

## Supplementary Information

### **MWCNT based monolith for the analysis of antibiotics and pesticides in milk and honey by an integrated nano liquid chromatography-high resolution orbitrap mass spectrometry**

Cemil Aydoğan<sup>1\*</sup> and Ziad El Rassi<sup>2</sup>

<sup>1</sup>Department of Food Engineering, Bingöl University, 12000 Bingöl, Turkey

<sup>2</sup>Department of Chemistry, Oklahoma State University, Stillwater, OK, USA

#### **Table of Contents**

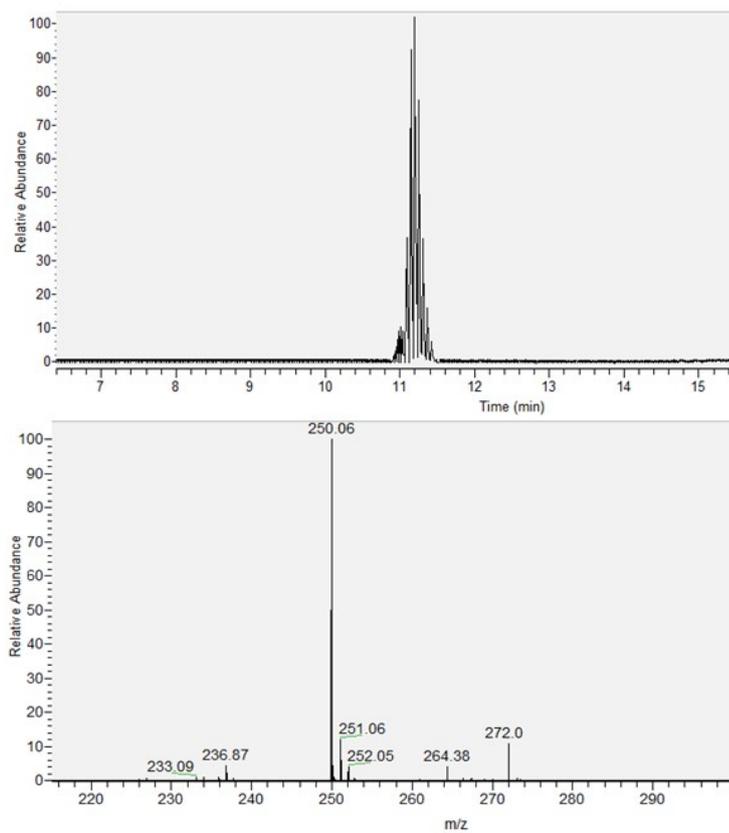
Figure S1: Total ion chromatogram and MS spectra of sulfapyridine using nano LC-HR Orbitrap MS.

Figure S2: Total ion chromatograms of pesticides

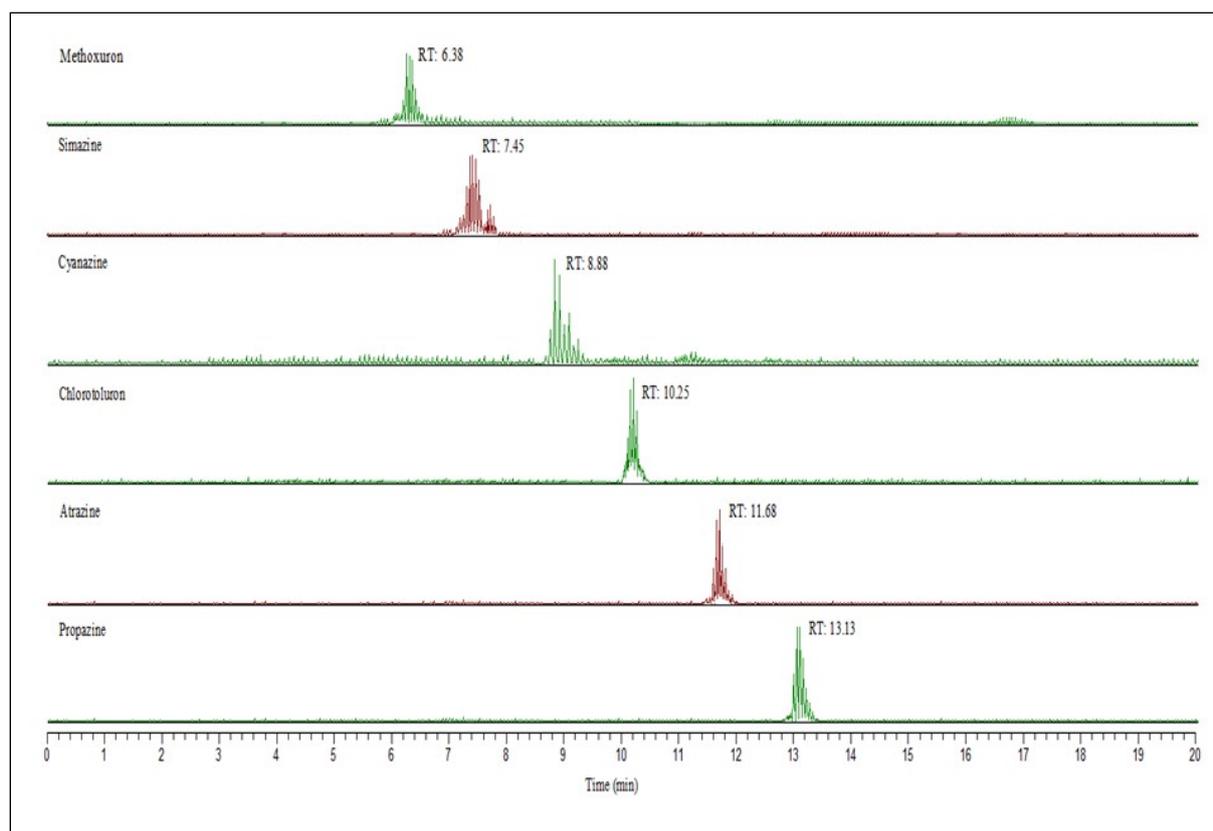
Table S1: Exact mass database of the studied eight antibiotics including experimental and theoretical masses, retention time, and accurate mass error.

Table S2: Exact mass database of the studied six pesticides including experimental and theoretical masses, retention time, and accurate mass error.

Table S3: Validation parameters of the developed method.



**Figure S1:** Total ion chromatogram and MS spectra of sulfapyridine using nano LC-HR Orbitrap MS.



**Figure S2:** Total ion chromatograms of pesticides

**Tables S1:** Exact mass database of the studied eight antibiotics including experimental and theoretical masses, retention time, and accurate mass error.

No	Compound	Theoretical mass <sup>a</sup> (m/z)	Experimental <sup>b</sup> (m/z)	Retention time (UV <sup>c</sup> - OrbitrapMS <sup>d</sup> )	Mass error ( $\Delta$ ppm)
1	Sulfacetamide	214.04121	214.04090	6.42 – 6.48	-1.4
2	Sulfanilamide	172.03065	172.03030	7.74 – 7.84	-2.0
3	Sulfadiazine	251.05972	251.06045	9.32 – 9.38	2.9
4	Sulfapyridine	250.06447	250.06420	11.20 – 11.25	-1.0
5	Sulfadoxine	311.08090	311.08025	12.66 – 12.72	-2.1
6	Sulfathiazole	256.02089	256.02062	14.52 – 14.67	-1.1
7	Sulfamethazine	279.09102	279.09024	16.80 – 16.85	-2.8
8	Sulfisoxazole	268.07504	268.07446	19.23 – 19.43	-2.2

<sup>a</sup> Theoretical mass m/z values were obtained from m/z cloud

([https://www.mzcloud.org/DataViewer#/Main/reference\\$1/T2%23Standard/Recalibrated/389606](https://www.mzcloud.org/DataViewer#/Main/reference$1/T2%23Standard/Recalibrated/389606))

<sup>b</sup> Experimental mass m/z values were obtained from the nano LC-HR Orbitrap MS system.

<sup>c</sup> These values were obtained using the nano LC-UV.

<sup>d</sup> These values were obtained using nano LC-HR Orbitrap MS system.

**Table S2:** Exact mass database of the studied six pesticides including experimental and theoretical masses, retention time, and accurate mass error.

No	Compound	Theoretical mass <sup>a</sup> (m/z)	Experimental <sup>b</sup> (m/z)	Retention time (UV <sup>c</sup> -MS <sup>d</sup> )	Mass error (Δppm)
1	Methoxuron	229.07383	229.07332	6.34 – 6.38	-2.2
2	Simazine	201.08540	201.08520	7.44 – 7.45	-1.0
3	Cyanazine	241.09630	241.09614	8.81 – 8.88	-0.6
4	Chlorotoluron	213.07890	213.07892	10.19 – 10.25	0.1
5	Atrazine	216.10100	216.10087	11.66 – 11.68	-0.6
6	Propazine	230.11670	230.11649	13.03 – 13.13	-0.3

<sup>a</sup> Theoretical mass m/z values were obtained from m/z cloud

([https://www.mzcloud.org/DataViewer#/Main/reference\\$1/T2%23Standard/Recalibrated/389606](https://www.mzcloud.org/DataViewer#/Main/reference$1/T2%23Standard/Recalibrated/389606))

<sup>b</sup> Experimental mass m/z values were obtained from the nano LC-HR Orbitrap MS system.

<sup>c</sup> These values were obtained using the nano LC-UV.

<sup>d</sup> These values were obtained using nano LC-HR Orbitrap MS system.

**Table S3**

Validation parameters of the developed method.

Antibiotics	SXZ	SDZ	SPRY	SMZ	STZ	SNM	SCM	SDX
Matrix <sup>a</sup> effect	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.0
Linearity	0.9971	0.9981	0.9980	0.9976	0.9992	0.9986	0.9976	0.9983
LOD(μg/kg)	0.10	0.10	0.14	0.10	0.10	0.12	0.12	0.10
LOQ(μg/kg)	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20
Recovery at 10 μg/kg	77	82	88	86	86	79	82	89
RSD at 10 μg/kg	8	11	11	9	8	10	7	4

<sup>a</sup>Matrix effects were calculated using the equation [(curve slope in matrix/ curve slope in solvent)-1]x100