

1 **Compositional, thermal and water sorption properties of wheat flour:**  
2 **comparing wild-relatives v/s elite wheat varieties used in current plant**  
3 **breeding**

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13 **Supplementary Data**

14 *Supplementary Tables:*

15 **Table T1:** *Assignments of the different absorbance bands in FTIR spectra of wheat flour*  
16 *(Gorgulu et al., 2007, Naumann et al., 2000, Yu et al., 2007, Singh et al., 2011, Liu et al., 2005,*  
17 *Robert et al., 2005, Moroi et al., 2011, Saulnier et al., 2009, Kizil et al., 2002, Akerholm et al.,*  
18 *2004).*

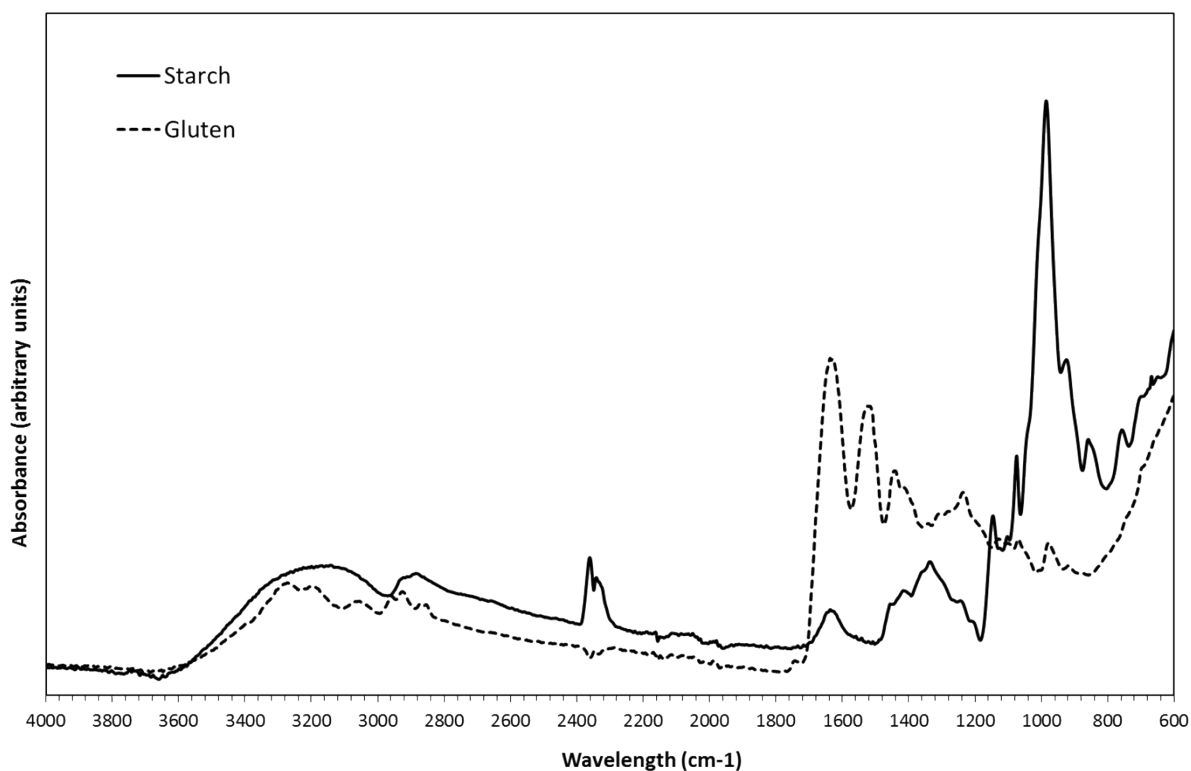
Wavelength (cm <sup>-1</sup> )	Band Assignments
3500–3300	OH-N-H stretching vibrations: water, carbohydrates, proteins
3008	Olefinic =CH
2959	CH <sub>3</sub> asymmetric stretching: mainly lipids with contribution from proteins, carbohydrates, nucleic acids
2923	CH <sub>2</sub> asymmetric stretching: mainly lipids with contribution from proteins, carbohydrates, nucleic acids
2872	CH <sub>3</sub> symmetric stretching: mainly proteins with contribution from lipids, carbohydrates, nucleic acids
2852	CH <sub>2</sub> symmetric stretching: mainly lipids with contribution from proteins, carbohydrates, nucleic acids
1745	C=O ester stretching, lipids, carbohydrates
1642	Amide I (C=O stretching): proteins
1540	Amide II (C-N stretching, N-H bending): mainly proteins
1514	Lignin

1446	C-H: cell wall polysaccharides
1414	O-H bending: cell wall polysaccharides, alcohols and carboxylic acids
1369, 1335, 1315, 1280	Cellulose
1239	Amide III (C-N and N-H stretching): mainly proteins
1205	Cellulose
1150	Starch
1124	Starch
1101	Pectin
1076	$\beta$ -(1 - >6) or $\beta$ -(1 - >3) linked galactan
1049	Arabinogalactorhamnoglycan, starch
990	Arabinoxylans
932	Starch
859	Starch

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20 *Supplementary Figures:*

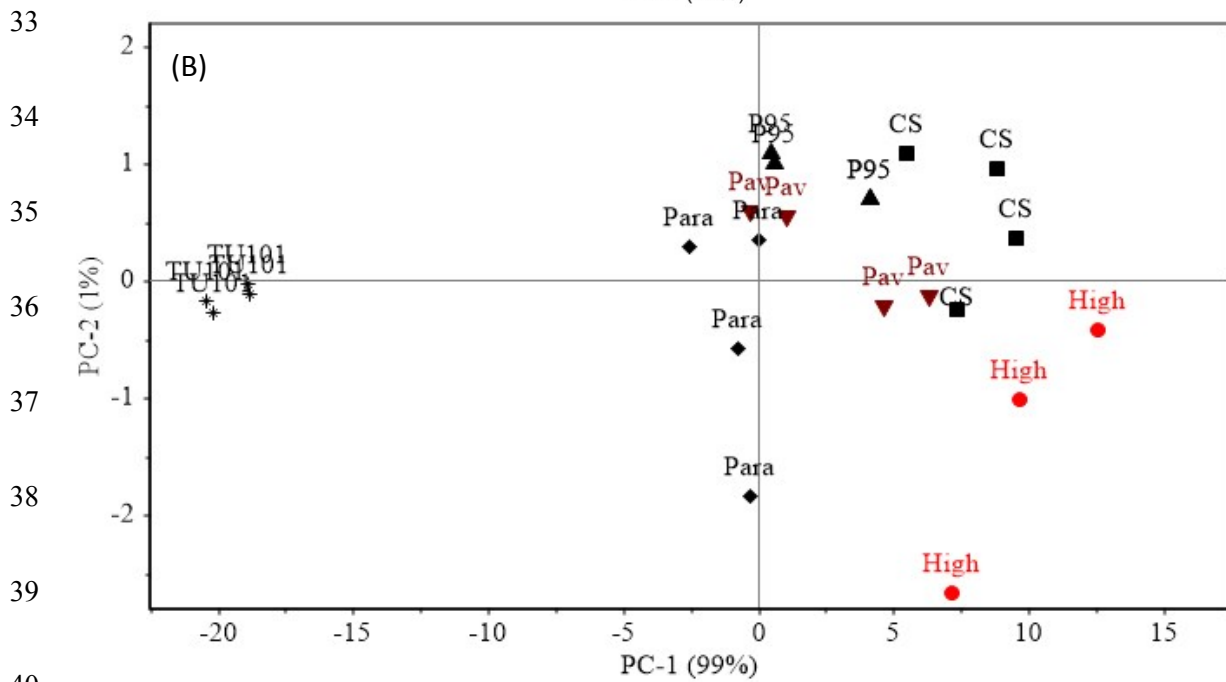
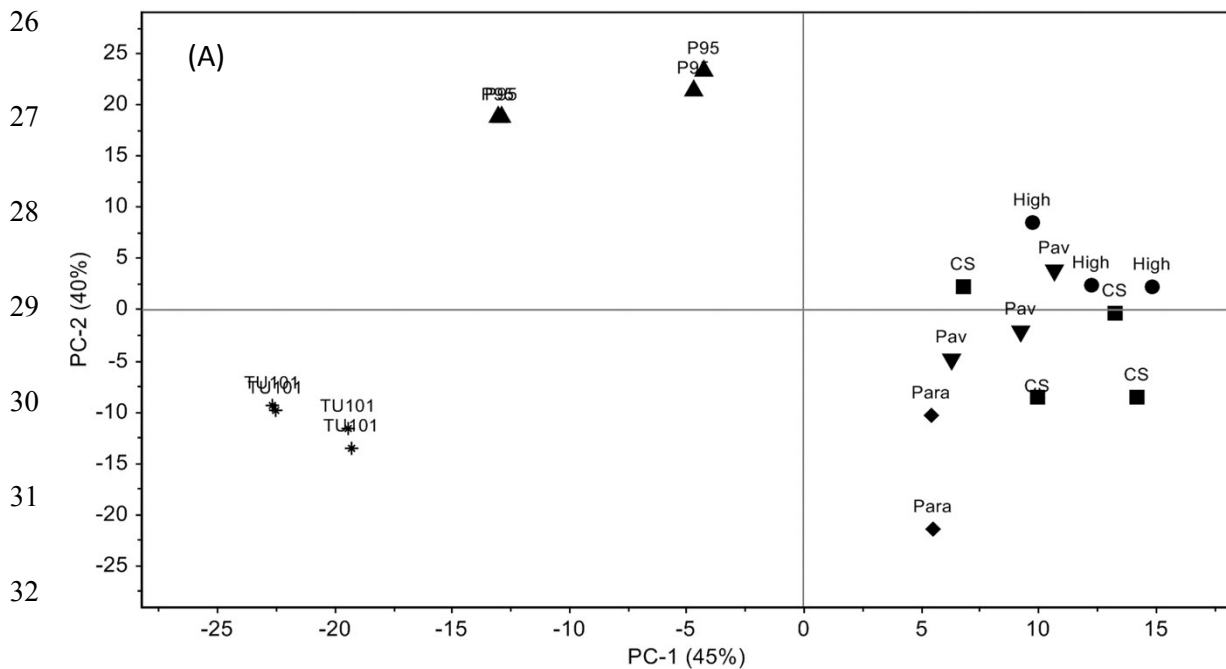


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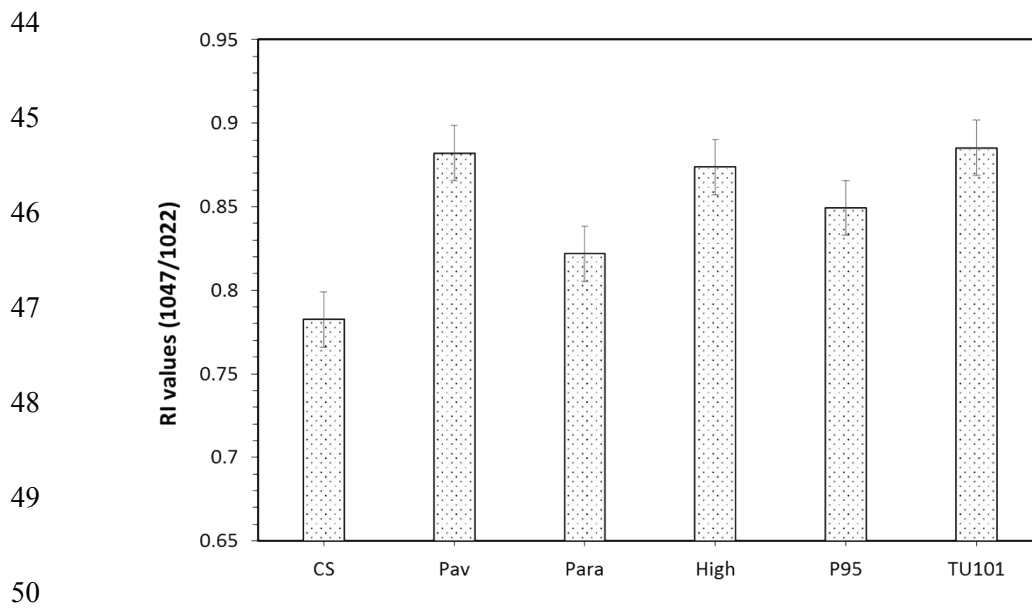
22 **Figure S1:** *The ATR-FTIR spectra (vector normalised) of wheat gluten (Sigma, UK) and native*  
 23 *wheat starch (Healy group, UK).*

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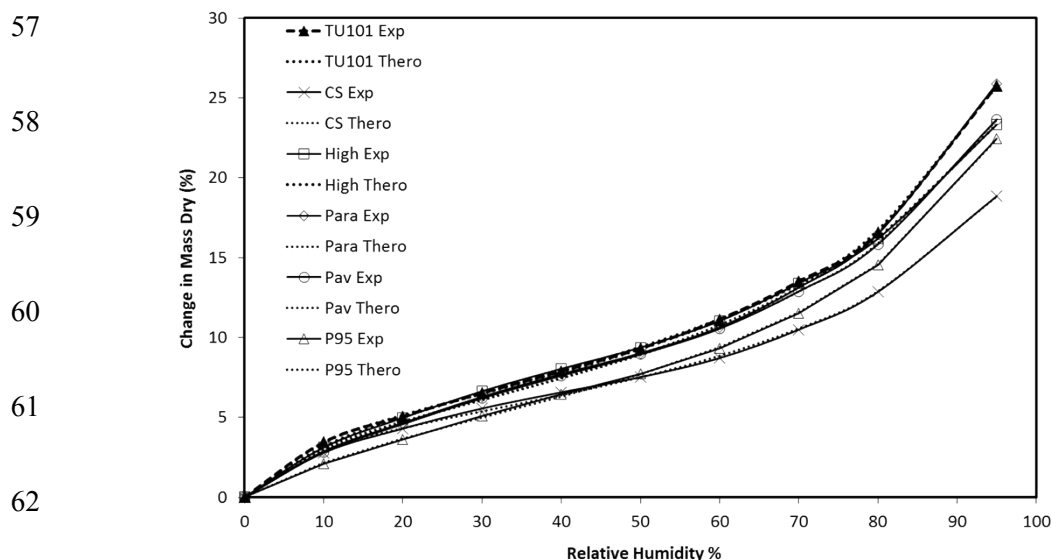
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41 **Figure S2:** Principal component analysis (PC2 versus PC1) scores plot of the vector  
42 normalised spectra in the (a) carbohydrate region: 1200-600  $\text{cm}^{-1}$  range, and (b) lignin  
43 region: 1570-1482  $\text{cm}^{-1}$  range.



51 **Figure S3:** IR ratio of the absorbances  $1047/1020\text{ cm}^{-1}$  for different wheat flours. IR ratio was  
 52 calculated by extracting IR absorbance values at  $1047$  and  $1022\text{ cm}^{-1}$  from the vector  
 53 normalised spectra after water subtraction, baseline correction and deconvolution. The bands  
 54 at  $1047$  and  $1022\text{ cm}^{-1}$  generally associated with the ordered and amorphous structures of  
 55 starch, respectively. The ratio of absorbance can be used to quantify the degree of “order” in  
 56 starch [ordered starch] samples (VanSoest et al., 1995).



63 **Figure S4:** GAB model fitting of sorption data for all wheat flours. The experimental sorption  
 64 data have been fitted with the three-parameter GAB model (Guggenheim-Andersen-de Boer  
 65 model). There is good agreement between experimental data and predicted values ( $R^2 =$   
 66  $0.997$ ).

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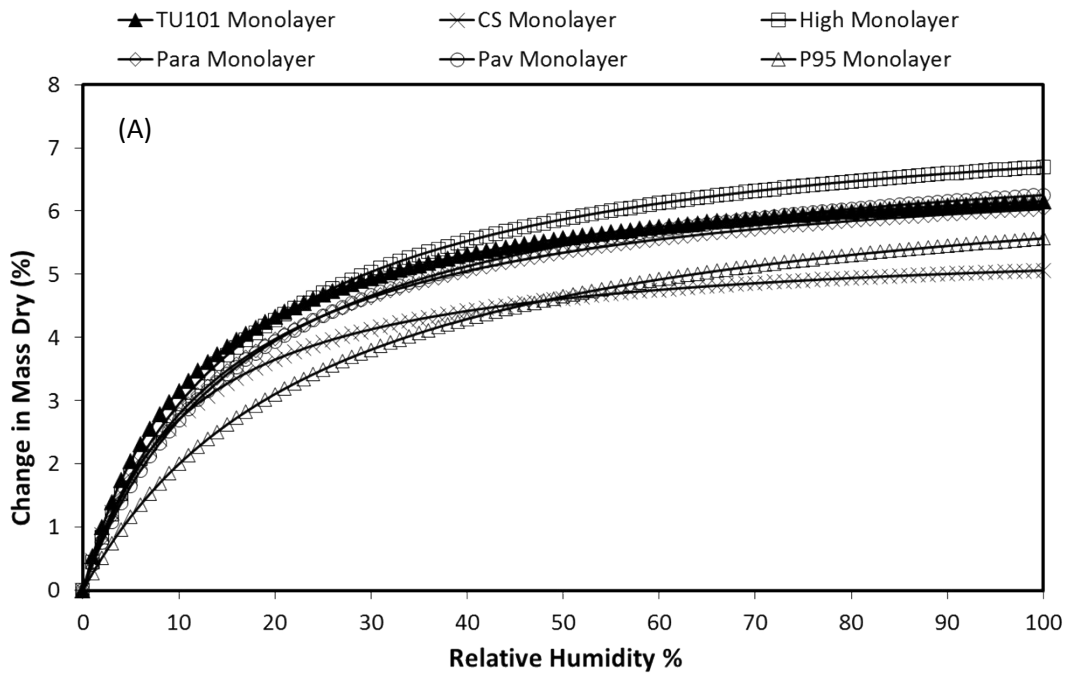
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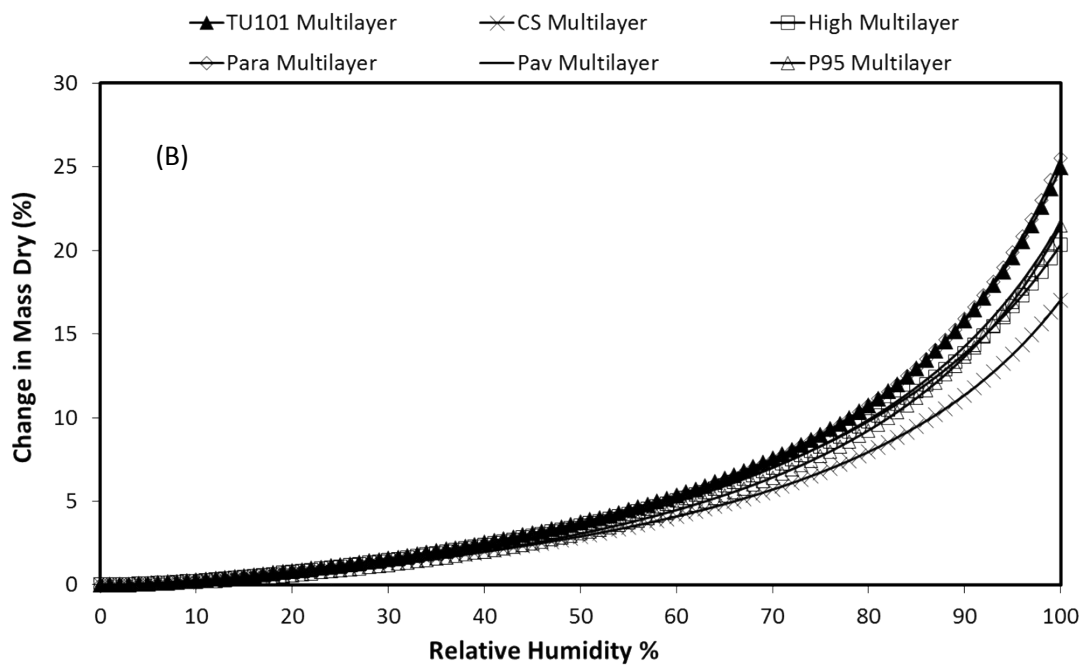
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82 **Figure S5:** GAB model fitting of sorption data for all wheat flours, (a) Monolayer sorption,

83 and (b) Multilayer sorption.