

## Electronic Supplementary Information

### Critical evaluation of spectral information of benchtop vs. portable near-infrared spectrometers: Quantum chemistry and two-dimensional correlation spectroscopy for a better understanding of PLS regression models of the rosmarinic acid content in *Rosmarini folium*

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Table S-1: NIR spectra recording parameters

spectrometer	NIRFlex N-500	microPHAZIR	MicroNIR 2200
wavenumber range / $\text{cm}^{-1}$	10000 - 4000	6266 - 4173	8864 - 4626
recording-resolution / $\text{cm}^{-1}$	8	21	33
spectra per sample	3	6	6
scans per spectrum	64	10	200 x 6500 $\mu\text{s}$
data points per spectrum	1501	100	128

Table S-2: Instrument specification NIRFlex N-500

<b>Spectrometer</b>	<b>NIRFlex N-500 FT-NIR spectrometer</b>
<b>Spectral range</b>	12500 - 4000 $\text{cm}^{-1}$ (standard 10000 - 4000 $\text{cm}^{-1}$ ) 800 - 2500 nm (standard 1000 - 2500 nm)
<b>Resolution</b>	8 $\text{cm}^{-1}$ (with boxcar apodization)
<b>Radiation source</b>	Tungsten halogen lamp
<b>Monochromator</b>	FT-NIR-Polarization interferometer with $\text{TeO}_2$ wedges
<b>Detector</b>	Extended range InGaAs (temperature controlled)
<b>Accessory</b>	NIRFlex Solids Cell with rotating Add-on XL
<b>Measuring mode</b>	Diffuse reflection
<b>Dimension</b>	350 x 250 x 450 mm (W x D x H) (Base Unit)
<b>Operating temperature</b>	5 to 35 °C

Table S-3: Instrument specification microPHAZIR

<b>Spectrometer</b>	<b>ThermoScientific microPHAZIR</b>
<b>Spectral range</b>	6266 - 4173 cm <sup>-1</sup> ; 1596 - 2396 nm
<b>Resolution (averaged)</b>	21 cm <sup>-1</sup> ; 8 nm
<b>Radiation source</b>	Tungsten halogen lamp
<b>Monochromator</b>	MEMS-technology
<b>Detector</b>	InGaAs
<b>Measuring mode</b>	Diffuse reflection
<b>Weight</b>	1,8 kg
<b>Dimensions</b>	25,4 cm × 29,2 cm × 15,2 cm
<b>Power requirement</b>	Lithium Ion rechargeable battery
<b>Operating temperature</b>	5°C to 40°C

Table S-4: Instrument specification MicroNIR 2200

<b>Spectrometer</b>	<b>MicroNIR 2200 spectrometer</b>
<b>Spectral range</b>	8864 - 4626 cm <sup>-1</sup> ; 1128 - 2162 nm
<b>Geometric resolution</b>	33 cm <sup>-1</sup> (averaged); 8 nm
<b>Optical resolution</b>	<1.25% of center wavelength
<b>Radiation source</b>	Two integrated vacuum tungsten lamps
<b>Monochromator</b>	Linear Variable Filter (LVF)
<b>Detector</b>	128 pixel InGaAs photodiode array
<b>Measuring mode</b>	Diffuse reflection
<b>Weight</b>	60 g
<b>Dimensions</b>	45 mm diameter x 42 mm height
<b>Power requirement</b>	USB, <500mA at 5V
<b>Operating temperature</b>	-20°C to 40°C
<b>additional temperature controller</b>	thermoelectric cooling (TEC) appliance

Table S-5: DFT-B3LYP/N07D optimized structural parameters of RA molecule in Cartesian coordinates

	x / Å	y / Å	z / Å
C	9.136913964	1.993409388	2.319143744
C	10.49089596	1.670381388	2.426721744
C	10.86730596	0.386307388	2.809316744
C	9.885627964	-0.586724612	3.087929744
C	8.541710964	-0.258884612	2.979539744
C	8.141796964	1.037712388	2.593130744
H	8.848483964	2.997690388	2.020778744
H	11.25364196	2.417050388	2.213311744
H	7.813042964	-1.031969612	3.202817744
C	4.301342964	1.248451388	2.509665744
O	4.032789964	2.383325388	2.167985744
O	3.373747293	0.419562917	2.627054298
C	1.125591964	-0.519891612	2.810280744
H	1.506988964	-1.252443612	2.089868744
H	1.320827964	-0.918467612	3.811577744
C	-0.358585036	-0.305826612	2.601732744
C	-1.218479036	-0.167991612	3.700787744
C	-0.897227036	-0.231975612	1.310465744
H	-0.251502036	-0.345736612	0.442884744
C	-2.583695036	0.047075388	3.519635744
C	-2.265566036	-0.016241612	1.119642744
H	-2.677889036	0.037585388	0.113321744
C	-3.107363036	0.124985388	2.219101744
H	-0.839008036	-0.226232612	4.718048744
O	-3.395102036	0.176224388	4.607601744
H	-4.301741036	0.313967388	4.299478744
O	-4.465777036	0.335776388	2.139311744
H	-4.744111036	0.381497388	1.217730744
C	1.652042964	1.805356388	3.693142744
O	2.053499964	1.786484388	4.831138744
O	0.802487964	2.734155388	3.213704744
H	0.596430964	3.336961388	3.946933744
O	10.24514996	-1.845608612	3.462237744
H	11.21071096	-1.898075612	3.489665744
O	12.16506796	-0.035091612	2.945037744
H	12.77712996	0.682649388	2.744883744
C	1.982645964	0.749654388	2.633327744
H	1.839938964	1.192748388	1.643356744
C	6.740675964	1.431645388	2.465712744
H	6.564348964	2.461688388	2.155684744
C	5.645650964	0.676273388	2.687565744
H	5.692832964	-0.360654612	3.005558744

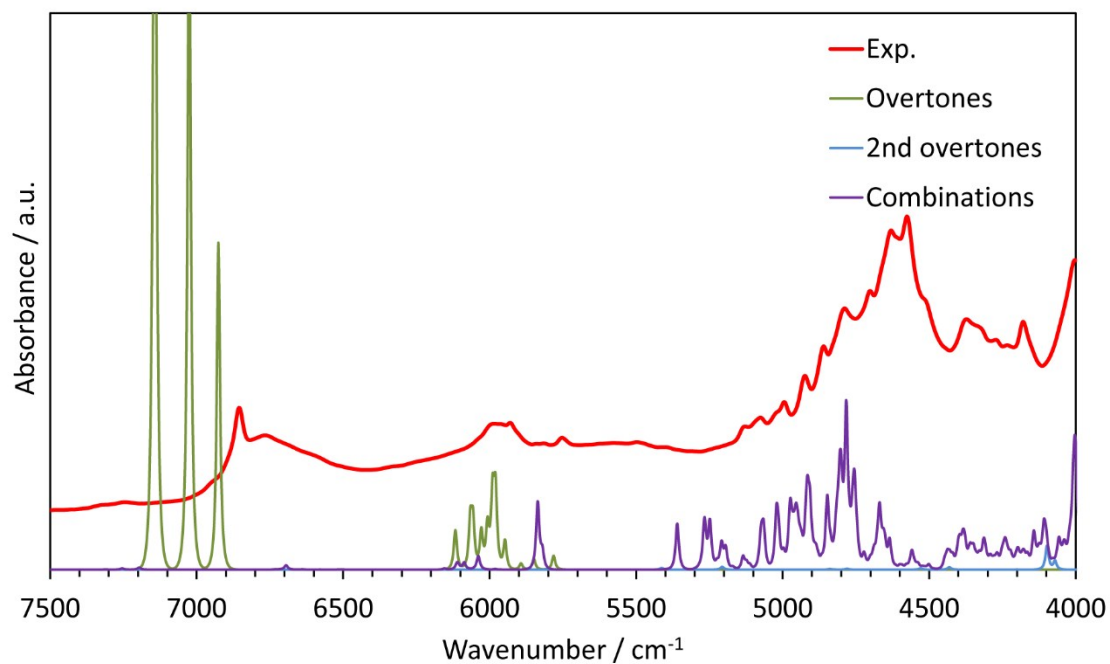


Fig. S-1: Contributions of first overtones, second overtones (estimated) and binary combination modes into NIR spectrum of RA. Plot based on unscaled DFT-B3LYP/N07D results. A lower FWHH parameter of modeled bands was applied here for better view of details.

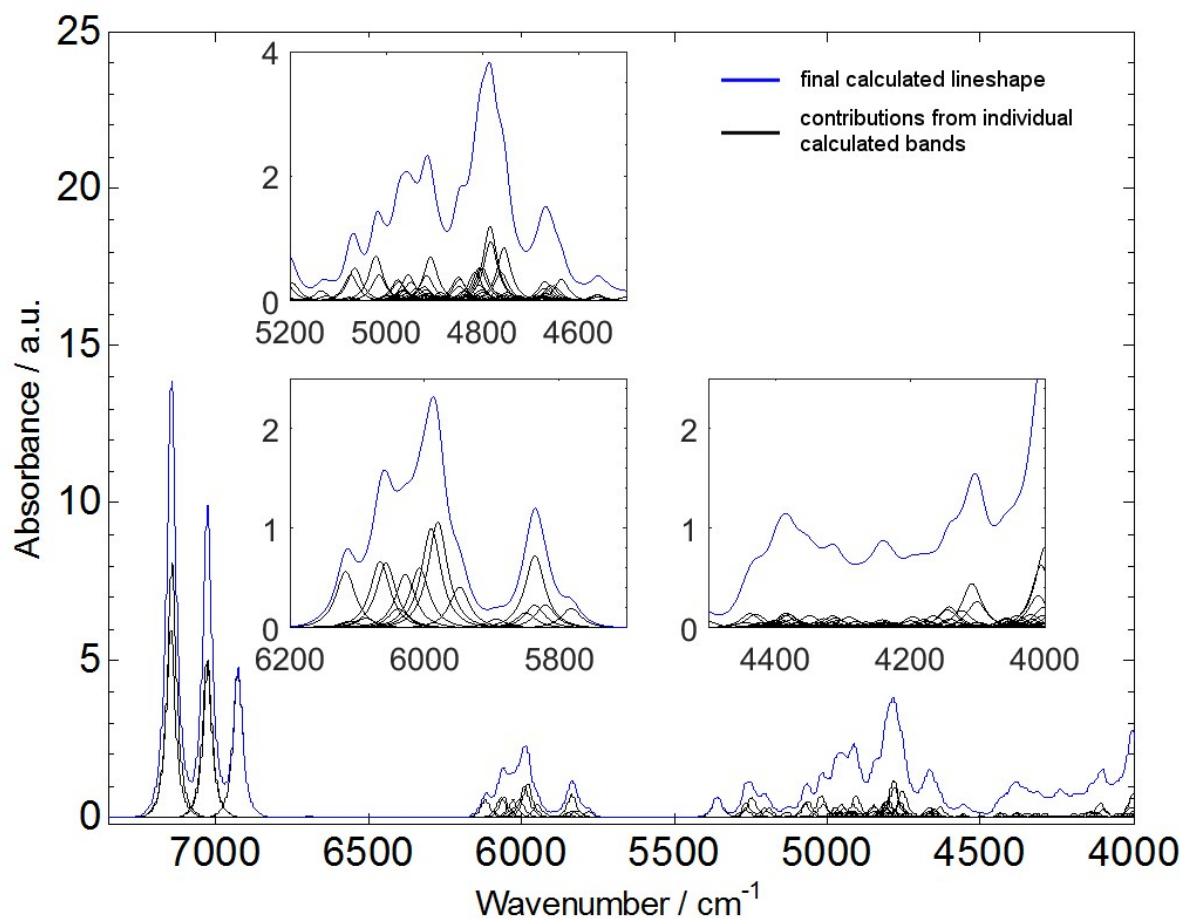


Fig. S-2: The contributions into the theoretical (DFT-B3LYP/N07D) NIR spectrum of rosmarinic acid stemming from each calculated band and the final theoretical spectrum. Raw unscaled theoretical data is presented here.