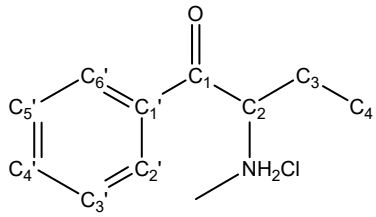
Synthesis and structural elucidation of NPS

Buphederone hydrochloride. Bromine (0.16 ml, 3.0 mmol) was added to a solution of butyrophenone (0.44 ml, 3.0 mmol) in dichloromethane (5 ml) and the mixture was stirred for 2 h. The solvent was removed and the crude was dissolved in THF (5 ml) and methylamine (40 wt. % in water, 1.04 ml, 12 mmol) was added. Flash chromatography (ethyl acetate/methanol, 99/1), formation of the hydrochloride salt with ethereal hydrogen chloride (1 M) and recrystallization from ethanol/acetone afforded the product as a white powder (0.51 g, 80%).



^{1}H NMR (300 MHz, DMSO-*d6*): 0.76 (t, 3H, J= 7.0 Hz, H_4), 1.85-2.04 (m, 1H, H_3), 2.06-2.14 (m, 1H, H_3), 2.56 (s, 3H, NCH_3), 5.27 (s, 1H, H_2), 7.60 (t, 2H, J= 7.6 Hz, $H_{3',5'}$) 7.74 (t, 1H, J= 7.6 Hz, $H_{4'}$) 8.04 (d, 2H, J= 7.6 Hz, $H_{2',6'}$), 9.34, (s (br), 1H, NH_2) 9.82 (s (br), 1H, NH_2). ^{13}C NMR (75 MHz, DMSO-d6): 8.6 (C_4), 23.1 (C_3), 31.7 (NCH_3), 63.2 (C_2), 129.2 ($C_{2',6'}$), 129.6 ($C_{3',5'}$), 134.4 ($C_{1'}$), 135.2 ($C_{4'}$), 196.5 (C_1).

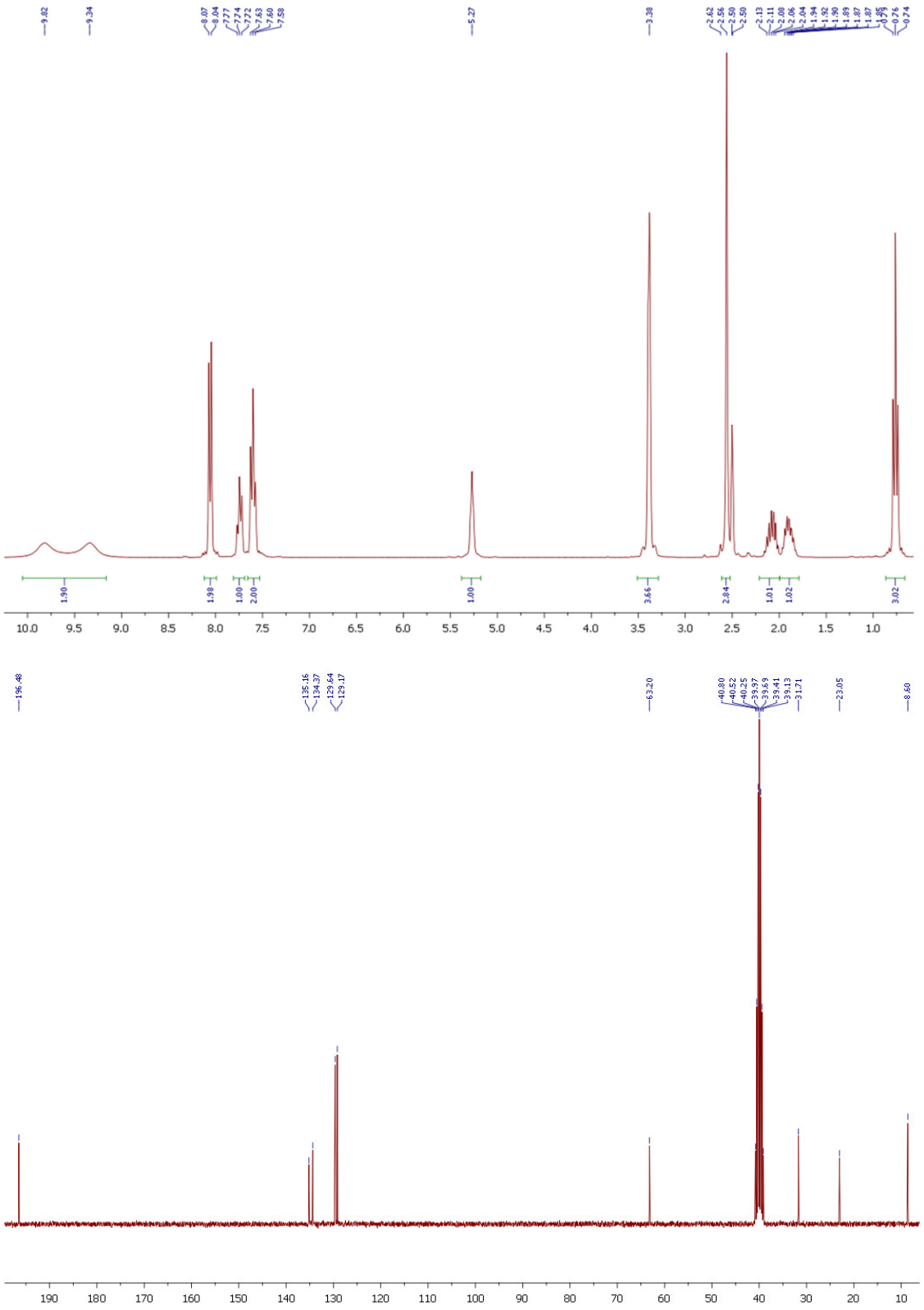


Figure 1. ^{1}H- (top) and ^{13}C- (bottom) NMR spectra of buphedrone hydrochloride in DMSO-*d6*.