Supporting Information

Chromane Helicity Rule – Scope and Challenges Based on ECD Study of Various Trolox Derivatives

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Figure S1. ECD spectrum of chromane 2 recorded in chloroform at room temperature. The symbol $\Delta \varepsilon$ denotes the difference of the molar decadic absorption coefficients of left and right circularly polarized light, and $\lambda$ – the wavelength.

Figure S2. Boltzmann averaged ECD spectra of chromane 2 calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) level of theory simulated with different values of the Gaussian band-width.
Figure S3. The experimental (pink line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) ECD spectra (blue line) for compound 1.
Figure S4. ECD spectra of individual conformers of compound 1 calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) level.

Figure S5. The experimental (green line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) ECD spectra (blue line) for compound 3.
Figure S6. ECD spectra of individual conformers of compound 3 calculated at B3LYP/6-311++G(d,p)/PCM(CH₃CN) level.

Figure S7. The experimental (orange line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH₃CN) ECD spectra (blue line) for compound 4.
Figure S8. ECD spectra of individual conformers of compound 4 calculated at B3LYP/6-311++G(d,p)/PCM(CH3CN) level.
**Figure S9.** The experimental (red line) and Boltzmann averaged calculated at B3LYP/TZVP/PCM(CH$_3$CN) ECD spectra (blue line) for compound 5.

**Figure S10.** ECD spectra of individual conformers of compound 5 calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) level.
**Figure S11.** The experimental (red line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) ECD spectra (blue line) for compound 6.

**Figure S12.** ECD spectra of individual conformers of compound 6 calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) level.
Figure S13. The experimental (red line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) ECD spectra (blue line) for compound 7.

Figure S14. ECD spectra of individual conformers of compound 7 calculated at B3LYP/6-311++G(d,p)/PCM(CH$_3$CN) level.
Figure S15. The experimental (red line) and Boltzmann averaged calculated at B3LYP/TZVP/PCM(CH$_3$CN) ECD spectra (blue line) using 0.3 and 0.4 eV Gaussian band-shape as a half-height width for compound 8.

Figure S16. ECD spectra of individual conformers of compound 8 calculated at B3LYP/TZVP/PCM(CH$_3$CN) level.
**Figure S17.** Simulated ECD spectra and structures of conformers of compound 9 calculated at the B3LYP/TZVP/PCM(CH$_3$CN) level of theory (remaining conformers and their spectra are given in main text).
Figure S18. MOs of compound 9 (for conformers 9a, 9c and 9d).
Figure S19. ECD spectra of individual conformers 9a, 10 (M-helicity) and 10 (P-helicity) calculated at CAM-B3LYP/TZVP/PCM(CH₃CN) level.
Table S1. Electric ($\mu_e$) and magnetic ($\mu_m$) transition dipole moments, and their angles ($\theta$) for two lowest transitions of most stable conformers of compounds 1-11 calculated at: B3LYP/6-311++G(d,p)/PCM(CH$_3$CN)$_n$\[a\] and B3LYP/TZVP/PCM(CH$_3$CN)$_n$\[b\] levels of theory.

| Comp.  | $|\mu_e|$ | $|\mu_m|$ | $\theta$ / deg | MO→MO*       |
|--------|----------|----------|----------------|--------------|
| 1a\[a\] | 0.50     | 0.36     | 51             | HOMO-LUMO   |
|        | 0.34     | 0.28     | 110            | HOMO-LUMO+1 |
| 2a\[a\] | 0.57     | 0.40     | 58             | HOMO-LUMO   |
|        | 0.29     | 0.28     | 115            | HOMO-LUMO+1 |
| 3a\[a\] | 0.37     | 0.23     | 61             | HOMO-LUMO   |
|        | 0.41     | 0.39     | 95             | HOMO-LUMO+1 |
| 4a\[a\] | 0.53     | 0.42     | 80             | HOMO-LUMO   |
|        | 0.28     | 0.32     | 109            | HOMO-LUMO+1 |
| 5a\[a\] | 0.83     | 0.45     | 74             | HOMO-LUMO   |
|        | 0.12     | 0.25     | 47             | HOMO-LUMO+1 |
| 6a\[a\] | 0.80     | 0.43     | 71             | HOMO-LUMO   |
|        | 0.07     | 0.28     | 69             | HOMO-LUMO+1 |
| 7a\[a\] | 0.51     | 0.38     | 72             | HOMO-LUMO   |
|        | 0.36     | 0.29     | 121            | HOMO-LUMO+1 |
| 8a\[b\] | 0.96     | 0.49     | 89.6           | HOMO-LUMO   |
|        | 0.06     | 0.39     | 80             | HOMO-LUMO+1 |
| 9a\[b\] | 0.95     | 0.47     | 93             | HOMO-LUMO   |
|        | 0.16     | 0.08     | 130            | HOMO-LUMO+1 |
| 10 P-helicity\[a\] | 0.39     | 0.49     | 60             | HOMO-LUMO   |
|        | 0.87     | 0.93     | 98             | HOMO-LUMO+1 |
| 10 M-helicity\[a\] | 0.26     | 0.32     | 136            | HOMO-LUMO   |
|        | 0.91     | 0.81     | 85             | HOMO-LUMO+1 |
| 10 P-helicity\[b\] | 0.96     | 1.00     | 90.2           | HOMO-LUMO   |
|        | 0.06     | 0.43     | 102            | HOMO-LUMO+1 |
| 10 M-helicity\[b\] | 0.95     | 0.83     | 90.4           | HOMO-LUMO   |
|        | 0.08     | 0.37     | 75             | HOMO-LUMO+1 |
| 11 P-helicity\[a\] | 0.45     | 0.46     | 58             | HOMO-LUMO   |
|        | 0.84     | 0.76     | 102            | HOMO-LUMO+1 |
| 11 M-helicity\[a\] | 0.24     | 0.35     | 45             | HOMO-LUMO   |
|        | 0.84     | 0.74     | 91             | HOMO-LUMO+1 |
| 11 P-helicity\[b\] | 0.96     | 0.83     | 90.3           | HOMO-LUMO   |
|        | 0.34     | 0.35     | 93             | HOMO-LUMO+1 |
| 11 M-helicity\[b\] | 0.87     | 0.76     | 84             | HOMO-LUMO   |
|        | 0.32     | 0.41     | 124            | HOMO-LUMO+1 |
Cartesian coordinates for individual conformers of compounds 1-11 calculated by means of DFT at B3LYP/6-31G(d) level of theory.

Compound 1

Conf. 1a

Imaginary frequencies = 0
Sum of electronic and thermal Enthalpies (Hartree) = -844.99381400

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**Compound 2**

**Conf. 2a**

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -884.27501600

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Conf. 2b

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Conf. 3a
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*Imaginary frequencies = 0*

*Sum of electronic and thermal Enthalpies (Hartree) = -997.62122100*

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**Conf. 4a**

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Sum of electronic and thermal Enthalpies (Hartree) = -1037.216356

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Conf. 5b

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**Conf. 5c**

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**Compound 7**

**Conf. 7a**

Imaginary frequencies = 0  
Sum of electronic and thermal Enthalpies (Hartree) = -901.310594

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Conf. 7b
Imaginary frequencies = 0
Sum of electronic and thermal Enthalpies (Hartree) =  -901.309166

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Conf. 7c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -901.307432

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Conf. 7d

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**Compound 8**

**Conf. 8a**

Imaginary frequencies = 0

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**Conf. 9b**

Sum of electronic and thermal Enthalpies (Hartree) = -733.80217800

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Conf. 9d

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Conf. 9e

Imaginary frequencies = 0

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Conf. 9f

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80074300
Conf. 9g

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.79981600
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**Conf. 9h**

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Sum of electronic and thermal Enthalpies (Hartree) = -733.79966300

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S48
Synthesis of Compound 11.

Scheme S1. Synthesis of (S)-2-(Z-hex-1-enyl)-6-hydroxy-2,5,7,8-tetramethylchromane (11). n-Pentyltriphenylphosphonium bromide (198 mg, 0.48 mmol) was dissolved in anhydrous THF (12 mL) under argon and a solution of LiHMDS (solution in THF, 1.0 M, 0.65 mL, 0.65 mmol) was added dropwise at room temperature. After stirring for 1 h, a solution of iii (150 mg, 0.43 mmol) in anhydrous THF (6 mL) was added and stirred for 6 h at room temperature. The reaction was quenched with saturated ammonium chloride and extracted with dichloromethane. The crude product was purified by flash chromatography over silica gel (hexane/dichloromethane v/v 3:1) to afford product (120 mg, 0.30 mmol, 69%) as oil. A solution of (S)-tert-butyldimethylsilyloxy-2-[(Z)-hex-1-enyl]-2,5,7,8-tetramethylchromane (100 mg, 0.25 mmol) in anhydrous THF (8 mL) was added dropwise via syringe to a stirred solution of TBAF (0.28 mL of a 1 M solution in 2 mL of THF). The mixture was stirred at room temperature until starting material was no longer detected by TLC. The reaction was diluted with ether, washed with water, dried and evaporated to afford light yellow oil. The crude product was purified by flash chromatography on silica gel (hexane/dichloromethane v/v 2:1) and provided 70 mg (97%) of 11. $^1$H NMR (400 MHz, CDCl$_3$): δ 5.37-5.37 (m, 2H), 4.21 (s, 1H), 2.65-2.62 (m, 2H), 2.36-2.33 (m, 1H), 2.18-2.13 (m, 1H), 2.18 (s, 6H), 2.12 (s, 3H), 2.05-2.00 (m, 1H), 1.82-1.75 (m, 1H), 1.50 (s, 3H), 1.31-1.28 (m, 4H), 0.92-0.89 (m, 3H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): δ 145.7, 144.7, 133.2, 132.7, 122.4, 121.0, 118.5,
117.7, 75.5, 33.4, 32.2, 27.8, 27.1, 22.5, 21.2, 14.0, 12.2, 12.0, 11.3 ppm; IR (ATR) $\nu_{\text{max}}$/cm$^{-1}$: 3501, 2927, 1639, 1449; MS(+EI): 164 (100), 288 (M$^+$, 63), HRMS (EI) calculated for C$_{19}$H$_{28}$O$_2$: 288.2089, found: 288.2082.
Copies of $^1$H and $^{13}$C NMR, IR and MS spectra for Compound 11.
S52
X-ray crystallographic data of (S)–Trolox methyl ester (2)

C₁₅H₂₀O₄, colorless crystal, temperature T=100K, formula weight M=264.31, monoclinic, P2₁ space group, a=7.1858(3) Å, b=21.2747(8) Å, c=8.7923(4) Å, β=97.085(4)°, V=1333.87(10) Å³, Z=4, D<sub>x</sub>=1.316 Mgm⁻³, absorption coefficient μ=0.094 mm⁻¹, F(000)= 568, crystal size = 0.15x0.12x0.11. The collected data range was 1.91<Θ<25.04 deg.(-8<h<8, -25<k<25, -10<l<10), 12743 reflections collected, 2429 reflections unique [R(int) = 0.0359], Data/restraints/parameters 2429/1/361, Goodness-of-fit on F²=1.120, Final R indices [I>2σ(I)] R1=0.0458, wR²=0.1211, R indices (all data) R1=0.0504, wR²=0.1246, maximum and minimum difference electron densities were 0.415 and -0.273 e. Å⁻³.

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S54
Refinement of \( F^2 \) against ALL reflections. The weighted R-factor wR and goodness of fit S are based on \( F^2 \); conventional R-factors R are based on F, with F set to zero for negative \( F^2 \). The threshold expression of \( F^2 > 2\sigma(F^2) \) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on \( F^2 \) are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

\[ \text{calc} = \frac{1}{\sigma^2(Fo^2) + (0.0710P)^2 + 0.5856P} \text{ where } P = \frac{(Fo^2 + 2Fc^2)}{3} \]

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**Sources:**
- S57

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**Note:** The table above represents the atomic coordinates and thermal parameters for a crystal structure, with columns for atom type, fractional coordinates (X, Y, Z), anisotropic thermal parameter (Uiso), and occupancy. The data is typical for crystallographic analysis, often used in materials science and chemistry to understand molecular structures and their properties.
S59

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are estimated using the full covariance matrix. The cell esds are taken
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treatment of cell esds is used for estimating esds involving l.s. planes.
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O1A C1A C2A 121.8(3) \_?
C9A C1A C2A 122.0(3) \_?
C1A C2A C3A 119.1(3) \_?
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