



## Supporting Information

for

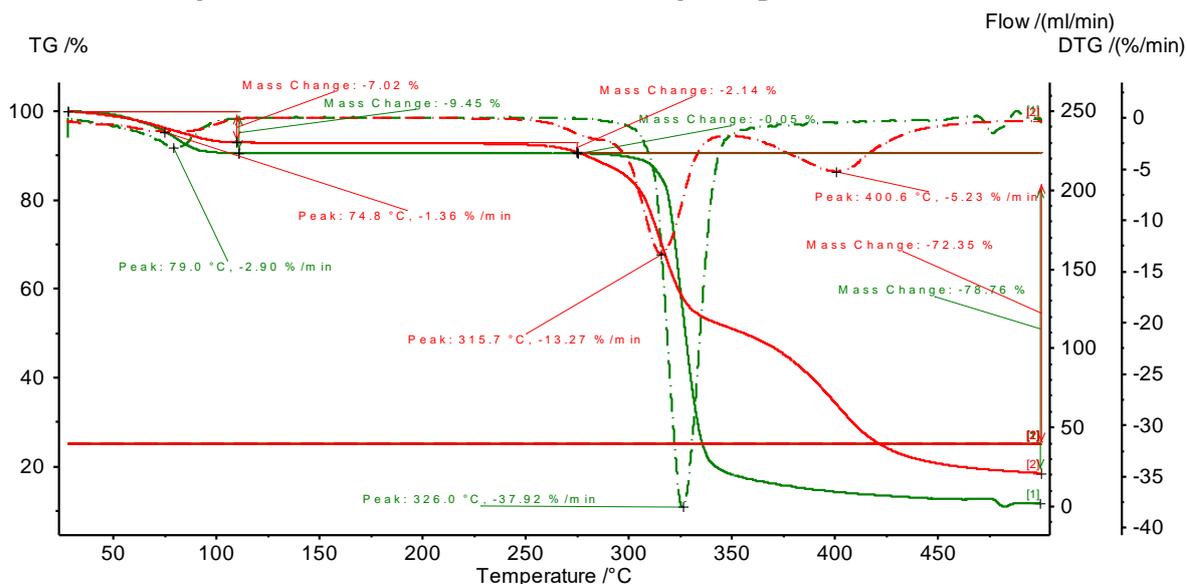
### **Discrimination of $\beta$ -cyclodextrin/hazelnut (*Corylus avellana* L.) oil/flavonoid glycoside and flavonolignan ternary complexes by Fourier-transform infrared spectroscopy coupled with principal component analysis**

Nicoleta G. Hădărugă, Gabriela Popescu, Dina Gligor (Pane), Cristina L. Mitroi, Sorin M. Stanciu and Daniel Ioan Hădărugă

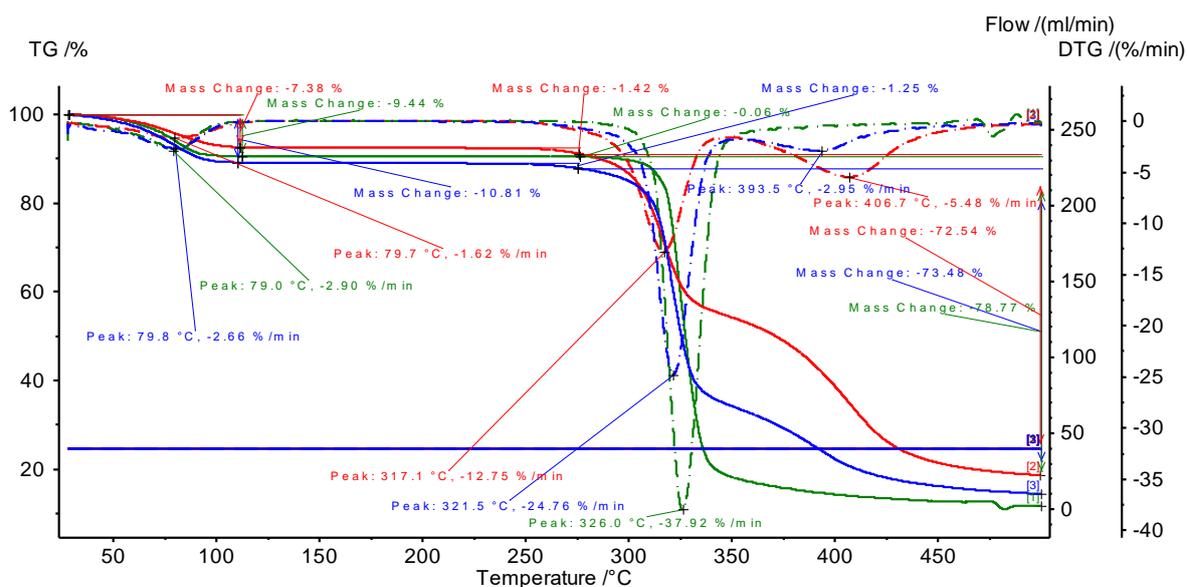
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### **Thermal analysis, FTIR and FTIR–PCA data for ternary complexes**

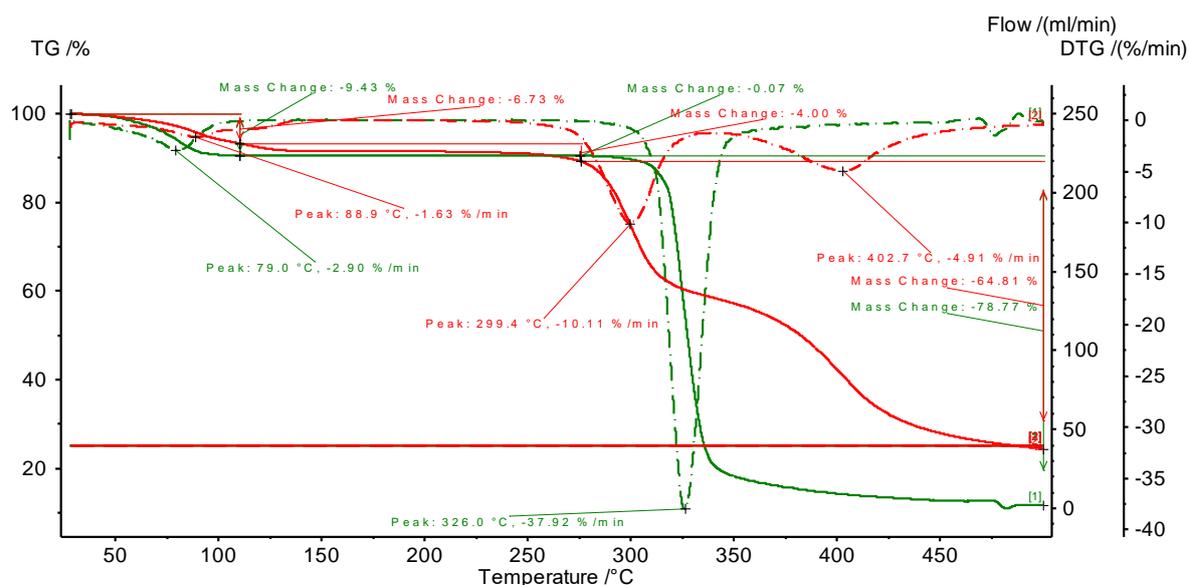
## 1. Thermal analyses (TG–DTG and DSC) of ternary complexes



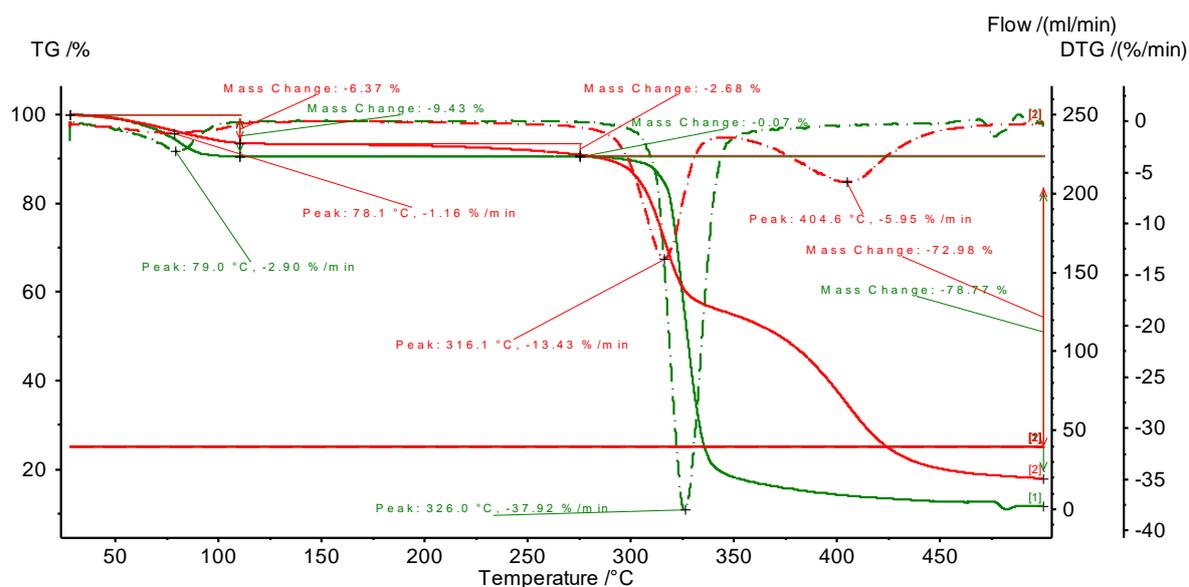
**Figure S1:** Superimposed TG–DTG thermograms for  $\beta$ -cyclodextrin/hazelnut oil/hesperidin ternary complex at a 1:1:1 molar ratio (code X1H, red) and  $\beta$ -cyclodextrin hydrate (green).



**Figure S2:** Superimposed TG–DTG thermograms for  $\beta$ -cyclodextrin/hazelnut oil/naringin ternary complex at 1:1:1 (code X1N, red) and 3:1:1 molar ratios (code X3N, blue), in comparison with the  $\beta$ -cyclodextrin hydrate (green).



**Figure S3:** Superimposed TG–DTG thermograms for  $\beta$ -cyclodextrin/hazelnut oil/rutin ternary complex at a 1:1:1 molar ratio (code X1R, red) and  $\beta$ -cyclodextrin hydrate (green).



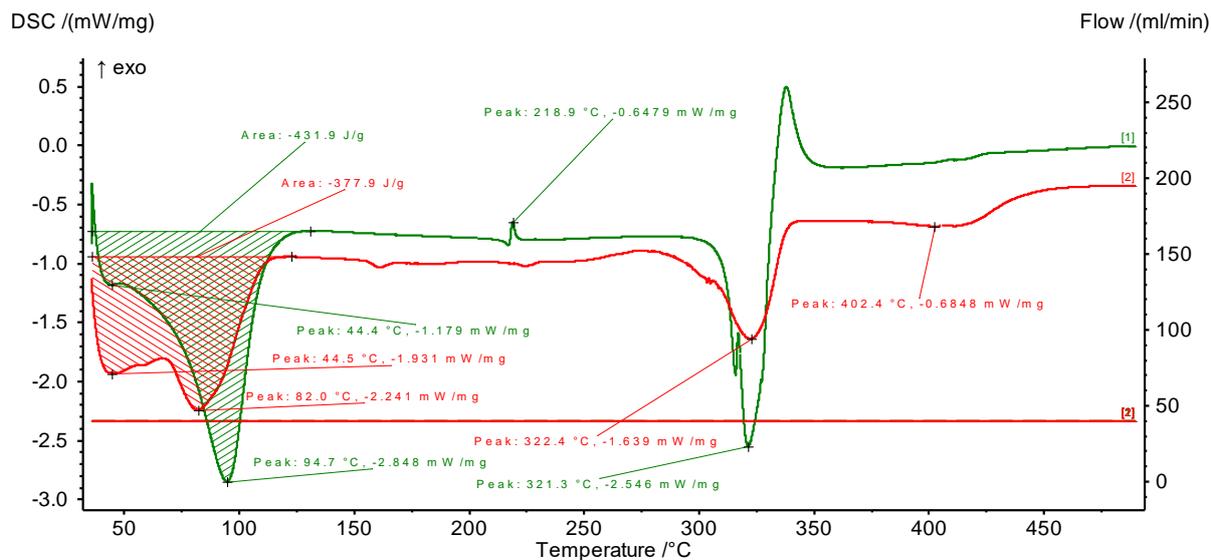
**Figure S4:** Superimposed TG–DTG thermograms for  $\beta$ -cyclodextrin/hazelnut oil/silymarin ternary complex at a 1:1:1 molar ratio (code X1S, red) and  $\beta$ -cyclodextrin hydrate (green).

**Table S1:** TG results (mass loss, %, for specific temperature ranges) for  $\beta$ -cyclodextrin hydrate ( $\beta$ -CD) and the  $\beta$ -cyclodextrin/hazelnut oil/flavonoid glycoside or flavonolignan ternary complexes at 1:1:1 or 3:1:1 molar ratios (codes X1H, X1N, X3N, X1R and X1S).

No	Code	Mass loss <sub>(&lt;110 °C)</sub> (%)	Mass loss <sub>(110–275 °C)</sub> (%)	Mass loss <sub>(&gt;275 °C)</sub> (%)
1	$\beta$ -CD	9.45	0.05	78.76
2	X1H	7.02	2.14	72.35
3	X1N	7.38	1.42	72.54
4	X3N	10.81	1.25	73.48
5	X1R	6.73	4.00	64.81
6	X1S	6.37	2.68	72.98

**Table S2:** DTG results (peak temperatures for the maximum mass loss rate, °C, for specific temperature ranges) for  $\beta$ -cyclodextrin hydrate ( $\beta$ -CD) and the  $\beta$ -cyclodextrin/hazelnut oil/flavonoid glycoside or flavonolignan ternary complexes at 1:1:1 or 3:1:1 molar ratios (codes X1H, X1N, X3N, X1R and X1S).

No	Code	$T_{DTG1(<110\text{ }^{\circ}\text{C})}$ (°C)	$T_{DTG2(275\text{--}350\text{ }^{\circ}\text{C})}$ (°C)	$T_{DTG3(>350\text{ }^{\circ}\text{C})}$ (°C)
1	$\beta$ -CD	79.0	326.0	-
2	X1H	74.8	315.7	400.6
3	X1N	79.7	317.1	406.7
4	X3N	79.8	321.5	393.5
5	X1R	88.9	299.4	402.7
6	X1S	78.1	316.1	404.6

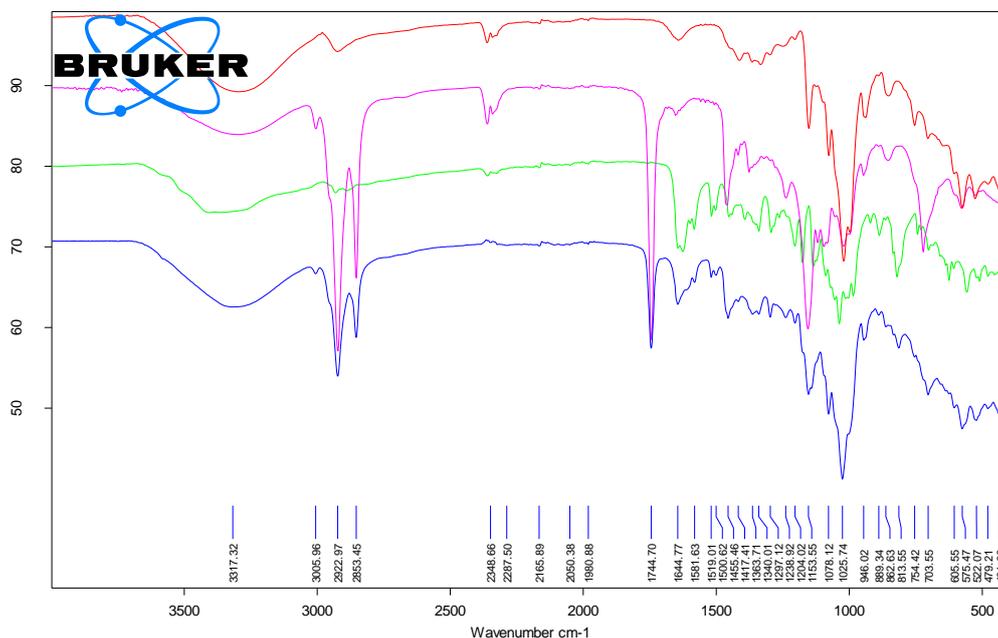


**Figure S5:** Superimposed DSC plots for the  $\beta$ -cyclodextrin/hazelnut oil/naringin ternary complex at 1:1:1 molar ratio (code X1N, red) and  $\beta$ -cyclodextrin hydrate (green).

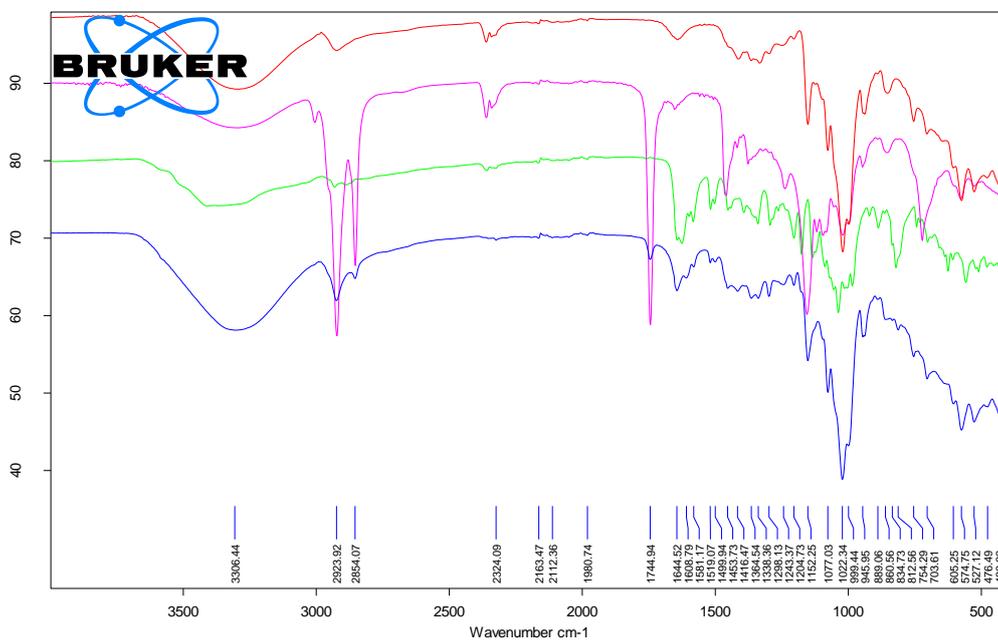
**Table S3:** DSC results (peak area, J/g, and peak temperatures for the maximum rate of the calorimetric effect, °C, for specific temperature ranges) for  $\beta$ -cyclodextrin hydrate ( $\beta$ -CD) and the  $\beta$ -cyclodextrin/hazelnut oil/naringin ternary complex at a 1:1:1 molar ratio (code X1N).

No	Code	$\text{Area}_{DSC(<110\text{ }^{\circ}\text{C})}$ J/g	$T_{DSC1(<110\text{ }^{\circ}\text{C})}$ (°C)	$T_{DSC2(<110\text{ }^{\circ}\text{C})}$ (°C)	$T_{DSC3(140\text{--}275\text{ }^{\circ}\text{C})}$ (°C)	$T_{DSC4(275\text{--}350\text{ }^{\circ}\text{C})}$ (°C)	$T_{DSC5(>350\text{ }^{\circ}\text{C})}$ (°C)
1	$\beta$ -CD	431.9	44.4	94.7	218.9	321.3	-
2	X1N	377.9	44.5	82.0	-	322.4	402.4

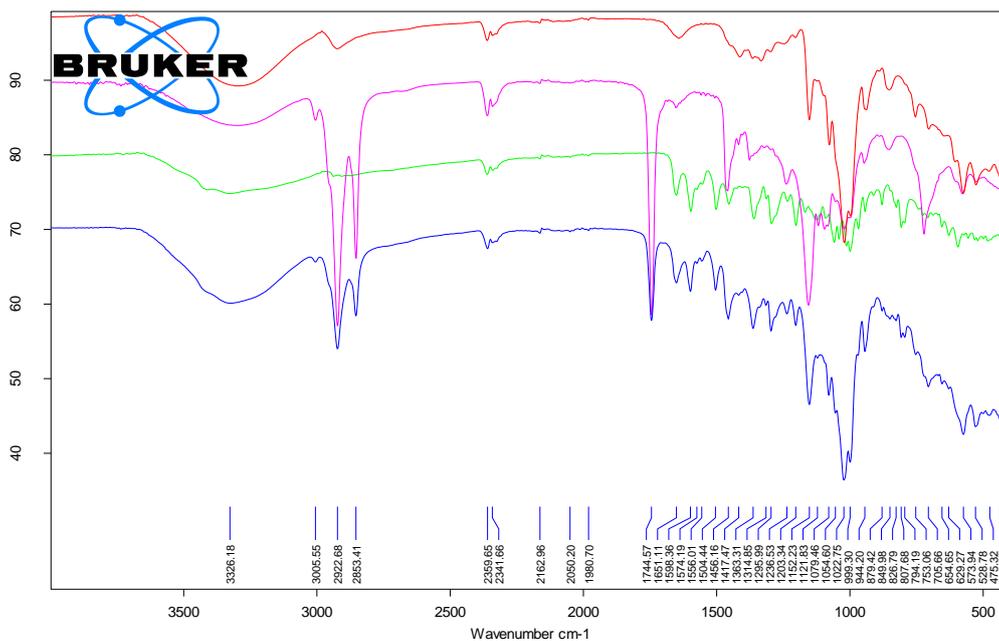
## 2. Fourier transform infrared spectroscopy (FTIR) of ternary complexes



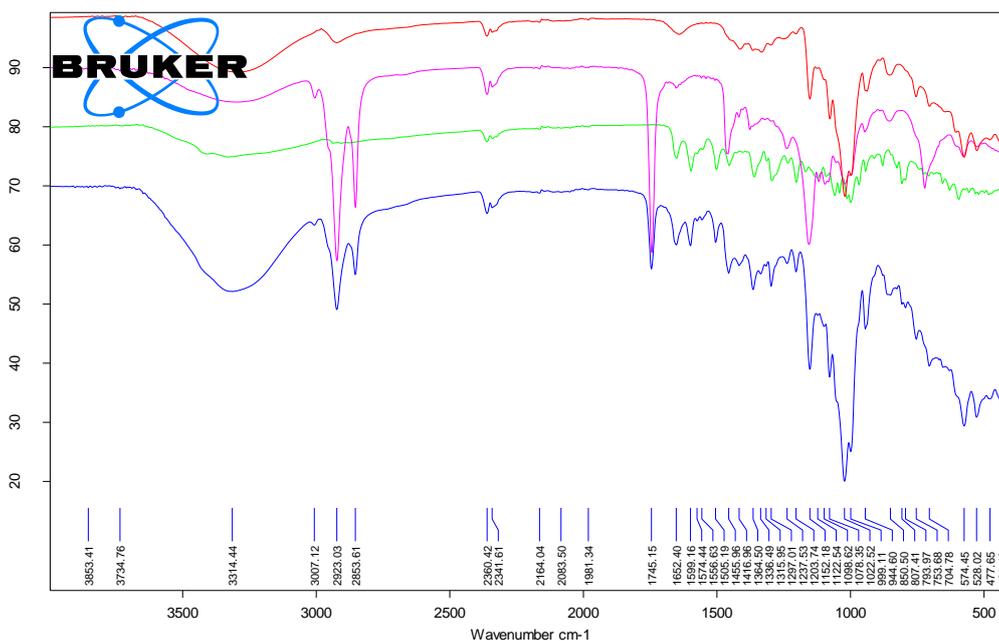
**Figure S6:** Superposition of the FTIR spectra for the  $\beta$ -cyclodextrin/*Corylus avellana* oil/naringin ternary complex at a 1:1:1 molar ratio (blue),  $\beta$ -cyclodextrin hydrate (red), *C. avellana* oil (pink), and naringin (green).



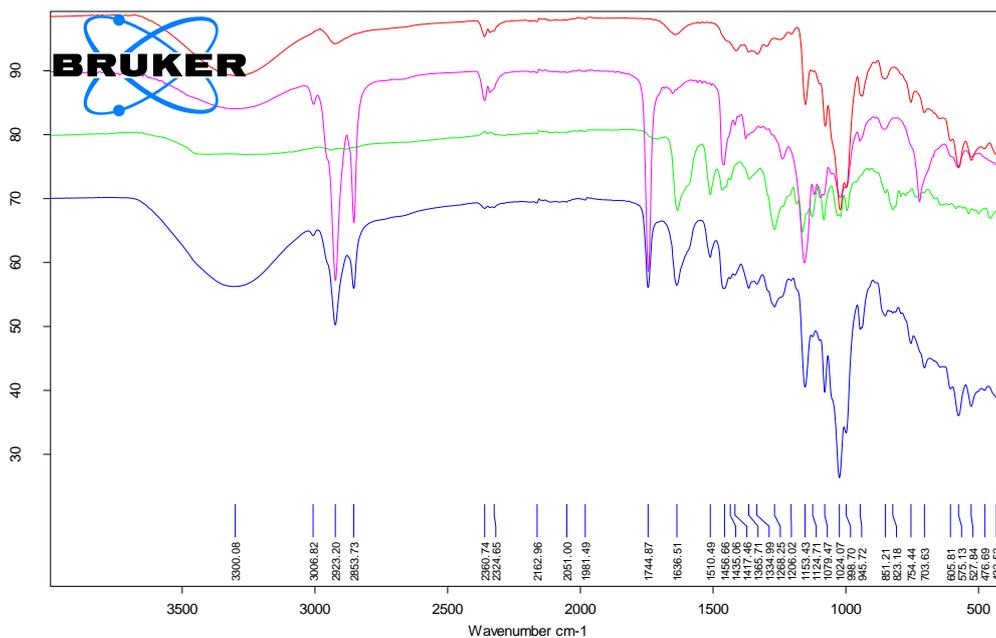
**Figure S7:** Superposition of the FTIR spectra for the  $\beta$ -cyclodextrin/*Corylus avellana* oil/naringin ternary complex at a 3:1:1 molar ratio (blue),  $\beta$ -cyclodextrin hydrate (red), *C. avellana* oil (pink), and naringin (green).



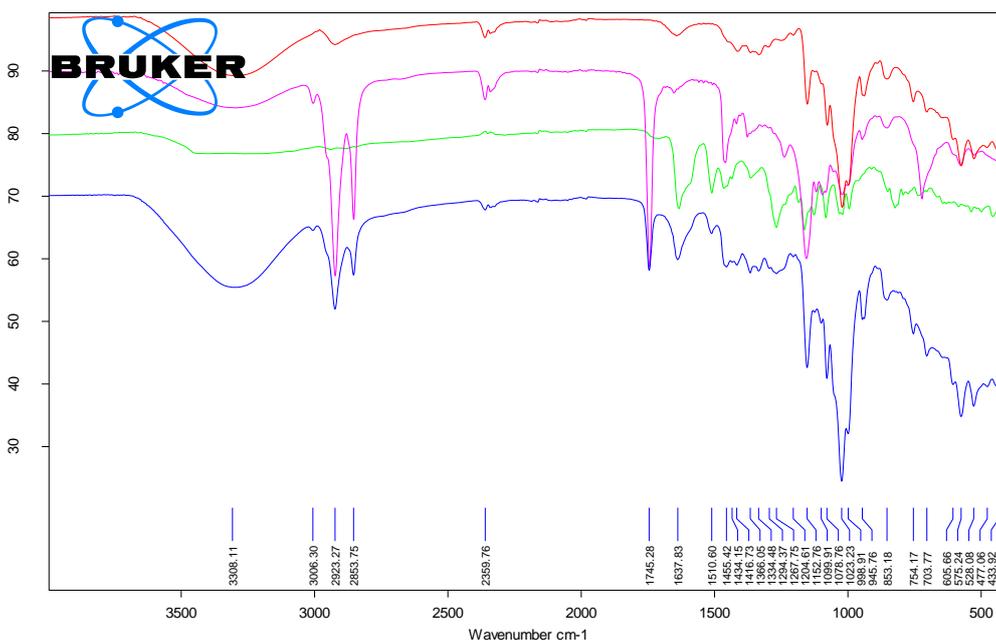
**Figure S8:** Superposition of the FTIR spectra for the  $\beta$ -cyclodextrin/*Corylus avellana* oil/rutin ternary complex at a 1:1:1 molar ratio (blue),  $\beta$ -cyclodextrin hydrate (red), *C. avellana* oil (pink), and rutin (green).



**Figure S9:** Superposition of the FTIR spectra for the  $\beta$ -cyclodextrin/*Corylus avellana* oil/rutin ternary complex at a 3:1:1 molar ratio (blue),  $\beta$ -cyclodextrin hydrate (red), *C. avellana* oil (pink), and rutin (green).



**Figure S10:** Superposition of the FTIR spectra for the  $\beta$ -cyclodextrin/*Corylus avellana* oil/silymarin ternary complex at a 1:1:1 molar ratio (blue),  $\beta$ -cyclodextrin hydrate (red), *C. avellana* oil (pink), and silymarin (green).



**Figure S11:** Superposition of the FTIR spectra for the  $\beta$ -cyclodextrin/*Corylus avellana* oil/silymarin ternary complex at a 3:1:1 molar ratio (blue),  $\beta$ -cyclodextrin hydrate (red), *C. avellana* oil (pink), and silymarin (green).

**Table S4:** FTIR band assignments for  $\beta$ -CD hydrate (mean( $\pm$ SD) of triplicate determinations).

Wavenumber ( $\text{cm}^{-1}$ )	Band assignment
3301.6( $\pm$ 8.5)	$\nu_{\text{OH}}$ , stretching vibration of the O-H groups in $\beta$ -CD and water
2924.8( $\pm$ 1.4)	$\nu^{\text{as}}_{\text{CH}}$ , stretching vibrations of the C-H groups
1643.3( $\pm$ 1.8)	$\delta_{\text{OH}}$ , bending vibrations of the O-H groups
1451( $\pm$ 0.2)	$\delta_{\text{CH}_2}$ , symmetric bending vibrations of the $\text{CH}_2$ groups
1413.7( $\pm$ 0.8)	$\delta_{\text{OH}}$ , in-plane bending vibrations of the O-H groups
1364.9( $\pm$ 0.3)	$\delta_{\text{CH}_2}$ , asymmetric bending vibrations of the $\text{CH}_2$ groups
1333.8( $\pm$ 0.2)	$\delta_{\text{OH}}$ , bending vibrations of the O-H groups
1297.9( $\pm$ 0.4)	$\delta_{\text{CH}}$ , in-plane bending vibrations of the C-H groups ( <i>tentative</i> )
1248( $\pm$ 0.9)	$\delta_{\text{CH}}$ , in-plane bending vibrations of the C-H groups ( <i>tentative</i> )
1204.7( $\pm$ 0.3)	$\delta_{\text{CH}}$ , in-plane bending vibrations of the C-H groups ( <i>tentative</i> )
1152.1( $\pm$ 0.1)	$\nu^{\text{s}}_{\text{COC}}$ , stretching vibrations of the C-O-C groups in glucosydic moieties
1077.2( $\pm$ 0.1)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups
1020.9( $\pm$ 0.3)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
997.7( $\pm$ 0.2)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups ( <i>tentative</i> )
939.2( $\pm$ 1.8)	$\nu_{\text{rgCH}}$ , stretching vibrations of the C-H groups from the $\beta$ -cyclodextrin ring
852.9( $\pm$ 0.8)	$\delta_{\text{CCH}}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds)
754.4( $\pm$ 0.3)	$\delta_{\text{CH}}$ , bending vibrations of the C-H groups ( <i>tentative</i> )
704( $\pm$ 0.7)	$\delta_{\text{CH}}$ , bending vibrations of the C-H groups ( <i>tentative</i> )
648.1( $\pm$ 0.9)	<i>not assigned</i>
574.2( $\pm$ 0.8)	$\delta_{\text{OCC}}$ , bending vibrations of the O-C-C groups ( <i>tentative</i> )
526.3( $\pm$ 1.3)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups ( <i>tentative</i> )

**Table S5:** FTIR band assignments for the hazelnut (*Corylus avellana* L.) oil (mean( $\pm$ SD) of triplicate determinations).

Wavenumber ( $\text{cm}^{-1}$ )	Band assignment
3287.8( $\pm$ 10)	$\nu_{\text{OH}}$ , stretching vibrations of the O-H groups from the free fatty acids and water
3005( $\pm$ 0.2)	$\nu^{\text{s}}_{=\text{CH}}$ , symmetric stretching vibrations of the $=\text{CH}$ groups
2952.5( $\pm$ 0.3)	$\nu^{\text{as}}_{\text{CH}}$ , asymmetric stretching vibrations of the CH groups
2922.5( $\pm$ 0)	$\nu^{\text{as}}_{\text{CH}}$ , symmetric stretching vibrations of the CH groups
2853.2( $\pm$ 0)	$\nu^{\text{s}}_{\text{CH}}$ , symmetric stretching vibrations of the CH groups
1744( $\pm$ 0)	$\nu_{\text{estC=O}}$ , stretching vibrations of the esteric C=O groups in triglycerides
1710.3( $\pm$ 0.7)	$\nu_{\text{faC=O}}$ , stretching vibrations of the C=O groups in free fatty acids (shoulder)
1652.7( $\pm$ 0.3)	$\nu_{\text{cC=C}}$ , stretching vibrations of the <i>cis</i> RHC=CHR' groups
1458.7( $\pm$ 0.2)	$\delta_{\text{CH}_2/3}$ , deformation vibrations of the $\text{CH}_2$ and $\text{CH}_3$ groups

1417.6(±0.1)	$\delta_{\text{rk}=\text{CH}}$ , rocking vibrations of the =C–H groups in <i>cis</i> RHC=CHR'
1376.7(±0)	$\delta_{\text{CH}_2}$ , bending vibrations of the CH <sub>2</sub> groups
1236.8(±1.3)	$\delta_{\text{CH}_2}$ , bending vibrations of the CH <sub>2</sub> groups
1158.1(±2.3)	$\delta_{\text{CH}_2}$ , bending vibrations of the CH <sub>2</sub> groups
1094.7(±0.7)	$\nu_{\text{CO}}$ , stretching vibrations of the C–O groups
1027.9(±5.7)	$\nu_{\text{CO}}$ , stretching vibrations of the C–O groups
956.7(±8.7)	$\delta_{\text{C}=\text{C}}$ , bending vibrations of the C=C groups in <i>trans</i> RHC=CHR'
722(±0.1)	$\delta_{\text{opCH}}$ , out-of-plane deformation vibrations in the C–H groups

**Table S6:** FTIR band assignments for hesperidin and the corresponding  $\beta$ -cyclodextrin/hazelnut oil/hesperidin 1:1:1 and 3:1:1 ternary complexes (codes “X1H and X3H); bands associated to  $\beta$ -CD or hazelnut oil are also specified; wavenumbers (cm<sup>-1</sup>) are expressed as mean(±SD) of triplicate determinations for hesperidin and duplicate determinations for the ternary complexes.

Hesperidin	Wavenumber (cm <sup>-1</sup> )		Band assignment
	X1H	X3H	
3540.5(±1)	–	–	$\nu_{\text{OH}}$ , stretching vibrations of the O–H groups (phenolic, glycosidic, water)
3467.5(±1.3)	–	–	$\nu_{\text{OH}}$ , stretching vibrations of the O–H groups (phenolic, glycosidic, water)
3411.3(±0.5)	3312.1(±2.8)	3306.2(±2.1)	$\nu_{\text{OH}}$ , stretching vibrations of the O–H groups (phenolic, glycosidic, water) (also from $\beta$ -CD)
–	3006.5(±1)	3009.6(±0.8)	$\nu^{\text{s}}_{=\text{CH}}$ , symmetric stretching vibrations of the =CH groups (from hazelnut oil)
2982(±0.5)	–	–	$\nu^{\text{as}}_{\text{CH}}$ , stretching vibrations of the C–H bonds in the aliphatic CH <sub>3</sub> /CH groups
2940.8(±0.8)	–	–	$\nu^{\text{as}}_{\text{CH}}$ , stretching vibrations of the C–H bonds in the aliphatic CH <sub>3</sub> /CH groups
2914.2(±0.9)	2922.4(±0.1)	2922.6(±0.1)	$\nu^{\text{as}}_{\text{CH}}$ , stretching vibrations of the C–H bonds in the aliphatic CH <sub>3</sub> /CH groups (also from hazelnut oil)
2895.6(±0.4)	–	–	$\nu^{\text{s}}_{\text{CH}}$ , stretching vibrations of the C–H bonds in the aliphatic CH <sub>2</sub> groups
–	2853.4(±0)	2853.5(±0.2)	$\nu^{\text{s}}_{\text{CH}}$ , symmetric stretching vibrations of the CH groups (from hazelnut oil)
–	1745(±0.1)	1745(±0.1)	$\nu_{\text{estC}=\text{O}}$ , stretching vibrations of the esteric C=O groups in triglycerides (from hazelnut oil)
1644.8(±0.5)	1647.2(±0.1)	1647.2(±0.1)	$\nu^{\text{as}}_{\text{C}=\text{O}/\text{C}=\text{C}}$ , asymmetric stretching vibrations of the C=O/C=C groups
1604.4(±0.1)	1605.9(±0.1)	1606.8(±0.3)	$\nu_{\text{CC}}/\delta_{\text{ar}\#\text{C}}$ , stretching vibrations of the C–C group in the ring C / bending vibrations of the aromatic C#C groups
1518.3(±0.6)	1519.7(±0.1)	1519.7(±0.1)	$\delta_{\text{ar}\#\text{C}}$ , bending vibrations of the aromatic C#C groups
1504.1(±0.3)	1505.8(±0.7)	1505.1(±1.2)	$\nu_{\text{CC}}$ , stretching of C–C group in the ring C
1467.5(±1.1)	1457.6(±0.7)	1456.5(±0.3)	$\delta_{\text{CH}_3}$ , asymmetric bending vibrations of the CH <sub>3</sub> groups
1442.5(±0.4)	1445(±0.3)	1446.5(±0.1)	$\delta_{\text{CH}_3}$ , asymmetric bending vibrations of the CH <sub>3</sub> groups
–	1416.6(±0.5)	1416.1(±0.2)	$\delta_{\text{OH}}$ , in-plane bending vibrations of the O–H groups (from $\beta$ -CD)
1404(±1)	–	–	$\delta_{\text{CH}_3}/\delta_{\text{HOC}}$ , symmetric bending vibrations of the CH <sub>3</sub> groups/in-plane bending vibrations of the H–O–C groups
1356.6(±0.5)	1357(±0)	1365(±0.4)	$\nu_{\text{CO}}$ , stretching vibrations of the C–O groups
1339.9(±0.6)	1339.1(±0.3)	1336.9(±0.3)	$\delta_{\text{CH}_3}/\delta_{\text{OCC}}$ , symmetric bending vibrations of the CH <sub>3</sub> /OCC groups (also from $\beta$ -CD)
1298.2(±0.2)	1299(±0.1)	1298.9(±0)	$\delta_{\text{CH}}/\delta_{\text{OCH}}/\nu_{\text{CC}}$ , in-plane bending vibrations of the C–H/OCH groups / stretching vibrations of the C–C groups
1275.7(±0.3)	1276.8(±0)	1277.3(±0.2)	$\nu_{\text{CO}}$ , stretching vibrations of the C–O groups (carbohydrates and phenolics)

–	1241.4(±0.1)	1242.5(±0.4)	$\delta_{\text{CH}_2}$ , bending vibrations of the $\text{CH}_2$ groups (from hazelnut oil)
1203.3(±0.6)	1204.4(±0)	1204.6(±0)	$\nu_{\text{CC}}/\nu_{\text{CO}}$ , stretching vibrations of the C-C groups in ring B / stretching vibrations of the C-O groups (carbohydrates and phenolics)
1182.4(±0.1)	1182.3(±0.1)	1182.3(±0.2)	$\nu_{\text{CO}}/\delta_{\text{HCC/HOC}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O groups (carbohydrates and phenolics)/in-plane bending vibrations of the HCC or HOC groups / stretching vibrations of the C-C groups in the ring A
–	1153.5(±0.3)	1152.6(±0.1)	$\nu_{\text{COC}}$ , stretching vibrations of the C-O-C groups in glucosidic moieties (from $\beta$ -CD)
1130(±0.1)	1131.9(±0.4)	1130.5(±0.3)	$\nu_{\text{CO}}/\delta_{\text{CCH}}/\tau_{\text{CH}_2}$ , stretching vibrations of the C-O groups/ bending vibrations of the C-C-H groups/“twisting” bending vibrations of the $\text{CH}_2$ groups
1093.9(±0.2)	1095(±0.1)	1096.5(±0.3)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups
–	1077.9(±0.2)	1077.4(±0)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups (from $\beta$ -CD)
1065.5(±1.2)	–	–	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
1053.3(±2.7)	1049.5(±0.3)	1050.4(±0.6)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
1030.8(±2.3)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups in the ring B
–	1023.9(±0.5)	1022.3(±0.2)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups (from $\beta$ -CD)
1010.5(±1.5)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups ( <i>tentative</i> )
971.7(±0.9)	–	–	$\nu_{\text{OC}}$ , stretching vibrations of the O-C groups
–	946.1(±0.1)	946(±0)	$\nu_{\text{rgCH}}$ , stretching vibrations of the C-H groups from the $\beta$ -cyclodextrin ring (from $\beta$ -CD)
911.5(±0.6)	911.6(±0.1)	911.7(±0.6)	$\tau_{\text{HCCC}}$ , “twisting” bending vibrations of the H-C-C-C groups
–	861.8(±0.2)	861.9(±0.6)	$\delta_{\text{CCH}}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds) (from $\beta$ -CD)
–	847.6(±0)	848.1(±0)	$\delta_{\text{CCH}}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds) (from $\beta$ -CD) ( <i>tentative</i> )
814.1(±0.8)	815.2(±0)	815(±0.1)	$\delta_{\text{CH}}$ , out-of-plane bending vibrations of the C-H groups
741.5(±1.4)	743.1(±0)	743.5(±0)	$\tau_{\text{COH}}$ , “twisting” bending vibrations of the C-O-H groups
–	576.1(±0.1)	575.3(±0.4)	$\delta_{\text{OCC}}$ , bending vibrations of the O-C-C groups (from $\beta$ -CD) ( <i>tentative</i> )
–	526.6(±0.2)	527.4(±0.2)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups (from $\beta$ -CD) ( <i>tentative</i> )

**Table S7:** FTIR band assignments for naringin and the corresponding  $\beta$ -cyclodextrin/hazelnut oil/naringin 1:1:1 and 3:1:1 ternary complexes (codes “X1N and X3N”); bands associated to  $\beta$ -CD or hazelnut oil are also specified; wavenumbers ( $\text{cm}^{-1}$ ) are expressed as mean(±SD) of triplicate determinations for naringin and duplicate determinations for the ternary complexes (\* observed in one duplicate).

Naringin	Wavenumber ( $\text{cm}^{-1}$ )		Band assignment
	X1N	X3N	
3405.3(±4)	3321(±5.2)	3295.8(±15)	$\nu_{\text{OH}}$ , stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from $\beta$ -CD)
–	3006.4(±0.6)	3008.8(±0.8)	$\nu_{\text{OH}}$ , stretching vibrations of the O-H groups (phenolic, glycosidic, water)
2930.8(±0.6)	2923.1(±0.2)	2923.6(±0.4)	$\nu_{\text{CH}}^{\text{as}}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_3/\text{CH}$ groups (also from hazelnut oil)
2889.9(±0.2)	–	–	$\nu_{\text{CH}}^{\text{s}}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_2$ groups
–	2853.5(±0.1)	2853.7(±0.6)	$\nu_{\text{CH}}^{\text{s}}$ , symmetric stretching vibrations of the CH groups (from hazelnut oil)
–	1745(±0.4)	1743.6(±1.9)	$\nu_{\text{estC=O}}$ , stretching vibrations of the esteric C=O groups in triglycerides (from hazelnut oil)

1643.5(±0.6)	1644.8(±0.1)	1643.7(±1.1)	$\nu^{\text{as}}_{\text{C=O/C=C}}$ , asymmetric stretching vibrations of the C=O/C=C groups
1625.8(±0.1)	1606.6(±0.1)	1608.8*	$\nu_{\text{CC}}/\delta_{\text{arC}\#C}$ , stretching vibrations of the C-C group in the ring C / bending vibrations of the aromatic C#C groups
1583.2(±0.1)	–	–	$\nu_{\text{CC}}/\delta_{\text{arC}\#C}$ , stretching vibrations of the C-C group in the ring C / bending vibrations of the aromatic C#C groups
1518.1(±0.1)	1519(±0)	1519(±0)	$\delta_{\text{arC}\#C}$ , bending vibrations of the aromatic C#C groups
1502.6(±0.1)	1500.5(±0.2)	1501.3(±2)	$\nu_{\text{CC}}$ , stretching of C-C group in the ring C
1452.6(±0.1)	1455.1(±0.5)	1453.4(±0.4)	$\delta_{\text{CH}_3}$ , asymmetric bending vibrations of the CH <sub>3</sub> groups
1441.9(±0.1)	1444.3(±0.1)	1444.4*	$\delta_{\text{CH}_3}$ , asymmetric bending vibrations of the CH <sub>3</sub> groups
–	1417.4(±0)	1415.5(±1.4)	$\delta_{\text{OH}}$ , in-plane bending vibrations of the O-H groups (from $\beta$ -CD)
1392.6(±0.1)	–	–	$\delta_{\text{CH}_3}/\delta_{\text{HOC}}$ , symmetric bending vibrations of the CH <sub>3</sub> groups/in-plane bending vibrations of the H-O-C groups
1339.9(±0)	1339.7(±0.4)	1339.4(±1.5)	$\delta_{\text{CH}_3}/\delta_{\text{OCC}}$ , symmetric bending vibrations of the CH <sub>3</sub> /OCC groups (also from $\beta$ -CD)
1294.1(±0.1)	1297.1(±0)	1297.7(±0.7)	$\delta_{\text{CH}}/\delta_{\text{OCH}}/\nu_{\text{CC}}$ , in-plane bending vibrations of the C-H/OCH groups / stretching vibrations of the C-C groups
1204.1(±0.2)	1204.1(±0.2)	1206.3(±2.2)	$\nu_{\text{CC}}/\nu_{\text{CO}}$ , stretching vibrations of the C-C groups in ring B / stretching vibrations of the C-O groups (carbohydrates and phenolics)
1175.8(±0.2)	1177.1(±1)	1178.5(±1.8)	$\nu_{\text{CO}}/\delta_{\text{HCC/HOC}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O groups (carbohydrates and phenolics)/in-plane bending vibrations of the HCC or HOC groups / stretching vibrations of the C-C groups in the ring A
–	1153.2(±0.5)	1152.6(±0.4)	$\nu^{\text{s}}_{\text{COC}}$ , stretching vibrations of the C-O-C groups in glucosydic moieties (from $\beta$ -CD)
1135(±0.1)	1141.1(±0.2)	–	$\nu_{\text{CO}}/\delta_{\text{CCH}}/\tau_{\text{CH}_2}$ , stretching vibrations of the C-O groups/ bending vibrations of the C-C-H groups/“twisting” bending vibrations of the CH <sub>2</sub> groups
1088.2(±0.3)	1095.1(±0.5)	1096.5(±0.2)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups
–	1077.7(±0.7)	1077(±0.1)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups (from $\beta$ -CD)
1054.9(±0)	1048.1(±0.8)	1051.1(±1.3)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
1037.4(±0.2)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups in the ring B
–	1025.7(±0.1)	1022(±0.5)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups (from $\beta$ -CD)
1014.3(±0.3)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups ( <i>tentative</i> )
985.1(±0.1)	–	–	$\nu_{\text{OC}}$ , stretching vibrations of the O-C groups
–	945.9(±0.1)	946.4(±0.6)	$\nu_{\text{rgCH}}$ , stretching vibrations of the C-H groups from the $\beta$ -cyclodextrin ring (from $\beta$ -CD)
920.8(±0)	911.4(±0.2)	–	$\tau_{\text{HCCC}}$ , “twisting” bending vibrations of the H-C-C-C groups
–	862.9(±0.4)	858.2(±3.4)	$\delta_{\text{CCH}}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds) (from $\beta$ -CD)
820.8(±0)	813.5(±0.1)	813.9(±1.8)	$\delta_{\text{CH}}$ , out-of-plane bending vibrations of the C-H groups
743.4(±0.1)	–	–	$\tau_{\text{COH}}$ , “twisting” bending vibrations of the C-O-H groups
–	575.5(±0)	574.7(±0)	$\delta_{\text{OCC}}$ , bending vibrations of the O-C-C groups (from $\beta$ -CD) ( <i>tentative</i> )
–	524.2(±3)	526.4(±1)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups (from $\beta$ -CD) ( <i>tentative</i> )

**Table S8:** FTIR band assignments for naringin and the corresponding  $\beta$ -cyclodextrin/hazelnut oil/rutin 1:1:1 and 3:1:1 ternary complexes (codes “X1R and X3R”); bands associated to  $\beta$ -CD or hazelnut oil are also specified; wavenumbers ( $\text{cm}^{-1}$ ) are expressed as mean( $\pm$ SD) of triplicate determinations for rutin and duplicate determinations for the ternary complexes.

	Wavenumber ( $\text{cm}^{-1}$ )		Band assignment
	Rutin	X1R	
3407.4( $\pm$ 2.2)	–	–	$\nu_{\text{OH}}$ , stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from $\beta$ -CD)
3325( $\pm$ 7.3)	3325.1( $\pm$ 1.5)	3310.8( $\pm$ 5.1)	$\nu_{\text{OH}}$ , stretching vibrations of the O-H groups (phenolic, glycosidic, water)
–	3006.3( $\pm$ 1.1)	3007.5( $\pm$ 0.5)	$\nu^{\text{s}}_{\text{CH}}$ , symmetric stretching vibrations of the =CH groups (from hazelnut oil)
2938( $\pm$ 0)	–	–	$\nu^{\text{as}}_{\text{CH}}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_3/\text{CH}$ groups
2907.3( $\pm$ 0.2)	2922.8( $\pm$ 0.2)	2923.1( $\pm$ 0)	$\nu^{\text{as}}_{\text{CH}}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_3/\text{CH}$ groups (also from hazelnut oil)
2875.9( $\pm$ 0.4)	–	–	$\nu^{\text{s}}_{\text{CH}}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_2$ groups
–	2853.5( $\pm$ 0.2)	2853.7( $\pm$ 0.1)	$\nu^{\text{s}}_{\text{CH}}$ , symmetric stretching vibrations of the CH groups (from hazelnut oil)
–	1744.7( $\pm$ 0.2)	1745.1( $\pm$ 0)	$\nu_{\text{estC=O}}$ , stretching vibrations of the esteric C=O groups in triglycerides (from hazelnut oil)
1651( $\pm$ 0.1)	1651.7( $\pm$ 0.8)	1651.8( $\pm$ 0.9)	$\nu^{\text{as}}_{\text{C=O/C=C}}$ , asymmetric stretching vibrations of the C=O/C=C groups
1596.8( $\pm$ 0.1)	1598.4( $\pm$ 0.1)	1599.2( $\pm$ 0.1)	$\nu_{\text{CC}}/\delta_{\text{arC}\#C}$ , stretching vibrations of the C-C group in the ring C / bending vibrations of the aromatic C#C groups
1554.1( $\pm$ 0.1)	–	–	$\delta_{\text{arC}\#C}$ , bending vibrations of the aromatic C#C groups
1502( $\pm$ 0.1)	1504.6( $\pm$ 0.2)	1504.9( $\pm$ 0.4)	$\nu_{\text{CC}}$ , stretching of C-C group in the ring C
1454.3( $\pm$ 0.2)	1456.2( $\pm$ 0.1)	1455.6( $\pm$ 0.6)	$\delta_{\text{CH}_3}$ , asymmetric bending vibrations of the $\text{CH}_3$ groups
–	1417.7( $\pm$ 0.4)	1416.5( $\pm$ 0.6)	$\delta_{\text{OH}}$ , in-plane bending vibrations of the O-H groups (from $\beta$ -CD)
1402.6( $\pm$ 0.4)	–	–	$\delta_{\text{CH}_3}/\delta_{\text{HOC}}$ , symmetric bending vibrations of the $\text{CH}_3$ groups/in-plane bending vibrations of the H-O-C groups
1360( $\pm$ 0.1)	1363.3( $\pm$ 0)	1364.6( $\pm$ 0.1)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
–	1339.4( $\pm$ 0.1)	1336.1( $\pm$ 0.5)	$\delta_{\text{CH}_3}/\delta_{\text{OCC}}$ , symmetric bending vibrations of the $\text{CH}_3/\text{OCC}$ groups (also from $\beta$ -CD)
1294.7( $\pm$ 0)	1295.9( $\pm$ 0.1)	1296.9( $\pm$ 0.1)	$\delta_{\text{CH}}/\delta_{\text{OCH}}/\nu_{\text{CC}}$ , in-plane bending vibrations of the C-H/OCH groups / stretching vibrations of the C-C groups
–	1279.5( $\pm$ 0.7)	1280.5( $\pm$ 0.2)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups (carbohydrates and phenolics)
–	1236.4( $\pm$ 0.1)	1237.8( $\pm$ 0.4)	$\delta_{\text{CH}_2}$ , bending vibrations of the $\text{CH}_2$ groups (from hazelnut oil)
1202.5( $\pm$ 0.1)	1203.5( $\pm$ 0.2)	1203.9( $\pm$ 0.2)	$\nu_{\text{CC}}/\nu_{\text{CO}}$ , stretching vibrations of the C-C groups in ring B / stretching vibrations of the C-O groups (carbohydrates and phenolics)
1168.4( $\pm$ 0.2)	–	–	$\nu_{\text{CO}}/\delta_{\text{HCC/HOC}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O groups (carbohydrates and phenolics)/in-plane bending vibrations of the HCC or HOC groups / stretching vibrations of the C-C groups in the ring A
–	1152.4( $\pm$ 0.3)	1152.1( $\pm$ 0.1)	$\nu^{\text{s}}_{\text{COC}}$ , stretching vibrations of the C-O-C groups in glucosidic moieties (from $\beta$ -CD)
–	1121.7( $\pm$ 0.1)	1123( $\pm$ 0.6)	$\nu_{\text{CO}}/\nu_{\text{CC}}/\delta_{\text{HCC/HOC}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups (phenolics)/ in-plane bending vibrations of the HCC or HOC groups / stretching vibrations of the C-C groups in the ring A
1092.1( $\pm$ 0.3)	–	–	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups
–	1079.7( $\pm$ 0.3)	1078.1( $\pm$ 0.3)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups (from $\beta$ -CD)
1058.6( $\pm$ 0.1)	1054.9( $\pm$ 0.4)	1053.6( $\pm$ 0.3)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
1041.1( $\pm$ 0)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups in the ring B
–	1023.2( $\pm$ 0.7)	1022.4( $\pm$ 0.2)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups (from $\beta$ -CD)
1013.1( $\pm$ 0)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups ( <i>tentative</i> )

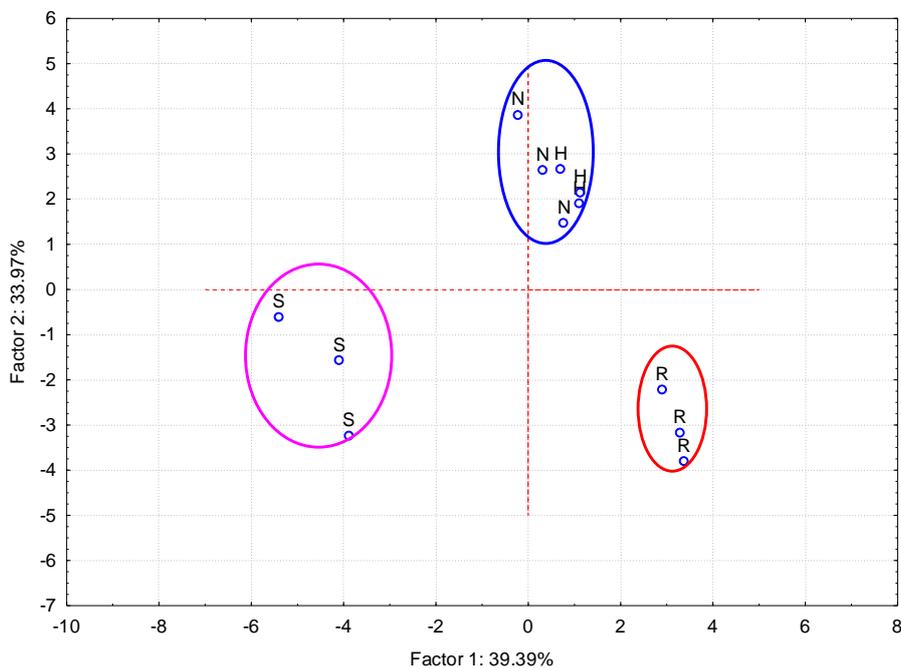
968(±0.2)	–	–	$\nu_{OC}$ , stretching vibrations of the O-C groups
–	944.2(±0)	944.7(±0.1)	$\nu_{rgCH}$ , stretching vibrations of the C-H groups from the $\beta$ -cyclodextrin ring (from $\beta$ -CD)
911.1(±0.2)	912.1(±0.1)	911.4(±0.1)	$\tau_{HCCC}$ , “twisting” bending vibrations of the H-C-C-C groups
–	863.7(±1.3)	862.1(±0)	$\delta_{CCH}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds) (from $\beta$ -CD)
–	849.7(±0.4)	850.6(±0.1)	$\delta_{CCH}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds) (from $\beta$ -CD) ( <i>tentative</i> )
807.6(±0)	807.6(±0.2)	807.4(±0)	$\delta_{CH}$ , out-of-plane bending vibrations of the C-H groups
742.2(±0.1)	752.8(±0.3)	753.7(±0)	$\tau_{COH}$ , “twisting” bending vibrations of the C-O-H groups
–	574.2(±0.4)	574.7(±0.3)	$\delta_{OCC}$ , bending vibrations of the O-C-C groups (from $\beta$ -CD) ( <i>tentative</i> )
–	528.6(±0.2)	527.9(±0.1)	$\nu_{CC}$ , stretching vibrations of the C-C groups (from $\beta$ -CD) ( <i>tentative</i> )

**Table S9:** FTIR band assignments for naringin and the corresponding  $\beta$ -cyclodextrin/hazelnut oil/naringin 1:1:1 and 3:1:1 ternary complexes (codes “X1N and X3N”); bands associated to  $\beta$ -CD or hazelnut oil are also specified; wavenumbers ( $\text{cm}^{-1}$ ) are expressed as mean ( $\pm$ SD) of triplicate determinations for naringin and duplicate determinations for the ternary complexes.

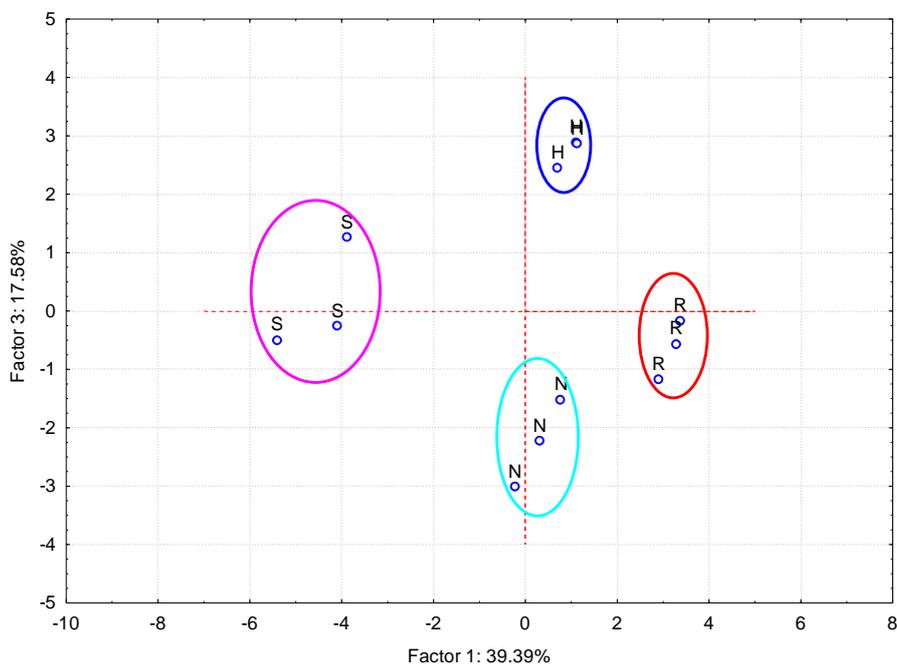
Silymarin	Wavenumber ( $\text{cm}^{-1}$ )		Band assignment
	X1S	X3S	
3400.3(±4.2)	3298.1(±6.2)	3302.4(±8.1)	$\nu_{OH}$ , stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from $\beta$ -CD)
3263.1(±1.3)	–	–	$\nu_{OH}$ , stretching vibrations of the O-H groups (phenolic, glycosidic, water)
–	3006.6(±1.6)	3007.6(±1.8)	$\nu^s_{=CH}$ , symmetric stretching vibrations of the =CH groups (from hazelnut oil)
2938.4(±3)	–	–	$\nu^{as}_{CH}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_3/\text{CH}$ groups
–	2922.9(±0.2)	2923.3(±0)	$\nu^{as}_{CH}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_3/\text{CH}$ groups (also from hazelnut oil)
2882(±1.8)	–	–	$\nu^s_{CH}$ , stretching vibrations of the C-H bonds in the aliphatic $\text{CH}_2$ groups
–	2853.5(±0.1)	2853.7(±0.1)	$\nu^s_{CH}$ , symmetric stretching vibrations of the CH groups (from hazelnut oil)
–	1744.7(±0)	1745.2(±0.2)	$\nu_{estC=O}$ , stretching vibrations of the esteric C=O groups in triglycerides (from hazelnut oil)
1634.1(±0.4)	1637.5(±0.2)	1637.5(±0.5)	$\nu^{as}_{C=O/C=C}$ , asymmetric stretching vibrations of the C=O/C=C groups
1509.9(±0.6)	1510.4(±0.2)	1510.1(±0.6)	$\nu_{CC}$ , stretching of C-C group in the ring C
1464.3(±0.7)	1455.7(±0.7)	1455.7(±0.4)	$\delta_{CH_3}$ , asymmetric bending vibrations of the $\text{CH}_3$ groups
–	1416.9(±0.1)	1417.1(±0.6)	$\delta_{OH}$ , in-plane bending vibrations of the O-H groups (from $\beta$ -CD)
1364(±0.4)	1365.9(±0)	1365.7(±0.5)	$\nu_{CO}$ , stretching vibrations of the C-O groups
–	1335(±0)	1335(±0.7)	$\delta_{CH_3}/\delta_{OCC}$ , symmetric bending vibrations of the $\text{CH}_3/\text{OCC}$ groups (also from $\beta$ -CD)
1268.1(±0.1)	1268.3(±0.2)	1268(±0.3)	$\nu_{CO}$ , stretching vibrations of the C-O groups (carbohydrates and phenolics)
–	1243.5(±0.7)	1242.9(±0.8)	$\delta_{CH_2}$ , bending vibrations of the $\text{CH}_2$ groups (from hazelnut oil)
–	1204.6(±0.3)	1205.2(±0.4)	$\nu_{CC}/\nu_{CO}$ , stretching vibrations of the C-C groups in ring B / stretching vibrations of the C-O groups (carbohydrates and phenolics)
1184.7(±0.8)	–	–	$\nu_{CO}/\delta_{HCC/HOC}/\nu_{CC}$ , stretching vibrations of the C-O groups (carbohydrates and phenolics)/in-plane bending vibrations of the HCC or HOC groups / stretching vibrations of the C-C groups in the ring A
–	1152.8(±0.1)	1152.8(±0)	$\nu^s_{COC}$ , stretching vibrations of the C-O-C groups in glucosydic moieties (from $\beta$ -CD)

1163.3(±0.2)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}/\delta_{\text{HCC/HOC}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups (phenolics)/ in-plane bending vibrations of the HCC or HOC groups / stretching vibrations of the C-C groups in the ring A
1082.5(±0.1)	1078.6(±0.2)	1078.6(±0.3)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups
–	1050.9(±0.2)	1051.4(±0.3)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups
1031.7(±0.2)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups in the ring B
–	1023.1(±0.3)	1023.1(±0.1)	$\nu_{\text{CO}}$ , stretching vibrations of the C-O groups (from $\beta$ -CD)
1020.3(±0.1)	–	–	$\nu_{\text{CO}}/\nu_{\text{CC}}$ , stretching vibrations of the C-O/C-C groups ( <i>tentative</i> )
995.2(±0)	–	–	$\nu_{\text{OC}}$ , stretching vibrations of the O-C groups
–	946(±0.1)	945.9(±0.2)	$\nu_{\text{rgCH}}$ , stretching vibrations of the C-H groups from the $\beta$ -cyclodextrin ring (from $\beta$ -CD)
–	852.6(±0.2)	852.6(±0.9)	$\delta_{\text{CCH}}$ , bending vibrations of the C-C-H groups (the $\alpha$ -type glycosidic bonds) (from $\beta$ -CD) ( <i>tentative</i> )
819.7(±5.9)	812.7(±0.7)	812.3(±0.8)	$\delta_{\text{CH}}$ , out-of-plane bending vibrations of the C-H groups
–	575.5(±0.3)	574.9(±0.4)	$\delta_{\text{OCC}}$ , bending vibrations of the O-C-C groups (from $\beta$ -CD) ( <i>tentative</i> )
–	528(±0.2)	528.1(±0)	$\nu_{\text{CC}}$ , stretching vibrations of the C-C groups (from $\beta$ -CD) ( <i>tentative</i> )

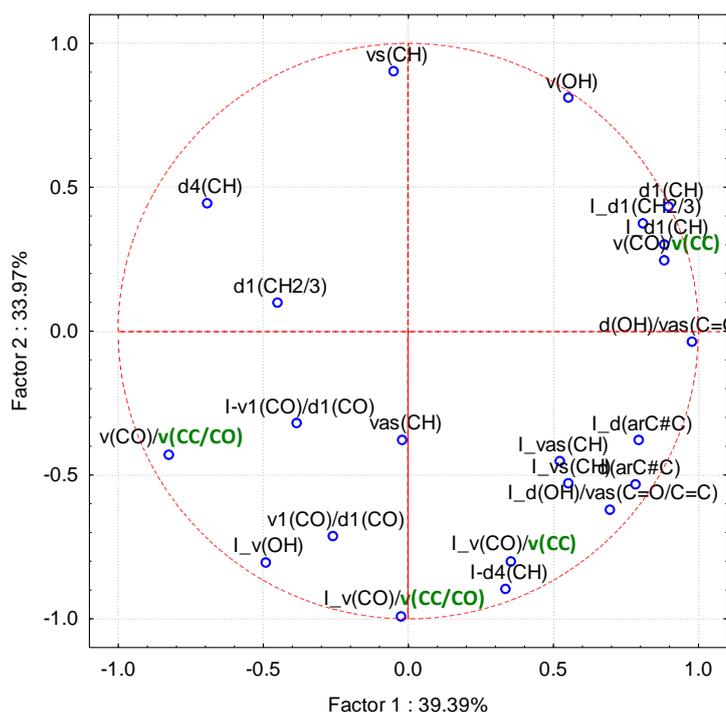
### 3. Fourier transform infrared spectroscopy–principal component analysis (FTIR–PCA) of ternary complexes.



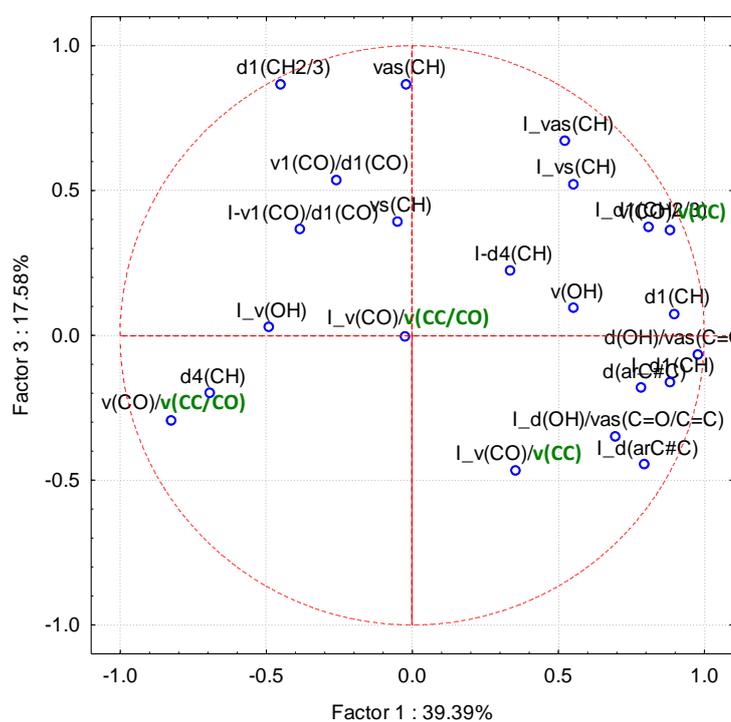
**Figure S12:** PC<sub>2</sub> versus PC<sub>1</sub> scores plot from the FTIR–PCA analysis of the flavonoid glycoside and flavanolignan antioxidants (codes: “H” – hesperidin, “N” – naringin, “R” – rutin and “S” – silymarin); all wavenumber and intensity of the FTIR bands were used as input variables.



**Figure S13:** PC<sub>3</sub> versus PC<sub>1</sub> scores plot from the FTIR–PCA analysis of the flavonoid glycoside and flavanolignan antioxidants (codes: “H” – hesperidin, “N” – naringin, “R” – rutin and “S” – silymarin); all wavenumber and intensity of the FTIR bands were used as input variables.



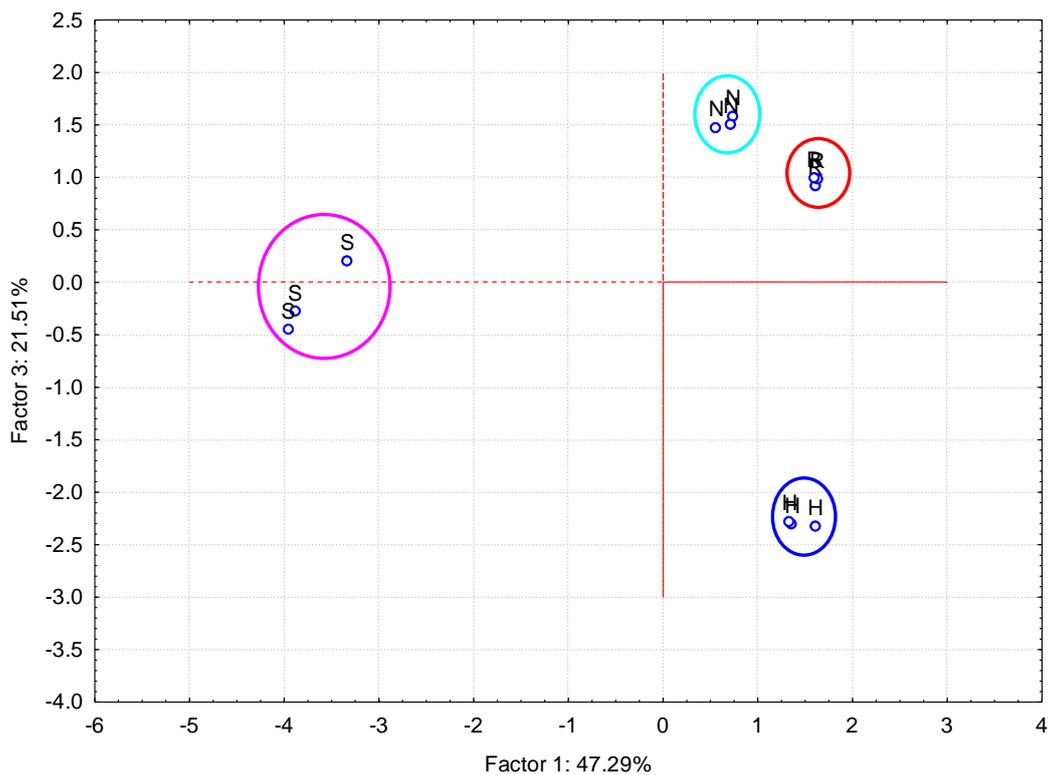
**Figure S14:** PC<sub>2</sub> versus PC<sub>1</sub> loadings plot from the FTIR–PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S10 for codes).



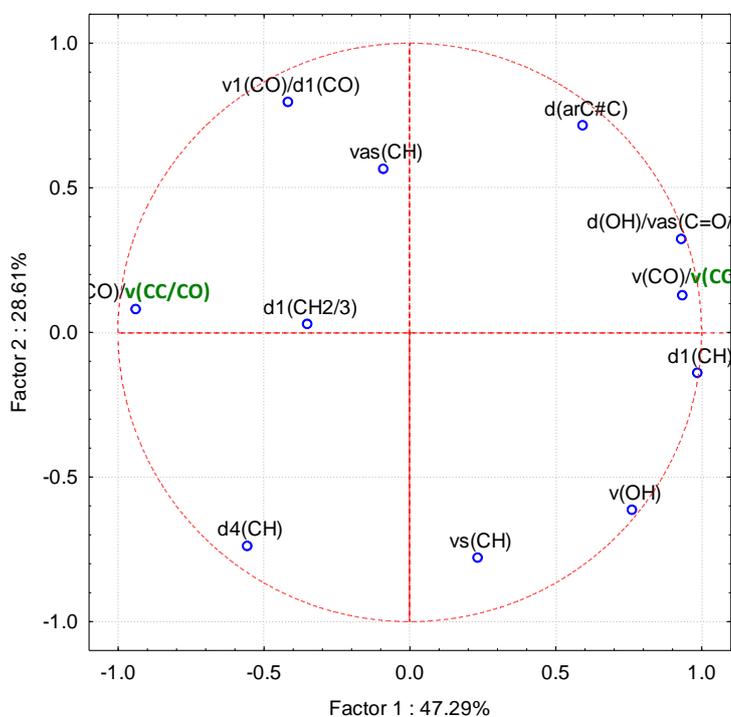
**Figure S15:** PC<sub>3</sub> versus PC<sub>1</sub> loadings plot from the FTIR–PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S10 for codes).

**Table S10:** Factor coordinates (principal components, PCs) of the variables, based on correlations, from the FTIR–PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; all wavenumber (“v” – for stretching vibrations, “d” – for bending vibrations) and intensity (designed as “I\_v/d”) of the FTIR bands were used as input variables.

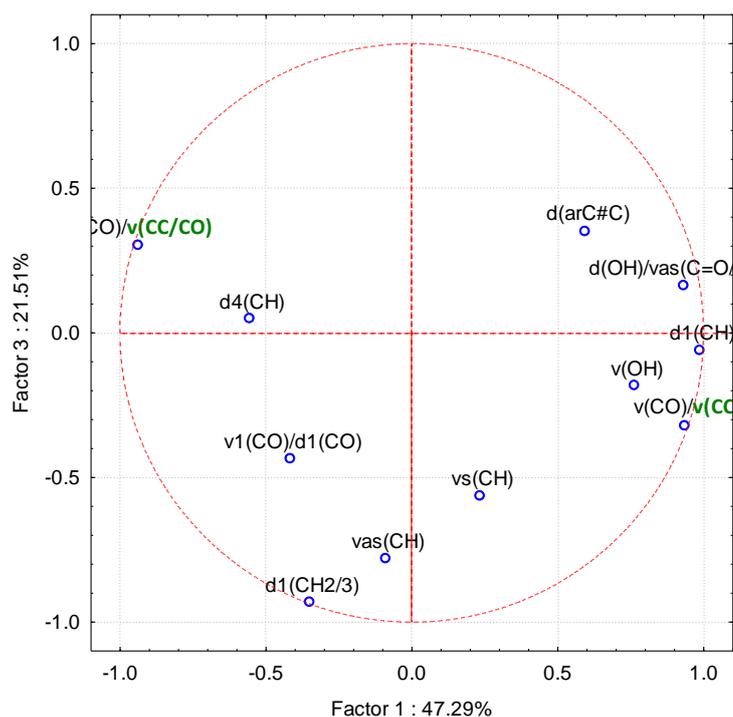
	<b>PC<sub>1</sub></b>	<b>PC<sub>2</sub></b>	<b>PC<sub>3</sub></b>
<b>v(OH)</b>	0.555	0.809	0.093
<b>I_v(OH)</b>	-0.492	-0.805	0.027
<b>vas(CH)</b>	-0.019	-0.379	0.866
<b>I_vas(CH)</b>	0.524	-0.452	0.670
<b>vs(CH)</b>	-0.049	0.902	0.392
<b>I_vs(CH)</b>	0.552	-0.531	0.521
<b>d(OH)/vas(C=O/C=C)</b>	0.980	-0.039	-0.068
<b>I_d(OH)/vas(C=O/C=C)</b>	0.696	-0.621	-0.349
<b>d(arC#C)</b>	0.786	-0.533	-0.183
<b>I_d(arC#C)</b>	0.797	-0.380	-0.448
<b>d1(CH<sub>2</sub>/3)</b>	-0.450	0.099	0.867
<b>I_d1(CH<sub>2</sub>/3)</b>	0.809	0.374	0.375
<b>v1(CO)/d1(CO)</b>	-0.259	-0.714	0.536
<b>I-v1(CO)/d1(CO)</b>	-0.383	-0.323	0.365
<b>d1(CH)</b>	0.898	0.430	0.073
<b>I_d1(CH)</b>	0.883	0.300	-0.163
<b>v(CO)/v(CC)</b>	0.882	0.243	0.364
<b>I_v(CO)/v(CC)</b>	0.356	-0.801	-0.469
<b>v(CO)/v(CC/CO)</b>	-0.826	-0.430	-0.296
<b>I_v(CO)/v(CC/CO)</b>	-0.023	-0.992	-0.004
<b>d4(CH)</b>	-0.693	0.444	-0.202
<b>I-d4(CH)</b>	0.337	-0.897	0.223



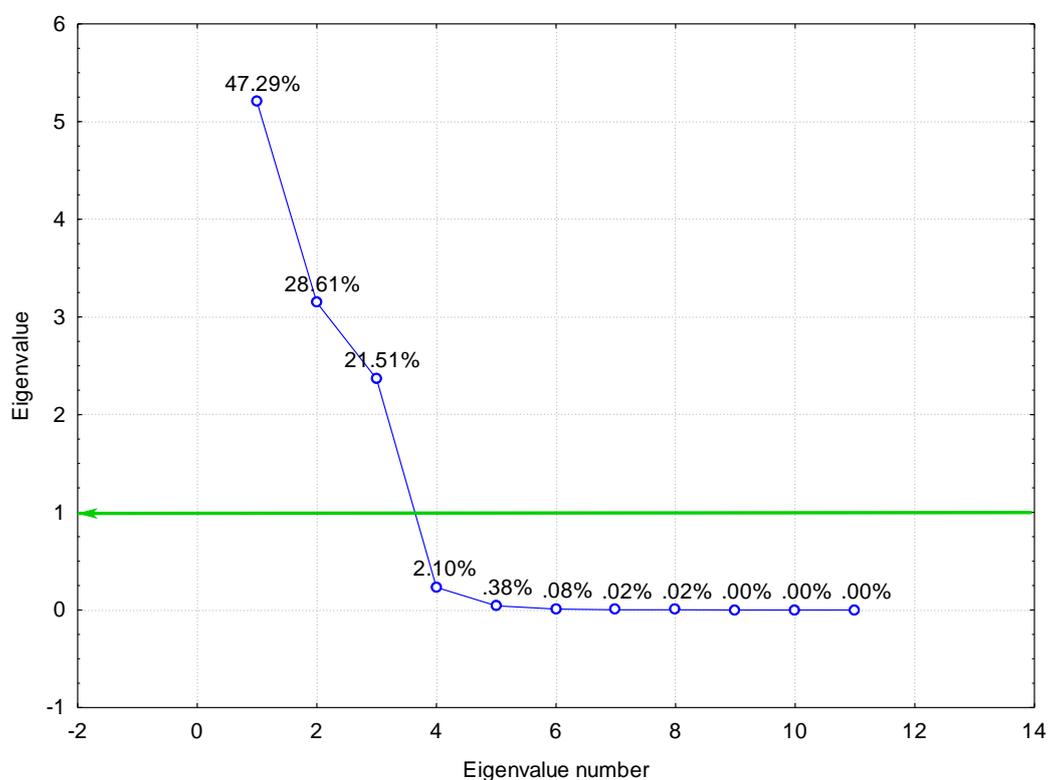
**Figure S16:** PC<sub>3</sub> versus PC<sub>1</sub> scores plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants (codes: “H” – hesperidin, “N” – naringin, “R” – rutin and “S” – silymarin); only wavenumbers of the FTIR bands were used as input variables.



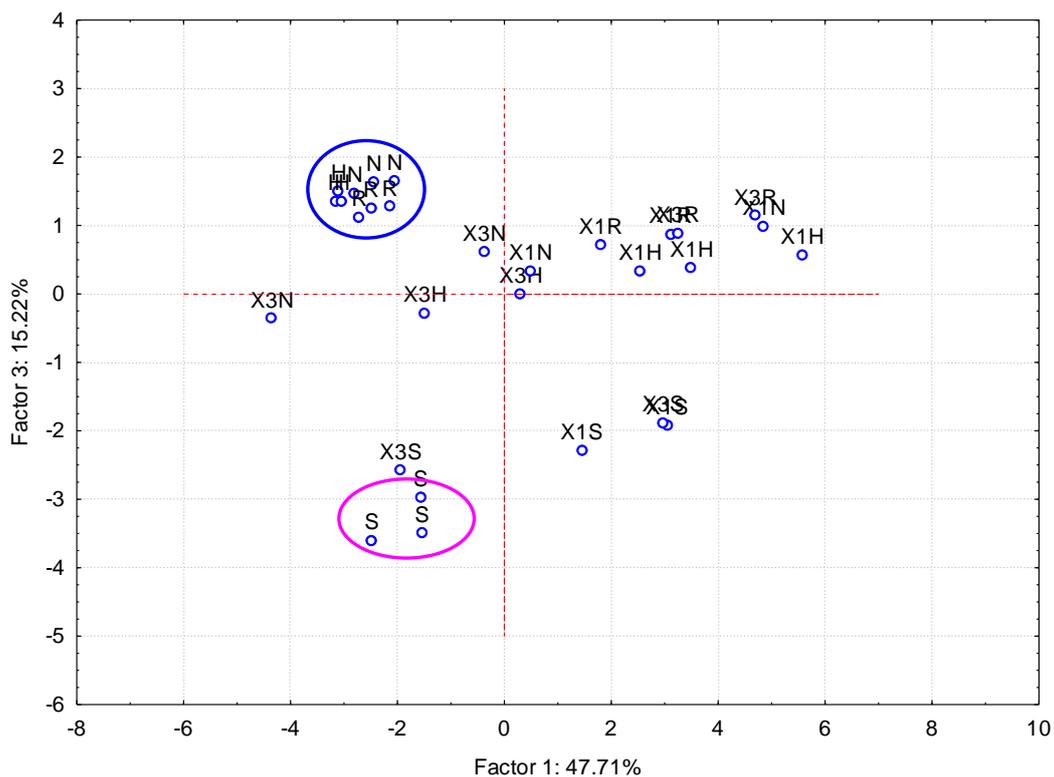
**Figure S17:** PC<sub>2</sub> versus PC<sub>1</sub> loadings plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; only wavenumbers of the FTIR bands were used as input variables (see Table S11 for codes).



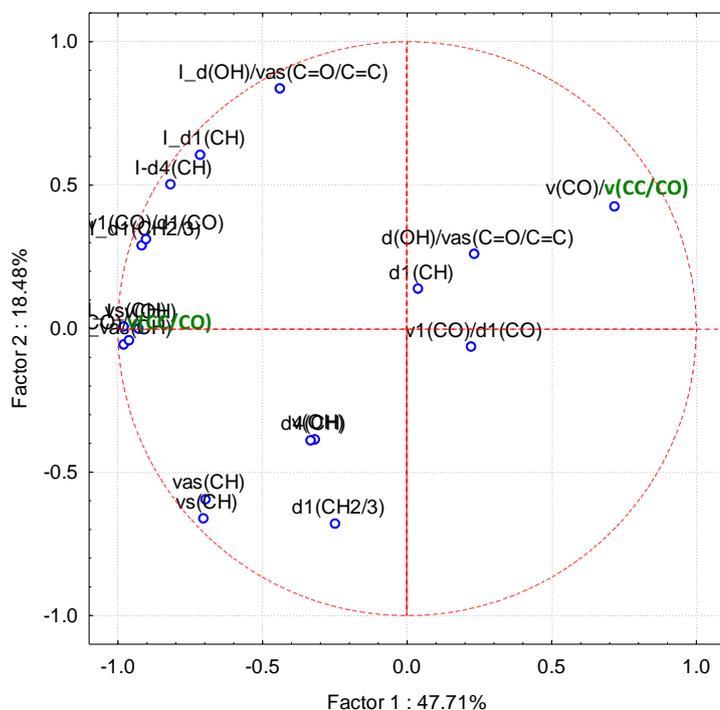
**Figure S18:** PC<sub>3</sub> versus PC<sub>1</sub> loadings plot from the FTIR–PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; only wavenumbers of the FTIR bands were used as input variables (see Table S11 for codes).



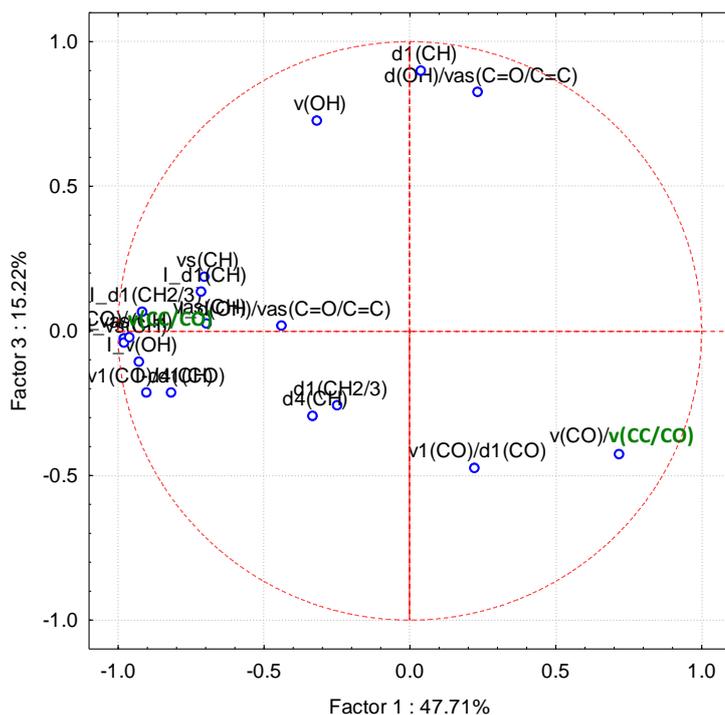
**Figure S19:** Eigenvalues of the correlation matrix from the FTIR–PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; only wavenumbers of the FTIR bands were used as input variables (see Table S11 for codes); the first three PCs can be retained, which explain 97.41% from the variance of the data.



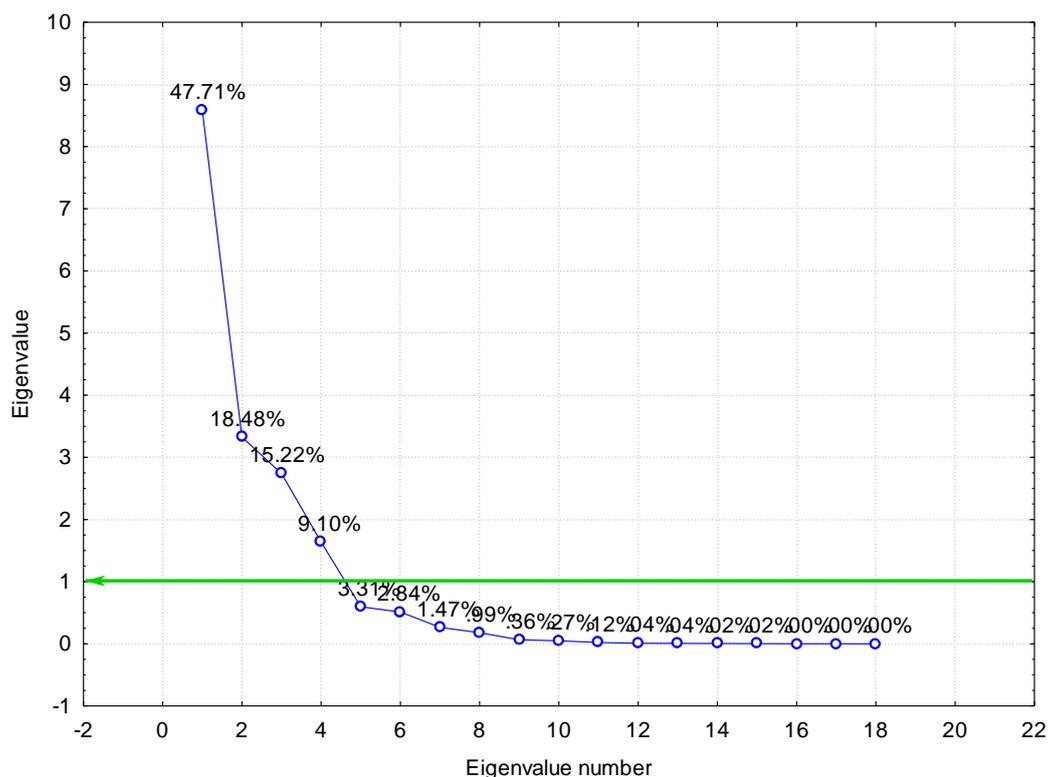
**Figure S20:** PC<sub>3</sub> versus PC<sub>1</sub> scores plot from the FTIR-PCA analysis of the  $\beta$ -CD/hazelnut oil/flavonoid 1:1:1 and 3:1:1 ternary complexes (codes: “X1H/N/R/S” and “X3H/N/R/S”) with hesperidin/naringin/rutin/silymarin, respectively) and flavonoids (codes: “H” – hesperidin, “N” – naringin, “R” – rutin and “S” – silymarin); all wavenumber and intensity of the FTIR bands were used as input variables.



**Figure S21:** PC<sub>2</sub> versus PC<sub>1</sub> loadings plot from the FTIR-PCA analysis of the  $\beta$ -CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S12 for codes).



**Figure S22:** PC<sub>3</sub> versus PC<sub>1</sub> loadings plot from the FTIR–PCA analysis of the β-CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S12 for codes).



**Figure S23:** Eigenvalues of the correlation matrix from the FTIR–PCA analysis of the β-CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S12 for codes); the first four PCs can be retained, which explain 90.51% from the variance of the data.

**Table S11:** Factor coordinates (principal components, PCs) of the variables, based on correlations, from the FTIR–PCA analysis of the  $\beta$ -CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber (“v” – for stretching vibrations, “d” – for bending vibrations) and intensity (designed as “I\_v/d”) of the FTIR bands were used as input variables.

	PC <sub>1</sub>	PC <sub>2</sub>	PC <sub>3</sub>	PC <sub>4</sub>
v(OH)	-0.318	-0.387	0.727	0.169
I_v(OH)	-0.928	-0.001	-0.109	-0.015
vas(CH)	-0.695	-0.595	0.023	-0.305
I_vas(CH)	-0.979	-0.056	-0.026	-0.056
vs(CH)	-0.702	-0.662	0.185	-0.014
I_vs(CH)	-0.979	0.005	-0.042	-0.043
d(OH)/vas(C=O/C=C)	0.235	0.258	0.824	-0.372
I_d(OH)/vas(C=O/C=C)	-0.437	0.834	0.016	-0.246
d1(CH <sub>2</sub> /3)	-0.247	-0.680	-0.259	-0.298
I_d1(CH <sub>2</sub> /3)	-0.914	0.290	0.063	0.067
v1(CO)/d1(CO)	0.222	-0.065	-0.475	-0.758
I-v1(CO)/d1(CO)	-0.901	0.310	-0.215	0.146
d1(CH)	0.040	0.136	0.899	0.035
I_d1(CH)	-0.712	0.605	0.135	0.178
v(CO)/v(CC/CO)	0.718	0.426	-0.426	0.223
I_v(CO)/v(CC/CO)	-0.961	-0.044	-0.022	-0.075
d4(CH)	-0.334	-0.390	-0.294	0.717
I-d4(CH)	-0.817	0.501	-0.213	-0.148

**Table S12:** Factor coordinates (principal components, PCs) of the variables, based on correlations, from the FTIR–PCA analysis of the  $\beta$ -CD/hazelnut oil/flavonoid ternary complexes and flavonoids; only wavenumbers (“v” – for stretching vibrations, “d” – for bending vibrations) of the FTIR bands were used as input variables.

	PC <sub>1</sub>	PC <sub>2</sub>	PC <sub>3</sub>
v(OH)	0.683	-0.551	0.141
vas(CH)	0.888	0.177	-0.270
vs(CH)	0.981	0.048	0.009
d(OH)/vas(C=O/C=C)	-0.153	-0.890	-0.370
d1(CH <sub>2</sub> /3)	0.562	0.441	-0.372
v1(CO)/d1(CO)	-0.216	0.461	-0.787
d1(CH)	0.073	-0.916	0.011
v(CO)/v(CC/CO)	-0.904	0.236	0.190
d4(CH)	0.411	0.410	0.703