

Exploring the 2'-hydroxy-chalcone framework for the development of dual antioxidant and soybean lipoxygenase inhibitory agents

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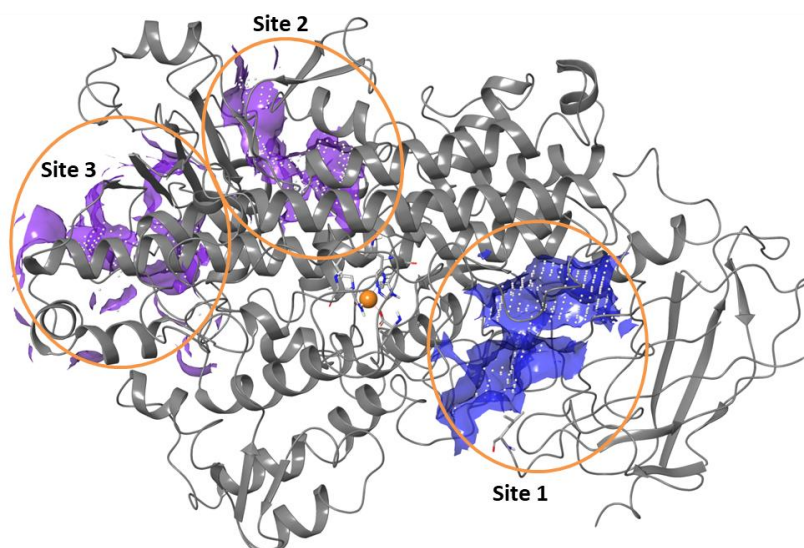


Figure S1: Predicted binding sites of Soybean Lipoxxygenase seed isoform 1 (LOX-1).

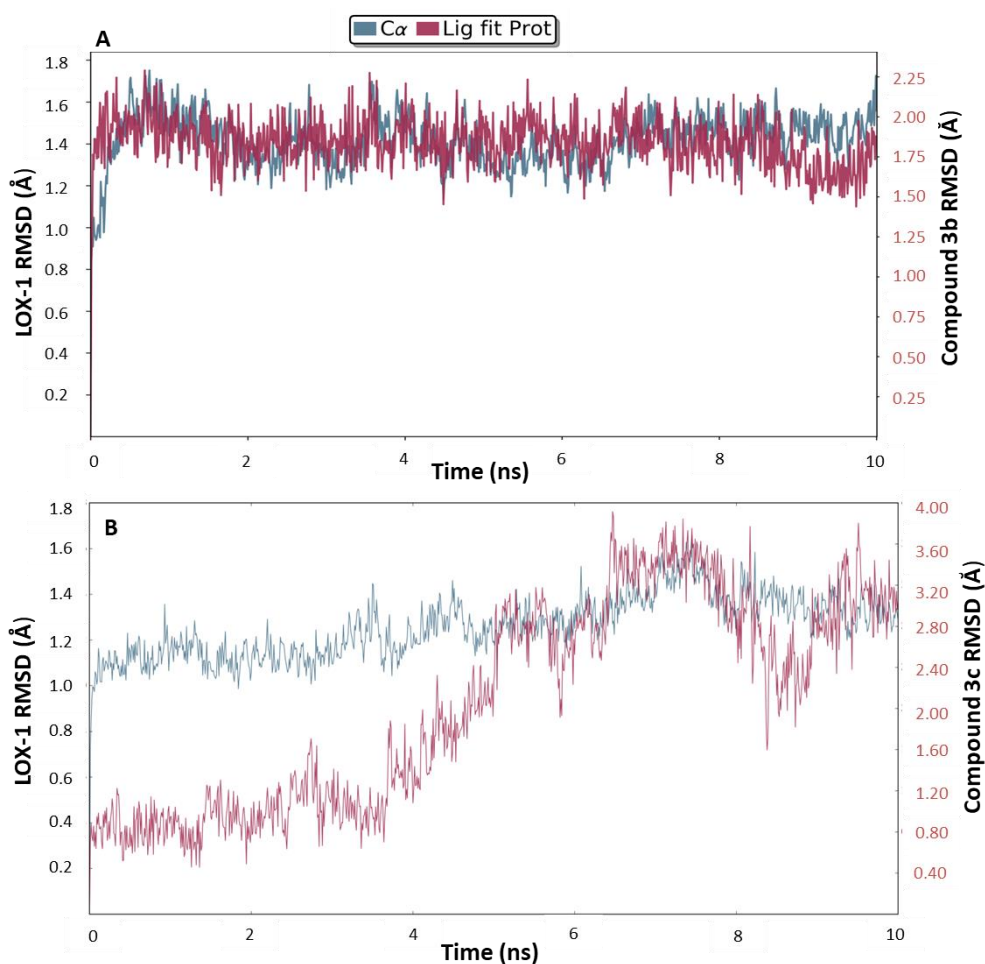


Figure S2: RMSD calculations for (A) all Ca enzyme atoms (blue) in LOX-1-Compound **3b** complex and for all atoms of compound **3b** (red), (B)) all C_a enzyme atoms (blue) in LOX-1-Compound **3c** complex and for all atoms of compound **3c** (red).

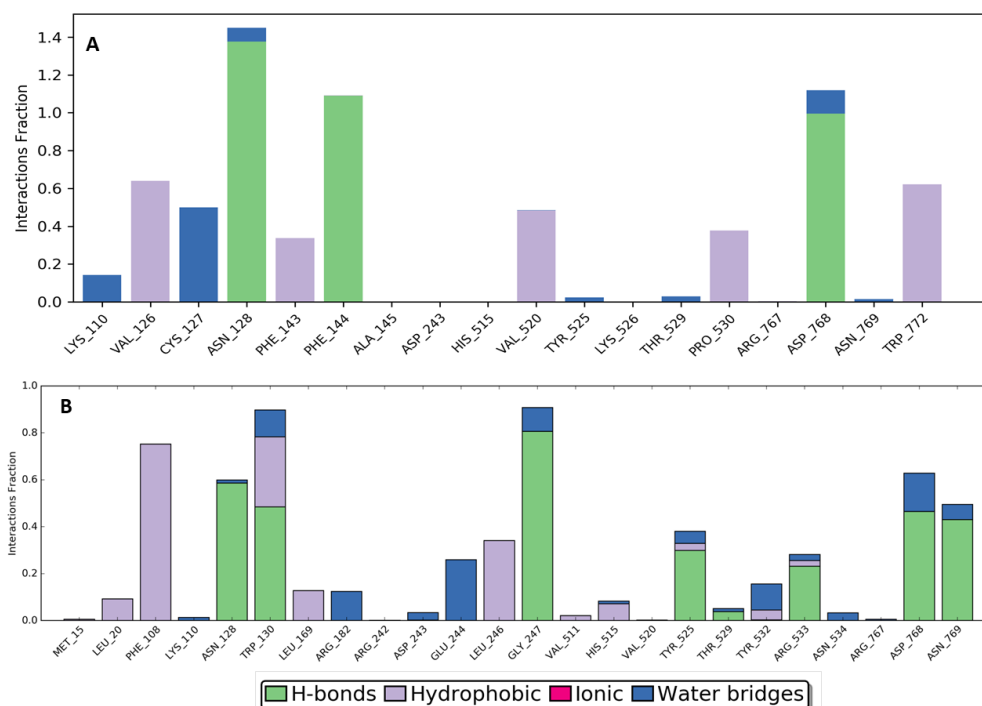
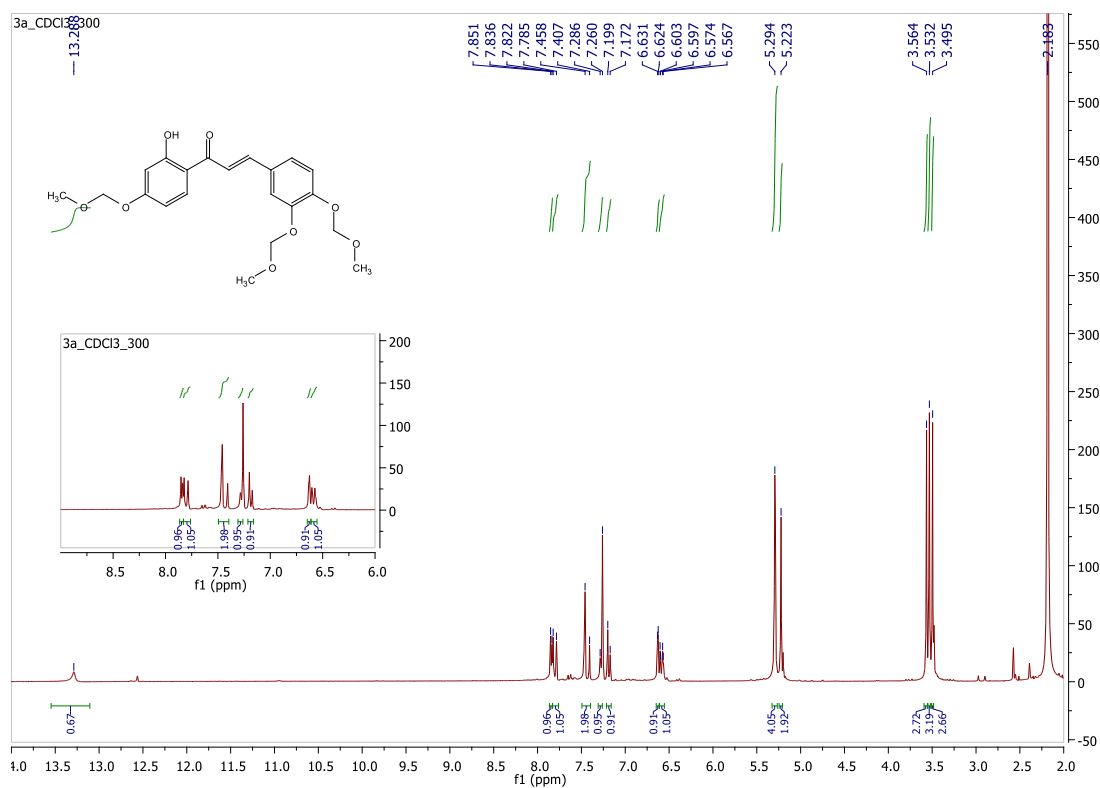


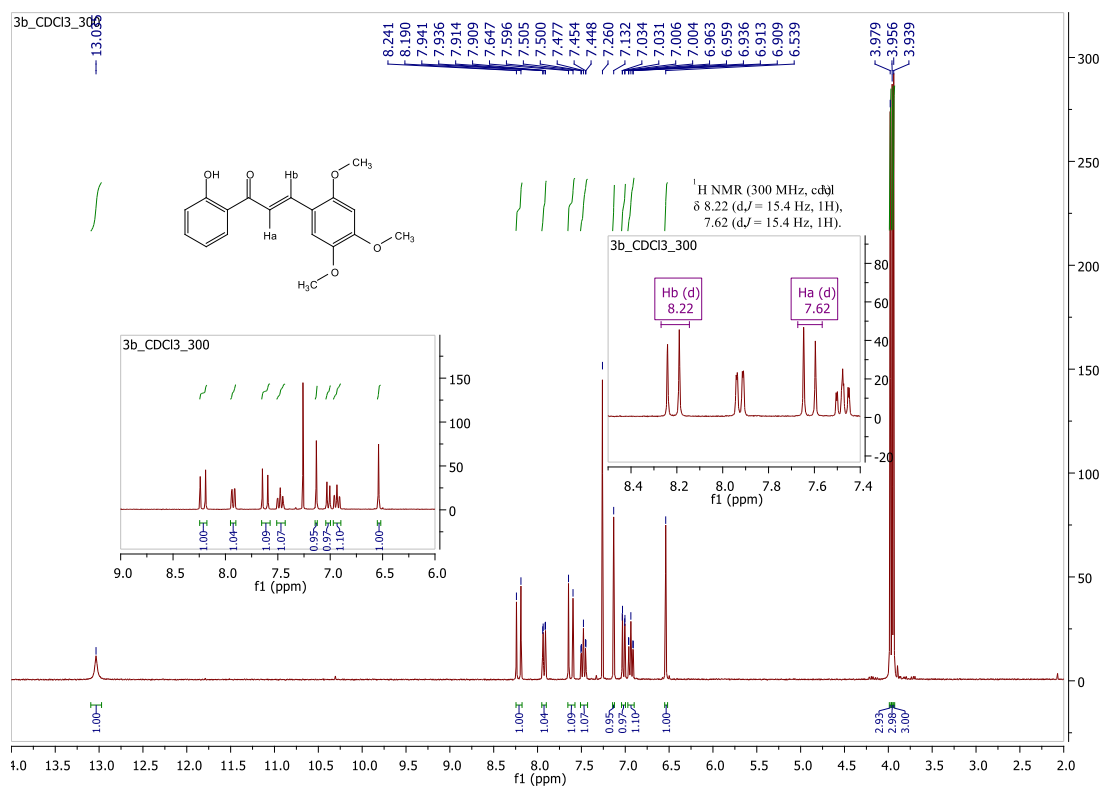
Figure S3: Categorization of (A) LOX-1-Compound **3b** and (B) LOX-1-Compound **3c** interactions, during the molecular dynamics simulation (10 ns).

¹H NMR spectra of all the synthesized compounds and ¹³C NMR spectra of the novel synthesized compounds

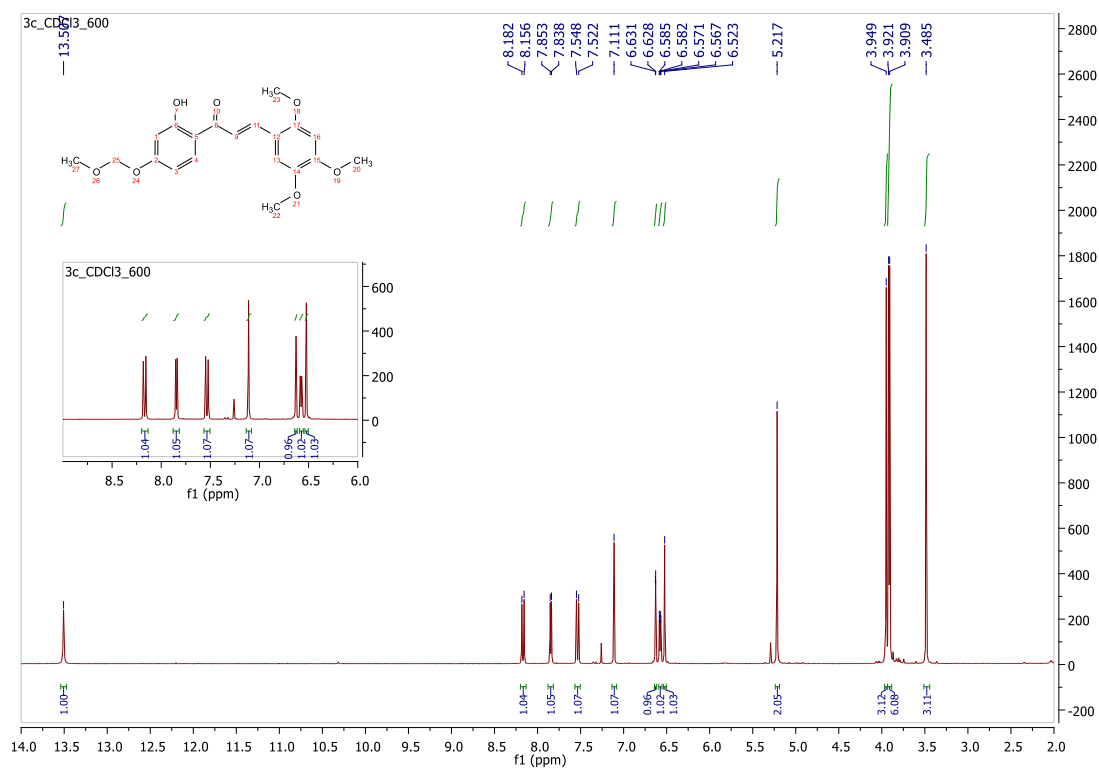
¹H NMR of compound 3a



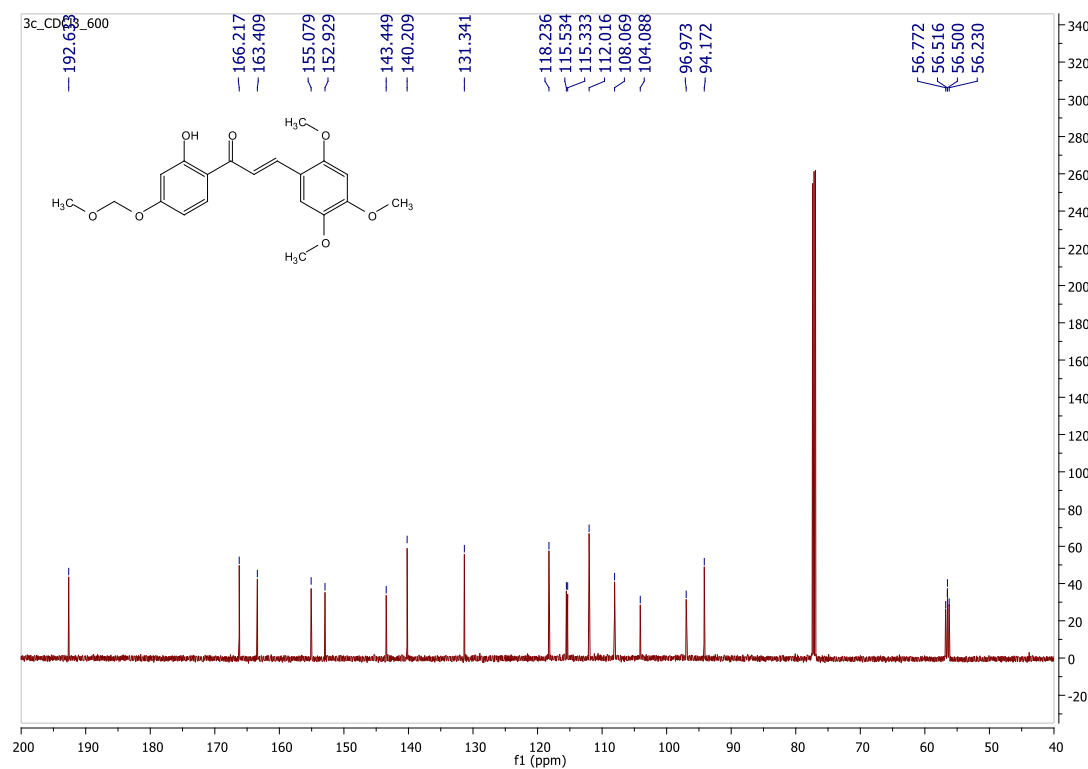
¹H NMR of compound 3b



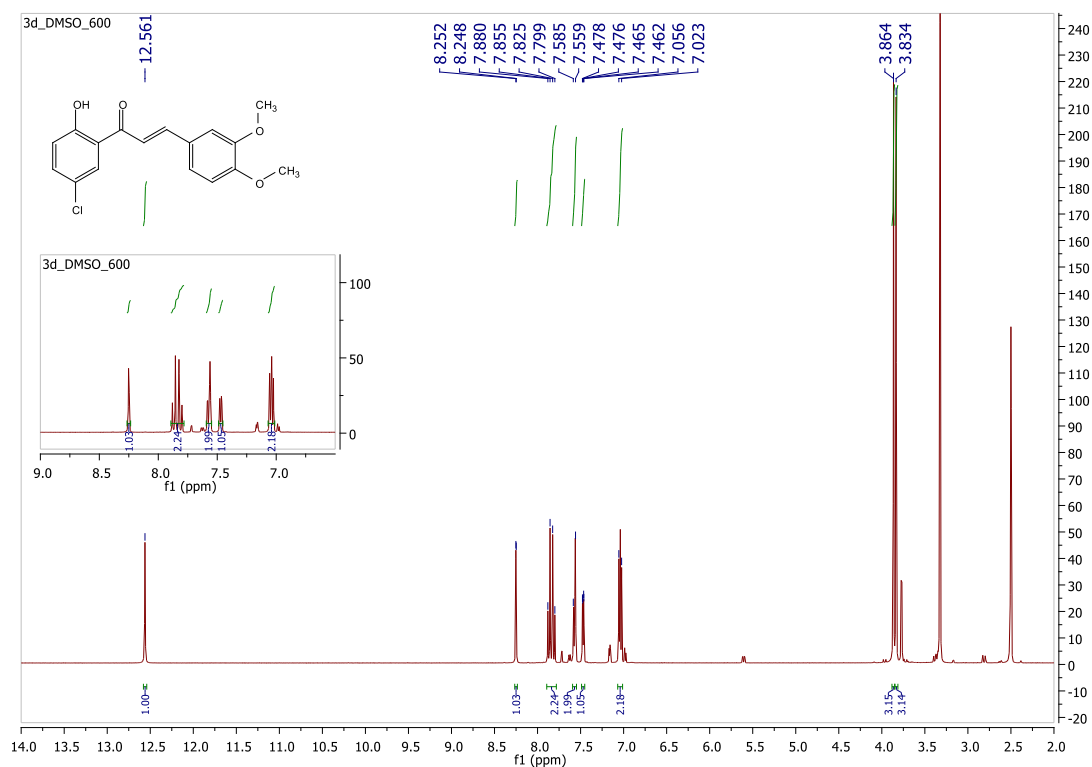
¹H NMR of compound **3c**



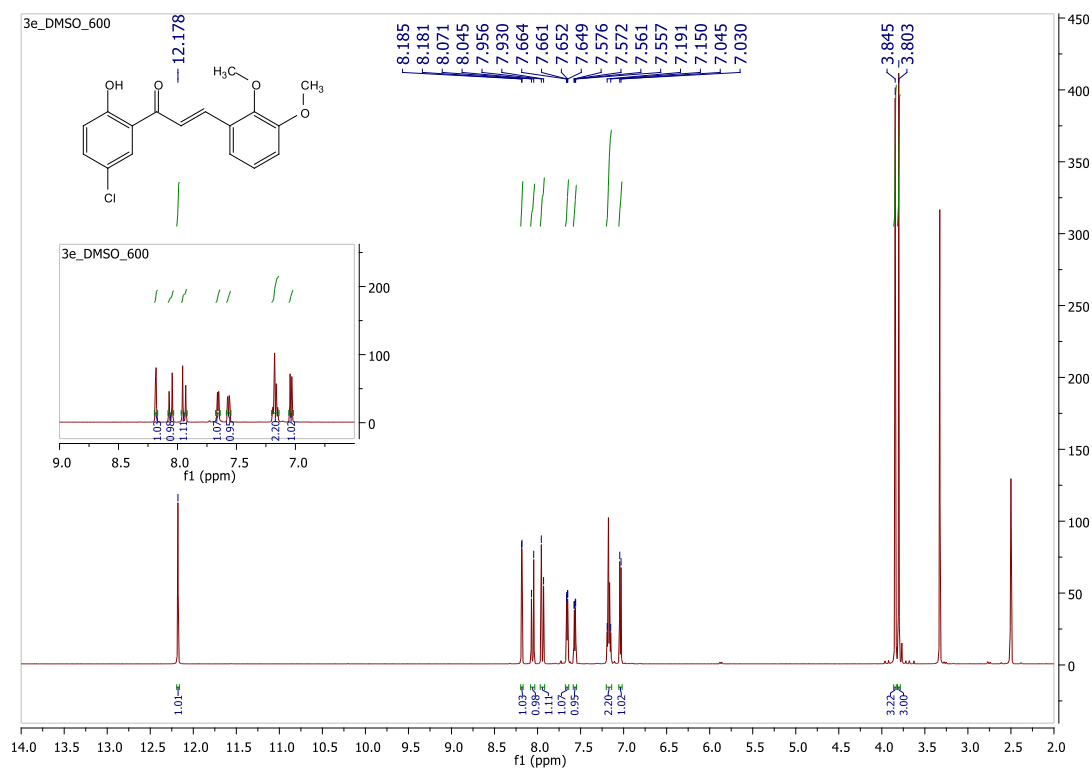
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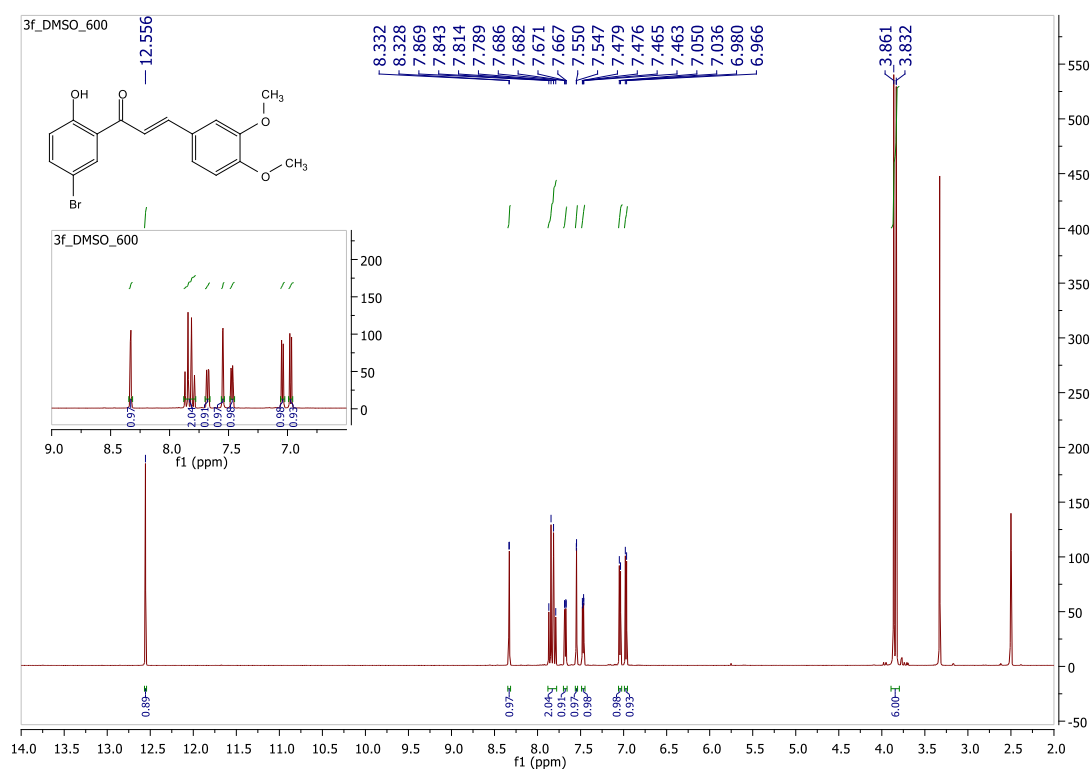
¹H NMR of compound **3d**



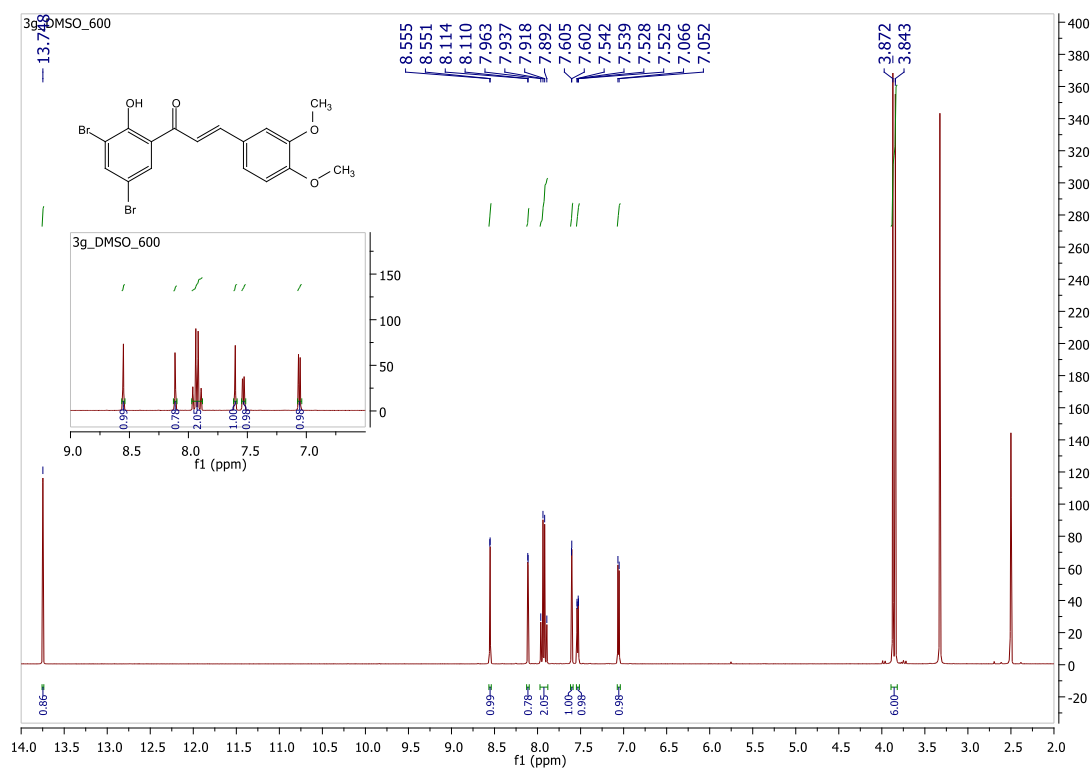
¹H NMR of compound **3e**



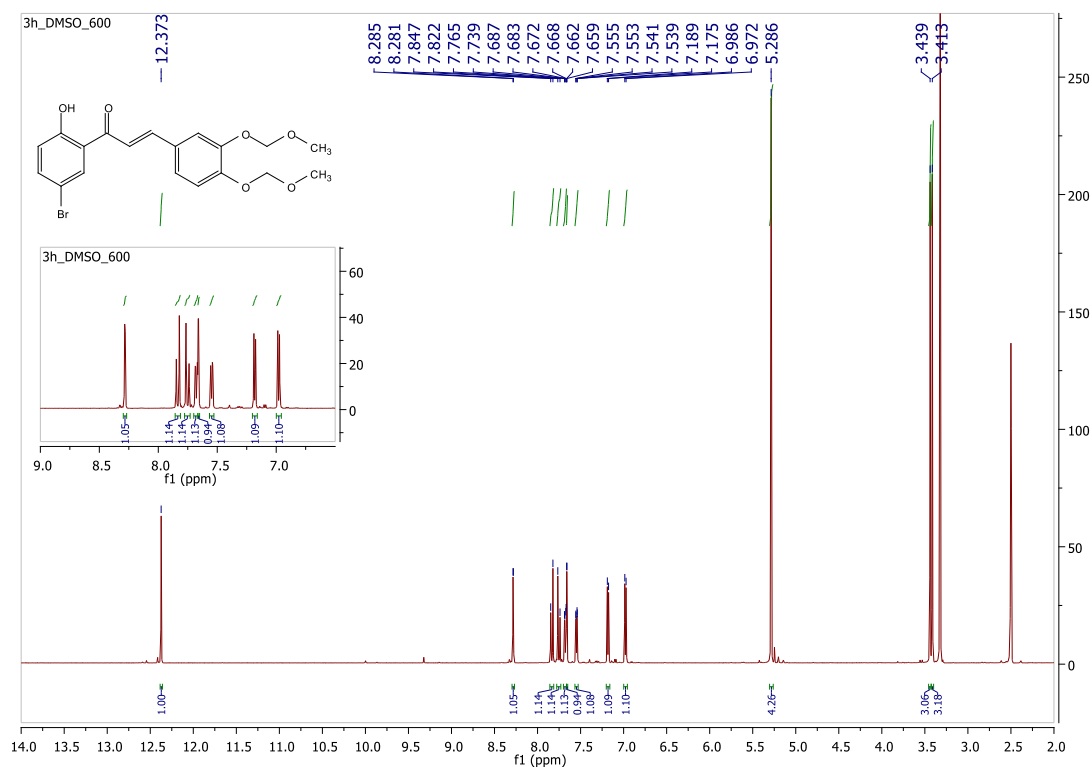
¹H NMR of compound **3f**



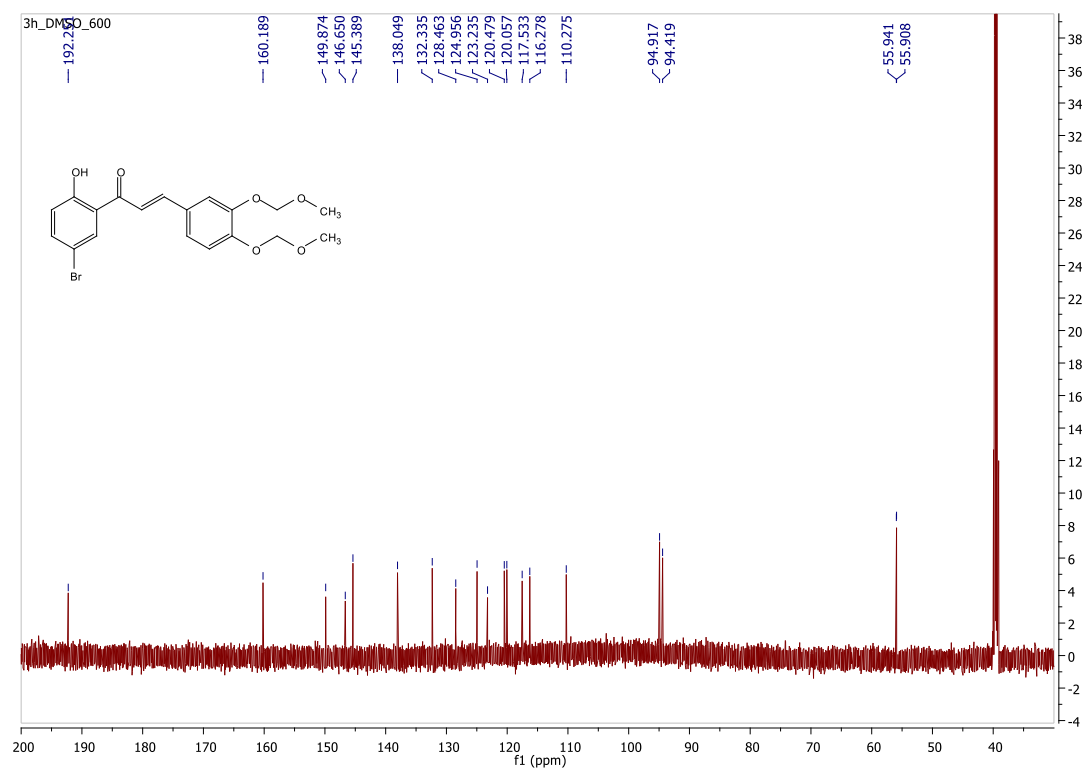
¹H NMR of compound **3g**



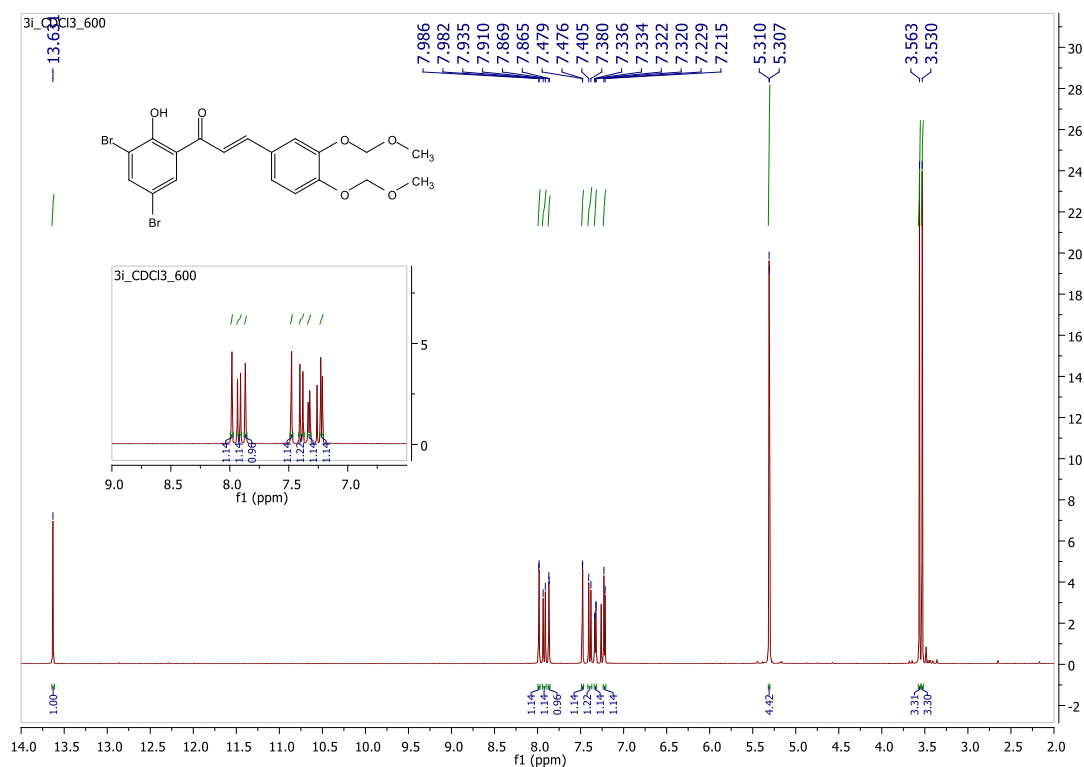
¹H NMR of compound **3h**



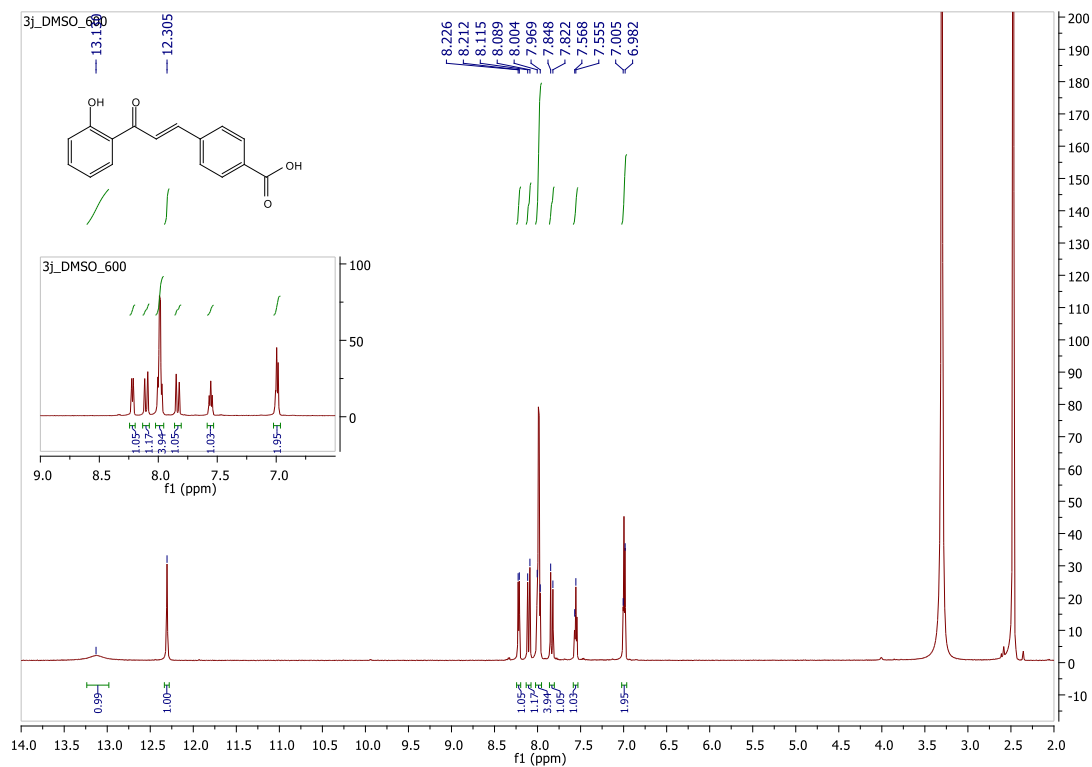
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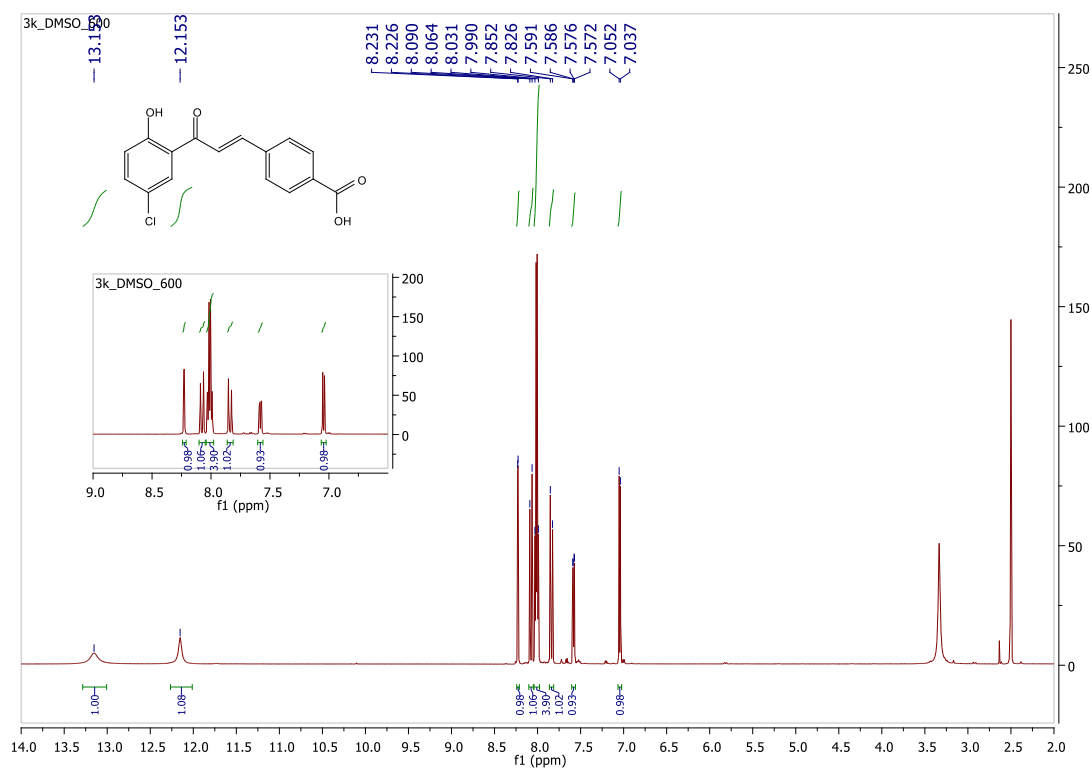
¹H NMR of compound **3i**



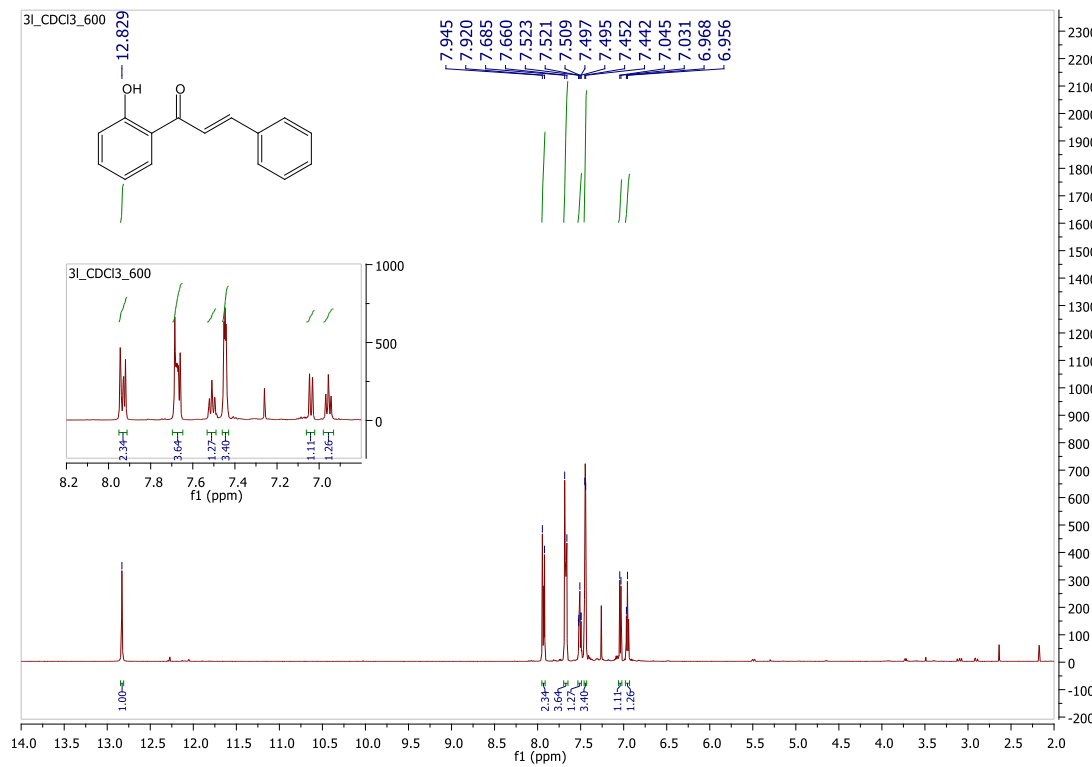
¹H NMR of compound **3j**



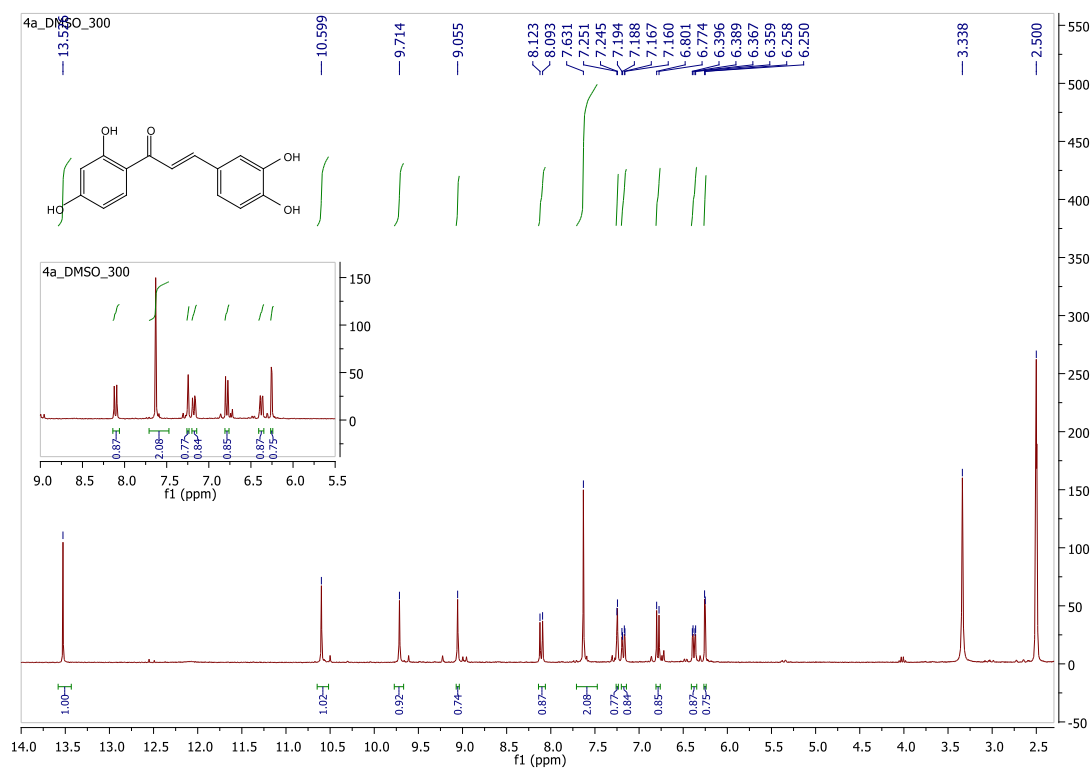
¹H NMR of compound **3k**



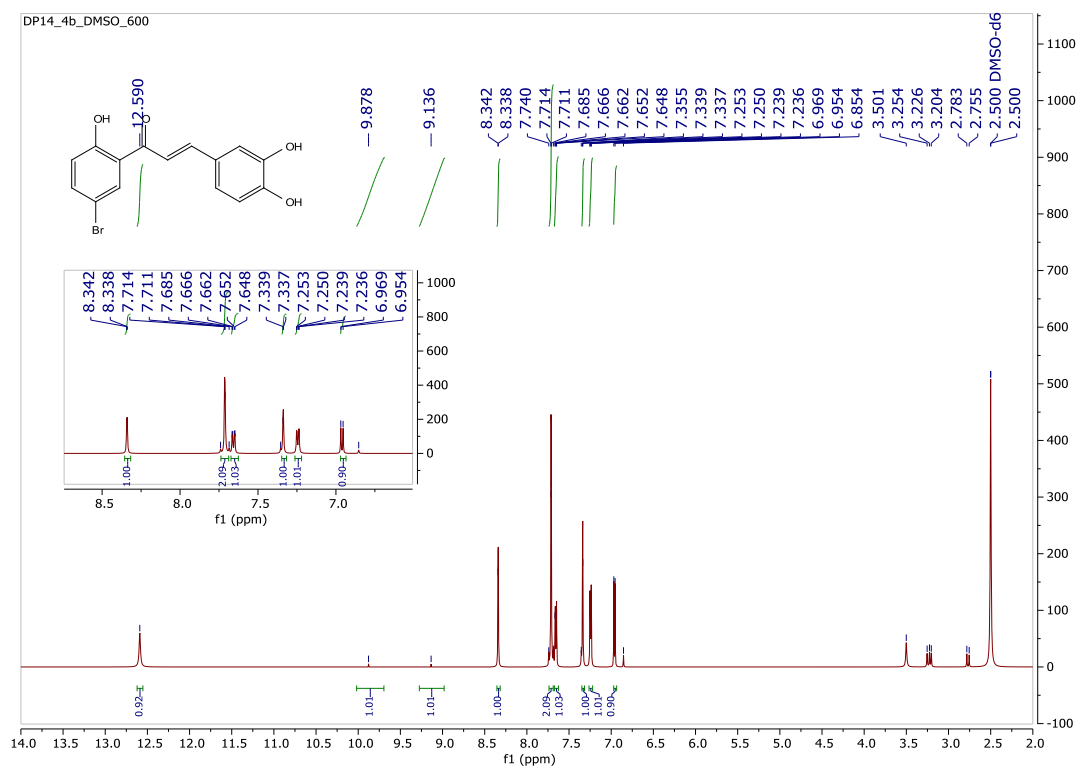
¹H NMR of compound **3l**



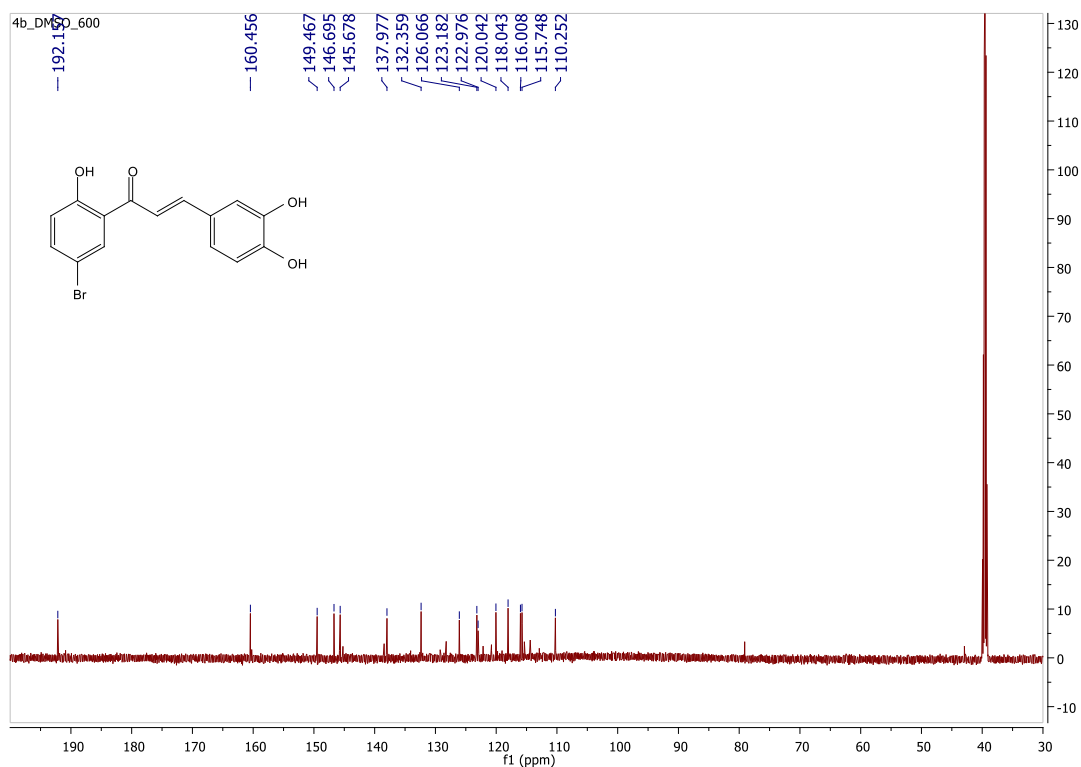
¹H NMR of compound **4a**



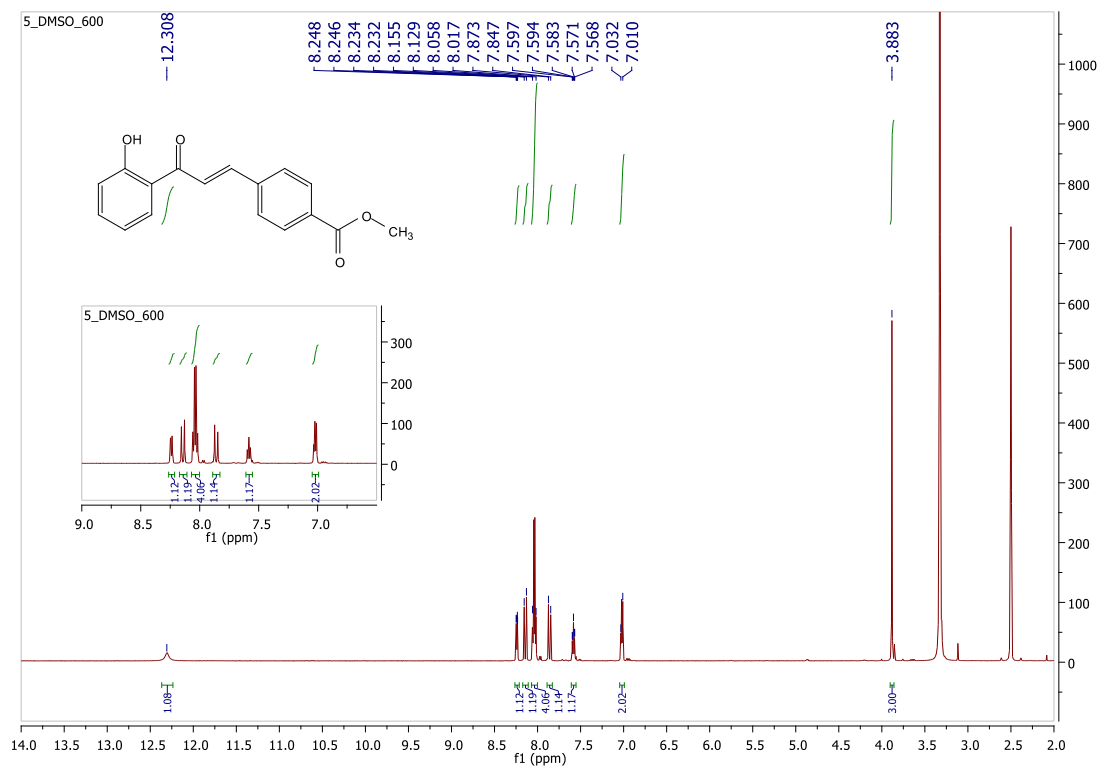
¹H NMR of compound **4b**



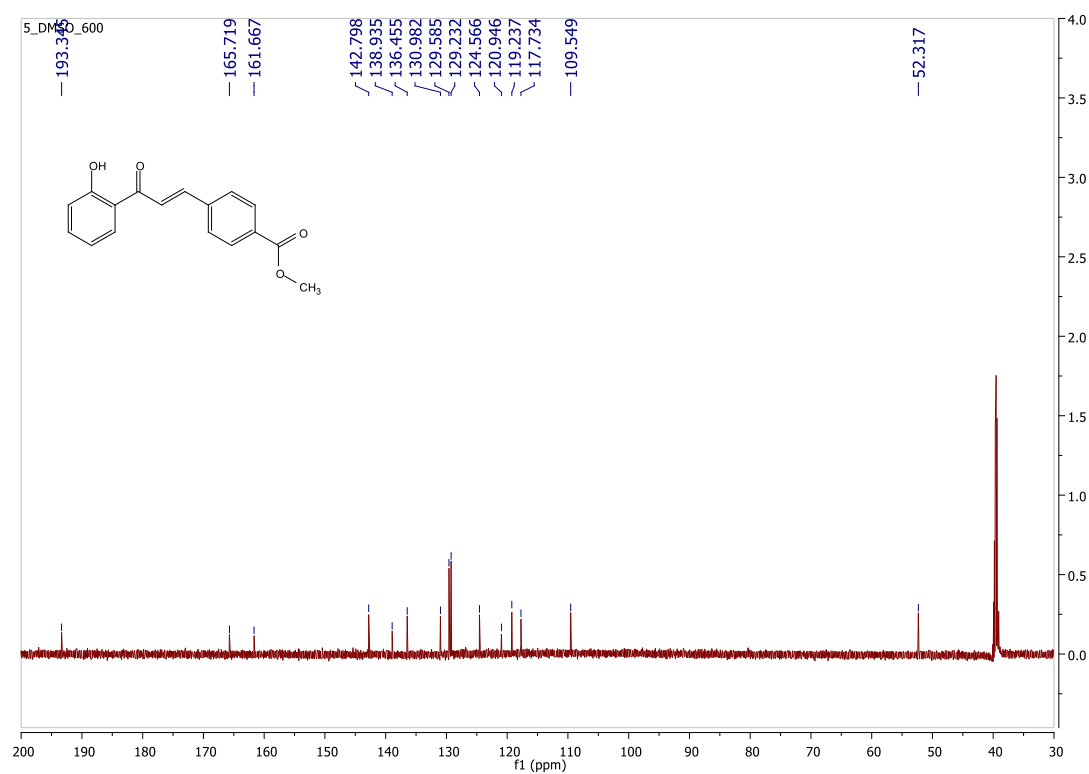
¹³C NMR of compound **4b**



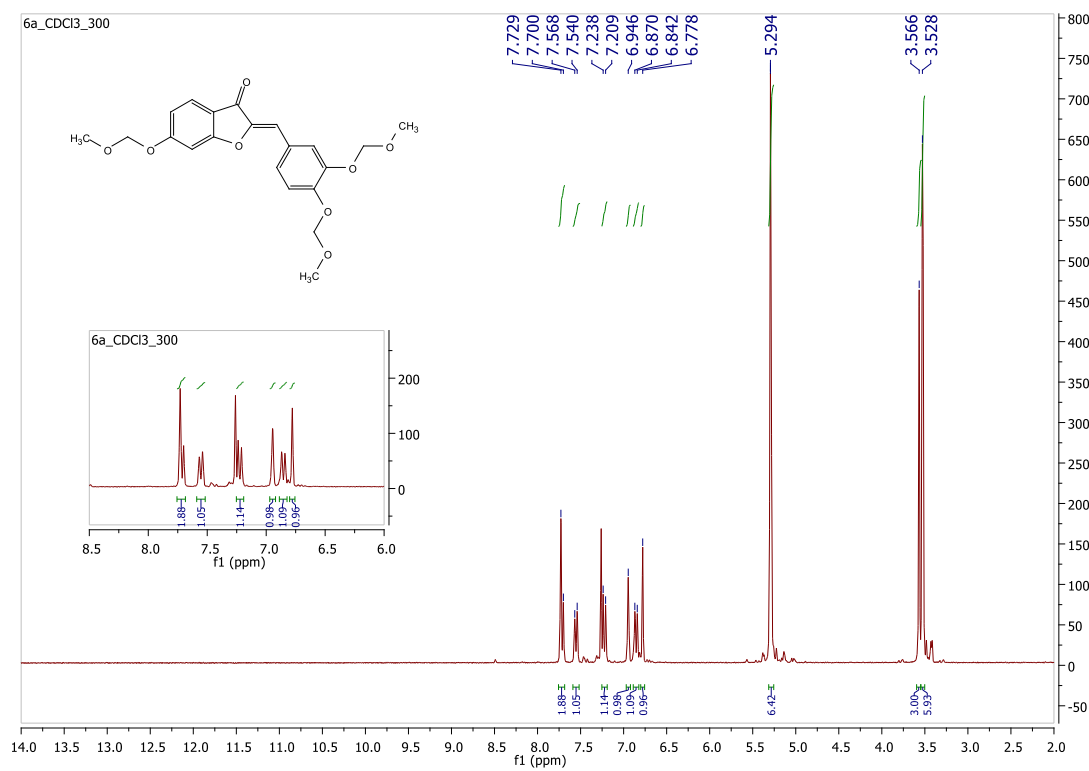
¹H NMR of compound **5**



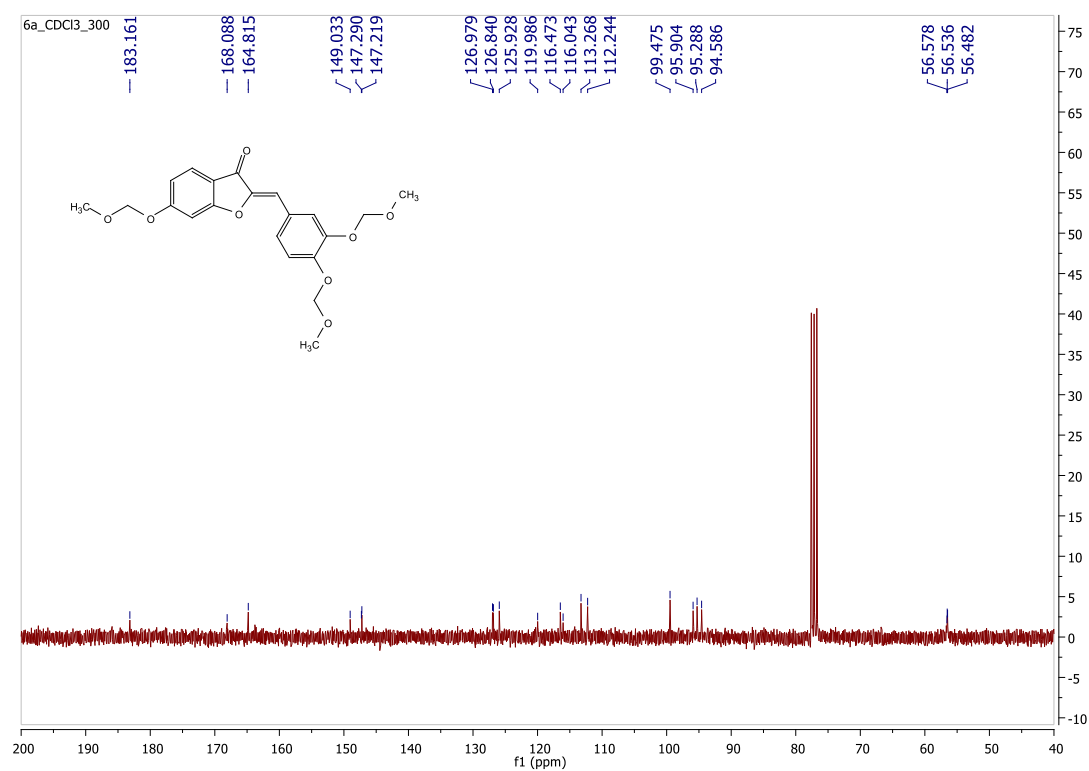
¹³C NMR of compound **5**



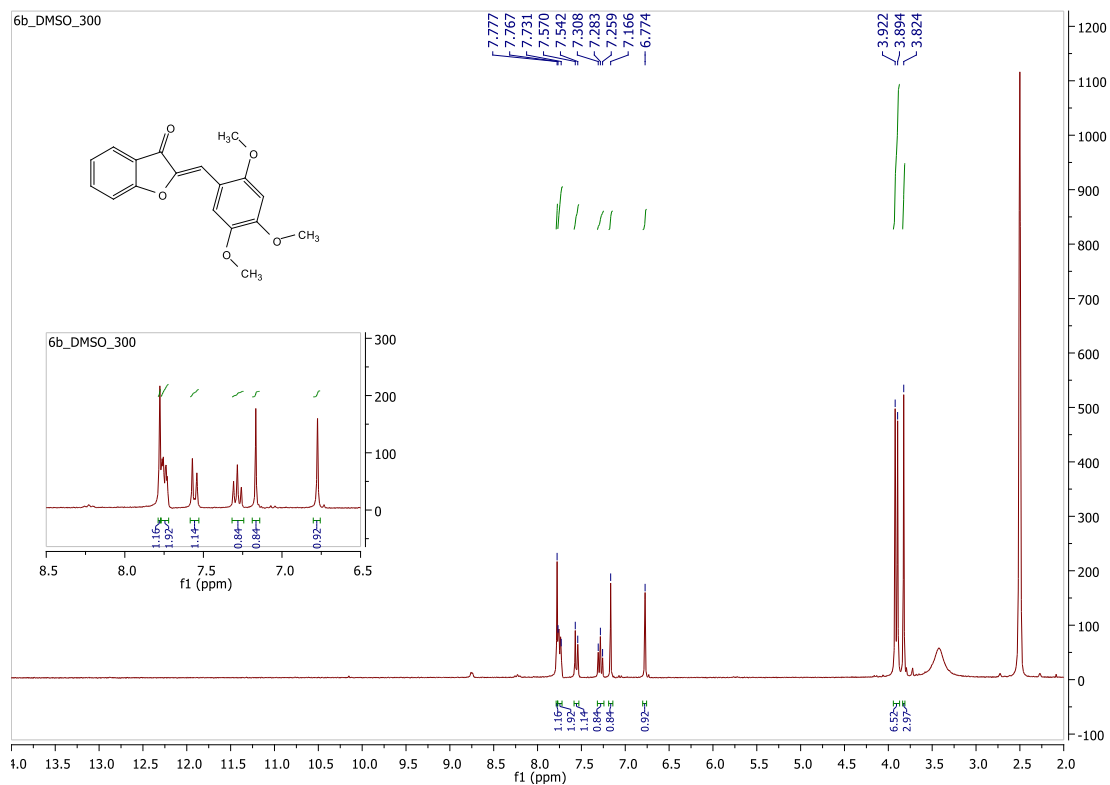
¹H NMR of compound **6a**



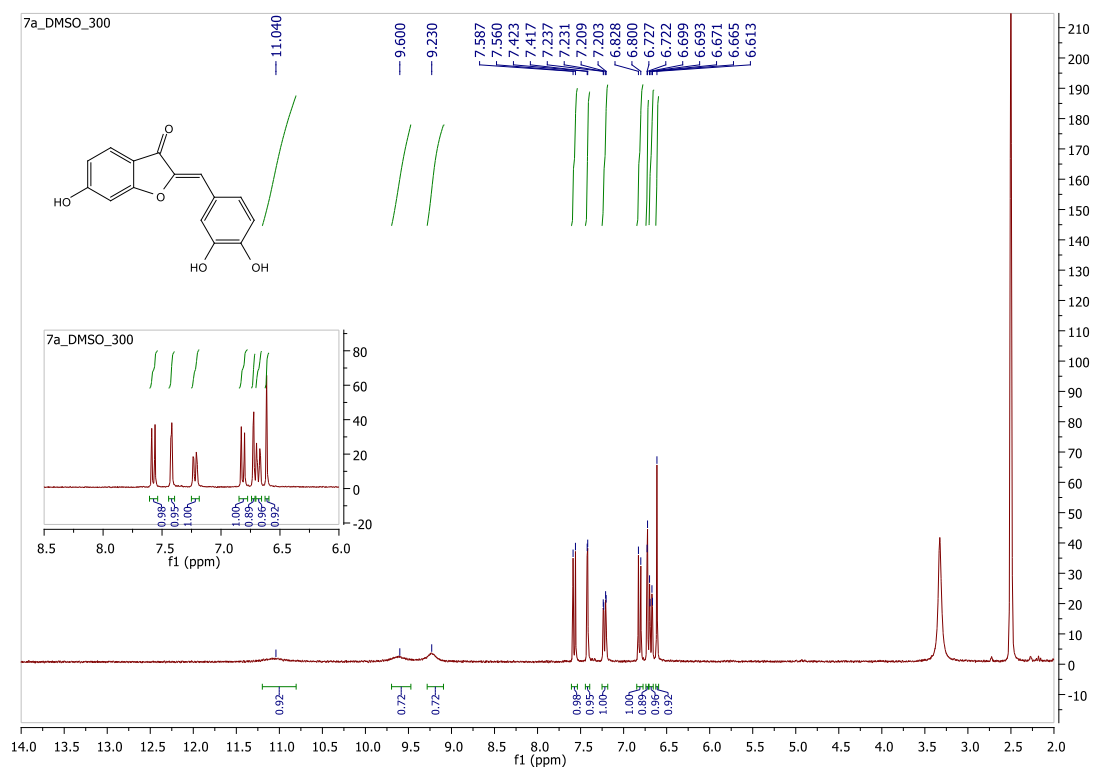
¹³C NMR of compound **6a**



¹H NMR of compound **6b**



¹H NMR of compound **7a**



¹H NMR of compound **7b**

