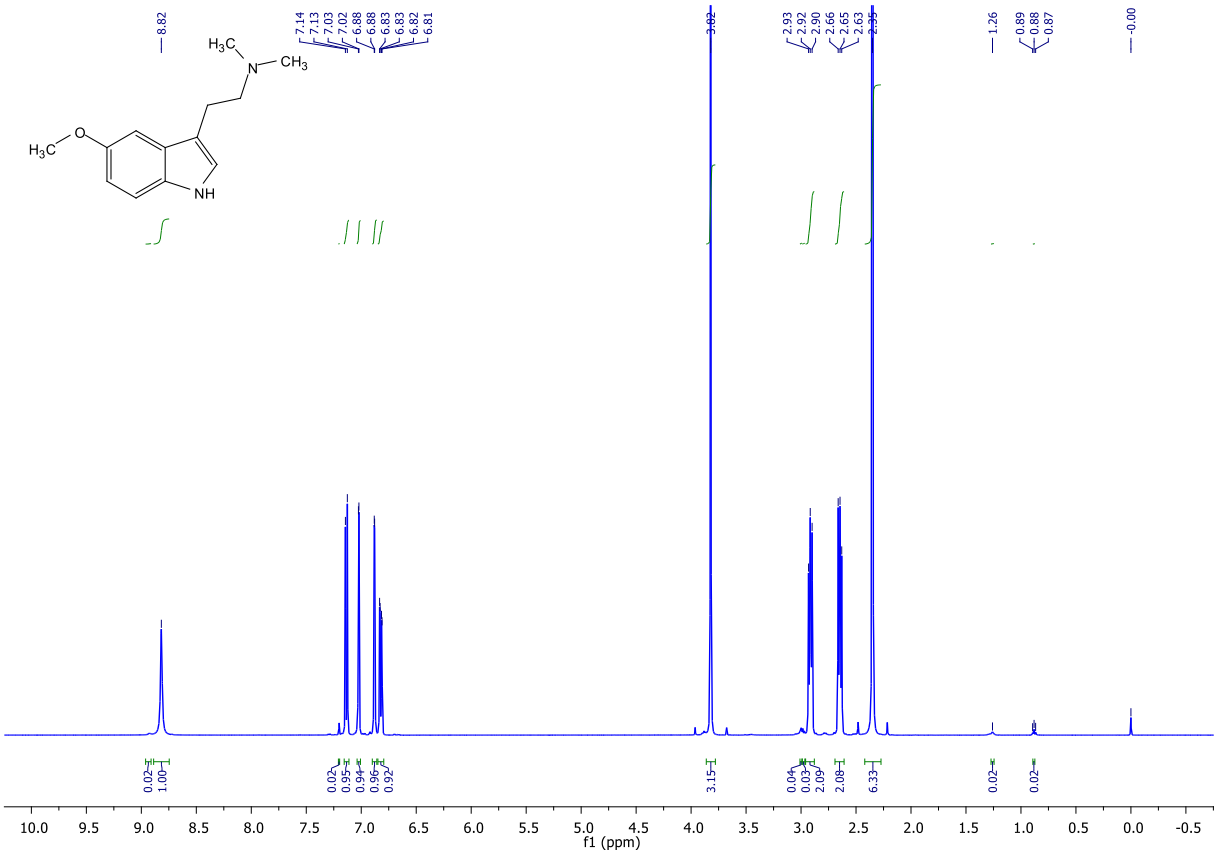
^{1}H NMR analysis report

Batch No.: 5MMMTFB_2 **Date:** 02/11/2026

Instrument: Bruker 500 MHz
Solvent: $CDCl_3$; spectra calibrated to internal standard - tetramethylsilane (TMS; δ = 0 ppm)

Expected structure: 5-Methoxy-*N*,*N*-dimethyltryptamine, freebase (5-MeO-DMT freebase)

Results:
Data consistent with the proposed structure: Yes
Estimated purity: 98%



^{1}H NMR ($CDCl_3$), cmpd and imp integrated.

^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 8.82 (s, 1H, NH), 7.14 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.02 (d, *J* = 2.2 Hz, 1H, Ar-H), 6.88 (d, *J* = 1.7 Hz, 1H, Ar-H), 6.82 (dd, *J* = 8.7, 2.3 Hz, 1H, Ar-H), 3.82 (s, 3H, OCH_3), 2.95 – 2.88 (m, 2H, CH_2), 2.69 – 2.62 (m, 2H, CH_2), 2.35 (s, 6H, 2 × CH_3).

Notes:

The relatively simple ^{1}H NMR spectrum exhibits signals corresponding to all four aromatic protons, along with a characteristic broad NH singlet at δ = 8.82 ppm. The methoxy group gives rise to a singlet at δ = 3.82 ppm, while the CH_2CH_2 bridge is represented by two multiplets at δ = 2.92 and 2.65 ppm, respectively. The equivalent *N*-methyl groups appear as a singlet (δ = 2.35 ppm, I = 6H).

NMR-active impurity is present at approximately 2 mol%. Its spectral features suggest a structure closely related to that of the main analyte, as evidenced by the presence of an NH proton, aromatic resonances, and a corresponding set of signals in the aliphatic region. Notably, the characteristic methoxy resonance at approximately δ = 3.8 ppm is absent from the impurity's signal pattern, suggesting that the contaminant may be the corresponding 5-hydroxy derivative (5-HO-DMT). However, owing to the low concentration of this impurity, its identity cannot be conclusively established from the available NMR data alone.