

Vapor detection and vapor pressure measurements of fentanyl and fentanyl hydrochloride salt at ambient temperatures

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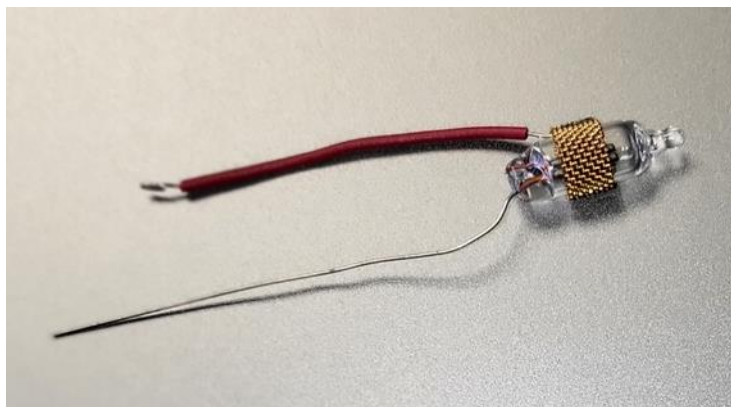


Figure S1. Photograph of dielectric barrier discharge ionization source. The inner and outer leads were connected to a radiofrequency power supply, which produced a ~42 kHz waveform with a ~2.5 kV peak-to-peak voltage.

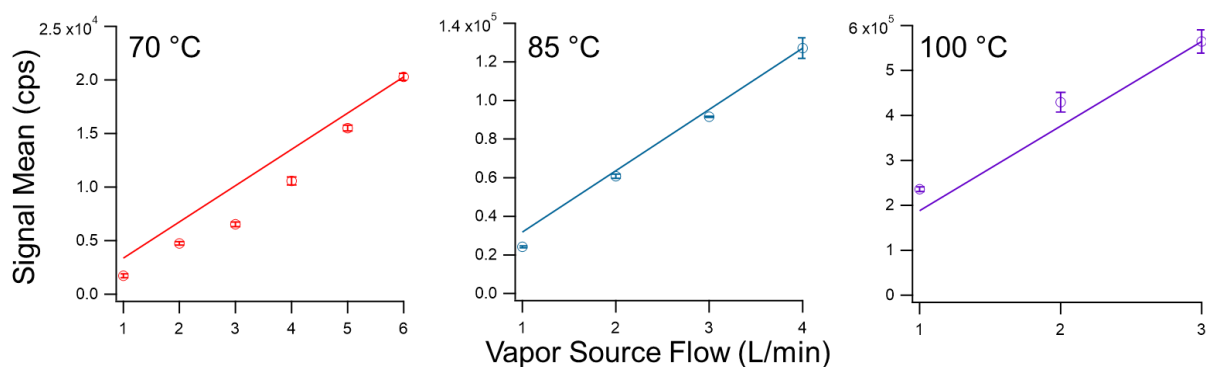


Figure S2. Direct vapor measurements of the fentanyl-HCl saturated vapor source at 70 °C, 85 °C, and 100 °C. The solid line in each plot indicates where points should fall based on ideal proportional scaling between signal intensity and flow rate. The circles represent average peak height at a given flow.

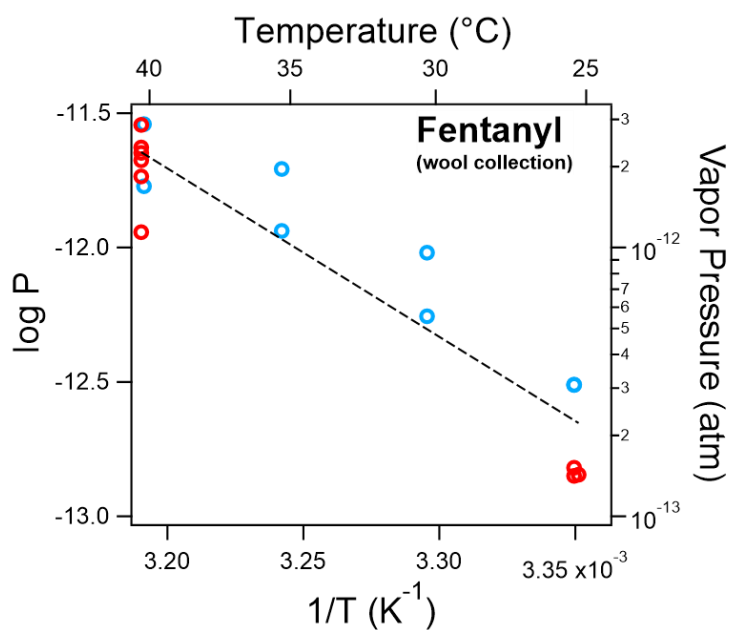


Figure S3. Clausius-Clapeyron relations of log P as a function of temperature for fentanyl using the wool collection and extraction method. Circle colors indicate data collected on different days.

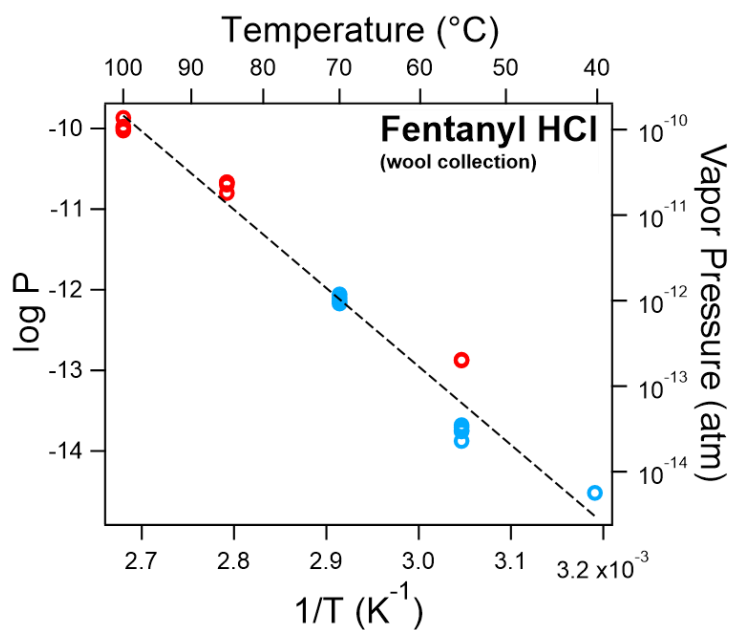


Figure S4. Clausius-Clapeyron relations of log P as a function of temperature for fentanyl hydrochloride salt using the wool collection and extraction method. Circle colors indicate data collected on different days.

Table S1. Individual measurements of fentanyl free base vapor pressures, log (P/atm), obtained from the filter collection experiments on two different days.

Day	Temperature (°C)	Temperature (K)	Fentanyl Log (P/atm)
1	14.6	287.75	-13.83
1	14.6	287.75	-13.70
1	14.8	287.95	-13.84
1	19.5	292.65	-13.44
1	19.9	293.05	-13.43
1	20.0	293.15	-13.45
1	20.1	293.25	-13.47
1	20.1	293.25	-13.19
1	25.4	298.55	-13.19
1	25.4	298.55	-13.10
1	25.4	298.55	-13.00
1	25.4	298.55	-13.06
1	30.4	303.55	-12.77
1	30.4	303.55	-12.72
1	30.4	303.55	-12.69
1	35.3	308.45	-12.35
1	35.3	308.45	-12.35
1	35.3	308.45	-12.32
1	40.3	313.45	-11.98
1	40.3	313.45	-11.87
1	40.3	313.45	-11.89
2	12.6	285.70	-14.17
2	12.6	285.75	-14.22
2	12.7	285.80	-14.32
2	15.1	288.20	-13.95
2	15.0	288.15	-13.99
2	15.0	288.15	-13.93
2	18.9	292.00	-13.59
2	18.7	291.85	-13.53
2	18.7	291.80	-13.47
2	19.6	292.75	-13.46
2	19.7	292.80	-13.53
2	19.7	292.80	-13.48
2	25.6	298.70	-12.96
2	25.4	298.55	-12.98
2	25.4	298.55	-12.93
2	30.3	303.45	-12.60
2	30.3	303.45	-12.57
2	30.3	303.45	-12.47
2	35.3	308.45	-12.15
2	35.3	308.45	-12.14
2	35.3	308.45	-12.18
2	40.2	313.35	-11.77
2	40.2	313.35	-11.79
2	40.2	313.35	-11.80

Table S2. Individual measurements of fentanyl hydrochloride vapor pressures, log (P/atm), obtained from the filter collection experiments on two different days.

<u>Day</u>	<u>Temperature (°C)</u>	<u>Temperature (K)</u>	<u>Fentanyl HCl Log (P/atm)</u>
1	40.2	313.35	-15.23
1	40.2	313.35	-15.22
1	40.2	313.35	-15.29
1	55.1	328.25	-13.83
1	55.1	328.25	-13.76
1	55.1	328.25	-13.78
1	70.0	343.15	-12.40
1	70.0	343.15	-12.36
1	70.0	343.15	-12.32
1	85.0	358.15	-11.15
1	85.0	358.15	-11.14
1	85.0	358.15	-11.09
2	40.3	313.40	-15.25
2	40.3	313.40	-14.94
2	40.3	313.45	-14.96
2	55.1	328.25	-13.62
2	55.2	328.35	-13.54
2	55.2	328.30	-13.53
2	70.1	343.20	-12.36
2	70.0	343.15	-12.35
2	70.0	343.15	-12.31
2	85.0	358.15	-11.29
2	85.0	358.15	-11.32
2	85.0	358.15	-11.27

Table S3. Individual measurements of fentanyl free base vapor pressures, log (P/atm), obtained from the wool collection and extraction experiments on two different days.

Day	Temperature (°C)	Temperature (K)	Fentanyl Log (P/atm)
1	25.4	298.55	-12.51
1	30.3	303.45	-12.02
1	35.3	308.45	-11.71
1	40.2	313.35	-11.77
1	25.4	298.55	-12.51
1	30.3	303.45	-12.26
1	35.3	308.45	-11.94
1	40.2	313.35	-11.54
2	25.3	298.40	-12.84
2	25.4	298.55	-12.82
2	25.4	298.55	-12.85
2	40.3	313.45	-11.94
2	40.3	313.45	-11.65
2	40.3	313.45	-11.74
2	40.3	313.45	-11.63
2	40.3	313.45	-11.68
2	40.3	313.45	-11.54

Table S4. Individual measurements of fentanyl hydrochloride vapor pressures, log (P/atm), obtained from the wool collection and extraction experiments on two different days.

Day	Temperature (°C)	Temperature (K)	Fentanyl HCl Log (P/atm)
1	40.3	313.40	-14.52
1	55.1	328.25	-13.76
1	55.1	328.25	-13.71
1	55.1	328.25	-13.68
1	55.1	328.25	-13.88
1	55.1	328.25	-13.74
1	70.0	343.15	-12.14
1	70.0	343.15	-12.17
1	70.0	343.15	-12.10
1	70.0	343.15	-12.06
2	55.1	328.25	-12.88
2	55.1	328.25	-12.87
2	85.0	358.15	-10.67
2	85.0	358.15	-10.70
2	85.0	358.15	-10.80
2	85.0	358.15	-10.67
2	100.0	373.15	-9.98
2	100.0	373.15	-10.02
2	100.0	373.15	-9.87
2	100.0	373.15	-10.00

Table S5. Results using the wool collection method for fentanyl and fentanyl hydrochloride vapor pressure values, Clausius-Clapeyron equations, and enthalpy of sublimation values.

Species	Temperature Range (°C)	Clausius-Clapeyron Equation	Vapor Pressure at 25 °C (atm)	Enthalpy of sublimation (kJ/mol)
Fentanyl Free Base	25-40	$\log P = 8.34 - 6264.3/T$	2.1×10^{-13}	-120
Fentanyl Hydrochloride	40-100	$\log P = 16.22 - 9724.9/T$	4.0×10^{-17}	-186