

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.

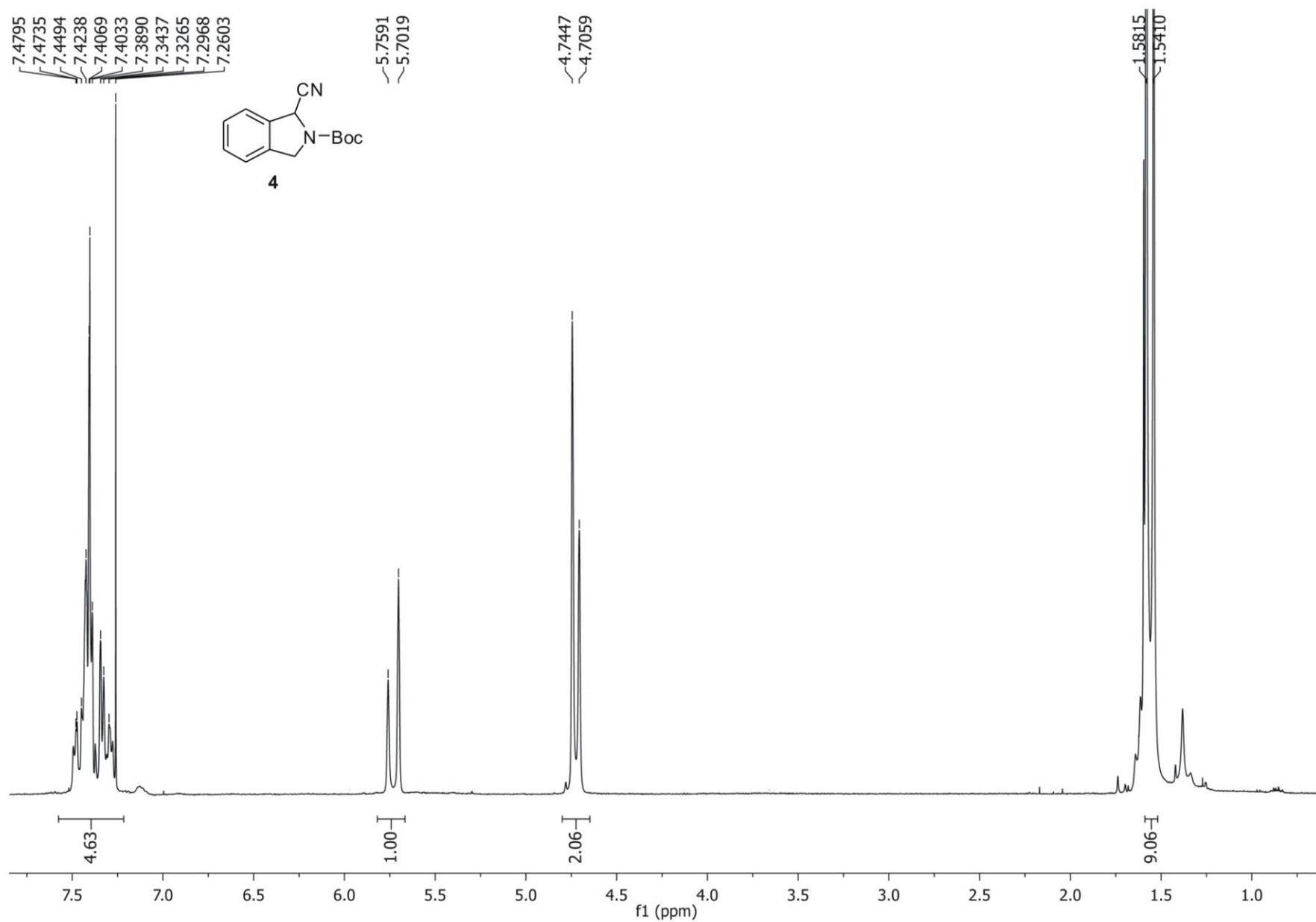
Fax: +34-985103448. vgs@uniovi.es

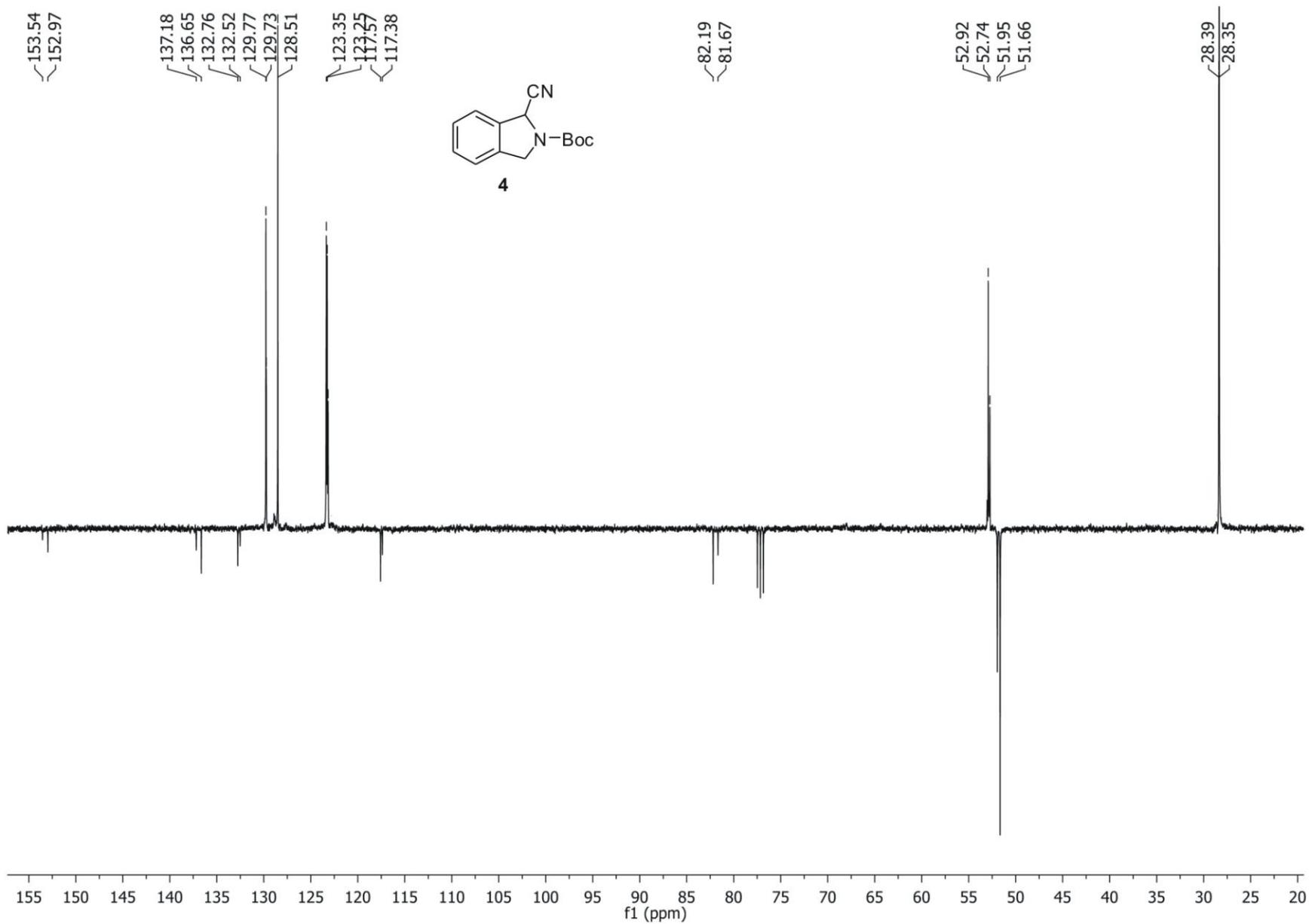
NMR SPECTRA (page 1 of 17 pages)

Table of Contents

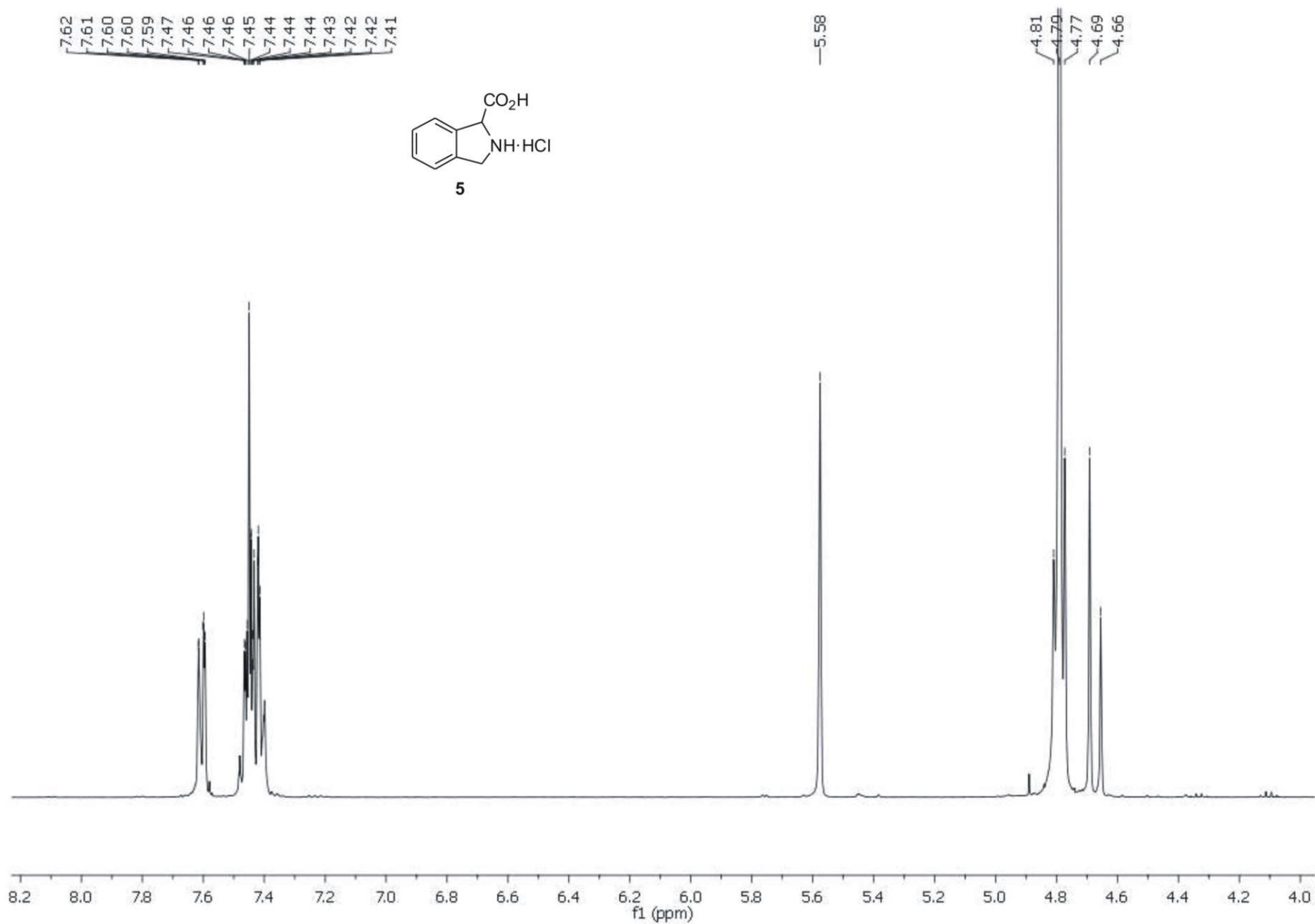
<i>tert</i> -Butyl 1-cyano-1,3-dihydro-2 <i>H</i> -isoindole-2-carboxylate (4)	S2
¹ H NMR spectrum	S2
APTC spectrum	S3
1,3-Dihydro-2 <i>H</i> -isoindole-1-carboxylic hydrochloride salt (5)	S4
¹ H NMR spectrum	S4
APTC spectrum	S5
Methyl 1,3-Dihydro-2 <i>H</i> -isoindole-1-carboxylate (6)	S6
¹ H NMR spectrum	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> /S, 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

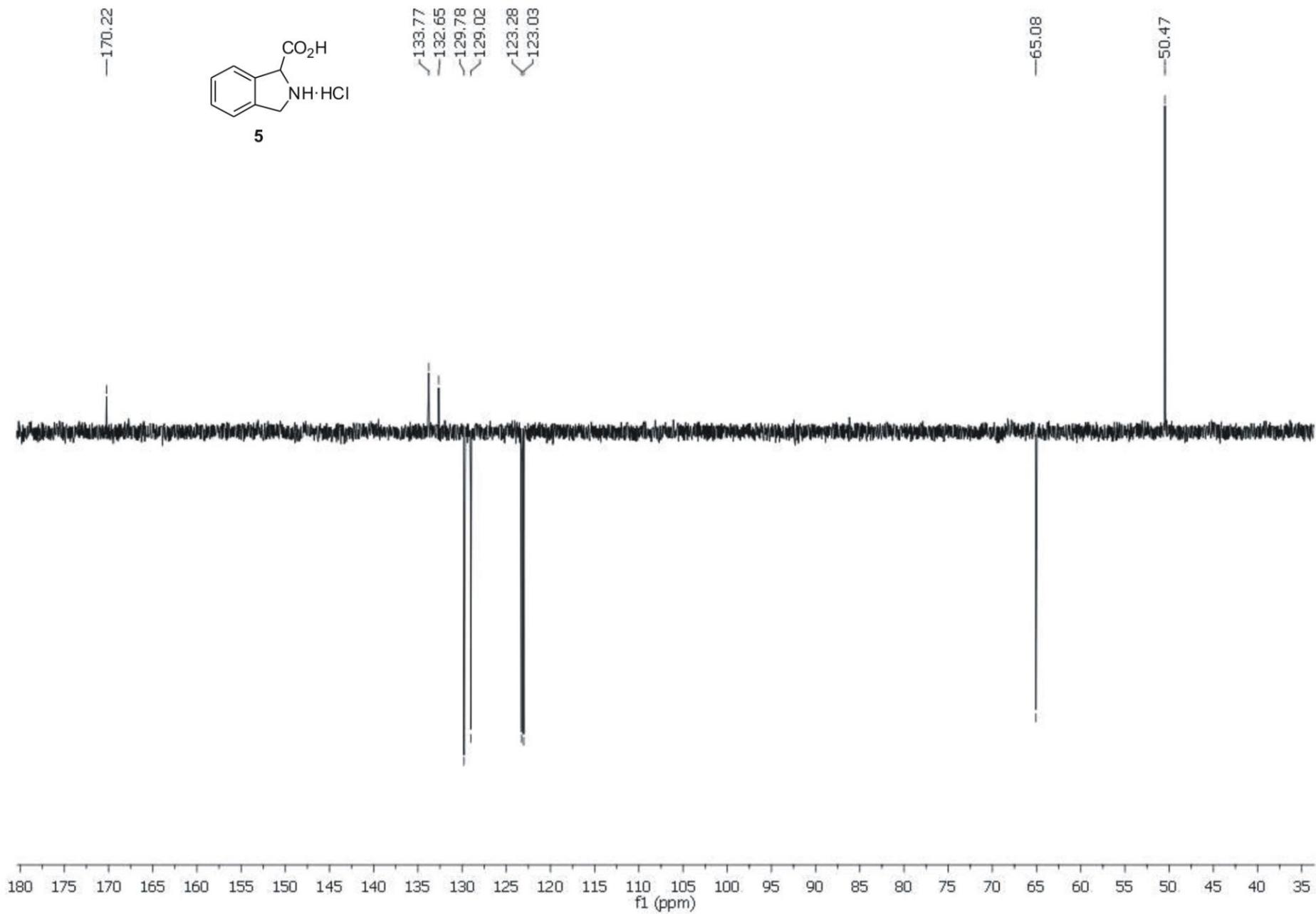
***tert*-Butyl 1-cyano-1,3-dihydro-2*H*-isoindole-2-carboxylate (4)**



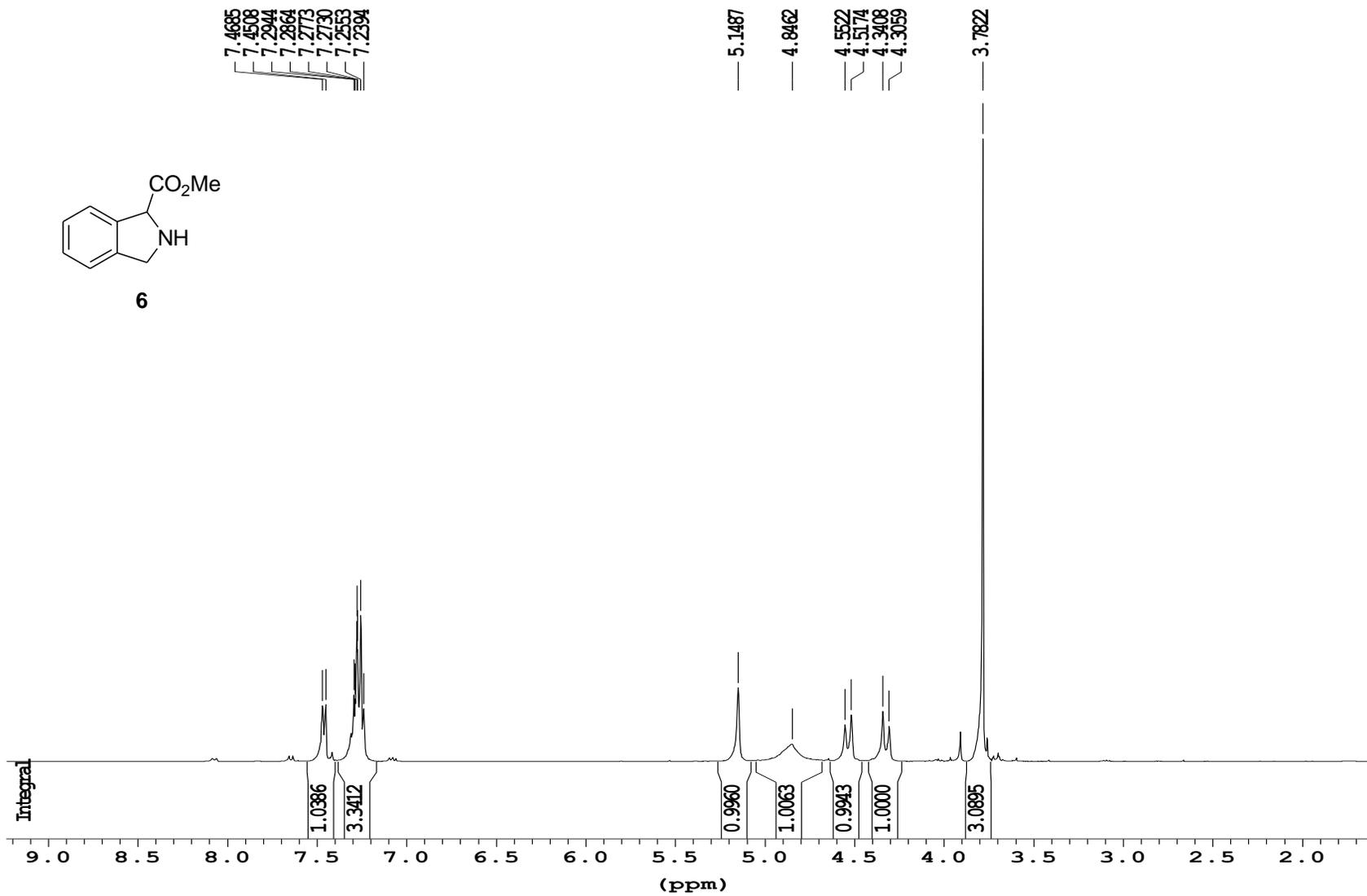
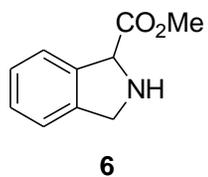


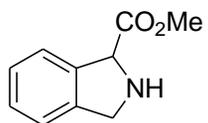
1,3-Dihydro-2*H*-isoindole-1-carboxylic acid hydrochloride salt (5)





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





6

— 172.4583

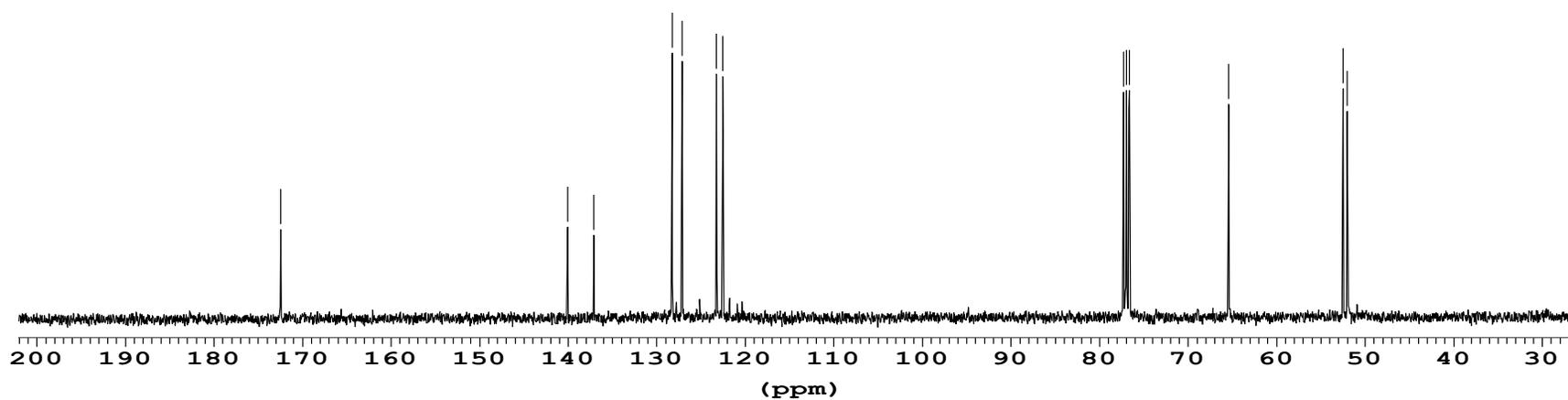
— 140.0531
— 137.0932

128.2282
127.1365
123.2168
122.5282

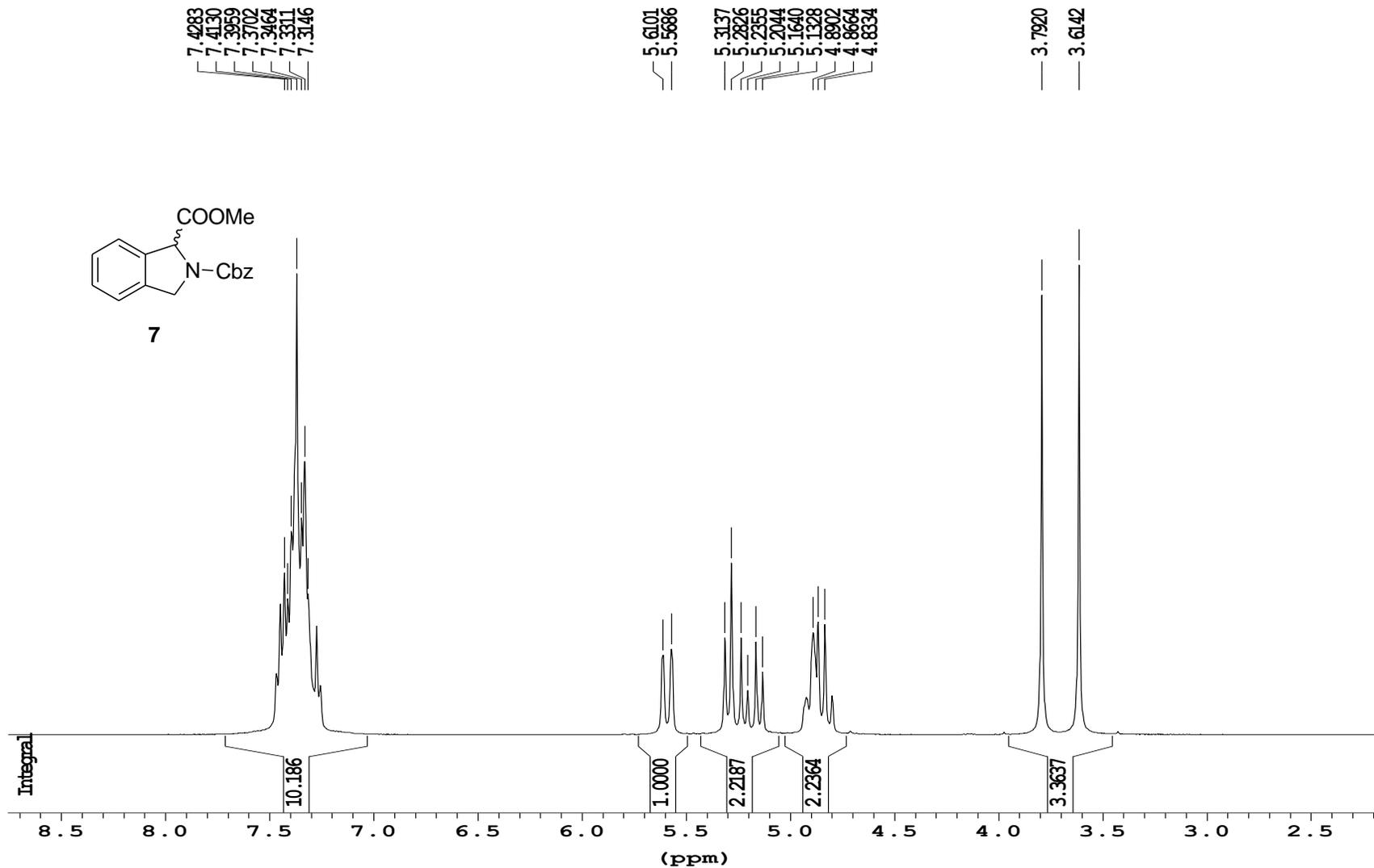
77.2724
76.9500
76.6350

— 65.4034

52.4941
51.9886



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



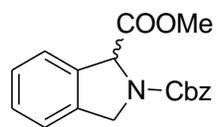
170.6766
170.3590

154.6532
154.1609
137.2243
136.7717
136.3747
136.2874
134.9376
134.5961
128.7759
128.7203
128.4186
128.3630
128.0057
127.9660
127.8549
127.7755
127.7278
122.9716
122.9319
122.8525
122.7890

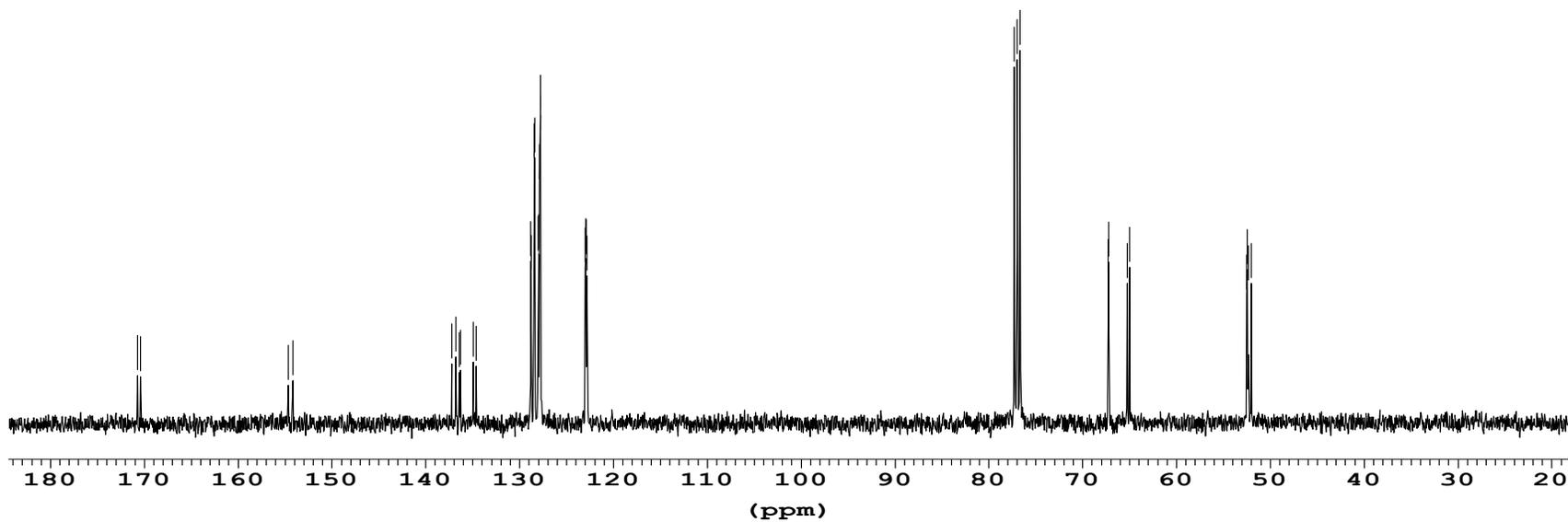
77.2676
76.9500
76.6324

67.2788
67.1914
66.2461
64.9761

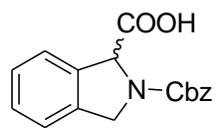
52.5099
52.4305
52.3353
52.0097



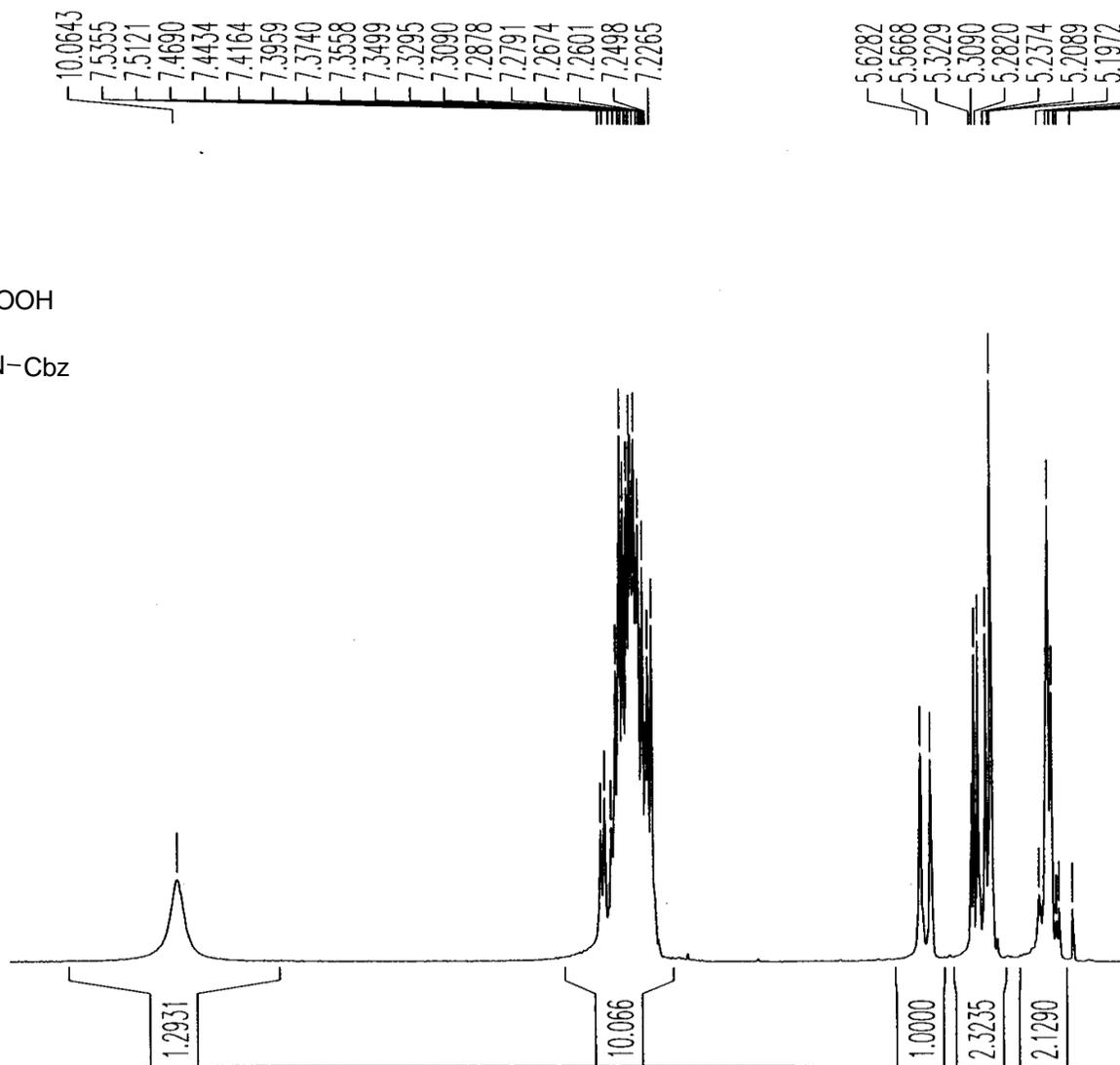
7



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



8

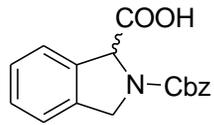


175.5174
174.7745

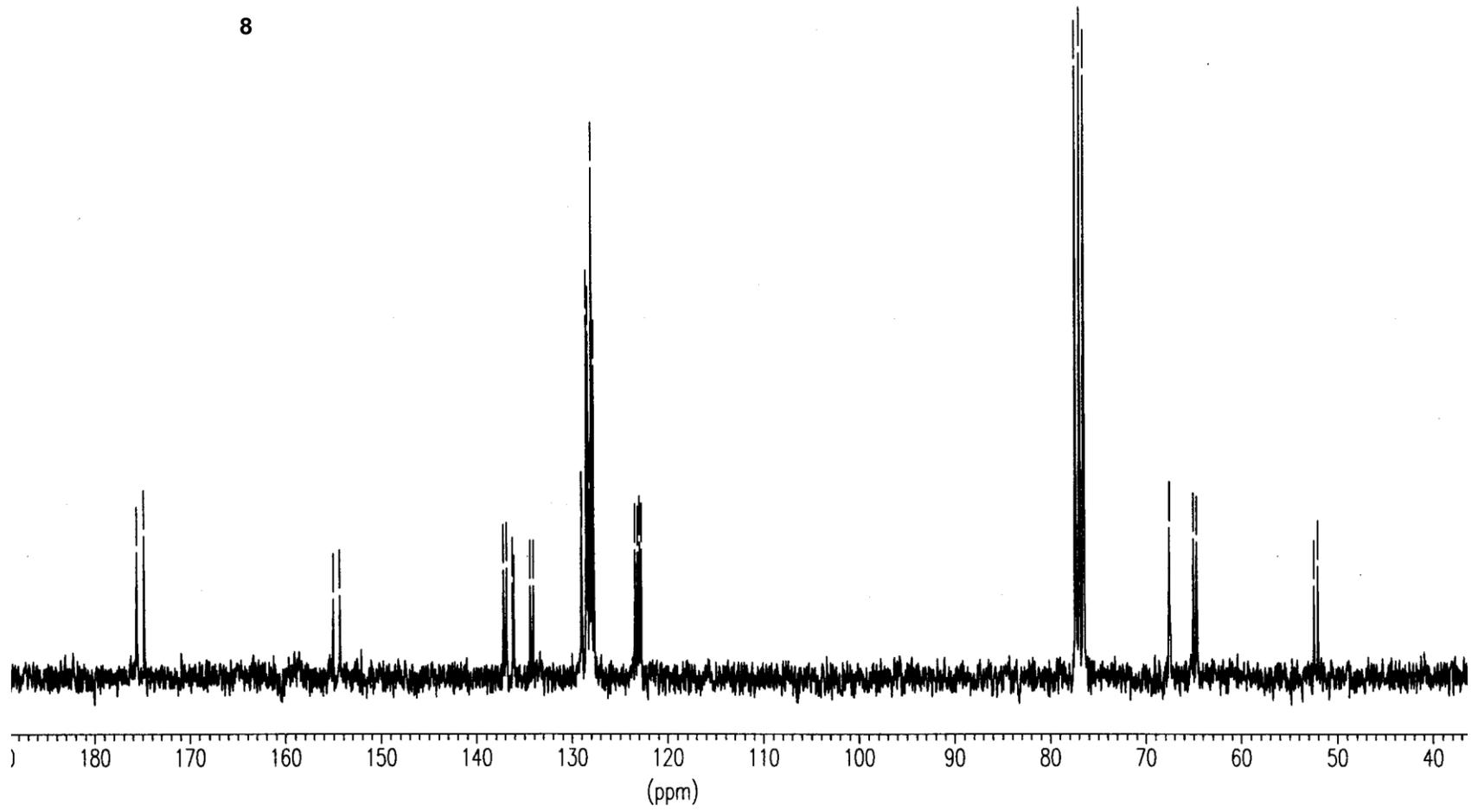
154.9921
154.3105
137.1397
136.8180
136.1517
136.0292
134.3442
134.0302
128.9755
128.9142
128.4470
128.3168
128.0794
127.9109
127.6735
123.3770
123.1396
122.9481
122.7413

77.3712
77.1568
76.9500
76.5288
67.5528
67.4379
65.0407
64.6654

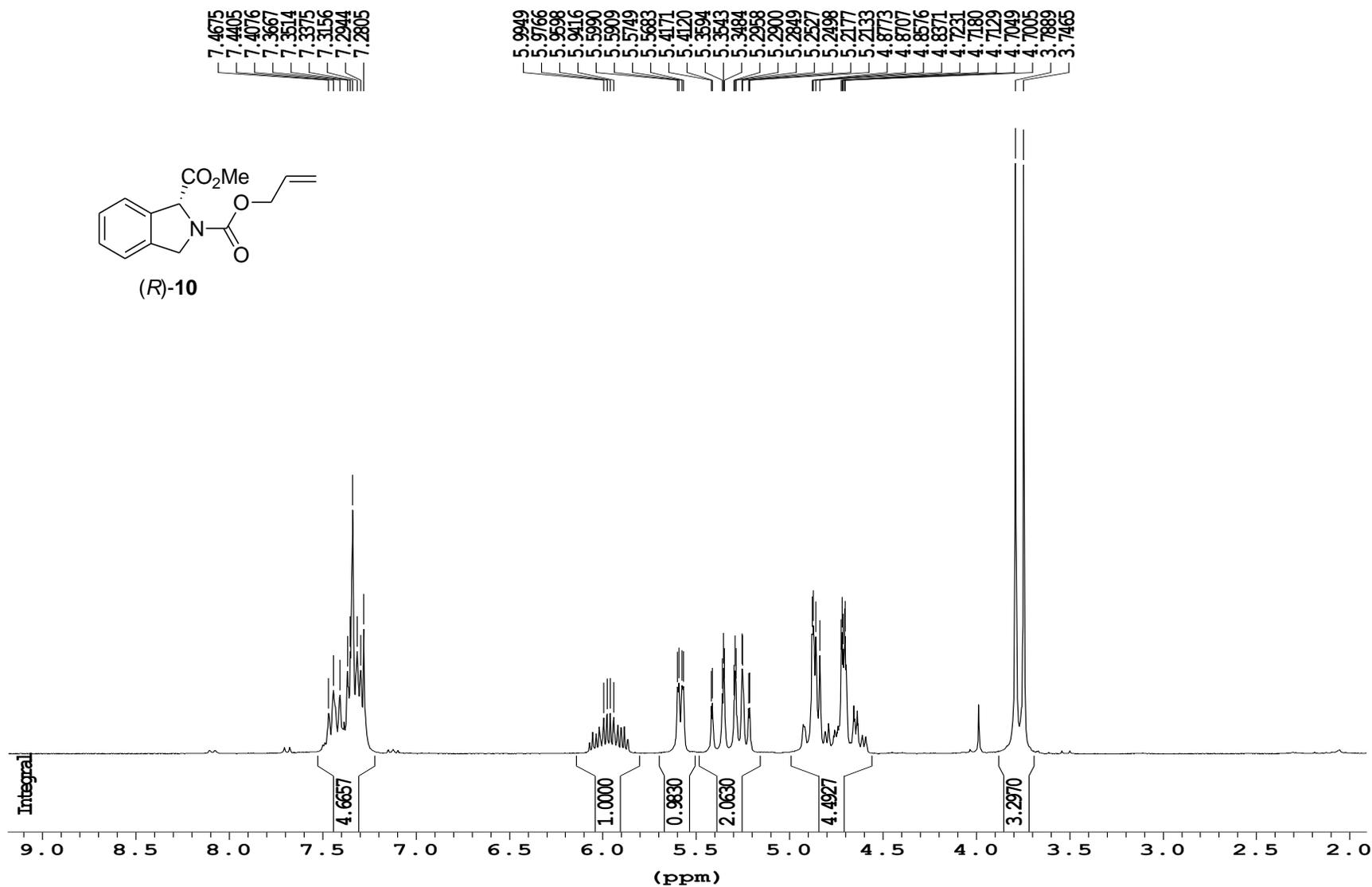
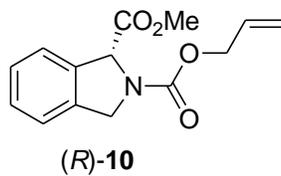
52.4345
52.0363



8



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



170.7307
170.3937

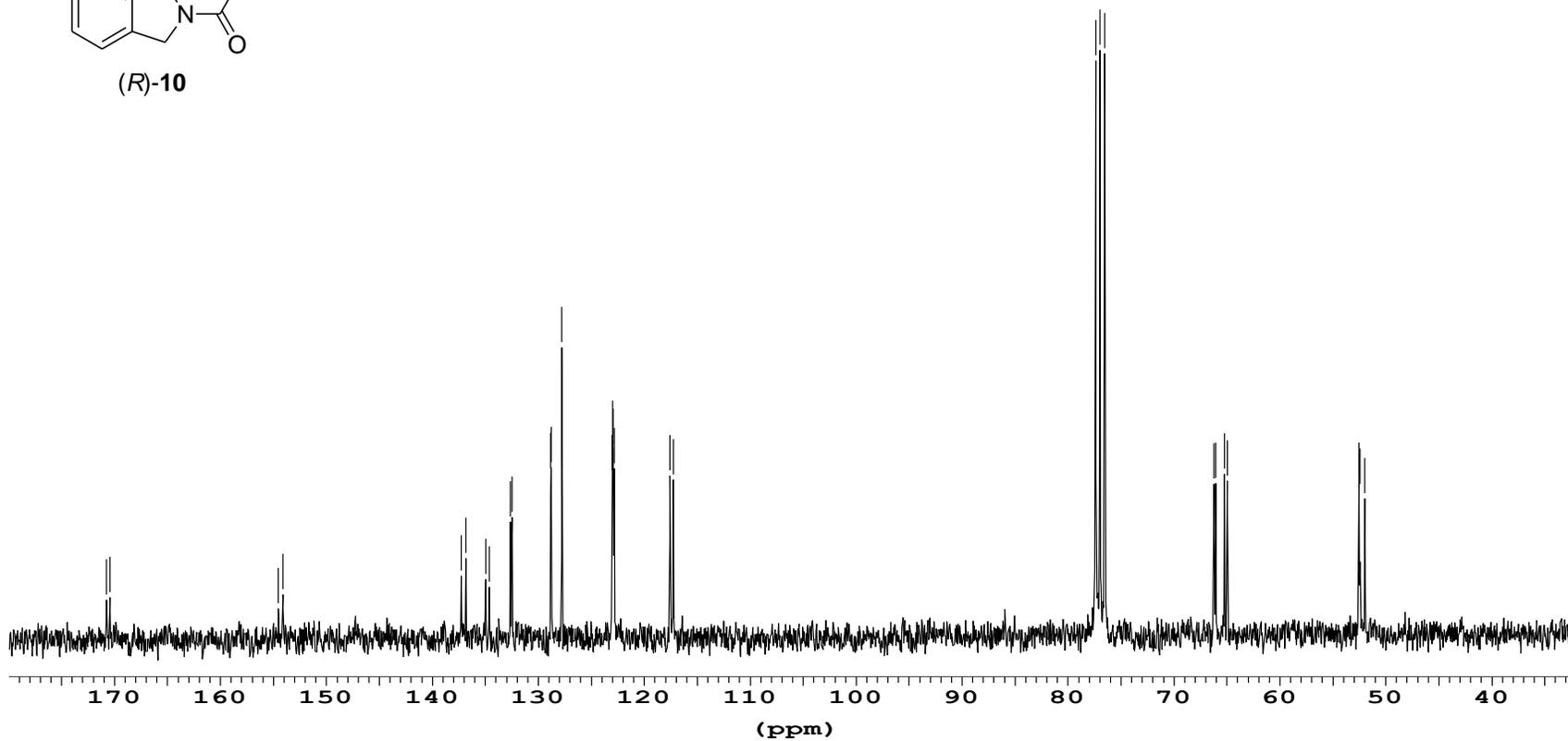
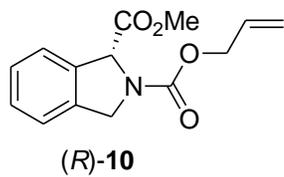
154.5172
154.0884

137.2469
136.7950
134.9416
134.5970
132.6287
132.4755
128.7993
128.7381
127.7501
123.0017
122.9558
122.8945
122.8256
117.5334
117.2424

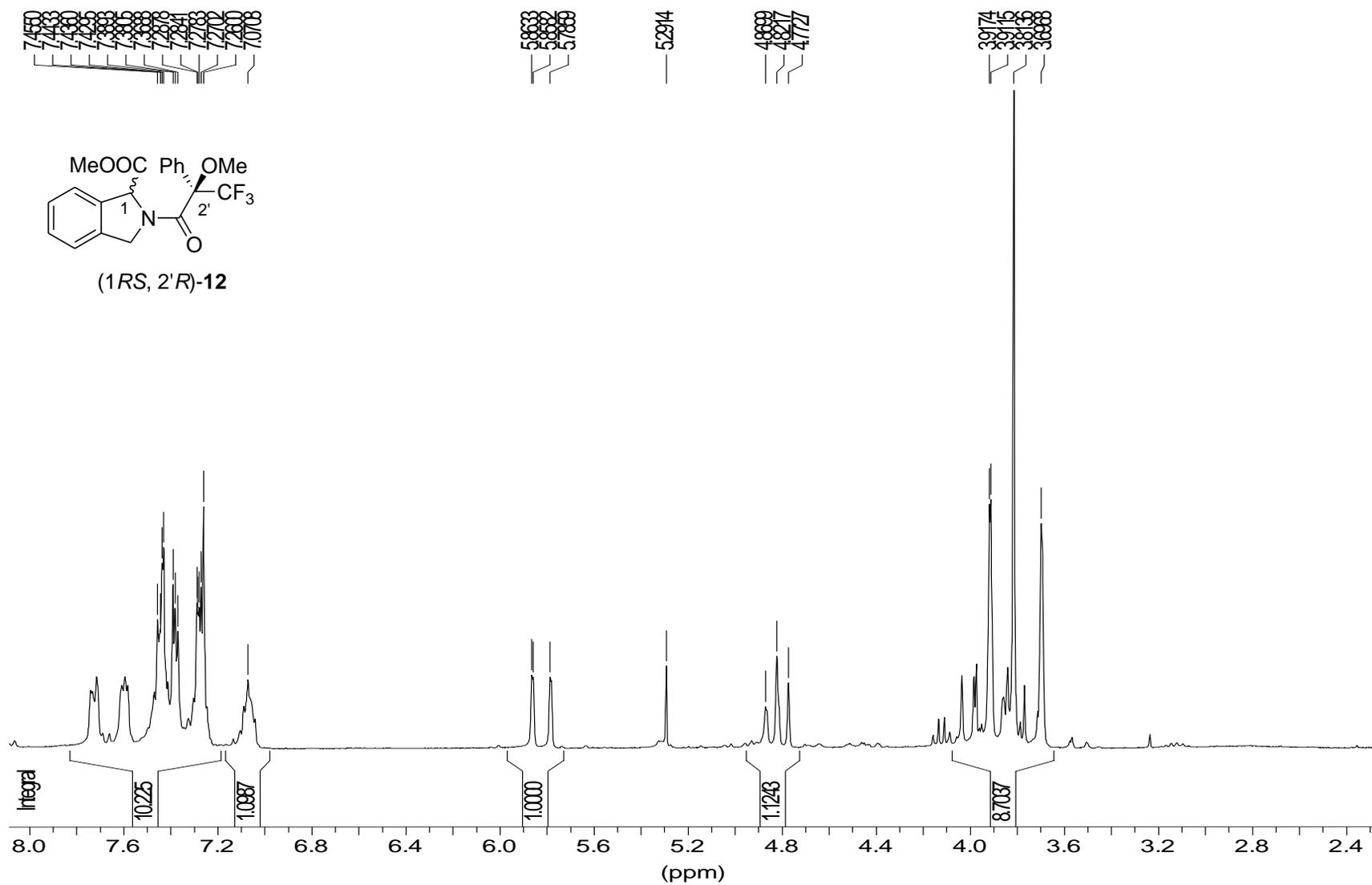
77.3712
76.9500
76.5288

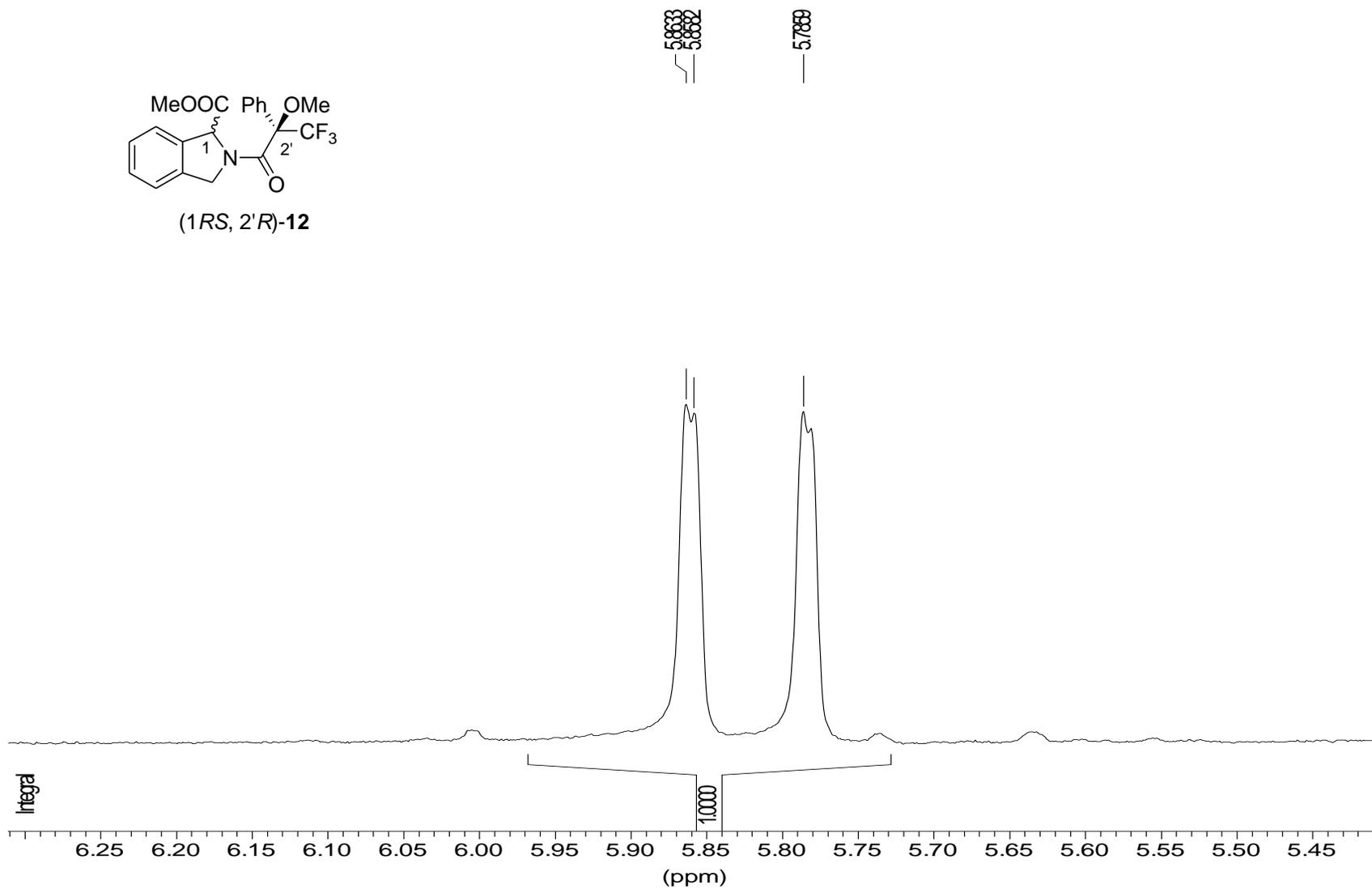
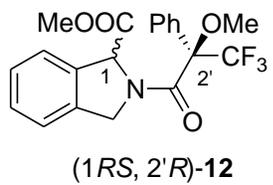
66.2048
66.0517
65.1939
64.9335

52.5494
52.5034
52.4269
51.9597



Methyl (1*R*, 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]

