Valorisation of Tomato Pomace: Bioactive Compounds, Antimicrobial Activity and Photodynamic Inactivation

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Supplementary Information

1.HPLC-DAD-ESI-MS/MS individual polyphenol quantification

Table A.1. Mass spectrophotometry polyphenol tentative identification. Concentration of polyphenols in mg of polyphenol equivalents (PE) per g of dry weight (DW). In white: catechin equivalents, maximum absorbance at 280nm; In blue: chlorogenic acid equivalents, maximum absorbance at 320nm; In purple: quercetin equivalents, maximum absorbance at 353 nm. rt: retention time, nd: not-determined, nd*: not-detected

Peak number	Wavelength	Tentative Identification	rt	$[M-H]^-$	MS/MS Fragments	ST	HL
1	280	Cinnamic acid	4.18	193.24	130.87,113.03,89.02,174.89,148.89	0.0174	0.0070
2	320	Chlorogenic acid	4.56	191.28	190.92,126.93,173,84.98	0.0040	nd*
	320		4.62	191.23	126.94,173.84		
3	280	Quinic acid	6.06	191.00	110.81,172.88	0.0048	nd*
4	280	nd	7.07	323.20	210.88, 279.89	0.0509	0.0071
5	280	nd	8.37	243.02	199.96,110.91,151.96	0.0612	0.0483
6	280	nd	11.21	134.01	133.92,106.85	0.0791	0.0770
7	280	nd	12.16	282.11	149.92,133	0.1364	0.0863
8	280	nd	15.40	233.00	188.88	0.0469	0.0363
9			18.53			0.0496	0.0155
10	280	nd	23.78	203.00		0.0693	0.0280
11	280	*p*-coumaric acid	25.70	162.99		0.1162	0.0404

12	280	Caffeic acid-hexose	26.07	341.18		0.0165	0.0222
13	280	nd	29.23	443.34	237.10,160.95,425.15,219.50,142.80	0.0480	0.0457
14	280	Homovanillic acid-*O* hexoside	30.54	343.16	180.9,136.0	0.0258	0.0147
15	280	Coumaric acid-hexose	31.38	325.21	162.84	0.2789	0.1095
16	353	Rutin-*O*-hexoside-pentoside	32.63	903.27	741.20	0.0110	0.0180
17	280	Naringenin chalcone-dihexoside	34.48	595.23	355.07,475.05,385.16,505.16	0.1981	0.0774
18	353	Rutin-*O*-hexoside	35.31	771.33	609.12, 463.11,301.03	0.0999	0.0698
19			35.92	771.40	609.63,301,21,463.43,652.23		
20	280	Naringenin-*O*-glucoside (1)	39.15	433.22	271.00	0.0258	0.0232
21	353	Quercetin-3-galactoside	40.41	463.26	301.06	0.0017	nd*
22	280	Eriodictyol-*O*-dihexoside	42.33	611.27	449.02	0.0124	0.0092
23	280	Naringenin-*O*-glucoside (2)	44.47	433.22		0.0163	0.0088
24	280	Eriodictyol-7-*O*-glucoside	45.73	449.21	286.96	0.0738	0.0787
25	280	Naringenin-*O*-dihexoside	46.24	595.30	270.90	0.0084	0.0154
26	353	Rutin-*O*-pentoside	48.48	741.60	300.32,609.21,591.27	0.1276	0.0946
27	280	Phloretin-*C*-diglycoside	50.10	597.42	357.53,477.24	0.0656	0.0401
28	353	Querecetin derivative	50.57	1328.80	1268.67	0.0161	0.0127
29	353	Rutin	51.77	609.97	300.92	0.8636	1.1017
30	353	Rutin derivative (1)	53.16	917.36	741.18, 723.26	nd*	nd*
31	320	Tricaffeoylquinic acid derivative	53.50	713.78	677.47	0.0023	0.0028
32	280	Naringenin derivate	54.20	475.35	270.93	0.0349	0.0171
33	320	Tricaffeoylquinic acid derivative	54.98	827.00	790.56	0.0644	0.0740
34	353	Rutin derivative (2)	55.56	921.45	741.19,877.24,723.22,609.27	0.0204	0.0094
35	280	Naringenin Chalcone	57.67	271.32	151.08,271.05,272,177.05,165.01	0.2981	0.7108

2. HPLC-DAD polyphenols

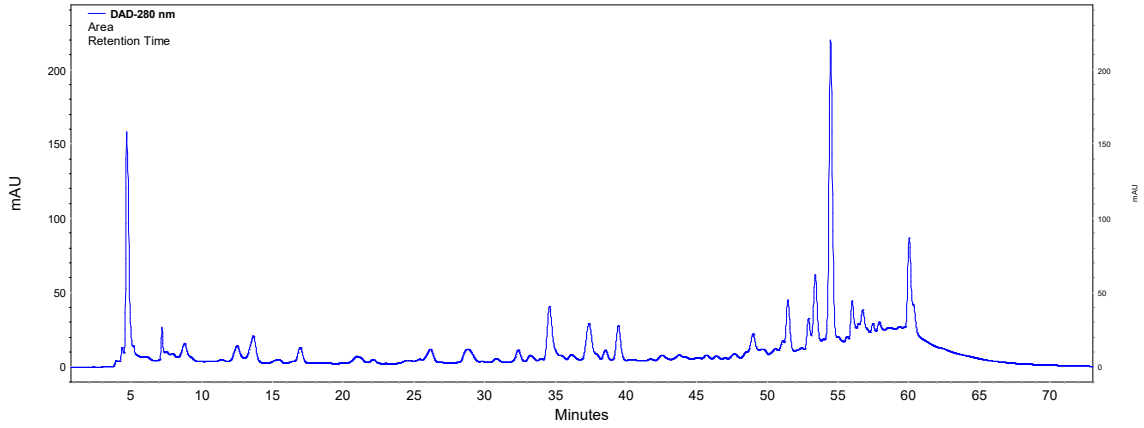

Figure A.1. Chromatogram HPLC-DAD of tomato pomace polyphenol extracts of ST variety at 280 nm.

3. HPLC-DAD carotenoids

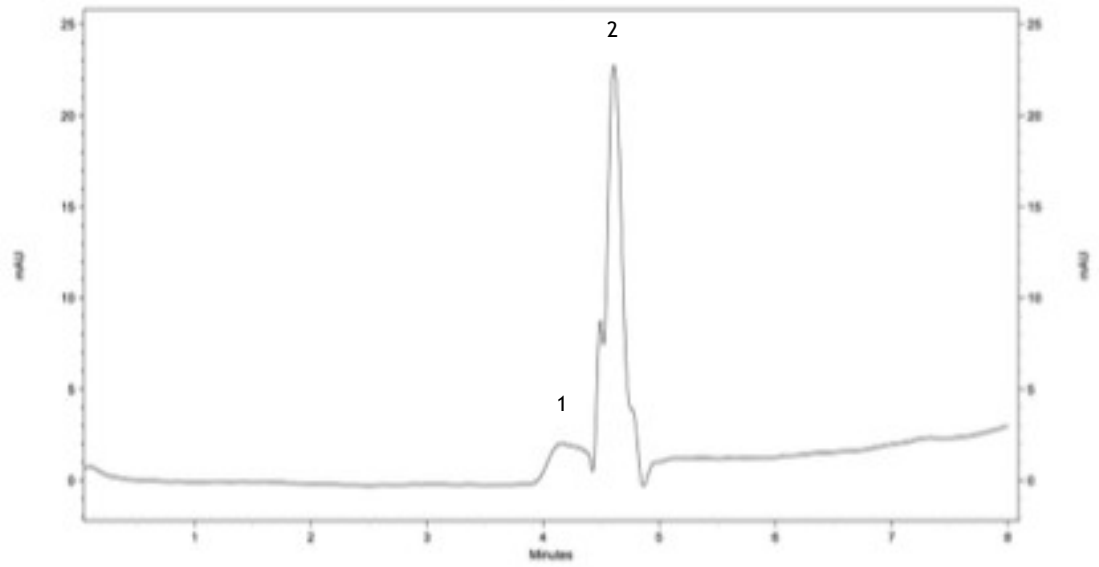

Figure A.2. Chromatogram HPLC-DADof tomato pomace carotenoid extract from ST variety. 1.*β*-carotene, 2.Lycopene.

4. Absorption spectrums of polyphenol and carotenoid extracts

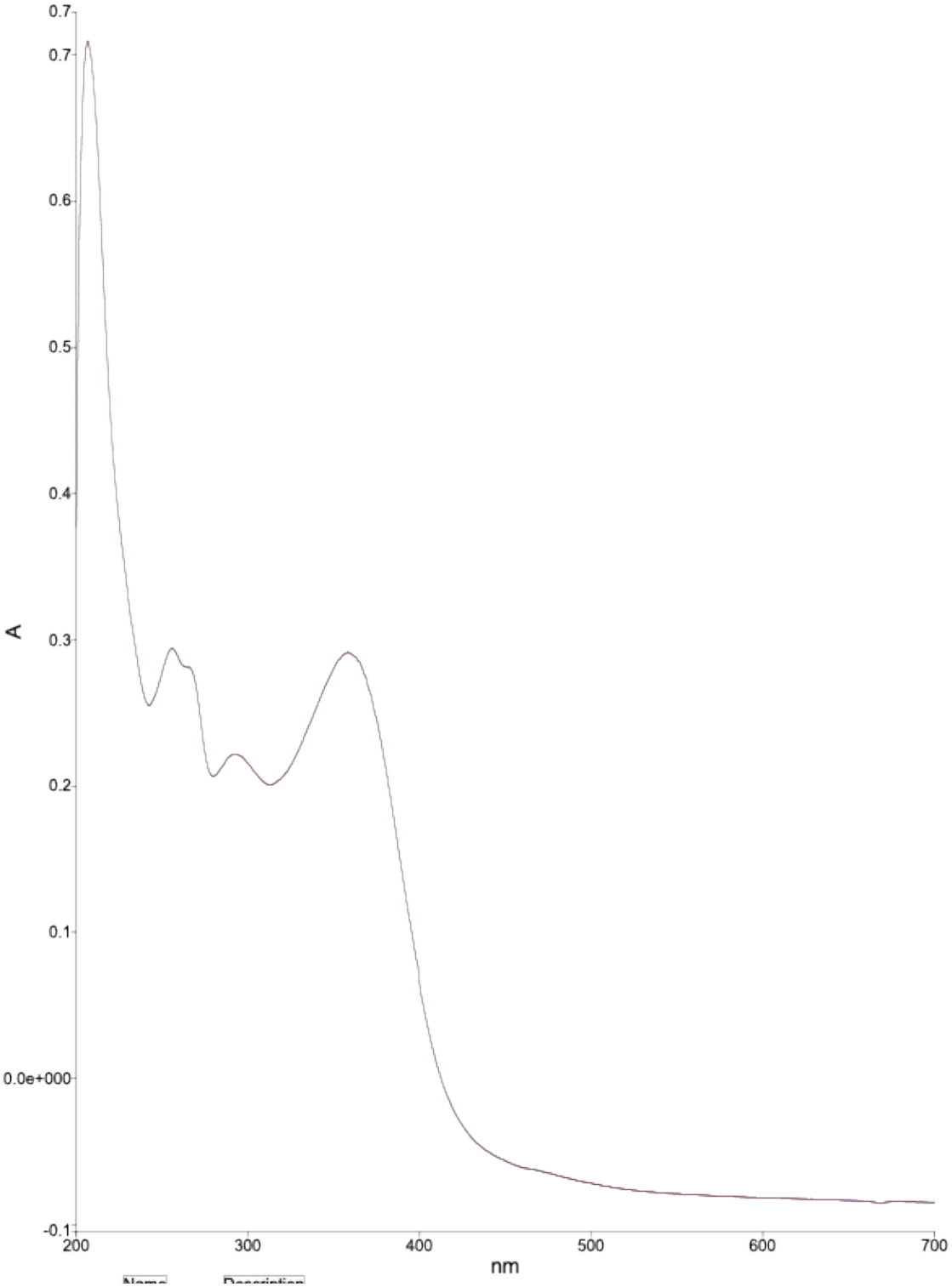

Figure A.3. Absorption spectrum of polyphenol extract of HL variety

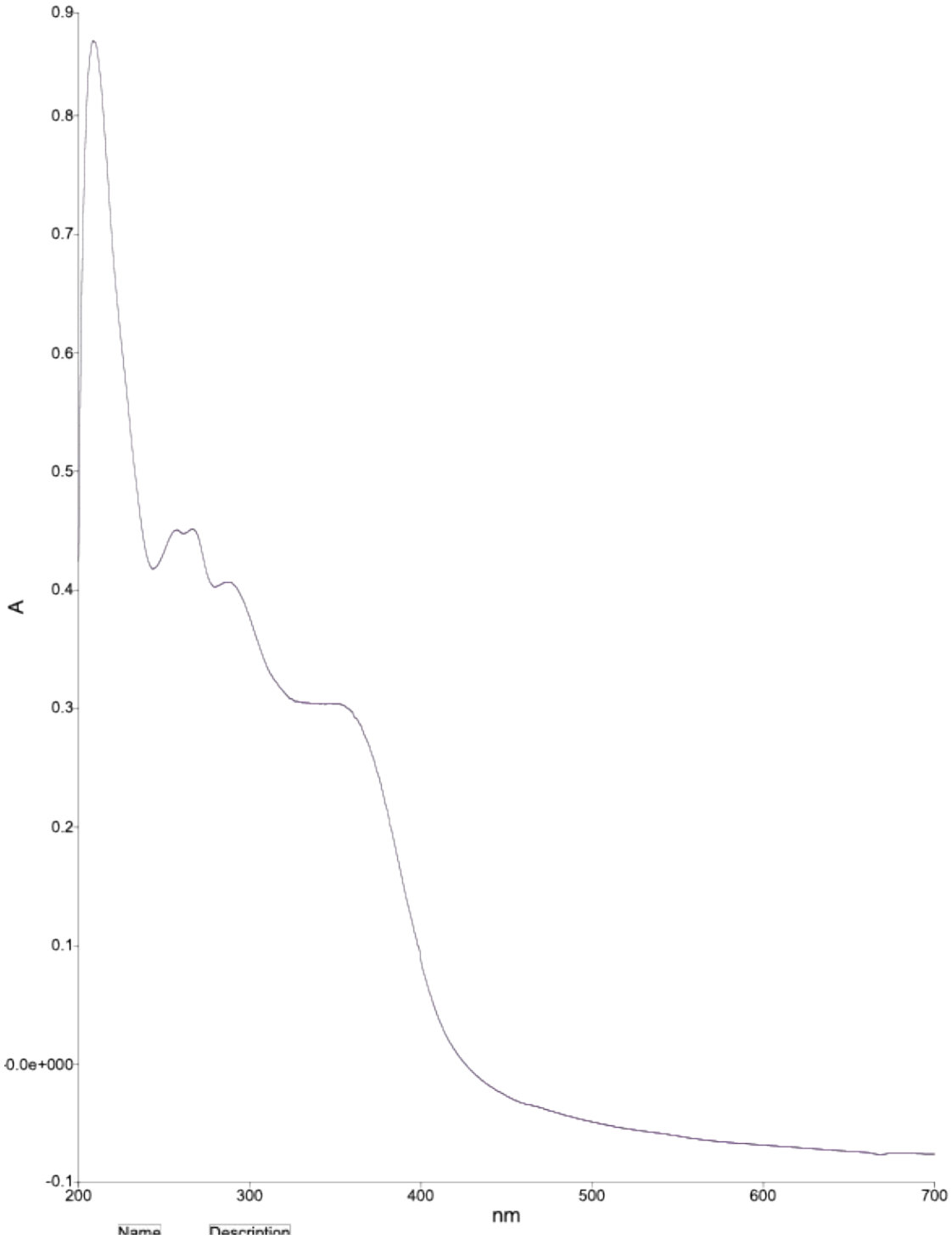

Figure A.4. Absorption spectrum of polyphenol extract of ST variety

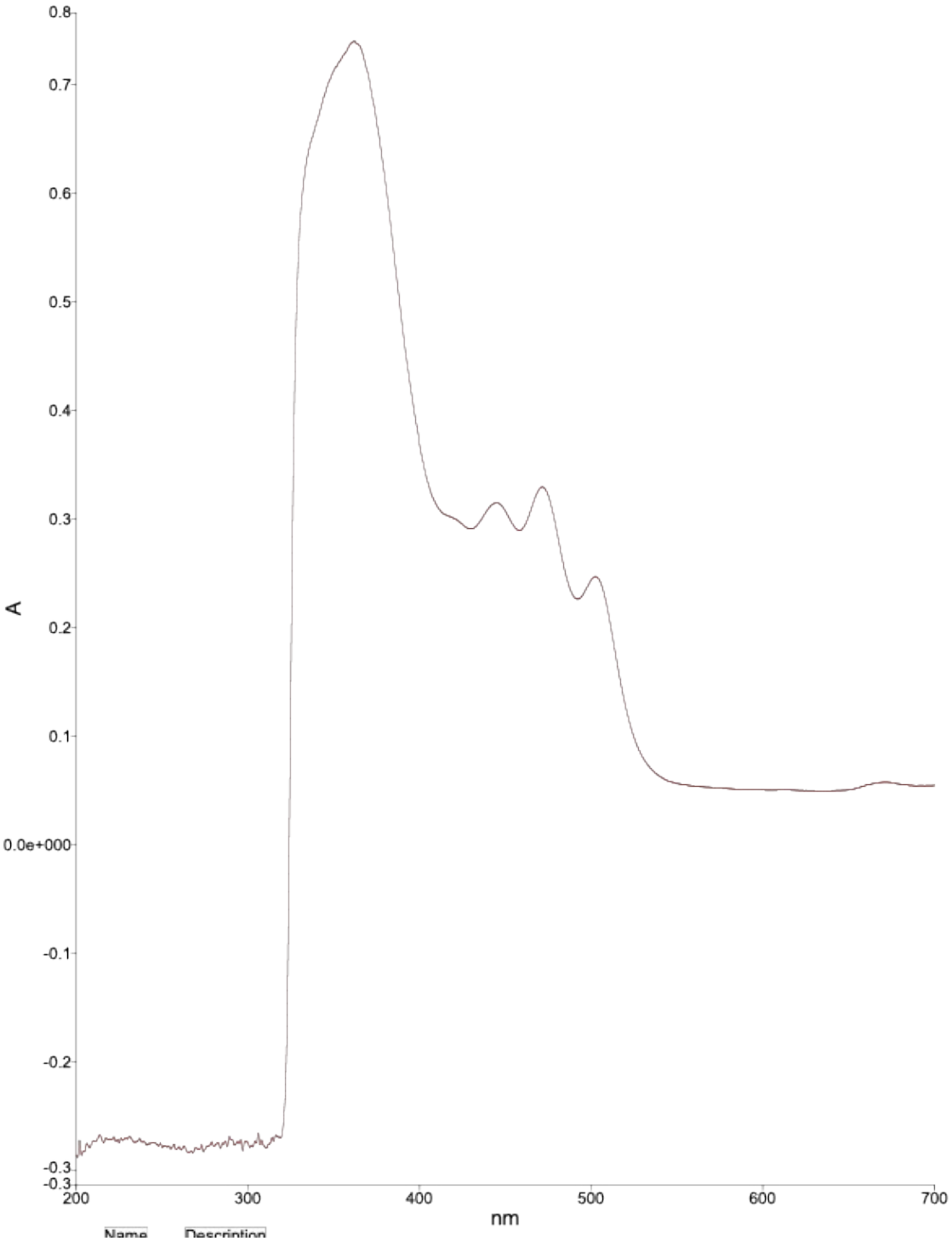

Figure A.5. Absorption spectrum of carotenoid extract of ST variety

Note: The negative absorbance values from 325nm and below are from the acetone present in the extraction solvent.

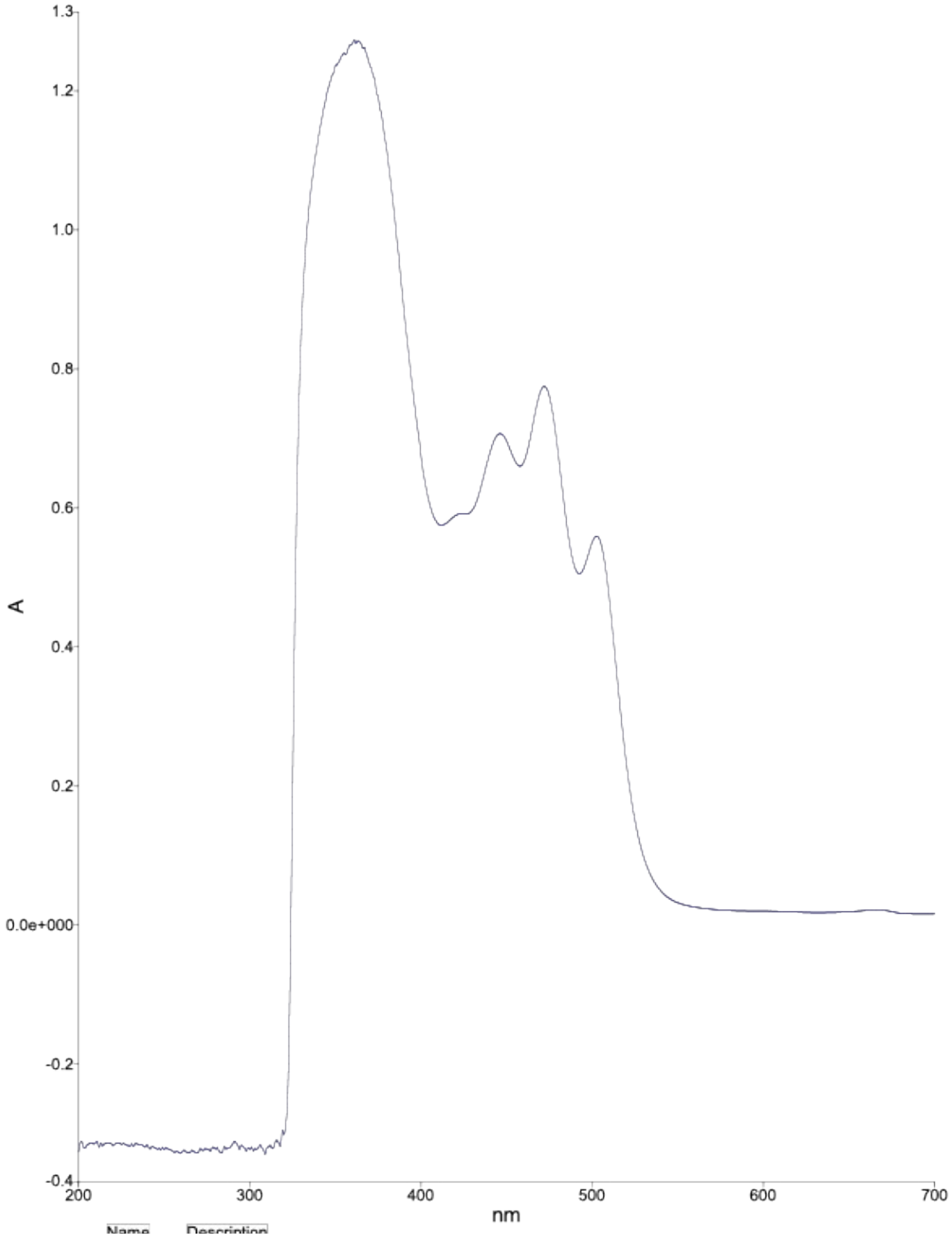

Figure A.6. Absorption spectrum of carotenoid extract of HL variety