

Supplementary Data

An efficient route to N-alkylated 3,4-dihydroisoquinolinones with substituents at the 3-position

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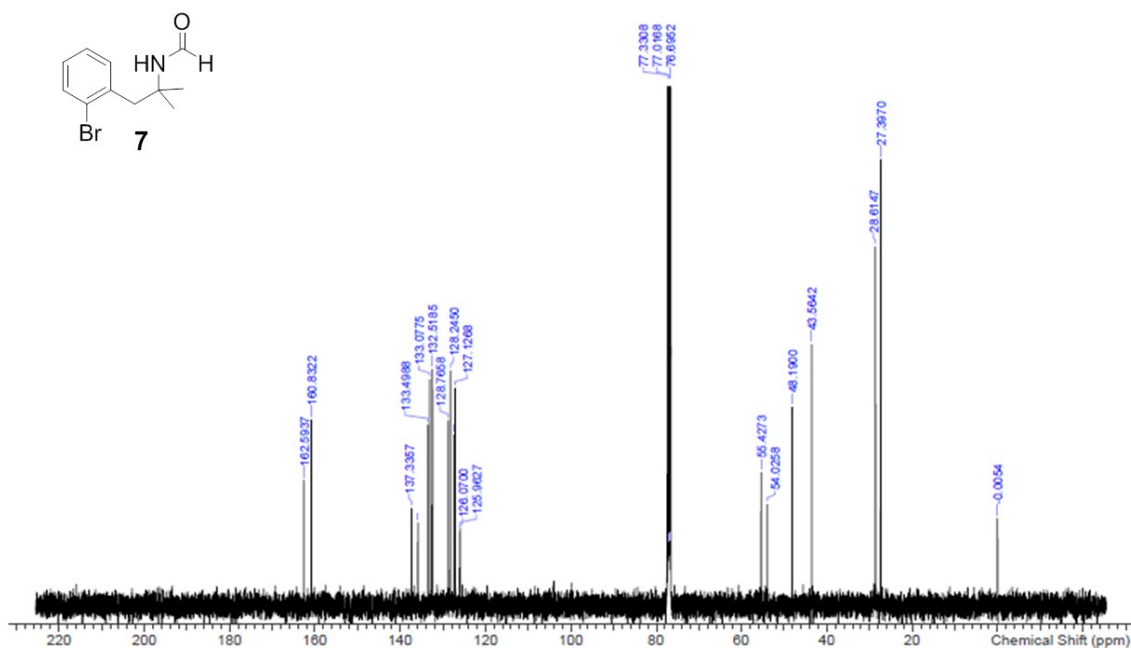
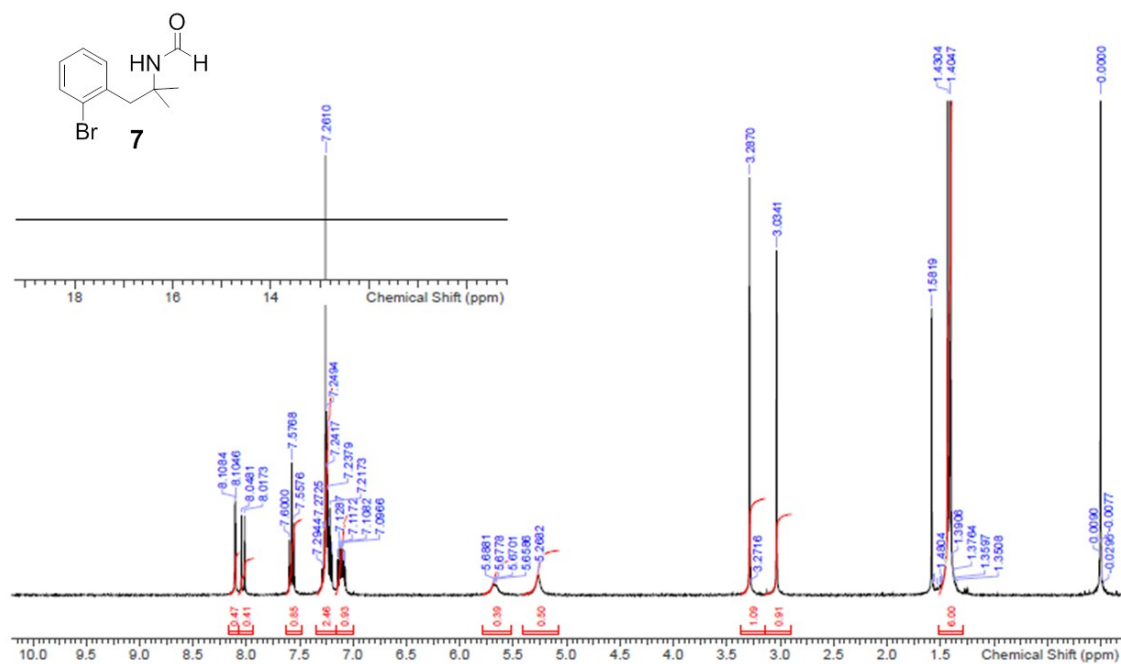
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S2 General Information

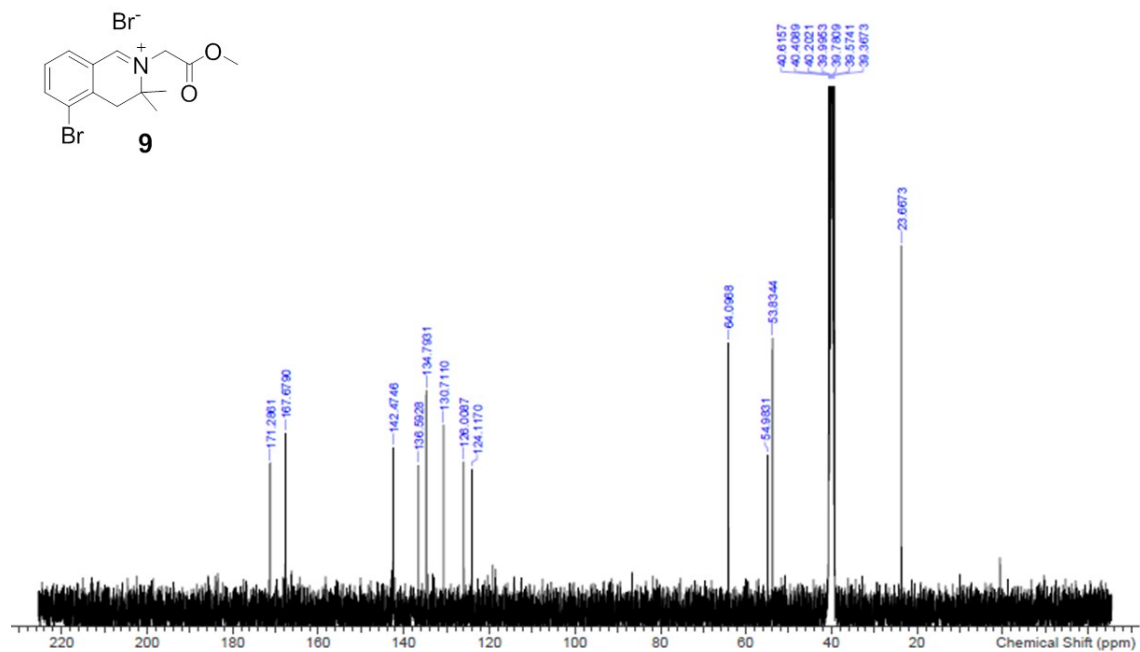
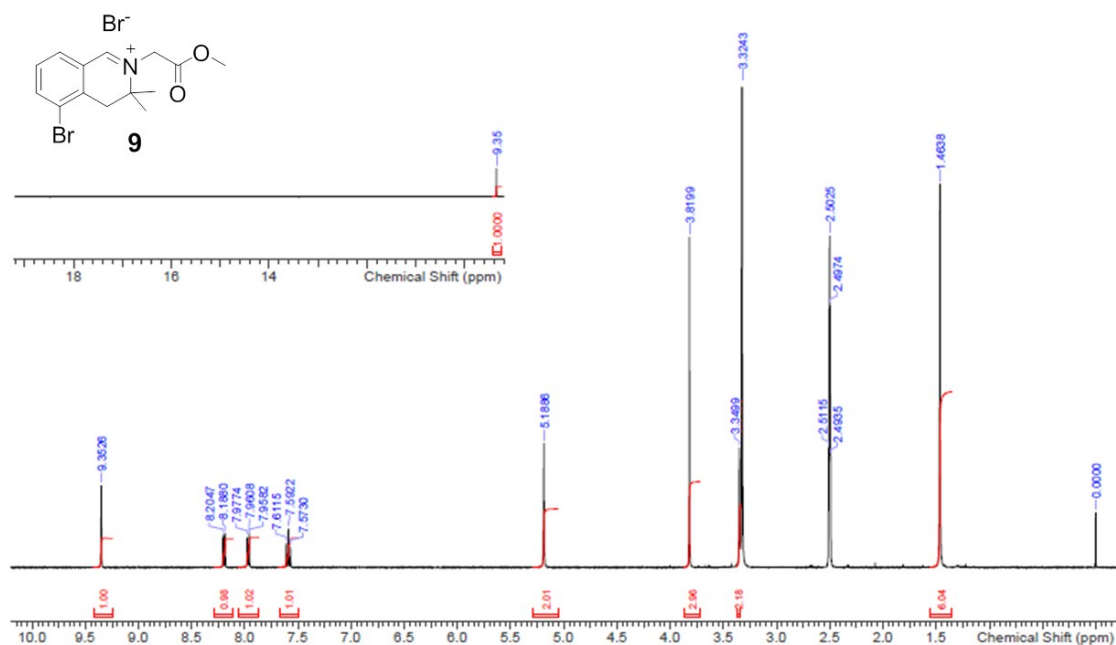
S3-S11 NMR Spectra of compounds

General Information. ^1H and ^{13}C NMR spectra were recorded on a Bruker 400 ULTRASHIELD PLUS. ^1H and ^{13}C chemical shifts are reported in ppm downfield from tetramethylsilane (TMS, δ scale) with the solvent resonances as internal standards. The following abbreviations were used to explain the multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; band, several overlapping signals; br, broad. IR spectra were recorded on a PerkinElmer Spectrum One FT-IR Spectrometer using attenuated total reflection (ATR). Melting points (m.p.) were recorded on a BÜCHI Melting Point B-545. Mass spectra were provided at the DMPK Research Laboratory, Mitsubishi Tanabe Pharma Corporation.

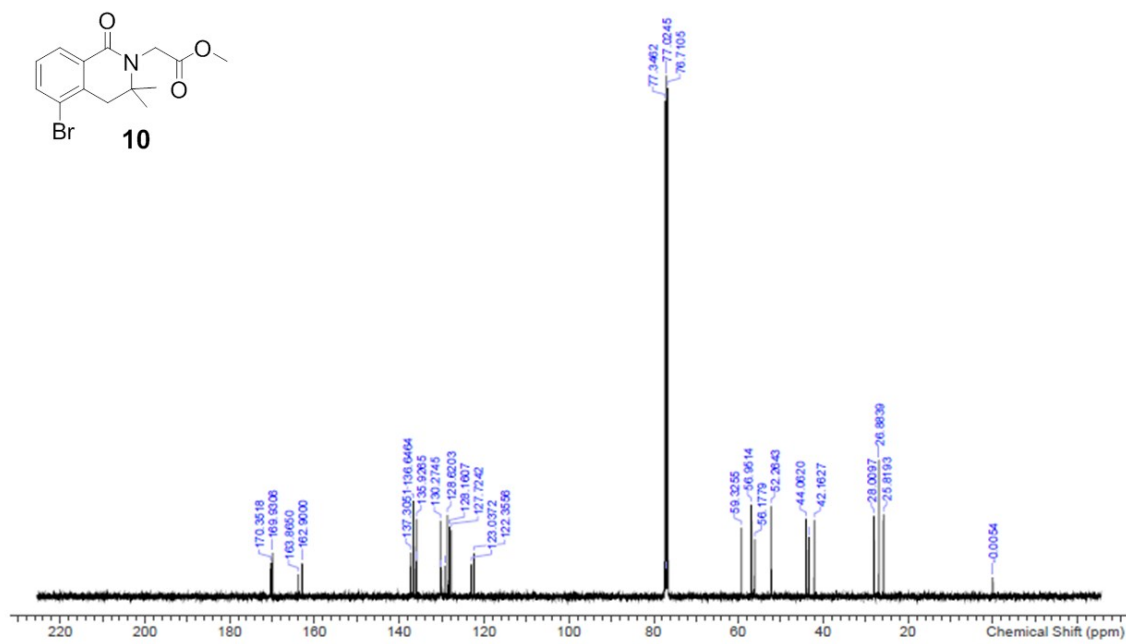
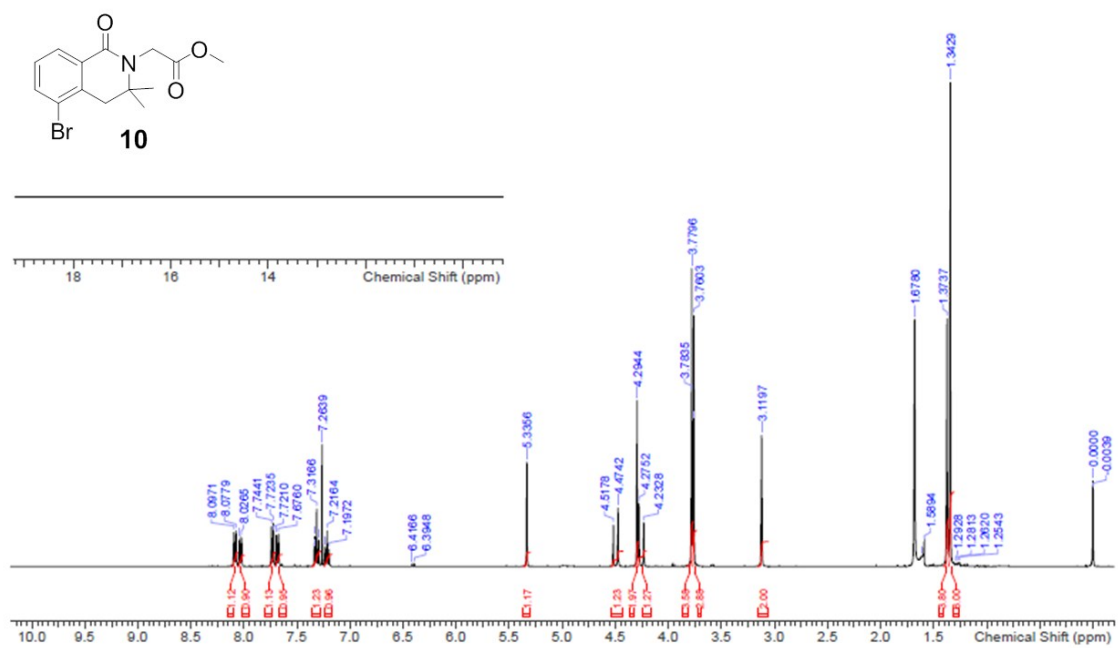
***N*-(1-(2-Bromophenyl)-2-methylpropan-2-yl)formamide (7).**



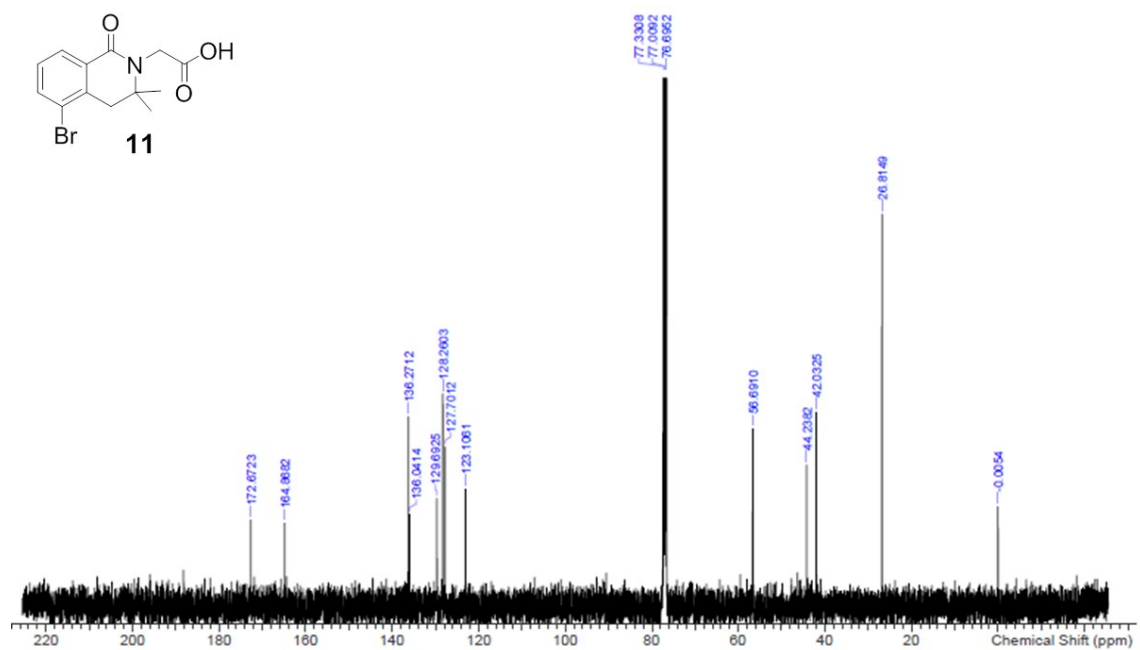
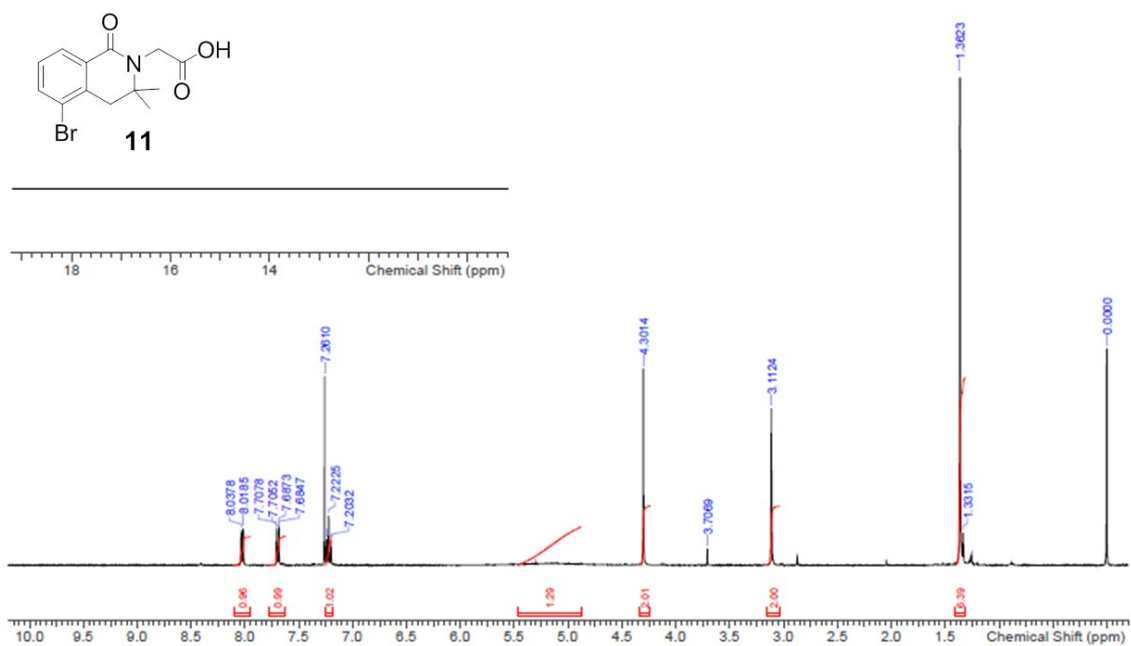
5-Bromo-2-(2-methoxy-2-oxoethyl)-3,3-dimethyl-3,4-dihydro-isoquinolin-2-ium bromide (9).



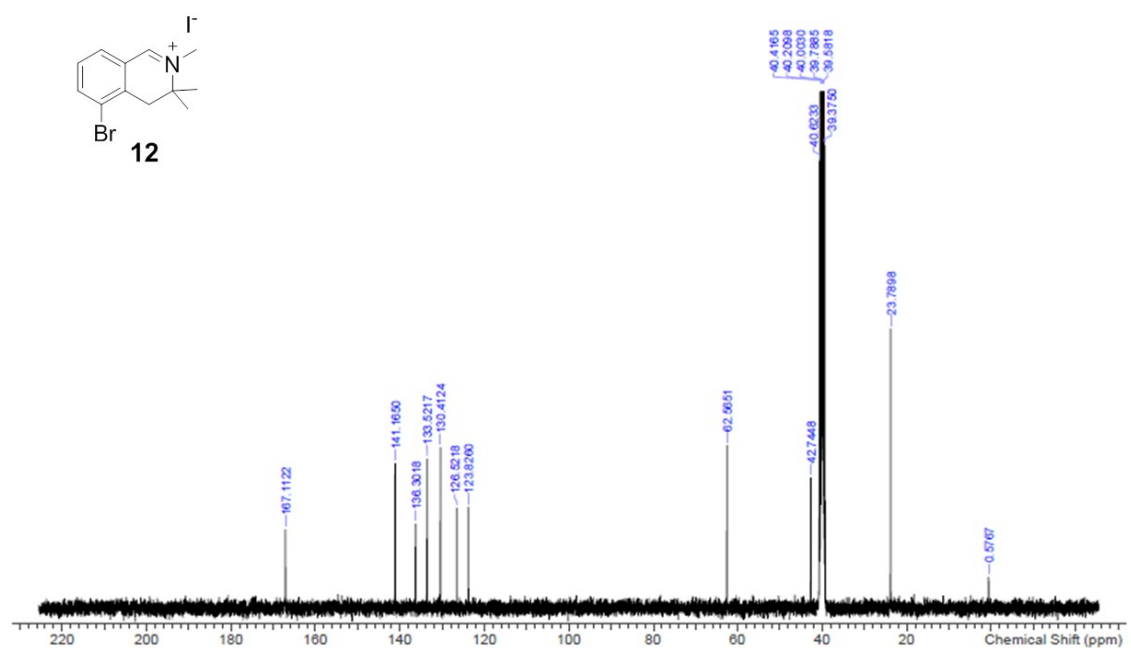
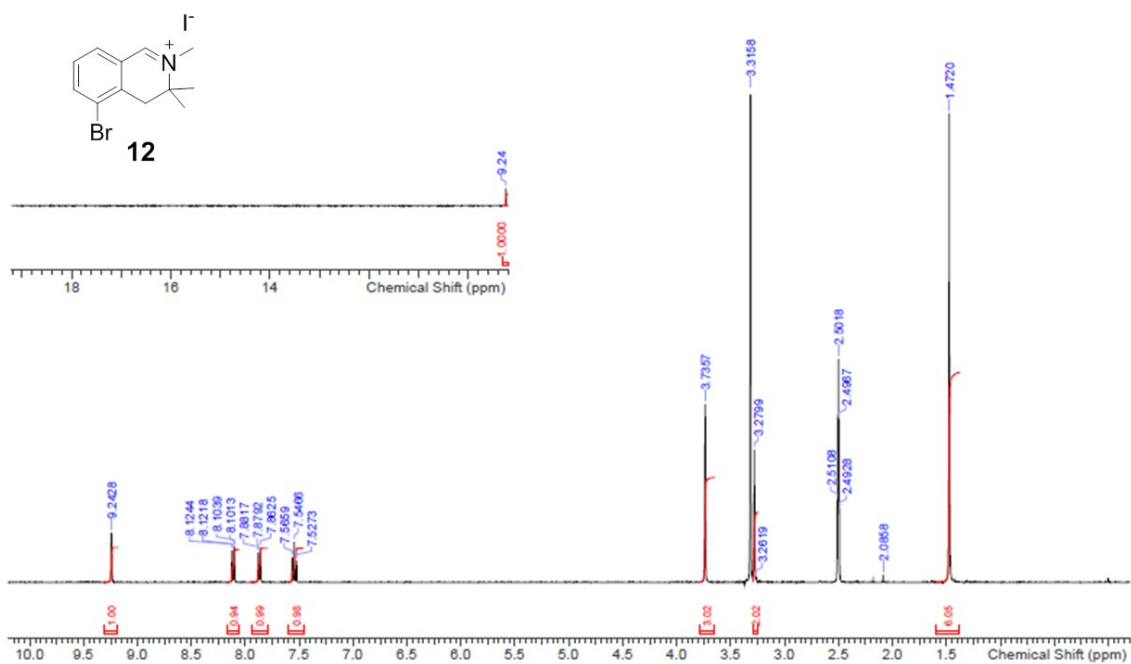
Methyl 2-(5-bromo-3,3-dimethyl-1-oxo-3,4-dihydroisoquinolin-2(1H)-yl)acetate (10).



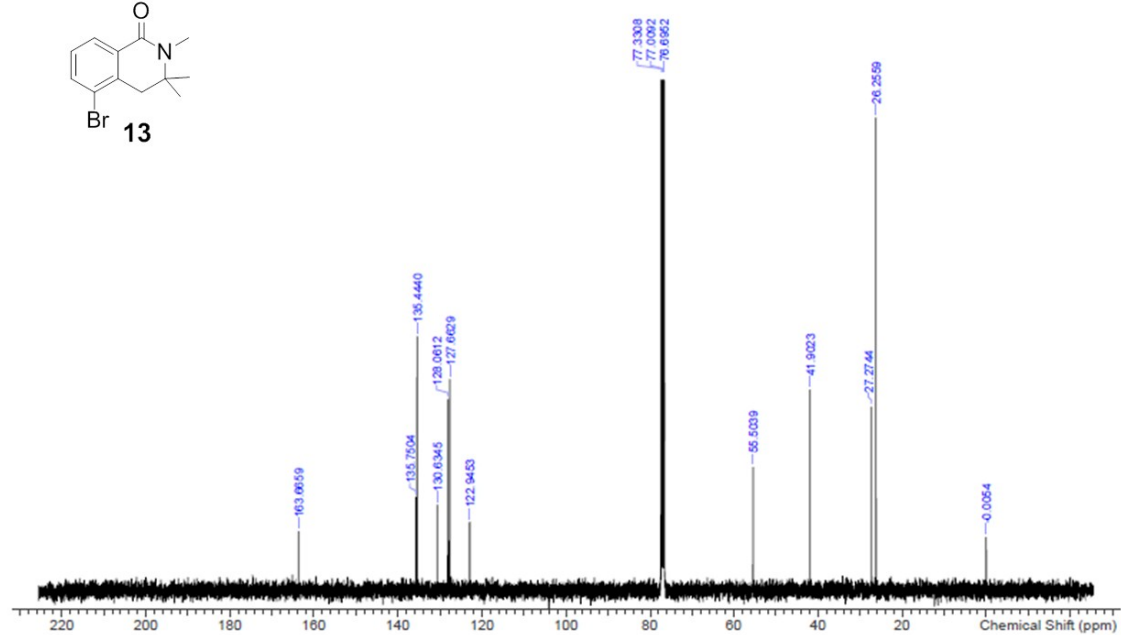
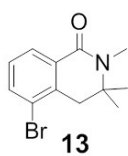
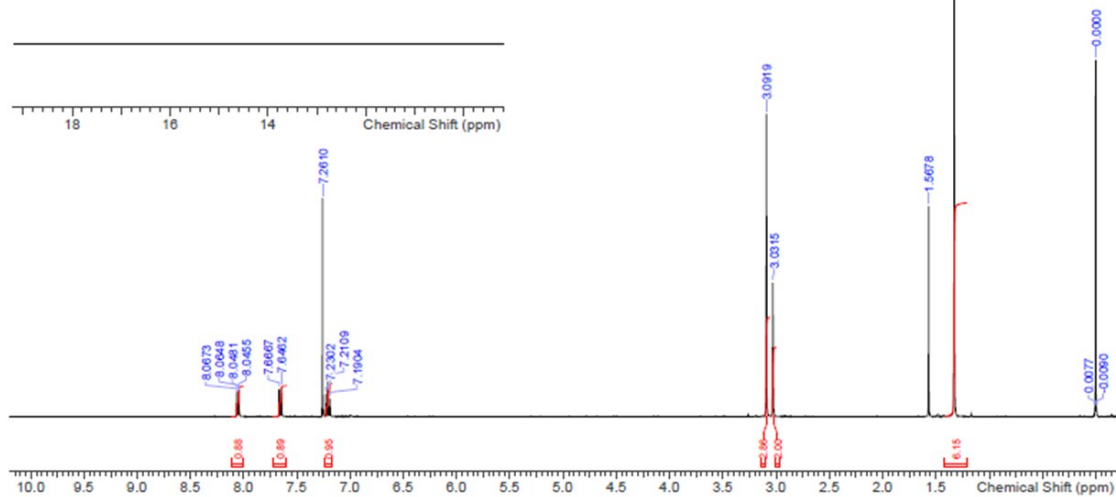
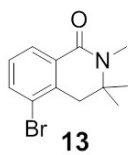
2-(5-Bromo-3,3-dimethyl-1-oxo-3,4-dihydroisoquinolin-2(1H)-yl)acetic acid (11).



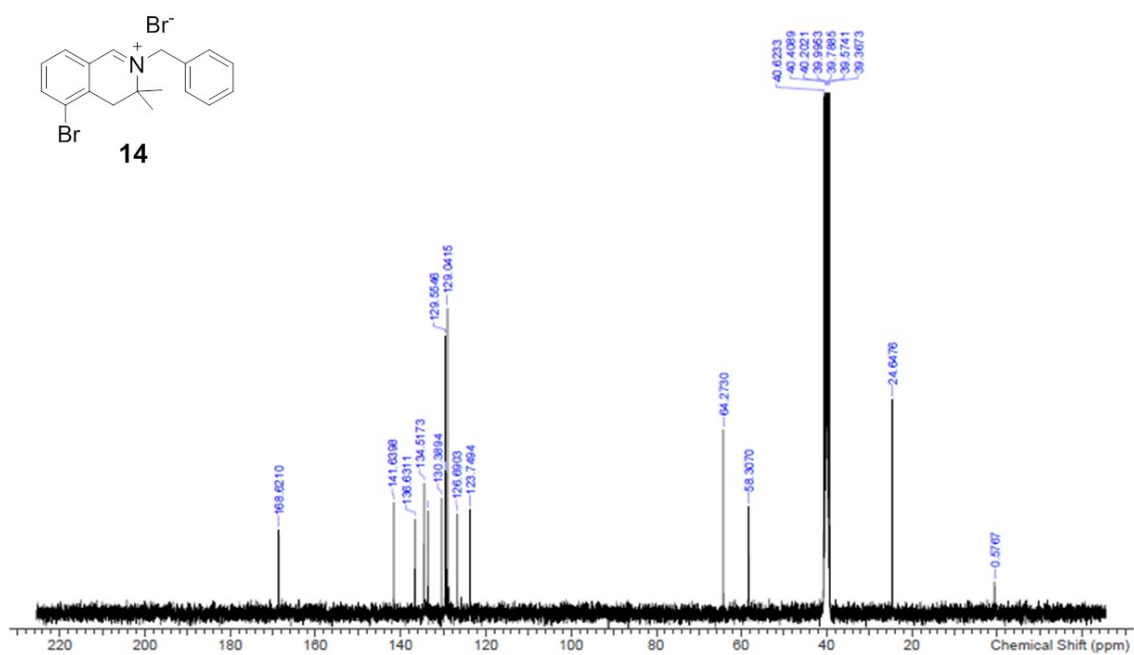
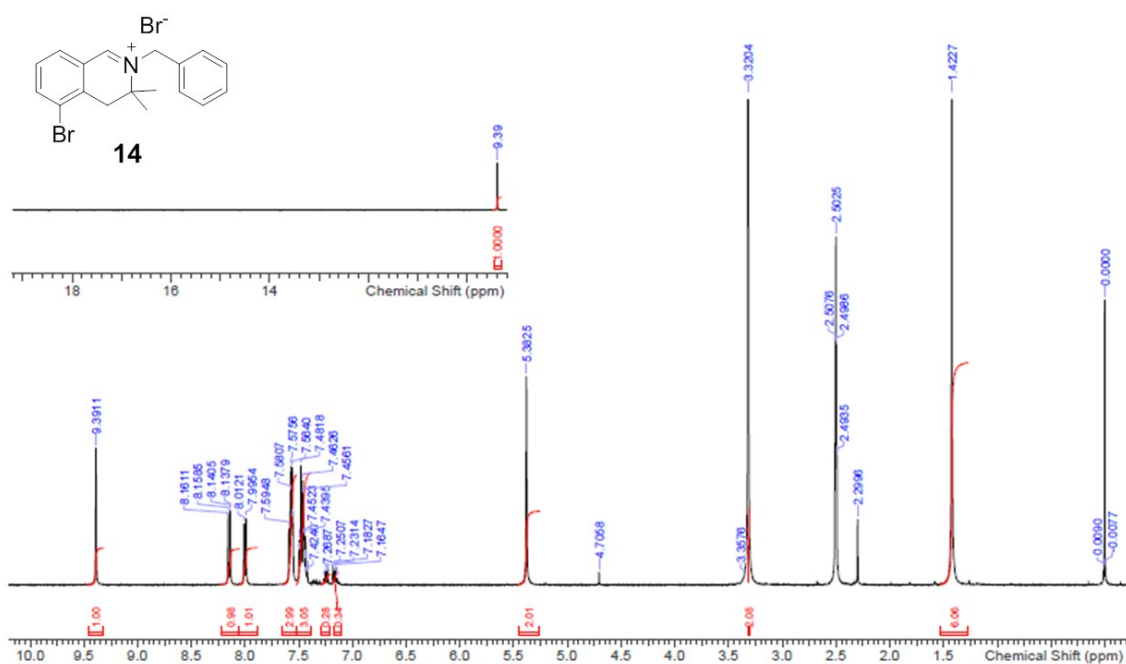
5-Bromo-2,3,3-trimethyl-3,4-dihydroisoquinolin-2-ium iodide (12).



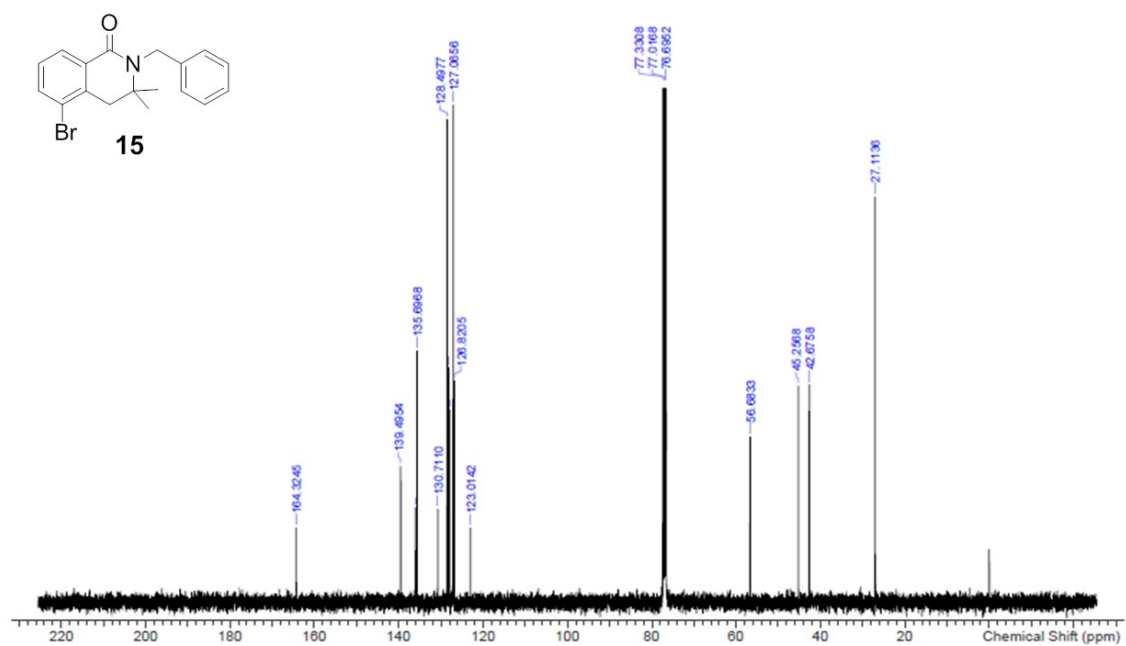
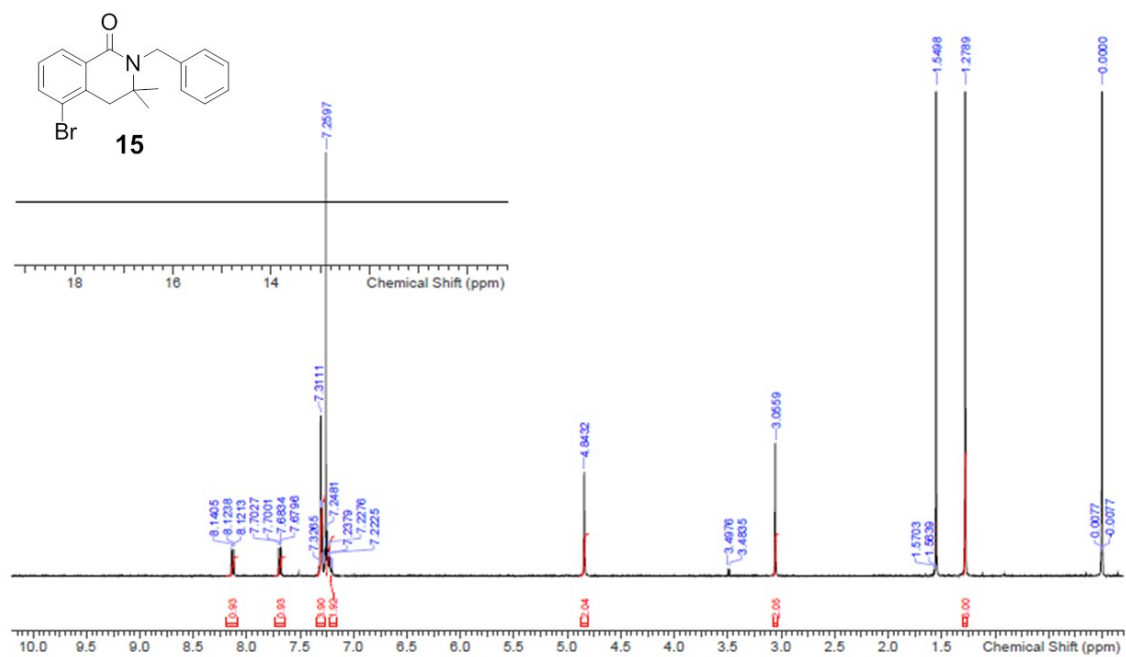
5-Bromo-2,3,3-trimethyl-3,4-dihydroisoquinolin-1(2H)-one (13).



2-Benzyl-5-bromo-3,3-dimethyl-3,4-dihydroisoquinolin-2-ium bromide (14).



2-Benzyl-5-bromo-3,3-dimethyl-3,4-dihydroisoquinolin-1(2H)-one (15).



1,2,3,4-tetrahydro-2-methyl-isoquinolinol intermediate(**18**).

