R E V I S E D !

Supporting Information (2 pages)

Diastereoselective Epoxidation of Oxazolidine-Substituted Alkenes by Dimethyldioxirane and *m*-Chloroperbenzoic Acid: π-Facial Control through Hydrogen Bonding by the Urea Functionality

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Experimental Section

General Aspects. The elemental analyses were performed at the Microanalytical Department of the Institute of Inorganic Chemistry, University of Würzburg. ^{1}H- and ^{13}C-NMR spectra were recorded in $CDCl_3$ on a Bruker AC 200 or a AC 250 (^{1}H: 200 MHz or 250 MHz; ^{13}C: 50 MHz or 63 MHz) spectrometer by using $CHCl_3$ as standard. The multiplicity of the ^{13}C signals is only given, when determined by DEPT spectroscopy. IR spectra were recorded on a FT-IR Perkin Elmer 1600 spectrophotometer. TLC analysis was conducted on precoated silica-gel foils Polygram SIL G/UV254 (40 × 80 mm) from Machery and Nagel. Spots were visualized by UV light or spray tests with phosphomolybdic acid. Flash chromatography was performed on silica gel (20 – 63 μm, Woelm) or on a Harrison Research Chromatotron (model 7924T), equipped with plates coated with Merck 60 PF_{254} silica gel. GC analyses were

performed on a HRGC Mega 2 series 8560, equipped with an achiral Permabond CW20M-DF-0.25 column and a chiral Cyclodex B in DB 1701 column.

Materials. All commercially available reagents were used without further purification. Solvents were purified by the standard procedures. The DMD solution in acetone was prepared by the standard procedure.[16] Commercially available 3-chloroperbenzoic acid (*m*CPBA, 70-75% purity) was washed with phosphate buffer (pH 7) and dried in an exsiccator to remove water and 3-chlorobenzoic acid.[17] The enantiomerically pure *S*-phenylglycinol was a generous gift from Degussa-Hüls AG, Germany. The synthesis of alkenes **1a**-**c** was described earlier.[8] The racemic aldehyde **3** was synthesized by epoxidation of *E*-2-methyl-2-buten-1-ol with *m*CPBA, followed by oxidation with chromium trioxide dipyridine complex.[10] Optically active 2*R*,3*S*-**3** (ee 64%, determined by GC on a chiral phase) was prepared by the Sharpless-Katsuki epoxidation of *E*-2-methyl-2-buten-1-ol, followed by oxidation with chromium trioxide dipyridine complex.[10]

Preparation of [*2S*-[*cis*-(*E*)]]-2-(1-Methyl-1-propenyl)-4,*N*-diphenyl-3-oxazolidine-carboxamide (1d). A sample of 1.37 g (10.0 mmol) of *S*-phenylglycinol was dissolved in dichloromethane (20 mL) and molecular sieves 4 Å (5 g) and 0.97 mL (840 mg, 10 mmol) of *E*-2-methyl-2-butenal were added. After stirring at 20 °C for 3 h, the molecular sieves were removed by filtration. A solution of 2.20 mL (2.40 g, 20.1 mmol) of phenyl isocyanate in ethyl ether (10 mL) was added slowly (10 min), and the solution was stirred for 16 h at 20 °C. A 2-M aqueous solution of sodium hydroxide (15 mL) was added and the resulting mixture was stirred vigorously for 30 min. The phases were separated and the aqueous layer was extracted with ether (3 × 15 mL). The combined organic phases were washed with water (2 × 20 mL), dried over anhydrous magnesium sulfate, and the solvent was removed (30 °C, 800 mbar). The crude product was purified by column chromatography (5:1 petroleum ether/

ethyl ether as eluent) and 2.15 g (67%) of [*2S*-[*cis*-(*E*)]]-2-(1-Methyl-1-propenyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide (**1d**) were obtained as yellow oil.

$[\alpha]^{25}_{D}$ = +1.25° (c 1.13, $CHCl_3$); IR (NaCl): 3381, 3061, 3031, 2984, 2921, 2861, 1682, 1599, 1538, 1504, 1445, 1316, 1246, 1152, 1064, 963; ^{1}H NMR δ 1.75 (s, 3 H), 1.83 (dd, *J* =7.5, 0.6 Hz, 3 H), 4.23 (dd, *J* = 9.0, 4.3 Hz, 1 H), 4.33 (dd, *J* = 9.0, 6.72 Hz, 1 H), 5.22 (dd, *J* = 6.4, 4.1 Hz, 1 H), 5.52 (s, 1 H), 6.09 (q, *J* = 6.7 Hz, 1 H), 6.69 (s, 1 H), 6.9-7.6 (m, 10 H); ^{13}C NMR δ 11.1 (q), 13.6 (q), 60.2 (d), 72.6 (t), 94.8 (d), 119.0 (d), 123.1 (d), 127.2 (d), 127.9 (d), 128.1(d), 128.8(d), 128.9 (d), 134.9 (s), 138.5 (s), 140.3 (s), 154.1 (s); Anal. Calcd. for $C_{20}H_{22}N_2O_2$ (322.4): C, 74.51; H, 6.88; N, 8.69. Found: C, 74.26; H, 6.51; N, 8.65.

General Procedure for the Epoxidation with Dimethyldioxirane. A sample of the olefin was dissolved in acetone and 1.1 equiv. of a 0.05 - 0.08 M solution of dimethyldioxirane in acetone were added. After stirring at 20 °C for 5 h, the solvent was removed (20 °C, 30 mbar) and the product distribution was determined by ^{1}H-NMR spectroscopy. The spectral data are given below and the individual results are listed in Table 1 (see main text).

DMD Epoxidation of (*2S*-*cis*)-2-(2-Methyl-1-propenyl)-4,*N*-diphenyl-3-oxazolidine-carboxamide (1a). According to the general procedure, 92.6 mg (287 μmol) of **1a** was epoxidized by DMD. The crude product was recrystallized from a dichloromethane/petroleum ether mixture to yield 86.6 mg (89%) of [2*S*-[2α(*R**),4α]]-2-(3,3-dimethyloxiranyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide (*lk*-**2a**) as white needles (mp 154-155 °C).

$[\alpha]^{25}_{D}$ = +0.54° (c 0.96 $CHCl_3$); IR (KBr) 4028, 3013, 1682, 1600, 1556, 1504, 1446, 1320, 1253, 1177, 1083, 907; ^{1}H NMR δ 1.46 (s, 3 H), 1.56 (s, 3 H), 3.04 (d, *J* = 8.2 Hz, 1 H), 4.23

(dd, *J* = 8.7, 4.2 Hz, 1 H), 4.31 (dd, *J* = 8.7, 6.4 Hz, 1 H), 5.01 (d, *J* = 8.2 Hz, 1 H), 5.47 (dd, *J* = 6.3, 4.1 Hz, 1 H), 7.01 (t, *J* = 7.2 Hz, 1 H), 7.1-7.5 (m, 9 H), 8.04 (s, 1 H); ^{13}C NMR δ 18.8 (q), 24.5 (q), 59.6 (d), 61.5 (s), 64.2 (d), 73.2 (t), 88.6, (d), 119.2 (d), 122.9 (d), 126.3 (d), 127.6 (d), 128.7 (d), 128.8 (d), 139.0 (s), 140.4 (s), 153.7 (s); Anal. Calcd. for $C_{20}H_{22}N_2O_3$ (338.4): C, 70.99; H, 6.55; N, 8.28. Found: C, 70.59; H, 6.63; N, 8.17.

DMD Epoxidation of (*2S-cis*)-2-(2-Methyl-1-propenyl)-*N*-(4-nitrophenyl)-4-phenyl-3-oxazolidinecarboxamide (1b). According to the general procedure, 100 mg (273 μmol) of **1b** was epoxidized by DMD. The crude product was recrystallized from dichloromethane/petroleum ether to yield 87.0 mg (83%) of [2*S*-[2α(*R**),4α]]-2-(3,3-dimethyloxiranyl)-*N*-(4-nitrophenyl)-4-phenyl-3-oxazolidinecarboxamide (*lk*-**2b**) as yellow plates; mp 179-180 °C.

$[\alpha]^{25}_D$= +75° (c 1.04, $CHCl_3$); IR (KBr) 3345, 3090, 3030, 2960, 1695, 1630, 1610, 1570, 1525, 1450, 1420, 1380, 1440, 1260, 1185, 1115, 1085; ^{1}H NMR δ 1.50 (s, 3 H), 1.59 (s, 3 H), 3.08 (d, *J* = 8.2 Hz, 1 H), 4.26 (dd, *J* = 8.8, 4.0 Hz, 1 H), 4.33 (dd, *J* = 8.8, 6.4, 1 H), 5.00 (d, *J* = 8.2 Hz, 1 H), 5.44 (dd, *J* = 6.1, 3.8 Hz, 1 H), 7.3-7.7 (m, 7 H), 8,14 (d, *J* = 9.3 Hz, 2 H), 8.55 (s, 1 H); ^{13}C NMR δ 18.8 (q), 24.6 (q), 59.8 (d), 62.3 (s), 64.1 (d), 73.4 (t), 88.5 (d), 118.3 (d), 125.0 (d), 126.3 (d), 127.9 (d), 128.9 (d), 139.9 (s), 142.5 (s), 145.3 (s), 152.8 (s); Anal. Calcd. for $C_{20}H_{21}N_3O_5$ (383.4): C, 62.65; H, 5.52; N, 10.96. Found: C, 62.95; H 5.60; N, 10.81.

DMD Epoxidation of (*2S-cis*)-*N*-Methyl-2-(2-methyl-1-propenyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide (1c). According to the general procedure, 67.7 mg (201 μmol) of olefin **1c** was epoxidized by DMD. Chromatography on the Chromatotron (10:1 petroleum

ether/ethyl ether as eluent) yielded 58.3 mg (82%) of a diastereomeric mixture of [2*S*-[2α(S*),4α]]- and [2*S*-[2α(R*),4α]]-*N*-Methyl-2-(3,3-dimethyloxiranyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide (**2c**).

IR (NaCl) 3062, 3030, 2963, 2927, 2873, 1716, 1660, 1596, 1495, 1455, 1422, 1372, 1311, 1247, 1171, 1114, 1077, 1045, 1029, 983, 950, 917; Anal. Calcd. for $C_{21}H_{24}N_2O_3$ (352.4): C, 71.57; H, 6.86; N, 7.95. Found: C, 71.57; H, 6.45; N, 7.72.

{2*S*-[2α(*R),4α]} (*like*) Diastereomer 2c.** ^{1}H NMR δ 1.34 (s, 3 H), 1.45 (s, 3 H), 2.96 (d, *J* = 7.0 Hz, 1 H), 3.17 (s, 3 H), 3.81 (dd, *J* = 8.4, 2.4 Hz, 1 H), 4.05 (dd, *J* = 8.3, 6.1 Hz, 1 H), 4.77 (dd, *J* = 6.1, 2.3 Hz, 1 H), 5.41 (d, *J* = 7.02 Hz, 1 H), 6.9-7.2 (m, 10 H); ^{13}C NMR δ 19.3 (q), 24.5 (q), 40.5 (q), 58.7 (d), 62.5 (s), 63.8 (d), 74.2 (t), 90.0, (d), 125.5 (d), 125.9 (d), 126.5 (d), 126.6 (d), 127.8 (d), 129.1 (d), 140.4 (s), 144.2 (s), 160.2 (s).

{2*S*-[2α(*S),4α]} (*unlike*) Diastereomer 2c.** ^{1}H NMR δ 1.28 (s, 3 H), 1.41 (s, 3 H), 2.86 (d, *J* = 4.5 Hz, 1 H), 3.11 (s, 3 H), 3.83 (dd, *J* = 8.8, 6.3 Hz, 1 H), 4.13 (dd, *J* = 8.6, 7.0 Hz, 1 H), 4.61 (t, *J* = 6.6 Hz, 1 H), 5.38 (d, *J* = 4.6 Hz, 1 H), 6.8-7.2 (m, 10 H); ^{13}C NMR δ 18.8 (q), 24.7 (q), 40.2 (q), 59.0 (s), 61.2 (d), 63.3 (d), 73.8 (t), 88.4 (d), 126.0 (d), 126.1 (d), 126.2 (d), 127.2 (d), 127.8 (d), 129 (d), 139.7 (s), 144.6 (s), 159.2 (s).

DMD Epoxidation of {2*S*-[*cis*-(*E*)]}-2-(1-Methyl-1-propenyl)-4,*N*-diphenyl-3-oxazolidine-carboxamide (1d). A sample of 106 mg (329 μmol) of **1d** was epoxidized by DMD according to the general procedure. The crude product was purified on the Chromatotron (5:1 petroleum ether/ether as eluent) to yield 80.4 mg (73%) of {2*S*-[2α(2*R**,3*R**),4α]}- and {2*S*-[2α(2*S**,3*S**),4α]}-2-(2,3-dimethyloxiranyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide (**1d**) as diastereomeric mixture.

IR (NaCl): 3309, 3267, 3140, 3096, 3015, 2925, 1676, 1619, 1590, 1561, 1531, 1502, 1437, 1384, 1331, 1320, 1279, 1255, 1155, 1102, 1073, 1032, 997, 967, 903; Anal. Calcd. for $C_{20}H_{22}N_2O_3$ (338.4): C, 70.99; H, 6.55; N, 8.28. Found: C, 70.92; H, 6.68; N, 8.22.

{2*S*-[2α(2*R,3*R**),4α]} (*like*) Diastereomer 2d.** ^{1}H NMR δ 1.28 (d, *J* = 5.6 Hz, 3 H), 1.49 (s, 3 H), 3.33 (q, *J* = 5.6 Hz, 1 H), 4.20 (dd, *J* = 8.8, 6.1 Hz, 1 H), 4.30 (dd, *J* = 8.8, 6.7 Hz, 1 H), 5.32 (t, *J* = 6.4 Hz, 1 H), 6.9-7.5 (m, overlap with signals of the other diastereomer), 7.80 (s, 1 H); ^{13}C NMR δ 13.2 (q), 14.1 (q), 56.7 (d), 60.2 (d), 63.1 (s), 72.6 (t), 91.5 (d), 119.2 (d), 123.0 (d), 127.1 (d), 128.2 (d), 128.8 (d), 129.0 (d), 138.7 (s), 139.0 (s), 155.5 (s).

{2*S*-[2α(2*S,3*S**),4α]} (*unlike*) Diastereomer 2d.** ^{1}H NMR δ 1.27 (s, 3 H), 1.54 (d, *J* = 5.8 Hz, 3 H), 3.27 (q, *J* = 5.5 Hz, 1 H), 4.23 (dd, *J* = 8.8, 5.9 Hz, 1 H), 4.40 (dd, *J* = 8.8, 4.9 Hz, 1 H), 4.85 (s, 1 H), 5.37 (t, *J* = 5.3 Hz, 1 H), 6.9-7.5 (m, overlap with signals of the other diastereomer), 8.24 (s, 1 H); ^{13}C NMR δ 13.4, 15.8, 48.3, 60.5, 61.7, 72.4, 94.5, 120.6, 124.5, 127.9, 129.8, 130.5, 136.5, 137.2, 139.4, 153.4.

General Procedure for the Epoxidation with *meta*-Chloroperbenzoic acid (*m*CPBA). A sample of the alkene was dissolved in $CDCl_3$ and 1.1 equiv. *m*CPBA was added. After 2 h (complete conversion of the olefin), the solution was filtered, potassium carbonate (ca. 200 mg) was added, and stirred at 20 °C for 30 min. The solids were removed by filtration and the product distribution was determined by ^{1}H-NMR spectroscopy. The individual results are listed in Table 1 (see main text).

***m*CPBA Epoxidation of Olefin 1a.** According to the general procedure, 51.3 mg (159 μmol) of **1a** was epoxidized by *m*CPBA to afford 49.5 mg (92%) of {2*S*-[2α(*R**),4α]}- and

{2*S*-[2α(*S**),4α]}-2-(3,3-dimethyloxiranyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide **2a** as diastereomeric mixture.

{2*S*-[2α(*S),4α]} (*unlike)* Diastereomer 2a.** ^{1}H NMR δ 1.42 (s, 3 H), 1.57 (s, 3 H), 3.20 (d, *J* = 5.3 Hz, 1 H), 4.16 (dd, *J* = 8.8, 7.6 Hz, 1 H), 4.48 (dd, *J* = 8.8, 6.8 Hz, 1 H), 4.85 (t, *J* = 7.2 Hz, 1 H), 5.64 (d, *J* = 5.2 Hz, 1 H), 6.16 (s, 1 H), 6.9-7.6 (m, overlap with signals of the other diastereomer); ^{13}C NMR δ 19.1, 25.0, 60.0, 61.1, 63.7, 75.1, 87.9, 119.5, 123.4, 126.9, 128.8, 129.4, 129.8, 137.9, 138.0, 153.7.

The spectral data for the *like* diastereomer *lk*-**2a** are given above.

***m*CPBA Epoxidation of Olefin 1b.** According to the general procedure, 79.2 mg (216 μmol) of **1b** was epoxidized by *m*CPBA to yield 78.6 mg (95%) {2*S*-[2α(*R**),4α]}- and {2*S*-[2α(*S**),4α]}-2-(3,3-dimethyloxiranyl)-*N*-(4-nitrophenyl)-4-phenyl-3-oxazolidinecarbox-amide (**2b**) as diastereomeric mixture.

{2*S*-[2α(*S),4α]} (*unlike*) Diastereomer *ul*-2b.** ^{1}H NMR δ 1.42 (s, 3 H), 1.57 (s, 3 H), 3.22 (d, *J* = 5.0 Hz, 1 H), 4.20 (dd, *J* = 8.8, 7.5 Hz, 1 H), 4.50 (dd, *J* = 9.0, 7.0 Hz, 1 H), 4.88 (t, *J* = 7.3 Hz, 1 H), 5.65 (d, *J* = 5.0 Hz, 1 H), 6.74 (s, 1 H), 7.3-8.3 (m, overlap with signals of the other diastereomer); ^{13}C NMR δ 18.4, 24.9, 60.2, 60.9, 63.4, 75.0, 87.8, 118.0, 126.5, 128.1, 129.7, 130.0, 137.2, 144.2, 144.5, 152.3.

The spectral data for the *like* diastereomer *lk*-**2b** are given above.

***m*CPBA Epoxidation of Olefin 1d.** According to the general procedure, 40.7 mg (126 μmol) of alkene **1d** was epoxidized by *m*CPBA to afford 38.4 mg (90%) of epoxide **2d** as diastereomeric mixture (spectral data are given above).

***m*CPBA Epoxidation of Olefin 1c in a Buffered Two-Phase System.**[18] A sample of 44.0 mg (131 μmol) of olefin **1c** was dissolved in dichloromethane (1.3 mL) and 0.5 M aqueous solution of sodium hydrogen carbonate (390 μL) were added, followed by 22.9 mg (131 μmol) of *m*CPBA (added in small portions), and the resulting mixture was stirred vigorously for 2 h at 20 °C. The phases were separated and the organic layer was washed with 1 M aqueous NaOH solution (0.5 mL) and water (0.5 mL), and dried over sodium sulfate. Removal of the solvent (20 °C, 30 mbar) yielded 41.7 mg (90%) of the crude product mixture that consisted of the diastereomers of *lk*-**2c** and *ul*-**2c** and unreacted olefin **1c** (spectral data are given above).

Structural Assignments.

Base-Catalyzed Rearrangement of the Epoxide *lk*-2a. A sample of 21.0 mg (62.1 μmol) of the epoxide *lk*-**2a** was dissolved in dichloromethane (2 mL) and 400 mg activated aluminum oxide[9] were added. The solvent was removed (30 °C, 30 mbar), n-hexane (10 mL) was added, and the resulting suspension was stirred at 20 °C for 16 h. The solid was removed by filtration and washed with ethyl ether (2 × 5 mL). Removal of the solvent (40 °C, 300 mbar) afforded 17.3 mg (82%) of crude product, that consisted of 10% of the rearranged product {2*S*-[2α(*S**),4α]}-2-(1-hydroxy-2-methyl-2-propenyl)-4,*N*-diphenyl-3-oxazolidinecarboxamide (*lk*-**3a**).[9]

Methylation of the Epoxide *lk*-2a. A sample of 58.3 mg (1.04 mmol) of powdered potassium hydroxide was suspended in DMSO (1 mL) and a solution of 88.0 mg (259 μmol) of epoxide *lk*-**2a** in DMSO (0.5 mL) was added. After stirring at 20 °C for 20 min, 33 μL (74.6 mg, 526 μmol) methyl iodide was added and stirring was continued for 20 h. The solution was

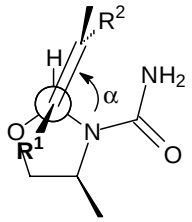
poured into water (5 mL) and extracted with ethyl ether (4 × 15 mL). The combined organic layers were washed with water (3 × 20 mL) and dried ($MgSO_4$). The solvent was removed (35 °C, 800 mbar) and the crude product was purified by chromatography on the Chromatotron (10:1 ethyl ether/petroleum ether as eluent) to afford 65.3 mg (72%) *lk*-**2c** (spectral data are given above).

Condensation of the Racemic Epoxy Aldehyde 3 with *S*-Phenylglycinol. A sample of 60.1 mg (612 μmol) of racemic epoxy aldehyde **3** was dissolved in $CDCl_3$ (2 mL) and 84.3 mg (615 μmol) of *S*-phenylglycinol and 0.2 g of potassium carbonate were added. After stirring for 2 h at 20 °C, the solids were removed by filtration through a pad of Celite and 67.1 μL (73.2 mg, 615 μmol) of phenyl isocyanate were added. After 1 h, the mixture was submitted to ^{1}H-NMR analysis and found to consist of a 1:1 diastereomeric mixture of *lk*-**2d** and *ul*-**2d**.

Condensation of the Optically Active Epoxy Aldehyde 2*R*,3*S*-3 with *S*-Phenylglycinol. A sample of 21.1 mg (215 μmol) of optically active epoxy aldehyde 2*R*,3*S*-**3** (ee 64%) was dissolved in $CDCl_3$ (1 mL) and 29.5 mg (215 μmol) of *S*-phenylglycinol and 0.1 g of potassium carbonate were added. After stirring for 2 h at 20 °C, the solids were removed by filtration through a pad of Celite and 23.5 μL (25.6 mg, 215 μmol) of phenyl isocyanate were added. After stirring for 1 h, ^{1}H-NMR analysis showed a 81:19 mixture of *ul*-**2d** and *lk*-**2d**.

Semiempirical (PM3) and DFT Calculations for the Determination of the Preferred Ground-state Conformers. The PM3[19] calculations were performed to examine the energy profile for the rotation about the α angle in the olefins **4a**,**d**, which were chosen as model

compounds for the substrates **1a**,**d**. Two minima were detected for each isomer and they were



4a: R^1=H, R^2=Me
4d: R^1=Me, R^2=H

refined at the B3LYP/3-21G* level.[20] The refined structures were further optimized and their energies were calculated by the B3LYP/6-31G* method. The α angles and relative energies are given in Table 2.

Table 2: The α Angle and Relative Energies (B3LYP/6-31G*) for the Conformational Minima of the Model Olefins **4a** and **4d**.

conformer	α angle [°]	rel. energy [kcal/mol]
4a'	131	0.0
4a"	-1	3.2[a]
4d'	124	0.36[b]
4d"	-1	0.0

[a]Relative to the lower-energy conformer **4a'**. [b]Relative to the lower-energy conformer **4d"**.

Additional References

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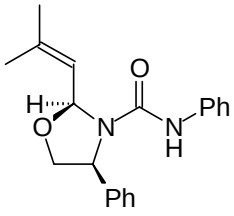
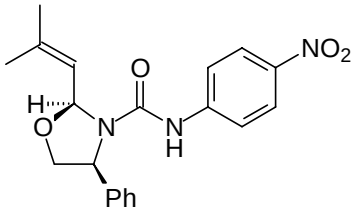
[19] (a) Semiempirical calculations were performed with the VAMP 6.1 program package: VAMP 6.1; Rauhut, G.; Alex, A.; Chandrasekhar, J.; Steinke, T.; Sauer, W.; Beck, B.; Hutter, M.; Gedeck P.; Clark, T. Erlangen 1996. (b) Stewart, J. J. P. *J. Comput. Chem.* **1989**, *10*, 209-221. (c) Stewart, J. J. P. *J. Comput. Chem.* **1991**, *12*, 320.

[20] Density functional calculations were carried out by using the Gaussian 98 package: Gaussian 98, Revision A.7, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A.; Gaussian, Inc., Pittsburgh PA, 1998.

Structure Matrix



1a



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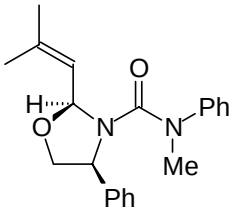
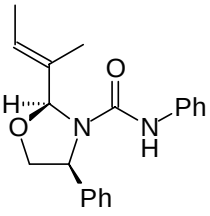


1c



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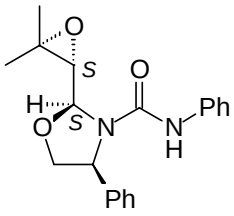
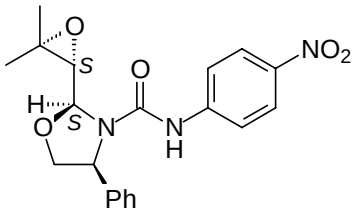


lk-**2a**



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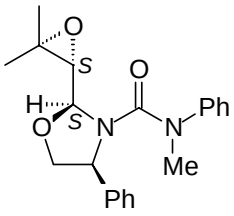

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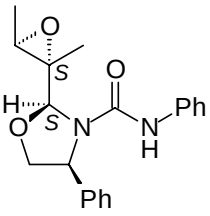

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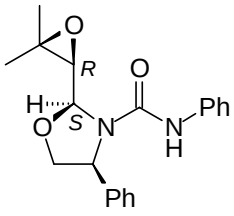

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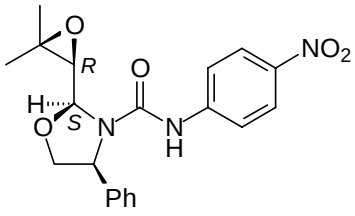

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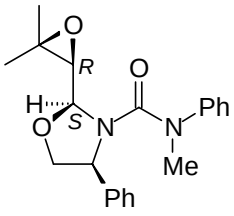

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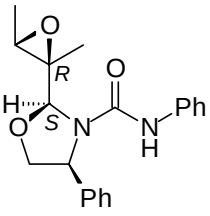

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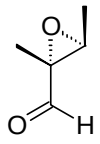
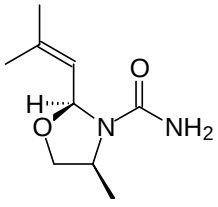
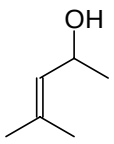


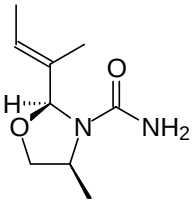
2*R*,3*S*-**3**



4a



5



4d