Supplementary material: Karl Fischer water titration—principal component analysis approach on bread products

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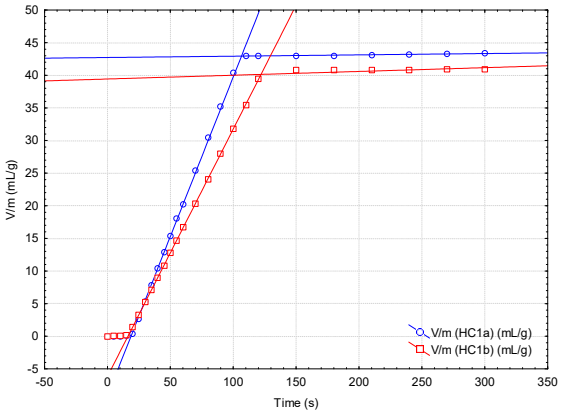
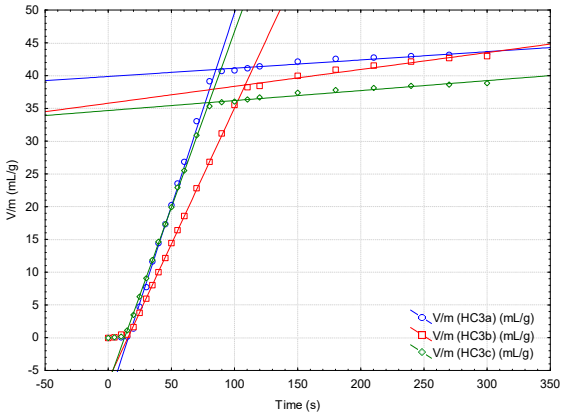
1. Karl Fischer water titration (KFT)



(**a**)



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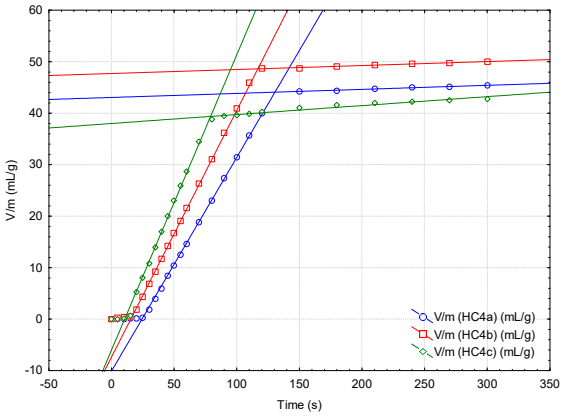

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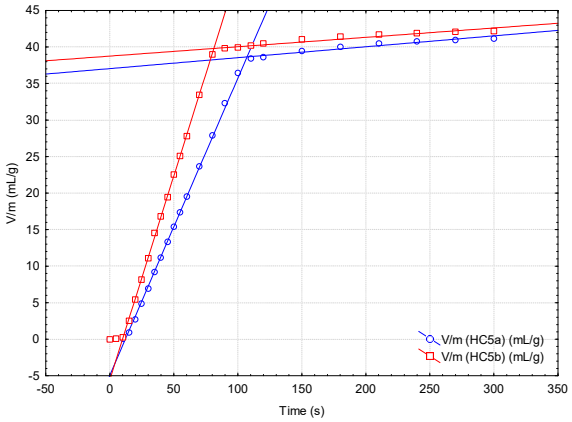

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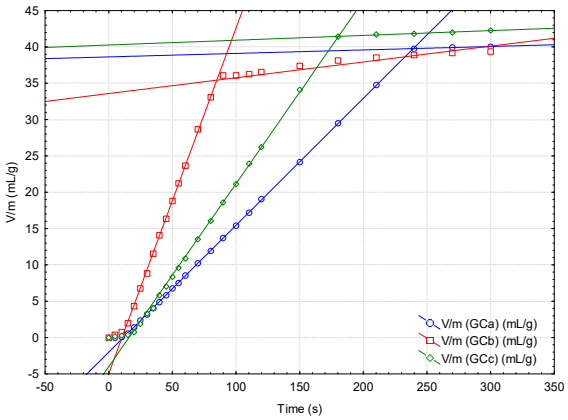

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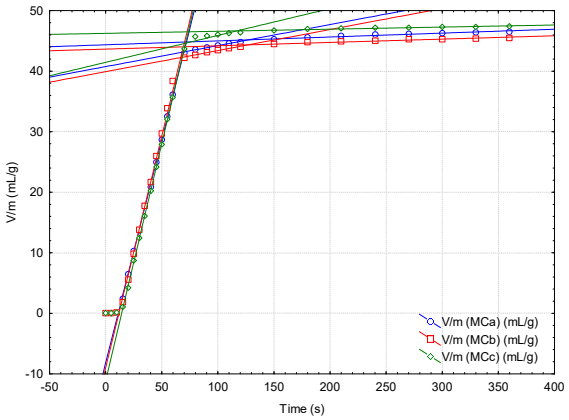

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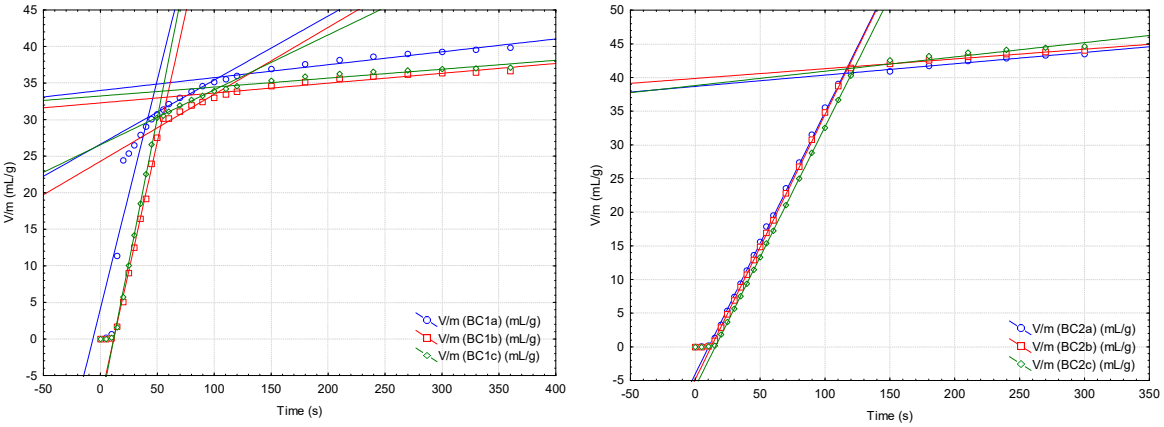


(**g**) (**h**)

Figure S1. The *Volume/sample mass (V/m) versus Time* titration curves from KFT analysis of the bread samples (triplicates, excepting *): (**a**) white wheat bread, non-packed (core) – code "*HC1*"; (**b**) white wheat bread roll, non-packed (core) – code "*HC3*" ; (**c**) white wheat bread roll, topped with various seeds, non-packed (core) – code "*HC4*"; (**d**) homemade white wheat bread (core) – code "*HC5*"; (**e**) Graham bread (core) – code "*GC*"; (**f**) whole meal bread (core) – code "*MC*"; (**g**) brown wheat bread, non-packed, from the market (core) – code "*BC1*"; (**h**) brown wheat bread, non-packed, from the manufacturer (core) – code "*BC2*".

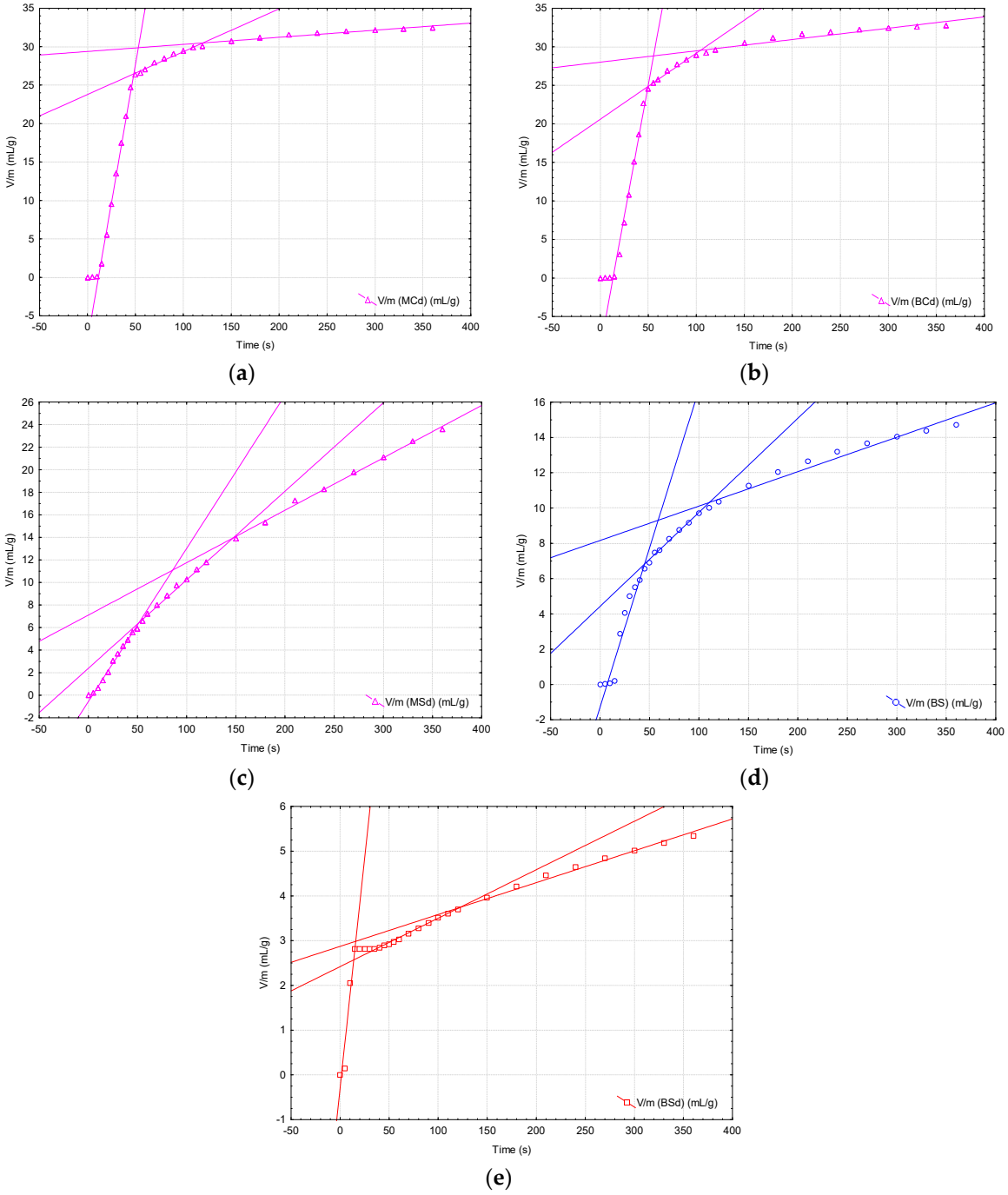


Figure S2. The *Volume/sample mass (V/m) versus Time* titration curves from KFT analysis of the pre-dried core, raw and pre-dried bread shell samples: (**a**) pre-dried whole meal bread (core) – code "*MCd*"; (**b**) pre-dried brown wheat bread, non-packed, from the market (core) – code "*BCd*"; (**c**) pre-dried whole meal bread (shell) – code "*MSd*"; (**d**) brown wheat bread, non-packed, from the market (shell) – code "*BS*"; (**e**) pre-dried brown wheat bread, non-packed, from the market (shell) – code "*BSd*".

Table S1. The mean KFT water reaction rates on the third time range (pseudolinear, the "normal" drift) for the core, pre-dried core, shell and pre-dried shell of bread samples. Values are expressed as mean (±standard deviation, SD) of triplicate analysis (excepting *).

Nº	Code	Mean KFT reaction rate v_3 (mM/s)	Nº	Code	Mean KFT reaction rate v_3 (mM/s)
1	*HC1*	0.022(±0.015)	1	*MCd* *	0.051
2	*HC2*	0.050(±0.004)	2	*BCd2* *	0.082
3	*HC3*	0.099(±0.039)	3	*MS*	0.083(±0.010)
4	*HC4*	0.061(±0.031)	4	*MSd* *	0.259
5	*HC5*	0.077(±0.008)	5	*BS* *	0.108
6	*GC* *	0.062	6	*BSd* *	0.039
7	*MC*	0.028(±0.009)			
8	*BC1*	0.080(±0.016)			
9	*BC2*	0.097(±0.019)			

Table S2. Significance levels (*p*-level) from the Tukey's HSD (honestly significant difference) test for the KFT volume/sample mass ratio – *V*/*m* (mL/g) in the case of KFT analysis of all bread samples (*p*-level values lower than 0.05 are bolded).

	HC1	***HC2***	***HC3***	***HC4***	***HC5***	***GC***	***MC***	***BC1***	***BC2***	***MCd***	***BCd***	***MS***	***MSd***	***BS***	***BSd***
HC1		0.957545	1.000000	0.581029	1.000000	0.999278	0.427987	0.995770	0.426622	**0.018850**	**0.024766**	**0.000157**	**0.000161**	**0.000157**	**0.000157**
HC2			0.777386	0.999571	0.870528	0.339460	0.993117	1.000000	**0.012374**	**0.001109**	**0.001444**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
HC3				0.275186	1.000000	0.999936	0.171748	0.940804	0.424537	**0.017008**	**0.022735**	**0.000157**	**0.000159**	**0.000157**	**0.000157**
HC4					0.416283	0.073231	1.000000	0.984959	**0.002046**	**0.000412**	**0.000498**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
HC5						0.999987	0.288013	0.971741	0.592498	**0.028664**	**0.037492**	**0.000157**	**0.000163**	**0.000157**	**0.000157**
GC							**0.041874**	0.564966	0.857321	**0.049571**	0.065388	**0.000157**	**0.000164**	**0.000157**	**0.000157**
MC								0.932271	**0.001190**	**0.000321**	**0.000383**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
BC1									**0.027790**	**0.001878**	**0.002475**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
BC2										0.427395	0.510429	**0.000157**	**0.000283**	**0.000157**	**0.000157**
MCd											1.000000	**0.013960**	0.113094	**0.000259**	**0.000157**
BCd												**0.010436**	0.091172	**0.000237**	**0.000157**
MS													1.000000	**0.045026**	**0.000160**
MSd														0.107215	**0.000224**
BS															0.077434
BSd															

Table S3. Significance levels (*p*-level) from the Tukey's HSD (honestly significant difference) test for the water content – *W* (%) in the case of KFT analysis of all bread samples (*p*-level values lower than 0.05 are bolded).

	HC1	***HC2***	***HC3***	***HC4***	***HC5***	***GC***	***MC***	***BC1***	***BC2***	***MCd***	***BCd***	***MS***	***MSd***	***BS***	***BSd***
HC1		0.881592	0.357435	0.998673	0.999472	0.148974	0.999999	1.000000	**0.043542**	**0.016105**	**0.019198**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
HC2			0.997780	0.999838	0.999957	0.907946	0.428128	0.465221	0.513290	0.137353	0.161401	**0.000158**	**0.000157**	**0.000157**	**0.000157**
HC3				0.819101	0.904697	0.999995	0.075213	0.085053	0.979897	0.438676	0.491905	**0.000163**	**0.000157**	**0.000158**	**0.000157**
HC4					1.000000	0.461024	0.886738	0.910420	0.150026	**0.046057**	0.055098	**0.000157**	**0.000157**	**0.000157**	**0.000157**
HC5						0.621559	0.943758	0.957130	0.265445	0.070834	0.083463	**0.000158**	**0.000157**	**0.000157**	**0.000157**
GC							**0.022623**	**0.025787**	0.999956	0.698909	0.752138	**0.000182**	**0.000157**	**0.000160**	**0.000157**
MC								1.000000	**0.005106**	**0.003954**	**0.004759**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
BC1									**0.005827**	**0.004337**	**0.005223**	**0.000157**	**0.000157**	**0.000157**	**0.000157**
BC2										0.935670	0.957716	**0.000296**	**0.000157**	**0.000167**	**0.000157**
MCd											1.000000	0.175957	**0.000157**	**0.003853**	**0.000160**
BCd												0.150072	**0.000157**	**0.003318**	**0.000160**
MS													**0.000159**	0.185552	**0.000220**
MSd														**0.016865**	0.994571
BS															0.155989
BSd															

Table S4. Significance levels (p-level) from the Tukey's HSD (honestly significant difference) test for the mean KFT reaction rate for the first time range – v_1 (mM/s) in the case of KFT analysis of all bread samples (p-level values lower than 0.05 are bolded).

	HC1	***HC2***	***HC3***	***HC4***	***HC5***	***GC***	***MC***	***BC1***	***BC2***	***MCd***	***BCd***	***MS***	***MSd***	***BS***	***BSd***
HC1		0.785901	0.997583	0.999957	0.999997	0.875362	**0.017979**	0.999997	0.073219	0.309183	0.492114	0.999972	0.246470	0.457746	0.605495
HC2			0.998912	0.979411	0.984691	**0.026717**	0.364050	0.287147	0.821918	0.970599	0.997883	0.233187	**0.009534**	**0.024130**	**0.040507**
HC3				1.000000	1.000000	0.170953	0.068656	0.833777	0.276553	0.691457	0.879164	0.765541	**0.038612**	0.093214	0.149312
HC4					1.000000	0.309183	**0.033463**	0.958914	0.150474	0.532766	0.751898	0.925723	0.064142	0.149312	0.231588
HC5						0.518421	0.063762	0.990760	0.227752	0.572359	0.776254	0.979921	0.108653	0.229522	0.334713
GC							**0.000258**	0.984786	**0.000711**	**0.017719**	**0.036802**	0.994054	0.888717	0.988387	0.998688
MC								**0.001740**	0.999890	1.000000	0.999805	**0.001358**	**0.000339**	**0.000642**	**0.000984**
BC1									**0.008436**	0.106636	0.202050	1.000000	0.378413	0.647415	0.797017
BC2										1.000000	1.000000	**0.006442**	**0.000756**	**0.001709**	**0.002827**
MCd											1.000000	0.089668	**0.005161**	**0.011025**	**0.016972**
BCd												0.172496	**0.009439**	**0.020158**	**0.030893**
MS													0.429069	0.703824	0.843125
MSd														1.000000	0.999997
BS															1.000000
BSd															

Table S4. Significance levels (*p*-level) from the Tukey's HSD (honestly significant difference) test for the mean KFT reaction rate for the second time range – v_2 (mM/s) in the case of KFT analysis of all bread samples (*p*-level values lower than 0.05 are bolded).

	HC1	***HC2***	***HC3***	***HC4***	***HC5***	***GC***	***MC***	***BC1***	***BC2***	***MCd***	***BCd***	***MS***	***MSd***	***BS***	***BSd***
HC1		0.999111	0.379041	0.980548	0.890003	0.979031	**0.000383**	0.416166	**0.000157**	**0.000188**	**0.000157**	**0.000157**	**0.000157**	**0.000229**	0.999030
HC2			0.821287	1.000000	0.999476	1.000000	**0.000588**	0.857388	**0.000157**	**0.000227**	**0.000157**	**0.000157**	**0.000157**	**0.000309**	1.000000
HC3				0.964331	0.999936	0.966843	**0.021222**	1.000000	**0.000157**	**0.001307**	**0.000157**	**0.000160**	**0.000158**	**0.002577**	0.997751
HC4					0.999999	1.000000	**0.001199**	0.976578	**0.000157**	**0.000292**	**0.000157**	**0.000157**	**0.000157**	**0.000443**	1.000000
HC5						0.999999	**0.011313**	0.999979	**0.000157**	**0.000850**	**0.000157**	**0.000161**	**0.000158**	**0.001558**	1.000000
GC							**0.001233**	0.978415	**0.000157**	**0.000294**	**0.000157**	**0.000157**	**0.000157**	**0.000449**	1.000000
MC								**0.018150**	**0.000157**	0.373858	**0.000208**	**0.031956**	**0.000656**	0.580742	**0.030947**
BC1									**0.000157**	**0.001179**	**0.000157**	**0.000160**	**0.000158**	**0.002316**	0.998681
BC2										**0.017316**	1.000000	**0.000913**	0.999306	**0.008372**	**0.000157**
MCd											0.067525	1.000000	0.309123	1.000000	**0.001811**
BCd												**0.020138**	0.999669	**0.038210**	**0.000158**
MS													0.157500	0.999998	**0.000236**
MSd														0.194309	**0.000160**
BS															**0.003197**
BSd															

2. Principal component analysis (PCA)

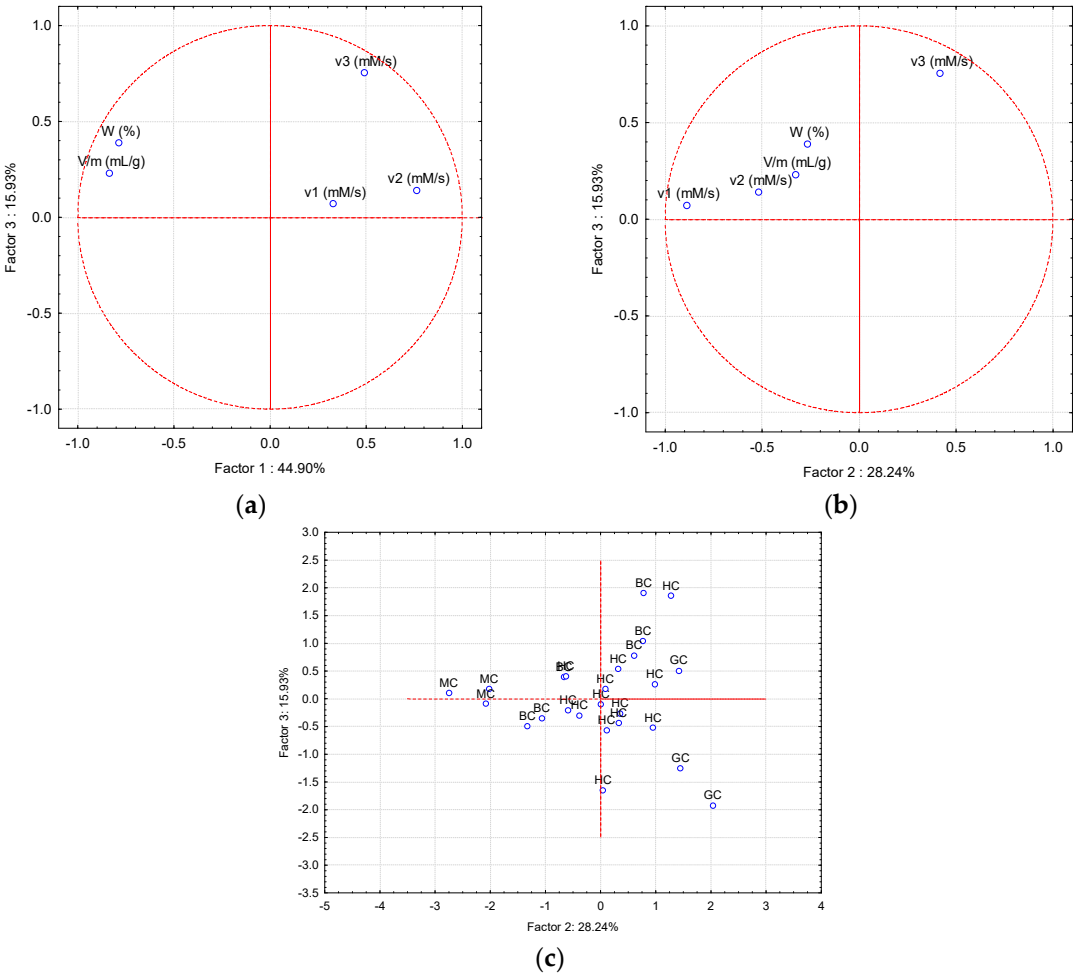
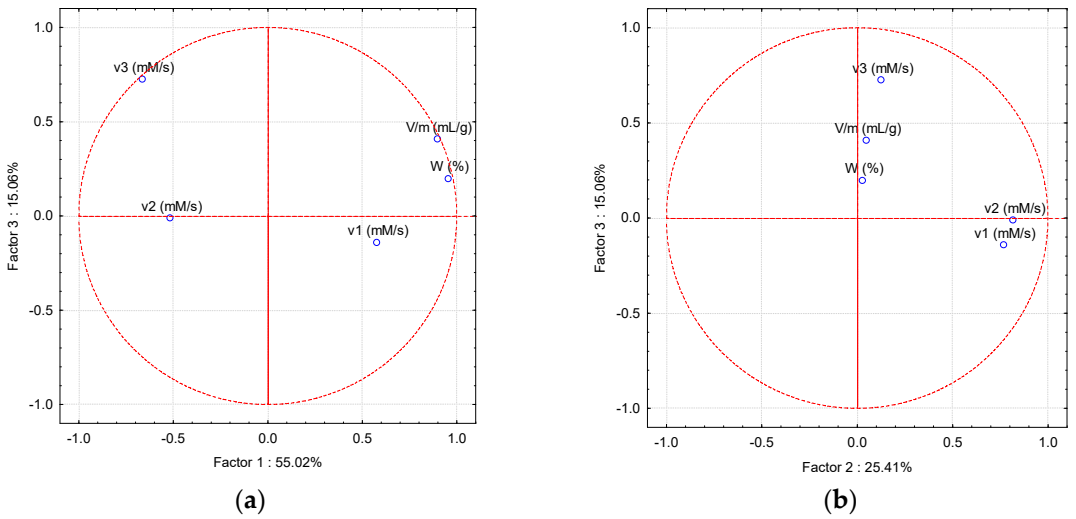
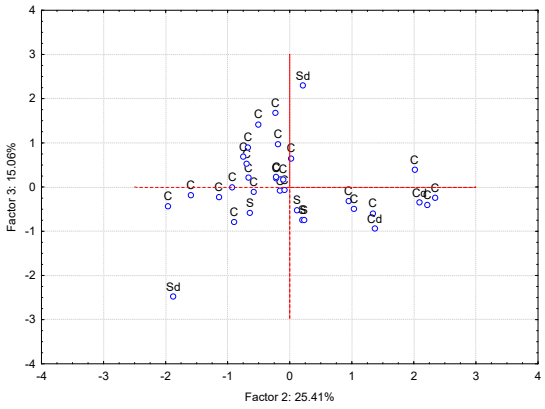


Figure S3. PCA results for the KFT data of bread core samples: (**a**) *PC*₃ *versus PC*₁ loadings plot; (**b**) *PC*₃ *versus PC*₂ loadings plot; (**c**) *PC*₃ *versus PC*₂ scores plot.





(**c**)

Figure S4. PCA results for the KFT data of all bread core and shell samples: (**a**) *PC₃ versus PC₁* loadings plot; (**b**) *PC₃ versus PC₂* loadings plot; (**c**) *PC₃ versus PC₂* scores plot.