

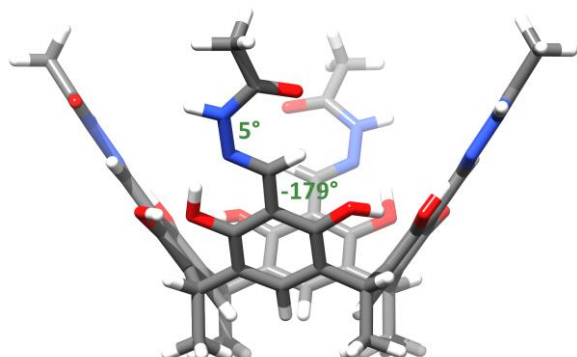
SUPPLEMENTARY INFORMATION

Amplification of electronic circular dichroism— a tool to follow self-assembly of chiral molecular capsules

Marek P. Szymański, Marcin Grajda and Agnieszka Szumna*

Atomic Cartesian coordinates for all calculated geometries:

(*M*, *s-cis*, *s-cis*)-**3** $\alpha = -179^\circ$ $\beta = 5^\circ$

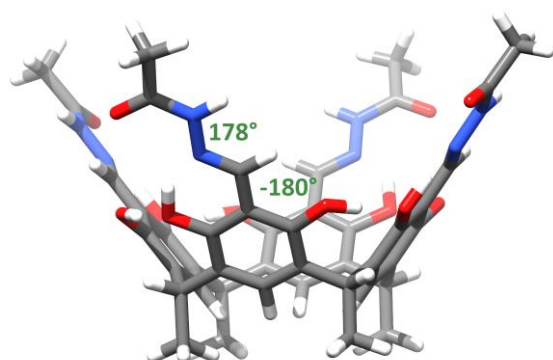


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H	3.56178200	-2.25344700	-4.59343100
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(*M*, *s-trans*, *s-cis*)-**3** $\alpha = -180^\circ$ $\beta = 178^\circ$

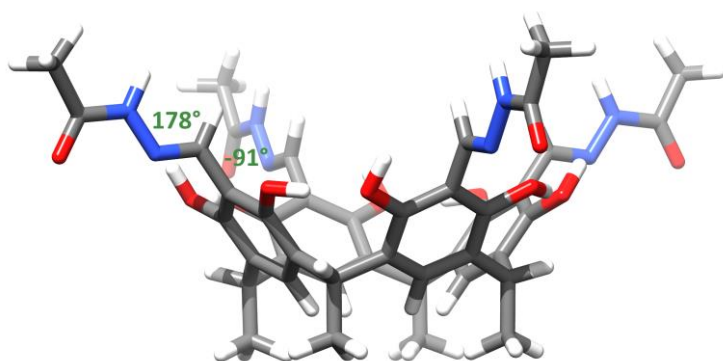


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(*M*, *s*-90, *s*-*cis*)-**3** $\alpha = -91^\circ$ $\beta = 178^\circ$

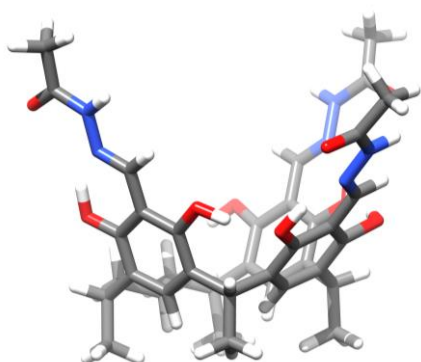


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O	3.37233073	-9.74862809	1.45001881
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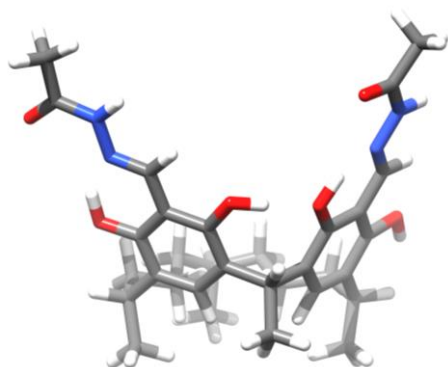
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C	1.82652000	-3.44011700	-1.12877800

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C	-3.33115300	2.61532100	-1.39325800
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H	-2.14847900	-6.43380600	2.01978900
H	-1.45844700	-4.97830600	2.72985700
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C	5.66237000	-1.98197500	-5.58277800
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H	5.68395500	-0.96569900	-5.98479600
O	5.72211200	-1.27904300	-3.27669300
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C	4.73601700	7.18625300	-0.12122900
H	4.34665100	7.67819300	-1.01637800
H	5.64418900	6.63686200	-0.38441100
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H	-3.63111800	4.00656800	-3.42274800
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H	-3.30425000	-5.19887800	0.11910600
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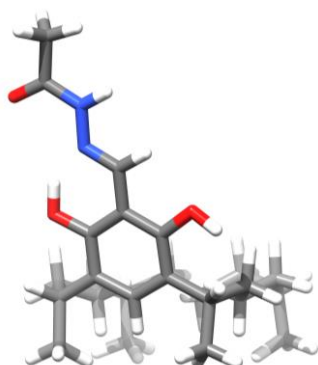


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C	-2.60936000	-0.49322900	-1.34310000
H	-2.46763600	-1.43228700	-1.86518800
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C	-3.20719000	3.17299300	0.68079000
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C	0.68945300	-0.10739300	-1.93549700
C	0.92362300	-1.48226100	-1.76910700
H	0.17993500	-2.17378300	-2.15059300
C	2.05980900	-2.01872300	-1.16727800
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C	1.66080800	0.77466100	-1.44465700
C	3.81976300	1.23845100	-0.34072900
H	3.58485000	2.29938400	-0.46197600
C	1.89536400	-3.99583000	0.43328400
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H	-1.36763700	3.60128600	-0.70087700
O	1.56075400	2.13057100	-1.55292900
H	0.62504700	2.41384400	-1.52715200
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H	-5.12912000	-2.04816600	-2.14000300
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C	1.67612400	-4.37649000	-2.09717900
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H	0.58244700	-4.33079400	-2.11327000
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C	7.84574100	2.58344500	1.69795900
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H	-3.70875700	-2.09648600	0.78909900
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