Supporting Information for

Asymmetric Reduction of β -Ketonitriles with a Recombinant Carbonyl Reductase and Cascade Enzymatic Transformation to Optically Pure β -Hydroxy Carboxylic Acids

Dunming Zhu, Haribabu Ankati, Chandrani Mukherjee, Yan Yang,
Edward R. Biehl and Ling Hua

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

Table of contents

1. General methods	S2
2. Carbonyl reductase-catalyzed reduction of β -ketonitriles	S2
3. Nitrilase-catalyzed hydrolysis of β -hydroxy nitriles	S2
4. NMR and specific rotation data for β -hydroxy nitriles and β -hydroxy carboxylic acids	S2-S5
5. References	S5
6. ^{13}C NMR spectra of β -hydroxy nitriles and β -hydroxy carboxylic acids	S6-S26

1. General methods. The chiral HPLC analysis was performed on an Agilent 1100 series high-performance liquid chromatography system with (S,S)-Whelk-O 1 column (25 cm × 4.6 mm, Regis Technologies Inc.). The chiral GC analysis was performed on a Hewlett Packard 5890 series II plus gas chromatograph equipped with autosampler, EPC, split/splitless injector, FID detector and CP-Chirasil-Dex CB chiral capillary column (25 m × 0.25 mm). Aromatic β -ketonitriles were prepared and purified as previously reported.¹ The carbonyl reductase from *Candida magnoliae* (**CMCR**),² nitrilases from cyanobacterium *Synechocystis* sp. strain PCC 6803 (**NIT6803**)³ and *Bradyrhizobium japonicum* strain USDA110 (**bnl6402**)⁴ were readily prepared at gram scale using our previously reported procedures.

2. Carbonyl reductase-catalyzed reduction of β -ketonitriles. The reaction was carried out as follows: D-glucose (400 mg), D-glucose dehydrogenase (10 mg), NADPH (10 mg) and carbonyl reductase (10 mg) were mixed in a potassium phosphate buffer (100 ml, 100 mM, pH 7.0). To the mixture was added a 3-oxo-3-phenylpropanenitrile (**1a**) solution (170 mg 1.17 mmole) in 5.0 ml DMSO. The mixture was stirred at room temperature and monitored by TLC until conversion was complete. The mixture was extracted with methyl *tert*-butyl ether. The organic extract was dried over anhydrous sodium sulfate and removal of the solvent gave (R)-3-hydroxy-3-phenylpropanenitrile (**2a**, 147 mg, 85% yield), which was identified by comparison of ¹H and ¹³C NMR with literature data.^{1,5-7} The absolute configurations of the product alcohols were determined by comparison of the sign of specific rotation data with those in the literature.^{1,8}

3. Nitrilase-catalyzed hydrolysis of β -hydroxy nitriles. The reaction was carried out as follows: (R)-3-Hydroxy-3-phenylpropanenitrile (**2a**, 70 mg, 0.34 mmole) was suspended in 50 ml of potassium phosphate buffer (100 mM, pH 7.2). Nitrilase NIT6803 (3 mg) was added to the mixture, which was stirred at 30°C. The reaction was monitored by TLC. After completion of the reaction, the reaction mixture was acidified with 2 N HCl, saturated with NaCl, and extracted with ethylacetate. The organic extract was dried over sodium sulfate and evaporated under reduced pressure to give crude product, which was purified by preparative TLC. The product (R)-3-hydroxy-3-phenylpropanoic acid (**3a**) was obtained as white crystalline solid (67 mg, 85% yield), which was identified by comparison of ¹H and ¹³C NMR with literature data.^{1,9,10} The absolute configurations of the product alcohols were determined by comparison of the sign of specific rotation data with those in the literature.^{1,11}

4. NMR and specific rotation data for β -hydroxy nitriles and β -hydroxy carboxylic acids:

(R)-3-Hydroxy-3-phenylpropanenitrile (2a).¹ viscous oil, 147 mg, 85% yield; ¹H NMR (CDCl₃) δ (ppm) 2.66 (d, *J* = 6.0 Hz, 2H, CH₂), 3.45 (br, 1H, OH), 4.93 (t, *J* = 8.0 Hz, 1H, CH), 7.29-7.37 (m, 5H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 27.7 (CH₂), 69.5 (CH), 117.5 (CN), 125.4 (CH), 128.5 (CH), 128.7 (CH), 140.9 (C); [α]_D²² +44.7 (c 2.50, CH₃OH); lit.¹¹ [α]_D²² +50.4 (c 4.945, CH₃OH).

(R)-3-Hydroxy-3-phenylpropanoic acid (3a).¹ white crystalline solid, 67 mg, 85% yield; m.p. 117-120°C. ¹H NMR (methanol-d₄) δ (ppm) 2.62-2.66 (m, 2H, CH₂), 5.04-

5.07 (m, 1H, CH), 7.20-7.25 (m, 5H, aromatic); ^{13}C NMR (methanol- d_4) δ (ppm) 42.3 (CH₂), 69.1 (CH), 124.4 (CH), 126.0 (C), 126.8 (CH), 142.6 (C), 172.4 (CO); $[\alpha]^{22}_{\text{D}} +23.8$ (c 0.5, CH₃OH); lit.¹¹ $[\alpha]^{22}_{\text{D}} +22.4$ (c 4.135, CH₃OH).

(R)-3-(4'-Fluorophenyl)-3-hydroxypropanenitrile (2b).¹ colorless oil, 155 mg, 90% yield; ^1H NMR (CDCl₃) δ (ppm) 2.75 (d, $J = 6.2$ Hz, 2H, CH₂), 2.85 (brs, 1H, OH), 5.02-5.05 (m, 1H, CH), 7.10 (d, $J = 8.6$ Hz, 2H, aromatic), 7.38 (d, $J = 8.6$ Hz, 2H, aromatic); ^{13}C NMR (CDCl₃) δ (ppm) 28.4 (CH₂), 69.7 (CH), 116.2 (d, $^2J_{\text{C-F}} = 21$ Hz, CH), 117.6 (CN), 127.8 (d, $^3J_{\text{C-F}} = 8$ Hz, CH), 137.2 (C), 163.2 (d, $^1J_{\text{C-F}} = 246$ Hz, C); $[\alpha]^{22}_{\text{D}} +38.43$ (c 0.75, CH₃OH).

(R)-3-(4'-Fluorophenyl)-3-hydroxypropanoic acid (3b).¹ white solid, 48 mg, 86% yield; m.p. 70-72°C. ^1H NMR (CDCl₃) δ (ppm) 2.72-2.86 (m, 2H, CH₂), 5.13-5.16 (m, 1H, CH), 7.03-7.07 (m, 2H, aromatic), 7.34-7.38 (m, 2H, aromatic); ^{13}C NMR (CDCl₃) δ (ppm) 42.9 (CH₂), 69.76 (CH), 115.6 (d, $^2J_{\text{C-F}} = 21$ Hz, CH), 127.4 (d, $^3J_{\text{C-F}} = 8$ Hz, CH), 137.8 (C), 163.2 (d, $^1J_{\text{C-F}} = 245$ Hz, C), 176.5 (CO); $[\alpha]^{22}_{\text{D}} +9.6$ (c 0.33, CH₃OH).

(R)-3-(2',4'-Difluorophenyl)-3-hydroxypropanenitrile (2c).⁵ colorless oil, 158 mg, 92% yield; ^1H NMR (CDCl₃) δ (ppm) 2.50 (brs, 1H, OH), 2.66-2.82 (m, 2H, CH₂), 5.26 (br, 1H, CH), 6.73-6.90 (m, 2H, aromatic), 7.49-7.53 (m, 1H, aromatic); ^{13}C NMR (CDCl₃) δ (ppm) 26.9 (CH₂), 63.8 (CH), 104.1 (t, $^2J_{\text{C-F}} = 25$ Hz, CH), 112.0 (dd, $^2J_{\text{C-F}} = 21$ Hz, $^3J_{\text{C-F}} = 3$ Hz, CH), 116.7 (CN), 123.9 (dd, $^2J_{\text{C-F}} = 13$ Hz, $^3J_{\text{C-F}} = 4$ Hz, C), 128.2 (dd, $^3J_{\text{C-F}} = 10$ Hz, $^3J_{\text{C-F}} = 5$ Hz, CH), 159.2 (dd, $^1J_{\text{C-F}} = 249$ Hz, $^3J_{\text{C-F}} = 12$ Hz, C), 163.2 (dd, $^1J_{\text{C-F}} = 249$ Hz, $^3J_{\text{C-F}} = 12$ Hz, C); $[\alpha]^{22}_{\text{D}} +46.85$ (c 1.67, CH₃OH).

(R)-3-(2',4'-Difluorophenyl)-3-hydroxypropanoic acid (3c).⁹ viscous oil, 89 mg, 89% yield; ^1H NMR (methanol- d_4) δ (ppm) 2.62-2.64 (m, 2H, CH₂), 5.28-5.32 (m, 1H, CH), 6.82-6.92 (m, 2H, aromatic), 7.46-7.50 (m, 1H, aromatic); ^{13}C NMR (methanol- d_4) δ (ppm) 41.0 (CH₂), 62.6 (CH), 101.8 (t, $^2J_{\text{C-F}} = 25$ Hz, CH), 109.7 (d, $^2J_{\text{C-F}} = 21$ Hz, CH), 125.8 (d, $^2J_{\text{C-F}} = 10$ Hz, C), 127.3 (t, $^3J_{\text{C-F}} = 9$ Hz, CH), 159.7 (d, $^1J_{\text{C-F}} = 257$ Hz, C), 162.4 (d, $^1J_{\text{C-F}} = 259$ Hz, C), 171.9 (CO); $[\alpha]^{22}_{\text{D}} +34.6$ (c 0.66, CH₃OH).

(R)-3-(4'-Chlorophenyl)-3-hydroxypropanenitrile (2d).¹ viscous oil, 155 mg, 90% yield; ^1H NMR (CDCl₃) δ (ppm) 2.63-2.65 (m, 2H, CH₂), 3.0 (brs, 1H, OH), 4.91 (br, 1H, CH), 7.18-7.29 (m, 4H, aromatic); ^{13}C NMR (CDCl₃) δ (ppm) 27.8 (CH₂), 69.1 (CH), 117.1 (CN), 126.9 (CH), 128.9 (CH), 134.4 (C), 139.4 (C); $[\alpha]^{22}_{\text{D}} +53.20$ (c 2.0, CH₃OH); lit.¹² $[\alpha]^{30}_{\text{D}} -54.5$ (c 2.0, CHCl₃) for (S)-enantiomer.

(R)-3-(4'-Chlorophenyl)-3-hydroxypropanoic acid (3d).¹ white crystalline solid, 67 mg, 86% yield; m.p. 80-81°C. ^1H NMR (CDCl₃) δ (ppm) 2.74-2.86 (m, 2H, CH₂), 5.14-5.17 (m, 1H, CH), 7.28-7.38 (m, 4H, aromatic); ^{13}C NMR (methanol- d_4) δ (ppm) 45.0 (CH₂), 71.1 (CH), 128.7 (CH), 129.6 (CH), 134.3 (C), 142.2 (C), 174.8 (CO); $[\alpha]^{22}_{\text{D}} +16.7$ (c 0.5, CH₃OH).

(R)-3-(4'-Bromophenyl)-3-hydroxypropanenitrile (2e).⁵ viscous oil, 151 mg, 88% yield; ^1H NMR (CDCl₃) δ (ppm) 2.69-2.75 (m, 2H, CH₂), 3.33 (brs, 1H, OH), 4.96 (br, 1H, CH), 7.25 (dd, $J = 2.0, 2.2$ Hz, 2H, aromatic), 7.50 (dd, $J = 4.7, 2.3$ Hz, 2H, aromatic); ^{13}C NMR (CDCl₃) δ (ppm) 28.3 (CH₂), 69.6 (CH), 117.6 (CN), 123.0 (C), 127.7 (CH), 132.3 (CH), 140.4 (C); $[\alpha]^{22}_{\text{D}} +41.90$ (c 1.0, CH₃OH).

(R)-3-(4'-Bromophenyl)-3-hydroxypropanoic acid (3e).⁹ white solid, 77 mg, 85% yield; m.p. 110-112°C. ^1H NMR (methanol- d_4) δ (ppm) 2.63-2.68 (m, 2H, CH₂), 5.04-5.06 (m, 1H, CH), 7.32 (d, $J = 7.9$ Hz, 2H, aromatic), 7.50 (d, $J = 7.9$ Hz, 2H, aromatic);

¹³C NMR (methanol-d₄) δ (ppm) 42.3 (CH₂), 68.5 (CH), 119.6 (CH), 126.4 (CH), 129.9 (CH), 142.1 (C), 172.1 (CO); [α]²²_D +7.5 (c 0.5, CH₃OH).

(R)-3-Hydroxy-3-(4'-methylphenyl)propanenitrile (2f).¹ colorless viscous oil; 155 mg, 90% yield; ¹H NMR (CDCl₃) δ (ppm) 2.37 (s, 3H, CH₃), 2.58-3.01 (m, 2H, CH₂), 2.97 (s, 1H, OH), 5.0 (br, 1H, CH), 7.20 (d, *J* = 7.9 Hz, 2H, aromatic), 7.25 (d, *J* = 7.9 Hz, 2H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 21.0 (CH₃), 27.7 (CH₂), 69.7 (CH), 117.4 (CN), 125.3 (CH), 129.4 (CH), 138.0 (C), 138.4 (C); [α]²²_D +48.4 (c 1.67, CH₃OH); lit.¹² [α]³⁰_D -52.6 (c 2.0, CHCl₃) for (S)-enantiomer.

(R)-3-Hydroxy-3-(4'-methylphenyl)propanoic acid (3f).¹ white solid, 66 mg, 85% yield; m.p. 88-91°C. ¹H NMR (methanol-d₄) δ (ppm) 2.33 (s, 3H, CH₃), 2.55-2.68 (m, 2H, CH₂), 4.98-5.01 (m, 1H, CH), 7.10 (d, *J* = 7.6 Hz, 2H, aromatic), 7.22 (d, *J* = 7.9 Hz, 2H, aromatic); ¹³C NMR (methanol-d₄) δ (ppm) 18.3 (CH₃), 41.9 (CH₂), 68.5 (CH), 123.9 (CH), 126.9 (CH), 135.3 (C), 139.1 (C), 171.9 (CO); [α]²²_D +18.6 (c 0.66, CH₃OH).

(R)-3-(4'-Cyanophenyl)-3-hydroxypropanenitrile (2g).⁶ light yellow solid, 155 mg, 90% yield; m.p. 80-82°C. ¹H NMR (CDCl₃) δ (ppm) 2.77-2.81 (m, 2H, CH₂), 2.97 (brs, 1H, OH), 5.11-5.14 (m, 1H, CH), 7.54 (d, *J* = 8.1 Hz, 2H, aromatic), 7.70 (d, *J* = 6.6 Hz, 2H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 27.9 (CH₂), 69.2 (CH), 112.5 (CN), 116.5 (CN), 118.2 (C), 126.3 (CH), 132.6 (CH), 145.9 (C); [α]²²_D +66.5 (c 1.67, CH₃OH).

(R)-3-(4'-Carboxyphenyl)-3-hydroxypropanoic acid (4g).¹⁰ white solid, 68 mg, 80% yield; ¹H NMR (methanol-d₄) δ (ppm) 2.67 (d, *J* = 7.8 Hz, 2H, CH₂), 5.15 (m, 1H, CH), 7.40 (d, *J* = 8.0 Hz, 2H, aromatic), 7.90 (d, *J* = 8.0 Hz, 2H, aromatic); ¹³C NMR (methanol-d₄) δ (ppm) 42.4 (CH₂), 68.7 (CH), 124.4 (CH), 128.3 (CH), 128.6 (C), 148.1 (C), 167.2 (CO), 172.2 (CO); [α]²²_D + 95.36 (c 0.5, CH₃OH).

(R)-3-(4'-Cyanophenyl)-3-hydroxypropanoic acid (3g).¹⁰ light yellow solid, 80 mg, 90% yield; ¹H NMR (CDCl₃) δ (ppm) 2.69 (d, *J* = 8.0 Hz, 2H, CH₂), 5.13-5.16 (m, 1H, CH), 7.49 (d, *J* = 8.0 Hz, 2H, aromatic), 7.98 (d, *J* = 8.0 Hz, 2H, aromatic); ¹³C NMR (acetone-d₆) δ (ppm) 42.2 (CH₂), 68.4 (CH), 109.6 (CN), 117.2 (C), 124.4 (CH), 125.4 (C), 128.4 (C), 130.8 (CH), 148.6 (C), 171.8 (CO); [α]²²_D + 12.27 (c 0.33, CH₃OH).

(R)-3-Hydroxy-3-(4'-nitrophenyl)propanenitrile (2h).⁷ light yellow solid, 147 mg, 86% yield; m.p. 95-98°C. ¹H NMR (CDCl₃) δ (ppm) 2.75-2.85 (m, 2H, CH₂), 3.05 (brs, 1H, OH), 5.17-5.20 (m, 1H, CH), 7.61 (d, *J* = 8.8 Hz, 2H, aromatic), 8.25 (d, *J* = 8.6 Hz, 2H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 28.5 (CH₂), 69.4 (CH), 116.9 (CN), 124.5 (CH), 127.0 (CH), 148.2 (C), 148.4 (C); [α]²²_D +12.33 (c 0.50, CH₃OH).

(R)-3-Hydroxy-3-(4'-nitrophenyl)propanoic acid (3h).¹⁰ light yellow solid, 77 mg, 88% yield; ¹H NMR (methanol-d₄) δ (ppm) 2.70-2.72 (m, 2H, CH₂), 5.20-5.22 (m, 1H, CH), 7.66 (d, *J* = 8.0 Hz, 1H, aromatic), 8.23 (d, *J* = 8.0 Hz, 1H, aromatic); ¹³C NMR (methanol-d₄) δ (ppm) 42.3 (CH₂), 68.3 (CH), 121.9 (CH), 125.5 (CH), 146.2 (C), 150.5 (C), 171.9 (CO); [α]²²_D +28.9 (c 0.5, CH₃OH).

(R)-3-Hydroxy-3-(3'-nitrophenyl)propanenitrile (2i).⁷ light yellow solid, 150 mg, 87% yield; m.p. 86-89°C; ¹H NMR (CDCl₃) δ (ppm) 2.81-2.83 (m, 2H, CH₂), 3.93 (brs, 1H, OH), 5.18 (br, 1H, CH), 7.59 (t, *J* = 8.0 Hz, 1H, aromatic), 7.76 (d, *J* = 8.0 Hz, 1H, aromatic), 8.20 (d, *J* = 8.0 Hz, 1H, aromatic), 8.30 (s, 1H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 28.1 (CH₂), 68.7 (CH), 116.7 (CN), 120.7 (CH), 123.5 (CH), 129.8 (CH), 131.7 (CH), 143.4 (C), 148.4 (C); [α]²²_D +22.3 (c 1.67, CH₃OH).

(R)-3-Hydroxy-3-(3'-nitrophenyl)propanoic acid (3i).¹⁰ light yellow solid, 76 mg, 87% yield; m.p. 110–113°C. ¹H NMR (methanol-d₄) δ (ppm) 2.72-2.74 (d, *J* = 8.1 Hz, 2H, CH₂), 5.20-5.23 (t, *J* = 7.6 Hz, 1H, CH), 7.59 (t, *J* = 7.7 Hz, 1H, aromatic), 7.80 (d, *J* = 8.2 Hz, 1H, aromatic), 8.14 (d, *J* = 8.2 Hz, 1H, aromatic), 8.30 (s, 1H, aromatic); ¹³C NMR (methanol-d₄) δ (ppm) 46.2 (CH₂), 72.0 (CH), 123.2 (CH), 124.7 (CH), 132.0 (CH), 134.7 (CH), 149.3 (C), 151.2 (C), 175.8 (CO); [α]_D²² +7.7 (c 0.5, CH₃OH).

(R)-3-Hydroxy-3-(3'-methoxyphenyl)propanenitrile (2j).¹ viscous oil, 153 mg, 89% yield; ¹H NMR (CDCl₃) δ (ppm) 2.68-2.71 (m, 2H, CH₂), 3.33 (brs, 1H, OH), 3.79 (s, 3H, OCH₃), 4.93 (br, 1H, CH), 6.84 (d, *J* = 8.0 Hz, 2H, aromatic), 6.92 (s, 1H, aromatic), 7.27 (d, *J* = 8.0 Hz, 2H, aromatic); ¹³C NMR (CDCl₃) δ (ppm) 27.3 (CH₂), 55.2 (OCH₃), 69.6 (CH), 111.0 (CH), 113.9 (CH), 117.4 (CN), 117.7 (CH), 129.8 (CH), 142.7 (C), 159.7 (C); [α]_D²² +26.5 (c 1.67, CH₃OH).

(R)-3-Hydroxy-3-(3'-methoxyphenyl)propanoic acid (3j).¹ white crystalline solid, 61 mg, 90% yield; m.p. 110–112°C. ¹H NMR (methanol-d₄) δ (ppm) 2.54-2.65 (m, 2H, CH₂), 3.71 (s, 3H, OCH₃), 4.99-5.02 (m, 1H, CH), 6.74 (s, 1H, aromatic), 6.88 (d, *J* = 8.1 Hz, 2H, aromatic), 7.15 (t, *J* = 8.1 Hz, 1H, aromatic); ¹³C NMR (methanol-d₄) δ (ppm) 42.5 (CH₂), 53.0 (OCH₃), 69.1 (CH), 109.8 (CH), 111.5 (CH), 116.5 (CH), 127.7 (CH), 144.3 (C), 158.7 (C), 172.4 (CO); [α]_D²² +17.7 (c 0.83, CH₃OH).

5. References

- (1) Kamila, S.; Zhu, D.; Biehl, E. R.; Hua, L. *Org. Lett.* **2006**, 8, 4429-4431.
- (2) Zhu, D.; Yang, Y.; Hua, L. *J. Org. Chem.* **2006**, 71, 4202-4205.
- (3) Mukherjee, C.; Zhu, D.; Biehl, E. R.; Hua, L. *Eur. J. Org. Chem.* **2006**, 5238-5242.
- (4) Zhu, D.; Mukherjee, C.; Biehl, E. R.; Hua, L. *J. Biotechnol.* **2007**, 129, 645-650.
- (5) Zhou, Z.; Shi, L.; Huang, Y. Z. *Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999)* **1991**, 1931-3.
- (6) Sun, P.; Shi, B. *J. Chem. Res., Synop.* **1999**, 318-319.
- (7) Araki, S.; Yamada, M.; Butsugan, Y. *Bull. Chem. Soc. Jpn.* **1994**, 67, 1126-9.
- (8) Liu, P. N.; Gu, P. M.; Wang, F.; Tu, Y. Q. *Org. Lett.* **2004**, 6, 169-172.
- (9) Leclercq, M.; Collet, A.; Jacques, J. *Tetrahedron* **1976**, 32, 821-8.
- (10) Washio, T.; Nakamura, S.; Anada, M.; Hashimoto, S. *Heterocycles* **2005**, 66, 567-578.
- (11) Meisterhans, C.; Linden, A.; Hesse, M. *Helv. Chim. Acta* **2003**, 86, 644-656.
- (12) Kamal, A.; Khanna, G. B. R.; Ramu, R. *Tetrahedron: Asymmetry* **2002**, 13, 2039-2051.

6. ¹³C NMR spectra of β-hydroxy nitriles and β-hydroxy carboxylic acids.

Current Data Parameters
NAME: nap1-H-ac10-13C
EXPNO: 7
PROCNO: 7

F2 - Acquisition Parameters
Date_: 20070214
Time: 14.47
INSTRUM: spect
PROBHD: 5 mm QNP 1H/2
PULPROG: zgpg30
TD: 65536
SOLVENT: MeOD
NS: 160
DS: 2
SWH: 23980.814 Hz
FIDRES: 0.365918 Hz
AQ: 1.3664756 sec
RG: 5160.6
DM: 20.850 usec
DE: 8.00 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
SFO1: 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
SFO2: 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: 17.73 cm
F1P: 219.169 ppm
F1: 22051.19 Hz
F2P: -19.179 ppm
F2: -1929.62 Hz
DPRCM: 11.91739 ppm/cm
HZCM: 1199.04077 Hz/cm

Current Data Parameters

NAME	nar-2-fluoro-13C
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20070108
Time	10.37
INSTRUM	spect
PROBHD	5 mm QNP 1H/2
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	69
DS	2
SWH	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	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
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters:

CX	20.00 cm
CY	9.22 cm
F1P	219.169 ppm
F1	22051.19 Hz
F2P	-19.179 ppm
F2	-1929.62 Hz
PRGCM	11.91739 ppm/cm
HZCM	1199.04077 Hz/cm

Current Data Parameters

NAME	nar1-4-F-act10-13C
EXPNO	7
PROCNO	7

F2 - Acquisition Parameters

Date_	20070210
Time	11:57
INSTRUM	SPECT
PROBHD	5 mm QNP 1H/2
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1219
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
R6	5792.6
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	100.6227898 MHz

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

CPDPRG2	waltz16
NUC2	¹ H
PCPD2	100.00 usec
PL2	-4.00 dB
PL12	16.00 dB
PL13	16.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

S1	32768
SF	100.6127702 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CX	20.00 cm
CV	51.64 cm
FAP	218.759 ppm
F1	22009.94 Hz
F2P	-19.589 ppm
F2	-1970.87 Hz
PPMCM	11.91738 ppm/cm
HZCM	1199.04077 Hz/cm

Current Data Parameters
NAME hmf-31fluoro-nitrile-13
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070108
Time 17:57
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TD 65536
SOLVENT DMS
NS 668
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 6502
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 100.627788 MHz

***** CHANNEL f2 *****
COPPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.00 dB
PL13 16.00 dB
SFO2 400.136005 MHz

F2 - Processing parameters
SI 32768
SF 100.612710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 38.42 cm
F1P 2715.000 ppm
F1 21631.75 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPHCH 11.00000 ppm/cm
HZCM 1106.74048 Hz/cm

Current Data Parameters
 NAME har1-2,4-di-fluoro-acid
 EXPNO 7
 PROCNO 7

F2 - Acquisition Parameters
 Date_ 20070213
 Time 17.32
 INSTRUM spect
 PROBRD 5 mm QNP 3H/2
 PULPROG zgpg30
 ID 65536
 SOLVENT MeOD
 NS 270
 DS 2
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.364756 sec
 RG 5792.6
 DM 20.890 usec
 DE 8.00 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 100.6227898 MHz

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

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

1D NMR Plot Parameters
 CX 20.00 cm
 CY 36.63 cm
 F1P 219.169 ppm
 F1 22051.19 Hz
 F2P -19.179 ppm
 F2 -1929.62 Hz
 PPMCM 11.91739 ppm/cm
 HZCM 1199.04077 Hz/cm

Current Data Parameters

NAME	nar1-chloro-nit11e
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20070109
Time	9.08
INSTRUM	spect
PROBHD	5 mm QNP 1H/2
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	51
DS	2
SWH	23880.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	6502
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	100.6227698 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	100.6127783 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	14.77 cm
F1P	215.000 ppm
F1	21631.75 Hz
F2P	-503.06 Hz
F2	-503.06 Hz
PPMCK	11.00000 ppm/cm
HZCM	1106.74048 Hz/cm

Current Data Parameters

NAME	EXPNO	PROCNO
1H-bromo-oltrile-13C	10	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DW	DE	TE	D1	D11	D12
20070111	16.52	spect	5 mm QNP 1H/2	zgpg30	65536	CDCl3	123	2	23980.814 Hz	0.365918 Hz	1.3664756 sec	3649.1	20.650 usec	8.00 usec	300.0 K	2.00000000 sec	0.03000000 sec	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
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CX	20.00 cm
CY <td>11.08 cm</td>	11.08 cm
F1P <td>215.000 ppm</td>	215.000 ppm
F1 <td>21631.74 Hz</td>	21631.74 Hz
F2P <td>-5.000 ppm</td>	-5.000 ppm
F2 <td>-503.06 Hz</td>	-503.06 Hz
PRCKM <td>11.00000 ppm/cm</td>	11.00000 ppm/cm
HZCM <td>1106.73999 Hz/cm</td>	1106.73999 Hz/cm

Current Data Parameters
 NAME: har-4-br-acid-13C
 EXPNO: 5
 PROCNO: 5

F2 - Acquisition Parameters
 Date_: 20070207
 Time: 10.56
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/2
 PULPROG: zgpg30
 TO: 65536
 SOLVENT: CDCl3
 NS: 415
 DS: 2
 SWH: 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 =====
 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: 62.45 cm
 F1P: 219.169 ppm
 F1: 22051.19 Hz
 F2P: -19.179 ppm
 F2: -1929.62 Hz
 PPMCH: 11.91739 ppm/cm
 HZCM: 1199.04077 Hz/cm

Current Data Parameters
NAME har-methyl-nitro-le-13c
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070108
Time 9.31
INSTRUM spect
PROBHD 5 mm DNP 1H/2
PULPROG zgpg30
TD 65536
SOLVENT DMS
NS 71
DS 2
SWH 23960.814 HZ
FIDRES 0.365918 HZ
AQ 1.3664756 sec
RG 2298.8
DM 20.850 usec
DE 8.00 usec
TE 300.0 K
D1 2.00000000 sec
D12 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
SFO1 100.6227698 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 100.6127812 MHz
WDW EM
SSB 0
LB 1.00 HZ
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 11.50 cm
F1P 215.000 ppm
F1 21631.75 HZ
F2P -503.06 HZ
F2 11.00000 ppm/cm
PPMCH 1106.74048 HZ/cm

Current Data Parameters

NAME nar1-4-Me-alc10

EXPNO 5

PROCNO 5

F2 - Acquisition Parameters

Date_ 20070207

Time 9.59

INSTRUM spect

PROBHD 5 mm QNP 1H/2

PULPROG zgpg30

TD 65536

SOLVENT MeOD

NS 61

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 0.0002000 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

SF 32768

SF 100.6127732 MHz

MDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 10.28 cm

FAP 218.730 ppm

F1 22007.02 Hz

F2P -19.618 ppm

F2 -1973.79 Hz

PPMCM 11.91738 ppm/cm

HZCM 1199.04077 Hz/cm

Current Data Parameters
NAME har1-cyano-nitrile-13C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070112
Time 12:52
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 138
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 6502
CK 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 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 100.6127724 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 16.58 cm
F1P 219.169 ppm
F1 22051.20 Hz
F2P -19.179 ppm
F2 -1929.62 Hz
PPMCH 11.91739 ppm/cm
HZCM 1199.04126 Hz/cm

Current Data Parameters

NAME	har-4-CN-acid
EXPNO	7
PROCNO	7

F2 - Acquisition Parameters

Date_	20070213
Time	14.25
INSTRUM	Spect
PROBHD	5 mm QNP 1H/2
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	763
DS	2
SWH	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	100.6227898 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>400.1316005 MHz</td>	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF <td>100.6127290 MHz</td>	100.6127290 MHz
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>68.08 cm</th>	68.08 cm
F1P <th>219.169 ppm</th>	219.169 ppm
F1 <th>22051.19 Hz</th>	22051.19 Hz
F2P <th>-19.179 ppm</th>	-19.179 ppm
F2 <th>-1929.62 Hz</th>	-1929.62 Hz
PPMCK <th>11.91739 ppm/cm</th>	11.91739 ppm/cm
HZCM <th>1199.04077 Hz/cm</th>	1199.04077 Hz/cm

Current Data Parameters

NAME	NAME	EXPNO	PROCNO
NAME	nar1-Cn-acid	5	5

F2 - Acquisition Parameters

Date_	Time
20070223	9.35

INSTRUM spect

PROBHD 5 mm QNP 1H/2

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 901

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 0.00002000 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
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CX	20.00 cm
CY <td>61.56 cm</td>	61.56 cm
FAP <td>219.169 ppm</td>	219.169 ppm
F1 <td>22051.19 Hz</td>	22051.19 Hz
F2P <td>-19.179 ppm</td>	-19.179 ppm
F2 <td>-1929.62 Hz</td>	-1929.62 Hz
PPMCM <td>11.91739 ppm/cm</td>	11.91739 ppm/cm
HZCM <td>1199.04077 Hz/cm</td>	1199.04077 Hz/cm

Current Data Parameters
NAME hart-nitro-nitrile
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070112
Time 12.42
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 108
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3654756 sec
RG 6502
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 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ID NMR plot parameters
CX 20.00 cm
CY 9.96 cm
F1P 219.169 ppm
F1 22051.19 Hz
F2P -19.179 ppm
F2 -1929.62 Hz
PPMCM 11.91739 ppm/cm
HZCM 1199.04077 Hz/cm

Current Data Parameters

NAME	NAME	EXPNO	PROCNO
NAME	narj-Nitro-acid	7	7

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DM	DE	TE	D1	D12
20070215	8.53	spect	5 mm QNP 1H/2	zgpg30	65536	CDCl3	901	2	23980.814 Hz	0.365918 Hz	1.3664756 sec	2896.3	20.850 usec	8.00 usec	300.0 K	2.00000000 sec	0.03000000 sec

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

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

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

CPDPRG2	WALTZ16	NUC2	PCPD2	PL2	PL12	PL13	SFO2
waltz16	1H	100.00 usec	-4.00 dB	16.00 dB	16.00 dB	16.00 dB	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127280 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	133.97 cm
F1P	219.169 ppm
F2P	-19.179 ppm
F2	-1929.62 Hz
PPMCK	11.91739 ppm/cm
HZCM	1199.04077 Hz/cm

Current Data Parameters

NAME har-1-3-nitro-ethyl-13

EXPNO 5

PROCNO 5

F2 - Acquisition Parameters

Date_ 20070207

Time 9.12

INSTRUM spect

PROBHD 5 mm QNP 1H/2

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 101

DS 2

SWH 23980.814 Hz

FIDRES 0.365918 Hz

AQ 1.3664756 sec

RG 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

SFO1 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

SFO2 400.1316005 MHz

F2 - Processing parameters

SF 32768

MDK EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 12.04 cm

F1P 200.340 DPM

F1 20156.79 Hz

F2P -868.47 Hz

F2 1044861 DPM/cm

PCNCH 1051.65318 Hz/cm

HZCM

```

Current Data Parameters
NAME      tw-1-3-OH-e-nitrile
EXPNO     5
PROCNO    5

F2 - Acquisition Parameters
Date_     20070207
Time      8.56
INSTRUM   spect
PROBHD    5 mm DNP 1H/2
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS         21
DS         2
SWH        23980.814 Hz
FIDRES     0.365918 Hz
AQ         1.3664756 sec
RG         2896.3
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       100.6227898 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         100.6127827 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
CY         8.05 cm
F1P        215.000 ppm
F1         21631.75 Hz
F2P        -5.000 ppm
F2         -503.06 Hz
PPMCH      11.00000 ppm/cm
HZCM       1106.74060 Hz/cm
  
```