Structural and spectroscopic properties of Magnolol and Honokiol – Experimental and theoretical studies

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Supplementary material

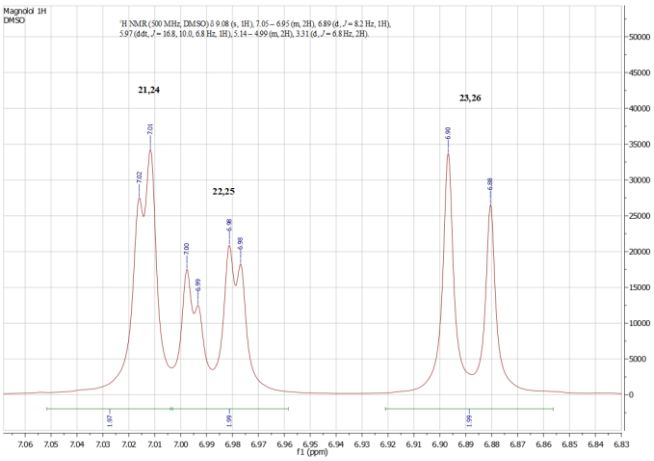


Figure S1. The ^{1}H spectrum of magnolol — aromatic region showing numeration and multiplets.

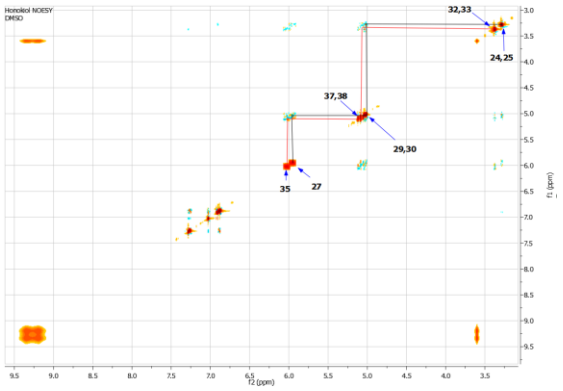
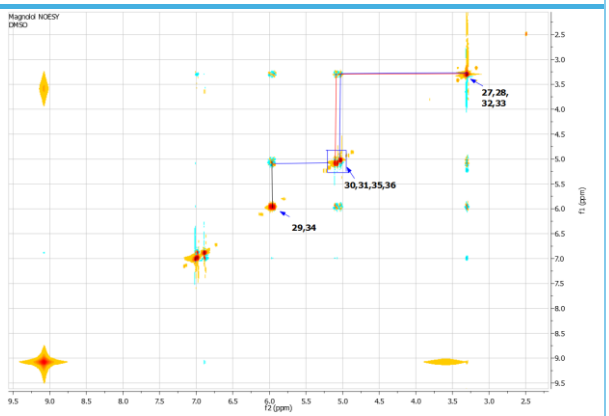
Honokiol – NOESY – allyl range	Magnolol - NOESY – allyl range
	

Figure S2. The NOESY spectra of magnolol and honokiol.

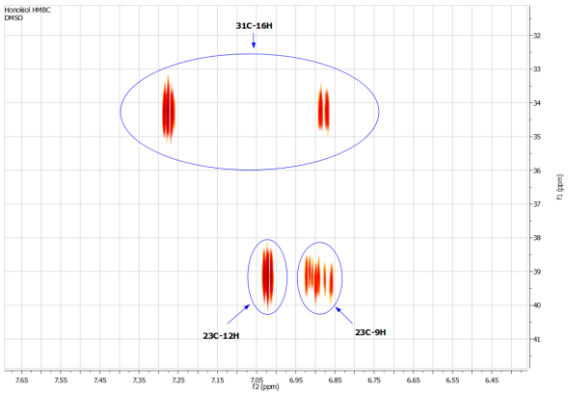


Figure S3. The HMBC spectrum of honokiol.

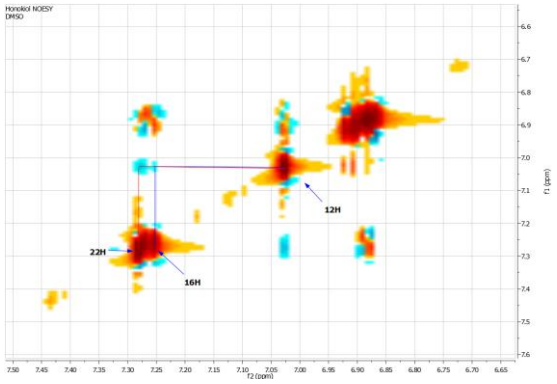


Figure S4. The NOESY spectrum of honokiol – aromatic region.

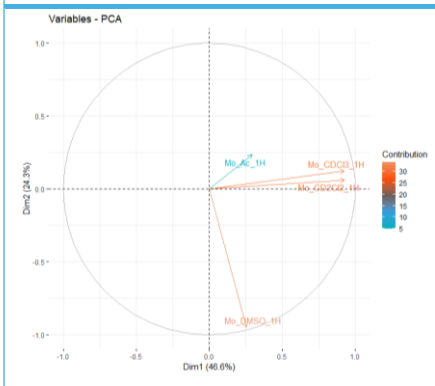
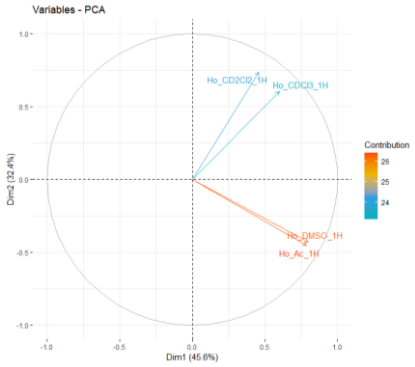
Magnolol – PCA - variables	**Honokiol – PCA - variables**
	
w~~W~~here~~:~~ Mo – Magnolol, Ho – Honokiol, Ac – acetone-d6, $CDCl_3$ – chloroform, CD_2Cl_2 – dichloromethane, DMSO – dimethylsulfoxide-d6	

Figure S5. The plot of the PCA variables computed for magnolol and honokiol.

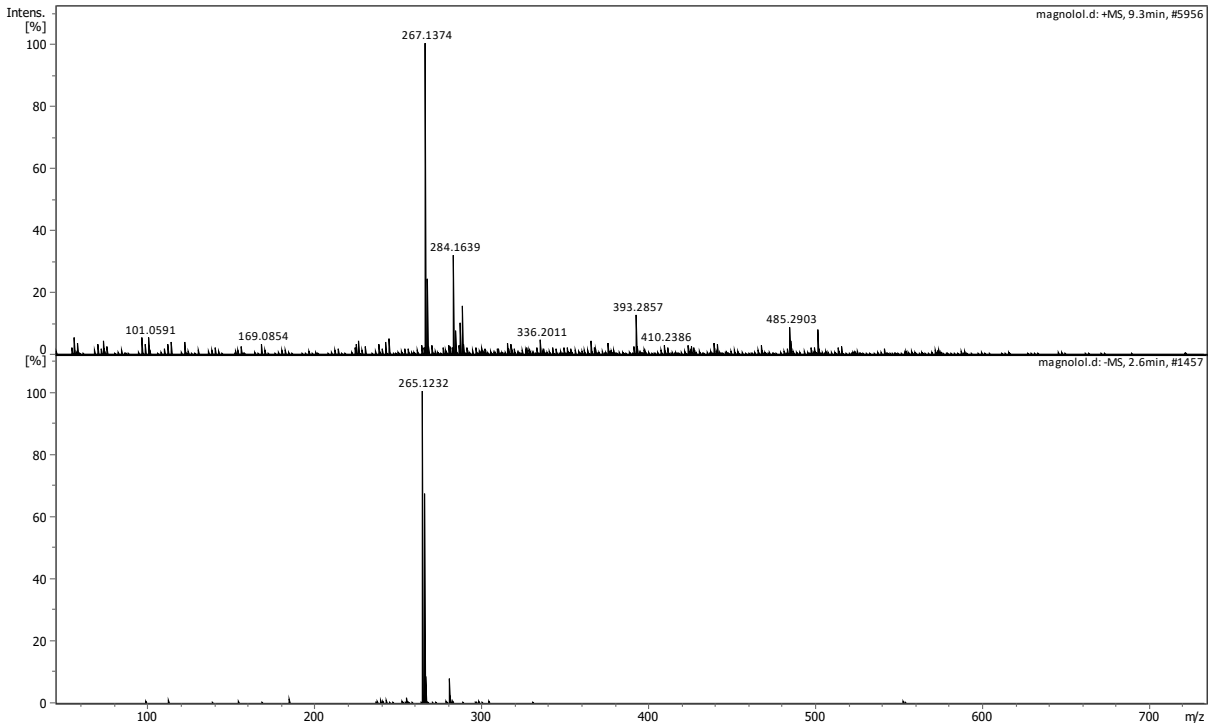


Figure S6. MS ESI spectra for magnolol.

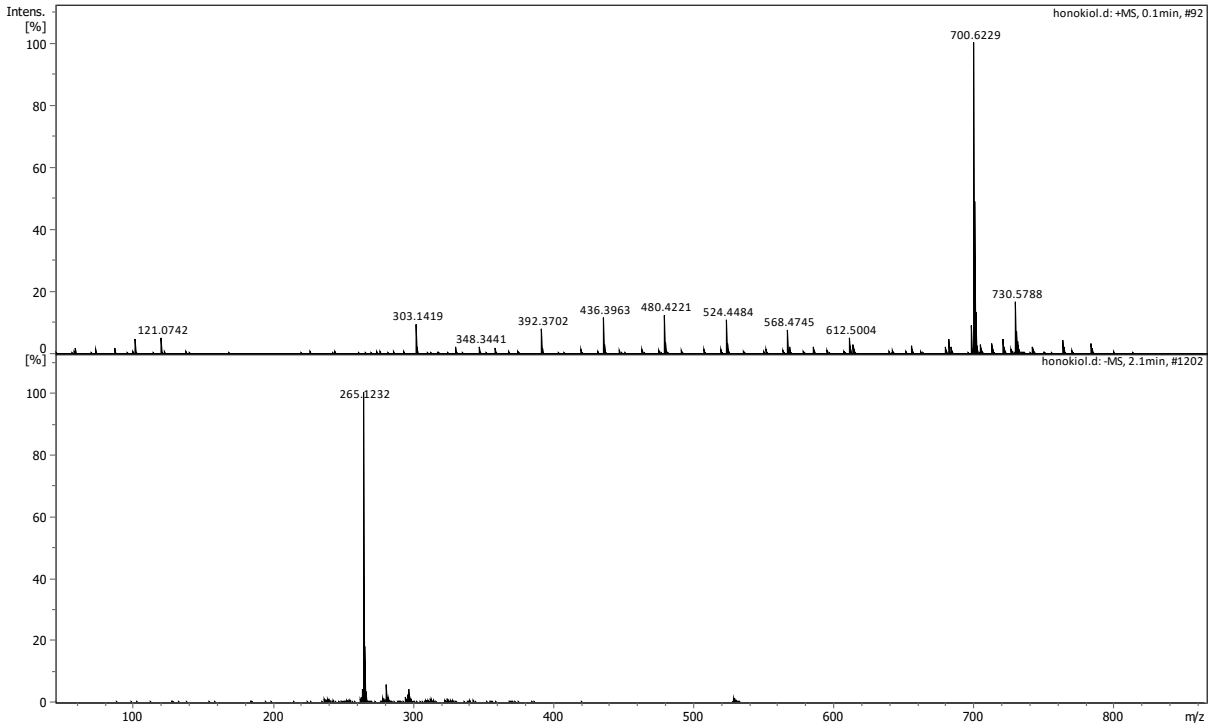


Figure S7. MS ESI spectra for honokiol.

Table S1. The atomic charges [e] for oxygen atoms within the structure of magnolol and honokiol (geometries optimized at the B3LYP/6-311+G(d,p) level of theory in gaseous phase, the Mulliken, CHelpG and NBO charges computations at the B3LYP/6-311++G(2d,3p) level of theory) estimated according to the Mulliken, CHelpG or NBO methodology (atoms numbering as in the Fig. 1).

Heteroatom	***Magnolol***		
	Calculated charges		
	Mulliken	**CHelpG**	**NBO**
O5	-0.242	-0.599	-0.707
O6	-0.128	-0.592	-0.709
Heteroatom	***Honokiol***		
	Calculated charges		
	Mulliken	**CHelpG**	**NBO**
O1	-0.560	-0.552	-0.681
O3	-0.624	-0.528	-0.696

Table S2. First excited states of the magnolol **1** computed using LR TD DFT approach in vacuum or in methanol; B3LYP/6-311++G(2d,3p)//B3LYP/6-311++G(d,p) level of theory.

Compound 1				
Environment	**Energy [eV]**	**Wavelength [nm]**	**Oscillator strength**	**Ground state–first excited state orbital transition**
Methanol	4.3844	282.79	0.2052	71 → 72

Table S3. First excited states of the honokiol **2** computed using LR TD DFT approach in vacuum or in methanol; wB97XD/6-311++G(2d,3p)//wB97XD/6-31G(d,p) level of theory.

Compound 2				
Environment	**Energy [eV]**	**Wavelength [nm]**	**Oscillator strength**	**Ground state–first excited state orbital transition**
Methanol	4.7471	261.18	0.3402	71 → 72

Table S4. Comparison of theoretical and experimental ^{1}H NMR shifts (atom~~s~~ numbering as in ~~the~~ Fig. 1) for magnolol and honokiol.

Magnolol.

Hydrogen	**Theoretical (ppm)**	**Experimental (ppm)**	**Error (ppm)**	**Relative Error**
21H	7.22	7.01	-0.21	-0.03
22H	7.16	6.99	-0.17	-0.02
23H	6.84	6.89	0.05	0.01
24H	7.31	7.01	-0.30	-0.04
25H	7.14	6.99	-0.15	-0.02
26H	6.75	6.89	0.14	0.02
27H	3.39	3.31	-0.08	-0.02
28H	3.11	3.31	0.20	0.06
29H	6.06	5.97	-0.09	-0.02
30H	5.03	5.07	0.04	0.01
31H	5.35	5.07	-0.28	-0.05
32H	3.15	3.31	0.16	0.05
33H	3.38	3.31	-0.07	-0.02

34H	6.17	5.97	-0.20	-0.03
35H	5.20	5.07	-0.13	-0.03
36H	5.41	5.07	-0.34	-0.06
37H	7.11	9.08	1.97	0.28
38H	4.80	9.08	4.28	0.89

Honokiol.

Hydrogen	Theoretical (ppm)	Experimental (ppm)	Error (ppm)	Relative Error
2H	4.23	9.19	4.96	1.17
4H	6.00	9.33	3.33	0.56
7H	6.65	6.87	0.21	0.03
9H	7.03	6.91	-0.13	-0.02
12H	7.10	7.02	-0.08	-0.01
16H	7.09	7.28	0.19	0.03
20H	6.75	6.88	0.13	0.02
22H	7.76	7.25	-0.51	-0.07
24H	3.20	3.28	0.08	0.03
25H	3.17	3.28	0.11	0.03
27H	6.35	5.95	-0.41	-0.06
29H	4.52	5.01	0.49	0.11
30H	5.17	5.01	-0.16	-0.03
32H	3.63	3.37	-0.26	-0.07
33H	3.29	3.37	0.08	0.02
35H	6.39	6.03	-0.36	-0.06
37H	5.76	5.08	-0.67	-0.12
38H	5.45	5.08	-0.37	-0.07