

Supplementary Material

Addition of Heteroatom Nucleophiles to Ketene Dimers

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Nessan J. Kerrigan^b

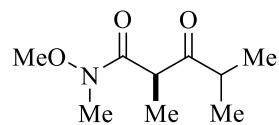
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^b School of Chemical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland

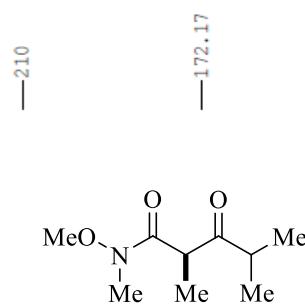
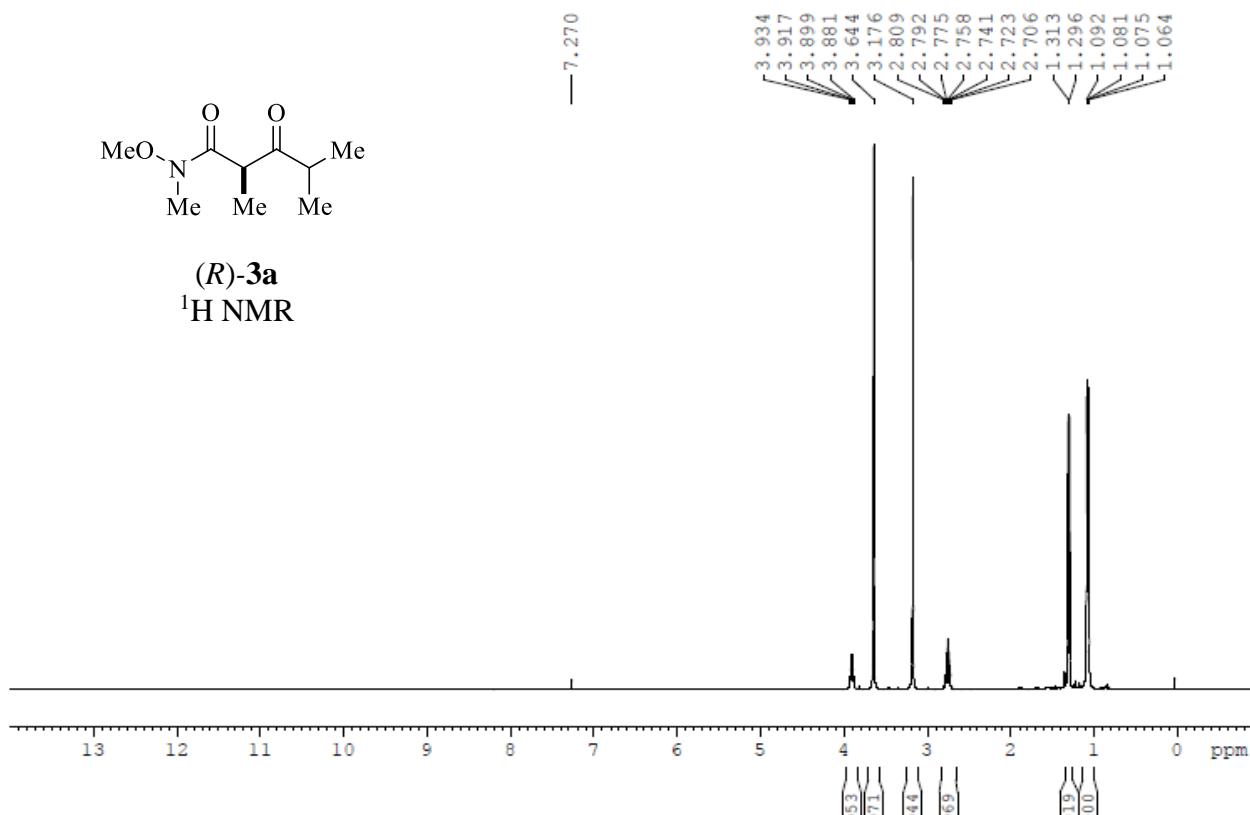
Email: nessan.kerrigan@dcu.ie

Table of Contents

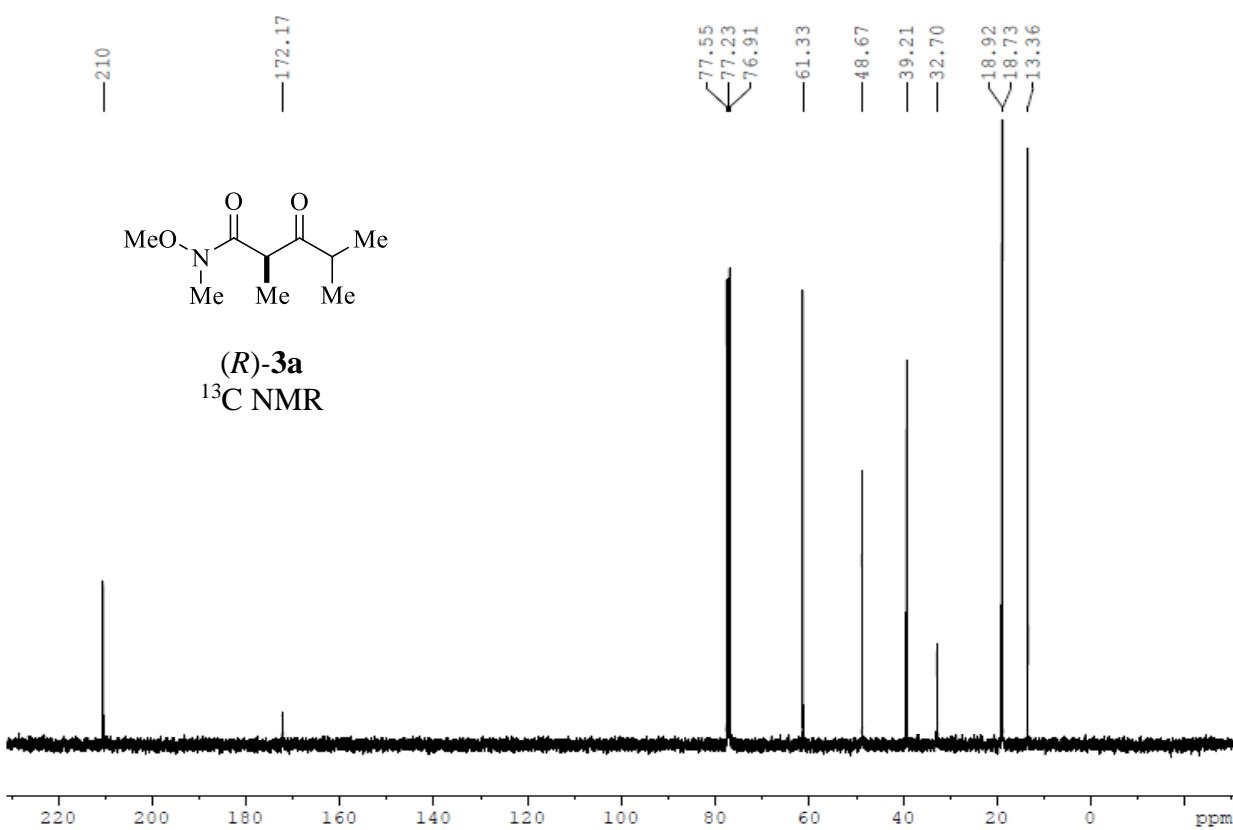
¹ H NMR and ¹³ C NMR for (<i>R</i>)-3a	S2
¹ H NMR and ¹³ C NMR for (<i>S</i>)-3a	S3
¹ H NMR and ¹³ C NMR for (<i>R</i>)-3b	S4
¹ H NMR and ¹³ C NMR for (<i>S</i>)-3b	S5
¹ H NMR and ¹³ C NMR for 3c	S6
¹ H NMR for 3d and 3e	S7
¹³ C NMR for 3e and ¹ H NMR for 4	S8
¹³ C NMR for 4 and ¹ H NMR for 5	S9
¹³ C NMR for 5	S10
¹ H NMR and ¹³ C NMR for 6a	S11
¹ H NMR for 6e	S12
¹ H NMR for 8e	S13
¹³ C NMR for 8e	S14

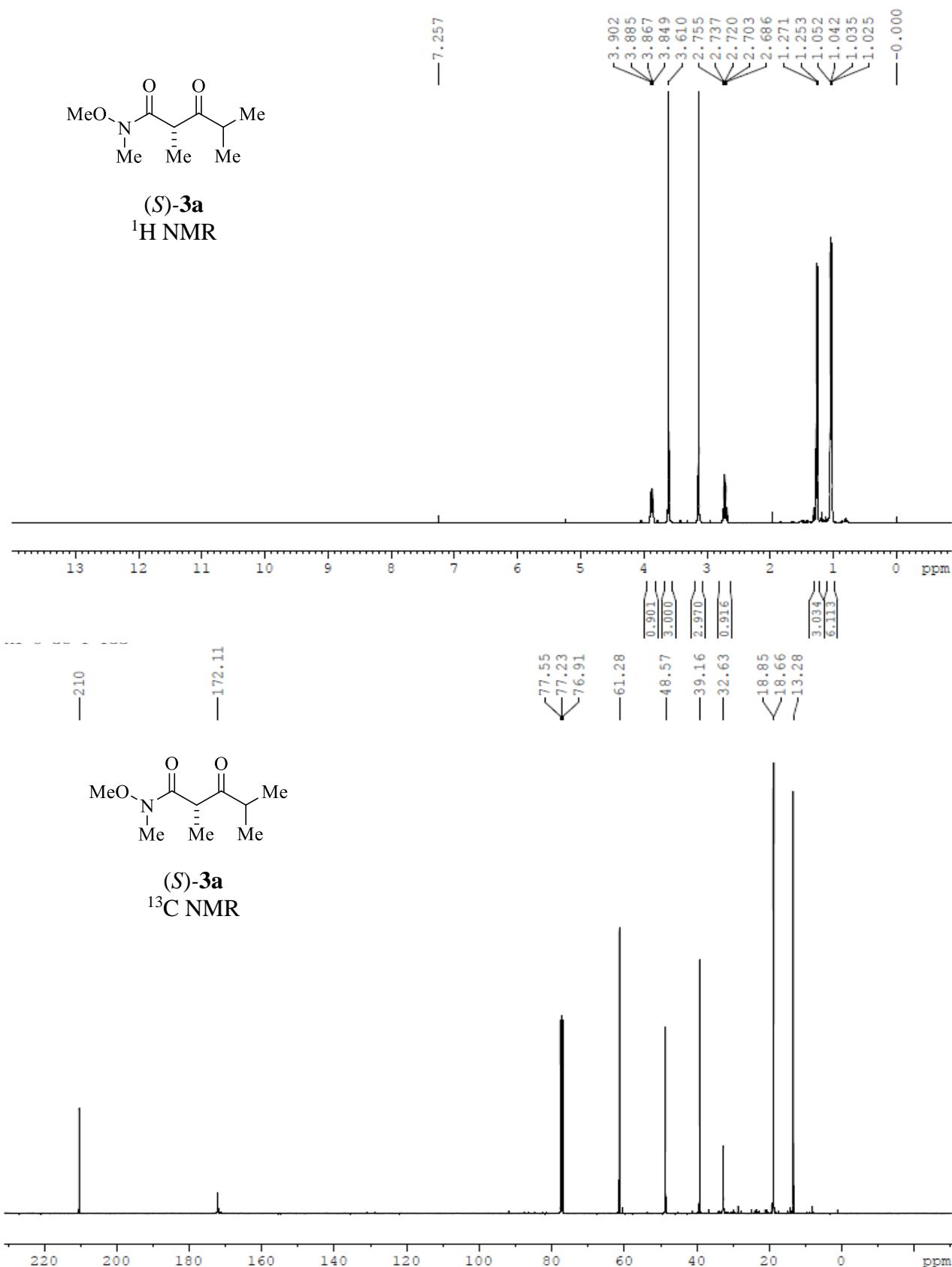


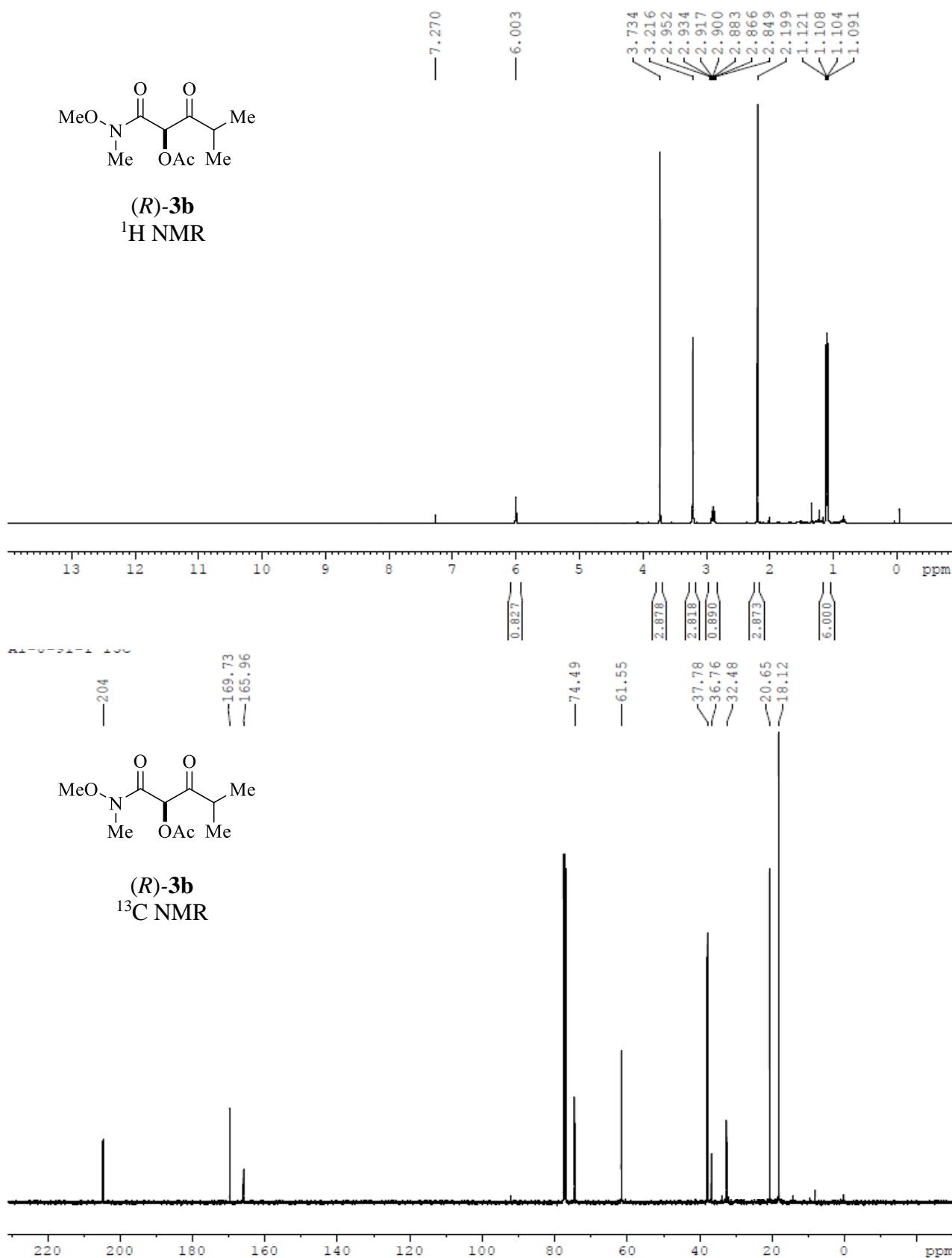
(R)-3a
 ^1H NMR

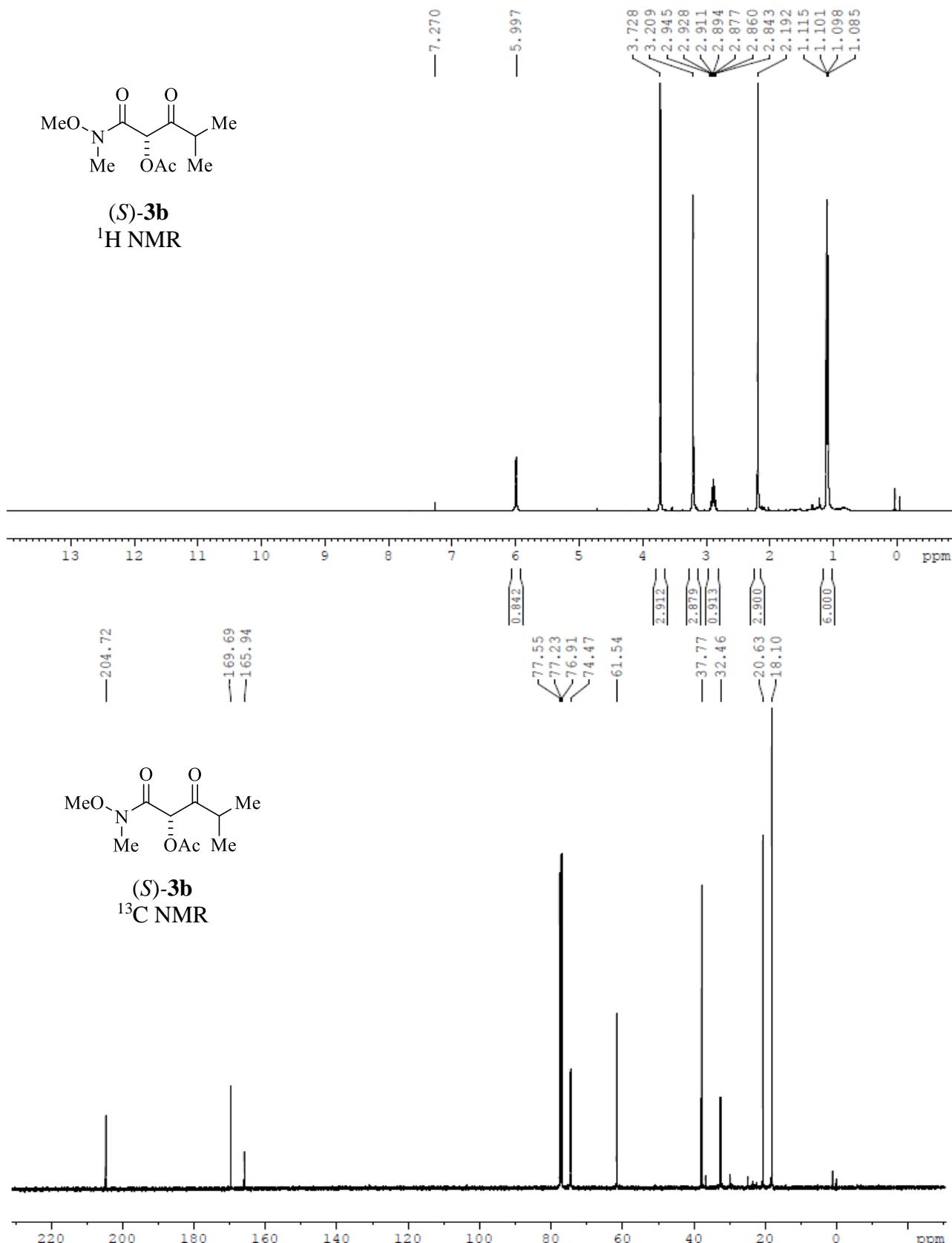


(R)-3a
 ^{13}C NMR

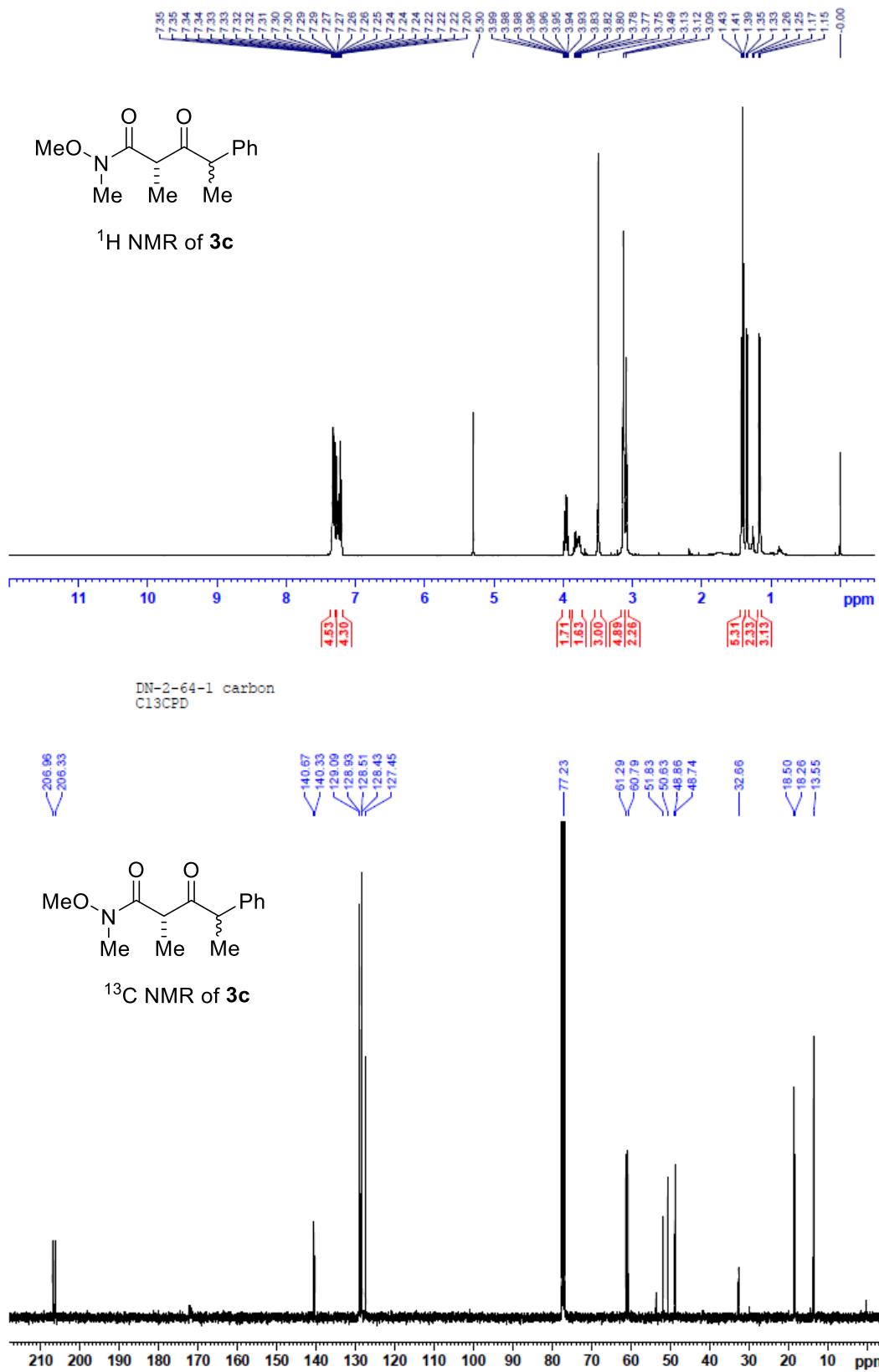




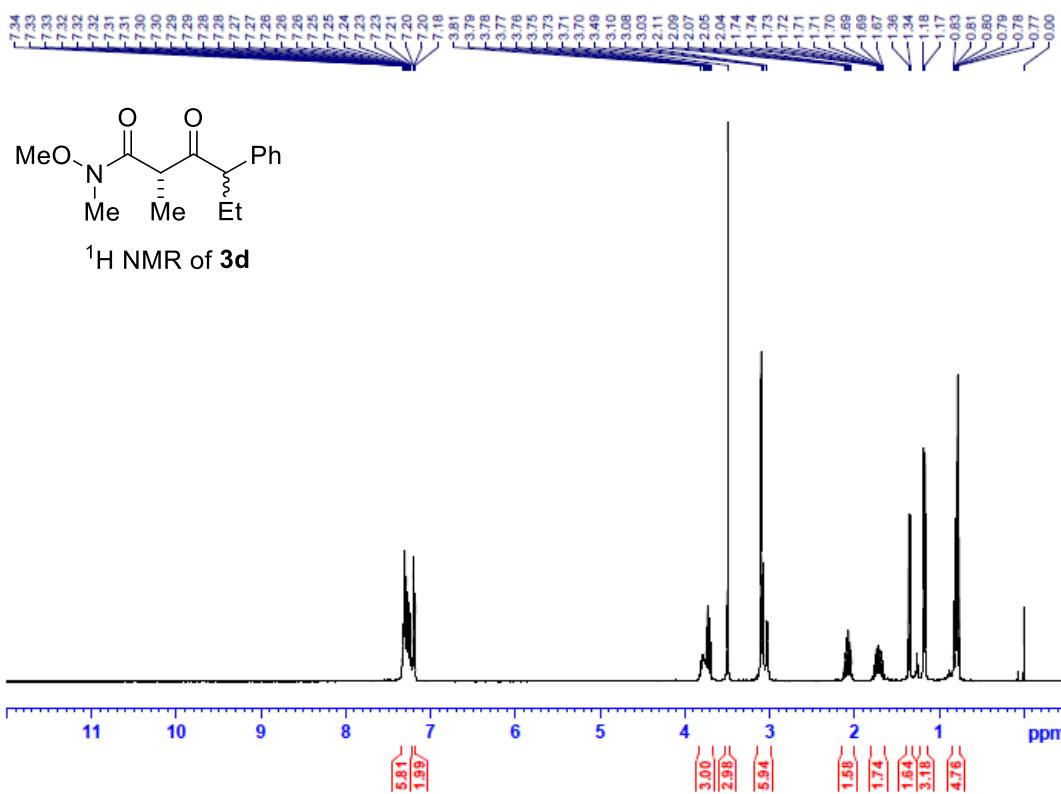
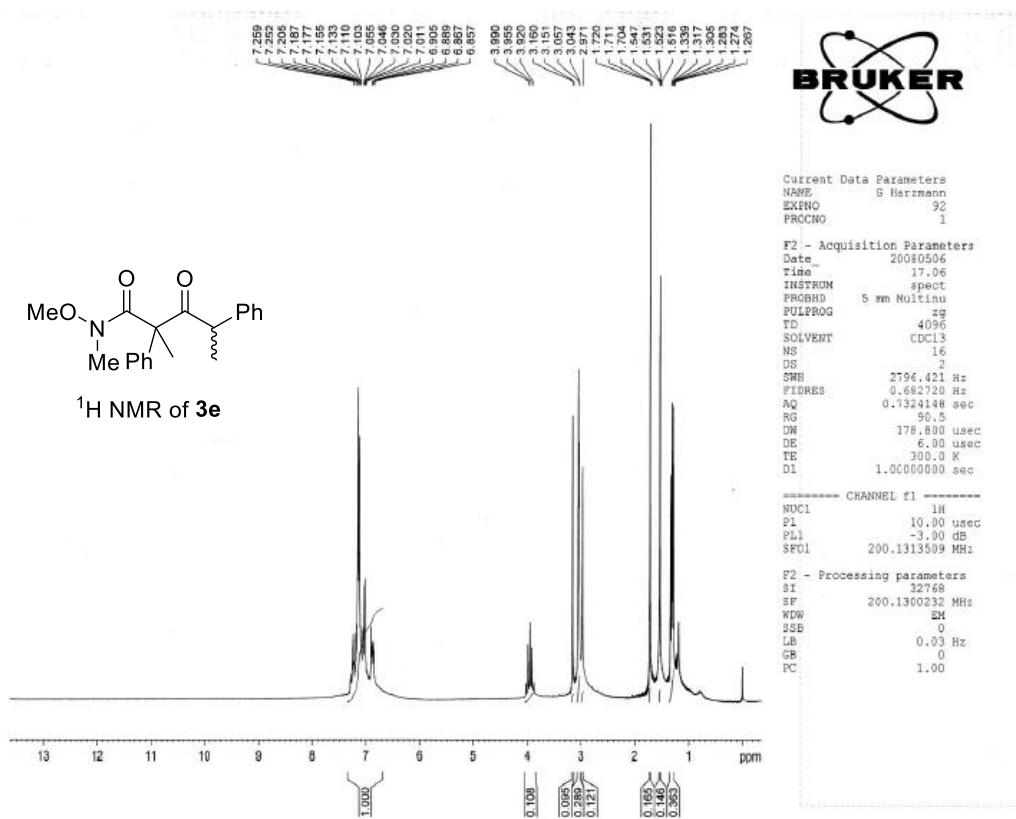




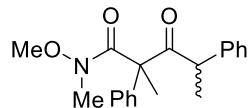
DN-2-64-1



DN-2-54-1

¹H NMR of 3e

GH1-99-1 (Carbon)

207.422
206.945141.723
141.183
139.624
138.558
128.715
128.419
128.297
128.142
128.055
127.832
127.566
127.1235
126.985
126.579
77.863
77.828
76.593
75.410
64.380
64.181
59.869
59.607
50.089
49.318
33.644
23.046
21.847
21.743
21.527¹³C NMR of 3e

220

200

180

160

140

120

100

80

60

40

20

ppm

Current Data Parameters

NAME G Harzmann

EXPNO 93

PROCNO 1

F2 - Acquisition Parameters

Date 20080507

Time 9.52

INSTRUM spect

PROBEHD 5 mm Multinu

PULPROG zgdc

TD 37686

SOLVENT CDCl₃

NS 9482

DS 4

SWH 12562.814 Hz

FIDRES 0.333355 Hz

AQ 1.4999528 sec

RG 71.8

DW 39.800 used

DE 6.00 used

TE 300.0 K

D1 4.0000000 sec

d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 ¹³C

PL1 6.00 used

PL1 1.00 dB

SFO1 50.3285046 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 ¹H

PCPDE2 100.00 used

PL2 -4.00 dB

PL12 16.72 dB

SFO2 200.1300000 MHz

F2 - Processing parameters

SI 32768

SF 50.3227197 MHz

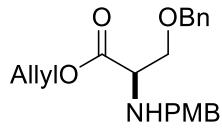
WDW EM

SSB 0

LB 3.00 Hz

GB 0

PC 1.40

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7.303
7.273
7.265
7.260
7.256
7.253
7.231
6.849
6.837
6.832
5.932
5.906
5.904
5.891
5.889
5.877
5.875
5.863
5.343
5.340
5.336
5.332
5.297
5.293
5.247
5.244
5.241
5.238
5.221
5.218
5.215
4.647
4.644
4.641
4.633
4.630
4.627
3.849
3.817
3.736
3.726
3.713
3.688
3.676
3.667
3.653
3.636
3.524
3.512
3.499

4

¹H NMR

12

11

10

9

8

7

6

5

4

3

2

1

0

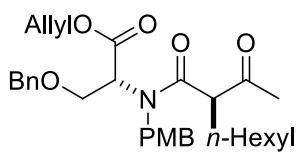
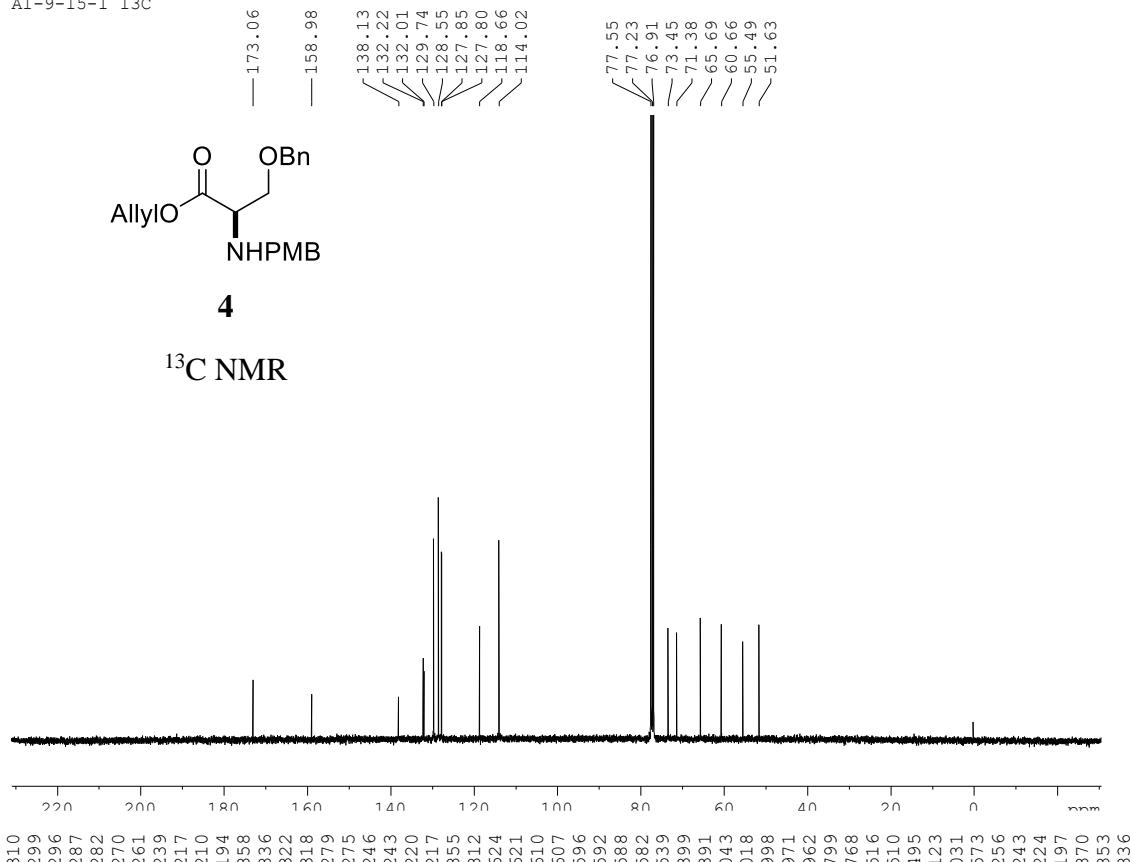
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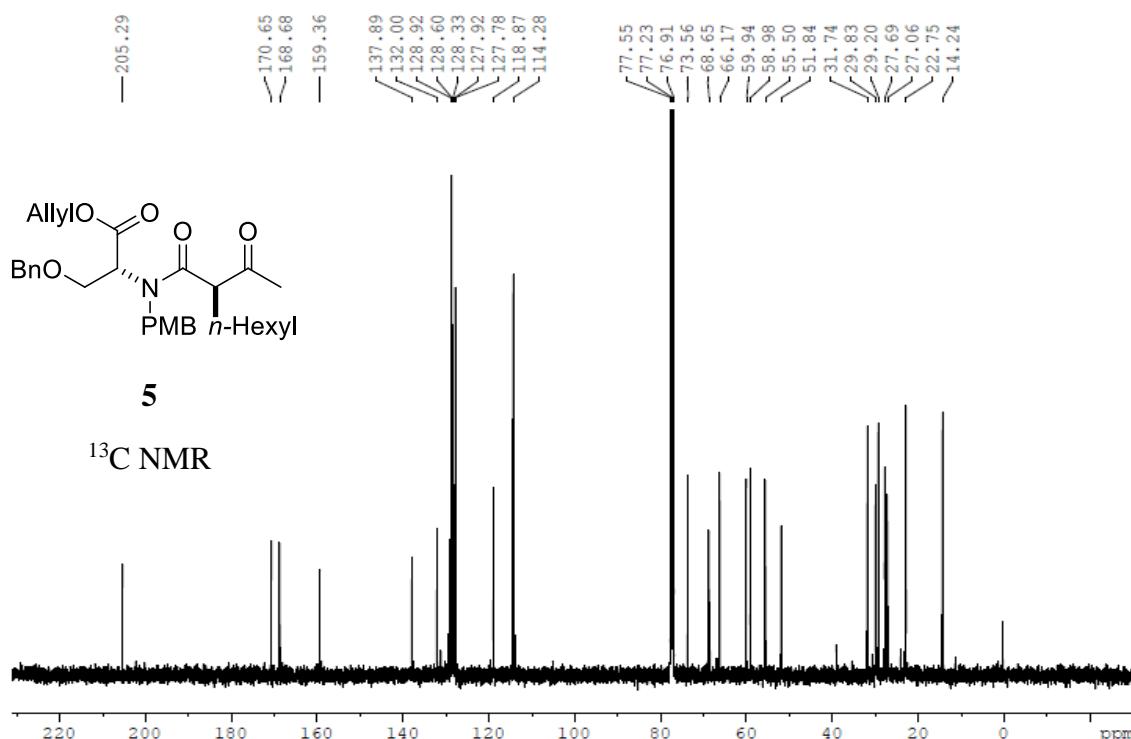
-2

ppm

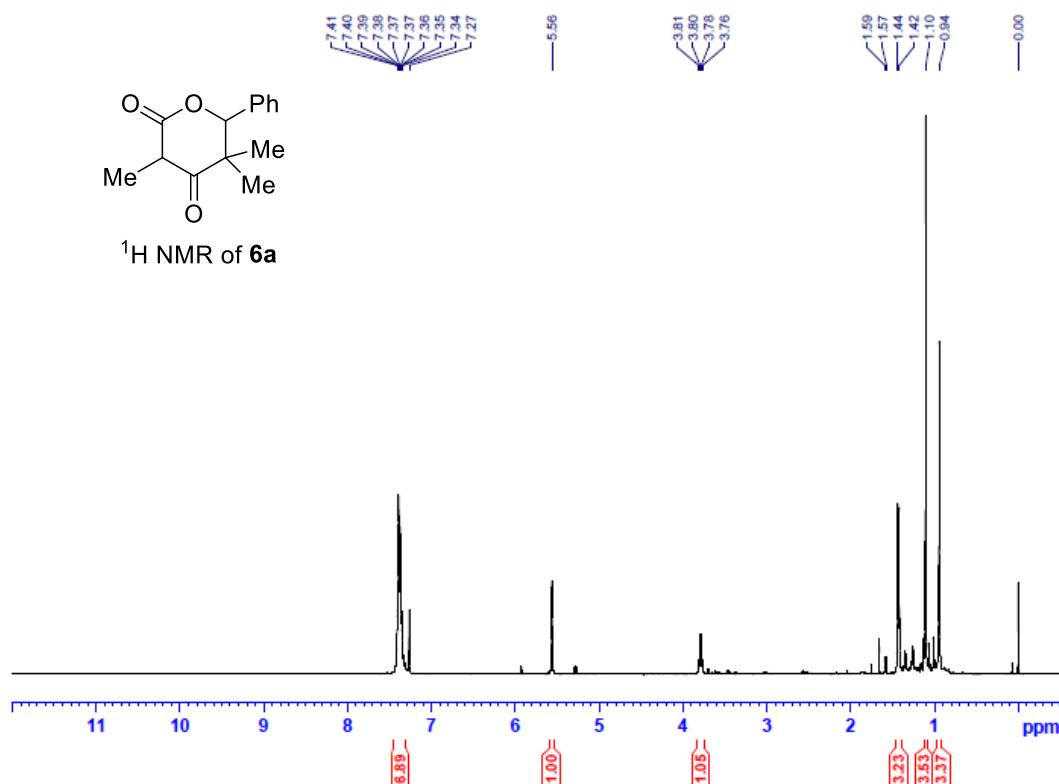
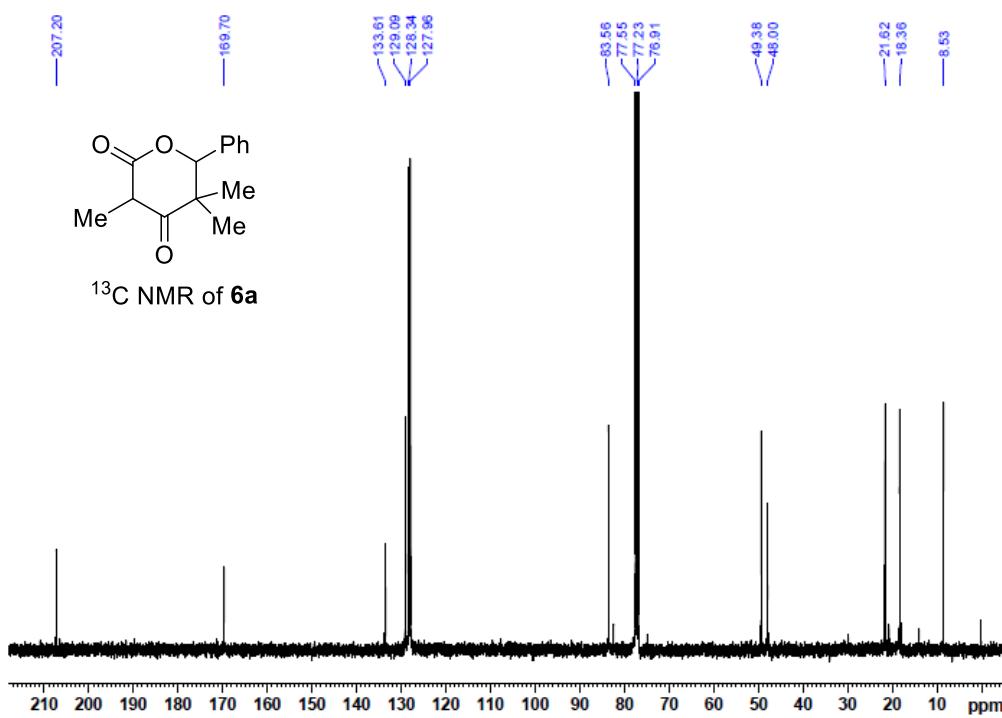
.941 .110 .000
.027 .122 .191
.152 .231 .332
.369

AI-9-15-1 13C

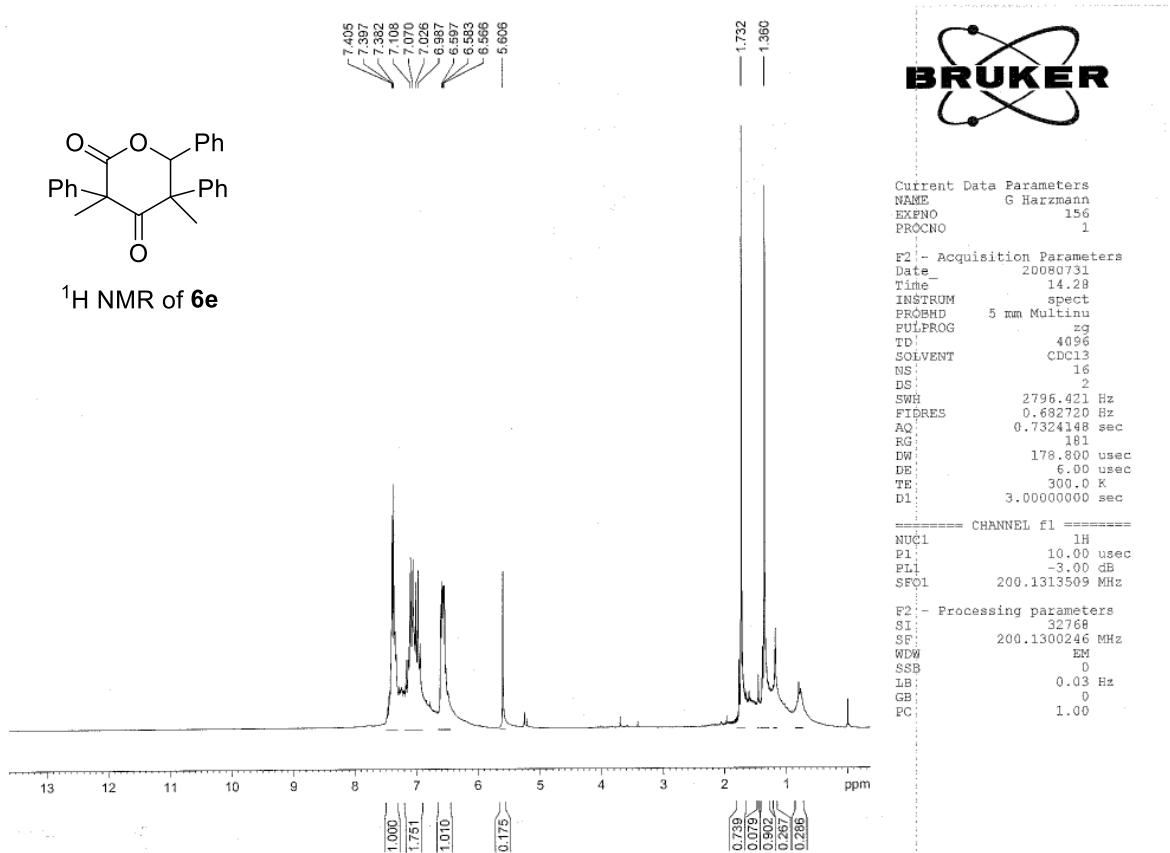




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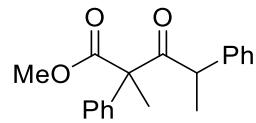
DN-2-79-2
C13CPD

GH2-69-1





AI-2-50-1

¹H NMR of 8e

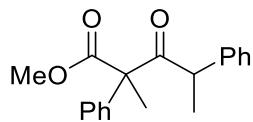
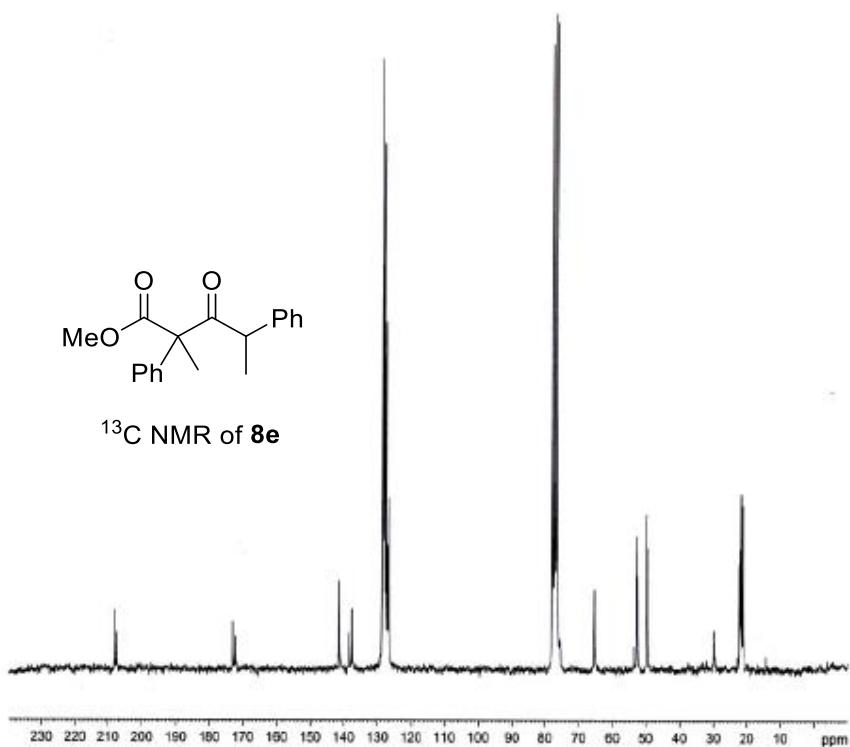
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EXPNO 248
PROCNO 1

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Time 15.16
INSTRUM spect
PROBHD 5 mm Multinu
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TD 4096
SOLVENT CDCl3
NS 16
DS 2
SWH 2796.421 Hz
FIDRES 0.582720 Hz
AQ 0.7324148 sec
RG 574.7
DW 178.800 usec
DE 6.00 usec
TE 300.0 K
D1 3.0000000 sec

----- CHANNEL f1 -----
NUC1 1H
F1 10.00 usec
PL1 -3.00 dB
SFQ1 200.13013509 MHz

F2 - Processing parameters
SI 32768
SF 200.1300233 MHz
WDW EM
SSB 0
LB 0.03 Hz
GB 0
PC 1.00

AI-2-50-1

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172.254141.349
136.274
137.528
128.603
128.477
128.145
127.957
127.489
127.031
126.70877.872
77.237
76.602
65.406
65.393
52.727
52.461
29.810
22.351
22.157
21.912
21.458¹³C NMR of **8e**

Current Data Parameters
 NAME Ahnad
 EXPNO 249
 PROCHD 1

F2 - Acquisition Parameters
 Date 20080422
 Time 10.38
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zgdc
 TD 37686
 SOLVENT DMSO
 NS 9500
 DS 4
 SWH 12562.114 Hz
 FIDRES 0.333355 Hz
 AQ 1.4999528 sec
 R2 57.9
 DW 39.800 usec
 DE 6.00 usec
 TS 300.0 K
 D1 4.0000000 sec
 D11 0.0300000 sec

CHANNEL f1 ======
 NUC1 J3C
 PL1 6.00 usec
 PL1 1.00 dB
 SPO1 50.3285046 MHz

CHANNEL f2 ======
 CPDPFG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.72 dB
 SPO2 200.1300000 MHz

F2 - Processing parameters
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 SF 50.3227193 MHz
 WDM EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PG 1.40