Supplementary information

Rapid characterisation of hypanthium and seed in wild and cultivated rosehip: application of Raman microscopy combined with multivariate analysis

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Content

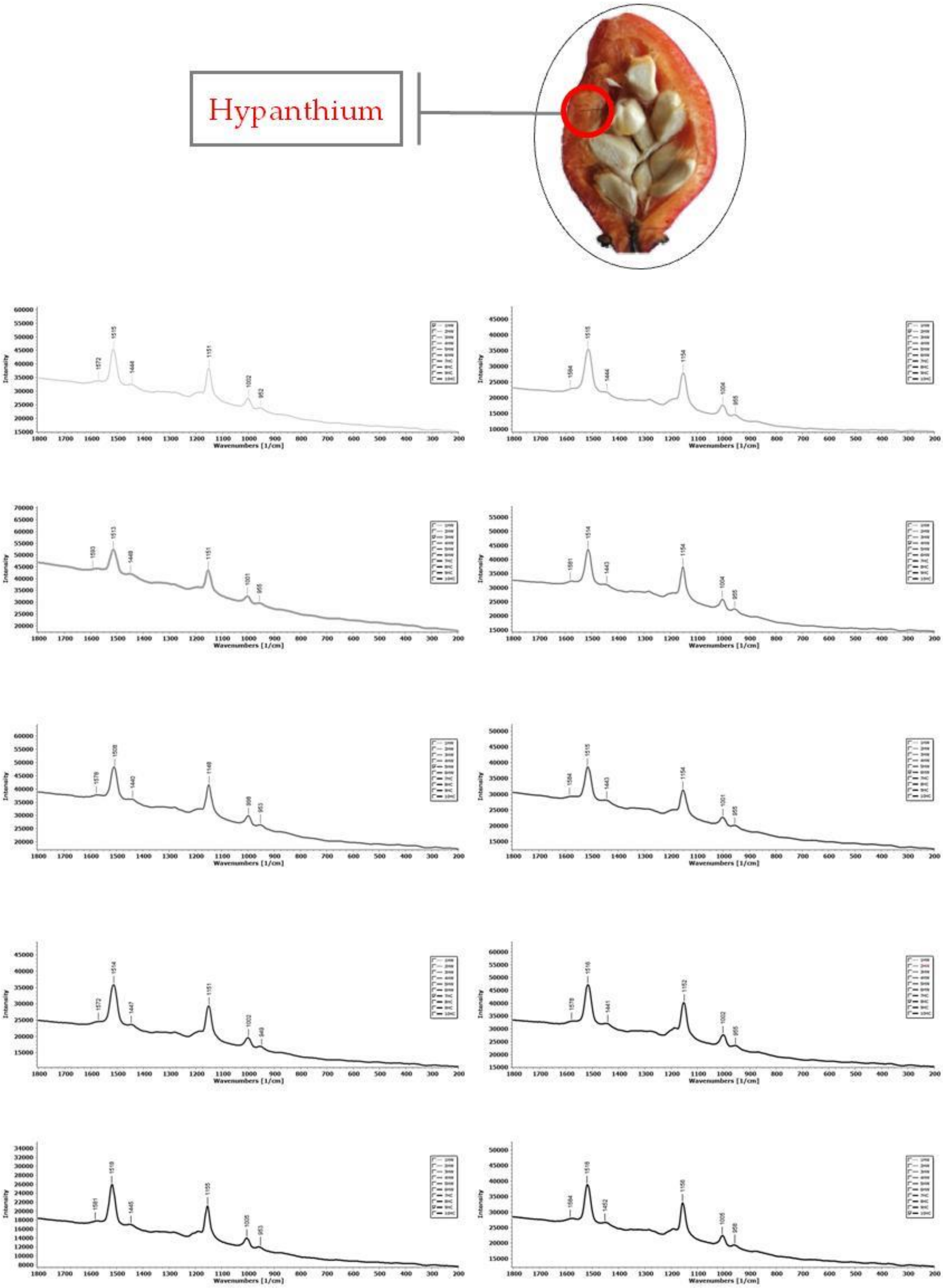

Figure S1. Raw average Raman spectra of the individual hypanthium samples 1H-10H

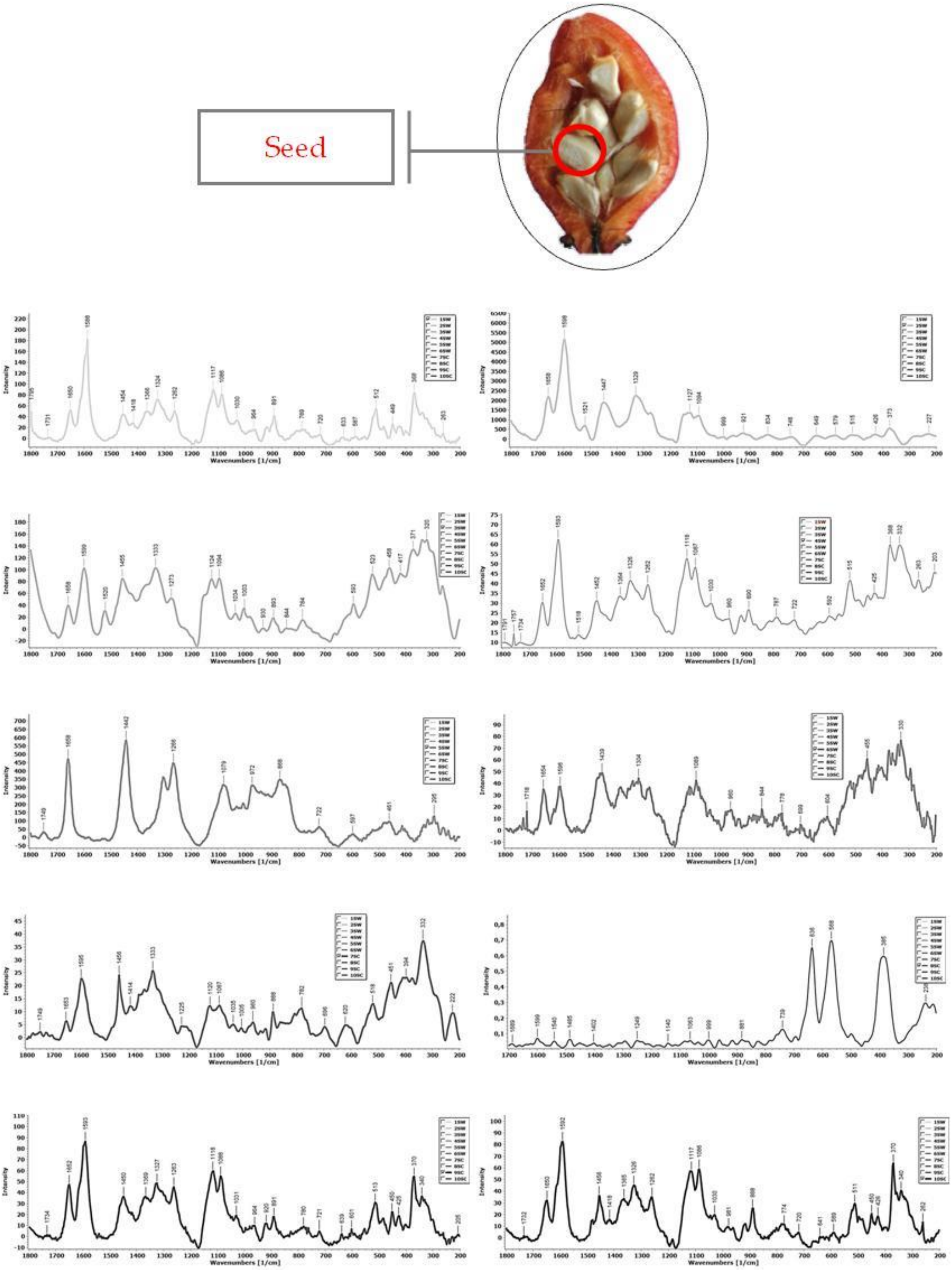

Figure S2. Raw average Raman spectra of the individual seed samples 1S-10S

Table S1. Vibrational bands and their assignments in average spectra (Figures 2 and 4) collected from tissue sections of studied rosehip hypanthium and seed samples and literature data.

Hypantium	Seed	Literature data	Vibrational mode	Chemical moiety	Reference
Wave number (cm^{-1})					
	328	336 (rosehip)	δ(C-C-C)	Glucosidic ring	[25]
		360 (black spruce milled-wood)		Lignin	[64]
	372	372 (orange peel)		Polygalacturonic (pectic) acid	[42]
		380 (pure compound)	δ(C-C-C) ring	Celulose	[46]
		378 (rosehip seed)	δ(C-C-C)	Glucosidic ring	[25]
	413	415 (pure compound)	δ(C2-C1-O1) bending	α-Glucose	[35]
	460	441 (orange peel)	T(C–O–C) def	Polygalacturonic (pectic) acid	[42]
		479 (pure compound)	C-C-O and C-O-C ν(C-O-C) Glycosidic	Glycosidic ring skeletal deformations Pectin	[46]
		480		Carbohydrates	[45]
	483	480	C-C-O and C-C-C Deformations; Related to glycosidic ring skeletal deformations δ(C-C-C) + τ(C-O) scissoring of C-C-C and out-of-plane bending of C-O	Carbohydrates	[26]
		486 (orange peel)		Polygalacturonic (pectic) acid	[42]
		520	ν(C-O-C) Glycosidic	Cellulose	[65, 45]
		522	δ$_{ip}$(COC)	Glucosidic ring	[25]
	523	527 (fructose)	CCO, CCC and OCO deformations	Fructopyranose	[48]
		537 (orange peel)		Polygalacturonic (pectic) acid	[42]
	610	620	Phenylalanine (skeletal)	Protein	[35]
	625-7	631, 634	Ring deformation	Fructose (pure compound)	[35]
		686 (orange peel)	Low frequency vibrations of pyranoid ring	Polygalacturonic (pectic) acid	[42]
	698,721				
		709	Skeletal vibration	Fructose	[35]
		710 (orange peel)	□γ(C–OH)$_{ring}$	Polygalacturonic (pectic) acid	[42]
		747	γ(C–O-H) of COOH	Pectin	[42, 45]
		789	ν(CO)$_{ring}$, β(COC), β(CCO), β(OCO)		[48]
	781				

		800	ν(C-C)	Fructose, sucrose	[35]
		840	νs(C-C)	Linoleic acid	[35]
		843	$\nu_s(CO)_{ring}$, ν(CC), ν(CO)	L(+)- Arabinose	[48]
	843	849–853	(C6–C5–O5–C1–O1)	Pectin	[66, 45]
		856 (tomato)	(COC) skeletal mode of α-anomers	Pectin	[46]
		890 (sea weed)	ν(CC)streching	β-Galactose	[48]
	894	899 (rosehip seed)		Glucosidic ring	[25]
		917	ν(C-O-C) in plane, symmetric	Cellulose, phenylpropanoids	[65]
		917		Carbohydrates	[45]
	931	922, 928	$\rho(CH_3)$	Methyl and acetyl ester groups respectively, in pectins	[42]
955		953 (orange peel)	δ(CCH), δ(COH)	Polygalacturonic (pectic) acid	[42]
	967	964	CH_2/CH_3 vibrations	Aliphatic groups	[45]
		971 (tomato)	$\rho(CH_2)$	Cellulose	[46]
1003		1000		Carotenoids	[45]
		1004 -1005 (rosehip carrot, pepper)	ν(C-C)	Carotene	[25] [37]
		1008	$(C–CH_3)$ rocking	β-Carotene (pure compound)	[35]
	1010	1000-1005	In-plane CH_3 rocking of polyene	Carotenoids	[67]
			aromatic ring of phenylalanine	Protein	[45]
	1037	1030 (orange peel)	ν(CC)(CO)	Polygalacturonic (pectic) acid	[42]
		1037 (black spruce)	ν(C-C), ν(C-O-C)	Carbohydrates	[68]
		1078	$\nu_{as}(C-C)$trans	Linoleic acid (pure compound)	[35]
		1086			[25]
	1092	1090 (tomato)	ν(C-O-C) glycosidic, asymetric	Cellulose	[46]
		1095 (rosehip)			[25]
		1090 (carrot)		Glycosidic bonds in cellulose	[69]
		1098 (tomato)	ν(C-O-C)		[46]
		1092 (cucumber)			[44]
		1115–1119	Sym ν(C-O-C), C-O-H bending	Cellulose	[65,45]
		1120 (tomato)	ν(C-O-C) glycosidic, symetric	Cellulose	[46]
	1119	1121 (tomato)	ν(C-O-C)		[46]
		1122 (carrot)			[69]
		1124 (rosehip)		Glycosidic bonds in cellulose	[25]
1153		1145	ν(COC)glycosidic bond, ring	Polygalacturonic (pectic) acid	[42]

		1048		Celulose	[45]
		1155		Carotenoids	[45]
		1156 (cucumber)			[44]
		1157 (pumpkin)	ν(C-C)	Carotene	[37]
		1156	ν (C–C)	β-Carotene (pure compound)	[35]
		1157 (rosehip)	ν_s(COC)		[25]
		1155	C-C Stretching; ν(C-O-C), ν(C-C) in glycosidic linkages, asymmetric ring breathing	Carotenoids , carbohydrates	[67] [48]
	1224	1218	δ(C-C-H)	Aliphatics, xylan	[68, 70]
		1254 (orange peel)	δ(CH)	Polygalacturonic (pectic) acid	[42]
	1264	1265,1270 (rosehip)	=C-H	*Cis-* Lipids	[25]
		1265	-C=C−	Unsaturated fatty acids	[45, 49]
1281		1286	CH_2/CH_3 vibrations	Aliphatic groups	[45]
	1300	1301	δ(C-C-H) + δ(O-C-H) + δ(C-O-H)	Carbohydrates	[26]
		1327	δCH_2 bending	Aliphatics, cellulose, phenylpropanoids	[45, 65]
	1330	1330 (orange peel)	δ(CH)	Polygalacturonic (pectic) acid	[42]
		1332		α-anomer of glucose	[35]
	1374	1375		α-anomer of glucose	[35]
		1378	δ_s(CH_3)	Methyl ester groups in pectins	[42]
		1440	ν(C-C)	Linoleic acid	[35]
1443		1443	CH_2/CH_3 vibrations	Aliphatic groups	[45]
		1444 (rosehip)	δ(CH_2)	Lipids and glucosidic signal	[25]
		1440	CH_2□Scissoring vibration	Carotenoids	[35]
		1451,1456 (rosehip)	δ(COH)	Glucosidic signal	[25]
	1453	1455 (apple/pear pulp)	δ_{as}(CH_3)	Fructose	[47]
		1458, 1440	δ(CH_2) + δ(CH_3)	Methyl and acetyl ester groups in pectins, respectively	[42]
		1513	ν□□C C□ Stretching	β-Carotene	[35]
1514		1520 (rosehip)	ν(C=C)	Carotene	[25]
		1524 (pumpkin)			[37]
		1526	-C=C- (in plane)	Carotenoids	[45,50]
1576		1576 (citrus fruit)	ν(C=C)	center of polyene chain	[71]

	1596	1601 (rosehip)	ν(C=C)	Phenolic compounds	[25]
		1598 (cucumber)			[44]
		1606-1632	ν(C-C) Aromatic ring + σ(CH)	Phenylpropanoids	[72, 73]
		1606		Phenylpropanoids (including lignin)	[45]
	1654	1658 (rosehip)	ν(C=C)	Unsaturated fatty acids assigned to *cis* isomer and lignin	[25]
		1656 (rapeseed)			[74]
		1656-1658 (coconut, babassu, peanut, grape)			[63]
		1658 (cucumber)			[44]
		1654–1660	-C=C-	Unsaturated fatty acids	[49]
		1654–1660	C=O Stretching, amide I	Proteins	[50]
1694		1600-1700 (soy and whey protein isolates)		Amide I band (predominantly β-sheet)	[35]
		1654–1660		Amide I band – proteins	[40]
		1660		Proteins	[45]
		1680–1715	C=O	in nucleic acids	[40]
		1682		Carboxylic acids	[45]

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