Structure Revision of Anti-inflammatory Indole Alkaloids with a 1,2-Benzisoxazole Ring

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Table S1. Gibbs free energies and Boltzmann distribution of conformers of original 2*S*-**1**.

Conformers	B3LYP/6-31G(d) Gibbs free energy (298.15 K)		
	G (Hartree)	ΔG (kcal/mol)	Boltzmann distribution (%)
original 2*S*-**1**_1	-916.1509323	0	61.8
original 2*S*-**1**_1	-916.1504762	0.286207083	38.2

Table S2. Gibbs free energies and Boltzmann distribution of conformers of revised 2*S*-**1**.

Conformers	B3LYP/6-31G(d) Gibbs free energy (298.15 K)		
	G (Hartree)	ΔG (kcal/mol)	Boltzmann distribution (%)
revised 2*S*-**1**_1	-916.2190744	0	36.6
revised 2*S*-**1**_2	-916.2195235	-0.281814517	58.9
revised 2*S*-**1**_3	-916.2170880	1.246484871	4.5

Table S3. Experimental (Exp.) and calculated (Cal.) ^{1}H NMR chemical shift values of original and revised (±)-**1** used for DP4+ analysis.

Proton	Exp.	Cal.	
	(±)-**1**	original (±)-**1**	revised (±)-**1**
4	7.80	7.60	7.83
5	7.32	7.49	7.32
6	7.80	7.62	7.84
7	8.44	8.61	8.40
8	2.05	2.07	2.01
9	0.75	0.74	0.78
4’	7.87	7.71	7.92
5’	6.88	6.90	6.77
6’	7.38	7.49	7.46
7’	6.96	7.03	6.91

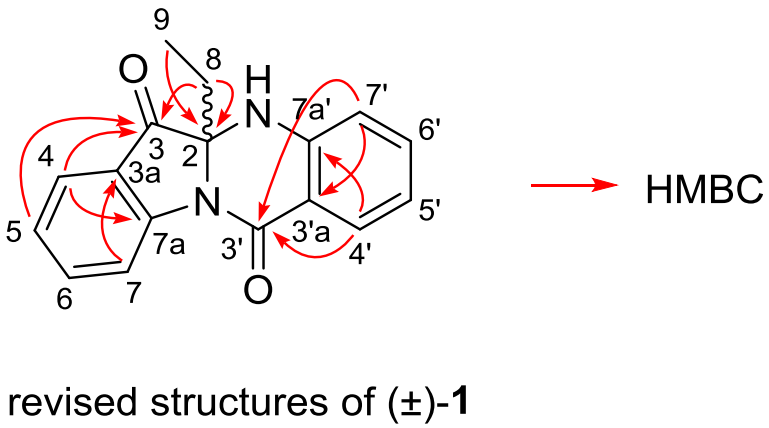

Figure S1. Key HMBC correlations of revised (±)-**1**.

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d)	Scaled Shifts

		DP4+	-	-	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	198.4	198.6	198.6			
C	x	162.1	164.0	161.0			
C	x	153.1	162.5	155.7			
C	x	149.0	159.0	148.3			
C	x	139.4	138.8	140.5			
C	x	136.0	131.2	136.7			
C	x	129.6	126.1	130.7			
C	x	126.1	126.1	126.8			
C	x	125.5	123.9	124.8			
C	x	124.0	120.8	122.5			
C	x	120.4	119.7	119.5			
C	x	118.4	119.3	117.5			
C	x	117.3	114.0	117.1			
C	x	117.3	110.2	115.7			
C		80.1	74.3	80.7			
C		30.2	35.7	31.1			
C		7.7	10.5	7.5			
H	x	8.44	8.61	8.40			
H	x	7.87	7.71	7.92			
H	x	7.80	7.62	7.84			
H	x	7.80	7.60	7.83			
H	x	7.38	7.49	7.46			
H	x	7.32	7.49	7.32			
H	x	6.96	7.03	6.91			
H	x	6.88	6.90	6.77			
H		2.05	2.07	2.01			
H		0.75	0.74	0.78			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d)	Scaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.15%	99.85%	-	-	-	-
sDP4+ (C data)	0.00%	100.00%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	-	-	-	-	-	-
uDP4+ (C data)	-	-	-	-	-	-
uDP4+ (all data)	-	-	-	-	-	-
DP4+ (H data)	-	-	-	-	-	-
DP4+ (C data)	-	-	-	-	-	-
DP4+ (all data)	-	-	-	-	-	-

Figure S2. Results for DP4+ analysis of **1** with chemical shifts calculated at mPW1PW91/6-311G(d) level (isomer 1 = original **1**, isomer 2 = revised **1**).

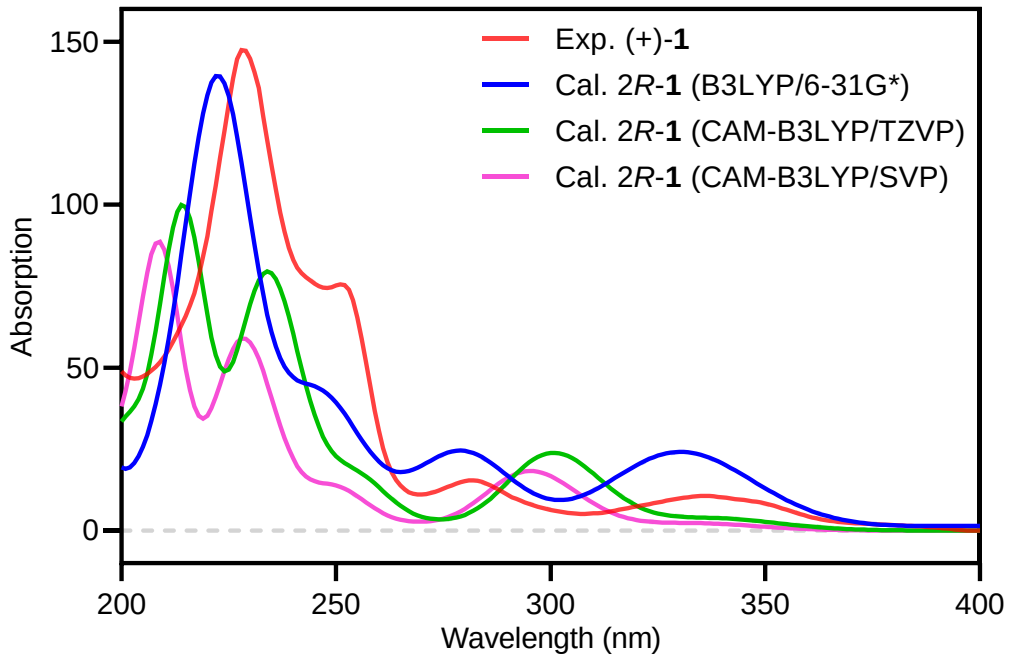

Figure S3. Experimental UV spectrum of (+)-**1** and calculated UV spectra of 2*R*-**1**.

Coordinates of the conformers

original 2*S*-**1**_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.496885	-1.634241	1.580339
2	6	0	1.032655	-0.765062	0.912507
3	6	0	0.412499	0.648124	0.638670
4	6	0	-0.815106	0.540855	-0.242132
5	7	0	-0.868329	1.252640	-1.339962
6	8	0	-2.118276	1.024523	-1.940122
7	6	0	-2.805991	0.155974	-1.155980
8	6	0	-2.034290	-0.204874	-0.044310
9	6	0	-2.549187	-1.112441	0.897933
10	6	0	-3.829357	-1.606079	0.683962
11	6	0	-4.588434	-1.219426	-0.441624
12	6	0	-4.091656	-0.331950	-1.389893
13	6	0	0.075984	1.310023	2.001459
14	6	0	-0.470480	2.734620	1.891953
15	7	0	1.494852	1.368590	-0.053416
16	6	0	2.529839	0.489899	-0.341646
17	6	0	3.687093	0.740093	-1.092586
18	6	0	4.627040	-0.281177	-1.198391
19	6	0	4.448928	-1.532981	-0.576063
20	6	0	3.296961	-1.781371	0.159266
21	6	0	2.338140	-0.767301	0.261310
22	1	0	-1.947625	-1.432073	1.740448
23	1	0	-4.255689	-2.310864	1.391657
24	1	0	-5.585619	-1.630154	-0.573694
25	1	0	-4.662152	-0.032025	-2.262042
26	1	0	1.000043	1.311297	2.591726
27	1	0	-0.633437	0.659007	2.524348
28	1	0	0.241845	3.390121	1.379734
29	1	0	-0.647094	3.148497	2.890639
30	1	0	-1.418197	2.767700	1.344008
31	1	0	1.197165	1.996240	-0.792691
32	1	0	3.846999	1.701357	-1.572315
33	1	0	5.529526	-0.104256	-1.778142
34	1	0	5.211826	-2.298472	-0.679305
35	1	0	3.120058	-2.738788	0.640936

original 2*S*-**1**_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.427399	1.637890	1.457263
2	6	0	0.951211	0.881369	0.655539
3	6	0	0.367000	0.552080	-0.760399
4	6	0	-0.892704	-0.284961	-0.636296
5	7	0	-0.969595	-1.406030	-1.307954
6	8	0	-2.244885	-1.952714	-1.087585
7	6	0	-2.922744	-1.113271	-0.264001
8	6	0	-2.120031	-0.016315	0.073015
9	6	0	-2.621426	0.978362	0.930883
10	6	0	-3.918708	0.827699	1.402695
11	6	0	-4.708296	-0.285497	1.041996
12	6	0	-4.226237	-1.283710	0.202504
13	6	0	0.050983	1.856424	-1.538557
14	6	0	1.253169	2.785945	-1.720458
15	7	0	1.443886	-0.223064	-1.399303
16	6	0	2.414510	-0.534943	-0.457318
17	6	0	3.528142	-1.372330	-0.612280
18	6	0	4.410341	-1.485675	0.458586
19	6	0	4.217015	-0.788507	1.667962
20	6	0	3.107307	0.032596	1.822325
21	6	0	2.205170	0.143297	0.758416
22	1	0	-1.998628	1.813710	1.228247
23	1	0	-4.335514	1.577070	2.069063
24	1	0	-5.718294	-0.367061	1.434126
25	1	0	-4.820837	-2.146158	-0.078042
26	1	0	-0.748770	2.377878	-1.001056
27	1	0	-0.354518	1.566928	-2.515993
28	1	0	1.614763	3.165589	-0.758964
29	1	0	0.970335	3.649228	-2.332434
30	1	0	2.077098	2.268733	-2.221428
31	1	0	1.133373	-0.968985	-2.013339
32	1	0	3.699668	-1.911345	-1.539533
33	1	0	5.278681	-2.131624	0.355471
34	1	0	4.934603	-0.901660	2.474749
35	1	0	2.919677	0.574574	2.744843

revised 2*S*-**1**_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.565346	2.640505	-0.850427
2	6	0	1.441666	1.504489	-0.425986
3	6	0	0.119489	0.935342	0.149156
4	6	0	-0.146034	1.527641	1.564982
5	6	0	-0.481170	3.022202	1.580036
6	7	0	0.403996	-0.507284	0.267383
7	6	0	-0.612917	-1.453481	0.365100
8	6	0	-1.963929	-0.917902	0.059572
9	6	0	-3.087028	-1.729725	0.262051
10	6	0	-4.351063	-1.303844	-0.127033
11	6	0	-4.491168	-0.054848	-0.746841
12	6	0	-3.389773	0.766771	-0.962201
13	6	0	-2.112499	0.349533	-0.554601
14	7	0	-0.975357	1.114078	-0.781813
15	8	0	-0.386027	-2.630611	0.621781
16	6	0	1.770774	-0.751403	0.084637
17	6	0	2.478688	-1.949391	0.228824
18	6	0	3.845897	-1.920421	-0.048908
19	6	0	4.508530	-0.749316	-0.457151
20	6	0	3.795925	0.436296	-0.601217
21	6	0	2.427431	0.427462	-0.321845
22	1	0	0.740575	1.329907	2.180385
23	1	0	-0.969071	0.955424	2.009047
24	1	0	-0.606796	3.364101	2.612742
25	1	0	0.305858	3.621193	1.113690
26	1	0	-1.421038	3.225871	1.054304
27	1	0	-2.931554	-2.702921	0.716869
28	1	0	-5.218820	-1.935064	0.036938
29	1	0	-5.473926	0.285522	-1.062674
30	1	0	-3.509414	1.734821	-1.442672
31	1	0	-1.104635	2.069078	-1.093728
32	1	0	1.972282	-2.853313	0.538062
33	1	0	4.416182	-2.839791	0.055890
34	1	0	5.575162	-0.775633	-0.658299
35	1	0	4.273264	1.357651	-0.921836

revised 2*S*-**1**_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.569281	-2.728329	-0.778371
2	6	0	-1.413789	-1.568794	-0.438050
3	6	0	-0.084119	-1.031190	0.150698
4	6	0	0.186024	-1.681527	1.532490
5	6	0	-0.879532	-1.433241	2.604648
6	7	0	-0.320376	0.419192	0.250804
7	6	0	0.730381	1.331622	0.341378
8	6	0	2.063295	0.746574	0.050835
9	6	0	3.213653	1.519810	0.252219
10	6	0	4.462755	1.048027	-0.131586
11	6	0	4.560016	-0.207803	-0.746102
12	6	0	3.430909	-0.990680	-0.961594
13	6	0	2.168142	-0.527471	-0.558257
14	7	0	1.005814	-1.254677	-0.783304
15	8	0	0.541951	2.519488	0.577237
16	6	0	-1.661007	0.716756	-0.032569
17	6	0	-2.318853	1.949819	0.029924
18	6	0	-3.664261	1.975979	-0.339242
19	6	0	-4.354949	0.824540	-0.756915
20	6	0	-3.692908	-0.396837	-0.817398
21	6	0	-2.345895	-0.442447	-0.449707
22	1	0	1.161238	-1.324672	1.883854
23	1	0	0.281474	-2.758738	1.344568
24	1	0	-0.577404	-1.904756	3.545722
25	1	0	-1.014226	-0.363775	2.796340
26	1	0	-1.850245	-1.854426	2.321855
27	1	0	3.091498	2.500055	0.702081
28	1	0	5.351878	1.648918	0.031855
29	1	0	5.530951	-0.584111	-1.057712
30	1	0	3.517496	-1.964424	-1.437541
31	1	0	1.111597	-2.224656	-1.058784
32	1	0	-1.791602	2.838571	0.348332
33	1	0	-4.194815	2.923803	-0.299178
34	1	0	-5.403675	0.893935	-1.029315
35	1	0	-4.192782	-1.305424	-1.140147

revised 2*S*-**1**_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.611546	-2.765429	-0.777332
2	6	0	-1.488022	-1.616756	-0.391806
3	6	0	-0.172603	-1.060893	0.219745
4	6	0	-0.028276	-1.720750	1.619912
5	6	0	1.180688	-1.312970	2.466040
6	7	0	-0.430394	0.388517	0.310596
7	6	0	0.588611	1.344895	0.302984
8	6	0	1.924109	0.815286	-0.059158
9	6	0	3.039798	1.659381	0.008483
10	6	0	4.284351	1.230883	-0.435600
11	6	0	4.409894	-0.056911	-0.974748
12	6	0	3.316123	-0.911383	-1.056256
13	6	0	2.059144	-0.490291	-0.588752
14	7	0	0.938205	-1.295458	-0.677030
15	8	0	0.360979	2.530115	0.516631
16	6	0	-1.791438	0.648588	0.078639
17	6	0	-2.484821	1.858679	0.188370
18	6	0	-3.841765	1.851165	-0.137742
19	6	0	-4.510394	0.688445	-0.558857
20	6	0	-3.813410	-0.509970	-0.667498
21	6	0	-2.455214	-0.521397	-0.341302
22	1	0	-0.017006	-2.804123	1.441491
23	1	0	-0.951795	-1.510589	2.175733
24	1	0	1.158878	-1.858384	3.416216
25	1	0	2.127428	-1.547252	1.970663
26	1	0	1.174271	-0.243589	2.698604
27	1	0	2.892604	2.658989	0.404959
28	1	0	5.146425	1.887786	-0.376592
29	1	0	5.376166	-0.401323	-1.334227
30	1	0	3.425173	-1.908894	-1.474965
31	1	0	1.054753	-2.260486	-0.960173
32	1	0	-1.975002	2.757556	0.505779
33	1	0	-4.398740	2.781341	-0.060216
34	1	0	-5.569110	0.730693	-0.795964
35	1	0	-4.294834	-1.426637	-0.995379