

**Electronic Supplementary Information For:**

**Trace Level Screening of Chemicals Related to Clandestine Desomorphine  
Production with Ambient Sampling, Portable Mass Spectrometry**

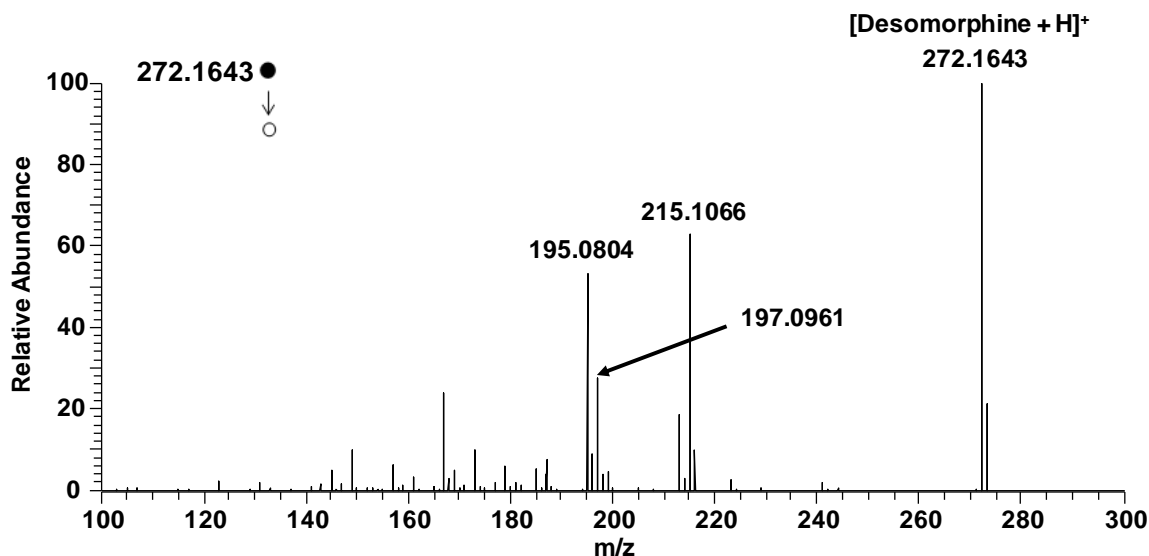
Seth E. Hall, Adam E. O’Leary, Zachary E. Lawton, Alessandra M. Bruno, and  
Christopher C. Mulligan\*

Department of Chemistry, Illinois State University, Normal, IL USA

\*Corresponding author: Email: [mulligan@ilstu.edu](mailto:mulligan@ilstu.edu)

## High Resolution Mass Spectrometric (HRMS) Investigation of Desomorphine

In an effort to confirm the suspected fragmentation pathways observed for MS/MS analysis of desomorphine using DESI and PSI-MS on the FLIR AI-MS 1.2, high resolution mass spectrometric investigation was conducted on a Thermo Fisher Q Exactive orbitrap mass spectrometer in-house. Positive-ion mode direct injection analysis electrospray ionization (DIA-ESI) was used to study a solution comprising of 10 ppm desomorphine in methanol. Protonated desomorphine was observed at  $m/z$  272.1643, yielding an error of 0.735 ppm compared to theoretical mass. MS/MS investigation of protonated desomorphine using high energy collisional dissociation (HCD, setting of 57%) yielded similar fragmentation as observed of the AI-MS 1.2 with both DESI and PSI, as seen in Figure S-1. Examining the accurate mass fragments observed allows the assignment of potential molecular losses with high accuracy. Suspected losses assigned to specific fragments and the associated error (in ppm) can be seen in Table S-1



**Figure S-1.** High resolution/accurate mass (HR/AM) DIA-ESI-MS/MS of 10 ppm of desomorphine in methanol, yielding transitions matching that of portable MS investigations via DESI and PSI-MS.

**Table S-1.** Proposed molecular losses via desomorphine MS/MS and associated error

Observed Ion ( $m/z$ ) and Difference	Proposed Assignment/Loss	Theoretical mas (Da)	Error (ppm)
272.1645	[Desomorphine + H] <sup>+</sup>	272.1645	0.735
215.1066 (- 57.0577)	Loss of C <sub>3</sub> H <sub>7</sub> N	57.0578	1.75
197.0961 (- 75.0682)	Loss of C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> O	75.0684	2.66
195.0804 (77.0839)	Loss of C <sub>3</sub> H <sub>9</sub> NH <sub>2</sub> O	77.0840	1.29