Supporting Information

Highly Selective Sulfoxidation of Allylic and Vinylic Sulfides by Hydrogen Peroxide using a Flavin as Catalyst

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LK-251

Pulse Sequence: s2pu1
 Solvent: CDCl₃
 Temp. 25.0 C / 298.1 K
 Mercury-4800B "nmr4"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 50.0 degrees
 Acq. time 1.139 sec
 Width 25000.0 Hz
 Spectrometer 500.5652137 MHz
 QNP/PROB 1H/13C
 DECOUPLE H1, 399.9428336 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FI size 65536
 Total time 41 min, 8 sec

all25
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp: 25.8 C / 298.1 K
 Mercury-40005 "nmr4"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse delay 2.751 sec
 Acq. delay 2.751 sec
 Width 5958.8 Hz
 16 repetitions
 OBSERVE 400.139.9400609 MHz
 DATA PROCESSING
 Line broadening 0.1 Hz
 F1 resolution 1.250 Hz
 Total time 11 min, 2 sec

13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Mercury-40066 "nmr4"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 50.8 degrees

Acq. time 1.199 sec

Width 25800.0 Hz

72 repetitions

OBSERVE C13, 100.6251846 MHz

DECOUPLE H1, 399.9426336 MHz

Power 42 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 42 min, 5 sec

LK-244.1

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Mercury-400BB "nmr4"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 44.3 degrees

Acq. time 2.731 sec

Width 5998.8 Hz

Observed F1

Observed F2 99.9408614 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 min, 2 sec

LK-244.1

Pulse Sequence: szpul
Solvent: CDCl₃
Temp: 25.0 °C / 298.1 K
Nuc1: 13C / "nuc4"
Nuc2: 1H / "nuc1"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 50.0 degrees
Acq. time 1.199 sec
F2 (Hz) 100.625000
F1 (Hz) 65536.00
OBSERVE C13, 100.625000 MHz
DECOUPLE H1, 399.942835 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 41 min, 8 sec

LK-264, new

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 25.0 C / 298.1 K

Mercury-300BB "nmr3"

PULSE SEQUENCE

Pulse: 9.00 sec

Pulse: 9.00 sec

Acq. time: 1.998 sec

Width: 4586.5 Hz

16 repetitions

OBSERVE H1, 299.9464283 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 8 min, 49 sec

LK-264, new

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 25.0 C / 298.1 K

Mercury-3000B "nuc3"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 71.8 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

1888 repetitions

OBSERVE C13, 75.4215935 MHz

DECOUPLE H1, 239.9479604 MHz

Power 42 dB

continuously on

VALT2-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 51 min, 52 sec

al153 product after kolomn

Pulse Sequence: s2pul
Solvent: CDCl3
Temp: 25.0 C / 298.1 K
File: al153_H1
Mercury-300BB "nuc3"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 57.3 degrees
Acq. time 1.988 sec
Width 4500.5 Hz
Observed F1 399.9464283 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 49 sec

Diethylaminosulfide after column

Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp: 25.8 C / 298.1 K
 Mercury-30088 "nmr3"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 75.4 degrees
 Width 18.617 Hz
 352 repetitions
 OBSERVE C13 75.4215771 MHz
 DECOUPLE H1 299.9479604 MHz
 Power 35 dB
 continuous wave on
 VOLTAGE-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131024
 Total time 53 min, 4 sec

13C OBSERVE

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Temp: 25.0 C / 298.1 K
 Mercury-4000 "nmr4"
 PULSE SEQUENCE
 Relax delay 1.000 sec
 Pulse 50.0 degrees
 Acq. time 1.199 sec
 Width 25000.0 Hz
 768 repetitions
 OBSERVE C13, 100.6251946 MHz
 DECOUPLE H1, 399.5428338 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulation
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 42 min, 5 sec