Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Accurate Prediction of the Optical Rotation and NMR Properties for Highly Flexible Chiral Natural Products

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Experimental Details

NMR spectra were recorded using a Varian DirectDrive spectrometer equipped with a triple resonance HCN cryogenic probe operating at 600 MHz and 150 MHz for ^{1}H and ^{13}C nuclei, respectively. Residual solvent peaks were used as an internal reference for chemical shifts (CD_2Cl_2: δ_H 5.32, δ_C 53.84).[1] NMR spectra were obtained using 3 mm Norell® Select Series™ and 5 mm WILMAD® NMR tubes, respectively.

Optical rotations were measured using a Rudolph Research Analytical Autopol II polarimeter at the sodium D-line (589 nm).

Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc. Optima® grade dichloromethane for measuring the optical rotation was purchased from Fisher Scientific.

Analysis Details

Analysis of the correlation between the relative energies of the conformers of **3** and the percentile rank of their antecedents in **2**. The correlation between the two values is 83%. This value rises to 95% once all conformers whose energy has risen by at least 10 percentage points have been excluded from the analysis.

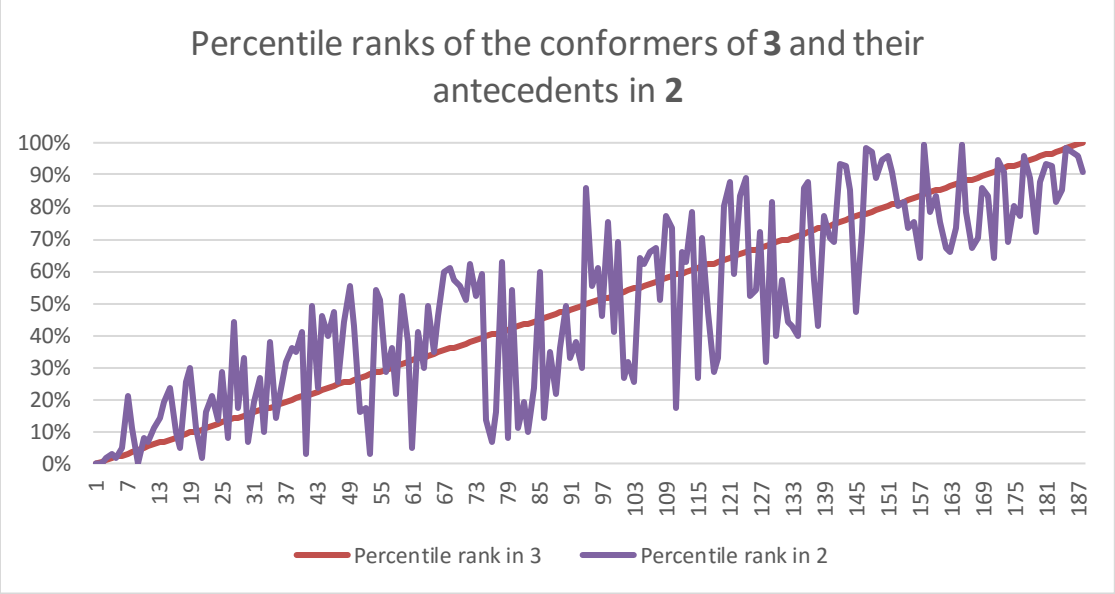

Figure S 1: Correlation analysis for all conformers of 3.

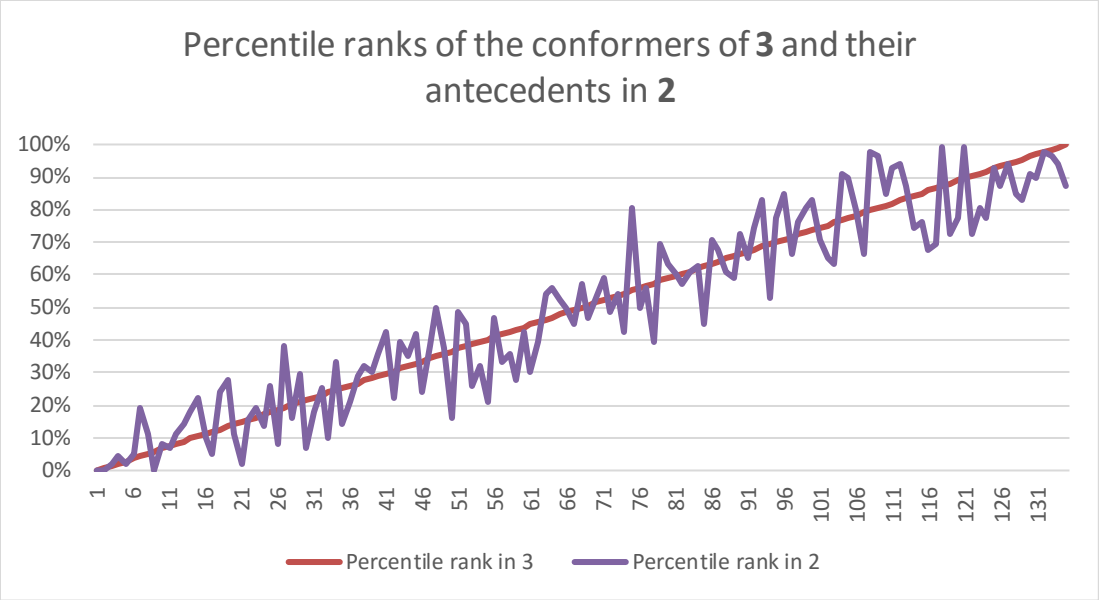

Figure S 2: Correlation for all conformers of 3 whose antecedents do not rise in energy more than 10 percentage points.

Conformer no (rank in 3)	percentile rank in 3	percentile rank in 2
1	0%	0%
2	1%	0%
3	1%	2%
4	2%	3%
5	2%	2%
6	3%	5%
7	3%	21%
8	4%	11%
9	4%	0%
10	5%	8%
11	5%	6%
12	6%	11%
13	6%	14%
14	7%	19%
15	7%	24%
16	8%	10%
17	9%	5%
18	9%	25%
19	10%	30%
20	10%	11%

21	11%	2%
22	11%	16%
23	12%	21%
24	12%	13%
25	13%	28%
26	13%	8%
27	14%	44%
28	14%	18%
29	15%	33%
30	16%	6%
31	16%	19%
32	17%	27%
33	17%	10%
34	18%	38%
35	18%	14%
36	19%	22%
37	19%	32%
38	20%	36%
39	20%	35%
40	21%	41%
41	21%	3%
42	22%	49%
43	22%	24%
44	23%	46%
45	24%	40%
46	24%	48%
47	25%	25%
48	25%	44%
49	26%	56%
50	26%	43%
51	27%	16%
52	27%	18%
53	28%	3%
54	28%	54%
55	29%	51%
56	29%	28%
57	30%	36%
58	30%	22%
59	31%	52%

60	32%	38%
61	32%	5%
62	33%	41%
63	33%	30%
64	34%	49%
65	34%	35%
66	35%	46%
67	35%	60%
68	36%	61%
69	36%	57%
70	37%	56%
71	37%	51%
72	38%	62%
73	39%	52%
74	39%	59%
75	40%	13%
76	40%	6%
77	41%	16%
78	41%	63%
79	42%	8%
80	42%	54%
81	43%	11%
82	43%	19%
83	44%	10%
84	44%	24%
85	45%	60%
86	45%	14%
87	46%	35%
88	47%	22%
89	47%	36%
90	48%	49%
91	48%	33%
92	49%	38%
93	49%	30%
94	50%	86%
95	50%	56%
96	51%	61%
97	51%	46%
98	52%	75%

99	52%	41%
100	53%	69%
101	53%	27%
102	54%	32%
103	55%	25%
104	55%	64%
105	56%	62%
106	56%	66%
107	57%	67%
108	57%	51%
109	58%	77%
110	58%	74%
111	59%	18%
112	59%	66%
113	60%	63%
114	60%	79%
115	61%	27%
116	61%	71%
117	62%	48%
118	63%	28%
119	63%	33%
120	64%	80%
121	64%	88%
122	65%	59%
123	65%	83%
124	66%	89%
125	66%	52%
126	67%	54%
127	67%	72%
128	68%	32%
129	68%	82%
130	69%	40%
131	70%	57%
132	70%	44%
133	71%	43%
134	71%	40%
135	72%	86%
136	72%	88%
137	73%	57%

138	73%	43%
139	74%	77%
140	74%	71%
141	75%	69%
142	75%	94%
143	76%	93%
144	76%	85%
145	77%	48%
146	78%	72%
147	78%	98%
148	79%	97%
149	79%	89%
150	80%	95%
151	80%	96%
152	81%	91%
153	81%	80%
154	82%	82%
155	82%	74%
156	83%	75%
157	83%	64%
158	84%	99%
159	84%	79%
160	85%	83%
161	86%	75%
162	86%	67%
163	87%	66%
164	87%	74%
165	88%	99%
166	88%	79%
167	89%	67%
168	89%	71%
169	90%	86%
170	90%	83%
171	91%	64%
172	91%	95%
173	92%	91%
174	93%	69%
175	93%	80%
176	94%	77%

177	94%	96%
178	95%	89%
179	95%	72%
180	96%	88%
181	96%	94%
182	97%	93%
183	97%	82%
184	98%	85%
185	98%	98%
186	99%	97%
187	99%	96%
188	100%	91%

xyz coordinates of the most stable conformer of 3-epixestoaminol (11)

47
xa01-1-2-2-1-1-1-1-1-1-2.log

C	-6.35526	1.63172	0.57825
C	-6.14489	0.32081	-0.15808
C	-4.83922	-0.38219	0.22757
C	-3.59601	0.36504	-0.20600
C	-2.30464	-0.32182	0.20654
C	-1.06272	0.41012	-0.27373
C	0.23384	-0.25786	0.15258
C	1.47748	0.44194	-0.36967
C	2.77338	-0.22183	0.06538
C	4.01741	0.46029	-0.47873
C	5.31211	-0.21052	-0.05025
C	6.55229	0.47828	-0.59810
C	7.86281	-0.22465	-0.26703
N	-7.22810	-0.64183	0.05202
O	-4.82619	-1.67044	-0.35893
H	-5.57921	2.36480	0.34711
H	-6.35660	1.46806	1.66110
H	-7.31813	2.06953	0.30253
H	-6.10105	0.51083	-1.23690
H	-4.82816	-0.48088	1.32847
H	-3.61761	1.37369	0.21822
H	-3.62486	0.47504	-1.29730
H	-5.76858	-1.91639	-0.37364
H	-7.47760	-0.67425	1.03613
H	-8.05964	-0.35804	-0.45154
H	-2.29819	-1.34434	-0.18402
H	-2.27623	-0.40855	1.30028
H	-1.07885	1.44231	0.09920
H	-1.08875	0.48202	-1.36851
H	0.27511	-0.30210	1.24833
H	0.23389	-1.29914	-0.19360
H	1.43874	0.47486	-1.46592
H	1.47480	1.48678	-0.03393
H	2.82042	-0.24078	1.16162
H	2.76730	-1.27099	-0.25644
H	3.96739	0.48271	-1.57479
H	4.02763	1.50851	-0.15370
H	5.35277	-0.23953	1.04440
H	5.30503	-1.25657	-0.38337
H	6.45776	0.55700	-1.68774
H	6.58983	1.50823	-0.22023
H	8.67874	0.28718	-0.78885

C	8.18187	-0.27789	1.21815
H	7.83457	-1.24375	-0.67144
H	9.16031	-0.73257	1.39565
H	8.20015	0.72731	1.65159
H	7.44451	-0.86330	1.77319

References

1. G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176-2179.