Electronic Supplementary Material (ESI) for Chemical Science.

Chirality sensing of tertiary alcohols by a novel strong hydrogen-bonding donor−selenourea

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Genenal information:

^{1}H NMR spectra were recorded on a Bruker Avance 400 (400 MHz) spectrometer, and chemical shifts were reported in ppm using TMS (δ H=0, in $CDCl_3$) or C_6D_6 (δ H=7.16, in C_6D_6) as internal standards. ^{13}C NMR spectra were recorded on a Bruker Avance 400 (100 MHz) spectrometer with complete proton decoupling, and chemical shifts were reported in ppm from the solvent resonance as the internal standard ($CDCl_3$; 77.16 ppm). 2D COSY and NOESY spectra were recorded on a Bruker Avance 500 MHz spectrometer, using C_6D_6 (δ H=7.16) as internal standards. ^{19}F NMR spectra were recorded on a Bruker Avance 400 (376 MHz) spectrometer. ^{77}Se NMR spectra were recorded on a Bruker Avance 500 (95 MHz) spectrometer, and chemical shifts are reported in ppm from PhSeSePh (δ Se=464 ppm, in $CDCl_3$) resonance as the external standard. Optical rotations were measured on a SGW-1 automatic polarimeter. Electrospray ionization mass spectrometry (ESI-MS) spectra were obtained on a 1290UHPLC/6538QTOF spectrometer giving fragment ions in m/z with relative intensities (%) in parentheses. All air- and moisture-sensitive reactions were performed under an atmosphere of argon (Ar) in dried glassware.

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) of (*S*, *S*)-CSA-2

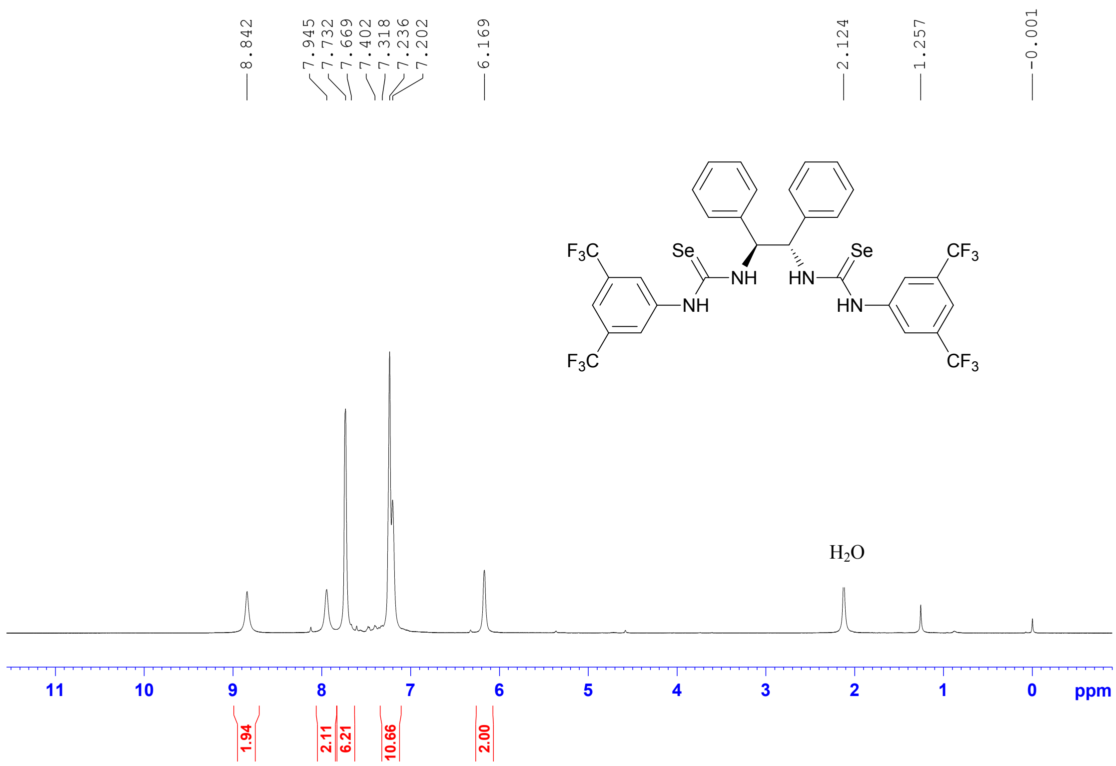


Figure S2. 13C NMR (400 MHz, $CDCl_3$) of (*S*, *S*)-CSA-2

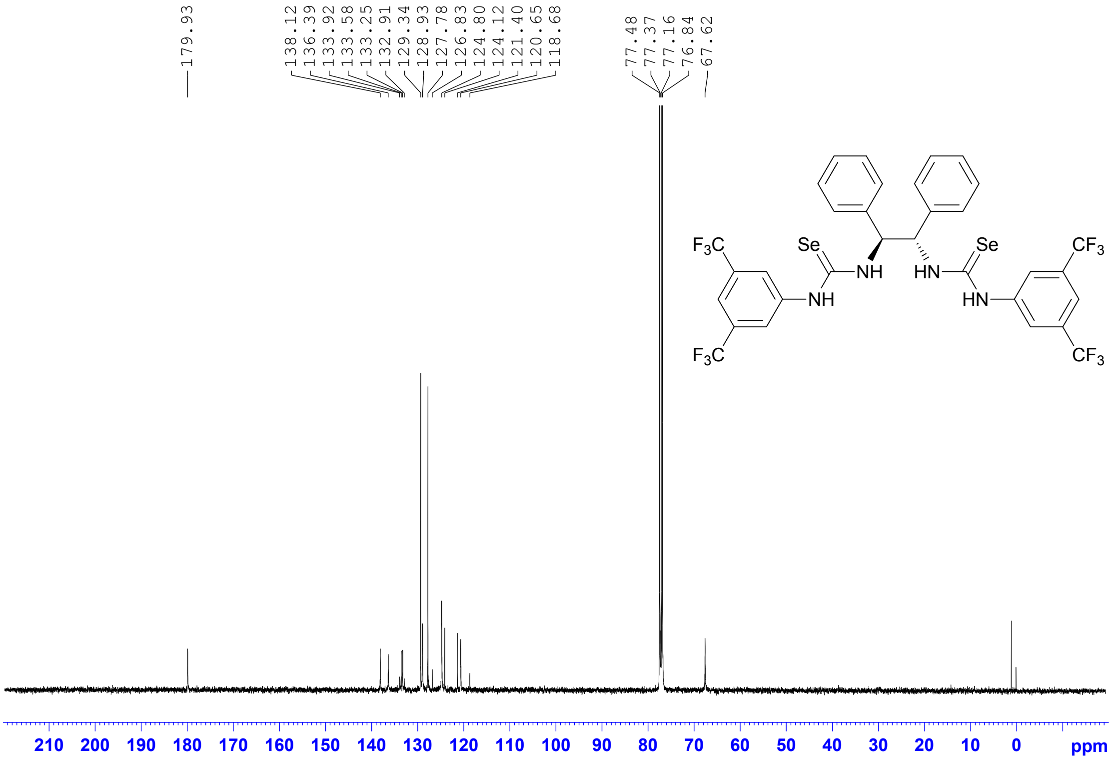


Figure S3. 77Se NMR (95 MHz, $CDCl_3$) of (*S*, *S*)-CSA-2

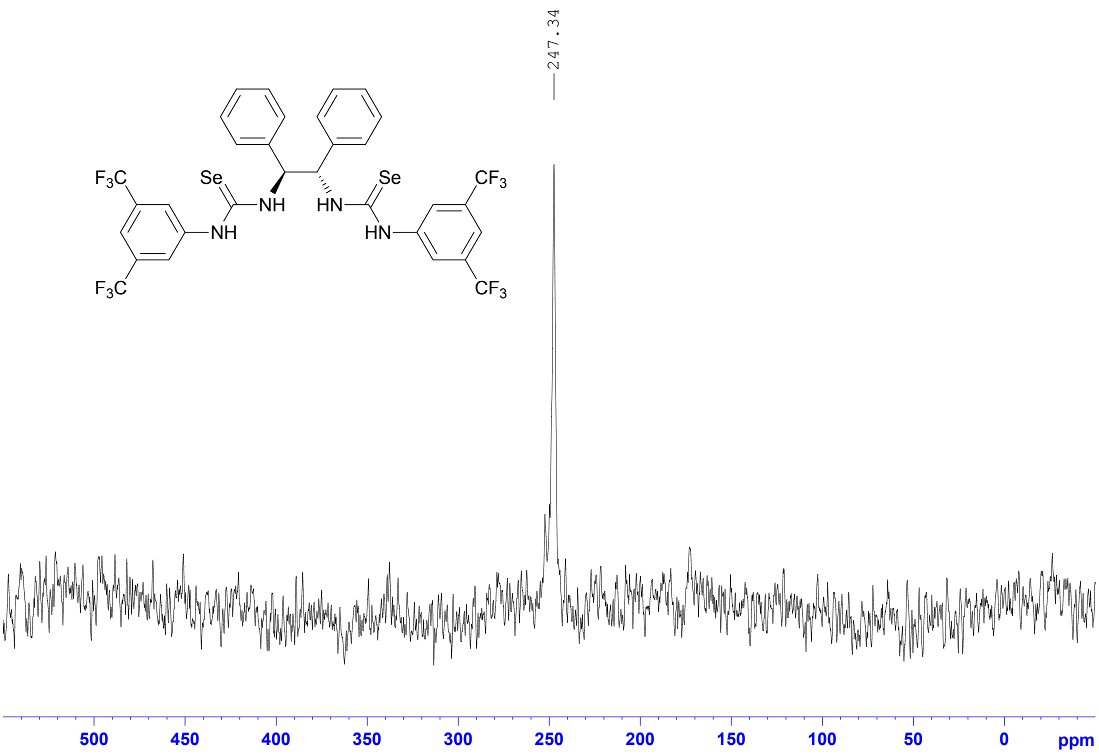


Figure S4. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2

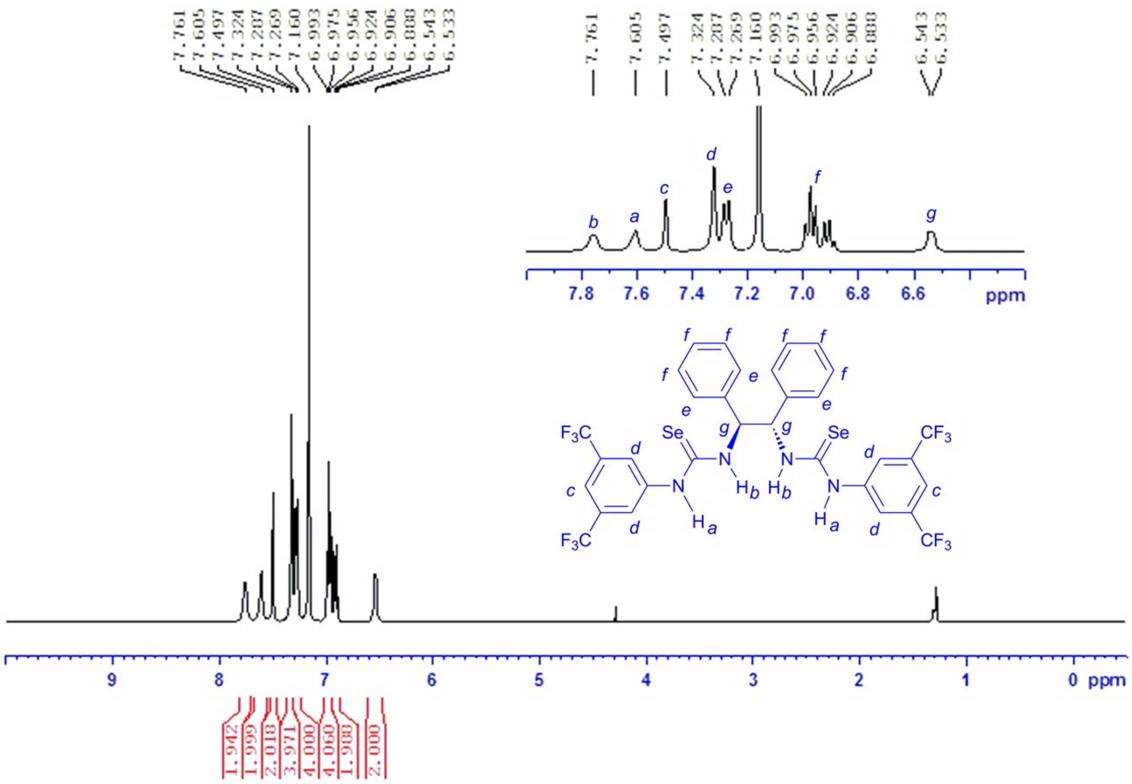


Figure S5. COSY NMR (500 MHz, C_6D_6) of (*S*, *S*)-CSA-2

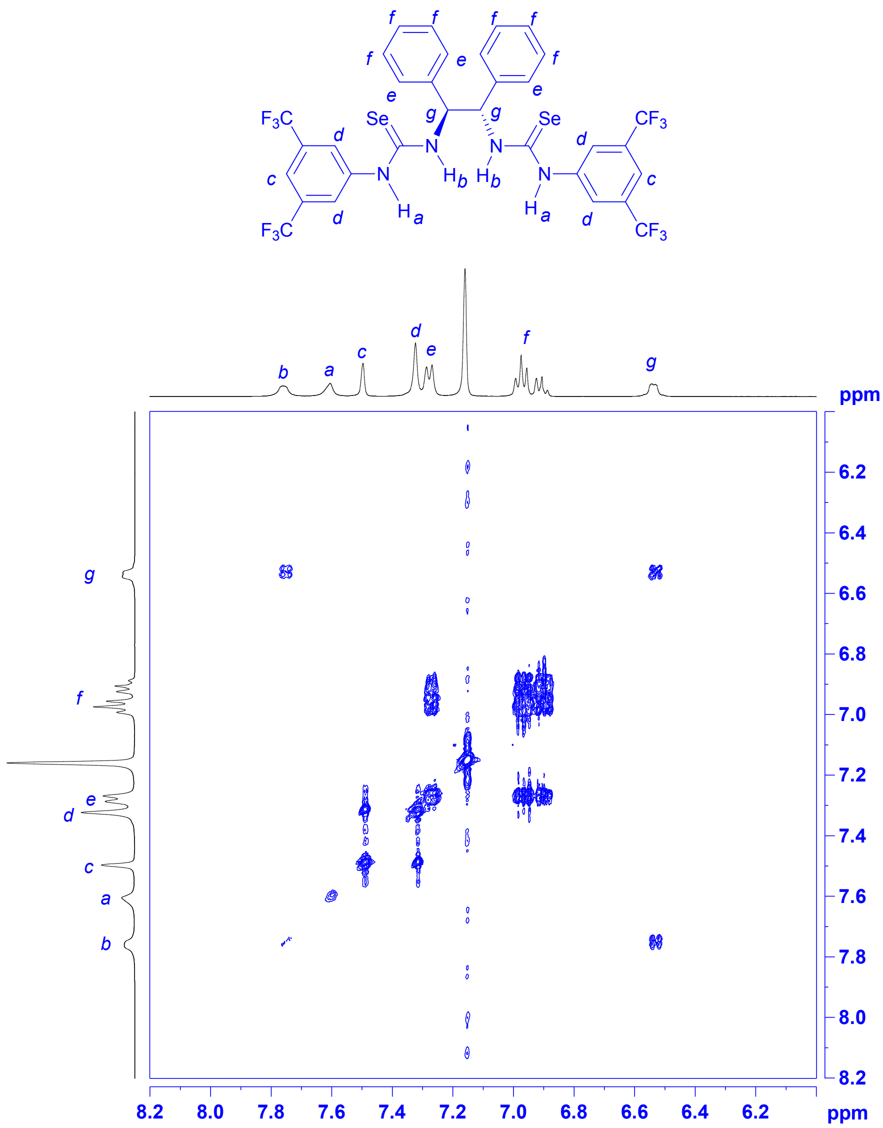


Figure S6. Contrasted ^{1}H NMR (400 MHz, $CDCl_3$) of A/(*S*, *S*)-CSA-2 and A/(*S*, *S*)-CSA-1.

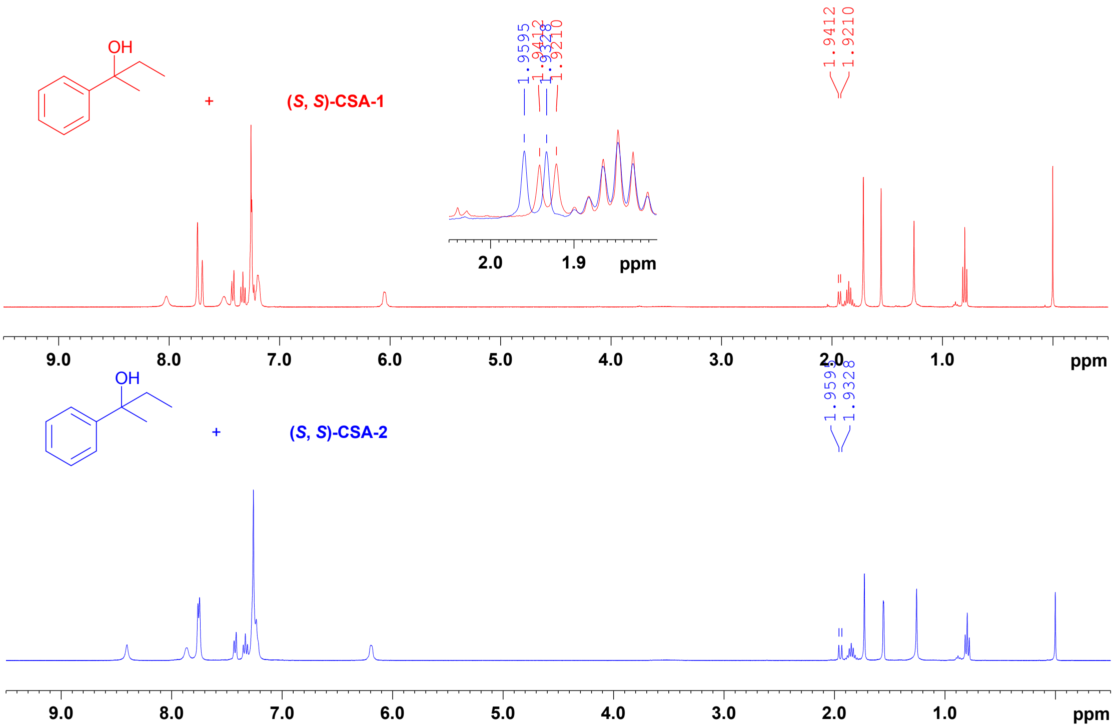


Figure S7. Contrasted ^{1}H NMR (400 MHz, $CDCl_3$) of B/(*S*, *S*)-CSA-2 and B/(*S*, *S*)-CSA-1.

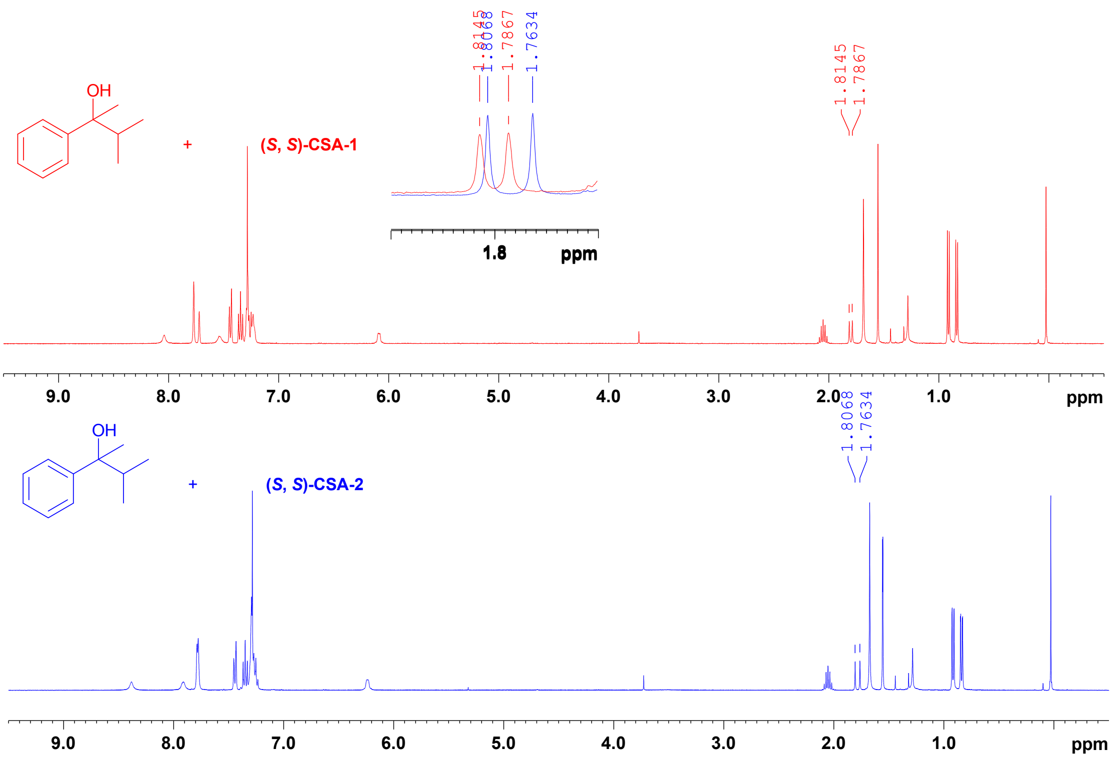


Figure S8. Contrasted ^{1}H NMR (400 MHz, $CDCl_3$) of D/(*S*, *S*)-CSA-2 and D/(*S*, *S*)-CSA-1.

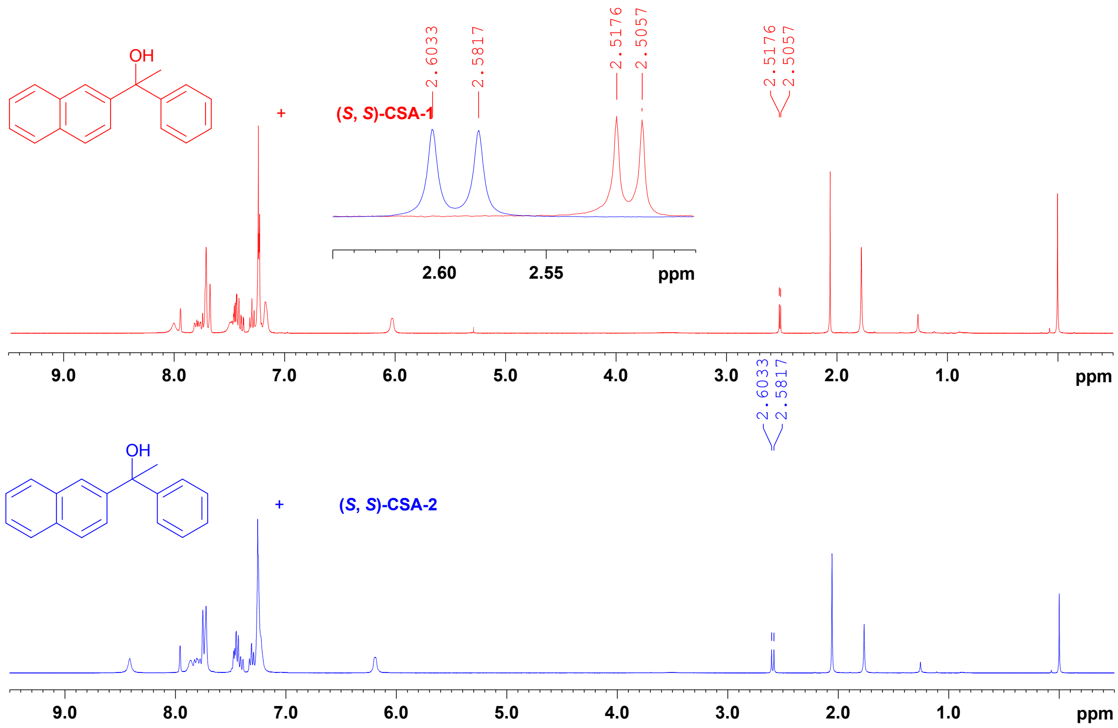


Figure S9. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and racemic guest A

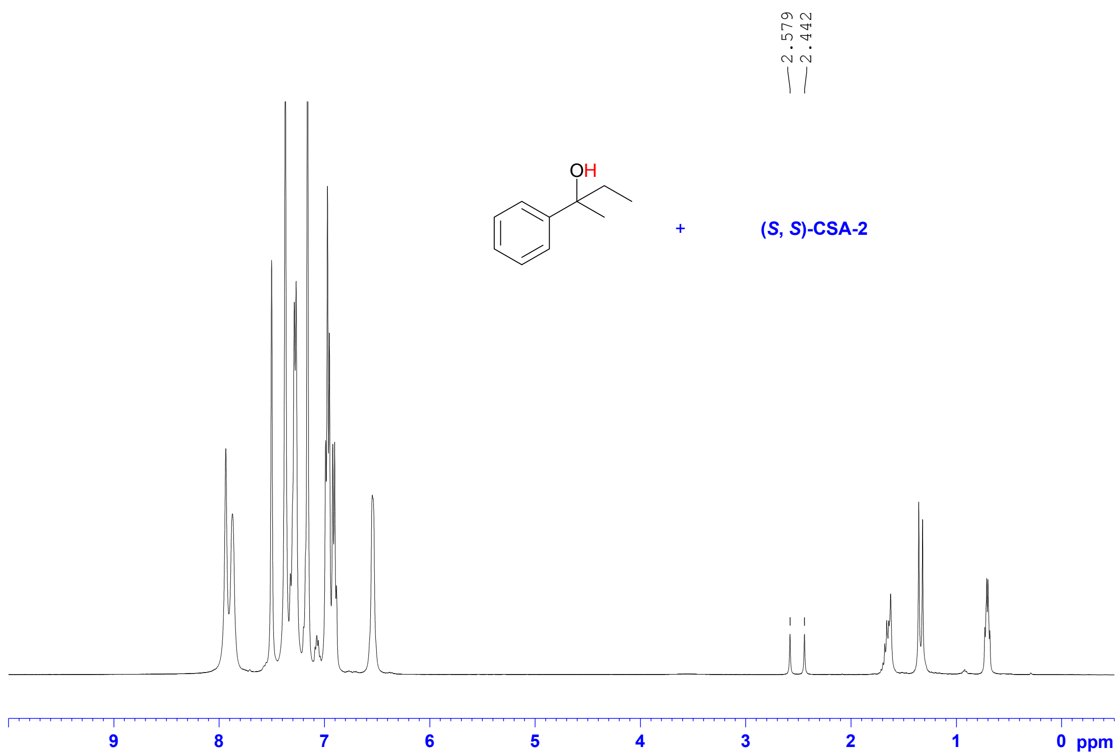


Figure S10. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2 and enantiomeric excess of guest A**

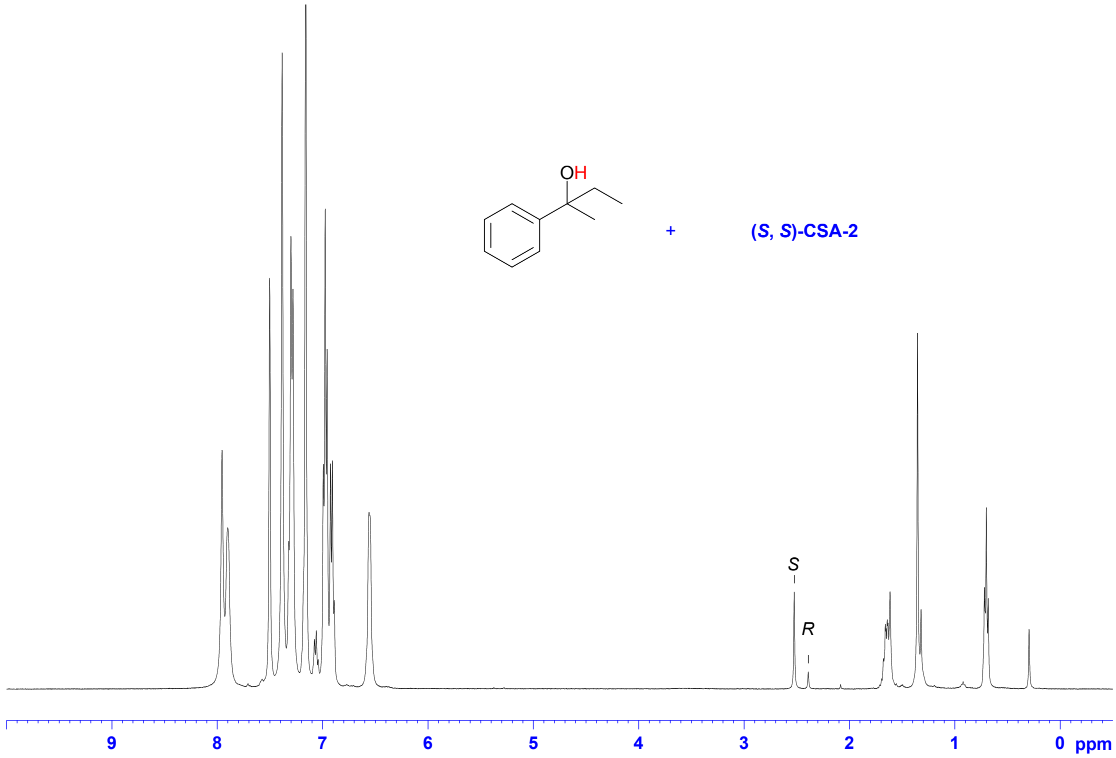


Figure S11. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2 and racemic tertiary alcohol B**

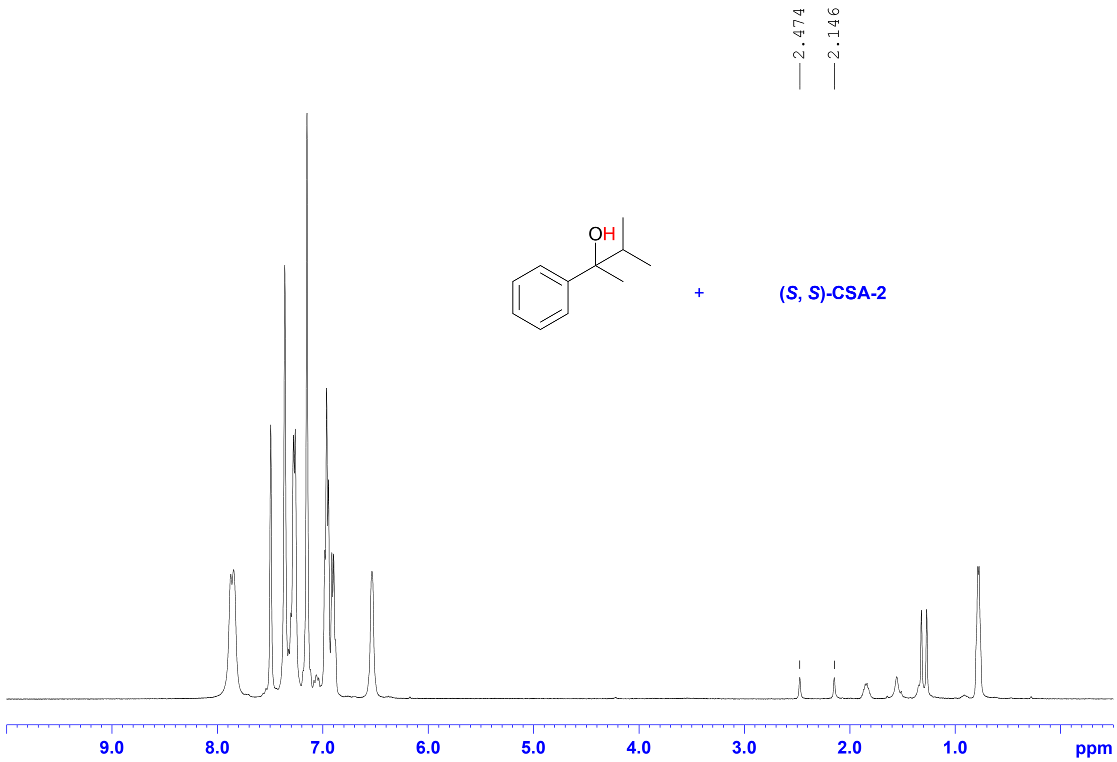


Figure S12. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and enantiomeric excess of guest B

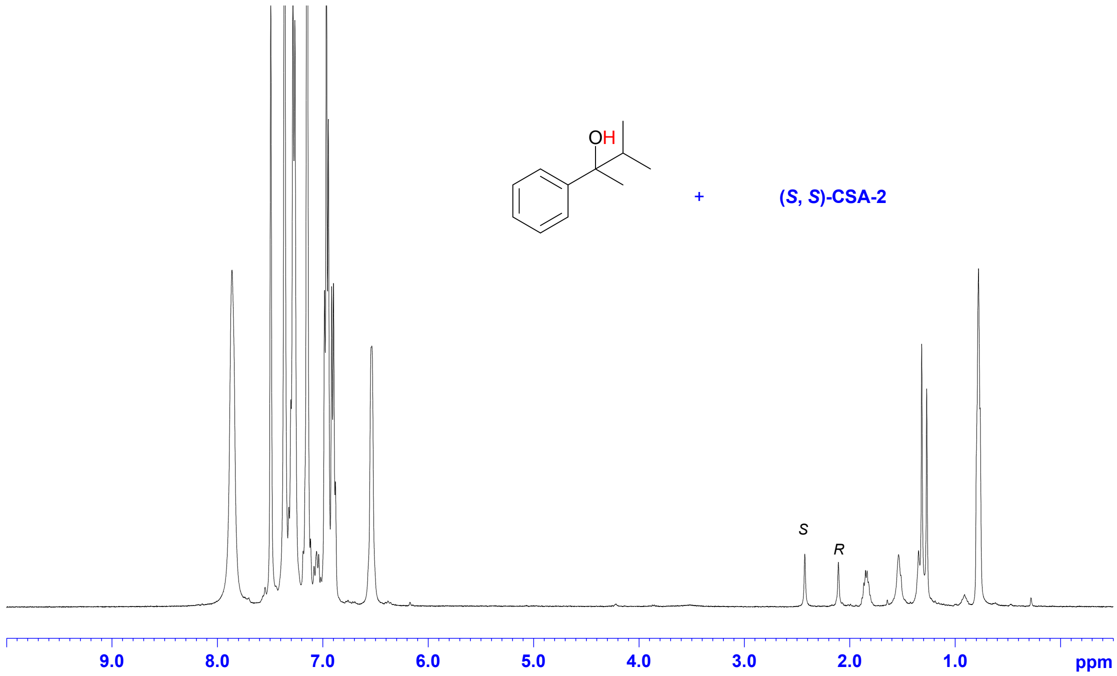


Figure S13. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and racemic guest C

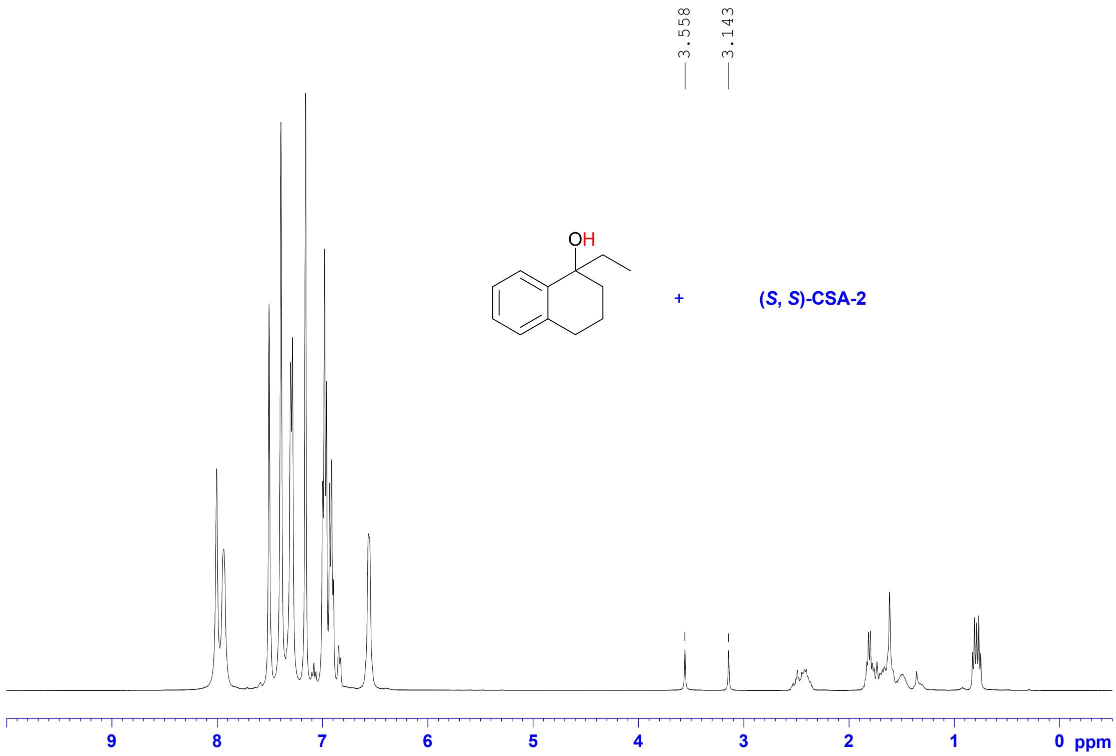


Figure S14. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and enantiomeric excess of guest C

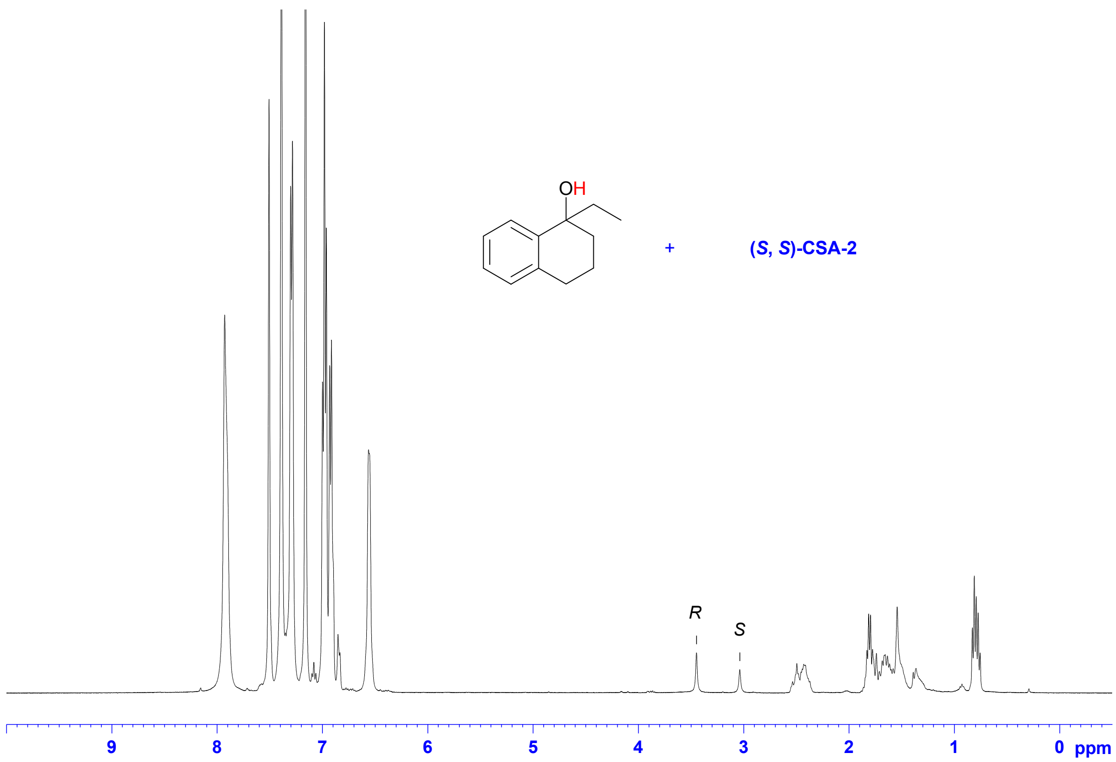


Figure S15. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and racemic guest D

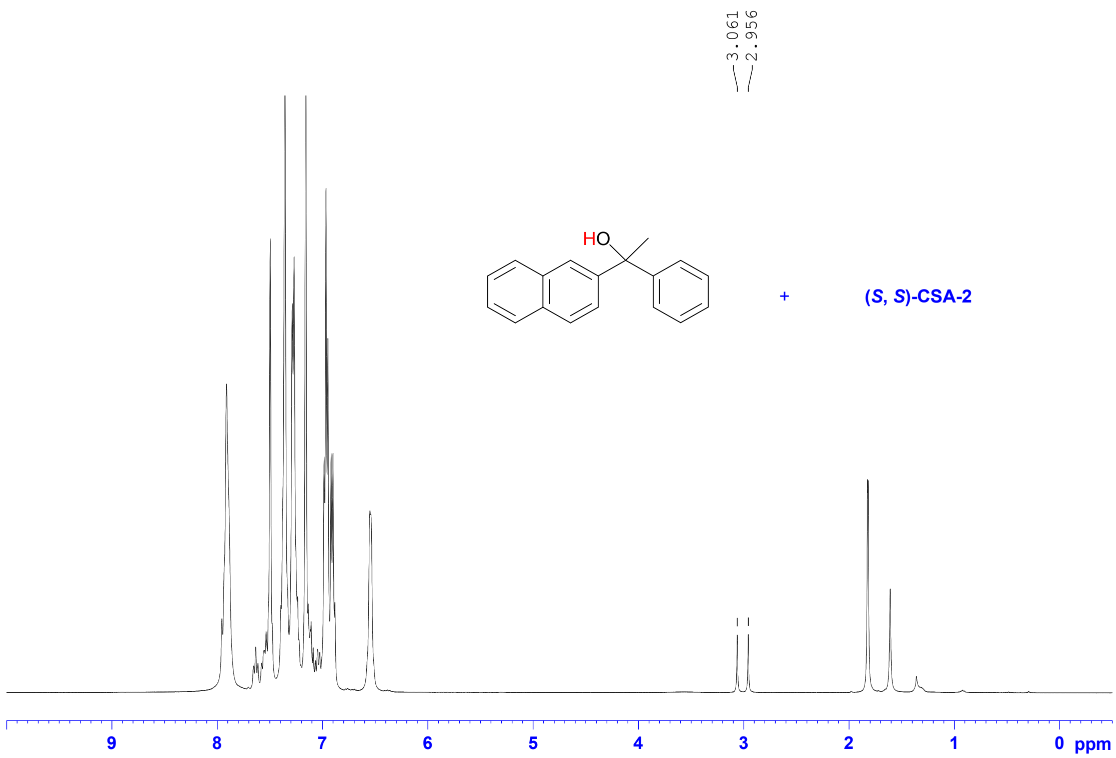


Figure S16. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and enantiomeric excess of guest D

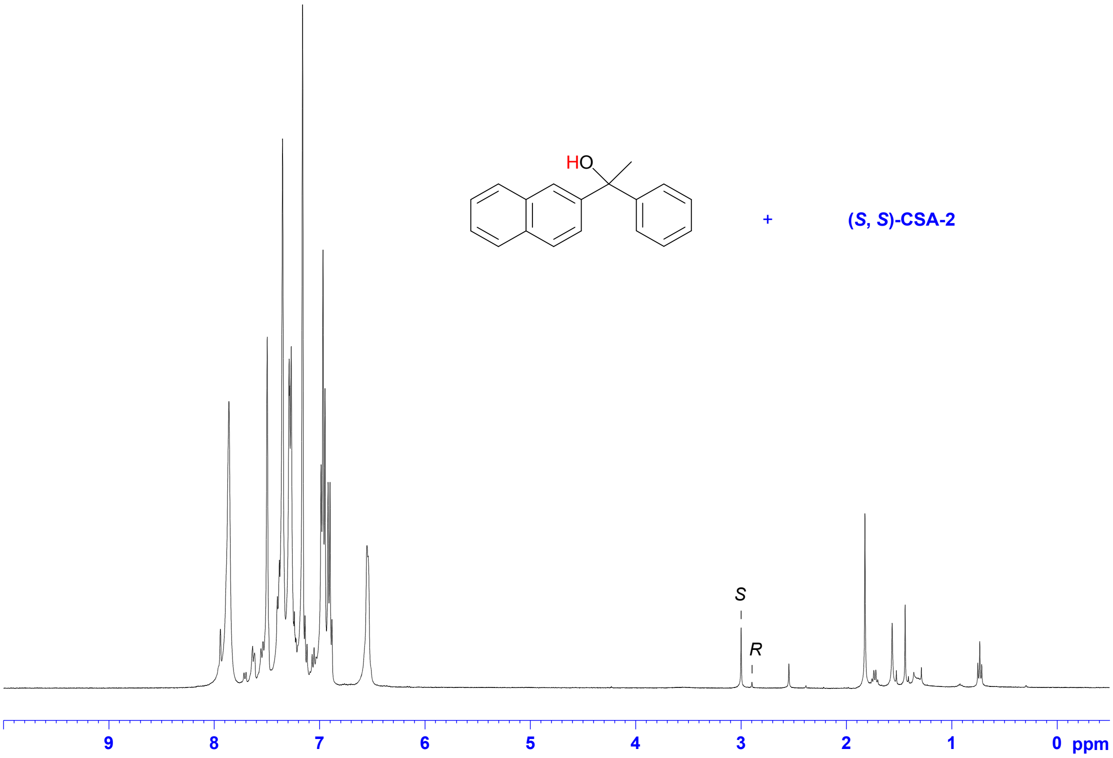


Figure S17. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and racemic guest E

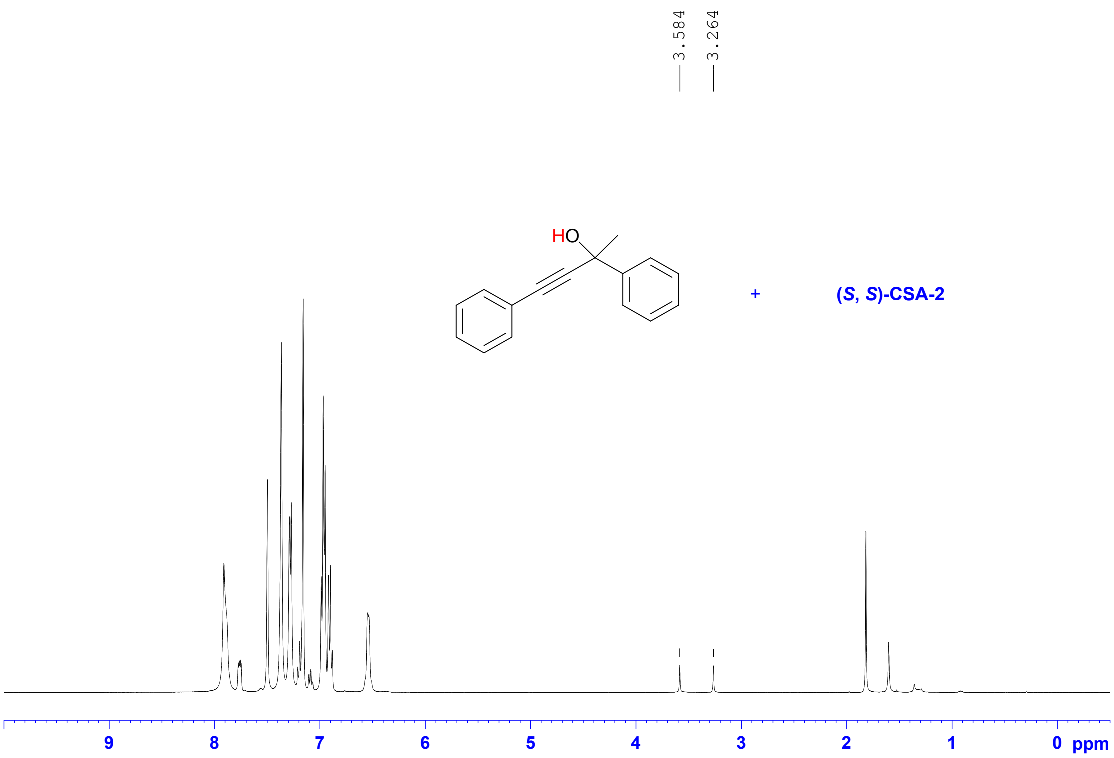


Figure S18. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2and enantiomeric excess of guest E**

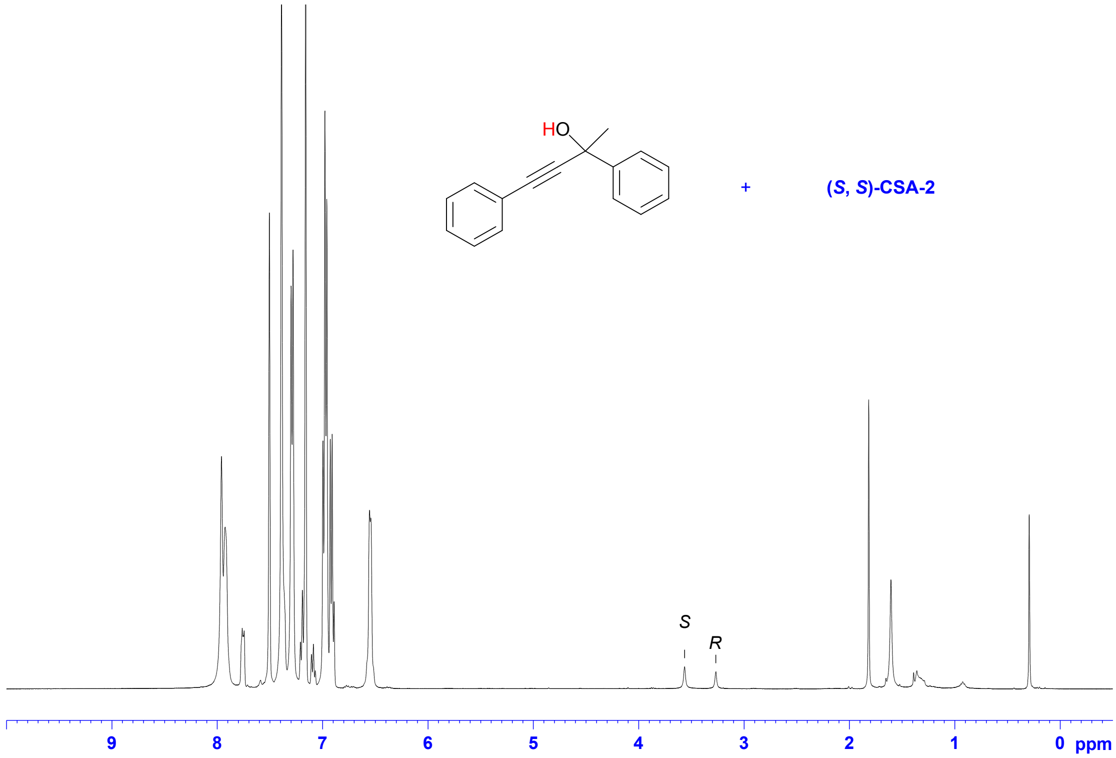


Figure S19. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2and racemic guest F**

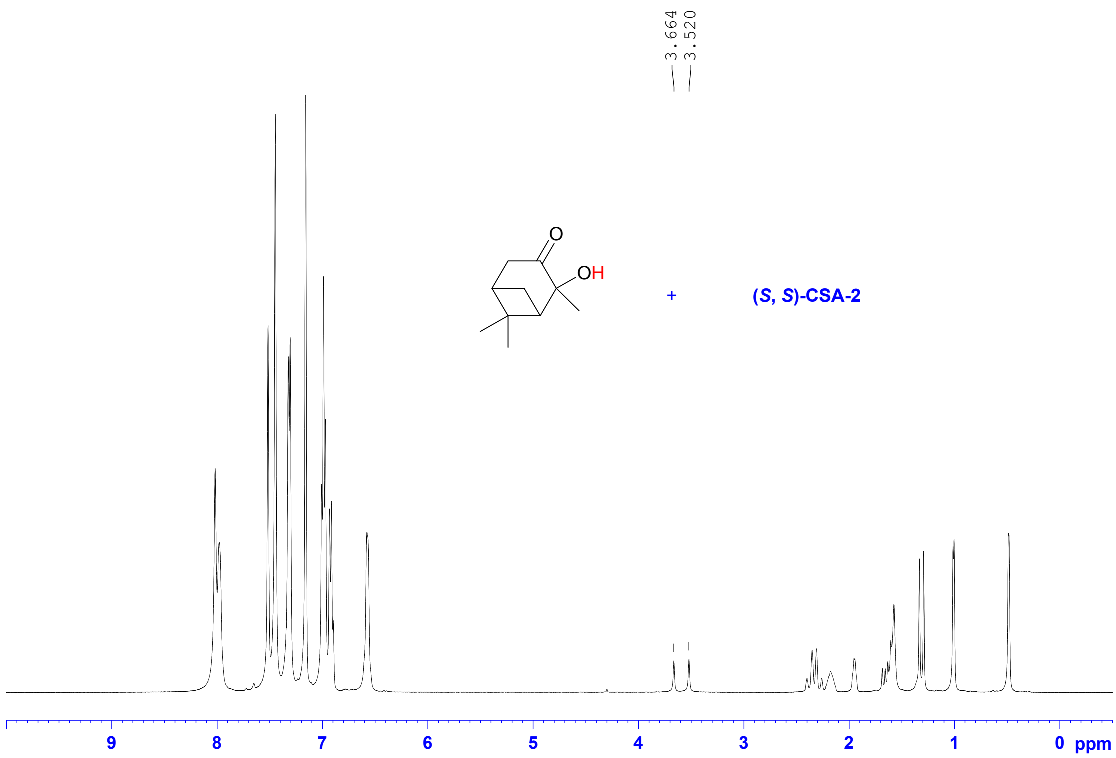


Figure S20. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and enantiomeric excess of guest F

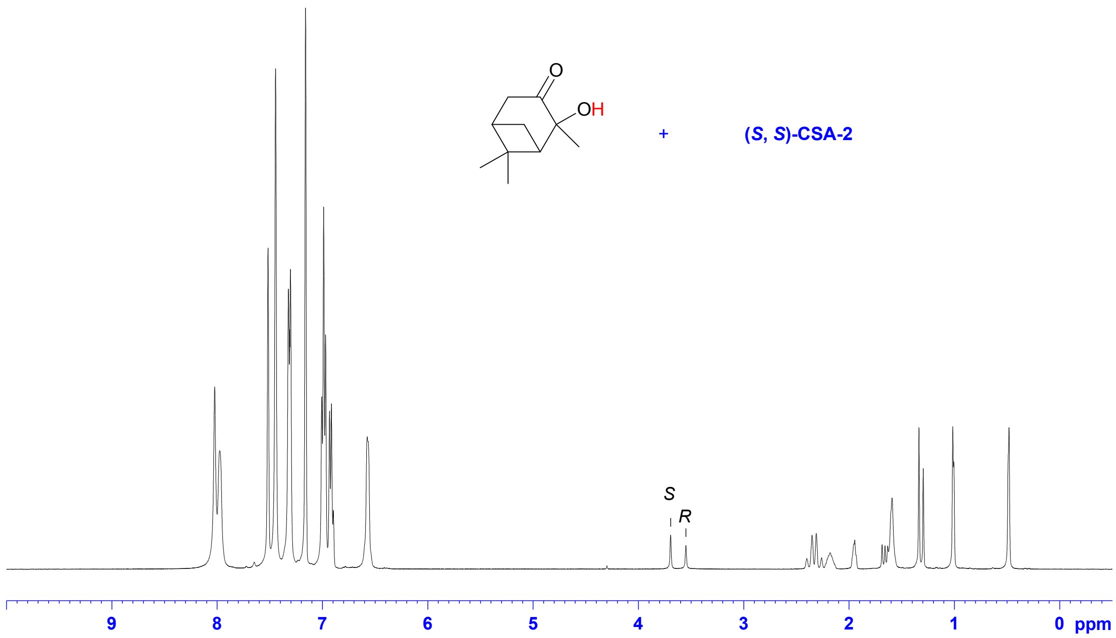


Figure S21. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and racemic guest G

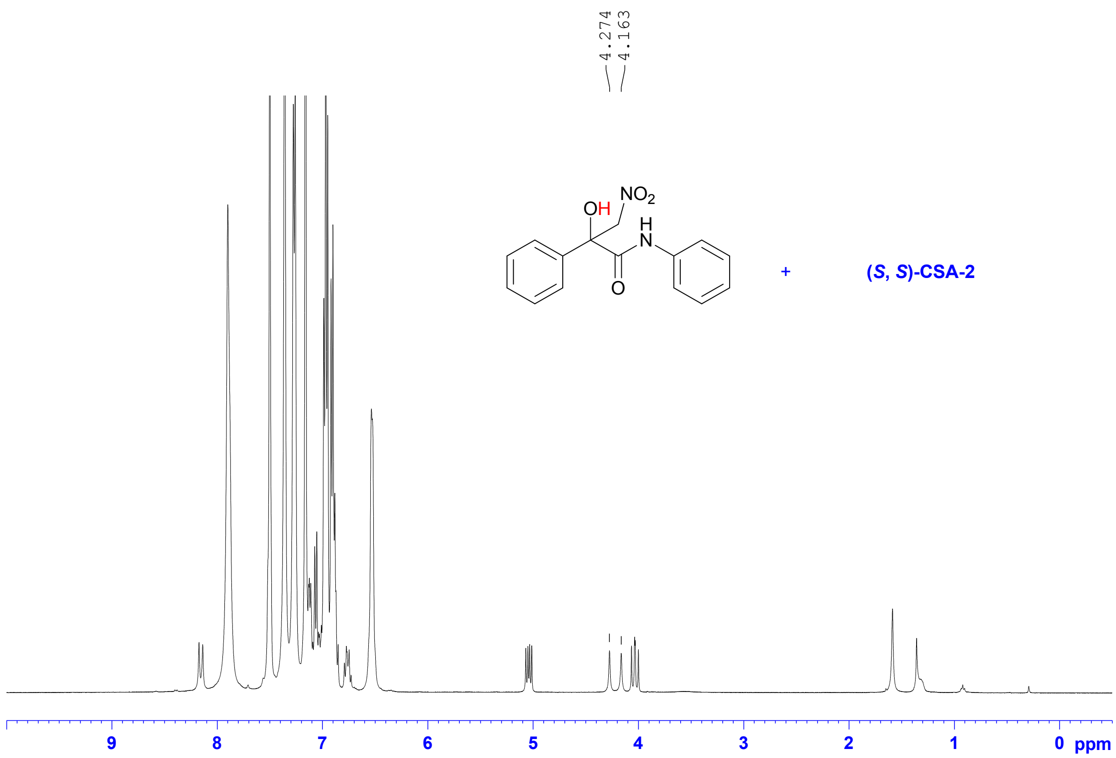


Figure S22. **^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and enantiomeric excess of guest G**

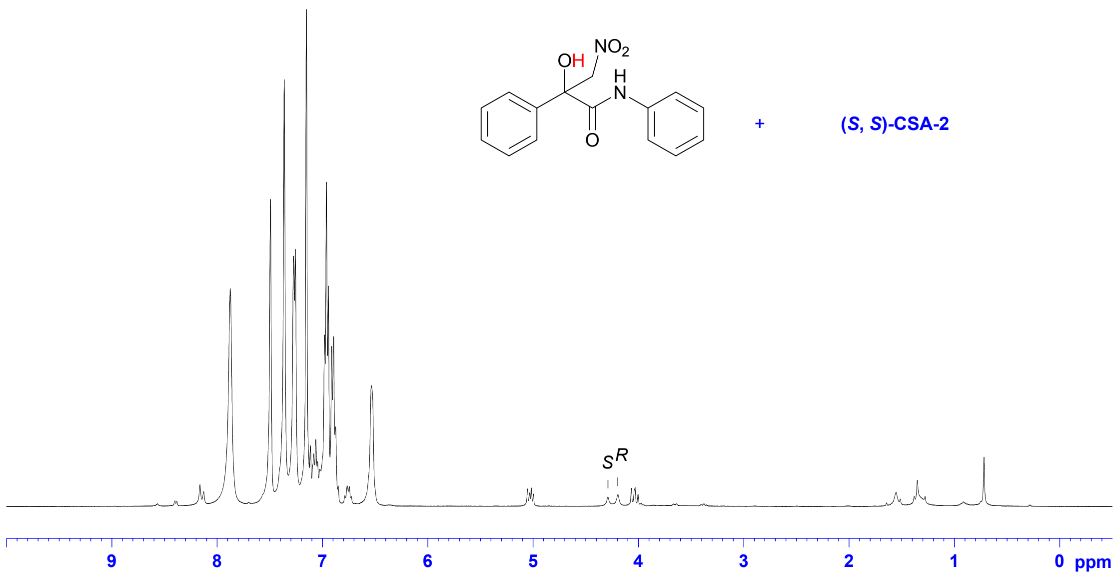


Figure S23. **^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and racemic guest H**

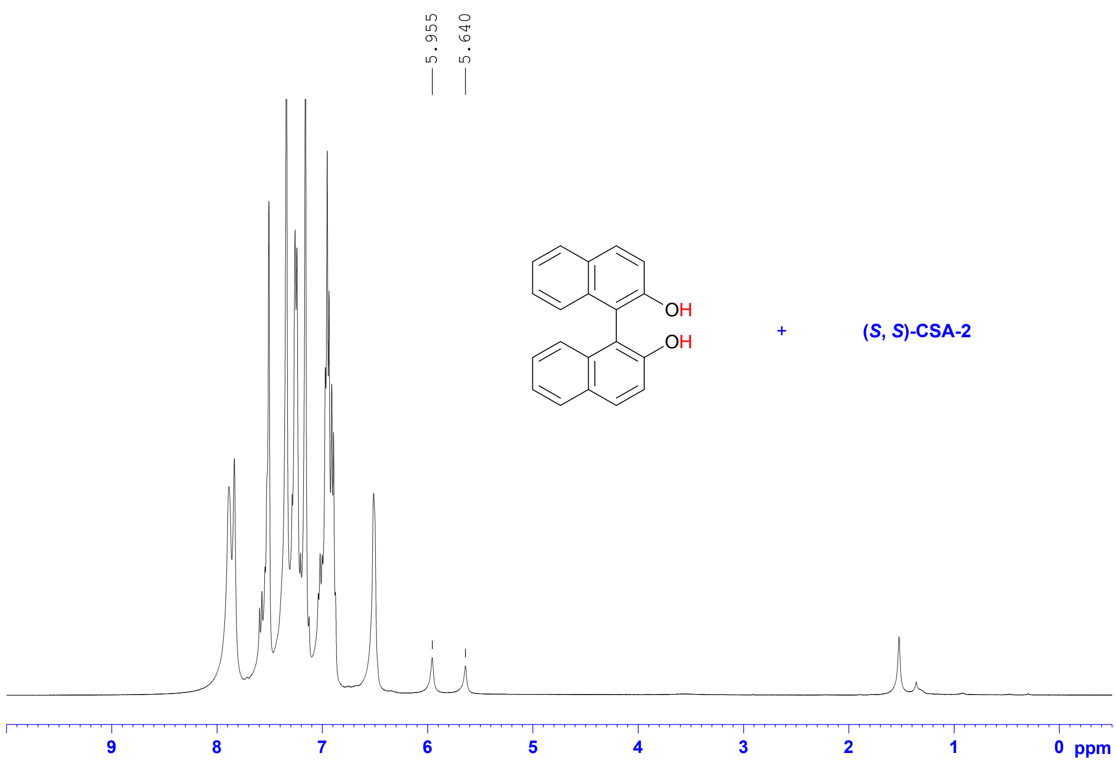


Figure S24. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2and enantiomeric excess of guest H**

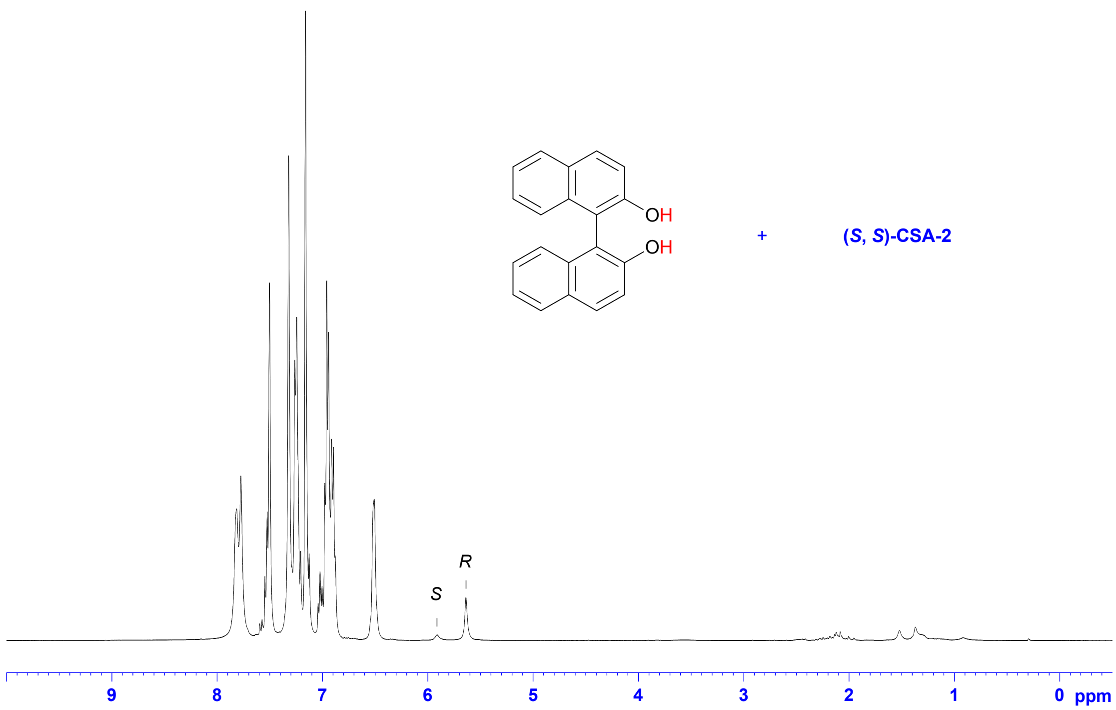


Figure S25. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2and racemic guest I**

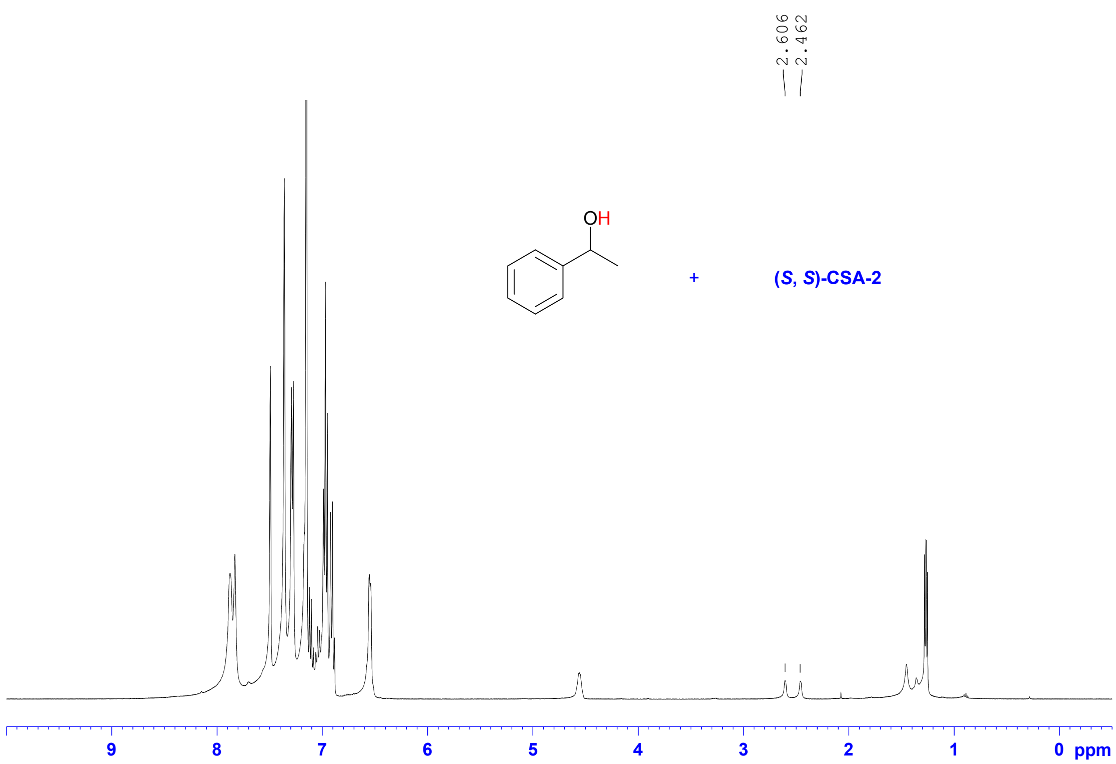


Figure S26. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2and enantiomeric excess of guest I**

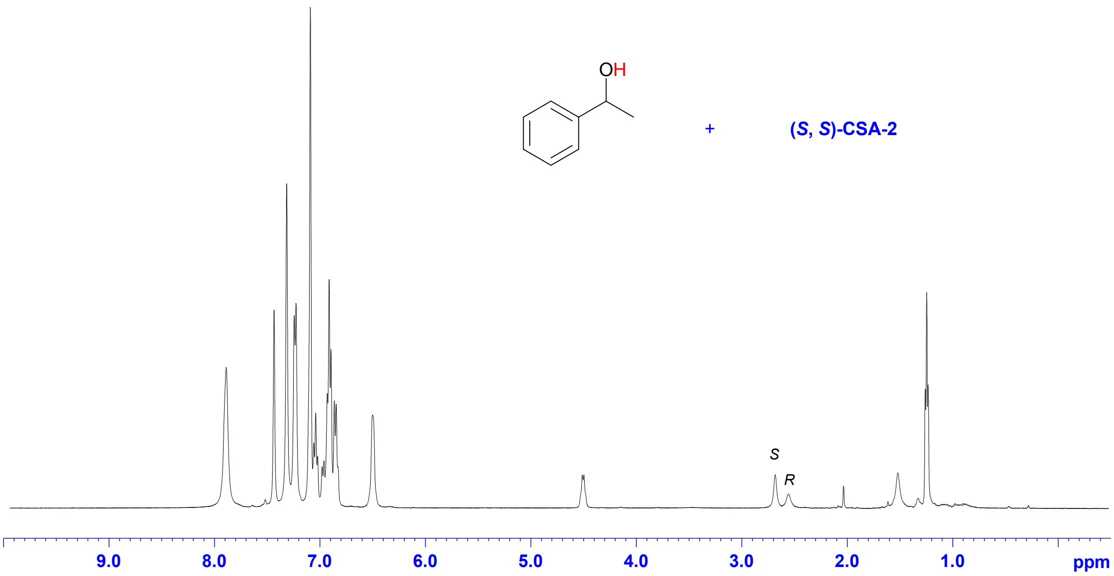


Figure S27. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2 and racemic guest J**

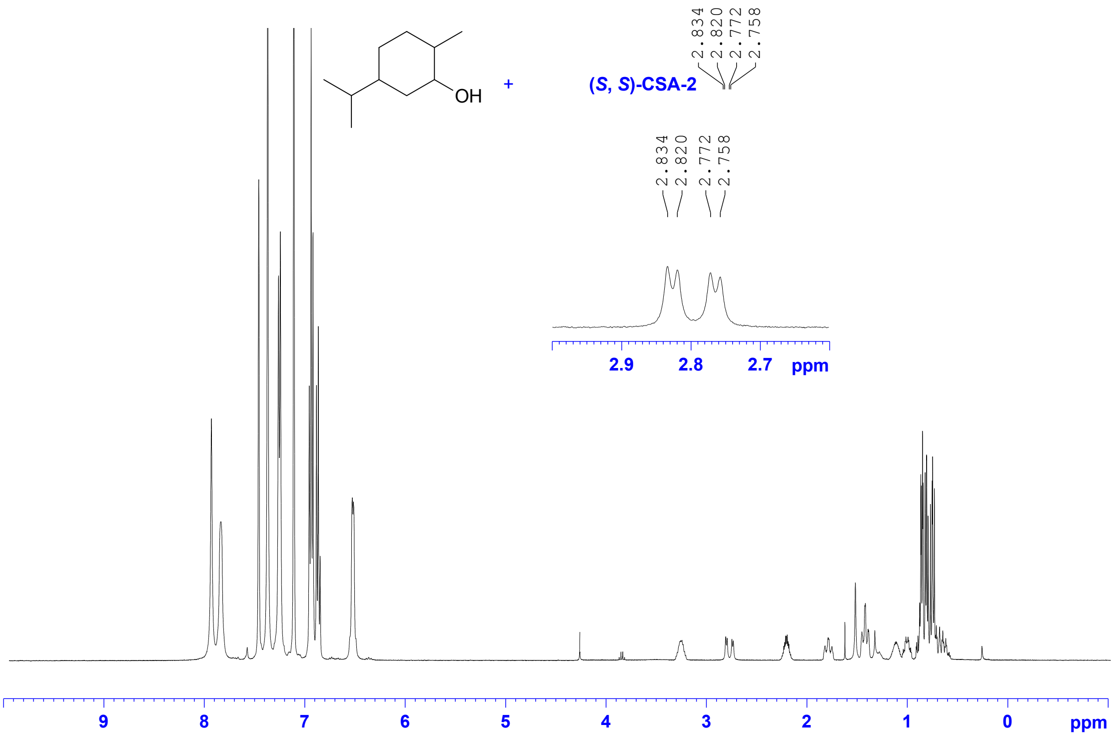


Figure S28. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and enantiomeric excess of guest J

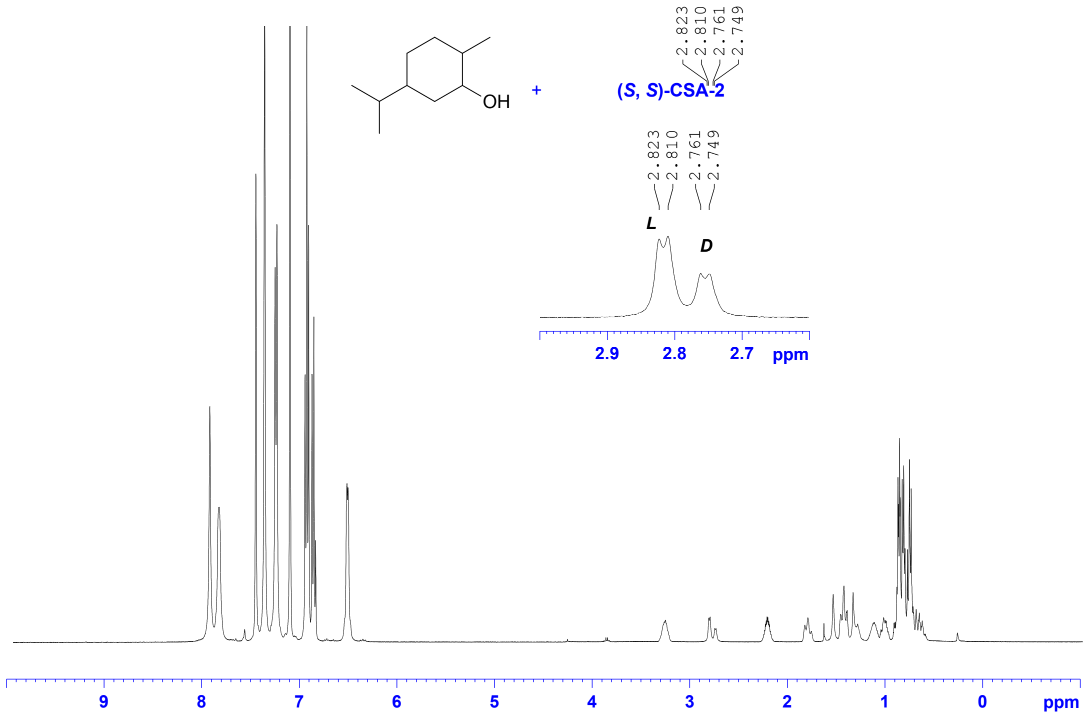


Figure S29. ^{19}F NMR (376 MHz, C_6D_6, with proton decoupling) of (*S*, *S*)-CSA-2 and racemic guest K

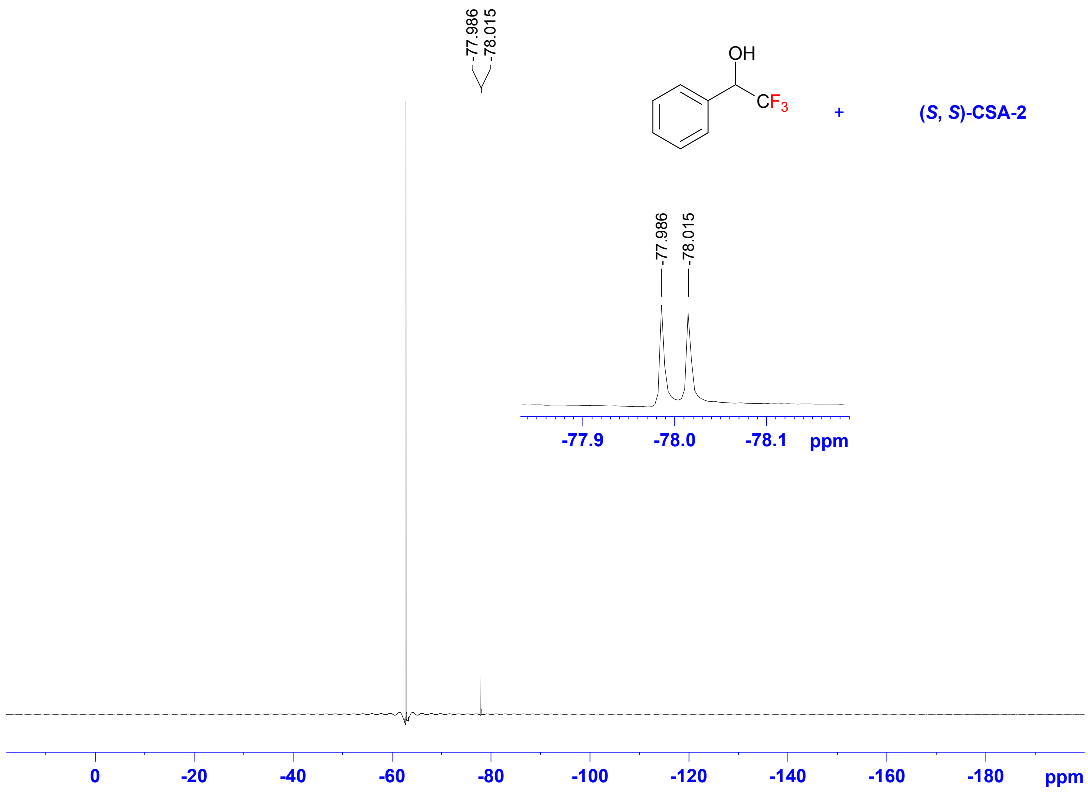


Figure S30. ^{19}F NMR (376 MHz, C_6D_6, with proton decoupling) of (*S*, *S*)-CSA-2 and enantiomeric excess of guest K

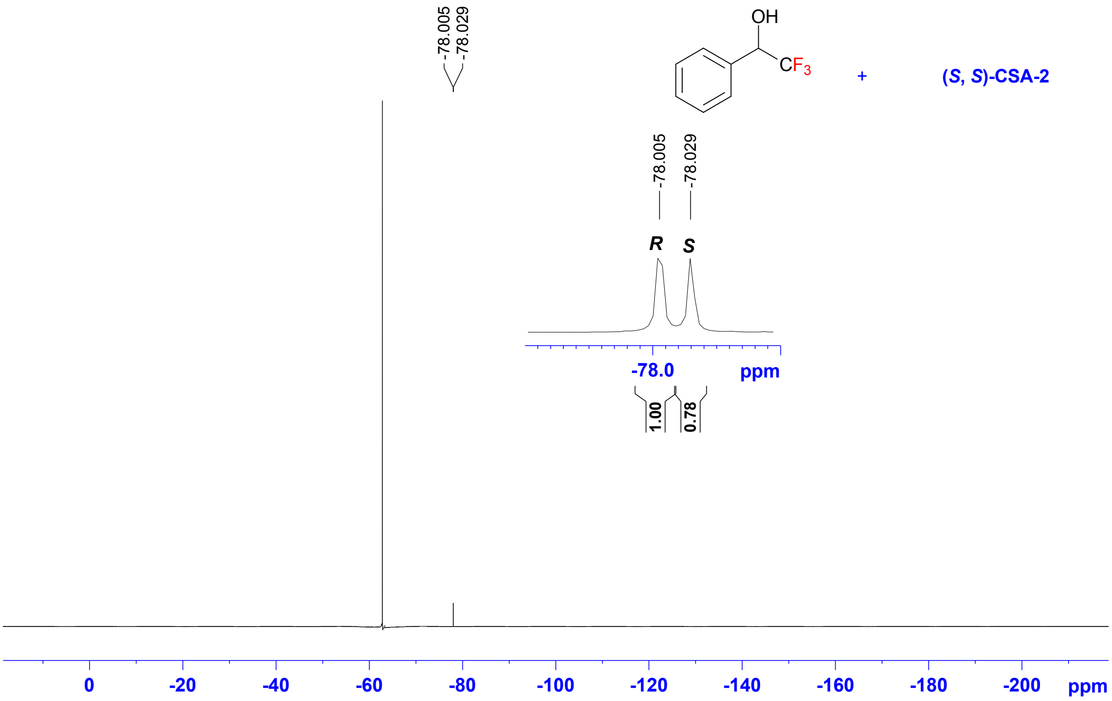


Figure S31. ^{19}F NMR (376 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and racemic guest L

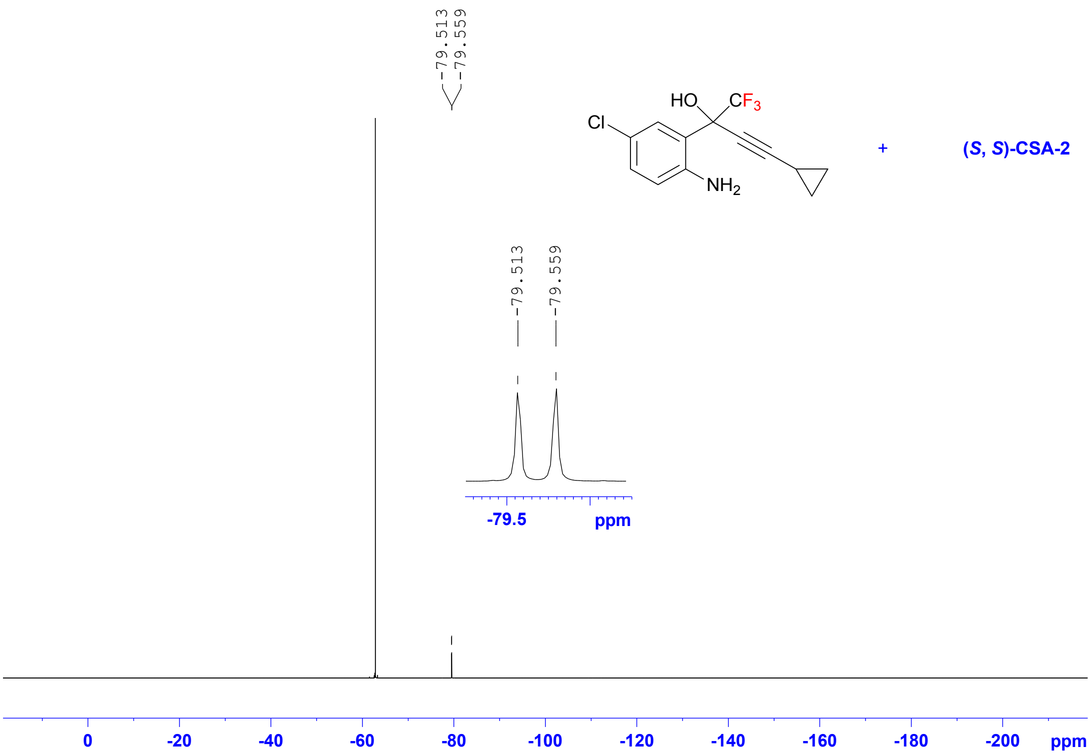


Figure S32. ^{19}F **NMR (376 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2 and enantiomeric excess of guest L**

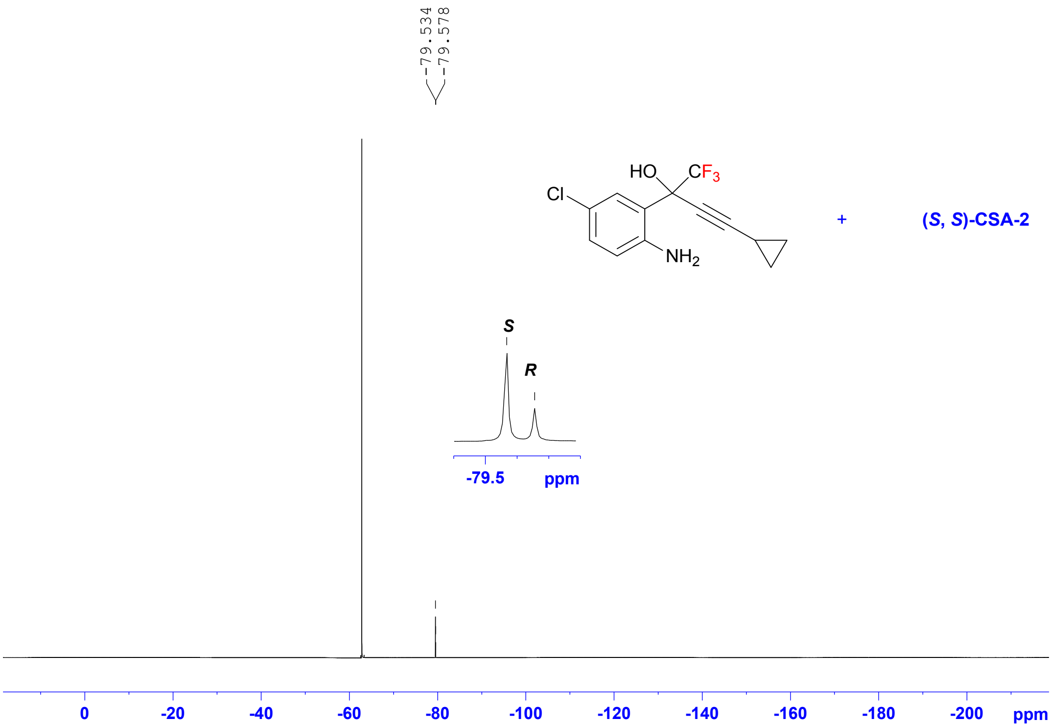


Figure S33. 2D NOESY (500 MHz, C_6D_6**) of racemic A (100 mM) and (*S*, *S*)-CSA-2 (100 mM).**

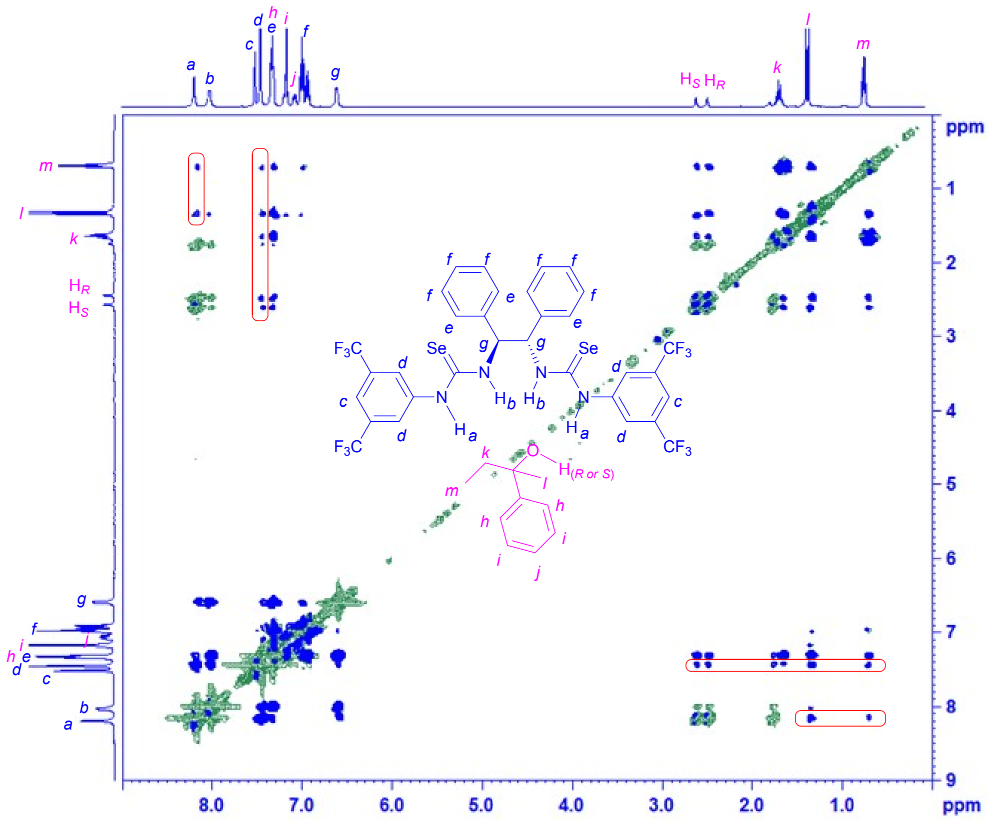


Figure S34. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest I at different time point (ee 34% (*S*)).

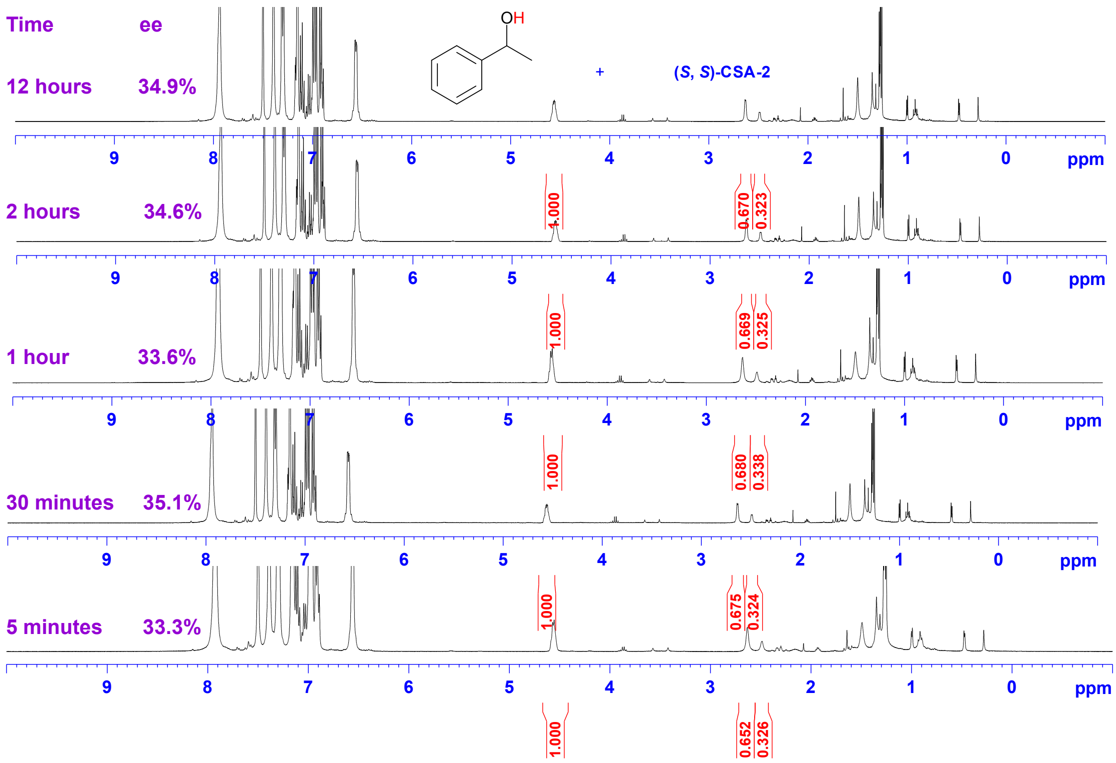


Figure S35. ^{1}H NMR (400 MHz, Toluene-d8) of (*S*, *S*)-CSA-2 and guest I at different temperatures (ee 30% (*S*)).

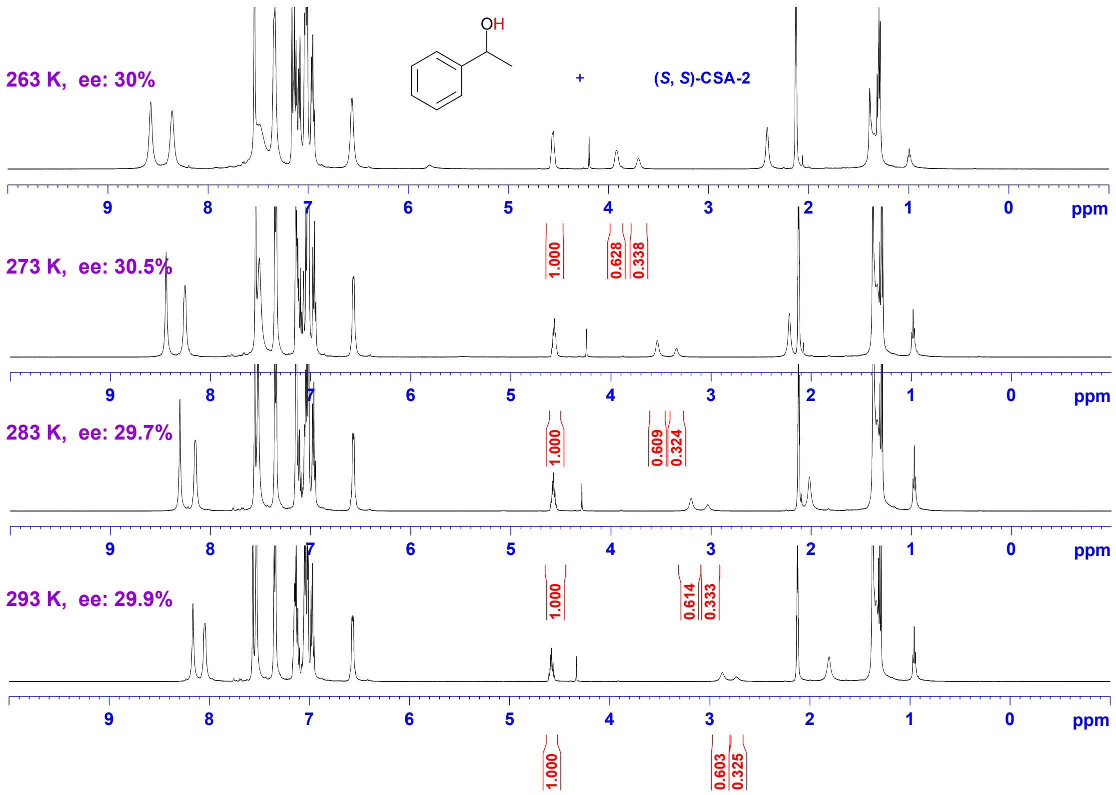


Figure S36. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest F (Sample 1, ee 90.0% (*S*))

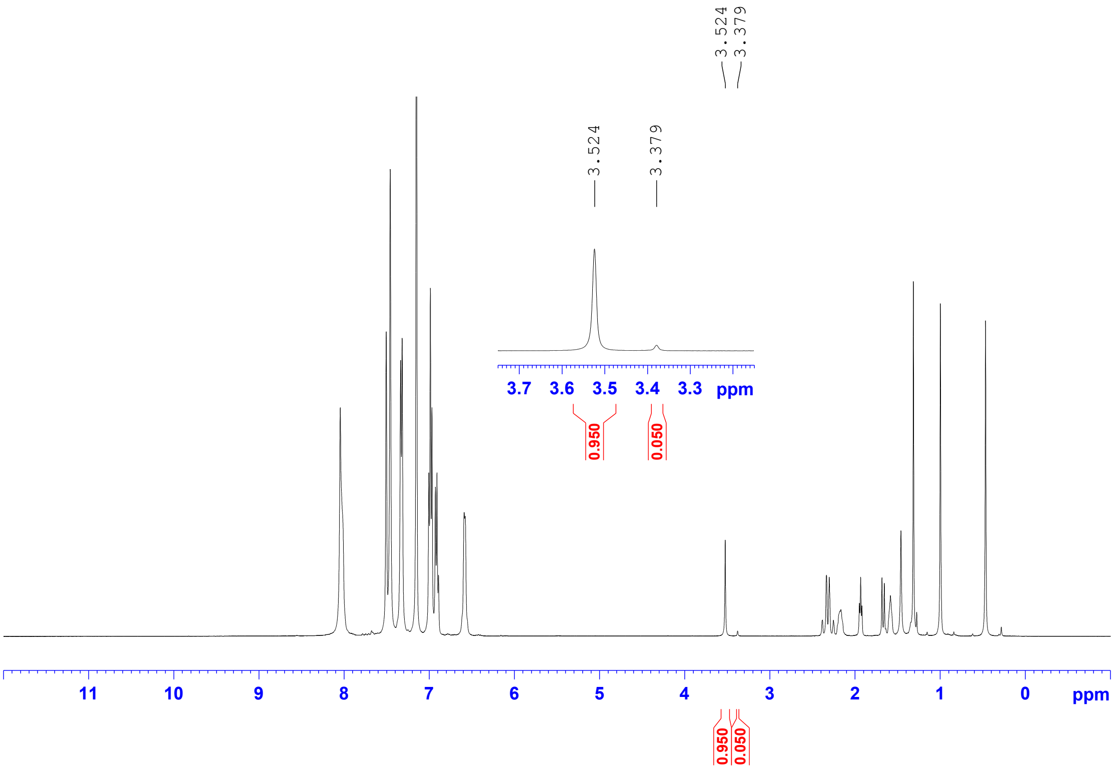
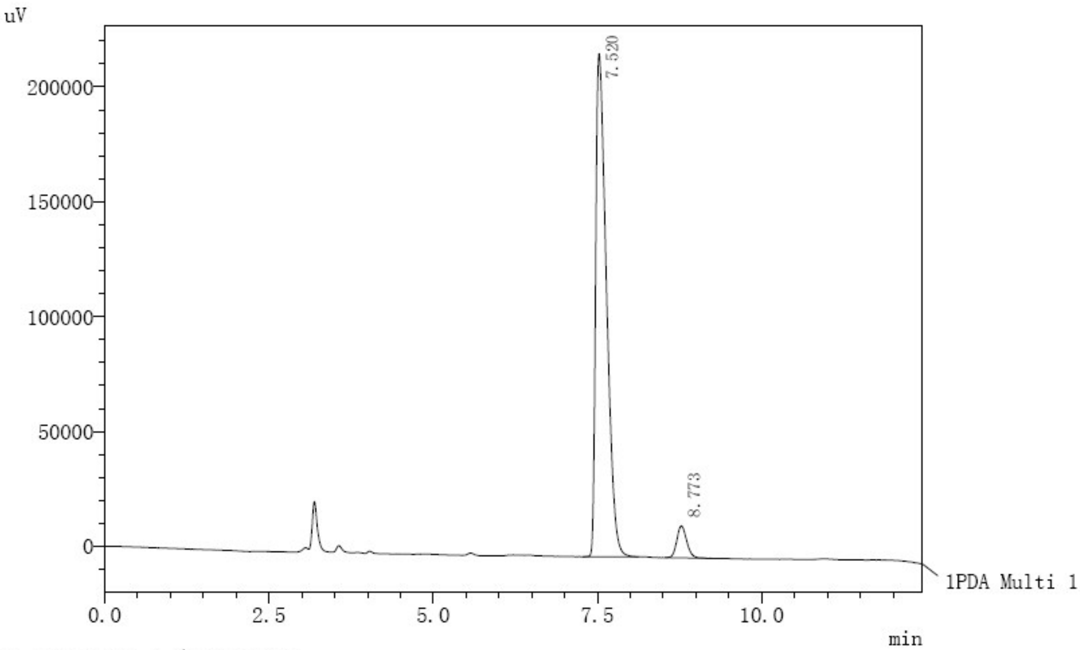


Figure S37. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 1, ee 88.9% (*S*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.520	2484021	218974	94.438	94.438
2	8.773	146300	13981	5.562	5.562
Total		2630321	232955	100.000	

Figure S38. ¹H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest F (Sample 2, ee 84.6% (*S*))

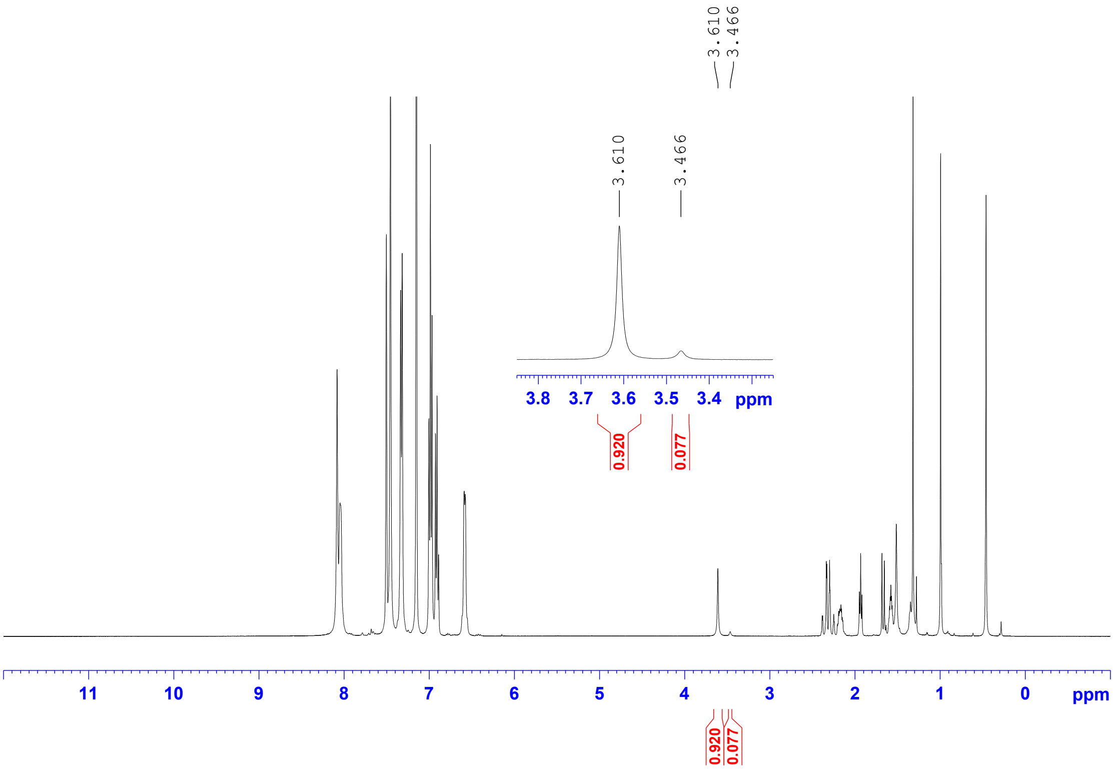
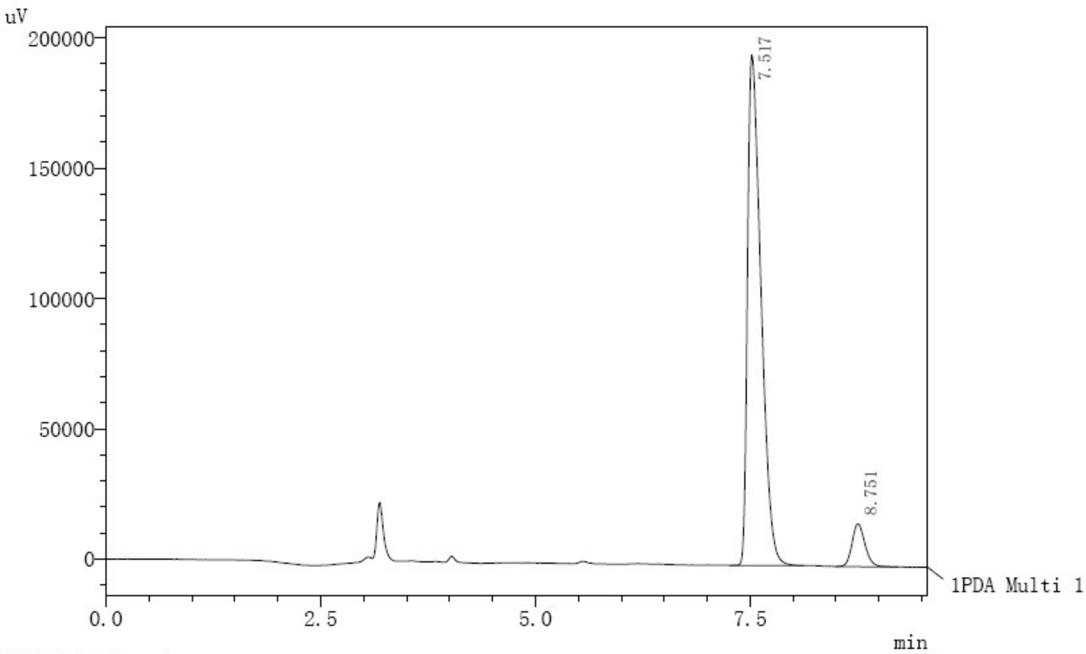


Figure S39. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 2, ee 85.1% (*S*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.517	2136187	195922	92.540	92.540
2	8.751	172209	16424	7.460	7.460
Total		2308396	212347	100.000	

Figure S40. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest F (Sample 3, ee 69.7% (*S*))

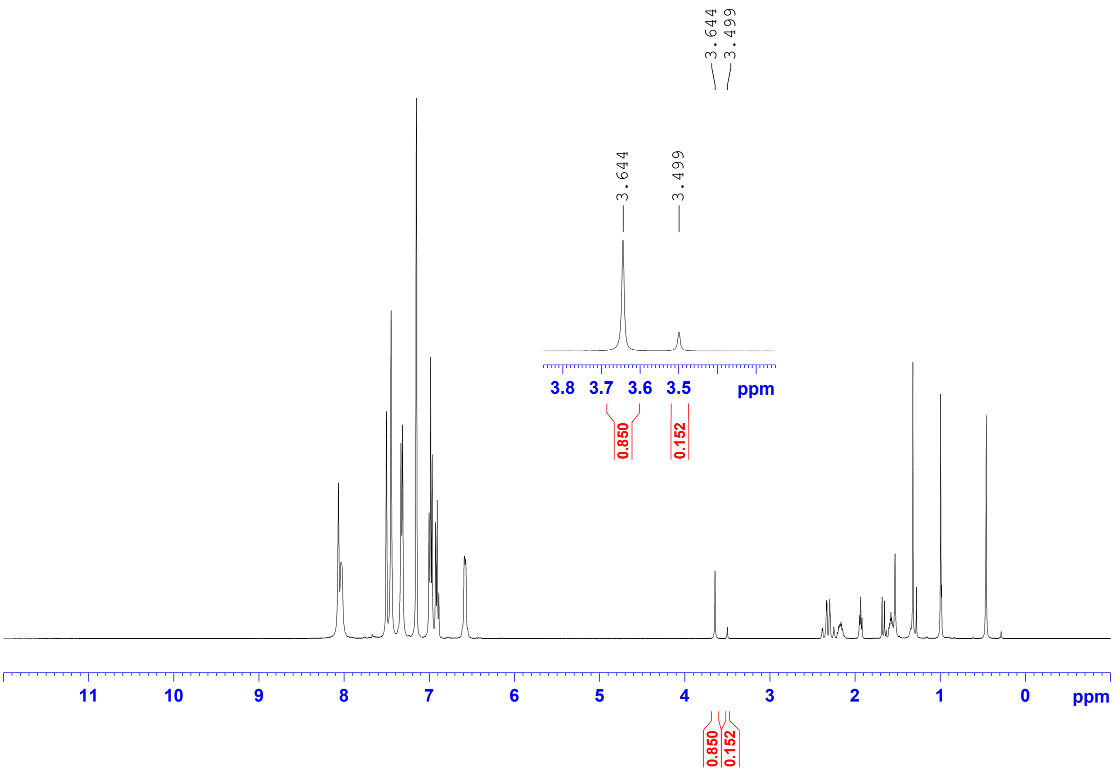
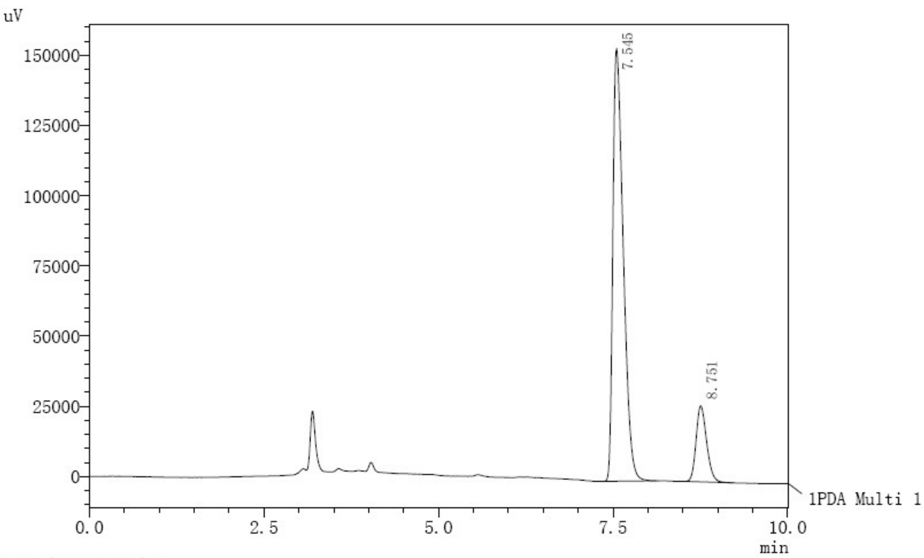


Figure S41. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 3, ee 69.7% (*S*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.545	1592167	154136	84.846	84.846
2	8.751	284363	27100	15.154	15.154
Total		1876531	181236	100.000	

Figure S42. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest F (Sample 4, ee 52.4% (*S*))

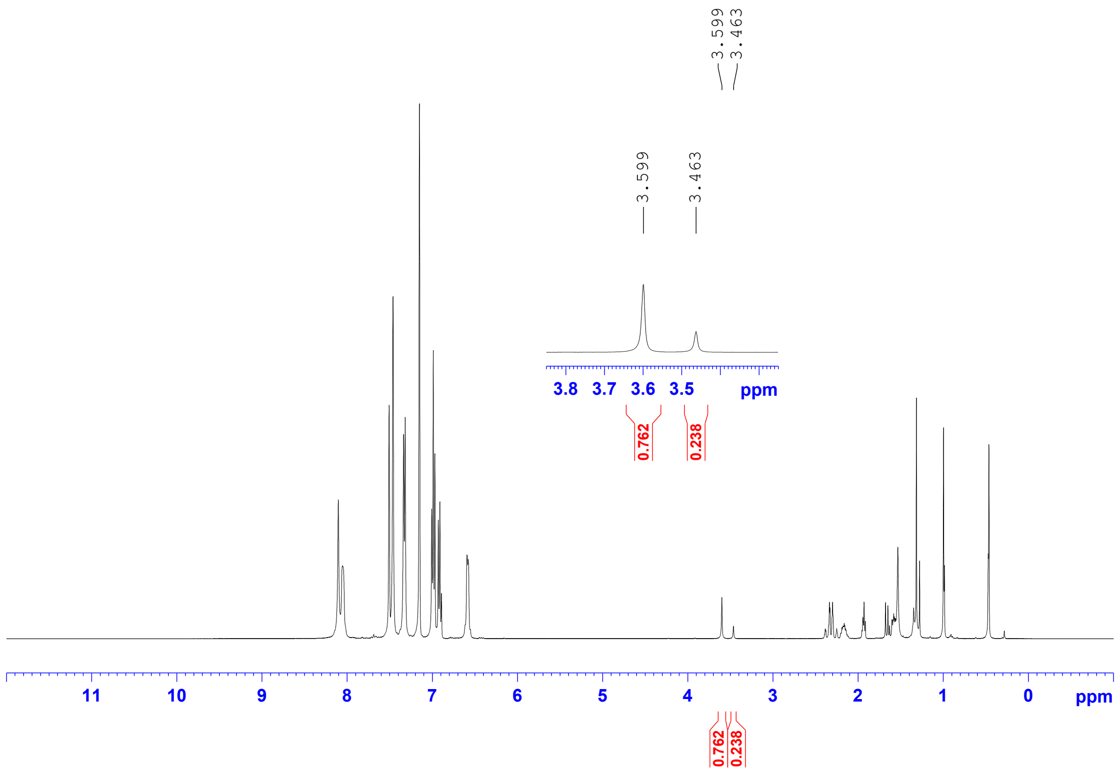
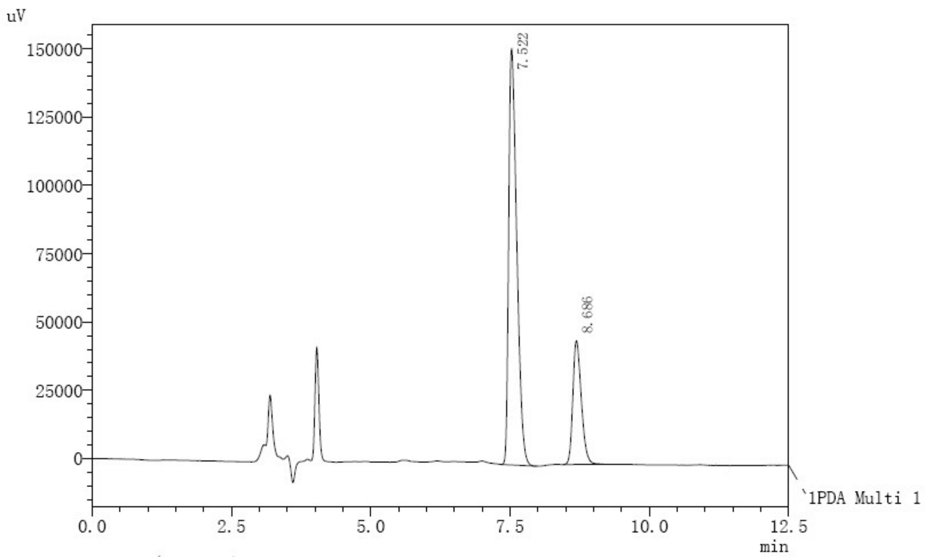


Figure S43. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 4, ee 52.3% (*S*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.522	1534393	152437	76.126	76.126
2	8.686	481213	45370	23.874	23.874
Total		2015606	197807	100.000	

Figure S44. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest F (Sample 5, ee 33.0% (*S*))

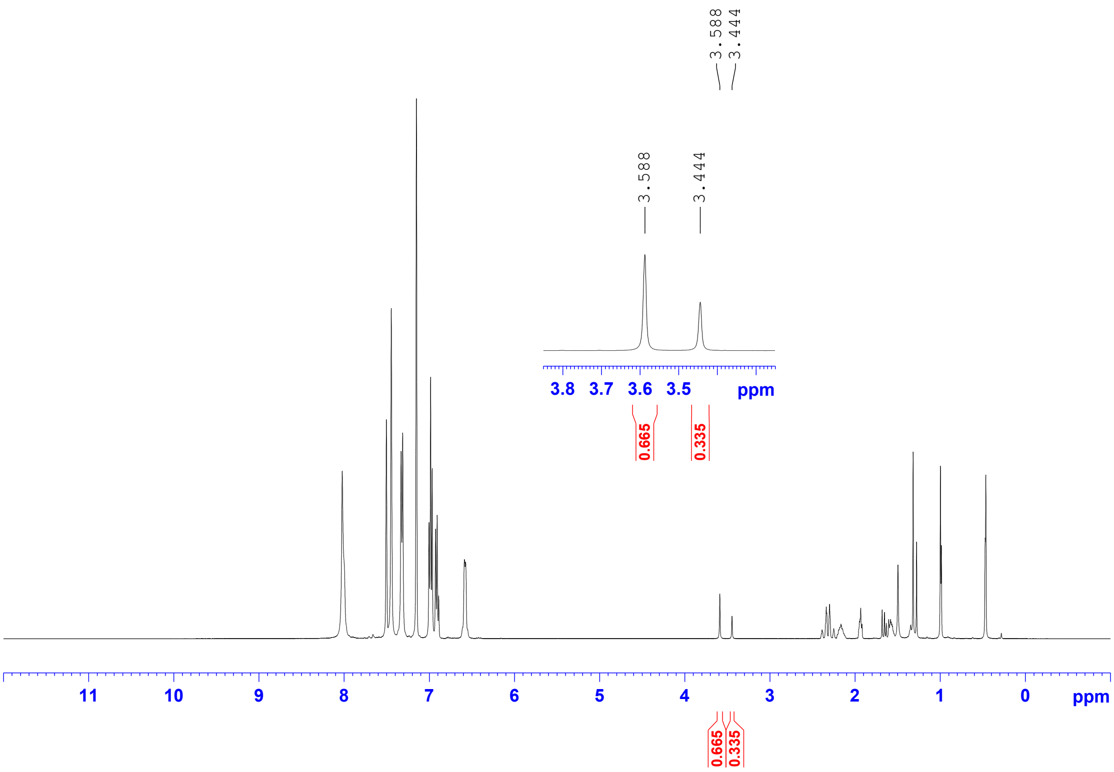
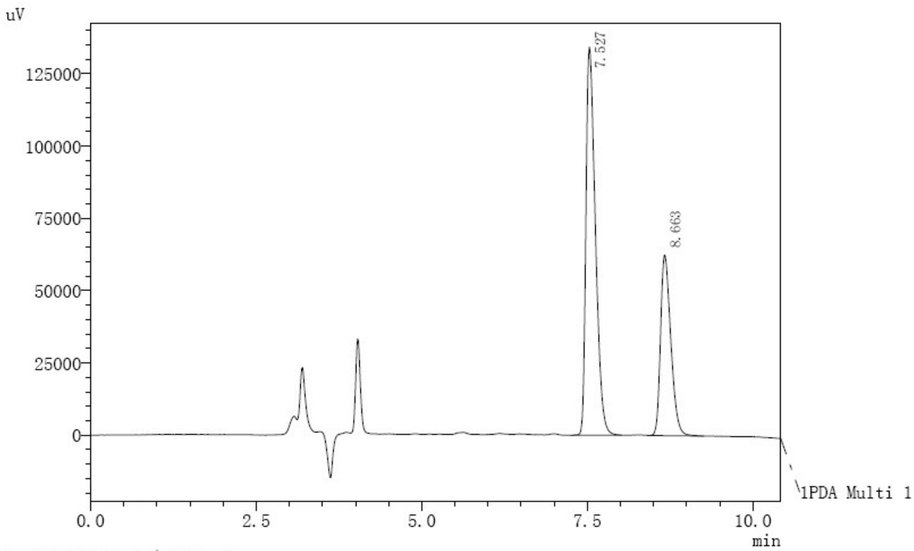


Figure S45. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 5, ee 32.7% (*S*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.527	1328771	134289	66.339	66.339
2	8.663	674232	62515	33.661	33.661
Total		2003003	196805	100.000	

Figure S46. ^{1}H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and guest F (Sample 6, ee 10.8% (*S*))

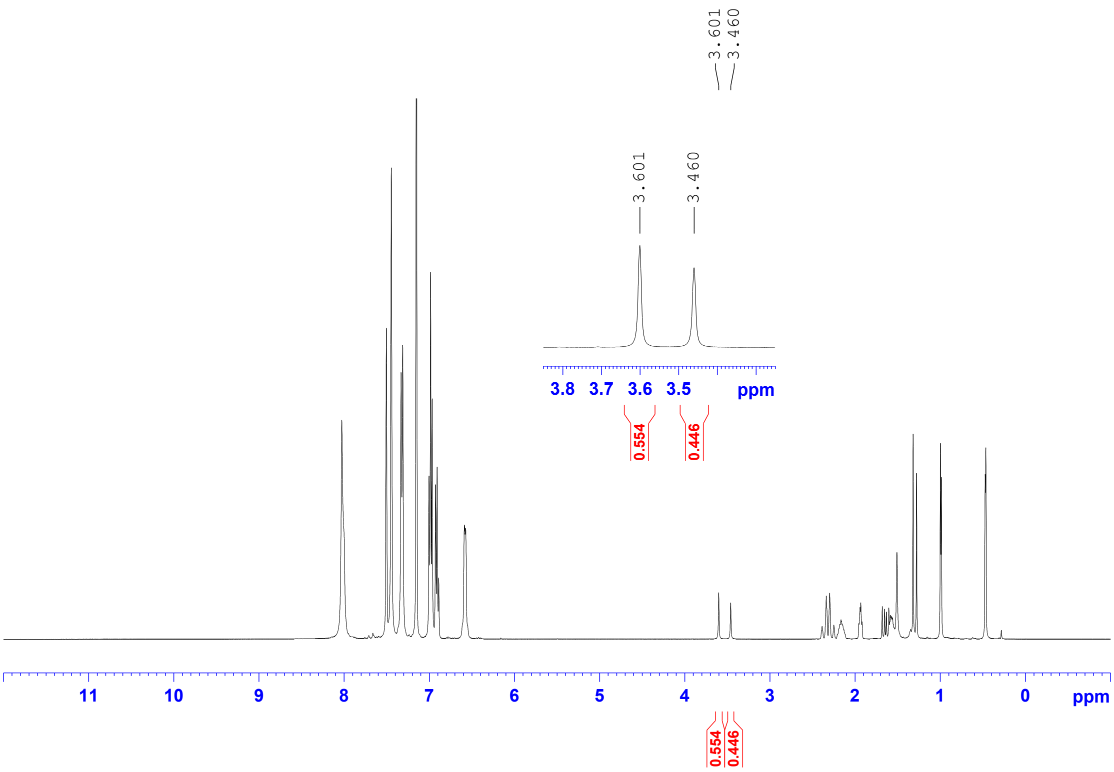
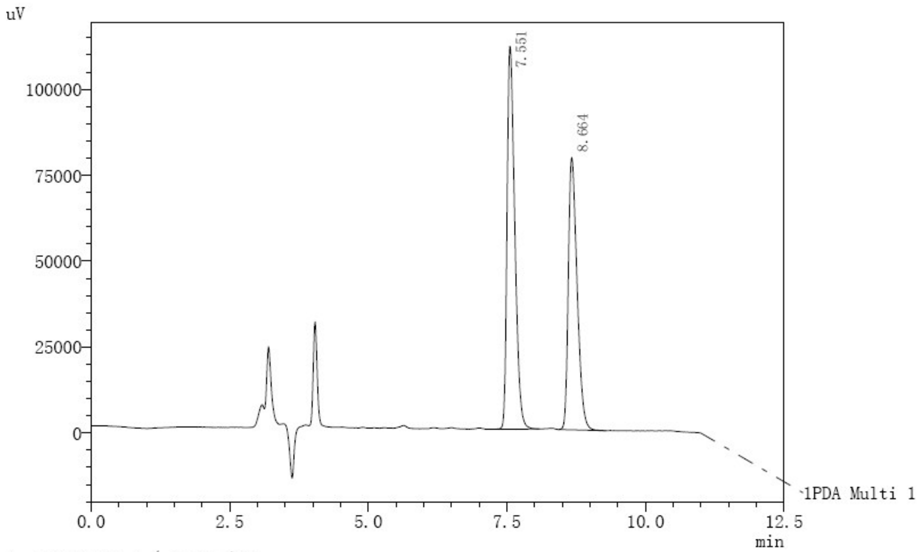


Figure S47. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 6, ee 10.5% (*S*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.551	1077738	111422	55.242	55.242
2	8.664	873200	79246	44.758	44.758
Total		1950938	190668	100.000	

Figure S48. ¹H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2 and guest F (Sample 7, ee 9.8% (*R*))

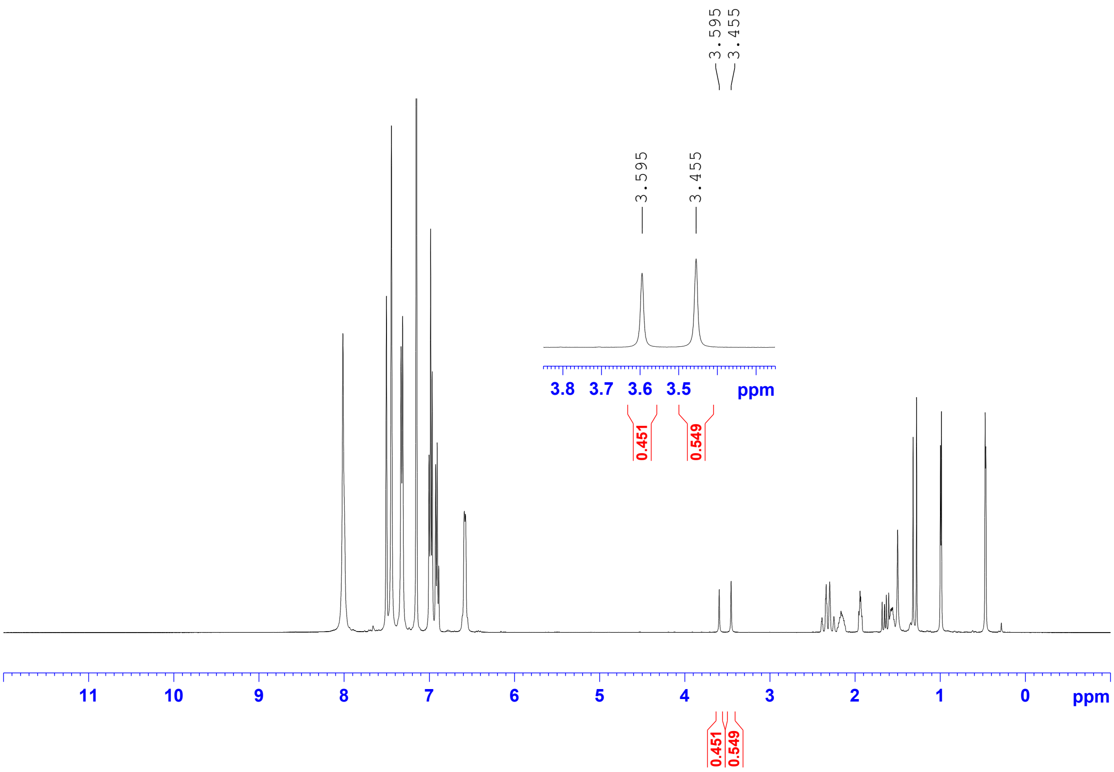
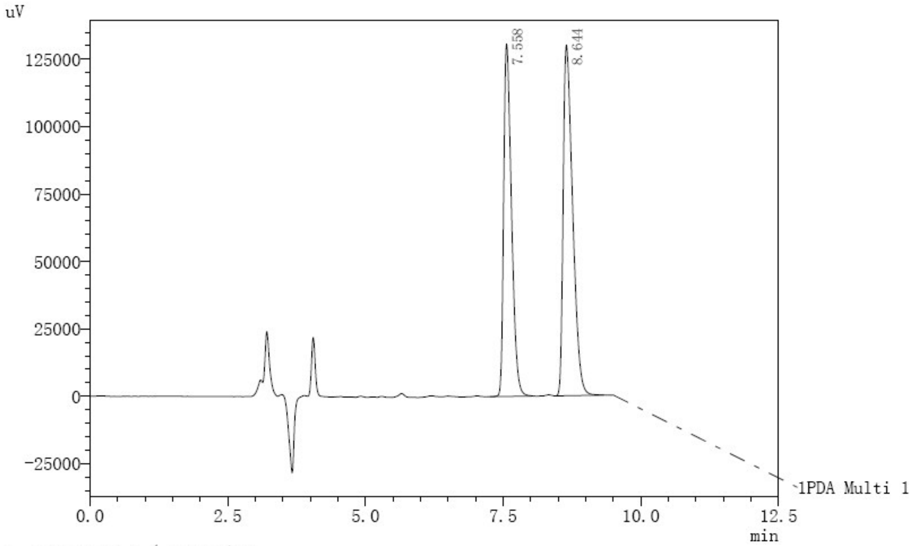


Figure S49. HPLC of (*S*, *S*)-CSA-2and guest F (Sample 7, ee 9.5% (*R*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.558	1286975	130785	45.259	45.259
2	8.644	1556597	130168	54.741	54.741
Total		2843572	260952	100.000	

Figure S50. ^{1}**H NMR (400 MHz, C_6D_6) of (*S*, *S*)-CSA-2and guest F (Sample 8, ee 31.2% (*R*))**

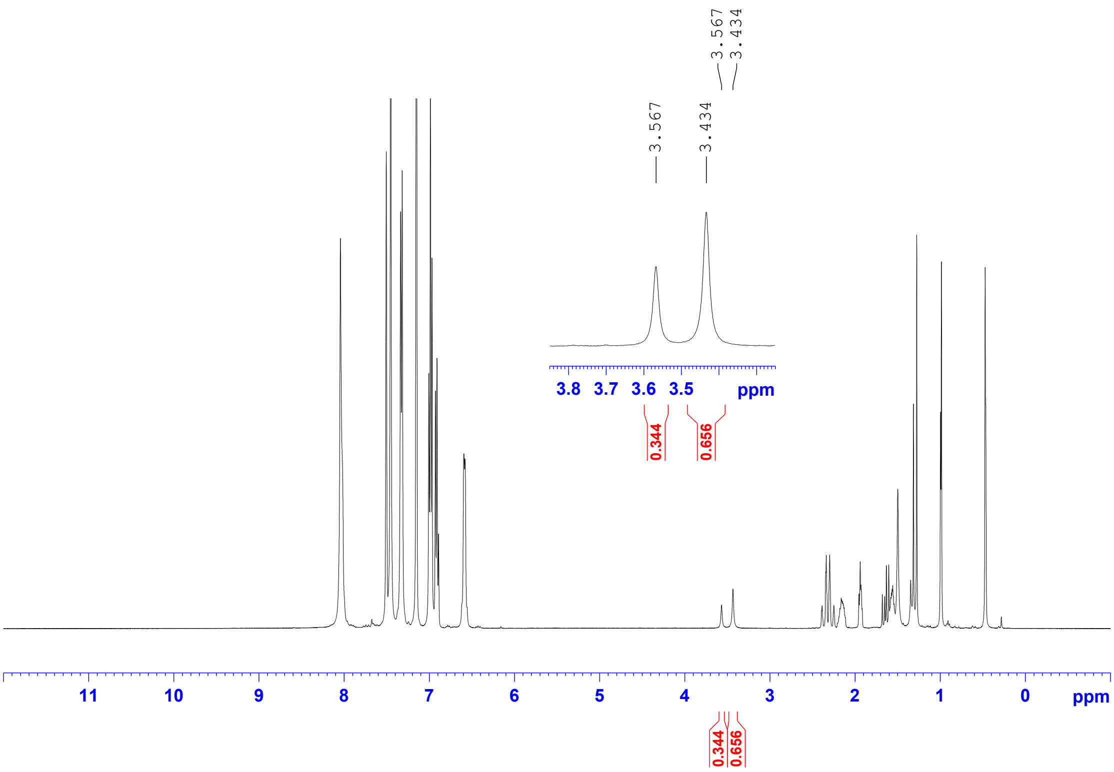
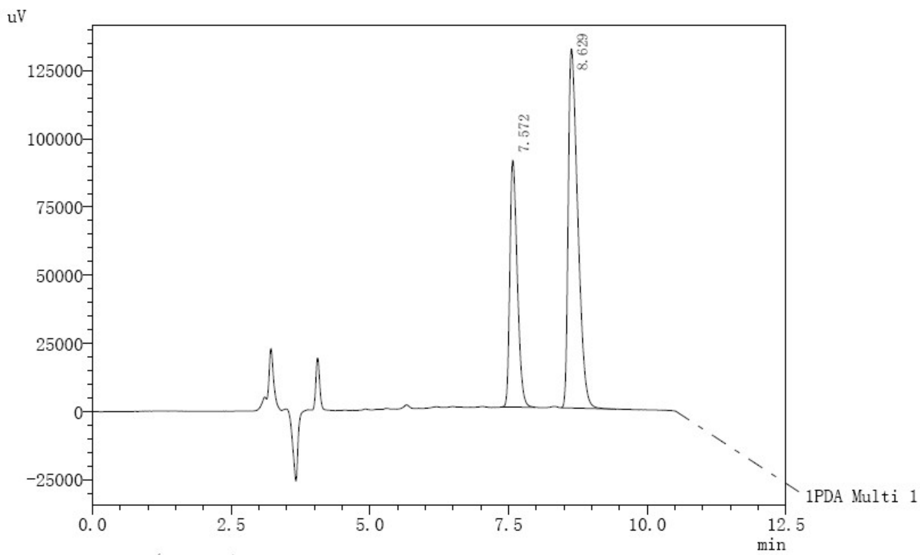


Figure S51. HPLC of (*S*, *S*)-CSA-2and guest F (Sample 8, ee 30.3% (*R*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.572	843461	90429	34.874	34.874
2	8.629	1575153	131524	65.126	65.126
Total		2418614	221954	100.000	

Figure S52. ^{1}**H NMR (400 MHz,** C_6D_6**) of (*S*, *S*)-CSA-2and guest F (Sample 9, ee 51.1% (*R*))**

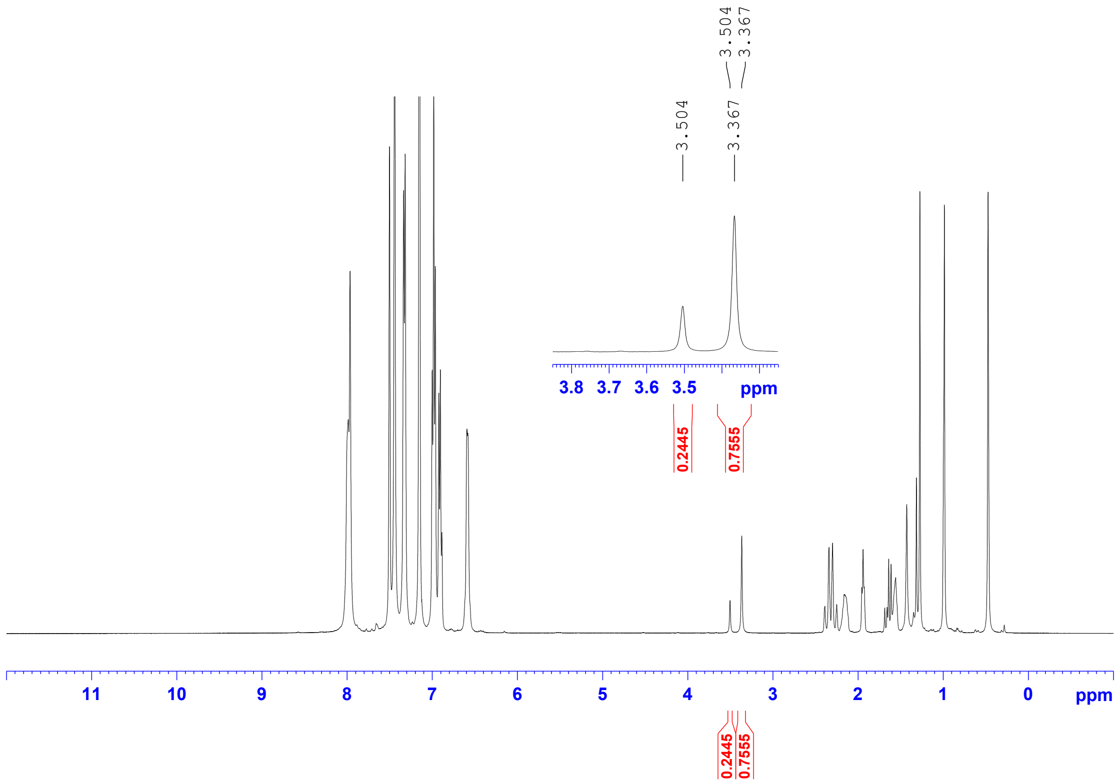
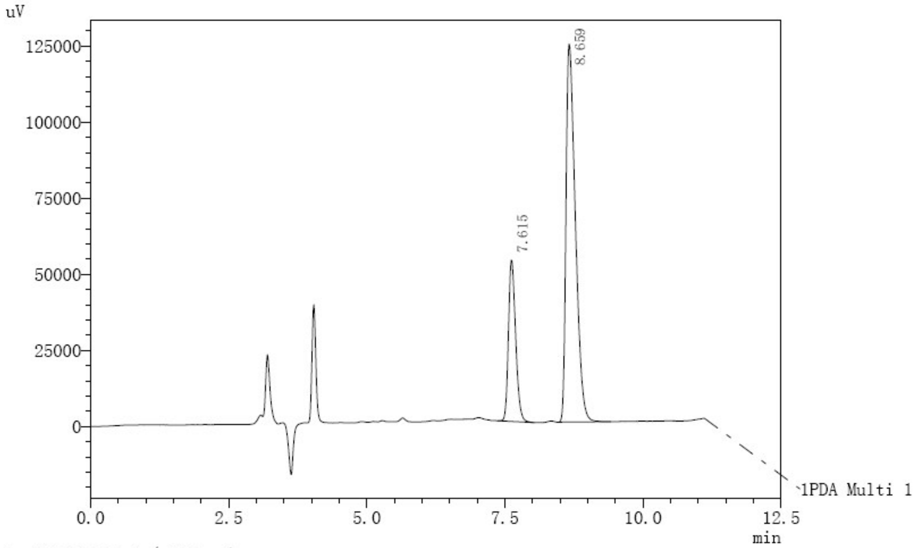


Figure S53. HPLC of (*S*, *S*)-CSA-2 and guest F (Sample 9, ee 50.8% (*R*))

Column: CHIRALPAK OJ-H

Mobile Phase: n-Hexane/iPrOH = 97/3

Flow Rate: 1 ml/min



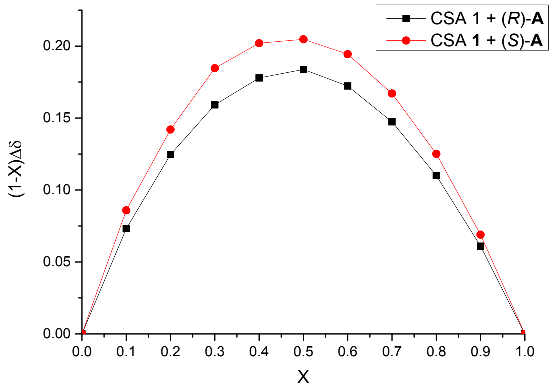
1 PDA Multi 1 / 207nm 4nm

PDA Ch1 207nm 4nm

Peak	Ret. time	Area	Heigh	Area %	Conc.
1	7.615	478715	53015	24.608	24.608
2	8.659	1466629	124252	75.392	75.392
Total		1945344	177267	100.000	

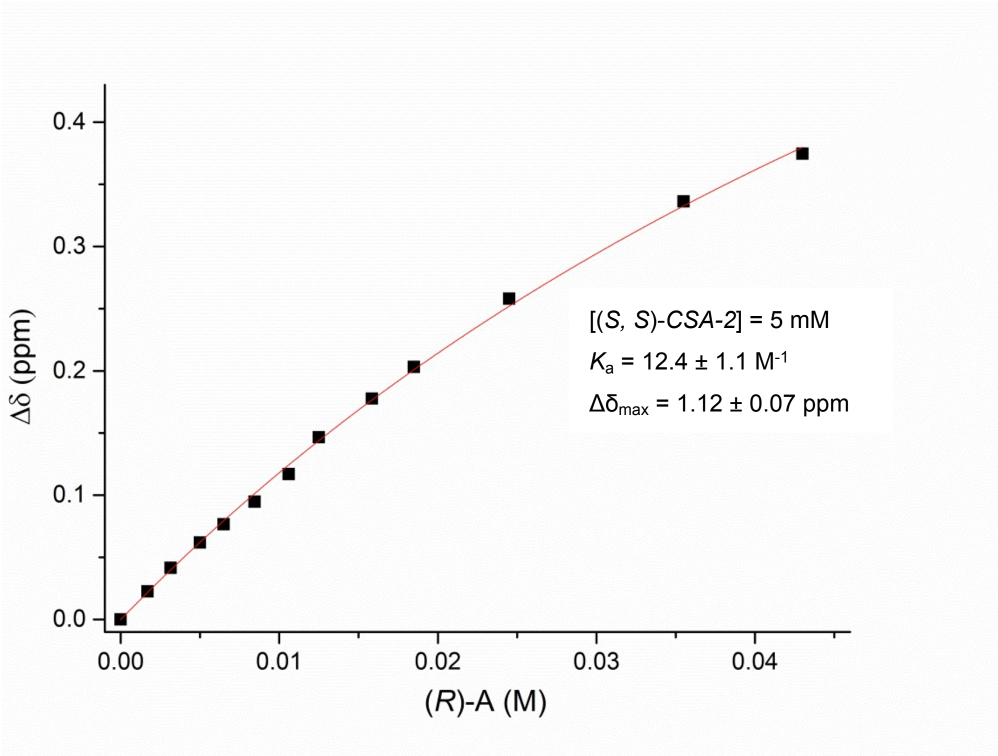
Studies of the stoichiometry of the guest A/(*S*, *S*)-CSA-2 complex (Job Plots).

Nine samples with a constant concentration (30 mM in C_6D_6) were prepared containing variable ratios of (*S*, *S*)-CSA-2 and (*R*)-**A** or (*S*)-**A**. The ^{1}H NMR spectra of these samples were recorded and the corresponding chemical shift variations were observed for the hydroxy proton of (*R*)-**A** or (*S*)-**A**. It was found that the recorded Job Plots for (*S*, *S*)-CSA-2 exhibited maxima at 0.5 ± 0.05. This indicates that (*S*, *S*)-CSA-2 forms a 1:1 complex with (*R*)-**A** or (*S*)-**A**. (x = [(*S*, *S*)-CSA-2] / ([(*S*, *S*)-CSA-2] + [A]); Δδ = variation of the chemical shift of the observed proton (OH))

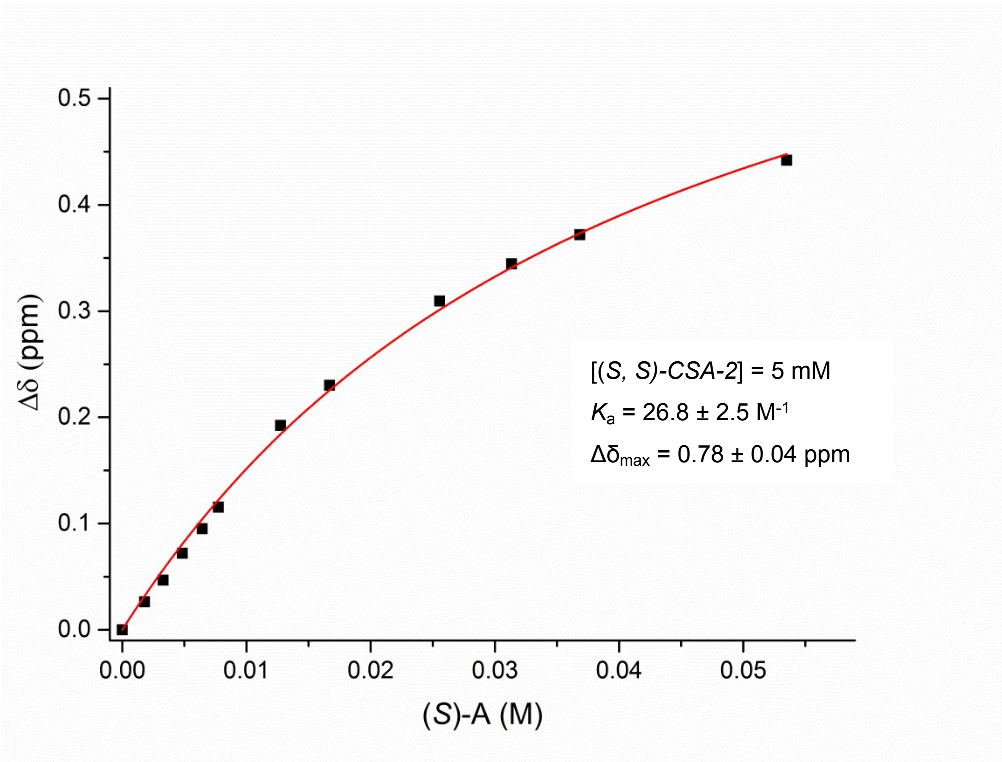


Determination of binding constants by ^{1}H NMR titrations.

The (*S*, *S*)-CSA-2(8 mM) was titrated by the addition of (*R*)-A or (*S)*-A in C_6D_6 and ^{1}H NMR was then measured at 25 ºC. The change in the N-H resonances of (*S*, *S*)-CSA-2 was monitored. The data were fit to a 1:1 binding profile and the binding constant was calculated by the nonlinear least-squares curve-fitting method.



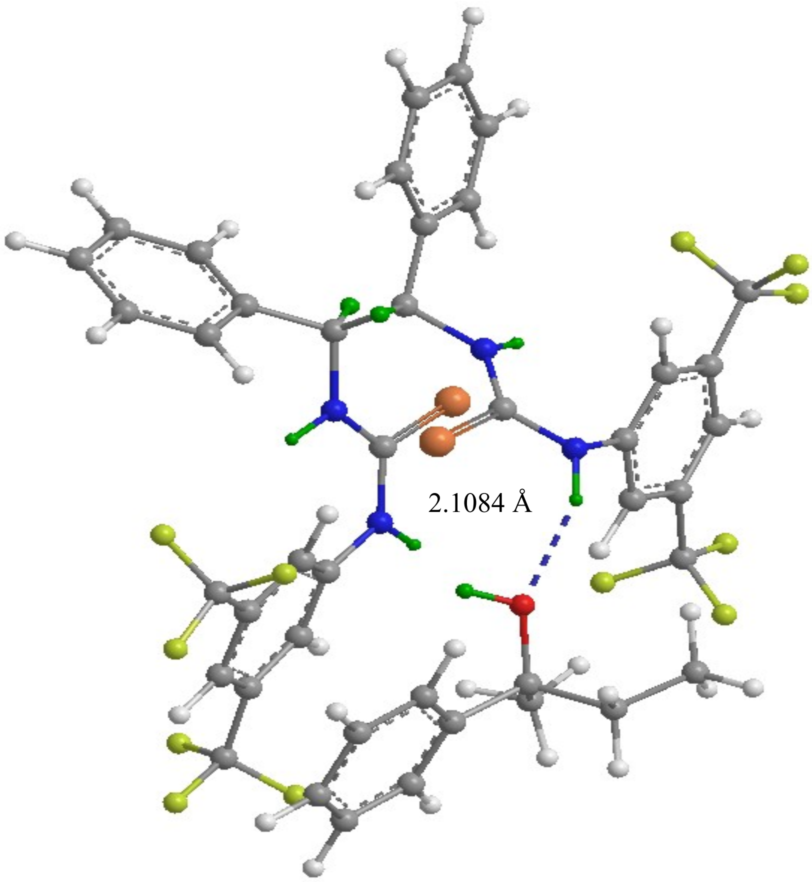
0.4
0.3
0.2
0.1
0.0
Δδ (ppm)
0.00
0.01
0.02
0.03
0.04
(R)-A (M)
[(S, S)-CSA-2] = 5 mM
Ka = 12.4 ± 1.1 M-1
Δδmax = 1.12 ± 0.07 ppm



0.5
0.4
0.3
0.2
0.1
0.0
Δδ (ppm)
0.00
0.01
0.02
0.03
0.04
0.05
(S)-A (M)
[(S, S)-CSA-2] = 5 mM
Ka = 26.8 ± 2.5 M-1
Δδmax = 0.78 ± 0.04 ppm

Computational models of complexes.

Ball-cylinder model for (*S*)-A/(*S*, *S*)-CSA-2 complex and cartesian coordinates.

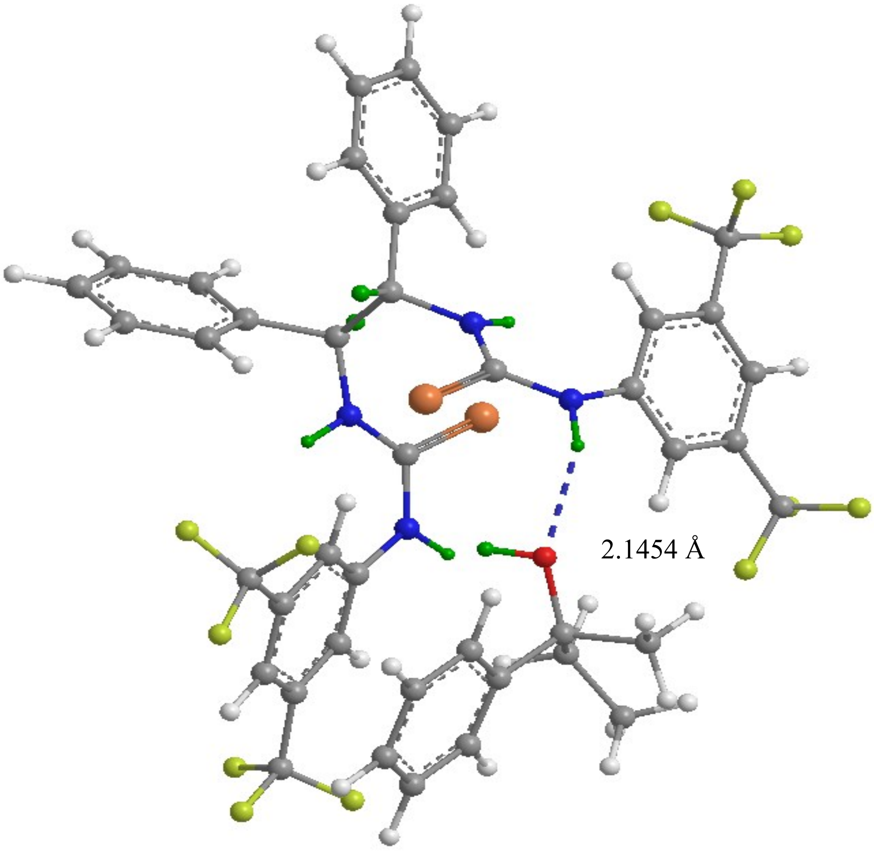


C	-6.224768	2.111209	0.279706
C	-0.438655	5.909407	0.439551
C	-1.887918	2.430421	0.871811
C	-2.519226	2.170937	-0.536157
C	-2.113486	5.989762	2.159777
N	-2.342311	0.790568	-0.951243
C	-1.351194	0.342077	-1.719741
N	-1.243167	-1.003167	-1.877489
C	-1.953998	-1.984731	-1.150834
C	-3.341815	-2.037541	-1.154769
C	-3.987856	-2.974645	-0.363240
C	-3.278134	-3.892889	0.392797
C	-6.683447	3.217832	-0.422882
C	-1.059657	-4.815849	1.143385
F	-1.797196	-5.643198	1.882418
F	-0.283989	-5.568952	0.349207
F	-0.230826	-4.164180	1.972275

C	-5.490144	-2.942220	-0.321563
F	-5.930307	-1.831184	0.287429
F	-6.000712	-3.984283	0.336084
F	-6.017799	-2.941031	-1.550595
Se	-0.107553	1.418723	-2.575939
C	-1.894236	-3.859583	0.340612
C	-1.229853	-2.910618	-0.412085
N	-0.650143	1.685954	1.058778
C	-0.566688	0.448694	1.539233
N	0.662542	-0.146195	1.575253
C	1.940388	0.372238	1.296482
C	3.008302	-0.085246	2.068392
C	4.290963	0.362349	1.815158
C	4.548122	1.303604	0.829415
C	3.676961	2.794797	-0.997539
F	3.093681	3.946579	-0.630703
F	3.120580	2.439367	-2.159511
F	4.964339	3.059446	-1.226226
C	5.409372	-0.202856	2.646688
F	6.597260	0.298205	2.305426
F	5.226869	0.043075	3.948377
F	5.484429	-1.535748	2.514950
Se	-2.001172	-0.507000	2.210916
C	-5.793241	3.985930	-1.158124
C	3.486072	1.745459	0.065489
C	2.197850	1.269214	0.263234
C	-1.155799	6.628556	1.386884
C	-1.630565	3.905925	1.053477
C	-3.984151	2.536772	-0.503146
C	-2.346927	4.631494	1.995931
C	-0.681918	4.555619	0.266012
C	-4.448451	3.643866	-1.200724
C	-4.879819	1.777646	0.247268
H	-2.000230	2.782887	-1.269309
H	-4.527157	0.924571	0.819674
H	-3.753916	4.239474	-1.780050
H	-6.912352	1.507933	0.856657
H	-0.138806	4.007127	-0.499422
H	0.306490	6.402617	-0.169470
H	-3.091206	4.129556	2.601156
H	-2.677506	6.546747	2.895297
H	-7.732272	3.480250	-0.395748
H	-6.144476	4.850571	-1.704633
H	-2.830043	0.109656	-0.379196

H	-0.343971	-1.293203	-2.245564
H	-3.915053	-1.346040	-1.759644
H	-0.149831	-2.838415	-0.407420
H	-3.792366	-4.616886	1.006466
H	-2.584741	2.078762	1.630269
H	-0.968957	7.685422	1.519481
H	0.197137	2.181035	0.827555
H	0.637332	-1.036736	2.051763
H	2.831583	-0.796162	2.866572
H	5.549554	1.664414	0.653666
H	1.423720	1.558842	-0.439158
C	2.776436	-2.472477	-1.354647
O	1.586004	-1.674978	-1.487381
C	5.149679	-1.821888	-0.694038
C	5.192292	0.202452	-2.580034
C	4.052461	-0.570575	-2.415327
C	2.703535	-3.200691	-0.016384
C	4.015462	-1.595757	-1.469708
C	6.292564	-1.051436	-0.860508
C	6.318173	-0.036451	-1.804646
C	2.769702	-3.467253	-2.526653
H	3.470893	-3.970294	0.064149
H	5.152500	-2.601799	0.053613
H	5.195244	0.999584	-3.310964
H	3.182242	-0.369616	-3.030532
H	7.206045	0.567716	-1.934101
H	7.158966	-1.244490	-0.241553
H	1.739044	-3.692295	0.087997
H	2.829776	-2.498138	0.808300
H	2.816219	-2.882281	-3.446960
H	3.688930	-4.055121	-2.476944
H	1.790403	-0.736767	-1.394520
C	1.554643	-4.384895	-2.558574
H	1.567267	-4.998407	-3.458387
H	0.630025	-3.806720	-2.566480
H	1.526537	-5.057492	-1.701891

Ball-cylinder model for (*R*)-A/(*S*, *S*)-CSA-2 complex and cartesian coordinates.



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C	0.049315	5.975262	0.212516
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C	-2.323640	2.370533	-0.445531
C	-1.426072	6.207633	2.094107
N	-2.300356	0.973271	-0.831190
C	-1.409397	0.418542	-1.649816
N	-1.459793	-0.930758	-1.799521
C	-2.318377	-1.843525	-1.160776
C	-3.684142	-1.628630	-1.040029
C	-4.464745	-2.555484	-0.360843
C	-3.922165	-3.714630	0.156331
C	-6.364268	3.765099	-0.021008
C	-1.971834	-5.228000	0.484377
F	-2.402772	-5.516367	1.715004
F	-2.304143	-6.262161	-0.297636
F	-0.633476	-5.183967	0.527063
C	-5.924195	-2.239400	-0.188925
F	-6.095382	-1.171094	0.604458

F	-6.603868	-3.250405	0.353224
F	-6.502295	-1.944311	-1.358574
Se	-0.106952	1.348462	-2.582926
C	-2.562853	-3.943672	-0.025684
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C	3.306714	0.052821	2.002881
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H	-4.336409	1.271209	1.035305
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H	-6.652048	2.054589	1.245973
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H	-4.146793	-0.749806	-1.469898

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H	3.133229	-0.530190	2.899216
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C	2.320296	-2.745323	-0.943098
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C	3.762184	-1.272011	-2.388781
C	2.171462	-3.172506	0.530975
C	3.658092	-2.080269	-1.255281
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H	2.882760	-1.089172	-2.994354
H	7.041924	-0.442086	-2.230030
H	6.875395	-1.854384	-0.200006
H	1.101590	-3.145106	0.749997
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