Electronic supporting information

Chiral hydrogen-bonded supramolecular capsules: Synthesis, characterization and complexation of C_{70}

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1. General information

1.1. Analytical methods

Melting points were measured with a Büchi Melting-Point B-540 apparatus with open end glass capillary tubes.

IR spectra were measured on a Jasco FT/IR-430 spectrometer.

NMR spectra were recorded with a Bruker DMX 300 spectrometer [^{1}H: 300 MHz, ^{13}C: 75.5 MHz, ^{31}P: 121.5 MHz] or with a Bruker DMX 600 spectrometer [^{1}H: 600 MHz, ^{13}C: 151 MHz, ^{31}P: 243 MHz]. All measurements were performed at room temperature, using [D_1]-chloroform, [D_6]-dimethylsulfoxide or [D_4]-methanol as solvents. The chemical shifts are referenced relative to the residual proton signals of the solvents in the ^{1}H-NMR ([D_1]-chloroform: δ = 7.24 ppm, [D_4]-methanol: δ = 3.31 ppm, [D_6]-dimethylsulfoxide: δ = 2.50 ppm) or relative to the solvent signal in the ^{13}C-NMR ([D_1-chloroform: δ = 77.16 ppm, [D_4]-methanol: δ = 49.15 ppm, [D_6]-dimethylsulfoxide: δ = 39.51 ppm). In case of the [D_1]-chloroform/[D_4]-methanol mixtures, the [D_1]-chloroform signals were used for referencing. The apparent coupling constants are given in Hertz. The description of the fine structure means: s = singlet, bs = broad singlet, d = doublet, ps d = pseudo doublet, dd = doublet of doublets, dt = doublet of triplets, t = triplet, m = multiplet.

DOSY-spectra were recorded on a Bruker DRX 500 or on a Bruker Avance Neo 500 spectrometer equipped with a gradient unit (maximum z-gradient of 1200 G/cm) and a DIFF30 probe equipped with a ^{1}H/^{2}H coil. Analysis of the data was performed using the Stejskal-Tanner-equation for relevant integral areas. Hydrodynamic radii were calculated using the Stokes-Einstein equation using the correction for cylindrical particles. Diameters and heights of the capsules **1** and **2** were estimated from their DFT-calculated structures.

Low resolution ESI mass spectra were recorded on a Bruker Amazon SL spectrometer. High resolution ESI mass spectra were recorded on a Bruker Maxis 4G spectrometer.

Mass spectra of the capsule (*all-R*)-**2** were measured with an ESI-Q/TOF instrument (Bruker micrOTOF-Q) in positive and negative mode. Samples in varying concentrations in the range of 10^{-5} - $5*10^{-4}$ M in a mixture $CHCl_3$/CH_3OH 8/2 were introduced into the ESI source with flow rates of 3-7 µL/min. Other solvents (acetonitrile, acetone) did not lead to better results. Ionizing parameters were tuned from normal to very soft ionization conditions (source temperature 30 - 200 °C, quadrupole voltage 1-4 V, collision energy voltage 1-6 V).

The UV-VIS and CD spectra were recorded on a JASCO J-815 spectropolarimeter at 20 °C. The quartz cuvettes were from Hellma®Analytics type 100-QS (1 mm light path) for UV-VIS and CD. All solvents used were of spectrometric grade.

The fluorescence spectra were recorded on a Shimadzu RF-6000 spectro fluorometer at 25 °C. The quartz cuvettes were from Hellma®Analytics type 101-QS (10 mm light path) for fluorescence. All solvents used were of spectrometric grade.

1.2. Materials and Methods

Materials

For thin layer chromatography (TLC) analysis throughout this work, Polygram® SIL G/UV254 TLC plates (silica gel 0.2 mm, 40 × 80 mm) were used. Visualization of the spots was carried under a 254 nm UV light source. The products were purified by flash column chromatography on silica gel 60M (40-63 μm) which was purchased from MACHEREY-NAGEL GmbH & Co. KG. Eppendorf Research® Plus pipettes were used with epT.I.P.S. pipette tips for exact volumes.

Solvents

Dry pyridine was distilled from KOH and stored over molecular sieves under argon. Aqueous sodium carbonate solution (2 M) was degassed by bubbling with argon for 15 minutes. Phosphoryl chloride ($POCl_3$) was distilled under vacuum and stored in a Schlenk flask under argon. Aqueous work-ups and column chromatographies were carried out using technical grade solvents. Ethyl acetate was distilled prior to use. Dry tetrahydrofuran was distilled freshly from Na/benzophenone prior to use. Dimethoxyethane (DME) was distilled and stored under argon prior to use.

Chemicals

Copper(I) iodide, tetrabutylammonium fluoride and $Pd(PPh_3)_4$ were purchased from Sigma-Aldrich and used without further purification.

Sodium hydride (60% dispersion in mineral oil), triisopropylborate, terephthaloyl dichloride and bromoethane were purchased from TCI and used without further purification.

Bromine, boron tribromide, *n*-butyllithium (2.5 M in hexane), 1-bromo-4-iodobenzene, sodium iodide, ethylamine solution (70 % in water) and [1,1'-Bis(diphenyl-phosphino)ferrocene]palladium(II) dichloride [(dppf)$PdCl_2$] were purchased from ACROS Organics and used without further purification.

Sodium chloride, potassium chloride and hydrochloric acid (12 M) were purchased from Bernd Kraft GmbH and used without further purification.

Thionyl chloride, ethylamine solution (2M in tetrahydrofuran) and hexachloroethane were purchased from Alfa Aesar and used without further purification.

1,1'-Bis(diphenylphosphino)palladium(II) dichloride was purchased from Fluorochem and used without further purification.

(*S*)- and (*R*)-1,1′-Binaphthyl-2,2′-diol (>99.9% ee) were purchased from RCA Separations and used without further purification.

2. Synthetic procedures

2.1. Overview

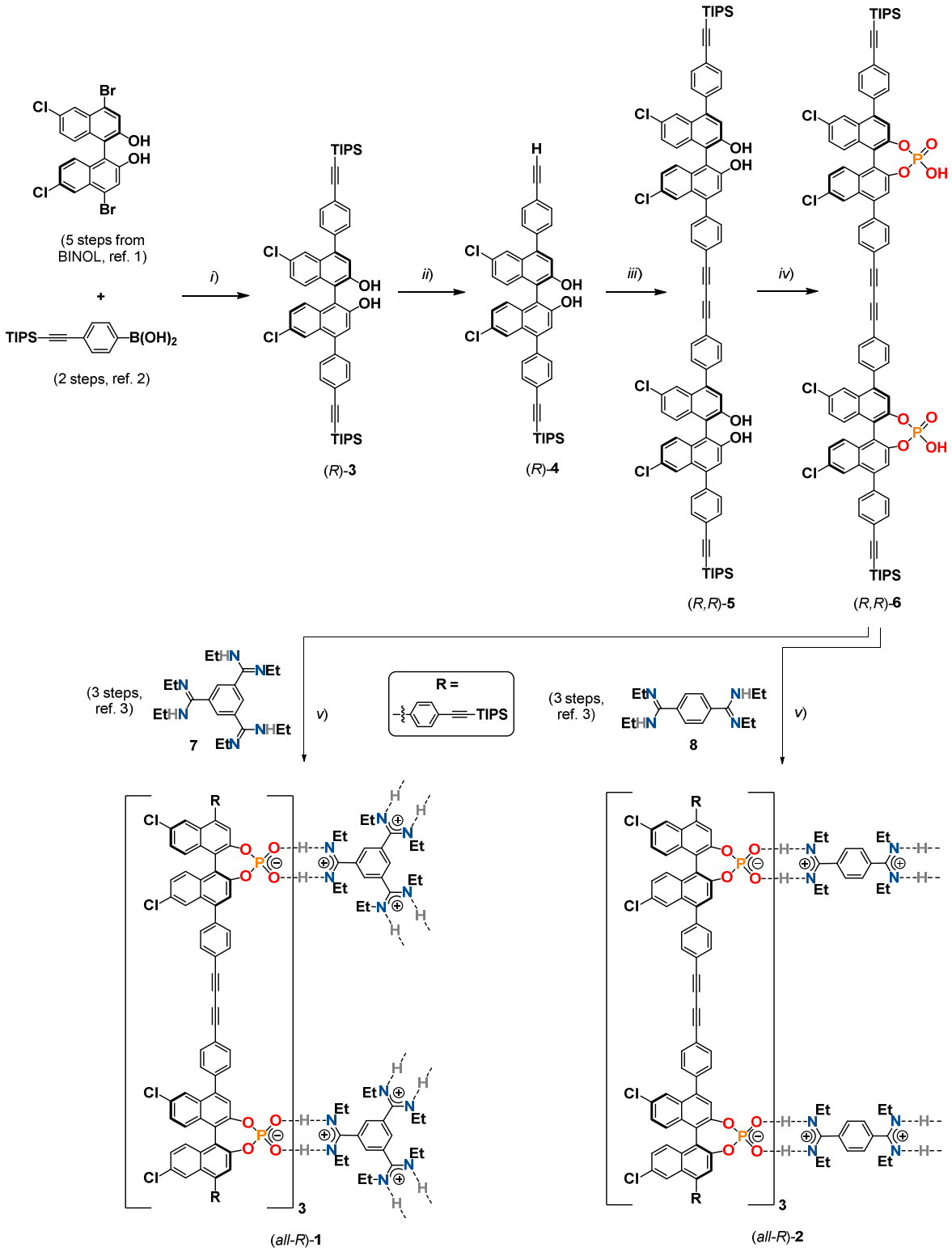
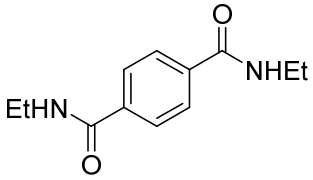


Figure S 1: Synthesis of the capsules **1** and **2**. Reagents and conditions: *i*) 2.4 equiv. of boronic acid, (dppf)$PdCl_2$, Na_2CO_3, 85 °C, DME/Na_2CO_3 (2 M), 91%; *ii*) TBAF (0.8 equiv.), 25 °C, RT, THF, 34% (alongside with 57% reisolated (*R*)-**3**); *iii*) $(PPh_3)_2PdCl_2$, CuI, 25 °C, THF/$CHCl_3$, 98%; *iv*) $POCl_3$, pyridine, 60°C, then H_2O, 26%; *v*) [D_1]-chloroform / [D_4]-methanol = 8 / 2 (v/v), 25 °C, 5 min.

2.2. Synthesis of the amidines

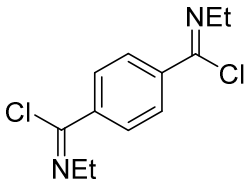
2.2.1. *N*,*N*′-diethylterephthalamide[1]



Terephthaloyl dichloride (3.00 g, 14.8 mmol, 1 eq.) was added to ethylamine (70% in water, 17.8 ml, 222 mmol, 15 eq.) at 0° C and stirred at 0° C for 30 minutes. After the reaction was completed, water (2 ml) were added alongside with concentrated hydrochloric acid (3 ml), ensuring that the pH stays basic. The product was filtered off and washed with water (2 x 15 ml) and methanol (2 x 15 ml), then dried under vacuum. This work up yielded analytically pure product (2.92 g, 13.3 mmol, 90.0 %).

$C_{12}H_{16}N_2O_2$ (220.27 g/mol)

^{1}H NMR (300 MHz, [D$_6$]-dimethylsulfoxide) δ = 8.55 (t, *J* = 5.5 Hz, 2H), 7.88 (s, 2H), 3.29 (d, *J* = 7.3 Hz, 4H), 1.12 (t, *J* = 7.2 Hz, 6H).



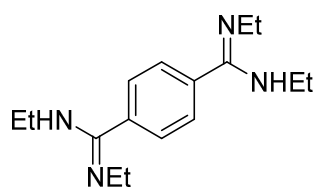
2.2.2. *N*,*N*′-diethylterephthalimidoyl dichloride[1]

N,*N*′-diethylterephthalamide (2.90 g, 13.2 mmol, 1 eq.) was placed under argon, and thionyl chloride (19.1 ml, 263 mmol, 20 eq.) was added dropwise. The reaction mixture was heated under reflux for three hours and stirred at room temperature overnight. After the reaction was completed, the excess thionyl chloride was removed under reduced pressure, then the crude oil was extracted with *n*-hexane (3 x 30 ml) and the solvent removed under reduced pressure. The work up yielded analytically pure product as a yellow oil (3.38 g, 11.3 mmol, 85.6 %).

$C_{12}H_{14}Cl_2N_2$ (257.16 g/mol)

^{1}H NMR (300 MHz, [D$_1$]-chloroform, 298 K) δ = 8.04 (q, *J* = 0.8 Hz, 4H), 3.78 (q, *J* = 7.3 Hz, 4H), 1.36 (t, *J* = 7.3 Hz, 6H).

2.2.3. *N*,*N*,*N*′,*N*′-tetraethyl-terephthalimidamide[1] (8)



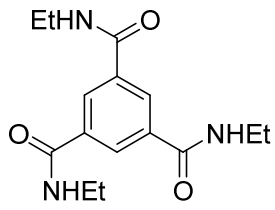
N,*N*′-diethylterephthalimidoyl dichloride (3.25 g, 12.6 mmol, 1 eq.) was dissolved in dichloromethane (20 ml) and added dropwise to a solution of ethylamine in tetrahydrofuran (2.0 M, 34.8 ml, 69.5 mmol, 5.5 eq.) at -10° C. The resulting solution was stirred at -10° C for an hour and overnight at room temperature. After the reaction was completed, the solvent was removed under reduced pressure and the remaining precipitate dissolved in water (30 ml). Sodium hydroxide (5

g, 125 mmol, 10 eq.) was added and the solution extracted with ethyl acetate (3 x 40 ml). The combined organic phases were dried over sodium sulfate, filtered and the solvent removed under reduced pressure. The crude product was purified using *Kugelrohr* distillation at 0.15 mbar and 220° C to give the analytically pure product **9** as a white solid (1.63 g, 5.95 mmol, 47.2 %).

$C_{16}H_{26}N_4$ (274.41 g/mol)

^{1}H NMR (600 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ = 7.16 (s, 4H, Ar-H), 2.96 (bs, 8H, CH_2), 0.98 (bs, 12H, CH_3).

2.2.4. *N*,*N*′,*N*′′-triethylbenzene-1,3,5-tricarboxamide[1]

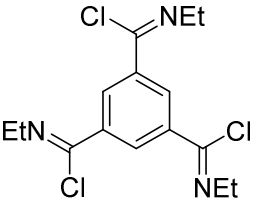


1,3,5-tricarboxybenzene (3.00 g, 14.3 mmol, 1 eq.) was dissolved in thionyl chloride (51.8 ml, 714 mmol, 50 eq.) alongside with dimethylformamide (one drop). The resulting mixture was heated under reflux for three hours and then the solvent removed under reduced pressure. A yellow oil was obtained, which was slowly added to ethylamine (70 % in water, 17.2 ml, 214 mmol, 15 eq.) at 0° C. The solution was stirred for 30 minutes, then diluted with water (30 ml). Concentrated hydrochloric acid (3 ml) was added and the mixture filtrated, washing the filtrate with water (2 x 5 ml) and methanol (2 x 5 ml). The workup yielded analytically pure product (3.07 g, 10.5 mmol, 73.4 %).

$C_{15}H_{21}N_3O_3$ (291.35 g/mol)

^{1}H NMR (300 MHz, [D$_6$]-dimethylsulfoxide) δ = 8.66 (t, *J* = 5.5 Hz, 1H), 8.36 (s, 1H), 3.30 (qd, *J* = 7.2, 5.4 Hz, 2H), 1.13 (t, *J* = 7.2 Hz, 3H).

2.2.5. *N*,*N*′,*N*′′-triethylbenzene-1,3,5-tris(carbonimidoyl trichloride)[1]

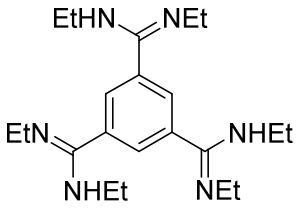


N,*N*′,*N*′′-Triethylbenzene-1,3,5-tricarboxamide (2.72 g, 9.32 mmol, 1 eq.) was dissolved in thionyl chloride (13.5 ml, 187 mmol, 20 eq.) and heated for three hours under reflux, then overnight at room temperature. After the reaction was completed, the excess thionyl chloride was removed under reduced pressure and the remaining solid extracted with *n*-hexane (3 x 10 ml). The combined organic phases were dried over magnesium sulfate, filtered and the solvent removed under reduced pressure. The workup yielded analytically pure solid (1.23 g, 3.57 mmol, 38.3 %).

$C_{15}H_{18}Cl_3N_3$ (346.68 g/mol)

^{1}H NMR (300 MHz, [D$_1$]-chloroform, 298 K) δ = 8.66 (s, 3H), 3.79 (q, *J* = 7.3 Hz, 6H), 1.36 (t, *J* = 7.3 Hz, 9H).

2.2.6. *N,N,N′,N′,N′′,N′′*-hexaethylbenzene-1,3,5-tris(carboximidamide)[1] (7)



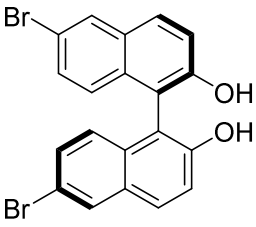
N,N′,N′′-triethylbenzene-1,3,5-tris(carbonimidoyl trichloride) (1.23 g, 3.55 mmol, 1 eq.) was dissolved in dichloromethane (20 ml) and added dropwise to ethylamine solution (2.0 M in tetrahydrofuran, 21.3 ml, 42.5 mmol, 12 eq.) at -10° C. The solution was stirred at -10° C for an hour and overnight at room temperature. After the reaction went to completion, the solvent was removed under reduced pressure and the remaining solid dissolved in water (30 ml). Sodium hydroxide (1.4 g, 35.0 mmol, 10 eq.) was added and the solution extracted with ethyl acetate (3 x 50 ml), dried over sodium sulfate, filtered and the solvent removed under reduced pressure.

The crude product was purified *via Kugelrohr* distillation at 0.35 mbar and 295° C. This workup yielded analytically pure product **8** as a white solid (1.06 g, 2.85 mmol, 80.3 %).

$C_{21}H_{36}N_6$ (372.56 g/mol)

^{1}H NMR (300 MHz, [D$_1$]-chloroform, [D$_4$]-methanol , 298 K) δ = 7.11 (s, 3H, Ar-H), 2.99 (bs, 8H, CH_2), 0.99 (bs, 12H, CH_3).

2.3. Synthesis of BINOL-precursors



2.3.1. (*R*)-6,6'-Dibromo-1,1'-binaphthalene-2,2'-diol[2]

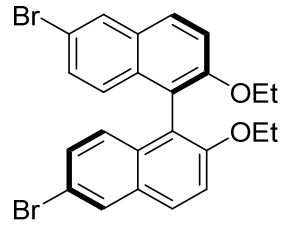
1,1'-Binapthyl-2,2'-diol (20.0 g, 69.9 mmol, 1 eq.) was suspended in dichloromethane (400 ml) and cooled to -78° C. Bromine (9.72 ml, 30.1 g, 189 mmol, 2.7 eq.) was dissolved in dichloromethane (100 ml) and was added dropwise to the suspension. The mixture was stirred for two hours at -78° C, then overnight at room temperature.

After the reaction was completed, sodium bisulfite (3.65 M, 37 %, 5 eq., 349 mmol, 95.6 ml) was added at 0° C and the biphasic mixture was stirred for two hours. Dichloromethane (100 ml) and water (100 ml) were added and the phases separated. The aqueous phase was extracted with dichloromethane (100 ml), the organic phase washed with water (100 ml), then the organic phase was dried over magnesium sulfate, filtered and the solvent removed under reduced pressure. This workup yielded analytically pure product (30.3 g, 68.1 mmol, 97.5 %).

$C_{20}H_{12}Br_2O_2$ (444.12 g/mol)

^{1}H NMR (300 MHz, [D$_1$]-Chloroform, 298 K) δ = 7.90 (d, *J* = 2.0 Hz, 2H), 7.73 (dt, *J* = 8.9, 0.6 Hz, 2H), 7.27 – 7.18 (m, 4H), 6.82 (dt, *J* = 8.9, 0.6 Hz, 2H), 4.87 (bs, 2H).

2.3.2. (*R*)-6,6'-dibromo-2,2'-diethoxy-1,1'-binaphthalene[2]



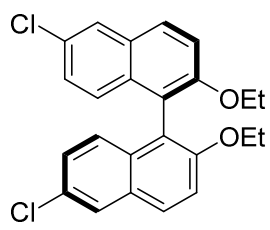
(*R*)-6,6'-Dibromo-1,1'-binaphthalene-2,2'-diol (30.3 g, 68.0 mmol, 1 eq.) was suspended in acetone (300 ml) alongside with sodium iodide (510 mg, 3.41 mmol, 0.05 eq.) and potassium carbonate (33.5 g, 241 mmol, 4 eq.). The suspension was refluxed for one hour, then bromoethane (31.5 ml, 408 mmol, 6 eq.) was added in four parts over a four hour period. The resulting solution was refluxed overnight.

After the reaction was completed, the solution was filtered and the solvent was removed under reduced pressure. The remaining solid was taken up in *n*-hexane (100 ml) and stirred for two hours at room temperature, then the supernatant was filtered off and the filtrate washed with *n*-hexane (2 x 10 ml), then dried under high vacuum. This workup yielded analytically pure product. (25.9 g, 51.7 mmol, 76.0 %).

$C_{24}H_{20}Br_2O_2$ (500.23 g/mol)

^{1}H NMR (300 MHz, [D_1]-chloroform, 298 K) δ = 7.99 (d, *J* = 2.1 Hz, 2H, Ar-H), 7.83 (d, *J* = 9.0 Hz, 2H, Ar-H), 7.40 (d, *J* = 9.0 Hz, 2H, Ar-H), 7.25 (dd, *J* = 9.0, 2.1 Hz, 2Hz, Ar-H), 6.95 (dt, *J* = 9.1, 0.6 Hz, 2H, Ar-H), 4.09-3.95 (m, 4H, CH_2), 1.05 (t, *J* = 7.0 Hz, 6H, CH_3).

2.3.3. (*R*)-6,6'-dichloro-2,2'-diethoxy-1,1'-binaphthalene[2]



(*R*)-6,6'-dibromo-2,2'-diethoxy-1,1'-binaphthalene (25.9 g, 51.7 mol, 1 eq.) was dissolved in dry tetrahydrofuran (160 ml) in a Schlenk flask and cooled to -78° C. *N*-butyllithium (2.5 M in hexane, 62.0 ml, 155 mmol, 3 eq.) was added to the solution and the mixture was stirred for 30 minutes. Hexachloroethane (24.5 g, 103 mmol, 2 eq.) was dissolved in dry tetrahydrofuran (50 ml) and added dropwise at -78° C. The solution was stirred for two hours at -78° C, then warmed to room temperature overnight.

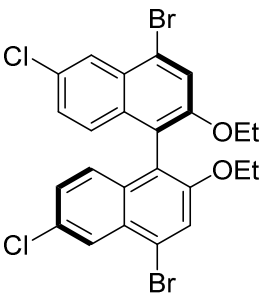
After the reaction was completed, ammonium chloride (100 ml) was added and the phases separated. The aqueous phase was extracted with ethyl acetate (2 x 200 ml), the combined organic phases were dried over magnesium sulfate, filtered and the solvent removed under reduced pressure.

The remaining solid was suspended in *n*-hexane (50 ml) and stirred for one hour. The supernatant was filtered off and the filtrate was washed with *n*-hexane (3 x 10 ml) and dried under high vacuum. This workup yielded analytically pure product (11.3 g, 27.5 mmol, 53.3 %).

$C_{24}H_{20}Cl_2O_2$ (411.32 g/mol)

^{1}H NMR (300 MHz, [D_1]-chloroform, 298 K) δ = 7.83 (d, *J* = 9.0 Hz, 2H, Ar-H), 1H), 7.81 (d, *J* = 2.2 Hz, 2H, Ar-H), 7.41 (d, *J* = 9.0 Hz, 2H, Ar-H), 7.12 (dd, *J* = 9.1, 2.2 Hz, 2H, Ar-H), 7.00 (d, *J* = 9.0 Hz, 2H, Ar-H), 4.07-3.97 (m, 4H, CH_2), 1.04 (t, *J* = 7.0 Hz, 6H, CH_3).

2.3.4. (*R*)-4,4'-dibromo-6,6'-dichloro-2,2'-diethoxy-1,1'- binaphthalene[2]



(*R*)-6,6'-dichloro-2,2'-diethoxy-1,1'-binaphthalene (11.3 g, 27.6 mmol, 1 eq.) was dissolved in dichloromethane (400 ml) and cooled to -78° C. Bromine (21.3 ml, 66.0 g, 413 mmol, 15 eq.) was dissolved in dichloromethane (50 ml) and added dropwise to the solution over the course of an hour, then stirred at room temperature overnight.

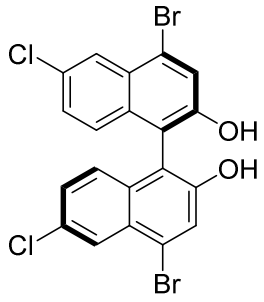
After the reaction was completed, sodium bisulfite (3.65 M, 37 %, 151 ml, 20 eq.) was added and the solution stirred for two hours at room temperature. The phases were then separated and the aqueous phase was extracted with dichloromethane (2 x 100 ml) and the organic phase washed with sodium chloride solution (2 x 100 ml), then the combined organic phases were dried over magnesium

sulfate, filtered, and the solvent removed under reduced pressure. The remaining solid was taken up in acetone (10 ml) and precipitated with *n*-hexane (75 ml). The solvent was removed, the solid suspended in *n*-hexane (50 ml) and stirred for one hour. After stirring, the supernatant was filtered off and the filtrate dried under high vacuum. This workup yielded analytically pure product (11.6 g, 20.4 mmol, 73.9 %).

$C_{24}H_{18}Br_2Cl_2O_2$ (569.11 g/mol)

^{1}H NMR (300 MHz, [D_1]-chloroform, 298 K) δ = 8.21 (d, *J* = 2.1 Hz, 2H, Ar-H), 7.71 (s, 2H, Ar-H), 7.16 (dd, *J* = 9.0, 2.1 Hz, 2H, Ar-H), 6.99 (d, *J* = 9.0 Hz, 2H, Ar-H), 4.07-3.97 (m, 4H, CH_2), 1.06 (t, *J* = 7.0 Hz, 6H, CH_3).

2.3.5. (*R*)-4,4'-dibromo-6,6'-dichloro-[1,1'-binaphthalene]-2,2'-diol[2]



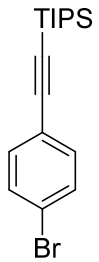
(*R*)-4,4'-dibromo-6,6'-dichloro-2,2'-diethoxy-1,1'- binaphthalene (11.6 g, 20.4 mmol, 1 eq.) was dissolved in dichloromethane (150 ml) and cooled to -78° C. Boron tribromide (4.83 ml, 12.5 g, 50.9 mmol, 2.5 eq.) was added and the solution was stirred at -78° C for two hours, then warmed up to room temperature overnight.

After the reaction was completed, sodium hydrogen carbonate (50 ml) was added, the phases were separated and the organic phase washed with sodium chloride solution (2 x 50 ml). The combined organic phases were dried over magnesium sulfate, filtered and the solvent removed under reduced pressure. This workup yielded analytically pure product (*R*)-**3** (9.65 g, 18.8 mmol, 92.2%).

$C_{20}H_{10}Br_2Cl_2O_2$ (513.01 g/mol)

^{1}H NMR (300 MHz, [D_1]-chloroform, 298 K) δ = 8.28 (d, *J* = 2.1 Hz, 1H, Ar-H), 7.74 (s, 1H, Ar-H), 7.28 (dd, *J* = 8.9, 2.1 Hz, 1H, Ar-H), 7.02 (d, *J* = 9.0 Hz, 1H, Ar-H), 4.96 (s, 2H, OH).

2.3.6. ((4-bromophenyl)ethynyl)triisopropylsilane[3]



Commercially available 1-bromo-4-iodobenzene (12.9 g, 45.7 mmol, 1 eq) and (triisopropylsilyl)acetylene (10.0 g, 12.3 ml, 54.8 mmol, 1.2 eq) were dissolved in piperidine (60 ml) in a Schlenk flask flushed with argon. The solution was degassed by bubbling argon through it for 15 minutes. The solution was cooled to 0° C and copper(I)iodide (0.17 g, 0.91 mmol, 0.02 eq) and bis(triphenylphosphine)palladium(II) dichloride (0.32 g, 0.46 mmol, 0.01 eq) were added. The solution was stirred under argon for two hours at 0° C and then for twelve hours at room temperature.

After the reaction was completed, the solution was poured into cold 2 M hydrochloric acid (300 ml). The resulting mixture was extracted with diethyl ether (300 ml), and the resulting organic phases were washed with 2 M hydrochloric acid (2 x 50 ml). The

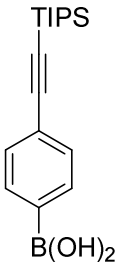
combined aqueous phases were extracted with diethyl ether (3 x 150 ml). The combined organic phases were dried over magnesium sulfate, filtered and the solvent was removed under vacuum. The resulting black oil was distilled using *via* Kugelrohr at 2.5 mbar and 150-170° C. The resulting yellow oil was obtained analytically pure (9.65 g, 28.6 mmol, 62.6 %).

Comment: The product contains a small amount (10%) of the disubstituted product (1,4-Bis(triisopropylsilylethynyl)benzene) as an impurity (^{1}H NMR: δ = 7.37 ppm). This can be removed in the next step because it cannot be transformed into the more polar boronic acid and elutes more quickly during column chromatography.

$C_{17}H_{25}BrSi$ (337.38 g/mol)

^{1}H NMR (300 MHz, [D_1]-chloroform, 298 K**)** δ = 7.41 (ps d, *J* = 8.6 Hz, 2H), 7.31 (ps d, *J* = 8.6 Hz, 2H, 2H), 1.11 (s, 3 H, TIPS-CH), 1.10 (s, 18 H, TIPS-CH_3).

2.3.7. (4-((triisopropylsilyl)ethynyl)phenyl) boronic acid[3]



The synthesized ((4-bromophenyl)ethynyl)triisopropylsilane (9.65 g, 28.6 mmol, 1 eq.) was dissolved in dry tetrahydrofuran (300 ml) and cooled to -78° C in a multinecked flask under argon. After cooling, *n*-butyllithium was added (2.5 M in hexane, 14.9 ml, 37.2 mmol, 1.3 eq) and the solution stirred for 30 minutes. It was then transferred into a solution of triisopropylborate (19.8 ml, 85.8 mmol, 3 eq.) in dry tetrahydrofuran (50 ml) at -78° C in a multinecked flask under argon. Following the transfer, the resulting solution was stirred at room temperature overnight.

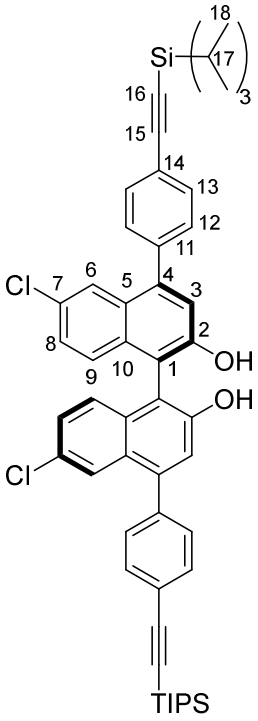
After the reaction was completed, hydrochloric acid (2 M, 200 ml) was added alongside with tetrahydrofuran (400 ml), and the reaction stirred for an additional hour. The phases were separated, sodium chloride solution (150 ml) was added, and the organic phase washed with sodium chloride solution (2 x 50 ml). The combined organic phases were dried over magnesium sulfate, filtered and the solvent removed under reduced pressure. The resulting white powder was purified using column chromatography (Cy: Et_2O: MeOH 1 : 2 : 1) and obtained as analytically pure product (6.79 g, 22.5 mmol, 78.5 %).

$C_{17}H_{27}BO_2Si$ (302.30 g/mol)

^{1}H NMR (300 MHz, [D_6]- dimethylsulfoxide**)** δ = 8.17 (s, 2H, OH), 7.78 (ps d, *J* = 8.1 Hz, 2H, Ar-H), 7.41 (ps d, *J* = 8.1 Hz, 2H, Ar-H), 1.10 (s, 21 H, TIPS).

2.4. Synthesis of the bisphosphoric acid (*R*,*R*)-6

2.4.1. Synthesis of (*R*)-3



(*R*)-4,4'-dibromo-6,6'-dichloro-[1,1'-binaphthalene]-2,2'-diol (4.00 g, 7.80 mmol, 1 eq.) was dissolved in distilled dimethoxyethane (80 ml) alongside with (4-((triisopropylsilyl)ethynyl)phenyl)boronic acid (5.66 g, 18.7 mmol, 2.4 eq.) and [1,1'-Bis(diphenylphosphino)-ferrocene]palladium(II) dichloride (318 mg, 0.390 mmol, 0.05 eq). Degassed sodium carbonate solution (2 M, 25.7 ml, 51.5 mmol, 6.6 eq.) was added and the reaction heated to reflux under argon overnight.

After the reaction was completed, saturated ammonium chloride solution (100 ml) and tetrahydrofuran (300 ml) were added. The phases were separated and the aqueous phase was extracted with tetrahydrofuran (2 x 100 ml). The combined organic phases were dried over magnesium sulfate, filtered and the solvent removed under reduced pressure. The resulting black solid was purified using column chromatography (Cy : EA = 4 : 1) and the product (*R*)-**3** was obtained as a yellowish solid (6.77 g, 7.80 mmol, 90.8%).

Comment: For some batches of the starting dibromide, we observed that the coupling only worked at higher catalyst loadings (i.e. 20%-50%). Repurification of the dibromide by column chromatography did not alleviate this problem, only the synthesis of a new batch of the dibromide starting from BINOL was found to be helpful.

$C_{54}H_{60}Cl_2O_2Si_2$ (868.14 g/mol)

^{1}H NMR (600 MHz, [D_1]-chloroform, 298 K) δ = 7.85 (d, ^4J = 2.2 Hz, 2H, H-6), 7.68 (ps d, ^3J = 8.4 Hz, 4H, H-13), 7.51 (ps d, ^3J = 8.4 Hz, 4H, H-12), 7.35 (s, 2H, H-3), 7.27 (dd, ^3J = 9.0 Hz, ^4J = 2.2 Hz, 2H, H-8), 7.17 (dd, ^3J = 9.0 Hz, ^5J = 0.5 Hz, 2H, H-9), 5.11 (s, 2H, OH), 1.17 (s, 36H, H-18), 1.16 (s, 6H, H-17).

^{13}C NMR (151 MHz, [D_1]-chloroform, 298 K) δ = 152.4 (C-2), 142.8 (C-4), 139.1 (C-11) , 132.5 (C-13), 132.4 (C-10) , 130.7 (C-7) , 129.8 (C-12), 128.7 (C-5), 128.6 (C-8) , 126.4 (C-9), 125.7 (C-6) , 123.6 (C-14), 119.7 (C-3), 110.6 (C-1), 106.7 (C-15), 92.1 (C-16), 18.9 (C-18), 11.5 (C-17).

COSY (600 MHz, [D_1]-chloroform, 298 K) δ (^{1}H) / δ (^{1}H) = 7.85/7.27 (H-6/H-8), 7.68/7.51 (H-13/H-12), 7.51/7.68 (H-12/H-13), 7.27/7.85, 7.17 (H-8/H-6, H-9), 7.17/7.27 (H-9/H-8).

HSQC (600/151 MHz, [D_1]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.85/125.7 (H-6/C-6), 7.68/132.5 (H-13/C-13), 7.51/129.8 (H-12/C-12), 7.35/119.7 (H-3/C-3), 7.27/128.6 (H-8/C-8), 7.17/126.4 (H-9/C-9), 1.17/18.9 (TIPS-C*H*$_3$/TIPS-*C*H$_3$), 1.16/11.5 (TIPS-C*H*/TIPS-*C*H).

HMBC (600/151 MHz, [D_1]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.85/142.8, 132.4, 130.7, 128.6 (H-6/C-4, C-10, C-7, C-8), 7.68/139.1, 132.5, 129.8, 106.7 (H-13/C-11, C-13, C-12, C-15), 7.51/142.8, 132.5, 129.8, 123.6 (H-12/C-4, C-13, C-12, C-14), 7.35/152.4, 142.8, 139.1, 110.6 (H-3/C-2, C-4, C-11, C-1), 7.27/132.4; 130.7, 125.7 (H-8/C-10, C-7, C-6), 7.17/132.4, 130.7, 128.7, 125.7 (H-9/ C-10, C-7, C-5, C-6), 5.11/152.4, 142.8, 119.7, 110.6 (OH/C-2, C-4, C-3, C-1), 1.17, 1.16/92.1, 18.9, 11.5 (H-18, H-17/C-16, C-18, C-17).

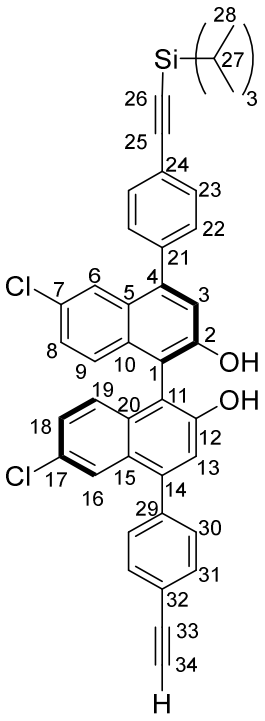
Melting point: 168°C

MS (ESI, -Mode): m/z = 865.3404 ([M-H]$^-$, calculated: m/z= 865.3436 for [$C_{54}H_{60}Cl_2O_2Si_2$]$^-$).

IR (ATR) υ bar: 3526, 2941, 2863, 2360, 2156, 1588, 1496, 1461, 1379, 1140 cm^{-1}.

Elemental analysis calcd. for $C_{54}H_{60}Cl_2O_2Si_2$: C, 74.71; H, 6.97. Found: C, 74.5; H, 7.14.

2.4.2. Synthesis of (*R*)-4



The Suzuki-coupling product (*R*)-**3** (925 mg, 1.07 mmol, 1 eq.) was dissolved in tetrahydrofuran (30 ml). A solution of tetrabutylammonium fluoride (209 mg, 0.799 mmol, 0.7 eq.) in tetrahydrofuran (20 ml) was added dropwise *via* an addition funnel, then the solution was stirred overnight at room temperature.

The reaction was followed by TLC, and stopped after ca. 50% conversion. The solvent was removed under reduced pressure and the resulting yellow oil was purified *via* column chromatography (Cy : EA = 10 : 1). As a first fraction, reisolated starting material (*R*)-**4** was obtained (529 mg, 0.609 mmol, 56.9%). As a second fraction, the desired product (*R*)-**5** was obtained as a yellow solid (255 mg, 0.359 mmol, 33.6 %).

$C_{45}H_{40}Cl_2O_2Si$ (711.80 g/mol)

^{1}H NMR (600 MHz, [D_1]-chloroform, 298 K) δ = 7.85, 7.84 (each d, each ^4J = 2.1 Hz, each 1H, H-6 and H-16), 7.69 (ps d, ^3J = 8.2 Hz, 2H, H-31), 7.68 (ps d, ^3J = 8.2 Hz, 2H, H-23), 7.52 (ps d, ^3J = 8.2 Hz, 2H, H-30), 7.51 (ps d, ^3J = 8.2 Hz, 2H, H-22), 7.353 (s, 1H, H-13), 7.347 (s, 1H, H-3), 7.275, 7.271 (each dd, each ^3J = 9.0 Hz, ^4J = 2.1 Hz, each 1H, H-8 and H-18), 7.17, 7.16 (each d, each ^3J = 9.0 Hz,

each 1H, H-9 and H-19), 5.12 (bs, 2H, OH), 3.18 (s, 1H, H-34), 1.164 (s, 18H, H-28), 1.162 (s, 3H, H-27).

^{13}C NMR (151 MHz, [D$_1$]-chloroform, 298 K) δ = 152.43, 152.42 (C-2, C-12), 142.8, 142.6 (C-4, C-14), 139.7 (C-29), 139.1 (C-21), 132.6, 132.5 (C-23, C-31), 132.40 132.37 (C-10, C-20), 130.78, 130.76 (C-7, C-17), 129.9, 129.8 (C-22, C-30), 128.7, 128.6 (C-8, C-18), 128.62, 128.60 (C-5, C-15), 126.4, 126.3 (C-9, C-19), 125.7, 125.6 (C-6, C-16), 123.6 (C-24), 122.2 (C-32), 119.84, 119.75 (C-3, C-13), 110.7, 110.6 (C-1, C-11), 106.7 (C-25), 92.1 (C-26), 83.4 (C-33), 78.0 (C-34), 18.9 (C-28), 11.5 (C-27).

COSY (600 MHz, [D$_1$]-chloroform, 298 K) δ (^{1}H) / δ (^{1}H) = 7.85, 7.84 / 7.275, 7.271 (H-6, H-16 / H-8, H-18), 7.69, 7.68 / 7.52, 7.51 (H-31, H-23 / H-22, H-30), 7.52, 7.51 / 7.69, 7.68 (H-30, H-22 / H-23, H-31), 7.275, 7.271 / 7.85, 7.84, 7.17, 7.16 (H-8, H-18 / H-6, H-16, H-9, H-19), 7.17, 7.16 / 7.85, 7.84 (H-9, H-19 / H-8, H-18).

HSQC (600/151 MHz, [D$_1$]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.85, 7.84 / 125.7, 125.6 (H-6, H-16 / C-6, C-16), 7.69, 7.68 / 132.6, 132.5 (H-23, H-31 / C-23, C-31), 7.52, 7.51 /129.9, 129.8 (H-22, H-30 / C-22, C-30), 7.353, 7.347 / 119.84, 119.75 (H-3, H-13 / C-3, C-13), 7.275, 7.271 / 128.7, 128.6 (H-8, H-18 / C-8, C-18), 7.17, 7.16 / 126.4, 126.3 (H-9, H-19 / C-9, C-19), 3.18 / 78.0 (H-34 / C-34), 1.164 / 18.9 (H-28 / C-28), 1.162 / 11.5 (H-27 / C-27).

HMBC (600/151 MHz, [D$_1$]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.85, 7.84 / 142.8, 142.6, 132.40, 132.37, 130.78, 130.76, 128.7, 128.6 (H-6, H-16 / C-4, C-14, C-10, C-20, C-7, C-17, C-8, C-18), 7.69 / 139.7, 132.6, 132.5, 129.9, 129.8, 83.4 (H-31 / C-29, C-31, C-30, C-33), 7.68 / 139.1, 132.6, 132.5, 129.9, 129.8, 106.7 (H-23 / C-21, C-23, C-22, C-25), 7.52 / 142.8, 142.6, 132.6, 132.5, 129.9, 129.8, 122.2 (H-30 / C-4, C-14, C-23, C-31, C-22, C-30, C-32), 7.51 / 142.8, 142.6 132.6, 132.5 129.9, 129.8 123.6 (H-22 / C-4, C-14, C-23, C-31, C-22, C-30, C-24), 7.353 / 152.43, 152.42, 139.7, 128.62, 128.60, 110.7, 110.6 (H-13 / C-12, C-29, C-15, C-11), 7.347 / 152.43, 152.42, 139.1, 128.62, 128.60, 110.7, 110.6 (H-3 / C-2, C-21, C-5, C-1), 7.275, 7.271 / 132.40, 132.37, 130.78, 130.76, 125.7, 125.6 (H-8, H-18 / C-10, C-20, C-7, C-17, C-6, C-16), 7.17, 7.16 / 130.78, 130.76, 128.62, 128.60, 110.7, 110.6 (H-9, H-19 / C-7, C-17, C-5, C-15, C-1, C-11), 3.18 / 132.6, 132.5, 122.2 (H-34 / C-31, C-32), 1.164, 1.162 / 18.9, 11.5 (H-28, H-27 / C-28, C-27).

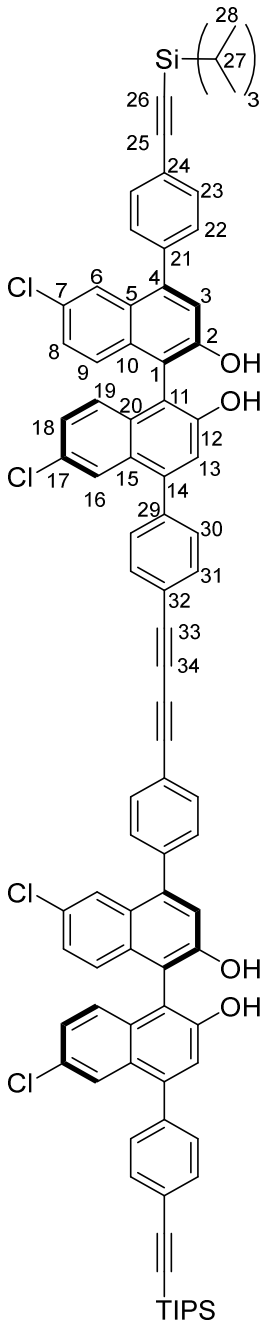
MS (ESI, -Mode): m/z = 709.2091 ([M-H]$^-$, calculated: m/z = 709.2102)

IR (ATR) υ bar: 2940, 2863, 2360, 2156, 1587, 1496, 1461, 1379, 1263, 1140 cm^{-1}

Melting point: 189°C

Elemental analysis: expected C = 75.93 %, H = 5.66 %, found C = 76.9 %, H = 6.22 %

2.4.3. Synthesis of (*R*,*R*)-5



The monodeprotected product (*R*)-**4** (866 mg, 1.22 mmol, 1 eq.) was dissolved in a chloroform : tetrahydrofuran 1:2 mixture (135 ml) alongside with bis(triphenylphosphine)palladium(II) dichloride (42.8 mg, 0.06 mmol, 0.05 eq.) and copper(I)iodide (11.6 mg, 0.06 mmol, 0.05 eq.). To this was added triethylamine (1.25 ml, 9.76 mmol, 8 eq.) and the resulting solution was stirred at room temperature overnight.

After the reaction was completed, the solvent was removed under reduced pressure, then the resulting solid was taken up in dichloromethane (400 ml) and washed with hydrochloric acid (1 M, 3 x 100 ml). The combined organic phases were dried over sodium sulfate, filtered, and the solvent removed under reduced pressure. This workup yielded (*R*)-**5** as a brown solid, containing minor impurities stemming from the catalysts (850 mg, 0.60 mmol, 98.0%). An analytically pure sample can be obtained by column chromatography (Cy : EA = 4 : 1).

$C_{90}H_{78}Cl_4O_4Si_2$ (1421.58 g/mol)

^{1}H NMR (600 MHz, [D$_1$]-chloroform, 298 K) δ = 7.87, 7.86 (each d, each ^4J = 2.1 Hz, each 2H, H-6 and H-16), 7.77 (ps d, ^3J = 8.2 Hz, 4H, H-31), 7.69 (ps d, ^3J = 8.2 Hz, 4H, H-23), 7.58 (ps d, ^3J = 8.2 Hz, 4H, H-30), 7.52 (ps d, ^3J = 8.2 Hz, 4H, H-22), 7.38 (s, 2H, H-13), 7.36 (s, 2H, H-3), 7.29, 7.28 (each dd, each ^3J = 9.0 Hz, ^4J = 2.1 Hz, each 2H, H-8 and H-18), 7.19 (d, ^3J = 8.7 Hz, 2H, H-19), 7.18 (d, ^3J = 8.7 Hz, 2H, H-9), 5.14 (bs, 4H, OH), 1.167 (s, 36H, H-28), 1.165 (s, 6H, H-27).

^{13}C NMR (151 MHz, [D$_1$]-chloroform, 298 K) δ = 152.45, 152.43 (C-2, C-12), 142.9 (C-4) 142.4 (C-14), 140.2 (C-29), 139.1 (C-21), 133.0 (C-31), 132.5 (C-23), 132.44 132.37 (C-10, C-20), 130.9, 130.8 (C-7, C-17), 130.1 (C-30), 129.8 (C-22), 128.73, 128.68, 128.63, 128.56 (C-8, C-18, C-5, C-15), 126.5, 126.3 (C-9, C-19), 125.7, 125.5 (C-6, C-16), 123.7 (C-24), 121.9 (C-32), 119.9, 119.8 (C-3, C-13), 110.9 (C-11), 110.5 (C-1), 106.7 (C-25), 92.2 (C-26), 81.8 (C-33), 75.1 (C-34), 18.9 (C-28), 11.5 (C-27).

COSY (600 MHz, [D$_1$]-chloroform, 298 K) δ (^{1}H) / δ (^{1}H) = 7.87, 7.86 / 7.29, 7.28 (H-6, H-16 / H-8, H-18), 7.77 / 7.58 (H-31 / H-30), 7.69 / 7.52 (H-23 / H-22), 7.58 / 7.77 (H-30 / H-31), 7.52 / 7.69 (H-22 / H-23), 7.29, 7.28 / 7.87, 7.86, 7.19, 7.18 (H-8, H-18 / H-6, H-16, H-9, H-19), 7.19, 7.18 / 7.87, 7.86 (H-9, H-19 / H-8, H-18).

HSQC (600/151 MHz, [D1]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.87, 7.86 / 125.7, 125.5 (H-6, H-16 / C-6, C-16), 7.77 / 133.0 (H-31 / C-31), 7.69 / 132.5 (H-23 / C-23), 7.52 / 130.1 (H-30 / C-30), 7.38 / 129.8 (H-22 / C-22), 7.38, 7.36 / 119.9, 119.8 (H-3, H-13 / C-3, C-13), 7.29, 7.28 / 128.73, 128.68, 128.63, 128.56 (H-8, H-18 / C-8, C-18), 7.19, 7.18 / 126.5, 126.3 (H-9, H-19 / C-9, C-19), 1.167 / 18.9 (H-28 / C-28), 1.165 / 11.5 (H-27 / C-27).

HMBC (600/151 MHz, [D1]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.87, 7.86 / 142.9, 142.4, 132.44, 132.37, 130.9, 130.8, 128.73, 128.68, 128.63, 128.56 (H-6, H-16, C-4, C-14, C-10, C-20, C-7, C-17, C-8, C-18, C-5, C-15), 7.77 / 140.2, 133.0, 81.8 (H-31 / C-29, C-31, C-33), 7.69 / 139.1, 132.5, 106.7 (H-23 / C-21, C-23, C-25), 7.58 / 142.4, 130.1, 121.9 (H-30 / C-14, C-30, C-32), 7.52 / 142.9, 129.8, 123.7 (H-22 / C-4, C-22, C-24), 7.38 / 152.45, 152.43, 140.2, 128.73, 128.68, 128.63, 128.56, 110.9 (H-13 / C-12, C-29, C-15, C-11), 7.36 / 152.45, 152.43, 139.1, 128.73, 128.68, 128.63, 128.56, 110.5 (H-3 / C-2, C-21, C-5, C-1), 7.29, 7.28 / 132.44, 132.37, 125.7, 125.5 (H-8, H-18 / C-10, C-20, C-6, C-16), 7.19 / 130.9, 130.8, 128.73, 128.68, 128.63, 128.56, 110.9 (H-19 / C-17, C-15, C-11), 7.18 / 130.9, 130.8, 128.73, 128.68, 128.63, 128.56, 110.5 (H-9 / C-7, C-5, C-1), 1.167, 1.165 / 92.2, 18.9, 11.5 (H-28, H-27 / C-26, C-28, C-27).

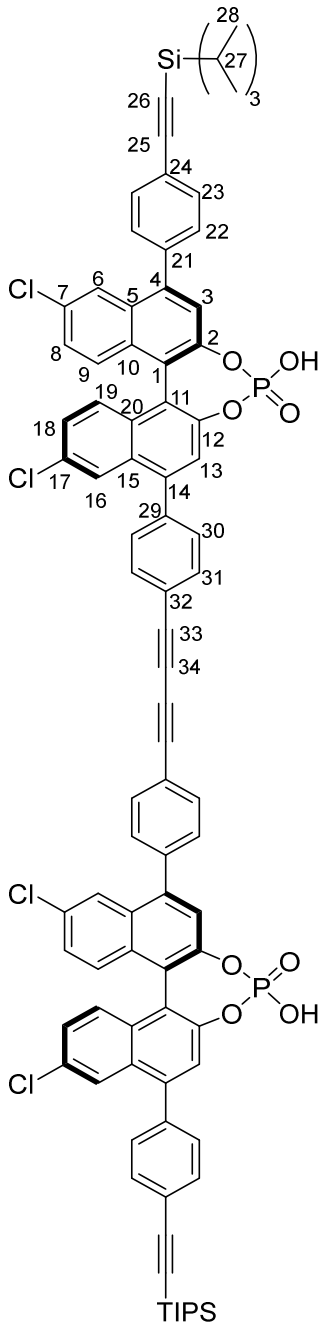
MS (ESI, -Mode): m/z = 1417.4151 ([M-H]$^{-}$, calculated: m/z = 1417.4120)

IR (ATR) υ bar: 2924, 2862, 2360, 2341, 2157, 1717, 1588, 1495, 1460, 1379, 1263, 1140 cm^{-1}

Melting point: 172°C

Elemental analysis: expected C = 76.04 %, H = 5.53 %, found C = 75.4 %, H = 6.06 %

2.4.4. Synthesis of (*R,R*)-6



The Glaser-coupling product (*R,R*)-**5** (274 mg, 0.193 mmol, 1 eq.) was dissolved in dry pyridine (4 ml). Phosphorus oxychloride (141 µl, 237 mg, 1.54 mmol, 8 eq.) was added to the solution and the reaction stirred at 60° C overnight.

After the reaction was completed, water (1.5 ml) was added to the solution and the reaction stirred for two hours at 60° C. The solvent was then removed under reduced pressure and the remaining solid taken up in dichloromethane (100 ml), then washed with hydrochloric acid (1 M, 5 x 10 ml). The combined organic phases were dried over sodium sulfate, filtered and the solvent removed under reduced pressure. The resulting solid was purified *via* column chromatography (DCM : MeOH = 10:1 to 1:1). The solvent was removed under reduced pressure, the solid taken up in a 10:1 mixture of dichloromethane : methanol (30 ml) and washed with hydrochloric acid (1 M, 3 x 10 ml). This yielded analytically pure product (*R,R*)-**6** (77.9 mg, 50.4 µmol, 26.1 %).

$C_{90}H_{76}Cl_4O_8P_2Si_2$ (1545.51 g/mol)

^{1}H NMR (600 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ = 7.81, 7.80 (each d, each ^4J = 2.1 Hz, each 2H, H-6 and H-16), 7.65 (ps d, ^3J = 8.2 Hz, 4H, H-31), 7.56 (ps d, ^3J = 8.2 Hz, 4H, H-23), 7.48 (ps d, ^3J = 8.2 Hz, 4H, H-30), 7.43 (s, 2H, H-13), 7.41 (ps d, ^3J = 8.2 Hz, 4H, H-22), 7.40 (s, 2H, H-3), 7.30 (d, ^3J = 9.0 Hz, 2H, H-19), 7.28 (d, ^3J = 9.0 Hz, 2H, H-9), 7.18, 7.17 (each dd, each ^3J = 9.0 Hz, ^4J = 2.1 Hz, each 2H, H-8 and H-18), 1.05 (s, 36H, H-28), 1.04 (s, 6H, H-27).

^{13}C NMR (151 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ = 146.95, 146.94 (each d, each $^2J_{C\text{-}P}$ = 9.2 Hz, C-2 and C-12), 142.3 (C-4), 141.9 (C-14), 139.6 (C-29), 138.5 (C-21), 132.8 (C-31), 132.26 (C-23), 132.28, 132.19 (C-7, C-17), 131.05, 131.00 (C-10, C-20), 130.7 (C-5), 130.5 (C-15), 130.0 (C-30), 129.7 (C-22), 128.9, 128.8 (C-9, C-19), 127.75, 127.71 (C-8, C-18), 125.3, 125.2 (C-6, C-16), 123.5 (C-24), 122.5 (d, $^3J_{C\text{-}P}$ = 2.0 Hz, C-13), 122.4 (d, $^3J_{C\text{-}P}$ = 2.0 Hz, C-3), 121.7 (C-32), 121.0 (d, $^4J_{C\text{-}P}$ = 1.7 Hz, C-11), 120.7 (d, $^4J_{C\text{-}P}$ = 1.7 Hz, C-1), 106.5 (C-25), 92.0 (C-26), 81.5 (C-33), 74.9 (C-34), 18.5 (C-28), 11.3 (C-27).

^{31}P NMR (243 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ = 3.6 ($\nu_{1/2}$ = 19.5 Hz).

COSY (600 MHz, [D1]-chloroform, [D4]-methanol, 298 K) δ (^{1}H) / δ (^{1}H) = 7.65 / 7.48 (H-31 / H-30), 7.56 / 7.41 (H-23 / H-22), 7.48 / 7.65 (H-30 / H-31), 7.41 / 7.56 (H-22 / H-23), 7.30, 7.28 / 7.18, 7.17 (H-9, H-19 / H-8, H-18), 7.18, 7.17 / 7.30, 7.28 (H-8, H-18 / H-9, H-19).

HSQC (600/151 MHz, [D1]-chloroform, [D4]-methanol, 298 K) δ (^{1}H) / δ (^{13}C) = 7.81, 7.80 / 125.3, 125.2 (H-6, H-16 / C-6, C-16), 7.65 / 132.8 (H-31 / C-31), 7.56 / 132.26 (H-23 / C-23), 7.48 / 130.0 (H-30 / C-30), 7.43 / 122.5 (H-13 / C-13), 7.41 / 129.7 (H-22 / C-22), 7.40 / 122.4 (H-3 / C-3), 7.30, 7.28 / 128.9, 128.8 (H-9, H-19 / C-9, C-19), 7.18, 7.17 / 127.75, 127.71 (H-8, H-18 / C-8, C-18), 1.05 / 18.5 (H-28 / C-28), 1.04 / 11.3 (H-27 / C-27).

HMBC (600/151 MHz, [D1]-chloroform, [D4]-methanol, 298 K) δ (^{1}H) / δ (^{13}C) = 7.81, 7.80 / 142.3, 141.9, 132.28, 132.19, 131.05, 131.00, 127.75, 127.71 (H-6, H-16 / C-4, C-14, C-7, C-17, C-10, C-20, C-8, C-18), 7.65 / 139.6, 132.8, 81.5 (H-31 / C-29, C-31, C-33), 7.56 / 138.5, 132.26, 129.7, 106.5 (H-23 / C-21, C-23, C-22, C-25), 7.48 / 141.9, 130.0, 121.7 (H-30 / C-14, C-30, C-32), 7.43 / 146.95, 146.94, 139.6, 130.7, 121.0 (H-13 / C-2, C-12, C-29, C-15, C-11), 7.41 / 142.3, 132.26, 129.7, 123.5 (H-22 / C-4, C-23, C-22, C-24), 7.40 / 146.95, 146.94, 138.5, 130.5, 120.7 (H-3 / C-2, C-12, C-21, C-5, C-1),7.30, 7.28 / 132.28, 132.19, 130.7, 130.5, 121.0, 120.7 (H-9, H-19 / C-7, C-17, C-15, C-5, C-11, C-1), 7.18, 7.17 /131.05, 131.00, 125.3, 125.2 (H-8, H-18 / C-10, C-20, C-6, C-16), 1.05, 1.04 / 92.0, 18.5, 11.3 (H-28, H-27 / C-26, C-28, C-27).

IR (ATR) υ bar: 2940, 2863, 2360, 2156, 1583, 1493, 1320, 1259, 1180, 1149 cm^{-1}

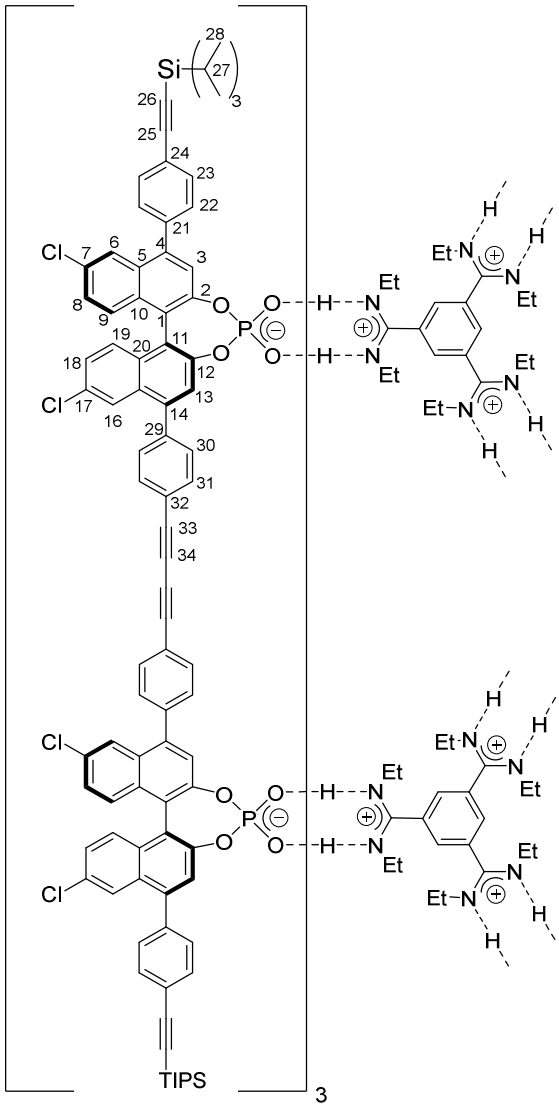
MS (ESI, -Mode): m/z = 770.1535 ([M-H]$^{2-}$, calculated: m/z = 770.1581)

Melting point: 153-154°C

Elemental analysis: expected C = 69.94 %, H = 4.96 %, found C = 69.3 %, H = 5.33 %

2.5. Synthesis of the supramolecular capsules

2.5.1. Capsule (*all-R*)-1



The bisphosphoric acid (*R,R*)-**7** (9.27 mg, 6.00 µmol, 3 eq.) was weighed into a vial. A stock solution of trisamidine **7** (500 µL of an 8 mM solution in [D_1]-chloroform : [D_4]-methanol (8/2 v/v), containing 4.00 µmol, 2 eq). The resulting solution (4 mM in capsule **1**) was analyzed by NMR.

$C_{312}H_{300}Cl_{12}N_{12}O_{24}P_6Si_6$ (5381.65 g/mol)

^{1}H NMR (600 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ = 7.78 (bs, 6H, H-35), 7.74, 7.72 (each d, each ^4J = 1.8 Hz, each 6H, H-6 and H-16), 7.56 (ps d, ^3J = 7.8 Hz, 12H, H-31), 7.49 (ps d, ^3J = 7.8 Hz, 12H, H-23), 7.42 (ps d, ^3J = 7.8 Hz, 12H, H-30), 7.33 (ps d, ^3J = 7.8 Hz, 12H, H-22), 7.27 (s, 6H, H-13), 7.25 (s, 6H, H-3), 7.23, 7.21 (each d, each ^3J = 9.0 Hz, each 6H, H-9, H-19), 7.09, 7.07 (each dd, each ^3J = 9.0 Hz, ^4J = 1.8 Hz, each 6H, H-8 and H-18), 3.13, 3.10 (each bs, each 12H, H-38, H-40), 1.05 (s, 126H, H-28, H-27), 0.95, 0.90 (each bs, each 18H, H-39, H-41).

^{13}C NMR (151 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ = 160.7 (C-37), 148.6 (d, $^2J_{C\text{-}P}$ = 8.9 Hz, C-2, C-12 (isochronous signals)), 141.3 (C-4), 140.8 (C-14), 140.0 (C-29), 138.9 (C-21), 132.7 (C-31), 132.3 (C-23), 131.5, 131.4 (C-7, C-17), 131.2, 131.1 (C-10, C-20), 130.6 (C-35), 130.0, 129.8 (C-5, C-15), 130.0 (C-30), 129.6 (C-22), 128.8, 128.7 (C-9, C-19), 127.24, 127.20 (C-8, C-18), 125.0, 124.9 (C-6, C-16), 123.4 (C-13), 123.3 (C-3), 123.2 (C-24), 121.7 (C-11), 121.39 (C-1), 121.36 (C-32), 106.5 (C-25), 91.8 (C-26), 81.5 (C-33), 74.9 (C-34), 40.8, 38.2 (C-38, C-40), 18.5 (C-28), 14.9, 12.2 (C-39, C-41), 11.2 (C-27). C-36 was not observed.

^{31}P NMR (243 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ = 4.7 ($\nu_{1/2}$ = 15 Hz).

COSY (600 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ (^{1}H) / δ (^{1}H) = 7.74, 7.72 / 7.09, 7.07 (H-6, H-16 / H-8, H-18), 7.56 / 7.42 (H-31 / H-30), 7.49 / 7.33 (H-23 / H-22), 7.42 / 7.56 (H-30 / H-31), 7.33 / 7.49 (H-22 / H-23), 7.23, 7.21 / 7.09, 7.07 (H-9, H-19 / H-8, H-18), 7.09, 7.07 / 7.74, 7.72, 7.23, 7.21 (H-8, H-18 / H-6, H-16, H-9, H-19), 3.13,

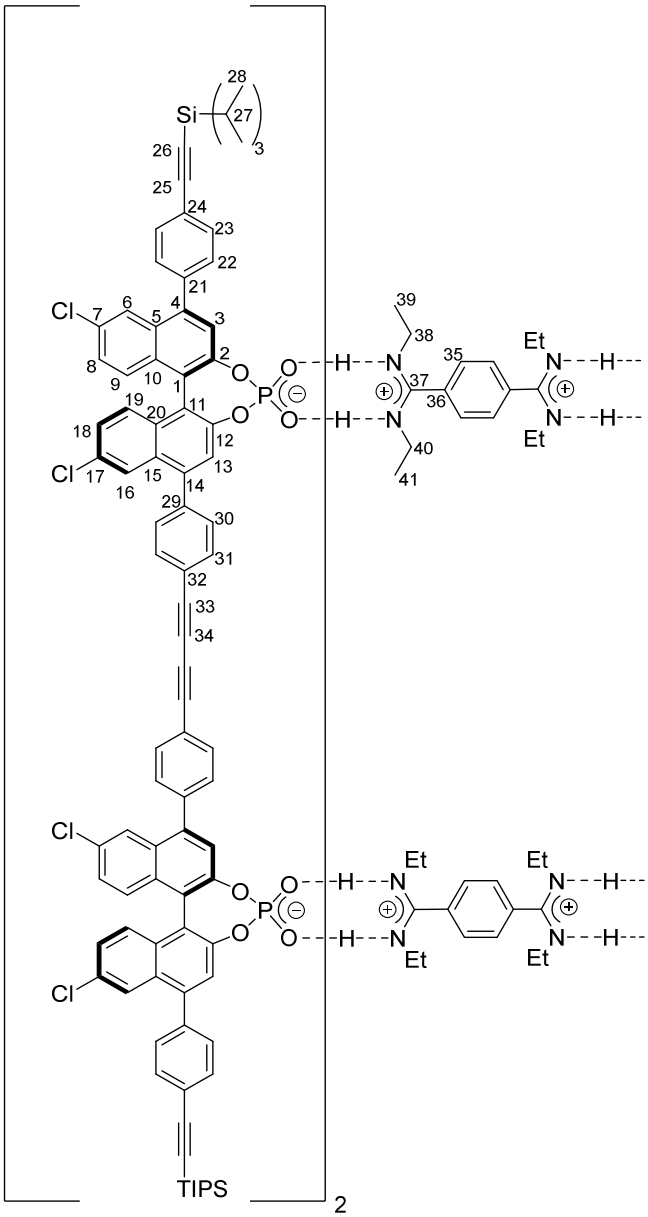
3.10 / 0.95, 0.90 (H-38, H-40 / H-39, H-41), 0.95, 0.90 / 3.13, 3.10 (H-39, H-41 / H-38, H-40).

HSQC (600/151 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ (^{1}H) / δ (^{13}C) = 7.78 / 130.6 (H-35 / C-35), 7.74, 7.72 / 125.0, 124.9 (H-6, H-16 / C-6, C-16), 7.56 / 132.7 (H-31 / C-31), 7.49 / 132.3 (H-23 / C-23), 7.42 / 130.0 (H-30 / C-30), 7.33 / 129.6 (H-22 / C-22), 7.27 / 123.4 (H-13 / C-13), 7.25 / 123.3 (H-3 / C-3), 7.23, 7.21 / 128.8, 128.7 (H-9, H-19 / C-9, C-19), 7.09, 7.07 / 127.24, 127.20 (H-8, H-18 / C-8, C-18), 3.13, 3.10 / 40.8, 38.2 (H-38, H-40 / C-38, C-40), 1.05 / 18.5, 11.2 (H-28, H-27 / C-28, C-27), 0.95, 0.90 / 14.9, 12.2 (H-39, H-41 / C-39, C-41).

HMBC (600/151 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ (^{1}H) / δ (^{13}C) = 7.74, 7.72 / 141.3, 140.8, 131.5, 131.4, 131.2, 131.1, 127.24, 127.20 (H-6, H-16 / C-4, C-14, C-7, C-17, C-10, C-20, C-8, C-18), 7.56 / 140.0, 132.7, 130.0, 81.5 (H-31 / C-29, C-31, C-30, C-33), 7.49 / 138.9, 132.3, 129.6, 106.5 (H-23 / C-21, C-23, C-22, C-25), 7.42 / 140.8, 132.7, 130.0, 121.36 (H-30 / C-14, C-31, C-30, C-32), 7.33 / 141.3, 132.3, 129.6, 123.2 (H-22 / C-4, C-23, C-22, C-24), 7.27 / 148.6, 140.0, 130.0, 129.8, 121.7 (H-13 / C-12, C-29, C-15, C-11), 7.25 / 148.6, 138.9, 130.0, 129.8, 121.39 (H-3 / C-2, C- 21, C-5, C-1), 7.23, 7.21 / 131.5, 131.4, 130.0, 129.8, 121.7, 121.39 (H-9, H-19 / C-7, C-17, C-5, C-15, C-1, C-11), 7.09, 7.07 / 131.2, 131.1, 125.0, 124.9 (H-8, H-18 / C-10, C-20, C-6, C-16), 1.05 / 91.8, 18.5, 11.2 (H-28, H-27 / C-26, C-28, C-27).

NOESY (600 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ (^{1}H) / δ (^{1}H) = 7.78 / 3.13, 3.10, 0.95, 0.90 (H-35 / H-38, H-40, H-39, H-41), 7.74, 7.72 / 7.42, 7.33 (H-6, H-16 / H-30, H-22), 7.56 / 7.42, 0.95, 0.90 (H-31 / H-30, H-39, H-41), 7.49 / 7.33, 0.95, 0.90 (H-23 / H-22, H-39, H-41), 7.42 / 7.74, 7.72, 7.56, 7.27, 7.25, 0.95, 0.90 (H-30 / H-16, H-31, H-13, H-39, H-41), 7.33 / 7.74, 7.72 7.49, 0.95, 0.90 (H-22 / H-6, H-23, H-39, H-41), 7.27, 7.25 / 7.42, 3.13, 3.10, 0.95, 0.90 (H-3, H-13 / H-30, H-38, H-40, H-39, H-41), 7.23, 7.21 / 7.09, 7.07 (H-9, H-19 / H-8, H-18), 7.09, 7.07 / 7.23, 7.21 (H-8, H-18 / H-9, H-19), 3.13, 3.10 / 7.78, 7.27, 7.25, 0.95, 0.90 (H-38, H-40 / H-35, H-3, H-13, H-39, H-41), 0.95, 0.90 / 7.56, 7.49, 7.42, 7.33, 7.27, 7.25, 3.13, 3.10 (H-39, H-41 / H-31, H-23, H-30, H-22, H-13, H-3, H-38, H-40).

2.5.2. Capsule (*all-R*)-2



The bisphosphoric acid (*R,R*)-**6** (2.16 mg, 1.40 µmol, 2 eq.) was weighed into a vial. A stock solution of bisamidine **8** (175 µL of an 8 mM solution in [D_1]-chloroform : [D_4]-methanol (8/2 v/v), containing 1.40 µmol, 2 eq). The resulting solution (4 mM in capsule **2**) was analyzed by NMR.

$C_{212}H_{204}Cl_8N_8O_{16}P_4Si_4$ (3639.84 g/mol)

^{1}H NMR (600 MHz, [D_1]-chloroform, 298 K) δ = 7.70, 7.69 (each d, each ^4J = 1.8 Hz, each 4H, H-6 and H-16), 7.55 (ps d, ^3J = 7.8 Hz, 8H, H-31), 7.47 (ps d, ^3J = 7.8 Hz, 8H, H-23), 7.44 (s, 8H, H-35), 7.41 (ps d, ^3J = 7.8 Hz, 8H, H-30), 7.38 (ps d, ^3J = 7.8 Hz, 8H, H-22), 7.30, 7.28 (each s, each 4H, H-3 and H-13), 7.22, 7.20 (each d, each ^3J = 9.0 Hz, each 4H, H-9, H-19), 7.05, 7.04 (each dd, each ^3J = 9.0 Hz, ^4J = 1.8 Hz, each 4H, H-8 and H-18), 3.15, 3.02 (each q, each ^3J = 7.5 Hz, each 8H, H-38, H-40), 0.98 (s, 84H, H-28, H-27), 0.95, 094 (each t, each ^3J = 7.5 Hz, each 12H, H-39, H-41).

^{13}C NMR (151 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ = 162.3 (C-37), 148.6 (d, $^2J_{C\text{-}P}$ = 9.1 Hz, C-2, C-12 (isochronous signals)), 141.3 (C-4), 140.9 (C-14), 140.0 (C-29), 138.9 (C-21), 132.6 (C-31), 132.1 (C-23), 131.39, 131.35 (C-7, C-17), 131.29 (C-36), 131.13, 131.08 (C-10, C-20), 129.96, 129.8 (C-5, C-15), 129.93 (C-30), 129.6 (C-22), 128.8, 128.6 (C-9, C-19), 128.7 (C-35), 127.11, 127.07 (C-8, C-18), 125.0, 124.8 (C-6, C-16), 123.5, 123.3 (C-3, C-13), 123.1 (C-24), 121.6, 121.35 (C-1, C-11), 121.27 (C-32), 106.5 (C-25), 91.6 (C-26), 81.4 (C-33), 74.7 (C-34), 40.6, 38.0 (C-38, C-40), 18.4 (C-28), 15.0, 12.1 (C-39, C-41), 11.2 (C-27).

^{31}P NMR (243 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ = 5.4 ($\nu_{1/2}$ = 99 Hz).

COSY (600 MHz, [D_1]-chloroform, [D_4]-methanol, 298 K) δ (^{1}H) / δ (^{1}H) = 7.70, 7.69 / 7.05, 7.04 (H-6, H-16 / H-8, H-18), 7.47 / 7.38 (H-23 / H-22), 7.38 / 7.47 (H-22 / H-23),

7.22, 7.20 / 7.05, 7.04 (H-9, H-19 / H-8, H-18), 7.05, 7.04 / 7.70, 7.69, 7.22, 7.20 (H-8, H-18 / H-6, H-16, H-9, H-19).

HSQC (600/151 MHz, [D$_1$]-chloroform, 298 K) δ (^{1}H) / δ (^{13}C) = 7.70, 7.69 / 125.0, 124.8 (H-6, H-16 / C-6, C-16), 7.55 / 132.6 (H-31 / C-31), 7.47 / 132.1 (H-23 / C-23), 7.44 / 128.7 (H-35 / C-35), 7.41 / 129.93 (H-30 / C-30), 7.38 / 129.6 (H-22 / C-22), 7.30, 7.28 / 123.5, 123.3 (H-3, H-13 / C-3, C-13), 7.22, 7.20 / 128.8, 128.6 (H-9, H-19 / C-9, C-19), 7.05, 7.04 / 127.11, 127.07 (H-8, H-18 / C-8, C-18), 3.15, 3.02 / 40.6, 38.0 (H-38, H-40 / C-38, C-40), 0.98 / 18.4, 11.2 (H-28, H-27 / C-28, C-27), 0.95, 094 / 15.0, 12.1 (H-39, H-41 / C-39, C-41).

HMBC (600/151 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ (^{1}H) / δ (^{13}C) = 7.70, 7.69 / 141.3, 140.9, 131.39, 131.35, 131.13, 131.08, 127.11, 127.07 (H-6, H-16 / C-4, C-14, C-7, C-17, C-10, C-20, C-8, C-18), 7.55 / 140.0, 132.6, 81.4 (H-31 / C-29, C-31, C-33), 7.47 / 138.9, 132.1, 106.5 (H-23 / C-21, C-23, C-25), 7.44 / 131.29 (H-35 / C-36), 7.41 / 129.93, 121.27 (H-30 / C-30, C-32), 7.38 / 129.6, 123.1 (H-22 / C-22, C-24), 7.30, 7.28 / 129.96, 129.8 (H-3, H-13 / C-5, C-15), 7.22, 7.20 / 131.39, 131.35, 129.96, 129.8, 121.6, 121.35 (H-9, H-19 / C-7, C-17, C-5, C-15, C-1, C-11), 7.05, 7.04 / 131.39, 131.35, 131.13, 131.08, 125.0, 124.8 (H-8, H-18 / C-7, C-17, C-10, C-20, C-6, C-16), 0.98 / 18.4, 11.2 (H-28, H-27 / C-28, C-27), 0.95, 094 / 40.6, 38.0 (H-39, H-41 / C-38, C-40).

NOESY(600 MHz, [D$_1$]-chloroform, [D$_4$]-methanol, 298 K) δ (^{1}H) / δ (^{1}H) = 7.70, 7.69 / 7.41, 7.38 (H-6, H-16 / H-30, H-22), 7.55 / 7.41 (H-31 / H-30), 7.47 / 7.38, 0.95, 0.94 (H-23 / H-22, H-39, H-41), 7.41 / 7.55, 7.70, 7.69 (H-30 / H-31, H-16), 7.38 / 7.47, 7.70, 7.69 (H-22 / H-23, H-6), 7.22, 7.20 / 7.05, 7.04 (H-9, H-19 / H-8, H-18), 7.05, 7.04 / 7.22, 7.20 (H-8, H-18 / H-9, H-19), 0.95, 0.94 / 7.47 (H-39, H-41 / H-23).

3. Characterization of the capsules

3.1. Structure calculations

C_3- and C_2-symmetric input structures of the (*all-R*)-**1** and (*all-R*)-**2** were generated and pre-optimized on force field level (Schrödinger MacroModel 10.1, OPLS 2005 force field, chloroform solvent) to remove any large structural constraints. Afterwards, two FF-optimized structures of (*all-R*)-**1** were obtained, which represent a right- and a left-handed helical assembly (cf. Figures S2 and S3). The left-handed helical form was found to be about 3 kcal/mol more stable than the right-handed structure. For (*all-R*)-**2**, a single almost planar and rectangular structure was obtained (Fig. S4).

In order to further refine the structures, the FF-optimized geometries were subject to density functional theory (DFT) calculations at the B3LYP/6-31G(d,p)/IEFPCM(chloroform) level of theory.[4] During the course of the DFT-based geometry optimization, the almost planar structure of (*all-R*)-**2** changed to a notably twisted structure with the ≡C-**C**-**C**-C≡ bonds on the opposing sides featuring a tilt angle of ~39°. Interestingly, the left-handed helical structure of (*all-R*)-**1** was found to be unfavorable on DFT level. In fact, it converted to the right-handed structure in any of the attempts to optimize it. This is particularly important to note, as DFT therefore suggests the former higher-energy conformer to actually be the only structure that is adopted by (*all-R*)-**1**. It moreover suggests that there might be structural or steric effects that are not accurately captured by the force field, which render the left-handed structure energetically so unfavorable that it is no longer a minimum on the potential energy surface. As the structural change occurred within the first ten steps of the geometry optimization, this observation leads to the suggestion that force-field optimized structures should always be further refined on low DFT level in order to confirm the stability of the structure and to exclude large destabilizing effects that the force field may not capture accurately.

Cartesian coordinates and figures of the structures are provided below. It should be noted that the final DFT structure of (*all-R*)-**1** was not optimized to full convergence of the electronic structure, but geometrical changes between subsequent optimization steps were very small and only involving the exact position of the TIPS groups.

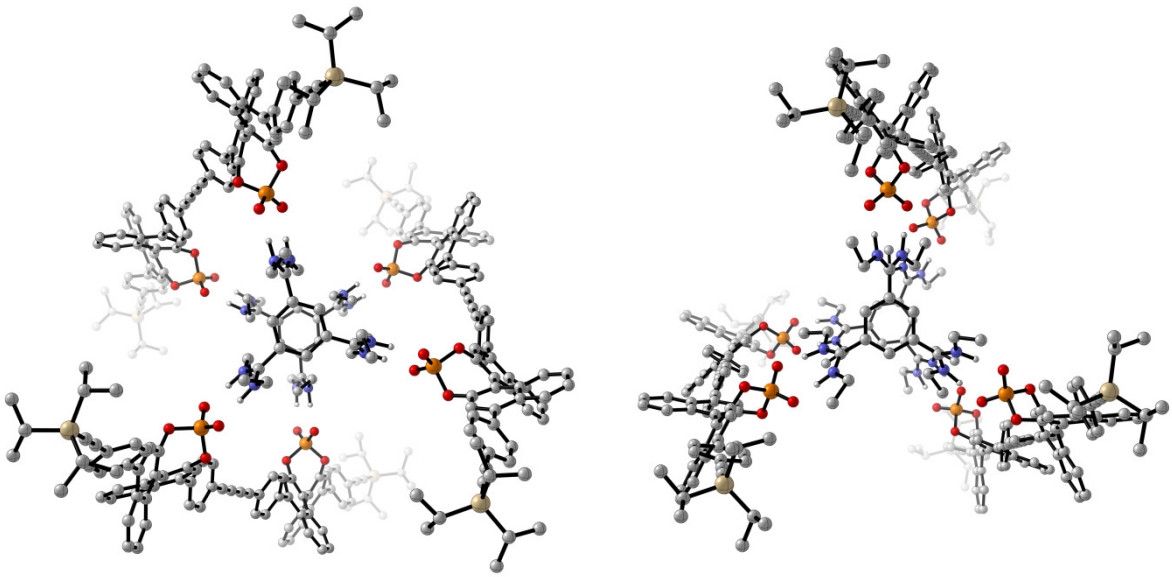


Figure S 2: View along the C3-axis of the DFT-optimized (*all-R*)-**1** in its right-handed helical structure (left) and of the OPLS-force field optimized left-handed structure (right) which is not stable on DFT level.

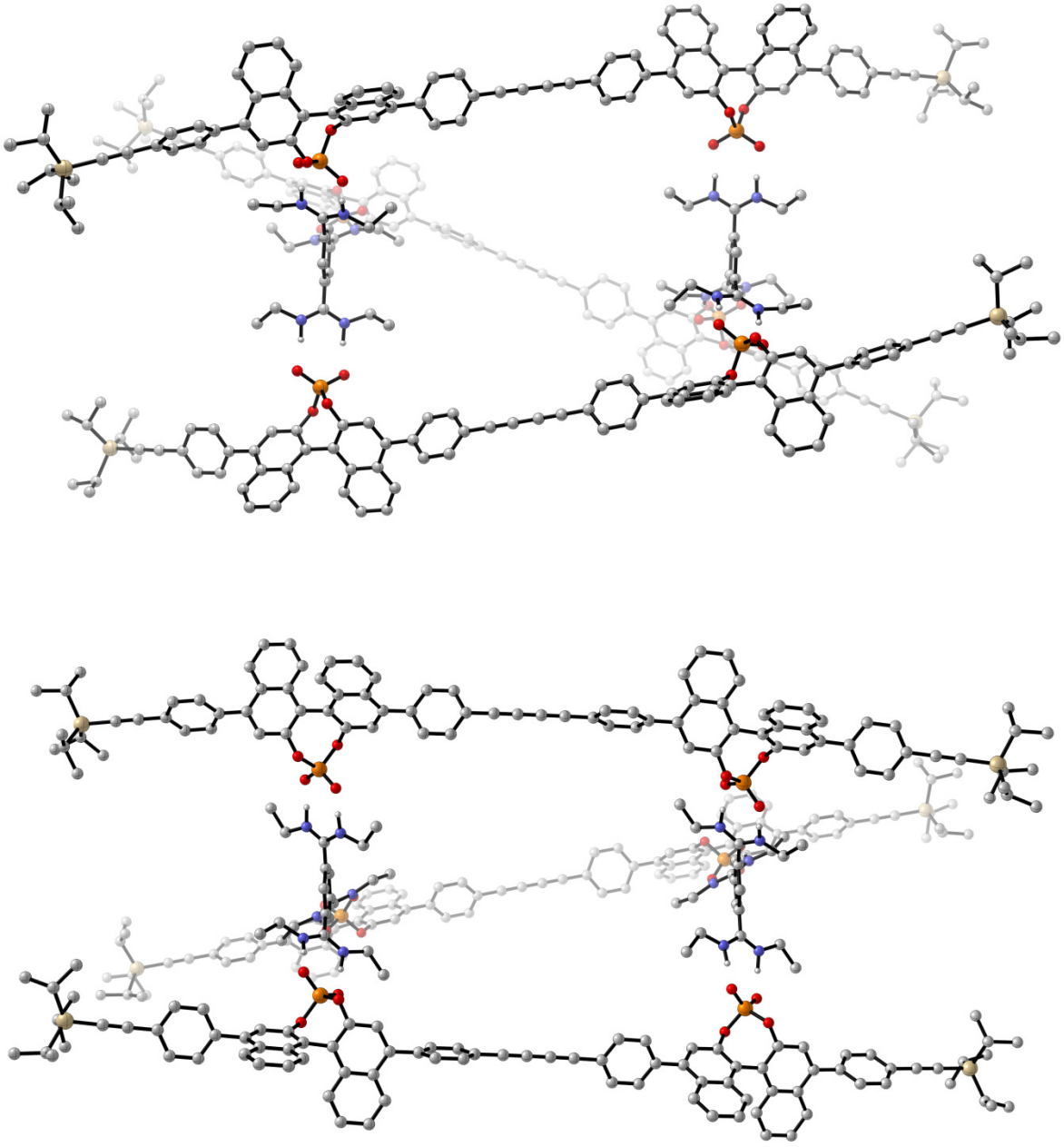


Figure S 3: Side-view of (*all-R*)-**1** in its right-handed helical structure obtained from DFT calculations (top) and in its left-handed structure obtained on force field level (bottom).

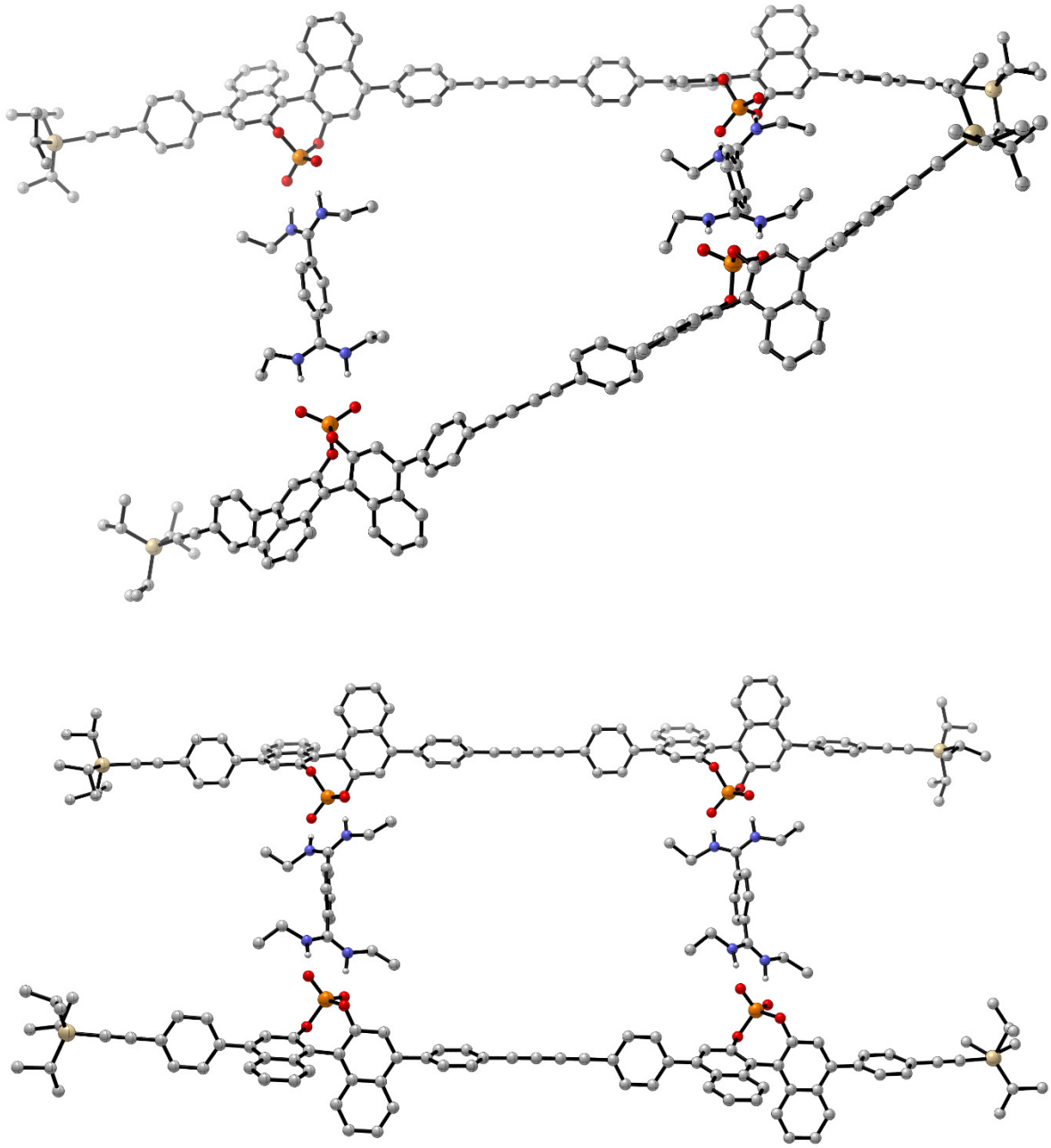


Figure S 4: DFT-optimized (top) and force-field optimized (bottom) structure of (*all-R*)-**2**

Cartesian coordinates

(*all-R*)-**1**, DFT optimized right-handed structure				(*all-R*)-**1**, OPLS-optimized left-handed structure			
C	-0.92742700	10.75626400	0.40963400	C	-10.98710000	0.13920000	1.48310000
C	-1.63823800	10.58408600	1.60225900	C	-11.06650000	1.25370000	0.61860000
C	-0.95047900	10.44989500	2.81294600	C	-11.08070000	1.07180000	-0.78180000
C	0.44767600	10.48817300	2.83162400	C	-11.02190000	-0.23430000	-1.31660000
C	1.15776900	10.65767300	1.63818800	C	-10.94480000	-1.35470000	-0.45980000
C	0.47060900	10.79617000	0.42781400	C	-10.92500000	-1.16300000	0.93920000
C	-1.71290500	10.25203100	4.08966800	C	-11.14790000	2.23640000	-1.67880000
N	-1.82835600	11.25190800	4.95187400	N	-12.16080000	2.37470000	-2.56210000
N	-2.26822200	9.07702900	4.34395400	N	-10.19620000	3.19460000	-1.64060000
H	-2.85021500	8.97502900	5.21015100	H	-10.33000000	4.08260000	-2.18640000
C	-2.16811400	7.85011000	3.54629500	C	-8.98560000	3.23380000	-0.80750000
H	-2.31264600	11.07224500	5.86522900	H	-12.09950000	3.10940000	-3.31090000
C	-1.35342600	12.63104200	4.79041600	C	-13.34270000	1.51630000	-2.72300000
H	-2.72264800	10.55030600	1.58710200	H	-11.11330000	2.25240000	1.03270000
H	0.98119500	10.38058700	3.77045400	H	-11.03450000	-0.37700000	-2.38800000
H	1.02202400	10.93068200	-0.49703500	H	-10.86290000	-2.01850000	1.59920000
C	1.25130000	-10.57527200	-2.40551600	C	11.05430000	-0.89010000	-1.10500000
C	1.57144500	-10.72128300	-1.05188900	C	11.00290000	0.47290000	-1.47260000
C	0.55259500	-10.86712600	-0.10448000	C	10.99140000	1.48080000	-0.48350000
C	-0.78598000	-10.86895100	-0.51062100	C	11.02870000	1.11860000	0.88150000
C	-1.10495100	-10.72130300	-1.86461200	C	11.07790000	-0.24180000	1.25920000
C	-0.08683600	-10.57532100	-2.81270400	C	11.09320000	-1.24150000	0.26240000
H	2.60927600	-10.71592000	-0.73495800	H	10.97560000	0.74420000	-2.51970000
H	-1.57679200	-10.97551400	0.22489900	H	11.01750000	1.88680000	1.64180000
H	-0.33579700	-10.45565100	-3.86213100	H	11.12860000	-2.28520000	0.54560000
C	0.89703200	-11.00323800	1.34846300	C	10.93590000	2.89920000	-0.87330000
N	1.34795700	-9.95080300	2.01537300	N	9.91840000	3.37310000	-1.62530000
N	0.75176900	-12.17107700	1.95744700	N	11.90090000	3.76330000	-0.49010000
H	0.92202600	-12.21889000	2.99167600	H	11.75120000	4.79540000	-0.62080000
C	0.40202400	-13.46039500	1.35050900	C	13.14030000	3.46970000	0.24270000
H	1.65039200	-10.08211400	3.01066000	H	9.98230000	4.33980000	-2.03200000
C	1.43537200	-8.56288300	1.54751700	C	8.73480000	2.64610000	-2.10590000
C	2.34569900	-10.39788400	-3.41599600	C	11.06610000	-1.93850000	-2.13860000
N	3.07466500	-11.43981200	-3.78852800	N	12.01430000	-1.94990000	-3.08710000
N	2.57731600	-9.19526300	-3.92060700	N	10.12850000	-2.89780000	-2.14510000
C	2.65696100	10.68624800	1.65365100	C	-10.89010000	-2.71430000	-1.02040000
N	3.29456000	11.83123700	1.46206800	N	-11.83030000	-3.63160000	-0.70490000
N	3.33428700	9.56447000	1.85363900	N	-9.89950000	-3.07860000	-1.86360000
C	2.70609500	13.17020300	1.35141800	C	-13.02240000	-3.45140000	0.13590000
H	4.34137100	11.81346400	1.39317600	H	-11.69580000	-4.63260000	-0.99510000
C	2.80276700	8.19913000	1.93534100	C	-8.73010000	-2.29190000	-2.27940000
H	4.37781300	9.61823200	1.93666400	H	-9.98360000	-3.97770000	-2.40100000
H	3.88932100	-11.27604200	-4.42810900	H	11.96110000	-2.65600000	-3.87680000
C	2.92064900	-12.83168000	-3.34694900	C	13.21150000	-1.11060000	-3.22720000
C	1.89380600	-7.94389900	-3.57059600	C	8.91950000	-3.03470000	-1.32230000
H	3.29446100	-9.09921400	-4.68078600	H	10.20910000	-3.70920000	-2.82340000
C	-2.54035700	-10.70264200	-2.29801600	C	11.11020000	-0.61760000	2.68190000
N	-3.04799300	-11.74208100	-2.94389000	N	12.12680000	-1.35350000	3.18180000
N	-3.29125900	-9.64448800	-2.03135500	N	10.12180000	-0.23980000	3.52200000
C	-1.66409600	10.88726500	-0.88999400	C	-10.96690000	0.33380000	2.94170000
N	-1.63456000	9.89164500	-1.76366800	N	-9.94170000	-0.12510000	3.67350000
N	-2.33359000	11.99844500	-1.16005200	N	-11.97220000	0.97280000	3.55660000
H	-2.09351900	10.03071500	-2.69641000	H	-10.04510000	-0.17040000	4.72790000
C	-1.06530700	8.55224200	-1.57574700	C	-8.70300000	-0.76840000	3.21690000
H	-2.89981400	12.03826900	-2.04192300	H	-11.84280000	1.28320000	4.56210000
C	-2.35900600	13.23936200	-0.37769300	C	-13.22450000	1.48100000	2.98170000
H	-4.02920200	-11.67327900	-3.30765000	H	12.04640000	-1.75600000	4.14920000
C	-2.40837800	-13.03862500	-3.19269800	C	13.32900000	-1.82660000	2.48110000
C	-2.85988800	-8.36752500	-1.45257800	C	8.88240000	0.47870000	3.19480000
H	-4.31233500	-9.68073300	-2.27070800	H	10.24120000	-0.37380000	4.55730000
C	6.07827600	-23.92726700	8.46423500	C	22.82110000	13.16630000	-0.06470000
C	-6.45533900	12.17655800	13.88252300	C	-13.78840000	8.51020000	-10.16780000
C	7.28788900	-23.80522300	7.51887400	C	23.51350000	12.12640000	-0.96150000
C	-5.99704200	10.84297200	13.95504200	C	-12.40650000	8.67250000	-9.98270000
O	-5.44139800	10.01121900	7.92440100	O	-12.30740000	6.68910000	-4.18450000
C	8.01720500	-25.15637700	7.38778800	C	25.04180000	12.26130000	-0.88040000
C	-5.76748800	10.12536500	12.80320900	C	-11.82970000	8.39090000	-8.73160000
Si	6.83387000	-23.00545800	5.83638000	Si	22.92620000	10.34760000	-0.56430000
C	-5.99021600	10.69181500	11.51685000	C	-12.62050000	7.95060000	-7.63980000
C	8.41036700	-22.74819300	4.77938500	C	23.75070000	9.10640000	-1.76920000
P	-3.85035400	9.70233200	7.59451000	P	-11.27100000	5.36720000	-4.20940000
C	8.13094600	-22.00647600	3.45830000	C	23.21800000	7.67690000	-1.57680000
C	-6.44543000	12.05455200	11.44281700	C	-14.02090000	7.77150000	-7.83670000
C	9.52718200	-22.03778100	5.56817000	C	23.57790000	9.55700000	-3.22900000
C	-6.66502700	12.76514500	12.65608600	C	-14.58740000	8.05880000	-9.10300000
C	5.48862000	-24.02631600	4.91932000	C	23.28130000	9.90190000	1.26980000
C	4.54880000	-23.18824600	4.03180700	C	22.26430000	8.89640000	1.83850000
C	-5.71465500	9.95400400	10.31180600	C	-12.02700000	7.67760000	-6.37250000
C	6.07946700	-25.20538700	4.11877600	C	24.71920000	9.39020000	1.46150000
O	-3.84929700	8.63956600	6.52461500	O	-10.45650000	5.36190000	-2.97580000
C	-5.76741700	10.64693100	9.11281800	C	-12.84600000	7.12080000	-5.36150000

C	6.14332400	-21.33695600	6.22979200	C	21.11370000	10.31100000	-0.85810000
O	-3.06379500	10.96998500	7.37256200	O	-12.06090000	4.13500000	-4.41850000
C	5.70282600	-20.22916800	6.50218700	C	19.91120000	10.28120000	-1.06630000
C	5.17645300	-18.94871000	6.85215600	C	18.47910000	10.24110000	-1.30280000
C	-6.21618900	11.97892100	9.02892700	C	-14.22720000	6.95910000	-5.55680000
C	-6.59726800	12.67877100	10.15614300	C	-14.83670000	7.29540000	-6.77810000
C	4.14139900	-18.36443200	6.09694900	C	17.64060000	9.50280000	-0.44460000
O	-3.34853600	9.10518400	9.05318400	O	-10.26080000	5.60530000	-5.53080000
C	3.63493300	-17.11565100	6.44045000	C	16.25110000	9.46650000	-0.67600000
C	-4.38726800	5.80481600	10.26116000	C	-7.77780000	8.30830000	-5.67570000
C	5.68642800	-18.23863900	7.95714300	C	17.92260000	10.93980000	-2.39200000
C	5.17177300	-16.99242400	8.29518600	C	16.53260000	10.90000000	-2.61890000
C	-3.66803600	6.82202100	9.66683600	C	-8.36410000	7.03520000	-5.56940000
C	-4.13464900	8.15003000	9.67960700	C	-9.74530000	6.85070000	-5.74380000
C	4.13429300	-16.40841900	7.54693000	C	15.68260000	10.16750000	-1.76150000
C	3.61574500	-15.04893900	7.86396000	C	14.22960000	10.11940000	-2.00250000
C	-5.31336800	8.51997200	10.30724400	C	-10.58790000	7.93430000	-6.08800000
C	-6.11854100	7.47353600	10.88047900	C	-10.01540000	9.23920000	-6.13460000
C	3.10239500	-14.69631200	9.16009700	C	13.36920000	11.22940000	-1.79990000
C	2.68012200	-13.34349800	9.40784300	C	11.97530000	11.11780000	-2.07660000
C	-5.64183200	6.11576500	10.88928400	C	-8.61400000	9.42180000	-5.94780000
C	-7.40916400	7.73506700	11.42034100	C	-10.82740000	10.37990000	-6.35920000
C	2.93604800	-15.66092600	10.19293200	C	13.88400000	12.45370000	-1.30670000
C	2.38786500	-15.32444200	11.40982300	C	13.04040000	13.55540000	-1.08120000
C	-8.16378800	6.73835800	11.99610400	C	-10.26930000	11.66840000	-6.43370000
C	1.96236800	-13.99946500	11.64883000	C	11.66490000	13.44480000	-1.33860000
C	-7.66060200	5.42114400	12.07530400	C	-8.88450000	11.84030000	-6.28190000
C	-6.43228300	5.12178800	11.53144300	C	-8.06460000	10.72440000	-6.03970000
C	2.10183800	-13.03973000	10.67210200	C	11.13910000	12.23580000	-1.82760000
C	3.61110600	-14.09612900	6.86522700	C	13.66970000	8.90220000	-2.42850000
C	-7.12630100	14.06079800	9.99036500	C	-16.29270000	7.10600000	-6.90100000
C	3.19267200	-12.77564100	7.11695600	C	12.29490000	8.78280000	-2.68940000
C	-8.38311900	14.43218900	10.50045000	C	-17.16240000	8.21670000	-6.96430000
C	2.79510600	-12.34834900	8.37391700	C	11.43280000	9.89970000	-2.58080000
C	-8.89196400	15.70929300	10.29490600	C	-18.55520000	8.03430000	-7.07350000
C	-8.15544700	16.66602500	9.56842700	C	-19.09440000	6.73360000	-7.11690000
C	2.44841300	-10.91568500	8.58088300	C	10.00330000	9.75920000	-2.97210000
C	-6.89889000	16.29594800	9.05178500	C	-18.23560000	5.61880000	-7.04980000
C	1.53129200	-10.31105900	7.73625100	C	9.18480000	8.82780000	-2.28980000
C	-6.39945400	15.01459300	9.25861400	C	-16.84350000	5.80690000	-6.94040000
O	0.94964500	-11.03299100	6.70532800	O	9.71960000	7.96150000	-1.38100000
P	1.85592100	-11.36119600	5.36113900	P	10.78420000	6.78020000	-1.92340000
C	-8.67134000	17.98211500	9.36529400	C	-20.52950000	6.54260000	-7.23080000
C	-9.11314800	19.10699100	9.17967400	C	-21.73480000	6.38180000	-7.33990000
O	3.26195600	-11.87648100	6.06330200	O	11.80410000	7.55120000	-3.01310000
Si	-9.76960800	20.80560400	8.84238900	Si	-23.54260000	6.13690000	-7.53170000
O	1.14059200	-12.47734600	4.64181100	O	11.58580000	6.28490000	-0.78400000
C	-10.46000800	20.73836500	7.05368300	C	-24.19690000	5.69440000	-5.78290000
O	2.20914800	-10.10659600	4.60241200	O	10.02190000	5.72820000	-2.62940000
C	-11.12307500	21.09228000	10.17078900	C	-24.22540000	7.80650000	-8.18650000
C	1.09799000	-8.98377300	7.91748700	C	7.80890000	8.74230000	-2.55740000
C	-8.26057800	21.97473200	9.02978000	C	-23.73880000	4.70120000	-8.78980000
C	1.59693800	-8.19949600	8.93834300	C	7.20580000	9.53950000	-3.54560000
C	-11.60564800	22.54750700	10.32558500	C	-25.65940000	7.71050000	-8.73370000
C	2.63755800	-8.73263700	9.77537600	C	8.02390000	10.41440000	-4.30620000
C	3.06931000	-10.09177600	9.58497700	C	9.41840000	10.51600000	-4.02920000
C	-12.31573300	20.13392000	9.98366800	C	-24.10780000	8.90580000	-7.11760000
C	-11.35607700	21.92207800	6.64086100	C	-25.72760000	5.77880000	-5.66130000
C	4.15520300	-10.56929200	10.37078600	C	10.21260000	11.37270000	-4.83320000
C	4.77293400	-9.77018900	11.30593100	C	9.64450000	12.13030000	-5.87270000
C	-9.33854900	20.51003500	6.02122300	C	-23.67620000	4.31940000	-5.33250000
C	4.34216300	-8.43965500	11.50006500	C	8.26830000	12.03870000	-6.13290000
C	-8.45538500	23.40461500	8.48948100	C	-25.16120000	4.11880000	-8.83950000
C	-7.73938700	22.00076000	10.48008900	C	-23.25970000	5.12640000	-10.18790000
C	3.30613000	-7.93614700	10.74646500	C	7.46620000	11.18360000	-5.35710000
C	-1.98741400	2.88162900	10.54510900	C	-4.03150000	8.02100000	-6.23900000
C	1.04850900	-6.82620200	9.11002200	C	5.75400000	9.40250000	-3.75600000
C	0.99684700	-5.94550900	8.01566000	C	5.22050000	8.22190000	-4.31650000
C	-2.54148600	4.15201100	10.65301000	C	-5.42350000	7.93000000	-6.43770000
C	-3.84091000	4.42045400	10.19073400	C	-6.32360000	8.41860000	-5.46650000
C	0.44425100	-4.67648400	8.13864100	C	3.83200000	8.08190000	-4.51220000
C	-0.08336000	-4.24388300	9.37215100	C	2.95950000	9.12540000	-4.14420000
C	-4.56969500	3.36954800	9.60549300	C	-5.80520000	8.99330000	-4.28540000
C	-4.02457500	2.09673000	9.48929100	C	-4.41420000	9.08710000	-4.08140000
C	-0.03981300	-5.12587500	10.47150600	C	3.48170000	10.30570000	-3.57910000
C	0.51741900	-6.39191100	10.33788200	C	4.87070000	10.44000000	-3.38550000
C	-2.72172300	1.83090300	9.95945700	C	-3.52400000	8.60090000	-5.05940000
C	-0.64913500	-2.94563400	9.50110200	C	1.52750000	8.98570000	-4.34570000
C	-2.15838100	0.53087900	9.83600600	C	-2.08920000	8.69610000	-4.85200000
C	-1.67484600	-0.58609600	9.72548400	C	-0.88310000	8.78590000	-4.68260000
C	-1.13409300	-1.82869700	9.60576300	C	0.32240000	8.88200000	-4.51420000
H	5.57385200	-22.96649600	8.60784800	H	21.73570000	13.10510000	-0.15170000
H	5.33682900	-24.63758500	8.07950800	H	23.07720000	13.02400000	0.98520000
H	6.39025100	-24.29165400	9.45127300	H	23.11250000	14.18000000	-0.34070000
H	-6.62205100	12.74408200	14.79308000	H	-14.23540000	8.72230000	-11.12840000
H	7.98997300	-23.09327600	7.97742600	H	23.21990000	12.34080000	-1.98940000
H	-5.80775600	10.38658000	14.92208200	H	-11.78590000	9.01020000	-10.80030000
H	8.90353100	-25.09382300	6.74735200	H	25.54050000	11.50680000	-1.48920000
H	8.34798100	-25.51544600	8.37060800	H	25.36780000	13.23800000	-1.23880000

H	7.36034900	-25.92824800	6.97070700	H	25.39780000	12.15590000	0.14390000
H	-5.38951100	9.11256800	12.87005900	H	-10.76230000	8.51660000	-8.62940000
H	8.76753800	-23.75815800	4.52743500	H	24.81950000	9.09120000	-1.55550000
H	9.05491800	-21.88317800	2.87895800	H	23.68570000	6.98420000	-2.27680000
H	7.41644800	-22.54067600	2.82415400	H	23.42550000	7.30720000	-0.57370000
H	7.72478500	-21.00570200	3.64423300	H	22.13970000	7.62830000	-1.73290000
H	10.42471700	-21.91878800	4.94800200	H	24.06390000	8.86480000	-3.91690000
H	9.21420200	-21.03583200	5.88410300	H	22.52420000	9.61470000	-3.50480000
H	9.82042200	-22.59168500	6.46568900	H	24.01800000	10.54050000	-3.39500000
H	-6.98098600	13.80026600	12.60601500	H	-15.64430000	7.92640000	-9.28090000
H	4.87335800	-24.45306400	5.72557700	H	23.18000000	10.81640000	1.85360000
H	3.75442800	-23.81766100	3.61038800	H	22.48820000	8.65560000	2.87800000
H	4.07393600	-22.37802300	4.59234500	H	21.25220000	9.30130000	1.81510000
H	5.08302100	-22.73526100	3.18907400	H	22.25800000	7.96290000	1.27730000
H	5.27799800	-25.82294800	3.69402300	H	24.93920000	9.22180000	2.51600000
H	6.69381800	-24.85473700	3.28180900	H	24.88160000	8.44820000	0.93810000
H	6.70528300	-25.86063700	4.73288300	H	25.45320000	10.10170000	1.08710000
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H	3.73868400	-18.89936300	5.24313300	H	18.05970000	8.96360000	0.39290000
H	2.83159000	-16.68242400	5.85253900	H	15.61370000	8.89890000	-0.01320000
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O	-3.20917400	11.90625400	-5.90935500	O	-11.95060000	0.13630000	8.02900000
C	-12.26342300	-24.65110500	-2.24589500	C	25.66540000	-4.59230000	10.42540000
C	-7.30123000	12.70664200	-8.46841200	C	-11.32800000	3.02600000	11.90920000
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O	-2.77587300	10.06263900	-4.23750300
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C	-8.76779200	-16.26620400	-3.86644600
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H	23.99600000	-7.03550000	-11.07930000
H	-13.58540000	-14.15040000	-2.58660000

H	6.67275400	-20.40215100	-14.61074500	H	23.87860000	-7.76270000	-8.71950000
H	13.80256800	12.62886500	-0.69725200	H	-11.16360000	-13.91700000	-3.10810000
H	5.43292700	-22.52326300	-15.17484000	H	26.15860000	-7.00950000	-7.96750000
H	7.17885700	-22.70584500	-15.37419900	H	26.12380000	-7.50540000	-9.65360000
H	6.38096500	-23.39202600	-13.96076300	H	26.15560000	-5.79730000	-9.24790000
H	12.05582700	11.03324500	-0.05590500	H	-10.21930000	-11.71940000	-3.64040000
H	3.32236300	-21.56336600	-14.00946700	H	25.26620000	-6.04230000	-5.81910000
H	1.48564900	-19.96707400	-13.38949800	H	23.94750000	-5.78900000	-3.71070000
H	2.19920400	-20.70805400	-11.95363400	H	23.81060000	-4.37240000	-4.73350000
H	2.61769000	-19.04748400	-12.39092500	H	22.48490000	-5.52860000	-4.65600000
H	2.78937000	-19.59063700	-15.46860600	H	24.36300000	-8.07360000	-4.69740000
H	4.02766600	-18.63909100	-14.64272400	H	22.90570000	-7.97930000	-5.68230000
H	4.49058500	-20.04619800	-15.60833300	H	24.46440000	-8.30190000	-6.43510000
H	12.09116500	15.59487100	1.88508900	H	-15.04540000	-12.17580000	-2.58850000
H	6.10048400	-22.27614800	-11.03254400	H	23.94240000	-3.63340000	-8.94190000
H	4.57515400	-22.05084200	-9.09476700	H	23.16150000	-1.78430000	-7.46960000
H	5.15327800	-20.45733900	-9.61041500	H	21.91640000	-2.99380000	-7.71660000
H	3.51405400	-20.97638300	-10.00821400	H	22.79820000	-2.94240000	-6.19620000
H	4.27162800	-23.93023300	-10.74764600	H	25.62220000	-2.40190000	-7.62270000
H	3.19246500	-22.96305700	-11.75335700	H	25.42610000	-3.51090000	-6.27230000
H	4.62046300	-23.71875200	-12.46551100	H	26.11630000	-4.07800000	-7.78380000
H	8.15732600	13.47775900	3.67517800	H	-14.37800000	-7.47890000	-3.32110000
H	5.58330200	-17.08462900	-9.07705000	H	18.62800000	-4.05490000	-7.26530000
H	6.18806100	-14.86337700	-8.17846900	H	16.16590000	-4.34970000	-7.23360000
H	7.06115300	-15.91435900	-12.94456200	H	19.12530000	-8.31270000	-7.75470000
H	7.65599500	-13.69541800	-12.04492000	H	16.66250000	-8.60060000	-7.72000000
H	7.90516800	8.00078700	-0.56549800	H	-7.27340000	-7.66540000	-3.07890000
H	12.19760900	10.39688200	2.73732200	H	-11.50160000	-10.55800000	-6.10060000
H	9.57051500	-13.90900900	-10.42425200	H	15.69220000	-7.12030000	-9.95140000
H	11.81281400	-12.91003700	-10.47243400	H	14.36660000	-7.74680000	-11.92130000
H	13.98156100	8.78041200	3.19971500	H	-10.58550000	-11.58310000	-8.12920000
H	12.16881600	-10.59898300	-9.59474100	H	11.89910000	-8.01010000	-11.73770000
H	13.87751500	6.48269300	2.22585500	H	-8.16200000	-11.38070000	-8.65450000
H	11.97666600	5.83218800	0.81704300	H	-6.67080000	-10.13950000	-7.14840000
H	10.28076600	-9.31323900	-8.70541900	H	10.77430000	-7.65880000	-9.58830000
H	5.28139300	-12.49151300	-8.76521700	H	14.66390000	-6.07070000	-5.37950000
H	11.94653300	15.23298000	4.36434000	H	-16.30080000	-10.63940000	-4.70100000
H	11.83793100	17.39925300	5.53895500	H	-18.72760000	-10.74460000	-4.20290000
H	7.89913700	18.06641500	3.94219800	H	-18.02090000	-8.84940000	-0.39160000
H	8.01648000	15.90032800	2.75858400	H	-15.59480000	-8.74850000	-0.89580000
H	9.46351000	20.58144100	9.05047000	H	-23.32940000	-8.14670000	-2.87530000
H	11.74659800	22.43078600	6.05051100	H	-22.95010000	-12.34580000	-2.17650000
H	7.32499800	-6.91373400	-5.20671200	H	7.64810000	-5.49330000	-6.24660000
H	7.56454800	22.24007100	5.69106100	H	-22.38990000	-9.58630000	1.03830000
H	12.54745200	24.31358900	7.47856500	H	-25.38680000	-12.77470000	-2.53990000
H	10.96004800	24.66316400	6.79184300	H	-25.01280000	-12.34170000	-0.88700000
H	11.10706400	24.19259000	8.48799900	H	-25.75540000	-11.15880000	-1.95540000
H	13.31257900	21.96529000	7.92085400	H	-23.89560000	-12.05890000	-4.44240000
H	11.96327000	21.67875000	9.02136500	H	-24.24110000	-10.36540000	-4.10990000
H	12.23843400	20.58395600	7.66010100	H	-22.57660000	-10.92940000	-4.17410000
H	8.48640700	22.17885700	10.69983100	H	-25.60330000	-7.35460000	-2.19640000
H	9.92954000	22.85051100	9.93825900	H	-25.58590000	-9.03270000	-2.68930000
H	8.32777400	23.41120100	9.44892900	H	-25.67790000	-8.62270000	-0.98180000
H	8.32262000	-8.79693500	-10.73300400	H	11.75610000	-9.59870000	-7.53040000
H	9.00453700	-6.95417100	-12.19886200	H	10.73160000	-11.80500000	-7.82460000
H	7.02850500	20.50399300	9.52984200	H	-23.52200000	-6.23380000	-1.32150000
H	6.70081100	21.63308000	8.21393000	H	-23.48560000	-7.32250000	0.06100000
H	7.34152500	20.02366700	7.85614500	H	-22.07450000	-7.16880000	-0.97740000
H	9.28942300	-4.65201400	-11.27226000	H	8.26630000	-12.08100000	-7.63020000
H	7.18489200	24.69971100	5.86793800	H	-24.47190000	-10.31210000	2.21910000
H	7.30670700	23.95609000	7.46367400	H	-24.76440000	-9.05890000	1.03450000
H	8.66140000	24.88415500	6.81344700	H	-25.20070000	-10.72390000	0.67390000
H	8.34158200	23.72955500	3.86231000	H	-22.48590000	-11.85210000	2.02150000
H	9.92161600	23.89992500	4.62905200	H	-23.11220000	-12.50670000	0.51240000
H	9.40919800	22.32598000	4.00687200	H	-21.48400000	-11.84540000	0.57790000
H	8.86774500	-4.22624000	-8.89293700	H	6.84230000	-10.14430000	-7.12890000
H	11.33553500	4.03589500	-2.79650200	H	-2.99410000	-10.54740000	-5.01140000
H	6.27020200	-4.60004500	-5.62424700	H	6.19180000	-7.40580000	-4.47210000
H	11.59286000	6.19308500	-1.63236000	H	-5.42950000	-10.80590000	-4.62920000
H	6.58190400	-2.44582600	-4.45744900	H	3.73030000	-7.56610000	-4.22650000
H	7.81939100	5.58963200	0.33623800	H	-6.02940000	-6.64980000	-5.58720000
H	7.54787000	3.43473500	-0.83921000	H	-3.59430000	-6.38240000	-5.97020000
H	10.68294500	-2.34199700	-5.76523500	H	3.34980000	-8.13400000	-8.48820000
H	10.36960400	-4.49975900	-6.91403500	H	5.81260000	-7.97120000	-8.72470000
H	-1.46234600	8.00588700	2.72878900	H	-8.37410000	2.38370000	-1.02680000
H	-3.14913800	7.64903600	3.10069700	H	-9.26300000	3.21670000	0.22580000
H	-0.98462100	12.77197400	3.77341000	H	-13.90170000	1.50440000	-1.81080000
H	-0.50856000	12.78724300	5.47112400	H	-13.03090000	0.52140000	-2.96330000
H	0.35834100	-13.35195000	0.26588700	H	13.73320000	2.78020000	-0.32110000
H	-0.59978600	-13.74218700	1.69441600	H	12.89970000	3.03970000	1.19250000
H	1.01702400	-8.48964100	0.54247900	H	8.18060000	2.27450000	-1.26950000
H	2.49500600	-8.29096700	1.48363800	H	9.04470000	1.82710000	-2.72070000
H	1.63446200	13.11228000	1.54841900	H	-13.64740000	-2.69400000	-0.28910000
H	2.83327700	13.51630400	0.31927400	H	-12.72340000	-3.15640000	1.12000000
H	1.73138000	8.21201000	1.73017100	H	-8.14690000	-2.03790000	-1.41910000
H	2.93737500	7.83962200	2.96176700	H	-9.05720000	-1.39660000	-2.76560000
H	1.94155600	-12.95659900	-2.88096800	H	13.84000000	-1.24000000	-2.37090000
H	1.36619600	-8.07383500	-2.62383100	H	8.28360000	-2.18860000	-1.47910000
H	-0.71126200	8.44747700	-0.54909600	H	-8.16880000	-0.09880000	2.57580000

H	-0.19596200	8.45356700	-2.23575000
H	-1.66137800	13.15638800	0.45706700
H	-3.36357300	13.35996200	0.04370300
H	-1.43686500	-13.06477500	-2.69683800
H	-2.23128300	-13.13190000	-4.27016500
H	-1.77444700	-8.36707200	-1.34236200
H	-3.29338500	-8.28115900	-0.44972600
H	1.14410900	-7.72140500	-4.33953400
H	3.67902200	-13.04768500	-2.58466000
C	-1.73803200	6.67292100	4.42163900
H	-2.42221300	6.55218900	5.26560300
H	-1.74801700	5.75106600	3.83309200
H	-0.72860200	6.82466400	4.81478100
C	-2.47061500	13.62568200	5.10590700
H	-2.86519400	13.45377800	6.11082900
H	-2.08160300	14.64673600	5.05698800
H	-3.29341600	13.53125000	4.39132800
C	-2.01210700	14.43943700	-1.25905800
H	-2.68794100	14.49340200	-2.11658700
H	-2.11042100	15.36346900	-0.68210800
H	-0.98630700	14.36860700	-1.63223600
C	-2.09933500	7.47537400	-1.90562200
H	-2.48563300	7.61261000	-2.91901000
H	-1.63675500	6.48624400	-1.84161300
H	-2.94063500	7.51273900	-1.20743700
C	3.53179100	7.27709000	0.95798400
H	4.60973000	7.30441700	1.13796700
H	3.18422200	6.24841100	1.09009500
H	3.34668600	7.57779400	-0.07732400
C	3.38584200	14.14031600	2.31788200
H	4.46496800	14.16297800	2.14385400
H	2.99038800	15.14902300	2.16796800
H	3.20969400	13.84761400	3.35702600
C	3.08053100	-13.78431800	-4.53093100
H	4.04410500	-13.62932800	-5.02339800
H	3.03269700	-14.81919300	-4.18073200
H	2.28790600	-13.62890800	-5.26845800
C	2.90167100	-6.79954100	-3.47181900
H	3.46967000	-6.70434500	-4.40074100
H	2.37461700	-5.85923500	-3.28761600
H	3.60726300	-6.96948500	-2.65336500
C	-3.31895500	-7.19862200	-2.32472600
H	-3.06033800	-6.25202600	-1.84151700
H	-2.84042700	-7.23065900	-3.30781400
H	-4.40238000	-7.23033400	-2.46751600
C	-3.29883800	-14.18239100	-2.70611400
H	-2.84561100	-15.14243900	-2.96945300
H	-3.42916300	-14.14419900	-1.62074300
H	-4.28542600	-14.12598500	-3.17372200
C	1.41490900	-14.53395300	1.74945400
H	1.10007200	-15.50477000	1.35620600
H	2.40801800	-14.30257300	1.35352600
H	1.48648100	-14.60830000	2.83789500
C	0.70881300	-7.62127300	2.50858500
H	0.85172100	-6.58467000	2.18985000
H	-0.36385700	-7.83451700	2.53071400
H	1.10301700	-7.72912700	3.52257100
H	-8.94250000	-1.66210000	2.67940000
H	-13.77470000	0.67010000	2.55200000
H	-13.00190000	2.20230000	2.22330000
H	13.88060000	-0.98700000	2.11240000
H	13.04150000	-2.45200000	1.66180000
H	8.31160000	-0.09510000	2.49480000
H	9.12350000	1.42840000	2.76490000
H	9.19500000	-3.08740000	-0.28970000
H	12.92030000	-0.08390000	-3.30410000
C	-8.19840000	4.52330000	-1.10630000
H	-8.78160000	5.37240000	-0.81680000
H	-7.28080000	4.51650000	-0.55610000
H	-7.98590000	4.57680000	-2.15360000
C	-14.22550000	2.06600000	-3.85890000
H	-13.68810000	2.01910000	-4.78290000
H	-15.11660000	1.47840000	-3.93430000
H	-14.48530000	3.08250000	-3.64860000
C	-14.06610000	2.14290000	4.08860000
H	-13.50870000	2.94210000	4.53070000
H	-14.97010000	2.52950000	3.66630000
H	-14.30420000	1.41710000	4.83770000
C	-7.82850000	-1.12050000	4.43460000
H	-8.35230000	-1.81100000	5.06220000
H	-6.91430000	-1.56490000	4.10060000
H	-7.61140000	-0.23030000	4.98720000
C	-7.87340000	-3.12150000	-3.25370000
H	-8.42850000	-3.30430000	-4.15000000
H	-6.98010000	-2.58240000	-3.49110000
H	-7.61630000	-4.05440000	-2.79700000
C	-13.80200000	-4.77730000	0.21210000
H	-13.20790000	-5.51210000	0.71410000
H	-14.71280000	-4.62490000	0.75270000
H	-14.02710000	-5.11610000	-0.77760000
C	13.98140000	-1.52220000	-4.49590000
H	13.37010000	-1.34740000	-5.35650000
H	14.87840000	-0.94390000	-4.57210000
H	14.23060000	-2.56130000	-4.44050000
C	8.17080000	-4.32030000	-1.72000000
H	8.79160000	-5.16960000	-1.52470000
H	7.26900000	-4.39890000	-1.14950000
H	7.93150000	-4.28570000	-2.76230000
C	8.05780000	0.69060000	4.47810000
H	7.14660000	1.19700000	4.23700000
H	7.83280000	-0.25840000	4.91820000
H	8.62120000	1.28040000	5.17070000
C	14.20880000	-2.63050000	3.45650000
H	15.09080000	-2.96300000	2.95000000
H	14.48480000	-2.00920000	4.28270000
H	13.66210000	-3.47780000	3.81430000
C	13.93200000	4.77340000	0.45520000
H	14.84320000	4.55700000	0.97260000
H	14.15670000	5.21300000	-0.49420000
H	13.34630000	5.45600000	1.03460000
C	7.84660000	3.59810000	-2.92830000
H	6.97470000	3.07440000	-3.26060000
H	7.55380000	4.42790000	-2.31940000
H	8.39400000	3.95340000	-3.77620000

(*all-R*)-**2**, DFT optimized twisted structure				(*all-R*)-**2**, OPLS-optimized flat structure			
C	10.60850000	2.02480000	0.55940000	C	11.04695900	1.42560200	0.12211500
C	10.46510000	1.76690000	1.92850000	C	11.14642800	0.63064600	1.28576700
C	10.51890000	0.45740000	2.40100000	C	11.14151400	-0.77610200	1.18596400
C	10.73460000	-0.60170000	1.51000000	C	11.04401700	-1.39672100	-0.07820100
C	10.88680000	-0.34280000	0.14190000	C	10.94512600	-0.60355600	-1.24162100
C	10.81500000	0.96510000	-0.33290000	C	10.94297700	0.80299400	-1.14183700
C	10.80450000	-2.00690000	2.01910000	C	11.04906000	-2.86179500	-0.18314700
N	11.95210000	-2.67060000	1.97290000	N	12.03582500	-3.49857700	-0.85112300
N	9.71950000	-2.58550000	2.51770000	N	10.06788300	-3.59470400	0.38700200
H	9.80740000	-3.54770000	2.91920000	H	10.13645900	-4.64175500	0.40697900
C	8.33360000	-2.11760000	2.40410000	C	8.88939200	-3.08943000	1.10564300
C	13.28620000	-2.12100000	1.70670000	C	13.21053400	-2.88745400	-1.48916600
H	11.96380000	-3.67070000	2.28000000	H	11.97902300	-4.53344600	-1.01561100
H	10.30730000	2.58590000	2.62240000	H	11.22025900	1.10441600	2.25580200
H	10.92510000	1.16220000	-1.39410000	H	10.87272000	1.40913400	-2.03555000
C	-10.55750000	-0.99630000	-2.46150000	C	-11.05460300	-0.77486300	-1.16248500
C	-10.57760000	-2.05540000	-1.54500000	C	-11.12506600	-1.39334100	0.10566800
C	-10.75380000	-1.79400000	-0.18010000	C	-11.18799200	-0.59505200	1.26949400
C	-10.89660000	-0.48230000	0.26640000	C	-11.17716400	0.81119900	1.16563900
C	-10.88380000	0.57640000	-0.65080000	C	-11.11102000	1.42807100	-0.10241500
C	-10.71950000	0.31410000	-2.01690000	C	-11.05149500	0.63149600	-1.26623900
H	-11.02280000	-0.28220000	1.32530000	H	-11.23104900	1.41989400	2.05755200
H	-10.71090000	1.13170000	-2.73000000	H	-10.99280400	1.10212500	-2.23792300
C	-10.40770000	-3.46390000	-2.01980000	C	-11.13376300	-2.86139700	0.21339700
N	-9.24700000	-3.85450000	-2.53070000	N	-10.09781100	-3.57965100	-0.24539900
N	-11.41670000	-4.32020000	-1.92760000	N	-12.17762700	-3.49302100	0.77123800

H	-11.24850000	-5.31860000	-2.19230000
C	-12.82380000	-4.00700000	-1.65500000
C	-7.96160000	-3.15180000	-2.45020000
H	-9.17110000	-4.82510000	-2.91340000
C	-11.04050000	1.98440000	-0.17000000
N	-12.12510000	2.67840000	-0.49010000
N	-10.09370000	2.53610000	0.57810000
C	10.54330000	3.43030000	0.04960000
N	9.51130000	3.81910000	-0.68780000
N	11.51890000	4.28250000	0.33450000
H	9.51590000	4.78880000	-1.08110000
C	8.23820000	3.11300000	-0.86910000
H	11.42590000	5.27440000	0.01440000
C	12.83650000	3.96530000	0.89610000
H	-12.17830000	3.68170000	-0.19900000
C	-13.37530000	2.15930000	-1.05580000
C	-8.72670000	2.04410000	0.78290000
H	-10.25550000	3.49710000	0.95980000
C	-21.37450000	-12.70630000	-8.48990000
C	14.80330000	-11.90940000	4.85220000
C	-21.44550000	-11.55910000	-9.51490000
C	13.52400000	-12.17500000	4.31680000
O	11.36090000	-6.49200000	4.93990000
C	-22.76910000	-11.61110000	-10.30220000
C	12.56680000	-11.18620000	4.28610000
Si	-21.07730000	-9.84680000	-8.73460000
C	12.82640000	-9.88270000	4.79470000
C	-21.02460000	-8.49800000	-10.09390000
P	11.00720000	-5.91350000	3.42910000
C	-20.61760000	-7.11540000	-9.54980000
C	14.13330000	-9.60950000	5.33070000
C	-20.11810000	-8.89920000	-11.27340000
C	15.09760000	-10.65560000	5.33850000
C	-22.32590000	-9.43570000	-7.33310000
C	-21.74850000	-8.55990000	-6.20500000
C	11.83830000	-8.83800000	4.72670000
C	-23.64290000	-8.83360000	-7.86530000
O	9.73810000	-5.11450000	3.57940000
C	12.24310000	-7.55420000	5.05750000
C	-19.38630000	-9.97070000	-7.99940000
O	12.20930000	-5.28030000	2.77640000
C	-18.26080000	-10.06130000	-7.52980000
C	-16.94760000	-10.17050000	-6.97970000
C	13.51640000	-7.27840000	5.59140000
C	14.44950000	-8.27940000	5.77660000
C	-16.54880000	-9.36050000	-5.89880000
O	10.74520000	-7.33370000	2.61810000
C	-15.26950000	-9.47370000	-5.36580000
C	7.79230000	-9.42080000	3.21780000
C	-16.02130000	-11.09200000	-7.50680000
C	-14.74530000	-11.20010000	-6.96600000
C	8.65490000	-8.48120000	2.68860000
C	9.94860000	-8.29930000	3.21260000
C	-14.34420000	-10.39600000	-5.88400000
C	-12.96300000	-10.46350000	-5.33350000
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C	-12.53990000	-14.06030000	-4.31230000
C	9.07060000	-11.65820000	6.61090000
C	-11.20190000	-14.05480000	-3.86170000
C	7.81020000	-11.92080000	6.03030000
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C	-10.45720000	-12.89820000	-3.91590000
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C	16.22160000	-8.61760000	7.54600000
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C	17.40740000	-8.24550000	8.16880000
C	18.16810000	-7.16660000	7.67640000
C	-8.79580000	-10.40410000	-4.07040000
C	17.69750000	-6.47510000	6.54330000
C	-8.39560000	-9.51770000	-3.08280000
C	16.50890000	-6.85250000	5.92830000
O	-9.32480000	-8.69690000	-2.46370000
P	-9.90600000	-7.38800000	-3.29560000
C	19.38620000	-6.78040000	8.31400000
C	20.42780000	-6.44750000	8.86110000
O	-10.23280000	-8.08550000	-4.76110000
Si	21.99900000	-5.93730000	9.69800000
O	-11.16660000	-6.97050000	-2.58240000
C	21.56090000	-4.33630000	10.66010000
O	-8.82770000	-6.36660000	-3.55350000
C	22.46220000	-7.40690000	10.83960000

H	-12.10583100	-4.52567300	0.99110400
C	-13.42571100	-2.89828400	1.26657200
C	-8.84175700	-3.07815000	-0.81759500
H	-10.19207700	-4.62977400	-0.33659500
C	-11.10466600	2.89288200	-0.21005000
N	-12.10109100	3.53915000	-0.85360200
N	-10.10219200	3.61737500	0.33340700
C	11.05576400	2.89400500	0.22520200
N	10.01084400	3.61111100	-0.21439100
N	12.11024600	3.52913000	0.75867800
H	10.10611900	4.66046800	-0.31344900
C	8.74146900	3.10990500	-0.75634800
H	12.03594600	4.55968700	0.98724200
C	13.37240400	2.94053800	1.22436600
H	-12.02862300	4.57074900	-1.03222900
C	-13.30050100	2.94226500	-1.45814300
C	-8.90678900	3.10243800	1.01603200
H	-10.16799200	4.66417900	0.36555000
C	-23.82208200	-11.97429500	2.61836000
C	13.88756000	-12.94615100	-3.14212200
C	-24.31377700	-11.20349700	1.38181000
C	12.48654000	-12.95945200	-3.05712500
O	12.01648500	-7.95383000	0.44696600
C	-25.84782900	-11.22253500	1.29721600
C	11.82290000	-11.99467200	-2.27854900
Si	-23.61048000	-9.42288000	1.33289500
C	12.54351800	-11.00388300	-1.56418800
C	-24.20114700	-8.53587500	-0.26005000
P	11.08089800	-6.89131200	-0.45882300
C	-23.56926400	-7.14249000	-0.41242800
C	13.96522000	-10.98421100	-1.66601900
C	-23.92438100	-9.39545800	-1.50450600
C	14.61966400	-11.96269400	-2.45426200
C	-24.09757000	-8.44745000	2.91424000
C	-23.05885600	-7.37476300	3.28774200
C	11.86117000	-10.03667500	-0.76936100
C	-25.49990000	-7.82784900	2.79013400
O	10.17302700	-6.15491800	0.44591400
C	12.62514600	-8.99703300	-0.18788600
C	-21.78185300	-9.57725700	1.25657900
O	11.97122200	-6.02839800	-1.26382600
C	-20.56480900	-9.65988900	1.20686100
C	-19.11579500	-9.73906900	1.15325200
C	14.02657700	-8.99034700	-0.28040600
C	14.71640200	-9.98460900	-0.99558900
C	-18.33074700	-8.80190100	1.85325300
O	10.16918400	-7.85618300	-1.49000400
C	-16.92475600	-8.87902700	1.79933400
C	7.53367300	-10.12955900	-0.31514100
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C	-17.08271800	-10.82414100	0.35003600
C	8.19244500	-9.03464100	-0.90081300
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C	-16.28698200	-9.89246700	1.05205800
C	-14.81633800	-9.96415200	0.99444200
C	10.38848100	-10.07250400	-0.54968300
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C	-14.06092600	-10.97897800	1.63673600
C	-12.64051900	-11.00131600	1.51821700
C	8.31443000	-11.19371200	0.20571700
C	10.48632900	-12.21570600	0.67901200
C	-14.70952500	-11.97026600	2.41370600
C	-13.97291800	-12.96948800	3.07356600
C	9.85206800	-13.30408300	1.30373400
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C	8.45083600	-13.35271300	1.36964500
C	7.68930400	-12.30388800	0.82526000
C	-11.91509400	-12.00797100	2.20494300
C	-14.13142600	-8.95934000	0.28910600
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C	18.37688600	-10.79811600	-0.36386400
C	19.01860700	-9.77448500	-1.08834200
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C	18.24764900	-8.82125900	-1.78253600
C	-9.69744000	-8.97372700	0.95351500
C	16.84072800	-8.89384800	-1.75082300
O	-10.27304900	-7.85050200	1.47205600
P	-11.18151500	-6.86269800	0.45705300
C	20.46869200	-9.70177100	-1.11870100
C	21.68790400	-9.64856700	-1.15388100
O	-12.12630700	-7.91982600	-0.44909700
Si	23.51955300	-9.58345600	-1.23106900
O	-12.06609600	-6.00842100	1.27757800
C	24.04464700	-8.20507200	-0.00354400
O	-10.26889400	-6.13348200	-0.44917400
C	24.12289700	-11.32670700	-0.70242800

C	-7.06910000	-9.45880000	-2.61460000	C	-8.29760700	-9.01414600	0.84827400
C	23.25760000	-5.64800000	8.27980000	C	23.94498700	-9.16390800	-3.05445600
C	-6.08330000	-10.26580000	-3.14770000	C	-7.64073500	-10.10142400	0.24596600
C	23.89450000	-7.38250000	11.40730000	C	25.60391400	-11.58691600	-1.02435300
C	-6.41210000	-11.11780000	-4.25860000	C	-8.42478600	-11.15170100	-0.29827300
C	-7.77210000	-11.17630000	-4.72440000	C	-9.84519300	-11.12271500	-0.18158700
C	21.42710000	-7.59950000	11.96530000	C	23.82034500	-11.58650800	0.78287500
C	22.60070000	-3.87940000	11.70160000	C	25.54604700	-8.21930000	0.32888800
C	-8.05650000	-11.96550000	-5.87390000	C	-10.59923000	-12.16990700	-0.76994300
C	-7.07070000	-12.67400000	-6.52280000	C	-9.96975200	-13.23481100	-1.43839000
C	21.19410000	-3.18300000	9.70560000	C	23.59737000	-6.82200700	-0.50549000
C	-5.73750000	-12.62280000	-6.06080000	C	-8.57008400	-13.26749000	-1.53844900
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C	-5.42030000	-11.85720000	-4.96150000	C	-7.80527000	-12.23074000	-0.97582500
C	5.02820000	-9.83560000	0.65410000	C	3.88495500	-10.23476300	-1.36857800
C	-4.71770000	-10.20230000	-2.55970000	C	-6.16820100	-10.07656900	0.18960300
C	-4.07680000	-8.96260000	-2.39010000	C	-5.49893300	-9.13700100	-0.62397800
C	6.28550000	-9.76490000	1.24260000	C	5.29254700	-10.27075900	-1.42073000
C	6.43250000	-9.54460000	2.62300000	C	6.06200500	-10.09758300	-0.25014100
C	-2.82110000	-8.87580000	-1.80080000	C	-4.09106600	-9.10282100	-0.67541800
C	-2.16010000	-10.03780000	-1.35380000	C	-3.33514800	-10.01006500	0.09319800
C	5.26920000	-9.38500000	3.39750000	C	5.39652400	-9.87606400	0.97542500
C	4.00740000	-9.45050000	2.81930000	C	3.98909000	-9.83924100	1.03355100
C	-2.80200000	-11.28320000	-1.51460000	C	-3.99348100	-10.94755800	0.91343400
C	-4.05630000	-11.35860000	-2.10750000	C	-5.40122900	-10.97691100	0.96109200
C	3.86520000	-9.68100000	1.43540000	C	3.22995000	-10.02005600	-0.13971500
C	-0.87290000	-9.95720000	-0.75440000	C	-1.88320000	-9.98027300	0.04106000
C	2.57540000	-9.75400000	0.84040000	C	1.77831300	-9.98689700	-0.08328900
C	1.46720000	-9.81810000	0.32900000	C	0.55779400	-9.97394300	-0.04079300
C	0.23420000	-9.89090000	-0.24110000	C	-0.66260700	-9.97165100	0.00001500
H	-20.42000000	-12.71630000	-7.95410000	H	-22.73265700	-11.99890100	2.66246300
H	-22.17390000	-12.62930000	-7.74330000	H	-24.18026200	-11.52032600	3.54231700
H	-21.48990000	-13.67890000	-8.98490000	H	-24.17032300	-13.00738800	2.60203900
H	15.56110000	-12.68700000	4.86090000	H	14.40167900	-13.68355600	-3.74176600
H	-20.62670000	-11.71220000	-10.23310000	H	-23.93118000	-11.72435900	0.50376000
H	13.29890000	-13.15700000	3.91160000	H	11.91806400	-13.70739000	-3.59111500
H	-22.83550000	-10.82570000	-11.06270000	H	-26.20643100	-10.65008500	0.44140900
H	-22.87700000	-12.57470000	-10.81600000	H	-26.22046600	-12.24128200	1.18777100
H	-23.63510000	-11.50450000	-9.63890000	H	-26.30257000	-10.80555800	2.19502900
H	11.59820000	-11.39230000	3.84730000	H	10.74424200	-12.02897600	-2.24552300
H	-22.05430000	-8.41850000	-10.47380000	H	-25.28051300	-8.40156500	-0.18809600
H	-20.60850000	-6.36870000	-10.35400000	H	-23.90143300	-6.65700100	-1.33030000
H	-21.30270000	-6.75450000	-8.77630000	H	-23.84566400	-6.48849500	0.41317400
H	-19.61170000	-7.14100000	-9.11550000	H	-22.48052600	-7.19878100	-0.44264300
H	-20.11720000	-8.11860000	-12.04480000	H	-24.27879500	-8.90459200	-2.41123500
H	-19.08050000	-9.03670000	-10.94770000	H	-22.85751200	-9.58687900	-1.62561300
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H	-22.56860000	-10.41290000	-6.88940000	H	-24.12645600	-9.15758600	3.74027900
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H	13.72970000	-6.25870000	5.89220000	H	14.57919600	-8.19404800	0.19607200
H	-17.25220000	-8.64860000	-5.47960000	H	-18.80339200	-8.02132900	2.43218000
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H	8.34320000	-7.84000000	1.87160000	H	7.61608300	-8.19591900	-1.26252600
H	10.88170000	-10.54170000	6.49270000	H	11.56564100	-12.21088500	0.64904700
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H	-13.12970000	-14.97000000	-4.25340000	H	-14.48263400	-13.71661300	3.66490600
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H	-10.76310000	-14.96080000	-3.45450000	H	-12.00092300	-13.74553300	3.48484200
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H	6.43370000	-11.41450000	4.48440000	H	6.61353800	-12.36678300	0.89572600
H	-9.44090000	-12.89820000	-3.54140000	H	-10.83705700	-12.04449700	2.15879000
H	-12.65990000	-8.34770000	-5.54680000	H	-14.68589100	-8.15198800	-0.16606400
H	15.64180000	-9.43960000	7.95360000	H	16.48409000	-11.65287200	0.22330300
H	17.75130000	-8.78120000	9.04740000	H	18.96021400	-11.53240800	0.17287800
H	18.27430000	-5.64480000	6.14940000	H	18.73163100	-8.03221300	-2.33995500
H	16.16660000	-6.31510000	5.04940000	H	16.25550800	-8.15893500	-2.28511500
H	20.64710000	-4.60490000	11.21060000	H	23.51419700	-8.39207500	0.93076400
H	22.39040000	-8.28350000	10.17860000	H	23.54465000	-12.05113700	-1.27698500
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H	24.08020000	-8.27760000	12.01470000	H	25.91516500	-12.56954900	-0.66886200
H	24.65190000	-7.36310000	10.61790000	H	25.78214200	-11.57051000	-2.09838500
H	24.06770000	-6.51510000	12.05300000	H	26.26123600	-10.84923900	-0.56771100
H	21.63620000	-8.51470000	12.53350000	H	24.09050600	-12.60311800	1.06963700
H	21.44580000	-6.76630000	12.67740000	H	24.36936000	-10.90307900	1.43021300
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H	22.24890000	-2.98010000	12.22340000	H	25.80764600	-7.39644900	0.99449500
H	22.78750000	-4.64340000	12.46240000	H	25.82768600	-9.13859000	0.84012700
H	23.56270000	-3.62830000	11.24240000	H	26.16654500	-8.13151300	-0.56102500
H	-9.07060000	-11.98890000	-6.25360000	H	-11.67791000	-12.17139500	-0.72276700

H	-7.31720000	-13.25960000	-7.40350000
H	20.82720000	-2.31500000	10.26790000
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H	24.20890000	-6.75670000	6.65380000
H	24.14350000	-7.65440000	8.17140000
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H	-4.38930000	-11.79240000	-4.63490000
H	4.93400000	-10.01500000	-0.41170000
H	-4.56670000	-8.05970000	-2.74090000
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H	5.35730000	-9.18740000	4.46080000
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H	-4.54040000	-12.32480000	-2.20610000
C	-24.47650000	9.26830000	3.44220000
C	13.28480000	13.92600000	-2.10270000
C	-24.58650000	8.22540000	4.57000000
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O	10.95220000	7.98270000	-2.77700000
C	-26.04730000	8.07930000	5.03800000
C	11.13970000	12.81310000	-2.02820000
Si	-23.74900000	6.55970000	4.12220000
C	11.73230000	11.57860000	-2.41550000
C	-23.79340000	5.37310000	5.62530000
P	10.37130000	7.33240000	-1.36960000
C	-23.03980000	4.05400000	5.36950000
C	13.15390000	11.54530000	-2.63460000
C	-23.27520000	6.04670000	6.91060000
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C	-25.81540000	4.98610000	2.85110000
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C	11.63930000	9.18490000	-2.72360000
C	-21.97820000	6.95200000	3.76760000
O	11.48580000	6.91050000	-0.44670000
C	-20.80590000	7.22120000	3.54680000
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C	-18.70920000	6.82720000	2.31060000
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C	-10.26810000	8.23200000	1.25330000
C	16.04700000	9.26070000	-2.57910000
O	-10.92270000	7.30350000	0.45980000
P	-11.45550000	5.90090000	1.16080000
C	19.36400000	9.72260000	-4.24060000
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Si	22.33640000	9.38810000	-4.95190000
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C	22.40060000	7.90430000	-6.16640000

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C	11.92514300	10.04729900	0.69513900
C	-25.48952700	7.73150800	-2.54106200
O	10.18978900	6.16226200	-0.43625600
C	12.68030700	8.98166100	0.15020900
C	-21.71612900	9.54139600	-1.22719600
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C	14.77685800	9.96379200	0.95067100
C	-18.26050600	8.77828600	-1.84343600
O	10.21756300	7.90211200	1.46435800
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C	18.27726000	8.78383700	1.84055500
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O	-10.19177900	7.89560600	-1.49536200
P	-11.10547400	6.91929800	-0.47710200
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H	-7.03260000	11.00920000	3.58790000
H	2.58780000	12.24310000	-0.69720000
H	-6.28810000	7.34020000	1.68240000
H	4.96640000	12.35350000	-1.33540000
H	-3.89970000	7.53160000	1.08440000
H	5.06330000	8.07510000	-1.74240000
H	2.68430000	7.95640000	-1.09060000
H	-4.36960000	11.78480000	0.60630000
H	-6.75610000	11.58520000	1.19080000
H	10.39980000	0.25990000	3.46110000
H	11.05570000	-1.16060000	-0.55070000
H	-10.42120000	-1.19530000	-3.51930000
H	-10.77230000	-2.61270000	0.53170000
C	14.18650000	-2.24560000	2.93700000
C	13.94450000	4.18490000	-0.13550000
C	7.09860000	3.82440000	-0.13740000
C	7.51750000	-3.01760000	1.47440000
C	-7.70440000	2.95190000	0.09660000
C	-14.52130000	2.25500000	-0.04710000
C	-6.98120000	-3.89470000	-1.54060000
C	-13.70230000	-4.31170000	-2.86960000
H	-12.91230000	-2.96030000	-1.36280000
H	-13.13880000	-4.61500000	-0.80060000
H	-8.12530000	-2.13300000	-2.09820000
H	-7.55860000	-3.08790000	-3.46600000
H	-13.22640000	1.12930000	-1.38070000
H	-13.60570000	2.75480000	-1.94520000
H	-8.64930000	1.02090000	0.41460000
H	-8.54500000	2.01980000	1.86220000
H	-6.69030000	2.61240000	0.32790000
H	-7.83570000	2.93870000	-0.98950000
H	-7.81200000	3.98270000	0.44530000
H	-15.45650000	1.93420000	-0.51550000
H	-14.33230000	1.61880000	0.82260000
H	-14.64380000	3.28510000	0.29830000
H	-6.00650000	-3.39810000	-1.55970000
H	-7.34140000	-3.91300000	-0.50770000
H	-6.85060000	-4.92600000	-1.87940000
H	-14.75370000	-4.14090000	-2.61960000
H	-13.43790000	-3.67050000	-3.71560000
H	-13.58570000	-5.35460000	-3.17670000
H	8.32590000	-1.08520000	2.05370000
H	7.90290000	-2.12630000	3.41040000
H	13.19460000	-1.08090000	1.39300000
H	13.71460000	-2.68100000	0.86880000
H	8.34090000	2.08390000	-0.52410000
H	8.03430000	3.08060000	-1.94400000
H	12.83860000	2.93750000	1.25990000
H	12.99090000	4.62020000	1.75970000
H	15.19750000	-1.90560000	2.69380000
H	13.80570000	-1.63950000	3.76440000
H	14.24090000	-3.28640000	3.26740000
H	14.92210000	4.02080000	0.32750000
H	13.83860000	3.49440000	-0.97760000
H	13.91150000	5.20760000	-0.52080000
H	6.14970000	3.32230000	-0.34850000
H	7.26270000	3.81630000	0.94430000
H	7.01990000	4.86390000	-0.46740000
H	6.47200000	-2.69530000	1.46830000
H	7.90020000	-2.97320000	0.45040000
H	7.55590000	-4.05630000	1.81340000

H	26.20930800	8.00069600	0.60627200
H	-11.62671800	12.22848200	0.66206400
H	-10.52378000	14.09830200	1.79888800
H	23.86147200	6.05908500	-0.47618500
H	24.08294000	6.37523000	1.24125500
H	22.54210800	6.72990400	0.47100100
H	-8.04295300	14.17373800	1.97507000
H	25.55060100	8.00669100	4.36547100
H	25.59935600	7.45200300	2.70730300
H	26.10208500	9.09144200	3.09739500
H	23.66859000	9.46348400	5.19580400
H	24.13833900	10.74734700	4.08712900
H	22.49033300	10.13362900	4.07763300
H	-6.68112900	12.36602100	1.02159800
H	3.39666800	11.74316500	1.47788000
H	-6.00182300	8.55161200	1.20988300
H	5.87394000	11.77899800	1.55692500
H	-3.52475700	8.50402000	1.30059500
H	6.01898500	8.49803800	-1.22938500
H	3.54144100	8.45439400	-1.31350000
H	-3.36507400	11.71267100	-1.58158700
H	-5.84206500	11.75276500	-1.66740200
H	11.22543800	-1.38187700	2.07753500
H	10.86211200	-1.07725300	-2.21007200
H	-11.01229200	-1.38373300	-2.05608900
H	-11.23614700	-1.06604700	2.24256800
C	14.39843200	-3.85378100	-1.51545600
C	14.52353300	3.94393000	1.11399100
C	7.60870800	4.11447600	-0.52745000
C	7.71464300	-4.06769500	1.01035000
C	-7.72423100	4.06534500	0.87334700
C	-14.47677400	3.92348600	-1.45025000
C	-7.70326200	-4.08212900	-0.61634500
C	-14.57968200	-3.90249400	1.20454700
H	-13.68735000	-2.02643100	0.66536900
H	-13.28302900	-2.55412900	2.29165700
H	-8.56625500	-2.13526400	-0.34306500
H	-8.98081800	-2.87767100	-1.88065600
H	-13.58430600	2.04856600	-0.90239800
H	-13.07496800	2.63308700	-2.47916100
H	-8.62901500	2.13847200	0.58974300
H	-9.13428200	2.93932200	2.06985800
H	-6.81948700	3.64012000	1.30819100
H	-7.51676700	4.29055500	-0.17335600
H	-7.92307100	5.01039000	1.38154200
H	-15.38435400	3.44828000	-1.82290800
H	-14.68247300	4.29204600	-0.44471300
H	-14.27189200	4.78821100	-2.08364300
H	-6.75591900	-3.67436700	-0.96924800
H	-7.58345100	-4.34140800	0.43607400
H	-7.89173300	-5.00580400	-1.16556400
H	-15.52111500	-3.43403200	1.49151600
H	-14.70113800	-4.30687300	0.19914400
H	-14.40755700	-4.74183100	1.88019900
H	8.58570800	-2.13274300	0.68057800
H	9.14945000	-2.91407600	2.14991100
H	13.49948500	-1.99142000	-0.93967800
H	12.95318200	-2.57901700	-2.50287600
H	8.47720200	2.16692700	-0.27549400
H	8.85501400	2.90964600	-1.82248400
H	13.61682500	2.06031700	0.62802600
H	13.26020200	2.61101500	2.25791800
H	15.29317200	-3.36276600	-1.89849100
H	14.62700200	-4.23297400	-0.51885900
H	14.19220600	-4.71271400	-2.15609600
H	15.47251800	3.48112500	1.38481700
H	14.61842400	4.32973500	0.09835600
H	14.36837000	4.79538700	1.77842600
H	6.65303300	3.70756300	-0.85837100
H	7.51390900	4.37274100	0.52770900
H	7.78492300	5.03859200	-1.08016300
H	6.81735800	-3.64642000	1.46391800
H	7.48105700	-4.31148000	-0.02661900
H	7.93865200	-5.00262600	1.52655500

3.2. CD- and VCD-measurements

In order to further characterize the structures of **1** and **2**, we carried out ECD and VCD measurements. The results of these experiments are summarized in Figure S5. In comparison to the free bisphosphoric acid **6**, neither ECD or VCD show any additional spectral signatures. While one may argue that the UV chromophore of the phosphoric acid must dominate the UV/ECD spectra and thus overlap with any small contributions of the amidines, the lack of any additional VCD signatures is unexpected. In particular the strong amidine band at around 1650 cm^{-1} is a nicely isolated chromophore which we expected to feature a VCD signature due to the chiral twist or tilt of the trisamidine core. Due to the size of the capsules and the lack of additional spectral signatures, we have not attempted any VCD spectra calculations. It is, however, possible that the structural flexibility that was indicated by the geometry optimizations and the resulting conformational changes between the right- and left-handed forms of **1** may lead to a cancelation of the amidine VCD signatures.

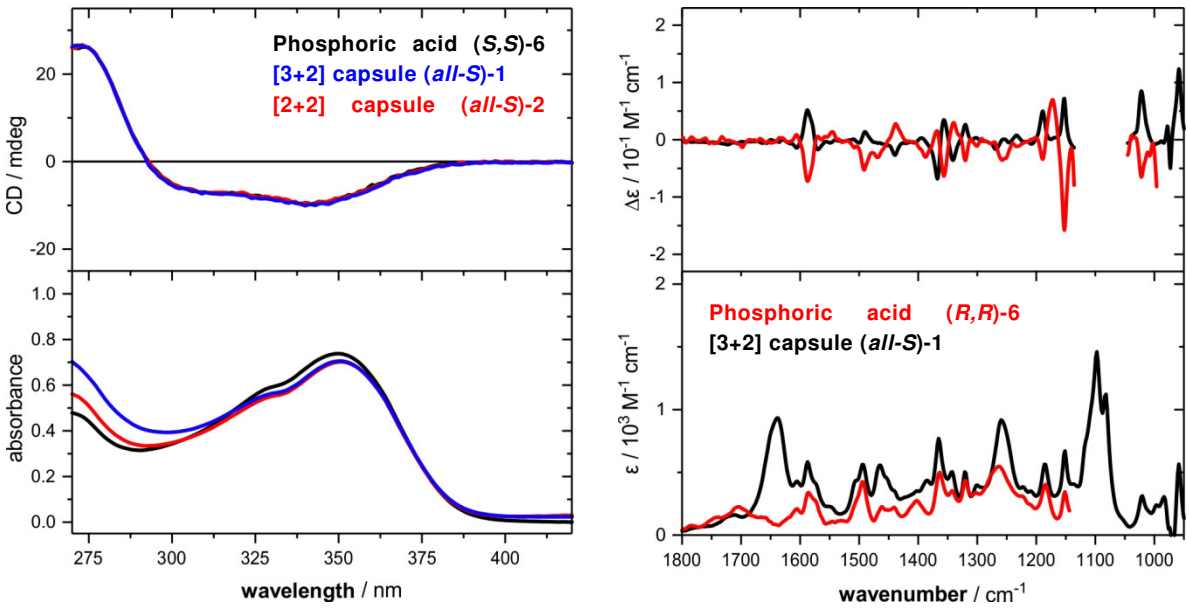

Figure S 5: Experimental UV/ECD spectra of phosphoric acid (*R,R*)-**6** and capsules (*all-R*)-**1/2** (left, each 100 µM in [D_1]-chloroform/[D_4]-methanol = 8/2) and IR/VCD spectra (right) of phosphoric acid (*S,S*)-**6** and capsule (*all-R*)-**1** (30 mM, chloroform/[D_4]-methanol = 8/2, 100 µm path length).

3.3. MS-Measurements

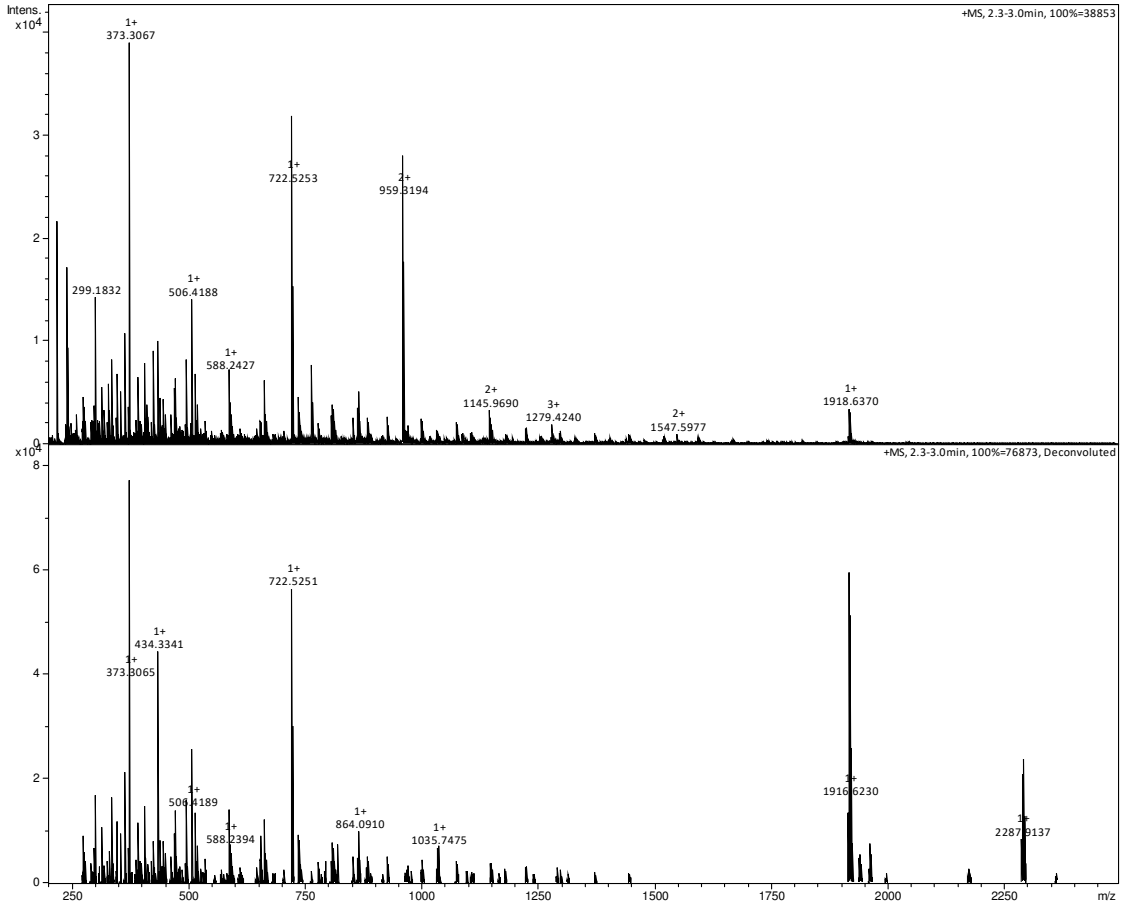

Figure S 6: ESI-MS spectrum of the [3+2]-capsule (*all-R*)-**1** (full range, top: as recorded, bottom: deconvoluted).

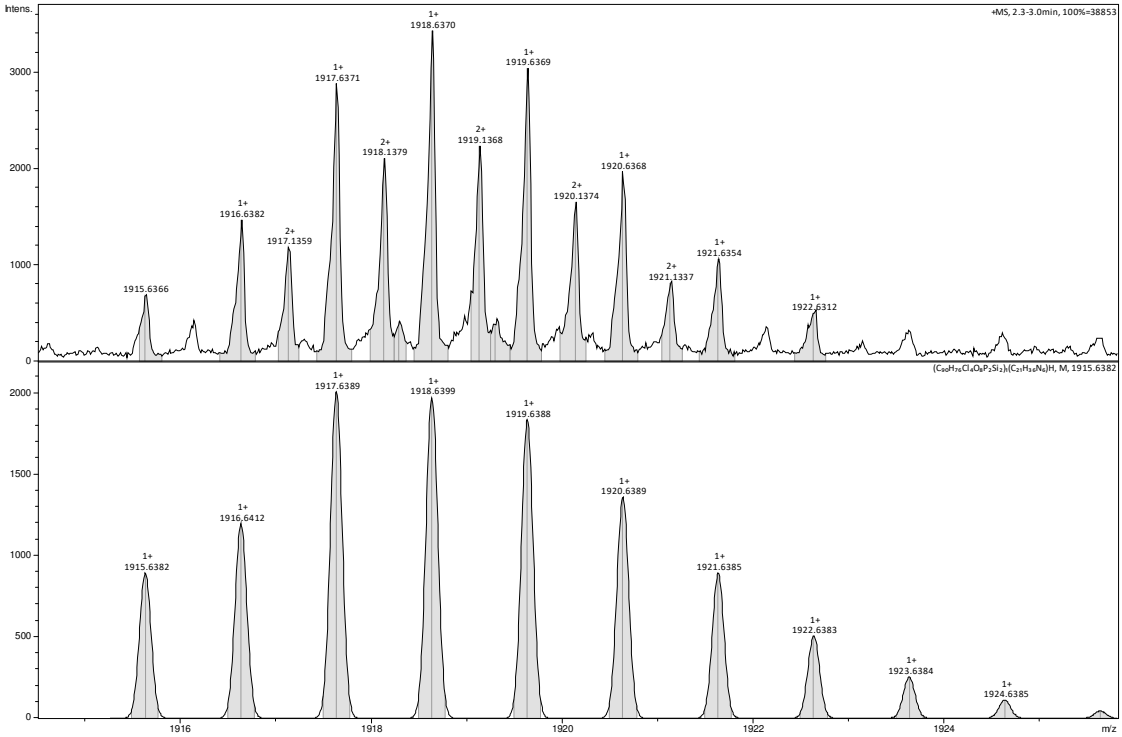

Figure S 7: ESI-MS spectrum of the [3+2]-capsule (*all-R*)-**1**, showing the aggregates [**6**+**7**+H]$^+$ and [(**6**)$_2$+(**7**)$_2$+2H]$^{2+}$ (top: measured spectrum, bottom: simulated spectrum of [**6**+**7**+H]$^+$).

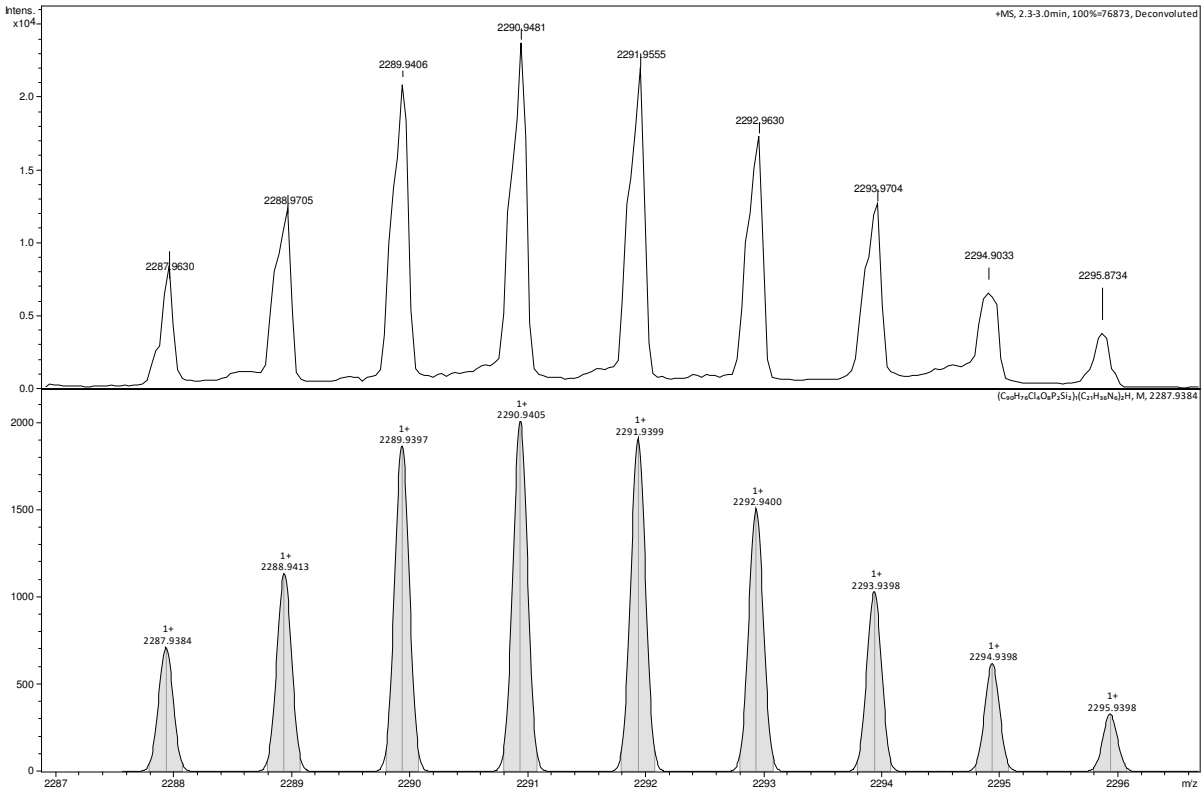

Figure S 8: ESI-MS spectrum of the [3+2]-capsule (*all-R*)-**1**, showing the aggregate [**6**+(**7**)$_2$+H]$^+$ (top: measured spectrum (deconvoluted), bottom: simulated spectrum).

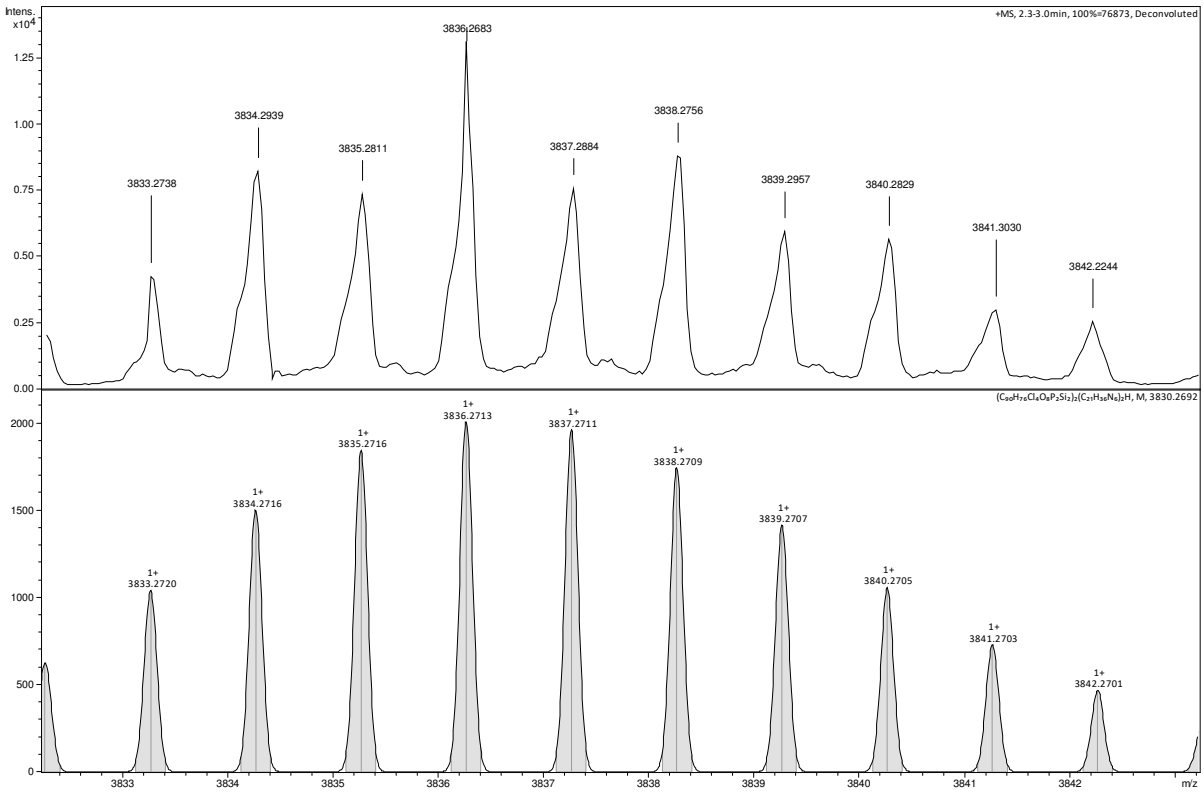

Figure S 9: ESI-MS spectrum of the [3+2]-capsule (*all-R*)-**1**, showing the aggregate [(**6**)$_2$+(**7**)$_2$+H]$^+$ (top: measured spectrum (deconvoluted), bottom: simulated spectrum).

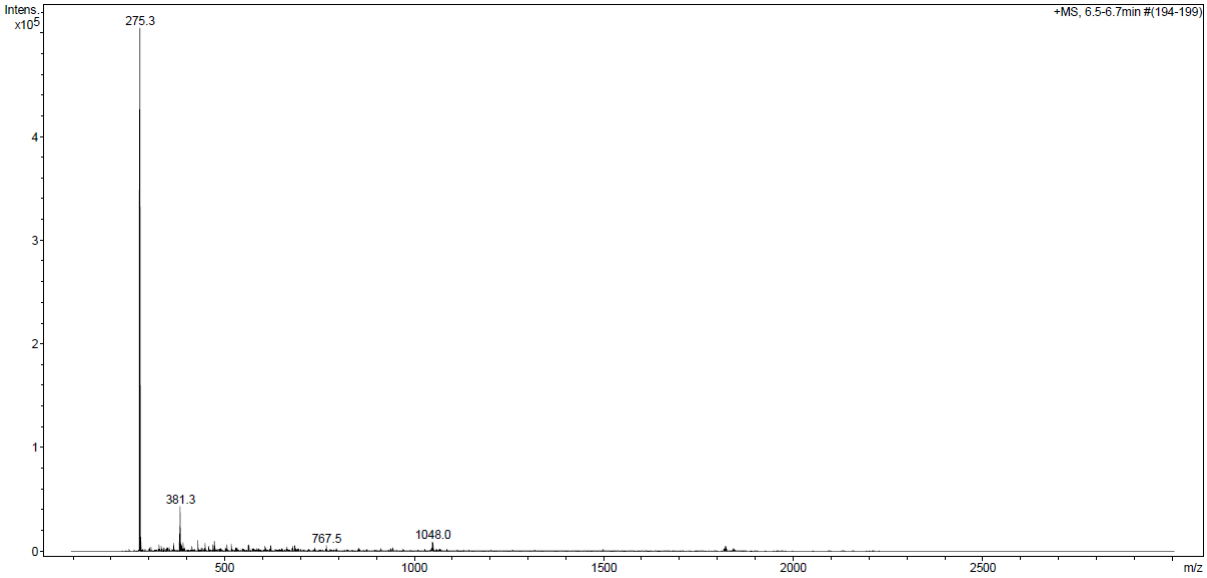

Figure S 10: ESI-MS spectrum of the [2+2]-capsule (*all-R*)-**2** (full range).

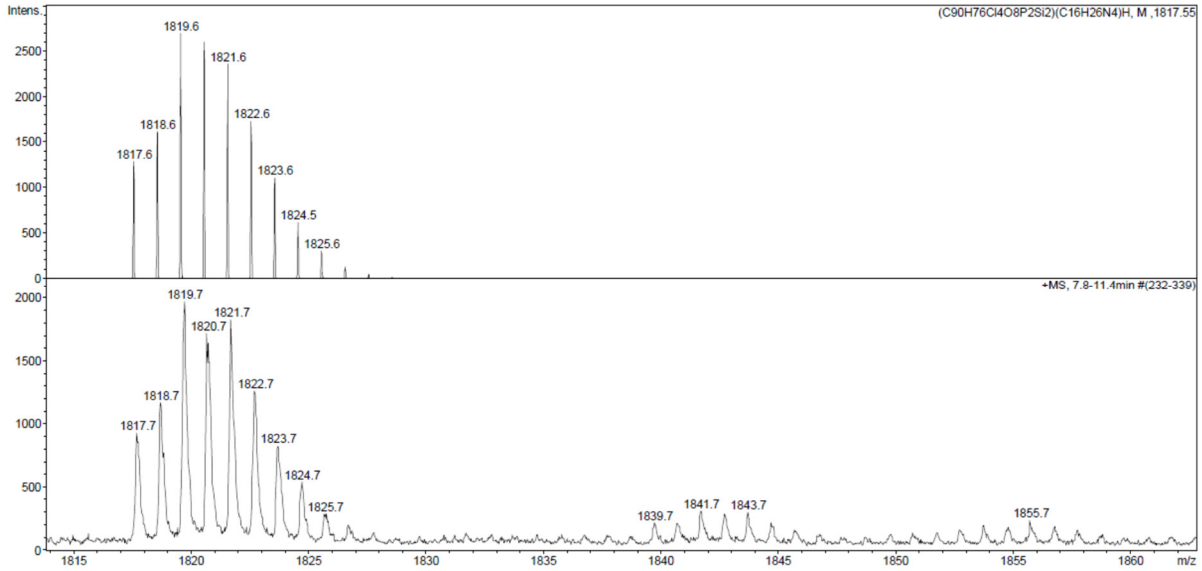

Figure S 11: ESI-MS spectrum of the [2+2]-capsule (*all-R*)-**2**, showing the aggregates [**6**+**8**+H]$^+$ and [**6**+**8**+Na]$^+$ (top: simulated spectrum, bottom: measured spectrum).

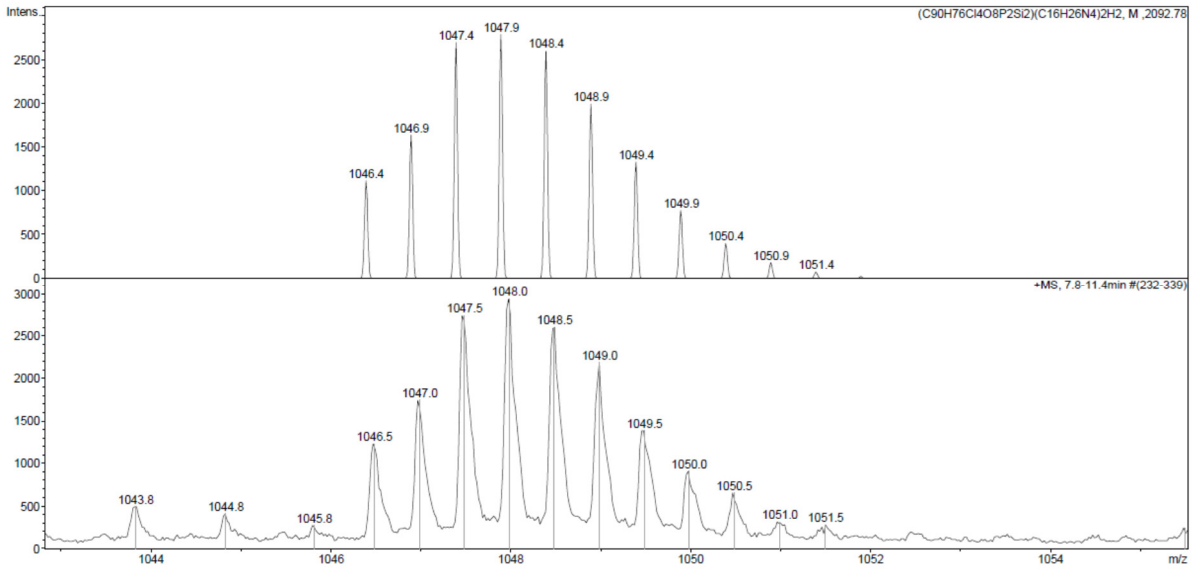

Figure S 12: ESI-MS spectrum of the [2+2]-capsule (*all-R*)-**2**, showing the aggregate [**6**+(**8**)$_2$+2H]$^{2+}$ (top: simulated spectrum, bottom: measured spectrum).

3.4. DOSY-Measurements

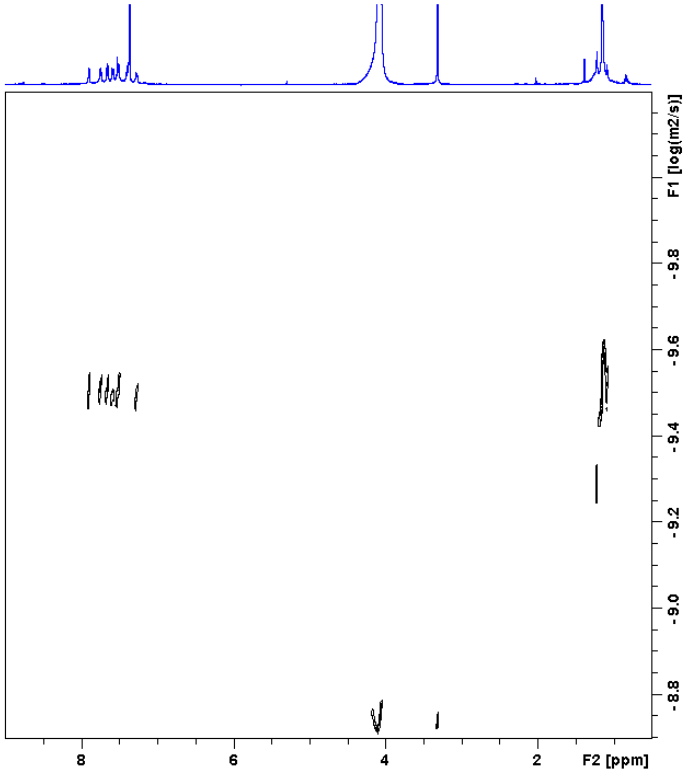

Figure S 13: DOSY-NMR spectrum of bisphosphoric acid (*R,R*)-**6** (12 mM) (500 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

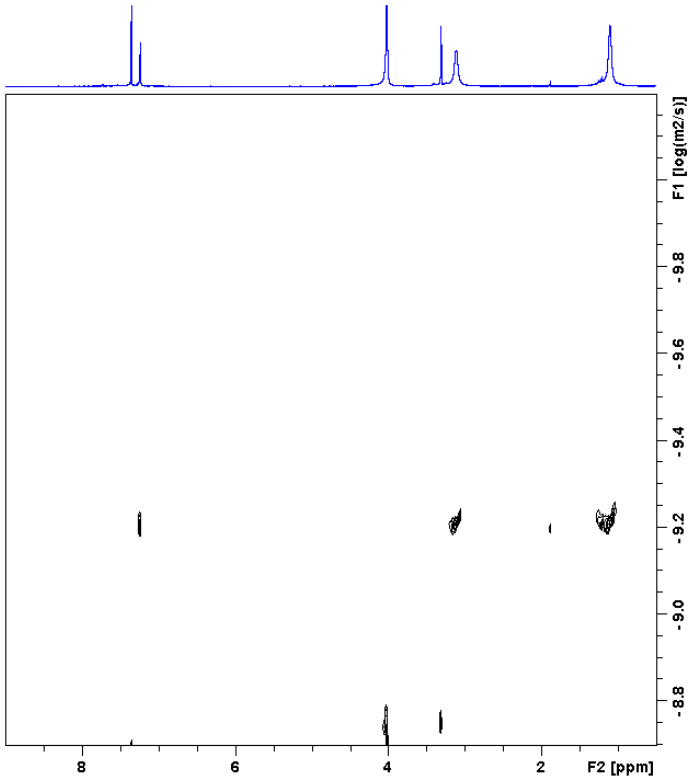

Figure S 14: DOSY-NMR spectrum of trisamidine **7** (500 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

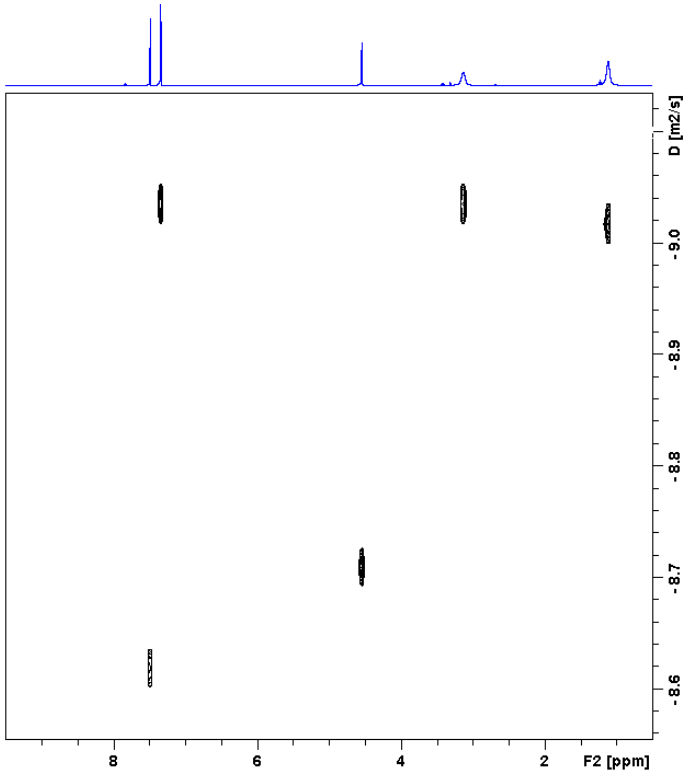

Figure S 15: DOSY-NMR spectrum of bisamidine **8** (500 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

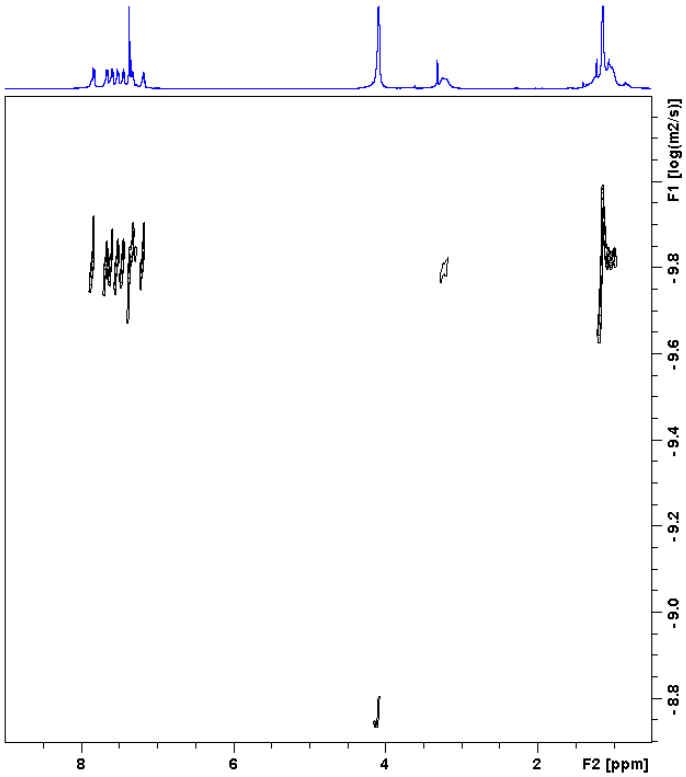

Figure S 16: DOSY-NMR spectrum of [3+2]-capsule (*all-R*)-**1** (4 mM) (500 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

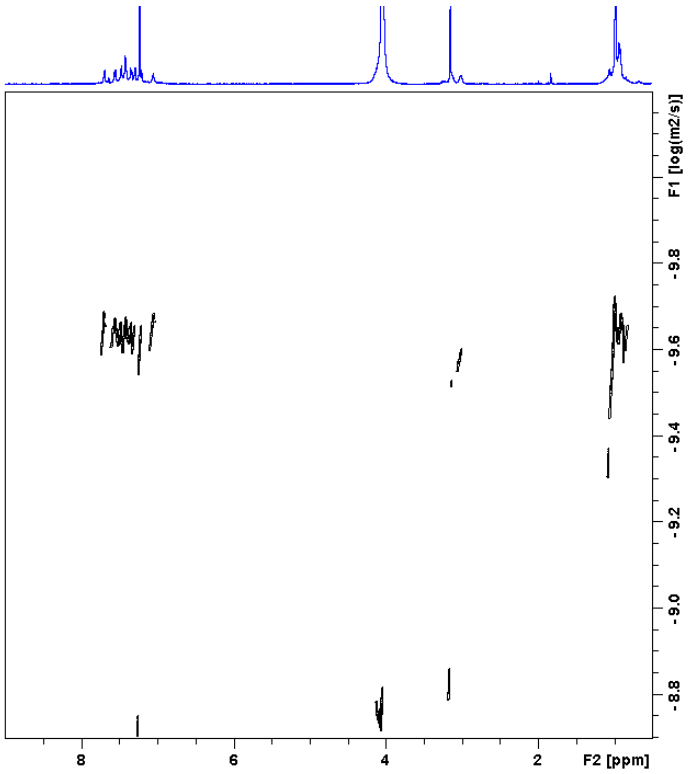

Figure S 17: DOSY-NMR spectrum of [2+2]-capsule (*all-R*)-**2** (4 mM) (500 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

Table S 1: Diffusion coefficients as determined per DOSY-NMR and calculated molecular diffusion coefficients. All measurements were performed in [D_1]-chloroform/[D_4]-methanol (8/2 v/v) at 298 K. Theoretical values were calculated based on the DFT-optimized structures using the Stokes-Einstein equation using the approximation for cylindrical particles.

Trisamidine 7

Integral region (ppm)	7.2	3.2	1.1	Mean value	Calculated value
D	6.10	5.99	5.97	**6.02**	-
SD (%)	0.23	0.23	0.21	**0.22**	-

Bisamidine 8

Integral region (ppm)	7.3	3.2	1.1	Mean value	Calculated value
D	8.81	8.79	8.90	**8.83**	-
SD (%)	0.02	0.01	0.01	**0.01**	-

Bisphosphoric acid (*R,R*)-6

Integral region (ppm)	7.9	7.8	7.7	7.6	7.5	7.3	1.1	Mean value	Calculated value
D	3.17	3.18	3.17	3.28	3.21	3.26	3.19	**3.21**	-
SD (%)	0.05	0.05	0.05	0.07	0.06	0.06	0.06	**0.06**	-

[3+2]-capsule (*all-R*)-1

Integral region (ppm)	7.9	7.7	7.6	7.5	7.4	7.2	3.2	1.1	Mean value	Calculated value
D	1.57	1.59	1.55	1.58	1.56	1.54	1.55	1.61	**1.57**	**1.58**
SD (%)	0.07	0.09	0.07	0.09	0.11	0.07	0.07	0.10	**0.08**	-

[2+2]-capsule (*all-R*)-2

Integral region (ppm)	7.7	7.6	7.5	7.4	7.3	3.2	1.1	Mean value	Calculated value
D	2.30	2.28	2.30	2.35	2.34	2.68	2.29	**2.36**	**1.84**
SD (%)	0.02	0.02	0.02	0.02	0.03	0.05	0.02	**0.03**	-

4. Encapsulation of C_{70}-IPH

4.1. UV-/CD-and fluorescence measurements

4.1.1. Sample preparation for 1:3 mixtures

Mixtures with a fixed 1:3 host:guest ratio were prepared as follows: Bisphosphoric acid (*R,R*)-**6**, [3+2] capsule (*all-R*)-**1** or [2+2] capsule (*all-R*)-**2** were dissolved in [D_1]-chloroform/[D_4]-methanol = 8/2 (2 ml, each 100 µM final concentration). C_{70}-IPH (2.39 mg, 300 µM, 3 eq for each substrate) was added into the solution and the mixture was stirred for 72 hours. The suspension was then centrifuged for one hour at 1200 rpm before being filtered through a syringe filter (0.2 µm) and measured directly.

4.1.2. Fluorescence titrations

Fluorescence titrations were performed as follows: Bisphosphoric acid (*R,R*)-**6**, [3+2] capsule (*all-R*)-**1** or [2+2] capsule (*all-R*)-**2** were dissolved in [D_1]-chloroform/[D_4]-methanol = 8/2 (2 ml, each 100 µM final concentration). C_{70}-IPH (5 mM, in [D_1]-chloroform/[D_4]-methanol = 8/2) was titrated into the solution in a stepwise fashion and the corresponding fluorescence spectra were recorded.

Fitting of the fluorescence data was performed as follows:

Software: The data was fitted using Microsoft Excel. The RGP-function was used for linear curve fitting and statistical values. The SOLVER plugin was used for nonlinear curve fitting. The sum of square residues for the calculated F_0/F was minimized by changing K_{11} . The cubic equation for the 1:2 binding was solved using the CUBIC macro.[4] Statistical values were obtained from the SOLVSTAT Macro written by E. J. Billo.[5]

Quenching components: Both dynamic and static quenching components were considered. For the dynamic quenching component, the F_0/F-values for low C_{70}-IPH concentrations [≤ 0.2 eq for (*all-R*)-**1**, ≤ 1 eq for (*all-R*)-**2** and (*R,R*)-**6**] were fitted with a linear fit according to the Stern-Volmer equation to determine K_{SV}.

Definitions:

H: Host (**1**/**2**/**6**)	[X]: Equilibrium conc. of X	F_0: Fluorescence in absence of G
G: Guest (C_{70}-IPH)	[X_0]: Total (added) conc. of X	F: Fluorescence for each [G]
HG: 1:1 complex		
HGG: 1:2 complex		

Dynamic quenching (K_{SV} determined as the slope in an F0/F vs. [G] plot for low C_{70}-IPH concentrations):	F0/F = 1 + K_{SV}*[G0]

The fluorescence data was then fitted using both dynamic and static quenching in a F0/F vs. [C_{70}-IPH] plot, assuming a nonfluorescent complex between C_{70}-IPH and (*all-R*)-**1**/(*all-R*)-**2**/(*R,R*)-**6**.[6]

Total fluorescence	F/F0 = [F/F0]dyn * [H]/[H0] with [F/F0]dyn = 1/(1 + K_{SV}*[G0])

Since only small excesses of C_{70}-IPH are used, the static quenching component cannot be abbreviated as $F_0/F = 1 + K_a*[G_0]$ (because [G] is not equal [G_0]). Instead, the equilibrium concentrations of the components have to be expressed via the full equations. For this, 1:1 and 1:2 equilibria were used as follows:

1:1 case

Host:	H
Guest:	G
1:1-complex:	HG
Reaction:	H + G => HG
Equilibrium constant K:	K = [HG]/([H]*[G])
Total conc. of H:	[H0] = [H] + [HG]
Total conc. of G:	[G0] = [G] + [HG]
Equilibrium conc. of HG:	[HG]=0.5*([G0]+[H0]+1/K)-(([G0]+[H0]+1/K)^2 - 4*[H0]*[G0])^(0.5)

1:2 case

Host:	H
Guest:	G
Complex:	HGG
Reaction step 1:	H + G => HG
Reaction step 2:	HG + G => HGG
Total reaction:	H + 2 G => HGG
Equilibrium constant K1:	K1 = [HG]/([G]*[H])
Equilibrium constant K1:	K2 = [HGG]/([HG]*[H])
Total equilibrium constant:	K1*K2 = [HHG]/([H]*[G]^2)
Total conc. of H:	[H0] = [H] + [HG] + [HGG]
Total conc. of G:	[G0] = [G] + [HG] + 0.5[HGG]
Equilibrium conc. of G: (G is obtained by solving the cubic equation)	$K11*K21*[G]^3+(2*K11*K21*[H0]-K11*K21*[G0]+K11)*[G]^2+$ $(1-K11*[G0]+K11[H0])*[G]-[G0] = 0$ $A*[G]^3+B*[G]^2+C*[G]+D=0$

	A = K11*K21
	B = 2*K11*K21*[H0]-K11*K21*[G0]+K11
	C = 1-K11*[G0]+K11[H0]
	D = -[G0]
	$K11*K21*[G]^3+(2*K11*K21*[H0]-K11*K21*[G0]+K11)*[G]^2+(1-K11*[G0]+K11[H0])*[G]-[G0]=0$
Equilibrium conc. of HG:	$[HG]=(K11*[H0]*[G])/(1+K11*[G]+K11*K21*[G]^2)$
Equilibrium conc. of HGG:	$[HGG]=K21*[HG]*[G]=(K11*K21*[H0]*[G]^2)/(1+K11*[G]+K11*K21*[G]^2)$

This results in the following equations for fitting of the total fluorescence change:

1:1 case	
Total fluorescence	F/F0 = [F/F0]dyn * [H]/[H0]
Conc. of HG:	[HG]=0.5*([G0]+[H0]+1/K)-(([G0]+[H0]+1/K)^2 - 4*[H0]*[G0])^(0.5)
Conc. of H:	[H] = [H0] - [HG]
	[H] = [H0] - 0.5*([G0]+[H0]+1/K)-(([G0]+[H0]+1/K)^2 - 4*[H0]*[G0])^(0.5)
Stern-Volmer plot (Fitting carried out by variation of K in least-square analysis (SOLVER))	F0/F = [F0/F]dyn * [H0]/[H]
	F0/F = (1+ Ksv[G]) * [H0]/[H]
	F0/F = (1+ Ksv[G]) * [H0]/([H0] - 0.5*([G0]+[H0]+1/K)-(([G0]+[H0]+1/K)^2 - 4*[H0]*[G0])^(0.5))

1:2 case	
Total fluorescence	F/F0 = [F/F0]dyn * [H]/[H0]
Conc. of HG:	$[HG]=(K11*[H0]*[G])/(1+K11*[G]+K11*K21*[G]^2)$
Conc. of HGG:	$[HGG]=K21*[HG]*[G]=(K11*K21*[H0]*[G]^2)/(1+K11*[G]+K11*K21*[G]^2)$
Conc. of H:	[H] = [H0] - [HG] - [HGG]
Stern-Volmer plot (Fitting carried out by variation of K11 and K12 in least-square analysis (SOLVER))	F0/F = [F0/F]dyn * [H0]/[H]
	F0/F = (1+ Ksv[G]) * [H0]/([H0] - [HG] - [HGG])

Fitting was carried out both for the 1:1 case and for the 1:2 case and the results were compared. For the 1:2 case, different fitting routines were used (independent K_{11} and K_{12}, equal K_{11} and K_{12}, noncooperative case with $K_{11} = 4*K_{12}$).

The best results were obtained for the noncooperative 1:2 case, which was thus applied for all cases.

Table S 2: Fitting results for fluorescence quenching of the different host-molecules by C_{70}-IPH [based on dynamic and static quenching, static quenching based on 1:2 complex stoichiometry in a noncooperative binding mode (K_{11} = 4* K_{12}, only K_{11} reported)].

	Phosphoric acid (*R,R*)-**6**	[3+2]capsule (*all-R*)-**1**	[2+2]capsule (*all-R*)-**2**
K_{SV} [M^{-1}]	4700 ± 770	20 300 ± 690	5000 ± 60
R^2	0.974	0.999	0.999
K_{11} [M^{-1}]	2100 ± 1500	20200 ± 4500	4600 ± 2100
R^2	0.893	0.917	0.936

4.1.3. UV- and fluorescence spectra for the 1:3 mixtures

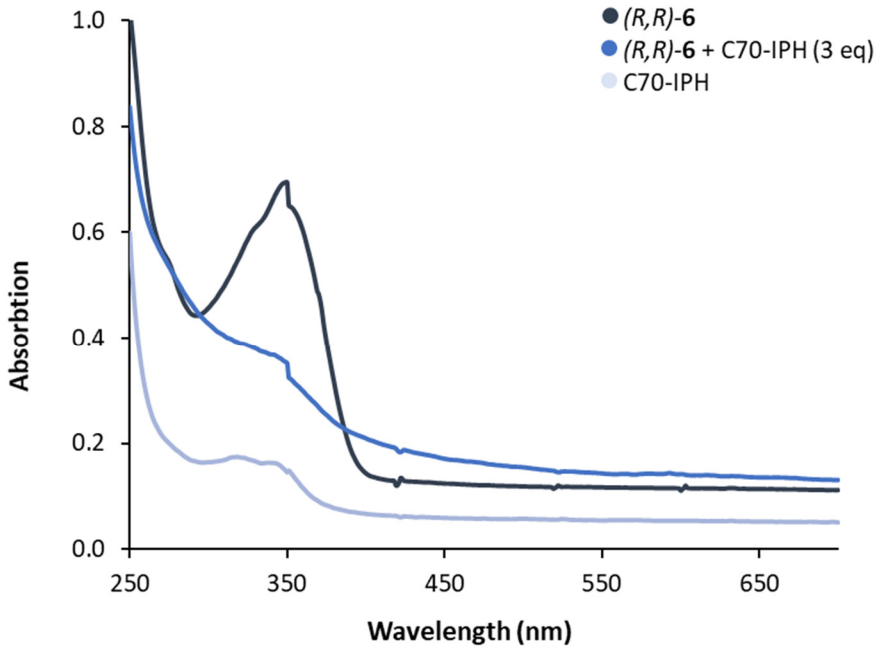

Figure S 18: UV absorption spectra of (*R,R*)-**6** (100 µM), C_{70}-IPH (300 µM), and a mixture of (*R,R*)-**6** (100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2).

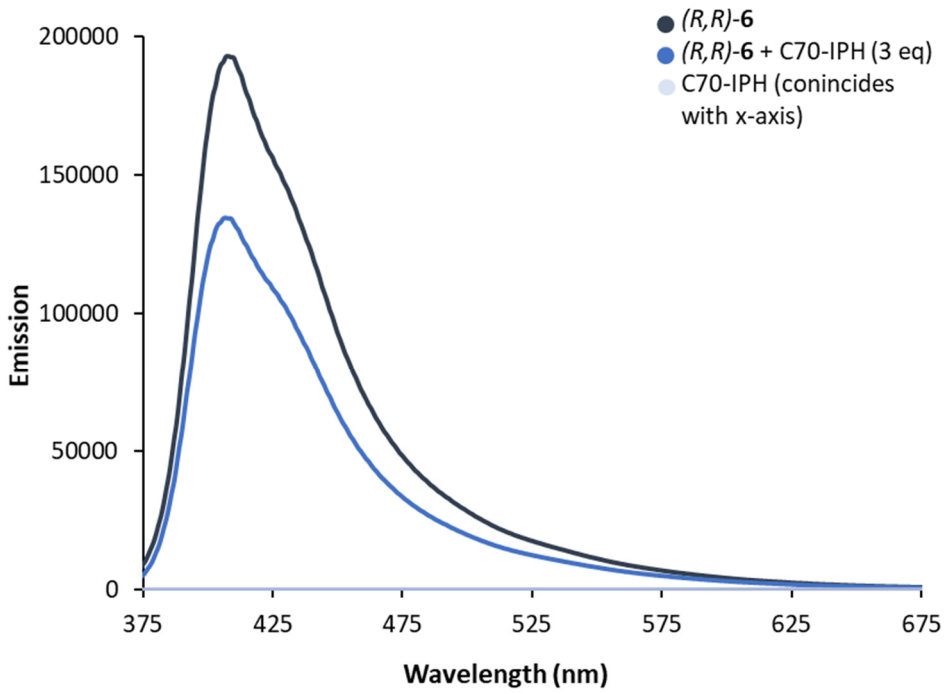

Figure S 19: Fluorescence emission spectra of (*R,R*)-**6** (100 µM), C_{70}-IPH (300 µM), and a mixture of (*R,R*)-**6** (100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2, λ_{exc} = 350 nm).

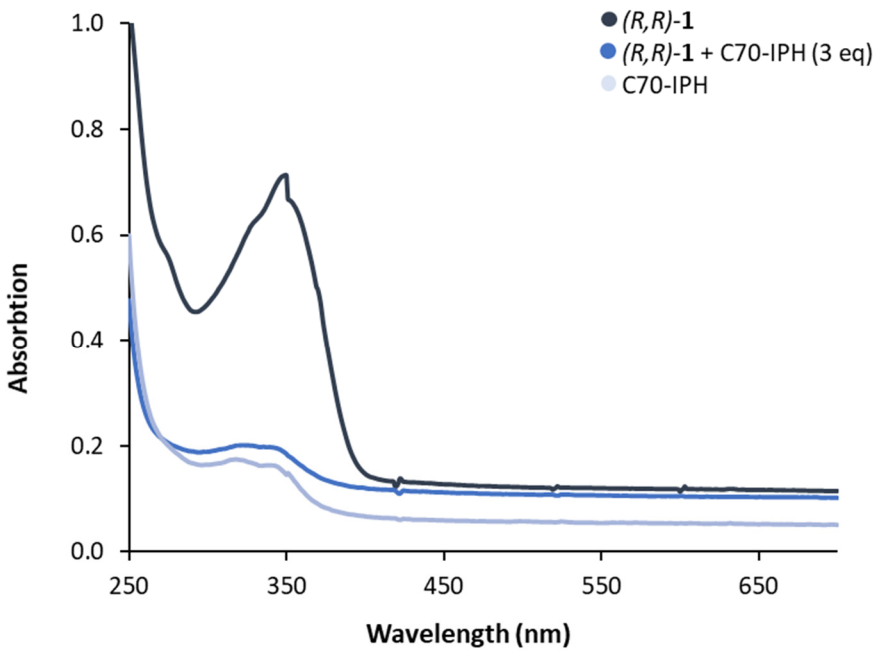

Figure S 20: UV absorption spectra of (*R,R*)-**1** (100 µM), C_{70}-IPH (300 µM), and a mixture of (*R,R*)-**1** (100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2).

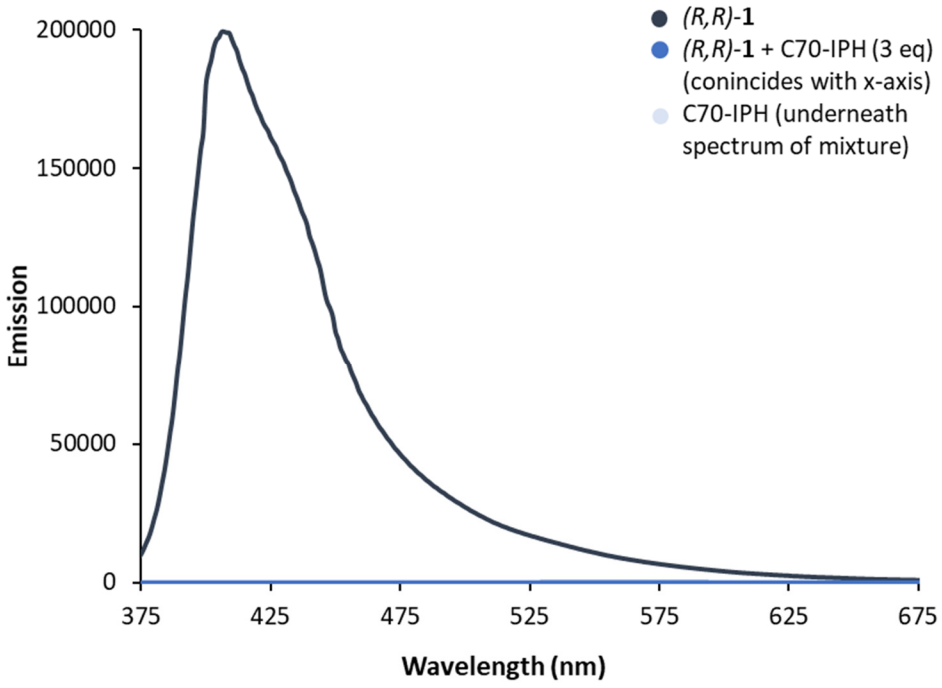

Figure S 21: Fluorescence emission spectra of (*R,R*)-**1** (100 µM), C_{70}-IPH (300 µM), and a mixture of (*R,R*)-**1** (100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2, λ_{exc} = 350 nm).

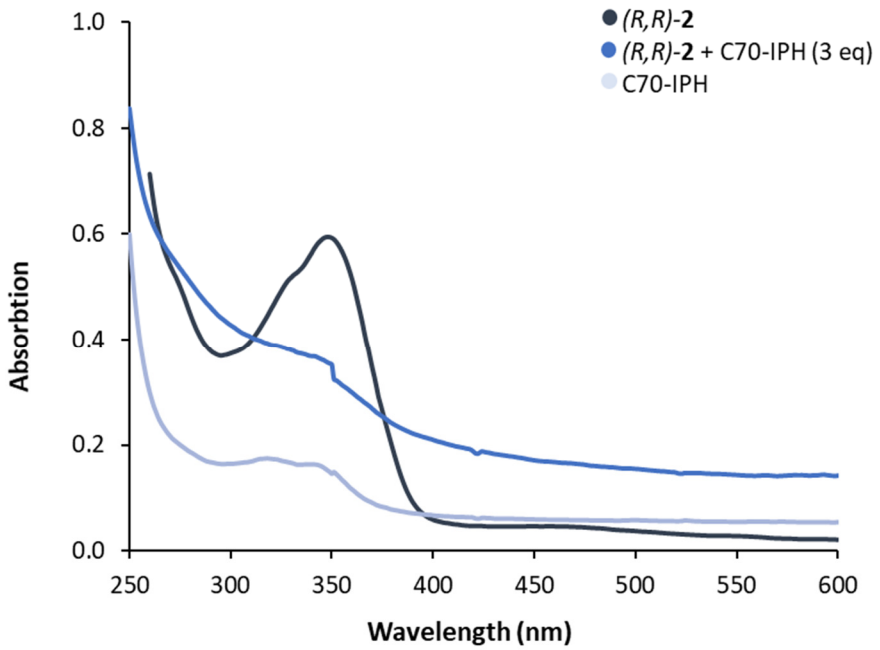

Figure S 22: UV absorption spectra of (*R,R*)-**2** (100 µM), C_{70}-IPH (300 µM), and a mixture of (*R,R*)-**2** (100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2).

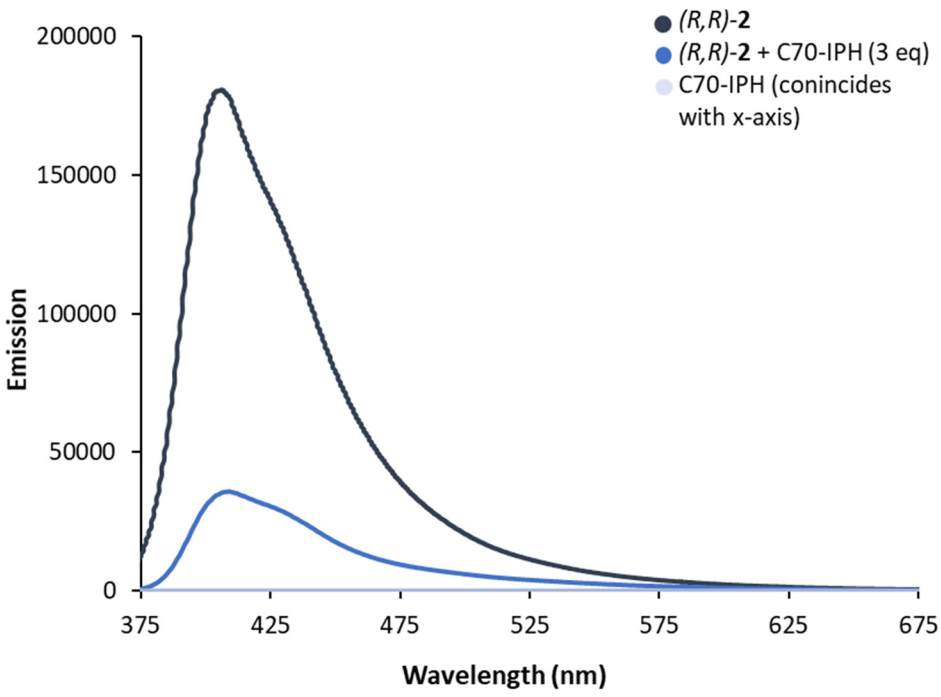

Figure S 23: Fluorescence emission spectra of (*R,R*)-**2** (100 µM), C_{70}-IPH (300 µM), and a mixture of (*R,R*)-**1** (100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2, λ_{exc} = 350 nm).

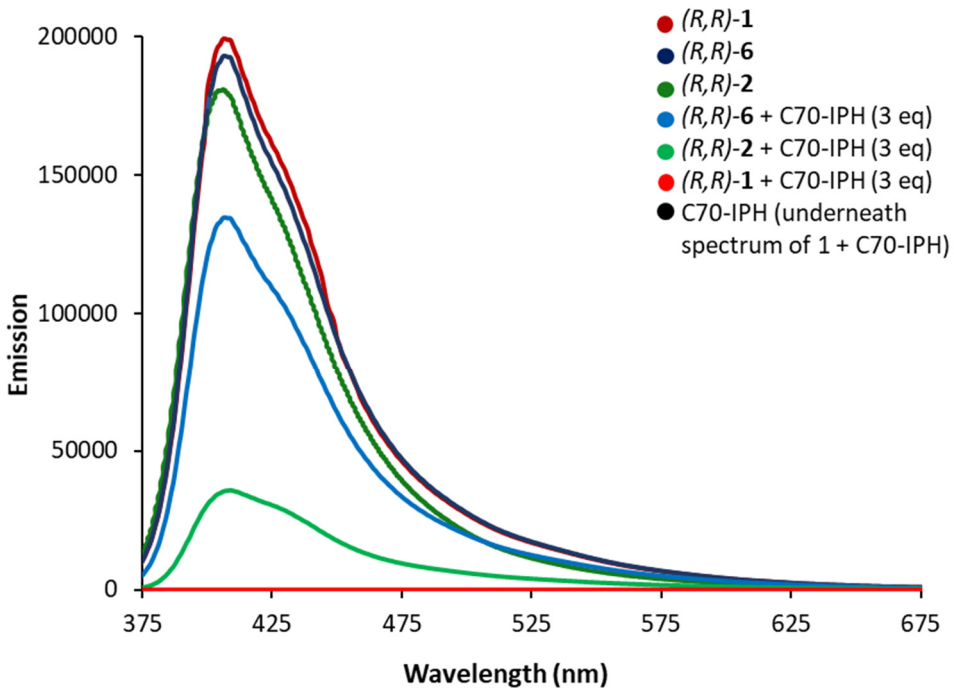

Figure S 24: Fluorescence emission spectra of (*R,R*)-**6**/(*R,R*)-**1**/(*R,R*)-**2** (each 100 µM), C_{70}-IPH (300 µM), and of mixtures of (*R,R*)-**6**/(*R,R*)-**1**/(*R,R*)-**2** (each 100 µM) and C_{70}-IPH (300 µM) (all: [D_1]-chloroform/[D_4]-methanol = 8/2, λ_{exc} = 350 nm).

4.1.4. Fluorescence spectra and fitting data for the titrations

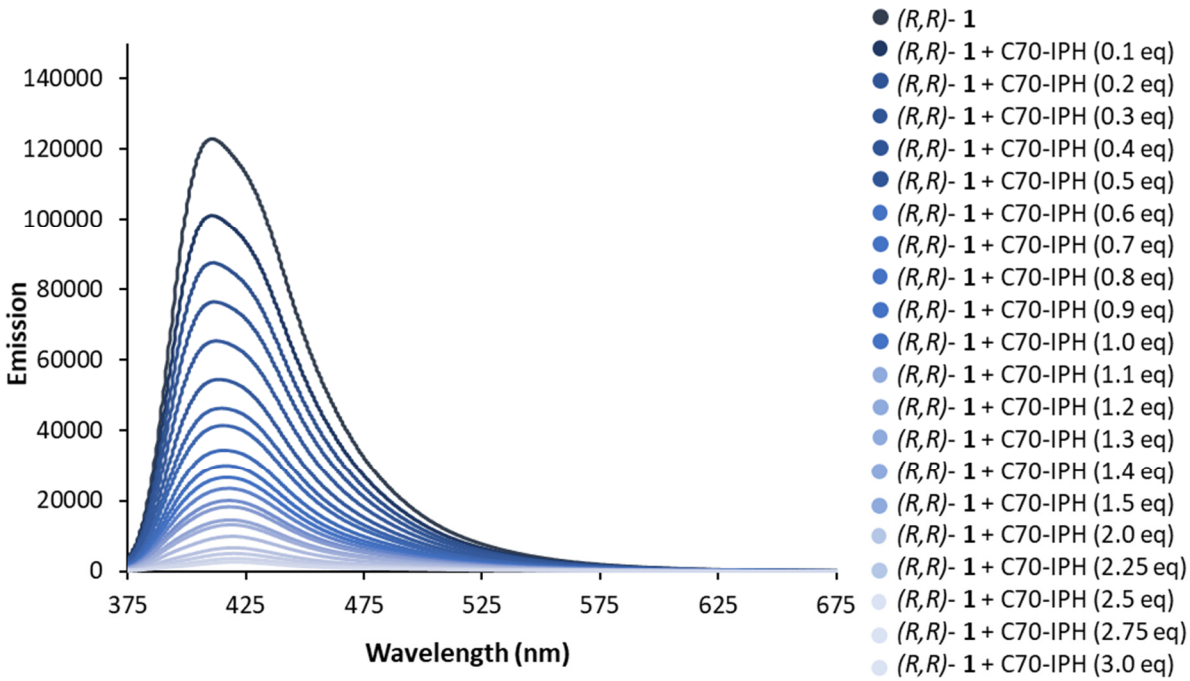

Figure S 25: Fluorescence emission spectra of a titration of (*R,R*)-**1** (100 µM), to which C_{70}-IPH (5 mM) was added in a stepwise fashion (both: $[D_1]$-chloroform/$[D_4]$-methanol = 8/2, λ_{exc} = 350 nm).

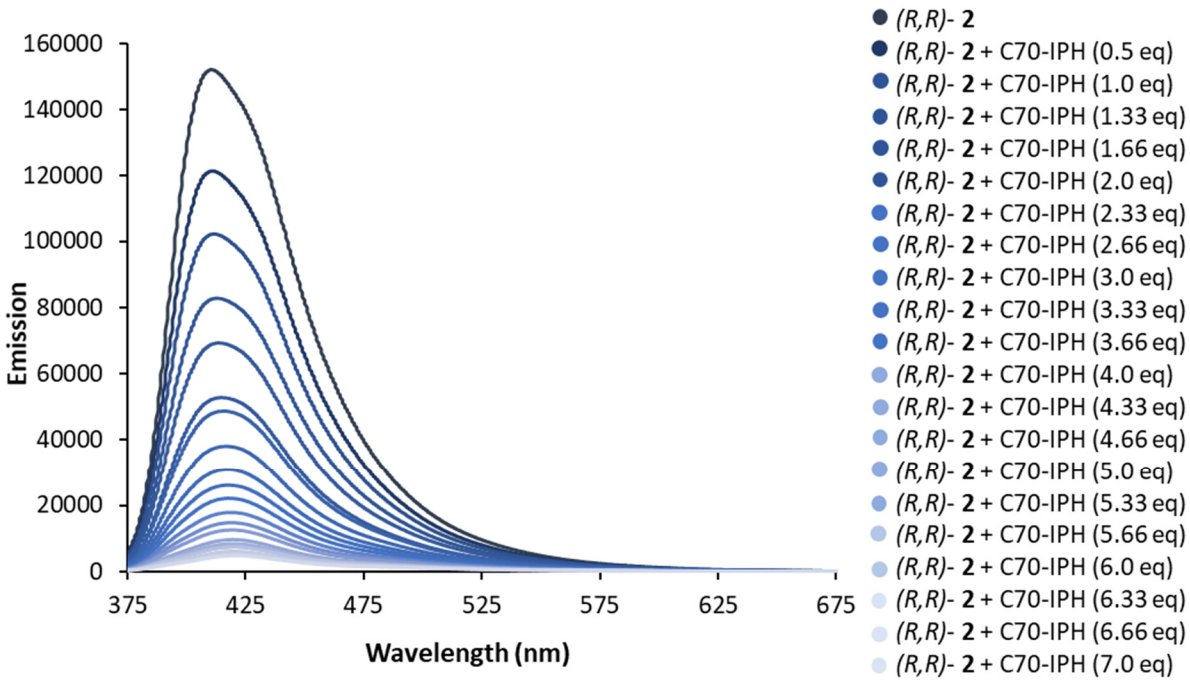

Figure S 26: Fluorescence emission spectra of a titration of (*R,R*)-**2** (100 µM), to which C_{70}-IPH (5 mM) was added in a stepwise fashion (both: $[D_1]$-chloroform/$[D_4]$-methanol = 8/2, λ_{exc} = 350 nm).

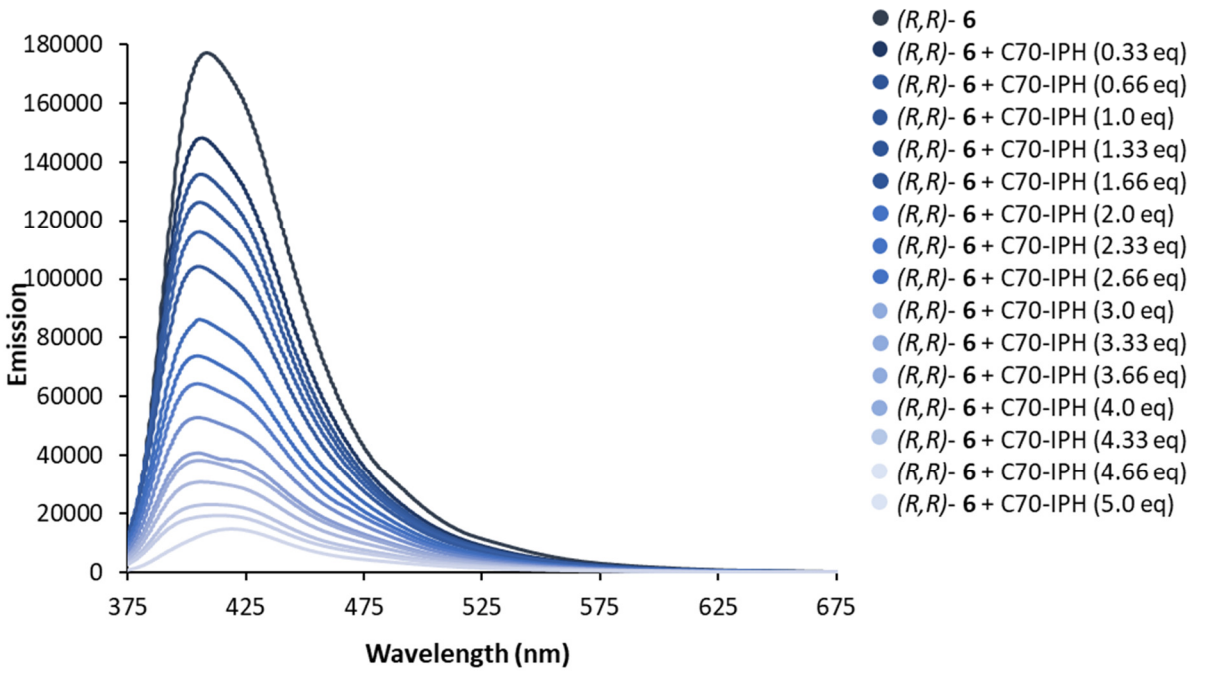

Figure S 27: Fluorescence emission spectra of a titration of (*R,R*)-**6** (100 µM), to which C_{70}-IPH (5 mM) was added in a stepwise fashion (both: [D_1]-chloroform/[D_4]-methanol = 8/2, λ_{exc} = 350 nm).

5. NMR-Spectra

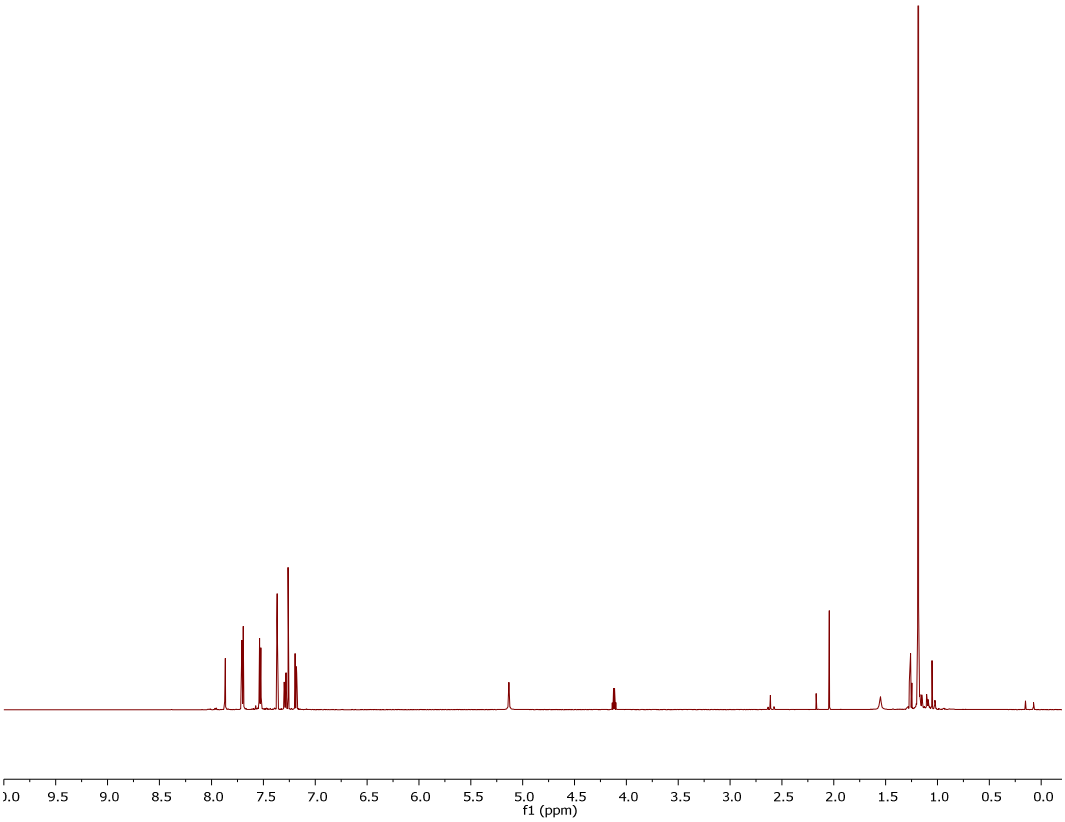

Figure S 28: ^{1}H-NMR spectrum of (*R*)-**3** (600MHz, [D_1]-chloroform, 298 K).

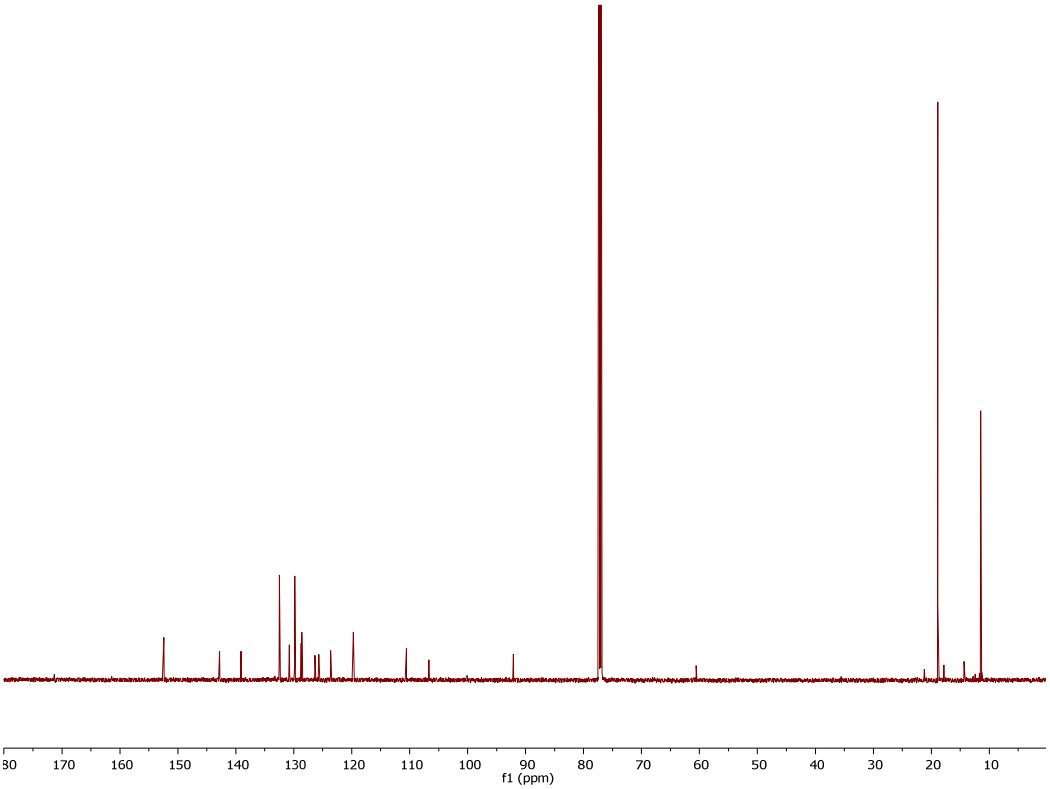

Figure S 29: ^{13}C-NMR Spectrum of (*R*)-**3** (150 MHz, [D_1]-chloroform, 298 K).

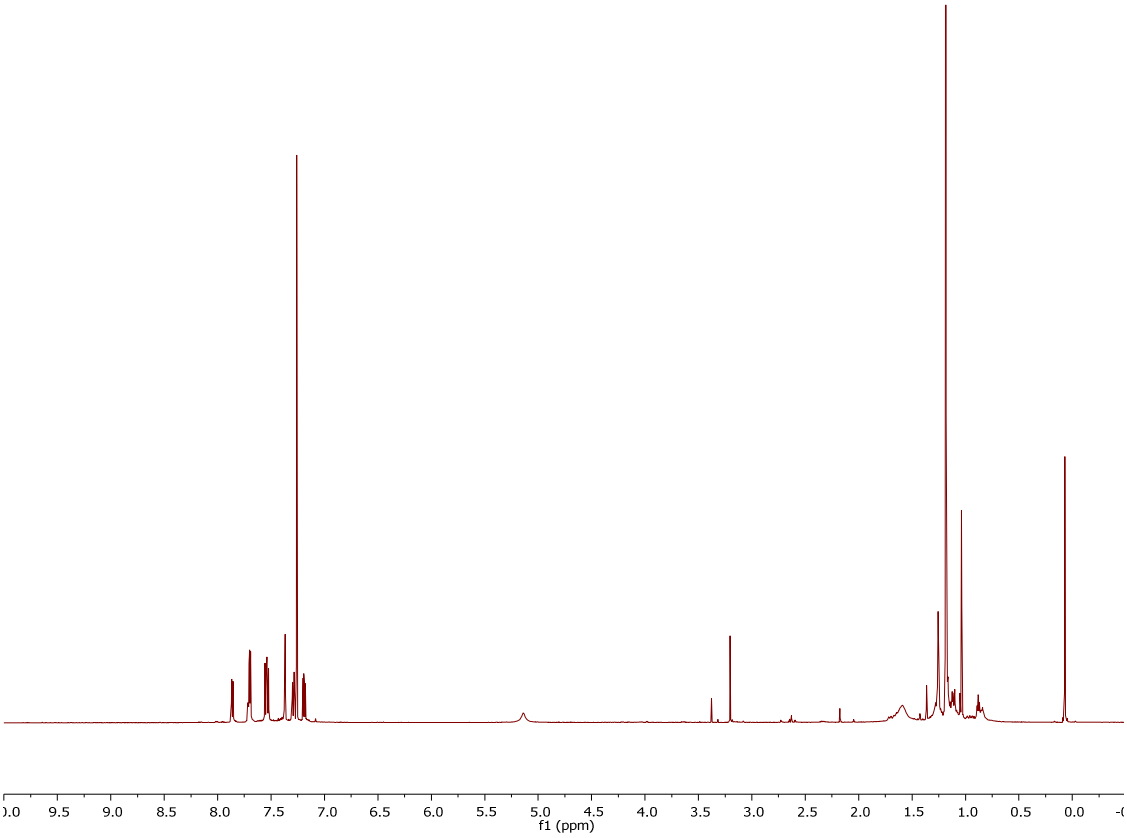

Figure S 30: ^{1}H- NMR Spectrum of (*R*)-**4** (600MHz, [D_1]-chloroform, 298 K).

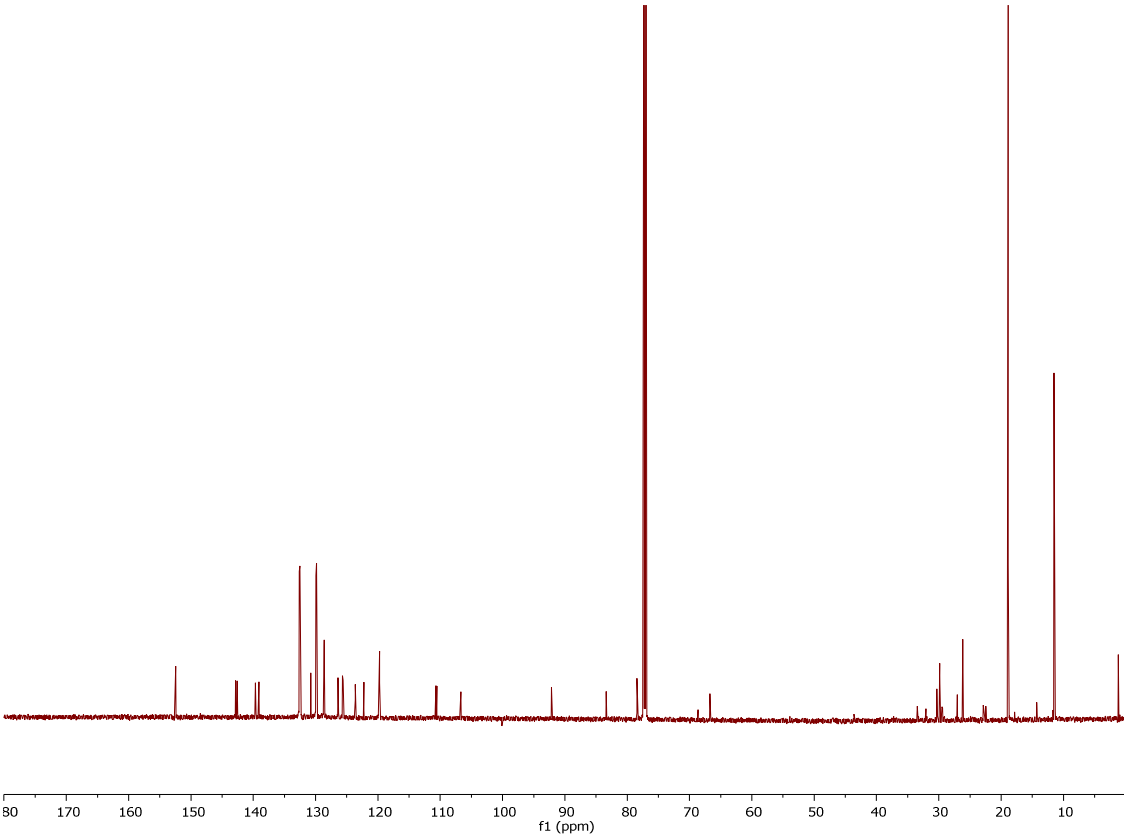

Figure S 31: ^{13}C-NMR Spectrum of (*R*)-**4** (150 MHz, [D_1]-chloroform, 298 K).

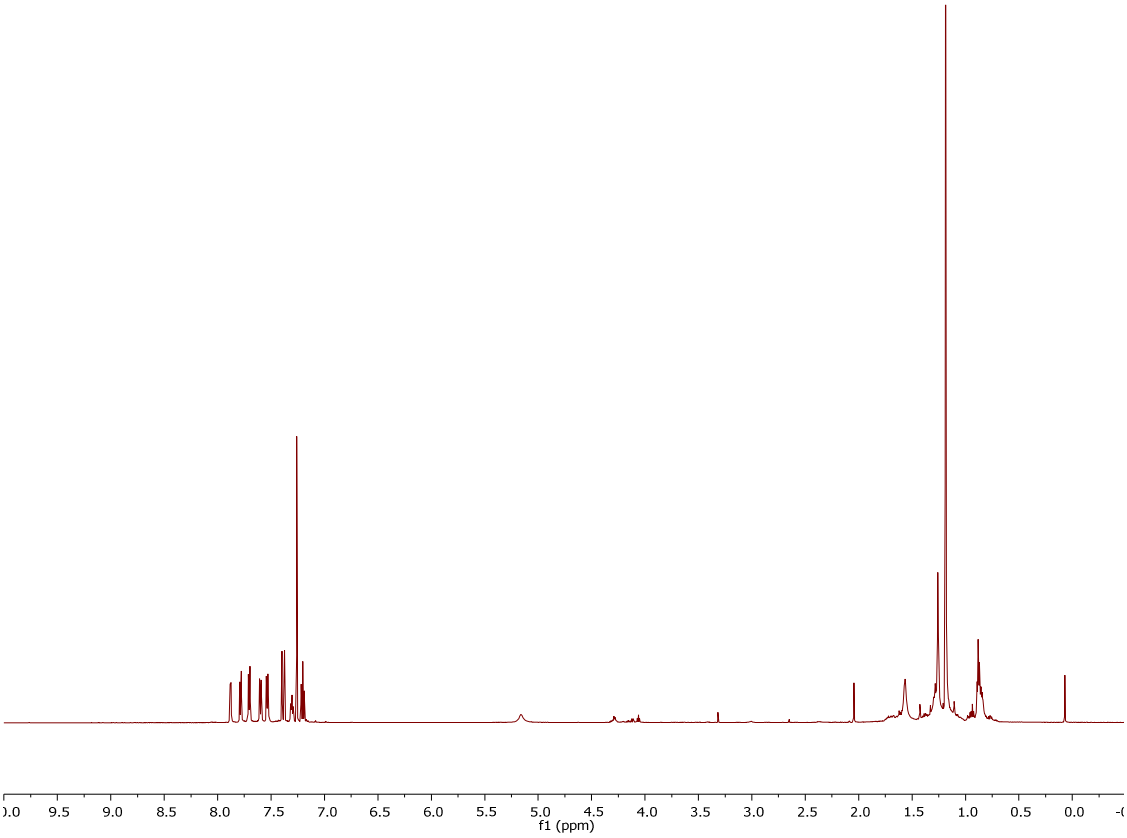

Figure S 32: ^{1}H-NMR spectrum of (*R*)-**5** (600MHz, [D_1]-chloroform, 298 K).

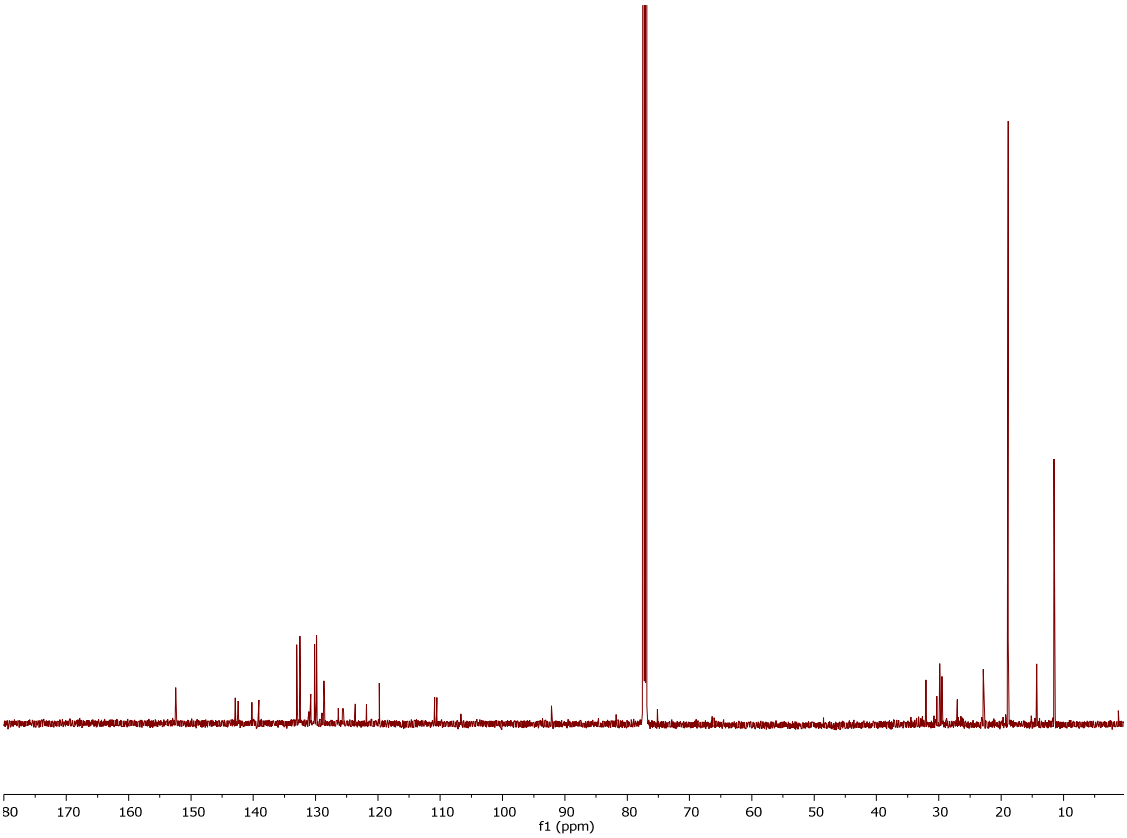

Figure S 33: ^{13}C-NMR Spectrum of (*R*)-**5** (150 MHz, [D_1]-chloroform, 298 K).

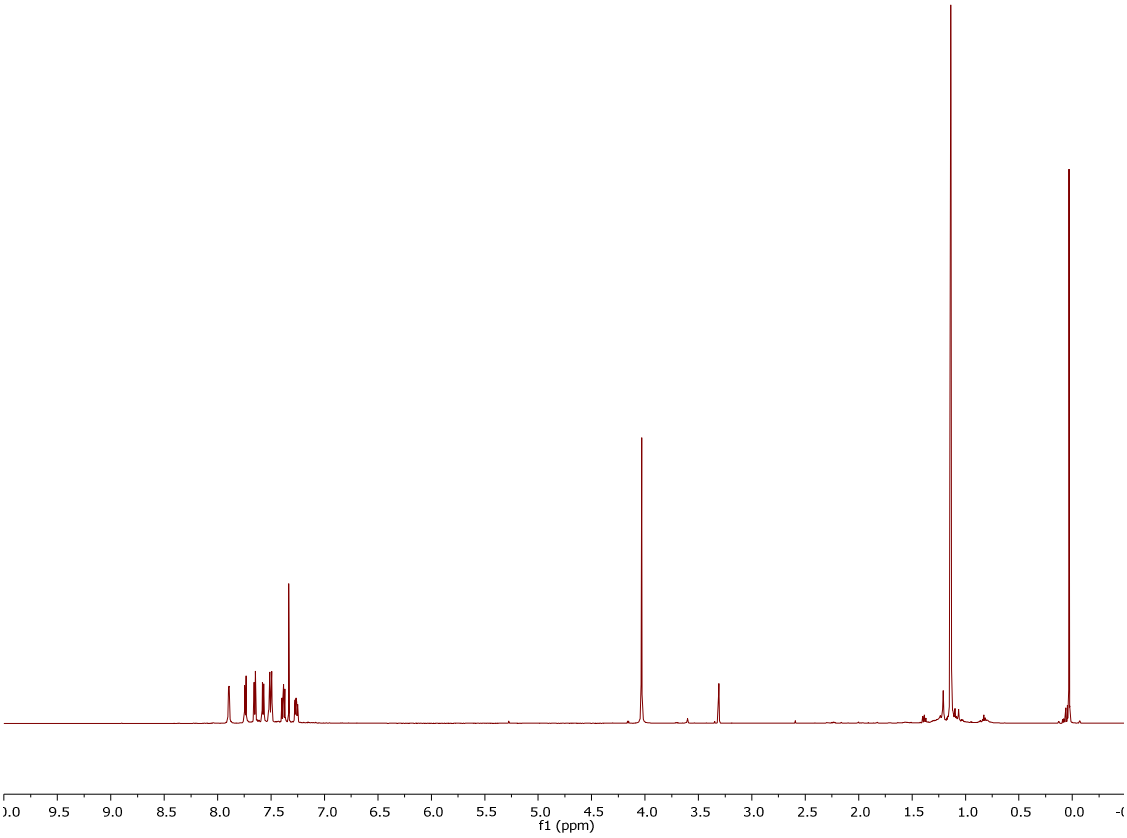

Figure S 34: ^{1}H-NMR Spectrum of (*R,R*)-**6** (600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

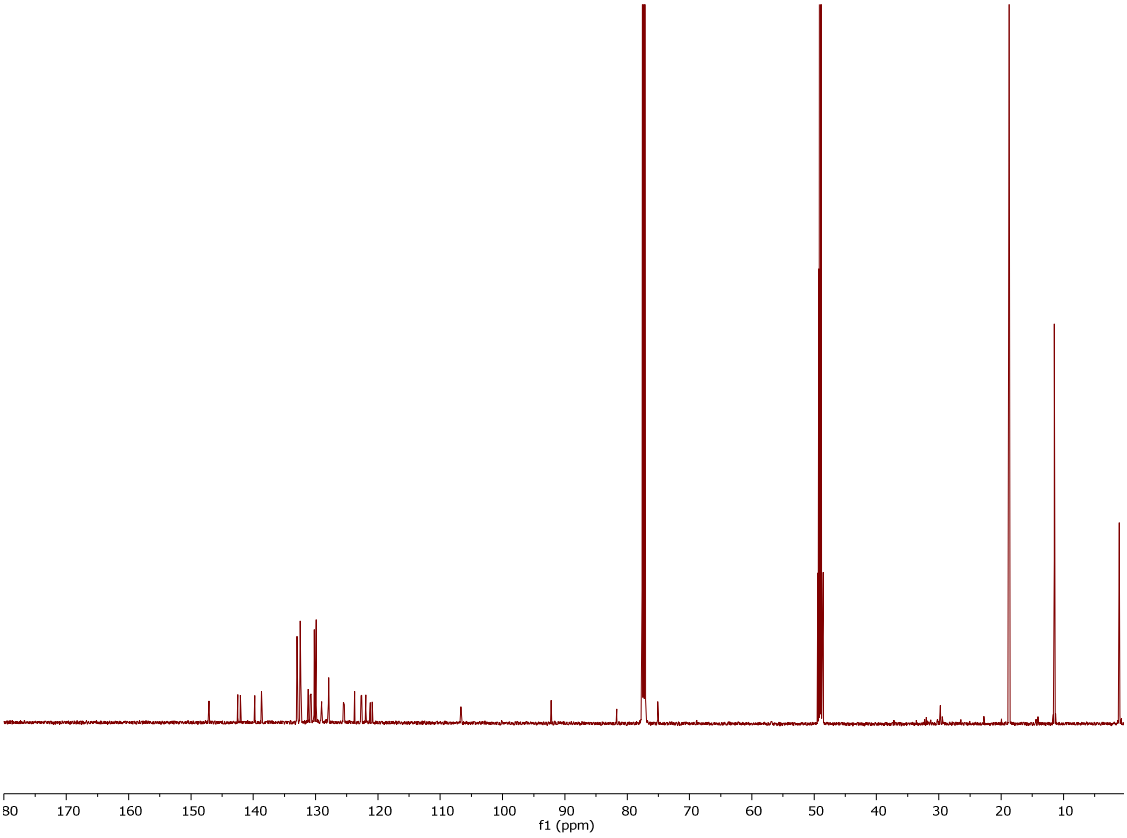

Figure S 35: ^{13}C-NMR Spectrum of (*R,R*)-**6** (150 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

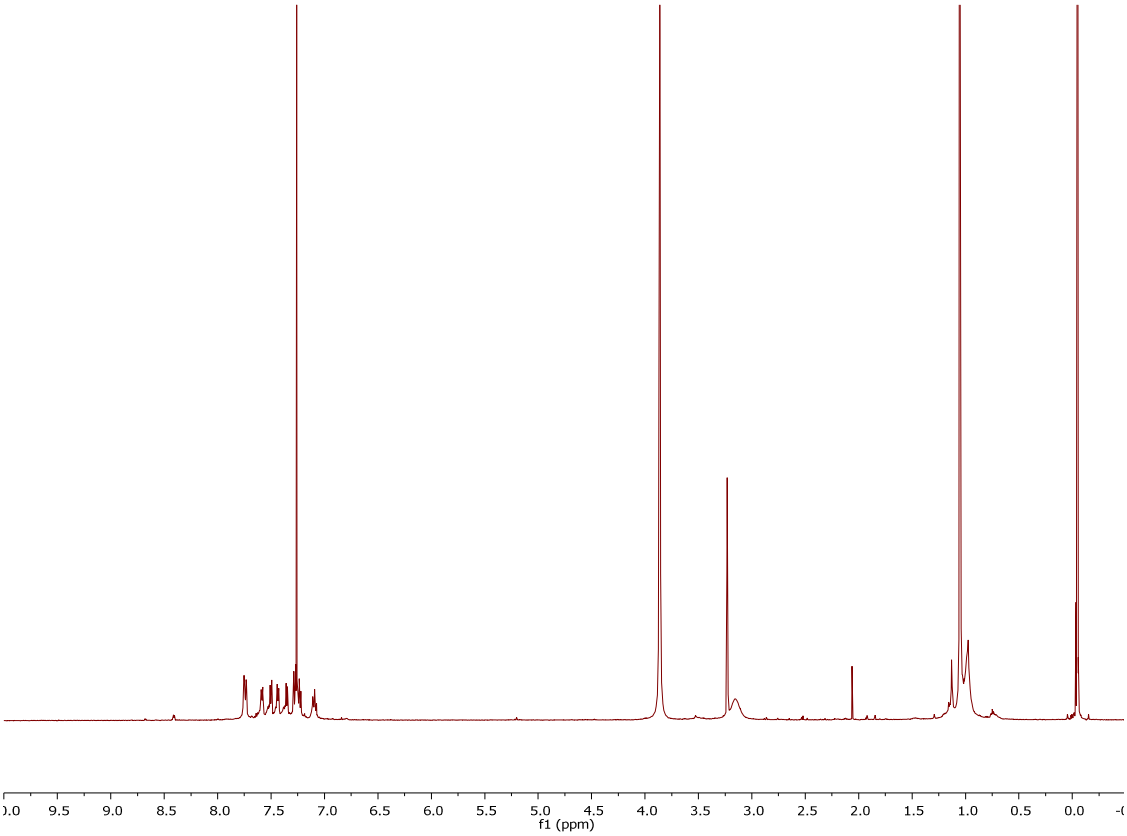

Figure S 36: ^{1}H-NMR spectrum of (*all-R*)-**1** (600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

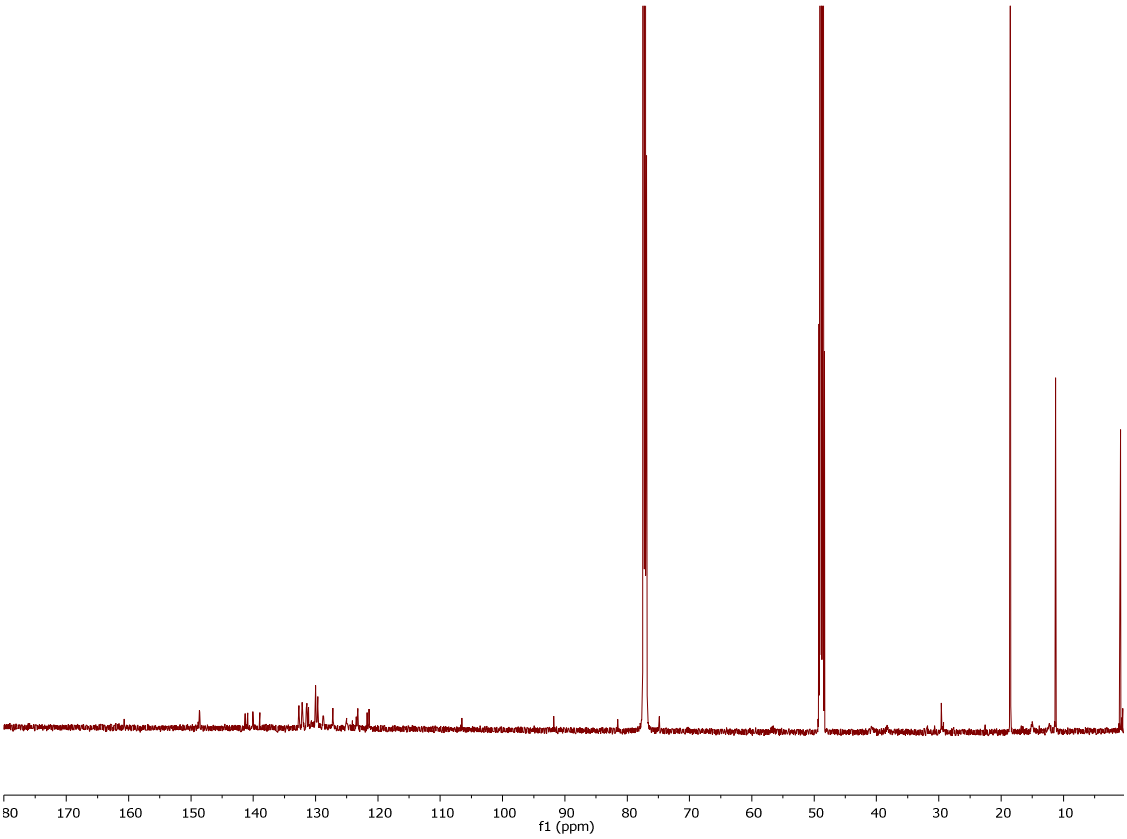

Figure S 37: ^{13}C-NMR spectrum of (*all-R*)-**1** (150 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

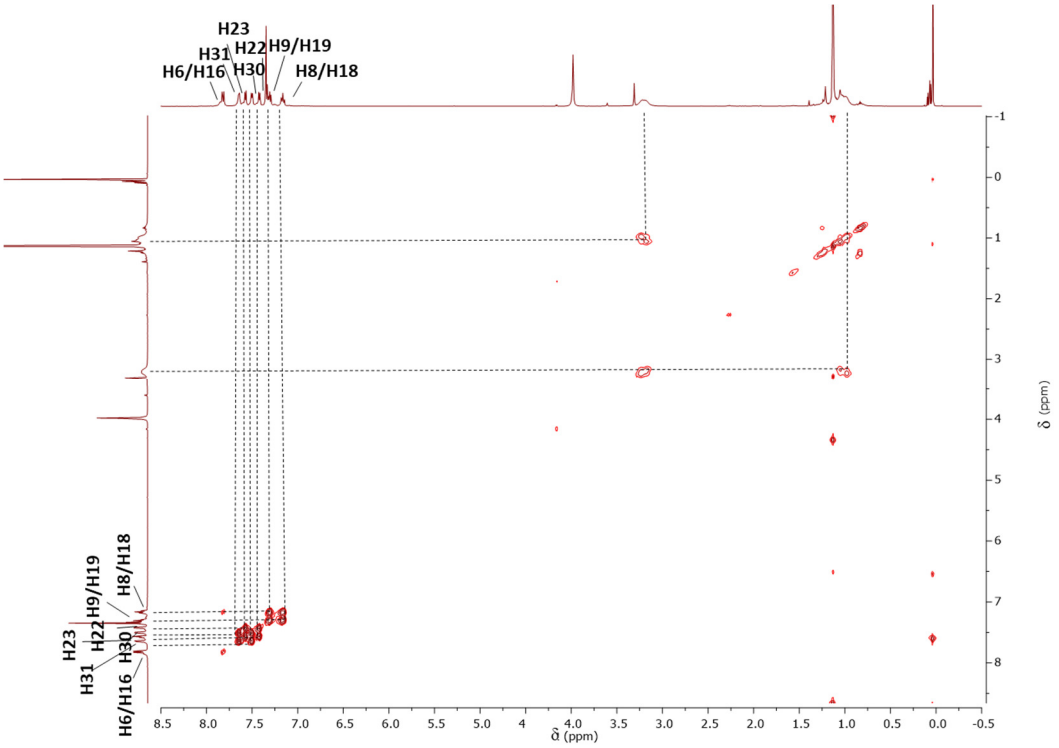

Figure S 38: ^{1}H-COSY NMR spectrum of (*all-R*)-**1** (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

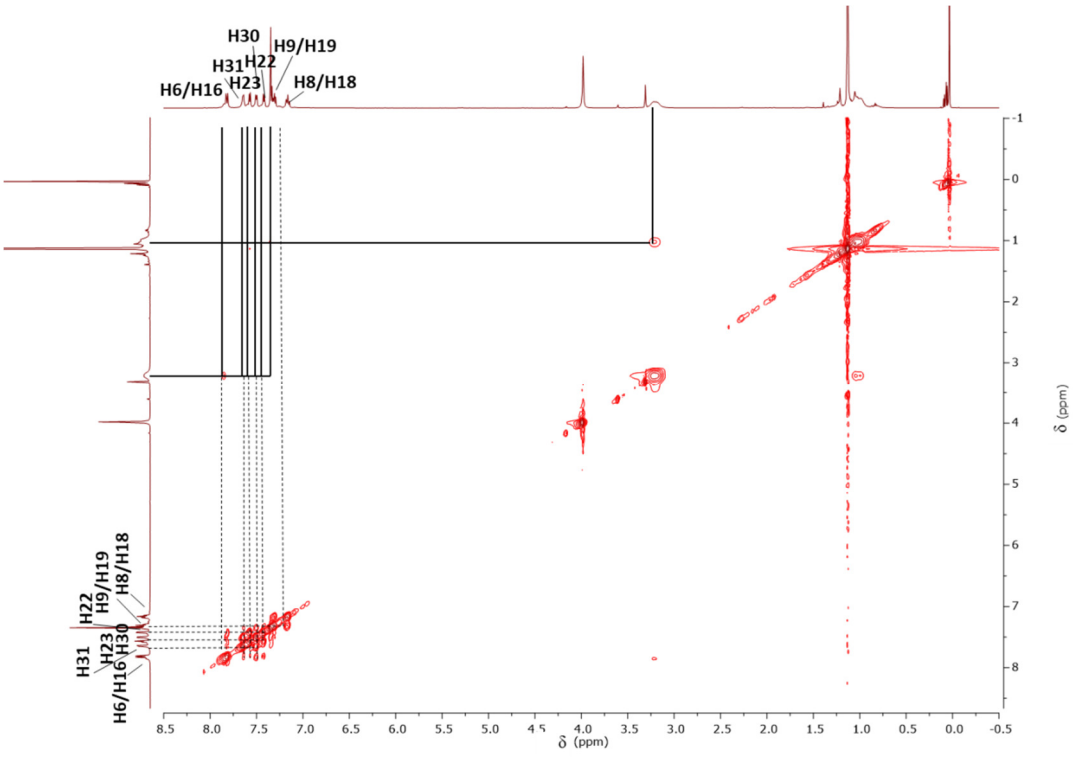

Figure S 39: ^{1}H-NOESY NMR spectrum of (*all-R*)-**1** (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions. For enlargement see the main paper.

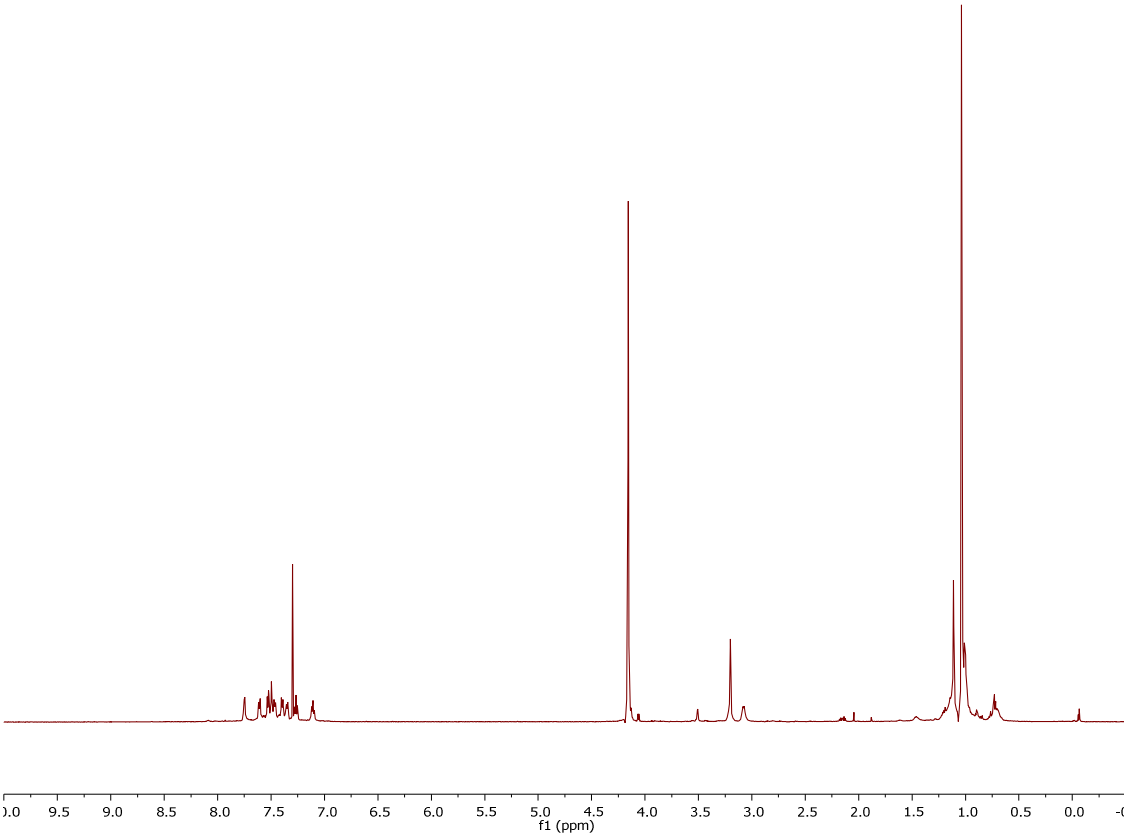

Figure S 40: ^{1}H-NMR Spectrum of (*all-R*)-**2** (600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

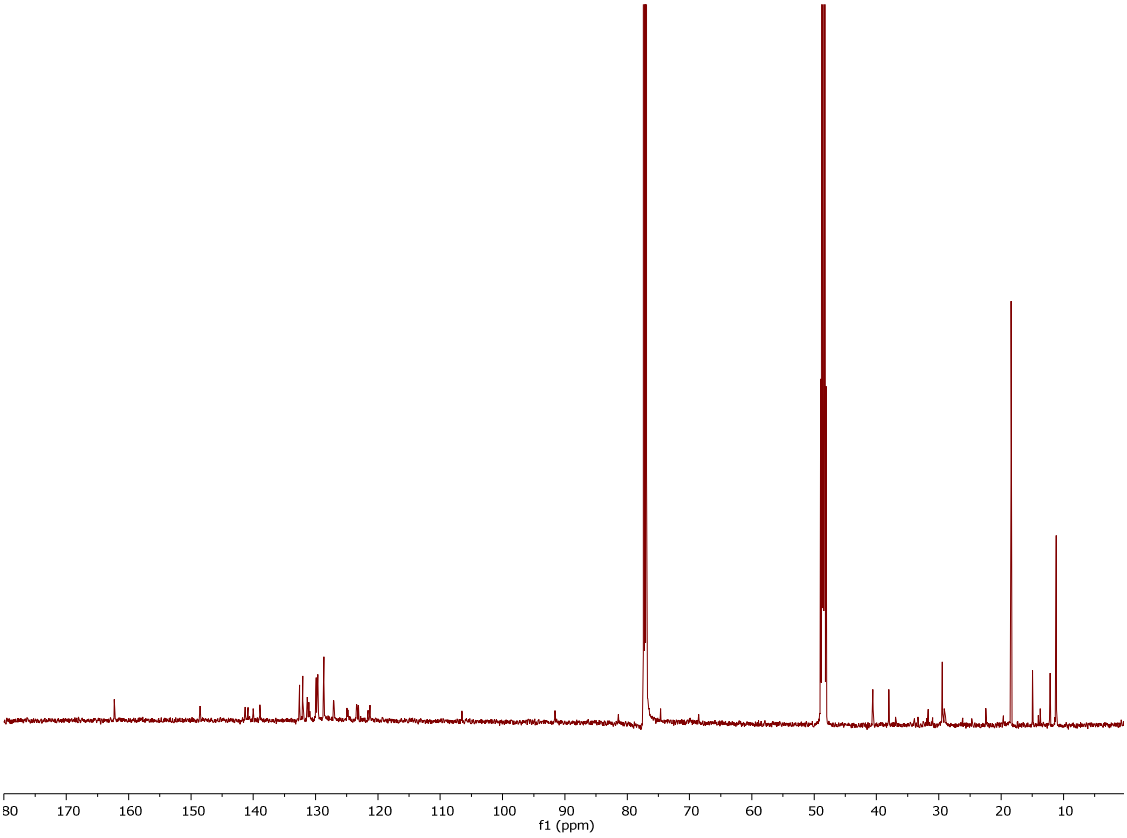

Figure S 41: ^{13}C-NMR Spectrum of (*all-R*)-**2** (150 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

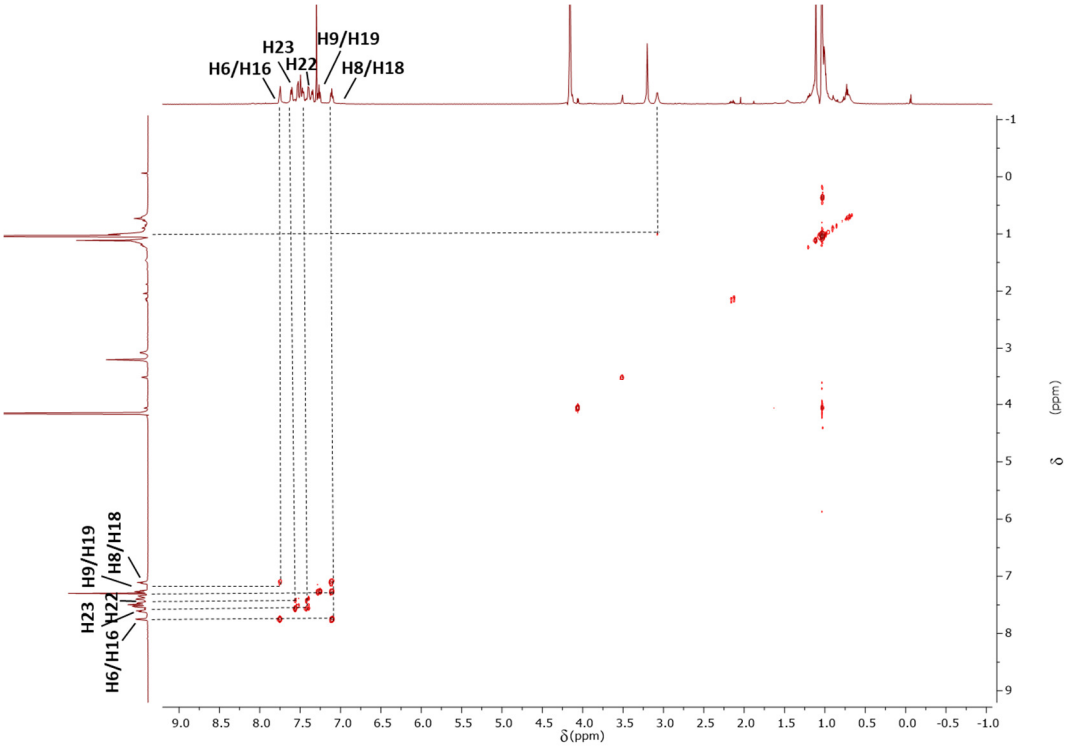

Figure S 42: ^{1}H-COSY NMR spectrum of (*all-R*)-**2** (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

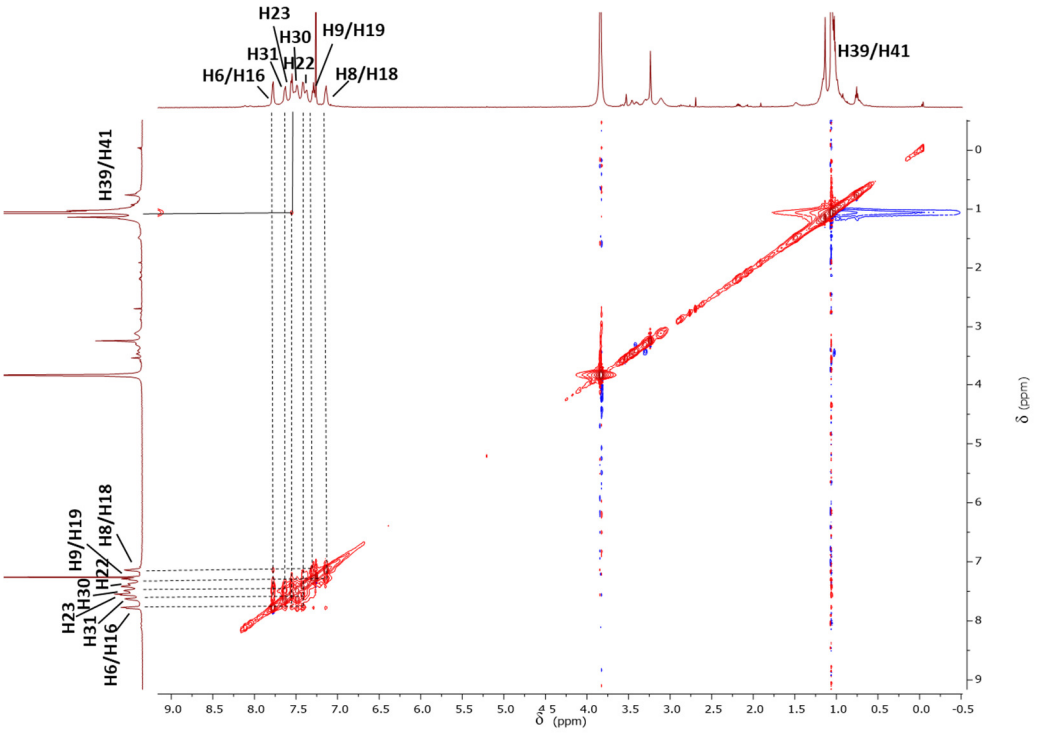

Figure S 43: ^{1}H-NOESY NMR spectrum of (*all-R*)-**2** (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

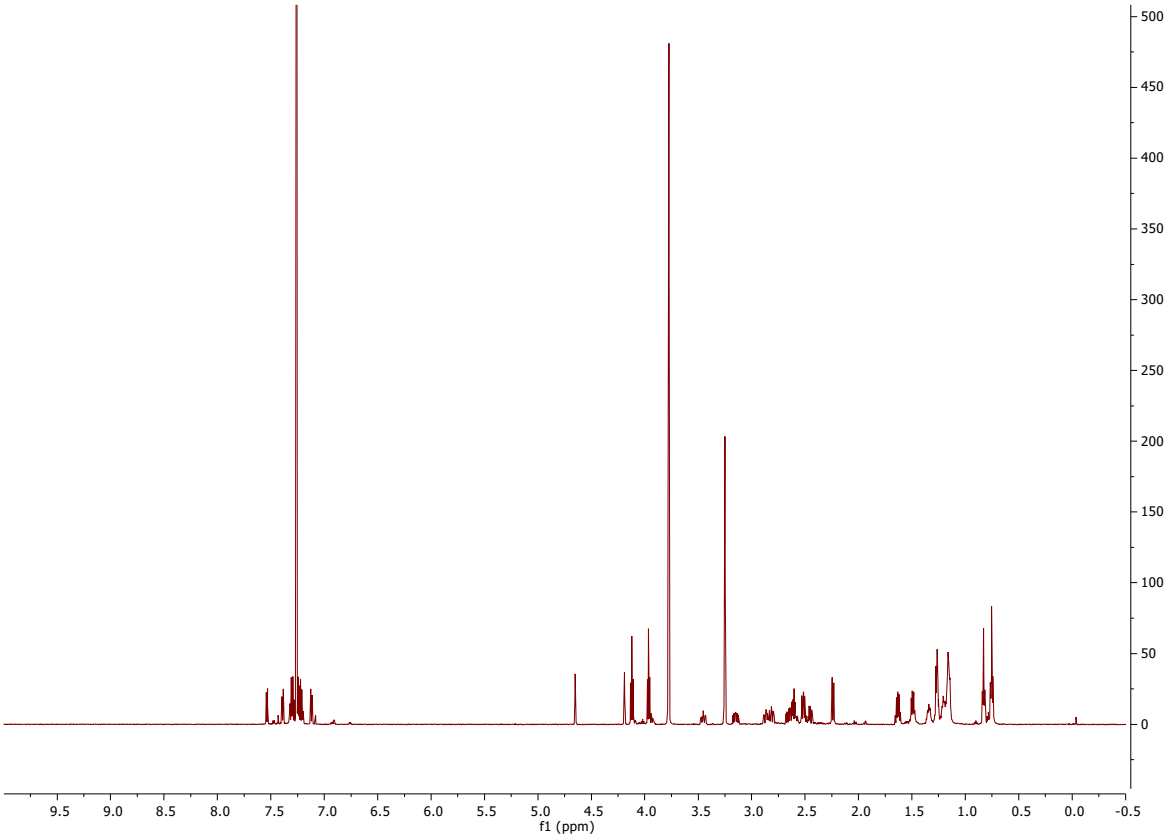

Figure S 44: ^{1}H-NMR spectrum of C_{70}-IPH (600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

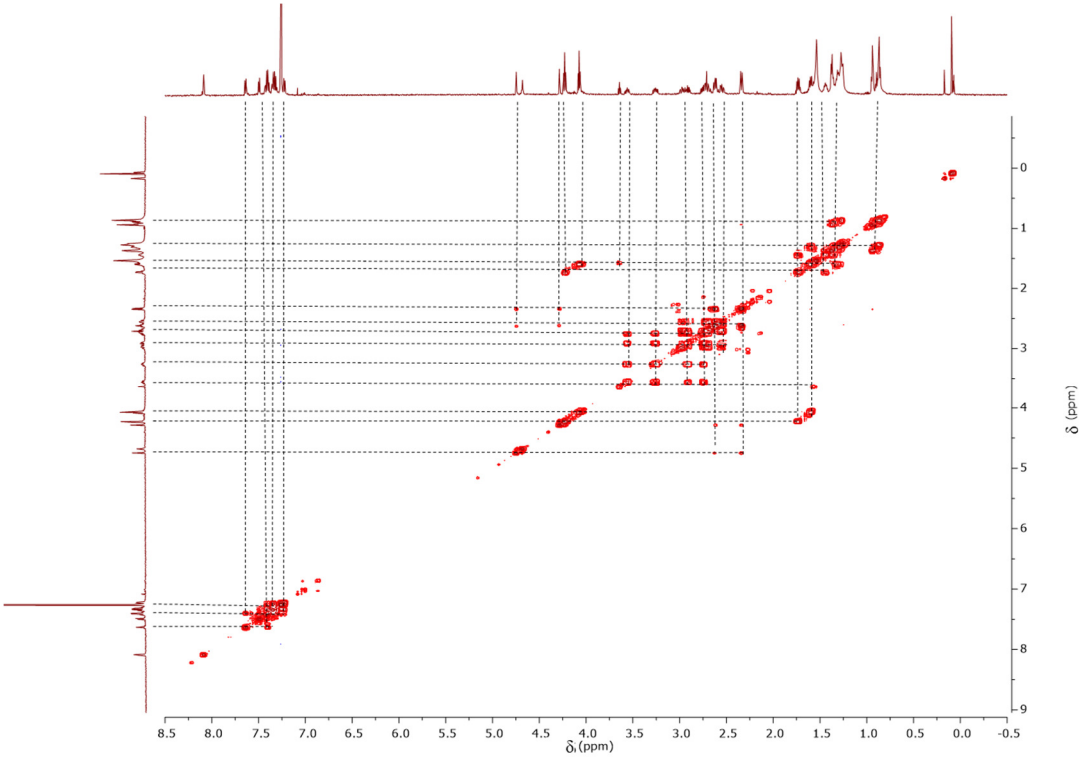

Figure S 45: ^{1}H-COSY NMR spectrum of C_{70}-IPH (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

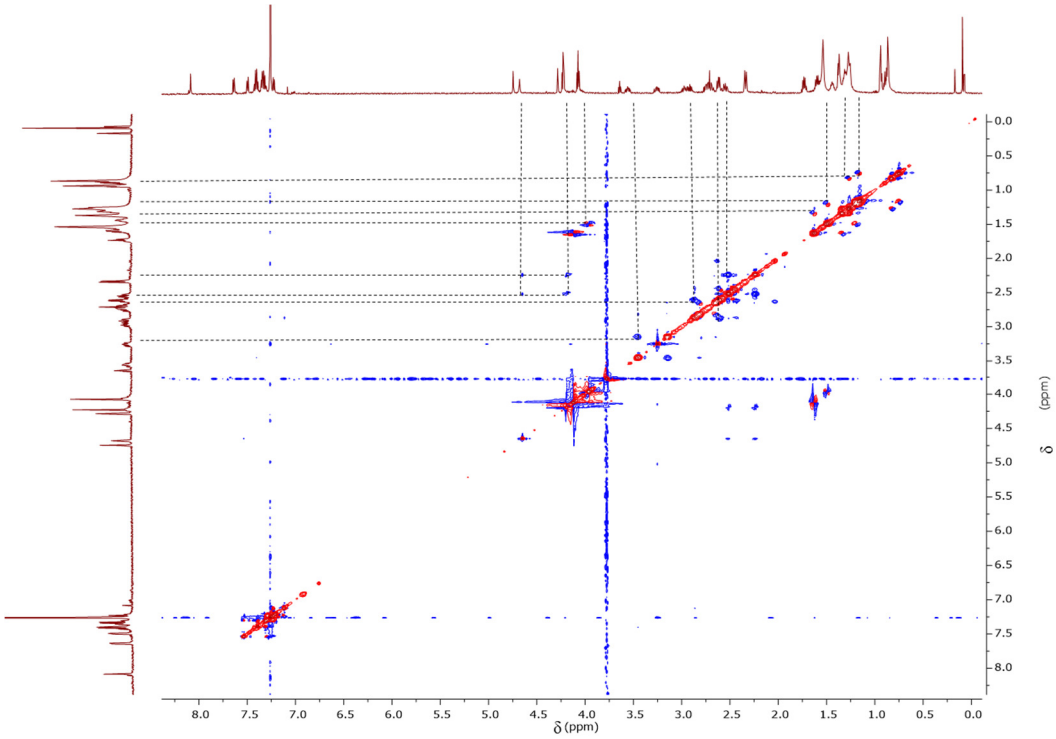

Figure S 46: ^{1}H-NOESY NMR spectrum of C_{70}-IPH (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

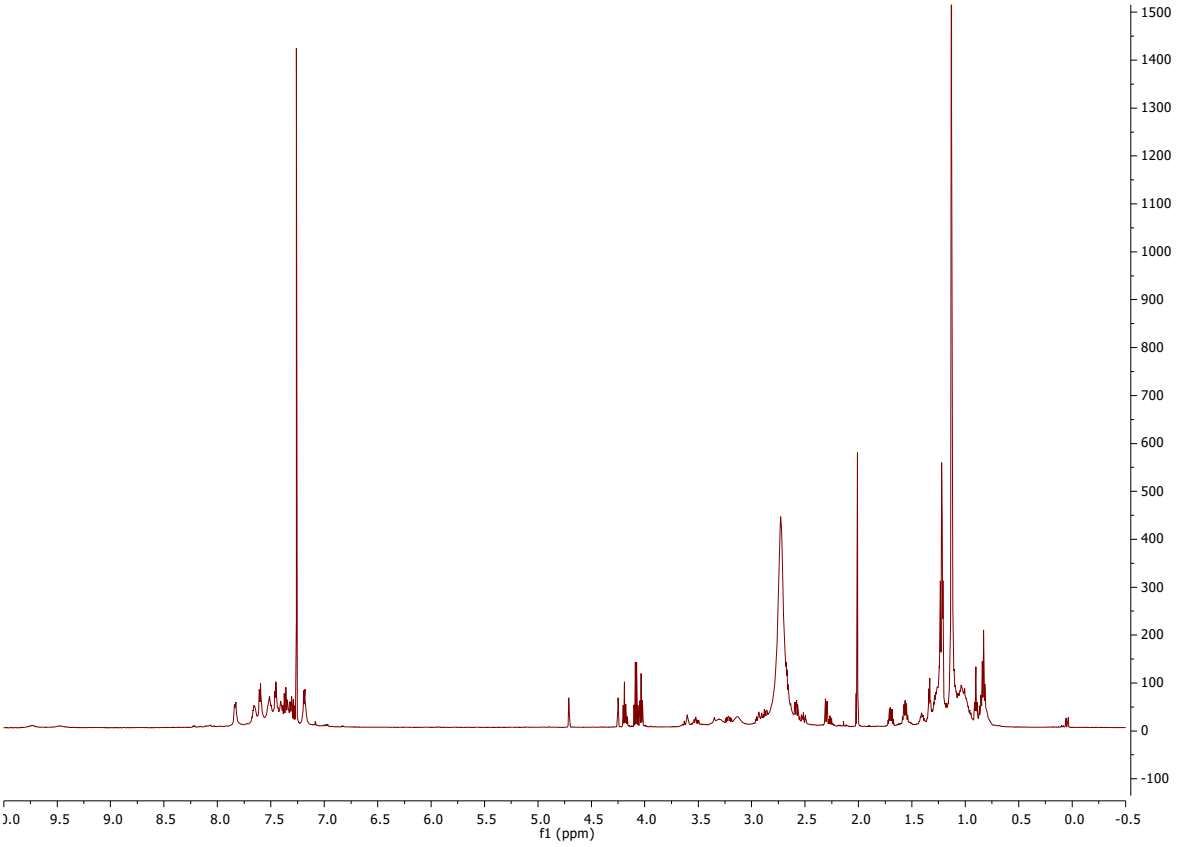

Figure S 47: ^{1}H-NMR spectrum of a mixture of the [3+2]-capsule (*all-R*)-**1** (4 mM) and C_{70}-IPH (ca. 10.6 mM by integration) (600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

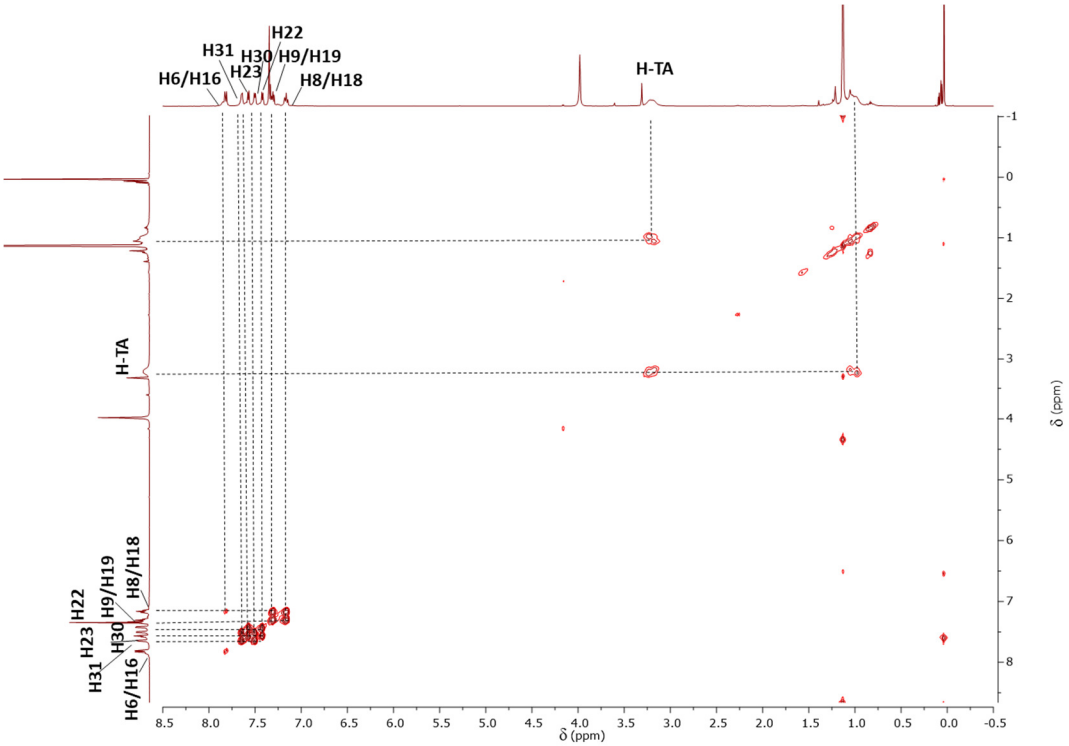

Figure S 48: ^{1}H-COSY NMR spectrum of a mixture of the [3+2]-capsule (*all-R*)-**1** (4 mM) and C_{70}-IPH (ca. 10.6 mM by integration) (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

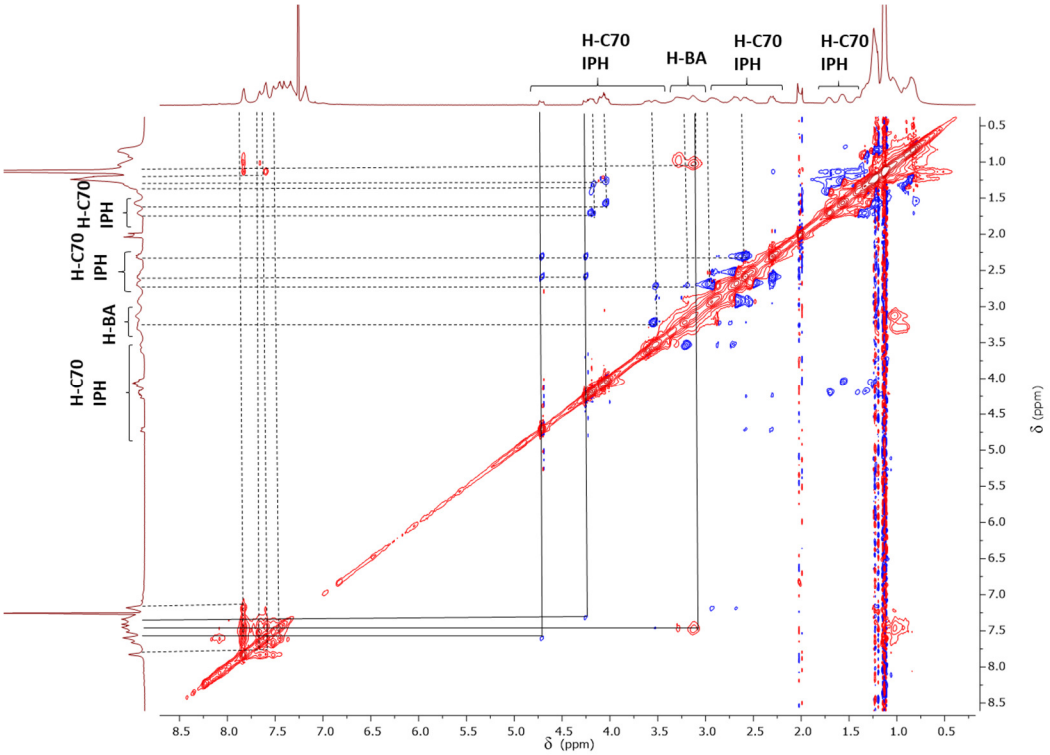

Figure S 49: ^{1}H-NOESY NMR spectrum of a mixture of the [3+2]-capsule (*all-R*)-**1** (4 mM) and C_{70}-IPH (ca. 10.6 mM by integration) (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

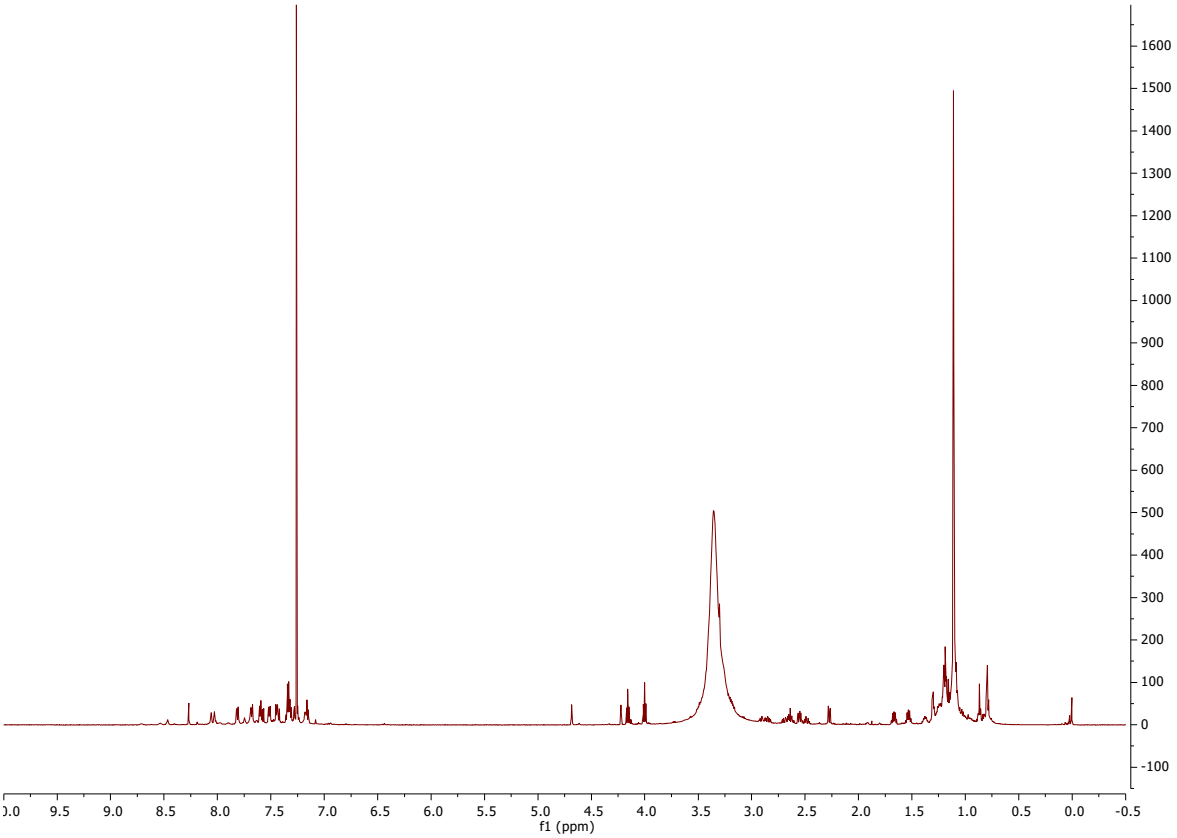

Figure S 50: ^{1}H-NMR spectrum of a mixture of the [2+2]-capsule (*all-R*)-**2** (4 mM) and C_{70}-IPH (ca. 10.2 mM by integration) (600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K).

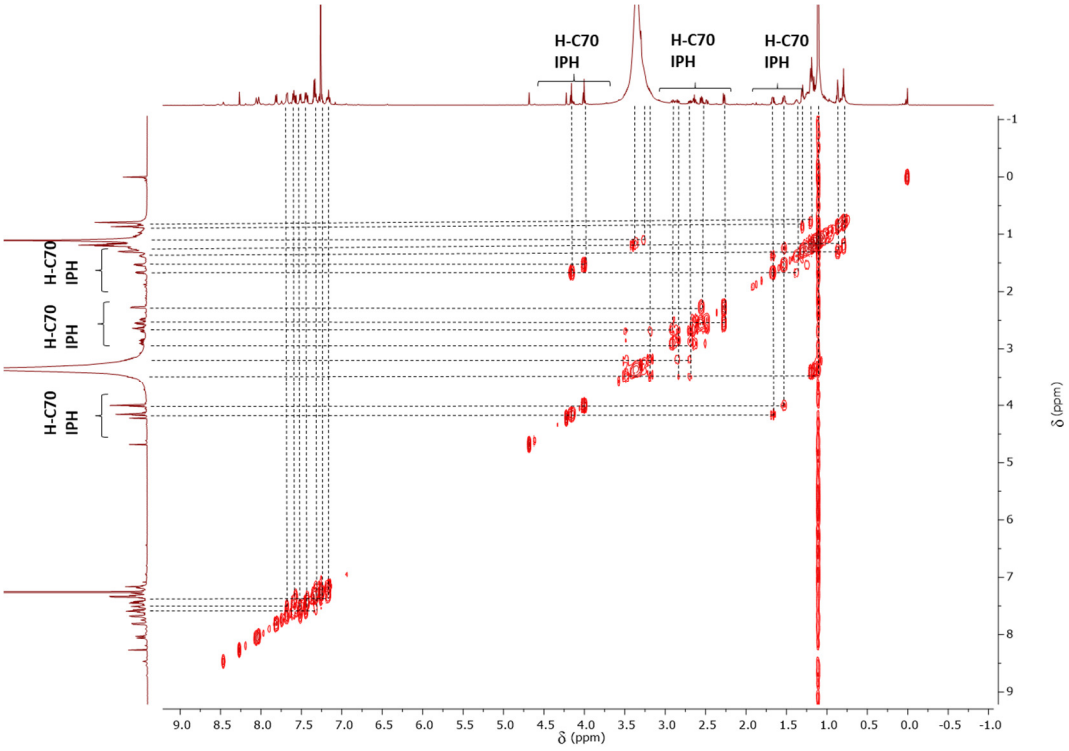

Figure S 51: ^{1}H-COSY NMR spectrum a mixture of the [2+2]-capsule (*all-R*)-**2** (4 mM) and C_{70}-IPH (ca. 10.2 mM by integration) (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

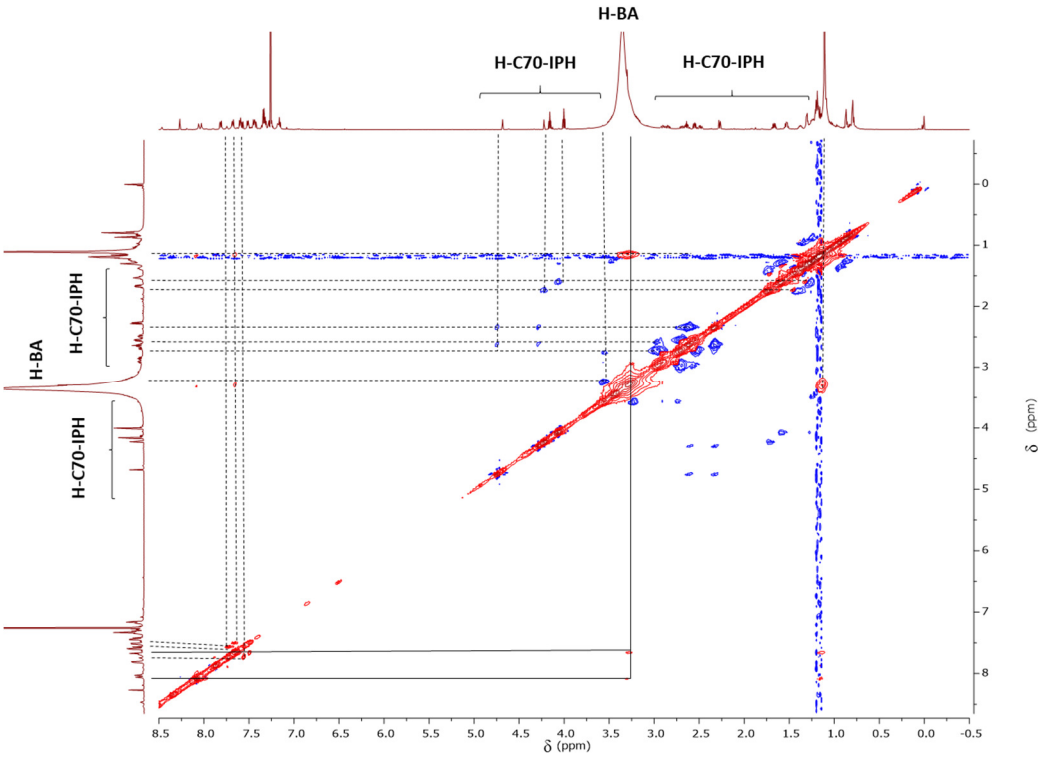

Figure S 52: ^{1}H-NOESY NMR spectrum a mixture of the [2+2]-capsule (*all-R*)-**2** (4 mM) and C_{70}-IPH (ca. 10.2 mM by integration) (600/600 MHz, [D_1]-chloroform/[D_4]-methanol = 8/2 (v/v), 298 K). Dashed lines indicate intramolecular interactions, while solid lines represent intermolecular interactions.

6. References

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