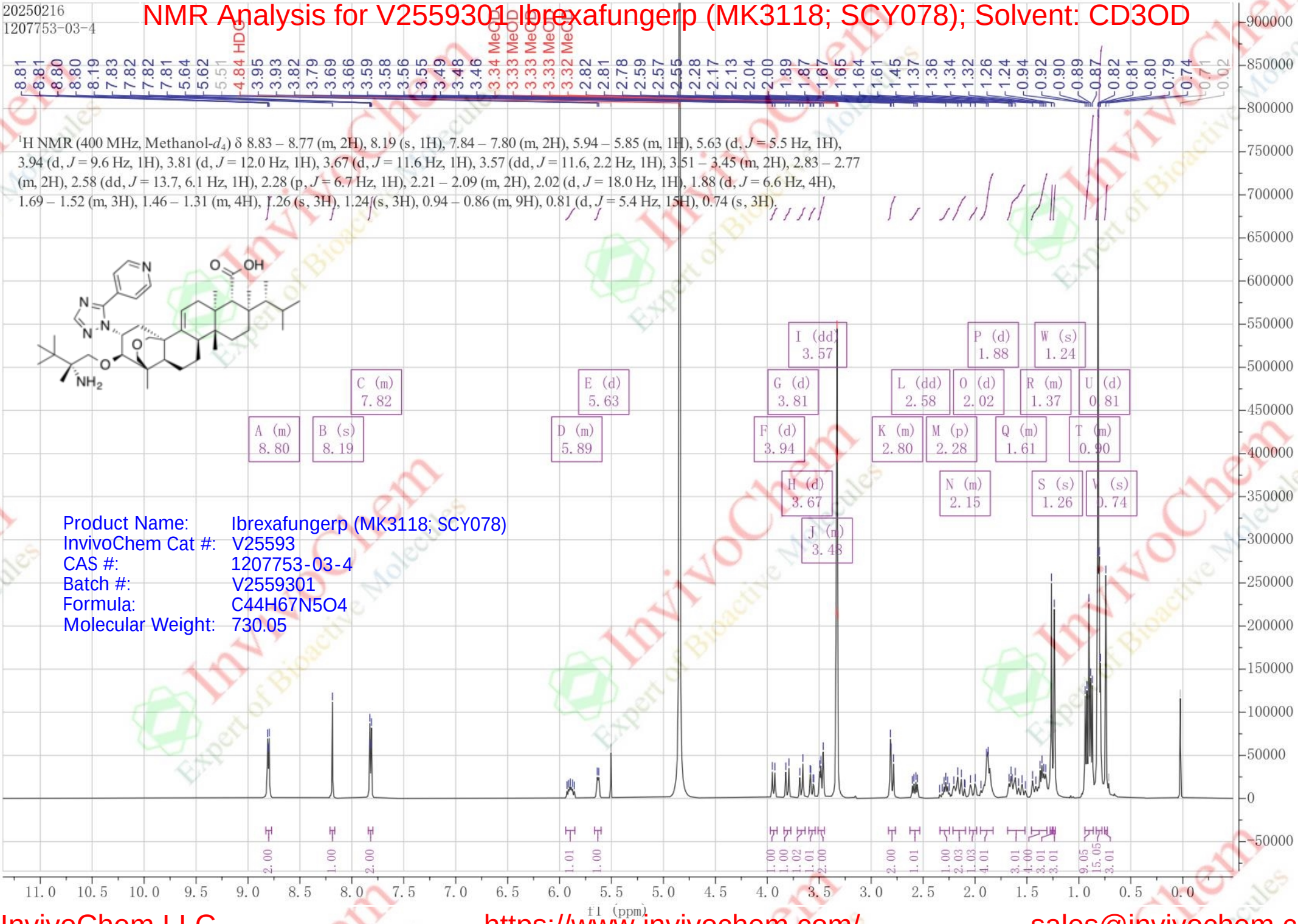
20250216
1207753-03-4

NMR Analysis for V2559301 Ibrexafungerp (MK3118; SCY078); Solvent: CD3OD

^{1}H NMR (400 MHz, Methanol-d_4) δ 8.83 – 8.77 (m, 2H), 8.19 (s, 1H), 7.84 – 7.80 (m, 2H), 5.94 – 5.85 (m, 1H), 5.63 (d, J = 5.5 Hz, 1H), 3.94 (d, J = 9.6 Hz, 1H), 3.81 (d, J = 12.0 Hz, 1H), 3.67 (d, J = 11.6 Hz, 1H), 3.57 (dd, J = 11.6, 2.2 Hz, 1H), 3.51 – 3.45 (m, 2H), 2.83 – 2.77 (m, 2H), 2.58 (dd, J = 13.7, 6.1 Hz, 1H), 2.28 (p, J = 6.7 Hz, 1H), 2.21 – 2.09 (m, 2H), 2.02 (d, J = 18.0 Hz, 1H), 1.88 (d, J = 6.6 Hz, 4H), 1.69 – 1.52 (m, 3H), 1.46 – 1.31 (m, 4H), 1.26 (s, 3H), 1.24 (s, 3H), 0.94 – 0.86 (m, 9H), 0.81 (d, J = 5.4 Hz, 15H), 0.74 (s, 3H).



Product Name: Ibrexafungerp (MK3118; SCY078)
InvivoChem Cat #: V25593
CAS #: 1207753-03-4
Batch #: V2559301
Formula: C44H67N5O4
Molecular Weight: 730.05