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SUPPLEMENTARY MATERIAL TO

Stability and computational analyses of selected pesticides in use in the Republic of Serbia

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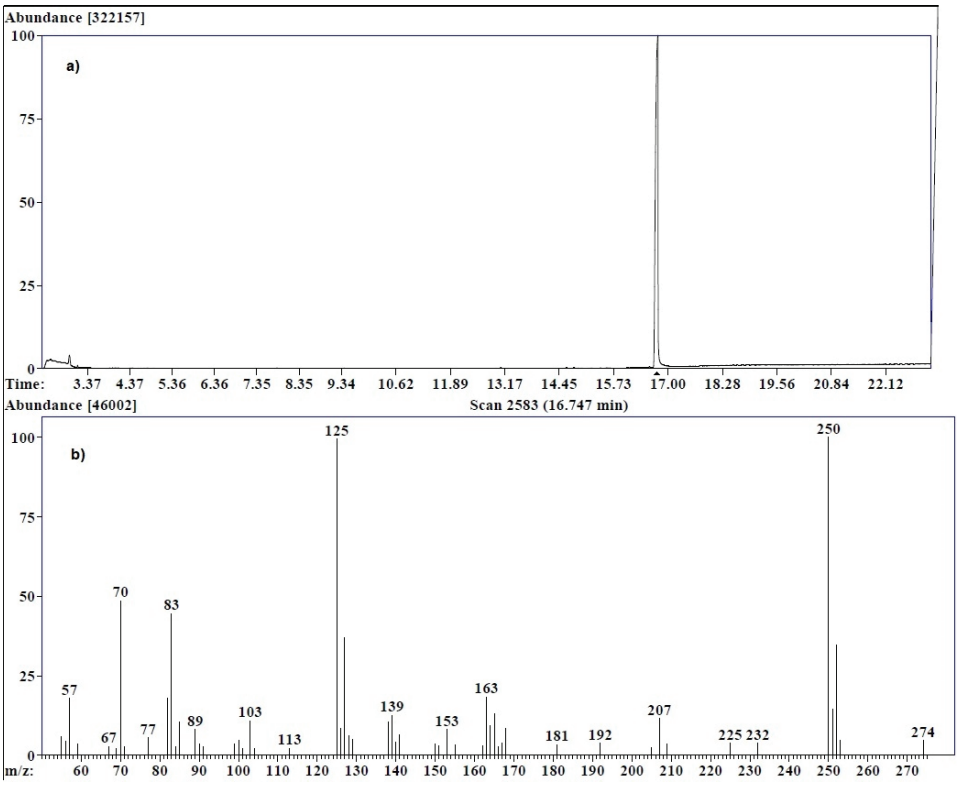

Fig S-1. a) Total-Ion Chromatogram (TIC) of tebuconazole solution, b) Mass spectrum of tebuconazole.

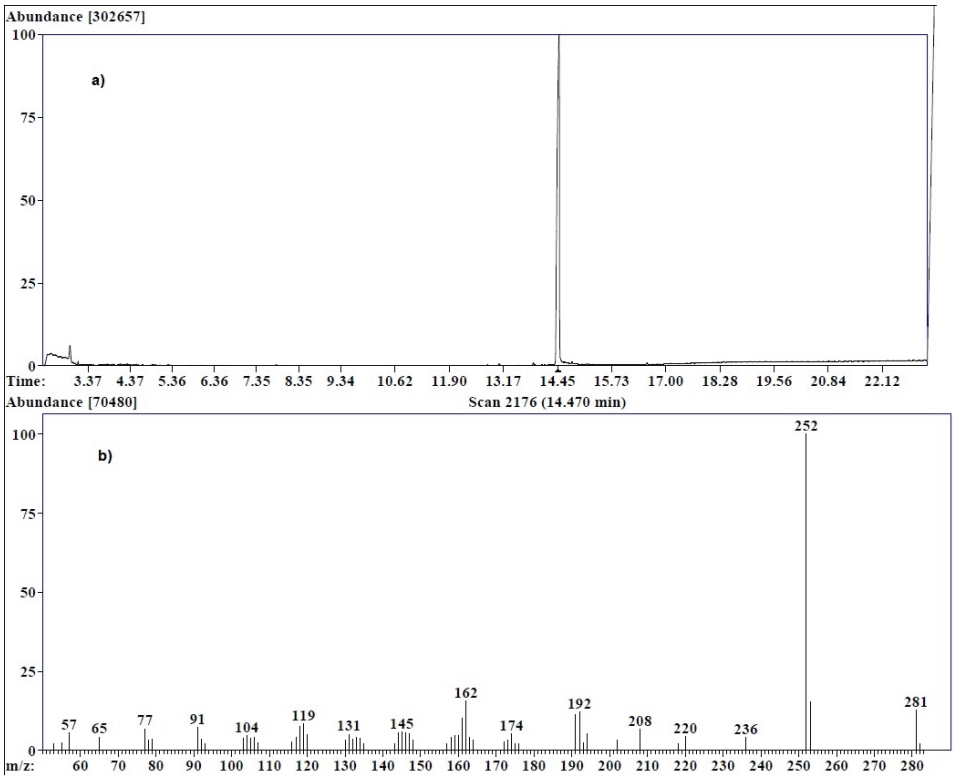

Fig S-2. a) Total-Ion Chromatogram (TIC) of pendimethalin solution, b) Mass spectrum of pendimethalin.

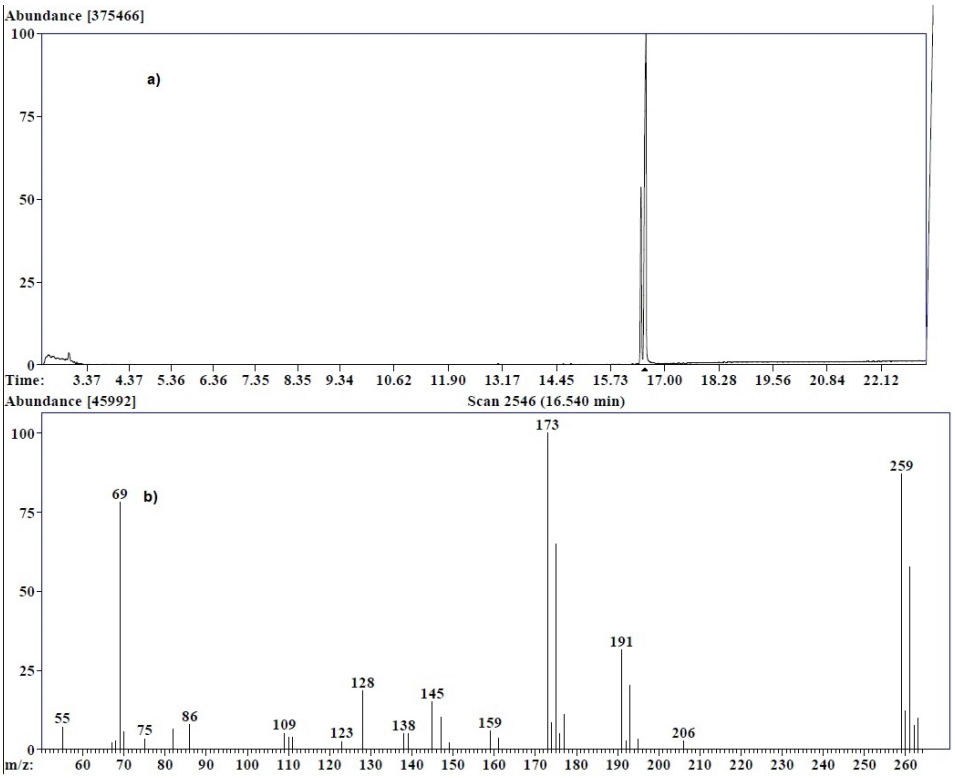

Fig S-3. a) Total-Ion Chromatogram (TIC) of propiconazole solution, b) Mass spectrum of propiconazole.

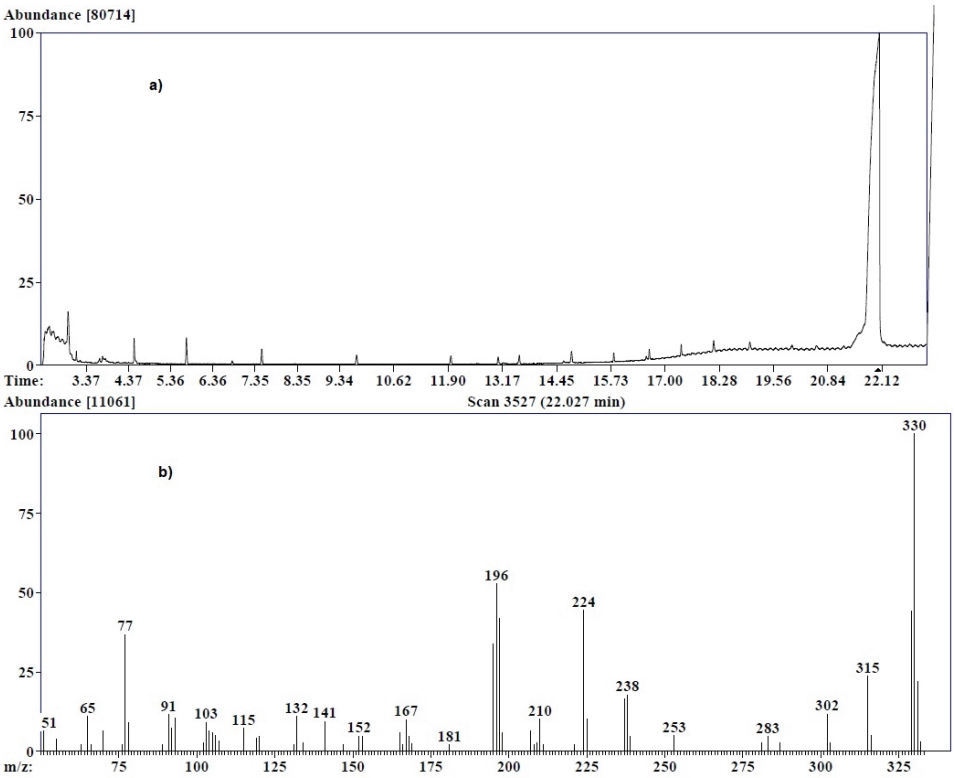

Fig S-4. a) Total-Ion Chromatogram (TIC) of famoxadone solution, b) Mass spectrum of famoxadone.

Table S-I. Calculated absorption, distribution, metabolism, elimination, and toxicity (ADMET) parameters of the compounds using QikProp v7.0.

Compound	MW	DM	MV	DHB	AHB	PSA	logP	logS	PCaco	PM	%HOA	VRF	VRT
Tebuconazole	307.8	3.4	978.7	1	3.7	41.4	4.1	-4.5	2515.3	2	100	0	0
Pendimetalin	281.3	4.6	918.5	1	3	83.8	2.9	-3.8	625.9	6	94	0	0
Pyraclostrobin	387.8	1.5	1194.8	0	5.2	71.6	4.9	-5.9	3362.1	3	100	0	1
Propiconazole	342.2	3.7	1002.8	0	4.5	115.5	3.9	-4.5	3382.5	0	100	0	0
Famoxadone	374.4	7.1	1131.4	2	0	75.6	3.7	-5.4	1523.7	2	100	0	0

MW: Molecular weight; DM: computed dipole moment; MV: total solvent-accessible volume; DHB: estimated number of hydrogen-bond donors; AHB: estimated number of hydrogen-bond acceptors; PSA: van der Waals surface area of polar nitrogen and oxygen atoms and carbonyl carbon atoms; logP: predicted octanol/water partition coefficient; log S: predicted aqueous solubility; PCaco: predicted apparent Caco-2 cell permeability; PM: number of likely metabolic reactions; % HOA: predicted human oral absorption percentage; VRF: number of violations of Lipinski rule of five (the rules are as follows: MW< 500, log P < 5, DHB ≤ 5, AHB ≤ 10, positive PSA value); VRT: number of violations of Jorgensen rule of three (the rules are as follows: log S > -5.7, PCaco > 22 nm s^{-1}, PM < 7).

Table S-II. ADME and drug safety profiling of the selected pesticides using Percepta 14.53.0 (Build 3577).

Pesticides	Caco-2 / cm s^{-1}	PPB / %	CNS	HIA / %	Metabolic stability	p-gp substrate	CYP1A2 inhibitor	CYP2C9 inhibitor	CYP2C19 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Ames	hERG
Tebuco-nazole	142 x 10^{-6}	91	-2.20	100	0.33	0.48	0.41	0.42	0.45	0.45	0.72	0.19	0.36
Pendi-methalin	79 x 10^{-6}	93	-2.29	100	0.37	0.42	0.52	0.37	0.37	0.47	0.46	0.68	0.42
Pyraclo-strobin	174 x 10^{-6}	97	-2.75	100	0.48	0.43	0.56	0.41	0.51	0.47	0.54	0.52	0.54
Propicon-azole	196 x 10^{-6}	92	-2.24	100	0.43	0.32	0.50	0.40	0.52	0.41	0.72	0.20	0.42
Famox-adone	109 x 10^{-6}	98	-2.80	100	0.40	0.47	0.30	0.45	0.50	0.37	0.59	0.34	0.40