



Supplementary Material

Discovery of New Hydrazone-Thiazole Polyphenolic Antioxidants through Computer-Aided Design and In Vitro Experimental Validation

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1. Figures

1.1. The IR spectra of the compounds

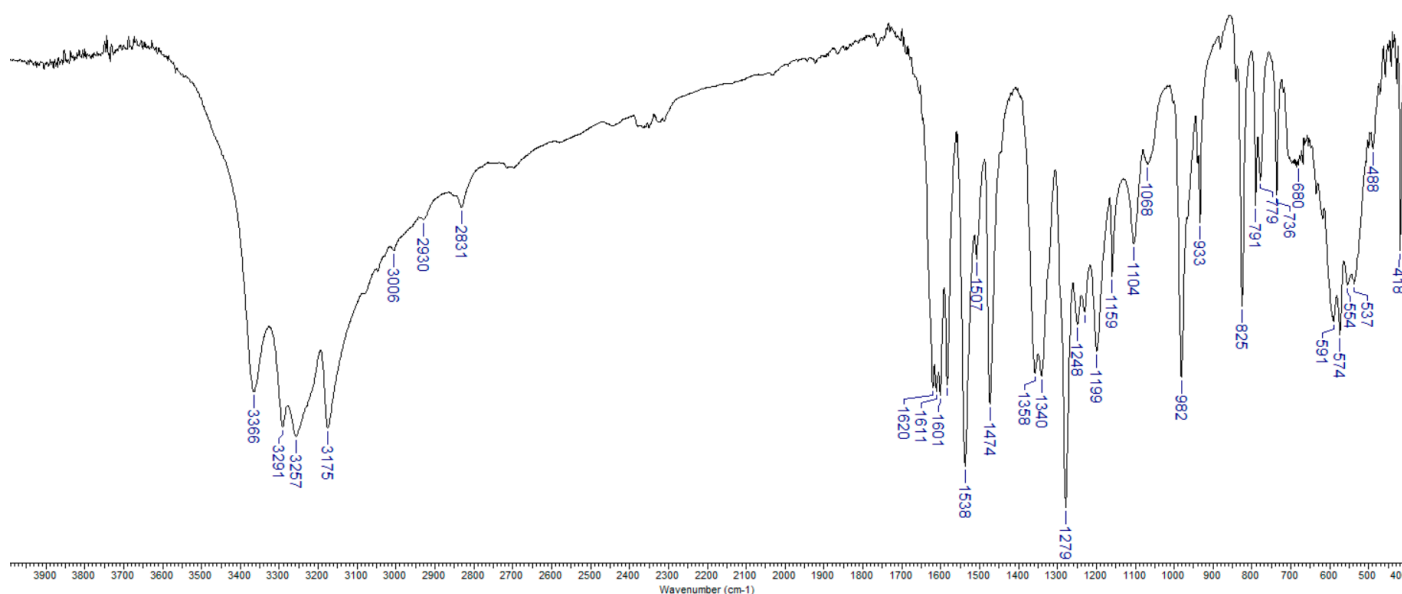


Figure S1. The IR spectrum for the compound 3b.

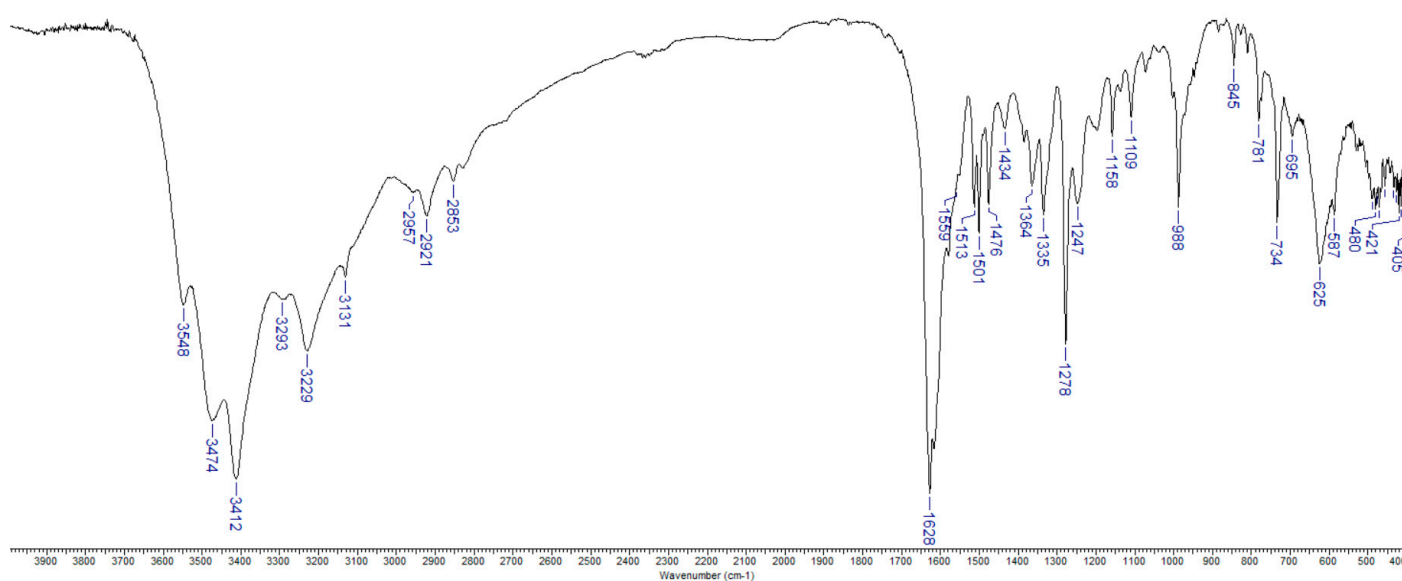


Figure S2. The IR spectrum of the compound 6b.

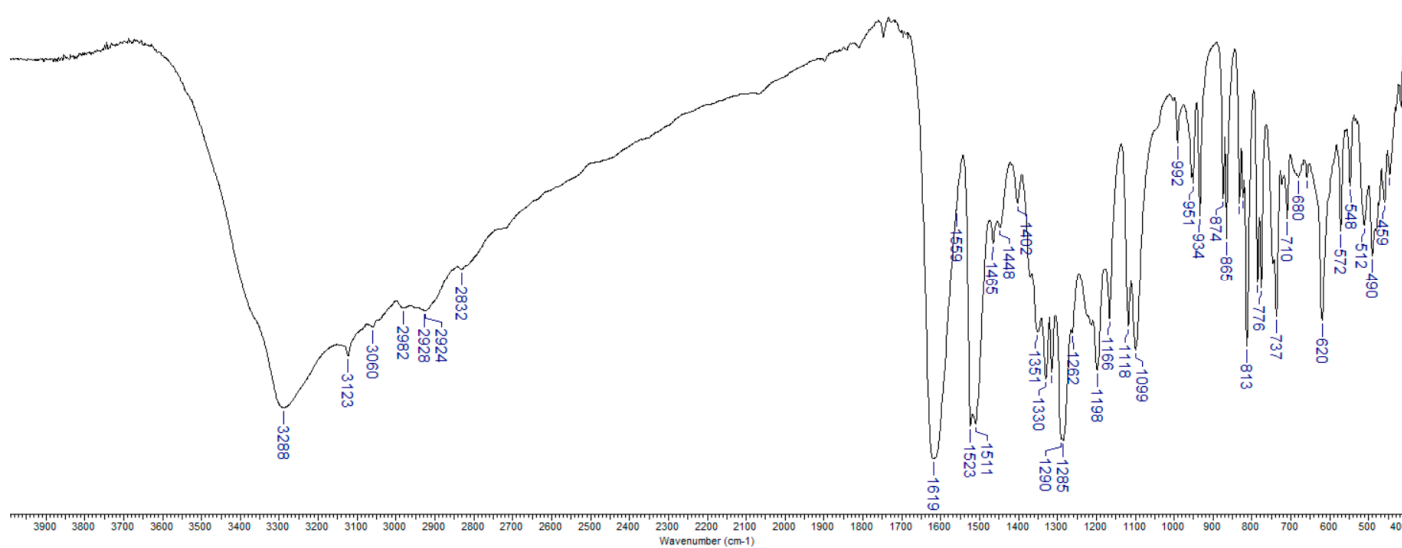


Figure S3. The IR spectrum of the compound 7a.

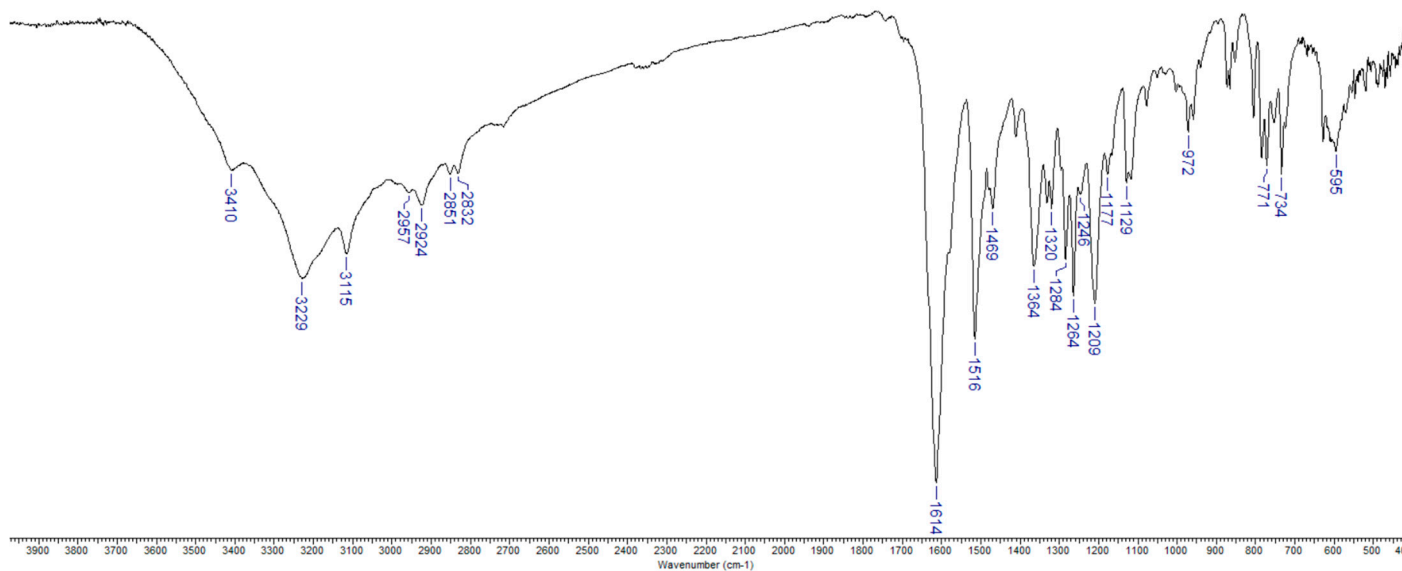


Figure S4. The IR spectrum of the compound 7b.

1.2. The mass spectra of the compounds

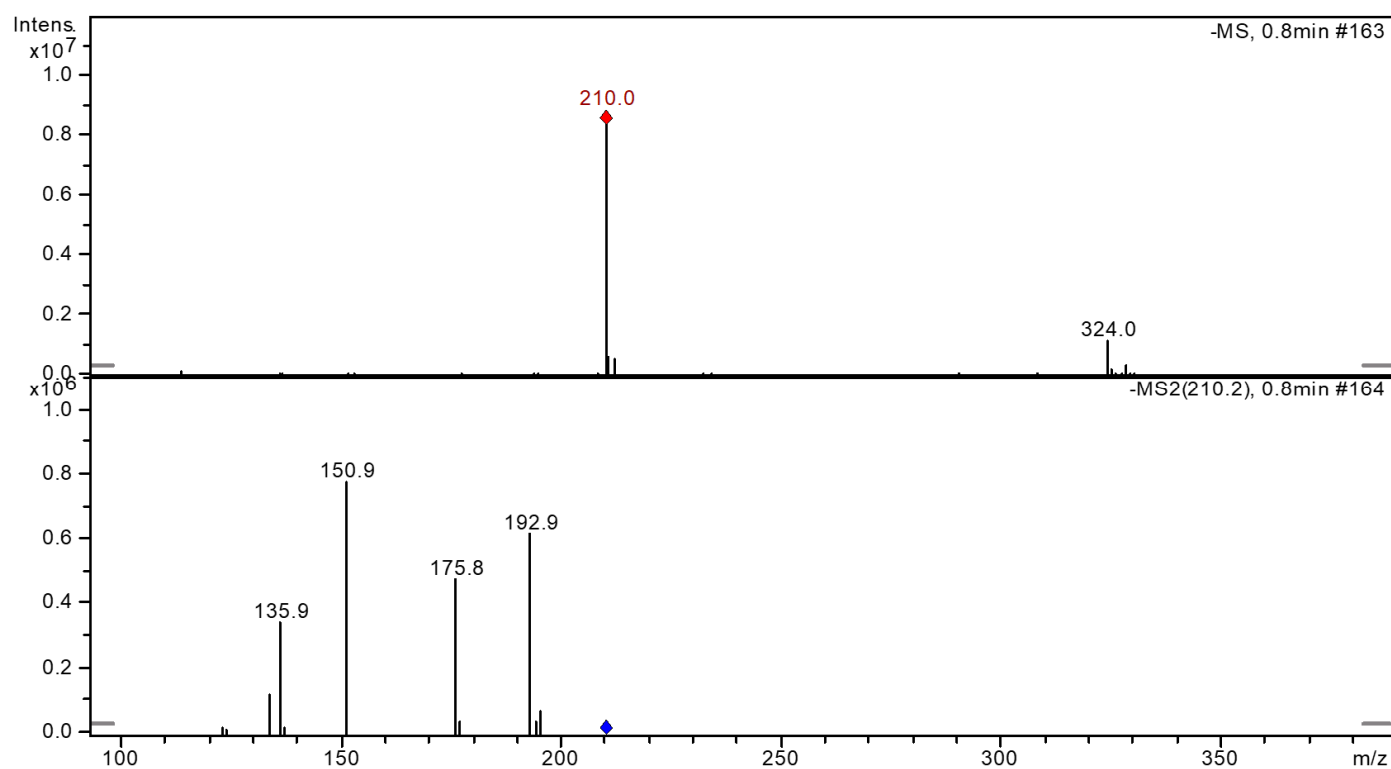


Figure S5. The mass spectrum of the compound 3b.

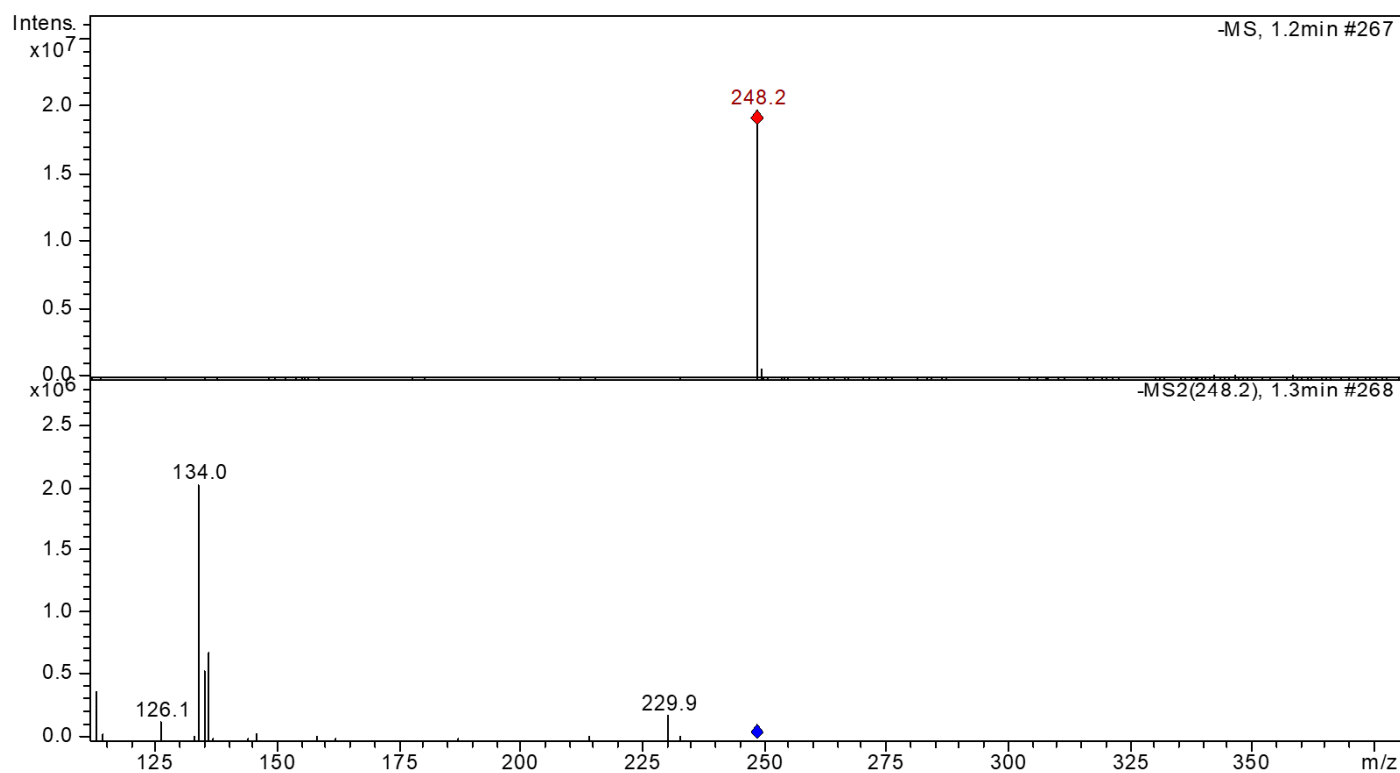


Figure S6. The mass spectrum of the compound 6b.

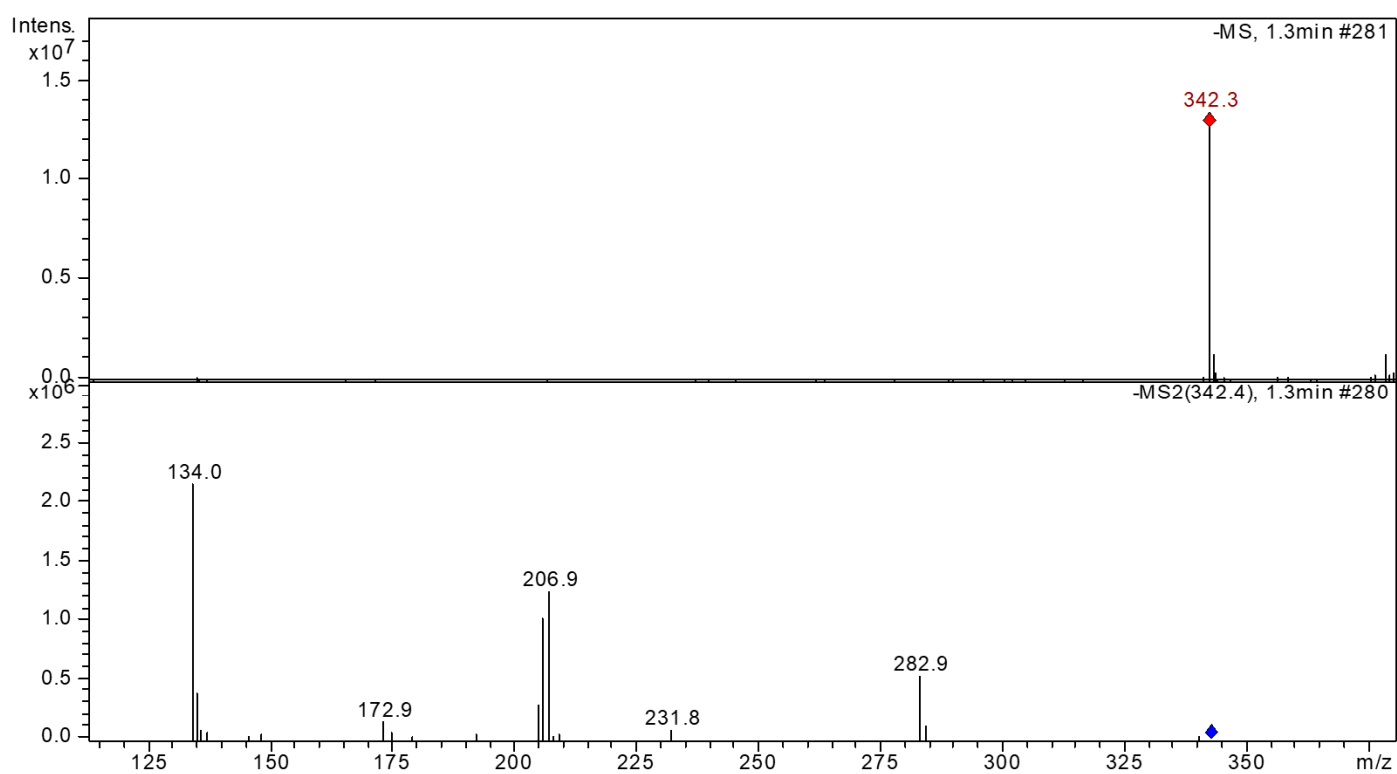


Figure S7. The mass spectrum of the compound 7a.

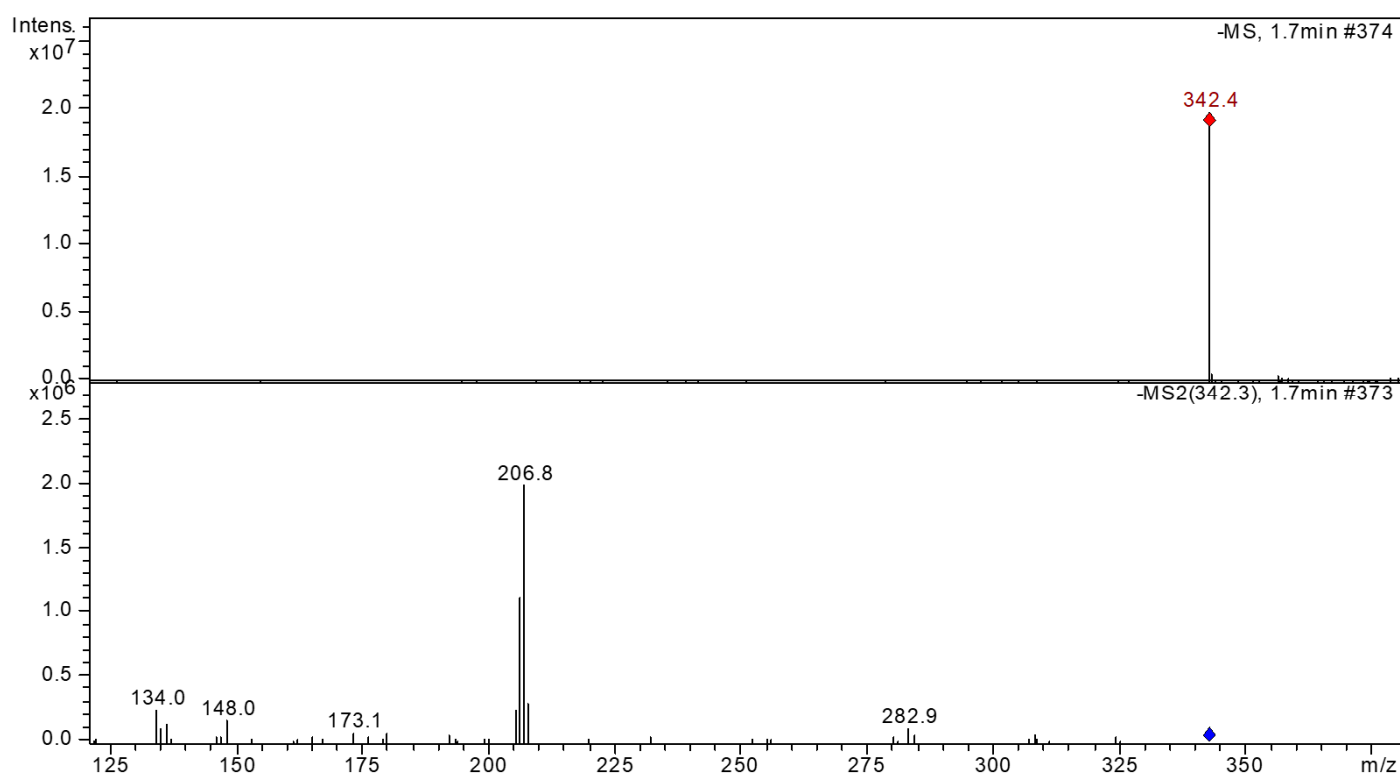


Figure S8. The mass spectrum of the compound 7b.

1.3. The ^1H NMR spectra of the compounds

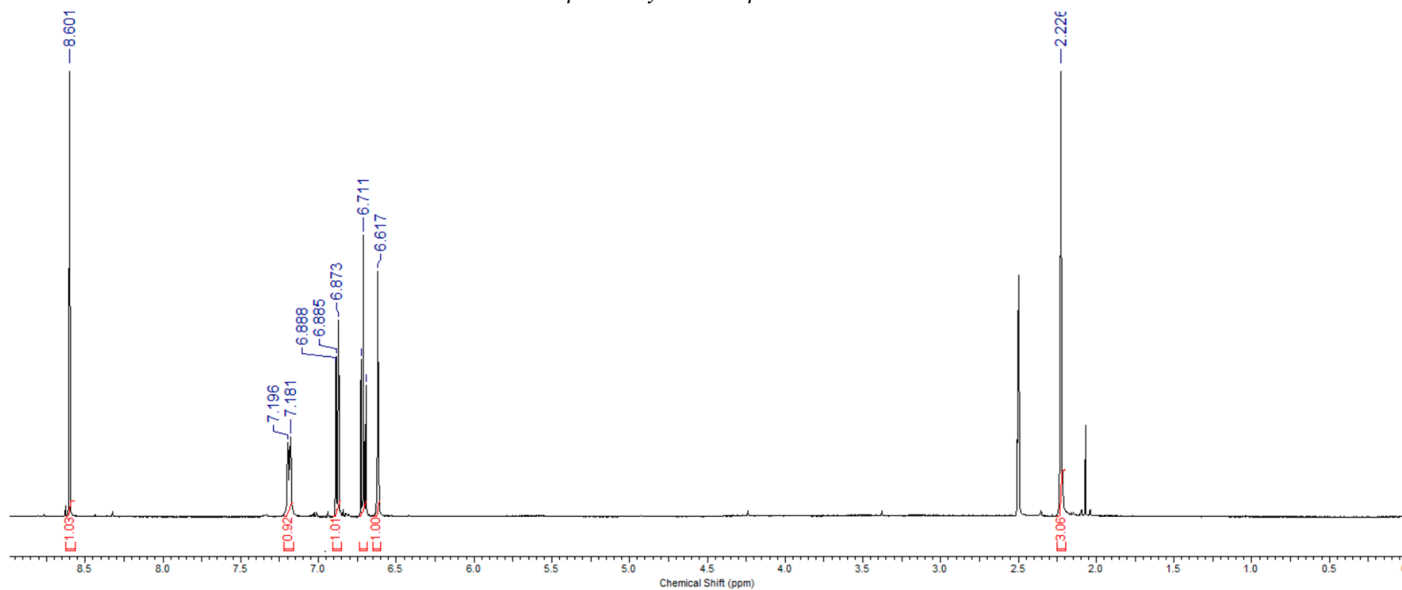


Figure S9. The ^1H NMR spectrum of the compound **6b**.

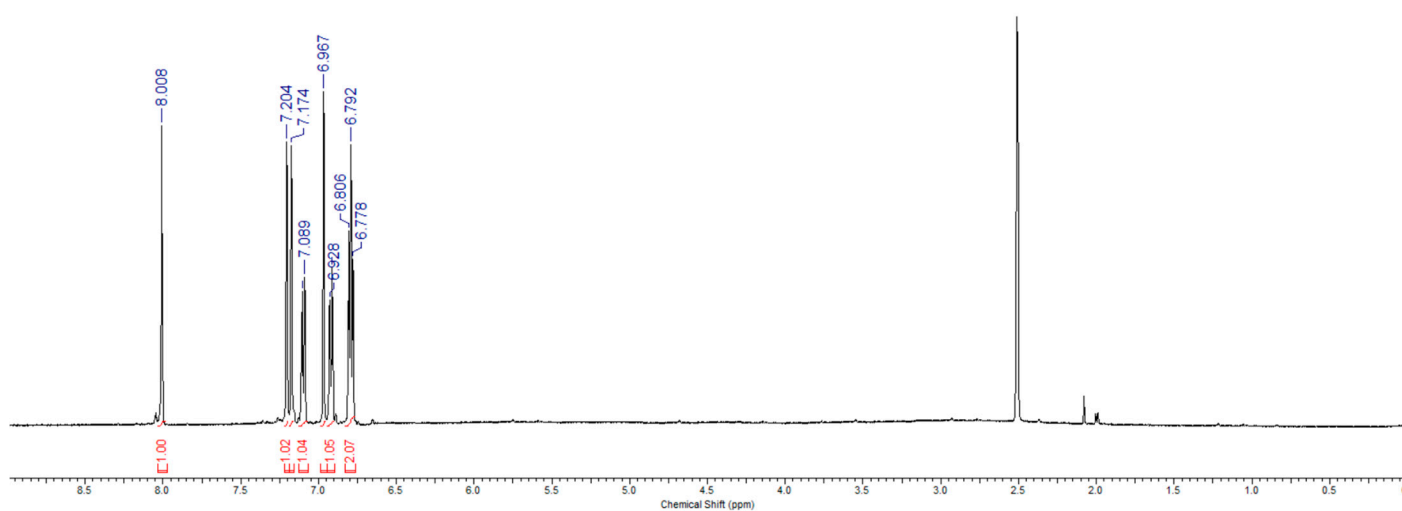


Figure S10. The ^1H NMR spectrum of the compound **7a**.

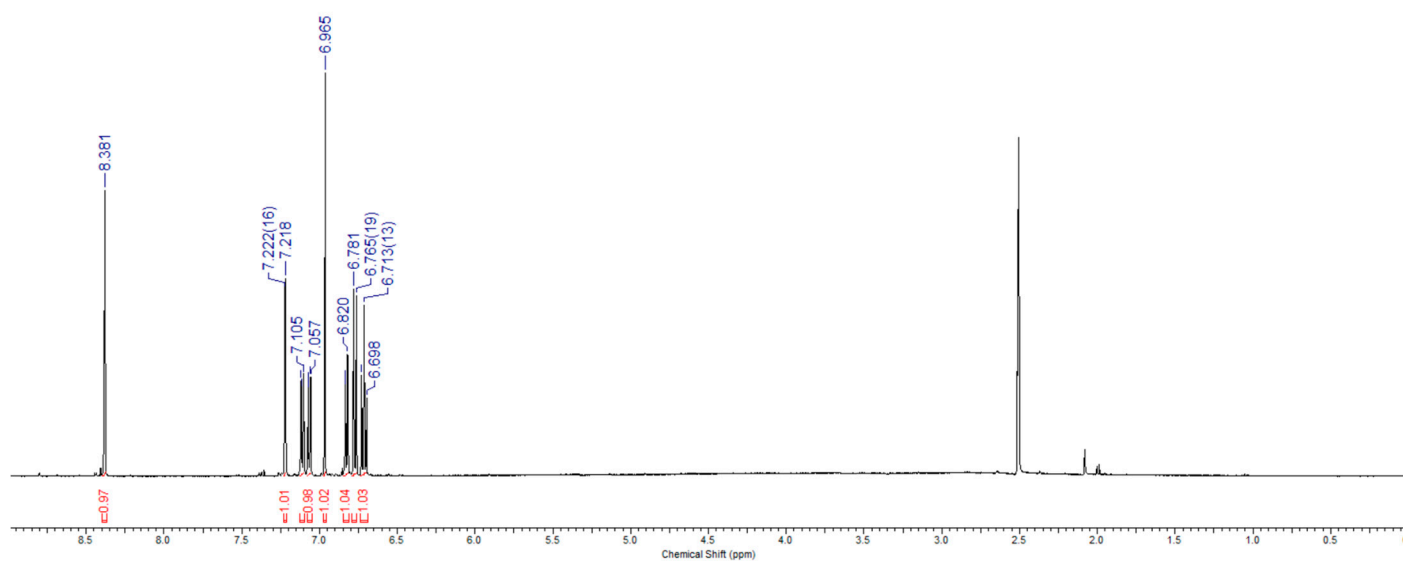


Figure S11. The ^1H NMR spectrum of the compound **7b**.

1.4. The ^{13}C NMR spectra of the compounds

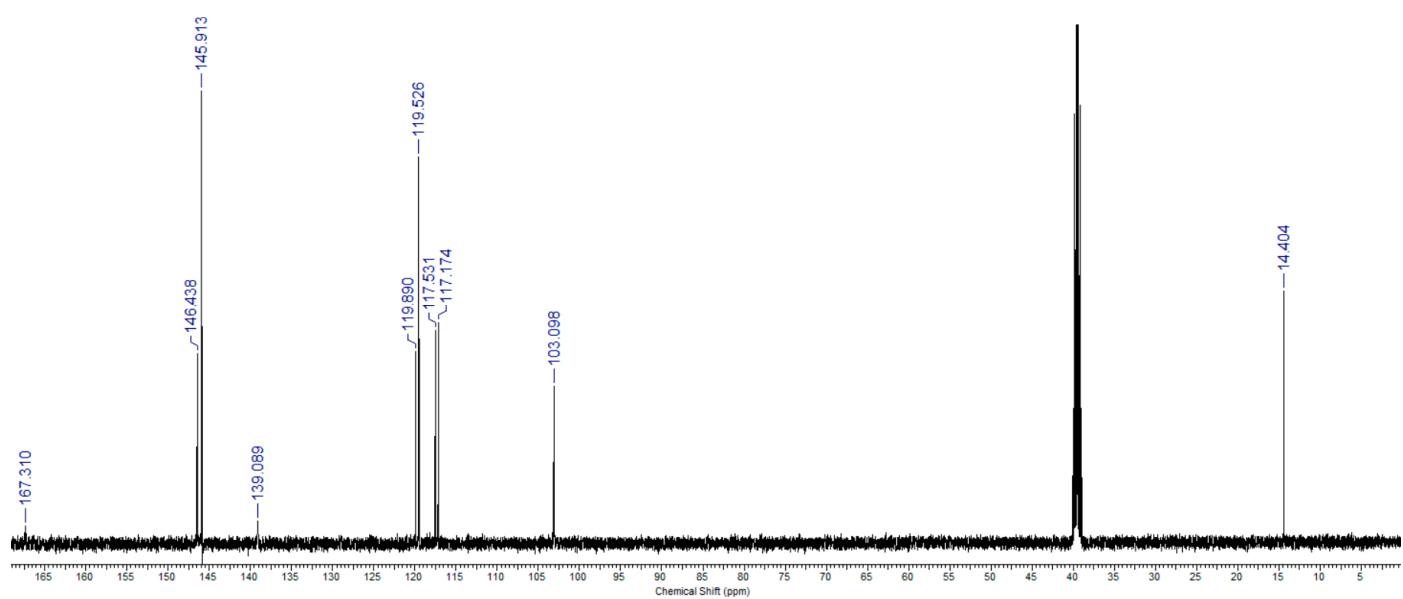


Figure S12. The ^{13}C NMR spectrum of the compound **6b**.

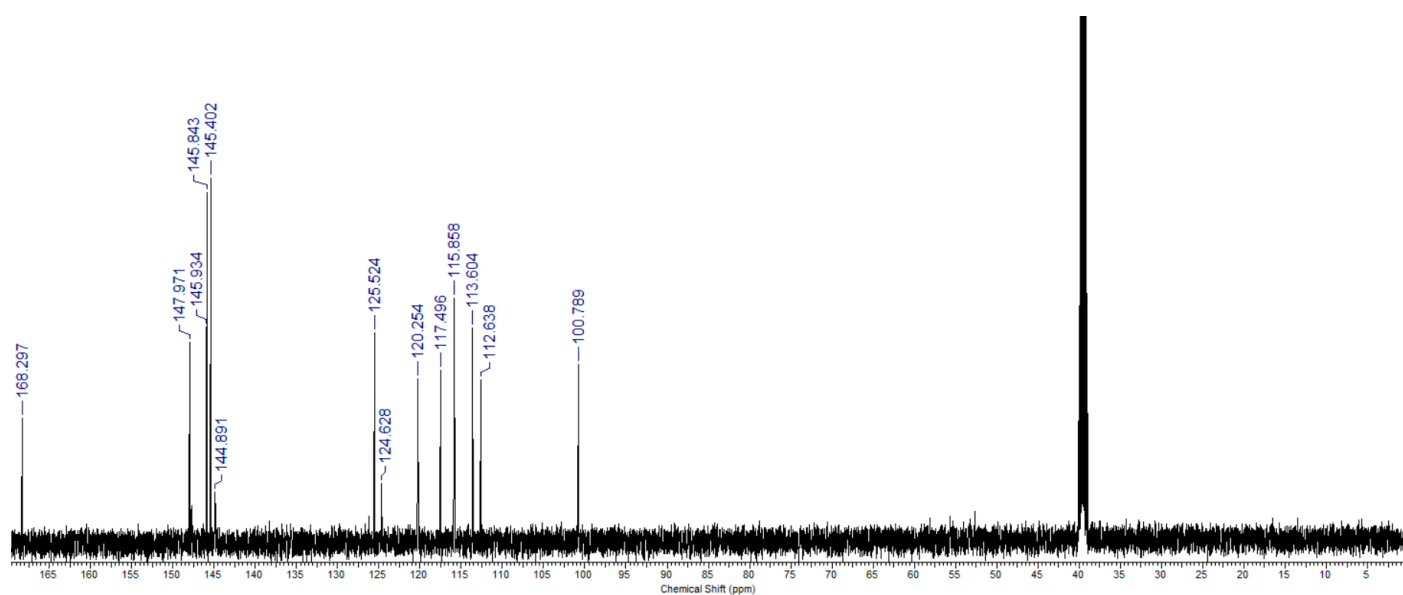


Figure S13. The ¹³C NMR spectrum of the compound 7a.

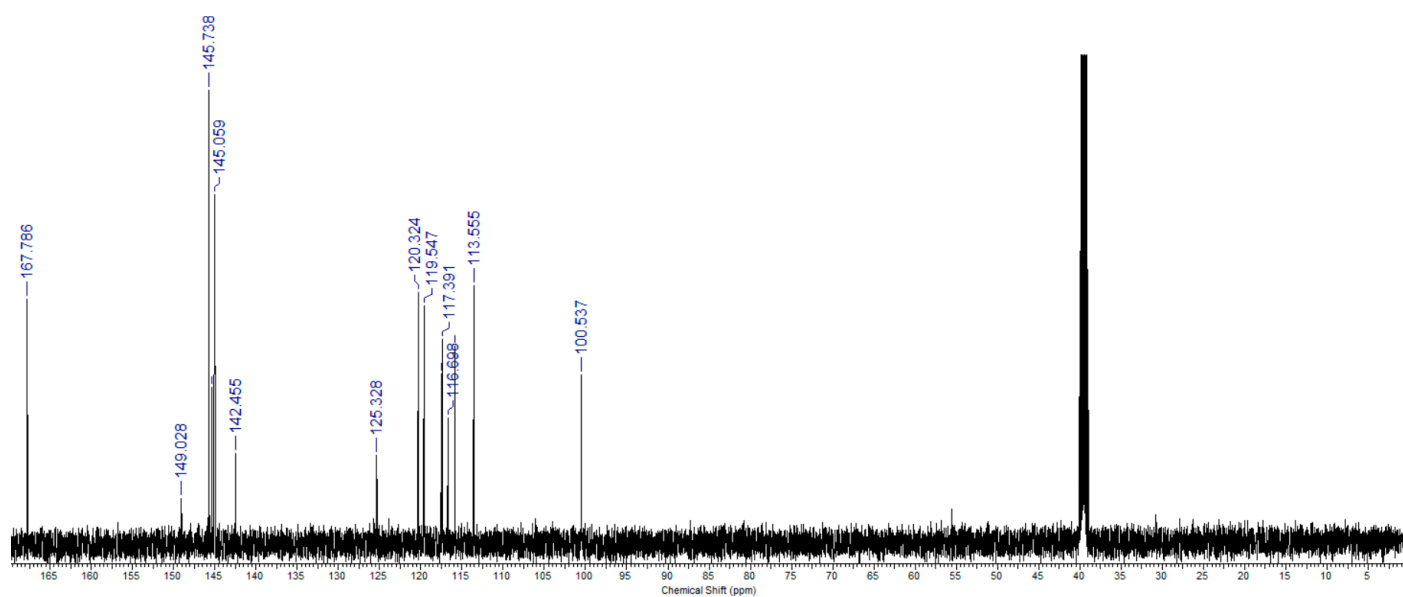


Figure S14. The ¹³C NMR spectrum of the compound 7b.

2. Tables

Table S1. HOMO and LUMO frontier orbitals of compounds 6a-b and 7a-b.

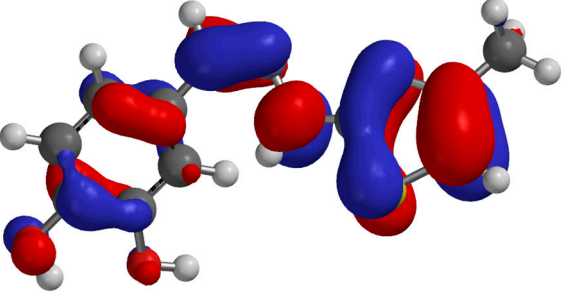
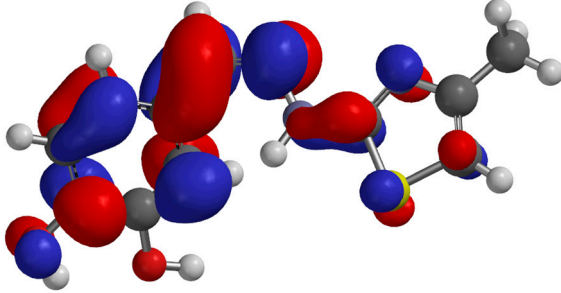
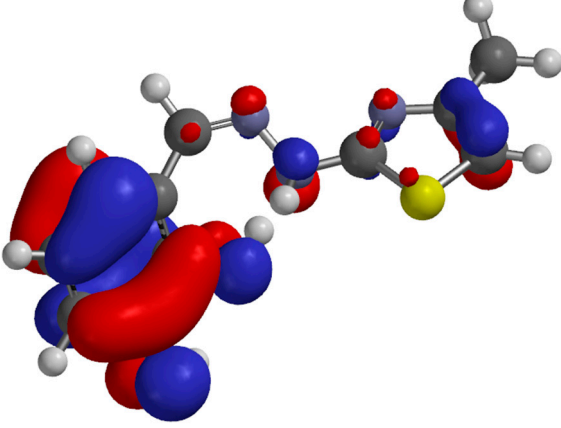
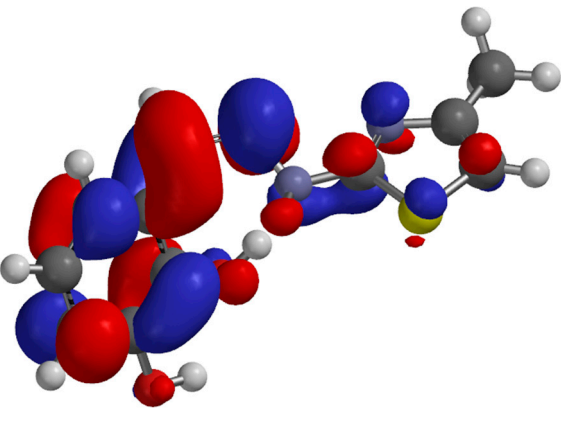
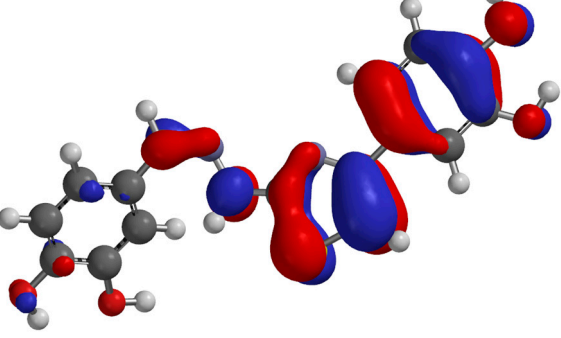
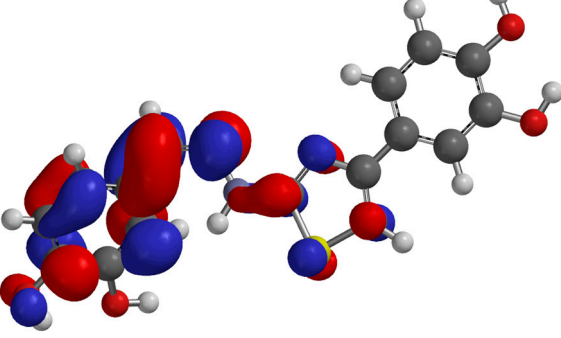
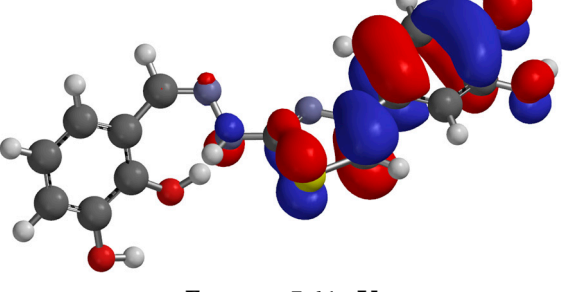
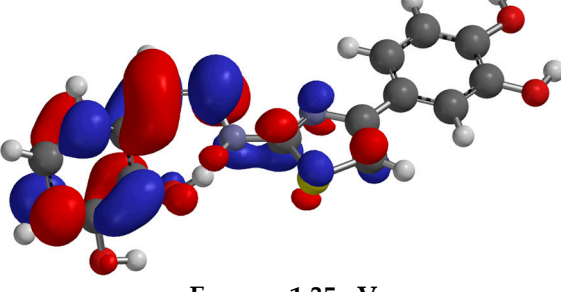
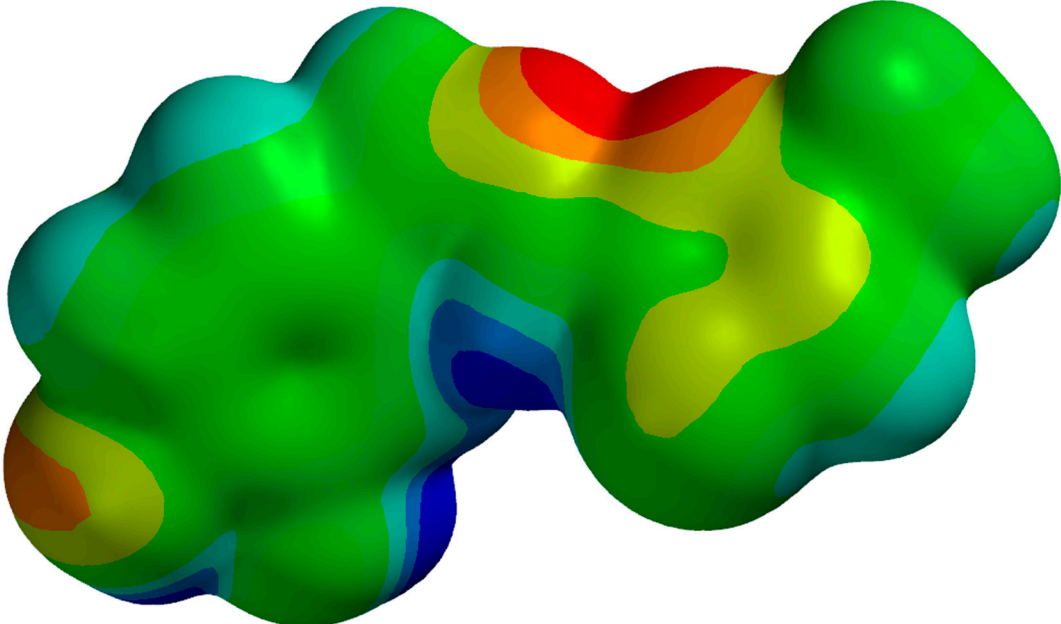
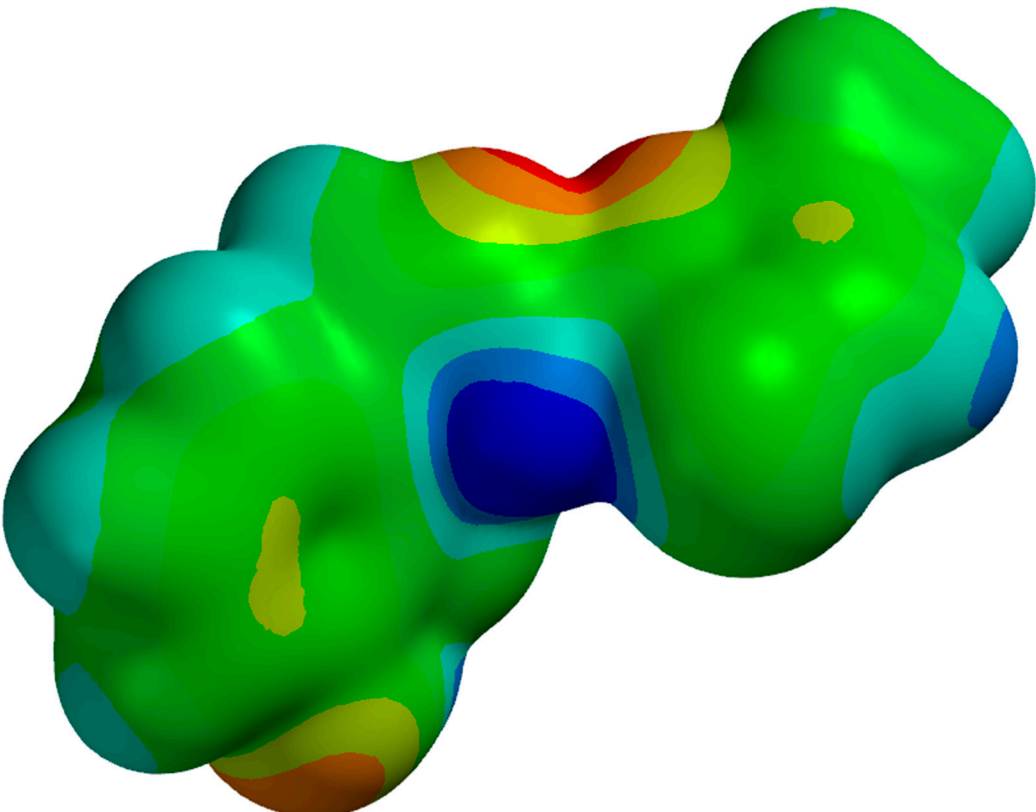
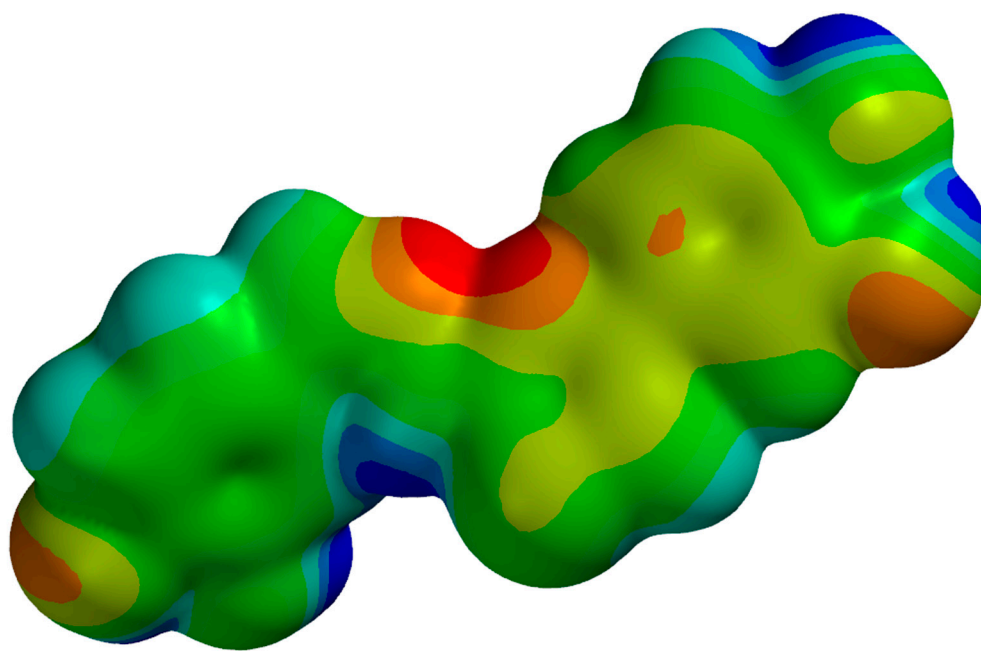
Compound	HOMO	LUMO
6a	 $E_{\text{HOMO}} = -5.30 \text{ eV}$	 $E_{\text{LUMO}} = -1.13 \text{ eV}$
6b	 $E_{\text{HOMO}} = -5.87 \text{ eV}$	 $E_{\text{LUMO}} = -1.33 \text{ eV}$
7a	 $E_{\text{HOMO}} = -5.08 \text{ eV}$	 $E_{\text{LUMO}} = -1.16 \text{ eV}$
7b	 $E_{\text{HOMO}} = -5.41 \text{ eV}$	 $E_{\text{LUMO}} = -1.35 \text{ eV}$

Table S2. Electrostatic potential maps of compounds **6a-b** and **7a-b**.

Compound	Electrostatic potential map
6a	
6b	

7a



7b

