

Dynamic Kinetic Resolution of 1,3-Dihydro-2*H*-isoindole-1-carboxylic Acid Methyl Ester: Asymmetric Transformations Towards Isoindoline Carbamates

Roberto Morán-Ramallal,^a Vicente Gotor-Fernández,^a Pedro Laborda,^b
Francisco J. Sayago,^b Carlos Cativiela,^{b,*} and Vicente Gotor^{a,*}

Departamento de Química Orgánica e Inorgánica, Instituto Universitario de Biotecnología de Asturias, Universidad de Oviedo, 33006 Oviedo, Spain.

Departamento de Química Orgánica, Instituto de Síntesis Química y Catálisis Homogénea, Universidad de Zaragoza-CSIC, 50009 Zaragoza, Spain.

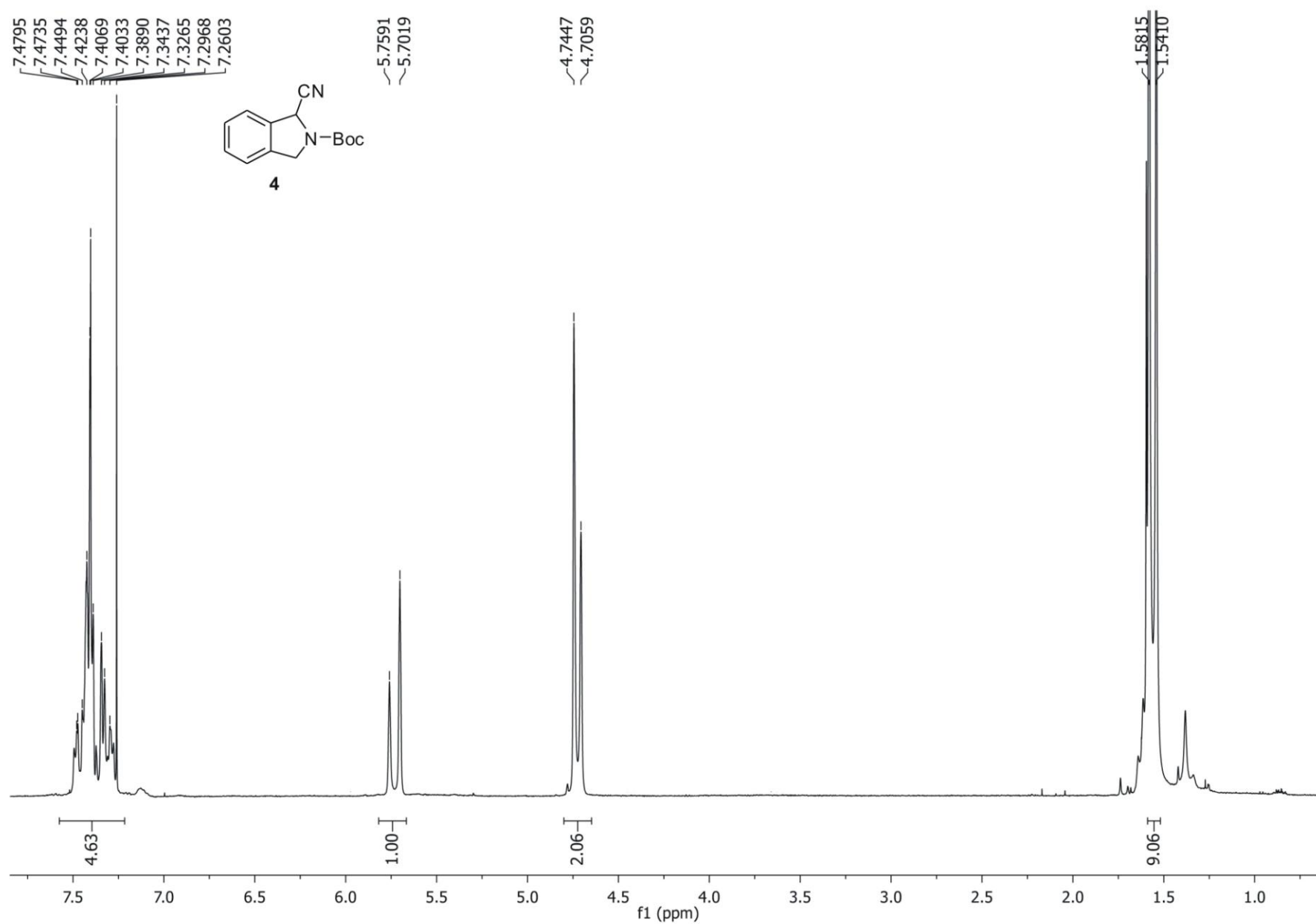
Fax: +34-985103448. vgs@uniovi.es

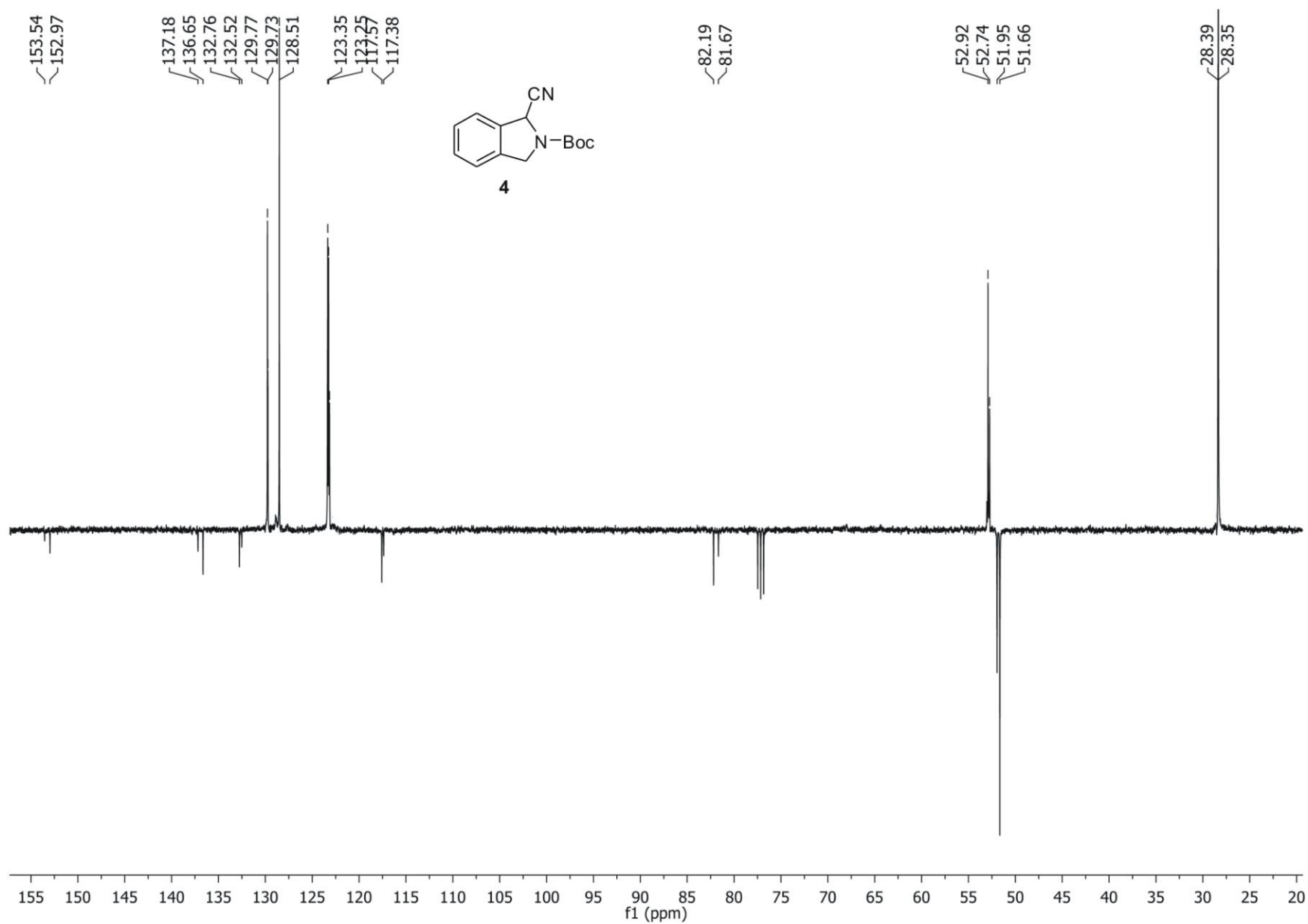
NMR SPECTRA (page 1 of 17 pages)

Table of Contents

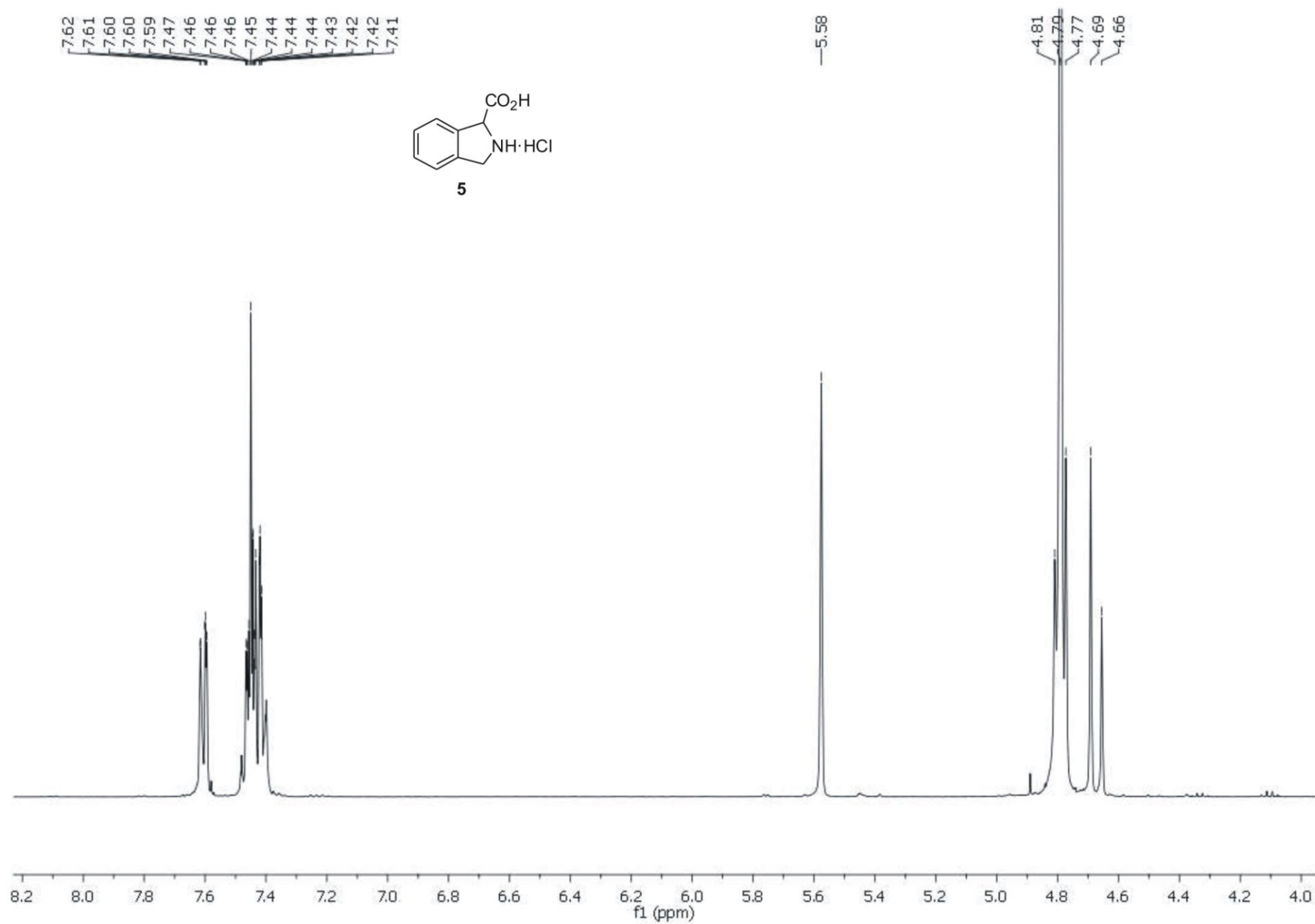
<i>tert</i> -Butyl 1-cyano-1,3-dihydro-2 <i>H</i> -isoindole-2-carboxylate (4)	S2
¹ H NMR spectrum	S2
APTC spectrum	S3
1,3-Dihydro-2 <i>H</i> -isoindole-1-carboxylic hydrochloride salt (5)	S4
¹ H NMR spectrum	S4
APTC spectrum	S5
Methyl 1,3-Dihydro-2 <i>H</i> -isoindole-1-carboxylate (6)	S6
¹ H NMR spectrum	S6
¹³ C NMR spectrum	S7
2-Benzyl-1-methyl 1,3-dihydro-2 <i>H</i> -isoindole-1,2-dicarboxylate (7)	S8
¹ H NMR spectrum	S8
¹³ C NMR spectrum	S9
2-[(Benzyloxy)carbonyl]-1,3-dihydro-2 <i>H</i> -isoindole-1-carboxylic acid (8)	S10
¹ H NMR spectrum	S10
¹³ C NMR spectrum	S11
2-Allyl-1-methyl 1,3-dihydro-2 <i>H</i> -isoindole-1,2-dicarboxylate (10)	S12
¹ H NMR spectrum	S12
¹³ C NMR spectrum	S13
¹ H NMR of Methyl (1 <i>R</i> / <i>S</i> , 2' <i>R</i>)-2-(3,3,3-trifluoro-2-methoxy-2-phenylpropanoyl)-1,3-dihydro-2 <i>H</i> - isoindole-1-carboxylate (<i>rac</i> -12)	S14
¹ H NMR of Methyl (1 <i>R</i> , 2' <i>R</i>)-2-(3,3,3-trifluoro-2-methoxy-2-phenylpropanoyl)-1,3-dihydro-2 <i>H</i> - isoindole-1-carboxylate [(<i>R</i>)-12]	S16

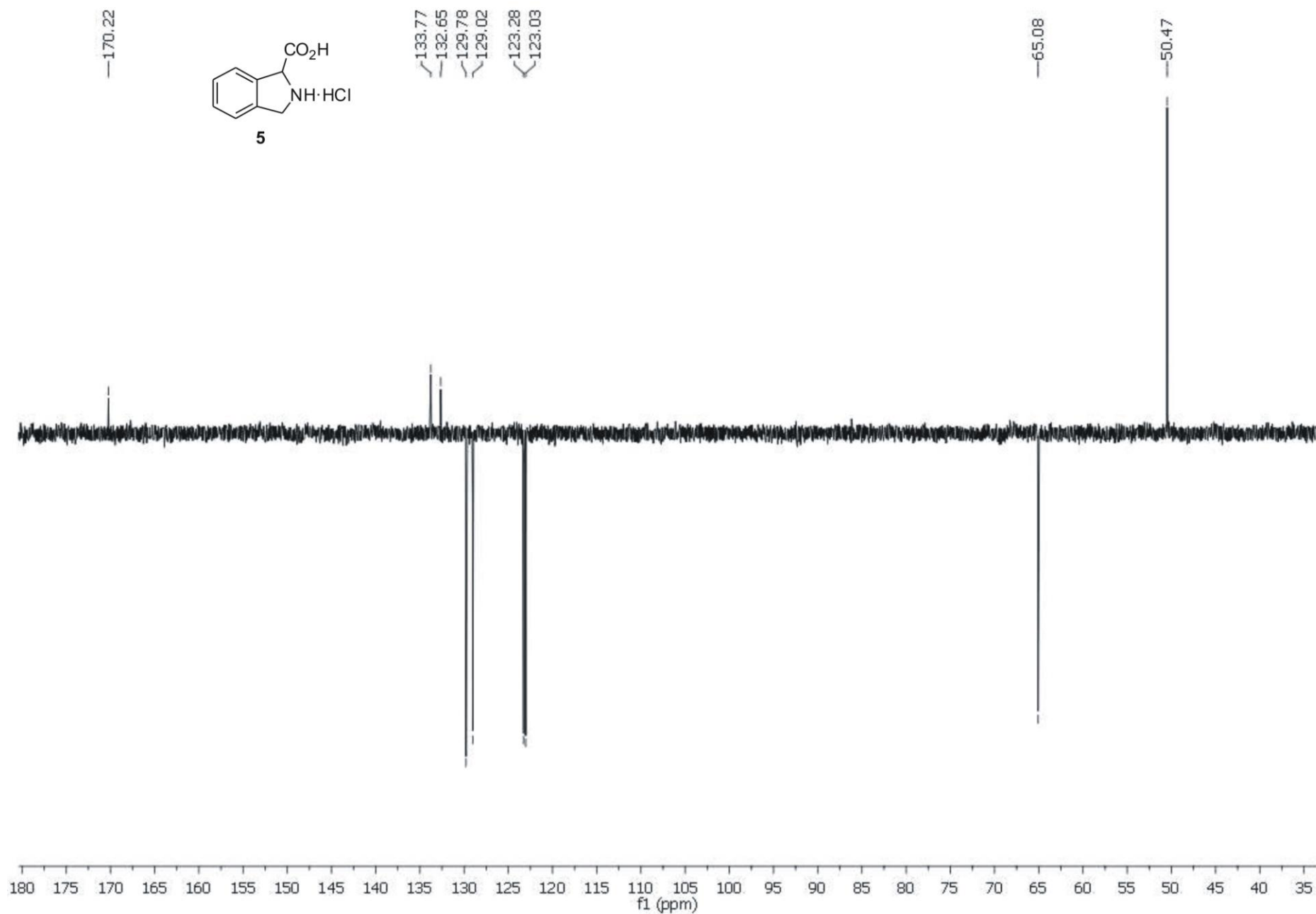
***tert*-Butyl 1-cyano-1,3-dihydro-2*H*-isoindole-2-carboxylate (4)**



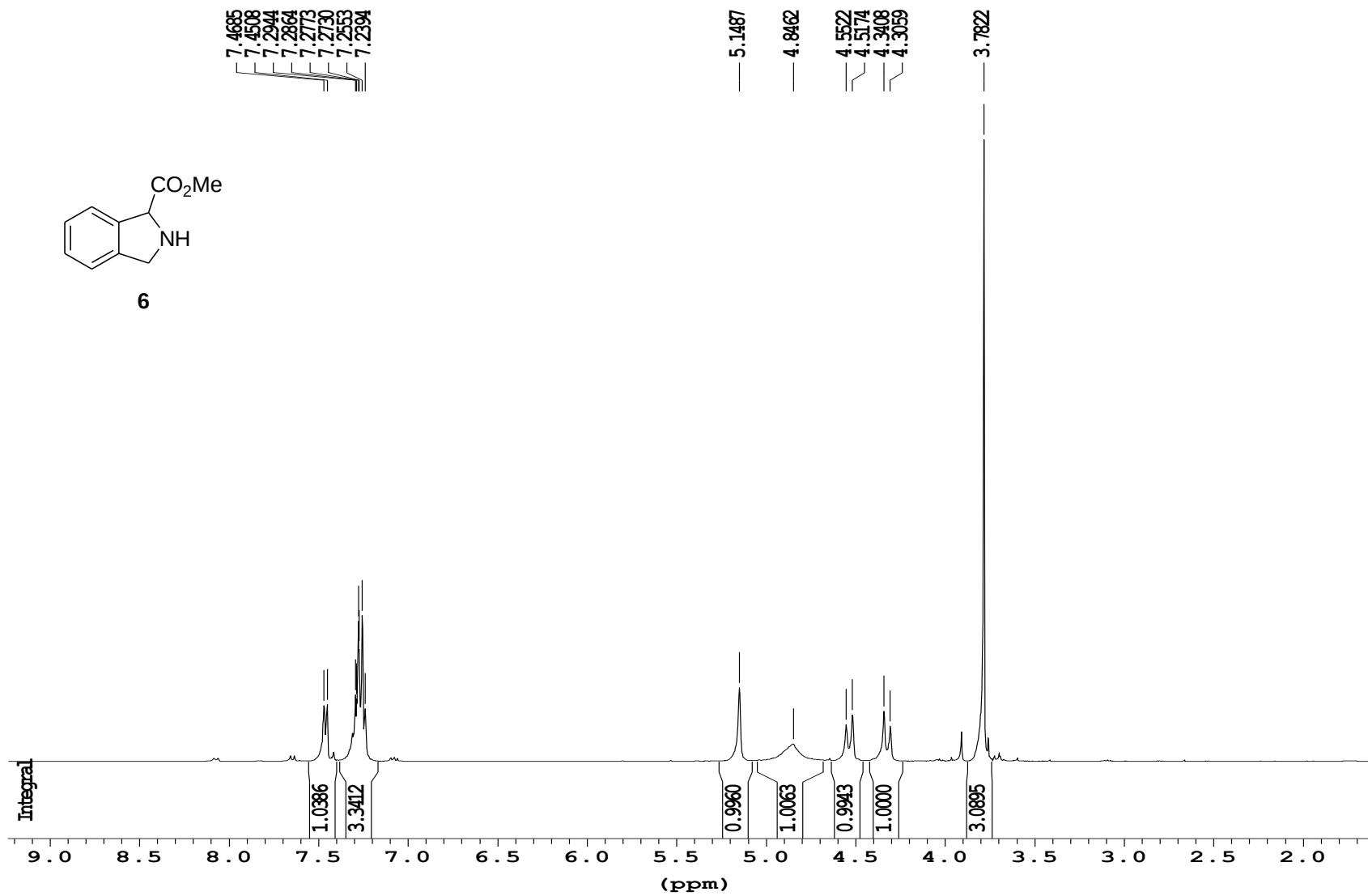


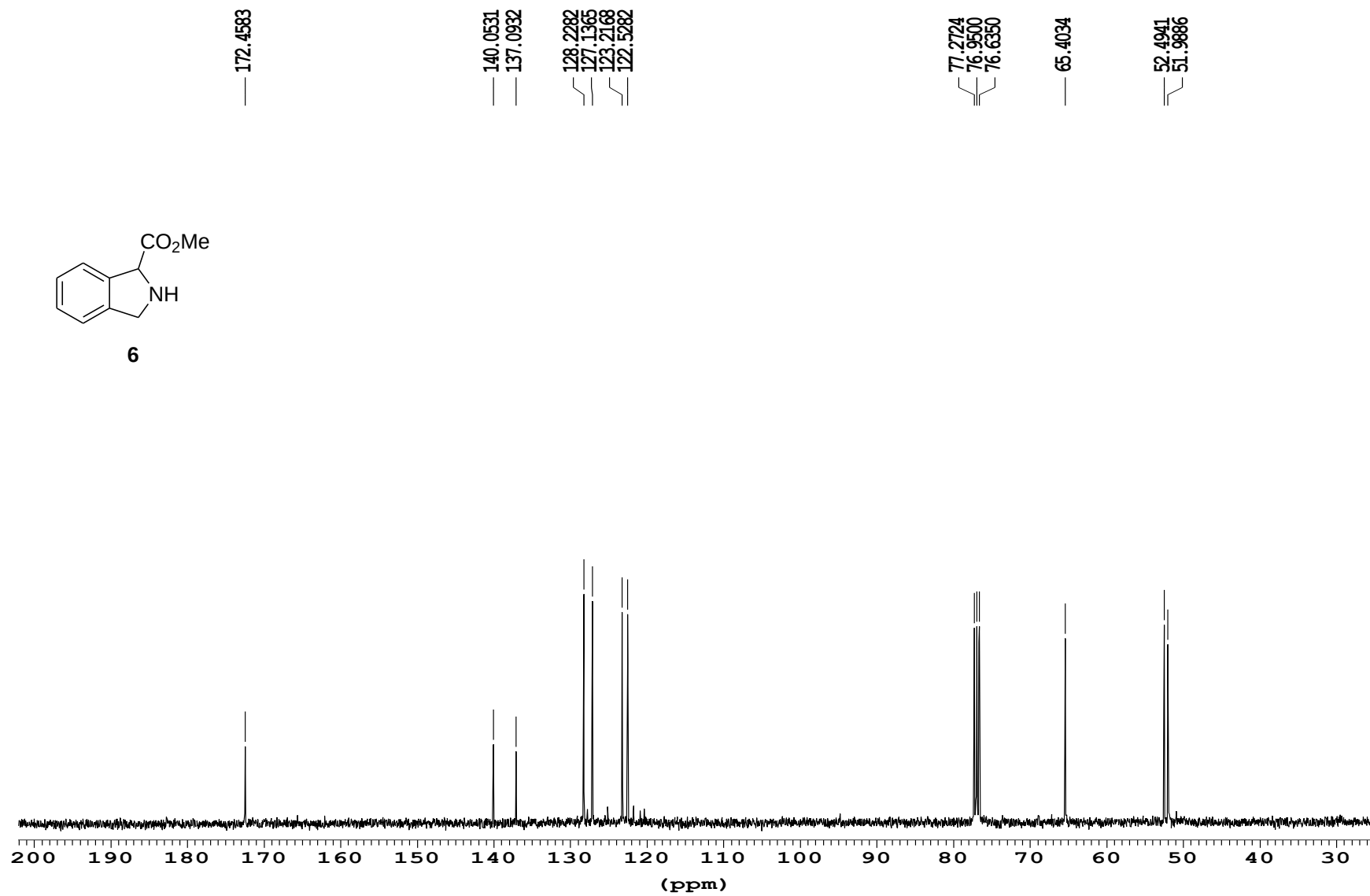
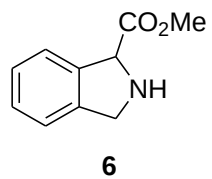
1,3-Dihydro-2*H*-isoindole-1-carboxylic acid hydrochloride salt (5)



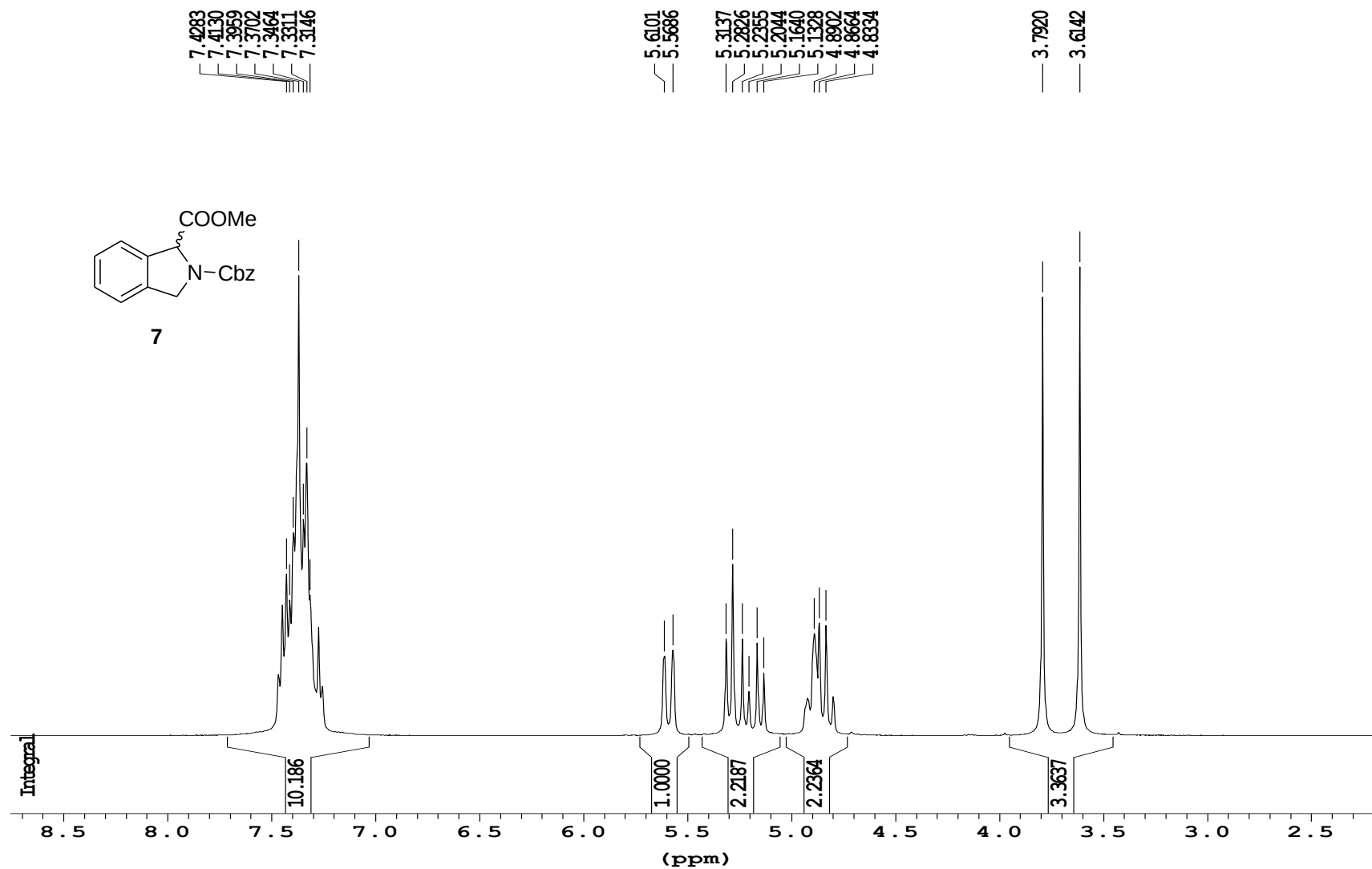


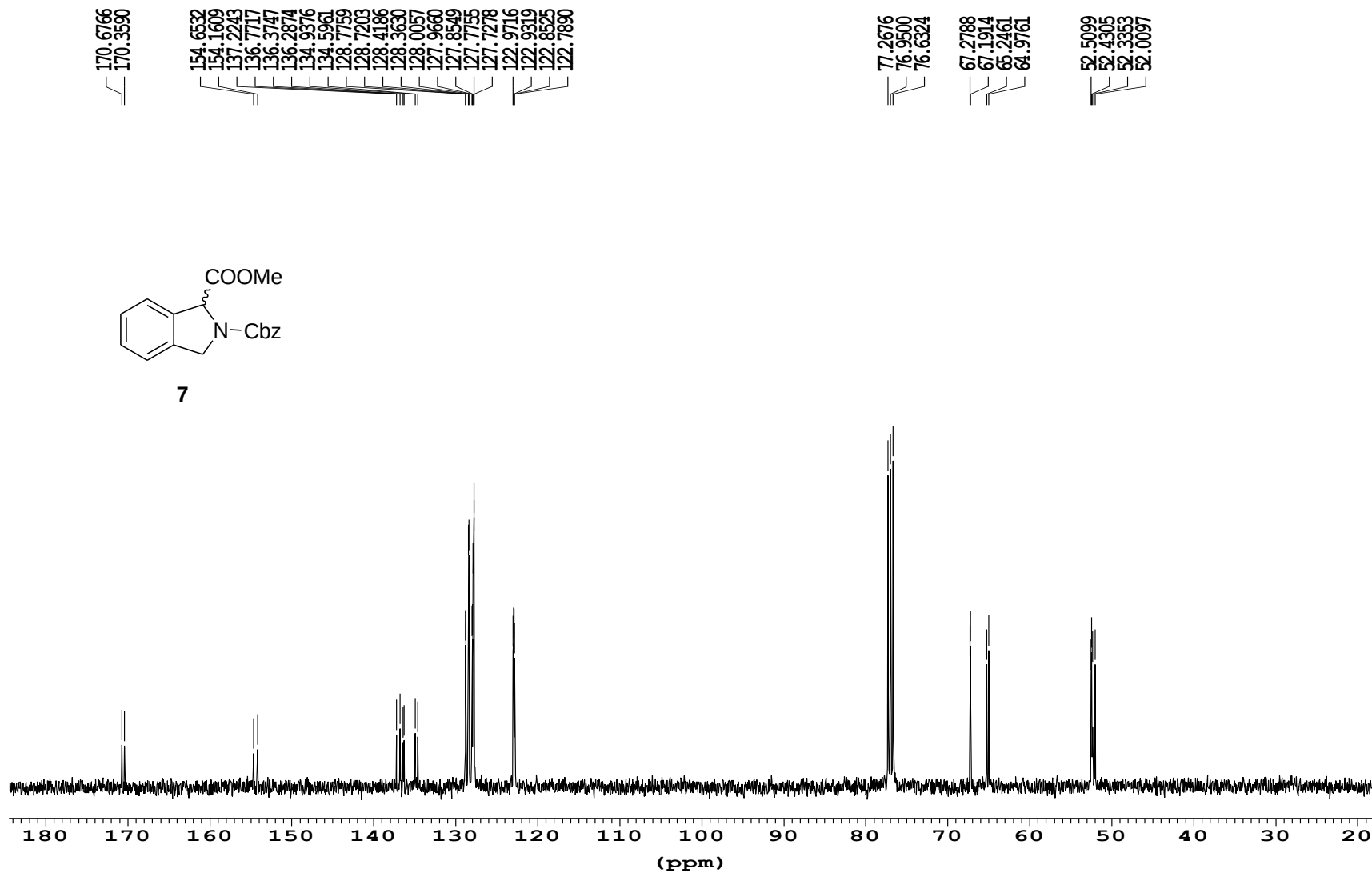
1,3-Dihydro-2*H*-isoindole-1-carboxylic acid methyl ester (6)



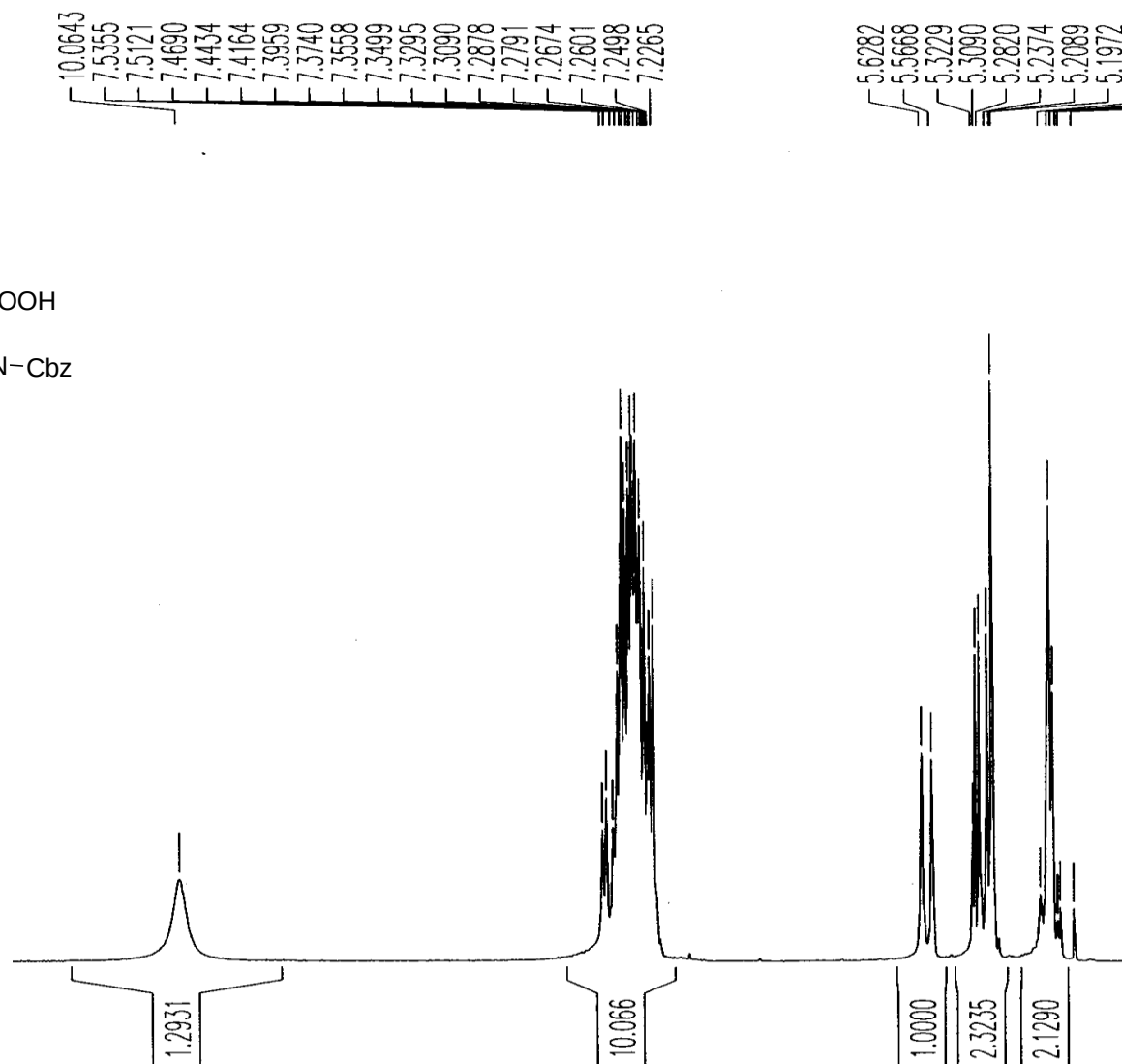
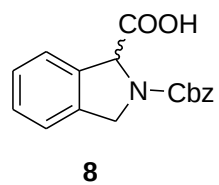


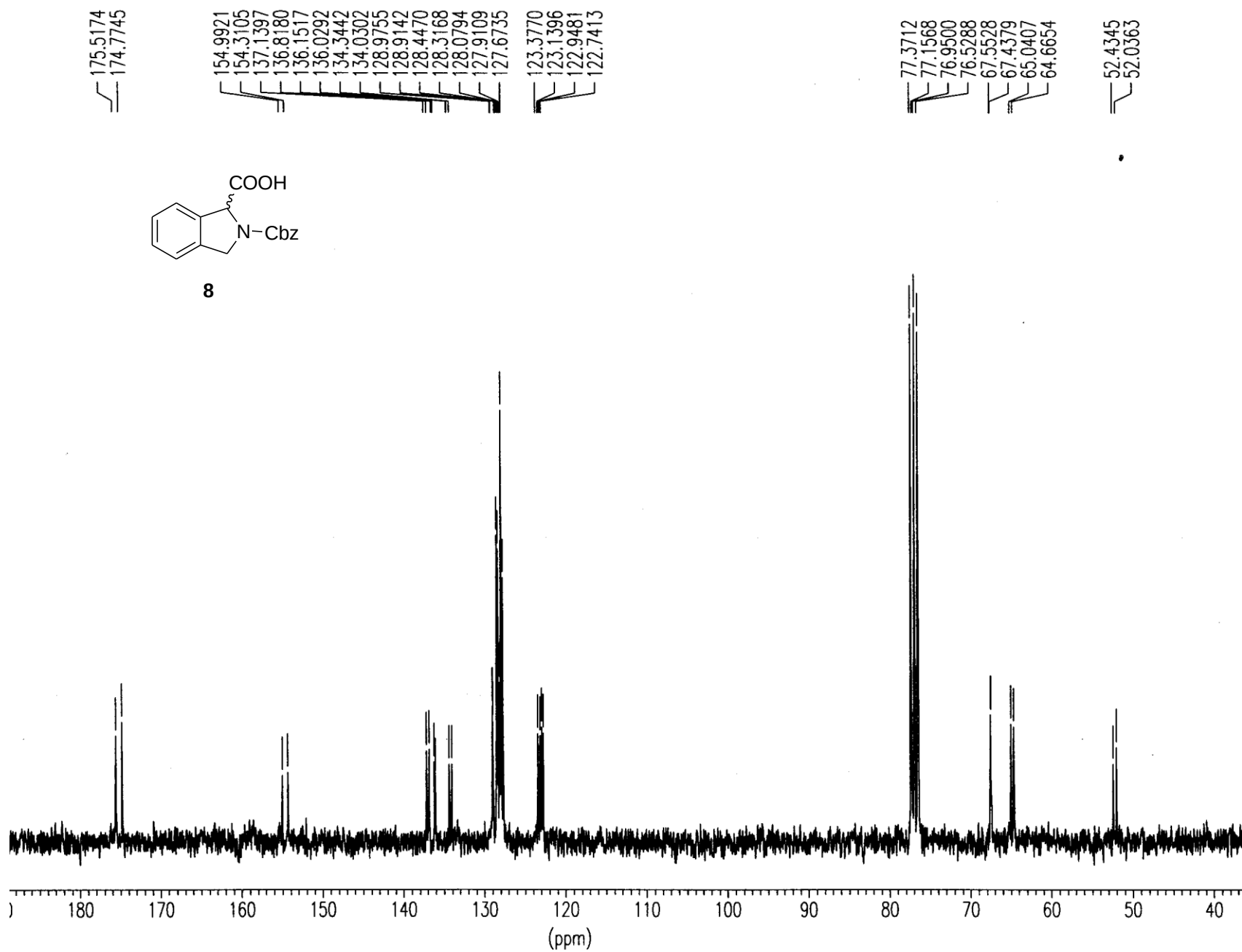
2-Benzyl-1-methyl 1,3-dihydro-2*H*-isoindole-1,2-dicarboxylate (7)



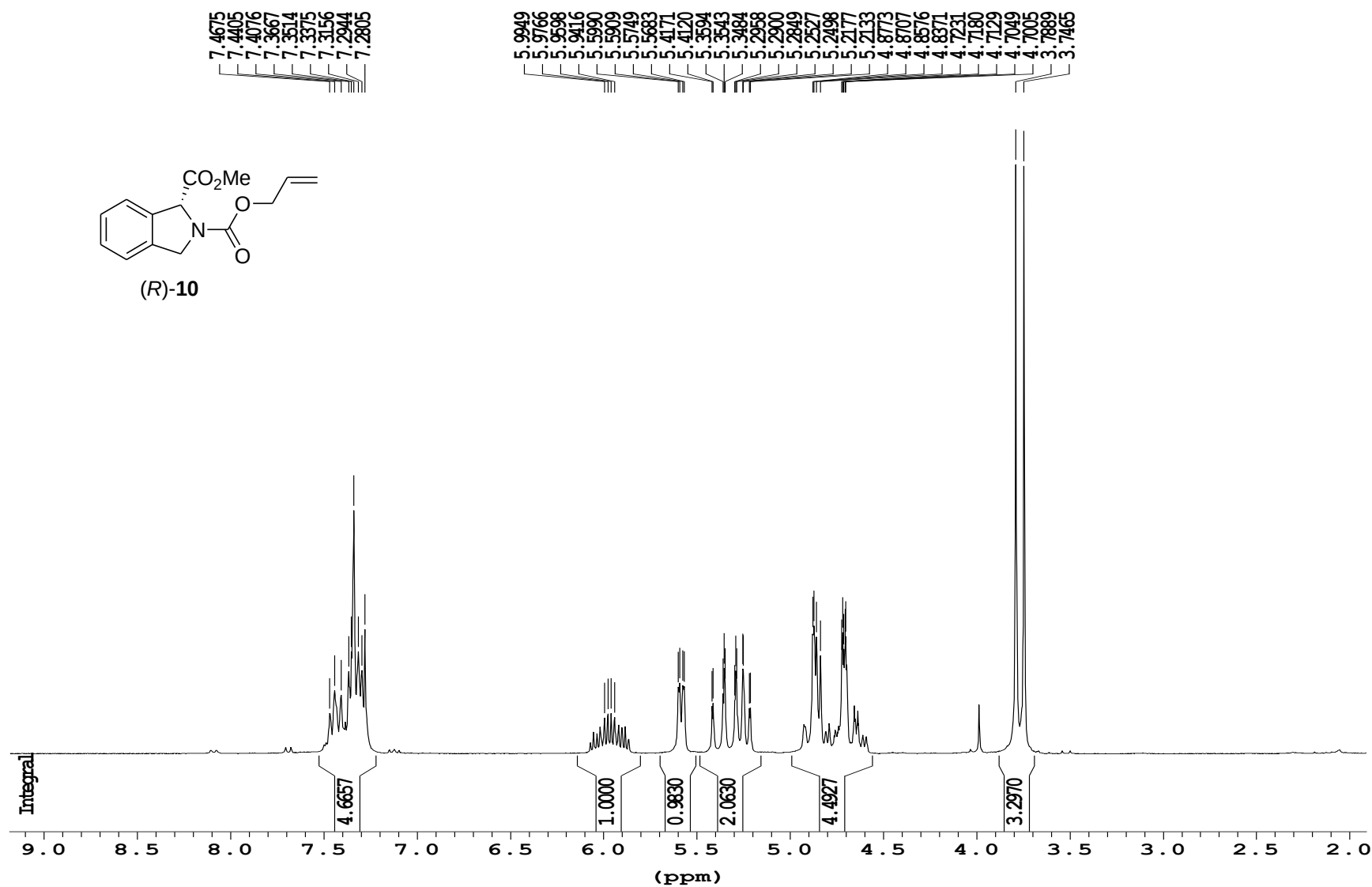


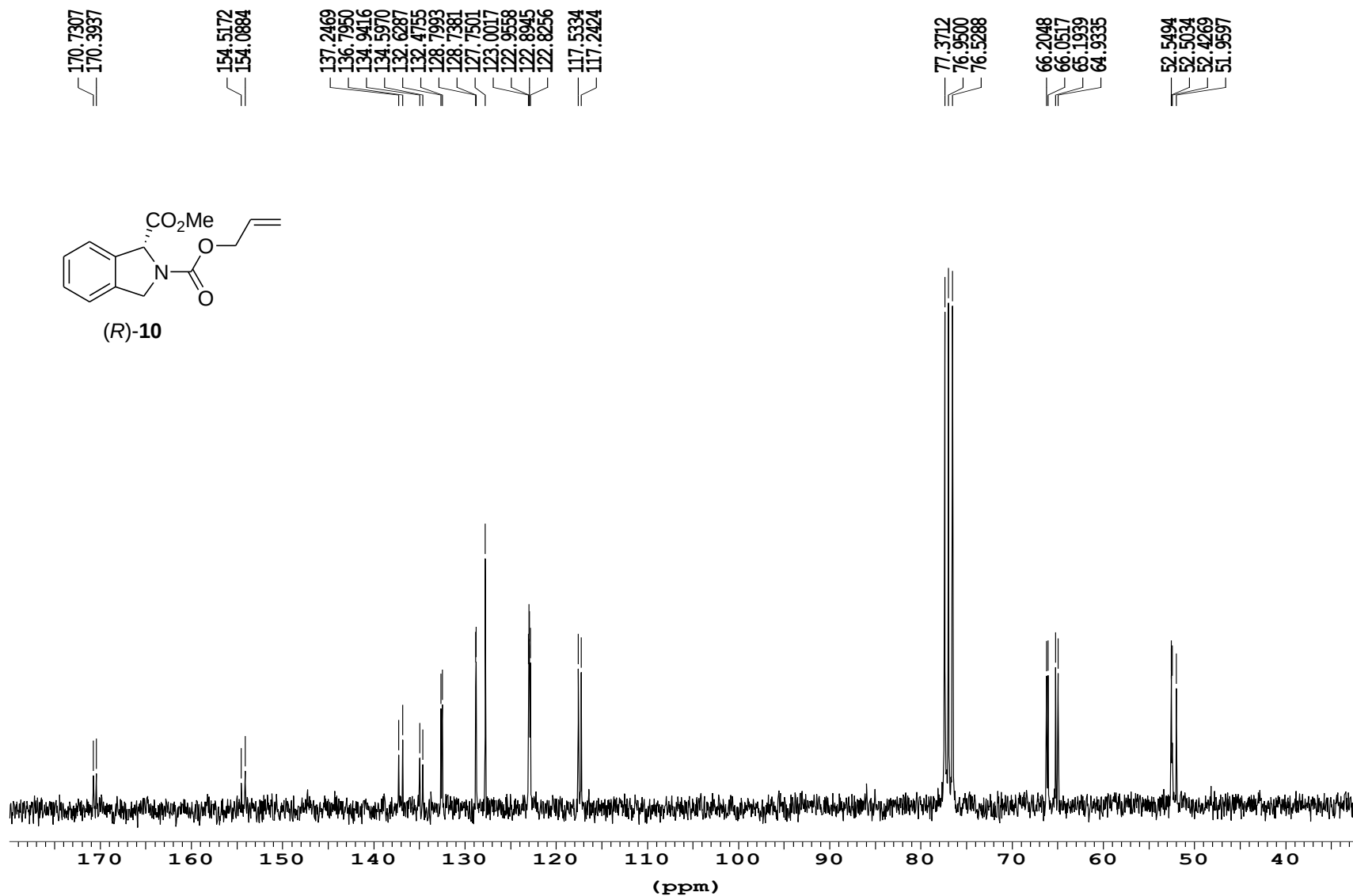
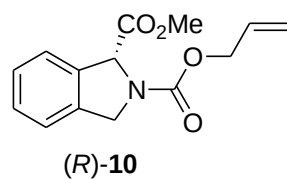
2-[(Benzyloxy)carbonyl]-1,3-dihydro-2*H*-isoindole-1-carboxylic acid (8)



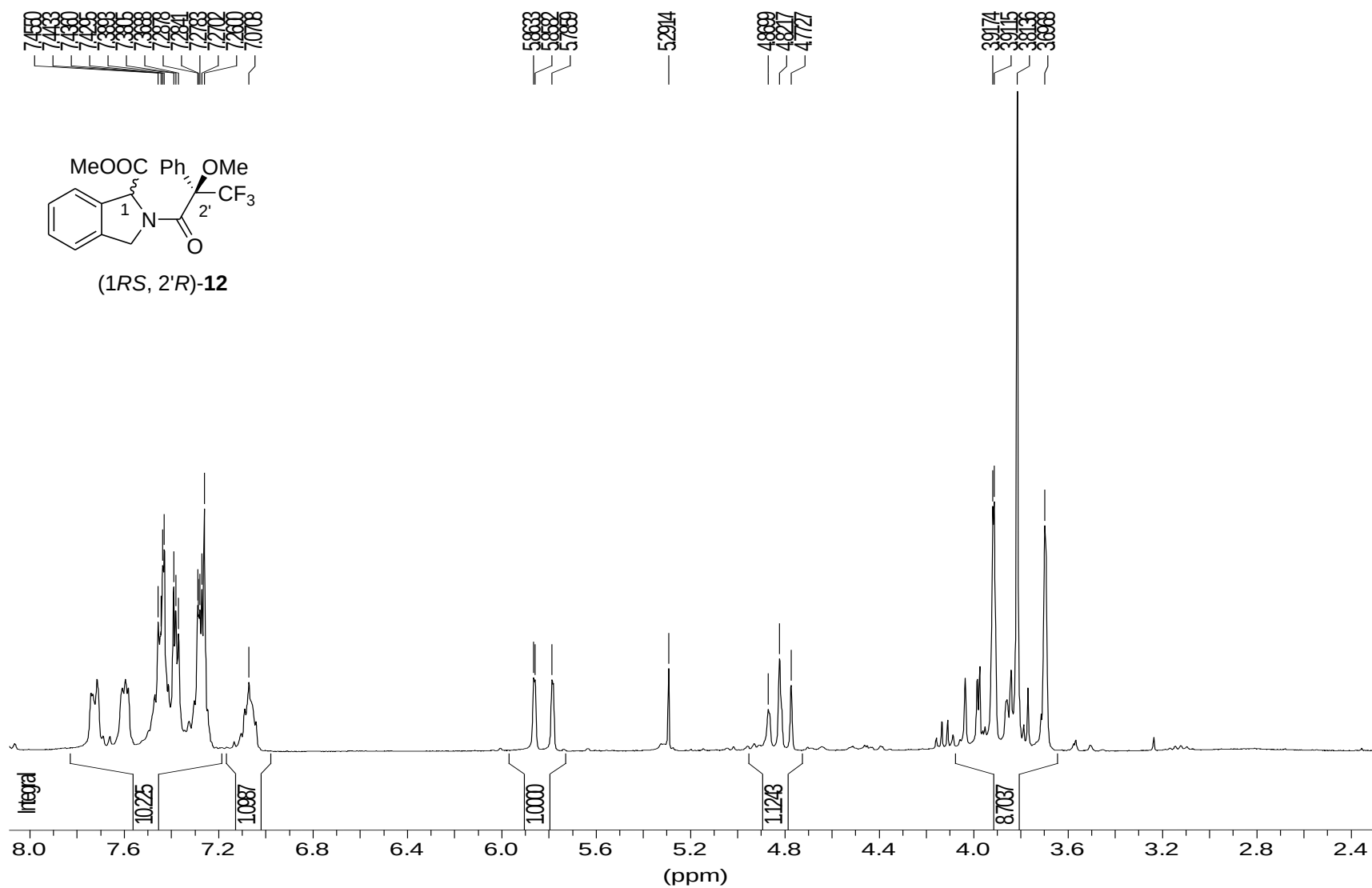


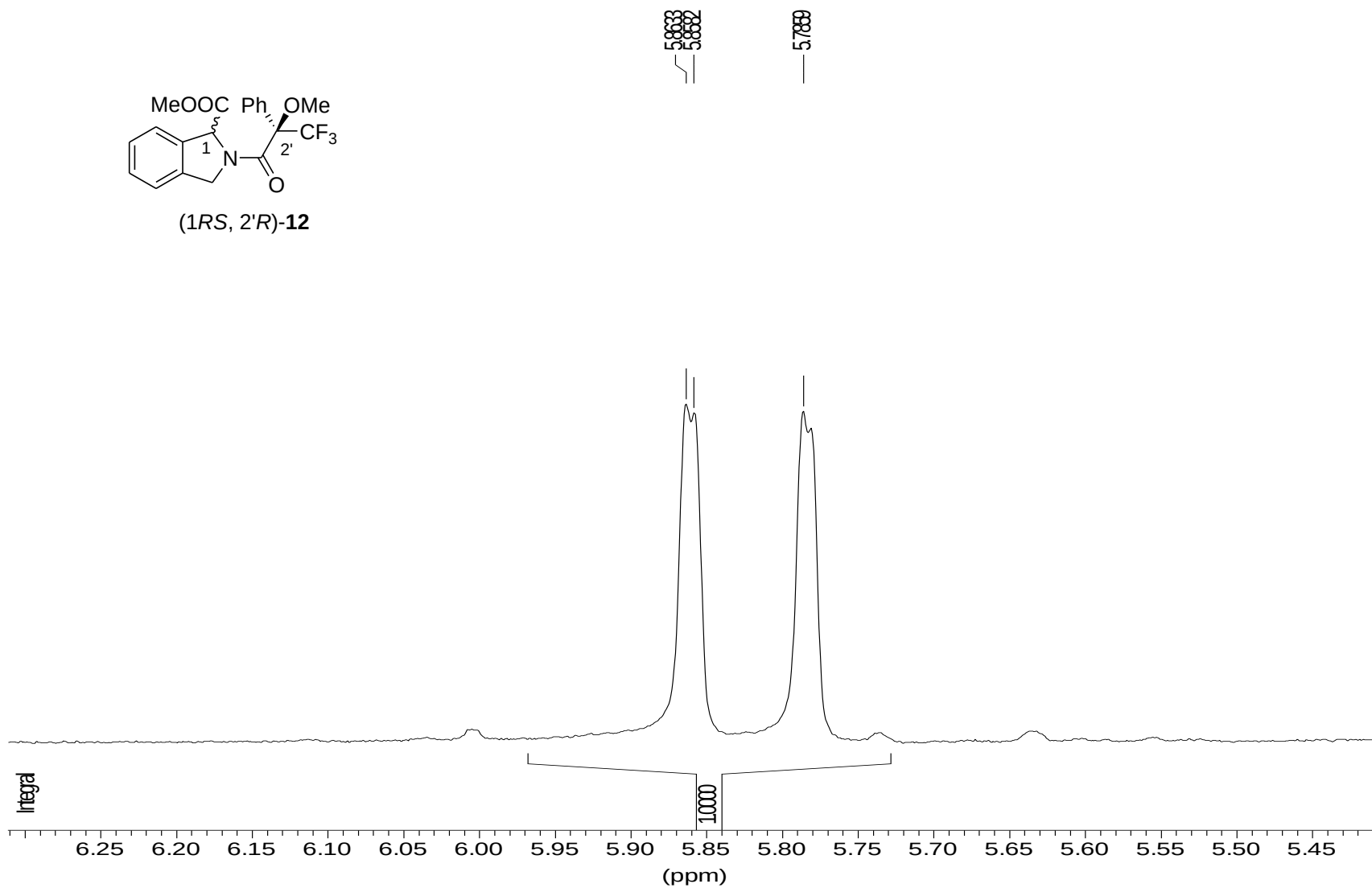
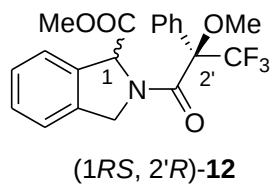
2-Allyl-1-methyl 1,3-dihydro-2*H*-isoindole-1,2-dicarboxylate (10)





Methyl (1*R*/*S*, 2'*R*)-2-(3,3,3-trifluoro-2-methoxy-2-phenylpropanoyl)-1,3-dihydro-2*H*-isoindole-1-carboxylate (*rac*-12)





Methyl (1*R*, 2'*R*)-2-(3,3,3-trifluoro-2-methoxy-2-phenylpropanoyl)-1,3-dihydro-2*H*-isoindole-1-carboxylate [(*R*)-12]

