

Supporting Information

Absolute Configuration of Verticillane Diterpenoids by Vibrational Circular Dichroism

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Table S1. DFT atomic Cartesian coordinates (Å) for conformer **1a**

Atom	X	Y	Z
C1	-1.407444	-1.939340	0.455247
C2	-0.057028	-2.636448	0.062955
C3	0.957920	-1.898101	-0.775481
C4	2.253597	-1.656605	-0.506027
C5	3.098719	-0.852041	-1.476080
C6	3.449447	0.582726	-0.983241
C7	2.226928	1.445719	-0.830399
C8	1.745216	2.069770	0.258217
C9	0.403672	2.775868	0.200446
C10	-0.772916	1.983094	0.842358
C11	-1.055198	0.599245	0.196223
C12	-2.085622	0.679745	-0.981830
C13	-2.185181	-0.693074	-1.678231
C14	-2.417336	-1.860723	-0.711549
C15	-1.302598	-0.572033	1.222200
C16	-2.578085	-0.375641	2.077852
C17	-0.131624	-0.651178	2.229565
C18	-3.485604	1.207904	-0.640151
C19	2.444677	2.111725	1.595550
C20	2.981087	-2.124198	0.731806
O12	-1.607404	1.641921	-1.948740
H1	-1.842783	-2.645785	1.177329
H2A	-0.345909	-3.550908	-0.477317
H2B	0.416561	-2.983152	0.984534
H3	0.595934	-1.540442	-1.737962
H5A	2.577893	-0.771102	-2.437801
H5B	4.041481	-1.381135	-1.674684
H6A	4.018914	0.524587	-0.050957
H6B	4.126535	1.027892	-1.726380
H7	1.637644	1.532136	-1.746561
H9A	0.138636	2.992706	-0.836976
H9B	0.476146	3.742229	0.718902
H10A	-0.568921	1.867340	1.910481
H10B	-1.658343	2.623510	0.784027
H11	-0.120925	0.304765	-0.295738
H12	-0.742776	1.334777	-2.254677
H13A	-2.984440	-0.654247	-2.427884
H13B	-1.256229	-0.854851	-2.238358
H14A	-2.406781	-2.806293	-1.267848
H14B	-3.429421	-1.777849	-0.297348
H16A	-3.505101	-0.529481	1.524505
H16B	-2.579586	-1.087026	2.911752
H16C	-2.613124	0.630686	2.508227
H17A	0.840295	-0.609635	1.735724
H17B	-0.175247	0.160898	2.960883
H17C	-0.189112	-1.586097	2.798740
H18A	-4.092180	0.468689	-0.116445
H18B	-3.449012	2.114051	-0.031659

H18C	-3.987897	1.458357	-1.578708
H19A	3.386920	1.560333	1.608727
H19B	2.664786	3.150961	1.872849
H19C	1.809434	1.706513	2.391560
H20A	2.355654	-2.712346	1.404668
H20B	3.381648	-1.279866	1.306287
H20C	3.842763	-2.744076	0.451452

Table S2. DFT atomic Cartesian coordinates (Å) for conformer **1b**

Atom	X	Y	Z
C1	-1.411997	-1.940241	0.462630
C2	-0.064505	-2.642783	0.072003
C3	0.948814	-1.908616	-0.771537
C4	2.245751	-1.669616	-0.507252
C5	3.085163	-0.865655	-1.482499
C6	3.424849	0.573724	-0.997495
C7	2.194369	1.423765	-0.833518
C8	1.745719	2.075745	0.252967
C9	0.401872	2.779982	0.207725
C10	-0.764690	1.980193	0.857531
C11	-1.045339	0.599734	0.203073
C12	-2.064258	0.680017	-0.978447
C13	-2.168528	-0.694261	-1.670951
C14	-2.419183	-1.858511	-0.705578
C15	-1.303143	-0.571153	1.225744
C16	-2.577912	-0.372872	2.082724
C17	-0.131159	-0.652421	2.232426
C18	-3.463374	1.227008	-0.647443
C19	2.475975	2.149677	1.572497
C20	2.977953	-2.134565	0.728637
O12	-1.450493	1.602606	-1.908825
H1	-1.852048	-2.642805	1.185779
H2A	0.409512	-2.986639	0.994516
H2B	-0.356986	-3.559349	-0.463145
H3	0.584200	-1.546388	-1.730681
H5A	4.030952	-1.390267	-1.679617
H5B	2.560994	-0.792250	-2.442639
H6A	4.087314	1.023321	-1.751663
H6B	4.009146	0.525207	-0.073388
H7	1.564787	1.472052	-1.723551
H9A	0.476062	3.743923	0.731194
H9B	0.130617	2.991352	-0.827824
H10A	-1.654887	2.616633	0.822924
H10B	-0.545696	1.853147	1.921466
H11	-0.113690	0.311675	-0.291550
H12	-2.042567	1.677576	-2.670036

H13A	-1.235812	-0.845705	-2.221091
H13B	-2.968373	-0.660093	-2.424698
H14A	-3.432390	-1.767826	-0.295210
H14B	-2.412423	-2.804471	-1.261256
H16A	-3.505880	-0.539613	1.533777
H16B	-2.618129	0.637372	2.503349
H16C	-2.574034	-1.076167	2.923451
H17A	0.839788	-0.604264	1.737234
H17B	-0.185795	-1.590840	2.795995
H17C	-0.176173	0.155137	2.968442
H18A	-4.061564	0.536027	-0.051790
H18B	-4.010383	1.396538	-1.583748
H18C	-3.414662	2.181814	-0.119628
H19A	3.416106	1.594075	1.579295
H19B	1.856449	1.765645	2.392091
H19C	2.706447	3.193895	1.822068
H20A	2.352800	-2.713023	1.410396
H20B	3.833276	-2.762890	0.447273
H20C	3.388727	-1.288556	1.293440

Table S3. DFT atomic Cartesian coordinates (\AA) for conformer **1c**

Atom	X	Y	Z
C1	-1.375960	-1.950975	0.462953
C2	-0.020816	-2.637292	0.073079
C3	0.982294	-1.891302	-0.771414
C4	2.279333	-1.648603	-0.511024
C5	3.111223	-0.833507	-1.483280
C6	3.431248	0.608238	-0.992719
C7	2.188815	1.441049	-0.835331
C8	1.725991	2.088606	0.247439
C9	0.375628	2.779368	0.187675
C10	-0.792844	1.978710	0.836860
C11	-1.065341	0.590109	0.194856
C12	-2.106403	0.651833	-0.975352
C13	-2.171001	-0.714849	-1.674755
C14	-2.384184	-1.883899	-0.706588
C15	-1.284237	-0.580647	1.227019
C16	-2.552589	-0.408187	2.098967
C17	-0.099307	-0.635287	2.220031
C18	-3.519345	1.143807	-0.619044
C19	2.445402	2.177818	1.571550
C20	3.019268	-2.119465	0.718188
O12	-1.590300	1.538383	-1.997903
H1	-1.806933	-2.659316	1.185938
H2A	0.457939	-2.975777	0.995147
H2B	-0.302698	-3.557159	-0.461979
H3	0.609467	-1.524646	-1.725811

H5A	4.064067	-1.345353	-1.679080
H5B	2.588795	-0.763956	-2.444555
H6A	4.091463	1.069725	-1.741460
H6B	4.009739	0.565425	-0.064759
H7	1.564419	1.478728	-1.729718
H9A	0.437287	3.752658	0.694876
H9B	0.131928	2.979072	-0.858667
H10A	-1.688268	2.612079	0.801142
H10B	-0.577356	1.868239	1.902968
H11	-0.138405	0.315809	-0.315699
H12	-1.776665	2.445060	-1.721430
H13A	-1.237723	-0.835515	-2.232175
H13B	-2.971012	-0.693663	-2.424315
H14A	-3.398681	-1.819262	-0.293778
H14B	-2.357299	-2.828599	-1.263519
H16A	-3.482734	-0.594555	1.560385
H16B	-2.609822	0.600825	2.521379
H16C	-2.523777	-1.111161	2.939351
H17A	0.864775	-0.572677	1.713071
H17B	-0.129764	-1.570670	2.790406
H17C	-0.150761	0.175686	2.952474
H18A	-4.088377	0.420827	-0.033710
H18B	-4.063404	1.323867	-1.551459
H18C	-3.502903	2.081141	-0.052497
H19A	3.388398	1.627702	1.586910
H19B	1.823978	1.794839	2.389922
H19C	2.668461	3.225142	1.814835
H20A	2.396679	-2.695377	1.404332
H20B	3.868584	-2.752344	0.428868
H20C	3.439946	-1.277004	1.281178

Table S4. DFT atomic Cartesian coordinates (\AA) for conformer **1d**

Atom	X	Y	Z
C1	-1.253584	-2.040107	0.276096
C2	0.151943	-2.693549	0.048310
C3	1.153566	-1.899263	-0.753442
C4	2.419424	-1.557734	-0.457752
C5	3.219951	-0.716310	-1.435357
C6	3.423222	0.763543	-1.001504
C8	1.631036	2.168904	0.196824
C7	2.119977	1.503666	-0.863336
C9	0.221482	2.732701	0.173972
C10	-0.787572	1.845310	0.956792
C11	-1.126741	0.514599	0.237463
C12	-2.260452	0.667923	-0.848423
C13	-2.924294	-0.691263	-1.180980
C14	-1.953122	-1.866105	-1.102906
C15	-1.295759	-0.737556	1.171325

C16	-2.604720	-0.700681	1.998525
C17	-0.158812	-0.799808	2.217757
C18	-3.363153	1.680295	-0.520190
C19	2.386772	2.387265	1.486597
C20	3.144466	-1.941001	0.808901
O12	-1.664625	1.204893	-2.055292
H1	-1.818336	-2.796332	0.838381
H2A	-0.048269	-3.629587	-0.496410
H2B	0.577695	-2.999231	1.006100
H3	0.799662	-1.577493	-1.732940
H5A	2.722622	-0.723900	-2.412763
H5B	4.211822	-1.164837	-1.586842
H6A	4.046121	1.245242	-1.769285
H6B	4.003838	0.801059	-0.075055
H7	1.481524	1.452938	-1.747381
H9A	-0.129059	2.839807	-0.856255
H9B	0.222746	3.734209	0.625921
H10A	-1.692040	2.428106	1.149506
H10B	-0.364127	1.642522	1.942628
H11	-0.229597	0.264119	-0.340025
H12	-0.976112	0.588475	-2.339418
H13A	-3.334798	-0.603289	-2.193328
H13B	-3.779215	-0.863939	-0.520764
H14A	-1.197334	-1.726862	-1.885289
H14B	-2.466349	-2.796997	-1.370485
H16A	-3.512923	-0.790779	1.401130
H16B	-2.671948	0.233211	2.567782
H16C	-2.613157	-1.523917	2.722455
H17A	0.824356	-0.631317	1.773693
H17B	-0.151719	-1.778159	2.710651
H17C	-0.304180	-0.059041	3.008893
H18A	-3.816937	1.480097	0.454133
H18B	-4.144789	1.619052	-1.283627
H18C	-2.977093	2.701514	-0.526940
H19A	3.368463	1.910445	1.498759
H19B	1.823552	2.012533	2.349827
H19C	2.537573	3.461150	1.658676
H20A	4.056997	-2.502844	0.570199
H20B	2.541203	-2.555935	1.478533
H20C	3.465043	-1.054136	1.369845

Table S5. DFT atomic Cartesian coordinates (\AA) for conformer **1e**

Atom	X	Y	Z
C1	-1.281521	-2.035513	0.301578
C2	0.119237	-2.690065	0.057480
C3	1.113357	-1.886016	-0.743965
C4	2.394833	-1.587679	-0.469618

C5	3.190903	-0.732115	-1.439396
C6	3.399899	0.740550	-0.986649
C7	2.097357	1.482502	-0.847461
C8	1.633555	2.185157	0.199551
C9	0.221038	2.744177	0.186531
C10	-0.775538	1.846168	0.972981
C11	-1.107392	0.516807	0.249468
C12	-2.212665	0.666995	-0.859369
C13	-2.933162	-0.669831	-1.153688
C14	-1.995968	-1.868932	-1.070769
C15	-1.303622	-0.727287	1.186494
C16	-2.611326	-0.658977	2.014521
C17	-0.167155	-0.805558	2.233000
C18	-3.274428	1.747069	-0.599343
C19	2.412415	2.445623	1.467420
C20	3.143995	-2.034802	0.761779
O12	-1.456007	1.047293	-2.037413
H1	-1.839960	-2.785247	0.879143
H2A	-0.087979	-3.620043	-0.495467
H2B	0.551986	-3.007979	1.008386
H3	0.734989	-1.505539	-1.691814
H5A	2.685651	-0.722768	-2.412338
H5B	4.180272	-1.181514	-1.604769
H6A	4.027833	1.228474	-1.747006
H6B	3.978090	0.765876	-0.057647
H7	1.435163	1.392750	-1.709539
H9A	-0.131355	2.851377	-0.842946
H9B	0.218980	3.744467	0.641499
H10A	-1.682044	2.419910	1.186683
H10B	-0.335939	1.637208	1.950537
H11	-0.210621	0.263366	-0.321345
H12	-2.092544	1.231261	-2.743047
H13A	-3.359839	-0.600629	-2.164098
H13B	-3.788710	-0.794111	-0.483461
H14A	-1.251804	-1.741870	-1.862391
H14B	-2.537502	-2.790633	-1.313676
H16A	-3.522914	-0.725744	1.418893
H16B	-2.654881	0.276123	2.584220
H16C	-2.640679	-1.481773	2.738428
H17A	0.817986	-0.657730	1.785913
H17B	-0.178316	-1.782508	2.728668
H17C	-0.297023	-0.059295	3.021683
H18A	-3.792079	1.592929	0.352352
H18B	-4.033308	1.713031	-1.391704
H18C	-2.837667	2.747922	-0.600134
H19A	3.384390	1.949194	1.486346
H19B	1.854665	2.120413	2.354418
H19C	2.588010	3.522641	1.591332
H20A	4.011718	-2.646268	0.480578
H20B	2.531514	-2.623668	1.446692
H20C	3.539108	-1.177610	1.321646

Table S6. DFT atomic Cartesian coordinates (\AA) for conformer **1f**

Atom	X	Y	Z
C1	-1.293301	-2.021406	0.343619
C2	0.106865	-2.674315	0.095975
C3	1.087716	-1.876258	-0.726990
C4	2.377293	-1.589651	-0.479469
C5	3.160706	-0.740575	-1.464953
C6	3.399271	0.727461	-1.011345
C7	2.112232	1.490213	-0.850645
C8	1.654147	2.163200	0.217463
C9	0.256902	2.758658	0.216521
C10	-0.785239	1.868894	0.952103
C11	-1.105613	0.530650	0.235867
C12	-2.204817	0.656213	-0.894941
C13	-2.939058	-0.675285	-1.148514
C14	-2.028987	-1.892109	-1.021868
C15	-1.307674	-0.695131	1.199123
C16	-2.615832	-0.602101	2.023501
C17	-0.171552	-0.762474	2.247555
C18	-3.256884	1.754299	-0.671819
C19	2.423958	2.356847	1.502406
C20	3.149001	-2.047777	0.734040
O12	-1.540722	0.923122	-2.155962
H1	-1.838034	-2.759148	0.948868
H2A	-0.102121	-3.612455	-0.442031
H2B	0.551853	-2.977394	1.046246
H3	0.689268	-1.490425	-1.664491
H5A	2.634388	-0.722162	-2.426525
H5B	4.141211	-1.199702	-1.654053
H6A	4.021302	1.210478	-1.779177
H6B	3.990805	0.741574	-0.090861
H7	1.455994	1.438915	-1.721521
H9A	-0.063513	2.949838	-0.815409
H9B	0.276161	3.740580	0.708682
H10A	-1.691499	2.457287	1.120319
H10B	-0.387618	1.671438	1.949491
H11	-0.202347	0.263972	-0.318325
H12	-1.096559	1.777098	-2.077512
H13A	-3.344768	-0.618869	-2.164642
H13B	-3.799275	-0.758435	-0.478988
H14A	-1.297213	-1.827044	-1.832148
H14B	-2.601613	-2.807264	-1.213138
H16A	-3.525717	-0.674423	1.426389
H16B	-2.655629	0.343558	2.575938
H16C	-2.651534	-1.410766	2.762871
H17A	0.815228	-0.630394	1.798472
H17B	-0.189482	-1.730949	2.759378

H17C	-0.295407	-0.003573	3.025433
H18A	-3.771753	1.640463	0.287589
H18B	-4.002877	1.700644	-1.470507
H18C	-2.817606	2.756776	-0.699824
H19A	3.388968	1.847388	1.505358
H19B	1.854658	1.995439	2.367442
H19C	2.611142	3.424481	1.677947
H20A	3.993884	-2.681689	0.433561
H20B	2.541107	-2.618354	1.438171
H20C	3.579550	-1.197988	1.278911

Table S7. X-ray fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (1*S*,3*S*,4*S*,7*S*,8*S*,11*S*,12*R*)-(+)-3,4:7,8-diepoxiverticillan-12-ol (**4**).

Atom	x	y	z	U(eq)
C(1)	12154(4)	-416(3)	1604(2)	50(1)
C(2)	12826(4)	-1243(3)	1052(2)	53(1)
C(3)	11914(4)	-1643(2)	356(2)	44(1)
C(4)	12449(4)	-1617(2)	-473(2)	46(1)
C(5)	11255(5)	-1779(3)	-1119(2)	53(1)
C(6)	10537(5)	-832(3)	-1495(2)	60(1)
C(7)	9230(4)	-360(3)	-1016(2)	49(1)
C(8)	9001(5)	732(3)	-886(2)	55(1)
C(9)	8023(5)	1076(3)	-194(2)	60(1)
C(10)	8935(5)	1308(2)	563(2)	53(1)
C(11)	9707(4)	382(2)	965(2)	41(1)
C(12)	8636(4)	-62(3)	1615(2)	49(1)
C(13)	9389(5)	-1014(3)	1955(2)	52(1)
C(14)	11066(5)	-843(3)	2240(2)	57(1)
C(15)	11456(4)	553(3)	1224(2)	46(1)
C(16)	12470(5)	829(3)	505(2)	58(1)
C(17)	11611(6)	1449(3)	1808(2)	65(1)
C(18)	6976(4)	-326(4)	1334(2)	65(1)
C(19)	10131(7)	1499(3)	-1242(2)	84(2)
C(20)	13989(5)	-1138(3)	-726(2)	63(1)
O(1)	8484(4)	694(2)	2217(1)	63(1)
O(2)	12657(3)	-2526(2)	-3(2)	54(1)
O(3)	8061(3)	203(2)	-1465(1)	74(1)

$$U_{\text{eq}} = [1/(6\pi^2)] \sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

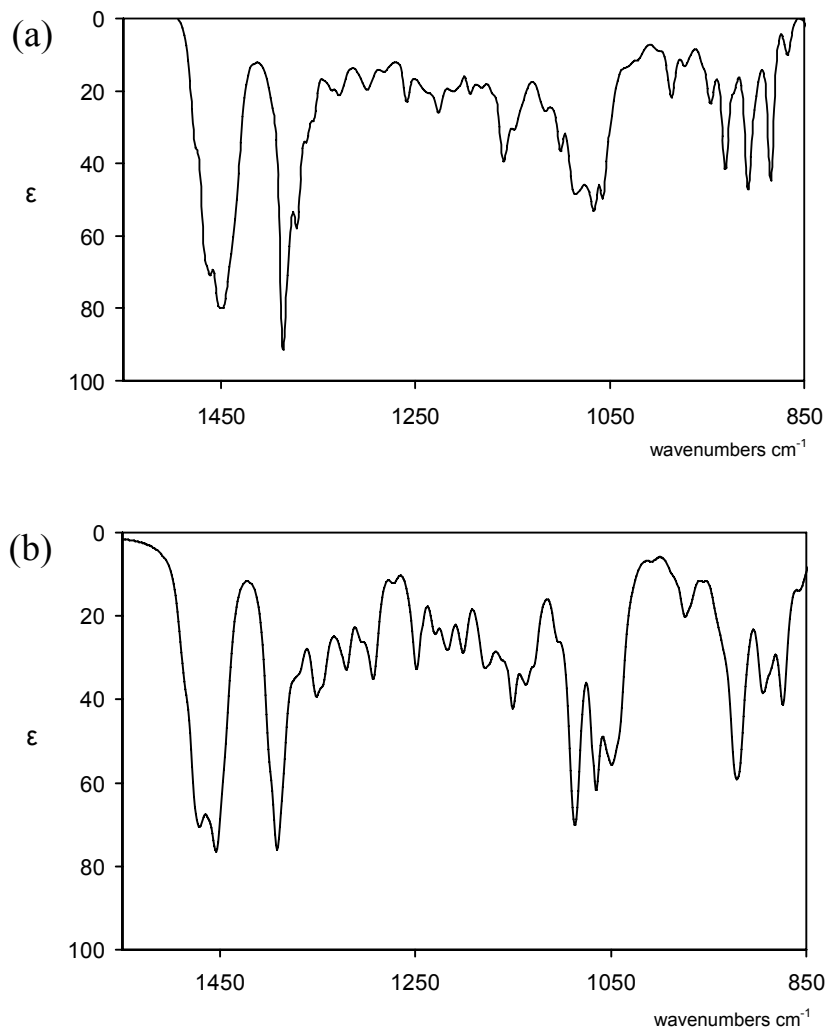


Figure 1S. (a) Experimental IR spectrum of (+)-verticillol (**1**) isolated from *Bursera suntui* and (b) B3LYP/6-31G(d,p) DFT Boltzmann-weighted IR spectra of (1*S*,11*S*,12*S*)-verticilla-3*E*,7*E*-dien-12-ol (**1**).