Supplementary information for:

Sniffing out camphor: the fine balance between hydrogen bonding and London dispersion in the chirality recognition with α-fenchol

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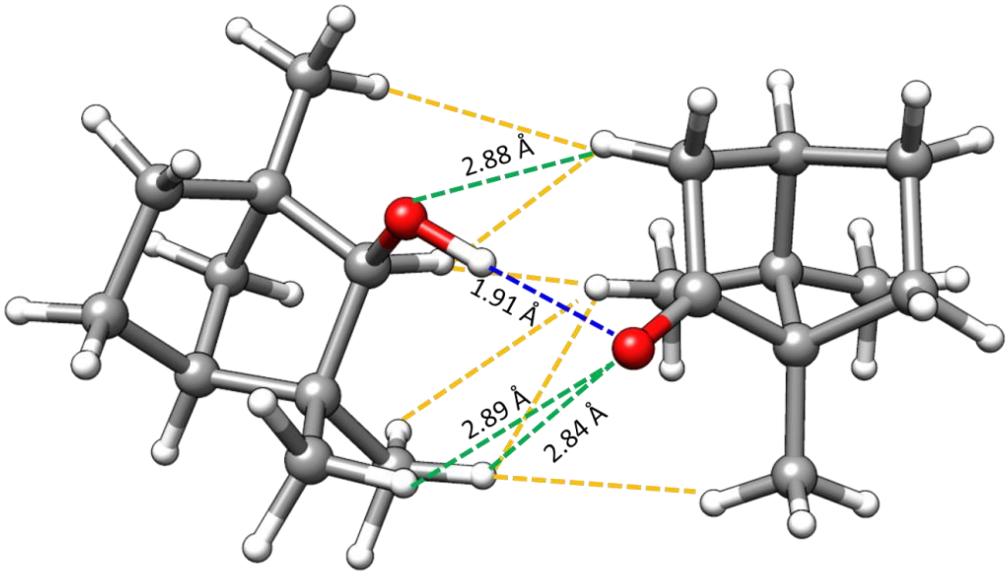
Contents:

Figure S1. *RR*-A-a-(I) and *SR*-A-b-(I) structures highlighting the main interactions between them.

***RR*-A-a-(I)**



***SR*-A-b-(I)**

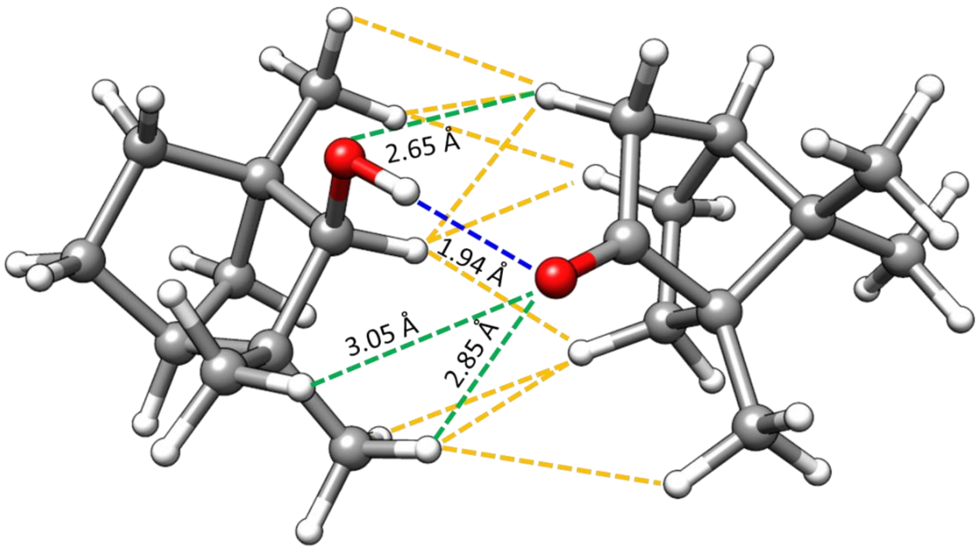
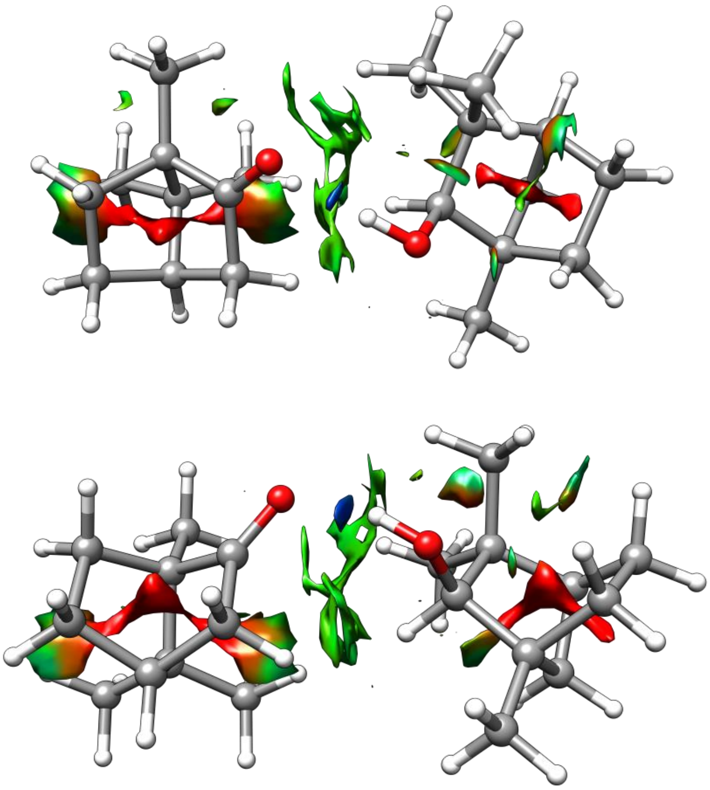
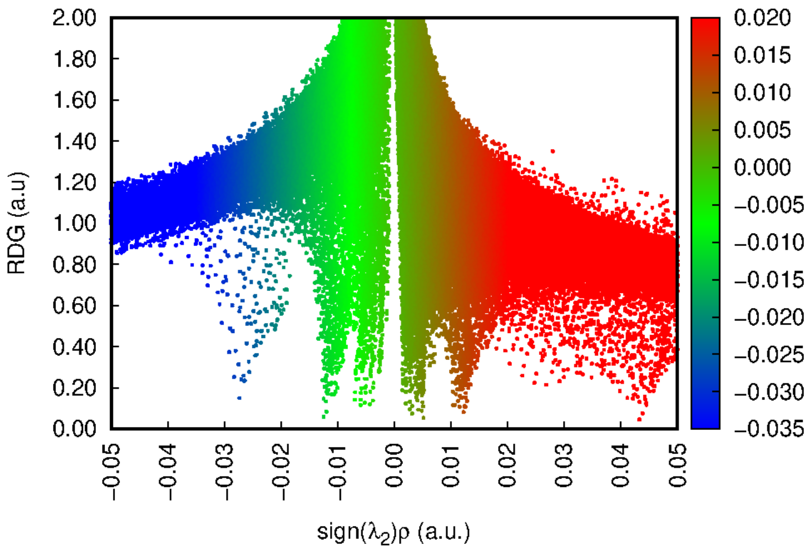


Figure S2. NCI plots and scatter graphs for the *RR* and *SR* complexes below 2.0 kJ/mol.

***RR*-A-a-(I)**





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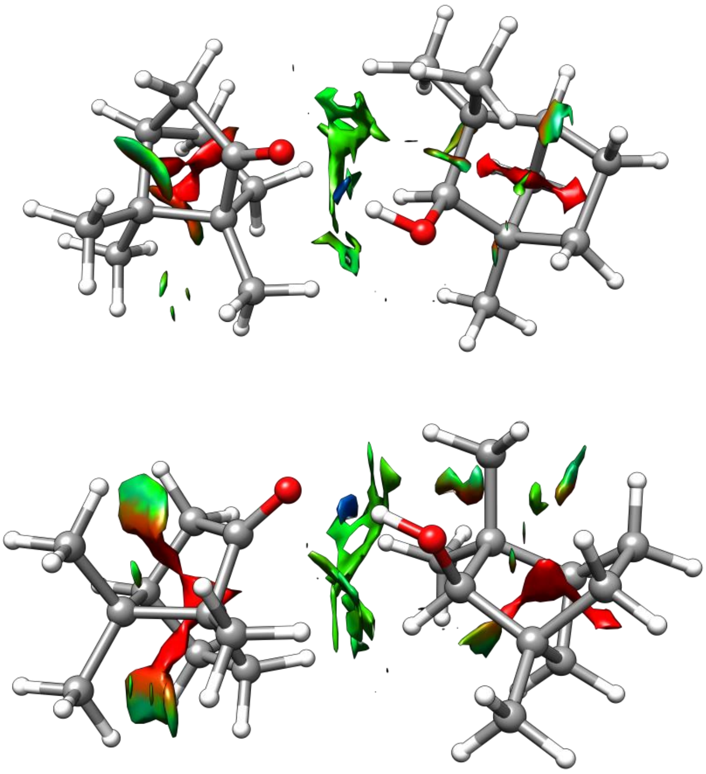
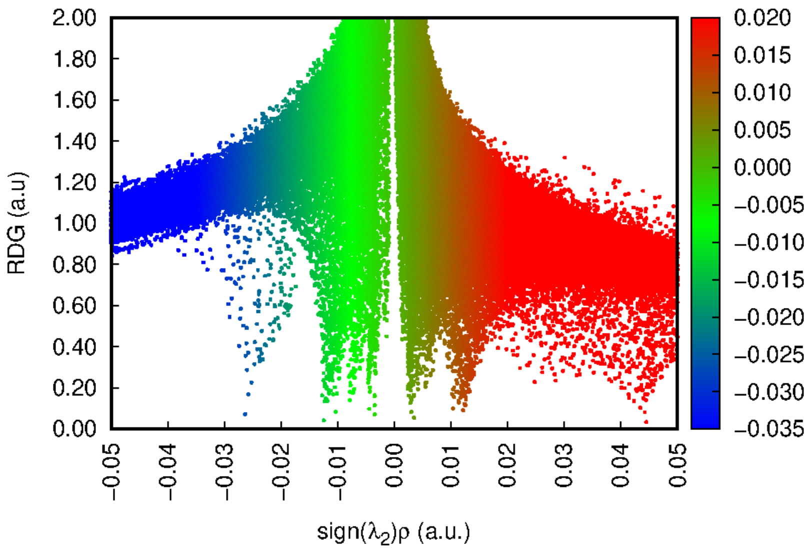
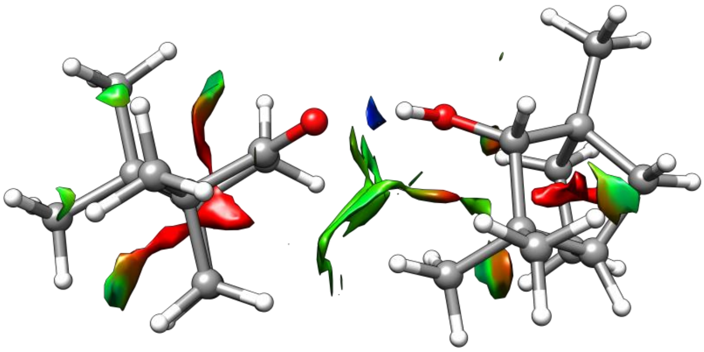
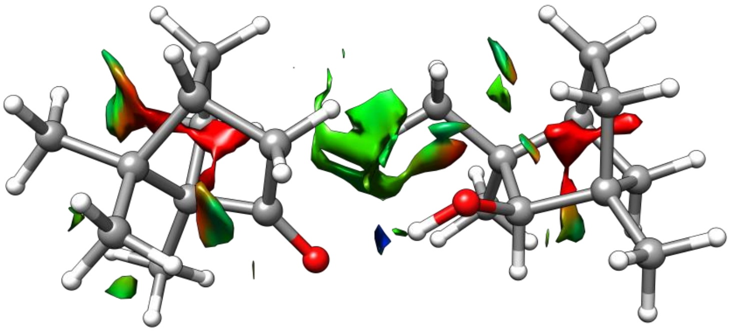
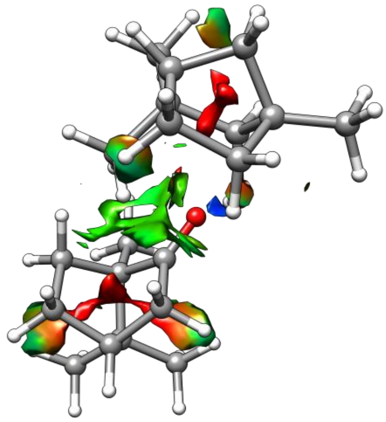


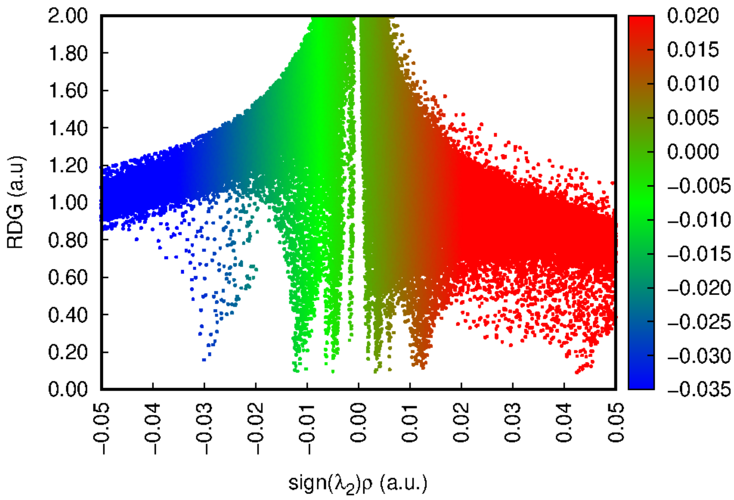

RDG (a.u)
sign(λ2)ρ (a.u.)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

***RR*-A-b-(III)**

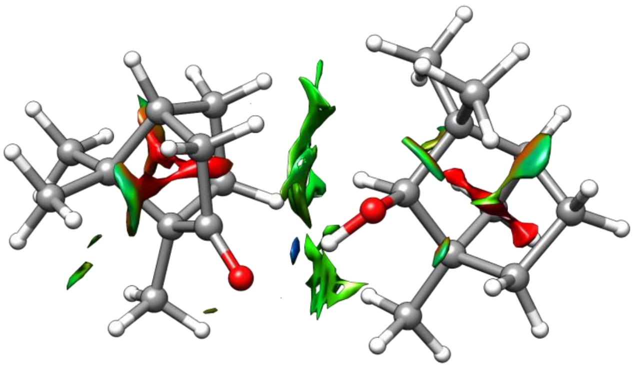


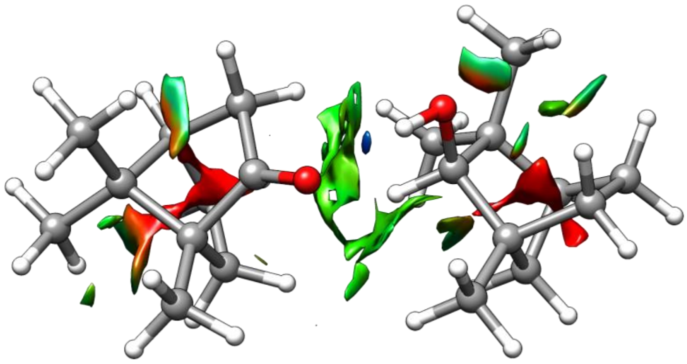


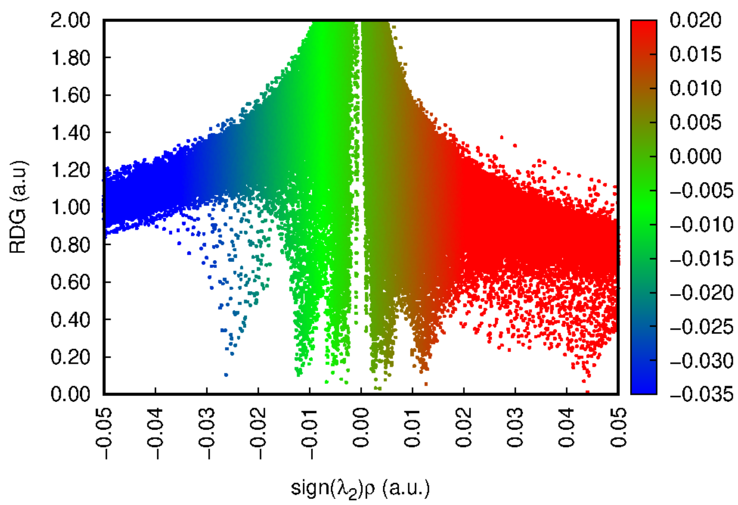



RDG (a.u)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ_2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

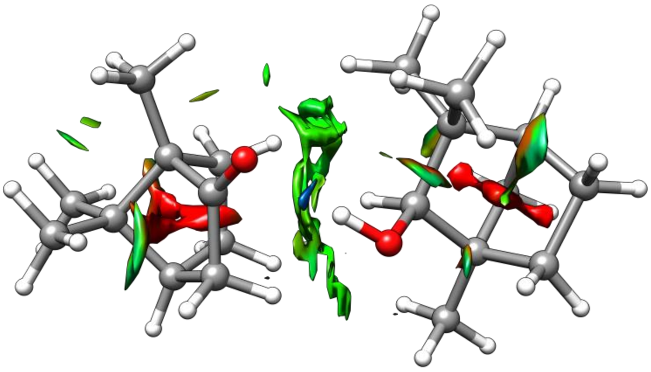
***RR*-B-b-(IV)**

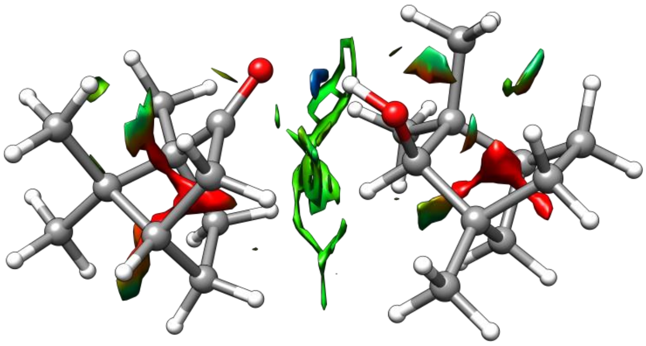


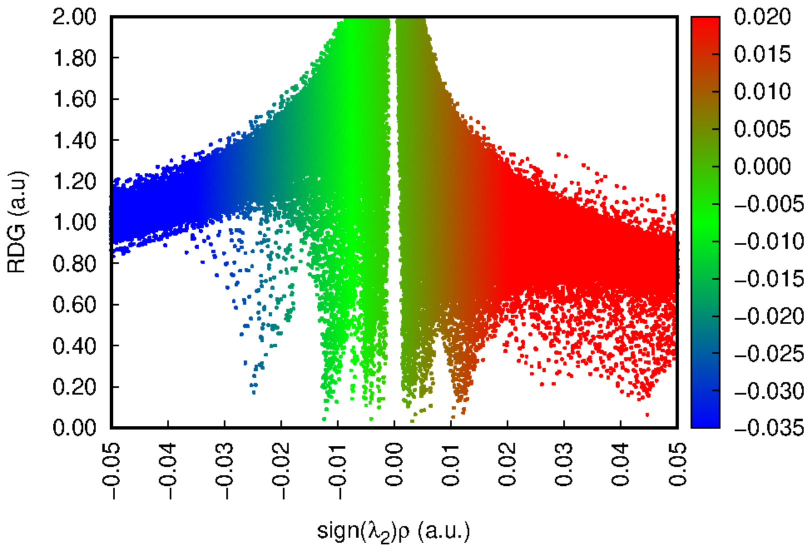



RDG (a.u)
sign(λ2)ρ (a.u.)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

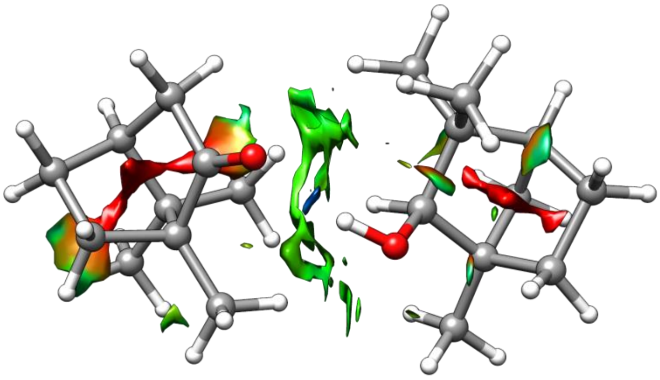
***SR*-A-b-(I)**

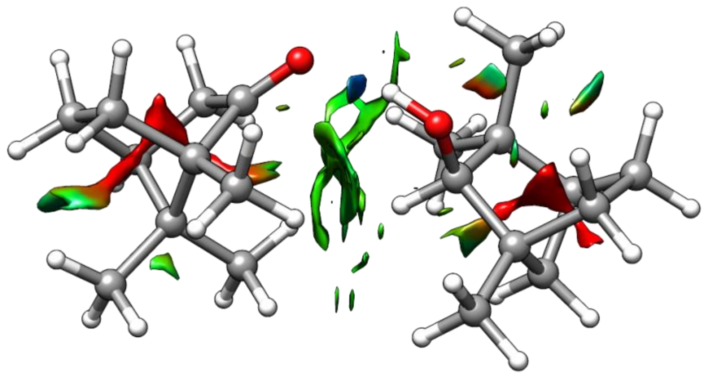


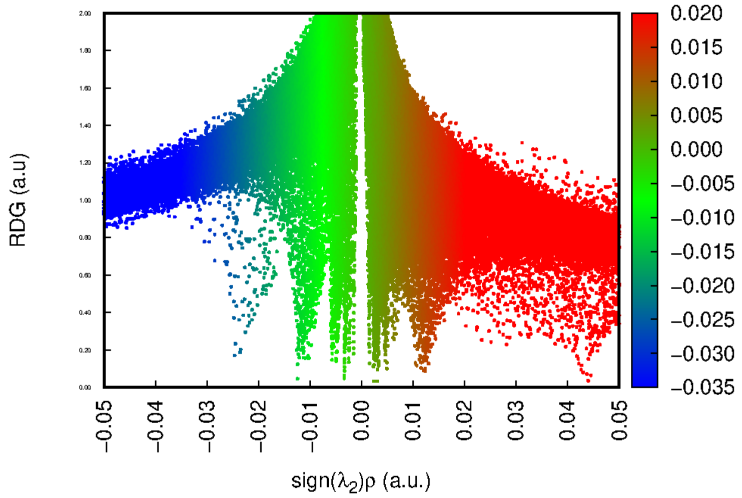



RDG (a.u)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

***SR*-A-d-(II)**






RDG (a.u)
sign(λ2)ρ (a.u.)
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

***SR*-A-a-(III)**

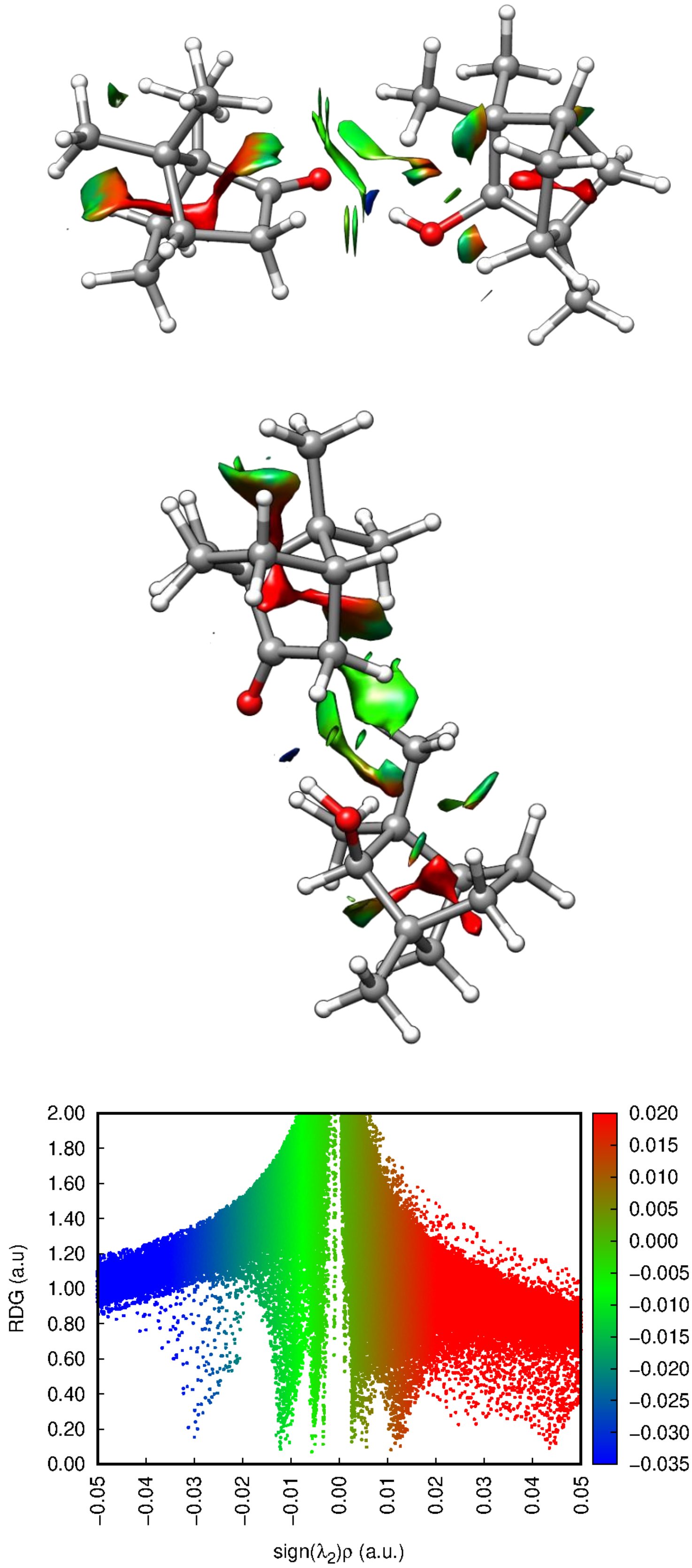

2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
RDG (a.u)
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

Table S1. Rotational parameters calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory for the *RR* complexes lower than 5.0 kJ/mol.

	Δ*E*[a]	***A*[b]**	***B*[b]**	***C*[b]**	***B*–*C*[c]**	**$\mu_a/\mu_b/\mu_c$[d]**
***RR*-A-a-(I)**	0.0	581.1	156.1	149.5	6.6	4.0/0.8/1.8
***RR*-A-c-(II)**	0.7	597.6	155.4	147.8	7.6	4.3/0.2/2.4
***RR*-A-b-(III)**	1.3	629.9	135.2	132.6	2.6	3.6/1.1/1.1
***RR*-B-b-(IV)**	2.0	593.9	160.4	151.0	9.4	3.5/1.3/2.1
***RR*-B-a-(V)**	2.4	598.3	145.2	141.2	4.0	3.3/1.0/1.1
***RR*-B-a-(VI)**	2.8	560.4	160.5	155.4	5.1	2.4/0.7/0.9
***RR*-A-d-(VII)**	3.0	625.0	135.3	132.4	2.9	4.7/1.2/0.1
***RR*-C-a-(VIII)**	3.1	580.0	152.4	145.6	6.8	2.6/0.4/0.1
***RR*-B-d-(IX)**	3.3	576.4	161.7	153.1	8.6	4.3/0.6/2.4
***RR*-A-a-(X)**	3.5	557.4	165.4	156.8	8.6	3.3/1.0/1.1
***RR*-B-c-(XI)**	3.5	612.9	145.0	140.3	4.7	3.5/1.7/0.6
***RR*-C-a-(XII)**	3.6	583.1	144.3	139.2	5.1	3.4/0.9/0.3
***RR*-B-c-(XIII)**	3.7	578.1	160.2	154.9	5.3	2.3/0.2/1.7
***RR*-C-c-(XIV)**	3.7	593.6	153.2	146.3	6.9	2.6/1.2/0.4
***RR*-A-b-(XV)**	4.5	661.8	131.3	126.5	4.8	3.5/0.8/1.3
***RR*-B-d-(XVI)**	4.5	584.1	155.2	144.4	10.7	3.5/0.9/1.5
***RR*-C-c-(XVII)**	4.8	588.9	146.8	139.9	6.9	3.0/0.2/0.1
***RR*-B-d-(XVIII)**	4.9	600.1	136.2	129.5	6.7	4.8/0.5/1.4

[a] Δ*E* is the calculated zero-point corrected energy difference to the global minimum isomer within the diastereomeric dimer in kJ/mol.
[b] *A*, *B* and *C* are the rotational constants in MHz.
[c] *B*–*C* is the difference between the rotational constants *B* and *C* in MHz.
[d] μ_α (α = a, b or c) are the absolute values of the electric dipole moment components in Debye.

Table S2. Rotational parameters calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory for the *SR* complexes lower than 5.0 kJ/mol.

	ΔE^a	A^b	B^b	C^b	$B–C^c$	$\mu_a/\mu_b/\mu_c{}^d$
***SR*-A-b-(I)**	0.0	598.5	161.5	152.0	9.5	3.5/1.1/1.9
***SR*-A-d-(II)**	1.4	581.1	163.2	153.9	9.3	4.3/0.5/2.2
***SR*-A-a-(III)**	1.8	600.8	135.8	131.7	4.1	3.7/0.5/1.1
***SR*-B-b-(IV)**	2.6	615.7	148.9	146.9	2.0	2.8/0.5/1.8
***SR*-A-a-(V)**	2.6	562.6	153.2	148.7	4.5	2.4/0.6/1.0
***SR*-B-a-(VI)**	2.6	575.1	154.2	146.7	7.6	3.8/1.3/1.6
***SR*-A-c-(VII)**	2.6	590.5	149.0	143.8	5.3	2.9/0.7/1.3
***SR*-B-b-(VIII)**	3.4	637.1	135.3	131.2	4.1	3.6/1.9/0.3
***SR*-B-a-(IX)**	3.4	580.4	153.4	144.2	9.3	3.2/1.1/0.7
***SR*-B-c-(X)**	3.5	588.3	153.5	145.5	8.0	4.2/0.2/2.4
***SR*-B-c-(XI)**	3.5	588.8	153.8	146.0	7.8	4.2/0.1/2.5
***SR*-C-a-(XII)**	3.7	581.3	156.2	149.5	6.7	3.0/1.0/0.3
***SR*-C-b-(XIII)**	3.9	599.5	146.1	141.0	5.2	3.1/1.2/0.5
***SR*-C-a-(XIV)**	4.7	583.4	148.8	144.0	4.8	3.4/1.4/0.7
***SR*-B-d-(XV)**	4.9	561.7	159.6	151.5	8.1	2.4/0.2/1.4

[a] ΔE is the calculated zero-point corrected energy difference to the global minimum isomer within the diastereomeric dimer in kJ/mol.
[b] *A*, *B* and *C* are the rotational constants in MHz.
[c] *B*–*C* is the difference between the rotational constants *B* and *C* in MHz.
[d] μ_α (α = a, b or c) are the absolute values of the electric dipole moment components in Debye.

Table S3. Experimental vibrational fundamental transitions in cm^{-1} and assignments.

Wavenumber (cm^{-1})	**Assignment**
3675	fenchol monomer
3666	fenchol monomer
3517	*SR*-A-b-(I)
3504	*RR*-A-a-(I)
3499	fenchol dimer

Table S4. Structural hydrogen bond parameters for camphor complexes at B3LYP-D3(BJ)/def2-TZVP level. Angles are given in °, distances in Å.

	α(C2=O··H)	β(O···H–O)	τ(C3–C2=O···H)	*d*(O···H)	*d*(H–O)
RR-A-a-(I)	113	159	19	1.905	0.972
RR-A-c-(II)	128	163	–156	1.908	0.971
RR-A-b-(III)	110	166	–16	1.873	0.972
RR-B-b-(IV)	110	159	–35	1.922	0.971
SR-A-b-(I)	109	155	31	1.940	0.971
SR-A-d-(II)	127	159	40	1.934	0.969
SR-A-a-(III)	110	166	–9	1.866	0.973

Table S5. A) SAPT(0) energies for the *RR* and *SR* complexes below 2.0 kJ/mol and comparison with the SAPT(0) energies from other works [refs. 18 and 20 in the manuscript]. The energies are given in kJ/mol. B) Percentage relative to the total energy for the electrostatic, induction and dispersion components of the SAPT energies. C) Percentage relative to the overall attractive interactions for the electrostatic, induction and dispersion components of the SAPT energies.

A)	ΔE_{elect}	ΔE_{ind}	ΔE_{disp}	ΔE_{exch}	ΔE_{tot}
RR-A-a-(I)	-47.78	-16.28	-32.52	56.51	-40.07
RR-A-c-(II)	-47.64	-15.87	-33.25	57.33	-39.44
RR-A-b-(III)	-51.79	-16.95	-27.45	56.77	-39.42
RR-B-b-(IV)	-44.24	-15.19	-34.30	56.08	-37.64
SR-A-b-(I)	-46.78	-15.00	-35.07	56.45	-40.40
SR-A-d-(II)	-43.88	-14.24	-34.74	53.31	-39.55
SR-A-a-(III)	-52.40	-17.20	-26.06	56.31	-39.35
Camphor-H_2O	-49.2	-14.6	-11.6	43.6	-31.8
Camphor-MeOH-I	-45.8	-14.1	-14.3	44.2	-30.0
Camphor-EtOH-I	-47.4	-14.3	-18.6	47.2	-33.1

B)	ΔE_{elect}	ΔE_{ind}	ΔE_{disp}	ΔE_{exch}
RR-A-a-(I)	1.19	0.41	0.81	1.41
RR-A-c-(II)	1.21	0.40	0.84	1.45
RR-A-b-(III)	1.31	0.43	0.70	1.44
RR-B-b-(IV)	1.18	0.40	0.91	1.49
SR-A-b-(I)	1.16	0.37	0.87	1.40
SR-A-d-(II)	1.11	0.36	0.88	1.35
SR-A-a-(III)	1.33	0.44	0.66	1.43
Camphor-H_2O	1.55	0.46	0.36	1.37
Camphor-MeOH-I	1.53	0.47	0.48	1.47
Camphor-EtOH-I	1.43	0.43	0.56	1.43

C)	ΔE_{elect}	ΔE_{ind}	ΔE_{disp}
RR-A-a-(I)	49	17	34
RR-A-c-(II)	49	16	34
RR-A-b-(III)	54	18	29
RR-B-b-(IV)	47	16	37
SR-A-b-(I)	48	15	36
SR-A-d-(II)	47	15	37
SR-A-a-(III)	55	18	27
Camphor-H_2O	65	19	15
Camphor-MeOH-I	62	19	19
Camphor-EtOH-I	59	18	23

Table S6. Observed frequencies and residuals (MHz) for the *R*-camphor - *R*-fenchol complex for $J'K'_{-1}K'_{+1} \leftarrow J''K''_{-1}K''_{+1}$ transitions.

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
7 1 7	6 1 6	2077.96381	-0.00281
7 0 7	6 0 6	2097.87041	-0.00265
7 2 6	6 2 5	2101.52369	0.00037
7 5 2	6 5 1	2102.39049	0.01084
7 5 3	6 5 2	2102.39049	0.01084
7 3 5	6 3 4	2102.73706	0.02083
7 1 6	6 1 5	2124.25888	-0.00548
7 3 4	7 2 6	2155.82650	-0.01382
6 1 6	5 0 5	2164.43388	-0.00073
6 1 5	5 0 5	2303.48883	-0.00201
8 1 8	7 1 7	2374.45720	-0.00515
8 0 8	7 0 7	2396.07818	-0.00498
8 2 7	7 2 6	2401.48342	0.00079
8 5 3	7 5 2	2402.78582	0.00639
8 5 4	7 5 3	2402.78582	0.00639
8 4 5	7 4 4	2402.92626	-0.02015
8 4 4	7 4 3	2402.92626	-0.02124
8 3 6	7 3 5	2403.25908	-0.00320
8 2 6	7 2 5	2407.81167	-0.00485
8 1 7	7 1 6	2427.31056	-0.00392
4 2 3	3 1 3	2512.93161	-0.00371
9 1 9	8 1 8	2670.82429	-0.00184
10 0 10	9 1 9	2689.96287	0.01266
9 0 9	8 0 8	2693.74219	0.00701
9 2 8	8 2 7	2701.34282	0.00396
9 2 7	8 2 6	2710.31335	-0.00321
9 1 8	8 1 7	2730.18554	-0.00105
5 2 4	4 1 4	2826.46347	-0.00248
8 1 7	7 0 7	2958.04718	0.00623
10 1 10	9 1 9	2967.04933	0.00147
10 0 10	9 0 9	2990.78667	-0.00617
10 4 6	9 4 5	3003.97144	-0.00949
10 3 8	9 3 7	3004.51347	0.00146
10 3 7	9 3 6	3004.94475	-0.00155
10 1 9	9 1 8	3032.85969	0.00850
6 2 4	5 1 4	3049.30155	0.00055
3 3 1	2 2 0	3053.97293	-0.01222
3 3 0	2 2 0	3053.97293	-0.01277
11 1 11	10 1 10	3263.11446	-0.00508
11 0 11	10 0 10	3287.23743	-0.00063
9 1 8	8 0 8	3292.14246	-0.00192
11 2 10	10 2 9	3300.69115	-0.00057
11 6 5	10 6 4	3303.89582	-0.00909
11 6 6	10 6 5	3303.89582	-0.00909
11 5 7	10 5 6	3304.13605	0.00165
11 5 6	10 5 5	3304.13605	0.00156
11 4 8	10 4 7	3304.56175	0.00238
11 4 7	10 4 6	3304.56175	-0.00891
11 3 9	10 3 8	3305.20382	-0.01011
7 2 5	6 1 5	3334.00464	-0.00201
11 1 10	10 1 9	3335.27610	-0.00018
12 0 12	11 0 11	3583.07424	0.00055
12 2 11	11 2 10	3600.17313	0.00950
12 4 8	11 4 7	3605.22041	0.00370
12 3 10	11 3 9	3605.96657	0.00401
12 3 9	11 3 8	3607.06474	0.01021
8 2 6	7 1 6	3617.55476	-0.00404
10 1 9	9 0 9	3631.26165	0.00126
12 1 11	11 1 10	3637.42451	-0.00264
5 3 3	4 2 2	3653.99940	0.01358
5 3 2	4 2 2	3653.99940	-0.00184
5 3 3	4 2 3	3655.13802	0.00665
5 3 2	4 2 3	3655.13802	-0.00877
8 2 7	7 1 7	3786.99582	-0.00333
13 1 13	12 1 12	3854.79076	-0.00044
20 5 15	20 4 16	3860.05639	0.01822
13 0 13	12 0 12	3878.32664	0.00193
13 2 12	12 2 11	3899.49002	0.00687
9 2 7	8 1 7	3900.56012	-0.00077
13 2 11	12 2 10	3925.00884	0.00230
13 1 12	12 1 11	3939.26415	-0.00210
6 3 3	5 2 3	3953.38364	0.00266
6 3 4	5 2 4	3956.00650	0.00103
6 4 3	5 3 2	4816.18244	0.00969
6 4 2	5 3 2	4816.18244	0.00954
6 4 3	5 3 3	4816.18244	-0.00574
6 4 2	5 3 3	4816.18244	-0.00588
7 4 4	6 3 3	5116.43472	0.02090
7 4 3	6 3 3	5116.43472	0.02035
7 4 4	6 3 4	5116.43472	-0.02537
7 4 3	6 3 4	5116.43472	-0.02591
14 1 14	13 1 13	4150.37565	-0.01010
14 0 14	13 0 13	4173.04018	0.00317
10 2 8	9 1 8	4183.66073	-0.00558
14 2 13	13 2 12	4198.63640	-0.00231
14 7 7	13 7 6	4205.03571	-0.00093
14 7 8	13 7 7	4205.03571	-0.00093
14 6 8	13 6 7	4205.30526	-0.01317
14 6 9	13 6 8	4205.30526	-0.01317
14 5 10	13 5 9	4205.78312	-0.00267
14 5 9	13 5 8	4205.78312	-0.00354
14 4 10	13 4 9	4206.69349	-0.00990
14 3 12	13 3 11	4207.57322	0.00009
4 4 0	3 3 0	4215.56614	-0.00211
4 4 1	3 3 0	4215.56614	-0.00211
4 4 0	3 3 1	4215.56614	-0.00267

Table S6. Continued.

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
4 4 1	3 3 1	4215.56614	-0.00266
7 3 4	6 2 4	4252.05878	0.02910
7 3 5	6 2 5	4257.24562	-0.00241
7 3 4	6 2 5	4257.36565	0.00202
12 1 11	11 0 11	4325.94568	0.01276
15 1 15	14 1 14	4445.81751	-0.00180
11 2 9	10 1 9	4467.55757	-0.00472
15 2 14	14 2 13	4497.62097	0.00178
15 7 8	14 7 7	4505.50407	0.00618
15 7 9	14 7 8	4505.50407	0.00618
15 6 9	14 6 8	4505.83753	-0.00525
15 6 10	14 6 9	4505.83753	-0.00524
15 5 11	14 5 10	4506.41518	-0.00092
15 5 10	14 5 9	4506.41518	-0.00256
5 4 2	4 3 1	4515.88816	0.00494
5 4 1	4 3 1	4515.88816	0.00491
5 4 1	4 3 2	4515.88816	0.00105
5 4 2	4 3 2	4515.88816	0.00108
8 3 6	7 2 6	4558.98840	0.00142
8 3 5	7 2 6	4559.24908	0.00790
13 6 7	13 5 8	4735.28978	-0.00224
13 6 8	13 5 8	4735.28978	-0.00223
13 6 7	13 5 9	4735.28978	-0.00302
13 6 8	13 5 9	4735.28978	-0.00301
12 6 6	12 5 7	4735.66195	-0.00589
12 6 7	12 5 7	4735.66195	-0.00588
12 6 6	12 5 8	4735.66195	-0.00623
12 6 7	12 5 8	4735.66195	-0.00623
11 6 5	11 5 6	4735.96444	-0.00003
11 6 6	11 5 6	4735.96444	-0.00003
11 6 5	11 5 7	4735.96444	-0.00018
11 6 6	11 5 7	4735.96444	-0.00018
10 6 4	10 5 5	4736.20034	0.00627
10 6 5	10 5 5	4736.20034	0.00627
10 6 4	10 5 6	4736.20034	0.00622
10 6 5	10 5 6	4736.20034	0.00622
9 6 3	9 5 4	4736.37166	0.00397
9 6 3	9 5 5	4736.37166	0.00395
9 6 4	9 5 4	4736.37166	0.00397
9 6 4	9 5 5	4736.37166	0.00395
8 6 2	8 5 3	4736.49603	0.00062
8 6 2	8 5 4	4736.49603	0.00062
8 6 3	8 5 3	4736.49603	0.00062
8 6 3	8 5 4	4736.49603	0.00062
16 1 16	15 1 15	4741.07972	-0.01447
12 2 10	11 1 10	4752.95119	0.00000
16 0 16	15 0 15	4761.12409	0.01314
16 2 15	15 2 14	4796.42048	0.00640
16 3 13	15 3 12	4813.83556	-0.00229
6 4 3	5 3 2	4816.18244	0.00969
6 4 2	5 3 2	4816.18244	0.00954
6 4 3	5 3 3	4816.18244	-0.00574
6 4 2	5 3 3	4816.18244	-0.00588
9 3 7	8 2 6	4845.44934	-0.00221
9 3 6	8 2 6	4845.95777	-0.00174
9 3 7	8 2 7	4861.36252	-0.00266
9 3 6	8 2 7	4861.87254	-0.00059
13 2 11	12 1 11	5040.52316	-0.00742
17 0 17	16 0 16	5054.62969	0.00087
12 2 11	11 1 11	5114.82001	0.00315
7 4 4	6 3 3	5116.43472	0.02090
7 4 3	6 3 3	5116.43472	0.02035
7 4 4	6 3 4	5116.43472	-0.02537
7 4 3	6 3 4	5116.43472	-0.02591
10 3 7	9 2 7	5140.59235	0.00311
10 3 8	9 2 8	5164.53567	-0.00265
14 2 12	13 1 12	5330.97362	-0.00107
18 1 18	17 1 17	5331.18822	0.00258
18 0 18	17 0 17	5347.89910	-0.00836
5 5 0	4 4 0	5377.10457	-0.00546
5 5 0	4 4 1	5377.10457	-0.00546
5 5 1	4 4 0	5377.10457	-0.00546
5 5 1	4 4 1	5377.10457	-0.00546
18 2 17	17 2 16	5393.41495	0.00637
18 4 14	17 4 13	5410.66110	-0.01062
11 3 9	10 2 8	5431.57428	0.00536
11 3 8	10 2 8	5433.22062	0.00536
18 1 17	17 1 16	5442.30152	0.00217
11 3 9	10 2 9	5468.67161	-0.00126
16 7 9	16 6 10	5596.03222	-0.00217
16 7 10	16 6 10	5596.03222	-0.00217
16 7 9	16 6 11	5596.03222	-0.00223
16 7 10	16 6 11	5596.03222	-0.00223
15 7 8	15 6 9	5596.44724	-0.00409
15 7 8	15 6 10	5596.44724	-0.00411
15 7 9	15 6 9	5596.44724	-0.00409
15 7 9	15 6 10	5596.44724	-0.00411
14 7 7	14 6 8	5596.79579	-0.00043
14 7 7	14 6 9	5596.79579	-0.00044
14 7 8	14 6 8	5596.79579	-0.00043
14 7 8	14 6 9	5596.79579	-0.00044
13 7 6	13 6 7	5597.08346	0.00545
13 7 6	13 6 8	5597.08346	0.00544
13 7 7	13 6 7	5597.08346	0.00545
13 7 7	13 6 8	5597.08346	0.00544
12 7 5	12 6 6	5597.29771	-0.00732

Table S6. Continued.

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
12 7 5	12 6 7	5597.29771	-0.00732
12 7 6	12 6 6	5597.29771	-0.00732
12 7 6	12 6 7	5597.29771	-0.00732
11 7 4	11 6 5	5597.48269	-0.00230
11 7 4	11 6 6	5597.48269	-0.00230
11 7 5	11 6 5	5597.48269	-0.00230
11 7 5	11 6 6	5597.48269	-0.00230
10 7 3	10 6 4	5597.62467	-0.00032
10 7 3	10 6 5	5597.62467	-0.00032
10 7 4	10 6 4	5597.62467	-0.00032
10 7 4	10 6 5	5597.62467	-0.00032
9 7 2	9 6 3	5597.72105	-0.01051
9 7 2	9 6 4	5597.72105	-0.01051
9 7 3	9 6 3	5597.72105	-0.01051
9 7 3	9 6 4	5597.72105	-0.01051
8 7 1	8 6 2	5597.82098	0.01037
8 7 1	8 6 3	5597.82098	0.01037
8 7 2	8 6 2	5597.82098	0.01037
8 7 2	8 6 3	5597.82098	0.01037
15 2 13	14 1 13	5624.91649	-0.00249
19 1 19	18 1 18	5626.01415	-0.00051
19 0 19	18 0 18	5641.02240	0.00193
6 5 1	5 4 1	5677.43412	0.00578
6 5 2	5 4 1	5677.43412	0.00578
6 5 1	5 4 2	5677.43412	0.00575
6 5 2	5 4 2	5677.43412	0.00575
19 7 12	18 7 11	5707.55981	-0.00740
19 7 13	18 7 12	5707.55981	-0.00740
19 6 14	18 6 13	5708.25824	-0.00158
19 6 13	18 6 12	5708.25824	-0.00180
19 5 15	18 5 14	5709.42105	0.00540
19 5 14	18 5 13	5709.42105	-0.00905
19 4 16	18 4 15	5711.37557	-0.00100
19 3 17	18 3 16	5711.74648	0.00685
19 4 15	18 4 14	5711.93741	0.00966
19 3 16	18 3 15	5722.21636	-0.00625
12 3 9	11 2 9	5723.53328	0.01068
19 1 18	18 1 17	5741.36155	0.00310
12 3 10	11 2 10	5773.94474	0.00104
20 1 20	19 1 19	5920.70345	-0.00589
16 2 14	15 1 14	5922.95085	0.00102
20 0 20	19 0 19	5934.01533	-0.01604
7 5 2	6 4 2	5977.73351	-0.00150
7 5 3	6 4 2	5977.73351	-0.00150
7 5 2	6 4 3	5977.73351	-0.00165
7 5 3	6 4 3	5977.73351	-0.00165
13 3 11	12 2 10	6006.86515	-0.00569
20 8 12	19 8 11	6007.64436	0.02121
20 8 13	19 8 12	6007.64436	0.02121
20 7 13	19 7 12	6008.14163	-0.00608
20 7 14	19 7 13	6008.14163	-0.00608
20 6 15	19 6 14	6008.95713	0.00296
20 6 14	19 6 13	6008.95713	0.00256
20 5 16	19 5 15	6010.30853	0.00902
20 5 15	19 5 14	6010.30853	-0.01405
13 3 10	12 2 10	6011.24069	-0.00006
20 3 18	19 3 17	6012.50248	0.02433
20 4 16	19 4 15	6013.31754	0.00340
10 4 7	9 3 6	6016.47689	0.00327
10 4 6	9 3 6	6016.47689	-0.00662
20 3 17	19 3 16	6025.82507	-0.00032
20 1 19	19 1 18	6039.80228	0.00042
13 3 11	12 2 11	6080.53493	0.00314
17 2 15	16 1 15	6225.61199	0.01192
21 0 21	20 0 20	6227.00096	0.00914
8 5 3	7 4 3	6278.01950	-0.00198
8 5 4	7 4 3	6278.01950	-0.00198
8 5 3	7 4 4	6278.01950	-0.00253
8 5 4	7 4 4	6278.01950	-0.00252
21 2 20	20 2 19	6287.30117	0.00946
14 3 11	13 2 11	6296.16349	-0.00536
21 8 13	20 8 12	6308.14966	-0.00122
21 8 14	20 8 13	6308.14966	-0.00122
21 7 14	20 7 13	6308.76080	0.00447
21 7 15	20 7 14	6308.76080	0.00448
21 6 16	20 6 15	6309.68211	-0.00656
21 6 15	20 6 14	6309.68211	-0.00725
21 5 17	20 5 16	6311.26562	0.02316
21 5 16	20 5 15	6311.26562	-0.01280
21 3 19	20 3 18	6313.15126	0.00688
11 4 8	10 3 7	6316.09947	0.01278
11 4 7	10 3 7	6316.09947	-0.00840
11 4 8	10 3 8	6317.02095	-0.00798
21 3 18	20 3 17	6329.87465	0.00027
21 1 20	20 1 19	6337.59908	0.00256
14 3 12	13 2 12	6388.62335	0.00157
15 8 7	15 7 8	6458.18838	0.00749
15 8 7	15 7 9	6458.18838	0.00749
15 8 8	15 7 8	6458.18838	0.00749
15 8 8	15 7 9	6458.18838	0.00749
12 8 4	12 7 5	6458.76299	0.01781
12 8 4	12 7 6	6458.76299	0.01781
12 8 5	12 7 5	6458.76299	0.01781
12 8 5	12 7 6	6458.76299	0.01781
11 8 3	11 7 4	6458.86628	0.00084
11 8 3	11 7 5	6458.86628	0.00084

Table S6. Continued.

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
11 8 4	11 7 4	6458.86628	0.00084	8 6 2	7 5 3	7139.27384	-0.00100	11 9 3	11 8 3	7320.18610	0.00254
11 8 4	11 7 5	6458.86628	0.00084	8 6 3	7 5 2	7139.27384	-0.00100	11 9 3	11 8 4	7320.18610	0.00254
18 2 16	17 1 16	6533.34887	-0.00105	8 6 3	7 5 3	7139.27384	-0.00100	17 3 15	16 2 15	7323.74963	-0.00418
6 6 0	5 5 0	6538.65245	0.00346	11 5 7	10 4 6	7178.64526	0.00256	25 1 25	24 1 24	7392.47997	-0.00153
6 6 0	5 5 1	6538.65245	0.00346	11 5 6	10 4 6	7178.64526	0.00242	18 3 15	17 2 15	7407.63293	0.01309
6 6 1	5 5 0	6538.65245	0.00346	11 5 7	10 4 7	7178.64526	-0.00733	9 6 3	8 5 3	7439.56456	-0.00631
6 6 1	5 5 1	6538.65245	0.00346	11 5 6	10 4 7	7178.64526	-0.00747	9 6 3	8 5 4	7439.56456	-0.00631
15 3 12	14 2 12	6578.21874	0.01899	14 4 11	13 3 10	7212.45648	0.00262	9 6 4	8 5 3	7439.56456	-0.00631
9 5 5	8 4 4	6578.28864	0.01151	14 4 10	13 3 10	7212.59694	-0.00052	9 6 4	8 5 4	7439.56456	-0.00631
9 5 4	8 4 4	6578.28864	0.01149	14 4 11	13 3 11	7216.82216	-0.00160	12 5 8	11 4 7	7478.72630	0.00632
9 5 4	8 4 5	6578.28864	0.00986	16 9 7	16 8 8	7319.48740	-0.01538	12 5 7	11 4 7	7478.72630	0.00597
9 5 5	8 4 5	6578.28864	0.00988	16 9 7	16 8 9	7319.48740	-0.01538	12 5 8	11 4 8	7478.72630	-0.01486
12 4 8	11 3 8	6615.40419	-0.00236	16 9 8	16 8 8	7319.48740	-0.01538	12 5 7	11 4 8	7478.72630	-0.01520
12 4 9	11 3 9	6617.01391	0.00334	16 9 8	16 8 9	7319.48740	-0.01538	15 4 11	14 3 11	7510.23264	0.01160
15 3 13	14 2 13	6698.39243	-0.00709	15 9 6	15 8 7	7319.70081	0.00529	15 4 12	14 3 12	7516.70974	0.00499
16 2 14	15 1 15	6707.73625	-0.00081	15 9 6	15 8 8	7319.70081	0.00529	19 3 16	18 2 16	7679.42256	-0.00560
7 6 1	6 5 1	6838.96511	-0.00076	15 9 7	15 8 7	7319.70081	0.00529	26 0 26	25 0 25	7692.06161	-0.00162
7 6 1	6 5 2	6838.96511	-0.00076	15 9 7	15 8 8	7319.70081	0.00529	7 7 0	6 6 0	7700.19209	0.00691
7 6 2	6 5 1	6838.96511	-0.00076	14 9 5	14 8 6	7319.84936	-0.00688	7 7 0	6 6 1	7700.19209	0.00691
7 6 2	6 5 2	6838.96511	-0.00076	14 9 5	14 8 7	7319.84936	-0.00688	7 7 1	6 6 0	7700.19209	0.00691
19 2 17	18 1 17	6846.63312	0.00141	14 9 6	14 8 6	7319.84936	-0.00688	7 7 1	6 6 1	7700.19209	0.00691
16 3 13	15 2 13	6857.34146	0.00144	14 9 6	14 8 7	7319.84936	-0.00688	10 6 4	9 5 4	7739.83836	-0.00956
10 5 6	9 4 5	6878.48845	-0.00078	13 9 4	13 8 5	7319.99556	0.00678	10 6 4	9 5 5	7739.83836	-0.00958
10 5 5	9 4 5	6878.48845	-0.00084	13 9 4	13 8 6	7319.99556	0.00678	10 6 5	9 5 4	7739.83836	-0.00956
10 5 5	9 4 6	6878.48845	-0.00507	13 9 5	13 8 5	7319.99556	0.00678	10 6 5	9 5 5	7739.83836	-0.00958
10 5 6	9 4 6	6878.48845	-0.00502	13 9 5	13 8 6	7319.99556	0.00678	13 5 9	12 4 8	7778.72158	0.02092
13 4 10	12 3 9	6914.18998	-0.00755	12 9 3	12 8 4	7320.09030	-0.00647	13 5 8	12 4 8	7778.72158	0.02014
13 4 9	12 3 9	6914.28275	0.00536	12 9 3	12 8 5	7320.09030	-0.00647	13 5 9	12 4 9	7778.72158	-0.02140
16 3 14	15 2 14	7010.04039	-0.00938	12 9 4	12 8 4	7320.09030	-0.00647	13 5 8	12 4 9	7778.72158	-0.02218
16 3 13	15 2 14	7024.65099	-0.02341	12 9 4	12 8 5	7320.09030	-0.00647	16 4 12	15 3 12	7806.97161	-0.00634
17 3 14	16 2 14	7133.72243	-0.00154	11 9 2	11 8 3	7320.18610	0.00254	26 1 25	25 1 24	7816.52347	-0.00472
8 6 2	7 5 2	7139.27384	-0.00100	11 9 2	11 8 4	7320.18610	0.00254	16 4 13	15 3 13	7816.61851	-0.00350

Table S6. Continued.

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
26 7 20	25 7 19	7812.28249	0.01064
26 7 19	25 7 18	7812.28249	0.01049
26 6 21	25 6 20	7814.02867	-0.00749
26 6 20	25 6 19	7814.02880	-0.01491
26 5 21	25 5 20	7817.17331	0.00140
26 4 23	25 4 22	7820.59011	-0.00378
26 3 23	25 3 22	7856.71439	0.00069
27 0 27	26 0 26	7985.22097	0.00240

Table S7. Observed frequencies and residuals (MHz) for the *S*-camphor - *R*-fenchol complex for $J'K'_{-1}K'_{+1} \leftarrow J''K''_{-1}K''_{+1}$ transitions.

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
5 1 4	4 0 4	2057.77177	0.01677	13 1 12	12 2 10	2937.51953	0.00721	12 7 6	11 7 5	3705.70307	0.00496
7 1 7	6 1 6	2126.59135	-0.00204	9 1 9	8 0 8	3031.92668	-0.00559	12 6 6	11 6 5	3706.04636	0.01793
7 0 7	6 0 6	2152.90822	-0.00237	10 1 10	9 1 9	3035.28913	0.00360	12 6 7	11 6 6	3706.04636	0.01794
7 2 6	6 2 5	2159.86303	0.00272	10 0 10	9 0 9	3064.29996	0.01355	12 5 8	11 5 7	3706.59063	0.00624
7 3 4	6 3 3	2162.30986	0.00097	10 2 9	9 2 8	3083.43156	0.00008	12 5 7	11 5 6	3706.59063	0.00525
7 2 5	6 2 4	2167.95023	0.00168	10 3 8	9 3 7	3089.87467	0.00221	12 4 9	11 4 8	3707.62227	0.01290
7 1 6	6 1 5	2191.55865	0.00134	10 3 7	9 3 6	3091.00764	0.00309	12 3 10	11 3 9	3708.74245	0.00293
6 1 6	5 0 5	2200.77852	0.00055	8 1 7	7 0 7	3091.36568	0.00225	12 3 9	11 3 8	3711.57404	0.00130
6 1 5	5 0 5	2396.09483	0.00059	10 2 8	9 2 7	3106.23801	-0.01535	12 2 10	11 2 9	3735.39886	-0.00985
8 1 8	7 1 7	2429.73384	0.00177	6 2 4	5 1 4	3122.33526	0.00138	12 1 11	11 1 10	3748.64523	-0.00305
8 0 8	7 0 7	2457.69408	-0.00158	10 1 9	9 1 8	3127.21633	-0.00035	8 2 7	7 1 7	3929.64602	0.00704
8 2 7	7 2 6	2467.91015	-0.01060	3 3 1	2 2 0	3142.26564	0.01799	9 2 8	8 1 7	3941.33507	0.01194
8 2 6	7 2 5	2479.93193	-0.00037	3 3 0	2 2 0	3142.26564	0.01655	13 1 13	12 1 12	3941.67815	0.00301
7 1 7	6 0 6	2480.16684	-0.00564	6 2 5	5 1 5	3251.68391	-0.00343	13 0 13	12 0 12	3967.17057	-0.00711
8 1 7	7 1 6	2503.83208	0.01075	6 2 4	5 1 5	3261.88695	-0.00487	9 2 7	8 1 7	3988.53985	-0.00531
4 2 2	3 1 2	2538.81069	0.00131	11 1 11	10 1 10	3337.68453	0.00644	13 2 12	12 2 11	4004.82762	-0.00098
4 2 3	3 1 3	2592.45300	0.00135	11 0 11	10 0 10	3366.10407	-0.00135	13 7 6	12 7 5	4014.66886	0.00654
9 1 9	8 1 8	2732.62691	-0.00705	11 2 10	10 2 9	3390.82886	-0.00635	13 7 7	12 7 6	4014.66886	0.00654
7 1 6	6 0 6	2740.45214	-0.00053	11 5 7	10 5 6	3397.46498	0.01296	13 6 7	12 6 6	4015.08769	0.00596
9 0 9	8 0 8	2761.49650	0.00304	11 5 6	10 5 5	3397.46498	0.01252	13 6 8	12 6 7	4015.08769	0.00598
9 2 8	8 2 7	2775.78233	-0.00333	11 3 9	10 3 8	3399.27301	-0.00417	13 5 9	12 5 8	4015.80197	0.01394
9 6 3	8 6 2	2779.13558	-0.00627	11 3 8	10 3 7	3401.10283	-0.00612	13 5 8	12 5 7	4015.80197	0.01183
9 6 4	8 6 3	2779.13558	-0.00627	7 2 5	6 1 5	3411.28993	0.00187	13 4 10	12 4 9	4017.07486	0.00028
9 5 5	8 5 4	2779.37225	-0.00508	9 1 8	8 0 8	3449.39780	0.00112	13 4 9	12 4 8	4017.19932	-0.00895
9 5 4	8 5 3	2779.37225	-0.00514	11 1 11	10 0 10	3579.12838	0.01234	13 3 11	12 3 10	4018.23861	-0.00147
9 4 6	8 4 5	2779.82917	0.00893	7 2 6	6 1 6	3588.31446	0.00284	13 3 10	12 3 9	4022.46332	0.00476
9 4 5	8 4 4	2779.82917	-0.00039	12 1 12	11 1 11	3639.81199	0.00425	13 2 11	12 2 10	4050.75064	-0.00762
9 3 7	8 3 6	2780.54896	0.00887	12 0 12	11 0 11	3667.02438	-0.00506	13 1 12	12 1 11	4058.45132	0.01658
9 3 6	8 3 5	2781.19906	-0.00351	8 2 6	7 1 6	3699.66583	0.00277	6 3 4	5 2 3	4065.39844	-0.00322
9 1 8	8 1 7	2815.72912	0.00021	12 8 4	11 8 3	3705.45912	-0.02550	6 3 3	5 2 3	4065.52066	-0.00206
5 2 3	4 1 3	2831.80066	-0.00090	12 8 5	11 8 4	3705.45912	-0.02550	6 3 4	5 2 4	4070.51299	-0.00427
5 2 4	4 1 4	2919.74252	0.00100	12 7 5	11 7 4	3705.70307	0.00496	6 3 3	5 2 4	4070.63871	0.00038

Table S7. Continued.

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
14 0 14	13 0 13	4266.69266	-0.00326
10 2 8	9 1 8	4279.06657	-0.00304
14 2 13	13 2 12	4311.39217	0.01496
14 5 10	13 5 9	4325.04547	-0.02336
14 5 9	13 5 8	4325.04547	-0.02757
14 4 11	13 4 10	4326.65654	0.00656
14 4 10	13 4 9	4326.87787	0.00126
14 3 12	13 3 11	4327.75476	-0.00050
14 3 11	13 3 10	4333.82931	-0.00404
4 4 1	3 3 0	4337.50033	-0.00100
4 4 0	3 3 0	4337.50033	-0.00102
4 4 0	3 3 1	4337.50033	-0.00246
4 4 1	3 3 1	4337.50033	-0.00245
14 2 12	13 2 11	4366.40384	0.00826
14 1 13	13 1 12	4367.47241	-0.01597
7 3 5	6 2 4	4370.80822	-0.00380
7 3 4	6 2 4	4371.11320	-0.00124
7 3 5	6 2 5	4381.01073	-0.00577
7 3 4	6 2 5	4381.31455	-0.00437
11 2 10	10 1 9	4472.63507	-0.00916
15 1 15	14 1 14	4544.64861	0.00163
15 0 15	14 0 14	4565.73353	-0.00597
11 2 9	10 1 9	4572.38579	0.00872
15 6 10	14 6 9	4633.35777	0.00843
15 6 9	14 6 8	4633.35777	0.00833
15 5 11	14 5 10	4634.44729	0.01465
15 5 10	14 5 9	4634.44729	0.00667
15 3 13	14 3 12	4637.21656	-0.04110
15 3 12	14 3 11	4645.76016	-0.00590
5 4 2	4 3 1	4646.24635	0.00385
5 4 1	4 3 1	4646.24635	0.00375
5 4 2	4 3 2	4646.24635	-0.00624
5 4 1	4 3 2	4646.24635	-0.00635
8 3 6	7 2 5	4674.15174	-0.00179
8 3 5	7 2 5	4674.81711	-0.00101
15 2 13	14 2 12	4682.12910	-0.00237
8 3 6	7 2 6	4692.44278	-0.00347
8 3 5	7 2 6	4693.10727	-0.00357
16 1 16	15 1 15	4845.77814	0.00592
16 0 16	15 0 15	4864.44078	-0.01645
12 2 10	11 1 10	4869.57344	0.00273
16 2 15	15 2 14	4923.48814	0.00098
16 6 11	15 6 10	4942.57216	0.00032
16 6 10	15 6 9	4942.57216	0.00011
16 4 13	15 4 12	4946.14944	0.00727
16 3 14	15 3 13	4946.72278	0.00602
16 4 12	15 4 11	4946.72278	-0.00209
6 4 3	5 3 2	4954.95522	0.02168
6 4 2	5 3 2	4954.95522	0.02115
6 4 3	5 3 3	4954.95522	-0.01869
6 4 2	5 3 3	4954.95522	-0.01922
16 3 13	15 3 12	4958.32142	-0.00233
13 1 12	12 0 12	4962.99458	-0.00214
9 3 7	8 2 6	4974.76393	0.00261
9 3 6	8 2 6	4976.08745	-0.00094
11 2 10	10 1 10	4982.04971	0.00993
16 1 15	15 1 14	4983.04664	0.00071
13 2 12	12 1 11	4988.58894	0.00483
16 2 14	15 2 13	4997.76924	-0.01114
9 3 7	8 2 7	5005.06891	0.00332
17 4 14	16 4 13	5256.08998	0.03077
17 3 15	16 3 14	5256.08998	-0.00962
17 4 13	16 4 12	5256.95795	0.00688
17 3 14	16 3 13	5271.56910	0.00275
10 3 7	9 2 7	5274.38949	-0.00002
10 3 8	9 2 8	5319.15448	0.00211
10 3 7	9 2 8	5321.61948	0.00794
12 2 11	11 1 11	5342.32732	-0.00899
14 2 12	13 1 12	5479.64012	-0.00139
5 5 0	4 4 0	5532.67589	-0.00183
5 5 0	4 4 1	5532.67589	-0.00184
5 5 1	4 4 0	5532.67589	-0.00183
5 5 1	4 4 1	5532.67589	-0.00184
18 2 17	17 2 16	5534.18523	0.00189
18 3 16	17 3 15	5565.36034	-0.01121
11 3 8	10 2 8	5569.23362	-0.01148
18 3 15	17 3 14	5585.54152	0.00162
18 1 17	17 1 16	5594.65902	-0.00748
11 3 9	10 2 9	5635.00193	0.00385
11 3 8	10 2 9	5639.29448	0.00546
19 0 19	18 0 18	5759.83763	0.01089
15 2 13	14 1 13	5794.28293	-0.00166
19 2 18	18 2 17	5838.97177	-0.00262
6 5 1	5 4 1	5841.42762	-0.00228
6 5 2	5 4 1	5841.42762	-0.00228
6 5 1	5 4 2	5841.42762	-0.00239
6 5 2	5 4 2	5841.42762	-0.00239
12 3 9	11 2 9	5860.29877	0.00505
19 4 16	18 4 15	5876.22235	0.00571
9 4 6	8 3 5	5880.12440	0.00315
9 4 5	8 3 5	5880.12440	-0.01199
9 4 6	8 3 6	5880.78921	0.00337
9 4 5	8 3 6	5880.78921	-0.01177
19 1 18	18 1 17	5898.84992	-0.00037
19 3 16	18 3 15	5900.26685	-0.00177
19 2 17	18 2 16	5942.61286	0.00177

Table S7. Continued.

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
12 3 10	11 2 10	5952.90514	0.00274
20 0 20	19 0 19	6058.27159	-0.01061
16 2 14	15 1 14	6116.35479	0.01082
13 3 10	12 2 10	6147.34689	0.00333
7 5 2	6 4 2	6150.16145	-0.00029
7 5 3	6 4 2	6150.16145	-0.00028
7 5 2	6 4 3	6150.16145	-0.00082
7 5 3	6 4 3	6150.16145	-0.00081
20 3 18	19 3 17	6183.43585	-0.00488
20 4 17	19 4 16	6186.44594	0.00522
10 4 7	9 3 7	6189.23331	-0.00130
20 3 17	19 3 16	6215.74460	-0.00224
13 3 11	12 2 11	6273.15947	-0.00837
13 3 10	12 2 11	6284.51314	0.00266
21 0 21	20 0 20	6356.80331	-0.00477
14 3 12	13 2 11	6412.98965	-0.00829
17 2 15	16 1 15	6446.47236	0.00226
8 5 3	7 4 3	6458.86247	0.00565
8 5 4	7 4 3	6458.86247	0.00568
8 5 4	7 4 4	6458.86247	0.00374
8 5 3	7 4 4	6458.86247	0.00371
11 4 8	10 3 7	6495.15884	0.00634
11 4 7	10 3 7	6495.22384	-0.00421
11 4 8	10 3 8	6497.61159	-0.00008
21 2 19	20 2 18	6569.52463	0.01390
14 8 6	14 7 7	6646.81539	-0.01159
14 8 6	14 7 8	6646.81539	-0.01159
14 8 7	14 7 7	6646.81539	-0.01159
14 8 7	14 7 8	6646.81539	-0.01159
13 8 5	13 7 6	6647.17279	0.00844
13 8 5	13 7 7	6647.17279	0.00844
13 8 6	13 7 6	6647.17279	0.00844

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
13 8 6	13 7 7	6647.17279	0.00844
12 8 4	12 7 5	6647.44008	0.00504
12 8 4	12 7 6	6647.44008	0.00504
12 8 5	12 7 5	6647.44008	0.00504
12 8 5	12 7 6	6647.44008	0.00504
15 3 12	14 2 12	6709.79908	0.00993
6 6 0	5 5 0	6727.84794	-0.00268
6 6 0	5 5 1	6727.84794	-0.00268
6 6 1	5 5 0	6727.84794	-0.00268
6 6 1	5 5 1	6727.84794	-0.00268
9 5 5	8 4 4	6767.49817	0.00361
9 5 4	8 4 4	6767.49817	0.00352
9 5 4	8 4 5	6767.49817	-0.00230
9 5 5	8 4 5	6767.49817	-0.00221
12 4 9	11 3 8	6801.64733	-0.00559
12 4 8	11 3 8	6801.80054	-0.00330
12 4 9	11 3 9	6805.94383	-0.00003
12 4 8	11 3 9	6806.08935	-0.00542
15 3 13	14 2 13	6921.97293	-0.00203
7 6 1	6 5 1	7036.60351	-0.00083
7 6 1	6 5 2	7036.60351	-0.00083
7 6 2	6 5 1	7036.60351	-0.00083
7 6 2	6 5 2	7036.60351	-0.00083
10 5 6	9 4 5	7076.05772	0.00774
10 5 5	9 4 5	7076.05772	0.00747
10 5 6	9 4 6	7076.05772	-0.00740
10 5 5	9 4 6	7076.05772	-0.00766
13 4 9	12 3 9	7107.43650	-0.00286
13 4 10	12 3 10	7114.26832	-0.01060
24 1 24	23 1 23	7248.24534	0.00431
16 3 14	15 2 14	7251.10452	0.01498
17 3 14	16 2 14	7259.78795	0.02054

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
8 6 2	7 5 2	7345.35862	0.01334
8 6 2	7 5 3	7345.35862	0.01333
8 6 3	7 5 2	7345.35862	0.01334
8 6 3	7 5 3	7345.35862	0.01333
11 5 7	10 4 6	7384.51027	0.01728
11 5 6	10 4 6	7384.51027	0.01658
11 5 7	10 4 7	7384.51027	-0.01802
11 5 6	10 4 7	7384.51027	-0.01871
14 4 10	13 3 10	7411.86265	0.00524
24 3 22	23 3 21	7416.73038	0.01483
24 6 19	23 6 18	7419.05327	0.02484
24 6 18	23 6 17	7419.05327	0.00442
14 4 11	13 3 11	7422.68541	-0.00340
24 5 19	23 5 18	7423.87441	-0.00239
24 4 21	23 4 20	7427.95913	0.00081
24 4 20	23 4 19	7437.42920	-0.00802
24 2 22	23 2 21	7503.60183	-0.00421
18 3 15	17 2 15	7532.11561	-0.01967
25 1 25	24 1 24	7547.99109	0.00229
25 0 25	24 0 24	7551.79540	0.00377
17 3 15	16 2 15	7583.69581	-0.00616
9 6 3	8 5 3	7654.06984	0.00583
9 6 4	8 5 3	7654.06984	0.00583
9 6 3	8 5 4	7654.06984	0.00580
9 6 4	8 5 4	7654.06984	0.00580
25 2 24	24 2 23	7659.79654	0.00190
25 1 24	24 1 23	7702.49702	-0.02041
15 4 12	14 3 12	7731.26585	-0.00646
25 4 21	24 4 20	7750.78336	-0.00135
25 3 22	24 3 21	7801.51669	-0.00442
25 2 23	24 2 22	7813.01921	0.00748
18 3 16	17 2 16	7920.04057	-0.01491

Table S7. Continued.

$J^{'}K_{-1}^{'}K_{+1}^{'}$	$J^{''}K_{-1}^{''}K_{+1}^{''}$	Obs.	Res.
7 7 0	6 6 0	7923.01913	-0.00158
7 7 0	6 6 1	7923.01913	-0.00158
7 7 1	6 6 0	7923.01913	-0.00158
7 7 1	6 6 1	7923.01913	-0.00158
10 6 4	9 5 4	7962.75412	0.00497
10 6 4	9 5 5	7962.75412	0.00488
10 6 5	9 5 4	7962.75412	0.00497
10 6 5	9 5 5	7962.75412	0.00488

%nprocshared=12
%mem=24GB
b3lyp empiricaldispersion=gd3bj def2tzvp density=current geom=connectivity int=ultrafine output=pickett opt=tight freq=vibrot

Gaussian input and optimized coordinates for *SR*-A-b-(I)

```
0 1
 C     2.07004100   -0.01772100    1.53276800
 C     2.72974100    0.70860200    0.31742900
 C     2.84503800   -1.51028100   -0.20187400
 C     2.18811400   -1.52730300    1.19213700
 H     1.04111700    0.30792700    1.68015100
 H     2.61768500    0.24195100    2.43846400
 H     1.21813900   -2.02344200    1.16708400
 H     2.80050000   -2.05531600    1.92138400
 C     3.83737600   -0.31329400   -0.10324200
 C     1.78035200   -0.98290500   -1.17504800
 H     3.29541200   -2.45580100   -0.50117700
 C     3.10344300    2.15074100    0.55972100
 H     3.80420900    2.23698500    1.39162800
 H     2.21691400    2.73934500    0.79871000
 H     3.56051400    2.59689000   -0.32456200
 C     1.70838400    0.48945600   -0.78837200
 O     0.95614000    1.32011400   -1.24789600
 C    -4.03218400   -1.08416600   -0.82841200
 C    -2.79105500   -1.26819000    0.07641100
 C    -3.79773400    0.59263700    0.89768100
 C    -4.76771000    0.13372300   -0.20486400
 H    -3.73892700   -0.91918700   -1.86336000
 H    -4.65180700   -1.98223000   -0.79748800
 H    -4.99643500    0.91258100   -0.92899700
 H    -5.71376600   -0.17192000    0.24595700
 C    -3.32544400   -0.77115900    1.43141300
 H    -2.55343400   -0.71213100    2.19974600
 H    -4.14299000   -1.38768600    1.81051100
 C    -1.79302500   -0.14118700   -0.24902900
 H    -0.88805400   -0.31129900    0.34929000
 C    -2.49361300    1.17276000    0.27730900
 H    -4.25133900    1.26566900    1.62670700
 C    -2.17518600   -2.65095100    0.02963700
 H    -2.90560000   -3.41743900    0.29847700
 H    -1.80561600   -2.87357400   -0.97330000
 H    -1.33427800   -2.73043100    0.72449100
 C    -1.63706200    1.83655200    1.36108800
 H    -0.66804400    2.12894300    0.95094200
 H    -2.12518600    2.73702500    1.74190800
 H    -1.45801500    1.17320900    2.20882900
 C    -2.73243500    2.19751200   -0.83029300
 H    -3.37162500    3.00496800   -0.46436200
 H    -1.78704300    2.64071800   -1.14837700
 H    -3.19628600    1.76030000   -1.71082900
 O    -1.44841900   -0.15957100   -1.61904300
 H    -0.70398200    0.44993200   -1.74876900
 H     0.80192600   -1.45417200   -1.08187000
 H     2.07222000   -1.06370800   -2.22291800
 C     4.51412400    0.04810100   -1.42895000
 H     5.17837700    0.90323100   -1.29417700
 H     5.12244000   -0.78615900   -1.78472500
 H     3.81218100    0.30871200   -2.22036300
 C     4.93449600   -0.50822000    0.94226900
 H     5.59338600   -1.32546400    0.63997500
 H     5.54744100    0.39095300    1.02587400
 H     4.55422500   -0.74196600    1.93398000
```

```
%nprocshared=12
%mem=24GB
# b3lyp empiricaldispersion=gd3bj def2tzvp density=current geom=connectivity int=ultrafine
output=pickett opt=tight freq=vibrot
```

Gaussian input and optimized coordinates for *RR*-A-a-(I)

```
0 1
 C          4.16470100   0.43741600  -1.12977100
 C          3.01267400   0.77553200  -0.13219600
 C          3.08627500  -1.50512000  -0.18090400
 C          4.24246400  -1.11356600  -1.12068900
 H          3.96603900   0.84911200  -2.11950100
 H          5.08762700   0.89572800  -0.77523900
 H          4.11130300  -1.54219700  -2.11409000
 H          5.20302100  -1.46284200  -0.74525000
 C          3.13337200  -0.39055600   0.90630200
 C          1.78437100  -1.18405500  -0.93164700
 H          3.14015000  -2.52290900   0.20323400
 C          2.98367500   2.20209000   0.36029500
 H          3.91709700   2.45944300   0.86327100
 H          2.84322700   2.89139700  -0.47315900
 H          2.16034800   2.36415200   1.05719600
 C          1.77023700   0.33948300  -0.89160900
 O          0.93478100   1.06767500  -1.37967600
 C         -4.15957900  -1.02604600  -0.76447000
 C         -2.95028300  -1.25351400   0.17298900
 C         -3.80203700   0.73851700   0.84907300
 C         -4.79497500   0.28966100  -0.23696100
 H         -3.83978700  -0.95703100  -1.80241300
 H         -4.85483200  -1.86382200  -0.68553900
 H         -4.94733100   1.03392700  -1.01557100
 H         -5.76906500   0.09706600   0.21673700
 C         -3.45593200  -0.62078600   1.48173500
 H         -2.69085400  -0.57525200   2.25788500
 H         -4.32830000  -1.13759800   1.88688400
 C         -1.85468400  -0.24119100  -0.20996200
 H         -0.97743300  -0.44504600   0.41921600
 C         -2.44564900   1.16119200   0.21341100
 H         -4.20421100   1.49652900   1.52289000
 C         -2.45535700  -2.68361600   0.22976400
 H         -3.25234900  -3.36497300   0.53638200
 H         -2.09381700  -3.00368500  -0.74931900
 H         -1.63240300  -2.78634900   0.94289500
 C         -1.54686500   1.82176800   1.26479300
 H         -0.55295300   2.00495700   0.85103800
 H         -1.96130600   2.78305500   1.57857000
 H         -1.43082300   1.20278500   2.15575400
 C         -2.58303300   2.12416600  -0.96481600
 H         -3.15583900   3.00554000  -0.66532400
 H         -1.59972900   2.46282800  -1.29551400
 H         -3.07226500   1.66793600  -1.82173100
 O         -1.49141100  -0.38524900  -1.56634300
 H         -0.70823400   0.16727800  -1.72548400
 H          0.88763300  -1.56983700  -0.44705000
 H          1.76218000  -1.54141500  -1.96208700
 C          1.96644700  -0.43752500   1.89682300
 H          1.99086200  -1.36844900   2.46715200
 H          2.03897500   0.38574100   2.60916100
 H          0.98857500  -0.36466900   1.42389500
 C          4.43033000  -0.36970800   1.71393100
 H          4.43464200   0.47352100   2.40672900
 H          4.51051300  -1.28194200   2.30955000
 H          5.32546300  -0.29723800   1.10044000
```

Number of isomers found with each conformational search

The number of species found with each method was the following:

• ABC Cluster: We ran this program three times for each complex (*RR* and *RS*) using the three different fenchol conformations A, B, and C as inputs. Thus, we obtained 100 isomers each time and selected the 20 lowest-energy ones for further optimization. Number of optimized isomers: 20 * 3 * 2 = 120 isomers.

• GFN-xTB: We did the same as before. This time we obtained around 140 isomers each time, and we optimized the 20 lowest-energy ones. Number of optimized isomers: 20 * 3 * 2 = 120 isomers.

• GFN-xTB with its CREST driver: We ran this program once for each *RR* and *SR* complex, and we obtained 297 and 319 isomers, respectively. We optimized the 30 lowest-energy isomers for each *RR* and *SR* complex. Number of optimized isomers: 30 * 2 = 60.

• Manual conformational search: We focused the manual search mainly on complexes involving the most stable alcohol conformer (A fenchol). This search was supplemented by reoptimization of modified structures of the closely related fenchol-fenchone complex, which is another work in progress carried out by some of us.