








A Method for Monitoring Pesticide Transformation Products in Water environments (PTPWs) without their Authentic Standards

Fumi HASHIMOTO¹, Hirokazu TAKANASHI¹, Tsunenori NAKAJIMA¹, Akira OHKI¹,
Takehiko UEDA¹, Jun-ichi KADOKAWA¹, Nobukazu MIYAMOTO², Hidenori ISHIKAWA²

Abstract

Pesticides are ubiquitous contaminants in water environments, so many researchers have reported their concentrations in surface waters. As well as the pesticides, Pesticide Transformation Products in Water environments (PTPWs) can be detected in the surface waters. In order to detect the PTPWs, authentic standards are needed. But the number of commercially available standards has been still limited. Thus in this study, a technique to detect the PTPWs without any of authentic standards was developed by coupling a LC-MS/MS with a high resolution LC-MS. A neonicotinoid pesticide imidacloprid was used as a model compound. Five purchasable PTPWs were detected in the irradiated aqueous solutions of imidacloprid by the analysis with the high resolution LC-MS, being acquired their retention times and m/z values. The product ion scan of the solution was conducted with the LC-MS/MS using the same chromatographic conditions, which resulted in the detection of five chromatographic peaks whose retention times are almost identical with those in the LC-MS analysis. Given this fact, SRM conditions were developed for each of these five compounds using the irradiated samples (Table 1). The developed conditions were verified by using the authentic standards, which indicates that the developed method in this study was shown to be effective (Figure 1).

Table 1. SRM conditions for imidacloprid and its PTPWs

Chemical name	CAS RN	Structure	Molecular formula	Precursor ion m/z	Target ion m/z	Qualifier ion m/z
imidacloprid	138261-41-3		$C_9H_{10}ClN_3O_2$	256	175	209
			Adduct ion	RF lens [V]	CE [V]	CE [V]
			$[M+H]^+$	40	20	18
5-(aminomethyl)-2-chloropyridine	97004-04-1		$C_6H_7ClN_2$	143	78	107
			$[M+H]^+$	50	28	22
1-((6-chloropyridin-3-yl)methyl)imidazolidine-2-imine	127202-53-3 (115970-17-7)		$C_9H_{11}ClN_4$	211	126	99
			$[M+H]^+$	60	26	40
6-chloronicotinaldehyde	23100-12-1		C_6H_4ClNO	142	78	106
			$[M+H]^+$	80	23	18
N-(1-((6-chloropyridin-3-yl)methyl)-1,3-dihydro-2H-imidazol-2-ylidene)nitramide	115086-54-9		$C_9H_8ClN_5O_2$	254	171	236
			$[M+H]^+$	40	18	10
1-((6-chloropyridin-3-yl)methyl)imidazolidine-2-one	120868-66-8		$C_9H_{10}ClN_3O$	212	128	99
			$[M+H]^+$	60	21	21
6-chloronicotinic acid	5326-23-8		$C_6H_4ClNO_2$	158	122	78
			$[M+H]^+$	28	19	23

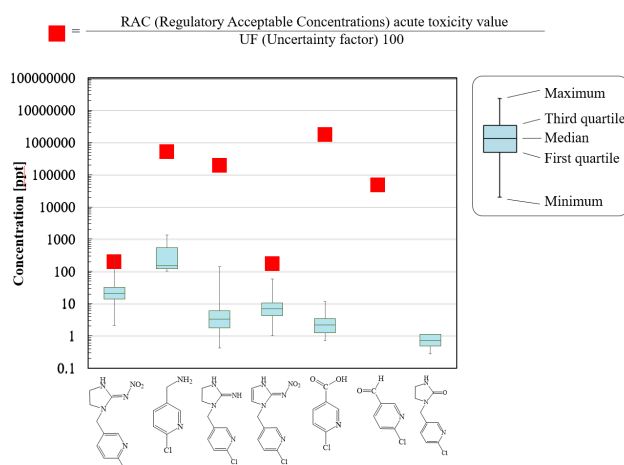


Figure 1. PTPW concentrations in the river water samples and their risk assessments

¹ Graduate School of Science and Engineering, Kagoshima University, Kagoshima 890-0065 Japan

² Institute of Environmental Ecology, IDEA Consultants, Inc., Shizuoka 421-0212, Japan