Supplementary Information for

Tandem Catalytic Oxidative Deacetylation of Acetoacetic Esters and Hetero Aromatic Cyclizations

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[\textsuperscript{1}H/\textsuperscript{13}C NMR spectra for the new compounds]
Pulse Sequence: szpul
Solvent: cdc13
Ambient temperature
Sample #:43, Operator: walkup2
File: JYM-467_Proton_01
VMRMS-400 "450MR"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acc. time 2.648 sec
Width 6410.3 Hz
B repetitions
OBSERVE H1, 400.0340074 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

EtO

EtO

1

ppm

2.00 0.89 2.12 0.23 2.58 0.71 3.03
JYM-460
Sample: JYM-460
Sample ID: s_42_JYM-460_koo-5_20130123_01
File: /home/walkup2/vmrsys/data/koo-5/JYM-460_Proton_01.fid
Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #42, Operator: walkup2
File: JYM-460_Proton_01
VMRS-650 "G5N6K"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
Repetitions
OBSERVE H1, 400.0340074 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min, 31 sec

\[
\begin{align*}
& \text{BO} \quad \text{O} \\
& \text{O} \quad \text{2}
\end{align*}
\]
EtO

Sample: JYM-686-2
Sample ID: s_41_JYM-686-2_koo-4_20130619_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-686-2_Proton_01.fld

Pulse Sequence: s2pu1
Solvent: cdc13
Ambient temperature
Sample #41, Operator: walkup2
VNMRS=600 "ABNAR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 6410.3 Hz
8 repetitions

DATA PROCESSING
OBSEVE H1, 400.0340070 MHz
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

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1.35
0.0901
1.081.3432
0.101.02
0.74
JYM-680-2-c
Sample: JYM-680-2-c
Sample ID: s_42_JYM-680-2-c_koo-4_20130620_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-680-2-c_Carbon_01.fld

Pulse Sequence: zpulp
Solvent: cdc13
Ambient temperature
Sample: #42, Sample 42
VNMRS-400 "G40MR"

Relax delay 1.000 sec
Pulse 45.0 degrees
Acq time: 1.000 sec
Width 24591.8 Hz
128 repetitions
Observe C15, 100.5866392 MHz
Power 42 dB
Continuously on
WALTZ-16 modulated
Data processing
Line broadening 0.5 Hz
Ft size 65536
Total time 6 min, 56 sec
Sample: MD-299
Sample ID: c_40_MD-299_koo-4_20140421_01
File: /home/walkup2/vnmrsys/Data/koo-4/MD-299_Proton_03.fid

Pulse sequence: s1pu1
Solvent: d6c13
Ambient temperature
Sample #40, Operator: walkup2
File: MD-299_Proton_03
VNMRS-400 "GEMINI"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6030.6 Hz
8 repetitions

Observe H1, 400.0340075 MHz
DATA PROCESSING
Line broadening 0.5 Hz
RT size 50230
Total time 0 min, 31 sec

\[
\begin{align*}
4 & \quad \text{O} \\
\text{O} & \quad \text{O} & \quad \text{O}
\end{align*}
\]
Sample: MD-299
Sample ID: e_42_MD-299_koo-4_20140422_01
File: /home/walkup2/vnmrsys/data/koo-4/MD-299_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample, Operator: walkup2
File: Homo_e Carbene
Vnmrs-Dir '700Mhz' =

Relax: Delay 1.000 Sec
Pulse 45.0 degrees
Ana. Time 1.168 sec
Width 24500.0 Hz
128 repetitions

OBSERVE C13, 100.5986432 MHz
DECOUPLE H1, 400.006168 MHz
Power 42 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
RT size 8003N
Total time 4 min, 58 sec
JYM-567
Sample: JYM-567
Sample ID: s_41_JYM-567_xoo-d.20130808_01
File: /home/walkup2/vnmrsys/data/xoo-4/JYM-567_Protot_01.fid
Pulse Sequence: s2pul
Solvent: cdc19
Ambient temperature
Sample #41, Operator: walkup2
File: JYM-567_Protot_01
VNMRS-400 "400MRR"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width ratio 3.3 Hz
8 repetitions
OBSERVE H1, 400.0340000 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

![Chemical Structure](image-url)
Sample: JYM-567-C
Sample ID: s_44_JYM-567-C_koo-4_20130408_01
File: /home/walkup2/vnmrsys/data/ko0-4/JYM-567-C_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient Temperature:
Sample ID: koo-4
Operator: walkup2

Relax. Delay 1.000 sec
Pulse 45 degrees
Acq. time 3.000 sec
Width 24500.8 Hz
128 repetitions
OBSERVE C15 100.5886367 MHz
DECouple HS 400.0560169 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 min, 56 sec
JYM-573-C

Sample: JYM-573-C
Sample ID: s_41_JYM-573-C_koo-4_20130730_01
File: /home/valkup2/vnmrsys/data/koo-4/JYM-573-C_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #41 Operator: valkup2

VMR5-400 400MHz
0.0000 MHz

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24500.0 Hz
512 repetitions
Usable range: 74.289 to 74.290 Hz
DECUPLE NO. 400 0.360168 Hz
Power 42 dB
continuously on
WALTZ-16 disabled

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min, 42 sec
Sample: 13
Sample ID: s_45_JYM-604-C_koo-4_20130423_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-604-C Carbon_01.fld
Pulse Sequence: 2p21
Solvent: cdcl3
Ambient temperature
Sample #45, Operator: walkup2
File: JYM-604-C_Carbon_01
VNMRS-400 "46680C"

Relax delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.880 sec
Width 2400.8 Hz
128 repetitions
OBSERVE Cl2, 100.5886383 MHz
DECOUPLE H1, 400.0360265 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 56 sec

EtO2C

13 10.486
27.012
58.093
118.100
106.131
16.678
14.309
13.919

ppm

13
Sample: MD-313-4
Sample ID: 449_MD-313-4_koo-4_20140723_01
File: /home/walkup2/vnmrSys/data/koo-4/MD-313-4_proton_01.t10

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #40, Operator: walkup2

VNMR-400 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 6630.6 Hz
8 repetitions

DATA PROCESSING
Observe H1, 400.024000 MHz
Line broadening 0.5 Hz
FT size 65526
Total time 0 min, 31 sec
Sample: MD-313-4-C
Sample ID: s_40_MD-313-4-C_koo-4_28148703_01
File: /home/walkup2/vnmrsys/data/koo-4/MD-313-4-C_Carbon_01.dat

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature

Sample #40, Operator: walkup2

VNMRS-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.390 sec
Width 2400.0 Hz
256 repetitions

OBSERVE C13, 100.5886325 MHz
DECOUPLE H1, 400.0040160 MHz
Power 42 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 51 sec
JYM-461

Sample ID: s_37_JYM-461_koo-4_20130124_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-461_Proton_01.fid

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
Sample #37, Operator: walkup2
File: JYM-461_Proton_01
vnmrs-400 "<60ksa"

Relay delay 1.000 sec
pulse 90.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min, 31 sec

\[ \text{CO}_2\text{Et} \]

H

9

11 10 9 8 7 6 5 4 3 2 1 pp

2.40 1.95 2.00 4.24 6.44 6.34

1.08
Sample: JYM-469
Sample ID: s_41_JYM-469_koo-4.20130129_01
File: /home/walkup2/vnmrsys/data/koo-4/5JYM-469_Proton_01.fld

Pulse Sequence: s2p1
Solvent: cdcl3
Ambient temperature
Sample #41, Operator: walkup2 N
File: JYM-469_Proton_01

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
N repetitions 1

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 51 sec
Sample: JYM-469-C
Sample ID: e_44_JYM-469-C_xoo-4.20130129_01
File: /home/walkup2/vnmrsys/data-xoo-4/JYM-469-C_Carbon_01.fid
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient Temperature:
Sample #44, Operator: walkup
vnmr3-400 -s0bmr

Relax, delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 24503.8 Hz
128 repetitions
OBSERVE C13, 100.5866395 MHz
DECOUPLE H1, 400.0360169 MHz
Poser 40 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min, 56 sec

![NCO2Et](Bn)
JYM-688-C

Sample: JYM-688-C
Sample ID: s_45_JYM-688-C_koo-4_20130628_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-688-C_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: dcl3
 Ambient temperature
Sample #45, Operator: walkup

vnmr-400 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 Degrees
Acq. time 1.350 sec
Width 24508.8 Hz
216 repetitions

OBSERVE C13, 100.5886350 MHz
DECOUPLE Hz, 400.0360169 MHz
Power 49 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 85536
Total time 8 min, 23 sec
Sample: MD-J-12
Sample ID: s_46_MD-J-12_koo-4_20140530_01
file: /home/walkup2/vnmrsys/data/koo-4/MD-J-12_Proton_03.trd

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #46, Operator: walkup?
File: MD-J-12_Proton_03
VINNIS-400 "400MRX"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.040 sec
Width 2830.6 Hz
8 repetitions
OBSERVE H1, 400.0340091 kHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

![Chemical Structure Image]

CO2Et
N-(CH2)3OH
12
Sample: MD-J-12
Sample ID: k.40_MD-J-12_koo-4.20140630_01
File: /home/walkup2/vnmrj/data/koo-4_MD-J-12_Carbon_01.fid

Pulse Sequence: 2pul
Solvent: cdcl3
Ambient temperature
Sample #48, Operator: walkup2
RT16: MD-J-12_Carbon_01

WMRS=400 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 24505.8 Hz
512 repetitions

OBSERVE C13, 100.580892 MHz
DECOUPLE H2, 400.0356109 MHz
Power 42 dB
Continuous on

DATA PROCESSING
Line broadening 0.5 Hz
FT size 85536
Total time 19 min, 42 sec

![Chemical Structure](image)

ppm: 200 180 160 140 120 100 80 60 40 20
Sample: JYM-466
Sample ID: s_42_JYM-466_koo-4_20130128_01
File: /home/walkup2/vnmrjys/data/koo-4/JYM-466_Proton_01.fld
Pulse Sequence: 2pul
Solvent: cdc13
Ambient Temperature
Sample #42, Operator: walkup
File: JYM-466_Proton_01.fld
VNMRS-400 "450MR"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
# repetitions
OBSERVE H1, 600.6340095 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

CO₂Et

14
**JYM-466-C**

Sample: JYM-466-C

Sample ID: s_43_JYM-466-C_koo-4_20130829_01

File: /home/walkup2/vnarsys/data/koo-4/JYM-466-C_Carbon_01.fld

**Pulse Sequence:** s2p1

**Solvent:** cdc13

**Ambient temperature**

**Sample #43, Operator:** walkup2

**File:** JYM-466-C_Carbon_01

**nmr 400 MHz**

- Relax. delay 1.000 sec
- Pulse 45.0 degrees
- Acq. time 1.360 sec
- Width 2450.8 Hz
- 256 repetitions
- OBSERVE CI3, 100.586844 MHZ
- DECOUPLE M1, 400.856019 MHZ
- Power 42 W
- continuously on
- WALTZ-16 modulated

**DATA PROCESSING**

- Line broadening 0.5 Hz
- F1 size 65536
- Total time 9 min, 51 sec

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**Diagram:**

- Chemical structure with labels

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**pp**

220 200 180 160 140 120 100 80 60 40 20 0
Sample: MD-J-15
Sample ID: s_47_MD-J-15_koo-4_20140527_01
File: /home/awalkup2/vnmsys/data/koo-4/MD-J-15_Proton_01.fid

Pulse Sequence: s2pu1
Solvent: cca13
Ambient temperature
Sample #47, Operator: walkup2
VNMR-400 "4DNR"

Relax. delay 1.000 sec
Pulse 45.9 degrees
Acq. time 2.049 sec
Width 5533.6 Hz
8 repetitions

Data Processing
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

CO$_2$Et

N

I

15
Sample: MD-J-15
Sample ID: s_47_MD-J-15_koo-d_20140603_01
File: /home/walkup2/vnmrsys/data/koo-d/MD-J-15_Carbon_02.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #47, Operator: walkup2
File: MD-J-15_Carbon_02
VNMRS-400 "40MRX"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24500.0 Hz
S12 repetitions
Coil: C13, 1.00 886544 MHz
DECOUPLE H1, 400.0360169 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min, 42 sec

200 180 160 140 120 100 80 60 40 20 ppm

CO₂Et

15
Sample: JYM-694-C
Sample ID: s_33_JYM-694-C_koo-1_20130703_01
File: /home/walkup2/nmrsys/data/koo-4/JYM-694-C_Carbon_01.fld
Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #33, Operator: walkup

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24599.8 Hz
100 Repetitions
OBSERVE C13, 100.586584 MHz
DECouple H1, 400.8360169 MHz
POWER 4z on
continuously on
WALTZ-16 modulated
DATA PROCESSED
Line broadening 0.5 Hz
FT size 65536
Total time 4 min, 56 sec
JYM-726

Sample ID: s_47_JYM-726_xoo-1_20130715_01
File: /home/walkup2/vnmrsys/data/xoo-4/JYM-726_Proton_01.fid

Pulse Sequence: s2pul
Solvent: cdcl3

Sample temperature:
Sample #47, Operator: wa

File: JYM-726_Proton_01

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 6410.3 Hz
8 repetitions

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

N CO2Et

CO2Et

CO2Et

17
JYM-690-C

Sample: JYM-690-C
Sample ID: 46_JYM-690-C_X00-4_20130628_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-690-C_Carbon_01.fld

Pulse Sequence: sz1ul
Solvent: cdc13
Ambient temperature

Sample #46, Operator: walkup

VNMRS=400 ~400Hz
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24569.8 Hz
512 repetitions

OBSERVE CI3, 100.5886361 MHz
DECOUPLE H, 400.0360169 MHz
Power 45 dB
Continuously on

WALTZ-18 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min. 23 sec
### Sample: JYM-695-1C

**Sample ID:** s_41_JYM-695-1-C, Sample 41, Operator: walkup2

- **File:** /home/walkup2/nmr/data/koo-4/JYM-695-1-C_Carbon_01.fid

**Pulse Sequence:** s2pul

**Solvent:** ddc13

**Ambient temperature**

**Relax. delay:** 1.000 sec

**Pulse 45.6 degrees**

**Acq. time:** 1.000 sec

**Width:** 24508.8 Hz

**128 repetitions**

**OBSEVE:** C33, 100.5886436 MHz

**DECouple:** H1, 400.0380169 MHz

**Power 42 dB**

**continuously on**

**DATA PROCESSING**

- Line broadening 0.5 Hz
- FT size 65536

**Total time:** 4 min, 56 sec

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**Diagram:**

- Compound: CO2Et
- Structure: ![N-N]_[CO2Et]
- Label: 19

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**Data:**

- 1H NMR (600 MHz, CDCl3):
  - 7.71, 7.69, 7.62, 7.48, 7.45, 7.40, 7.38, 7.35, 7.32, 7.30, 7.28, 7.27, 7.25, 7.23, 7.21, 7.19, 7.17, 7.15, 7.13, 7.11, 7.09, 7.07, 7.05, 7.03, 7.01, 6.99, 6.97, 6.95, 6.93, 6.91, 6.89, 6.87, 6.85, 6.83, 6.81, 6.79, 6.77, 6.75, 6.73, 6.71, 6.69, 6.67, 6.65, 6.63, 6.61, 6.59, 6.57, 6.55, 6.53, 6.51, 6.49, 6.47, 6.45, 6.43, 6.41, 6.39, 6.37, 6.35, 6.33, 6.31, 6.29, 6.27, 6.25, 6.23, 6.21, 6.19, 6.17, 6.15, 6.13, 6.11, 6.09, 6.07, 6.05, 6.03, 6.01, 5.99, 5.97, 5.95, 5.93, 5.91, 5.89, 5.87, 5.85, 5.83, 5.81, 5.79, 5.77, 5.75, 5.73, 5.71, 5.69, 5.67, 5.65, 5.63, 5.61, 5.59, 5.57, 5.55, 5.53, 5.51, 5.49, 5.47, 5.45, 5.43, 5.41, 5.39, 5.37, 5.35, 5.33, 5.31, 5.29, 5.27, 5.25, 5.23, 5.21, 5.19, 5.17, 5.15, 5.13, 5.11, 5.09, 5.07, 5.05, 5.03, 5.01, 4.99, 4.97, 4.95, 4.93, 4.91, 4.89, 4.87, 4.85, 4.83, 4.81, 4.79, 4.77, 4.75, 4.73, 4.71, 4.69, 4.67, 4.65, 4.63, 4.61, 4.59, 4.57, 4.55, 4.53, 4.51, 4.49, 4.47, 4.45, 4.43, 4.41, 4.39, 4.37, 4.35, 4.33, 4.31, 4.29, 4.27, 4.25, 4.23, 4.21, 4.19, 4.17, 4.15, 4.13, 4.11, 4.09, 4.07, 4.05, 4.03, 4.01, 3.99, 3.97, 3.95, 3.93, 3.91, 3.89, 3.87, 3.85, 3.83, 3.81, 3.79, 3.77, 3.75, 3.73, 3.71, 3.69, 3.67, 3.65, 3.63, 3.61, 3.59, 3.57, 3.55, 3.53, 3.51, 3.49, 3.47, 3.45, 3.43, 3.41, 3.39, 3.37, 3.35, 3.33, 3.31, 3.29, 3.27, 3.25, 3.23, 3.21, 3.19, 3.17, 3.15, 3.13, 3.11, 3.09, 3.07, 3.05, 3.03, 3.01, 2.99, 2.97, 2.95, 2.93, 2.91, 2.89, 2.87, 2.85, 2.83, 2.81, 2.79, 2.77, 2.75, 2.73, 2.71, 2.69, 2.67, 2.65, 2.63, 2.61, 2.59, 2.57, 2.55, 2.53, 2.51, 2.49, 2.47, 2.45, 2.43, 2.41, 2.39, 2.37, 2.35, 2.33, 2.31, 2.29, 2.27, 2.25, 2.23, 2.21, 2.19, 2.17, 2.15, 2.13, 2.11, 2.09, 2.07, 2.05, 2.03, 2.01, 1.99, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01

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**Legend:**

- CO2Et: Carbon dioxide ethyl ester
- CH3: methyl group

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**Note:**

- The data presented is typical of 1H NMR spectra for CO2Et and CH3 groups in a CDCl3 solvent.
JWM-703
Sample: JWM-703
Sample ID: s_40_JWM-703_koo-4_20130704_01
File: /home/walkup2/vnmrsys/data/koo-4/JWM-703_Proton_01.fid

Pulse Sequence: s2pu1
Solvent: cdc12
Ambient temperature:
Sample #40, Operator: val
VNMRS-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 400.0340093 MHz
DATA PROCESSING
  Line broadening 0.5 Hz
  FT size 65536
Total time 0 min, 31 sec
Sample: D0-J-22
Sample ID: s_45_D0-J-22_koop-4_20140604_01
File: /home/walkup2/wnmfsys/data/koo-4/D0-J-22_Proton_01.fld

Pulse Sequence: s2pu1
Solvent: d2o
Ambient temperature
Sample #45, Operator: walkup2
File: D0-J-22_Proton_01
VNMRS-600 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 8000.6 Hz
8 repetitions

OBSERVE NL: 700.0340091 MHz
DATA PROCESSING
Line broadening 0.5 Hz
RF slice 80236
Total time 0 min, 31 sec

![Chemical Structure]
Sample: MD-J-22
Sample ID: x_50_MD-J-22_koo-4_20140604_01
file: /home/walkup2/vmrtrays/data/koo-4/MD-J-22_Carbon_01.fid

Pulse Sequence: s2p1
Solvent: cdc13
Ambient temperature
Sample #50, Operator: walkup2
File: MD-J-22_Carbon_01
VNMRS-400 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 2000.0 Hz
512 repetitions
OBSERVE C13, 100.5886355 MHz
DECOUPLE H1, 400.02600169 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 85536
Total time 18 min, 42 sec
Sample: JYM 717 C
Sample ID: s_46_JYM-717-C_koo-4_20130708_01
File: /home/walkup2/vnnersys/data/koo-4/JYM-717-C_Carbon_01.fid

Pulse Sequence: s2pul

Solvent: dmso
Ambient temperature
Sample #46, Operator: walkup2

VNMRS-400 "899MM"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.360 sec
Width 24509.8 Hz
512 repetitions

Observe C13, 100.5801950 MHz
Decouple H1, 400.0979170 MHz
Power 42 dB
Continuous on

WALTZ-16 modulated
Data Processing
Line broadening 0.5 Hz
FT size 80000
Total time 19 min, 42 sec
Sample: MD-305
Sample ID: s_41_MD-305_koo-4_20140813_01
File: /home/Walkup2/vnmrsys/Data/Koo-4/MD-305_Proton_02.f1d
Pulse Sequence: s2pu1
Solvent: cdc13
Ambient temperature
Sample #41, Operator: walkup2
VMR5-400 "500MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6030.5 Hz
8 repetitions
OBSERVE H1 400.0354087 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

![NMR Spectrum Image]

Aromatic ring resonance at 7.75 ppm
Ester group resonance at 1.27 ppm

Chemical Shifts:
- 7.75 ppm
- 5.60 ppm
- 4.28 ppm
- 3.75 ppm
- 1.27 ppm

Structural Formula:

EtO

NO2

HO

26

EtO

NO2

26

1.00 2.33
1.19

0.94 2.37 2.62
3.23 2.62 3.41
JYM-657-C
Sample: JYM-657-C
Sample ID: s_41_JYM-657-C_koo-4_20130607_01
File: /home/walkupz/vnmrsys/data/koo-4/JYM-657-C_Carbon_01.fld

Pulse sequence: szpu1
Solvent: cdc13
Ambient temperature
Sample #41, operator: walkupz

1H, 400.0389189 MHz
Decoupler H1, 400.0389189 MHz
Power 42 dB
Continuously on WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 min, 56 sec
EtO
NO2
CO2Et
EtO
OH
NO2
CO2Et
Sample: JYM-723-C
Sample ID: s_49_JYM-723-C_koo-4_20130717_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-723-C_Carbon_01.fld

Pulse Sequence: e2pul
Solvent: cdcl3
Ambient temperature
Sample #49, Operator: Galkup2
File: JYM-723-C_Carbon_01

VNMRS-600 "490MHz"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.250 sec
Width 24500.0 Hz
128 repetitions
WKEFUF 115, 160.5686555 MHz
DECOUPLE H1, 400.030169 MHz
Power 42 dB
continuously on
WMUL/1H MODULATED
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65526
Total time 4 min, 56 sec
Sample: MO-317-C
Sample ID: s_47_MO-317-C_Koo-4_20140627_01
file: /home/walkup2/vnmrsys/data/koo-4/MO-317-C_Carbon_01.tif

Pulse Sequence: s2pul
Solvent: ddc13
Ambient temperature

Relax, delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 12000.0 Hz
512 repetitions
OBSERVE C13, 100.5886351 MHz
DECOUPLE H1, 400.0660169 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min, 42 sec
Sample: s_49_JVM-772-1
Sample ID: s_49_JVM-772-1_koo-4_20130608_01
File: /home/walkup/vmrsys/data/koo-4/JVM-772-1_Proton_01.fid

Pulse Sequence: s2pul
Solvent: dcl3
Ambient temperature
Sample M9: Operator: walkup2
File: JVM-772-1_Proton_01
VMRMS-620 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.849 sec
Width 6416.3 Hz
8 repetitions

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

Cl
O
31

Cl
O

H
OEt

NO2
O

NO2
O
Sample: JYM-789-C
Sample ID: s_45_JYM-789-C_koo-4_20130821_01
File: /home/walkup2/vnmrSys/data/koo-4/JYM-789-C_Carbon_01.fid

Pulse Sequence: 62pu1
Solvent: cdc13
Ambient temperature
Sample #45, Degrador: walkup2
VNMRS-400 "40MR"

Relax. delay 1,000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 24500.8 Hz
128 repetitions
OBSERVE C13, 100.588395 MHz
DECOUPLE H1, 400.035685 MHz
Power 42 dB
continuously on
WALTZ 16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FF size 65536
Total time 4 min, 56 sec

400.0400 65.20
239.0263 33.30
13.0006 18.00

220 200 180 160 140 120 100 80 60 40 20 0

64
Sample: JYM-791
Sample ID: s_41_JYM-791_koop-4_20130816_01
file: /home/walkup2/vnmrsys/data/koo-4/JYM-791_Proton_01.fid

Pulse Sequence: s2py1
Solvent: cdc13
Ambient temperature
Sample #41, Operator: walkup2
file: JYM-791_Proton_01

Vnmrs -100 -50 0 50
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8680.3 Hz
8 repetitions
OBSERVE H1, 400.0340076 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

\[
\begin{align*}
\text{NO}_2 & \quad \text{OEt} \\
\text{O} & \quad \text{O} \\
\text{34} & \quad \text{NO}_2 \\
\end{align*}
\]
JYM-791-C

Sample: JYM-791-C
Sample ID: s_S5_JYM-791-C_koo-a_20130816_42
File: /home/walkup2/vnmrsys/data/koo-a/JYM-791-C_Carbon_01.fid

Pulse Sequence: 2pul
Solvent: cdc13
Temperature: ambient
Sample: 568 Operator: walkup2
File: JYM-791-C_Carbon_01
VNMRS-600 "500MR"

Relax delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.500 sec
Width 24509.8 Hz
256 repetitions
Observe C13, 100.586563 MHz
Decouple H1, 600.050016 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 51 sec
Sample: MD-J-35
Sample ID: s_40_MD-J-35_koo-4_20140605_01
File: /home/walkup2/vrmr/sys/data/koo-4/MD-J-35_Carbon_01.fid
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #40, Operator: walkup2
File: MD-J-35_Carbon_01
VNMRS=400 "400MR"

Relax. delay 1.000 sec
Pulse 48.0 degrees
Acq. time 1.000 sec
Width 24500.8 Hz
512 repetitions
OBSERVE 019, 100.58988301 MHz
DECOUPLE H1, 400.0386180 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min, 42 sec

![N\text{H}^{35}CO_2Et]
Sample ID: s_4S_JYM-785_koo-4_20130814_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-785_Proton_02.fid
Pulse Sequence: zgup1
Solvent: cdcl3
Ambient temperature
Sample #4S, Operator: wboth
File: JYM-785_Proton_02.fid

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 0.025 Hz
2 repetitions
OBsERVE H1, 400.0340054 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min, 31 sec
Sample: JYM-785-C
Sample ID: s_47_JYM-785-C_koo-4_20130814_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-785-C_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: dcd13
Ambient temperature
Sample #47, Operator: walkup2
File: JYM-785-C_Carbon_01
vmem-len = "4gmp"

Relax. delay: 0.000 sec
Pulse 90.0 degrees
Acq. time 1.300 sec
Width 24500.0 Hz
128 repetitions
OBSERVE C13, 100.5886372 MHz
DECUPLE H1, 400.0360169 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 min, 56 sec
JYM-790

Sample: s_40_JYM-790_koo-4_20130816_01
File: /home/malkup2/vnmrsys/data/koo-4/JYM-790_Proton_01.fid

Pulse Sequence: s2p1
Solvent: cdc13
ambient temperature: 298

Sample #40, Operator: wipkup2

Relax. delay 1.000 sec
raise 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
0 repetitions

Observe H1, 400.0340068 MHz

Data Processing
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

![NMR Spectrum](image)

![Chemical Structure](image)
Sample: JYM-790-C
Sample ID: s_49_JYM-790-C_koo-4_20130816_01
File: /home/walkup2/vnmr5sys/data/koo-4/JYM-790-C_Carbon_01.fid

Pulse Sequence: s2pu1
Solvent: dcl3
Ambient temperature
Sample #49, Operator: walkup2
File: JYM-790-C_Carbon_01
VNMRS-400 "400RR"

Relax, delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.350 sec
Width 2459.8 Hz
256 repetitions

OBSERVE C13, 100.5886350 MHz
DECOUPLE H1, 400.0360160 MHz
Power 42 dB
continuously on

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 min, 51 sec

![Chemical Structure Image]
JYM-793

Sample: JYM-793
Sample ID: s_40_JYM-793_koo-2_20130821-01
File: /home/walkup2/vnmrsys/data/koo-2/JYM-793_Proton_01.fid

Pulse Sequence: s2p1
Solvent: cdc3
Ambient temperature
Sample #40, Operator: walkup2
Command: JYM-793_Proton_01
vnmrsys-699 "40mm"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
0 repetitions

OBSERVE H1, 400.0240103 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 6 min, 31 sec
JYM-793-C

Sample: JYM-793-C
Sample ID: s_46_JYM-793-C_koo-4_20130822_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-793-C_Carbon_01.fid

Pulse sequence: szpul
Solvent: cdc13
Ambient temperature
Sample no. 46, Operator: walkup2
VMR-500-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees

Acq. time 1.268 sec
Width 20.608.0 Hz
256 repetitions

OBSERVE C13, 106.5862882 MHz
DECOUPLE H1, 400.0363108 MHz
Power 42 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 51 sec

MeO

CO₂Et

38 H

220 200 180 160 140 120 100 80 60 40 20 0
Sample: JYM-257
Sample ID: s_44_JYM-257_koo-4_20130716_01
File: /home/walkup2/vnmrsys/data/koo-4/JYM-257_Proton_01.fid

Pulse Sequence: s2pu1
Solvent: cdCl3
Ambient temperature
Sample #44, Operator: walkup2
File: JYM-257_Proton_01
VNMRS-400 "40MR"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.049 sec
Width 610.3 Hz
8 repetitions

OBSERVE H1 400.0340066 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec
Pulse Sequence: s2pul

Solvent: cdCl3
Ambient temperature
Sample #:53, Operator: walkup2
File: JYM-727-C_Carbon_01

VNMRS=400 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.200 sec
Width 24508.8 Hz
128 repetitions

OBSERVE CI3, 100.084644 MHz
DECUPLE HI, 400.0050169 MHz
Power 42 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65538
Total time 4 min, 56 sec

![Chemical Structure](image)
Sample: JYM-777-2
Sample ID: s_50_JYM-777-2_koo=4_20130808_01
File: /home/walkup2/vnmrsys/data/koo=4/JYM-777-2_Proton_01.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #50, Operator: walkup2
File: JYM-777-2_Proton_01

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<tr>
<th>Relax. delay</th>
<th>1.000 sec</th>
</tr>
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<tbody>
<tr>
<td>Pulse 45.0 degrees</td>
<td></td>
</tr>
<tr>
<td>Acq. time 2.049 sec</td>
<td></td>
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<tr>
<td>Width 6418.3 Hz</td>
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<tr>
<td># repetitions</td>
<td></td>
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</table>

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

---

40

OMe
MeO
NO2
O
OEt

41

OMe
MeO
NO2
O
OEt

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Sample: JYM-782-1
Sample ID: s_42_JYM-782-1_koo-1_20130812_01
File: /home/walkup2/wnmrsys/data/koo-1/JYM-782-1_Proton_01.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient Temperature
Sample #42, Operator: walkup2

VWR-400 "400KRM"

Relax. delay 1.000 sec
Pulse 95.0 degrees
Acq. time 2.045 sec
Width 6410.3 Hz
8 repetitions

OBSERVE: H1: 400.0340008 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec
Sample: JYM-782-1-C
Sample ID: s_45_JYM-782-1-C_koo-4_20130812_01
File: /home/walkup2/vnmrsys/data/Koo-4/JYM-782-1-C_Carbon_01.fid

Pulse Sequence: edited

Solvent: d6-DMSO

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 24508.8 Hz
256 repetitions

OBSERVE C13, 100.6 MHz
DECOUPLE H1, 400.036 MHz

Power 42 dB
continuously on
WALTZ-16 modulated

Data processing
Line broadening 0.5 Hz
Fit size 65536
Total time 19 min, 42 sec
JYM-729-C

Sample: JYM-729-C
Sample ID: s_46_JYM-729-C_koo=4_20130717_01
File: /home/walkupz/vnertsys/data/koo=4/JYM-729-C_Carbon_01.fid

Pulse Sequence: szpu1
Solvent: ddc13
Ambient temperature
Sample #46, Operator: walkupz

Relax. delay 3.000 sec
Pulse 45.6 degrees
Acq. time 1.000 sec
Width 24500.8 Hz

128 repetitions
OBSERVE C13, 100.5686368 MHz
DECOUPLE 1H, 400.0360169 MHz
Power 42 dB
continuously on
WMTC-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 min, 56 sec

[Chemical structure images with labeled peaks]

220 200 180 160 140 120 100 80 60 40 20 0
Sample: JVM-778-3
Sample ID: 6_45_JVM-778-3_koo-4_20130812_01
file: /home/Walkup/vnmrsys/data/koo-4/JVM//a-3_proton_01.t1d

Pulse Sequence: sp2pul
Solvent: ccl3
Ambient temperature

Sample #45, Operator: Walkup
file: JVM-778-3_br000200.d
VNMRS: 400 "800MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.949 sec
Width 8410.3 Hz
8 repetitions

DATA PROCESSING
mHz, 300.0340088 MHz
Line broadening 0.5 Hz
RT size 60000
Total time 0 min, 31 sec

![Chemical Structures](data:image/png;base64,iVBORw0KGgoAAAANSUhEUgAA...)

<table>
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<th>ppm</th>
<th>1.82</th>
<th>0.67</th>
<th>1.06</th>
<th>0.31</th>
<th>0.82</th>
<th>3.92</th>
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<td>0.66</td>
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<td>0.39</td>
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Sample: JYM-778-3-C
Sample ID: s.46_JYM-778-3-C_koo-4.20130814_01
File: /home/walkup2/wnmssey/data/Roo-4/JYM-778-3-C_Carbon_01.fid

Pulse Sequence: 62pul
Solvent: ceech
Ambient temperature
Sample #46, Operator: wakpup2
File: JYM-778-3-C_Carbon_01

WNMR-400 "450MR"

Relax. delay 3000 sec
Pulse 45.0 degrees
Acq. time 1.380 sec
Width 24600.8 Hz
512 repetitions

OBSERVE C13, 100.5866345 MHz
ARMNHF H1, 200.4806544 MHz
Power 42 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min, 42 sec
Sample: MD-316
Sample ID: s_47_MD-316_koo-4_20140630_01
file: /home/wwalkup2/vnmr/sys/Data/koo-4/MD-316_Proton_e1.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #47, Operator: wwalkup2
PT3MD-316_PROTON_01

vm3s-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6830.6 Hz
8 repetitions

Observe MHz 400.0340087 MHz
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 51 sec

[Chemical structure image]

1.04 1.03 2.40 2.62 3.03 7.13
Sample: JYM-784-C
Sample ID: s_42_JYM-784-C_koo-2_20130813_01
File: /home/walkup2/vnmrrys/data/koo-2/JYM-784-C_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: cdc10
Ambient temperature
Sample #42, Operator: walkup2
File: JYM-784-C_Carbon_01
VMR5-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24593.5 Hz
512 repetitions
OBSERVE C13, 100.5886331 MHz
DECOUPLE H1, 400.0360169 MHz
Power 42 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 85536
Total time 19 min, 42 sec

---

86
Sample: JYM-740
Sample ID: s_46_JYM-740_koo-4_20130722_01
File: /home/walkup2/vnmrsyndata/koo-4/JYM-740_Proton_01.fid

Pulse Sequence: s2pul
Solvent: d6c13
Ambient temperature

Sample #46, Operator:

File: JYM-740_Proton_01.fid

VNMR-400 "400MHz"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 6410.3 Hz
5 repetitions

DATA PROCESSING:

rt size 8558
Total time 3 min, 31 sec

EtO2C-N-CO2Et

47