

Compound Characterisation Checklist

Structural formula:

Molecular formula:

Molecular weight:

Notebook entry ref:

IUPAC name (use Autonom):

Trivial name:

Literature reference:

Physical Property:

Appearance:

Mpt/bpt (quote lit. value):

Method of purification (include description):

Structural data

(solvent/field strength/temperature):

^1H NMR (δ , integral, multiplet, J value, assignment):

^{13}C NMR (δ , integral, multiplet, J value, assignment):

Other nuclei:

Other experiments to confirm assignment: DEPT135, COSY, HMQC, HMBC, NOESY?

Elemental analysis (within $\pm 0.2\%$)

Calculated:

Observed:

Mass Spectrometry (technique, fragmentation ion, relative intensity)

Infrared (sample preparation, absorption band, signal strength):

UV (solvent, wavelength and extinction coefficient):

Chiral Compound

$[\alpha]_D^{20}$ (solvent, concentration, sign, specific rotation):

Optical purity:

Chiral HPLC/GC (column, solvent, R_t):

Chiral shift reagent (reagent, solvent, chemical shifts):