



Data Article

Data on the characterization of seaweed, wheat bran, and other food processing byproducts as feasible biosorbents



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ABSTRACT

Traditionally, biosorbents have been used to remove contaminants from polluted water, such as wastewater, landfill leachate, rainwater or drinking water. However, two alternative uses of biosorbents have been proposed relatively recently: the removal of heavy metals from fruit juices by biosorption and the use of saturated biosorbents as animal feed. Because these biosorbents are in contact with food or are used as animal feed, the concentration of contaminants in biosorbents must be known. In addition, the characterization of biosorbents is crucial because biosorbent properties affect both adsorption efficiency and the performance of full-scale biosorbent systems. This article presents data from Fourier transform infrared spectroscopy (FTIR) analysis, and the concentration of toxic metals (determined by ICP-MS) as well as pesticide residues was determined in ten biomass samples, namely, pea skins, straw, seaweed *Fucus vesiculosus*, wheat bran, rye bran, raspberry seeds, peat,

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buckwheat husks, highbush blueberry pulp, and blackcurrant pulp. Selected biomass samples were also characterized by scanning electron microscopy (SEM), nitrogen physisorption analysis, and pyrolysis-gas chromatography-mass spectrometry (Py-GC/ MS/FID) analysis.

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Specifications Table

Subject	Environmental science, materials science.
Specific subject area	Environmental science, environmental chemistry, material characterization.
Data format	Raw and analyzed.
Type of data	Tables and figures.
Data collection	Ten biosorbents (pea skins (outer layer of peas), raspberry seeds, highbush blueberry pulp, blackcurrant pulp, wheat straw, seaweed <i>Fucus vesiculosus</i> , wheat bran, rye bran, peat, and buckwheat husks) were analyzed. Main analysis: 1) metal content was determined by ICP-MS (Agilent 7700 ICP-MS instrument); 2) pesticide residues were determined by GC-MS/MS (Shimadzu gas chromatograph GC-2010 Plus coupled with a TQ8040 mass spectrometer) and UHPLC-MS/MS (UltiMate 3000 UHPLC system coupled to TSQ Quantiva mass spectrometer equipped with an electrospray ionization source); 3) functional groups were determined by FTIR (Nicolet iS50 spectrometer); 4) surface morphology was determined by SEM (apparatus Thermo Scientific™ Helios™ 5 UX); 5) structural identification and quantitation of pyrolysis products were determined by Py-GC/ MS/FID (Frontier Lab MicroDouble-shot Pyrolyser Py-3030D directly coupled to a Shimadzu 2D FID/MS gas chromatography system MS-GC/GC-MS-2010 with a RTX-1701 capillary column). Nitrogen physisorption was performed using Micromeritics Tristar II equipment.
Data source location	Institute of Food Safety, Animal Health and Environment “BIOR”, Riga, Latvia.
Data accessibility	Repository name: Mendeley Data Data identification number: doi: 10.17632/fysfntftzf.2 Direct URL to data: https://data.mendeley.com/datasets/fysfntftzf/2

1. Value of the Data

- Data on the concentration of toxic metals and pesticide residues are vital when biosorbents come into contact with food (e.g., when used for the removal of toxic metals from fruit juice), as washout of these substances can occur.
- Many of the adsorption studies do not include characterization of the tested biosorbents; however, this should be a mandatory requirement, as properties of the biosorbents strongly affect the adsorption performance.
- The concentration of metals in biomass matrices is a crucial parameter in biomass conversation (such as gasification and combustion), production of biogas, and animal feed.

2. Data Description

Altogether, 10 biosorbent samples were collected and analyzed by various methods. Provided characterization, i.e., tables and figures in this article are based on raw data given in the repository [1].

Table 1 presents the bulk density, ash content, and pH values of various biosorbents. Table 2 further explores the physical characteristics by presenting the average hydraulic conductivity and density of the selected biosorbents, offering insights into their water filtration potential.

Table 1

Bulk density, ash content, and pH of biosorbents (raw data is not provided in the repository, which is related to the simplicity of data acquisition).

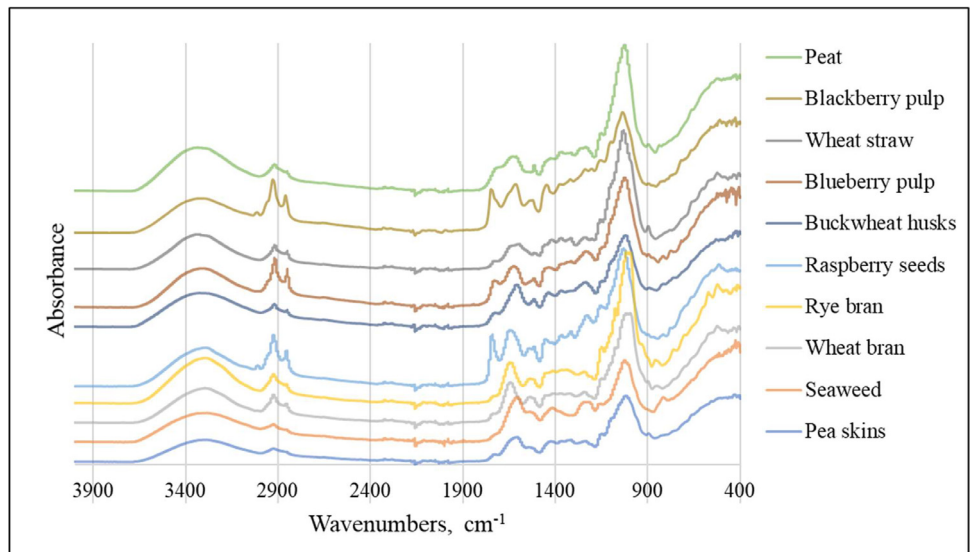
Biosorbent	Bulk density, g cm ⁻³	Ash content, %	pH
Pea skins	0.637	2.27	5.25
Wheat straw	0.141	7.23	8.12
Seaweed <i>Fucus vesiculosus</i>	0.744	15.16	5.72
Wheat bran	0.352	5.22	6.62
Rye bran	0.388	4.26	6.57
Raspberry seeds	0.390	1.50	3.93
Peat	0.145	0.33	4.01
Buckwheat husks	0.333	0.93	5.76
Highbush blueberry pulp*	0.307	0.73	3.01
Blackcurrant pulp*	0.471	2.88	3.34

* Sometimes called pomace

Table 2

Average hydraulic conductivity and density of the selected biosorbents.

Parameter	Raspberry seeds	Pea skins	Wheat bran	Buckwheat husks
Average K, cm s ⁻¹	0.10	0.11	0.17	3.03
Average K, cm h ⁻¹	360	396	612	10908
Density, g cm ⁻³	0.370	0.220	0.139	0.127

**Fig. 1.** FTIR spectra of the analyzed biosorbents.

The concentration of toxic and other metals within the biosorbents is quantitatively analysed in Table 3, while Table 4 focuses on the concentration of pesticide residues. Fig. 1 and Table 5 complement each other by illustrating and detailing the Fourier-transform infrared (FTIR) spectroscopy analysis of the biosorbents. They provide FTIR spectra and the absorption maxima that help in identifying the functional groups responsible for adsorption processes and highlight the differences in these functional groups. The specific surface area (SSA) of the samples is determined using nitrogen physisorption and presented through the Brunauer–Emmett–Teller (BET) theory in Table 6, with Fig. 2 displaying the corresponding nitrogen physisorption isotherms

Table 3
Concentration of toxic and other metals.

		Pea skins	Wheat straw	Seaweed Fucus vesiculosus	Wheat bran	Rye bran	Raspberry seeds	Peat	Buck-wheat husks	Highbush blueberry pulp	Blackcurrant pulp
Concentration, mg/kg	Na	ND	33.5 ± 3.3	6250 ± 610	30.3 ± 3.0	ND	ND	139 ± 14	ND	ND	10.1*
	Mg	2560 ± 250	853 ± 84	10000 ± 1000	5830 ± 570	4030 ± 400	1330 ± 130	205 ± 20	1230 ± 120	224 ± 22	874 ± 86
	Al	36.8 ± 3.6	61.7 ± 6.0	424 ± 42	6.85 ± 0.67	0.705 ± 0.069	3.48 ± 0.34	239 ± 23	44.7 ± 4.4	20.8 ± 2.0	22.3 ± 2.2
	K	5940 ± 580	6510 ± 640	19400 ± 1900	16700 ± 1600	13300 ± 1300	2350 ± 230	155 ± 15	2130 ± 210	2170 ± 210	5410 ± 530
	Ca	2440 ± 240	13400 ± 1300	23100 ± 2300	687 ± 67	847 ± 83	1170 ± 110	345 ± 34	1140 ± 110	421 ± 41	2670 ± 260
	V	0.0625 ± 0.0061	0.147 ± 0.014	1.18 ± 0.12	0.00896 ± 0.00088	ND	0.00724 ± 0.00071	0.426 ± 0.042	0.0507 ± 0.0050	0.0156 ± 0.0015	0.0336 ± 0.0033
	Cr	0.473 ± 0.046	1.27 ± 0.12	1.09 ± 0.11	0.0666*	0.0529*	0.694 ± 0.068	1.40 ± 0.14	0.300 ± 0.029	0.231 ± 0.023	0.501 ± 0.049
	Mn	4.93 ± 0.48	23.8 ± 2.3	1020 ± 100	92.1 ± 9.0	65.8 ± 6.4	23.8 ± 2.3	2.83 ± 0.28	53.7 ± 5.3	17.2 ± 1.7	10.8 ± 1.1
	Fe	72.0 ± 7.1	70.1 ± 6.9	618 ± 61	165 ± 16	106 ± 10	42.0 ± 4.1	102 ± 10	49.9 ± 4.9	45.7 ± 4.5	30.4 ± 3.0
	Co	0.0280 ± 0.0027	0.176 ± 0.017	1.01 ± 0.10	0.0317 ± 0.0031	0.0483 ± 0.0047	0.0205*	0.0885 ± 0.0087	0.235 ± 0.023	ND	0.0557 ± 0.0055
	Ni	ND	0.782 ± 0.077	3.05 ± 0.30	0.503*	0.318*	0.636*	1.05 ± 0.10	ND	0.306*	0.602*
	Cu	1.40 ± 0.14	3.77 ± 0.37	4.09 ± 0.40	13.5 ± 1.3	8.47 ± 0.83	6.05 ± 0.59	0.746 ± 0.073	5.82 ± 0.57	5.62 ± 0.55	11.2 ± 1.1
	Zn	110 ± 11	48.1 ± 4.7	23.2 ± 2.3	80.3 ± 7.9	57.5 ± 5.6	19.2 ± 1.9	5.46 ± 0.54	8.85 ± 0.87	8.20 ± 0.80	8.58 ± 0.84
	As	ND	0.0213 ± 0.0021	12.1 ± 1.2	ND	ND	ND	0.286 ± 0.028	ND	0.0104*	0.0112*
	Rb	4.56 ± 0.45	2.98 ± 0.29	8.71 ± 0.85	3.48 ± 0.34	7.83 ± 0.77	1.67 ± 0.16	0.381 ± 0.037	5.74 ± 0.56	1.80 ± 0.18	3.43 ± 0.34
	Sr	5.43 ± 0.53	8.36 ± 0.82	947 ± 93	5.99 ± 0.59	3.18 ± 0.31	3.56 ± 0.35	2.87 ± 0.28	3.23 ± 0.32	1.12 ± 0.11	3.87 ± 0.38
	Mo	0.117 ± 0.011	0.401 ± 0.039	0.227 ± 0.022	1.02 ± 0.10	0.802 ± 0.079	1.00 ± 0.10	0.0718 ± 0.0070	0.221 ± 0.022	0.0820 ± 0.0080	0.294 ± 0.029
	Cd	0.0199 ± 0.0020	0.0799 ± 0.0078	0.427 ± 0.042	0.0949 ± 0.0093	0.0174 ± 0.0017	0.0181 ± 0.0018	0.0213 ± 0.0021	0.0109 ± 0.0011	0.00286*	0.00488*
	Ba	4.67 ± 0.46	23.4 ± 2.3	326 ± 32	11.9 ± 1.2	3.30 ± 0.32	1.22 ± 0.12	3.85 ± 0.38	1.46 ± 0.14	2.14 ± 0.21	1.77 ± 0.17
	Tl	0.0152 ± 0.0015	0.00387 ± 0.00038	0.0216 ± 0.0021	ND	ND	ND	0.00280 ± 0.00027	0.00176 ± 0.00017	ND	ND
	Pb	0.0611 ± 0.0060	0.236 ± 0.023	0.257 ± 0.025	ND	ND	ND	4.92 ± 0.48	0.0746 ± 0.0073	0.0219*	0.0375 ± 0.0037

* Value below the limit of quantification (but above the limit of detection)

ND – not detected (value is below the limit of detection)

Table 4

Concentration of pesticide residues.

Biosorbent	Pesticide	Concentration, mg/kg
Pea skins	ND	
Wheat straw	Azoxystrobin	0.054 ± 0.027
	Cyfluthrin	0.011 ± 0.006
	Deltamethrin (cis-deltamethrin)	0.024 ± 0.012
	Difenoconazole	0.26 ± 0.13
	Epoxiconazole	0.037 ± 0.019
	Fenvalerate*	0.18 ± 0.09
	Lambda-cyhalothrin	0.046 ± 0.023
	Metrafenone	0.048 ± 0.024
	Propiconazole	0.19 ± 0.10
	Prothioconazole**	0.040 ± 0.020
	Tebuconazole	0.75 ± 0.38
	Seaweed <i>Fucus vesiculosus</i>	ND
Wheat bran	ND	
Rye bran	Pirimiphos-methyl	0.030 ± 0.015
Raspberry seeds	Fenhexamid	0.17 ± 0.09
Peat	Tolyfluanid	0.056 ± 0.028
Buckwheat husks	Tolyfluanid	0.012 ± 0.006
Highbush blueberry pulp	Boscalid	0.12 ± 0.06
	Diphenylamine	0.025 ± 0.013
Blackcurrant pulp	Cypermethrin***	0.026 ± 0.013
	Cyprodinil	0.016 ± 0.008
	Difenoconazole	0.079 ± 0.040
	Diphenylamine	0.012 ± 0.006
	Trifloxystrobin	0.38 ± 0.19

ND - not detected.

* Fenvalerate (any ratio of constituent isomers (RR, SS, RS and SR) including esfenvalerate)

** Prothioconazole: prothioconazole–desthio (sum of isomers)

*** Cypermethrin (cypermethrin including other mixtures of constituent isomers (sum of isomers))

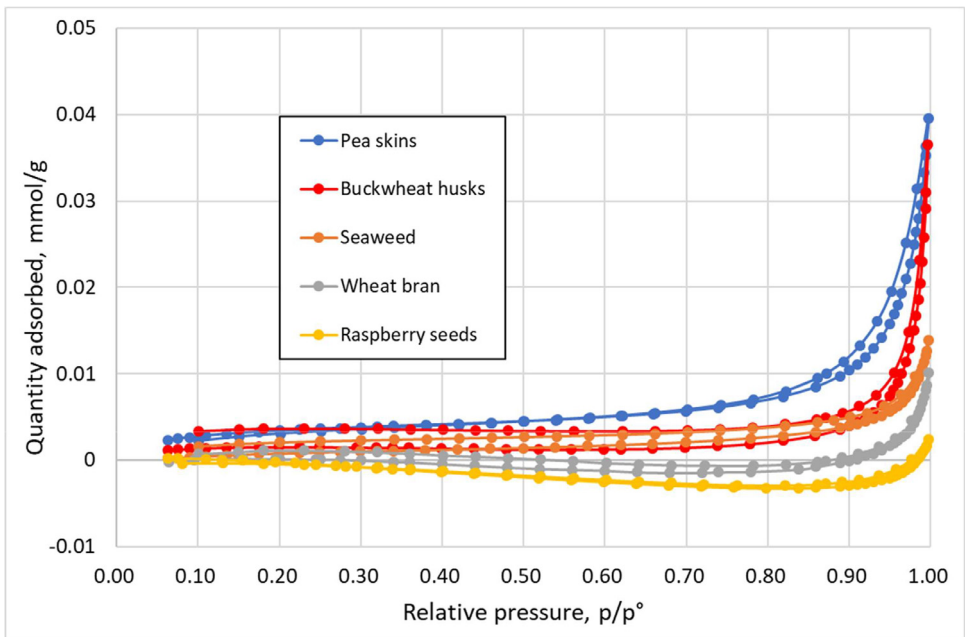
**Fig. 2.** Nitrogen physisorption isotherms of pea skins, seaweed, wheat bran, raspberry seeds, and buckwheat husks.

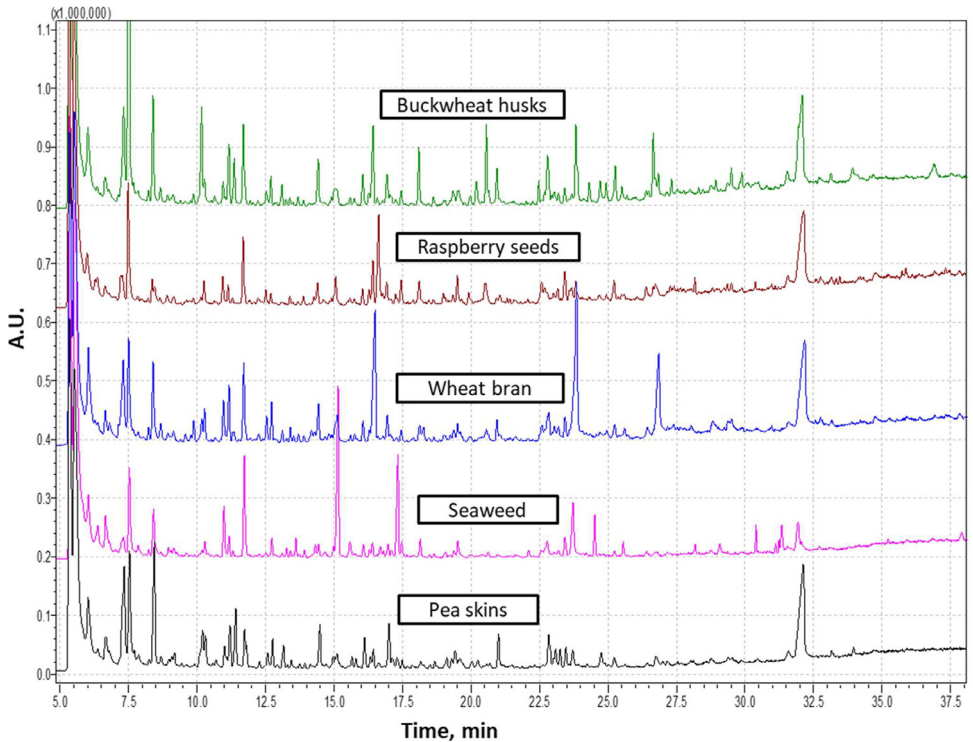
Table 5
FTIR peaks of the analyzed biosorbents and their characterization.

Wave numbers, cm ⁻¹ / absorbance	Pea skins	Wheat straw	Sea- weed	Wheat bran	Rye bran	Rasp-berry seeds	Peat	Buck-wheat husks	Blue-berry pulp	Black-berry pulp	Characteristics of the adsorption
770–700					0.152	0.158			0.186	0.196	Aromatic rings, C–H
880–800			0.127			0.141		0.123	0.145		
910–880	0.083	0.123				0.141	0.137	0.113	0.150	0.135	Vinyl C–H, R ₂ C=CH ₂
1190–910	0.181	0.374	0.223	0.296	0.406	0.366	0.396	0.250	0.350	0.322	Polysaccharides C–O, O–H
1073			0.110	0.207	0.258						Aliphatic ethers C–O, alcohols, carboxylic acids
1190–1120	0.082	0.141		0.127	0.159	0.216	0.167	0.131		0.195	Aliphatic amines C–N, ethers C=O
1290–1190	0.063	0.094		0.091	0.094	0.191	0.130	0.127	0.158	0.172	Carboxylic acids C–O
1360–1290	0.066	0.093		0.087	0.099	0.149	0.115		0.132	0.146	Aromatic amine, C–N stretch
1390–1360	0.063	0.093		0.087		0.139	0.117	0.106		0.134	Alkenes CH ₃ and CH ₂
1490–1400	0.062	0.088	0.100	0.087	0.096	0.129	0.101	0.101	0.116	0.133	Amide II band and carboxylic acids, sulfur (S–O) and phosphorous (–PO–) groups. Aliphatic compounds C–H
1560–1490	0.047	0.053	0.089	0.078	0.076	0.109	0.083	0.073	0.087	0.092	Aromatic rings C–C, Alkenes C=C
1690–1570	0.073	0.077	0.127	0.116	0.118	0.152	0.106	0.121	0.119	0.133	Conjugated C=C, Amide I band –NH ₂ , ketones C=O
1770–1700	0.028	0.033				0.141		0.048	0.082	0.125	Aliphatic aldehydes, aromatic esters, and ketones C=O
2923–2854	0.043	0.075	0.056	0.083	0.087	0.139	0.086	0.071	0.141	0.148	Aliphatic, methoxy CH ₃ , CH ₂ , methyl ether O–CH ₃ , C–H
3500–3000	0.066	0.102	0.086	0.101	0.129	0.106	0.129	0.099	0.113	0.096	Carbonyl, fatty acid, hydroxy groups, O–H, Aromatic compounds C–H, and/or amino groups N–H stretching

Table 6

Specific surface area (SSA) of the samples determined by nitrogen physisorption using Brunauer–Emmett–Teller (BET) theory.

Sample	SSA, m ² /g
Pea skins	0.2748 ± 0.0048
Seaweed	0.1484 ± 0.0373
Wheat bran	−0.0529 ± 0.6565
Raspberry seeds	−0.0168 ± 0.0242
Buckwheat husks	0.1064 ± 0.0056

**Fig. 3.** Analytical pyrogram of the biosorbents.

for selected biosorbents such as pea skins, seaweed, wheat bran, raspberry seeds, and buckwheat husks. Table 7 offers a comprehensive summary of the Py-GC/MS/FID analysis, detailing the relative contents of carbohydrates, lipids, lignin, and other polyphenols, alkaloids, and protein-derived products detected in volatiles. Fig. 3 and Fig. 4 visually represent the analytical pyrograms and microstructural characteristics of the biosorbents, respectively.

Table 7

Summary of biosorbent samples Py-GC/MS/FID analysis, including GC diagnostic peaks assignments and relative contents (%) of carbohydrates (CH), lipids (Lip), lignin (Lig), and other polyphenols (Pph), alkaloids, and proteins (Pr) derived products detected in volatiles.

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
Formic acid	CH	0.15		0.09		0.12
Acetic acid	CH	4.24	3.69	3.17	5.08	10.30
(S)-2-Hydroxypropanoic acid	CH	0.11		0.05		0.07
Formic acid, methyl ester	CH	0.32		0.55	0.08	0.40
Propanoic acid, 2-oxo-	CH	0.10				
Propanoic acid	CH	0.29	0.22	0.27	0.40	0.18
2-Propenoic acid	CH	0.12	0.10			0.08
2-Propenoic acid, methyl ester	CH	0.09	0.06	0.46	0.16	0.23
Acetic acid, methyl ester	CH	0.95	0.12	0.48	0.12	2.34
Propanoic acid, 2-oxo-, ethyl ester	CH		0.03	0.05		
Propanoic acid, 2-oxo-, methyl ester	CH	1.48	0.71	1.65	0.66	1.68
Acetic acid ethenyl ester	CH			0.05		0.07
Butanoic acid	CH		0.04			
Butanoic acid, 2-methyl-	CH			0.06		
(2E)-But-2-enoic acid	CH		0.13			
Propanoic acid, ethenyl ester	CH	0.12		0.41		0.08
2-Propenoic acid, 2-hydroxyethyl ester	CH			0.12		0.07
Crotonic acid, vinyl ester	CH	0.16		0.23	0.13	0.22
Propanoic acid, 2-methylpropyl ester	CH	0.16		0.08	0.13	0.09
2-Propenoic acid, 2-hydroxypropyl ester	CH			0.72		0.17
Pentanoic acid, 3-methyl-2-oxo-, methyl ester	CH					0.07
1,2-Ethanediol	CH	0.18				
1-Heptanol, 2-propyl-	CH	0.28	0.31	0.41		0.37
Methylglyoxal	CH	2.37		2.69	1.41	2.30
Acetone	CH		1.26			

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Table 7 (continued)

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
Propanal, 2-methyl-	CH			0.09	0.42	
2,3-Butanedione	CH	1.24	1.12	0.78	0.49	0.69
2-Butanone, 1-hydroxy-	CH	0.20	0.16	0.25	0.11	0.10
Butanal, 3-methyl-	CH		0.22		0.51	
Butanal, 2-methyl-	CH		0.22		0.53	
Acetaldehyde, hydroxy-	CH	5.25	0.21	3.02	0.55	2.96
2,3-Pentanedione	CH	0.17	0.18	0.13	0.15	0.07
2-Propanone, 1-hydroxy-	CH	5.15	1.60	2.70	1.04	2.83
2-Butanone, 3-hydroxy-	CH		0.07	0.03		
Hexanal	CH			0.23		
Propanal and Butanedial	CH	2.25		0.18		1.25
2-Butanone, 1-hydroxy-, derivative	CH	0.76	0.20	0.90		0.46
3-Hexanone, 4-ethyl-	CH	0.22		0.23		0.14
2-Propanone, 1-(acetyloxy)-	CH	0.82	0.58	1.19	0.36	0.62
2-Heptanone, 3-methyl-	CH	0.70		0.33		0.57
2-Pentanone, 3-methylene-	CH			0.08		
2,5-Hexanedione	CH	0.06	0.15	0.08		
2-Butanone, 1-(acetyloxy)-	CH	0.11		0.19	0.11	
2,4-Hexanedione	CH					0.17
Pentanal and Pentanadial	CH	1.20		0.70	0.16	0.88
4-Butoxy-2-butanone	CH	0.45	0.17	0.21	0.57	0.53
4-sec-Butoxy-2-butanone	CH	0.30			0.32	0.35
2-Cyclopenten-1-one	CH	0.41	0.17	0.21	0.19	0.23
2-Cyclopenten-1-one, 2-methyl-	CH	0.17	0.16		0.12	
4-Cyclopentene-1,3-dione	CH	0.15	0.26	0.17	0.27	0.13
1,3-Cyclopentanedione	CH	1.58	0.34	1.21	0.74	1.25
Cyclopentanone, 2-acetyl-	CH				0.13	
2-Cyclopenten-1-one, 2,3-dimethyl-	CH	0.07				
2-Cyclopenten-1-one, 3-methyl-	CH	0.30		0.16	0.14	0.17
Cyclopentanone, 2,3-dimethyl-	CH		0.13			

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Table 7 (continued)

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
1,2-Cyclopentanedione, 3-methyl-	CH	1.66	0.47	0.77	0.70	0.78
2-Cyclopenten-1-one,2-hydroxy-3-methyl-	CH	0.13	0.20	0.06		0.07
1,3-Cyclopentanedione, 4-hydroxy-5-methyl-	CH	0.31	4.37	0.14	0.18	0.16
2-Cyclopenten-1-one, 3,4-dimethyl-	CH	0.07				
2-Cyclopenten-1-one, 3-ethyl-	CH	0.17				
2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	CH	0.20	0.12	0.12		0.09
Furan, 2-methyl-	CH	0.20	0.53	0.14	0.42	0.17
Furan, 2,5-dihydro-3-methyl-	CH	0.12				0.14
Furan, 3-methyl-	CH	0.10	0.05	0.07	0.07	0.06
Furan, 2-(2-propenyl)-	CH				0.08	
3(2H)-Furanone, dihydro-5-methyl-	CH		0.06			
2(3H)-Furanone	CH	0.21	0.06	0.10	0.11	0.16
3(2H)-Furanone	CH	0.50	1.87	1.12	1.01	0.43
Furfural	CH	1.24	3.92	2.33	2.41	2.01
Furan, 2-propyl-	CH		0.05			
Furan, 2,3-dihydro-4-methyl-	CH					0.05
2-Furanmethanol	CH	0.51		0.72	0.41	0.31
2-Furancarboxaldehyde, 5-methyl-, isomer	CH		0.27			
Furan, 2,3-dihydro-2,5-dimethyl-	CH	0.07				0.12
Acetyl furan	CH	0.12	0.21		0.27	0.08
2-Furancarboxaldehyde, 5-methyl-, isomer	CH		0.50			
2(3H)-Furanone, dihydro-4-hydroxy-	CH			0.15		
2(3H)-Furanone, dihydro-3-methylene-	CH			0.08	0.14	
2,5-Furandione, dihydro-3-methylene-	CH		0.31			
2-Furancarboxaldehyde, 5-methyl-	CH	0.24	7.86		0.63	
2(3H)-Furanone, 3-acetyldihydro-	CH		0.65			
2(3H)-Furanone, dihydro-	CH	0.26		0.15	0.14	0.14
2(5H)-Furanone	CH	1.21	0.50	0.66	0.63	0.92
2(5H)-Furanone, 3-methyl-	CH					0.08
2-Furanone, 2,5-dihydro-3,5-dimethyl	CH	0.12				
2,5-Furandione, 3-methyl-	CH	0.18		0.05	3.30	0.16

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Table 7 (continued)

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
3(2H)-Furanone, 4-hydroxy-2,5-dimethyl-Methyl 2-furoate	CH	0.14	0.69	0.44	0.69	0.10
	CH		0.14	0.15	0.34	0.10
3-Hydroxydihydro-2(3H)-furanone	CH	0.26		0.14		0.12
4-Metyl-5H-furan-2-one	CH	0.33		0.11		0.31
5-(Hydroxymethyl)dihydro-2(3H)-furanone	CH	0.41		0.07		0.85
2-Furanone, 2,5-dihydro-3,5-dimethyl	CH	0.09				
2(3H)-Furanone, 5-acetyldihydro-	CH	0.05				0.10
Furan, 4-methyl-2-propyl-	CH		0.26			
2-Furancarboxylic acid, 2-propenyl ester	CH			0.25	0.58	
2,4(3H,5H)-Furandione, 3-methyl-	CH	1.07	0.08	0.44	0.23	1.06
2,5-Furandione, dihydro-3-methyl-	CH	0.09		0.06		0.10
2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (+/-)-	CH		2.79			
2(5H)-Furanone, 5-(acetyloxy)-	CH		1.33			
2-Furancarboxaldehyde, 5-(hydroxymethyl)-	CH	0.56				0.58
5-Hydroxymethyldihydrofuran-2-one	CH	0.28				
2H-Pyran, 3,4-dihydro-	CH	0.05	0.07			
4-Hydroxy-,5,6-dihydro-(2H)-pyran-2-one	CH	0.56	0.35	5.23	1.65	2.31
4H-Pyran-4-one, 3-hydroxy-2-methyl-	CH	0.29	0.18	0.14	0.22	0.25
4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-	CH			0.12	0.19	0.09
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	CH				0.60	
2H-Pyran-3(4H)-one, dihydro-	CH	0.29		0.20		0.18
2H-Pyran-2-one, tetrahydro-4-hydroxy-4-methyl-	CH		0.45			
2-Hydroxymethyl-5-hydroxy-2,3-dihydro-(4H)-pyran-4-one	CH	0.15	0.17	0.26	0.51	0.19
1,4;3,6-Dianhydro- α -D -glucopyranose	CH	0.68	1.18	0.71	1.50	0.40
D-Erythro-Pentose, 2-deoxy-	CH	0.63		6.46	0.35	0.13
β -D-Ribopyranoside, methyl, 3-acetate	CH					0.49
1,3-Di-O-acetyl- α - β -D-ribopyranose	CH					0.77
Lyxopyranose, tetraacetate	CH					0.10

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Table 7 (continued)

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
2-Deoxy-D-galactose	CH	0.36		4.13	0.37	0.16
1,6-Anhydro-β-D-glucopyranose	CH	8.62	1.41	7.67	9.30	5.59
Phenyl and benzyl derivatives, including:	Lignin (Lig) & Polyphenols (Pph)	0.86	1.31	2.99	4.90	12.10
Benzene, methyl-	PPH				0.42	
Benzene, ethenyl-	PPH		0.09	0.13	0.19	
Phenol	PPH, LIG	0.24	0.44	0.39	0.91	0.38
Phenol, 2-methyl-	PPH, LIG	0.19	0.14	0.10	0.19	0.20
Phenol, 3- and 4-methyl-	PPH, LIG	0.12	0.54	0.33	0.93	0.50
Phenol, 2-methoxy-6-methyl-	PPH, LIG					0.07
Phenol, 3,4-dimethyl-	PPH, LIG	0.12	0.10	0.11		0.15
Phenol, 4-ethyl-	PPH, LIG				0.06	
3,4-Dihydroxyacetophenone	PPH					0.08
Benzene, heptyl-	PPH				0.10	
1,2-Benzenediol	PPH					0.08
Phenol, 3-methoxy-5-methyl-	PPH					0.09
1,4-Benzenediol	PPH	0.19		0.09		0.12
1,4-Benzenediol, 2-methyl-	PPH					0.08
Guaiacol	LIG				0.25	1.30
p-Methylguaiacol	LIG			0.24	0.22	1.80
p-Ethylguaiacol	LIG					0.46
p-Vinylguaiacol	LIG			1.39	0.47	1.64
Eugenol and p-Propylguaiacol	LIG				0.13	0.52
cis-iso Eugenol	LIG					0.30
trans-Isoeugenol	LIG				0.36	1.49
Vanillin	LIG					0.37
Homovanillin	LIG					0.10
Acetoguaiacon	LIG					0.18
Propioguiaiacone	LIG					0.08

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Table 7 (continued)

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
Guacylacetone	LIG				0.19	0.24
Coniferyl aldehyde	LIG					0.10
Syringol	LIG			0.07	0.18	0.30
Syringol, 4-methyl-	LIG					0.25
Syringol, 4-ethyl-	LIG					0.13
Syringol, 4-vinyl-	LIG			0.14	0.30	0.37
Syringol, 4-allyl- and 4-propyl-	LIG					0.11
Syringol, 4-propenyl-(<i>cis</i>)	LIG					0.12
Syringol, 4-propenyl-(<i>trans</i>)	LIG					0.29
Syringaldehyde	LIG					0.11
Syringylacetone	LIG					0.09
N-containing			0.80	0.99	2.66	0.05
	Alkaloids + Proteins (PR)					
Pyridine	PR		0.19	0.15	0.37	
Pyrrrole	PR		0.20		0.79	
1H-Pyrrrole, 1-methyl-	PR		0.06		0.14	
1H-Pyrrrole, 3-methyl-	PR		0.04		0.17	
1H-Pyrrrole-2-carboxaldehyde	PR			0.07	0.13	0.05
2-Pentenenitrile, 4,4-dimethyl-	PR		0.14	0.11	0.16	
Indole	PR		0.17	0.49	0.90	
Pidolic Acid	PR			0.17		
Aliphatic, aromatic, and cyclic monomers	Lipids (LIP)	0.81	1.73	1.93	2.56	0.69
1-Nonene	LIP				0.08	

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Table 7 (continued)

Compound/ group of compounds	Compounds precursors	Compound proportion in volatiles from analytical pyrolysis, %				
		Pea skins	Seaweed	Wheat bran	Raspberry seeds	Buckwheat husks
Acids, alcohol, esters, aldehydes, ketones, cyclopentane deriv., furan derive., sugars, including:	Carbohydrates (CH)	55.21	43.71	57.85	42.11	52.15
1,4-Dioxin, 2,3-dihydro-	LIP	0.17	0.20	0.33	0.15	0.24
2-Decene	LIP				0.09	
D-Limonene	LIP				0.07	
1,3-Dioxol-2-one,4,5-dimethyl-	LIP			0.28		
Butane, 1,4-bis(2,3-epoxypropoxy)-	LIP		0.16			
1,4-Dioxin, 2,3-dihydro-5,6-dimethyl-	LIP					0.08
1-Dodecene	LIP				0.12	
1,4-Cyclohex-2-enedione	LIP	0.07				
Tridecane	LIP				0.14	
1-Tridecene	LIP	0.19		0.10	0.06	
Tetradecane	LIP				0.14	
1-Tetradecene	LIP				0.12	
Hexanoic acid, ethenyl ester	LIP			0.13		
Hexadecane	LIP				0.13	
1-Hexadecene	LIP			0.20	0.15	
8-Heptadecene	LIP				0.15	
1,15-Hexadecadiene	LIP			0.18		
1-Heptadecene	LIP				0.19	
Naphthalene, 1,4,6-trimethyl-	LIP				0.06	
Cycloundecane, 1,1,2-trimethyl-	LIP		0.21		0.38	
1,3-Dioxan-5-ol	LIP	0.12		0.36		0.18
1-Pentadecanol	LIP			0.21		
1,3-Dioxan-5-ol	LIP	0.15				0.19
Octadecanal	LIP		0.68		0.17	
1H-Indene-1,5(6H)-dione,	LIP	0.11				
2,3,7,7a-tetrahydro-7a-methyl-						
Octadecane	LIP			0.14	0.15	
Eicosane	LIP				0.12	
9-Eicosene, (E)-	LIP				0.09	
1-Octadecyne	LIP		0.24			
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	LIP		0.24			

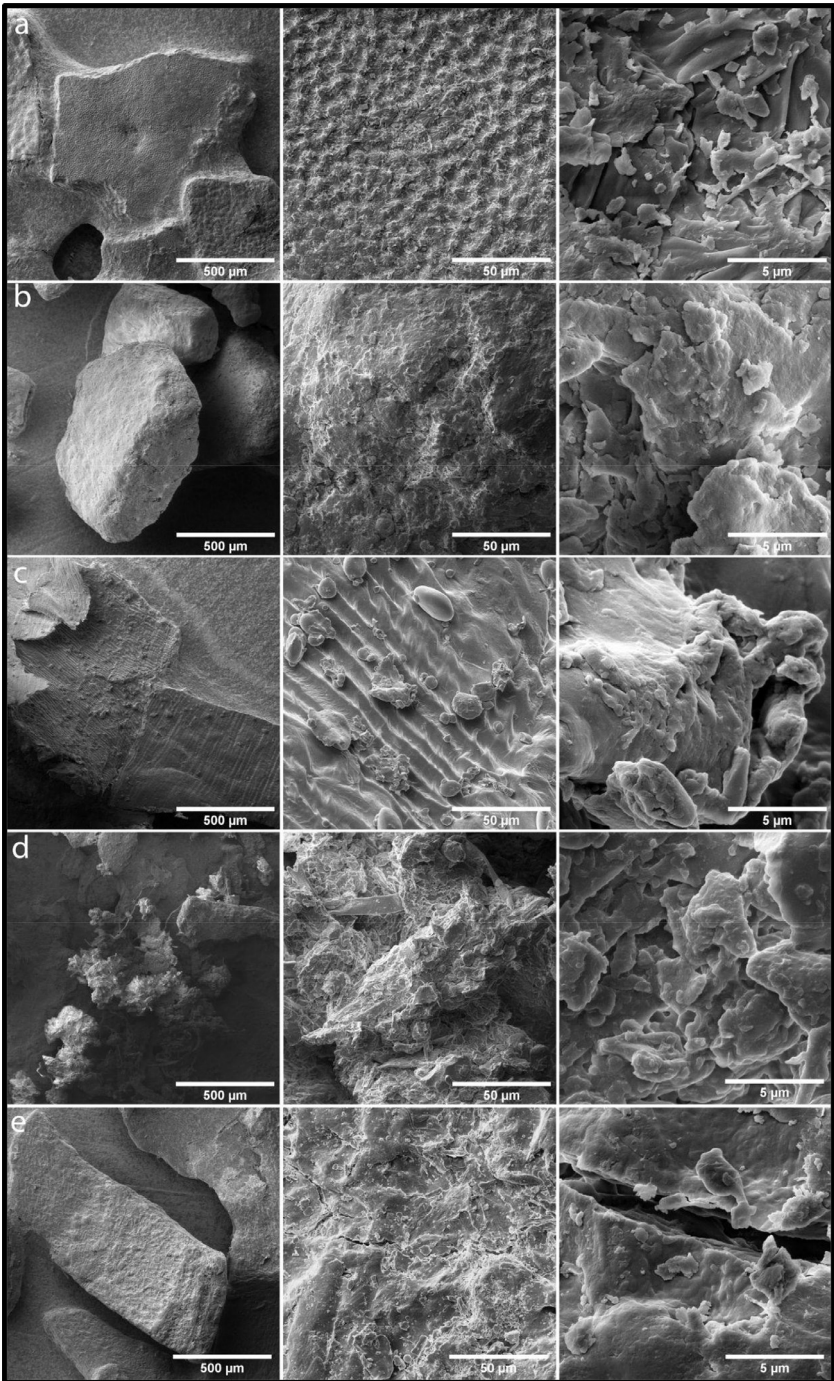


Fig. 4. Micrographs of (a) pea skins, (b) seaweed, (c) wheat bran, (d) raspberry seeds, e) buckwheat husks.

3. Experimental Design, Materials and Methods

3.1. Collection and pretreatment of the samples

Altogether, 10 biosorbent samples were collected and analyzed. Pea skins (outer layer of peas), raspberry seeds, highbush blueberry, and blackcurrant pulp were collected as byproducts from food production companies. Wheat straws were collected from the field after grain harvest. Seaweed *Fucus vesiculosus* was collected from the seashore. Wheat bran and rye bran were purchased from a local grocery store. Peat was collected from a harvested peatland (peat extraction site). Buckwheat husks were purchased from a local store (as a material for pillow filling). All samples were oven-dried (at 40 °C) and kept in airtight containers before analysis. The seaweed *Fucus vesiculosus* was washed with deionized water before drying.

3.2. Determination of the bulk density, ash content and pH

To determine bulk density, a cylindrical container with a predetermined volume was filled with the sample and tapped gently. After leveling off the excess sample material, the container's content was weighed. The bulk density was then calculated by dividing the mass of the contents by the volume of the container. The reported value is an average based on five replications [2]. A Nabertherm B180 muffle furnace and porcelain crucibles were used to measure the ash content after incineration at 550 ± 10 °C according to ISO 2171:2023 standard [3]. The reported value is an average based on three replications. The pH was determined according to the ISO 10390:2021 standard [4]. The reported value is an average based on three replications.

3.3. Determination of the hydraulic conductivity

The hydraulic conductivity of the tested biosorbents was tested using a permeameter [5,6], where water flow through the sample material due to the hydraulic head difference was measured. Hydraulic conductivity is calculated from Darcy's law [7] using the measured time spent for filtration of a fixed water volume through the sample (Eq. 1).

$$Q = K \cdot A \cdot \frac{h}{L} \quad (1)$$

where:

Q – water flow through porous medium, cm³ s⁻¹,

K – hydraulic conductivity, cm s⁻¹,

A – transverse section of the sample cylinder, cm²

h – hydraulic load as the difference between the water level in the tank and that in the sample, cm

L – sample length, cm.

Biosorbent samples were soaked in water for 24 h before the test. Wet samples were filled in the sample cylinder (height 5.00 cm, inner diameter 5.00 cm) and compacted manually. To characterize the compaction degree of the samples, the density of the sample was measured after the test. Cylinders with the samples were placed in the permeameter, and the water flow through the sample was tested. The time in which a constant volume of 40 cm³ seeps through the sample was measured. 10 repetitive test runs were made for each sample. Hydraulic conductivity was calculated using Eq. (2) for each test run, and the average K value was obtained for each sample.

$$K = \frac{Q \cdot L}{h \cdot A} = \frac{V \cdot L}{t \cdot h \cdot \pi r^2} \quad (2)$$

where:

Q – water flow through porous medium, $\text{cm}^3 \text{ s}^{-1}$,

K – hydraulic conductivity, cm s^{-1} ,

A – transverse section of the sample cylinder, cm^2

h – hydraulic load as the difference between the water level in the tank and that in the sample, cm

L – sample length, cm,

V – volume of water filtered through the sample at time t, cm^3 ,

t – filtration time, s,

r – radius of sample cylinder, cm.

After the test samples were oven dried at 105 °C temperature for 24 h, the mass of the samples was measured using analytical scales Sartorius TE1502S. Using the sample volume in the cylinder and the sample mass, the density of the sample used in the test was calculated.

3.4. Determination of toxic and other metals

A wet digestion procedure was applied to determine toxic and other biosorbents using ICP-MS. More details can be found in the work by Reinholds et al. [8]. In short, 0.5 (± 0.05) g of biosorbent sample was weighed in a PTFE digestion vessel. Then, deionized water (2 mL), 65% nitric acid (5 mL), and 30% hydrogen peroxide (3 mL) were added to the sample. The vessels were maintained at room temperature for 20 min to complete the reaction. The mixture was then capped and transferred to a Mars 6 microwave oven (CEM corporation, Matthews, NC, USA) for digestion. The temperature was raised to 150 °C for 15 min and maintained for 15 min. Then, it was raised to 180 °C in 10 min, maintained for 20 min, and finally allowed to cool down to room temperature. The digest was filtered, transferred to a 50 mL volumetric flask, and filled with deionized water to the mark. All samples and blanks were prepared in triplicate. The limits of detection and quantification (LOD and LOQ) were determined by the 3σ and 10σ approach. The concentration of metals in the digests was measured using an Agilent 7700 ICP-MS instrument with Mass Hunter Workstation software for ICP-MS, version B.01.03 (Tokyo, Japan).

3.5. Determination of pesticide residues

HPLC grade acetonitrile was purchased from Merck-Millipore (Darmstadt, Germany). Pesticide grade ethyl acetate was purchased from Chem-Lab (Zedelgem, Belgium). LC-MS grade acetic acid ($\geq 99.8\%$) and ammonium formate (99%) were purchased from Sigma-Aldrich (St. Louis, MO, USA). Ultrapure deionized water was generated using a Millipore Milli-Q™ system (Billerica, MA, USA). A buffer-salt mixture (1 g trisodium citrate dihydrate, 1 g sodium chloride, 0.5 g disodium hydrogen citrate sesquihydrate and 4 g of anhydrous magnesium sulfate) and a mixture of dSPE (900 mg anhydrous magnesium sulfate, 150 mg PSA and 150 mg C18E) were obtained from Phenomenex (Torrance, CA, USA).

3.6. Pesticide analytical standards

A total of 178 certified pesticide standards were obtained from Dr. Ehrenstorfer (Augsburg, Germany), AccuStandard (New Haven, USA), or Sigma-Aldrich (St. Louis, MO, USA). Stock solutions (approximately $1000 \text{ ng } \mu\text{L}^{-1}$) were prepared in acetonitrile or toluene. Purity of the standards were considered when calculating the concentration of each stock solution. A working standard solution of all pesticides at a concentration of $4 \text{ ng } \mu\text{L}^{-1}$ was prepared in acetonitrile. Quantification was performed by procedural calibration in the range of $0.01\text{--}1 \text{ mg kg}^{-1}$.

3.7. Sample preparation procedure

Analysis of pesticide residues was performed by an analytical method accredited under ISO 17025. 1.0 ± 0.1 g of the sample was weighed into a 50 mL polypropylene centrifuge tube. For calibration and quality control samples, standard solutions were added at the appropriate spiking level. Deionized water (10 mL) and acetonitrile (10 mL) were both added, and the tubes were shaken vigorously by hand for 1 min. Then, a salt mixture of 4 g of magnesium sulfate, 1 g of sodium chloride, 1 g of trisodium citrate dihydrate, and 0.5 g of disodium hydrogen citrate sesquihydrate was added. The tubes were closed and immediately shaken on an automatic shaker for 10 min and centrifuged for 5 min at 4500 rpm. An 8 mL aliquot of supernatant was transferred into a 15 mL PP centrifuge tube and frozen at $80\text{ }^{\circ}\text{C}$ for 30 min using a Heto Ultra freeze (Thermo Fisher Scientific, USA), followed by centrifugation of the resulting organic sample fraction for 15 min at 4500 rpm. For further cleaning, 7 mL of the extract was transferred into 15 mL PP tubes containing 900 mg anhydrous magnesium sulfate, 150 mg PSA, and 150 mg C18E. The tubes were shaken vigorously for 30 s and centrifuged for 5 min at 4500 rpm. For analysis with GC-MS/MS, 5 mL of the cleaned extract were evaporated in a water bath ($40\text{ }^{\circ}\text{C}$) under a gentle nitrogen stream. The samples were reconstituted in 200 μL of ethyl acetate and transferred into vials with inserts. For UHPLC-MS/MS analysis, an aliquot of 250 μL of cleaned extract was mixed with 500 μL of the mobile phase A. The final sample extracts were filtered through 0.22 μm PVDF centrifuge filters before being transferred into autosampler vials for analysis.

3.8. GC-MS/MS conditions

The sample extracts in ethyl acetate were analyzed using a Shimadzu gas chromatograph GC-2010 Plus coupled with a TQ8040 mass spectrometer (Shimadzu, Kyoto, Japan) operating in MRM mode. The capillary column used was Zebron ZB-50 (30 m \times 0.25 mm \times 0.25 μm) (Phenomenex, Torrance, CA, USA). The carrier gas was helium at a constant flow rate of 1.3 mL min^{-1} . The initial injector temperature was $70\text{ }^{\circ}\text{C}$, then increased to $150\text{ }^{\circ}\text{C}$ at a rate of 14 $^{\circ}\text{C min}^{-1}$ (held for 10 min) for the transfer step, then increased to $300\text{ }^{\circ}\text{C}$ at a rate of 10 $^{\circ}\text{C min}^{-1}$ and held for 25 min for cleaning. The interface temperature was $250\text{ }^{\circ}\text{C}$. The initial oven temperature was $65\text{ }^{\circ}\text{C}$ (held for 1.5 min), then increased to $150\text{ }^{\circ}\text{C}$ at a rate of 30 $^{\circ}\text{C min}^{-1}$ (held for 2 min), then increased to $290\text{ }^{\circ}\text{C}$ at a rate of 5 $^{\circ}\text{C min}^{-1}$, afterwards increased to $320\text{ }^{\circ}\text{C}$ at a rate of 30 $^{\circ}\text{C min}^{-1}$ and held for 5 min. The total analysis time was 38 min. The injection volume was 2 μL .

3.9. UHPLC-MS/MS conditions

The UHPLC-MS/MS analysis was carried out using an UltiMate 3000 UHPLC system coupled to a TSQ Quantiva mass spectrometer (Thermo Fisher Scientific, MA, USA) equipped with an electrospray ionization source. The separation of analyses was achieved using a Kinetex C18 analytical column (50 mm \times 3.0 mm \times 1.7 μm) (Phenomenex, CA, USA). The column was eluted with the following mobile phases: water with 5 mM ammonium formate and 0.01% acetic acid (A) and acetonitrile (B) at a flow rate of 0.4 mL min^{-1} using gradient mode. The gradient was programmed to hold the initial 20% of B for 1 min, then increase the amount of B to 90% in 9 min, hold for 1 min, and return to the initial conditions (20% B) in 5 min. The total run time was 16 min. Sample extract volumes of 10 μL were injected into the system. The temperature of the autosampler was thermostated at $15\text{ }^{\circ}\text{C}$. The parameters of the ion source were as follows: source temperature was set at $380\text{ }^{\circ}\text{C}$, ion spray voltage 3.50 kV for positive ionization mode and 2.50 kV for negative, sheath gas 45 arb, aux gas 25 arb, and sweep gas 5 arb. Analysis was performed by multiple reaction monitoring (MRM) in the positive and negative ionization modes.

3.10. Fourier transform infrared (FTIR) spectroscopy

FTIR spectra of biomass were recorded using a Nicolet iS50 spectrometer (Thermo Fisher Scientific, MA, US) in the range 4000–400 cm^{-1} (resolution: 4 cm^{-1} , number of scans: 64). FTIR data were collected using the attenuated total reflectance (ATR) method with a diamond crystal. Freeze-dried homogeneous samples were used for analysis. The crystal was cleaned with analytical-grade acetone between measurements. To identify dominant functional groups for potential biosorbents [9], peaks and their ranges were determined in FTIR spectra, along with the maximum absorbance of these peaks.

3.11. Nitrogen physisorption analysis

Before the analysis, the samples were vacuum dried for 24 h at 105 °C. Next, the samples were outgassed using a vacuum at 90 °C for 16 h. Nitrogen physisorption was performed using Micromeritics Tristar II equipment. The specific surface area (SSA) was calculated using the Brunauer–Emmett–Teller (BET) theory [10]. The relative pressure range (p/p_0) of 0.05–0.30 was selected for the derivation of the specific monolayer capacity using the BET equation with a consequent specific surface area calculation. The total pore volume was calculated using the Gurvich rule at the relative pressure $p/p_0 = 0.95$ [11].

3.12. Analytical pyrolysis

Pyrolysis-gas chromatography-mass spectrometry (Py-GC/MS/FID) analysis was carried out using a Frontier Lab (Japan) MicroDouble-shot Pyrolyser Py-3030D (pyrolysis temperature 500 °C, heating rate 600 °C/s) that was directly coupled to a Shimadzu 2D FID/MS gas chromatography system MS-GC/GC-MS-2010 with an RTX-1701 capillary column (Restek, 60 m x 0.25 mm x 0.25 μm film). The injector temperature was 250 °C, the ion source temperature was 250 °C (EI 70 eV), the MS scan range m/z was 15–350, the carrier gas was helium (flow rate 1 mL min^{-1}) and the split ratio was 1:30. The amount of sample was 1.00–2.00 mg. The oven temperature was maintained at 60 °C for 1 min, increased at 6 °C/min to 270 °C, and finally held at 270 °C for 10 min. The identification of individual compounds was performed using GC/MS chromatograms from the LibraryMSNIST14, whereas the relative peak area of individual compounds was calculated using Shimadzu software based on GC/FID data. The summed molar areas of the relevant peaks were normalized to 100%, and the data for 5 repetitive pyrolysis experiments were averaged. Relative peak areas, calculated as percentages, for pyrolysis products of different origins were used to assess biomass sample composition. The measurement error did not exceed 5% of the mean area value.

3.13. Scanning electron microscopy analysis

The samples were coated with a gold layer in a vacuum thermal evaporator Edwards Auto 306. The morphology of the samples was characterized by high-resolution field emission scanning electron microscopy (SEM) apparatus Thermo Scientific™ Helios™ 5 UX operated at 5 kV voltage and 0.1 nA current. The distance between the top of the specimen and the SEM column during the measurements was set to 4 mm. The images were obtained from secondary electron detection using an Everhart–Thornley detector (ETD) or an ion conversion and electron (ICE) detector.

Limitations

None.

Ethics Statement

The authors confirm that they have read and followed the ethical requirements for publication in Data in Brief and confirming that the current work does not involve human subjects, animal experiments, or any data collected from social media platforms.

Data Availability

[Characterization of seaweed, wheat bran and other biosorbents \(Original data\)](#) (Mendeley Data).

CRediT Author Statement

Artis Robalds: Funding acquisition, Supervision, Visualization, Writing – original draft, Resources, Investigation, Methodology, Conceptualization, Writing – review & editing; **Oskars Bikovens:** Resources, Visualization, Writing – review & editing; **Aija Dēliņa:** Resources, Formal analysis, Writing – review & editing; **Nikolai P. Ponomarev:** Resources, Investigation, Writing – review & editing; **Oskars Purmalis:** Visualization, Writing – review & editing; **Laura Elīna Tomšone:** Investigation, Writing – review & editing; **Edgars Vanags:** Resources, Investigation, Visualization, Writing – review & editing.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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