SUPPORTING INFORMATION

DFT Study of the Antiradical Properties of Some Aromatic Compounds Derived from Antioxidant Essential Oils: C-H Bond vs O-H Bond

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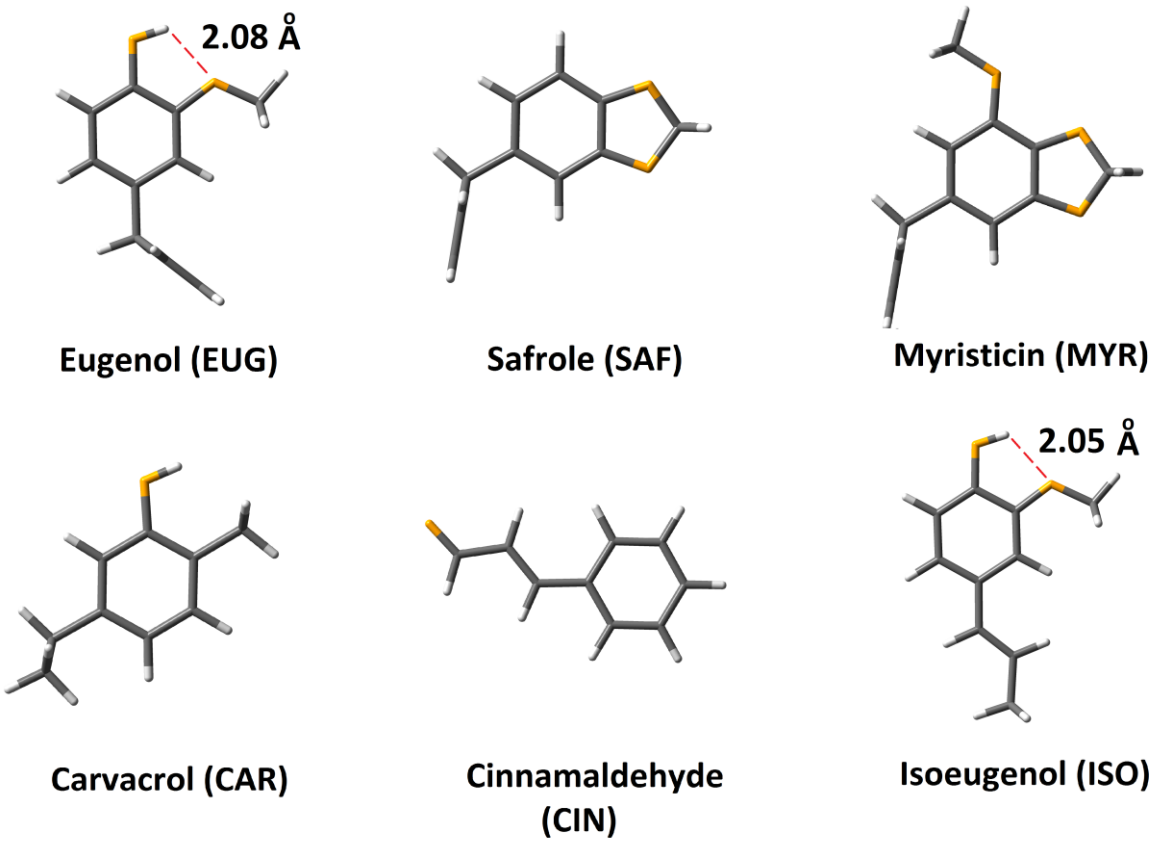

Fig. S1. Optimized molecular geometries with intramolecular hydrogen-bonds of **EUG**, **SAF**, **MYR**, **CAR**, **CIN** and **ISO** obtained at B3LYP/6-311G(d,p) level of theory.

Table S1. BDE values in kcal/mol of the potential hydrogens of **EUG**, **SAF**, **MYR**, **CAR**, **CIN** and **ISO** calculated at B3LYP/6-311G(d,p) level of theory.

Compound	BDE in kcal/mol		
	Gas	Water	Benzene
EUG (OH)	81.07	78.72	77.96
EUG (CH)	72.47	72.56	69.80
SAF (CH)	72.46	72.61	70.77
CIN (CH)	87.40	88.90	86.02
MYR (CH)	72.20	72.48	70.55
CAR (OH)	79.47	79.65	77.73
CAR (C1H)	86.66	87.38	85.22
CAR (C2H)	82.72	83.05	81.11
ISO (CH)	78.76	79.14	77.17
ISO (OH)	73.85	73.06	71.73

Table S2. Calculated Gibbs free energies (ΔG kcal/mol) of the reaction of **EUG**, **SAF**, **MYR**, **CAR**, **CIN** and **ISO** with HO• and HOO• at 298.15 K

Compound	Gibbs free energies kcal/mol (HOO•)			Gibbs free energies kcal/mol (HO•)		
	Gas	Water	Benzene	Gas-phase	Water	Benzene
EUG (OH)	-8.33	-4.42	-1.90	-41.05	-37.36	-34.53
EUG (CH)	-8.24	-9.30	-8.82	-40.97	-42.24	-41.45
SAF (CH)	-8.28	-9.56	-8.87	-41.00	-42.50	-41.50
CIN (CH)	8.70	5.97	6.92	-24.03	-26.97	-25.72
MYR (CH)	-8.56	-9.53	-9.02	-41.28	-42.46	-41.65
CAR (OH)	-2.13	-3.06	-2.72	-34.85	-35.99	-35.35
CAR (C1H)	5.24	5.16	5.17	-27.49	-27.78	-27.46
CAR (C2H)	0.25	-0.73	-0.13	-32.48	-33.66	-32.77
ISO (CH)	-1.57	-2.16	-1.83	-34.30	-35.09	-34.47
ISO (OH)	-6.90	-8.83	-7.83	-39.62	-41.77	-40.46