

Supplementary Materials: Modification of 6,7-Dichloro-5,8-Quinolinedione at C2 Position: Synthesis, Quantum Chemical Properties, and Activity against DT-Diaphorase Enzyme

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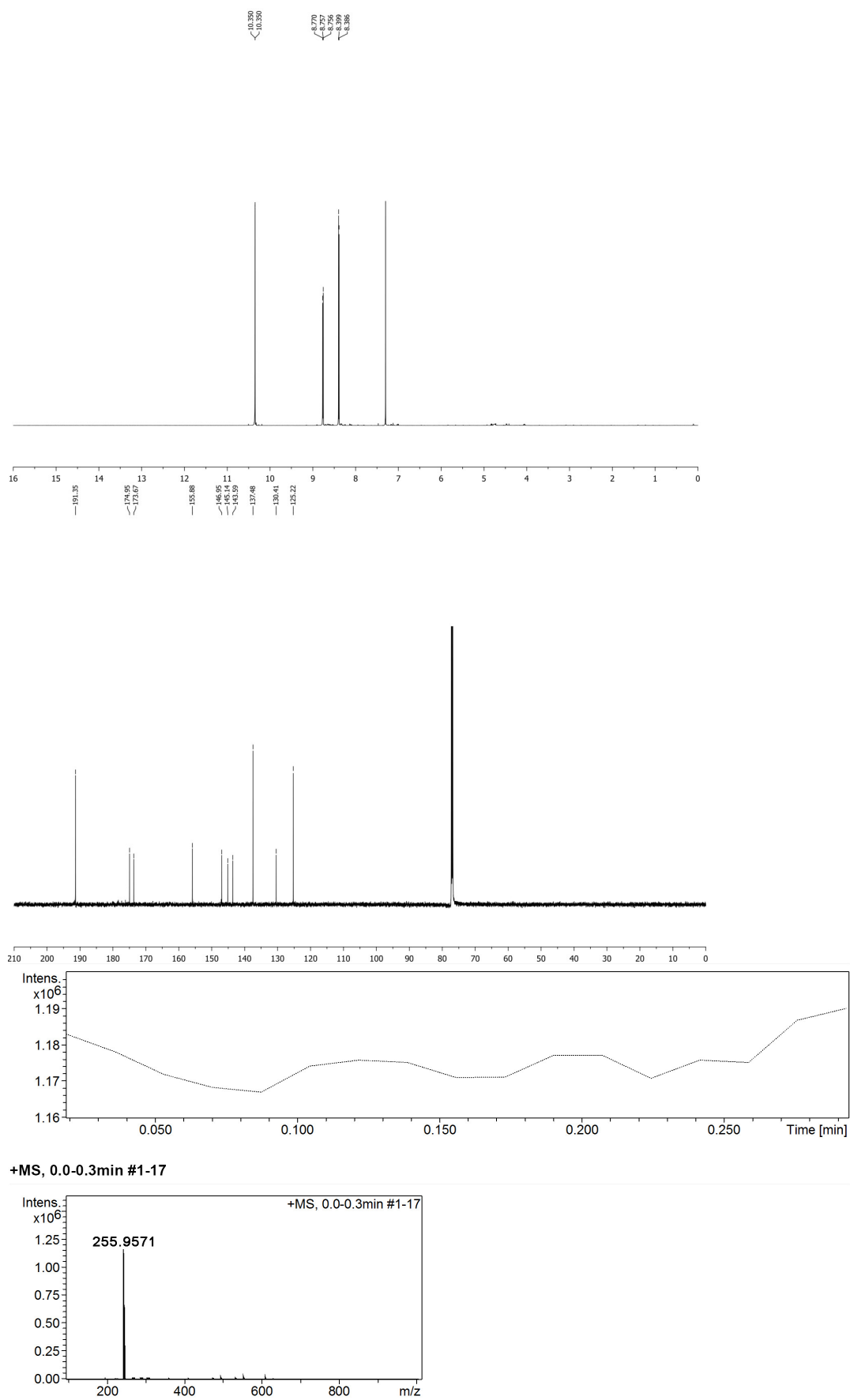


Figure S1. Spectra of 6,7-dichloro-5,8-dioxo-5,8-dihydroquinoline-2-carbaldehyde **3**.

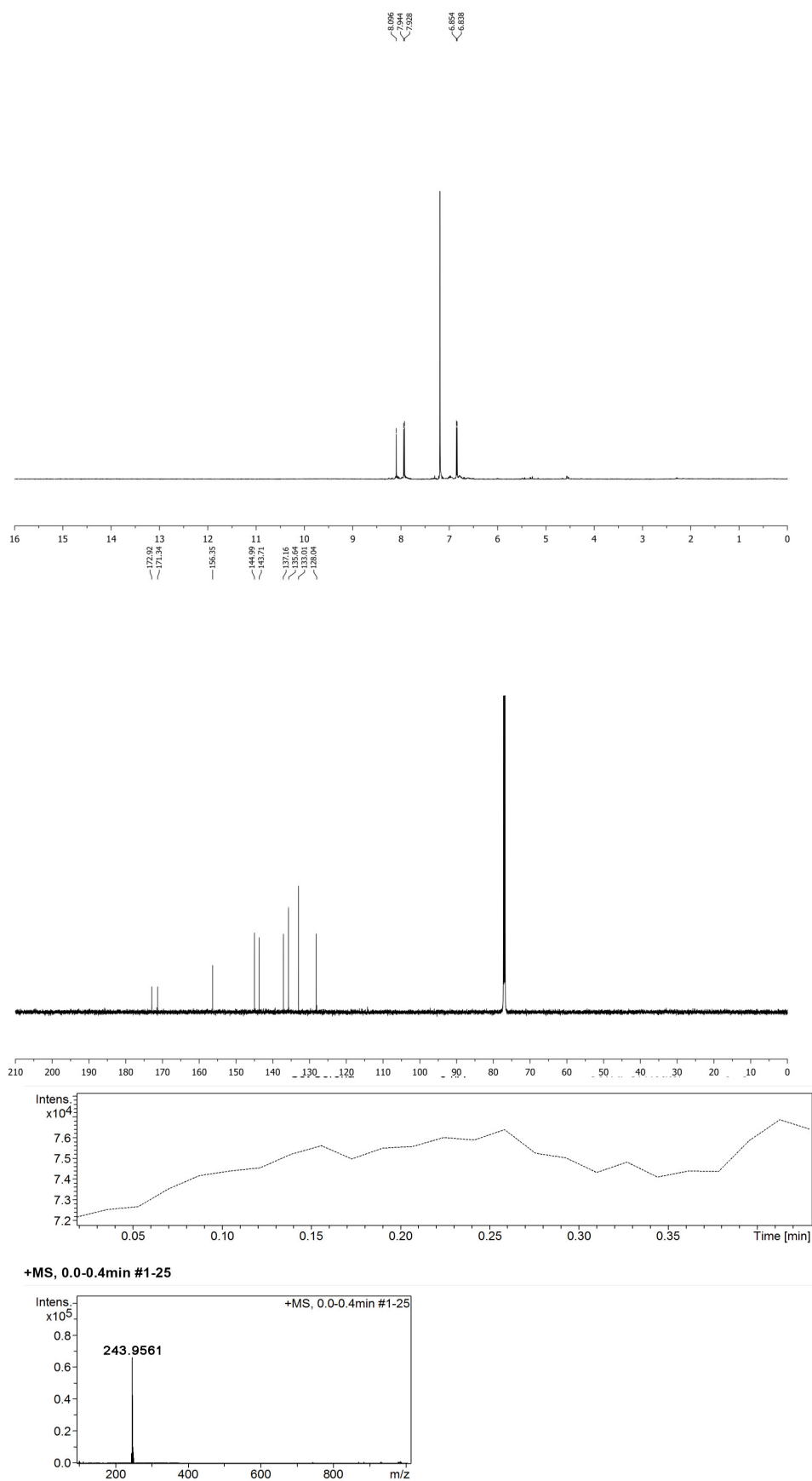


Figure S2. Spectra of 6,7-dichloro-2-hydroxy-5,8-quinolinedione 6.

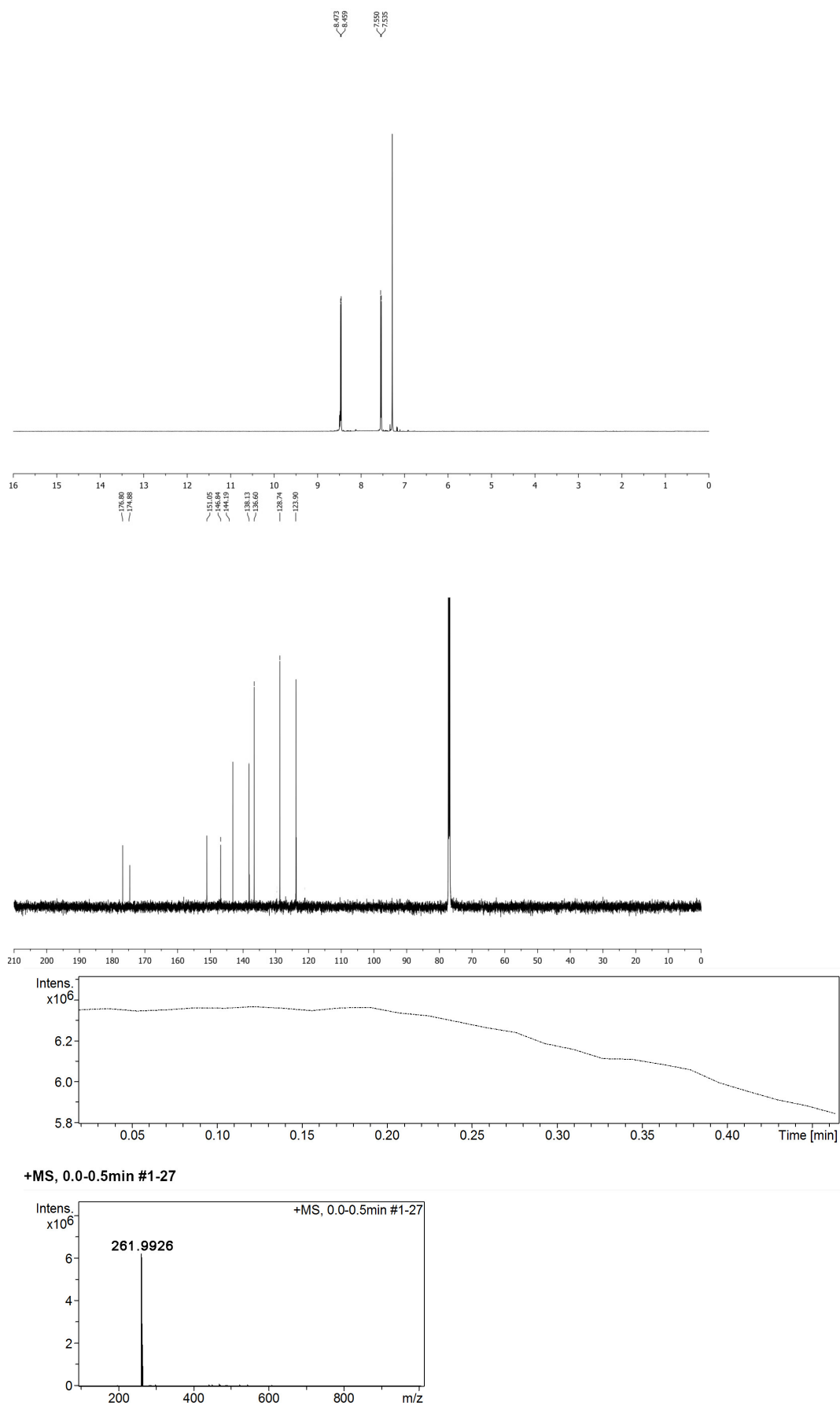


Figure S3. Spectra of 2,6,7-trichloro-5,8-chinolinodion 7.

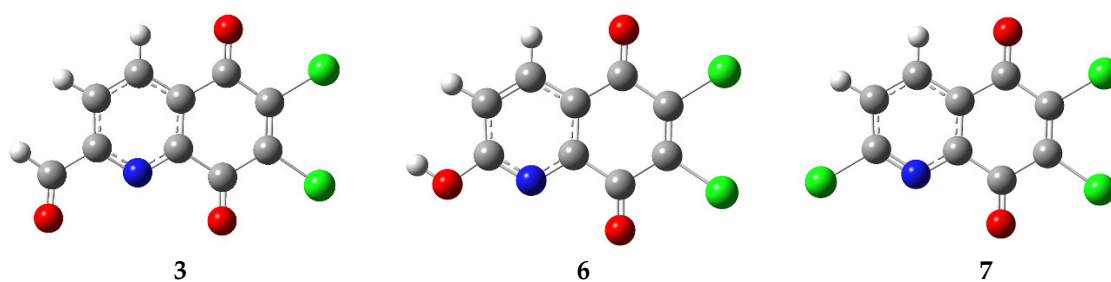


Figure S4. The optimized structure of 5,8-quinolinedione compounds 3 and 6-7.

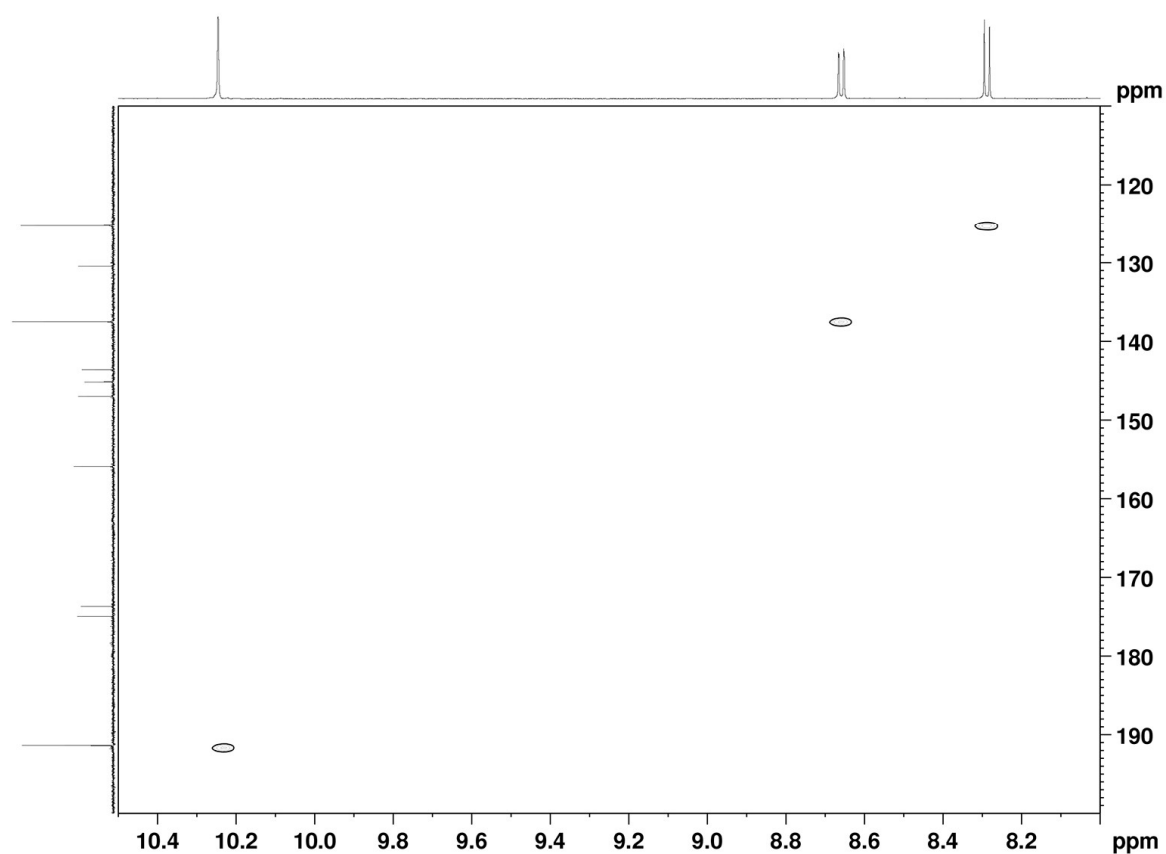


Figure S5. The ^1H - ^{13}C HSQC spectrum (600 MHz, CDCl_3) of compound 3.

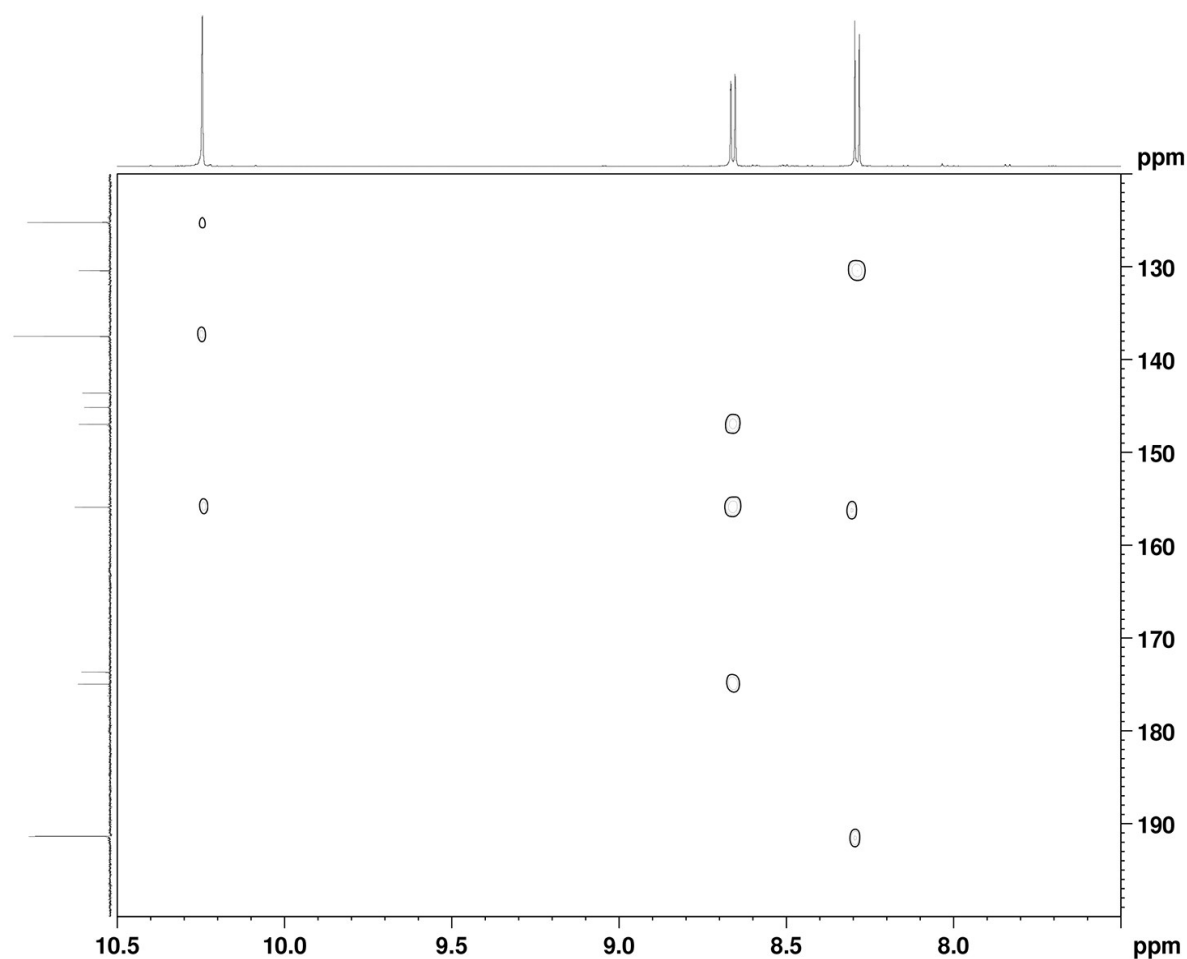


Figure S6. The ^1H - ^{13}C HMBC spectrum (600 MHz, CDCl_3) of compound **3**.

Table S1. Interaction of compounds **1-3** and **6-7** with active site of NQO1 protein.

Compound	π -interaction residues and lenght (Å)	H-bonding residues and lenght (Å)
1	PHE178 (5.11)	
	TYR128 (4.90)	TYR126 (3.22)
	FAD (3.59, 4.18, 4.06, 5.18)	
2	PHE178 (5.06)	
	TYR128 (4.76, 4.80)	TYR126 (3.14)
	FAD (4.31, 3.62, 5.27, 4.12)	TYR128 (2.90)
3	PHE178 (5.11)	
	TYR128 (4.77)	TYR126 (3.13)
	FAD (4.31, 3.63, 5.27, 4.12)	TYR128 (2.90)
6	PHE178 (5.08)	
	TYR128 (4.83)	TYR126 (3.12)
	FAD (4.24, 3.62, 5.22, 4.10)	TYR128 (2.95, 3.39)
7	PHE178 (5.10)	
	TYR128 (4.78, 4.96)	TYR126 (3.10)
	FAD (4.27, 3.62, 5.22, 4.10)	TYR128 (2.89)