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Diastereomeric Preference of a Triply Axial Chiral Binaphthyl Based Molecule: a Concentration Dependent Study by Chiroptical Spectroscopies

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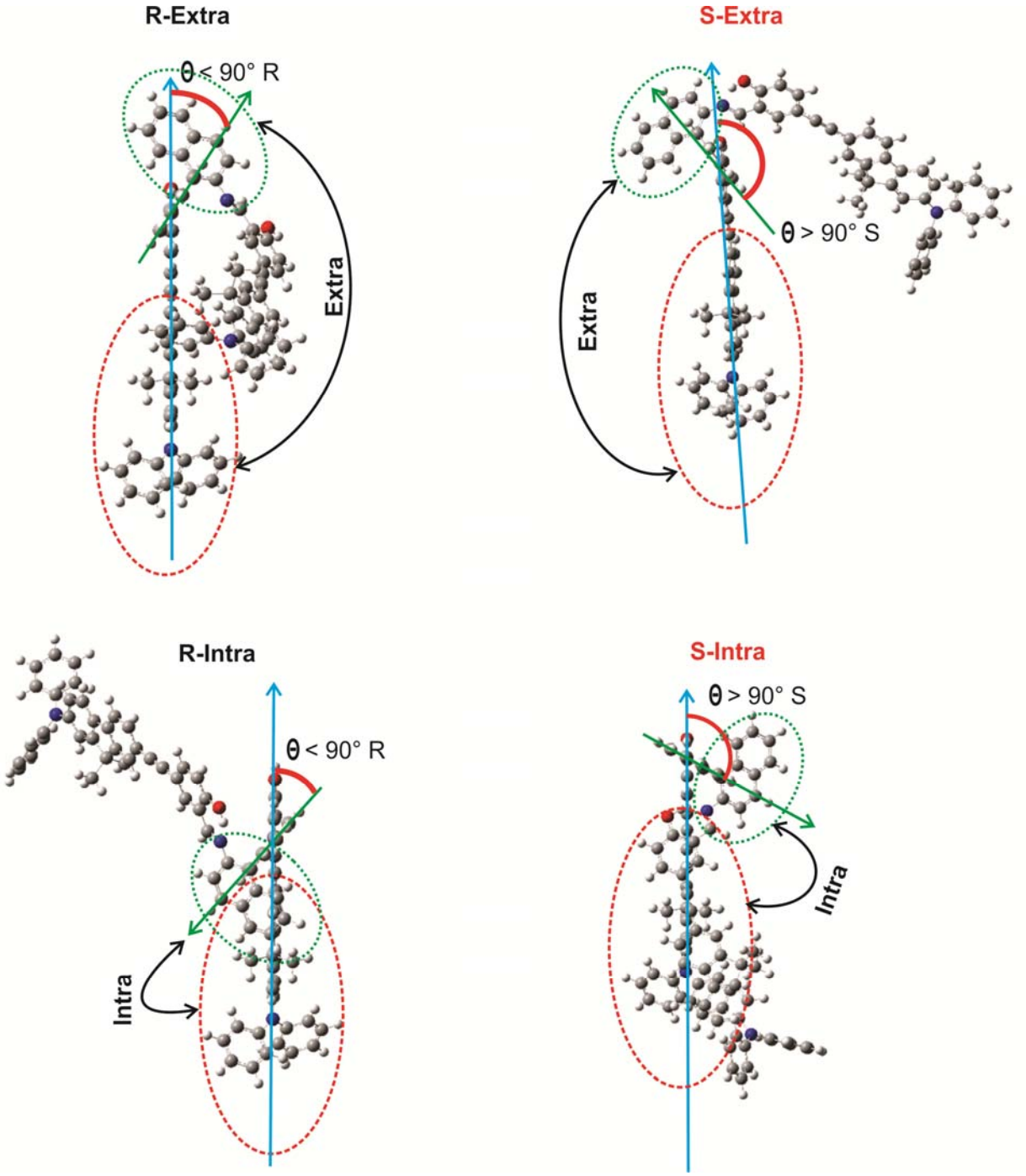

Figure S1. Illustrations of naming schemes used for R and S for axial chirality around the ─C-N bond and for the *intra* and *extra* labels for the relative position of the bulky group (in red dashed circle) with respect to the binaphthyl half (in green circle) which is not directly connected to it. Place the binaphthyl ring under consideration closer to the viewer and view the chiral axis ─C-N end-on. Align the blue arrow from the bulky group to the –O-H group up. Look at θ at the right side of the blue line from the blue arrow to the green line. The green arrow is used to aim the identification of *intra* and *extra* labels.

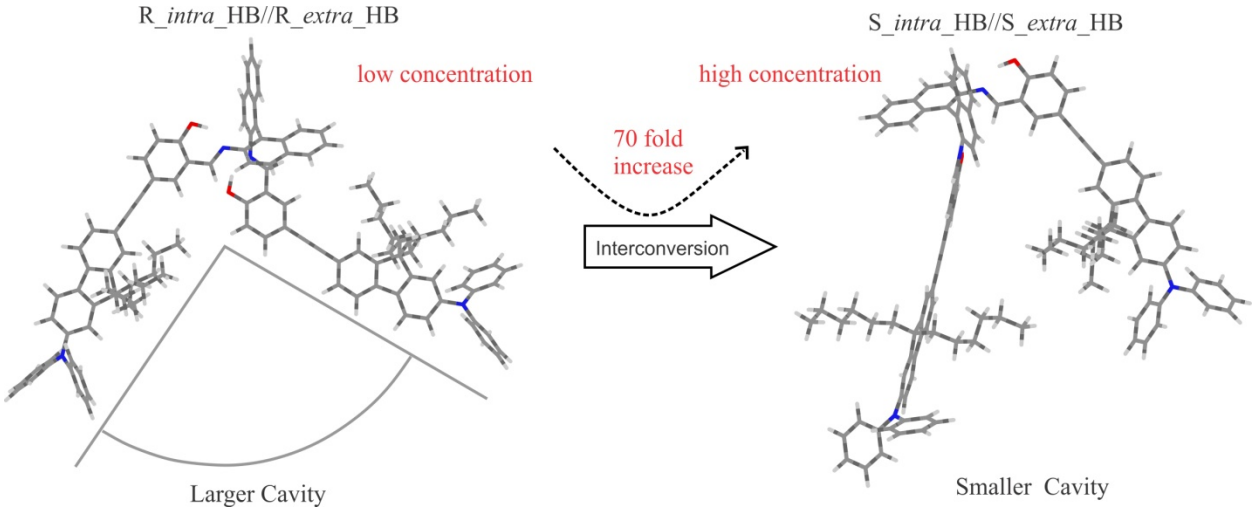

Figure S2. Illustration of the different cavity sizes provided by S-*intra*-HB//S-*extra*-HB (R-SS), and R-*intra*-HB//R-*extra*-HB for solvent molecules. This may influence their stabilities in highly concentrated and highly diluted solutions,

Table S1. Relative energies (in kcal/mol) of AXF-155 conformers using PCM for $CHCl_3$.

Conformers	6-31G(d)		cc-pVTZ//6-31G(d)	6-31G(d)-D[a]
	ΔE^b	ΔG^b	ΔE^b	ΔE^b
R_*intra*_HB//R_*extra*_HB	0.0[c]	0.0[c]	0.0[f]	0.0[g]
R_*extra*_HB//R-*extra*_HB	5.65	5.06	5.40	6.50
R_*intra*_HB//S_*extra*_HB	0.28	2.46	0.29	20.50
R_*extra*_HB//S_*extra*_HB	0.90	1.29	1.06	0.94
R_*extra*_HB//S_*intra*_HB	4.69	7.53	6.47	0.0[i]
R_*intra*_HB//S_*intra*_HB	0.0[d]	0.0[d]	0.0[h]	16.0
S_*extra*_HB//S_*extra*_HB	0.0[e]	0.0[e]	0.0[j]	18.66
S_*intra*_HB//S_*extra*_HB	3.80	4.77	3.70	0.0[k]
S_*intra*_HB//S_*intra*_HB	5.63	6.93	5.66	15.80

[a] Grimme's D3 dispersion-corrected DFT optimization.
[b] ΔE (conformer) = E (conformer) – E (most stable one) and ΔG values are similarly defined.
[c] E= -4699.383299 H, G= -4699.555561 H.
[d] E= -4699.378542 H, G= -4699.553524 H.
[e] E= -4699.381303 H, G= -4699.556087 H.
[f] E= -4702.855238 H.
[g] E= -4701.566950 H.
[h] E= -4702.851107 H.
[i] E= -4701.565878 H.
[j] E= -4702.85403 H.
[k] E= -4701.55732 H.