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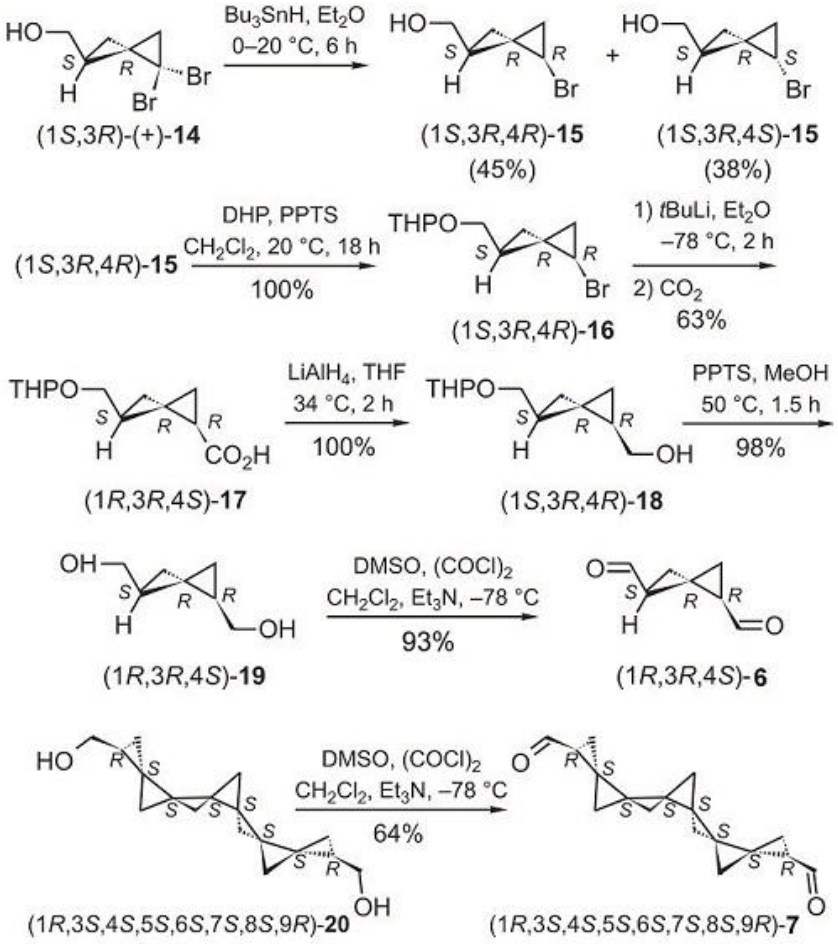
Supporting Information

Chiral Macrocyclic Aliphatic Oligoimines Derived from *trans*-1,2-Diaminocyclohexane

M. Kwit, A. Plutecka, U. Rychlewska, J. Gawronski, A. F. Khlebnikov, S. I. Kozhushkov, K. Rauch and A. de Meijere*

Enantiomerically pure [(1*R*,3*R*,4*S*)-spiropentane-1,4-diyl]dimethanol [(1*R*,3*R*,4*S*)-**19**] was prepared in five steps in 28% overall yield starting from the known [(1*S*,3*R*)-4,4-dibromospiropent-1-yl]methanol [(1*S*,3*R*)-**14**] (Scheme 1).[1]



Scheme 1. Preparation of [(1*R*,3*R*,4*S*)-spiropen-1,4-diyl]dimethanol [(1*R*,3*R*,4*S*)-**19**] from enantiomerically pure [(1*S*,3*R*)-4,4-dibromospiropent-1-yl]methanol [(1*S*,3*R*)-**14**] and of the corresponding dialdehydes **6** and **7** from diols **19** and **20**.

Thus, [(1*S*,3*R*)-**14**] was monodebrominated with tributyltin hydride to give a mixture of diastereomeric monobromides **15** which were separated by column chromatography. The bromospiropentylmethanol with (1*S*,3*R*,4*R*)-configuration[2] was, after tetrahydropyranyl protection, subjected to bromine-lithium exchange with tert-butyllithium, and the reaction mixture was treated with carbon dioxide to give the corresponding carboxylic acid (1*R*,3*R*,4*S*)-**17** in 63% yield over two steps.[3] Reduction and deprotection of the latter

furnished the diol (1*R*,3*R*,4*S*)-**19** in almost quantitative yield. This was oxidised (Swern procedure) to dialdehyde (1*R*,3*R*,4*S*)-**6**.

1,9-Diformyl-(–)-[7]triangulane [(1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-**7**] was prepared from the known (–)-[7]triangulane-1,9-dimethanol [(1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-**20**][1] applying Swern oxidation procedure in 64% yield (Scheme 1).

Experimental Section

General remarks: Starting materials: [(1*S*,3*R*)-4,4-dibromospiropent-1-yl]methanol [(1*S*,3*R*)-**14**][1] and (1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-(9-hydroxymethylhexaspiro[2.0.0.0.0.0.2.1.1.1.1.1.1]-pentadec-1-yl)methanol [(1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-**20**][1] were prepared according to previously published procedures. Bicyclo[2.2.2]octane-1,4-dicarbaldehyde (**5**) was obtained by oxidation of the known (4-hydroxymethyl-bicyclo[2.2.2]oct-1-yl)methanol[4] according to the published procedure.[5] All operations in anhydrous solvents were performed under an argon atmosphere in flame-dried glassware. Diethyl ether and THF were dried by distillation from sodium benzophenone ketyl, DMSO from CaH_2, and dichloromethane from P_4O_{10}. All other chemicals were used as commercially available. Organic extracts were dried over $MgSO_4$. ^1H and ^{13}C NMR spectra were recorded on a Bruker AM 250 (250 MHz for ^1H and 62.9 MHz for ^{13}C NMR) instrument in $CDCl_3$. Multiplicities were determined by DEPT (Distortionless Enhancement by Polarization Transfer), chemical shifts refer to $\delta_{TMS} = 0.00$ according to the chemical shifts of residual $CHCl_3$ signals. Mass spectra were measured with a Finnigan MAT 95 (CI at 70 eV) spectrometer. Optical rotations were measured on a Perkin-Elmer 241 digital polarimeter in a 1 dm cell. Melting points were determined with a Büchi 510 capillary melting point apparatus, values are uncorrected. TLC analyses were performed on precoated sheets, 0.25 mm Sil G/UV_{254} (Macherey-Nagel). Silica gel grade 60 (230–400 mesh) (Merck) was used for column chromatography.

(1*S*,3*R*,4*R*)- and (1*S*,3*R*,4*S*)-4-Bromospiropent-1-yl]methanol [(1*S*,3*R*,4*R*)-15 and (1*S*,3*R*,4*R*)-15]: Under vigorous stirring, a solution of tributyltin hydride (23.05 g, 21.3 mL, 79.18 mmol) in anhydrous diethyl ether (30 mL) was added dropwise to a solution of [(1*S*,3*R*)-4,4-dibromospiropent-1-yl]methanol [(1S,3R)-**14**] (19.30 g, 75.41 mmol) in Et_2O (60 mL) at 0 °C over a period of 10 min. The resulting solution was allowed to warm up to ambient temp. over a period of 6 h and then concentrated under reduced pressure. Column chromatography of the residue (750 g of silica gel, 70 × 5.5 cm column, hexane/THF 5:1, then

3:1) furnished the bromoalcohols (1*S*,3*R*,4*R*)-**15** (6.06 g, 45%, R_f = 0.18, hexane/THF 4:1) and (1*S*,3*R*,4*S*)-**15** (5.12 g, 38%, R_f = 0.14, hexane/THF 4:1) as colorless oils.

(1*S*,3*R*,4*R*)-**15**: ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.68–3.60 (m, 2 H; CH_2O), 3.31 (dd, *J* = 3.3, 6.5 Hz, 1 H; CHBr), 1.60–1.46 (m, 2 H; cPr-H + OH), 1.32 (dd, *J* = 4.6, 8.1 Hz, 1 H; cPr-H), 1.27 (dd, *J* = 3.3, 6.0 Hz, 1 H; cPr-H), 1.00 (t, *J* = 5.0, 1 H; cPr-H); ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ = 65.1 (CH_2), 22.7 (CH), 21.0 (C), 20.7 (CH), 13.9 (CH_2), 13.4 (CH_2).

(1*S*,3*R*,4*S*)-**15**: ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.64–3.48 (m, 2 H, CH_2O), 3.31 (ddd, *J* = 1.0, 3.3, 6.9 Hz, 1 H; CHBr), 1.77–1.65 (m, 1 H; cPr-H), 1.58–1.53 (m, 2 H; cPr-H + OH), 1.20 (dd, *J* = 3.3, 5.8 Hz, 1 H; cPr-H), 1.13 (dd, *J* = 3.2, 8.2 Hz, 1 H; cPr-H), 0.87 (t, *J* = 4.7, 1 H; cPr-H); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 64.7 (CH_2), 22.8 (CH), 22.1 (CH), 21.1 (C), 14.0 (CH_2), 11.5 (CH_2).

(1*S*,3*R*,4*R*)-2-(4-Bromospiropent-1-ylmethoxy)tetrahydropyran [(1*S*,3*R*,4*R*)-16]: A solution of bromospiropentylmethanol (1*S*,3*R*,4*R*)-**15** (6.06 g, 34.23 mmol), 3,4-dihydro-2*H*-pyran (DHP, 4.32 g, 4.64 mL, 51.34 mmol) and pyridinium *p*-toluenesulfonate (PPTS, 860 mg, 3.42 mmol) in anhydrous dichloromethane (50 mL) was stirred at ambient temp. for 18 h and then concentrated under reduced pressure. The residue was taken up with Et_2O (100 mL), the solution washed with sat. aq. $NaHCO_3$ solution (2 × 50 mL), water (50 mL), dried and concentrated again. Column chromatography (220 g of silica gel, 4 × 40 cm column, hexane/THF 6:1, R_f = 0.46) of the residue afforded (1*S*,3*R*,4*R*)-**16** (8.939 g, 100%) as a 1:1 mixture of two diastereomers (colorless oil). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 4.70 (t, *J* = 3.0 Hz, 0.5 H; OCHO), 4.65 (t, *J* = 3.0 Hz, 0.5 H; OCHO), 3.90–3.84 (m, 1 H; CH_2O), 3.72 (dd, *J* = 6.0, 10.8 Hz, 0.5 H; CH_2O), 3.56 (d, *J* = 7.0 Hz, 1 H; CH_2O), 3.51–3.83 (m, 1 H; CH_2O), 3.43 (dd, *J* = 7.3, 10.8 Hz, 0.5 H; CH_2O), 3.30 (dd, *J* = 3.3, 6.5 Hz, 1 H; CHBr), 1.85–1.71 (m, 1 H), 1.70–1.42 (m, 6 H), 1.37–1.20 (m, 3 H; *c*Pr-H), 1.02–0.98 (m, 1 H; *c*Pr-H); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 98.2/97.8 (CH), 69.8/69.6 (CH_2), 62.1/62.0 (CH_2), 30.5 (CH_2), 25.4 (CH_2), 23.0/22.9 (CH), 21.0/20.7 (C), 19.4/19.3 (CH_2), 18.4/18.0 (CH), 14.3/14.2 (CH_2), 14.1/13.9 (CH_2); MS (CI): *m/z* (%): 542/540/538 (9/16/9) [$2M^+$ + NH_4], 281/279/277 (52/100/52) [M^+ + NH_4].

(1*R*,3*R*,4*S*)-4-(Tetrahydropyran-2-yloxymethyl)spiropentane-1-carboxylic acid [(1*R*,3*R*,4*S*)-17]: Under vigorous stirring, to a solution of (1*S*,3*R*,4*R*)-**16** (8.932 g, 34.2 mmol) in anhydrous diethyl ether (200 mL) was added dropwise a solution of *tert*-butyllithium (34.2 mmol, 22.8 mL of a 1.50 N solution in pentane) at –78 °C over a period of 1 h. After stirring

for an additional 1 h at the same temp., an excess of powdered carbon dioxide (ca. 10 g) was added in one portion, the reaction mixture was allowed to warm up to ambient temp. over a period of 2 h and thoroughly extracted with water (150 mL). The aqueous solution was washed with Et_2O (100 mL), acidified to pH ≈ 3 by adding 2 N aq. HCl solution (21 mL) at 0 °C and then extracted with Et_2O (5 × 50 mL). The combined organic extracts were dried and evaporated under reduced pressure to afford the acid (1*S*,3*R*,4*R*)-**17** (4.874 g, 63%) as a 1:1 mixture of two diastereomers (colorless oil) which was used without further purification.
^{1}H NMR (250 MHz, $CDCl_3$): δ = 8.65 (br. s, 1 H; OH), 4.69–4.65 (m, 1 H; OCHO), 3.89–3.81 (m, 1 H; CH_2O), 3.76–3.65 (m, 1 H; CH_2O), 3.56–3.43 (m, 2 H; CH_2O), 2.06–2.02 (m, 1 H; *c*Pr-H), 1.81–1.45 (m, 6 H), 1.42–1.37 (m, 1 H; *c*Pr-H), 1.27–1.18 (m, 3 H; *c*Pr-H), 0.96–0.91 (m, 1 H; *c*Pr-H); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 179.1/179.0 (C), 98.3/97.8 (CH), 69.8/69.4 (CH_2), 62.0/61.9 (CH_2), 30.4/30.3 (CH_2), 25.2 (CH_2), 22.8/22.4 (C), 19.7/19.6 (CH), 19.3/19.1 (CH_2), 16.5/16.2 (CH), 13.5/13.3 (CH_2), 12.0/11.9 (CH_2).

(1*S*,3*R*,4*R*)-[4-(Tetrahydropyran-2-yloxymethyl)spiropent-1-yl]methanol [(1*S*,3*R*,4*R*)-18]: A solution of the crude acid (1*S*,3*R*,4*R*)-**17** (2.05 g, 9.06 mmol) in anhydrous diethyl ether (15 mL) was added dropwise to a vigorously stirred suspension of $LiAlH_4$ (515 mg, 13.58 mmol) in Et_2O (20 mL) over a period of 1 h. After stirring for an additional 1 h at 34 °C, the reaction mixture was cooled to 10 °C, the reaction was quenched by adding sat. aq. Na_2SO_4 solution (2.5 mL), and the reaction mixture was stirred at 34 °C for 1 h. After being cooled to ambient temp., the reaction mixture was filtered, dried, filtered again and concentrated under reduced pressure to give the alcohol (1*S*,3*R*,4*R*)-**18** (1.923 g, 100%) as a 1:1 mixture of two diastereomers (colorless oil) which was used without further purification.
^{1}H NMR (250 MHz, $CDCl_3$): δ = 4.65 (t, *J* = 3.0 Hz, 0.5 H; OCHO), 4.58 (t, *J* = 3.0 Hz, 0.5 H; OCHO), 3.90 (dd, *J* = 6.0, 10.0 Hz, 0.5 H; CH_2O), 3.85–3.82 (m, 1 H; CH_2O), 3.81–3.58 (m, 2.5 H; CH_2O), 3.52–3.43 (m, 1.5 H; CH_2O), 3.19 (dd, *J* = 8.3, 10.0 Hz, 0.5 H; CH_2O), 1.80–1.68 (m, 2 H; *c*Pr-H), 1.67–1.40 (m, 6 H), 1.07–1.02 (m, 1 H; *c*Pr-H), 1.07–1.02 (m, 1 H; *c*Pr-H), 0.92–0.83 (m, 2 H; *c*Pr-H), 0.72–0.67 (m, 1 H; *c*Pr-H); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 98.6/98.0 (CH), 71.2/70.9 (CH_2), 64.2 (CH_2), 62.0/61.6 (CH_2), 30.3/30.2 (CH_2), 25.14/25.10 (CH_2), 19.2/18.9 (CH_2), 18.3/18.2 (CH), 17.4/17.3 (C), 14.3/14.2 (CH), 10.2 (CH_2), 7.2/7.1 (CH_2).

(1*R*,3*R*,4*S*)-(4-Hydroxymethylspiropent-1-yl)methanol [(1*R*,3*R*,4*S*)-19]: A solution of the crude monoprotected diol (1*S*,3*R*,4*R*)-**18** (1.923 g, 9.06 mmol) in methanol (40 mL) was

stirred with PPTS (228 mg, 0.906 mmol) 50 °C for 1.5 h. The reaction mixture was cooled to ambient temp. and, after addition of H_2O (0.8 mL), concentrated under reduced pressure. Column chromatography (100 g of silica gel, 2.8 × 40 cm column, hexane/THF 1:1, R_f = 0.22) of the residue afforded (1*R*,3*R*,4*S*)-**19** (1.138 g, 98%) as a colorless oil. ^{1}H NMR (250 MHz, $CDCl_3$): 3.75 (dd, *J* = 6.0, 11.3 Hz, 1 H; CH_2O), 3.70 (dd, *J* = 5.5, 11.3 Hz, 1 H; CH_2O), 3.61 (dd, *J* = 5.5, 10.8 Hz, 1 H; CH_2O), 3.45 (dd, *J* = 7.8, 10.8 Hz, 1 H; CH_2O), 1.73 (s, 2 H; 2 OH), 1.49–1.40 (m, 2 H, *c*Pr-H), 1.02 (dd, *J* = 4.3, 7.8 Hz, 1 H; *c*Pr-H), 0.90 (dd, *J* = 4.3, 7.8 Hz, 1 H; *c*Pr-H), 0.82 (t, *J* = 4.3 Hz, 1 H; *c*Pr-H), 0.67 (t, *J* = 4.3 Hz, 1 H; *c*Pr-H); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 66.0 (CH_2), 64.3 (CH_2), 18.2 (CH), 17.9 (C), 16.8 (CH), 9.9 (CH_2), 7.0 (CH_2); $[\alpha]_D^{20}$ = –26.2 (*c* = 0.875 in $CHCl_3$).

(1*R*,3*R*,4*S*-(4-Formylspiropent-1-yl)carbaldehyde[(1*R*,3*R*,4*S*-6]: Under vigorous stirring, a solution of anhydrous DMSO (0.36 mL) in anhydrous CH_2Cl_2 (4.5 mL) was added dropwise to a solution of oxalyl chloride (0.31 g, 2.46 mmol) in anhydrous CH_2Cl_2 (11 mL) at –78 °C, and the reaction mixture was stirred at this temperature for an additional 15 min. A solution of the diol (1*R*,3*R*,4*S*)-**19** (70 mg, 0.55 mmol) in a mixture of anhydrous DMSO (2 mL) and anhydrous CH_2Cl_2 (4.5 mL) was added dropwise at the same temp., and the reaction mixture was stirred at this temperature for an additional 1 h. After this, triethylamine (1.6 mL) was added dropwise, the mixture was allowed to warm up to r.t., and then water (10 mL) was added. The two phases were separated, the organic one was washed with 5% aq HCl, water, 5% aq $NaHCO_3$ solution, and water again (25 mL each), dried and concentrated under reduced pressure. This furnished 63 mg (93%) of (1*R*,3*R*,4*S*)-**6** as a yellow oil which was pure according to NMR spectrum. Due to its instability the crude product was used directly for further reaction; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.26 (d, *J* = 5.5 Hz, 1 H; CHO), δ = 9.06 (d, *J* = 5.8 Hz, 1 H; CHO) 2.37–2.23 (m, 2 H; CH(CHO)), 1.80–1.61 (m, 4 H; CH_2); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 199.8/199.5 (CHO), 27.0/26.9 (CH), 24.3 (C), 12.4/11.9 (CH_2); $[a]_D^{20}$ = 139 (*c* = 1 in CH_2Cl_2).

(1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-(9-Formylhexaspiro[2.0.0.0.0.0.2.1.1.1.1.1]pentadec-1-yl)carbaldehyde [(1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-7]: Under vigorous stirring, a solution of anhydrous DMSO (0.80 mL) in anhydrous CH_2Cl_2 (10 mL) was added dropwise to a solution of oxalyl chloride (0.697g, 5.46 mmol) in anhydrous CH_2Cl_2 (25 mL) at –78 °C, and the reaction mixture was stirred at this temperature for an additional 15 min. A solution of the diol (1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-**20** (330 mg, 1.277 mmol) in a mixture of anhydrous DMSO (4

mL) and anhydrous CH_2Cl_2 (10 mL) was added dropwise at the same temp., and the reaction mixture was stirred at this temperature for an additional 1 h. After this, triethylamine (3.54 mL) was added dropwise, the mixture was allowed to warm up to r.t., and then water (15 mL) was added. The two phases was separated, the organic one was washed with 5% aq HCl, water, 5% aq $NaHCO_3$ solution, and water again (50 mL each), dried and concentrated under reduced pressure. Column chromatography of the residue (10 g of silica gel, pentane/ether 4:1) furnished the dialdehyde (1*R*,3*S*,4*S*,5*S*,6*S*,7*S*,8*S*,9*R*)-**6** (0.280 g, 86%) as white solid which was pure according to its NMR spectra. Attempted recrystallization of **6** gave only 75 mg of crystals, and a part of the compound had decomposed. Repeated chromatography of the concentrated mother liquor gave an additional 173 mg of crystals (in total 0.208 g, i. e. 64% yield) with m.p. 100–102 °C (hexane-ether); $[\alpha]_D^{20}$ = –711.2, $[\alpha]_{578}^{20}$ = –741.7, $[\alpha]_{546}^{20}$ = –841.9, $[\alpha]_{436}^{20}$ = –1383.3, $[\alpha]_{365}^{20}$ = –1845.8 (*c* = 0.52 in $CHCl_3$); ^{1}H NMR (250 MHz, $CDCl_3$): δ = 9.01 (d, *J* = 6.6 Hz, 2 H, 2 CHO), 2.07–2.00 (m, 2 H, cPr-H), 1.63 (t, *J* = 4.4 Hz, 2 H, cPr-H), 1.55 (dd, *J* = 4.7, 7.5 Hz, 2 H, cPr-H), 1.38 (dd, *J* = 4.6, 8.1 Hz, 4 H, cPr-H), 1.29 (d, *J* = 4.3 Hz, 2 H, cPr-H), 1.10 (s, 2 H, cPr-H), 1.08 (d, *J* = 4.3 Hz, 2 H, cPr-H); ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 9.2 (0.5 intensity), 9.5, 10.6, (each –, cPr-C), 201.5 (2 CHO), 28.5 (2 CH), 22.1 (2 C), 18.3 (2 C), 16.2 (2 C), 12.5 (2 CH_2), 10.6 (2 CH_2), 9.5 (2 CH_2), 9.2 (CH_2).

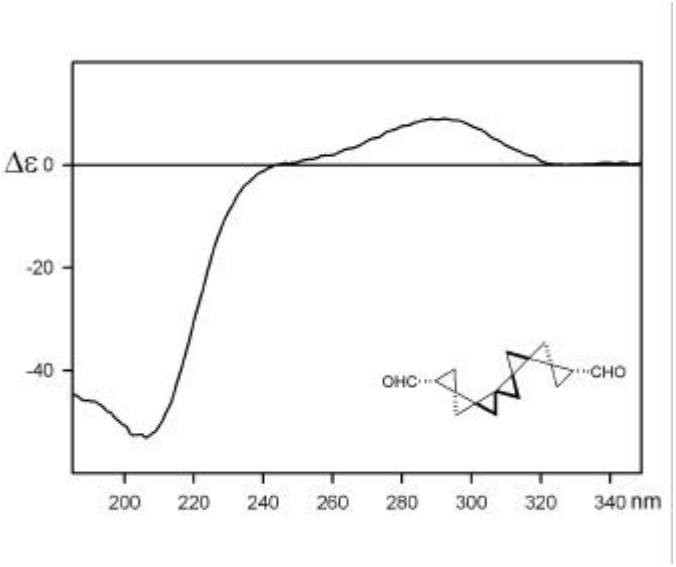


Figure A1. Measured in acetonitrile solution CD spectrum of dialdehyde **7**.

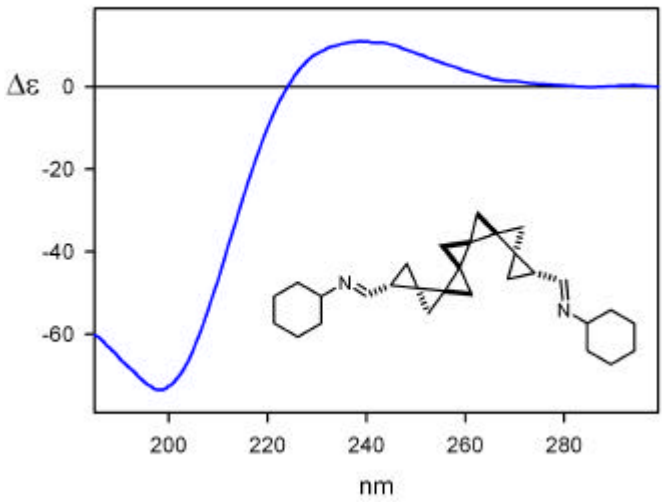


Figure A2. Measured in acetonitrile solution CD spectrum of diimine **11a**.

Computational Methods. In our computations all excited-state calculations have been performed at B3LYP/6-311++g(2d,2p) level based upon the ground state geometries of single model molecules with the use of a Gaussian program package.[7] Thus the results correspond to vertical transitions, and the excitation energies can be compared with the band maxima in the experimental spectra. Rotatory strengths were calculated using length and velocity representations. Length and velocity rotatory strengths are equal and origin-independent at the complete basis set limit. In the present study the differences between the length and velocity calculated values of rotatory strengths were quite small. The CD spectra were simulated by overlapping Gaussian functions for each transition according to the procedure described by Grimme *et al*. [8]

Dialdehydes **4-7** as well as model molecules **11b**, **12**, **13a-13d** were optimized at B3LYP/6-31g(d) level.

Macrocycles **8-10** were fully optimized with the use of PM3 Hamiltonian implemented in the gaussian package, additionally both conformers of macrocycle **10** were re-optimized at the B3LYP/6-31g(d) level. In all cases starting structures were those of the highest symmetry available for a given macrocycle. For all investigated structures frequency calculations were performed.

Table A1. Cartesian coordinates of the most stable conformer of **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.381384	2.840112	0.000000
2	6	0	-0.485557	1.329562	0.000000
3	6	0	0.180552	0.753089	1.269266
4	6	0	0.180552	-0.781701	1.268288
5	6	0	0.851293	-1.356586	0.000000
6	6	0	0.180552	-0.781701	-1.268288
7	6	0	0.180552	0.753089	-1.269266
8	1	0	0.666210	3.227732	0.000000
9	1	0	-1.553645	1.079129	0.000000
10	1	0	1.216008	1.119840	1.333458
11	1	0	-0.338680	1.122030	2.162213
12	1	0	0.691724	-1.150725	2.166434
13	1	0	-0.848334	-1.159443	1.312153
14	1	0	1.915152	-1.079027	0.000000
15	6	0	0.755232	-2.875002	0.000000
16	1	0	0.691724	-1.150725	-2.166434
17	1	0	-0.848334	-1.159443	-1.312153
18	1	0	1.216008	1.119840	-1.333458
19	1	0	-0.338680	1.122030	-2.162213
20	1	0	1.717452	-3.435308	0.000000
21	8	0	-1.319955	3.604867	0.000000
22	8	0	-0.299715	-3.472505	0.000000

Table A2. Cartesian coordinates of the most stable conformer of **5**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012143	-2.836471	0.000000
2	1	0	0.976988	-3.351619	0.000000
3	6	0	0.025955	-1.314456	0.000000
4	6	0	-0.713310	-0.783390	1.254751
5	1	0	-0.222220	-1.163349	2.158675
6	1	0	-1.731714	-1.184016	1.256933
7	6	0	-0.713310	0.772256	1.254945

8	1	0	-1.740452	1.157943	1.266510
9	1	0	-0.222172	1.156660	2.156555
10	6	0	0.029204	1.302572	0.000000
11	6	0	1.474744	0.774349	0.000000
12	1	0	2.003273	1.169095	-0.873892
13	1	0	2.003273	1.169095	0.873892
14	6	0	1.472390	-0.781084	0.000000
15	1	0	2.005138	-1.168109	0.878139
16	1	0	2.005138	-1.168109	-0.878139
17	6	0	-0.713310	-0.783390	-1.254751
18	1	0	-1.731714	-1.184016	-1.256933
19	1	0	-0.222220	-1.163349	-2.158675
20	6	0	-0.713310	0.772256	-1.254945
21	1	0	-0.222172	1.156660	-2.156555
22	1	0	-1.740452	1.157943	-1.266510
23	6	0	-0.023351	2.815821	0.000000
24	1	0	-1.056935	3.237402	0.000000
25	8	0	0.938882	3.552199	0.000000
26	8	0	-1.037021	-3.483826	0.000000

Table A3. Cartesian coordinates of the most stable conformer of **6**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.895414	1.457382	-0.923432
2	6	0	-1.123953	-0.041320	-0.615596
3	6	0	0.012360	0.750217	-0.019893
4	1	0	-0.911799	-0.748125	-1.417308
5	6	0	0.613312	0.935203	1.310246
6	6	0	1.495832	0.564598	0.097325
7	1	0	0.456418	0.168999	2.066413
8	1	0	0.729381	1.940811	1.703474
9	1	0	2.143029	1.334818	-0.312886
10	6	0	2.055940	-0.809730	0.048053
11	8	0	3.136765	-1.086206	-0.425364
12	1	0	1.404566	-1.595695	0.491575
13	6	0	-2.288993	-0.398429	0.244875
14	1	0	-2.509506	0.386175	1.017513
15	8	0	-2.928942	-1.425347	0.181084

16	1	0	-0.573101	1.699207	-1.929698
17	1	0	-1.616074	2.158701	-0.514303

Table A4. Cartesian coordinates of the most stable conformer of **7**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.306998	0.031811
2	6	0	-0.691508	4.562981	0.475209
3	6	0	0.617081	4.062631	1.129443
4	6	0	0.420280	2.709262	-1.283794
5	6	0	-0.397348	1.936694	-0.287786
6	1	0	-1.609179	4.471682	1.046408
7	6	0	-0.612628	5.759758	-0.391970
8	1	0	0.527697	3.692581	2.144243
9	1	0	1.517418	4.635426	0.928912
10	1	0	1.465969	2.443259	-1.404792
11	1	0	-0.072722	3.054797	-2.187339
12	6	0	-1.661664	1.124985	-0.299063
13	6	0	-0.399551	0.613007	0.338108
14	1	0	-1.973795	0.684823	-1.241280
15	1	0	-2.473335	1.438909	0.351064
16	6	0	0.000000	0.000000	1.652016
17	6	0	0.399551	-0.613007	0.338108
18	8	0	-1.491491	6.577064	-0.519331
19	1	0	0.349073	5.859264	-0.946035
20	1	0	-0.768373	-0.498358	2.235670
21	1	0	0.768373	0.498358	2.235670
22	6	0	1.661664	-1.124985	-0.299063
23	6	0	0.397348	-1.936694	-0.287786
24	1	0	2.473335	-1.438909	0.351064
25	1	0	1.973795	-0.684823	-1.241280
26	6	0	-0.420280	-2.709262	-1.283794
27	6	0	0.000000	-3.306998	0.031811
28	1	0	0.072722	-3.054797	-2.187339
29	1	0	-1.465969	-2.443259	-1.404792
30	6	0	-0.617081	-4.062631	1.129443
31	6	0	0.691508	-4.562981	0.475209
32	1	0	-1.517418	-4.635426	0.928912

33	1	0	-0.527697	-3.692581	2.144243
34	1	0	1.609179	-4.471682	1.046408
35	6	0	0.612628	-5.759758	-0.391970
36	8	0	1.491491	-6.577064	-0.519331
37	1	0	-0.349073	-5.859264	-0.946035

Table B1. Cartesian coordinates of calculated structure of macrocycle **8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.421667	-5.123365	-0.224105
2	6	0	8.147798	-3.865669	0.224105
3	6	0	7.427018	-2.619795	-0.264778
4	6	0	5.978196	-2.601177	0.241627
5	6	0	5.241783	-3.876682	-0.241627
6	6	0	5.982319	-5.122089	0.264778
7	1	0	7.448452	-5.201823	-1.329506
8	1	0	7.946743	-6.021074	0.155066
9	1	0	8.229137	-3.849637	1.329506
10	1	0	9.187774	-3.871544	-0.155066
11	1	0	7.964156	-1.715239	0.081729
12	1	0	7.451328	-2.580349	-1.372826
13	1	0	5.987062	-2.585060	1.364772
14	7	0	5.301491	-1.412202	-0.315719
15	7	0	3.873748	-3.885125	0.315719
16	1	0	5.232258	-3.892418	-1.364772
17	1	0	5.960312	-5.162865	1.372826
18	1	0	5.467519	-6.039542	-0.081729
19	6	0	4.779123	-0.514730	0.445231
20	6	0	4.089366	0.673427	-0.169924
21	6	0	2.626656	0.699998	0.278985
22	6	0	4.802134	1.953191	0.271583
23	6	0	4.092580	3.182174	-0.271583
24	6	0	2.627888	3.204782	0.169924
25	6	0	1.919544	1.924752	-0.278985
26	6	0	2.835331	-3.881477	-0.445231
27	6	0	1.461479	-3.878209	0.169924
28	6	0	0.709554	-5.135365	-0.271583
29	6	0	-0.709554	-5.135365	0.271583

30	6	0	-1.461479	-3.878209	-0.169924
31	6	0	-0.707112	-2.624750	0.278985
32	6	0	0.707112	-2.624750	-0.278985
33	1	0	4.797370	-0.560729	1.547527
34	1	0	4.116890	0.618223	-1.287339
35	1	0	2.106063	-0.227824	-0.049781
36	1	0	2.567854	0.698570	1.386373
37	1	0	4.848384	2.000560	1.378560
38	1	0	5.852929	1.939550	-0.076313
39	1	0	4.606164	4.099010	0.076313
40	1	0	4.156728	3.198544	-1.378560
41	1	0	2.593842	3.256220	1.287339
42	1	0	0.855730	1.937816	0.049781
43	1	0	1.888906	1.874542	-1.386373
44	1	0	2.884290	-3.874280	-1.547527
45	1	0	1.523048	-3.874443	1.287339
46	1	0	0.691656	-5.199104	-1.378560
47	1	0	1.246765	-6.038560	0.076313
48	1	0	-1.246765	-6.038560	-0.076313
49	1	0	-0.691656	-5.199104	1.378560
50	1	0	-1.523048	-3.874443	-1.287339
51	6	0	-2.835331	-3.881477	0.445231
52	1	0	-1.250333	-1.709992	-0.049781
53	1	0	-0.678948	-2.573112	1.386373
54	1	0	0.678948	-2.573112	-1.386373
55	1	0	1.250333	-1.709992	0.049781
56	7	0	-3.873748	-3.885125	-0.315719
57	6	0	-5.241783	-3.876682	0.241627
58	6	0	-5.982319	-5.122089	-0.264778
59	6	0	-5.978196	-2.601177	-0.241627
60	6	0	-7.421667	-5.123365	0.224105
61	6	0	-8.147798	-3.865669	-0.224105
62	6	0	-7.427018	-2.619795	0.264778
63	1	0	-2.884290	-3.874280	1.547527
64	1	0	-5.232258	-3.892418	1.364772
65	1	0	-5.960312	-5.162865	-1.372826
66	1	0	-5.467519	-6.039542	0.081729
67	7	0	-5.301491	-1.412202	0.315719
68	1	0	-5.987062	-2.585060	-1.364772
69	1	0	-7.946743	-6.021074	-0.155066
70	1	0	-7.448452	-5.201823	1.329506

71	1	0	-8.229137	-3.849637	-1.329506
72	1	0	-9.187774	-3.871544	0.155066
73	1	0	-7.964156	-1.715239	-0.081729
74	1	0	-7.451328	-2.580349	1.372826
75	6	0	-4.779123	-0.514730	-0.445231
76	6	0	-4.089366	0.673427	0.169924
77	6	0	-4.802134	1.953191	-0.271583
78	6	0	-4.092580	3.182174	0.271583
79	6	0	-2.627888	3.204782	-0.169924
80	6	0	-1.919544	1.924752	0.278985
81	6	0	-2.626656	0.699998	-0.278985
82	1	0	-4.797370	-0.560729	-1.547527
83	1	0	-4.116890	0.618223	1.287339
84	1	0	-4.848384	2.000560	-1.378560
85	1	0	-5.852929	1.939550	0.076313
86	1	0	-4.606164	4.099010	-0.076313
87	1	0	-4.156728	3.198544	1.378560
88	1	0	-2.593842	3.256220	-1.287339
89	6	0	-1.943792	4.396207	0.445231
90	1	0	-0.855730	1.937816	-0.049781
91	1	0	-1.888906	1.874542	1.386373
92	1	0	-2.567854	0.698570	-1.386373
93	1	0	-2.106063	-0.227824	0.049781
94	7	0	-1.427743	5.297327	-0.315719
95	6	0	-0.736413	6.477858	0.241627
96	6	0	-1.444700	7.741884	-0.264778
97	6	0	-0.726131	8.989035	0.224105
98	6	0	0.726131	8.989035	-0.224105
99	6	0	1.444700	7.741884	0.264778
100	6	0	0.736413	6.477858	-0.241627
101	1	0	-1.913079	4.435009	1.547527
102	1	0	-0.754804	6.477478	1.364772
103	1	0	-1.491016	7.743214	-1.372826
104	1	0	-2.496637	7.754782	0.081729
105	1	0	-1.241032	9.892618	-0.155066
106	1	0	-0.780685	9.051460	1.329506
107	1	0	0.780685	9.051460	-1.329506
108	1	0	1.241032	9.892618	0.155066
109	1	0	2.496637	7.754782	-0.081729
110	1	0	1.491016	7.743214	1.372826
111	1	0	0.754804	6.477478	-1.364772

112	7	0	1.427743	5.297327	0.315719
113	6	0	1.943792	4.396207	-0.445231
114	1	0	1.913079	4.435009	-1.547527

Table B2. Cartesian coordinates of calculated structure of macrocycle **9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.988342	8.709200	-0.375952
2	6	0	-2.337009	8.483969	0.288513
3	6	0	-2.895401	7.112473	-0.057790
4	6	0	-1.909062	6.013799	0.357800
5	6	0	-0.554226	6.239845	-0.364549
6	6	0	0.000000	7.619915	0.010218
7	1	0	-1.110383	8.738195	-1.477358
8	1	0	-0.585328	9.699988	-0.090854
9	1	0	-2.237902	8.587447	1.387751
10	1	0	-3.050037	9.270357	-0.025354
11	1	0	-3.869134	6.964054	0.448530
12	1	0	-3.108386	7.052782	-1.144397
13	1	0	-1.747332	6.074854	1.467564
14	7	0	-2.471598	4.702029	-0.028250
15	7	0	0.391537	5.195415	0.078016
16	1	0	-0.718625	6.206183	-1.475423
17	1	0	0.213992	7.671088	1.097090
18	1	0	0.968904	7.793934	-0.497413
19	6	0	-2.357324	3.677913	0.745235
20	6	0	-2.890164	2.322988	0.337732
21	6	0	-2.146759	1.799710	-0.901957
22	6	0	-4.394047	2.385134	0.029438
23	6	0	-4.907839	1.006052	-0.381019
24	6	0	-3.773464	-0.027811	-0.305728
25	6	0	-2.638667	0.398557	-1.255462
26	6	0	0.963124	4.406674	-0.763210
27	6	0	1.862647	3.281821	-0.305728
28	6	0	3.325186	3.747287	-0.381019
29	6	0	4.262610	2.612789	0.029438
30	6	0	3.456849	1.341461	0.337732
31	6	0	2.631974	0.959293	-0.901957

32	6	0	1.664494	2.085874	-1.255462
33	1	0	-1.849298	3.728464	1.725130
34	1	0	-2.302056	2.491276	-1.752560
35	1	0	-1.047745	1.793438	-0.717502
36	1	0	-4.940259	2.754566	0.918634
37	1	0	-4.586645	3.123860	-0.772460
38	1	0	-5.745214	0.692620	0.271536
39	1	0	-5.319540	1.033615	-1.408534
40	1	0	-1.808800	-0.342046	-1.190366
41	1	0	-2.986691	0.368053	-2.306388
42	1	0	0.824949	4.497295	-1.855288
43	1	0	3.554907	4.090049	-1.408534
44	1	0	3.472434	4.629191	0.271536
45	1	0	4.998665	2.410221	-0.772460
46	1	0	4.855654	2.901107	0.918634
47	6	0	4.363828	0.202546	0.745235
48	1	0	3.308536	0.748001	-1.752560
49	1	0	2.077035	0.010655	-0.717502
50	1	0	1.812089	2.402524	-2.306388
51	1	0	0.608180	1.737490	-1.190366
52	7	0	5.307876	-0.210548	-0.028250
53	6	0	6.162634	-1.353603	0.357800
54	6	0	7.607283	-1.048746	-0.057790
55	6	0	5.680977	-2.639949	-0.364549
56	6	0	8.515837	-2.218075	0.288513
57	6	0	8.036559	-3.498671	-0.375952
58	6	0	6.599040	-3.809958	0.010218
59	1	0	4.153594	-0.262693	1.725130
60	1	0	6.134644	-1.524193	1.467564
61	1	0	7.662081	-0.834450	-1.144397
62	1	0	7.965615	-0.131259	0.448530
63	7	0	4.303593	-2.936789	0.078016
64	1	0	5.734025	-2.480744	-1.475423
65	1	0	9.553383	-1.993769	-0.025354
66	1	0	8.555898	-2.355644	1.387751
67	1	0	8.122690	-3.407478	-1.477358
68	1	0	8.693100	-4.343085	-0.090854
69	1	0	6.265293	-4.736063	-0.497413
70	1	0	6.536361	-4.020867	1.097090
71	6	0	3.334730	-3.037427	-0.763210
72	6	0	1.910817	-3.254010	-0.305728

73	6	0	1.582653	-4.753339	-0.381019
74	6	0	0.131437	-4.997923	0.029438
75	6	0	-0.566685	-3.664449	0.337732
76	6	0	-0.485215	-2.759003	-0.901957
77	6	0	0.974173	-2.484431	-1.255462
78	1	0	3.482297	-2.963074	-1.855288
79	1	0	1.764633	-5.123664	-1.408534
80	1	0	2.272780	-5.321811	0.271536
81	1	0	-0.412020	-5.534081	-0.772460
82	1	0	0.084605	-5.655673	0.918634
83	6	0	-2.006504	-3.880459	0.745235
84	1	0	-1.006480	-3.239277	-1.752560
85	1	0	-1.029290	-1.804093	-0.717502
86	1	0	1.174602	-2.770577	-2.306388
87	1	0	1.200620	-1.395444	-1.190366
88	7	0	-2.836278	-4.491481	-0.028250
89	6	0	-4.253572	-4.660196	0.357800
90	6	0	-4.711882	-6.063727	-0.057790
91	6	0	-6.178828	-6.265894	0.288513
92	6	0	-7.048217	-5.210529	-0.375952
93	6	0	-6.599040	-3.809958	0.010218
94	6	0	-5.126751	-3.599896	-0.364549
95	1	0	-2.304296	-3.465771	1.725130
96	1	0	-4.387312	-4.550661	1.467564
97	1	0	-4.553695	-6.218332	-1.144397
98	1	0	-4.096481	-6.832795	0.448530
99	1	0	-6.503346	-7.276588	-0.025354
100	1	0	-6.317996	-6.231804	1.387751
101	1	0	-7.012307	-5.330717	-1.477358
102	1	0	-8.107772	-5.356903	-0.090854
103	1	0	-7.234197	-3.057872	-0.497413
104	1	0	-6.750353	-3.650222	1.097090
105	1	0	-5.015400	-3.725439	-1.475423
106	7	0	-4.695130	-2.258627	0.078016
107	6	0	-4.297854	-1.369247	-0.763210
108	1	0	-4.307246	-1.534221	-1.855288
109	6	0	1.564744	2.807524	1.124298
110	1	0	1.698420	3.643579	1.837737
111	1	0	0.498993	2.507738	1.207629
112	6	0	2.481965	1.642611	1.490668
113	1	0	1.887070	0.735243	1.721027

114	1	0	3.049203	1.872418	2.413500
115	6	0	1.649015	-2.758870	1.124298
116	1	0	2.306222	-3.292664	1.837737
117	1	0	1.922268	-1.686010	1.207629
118	6	0	0.181560	-2.970750	1.490668
119	1	0	-0.306796	-2.001872	1.721027
120	1	0	0.096960	-3.576896	2.413500
121	6	0	-2.663525	1.328139	1.490668
122	1	0	-1.580274	1.266629	1.721027
123	1	0	-3.146163	1.704478	2.413500
124	6	0	-3.213759	-0.048654	1.124298
125	1	0	-4.004642	-0.350915	1.837737
126	1	0	-2.421261	-0.821728	1.207629

Table B3. Cartesian coordinates of calculated structures of macrocycle **10**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.994569	7.524480	-0.508452
2	1	0	-1.211305	7.320545	-1.572803
3	6	0	-2.324146	7.383031	0.274812
4	1	0	-2.072209	7.419030	1.350301
5	6	0	-3.302170	8.528747	-0.060381
6	1	0	-4.196140	8.415854	0.565472
7	1	0	-3.633587	8.397222	-1.099284
8	6	0	-2.685139	9.920118	0.113723
9	1	0	-2.439200	10.090286	1.172176
10	1	0	-3.416387	10.689319	-0.165330
11	6	0	-1.412043	10.051807	-0.730128
12	1	0	-0.948117	11.035394	-0.582658
13	1	0	-1.673945	9.985192	-1.796301
14	6	0	-0.411354	8.948307	-0.370566
15	1	0	0.487048	9.016084	-0.996755
16	1	0	-0.075294	9.076206	0.667333
17	7	0	0.005034	6.607583	0.028208
18	6	0	0.605711	5.813984	-0.764383
19	1	0	0.347018	5.739364	-1.835478
20	6	0	1.724336	4.962173	-0.299068
21	1	0	2.036582	5.172493	0.721744

22	6	0	2.829151	4.559229	-1.297116
23	1	0	3.853218	4.567950	-0.930843
24	1	0	2.715331	4.898913	-2.325359
25	6	0	1.886175	3.549665	-0.777228
26	6	0	0.963322	2.478094	-1.284356
27	1	0	1.219172	1.991771	-2.225262
28	1	0	-0.104890	2.584815	-1.110395
29	6	0	1.883939	2.241423	-0.115513
30	6	0	1.815579	1.761010	1.310354
31	1	0	0.990858	1.116500	1.610987
32	1	0	2.157414	2.446961	2.085289
33	6	0	2.818642	1.205196	0.338096
34	7	0	-2.988662	6.136080	-0.083435
35	6	0	-3.177696	5.256482	0.815461
36	1	0	-2.809563	5.378912	1.849123
37	6	0	-3.910874	4.003020	0.524076
38	1	0	-4.451827	4.016655	-0.419747
39	6	0	-4.520181	3.184240	1.675621
40	1	0	-5.485840	2.717921	1.493973
41	1	0	-4.390042	3.571128	2.685211
42	6	0	-3.333160	2.686041	0.951626
43	6	0	-1.937179	2.209278	1.226882
44	1	0	-1.749265	1.691812	2.167152
45	1	0	-1.107258	2.819783	0.878267
46	6	0	-2.829151	1.515041	0.229185
47	6	0	-2.808234	1.066377	-1.209273
48	1	0	-1.850873	0.885937	-1.695903
49	1	0	-3.578670	1.468863	-1.866623
50	6	0	-3.214279	0.137690	-0.098794
51	6	0	-4.282469	-0.864817	0.247564
52	1	0	-4.859979	-1.310904	-0.561248
53	1	0	-4.841155	-0.715471	1.170709
54	6	0	3.214279	-0.137690	-0.098794
55	6	0	4.282469	0.864817	0.247564
56	6	0	-2.818642	-1.205196	0.338096
57	6	0	2.829151	-1.515041	0.229185
58	6	0	2.808234	-1.066377	-1.209273
59	1	0	4.841155	0.715471	1.170709
60	1	0	4.859979	1.310904	-0.561248
61	6	0	-1.883939	-2.241423	-0.115513
62	6	0	-1.815579	-1.761010	1.310354

63	6	0	3.333160	-2.686041	0.951626
64	6	0	1.937179	-2.209278	1.226882
65	1	0	1.850873	-0.885937	-1.695903
66	1	0	3.578670	-1.468863	-1.866623
67	6	0	-1.886175	-3.549665	-0.777228
68	6	0	-0.963322	-2.478094	-1.284356
69	1	0	-0.990858	-1.116500	1.610987
70	1	0	-2.157414	-2.446961	2.085289
71	6	0	3.910874	-4.003020	0.524076
72	6	0	4.520181	-3.184240	1.675621
73	1	0	1.749265	-1.691812	2.167152
74	1	0	1.107258	-2.819783	0.878267
75	6	0	-1.724336	-4.962173	-0.299068
76	6	0	-2.829151	-4.559229	-1.297116
77	1	0	-1.219172	-1.991771	-2.225262
78	1	0	0.104890	-2.584815	-1.110395
79	6	0	3.177696	-5.256482	0.815461
80	1	0	4.451827	-4.016655	-0.419747
81	1	0	5.485840	-2.717921	1.493973
82	1	0	4.390042	-3.571128	2.685211
83	6	0	-0.605711	-5.813984	-0.764383
84	1	0	-2.036582	-5.172493	0.721744
85	1	0	-3.853218	-4.567950	-0.930843
86	1	0	-2.715331	-4.898913	-2.325359
87	7	0	2.988662	-6.136080	-0.083435
88	1	0	2.809563	-5.378912	1.849123
89	7	0	-0.005034	-6.607583	0.028208
90	1	0	-0.347018	-5.739364	-1.835478
91	6	0	2.324146	-7.383031	0.274812
92	6	0	0.994569	-7.524480	-0.508452
93	1	0	2.072209	-7.419030	1.350301
94	6	0	3.302170	-8.528747	-0.060381
95	1	0	1.211305	-7.320545	-1.572803
96	6	0	0.411354	-8.948307	-0.370566
97	1	0	4.196140	-8.415854	0.565472
98	1	0	3.633587	-8.397222	-1.099284
99	6	0	2.685139	-9.920118	0.113723
100	6	0	1.412043	-10.051807	-0.730128
101	1	0	-0.487048	-9.016084	-0.996755
102	1	0	0.075294	-9.076206	0.667333
103	1	0	2.439200	-10.090286	1.172176

104	1	0	3.416387	-10.689319	-0.165330
105	1	0	0.948117	-11.035394	-0.582658
106	1	0	1.673945	-9.985192	-1.796301

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.682338	7.626052	-0.681562
2	1	0	-0.391117	7.698955	-0.428944
3	6	0	1.461746	7.497672	0.651358
4	1	0	2.509305	7.252962	0.397926
5	6	0	1.426795	8.816156	1.454916
6	1	0	2.047182	8.691320	2.351144
7	1	0	0.398539	8.969285	1.809508
8	6	0	1.880234	10.032541	0.641600
9	1	0	2.939982	9.924888	0.367629
10	1	0	1.805964	10.939023	1.255692
11	6	0	1.038764	10.170445	-0.632542
12	1	0	1.381460	11.022114	-1.233843
13	1	0	-0.005445	10.380227	-0.357903
14	6	0	1.110166	8.885814	-1.464894
15	1	0	0.483168	8.965394	-2.361686
16	1	0	2.138099	8.730219	-1.819196
17	7	0	0.962391	6.479087	-1.537254
18	6	0	0.000000	5.741731	-1.922243
19	1	0	-1.038896	5.899612	-1.583168
20	6	0	0.219622	4.627224	-2.872805
21	1	0	1.211887	4.623089	-3.319140
22	6	0	-0.944821	4.129811	-3.750353
23	1	0	-0.710539	3.864174	-4.778699
24	1	0	-1.908881	4.619139	-3.620180
25	6	0	-0.425142	3.290748	-2.652210
26	6	0	-0.923101	2.546586	-1.447065
27	1	0	-1.934355	2.142093	-1.480679
28	1	0	-0.608992	2.885223	-0.462505
29	6	0	0.089198	1.943770	-2.386995
30	6	0	1.455382	1.310260	-2.340773
31	1	0	1.792533	0.844657	-1.415994
32	1	0	2.245622	1.789240	-2.918605

33	6	0	0.310836	0.664258	-3.070779
34	6	0	0.000000	0.000000	-4.385527
35	1	0	0.824346	-0.399011	-4.975397
36	1	0	-0.824346	0.399011	-4.975397
37	7	0	0.854226	6.475339	1.494689
38	6	0	1.572190	5.511209	1.910769
39	1	0	2.623615	5.379898	1.599581
40	6	0	1.040046	4.510177	2.863574
41	1	0	0.076972	4.780903	3.291237
42	6	0	2.012361	3.724120	3.763711
43	1	0	1.699511	3.541443	4.789249
44	1	0	3.074812	3.932463	3.647459
45	6	0	1.300074	3.046766	2.662073
46	6	0	1.586962	2.184109	1.467146
47	1	0	2.446863	1.516514	1.515045
48	1	0	1.388456	2.587976	0.477132
49	6	0	0.439484	1.890206	2.399043
50	6	0	-1.047057	1.648898	2.348077
51	1	0	-1.494511	1.285269	1.424203
52	1	0	-1.680650	2.327636	2.918821
53	6	0	-0.122046	0.722826	3.087627
54	6	0	0.000000	0.000000	4.402511
55	1	0	-0.900755	-0.165732	4.992278
56	1	0	0.900755	0.165732	4.992278
57	6	0	-0.310836	-0.664258	-3.070779
58	6	0	0.122046	-0.722826	3.087627
59	6	0	-0.089198	-1.943770	-2.386995
60	6	0	-1.455382	-1.310260	-2.340773
61	6	0	-0.439484	-1.890206	2.399043
62	6	0	1.047057	-1.648898	2.348077
63	6	0	0.425142	-3.290748	-2.652210
64	6	0	0.923101	-2.546586	-1.447065
65	1	0	-1.792533	-0.844657	-1.415994
66	1	0	-2.245622	-1.789240	-2.918605
67	6	0	-1.300074	-3.046766	2.662073
68	6	0	-1.586962	-2.184109	1.467146
69	1	0	1.680650	-2.327636	2.918821
70	1	0	1.494511	-1.285269	1.424203
71	6	0	-0.219622	-4.627224	-2.872805
72	6	0	0.944821	-4.129811	-3.750353
73	1	0	1.934355	-2.142093	-1.480679

74	1	0	0.608992	-2.885223	-0.462505
75	6	0	-1.040046	-4.510177	2.863574
76	6	0	-2.012361	-3.724120	3.763711
77	1	0	-2.446863	-1.516514	1.515045
78	1	0	-1.388456	-2.587976	0.477132
79	6	0	0.000000	-5.741731	-1.922243
80	1	0	-1.211887	-4.623089	-3.319140
81	1	0	0.710539	-3.864174	-4.778699
82	1	0	1.908881	-4.619139	-3.620180
83	6	0	-1.572190	-5.511209	1.910769
84	1	0	-0.076972	-4.780903	3.291237
85	1	0	-1.699511	-3.541443	4.789249
86	1	0	-3.074812	-3.932463	3.647459
87	7	0	-0.962391	-6.479087	-1.537254
88	1	0	1.038896	-5.899612	-1.583168
89	7	0	-0.854226	-6.475339	1.494689
90	1	0	-2.623615	-5.379898	1.599581
91	6	0	-0.682338	-7.626052	-0.681562
92	6	0	-1.461746	-7.497672	0.651358
93	1	0	0.391117	-7.698955	-0.428944
94	6	0	-1.110166	-8.885814	-1.464894
95	1	0	-2.509305	-7.252962	0.397926
96	6	0	-1.426795	-8.816156	1.454916
97	6	0	-1.038764	-10.170445	-0.632542
98	1	0	-0.483168	-8.965394	-2.361686
99	1	0	-2.138099	-8.730219	-1.819196
100	1	0	-2.047182	-8.691320	2.351144
101	1	0	-0.398539	-8.969285	1.809508
102	6	0	-1.880234	-10.032541	0.641600
103	1	0	-1.381460	-11.022114	-1.233843
104	1	0	0.005445	-10.380227	-0.357903
105	1	0	-2.939982	-9.924888	0.367629
106	1	0	-1.805964	-10.939023	1.255692

Table B3. Cartesian coordinates of calculated structures of model compounds **11b, 12** and **13a-13d**

11b

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	0.664647	3.239519	0.193668
2	6	0	0.239679	4.608854	0.637066
3	6	0	1.421004	3.855711	1.291300
4	6	0	0.956217	2.569510	-1.121937
5	6	0	0.000000	1.977035	-0.125929
6	1	0	-0.677616	4.703853	1.208265
7	6	0	0.557479	5.765357	-0.230113
8	1	0	1.259071	3.511176	2.306100
9	1	0	2.418092	4.235866	1.090769
10	1	0	1.927107	2.098771	-1.242935
11	1	0	0.542721	3.007079	-2.025482
12	6	0	-1.401656	1.435994	-0.137206
13	6	0	-0.268195	0.680801	0.499965
14	1	0	-1.795883	1.067547	-1.079423
15	1	0	-2.133672	1.906644	0.512921
16	6	0	0.000000	0.000000	1.813873
17	6	0	0.268195	-0.680801	0.499965
18	1	0	1.519556	5.669549	-0.784178
19	1	0	-0.852855	-0.333760	2.397527
20	1	0	0.852855	0.333760	2.397527
21	6	0	1.401656	-1.435994	-0.137206
22	6	0	0.000000	-1.977035	-0.125929
23	1	0	2.133672	-1.906644	0.512921
24	1	0	1.795883	-1.067547	-1.079423
25	6	0	-0.956217	-2.569510	-1.121937
26	6	0	-0.664647	-3.239519	0.193668
27	1	0	-0.542721	-3.007079	-2.025482
28	1	0	-1.927107	-2.098771	-1.242935
29	6	0	-1.421004	-3.855711	1.291300
30	6	0	-0.239679	-4.608854	0.637066
31	1	0	-2.418092	-4.235866	1.090769
32	1	0	-1.259071	-3.511176	2.306100
33	1	0	0.677616	-4.703853	1.208265
34	6	0	-0.557479	-5.765357	-0.230113
35	1	0	-1.519556	-5.669549	-0.784178
36	7	0	0.189232	-6.812824	-0.366623
37	7	0	-0.189232	6.812824	-0.366623
38	6	0	0.189612	7.802519	-1.182970
39	1	0	0.291683	8.708072	-0.622207

40	1	0	1.127975	7.554081	-1.633142
41	1	0	-0.547791	7.937040	-1.946541
42	6	0	-0.189612	-7.802519	-1.182970
43	1	0	-0.291683	-8.708072	-0.622207
44	1	0	-1.127975	-7.554081	-1.633142
45	1	0	0.547791	-7.937040	-1.946541

12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.644504	0.416436	2.998165
2	6	0	0.644504	-0.416436	2.998165
3	6	0	0.750917	-1.269061	1.726800
4	6	0	0.650513	-0.419486	0.445987
5	6	0	-0.650513	0.419486	0.445987
6	6	0	-0.750917	1.269061	1.726800
7	1	0	-0.684603	1.061924	3.884635
8	1	0	-1.511611	-0.257043	3.062597
9	1	0	0.684603	-1.061924	3.884635
10	1	0	1.511611	0.257043	3.062597
11	1	0	-0.051586	-2.018788	1.707966
12	1	0	1.696821	-1.824738	1.709701
13	1	0	1.498696	0.288620	0.413668
14	7	0	0.650513	-1.305943	-0.710493
15	7	0	-0.650513	1.305943	-0.710493
16	1	0	-1.498696	-0.288620	0.413668
17	1	0	-1.696821	1.824738	1.709701
18	1	0	0.051586	2.018788	1.707966
19	6	0	1.582876	-1.181072	-1.563398
20	6	0	-1.582876	1.181072	-1.563398
21	6	0	-1.673520	2.050178	-2.783916
22	6	0	1.673520	-2.050178	-2.783916
23	1	0	2.376626	-0.422653	-1.447557
24	1	0	-2.376626	0.422653	-1.447557
25	1	0	-0.846767	2.764460	-2.804142
26	1	0	-1.646312	1.438734	-3.695648
27	1	0	-2.625081	2.598122	-2.799600
28	1	0	0.846767	-2.764460	-2.804142

29	1	0	1.646312	-1.438734	-3.695648
30	1	0	2.625081	-2.598122	-2.799600

13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.585429	-0.542569	-0.656165
2	6	0	-1.925735	-1.170623	0.570118
3	6	0	-1.431188	0.114003	0.007917
4	1	0	-1.331997	-2.069514	0.419031
5	1	0	-2.474161	-1.149320	1.509494
6	6	0	-1.070567	1.454605	0.507124
7	6	0	-0.111538	0.678075	-0.419406
8	1	0	-0.776215	1.565245	1.549475
9	1	0	-1.557913	2.329409	0.082366
10	1	0	-0.019503	1.035589	-1.442291
11	6	0	1.138361	0.128843	0.146499
12	1	0	1.074164	-0.231460	1.189734
13	1	0	-2.427325	-1.024198	-1.618612
14	1	0	-3.572248	-0.101412	-0.532012
15	7	0	2.216624	0.070710	-0.524844
16	6	0	3.388069	-0.487198	0.124671
17	1	0	4.191579	0.259918	0.126137
18	1	0	3.212981	-0.817127	1.163412
19	1	0	3.752434	-1.342923	-0.457368

13b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.344356	-0.032811	-0.242596
2	6	0	-2.599002	-1.313160	-0.617540
3	6	0	-1.939369	-0.254223	0.189700
4	1	0	-2.294888	-1.440083	-1.654548
5	1	0	-2.893201	-2.236163	-0.122522

6	6	0	-1.148235	-0.170931	1.463845
7	6	0	-0.674666	0.483674	0.193962
8	1	0	-0.630273	-1.065880	1.806642
9	1	0	-1.519310	0.469589	2.263260
10	6	0	-0.151162	1.800297	-0.219940
11	6	0	0.590881	0.505246	-0.609755
12	1	0	0.316884	2.437943	0.528156
13	1	0	-0.648763	2.341001	-1.022249
14	1	0	0.532940	0.197263	-1.651329
15	6	0	1.879228	0.194276	0.043549
16	1	0	1.970434	0.511898	1.098700
17	1	0	-3.537441	0.692652	-1.030470
18	1	0	-4.134978	-0.103944	0.501489
19	7	0	2.820132	-0.405079	-0.566580
20	6	0	4.043837	-0.666150	0.168083
21	1	0	4.028473	-0.306362	1.211497
22	1	0	4.239671	-1.745702	0.173649
23	1	0	4.886609	-0.193973	-0.352061

13c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.454266	-0.737971	0.045054
2	6	0	3.904865	-0.279192	-1.275995
3	6	0	3.231365	0.066966	0.023085
4	1	0	3.433806	-1.020235	-1.914666
5	1	0	4.437643	0.507358	-1.802787
6	6	0	2.698615	1.304449	0.691356
7	6	0	1.881735	0.045915	0.588532
8	1	0	2.423643	2.144958	0.061002
9	1	0	3.099800	1.572701	1.664239
10	6	0	1.070448	-0.818354	1.513675
11	6	0	0.523485	-0.338151	0.199244
12	1	0	0.678258	-0.369865	2.422008
13	1	0	1.337754	-1.867230	1.599386
14	6	0	-0.180239	-0.941328	-0.983279
15	6	0	-0.701904	0.289758	-0.292604
16	1	0	-0.709879	-1.877674	-0.836384

17	1	0	0.267491	-0.816548	-1.964519
18	6	0	-1.201360	1.618469	-0.668951
19	6	0	-2.012101	0.723621	0.296824
20	1	0	-1.608305	1.761497	-1.665371
21	1	0	-0.747937	2.499613	-0.229932
22	1	0	-2.038021	1.004328	1.344324
23	6	0	-3.257897	0.110921	-0.216097
24	1	0	-3.229649	-0.140341	-1.301374
25	7	0	-4.308452	-0.133796	0.497939
26	6	0	-5.383376	-0.697016	-0.064879
27	1	0	-5.191990	-0.872047	-1.102971
28	1	0	-5.594232	-1.626902	0.420663
29	1	0	-6.223716	-0.042607	0.037484
30	1	0	4.321524	-1.776339	0.266578
31	1	0	5.335569	-0.232629	0.380961

13d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.458294	-0.385029	-0.126075
2	6	0	-5.813097	0.168039	0.206948
3	6	0	-5.226923	0.217061	-1.223008
4	6	0	-3.716186	-1.666419	0.142360
5	6	0	-3.118289	-0.324122	0.455681
6	1	0	-5.867527	1.097851	0.763014
7	1	0	-4.950270	1.199437	-1.587900
8	1	0	-5.680843	-0.434872	-1.963181
9	1	0	-3.329426	-2.212794	-0.712482
10	1	0	-4.040617	-2.284962	0.973617
11	6	0	-2.450396	0.333179	1.630145
12	6	0	-1.856398	0.389450	0.249915
13	1	0	-1.973551	-0.306752	2.366385
14	1	0	-2.901106	1.236381	2.031531
15	6	0	-1.309557	1.445220	-0.671002
16	6	0	-0.554703	0.176508	-0.384058
17	1	0	-0.945390	2.367638	-0.228353
18	1	0	-1.766126	1.555366	-1.650197
19	6	0	0.140170	-0.894464	-1.178544

20	6	0	0.806277	-0.217212	-0.014447
21	1	0	0.487954	-0.647502	-2.177584
22	1	0	-0.187507	-1.921443	-1.048614
23	6	0	1.561858	-0.636990	1.214493
24	6	0	2.095685	0.409106	0.273507
25	1	0	2.029335	-1.616941	1.213855
26	1	0	1.194254	-0.304677	2.180567
27	6	0	2.690541	1.748877	0.361400
28	6	0	3.380290	0.640470	-0.467126
29	1	0	3.176208	2.046042	1.285919
30	1	0	2.253228	2.561821	-0.206602
31	1	0	3.344291	0.721186	-1.548288
32	6	0	4.626283	0.052637	0.073662
33	1	0	4.664275	0.007906	1.186458
34	7	0	5.607486	-0.387483	-0.645320
35	6	0	6.689552	-0.906438	-0.054339
36	1	0	6.565632	-0.874437	1.007979
37	1	0	6.815123	-1.921586	-0.368357
38	1	0	7.553426	-0.338394	-0.329924
39	1	0	-6.614642	-0.516114	0.392314

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