

# Supplementary Materials: Analysis of drugs in saliva of USA military veterans treated for substance-related disorders using supported liquid extraction and surface-enhanced Raman spectral analysis

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Table S1. Subject demographics, saliva and urine sampling times, daily buprenorphine dose, urinalysis, and other drugs used.

Sub ID Number	Race	Gender	Age	Vet/ Non-Vet	Date of Saliva Sample	Time of Saliva Sample	Date Saliva Sample Sent for Analysis	Date of Urine Sample	Time of Urine Sample	Daily BUP Dose	Urinalysis	Drugs used within 4 days of collected sample
1	Caucasian	M	65	V	6/26/2018	3:45PM	6/29/2018	6/26/2018	2:45PM	24mg	Positive: BUP	BUP
2	Caucasian	M	65	V	6/26/2018	1:45PM	6/29/2018	6/26/2018	2:25PM	20mg	Positive: BUP, cannabinoids	BUP, marijuana
3	Caucasian	M	58	V	6/26/2018	1:35 PM	6/29/2018	6/26/2018	2:30PM	8mg	Positive: BUP, amphetamines, cannabinoids	BUP, klonopin, marijuana
4	Caucasian	M	59	V	6/26/2018	1:30PM	6/29/2018	6/26/2018	1:15PM	24mg	Positive: BUP	BUP
5	Caucasian	M	62	V	6/25/2018	12:00PM	6/29/2018	6/25/2018	10:00AM	20mg	Positive: BUP	BUP
6	Caucasian	M	45	V	6/25/2018	11:45AM	6/29/2018	6/25/2018	11:45AM	16mg	Positive: BUP	BUP
7	AA	M	63	V	6/25/2018	2:45PM	6/29/2018	6/25/2018	2:40PM	20mg	Positive: BUP	BUP
8	AA	M	58	V	6/25/2018	10:45 AM	6/29/2018	6/25/2018	10:45 AM	20mg	Positive: BUP	BUP
9	Hispanic	M	65	V	6/25/2018	9:40AM	6/29/2018	6/25/2018	9:00AM	16mg	Positive: BUP, cannabinoids	BUP, marijuana
10	Caucasian	M	42	V	6/25/2018	9:20AM	6/29/2018	6/25/2018	8:45AM	8mg	Positive: BUP, cannabinoids	BUP, marijuana
11	AA	M	63	V	6/25/2018	9:10AM	6/29/2018	6/25/2018	8:45AM	24mg	Positive: BUP	BUP
12	AA	M	59	V	6/22/2018	1:40PM	6/29/2018	6/22/2018	12:00PM	8mg	Positive: BUP, opiates, methadone	BUP, heroin
13	declined to state race	M	46	V	6/22/2018	12:26 PM	6/29/2018	6/22/2018	12:28PM	24mg	Positive: BUP, cannabinoids	BUP
14	Hispanic	M	60	V	6/21/2018	1:25PM	6/29/2018	6/21/2018		24mg	Positive: BUP	BUP
15	Caucasian	M	44	V	6/21/2018	12:25PM	6/29/2018	6/21/2018	11:30AM	8mg	Positive: BUP	BUP
16	Caucasian	M	44	V	6/21/2018	11:40AM	6/29/2018	6/21/2018		8mg (started day of sample)	Positive: opiates	BUP (started same day as
17	Caucasian	M	36	V	6/21/2018	11:35 AM	6/29/2018	6/21/2018	11:30AM	20mg	Positive: BUP, cocaine	BUP
18	AA	M	65	V	6/21/2018	10:40 AM	6/29/2018	6/21/2018	9:30 AM	8mg	Positive: BUP, opiates	BUP, heroin
19	Caucasian	M	30	V	6/21/2018	10:22 AM	6/29/2018	6/21/2018	10:25 AM	24mg	Positive: BUP	BUP
20	Caucasian	M	49	V	6/20/2018	1:55 PM	6/29/2018	6/20/2018	12:00 PM	12mg	Positive: BUP, cannabinoids, cocaine	BUP, marijuana, cocaine



Figure S1. Images of Chem-ID software comparing Sample 1 to A) the first “Hit” nicotine, and B) the second “Hit” buprenorphine; and S-Quant software indicating the percent contribution for these two drugs using C) first derivative spectra and D) normal (untreated spectra). Spectral range used for analysis for all samples: 400 to 1800  $\text{cm}^{-1}$ . Conditions: 100 mg/L sample in water, 40 mW at 785 nm, 1 sec acquisition.

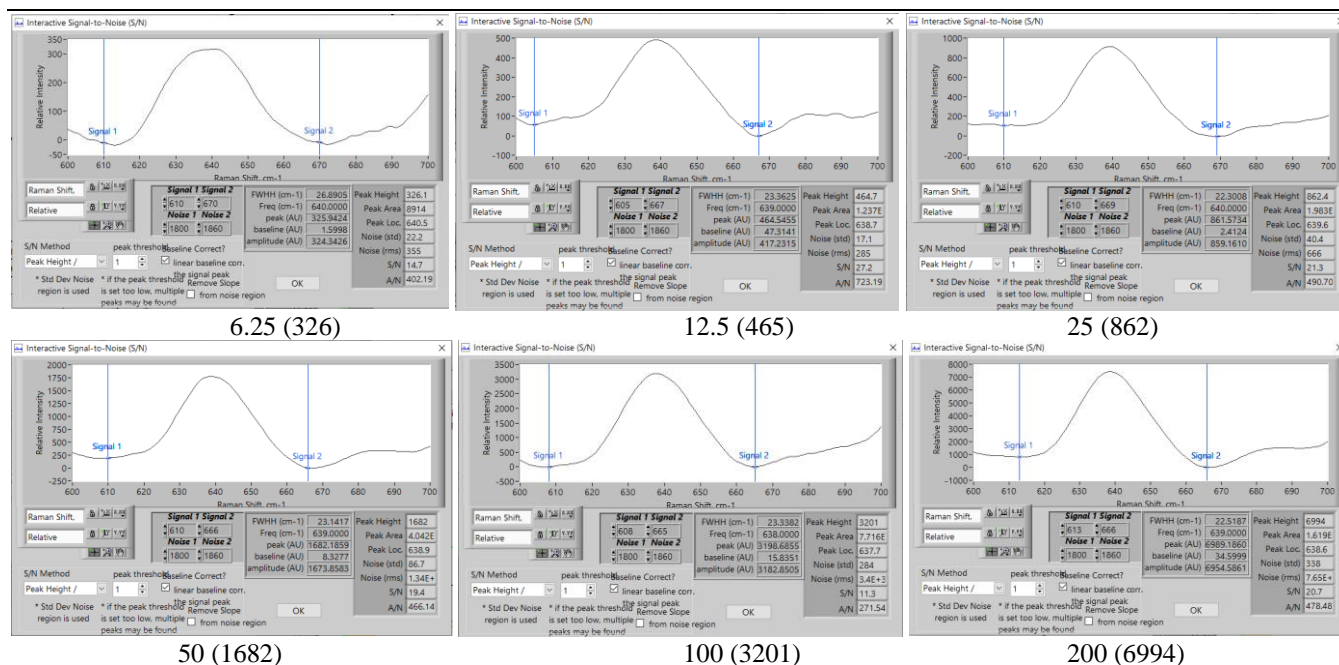


Figure S2. Spectra of samples for buprenorphine concentration calibration curve. Peak heights indicated in parentheses. Conditions as in Figure S1.

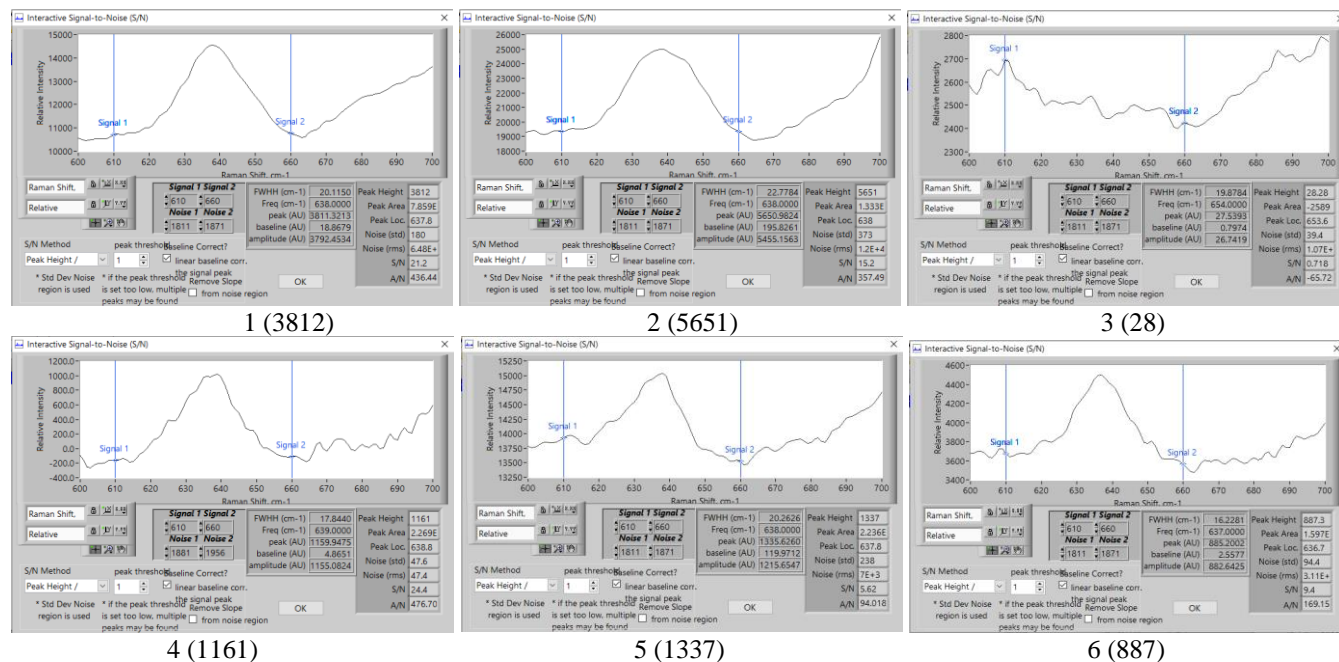


Figure S3a. Signal-to-noise software used to determine peak height with a baseline from 620 to 660  $\text{cm}^{-1}$  for Samples 1-6. Peak heights indicated in parentheses. Conditions as in Figure S1.

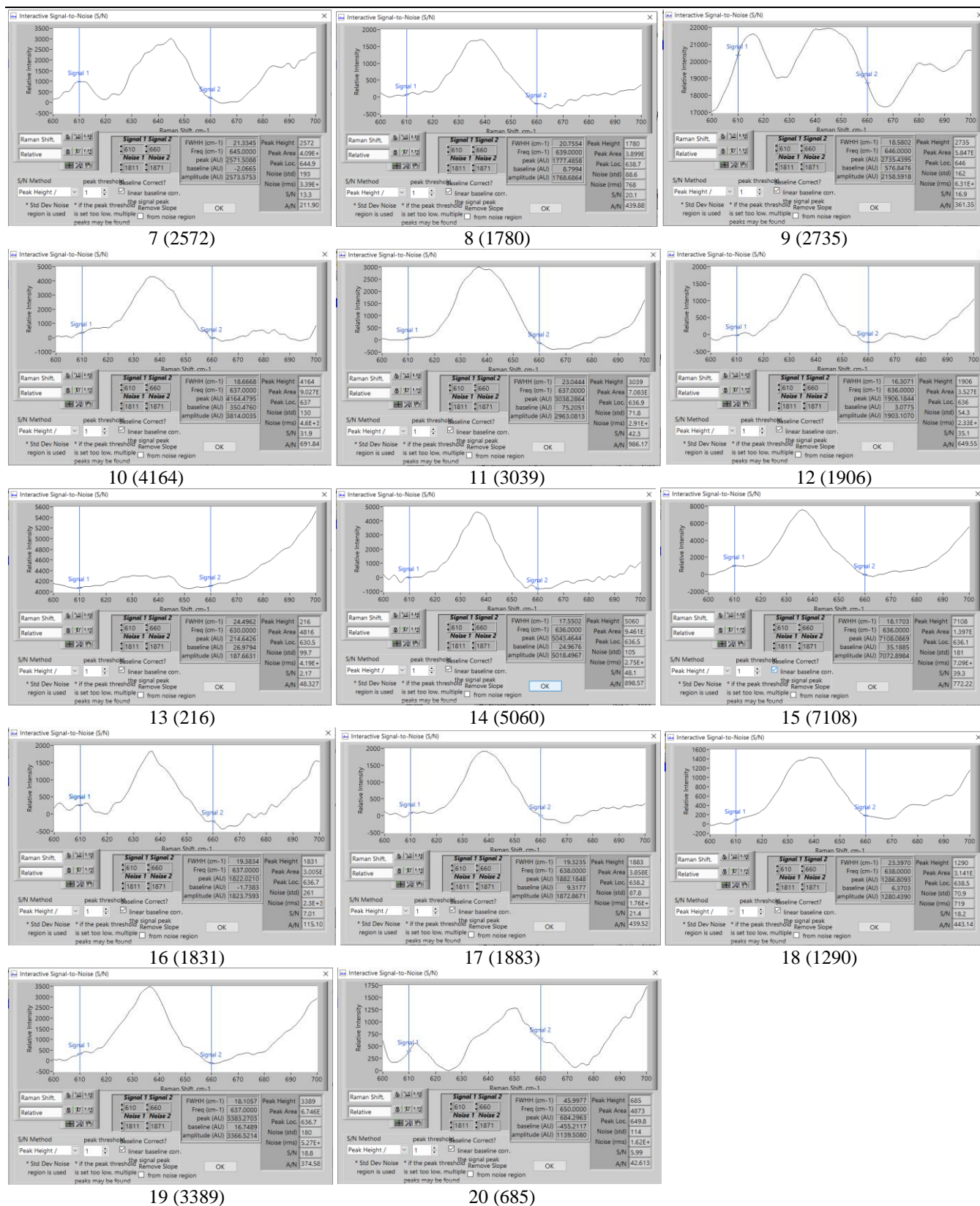


Figure S3b. Signal-to-noise software used to determine peak height with a baseline from 620 to 660 cm<sup>-1</sup> for Samples 7-20. Peak heights indicated in parentheses. Conditions as in Figure S1.



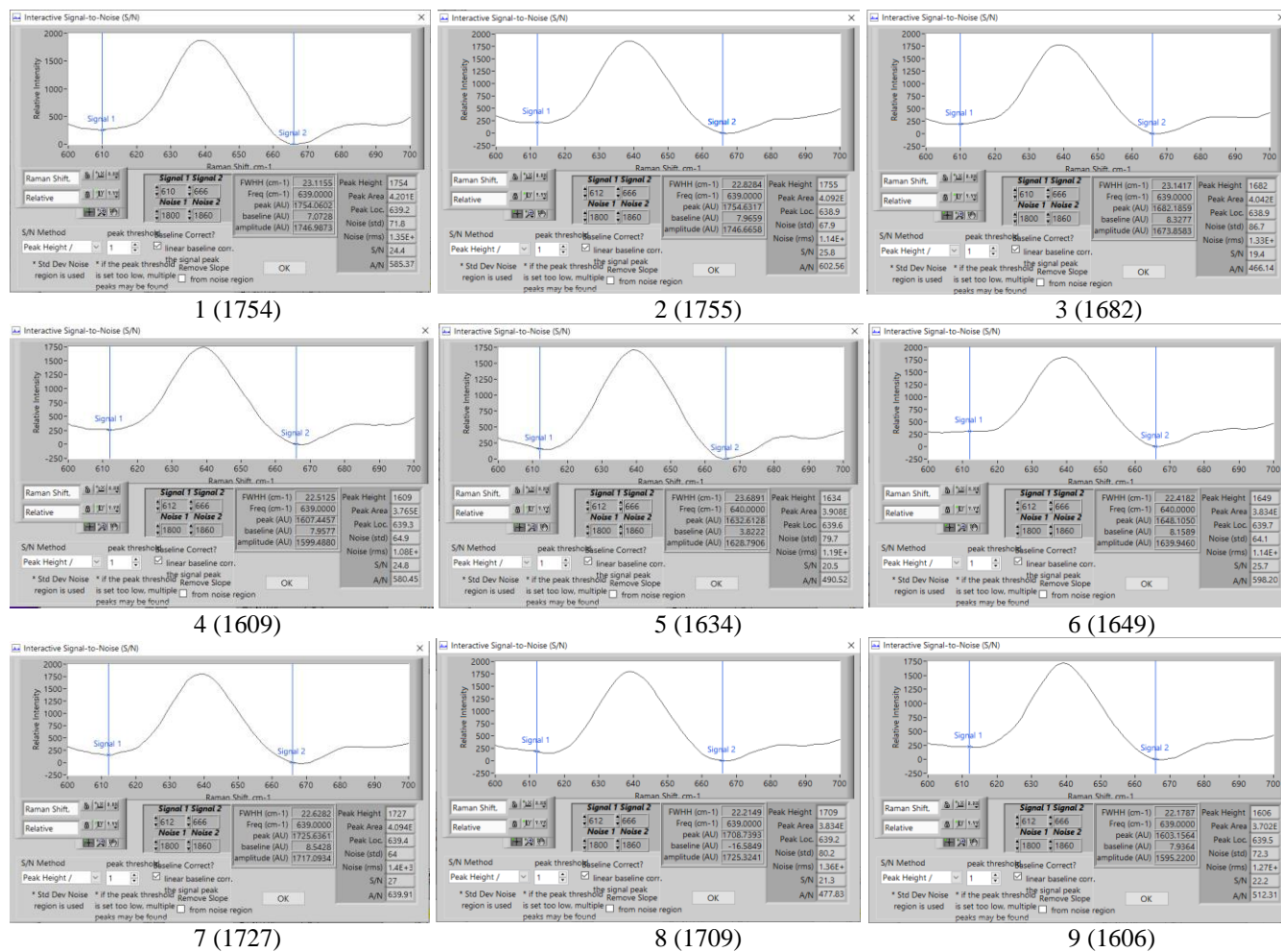


Figure S4. Nine repeat analyses for a 50 ng/mL prepared sample that included SLE preparation and SERS measurements. Peak heights indicated in parentheses. Conditions as in Figure S1.