

Structure–Activity Relationship Study of 3-Alkynyl-6-aryl-isothiazolo[4,3-*b*]pyridines as Dual Inhibitors of the Lipid Kinases PIKfyve and PIP4K2C

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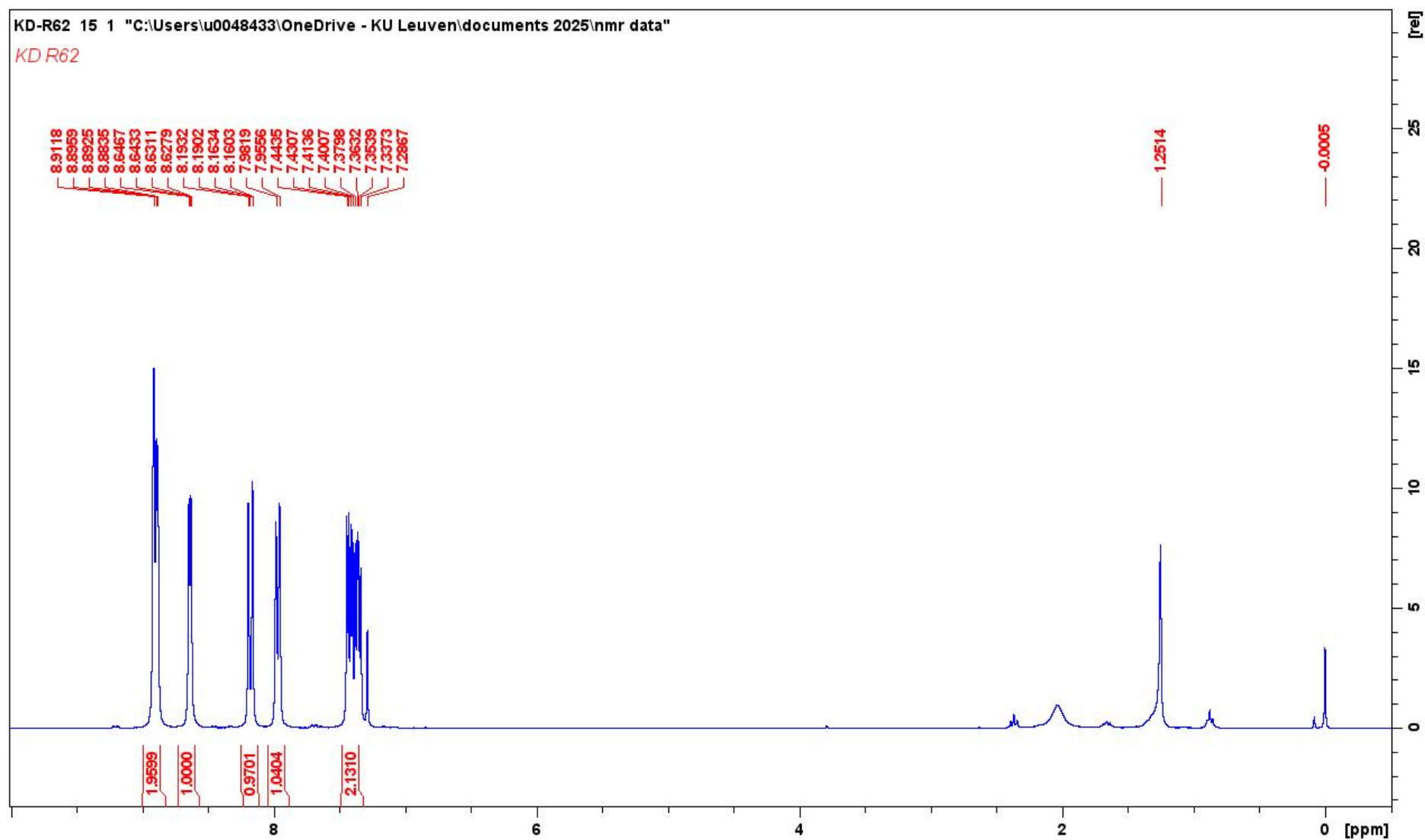
⁵ Molecular, Structural and Translational Virology Research Group, Department of Microbiology, Immunology and Transplantation, Rega Institute for Medical Research, KU Leuven, Herestraat 49, Box 1043, 3000 Leuven, Belgium; dominique.schols@kuleuven.be

⁶ Department of Microbiology and Immunology, Stanford University School of Medicine, Stanford, CA 94305, USA

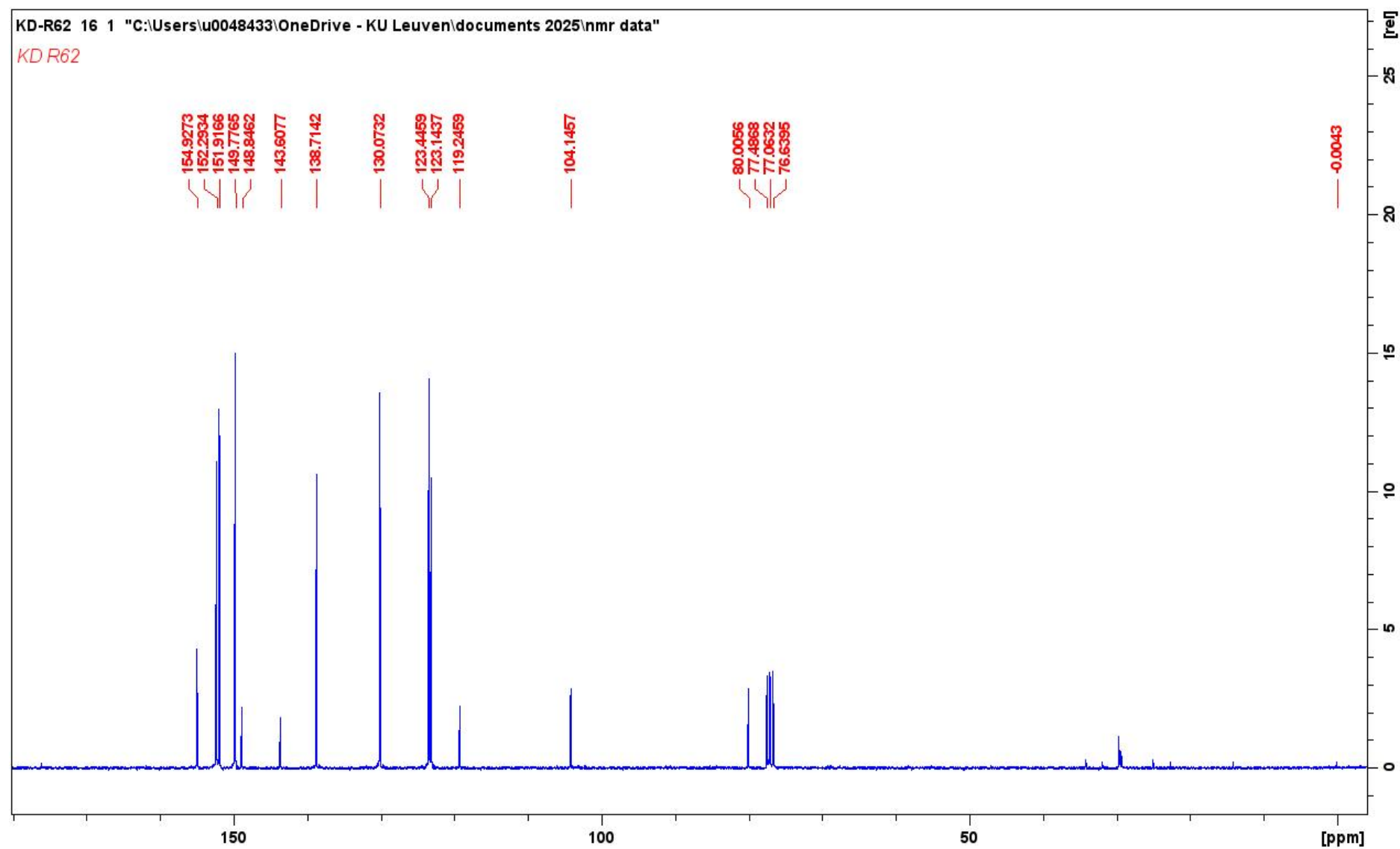
⁷ Chan Zuckerberg Biohub, San Francisco, CA 94305, USA

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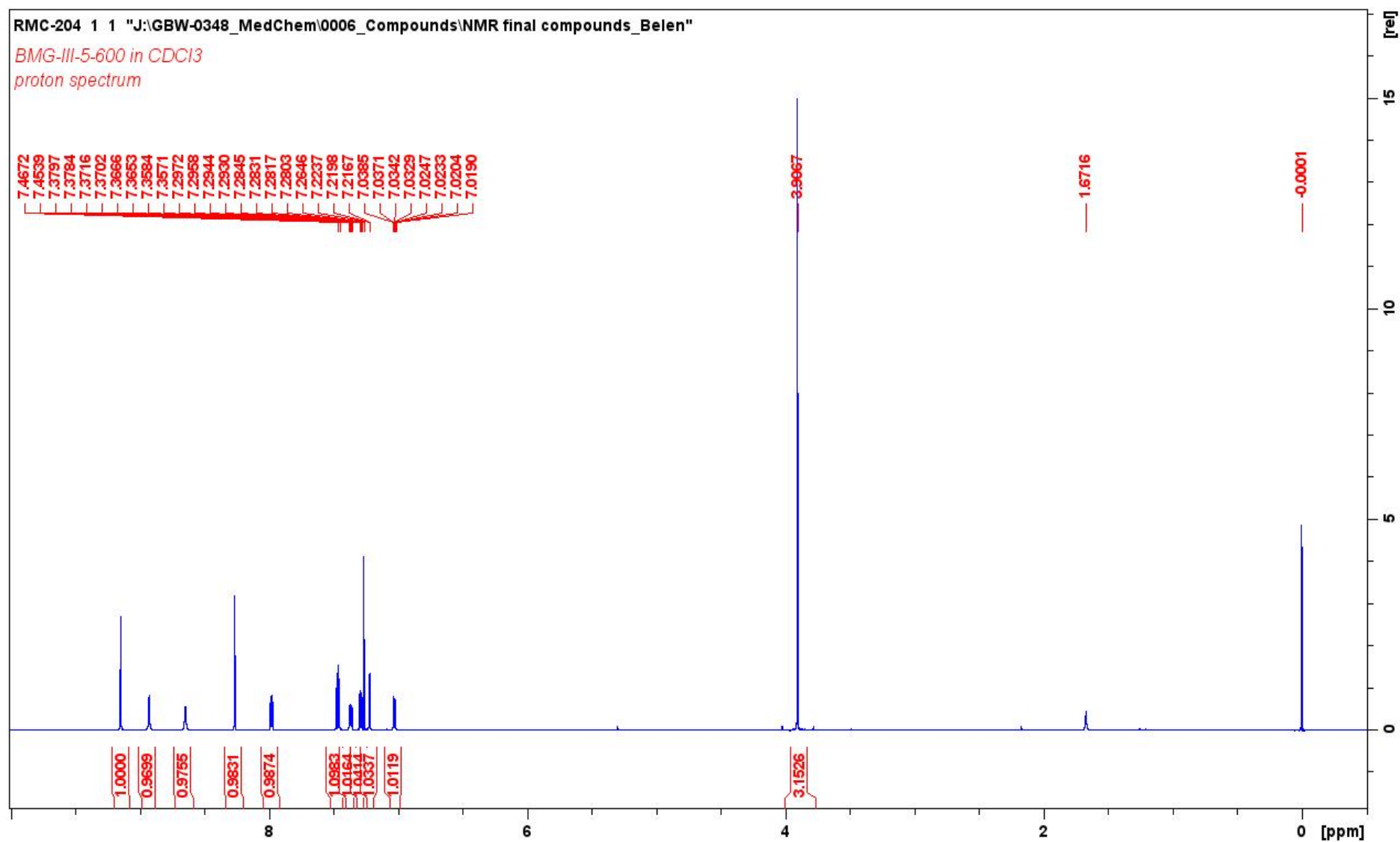
¹H NMR spectrum of 2a



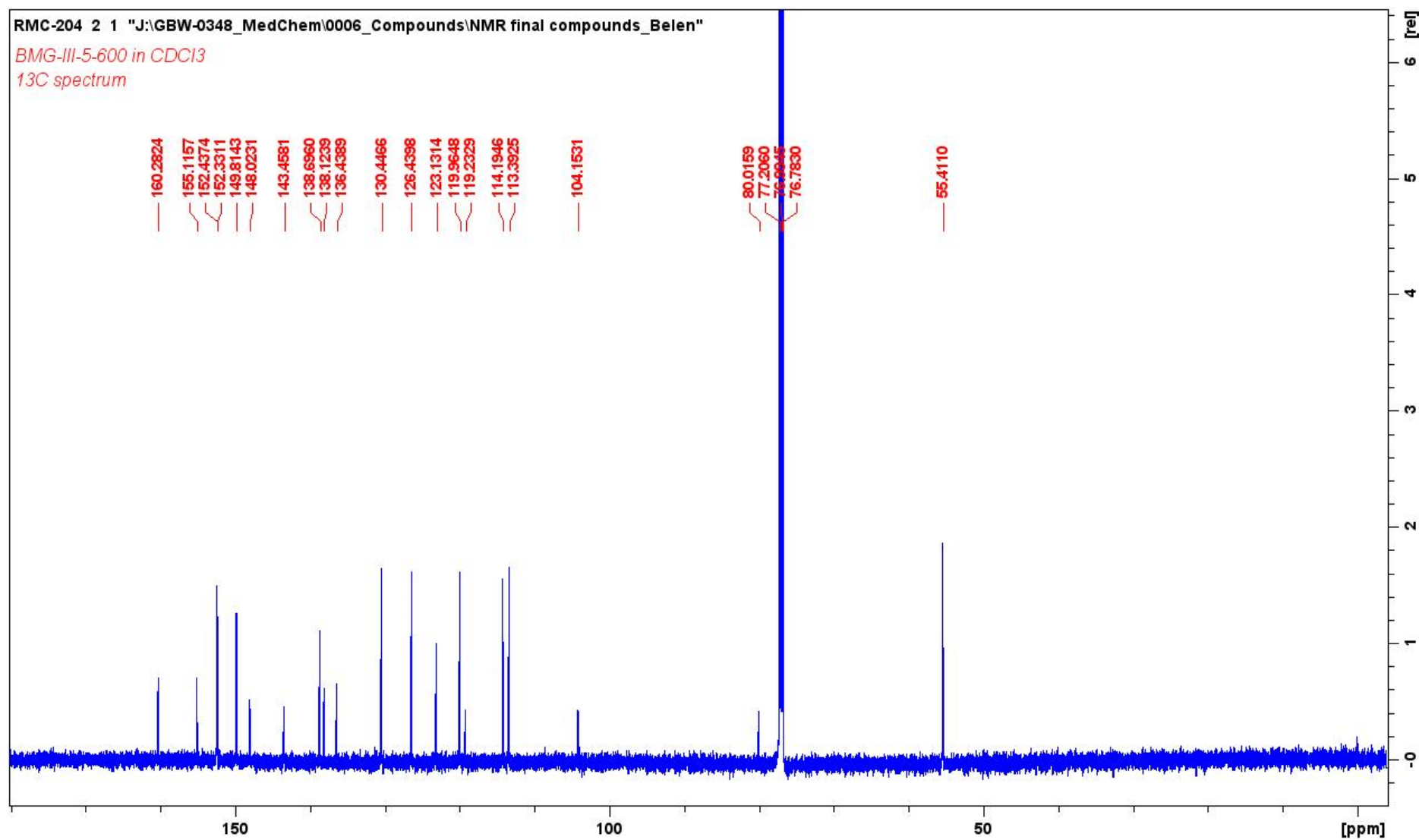
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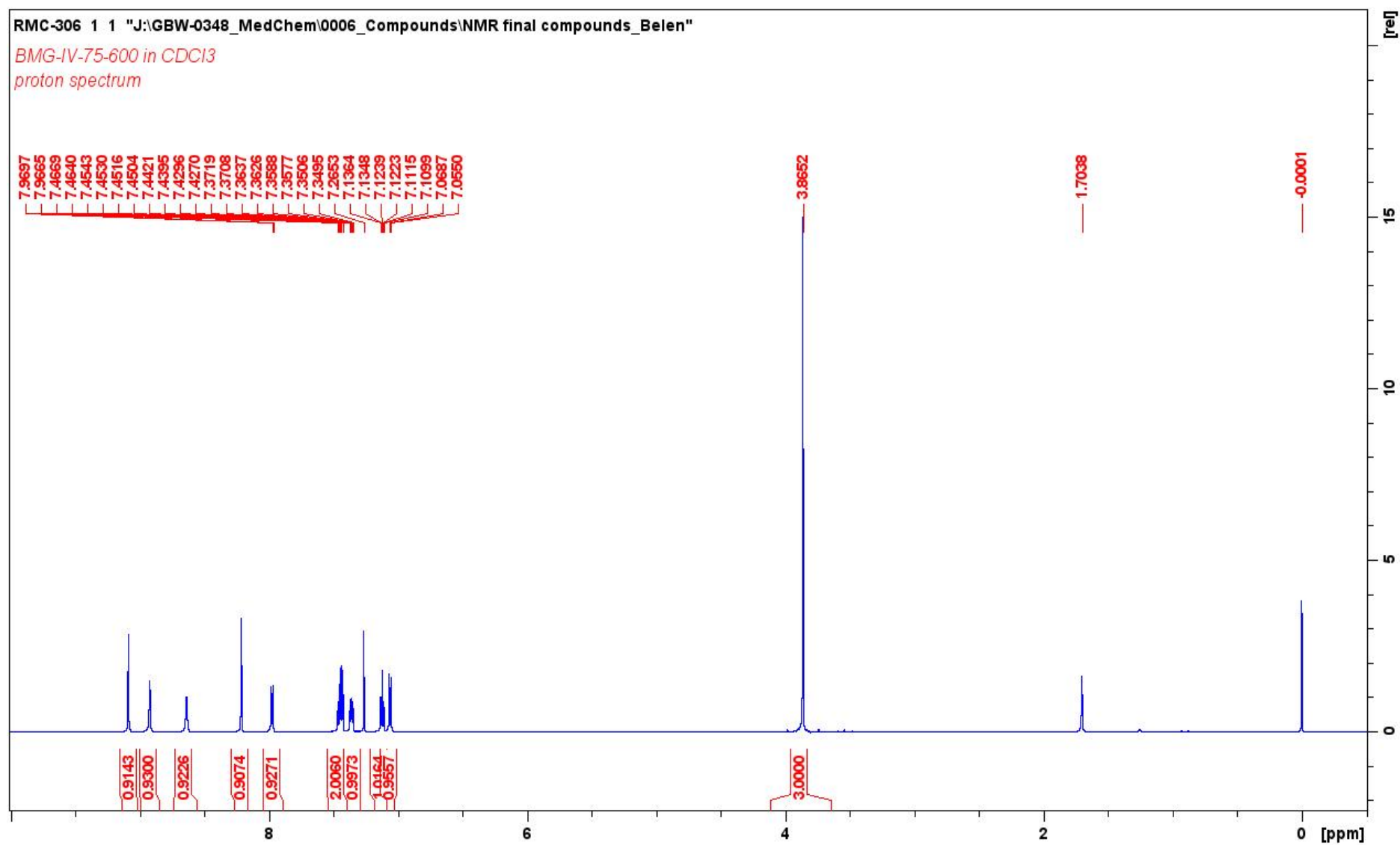
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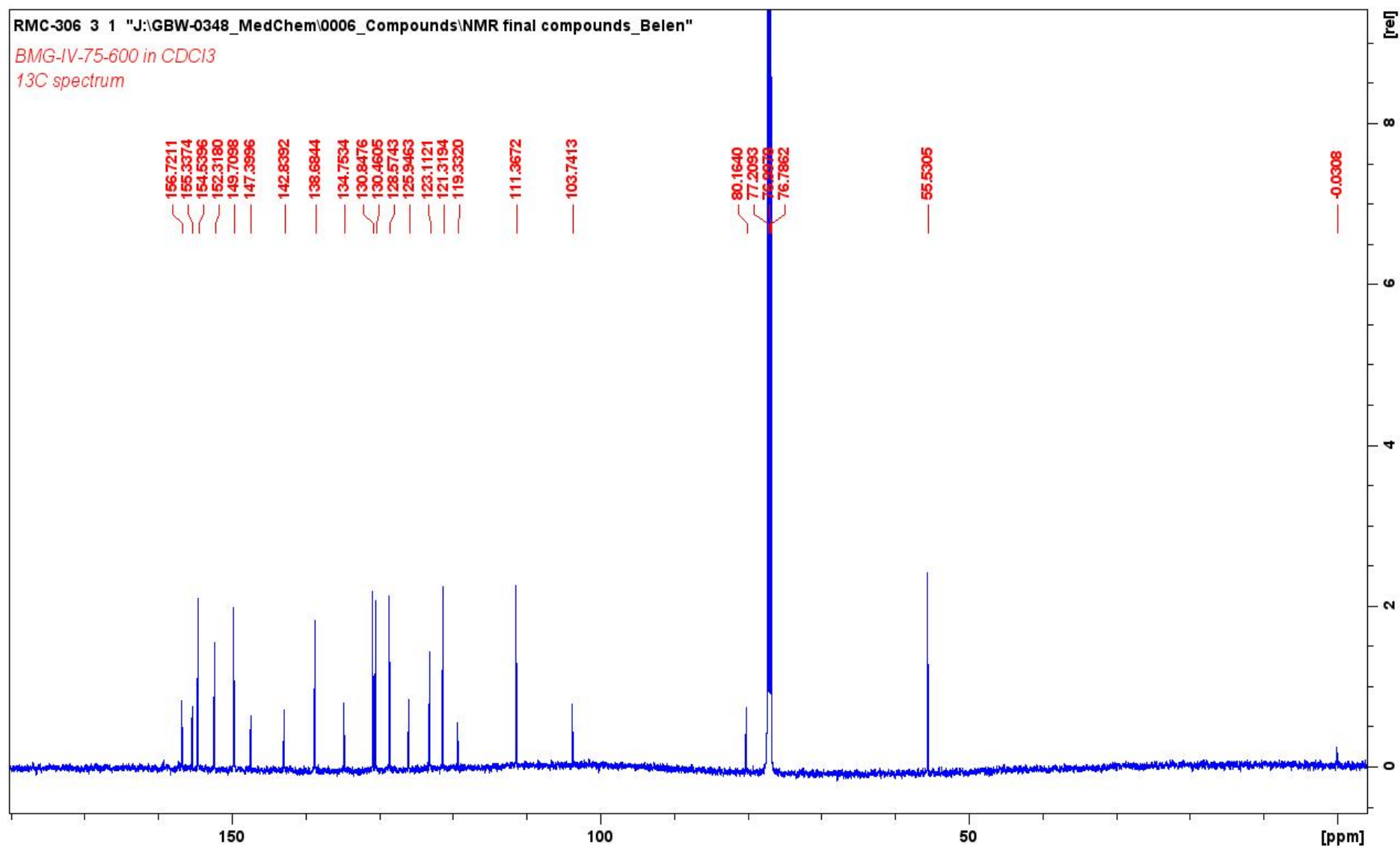
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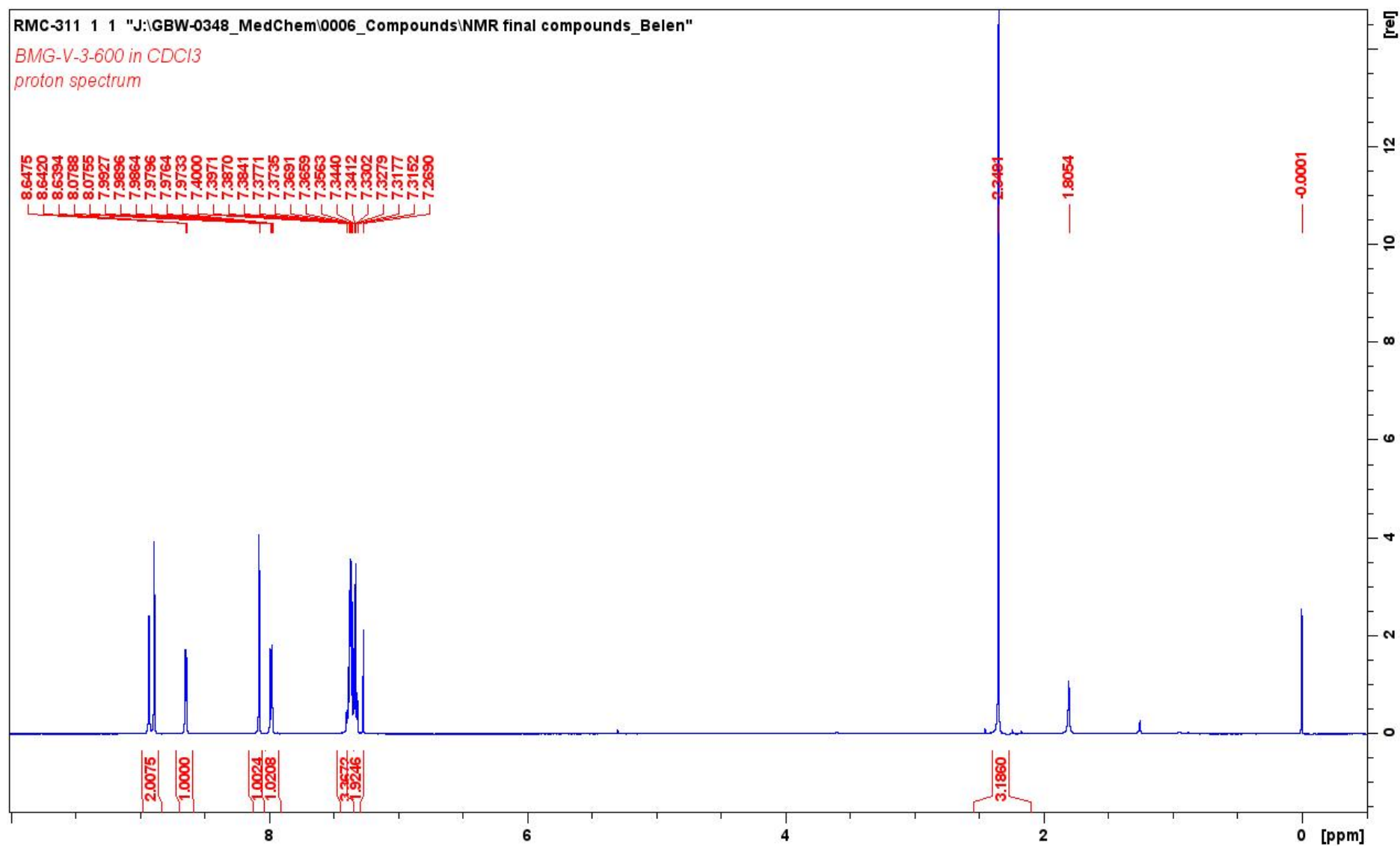
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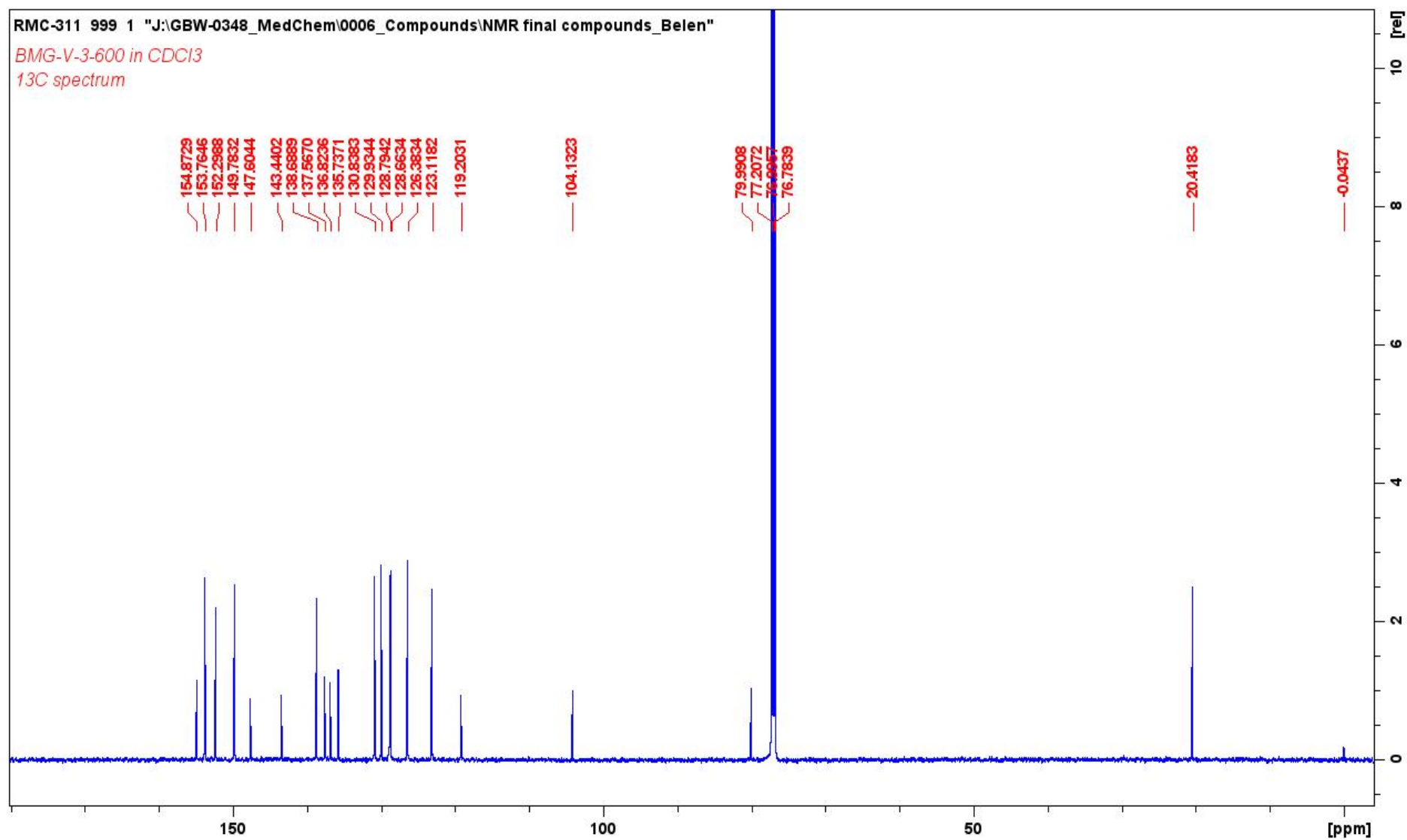
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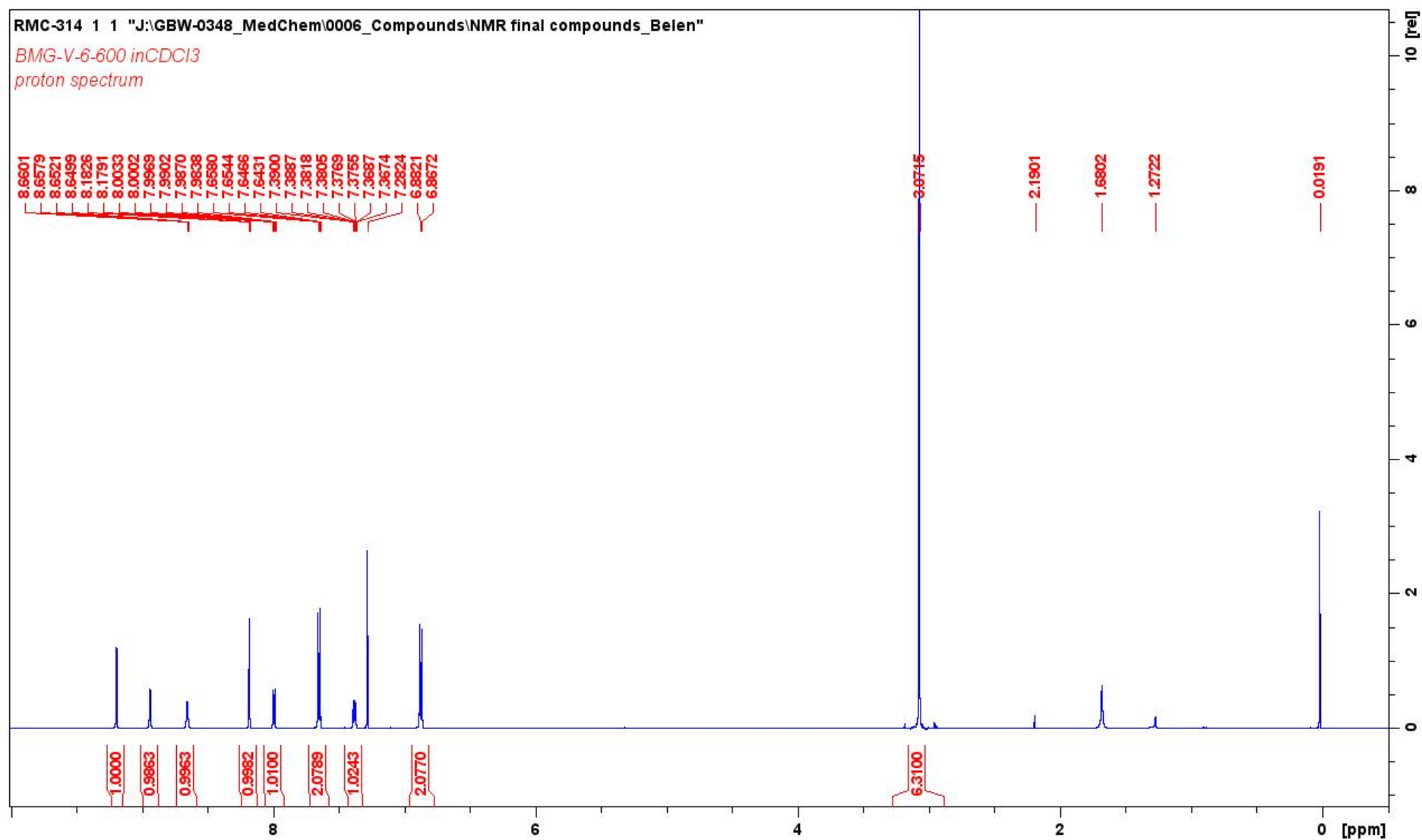
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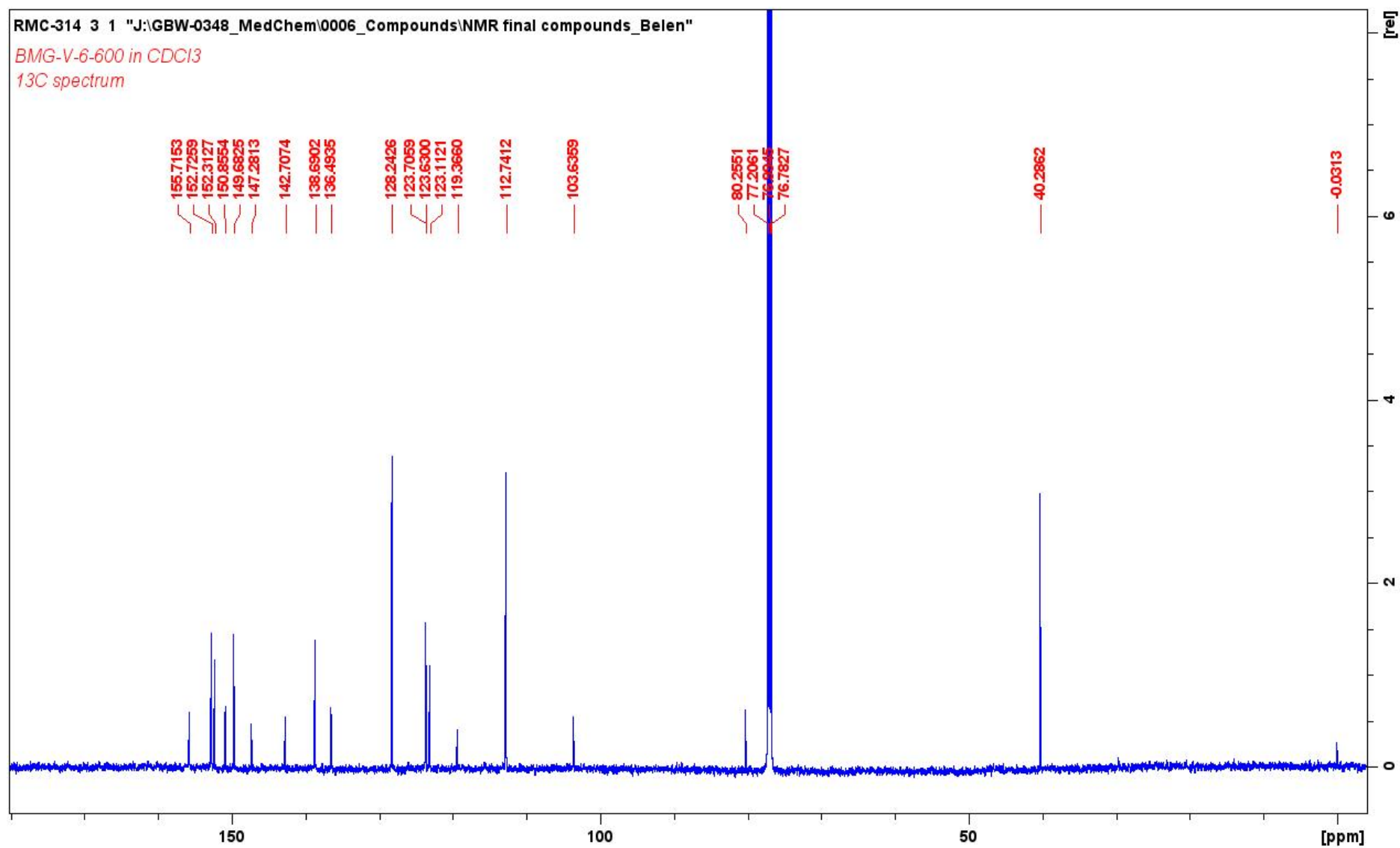
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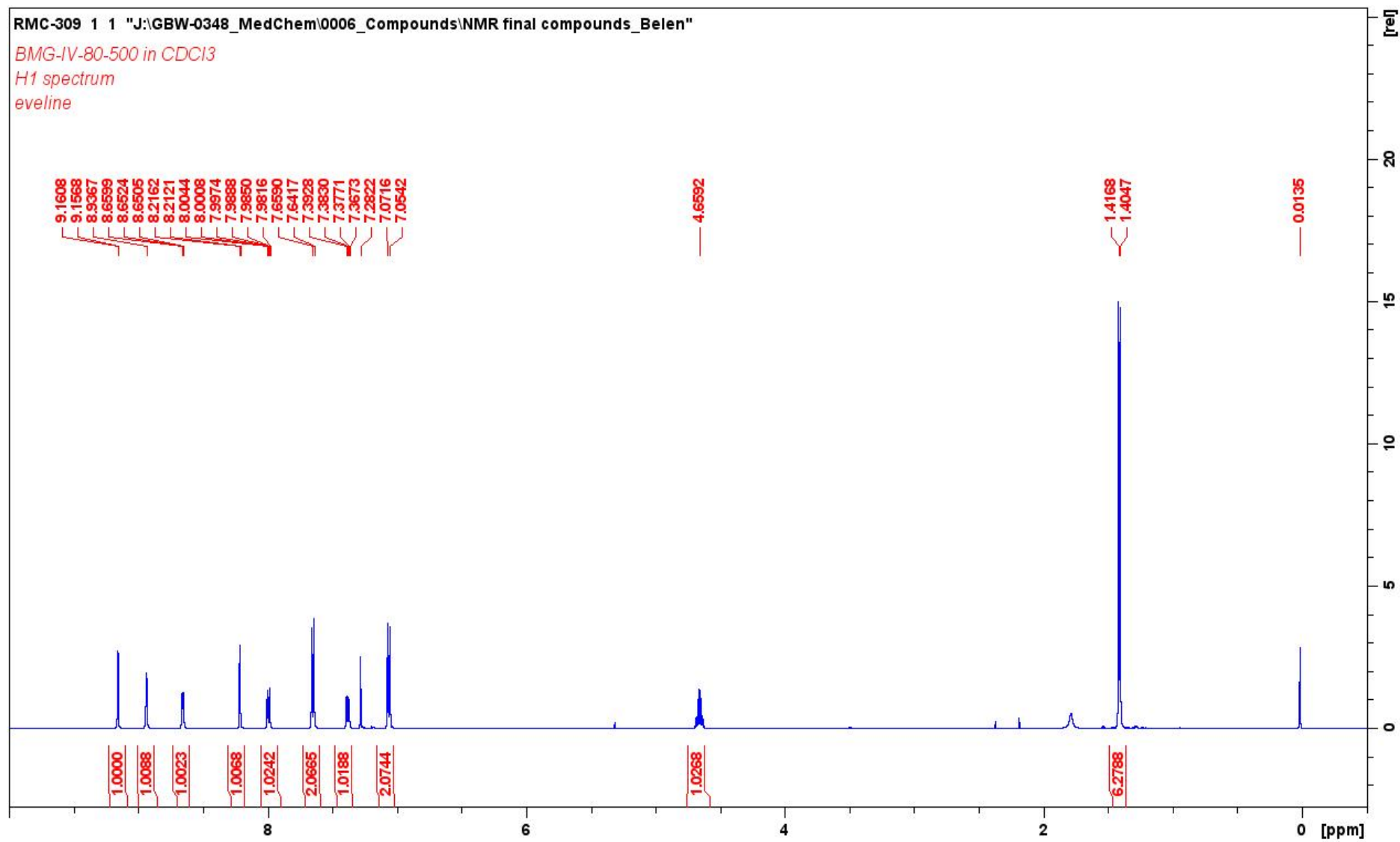
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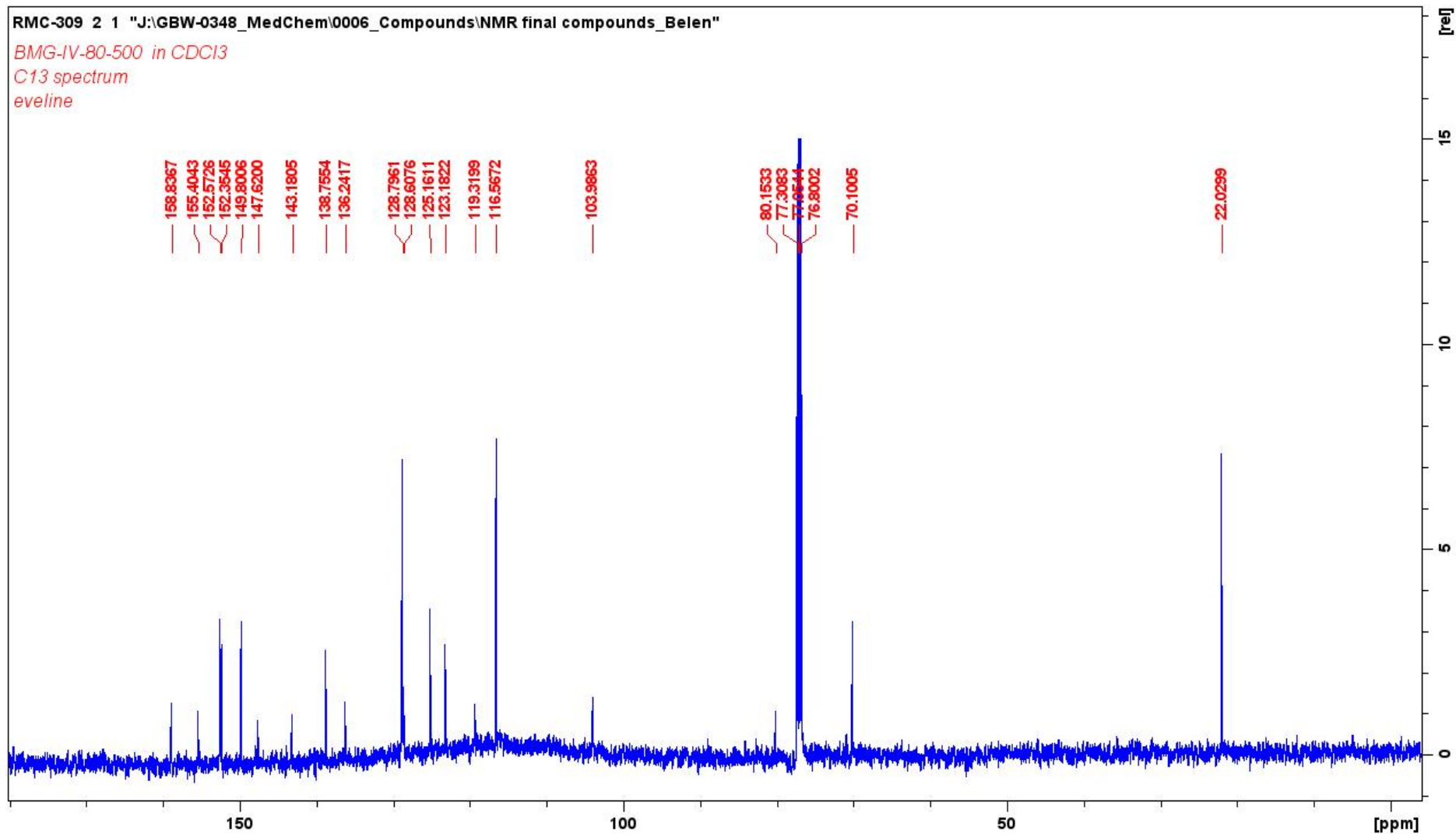
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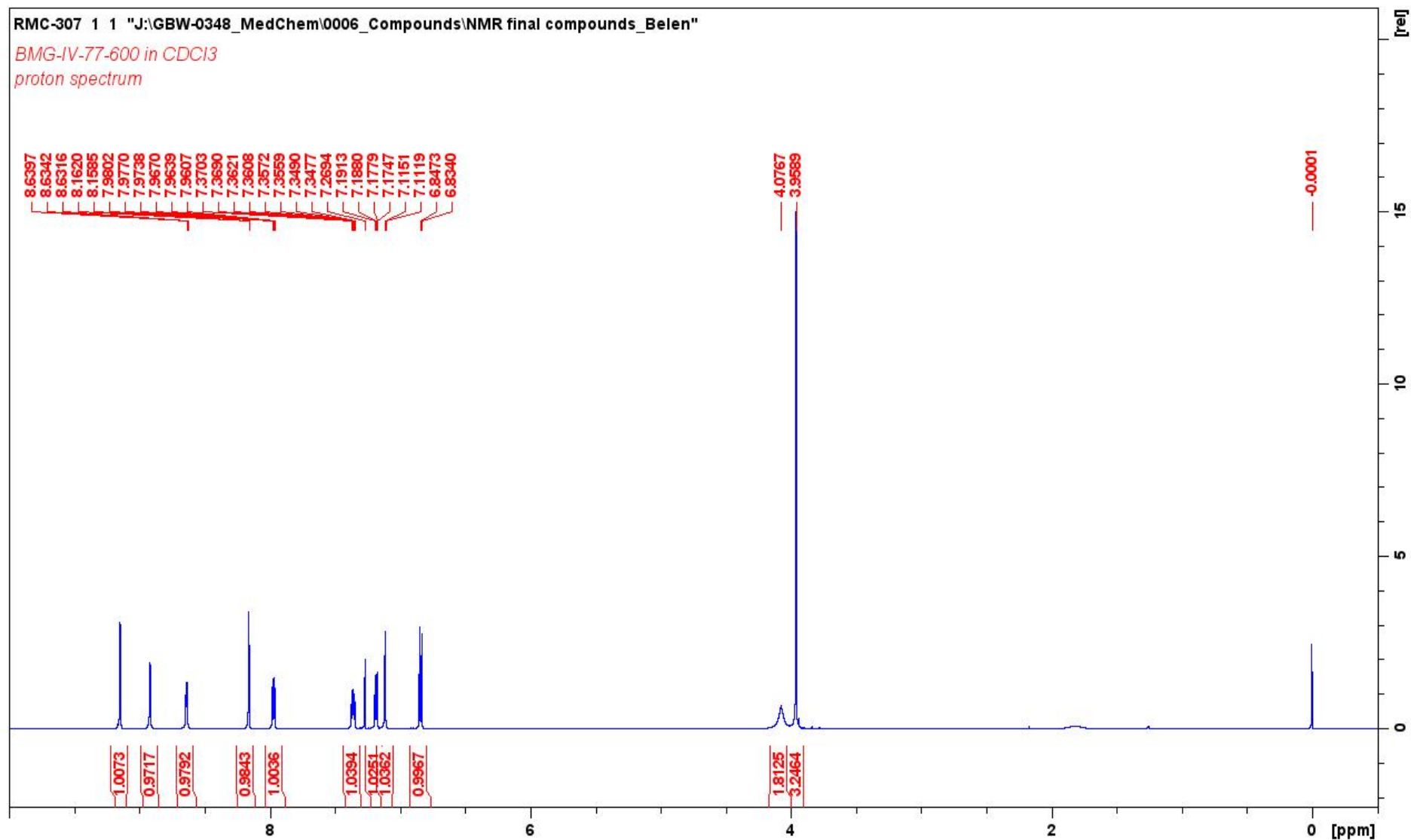
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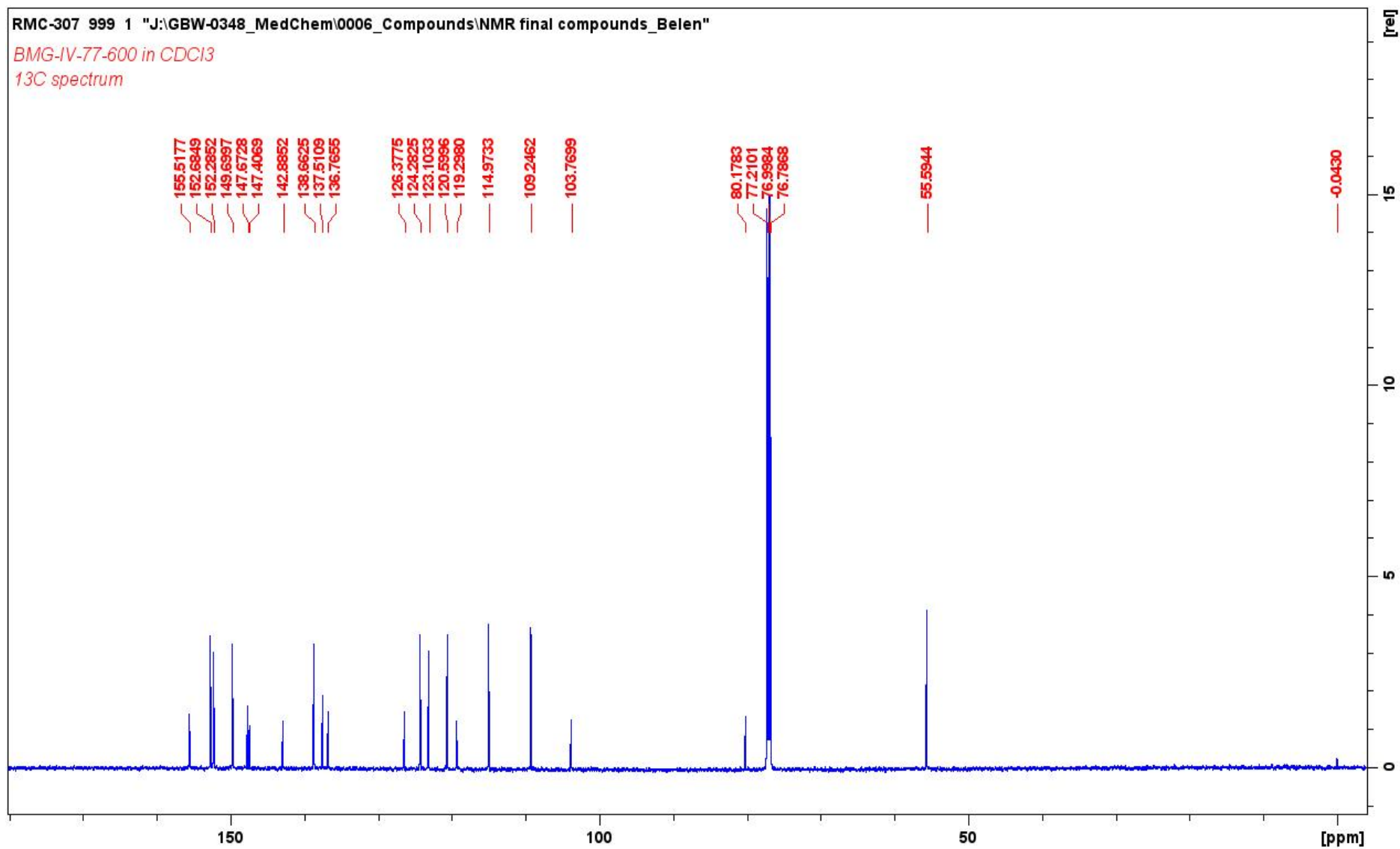
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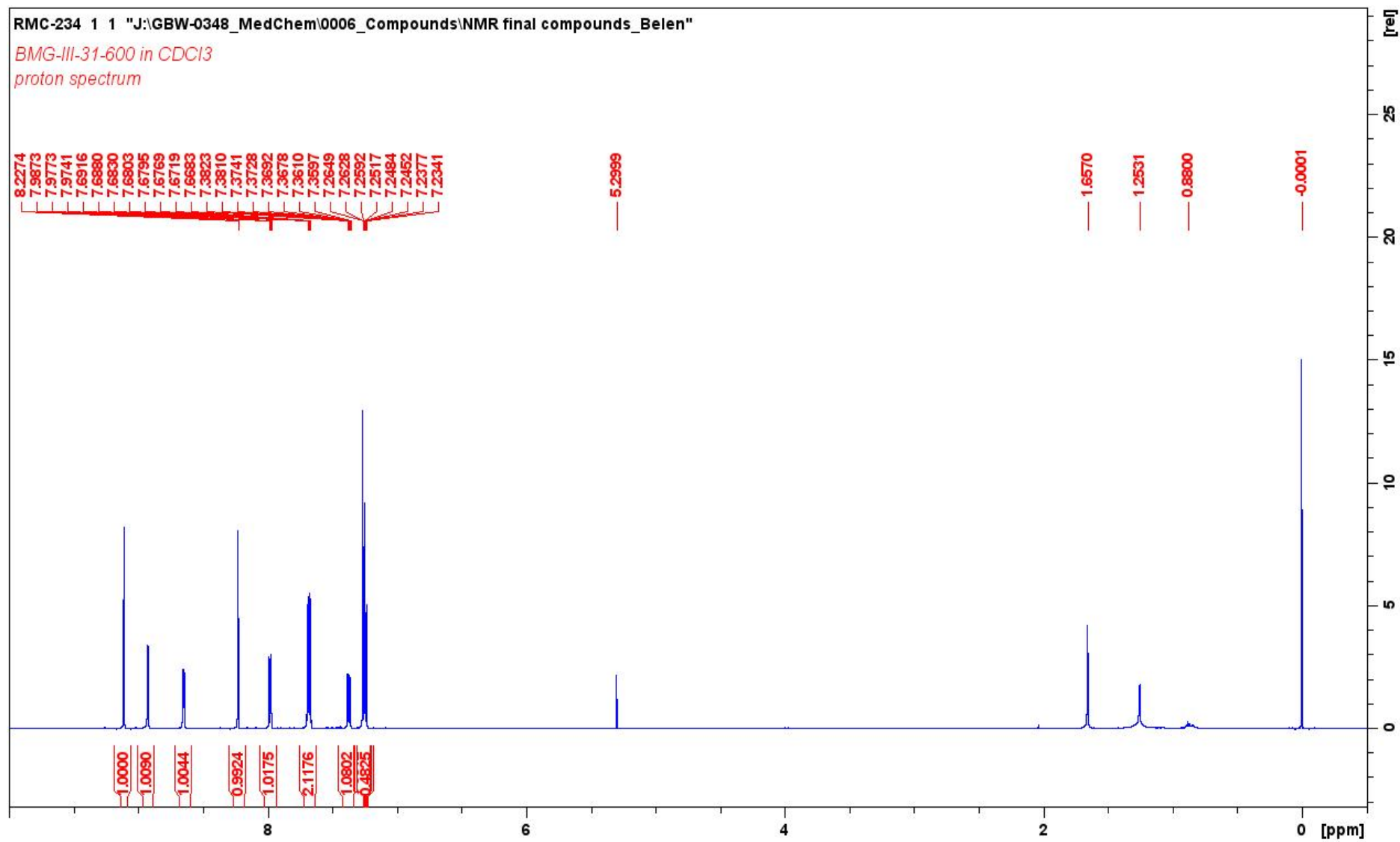
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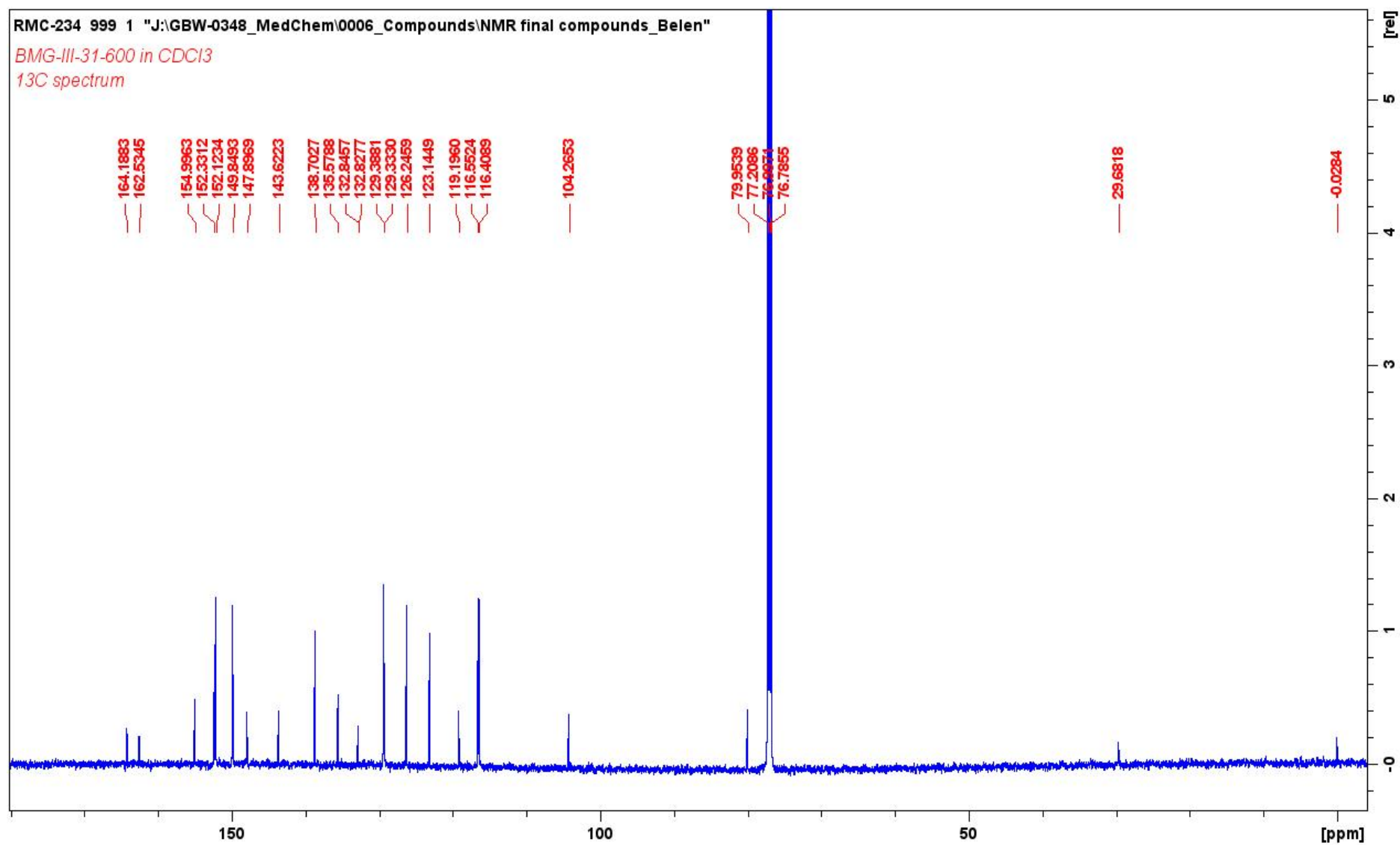
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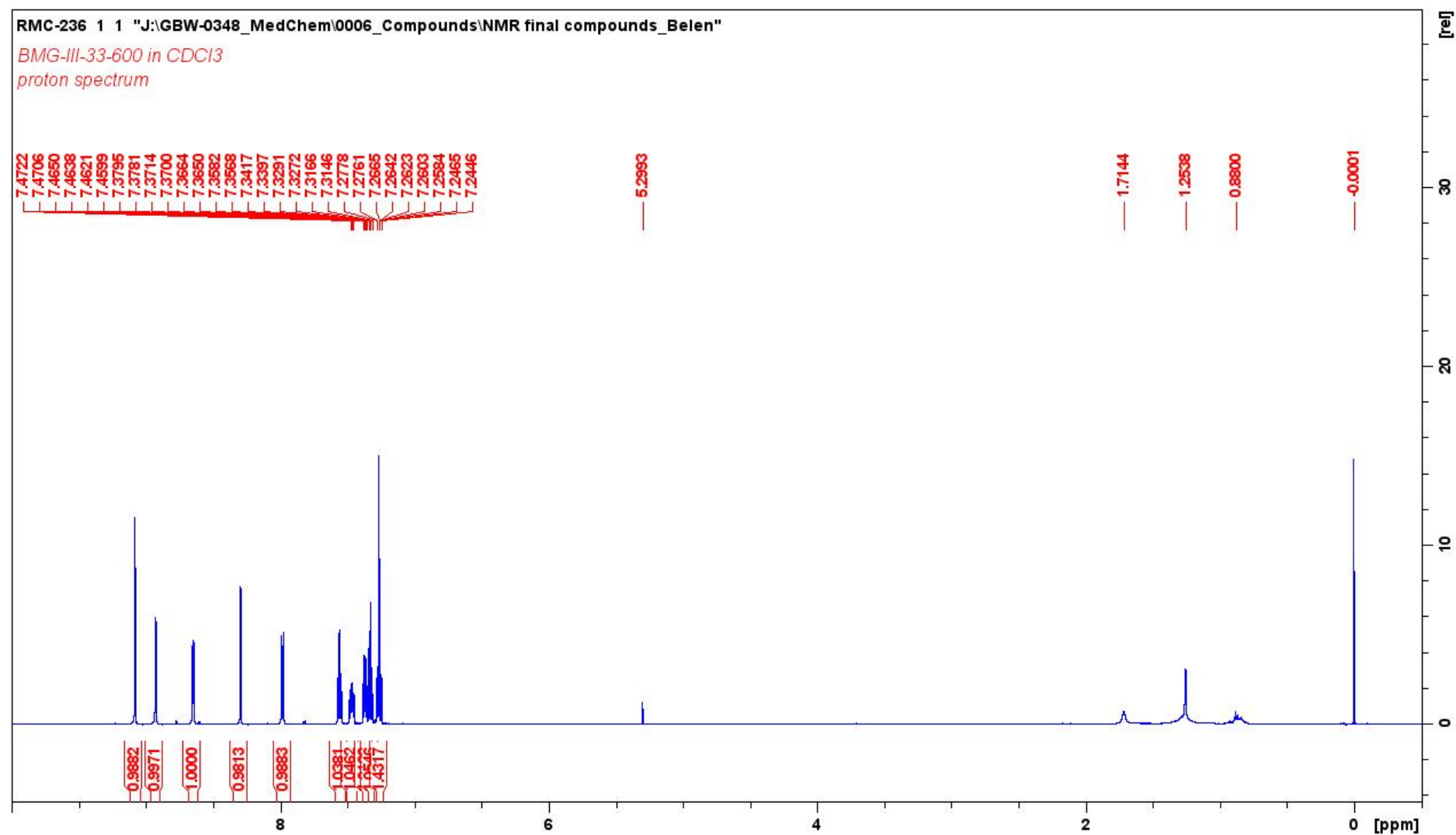
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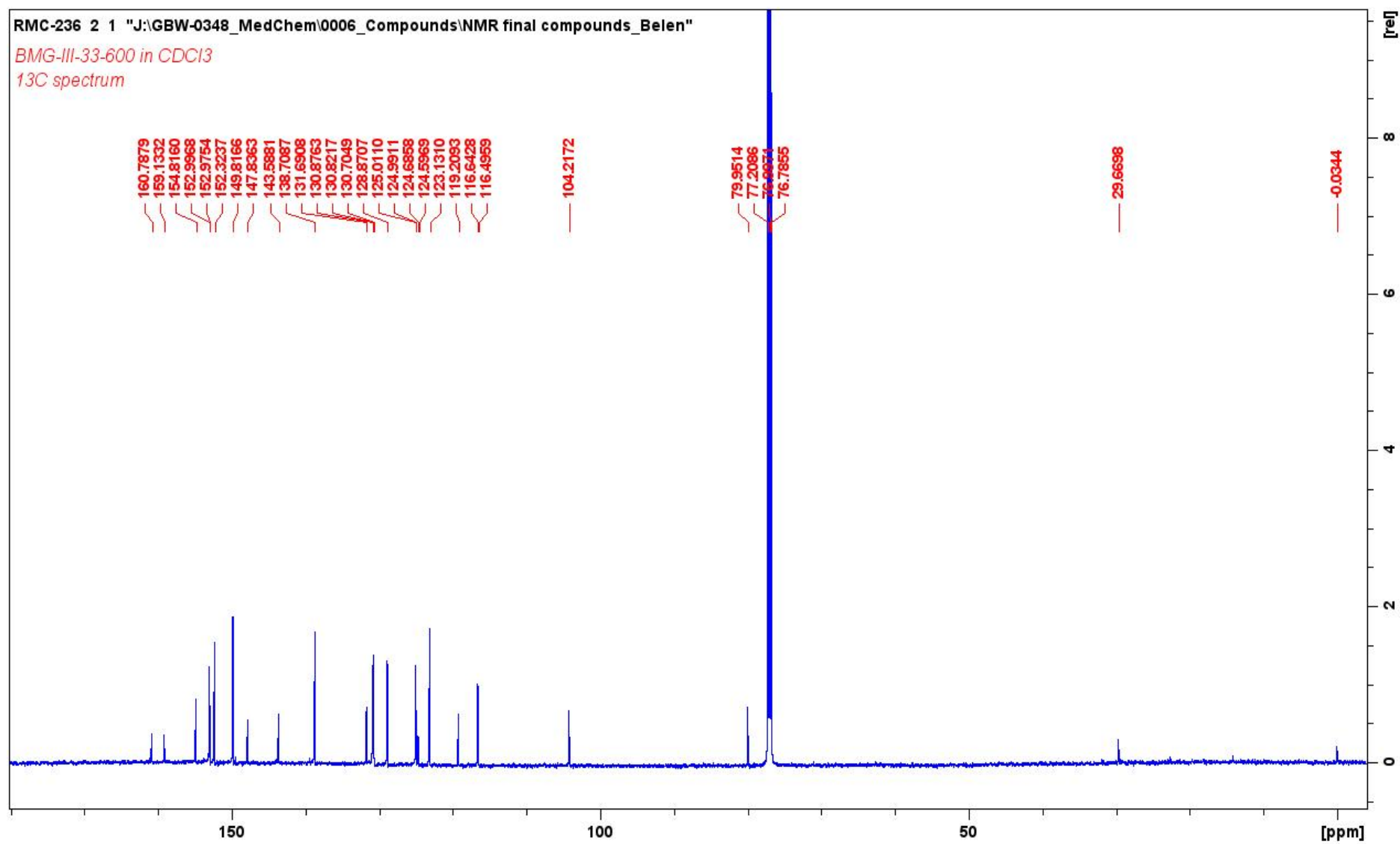
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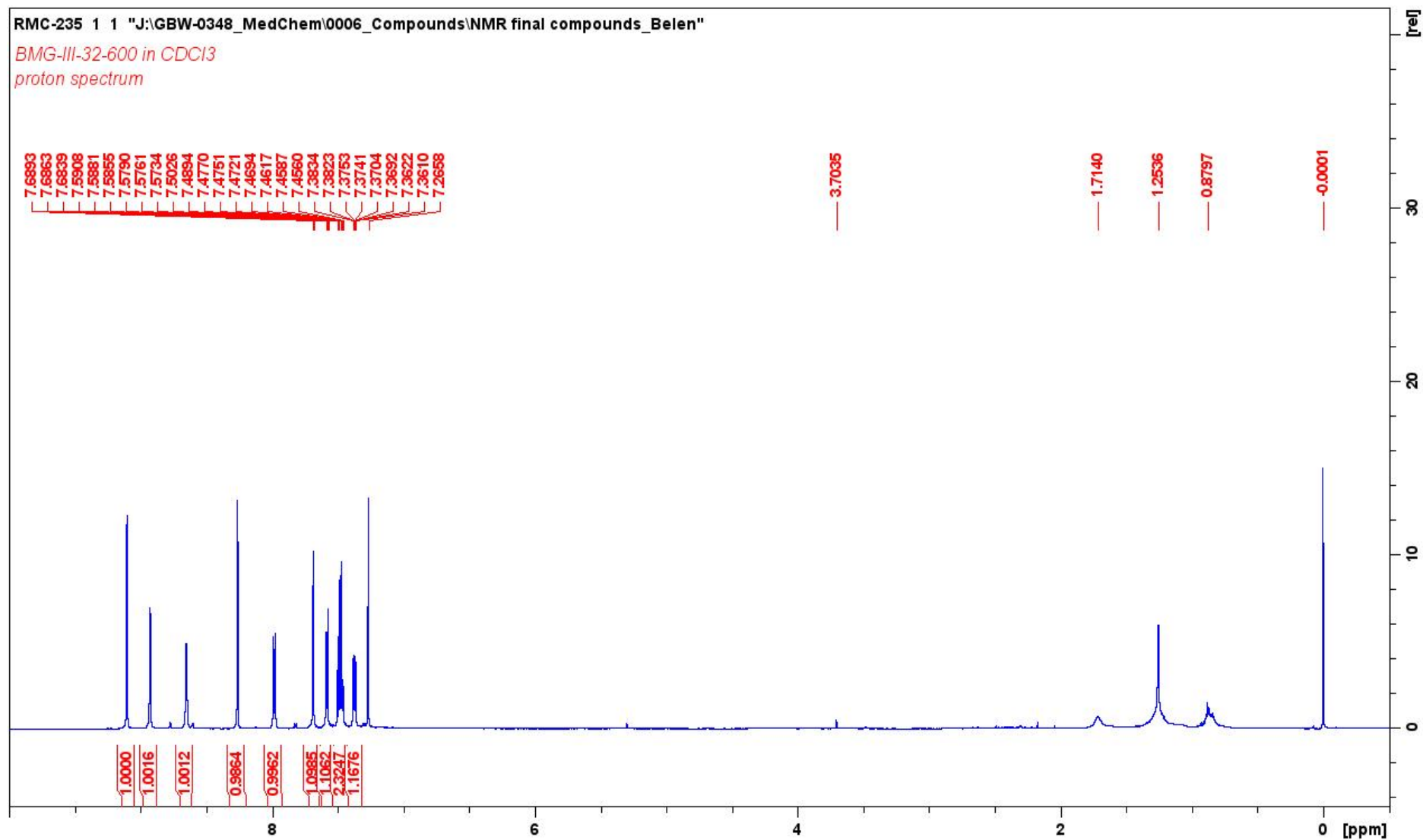
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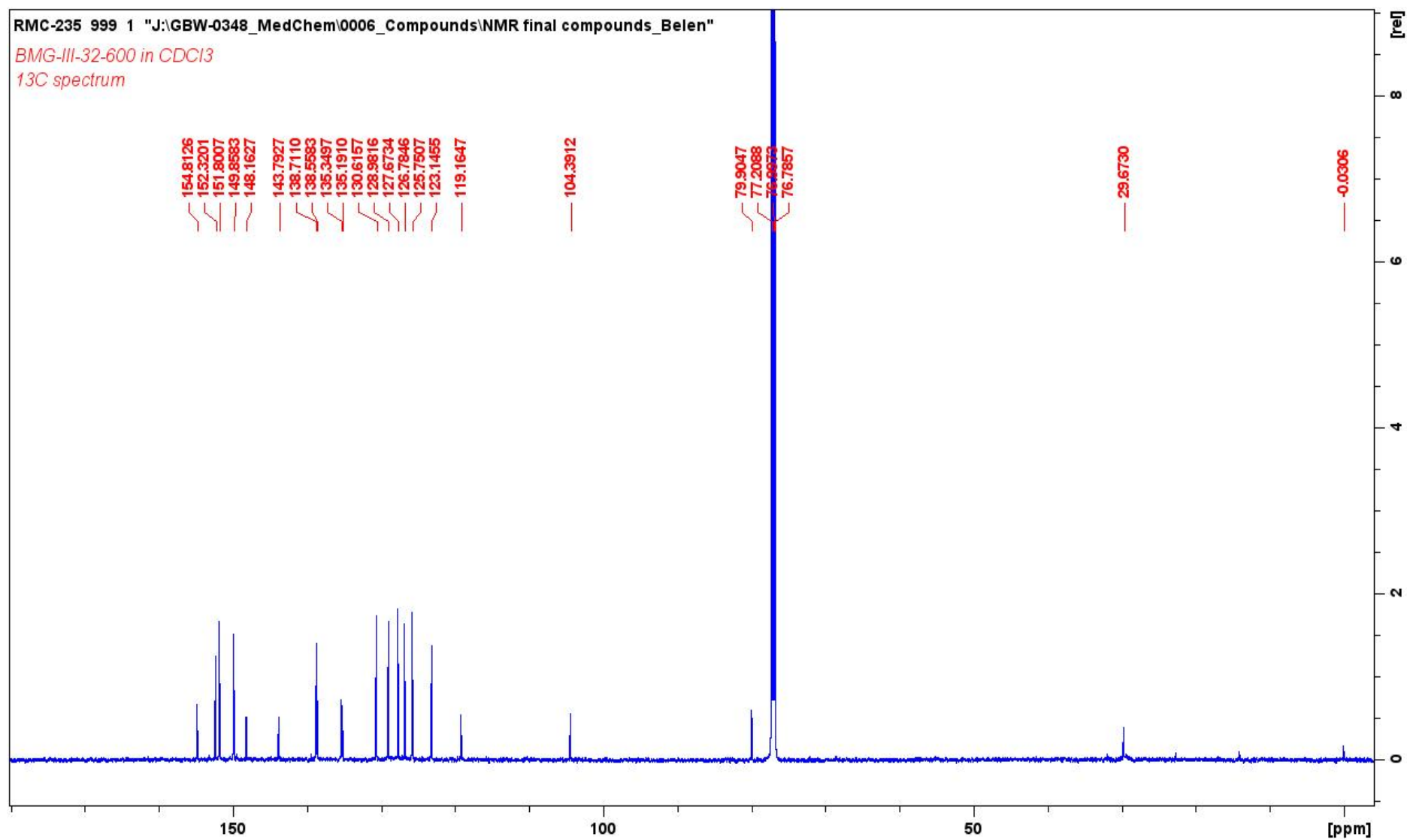
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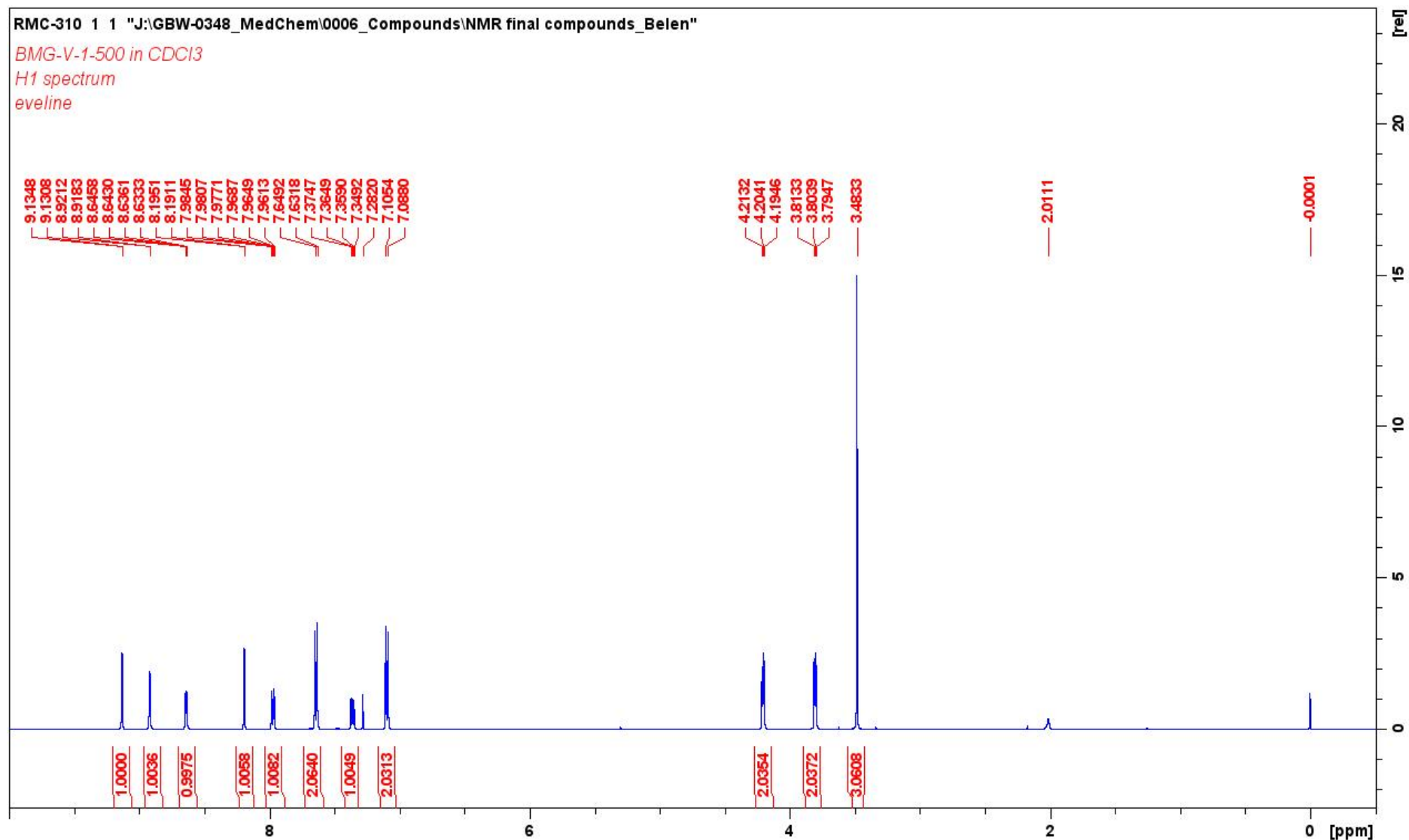
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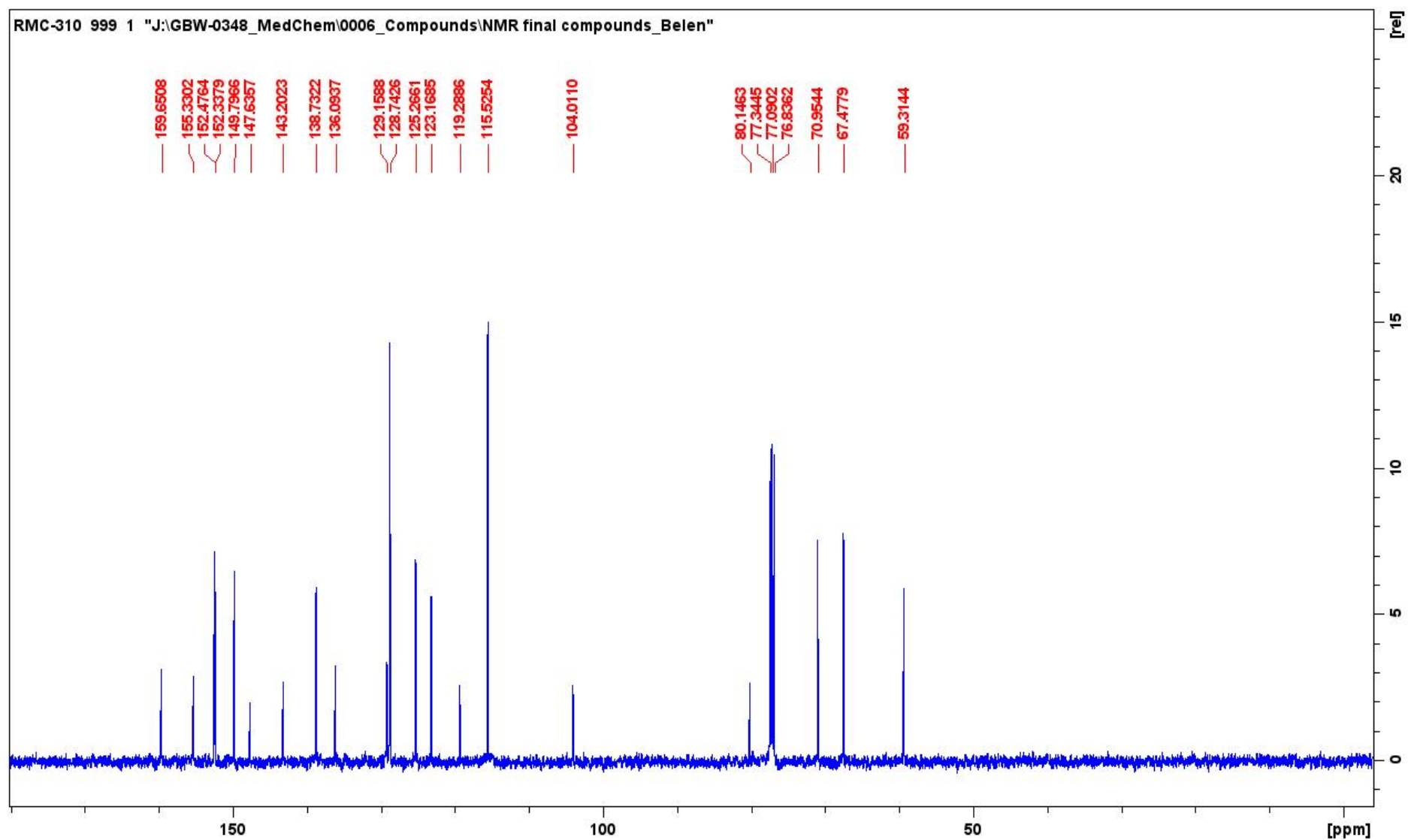
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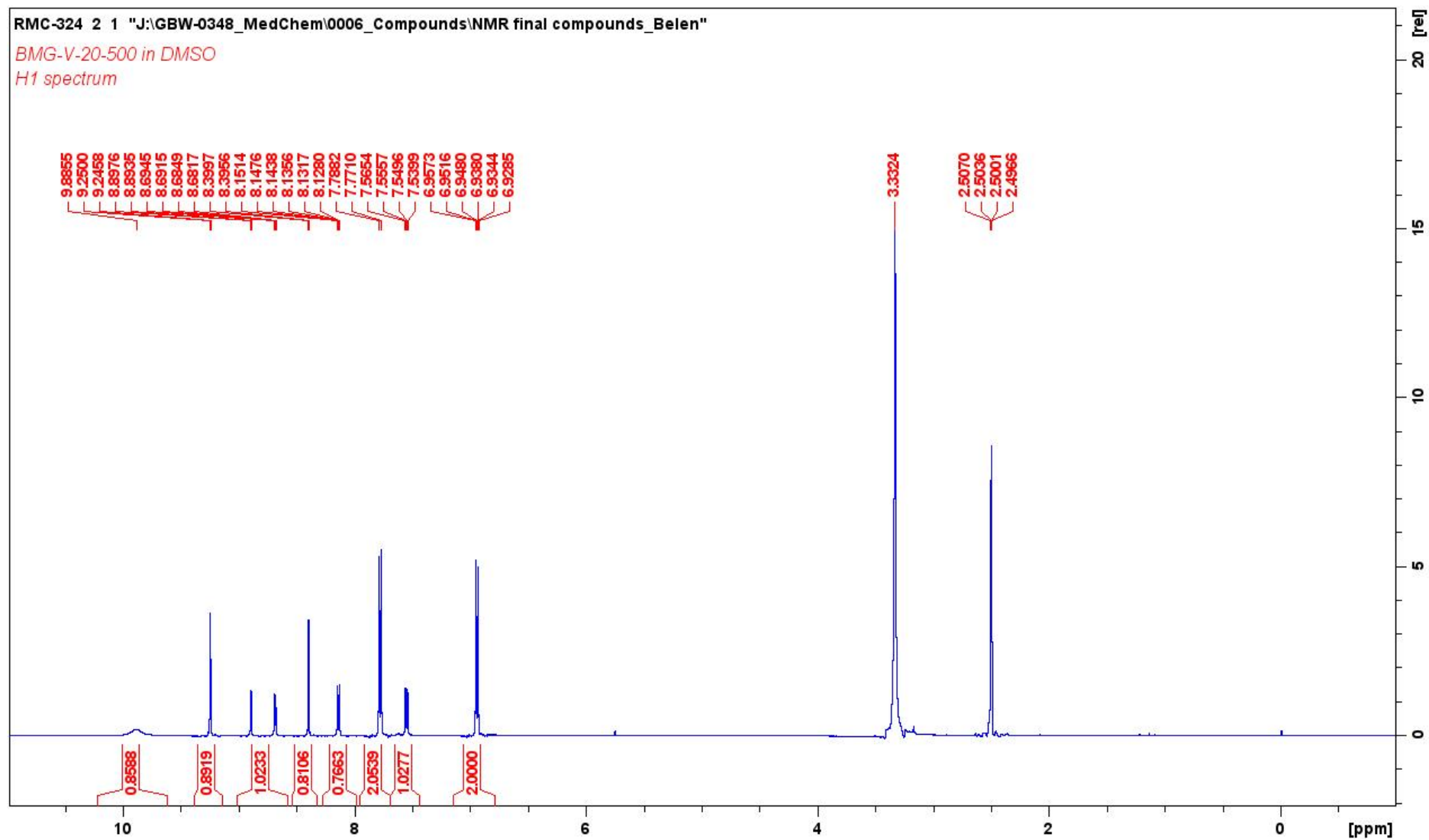
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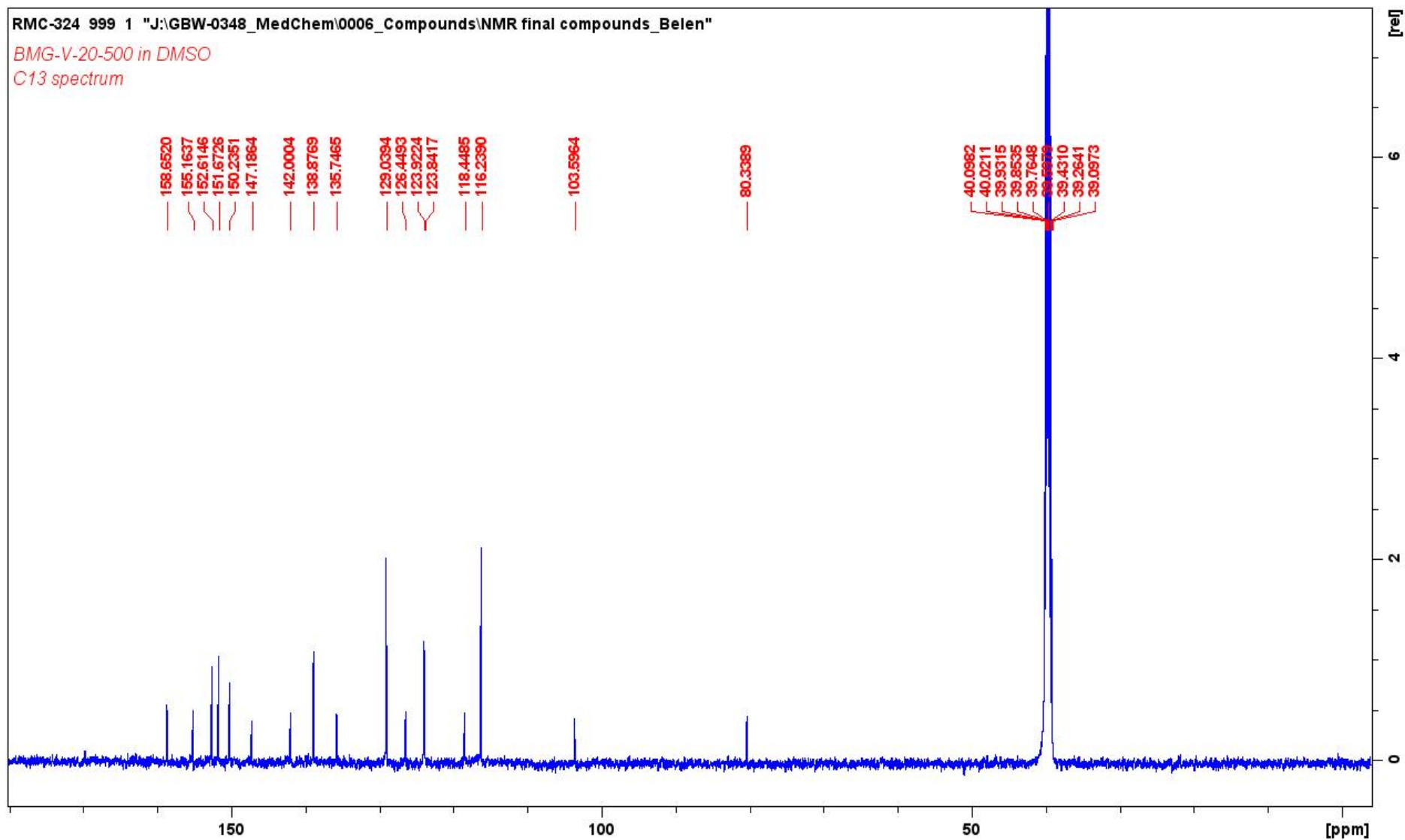
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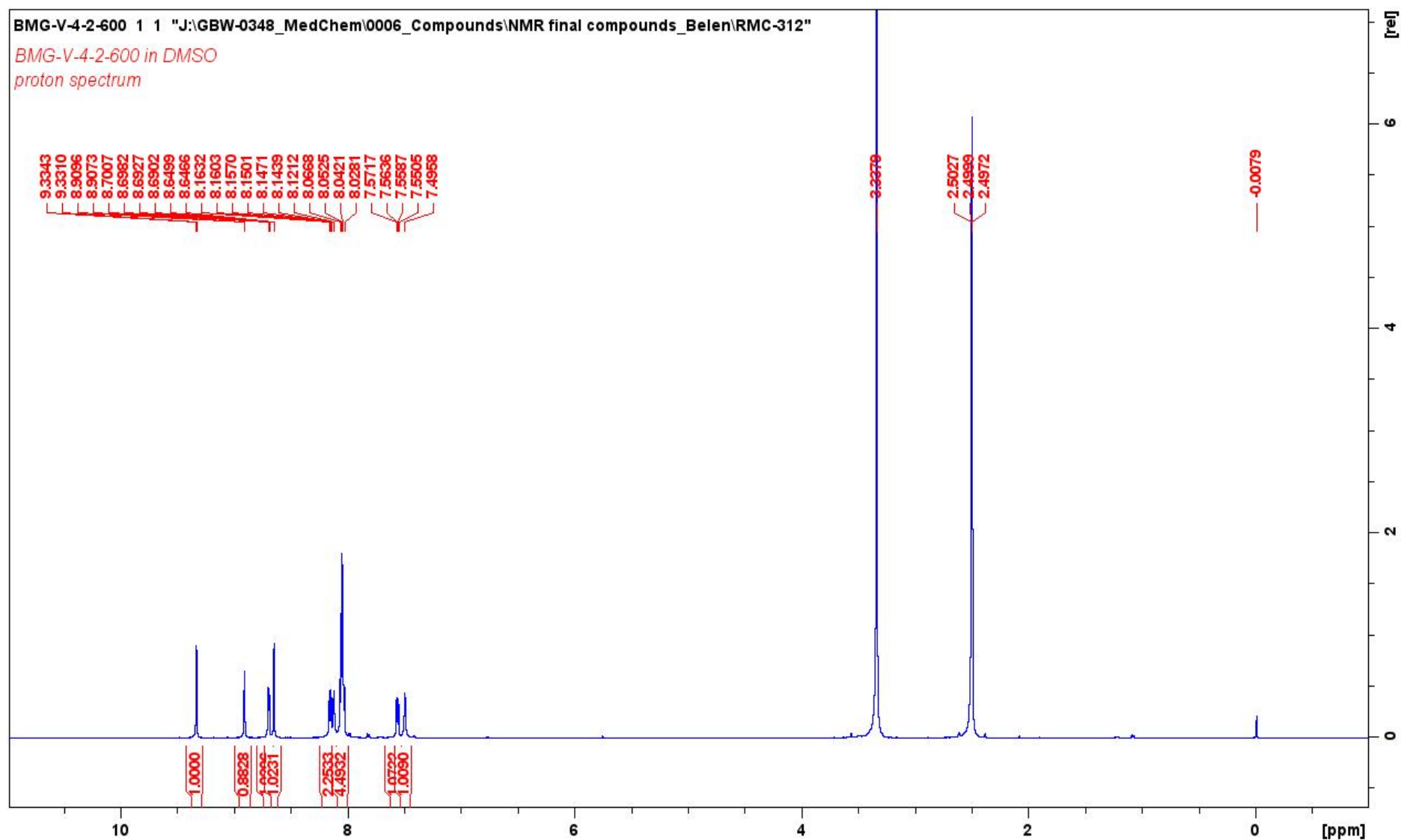
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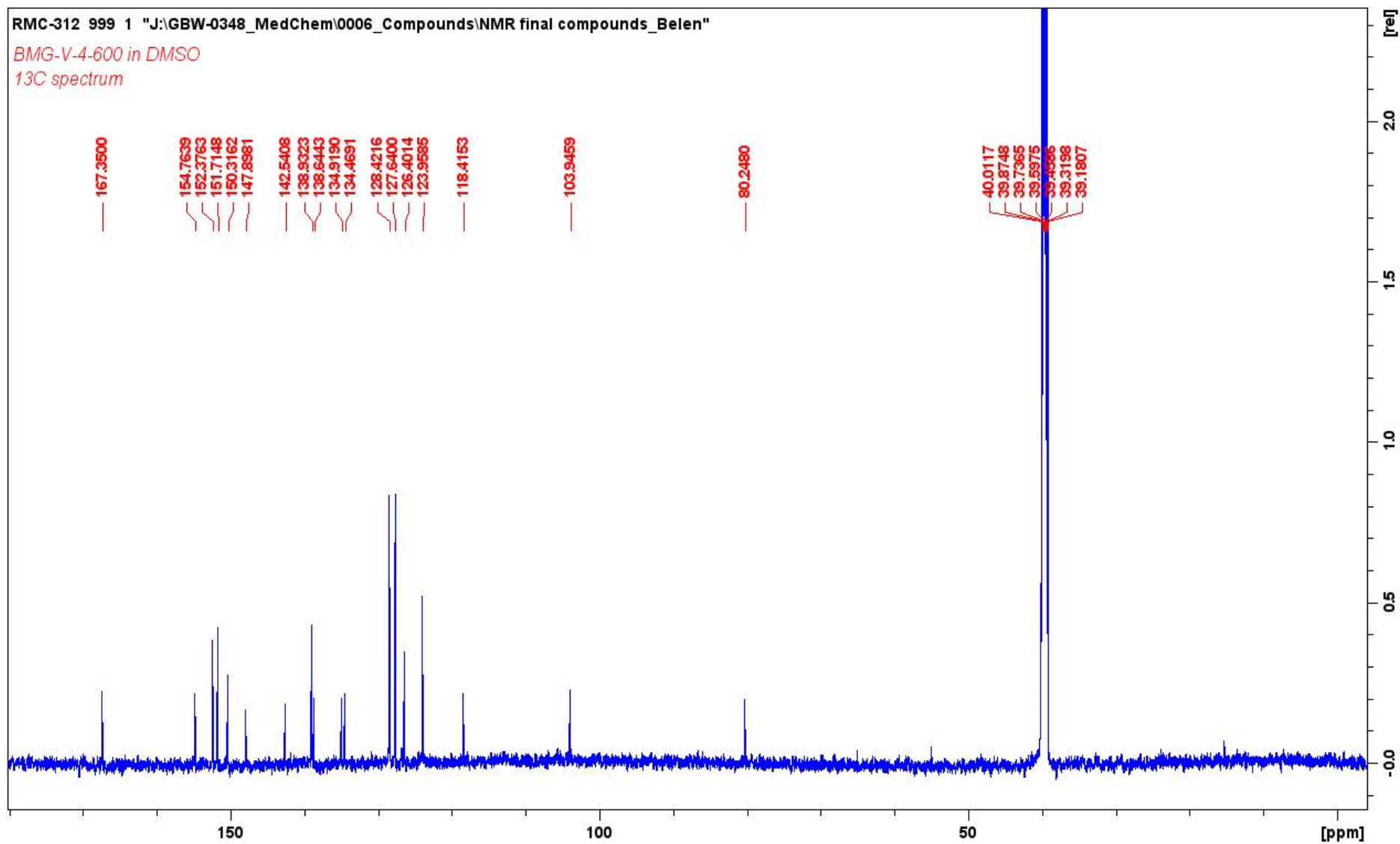
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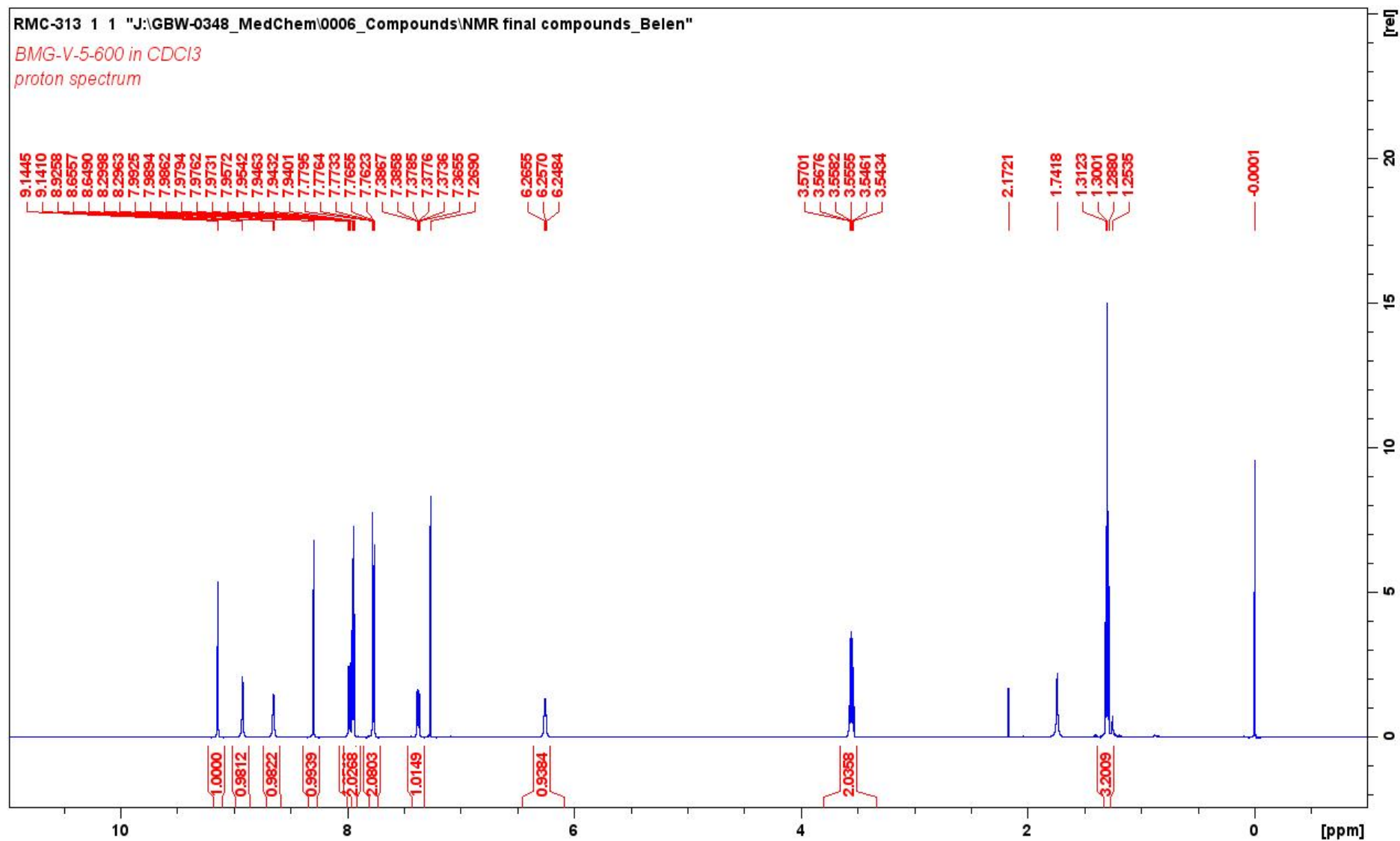
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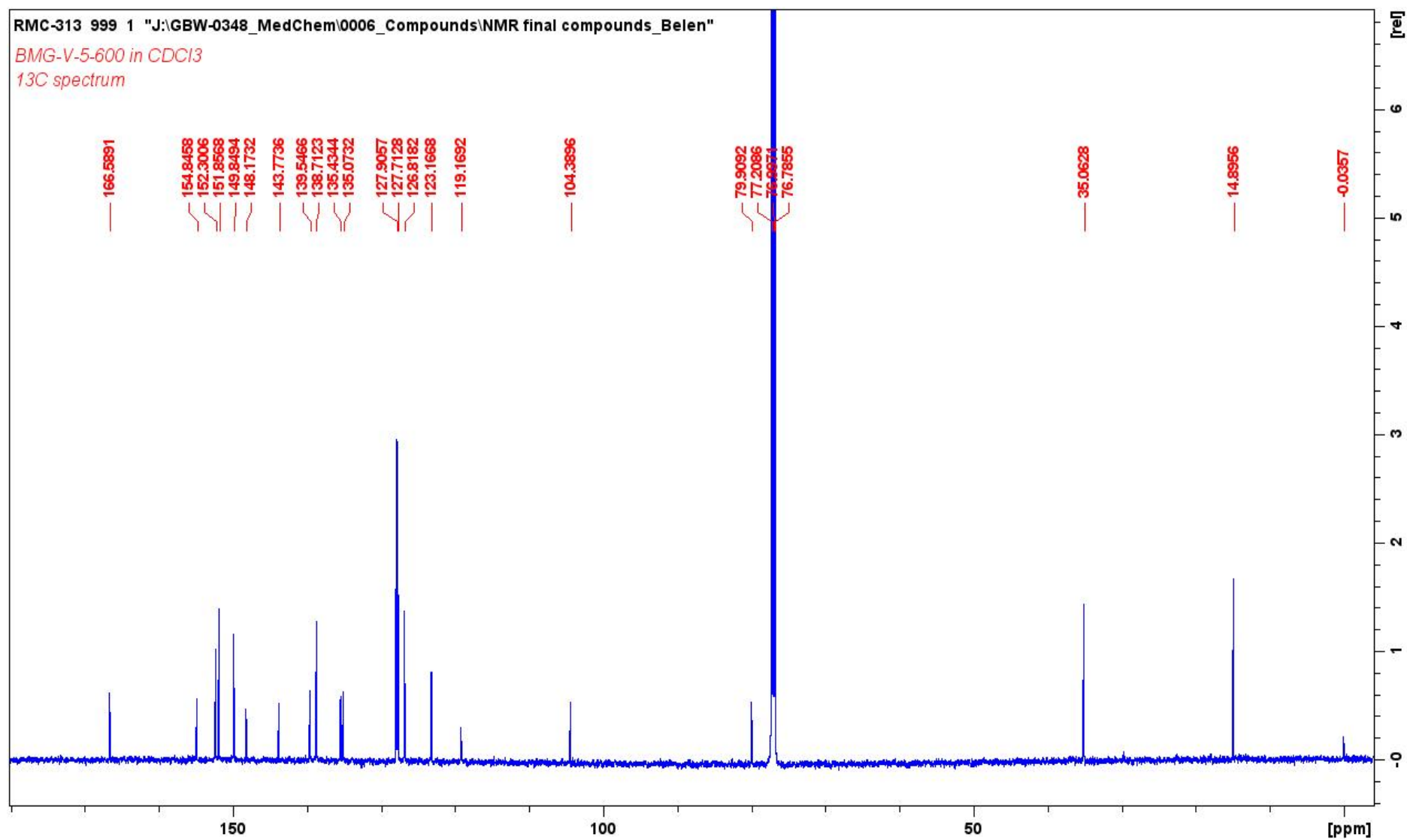
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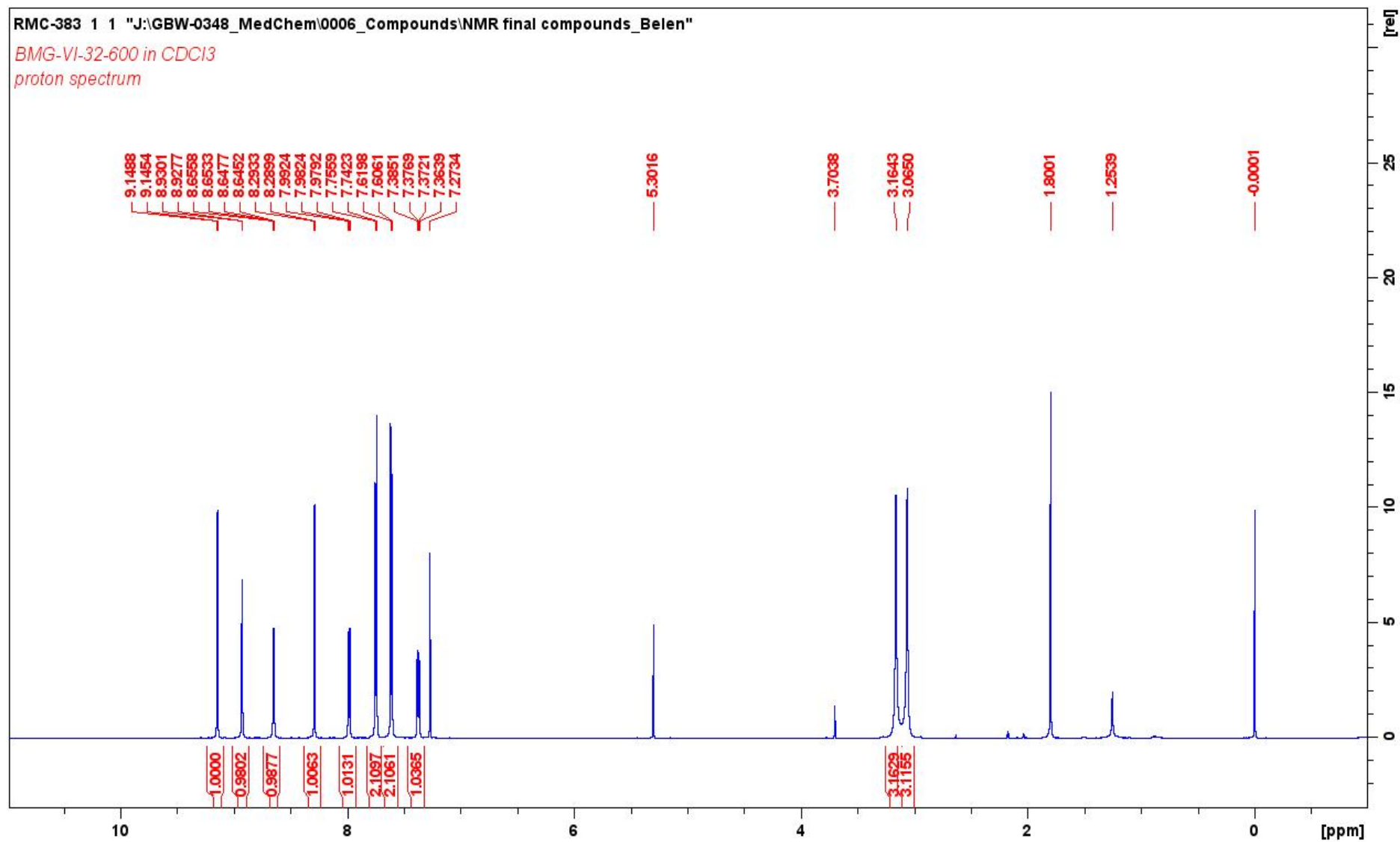
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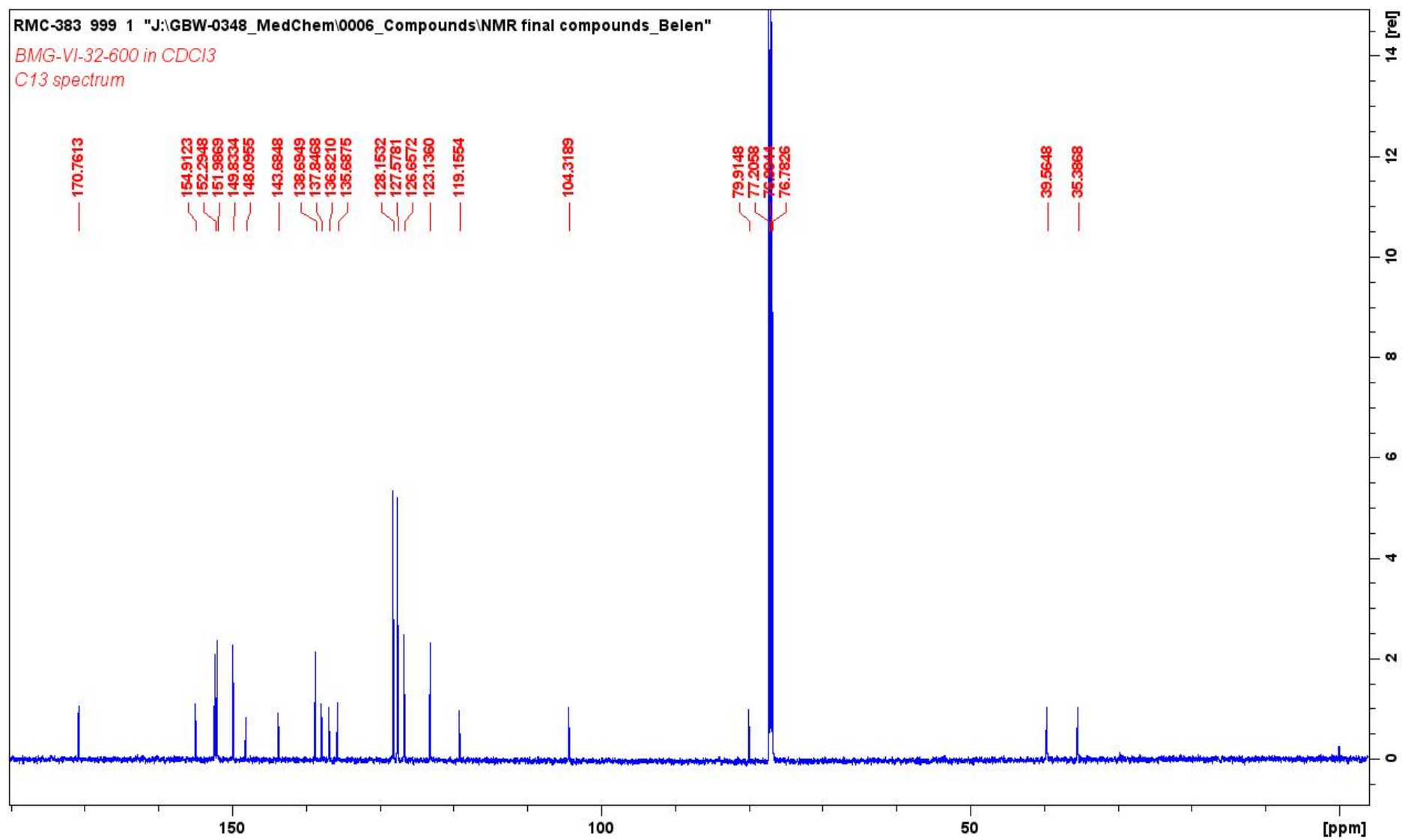
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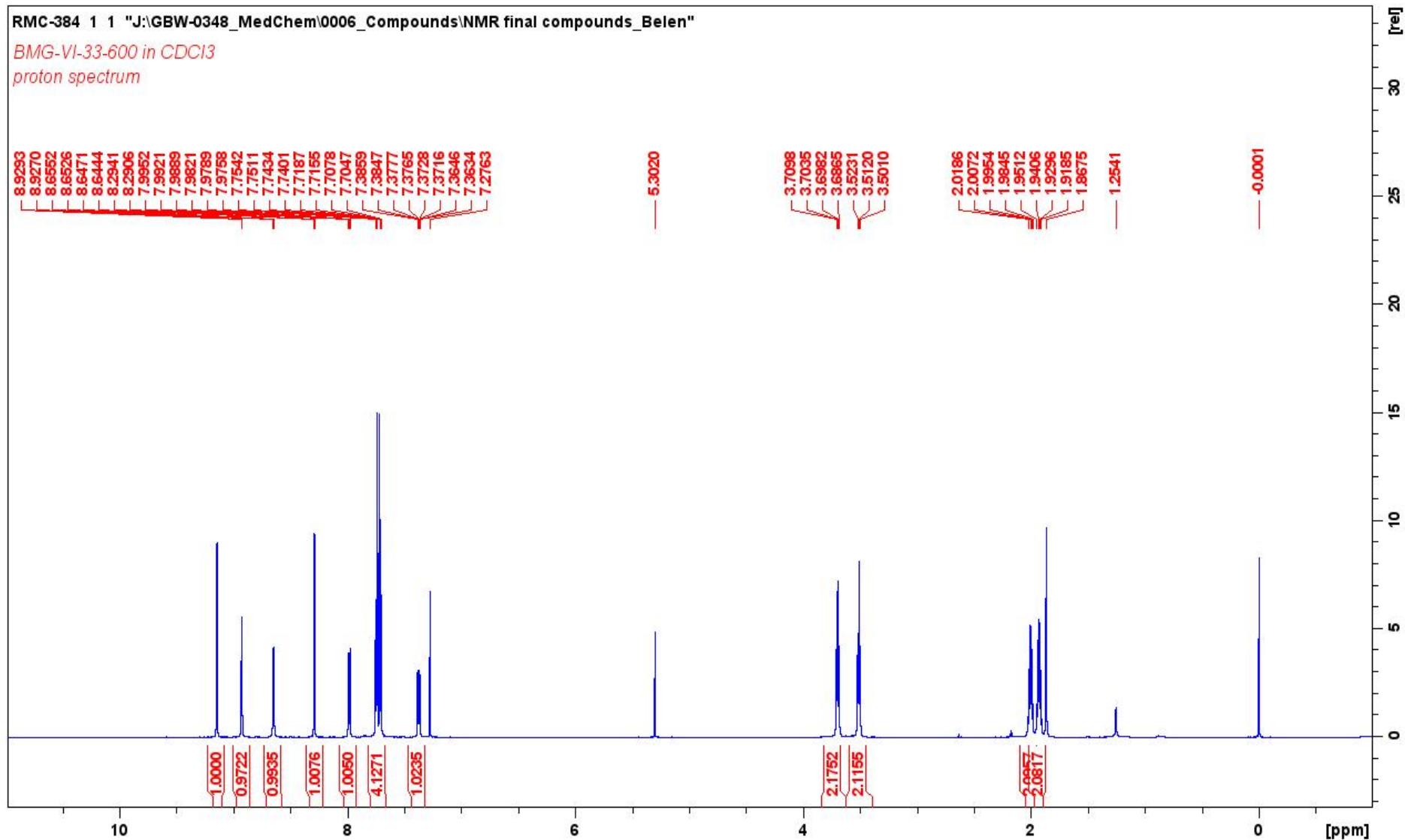
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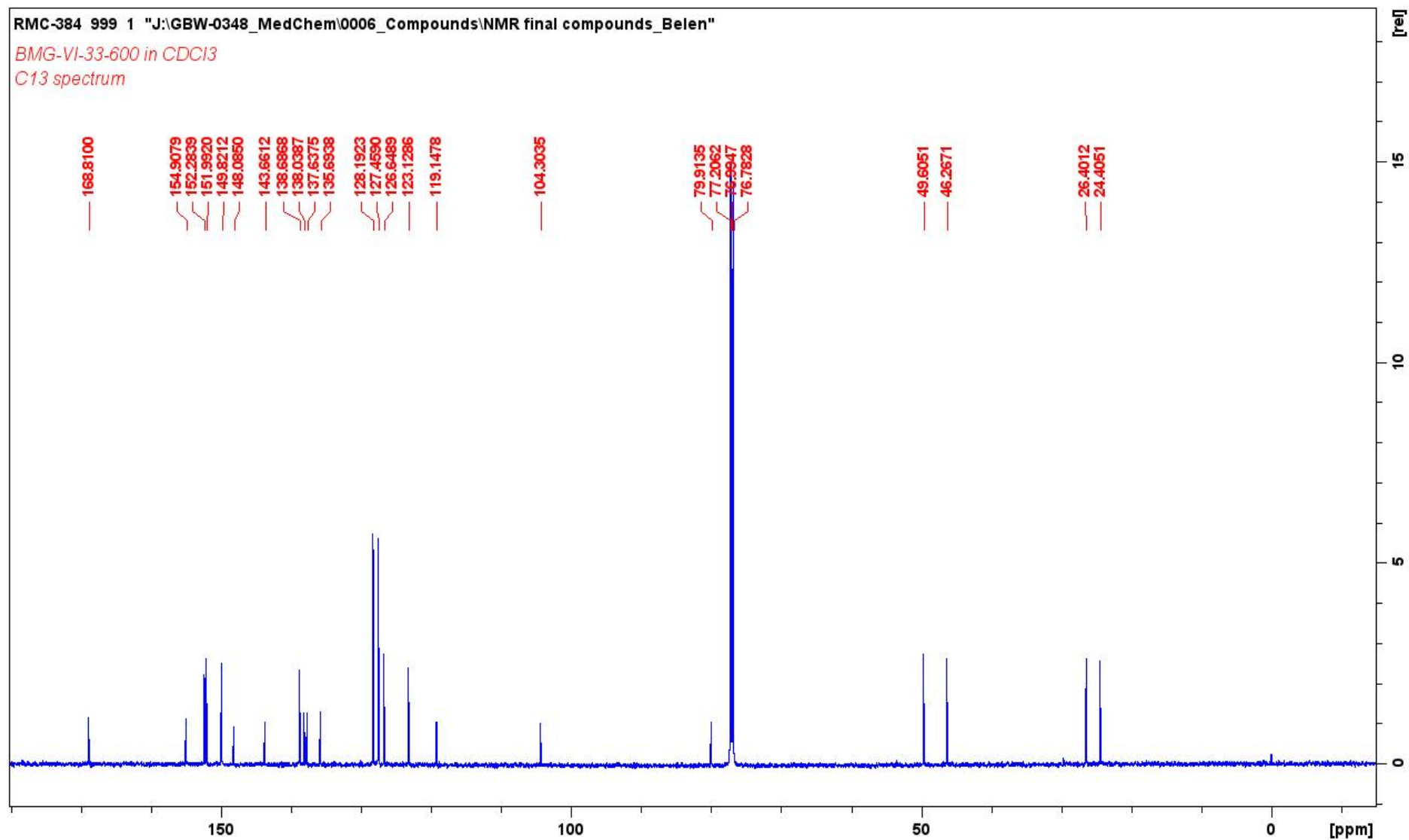
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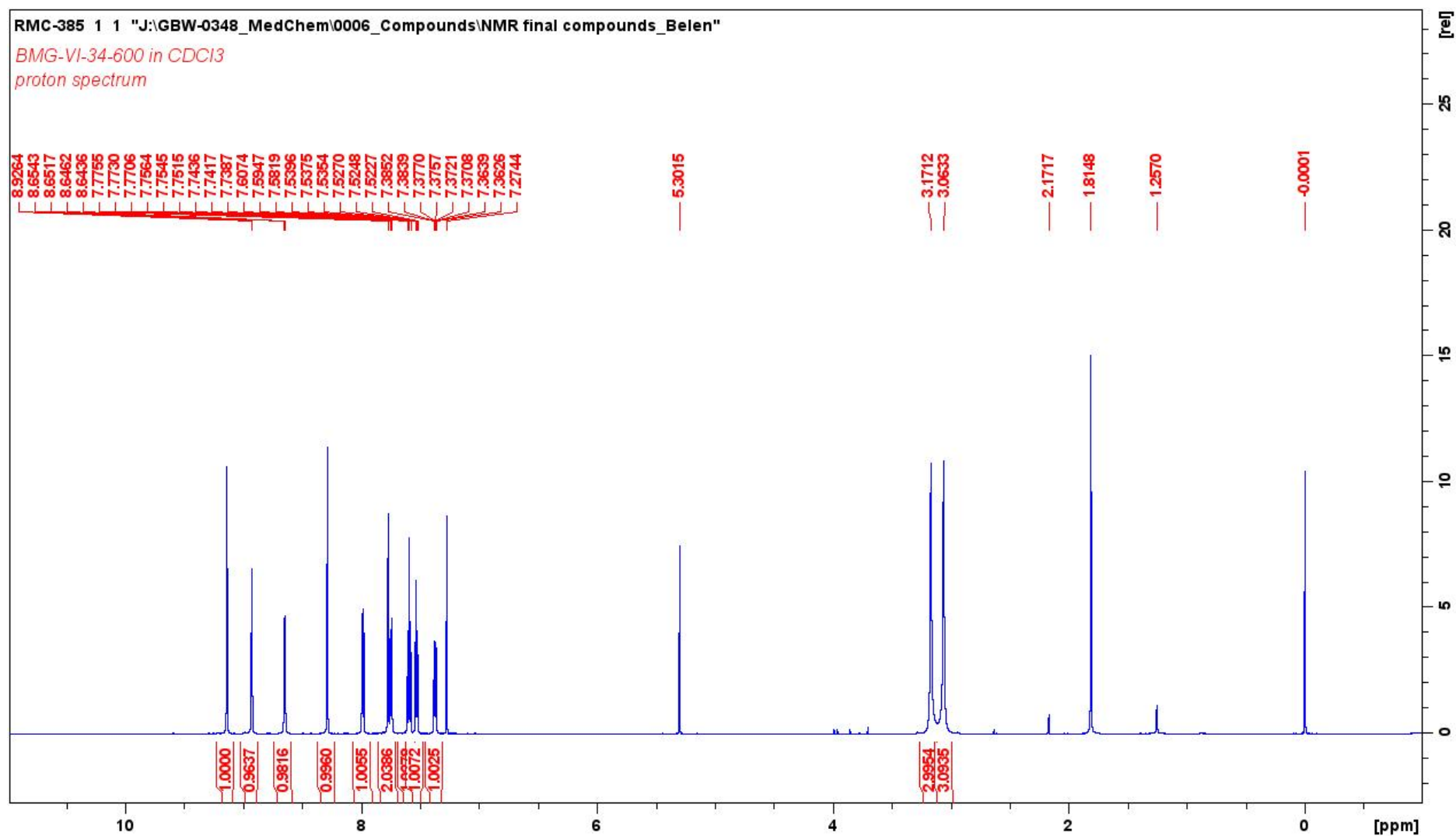
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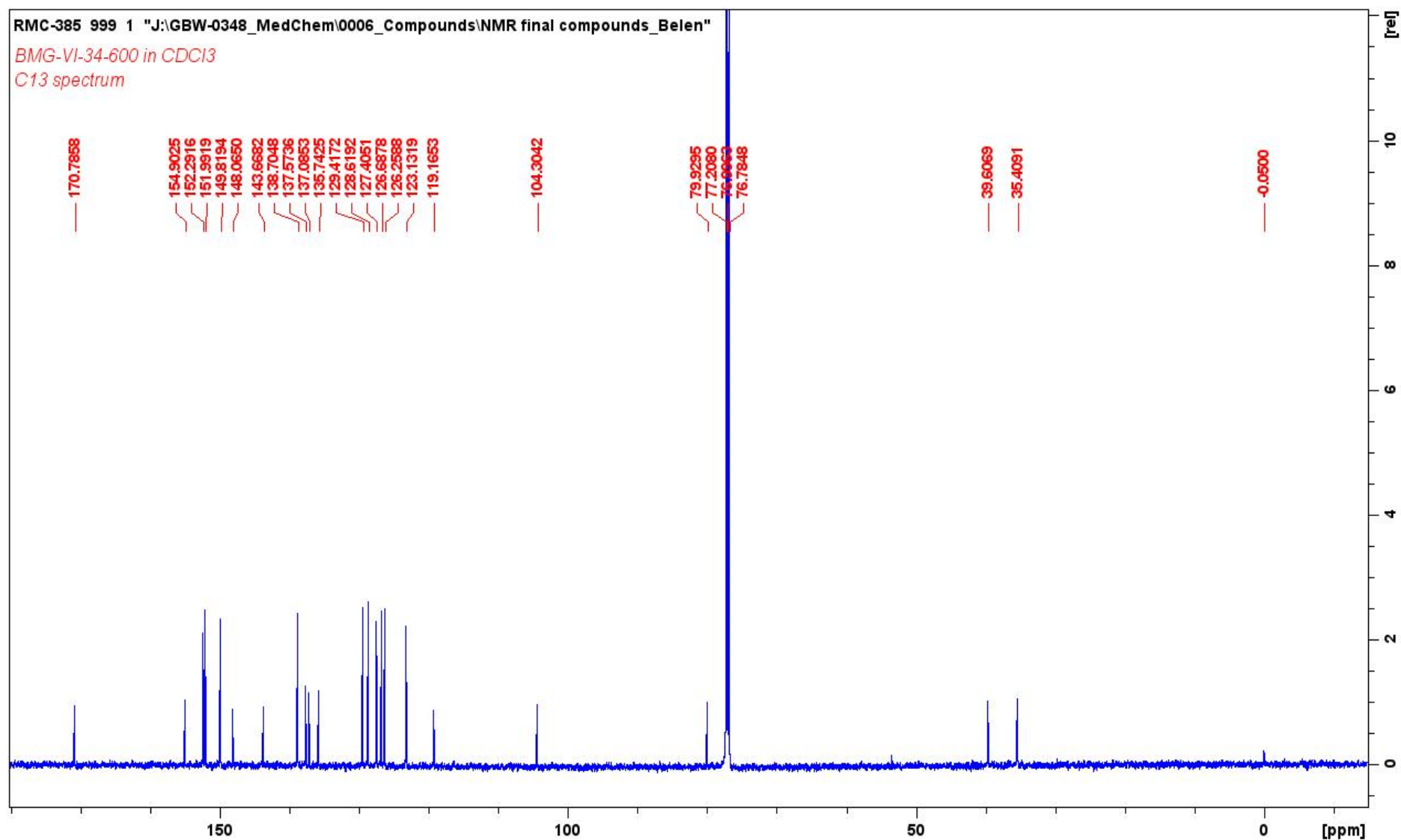
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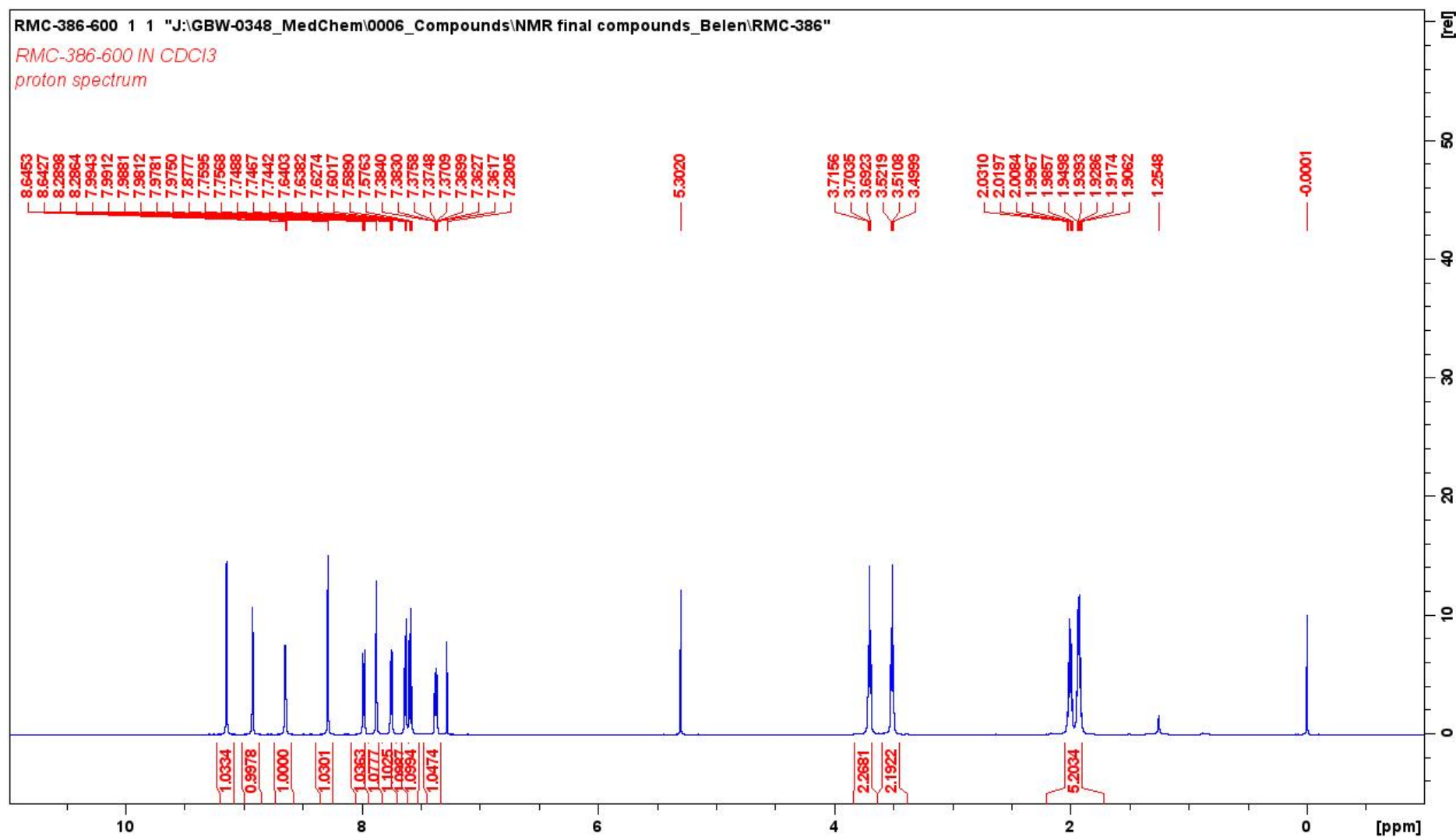
¹H NMR spectrum of **3q**



¹³C NMR spectrum of **3q**



¹H NMR spectrum of **3r**

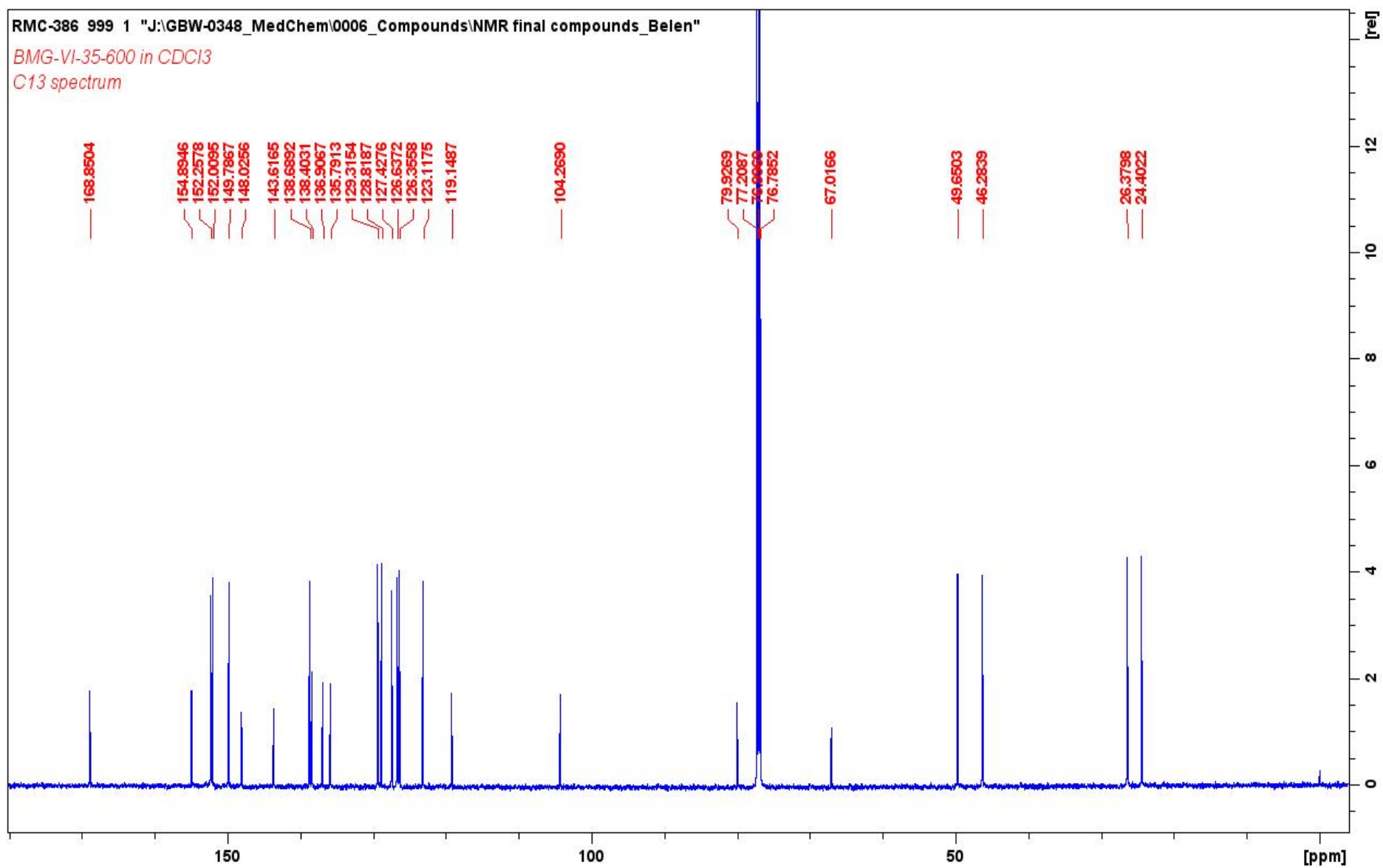


¹³C NMR spectrum of **3r**

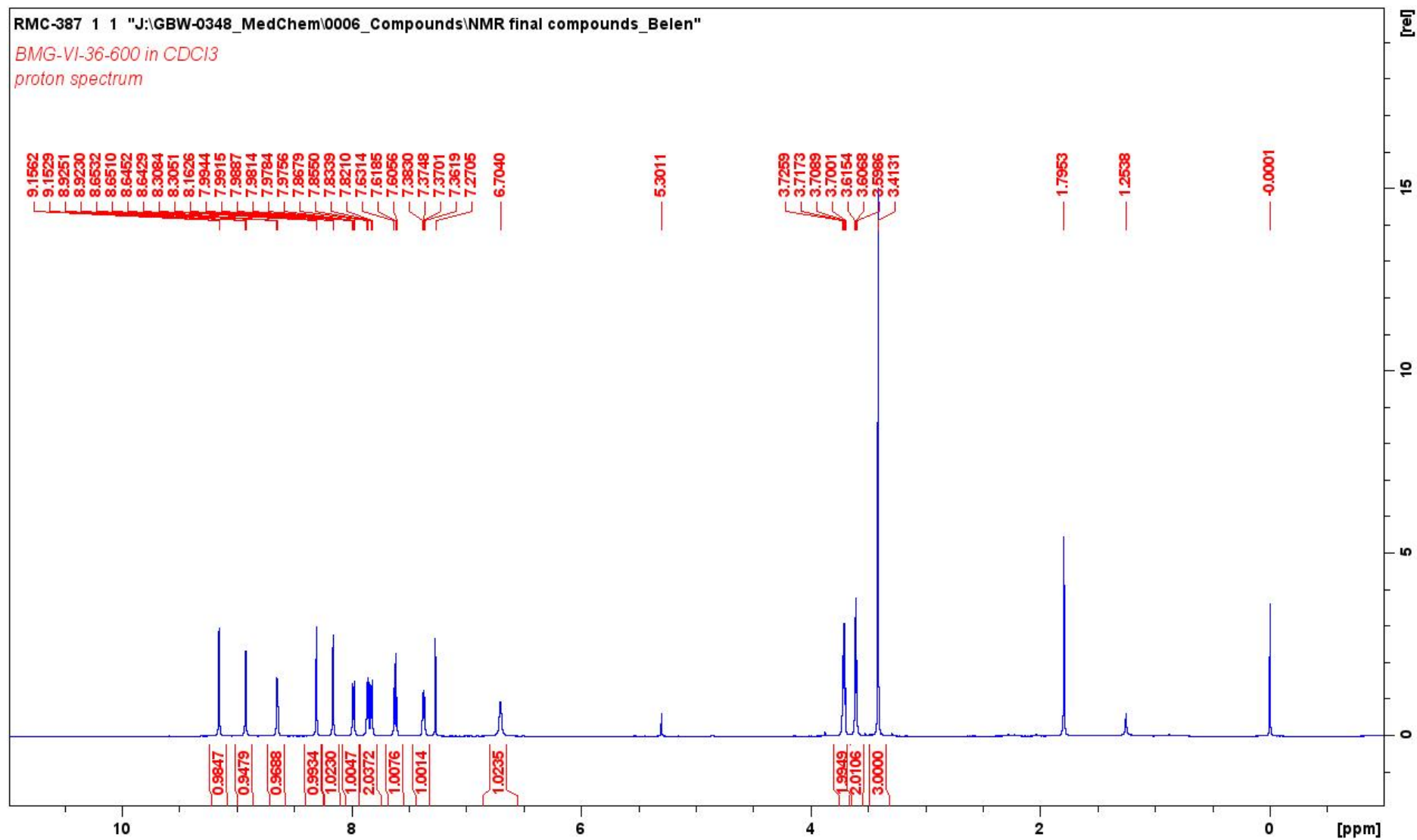
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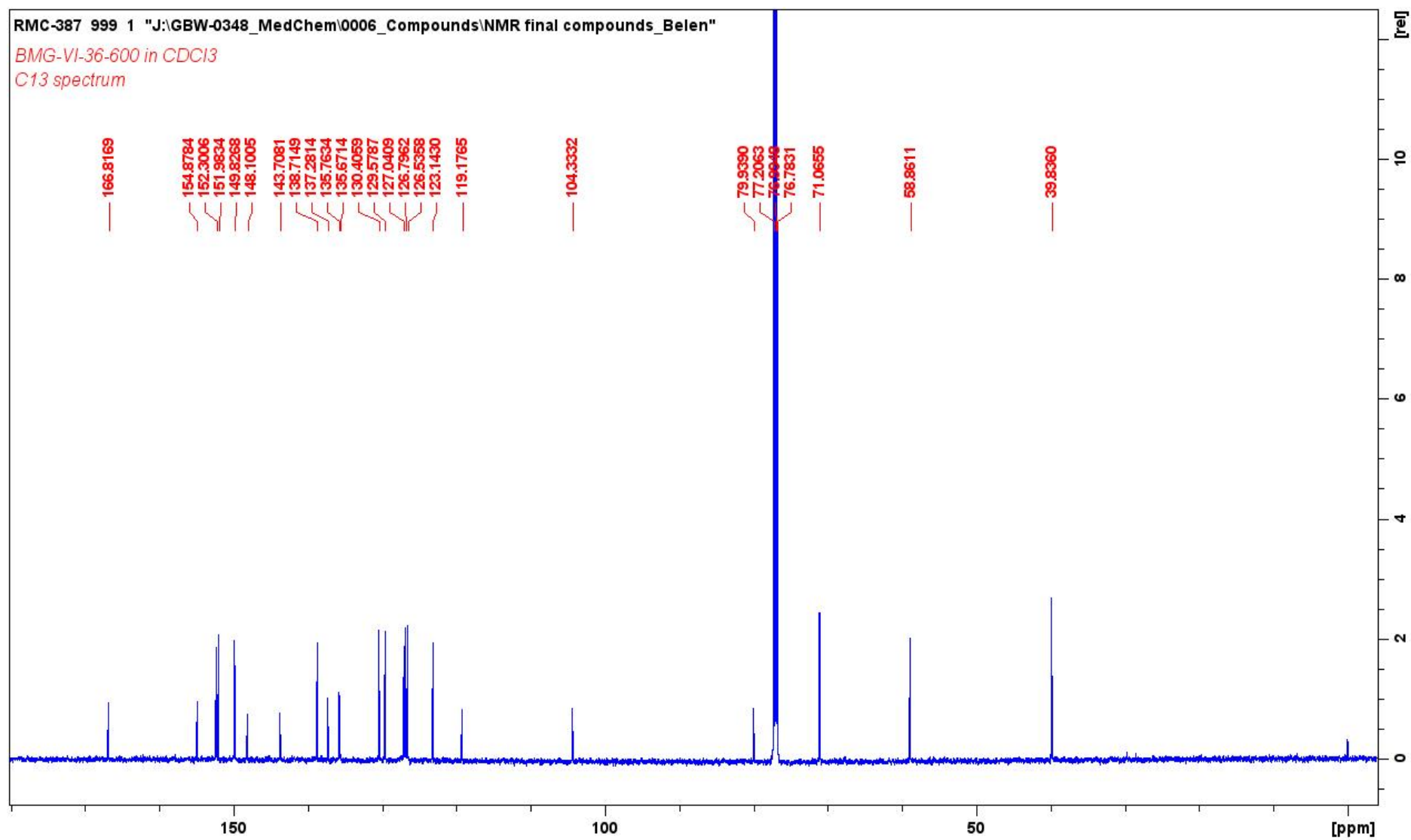
C13 spectrum



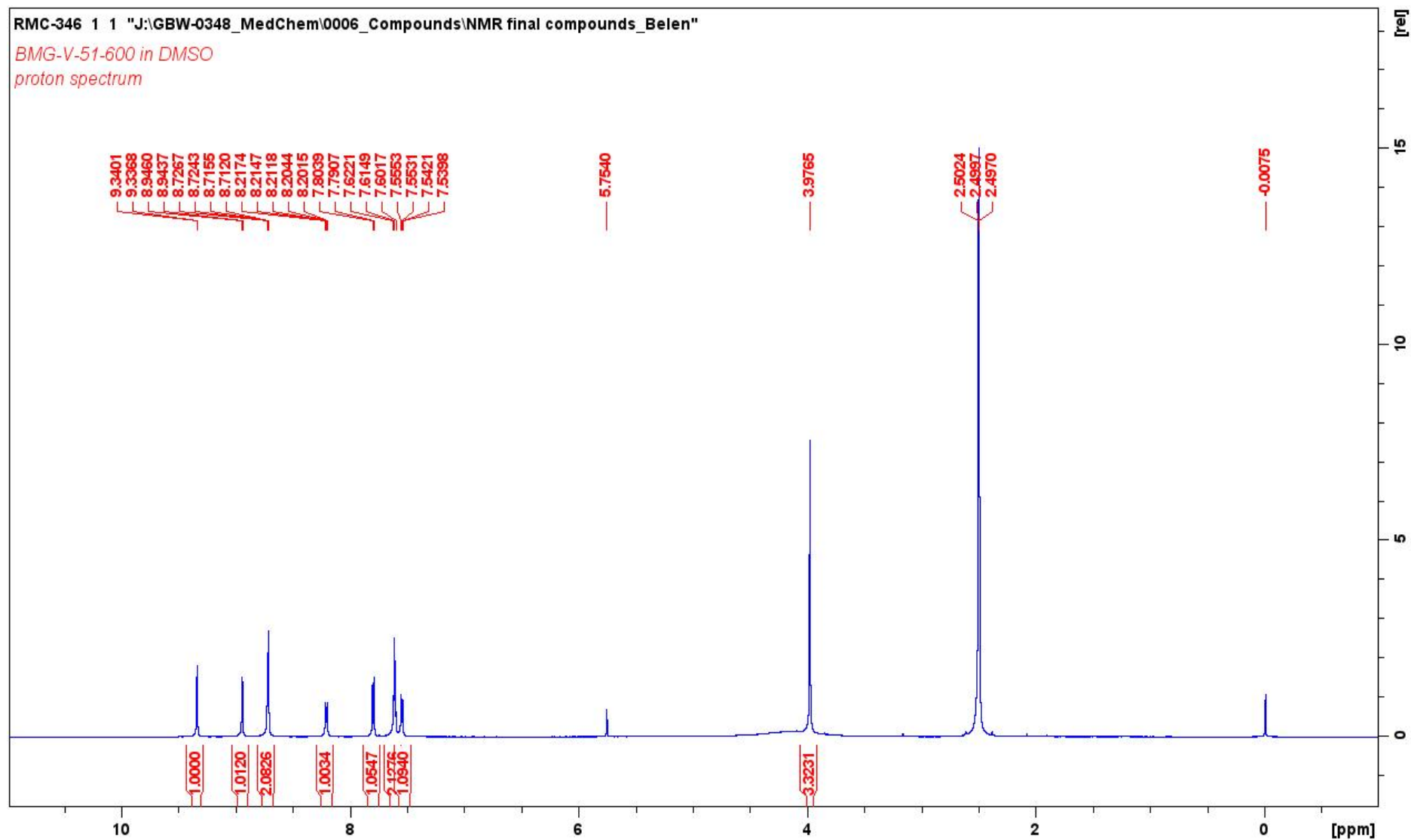
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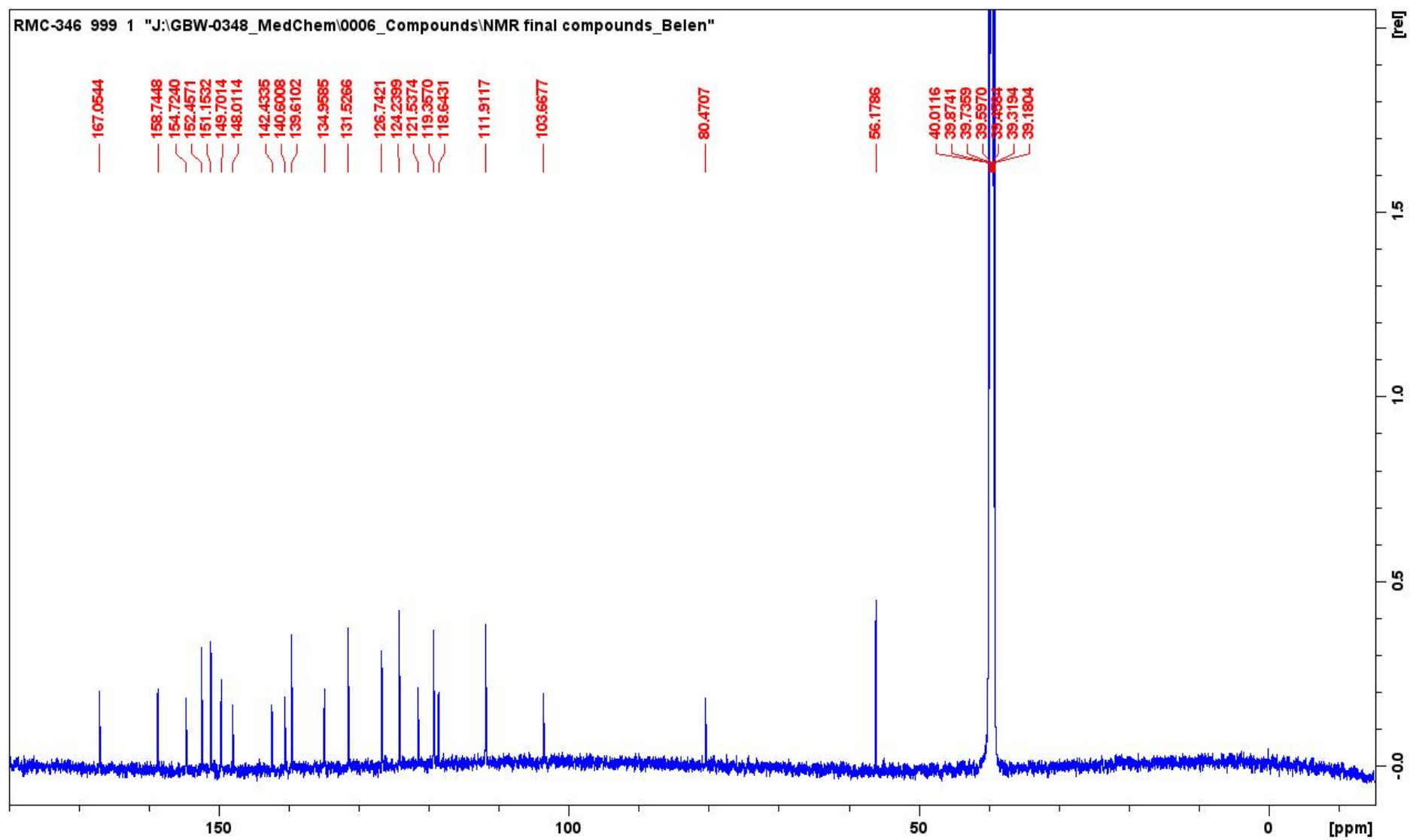
^{13}C NMR spectrum of **3s**



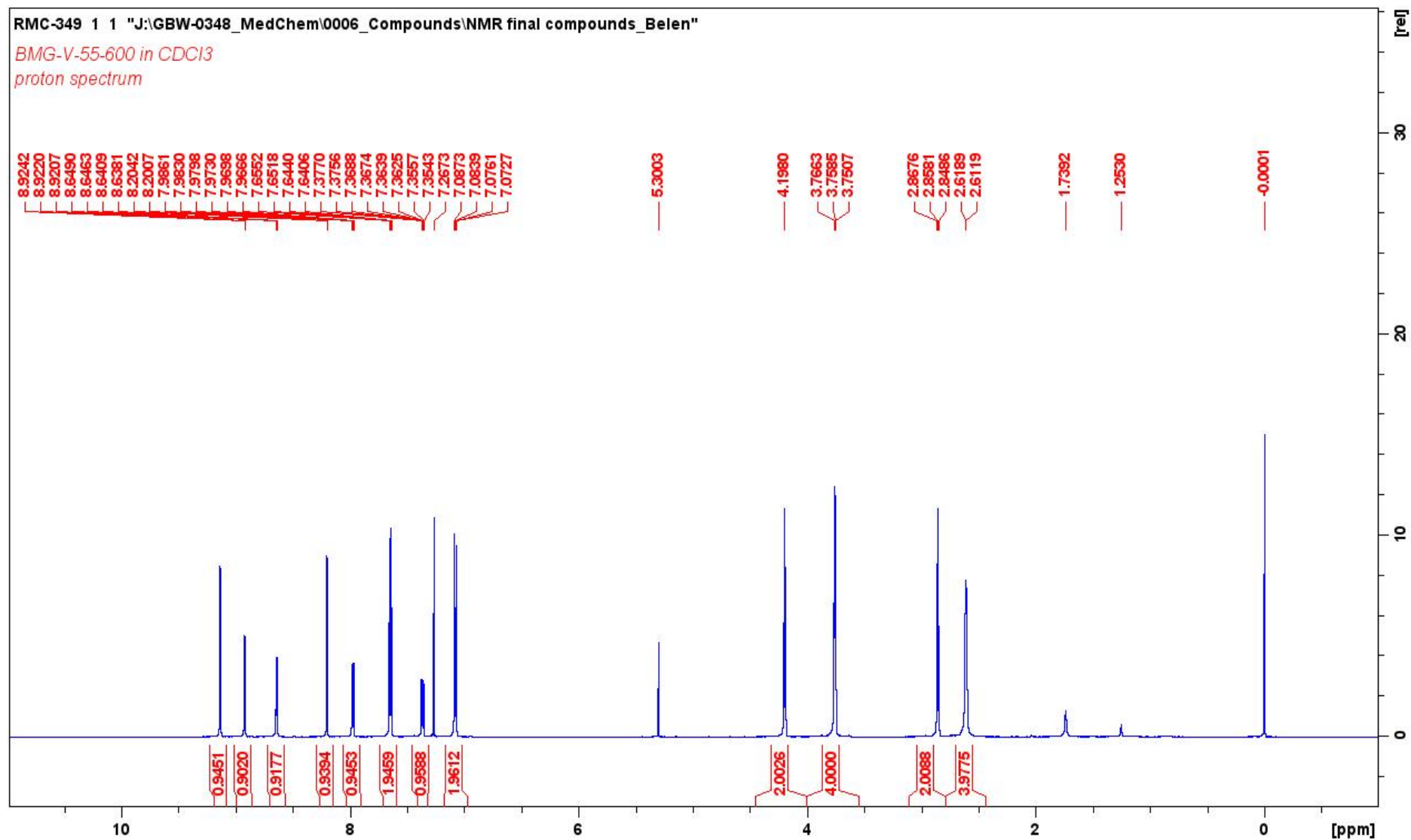
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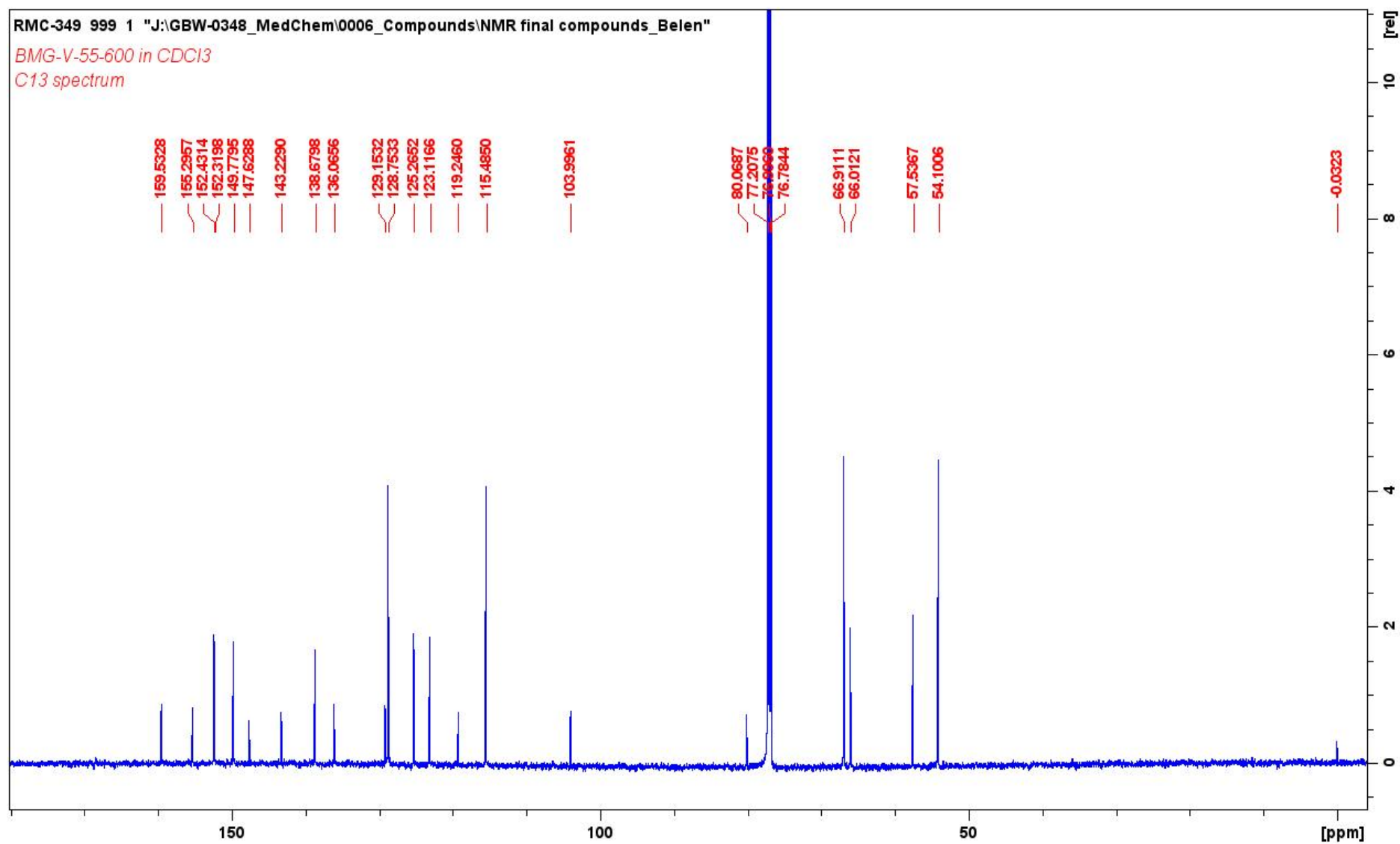
^{13}C NMR spectrum of **4**



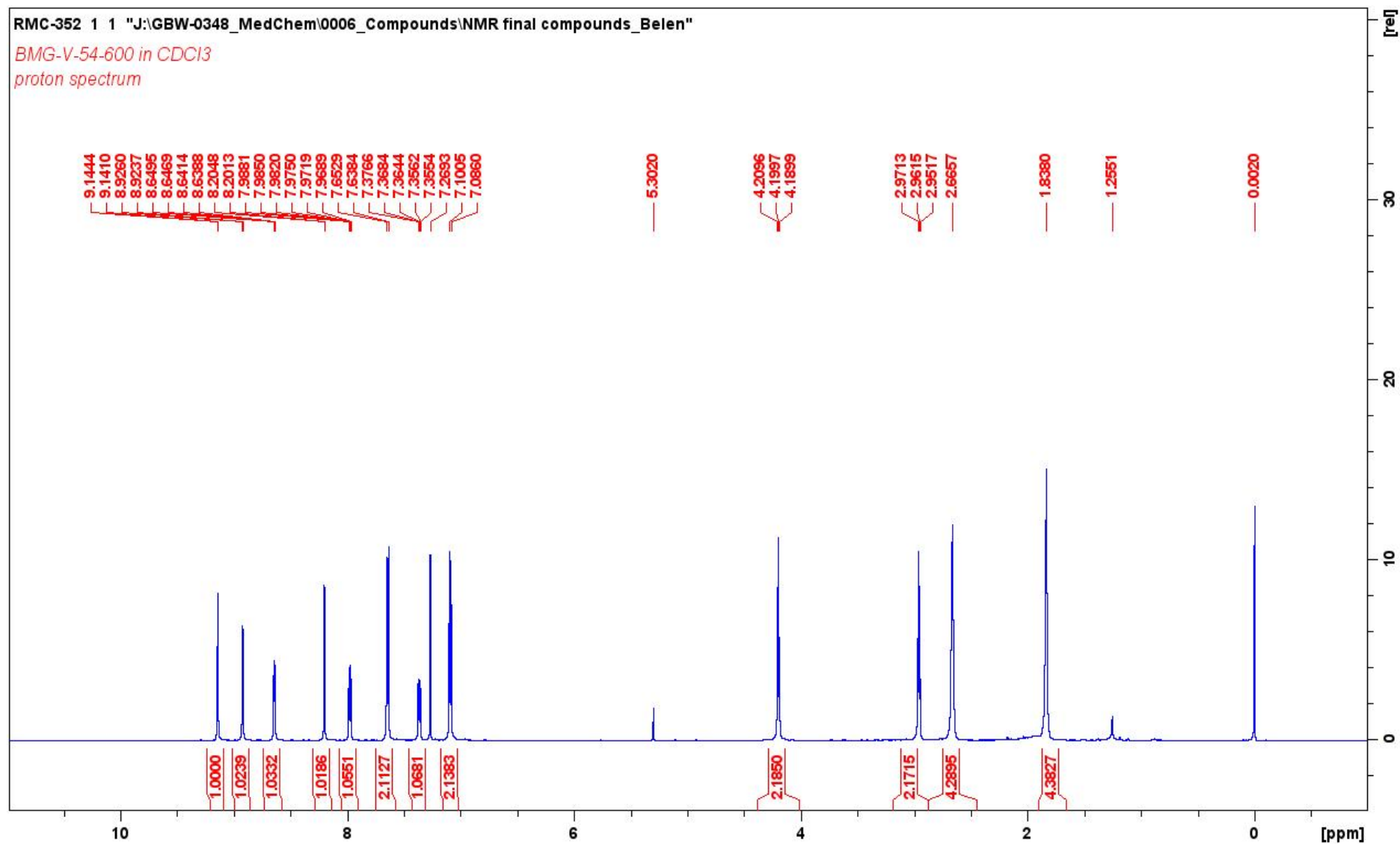
¹H NMR spectrum of 5a



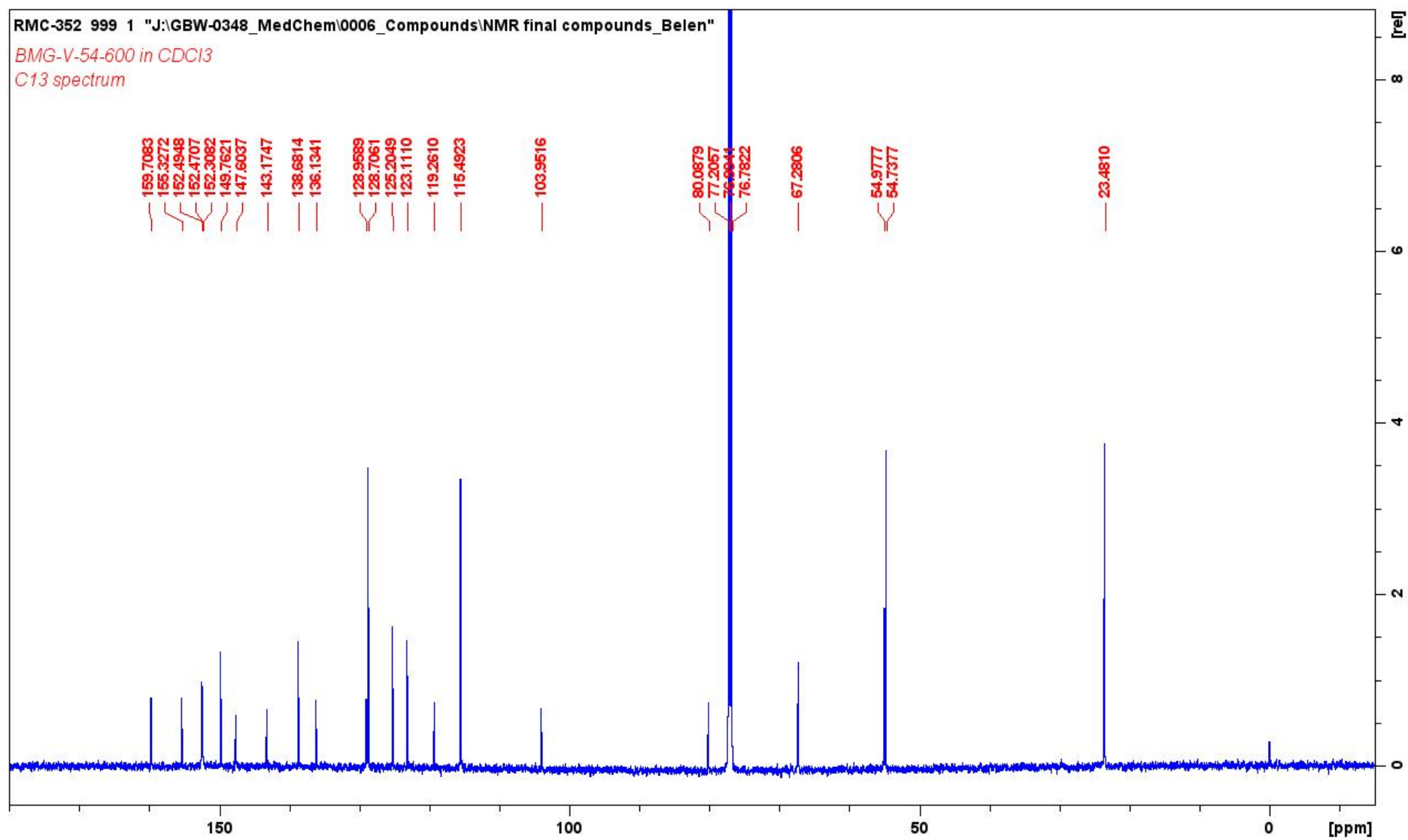
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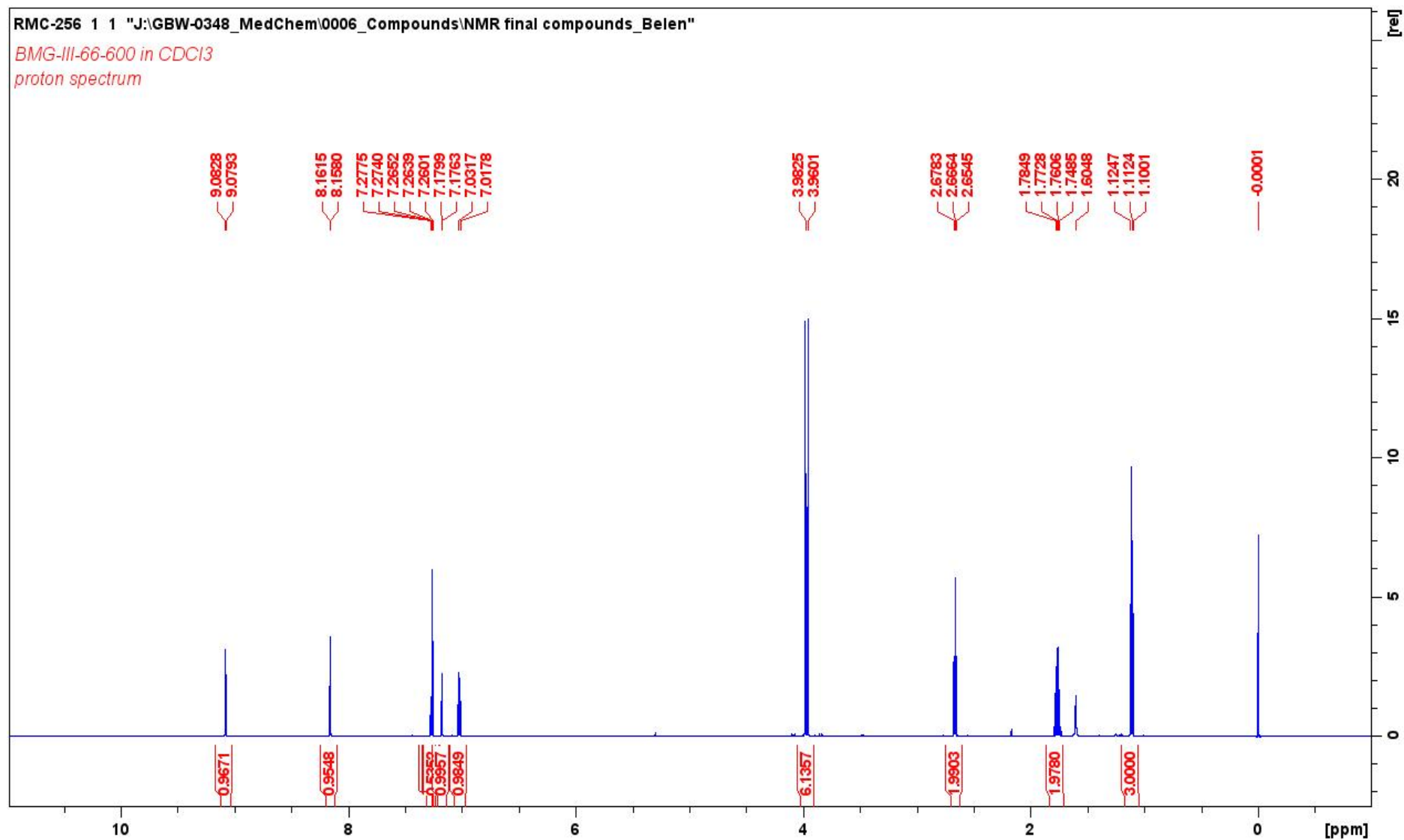
¹H NMR spectrum of **5b**



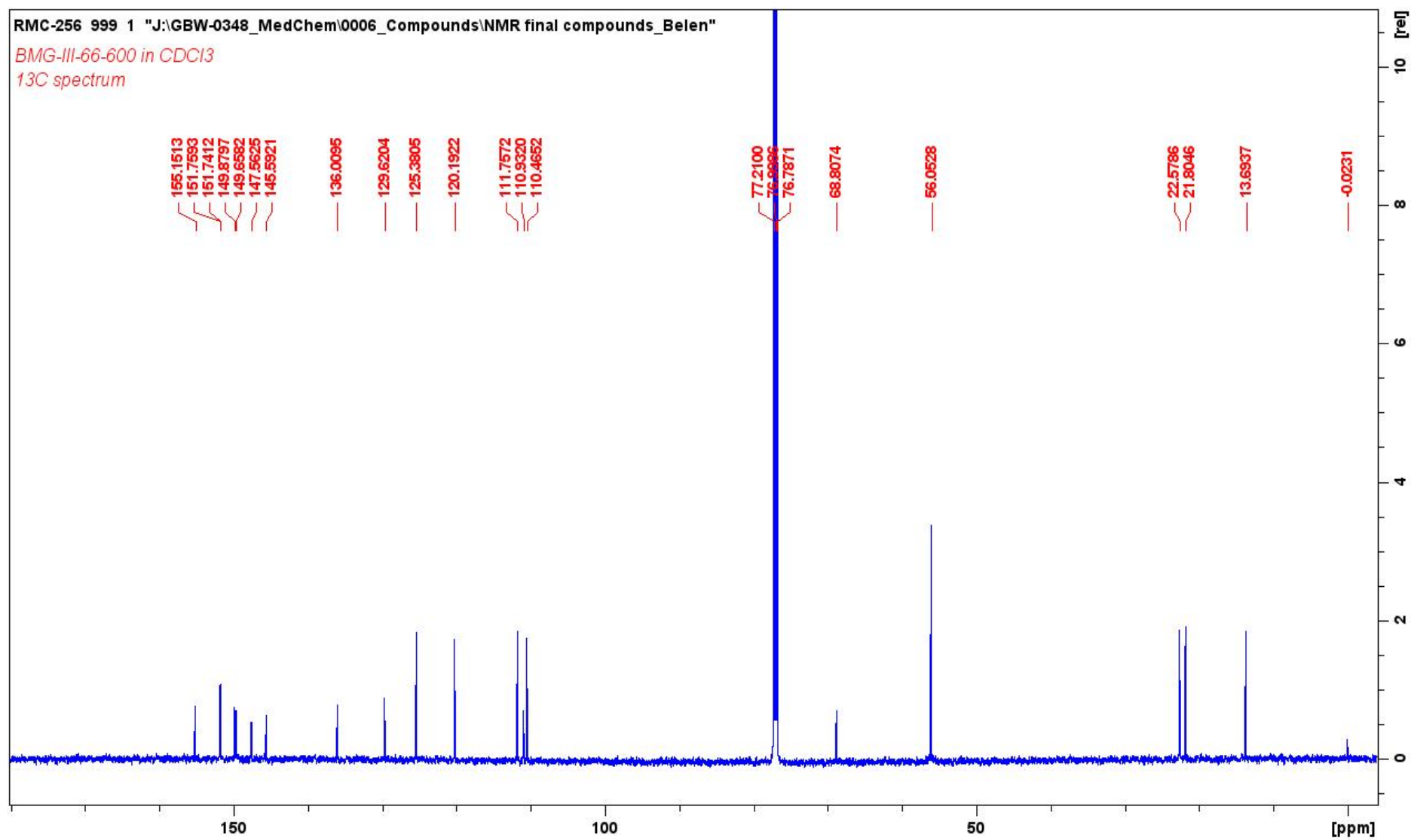
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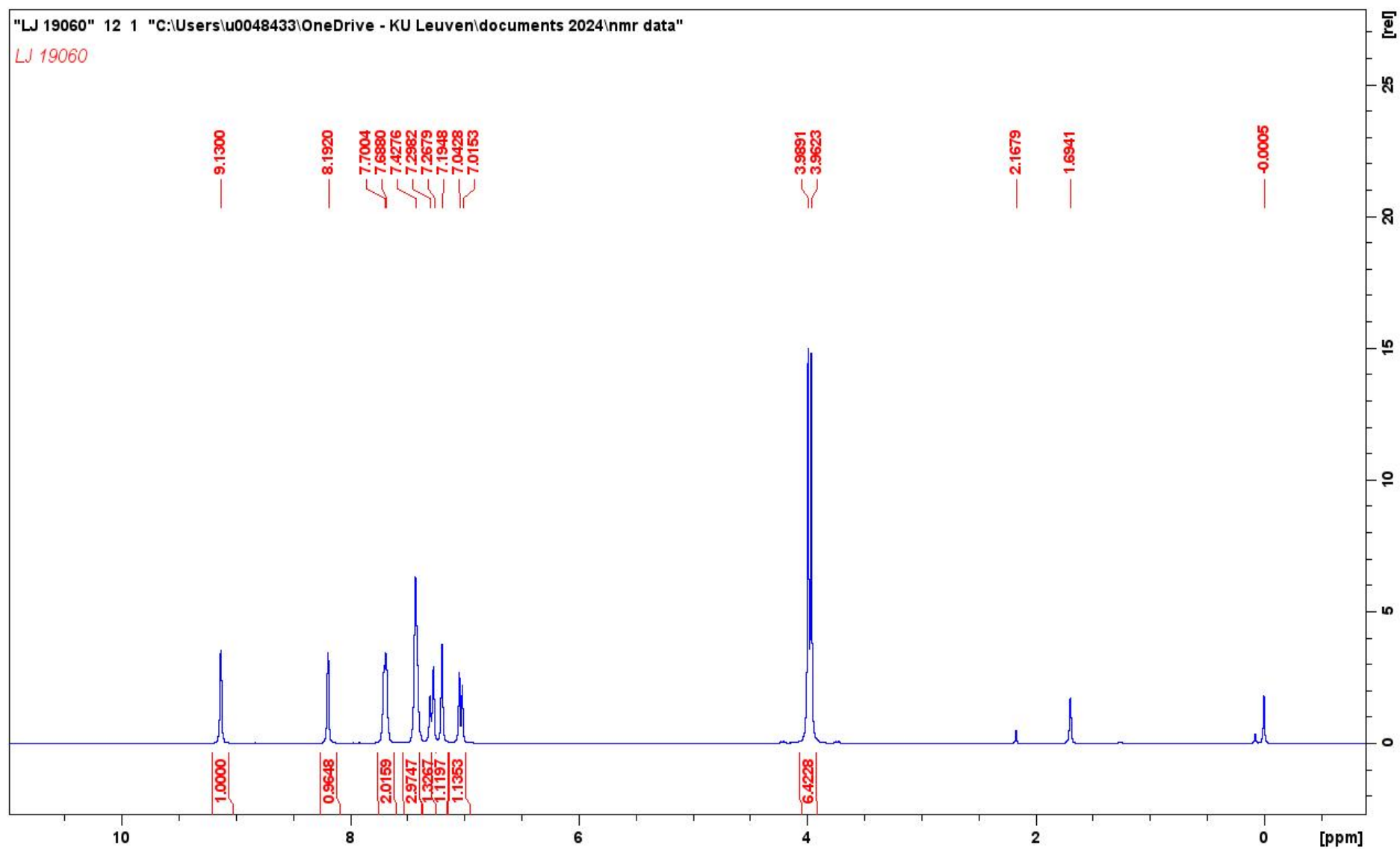
¹H NMR spectrum of 7a



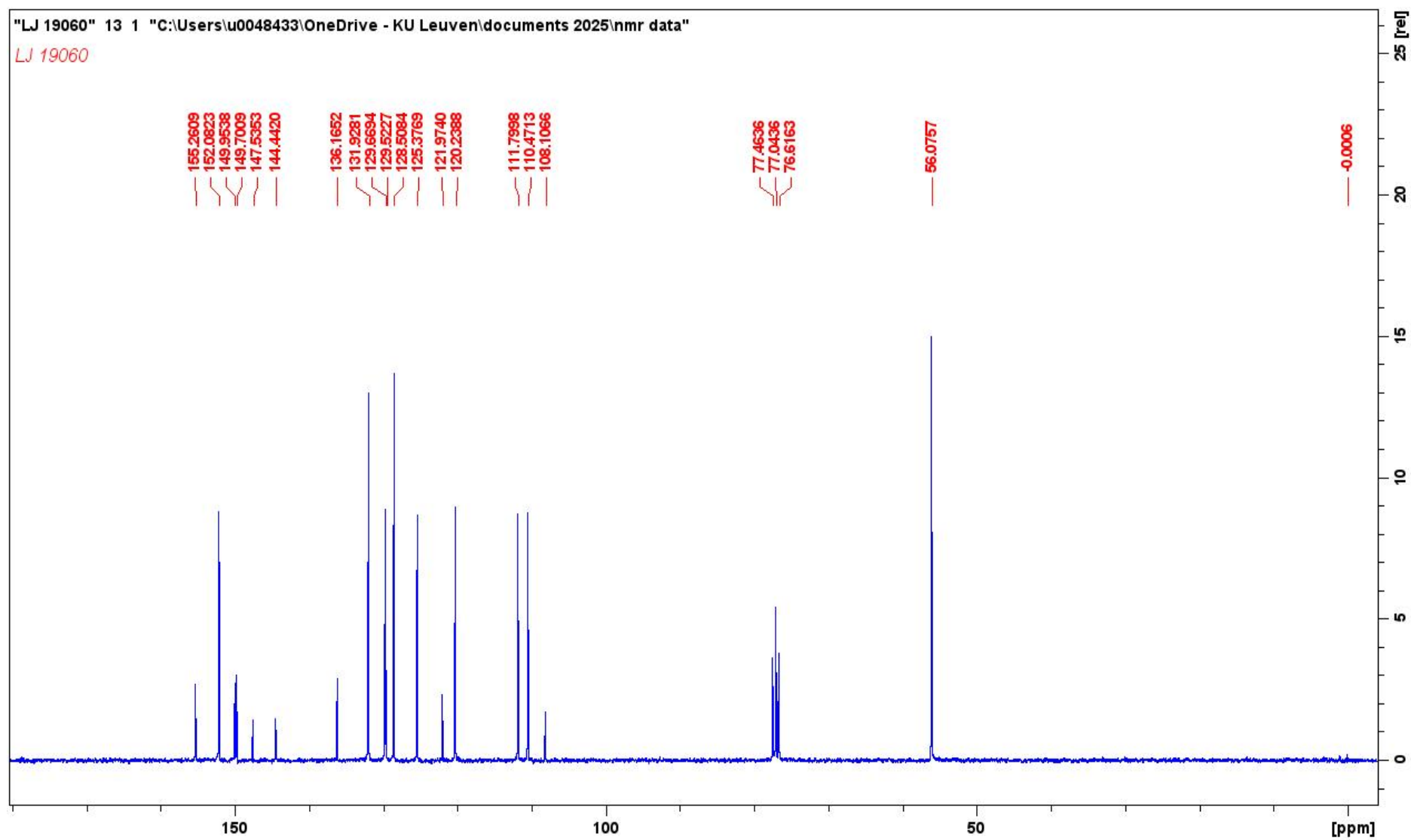
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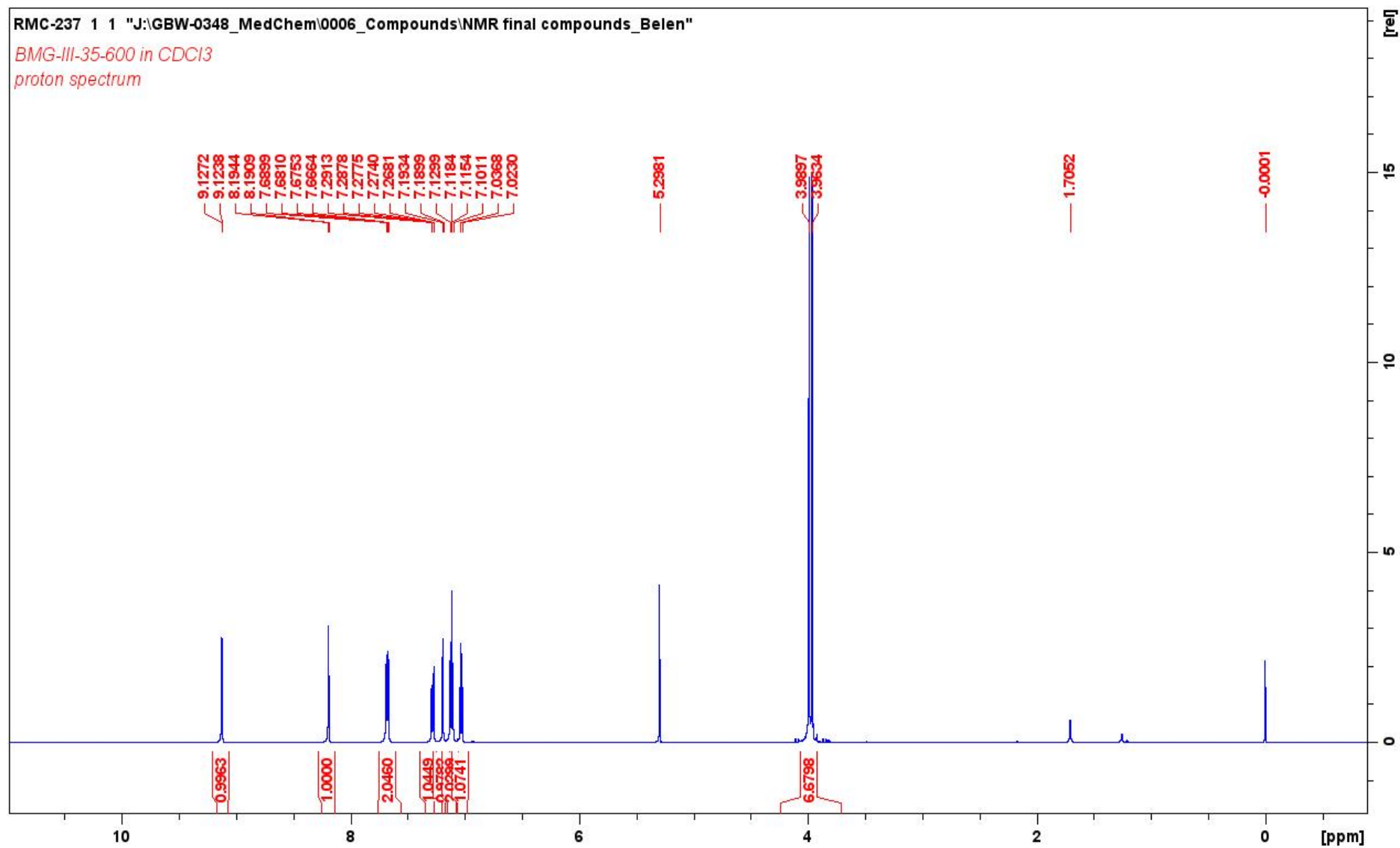
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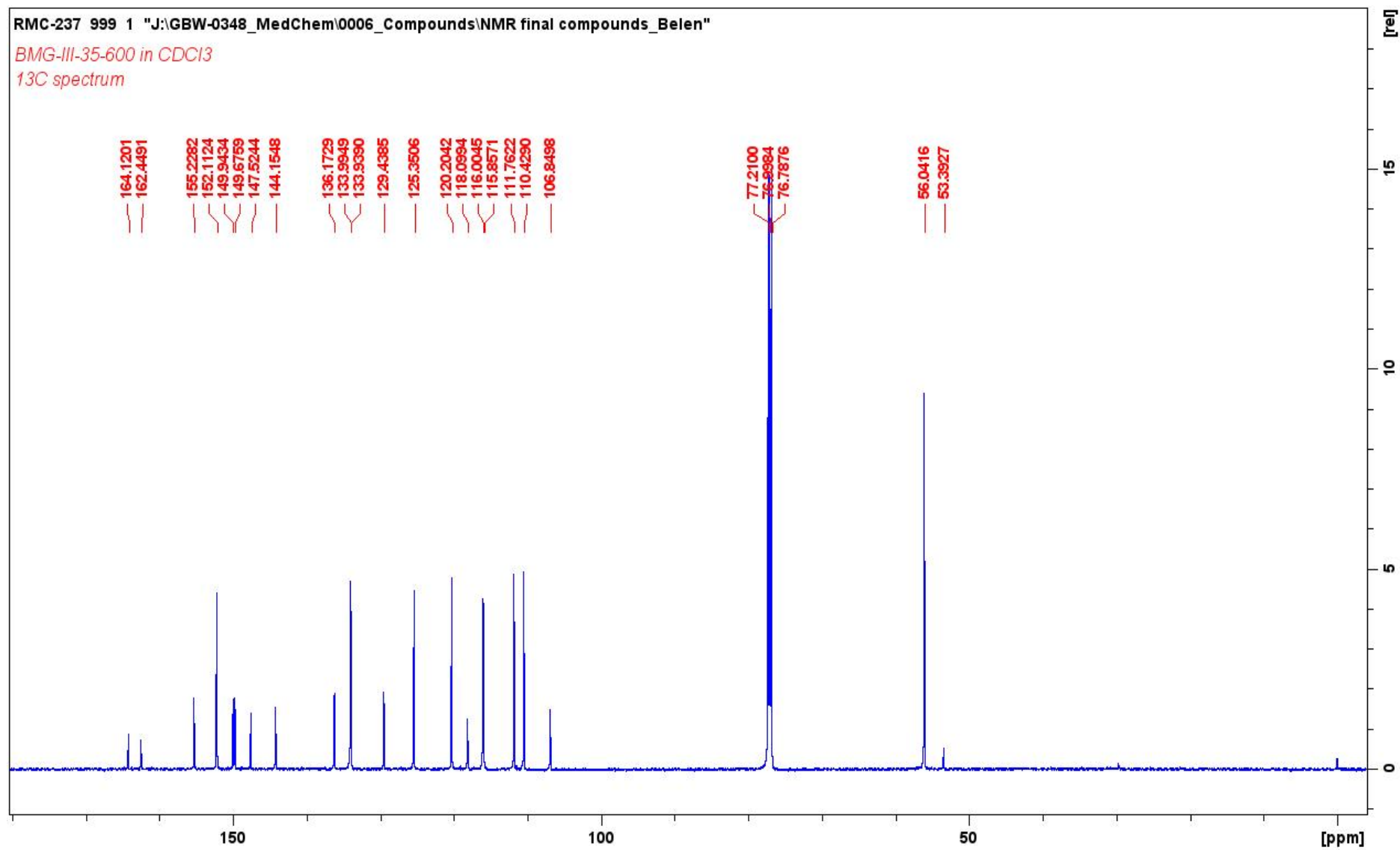
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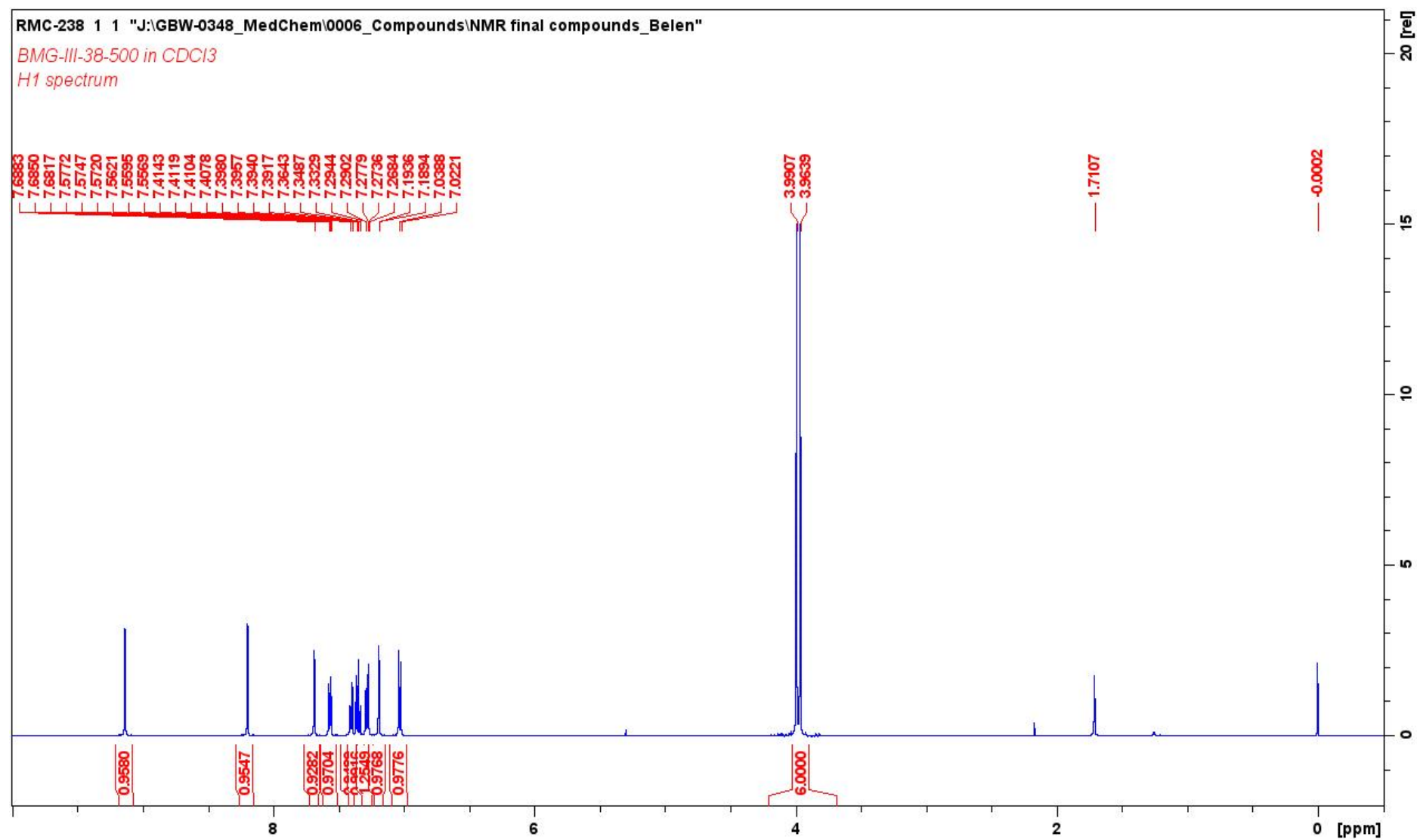
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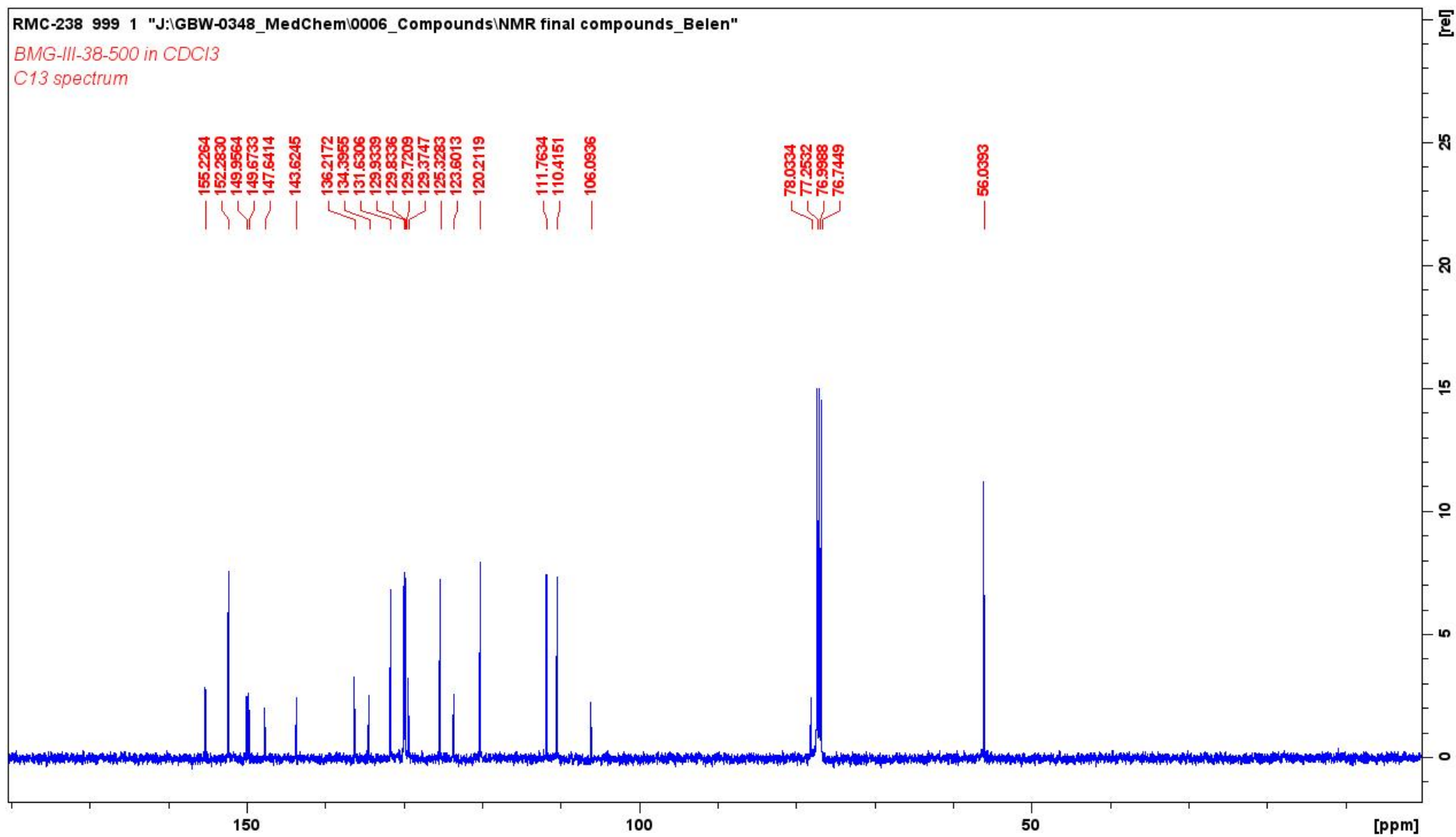
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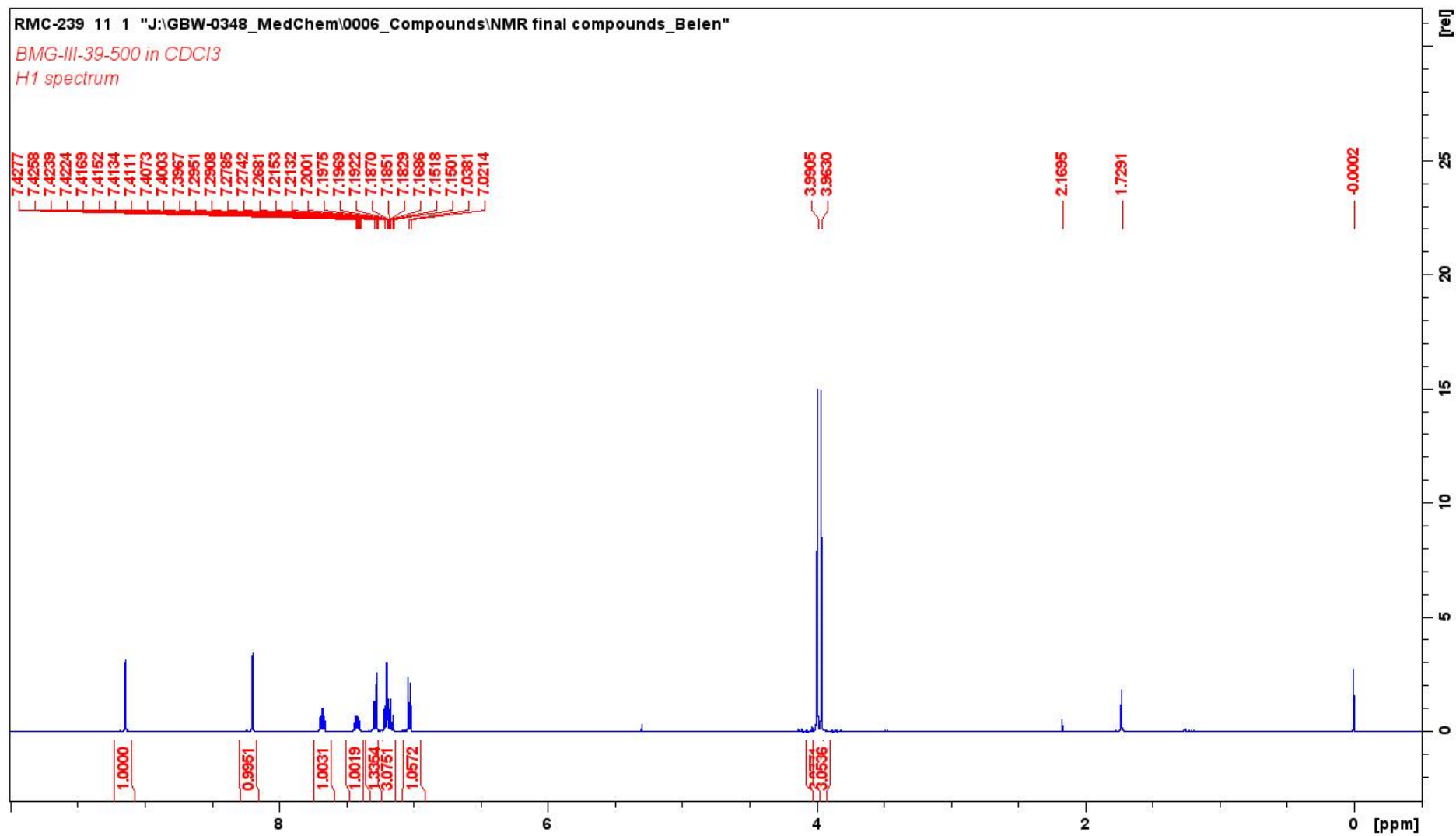
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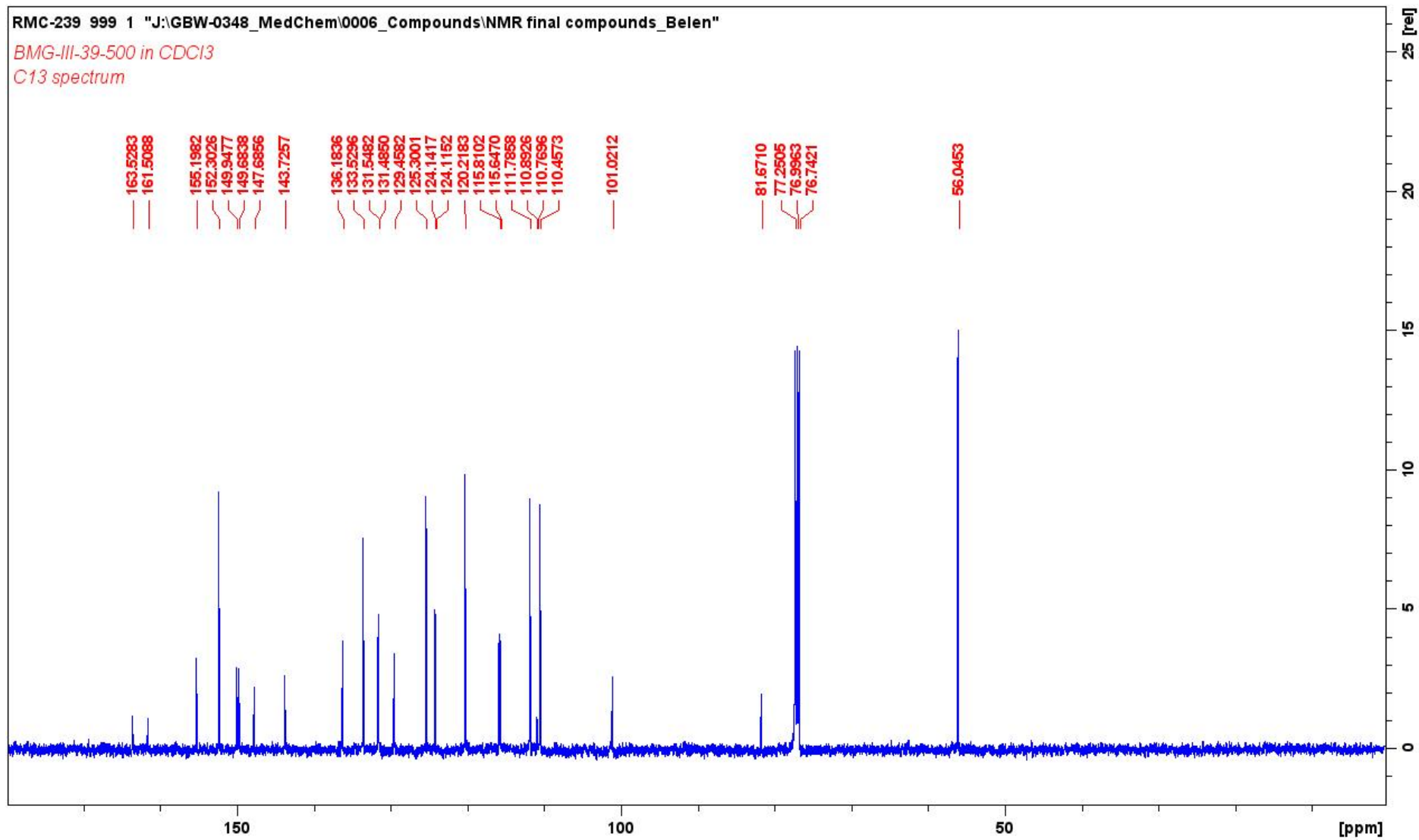
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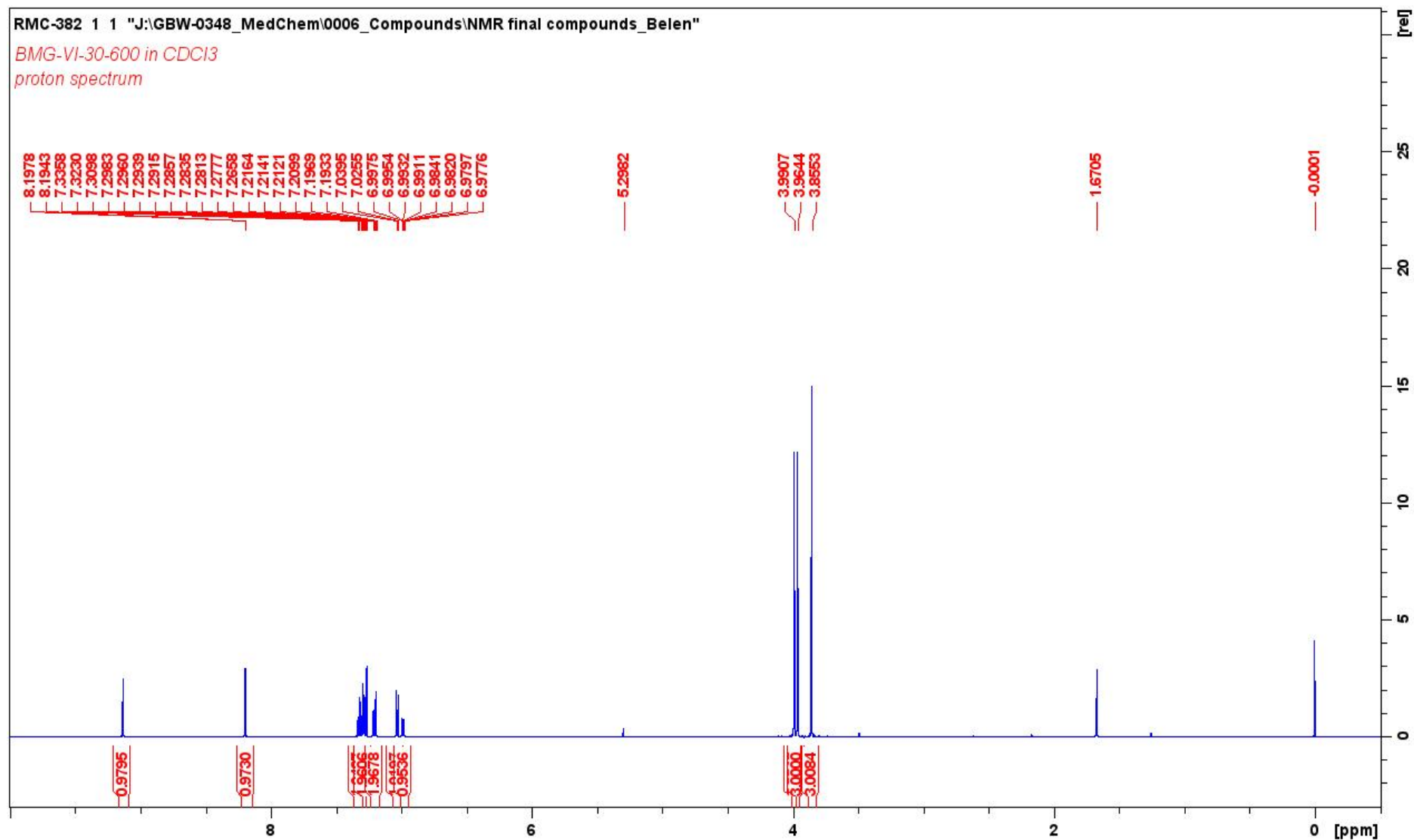
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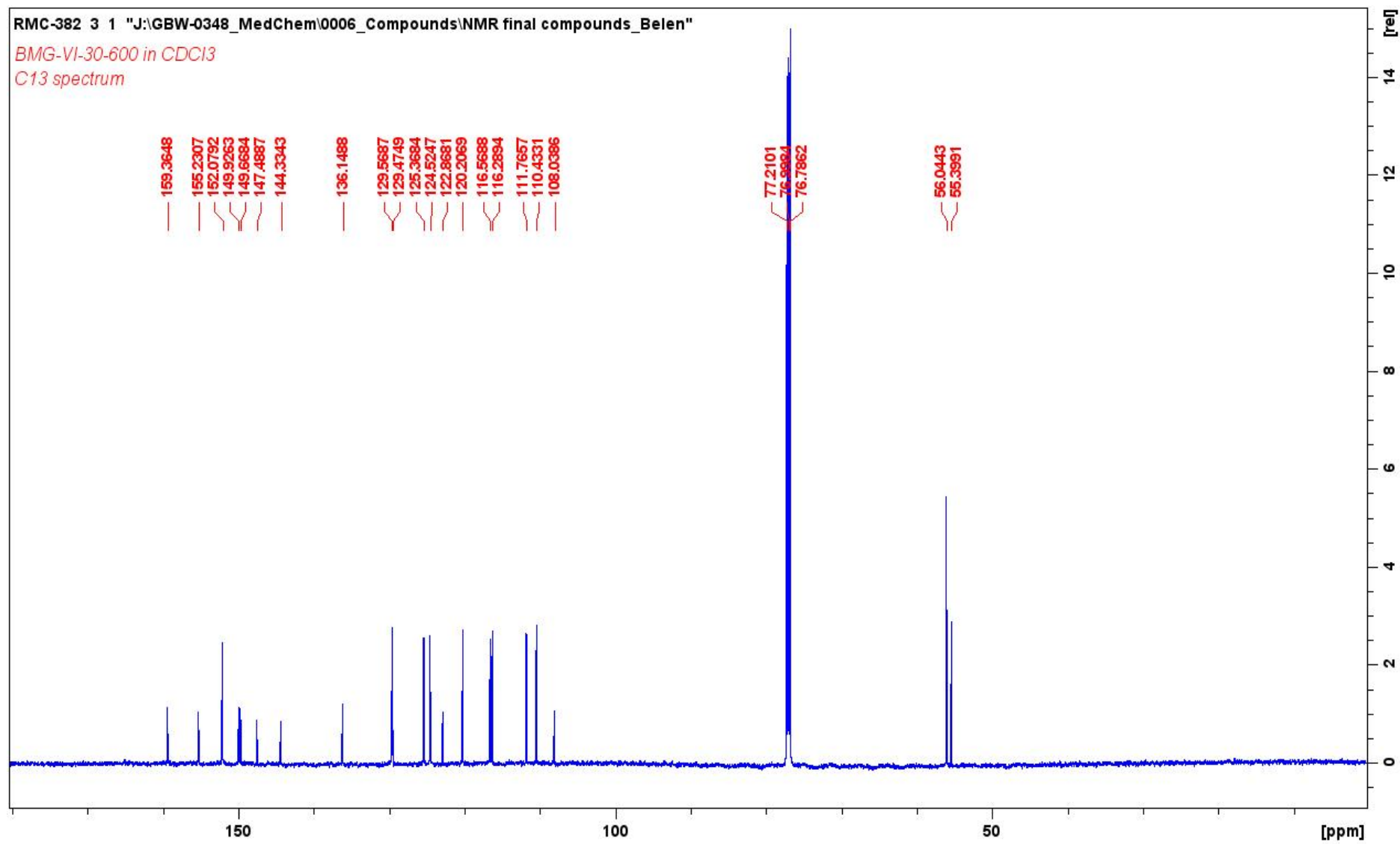
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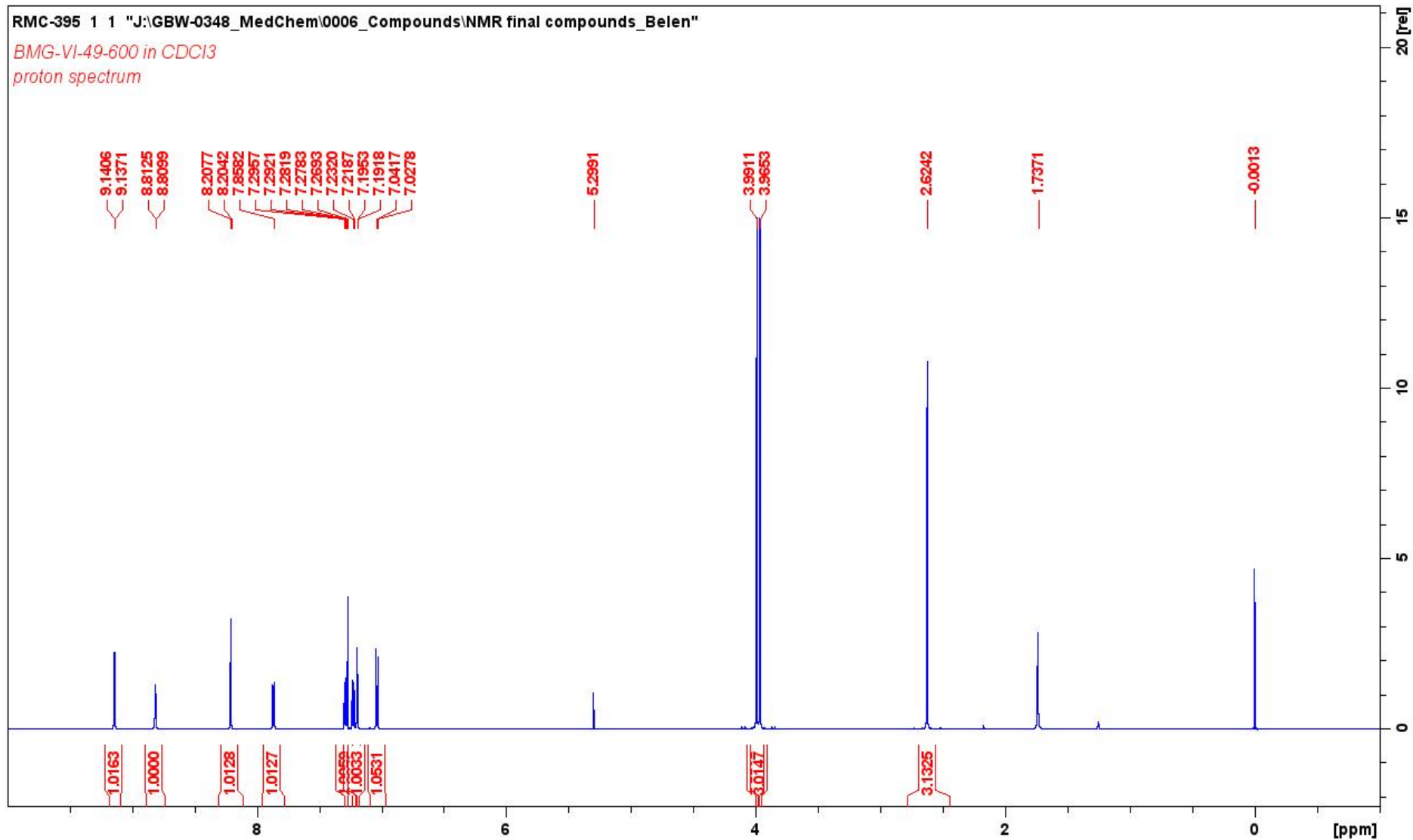
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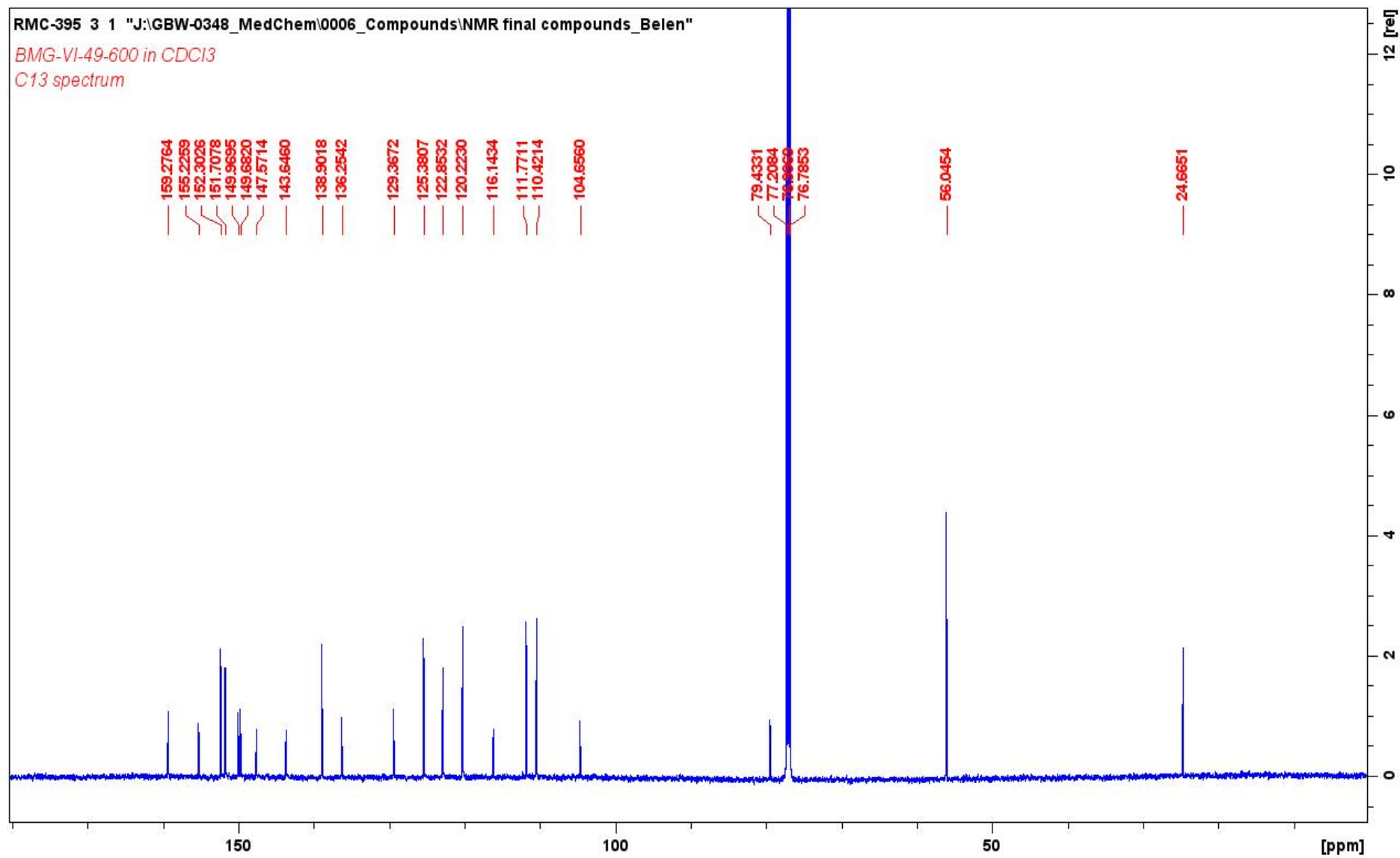
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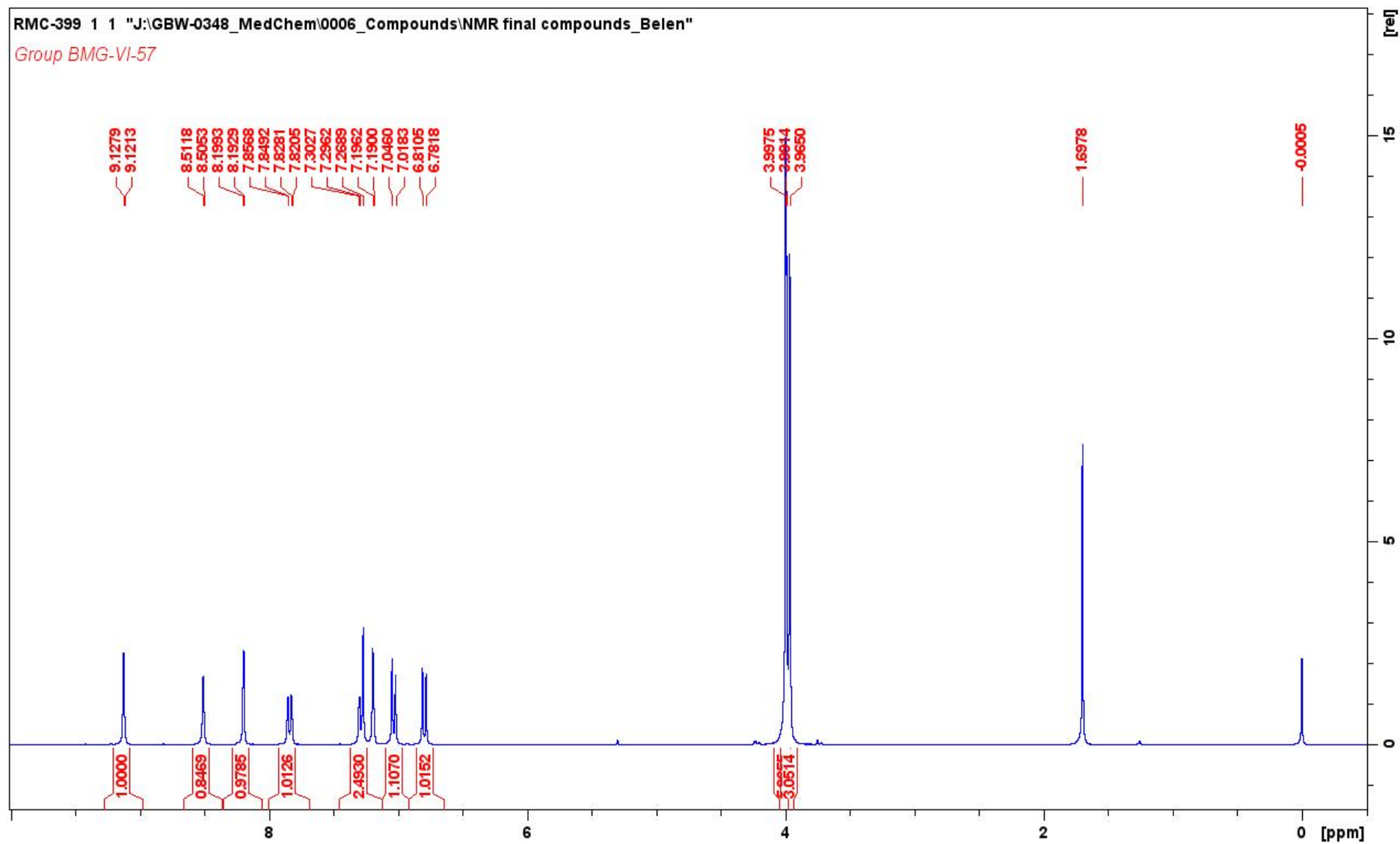
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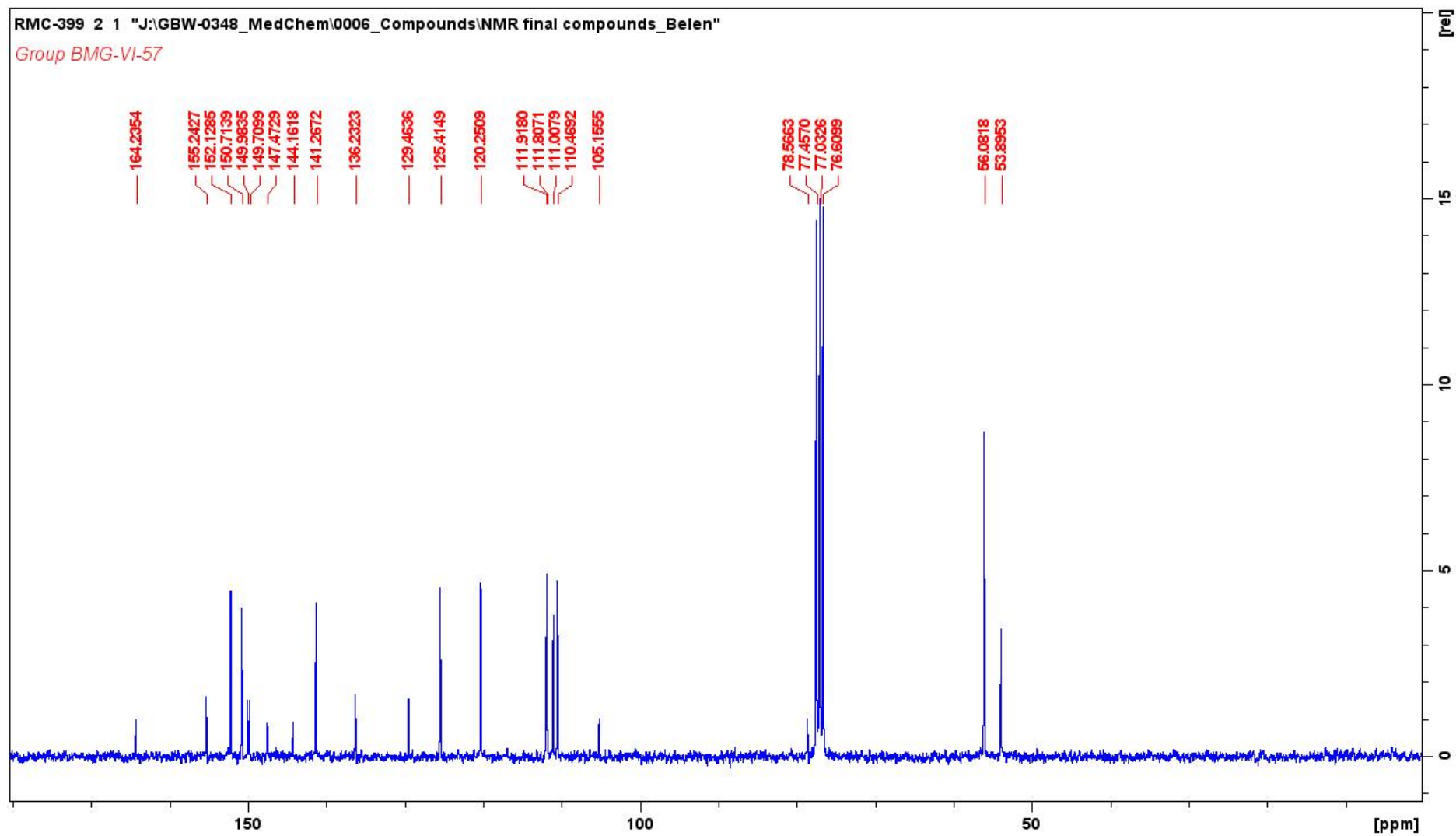
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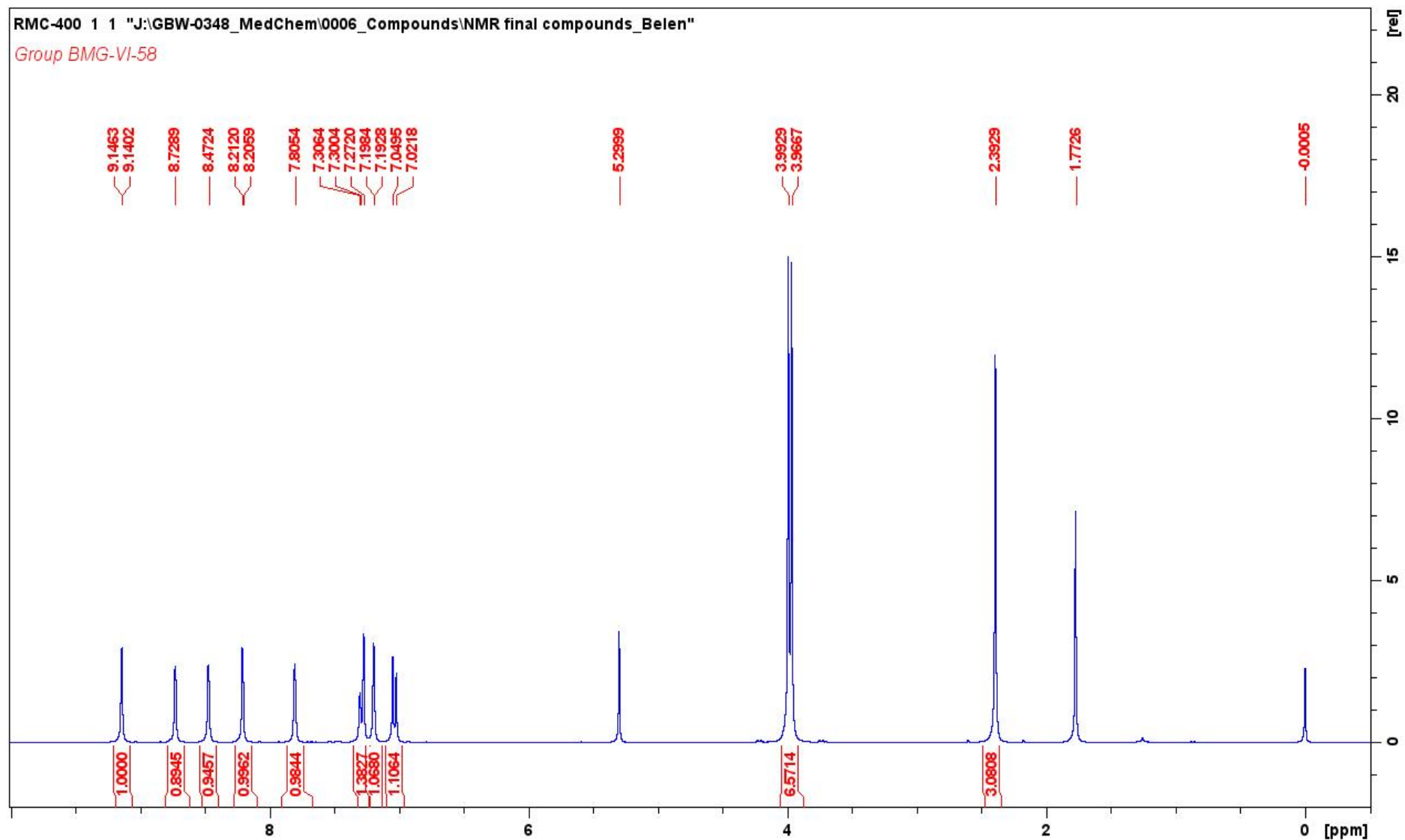
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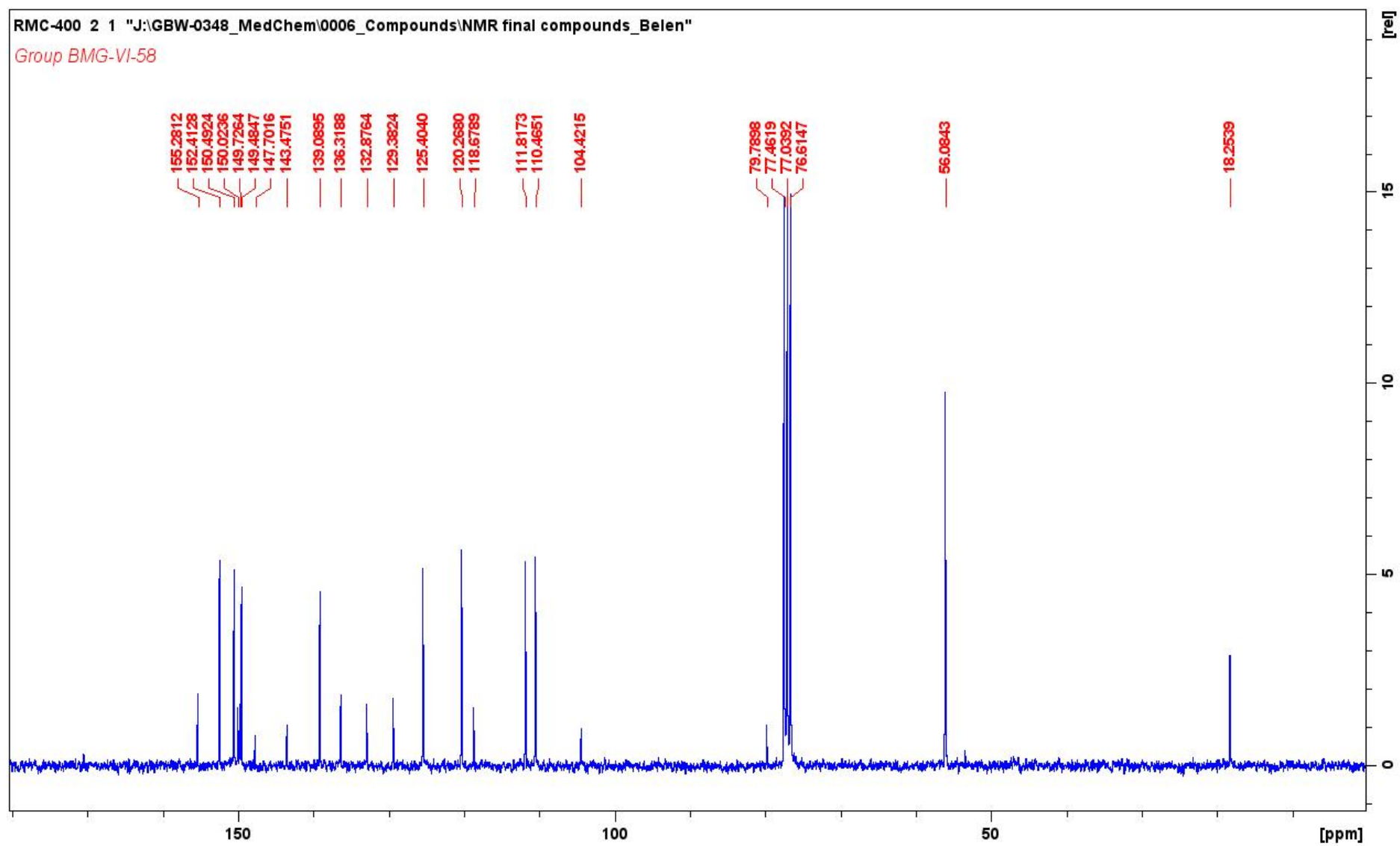
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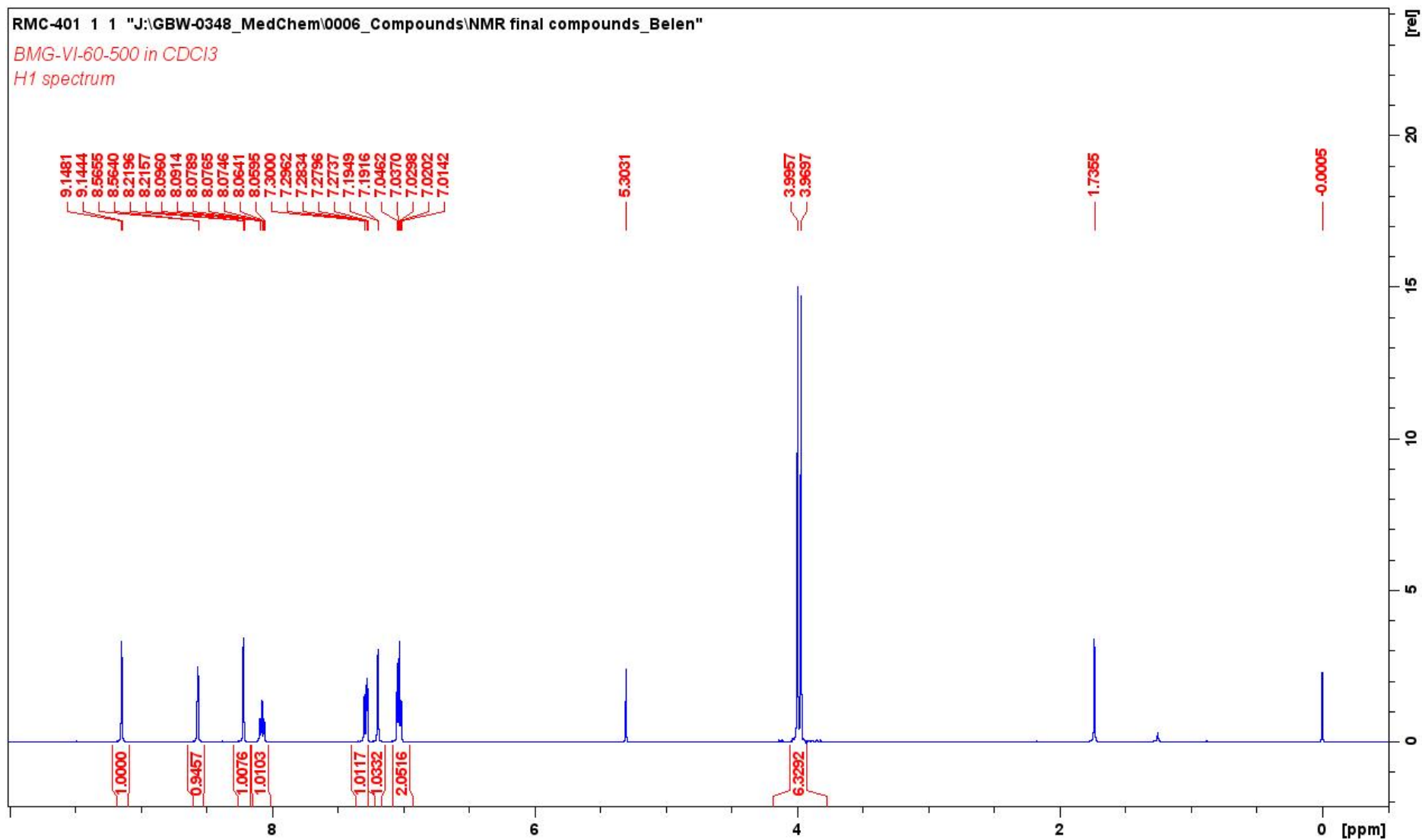
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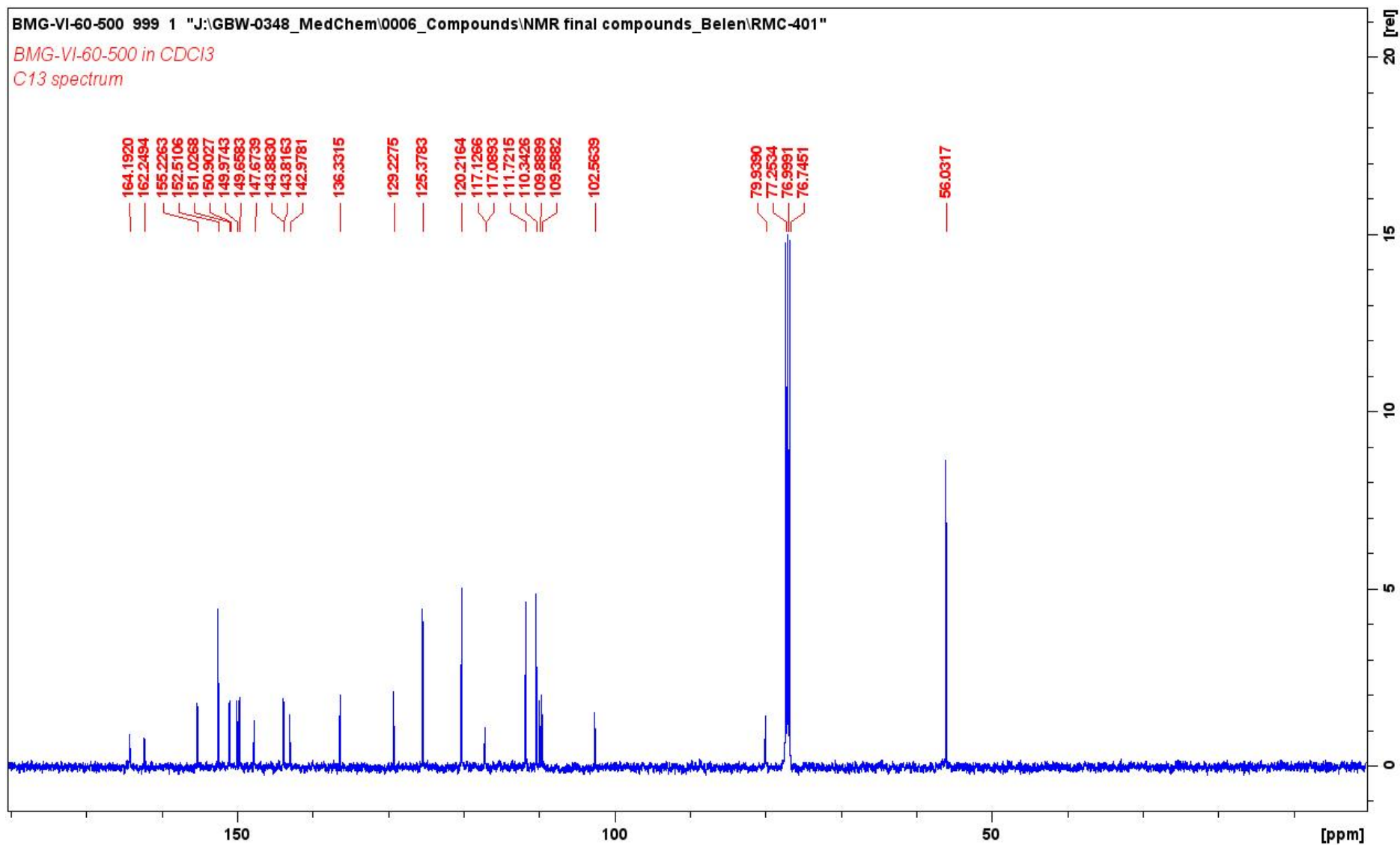
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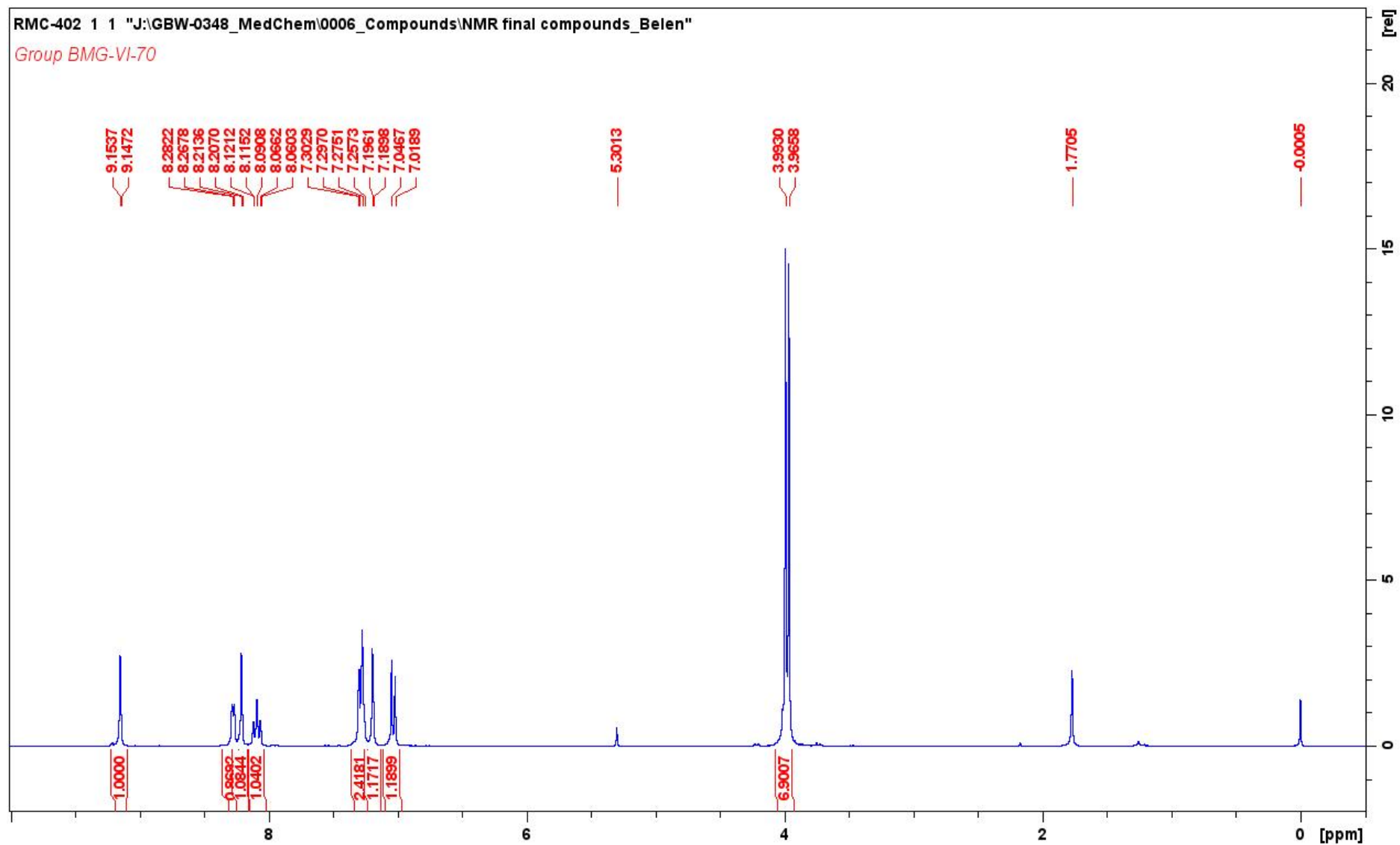
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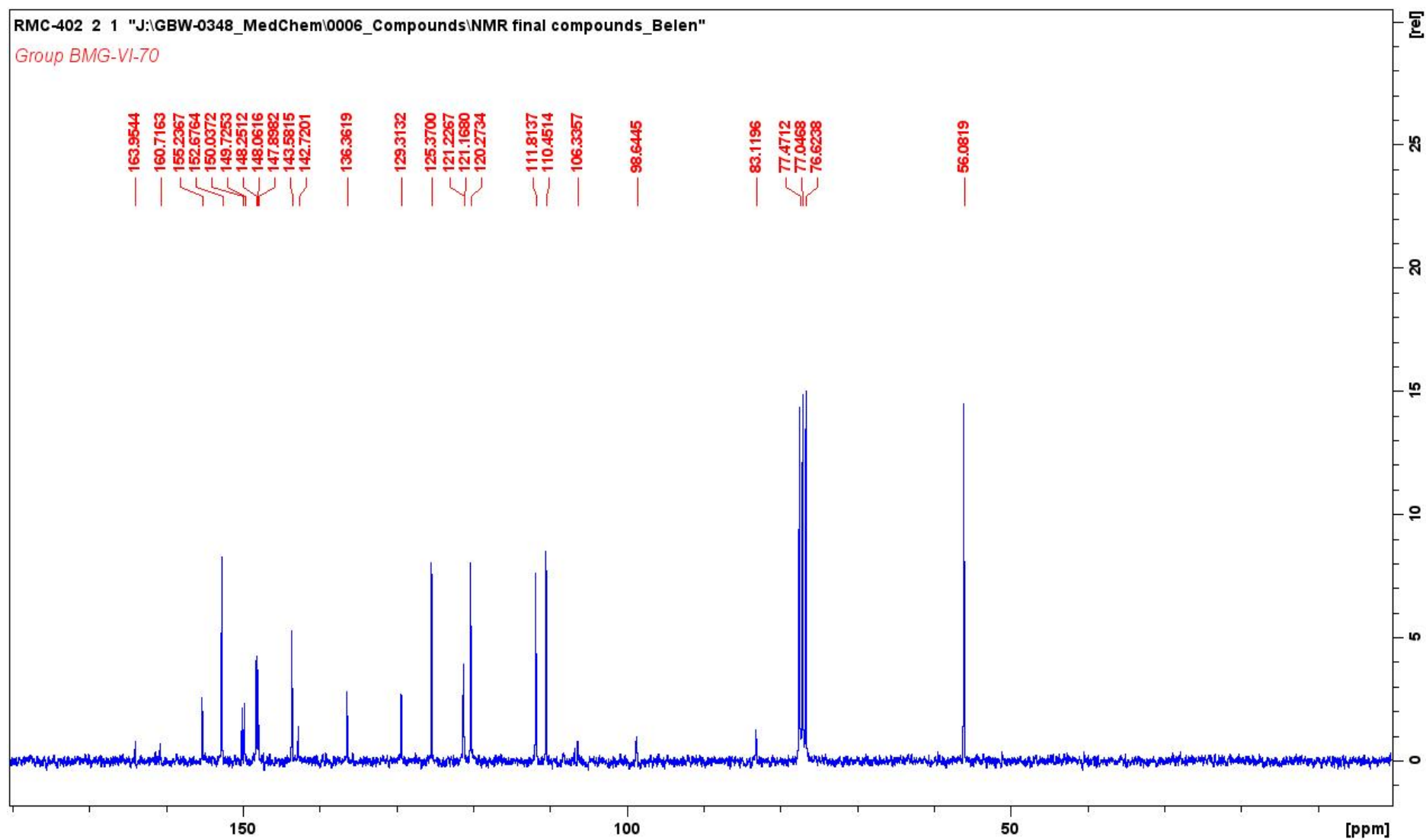
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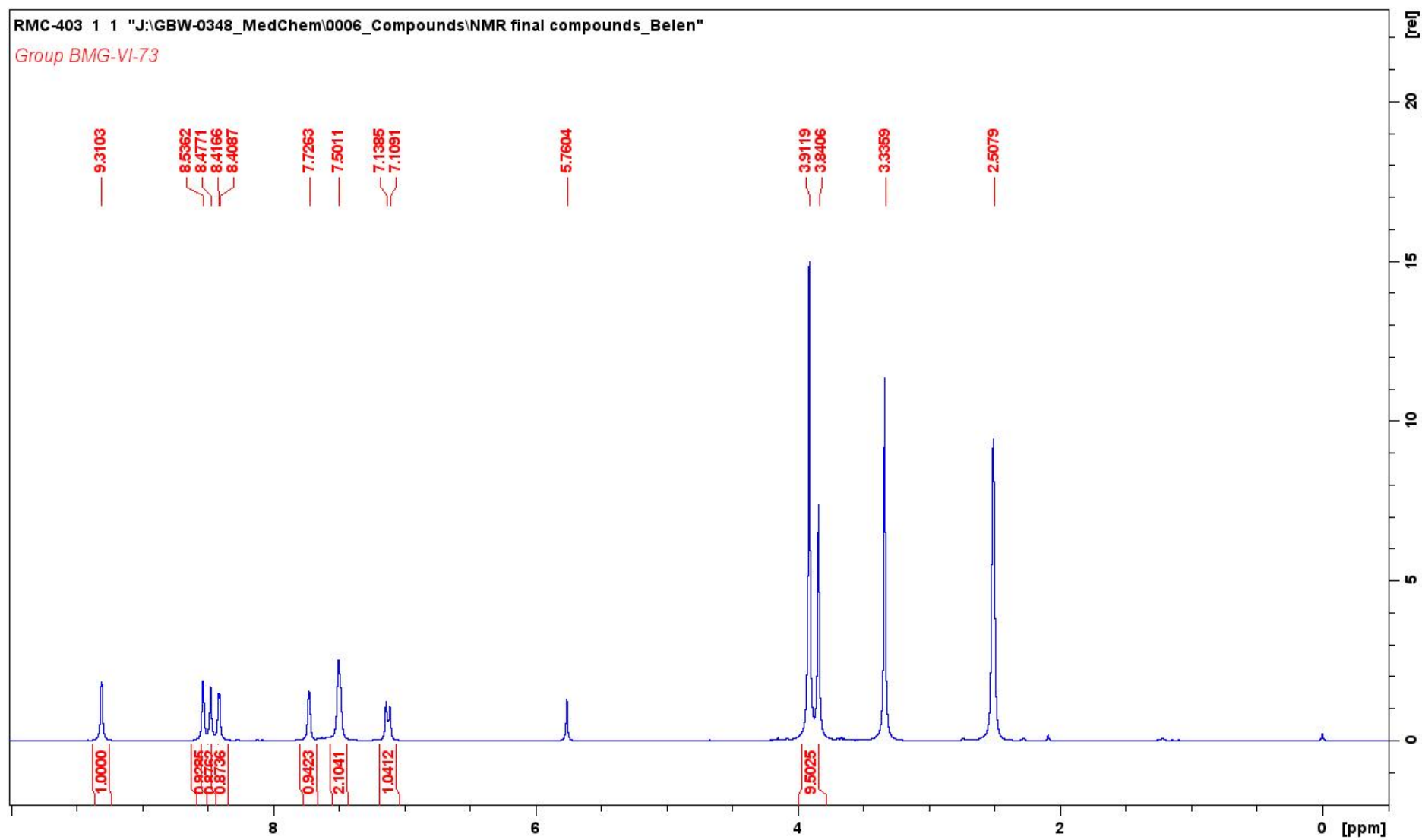
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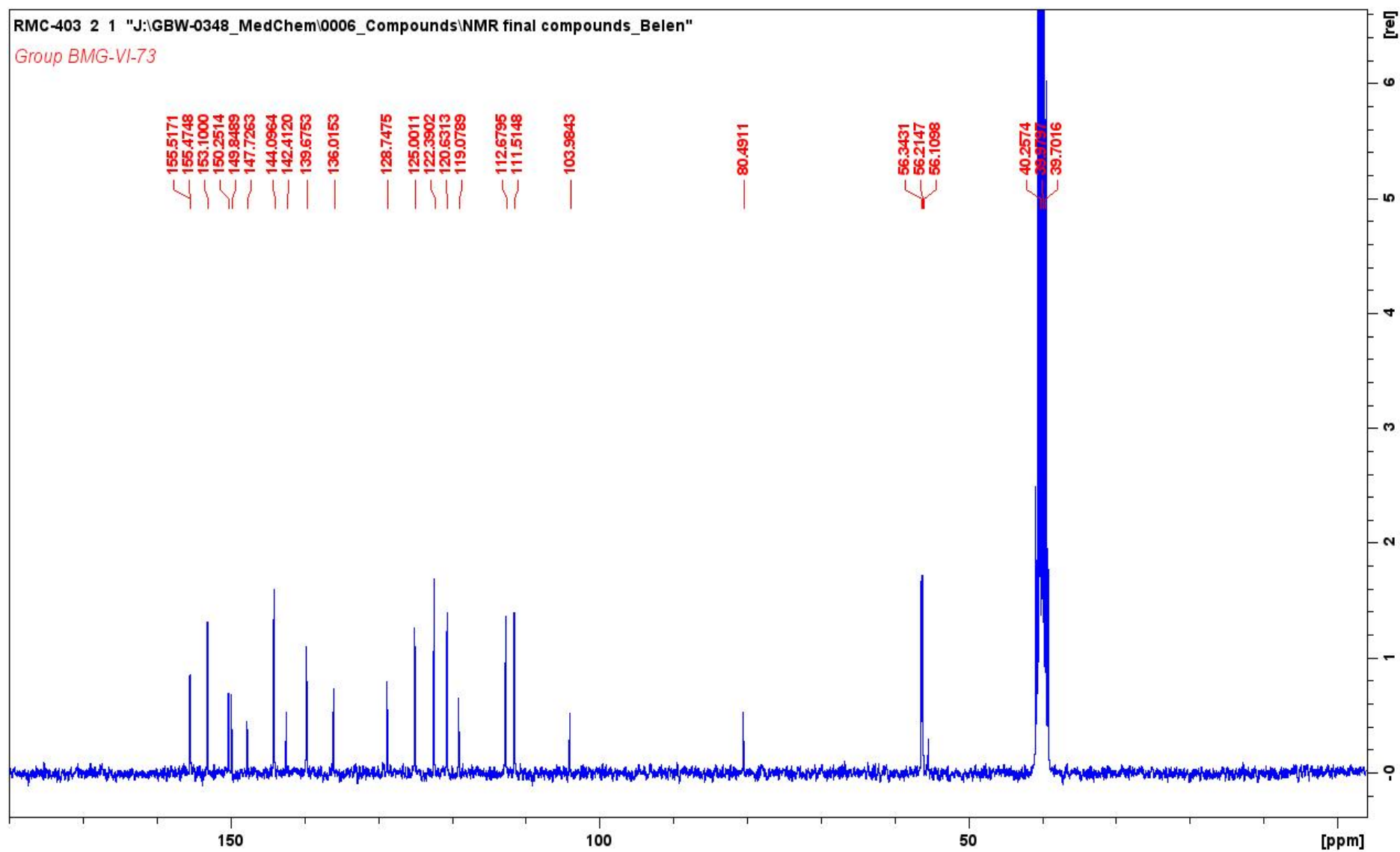
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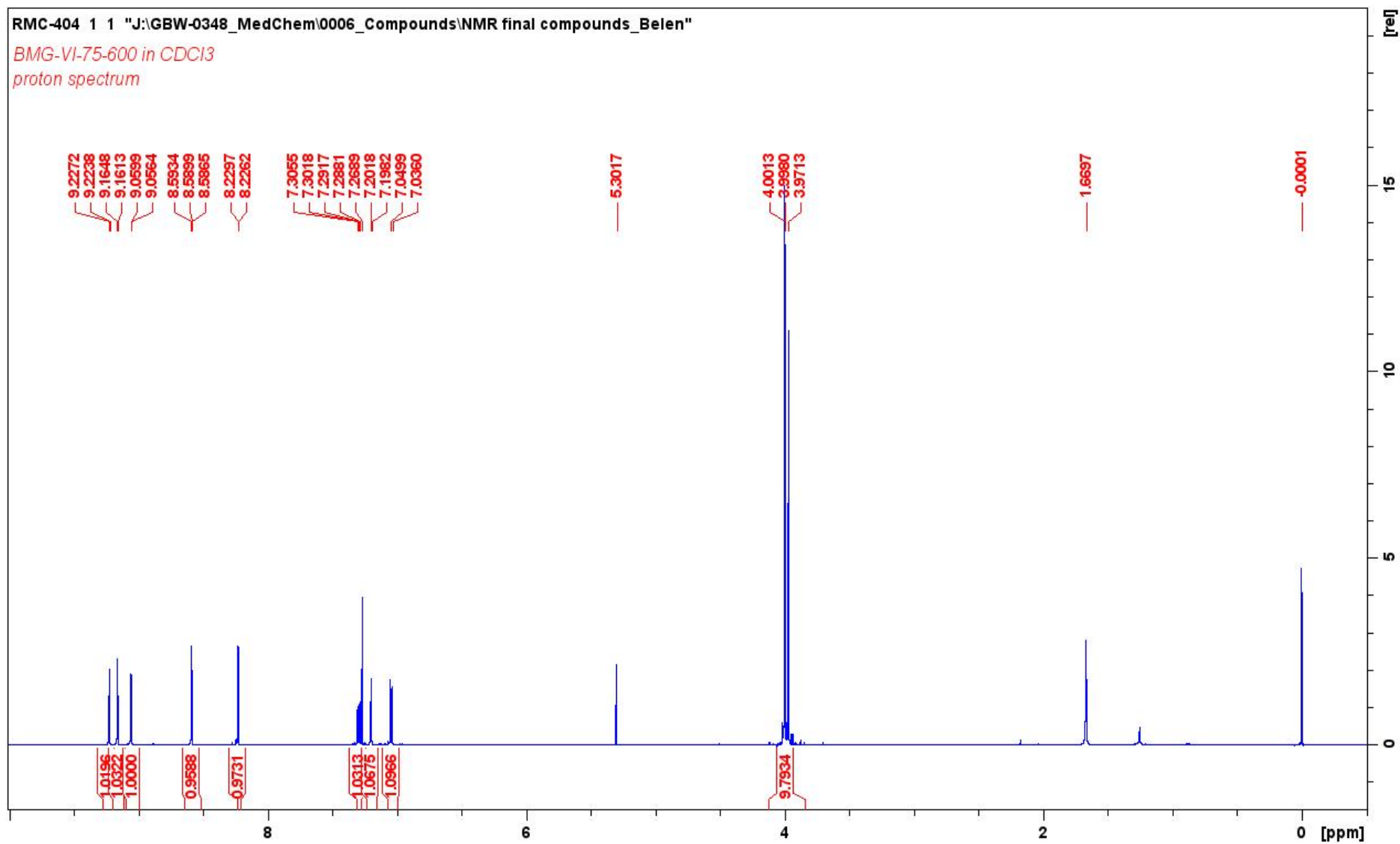
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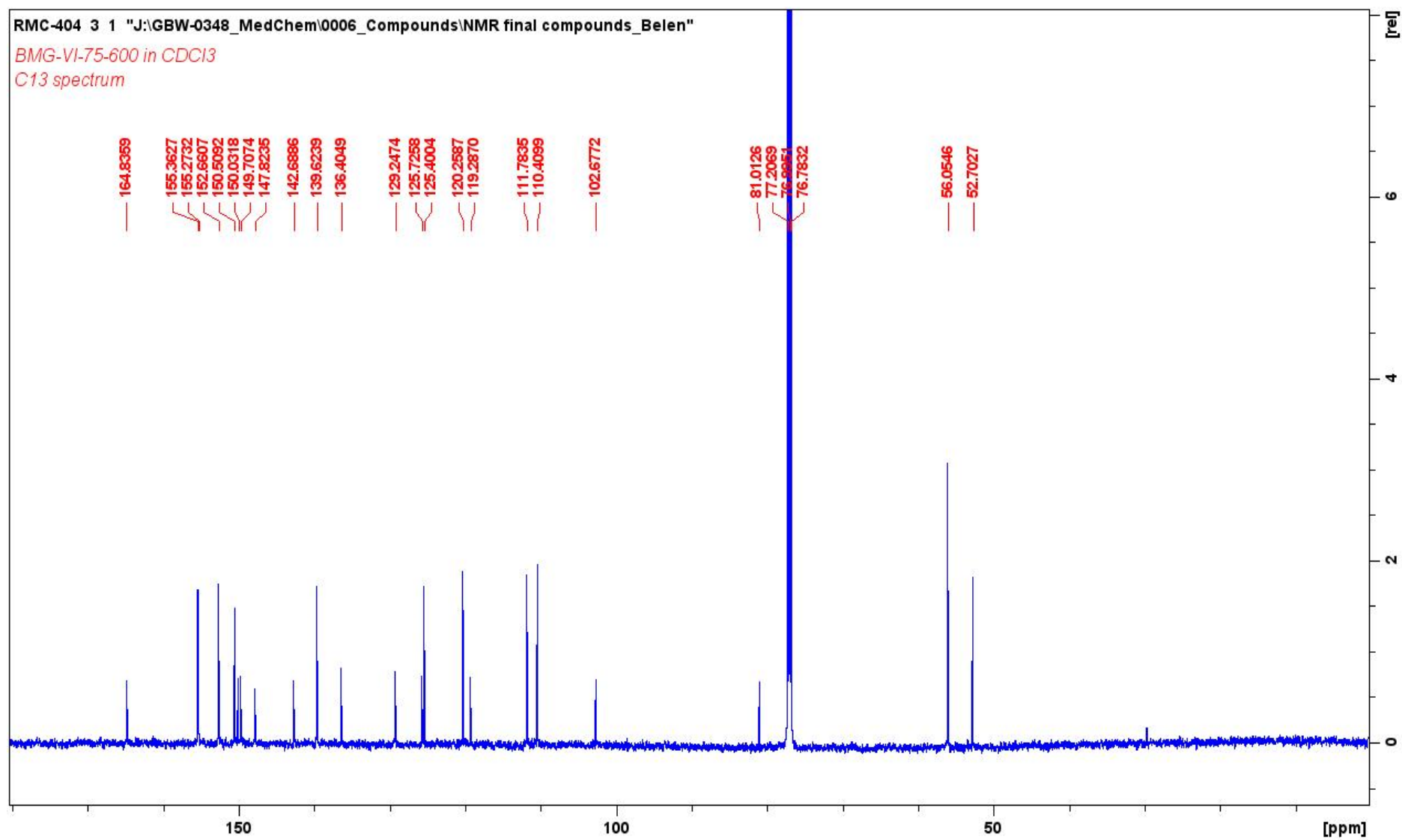
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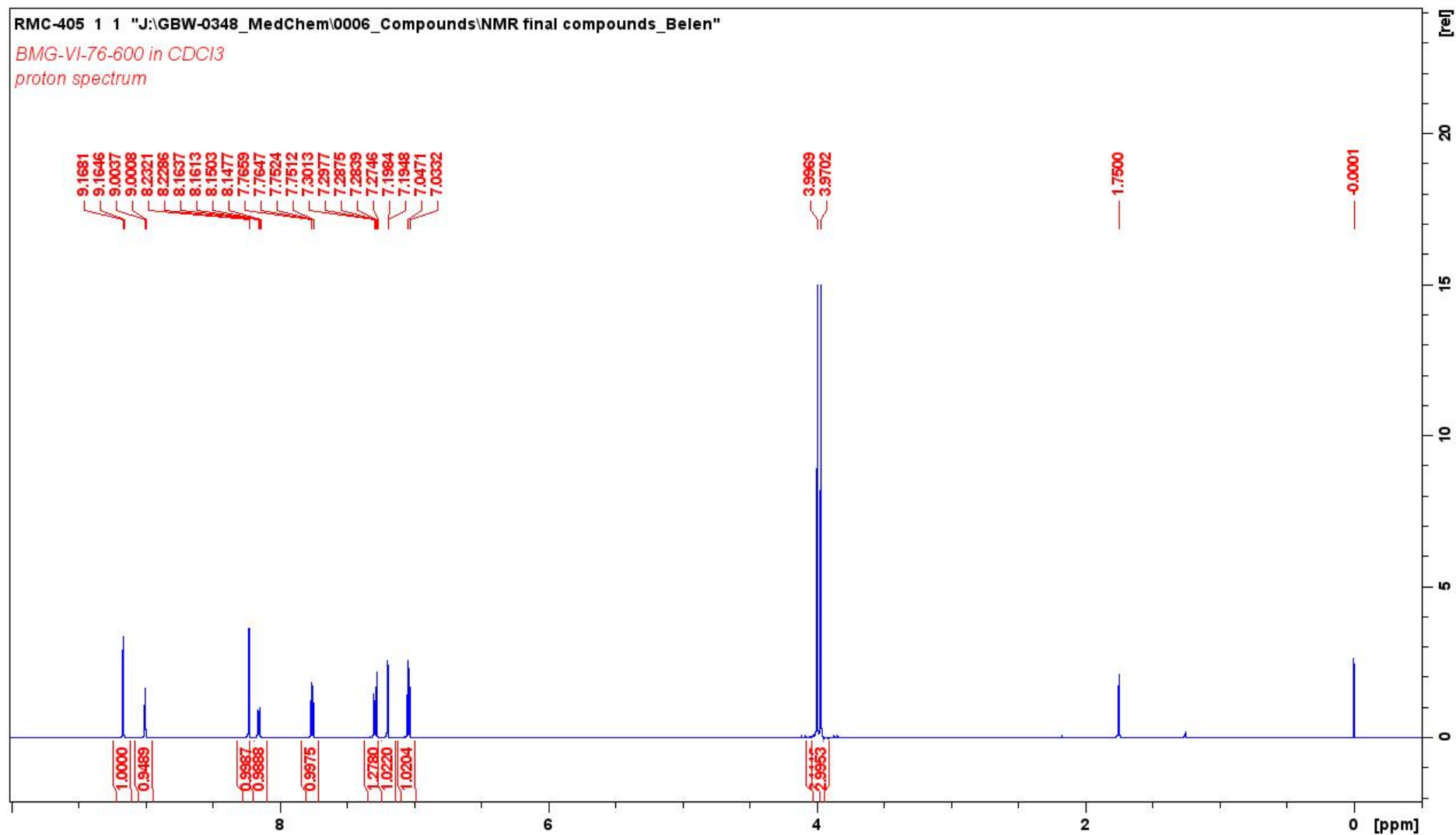
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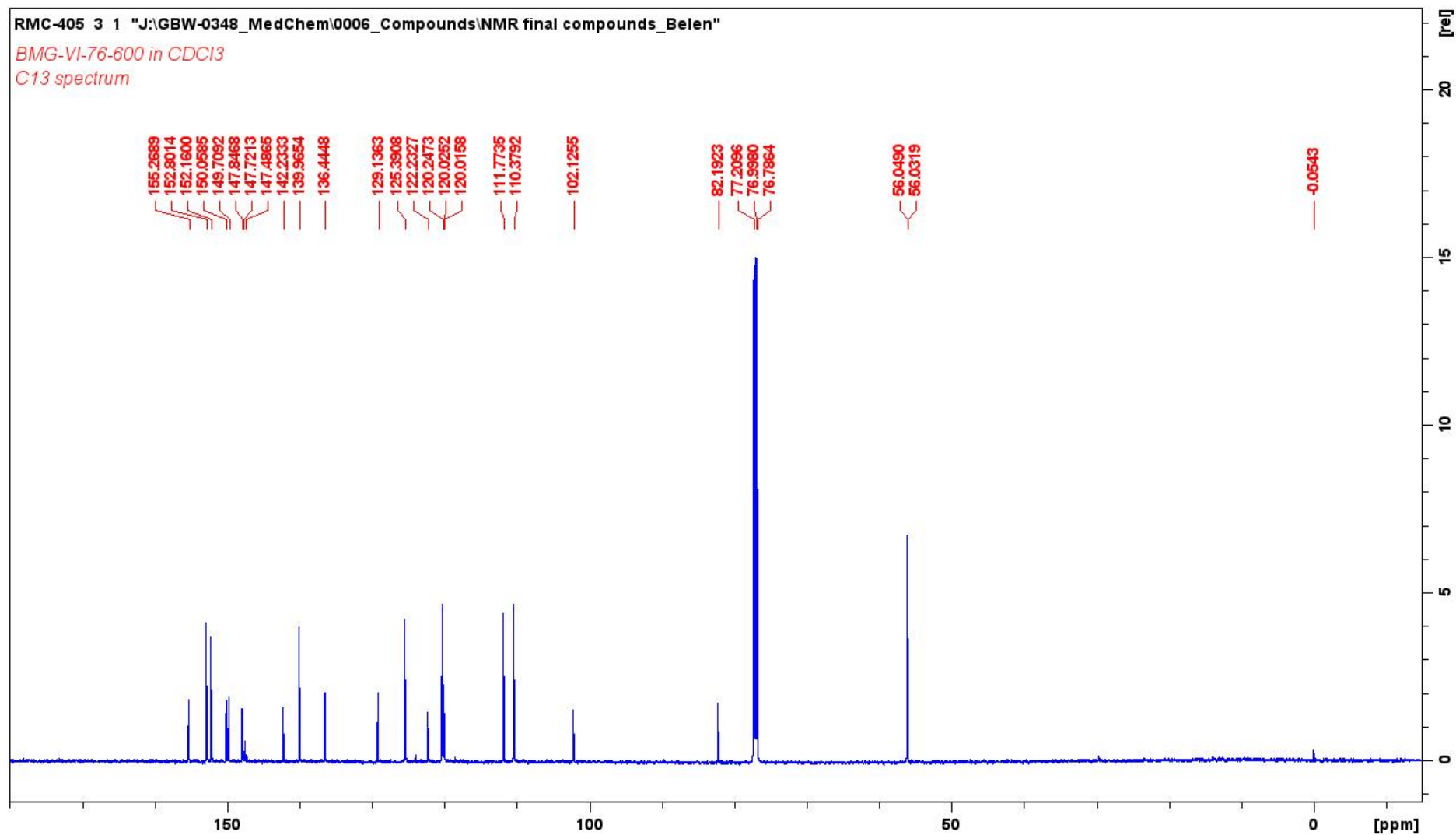
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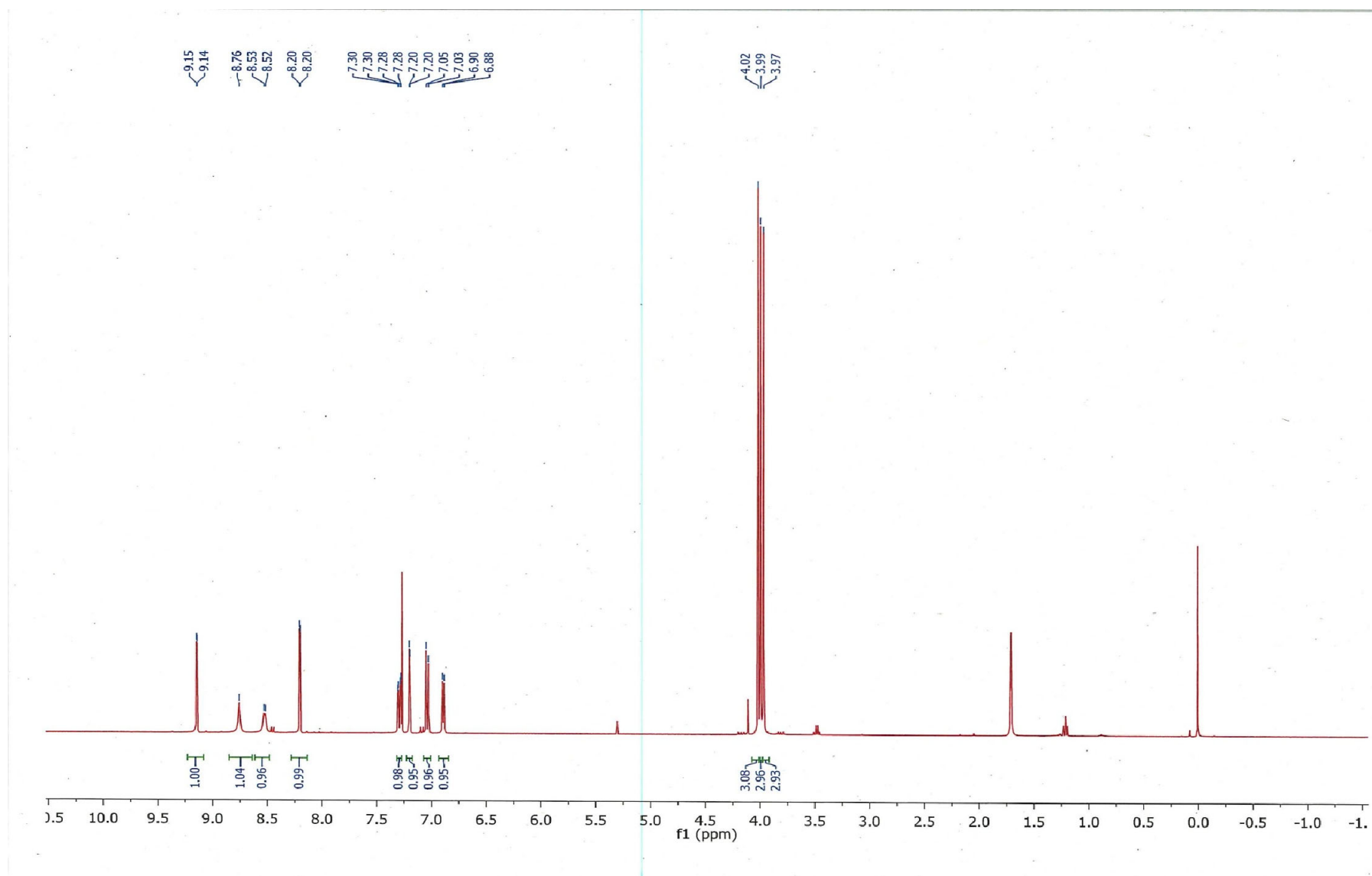
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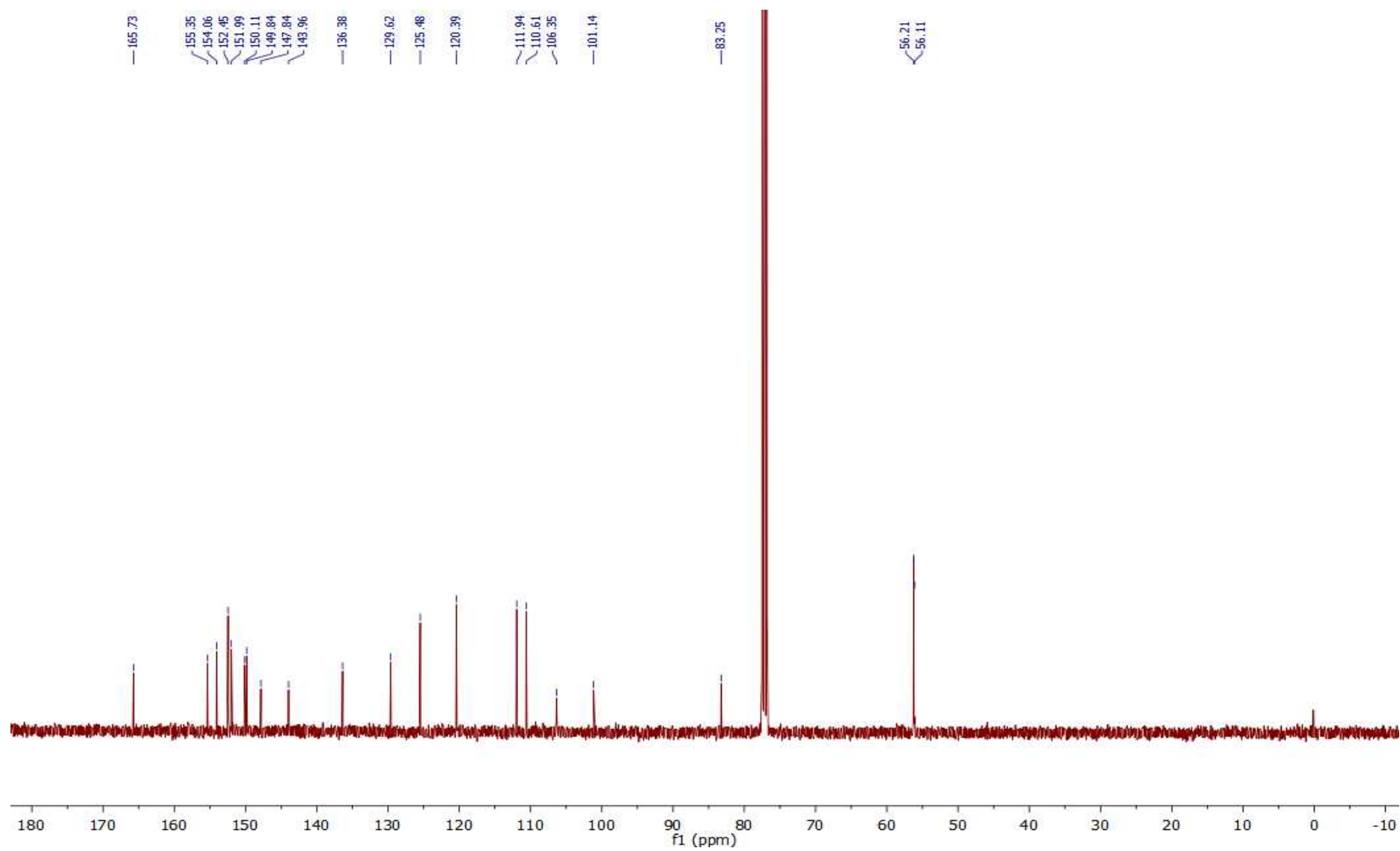
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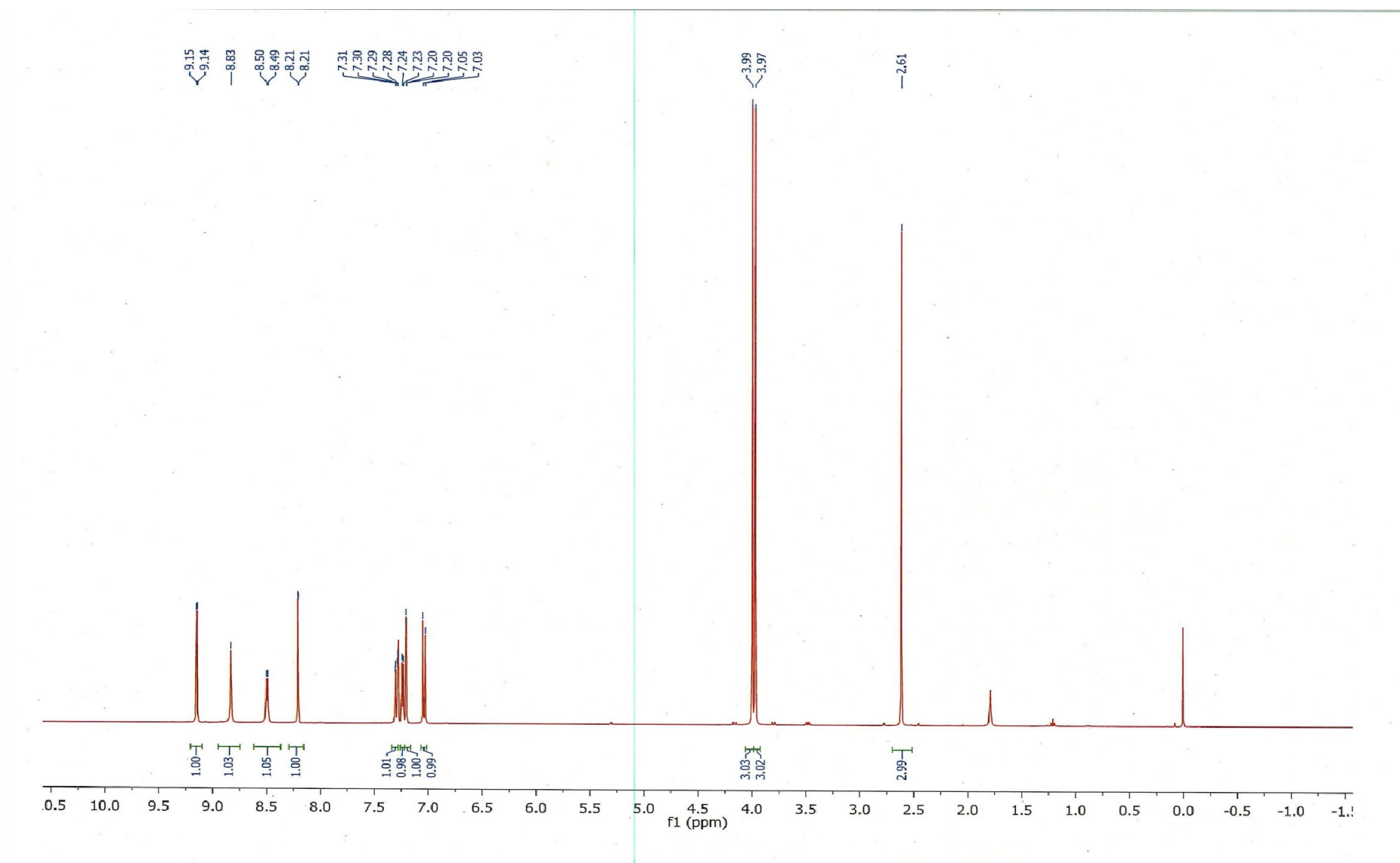
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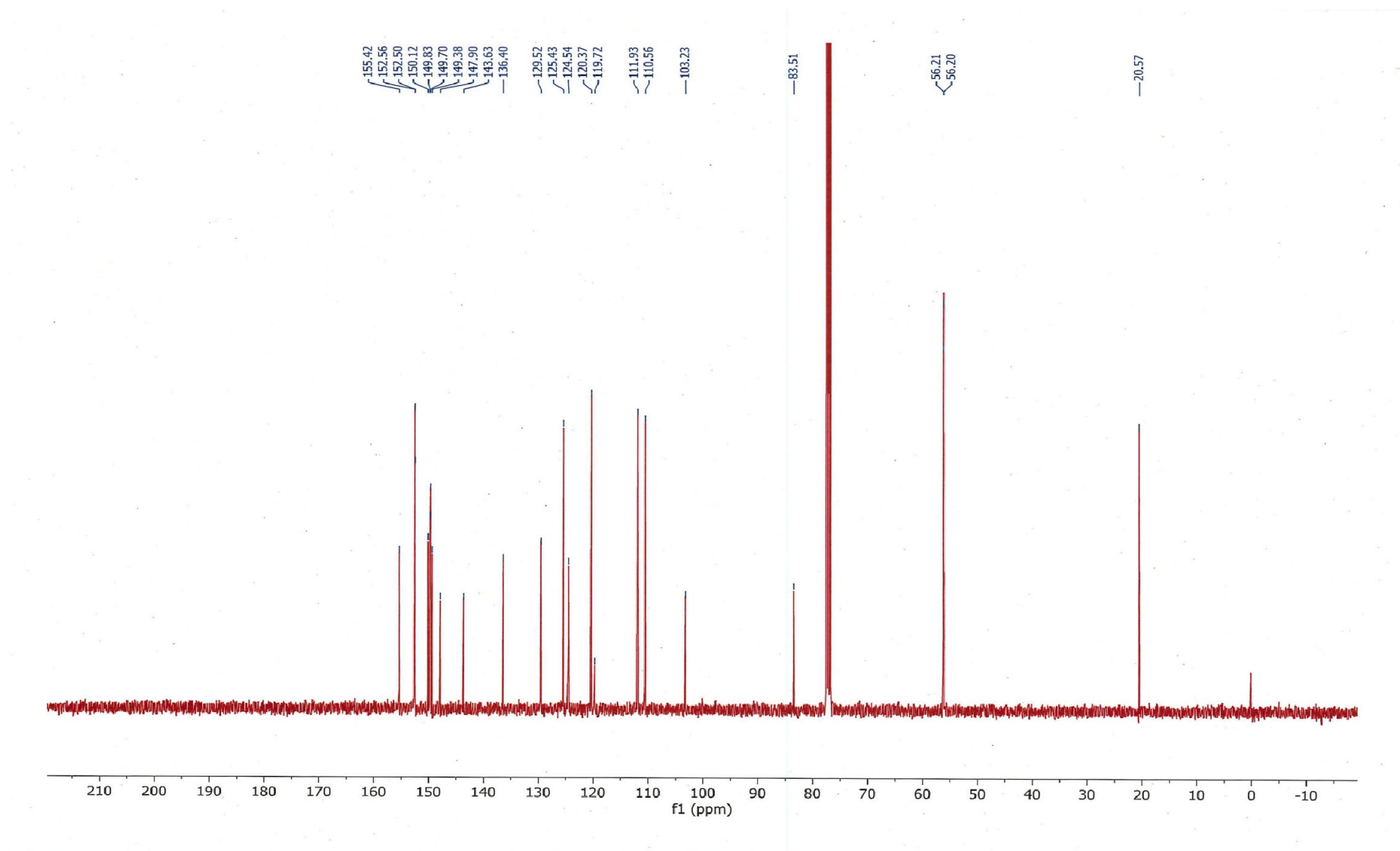
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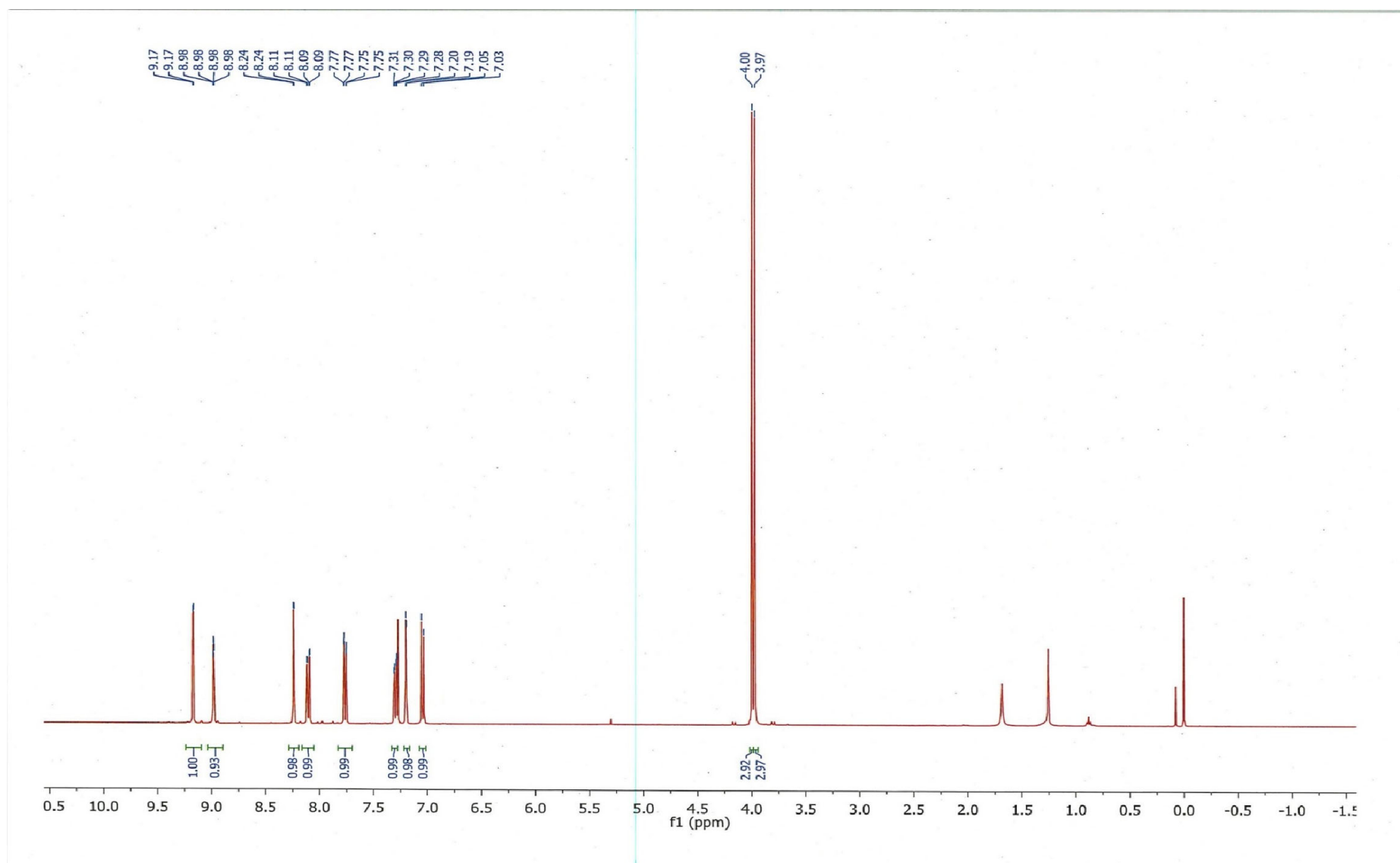
^1H NMR spectrum of **7p**



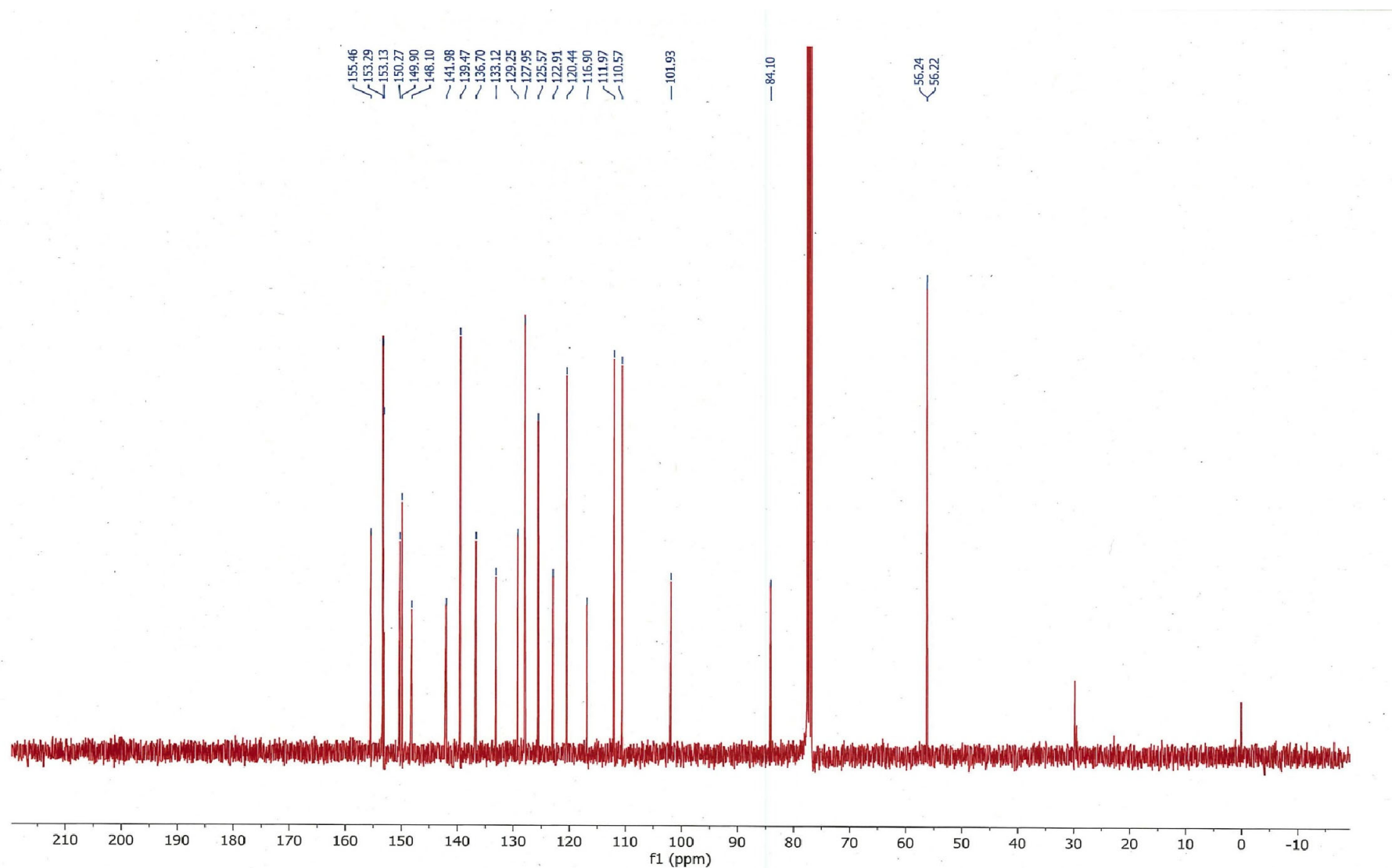
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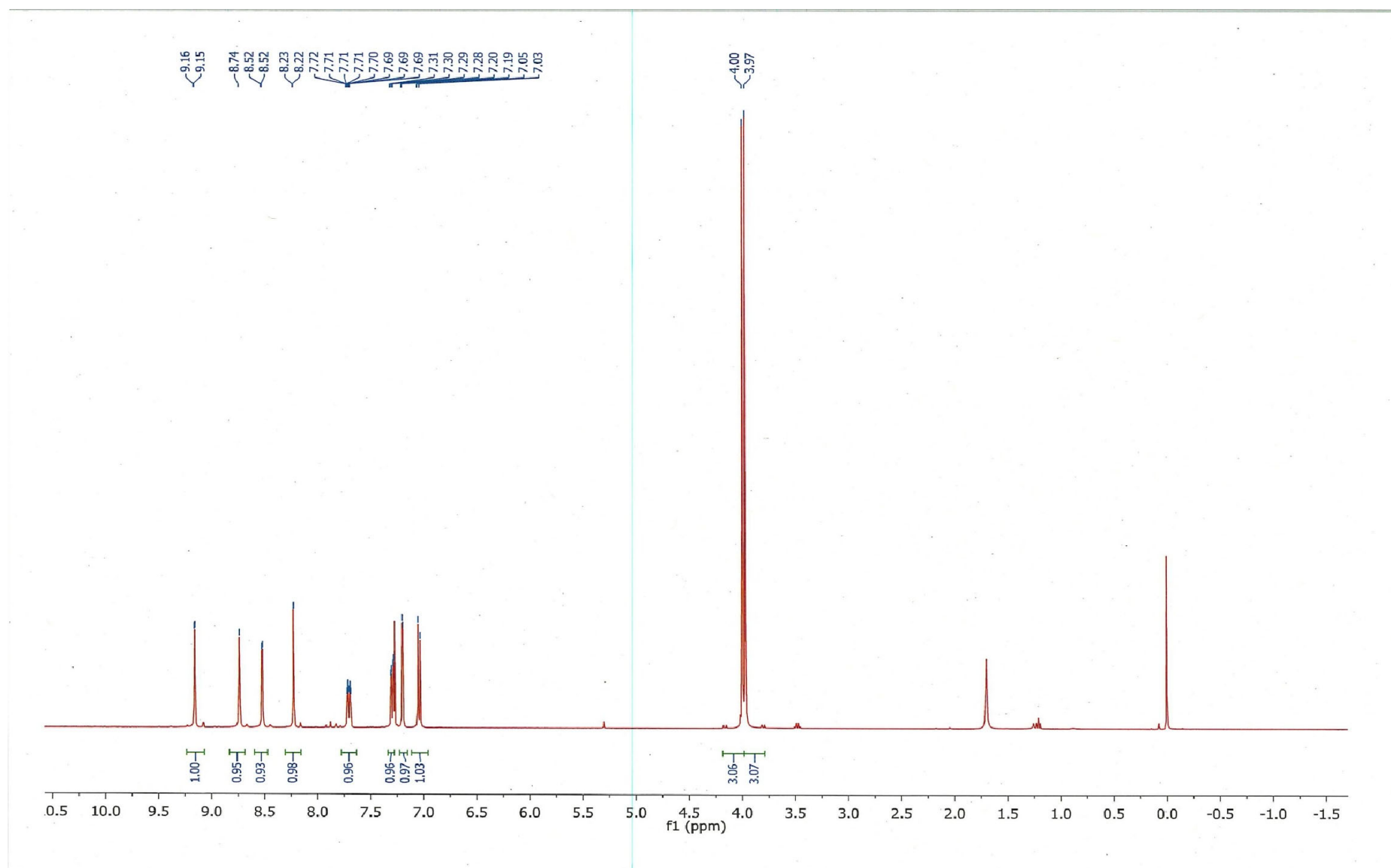
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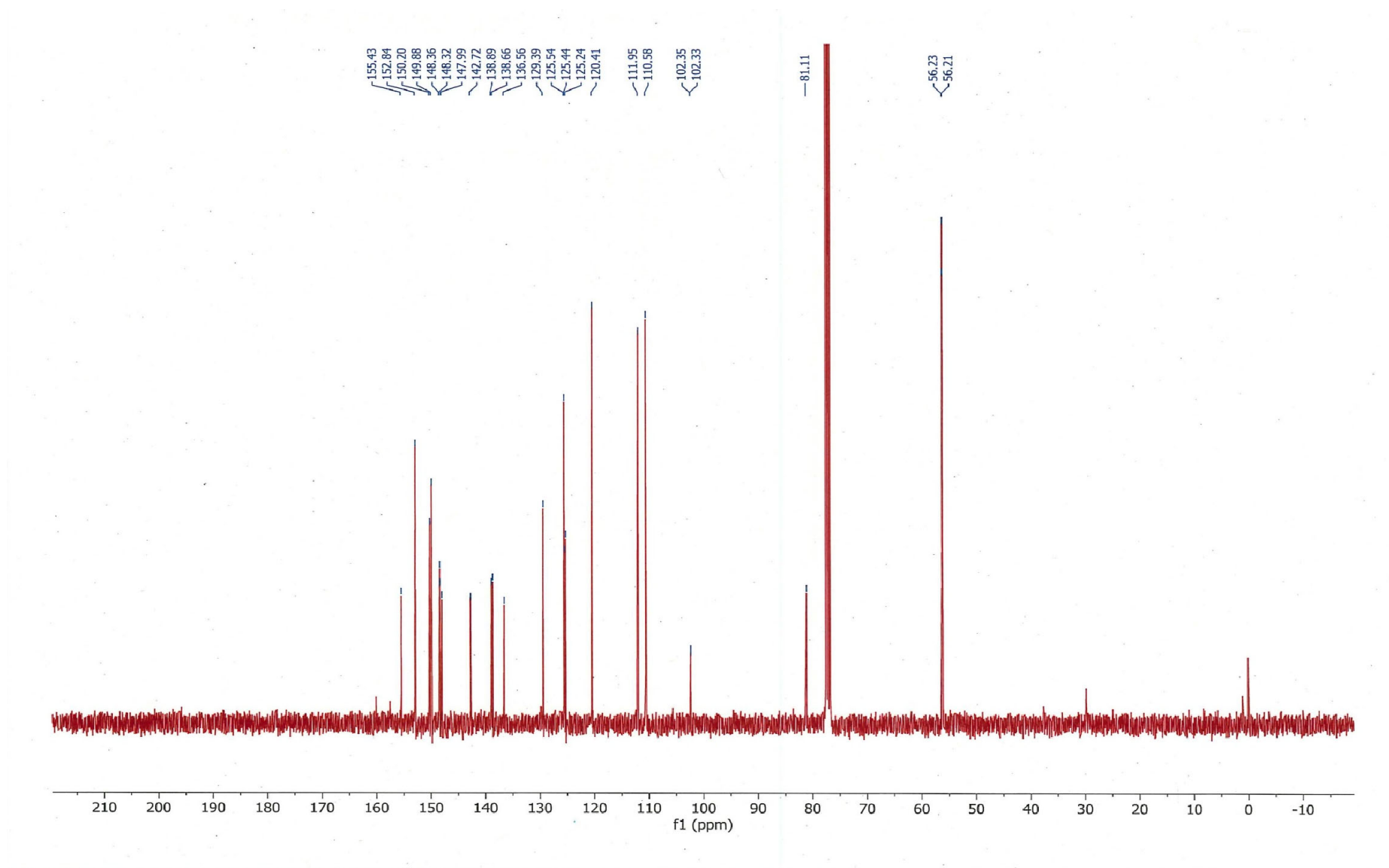
^{13}C NMR spectrum of **7q**



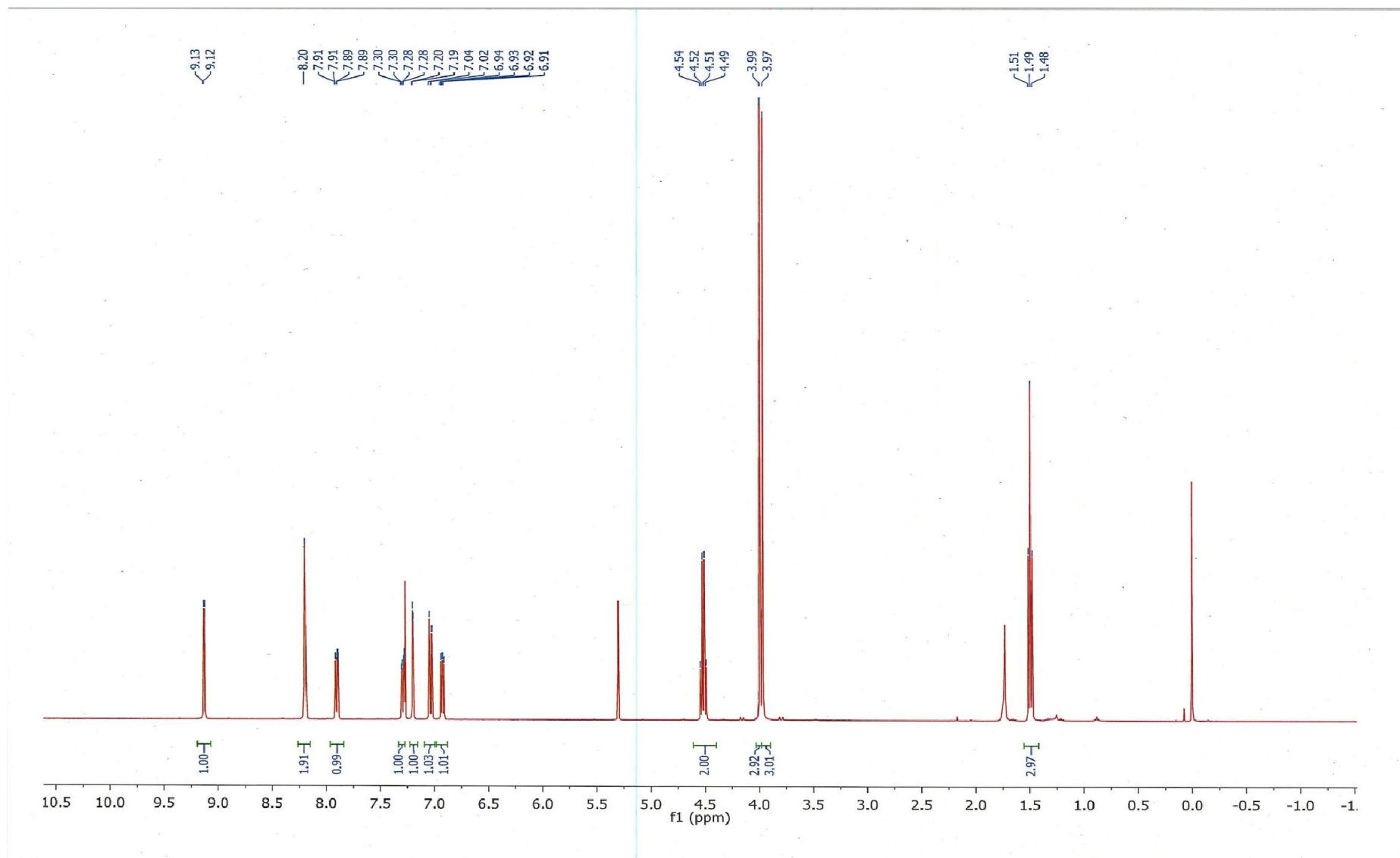
^1H NMR spectrum of **7r**



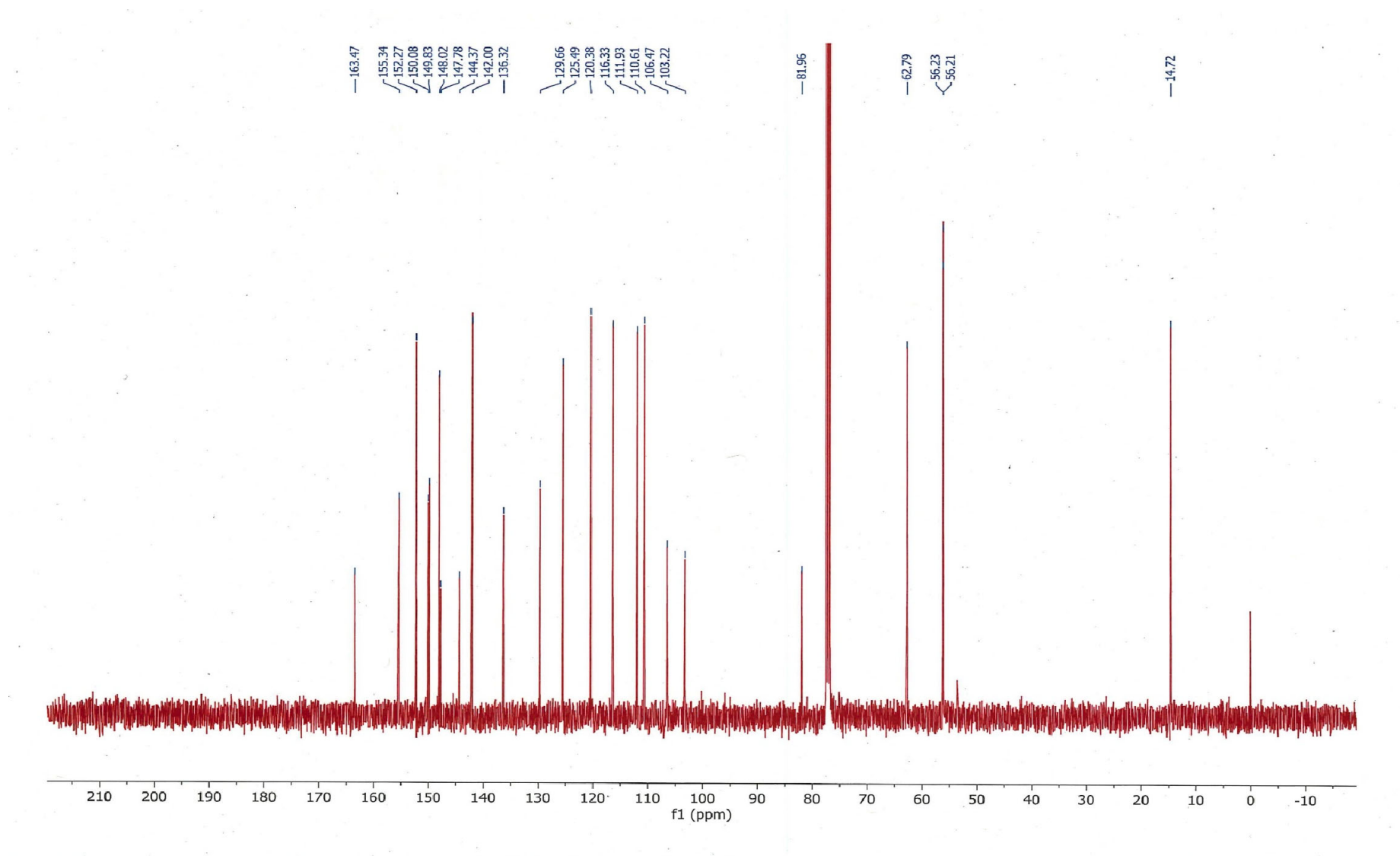
^{13}C NMR spectrum of **7r**



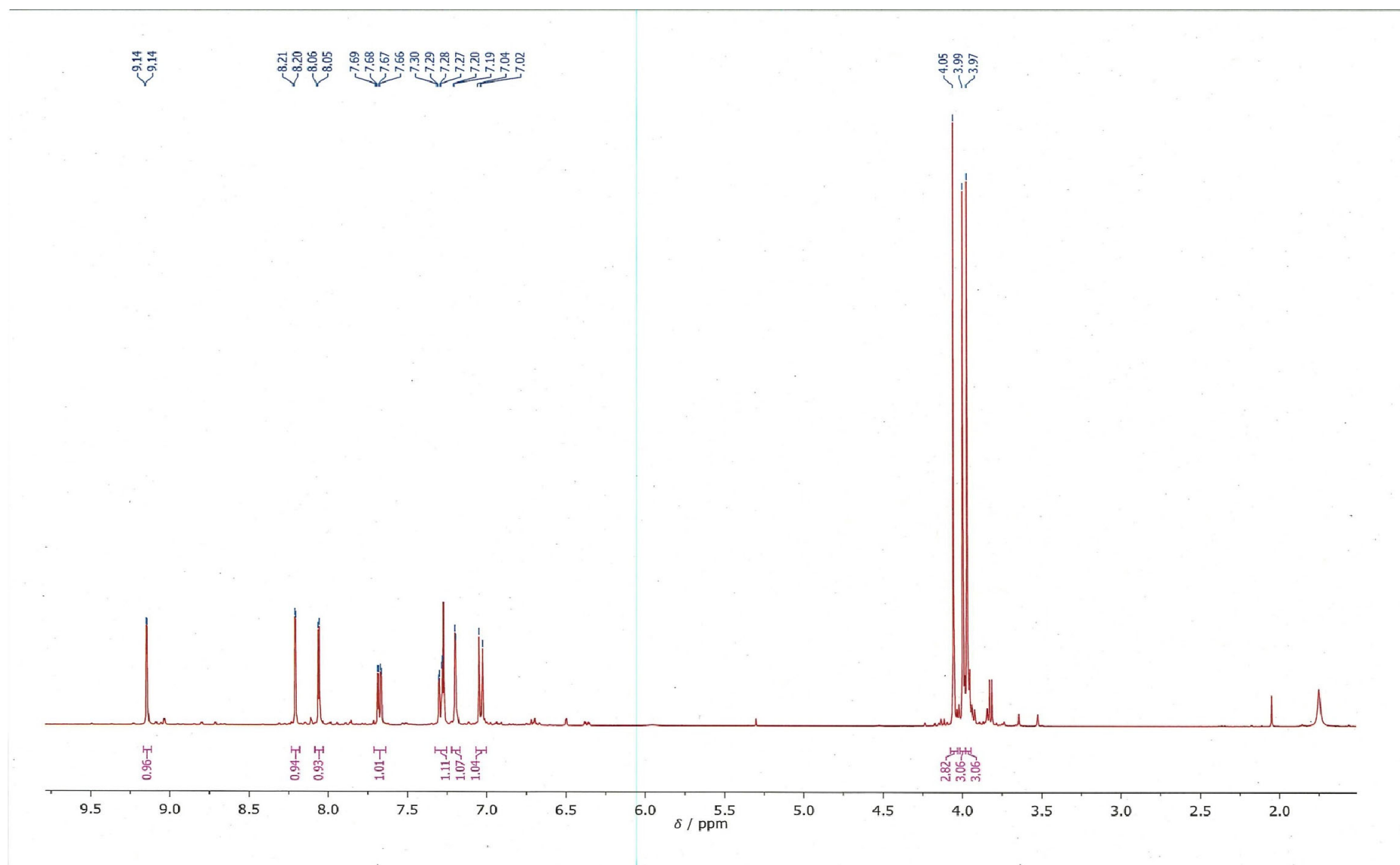
^1H NMR spectrum of **7s**



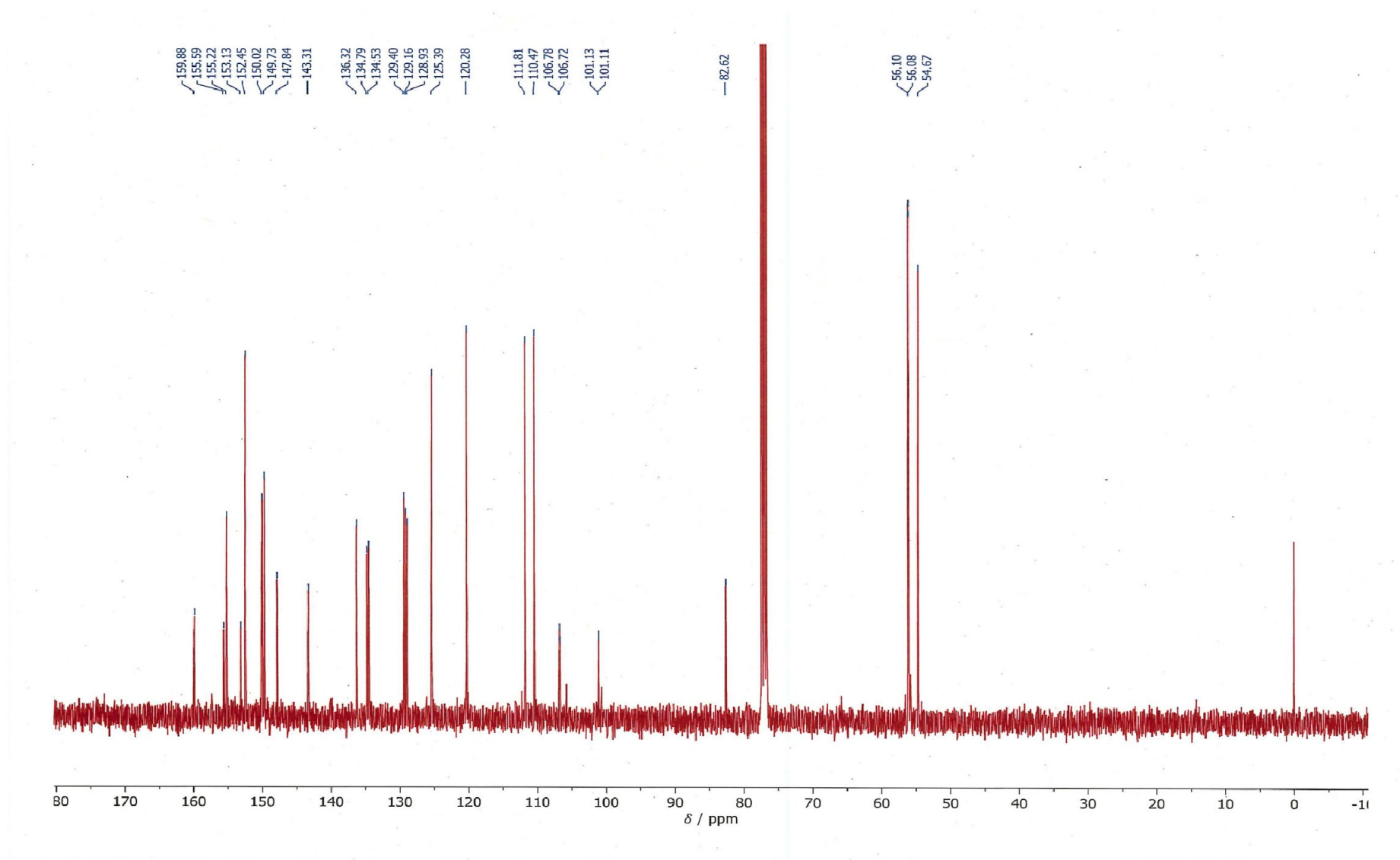
^{13}C NMR spectrum of **7s**



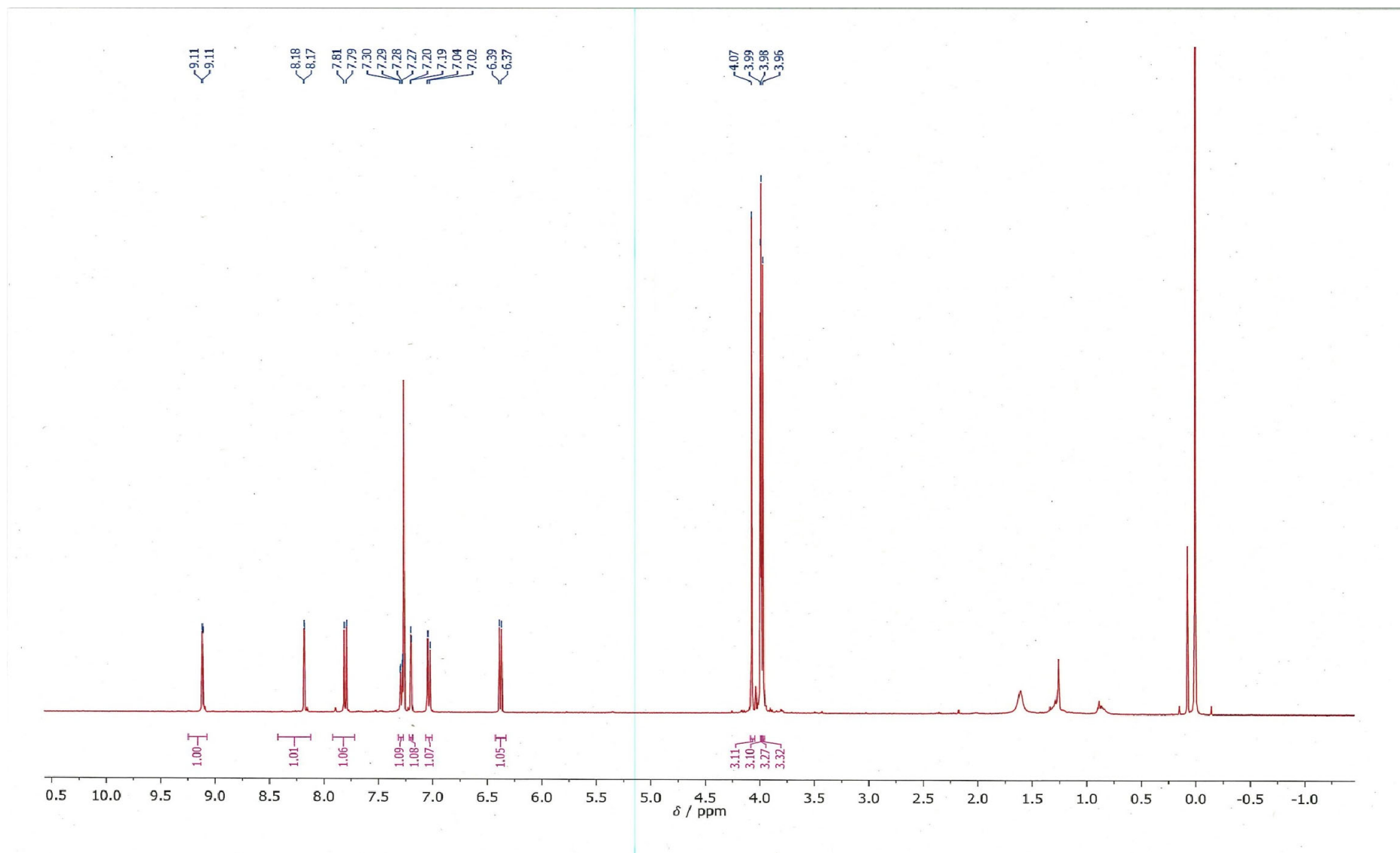
^1H NMR spectrum of **7t**



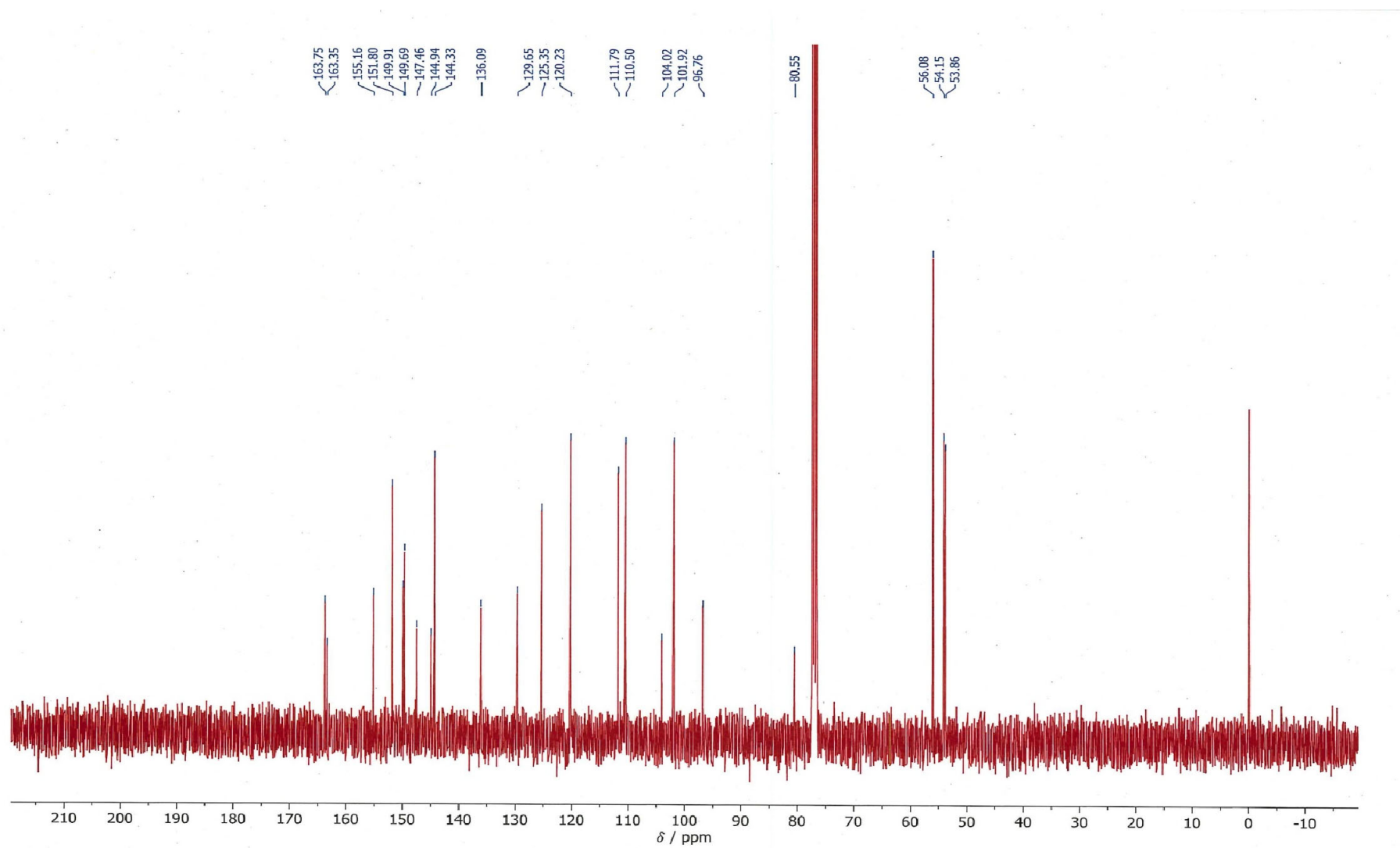
^{13}C NMR spectrum of **7t**



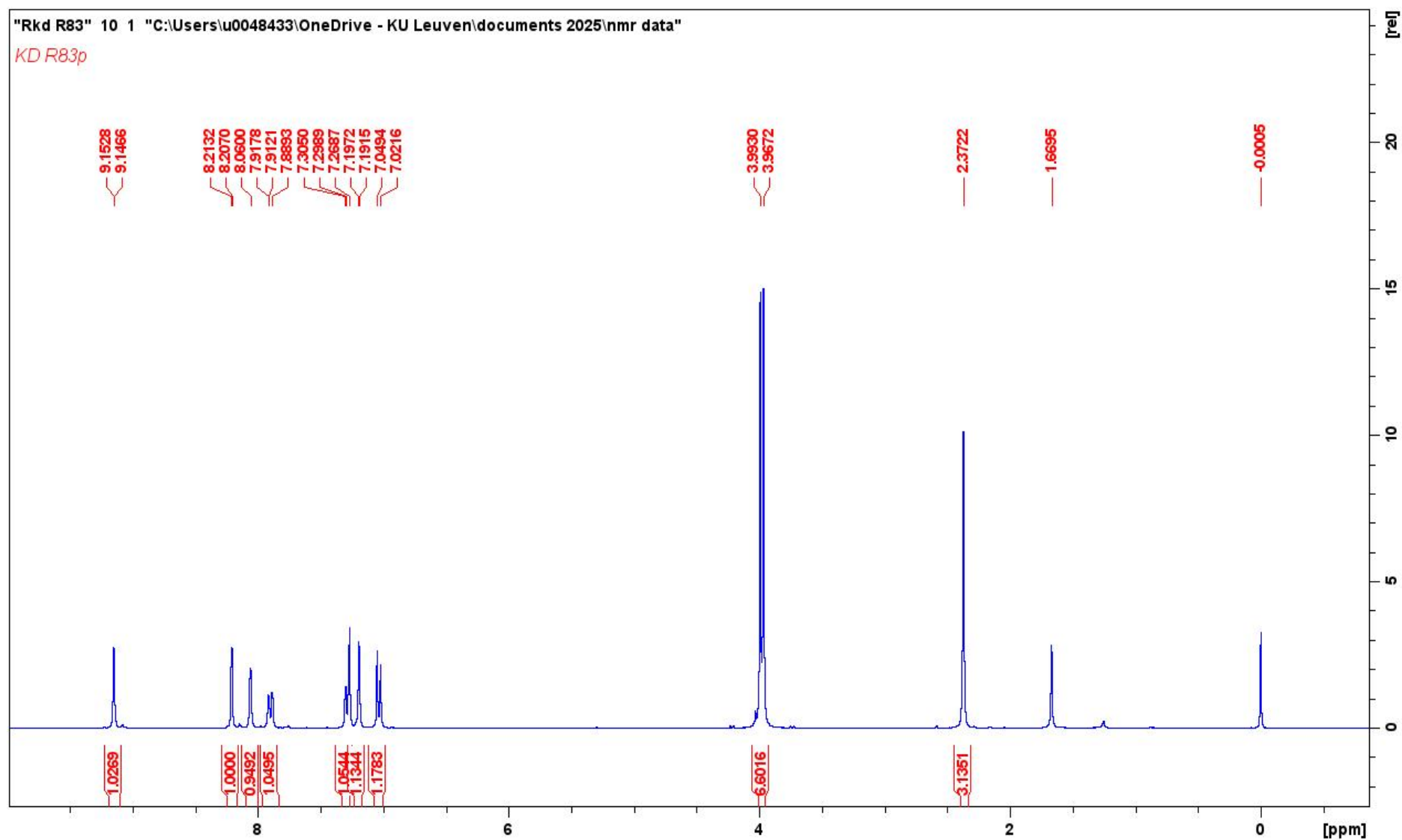
^1H NMR spectrum of **7u**



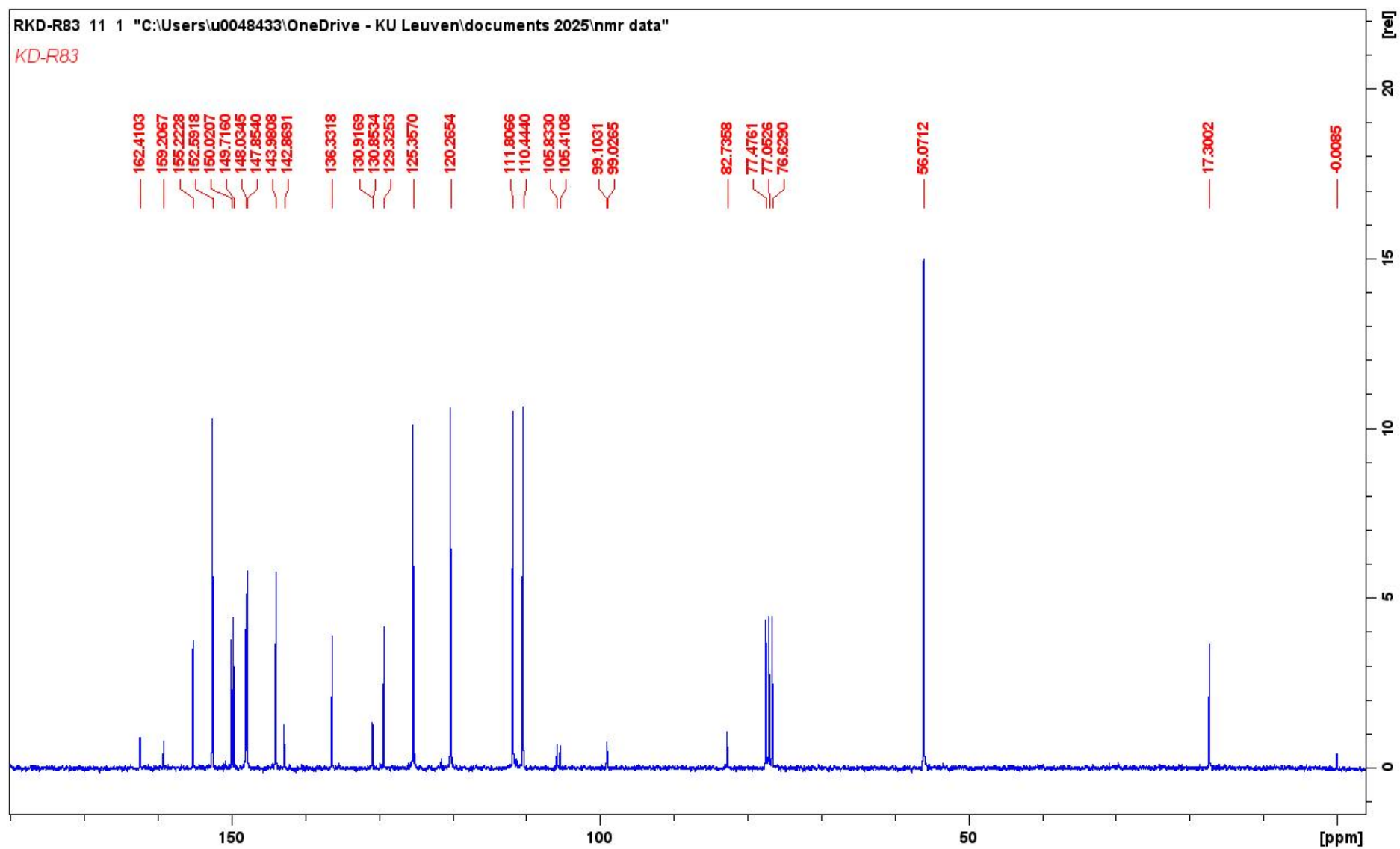
^{13}C NMR spectrum of **7u**



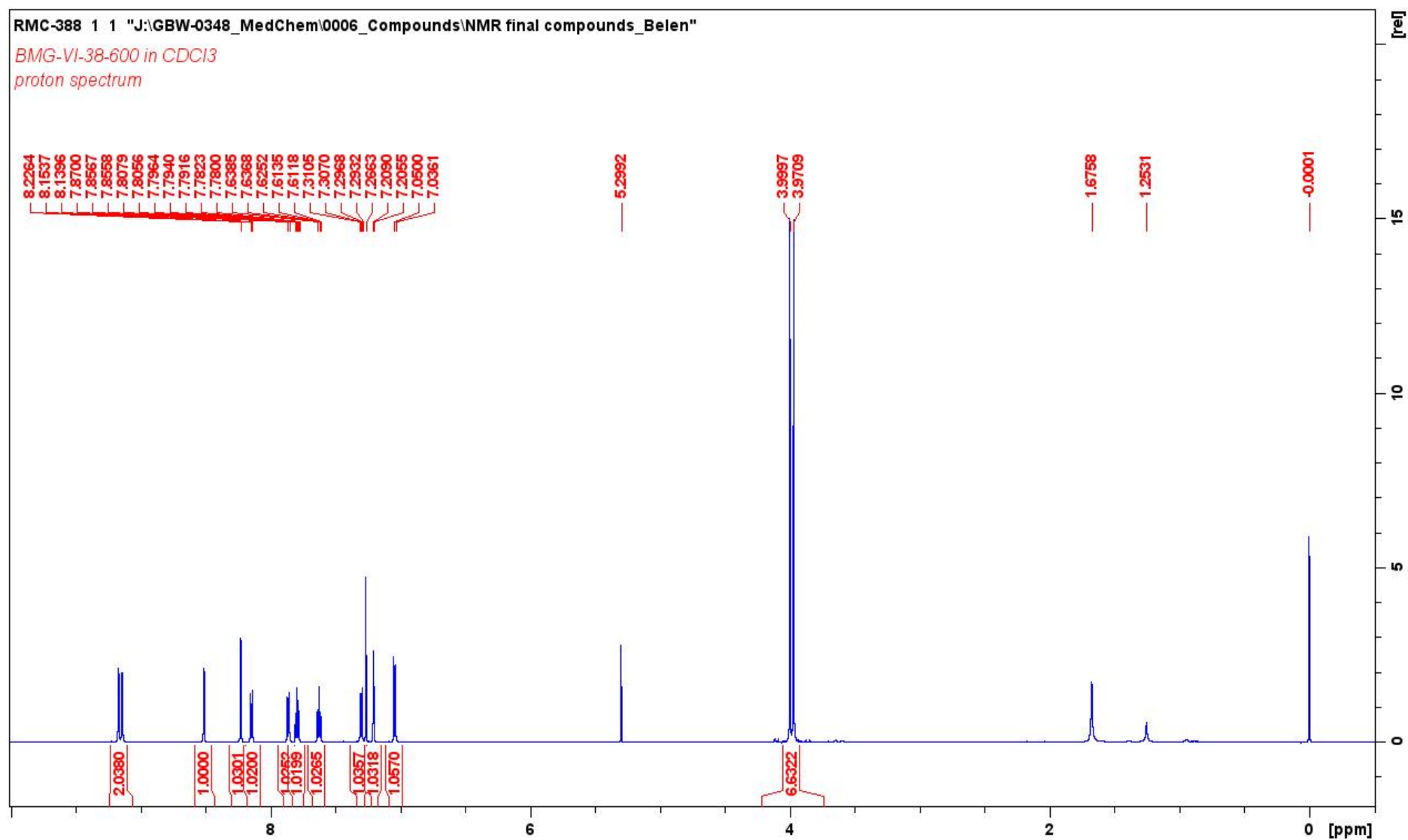
¹H NMR spectrum of 7v



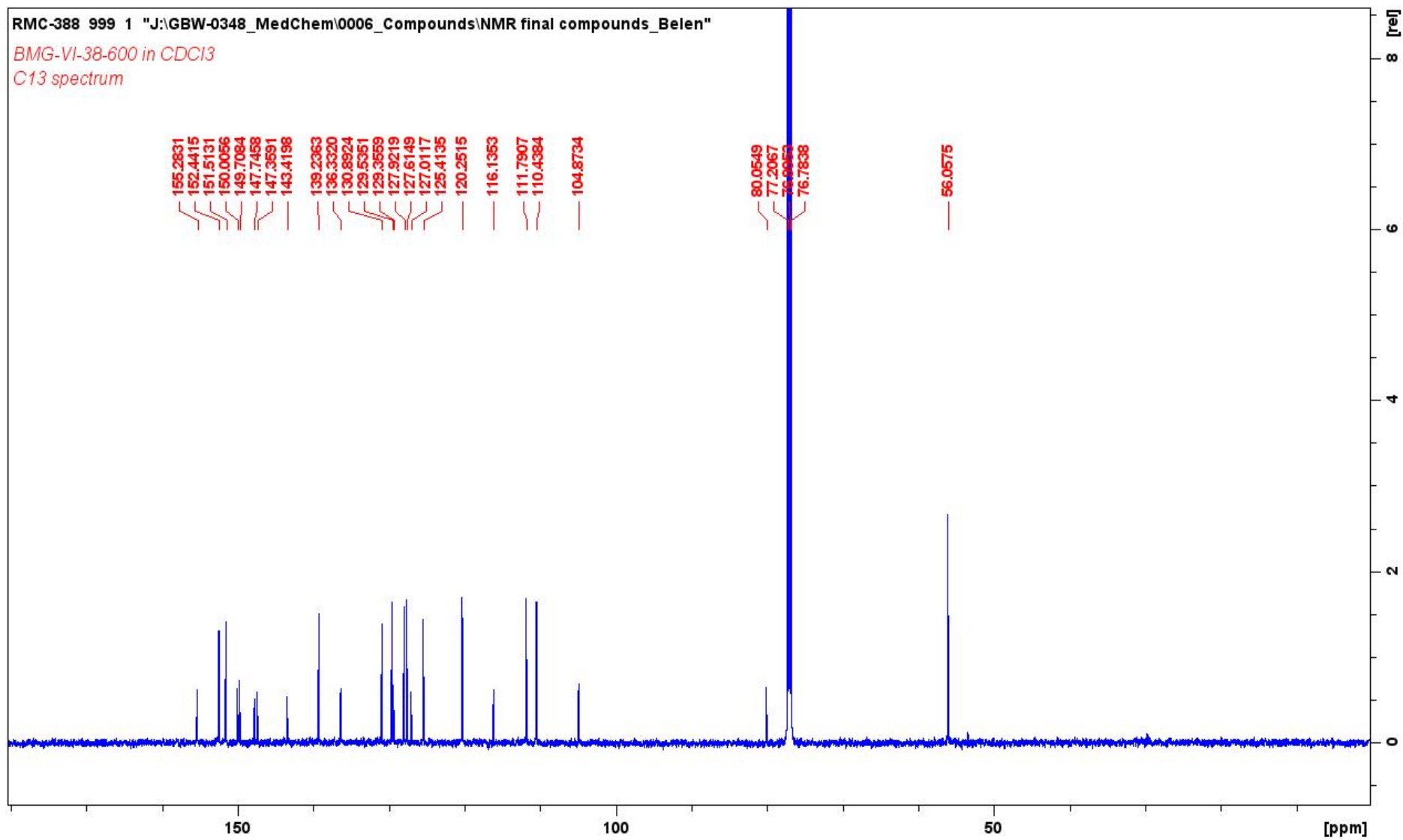
^{13}C NMR spectrum of **7v**



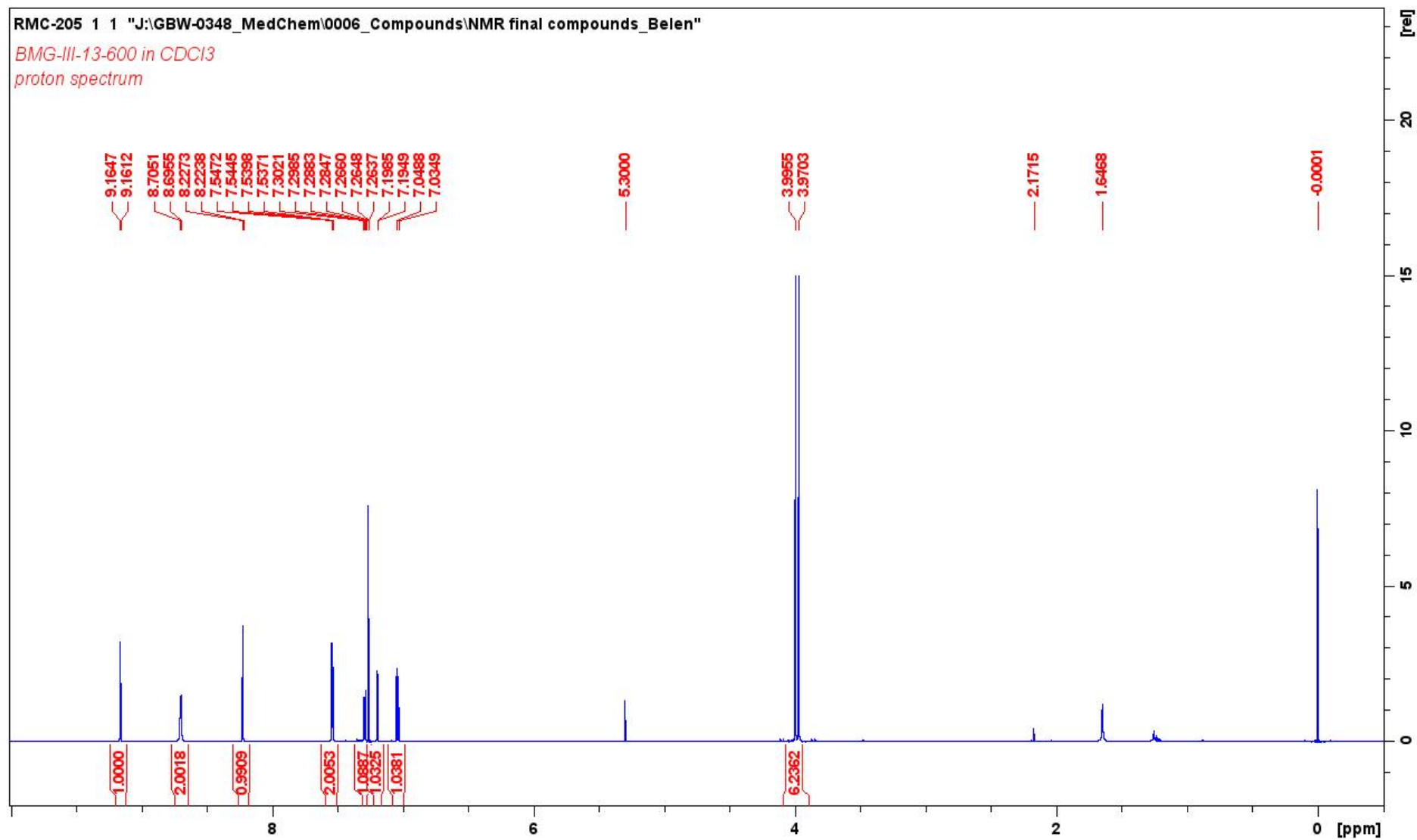
¹H NMR spectrum of 7w



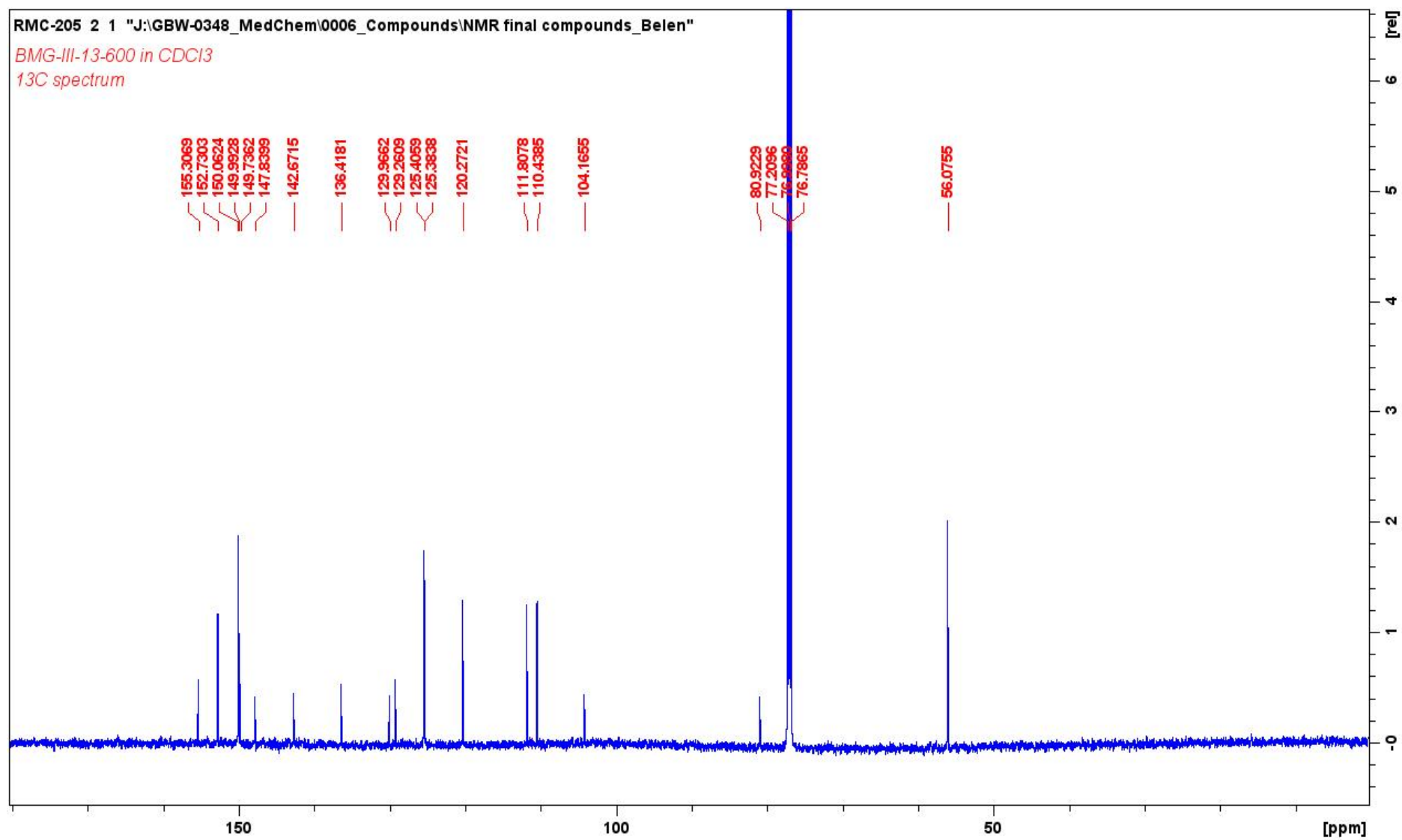
^{13}C NMR spectrum of **7w**



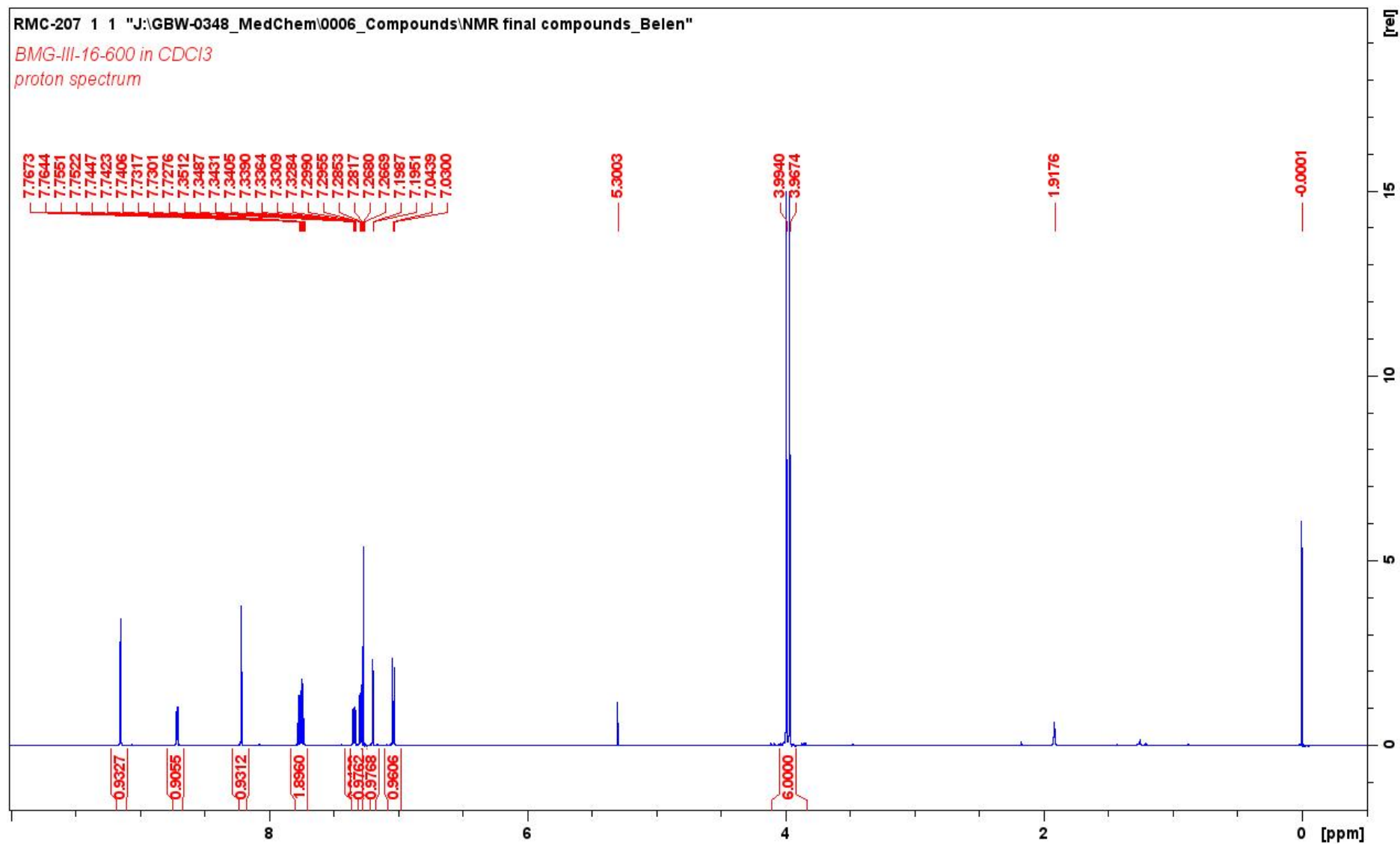
¹H NMR spectrum of 7x



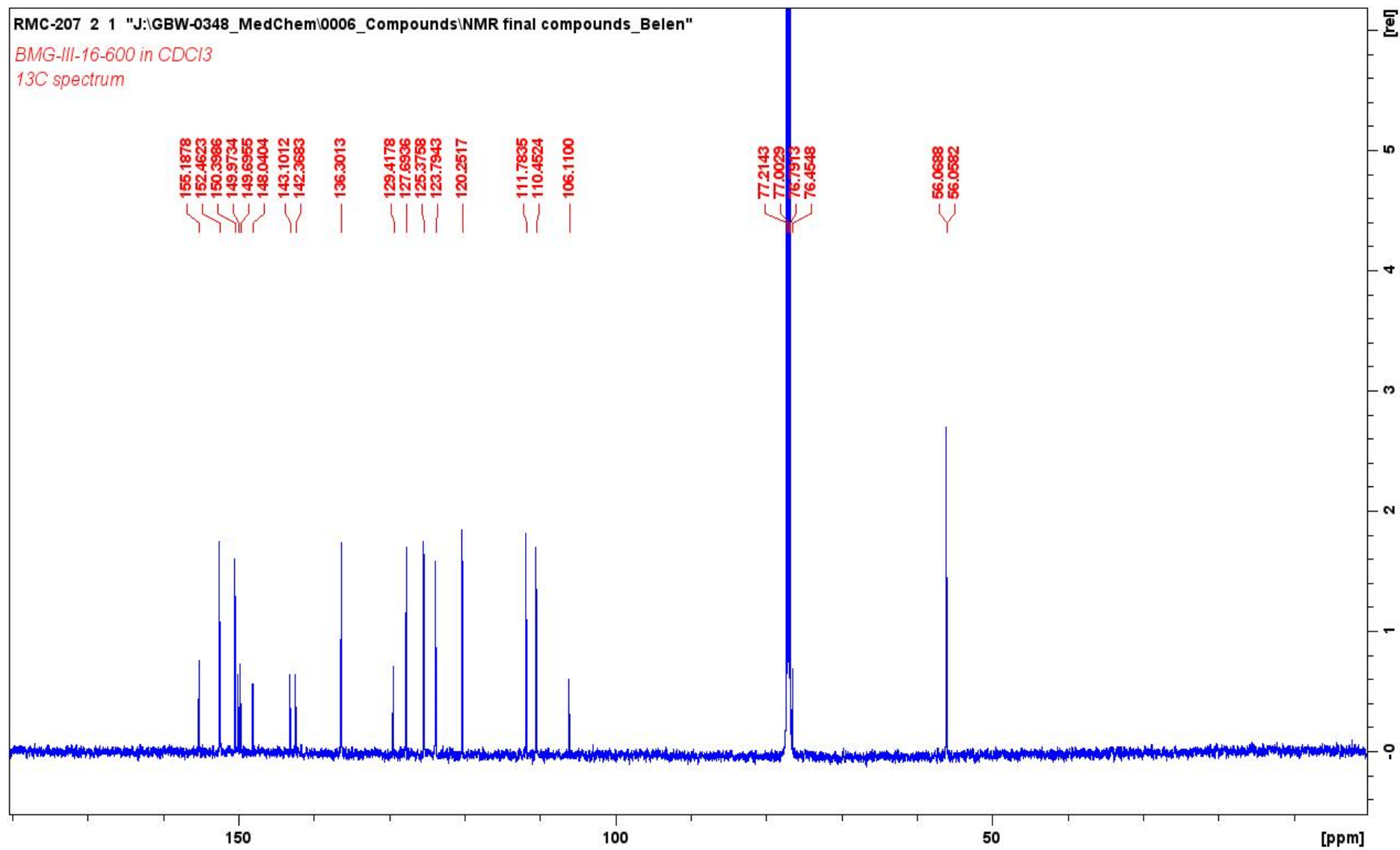
^{13}C NMR spectrum of **7x**



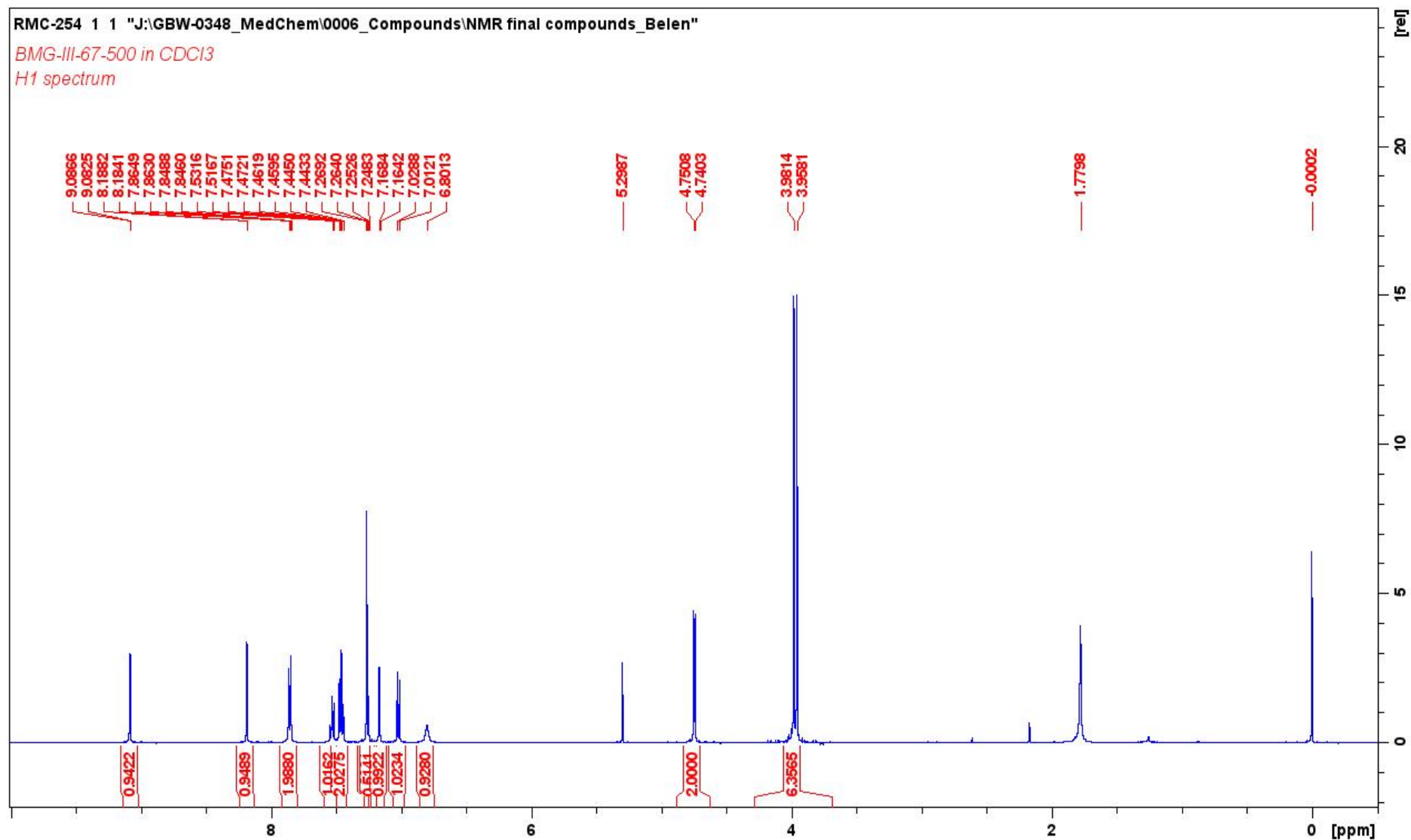
¹H NMR spectrum of 7y



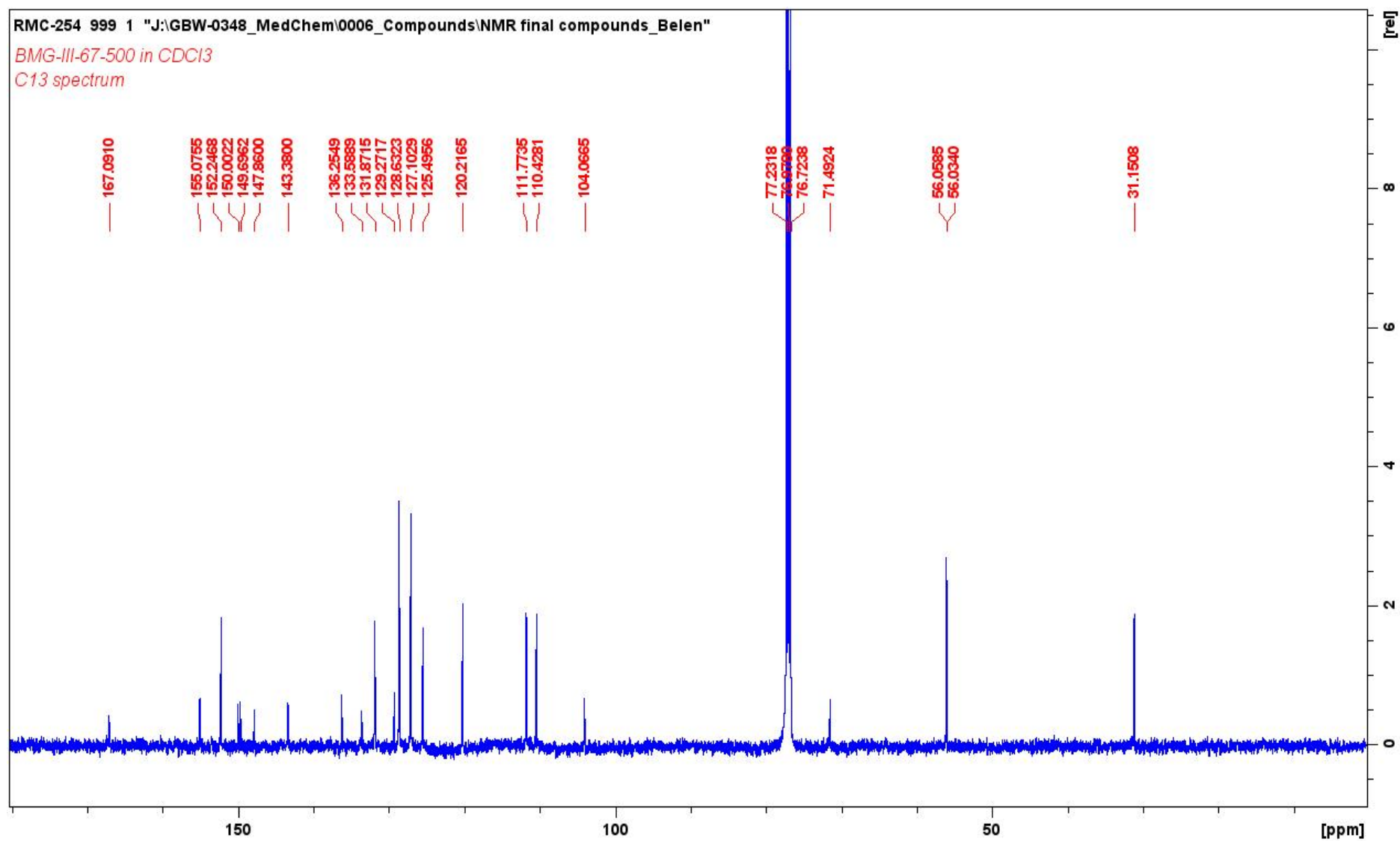
^{13}C NMR spectrum of **7y**



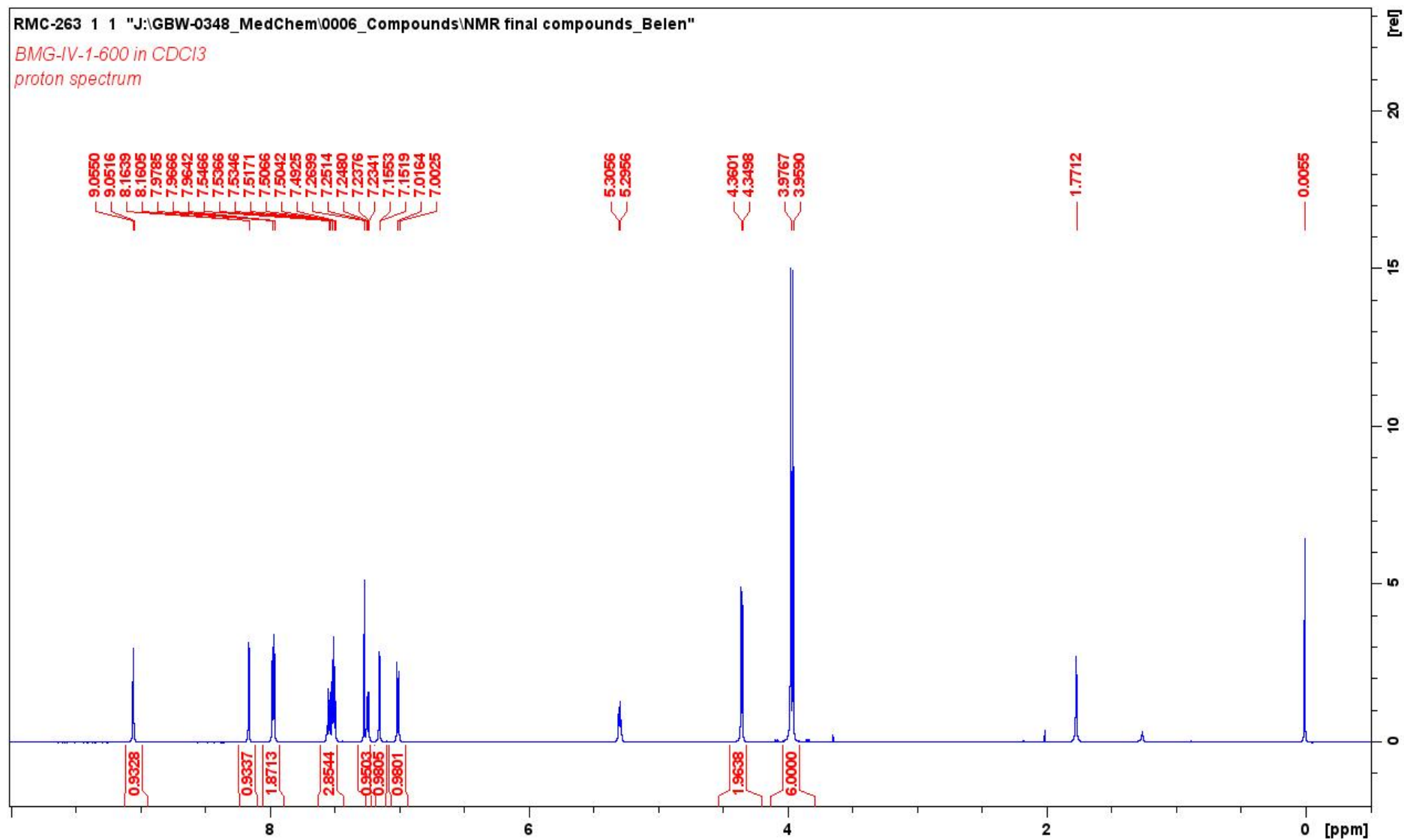
¹H NMR spectrum of **11a**



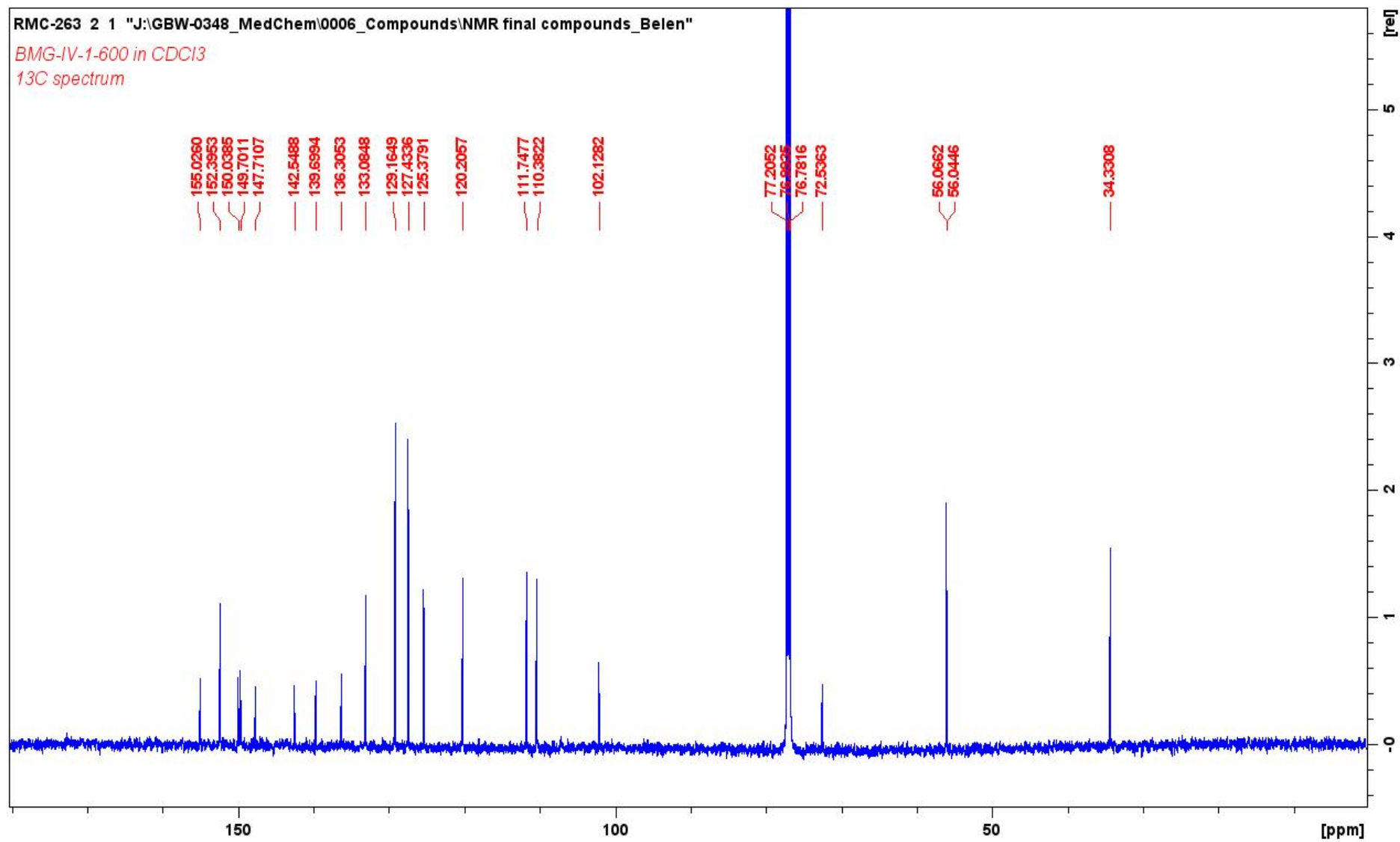
^{13}C NMR spectrum of **11a**



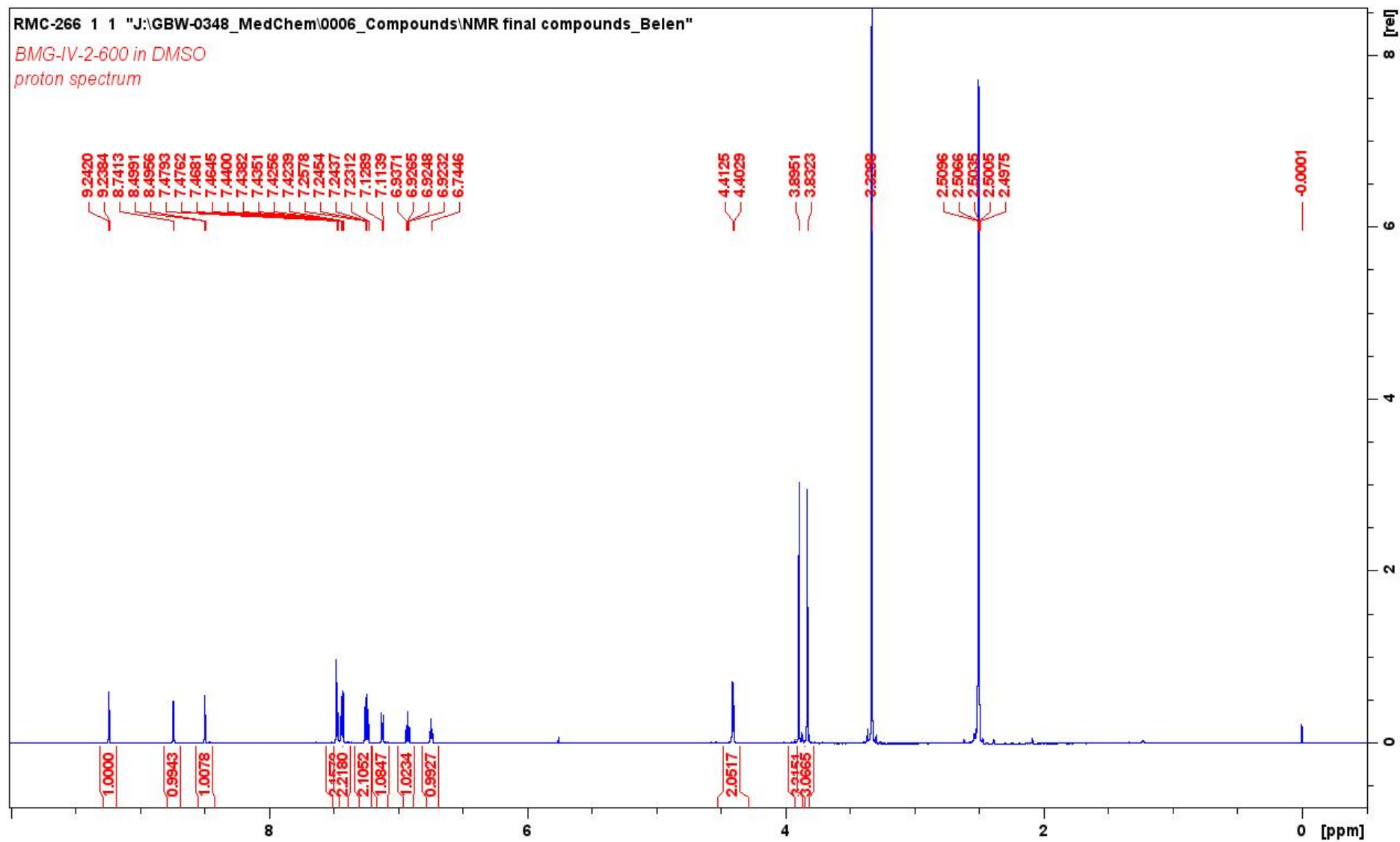
¹H NMR spectrum of **11b**



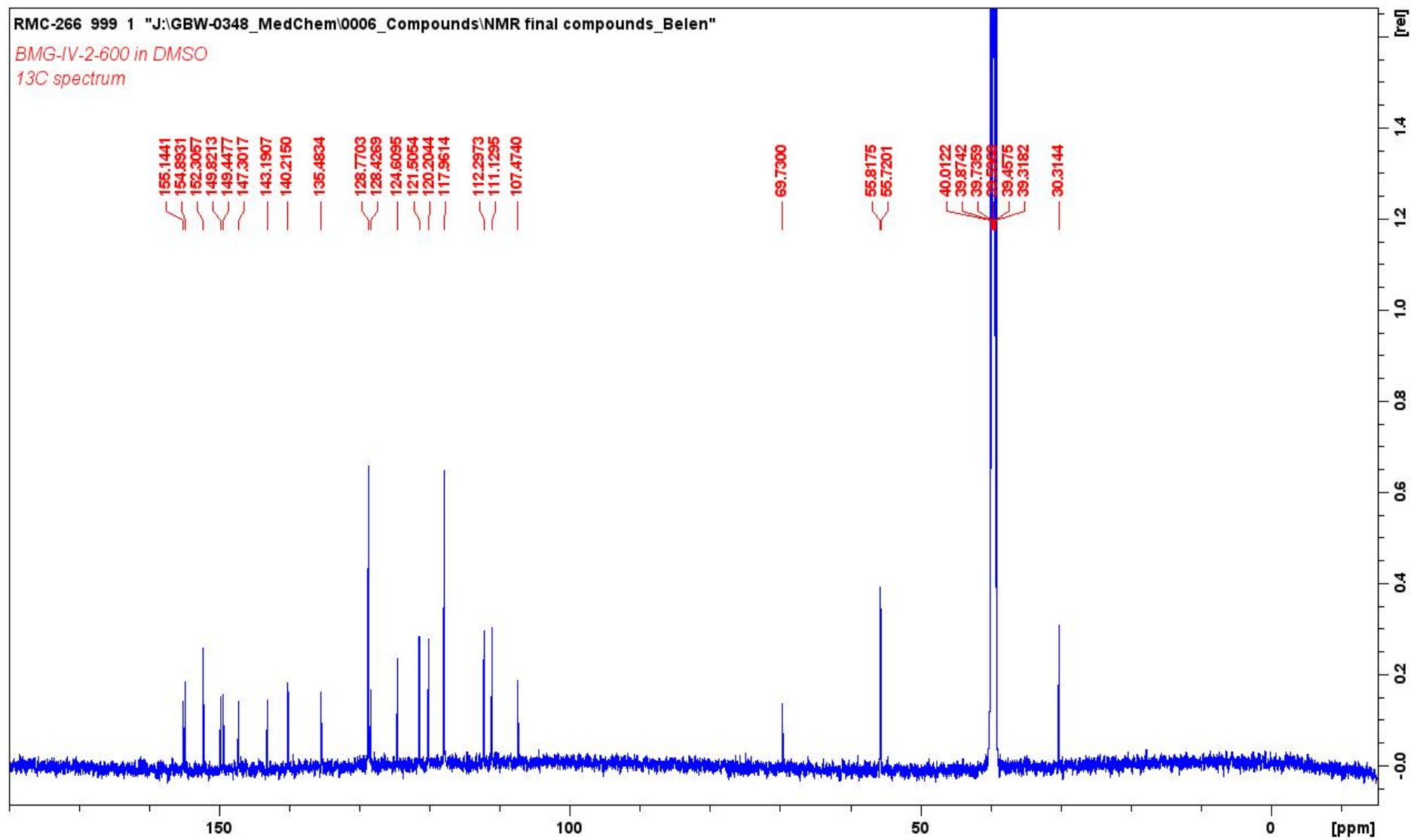
^{13}C NMR spectrum of **11b**



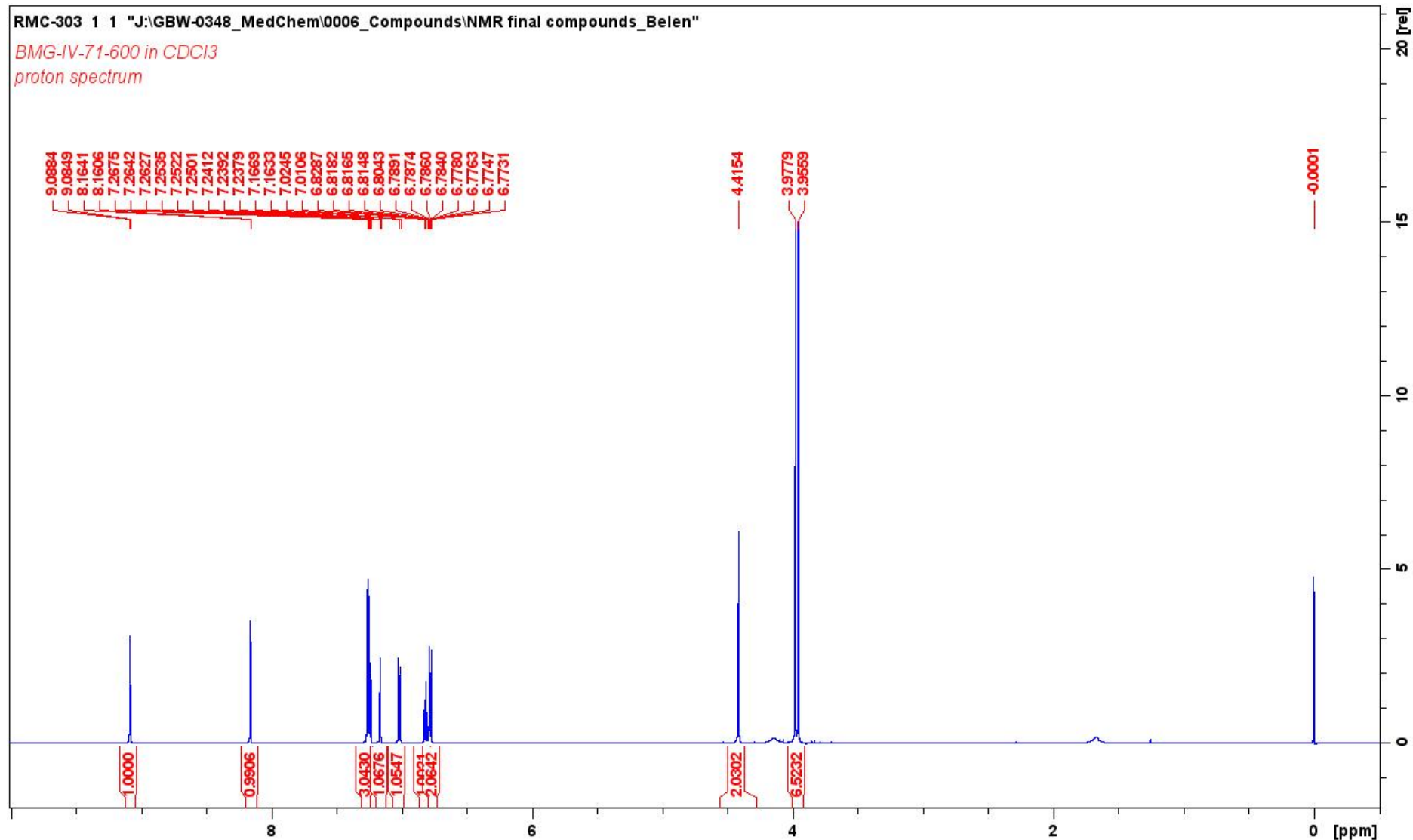
¹H NMR spectrum of **11c**



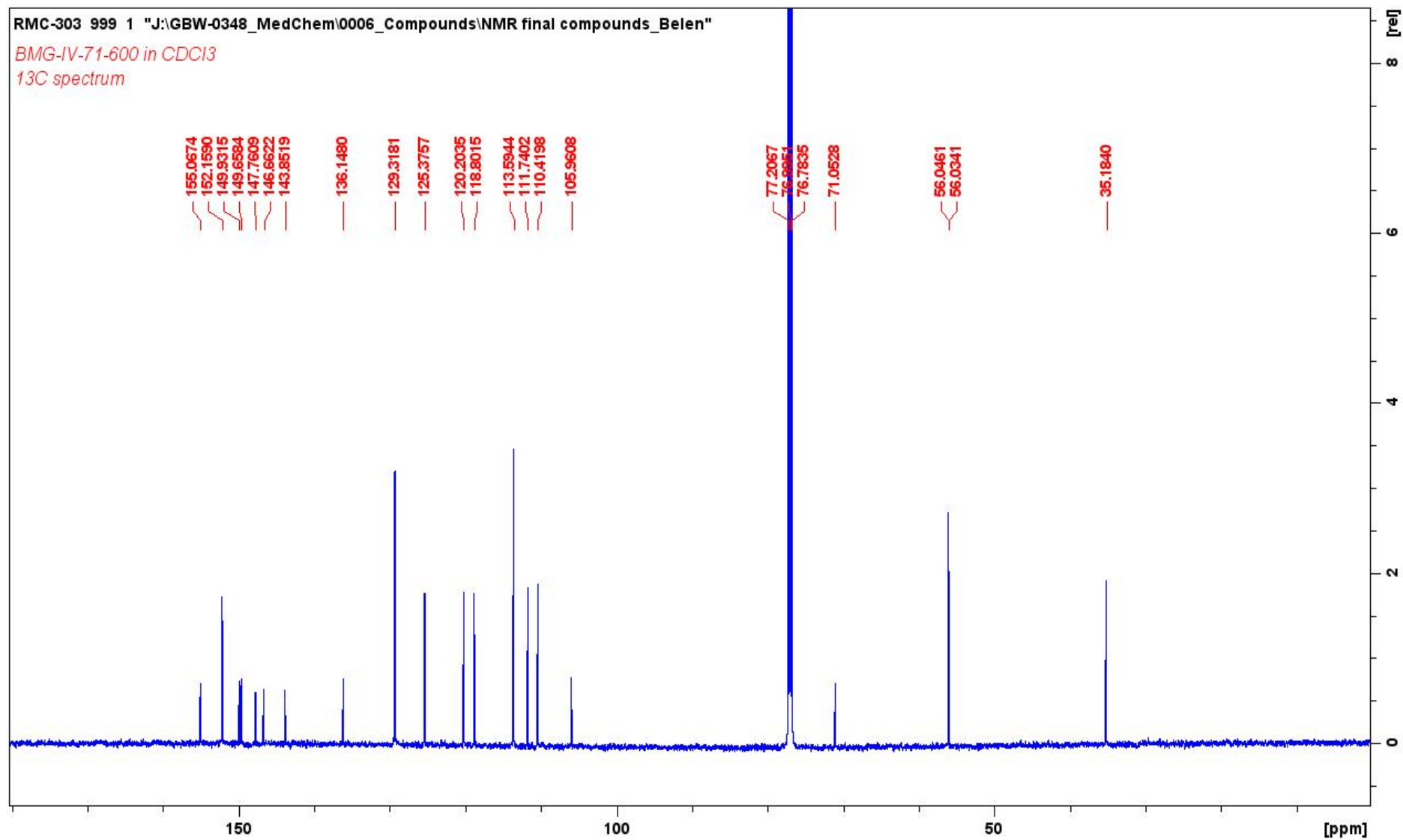
¹³C NMR spectrum of **11c**



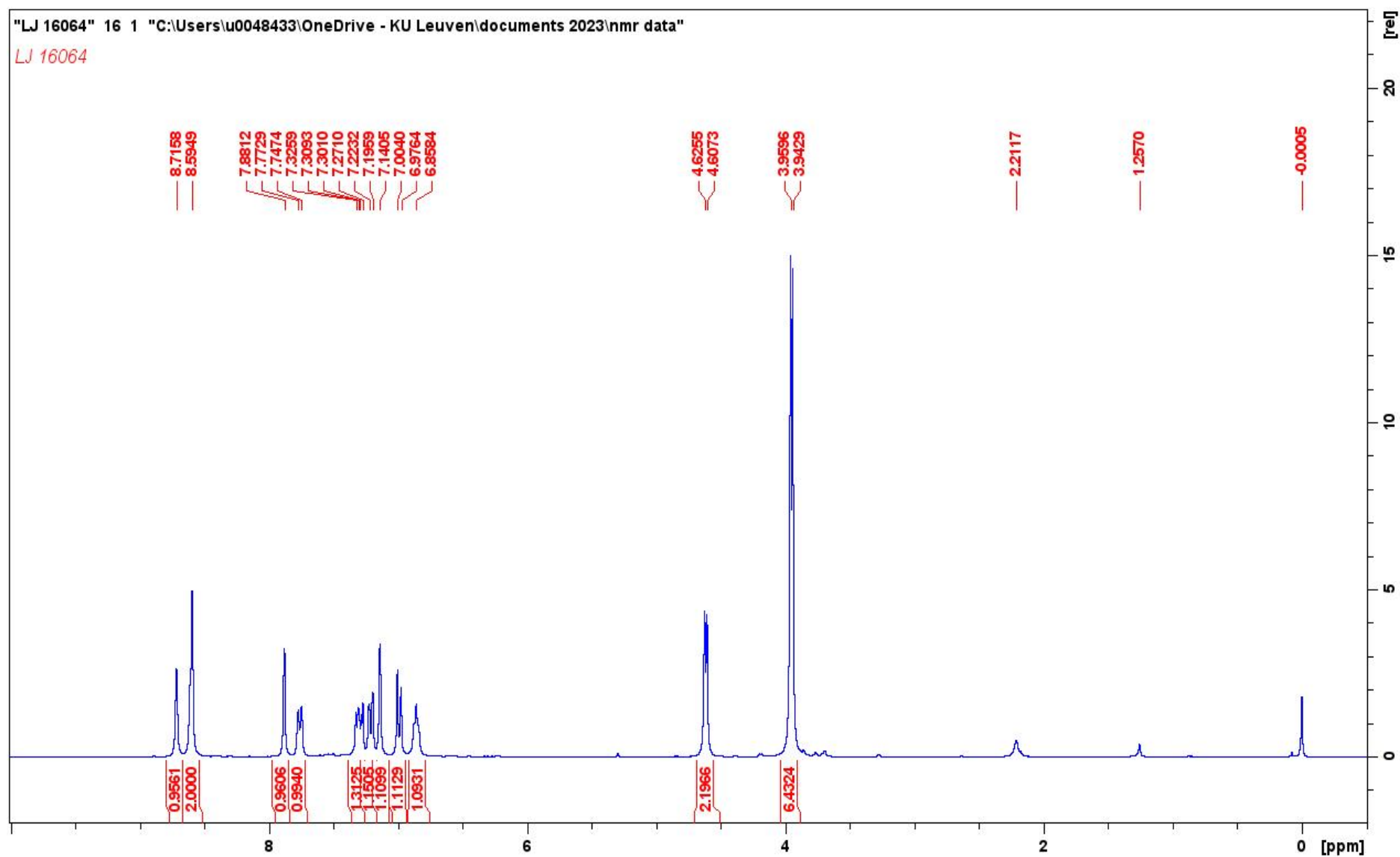
¹H NMR spectrum of **13**



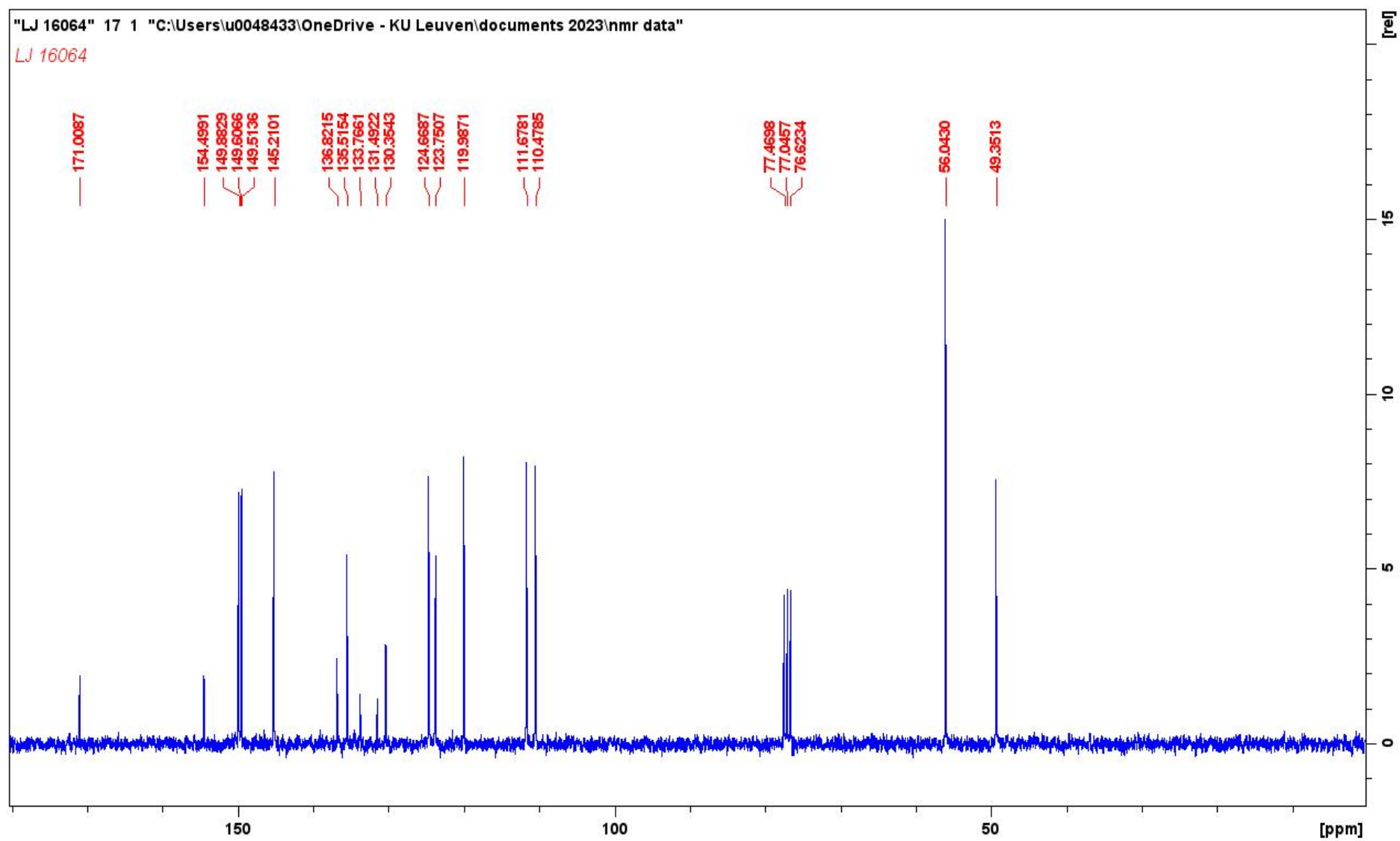
^{13}C NMR spectrum of **13**



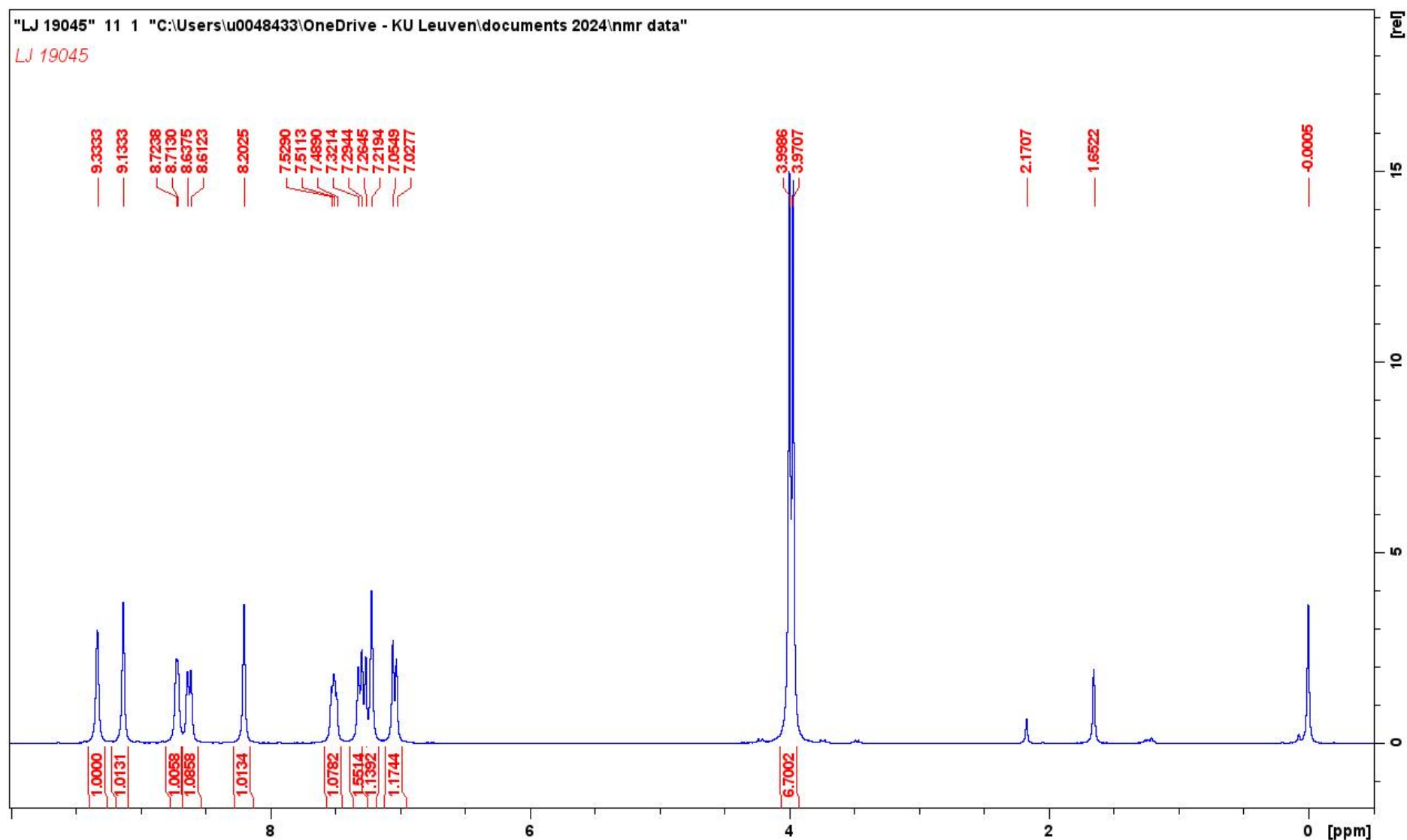
¹H NMR spectrum of **15**



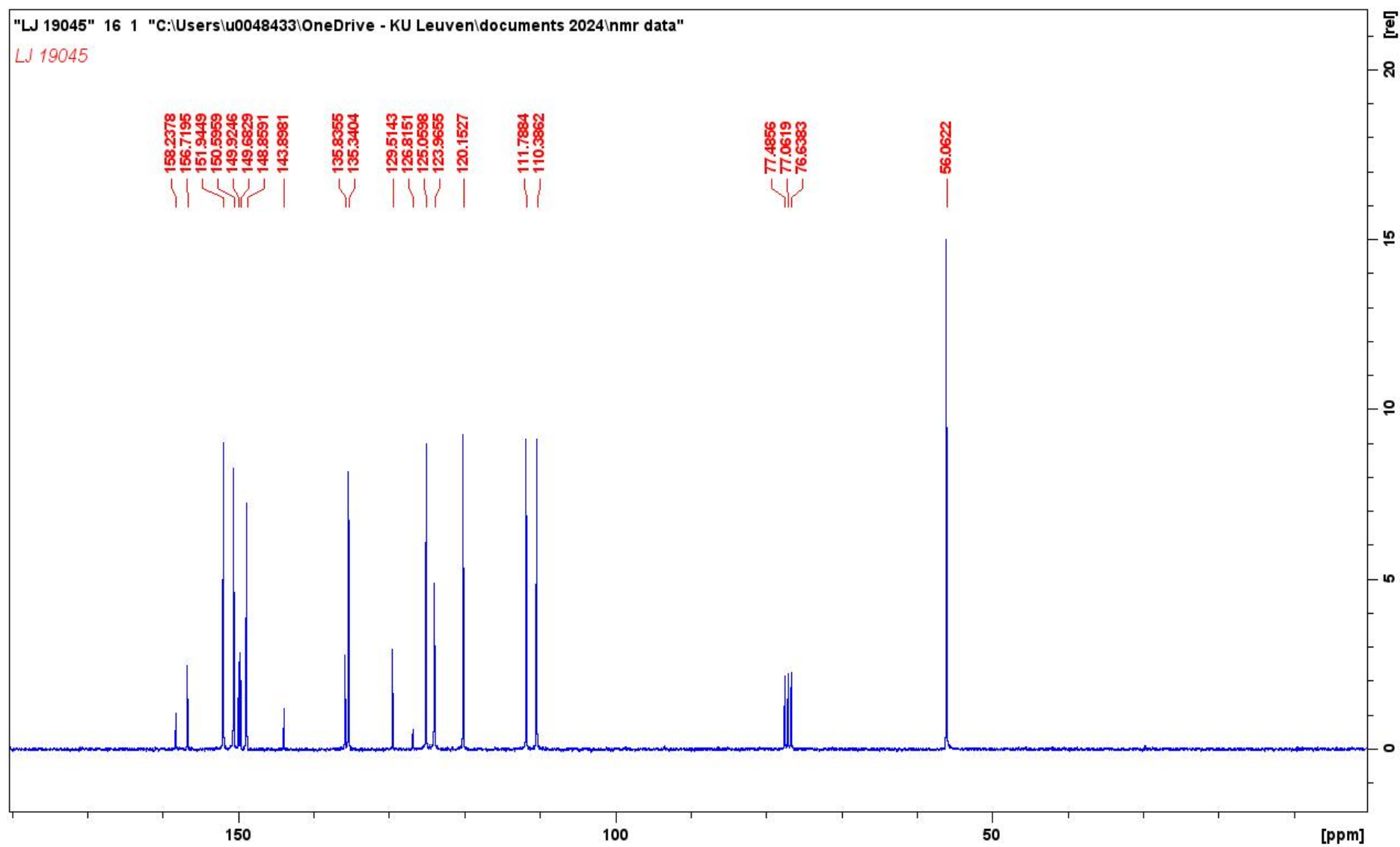
^{13}C NMR spectrum of **15**



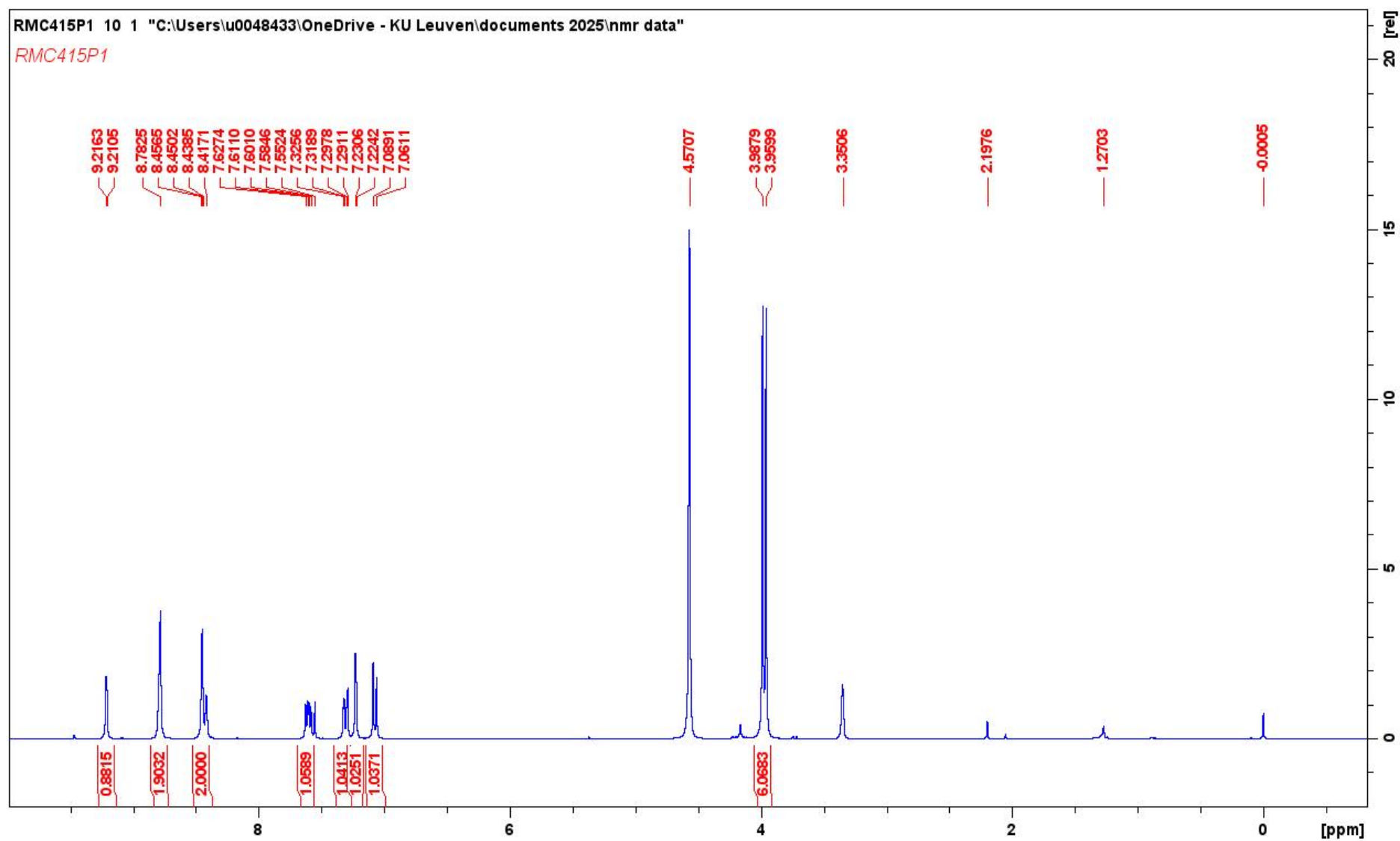
¹H NMR spectrum of **17**



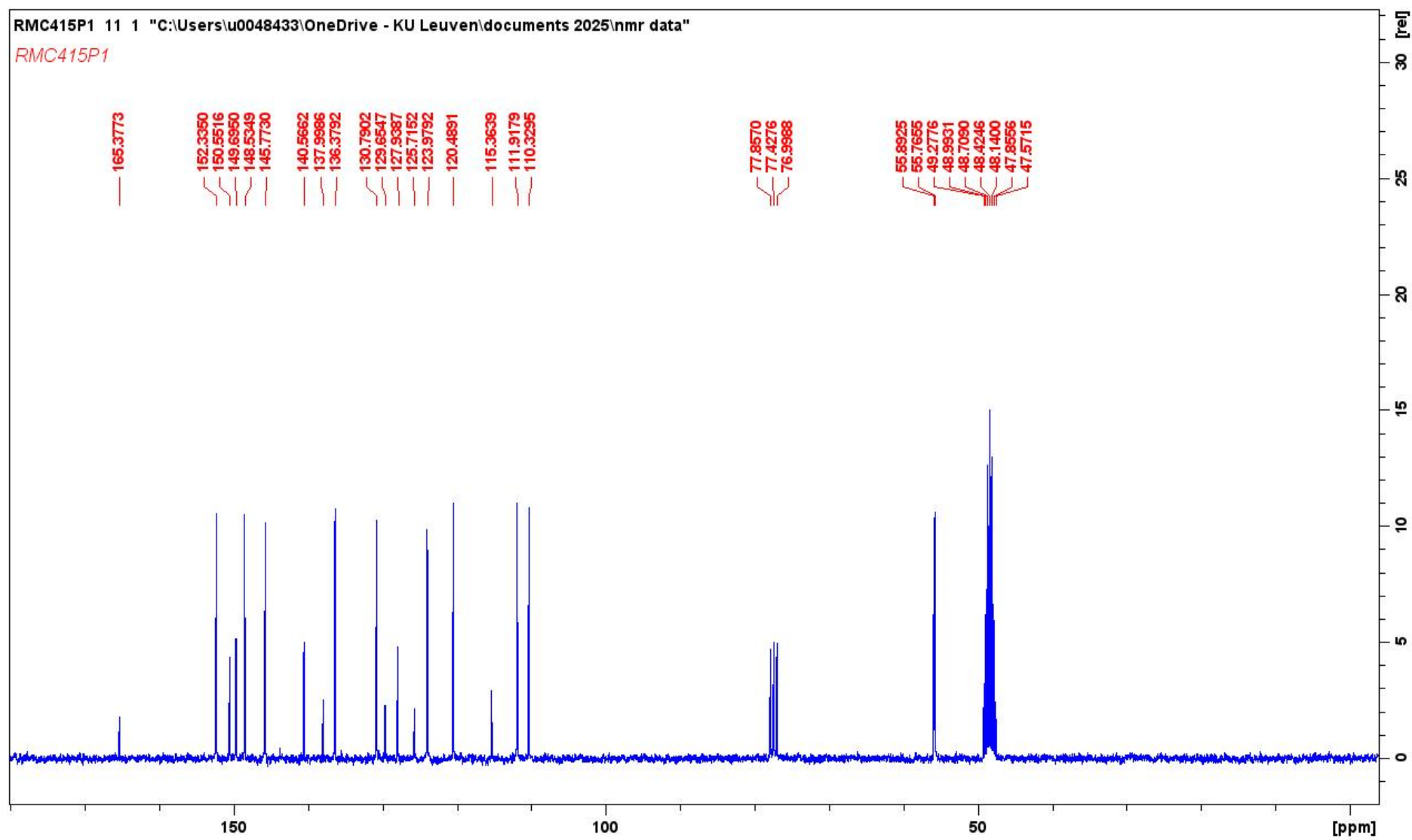
^{13}C NMR spectrum of **17**



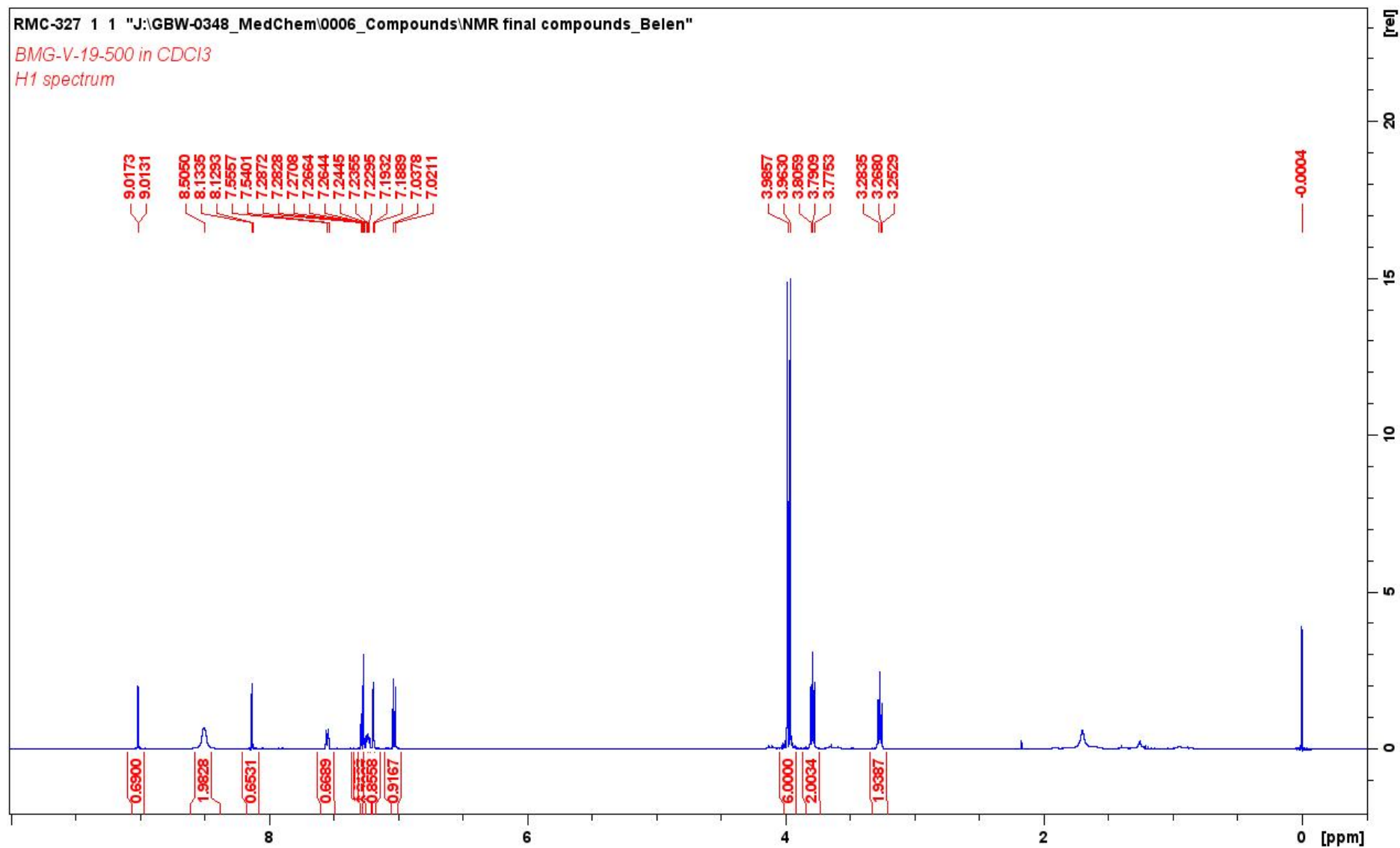
¹H NMR spectrum of **20**



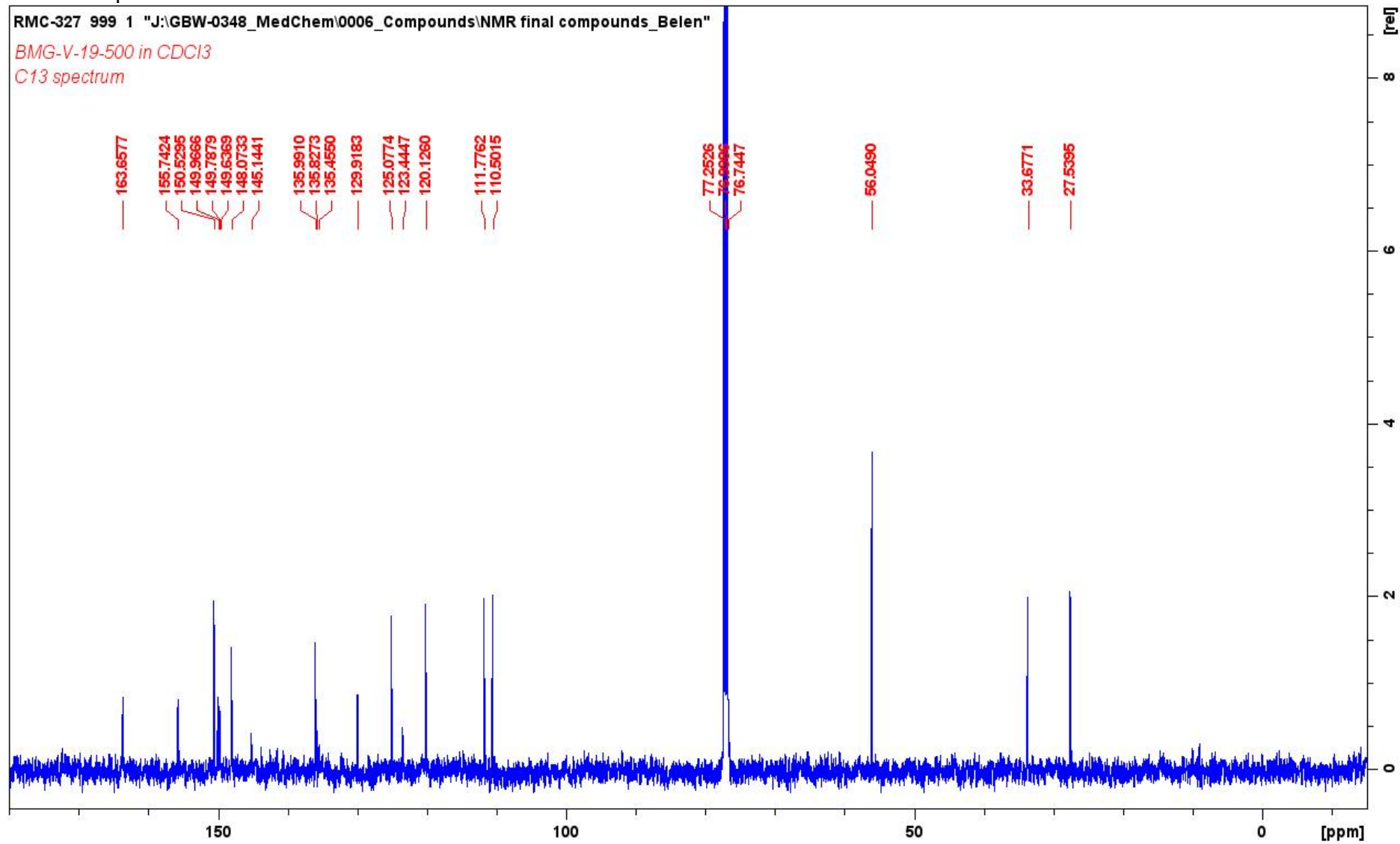
^{13}C NMR spectrum of **20**



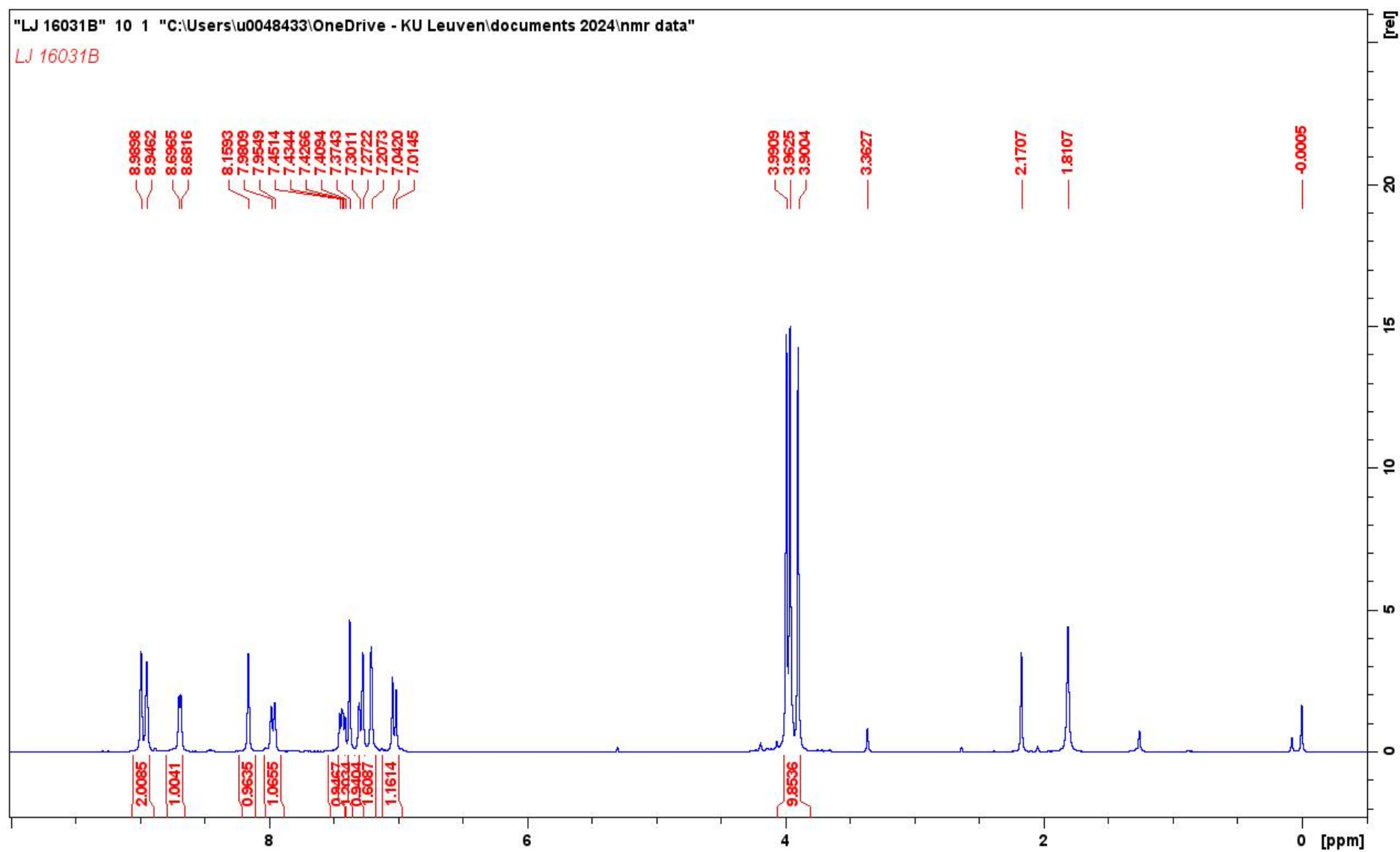
¹H NMR spectrum of 22



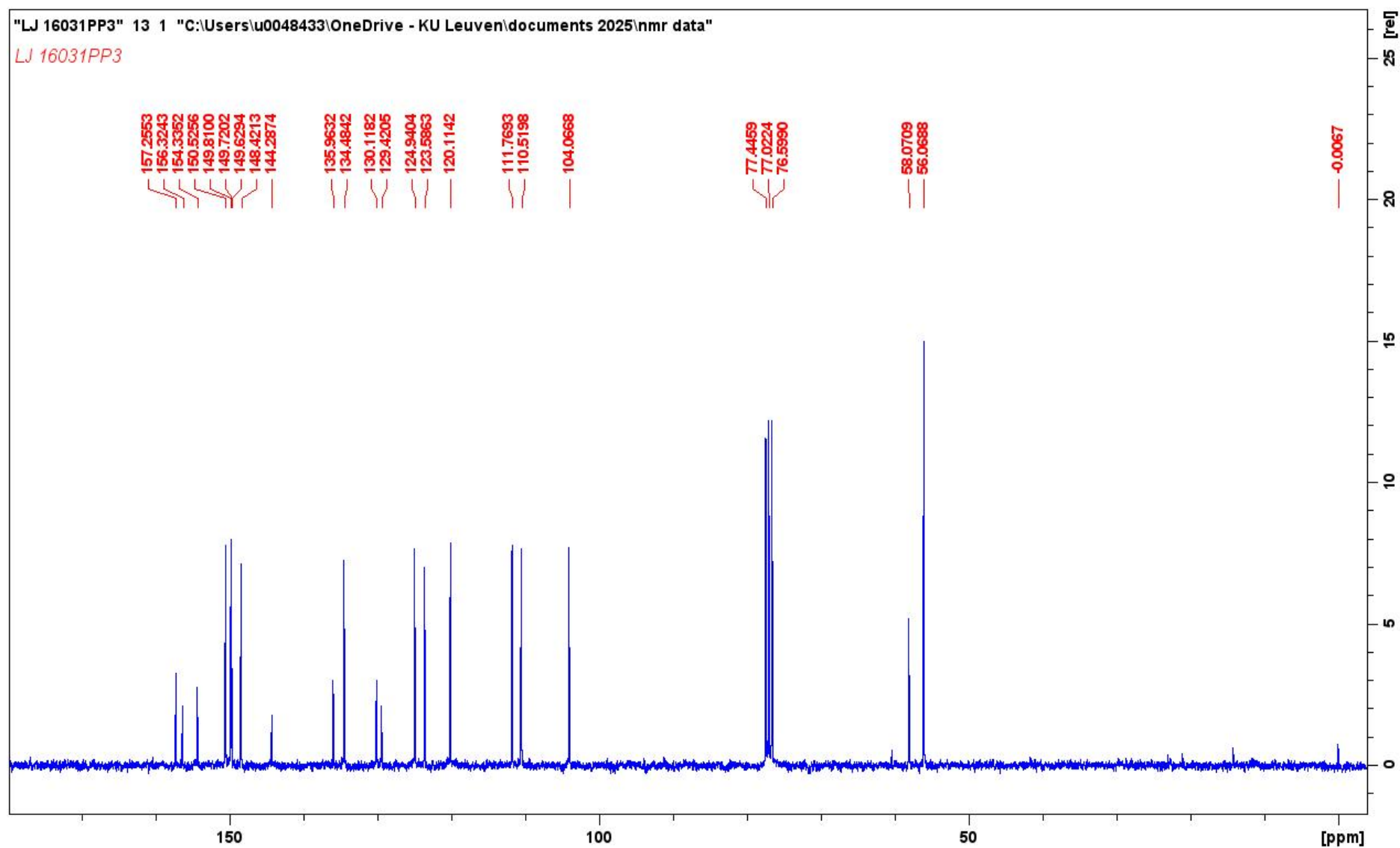
¹³C NMR spectrum of **22**



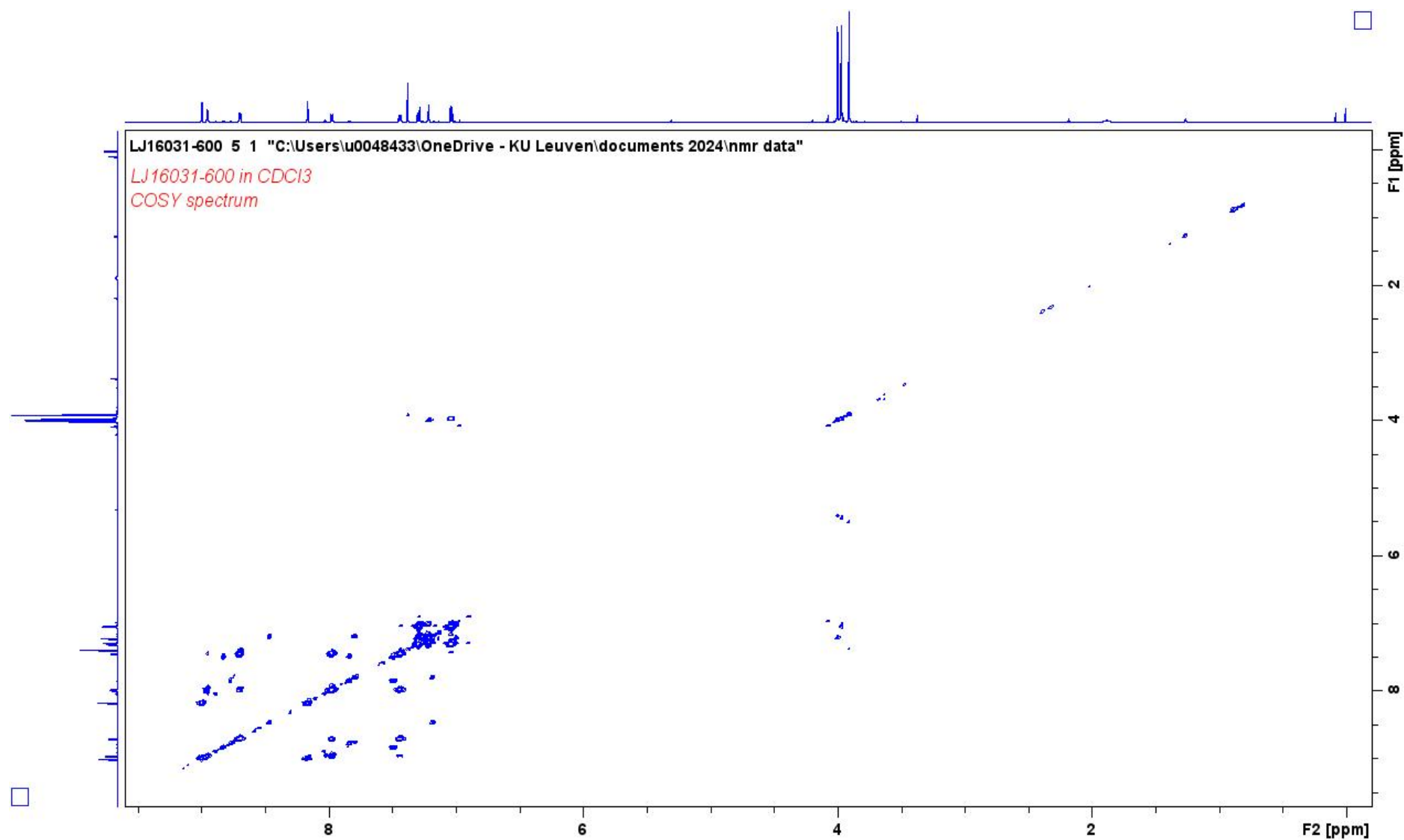
¹H NMR spectrum of **23a**



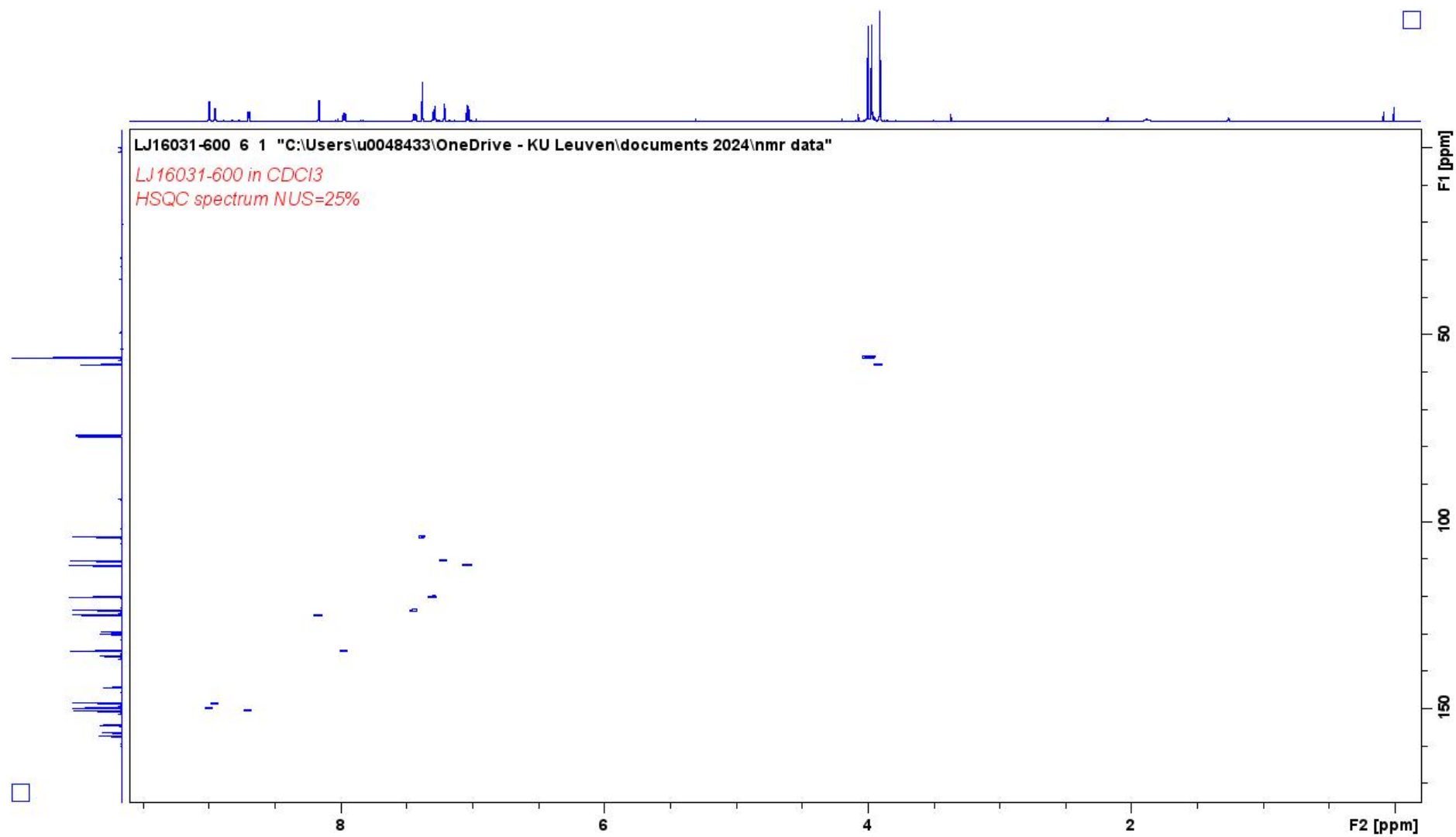
^{13}C NMR spectrum of **23a**



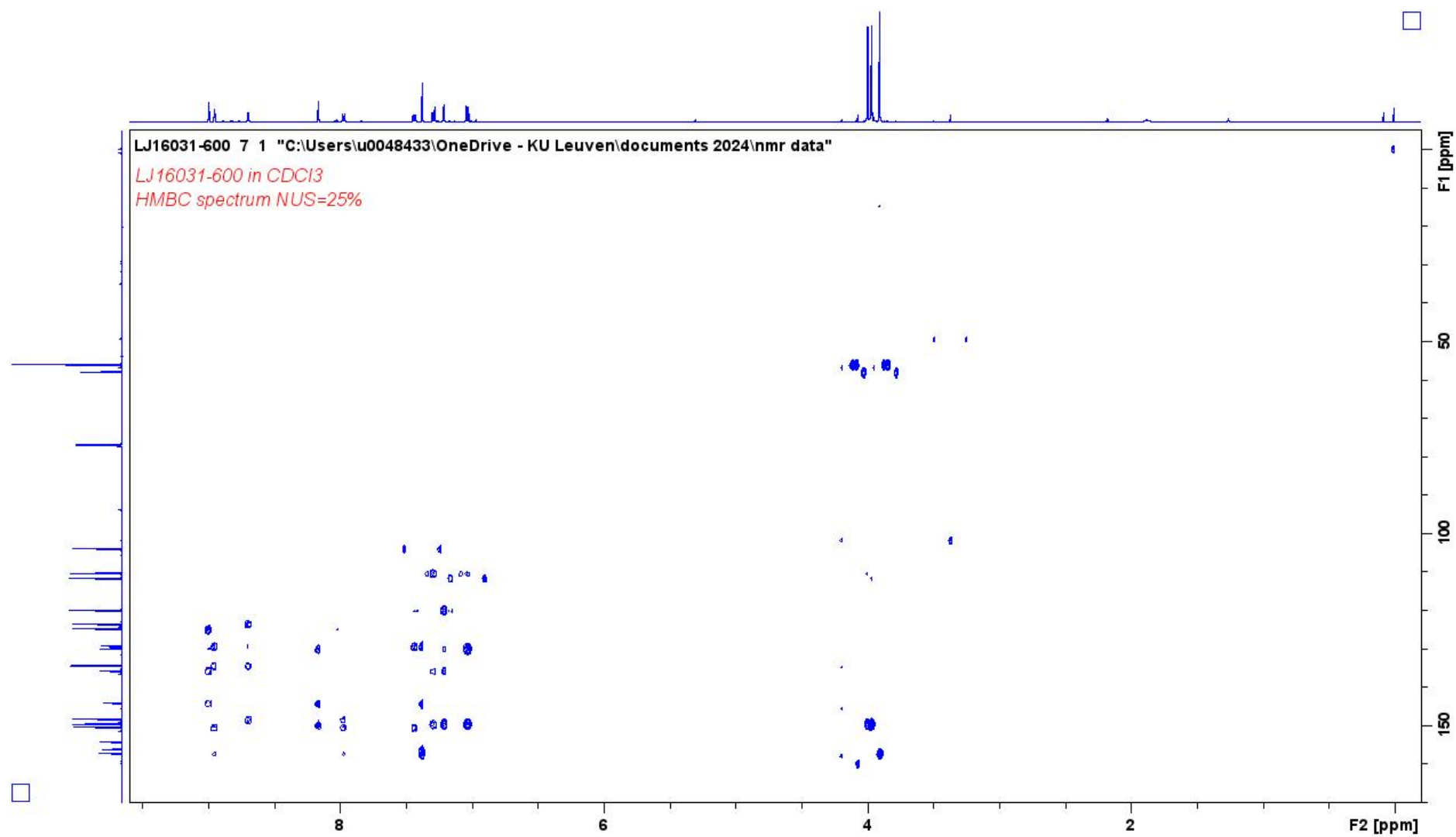
H-H COSY NMR spectrum of **23a**



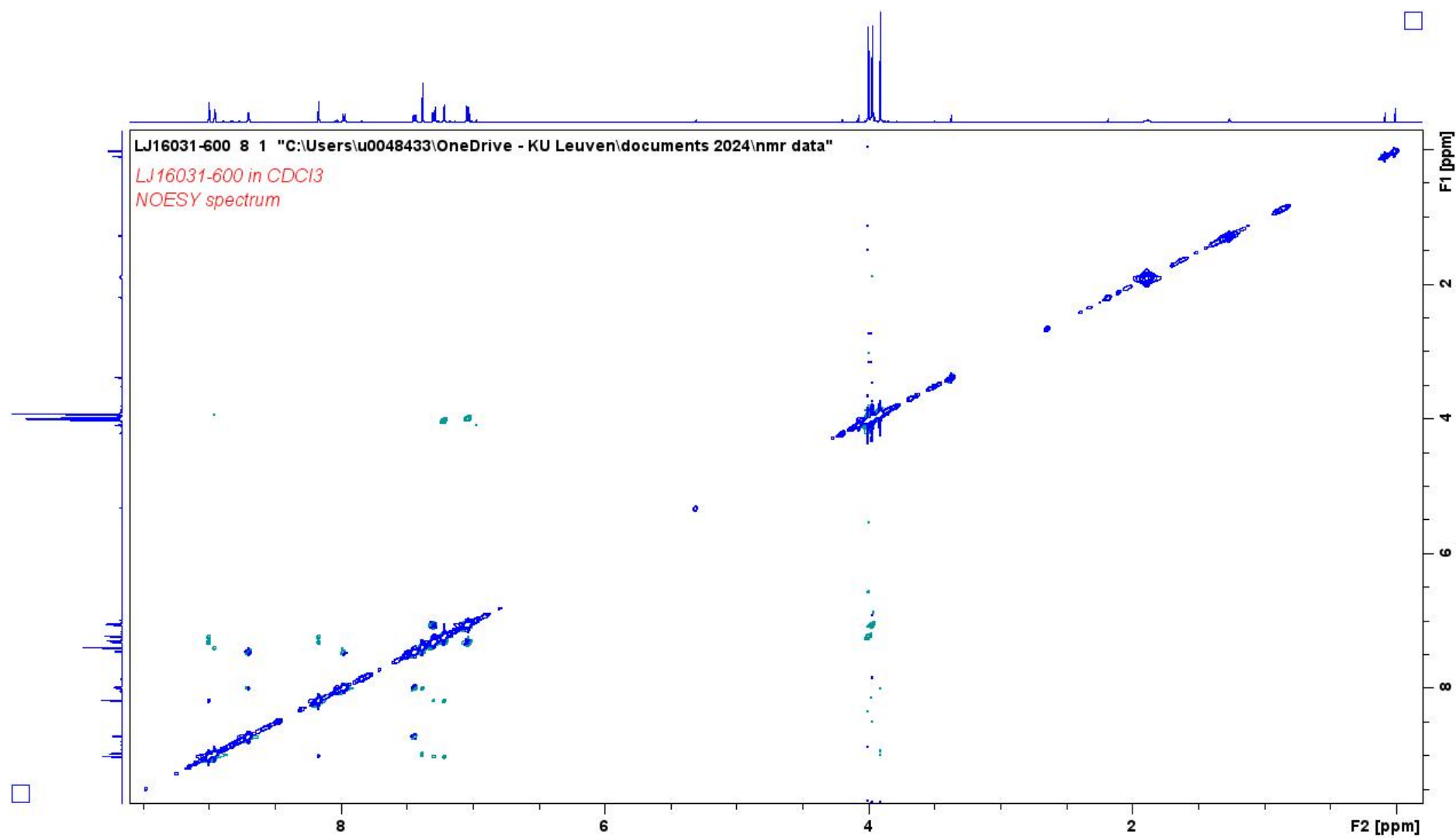
HSQC NMR spectrum of **23a**



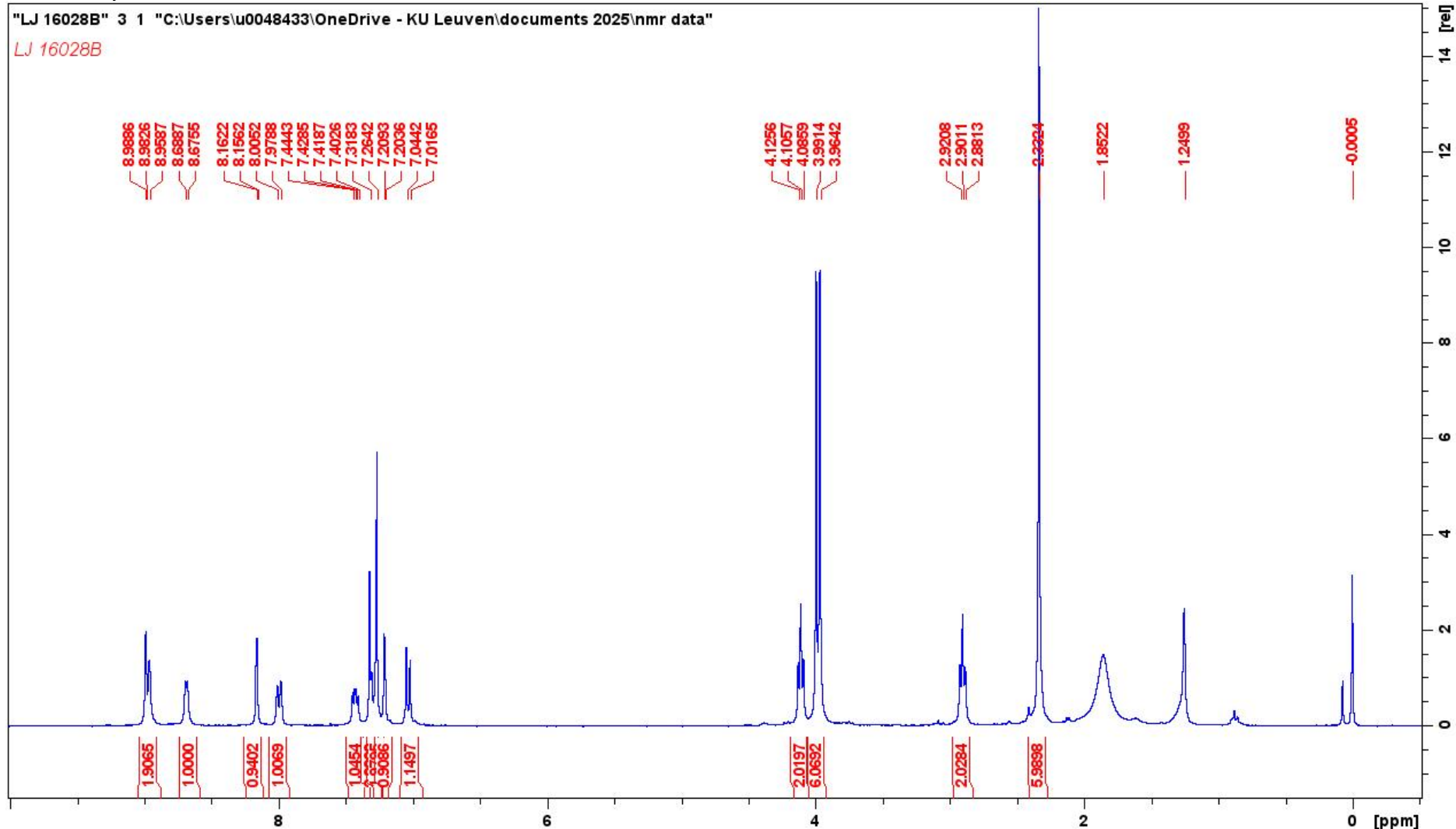
HMBC NMR spectrum of **23a**



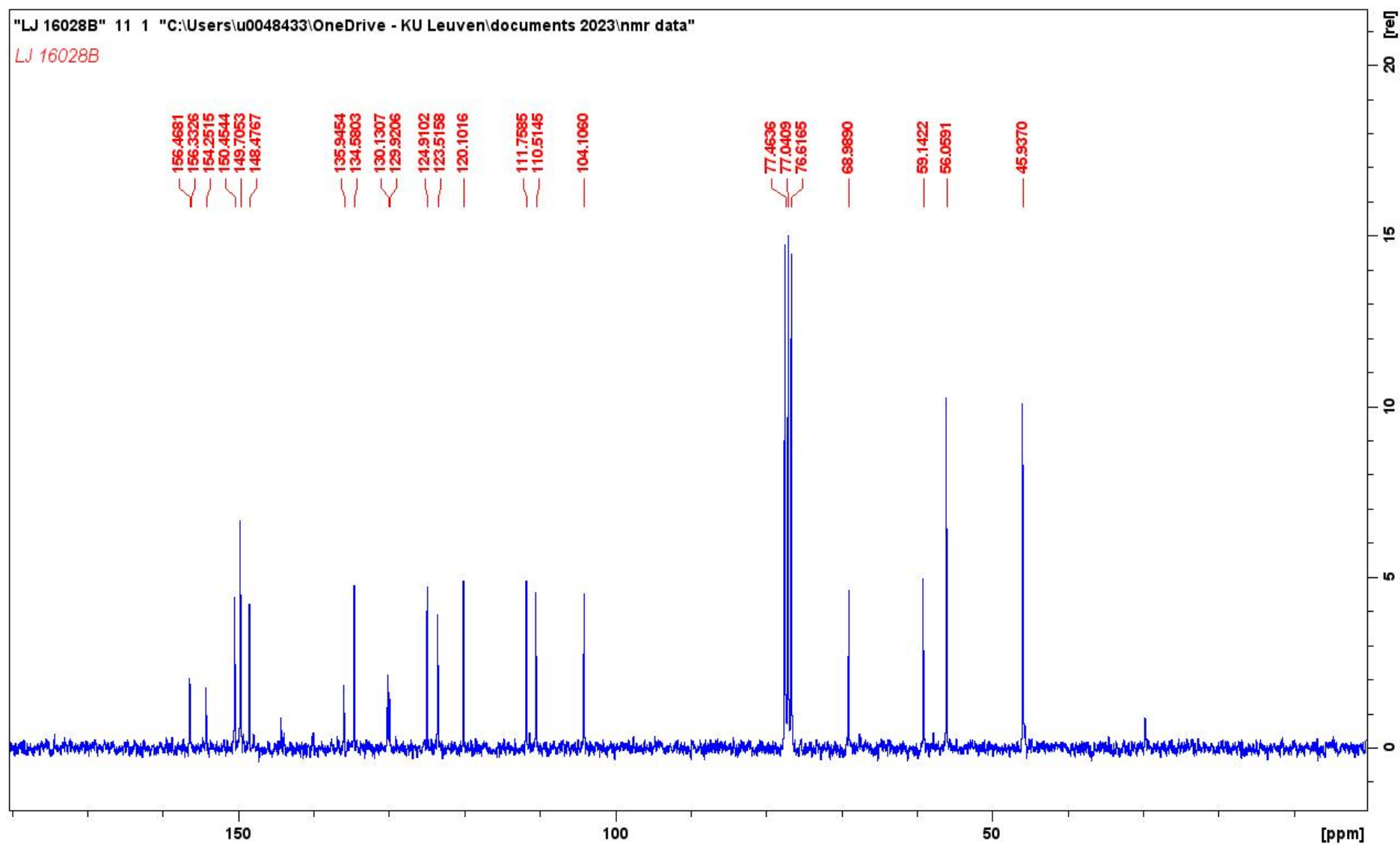
NOESY NMR spectrum of **23a**



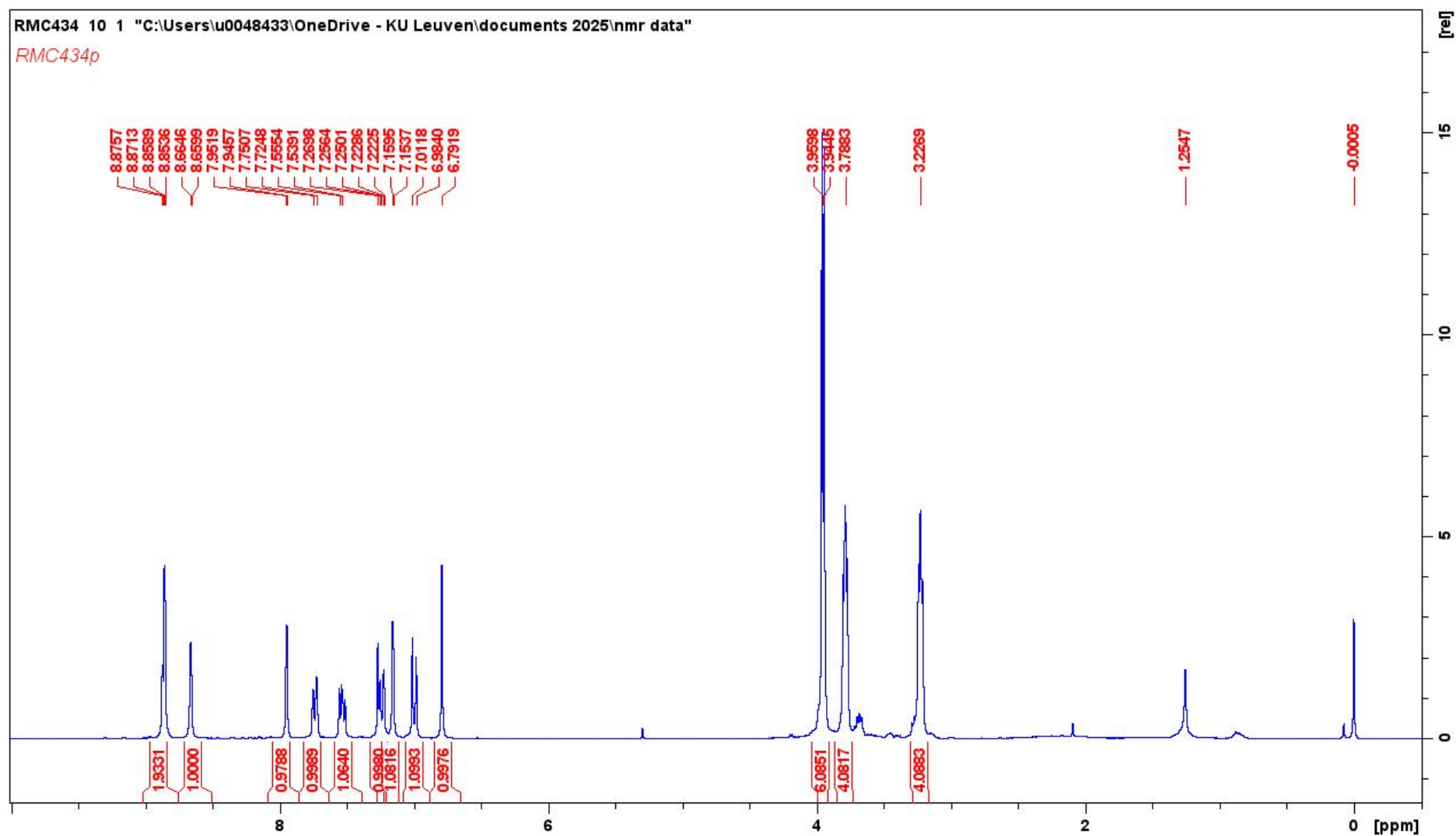
¹H NMR spectrum of **23b**



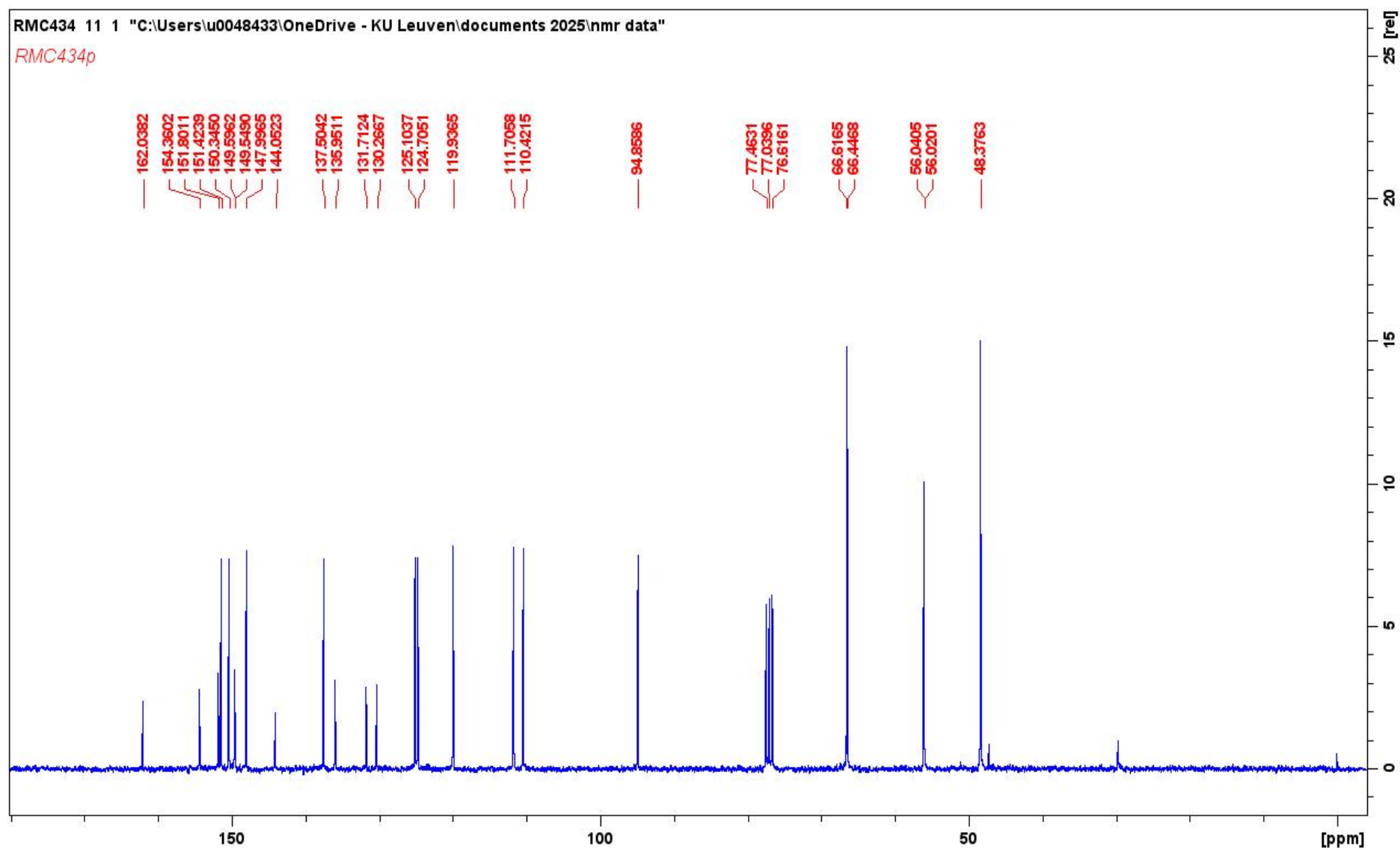
^{13}C NMR spectrum of **23b**



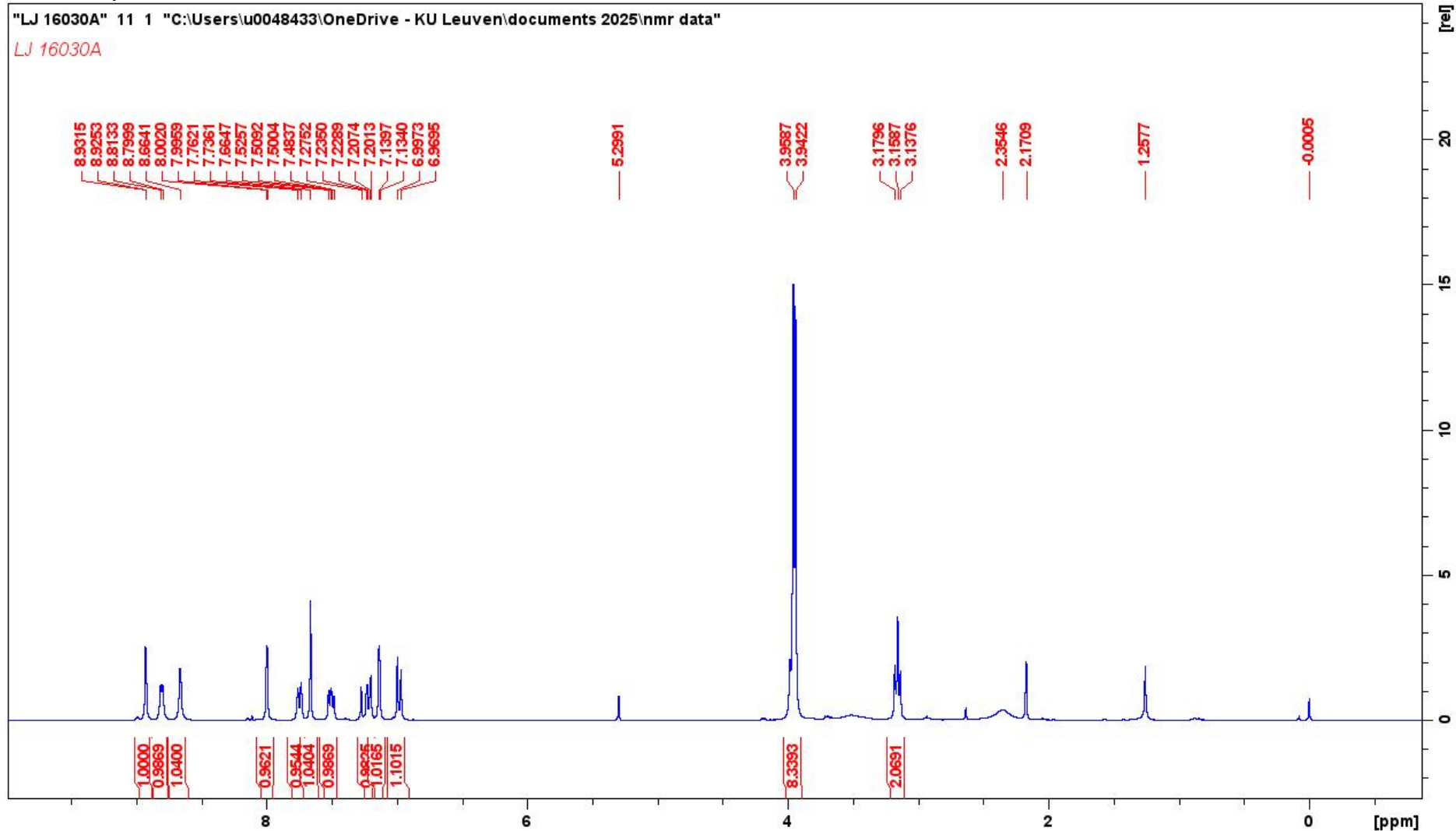
¹H NMR spectrum of **23c**



^{13}C NMR spectrum of **23c**



¹H NMR spectrum of **23d**



^{13}C NMR spectrum of **23d**

