SUPPORTING INFORMATION

Distinguishing Between Isobaric Ions Using Microdroplet Hydrogen-Deuterium Exchange Mass Spectrometry

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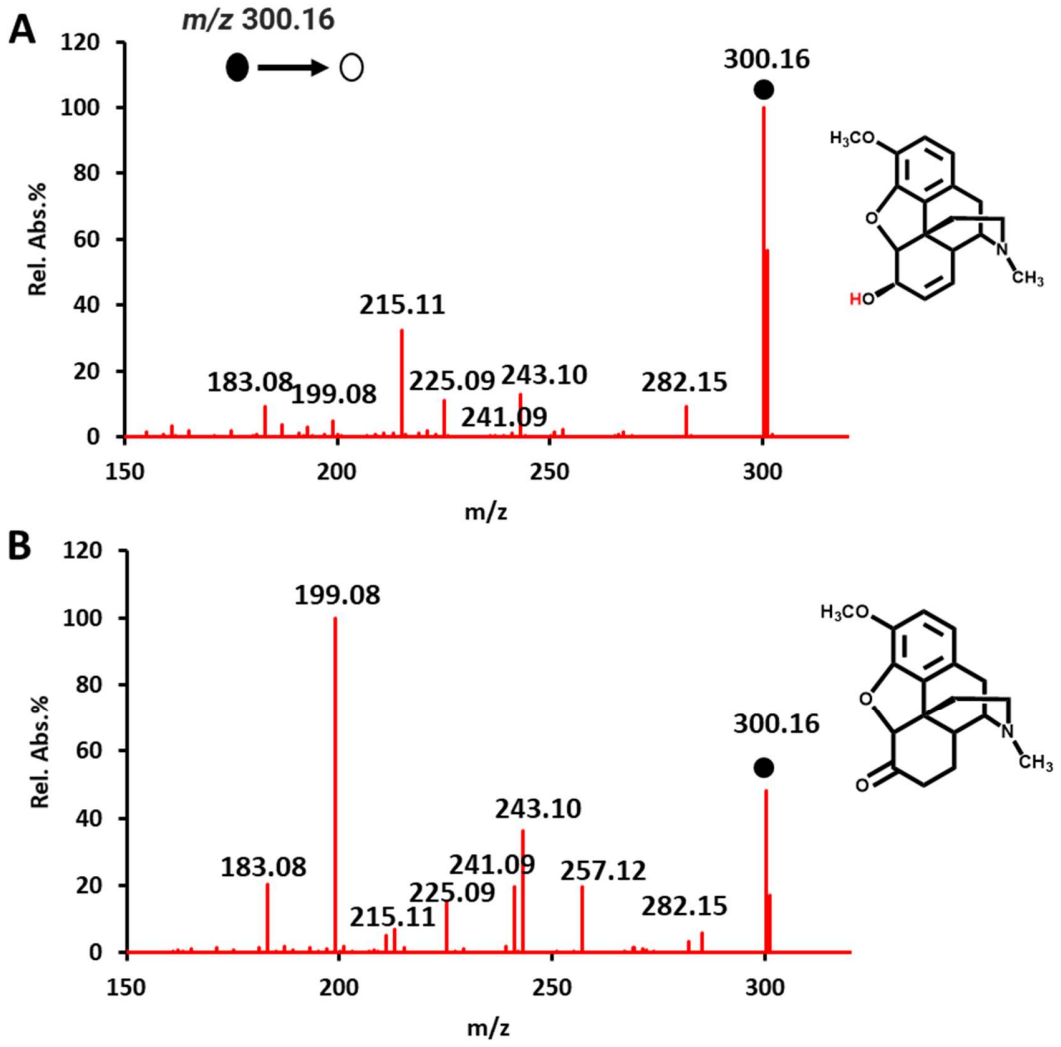

Figure S1. CID-MS/MS spectra of (A) codeine and (B) hydrocodone. The black dot indicates the precursor ion.

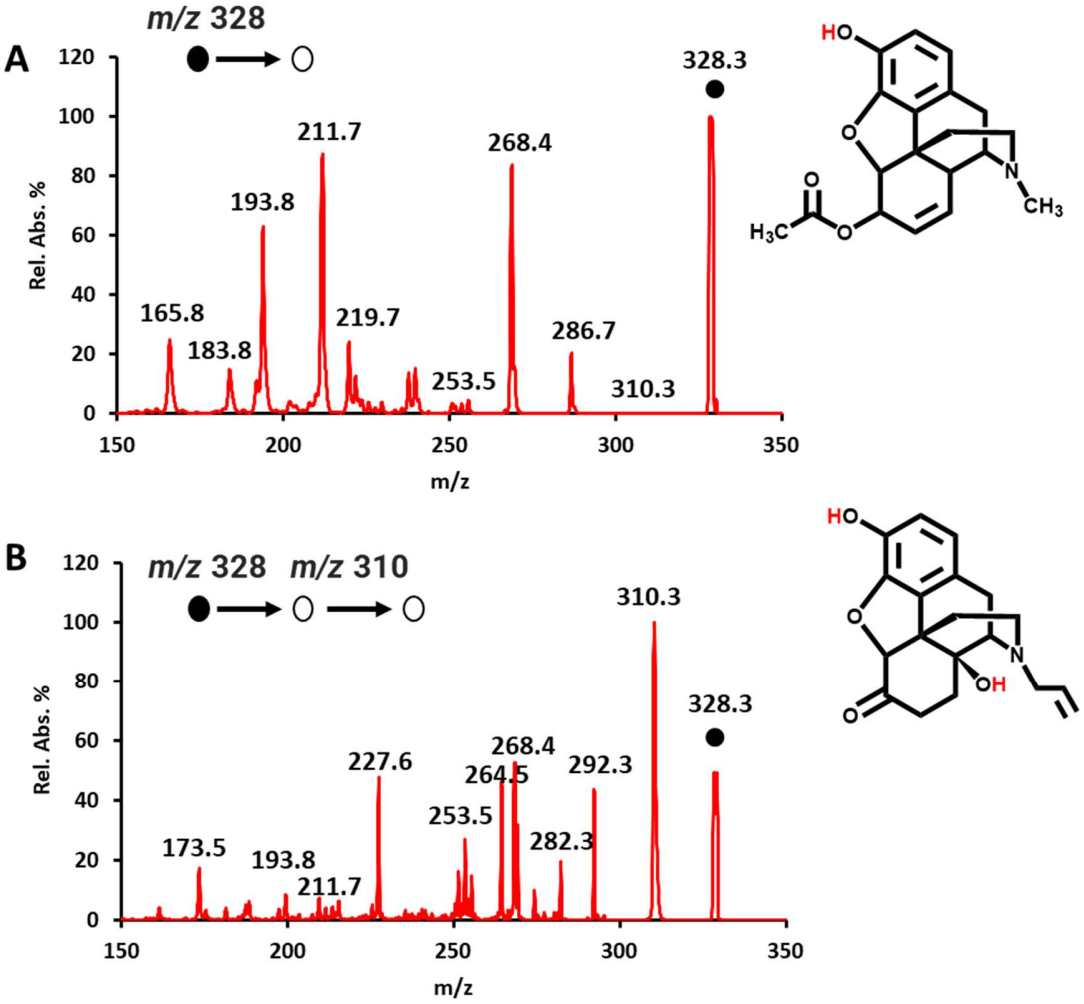

Figure S2. CID-MS/MS spectra for (A) 6-acetyl morphine and CID-MS3 experiment for (B) naloxone. The black dot indicates the precursor ion.

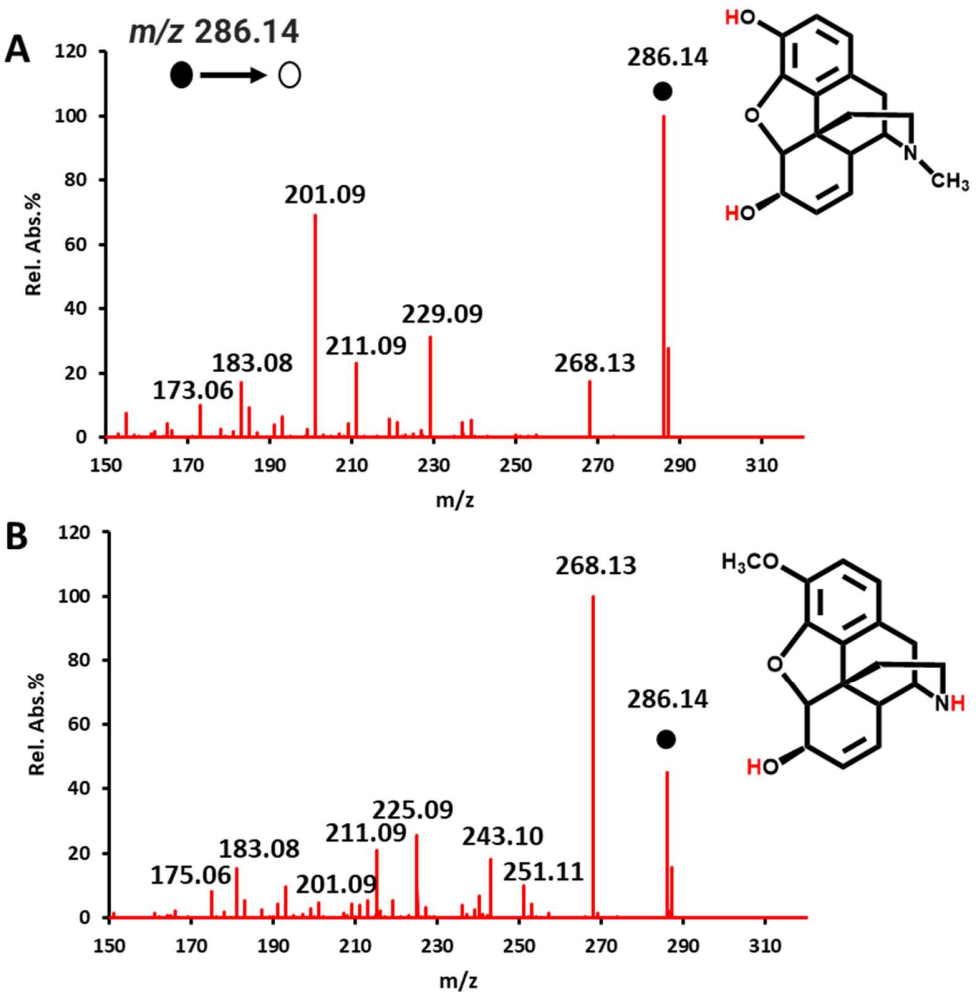

Figure S3. CID-MS/MS spectra of (A) morphine and (B) norcodeine. The black dot indicates the precursor ion.

Table S1. Isobaric ions that were frequently detected in saliva or serum and successfully distinguished by HDX-CPSI-MS.

No	Exact *m/z*	Adduct Ions	Formulae	Metabolites	Number of Exchangeable proton sites	Base peaks
1	118.0862	$[M+H]^+$	$C_5H_{11}NO_2$	Betaine	1	D_0
				5-Aminopentanoic acid	3	D_1
				Valine	3	D_0
2	141.0789	$[M+K]^+$	$C_5H_{14}N_2$	Cadaverine	4	D_2
				N-methyl putrescine	3	D_2
3	146.0459	$[M-H]^-$	$C_5H_9NO_4$	Glutamate	3	D2
				O-acetyl serine	2	D_0
				N-acetyl serine	2	D_1
4	280.0904	$[M+Na]^+$	$C_{10}H_{15}N_3O_5$	5-Methylcytidine	5	D_2
				3-methylcytidine	4	D_2
	280.0920	$[M+H]^+$	$C_8H_{20}NO_6P$	glycerophosphocholine	3	D_2
5	112.0369	$[M+Na]^+$	$C_3H_7NO_2$	Alanine	3	D_1
				Sarcosine	2	D_1
6	126.0520	$[M+Na]^+$	$C_4H_9NO_2$	aminobutyric acid	3	D_1
				N, N-dimethylglycine	1	D_0
7	137.0706	$[M+H]^+$	$C_7H_8N_2O$	2-aminobenzamide	4	D_1
				N-methylnicotinamide	1	D_0

Table S2. The relative intensities in HDX patterns acquired from samples of glucose (G) and inositol (I) at different molar ratios.

m/z	G:I Simulated HDX Patterns			G:I Observed HDX Patterns		
	1:1	3:1	1:3	1:1	3:1	1:3
203.05	46	55	33	41	55	38
204.06	73	82	57	72	78	63
205.07	100	100	91	100	100	95
206.08	95	83	100	87	91	100
207.09	64	49	74	52	51	79
208.10	28	19	35	17	18	40
209.11	4	2	6	5	6	7