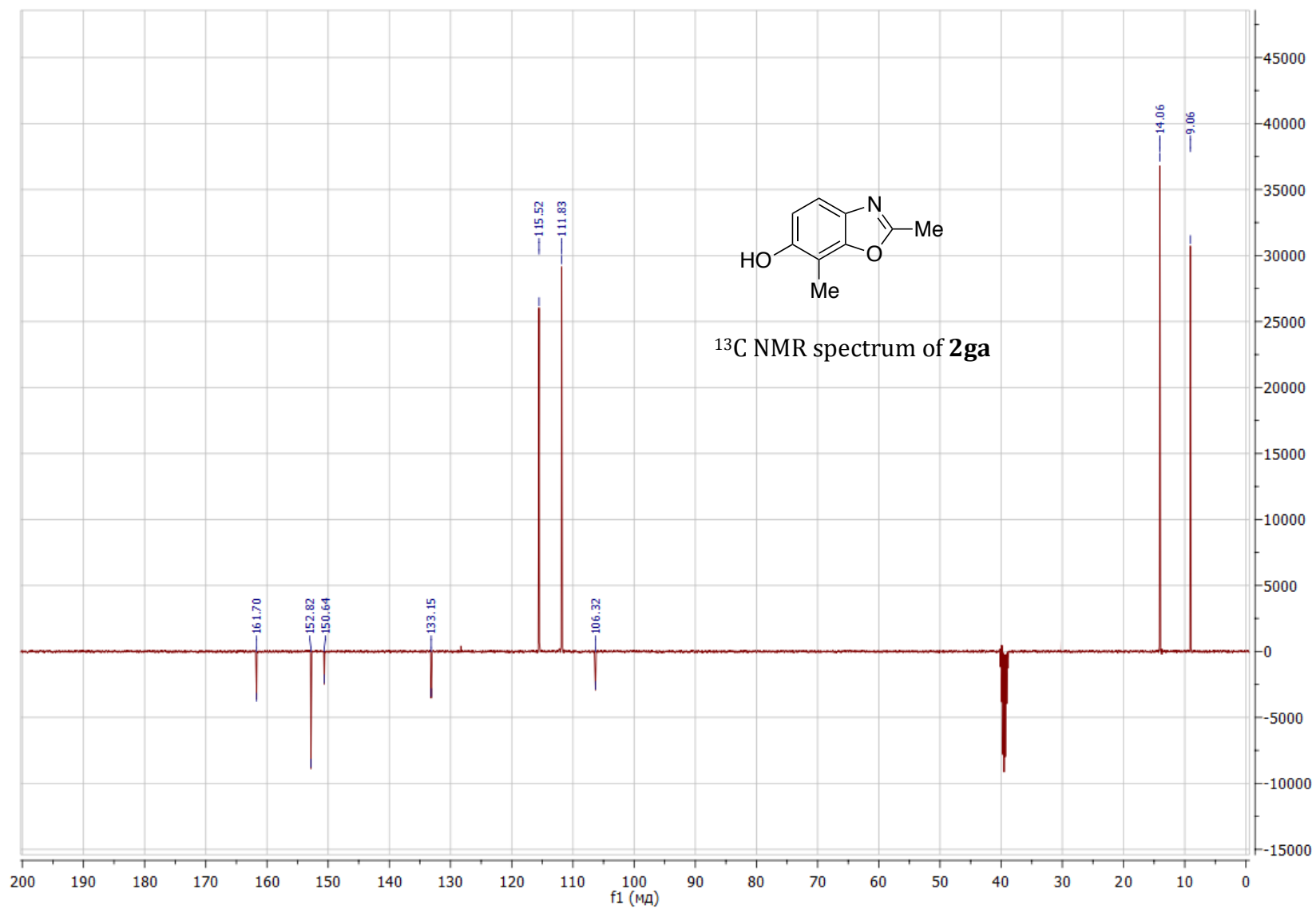


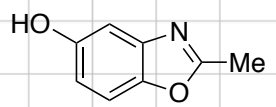


^{13}C NMR spectrum of **2fa**

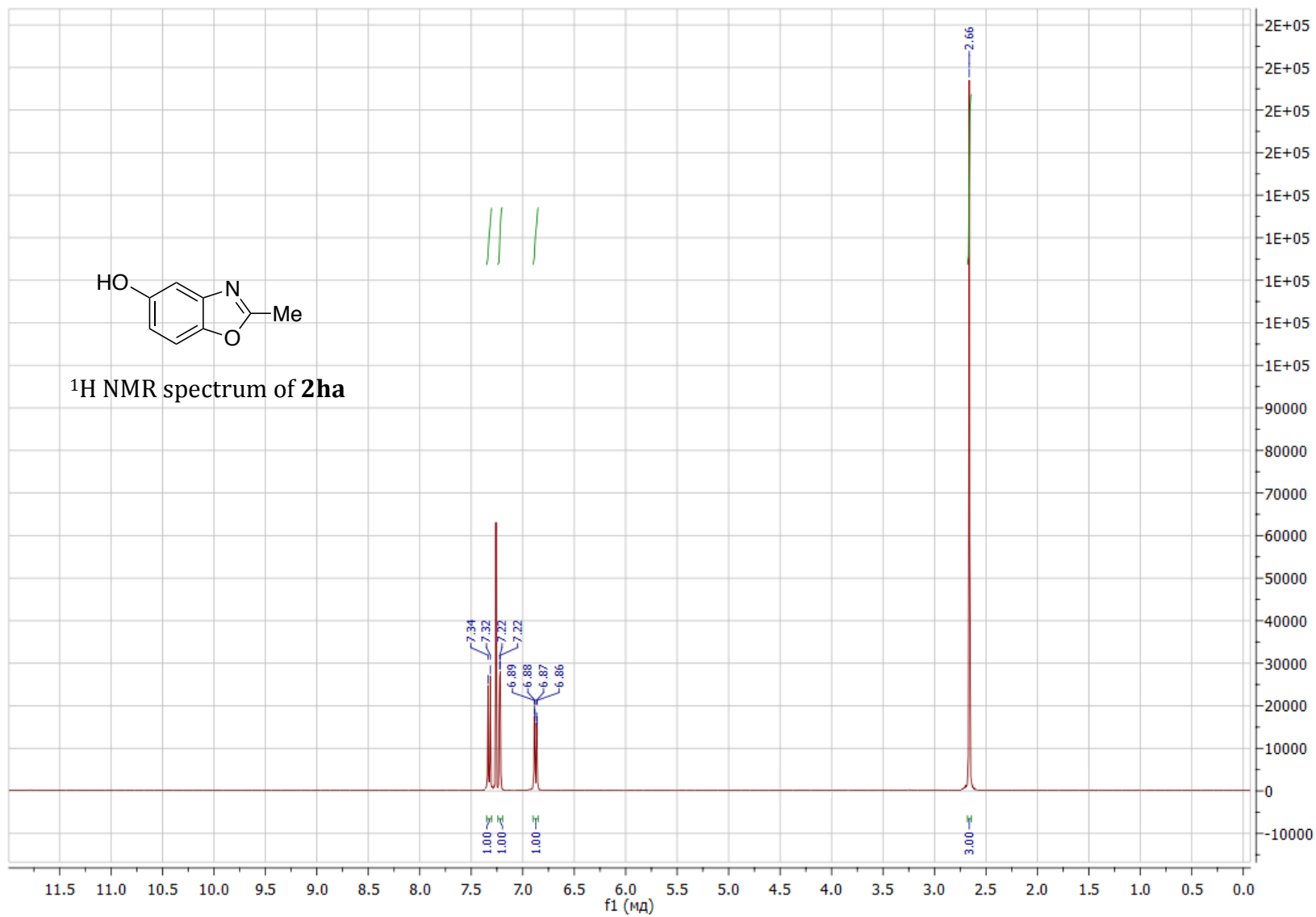


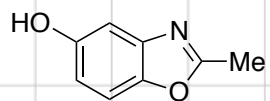




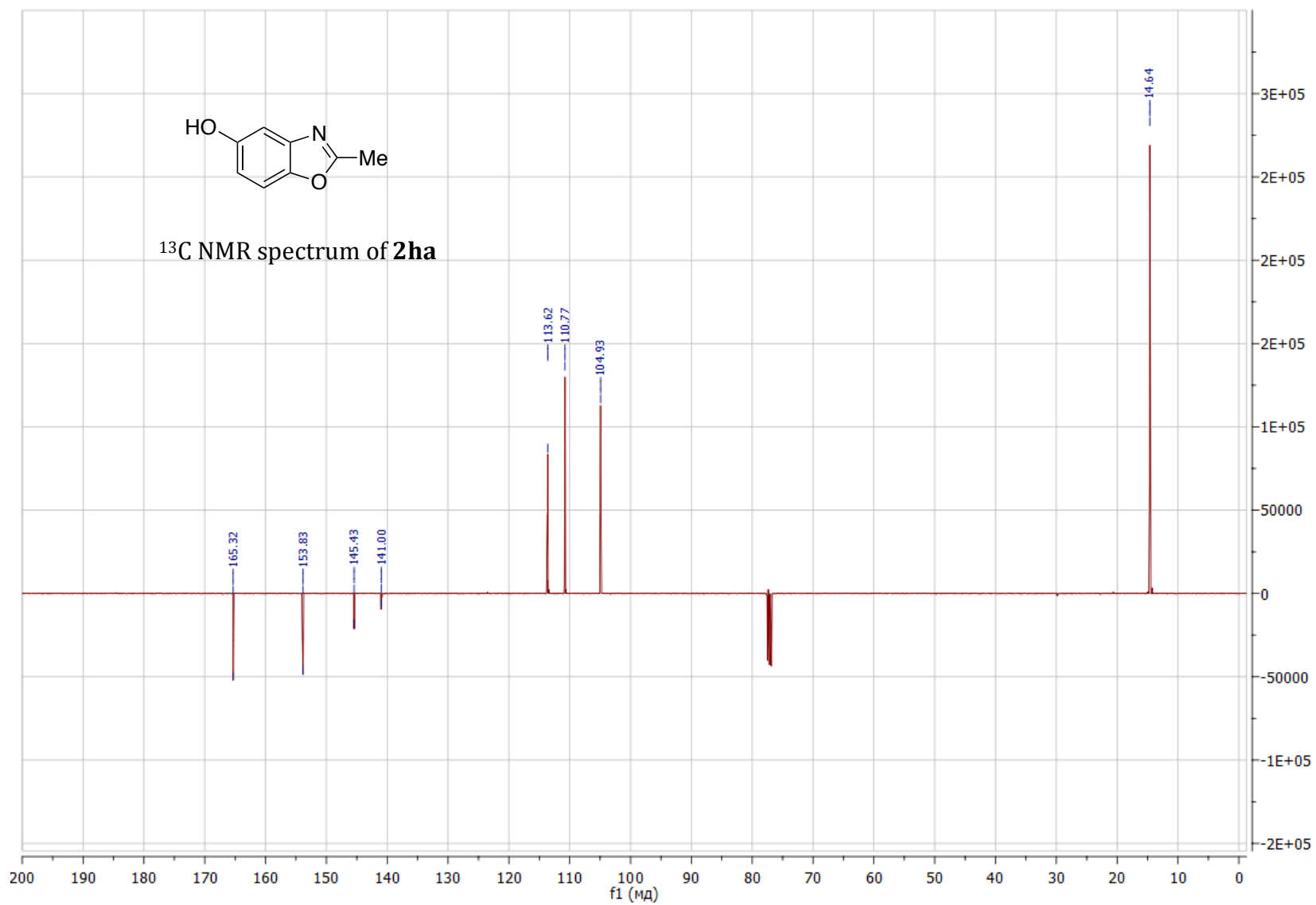


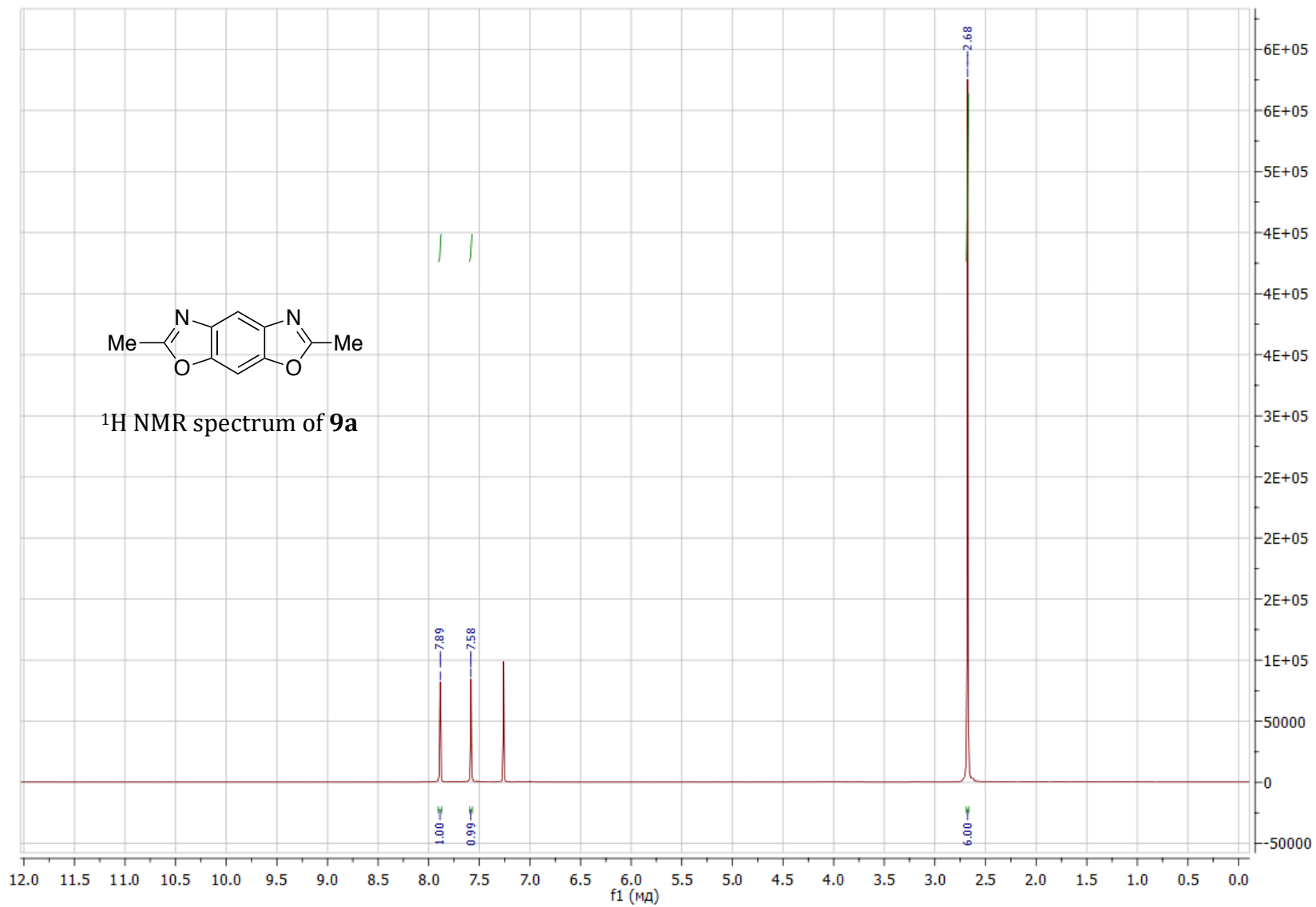
¹H NMR spectrum of **2ha**

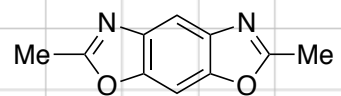




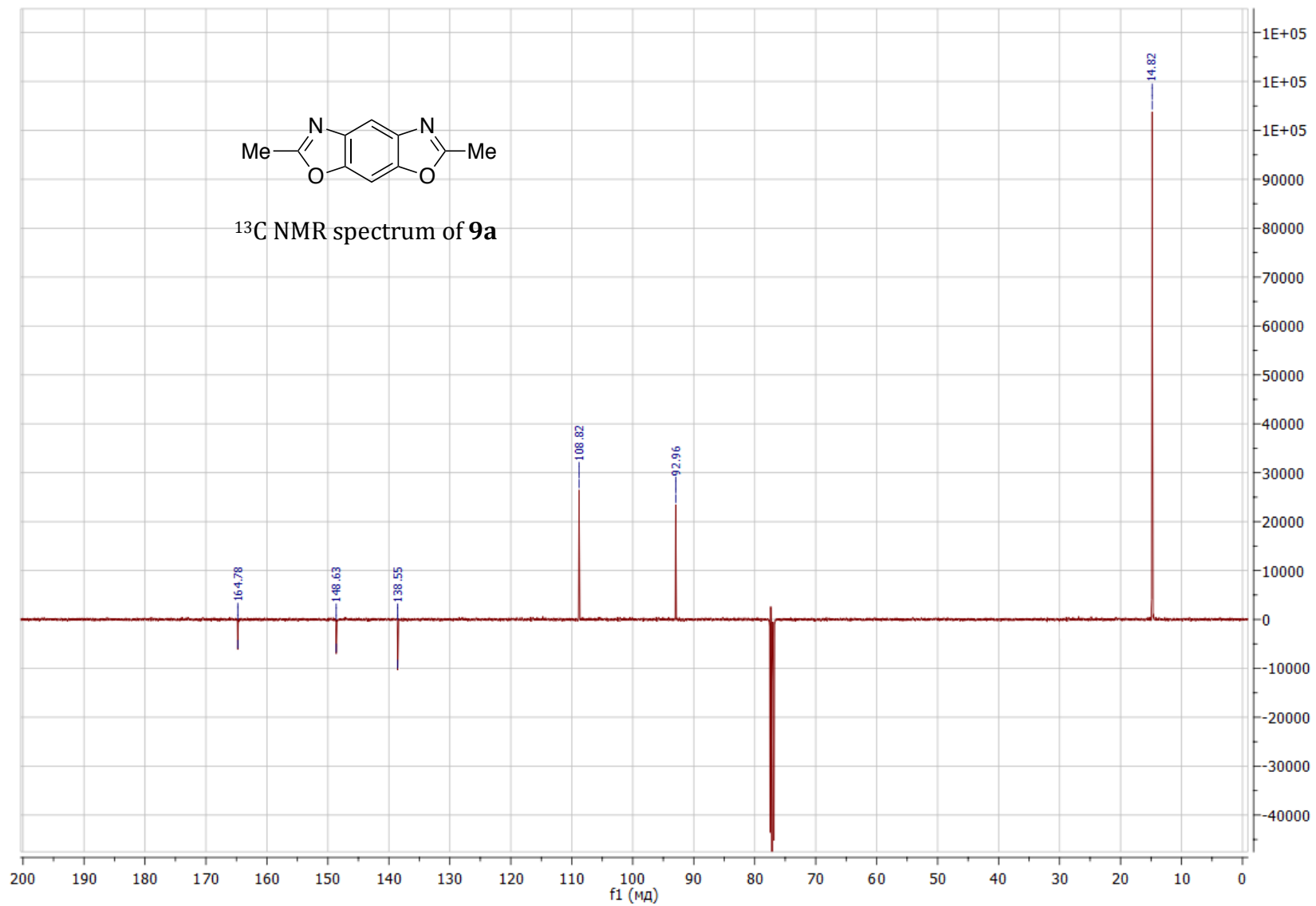
¹³C NMR spectrum of **2ha**

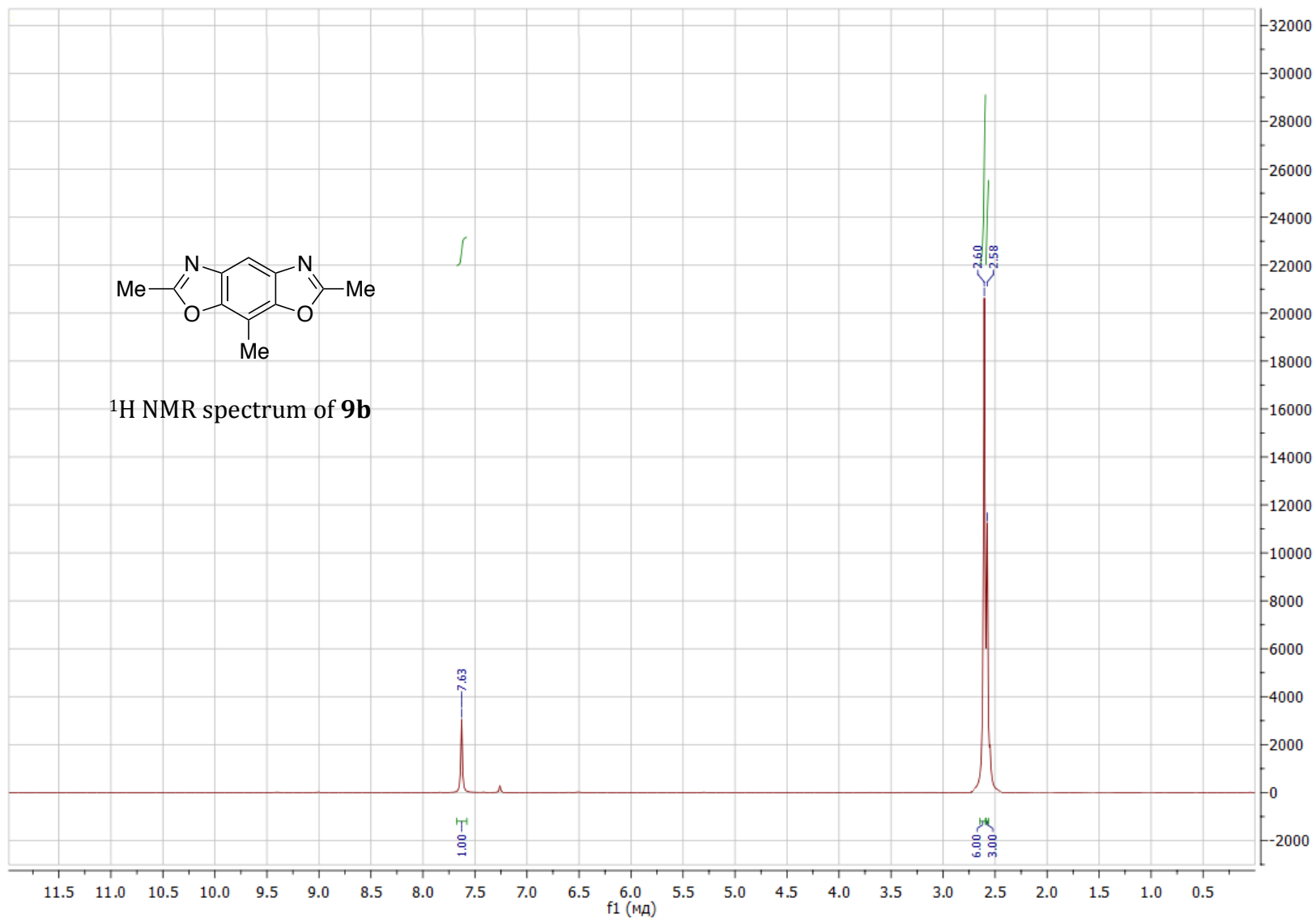


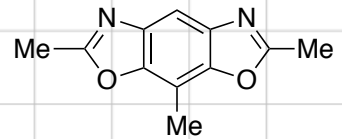




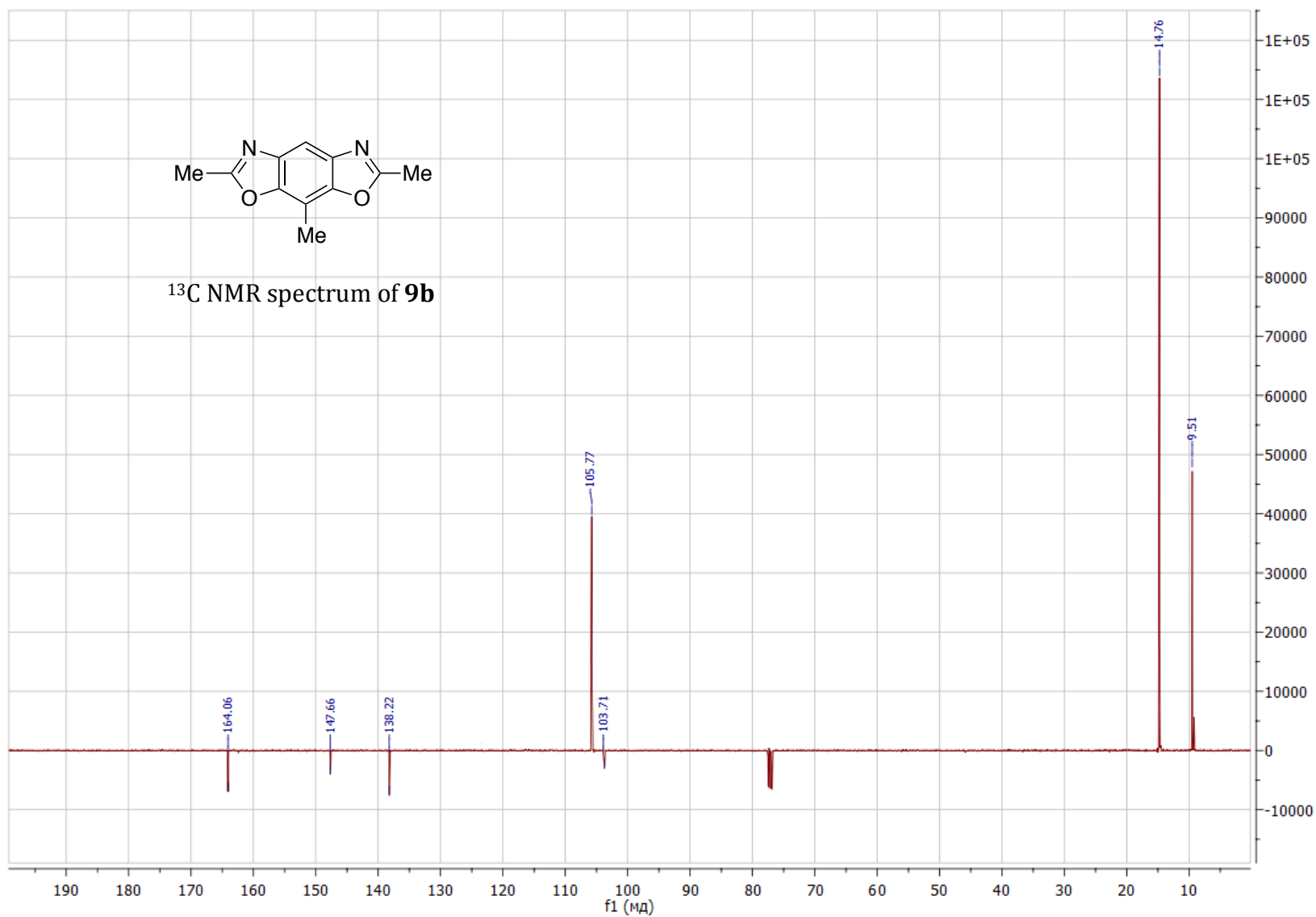
^{13}C NMR spectrum of **9a**

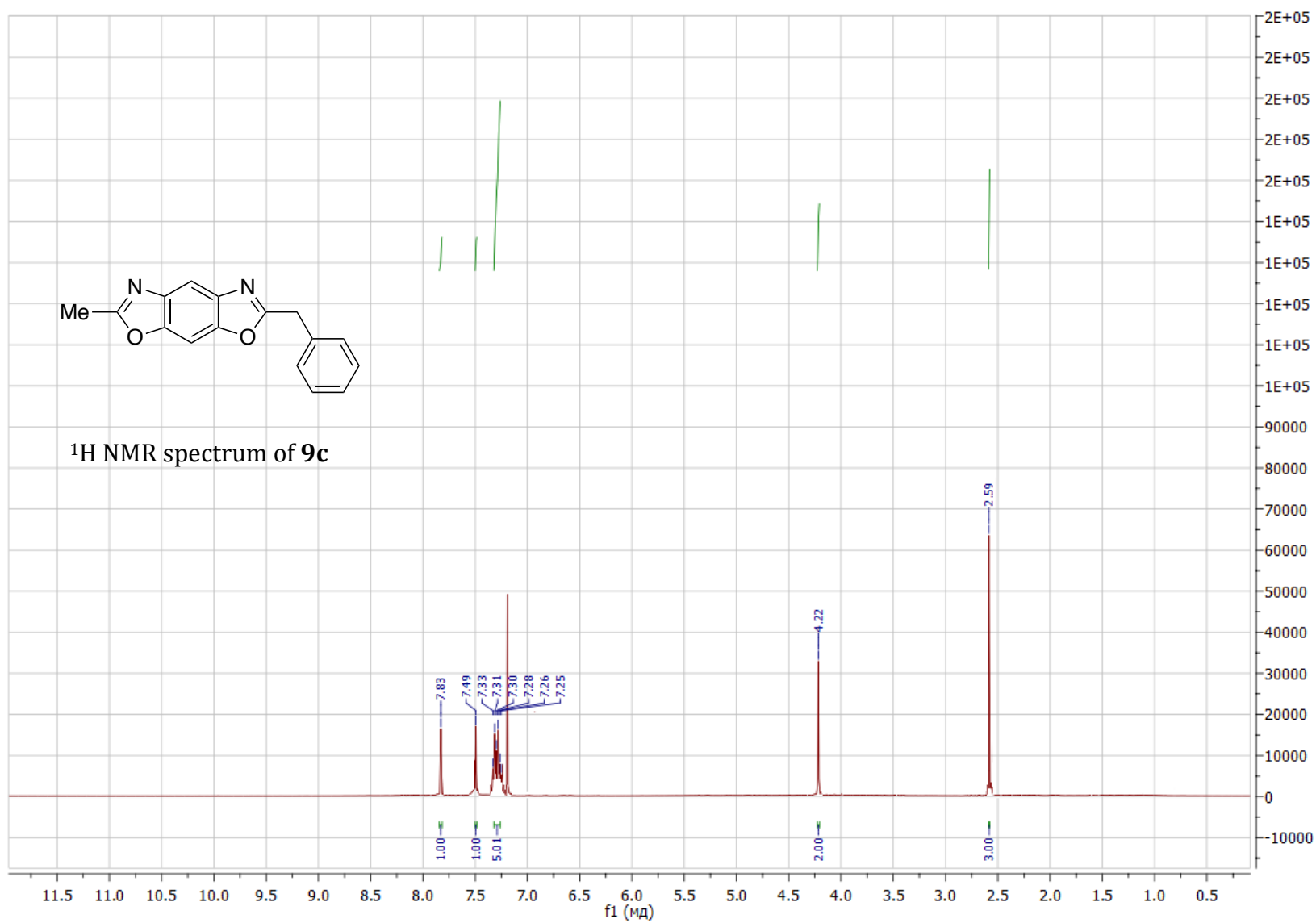


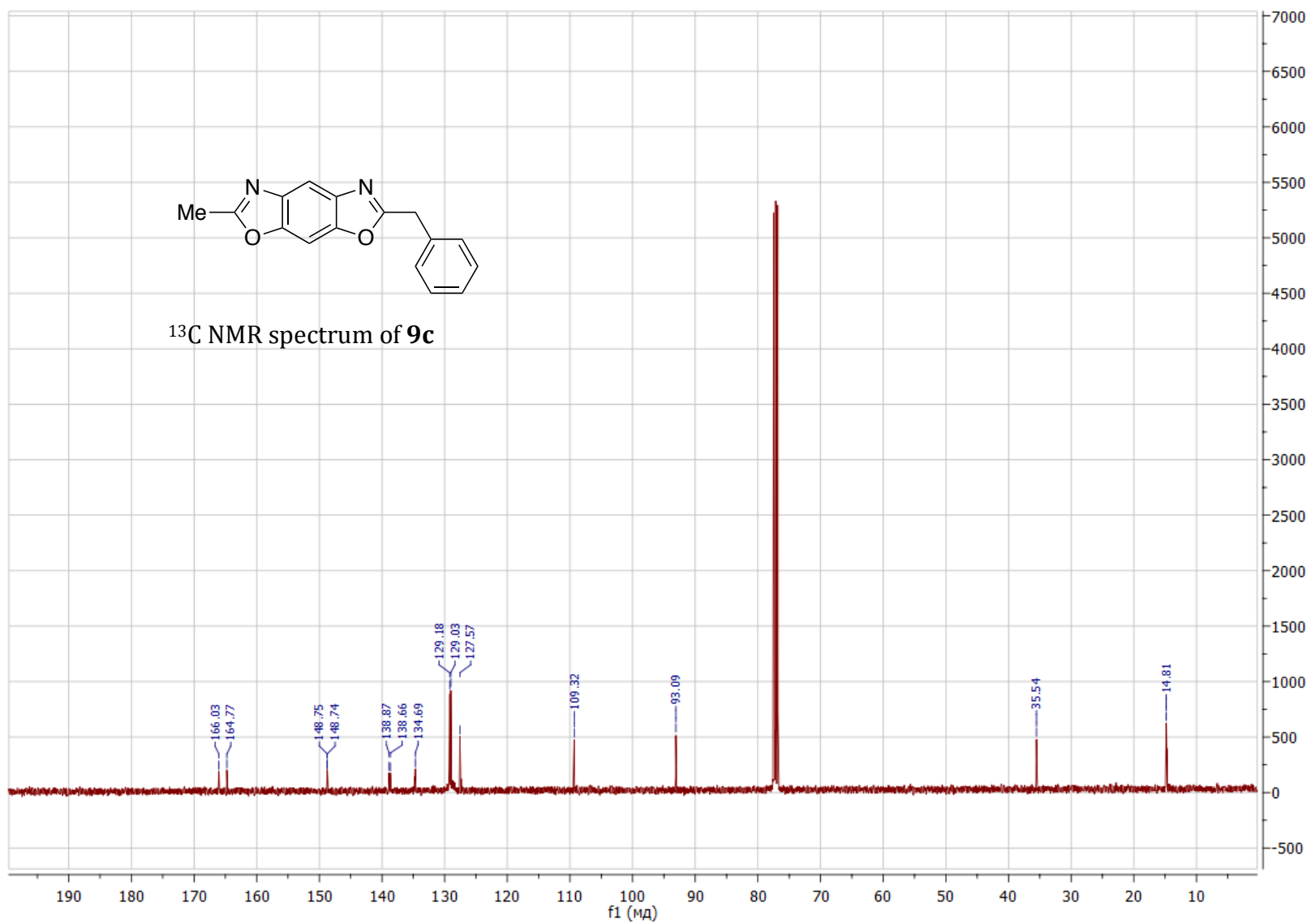


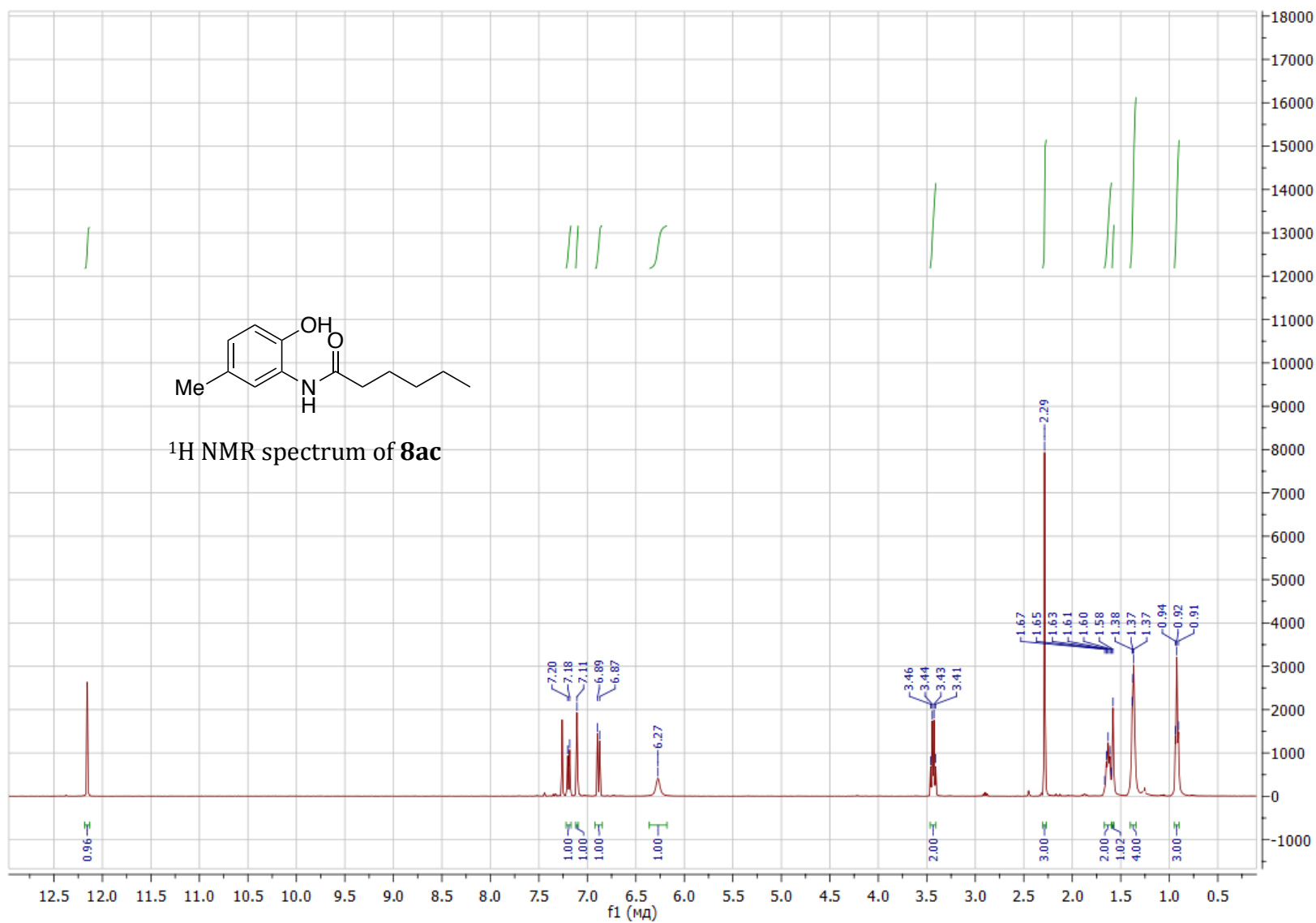


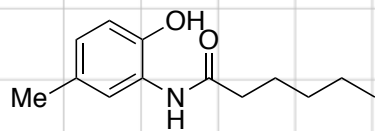
^{13}C NMR spectrum of **9b**



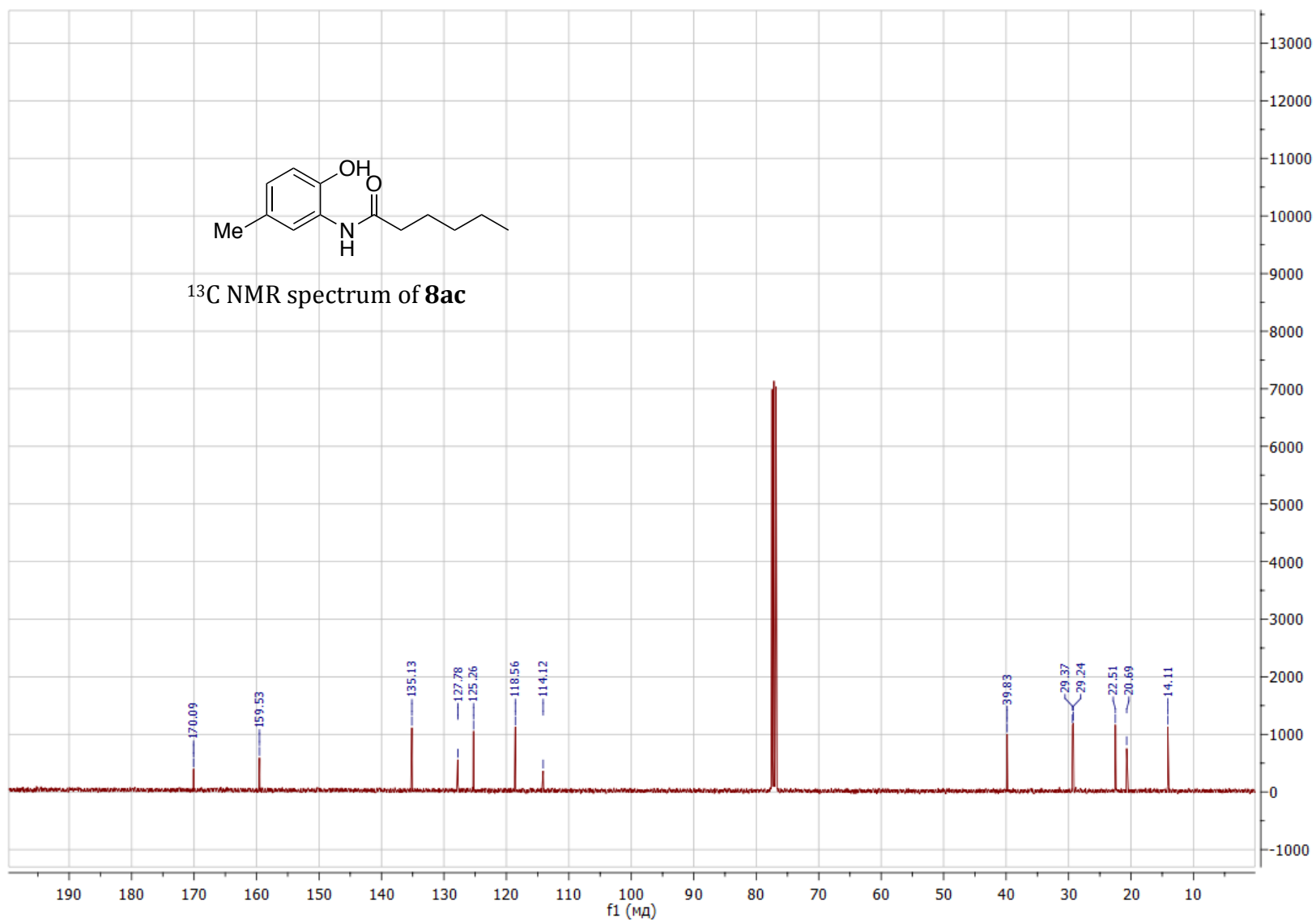


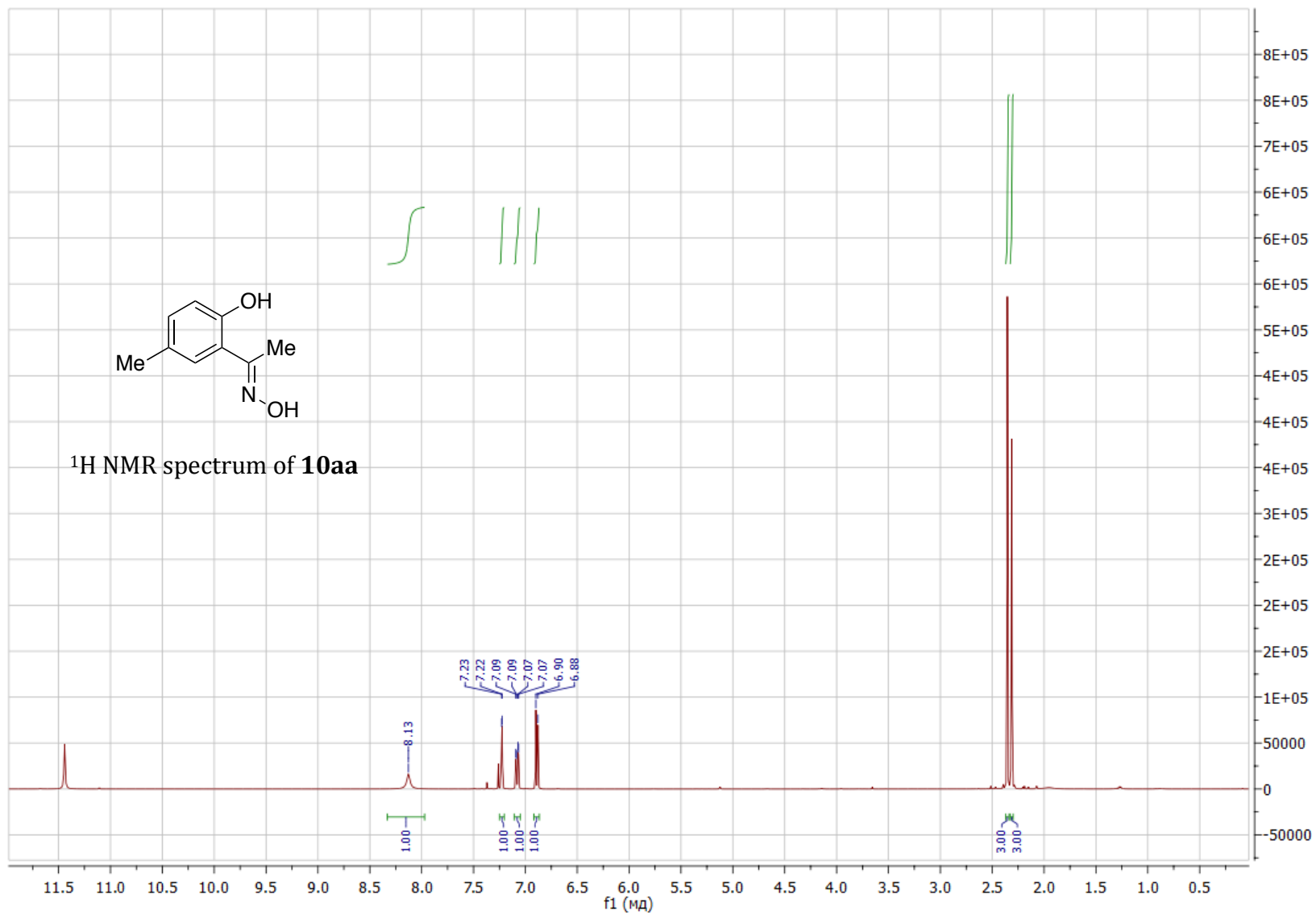


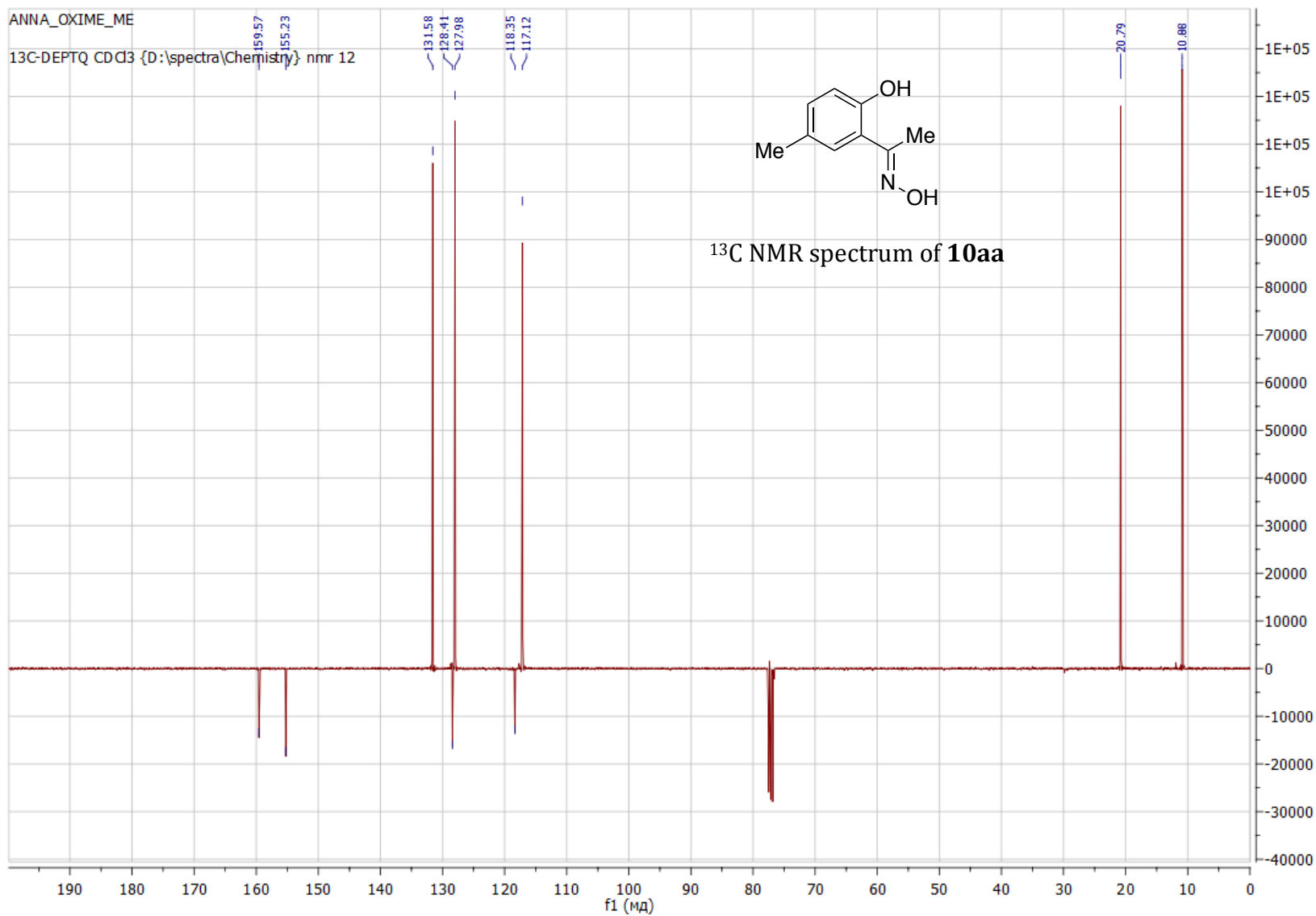


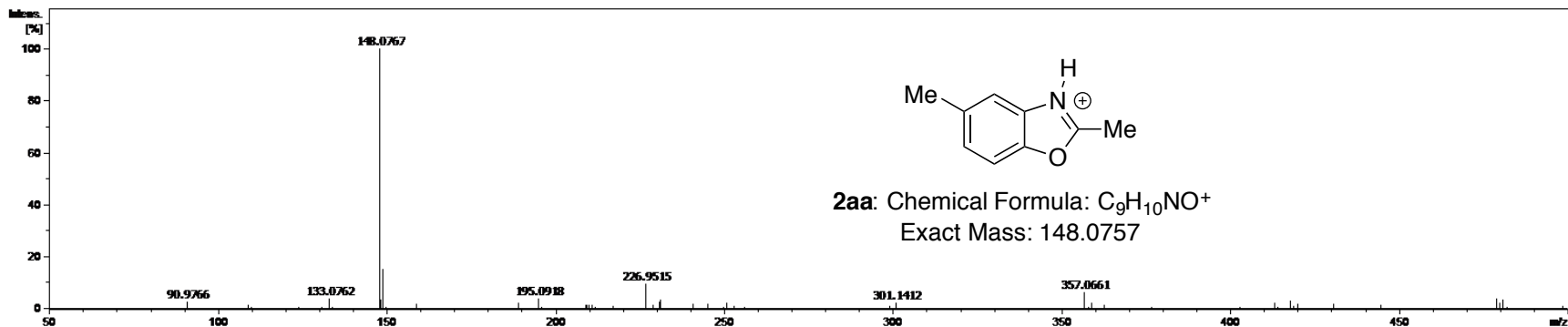


^{13}C NMR spectrum of **8ac**







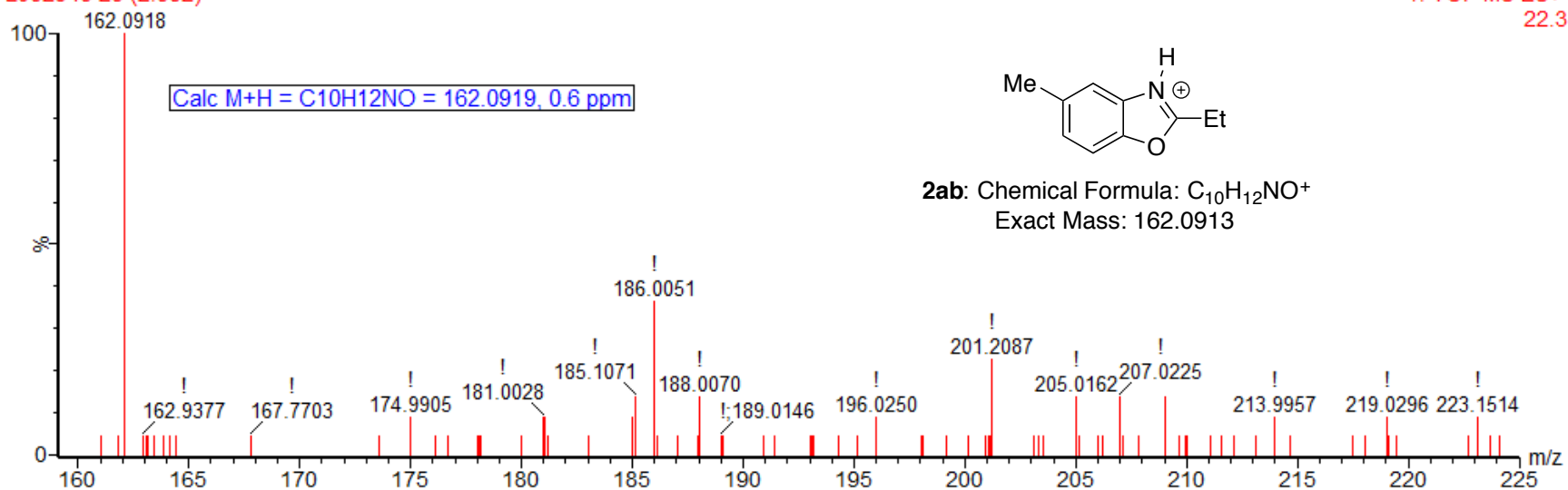


HRMS (ES TOF) Spectral Charts

NA034

L052945 25 (2.582)

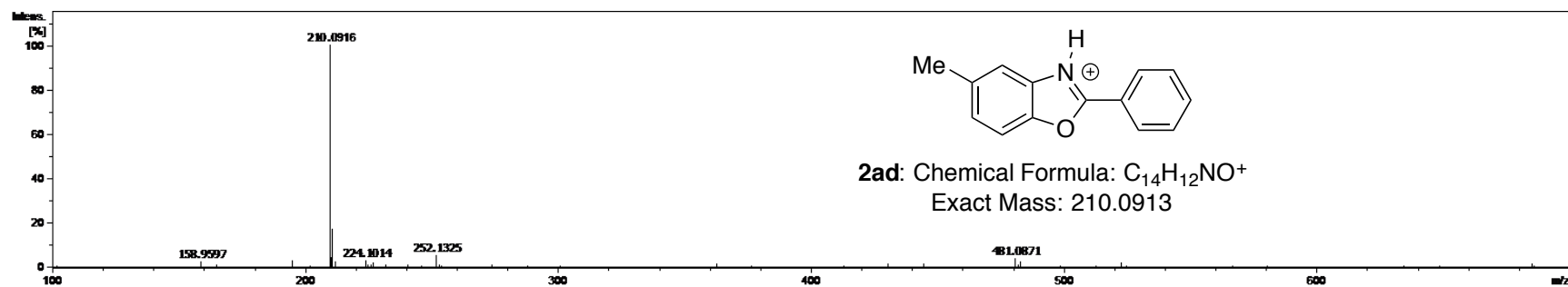
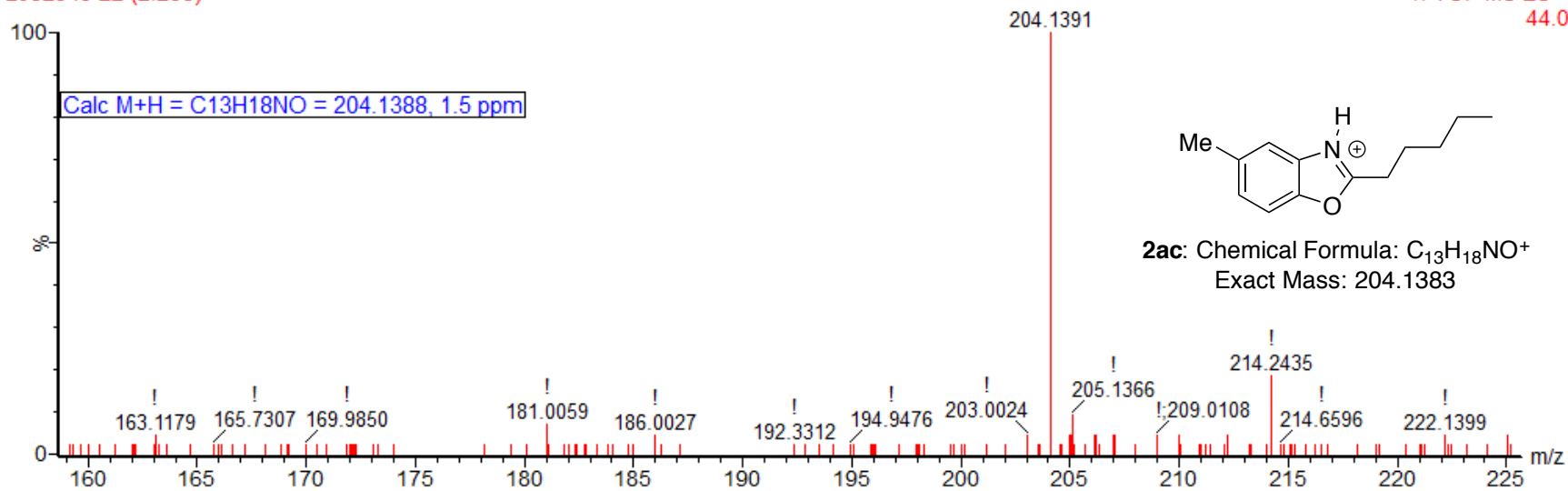
1: TOF MS ES+
22.3

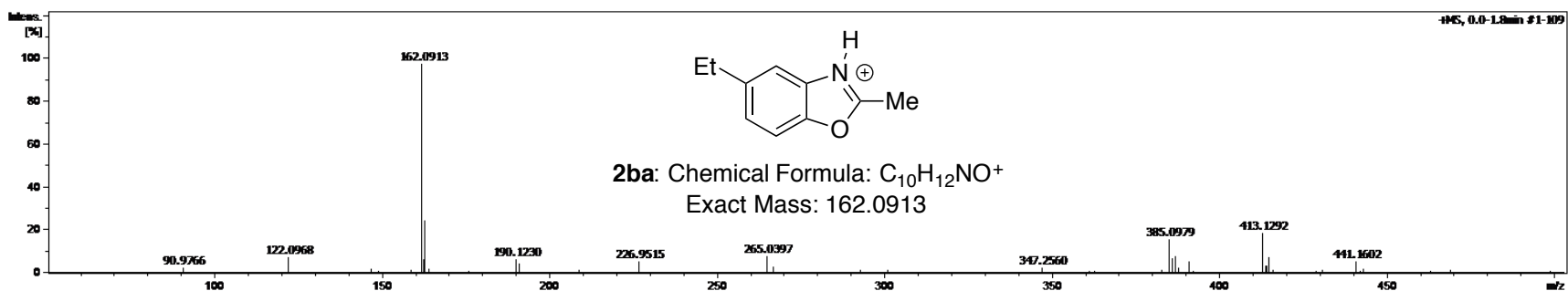
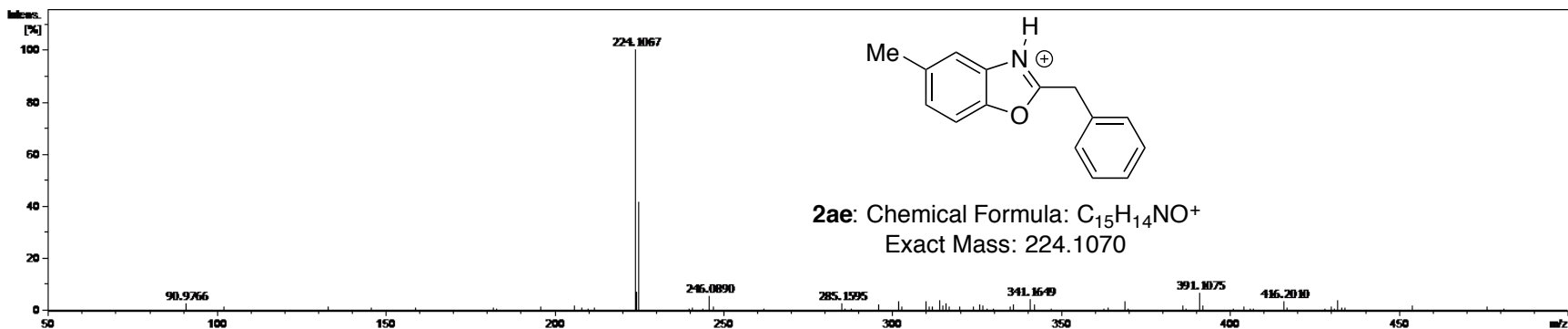


NA064

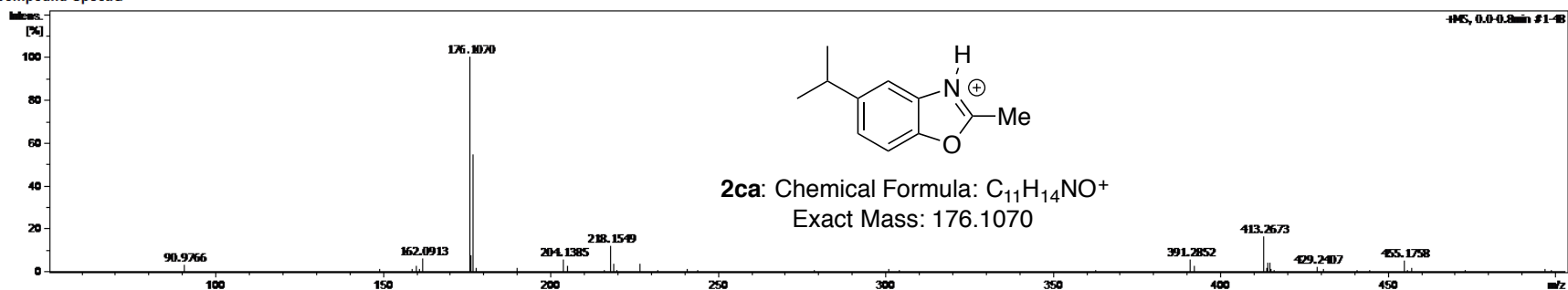
L052949 22 (2.236)

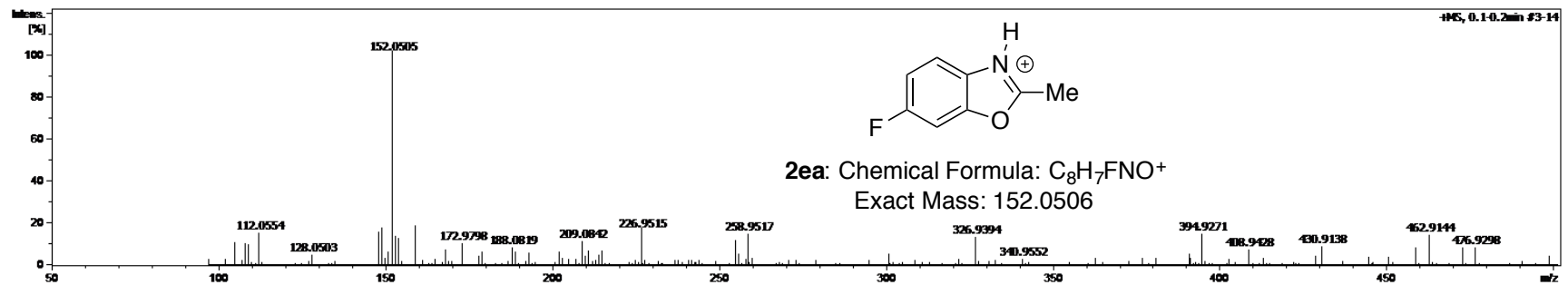
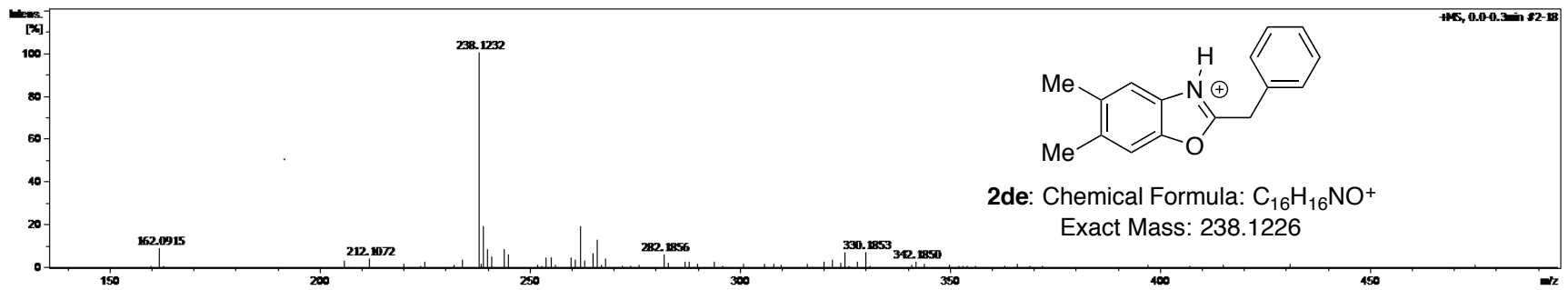
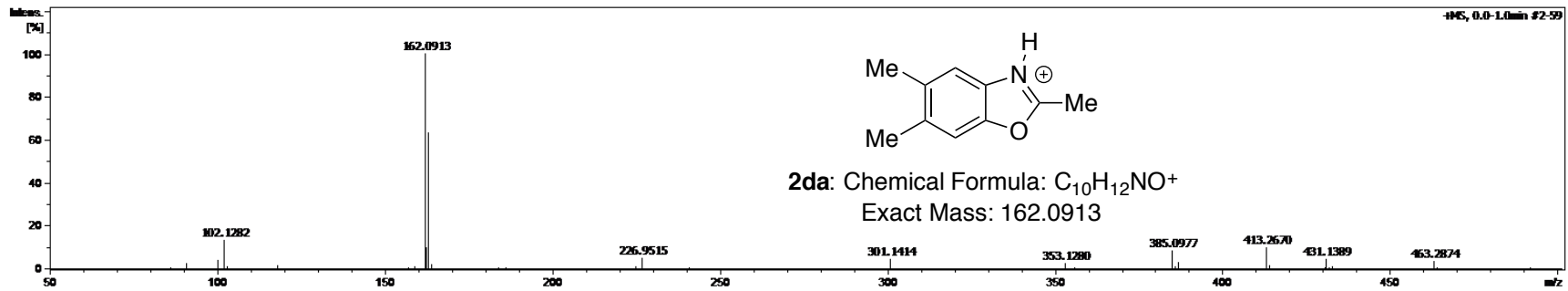
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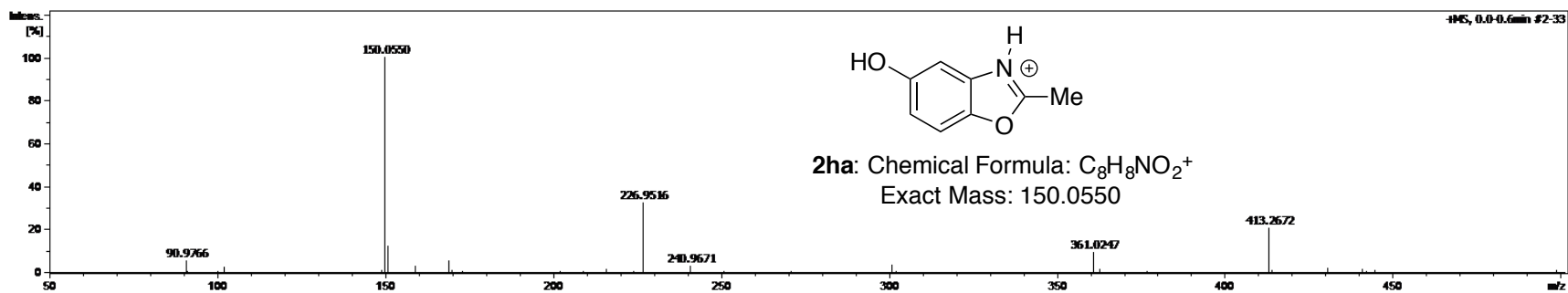
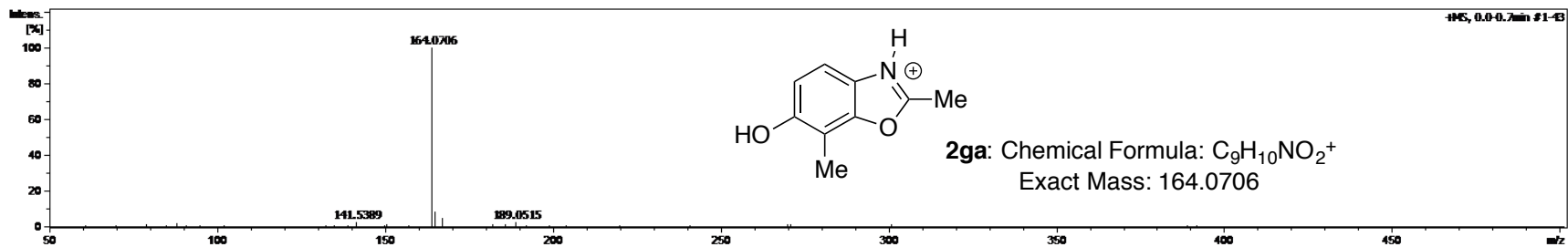
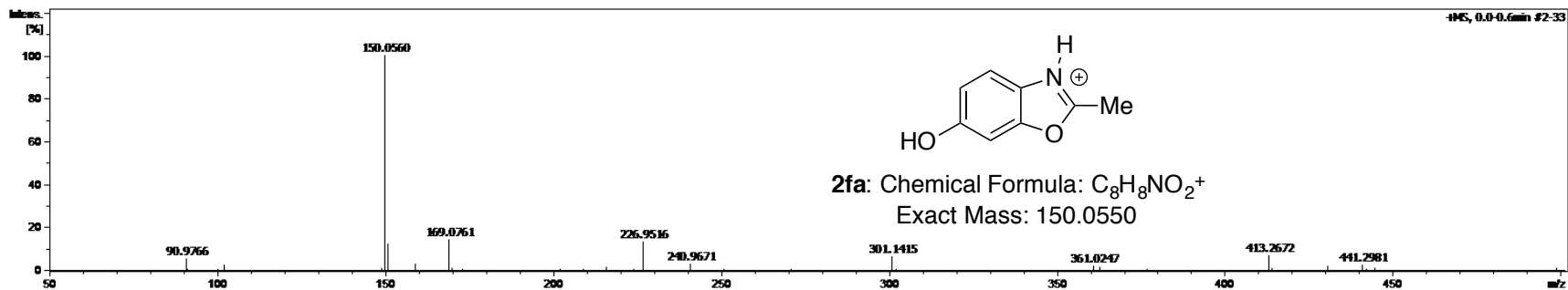


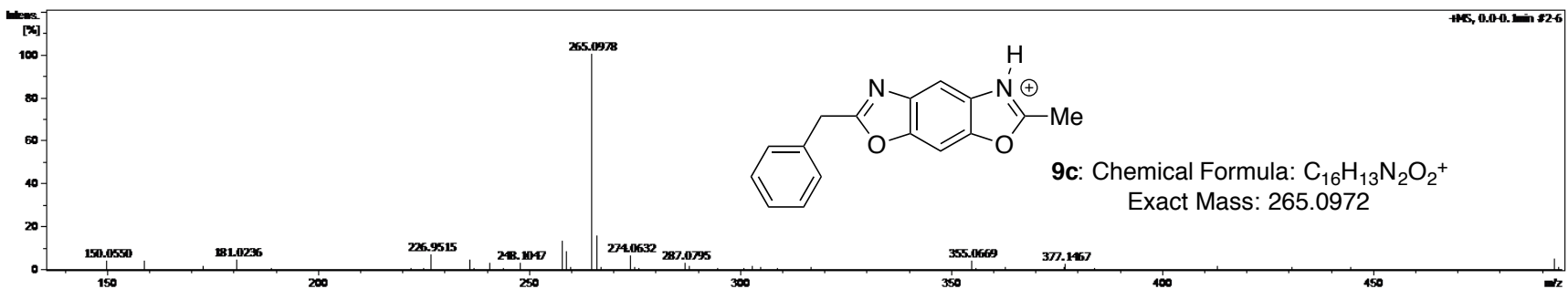
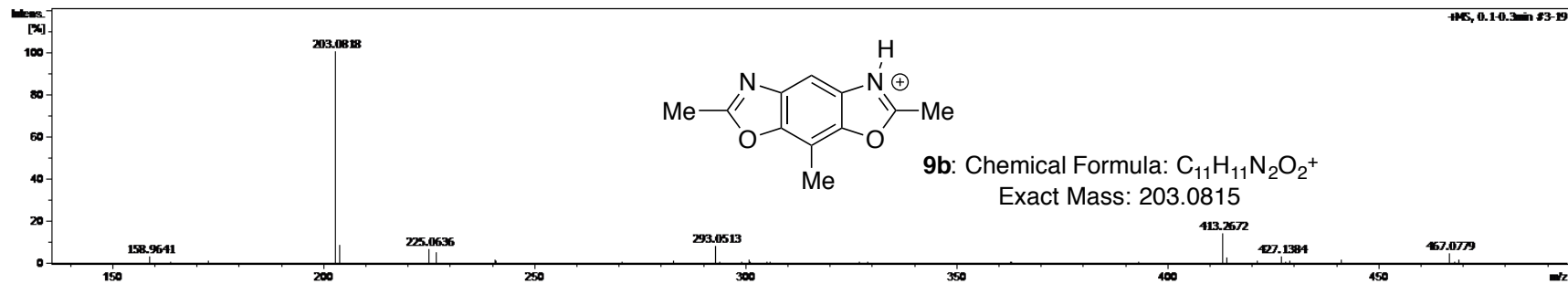
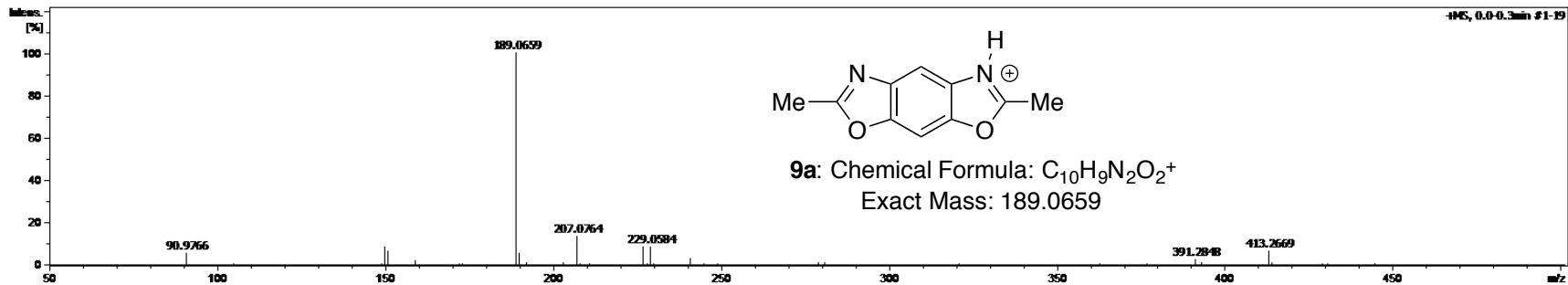


Compound Spectra





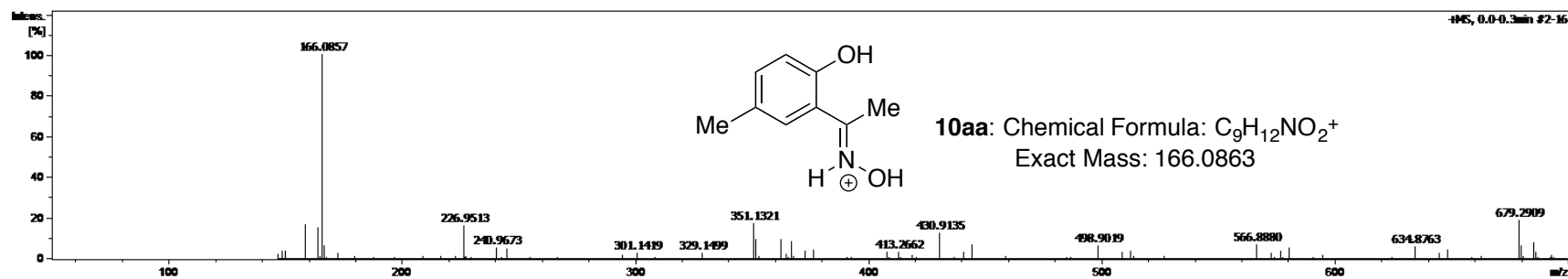
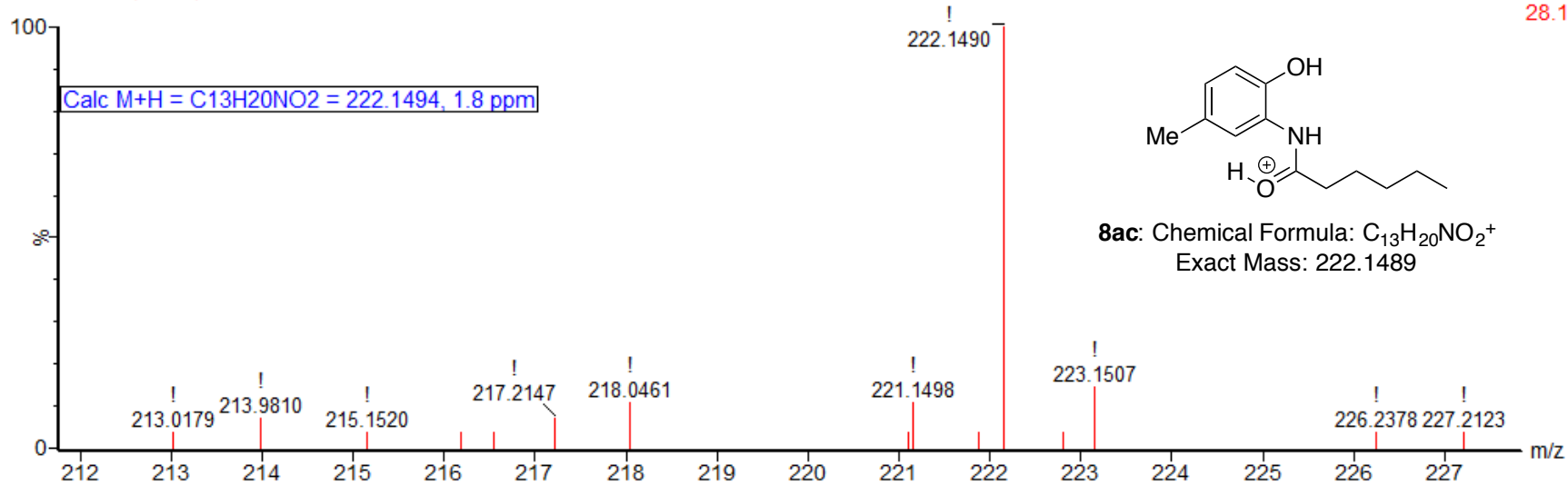




NA042

L052947 33 (3.409)

1: TOF MS ES+
28.1



ORTEP Drawings of Crystal Structures

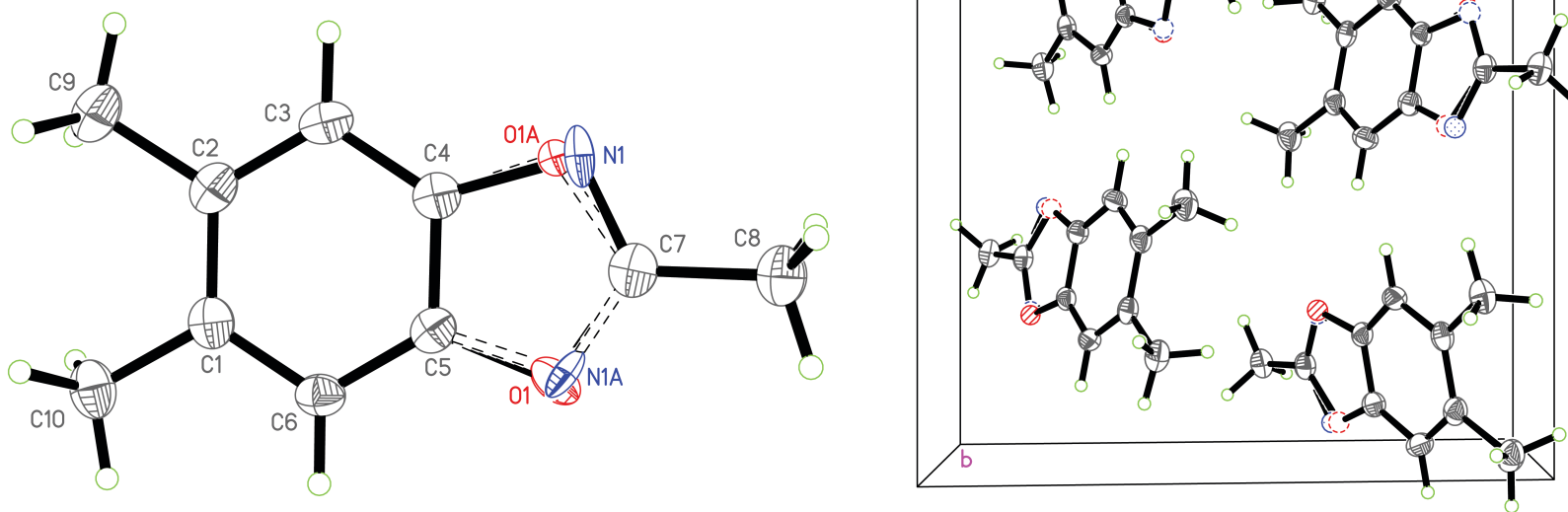


Figure 1. ORTEP drawing of 2,5,6-trimethylbenzo[d]oxazole (**2da**) showing 50% probability amplitude displacement ellipsoids. Oxygen and nitrogen atoms are shown disordered as this planar molecule can pack in two different ways occupying practically the same space in the crystalline lattice. Packing of the molecules in crystalline lattice cell is also shown.

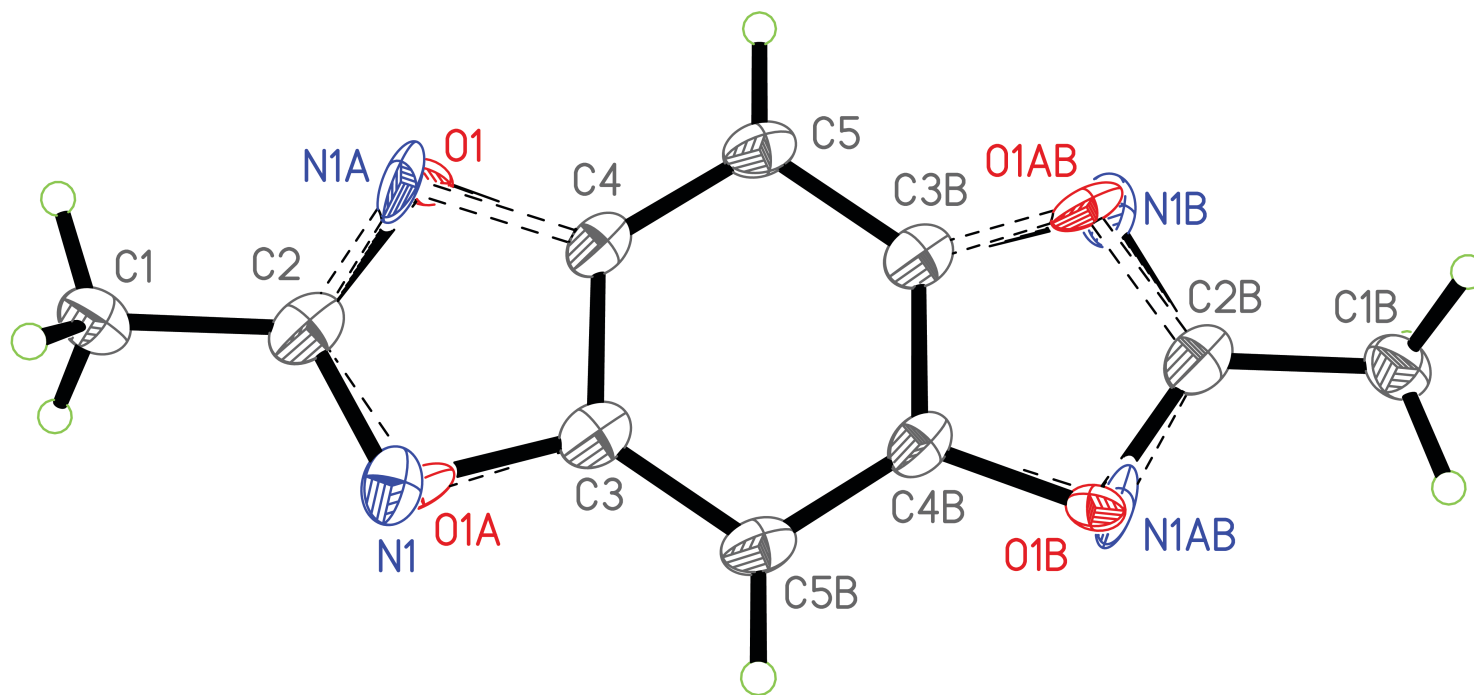


Figure 2. ORTEP drawing of 2,6-dimethylbenzo[1,2-d:5,4-d']bis(oxazole) (**9a**) showing 50% probability amplitude displacement ellipsoids. Oxygen and nitrogen atoms are shown disordered as this planar molecule can pack in two different ways occupying practically the same space in the crystalline lattice.

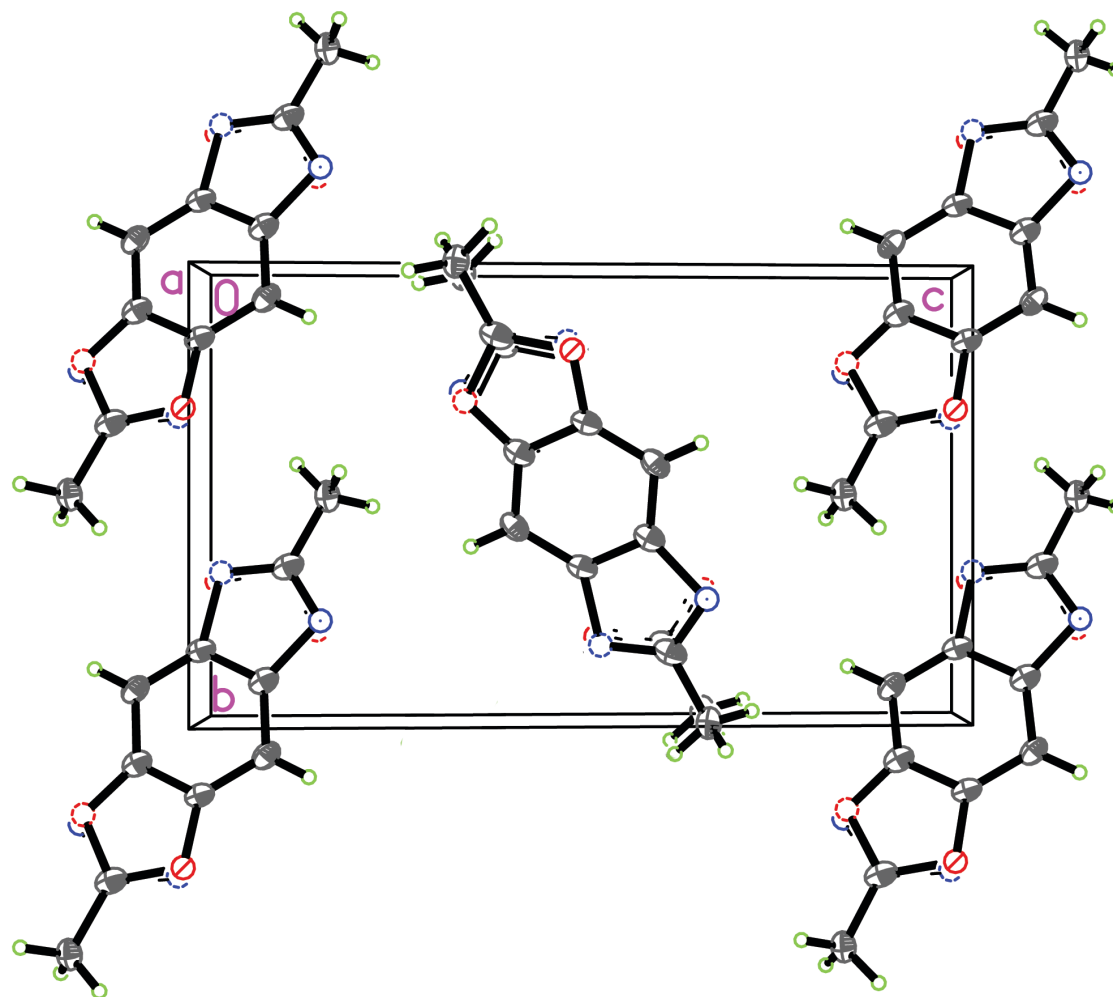


Figure 3. Packing of the molecules of 2,6-dimethylbenzo[1,2-d:5,4-d']bis(oxazole) (**9a**) in crystalline lattice cell is also shown.