Mild Conversion of β -Diketones and β -Ketoesters to Carboxylic Acids

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General procedure for the preparation of 2,4-diones

The β -dicarbonyl compound (21 mmol) was slowly added to a suspension of 1.04g NaH in THF (50 mL) at 0°C. After the mixture was stirred for 10 minutes, 13.2 mL n-BuLi (1.6 M in hexane) was added drop wise over a period of 15 min. The mixture was stirred for 20 minutes at 0°C. The corresponding halides (23 mmol) in 3 mL THF were added dropwise. After 2 hrs, the reaction was quenched with 4 mL concentrated HCl in 5 mL H₂O and 20 mL of Et₂O. The organic layer was washed with brine and dried with anhydrous MgSO₄ followed by filtration and removal of solvent with rotary evaporation. The crude products were purified with column chromatography using silica gel as the stationary phase and 3:1 Hexane/Et₂O as mobile phase.

Synthesis and NMR data for the 2,4-diones

1-Phenyl-1,3-butanedione (1): CAS No.: 93-91-4

7-Phenylheptane-2,4-dione (2)¹

7-Phenyl-heptane-2,4-dione was prepared by the reaction of 2,4-pentadione and (3-bromo-propyl)-benzene following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 1.95 (m, 2H); 2.03 (s, 3H); 2.28 (t, 2H, $J=7.6$ Hz); 2.63 (t, 2H, $J=7.6$ Hz); 5.46 (s, 1H); 7.31-7.15 (m, 5H); 15.47 (s, 1H)

6-Methyl-2,4-heptanedione (4): CAS No.: 3002-23-1

Nonane-2,4-dione (5)²

Nonane-2,4-dione was prepared by the reaction of 2,4-pentadione and 1-bromo-butane following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ

0.86 (t, 3H, $J=7$ Hz); 1.29 (m, 4H); 1.58 (m, 2H); 2.02 (s, 3H); 2.24 (t, 2H, $J=7.5$ Hz); 3.54 (s, 0.49H); 5.47 (s, 1.2 H); 15.31 (s, 1H).

Decane-2,4-dione (6)³: See reference 3.

Undecane-2,4-dione (7)⁴

Undecane-2,4-dione was prepared by the reaction of 2,4-pentadione and 1-bromohexane following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 0.88 (t, 3H, $J=7.0$ Hz); 1.27 (m, 8H); 1.56 (m, 2H); 2.03 (s, 3H); 2.25 (t, 2H, $J=7.5$ Hz); 3.53 (s, 0.29H); 5.46 (s, 1H); 15.33 (s, 1H).

Dodecane-2,4-dione (8)⁵

Dodecane-2,4-dione was prepared by the reaction of 2,4-pentadione and 1-bromohexane following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 0.88 (t, 3H, $J=7.0$ Hz); 1.29-1.25 (m, 8H); 1.57-1.56 (m, 2H); 2.03 (s, 3H); 2.25 (t, 2H, $J=7.5$ Hz); 5.46 (s, 1H); 15.30 (s, 1H).

Tridecane-2,4-dione (9)⁶

Tridecane-2,4-dione was prepared by the reaction of 2,4-pentadione and 1-bromooctane following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 0.86 (t, 3H, $J=7.0$ Hz); 1.29-1.25 (m, 10H); 1.57 (t, 2H, $J=7.2$ Hz); 2.03 (s, 3H); 2.24 (t, 2H, $J=7.6$ Hz); 5.47 (s, 1H); 15.42 (s, 1H).

3-Oxononanoic acid methyl ester (10)⁷

3-Oxo-nonanoic acid methyl ester was prepared by the reaction of methyl acetoacetate and 1-bromo-pentane following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 0.85 (t, 3H, *J*=7 Hz); 1.26 (m, 6H); 1.56 (m, 2H); 2.48 (t, 2H, *J*=7.5 Hz); 3.42 (s, 2H); 3.70 (s, 3H).

Methyl 4,4-dimethyl-3-oxopentanoate (11): CAS No.: 55107-14-7

4,4,4-Trifluoro-1-phenyl-1,3-butanedione (12): CAS No.: 326-06-7

3-Oxo-5-phenyl-pentanoic acid methyl ester (13)⁸

3-Oxo-5-phenyl-pentanoic acid methyl ester was prepared by the reaction of methyl acetoacetate and (2-bromo-ethyl)-benzene following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 2.84 (t, 3H, *J*=7.5 Hz); 2.90 (t, 3H, *J*=7.5 Hz); 3.41 (s, 2H); 3.69 (s, 3H); 7.17 (m, 3H); 7.28 (m, 2H).

1H-indene-1,3(2H)-dione (14): CAS No.: 606-23-5

1,5-Diphenyl-pentane-1,3-dione (15)⁹

1,5-Diphenyl-pentane-1,3-dione was prepared by the reaction of 1-phenyl-butane-1,3-dione and benzyl bromide following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. ¹H NMR (500MHz, CDCl₃): δ 2.73-2.76 (m, 2H); 3.00-3.03 (m, 2H); 6.13 (s, 1H); 7.13-7.88 (m, 10H); 16.13 (s, 1H).

2-Methyl-1-phenyl-butane-1,3-dione (16)¹⁰

In a three-neck flask was added toluene (60mL), potassium carbonate (22g), 1-phenyl-butane-1,3-dione (8.5g), and tetrabutylammonium bromide (0.65g) under nitrogen with stirring. The mixture was heated to reflux for 2hr and then cooled down to 40-50°C. Methyl iodine (6g) was added slowly in 1hr. After stirring for 2hr at 40-50°C, potassium carbonate (11g) and tetrabutylammonium bromide (0.6g) was added. The mixture was refluxed for 10hr and then cooled down to room temperature. The reaction was worked up with water and the mixture was filtered, extracted with ether, and dried over MgSO₄. The organic layer was concentrated and purified with column chromatograph to afford **16** as a yellow liquid. ¹H NMR (500MHz, CDCl₃): δ 1.43 (d, *J*=7.0Hz, 3H); 2.14 (s, 3H); 4.46 (q, *J*=7.0Hz, 1H); 7.46-7.97 (m, 5H).

Dodec-11-ene-2,4-dione (20)¹¹

Dodec-11-ene-2,4-dione was prepared by the reaction of 2,4-pentadione and 7-bromo-heptene following the general procedure for the preparation of 2,4-dione derivatives described in the experimental section of the manuscript. **20**: ¹H NMR (500MHz, CDCl₃): δ 1.36 (m, 6H); 1.57 (m, 2H); 1.99-2.03 (m, 5H); 2.24 (t, 2H, *J*=7.5Hz); 4.91 (m, 2H); 5.46 (s, 1H); 5.77 (m, 1H); 15.05 (s, 1H).

11-Hydroxyundecane-2,4-dione (22)¹²

11-Hydroxy-undecane-2,4-dione was prepared by the hydrolysis of 11-Methoxy-undecane-2,4-dione. **22**: ¹H NMR (500MHz, CDCl₃): δ 1.30 (m, 6H); 1.45 (m, 2H); 1.67 (bs, 1H); 1.87 (m, 2H); 2.06 (s, 3H); 2.29 (t, 2H, *J*=7.5 Hz); 3.40 (t, 2H, *J*=7.5 Hz); 5.50 (s, 1H); 14.98 (s, 1H).

Synthesis and NMR data for the carboxylic acid products

Benzoic acid (1a): CAS No.: 74920-45-9

4-Phenylbutyric acid (2a)

The procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.21g substrate **2** and 1.1g CAN. Purification by flash chromatography (25 × 30cm, EtOAc/Hexane:1/3) provided 0.136g product **2a** as a white solid: ¹H NMR (500MHz, CDCl₃): δ 11.91 (s, 1H); 7.28-7.16 (m, 5H); 2.66 (t, 2H, *J*=7.6 Hz); 2.36 (t, 2H, *J*=7.5 Hz); 1.96 (m, 2H). ¹³C NMR (125MHz, CDCl₃): δ 180.96; 161.16; 129.25; 127.60; 36.21; 34.57; 27.86. CAS No.: 1821-12-1.

3-Naphthalen-2-yl-propionic acid (3a)¹³

The general procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.24g substrate **3** and 1.1g CAN. GC-MS showed that **3a** was formed with 87% yield. Purification by flash chromatography (25 × 30cm, EtOAc/Hexane:1/3) provided 0.144g **3a** as a white solid: ¹H NMR (500MHz, CDCl₃): δ 2.54 (t, 2H); 2.90 (t, 2H); 7.17-7.50 (m, 7H); 11.5 (bs, 1H).

3-Methylbutanoic acid (4a): CAS No.: 503-74-2

Hexanoic acid (5a): CAS No.: 142-62-1

Heptanoic acid (6a): CAS No.: 111-14-8

Octanoic acid (7a): CAS No.: 124-07-2

Nonanoic acid (8a): CAS No.: 112-05-0

Decanoic acid (9a): CAS No.: 334-48-5

Heptanoic acid (10a): CAS No.: 111-14-8

Pivalic acid (11a): CAS No.: 75-98-9

1-Phenyl-1,3-butanedione (12a): CAS No.: 93-91-4

3-Phenylpropionic acid (13a)

The general procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.38g substrate **13** and 2.2g CAN. Product **13a** (0.21g) was obtained as a light yellow solid: ¹H NMR (500MHz, CDCl₃): δ 2.67 (t, 2H); 2.93 (t, 2H); 7.18-7.29 (m, 5H); 10.98 (bs, 1H). CAS No.: 501-52-0.

Isobenzofuran-1,3-dione (14a)

The general procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.146g indandione and 1.1g CAN. GC-MS showed the Isobenzofuran-1,3-dione was formed in 100% yield as a light color solid: ¹H NMR (500MHz, CDCl₃): δ 7.61-8.15 (m, 4H). CAS No.: 85-44-9.

1-Phenylpropane-1,2-dione (16a): CAS No.: 579-07-7.

3-(2-Methoxyphenyl)-propionic acid (17a)

The optimized procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.22g substrate **17** and 1.1g CAN. Product **17a** (0.13g) was obtained after purification by flash column chromatography. ¹H NMR (500MHz, CDCl₃): δ 2.65 (t, 2H, *J*=7 Hz); 2.91 (t, 2H, *J*=7 Hz); 3.83 (s, 3H); 7.08-7.29 (m, 4H); 11.28 (bs, 1H). CAS No.: 6342-77-4.

3-(4-Methoxy-phenyl)-propionic acid (18a)

The optimized procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of

0.22g substrate **18** and 1.1g CAN. Product **18a** (0.146g) was obtained after purification with flash column chromatography. ¹H NMR (500MHz, CDCl₃): δ 2.63 (t, 2H, *J*=7 Hz); 2.90 (t, 2H, *J*=7 Hz); 3.81 (s, 3H); 7.12-7.29 (m, 4H); 11.10 (bs, 1H). CAS No.: 1929-29-9.

3-(3-Methoxy-phenyl)-propionic acid (19a)

The optimized procedure described in the experimental section of the manuscript for the oxidation of β-dicarbonyls using CAN in CH₃CN was followed with the use of 0.22g substrate **19** and 1.1g CAN. Product **19a** (0.143g) was obtained after purification with flash column chromatography. ¹H NMR (500MHz, CDCl₃): δ 2.65 (t, 2H, *J*=7 Hz); 2.91 (t, 2H, *J*=7 Hz); 3.81 (s, 3H); 7.13-7.27 (m, 4H); 10.91 (bs, 1H). CAS No.: 10516-71-9.

Non-8-enoic acid (20a)¹⁴

The optimized procedure described in the experimental section of the manuscript for the oxidation of β-dicarbonyls using CAN in CH₃CN was followed with the use of 0.196g substrate **20** and 1.1g CAN. Product **20a** was (0.139g) obtained without purification. ¹H NMR (500MHz, CDCl₃): δ 1.34 (m, 6H); 1.60 (m, 2H); 2.02 (m, 2H); 2.34 (t, 2H, *J*=7.5 Hz); 4.95 (m, 2H); 5.75 (m, 1H); 12.34 (bs, 1H).

8-Methoxy-octanoic acid (21a)¹⁵

The optimized procedure described in the experimental section of the manuscript for the oxidation of β-dicarbonyls using CAN in CH₃CN was followed with the use of 0.214g substrate **21** and 1.1g CAN. Product **21a** (0.16g) was obtained after purification with flash column chromatography. ¹H NMR (500MHz, CDCl₃): δ 1.31 (m, 6H); 1.54(m, 4H); 2.32 (t, 2H, *J*=7.5 Hz); 3.23 (s, 3H); 3.36 (t, 2H, *J*=7.5 Hz); 9.57 (s, 1H).

8-Hydroxy-octanoic acid (**22a**)

The optimized procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.2g substrate **22** and 1.1g CAN. Product **22a** (0.118g) was obtained after purification with flash column chromatography. ¹H NMR (500MHz, CDCl₃): δ 1.30-1.47 (m, 8H); 1.88 (m, 4H); 2.28 (t, 2H, $J=7.4$ Hz); 3.45 (t, 2H, $J=7.4$ Hz); 10.40 (bs, 1H). CAS No.: 764-89-6.

3-(4-Iodo-phenyl)-propionic acid (**23a**)¹⁶

The optimized procedure described in the experimental section of the manuscript for the oxidation of β -dicarbonyls using CAN in CH₃CN was followed with the use of 0.32g substrate **23** and 1.1g CAN. Pure product of **23a** (0.243g) was obtained without purification. ¹H NMR (500MHz, CDCl₃): δ 2.64 (t, 2H, $J=8.2$ Hz); 2.87 (t, 2H, $J=8.2$ Hz); 6.95 (d, 2H, $J=8.2$ Hz); 7.59 (d, 2H, $J=8.2$ Hz); 11.62 (bs, 1H).

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Compound 3

Compound 3

Current Data Parameters
NAME 0611
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040611
Time 14.18
INSTRUM spect
PROBHD 5 mm QNP 13C-1
PULPROG zgpg
TO 65536
SOLVENT CDCl3
NS 223
DS 0
SMH 34013.605 Hz
FIDRES 0.519006 Hz
AQ 0.9634439 sec
RG 5792.6
DM 14.700 usec
DE 10.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7746011 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 500.1319002 MHz

F2 - Processing parameters
SI 65536
SF 125.7577916 MHz
WDM EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00

1C NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 270.450 ppm
F1 34016.24 Hz
F2P 0.021 ppm
F2 2.63 Hz
PPMCM 13.52346 ppm/cm
HZCM 1700.66030 Hz/cm

Compound 17

Compound 17

Current Data Parameters
 NAME j0914
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040914
 Time 10.20
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 150
 DS 0
 SMH 35211.270 Hz
 FIDRES 0.537261 Hz
 AQ 0.9396754 sec
 RG 2048
 DM 14.200 usec
 DE 7.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7753451 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 500.1319002 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577916 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 40.00 cm
 FIP 279.578 ppm
 F1 35159.07 Hz
 F2 -0.415 ppm
 F2 13.95964 ppm/cm
 PPMCM 1760.56335 Hz/cm
 HZCM

Compound 18

Compound 18

Current Data Parameters
 NAME J100104
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041001
 Time 10.08
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 150
 DS 0
 SMH 35211.270 Hz
 FIDRES 0.537281 Hz
 AQ 0.9306754 sec
 RG 4096
 DM 14.200 usec
 DE 7.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7753451 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 500.1319002 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577916 MHz
 NDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 13.00 cm
 FIP 279.578 ppm
 F1 35159.07 Hz
 F2 -0.415 ppm
 F2 -52.19 Hz
 PPMCM 13.99364 ppm/cm
 HZCM 1760.56335 Hz/cm

Compound 19

15.4323
ppm

Current Data Parameters
NAME j100107
EXPNO 1
PROCNO 1

F2 - Acquisition Parameter
Date_ 20041007
Time 14.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110282 se
RG 406.4
DM 27.800 US
DE 7.00 US
TE 300.0 K
D1 1.00000000 se

===== CHANNEL f1 =====
NUC1 1H
P1 5.00 US
PL1 -4.00 dB
SF01 500.1319002 MHz

F2 - Processing parameters
SI 32768
SF 500.1300233 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 16.221 pp
F1 8112.59 Hz
F2P -1.092 pp
F2 -546.35 Hz
PPMCM 0.86567 pp
HZCM 432.94705 Hz

Compound 19

Current Data Parameters
 NAME j100125
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041025
 Time 11.47
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TO 65536
 SOLVENT CDCl₃
 NS 200
 DS 0
 SMH 35211.270 Hz
 FIDRES 0.537281 Hz
 AQ 0.9306754 sec
 RG 1824.6
 DW 14.200 usec
 DE 7.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7753451 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCDP2 100.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 500.1319002 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577916 MHz
 WDM EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
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 CY 80.00 cm
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 F1 35159.07 Hz
 F2P -0.415 ppm
 F2 -52.19 Hz
 PPMCM 13.95984 ppm/cm
 HZCM 1760.56335 Hz/cm

Compound 21

Current Data Parameters
 NAME Y21217
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameter
 Date_ 20041217
 Time 9.48
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SMH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0448356 se
 RG 28.5
 DW 62.400 us
 DE 7.00 us
 TE 300.0 K
 D1 1.00000000 se

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 us
 PL1 -4.00 dB
 SF01 500.1339813 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300233 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 13.00 cm
 F1P 15.925 pp
 F1 7964.37 Hz
 F2P -0.097 pp
 F2 -48.46 Hz
 PPMCM 0.80107 pp
 HZCM 400.64105 Hz

Compound 21

Current Data Parameters
 NAME yz1217
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041217
 Time 9.54
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 150
 DS 0
 SMH 35211.270 Hz
 FIDRES 0.537281 Hz
 AQ 0.9306754 sec
 RG 7296.2
 DM 14.200 usec
 DE 7.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7753451 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCD2 100.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 500.1319002 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577916 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 13.00 cm
 F1P 240.000 ppm
 F1 30181.87 Hz
 F2P -0.415 ppm
 F2 -52.415 Hz
 PPMCM 12.02075 ppm/cm
 HZCM 1511.70325 Hz/cm

Compound 23

Current Data Parameters
 NAME YZ1220
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameter
 Date_ 20041221
 Time 16.47
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 7507.507 Hz
 FIDRES 0.229111 Hz
 AQ 2.1824653 se
 RG 28.5
 DW 66.600 us
 DE 7.00 us
 TE 300.0 K
 D1 1.00000000 se

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 us
 PL1 -4.00 dB
 SF01 500.1337495 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300233 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 50.00 cm
 FIP 10.000 pp
 F1 5001.30 Hz
 F2P -0.055 pp
 F2 -27.59 Hz
 PPMCM 0.50276 pp
 HZCM 251.44441 Hz

Compound 23

Current Data Parameters
 NAME Y21220
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041221
 Time 16:52
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 67
 DS 0
 SWH 35211.270 Hz
 FIDRES 0.537261 Hz
 AQ 0.9306754 sec
 RG 7298.2
 DM 14.200 usec
 DE 7.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7753451 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 500.1319002 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577916 MHz
 NDM EN
 SS9 0
 LB 1.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 13.00 cm
 F1P 279.578 ppm
 F1 35159.07 Hz
 F2P -0.415 ppm
 F2 -52.19 Hz
 PPMCM 13.99964 ppm/cm
 HZCM 1760.56335 Hz/cm

React IR Study

React IR study