

A new LC-MS method for evaluating the efficacy of pesticide residues removal from apple surfaces by washing agents

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Table of content

Table S1. Mass spectrometer operating parameters used for the determination of selected pesticides.	2
Table S2. Isotopic distributions for individual pesticides and their deuterated analogues: (a) acetamiprid, (b) boscalid, (c) pyraclostrobin, (d) pendimethalin.....	3
Figure S1. Sample preparing procedure: (a) immersion in a pesticides solution, (b) detergent washing, (c) tap water washing for detergent removal, (d) QuEChERS extraction of the ground apples.....	4

Table S1. Mass spectrometer operating parameters used for the determination of selected pesticides.

Analyte	Precursor ion m/z, [M+H] ⁺ , Da	Main product ions MS ² m/z, Da	DP, V	EP, V	CE, V	CXP, V
PESTICIDE						
Acetamiprid – Qualification	223	126	71	10	31	10
Acetamiprid – Confirmation	223	99	71	10	51	10
Boscalid – Qualification	343	140	76	10	27	10
Boscalid – Confirmation	343	112	76	10	59	10
Pyraclostrobin – Qualification	388	105	56	10	59	10
Pyraclostrobin – Confirmation	388	120	56	10	69	8
Pendimethalin – Qualification	282	212	26	10	15	8
Pendimethalin – Confirmation	282	91	26	10	27	16
PESTICIDE IZOTOPE ANALOGUE						
Acetamiprid-d3 – Qualification	228	128	66	10	31	10
Acetamiprid-d3 – Confirmation	228	101	66	10	53	10
Boscalid-d – Qualification	349	142	86	10	27	10
Boscalid-d4 – Confirmation	349	114	86	10	61	8
Pyraclostrobin-d6 – Qualification	394	105	61	10	79	8
Pyraclostrobin-d6 – Confirmation	394	120	61	10	65	8
Pendimethalin-d5 – Qualification	287	212	61	10	17	14
Pendimethalin-d5 – Confirmation	287	91	61	10	39	8

DP-declustering potential, **EP**-entrance potential, **CE**-collision energy, **CXP**-collision cell exit potential

Table S2. Isotopic distributions for individual pesticides and their deuterated analogues: (a) acetamiprid, (b) boscalid, (c) pyraclostrobin, (d) pendimethalin.

m/z , Da	[M+H] ⁺ , Da	Acetamiprid	Acetamiprid-d3
222	223	100.0%	
223	224	12.7%	
224	225	32.7%	
225	226	4.0%	100.0%
226	227	0.2%	12.7%
227	228		32.7%
228	229		4.0%
229	230		0.2%

(a)

m/z, Da	[M+H] ⁺ , Da	Pyraclostrobin	Pyraclostrobin-d6
387	388	100.0%	
388	389	22.5%	
389	390	35.2%	
390	391	7.5%	
391	392	1.0%	
392	393	0.1%	
393	394	0.0%	100.0%
394	395		22.5%
395	396		35.2%
396	397		7.5%
397	398		1.0%
398	399		0.1%

(c)

m/z , Da	[M+H] ⁺ , Da	Boscalid	Boscalid-d4
342	343	100.0%	
343	344	20.9%	
344	345	66.2%	
345	346	13.5%	
346	347	11.6%	100.0%
347	348	2.2%	20.9%
348	349	0.2%	66.2%
	350		13.5%
	351		
	352		2.2%
	353		0.2%

(b)

m/z, Da	[M+H] ⁺ , Da	Pendimethalin	Pendimethalin-d5
281	282	100.0%	
282	283	15.9%	
283	284	1.9%	
284	285	0.1%	
285	286	0.0%	
286	287	0.0%	100.0%
287	288	0.0%	15.9%
288	289	0.0%	1.9%
289	290		0.1%

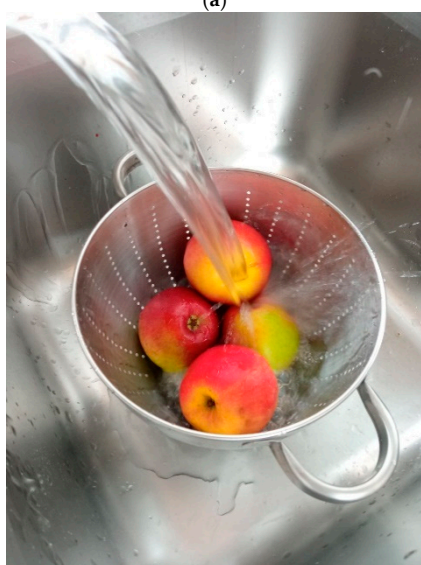
(d)



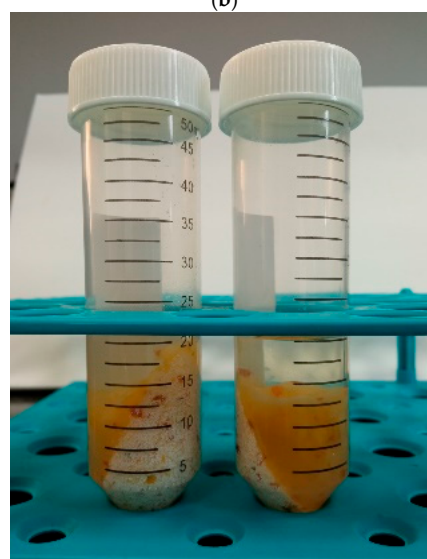
(a)



(b)



(c)



(d)

Figure S1. Sample preparing procedure: (a) immersion in a pesticides solution, (b) detergent washing, (c) tap water washing for detergent removal, (d) QuEChERS extraction of the ground apples.