Supplementary Materials

Switching from Aromatase Inhibitors to Dual Targeting Flavonoid-Based Compounds for Breast Cancer Treatment

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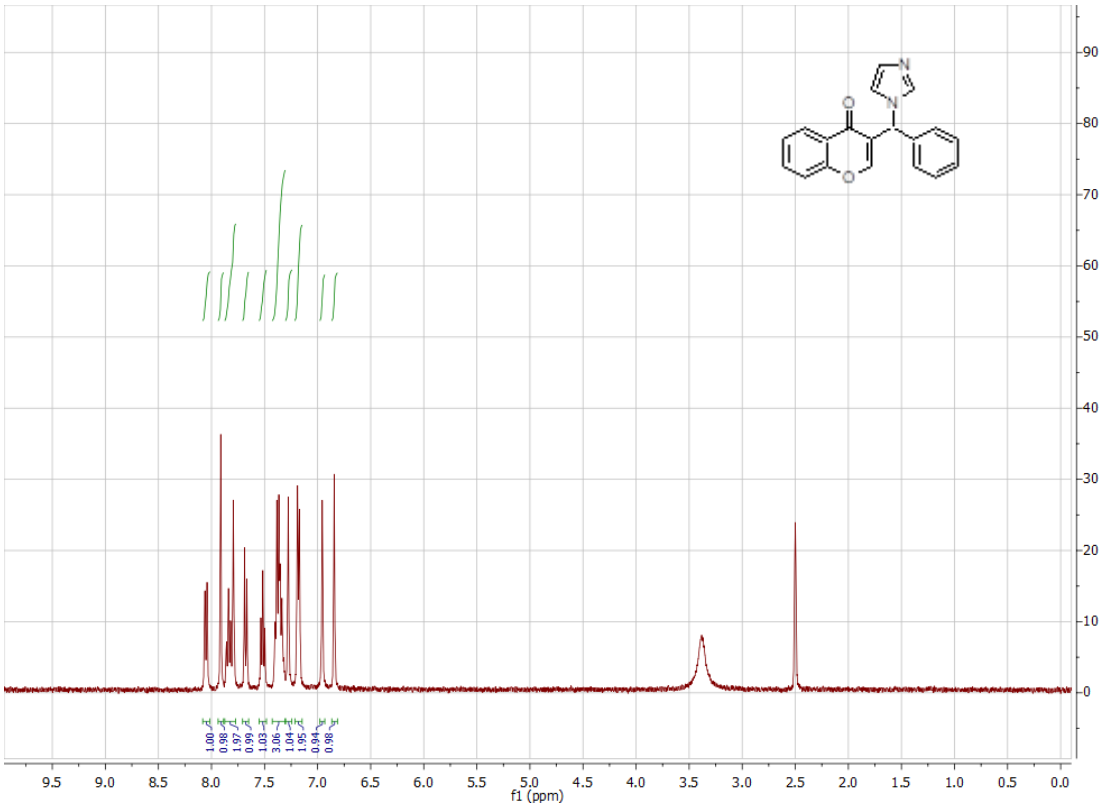
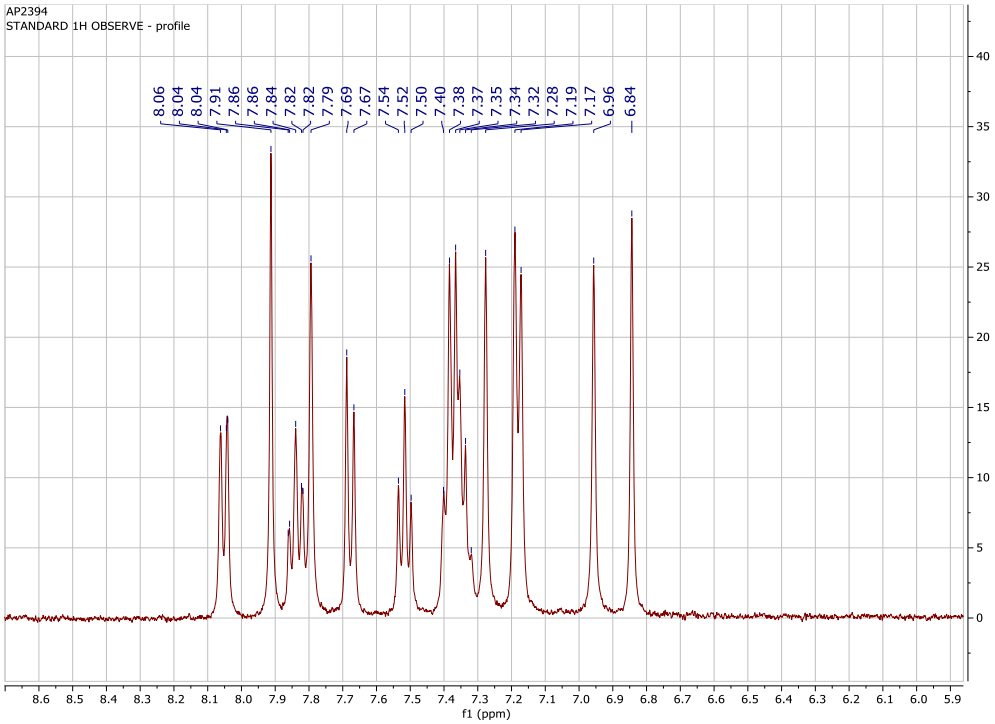
Figure S1. ^{1}H-NMR





Expansion

Figure S2. ^{13}C-NMR

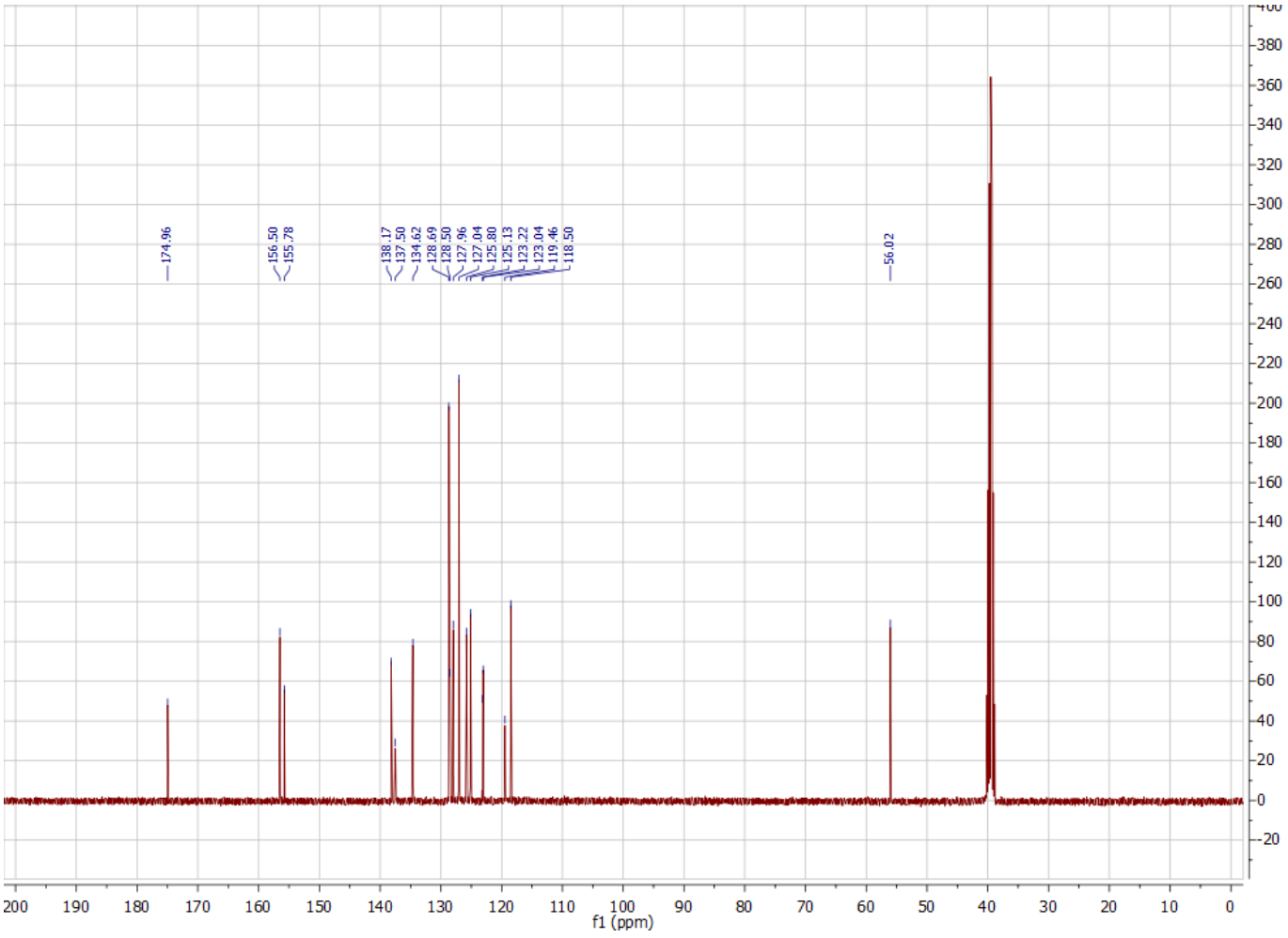


Figure S3. ^{1}H-^{1}H COSY

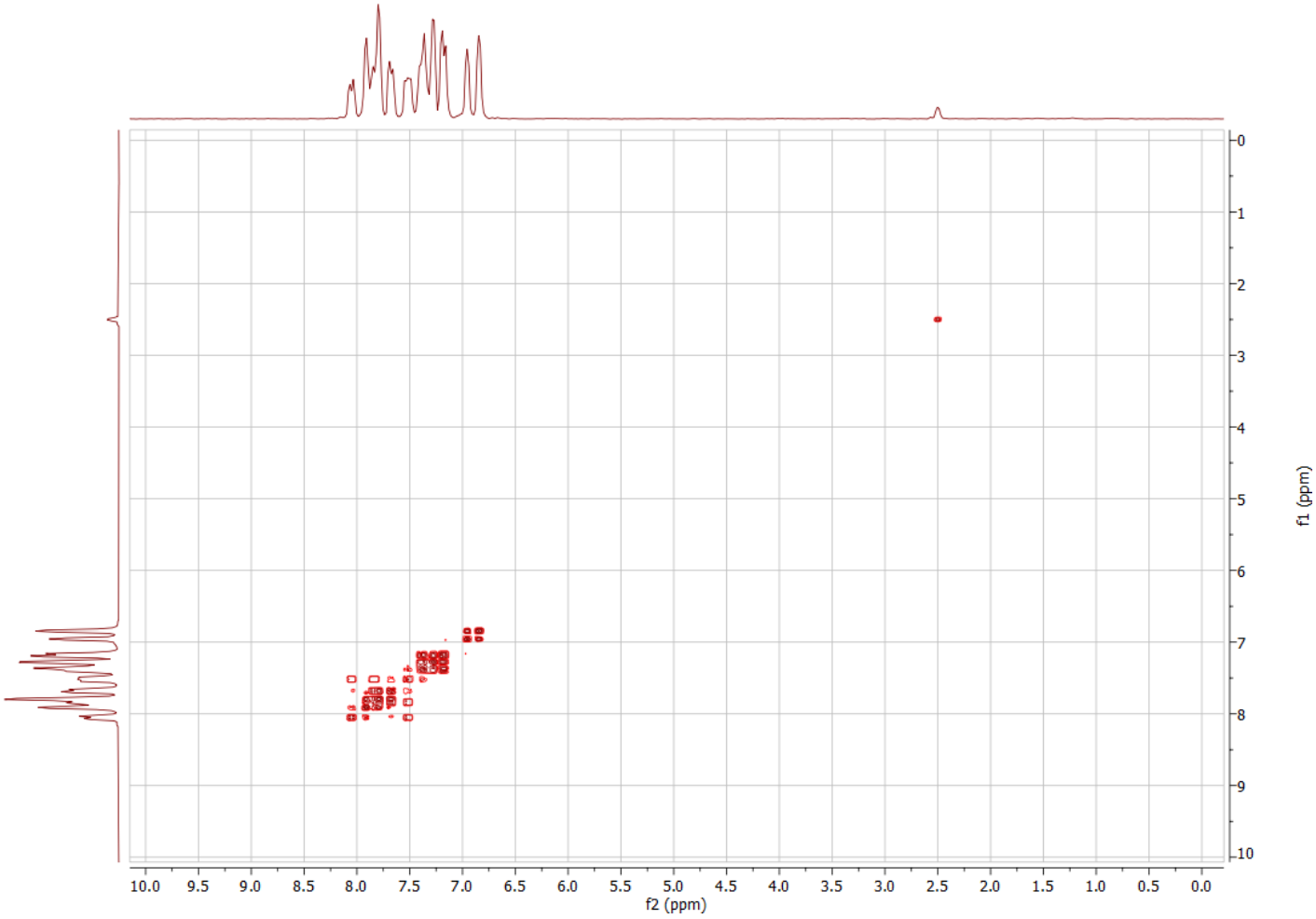


Figure S4. HMBC

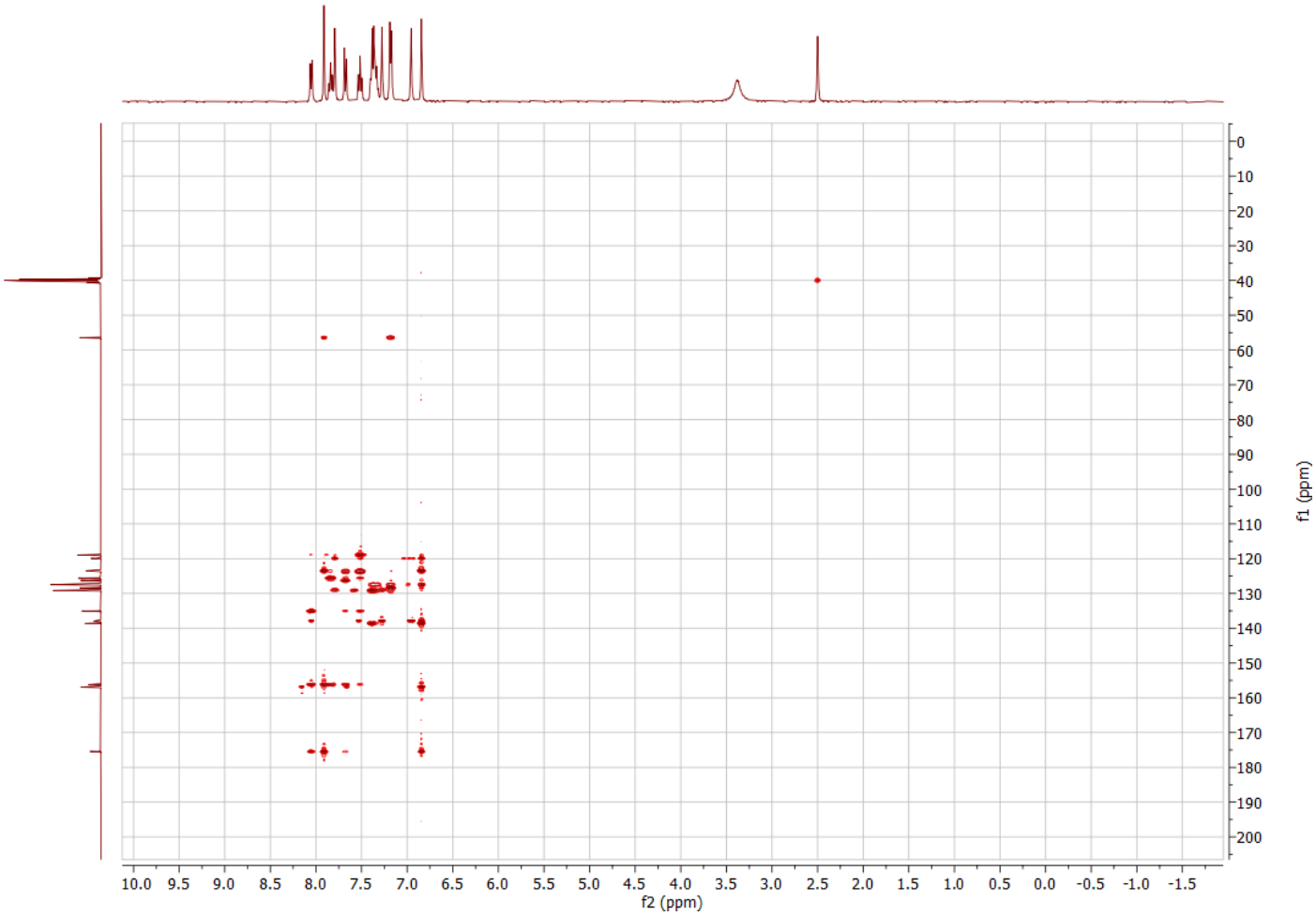


Figure S5. HSQC

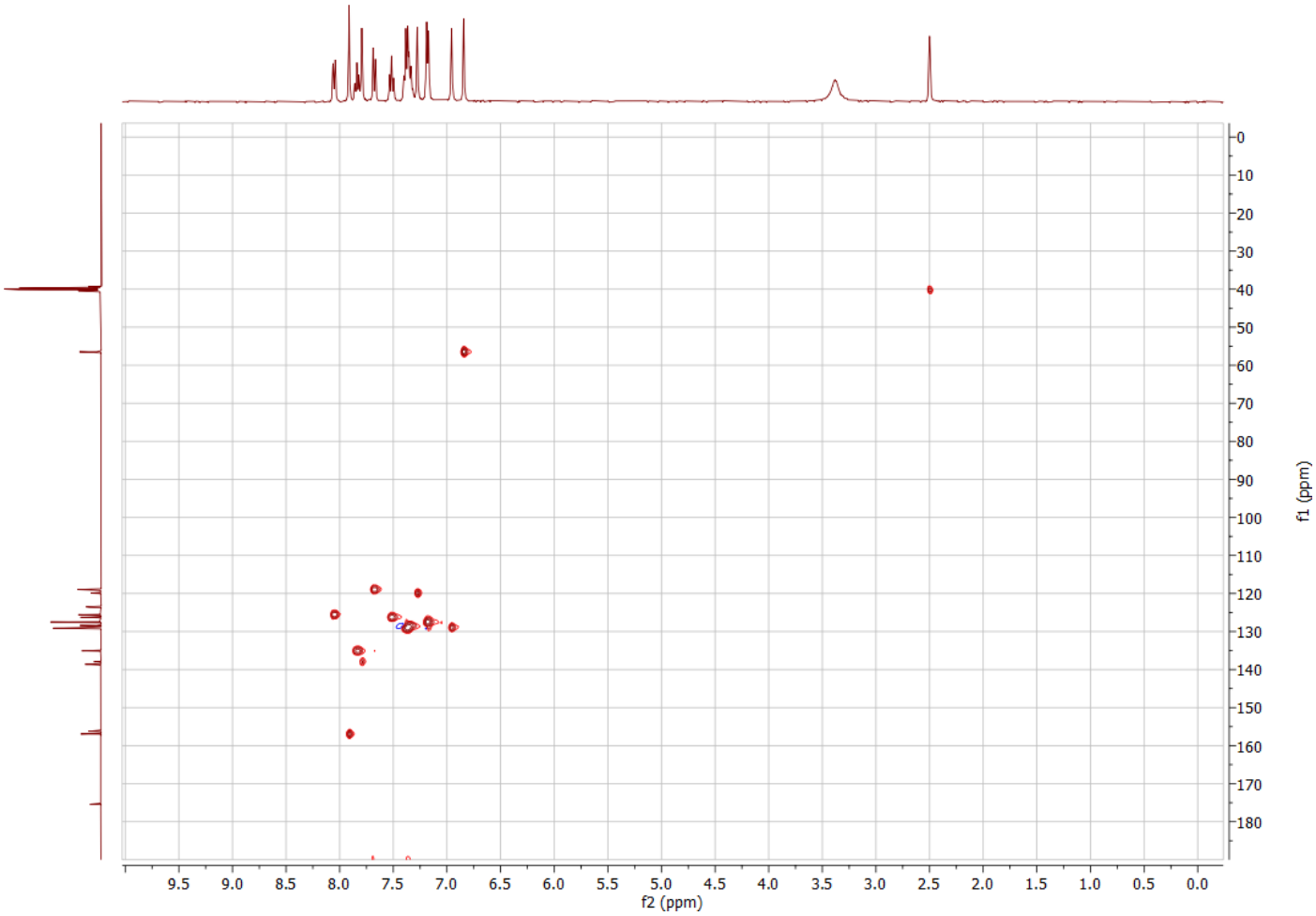


Figure S6. NMR spectra of 2a

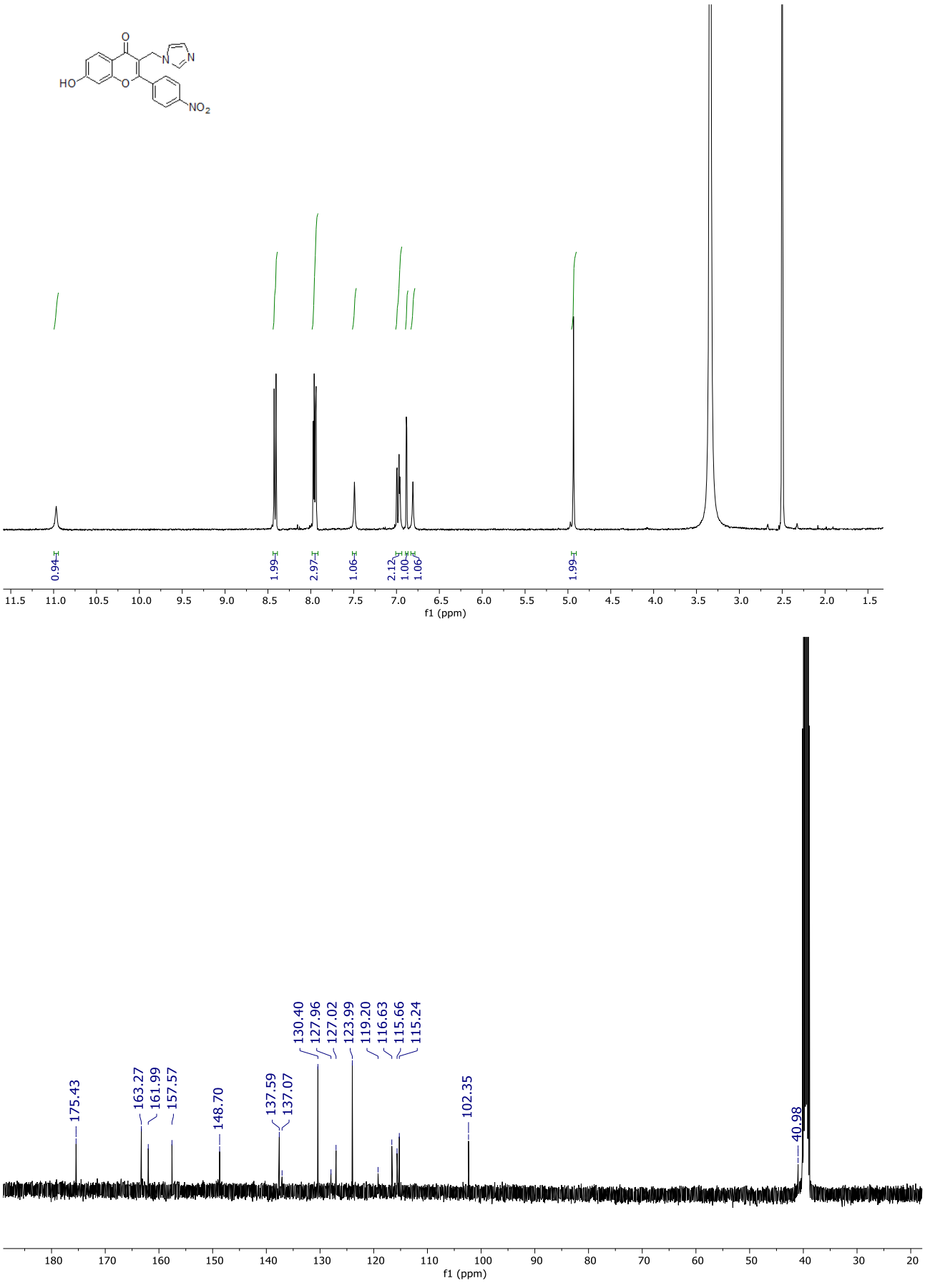
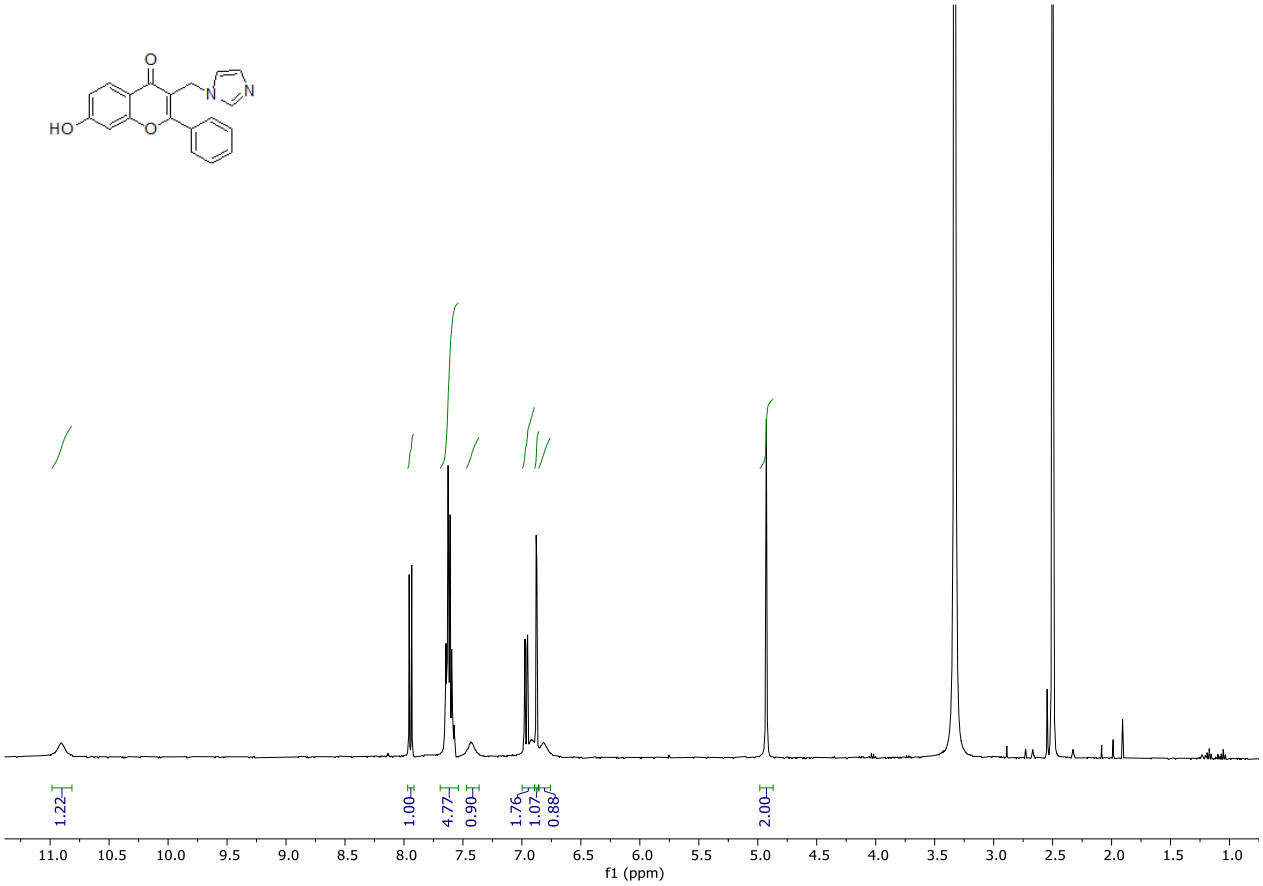


Figure S7. NMR spectra of 2b



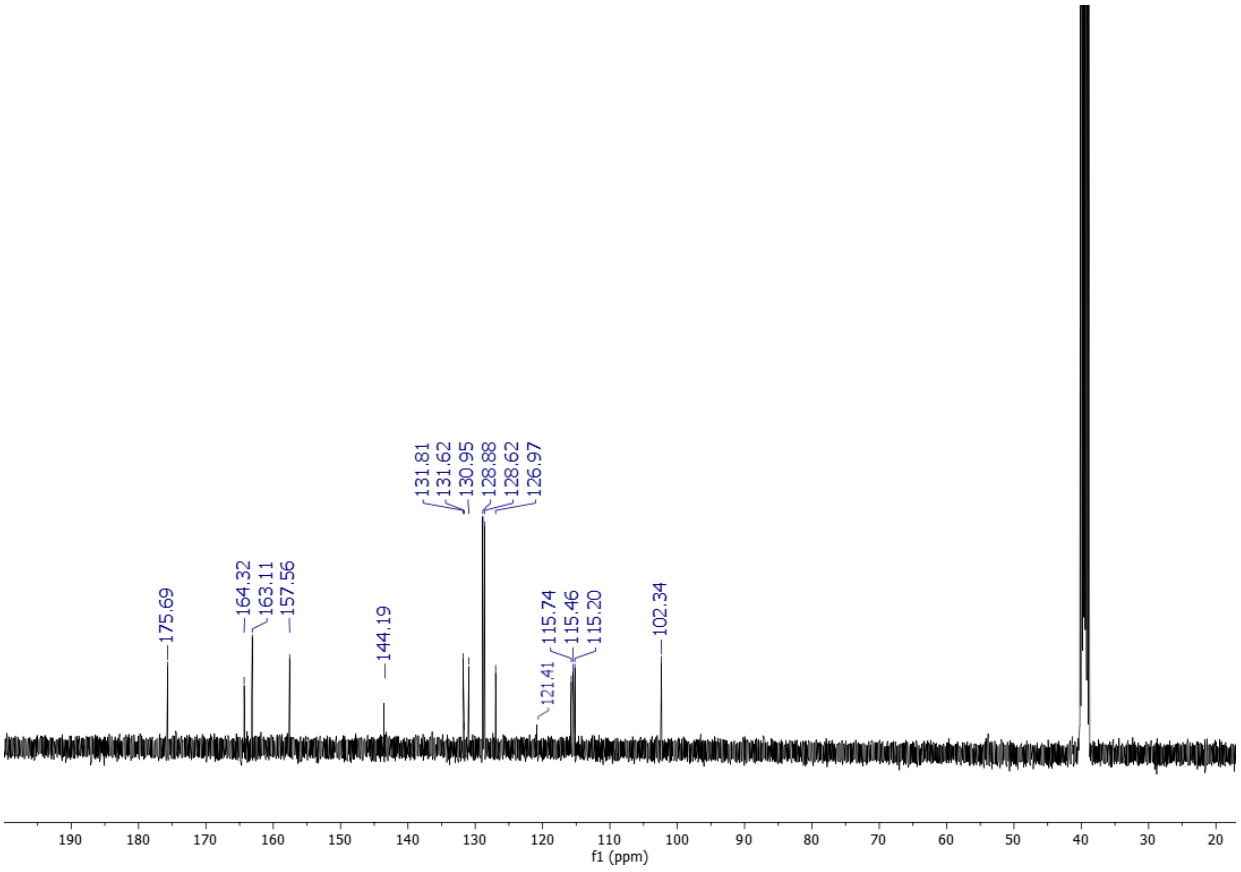


Figure S8. NMR spectra of 4a

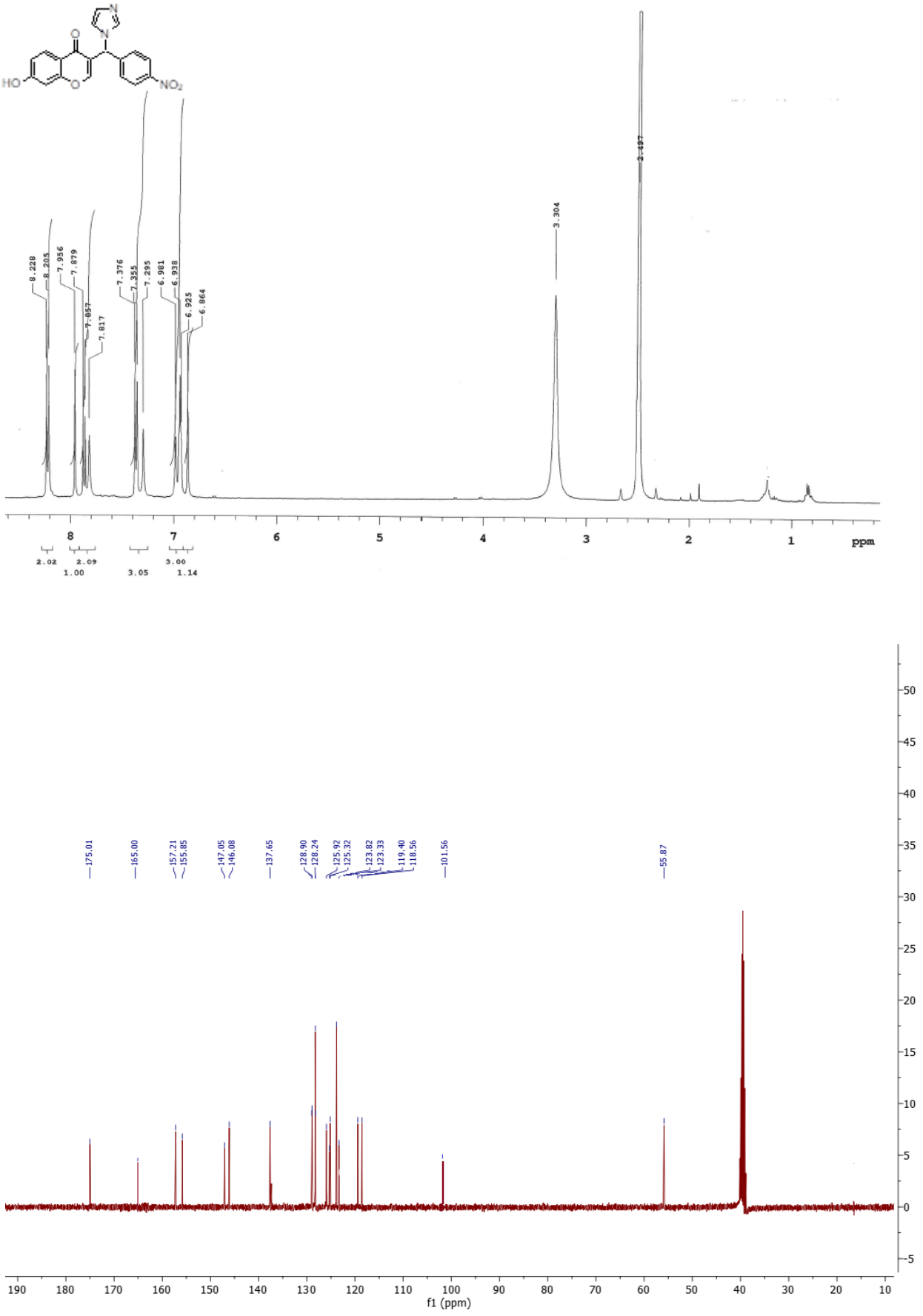
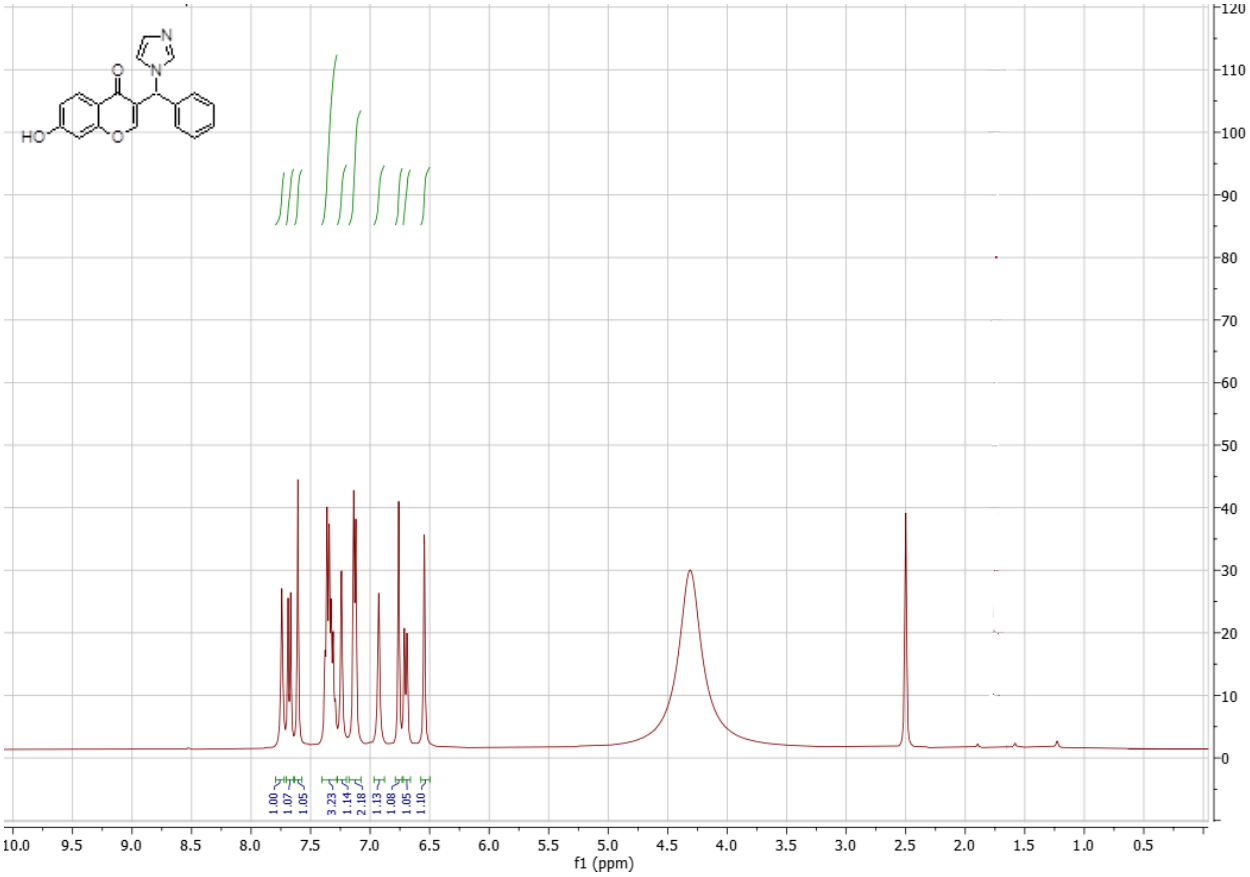


Figure S9. NMR spectra of 4b



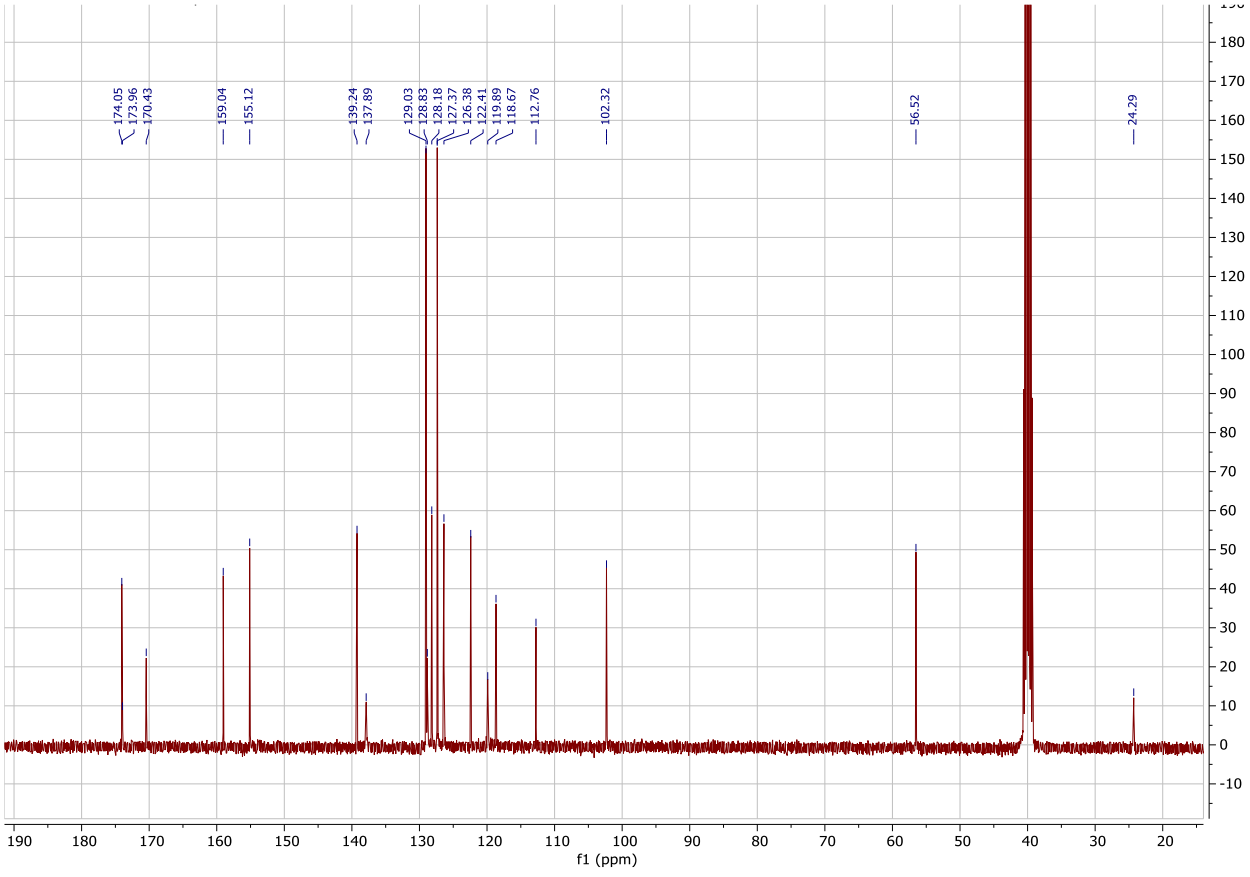
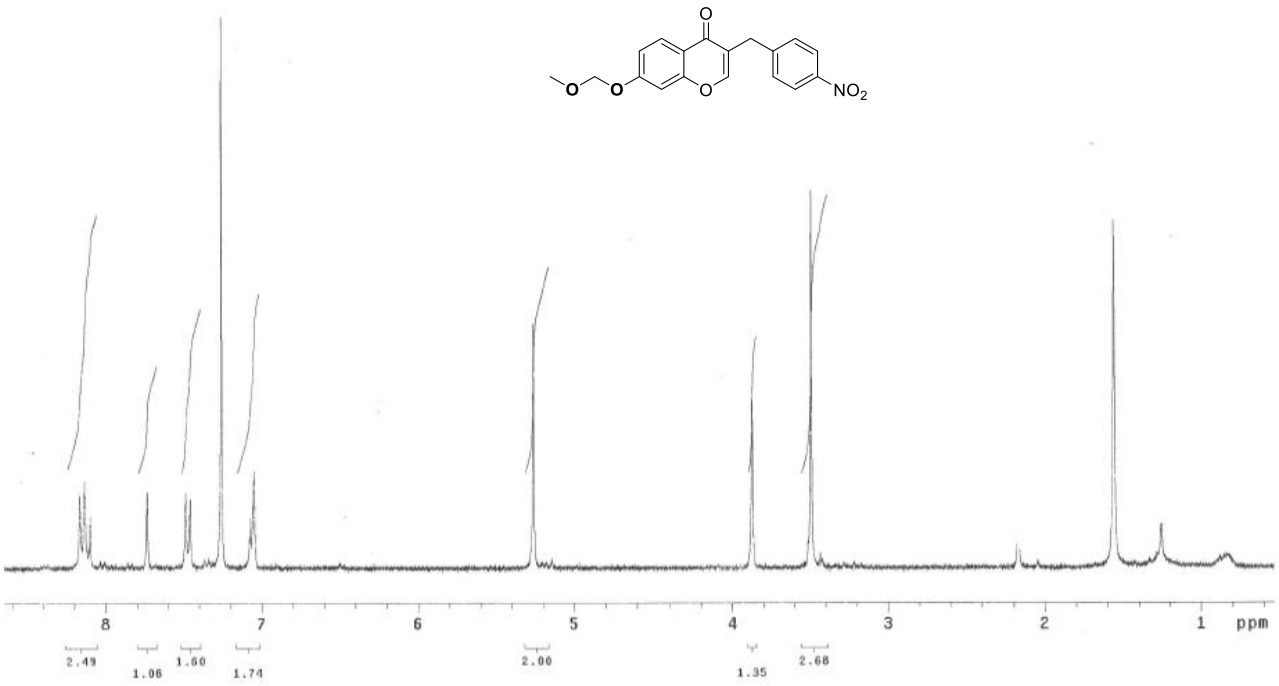


Figure S10. NMR spectra of intermediates 8a and 8b

8a



8b

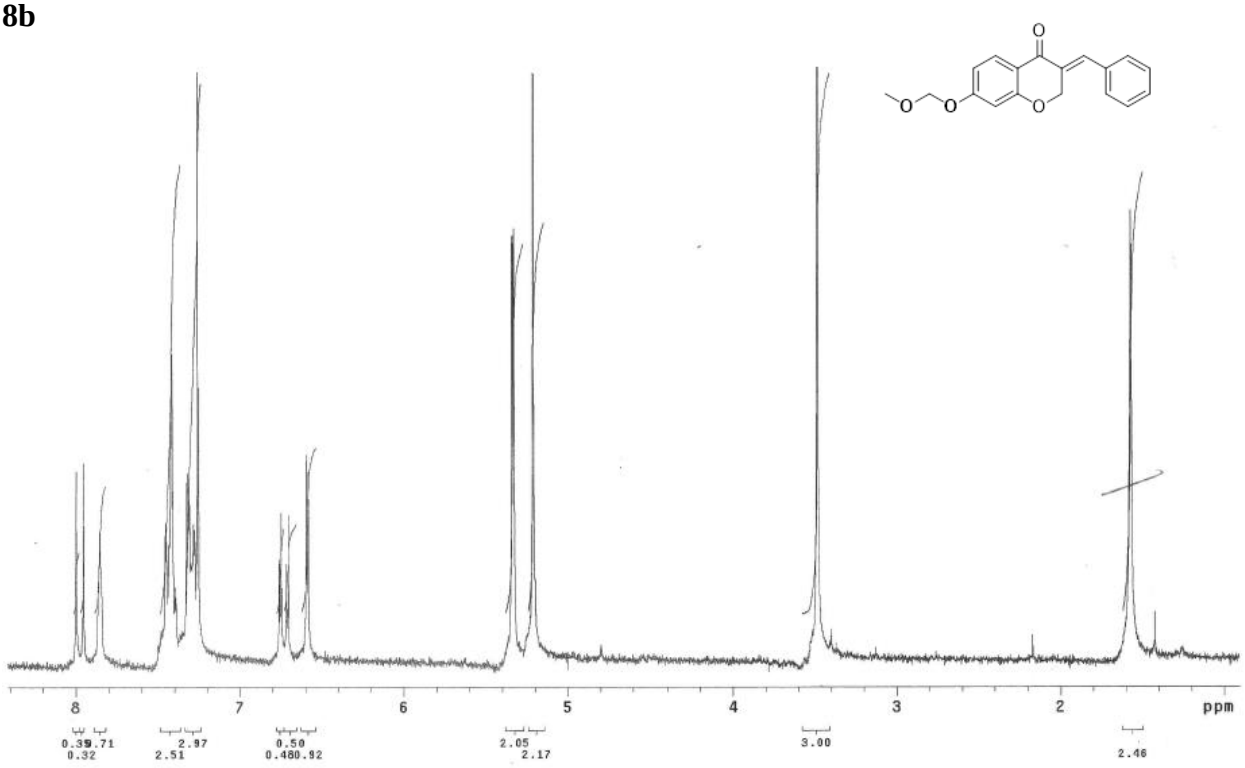


Table S1. Docking score (kcal/mol) to Estrogen Receptor α for the studied compounds. For compounds **3a,b** and **4a,b** we considered the R and S enantiomer in the docking simulations.

Compound	**Docking score**	**Docking score R**	**Docking score S**
1a	-9.76		
2a	-10.52		
1b	-9.85		
2b	-10.03		
3a		-9.53	-9.20
3b		-9.84	-8.68
4a		-10.49	-8.96
4b		-10.09	-10.38