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Supporting information for article:

(+)-Cedrol hemihydrate: a natural product derived from drying eastern red cedar (*Juniperus virginiana*) wood

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(+)-Cedrol hemihydrate: A natural product derived from drying eastern red cedar (*Juniperus virginiana*) wood

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Supporting information

Table S1 Fractional atomic coordinates and isotropic displacement parameters (Å^2), with standard deviations in the last significant digits in parentheses. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

	x/a	*y*/b	*z*/c	*U*(eq)
Molecule 1				
O(1)	0.0778(3)	0.37262(9)	0.07694(5)	0.0533(4)
H(1)	0.182(6)	0.353(2)	0.0599(11)	0.088(10)
C(1)	0.0831(4)	0.65872(13)	0.08169(7)	0.0474(5)
C(2)	0.0810(5)	0.76594(14)	0.08433(9)	0.0649(6)
H(2A).	-0.067022	0.784586	0.092597	0.092(10)
C(3)	0.2275(6)	0.78799(17)	0.12246(9)	0.0787(8)
H(3A)	0.379064	0.789311	0.113438	0.134(16)
H(3B)	0.190034	0.847706	0.135111	0.082(9)
C(4)	0.1884(6)	0.71133(16)	0.15440(9)	0.0759(8)
H(4A)	0.051703	0.720048	0.169818	0.110(13)
H(4B)	0.306124	0.707107	0.175457	0.116(13)
C(5)	0.1804(4)	0.62575(13)	0.12536(7)	0.0491(5)
H(5)	0.330804	0.605862	0.119881	0.050(6)
C(6)	0.0485(4)	0.53953(13)	0.13939(6)	0.0487(5)
C(7)	-0.0862(3)	0.51652(12)	0.09785(6)	0.0438(4)
H(7)	-0.220609	0.484153	0.106078	0.050(6)
C(8)	0.0270(3)	0.46414(13)	0.06118(6)	0.0450(4)
C(9)	0.2351(4)	0.51310(14)	0.04771(7)	0.0515(5)
H(9A)	0.282715	0.488452	0.019803	0.062(7)
H(9B)	0.347744	0.499521	0.069016	0.050(6)
C(10)	0.2105(4)	0.61814(14)	0.04380(7)	0.0536(5)
H(10A)	0.353917	0.646474	0.042809	0.073(8)
H(10B)	0.136229	0.632797	0.016678	0.063(7)

C(11)	-0.1400(3)	0.61380(13)	0.08172(8)	0.0511(5)
H(11A)	-0.202779	0.612504	0.052644	0.057(6)
H(11B)	-0.239145	0.645456	0.101423	0.056(7)
C(12)	0.1383(9)	0.81825(19)	0.04430(11)	0.1017(14)
H(12A)	0.123814	0.883686	0.049730	0.093(9)
H(12B)	0.042073	0.800457	0.021013	0.159(19)
H(12C)	0.286056	0.804546	0.036196	0.108(14)
C(13)	-0.1111(5)	0.55957(19)	0.17635(8)	0.0747(8)
H(13A)	-0.207037	0.609122	0.167865	0.080(9)
H(13B)	-0.031748	0.577432	0.202042	0.086(9)
H(13C)	-0.195160	0.504769	0.182419	0.085(9)
C(14)	0.1981(5)	0.46415(16)	0.15599(8)	0.0631(6)
H(14A)	0.267068	0.484465	0.182472	0.085(9)
H(14B)	0.307434	0.451109	0.134393	0.057(6)
H(14C)	0.114988	0.408897	0.161654	0.079(8)
C(15)	-0.1232(5)	0.45165(16)	0.02239(8)	0.0644(6)
H(15A)	-0.261720	0.428660	0.032227	0.080(9)
H(15B)	-0.059842	0.408040	0.002334	0.098(10)
H(15C)	-0.143247	0.510335	0.008016	0.077(8)
Molecule 2				
O(2)	0.7904(3)	0.22351(10)	0.07159(5)	0.0565(4)
H(2)	0.896(6)	0.269(2)	0.0768(10)	0.092(10)
C(16)	0.7290(3)	0.03607(12)	0.17296(6)	0.0426(4)
C(17)	0.7014(4)	-0.03382(14)	0.21057(7)	0.0527(5)
H(17)	0.818646	-0.021103	0.231489	0.065(7)
C(18)	0.4923(4)	-0.00440(17)	0.23210(8)	0.0597(6)
H(18A)	0.483791	-0.027480	0.261823	0.076(8)
H(18B)	0.366689	-0.026315	0.215840	0.072(8)
C(19)	0.5064(4)	0.09999(16)	0.23125(8)	0.0610(6)
H(19A)	0.611071	0.122752	0.252454	0.075(8)

H(19B)	0.365479	0.128176	0.236915	0.103(11)
C(20)	0.5818(3)	0.11896(13)	0.18485(7)	0.0472(4)
H(20)	0.453291	0.116434	0.165871	0.052(6)
C(21)	0.7102(4)	0.20785(14)	0.17309(7)	0.0528(5)
C(22)	0.9003(3)	0.16950(13)	0.14461(7)	0.0454(4)
H(22)	0.025059	0.211966	0.145996	0.059(6)
C(23)	0.8527(3)	0.14417(13)	0.09714(6)	0.0464(5)
C(24)	0.6650(4)	0.07661(15)	0.09405(7)	0.0526(5)
H(24A)	0.665044	0.048909	0.065163	0.065(7)
H(24B)	0.529497	0.110652	0.097373	0.050(6)
C(25)	0.6721(4)	-0.00077(14)	0.12801(6)	0.0508(5)
H(25A)	0.531090	-0.031242	0.129173	0.077(8)
H(25B)	0.779546	-0.046671	0.119335	0.063(7)
C(26)	0.9524(3)	0.08041(14)	0.16943(7)	0.0465(5)
H(26A)	0.052784	0.041314	0.153241	0.058(6)
H(26B)	0.013250	0.093598	0.198019	0.061(7)
C(27)	0.7155(6)	-0.13548(16)	0.19953(10)	0.0784(8)
H(27A)	0.598905	-0.151680	0.180028	0.077(9)
H(27B)	0.703671	-0.171561	0.225801	0.091(9)
H(27C)	0.852859	-0.148095	0.185699	0.121(14)
C(28)	0.8098(6)	0.25455(19)	0.21342(9)	0.0764(8)
H(28A)	0.695210	0.275691	0.232346	0.102(11)
H(28B)	0.897010	0.306576	0.204453	0.110(12)
H(28C)	0.899540	0.210646	0.228739	0.119(13)
C(29)	0.5644(5)	0.27917(17)	0.15182(10)	0.0746(8)
H(29A)	0.458457	0.300579	0.172605	0.083(9)
H(29B)	0.491120	0.251580	0.127331	0.069(8)
H(29C)	0.650875	0.330722	0.142003	0.101(11)
C(30)	0.0536(4)	0.10505(17)	0.07512(8)	0.0618(6)
H(30A)	0.024791	0.096276	0.044569	0.084(9)

H(30B)	0.090533	0.046459	0.088172	0.082(8)
H(30C)	0.172917	0.147600	0.078635	0.073(8)
Molecule 3				
O(3)	0.3991(3)	0.28423(12)	0.02900(6)	0.0679(5)
H(31)	0.529(6)	0.261(3)	0.0381(12)	0.126(14)
H(32)	0.383(7)	0.285(3)	0.0004(11)	0.134(16)

Table S2 Anisotropic atomic displacement parameters (Å^2 x 10^3) for **1**. The anisotropic displacement factor exponent takes the form $-2(\pi^2)(U_{11}(ha^*)^2 + U_{22}(kb^*)^2 + U_{33}(lc^*)^2 + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	58(1)	36(1)	66(1)	1(1)	8(1)	2(1)
C(1)	47(1)	37(1)	57(1)	4(1)	-3(1)	0(1)
C(2)	71(2)	39(1)	86(2)	7(1)	-8(1)	-1(1)
C(3)	115(3)	47(1)	75(2)	-6(1)	-5(2)	-13(1)
C(4)	108(2)	51(1)	68(2)	-9(1)	-10(2)	-9(1)
C(5)	51(1)	43(1)	54(1)	-1(1)	-3(1)	0(1)
C(6)	56(1)	44(1)	46(1)	1(1)	3(1)	2(1)
C(7)	35(1)	41(1)	56(1)	2(1)	5(1)	0(1)
C(8)	48(1)	38(1)	50(1)	1(1)	2(1)	0(1)
C(9)	51(1)	50(1)	54(1)	0(1)	12(1)	0(1)
C(10)	57(1)	49(1)	55(1)	9(1)	5(1)	-8(1)
C(11)	42(1)	43(1)	68(1)	2(1)	-3(1)	7(1)
C(12)	166(4)	47(1)	91(2)	18(1)	-12(3)	-12(2)
C(13)	94(2)	69(2)	61(2)	-2(1)	24(1)	2(2)
C(14)	77(2)	53(1)	59(1)	10(1)	-10(1)	4(1)
C(15)	76(2)	55(1)	63(1)	-3(1)	-13(1)	-7(1)
O(2)	53(1)	52(1)	65(1)	16(1)	-9(1)	-3(1)
C(16)	40(1)	40(1)	48(1)	3(1)	-4(1)	1(1)
C(17)	54(1)	51(1)	53(1)	10(1)	-3(1)	-1(1)
C(18)	55(1)	66(1)	58(1)	13(1)	3(1)	-6(1)
C(19)	58(1)	65(1)	61(1)	1(1)	11(1)	4(1)
C(20)	41(1)	48(1)	53(1)	2(1)	2(1)	2(1)
C(21)	56(1)	40(1)	62(1)	-2(1)	5(1)	2(1)
C(22)	38(1)	42(1)	57(1)	2(1)	-4(1)	-4(1)
C(23)	44(1)	43(1)	51(1)	8(1)	-4(1)	2(1)
C(24)	53(1)	53(1)	52(1)	4(1)	-9(1)	-8(1)
C(25)	57(1)	43(1)	53(1)	1(1)	-6(1)	-9(1)
C(26)	37(1)	49(1)	53(1)	3(1)	-5(1)	2(1)
C(27)	100(2)	50(1)	86(2)	19(1)	7(2)	2(1)
C(28)	101(2)	57(1)	71(2)	-15(1)	9(2)	-18(2)
C(29)	77(2)	53(1)	94(2)	14(1)	19(2)	22(1)
C(30)	58(1)	67(1)	61(1)	6(1)	10(1)	6(1)

O(3)	66(1)	68(1)	70(1)	0(1)	8(1)	12(1)

Table S3 Compounds containing isocedrol molecule.

Compound CID	IUPAC Name
90302351	(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol;2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undec-8-ene
130455335	decan-3-ol;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
146540682	(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol;(6E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol
23623850	methoxymethane;(1S,2R,5S,7R,8R)-2,6,6,8 tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
70150719	prop-1-ene;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
88052356	chromen-2-one;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
155090752	propan-2-one;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
131722851	prop-2-enoate;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
70454270	3-prop-2-enoxyprop-1-ene;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol
89157532	bromomethane;[cyano-(3-phenoxyphenyl)methyl] (1R,3S)-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane-1-carboxylate;(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.$0^{1,5}$]undecan-8-ol

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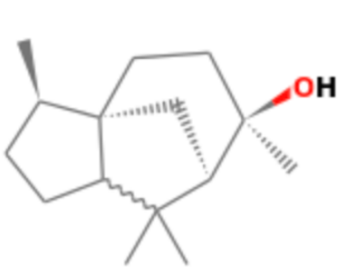
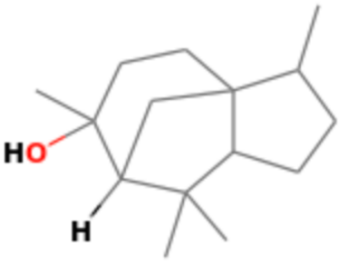
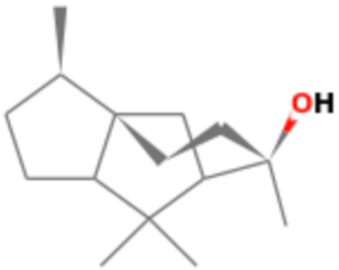
Table S4 Example isomers of cedrol (NIST Chemistry WebBook, SRM 69)



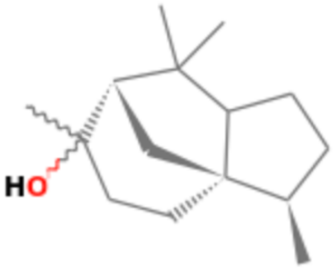
5-neo-Cedranol



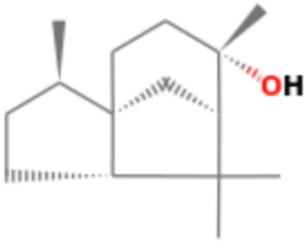
(3R,3aS,6S,7R)-3,6,8,8-Tetramethyloctahydro-1H-3a,7-methanoazulen-6-ol



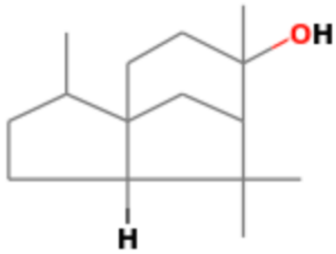
Isocedrol



Funebrol



Isocedranol



Epicedrol

Figure S1 Graph set analysis of the hydrogen bonding pattern in **1,** showing labeling scheme for the 1D spiral chain motif with the graph-set notation $C_3^3(6) > a > c > b$ in Mercury (2020). If the weak interaction between the two chains is considered, a 10-atom ring structure is formed with 5 donors and 4 acceptors along O1–H1⋯ O3 –H32⋯ $O2^{ii}$ ⋯ $H31^{ii}$–$O3^{ii}$–$H32^{ii}$ ⋯ O2–H ⋯ O1, which is consistent with the notation $R_5^4(10) > a > d > c > d > b$.

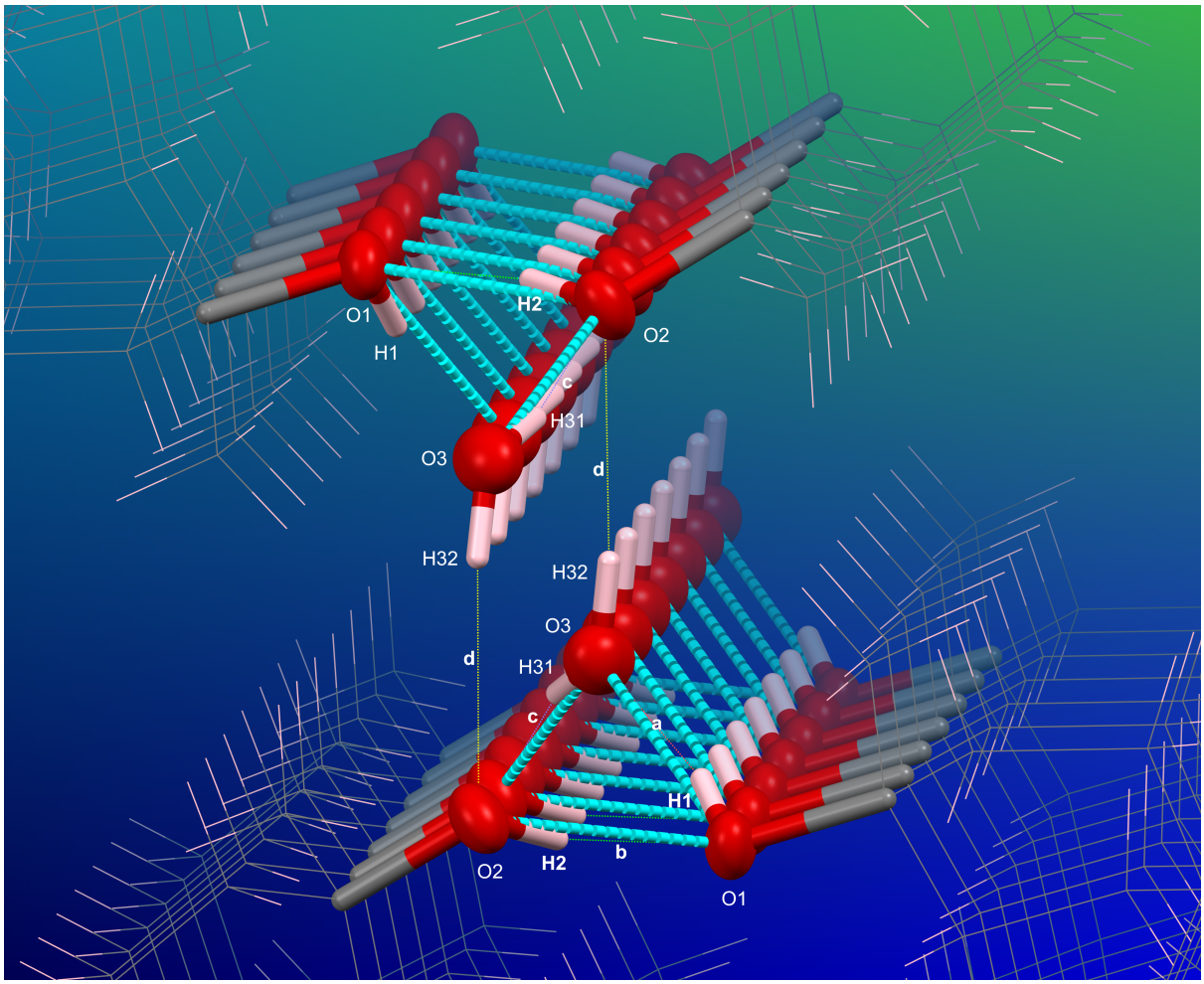
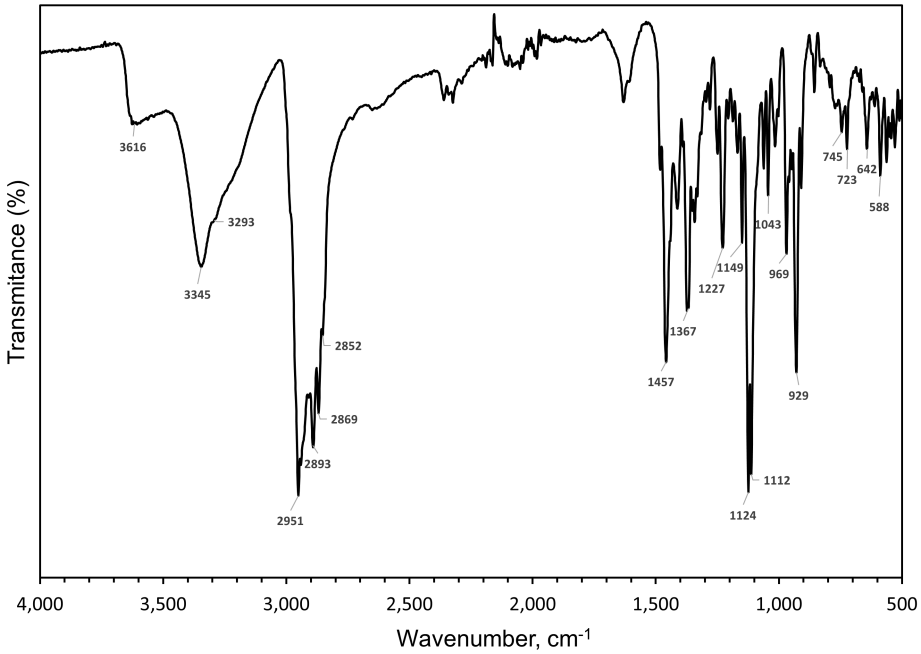


Figure S2 FT-IR spectrum of **1** recorded from a polycrystalline sample.



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