Supporting Information

Valorization of Pomegranate Waste through Green Solvent Extraction and Biochar Production: A Zero-Waste Biorefinery Approach

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TABLES

Table S1. List of HBAs used in the COSMO-RS screening.

Code	HBA	Code	HBA
1	Urea	38	Guanidine hydrochloride
2	Lactic acid	39	Cholinium dihydrogen citrate
3	Malic acid	40	Cholinium dihydrogen phosphate
4	Citric acid	41	Benzyl (2-hydroxyethyl) dimethylammonium chloride
5	Octanoic acid	42	D-Glucose
6	Nonanoic acid	43	L-Glucose
7	Decanoic acid	44	Fructose
8	Dodecanoic acid	45	Sucrose
9	Oxalic acid	46	Maltose
10	Acetamide	47	Xylose
11	Nicotinamide	48	Sodium acetate
12	Threonine	49	Ammonium acetate
13	Ornithine	50	Sodium propionate
14	Citrulline	51	Trimethylglycin
15	Glycine	52	Betaine
16	Proline	53	Thereonine
17	Serine	54	Tetrapropylammonium chloride
18	Alanine	55	Tetrabutylammonium chloride
19	Histidine	56	Tetraheptylammonium chloride
20	Lysine	57	Tetraoctylammonium chloride
21	Arginine	58	Methyltrioctyl ammonium chloride
22	Glycerol	59	Triethylmethylammonium chloride
23	1-propanol	60	Benzyltriethylammonium chloride
24	Ethylene glycol	61	Benzyltrimethylammonium chloride
25	Phenol	62	Phenyltrimethylammonium chloride
26	o-cresol	63	N-ethyl-2-hydroxy-N,N-dimethylethanaminium chloride
27	Cholinium acetate	64	2-(chlorocarbonyloxy)-N,N,N-trimethylethanaminium chloride
28	Cholinium chloride	65	Methyltrioctylammonium bromide
29	Cholinium bitartrate	66	Alyltriphenylphosphonium bromide
30	Acetylcholinium chloride	67	Ethylammonium chloride
31	Carnitine hydrochloride	68	N,N-Diethylethanolammonium chloride
32	Tetraethylammonium chloride	69	Tetraethylammonium chloride
33	Tetramethylammonium bromide	70	Tetramethylammonium bromide
34	Tetrapropylammonium bromide	71	Methyltriphenylphosphonium bromide
35	Tetrabutylammonium bromide	72	Menthol

36	Methyltriphenyl phosphonium bromide	73	Thymol
37	Benzyltriphenylphosphonium bromide		

Table S2. List of HBDs used in the COSMO-RS screening.

Code	HBD	Code	HBD
1	Urea	73	Benzoic acid
2	Dimethylurea	74	Salicylic acid
3	N-methylurea	75	Acetylsalicylic Acid
4	N,N-Dimethylformamide	76	Phenylacetic acid
5	Acetamide	77	p-Coumaric acid
6	Thiourea	78	Gallic Acid
7	1-Hexanol	79	p-Hydroxy benzoic acid
8	1-Octanol	80	Nicotinic acid
9	1-Decanol	81	p-Toluenesulfonic acid
10	1-Dodecanol	82	Phenylpropionic acid
11	1-Tetradecanol	83	Itaconic acid
12	1-Hexadecanol	84	3-Phenyl-propionic acid
13	Cyclohexanol	85	4-Phenyl-butyric acid
14	Glycerol	86	5-Phenyl-valeric acid
15	Ethylene glycol	87	Butyric acid
16	1,2-Propanediol	88	Valeric acid
17	1,3-Butanediol	89	Phenylacetic acid
18	2,3-Butanediol	90	Glutaric acid
19	1,5-Pentaneiol	91	Leucine
20	1,6_Hexanediol	92	Vanillic acid
21	1,7-Heptanediol	93	Geranic acid
22	1,8-Octanediol	94	Pyruvic acid
23	1,9-Nonanediol	95	Octanoicacid
24	1,10-Decanediol	96	Nonanoic acid
25	1,15-Pentadecanediol	97	Decanoic acid
26	1,4-Butanediol	98	Dodecanoic acid
27	Diethylene glycol	99	Caproic acid
28	Triethylene glycol	100	Glutamic acid
29	Furfuryl alcohol	101	Hexanoic acid
30	2,4,6-Trimethyl phenol	102	Ricinoleic acid
31	2-Methyl-phenol	103	Hexadecanoic acid
32	3,4-Dimethyl-phenol	104	Tetradecanoic acid
33	4-Chloro phenol	105	Oleic acid
34	4-Methoxy phenol	106	Lauric acid
35	Erythritol	107	Alanine
36	Inositol	108	Arginine
37	Mannitol	109	Glycine
38	Sorbitol	110	Histidine

39	Xylitol	111	Lysine
40	Arabinose	112	Proline
41	Fructose	113	Serine
42	Galactose	114	Thereonine
43	S-Glucose	115	Gulonolactone
44	L-Glucose	116	Fucose
45	Isosorbide	117	Menthol
46	Maltose	118	Thymol
47	Mannose	119	α-Naftol
48	Raffinose	120	Resorcinol
49	Rhamnose	121	Phenol
50	Sorbose	122	p-Chlorophenol
51	Sucrose	123	Guaiacol
52	Trehalose	124	p-Hydroxybenzyl alcohol
53	Xylose	125	p-Hydroxy benzaldehyde
54	D-Ribose	126	Vanillin
55	Formic acid	127	o-Cresol
56	Acetic acid	128	Ethanolamine
57	Aconitic acid	129	Camphor
58	Ascorbic acid	130	Pyridine
59	Citric acid	131	Quinoline
60	Fumaric acid	132	Trioctylphosphine oxide
61	Glycolic acid	133	Benzamide
62	Lactic acid	134	Catechol
63	Levulinic acid	135	Hydroquinone
64	Maleic acid	136	Paracetamol
65	Malic acid	137	Pyrrole
66	Malonic acid	138	Aspirin
67	Oxalic acid	139	2-Methylimidazole
68	Propionic acid	140	Chimaphilin
69	Succinic acid	141	Dihydroquercetin
70	Tartaric acid	142	Quercetin
71	Mandelic acid	143	Zinc Chloride
72	Aspartic acid	144	Ferric chloride

Table S3. Experimental and encoded values for extraction of anthocyanins from pomegranate waste extracted with gamma-valerolactone (GVL) in the CCRD (2^4) assays.

CCRD	**Assay**	**Solid-liquid ratio ($g_{biomass}.mL_{solvent}^{-1}$)**	**Concentration (M)**	**pH**	**Time of extraction (min)**	**Yield of anthocyanins ($mg_{anthocyanis}.g_{biomass}^{-1}$)**
		X_1	***X_2***	***X_3***	***X_4***	***Y***
Factorial points	**1**	0.045 (**-1**)	1.1 (**-1**)	3 (**-1**)	30 (**-1**)	23.00
	2	0.095 (**1**)	1.1 (**-1**)	3 (**-1**)	30 (**-1**)	19.41
	3	0.045 (**-1**)	2.9 (**1**)	3 (**-1**)	30 (**-1**)	23.53
	4	0.095 (**1**)	2.9 (**1**)	3 (**-1**)	30 (**-1**)	20.66
	5	0.045 (**-1**)	1.1 (**-1**)	5 (**1**)	30 (**-1**)	19.03
	6	0.095 (**1**)	1.1 (**-1**)	5 (**1**)	30 (**-1**)	10.64
	7	0.045 (**-1**)	2.9 (**1**)	5 (**1**)	30 (**-1**)	13.22
	8	0.095 (**1**)	2.9 (**1**)	5 (**1**)	30 (**-1**)	17.66
	9	0.045 (**-1**)	1.1 (**-1**)	3 (**-1**)	70 (**1**)	10.57
	10	0.095 (**1**)	1.1 (**-1**)	3 (**-1**)	70 (**1**)	12.15
	11	0.045 (**-1**)	2.9 (**1**)	3 (**-1**)	70 (**1**)	35.69
	12	0.095 (**1**)	2.9 (**1**)	3 (**-1**)	70 (**1**)	21.04
	13	0.045 (**-1**)	1.1 (**-1**)	5 (**1**)	70 (**1**)	11.90
	14	0.095 (**1**)	1.1 (**-1**)	5 (**1**)	70 (**1**)	13.02
	15	0.045 (**-1**)	2.9 (**1**)	5 (**1**)	70 (**1**)	34.37

	16	0.095 (**1**)	2.9 (**1**)	5 (**1**)	70 (**1**)	21.16
Axial points	**17**	0.020 (**-2**)	2.0 (**0**)	4 (**0**)	55 (**0**)	9.52
	18	0.120 (**2**)	2.0 (**0**)	4 (**0**)	55 (**0**)	2.38
	19	0.070 (**0**)	0.2 (**-2**)	4 (**0**)	55 (**0**)	16.14
	20	0.070 (**0**)	3.8 (**2**)	4 (**0**)	55 (**0**)	19.37
	21	0.070 (**0**)	2.0 (**0**)	2 (**-2**)	55 (**0**)	33.82
	22	0.070 (**0**)	2.0 (**0**)	6 (**2**)	55 (**0**)	1.53
	23	0.070 (**0**)	2.0 (**0**)	4 (**0**)	5 (**-2**)	21.92
	24	0.070 (**0**)	2.0 (**0**)	4 (**0**)	85 (**2**)	27.87
Central points	**25**	0.070 (**0**)	2.0 (**0**)	4 (**0**)	55 (**0**)	24.81
	26	0.070 (**0**)	2.0 (**0**)	4 (**0**)	55 (**0**)	23.79
	27	0.070 (**0**)	2.0 (**0**)	4 (**0**)	55 (**0**)	23.45
	28	0.070 (**0**)	2.0 (**0**)	4 (**0**)	55 (**0**)	24.47

Table S4. Experimental and encoded values for extraction of ellagic acid derivatives from pomegranate waste extracted with choline acetate ([Ch][Act]) in the CCRD (2^4) assays.

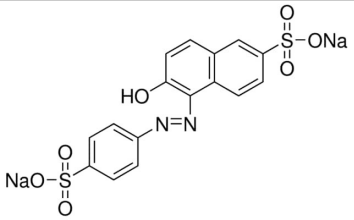
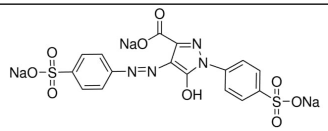
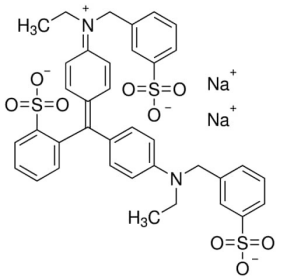
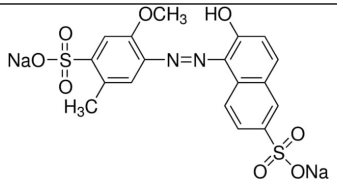
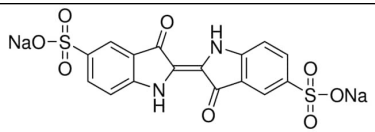
CCRD	**Assay**	**Solid-liquid ratio ($g_{biomass}.mL_{solvent}^{-1}$)**	**Concentration (M)**	**pH**	**Time of extraction (min)**	**Yield of anthocyanins ($mg_{anthocyanis}.g_{biomass}^{-1}$)**
		X_1	X_2	X_3	X_4	Y

Linear points	**1**	0.045 (**-1**)	1.1 (**-1**)	4 (**-1**)	30 (**-1**)	5.56
	2	0.095 (**1**)	1.1 (**-1**)	4 (**-1**)	30 (**-1**)	5.88
	3	0.045 (**-1**)	2.9 (**1**)	4 (**-1**)	30 (**-1**)	13.30
	4	0.095 (**1**)	2.9 (**1**)	4 (**-1**)	30 (**-1**)	12.51
	5	0.045 (**-1**)	1.1 (**-1**)	10 (**1**)	30 (**-1**)	14.96
	6	0.095 (**1**)	1.1 (**-1**)	10 (**1**)	30 (**-1**)	13.73
	7	0.045 (**-1**)	2.9 (**1**)	10 (**1**)	30 (**-1**)	14.19
	8	0.095 (**1**)	2.9 (**1**)	10 (**1**)	30 (**-1**)	20.82
	9	0.045 (**-1**)	1.1 (**-1**)	4 (**-1**)	70 (**1**)	4.41
	10	0.095 (**1**)	1.1 (**-1**)	4 (**-1**)	70 (**1**)	5.51
	11	0.045 (**-1**)	2.9 (**1**)	4 (**-1**)	70 (**1**)	12.62
	12	0.095 (**1**)	2.9 (**1**)	4 (**-1**)	70 (**1**)	19.60
	13	0.045 (**-1**)	1.1 (**-1**)	10 (**1**)	70 (**1**)	13.12
	14	0.095 (**1**)	1.1 (**-1**)	10 (**1**)	70 (**1**)	13.49
	15	0.045 (**-1**)	2.9 (**1**)	10 (**1**)	70 (**1**)	14.72
	16	0.095 (**1**)	2.9 (**1**)	10 (**1**)	70 (**1**)	22.14
Axial points	**17**	0.020 (**-2**)	2.0 (**0**)	7 (**0**)	55 (**0**)	13.45
	18	0.120 (**2**)	2.0 (**0**)	7 (**0**)	55 (**0**)	19.93

	19	0.070 (**0**)	0.2 (**-2**)	7 (**0**)	55 (**0**)	10.04
	20	0.070 (**0**)	3.8 (**2**)	7 (**0**)	55 (**0**)	13.07
	21	0.070 (**0**)	2.0 (**0**)	1 (**-2**)	55 (**0**)	20.69
	22	0.070 (**0**)	2.0 (**0**)	13 (**2**)	55 (**0**)	23.78
	23	0.070 (**0**)	2.0 (**0**)	7 (**0**)	5 (**-2**)	18.44
	24	0.070 (**0**)	2.0 (**0**)	7 (**0**)	85 (**2**)	16.78
Central points	**25**	0.070 (**0**)	2.0 (**0**)	7 (**0**)	55 (**0**)	19.76
	26	0.070 (**0**)	2.0 (**0**)	7 (**0**)	55 (**0**)	19.85
	27	0.070 (**0**)	2.0 (**0**)	7 (**0**)	55 (**0**)	18.92
	28	0.070 (**0**)	2.0 (**0**)	7 (**0**)	55 (**0**)	20.88

Table S5. List of synthetic food and textile dyes used in the adsorption experiments using the produced pomegranate biochar material.

Dye	**Compound**	**Structure**	**Purity**	**Molar mass ($g.mol^{-1}$)**	**Source**

Food dyes	Sunset Yellow		90%	452.37	Sigma Aldrich
	Tartrazine yellow		>85%	534.36	Sigma Aldrich
	Brilliant blue		95%	792.85	Sigma Aldrich
	Allura red (red 40)		80%	496.42	Sigma Aldrich
Textile dyes	Indigo carmine blue		95%	466.35	Sigma Aldrich

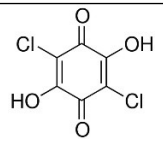
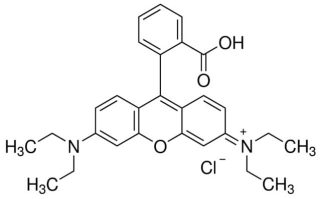
	Chloranilic acid		99%	208.98	Sigma Aldrich
	Rhodamine B		99%	479.01	Merck

Table S6. Retention time (RT), molecular ion ($[M]^+$ – *m/z*), fragmentation pattern (MS^2), and putative identification of the anthocyanins-rich fraction, recorded at 520 nm, and ellagic acid-rich fraction and derivatives recorded at 350 nm.

Extract	**Peak**	**Time (min)**	**$[M]^+$ (m/z)**	**MS^2**	**Compound**
Anthocyanins fraction – chromatogram recorded at 520 nm – Figure 1A	**1**	1.91	627	465,303	delphinidin-3,5-*O*-diglucoside
	2	2.07	595	449, 287	cyanidin-3-*O*-rutinoside
	3	2.25	433	271	pelargonidin-3-*O*-glucoside
	4	2.50	465	303	delphinidin-3-*O*-glucoside
	5	2.85	449	287	cyanidin 3-*O*-glucoside

Ellagic acid fraction – chromatogram recorded at 350 nm – Figure 1B	**1**	2.53	1083	781, 601, 301	α-punigalagin
	2	2.63	1083	781, 601, 301	β-punigalagin
	3	3.35	301	283, 257	ellagic acid

Table S7. Summary of the average macro-composition (ash, protein, fiber, fat, carbohydrates, and moisture) of pomegranate wastes reported in the literature.

Ash (%)	Protein (%)	Fiber (%)	Fat (%)	Carbohydrates (%)	Moisture (%)	Reference
6.80	5.10	12.61	1.50	30.50	43.49	[1]
3.71	3.96	28.10	0.00	30.65	33.58	[2]
4.41	5.59	31.03	0.00	33.02	25.96	[3]
4.85	4.18	18.48	0.80	26.70	44.99	[4]
3.40	4.90	16.30	1.26	17.70	56.44	[5]
4.22	3.96	28.10	0.00	30.65	33.07	[6]
3.40	4.90	19.41	1.26	17.70	53.33	[7]
4.40 ± 1.19	**4.66 ± 0.63**	**22.00 ± 7.02**	**0.69 ± 0.69**	**26.70 ± 6.42**	**41.55 ± 11.21**	**Mean ± SD**

Table S8. The activity coefficients at infinite dilution (ln γ∞) of delphinidin-3-*O*-glucoside and ellagic acid in bio-based solvents in aqueous solution (50 % molar fraction) at 35 °C.

Code	Bio-based solvent	ln γ∞ - delphinidin-3-*O*-glucoside	ln γ∞ - ellagic acid
1	Water	0.78	-1.09
2	Ethanol	-6.02	-8.07
3	1,3-Propanediol	-6.21	-8.99
4	Glycerol	-4.60	-7.31
5	1-Butanol	-3.30	-7.00
6	2-Butanol	-3.50	-7.36
7	Tert-butanol	-3.84	-7.68
8	1,2-Butanediol	-3.44	-6.50
9	1,3-Butanediol	-4.99	-8.45
10	1-Octanol	0.51	-5.69
11	2,3-Butanediol	-4.04	-7.23
12	2-Octanol	0.57	-5.88
13	Octan-4-ol	0.96	-5.49
14	Ethylacetate	-5.65	-9.41
15	Cyrene	-4.20	-8.26
16	Dimethyl isosorbide	-5.20	-9.28
17	γ-valerolactone	-7.20	-10.25
18	Lactic acid	-2.47	-2.72
19	Limonene	3.27	-3.79
20	Solketal	-5.31	-8.95
21	β-Pinene	3.56	-3.48
22	α-Pinene	4.38	-2.98
23	Dimethyl carbonate	-6.57	-9.72
24	Ethyl lactate	-4.80	-8.25
25	Succinic acid	-2.48	-1.56
26	Butyl levulinate	-2.80	-8.60
27	Cyclopentyl methyl ether	-2.52	-8.37
28	Dibutyl succinate	-1.46	-8.44
29	Ethyl levulinate	-5.94	-10.26
30	Furfuryl alcohol	-4.16	-6.60
31	γ-Butyrolactone	-7.85	-10.38
32	Levulinic acid	-2.65	-4.74
33	Propyl guaiacol	-1.18	-7.79
34	Propyl syringol	1.57	-4.29
35	1,2,3-Tributoxypropane	3.27	-6.68
36	1,3-Dibutoxy-2-propanol	0.23	-7.60
37	1,3-Diethoxy-2-propanol	-3.32	-9.08
38	3-Butoxy-1,2-propanediol	-1.62	-6.39
39	3-Ethoxy-1,2-propanediol	-3.00	-6.79
40	2,5-Dimethylfuran	-0.99	-5.60
41	Gluconic acid	0.37	-1.78
42	Glycerol triacetate	-4.34	-8.25
43	Propylene carbonate	3.42	-7.95
44	Terpinolene	-4.56	-3.72

45	1,3-Dioxane-5-ol	-5.98	-7.30
46	4-Hydroxymethyl-1,3-dioxolane	-4.61	-8.75
47	Diethyl succinate	-4.34	-9.70
48	Methyl isobutyl ketone	-5.08	-10.31
49	Triacetin	-3.42	-8.52

Table S9. Predicted results found through the mathematical model developed for the optimization of anthocyanins recovery and the respective relative deviation from the independent variables: solid-liquid ratio (SLR), concentration of gamma-valerolactone - GVL (C - M), pH, and time of extraction (t_{ext}) to define the 2^4 CCRD. V1, V2, and V3 represent the validation experimental assays.

Assays	**SLR (X_1) ($g_{biomass}.mL_{solvent}^{-1}$)**	**C (X_2) M**	**pH (X_3)**	**t_{ext} (X_4) min**	**Predicted values ($mg_{anthocyanins}.g_{biomass}^{-1}$)**	**Experimental values ($mg_{anthocyanins}.g_{biomass}^{-1}$)**	**Relative deviation (%)**
V1	0.07	2.9	3	30	37.4	38.5	3.0
V2						38.6	3.3
V3						38.5	2.9
					Final Validation	**38.52 ± 0.06**	**3.06 ± 0.21**

Table S10. Predicted results found through the mathematical model developed for the optimization of ellagic acid and derivatives and the respective relative deviation from the independent variables: solid-liquid ratio (SLR), concentration of cholinium acetate - [Ch][Act] (C - M), pH, and time of extraction (t_{ext}) to define the 2^4 CCRD. V1, V2, and V3 represent the validation experimental assays.

Assays	**SLR (X_1) ($g_{biomass}.mL_{solvent}^{-1}$)**	**C (X_2) M**	**pH (X_3)**	**t_{ext} (X_4) min**	**Predicted values ($mg_{anthocyanins}.g_{biomass}^{-1}$)**	**Experimental values ($mg_{anthocyanins}.g_{biomass}^{-1}$)**	**Relative deviation (%)**
V1	0.07 $g_{biomass}.mL_{solvent}^{-1}$	2900 mM	13	55 min	21.5	21.4	-0.32
V2						21.9	2.3
V3						22.1	3.2
					Final Validation	**21.82 ± 0.36**	**1.73 ± 1.83**

Table S11. Elemental analysis of the biochar produced by the (D)ES-mediated process.

Sample	**$\%_{carbon}$**	**$\%_{oxygen}$**	**$\%_{hydrogen}$**	**$\%_{nitrogen}$**	**$\%_{sulfur}$**
Pomegranate biochar	43.96	47.90	5.48	2.66	n.d.
Pomegranate biochar after indigo blue adsorption (textile dye)	42.87	48.37	5.26	2.69	0.81

Pomegranate biochar after sunset yellow adsorption (food dye)	43.26	48.13	5.38	2.55	0.68

Table S12. Detailed scores of each principle from *Path2Green* metric that is rooted in the 12 principles of green extraction.

Green Extraction Principles	Attributed Weight[a]	Score	Reason
Principle 1 – Biomass: Select biomass that is naturally sourced or requires minimal resource usage for production.	**6.00**	**+1.00**	The pomegranate used in this work is considered a waste from the juicy industry.
Principle 2 – Transport: Preserving biomass integrity while minimizing transport's environmental impact.	**5.00**	**-1.00**	The biomass used in this work, despite being industrial waste, was transported from California, USA, to the extraction site in Portugal**.** However, this score can be better considering the need to perform the biorefinery approach near the biomass origin site.
Principle 3 – Pre-treatment: Pre-treatment: Optimization for pre-treatment avoidance and cost-effective techniques.	**2.50**	**-0.20**	Only physical pretreatments were used to pre-treat the used biomass.
Principle 4 – Solvent: Minimize solvent usage, prioritizing those of biological origin, biodegradable and non-toxic.	**6.00**	**0.00**	A three-step biorefinery approach was developed to recover three valuable products from pomegranate waste: anthocyanins, an ellagic acid-rich fraction, and biochar material. This process utilized three solvents: bio-based gamma-valerolactone (scoring 0.00 in the CHEM21 database), cholinium acetate (which can be produced as a bio-based ionic liquid but is predominantly commercialized via synthetic routes, also scoring 0.00), and an eutectic solvent formulated from cholinium chloride and oxalic acid. While these solvents offer a sustainable alternative to traditional fossil-fuel-based volatile organic

			solvents, concerns about their production remain. As such, a neutral score (0.00) was applied in this metric to reflect these considerations.
Principle 5 – Scaling: Ensure reproducibility and a continuous extraction flow.	**5.00**	**-1.00**	A batch biorefinery process was employed, which poses challenges for scaling up.However, the operational units performed in this process can be replaced for at least semi-continuous mode.
Principle 6 – Purification: Final application dictates the extent of purification.	**2.50**	**+1.00**	Ready-to-use extracts were obtained (anthocyanins, and ellagic acid-rich fractions) without needing purification.
Principle 7 – Yield: Maximize the utilization and valorization of the biomass.	**4.00**	**+1.00**	Complete valorization of the biomass. No residual biomass obtained in the end of the process.
Principle 8 – Post-treatment: Functionalization of natural products post-extraction to maximize their benefits.	**2.50**	**+1.00**	Ready-to-use extracts were obtained (anthocyanins, and ellagic acid-rich fractions) without the need to purification – without the need to perform a post-treatment strategy.
Principle 9 – Energy: Prioritize using clean energy sources and high-efficiency extraction techniques.	**5.00**	**+0.50**	A low-dependent extraction technique was performed using renewable energy.
Principle 10 – Application: Ensure safety for applications in several domains.	**4.5**	**+1.00**	The obtained anthocyanins, ellagic acid and its derivatives can be applied in several sectors, which include pharma, nutraceutic, cosmetic, nutritional, food, biomedical, consumer products.
Principle 11 – Repurposing: Trace strategies to perform closed-loop extraction systems, preferably	**6.00**	**+1.00**	Non-virgin raw materials were employed.

using non-virgin materials.			
Principle 12 – Waste management: Refine waste reduction and ensure effective waste management.	**6.00**	**+1.00**	A zero waste biorefinery approach was developed culminating in the biochar production (zero waste).

[a]Weight selected according to preconized in Path2Green original article.

Figures

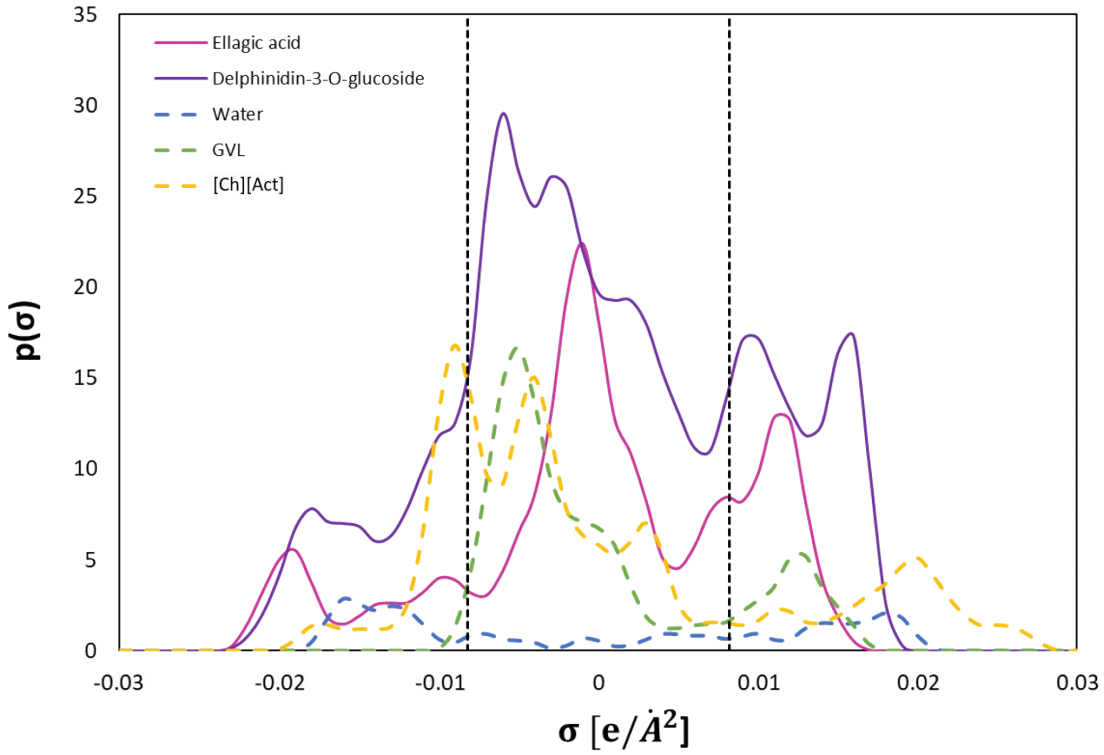


Figure S1. The σ-profiles and σ-potential - μ(σ) – from COSMO-RS of delphinidin-3-O-glucoside (—), ellagic acid (—), GVL (---), water (---) and [Ch][Act] (---) at 35 °C.

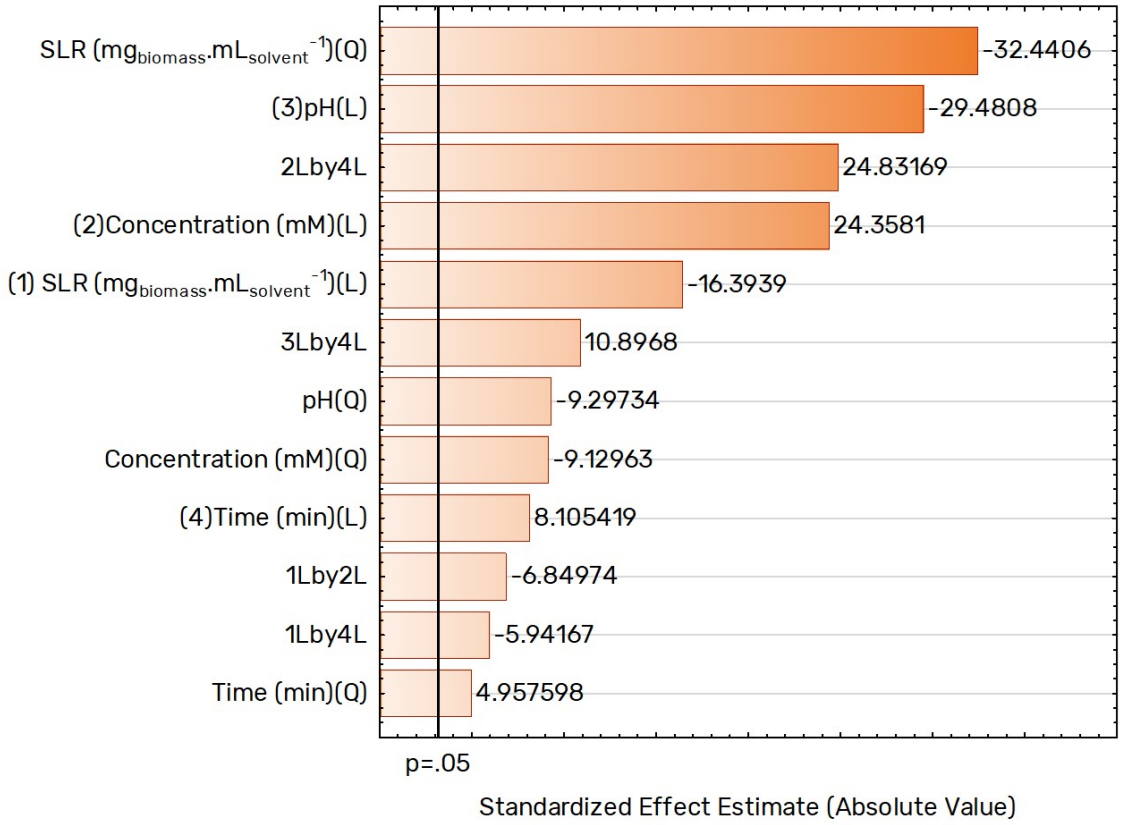


Figure S2. Pareto chart of the CCRD (2^4 + axial points) regarding the anthocyanins extraction yield from pomegranate wastes using gamma-valerolactone (GVL) as solvent. The point at which the estimated effects are statistically significant ($p < 0.05$) is indicated by the continuous vertical line

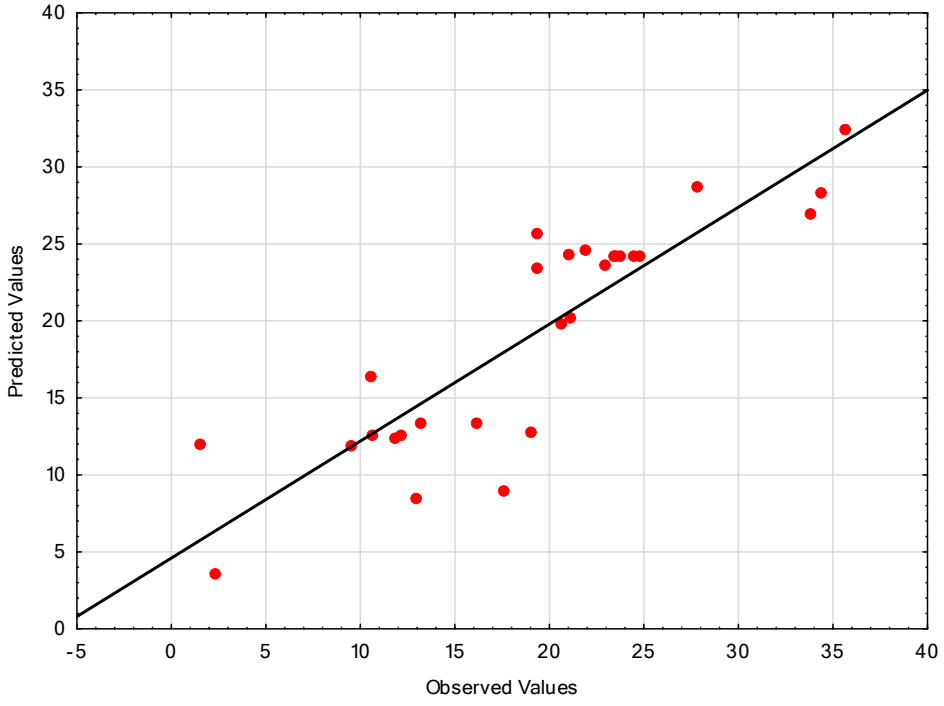


Figure S3. Predicted *vs*. Experimental values of the CCRD (2^4 + axial points) regarding the anthocyanins extraction yield from pomegranate wastes using gamma-valerolactone (GVL) as solvent.

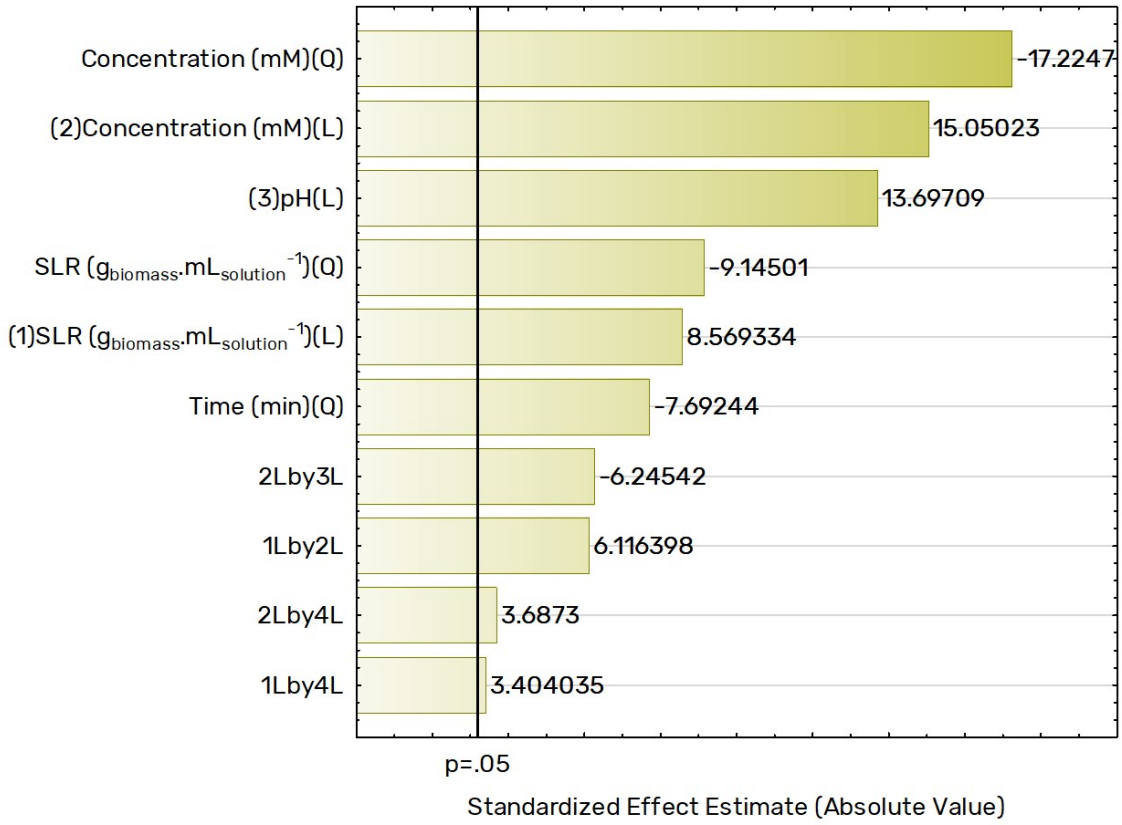


Figure S4. Pareto chart of the CCRD (2^4 + axial points) regarding the extraction yield of ellagic acid and derivatives from pomegranate using cholinium acetate [Ch][Act] as solvent. The point at which the estimated effects are statistically significant ($p < 0.05$) is indicated by the continuous vertical line.

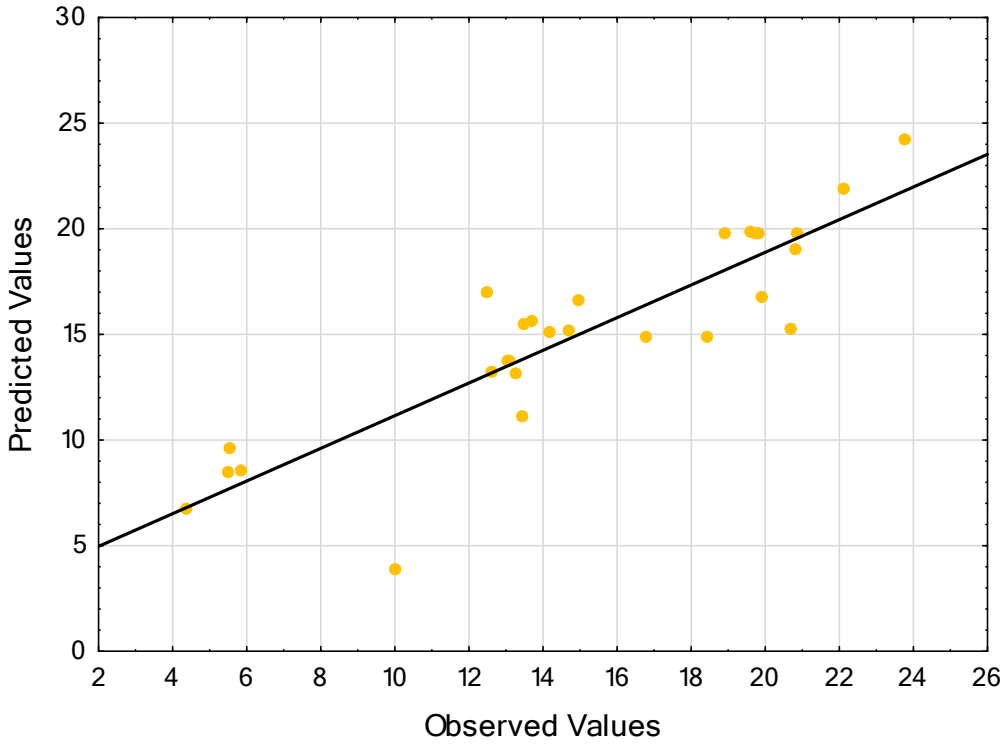


Figure S5. Predicted *vs*. Experimental values of the CCRD (2^4 + axial points) regarding the ellagic acid-rich fraction extraction yield from pomegranate wastes using cholinium acetate [Ch][Act] as solvent.

SECTION 1 – KINETIC MODELS AND BIOCHAR APPLICATION

- Non-linear forms of the pseudo first order and pseudo second order kinetic equations:

$$\log (Q_e - Q_t) = logQ_e - (\frac{k_1}{2.303})t$$

- Non-linear forms of the pseudo-second order kinetic equation:

$$Q_t - (\frac{k_2 {Q_e}^2 t}{1 + k_2 Q_e t})t$$

Where Q_t is the amount of dye adsorbed at time "t", Q_e is the amount of dye adsorbed at equilibrium, t is the time in minutes, k_1 is the rate constant of the first order model (min^{-1}) and k_2 is the rate constant of the second order model ($g.mg^{-1}.min^{-1}$).

As a proof of concept, adsorption experiments of synthetic food and textile dyes in the biochar material were proposed. Initially, the absorption of the food dye sunset yellow was tested, with the kinetic adsorption model being presented in Figure S6. After 75 min of contact between the biochar and the aqueous solution of sunset yellow (E 110), at circa 99.2% (0.023 $mg_{dye}.mL_{solution}^{-1}$) of the dye is remediated (adsorbed in the biochar). Afterward, the same condition was tested to investigate if the biochar material could be useful in the remediation of other synthetic dyes (used in food and textiles), as shown in Figure S8. After 75 min of contact, 100% of the colorant brilliant blue was adsorbed. Brilliant blue is a triarylmethane dye, denoted by E-number 133 (E133). It is approved for use in food, pharmaceutical, and cosmetic formulations. Regarding the azo

dyes, 100% of Red 40 (Allura red – E129) and 69.7% of tartrazine yellow (E102) were adsorbed into the biochar after 95 min of contact. It is unclear why, after 75 min, tartrazine yellow had a lower uptake than other dyes, but in a second test with 120 min of contact, it was possible to recover 100% of this colorant.

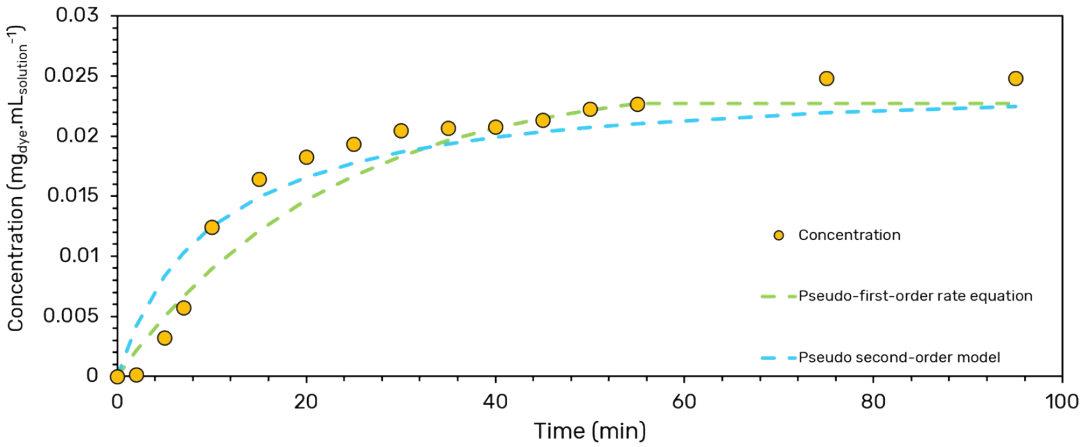


Figure S6. Pseudo first order and pseudo second order sorption kinetics of yellow sunset - food dye – using the biochar produced from the residual biomass obtained after the sequential extraction of anthocyanins and ellagic acid and derivatives.

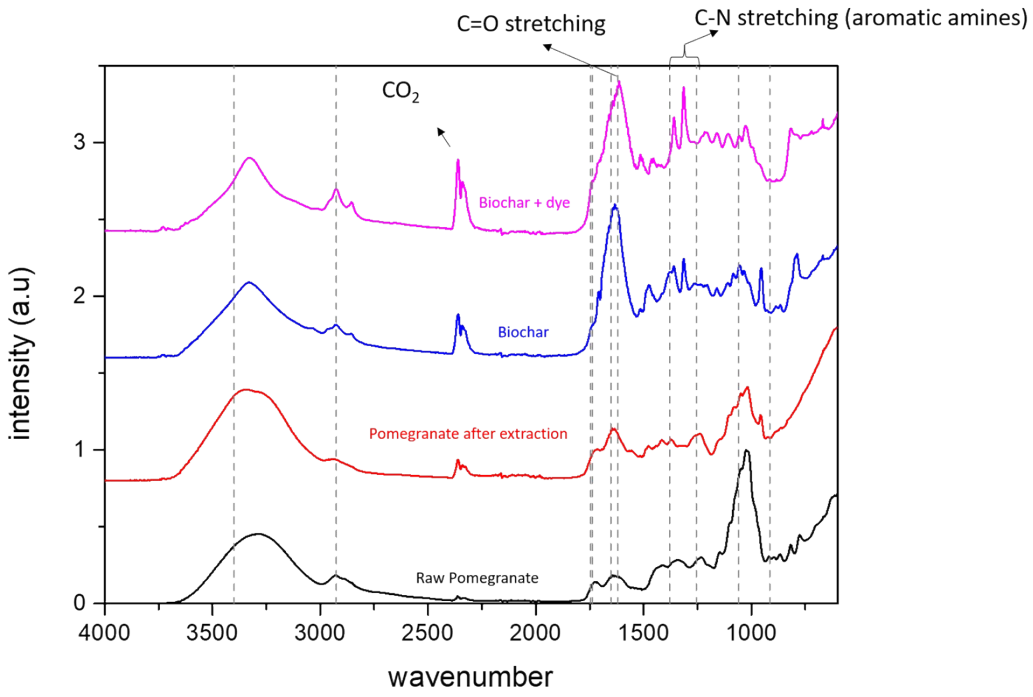


Figure S7. FTIR spectra of the raw pomegranate (before extraction) and post-extraction, biochar, and biochar after adsorption of sunset yellow dye.

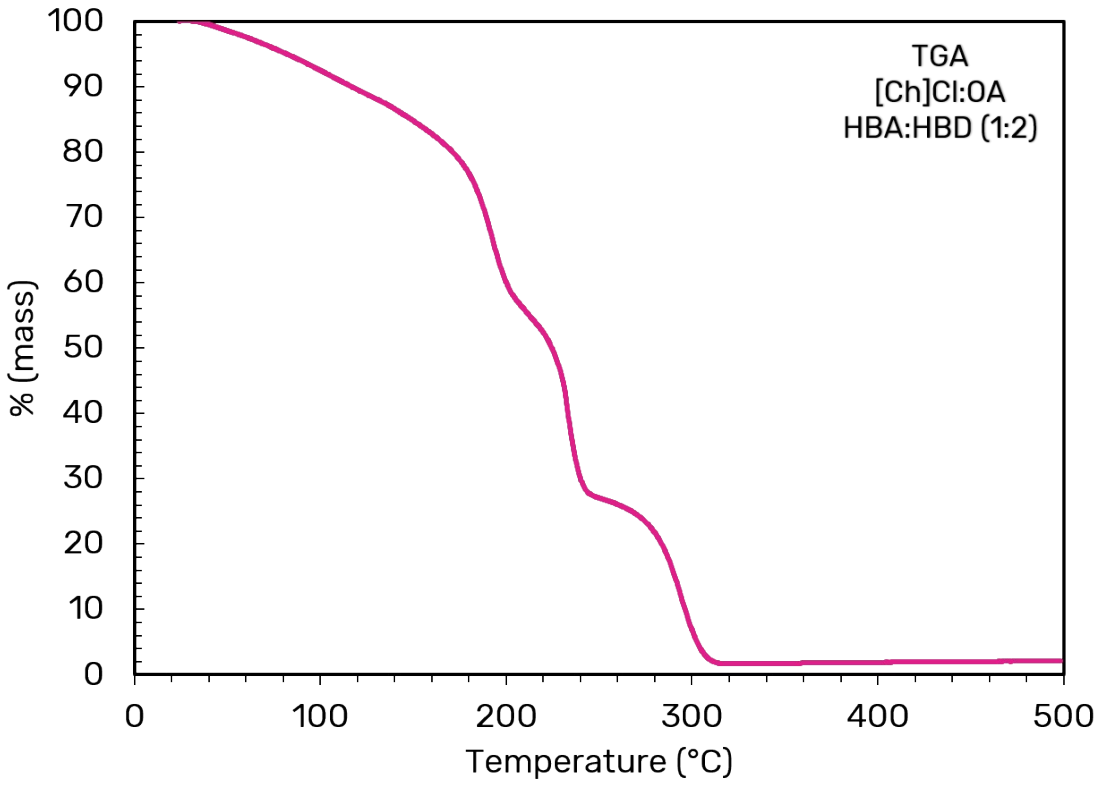


Figure S8. Thermogravimetric Analysis (TGA) of the eutectic solvent composed of cholinium chloride and oxalic acid ([Ch]Cl:OA, with a molar ratio of HBA:HBD (1:2), confirming its decomposition starting at temperatures exceeding 180°C.

Regarding the adsorption of textile dyes into the biochar material prepared with pomegranate wastes, by analysing Figure S9 it is possible to see adsorption values around 75-80% after 75 min of contact between the biochar and the aqueous dye solutions (indigo blue – 82.3%, chloranilic acid – 89.1%, and rhodamine – 78.3%). Another point that demonstrates the adsorption of synthetic dyes into biochar is the elemental composition of the samples after the remediation experiments. Table S10 shows the presence of sulfur elements, which are only detected after the adsorption of indigo blue and sunset yellow dyes. These dyes were specifically selected as evidence of the adsorption process. Even with lower efficiency in the adsorption of textile dyes than

food dyes, the biochar produced here is highly efficient. Thus, this carbon material may also be explored to produced filters or membranes, mixing more specific adsorbent materials that could assist the adsorption potential of the biochar, like ion exchange resins. Just to note that the production of this material was not optimize, which means that with the proper optimization of the material production, higher adsorption potential may be assessed.

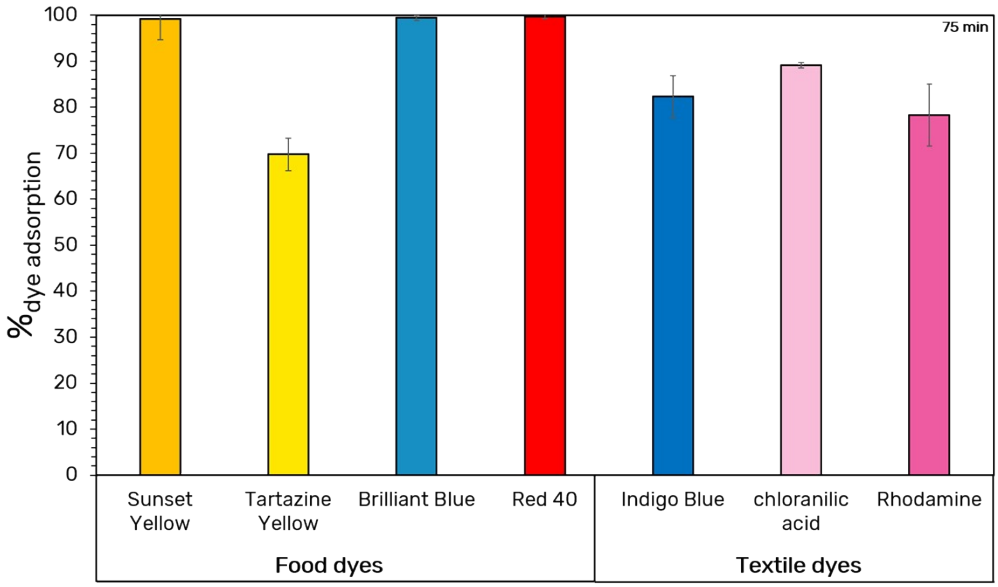


Figure S9. Evaluation of the dye adsorption (%) considering sunset yellow, tartazine yellow, brilliant blue, red 40, indigo blue, chloranilic acid, and rhodamine, into the biochar material developed through a eutectic solvent-mediated process from the residual biomass obtained after the sequential extraction of anthocyanins and ellagic acid and derivatives.

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