Supplementary Information

TD-DFT Analysis of the Dissymmetry Factor in Camphor

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The stable molecular geometries, corresponding to the energy minima on potential energy surface (PES), were obtained at the B3LYP/6-311++G(2d,p) level of theory. The results of all molecular geometries, electronic energies and the fractional populations of all systems and conformers are given in Tables S1 to S16.

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Table S1. Cartesian coordinates of *R*-3,3'-dibromo-1,1'-bi-2-naphthol

EE = −6068.17223531 a.u.[a] - 39.05%[b]

Atom	X / Å	Y / Å	Z / Å
C	2.44216	2.95720	−2.94686
C	3.24130	2.04816	−2.29562
C	2.68691	1.13781	−1.36189
C	1.28267	1.16860	−1.10113
C	0.48516	2.11667	−1.78978
C	1.05300	2.98893	−2.68913
C	3.49406	0.19507	−0.67854
C	2.94196	−0.67255	0.22379
C	1.54975	−0.65236	0.49976
C	0.72860	0.25177	−0.15779
C	−0.72860	0.25177	0.15779
C	−1.28267	1.16860	1.10113
C	−2.68691	1.13781	1.36189
C	−3.49406	0.19507	0.67854
C	−2.94196	−0.67255	−0.22379
C	−1.54975	−0.65236	−0.49976
C	−3.24130	2.04816	2.29562
C	−2.44216	2.95720	2.94686
C	−1.05300	2.98893	2.68913
C	−0.48516	2.11667	1.78978
O	−1.08186	−1.52989	−1.41444
O	1.08186	−1.52989	1.41444
Br	−4.03387	−1.92309	−1.13323
Br	4.03387	−1.92309	1.13323
H	0.58042	2.14460	1.59592
H	−0.58042	2.14460	−1.59592
H	−4.55935	0.16647	0.87570
H	4.55935	0.16647	−0.87570
H	−4.30930	2.01275	2.48472
H	4.30930	2.01275	−2.48472
H	−0.42911	3.70931	3.20712
H	0.42911	3.70931	−3.20712
H	−2.87377	3.65150	3.65913
H	2.87377	3.65150	−3.65913
H	−0.13159	−1.373292	−1.52855
H	0.13159	−1.37329	1.52855

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory; [b]fractional population.

Table S2. Cartesian coordinates of *R*-3,3'-dibromo-1,1'-bi-2-naphthol

EE = −6068.17205037 a.u. - 32.11%

Atom	X / Å	Y / Å	Z / Å
C	2.50763	3.06038	2.79827
C	3.29146	2.12498	2.16674
C	2.71794	1.17971	1.27964
C	1.30866	1.20477	1.04136
C	0.52733	2.18012	1.71293
C	1.11302	3.08384	2.56800
C	3.51004	0.20654	0.62357
C	2.93423	−0.69595	−0.22892
C	1.53857	−0.68134	−0.47994
C	0.73565	0.25720	0.14526
C	−0.72579	0.25567	−0.14449
C	−1.29783	1.21480	−1.03440
C	−2.70687	1.20414	−1.27343
C	−3.50762	0.23206	−0.62664
C	−2.93489	−0.68000	0.21533
C	−1.53659	−0.68408	0.47423
C	−3.27437	2.16084	−2.15189
C	−2.48304	3.09570	−2.77425
C	−1.08868	3.10612	−2.54287
C	−0.50929	2.19037	−1.69636
O	−0.96763	−1.57488	1.31579
O	1.05010	−1.60392	−1.34116
Br	−4.00243	−1.98822	1.08602
Br	4.00474	−1.99304	−1.10154
H	0.56004	2.20242	−1.52551
H	−0.54232	2.20220	1.54292
H	−4.57631	0.21547	−0.80497
H	4.57881	0.18144	0.80112
H	−4.34584	2.13844	−2.32218
H	4.36293	2.09342	2.33688
H	−0.46964	3.84498	−3.04027
H	0.49967	3.82253	3.07286
H	−2.92377	3.82533	−3.44434
H	2.95443	3.78032	3.47498
H	−1.65287	−2.17172	1.65501
H	0.09681	−1.45563	−1.43304

Table S3. Cartesian coordinates of *R*-3,3’-dibromo-1,1’-bi-2-naphthol

EE = −6068.17194910 a.u. - 28.84%

Atom	X / Å	Y / Å	Z / Å
C	2.10352	−3.55355	2.44198
C	2.98484	−2.82318	1.68150
C	2.54067	−1.70249	0.93657
C	1.16011	−1.33445	0.97728
C	0.27770	−2.10438	1.77753
C	0.73973	−3.18604	2.49023
C	3.43592	−0.93271	0.15479
C	2.98891	0.14708	−0.55716
C	1.62072	0.52111	−0.53743
C	0.71544	−0.20816	0.21975
C	−0.71544	0.20816	0.21975
C	−1.16011	1.33445	0.97728
C	−2.54067	1.70249	0.93657
C	−3.43592	0.93271	0.15479
C	−2.98891	−0.14708	−0.55715
C	−1.62072	−0.52111	−0.53743
C	−2.98484	2.82318	1.68151
C	−2.10351	3.55355	2.44198
C	−0.73973	3.18604	2.49023
C	−0.27770	2.10438	1.77753
O	−1.25862	−1.59568	−1.27134
O	1.25862	1.59568	−1.27134
Br	−4.19804	−1.16799	−1.59597
Br	4.19804	1.16799	−1.59597
H	0.76737	1.82249	1.82621
H	−0.76737	−1.82249	1.82621
H	−4.48406	1.20640	0.12356
H	4.48406	−1.20639	0.12356
H	−4.03564	3.09089	1.63964
H	4.03565	−3.09088	1.63963
H	−0.05124	3.76291	3.09821
H	0.05125	−3.76291	3.09821
H	−2.45105	4.40993	3.00893
H	2.45105	−4.40993	3.00892
H	−0.30248	−1.72360	−1.17723
H	0.30247	1.72360	−1.17724

Table S4. Cartesian coordinates of *S*-camphor

EE = −465.841478679 a.u.[a] - 100.00%[b]

Atom	X / Å	Y / Å	Z / Å
C	0.60081	1.78393	−0.84266
C	−0.05487	0.61255	−1.63088
C	0.60325	1.25765	0.60886
C	−0.29114	−0.49547	−0.55366
C	0.90989	−0.26159	0.42372
C	−1.43977	0.07282	0.27604
C	−0.53877	−1.88385	−1.10016
C	0.80236	−1.08332	1.71587
C	2.28195	−0.54356	−0.19616
C	−0.86566	1.24902	1.07359
O	−2.58365	−0.32232	0.29269
H	0.03271	2.71330	−0.92994
H	1.61221	1.98880	−1.19875
H	0.60477	0.22190	−2.40941
H	−0.99015	0.89820	−2.11941
H	1.28202	1.78453	1.28169
H	0.29720	−2.21458	−1.72336
H	−0.67347	−2.60972	−0.29264
H	−1.44660	−1.89805	−1.71037
H	1.00803	−2.13873	1.51274
H	1.53955	−0.73872	2.44830
H	−0.18290	−1.03160	2.18511
H	2.44502	−0.03235	−1.14551
H	3.07277	−0.22697	0.49243
H	2.40853	−1.61653	−0.37122
H	−0.98180	1.05775	2.14374
H	−1.40698	2.17228	0.84773

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory; [b]fractional population.

Table S5. Cartesian coordinates of (+)-menthone

EE = −467.058074556 a.u.[a] - 50.27%[b]

Atom	X / Å	Y / Å	Z / Å
O	−0.38587	1.98177	−0.81729
C	−0.70160	−0.17295	0.22782
C	0.08207	−1.37061	−0.36599
C	2.28708	−0.10263	−0.23632
C	1.53951	−1.39639	0.10227
H	−0.64570	−0.27357	1.32261
C	1.51580	1.10724	0.33650
C	0.07821	1.08678	−0.13592
H	2.29945	0.00404	−1.33029
C	−2.18099	−0.09119	−0.18846
H	0.04267	−1.31594	−1.46209
H	−0.41067	−2.30206	−0.07856
C	3.73099	−0.12162	0.26319
H	1.56793	−1.54996	1.19010
H	2.05806	−2.25006	−0.34802
H	1.97573	2.05206	0.03662
H	1.53027	1.04523	1.43280
H	4.25433	0.80294	−0.00031
H	3.76153	−0.22659	1.35383
H	4.28368	−0.96070	−0.17152
H	−2.20523	0.25182	−1.22986
C	−2.89671	−1.44407	−0.10608
C	−2.92222	0.94373	0.66892
H	−3.96031	1.04945	0.33773
H	−2.94003	0.62964	1.71965
H	−2.44543	1.92389	0.61208
H	−3.96194	−1.31962	−0.32554
H	−2.49599	−2.17138	−0.81642
H	−2.81436	−1.87328	0.89989

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory; [b]fractional population.

Table S6. Cartesian coordinates of (+)-menthone

EE = −467.057911305 a.u.[a] - 42.29%

Atom	X / Å	Y / Å	Z / Å
O	0.38068	2.23414	0.00706
C	0.69581	−0.11597	−0.43850
C	0.06480	−1.24323	0.40989
C	−2.21472	−0.14128	0.34276
C	−1.42134	−1.42960	0.09925
H	0.54499	−0.40158	−1.49194
C	−1.61203	1.00899	−0.48880
C	−0.11959	1.16003	−0.26988
H	−2.10451	0.12342	1.40402
C	2.20519	0.10108	−0.21935
H	0.18114	−1.00730	1.47384
H	0.60977	−2.17525	0.23335
C	−3.70316	−0.31224	0.04166
H	−1.54565	−1.73657	−0.94862
H	−1.83277	−2.23715	0.71482
H	−2.09677	1.96386	−0.27008
H	−1.77047	0.78724	−1.55406
H	−4.25637	0.61226	0.23551
H	−3.85677	−0.58139	−1.00981
H	−4.13854	−1.10450	0.65905
H	2.45653	1.02800	−0.74755
C	2.57728	0.30166	1.25521
C	3.02666	−1.03373	−0.84037
H	4.09811	−0.82988	−0.74564
H	2.83086	−1.99046	−0.34389
H	2.79905	−1.15539	−1.90469
H	3.63220	0.58039	1.34424
H	1.97760	1.09349	1.70984
H	2.43273	−0.61659	1.83392

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory.

Table S7. Cartesian coordinates of (+)-menthone

EE = −467.056271529 a.u.[a] - 7.45%[b]

Atom	X / Å	Y / Å	Z / Å
O	0.72992	−1.79573	−0.67950
C	0.65113	0.33749	0.47017
C	−0.20872	1.50527	−0.06975
C	−2.24473	0.01686	−0.30362
C	−1.69159	1.33004	0.26085
H	0.46509	0.30046	1.55498
C	−1.39865	−1.16957	0.20444
C	0.08043	−0.96879	−0.06645
H	−2.14021	0.05235	−1.39738
C	2.16469	0.55001	0.27015
H	−0.08814	1.57643	−1.15702
H	0.17233	2.44184	0.35090
C	−3.72229	−0.18061	0.03261
H	−1.83075	1.34016	1.35088
H	−2.26628	2.17327	−0.13792
H	−1.71260	−2.11105	−0.25315
H	−1.53701	−1.25659	1.29128
H	−4.10501	−1.11390	−0.39250
H	−3.86995	−0.22026	1.11805
H	−4.32600	0.64413	−0.35951
H	2.37795	1.52781	0.72479
C	2.98952	−0.49447	1.03280
C	2.59418	0.62899	−1.20132
H	3.66678	0.83868	−1.26765
H	2.39663	−0.31420	−1.71413
H	2.07047	1.42684	−1.73581
H	4.05642	−0.25405	0.98081
H	2.70437	−0.52676	2.09015
H	2.84272	−1.49064	0.60988

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory; [b]fractional population.

Table S8. Cartesian coordinates of *S*-naproxen

EE = −767.524562492 a.u.[a] - 51.39%[b]

Atom	X / Å	Y / Å	Z / Å
C	−1.14232	−0.47522	0.12199
C	−2.52358	−0.78653	0.02437
C	−3.45371	0.22489	−0.08663
O	−4.79649	0.04565	−0.18560
C	−5.28370	−1.28985	−0.17351
C	−3.03573	1.58264	−0.10463
C	−1.70803	1.90141	−0.01207
C	−0.71902	0.88833	0.10432
C	0.66105	1.18768	0.20123
C	1.60482	0.19248	0.31960
C	1.17941	−1.16051	0.33220
C	−0.15190	−1.48432	0.23551
C	3.08256	0.52674	0.45959
H	−0.46324	−2.52432	0.24346
H	−2.82030	−1.82723	0.03957
H	−1.39514	2.94068	−0.02660
H	−3.79739	2.34894	−0.19358
H	0.96933	2.22926	0.18651
H	1.92372	−1.94623	0.40751
H	−6.36763	−1.21725	−0.26124
H	−4.88543	−1.86457	−1.01729
H	−5.02497	−1.79757	0.76255
H	3.20022	1.60096	0.29455
C	3.63396	0.14588	1.83802
H	4.68946	0.41808	1.92428
H	3.07225	0.66861	2.61581
H	3.54541	−0.92922	2.00754
C	3.84328	−0.18485	−0.64486
O	3.77990	0.49062	−1.80767
O	4.41489	−1.24520	−0.53175
H	4.24479	−0.04136	−2.47370

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory; [b]fractional population.

Table S9. Cartesian coordinates of *S*-naproxen

EE = −767.524030589 a.u. - 29.26%

Atom	X / Å	Y / Å	Z / Å
C	−1.20341	0.69767	0.00928
C	−2.61901	0.71792	−0.09833
C	−3.33497	−0.45665	−0.01466
O	−4.68665	−0.55721	−0.10275
C	−5.42335	0.64332	−0.29525
C	−2.66197	−1.69362	0.17858
C	−1.29858	−1.73268	0.28425
C	−0.52406	−0.54363	0.20483
C	0.88543	−0.55405	0.31253
C	1.62064	0.61047	0.23166
C	0.94264	1.83634	0.03227
C	−0.42769	1.88090	−0.07297
C	3.13623	0.59460	0.38539
H	−0.93342	2.82961	−0.22363
H	−3.11169	1.67018	−0.24606
H	−0.79022	−2.68024	0.43193
H	−3.26093	−2.59522	0.23875
H	1.38987	−1.50537	0.45320
H	1.52024	2.75303	−0.03411
H	−6.47245	0.35103	−0.33783
H	−5.27036	1.33973	0.53694
H	−5.14153	1.13505	−1.23316
H	3.51339	1.57925	0.09670
C	3.56528	0.27263	1.82111
H	4.65382	0.30457	1.92097
H	3.12910	1.00139	2.50854
H	3.22382	−0.72419	2.10798
C	3.71061	−0.41152	−0.59384
O	3.83809	0.11167	−1.82792
O	3.99603	−1.55853	−0.33464
H	4.16385	−0.59653	−2.40677

Table S10. Cartesian coordinates of *S*-naproxen

EE = −767.523240251 a.u. - 12.67%

Atom	X / Å	Y / Å	Z / Å
C	−1.15331	−0.47113	0.11888
C	−2.53434	−0.78259	0.01930
C	−3.46420	0.22895	−0.09347
O	−4.80682	0.04975	−0.19465
C	−5.29406	−1.28574	−0.18425
C	−3.04620	1.58671	−0.11098
C	−1.71862	1.90542	−0.01645
C	−0.73002	0.89209	0.10126
C	0.64990	1.19081	0.20001
C	1.59568	0.19664	0.31999
C	1.16926	−1.15655	0.33302
C	−0.16237	−1.47922	0.23511
C	3.07013	0.54937	0.45333
H	−0.47351	−2.51931	0.24442
H	−2.83118	−1.82326	0.03433
H	−1.40557	2.94466	−0.03073
H	−3.80771	2.35299	−0.20122
H	0.95728	2.23263	0.18578
H	1.91021	−1.94400	0.40942
H	−6.37781	−1.21308	−0.27417
H	−4.89405	−1.85999	−1.02753
H	−5.03728	−1.79398	0.75206
H	3.16222	1.63344	0.35732
C	3.65618	0.10284	1.80113
H	4.71533	0.36543	1.87365
H	3.11857	0.60072	2.61205
H	3.56120	−0.97610	1.93690
C	3.82607	−0.01270	−0.73968
O	4.19927	−1.29601	−0.56101
O	4.05571	0.59554	−1.75869
H	4.63241	−1.58382	−1.38088

Table S11. Cartesian coordinates of *S*-naproxen

EE = −767.522637425 a.u. - 6.69%

Atom	X / Å	Y / Å	Z / Å
C	−1.21250	0.70419	0.01249
C	−2.62792	0.72366	−0.09779
C	−3.34258	−0.45234	−0.02442
O	−4.69390	−0.55397	−0.11648
C	−5.43154	0.64685	−0.30364
C	−2.66845	−1.68992	0.16135
C	−1.30528	−1.72800	0.26937
C	−0.53179	−0.53747	0.19993
C	0.87763	−0.54912	0.30948
C	1.61316	0.61648	0.23943
C	0.93259	1.84301	0.04838
C	−0.43750	1.88823	−0.05906
C	3.13021	0.61473	0.38376
H	−0.94303	2.83812	−0.20262
H	−3.12139	1.67643	−0.23952
H	−0.79607	−2.67603	0.41117
H	−3.26645	−2.59265	0.21377
H	1.37927	−1.50216	0.44156
H	1.50902	2.76096	−0.00951
H	−6.48012	0.35352	−0.35155
H	−5.28218	1.33809	0.53351
H	−5.14723	1.14496	−1.23742
H	3.48586	1.62636	0.17590
C	3.57730	0.19549	1.79202
H	4.66762	0.20639	1.87788
H	3.16439	0.89221	2.52599
H	3.22241	−0.80824	2.03325
C	3.73382	−0.24246	−0.71542
O	3.79282	−1.54832	−0.38384
O	4.10351	0.17282	−1.78885
H	4.14568	−2.02213	−1.15429

Table S12. Cartesian coordinates of L-tryptophan

EE = −686.303833110 a.u.[a] - 49.77%[b]

Atom	X / Å	Y / Å	Z / Å
C	3.67592	0.76530	0.58926
C	3.31911	−0.56334	0.39565
C	2.04498	−0.82109	−0.11342
C	1.13041	0.22258	−0.43135
C	1.52135	1.55437	−0.22613
C	2.78720	1.81404	0.28087
N	1.41948	−2.01217	−0.40600
C	0.15491	−1.75559	−0.89457
C	−0.06856	−0.40142	−0.93085
C	−1.33053	0.28881	−1.33845
H	−1.13084	1.11430	−2.02972
H	−1.99019	−0.41596	−1.85647
H	−0.49670	−2.56684	−1.18178
H	1.82515	−2.92746	−0.30210
H	0.84528	2.36931	−0.46453
H	4.00359	−1.37122	0.63100
H	3.10088	2.83974	0.44368
H	4.65866	0.99935	0.98461
C	−2.11386	0.88061	−0.14416
H	−1.49673	1.63164	0.35438
N	−3.33699	1.51625	−0.63050
H	−3.97302	0.77787	−0.92890
H	−3.80779	1.97383	0.14720
C	−2.39311	−0.24557	0.84359
O	−1.59343	−0.20645	1.92279
O	−3.23991	−1.09495	0.67723
H	−1.81587	−0.97415	2.47534

[a]Electronic energy at CAM-B3LYP/6-311++G(3df,2p)//B3LYP/6-311++G(2d,p) + SMD (ϵ = 24.852) level of theory; [b]fractional population.

Table S13. Cartesian coordinates of L-tryptophan

EE = −686.303145600 a.u. - 24.03%

Atom	X / Å	Y / Å	Z / Å
C	3.72828	0.71036	0.59191
C	3.33401	−0.61060	0.42004
C	2.05155	−0.84048	−0.08140
C	1.16540	0.22330	−0.41290
C	1.59392	1.54680	−0.22958
C	2.86806	1.77867	0.26985
N	1.39232	−2.01794	−0.35453
C	0.13354	−1.73404	−0.84233
C	−0.05179	−0.37454	−0.90059
C	−1.29480	0.34592	−1.31777
H	−1.06637	1.17883	−1.99117
H	−1.95790	−0.33597	−1.85962
H	−0.54266	−2.53074	−1.11227
H	1.76962	−2.94267	−0.22949
H	0.93952	2.37635	−0.47792
H	3.99626	−1.43364	0.66614
H	3.21067	2.79757	0.41614
H	4.71839	0.92302	0.98089
C	−2.06711	0.92684	−0.11707
H	−1.44378	1.66657	0.39098
N	−3.28933	1.58859	−0.57970
H	−3.92329	0.88415	−0.95147
H	−3.77336	2.00276	0.21362
C	−2.32648	−0.16805	0.91089
O	−3.10425	−1.14881	0.40455
O	−1.92229	−0.17700	2.05003
H	−3.24311	−1.79937	1.11090

Table S14. Cartesian coordinates of L-tryptophan

EE = −686.302457721 a.u. - 11.60%

Atom	X / Å	Y / Å	Z / Å
C	−3.85913	−1.16559	0.01700
C	−3.71595	0.18499	0.30688
C	−2.44687	0.74656	0.15371
C	−1.32487	−0.01609	−0.27992
C	−1.50300	−1.37990	−0.56465
C	−2.76379	−1.93993	−0.41460
N	−2.00940	2.03545	0.35561
C	−0.66489	2.11293	0.05852
C	−0.19658	0.88204	−0.33372
C	1.21405	0.55766	−0.72089
H	1.22628	−0.16165	−1.54738
H	1.71925	1.46339	−1.06326
H	−0.13974	3.05239	0.14323
H	−2.58402	2.80884	0.64734
H	−0.65848	−1.98328	−0.87718
H	−4.55695	0.78365	0.63954
H	−2.91196	−2.99294	−0.62999
H	−4.83220	−1.63271	0.12594
C	2.03325	−0.04276	0.44643
H	2.04660	0.71451	1.24954
N	1.47915	−1.32664	0.85862
H	2.09300	−1.74856	1.54927
H	0.58575	−1.16402	1.31303
C	3.48838	−0.23976	0.06199
O	4.03617	0.89130	−0.42197
O	4.11318	−1.26607	0.19518
H	4.96600	0.69593	−0.61988

Table S15. Cartesian coordinates of L-tryptophan

EE = −686.302337369 a.u. - 10.21%

Atom	X / Å	Y / Å	Z / Å
C	−3.92803	−1.08326	0.07373
C	−3.74329	0.27787	0.27754
C	−2.45316	0.78572	0.10978
C	−1.35115	−0.04019	−0.25165
C	−1.57086	−1.41234	−0.44608
C	−2.85218	−1.91993	−0.28577
N	−1.97533	2.07072	0.23370
C	−0.62512	2.08351	−0.04834
C	−0.19386	0.81374	−0.34731
C	1.20543	0.42731	−0.71167
H	1.19785	−0.34908	−1.48686
H	1.72568	1.29155	−1.13475
H	−0.07016	3.00926	−0.02053
H	−2.52746	2.88106	0.46087
H	−0.74458	−2.06417	−0.70496
H	−4.56841	0.92500	0.55524
H	−3.03241	−2.97958	−0.43429
H	−4.91808	−1.51013	0.19472
C	2.04305	−0.10065	0.48243
H	1.98856	0.64353	1.28249
N	1.51587	−1.36492	0.97372
H	1.75739	−2.08819	0.29838
H	2.01552	−1.62447	1.82112
C	3.49796	−0.19905	0.03624
O	4.09348	1.00791	−0.01518
O	4.05944	−1.22599	−0.26859
H	4.99616	0.87279	−0.34664

Table S16. Cartesian coordinates of L-tryptophan

EE = −686.301542892 a.u. - 4.40%

Atom	X / Å	Y / Å	Z / Å
C	−3.83504	−1.23109	0.02593
C	−3.71781	0.11286	0.35600
C	−2.46610	0.70993	0.19506
C	−1.33592	−0.01115	−0.28613
C	−1.48796	−1.36924	−0.61164
C	−2.73144	−1.96459	−0.45314
N	−2.05442	2.00171	0.42871
C	−0.71840	2.12060	0.10698
C	−0.22979	0.91452	−0.33401
C	1.17900	0.62839	−0.75729
H	1.19079	−0.08138	−1.59159
H	1.65854	1.54474	−1.10886
H	−0.21372	3.06923	0.21146
H	−2.64038	2.75168	0.75676
H	−0.63823	−1.94250	−0.96537
H	−4.56564	0.68001	0.72462
H	−2.85932	−3.01333	−0.69988
H	−4.79423	−1.72494	0.13969
C	2.03899	0.05014	0.37733
H	2.04875	0.78953	1.19869
N	1.53824	−1.26189	0.80036
H	2.09428	−1.59281	1.58356
H	0.59337	−1.13778	1.15445
C	3.49118	−0.07343	−0.05917
O	4.20184	−0.83794	0.79236
O	3.98588	0.46454	−1.02182
H	5.11699	−0.85558	0.46913

Camphor (1,7,7-trimethylbicyclo[2.2.1]heptan-2-one) is a well-known bicyclic terpenoid derived from the wood of the camphor laurel (*Cinnamomum camphora* tree). This chiral bicyclic ketone occurs naturally as the *R*-enantiomer (Figure S1, left). In this work we have studied the electronic and molecular properties of the *S*-enantiomer (Figure S1, right).

Figure S1. Molecular structures of *R*- (left) and *S*-camphor enantiomers.

Menthone is a monoterpene that occurs naturally in a number of essential oils. 2-Isopropil-5-methylcyclohexanone has two asymmetric carbon centers, resulting in four different stereoisomers described by two pairs of (+)-menthone and (−)-menthone and (+)-isomenthone and (−)-isomenthone enantiomers. Therefore, it is reasonable that these paired compounds (diastereoisomers) are isomers with each other (Figure S2). In this work we have studied the (+)-menthone, as shown at Figure S2b. And the three more stable conformations obtained for this molecular structure are described at Figure S3.

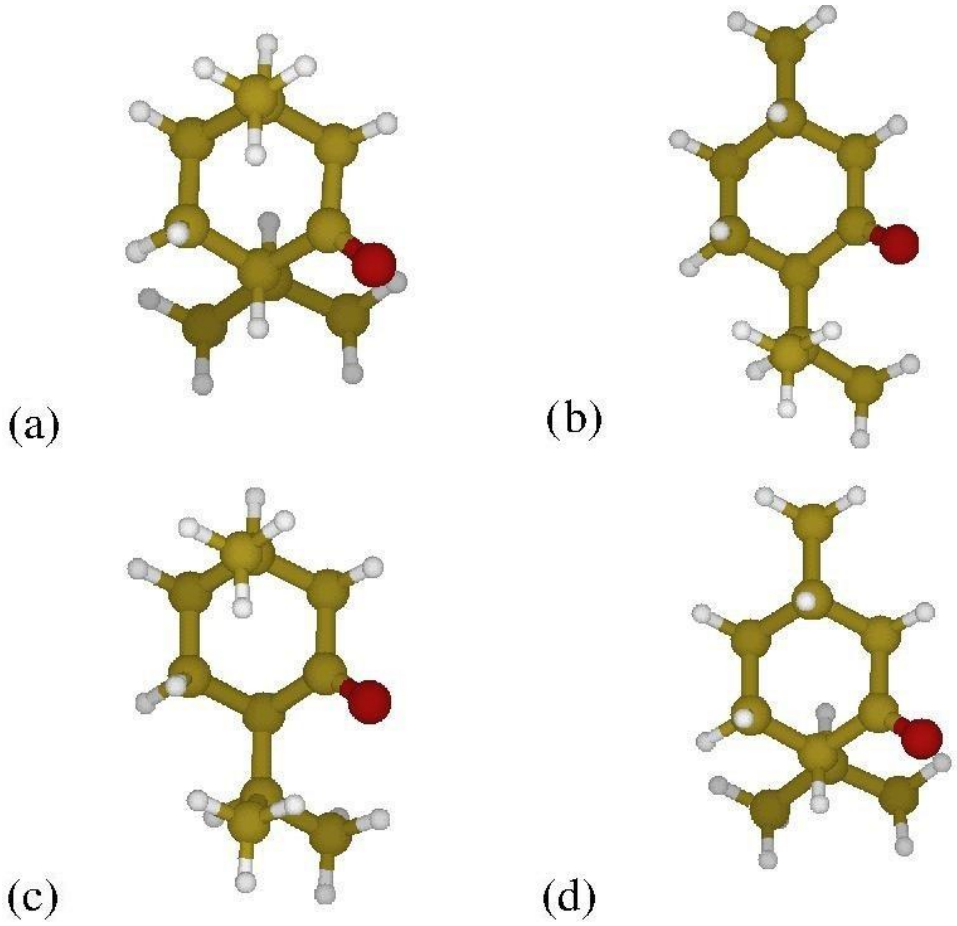

Figure S2. Molecular structures of (a) (−)-menthone; (b) (+)-menthone; (c) (+)-isomenthone; and (d) (−)-isomenthone.

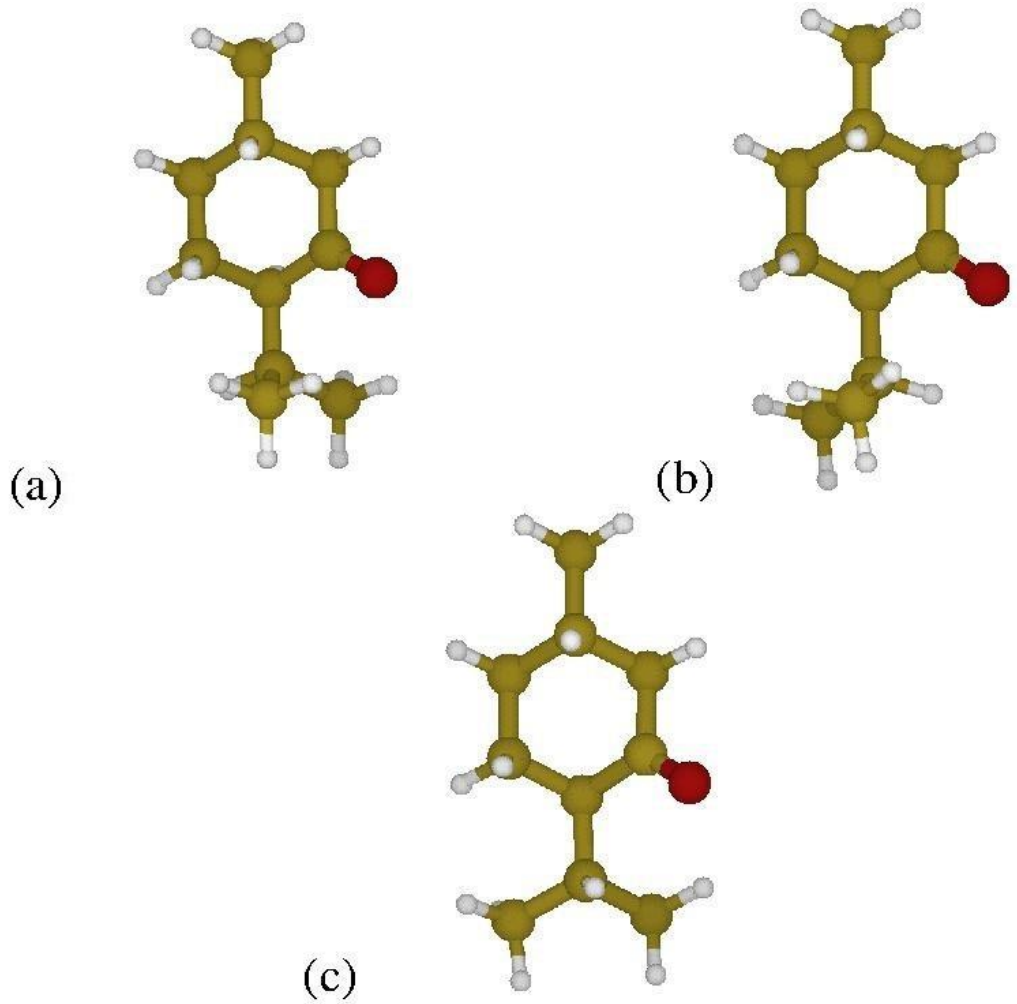

Figure S3. Conformational structures of (+)-menthone obtained after the dihedral angle rotation defined by the chemical bonds: O=C−C−C(H)(CH_3)(CH_3).

If there are several conformers which appear to be stable in terms of energy, ECD calculations generally involve two steps, first the conformational analysis of the compound to obtain the most relevant conformational structures, weighted considering the Boltzmann distribution law. The conformational search, employed for finding the stable conformers, was performed by varying selected dihedral angles, as described at Figure 4. The stable molecular geometries, corresponding to the energy minima on potential energy surface (PES), were obtained at the B3LYP/6-311++G(2d,p) level of theory.

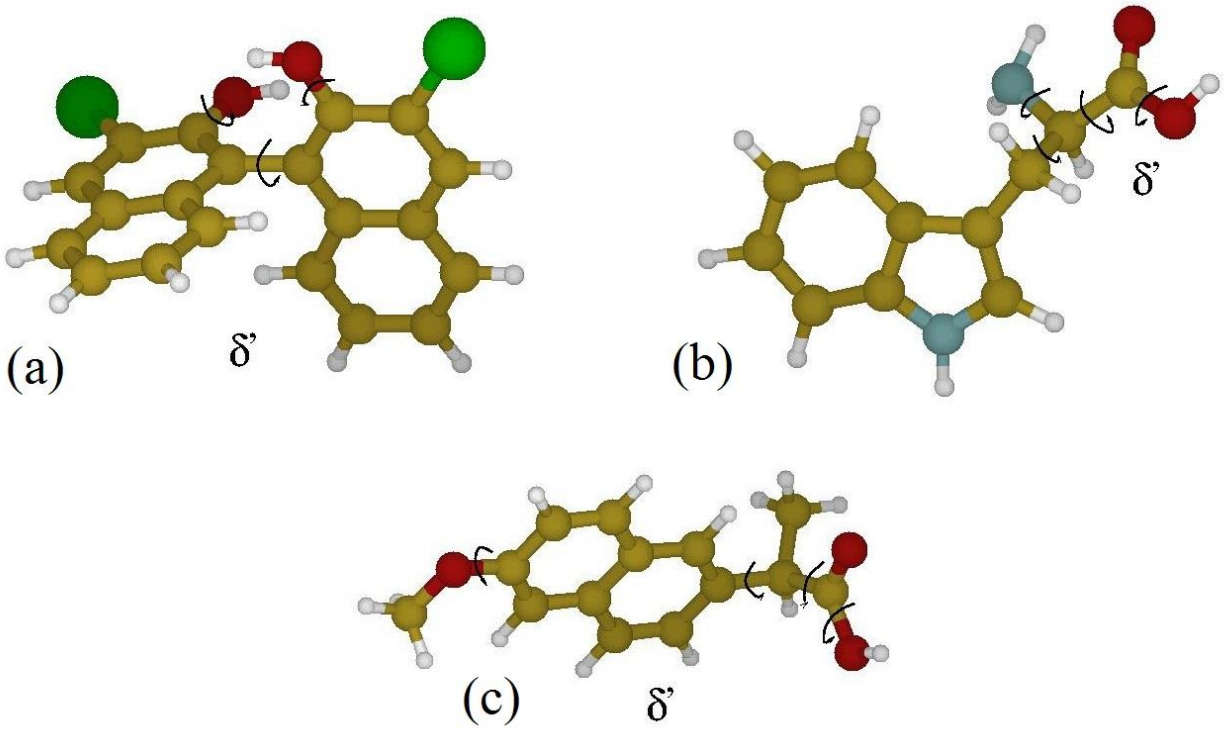

Figure S4. Dihedral angles selected for: (a) *R*-3,3'-dibromo-1,1'-bi-2-naphthol; (b) L-tryptophan; and (c) *S*-naproxen.

At Figures S5, S6 and S7, the absorbance, ECD and g-factor experimental spectra of S-camphor (CAM), L-tryptophan (TRY), *R*-3,3'-dibromo-1,1'-bi-2-naphthol (BIN), *S*-naproxen (NPX), and (+)-menthone (MEN) are shown.

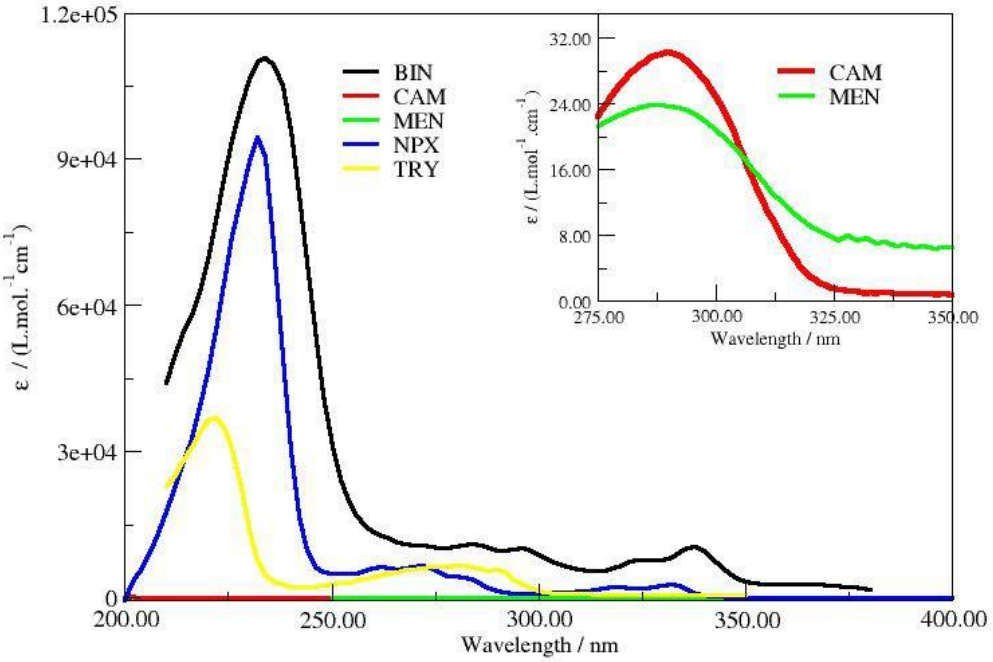

Figure S5. Experimental UV-Vis absorbance spectra of *S*-camphor (CAM), L-tryptophan (TRY), *R*-3,3'-dibromo-1,1'-bi-2-naphthol (BIN), *S*-naproxen (NPX), and (+)-menthone (MEN).

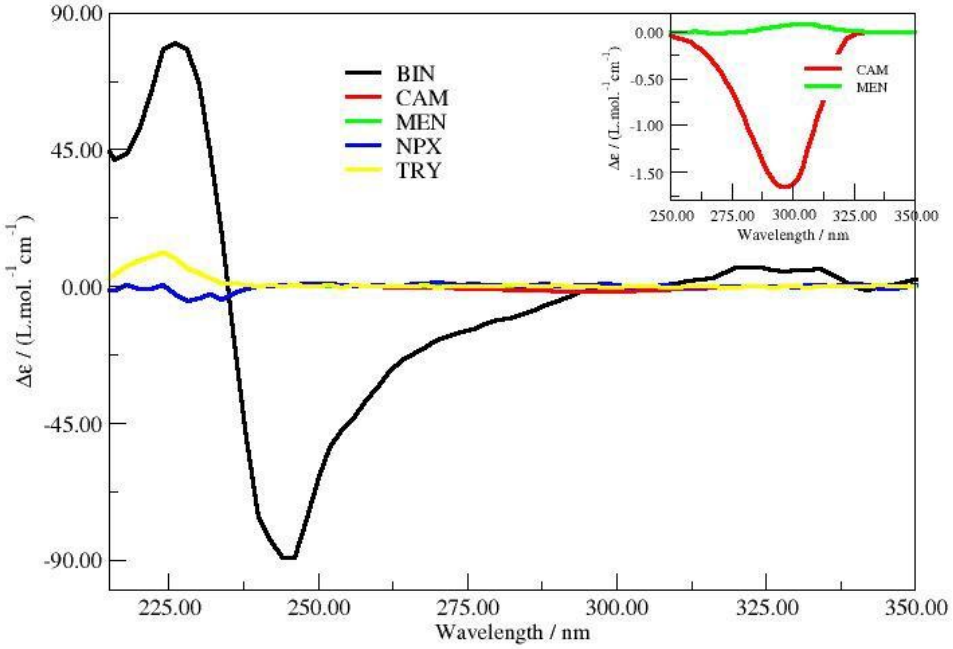

Figure S6. Experimental ECD spectra of *S*-camphor (CAM), L-tryptophan (TRY), *R*-3,3'-dibromo-1,1'-bi-2-naphthol (BIN), *S*-naproxen (NPX), and (+)-menthone (MEN).

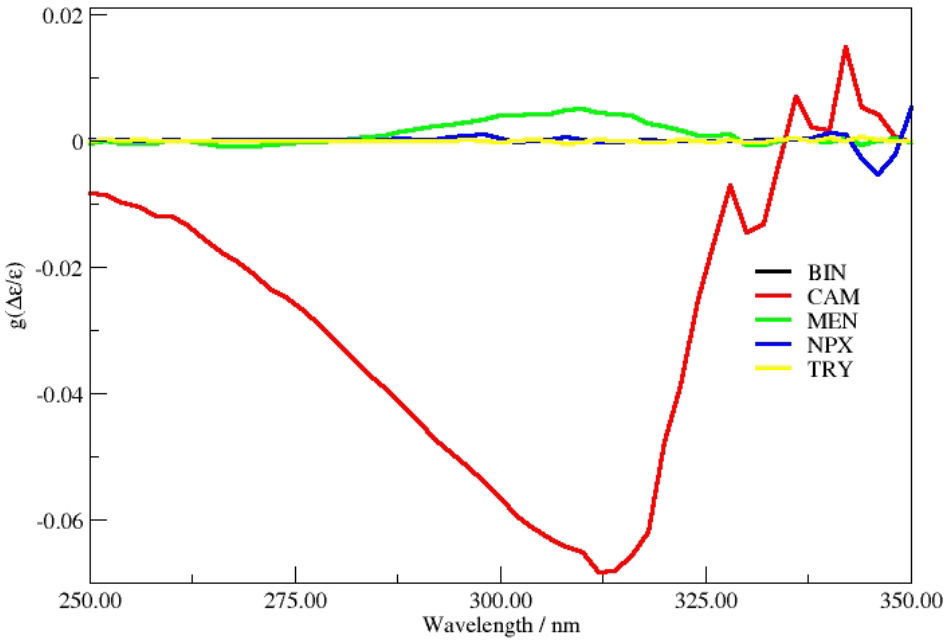

Figure S7. Experimental g-factor of *S*-camphor (CAM), L-tryptophan (TRY), *R*-3,3'-dibromo-1,1'-bi-2-naphthol (BIN), *S*-naproxen (NPX), and (+)-menthone (MEN).

For comparison purposes, λ_{max} and the molar absorptivity coefficient for all systems studied, i.e., quantities related to the UV-Vis and ECD spectra intensities, are given at Table S17.

Table S17. Maximum absorption, λ_{max}, molar absorptivity coefficient, ϵ_i, molar circular dichroism, $\Delta\epsilon$ for all systems studied.[a] All of these quantities are related to the UV-Vis and ECD spectra intensities

Molecule	λ_{max} / nm	ϵ / (M^{-1} cm^{-1})	$\Delta\epsilon$ / (M^{-1} cm^{-1})
R-3,3'-Dibromo-1,1'-bi-2-naphthol	298.0 (296.0)[b]	17,132.3 (10,188.7)	5.71 (−1.24)
S-Camphor	282.0 (290.0)	16.2 (30.2)	−1.44 (−1.51)
(+)-Menthone	281.0 (286.0)	12.0 (23.9)	0.02 (0.02)
S-Naproxen	292.0 (272.0)	4,392.3 (6,617.3)	−1.93 (1.00)
L-Tryptophan	263.0 (282.0)	11,609.0 (6,779.3)	−0.55 (0.41)

[a]The calculated intensity are weighted considering the Boltzmann distribution law; [b]the experimental values are between parentheses.

The results at Table S18 show, at its maximum intensity wavelengths, the g-factor of all systems. Specifically, the g-factors at their maximum were −0.0886 and −0.0001 for *S*-camphor and L-tryptophan, respectively. To reinforce that g-factors usually have low values, we also measured, for comparative purpose, the g-factor of *S*-naproxen (g = −0.0003) and *R*-3,3'-dibromo-1,1'-bi-2-naphthol (g = 0.0001). These values are in agreement with most of the published results.

Table S18. Dissymmetry factor for all systems studied

Molecule	g_{exper}	g_{calc}
R-3,3'-Dibromo-1,1'-bi-2-naphthol	0.0008	0.0003
S-Camphor	−0.0445	−0.0886
(+)-Menthone	0.0009	0.0013
S-Naproxen	0.0002	−0.0003
L-Tryptophan	0.0001	−0.0001

An explanation for the relatively high g-factor of camphor is due to the magnitude and the angle between the electric and magnetic transition dipole moments. These values were calculated at their maximum wavelengths. It is worth to note that the light absorption depends only on the electric transition dipole moments. Hence, as expected, the magnitude of electric component for *S*-camphor was lower as compared to L-tryptophan, which is in agreement with its lower molar absorptivity coefficient (Table S19).

Table S19. Electronic parameters calculated for all systems studies:[a] transition electric dipole moment, μ_{ele}, transition magnetic dipole moment, μ_{mag}, and angle between the electric and magnetic transition dipole moments. All of these quantities are related to the UV-Vis and ECD spectra intensities

Molecule	μ_{ele}	μ_{mag}	E-M angle / °
R-3,3'-Dibromo-1,1'-bi-2-naphthol	1.91	0.96	97.62
S-Camphor	0.06	1.18	104.89
(+)-Menthone	0.02	1.15	70.39
S-Naproxen	1.03	0.06	118.34
L-Tryptophan	1.35	0.97	90.54

[a]The calculated intensity are weighted considering the Boltzmann distribution law.