Supplementary Information:

A remarkably simple α-oximation of aldehydes *via* organo-SOMO catalysis

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General Procedures and Materials.

¹H-NMR and ¹³C-NMR spectra were recorded on a Bruker AC 300 spectrometer (300 MHz) using CDCl₃ and DMSO-d₆ as solvents. Chemical shifts are referred to the solvent signal and expressed in parts per million (δ scale); coupling constants are expressed in Hertz (Hz). Infrared (IR) spectra were obtained by using a Perkin–Elmer 1600 (FTIR) spectrometer; data are presented as wavenumbers $\bar{\nu}$ (cm⁻¹). GC analyses were run on a Varian CP 3800 instrument, equipped with 5% phenyl silicone 30m×0.25mm×25µm capillary column. GC–MS analyses have been run on a HP 5892 series II GC, equipped with a 5% phenyl silicone 30m×0.25mm×25µm capillary column and coupled to a HP 5972 MSD instrument operating at 70 eV. High-resolution mass spectra (HRMS) were performed with an Electrospray Ionisation Time of Flight Micromass spectrometer.

All chemicals were of highest commercially available quality and were used as received. Tetrahydrofuran (THF) was distilled over sodium benzophenone ketyl radical under an atmosphere of argon. Dimethylformamide (DMF) was distilled under reduced pressure and stored over 4\AA molecular sieves under argon atmosphere. Dichloromethane (CH₂Cl₂), acetonitrile (CH₃CN) and dimethylsulfoxide (DMSO) were purchased from Aldrich, stored over 4\AA molecular sieves and handled under an atmosphere of argon.

Experimental Procedures.

Preparation of the aldehydes 1e, **1f** and **1h**: aldehydes were prepared by TEMPO/BAIB oxidation of the corresponding alcohols in 50-78 % yield¹. The following are the ¹H NMR data of **1e-h**. *2-Cyclohexylethanal* **1e**^{2 1}H NMR (300 MHz; CDCl₃): δ 9.75 (1H, t, J=2.3 Hz, CHO); 2.28 (2H, dd, J=6.8 Hz, 2.3 Hz, CH₂CHO); 1.96-1.73 (1H, m, CH); 1.70-1.59 (5H, m, 5 HCH); 1.36-0.91

(5H, m, 5 HC*H*).

3,7-*dimethyl-6-octenal* **1f** ³ ¹H NMR (300 MHz; CDCl₃): δ 9.75 (1H, t, J=2.2 Hz, CHO); 5.12-5.03 (1H, m, CH=); 2.47-1.94 (5H, m); 1.64 (3H, d, J=15.8 Hz, CHCH₃); 1.39-1.23 (2H, m, CH₂); 0.98 (3H, s, CCH₃); 0.95 (3H, s, CCH₃).

(2*Z*)-3,7-dimethyl-2,6-octadienal **1h**⁴ ¹H NMR (300 MHz; CDCl₃): δ 9.88 (1H, d, J=8.2 Hz, CHO); 5.85 (1H, d, J=8.0 Hz, C=CHCHO); 5.11-5.05 (1H, m, CH=C(CH₃)₂); 2.57 (2H, t, J=7.5 Hz CH₂C(CH₃)); 2.25-2.15 (2H, m, CH₂CH=C); 1.96 (3H, d, J=1.3 Hz, CH₃); 1.66 (3H, s, CH₃); 1.58 (3H, s, CH₃).

General procedure for α-oximation of aldehydes.

Reactants were introduced in reaction vessel in the following order: pyrrolidine (0.4 mmol, 33 µL) was added to a solution of monohydrate *p*-TsOH (0.4 mmol, 76 mg) in 3 mL of anhydrous DMF, followed by addition of distilled water (4.0 mmol) and aldehyde (2.0 mmol). After mixing solution for 5 minutes, NaNO₂ (2.0 mmol, 138 mg) was added and then anhydrous FeCl₃ (2.0 mmol, 324 mg) was introduced in aliquotes (careful: reaction is exotermic). The reaction was monitored by thin layer cromatography. At the end of experiment (3 - 4.5 h), the internal standard was added, followed by addition of a saturated NaCl solution (5 mL). The mixture was extracted with ethyl acetate (30 mL); the organic phases were washed with a saturated solution of NaCl and dried over Na₂SO₄. The quantitative yields of α -oximation reaction were determined by GC analisys (error \pm 3%).

Characterization of α-oximation reaction products.

All 2-hydroxyimino-aldehydes were synthesized by following the general procedure. After evaporation of the solvent under reduced pressure, all products were isolated by chromatographic purification on silica gel using several mixtures of hexane/ethyl acetate as eluent and characterized by spectroscopic analysis. When injected to GC and GC-MS, all 2-hydroxyimino-aldehydes lose slightly HCOOH, giving the corresponding nitrile derivatives as confirmed by comparing with authentic samples.

2-hydroxyimino-3-phenylpropanal 2a: after column chromatography (eluent hexane/ethyl acetate 50/3) 276 mg (85%) of a yellow oil was obtained.¹H-NMR (300 MHz; CDCl₃): δ 9.52 (1H, s, CHO), 8.38 (1H, broad s, OH), 7.28-7.19 (5H, m, ArH), 3.86 (2H, s, CH₂). ¹³C-NMR (300 MHz; CDCl₃): δ 190.7, 159.8, 135.6, 129.4, 128.8, 126.9, 28.1. GC-MS: *m/z* 163 (M⁺, 48%), 117 (98), 91 (100). IR (CHCl₃): $\overline{\nu}$ / cm⁻¹ 3552 (OH), 1706 (conj. CO), 1602 (CN) and 1006 (NO). HRMS (ESI-TOF) calcd for [C₉H₉NO₂ - H⁺] 162.0550, found 162.05496.

2-hydroxyimino-2-phenylethanal $2b^5$: after column chromatography (eluent hexane/ethyl acetate 10/1) 192 mg (64%) of a yellow oil was obtained, from which the dimer crystallizes on standing as white solid. ¹H-NMR (300 MHz; DMSO-d₆): δ 9.61 (1H, s, CHO), 7.43-7.42 (5H, m, Ar*H*). ¹³C-NMR (300 MHz; CDCl₃): δ 190.7, 157.2, 132.5, 130.5, 129.6, 128.4. GC-MS: *m/z* 149 (M⁺, 40%),

119 (93), 103 (46), 77 (100). HRMS (ESI-TOF) calcd for $[C_8H_7NO_2 - H^+]$ 148.0393, found 148.0395.

2-hydroxyiminodecanal 2c: after column chromatography (eluent hexane/ethyl acetate 40/1) 253 mg (70%) of a white solid (mp 60-62°C from hexane/ethyl acetate) was obtained. ¹H-NMR (300 MHz; CDCl₃): δ 9.45 (1H, s, CHO), 8.64 (1H, broad s, NO*H*), 2.49 (2H, t, J=7.7 Hz, C*H*₂C=NOH), 1.49-1.44 (2H, m, C*H*₂CH₂C=NOH), 1.27-1.26 (10H, m), 0.87 (3H, t, J=6.7 Hz, C*H*₃). ¹³C-NMR: (300 MHz; CDCl₃) δ 191.3, 162.2, 32.2, 30.0, 29.5, 29.4, 25.8, 23.0, 22.2, 14.4. GC-MS: *m/z* 185 (M^+ , 2%), 168 (7), 156 (30), 138 (21), 124 (15), 110 (20), 96 (25), 87 (46), 81 (25), 71 (37), 69 (37), 55 (100). IR (CHCl₃): $\bar{\nu}$ /cm⁻¹ 3557 (OH), 1705 (conj. CO), 1603 (CN) and 1012 (NO). HRMS (ESI-TOF) calcd for [C₁₀H₁₉NO₂ - H⁺] 184.1338, found 184.1340.

2-hydroxyimino-3,5,5-trimethylhexanal 2d: after column chromatography (eluent hexane/ethyl acetate 50/3) 275 mg (80%) of a yellow oil was obtained. ¹H-NMR (300 MHz; CDCl₃): δ 9.397 and 9.392 (1H, s, CHO, *E* and *Z* isomers), 3.36-3.34 (1H, m, CH), 2.01 (1H, dd, J=14.3 Hz and 8.9 Hz, H_aCH_b), 1.35 (1H, dd, J=14.3 Hz and 3.9 Hz, H_bCH_a), 1.18 (3H, d, J=7.1 Hz, CHCH₃), 0.84 (9H, s, C(CH₃)₃). ¹³C-NMR (300 MHz; CDCl₃): δ 191.6, 165.5, 46.9, 31.5, 29.8, 26.0, 19.2. GC-MS: *m/z* 171 (M⁺,1%), 154 (2), 115 (10), 110 (10), 98 (30), 83 (20), 69 (25), 57 (100). IR (CHCl₃): $\bar{\nu}/cm^{-1}$ 3556 (OH), 1706 (conj. CO), 1610 (CN) and 1000 (NO). HRMS (ESI-TOF) calcd for [C₉H₁₇NO₂ - H⁺] 170.1181, found 170.1185.

2-cyclohexyl-2-hydroxyiminoethanal 2e: after column chromatography (eluent hexane/ethyl acetate 25/2) 251 mg (81%) of a yellow oil was obtained. ¹H-NMR (300 MHz, CDCl₃): δ 9.365 and 9.361 (1H, s, CHO, *E* and *Z* isomers), 3.09-3.01 (1H, m, CH), 1.91-1.27 (10H, m, 5CH₂). ¹³C-NMR (300 MHz; CDCl₃): δ 191.7, 163.6, 35.0, 27.6, 26.6, 26.1. GC-MS: *m/z* 155 (M⁺⁻, 5%), 138 (53), 126 (14), 108 (67), 81 (76), 67 (78), 55 (100). IR (CHCl₃): $\bar{\nu}$ /cm⁻¹ 3556 (OH), 1706 (conj. CO), 1607 (CN) and 1037 (NO). HRMS (ESI-TOF) calcd for [C₈H₁₃NO₂ - H⁺] 154.0868, found 154.0862.

2-hydroxyimino-3,7-dimethyl-oct-6-enal 2f: after column chromatography (eluent hexane/ethyl acetate 20/1) 190 mg (49%) of a yellow oil was obtained. ¹H-NMR (300 MHz; CDCl₃): δ 9.386 and 9.381 (1H, s, CHO, *E* and *Z* isomers), 5.08-4.91 (1H, m, CH=C), 3.28-3.18 (1H, m, CH₃CH), 1.95-1.75 4H, m, CH₂CH₂), 1.65 (3H, s, CCH₃), 1.55 (3H, s, CCH₃), 1.19 (3H, d, J=7.0 Hz, CHCH₃). ¹³C-NMR (300 MHz; CDCl₃): δ 190.7, 163.1, 131.6, 123.5, 32.2, 28.9, 26.0, 25.2, 17.2, 15.8. GC-

MS: m/z 183 (M^{+,} 2%), 166 (30), 101 (50), 83 (60), 69 (80), 55 (100). IR (CHCl₃): $\overline{\nu}/cm^{-1}$ 3559 (OH), 1703 (conj. CO), 1614 (CN) and 1015 (NO). HRMS (ESI-TOF) calcd for [C₁₀H₁₇NO₂ - H⁺] 182.1181, found 182.1184.

2-hydroxyimino-3,3-dimethyl-butanal 2g: after column chromatography (eluent hexane/ethyl acetate 40/1) 196 mg (76%) of a white solid (mp 102-104°C from hexane) was obtained, as a mixture of Z and E isomers (ratio 3/1). The diastereomeric ratio was determined by ¹H-NMR spectroscopy via integration of the aldehyde signals.

¹H-NMR (300 MHz; CDCl₃): *isomer Z* δ 10.29 (1H, s, CHO), 1.23 (9H, s, C(CH₃)₃); *isomer E* δ 9.35 (1H, s, CHO), 1.37 (9H, s, C(CH₃)₃). ¹³C-NMR (300 MHz; DMSO-d₆): *isomer Z* δ 192.0, 141.1, 37.2, 28.8, 28.5, 27.9; *isomer E* δ 193.3, 142.3, 35.9, 29.6, 29.0, 27.6. GC-MS: *m/z* 129 (M⁺, 32%), 112 (23), 100 (50), 84 (25), 68 (24), 57 (100). IR (CHCl₃): $\overline{\nu}$ /cm⁻¹ 3572 (OH), 1708 (conj. CO), 1614 (CN) and 1012 (NO). HRMS (ESI-TOF) calcd for [C₆H₁₁NO₂-H⁺] 128.0706, found 128.0712.

(E)-2-benzyl-5-phenylpent-2-enal 3^6 : was synthesized following the general procedure, but in absence of FeCl₃ and extending reaction time to 48 h. After column chromatography (eluent hexane/ethyl acetate 100/1) 100 mg (40%) of a colourless oil was obtained. ¹H-NMR (300 MHz; CDCl₃): δ 9.45 (1H, s, CHO), 7.29-7.10 (10H, m, 2 Ar*H*), 6.63 (1H, apparent t, J=6.33 Hz, C=C*H*), 3.59 (2H, s, C*H*₂), 2.76 (4H, m, C*H*₂C*H*₂). GC-MS: m/z 250 (M⁺, 6%), 232 (5), 159 (31), 145 (41), 131 (16), 115 (10), 91 (100).

2-methyl-5-(1-hydroxy-1-methylethyl)cyclopentanecarbaldehyde **4**: after column chromatography (eluent hexane/ethyl acetate 50/1) 75 mg (20%) of a colourless oil was obtained, as a mixture of **4a** and **4b** diastereomers (dr 2/1). The diastereomeric ratio was determined by ¹H-NMR spectroscopy via integration of the aldehyde signals.

HRMS (ESI-TOF) calcd for $[C_{10}H_{18}O_2-H^+]$ 169.1229, found 169.1228.

diastereomer 4a ¹H-NMR (300 MHz; CDCl₃): δ 9.66 (1H, d, J=3,5 Hz, CHO), 2.69-2.60 (1H, m, CHC(CH₃)₂OH); 2.46-2.40 (1H, dt, J=8.4 Hz and 3.5 Hz, CHCHO), 2.21-2.11 (1H, m, CHCH₃), 2.00-1.86 (2H, m, CH_aH_b-CH_aH_b),1.56 (3H, s, CH₃), 1.50 (3H, s, CH₃), 1.45-1.30 (2H, m, CH_aH_b-CH_aH_b), 1.10 (3H, d, J=6.7 Hz, CH₃). ¹³C-NMR (300 MHz; CDCl₃): δ 203.8, 73.8, 62.2, 53.0, 37.5, 34.3, 32.0, 31.0, 28.0, 19.0. GC-MS: *m*/*z* 152 (M⁺, 10%), 137 (11), 123 (84), 111 27), 109 (39), 95 (24), 93 (27), 91 (15), 82 (24), 81 (100), 79 (20), 77 (20), 70 (49), 67 (32), 55 (24), 53 (14).

diastereomer 4b ¹H-NMR (300 MHz; CDCl₃): δ 9.83 (1H, d, J=2.6 Hz, CHO), 2.92-2.98 (1H, m,

C*H*CHO), 2.82-2.74 (1H, dt, J=8.5 Hz and 6.1 Hz, C*H*C(CH₃)₂OH), 2.50-2.42 (1H, m, C*H*CH₃), 1.92-1.79 (2H, m, C*H*_aH_b-C*H*_aH_b), 1.55 (3H, s, C*H*₃), 1.47 (3H, s, C*H*₃), 1.45-1.27 (2H, m, CH_aH_b-CH_aH_b), 1.09 (3H, d, J=7.1 Hz, C*H*₃). ¹³C-NMR (300 MHz; CDCl₃): δ 205.2, 74.5, 57.1, 50.4, 38.8, 35.0, 32.3, 31.0, 28.3, 16.0. GC-MS: *m*/*z* 152 (M⁺, 12%), 137 (19), 133 (20), 123 (100), 111 (25), 109 (39), 97 (14), 95 (24), 93 (24), 91 (14), 83 (20), 81 (90), 79 (21), 77 (18), 70 (33), 69 (33), 67 (35), 55 (24), 53 (14).

3-phenyl-propionic acid ¹²: yield 67% (eluent hexane/ethyl acetate 10:1). white solid (mp 40-50°C from hexane). ¹H NMR (300 MHz; CDCl₃): δ 9.5 (1H, broad s, OH); 7.36-7.21 (5H, m, ArH); 2.97 (2H, t, J=7.8 Hz, CH₂CO₂H,); 2.70 (2H, t, J=7.7 Hz, CH₂Ph). ¹³C NMR (300 MHz; CDCl₃): δ 179.5, 140.5, 128.9, 128.6, 126.7, 35.9, 30.9.

General procedure for oxidative cyclization of citronellal 1f.

Reactants were introduced in reaction vessel in the following order: pyrrolidine (0.065 mmol, 5.4 μ L) was added to a solution of monohydrate *p*-TsOH (0.065 mmol, 12 mg) in 0.5 mL of anhydrous DMF, followed by addition of **1f** (0.33 mmol). After mixing solution for 5 minutes, the oxidant (0.65 mmol) was added. The mixture was stirred for 24 h at 80°C or room temperature. At the end of experiment, the internal standard was added, followed by addition of a saturated NaCl solution (1 mL). The mixture was extracted with ethyl acetate (5 mL); organic phases were washed with a saturated solution of NaCl and dried over Na₂SO₄. Quantitative yields of cyclization products were determined by GC analisys (error ± 3%).

Characterization of 2-methyl-5-(prop-1-en-2-yl)cyclopentanecarbaldehyde 8.

It was synthesized by following the general procedure. A crude product was obtained which, upon concentration and column chromatography on silica gel (hexane/ethyl acetate 80/1), produced 217 mg (44 %) of a yellow oil as a mixture of **8a**, **8b**, **8c** and **8d** diastereomers. The diastereomeric ratio (**8a**:**8b**:**8c**:**8d** = 29:5:1:1) was determined by ¹H-NMR spectroscopy via integration of the aldehyde signals.

diastereomer 8a^{7, 8, 9}: ¹H-NMR (300 MHz; CDCl₃): δ 9.56 (1H, d, J=3.6 Hz, CHO), 4.72 (1H, br s, C=CH_aH_b), 4.75 (1H, br s, C=CH_aH_b), 2.83 (1H, apparent q, J=8.7 Hz, CHC=CH₂), 2.30 – 2.20 (2H, m, CH₃CH-CHCHO), 2.00–1.86 (2H, m, CH_aH_b-CH_aH_b), 1.71 (3H, s, CH₃), 1.45–1.30 (2H, m, CH_aH_b-CH_aH_b), 1.06 (3H, d, J=6.4 Hz, CH₃).¹³C-NMR (300 MHz; CDCl₃): δ 204.4, 146.2,

110.4, 63.7, 49.1, 36.2, 33.5, 30.3, 20.4, 19.5. GC-MS: *m/z* 152 (M^{+,}, 2%), 137 (9), 123 (100), 109 (20), 95 (33), 81 (54), 67 (27), 55 (14).

diastereomer **8b**^{7, 8, 9, 10}: ¹H-NMR (300 MHz; CDCl₃): δ 9.75 (1H, d, J=3.4 Hz, CHO), 4.84 (1H, br s, C=CH_aH_b), 4.81 (1H, br s, C= CH_aH_b), 3.04 (1H, apparent q, J=8.5 Hz, CHC=CH₂), 2.69 (1H, ddd, J=8.8 Hz, 8.7 Hz and 3.4 Hz, CHCHO), 2.60–2.45 (1H, m, CHCH₃), 1.92–1.79 2H, m, CH_aH_b-CH_aH_b), 1.59 (3H, s, CH₃), 1.45–1.27 (2H, m, CH_aH_b-CH_aH_b), 1.05 (3H, d, J=7.0 Hz, CH₃). ¹³C-NMR (300 MHz; CDCl₃): δ 205.7, 146.8, 110.0, 58.5, 46.0, 37.3, 34.7, 30.6, 20.7, 16.7. GC-MS: *m*/*z* 152 (M⁺, 2%), 137 (9), 123 (100), 109 (20), 95 (33), 81 (54), 67 (27), 55 (14).

diastereomer **8c**^{8, 11}: partial data ¹H-NMR (300 MHz; CDCl₃): δ 9.50 (1H, d, J=3.7Hz, CHO). ¹³C-NMR (300 MHz; CDCl₃): *d* 201.2, 61.5, 52.0. GC-MS. *m/z* 152 (M^{+,}, 1%), 137 (7), 123 (8), 109 (47), 95 (25), 82 (42), 81 (100), 70 (93), 69 (49), 67 (58), 55 (30).

diastereomer **8d**^{8, 9}: partial data ¹H-NMR (300 MHz; CDCl₃): δ 9.30 (1H, d, J=4.5 Hz, CHO). ¹³C-NMR (300 MHz, CDCl₃): δ 202.9, 111.5, 60.4, 48.9, 36.3, 34.2, 30.7, 23.0, 21.2.

References

- 1 A. De Mico, G. Margarita, L. Parlanti, A. Vescovi and G. Piancatelli, J. Org Chem., 1997, 62, 6974.
- 2 (a) G. Righi and G. Rumboldt, J. Org. Chem., 1996, 61, 3557; (b) T. D. Beeson and D. W. C. MacMillan J. Am. Chem. Soc. 2005, 127, 8826.
- 3 E. Savoia, C. Tagliavine, A. Trombini and U. Ronchi. J. Org. Chem., 1981, 46, 5344.
- 4 M. J. Schultz; S. S. Hamilton; D. R. Jensen and M. S. Sigman, J. Org. Chem., 2005, 70, 3343.
- 5 J. M. Coustard, Tetrahedron, 1999, 55, 5809.
- 6 (a) O. Lifchits, C. M. Reisinger and B. List, J. Am. Chem. Soc., 2010, **132**,10227; (b) A.Erkkilä and P. M. Pihko, *Eur. J. Org. Chem.*, 2007, 4205.
- 7 P. V. Pham, K. Ashton and D. W. C. MacMillan, Chem. Sci., 2011, 2, 1470; (
- 8 B. B. Snider and E. Y. Kiselgof, Tetrahedron, 1996, 52, 6073.
- 9 T. Sakai, K. Morita, C. Matsumura, A. Sudo, S. Tsuboi and A. Takeda, J. Org. Chem., 1981, 46, 4774.
- V. Navickas, D. U. Ushakov, M. E. Maier, M. Ströbele and H.-J. Meyer, Org. Lett., 2010, 12, 3418.

11 R. Kaiser and D. Lamparsky Helv. Chim. Acta, 1976, 59, 1797.

12 J. Sedelmeier, S. V. Ley, I. R. Baxendale and M. Baumann, Org. Lett., 2010, 12, 3618.

NMR Spectra Data

¹H-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3-phenylpropanal 2a





¹³C-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3-phenylpropanal 2a







¹³C-NMR (300 MHz; CDCl₃) 2-hydroxyimino-2-phenylethanal 2b



¹H-NMR (300 MHz; CDCl₃) 2-hydroxyiminodecanal 2c







¹H-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3,5,5-trimethylhexanal 2d



¹³C-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3,5,5-trimethylhexanal 2d

¹H-NMR (300 MHz; CDCl₃) 2-cyclohexyl-2-hydroxyiminoethanal 2e





¹³C-NMR (300 MHz; CDCl₃) 2-cyclohexyl-2-hydroxyiminoethanal 2e

¹H-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3,7-dimethyl-oct-6-enal 2f





¹³C-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3,7-dimethyl-oct-6-enal 2f

¹H-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3,3-dimethyl-butanal 2g





¹³C-NMR (300 MHz; CDCl₃) 2-hydroxyimino-3,3-dimethyl-butanal 2g



¹H-NMR (300 MHz; CDCl₃) (E)-2-benzyl-5-phenylpent-2-enal 3





¹³C-NMR (300 MHz; CDCl₃) 2-methyl-5-(1-hydroxy-1-methylethyl)cyclopentanecarbaldehyde 4



DEPT-NMR (300 MHz; CDCl₃) 2-methyl-5-(1-hydroxy-1-methylethyl)cyclopentanecarbaldehyde





COSY-NMR (300 MHz; CDCl₃) 2-methyl-5-(1-hydroxy-1-methylethyl)cyclopentanecarbaldehyde







¹H-NMR (300 MHz; CDCl₃) 2-methyl-5-(prop-1-en-2-yl)cyclopentanecarbaldehyde 8



¹³C-NMR (300 MHz; CDCl₃) 2-methyl-5-(prop-1-en-2-yl)cyclopentanecarbaldehyde 8



DEPT-NMR (300 MHz; CDCl₃) 2-methyl-5-(prop-1-en-2-yl)cyclopentanecarbaldehyde 8