Supplementary Material

Highly Selective One-pot Coupling Reaction of Indole, Aromatic Aldehydes and 4-Hydroxycoumarin Using Copper Octoate as a Homogeneous Catalyst

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(4-hydroxycoumarin-3-yl)(3-indolyl)(phenyl)methane (4a).^[18] To a mixture of 4-hydroxycoumarin (1 mmol, 0.162 g), benzaldehyde (0.106 g, 1 mmol) and indole (1 mmol, 0.117 g) in n-hexane (2 ml), was added 0.58 g of a 6% solution of Copper octoate in xylene (10 mole%). The mixture was refluxed for 1 h. next, the solvent was evaporated and 10 ml of ethanol was added to the residue. The resulted mixture was steered for 15 minutes and filtered and washed with ethanol to give the crude product which was further purified by recrystallization from ethanol to give the pure product as Pale pink crystals with 88% Yield. mp: 198-199 °C. IR: 3336, 3275, 3056, 1689, 1617, 1570, 1493. ¹H-NMR (500 MHz, CDCl₃): 9.44 (s, 1H); 7.78 (s, 1H); 7.65 (dd, J = 7.90 Hz, J = 1.33 Hz, 1H); 7.45 (m, 2H); 7.38 (m, 3H); 7.28 (m, 4H); 7.18 (t, J = 7.42 Hz, 2H); 7.01 (t, J = 7.68 Hz, 1H); 6.71 (d, J = 1.1 Hz, 1H); 5.99 (s, 1H). ¹³C-NMR (500 MHz, CDCl₃): 163.1; 161.4; 152.8; 142.1; 137.1; 131.9; 128.6; 128.4; 127.3; 126.6; 124.7; 123.9; 123.6; 122.1; 119.3; 119.1; 116.6; 116.4; 115.2; 112.0; 107.8; 38.8. Ms: 367 (M⁺), 256, 204, 117, 69, 57, 43. Anal. Calcd. for C₂₄H₁₇NO₃: C, 78.46; H, 4.66; N, 3.81. Found: C, 78.42; H, 4.72; N, 3.83.

(4-hydroxycoumarin-3-yl)(3-indolyl)(4-methylphenyl)methane (4b). To a mixture of 4-hydroxycoumarin (1 mmol, 0.162 g), 4-tolylaldehyde (0.120 g, 1 mmol) and indole (1 mmol,

0.117 g) in n-hexane (2 ml), was added 0.58 g of a 6% solution of Copper octoate in xylene (10 mole%). The mixture was refluxed for 4 h. next, the solvent was evaporated and 10 ml of ethanol was added to the residue. The resulted mixture was steered for 15 minutes and filtered and washed with ethanol to give the crude product which was further purified by recrystallization from ethanol to give the pure product as Pale pink crystals with 86% Yield. mp: 169-170 °C. IR: 3324, 3279, 3052, 1690, 1620, 1425. ¹H-NMR (500 MHz, CDCl₃): 9.84 (s, 1H); 7.98 (s, 1H); 7.64 (d, J = 7.8 Hz, 1H); 7.44 (t, J = 7.76 Hz, 1H); 7.39 (d, J = 7.89 Hz, 1H); 7.34 (d, J = 8.09 Hz, 1H); 7.23 (d, J = 7.76 Hz, 3H); 7.14 (p, J = 7.71 Hz, 2H); 7.06 (d, J = 7.53 Hz, 2H); 6.96 (t, J = 7.50 Hz, 1H); 6.74 (s, 1H); 5.92 (s, 1H); 2.27 (s, 3H). ¹³C-NMR (500 MHz, CDCl₃): 163.4; 161.7; 153.0; 138.3; 137.6; 136.7; 132.1; 129.6; 128.6; 127.1; 124.8; 124.1; 123.6; 122.9; 120.0; 119.4; 116.6; 116.5; 115.7; 112.2; 107.1; 39.3; 21.4. Ms: 381 (M⁺), 347, 336, 249, 219, 162, 120, 92. Anal. Calcd. for C₂₅H₁₉NO₃: C, 78.72; H, 5.02; N, 3.67. Found: C, 78.73; H, 4.98; N, 3.59.

(4-hydroxycoumarin-3-yl)(3-indolyl)(4-nitrophenyl)methane (4c).^[18] To a mixture of 4-hydroxycoumarin (1 mmol, 0.162 g), 4-nitrobenzaldehyde (0.151 g, 1 mmol) and indole (1 mmol, 0.117 g) in n-hexane (2 ml), was added 0.58 g of a 6% solution of Copper octoate in xylene (10 mole%). The mixture was refluxed for 45 min. next, the solvent was evaporated and 10 ml of ethanol was added to the residue. The resulted mixture was steered for 15 minutes and filtered and washed with ethanol to give the crude product which was further purified by recrystallization from ethanol to give the pure product as Pale yellow crystals with 96% Yield. mp: 207 °C. IR: 3300, 3056, 1691, 1624, 1518, 1348. ¹H-NMR (500 MHz, CDCl₃): 9.48 (s, 1H); 8.84 (s, 1H); 8.16 (d, J = 8.42 Hz, 2H); 7.80 (d, J = 7.81 Hz, 1H); 7.58 (d, J = 8.38 Hz, 2H); 7.53 (t, J = 7.82 Hz, 1H); 7.47 (d, J = 7.91 Hz, 1H); 7.43 (d, J = 8.15 Hz, 1H); 7.31 (m, 1H); 7.24 (m, 2H); 7.07 (t, J = 7.62 Hz, 1H); 6.86 (s, 1H); 6.17 (s, 1H). ¹³C-NMR (500 MHz, CDCl₃): 163.3; 162.0; 153.1; 150.9; 146.7; 137.0; 132.3; 129.7; 127.3; 124.8; 124.2; 123.9; 123.6; 122.5; 119.7; 119.3; 116.8; 116.6; 114.0; 112.1; 107.2; 38.7. Ms: 412 (M⁺), 251, 217, 204, 176, 117, 92. Anal. Calcd. for C₂₄H₁₆N₂O₅: C, 69.90; H, 3.91; N, 6.79. Found: C, 69.75; H, 3.79; N, 6.92.

(4-hydroxycoumarin-3-yl)(3-indolyl)(2-methoxyphenyl)methane (4d). To a mixture of 4-hydroxycoumarin (1 mmol, 0.162 g), 2-methoxybenzaldehyde (0.136 g, 1 mmol) and indole (1 mmol, 0.117 g) in n-hexane (2 ml), was added 0.58 g of a 6% solution of Copper octoate in xylene (10 mole%). The mixture was refluxed for 2 h. next, the solvent was evaporated and 10 ml of ethanol was added to the residue. The resulted mixture was steered for 15 minutes and filtered and washed with ethanol to give the crude product which was further purified by recrystallization from ethanol to give the pure product as Pale pink crystals with 81% Yield. mp: 186-187 °C. IR: 3332, 3051, 1688, 1624, 1249. ¹H-NMR (500 MHz, CDCl₃): 8.21 (s, 1H); 7.93 (s, 1H); 7.74 (d, J = 7.86 Hz, 1H); 7.53 (t, J = 7.74 Hz, 1H); 7.46 (d, J = 7.39 Hz, 1H); 7.41 (d, J = 8.06 Hz, 2H); 7.34 (m, 2H); 7.25 (m, 2H); 7.07 (t, J = 7.71 Hz, 1H); 7.00 (m, 2H); 6.84 (s, 1H); 6.28 (s, 1H); 3.75 (s, 3H). ¹³C-NMR (500 MHz, CDCl₃): 163.5; 161.7; 157.6; 153.0; 137.7; 131.9; 130.1; 129.5; 128.7; 127.0; 124.2; 124.0; 123.6; 122.7; 121.3; 119.8; 119.5; 116.6; 116.5;

114.1; 112.1; 111.7; 106.2; 56.1; 35.4. Ms: 397 (M^+), 352, 249, 236, 162, 120, 92, 63. Anal. Calcd. for $C_{25}H_{19}NO_4$: C, 75.55; H, 4.82; N, 3.52. Found: C, 75.61; H, 4.79; N, 3.52.

(4-hydroxycoumarin-3-yl)(3-indolyl)(4-chlorophenyl)methane (4e). To a mixture of 4-hydroxycoumarin (1 mmol, 0.162 g), 4-chlorobenzaldehyde (0.141 g, 1 mmol) and indole (1 mmol, 0.117 g) in n-hexane (2 ml), was added 0.58 g of a 6% solution of Copper octoate in xylene (10 mole%). The mixture was refluxed for 3 h. next, the solvent was evaporated and 10 ml of ethanol was added to the residue. The resulted mixture was steered for 15 minutes and filtered and washed with ethanol to give the crude product which was further purified by recrystallization from ethanol to give the pure product as Pale pink crystals with 95% Yield. mp: 190 °C. IR: 3303, 3055, 1690, 1621, 1492, 1424. ^1H -NMR (500 MHz, $CDCl_3$): 9.78 (s, 1H); 8.40 (s, 1H); 7.70 (dd, $J = 7.95$ Hz, $J = 1.31$ Hz, 1H); 7.46 (t, $J = 7.07$ Hz, 1H); 7.42 (d, $J = 7.96$ Hz, 1H); 7.37 (d, $J = 8.19$ Hz, 1H); 7.31 (m, 2H); 7.25 (m, 3H); 7.17 (p, $J = 7.23$ Hz, 2H); 7.00 (t, $J = 7.29$ Hz, 1H); 6.77 (d, $J = 1.51$ Hz, 1H); 5.98 (s, 1H). ^{13}C -NMR (500 MHz, $CDCl_3$): 163.4; 162.0; 153.1; 140.4; 137.5; 132.7; 132.3; 130.2; 128.9; 127.0; 124.8; 124.2; 123.7; 123.0; 120.1; 119.4; 116.8; 116.5; 115.3; 112.2; 106.8; 39.1. MS: 401 (M^+), 356, 249, 239, 204, 162, 120, 91. Anal. Calcd. for $C_{24}H_{16}NO_3Cl$: C, 71.73; H, 4.01; N, 3.49. Found: C, 71.70; H, 3.98; N, 3.48.

(4-hydroxycoumarin-3-yl)(3-indolyl)(3-bromophenyl)methane (4f). To a mixture of 4-hydroxycoumarin (1 mmol, 0.162 g), 3-bromobenzaldehyde (0.185 g, 1 mmol) and indole (1 mmol, 0.117 g) in n-hexane (2 ml), was added 0.58 g of a 6% solution of Copper octoate in xylene (10 mole%). The mixture was refluxed for 4 h. next, the solvent was evaporated and 10 ml of ethanol was added to the residue. The resulted mixture was steered for 15 minutes and filtered and washed with ethanol to give the crude product which was further purified by recrystallization from ethanol to give the pure product as Pale pink crystals with 83% Yield. mp: 206 °C. IR: 3316, 3261, 1686, 1617, 1427, 1283. ^1H -NMR (500 MHz, $CDCl_3$): 9.97 (s, 1H); 9.16 (s, 1H); 7.74 (d, $J = 11.93$ Hz, 1H); 7.43 (s, 1H); 7.40 (t, $J = 7.78$ Hz, 1H); 7.35 (d, $J = 7.95$ Hz, 1H); 7.29 (m, 1H); 7.24 (d, $J = 7.81$ Hz, 2H); 7.18 (d, $J = 8.27$ Hz, 1H); 7.13 (t, $J = 7.61$ Hz, 1H); 7.05 (t, $J = 7.79$ Hz, 2H); 6.90 (t, $J = 7.49$ Hz, 1H); 5.95 (s, 1H). ^{13}C -NMR (500 MHz, $CDCl_3$): 163.3; 161.9; 153.1; 144.7; 137.3; 132.2; 131.7; 130.3; 129.9; 127.6; 127.2; 124.8; 124.1; 123.8; 122.7; 119.9; 119.3; 116.7; 116.6; 114.8; 112.2; 107.0; 39.0. Ms: 445 (M^+), 330, 204, 162, 120, 92, 63. Anal. Calcd. for $C_{24}H_{16}NO_3Br$: C, 64.59; H, 3.61; N, 3.14. Found: C, 64.48; H, 3.58; N, 3.16.

IR, ^1H -NMR, ^{13}C -NMR and Mass Spectra of 4a

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1D NMR plot parameters
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PROCNO 1

F2 - Acquisition Parameters
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SOLVENT CDCl3
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PCPD2 80.00 usec
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PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
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F1 27037.92 Hz
F2P -5.000 ppm
F2 -508.79 Hz
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HZCM 1383.33508 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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SOLVENT CDCl3
NS 74
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
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DM 16.650 usec
DE 6.50 usec
TE 298.0 K
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***** CHANNEL f1 *****
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PL1 3.00 dB
SFO1 125.7703643 MHz

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NUC2 1H
PCPD2 80.00 usec
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PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
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WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
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CY 6.02 cm
F1P 57.637 ppm
F1 7248.30 Hz
F2P 28.864 ppm
F2 3629.84 Hz
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HZCM 180.92418 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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AQ 0.5456539 sec
RG 6502
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SFO1 125.7703643 MHz

***** CHANNEL f2 *****
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NUC2 1H
PCPD2 80.00 usec
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PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 6.02 cm
F1P 144.754 ppm
F1 18205.21 Hz
F2P 102.545 ppm
F2 12895.84 Hz
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HZCM 265.46817 Hz/cm

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IR, ¹H-NMR, ¹³C-NMR and Mass Spectra of 4b

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24/10/2011

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Current Data Parameters
NAME Mousavizadeh
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111119
Time 10.05
INSTRUM spect
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1D NMR plot parameters
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CY 13.16 cm
F1P 13.586 ppm
F1 6754.68 Hz
F2P 0.629 ppm
F2 314.80 Hz
PPMCM 0.64782 ppm/cm
HZCM 323.99393 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
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Time 16.29
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PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 126
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
RG 7298.2
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
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SFO1 125.7703643 MHz

***** CHANNEL f2 *****
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PL13 15.50 dB
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F2 - Processing parameters
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SF 125.7577390 MHz
WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.45 cm
F1P 46.570 ppm
F1 5856.48 Hz
F2P 18.765 ppm
F2 2359.50 Hz
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HZCM 174.62870 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 126
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
RG 7298.2
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
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PL12 15.50 dB
PL13 15.50 dB
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F2 - Processing parameters
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SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.45 cm
F1P 142.840 ppm
F1 17963.21 Hz
F2P 102.585 ppm
F2 12900.81 Hz
PPMCM 2.01276 ppm/cm
HZCM 253.12007 Hz/cm

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IR, ¹H-NMR, ¹³C-NMR and Mass Spectra of 4c

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Current Data Parameters
NAME Mousavizadeh
EXPNO 1
PROCNO 1

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Time 13.46
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AQ 1.5860696 sec
RG 574.7
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DE 6.50 usec
TE 298.0 K
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MCREST 0.00000000 sec
MCWK 0.01500000 sec

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LB 0.30 Hz
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1D NMR plot parameters
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CY 6.29 cm
F1P 9.307 ppm
F1 4654.74 Hz
F2P 5.832 ppm
F2 2915.54 Hz
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HZCM 86.90598 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 13.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TO 32768
SOLVENT CDCl3
NS 93
DS 4
SWH 30030.020 Hz
FIDRES 0.516444 Hz
AQ 0.5456539 sec
RG 7298.2
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SF01 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
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PCPD2 80.00 usec
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PL12 15.50 dB
PL13 15.50 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.87 cm
F1P 209.841 ppm
F1 26389.07 Hz
F2P 6.813 ppm
F2 856.78 Hz
PPMCM 10.15138 ppm/cm
HZCM 1276.61438 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120505
Time 13.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 93
DS 4
SWH 30030.029 Hz
FIDRES 0.918444 Hz
AQ 0.545539 sec
RG 7298.2
DM 15.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.132005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.87 cm
F1P 53.840 ppm
F1 6770.82 Hz
F2P 23.991 ppm
F2 3017.07 Hz
PPWM 1.48245 ppm/cm
HZCM 187.68770 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120505
Time 13.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 93
DS 4
SWH 30030.029 Hz
FIDRES 0.918444 Hz
AQ 0.545539 sec
RG 7298.2
DM 15.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.132005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.87 cm
F1P 141.190 ppm
F1 17795.79 Hz
F2P 105.290 ppm
F2 13241.00 Hz
PPWM 1.79503 ppm/cm
HZCM 225.73941 Hz/cm

File : C:\MSDCHEM\4\DATA\SNAPSHOT\64008699.D
Operator :
Acquired : 14 Dec 2011 8:05 using AcqMethod TEST ARI
Instrument : Instrumen
Sample Name: A4
Misc Info :
Vial Number: 1

IR, ¹H-NMR, ¹³C-NMR and Mass Spectra of 4d

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23/10/2011

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Current Data Parameters
NAME: Housavizadeh
EXPNO: 3
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20111119
Time: 10.09
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 4
DS: 0
SWH: 10330.578 Hz
FIDRES: 0.315264 Hz
AQ: 1.5860096 sec
RG: 574.7
DM: 48.400 usec
DE: 6.50 usec
TE: 298.0 K
D1: 5.00000000 sec
WCREST: 0.00000000 sec
MCWIR: 0.01500000 sec
----- CHANNEL f1 -----
NUC1: 1H
P1: 10.50 usec
PL1: -3.00 dB
SF01: 500.1330885 MHz
F2 - Processing parameters
SI: 32768
SF: 500.1300049 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
1D NMR plot parameters
CX: 20.00 cm
CY: 13.16 cm
F1P: 11.069 ppm
F1: 500.03 Hz
F2P: 0.420 ppm
F2: 210.10 Hz
PQWCM: 0.55943 ppm/cm
HZCM: 279.76650 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111119
Time 10.09
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 574.7
DN 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 5.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.16 cm
F1P 8.766 ppm
F1 4394.29 Hz
F2P 5.838 ppm
F2 2919.74 Hz
PPMCH 0.14742 ppm/cm
HZCM 73.72750 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120502
Time 8.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 174
DS 4
SWH 30030.629 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
RG 728.2
DN 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPOPRG2 waitz16
NUC2 1H
P2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 27037.92 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCH 11.00000 ppm/cm
HZCM 1383.33508 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120502
Time 8.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 174
DS 4
SWH 30030.029 Hz
FIDRES 0.016444 Hz
AQ 0.545539 sec
RG 7298.2
DW 16.650 usec
DE 8.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999999 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 63.284 ppm
F1 7956.47 Hz
F2P 27.519 ppm
F2 3460.73 Hz
PWHM 1.78826 ppm/cm
HZCM 224.88705 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120502
Time 8.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 174
DS 4
SWH 30030.029 Hz
FIDRES 0.016444 Hz
AQ 0.545539 sec
RG 7298.2
DW 16.650 usec
DE 8.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999999 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 142.075 ppm
F1 17867.03 Hz
F2P 102.545 ppm
F2 12895.84 Hz
PWHM 1.97648 ppm/cm
HZCM 248.55539 Hz/cm

File : C:\MSDCHEM\4\DATA\SNAPSHOT\64008701.D
Operator :
Acquired : 14 Dec 2011 8:17 using AcqMethod TEST ARI
Instrument : Instrumen
Sample Name: A6
Misc Info :
Vial Number: 1

IR, ¹H-NMR, ¹³C-NMR and Mass Spectra of 4e

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Current Data Parameters
NAME Mousevazideh
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111119
Time 13.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 10330.576 Hz
FIDRES 0.315264 Hz
AQ 1.5860596 sec
RG 574.7
DW 46.400 usec
DE 6.50 usec
TE 299.0 K
D1 5.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 7.02 cm
F1P 12.772 ppm
F1 6387.50 Hz
F2P 0.676 ppm
F2 338.07 Hz
PPMCH 0.60479 ppm/cm
HZCM 302.47189 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111119
Time 13.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 574.7
DM 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 5.00000000 sec
MCREST 0.00000000 sec
MCWIR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 7.02 cm
F1P 8.699 ppm
F1 4350.74 Hz
F2P 6.216 ppm
F2 3108.87 Hz
PQCM 0.12415 ppm/cm
HZCM 62.08875 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120429
Time 15.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 116
DS 4
SWH 30030.029 Hz
FIDRES 0.316444 Hz
AQ 0.5456535 sec
RG 10321.3
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.00000000 sec
DELTA 1.80000000 sec
MCREST 0.00000000 sec
MCWIR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703543 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 27037.30 Hz
F2P -3.600 ppm
F2 -628.79 Hz
PQCM 11.00000 ppm/cm
HZCM 1383.33508 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120429
Time 15.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 116
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
RG 10321.3
DN 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.99999998 sec
WCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SF01 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 55.486 ppm
F1 6977.76 Hz
F2P 22.948 ppm
F2 2885.83 Hz
PPHCH 1.62691 ppm/cm
H2CH 204.59656 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120429
Time 15.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 116
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
RG 10321.3
DN 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.99999998 sec
WCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SF01 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 145.378 ppm
F1 18402.11 Hz
F2P 100.663 ppm
F2 12659.12 Hz
PPHCH 2.26574 ppm/cm
H2CH 287.44958 Hz/cm

File : C:\MSDCHEM\4\DATA\Snapshot\64008712.D
 Operator :
 Acquired : 14 Dec 2011 9:29 using AcqMethod TEST ARI
 Instrument : Instrumen
 Sample Name: A3
 Misc Info :
 Vial Number: 1

IR, ¹H-NMR, ¹³C-NMR and Mass Spectra of 4f

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24/06/2012

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Current Data Parameters
NAME Mousavizadeh
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120911
Time 9.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 148
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5450539 sec
RG 10321.3
DW 16.850 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.11 cm
F1P 51.066 ppm
F1 6673.41 Hz
F2P 30.477 ppm
F2 3832.73 Hz
PPMCH 1.12942 ppm/cm
HZCM 142.03392 Hz/cm

Current Data Parameters
NAME Mousavizadeh
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120911
Time 9.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 148
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5450539 sec
RG 10321.3
DW 16.850 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.11 cm
F1P 139.117 ppm
F1 17495.04 Hz
F2P 102.545 ppm
F2 12895.04 Hz
PPMCH 1.62859 ppm/cm
HZCM 229.95967 Hz/cm

File : C:\MSDCHEM\4\DATA\Snapshot\64010575.D
Operator :
Acquired : 18 Sep 2012 9:52 using AcqMethod TEST ARI
Instrument : Instrumen
Sample Name: A3
Misc Info :
Vial Number: 1