

## **Supplementary data**

**For**

### **Free radical scavenging potency of dihydroxybenzoic acids**

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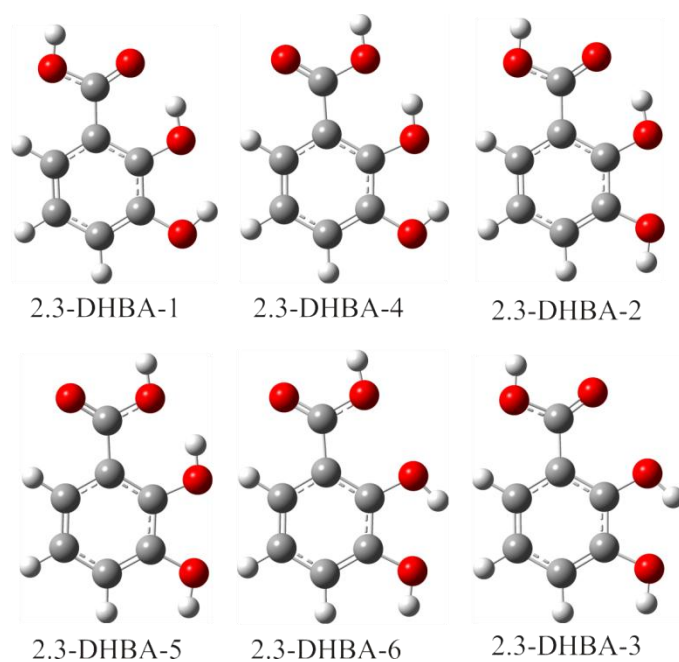
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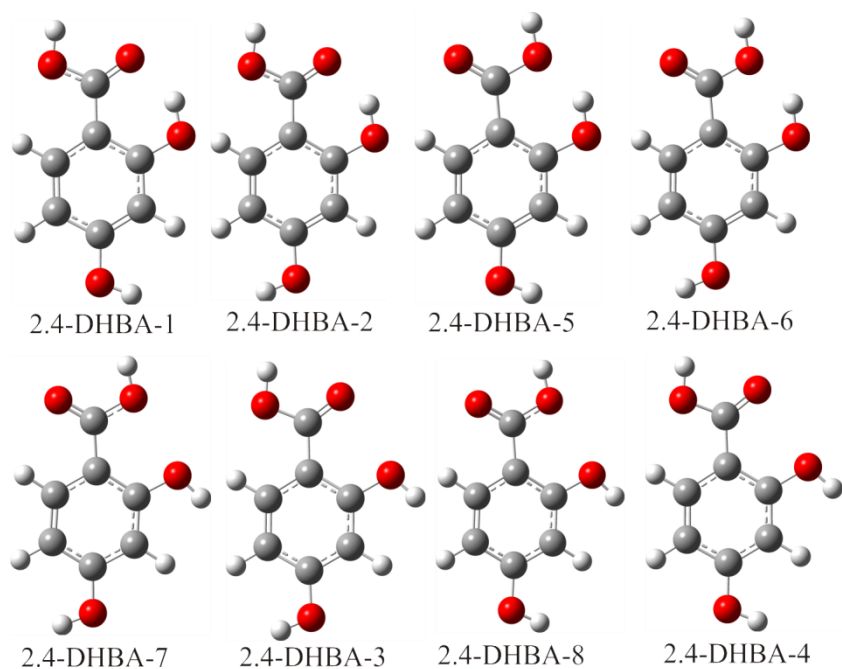
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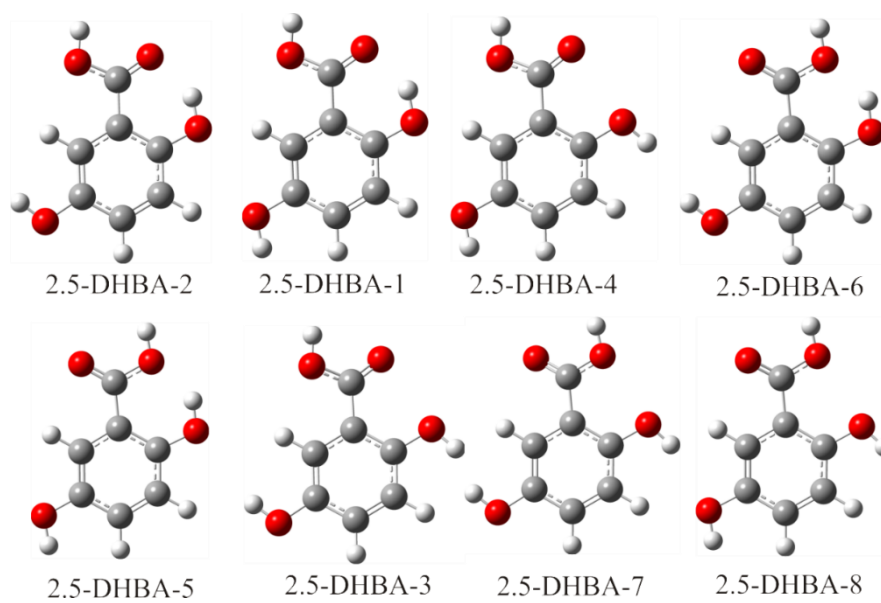
**FIGURES S1 - S6:** The structures of different rotamers of investigated DHBAs



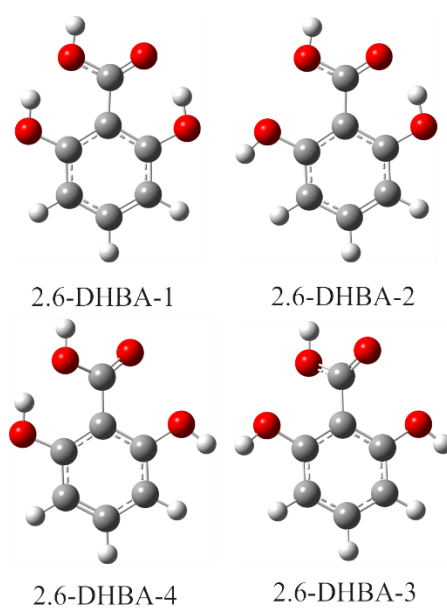
**Figure S1**



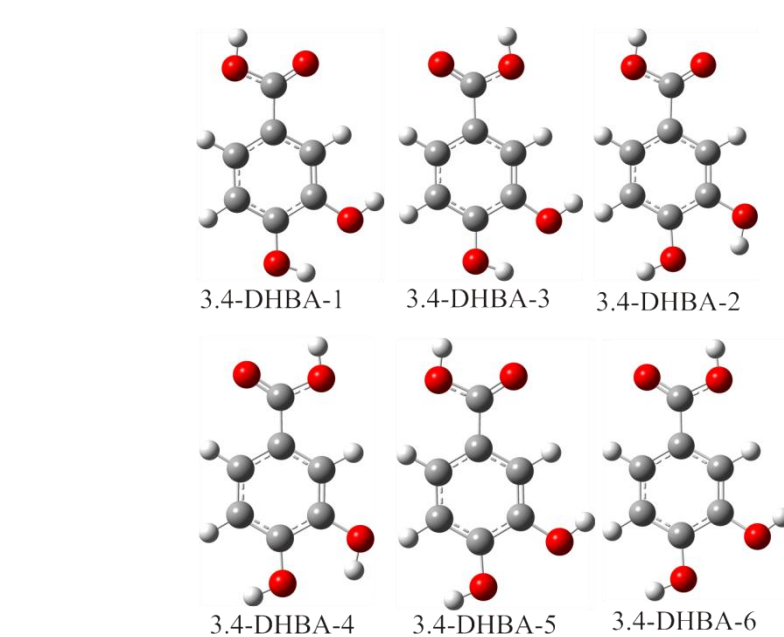
**Figure S2**



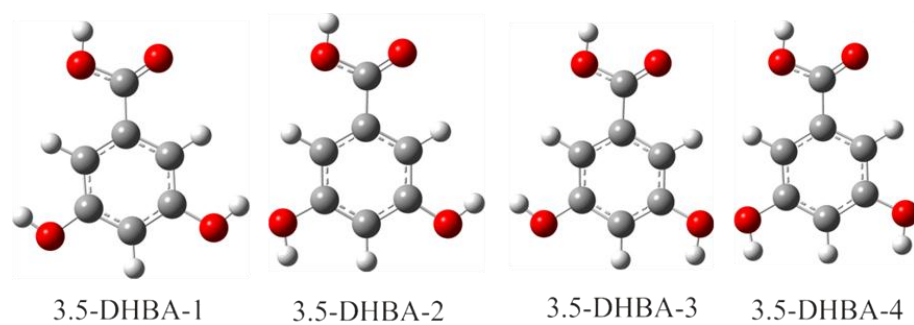
**Figure S3**



**Figure S4**



**Figure S5**



**Figure S6**

**TABLES S1 - S6 :** Relative energies kJ/mol ( $E$  = total energy,  $H$  = enthalpy, and  $G$  = free energy) for the examined DHBAs rotamers in different solvents. Calculations were performed at the M05-2X/6-311++G(d,p) level of theory. The abbreviations in tables  $PE$ ,  $W$  and  $B$  represents following solvents: penthylethanoate, water and benzene, respectively.

**Table S1**

<i>Rot</i>	$\Delta E^{SMD}$			$\Delta H^{SMD}$			$\Delta G^{SMD}$		
	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>
<i>2.3-DHBA</i>									
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	13.2	3.2	16.6	13.3	3.2	16.7	13.1	1.8	16.4
3	33.9	17.8	38.5	34.9	17.9	39.6	31.4	17.8	35.9
4	11.3	6.7	12.0	11.9	7.3	12.7	9.9	4.8	9.5
5	25.1	11.0	28.6	25.6	11.2	29.4	24.4	9.5	26.5
6	33.3	18.4	36.9	34.2	18.8	38.0	32.1	17.8	35.3

**Table S2**

<i>Rot</i>	$\Delta E^{SMD}$			$\Delta H^{SMD}$			$\Delta G^{SMD}$		
	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>
<i>2.4-DHBA</i>									
1	0.0	0.3	0.0	0.0	0.2	0.0	0.0	0.4	0.0
2	0.7	0.0	1.1	0.7	0.0	1.1	0.7	0.0	1.1
3	35.4	18.4	38.8	36.4	19.1	40.1	32.9	16.3	34.3
4	36.5	18.2	40.8	37.6	19.2	42.0	32.2	13.8	37.2
5	12.1	8.1	12.7	12.6	8.6	13.2	11.3	7.0	11.7
6	12.7	8.1	13.5	13.1	8.5	13.9	12.0	7.1	12.6
7	34.4	20.2	37.4	35.4	20.7	38.5	32.9	18.7	35.6
8	35.5	20.4	39.2	36.6	20.9	40.6	33.8	19.1	37.2

**Table S3**

<i>Rot</i>	$\Delta E^{SMD}$			$\Delta H^{SMD}$			$\Delta G^{SMD}$		
	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>
2.5-DHBA									
1	0.9	0.3	4.7	0.9	0.3	3.9	1.0	0.4	6.2
2	0.0	0.0	2.5	0.0	0.0	1.8	0.0	0.0	3.7
3	32.6	17.2	0.0	31.4	17.9	0.0	34.8	16.1	0.0
4	4.5	17.4	41.9	5.3	18.2	41.9	3.5	16.3	40.9
5	12.9	8.6	16.5	13.4	9.0	16.2	11.8	8.0	16.6
6	11.9	8.7	14.7	12.1	8.8	14.1	11.5	8.7	15.4
7	32.9	18.9	37.4	33.7	19.6	37.6	31.0	17.1	37.2
8	34.7	19.1	40.9	35.5	19.9	41.1	32.0	17.3	39.8

**Table S4:**

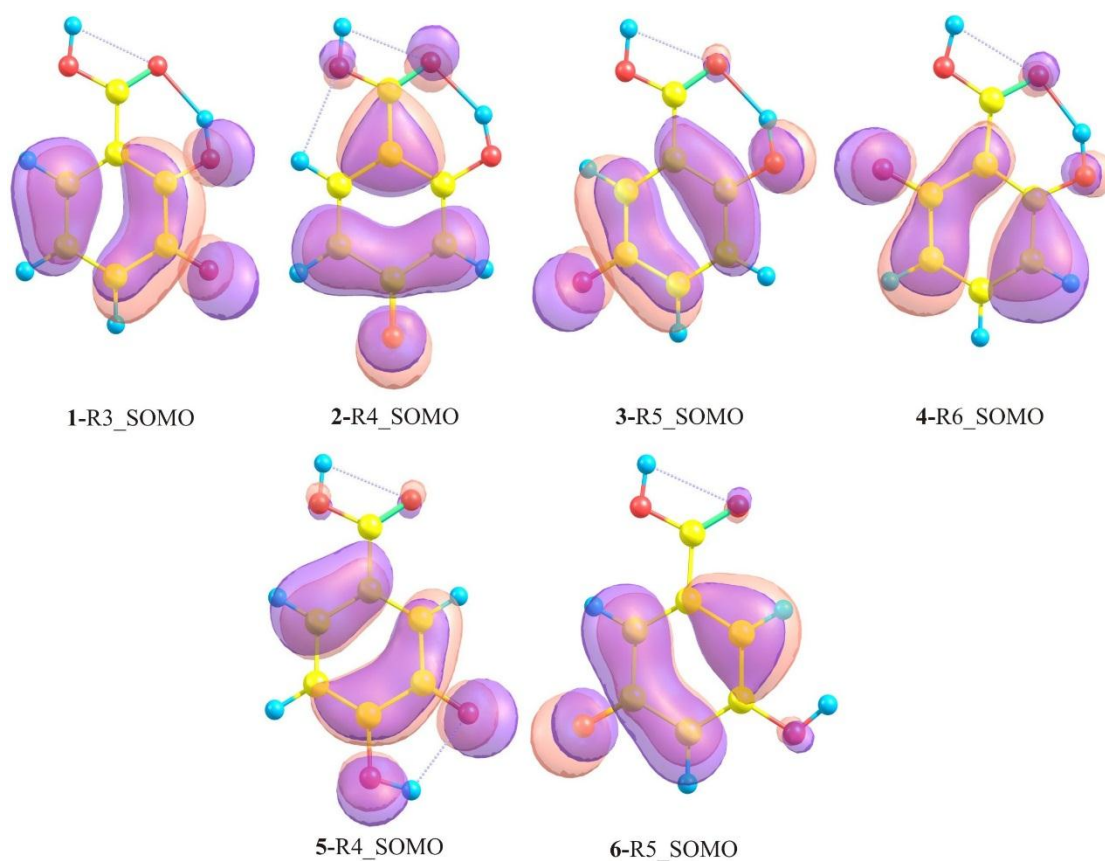
<i>Rot</i>	$\Delta E^{SMD}$			$\Delta H^{SMD}$			$\Delta G^{SMD}$		
	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>
2.6-DHBA									
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	16.9	9.7	18.7	17.0	9.6	18.9	16.7	9.9	18.4
3	39.2	23.3	45.7	42.1	24.4	48.9	34.1	22.5	39.4
4	32.1	19.2	35.5	32.8	19.3	36.1	30.0	19.3	34.1

**Table S5:**

<i>Rot</i>	$\Delta E^{SMD}$			$\Delta H^{SMD}$			$\Delta G^{SMD}$		
	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>
3.4-DHBA									
1	0.0	0.0	0.0	0.0	0.0	0.0	0.7	1.1	0.0
2	1.1	0.8	1.8	1.5	0.8	2.4	1.1	2.0	1.0
3	1.0	0.2	1.3	1.1	0.3	1.3	0.7	0.2	0.6
4	1.1	0.3	1.7	1.7	0.6	2.4	0.0	0.0	0.2
5	11.3	3.3	13.8	11.5	3.1	14.1	11.8	4.7	13.5
6	11.4	2.7	14.0	11.9	2.9	14.6	10.6	2.6	12.7

**Table S6**

<i>Rot</i>	$\Delta E^{\text{SMD}}$			$\Delta H^{\text{SMD}}$			$\Delta G^{\text{SMD}}$		
	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>	<i>PE</i>	<i>W</i>	<i>B</i>
<i>2,5-DHBA</i>									
1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.4	0.0
2	0.8	1.5	1.1	0.6	1.0	0.8	1.0	2.2	1.4
3	1.4	0.0	2.0	1.2	0.1	1.8	1.7	0.0	2.3
4	3.4	1.7	5.0	3.1	1.4	4.7	3.6	2.1	5.3



**FIGURE S7** SOMOs of the most stable radicals formed from the investigated DHBA in water.