SUPPORTING INFORMATION FOR:

Dielectric Barrier Discharge Ionization (DBDI) Enables Rapid Analysis of New Psychoactive Substances with Ion Mobility-Mass Spectrometry

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SUPPORTING TABLES

Table S1. Instrumental parameters for the Agilent 6560 IM-QTOF.

Instrument Region	Instrumental Parameter	Experimental Value
Source Region Plasmion SICRIT DBDI	Polarity	Positive
	Gas Temp	325 °C
	Drying Gas	12 L/min
	Nebulizer	30 psi
	VCap	0 V
	Fragmentor	400 V
	Oct 1 RF Vpp	750 V
High Pressure Funnel	High Pressure Funnel Delta	150 V
	High Pressure Funnel RF	150 V
Trapping Funnel	Trap Funnel Delta	180 V
	Trap Funnel RF	150 V
	Trap Funnel Exit	10 V
	Entrance Grid Delta	10 V
	Entrance Grid Low	97 V
	Entrance Grid High	107 V
	Trap Entrance	91 V
	Trap Exit	90 V
	Trap Fill Time	5000 µs
	Trap Release Time	150 µs
	Trap Exit Grid 1 Delta	4 V
	Trap Exit Grid 1 Low	85.7 V
	Trap Exit Grid 1 High	89.7 V
	Trap Exit Grid 2 Delta	8.5 V
	Trap Exit Grid 2 Low	84.9 V
	Trap Exit Grid 2 High	93.4 V
Drift Tube	Drift Tube Entrance Voltage	1700 V
	Drift Tube Exit Voltage	250 V
	Drift Tube Field Strength	18.6 V/cm

Table S2. Instrumental parameters for the MOBILion MOBIE SLIM & Agilent 6546 QTOF.

Instrument Region	Instrumental Parameter	Experimental Value
Ionization Source Plasmion SICRIT DBDI	Polarity	Positive
	Gas Temp	325 °C
	Drying Gas	12 L/min
	Nebulizer	30 psi
	VCap	0 V
	Fragmentor	400 V
	Oct 1 RF Vpp	750 V
SLIM Conditions	Funnel In	165 V
	Funnel Out	100 V
	Funnel Conductance Limit (CL)	95 V
	SLIM Bias	90 V
	SLIM Mode	HRIM (13 m)
	SLIM Wave Shape	Sine
	Fill Time	100 ms
	Trap Time	0.3 ms
	Release Time	3.2 ms
	IMS Frame Length	750 ms
	Fill TW Frequency	15 kHz
	Fill TW Amplitude	5 V_{pp}
	Release TW Frequency	15 kHz
	Release TW Amplitude	30 V_{pp}
	Separation TW Frequency	25 kHz
	Separation TW Speed	225 m/s
	Separation TW Amplitude	30 V_{pp}
	SLIM Exit CL	50 V
	Quad Bias	45 V
	Quad Pressure (Rough Vac)	2.5 Torr
	SLIM RF Amplitude	220 V
	SLIM RF Frequency	1200 kHz
	SLIM Board Spacing	3 mm

Table S3. $^{DT}CCS_{N2}$ measured for synthetic cannabinoids, benzodiazepines, and nitazenes using the single-field method with Agilent Tune Mix calibrant ions.

Compound	Formula	$[M+H]^+$ *m/z*	$^{DT}CCS_{N2}$ (Å^2)
JWH 018 4-hydroxyindole	$C_{24}H_{23}NO_2$	358.182	191.5 ± 0.1
JWH 018 N-(5-hydroxypentyl)			189.9 ± 0.1
JWH 018 6-hydroxyindole			190.0 ± 0.1
JWH 250 N-(4-hydroxypentyl)	$C_{22}H_{25}NO_3$	352.194	188.7 ± 0.1
JWH 250 N-(5-hydroxypentyl)			189.1 ± 0.1
JWH 250 5-hydroxyindole			193.0 ± 0.1
MDA-19 N-(4-hydroxyhexyl)	$C_{21}H_{23}N_3O_3$	366.181	198.0 ± 0.1
MDA-19 N-(5-hydroxyhexyl)			190.3 ± 0.1
4-cyano CUMYL-BUTINACA			189.6 ± 0.2
APP-BUTINACA phenylpropanoic acid			189.9 ± 0.1
Oxazepam	$C_{15}H_{11}ClN_2O_2$	287.062	164.6 ± 0.1
Demoxepam			170.6 ± 0.8
N-Desmethylclobazam			178.0 ± 0.1
Nimetazepam	$C_{16}H_{13}N_3O_3$	296.108	172.7 ± 0.1
(±)-3-methyl Nitrazepam			171.5 ± 0.1
4'-chloro Deschloroalprazolam	$C_{17}H_{13}ClN_4$	309.094	178.7 ± 0.1
Meclonazepam	$C_{16}H_{12}ClN_3O_3$	330.068	175.5 ± 0.1
(±)-Meclonazepam			175.5 ± 0.1
Nitazene	$C_{20}H_{24}N_4O_2$	353.199	189.2 ± 0.1
4'-hydroxy Nitazene	$C_{20}H_{24}N_4O_3$	369.192	194.2 ± 0.2
N-desethyl Etonitazene			198.6 ± 0.1
N-Piperidinyl 4'-hydroxy Nitazene	$C_{21}H_{24}N_4O_3$	381.191	199.0 ± 0.1
N-Pyrrolidino Metonitazene			197.7 ± 0.6
N-desethyl Protonitazene	$C_{21}H_{26}N_4O_3$	383.210	204.9 ± 0.1
Metonitazene			198.6 ± 0.1
Methylenedioxynitazene	$C_{21}H_{24}N_4O_4$	397.188	199.7 ± 0.1
Ethyleneoxynitazene	$C_{21}H_{26}N_4O_2$	395.209	202.1 ± 0.1
N-Pyrrolidino Etonitazene			205.2 ± 0.1
N-Piperidinyl Metonitazene			205.4 ± 0.7
Protonitazene	$C_{23}H_{30}N_4O_3$	411.241	211.4 ± 0.1
Isotonitazene			211.0 ± 0.1
Ethylene Etonitazene			204.5 ± 0.1
Protodesnitazene	$C_{23}H_{31}N_3O$	366.256	198.6 ± 0.1
Isotodesnitazene			198.3 ± 0.1
5-methyl Etodesnitazene			198.1 ± 0.1

SUPPORTING FIGURES

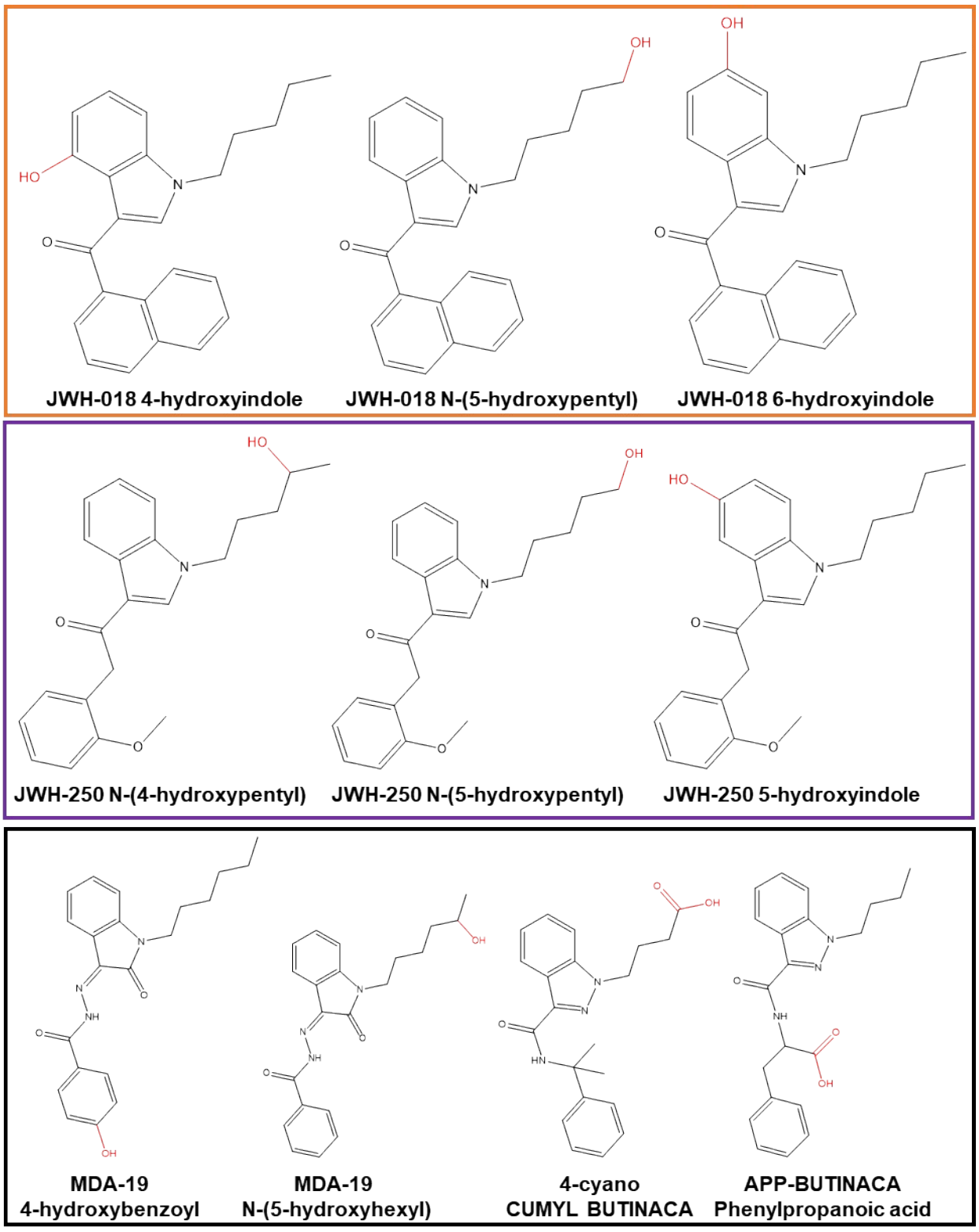

Figure S1. Chemical structures of surveyed synthetic cannabinoids.

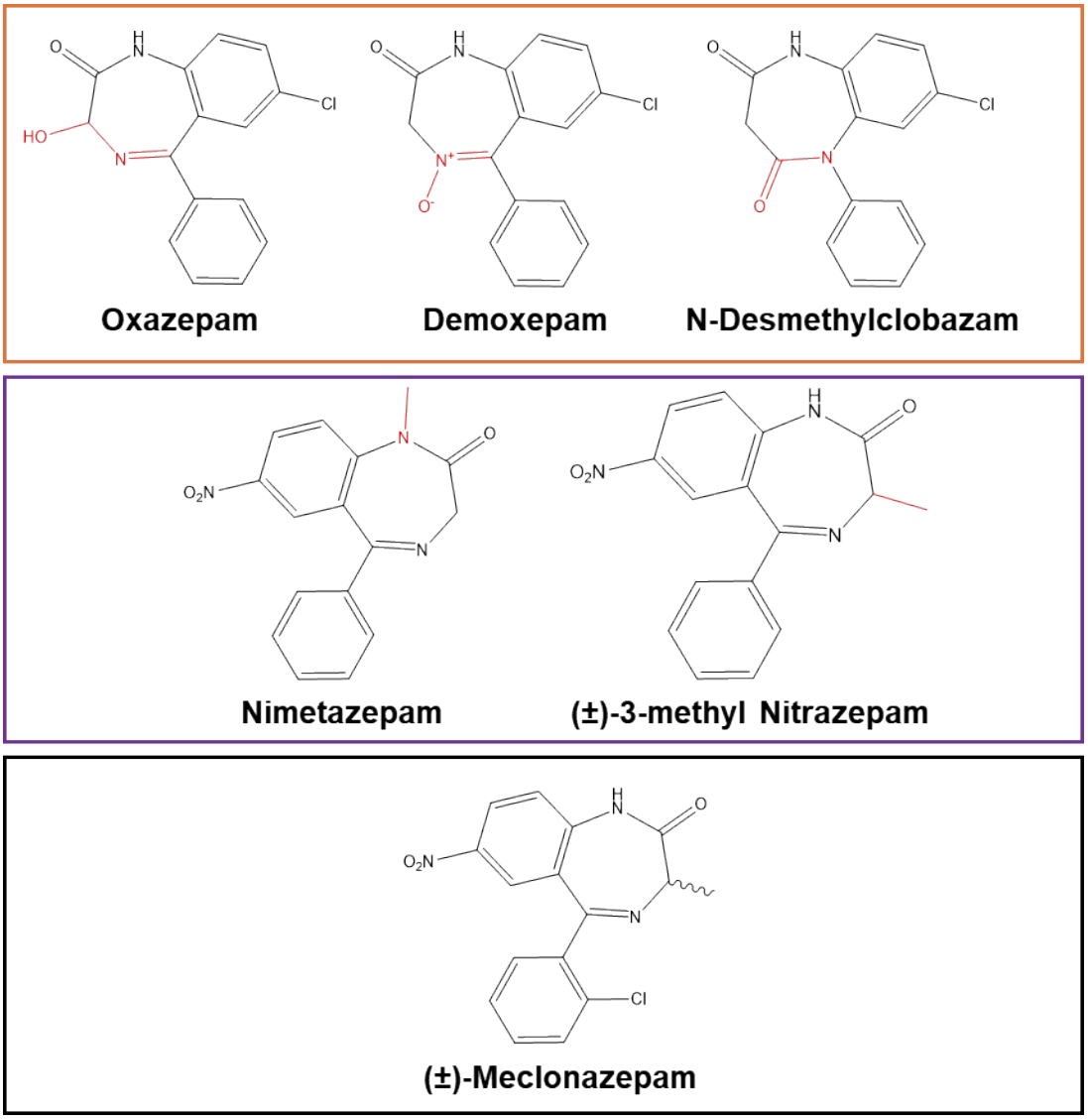

Figure S2. Chemical structures of surveyed benzodiazepines.

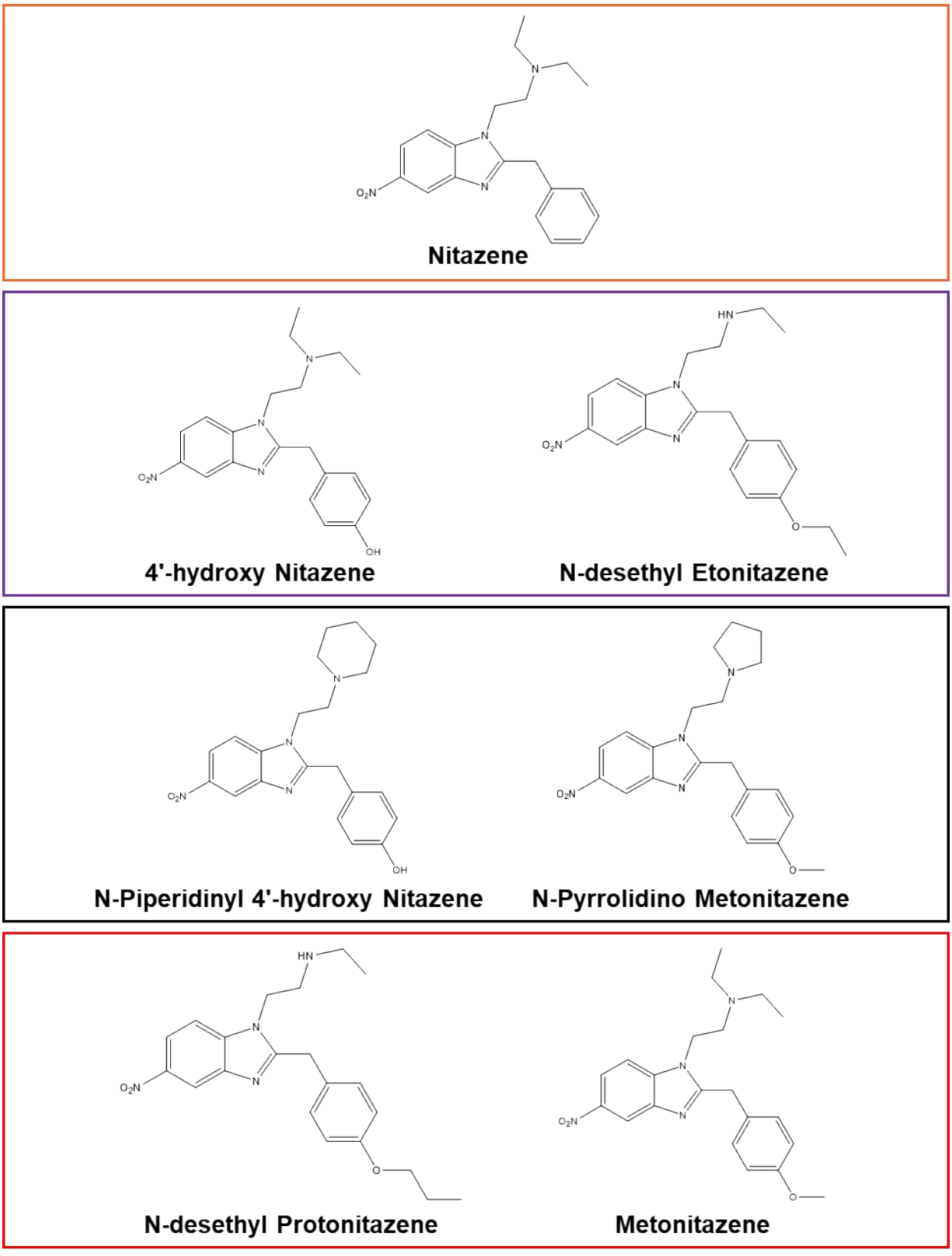

Figure S3. Chemical structures of surveyed nitazenes (continued on next page).

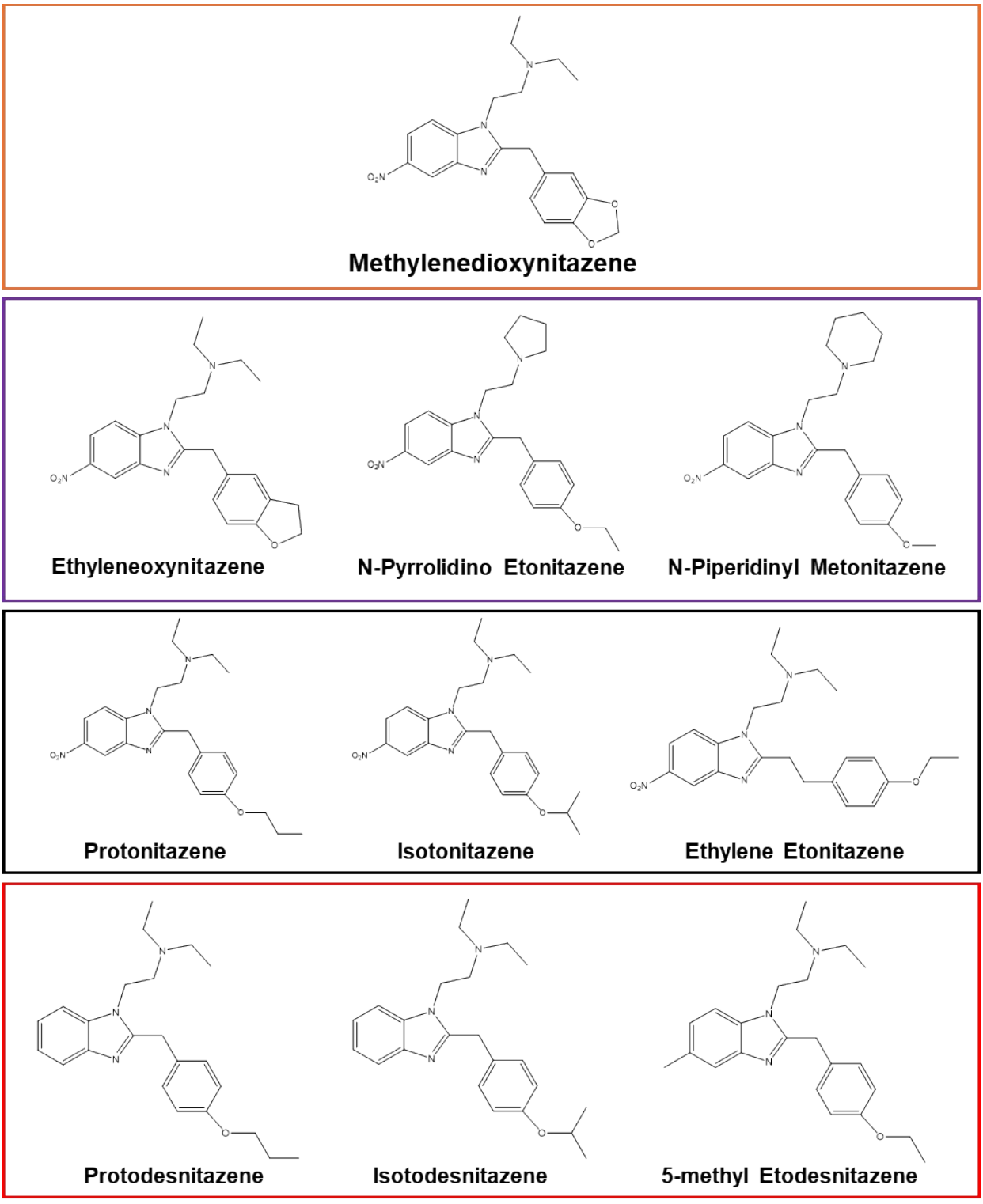

Figure S3 (continued). Chemical structures of surveyed nitazenes.

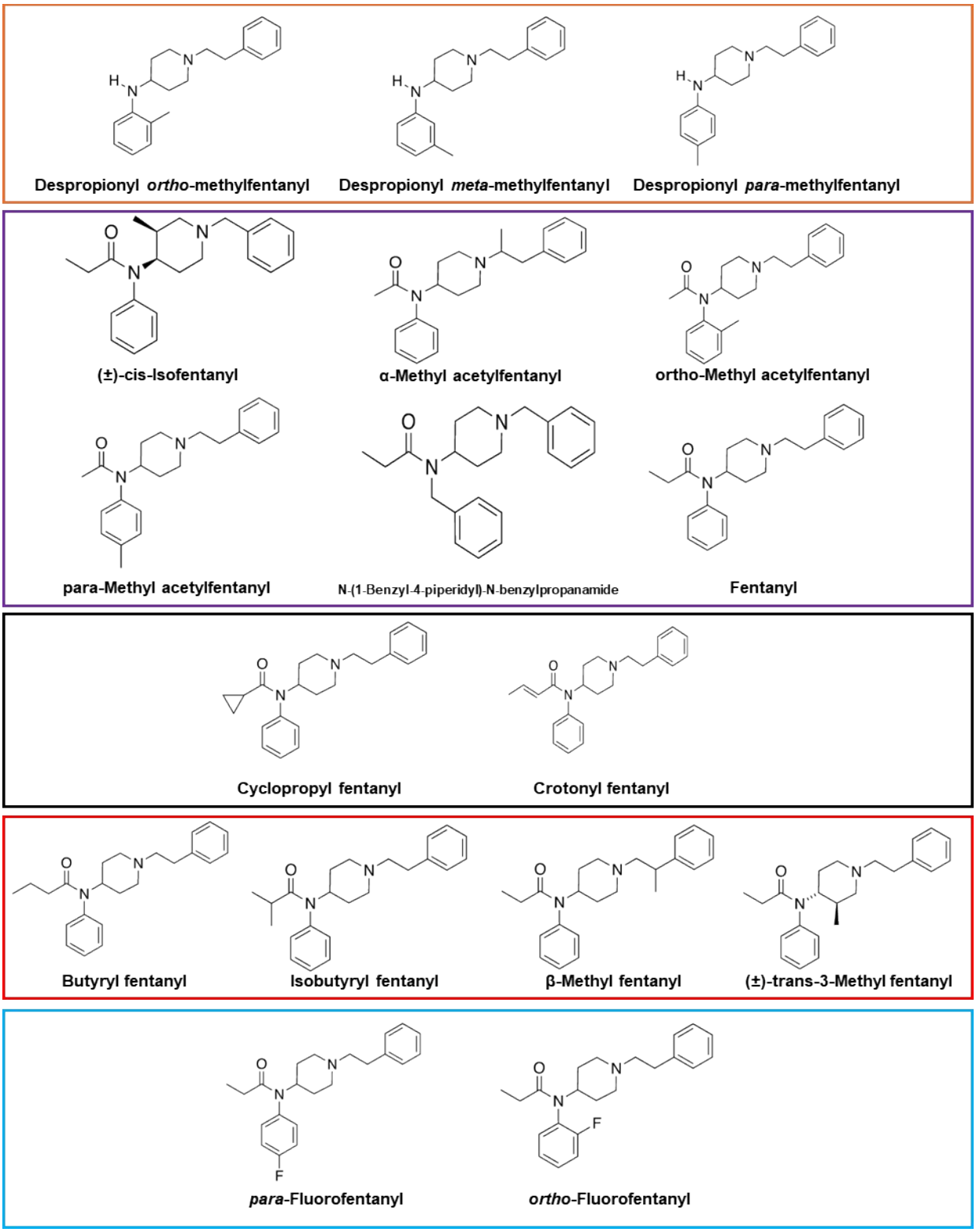

Figure S4. Chemical structures of surveyed fentanyl analogues.

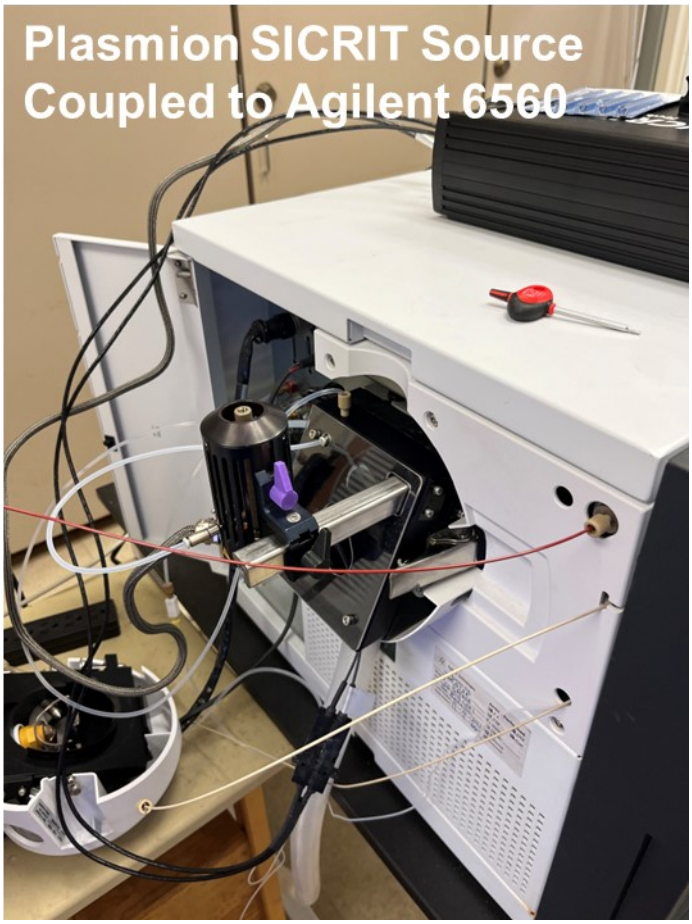

Figure S5. Image of the Plasmion SICRIT© source coupled to the front of an Agilent 6560 IM-QTOF.

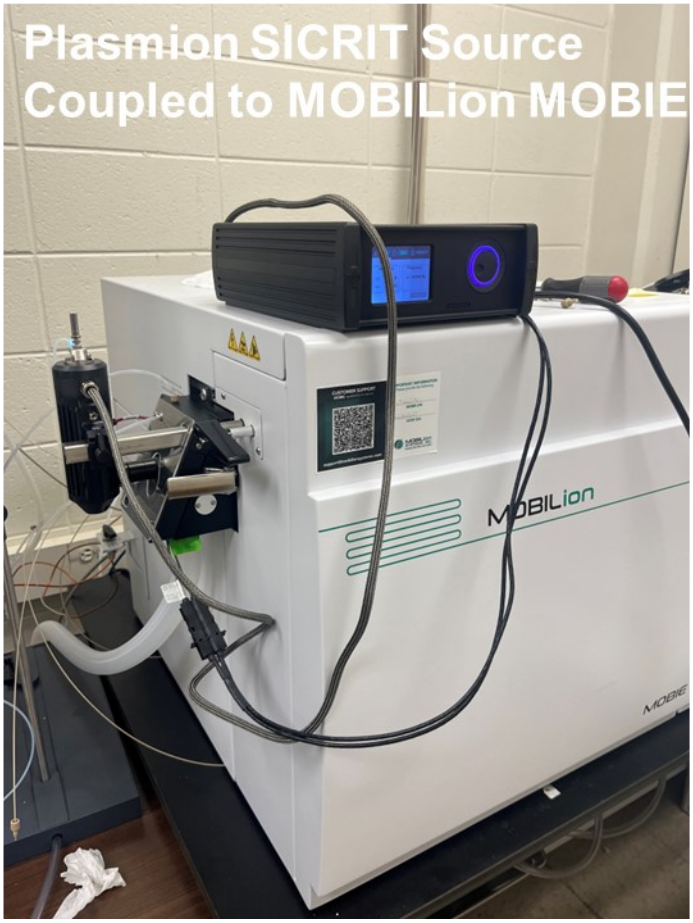

Figure S6. Image of the Plasmion SICRIT© source coupled to the front of a MOBILion MOBIE SLIM HRIM system (on an Agilent 6546 QTOF).

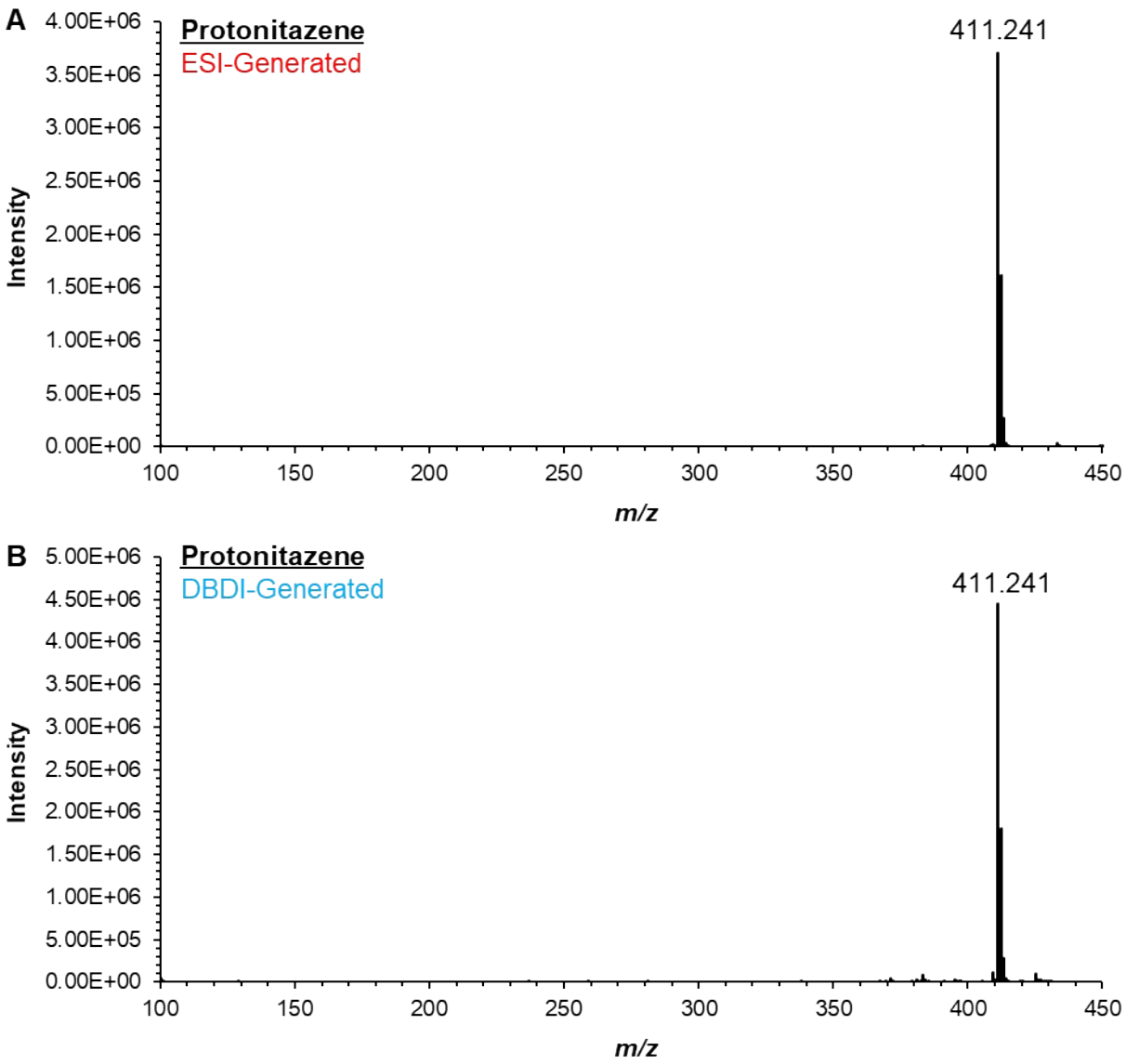

Figure S7. Comparative mass spectra (corresponding to the mobility data in Figure 3 of the main text) of protonitazene generated (A) ESI, and (B) DBDI, showing no major fragmentation for either ionization source.

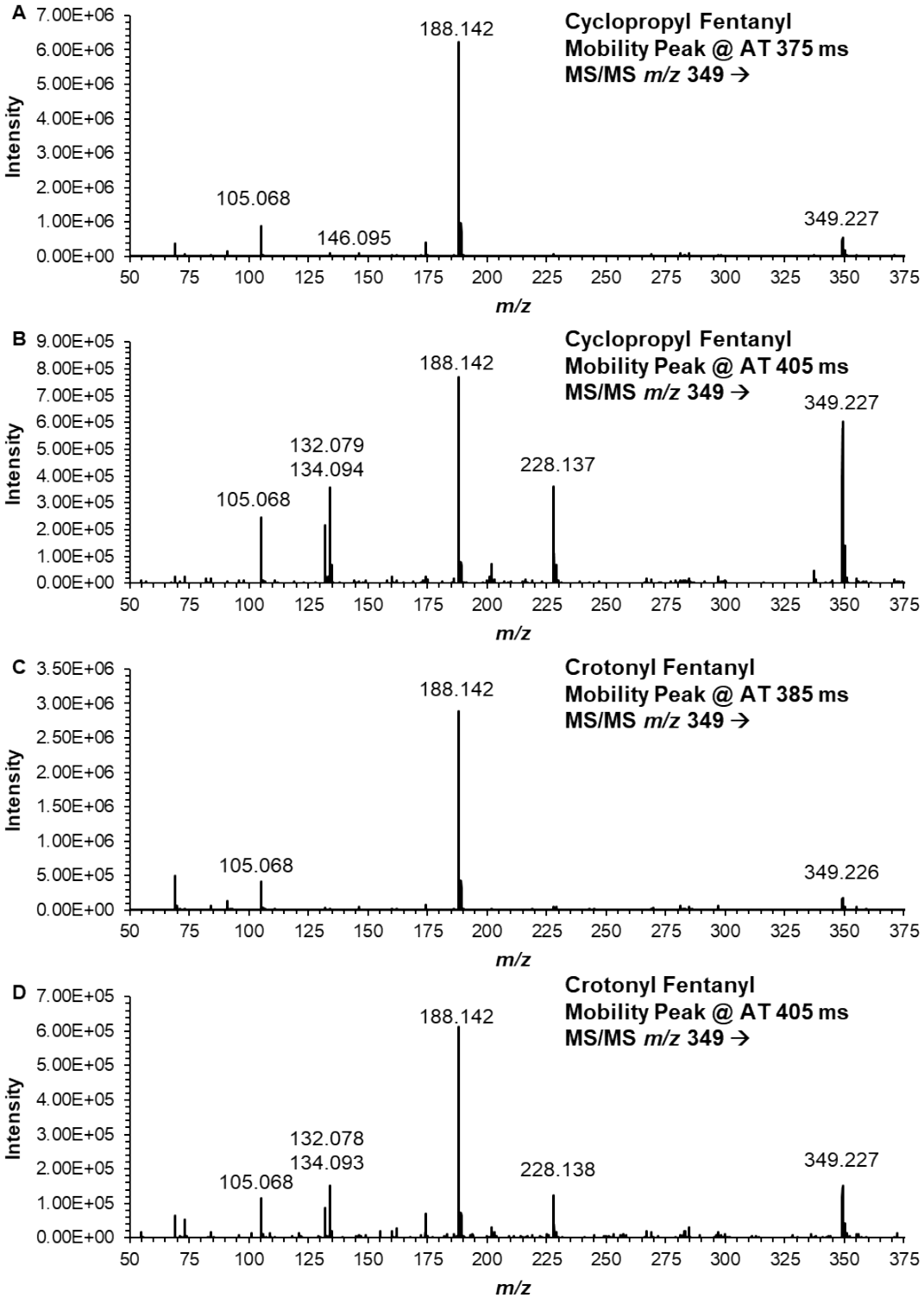

Figure S8. Comparison of MS/MS spectra obtained for the different mobility peaks of cyclopropyl and crotonyl fentanyl: (A) cyclopropyl fentanyl (*m/z* 349) MS/MS spectrum of higher mobility species (AT 375 ms); (B) cyclopropyl fentanyl (*m/z* 349) MS/MS spectrum of lower mobility species (AT 405 ms); (C) crotonyl fentanyl (*m/z* 349) MS/MS spectrum of higher mobility species (AT 385 ms); and (D) crotonyl fentanyl (*m/z* 349) MS/MS spectrum of lower mobility species (AT 405 ms).