

Electronic Supplementary Information For:

**A Low-Cost, Simplified Platform of Interchangeable, Ambient Ionization
Sources for Rapid, Forensic Evidence Screening on Portable Mass
Spectrometric Instrumentation**

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<u>Table of Contents</u>	<u>Page</u>
FLIR AI-MS 1.2 portable mass spectrometer	S-3
Factory-built ESI/DESI combination source	S-4
Part list and estimated cost for modular ionization sources	S-5
Estimated cost for swab and cone consumables	S-7
Photos of authentic evidence analyzed via modular ionization sources	S-8
Alternate and internal views of the modular sources	S-9
Absolute intensity obtained in reported MS spectra	S-11

FLIR AI-MS 1.2 Portable Mass Spectrometer

The FLIR AI-MS 1.2 portable MS system is a ruggedized CIT-based instrument capable of MS/MS chemical identification. The miniaturized vacuum system on-board the AI-MS 1.2 allows sampling of externally-generated ions in both positive and negative ion modes via a capillary-based atmospheric pressure inlet. All AC/DC voltages needed for instrument operation and modular ambient ionization sources described in this work are built in, as well as an on-board syringe pump for solvent delivery when necessary (i.e. ESI, DESI, STSI) and a cartridge-based helium supply for the CIT damping gas. The instrument is flexible in regards to input voltage, allowing the use of 110/220 VAC or 24V DAC service, and can be easily operated by a small, gas-powered generator. The size (24" x 20" x 15", L x W x H), weight (44 kg) and ruggedness of this instrument makes it an amenable platform for field-based applications like crime scene investigation, law enforcement and environmental monitoring.

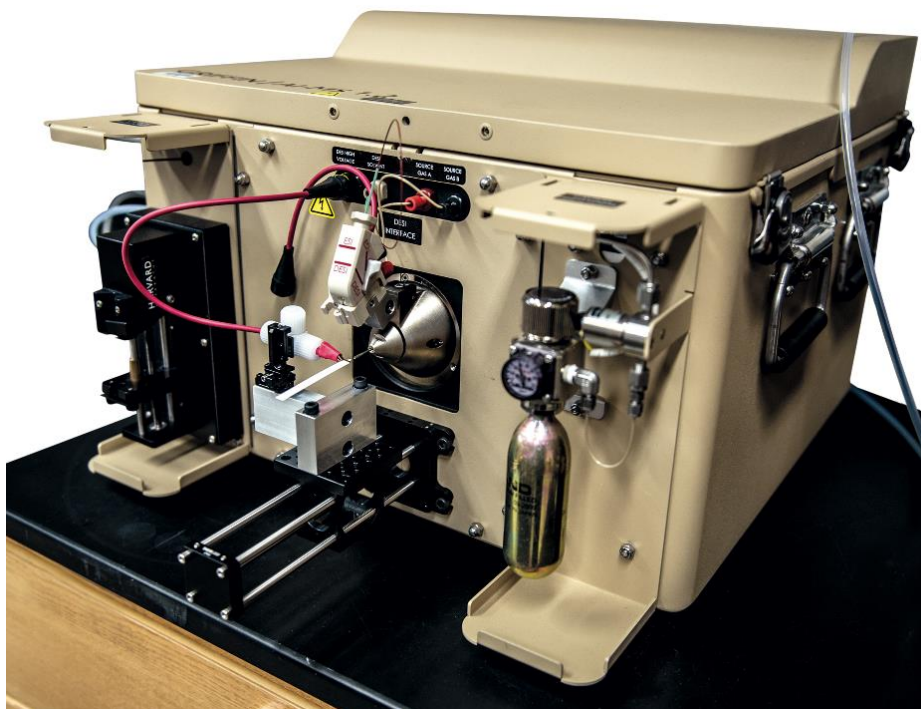


Figure S-1. FLIR Systems AI-MS 1.2 portable, cylindrical ion trap (CIT) mass spectrometer ruggedized for field usage. All required consumables for the modular ambient ionization sources, including flowed solvents and voltage, are on-board in shown form factor. Photo courtesy of Illinois State University

Factory-Built ESI/DESI Combination Source

The FLIR Systems AI-MS 1.2 includes a removable, factory-built combination source capable of both ESI-MS and DESI-MS (Figure S-2). This position-stationary source is mounted to fix both the DESI spray angle (55°) and sprayer tip-to-surface distance. The DESI sprayer is held in a hemispherical enclosure (Figure S-3), and once relatively-flat samples (such as glass slides, as seen in Figure S-4) are placed at the enclosure opening, they undergo desorption/ionization. As seen in Figure S-5, swabs can also be investigated with the source, allowing more geometrically complex samples to be screening via surface transfer experiments.



Figure S-2. Combination ESI/DESI source included with the FLIR AI-MS 1.2. ESI-MS is useful when examining extracts and dilute solution, while DESI-MS has proven is useful for the direct analysis of surfaces of simple geometry.



Figure S-3. Bottom-up view of the ESI/DESI emitter in relation to the inlet capillary of the AI-MS 1.2. The hemispherical enclosure allows placement of flat materials for sampling.



Figure S-4. DESI-MS analysis depicted from printed Teflon well slides (Omni Slides, Prosolia, Inc., Indianapolis, IN)



Figure S-5. DESI-MS analysis depicted directly from foam-based, surface-transfer swabs (Lab-Tips foam swab, Berkshire Corporation, Great Barrington, MA)

Table S-1: Part List and Estimated Cost for Modular Ionization Sources (as of 2/13/2018)

Company	Part Number	Part Description	Price
Rail Mount			Total = \$92.95
Thorlabs	CPVM	Vertical Mounting Plate for 30 mm and 60 mm Cage Systems	\$43.86
Thorlabs	ER6-P4	Cage Assembly Rod, 6" Long, Ø6 mm, 4 Pack	\$32.87
Thorlabs	CP01	Blank 30 mm Cage Plate, 0.35" Thick, 8-32 Tap	\$16.22
PSI			Total = \$462.92 – \$513.92
iPolymer	UC-F-4-HA	Union Cross, 1/4" Tube OD	\$61.08
Newark	82R5350	Toothless Solid Copper Alligator Clip	\$0.53
OptoSigma	123-7127*	Leadscrew Slide, 15 x 15 XYZ Metric	\$300.00 - \$351.00
Thorlabs	C6W	30 mm Cage Cube, Ø6 mm Through Holes	\$63.75
Thorlabs	UBP2	Universal Base Plate, 2.5" x 2.5" x 3/8"	\$36.47
Digi-Key	WM2953CT-ND	Terminal Connector Female, Receptacle (Socket) 18-22 AWG	\$0.57
Digi-Key	WM18267-ND	Terminal Connector Male, Pin (Plug) 18-22 AWG	\$0.52
PCSI			Total = \$151.01
Newark	82R5350	Toothless Solid Copper Alligator Clip	\$0.53
Thorlabs	AI25E8E	Adapter with Internal 1/4"-20 Threads and Internal 8-32 Threads	\$4.90
Thorlabs	RA180	Right-Angle End Clamp for Ø1/2" Posts, 1/4"-20 Stud and 3/16" Hex	\$10.81
Thorlabs	TR3C	Ø1/2" Optical Construction Post, SS, #8 Counterbores	\$16.73
Thorlabs	TR3T	Ø1/2" Optical Construction Post, SS, 8-32 Taps	\$16.73
Thorlabs	C6W	30 mm Cage Cube, Ø6 mm Through Holes	\$63.75
Thorlabs	UBP2	Universal Base Plate, 2.5" x 2.5" x 3/8"	\$36.47
Digi-Key	WM2953CT-ND	Terminal Connector Female, Receptacle (Socket) 18-22 AWG	\$0.57
Digi-Key	WM18267-ND	Terminal Connector Male, Pin (Plug) 18-22 AWG	\$0.52
STSI			Total = \$235.73
Agilent	160-1010-5	Deactivated Fused Silica, 5 m, 0.10 mm, 0.19 mm OD	\$112.00
IDEX	U-112	Stainless Steel Tubing 1/16" OD x .010 ID - 10cm	\$4.94
Newark	82R5350	Toothless Solid Copper Alligator Clip	\$0.53
Thorlabs	RA90	Right-Angle Clamp for Ø1/2" Posts, 3/16" Hex	\$9.76
Thorlabs	TR8	Ø1/2" Optical Post, SS, 8-32 Setscrew, 1/4"-20 Tap, L = 8"	\$8.28
Thorlabs	C6W	30 mm Cage Cube, Ø6 mm Through Holes	\$63.75
Thorlabs	UBP2	Universal Base Plate, 2.5" x 2.5" x 3/8"	\$36.47

APCI			Total = \$380.64
Hamilton	18304	Cleaning Wires for 22, 23, and Larger Gauge Needles	\$11.00
IDEX	U-102	Stainless Steel Tubing 1/16" OD x .020 ID - 10cm	\$4.56
iPolymer	FRT-F-42-HA	Female Run Tee, 1/4" Tube OD	\$47.63
iPolymer	MRT-F-42-HA	Male Run Tee, 1/4" Tube OD	\$47.63
KNF Neuberger	NMP830KNDC	Micro Diaphragm Gas Pump DC 12V, 3.1 L/min	\$146.00
Newark	66K6838	Through Hole Resistor, 100 M Ω , Mini-Mox Series, 7500 V, 1.5 W	\$8.11
Thorlabs	CL3/M	Compact Variable Height Clamp, M6 Tapped	\$5.15
Thorlabs	BA1	Mounting Base, 1" x 3" x 3/8"	\$5.60
Thorlabs	TR1	Ø1/2" Optical Post, SS, 8-32 Setscrew, 1/4"-20 Tap, L = 1"	\$4.74
Thorlabs	C6W	30 mm Cage Cube, Ø6 mm Through Holes	\$63.75
Thorlabs	UBP2	Universal Base Plate, 2.5" x 2.5" x 3/8"	\$36.47
Other			Total = \$112.79
Newark	63H2515	Test Lead Wire, Silicone, 18 AWG, 50 feet (15.2 Meter) Length, Red	\$26.99
McMaster-Carr	8975K213	Multipurpose 6061 Aluminum, 6" x 6" x 3/8"	\$11.22
McMaster-Carr	8975K244	Multipurpose 6061 Aluminum, 6" x 6" x 1"	\$24.58
McMaster-Carr	Various	Various Screws	\$50
Grand Total = \$1436.03 – \$1487.03 (plus S/H)			

*Product was discontinued by Thorlabs. Product TAS-24305L could be used alternatively

Table S-2: Estimated Cost (per Sample) for Swab and Cone Consumables (as of 2/13/2018)

Company	Part Number	Part Description	Price
Consumables			
Fisher Scientific	1118600001	Millipore MQuant Blank Strips (Without Reagent), Box of 100	\$0.60/Strip
Copan Diagnostics	160C	Plain Swab Sterile Aluminum Applicator Rayon Tipped, Case of 1000	\$3.12/Swab
Fisher Scientific	09-898-12B	Low-Nitrogen Weighing Paper, Pack of 500	\$0.09/Cone

Photos of Authentic Evidence Analyzed via Modular Ionization Sources on the AI-MS 1.2



Figure S-6. Seized heroin evidence analyzed via PSI-MS

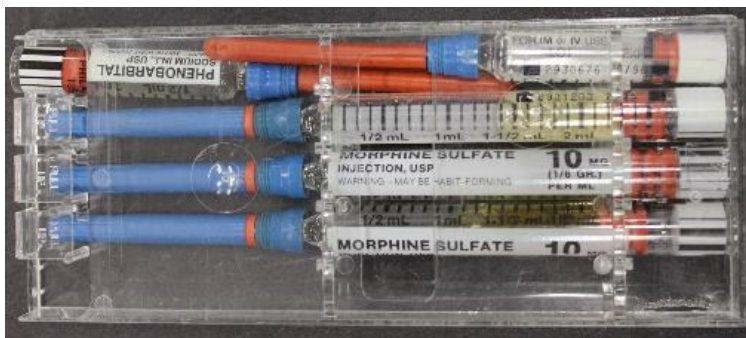


Figure S-7. Seized morphine sulphate injectable syringe analyzed via PSI-MS

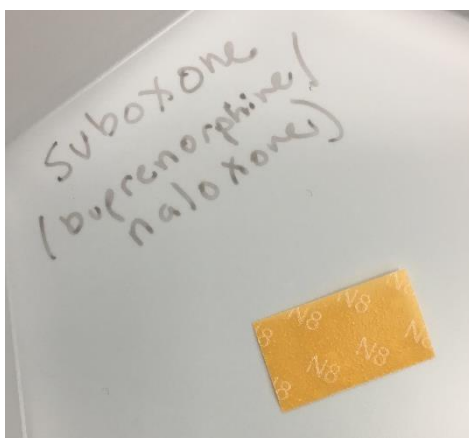


Figure S-8. Suboxone[®] sublingual film analyzed via PCSI-MS

Alternate and Internal Views of the Modular Sources

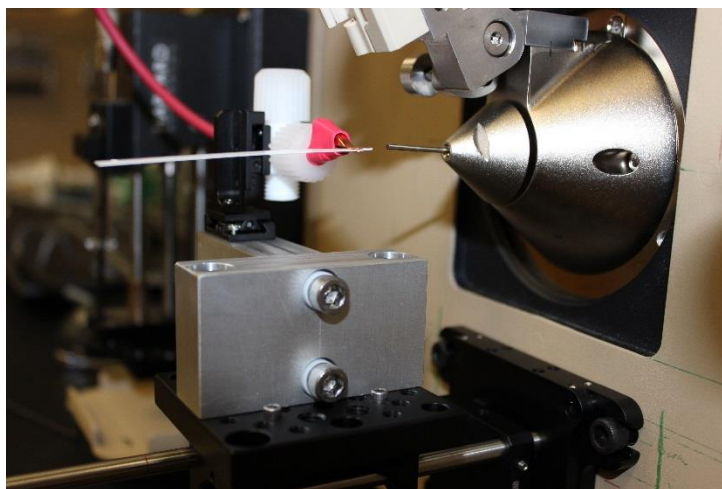


Figure S-9. Side-view of PSI source module

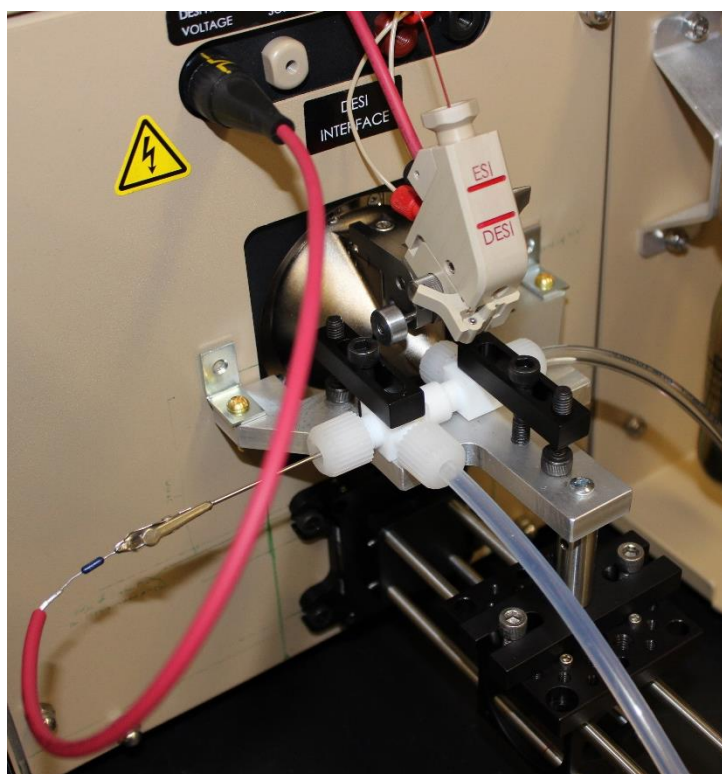


Figure S-10. Left-hand view of APCI source, including HV hookup and clamping

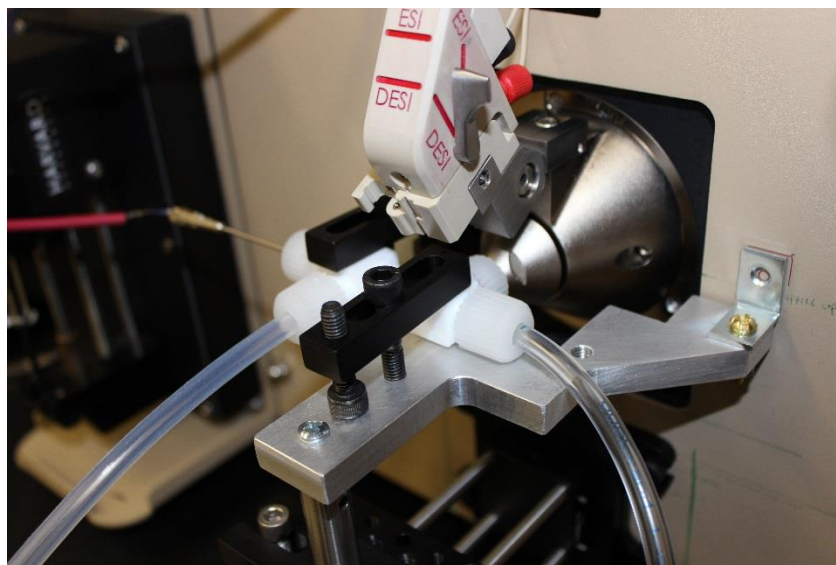


Figure S-11. Right-hand view of APCI source, including HV hookup and clamping

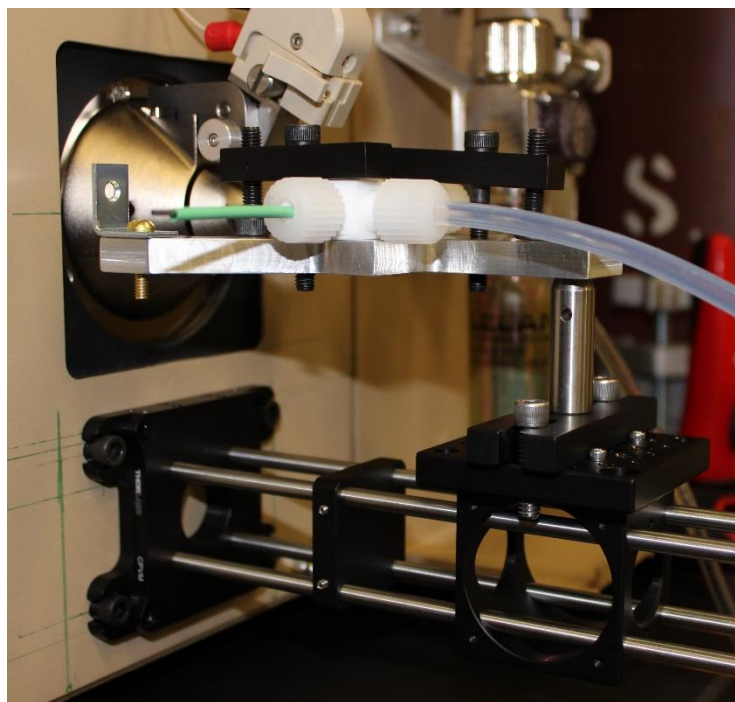


Figure S-12. Side view of APCI source module

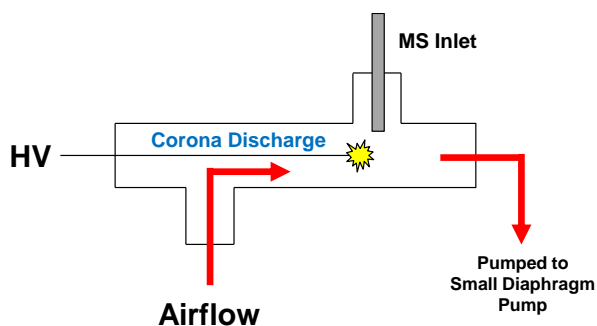


Figure S-13. Schematic of top, internal view of discharge region of the APCI source

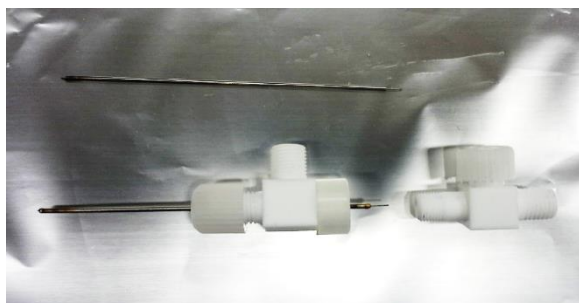


Figure S-14. Photo of simply-crafted discharge needle from syringe cleaning wire and stock SS LC capillary.

Absolute Intensity Obtained in Reported MS Spectra

Spectrum of Interest	Base Peak	Absolute Intensity (out of 4000)
Figure 3A	m/z 370 (Heroin)	3786
Figure 3C	m/z 286 (Morphine)	2842
Figure 5A	m/z 468 (Buprenorphine)	4950
Figure 7A	m/z 269 (Ethyl Centralite)	2469
Figure 9A	m/z 59 (Acetone)	1731
Figure 9C	m/z 114 (Caprolactam)	3012