Supporting Information
for
**An Unexpected Stereo-recognition in Nitrilase Catalysed Hydrolysis of
 β -Hydroxy Nitriles**

Sukanta Kamila, Dungming Zhu, Edward R. Biehl and Ling Hua

Department of Chemistry, Southern Methodist University, Dallas, Texas 75275

Contents

1. General methods.	S2
2. Experimental procedures and NMR data for β -hydroxy nitriles and β -hydroxy acids.	S2-S9
3. ^{13}C NMR spectra for β -hydroxy acids and β -hydroxy nitriles.	S10-S27

General methods.

Melting points were taken on a Mel-Temp capillary apparatus and are uncorrected with respect to stem correction. ^1H and ^{13}C NMR spectra were recorded on a 400 MHz Bruker AVANCE DRX-400 Multinuclear NMR spectrometer. Specific rotation $[\alpha]_{\text{D}}$ was measured in methanol. Chiral HPLC analysis was performed on Agilent 1100 series HPLC system with (S,S)-Whelk-O1 (25 cm $\times$ 4.6 mm) chiral column. All chemicals were purchased from Fisher Scientific or Aldrich chemicals. Nitrilase blt6402 was produced according to our previous report.¹

Synthesis of aromatic and aliphatic β -hydroxy nitriles.

β -Hydroxy nitriles were prepared by the reduction of β -ketonitriles with NaBH_4 (Scheme 1). A solution of β -ketonitrile² (1 equiv) in ethanol was cooled to 0°C , NaBH_4 (3.3 equiv) was added in one portion. After being stirred for 3 hrs at room temperature, the reaction mixture was acidified with 5% HCl solution. The mixture was extracted with ethyl acetate, and the extract was dried over anhydrous Na_2SO_4 . Evaporation of solvent afforded the crude products, which were purified by column chromatography using ethyl acetate-hexane mixture (80:10, v/v) as eluent. The obtained β -hydroxy nitriles were characterized by ^1H and ^{13}C NMR. The yields are summarized in Table S1.

Scheme 1

Table S1. Yields of β -ketonitriles and β -hydroxy nitriles.

α -bromoketone	β -ketonitrile ^a	yield (%)	β -hydroxy nitrile	yield (%)
		83		88
		89		82
		82		87
		82		90
		90		78
		88		87
		81		84
		89		80
		87		86

a. β -Ketonitriles were prepared by following literature method.²

Hydrolysis of aromatic and aliphatic β -hydroxy nitriles.

The reaction mixture of β -hydroxy nitrile (70 mg) and 5.6 mg of nitrilase bll6402 in 10 ml of potassium phosphate buffer (100 mM, pH 7.2) was incubated overnight at

30°C. The mixture was saturated with NaCl, and extracted with ethyl acetate. The extract was dried over sodium sulfate and evaporation of the solvent under reduced pressure afforded the crude products. The product β -hydroxy acid and unreacted β -hydroxy nitrile were separated by preparative thin layer chromatography (solvents: ethyl acetate/hexane = 40/60, v/v). The ee values of β -hydroxy acid and recovered β -hydroxy nitrile were determined by chiral HPLC analysis (Table S2). The absolute configuration was determined by comparing the sign of optical rotation with literature data.

Table S2. Details for Chiral HPLC and GC Analysis^a

β -hydroxy acid	t _S (min)	t _R (min)	β -hydroxy nitrile	t _S (min)	t _R (min)
2a	10.81	14.04	1a	16.63	19.01
2b	10.49	13.99	1b	15.82	17.89
2c	11.01	14.74	1c	16.84	19.61
2d	12.87	18.55	1d	17.54	20.68
2e	23.92	40.10	1e	31.23	36.64
2f	13.71	20.12	1f	11.80	13.79
2g^b	13.93	24.69	1g^b	19.29	24.27
2h	10.25	15.50	1h	17.29	19.49
2i	12.46	19.77	1i	19.78	23.15

a. HPLC, Column, (S,S)-Whelk O1 (25cm×4.5mm); Flow rate, 1 ml/min; Hexane/IPA(0.1% HOAc) = 95/5. b. Same as a, except Hexane/IPA(0.1% HOAc) = 90/10.

(R)-3-Hydroxy-3-phenylpropanenitrile. 29.0 mg (41%), gummy liquid. ¹H NMR (CDCl₃) δ (ppm) 2.5 (br, 1H, OH), 2.78 (d, *J* = 6.1 Hz, 2H, CH₂), 5.02-5.05 (m, 1H, CH), 7.37-7.42 (m, 5H, aromatic protons); ¹³C NMR (CDCl₃) δ (ppm) 23.1 (CH₂), 65.3 (CH), 112.4 (CN), 120.7 (CH), 124.0 (CH), 124.1 (CH), 136.2 (C); [α]_D²² +49.5 (c 0.55, CH₃OH); lit.³ [α]_D²² +50.4 (c 4.945, CH₃OH).

(S)-3-Hydroxy-3-phenyl-propionic acid. 28.5 mg (36%), white crystalline solid. m.p. 118-120°C. lit (Aldrich) m.p 117-120°C; ^1H NMR (acetone- d_6) δ (ppm) 2.70 (s, 2H, CH_2), 5.16 (br, 1H, CH), 7.20-7.50 (m, 5H, aromatic protons); ^{13}C NMR (acetone- d_6) δ (ppm) 44.2 (CH_2), 70.5 (CH), 126.2 (CH), 127.6 (CH), 128.6 (CH), 144.9 (C), 172.5 (CO); $[\alpha]_{\text{D}}^{22}$ -5.2 (c 0.65, CH_3OH); lit.³ $[\alpha]_{\text{D}}^{22}$ +22.4 (c 4.135, CH_3OH) for (R)-enantiomer.

(R)-3-(4-Fluorophenyl)-3-hydroxypropanenitrile. 25.9 mg (37%), colorless oil. ^1H NMR (CDCl_3) δ (ppm) 2.74 (d, $J = 6.09$, 2H, CH_2), 3.0 (s, 1H, OH), 5.02 (d, $J = 3.4$ Hz, 1H, CH), 7.09 (d, $J = 8.5$ Hz, 2H, aromatic protons), 7.39 (d, $J = 8.5$ Hz, 2H, aromatic protons); ^{13}C NMR (CDCl_3) δ (ppm) 28.4 (CH_2), 69.7 (CH), 116.1 (CH), 116.3 (CH), 117.6 (CN), 127.7 (CH), 127.8 (CH), 137.3 (C), 161.9 (C); $[\alpha]_{\text{D}}^{22}$ +40.7 (c 0.57, CH_3OH).

(S)-3-(4-Fluorophenyl)-3-hydroxypropionic acid. 30.2 mg (38%), white solid, m.p. 71-72°C. ^1H NMR (CDCl_3) δ (ppm) 2.71-2.84 (m, 2H, CH_2), 5.13-5.15 (m, 1H, CH), 6.84 (brs, 1H, -OH), 7.03-7.07 (m, 2H, aromatic), 7.34-7.35 (m, 2H, aromatic protons). ^{13}C NMR(CDCl_3) δ (ppm) 43.5 (CH_2), 70.0 (CH), 115.8 (CH), 116.0 (CH), 127.8 (CH), 127.9 (CH), 138.1 (C), 161.5 (C), 177.4 (C). $[\alpha]_{\text{D}}^{22}$ -12.5 (c 0.55, CH_3OH).

(R)-3-(4-Chlorophenyl)-3-hydroxypropanenitrile. 28.2 mg (40%), colorless gummy liquid. ^1H NMR (CDCl_3) δ (ppm) 2.63 (s, 1H, -OH), 2.76 (d, $J = 6.13$ Hz, 2H, CH_2), 5.04 (d, $J = 3.5$ Hz, 1H, CH), 7.35-7.40 (m, 4H, aromatic protons); ^{13}C NMR(CDCl_3) δ (ppm) 28.4 (CH_2), 69.8 (CH), 117.3 (CN), 127.3 (CH), 129.5 (CH), 135.0 (C), 139.8 (C); $[\alpha]_{\text{D}}^{22}$ +43.3 (c 0.45, CH_3OH); lit.⁴ $[\alpha]_{\text{D}}^{20}$ -52.1 (c 0.7, CHCl_3) for (S)-enantiomer.

(S)-3-(4-Chlorophenyl)-3-hydroxypropionic acid. 25.0 mg (32%), crystalline white solid. m.p. 79-81°C; ^1H NMR (CDCl_3) δ (ppm) 2.72-2.83 (m, 2H, CH_2), 5.12-5.14 (m, 1H, CH), 6.85 (brs, 1H, OH); ^{13}C NMR (CDCl_3) δ (ppm) 43.4 (CH_2), 69.9 (CH), 127.5 (CH), 129.2 (CH), 134.2 (C), 140.8 (C), 177.3 (C); $[\alpha]^{22}_{\text{D}}$ -15.8 (c 0.56, CH_3OH).

(R)-3-Hydroxy-3-(4-methylphenyl)propanenitrile. 24.5 mg (35%), colorless gummy liquid. ^1H NMR (CDCl_3) δ (ppm) 2.38 (s, 3H, CH_3), 2.60 (d, $J = 3.2$ Hz, 1H, OH), 2.76 (d, $J = 6.7$ Hz, 2H, CH_2), 5.00-5.02 (m, 1H, CH), 7.22 (d, $J = 7.9$ Hz, 2H, aromatic proton), 7.29 (d, $J=7.8$ Hz, 2H, aromatic proton); ^{13}C NMR (CDCl_3) δ (ppm) 21.5 (CH_3), 28.3 (CH_2), 70.3 (CH), 117.8 (CN), 125.8 (CH), 129.9 (CH), 138.5 (C), 139.1 (C); $[\alpha]^{22}_{\text{D}}$ +18.3 (c 0.55, CH_3OH); lit.⁴ $[\alpha]^{20}_{\text{D}}$ -53.4 (c 1.5, CHCl_3) for (S)-enantiomer.

(S)-3-Hydroxy-3-(4-methylphenyl)propionic acid. 31.0 mg (40%), white solid. m.p. 89-91°C. ^1H NMR (CDCl_3) δ (ppm) 2.37 (s, 3H, CH_3), 2.72-2.87 (m, 2H, CH_2), 5.13 (d, $J = 6.3$ Hz, 1H, CH), 7.18 (d, $J = 7.8$ Hz, 2H, aromatic proton), 7.27 (d, $J = 7.7$ Hz, 2H, aromatic proton); ^{13}C NMR (CDCl_3) δ (ppm) 21.5 (CH_3), 43.5 (CH_2), 70.5 (CH), 126.0 (CH), 129.7 (CH), 138.2 (C), 139.5 (C), 177.7 (C); $[\alpha]^{22}_{\text{D}}$ -22.4 (c 0.55, CH_3OH).

(R)-3-Hydroxy-3-(4-methoxyphenyl)propanenitrile. 40.1 mg (57%), colorless oil. ^1H NMR (CDCl_3) δ (ppm) 2.56 (s, 1H, OH), 2.74-2.76 (m, 2H, CH_2), 3.82 (s, 3H, OMe), 5.00 (s, 1H, CH), 6.92 (d, $J = 8.5$ Hz, 2H, aromatic proton), 7.33 (d, $J = 8.5$ Hz, 2H, aromatic protons); ^{13}C NMR(CDCl_3) δ (ppm) 28.3 (CH_2), 55.7 (OMe), 70.2 (CH), 114.6 (CH), 117.7 (CN), 127.2 (CH), 133.5 (C), 160.3 (C). $[\alpha]^{22}_{\text{D}}$ +24.5 (c 0.66, CH_3OH); lit.⁴ $[\alpha]^{20}_{\text{D}}$ -59.7 (c 0.6, CHCl_3) for (S)-enantiomer.

(S)-3-Hydroxy-3-(4-methoxyphenyl)propionic acid. 21 mg (27%), white solid. m.p. 75-77°C; ^1H NMR (CDCl_3) δ (ppm) 2.64-2.68 (m, 2H, CH_2), 3.77 (s, 3H, OMe), 5.08-5.09 (m, 1H, CH), 6.88 (d, $J = 8.4$ Hz, 2H, aromatic), 7.34 (d, $J = 8.5$ Hz, 2H, aromatic protons); ^{13}C NMR (CDCl_3) δ (ppm) 43.4 (CH_2), 55.7 (OMe), 70.3 (CH), 114.4 (CH), 127.4 (CH), 134.6 (C), 159.7 (C), 177.4 (C). $[\alpha]_D^{22}$ -22.2 (c 0.35, CH_3OH).

(R)-3-Hydroxy-3-(2-methoxyphenyl)propanenitrile. 32.6 mg (46%), off-white solid. m.p. 79-81°C. ^1H NMR (CDCl_3) δ (ppm) 2.75-2.91 (m, 2H, CH_2), 3.14 (brs, 1H, OH), 3.88 (s, 3H, OMe), 5.22-5.23 (m, 1H, CH), 6.91 (d, $J = 8.1$ Hz, 1H, aromatic), 7.00-7.03 (m, 2H, aromatic), 7.31-7.34 (m, 1H, aromatic), 7.43 (d, $J = 8.1$ Hz, 1H, aromatic); ^{13}C NMR (CDCl_3) δ (ppm) 28.3 (CH_2), 55.7 (OMe), 70.0 (CH), 114.6 (CH), 117.9 (CN), 127.3 (CH), 133.6 (C), 160.2 (C); $[\alpha]_D^{22}$ +23.5 (c 0.45, CH_3OH).

(S)-3-Hydroxy-3-(2-methoxyphenyl)propionic acid. 27.5 mg (36%), white solid. m.p. 123-124°C. ^1H NMR (CDCl_3) δ (ppm) 2.84-2.93 (m, 2H, CH_2), 5.38-5.40 (m, 1H, CH), 6.91 (d, $J = 8.1$ Hz, 1H, aromatic), 7.00 (dd, $J = 2.5, 8.1$ Hz, 1H, aromatic), 7.30 (dd, $J = 2.3, 8.1$ Hz, 1H, aromatic), 7.43 (dd, $J = 2.5, 8.1$ Hz, 1H, aromatic); ^{13}C NMR (CDCl_3) δ (ppm) 41.7 (CH_2), 55.6 (OMe), 62.7 (CH), 110.8 (CH), 121.3 (CH), 127.0 (CH), 129.3 (CH), 130.5 (C), 156.5 (C), 177.2 (C); $[\alpha]_D^{22}$ -22.1 (c 0.46, CH_3OH).

(R)-3-Hydroxy-3-(3-methoxyphenyl)propanenitrile. 32.0 mg (46%), colorless gummy liquid. ^1H NMR (CDCl_3) δ (ppm) 2.38 (brs, 1H, OH), 2.78 (d, $J = 6.3$ Hz, 2H, CH_2), 3.84 (s, 3H, OMe), 5.05 (brs, 1H, CH), 6.91 (d, $J = 8.2$ Hz, 1H, aromatic), 6.97-6.99 (m, 2H, aromatic), 7.33 (dd, $J = 7.5, 8.2$ Hz, 1H, aromatic); ^{13}C NMR (CDCl_3) δ (ppm) 28.3 (CH_2), 55.7 (OMe), 70.5 (CH), 111.4 (CH), 114.7 (CH), 117.5 (CN), 118.0 (CH), 130.4 (CH), 143.0 (C), 160.4 (C); $[\alpha]_D^{22}$ +17.8 (c 0.55, CH_3OH).

(S)-3-Hydroxy-3-(3-methoxyphenyl)propionic acid. 26.9 mg (35%), white crystalline solid. m.p. 111-112°C; ¹H NMR (Acetone-d₆) δ (ppm) 2.67 (d, *J* = 6.5 Hz, 2H, CH₂), 3.32 (brs, 1H, OH), 3.80 (s, 3H, OMe), 5.09-5.13 (m, 1H, CH), 6.82 (d, *J* = 8.1 Hz, 1H, aromatic), 6.98-7.03 (m, 2H, aromatic), 7.25 (dd, *J* = 7.8, 8.2 Hz, 1H, aromatic); ¹³C NMR (Acetone-d₆) δ (ppm) 41.7 (CH₂), 55.6 (OMe), 67.1 (CH), 110.8 (CH), 121.3 (CH), 127.0 (CH), 129.3 (CH), 130.3 (C), 156.5 (C), 177.2 (C). [α]²²_D -22.1 (c 0.45, CH₃OH).

(R)-3-(2-Chlorophenyl)-3-hydroxypropanenitrile. 28 mg (40%), colorless gummy liquid. ¹H NMR (CDCl₃) δ (ppm) 2.71-2.78 (m, 2H, CH₂), 2.89 (brs, 1H, OH), 5.49 (brs, 1H, CH), 7.35-7.50 (m, 4H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 26.8 (CH₂), 66.8 (CH), 117.8 (CN), 127.7 (CH), 128.8 (CH), 130.9 (C), 131.7 (CH), 133.8 (C); [α]²²_D +40.1 (c 0.49, CH₃OH).

(S)-3-(2-Chlorophenyl)-3-hydroxypropionic acid. 24.6 mg (32%), white powder. m.p. 89-90°C. ¹H NMR (CDCl₃) δ (ppm) 2.73-2.81 (m, 2H, CH₂), 3.01 (brs, 1H, OH), 5.51-5.53 (m, 1H, CH), 7.21-7.39 (m, 4H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 44.1 (CH₂), 67.9 (CH), 127.6 (CH), 128.9 (CH), 131.0 (C), 131.8 (CH), 134.1 (C), 177.5 (C); [α]²²_D -16.5 (c 0.41, CH₃OH).

(R)-3-(2,4-Dichlorophenyl)-3-hydroxypropanenitrile. 29.1 mg (42%), yellowish gummy liquid. ¹H NMR (CDCl₃) δ (ppm) 2.68-2.74 (m, 1H, CH₂), 2.87 (brs, 1H, OH), 2.88-2.94 (m, 1H, CH₂), 5.41 (brs, 1H, CH), 7.37 (dd, *J* = 2.4, 7.8 Hz, 1H, aromatic), 7.38-7.42 (m, 1H, aromatic), 7.65 (d, *J* = 7.8 Hz, 1H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 26.7 (CH₂), 66.4 (CH), 117.2 (CN), 128.3 (CH), 128.5 (CH), 131.3 (CH), 132.3 (C), 135.3 (C), 137.3 (C); [α]²²_D +14.5 (c 0.49, CH₃OH).

(S)-3-(2,4-Dichlorophenyl)-3-hydroxypropionic acid. 29.5 mg (39%), white solid. m.p. 129-130°C; ¹H NMR (CDCl₃) δ (ppm) 2.71-2.78 (m, 2H, CH₂), 3.01 (brs, 1H, OH), 5.51-5.56 (m, 1H, CH), 7.38 (dd, *J* = 2.5, 7.5 Hz, 1H, aromatic), 7.39-7.45 (m, 1H, aromatic), 7.68 (d, *J* = 7.5 Hz, 1H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 45.1 (CH₂), 67.4 (CH), 128.8 (CH), 129.1 (CH), 131.5 (CH), 132.9 (C), 135.3 (C), 138.1 (C), 178.1 (C); [α]_D²² -12.8 (c 0.49, CH₃OH).

References:

1. Zhu, D.; Mukherjee, C.; Biehl, E. R.; Hua, L. *Appl. Microbiol. Biotechnol.* **2006**, submitted.
2. Ridge, D.N.; Hanifin, J.W.; Harten, L.A.; Johnson, B.D.; Menschik, J.; Nicolau, G.; Sloboda, A.E.; Watts, D.E. *J. Med. Chem.* **1979**, 22, 1385-1389.
3. Meisterhans, C.; Linden, A.; Hesse, M. *Helv. Chim. Acta* **2003**, 86, 644-656.
4. Dehli, J. R.; Gotor, V. *Tetrahedron: Asymmetry* **2000**, 11, 3693-3700.
5. Palomo, C.; Oiarbide, M.; Aizpurua, J. M.; González, A.; Garcia, J. M.; Landa, C.; Odriozola, I.; Linden, A. *J. Org. Chem.* **1999**, 64, 8193-8200.

plottest

Current Data Parameters
 NAME SK-Bz-Acid-S-isomer
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20051108
 Time 17.01
 INSTRUM spect
 PROBO 5 mm QNP 1H/2
 PULPROG zgpg30
 TO 65536
 SOLVENT DMS
 NS 53
 DS 2
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3864756 sec
 RG 3649.1
 DM 20.850 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec
 ***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.627898 MHz
 ***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 MDM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 10 NMR plot parameters
 CX 20.00 cm
 CY 17.70 cm
 F1P 215.587 ppm
 F1 21690.76 Hz
 F2P -319.69 Hz
 F2 10.39820 ppm/cm
 PPMCH 1100.52234 Hz/cm
 H2CM

plottest

Current Data Parameters
 NAME SK-F-ACID-S-13C
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20051108
 Time 13.17
 INSTRUM spect
 PROBN 5 mm QNP 1H/2
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 53
 DS 2
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 3649.1
 DW 20.850 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec
 ***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.6227898 MHz
 ***** CHANNEL f2 *****
 CDPORG2 waitz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 S1 32768
 SF 100.6127290 MHz
 MVM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 20.00 cm
 CY 9.96 cm
 FIP 219.169 ppm
 F1 22051.19 Hz
 F2 -19.179 ppm
 F2 -1929.62 Hz
 PPMCM 11 91739 ppm/cm
 HZCM 1199.04077 Hz/cm

plottest

Current Data Parameters
 NAME SK-CI-Acid-enantiomer
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2005104
 Time 13.55
 INSTRUM spect
 PROBR0 5 mm QNP 1H/2
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 101
 DS 2
 SMH 23960.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3647756 sec
 R6 3649.1
 DE 20.850 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.0002000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.627898 MHz

***** CHANNEL f2 *****
 CPOPRG2 waltz16
 NUC2 1H
 PCPO2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 S1 32768
 SF 100.617290 MHz
 MCM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 CY 11.17 cm
 F1P 200.302 ppm
 F1 20152.91 Hz
 F2P -3.416 ppm
 F2 -343.71 Hz
 PPMCM 10.18590 ppm/cm
 HZCM 1024.83142 Hz/cm

plottest

Current Data Parameters
 NAME SK-enzyme-Me-2nd-13C
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20051101
 Time 13.35
 INSTRUM spect
 PROBHD 5 mm QNP 1H/2
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 123
 DS 2
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 3649.1
 DM 20.850 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec
 ***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.6227898 MHz
 ***** CHANNEL f2 *****
 CPOPRG2 waltz16
 NUC2 1H
 PCPO2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 10 NMR plot parameters
 CX 20.00 cm
 CY 12.18 cm
 F1P 203.884 ppm
 F1 20513.35 Hz
 F2P -3.415 ppm
 F2 -343.72 Hz
 PPMCM 10.36502 ppm/cm
 HZCM 1042.85315 Hz/cm

plottest

Current Data Parameters
 NAME SK--ONE-3C10-13C
 EXPNO 5
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20051110
 Time 14.26
 INSTRUM spect
 PROBHD 5 mm QNP 1H/2
 PULPROG zgpg30
 TD 65536
 FIDRES 0.364775 sec
 AQ 1.364775 sec
 RG 364.1
 DE 20.650 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec
 CHANNEL f1
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.6227898 MHz
 CHANNEL f2
 NUC2 1H
 P2 100.00 usec
 PL2 -4.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 NHM 64
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 20.00 cm
 CY 8.78 cm
 F1P 191.225 ppm
 F1 19239.81 Hz
 F2P -271.63 Hz
 F2 9.69631 ppm/cm
 HZCM 975.57220 Hz/cm

plottest

Current Data Parameters
NAME SK--2'-Ome-Acid-13C
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060311
Time 9.53
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TO 299.30
SOLVENT CDCl3
NS 15854
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.36647756 sec
RG 4096
DM 20.850 usec
DE 8.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
SF01 100.6271898 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.00 dB
PL13 16.00 dB
SF02 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
10 NMR plot parameters
CX 20.00 cm
CY 102.11 cm
F1P 191.754 ppm
F1 19292.88 Hz
F2P -3.508 ppm
F2 -352.96 Hz
PPHOM 9.76310 ppm/cm
HZCM 982.29205 Hz/cm

Current Data Parameters

NAME	SK-2-CHlor-13C
EXPNO	8
PROCNO	1

F2 - Acquisition Parameters

Date_	20060330
Time	17.51
INSTRUM	spect
PROBHD	5 mm QNP 1H/2
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	349
DS	2
SMH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	3649.1
DM	20.850 usec
DE	8.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec

***** CHANNEL f1 *****

NUC1	13C
P1	10.50 usec
PL1	0.00 dB
SFO1	100.627898 MHz

***** CHANNEL f2 *****

CPDPRG2	waltz16
NUC2 <td>1H</td>	1H
PCPD2 <td>100.00 usec</td>	100.00 usec
PL2 <td>-4.00 dB</td>	-4.00 dB
PL12 <td>16.00 dB</td>	16.00 dB
PL13 <td>16.00 dB</td>	16.00 dB
SFO2 <td>400.1316095 MHz</td>	400.1316095 MHz

F2 - Processing parameters

SF	32768
WDW <td>EM</td>	EM
SSB <td>0</td>	0
LB <td>1.00 Hz</td>	1.00 Hz
GB <td>0</td>	0
PC <td>1.40</td>	1.40

1D NMR plot parameters

CX	20.00 cm
CY <th>18.21 cm</th>	18.21 cm
F1P <th>196.481 ppm</th>	196.481 ppm
F1 <th>19768.45 Hz</th>	19768.45 Hz
F2P <th>-4.610 ppm</th>	-4.610 ppm
F2 <th>-463.86 Hz</th>	-463.86 Hz
PPMCK <th>10.05455 ppm/cm</th>	10.05455 ppm/cm
HZCM <th>1011.61554 Hz/cm</th>	1011.61554 Hz/cm

Current Data Parameters
NAME: SR-01CHloro-13C (2)-Acid
EXPNO: 12
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20060331
Time: 9.34
INSTRUM: spect
PROBHD: 5 mm QNP 1H/2
PULPROG: zgpg30
TO: 65536
SOLVENT: CDCl3
NS: 295
DS: 2
SWH: 23880.814 Hz
FIDRES: 0.385918 Hz
AQ: 1.3664756 sec
RG: 3649.1
DW: 20.850 usec
DE: 8.00 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
D12: 0.00020000 sec
----- CHANNEL f1 -----
NUC1: 13C
P1: 130
PL1: 0.00 dB
SFO1: 100.627098 MHz
----- CHANNEL f2 -----
CPOPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: -4.00 dB
PL12: 16.00 dB
PL13: 16.00 dB
SFO2: 400.1316005 MHz
F2 - Processing parameters
SI: 32768
SF: 100.617250 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 20.00 cm
CY: 16.29 cm
FID: 320.64 cm
F1: 20489.32 Hz
F2: -4.372 ppm
F3: -439.83 Hz
PPMCH: 10.40085 ppm/cm
HZCM: 1046.45740 Hz/cm

plottest

Current Data Parameters
 NAME SK-BZ-DN-R-150mer-13C
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 2005108
 Time 17 21
 INSTRUM spect
 PROBO 5 mm QNP 1H/2
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 52
 DS 2
 SWH 23980.814 Hz
 FIDRES 0.366918 Hz
 AQ 1.3664756 sec
 RG 5160.6
 DW 20.850 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SFO1 100.6227898 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SFO2 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 20.00 cm
 CY 10.94 cm
 F1P 161.134 ppm
 F1 16212.18 Hz
 F2P -2.939 ppm
 F2 -295.66 Hz
 PPMCH 8.20365 ppm/cm
 HZCM 825.39178 Hz/cm

plottest

ppm

Current Data Parameters
 NAME SK-F-QH-R-13C
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051108
 Time 13.33
 INSTRUM spect
 PROBRD 5 mm QNP 1H/2
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 59
 DS 2
 SWH 23960.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664776 sec
 RG 5792.6
 DE 20.650 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.0002000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.627898 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 9.56 cm
 F1P 208.183 ppm
 F1 20945.87 Hz
 F2P -3.416 ppm
 F2 -343.71 Hz
 PPMCN 10.57396 ppm/cm
 HZCN 1064.47390 Hz/cm

plottest

Current Data Parameters
 NAME SK-CI-CH-ene-13C
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20051104
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm QNP 1H/2
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 41
 DS 2
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 3649.1
 DM 20.850 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 ***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.6227898 MHz
 ***** CHANNEL f2 *****
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127280 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 10 NMR plot parameters
 CX 20.00 cm
 CY 11.47 cm
 F1P 186.605 ppm
 F1 18774.89 Hz
 F2P 6.743 ppm
 F2 678.40 Hz
 PPMCM 8.99314 ppm/cm
 HZCM 904.82428 Hz/cm

plottest

ppm

139.114
138.516
129.984
125.881
117.811

77.780
77.462
77.145
70.387

28.296
21.569

Current Data Parameters
NAME SK-enzyme-Me-Up-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 2005101
Time 13.16
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3647795 sec
RG 3849.1
DM 20.650 usec
DE 8.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
SF01 100.6227898 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.00 dB
PL13 16.00 dB
SF02 400.1316003 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CY 20.00 cm
CX 9.96 cm
F1P 209.616 ppm
F1 21090.04 Hz
F2P -848.32 ppm
F2 -848.32 Hz
PQCN 10.90238 ppm/cm
HZCN 1096.91809 Hz/cm

plottest

Current Data Parameters
 NAME SK-DIC-CH-R-13C
 EXPNO 5
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20051110
 Time 14.35
 INSTRUM spect
 PROBRD 5 mm QNP 1H/2
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 56
 DS 2
 SWH 23960.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 3649.1
 DW 20.650 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec
 ***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.627898 MHz
 ***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 MVM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 20.00 cm
 CY 9.96 cm
 F1P 180.718 ppm
 F1 18182.54 Hz
 F2P -151.49 Hz
 F2 9.11119 ppm/cm
 PPMCM 916.70142 Hz/cm
 HZCM

plottest

Current Data Parameters

NAME	SK-D-OH-CN (R)-isomer
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20060412
Time	16.01
INSTRUM	spect
PROBHD	5 mm QNP 1H/2
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	36
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3654756 sec
RG	2298.8
DM	20.850 usec
DE	8.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec

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

NUC1	¹³ C
P1	10.50 usec
PL1	0.00 dB
SFO1	100.627998 MHz

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

CPDPRG2	zgpg30
NUC2	¹ H
PCPD2	100.00 usec
PL2	-4.00 dB
PL12	16.00 dB
PL13	16.00 dB
SFO2	400.131605 MHz

F2 - Processing parameters

SF	32768
SF	100.6127290 MHz
MDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CV	11.48 cm
CP	176.808 ppm
F1	17789.13 Hz
F2	1.656 ppm
PC	166.66 Hz
PC	6.75/47 ppm/cm
PC	881.1134 Hz/cm

plotest

Current Data Parameters
NAME SK-3-Methoxy-R-nitrl18-13C
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060308
Time 18.03
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TD 65536
AQ 0.0213
RG 224
WE 2.24
DS 2
SMH 23960.814 Hz
FIDRES 0.365918 Hz
AQ 1.3684756 sec
RG 3649.1
WE 20.850 usec
TE 300.0 usec
TD 65536
F2 - Processing parameters
SI 32768
SF 100.6127260 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
10 NMR DOT Parameters
CX 20.00 cm
CY 20.00 cm
FIP 176.176 MHz
F1 17712.22 Hz
F2 -72.51 Hz
PPOCN 8.83921 ppm/cm
H2CN 889.23688 Hz/cm

plottest

Current Data Parameters
 NAME SK-13-CL
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060322
 Time 14.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/2
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 78
 DS 2
 SHH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664796 sec
 RG 9195.2
 DM 20.850 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 100.6227898 MHz

----- CHANNEL f2 -----
 CPROG2 wa1t216
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.00 dB
 PL13 16.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 10.91 cm
 F1P 154.300 ppm
 F1 15524.59 Hz
 F2P -0.652 ppm
 F2 -65.73 Hz
 PPMCH 7.75762 ppm/cm
 HZCH 780.51575 Hz/cm