

Supplementary Materials

Characterization and safety assessment of a novel antioxidant excipient from sustainable recovery of grape processing waste bentonite designed to develop a thermosensitive buccal spray for oral cavity wellness

Giulia Di Prima^{1,*}, Elena Belfiore², Cecilia La Mantia¹, Serena Indelicato¹, Giuseppe Avellone^{1,3}, Viviana De Caro^{1,3}

¹Dipartimento di Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche (STEBICEF), University of Palermo, Via Archirafi 32, 90123, Palermo, Italy. cecilialamantina000@gmail.com (CLM); serena.indelicato@unipa.it (SI); beppe.avellone@unipa.it (GA); viviana.decaro@unipa.it (VDC)

²Dipartimento di Medicina di Precisione in Area Medica, Chirurgica e Critica (Me.Pre.C.C.), University of Palermo, Via L. Giuffrè 5, 90127, Palermo, Italy. elena.belfiore@unipa.it (EB)

³Centro Interdipartimentale di Ricerca Riutilizzo Bio-Based Degli Scarti da Matrici Agroalimentari (RIVIVE), University of Palermo, 90128 Palermo, Italy

*Correspondance: Dr. Giulia Di Prima, giulia.diprima@unipa.it (GDP), +3909123896826

Data reported as supplementary material:

- **Table S1.** LC-MS/MS parameter and LOD values for polyphenols identification and quantification in the 5 extracts
- **Table S2.** LC-MS/MS parameters for organic acids identification and quantification in the 5 extracts
- **Video V1.** Ex vivo temperature-dependant gelation studies

Table S1. LC-MS/MS parameter and LOD values for polyphenols identification and quantification in the 5 extracts

	Precursor Ion (m/z) [M-H] ⁻	Product Ion (m/z)	Collision Energy (V)	RF Lens (V)	LOD (µg/L)
<i>Gallic Acid</i>	169	79	24	101	30
	169	125	14	101	
<i>Vanillic Acid</i>	177	123	20	105	32
	177	152	20	105	
<i>Ferulic Acid</i>	193	134	15	99	22
	193	178	13	99	
<i>Chlorogenic Acid</i>	353	179	45	180	26
	353	191	45	180	
<i>Catechin</i>	289	203	20	147	28
	289	245	15	147	
<i>Mandelic Acid</i>	151	77	18	65	26
	151	107	10	65	
<i>Gentisic Acid</i>	153	108	22	90	24
	153	109	14	90	
<i>Syringic Acid</i>	197	153	12	100	23
	197	182	14	100	
<i>Caffeic Acid</i>	179	107	25	101	26
	179	135	16	103	
<i>OH-Cynnamic</i>	163	93	31	90	27
	163	119	14	90	
<i>Rutin</i>	609	271	60	299	26
	609	300	38	299	
<i>Resveratrol</i>	227	143	27	156	25
	227	185	20	156	
<i>Apigenin-7Glu</i>	433	269	20	123	24
	433	271	20	123	
<i>Quercetin</i>	301	151	18	166	25
	301	179	21	166	
<i>Kaempferol</i>	285	202	20	195	26
	285	239	29	195	
<i>Cumaric Acid</i>	163	93	31	91	27
	163	119	13	91	
<i>Apigenin</i>	269	117	35	178	25
	269	151	25	178	

Table S2. LC-MS/MS parameters for organic acids identification and quantification in the 5 extracts

	Precursor Ion (m/z) [M-H] ⁻	Product Ion (m/z)	Collision Energy (V)	RF Lens (V)
<i>Lactic acid</i>	89	42.8	11	65
	89	44.8	12	165
<i>Tartaric Acid</i>	149	72.8	16	105
	149	86.8	13	105
<i>Malic Acid</i>	132.9	71	16	79
	132.9	114	19	79
<i>Citric Acid</i>	91	86.8	12	79
	91	110.8	17	79