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Scientific Report

Proton NMR Analyses of RD286 Treated Heroin

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1. Introduction

Aseptic Health, LLC (Aseptic) is developing products (Sanitize IT) to neutralize potent compounds such as opioids. Aseptic has previously confirmed the degradation of fentanyl via Sanitize IT (RD286 and RD500) through ^{1}H nuclear magnetic resonance (NMR) analysis (1) and requested the effectiveness of RD286 on heroin using ^{1}H NMR spectroscopy.

For the effectiveness testing, a heroin sample (~1 mg) was treated with RD286 for one minute at room temperature without sonication or vortexing to mimic the spraying of the product over heroin powder spilled on a surface (see the experimental section). The aliquot of the treated sample and reference materials (heroin and RD286) were analyzed by ^{1}H NMR to determine whether the treatment of RD286 was effective in degrading the potent compounds. **Table 1** contains details of the samples used to investigate the efficacy of RD286 on heroin.

Table 1. Summary of samples analyzed by ^{1}H NMR spectroscopy.

Sample Description	Lot Number of Triclinic Labs' Identifier	NMR Filename
RD286	08242022LAB1 TCL18313	N/A
Heroin·HCl	0559234 TCL18425	N/A
Heroin reference standard	1129-92-1	NMR1-2600
RD286 treated heroin sample (one minute incubation)	1129-92-3	NMR1-2602
Intact RD286	1129-33-1	NMR1-2103

2. Results

The ^{1}H NMR spectrum of heroin treated with RD286 is compared to reference spectra (RD 286 and heroin) in **Figures 1 - 3**. The ^{1}H NMR spectrum of RD286 treated heroin shows that the heroin signals at 6.7 and 6.8 ppm were shifted compared to those of the heroin reference standard (RS), and the signals in the 5.0 - 5.7 ppm range have interfered with the water peak centered at 4.79 ppm (**Figure 2**). The two peaks observed at 2.15 and 2.35 ppm in the heroin RS spectrum were converted to more than six peaks in the RD286 treated heroin spectrum, suggesting that RD286 structurally changed heroin (**Figure 3**).

3. Conclusion

The ^{1}H NMR analysis on the heroin reference standard and RD286 treated heroin sample showed evidence that the chemical structure of heroin was changed by treatment of RD286 after one-minute incubation.

4. References

1. Triclinic Labs non-GMP report for Aseptic Health, LLC, "1H NMR analyses of RD286 and RD500 Treated Samples of Fentanyl", R2022213.01, dated April 20, 2022.

5. Experimental

5.1. ^{1}H NMR Spectroscopy

The reference standard for heroin (Cayman Chemical Co.) was prepared for ^{1}H NMR analysis by dissolving 1.071 mg of heroin·HCl into 1 mL of D_2O. The intact RD286 sample was prepared by adding RD286 solution directly into coaxial tubes. The RD286 treated sample for heroin was initially exposed by weighing 1.0065 mg of heroin·HCl into a container, then 1 mL of RD286 was added and allowed to incubate at room temperature for one minute. After one minute of incubation, the RD286 treaded sample was filtered by a 0.45 µm (17mm diameter) nylon filter to collect the supernatant. The supernatant was then added to a 5-mm NMR tube and analyzed.

The ^{1}H NMR spectra were acquired on a Bruker NEO 400 MHz (9.4 T) spectrometer using TopSpin v4.1.4 software. Each spectrum was processed using TopSpin v4.1.4 and referenced to the chemical shift of the residual D_2O (4.79 ppm) peak. Detailed acquisition parameters are listed in **Table 2**.

Table 2. NMR acquisition parameters.

Parameter Name	Parameter Value
Transmitter Frequency	400.15 MHz
Acquisition Time	6 sec
Spectral Width	6250 Hz
Number of Scans	128 - 256
Sequence	ZG
P1 (pulse width)	13.7 µsec
PLW1 (pulse power)	14.3 W
D1 (relaxation delay)	4 sec
Line Broadening	0.1 Hz

6. Figures

Figure 1. Comparative analysis of the ^{1}H NMR spectra of the intact RD286, the heroin reference standard, and the RD286 treated heroin sample.

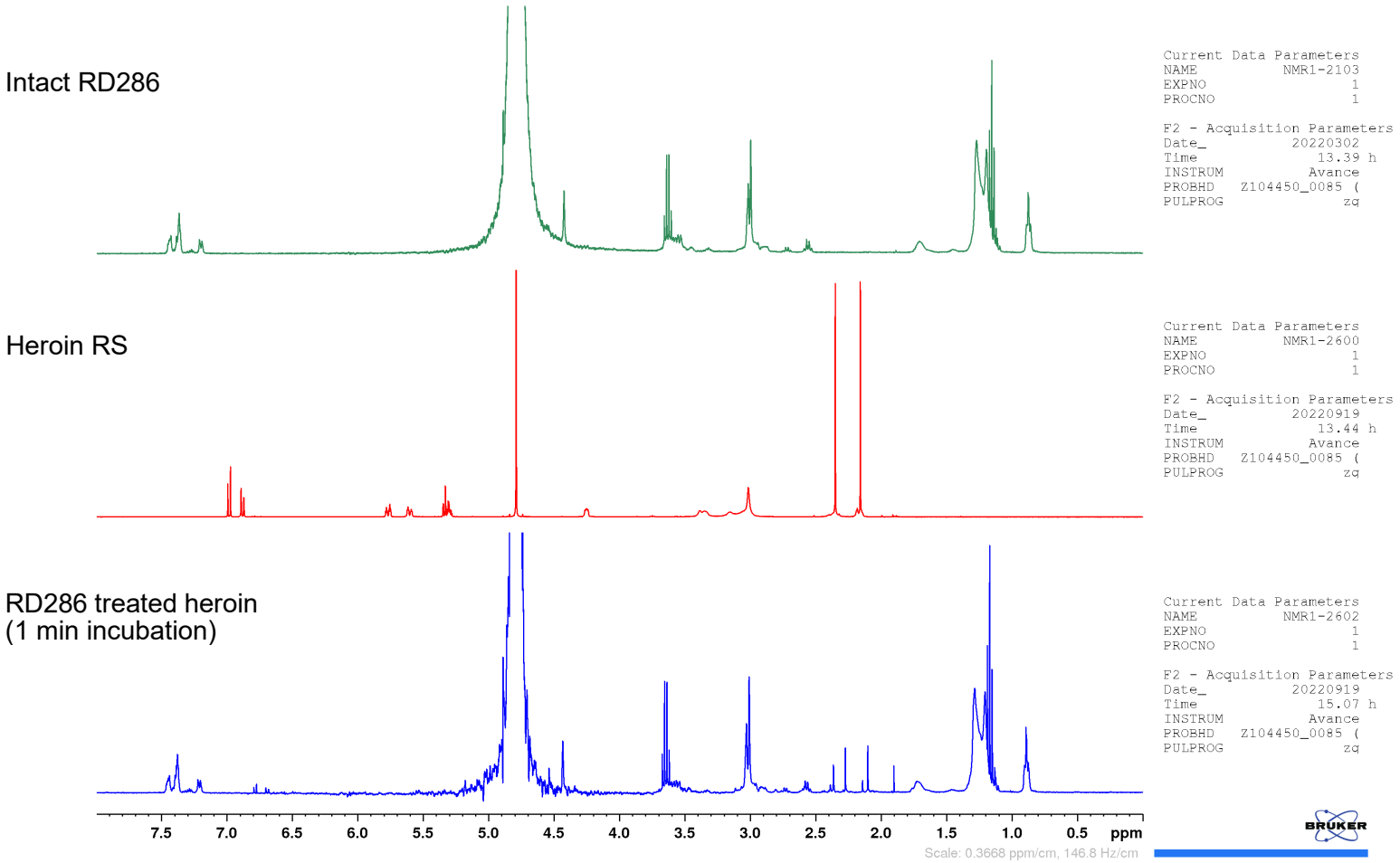

Figure 2. Comparative analysis of the ^{1}H NMR spectra (8 - 4 ppm) of the intact RD286, the heroin reference standard, and the RD286 treated heroin sample.

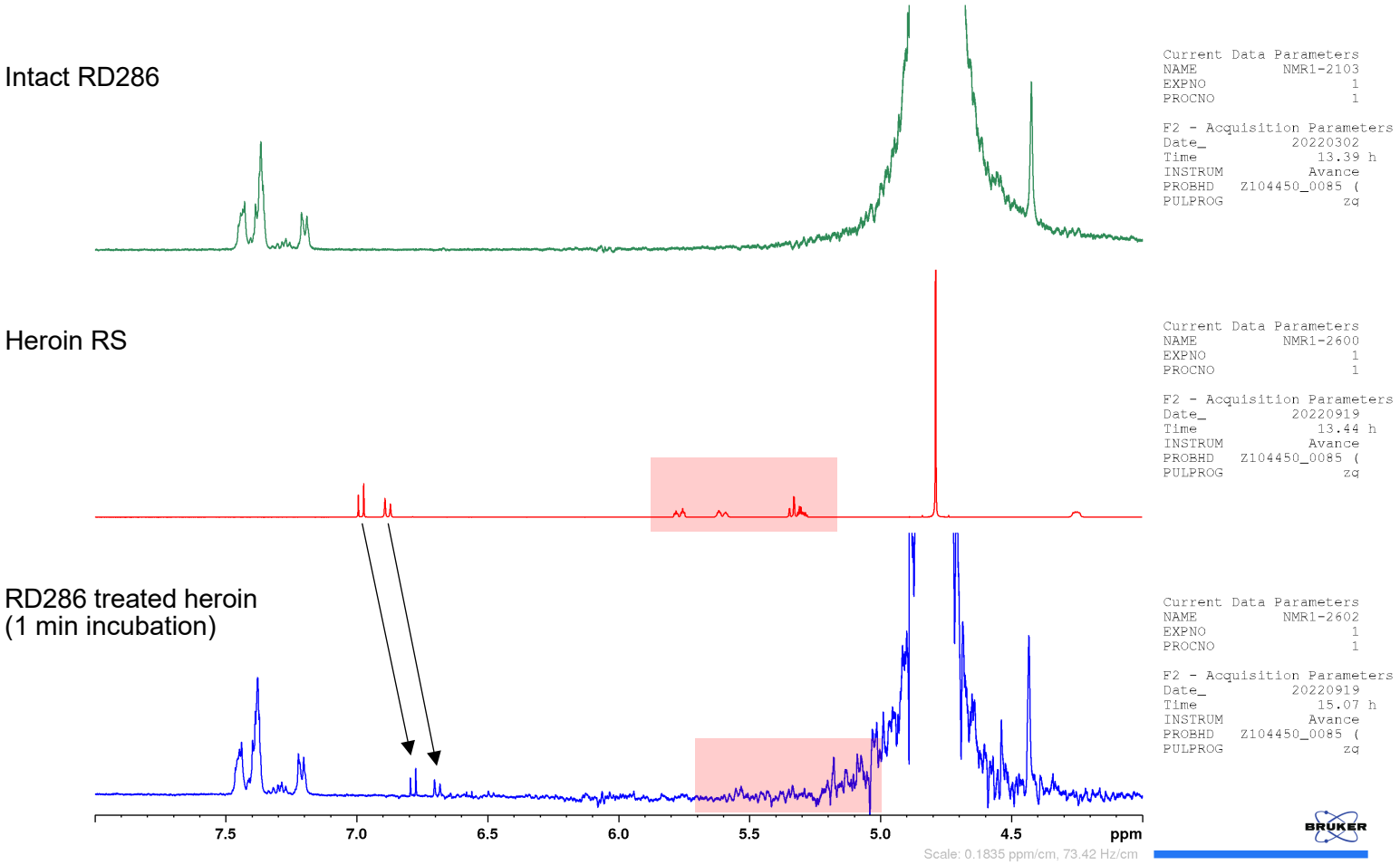

Figure 3. Comparative analysis of the ^{1}H NMR spectra (3.8 – 0.7 ppm) of the intact RD286, the heroin reference standard, and the RD286 treated heroin sample.