

Supplementary Data

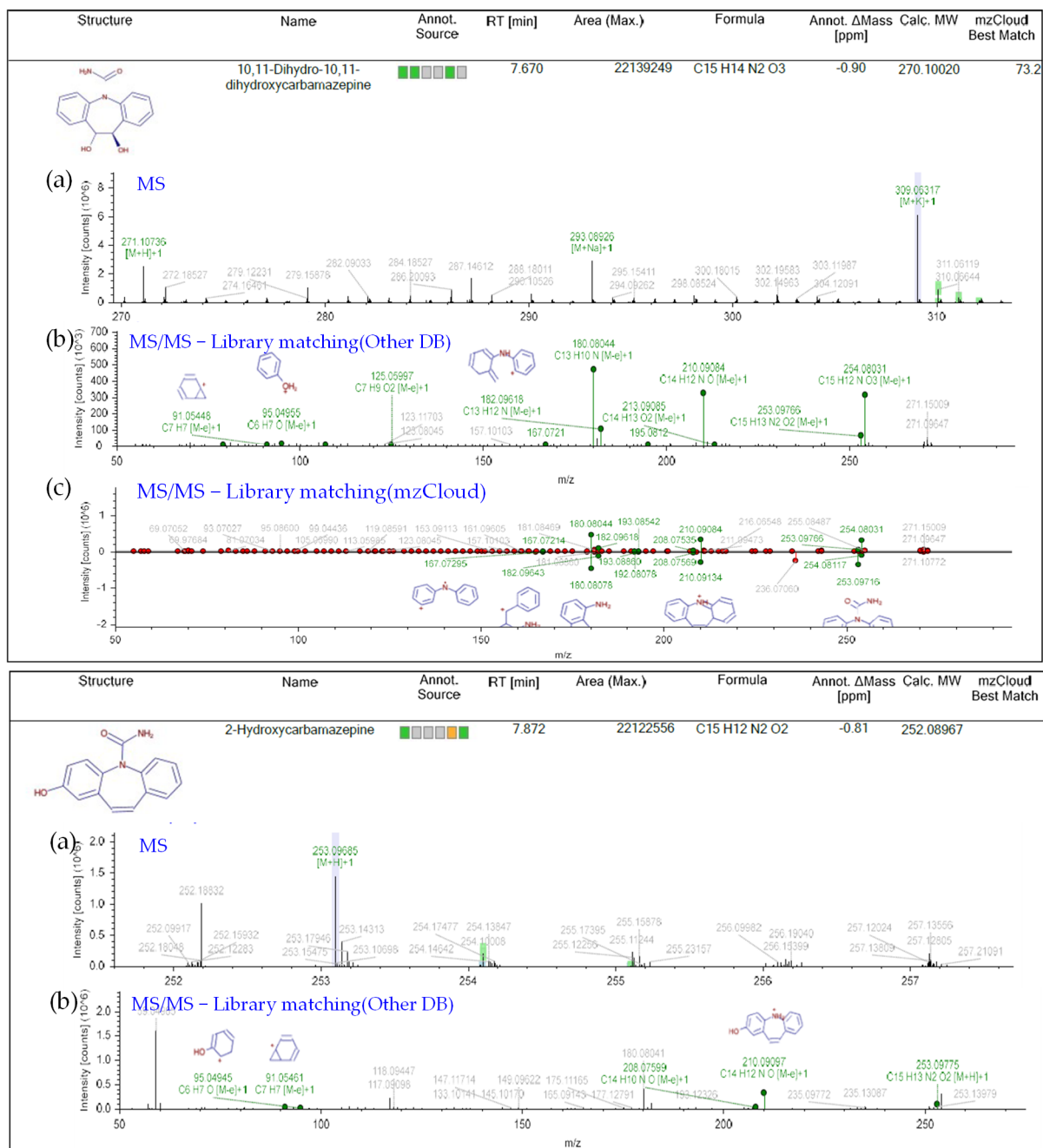
Non-Targeted Screening and Identification of the Transformation Pathway of Carbamazepine in the Saemangeum Watershed, Republic of Korea

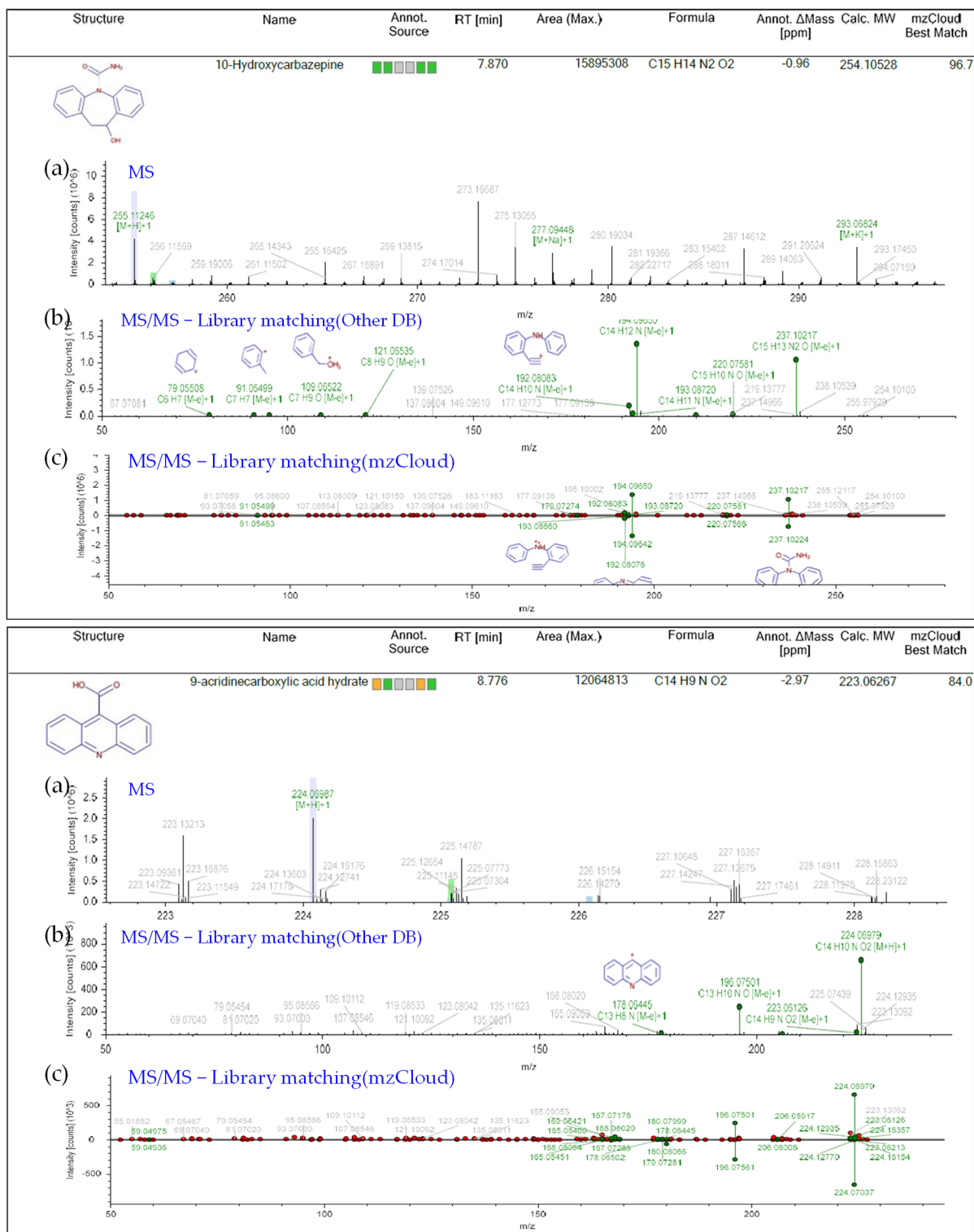
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Figure S1. Overview of compound identification workflow by Compound Discoverer3.3 showing the Level 2 identification of CBZ TPs in sample as an example (a) MS spectrum (b) Level 2b: MS2 spectrum matching – Other DB (c) Level 2a: MS2 spectrum matching–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





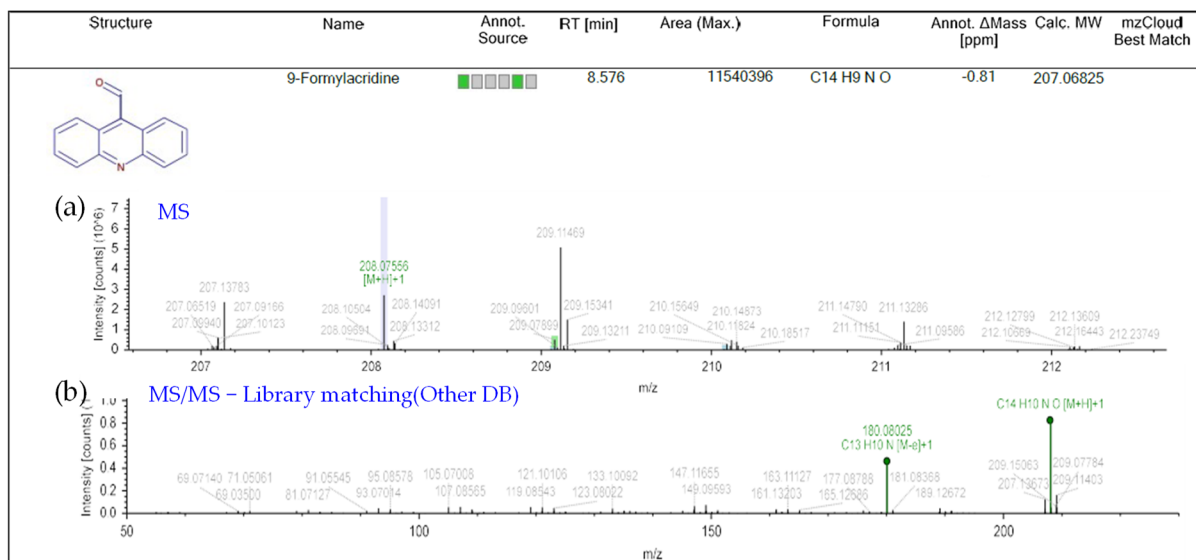


Table S1. On-line SPE & LC parameters

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	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 (m3/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: Complete nitrification reactor, CSBR: Cyclic sequencing batch reactor, MLE: Modified Ludzack-Ettinger process, AO: Anaerobic oxic process, Cl: Chlorination, UV: Ultraviolet disinfection