Supporting Information File 1

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

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

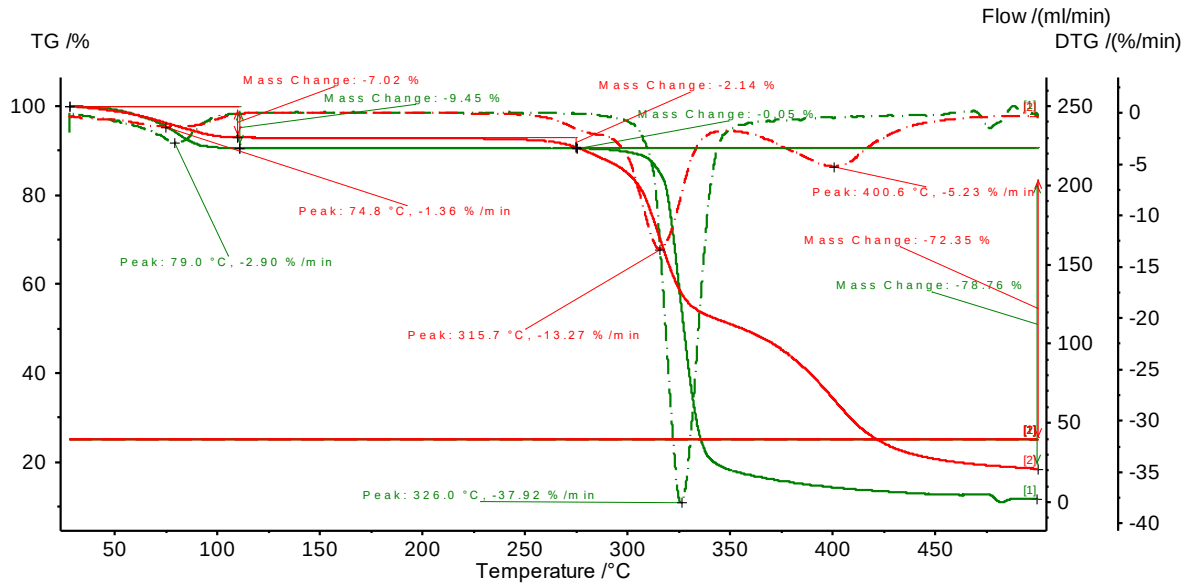

Figure S1: Superimposed TG-DTG thermograms for β-cyclodextrin/hazelnut oil/hesperidin ternary complex at 1:1:1 molar ratio (code X1H, red) and β-cyclodextrin hydrate (green)

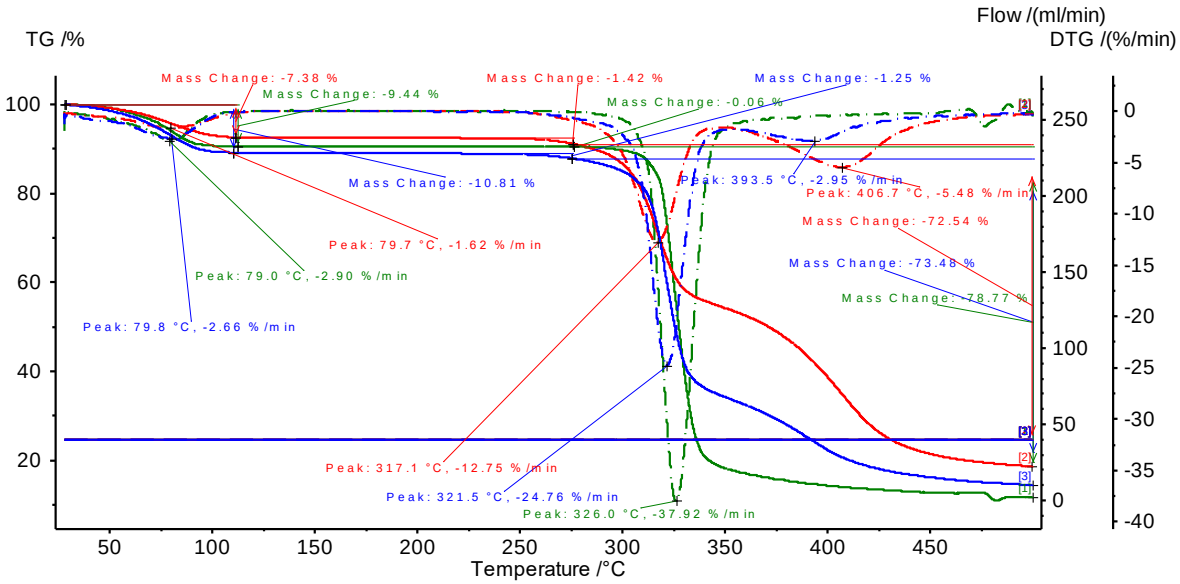

Figure S2: Superimposed TG-DTG thermograms for β-cyclodextrin/hazelnut oil/naringin ternary complex at 1:1:1 (code X1N, red) and 3:1:1 molar ratios (code X3N, blue), in comparison with the β-cyclodextrin hydrate (green)

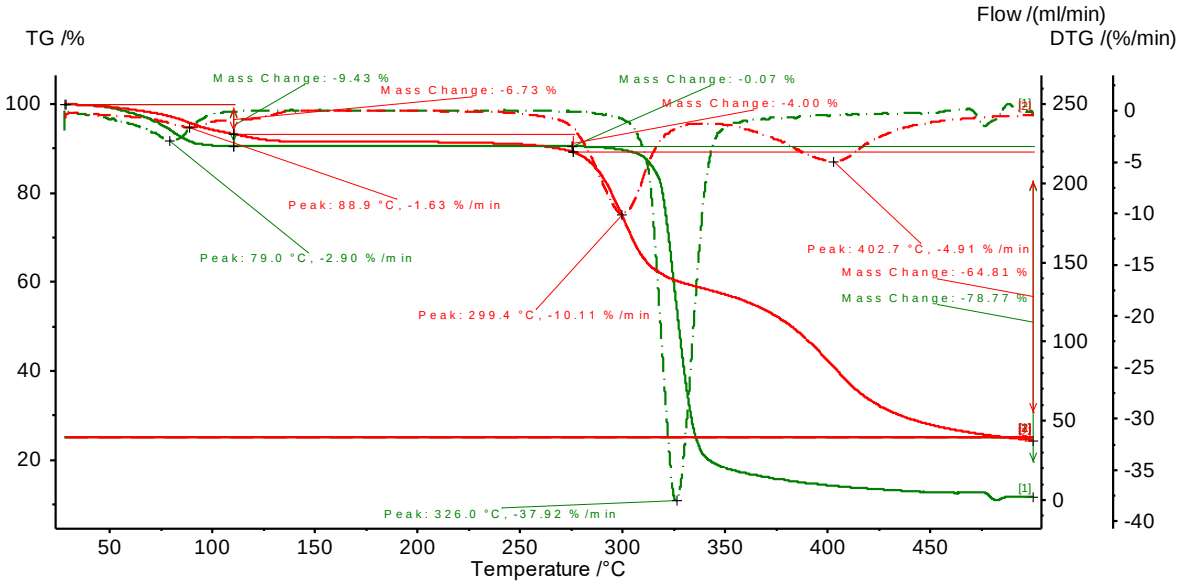

Figure S3: Superimposed TG-DTG thermograms for β-cyclodextrin/hazelnut oil/rutin ternary complex at 1:1:1 molar ratio (code X1R, red) and β-cyclodextrin hydrate (green)

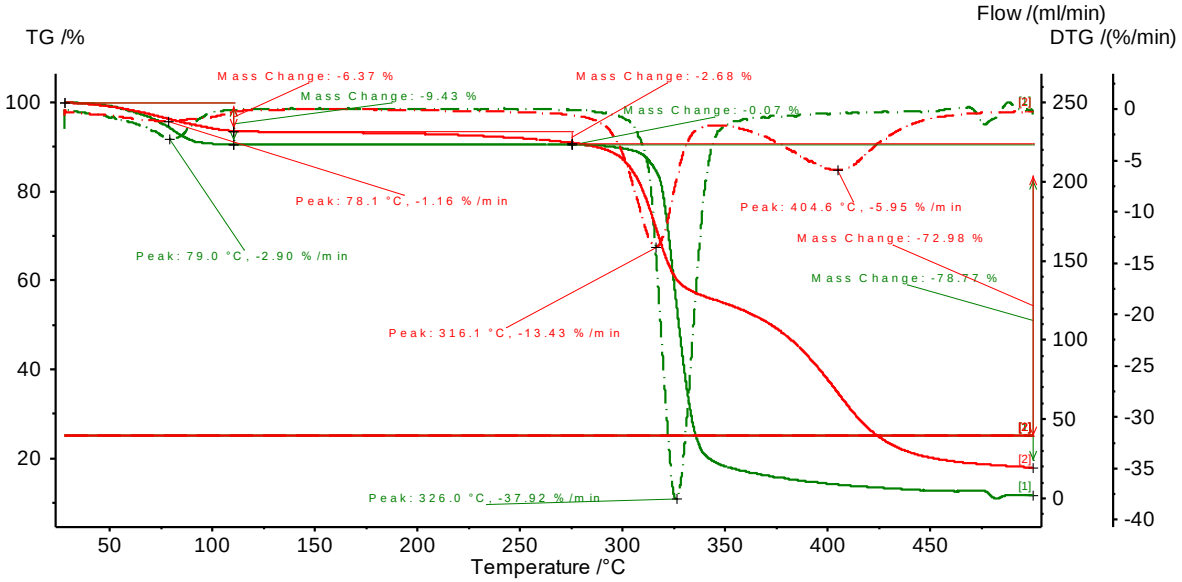

Figure S4: Superimposed TG-DTG thermograms for β-cyclodextrin/hazelnut oil/silymarin ternary complex at 1:1:1 molar ratio (code X1S, red) and β-cyclodextrin hydrate (green)

Table S1: TG results (mass loss, %, for specific temperature ranges) for the β-cyclodextrin hydrate (β-CD) and the β-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$_{(<110\ °C)}$ (%)	Mass loss$_{(110\text{-}275\ °C)}$ (%)	Mass loss$_{(>275\ °C)}$ (%)
1	β-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 the β-cyclodextrin hydrate (β-CD) and the β-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	$t_{DTG1(<110°C)}$ (°C)	$t_{DTG2(275\text{-}350°C)}$ (°C)	$t_{DTG3(>350°C)}$ (°C)
1	β-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

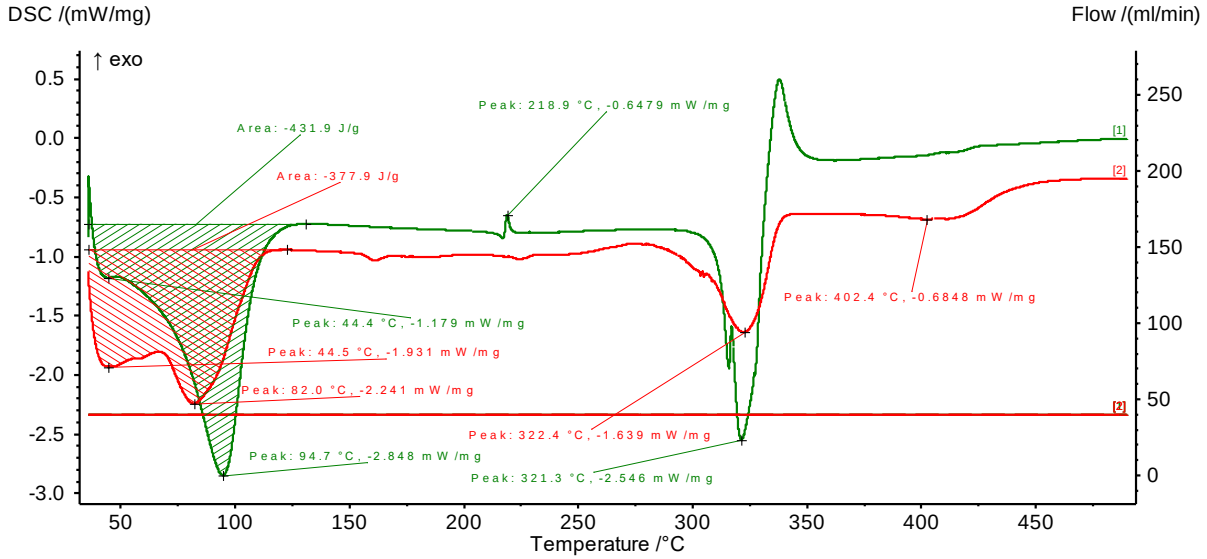

Figure S5: Superimposed DSC plots for β-cyclodextrin/hazelnut oil/naringin ternary complex at 1:1:1 molar ratio (code X1N, red) and β-cyclodextrin hydrate (green)

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 the β-cyclodextrin hydrate (β-CD) and the β-cyclodextrin/hazelnut oil/naringin ternary complex at 1:1:1 molar ratio (code X1N)

No	Code	$Area_{DSC(<110°C)}$ J/g	$t_{DSC1(<110°C)}$ (°C)	$t_{DSC2(<110°C)}$ (°C)	$t_{DSC3(140-275°C)}$ (°C)	$t_{DSC4(275-350°C)}$ (°C)	$t_{DSC5(>350°C)}$ (°C)
1	β-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

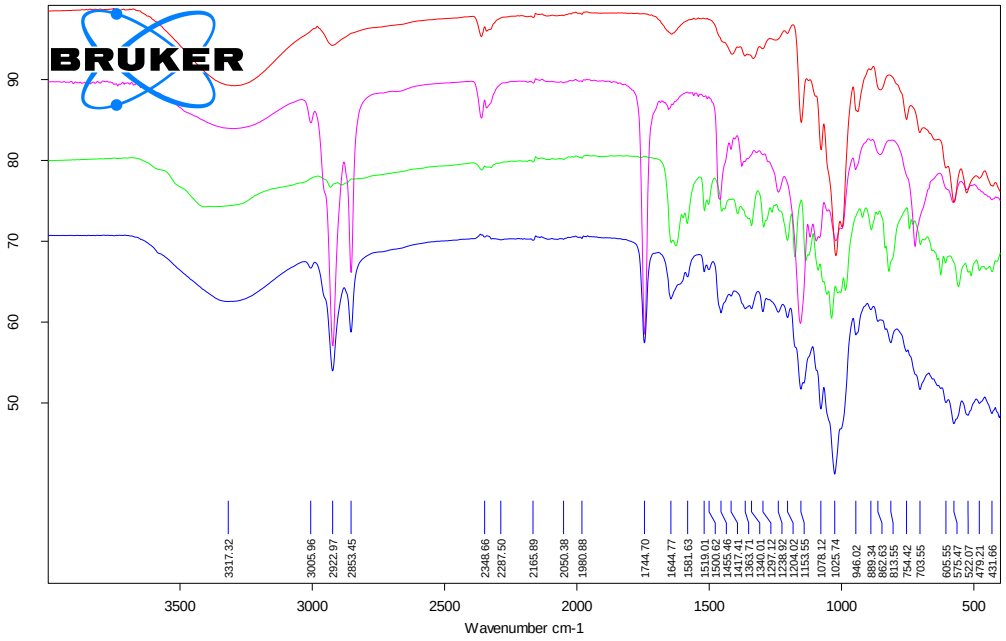

Figure S6: Superposition of the FTIR spectra for β-cyclodextrin/*Corylus avellana* oil/Naringin ternary complex at 1:1:1 molar ratio (blue), β-cyclodextrin hydrate (red), *C. avellana* oil (pink) and naringin (green)

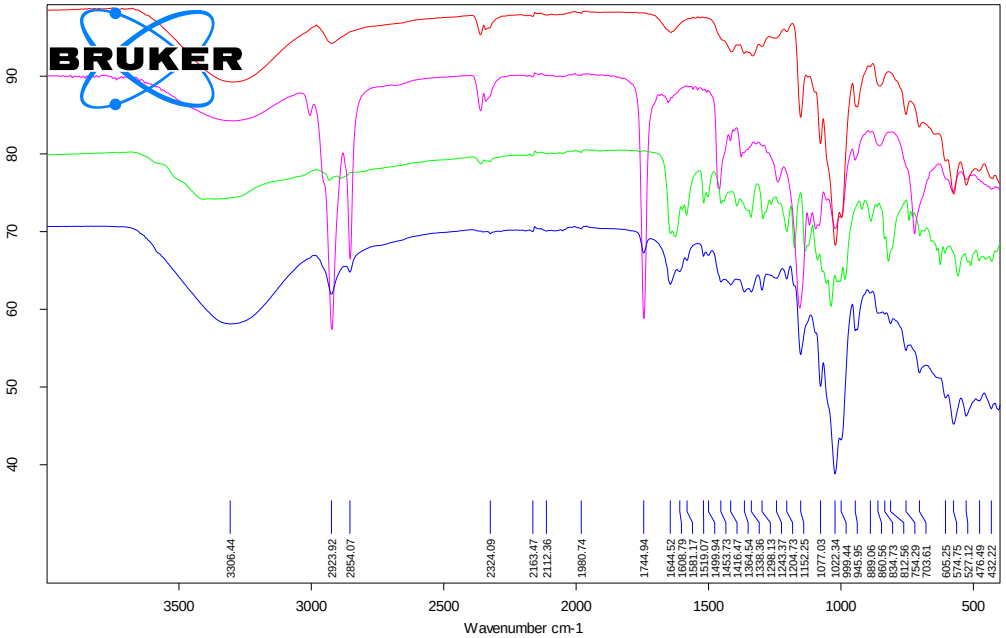

Figure S7: Superposition of the FTIR spectra for β-cyclodextrin/*Corylus avellana* oil/Naringin ternary complex at 3:1:1 molar ratio (blue), β-cyclodextrin hydrate (red), *C. avellana* oil (pink) and naringin (green)

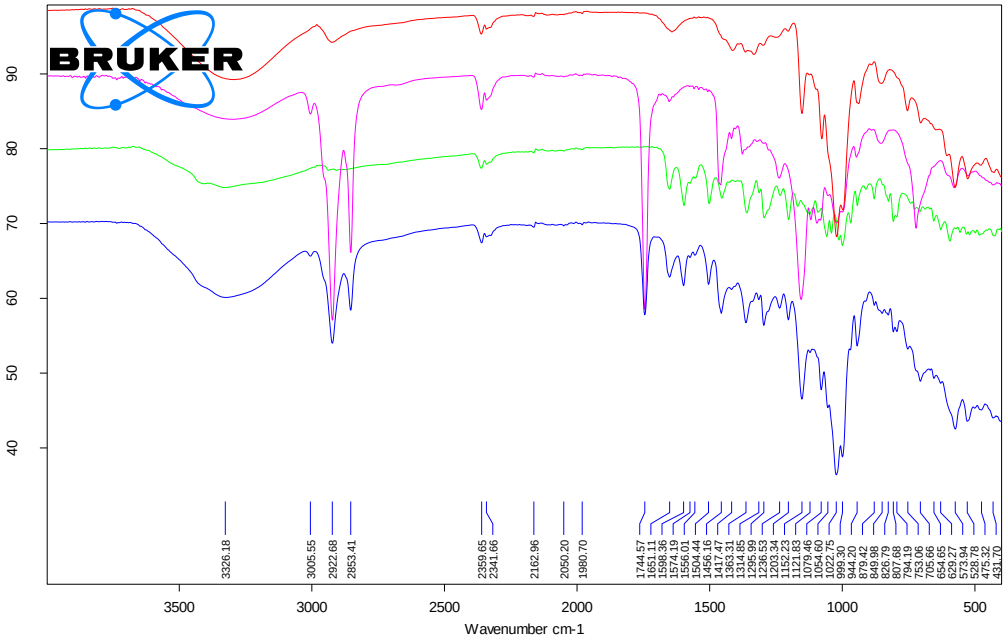

Figure S8: Superposition of the FTIR spectra for β-cyclodextrin/*Corylus avellana* oil/Rutin ternary complex at 1:1:1 molar ratio (blue), β-cyclodextrin hydrate (red), *C. avellana* oil (pink) and rutin (green)

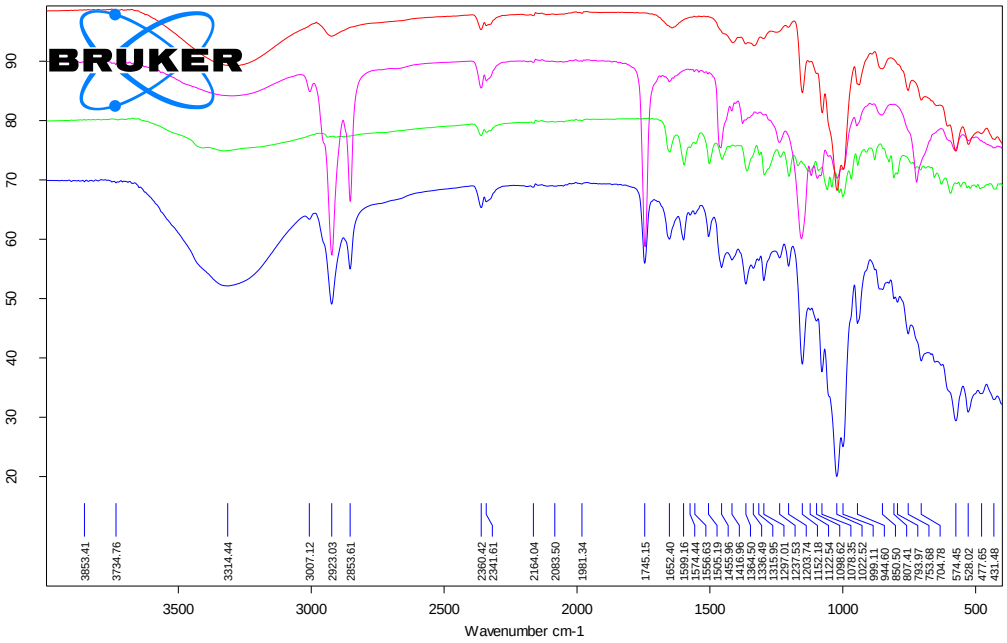

Figure S9: Superposition of the FTIR spectra for β-cyclodextrin/*Corylus avellana* oil/Rutin ternary complex at 3:1:1 molar ratio (blue), β-cyclodextrin hydrate (red), *C. avellana* oil (pink) and rutin (green)

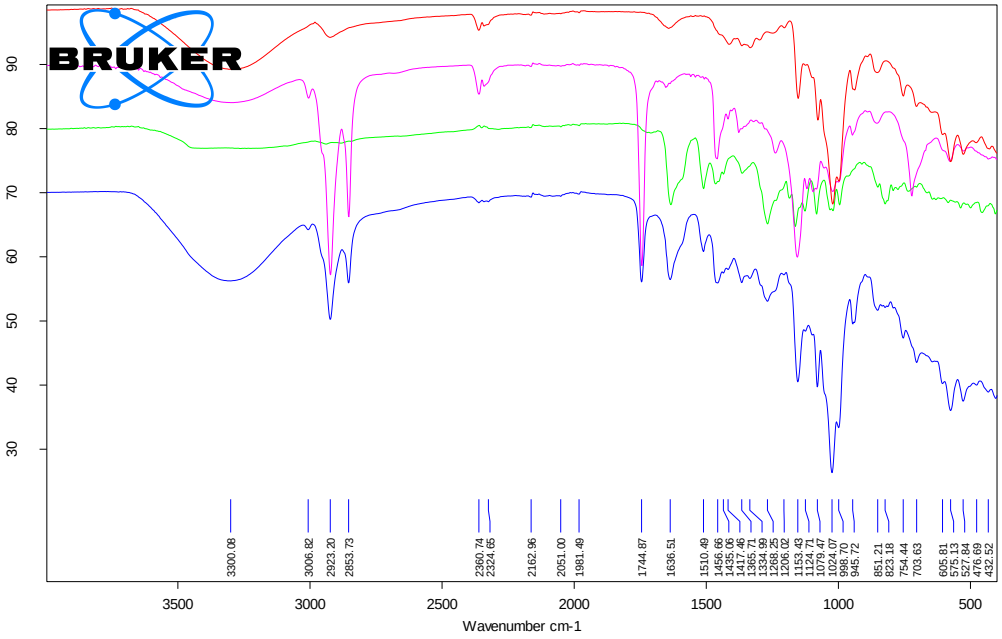

Figure S10: Superposition of the FTIR spectra for β-cyclodextrin/*Corylus avellana* oil/Silymarin ternary complex at 1:1:1 molar ratio (blue), β-cyclodextrin hydrate (red), *C. avellana* oil (pink) and silymarin (green)

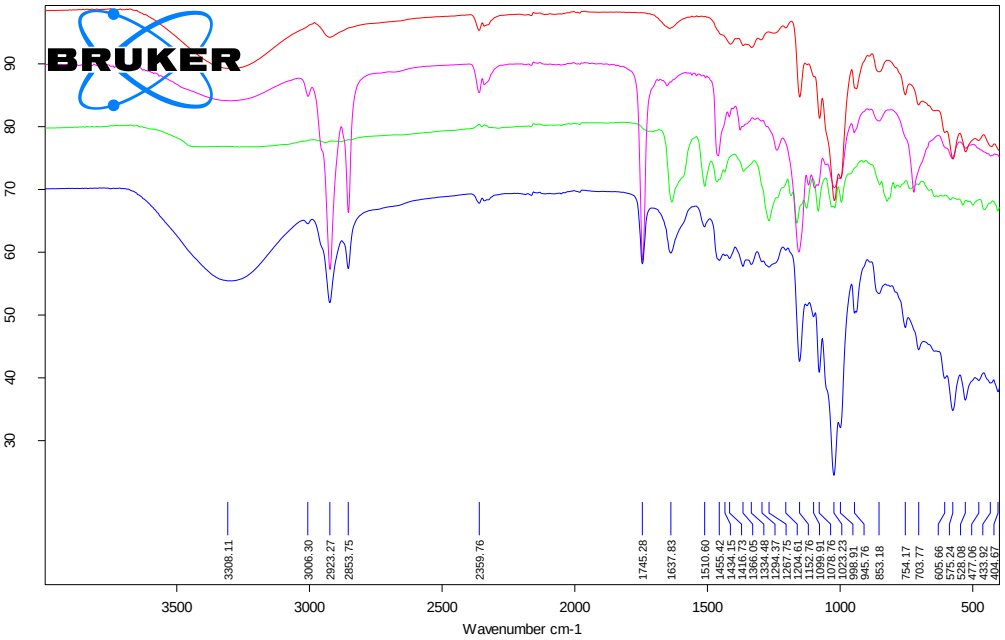

Figure S11: Superposition of the FTIR spectra for β-cyclodextrin/*Corylus avellana* oil/Silymarin ternary complex at 3:1:1 molar ratio (blue), β-cyclodextrin hydrate (red), *C. avellana* oil (pink) and silymarin (green)

Table S4: FTIR band assignments for β-CD hydrate (mean(±SD) of triplicate determinations)

Wavenumber (cm^{-1})	Band assignment
3301.6(±8.5)	ν_{OH}, stretching vibration of the O-H groups in β-CD and water
2924.8(±1.4)	ν^{as}_{CH}, stretching vibrations of the C-H groups
1643.3(±1.8)	δ_{OH}, bending vibrations of the O-H groups
1451(±0.2)	δ_{CH2}, symmetric bending vibrations of the CH_2 groups
1413.7(±0.8)	δ_{OH}, in-plane bending vibrations of the O-H groups
1364.9(±0.3)	δ_{CH2}, asymmetric bending vibrations of the CH_2 groups
1333.8(±0.2)	δ_{OH}, bending vibrations of the O-H groups
1297.9(±0.4)	δ_{CH}, in-plane bending vibrations of the C-H groups (*tentative*)
1248(±0.9)	δ_{CH}, in-plane bending vibrations of the C-H groups (*tentative*)
1204.7(±0.3)	δ_{CH}, in-plane bending vibrations of the C-H groups (*tentative*)
1152.1(±0.1)	ν^{s}_{COC}, stretching vibrations of the C-O-C groups in glucosydic moieties
1077.2(±0.1)	ν_{CC}, stretching vibrations of the C-C groups
1020.9(±0.3)	ν_{CO}, stretching vibrations of the C-O groups
997.7(±0.2)	ν_{CO}, stretching vibrations of the C-O groups (*tentative*)
939.2(±1.8)	ν_{rgCH}, stretching vibrations of the C-H groups from the β-cyclodextrin ring
852.9(±0.8)	δ_{CCH}, bending vibrations of the C-C-H groups (the α-type glycosidic bonds)
754.4(±0.3)	δ_{CH}, bending vibrations of the C-H groups (*tentative*)
704(±0.7)	δ_{CH}, bending vibrations of the C-H groups (*tentative*)
648.1(±0.9)	*not assigned*
574.2(±0.8)	δ_{OCC}, bending vibrations of the O-C-C groups (*tentative*)
526.3(±1.3)	ν_{CC}, stretching vibrations of the C-C groups (*tentative*)

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

Wavenumber (cm^{-1})	Band assignment
3287.8(±10)	ν_{OH}, stretching vibrations of the O-H groups from the free fatty acids and water
3005(±0.2)	$\nu^{s}_{=CH}$, symmetric stretching vibrations of the =CH groups
2952.5(±0.3)	ν^{as}_{CH}, asymmetric stretching vibrations of the CH groups
2922.5(±0)	ν^{as}_{CH}, symmetric stretching vibrations of the CH groups
2853.2(±0)	ν^{s}_{CH}, symmetric stretching vibrations of the CH groups
1744(±0)	$\nu_{estC=O}$, stretching vibrations of the esteric C=O groups in triglycerides
1710.3(±0.7)	$\nu_{faC=O}$, stretching vibrations of the C=O groups in free fatty acids (shoulder)
1652.7(±0.3)	$\nu_{cC=C}$, stretching vibrations of the *cis*RHC=CHR' groups
1458.7(±0.2)	$\delta_{CH2/3}$, deformation vibrations of the CH_2 and CH_3 groups

1417.6(±0.1)	$\delta_{rk,=CH}$, rocking vibrations of the =C–H groups in *cis*RHC=CHR'
1376.7(±0)	δ_{CH2}, bending vibrations of the CH_2 groups
1236.8(±1.3)	δ_{CH2}, bending vibrations of the CH_2 groups
1158.1(±2.3)	δ_{CH2}, bending vibrations of the CH_2 groups
1094.7(±0.7)	ν_{CO}, stretching vibrations of the C-O groups
1027.9(±5.7)	ν_{CO}, stretching vibrations of the C-O groups
956.7(±8.7)	$\delta_{tC=C}$, bending vibrations of the C=C groups in *trans*RHC=CHR'
722(±0.1)	δ_{opCH}, out-of-plane deformation vibrations in the C-H groups

Table S6: FTIR band assignments for hesperidin and the corresponding β-cyclodextrin/hazelnut oil/hesperidin 1:1:1 and 3:1:1 ternary complexes (codes "X1H and X3H); bands associated to β-CD or hazelnut oil are also specified; wavenumbers (cm^{-1}) are expressed as mean(±SD) of triplicate determinations for hesperidin and duplicate determinations for the ternary complexes

Wavenumber (cm^{-1})			**Band assignment**
Hesperidin	**X1H**	**X3H**	
3540.5(±1)	-	-	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water)
3467.5(±1.3)	-	-	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water)
3411.3(±0.5)	3312.1(±2.8)	3306.2(±2.1)	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from β-CD)
-	3006.5(±1)	3009.6(±0.8)	$\nu^{s}_{=CH}$, symmetric stretching vibrations of the =CH groups (from hazelnut oil)
2982(±0.5)	-	-	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups
2940.8(±0.8)	-	-	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups
2914.2(±0.9)	2922.4(±0.1)	2922.6(±0.1)	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups (also from hazelnut oil)
2895.6(±0.4)	-	-	ν^{s}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_2 groups
-	2853.4(±0)	2853.5(±0.2)	ν^{s}_{CH}, symmetric stretching vibrations of the CH groups (from hazelnut oil)
-	1745(±0.1)	1745(±0.1)	$\nu_{estC=O}$, 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)	$\nu^{as}_{C=O/C=C}$, asymmetric stretching vibrations of the C=O/C=C groups
1604.4(±0.1)	1605.9(±0.1)	1606.8(±0.3)	$\nu_{CC}/\delta_{arC\#C}$, 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)	$\delta_{arC\#C}$, bending vibrations of the aromatic C#C groups
1504.1(±0.3)	1505.8(±0.7)	1505.1(±1.2)	ν_{CC}, stretching of C-C group in the ring C
1467.5(±1.1)	1457.6(±0.7)	1456.5(±0.3)	δ_{CH3}, asymmetric bending vibrations of the CH_3 groups
1442.5(±0.4)	1445(±0.3)	1446.5(±0.1)	δ_{CH3}, asymmetric bending vibrations of the CH_3 groups
-	1416.6(±0.5)	1416.1(±0.2)	δ_{OH}, in-plane bending vibrations of the O-H groups (from β-CD)
1404(±1)	-	-	$\delta_{CH3}/\delta_{HOC}$, symmetric bending vibrations of the CH_3 groups/in-plane bending vibrations of the H-O-C groups
1356.6(±0.5)	1357(±0)	1365(±0.4)	ν_{CO}, stretching vibrations of the C-O groups
1339.9(±0.6)	1339.1(±0.3)	1336.9(±0.3)	$\delta_{CH3}/\delta_{OCC}$, symmetric bending vibrations of the CH_3/OCC groups (also from β-CD)
1298.2(±0.2)	1299(±0.1)	1298.9(±0)	$\delta_{CH}/\delta_{OCH}/\nu_{CC}$, 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)	ν_{CO}, stretching vibrations of the C-O groups (carbohydrates and phenolics)

-	1241.4(±0.1)	1242.5(±0.4)	δ_{CH2}, bending vibrations of the CH_2 groups (from hazelnut oil)
1203.3(±0.6)	1204.4(±0)	1204.6(±0)	ν_{CC}/ν_{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)	$\nu_{CO}/\delta_{HCC/HOC}/\nu_{CC}$, 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
-	1153.5(±0.3)	1152.6(±0.1)	ν^{s}_{COC}, stretching vibrations of the C-O-C groups in glucosydic moieties (from β-CD)
1130(±0.1)	1131.9(±0.4)	1130.5(±0.3)	$\nu_{CO}/\delta_{CCH}/\tau_{CH2}$, stretching vibrations of the C-O groups/ bending vibrations of the C-C-H groups/"twisting" bending vibrations of the CH_2 groups
1093.9(±0.2)	1095(±0.1)	1096.5(±0.3)	ν_{CC}, stretching vibrations of the C-C groups
-	1077.9(±0.2)	1077.4(±0)	ν_{CC}, stretching vibrations of the C-C groups (from β-CD)
1065.5(±1.2)	-	-	ν_{CO}, stretching vibrations of the C-O groups
1053.3(±2.7)	1049.5(±0.3)	1050.4(±0.6)	ν_{CO}, stretching vibrations of the C-O groups
1030.8(±2.3)	-	-	ν_{CO}/ν_{CC}, stretching vibrations of the C-O/C-C groups in the ring B
-	1023.9(±0.5)	1022.3(±0.2)	ν_{CO}, stretching vibrations of the C-O groups (from β-CD)
1010.5(±1.5)	-	-	ν_{CO}/ν_{CC}, stretching vibrations of the C-O/C-C groups (*tentative*)
971.7(±0.9)	-	-	ν_{OC}, stretching vibrations of the O-C groups
-	946.1(±0.1)	946(±0)	ν_{rgCH}, stretching vibrations of the C-H groups from the β-cyclodextrin ring (from β-CD)
911.5(±0.6)	911.6(±0.1)	911.7(±0.6)	τ_{HCCC}, "twisting" bending vibrations of the H-C-C-C groups
-	861.8(±0.2)	861.9(±0.6)	δ_{CCH}, bending vibrations of the C-C-H groups (the α-type glycosidic bonds) (from β-CD)
-	847.6(±0)	848.1(±0)	δ_{CCH}, bending vibrations of the C-C-H groups (the α-type glycosidic bonds) (from β-CD) (*tentative*)
814.1(±0.8)	815.2(±0)	815(±0.1)	δ_{CH}, out-of-plane bending vibrations of the C-H groups
741.5(±1.4)	743.1(±0)	743.5(±0)	τ_{COH}, "twisting" bending vibrations of the C-O-H groups
-	576.1(±0.1)	575.3(±0.4)	δ_{OCC}, bending vibrations of the O-C-C groups (from β-CD) (*tentative*)
-	526.6(±0.2)	527.4(±0.2)	ν_{CC}, stretching vibrations of the C-C groups (from β-CD) (*tentative*)

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

Wavenumber (cm^{-1})			**Band assignment**
Naringin	**X1N**	**X3N**	
3405.3(±4)	3321(±5.2)	3295.8(±15)	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from β-CD)
-	3006.4(±0.6)	3008.8(±0.8)	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water)
2930.8(±0.6)	2923.1(±0.2)	2923.6(±0.4)	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups (also from hazelnut oil)
2889.9(±0.2)	-	-	ν^{s}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_2 groups
-	2853.5(±0.1)	2853.7(±0.6)	ν^{s}_{CH}, symmetric stretching vibrations of the CH groups (from hazelnut oil)
-	1745(±0.4)	1743.6(±1.9)	$\nu_{estC=O}$, 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)	$\nu^{as}_{C=O/C=C}$, asymmetric stretching vibrations of the C=O/C=C groups
1625.8(±0.1)	1606.6(±0.1)	1608.8*	$\nu_{CC}/\delta_{arC\#C}$, stretching vibrations of the C-C group in the ring C / bending vibrations of the aromatic C#C groups
1583.2(±0.1)	-	-	$\nu_{CC}/\delta_{arC\#C}$, 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)	$\delta_{arC\#C}$, bending vibrations of the aromatic C#C groups
1502.6(±0.1)	1500.5(±0.2)	1501.3(±2)	ν_{CC}, stretching of C-C group in the ring C
1452.6(±0.1)	1455.1(±0.5)	1453.4(±0.4)	δ_{CH3}, asymmetric bending vibrations of the CH_3 groups
1441.9(±0.1)	1444.3(±0.1)	1444.4*	δ_{CH3}, asymmetric bending vibrations of the CH_3 groups
-	1417.4(±0)	1415.5(±1.4)	δ_{OH}, in-plane bending vibrations of the O-H groups (from β-CD)
1392.6(±0.1)	-	-	$\delta_{CH3}/\delta_{HOC}$, symmetric bending vibrations of the CH_3 groups/in-plane bending vibrations of the H-O-C groups
1339.9(±0)	1339.7(±0.4)	1339.4(±1.5)	$\delta_{CH3}/\delta_{OCC}$, symmetric bending vibrations of the CH_3/OCC groups (also from β-CD)
1294.1(±0.1)	1297.1(±0)	1297.7(±0.7)	$\delta_{CH}/\delta_{OCH}/\nu_{CC}$, 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)	ν_{CC}/ν_{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)	$\nu_{CO}/\delta_{HCC/HOC}/\nu_{CC}$, 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
-	1153.2(±0.5)	1152.6(±0.4)	ν^{s}_{COC}, stretching vibrations of the C-O-C groups in glucosydic moieties (from β-CD)
1135(±0.1)	1141.1(±0.2)	-	$\nu_{CO}/\delta_{CCH}/\tau_{CH2}$, stretching vibrations of the C-O groups/ bending vibrations of the C-C-H groups/"twisting" bending vibrations of the CH_2 groups
1088.2(±0.3)	1095.1(±0.5)	1096.5(±0.2)	ν_{CC}, stretching vibrations of the C-C groups
-	1077.7(±0.7)	1077(±0.1)	ν_{CC}, stretching vibrations of the C-C groups (from β-CD)
1054.9(±0)	1048.1(±0.8)	1051.1(±1.3)	ν_{CO}, stretching vibrations of the C-O groups
1037.4(±0.2)	-	-	ν_{CO}/ν_{CC}, stretching vibrations of the C-O/C-C groups in the ring B
-	1025.7(±0.1)	1022(±0.5)	ν_{CO}, stretching vibrations of the C-O groups (from β-CD)
1014.3(±0.3)	-	-	ν_{CO}/ν_{CC}, stretching vibrations of the C-O/C-C groups (*tentative*)
985.1(±0.1)	-	-	ν_{OC}, stretching vibrations of the O-C groups
-	945.9(±0.1)	946.4(±0.6)	ν_{rgCH}, stretching vibrations of the C-H groups from the β-cyclodextrin ring (from β-CD)
920.8(±0)	911.4(±0.2)	-	τ_{HCCC}, "twisting" bending vibrations of the H-C-C-C groups
-	862.9(±0.4)	858.2(±3.4)	δ_{CCH}, bending vibrations of the C-C-H groups (the α-type glycosidic bonds) (from β-CD)
820.8(±0)	813.5(±0.1)	813.9(±1.8)	δ_{CH}, out-of-plane bending vibrations of the C-H groups
743.4(±0.1)	-	-	τ_{COH}, "twisting" bending vibrations of the C-O-H groups
-	575.5(±0)	574.7(±0)	δ_{OCC}, bending vibrations of the O-C-C groups (from β-CD) (*tentative*)
-	524.2(±3)	526.4(±1)	ν_{CC}, stretching vibrations of the C-C groups (from β-CD) (*tentative*)

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

Wavenumber (cm^{-1})			Band assignment
Rutin	**X1R**	**X3R**	
3407.4(±2.2)	-	-	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from β-CD)
3325(±7.3)	3325.1(±1.5)	3310.8(±5.1)	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water)
-	3006.3(±1.1)	3007.5(±0.5)	$\nu^{s}_{=CH}$, symmetric stretching vibrations of the =CH groups (from hazelnut oil)
2938(±0)	-	-	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups
2907.3(±0.2)	2922.8(±0.2)	2923.1(±0)	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups (also from hazelnut oil)
2875.9(±0.4)	-	-	ν^{s}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_2 groups
-	2853.5(±0.2)	2853.7(±0.1)	ν^{s}_{CH}, symmetric stretching vibrations of the CH groups (from hazelnut oil)
-	1744.7(±0.2)	1745.1(±0)	$\nu_{estC=O}$, stretching vibrations of the esteric C=O groups in triglycerides (from hazelnut oil)
1651(±0.1)	1651.7(±0.8)	1651.8(±0.9)	$\nu^{as}_{C=O/C=C}$, asymmetric stretching vibrations of the C=O/C=C groups
1596.8(±0.1)	1598.4(±0.1)	1599.2(±0.1)	$\nu_{CC}/\delta_{arC\#C}$, stretching vibrations of the C-C group in the ring C / bending vibrations of the aromatic C#C groups
1554.1(±0.1)	-	-	$\delta_{arC\#C}$, bending vibrations of the aromatic C#C groups
1502(±0.1)	1504.6(±0.2)	1504.9(±0.4)	ν_{CC}, stretching of C-C group in the ring C
1454.3(±0.2)	1456.2(±0.1)	1455.6(±0.6)	δ_{CH3}, asymmetric bending vibrations of the CH_3 groups
-	1417.7(±0.4)	1416.5(±0.6)	δ_{OH}, in-plane bending vibrations of the O-H groups (from β-CD)
1402.6(±0.4)	-	-	$\delta_{CH3}/\delta_{HOC}$, symmetric bending vibrations of the CH_3 groups/in-plane bending vibrations of the H-O-C groups
1360(±0.1)	1363.3(±0)	1364.6(±0.1)	ν_{CO}, stretching vibrations of the C-O groups
-	1339.4(±0.1)	1336.1(±0.5)	$\delta_{CH3}/\delta_{OCC}$, symmetric bending vibrations of the CH_3/OCC groups (also from β-CD)
1294.7(±0)	1295.9(±0.1)	1296.9(±0.1)	$\delta_{CH}/\delta_{OCH}/\nu_{CC}$, in-plane bending vibrations of the C-H/OCH groups / stretching vibrations of the C-C groups
-	1279.5(±0.7)	1280.5(±0.2)	ν_{CO}, stretching vibrations of the C-O groups (carbohydrates and phenolics)
-	1236.4(±0.1)	1237.8(±0.4)	δ_{CH2}, bending vibrations of the CH_2 groups (from hazelnut oil)
1202.5(±0.1)	1203.5(±0.2)	1203.9(±0.2)	ν_{CC}/ν_{CO}, stretching vibrations of the C-C groups in ring B / stretching vibrations of the C-O groups (carbohydrates and phenolics)
1168.4(±0.2)	-	-	$\nu_{CO}/\delta_{HCC/HOC}/\nu_{CC}$, 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
-	1152.4(±0.3)	1152.1(±0.1)	ν^{s}_{COC}, stretching vibrations of the C-O-C groups in glucosydic moieties (from β-CD)
-	1121.7(±0.1)	1123(±0.6)	$\nu_{CO}/\nu_{CC}/\delta_{HCC/HOC}/\nu_{CC}$, 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(±0.3)	-	-	ν_{CC}, stretching vibrations of the C-C groups
-	1079.7(±0.3)	1078.1(±0.3)	ν_{CC}, stretching vibrations of the C-C groups (from β-CD)
1058.6(±0.1)	1054.9(±0.4)	1053.6(±0.3)	ν_{CO}, stretching vibrations of the C-O groups
1041.1(±0)	-	-	ν_{CO}/ν_{CC}, stretching vibrations of the C-O/C-C groups in the ring B
-	1023.2(±0.7)	1022.4(±0.2)	ν_{CO}, stretching vibrations of the C-O groups (from β-CD)
1013.1(±0)	-	-	ν_{CO}/ν_{CC}, stretching vibrations of the C-O/C-C groups (*tentative*)

968(±0.2)	-	-	ν_{OC}, stretching vibrations of the O-C groups
-	944.2(±0)	944.7(±0.1)	ν_{rgCH}, stretching vibrations of the C-H groups from the β-cyclodextrin ring (from β-CD)
911.1(±0.2)	912.1(±0.1)	911.4(±0.1)	τ_{HCCC}, "twisting" bending vibrations of the H-C-C-C groups
-	863.7(±1.3)	862.1(±0)	δ_{CCH}, bending vibrations of the C-C-H groups (the α-type glycosidic bonds) (from β-CD)
-	849.7(±0.4)	850.6(±0.1)	δ_{CCH}, bending vibrations of the C-C-H groups (the α-type glycosidic bonds) (from β-CD) (*tentative*)
807.6(±0)	807.6(±0.2)	807.4(±0)	δ_{CH}, out-of-plane bending vibrations of the C-H groups
742.2(±0.1)	752.8(±0.3)	753.7(±0)	τ_{COH}, "twisting" bending vibrations of the C-O-H groups
-	574.2(±0.4)	574.7(±0.3)	δ_{OCC}, bending vibrations of the O-C-C groups (from β-CD) (*tentative*)
-	528.6(±0.2)	527.9(±0.1)	ν_{CC}, stretching vibrations of the C-C groups (from β-CD) (*tentative*)

Table S9: FTIR band assignments for naringin and the corresponding β-cyclodextrin/hazelnut oil/naringin 1:1:1 and 3:1:1 ternary complexes (codes "X1N and X3N); bands associated to β-CD or hazelnut oil are also specified; wavenumbers (cm^{-1}) are expressed as mean(±SD) of triplicate determinations for naringin and duplicate determinations for the ternary complexes

Wavenumber (cm^{-1})			**Band assignment**
Silymarin	**X1S**	**X3S**	
3400.3(±4.2)	3298.1(±6.2)	3302.4(±8.1)	ν_{OH}, stretching vibrations of the O-H groups (phenolic, glycosidic, water) (also from β-CD)
3263.1(±1.3)	-	-	ν_{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)	-	-	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups
-	2922.9(±0.2)	2923.3(±0)	ν^{as}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_3/CH groups (also from hazelnut oil)
2882(±1.8)	-	-	ν^{s}_{CH}, stretching vibrations of the C-H bonds in the aliphatic CH_2 groups
-	2853.5(±0.1)	2853.7(±0.1)	ν^{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)	ν_{CC}, stretching of C-C group in the ring C
1464.3(±0.7)	1455.7(±0.7)	1455.7(±0.4)	δ_{CH3}, asymmetric bending vibrations of the CH_3 groups
-	1416.9(±0.1)	1417.1(±0.6)	δ_{OH}, in-plane bending vibrations of the O-H groups (from β-CD)
1364(±0.4)	1365.9(±0)	1365.7(±0.5)	ν_{CO}, stretching vibrations of the C-O groups
-	1335(±0)	1335(±0.7)	$\delta_{CH3}/\delta_{OCC}$, symmetric bending vibrations of the CH_3/OCC groups (also from β-CD)
1268.1(±0.1)	1268.3(±0.2)	1268(±0.3)	ν_{CO}, stretching vibrations of the C-O groups (carbohydrates and phenolics)
-	1243.5(±0.7)	1242.9(±0.8)	δ_{CH2}, bending vibrations of the CH_2 groups (from hazelnut oil)
-	1204.6(±0.3)	1205.2(±0.4)	ν_{CC}/ν_{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)	ν^{s}_{COC}, stretching vibrations of the C-O-C groups in glucosydic moieties (from β-CD)

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

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

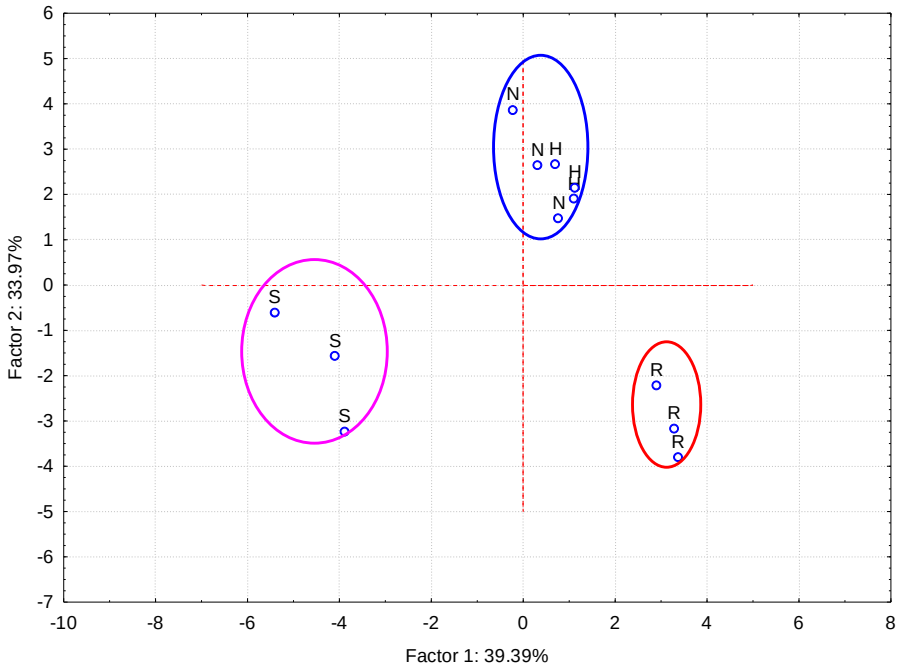

Figure S12: PC_2 *versus* PC_1 scores plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants (codes: "H" – hesperidin, "N" – naringin, "R" – rutin and "S" – silymarin); all wavenumber and intensity of the FTIR bands were used as input variables

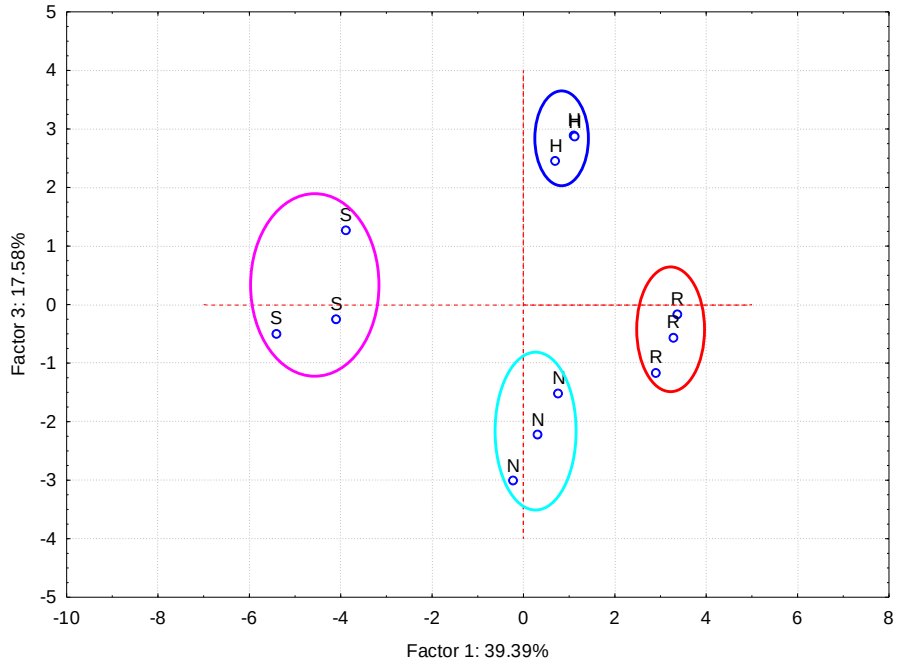

Figure S13: PC_3 *versus* PC_1 scores plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants (codes: "H" – hesperidin, "N" – naringin, "R" – rutin and "S" – silymarin); all wavenumber and intensity of the FTIR bands were used as input variables

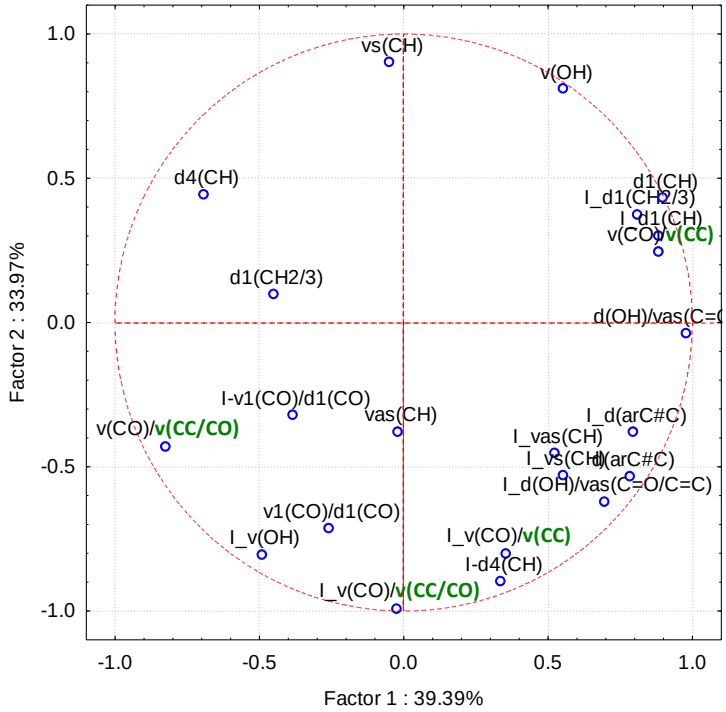

Figure S14: PC_2 *versus* PC_1 loadings plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S10 for codes)

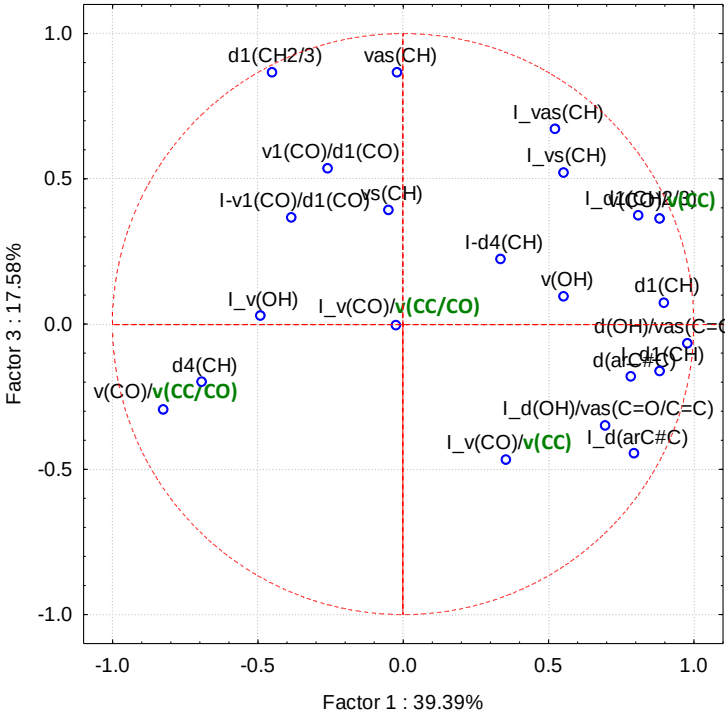

Figure S15: PC_3 *versus* PC_1 loadings plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S10 for codes)

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

	PC_1	**PC_2**	**PC_3**
v(OH)	0.555	0.809	0.093
I_v(OH)	-0.492	-0.805	0.027
vas(CH)	-0.019	-0.379	0.866
I_vas(CH)	0.524	-0.452	0.670
vs(CH)	-0.049	0.902	0.392
I_vs(CH)	0.552	-0.531	0.521
d(OH)/vas(C=O/C=C)	0.980	-0.039	-0.068
I_d(OH)/vas(C=O/C=C)	0.696	-0.621	-0.349
d(arC#C)	0.786	-0.533	-0.183
I_d(arC#C)	0.797	-0.380	-0.448
d1(CH2/3)	-0.450	0.099	0.867
I_d1(CH2/3)	0.809	0.374	0.375
v1(CO)/d1(CO)	-0.259	-0.714	0.536
I-v1(CO)/d1(CO)	-0.383	-0.323	0.365
d1(CH)	0.898	0.430	0.073
I_d1(CH)	0.883	0.300	-0.163
v(CO)/v(CC)	0.882	0.243	0.364
I_v(CO)/v(CC)	0.356	-0.801	-0.469
v(CO)/v(CC/CO)	-0.826	-0.430	-0.296
I_v(CO)/v(CC/CO)	-0.023	-0.992	-0.004
d4(CH)	-0.693	0.444	-0.202
I-d4(CH)	0.337	-0.897	0.223

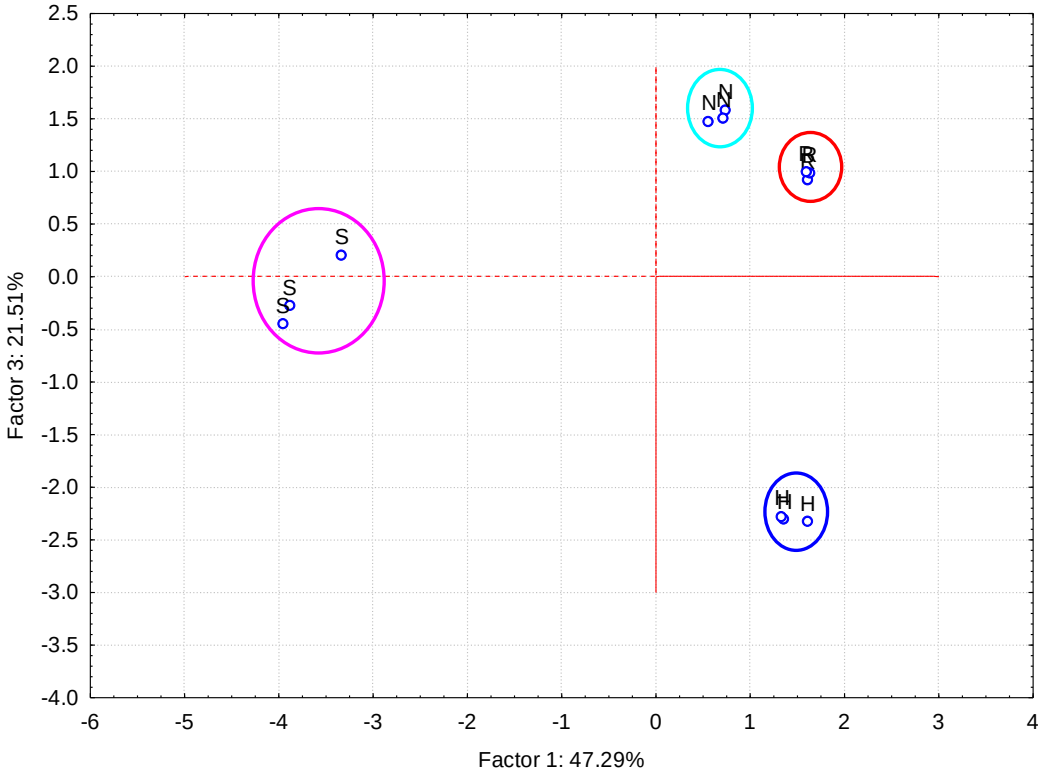

Figure S16: PC_3 *versus* PC_1 scores plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants (codes: "H" – hesperidin, "N" – naringin, "R" – rutin and "S" – silymarin); only wavenumbers of the FTIR bands were used as input variables

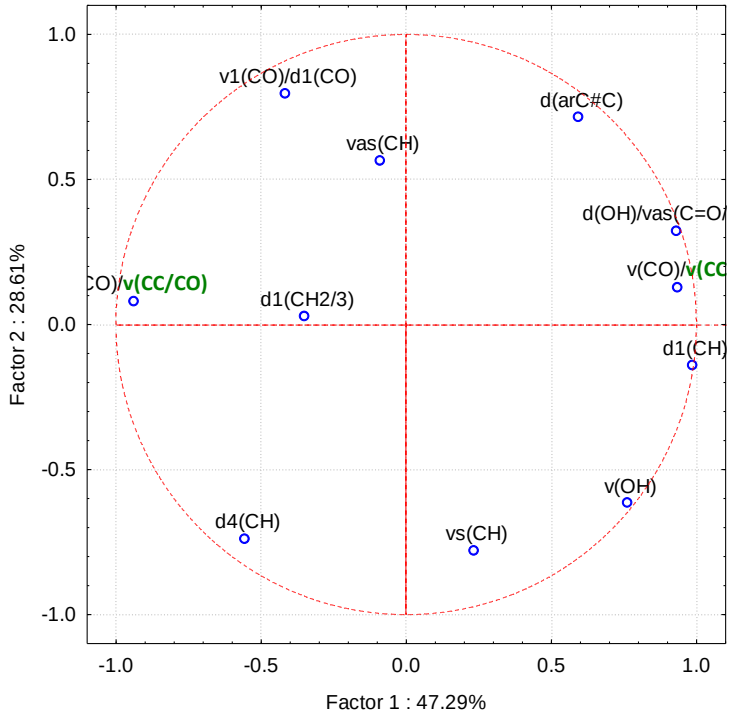

Figure S17: PC_2 *versus* PC_1 loadings plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; only wavenumbers of the FTIR bands were used as input variables (see Table S11 for codes)

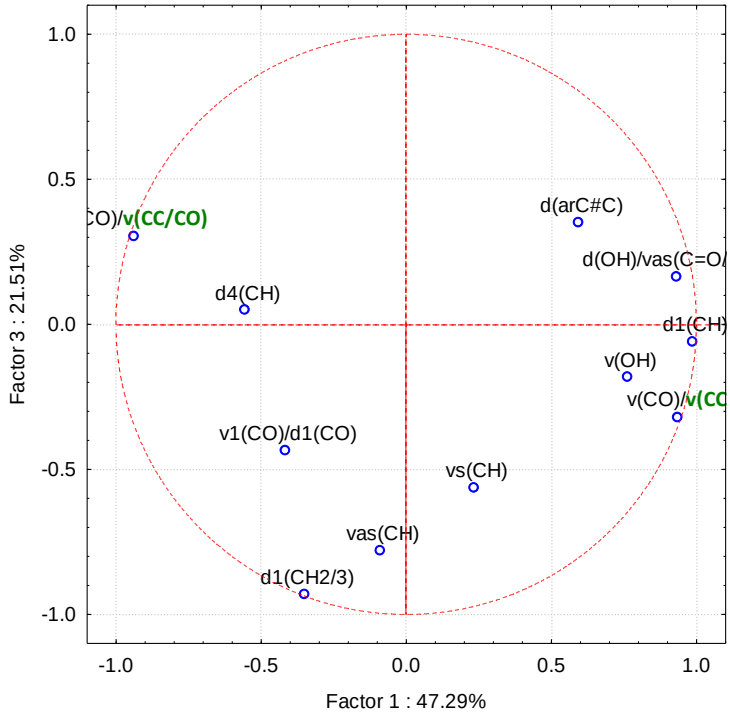

Figure S18: PC_3 *versus* PC_1 loadings plot from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; only wavenumbers of the FTIR bands were used as input variables (see Table S11 for codes)

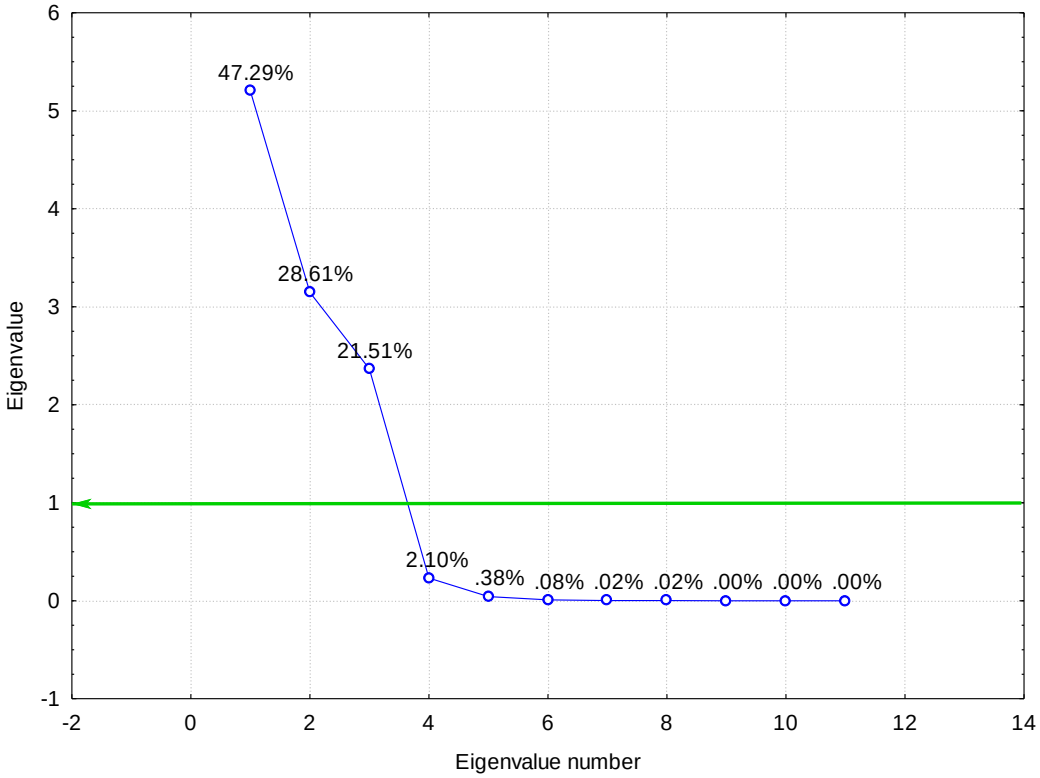

Figure S19: Eigenvalues of the correlation matrix from the FTIR-PCA analysis of the flavonoid glycoside and flavonolignan antioxidants; only wavenumbers of the FTIR bands were used as input variables (see Table S11 for codes); the first three PCs can be retained, which explain 97.41% from the variance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

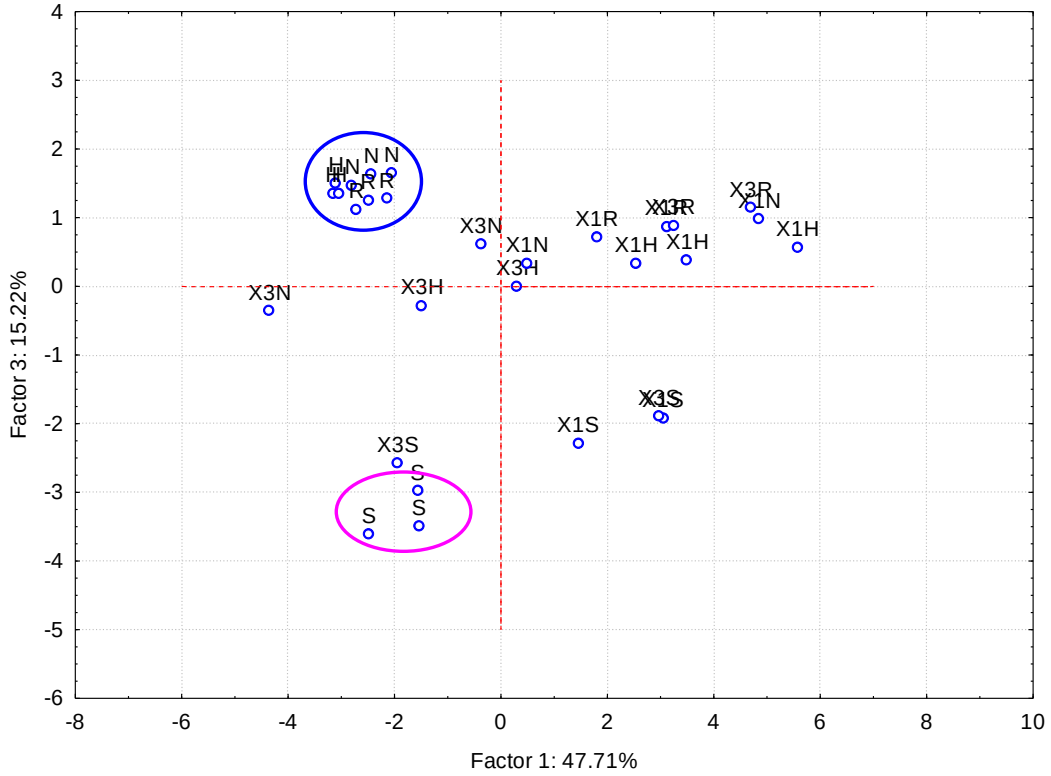

Figure S20: PC_3 *versus* PC_1 scores plot from the FTIR-PCA analysis of the β-CD/hazelnut oil/flavonoid ternary complexes (codes: "X1H/N/R/S" and "X3H/N/R/S" for the 1:1:1 and 3:1:1 ternary complexes with hesperidin/naringin/rutin/silymarin, respectively) and flavonoids (codes: "H" – hesperidin, "N" – naringin, "R" – rutin and "S" – silymarin); all wavenumber and intensity of the FTIR bands were used as input variables

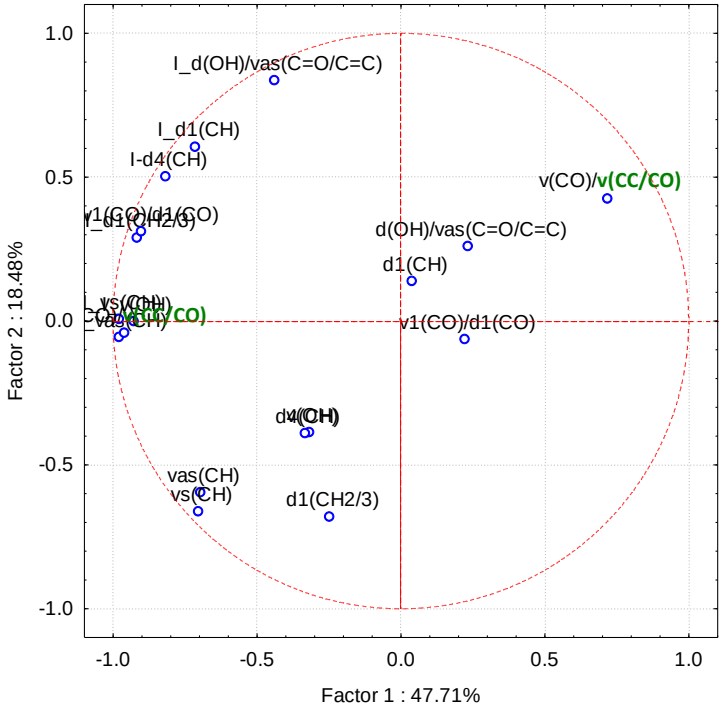

Figure S21: PC_2 *versus* PC_1 loadings plot from the FTIR-PCA analysis of the β-CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S12 for codes)

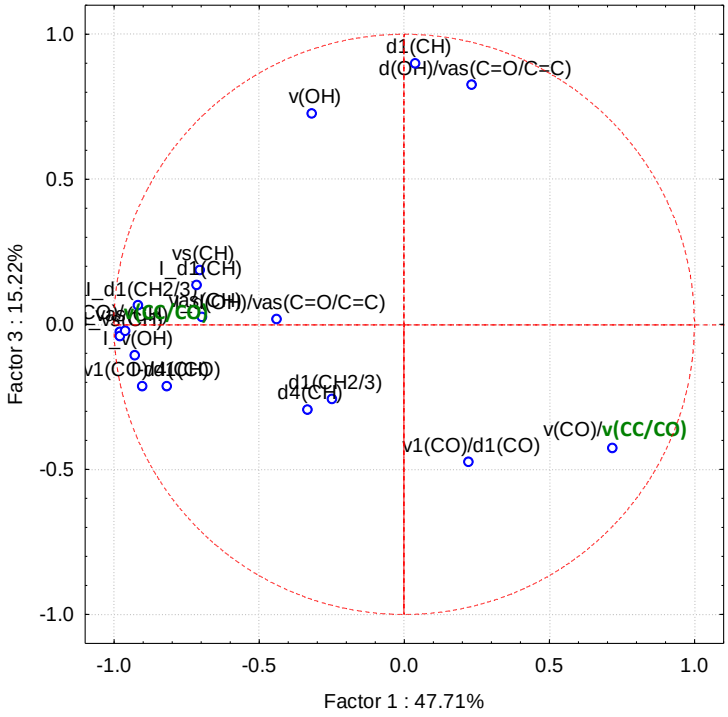

Figure S22: PC_3 *versus* PC_1 loadings plot from the FTIR-PCA analysis of the β-CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S12 for codes)

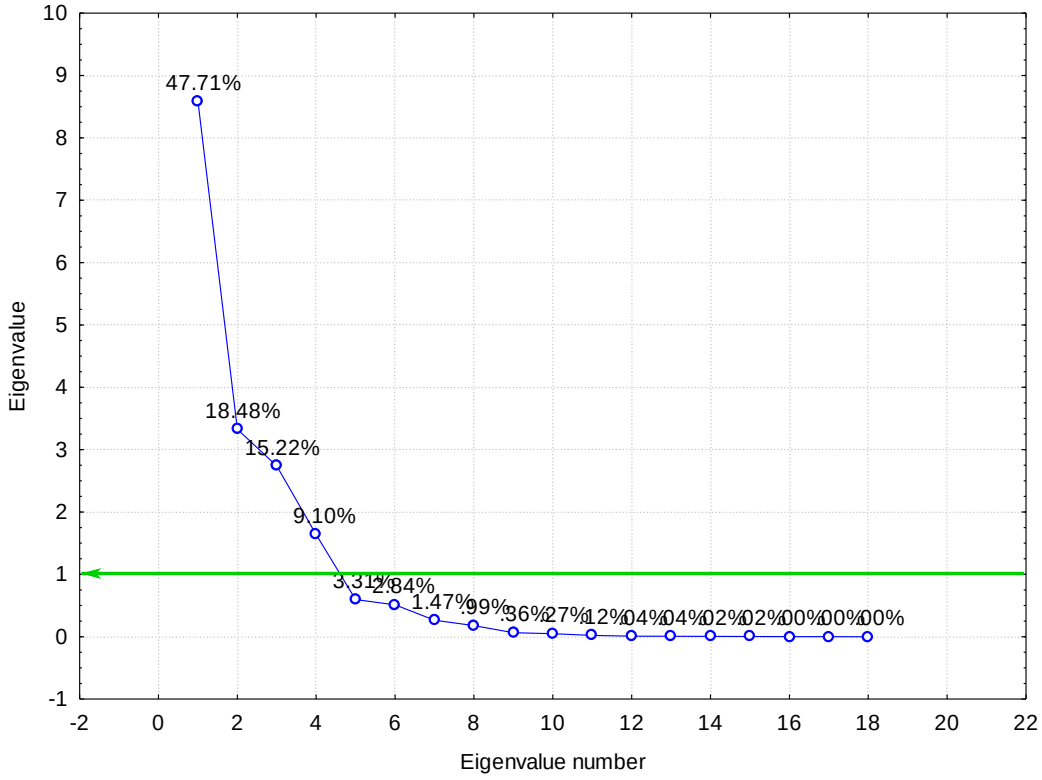

Figure S23: Eigenvalues of the correlation matrix from the FTIR-PCA analysis of the β-CD/hazelnut oil/flavonoid ternary complexes and flavonoids; all wavenumber and intensity of the FTIR bands were used as input variables (see Table S12 for codes); the first four PCs can be retained, which explain 90.51% 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 β-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_1	**PC_2**	**PC_3**	**PC_4**
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(CH2/3)	-0.247	-0.680	-0.259	-0.298
I_d1(CH2/3)	-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 β-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_1	**PC_2**	**PC_3**
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(CH2/3)	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