

## Supporting Information

# Synthesis, Biological, and Computational Evaluation of Antagonistic, Chiral Hydrobenzoin Esters of Arecaidine Targeting mAChR M1

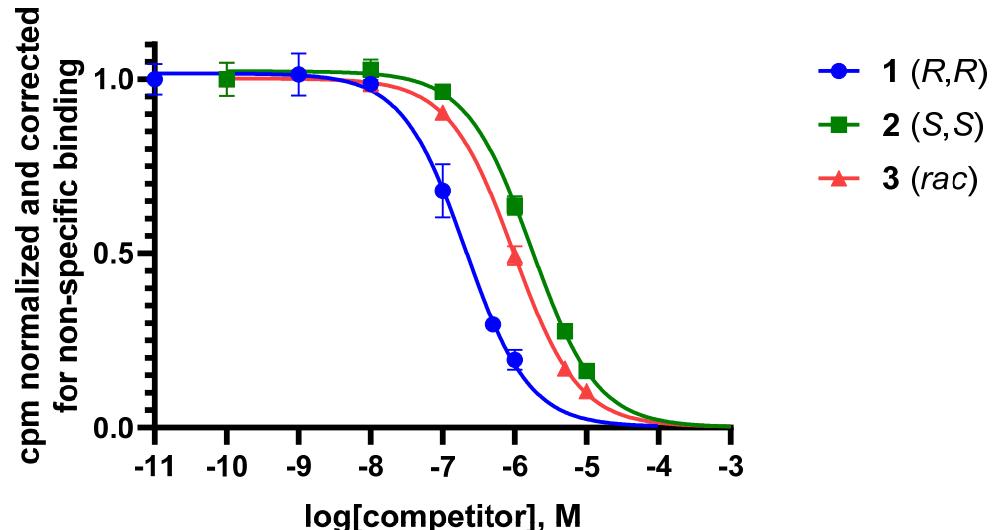
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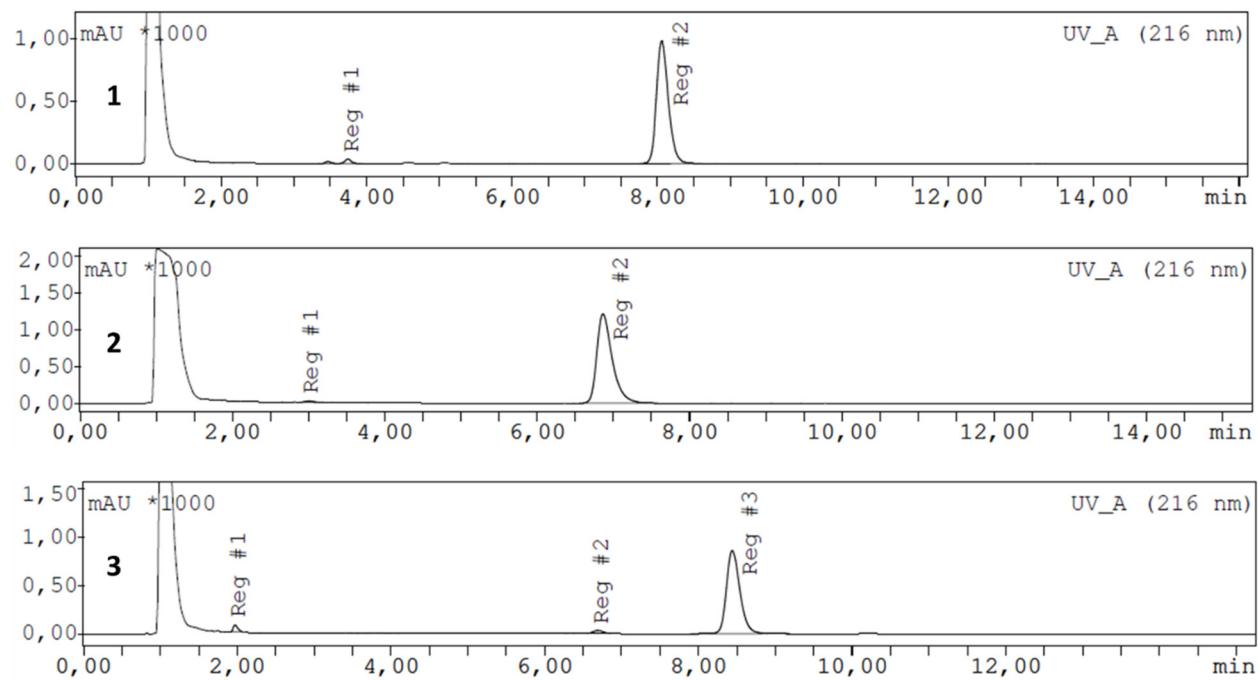
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### Content:

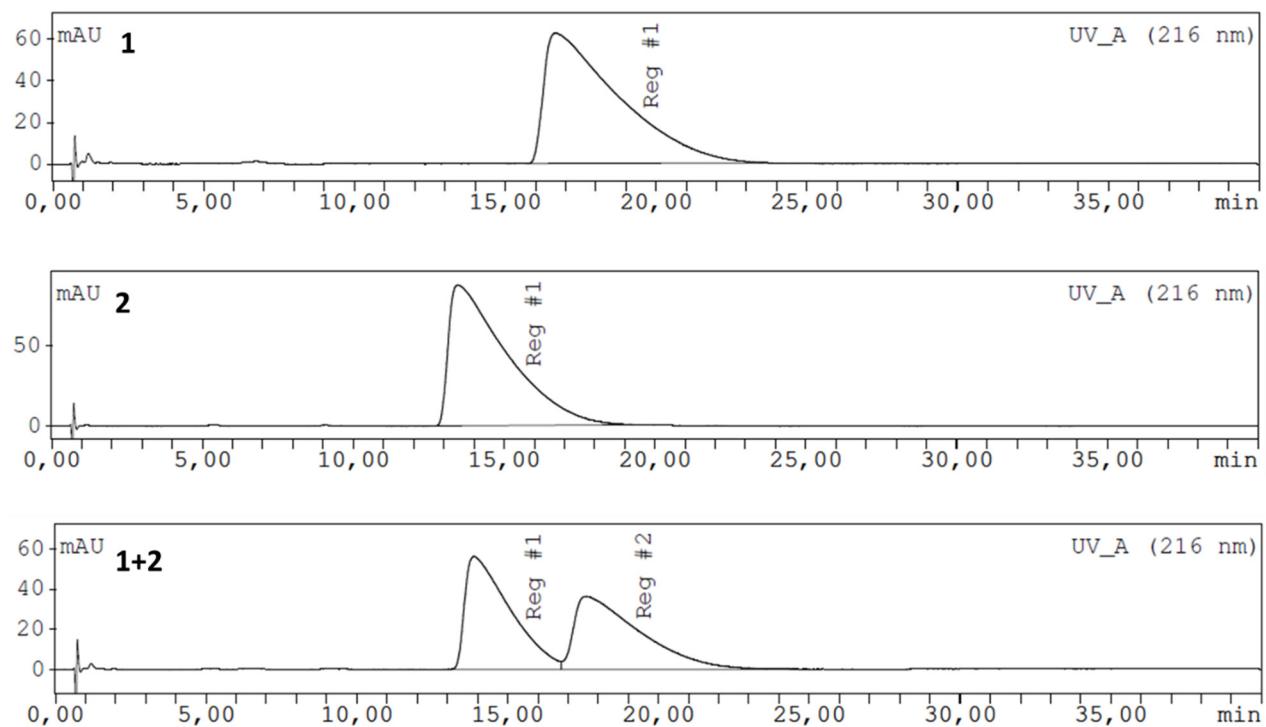
Exemplary competitive binding curves on human mAChR M1 (Figure S1)  
UV-HPLC chromatograms (Figure S2, Figure S3)  
NMR spectra (Figure S4, Figure S5, Figure S6)



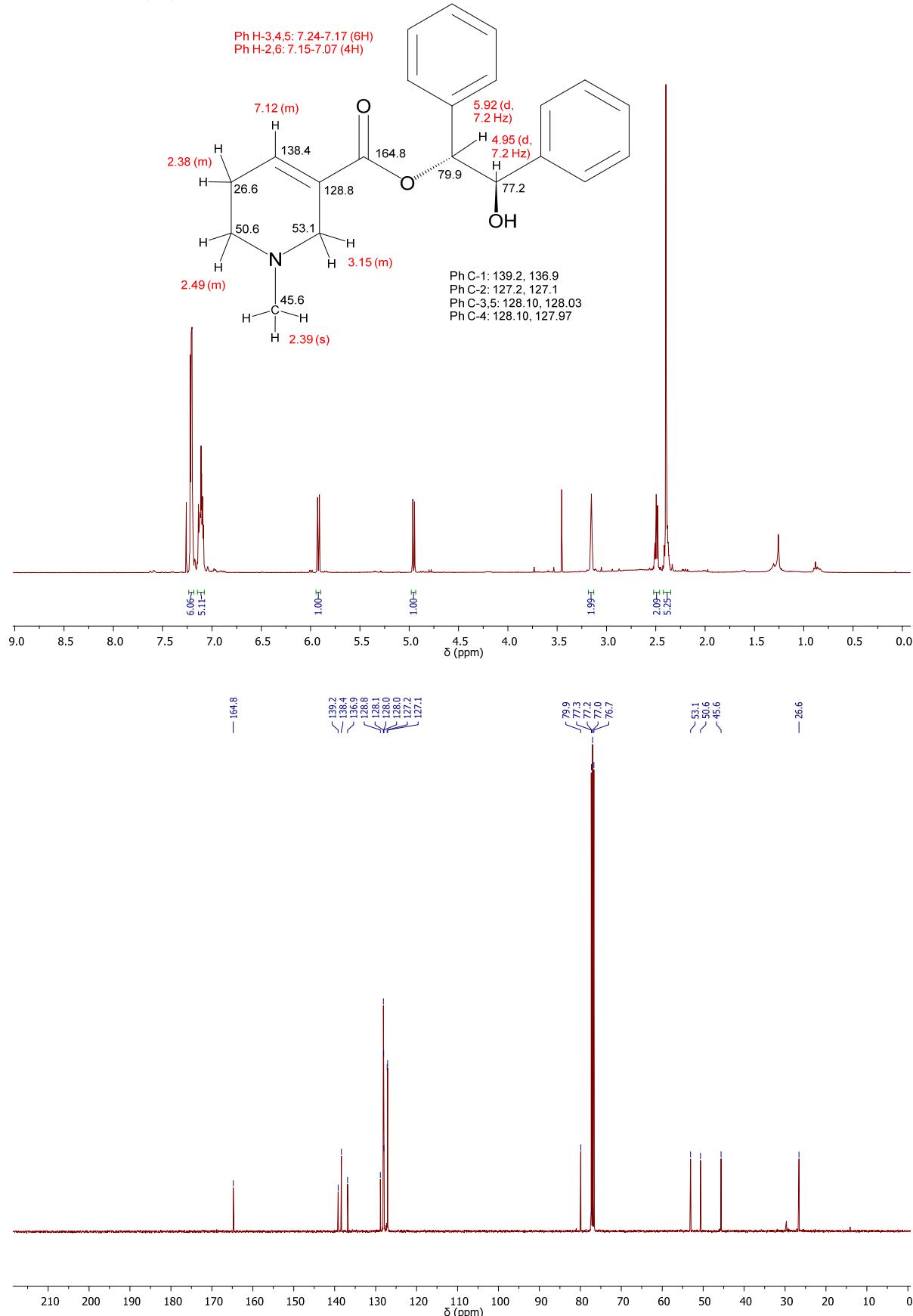
**Figure 1.** Exemplary competitive binding curves of **1**, **2**, and **3** on human mAChR M1 expressed on cell membranes of stably transfected CHO cells using [*N*-methyl-<sup>3</sup>H]scopolamine methyl chloride. Values at  $10^{-11}$  M and  $10^{-10}$  M represent full binding in absence of competitor.



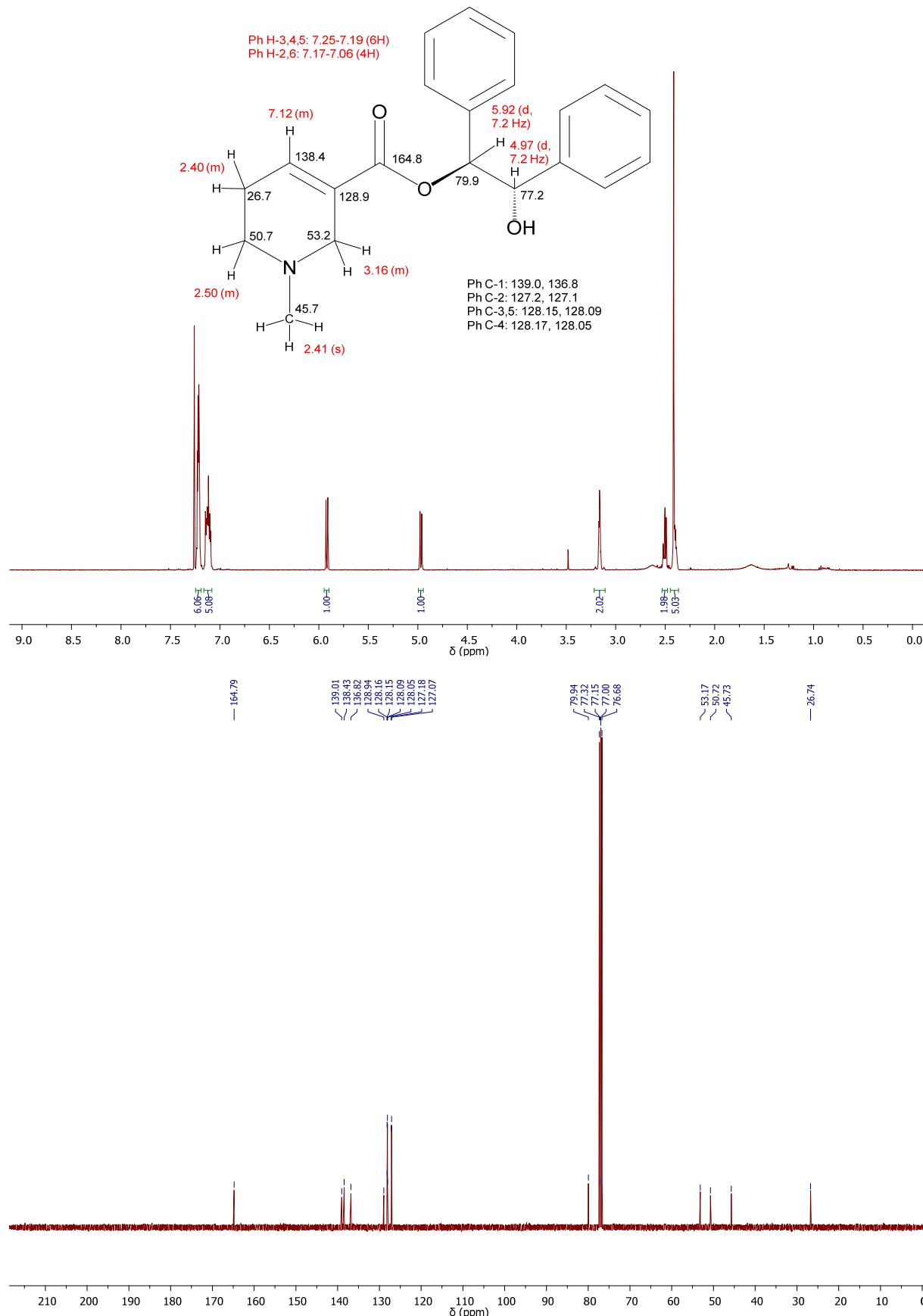
**Figure 2.** Isocratic HPLC chromatograms of compounds **1–3**. 35–40% ACN in 25 mM NH<sub>4</sub>H<sub>2</sub>PO<sub>4</sub> buffer pH 9.3 at a flow of 1 mL/min.



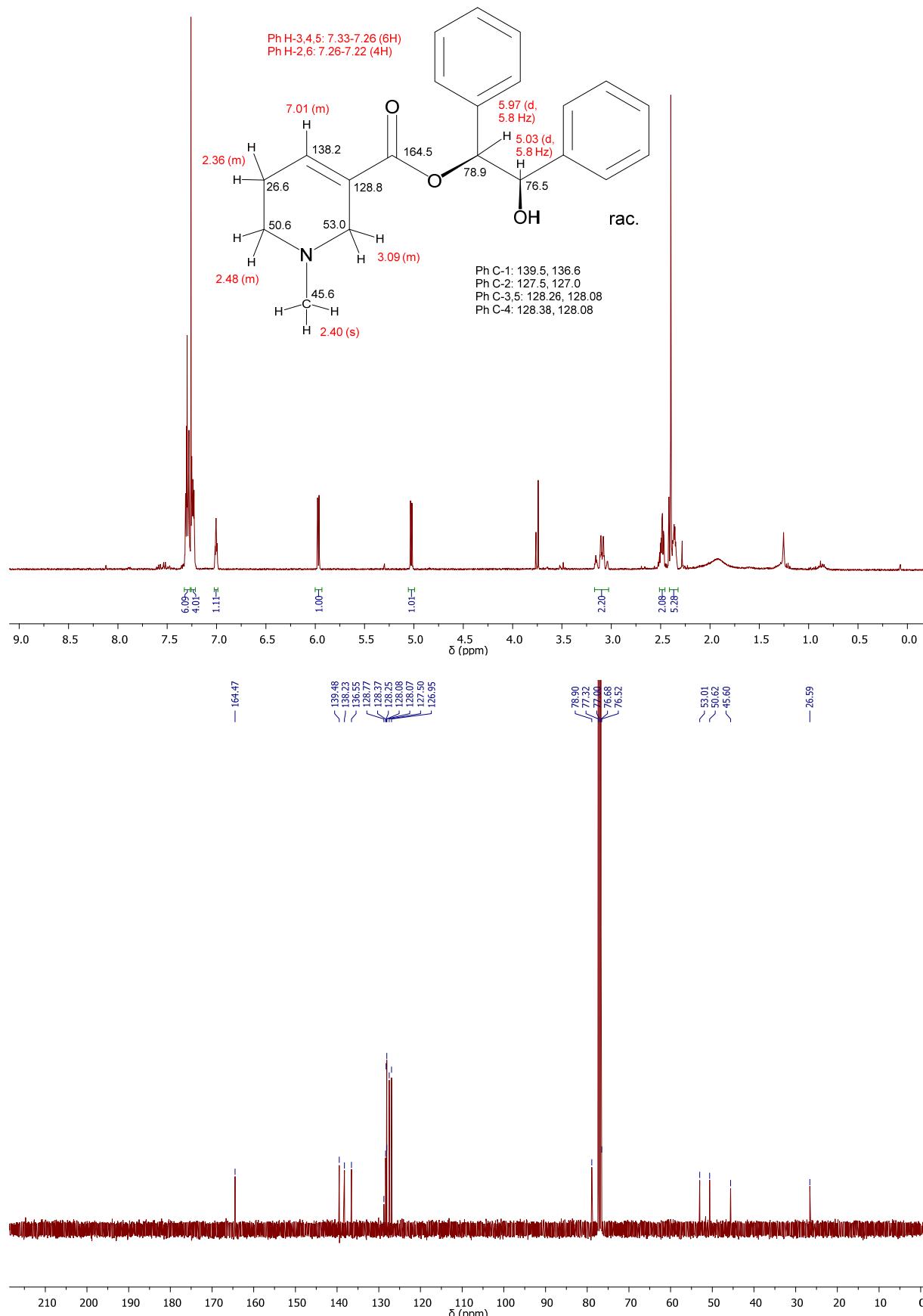
**Figure 3.** Chiral chromatography using a an AGP 0.3 cmØ × 5 cm 5 µM column operated with 2% IPA in 10 mM NH<sub>4</sub>Ac pH 5.8 at a flow of 0.5 mL/min.



**Figure 4.**  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectrum of **1**.



**Figure 5.** <sup>1</sup>H- and <sup>13</sup>C-NMR spectrum of 2.



**Figure 6.**  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectrum of **3**.