Supporting Materials

Spectroscopic Study of Phytosynthesized Ag Nanoparticles and Their Activity as SERS Substrate

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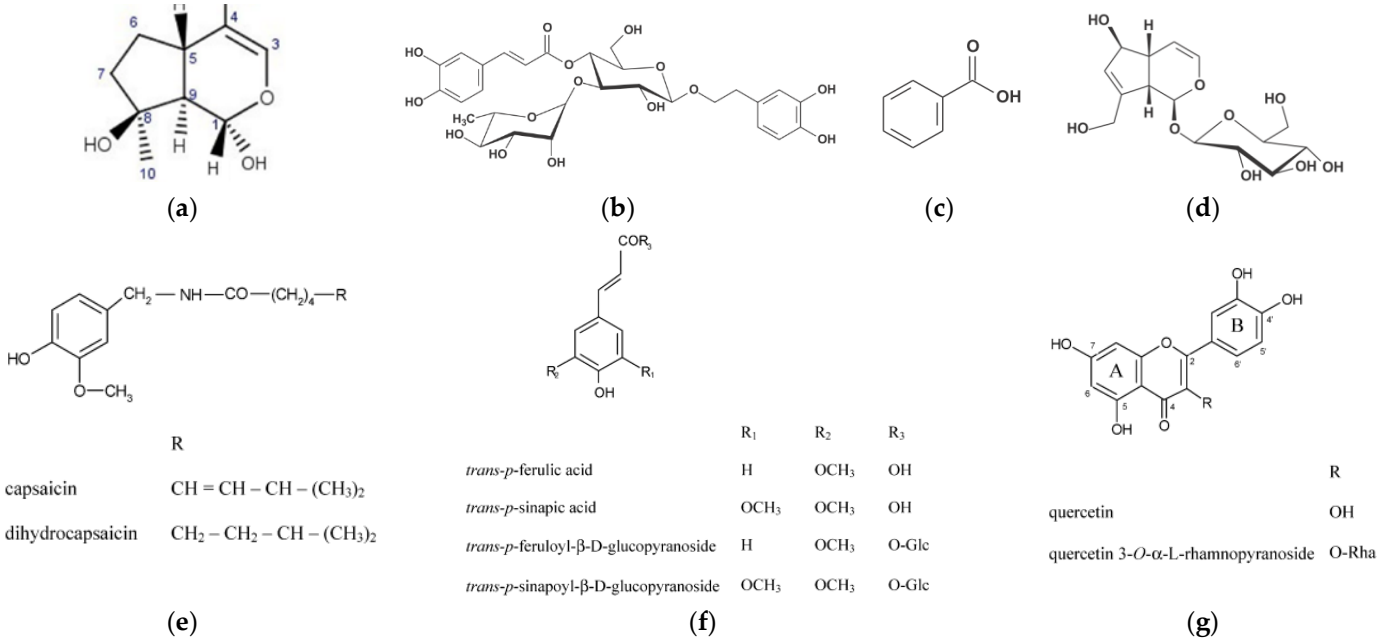

Figure S1. Schematic of the molecules reported in *L. squamaria*: (**a**) iridoid aglycones [24]; (**b**) acteoside [25]; (**c**) benzoic acid [25]; (**d**) aucubin [21,25]; and *Capsicum chinense*: (**e**–**g**) [22].

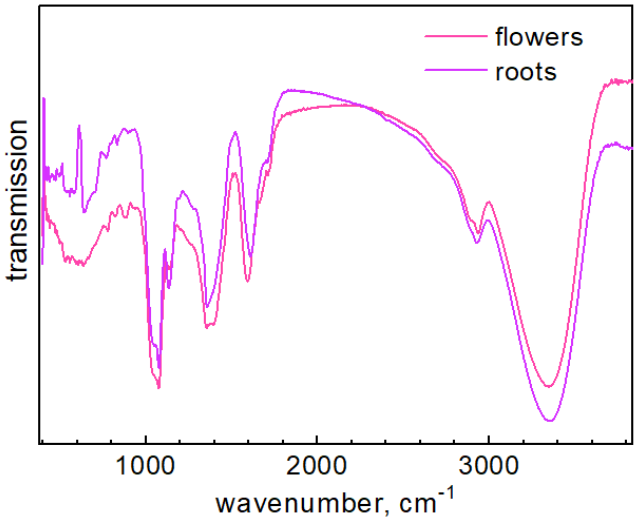

Figure S2. Spectra of IR absorption of common toothwort roots and flowers extracts.

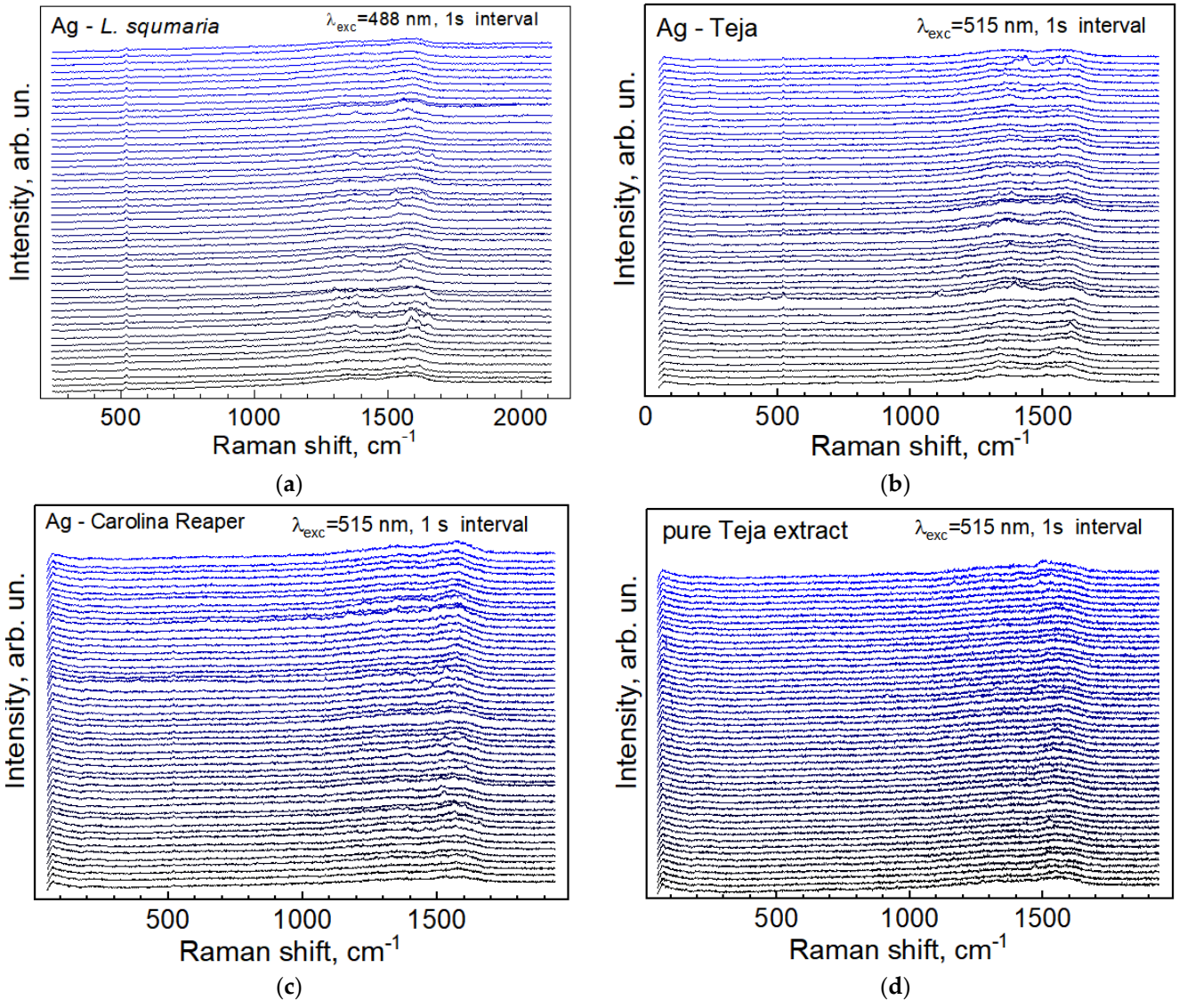

Figure S3. Variation of the Raman spectra with time (in 1 s intervals) for Ag–*L. Scuamaria* (**a**), Ag–Teja (**b**), Ag–Carolina Reaper (**c**), and pure Teja extract (**d**).

Table S1. Summary of the IR absorption features of phytosynthesized Ag NPs and their assignment based on the literature data. All numbers in the first column are observed for the pepper extracts, and the underlined ones only for common toothwort.

This work	Literature	Assignment	main compound, based on Ref [32]
1028	1030-1045 [30]	C–OH & C–OH stretch: cell wall polysaccarides (arabinan, cellulose) [30]	1030, Cellulose
1043, 1050	1050 [16] 1030-1045 [30]	C–O & C–OH stretch: cell wall polysaccarides (arabinan, cellulose) [16,30]	1043, Pectins, xyloglucan
1076, 1081	1077 [31,33],1090 [16] 1060−1065 [30] 1070−1075 [30] 1075−1085 [30]	C − O stretch of secondary alcohols [31] C–O stretch: cell wall polysaccarides (glucomannan) [30] C–O ring stretch: rhamnogalactorunan, β-galactan [30] C–O deformation: secondary alcohol, aliphatic ester [30]	1075, Xyloglucan
1134	1105−1110 [30] 1100−1105 [30]	C–O–C sym stretch: cutin [30] Antisymmetric in-phase: pectic substance[30]	1097, Pectins 1103-1015, Cellulose
1150	1140−1145 [30] 1160−1170 [30] 1150−1160 [30,33]	C–O–C asym stretch: cellulose (β-1.4 glucan) [30] C–O–C asym stretch: cutin [30] Symmetric bonding of aliphatic CH_2, OH, or C–O stretch of various groups: cell wall polysaccharide [30]	1147, Xyloglucan 1160, cellulose
1217	1235 [30] 1230−1235 [30] 1200−1205 [30]	Amide IV (C=N and N–H stretching): mainly protein [30] C–O stretch: lignin, xylan [30] O–H in plane bend: cellulose [30]	
1263	1249 [31] 1240−1250 [30]	C – N stretch [31] C=O stretch: pectic substances, lignin, hemicellulose, suberin/cutin esters [30]	1230-1368, Pectins
1355	1363 [31] 1365−1375 [30]	N = O of the aliphatic nitro group [31] C–H bend: cellulose and hemicellulose [30]	1316-1317, Xyloglucan 1320, Cellulose 1331, Pectins
1386	1395 [31], 1384 [33] 1370−1380 [30]	C − H bending of alkanes (CH_3) [31,33]; S=O [16] C–H sym bending of CH_2 and CH_3: cell wall polysaccharide, lipid and protein [30]	1367, Cellulose, hemicelluloses 1371, Xyloglucan, cellulose
1400	1395 [31] 1420−1430 [30]	C − H bend of alkanes (CH_3) [31] O–H bend: cell wall polysaccaride, alcohol, and carboxylic acid [30]	1400, Pectin ester group 1420, uronic acid 1430, Phenol; 1440, Pectins
1517	1505−1515 [30]	C=C aromatic stretch: lignin [30]	1515, Phenolic ring
1542, 1547	1510 – 1550 [31], 1515 – 1570 [31] 1540−1560 [30]	N − H bending in amides & the interaction between N − H bending and C − N stretching of C − N – H group [31] Amide II (C=N and N–H stretch): mainly protein [30]	1550, Amid II (proteins)
1597, 1610	1590-1620 [16,30,31]	C = C of aromatic group, N − H bending in amides [31] C - C skeletal vibrations/N = H deformations [16] C=O aromatic stretch: lignin, alkaloid [30]	1600, Non esterified uronic acid
1628	1620−1630 [30]	C=C stretch: phenolic compound [30]	1630, Phenolic ring, pectin ester group
1658	1630−1650 [30]	Amide I (C=O stretch): protein, pectin, water associated cellulose or lignin, alkaloids [30]	1650, Amid I (proteins)
1740	1730−1745 [30]	Saturated ester C=O stretch: phospholipid, cholesterol ester, hemicellulose, pectin, lignin, suberin/cutin esters [30]	1740, Esterified uronic acid, pectins
2854	2874 [31], 2851 [33] 2840−2860 [30]	C −H stretch of alkanes [31] CH_2 symmetric stretch: mainly lipids with a little contribution from protein, carbohydrate, and nucleic acid [30]	
	2870−2875 [30]	CH_3 symmetric stretch: mainly protein with a little contribution from lipid, carbohydrate, and nucleic acid [30]	

2926	2939 [31], 2922 [33] 2920−2930 [30]	C −H stretch of alkanes [31] CH_2 asymmetric stretch: mainly lipid with a little contribution from protein, carbohydrate, and nucleic acid [30]
2958	2950−2960 [30]	CH_3 asymmetric stretching: mainly lipid with a little contribution from protein, carbohydrate, and nucleic acid [30]
3290	3269 [31], 3197 & 3267 [34]	hydrogen-bonded OH [31] N-H of protein [34]
3345	3354 [34] 3200−3500 [30]	O-H and N-H stretch: carbohydrates, proteins, alcohols and phenolic compounds [30,34]

References

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