**Room Temperature Cu(II)-Catalyzed Chemo- and Regioselective *Ortho*-Nitration of
Arenes via C-H Functionalization**

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1. NMR (^1H and ^{13}C) Spectra of **4a-c**, **5a-b**, aniline- d_3 , **1r-d₃**, **2s-d** and **2r-d₂** S2-S15

SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degree Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509727	DATA PROCESSING FT size 32768 Total time 1 minute	SP-552 Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "HIT-800"
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EXPERIMENTAL Relax delay 1.000 sec Pulse 45.0 degree Acq time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVED 399.8509523	DATA PROCESSING FT size 32768 Total time 1 minutes	SP-392-401 Solvent: cdcl3 Temp: 25.0 C / 298.1 K Operator: chem File: SP-392-401 Mercury-400 *117G-MMR*
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PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 ACQ. time 2.561 sec
 Width 6398.0 Hz
 54 repetitions

COMMENTS: 1, 399-850701
 DATA PROCESSING
 FT size 32768
 Total time 3:minutes
 18074464.4085093
 Temp: 25.0 °C // 298.1 K
 Operator: chem
 Machine: J400 *IITC-3002*
 Sep-85-89

SP-2NO2-B-21-8-14-1H

Date: 11/11/2011
 Time: 13:03
 Name: 2-NO2-B-21-8-14-1H
 Sample: 5 mm 20000 Hz
 P1: 12.00
 P2: 12.00
 P3: 12.00
 P4: 12.00
 P5: 12.00
 P6: 12.00
 P7: 12.00
 P8: 12.00
 P9: 12.00
 P10: 12.00
 P11: 12.00
 P12: 12.00
 P13: 12.00
 P14: 12.00
 P15: 12.00
 P16: 12.00
 P17: 12.00
 P18: 12.00
 P19: 12.00
 P20: 12.00
 P21: 12.00
 P22: 12.00
 P23: 12.00
 P24: 12.00
 P25: 12.00
 P26: 12.00
 P27: 12.00
 P28: 12.00
 P29: 12.00
 P30: 12.00
 P31: 12.00
 P32: 12.00
 P33: 12.00
 P34: 12.00
 P35: 12.00
 P36: 12.00
 P37: 12.00
 P38: 12.00
 P39: 12.00
 P40: 12.00
 P41: 12.00
 P42: 12.00
 P43: 12.00
 P44: 12.00
 P45: 12.00
 P46: 12.00
 P47: 12.00
 P48: 12.00
 P49: 12.00
 P50: 12.00
 P51: 12.00
 P52: 12.00
 P53: 12.00
 P54: 12.00
 P55: 12.00
 P56: 12.00
 P57: 12.00
 P58: 12.00
 P59: 12.00
 P60: 12.00
 P61: 12.00
 P62: 12.00
 P63: 12.00
 P64: 12.00
 P65: 12.00
 P66: 12.00
 P67: 12.00
 P68: 12.00
 P69: 12.00
 P70: 12.00
 P71: 12.00
 P72: 12.00
 P73: 12.00
 P74: 12.00
 P75: 12.00
 P76: 12.00
 P77: 12.00
 P78: 12.00
 P79: 12.00
 P80: 12.00
 P81: 12.00
 P82: 12.00
 P83: 12.00
 P84: 12.00
 P85: 12.00
 P86: 12.00
 P87: 12.00
 P88: 12.00
 P89: 12.00
 P90: 12.00
 P91: 12.00
 P92: 12.00
 P93: 12.00
 P94: 12.00
 P95: 12.00
 P96: 12.00
 P97: 12.00
 P98: 12.00
 P99: 12.00
 P100: 12.00

ppm

SP-2NO2-21-8-14-13C

Current Data Parameters
NAME SP-2NO2-21-8-14-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140821
Time 12.44
INSTRUM spect
PROBHD 5 mm RABBO DD/2
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
CONC 11.2
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543029 sec
RG 65.24
DWT 13.0071 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 150.9279571 MHz
P1 13C
PL1 10.50 usec
PL12 95.00000000 W

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

NUC2 600.1704007 MHz
P2 1H
PL2 16.16 usec
PL22 70.00 usec
PL23 21.00000000 W
PL12 0.61714000 W
PL13 0.30239999 W

F2 - Processing parameters

SI 16384
SF 150.9128391 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.60

8F-13C-Cleavage-1H

Sample Name:

8F-13C-Cleavage-1H

Data Collected on:

11/10/2005-mwcrj400

Archive directory:

/home/mwcrj400/data/8f13c

Sample directory:

8F-13C-13C

FidFile: 8F-13C-Cleavage-13C

Pulse Sequence: CPMAS (42pul)

Solvent: dms-d6

Data collected on: Aug 12 2014

Temp: 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.304 sec

Width 25125.6 Hz

11470 repetitions

Current: 15, 100.5425817 MHz

Decouple: 15, 399.812994 MHz

Power 42 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

F2 size 63336

Total time 16 hr, 45 min

SP-ANILINE-D3

Sample Name:

SP-ANILINE-D3

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/export/home/chempack/vnmrns/data

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (e2pul)

Solvent: cdcl3

Data collected on: Jan 19 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

32 repetitions

OBSERVE H1, 399.8509687 MHz

DATA PROCESSING

FT size 32768

Total time 2 min 12 sec

<p>EXP. NO. 3</p> <p>EXP. DATE 11/10/00</p> <p>EXP. TIME 11:00</p> <p>EXP. OPERATOR S. K.</p> <p>EXP. INSTR. 400 MHz</p> <p>EXP. PULP. 1.000 sec</p> <p>EXP. PULS. 45.0 degrees</p> <p>EXP. ACQ. TIME 2.561 sec</p> <p>EXP. WIDTH 6398.0 Hz</p> <p>EXP. REPEATS 32</p>	<p>DATA PROCESSING</p> <p>FT size 32768</p> <p>Total time 1.1 minutes</p>	<p>SP-04-D3</p> <p>Solvent: cdcl3</p> <p>Temp: 25.0 C / 298.1 K</p> <p>Operator: chem</p> <p>Mercury-400 1H/13C-NMR</p>
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SP-564-D1-1H

Current Data Parameters
 NAME SP-564-D1-1H
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20161113
 Time 14:13
 INSTRUM spect
 PROBHD 5 mm TANGO BBO
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3531488 sec
 RG 327.5
 INU 41.620 usec
 DE 6.50 usec
 TE 300.3 K
 D1 1.00000000 sec
 T200 1
 ===== CHANNEL f1 =====
 NUC1 1H
 MDEL 600.1719143 MHz
 P1 12.00 usec
 PL1 21.00000000 W
 F2 - Processing parameters
 SI 32768
 SF 600.17015148 MHz
 WDW EM
 SSF 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1.586
 2.396
 2.059

10.092
 8.842
 8.827
 8.041
 7.581
 7.481
 7.468
 7.455
 7.328
 7.316
 7.260

<p>EXPERIMENTAL</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degrees</p> <p>Acq. time 5.122 sec</p> <p>Width 6398.0 Hz</p> <p>32 repetitions</p>	<p>ORIGIN: H1, 399.8509721</p>	<p>DATA PROCESSING</p> <p>Pr size 65536</p> <p>Total time 3 minutes</p>	<p>EXP: 555103</p> <p>Solvent: DMSO</p> <p>Temp: 25.0 °C / -298.1 K</p> <p>Operator: chm</p> <p>Machine: 400 *ITQ-MNO*</p>
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