

1 Headspace volatiles profiles of different spring varieties and a wild relative 2 of wheat flour.

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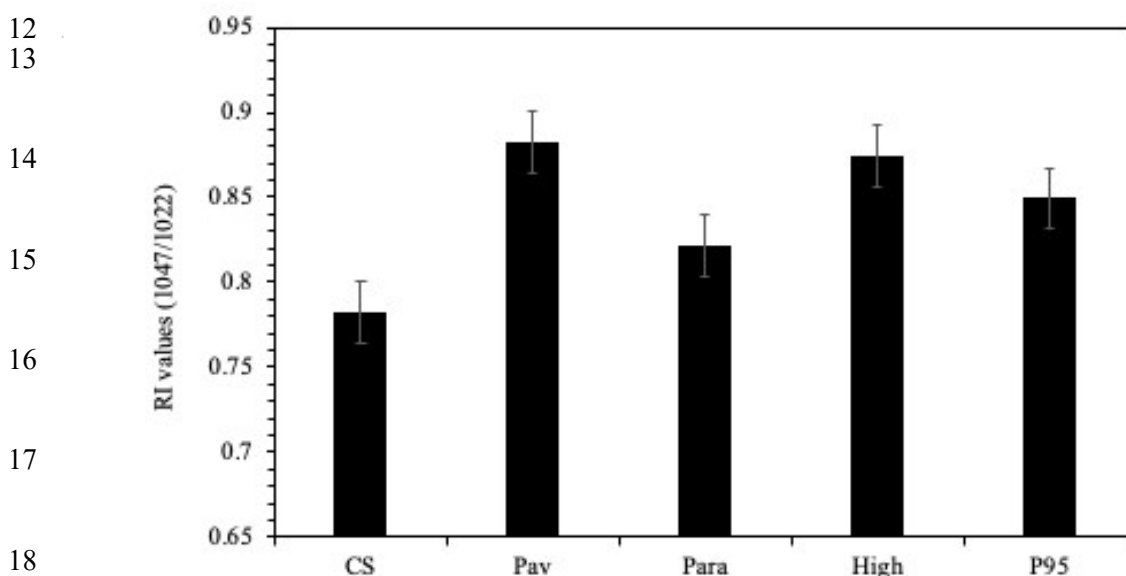
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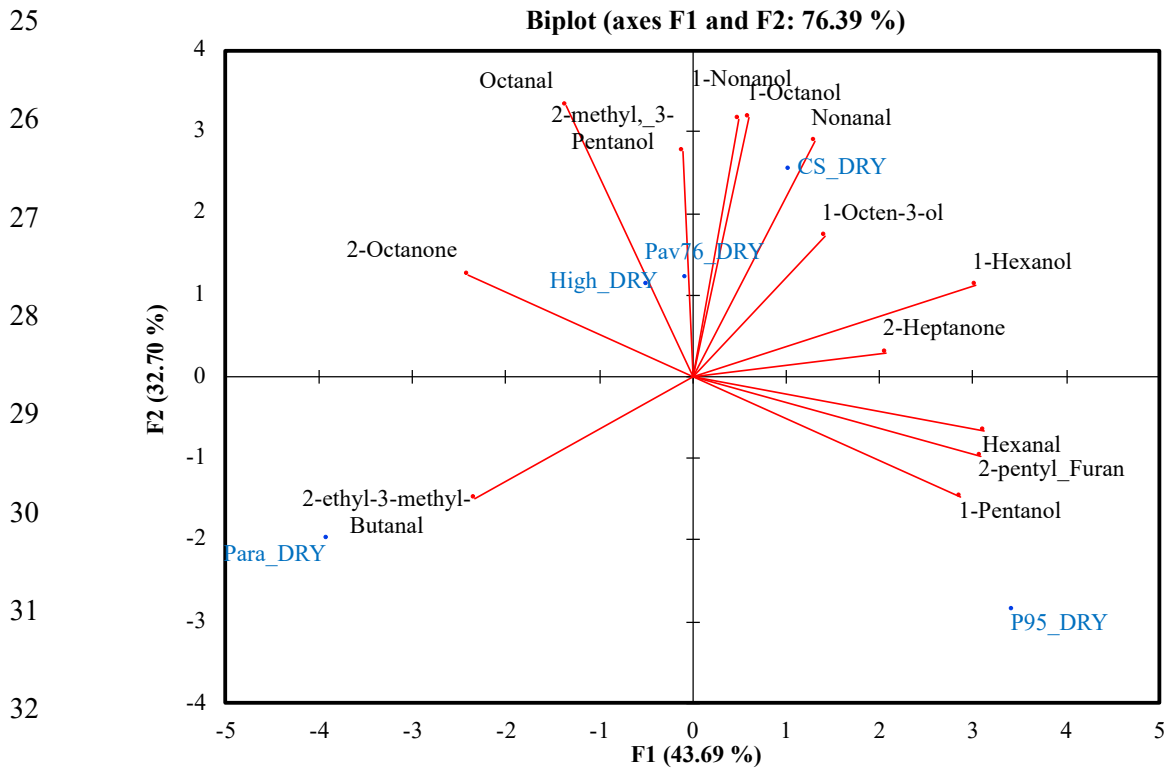
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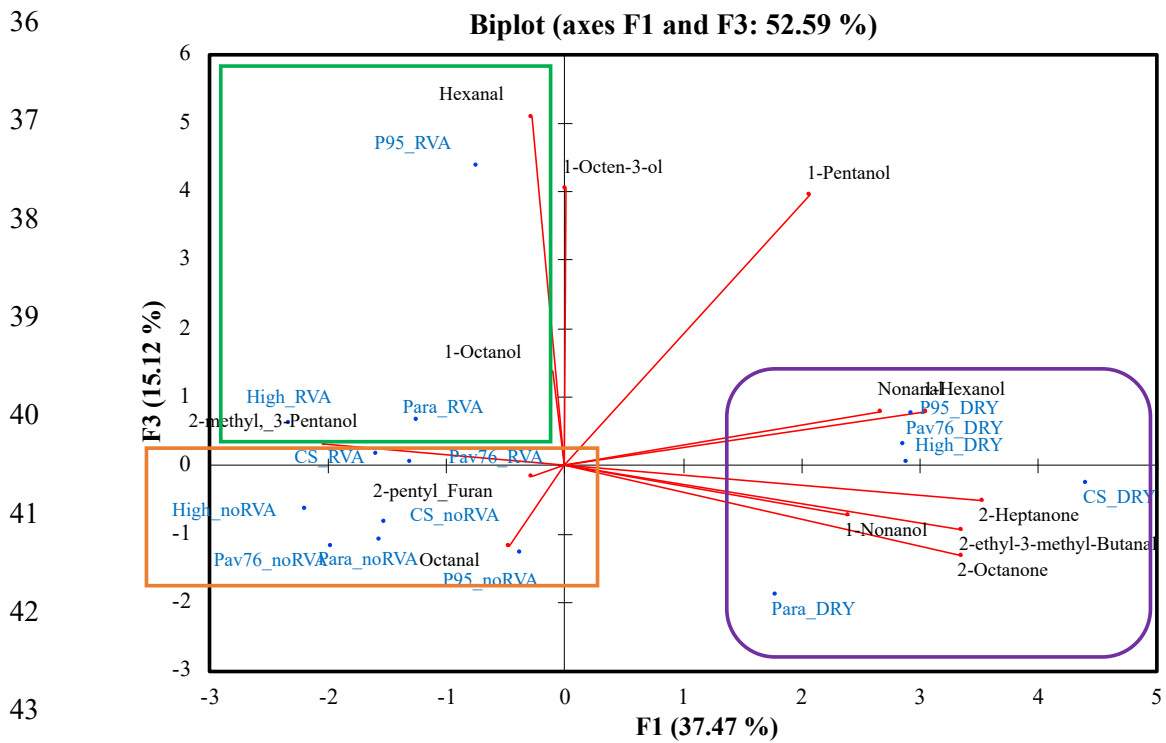
11 Supplementary Data



19 **Figure S1:** IR ratio of the absorbances $1047/1020\text{ cm}^{-1}$ for different wheat flours. IR ratio was
20 calculated by extracting IR absorbance values at 1047 and 1022 cm^{-1} from the vector
21 normalised spectra after water subtraction, baseline correction and deconvolution. The bands
22 at 1047 and 1022 cm^{-1} generally associated with the ordered and amorphous structures of
23 starch, respectively. The ratio of absorbance can be used to quantify the degree of “order” in
24 starch [ordered starch] samples (VanSoest et al., 1995).



33 **Figure S2:** The principal component analysis (PCA) based on the relative content of volatile
 34 compounds generated by different whole wheat dry flour (without water) of Chinese spring
 35 (CS), Pavon76 (Pav76), Highbury (High), Paragon (Para) and wild relative (P95).



44 **Figure S3:** *The principal component analysis (PCA) based on the relative content of volatile*
 45 *compounds generated by different whole wheat dry flour (without water), before and after RVA*
 46 *(flour with water) of Chinese spring (CS), Pavon76 (Pav76), Highbury (High), Paragon (Para)*
 47 *and wild relative P95.*

48 **Table S1:** Fatty acid composition (mg/g of wheat) of different wheat varieties such as Chinese
 49 spring (CS), Pavon76 (Pav76), Highbury (High), Paragon (Para) and a wild relative P95. A
 50 significant difference ($p < 0.05$) between the samples is indicated by different letters “abc” on
 51 the same column.

Wheat Variety	Pentadecanoic 14	Elaidic acid	Linoleic acid	Linolenic acid	11-Eicosenoate
CS	1.940 a	4.423 b	19.691 c	0.426 b	1.766 b
P95	2.019 a	6.700 a	14.483 d	0.258 d	2.939 a
High	1.771 b	4.309 b	20.684 c	0.467 a	0.829 c
Pav76	1.574 c	3.712 c	22.841 b	0.458 a	0.960 c
Para	0.487 d	3.113 d	30.528 a	0.312 c	0.860 c
Pr > F(Model)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

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