General experimental remarks

- All solvents and reagents were purified by standard techniques reported or used as supplied by commercial sources whatever appropriate.
- All recorded melting points are uncorrected.
- FT–IR spectra were recorded on Shimadzu FT–IR 8401 spectrometer using KBr disc, and are expressed in wave numbers (cm⁻¹).
- ¹H NMR and ¹³C NMR spectra were recorded on a Bruker Avance 400 spectrometer operating at 400 MHz for ¹H NMR, and 100 MHz for ¹³C NMR, as solutions in CDCl₃, or DMSO-d₆. Chemical shifts (δ) are expressed in parts per million (ppm) and referenced to the residual protic solvent.
- In ¹H NMR, δ of dissolved water in CDCl₃ and DMSO-d₆ are appeared at δ 1.5 and 3.35 ppm respectively. Residual proton of CDCl₃ appeared as a singlet at δ 7.26 ppm whereas quintet at δ 2.49 ppm for DMSO-d₆.
- ¹³C NMR chemical shift of CDCl₃ and DMSO-d₆ appeared at δ 77.0 and 39.7 ppm respectively.
- Coupling constant (J) is expressed in Hertz (Hz). Splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; br, broad; m, multiplet; comp, complex multiplet.
- The degree of substitution (C, CH, CH₂, and CH₃) was determined by the DEPT-135 method.
- Elemental analyses (% C, H, N) were carried out on a PerkinElmer 2400 Series-II elemental analyzer.
- The ESI mass spectra were recorded on Shimadzu LCMS-2010 spectrometer.
- TLC was performed on Merck 60 F₂₅₄ precoated silica plates. Spots were detected either by UV (254 nm, 366 nm) or dipping into a permanganate solution [KMnO₄ (3 g), K₂CO₃ (20 g), NaOH (5 mL, 5% in H₂O), H₂O (300 mL)] or anisaldehyde solution [3 % methoxybenzaldehyde and 1 % H₂SO₄ in methanol] or 2,4-dinitrophenyl hydrazine (2,4-DNP) solution [2,4-DNP (12 g), Conc. H₂SO₄ (6 mL), Water (8 mL), EtOH (20 mL)] followed by heating.
- The single X–ray intensity data were collected on using a CCD area-detector diffractometer (X’calibur system–Oxford diffraction make, U.K) at room temperature (293 K), equipped with graphite monochromated MoKα radiation (λ=0.71073 Å). The cell dimensions were determined by least-squares fit of angular settings of reflections in the appropriate θ range. Data
were corrected for Lorentz and polarization and absorption factors. The
crystal structure was solved by direct methods using SHELXS97 (Sheldrick,
1997). All non-hydrogen atoms of the molecule were located from the E-
map. Full-matrix least-squares refinement was carried out by using
SHELXL97 software (Sheldrick, 1997). All the hydrogen atoms were
positioned geometrically and were treated as riding on their parent atoms.
Atomic scattering factors were taken from International Tables for X—ray
Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4). The CIF for all
structures studied in the present work has been deposited at Cambridge
Crystal Data Centre. The geometry of the molecule was calculated using the
WinGX and PARST softwares.