

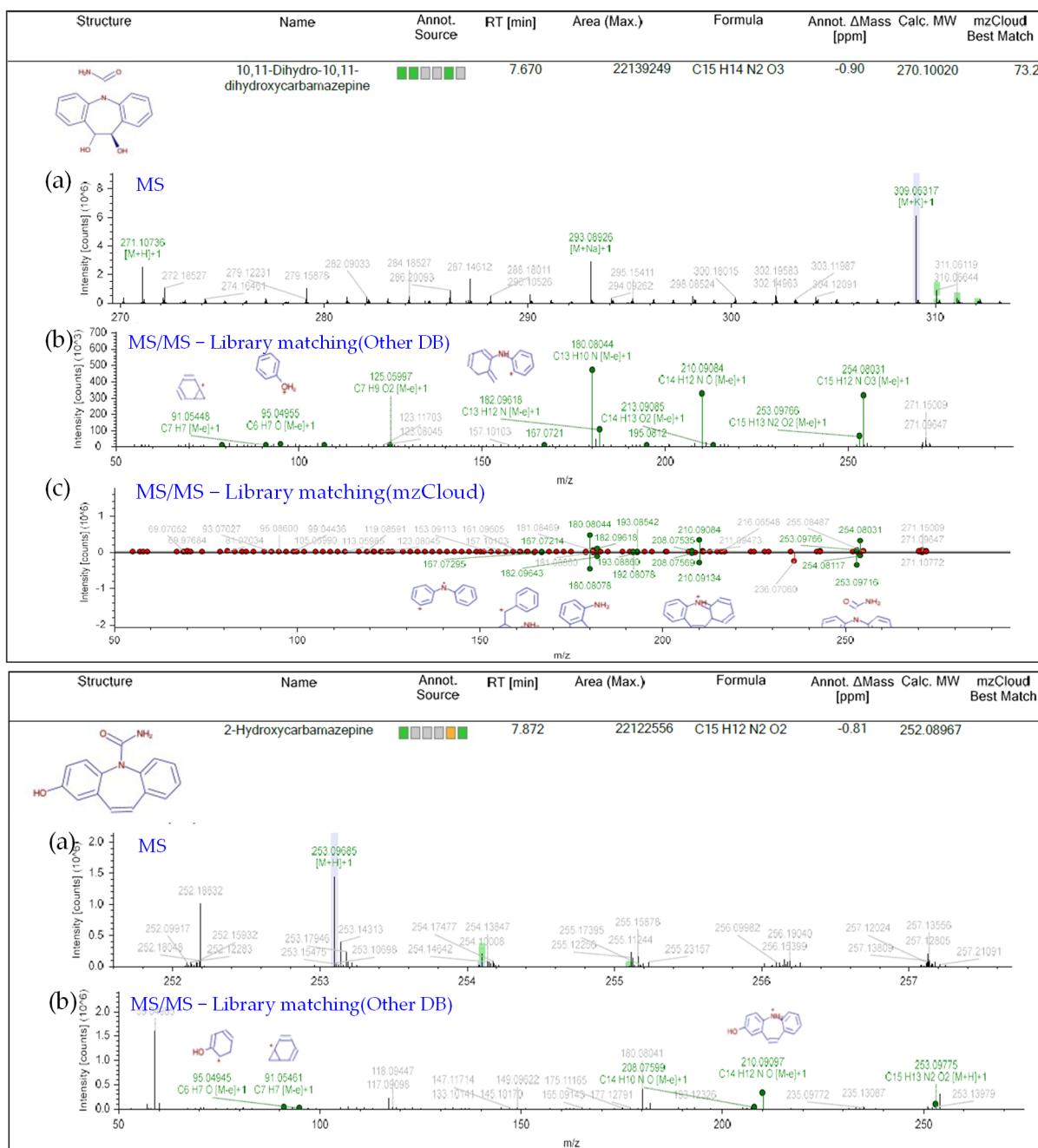
## **Supplementary Data**

# **Non-Targeted Screening and Identification of the Transformation Pathway of Carbamazepine in the Saemangeum Watershed, Republic of Korea**

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**Figure S1.** Overview of compound identification workflow by Compound Discoverer3.3 showing the Level 2 identification of CBZ TPs in sample as an example (a) MS spectrum (b) Level 2b: MS2 spectrum matching – Other DB (c) Level 2a: MS2 spectrum matching– mzCloud



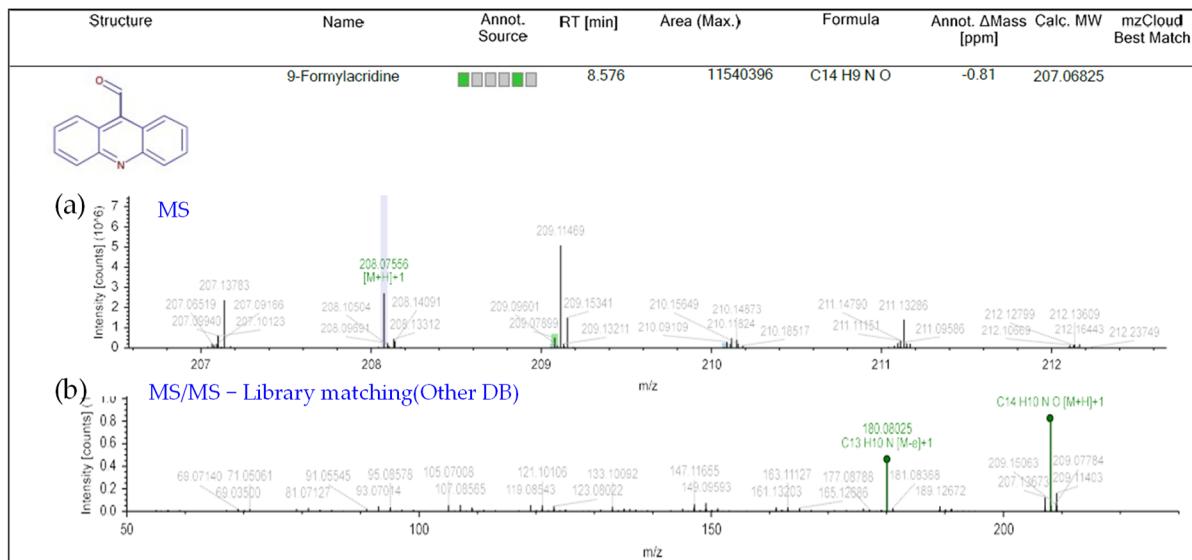
The figure displays three panels of mass spectral data for 10-Hydroxycarbazepine. Panel (a) shows the MS spectrum with major peaks at m/z 255.11246 [M+H]+, 273.16687, 275.13055, 277.09448 [M+Na]+, 280.19034, 281.19366, 282.22717, 283.15402, 285.18011, 287.14612, 289.14063, 291.20624, and 293.06824 [M+K]+. Panel (b) shows MS/MS library matching against other databases, with the base peak at m/z 192.00803 C14 H10 N [M-e]-1. Other significant peaks include m/z 121.06535 C8 H9 O [M-e]-1, 139.07526, 137.09604, 149.09610, 177.12773, 177.09130, 219.13777, 220.07581 C15 H10 N O [M-e]-1, 220.07581 C15 H10 N O [M-e]-1, 237.10217 C15 H13 N2 O [M-e]-1, 237.10217 C15 H13 N2 O [M-e]-1, 238.10539, 238.10539, 248.10100, 255.97929, and 257.07150. Panel (c) shows MS/MS library matching against mzCloud, with the base peak at m/z 192.00803 C15 H10 N O [M-e]-1. Other significant peaks include m/z 81.07059, 91.05469, 95.08600, 113.06009, 121.10150, 137.09604, 140.09610, 163.11163, 177.09138, 193.08860, 194.09650, 197.07274, 219.13777, 220.07581 C15 H10 N O [M-e]-1, 220.07581 C15 H10 N O [M-e]-1, 237.10217 C15 H13 N2 O [M-e]-1, 237.10224, 237.14065, 255.12117, 256.10100, 258.10539, and 255.97929.

The figure displays three panels showing the mass spectrum and library matching results for 9-acridinecarboxylic acid hydrate.

**(a) MS Spectrum:** The plot shows Intensity [counts] (10<sup>5</sup>) versus m/z. The base peak is at m/z 224.06987 [M+H]<sup>+</sup>. Other significant peaks are labeled at m/z 223.13213, 225.14787, and 227.16357.

**(b) MS/MS - Library matching(Other DB):** The plot shows Intensity [counts] versus m/z. The base peak is at m/z 224.06979 [M+H]<sup>+</sup>. Other labeled peaks include 199.07501 [M-e]<sup>-</sup>, 178.06445 [M-e]<sup>-</sup>, 168.08020 [M-e]<sup>-</sup>, 123.08042 [M-e]<sup>-</sup>, 119.08533 [M-e]<sup>-</sup>, 109.10112 [M-e]<sup>-</sup>, 95.03566 [M-e]<sup>-</sup>, 79.05454 [M-e]<sup>-</sup>, 69.07040 [M-e]<sup>-</sup>, 81.07020 [M-e]<sup>-</sup>, 93.07030 [M-e]<sup>-</sup>, 107.08546 [M-e]<sup>-</sup>, 110.08533 [M-e]<sup>-</sup>, 121.10092 [M-e]<sup>-</sup>, 135.11623 [M-e]<sup>-</sup>, 135.08011 [M-e]<sup>-</sup>, 165.03753 [M-e]<sup>-</sup>, 178.06445 [M-e]<sup>-</sup>, 186.08020 [M-e]<sup>-</sup>, 196.07501 [M-e]<sup>-</sup>, 223.06126 [M-e]<sup>-</sup>, 224.12935 [M-e]<sup>-</sup>, 225.07439 [M-e]<sup>-</sup>, 227.12675 [M-e]<sup>-</sup>, 227.14247 [M-e]<sup>-</sup>, 227.16357 [M-e]<sup>-</sup>, 227.17461 [M-e]<sup>-</sup>, 228.14911 [M-e]<sup>-</sup>, 228.15863 [M-e]<sup>-</sup>, 228.17955 [M-e]<sup>-</sup>, 228.23122 [M-e]<sup>-</sup>.

**(c) MS/MS - Library matching(mzCloud):** The plot shows Intensity [counts] (10<sup>3</sup>) versus m/z. The base peak is at m/z 224.06979 [M+H]<sup>+</sup>. Other labeled peaks include 59.04936, 60.04075, 67.05467, 70.05464, 83.07020, 93.07030, 95.03566, 107.08546, 109.10112, 110.08533, 121.10092, 123.08042, 135.11623, 135.08011, 156.09053, 165.05451, 165.05705, 165.06421, 165.08705, 165.09020, 165.09402, 165.09444, 165.09502, 165.09552, 165.09621, 165.09705, 165.09717, 165.09728, 165.09736, 165.09745, 165.09756, 165.09766, 165.09771, 165.09781, 165.09791, 165.09808, 165.09818, 165.09828, 165.09838, 165.09848, 165.09858, 165.09868, 165.09878, 165.09888, 165.09898, 165.09908, 165.09918, 165.09928, 165.09938, 165.09948, 165.09958, 165.09968, 165.09978, 165.09988, 165.09998, 166.07501, 166.07561, 166.07621, 166.07681, 166.07741, 166.07801, 166.07861, 166.07921, 166.07981, 166.08041, 166.08101, 166.08161, 166.08221, 166.08281, 166.08341, 166.08401, 166.08461, 166.08521, 166.08581, 166.08641, 166.08701, 166.08761, 166.08821, 166.08881, 166.08941, 166.08981, 166.09041, 166.09101, 166.09161, 166.09221, 166.09281, 166.09341, 166.09401, 166.09461, 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**Table S1.** On-line SPE & LC parameters

Dionex Ultimate 3000-Q						
Instrument	LC parameters			On-line SPE parameters		
Column	CORTECS T3 (100 × 2.1mm, 1.6 µm)			Hypersil GOLD aQ (20 × 2.1 mm, 12 µm)		
Mobile phase	A: Water (0.1% Formic acid, 5mM Ammonium formate) B: Methanol (0.1% Formic acid, 5mM Ammonium formate)					
Pump	Pump2 (HPG-3400RS)			Pump 1 (LPG-3400SD)		
Gradient	Retention (min)	%B	Flow (mL/min)	Retention (min)	%B	Flow (mL/min)
	0	5	0.2	0	2	1.0
	1.1	5	0.2	1.0	2	1.0
	5.0	70	0.2	1.1	2	0.05
	7.0	70	0.2	27.1	2	0.05
	22.0	100	0.2	28.0	2	1.0
	27.0	100	0.2	32.0	2	1.0
	28.0	5	0.2			
	32.0	5	0.2			
Column temperature	40 °C			Injection volume	1000 µL	
				Purification	2% MeOH	

**Table S2.** QA/QC results for carbamazepine compound

Compound	Formular	Precursor ion (Da)	Retention time (min)	Adduct	$r^2$	LOQ (ng/L)	Accuracy (n=7)	Precision (n=7)
Carbamazepine	C15H12N2O	237.10224	8.97	M+H	0.9993	40.6	100.7	2.5

**Table S3.** Information of the surveyed WWTPs

WWTP	River	Operation capacity (m <sup>3</sup> /day)	Treatment process	Effluent disinfection
Jeonju wastewater treatment plant (WM1)		403,000	CNR, CSBR	Cl, UV
Wanju industrial complex wastewater treatment plant (WM2)	Mangyeong	32,000	MLE	Cl, UV
Iksan wastewater treatment plant (WM3)		100,000	MLE	UV
Jeongeup wastewater treatment plant (WD1)	Dongjin	58,600	AO	Cl, UV

CNR: Comlete nitrification reactor, CSBR: Cyclic sequencing batch reactor, MLE: Modified Ludzack-Ettinger process, AO: Anaerobic oxic process, Cl: Chlorination, UV: Ultraviolet disinfection