

SUPPLEMENTAL INFORMATION

**Automated Flow Injection Method for the High Precision Determination
of Drift Tube Ion Mobility Collision Cross Sections**

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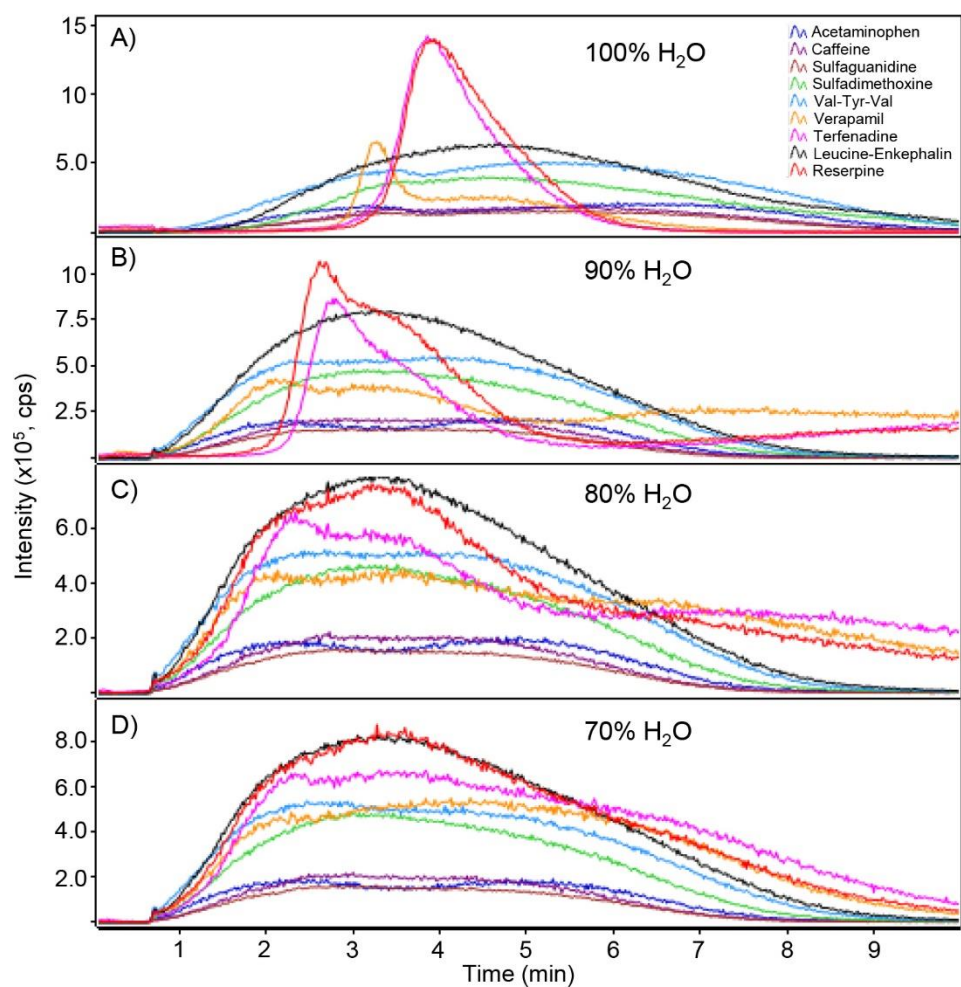


Figure S1. Extracted ion chromatograms illustrating the effects of solvent composition on FIA analyte elution shape. Mobile phase A and B are water and acetonitrile, respectively. A) 100% H₂O. B) 90% H₂O. C) 80% H₂O. D) 70% H₂O.

Table S1. Concentrations and commercial vendors of analyte.

Analyte	Conc. ($\mu\text{g/mL}$)	Vendors
Acetaminophen	10	Sigma-Aldrich
Caffeine	1.5	Sigma-Aldrich
Sulfaguanidine	5	Sigma-Aldrich
Sulfadimethoxine	1	Fluka
Val-Tyr-Val	2.5	Sigma
Verapamil	0.2	Sigma
Terfenadine	0.2	Sigma
Leucine-Enkephalin	2.5	Sigma
Reserpine	0.6	Sigma

The analytes were dissolved in 7:3 (water:acetonitrile) at the above concentrations. This mixture can also be purchased as a commercial sample (Part No. 186006963, Waters Corporation)

Table S2. Experiment time segment information for drift tube potentials

Time Segment ^a	Advanced Parameters			
	DT Ent. V. ^b	DT Exit V. ^c	R. Funnel Ent. ^d	R.Funnel Exit ^e
1.0	1074	224	217.5	217.5
1.5	1174	224	217.5	217.5
2.0	1274	224	217.5	217.5
2.5	1374	224	217.5	217.5
3.0	1474	224	217.5	217.5
3.5	1574	224	217.5	217.5
4.0	1674	224	217.5	217.5

^aExperimental time segment.

^bDrift Tube Entrance potential.

^cDrift Tube Exit potential.

^dRear Funnel Entrance potential.

^eRear Funnel Exit potential.

When using the “CCS Calculator (Multi-Field)” of IM-MS Browser (Agilent Technologies) to process the data, make sure that the “CCS Plot (Multi-Field)” captures all seven points of the method, otherwise the CCS will not be reproducible.

Table S3. Experimental LC flow rate timing.

Binary Pump	
Time	Flow [mL/min]
0.00	0.800
0.18	0.800
0.19	0.030
Stoptime = 4.30 min	
Posttime = 1.00 min	

Table S4. Experimental Source Conditions and Acquisition parameters for the measurements herein

ESI Source Conditions			IM-QTOF Acquisition Parameters		
Setting	value	units	Setting	value	units
Gas Temp	300	°C	Min Range	100	m/z
Drying Gas	8	l/min	Max Range	1000	m/z
Nebulizer	35	psig	Frame Rate	0.9	Tran./Frame
Sheath Gas Temp	350	°C	Max Drift Time	70	ms
Vcap	3500	V	TOF Transient		
Nozzle Voltage	800	V	Rate	751	Transients
Fragmentor	360	V	Trap Fill Time	20000	μs
Oct 1 RF Vpp	750	V	Trap Release Time	180	μs

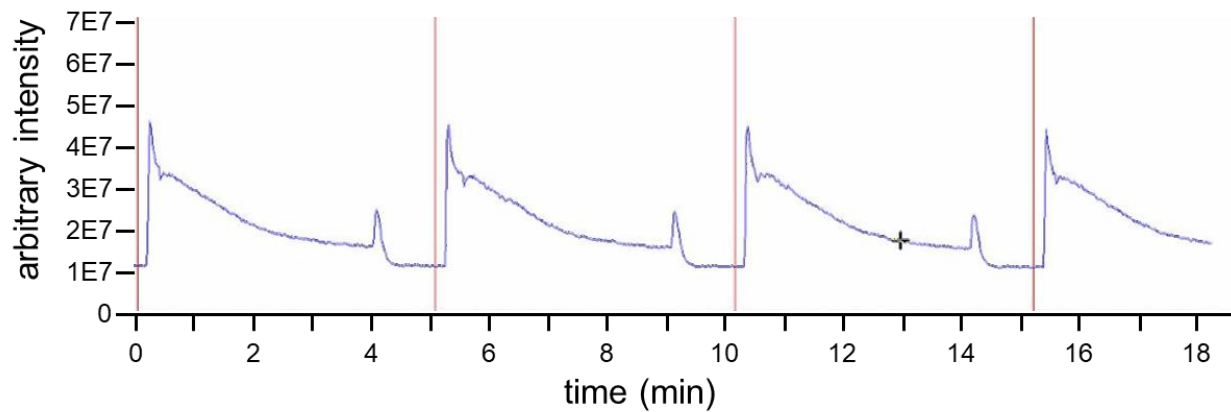


Figure S2 – A composite total ion chromatogram of three contiguous sample injections illustrating the stacking of multiple CCS measurements in the FIA-DTIM-MS method.