

Development and Optimisation of Solid-Phase Extraction of Extractable and Bound Phenolic Acids in Spelt (*Triticum spelta* L.) Seeds

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Table S1. Characteristics of phenolic acids from germinated spelt seeds by liquid chromatography–mass spectrometry in negative ion mode.

Phenolic acids	[M-H] ⁻ (m/z)	MS ² (m/z)	Expressed as (equivalents)	Standard curve	R ²	LOD (µg/g)	LOQ (µg/g)	Recovery (%)
<i>p</i> -Coumaric acid	163	119	<i>p</i> -Coumaric acid	y = 2327.3x	0.9911	0.176	0.534	93.49
<i>trans</i> -Ferulic acid	193	134, 149, 179	Ferulic acid	y = 1747.9x	0.9996	0.094	0.285	94.00
Caffeic acid	179	135	Caffeic acid	y = 1783.7x	1.0000	0.524	1.586	95.54
<i>p</i> -Hydroxybenzoic acid	137	93	<i>p</i> -Hydroxybenzoic acid	y = 607.04x	0.9994	0.269	0.814	89.51

LOD: limit of detection; LOQ: limit of quantitation.

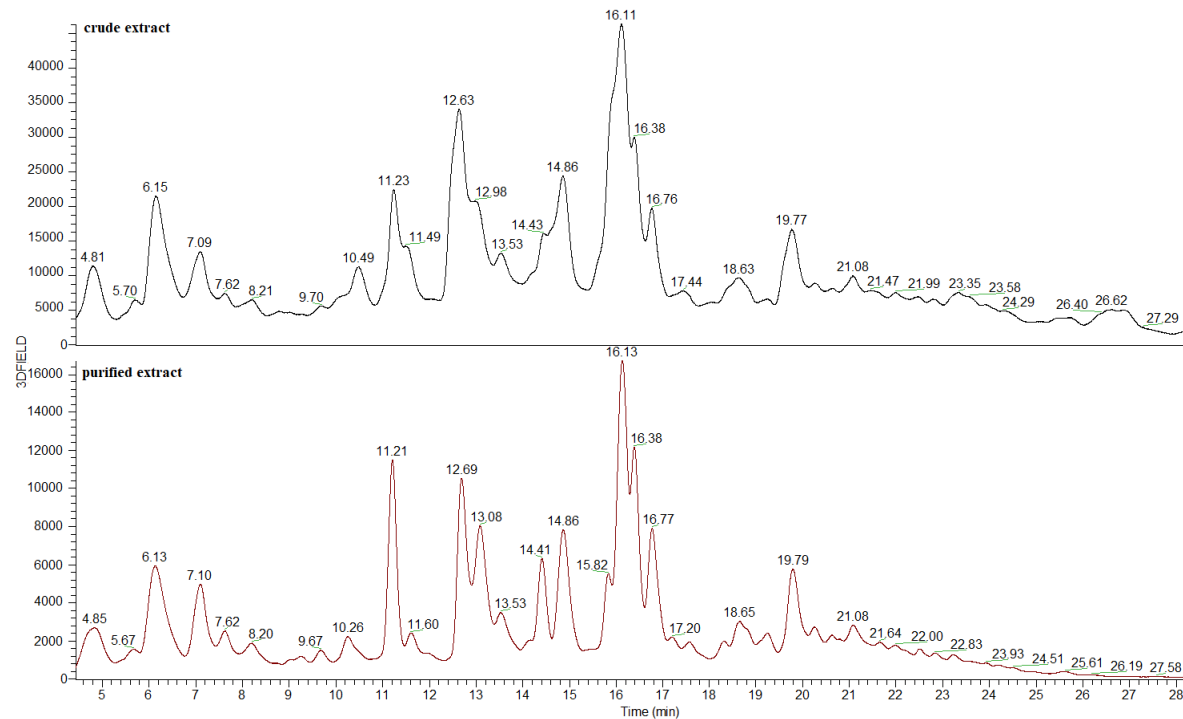


Figure S1. Representative HPLC chromatograms of the extractable phenolics of germinated spelt seeds in the crude extract without purification (Table 1, #1) and with purification through solid-phase extraction (Table 1, #2) (detected at 310 nm). Below: Peak times for purified sample corresponding to the defined phenolic acids determined in the present study.

Phenolic acid	Corresponding peak times (min)
<i>p</i> -Coumaric acid	18.65
<i>trans</i> -Ferulic acid	19.79
Caffeic acid derivatives	14.41
<i>p</i> -Hydroxybenzoic acid	12.69

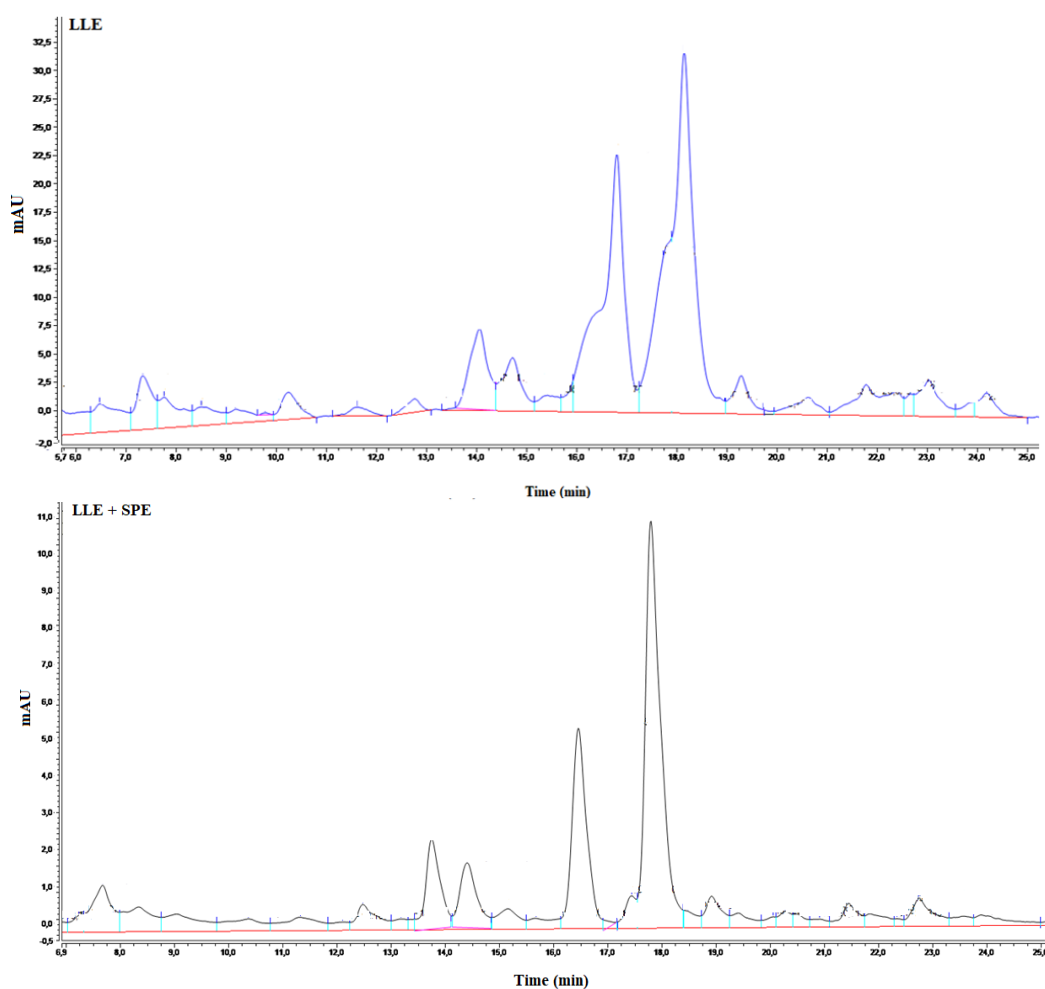


Figure S2. Representative HPLC chromatograms of free phenolics of germinated spelt seeds after liquid–liquid extraction without (LLE) and with solid phase extraction (LLE+SPE) (detected at 310 nm).

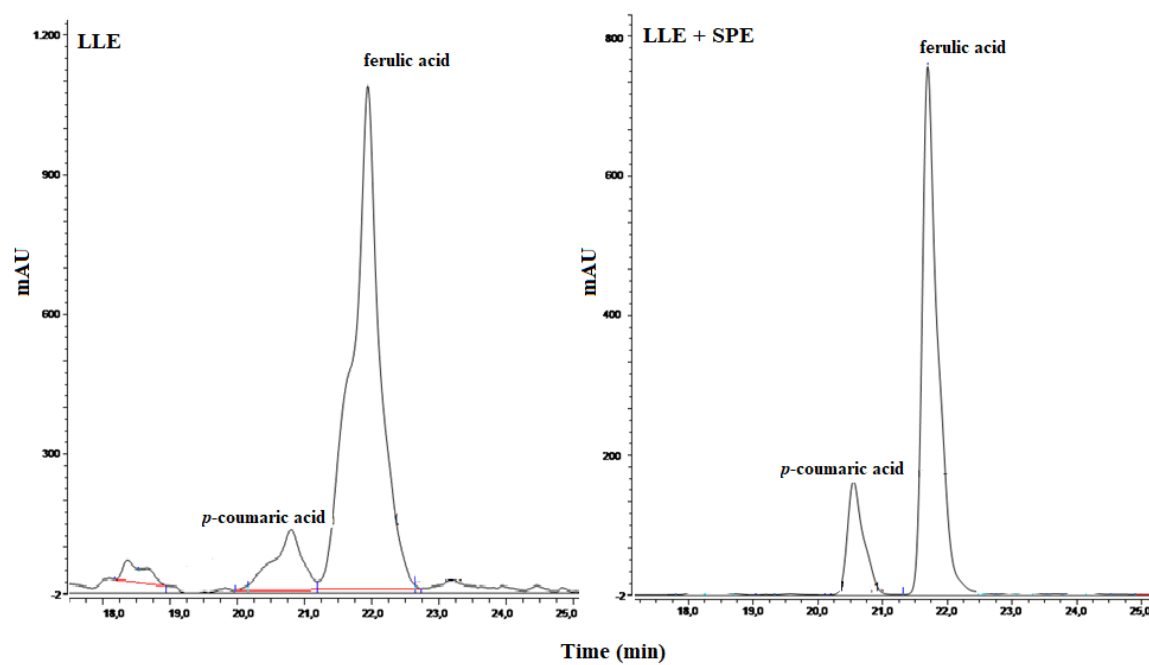


Figure S3. Representative HPLC chromatograms of bound phenolics of germinated spelt seeds after liquid-liquid extraction without (LLE) and with solid phase extraction (LLE+SPE) (detected at 310 nm).