Sui Generis Helicene Based Supramolecular Chirogenic System: Enantioselective Sensing, Solvent Control, and Application in Chiral Group Transfer Reaction

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Job's plot analysis of supramolecular complexes using UV-vis spectroscopy (Continuous variation method)

A series of solutions containing host 1 and guest 2 (CHD) were prepared such that the sum of the total host and guest concentration remained constant (6.9 x 10⁻⁵M) in benzene. The mole fraction (X) of guest 2 (CHD) was varied from 0.0, 0.1, 0.3, 0.5, 0.7, 0.9 to 1.0. The corrected absorption (at 347 nm x mole fraction (X) of guest 2 (CHD)) was plotted against the molar fraction (X) of the guest 2 (CHD), which confirmed 1:1 stoichiometry.

| Mole fraction of Guest (X) | Mole fraction of Host (Y) | Absorbance at 357 nm | Corrected absorbance (Abs. * X * 10⁻⁵) |
|---------------------------|---------------------------|----------------------|--------------------------------------|
| 1.0                       | 0.0                       | 0.0                  | 0.0                                  |
| 0.9                       | 0.1                       | 0.093                | 0.5775                               |
| 0.8                       | 0.2                       | 0.205                | 1.1316                               |
| 0.7                       | 0.3                       | 0.326                | 1.5746                               |
| 0.6                       | 0.4                       | 0.432                | 1.7885                               |
| 0.5                       | 0.5                       | 0.551                | 1.9010                               |
| 0.4                       | 0.6                       | 0.635                | 1.7526                               |
| 0.3                       | 0.7                       | 0.751                | 1.5546                               |
| 0.2                       | 0.8                       | 0.856                | 1.1835                               |
| 0.1                       | 0.9                       | 0.933                | 0.6438                               |
| 0.0                       | 1.0                       | 1.081                | 0.0                                  |

**Figure S7.** Job’s plot analysis of supramolecular complexes between host 1 and 2 using UV-visible spectroscopy
Fluorescence sensing studies:

Following guest molecules were evaluated for chiral molecular recognition studies.

![Figure S8: Chiral guests screened for molecular recognition studies](image)

**General Procedure.**

The stock solution of the host ($6.9 \times 10^{-5}$ M) was made by dissolving 0.9 mg of helicene-1-(S)-camphanate (1) in 25 ml of solvent. From this stock solution, 1 ml was pipetted out and transferred to various 10 ml standard flasks containing 0.0 (blank), 0.2, 0.4, 0.6, 0.8, 1.0 equivalents of (1R,2R) and (1S,2S)-cyclohexanediamine (CHD) in two separate set of experiments. The flasks were kept at room temperature for four hours prior to record their fluorescence responses.
Figure S9: a) UV and b) fluorescence spectra of host 1 in benzene solvent (6.9 x 10^{-5} M) (Slit width 7.5, 7.5)

  c) Comparative UV and d) fluorescence spectra of host 1 and 6 in toluene solvent
The following sensing experiments were repeated thrice to obtain consistence and reproducible results. The graphs were plotted using Origin-06 software.

**Figure S10:** Fluorescence response of host 1 with both the enantiomers of cyclohexanediamine in benzene (at 1:1 host: guest equivalence, c = 6.9 x 10^{-6} M, slit width (7.5, 7.5), \( \lambda_{\text{exci}} = 347 \) nm)
Figure S11: Fluorescence response of host 1 in benzene a) with \( R,R \)-CHD b) with \( S,S \)-CHD enantiomer

\[(\text{Host} = 6.9 \times 10^{-6} \text{ M}, \text{slit width (7.5, 7.5), } \lambda_{\text{exci}}=347 \text{ nm})\]
Binding Constant calculations using Benesi-Hildebrand equation:

As the system showed fluorescence enhancement for cyclohexane diamine enantiomers. Further calculations were performed using Benesi-Hildebrand equation.

\[
\frac{I_0}{(I-I_0)} = \frac{b}{(a-b)} \left[ \frac{1}{K[M]} + 1 \right]
\]

Where

- \(I_0\) is the fluorescence intensity of the sensor in the absence of substrates [guest];
- \(I\) is the fluorescence intensity of the sensor in the presence of substrates;
- \([M]\) is the concentration of the substrates; and
- \(K\) is the association constant between the sensor and the substrates.

Terms \(a\) and \(b\) are constants.

The \(\frac{b}{(a-b)}\) can be found out by plotting the \(\frac{I_0}{(I-I_0)}\) against the inverse of the concentration term, \(M^{-1}\).

The Benesi-Hildebrand equation is similar to equation for straight line, \(y = mx + C\). The intercept of the graph gives the \(\frac{b}{(a-b)}\); the \(I_0\) and \(I\) are found out experimentally and hence \(K\) can then be calculated.

The following table represents the tabulated form of the calculations. Readings were taken in triplet and the average readings (at 395 nm, \(I_0=283.75\) concentration of the Host: \(6.9 \times 10^{-6} M\)) were plotted and used for calculations.
| [M] x 10^{-6} | 1/[M] x 10^3 | I   | (I-I_0) | I_0 / (I-I_0) | log [M] | I/I_0 |
|--------------|-------------|-----|---------|---------------|---------|-------|
| 1.38         | 724         | 300.77 | 17.02   | 16.67         | -5.86   | 1.06  |
| 2.76         | 362         | 320.64 | 36.89   | 7.69          | -5.56   | 1.13  |
| 4.14         | 241         | 334.83 | 51.08   | 5.56          | -5.38   | 1.18  |
| 5.52         | 181         | 354.69 | 70.94   | 4.00          | -5.26   | 1.25  |
| 6.9          | 145         | 368.88 | 85.13   | 3.33          | -5.16   | 1.30  |

Table S1: For (1R,2R)-cyclohexanediamine guest

| [M] x 10^{-6} | 1/[M] x 10^3 | I   | (I-I_0) | I_0 / (I-I_0) | log [M] | I/I_0 |
|--------------|-------------|-----|---------|---------------|---------|-------|
| 1.38         | 724         | 354.68 | 70.93   | 4.00          | -5.86   | 1.25  |
| 2.76         | 362         | 425.63 | 141.88  | 2.00          | -5.56   | 1.50  |
| 4.14         | 241         | 505.08 | 221.33  | 1.28          | -5.38   | 1.78  |
| 5.52         | 181         | 581.69 | 297.94  | 0.95          | -5.26   | 2.05  |
| 6.9          | 145         | 641.28 | 537.53  | 0.53          | -5.16   | 2.26  |

Table S2: For (1S,2S)-cyclohexanediamine guest
Figure S12: a) Benesi-Hildebrand plot and b) Fluorescence enhancement of host 1 (c = 6.9 x 10^{-6} M) with enantiomers of cyclohexanediamine (c = 1.38 x 10^{-6} - 6.9 x 10^{-6} M) in benzene (slit width (7.5, 7.5), λ_{ex} = 347 nm)
The Gibbs free energy changes ($\Delta G^0$) related to the stability of the diastereomeric supramolecular complexes were calculated at 298K as shown in the following table.

| guest       | $K_{eq}$ M$^{-1}$ | $K_{SS}/K_{RR}$ | $\log_{10} K_{eq}$ | $2.303RT$ | $\Delta G^0$ Jmol$^{-1}$ | $\Delta G^0$ kcalmol$^{-1}$ | $\Delta \Delta G^0$ kcalmol$^{-1}$ |
|-------------|------------------|-----------------|-------------------|-----------|------------------------|-----------------------------|----------------------------------|
| (R,R)-CHD   | $4.0 \times 10^3$ | 7.25            | 3.6020            | 5705.84   | -20552                 | -4.91                       | -1.18                            |
| (S,S)-CHD   | $2.9 \times 10^4$ |                 | 4.4624            | 5705.84   | -25462                 | -6.09                       |                                  |

**Table S3:** Gibbs free energy calculations for diastereomeric complexes between host 1 and CHD enantiomers

$\text{T}=298 \text{ K (25°C)}, \text{R}=8.314 \text{ Jmol}^{-1} \text{ K}^{-1}, \Delta G_0 = -2.303 \text{ RT} (\log_{10} K_{eq})$ and $-\Delta \Delta G_0 = (\Delta G_0(R,R) - \Delta G_0(S,S))$

1 Joule = 0.000239006 kcal
Figure S13: Fluorescence response of 1 with both the enantiomers of cyclohexanediame in toluene (at 1:1 Host: Guest equivalence, c = 6.9 x 10^{-6} M, slit width (5.0, 5.0), \lambda_{exc} = 347 nm)
Figure S14: Fluorescence response of host 1 in toluene a) with $\text{R,R-CHD}$ b) with $\text{S,S-CHD}$ enantiomer

(Host = $6.9 \times 10^{-6}$ M, slit width (5.0, 5.0), $\lambda_{\text{exci}}$=347 nm)
The following table represents the tabulated form of the calculations. Readings were taken in triplet and the average readings (at 395 nm, $I_0=121.64$ concentration of the Host: $6.9 \times 10^{-6} \text{M}$) were plotted and used for calculations.

| [M] x $10^{-6}$ | 1/[M] x $10^3$ | I      | (I-I$_0$) | $I_0 / (I-I_0)$ | log [M] | I/I$_0$ |
|-----------------|-----------------|--------|-----------|-----------------|---------|---------|
| 1.38            | 724             | 207.33 | 85.69     | 1.4195355       | -5.86   | 1.7044558 |
| 2.76            | 362             | 293.02 | 171.38    | 0.7097678       | -5.56   | 2.4089115 |
| 4.14            | 241             | 378.71 | 257.07    | 0.4731785       | -5.38   | 3.1133673 |
| 5.52            | 181             | 435.51 | 313.87    | 0.387549        | -5.26   | 3.580319  |
| 6.9             | 145             | 505.2  | 383.56    | 0.3171342       | -5.16   | 4.1532391 |

Table S4: with (1R,2R)-cyclohexanediamine guest

| [M] x $10^{-6}$ | 1/[M] x $10^3$ | I      | (I-I$_0$) | $I_0 / (I-I_0)$ | log [M] | I/I$_0$ |
|-----------------|-----------------|--------|-----------|-----------------|---------|---------|
| 1.38            | 724             | 265.3  | 143.66    | 0.8467214       | -5.86   | 2.181026 |
| 2.76            | 362             | 409.13 | 287.49    | 0.4231104       | -5.56   | 3.3634495 |
| 4.14            | 241             | 528.5  | 406.86    | 0.2989726       | -5.38   | 4.3447879 |
| 5.52            | 181             | 696.43 | 574.79    | 0.2116251       | -5.26   | 5.7253371 |
| 6.9             | 145             | 864.37 | 742.73    | 0.1637742       | -5.16   | 7.1059684 |

Table S5: with (1S,2S)-cyclohexanediamine guest
Figure S15: a) Benesi-Hildebrand plot and b) Fluorescence enhancement of host 1 (c = 6.9 x 10^{-6} M) with enantiomers of cyclohexanediamine (c = 1.38 x 10^{-6} - 6.9 x 10^{-6} M) in toluene (slit width (5.0, 5.0), λ_ex=347 nm)
The Gibbs free energy changes ($\Delta G^0$) related to the stability of the diastereomeric supramolecular complexes were calculated at 298K as shown in the following table.

| guest    | $K_{eq}$ M$^{-1}$ | $K_{SS}/K_{RR}$ | $\log_{10} K_{eq}$ | $2.303RT$ | $\Delta G^0$ Jmol$^{-1}$ | $\Delta G^0$ kcalmol$^{-1}$ | $\Delta \Delta G^0$ kcalmol$^{-1}$ ($SS$ – $RR$) |
|----------|---------------------|------------------|---------------------|-----------|--------------------------|-----------------------------|----------------------------------|
| (R,R)-CHD | $2.47 \times 10^3$  | 6.36             | 3.3927              | 5705.84   | -19358                   | -4.63                       | -1.09                            |
| (S,S)-CHD | $1.57 \times 10^4$  | 4.1959           | 5705.84             | -23941    | -5.72                    |                             |                                  |

Table S6: Gibbs Free calculation for diastereomeric complexes

$T=298 \text{ K (25°C), } R=8.314 \text{ Jmol}^{-1} \text{ K}^{-1}, \Delta G_0 = -2.303 \text{ RT} \log_{10} K_{eq}$ and $-\Delta \Delta G_0 = (\Delta G_0^{(R,R)} - \Delta G_0^{(S,S)})$

1 Joule = 0.000239006 kcal
Figure S16: Fluorescence response of 1 with both the enantiomers of cyclohexanediamine in acetonitrile (at 1:1 Host: Guest equivalence, $c = 6.9 \times 10^{-6}$ M, slit width (10.0, 10.0), $\lambda_{excl}=347$ nm)
Figure S17: Fluorescence response of host 1 in acetonitrile a) with R,R-CHD b) with S,S-CHD enantiomer

(Host = 6.9 x 10^{-6} M, slit width (10.0, 10.0), \lambda_{exc}=347 \text{ nm})
Figure S18: Fluorescence response of 1 with both the enantiomers of cyclohexanediamine in cyclohexane (at 1:1 Host:Guest equivalence, $c = 6.9 \times 10^{-6}$ M, slit width (10.0, 10.0), $\lambda_{\text{exci}} = 347$ nm)
Figure S19: Fluorescence response of host 1 in cyclohexane  a) with R,R-CHD b) with S,S-CHD enantiomer

(Host = 6.9 x 10^-6 M, slit width (10.0, 10.0), λ_{exc}=347 nm)
**Figure S20:** Fluorescence response of 1 with both the enantiomers of cyclohexanediamine in THF (at 1:1 Host: Guest equivalence, $c = 6.9 \times 10^{-6}$ M, slit width (5.0, 5.0), $\lambda_{\text{exc}} = 347$ nm)
Figure S21: Fluorescence response of host 1 in THF a) with R,R-CHD b) with S,S-CHD enantiomer

(Host = 6.9 x 10^{-6} M, slit width (10.0, 10.0), \lambda_{exc}=347 \text{ nm})
Figure S22: Fluorescence response of 1 with both the enantiomers of cyclohexanediamine in chloroform (at 1:1 Host: Guest equivalence, c = 6.9 x 10^-6 M, slit width (10.0, 10.0), λ_{exci}=347 nm)
**Figure S23:** Fluorescence response of 1 with both the enantiomers of cyclohexanediamine in methanol (at 1:1 Host: Guest equivalence, $c = 6.9 \times 10^{-6}$ M, slit width (5.0, 5.0), $\lambda_{\text{exci}} = 347$ nm)
NMR studies:

**Experiment A.**

In a NMR sample vial containing 10.4 mg of helicene-(1S)-camphanate (1) in 0.5 ml of CDCl₃ was mixed 5.6 mg of (1R,2R)-cyclohexanediamine to obtain 1:1 host guest ratio. The clean solution obtain on mixing both (Host and Guest) components started to form precipitate on standing in NMR tube at 25 °C. The ¹H NMR of the mixture recorded at different time interval after mixing, indicated the possible group transfer reaction, presented in manuscript.

**Experiment B.**

In different experiments, we again dissolved 10.4 mg of helicene-(1S)-camphanate (1) in 0.5 ml of CDCl₃ and added 5.6 mg of (1S,2S)-cyclohexanediamine to obtain 1:1 host guest ratio. In another set of NMR tube 10.4 mg of helicene-(1S)-camphanate (1) in 0.5 ml of CDCl₃ at 25 °C and then their NMR spectra with precipitates was recorded.
**Figure S24:** Comparative NMR spectra for group transfer reaction of host 1 with CHD enantiomers
**Experiment 1-3.**

Following table shows the experiments performed towards the preliminary study of host 1 to behave as reagent for kinetic resolution for racemic CHD. Similar NMR studies for desymmetrization of meso-1,2-DPED was without much fruitful results.

The following 1-3 solutions were made by dissolving the weighed quantities of host and guest in 0.5 ml of CDCl₃ in NMR test tubes. After overnight incubation at RT, the ^1^H NMR of the solutions was recorded as it is without any further purification.

| xp. No. | Reagent (Quantity, mg) | Guest (Quantity, mg) | Solvent (0.5 ml) | Mole ratio (R:G) | Time (h) | NMR Code |
|---------|------------------------|----------------------|------------------|------------------|----------|----------|
| 1       | 1 (10.4)               | (R,R)-CHD (5.6)      | CDCl₃            | 1:1              | 12       | HN-386   |
| 2       | 1 (10.8)               | rac-CHD (4.7)        | CDCl₃            | 1:2              | 12       | HN-391   |
| 3       | 1 (11.6)               | meso-DPED (4.7)      | CDCl₃            | 1:2              | 12       | HN-388   |

**Table S7:** NMR samples prepared for studying preliminary group transfer reaction of host 1 with diamines
Figure S25a: $^1$H NMR of group transfer reaction between host 1 and R,R-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz
**Figure S25b**: Expanded $^1$H NMR of group transfer reaction between host 1 and R,R-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz
Figure S26a: $^1$H NMR of group transfer reaction between host 1 and rac-cyclohexanediamine (1:2), in CDCl$_3$ at 300 MHz
Figure S26b: Expanded $^1$H NMR of group transfer reaction between host 1 and rac-cyclohexanediamine (1:2), in CDCl$_3$ at 300 MHz
Figure S27a: $^1$H NMR of group transfer reaction between host 1 and meso-DPED (1:2), in CDCl$_3$ at 300 MHz
Figure S27b: Expanded $^1$H NMR of group transfer reaction between host 1 and meso-DPED (1:2), in CDCl$_3$ at 300 MHz
Reaction Kinetics:

Note. Starting material (SM)/ host 1 has disymmetric NMR pattern, which on reaction converts to parent helicene diol 6 (product 1/ P1) having symmetric NMR pattern. Thus the $^1$H integration is going to be doubled after reaction but actual concentration will remain the same. Thus correction factors needs to be taken in account to calculate exact concentration of the species.

Similarly, the reverse situation is for cyclohexanediamine, initially the $C_2$-symmetric CHD on chiral camphanate group transfer reaction gives disymmetric CHD camphanate amide product. As the sum of total concentration corresponding species will remains the same, thus corrected concentration is calculated for kinetic measurements.
Figure S28a: Overlay $^1$H NMR of group transfer reaction between host 1 and R,R-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz at different time scale
Figure S28b: Expanded aromatic region of overlay $^1$H NMR of group transfer reaction between host 1 and R,R-cyclohexediamine (1:1), in CDCl$_3$ at 300 MHz at different time scale.
Figure S28c: Expanded aliphatic region of overlay $^1$H NMR of group transfer reaction between host 1 and RR-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz at different time scale
For group transfer reaction with RR-CHD.

| Time | SM                  | P1                |
|------|---------------------|-------------------|
| h    | Helicene camphanate | Helicene diol     |

**Integration**

For 1H of SM

| Factors |                  |
|---------|------------------|
|         | 0.01998 mmol in 0.5 ml (4.0 *10^-2 M) |

**Molecular weight**

| 4.0 *10^-2 M solution in CDCl3 (0.5 ml) |
|----------------------------------------|

**δ**

| 8.8 ppm | 8.3-8.4 ppm | observed signal |
|---------|-------------|-----------------|

**Total integration**

| 1 | 0 | 1 | 0 | Distinguish signal Integration |
|---|---|---|---|---------------------------------|
| 1 |   |   | 0 | Corrected signals               |
|   |   |   | 0.0| Concentration *10^-2 M          |

| 1.145 | 1 | 1 | 0.29 | Distinguish signal Integration |
|-------|---|---|-----|---------------------------------|
| 1     |   |   | 0.87| Corrected signals               |
|       |   |   | 3.48| Concentration *10^-2 M          |

| 1.195 | 2 | 1 | 0.39 | Distinguish signal Integration |
|-------|---|---|-----|---------------------------------|
| 1     |   |   | 0.83 | Corrected signals               |
|       |   |   | 3.32 | Concentration *10^-2 M          |

| 4.74  | 3 | 1 | 7.48 | Distinguish signal Integration |
|-------|---|---|-----|---------------------------------|
| Time | Reactant concentration | Product concentration |
|------|------------------------|------------------------|
| T    | $C_{SM} \times 10^{-2}$ | $1/C_{SM}$             | $C_p \times 10^{-2}$ | $1/C_p$ |
| 0    | 4.05                   | 24.69                  | 0                     | 0       |
| 1    | 3.84                   | 26.04                  | 0.52                  | 192.31  |
| 2    | 3.32                   | 30.12                  | 0.65                  | 153.85  |
| 3    | 0.84                   | 119.048                | 3.16                  | 31.65   |
| 4    | 0.05                   | 123.02                 | 4.01                  | 24.93   |
| 5    | 0.05                   | 125.04                 | 4.01                  | 24.95   |
| 6    | 0.05                   | 127.01                 | 4.01                  | 24.95   |

Where $C$ represent concentration (obtained from 1H NMR data), $SM$=starting material, host 1, and $P$= Product, compound 6

**Table S8**: Calculations for chemical kinetics for group transfer reaction of 1 with $R,R$-2
**Figure S29**: Change in concentration of host 1 on group transfer reaction with R,R-cyclohexanediamine (1:1), with time, in chloroform solvent

Rate = negative slope

\[ k_{RR} = 2.1 \times 10^{-2} \text{ mol dm}^{-3} \text{ h}^{-1} = 5.83 \times 10^{-6} \text{ mol dm}^{-3} \text{ s}^{-1} \]
Figure S30a: Overlay $^1\text{H}$ NMR of group transfer reaction between host 1 and $S,S$-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz at different time scale
Figure S30b: Expanded aromatic region of overlay $^1$H NMR of group transfer reaction between host 1 and $S,S$-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz at different time scale
Figure S30c: Expanded aliphatic region of overlay $^1$H NMR of group transfer reaction between host 1 and $S,S$-cyclohexanediamine (1:1), in CDCl$_3$ at 300 MHz at different time scale
For group transfer reaction with $\delta$S-CHD.

| Time | SM   | P1     |
|------|------|--------|
| h    | Helicene camphanate | Helicene diol |

| Integration For 1H of SM | 10.4 mg |
|-------------------------|---------|
| Factors                | 520.52  |
| Molecular weight       |         |
| 0.01998 mmol in 0.5 ml (4.0 *10^{-2} M) |         |

| $\delta$ | 8.8 ppm | 8.3-8.4 ppm | observed signal |
|----------|---------|-------------|-----------------|

| Total integration | Distinguish signal Integration | Corrected signals | Concentration *10^{-2} M |
|-------------------|--------------------------------|-------------------|--------------------------|
| 1                 | 0 1                             | 0                 |                           |
| 1                 | 1 0                             | 0.605 (For 1H)    |                           |
|                    | 4.0 0.0                         | 0.62 0.38         |                           |
| 1.605              | 1 1                             | 0.605 (For 1H)    |                           |
|                    | 2.48 1.52                       | 0.45 0.55         |                           |
| 2.21               | 2 1                             | 1.21              | Distinguish signal Integration |
|                    | 1.8 2.2                         | 0.45 0.55         | Corrected signals         |
| 3.31               | 3 1                             | 2.21              | Distinguish signal Integration |
| Time | Reactant concentration | Product concentration |
|------|------------------------|------------------------|
| T    | \(M_{\text{SM}} \times 10^{-2}\) | \(1/M_{\text{SM}}\) | \(M_{\text{P}} \times 10^{-2}\) | \(1/M_{\text{P}}\) |
| 0    | 4.05                   | 24.69                  | 0                       | 0                   |
| 1    | 2.48                   | 40.32                  | 1.52                    | 65.79               |
| 2    | 1.8                    | 55.55                  | 2.2                     | 45.45               |
| 3    | 1.2                    | 83.33                  | 2.8                     | 35.71               |
| 4    | 1.08                   | 92.59                  | 2.92                    | 24.25               |

Where C represent concentration (obtained from 1H NMR data), SM=starting material, host 1, and P= Product, compound 6

**Table S9:** Calculations for chemical kinetics for group transfer reaction of 1 with \(S,S-2\)
Figure S31: Change in concentration of host 1 on group transfer reaction with S,S-cyclohexanediamine (1:1), with time, in chloroform solvent

Rate = negative slope

\[ K_{SS} = 0.21 \times 10^{-2} \text{ mol dm}^{-3} \text{ h}^{-1} = 5.97 \times 10^{-7} \text{ mol dm}^{-3} \text{ s}^{-1} \]
UV and CD spectra of host 1 in different solvent (Solvent dependent opposite helical conformations)

Figure S32. Overlay of a) UV and b) CD spectra of 1 in different solvent

(For CD measurements, parameters were Wavelength range = 400-280nm, Scan speed = 10nm per min, Accumulations = 5, Conc. = 5 x 10⁻⁵ M)
Table S10: CD data of 1 in different solvent

| Host   | Solvent      | CE at 350-360 nm | Amplitude | Δε (cm⁻¹ M⁻¹) |
|--------|--------------|------------------|-----------|---------------|
| 1      | Toluene      | -                | 4         | 2.426         |
|        | Benzene      | -                | 6         | 3.639         |
|        | Cyclohexane  | -                | 5         | 3.0321        |
|        | Dichloromethane | -             | 3         | 1.819         |
|        | Chloroform   | -                | 5         | 3.0321        |
|        | Tetrahydrofuran | +              | 3         | 1.819         |
|        | Acetonitrile | +                | 2         | 1.213         |
|        | Methanol     | NA               | NA        | NA            |

Table S11: Induced CD studies between stereodynamic parent helicene diol 6 and CHD enantiomers in chloroform

| Host | guest     | CE at 350-360 nm | Amplitude | Δε (cm⁻¹ M⁻¹) |
|------|-----------|------------------|-----------|---------------|
| 1:1 ratio | Blank | NA              | -         | -             |
| 6    | $\ddagger\ddagger$-CHD | +       | 1.4      | 0.425         |
|      | RR-CHD    | -                | 1.4      | 0.425         |

Job's plot analysis of supramolecular complexes between host 6 and 2 using Uv-Visible spectroscopy

A series of solutions containing host 6 and guest 2 (CHD) were prepared such that the sum of the total host and guest concentration remained constant (1 x 10⁻⁴ M) in chloroform. The mole fraction (X) of guest 2 (CHD) was varied from 0.0, 0.1, 0.3, 0.5, 0.7, 0.9 to 1.0. The corrected emission (at 345 nm x mole fraction (X) of guest 2 (CHD)) was plotted against the molar fraction (X) of the guest 2 (CHD), which confirmed 1:1 stoichiometry.
| Mole fraction of Guest (X) | Mole fraction of Host (Y) | Absorbance at 355 nm | Corrected absorbance (Abs. * X * 10^-4) |
|---------------------------|---------------------------|-----------------------|--------------------------------------|
| 1.0                       | 0.0                       | 0.0                   | 0.0                                  |
| 0.9                       | 0.1                       | 0.122                 | 0.1098                               |
| 0.8                       | 0.2                       | 0.274                 | 0.2192                               |
| 0.7                       | 0.3                       | 0.349                 | 0.2443                               |
| 0.6                       | 0.4                       | 0.451                 | 0.2706                               |
| 0.5                       | 0.5                       | 0.568                 | 0.2840                               |
| 0.4                       | 0.6                       | 0.690                 | 0.2760                               |
| 0.3                       | 0.7                       | 0.834                 | 0.2504                               |
| 0.2                       | 0.8                       | 1.101                 | 0.2202                               |
| 0.1                       | 0.9                       | 1.198                 | 0.1198                               |
| 0.0                       | 1.0                       | 0.566                 | 0                                   |

**Figure S33.** Job’s plot analysis of supramolecular complexes between host 6 and 2 using Uv-Visible spectroscopy.

**Figure S34:** Proposed favored supramolecular complex for Induced CD studies between stereodynamic parent helicene diol 6 and 2 in chloroform.
Figure S35. Theoretical UV and CD spectra of $P$-conformation of parent helicene diol 6, calculated at the RI-CC2/def2-TZVP//DFT-D3(BJ)-TPSS/def2-TZVP level.