Supplementary Material

Coumarin *N*-acylhydrazone derivatives: green synthesis and antioxidant potential - experimental and theoretical study

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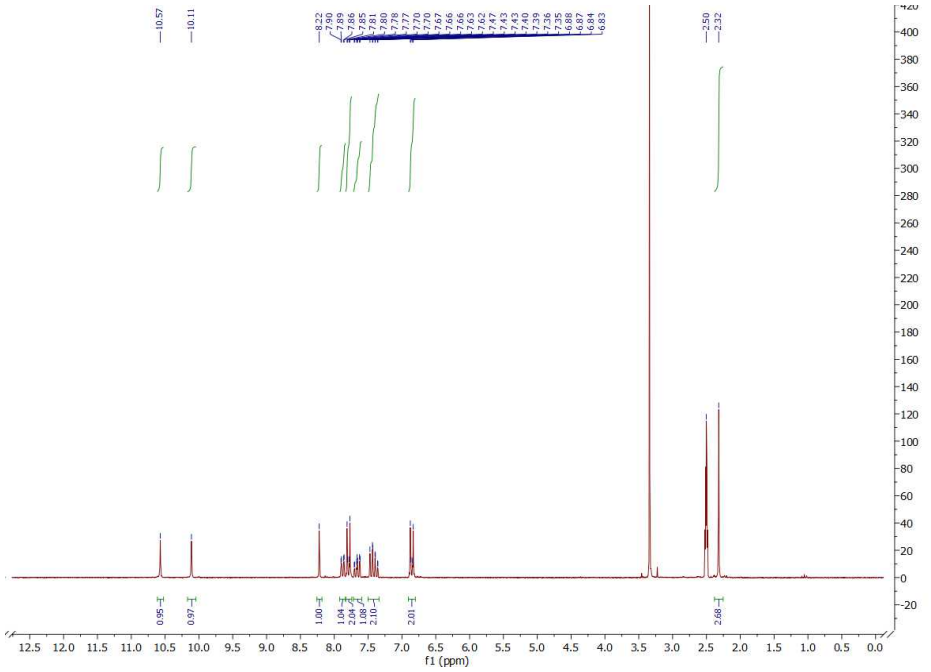
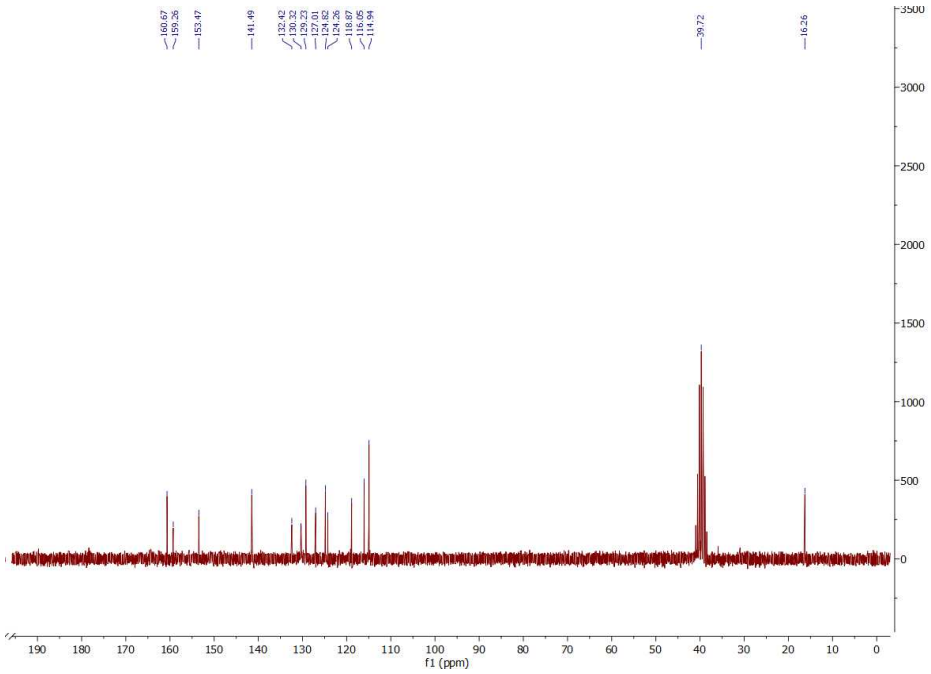
^{1}H NMR and ^{13}CNMR spectra of compound **3a**





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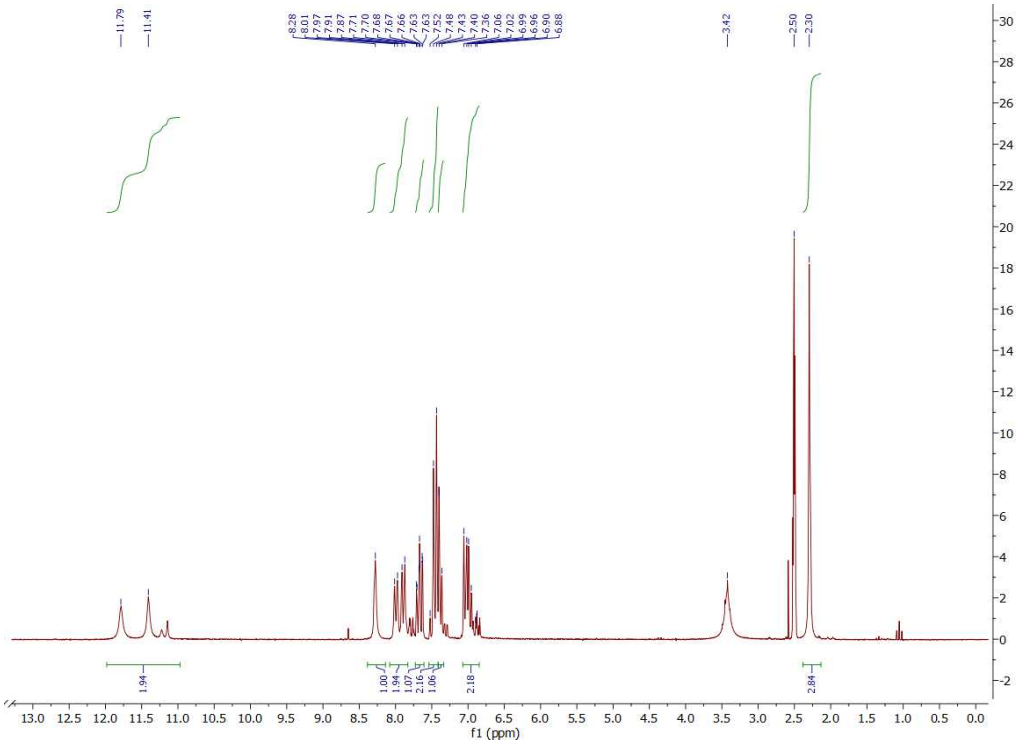

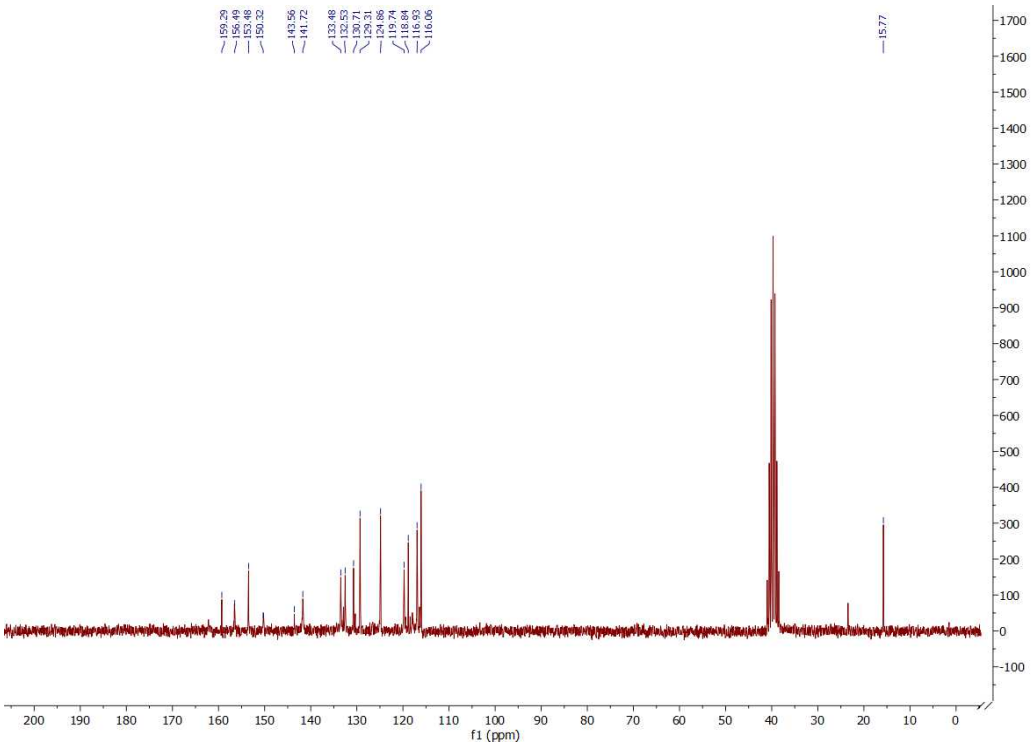

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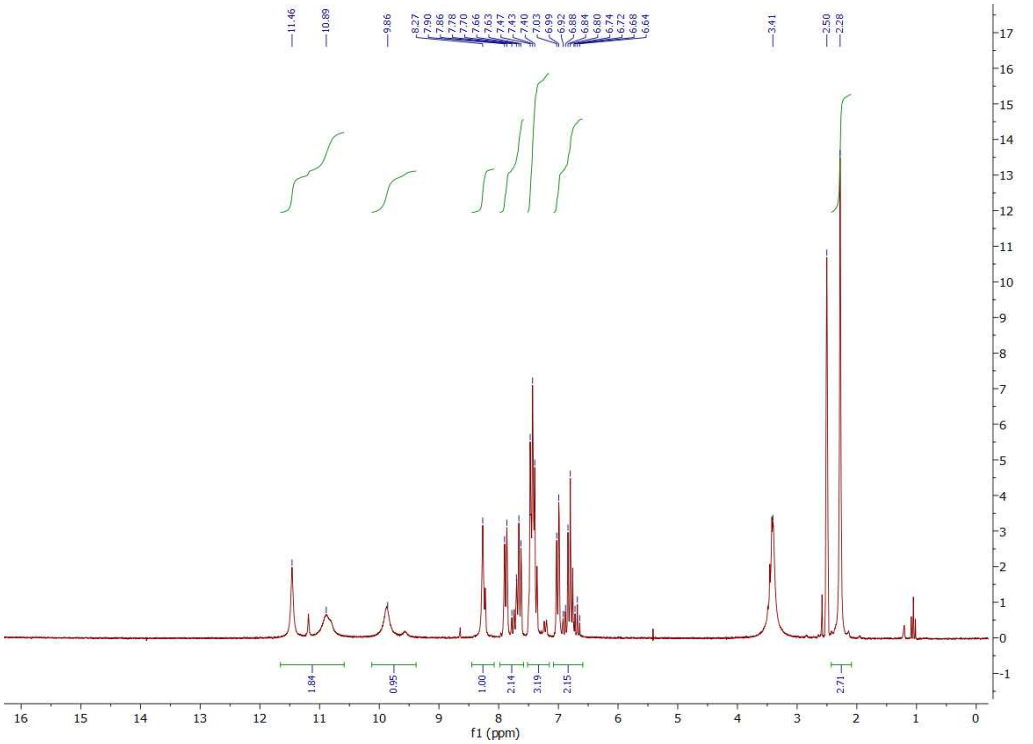

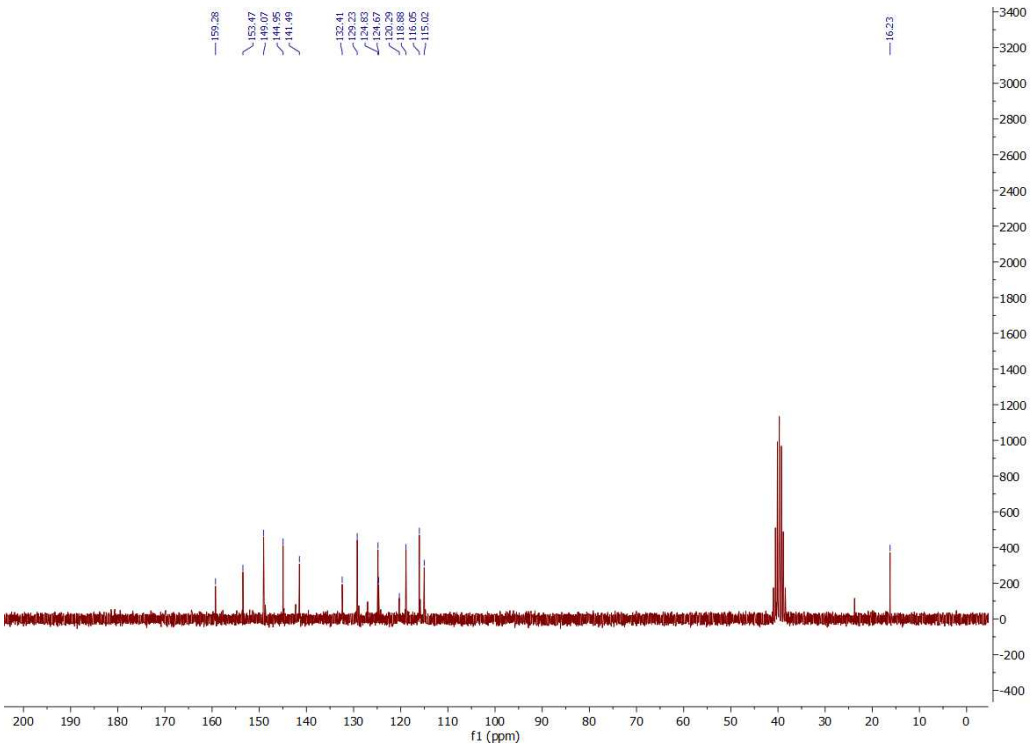

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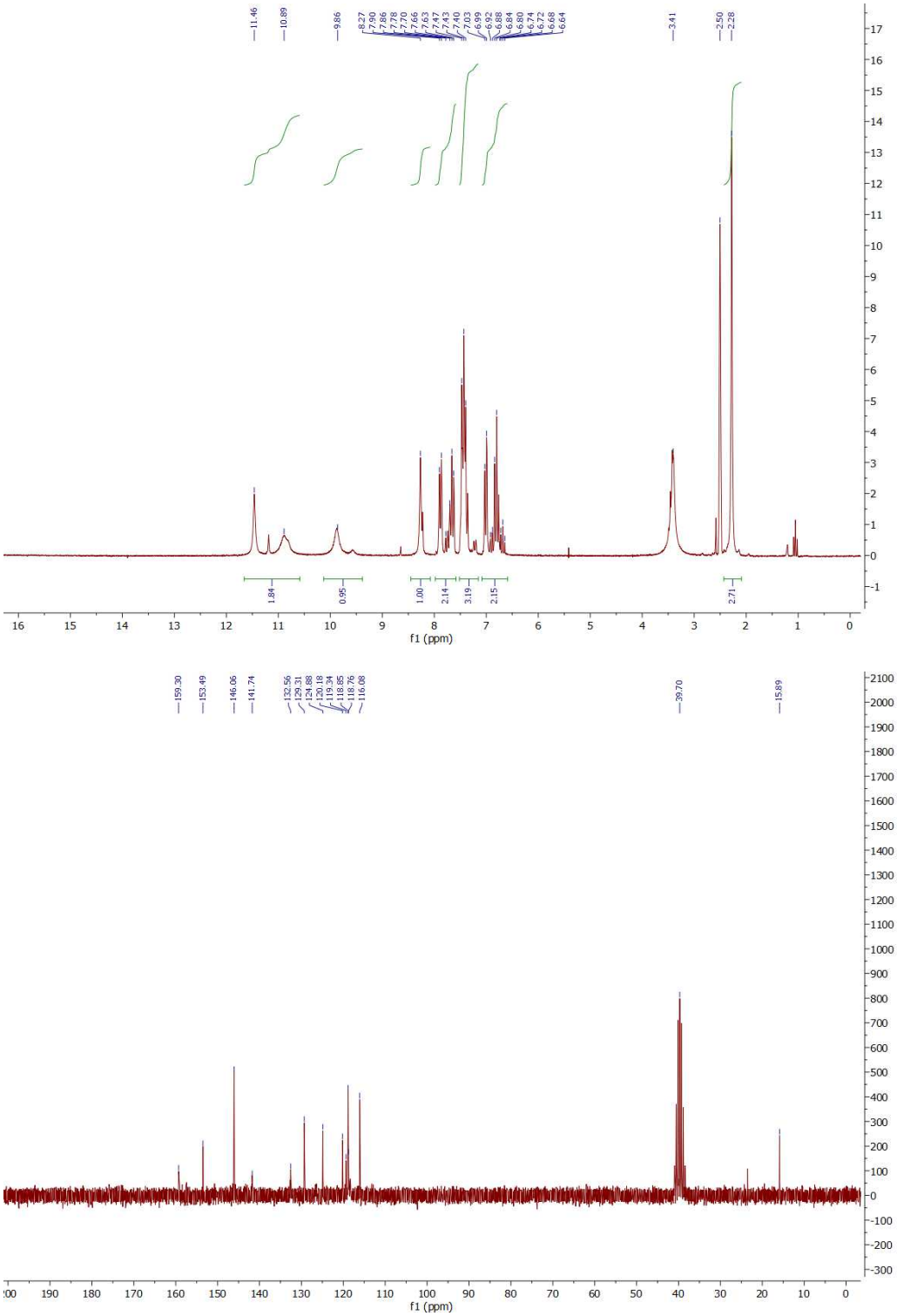

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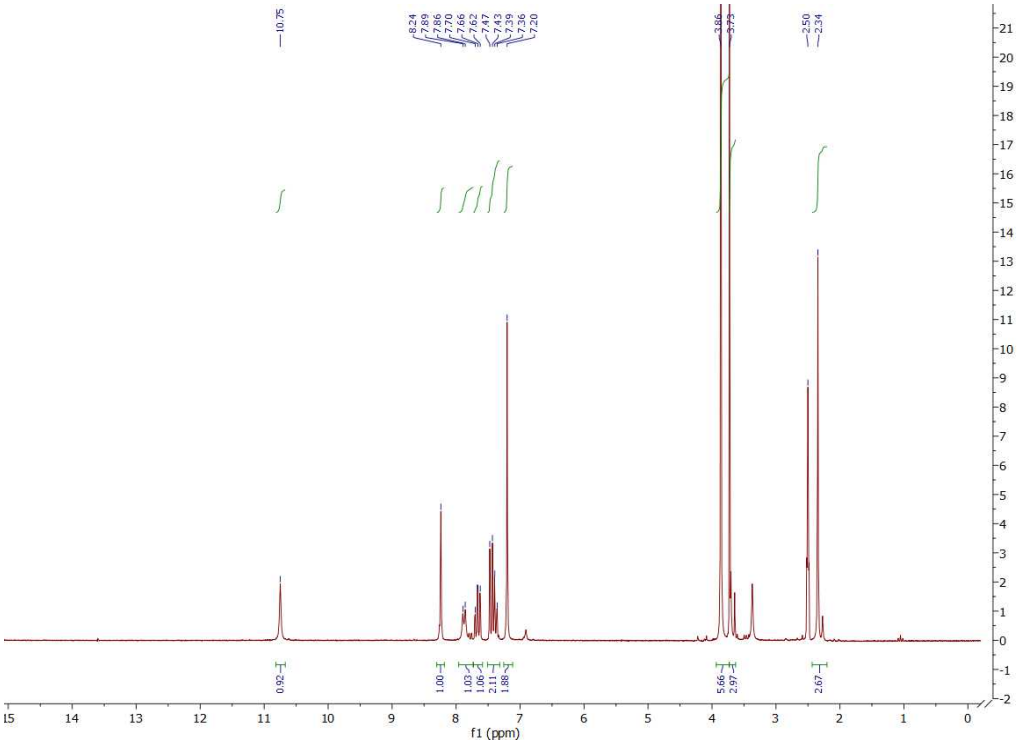

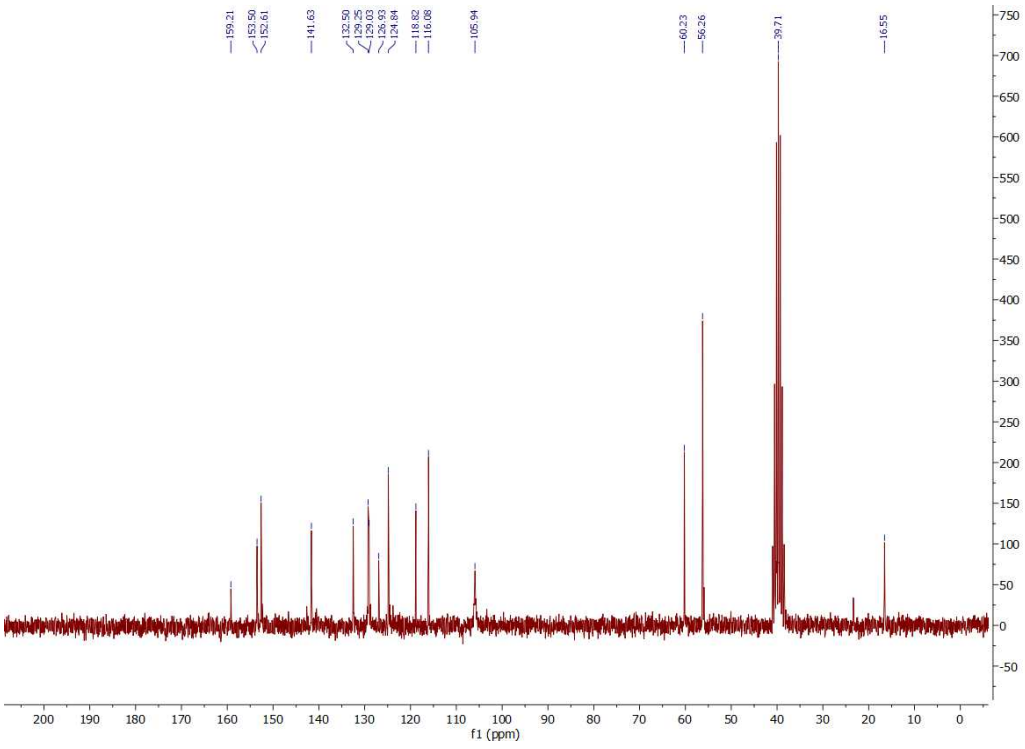

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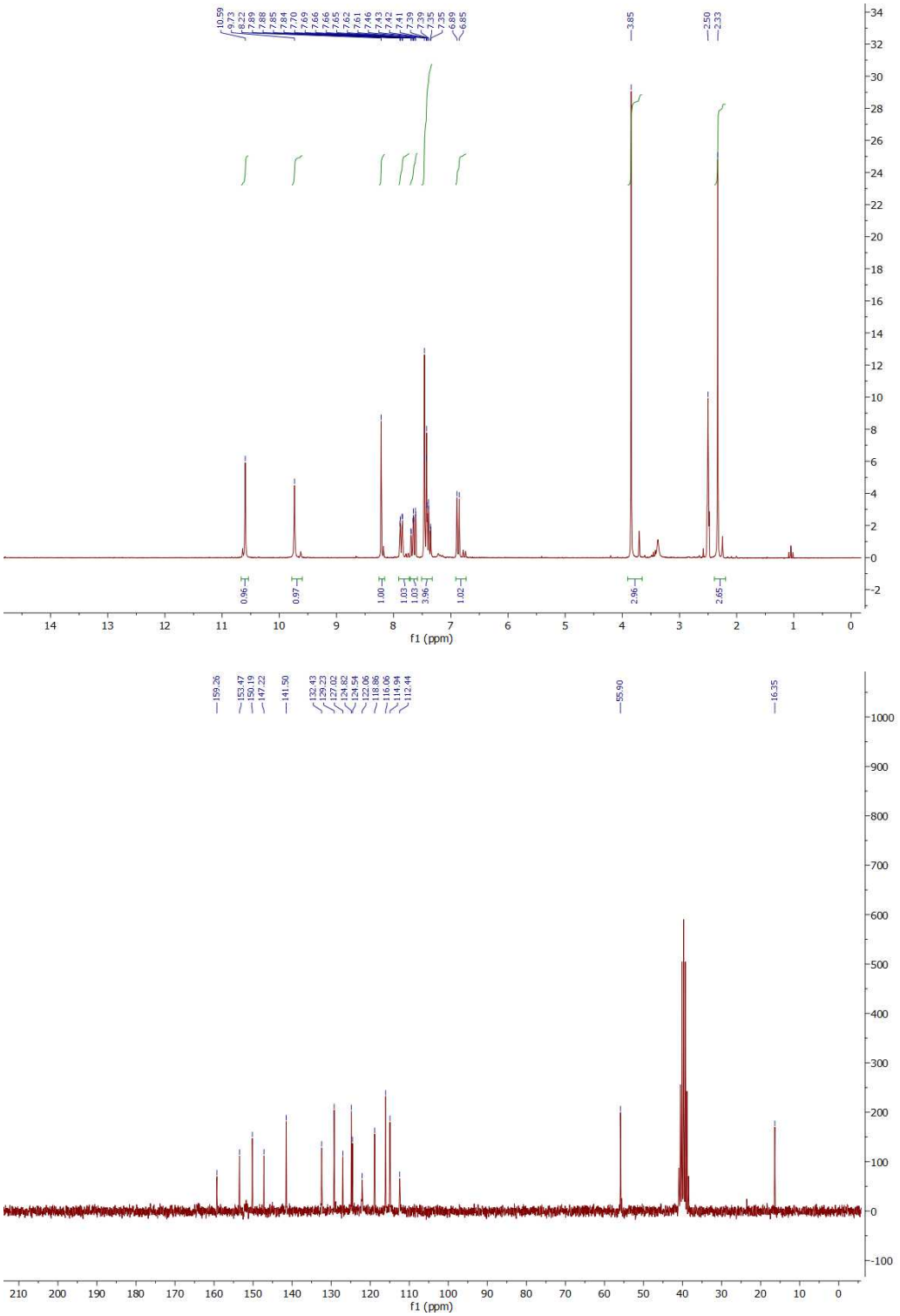
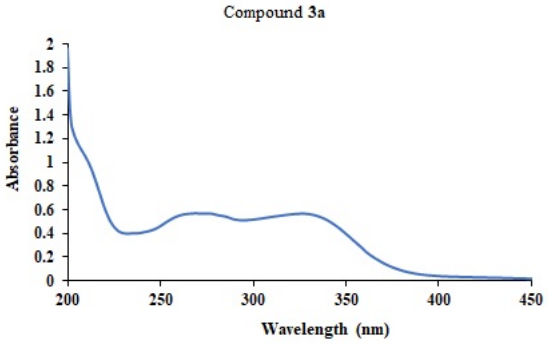
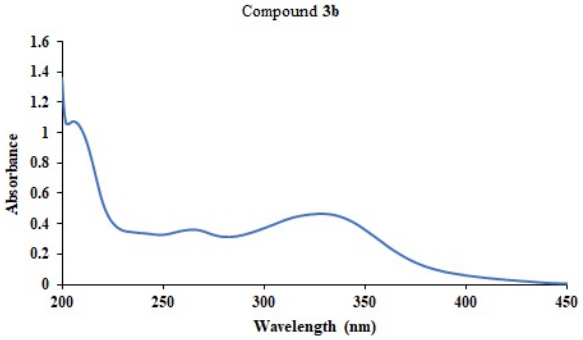
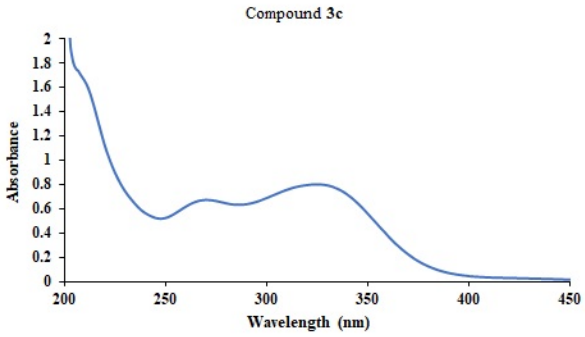
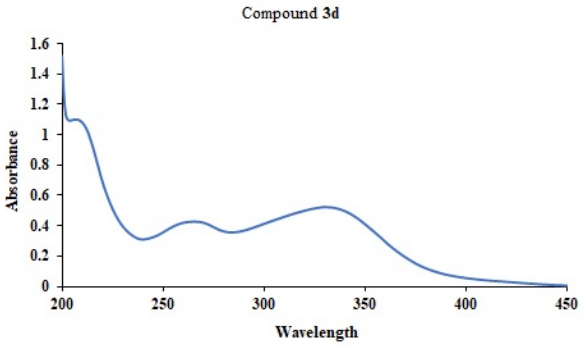


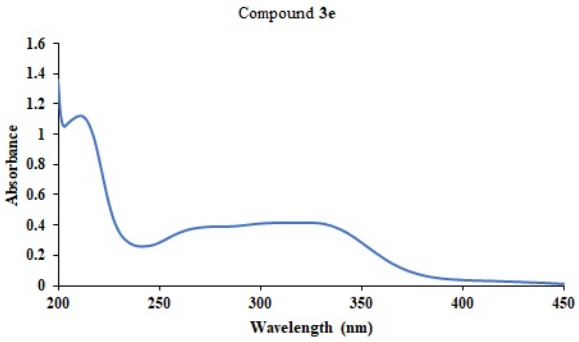
UV-Vis spectra of products **3a-f**

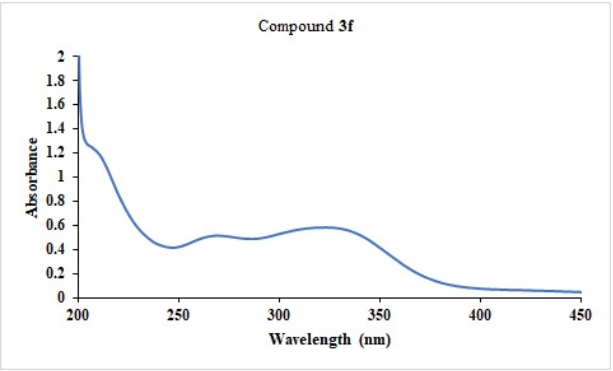












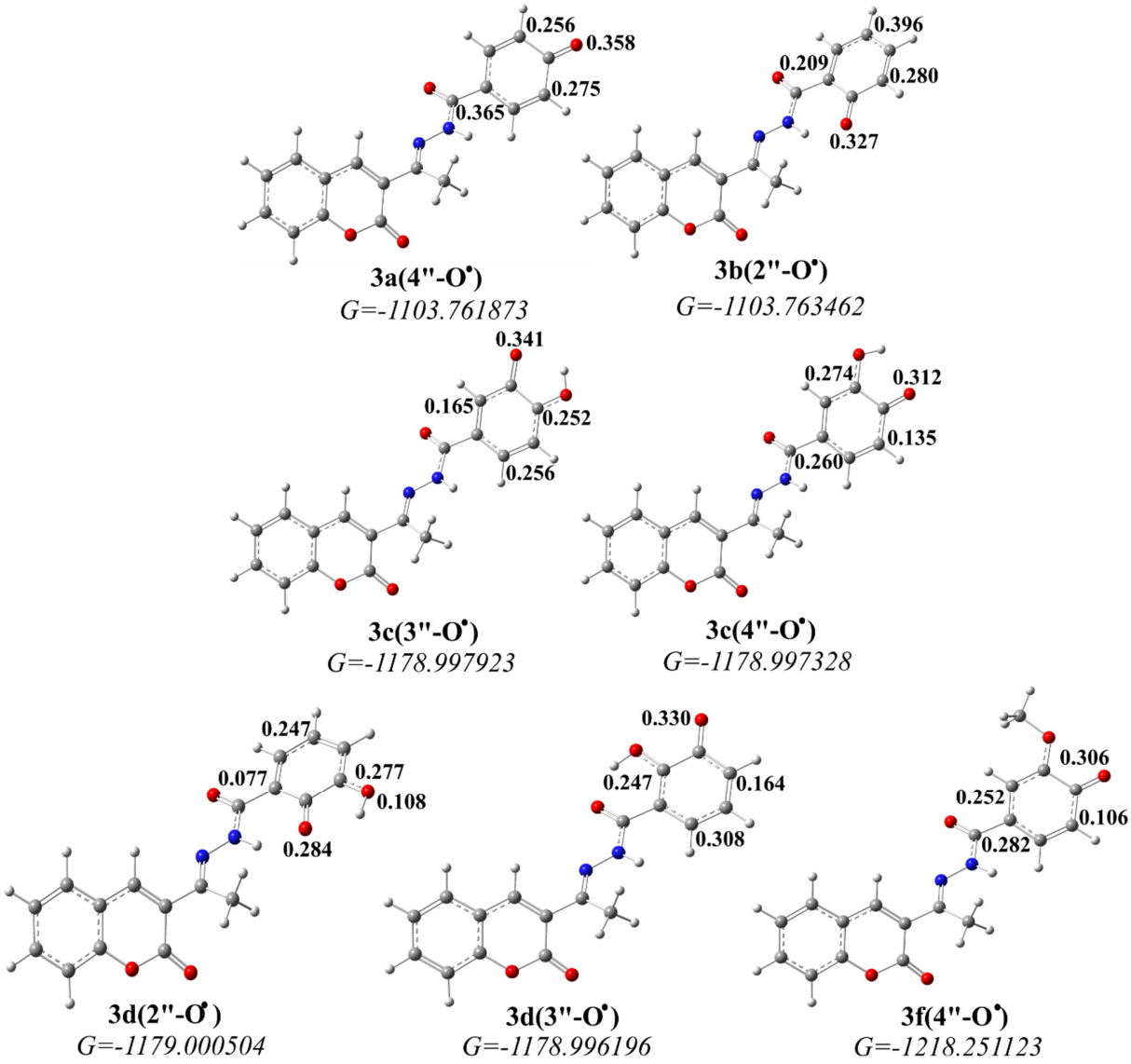


Figure S1. NBO spin distribution for formed O-centered radical species with the values of Gibbs free energy (a.u.)

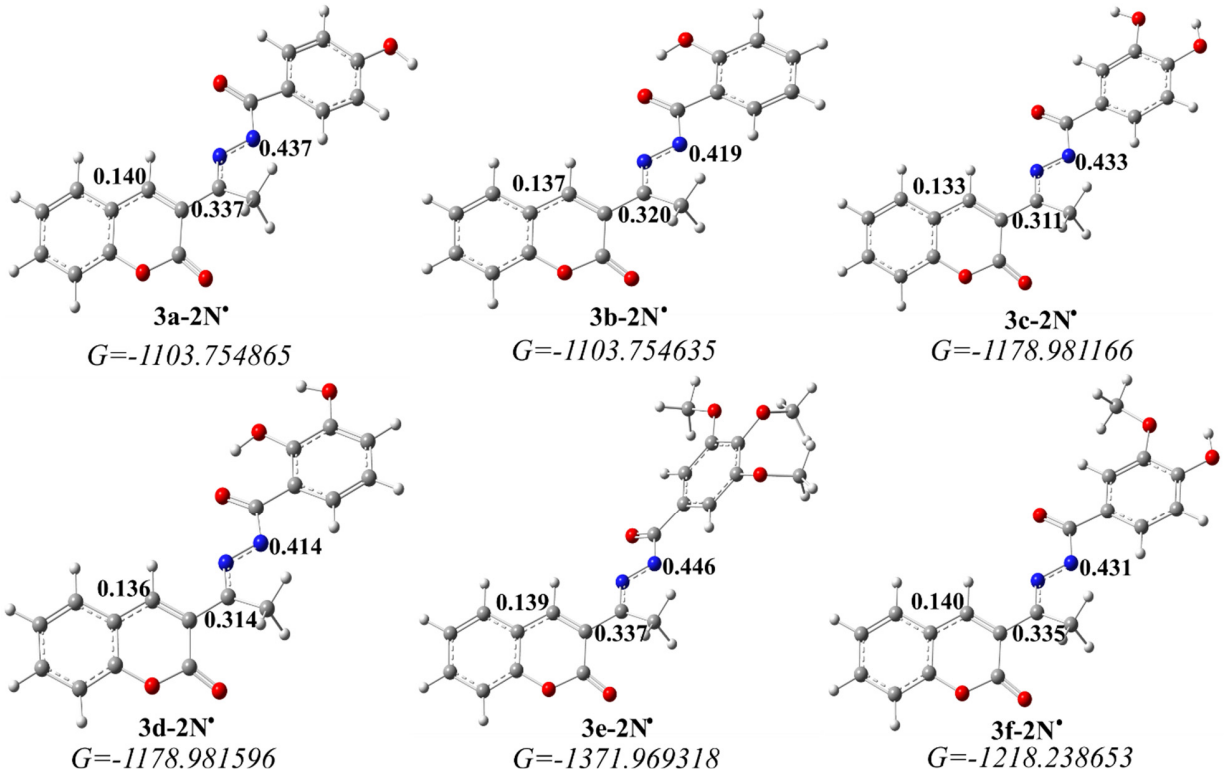


Figure S2. NBO spin distribution for formed N-centered radical species with the values of Gibbs free energy (a.u.)

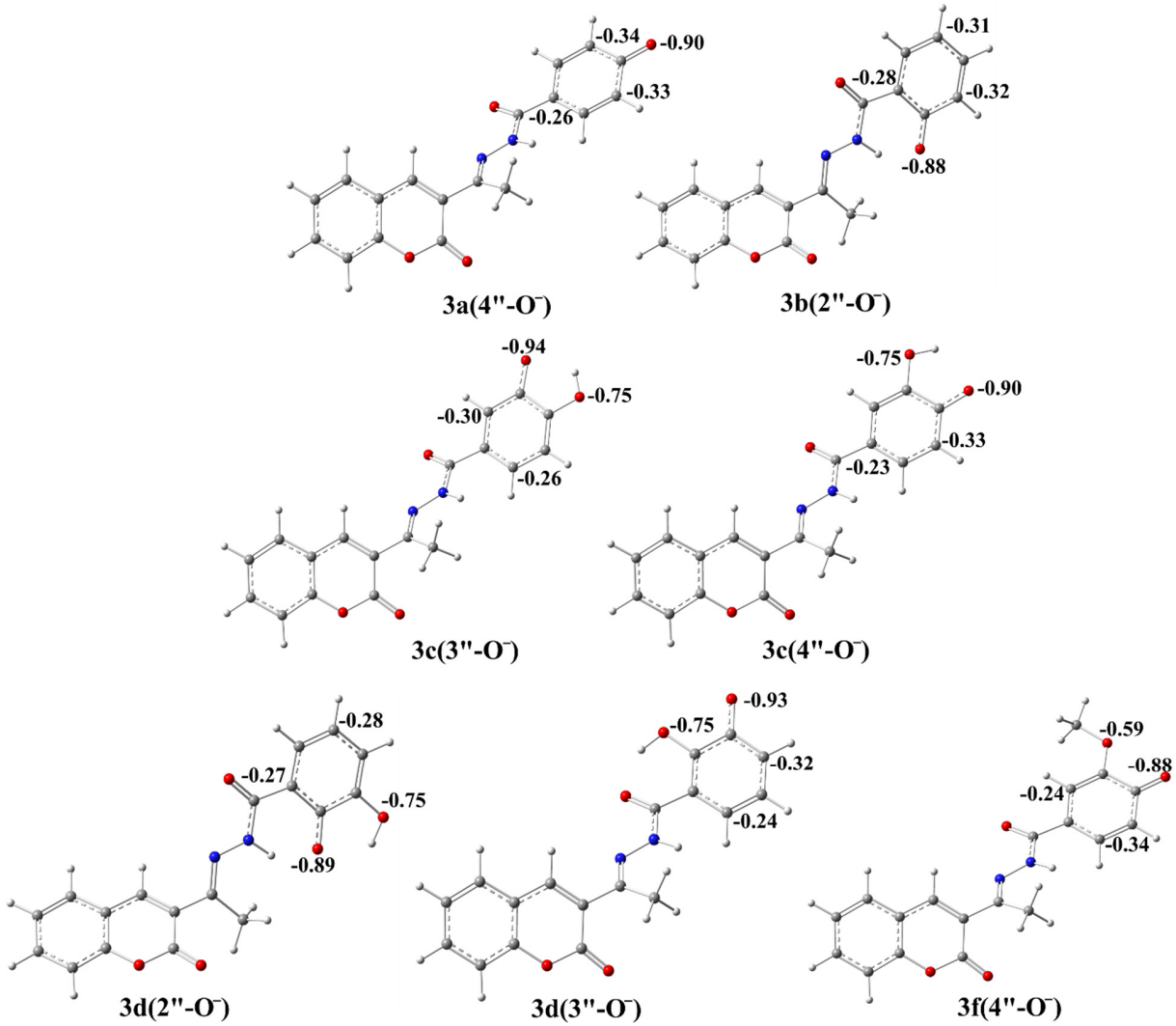


Figure S3. NBO charge distribution for formed O-centered anionic species

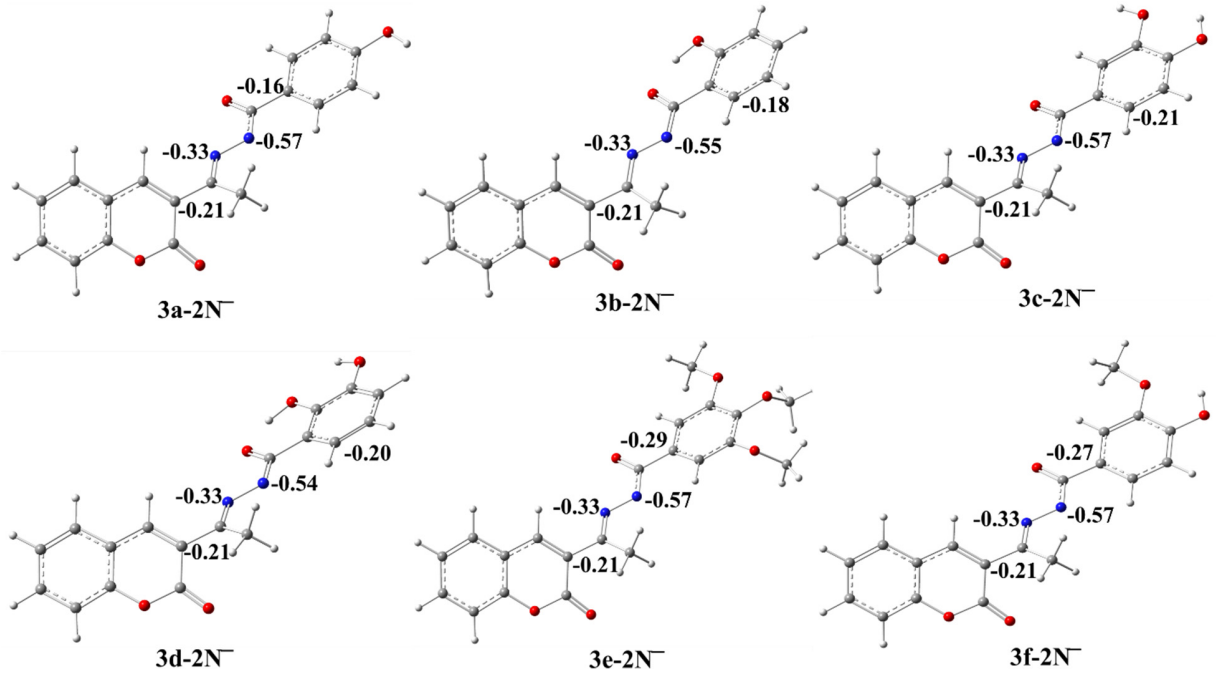


Figure S4. NBO charge distribution for formed N-centered anionic species

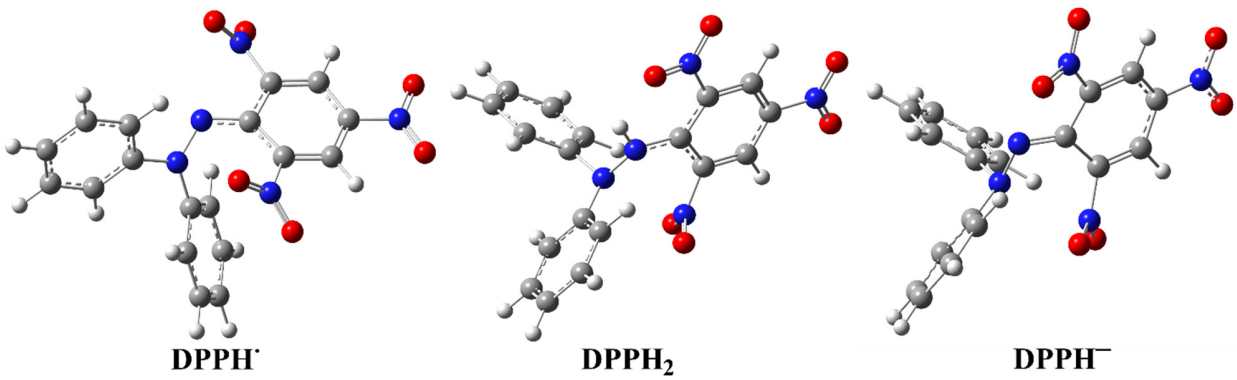


Figure S5. Optimized geometry of radical, neutral and anionic **DPPH** species at M06-2X/6-311++G(d,p) level of theory in methanol (SMD solvation model). Legend: gray-carbon atom, white-hydrogen atom, red-oxygen atom, blue-nitrogen atom.

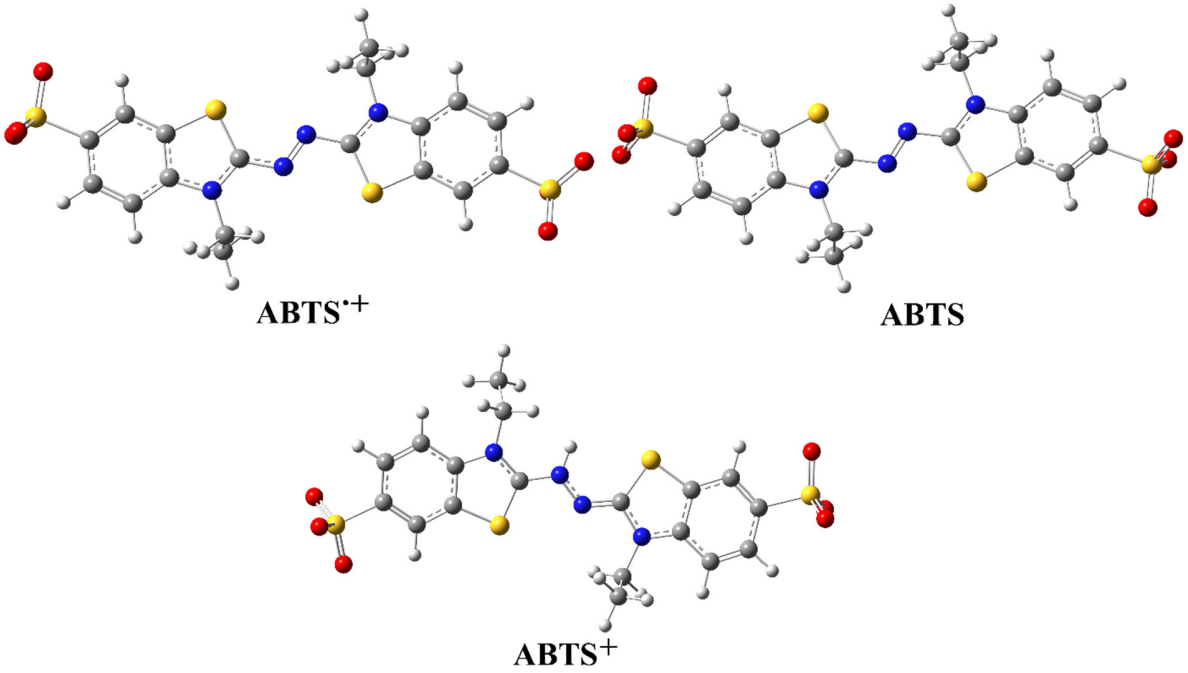


Figure S6. Optimized geometry of radical cation, neutral and cation **ABTS** species at M06-2X/6-311++G(d,p) level of theory in methanol (SMD solvation model). Legend: gray-carbon atom, white-hydrogen atom, red-oxygen atom, blue-nitrogen atom.

Table S1. DPPH scavenging activity of products **3c** and **3d**, as well as referent compounds at concentrations close to the IC_{50} value.

Compound	DPPH scavenging ability (%)					
	1 μM	1.5 μM	2 μM	2.5 μM	3 μM	5 μM
3c	16.1	39.3	42.6	64.3	72.1	-
3d	-	20.9	26.4	44.7	55.5	74.7
NDGA	40.2	42.2	56.3	59.9	79.52	-
Quercetin	30.7	45.1	53.9	60.9	77.6	-

Table S2. ABTS radical cation scavenging activity of products **3c, 3d**, and referent compound Trolox at concentrations close to the IC_{50} value.

Compound	ABTS radical cation scavenging activity (%)										
	1 μM	1.5 μM	2 μM	2.5 μM	3 μM	3.5 μM	4 μM	5 μM	6 μM	7 μM	8 μM
3c	29.5	39.4	46.4	55.1	65.5	68.8	-	-	-	-	-
3d	19.6	27.7	34.5	43.6	52.3	55.4	65.3	77.9	-	-	-
Trolox	-	-	-	-	-	-	38.8	48.8	55.3	64.8	71.9