Molecular Structure Characterization of the Extracts from Soybean Dreg

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Abstract. Soybean dreg was extracted with acetone in Soxhlet Extractor. The extracts were analyzed with GC/MS. In total, 53 kinds of organic compounds were detected in extracts, which can be divided into seven classes according to the difference of molecular structure and functional group: alkanes (As), unsaturated hydrocarbonaromatic (UHs), aromatic hydrocarbons (Ars), aldehydes (Als), acids, esters (Es) and other species (OS), respectively. The relative content (RC) of the above species decrease in the order: Als>> acids > Es>OS>Ars>UHs>As. Als are the most abundant, accounting for 51.4%. The study has important significance basic theory on the development of bean dreg with high added value utilization.

Introduction

Soybean dreg, as by-product of soybean processing industry, is about 16% ~ 25% of the whole soybean quality [1]. In China, nearly 20 million tons of soybean dreg as residue are produced every year [2]. According to the analysis, there are rich nutrients and physiological functions in soybean dreg [3-6]. Soybean dreg is susceptible to corruption due to the high content of the water, so soybean dreg is usually treated as a waste. At present, only a small part of the soybean dreg is consumed in a traditional way, such as animal feed, food production and extraction of functional components [7]. Until recently, the majority of soybean dreg has not been used and disposed off, causing environmental and public health problems [8]. Therefore, efficient utilization of which draws increasing attention in China.

In the present study, soybean dreg was extracted with acetone in a modified Soxhlet extractor. The extracts were analyzed with GC/MS and FTIR.

Experimental

Materials. Fresh wet soybean dreg was purchased from Xuzhou farmer market, in Jiangsu, China, which was dried in a vacuum at 65 ^{o}C for 24 h, and then cooled to room temperature under keeping vacuum state. The soybean dreg dried was pulverized to pass through a 150-mesh sieve, and kept in dryer. Acetone is commercially purchased analytical one and purified by distillation prior to use。

Methods. 5 g soybean and 120 mL acetone were put into Soxhlet extractor. The Soxhlet extractor was heated up to 56 ^{o}C and kept at the temperature for 5 h, then cooled down to room temperature. The extracts mixture was taken out from the extractor. The extract was distilled using a Büchi R-134 rotary evaporator to afford acetone extract (AE), which was analyzed with GC/MS.

Results and Discussion

GC/MS Analysis. Fig.1 show the total ion chromatograms (TICs) of extracts. The corresponding compounds identified are listed in Tables 1 to 5. In total, 53 kinds of organic compounds were detected in extracts, which can be divided into seven classes according to the difference of molecular structure and functional group: alkanes (As), unsaturated hydrocarbonaromatic (UHs), aromatic hydrocarbons (Ars), aldehydes (Als), acids, esters (Es) and other species (OS), respectively. The relative content (RC) of the above species is illustrated in fig. 2. As this figure shows, the yields of products decrease in the order: Als>> acids > Es>OS>Ars>UHs>As, and Als are the most abundant, accounting for 51.4%, indicating Als can be enriched by acetone from soybean dreg.

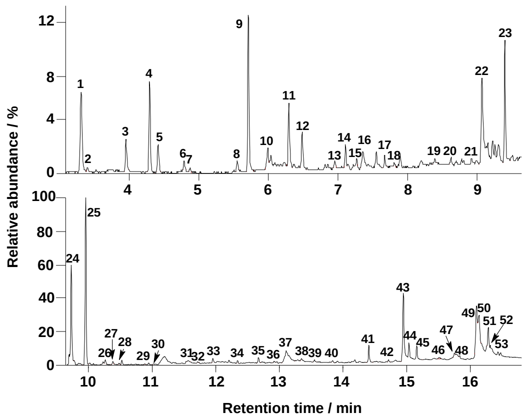

Figure 1. TIC of AE from soybean dreg.

Table 1 Alkanes and aromatic hydrocarbons identified in AE from soybean dreg

Peak	**Compounds**	**Peak**	**Compounds**
	Aromatic hydrocarbons		**Alkanes**
4	Ortho xylene	34	hexadecane
5	p-xylene	40	octadecane
6	Meta xylene	46	1-chlorooctadecane
29	1,5-dimethylnaphthalene		
30	1,6-dimethylnaphthalene		

Table 2 Unsaturated hydrocarbon identified in AE from soybean dreg

Peak	**Compounds**	**Peak**	**Compounds**
2	(E)-oct-2-ene	26	octadec-1-yne
8	(E)-2,4,6-trimethylhept-3-ene	27	tridec-1-ene
13	(E)-undec-1-ene	47	henicos-1-ene
20	(E)-dodec-3-ene		

Table 3 Aldehyde identified in AE from soybean dreg

Peak	**Compounds**	**Peak**	**Compounds**
1	(E)-hex-2-enal	21	(2E,4E)-nona-2,4-dienal
9	(E)-hept-2-enal	22	5-(hydroxymethyl)furan-2-carbaldehyde
11	(2E,4E)-hepta-2,4-dienal	23	(Z)-dec-2-enal
12	(2Z,4Z)-hepta-2,4-dienal	24	(2E,4E)-deca-2,4-dienal
14	(E)-oct-2-enal	25	(2Z,4Z)-deca-2,4-dienal
17	nonanal	36	(10Z,12Z)-hexadeca-10,12-dienal

Table 4 Acids and Ester identified in AE from soybean dreg

Peak	Acids	Peak	Ester
10	Hexanoic acid	28	dl-3,4-Dehydroproline methyl ester
19	Octanoic Acid	41	diisobutyl phthalate
31	11-bromoundecanoic acid	42	methyl palmitate
39	tetradecanoic acid	44	dibutyl phthalate
43	palmitic acid	45	ethyl palmitate
49	(9Z,12Z)-octadeca-9,12-dienoic acid	48	(9Z,12Z)-methyl octadeca-9,12-dienoate
52	oleic acid	51	(9Z,12Z)-ethyl octadeca-9,12-dienoate

Table 5 Other substances identified in AE from soybean dreg

Peak	Compounds	Peak	Compounds
3	2-methylhexan-2-ol	33	N-(4-chlorophenyl)-3-ethoxythiophene-2-carboxamide
7	dodec-11-en-2-one	35	diphenylamine
15	(3E,5E)-octa-3,5-dien-2-one	37	4,6-Di-O-methyl-.alpha.-d-galactose
16	6-butyl-3-methoxycyclohex-2-enone	38	2-hexyldecan-1-ol
18	Maltol	50	N-(2-hydroxyethyl)palmitamide
32	2-amino-4,6-dimethylphenol	53	(E)-octadec-9-enamide

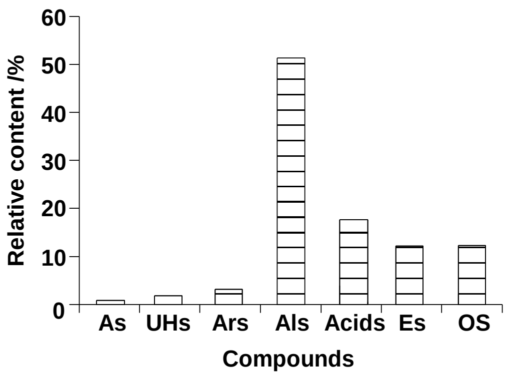

Figure 2. Distribution of different types of products in AE from bean dreg

As is shown in fig. 2, 3 As were detected with 0.9% of relative content, including hexadecane (peak 34), octadecane (peak 40), and 1-chlorooctadecane (peak 46). They may originally be present in wax layer of soybean. The Ars detected include 3 xylenes (peaks 4, 5, and 6), and 2 dimethylnaphthalene (peaks 29, and 30), with 3.3% of relative content. 7 UHs were identified as exhibited in table 2. Among the UHs, octadec-1-yne and henicos-1-ene is predominantly abundant.

These hydrocarbons are value-added chemicals in the application of many aspects, especially as raw materials for manufacturing chlorinated paraffin, senior spices, plastic, dyestuff, medicine and cosmetic. At present, they are mainly derived from fossil resources, such as oil, natural gas and coal. With the reduction of fossil resource reserves, the price will be affected. Therefore, further enriching and subsequently purifying the hydrocarbons is an important subject.

As were the most detected species with 51.4% of relative content in soybean dreg by GC/MS. As listed in Table 3, in total 12 As were identified in the products. Most of these As were unsaturated aldehydes, including 4 enal (peak 1, 9, 14, 23 in Fig. 2) and 6 dienal (peak 11,12, 21, 24,25, 36 in Fig. 2). The yields of (2E,4E)-deca-2,4-dienal and (2Z,4Z)-deca-2,4-dienal are much higher than other As, accounting for 14.2% and 22.7%, respectively. Enal, with special aroma, plays an important role in the flavor industry, such as (2E,4E)-hepta-2,4-dienal and (2E,4E)-deca-2,4-dienal.

As are mainly obtained from synthesized. If As can be isolated from soybean dreg will help reduce the material price, while improving the utilization value of soybean dreg.

As listed in Tables 4, 7 acids and 7 esters were detected in total. All of the acids are fatty acids accounting for 17.7%, consisting of 2 unsaturated fatty acids and 5 saturated fatty acids. Ester detected contained 2 phthalate esters and 5 aliphatic ester. These compounds have very important practical value at many fields such as Paints, adhesives, dyes, pesticides, spices, etc.

There are 12 OSs detected with 12.3% of RC, including 2 alcohols (peak 3, 38 in table 5), 3 ketones (peak 7, 15,16 in table 5), 2 phenols (peak 18, 32 in table 5),1 sugar(peak 37 in table 5), and 4 nitrogen containing compounds.

Summary

Soybean dreg was extracted with acetone in Soxhlet Extractor. A series of As, UHs, Ars, Als, acids, Es and OS were successively enriched, The relative content (RC) of the above species decrease in the order: Als>> acids > Es>OS>Ars>UHs>As. Als are the most abundant, accounting for 51.4%. The study has important significance basic theory on the development of bean dreg with high added value utilization.

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