

Linalool Supplemental Material

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Chiral Tag Geometries

Table S1. Spectroscopic parameters of candidate geometries of homochiral linalool / TFPO complexes. All complexes were calculated using B3LYP D3BJ / def2-TZVP.

	Isomer1	Isomer2	Isomer3	Isomer4	Isomer5
A / MHz	554.905	531.274	521.764	527.695	525.054
B / MHz	234.979	230.534	256.107	242.878	263.904
C / MHz	202.935	197.310	202.771	206.750	230.550
μ_A / D	-2.54	-2.50	1.81	-1.96	0.76
μ_B / D	-0.68	-0.67	0.79	-0.49	0.61
μ_C / D	0.33	0.39	-0.81	-0.15	-0.77
ΔE (cm ⁻¹)	0.0*	265.3	287.3	556.6	572.9
	Isomer6	Isomer7	Isomer8	Isomer9	Isomer10
A / MHz	633.645	559.913	495.873	512.764	550.475
B / MHz	168.071	228.792	288.368	258.866	209.950
C / MHz	153.738	192.582	219.637	222.672	171.287
μ_A / D	4.81	1.14	2.54	-0.86	0.36
μ_B / D	-0.78	-0.30	0.47	0.16	-2.97
μ_C / D	0.50	-1.21	1.88	-2.02	2.53
ΔE (cm ⁻¹)	578.0	593.2	607.4	1002.5	1645.8

*-958.3989444 hartree

Table S2. Spectroscopic parameters of candidate geometries of heterochiral linalool / TFPO complexes. All complexes were calculated using B3LYP D3BJ / def2-TZVP.

	Isomer1	Isomer2	Isomer3	Isomer4	Isomer5
A / MHz	531.806	554.437	547.703	495.274	530.116
B / MHz	240.944	215.972	197.211	281.244	244.683
C / MHz	199.451	184.832	171.057	215.528	199.740
μ_A / D	2.55	-2.52	4.52	-1.27	-0.87
μ_B / D	-0.13	-0.67	0.32	-0.53	0.57
μ_C / D	-1.08	-0.09	1.95	-0.77	0.83
ΔE (cm ⁻¹)	0.0	421.6	473.6	500.9	534.9
	Isomer6	Isomer7	Isomer8	Isomer9	Isomer10
A / MHz	502.369	518.207	492.989	508.533	719.800
B / MHz	256.326	224.319	280.652	266.818	161.381
C / MHz	214.299	188.545	217.547	222.341	147.770
μ_A / D	-3.43	-2.87	-2.49	-0.05	-0.34
μ_B / D	-1.98	0.03	-0.73	0.07	0.33
μ_C / D	1.00	-1.85	-1.77	0.69	-0.21
ΔE (cm ⁻¹)	641.1	672.2	733.6	869.6	1226.3

*-958.3988105 hartree

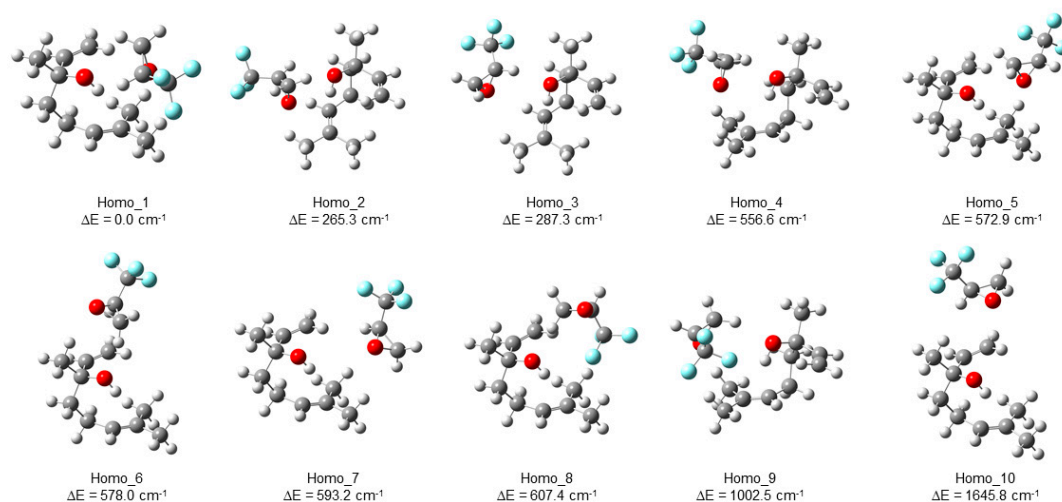


Figure S1. Optimized geometries of calculated linalool / TFPO homochiral complexes. All complexes were optimized at B3LYP-D3BJ/def2-TZVP level of theory.

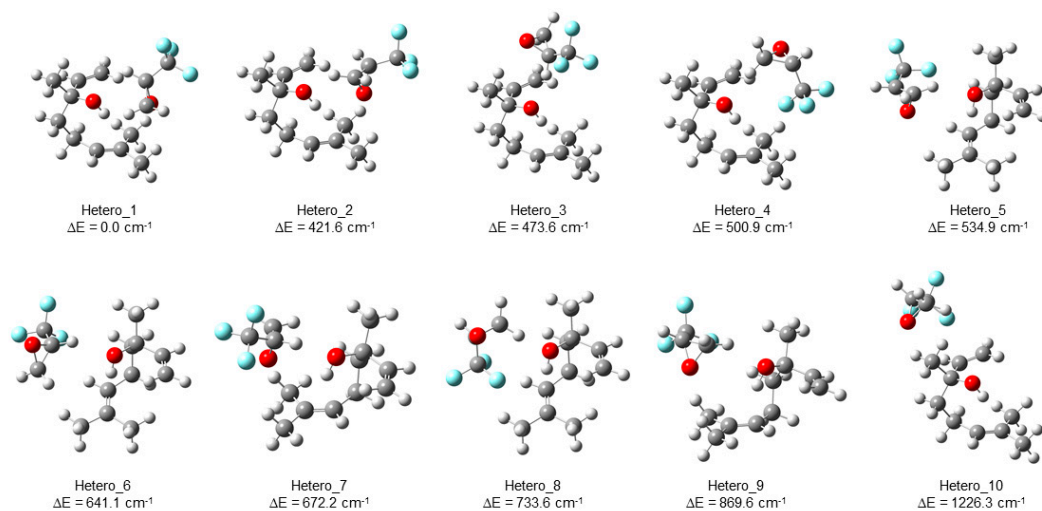


Figure S2. Optimized geometries of calculated linalool / TFPO heterochiral complexes. All complexes were optimized at B3LYP-D3BJ/def2-TZVP level of theory.

Table S3. Coordinates for optimized geometry of lowest energy linalool / TFPO homochiral complex (B3LYP-D3BJ/def2-TZVP).

Atom	Atomic Number	a-coordinate (Å)	b-coordinate (Å)	c-coordinate (Å)
1	8	-1.18186	-1.05873	-0.44091
2	6	-2.59133	-1.28004	-0.40685
3	6	-3.3256	-0.24139	-1.28141
4	6	-3.21482	1.216839	-0.8086
5	6	-2.79871	-2.68057	-0.98254
6	6	-3.12739	-1.23472	1.005516
7	6	-1.83537	1.796476	-0.93537
8	6	-1.06912	2.34681	0.012543
9	6	0.287229	2.902685	-0.32022
10	6	-1.45346	2.477536	1.458056
11	6	-2.41771	-0.9894	2.096927
12	1	-2.93303	-0.33143	-2.29811
13	1	-4.38259	-0.51772	-1.32313
14	1	-3.58279	1.296201	0.213989
15	1	-3.89439	1.812875	-1.42778
16	1	-2.44881	-2.71225	-2.01516
17	1	-2.23375	-3.40748	-0.39889
18	1	-3.85253	-2.96005	-0.95971
19	1	-4.19451	-1.42282	1.090982
20	1	-1.42757	1.764962	-1.94365
21	1	-1.01246	-0.12949	-0.22117
22	1	1.059062	2.428903	0.290364
23	1	0.326455	3.974872	-0.10365
24	1	0.539922	2.757807	-1.3704
25	1	-1.48543	3.532829	1.745978
26	1	-2.41601	2.029902	1.69063
27	1	-0.69658	2.00177	2.087335
28	1	-2.87969	-0.97578	3.075518
29	1	-1.35588	-0.78881	2.047725
30	6	1.480414	-1.4436	1.197925
31	6	1.839665	-0.69912	-0.00495
32	1	0.604547	-2.07837	1.149467
33	1	2.24637	-1.69243	1.922361
34	1	1.245352	-0.8169	-0.90479
35	6	3.263082	-0.28677	-0.27412
36	9	3.855907	-1.18267	-1.08981
37	9	4.001864	-0.19477	0.842201
38	9	3.312218	0.910747	-0.89084
39	8	1.205388	-0.03828	1.077342

Table S4. Coordinates for optimized geometry of lowest energy linalool / TFPO heterochiral complex (B3LYP-D3BJ/def2-TZVP).

Atom	Atomic Number	a-coordinate (Å)	b-coordinate (Å)	c-coordinate (Å)
1	8	1.044484	0.917417	-0.83926
2	6	2.106254	1.686579	-0.27499
3	6	3.471552	1.032593	-0.57678
4	6	3.703257	-0.34308	0.068077
5	6	2.025468	3.052032	-0.95715
6	6	1.938052	1.862306	1.216566
7	6	2.838686	-1.43425	-0.49406
8	6	1.991562	-2.24443	0.149411
9	6	1.227575	-3.305	-0.59329
10	6	1.714992	-2.20224	1.624432
11	6	0.964042	1.352664	1.955792
12	1	3.564582	0.952476	-1.66347
13	1	4.257099	1.714317	-0.23998
14	1	3.583212	-0.26313	1.148103
15	1	4.750753	-0.61288	-0.10647
16	1	2.182867	2.939789	-2.03066
17	1	1.041304	3.490375	-0.79135
18	1	2.779831	3.732166	-0.56034
19	1	2.707164	2.467851	1.689069
20	1	2.937736	-1.57488	-1.56851
21	1	1.136322	-0.00108	-0.54271
22	1	0.152472	-3.1772	-0.44525
23	1	1.483143	-4.29987	-0.21535
24	1	1.438788	-3.28269	-1.66259
25	1	1.999328	-3.15133	2.089212
26	1	2.23766	-1.39961	2.137621
27	1	0.643231	-2.07431	1.797691
28	1	0.916533	1.531543	3.021995
29	1	0.185625	0.737856	1.525089
30	6	-1.91339	0.187277	-0.48147
31	6	-1.568	-0.71656	-1.57415
32	8	-1.1773	-0.9972	-0.22071
33	1	-0.75743	-0.42604	-2.23146
34	1	-2.31896	-1.38595	-1.97596
35	1	-1.3624	1.113858	-0.3635
36	6	-3.30459	0.223853	0.093144
37	9	-3.98704	-0.91399	-0.11131
38	9	-3.27242	0.442677	1.421986
39	9	-4.00689	1.231754	-0.46408

Complex Assignments

Table S5. Spectroscopic constants determined for lowest energy linalool / TFPO heterochiral complex.

	Experimental
A / MHz	526.62456(17)
B / MHz	241.281240(95)
C / MHz	198.667830(95)
Δ_J / kHz	0.01643(15)
Δ_{JK} / kHz	0.0584(10)
δ_J / kHz	0.00331(11)
N	213
rms / kHz	7.4
$\mu_a^2 : \mu_b^2 : \mu_c^2$	1.00 : 0.05 : 0.19

Table S6. Spectroscopic constants determined for lowest energy linalool / TFPO homochiral complex.

	Experimental
A / MHz	550.2565(27)
B / MHz	236.05869(16)
C / MHz	202.98183(15)
Δ_J / kHz	0.01276(12)
Δ_{JK} / kHz	0.06520(74)
δ_J / kHz	0.00173(16)
N	161
rms / kHz	5.9
$\mu_a^2 : \mu_b^2 : \mu_c^2$	1.00 : 0.00 : 0.00

Enantiomeric Excess Calculation

Table S7. List of transitions and the relative intensity used to generate histogram analysis of (-)-Linalool / TFPO complexes.

Homochiral				Heterochiral			
Frequency (MHz)	Racemic Intensity (μ V)	Enantiopure Intensity (μ V)	Ratio	Frequency (MHz)	Racemic Intensity (μ V)	Enantiopure Intensity (μ V)	Ratio
4330.64	10.900	0.803	0.074	3973.82	9.854	17.420	1.767
4483.01	10.200	0.876	0.086	4850.5	9.331	15.980	1.713
4826.88	9.812	0.729	0.074	3982.89	8.785	15.850	1.804
5167.1	9.447	0.735	0.078	5698.7	7.873	13.200	1.676
4750.26	9.325	0.767	0.082	4368.42	7.803	14.680	1.881
4540.03	8.982	0.683	0.076	4758.12	7.682	13.050	1.699
5428.37	8.897	0.663	0.074	3569.74	7.642	13.600	1.780
3580.9	8.716	0.472	0.054	5045.36	7.605	12.870	1.692
4988.11	8.704	0.699	0.080	4418.91	7.450	12.890	1.730
4847.46	8.533	0.642	0.075	5009.55	7.405	12.940	1.747
4419.36	8.217	0.621	0.076	5277.16	7.366	12.390	1.682
4016.74	7.777	0.653	0.084	4564.56	7.269	12.640	1.739
3970.41	7.765	0.591	0.076	3153.2	7.262	14.220	1.958
4864.73	7.701	0.568	0.074	4296.84	7.149	13.290	1.858
5859.75	7.575	0.564	0.074	5519.45	7.050	12.110	1.718
5714.2	7.404	0.664	0.090	3884.25	7.044	12.700	1.803
4409.99	7.172	0.573	0.080	5427.28	6.937	11.890	1.714
4004.39	7.152	0.558	0.078	5983.09	6.770	11.700	1.728
3556.09	7.051	0.572	0.081	4705.5	6.742	11.520	1.709
3908.09	7.043	0.574	0.082	5830.96	6.735	11.590	1.720
5310.5	7.036	0.507	0.072	4446.35	6.631	11.720	1.767
5581.45	7.017	0.526	0.075	5341.68	6.382	10.310	1.616
5282.33	6.844	0.452	0.066	6115.23	6.303	10.340	1.641
3149.17	6.458	0.599	0.093	3467.3	6.287	11.150	1.773
4878.83	6.446	0.468	0.073	4887.58	6.240	10.270	1.645
5335.78	6.364	0.415	0.065	4487.82	6.209	11.150	1.796
3529.29	6.363	0.533	0.084	6078.24	6.191	10.180	1.644
6281.57	6.269	0.410	0.065	3543.2	6.172	10.990	1.781
4085.31	5.958	0.501	0.084	3210.58	6.005	11.830	1.970
3625.33	5.940	0.532	0.090	4894.81	5.847	9.626	1.646
2965.01	5.698	0.453	0.079	3604.11	5.846	9.859	1.687
5798.03	5.695	0.461	0.081	4491.12	5.828	10.440	1.792
6199.93	5.570	0.426	0.076	5785.84	5.713	9.321	1.631
3482.58	5.527	0.357	0.065	6078.52	5.486	8.953	1.632

3368.09	5.502	0.385	0.070	5416.51	5.440	8.794	1.617
6142.83	5.290	0.381	0.072	4132.15	5.358	10.060	1.878

Transition Frequencies

Table S8. Measured rotational transitions (ν_{obs} , MHz) of linalool / TFPO heterochiral complex and residuals ($\nu_{\text{obs}} - \nu_{\text{calc}}$, MHz).

J'	K _a '	K _c '	←	J''	K _a ''	K _c ''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{calc}}$
5	1	5	←	4	1	4	2076.6256	0.0004
5	0	5	←	4	0	4	2122.7343	-0.0005
5	2	4	←	4	2	3	2189.9097	-0.0003
5	3	3	←	4	3	2	2212.1468	0.0040
5	3	2	←	4	3	1	2218.0764	-0.0030
5	2	3	←	4	2	2	2266.7894	0.0017
5	1	4	←	4	1	3	2283.7528	0.0013
6	1	6	←	5	1	5	2483.6437	0.0019
6	0	6	←	5	0	5	2519.5715	-0.0056
6	2	5	←	5	2	4	2619.9135	0.0000
6	3	4	←	5	3	3	2656.7585	-0.0001
6	3	3	←	5	3	2	2672.1406	-0.0021
6	1	5	←	5	1	4	2723.9262	0.0013
6	2	4	←	5	2	3	2739.4608	0.0006
7	1	7	←	6	1	6	2887.9064	0.0055
7	0	7	←	6	0	6	2913.0204	-0.0111
7	2	6	←	6	2	5	3045.8253	0.0008
5	2	3	←	4	1	3	3046.3593	-0.0051
7	3	5	←	6	3	4	3100.7991	0.0020
7	4	4	←	6	4	3	3100.9584	0.0093
7	4	3	←	6	4	2	3102.7746	-0.0029
7	3	4	←	6	3	3	3133.7449	-0.0008
7	1	6	←	6	1	5	3153.1953	0.0001
7	2	5	←	6	2	4	3210.5861	0.0012
4	3	1	←	3	2	1	3283.9105	-0.0009
8	1	8	←	7	1	7	3289.8912	-0.0264
8	0	8	←	7	0	7	3306.1497	0.0086
8	2	7	←	7	2	6	3467.3037	0.0015
6	2	4	←	5	1	4	3502.0763	0.0032
8	7	1	←	7	7	0	3533.3448	-0.0033
8	6	2	←	7	6	1	3536.2986	-0.0067
8	3	6	←	7	3	5	3543.2031	0.0022
8	4	5	←	7	4	4	3548.6712	0.0039
8	4	4	←	7	4	3	3553.5877	0.0001
8	1	7	←	7	1	6	3569.7396	-0.0009
8	3	5	←	7	3	4	3604.1070	0.0008
8	2	6	←	7	2	5	3675.7981	0.0012

9	1	9	←	8	1	8	3690.2838	0.0285
9	0	9	←	8	0	8	3700.1466	-0.0035
5	3	2	←	4	2	2	3704.0173	-0.0010
5	3	3	←	4	2	3	3759.5170	-0.0050
6	2	5	←	5	1	5	3873.4397	-0.0035
9	2	8	←	8	2	7	3884.2507	0.0022
9	1	8	←	8	1	7	3973.8165	-0.0006
9	7	2	←	8	7	1	3977.3686	-0.0046
9	6	4	←	8	6	3	3981.5867	0.0026
9	3	7	←	8	3	6	3982.8959	0.0020
9	5	5	←	8	5	4	3988.5280	0.0012
9	5	4	←	8	5	3	3989.0561	-0.0013
9	4	6	←	8	4	5	3997.3467	0.0032
9	4	5	←	8	4	4	4008.7674	-0.0046
9	3	6	←	8	3	5	4082.3031	0.0004
10	1	10	←	9	1	9	4089.4221	-0.0002
10	0	10	←	9	0	9	4095.2170	-0.0015
6	3	3	←	5	2	3	4109.3712	-0.0021
9	2	7	←	8	2	6	4132.1517	0.0008
6	3	4	←	5	2	4	4226.3640	-0.0067
10	2	9	←	9	2	8	4296.8411	0.0035
5	4	1	←	4	3	1	4346.9881	-0.0025
5	4	2	←	4	3	2	4348.8609	-0.0008
10	1	9	←	9	1	8	4368.4182	0.0000
10	3	8	←	9	3	7	4418.9171	0.0046
10	7	4	←	9	7	3	4422.2333	-0.0026
10	6	5	←	9	6	4	4428.0410	0.0209
10	5	6	←	9	5	5	4437.3104	0.0081
10	5	5	←	9	5	4	4438.7601	-0.0006
10	4	7	←	9	4	6	4446.3533	0.0022
10	4	6	←	9	4	5	4469.9486	-0.0007
11	1	11	←	10	1	10	4487.8207	-0.0012
11	0	11	←	10	0	10	4491.1175	-0.0010
7	3	4	←	6	2	4	4503.6548	-0.0040
8	2	6	←	7	1	6	4511.3324	-0.0026
10	3	7	←	9	3	6	4564.5655	0.0008
10	2	8	←	9	2	7	4577.4057	0.0070
11	2	10	←	10	2	9	4705.5024	0.0057
7	3	5	←	6	2	5	4707.2507	-0.0036
11	1	10	←	10	1	9	4758.1141	-0.0045
6	4	2	←	5	3	2	4784.0047	-0.0042
6	4	3	←	5	3	3	4791.2523	-0.0081
11	3	9	←	10	3	8	4850.5011	0.0026
11	9	3	←	10	9	2	4859.7282	-0.0047

11	8	4	←	10	8	3	4863.0974	0.0058
11	7	5	←	10	7	4	4868.0359	0.0003
12	1	12	←	11	1	11	4885.7415	-0.0023
12	0	12	←	11	0	11	4887.5792	0.0016
11	5	6	←	10	5	5	4891.1220	0.0223
11	4	8	←	10	4	7	4894.8145	0.0024
8	3	5	←	7	2	5	4897.1756	-0.0046
11	4	7	←	10	4	6	4938.8405	-0.0005
11	2	9	←	10	2	8	5009.5543	0.0011
11	3	8	←	10	3	7	5045.3569	0.0012
9	2	7	←	8	1	7	5073.7478	0.0026
12	2	11	←	11	2	10	5110.8473	0.0113
12	1	11	←	11	1	10	5146.8904	-0.0106
8	3	6	←	7	2	6	5204.6290	-0.0017
7	4	3	←	6	3	3	5214.6326	-0.0112
7	4	4	←	6	3	4	5235.4512	0.0003
12	3	10	←	11	3	9	5277.1635	0.0040
13	1	13	←	12	1	12	5283.3722	-0.0088
13	0	13	←	12	0	12	5284.3796	-0.0035
12	8	5	←	11	8	4	5308.4330	-0.0035
12	7	6	←	11	7	5	5314.8801	0.0057
12	5	8	←	11	5	7	5339.0807	0.0068
12	5	7	←	11	5	6	5346.9181	-0.0053
6	5	1	←	5	4	1	5401.3789	0.0053
6	5	2	←	5	4	2	5401.4988	-0.0066
12	4	8	←	11	4	7	5416.5123	-0.0011
12	2	10	←	11	2	9	5427.2838	0.0003
13	2	12	←	12	2	11	5513.5210	-0.0268
12	3	9	←	11	3	8	5519.4550	0.0000
13	1	12	←	12	1	11	5536.9206	-0.0243
8	4	4	←	7	3	4	5634.4871	0.0015
10	2	8	←	9	1	8	5677.3346	0.0078
14	1	14	←	13	1	13	5680.8511	-0.0032
14	0	14	←	13	0	13	5681.3894	-0.0050
8	4	5	←	7	3	5	5683.3155	-0.0055
13	3	11	←	12	3	10	5698.7079	0.0063
9	3	7	←	8	2	7	5720.2175	-0.0049
10	3	7	←	9	2	7	5736.0953	-0.0045
13	8	6	←	12	8	5	5754.6416	0.0010
13	7	7	←	12	7	6	5762.8749	0.0179
13	6	8	←	12	6	7	5775.4629	0.0039
13	6	7	←	12	6	6	5776.4978	-0.0001
13	4	10	←	12	4	9	5785.8406	0.0025
13	5	9	←	12	5	8	5791.5127	0.0105

13	5	8	←	12	5	7	5807.4263	-0.0020
13	2	11	←	12	2	10	5830.9661	0.0016
13	4	9	←	12	4	8	5902.1902	-0.0016
14	1	13	←	13	1	12	5928.8645	-0.0004
13	3	10	←	12	3	9	5983.0873	0.0001
6	6	0	←	5	5	0	6013.5148	0.0067
9	4	5	←	8	3	5	6039.1484	-0.0030
15	1	15	←	14	1	14	6078.2287	-0.0073
15	0	15	←	14	0	14	6078.5096	-0.0141
14	3	12	←	13	3	11	6115.2420	0.0073
9	4	6	←	8	3	6	6137.4592	-0.0045
14	8	6	←	13	8	5	6201.7883	0.0008
14	2	12	←	13	2	11	6223.4665	0.0022
14	4	11	←	13	4	10	6226.2663	0.0032
14	6	9	←	13	6	8	6227.5658	-0.0085
14	6	8	←	13	6	7	6229.9580	-0.0161
14	5	10	←	13	5	9	6244.2103	0.0031
10	3	8	←	9	2	8	6254.8825	-0.0038
14	5	9	←	13	5	8	6274.1463	-0.0031
8	5	3	←	7	4	3	6280.3268	0.0038
8	5	4	←	7	4	4	6282.6308	-0.0016
15	2	14	←	14	2	13	6313.7007	0.0039
15	1	14	←	14	1	13	6322.4746	0.0033
14	4	10	←	13	4	9	6392.4108	-0.0037
10	4	6	←	9	3	6	6426.7956	-0.0026
14	3	11	←	13	3	10	6433.6828	-0.0005
7	6	2	←	6	5	2	6454.7761	0.0020
10	4	7	←	9	3	7	6600.9139	-0.0069
15	10	5	←	14	10	4	6635.2487	-0.0047
15	9	7	←	14	9	6	6641.3390	-0.0033
15	8	8	←	14	8	7	6649.9579	0.0074
15	6	10	←	14	6	9	6681.1408	0.0047
15	6	9	←	14	6	8	6686.2755	-0.0082
15	5	11	←	14	5	10	6696.3409	0.0021
16	2	15	←	15	2	14	6712.1839	0.0056
12	3	9	←	11	2	9	6713.9538	-0.0048
9	5	4	←	8	4	4	6715.7928	0.0000
16	1	15	←	15	1	14	6717.3336	-0.0032
9	5	5	←	8	4	5	6722.4837	-0.0082
15	5	10	←	14	5	9	6748.7167	-0.0042
11	4	7	←	10	3	7	6801.0738	-0.0006
11	3	9	←	10	2	9	6808.5454	-0.0018
15	3	12	←	14	3	11	6869.3494	0.0002
15	4	11	←	14	4	10	6881.6047	-0.0052

16	3	14	←	15	3	13	6935.0518	0.0130
12	2	10	←	11	1	10	6987.6378	0.0112
16	2	14	←	15	2	13	6993.8019	-0.0028
16	11	6	←	15	11	5	7075.8636	-0.0043
11	4	8	←	10	3	8	7076.8112	-0.0093
16	9	7	←	15	9	6	7088.7246	-0.0007
16	4	13	←	15	4	12	7092.7519	0.0059
17	2	16	←	16	2	15	7110.0913	0.0051
17	1	16	←	16	1	15	7113.0632	0.0040
16	6	11	←	15	6	10	7135.9393	0.0028
16	6	10	←	15	6	9	7146.2669	-0.0067
16	5	12	←	15	5	11	7146.8758	0.0017
12	4	8	←	11	3	8	7172.2295	-0.0027
16	5	11	←	15	5	10	7232.2083	-0.0082
16	3	13	←	15	3	12	7288.9400	0.0041
17	3	15	←	16	3	14	7339.6534	0.0194
16	4	12	←	15	4	11	7363.9430	-0.0052
18	2	17	←	17	2	16	7507.6664	0.0173
8	7	1	←	7	6	1	7508.0491	0.0170
18	1	17	←	17	1	16	7509.3370	0.0024
17	4	14	←	16	4	13	7517.9290	0.0103
17	9	9	←	16	9	8	7537.0271	-0.0020
13	4	9	←	12	3	9	7554.9659	-0.0031
11	5	6	←	10	4	6	7566.9393	0.0075
12	4	9	←	11	3	9	7567.9960	-0.0023
17	7	11	←	16	7	10	7568.2378	0.0108
17	7	10	←	16	7	9	7569.7742	-0.0077
17	6	12	←	16	6	11	7591.5857	0.0032
17	5	13	←	16	5	12	7594.7272	0.0156
11	5	7	←	10	4	7	7603.6422	-0.0024
17	6	11	←	16	6	10	7611.1171	-0.0028
19	0	19	←	18	0	18	7667.4383	-0.0248
17	3	14	←	16	3	13	7692.8328	0.0060
17	5	12	←	16	5	11	7724.0619	-0.0096
18	3	16	←	17	3	15	7741.6767	-0.0022
17	4	13	←	16	4	12	7834.8583	-0.0049
14	3	11	←	13	2	11	7872.4732	-0.0082
19	1	18	←	18	1	17	7905.9616	0.0051
18	4	15	←	17	4	14	7937.6554	0.0123
9	7	2	←	8	6	2	7949.1239	0.0239
14	4	10	←	13	3	10	7964.2874	-0.0090
12	5	7	←	11	4	7	7975.0200	0.0057
18	10	9	←	17	10	8	7975.6669	-0.0083
18	9	9	←	17	9	8	7986.3243	-0.0114

Table S9. Measured rotational transitions (ν_{obs} , MHz) of linalool / TFPO homochiral complex and residuals ($\nu_{\text{obs}} - \nu_{\text{calc}}$, MHz).

J'	K _a '	K _c '	←	J''	K _a ''	K _c ''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{calc}}$
5	1	5	←	4	1	4	2102.8239	0.0035
5	2	4	←	4	2	3	2189.6942	0.0008
5	3	3	←	4	3	2	2202.5533	0.0063
5	3	2	←	4	3	1	2204.9605	-0.0002
5	2	3	←	4	2	2	2235.4789	-0.0006
5	1	4	←	4	1	3	2265.7901	0.0011
6	1	6	←	5	1	5	2518.2038	0.0021
6	0	6	←	5	0	5	2559.6024	-0.0012
6	2	5	←	5	2	4	2623.1298	0.0005
6	3	4	←	5	3	3	2644.8252	0.0060
6	3	3	←	5	3	2	2651.1792	0.0150
6	2	4	←	5	2	3	2697.5976	0.0017
6	1	5	←	5	1	4	2710.3150	0.0016
7	1	7	←	6	1	6	2931.5787	0.0030
7	0	7	←	6	0	6	2965.0127	-0.0023
7	2	6	←	6	2	5	3054.1873	0.0005
7	5	2	←	6	5	1	3082.0538	-0.0077
7	4	4	←	6	4	3	3085.3749	-0.0008
7	4	3	←	6	4	2	3085.9107	-0.0007
7	3	5	←	6	3	4	3087.2369	0.0032
7	3	4	←	6	3	3	3101.1625	-0.0032
7	1	6	←	6	1	5	3149.1686	0.0003
7	2	5	←	6	2	4	3161.9006	-0.0015
8	1	8	←	7	1	7	3343.1376	0.0067
8	0	8	←	7	0	7	3368.0828	-0.0062
8	2	7	←	7	2	6	3482.5767	0.0007
8	6	2	←	7	6	1	3521.6216	-0.0043
8	5	4	←	7	5	3	3524.4206	0.0142
8	4	5	←	7	4	4	3529.0929	0.0050
8	3	6	←	7	3	5	3529.2951	0.0023
8	4	4	←	7	4	3	3530.5449	0.0000
8	3	5	←	7	3	4	3556.0918	-0.0012
8	1	7	←	7	1	6	3580.9046	0.0007
8	2	6	←	7	2	5	3625.3274	0.0000
9	1	9	←	8	1	8	3753.1577	0.0122
9	2	8	←	8	2	7	3908.0931	0.0002

9	8	1	←	8	8	0	3959.7528	-0.0114
9	7	3	←	8	7	2	3961.2794	0.0000
9	6	4	←	8	6	3	3963.6301	-0.0041
9	3	7	←	8	3	6	3970.4157	0.0010
9	4	6	←	8	4	5	3973.6717	-0.0063
9	4	5	←	8	4	4	3977.1139	-0.0051
9	1	8	←	8	1	7	4004.3882	-0.0002
9	3	6	←	8	3	5	4016.7398	-0.0014
9	2	7	←	8	2	6	4085.3095	-0.0005
10	1	10	←	9	1	9	4161.9357	0.0043
10	0	10	←	9	0	9	4173.6529	-0.0279
10	2	9	←	9	2	8	4330.6446	0.0012
10	8	2	←	9	8	1	4400.9731	-0.0038
10	7	3	←	9	7	2	4403.0512	-0.0018
10	6	5	←	9	6	4	4406.2863	0.0017
10	3	8	←	9	3	7	4409.9958	0.0008
10	5	6	←	9	5	5	4411.6378	-0.0032
10	5	5	←	9	5	4	4411.9514	-0.0004
10	1	9	←	9	1	8	4419.3638	0.0006
10	4	6	←	9	4	5	4426.2685	-0.0041
10	3	7	←	9	3	6	4483.0056	-0.0014
10	2	8	←	9	2	7	4540.0248	-0.0004
11	1	11	←	10	1	10	4569.7879	-0.0015
11	0	11	←	10	0	10	4577.4061	0.0023
11	2	10	←	10	2	9	4750.2626	0.0022
11	1	10	←	10	1	9	4826.8816	0.0002
11	9	2	←	10	9	1	4840.6929	-0.0047
11	8	4	←	10	8	3	4842.5805	-0.0018
11	7	5	←	10	7	4	4845.3431	-0.0019
11	3	9	←	10	3	8	4847.4639	0.0008
11	6	6	←	10	6	5	4849.6600	0.0101
11	5	7	←	10	5	6	4856.6682	0.0030
11	5	6	←	10	5	5	4857.4323	0.0000
11	4	8	←	10	4	7	4864.7358	0.0030
11	4	7	←	10	4	6	4878.8316	-0.0030
11	3	8	←	10	3	7	4953.4293	-0.0013
12	1	12	←	11	1	11	4976.9778	-0.0014
12	0	12	←	11	0	11	4981.7867	-0.0015
11	2	9	←	10	2	8	4988.1102	0.0001
12	2	11	←	11	2	10	5167.1068	0.0025
12	1	11	←	11	1	10	5229.1754	-0.0018
12	3	10	←	11	3	9	5282.3277	0.0015
12	8	4	←	11	8	3	5284.6195	-0.0011
12	7	6	←	11	7	5	5288.2103	0.0001

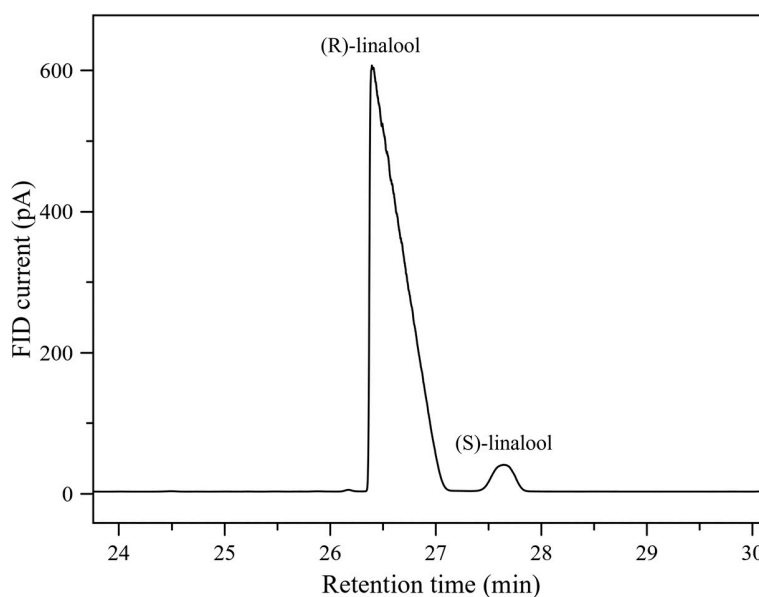
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12	5	7	←	11	5	6	5304.3924	0.0000
12	4	9	←	11	4	8	5310.4998	0.0017
12	4	8	←	11	4	7	5335.7735	-0.0022
13	1	13	←	12	1	12	5383.7045	-0.0028
13	0	13	←	12	0	12	5386.6821	-0.0025
12	3	9	←	11	3	8	5425.2993	-0.0019
12	2	10	←	11	2	9	5428.3741	0.0011
13	2	12	←	12	2	11	5581.4502	0.0038
13	1	12	←	12	1	11	5628.8760	-0.0041
13	3	11	←	12	3	10	5714.2032	0.0021
13	10	3	←	12	10	2	5721.8053	-0.0026
13	9	5	←	12	9	4	5724.0258	0.0005
13	8	6	←	12	8	5	5727.1331	0.0001
13	7	7	←	12	7	6	5731.7060	0.0018
13	5	8	←	12	5	7	5753.1902	-0.0068
13	4	10	←	12	4	9	5755.7630	0.0014
14	1	14	←	13	1	13	5790.1244	-0.0030
14	0	14	←	13	0	13	5791.9382	-0.0037
13	4	9	←	12	4	8	5798.0248	-0.0016
13	2	11	←	12	2	10	5859.7515	0.0012
13	3	10	←	12	3	9	5895.4092	-0.0009
14	2	13	←	13	2	12	5993.6424	0.0067
14	1	13	←	13	1	12	6028.1121	-0.0121
14	3	12	←	13	3	11	6142.8341	-0.0005
14	11	3	←	13	11	2	6161.4668	0.0052
14	10	4	←	13	10	3	6163.5063	-0.0037
14	9	5	←	13	9	4	6166.2787	0.0015
14	8	7	←	13	8	6	6170.1605	-0.0008
14	7	8	←	13	7	7	6175.8904	0.0057
15	1	15	←	14	1	14	6196.3405	-0.0074
14	5	9	←	13	5	8	6204.3389	-0.0096
14	4	10	←	13	4	9	6266.1027	-0.0031
14	2	12	←	13	2	11	6281.5678	0.0005
14	3	11	←	13	3	10	6360.9013	-0.0009
15	2	14	←	14	2	13	6404.0744	0.0172
15	1	14	←	14	1	13	6428.1675	0.0251
15	3	13	←	14	3	12	6568.1155	-0.0001
16	1	16	←	15	1	15	6602.4333	-0.0091
16	0	16	←	15	0	15	6603.0861	-0.0061
15	9	6	←	14	9	5	6608.9624	-0.0019
15	8	7	←	14	8	6	6613.7510	0.0009
15	7	9	←	14	7	8	6620.8051	-0.0053
15	6	10	←	14	6	9	6631.6535	-0.0012

15	6	9	←	14	6	8	6632.4832	0.0041
15	4	12	←	14	4	11	6642.3864	0.0001
15	5	11	←	14	5	10	6645.7714	0.0000
15	2	13	←	14	2	12	6694.0005	0.0008
15	4	11	←	14	4	10	6739.6115	-0.0030
16	2	15	←	15	2	14	6813.1002	0.0086
15	3	12	←	14	3	11	6819.6512	0.0011
16	3	14	←	15	3	13	6990.0787	0.0010
17	1	17	←	16	1	16	7008.4797	0.0211
16	11	5	←	15	11	4	7044.9413	0.0042
16	10	6	←	15	10	5	7047.9877	0.0000
16	9	7	←	15	9	6	7052.1204	0.0001
16	8	9	←	15	8	8	7057.9422	0.0012
16	6	11	←	15	6	10	7079.5511	0.0015
16	6	10	←	15	6	9	7081.2662	0.0227
16	4	13	←	15	4	12	7082.5421	-0.0011
16	5	12	←	15	5	11	7094.4423	0.0007
16	2	14	←	15	2	13	7098.4284	-0.0016
16	5	11	←	15	5	10	7116.5347	-0.0039
16	4	12	←	15	4	11	7216.8566	0.0012
17	2	16	←	16	2	15	7221.0801	-0.0027
16	3	13	←	15	3	12	7270.1309	-0.0040
17	3	15	←	16	3	14	7408.8909	0.0006
17	2	15	←	16	2	14	7497.3111	-0.0019
17	8	9	←	16	8	8	7502.7839	-0.0056
17	4	14	←	16	4	13	7519.8863	-0.0012
17	6	11	←	16	6	10	7531.7067	-0.0086
17	5	13	←	16	5	12	7542.9609	0.0004
17	5	12	←	16	5	11	7579.3450	-0.0031
18	2	17	←	17	2	16	7628.3122	-0.0089
18	1	17	←	17	1	16	7635.2586	-0.0058
17	4	13	←	16	4	12	7694.9497	0.0014
17	3	14	←	16	3	13	7711.1945	-0.0001
18	2	16	←	17	2	15	7893.4667	-0.0070
18	4	15	←	17	4	14	7954.0152	-0.0011
18	6	13	←	17	6	12	7978.1919	0.0140
18	5	14	←	17	5	13	7990.7924	-0.0039

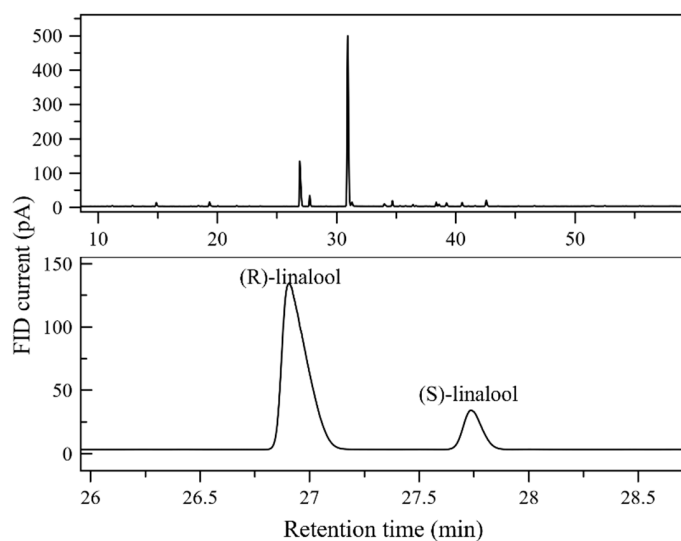
Chiral GC Measurements

The EE of linalool in the Aldrich standard, and two essential oils, was also measured using an Agilent 8890 gas chromatograph with a FID detector. The method parameters were as follows:

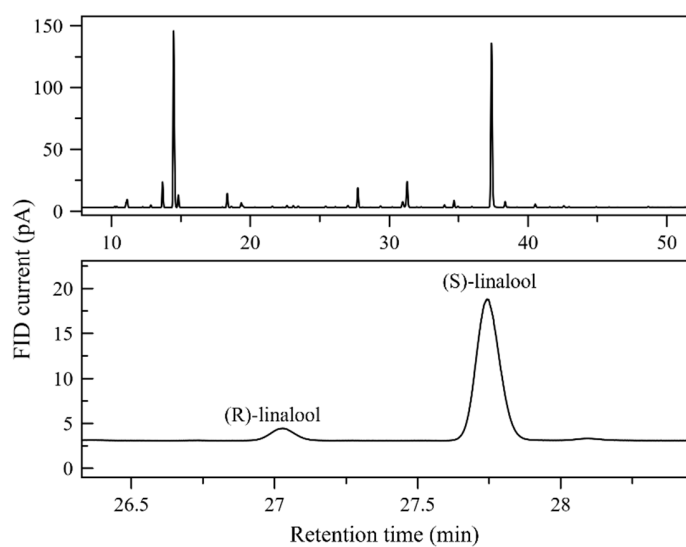
Column	Restek RT-BDEXse (30 m, 0.32 mm ID, 0.25 μ m film thickness)
Sample preparation	Diluted approximately 1:100 (v/v) in dichloromethane
Injection volume	2 μ L
Inlet temperature	275°C
Inlet mode	Split, 50:1, 3mL/min septum purge flow
Carrier gas velocity	80 cm/sec
Carrier gas	He
Oven temperature	40°C, increased by 2°C/min to 230°C
Detector temperature	325°C



Chromatogram of the Aldrich linalool standard.



Chromatogram of clary sage oil.



Chromatogram of cardamom essential oil.

Results:

Sample	Enantiomeric Excess (%R-%S)
Aldrich (-)-Linalool standard	92.01% (Average of 3 runs)
Clary sage oil	69.39%
Cardamom essential oil	-83.57%