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Scientific Report

Degradation Study of Cocaine by Liquid Chromatography – Mass Spectrometry After Exposure to SoRite® DECON

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1. Introduction

Aseptic Health requested that Triclinic Labs perform a degradation study on cocaine after treatment with their novel decontaminant product, SoRite® DECON (SoRite). Two experiments were performed. Experiment #1 was a “trace amounts test,” and experiment #2 was a “disposal test.” The protocols for these experiments are described in the experimental section of this report. The treated material was analyzed using liquid chromatography-mass spectrometry (LC-MS). The goal was to quantify the cocaine content in various timed pulls from the SoRite reaction in each experiment. A summary of the reference materials and submitted sample is given in Table 1. A summary of the analyte is shown in Table 2.

Table 1. Summary of as-received samples

Material Name	Sample ID or Lot #	TCL ID
Cocaine Hydrochloride CII	R067U0	TCL24180-24183
SoRite® DECON	N/A	TCL23805

Table 2. Analyte summary

Compound Name	Molecular Formula	Exact Mass (g/mol)	Quantitation Ion (m/z)
Cocaine	$C_{17}H_{21}NO_4$	303.14706	304.15492 $[M+H]^+$

2. Results and Discussion

Experiment #1 involved testing a trace amount of cocaine (~10 mg) dissolved in 6 mL of SoRite over a brief period, with 10 seconds of shaking, to imitate the agitation caused by the spray of SoRite from a spray bottle. Cocaine showed 54% degradation after 1 minute. No change was observed at the 5-minute pull with respect to the 1-minute pull. The extracted ion chromatograms (EICs) are shown in Figures 1 and 2.

Experiment #2 (disposal testing) involved testing 250 mg of cocaine with 2.5 mL of SoRite to produce a 100 mg/mL solution. The solution was continuously shaken for 5, 10, and 30 minutes. The results of this experiment are summarized in Table 3. The LC-MS results showed a gradual increase from 73% degradation to 88% over the 30-minute experiment. The extracted ion chromatograms from experiment #2 are shown in Figure 3.

Table 3. Degradation study (Experiment #2) results of cocaine in SoRite.

Time	Cocaine degradation (%)
5 min	73%
10 min	81%
30 min	88%

3. Experimental

3.1. Sample Preparation and Analysis

Experiment #1 was designed to mimic the action of spraying the SoRite product onto a trace amount of cocaine, with the goal of determining the amount of degradation of the trace cocaine over a short period. A small amount (~10 mg) of cocaine was weighed into a 20 mL scintillation vial and 6 mL was added. The vial was shaken briefly for 10 seconds to to imitate the agitation caused by the spray of SoRite from a spray bottle. After shaking, the vial was left to rest on the bench, and 200 µL aliquots were taken at 1 minute and 5 minutes and neutralized with a sodium thiosulfate solution. Each sample was subsequently diluted 1000x with water and analyzed for cocaine content by LC-MS.

Experiment #2 was designed to determine the efficiency of a larger-scale drug disposal method. For this experiment, 0.25 g of cocaine was mixed with 2.5 mL of SoRite to prepare a 100 mg/mL mixture and was then shaken on an orbital shaker for 30 minutes. Subsamples were pulled at various time points (5, 10, and 30 minutes) and neutralized with sodium thiosulfate solution. Each sample was subsequently diluted 100,000x with water and analyzed for cocaine content by LC-MS.

A cocaine reference standard mixture was analyzed along with the samples for quantification. The standard solution was diluted in LC-MS grade water to create calibration standards for linearity and precision. The analysis was performed with the built-in solution of fluoranthene as an internal calibration lock mass (Thermo Easy-IC). Instrument methods are described below in Table 4 and Table 5.

3.2. Liquid Chromatography Method

Table 4. LC instrument method

System	Thermo Vanquish UHPLC		
Mobile Phase A	0.1% Formic Acid in Water		
Mobile Phase B	0.1% Formic Acid in MeOH		
Needle Wash	Water/MeOH (90:10)		
Diluent	Water		
Column	Thermo Accucore C18 (4.6 mm x 100 mm, 2.6 µm)		
Injection Volume	2 µL		
Flow	0.400 mL/min		
Sampler Temp.	10°C		
Column Temp.	30°C		
Run Time	12 min		
Gradient	Time (min)	A (%)	B (%)
	0.00	90	10
	5.00	90	10
	8.00	10	90
	10.00	10	90
	10.10	90	10
	12.00	90	10

3.3. Mass Spectrometry Method

Table 3. MS instrument method

System	Thermo Orbitrap Exploris 120
Source	H-ESI
Scan Type	SIM
Ionization Mode:	Positive
Ion Spray Voltage	2200 V
Sheath Gas	35 arb
Aux Gas	5 arb
Sweep Gas	1 arb
Ion Transfer Tube Temp.	325°C
Vaporizer Temp.	350°C

4. Figures

Figure 1. Example extracted ion chromatogram (EIC) of cocaine (experiment #1, 1 min pull).

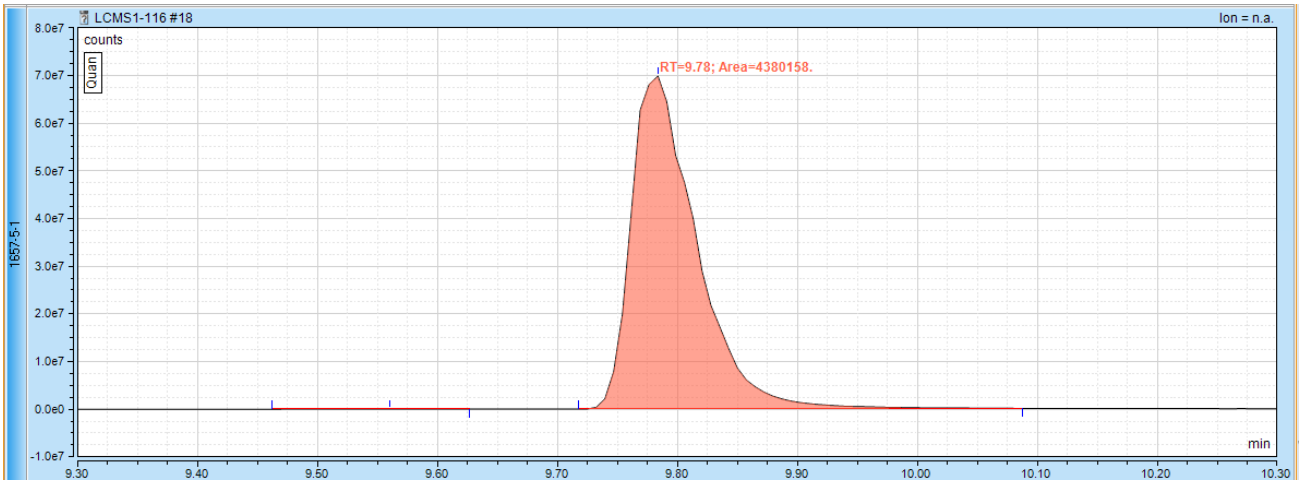

Figure 2. Example extracted ion chromatogram (EIC) of cocaine (experiment #1, 5 min pull).

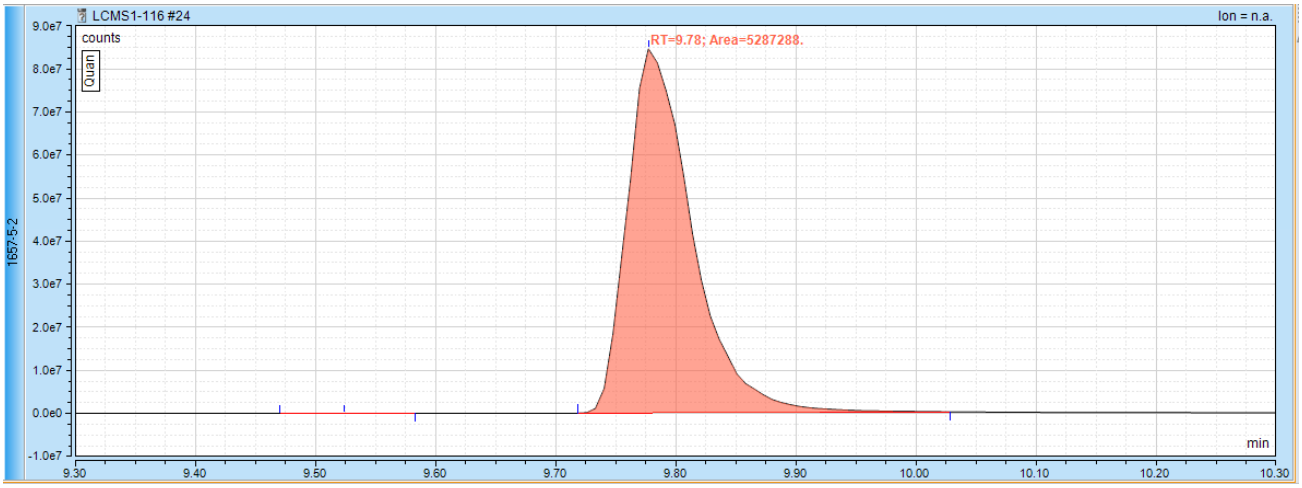

Figure 3. Overlaid extracted ion chromatograms of cocaine, experiment #2, at 5 min (blue), 10 min (black), and 30 min (magenta).