Supporting Information

Samarium-Promoted Coupling of Heteroaryl Analogues of Benzylic Acetates with Carbonyl Compounds

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[Supporting Information Table of Contents](#)

NMR spectra of compounds from Table 1.....S2-S15

STANDARD PROTON PARAMETERS

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 F2: 200.1363
 INOVA-500 "631A"
 Relax. delay 0.100 sec
 Pulse 9.000000 sec
 Acq time 4.989 sec
 Width 6568.1 Hz
 16 repetitions
 OBSERVE H1, 499.8611712 MHz
 DATA PROCESSING
 FT size 65536
 Total time 1 min, 21 sec

2-(2-ethyl-2-hydroxy-1-methylbutyl)-1,10-phenanthroline

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1
 Solvent: COCl₂
 Ambient temperature
 User: 1-14-87
 INOVA-500 "nova5"

Relax. delay 2.000 sec
 Pulse 90.0 degrees
 Acq. time 1.133 sec
 Nucleus 13C
 352 repetitions
 OBSERVE C13, 125.6901670 MHz
 DECOUPLE H1, 499.8639616 MHz
 Power 38 db
 Continuously on
 Lock 13C magnetized
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 8 hr, 46 min, 55 sec

STANDARD PROTON PARAMETERS

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient Temperature
 File: phenketbenz
 INOVA-500 "test1a"
 Relax. delay: 0.100 sec
 Pulse: 90.0 degrees
 Acq. time: 4.989 sec
 Width: 6568.1 Hz
 16 repetitions
 OBSERVE: N1 99.8611712 MHz
 N1 F1: 400.513 MHz
 N1 F2: 65536
 Total time: 5 min, 26 sec

2-(2,2-diphenyl-2-hydroxy-1-methylethyl)-1,10-phenanthroline

STANDARD CARBON PARAMETERS

Pulse Sequence: s2pu1

Solvent: CDCl3

Acquisition Temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 2.000 sec

Pulse 90.0 degrees

Acq. time 1.153 sec

Width 26429.3 Hz

Width 11109.3 Hz

OBSERVE C13 125.6901653 MHz

DECOUPLE H1 499.8639616 MHz

Power 38.48

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 8 hr, 46 min, 55 sec

2-(2,2-diphenyl-2-hydroxy-1-methylethyl)-1,10-phenanthroline

STANDARD PROTON PARAMETERS

Pulse Sequence: s2pul

Solvent: CDCl₃

Acquisition Temperature

File: 100-2-014

INOVA-500 "tesla"

Relax. delay 0.100 sec

Pulse program

Acq. time 4.989 sec

Width 6568.1 Hz

16 repetitions

OBSERVE H1, 499.8611714 MHz

DATA PROCESSING

FT size 65536

Total time 1 min, 21 sec

2-[(1-(1-hydroxycyclohexyl)ethyl)-1,10-phenanthroline]

STANDARD CARBON PARAMETERS

Pulse Sequence: szpul
 Solvent: CDCl3
 Ambient temperature
 User: 1-1-87
 INOVA-500 "INOVA5"

Relax. delay 2.009 sec
 Pulse 90.0 degrees
 Acq. time 1.153 sec
 32KHz 20429.3 Hz
 384KHz 20429.3 Hz
 OBSERVE C13 125.6901670 MHz
 DECOUPLE H1 489.8639616 MHz
 Power 38 dB
 continuously on
 VALTZ-16 modulated
 DATA PROCESSING
 1.0 Hz
 FT size 65536
 Total time 8 hr, 46 min, 55 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	20911.146	166.371	20.2
2	18946.915	150.743	71.7
3	18351.747	146.008	13.6
4	18238.960	145.110	14.5
5	17202.186	136.862	74.1
6	17078.120	135.875	71.7
7	16210.528	128.972	20.3
8	15964.939	127.019	18.5
9	15871.299	126.273	58.2
10	15855.682	126.149	61.8
11	15530.335	123.560	50.7
12	15481.750	123.174	66.7
13	9739.153	77.485	117.6
14	9707.052	77.230	117.1
15	9675.818	76.982	119.4
16	9189.099	73.109	26.1
17	6139.510	48.606	3.4
18	4808.020	38.237	60.9
19	4462.453	35.504	73.2
20	3285.129	26.137	60.8
21	2825.305	22.478	51.2
22	2797.542	22.257	61.2
23	2003.695	15.942	62.9

2-[1-(1-hydroxycyclohexyl)-ethyl]-1,10-phenanthroline

STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 UNITYplus-300 "echo-Chem.nd.edu"
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.337 sec
 Width 3508.0 Hz
 16 repetitions
 OBSERVATION 209.693028 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min, 53 sec

STANDARD 1H OBSERVE

Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
 UNITYplus-300 "echo.chem.nd.edu"
 Relax. delay 1.000 sec
 Pulse 86.2 degrees
 Acq. time 2.337 sec
 Width 3300 Hz
 16 repetitions
 OBSERVE H1 299.639032 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min, 53 sec

2-(2-hydroxy-1-methyl-2-phenylethyl)-1,10-phenanthroline

STANDARD PROTON PARAMETERS

Pulse Sequence: sgru1

Solvent: CDCl3

Acquisition Temperature

INNOVA-500 "INOVA5"

Relax: delay 1.000 sec

Pulse: 90.00 deg/sec

Acq time 2.022 sec

Width 8104.5 Hz

8 repetitions

OBSERVE H1, 499.861708 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 24 sec

1-(2-hydroxy-2-phenylethyl)-isoquinoline

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1
 Solvent: CDCl3
 Ambient temperature
 User: 1-14-87
 INOVA-500 "Inovas"

Relax. delay 2.000 sec
 Pulse: 0.000000 sec
 Acq. time 1.52 sec
 Width 29197.1 Hz
 288 Repetitions
 OBSERVE C13, 125.6301653 MHz
 DECOUPLE H1, 499.8641580 MHz
 Power 40.000000 W
 Lock 100.000000 Hz
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 8 hr, 41 min, 52 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	20134.135	160.189	23.0
2	18135.506	144.287	25.2
3	17721.168	140.591	66.0
4	17136.638	136.340	27.8
5	16408.649	130.548	82.6
6	16171.629	128.663	133.5
7	16050.466	127.639	104.7
8	16048.664	127.684	120.2
9	16037.972	127.539	88.2
10	16021.042	127.465	25.2
11	15885.108	126.124	146.9
12	15706.500	124.962	77.2
13	15682.566	120.878	80.3
14	9739.129	77.485	248.4
15	9707.052	77.430	263.3
16	9674.974	76.175	267.6
17	9120.740	72.365	78.6
18	5283.873	42.039	78.5

1-(2-hydroxy-2-phenylethyl)-isoquinoline

STANDARD PROTON PARAMETERS

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Acq. time: 4.389 sec
 Width: 6568.1 Hz
 4 repetitions
 OBSERVE H1, 499.861758 MHz
 DATA PROCESSING
 FI size 65536
 Total time 0 min, 20 sec

2-(2-hydroxybutyl)-quinoline

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1
 Solvent: CDCl3
 Sample Temperature: 125.2
 INOVA-500 "1HNOVA5"

Relax. delay 2.000 sec
 Pulse 90.0 degrees
 Acq. time 1.122 sec
 Width 28197.1 Hz
 OBSERVEPULSIONS 6901668 MHZ
 OBSERVEFREQ 125.761 MHz
 DECOUPLE H1. 499.8641580 MHZ
 Power 41 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Time 1.122 sec
 FT size 65538
 Total time 8 hr, 41 min, 52 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	20283.831	161.380	35.9
2	18508.748	147.265	21.8
3	17203.467	136.872	94.0
4	16328.454	129.810	111.4
5	16201.034	128.897	92.4
6	16035.793	127.741	108.5
7	15937.777	126.961	28.6
8	15873.127	126.268	93.9
9	15377.703	122.346	106.6
10	9738.129	77.485	153.1
11	9707.052	77.230	152.4
12	9674.974	76.975	144.3
13	9079.751	72.239	119.6
14	5466.538	43.492	111.4
15	3787.797	30.136	95.3
16	1292.853	10.286	76.4

2-(2-hydroxybutyl)-quinoline

STANDARD 1H OBSERVE

Pulse Sequence: zgpg30

Solvent: CDCl3

Acquisition Date: 10/10/2011

UNIT: plus-300 "echo.chem.nd.edu"

Relax: delay 1.000 sec

Pulse: zgpg30

Acq: time 2.337 sec

Width: 3506.0 Hz

16 repetitions

OBSERVE: H1, 299.6393026 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 53 sec

1-(2-hydroxybutyl)-isoquinoline

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1

Solvent: CDCl3

Ambient temperature

User: 1-14-97

File: JMW-2-93car

INOVN-500 16318

Relax. delay 2.000 sec

Pulse 90.0 degrees

Acq. time 1.153 sec

Width 28429.3 Hz

338 repetitions

0.33 sec

DECOUPLE H1, 499.863916 MHz

Power 33 db

continuously on

WALTZ-16 modulated

DATA ACQUISITION

1.0 Hz

FT size 65536

Total time 8 hr, 46 min, 55 sec

1-(2-hydroxybutyl)-isoquinoline