



INCOTIM

# Synthetic Strategies for Labeled Catecholamine-Based Compounds



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## Introduction

We present the recent results in synthesis and structural analysis of some isotopically labeled catecholamine derivatives, in order to elucidate aspects of their polymerization process. The selective labeled intermediates with <sup>15</sup>N and <sup>13</sup>C are required in order to reduce the obstacles encountered in deciphering the mechanism of polydopamine and its analogues formation. Consequently, it was proposed the selective synthesis of <sup>15</sup>N and <sup>13</sup>C labeled key-compound 3-amino-2-(3,4-dihydroxybenzyl)propionamide (**7**) using a multi-step strategy that follows both known literature data and also modified procedures<sup>1</sup>.

## Results

In order to obtain the target compound (**7**) the following synthetic route<sup>1</sup> was proposed (Scheme 1), with mention that we started from commercially available labeled derivative **1** (<sup>13</sup>C<sub>2</sub>-bromoacetic acid). All intermediates<sup>2,3</sup> were obtained in good yields and their structures were identified using NMR spectroscopy and mass spectrometry; also both **6** and **7** are new derivatives.

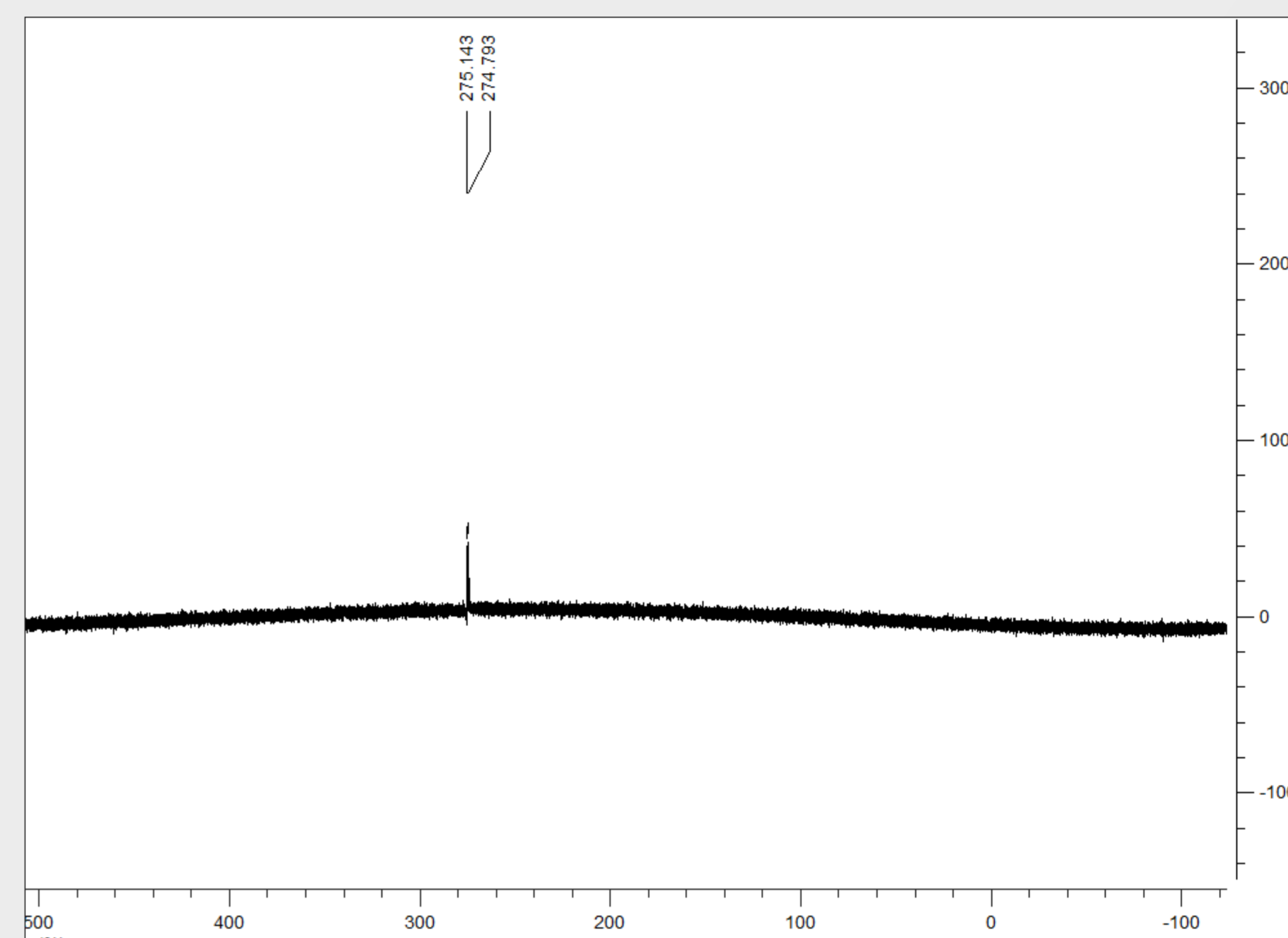
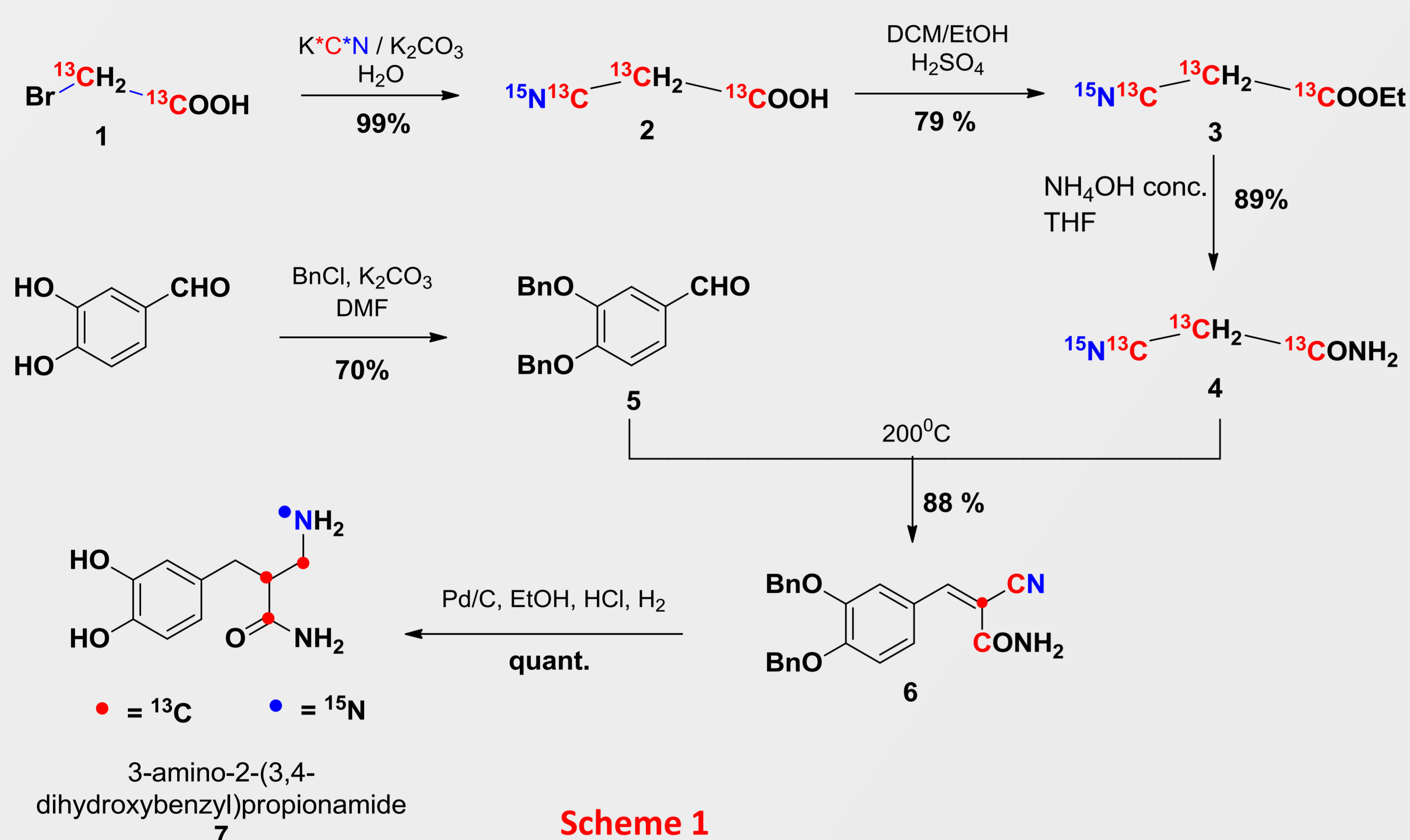


Figure 1. Fragment of <sup>15</sup>N NMR for monomer **6** (CDCl<sub>3</sub>, 500 MHz)

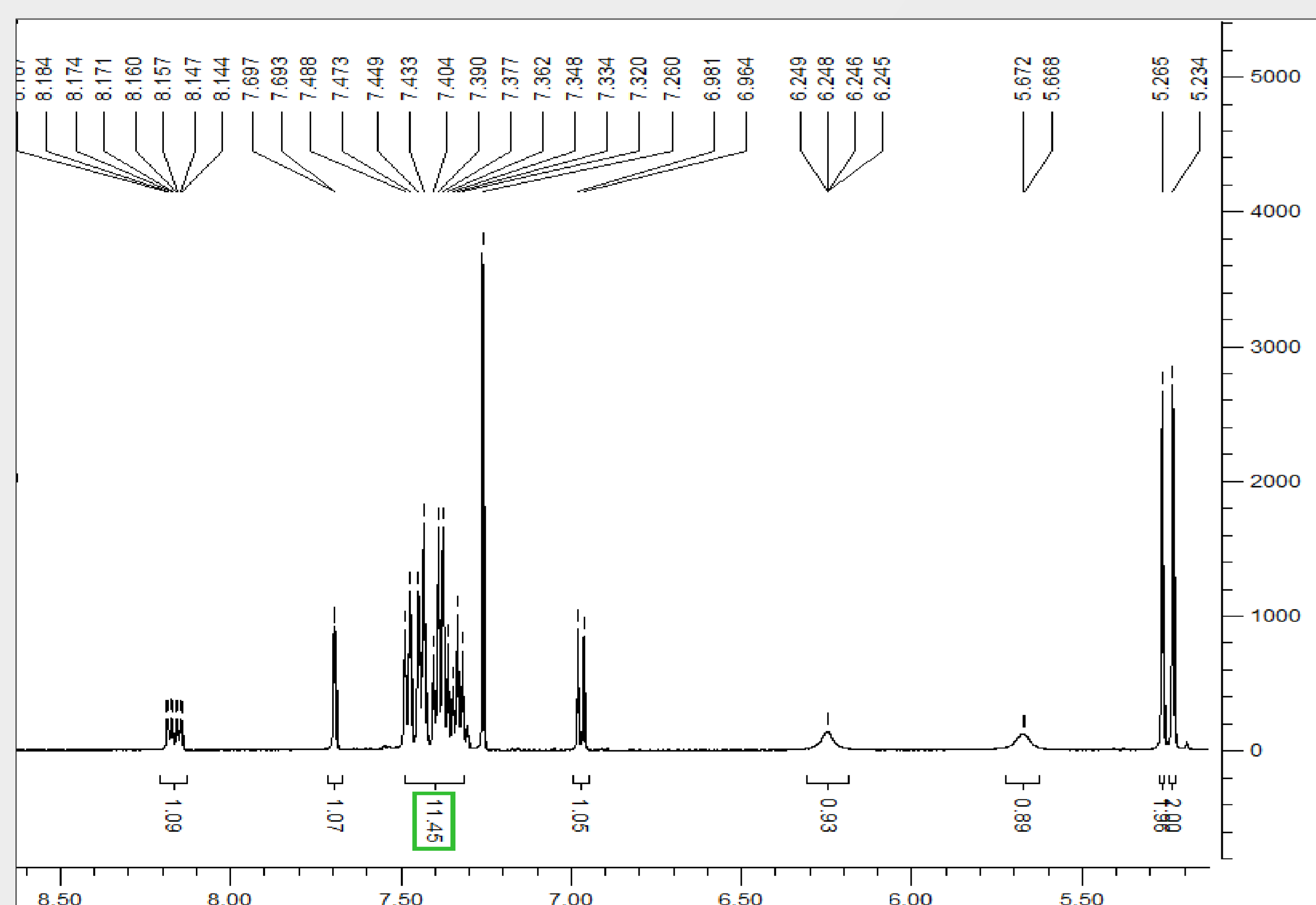


Figure 2. Fragment of <sup>1</sup>H NMR for monomer **6** (CDCl<sub>3</sub>, 500 MHz)

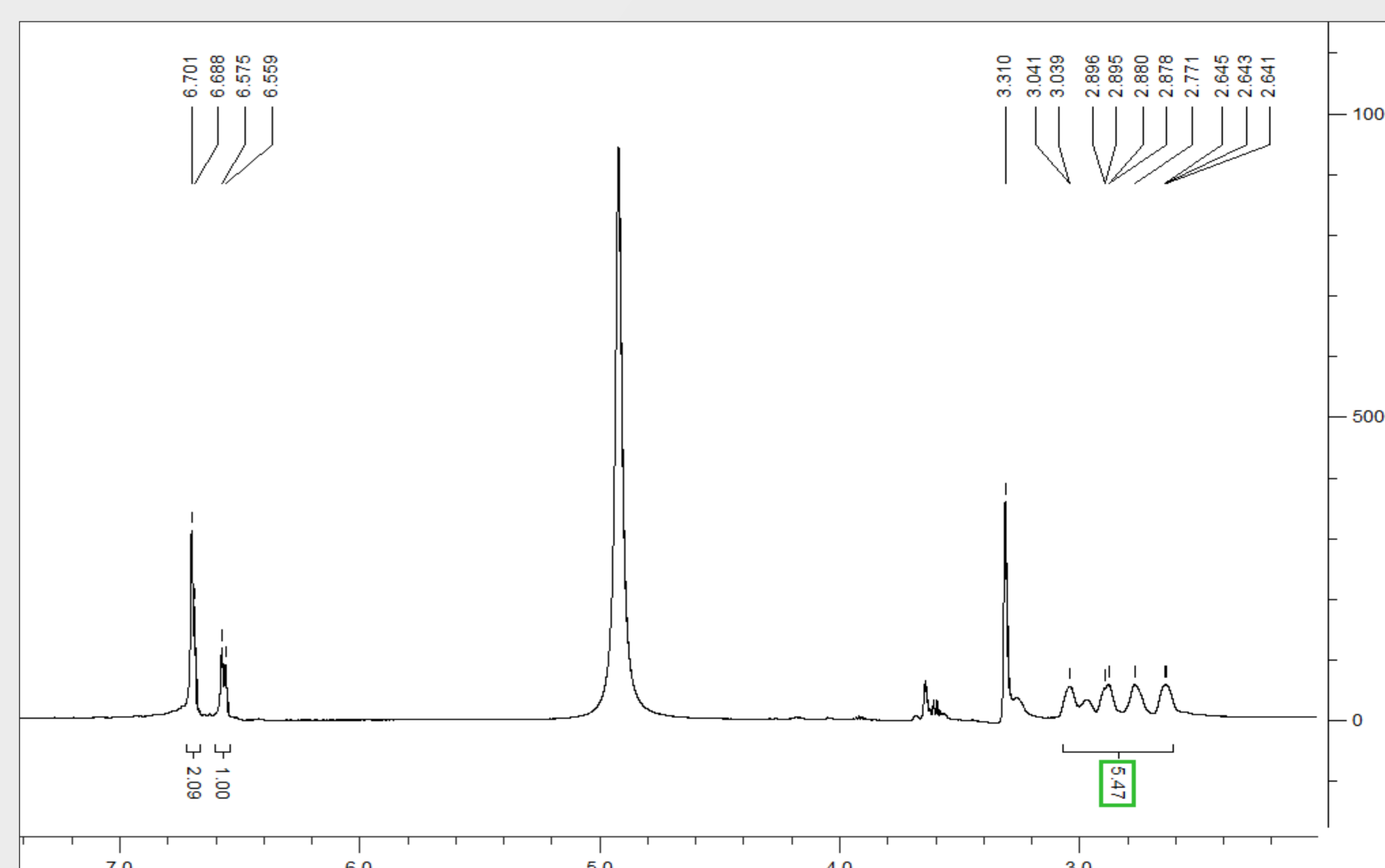


Figure 3. Fragment of <sup>1</sup>H NMR for monomer **7** (MeOD-*d*<sub>4</sub>, 500 MHz)

## Acknowledgements

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## References

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