# Supplementary Materials: Synthesis, Biological Evaluation and Molecular Modelling of 2′-Hydroxychalcones as Acetylcholinesterase Inhibitors

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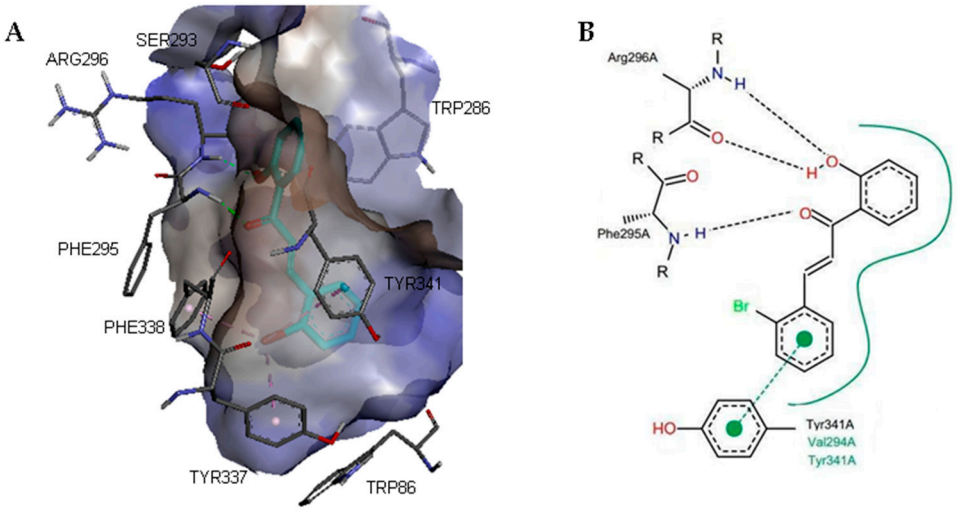


**Figure S1.** Representations of compound **7** in complex with human AChE (PDB ID: 4EY7). (**A**) 3D representation of the binding pose. The hydrophobic surfaces of the interacting residues are shown in blue relief. Hydrogen bonds and π-halogen interactions are depicted with green and purple dotted lines, respectively; (**B**) Schematic representation of the binding interactions. Hydrogen bonds and π-π stacking interactions are depicted with black and green dotted lines, respectively. The green curve represents other non-polar interactions.

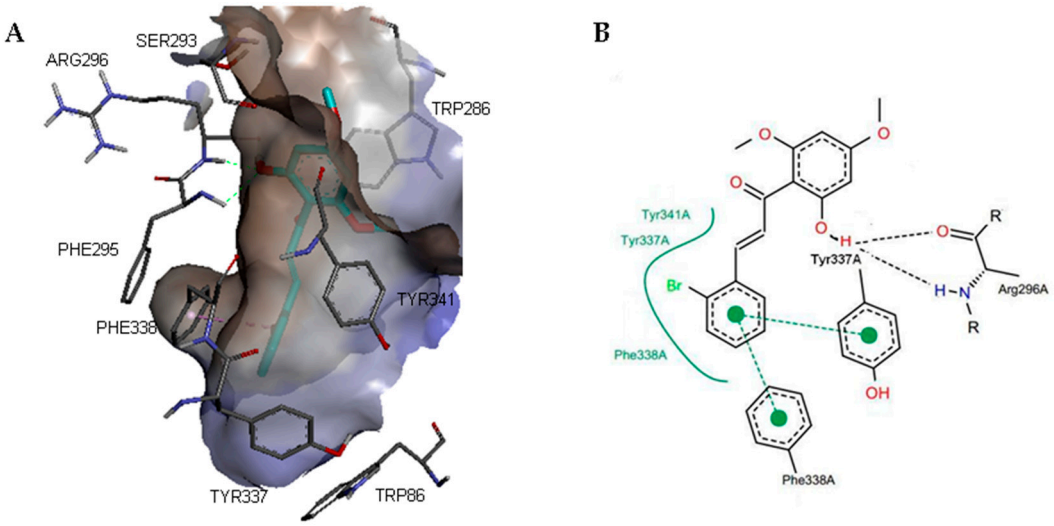


**Figure S2.** Representations of compound **13** in complex with human AChE (PDB ID: 4EY7). (**A**) 3D representation of the binding pose. The hydrophobic surfaces of the interacting residues are shown in blue relief. Hydrogen bonds and π-halogen interactions are depicted with green and purple dotted lines, respectively; (**B**) Schematic representation of the binding interactions. Hydrogen bonds and π-π stacking interactions are depicted with black and green dotted lines, respectively. The green curve represents other non-polar interactions.

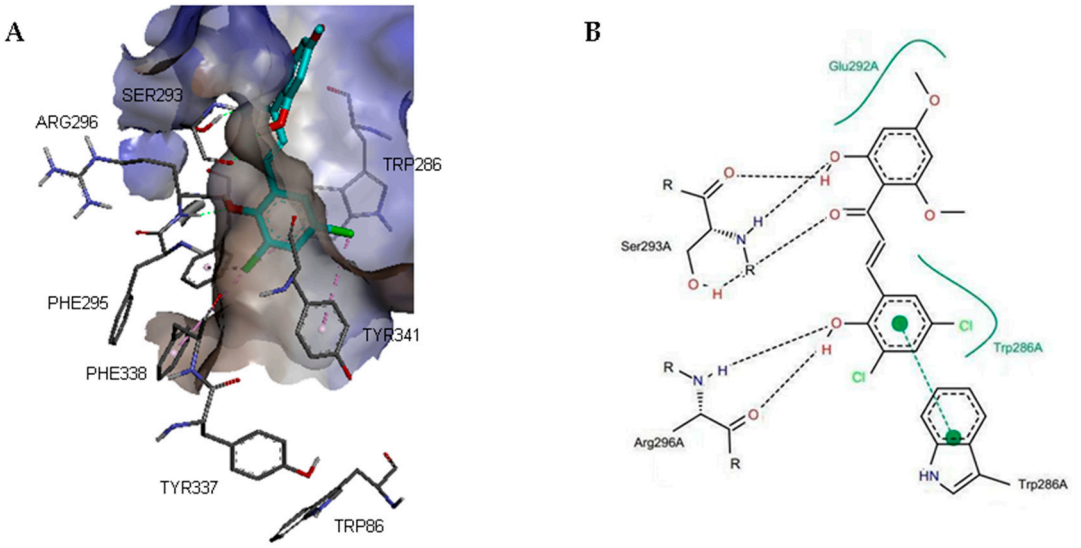


**Figure S3.** Representations of compound **14** in complex with human AChE (PDB ID: 4EY7). (**A**) 3D representation of the binding pose. The hydrophobic surfaces of the interacting residues are shown in blue relief. Hydrogen bonds and π-halogen interactions are depicted with green and purple dotted lines, respectively; (**B**) Schematic representation of the binding interactions. Hydrogen bonds and π-π stacking interactions are depicted with black and green dotted lines, respectively. The green curve represents other non-polar interactions.

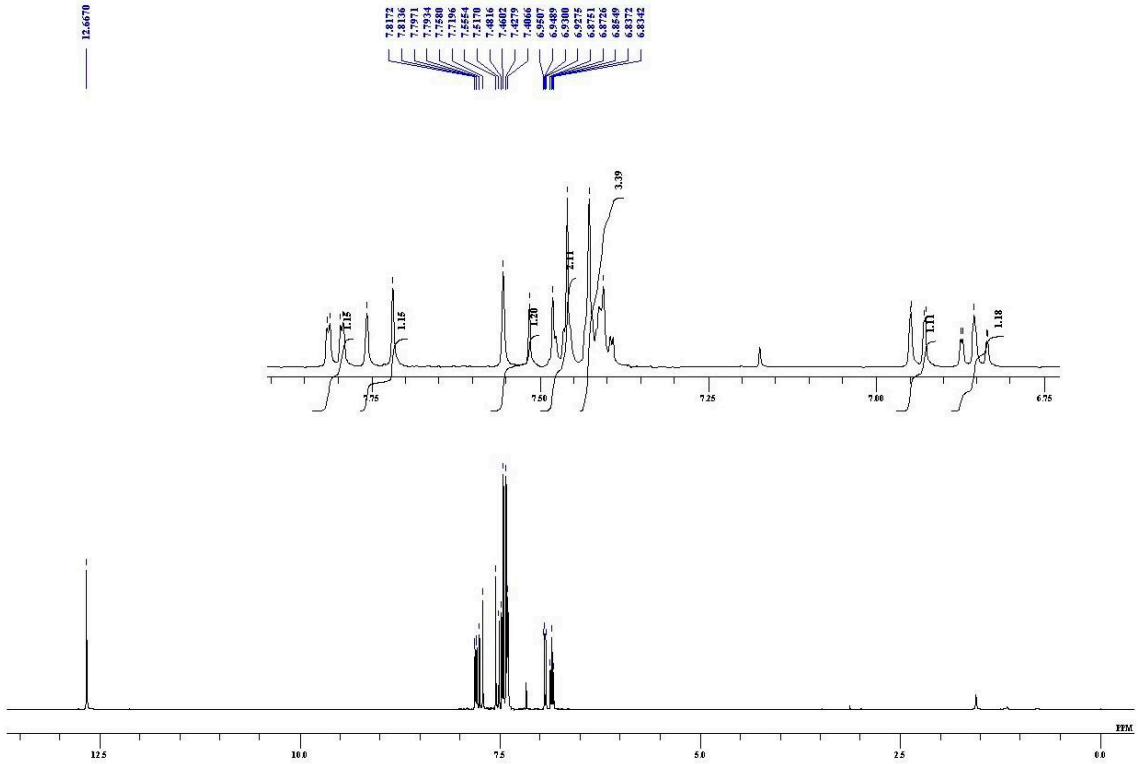

**Figure S4.** *Cont.*

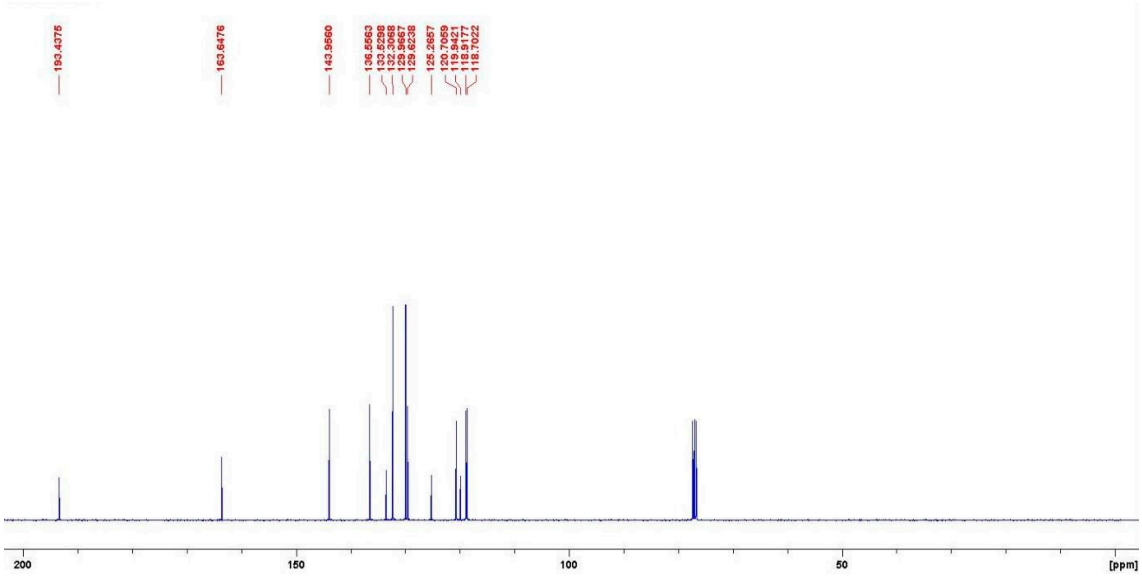


**Figure S4.** $^{1}$H-NMR and $^{13}$C-NMR spectra of 4-Bromo-2′-hydroxychalcone (**3**).

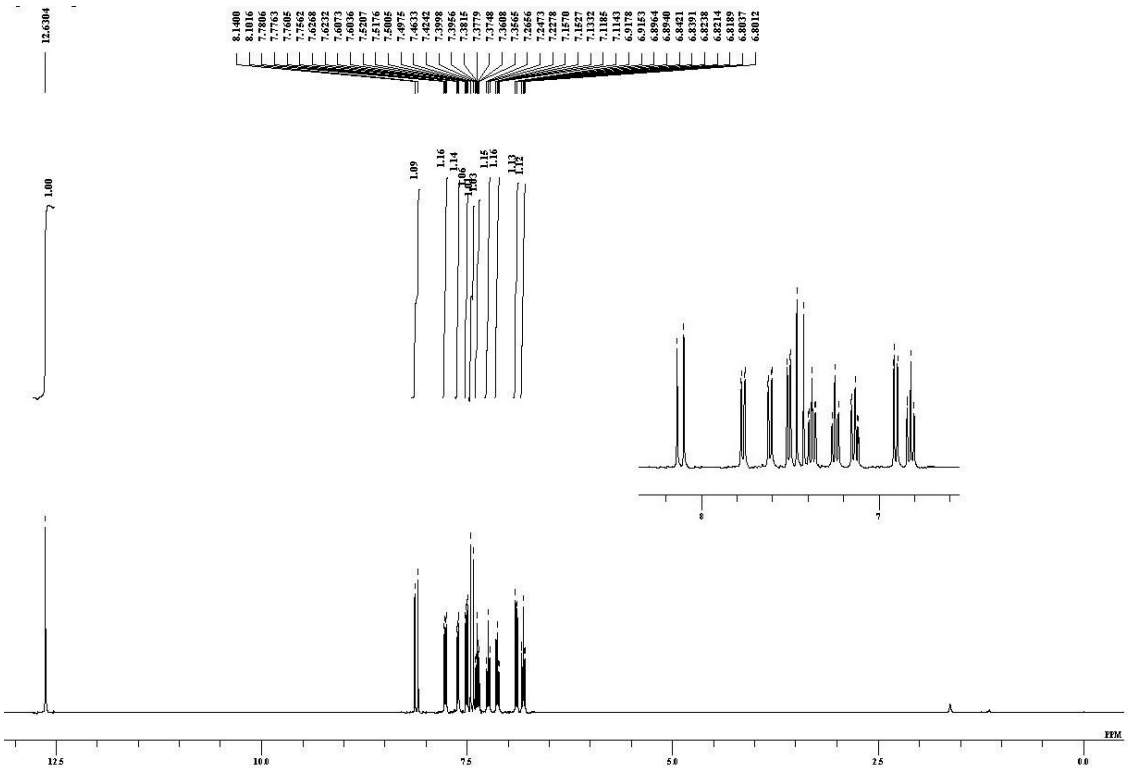


**Figure S5.** *Cont.*

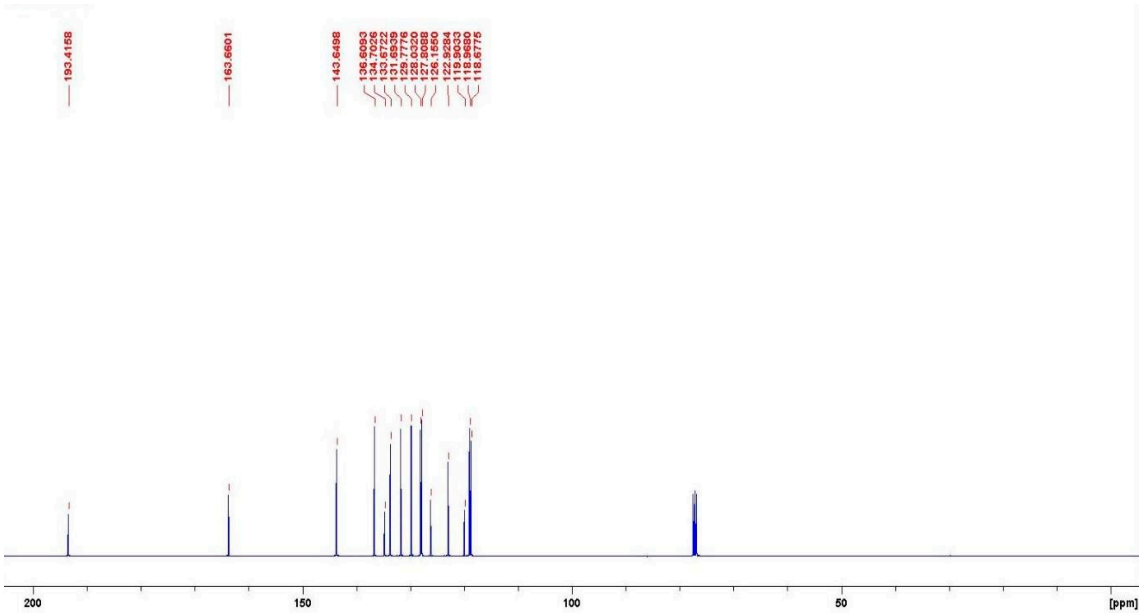


**Figure S5.** $^{1}$H-NMR and $^{13}$C-NMR spectra of 2-Bromo-2′-hydroxychalcone (**7**).

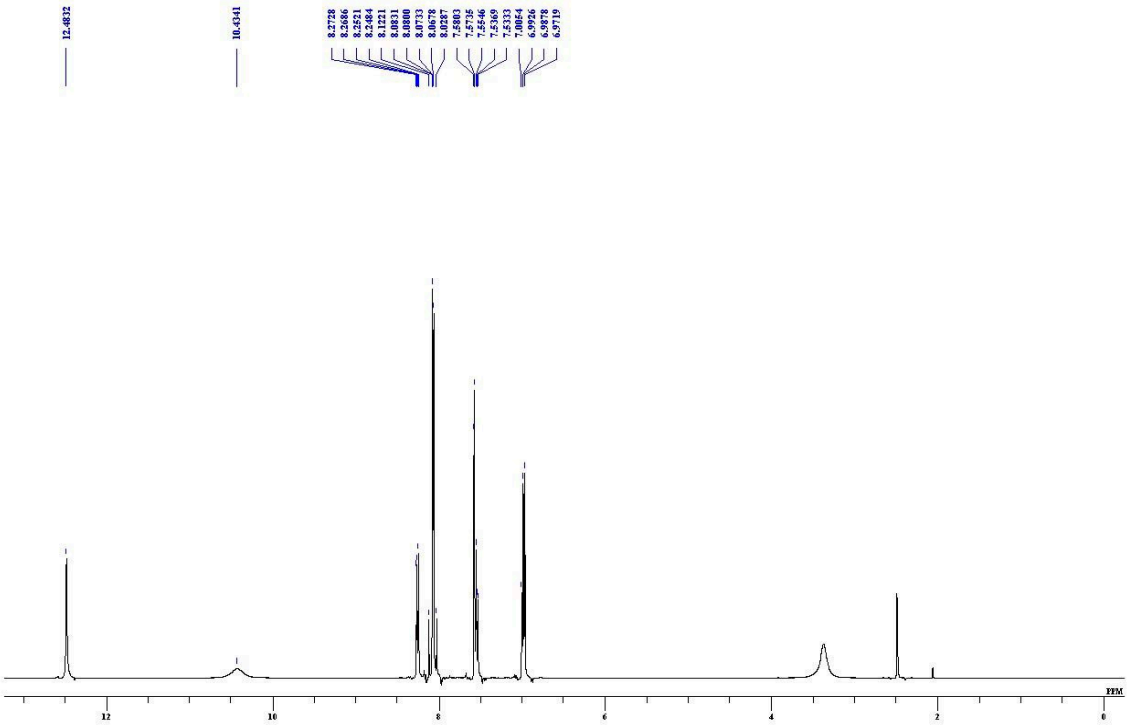


**Figure S6.** *Cont.*

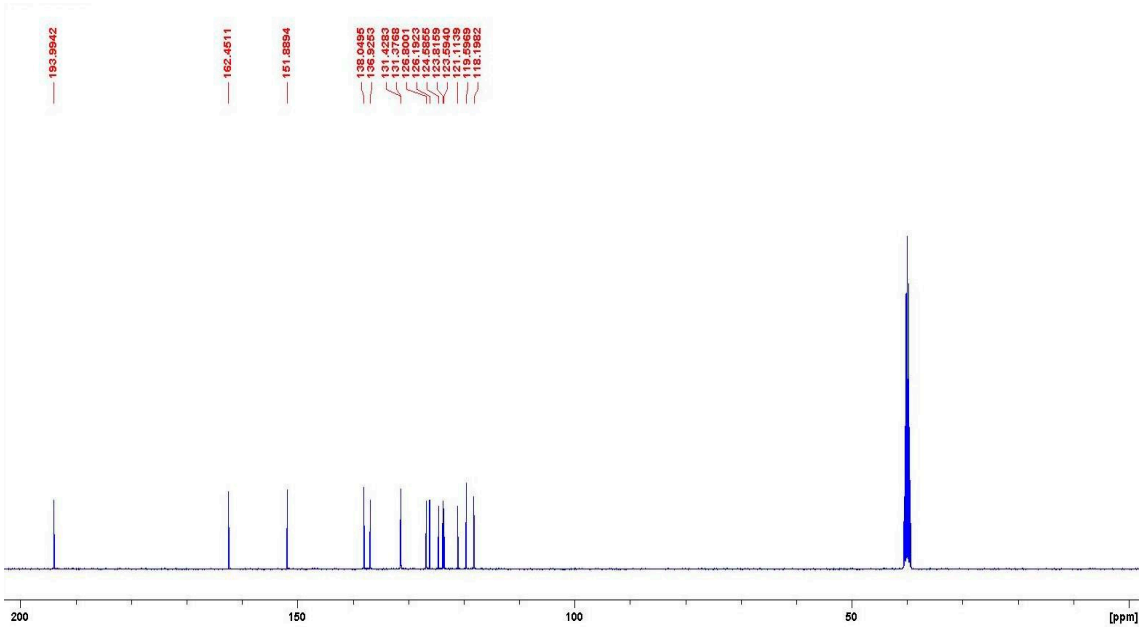


**Figure S6.** $^{1}$H-NMR and $^{13}$C-NMR spectra of 3,5-Dichloro-2,2′-dihydroxychalcone (**8**).

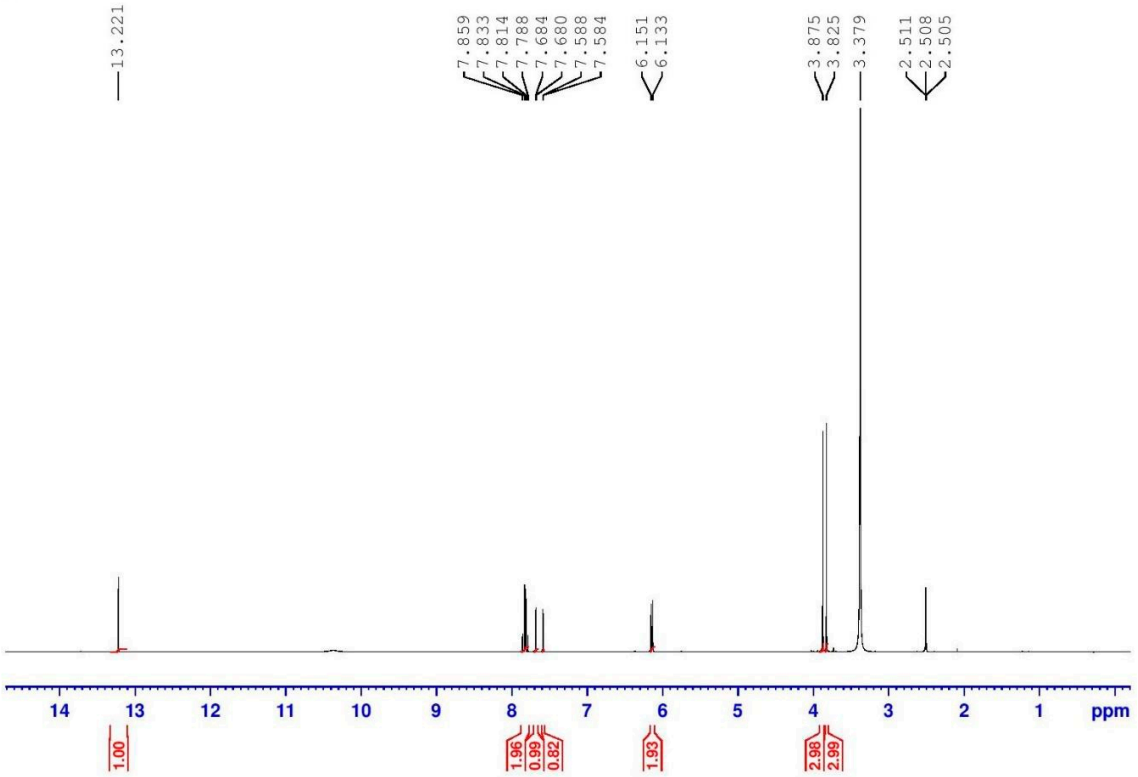


**Figure S7.** *Cont.*

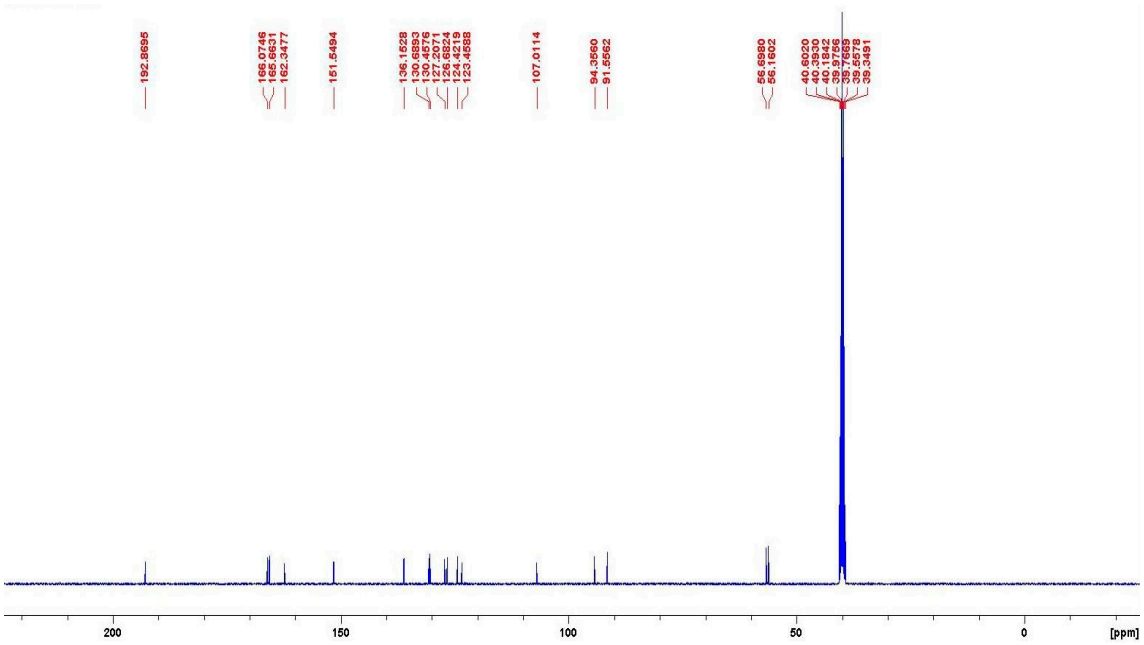


**Figure S7.** $^{1}$H-NMR and $^{13}$C-NMR spectra of 3,5-Dichloro-2,2′-dihydroxy-4′,6′-dimethoxychalcone (**14**).