

Supplementary Information:

Chiral sensors for determining the absolute configurations of α -amino acids derivatives

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Figure S1: ^1H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 1

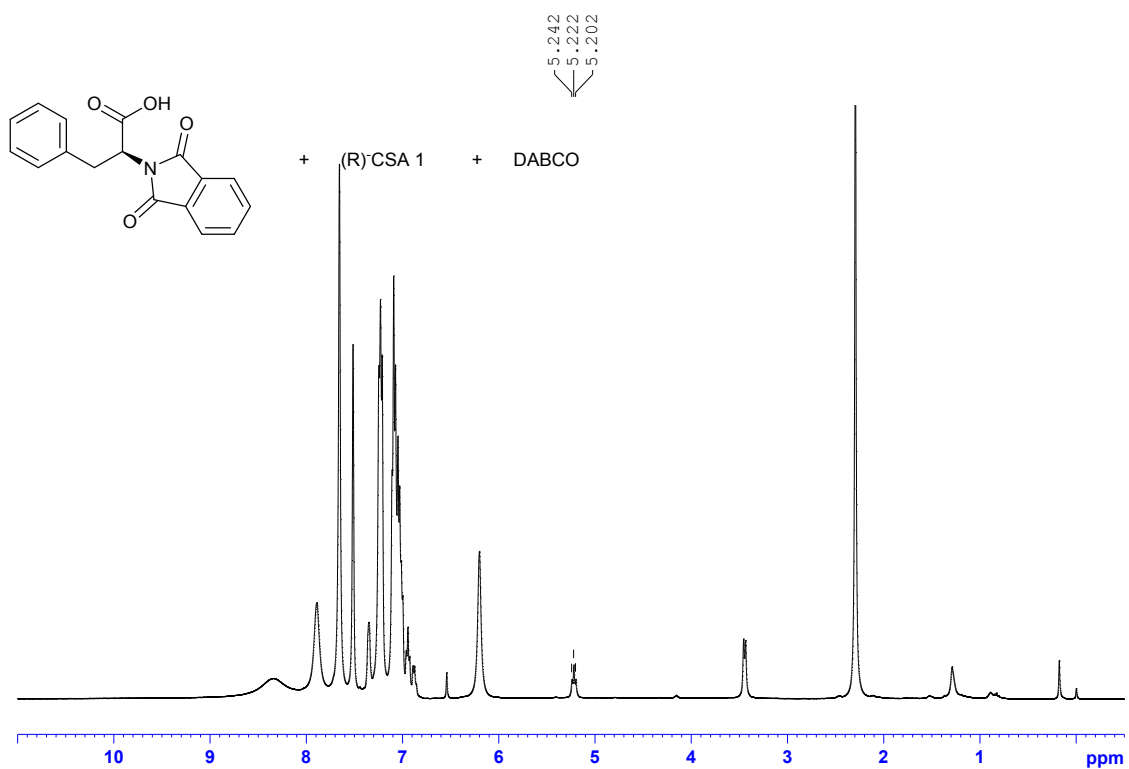


Figure S2: ^1H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 1

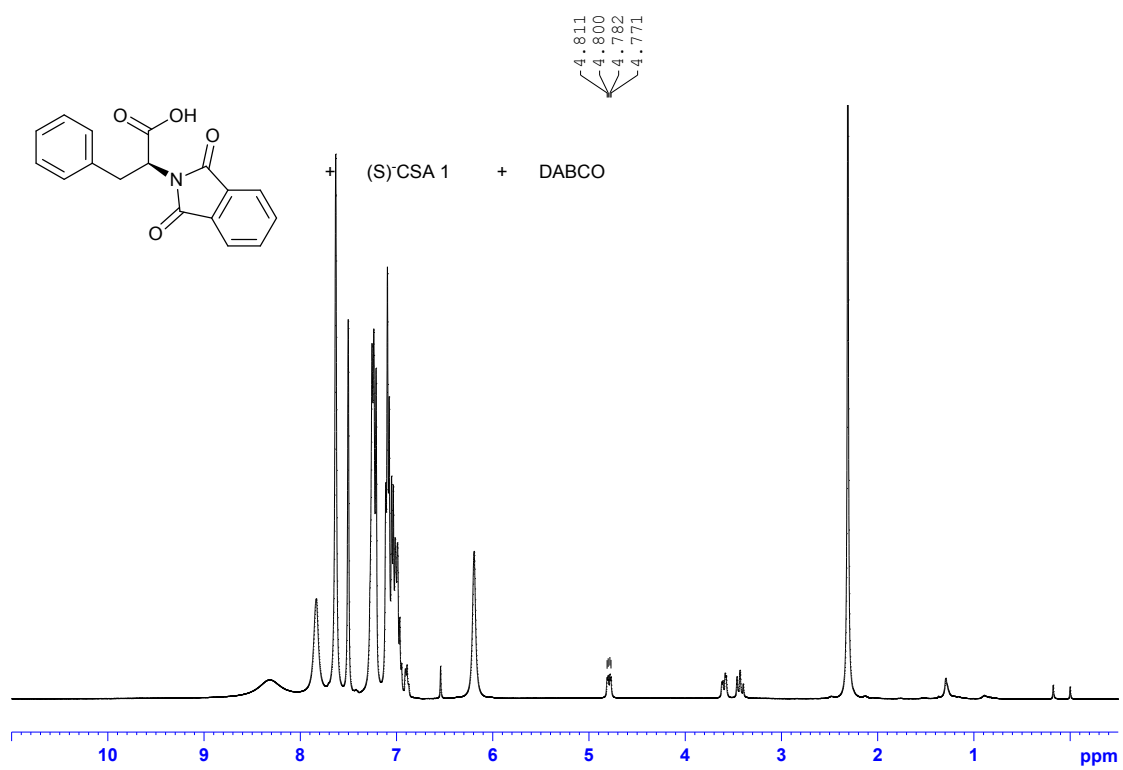


Figure S3: ^1H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 2

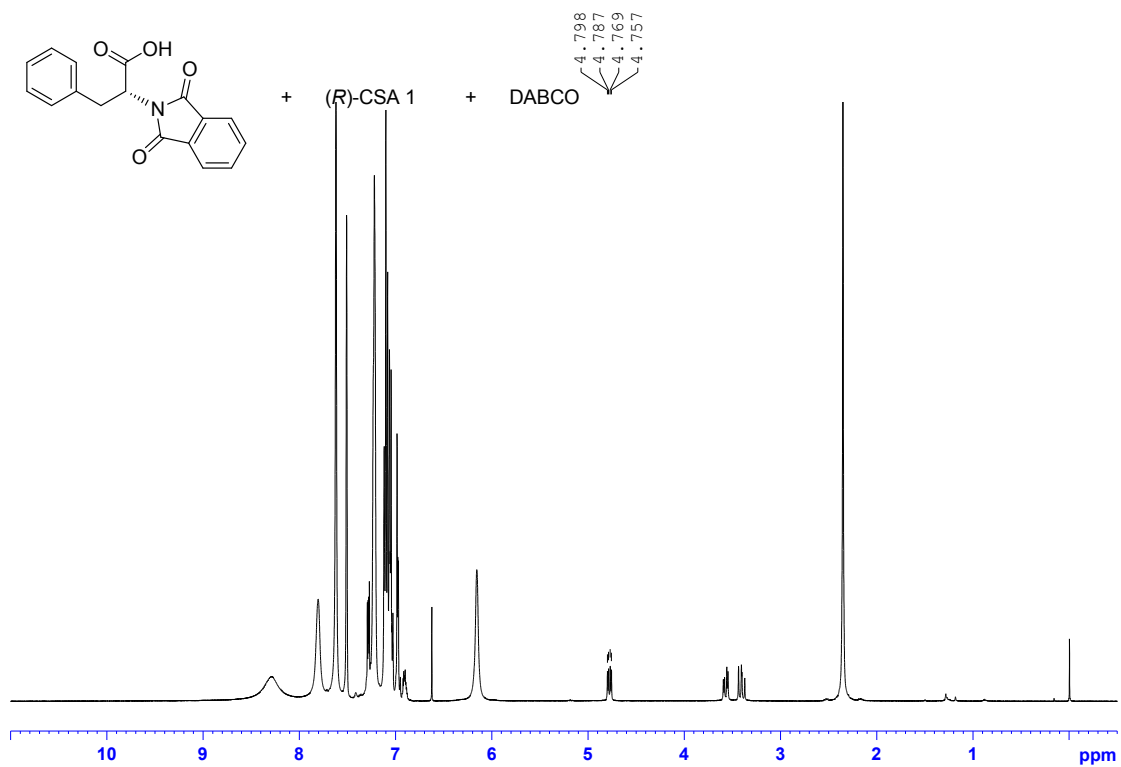


Figure S4: ^1H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 2

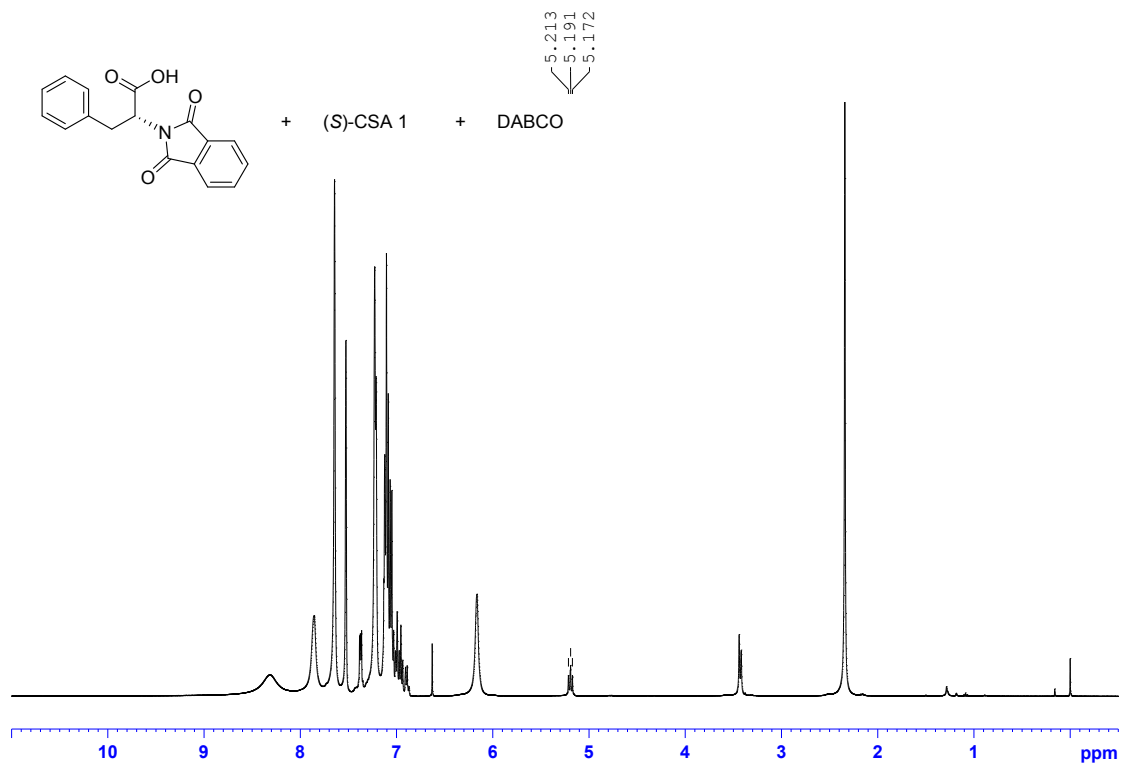


Figure S5. ^1H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 3

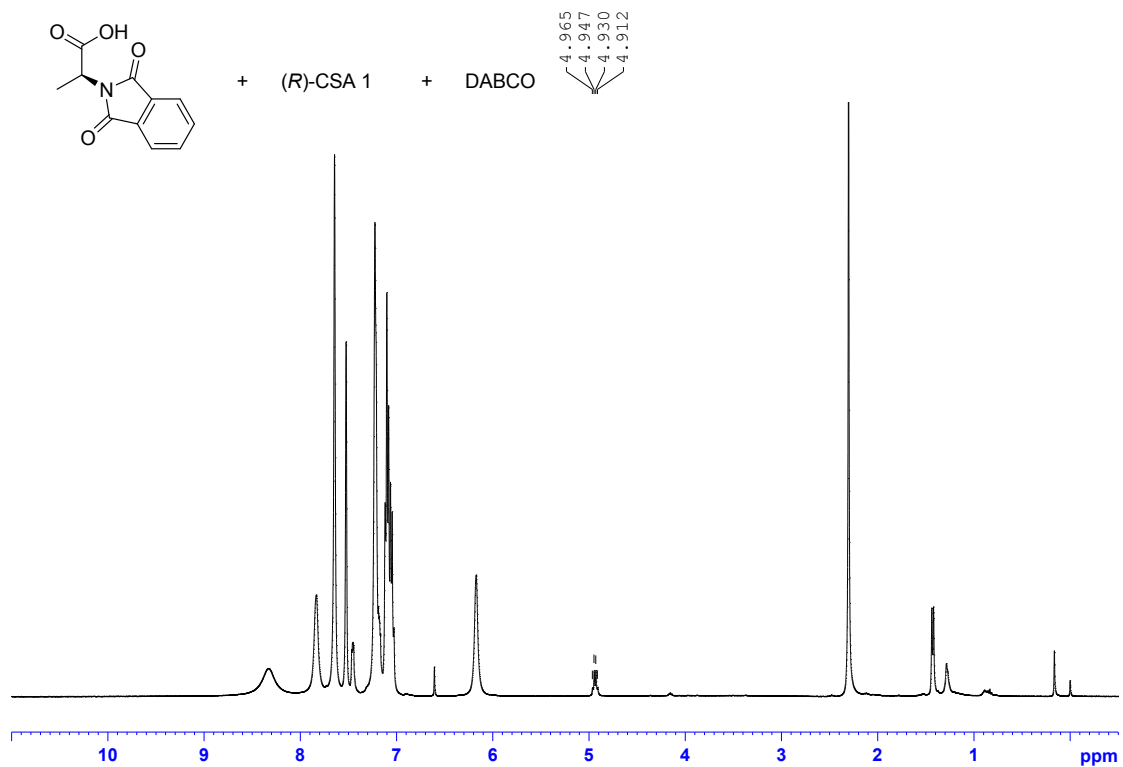


Figure S6. ^1H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 3

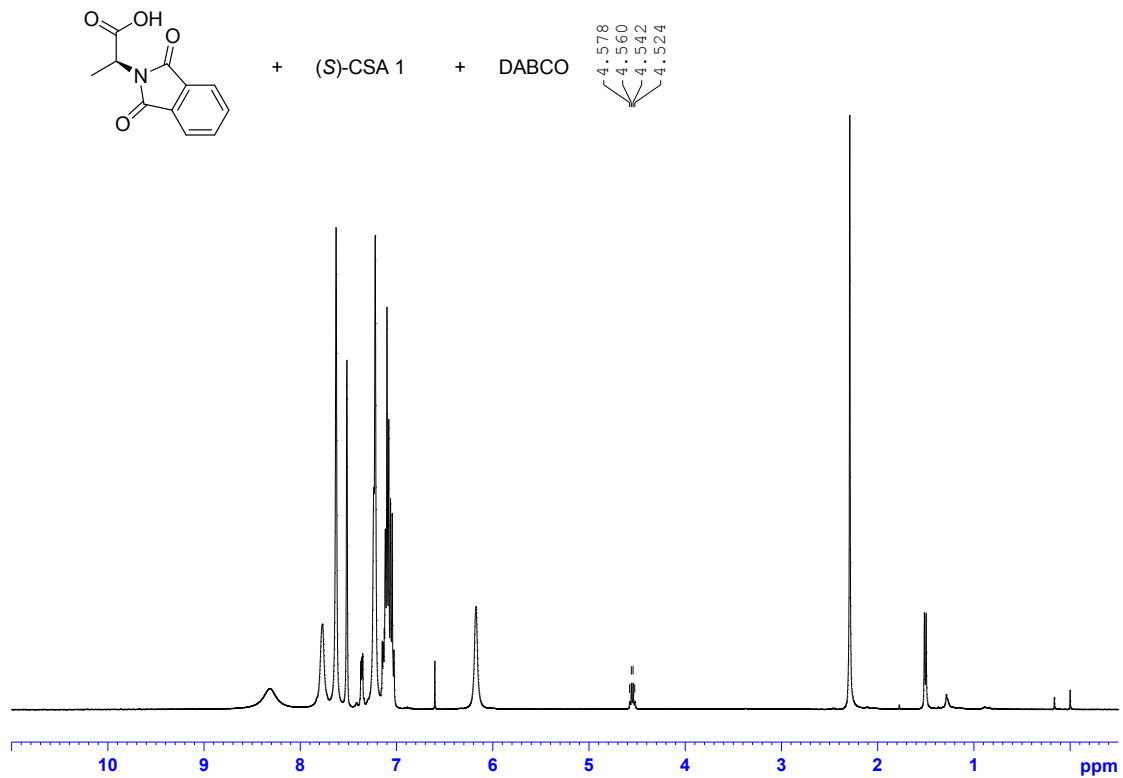


Figure S7. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 4

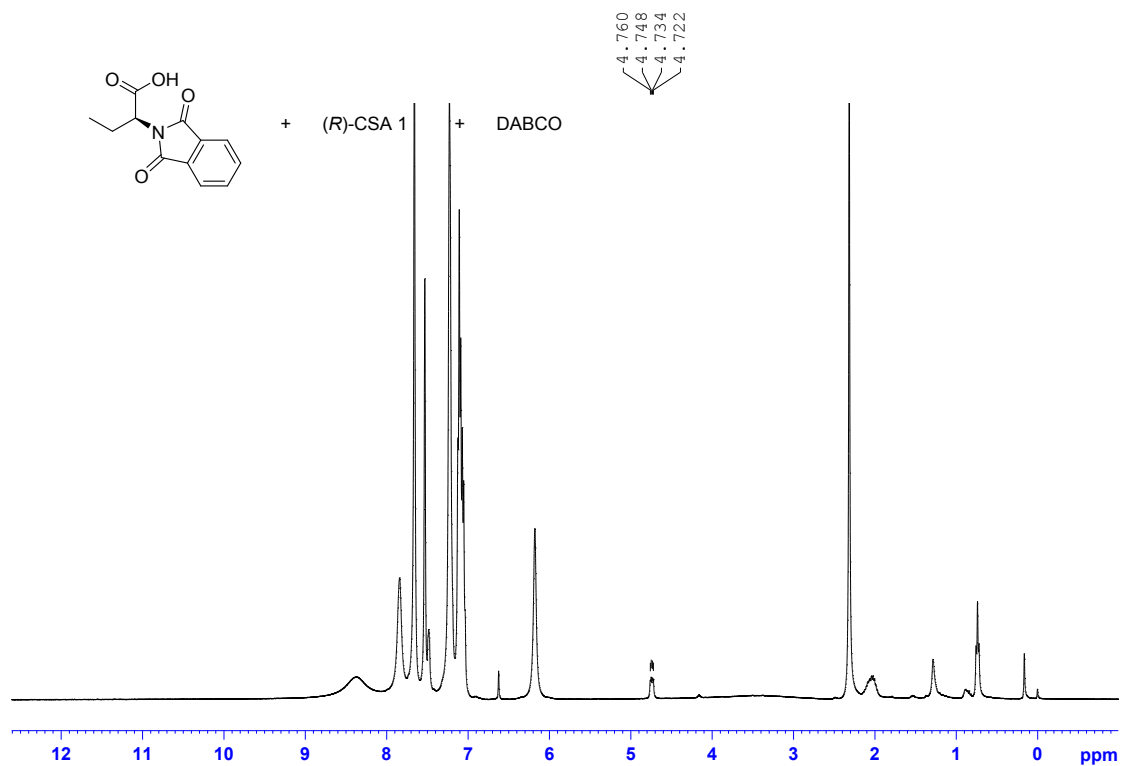


Figure S8. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 4

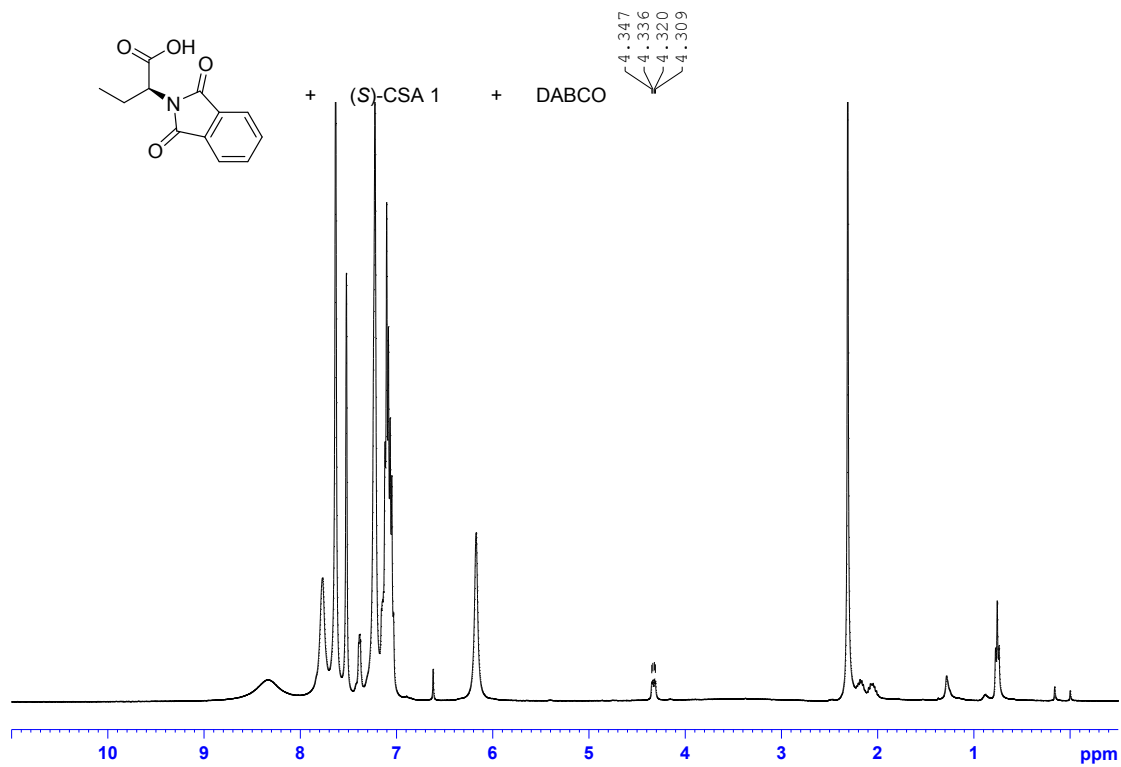


Figure S9. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 5

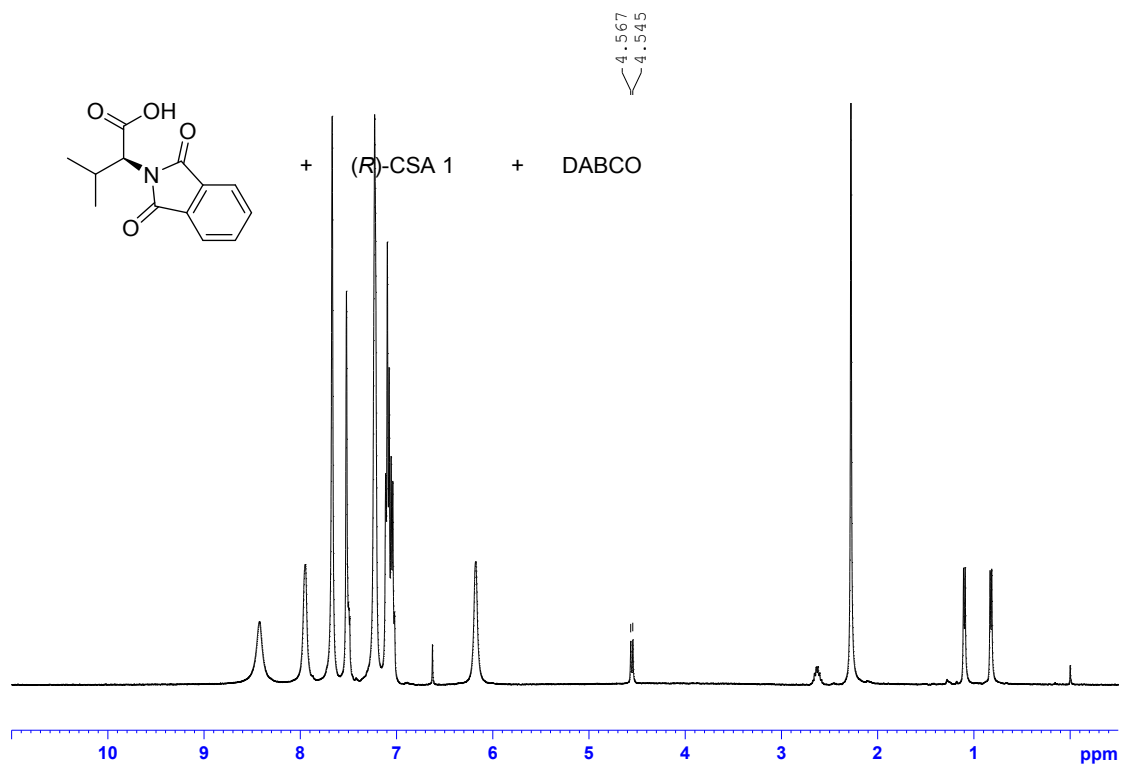


Figure S10. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 5

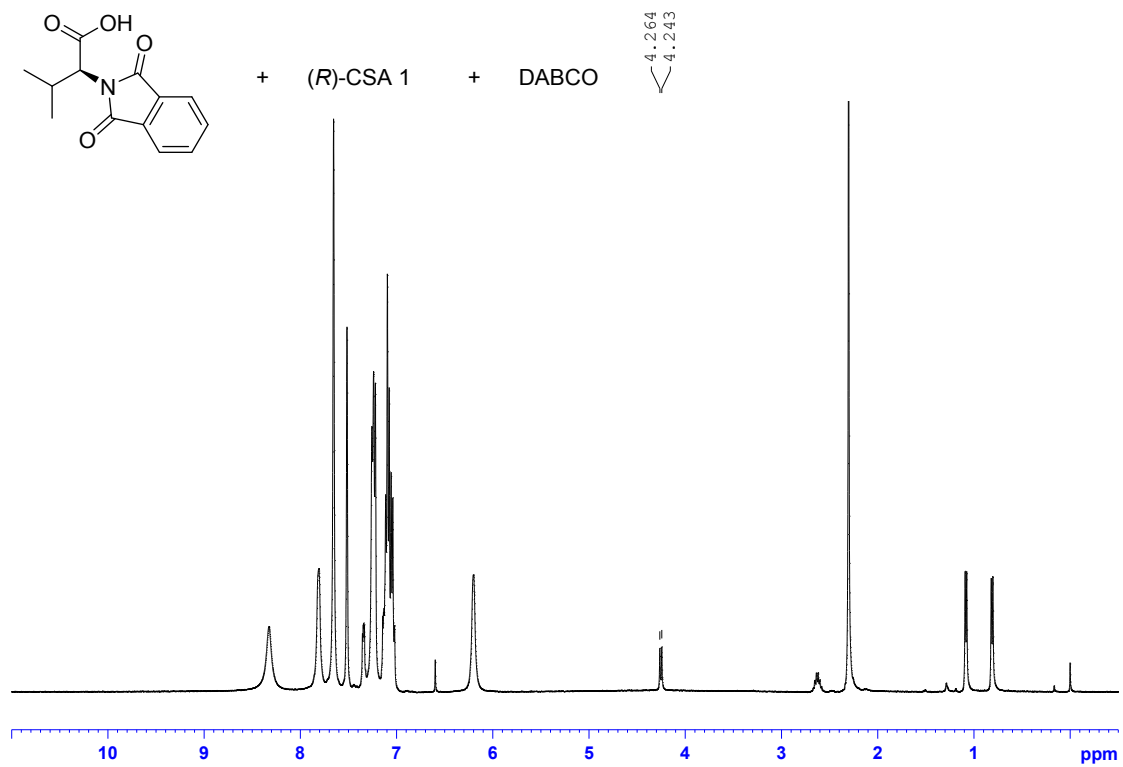


Figure S11. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 6

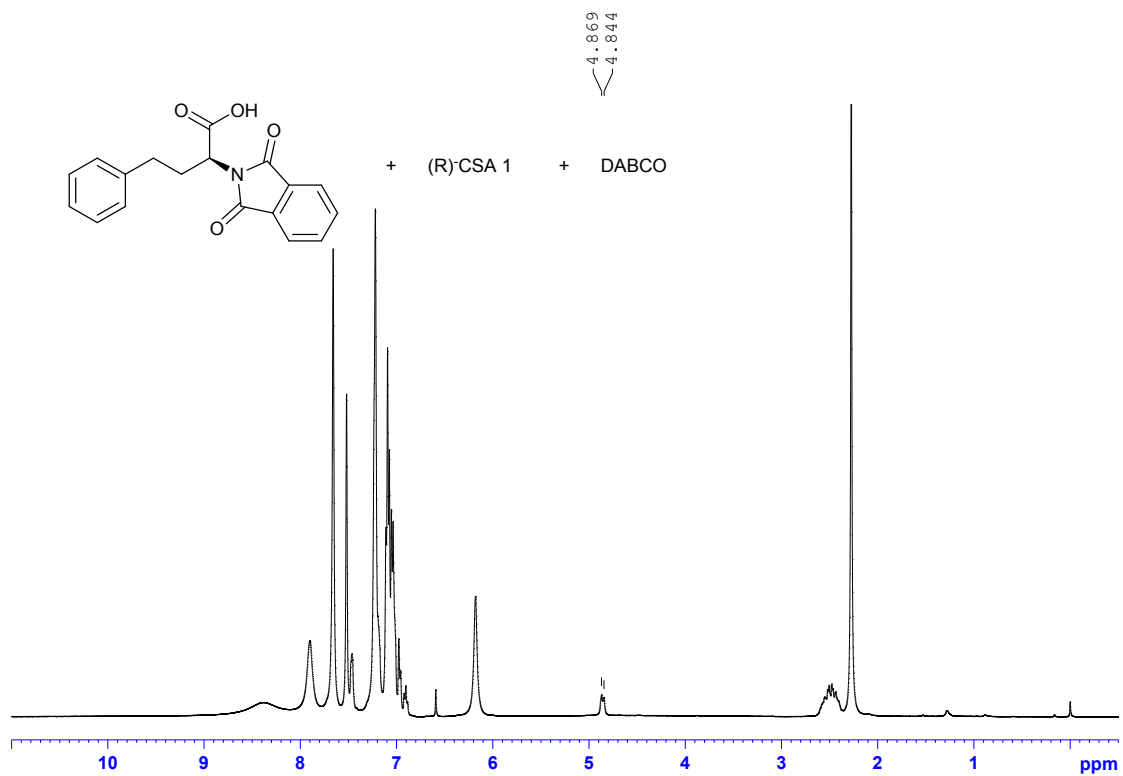


Figure S12. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 6

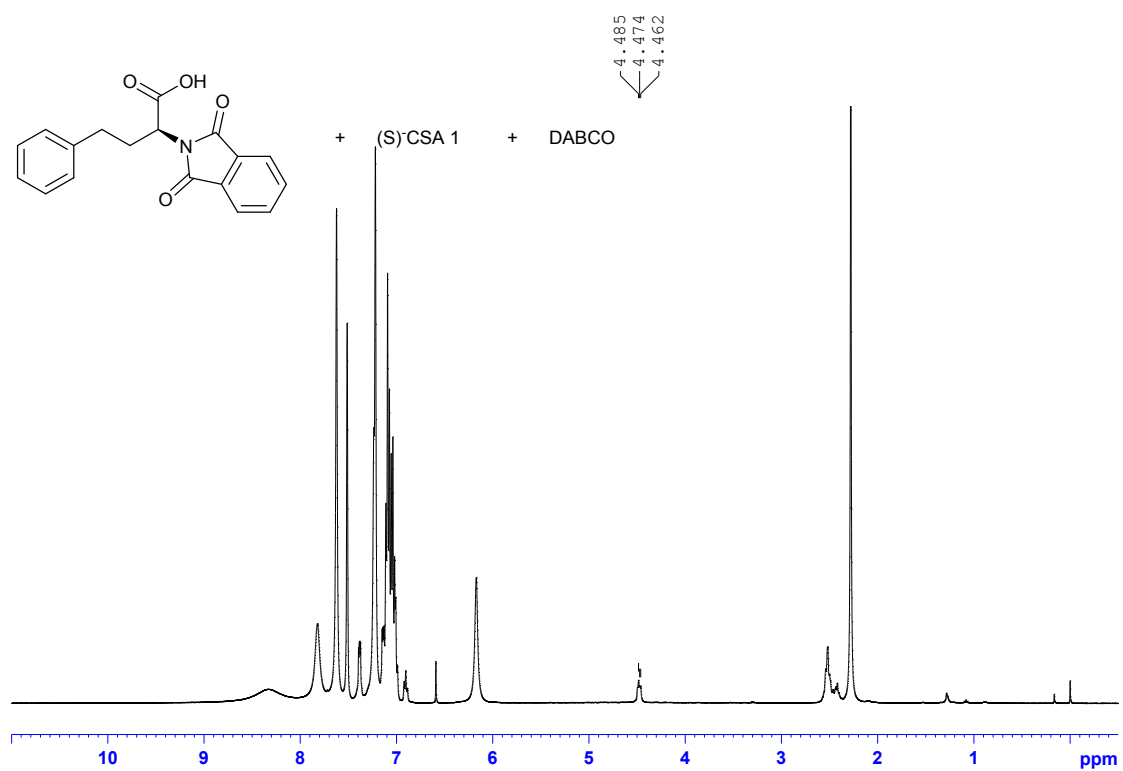


Figure S13. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 7

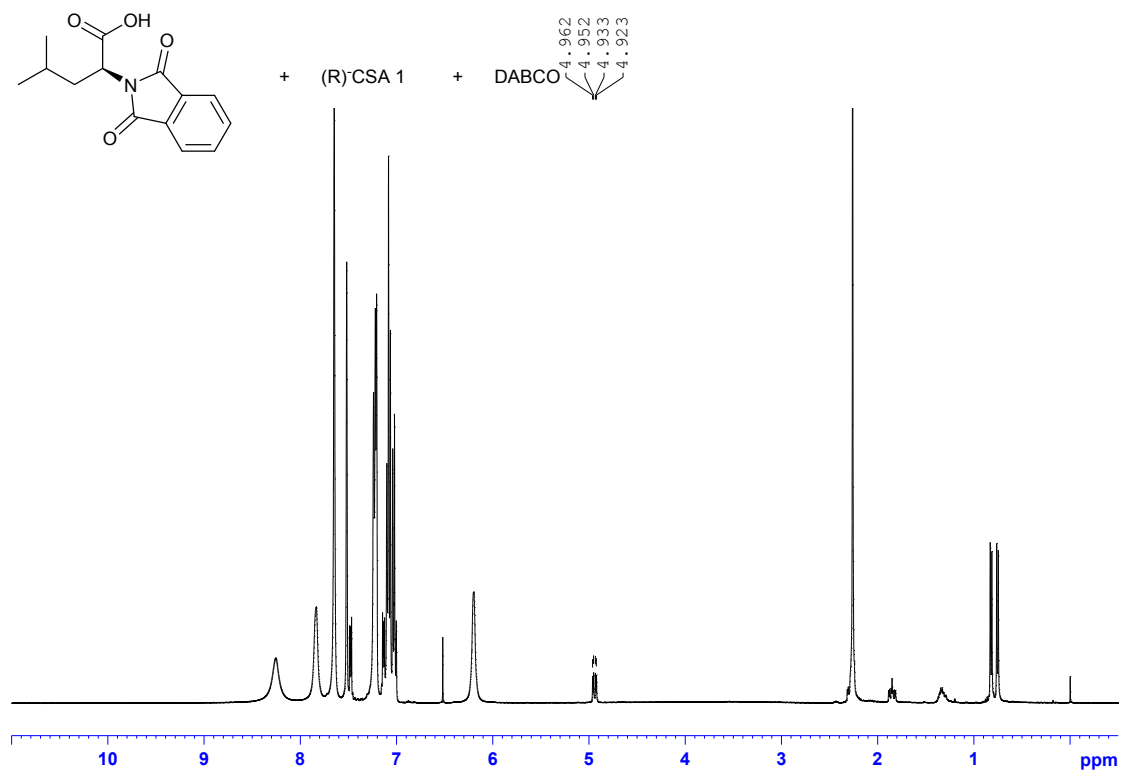


Figure S14. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 7

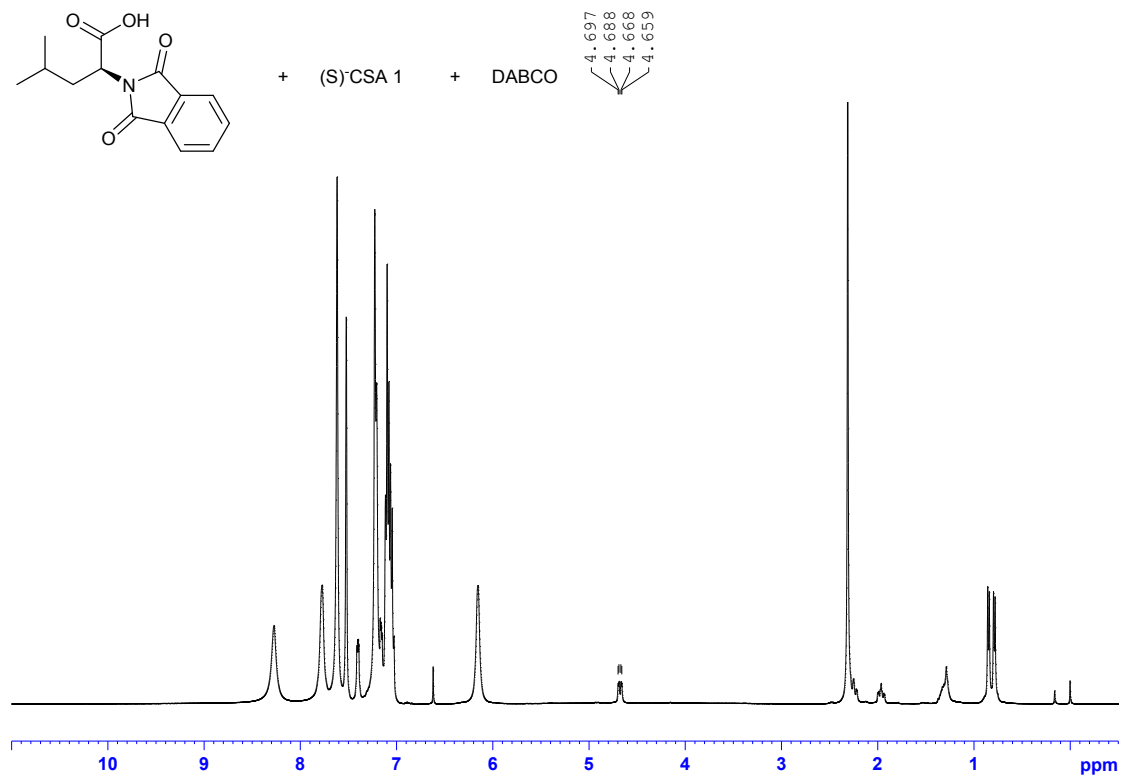


Figure S15. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 8

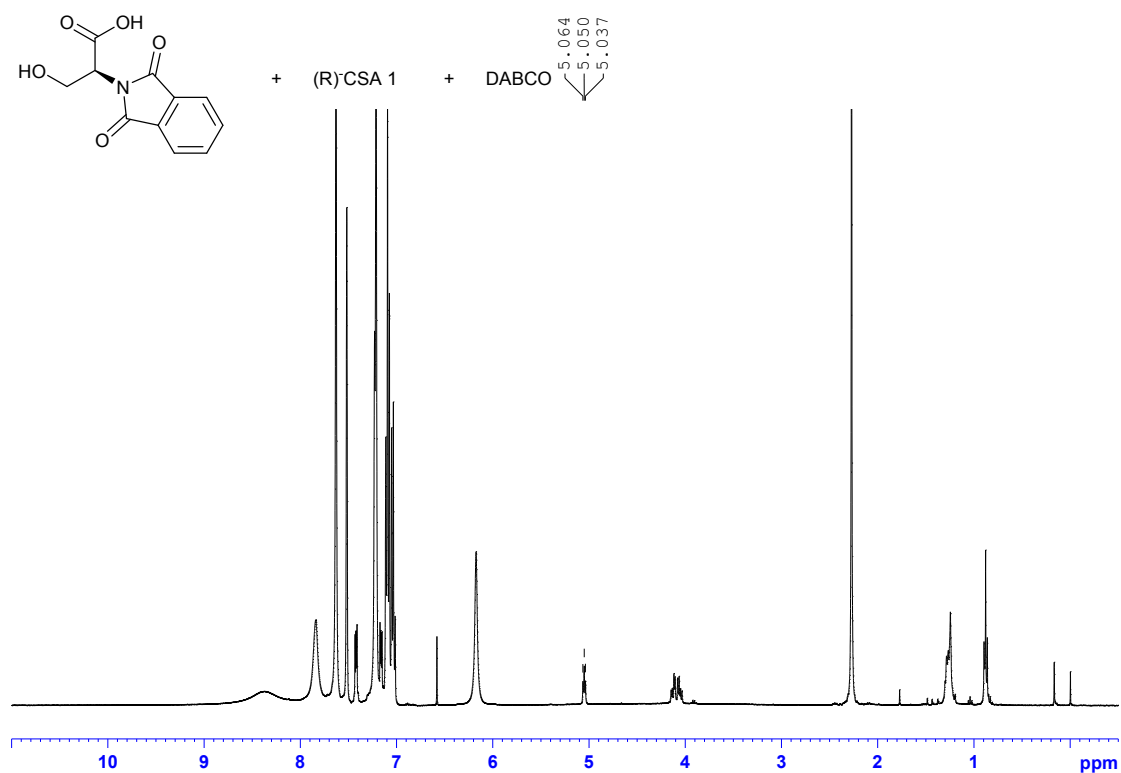


Figure S16. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 8

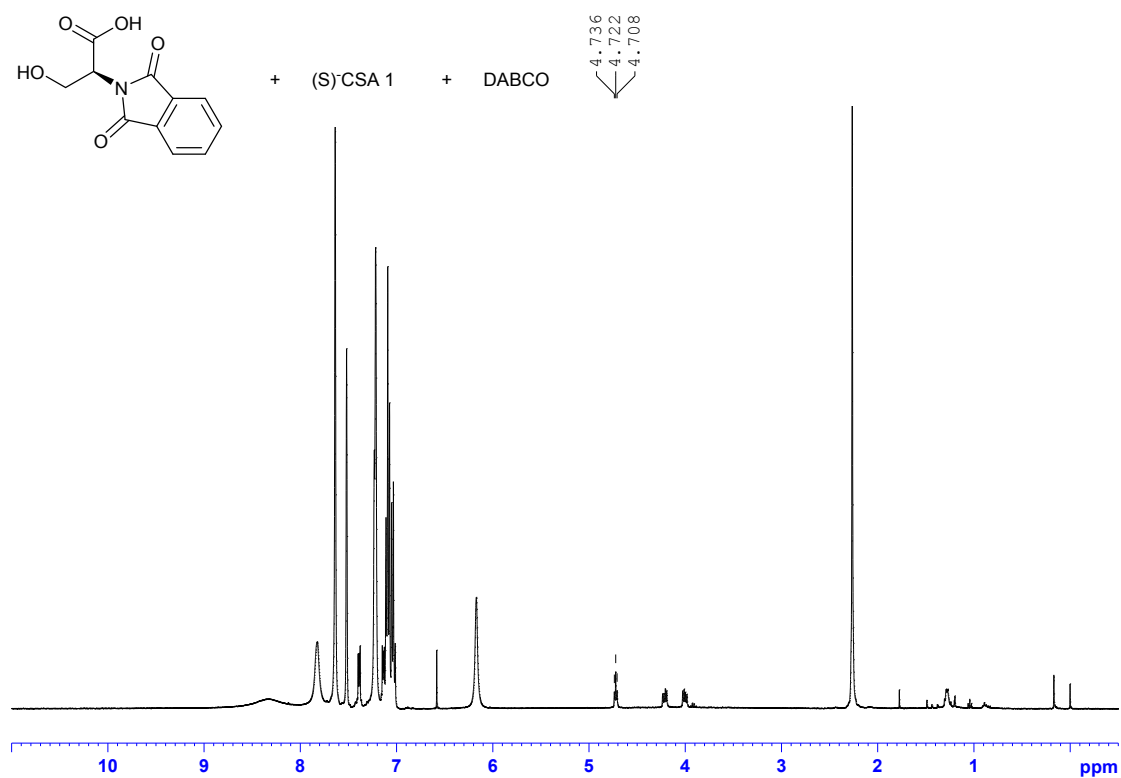


Figure S17. ^1H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 9

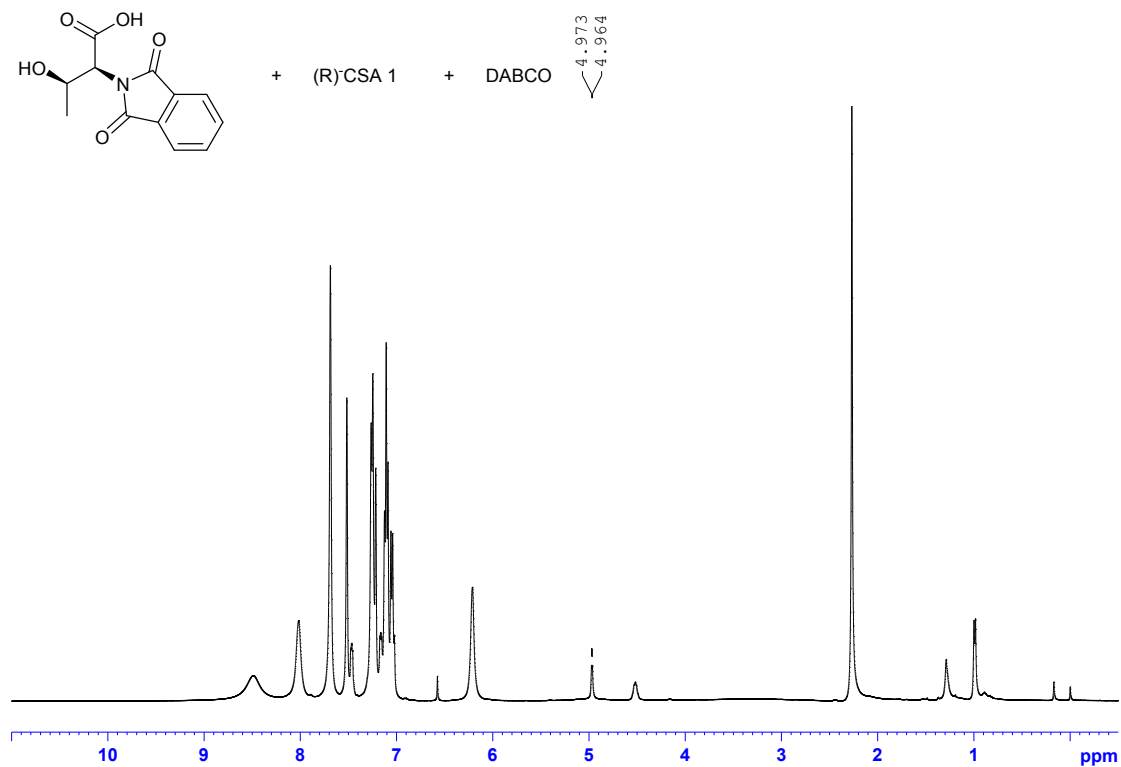


Figure S18. ^1H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 9

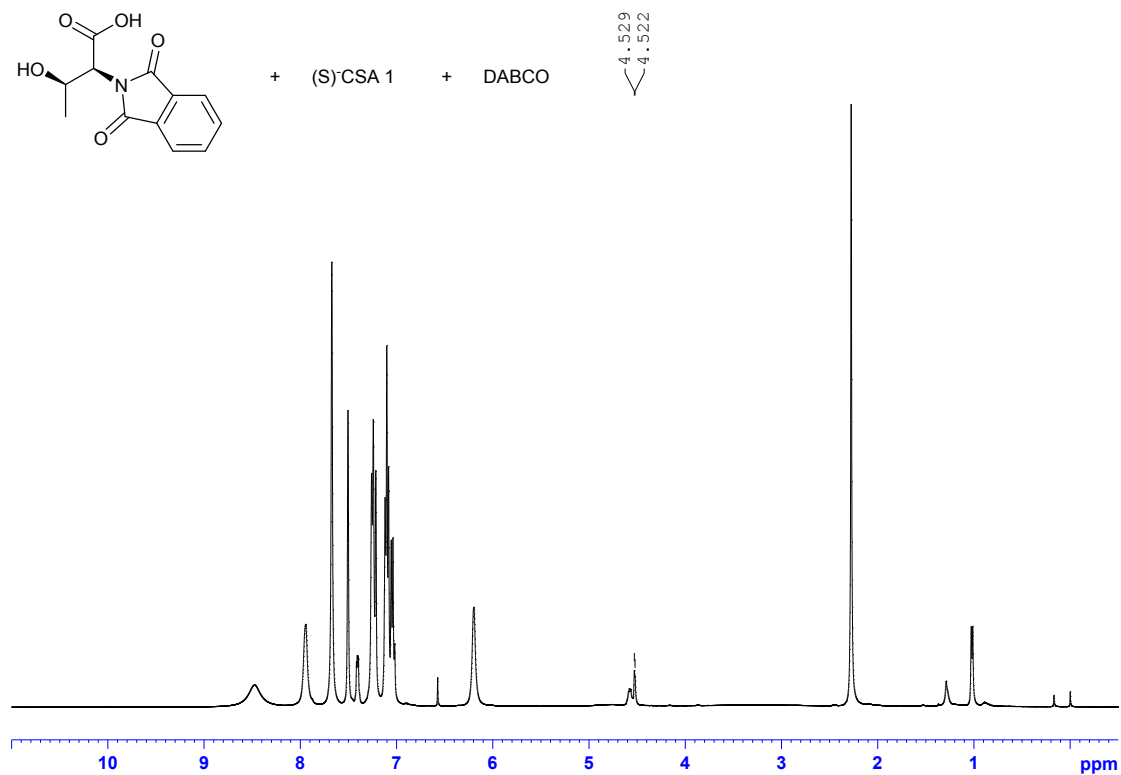


Figure S19. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 10

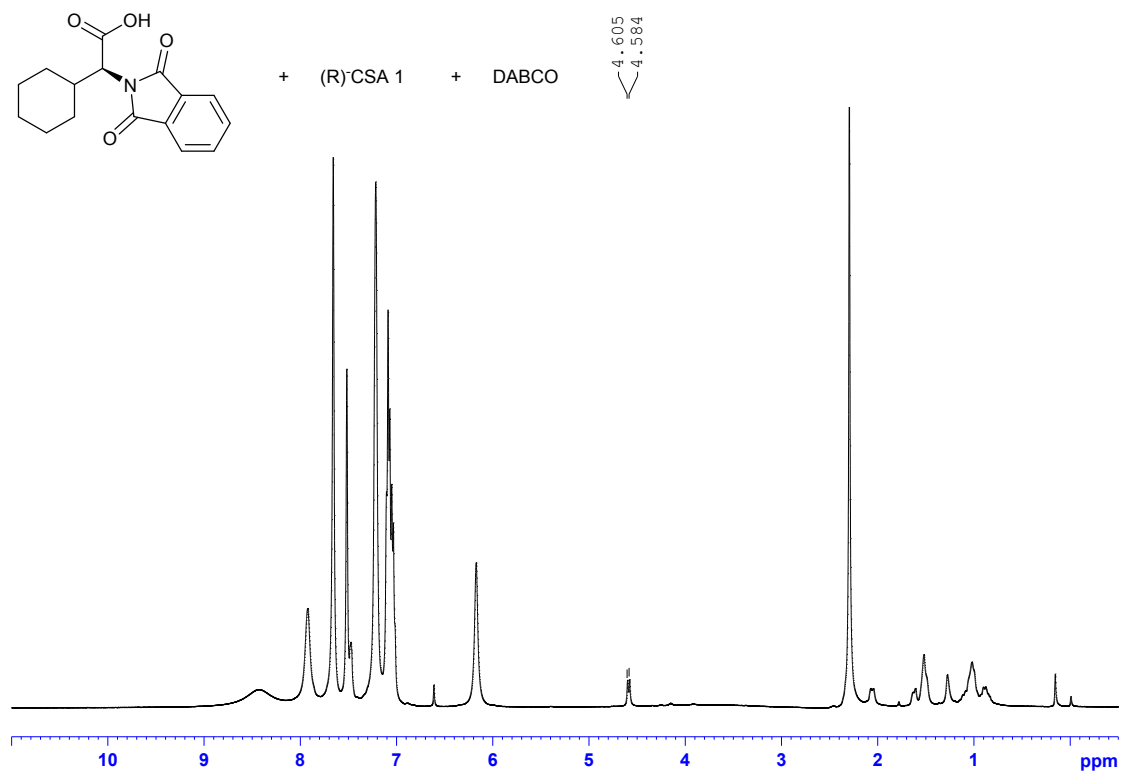


Figure S20. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 10

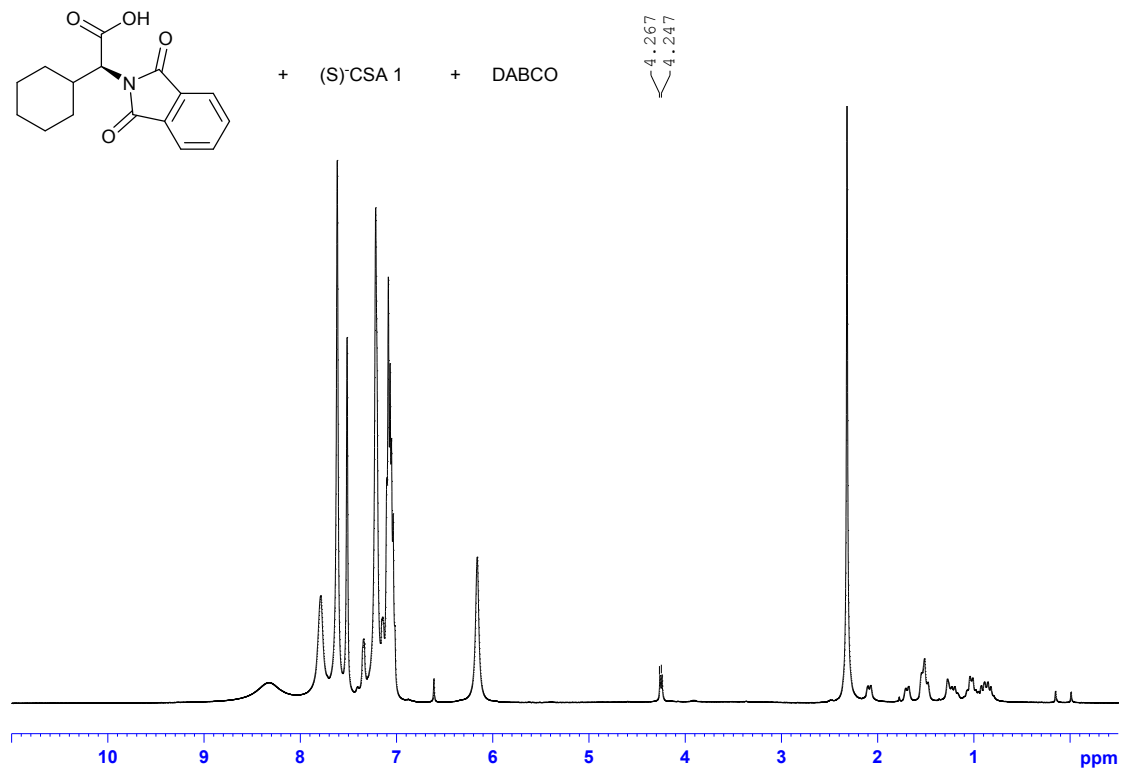


Figure S21. ¹H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 11

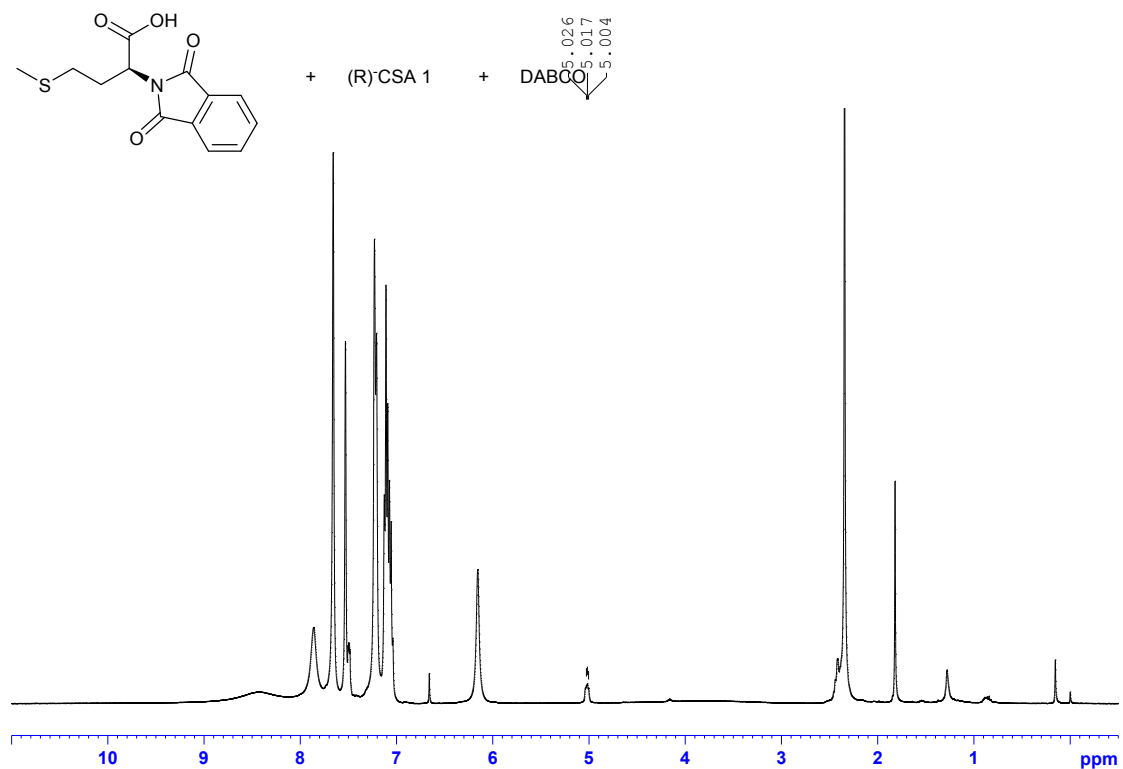


Figure S22. ¹H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 11

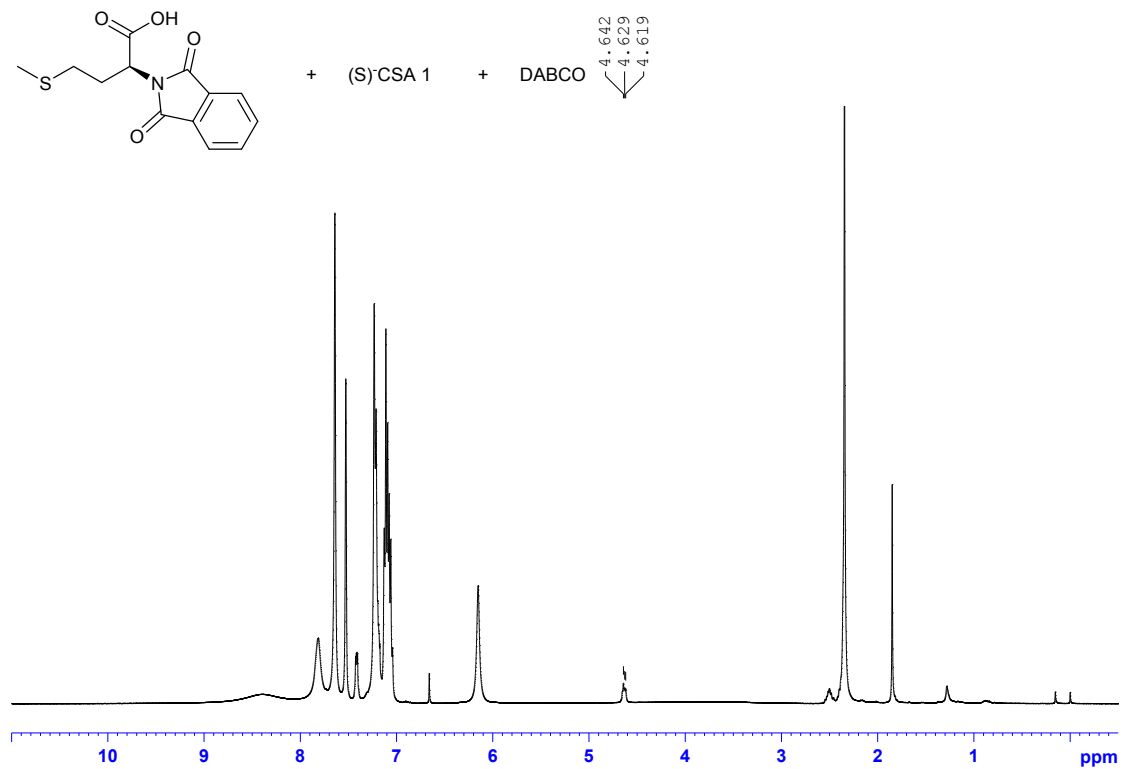


Figure S23. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 12

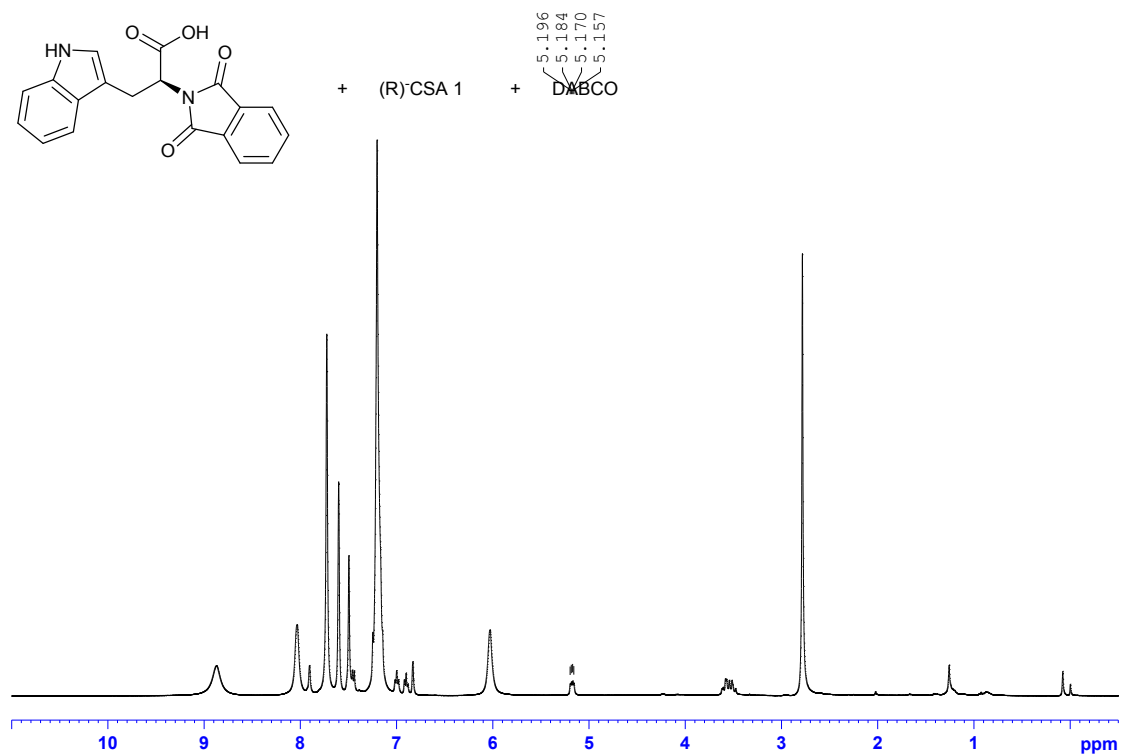


Figure S24. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 12

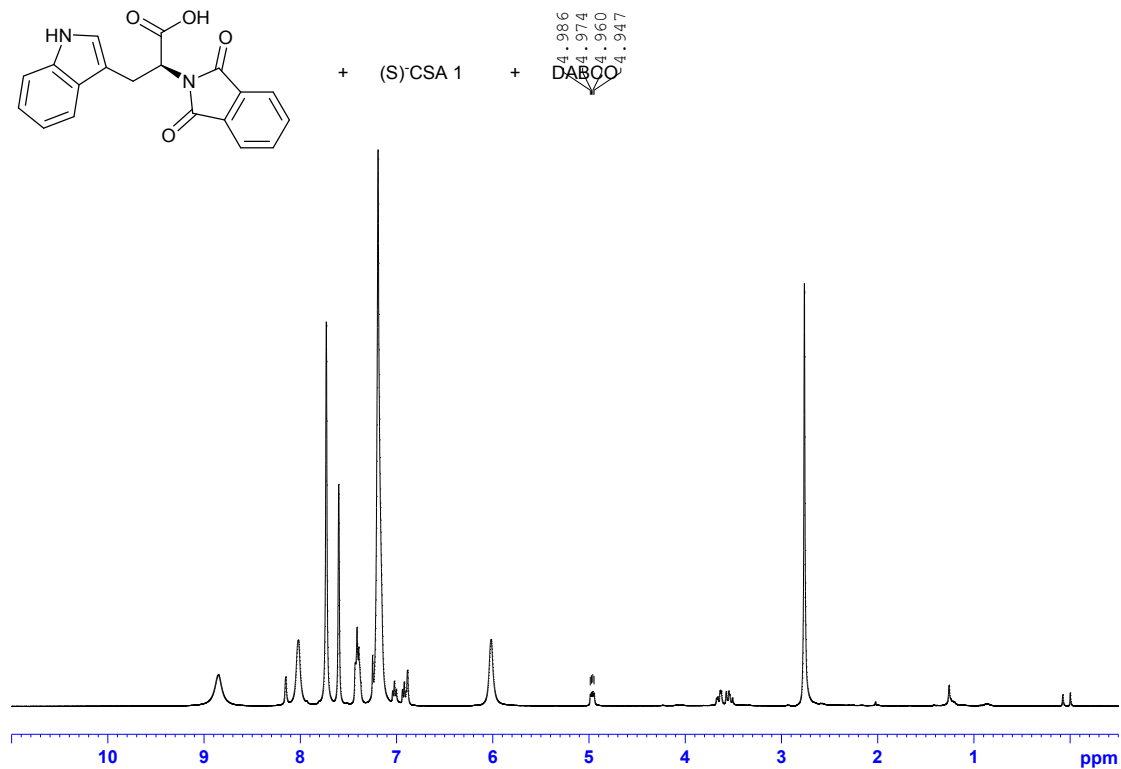


Figure S25. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 13

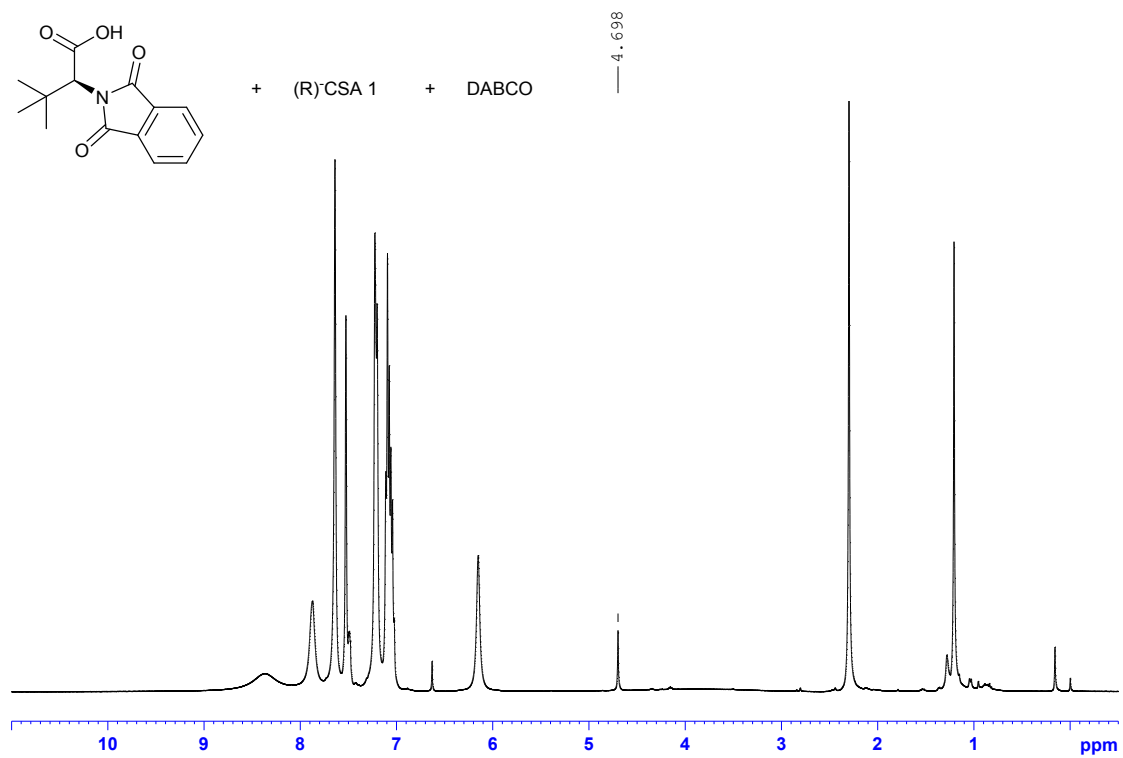


Figure S26. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 13

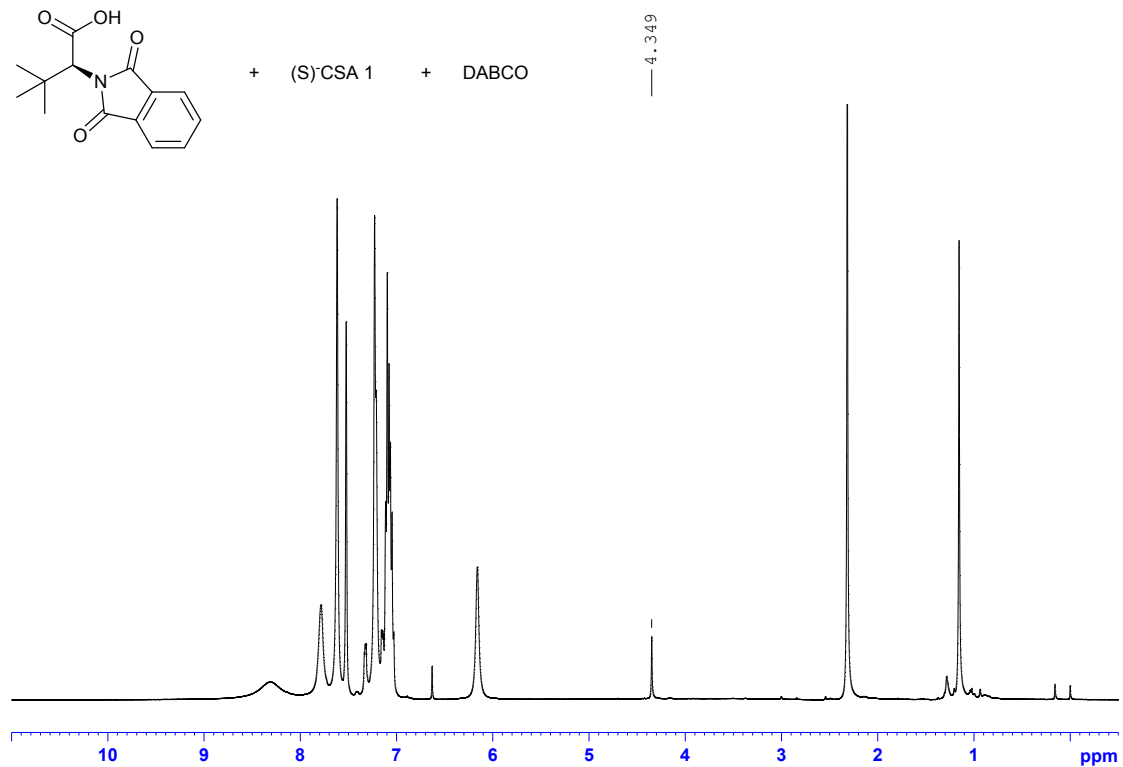


Figure S27. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 14

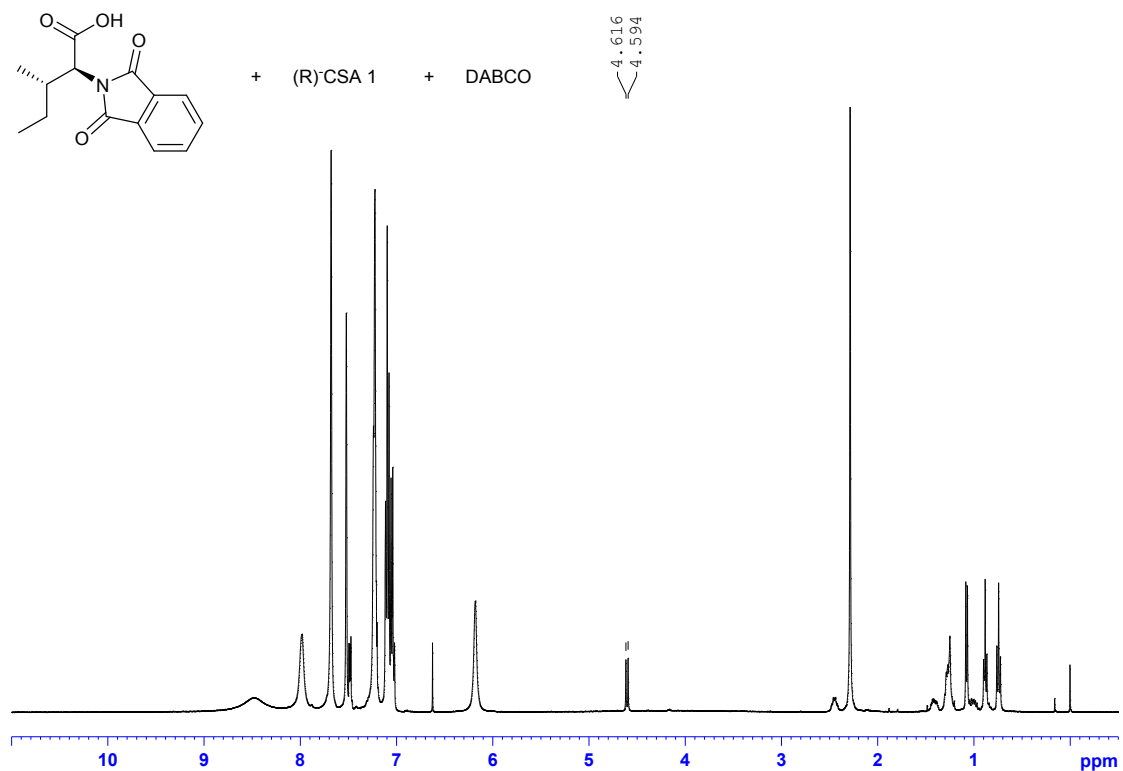


Figure S28. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 14

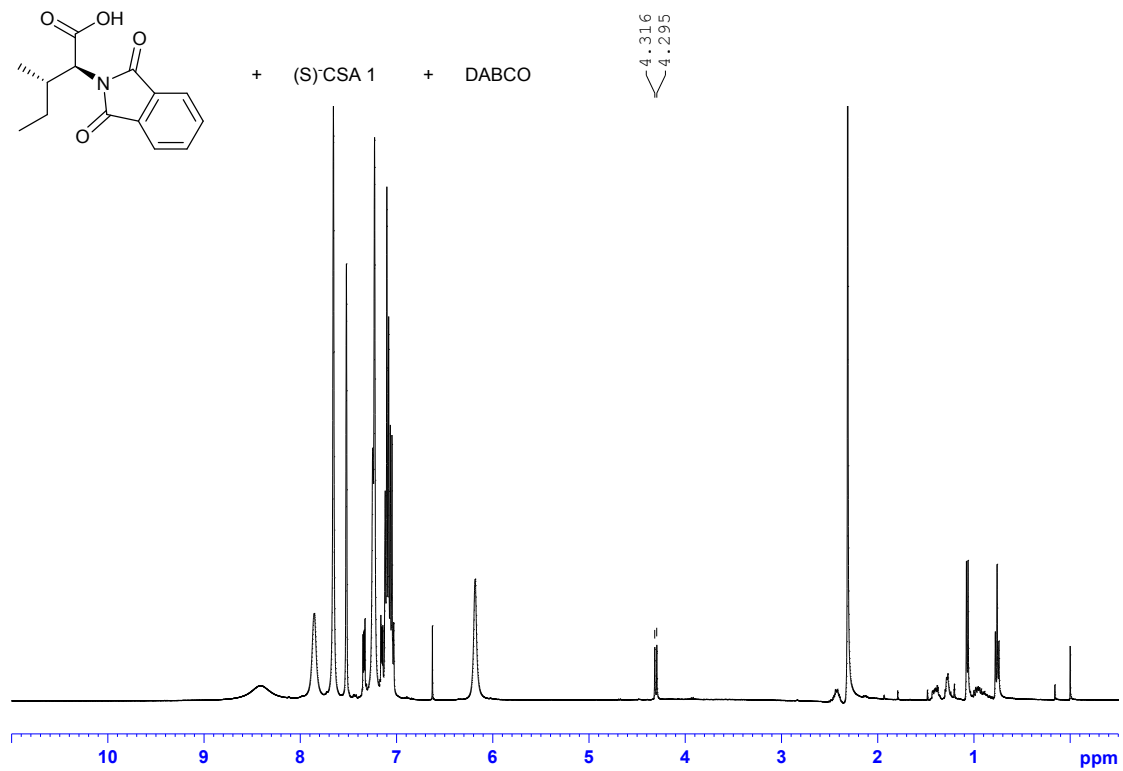


Figure S29. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 15

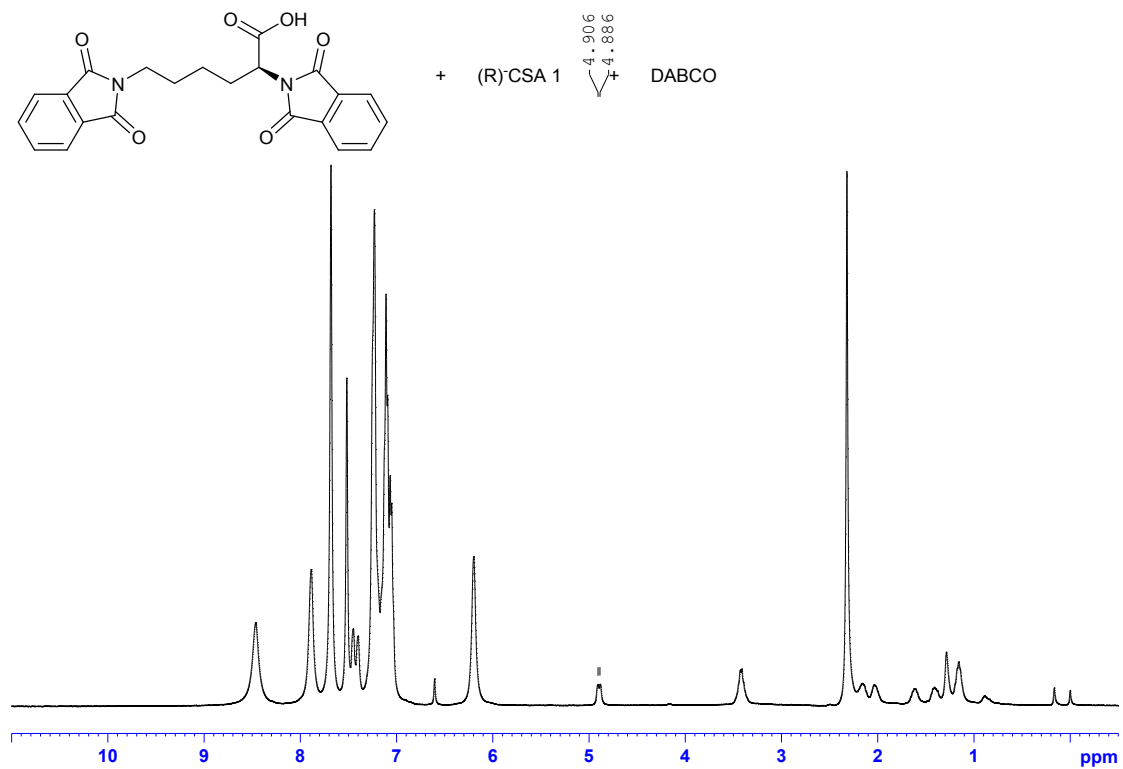


Figure S30. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 15

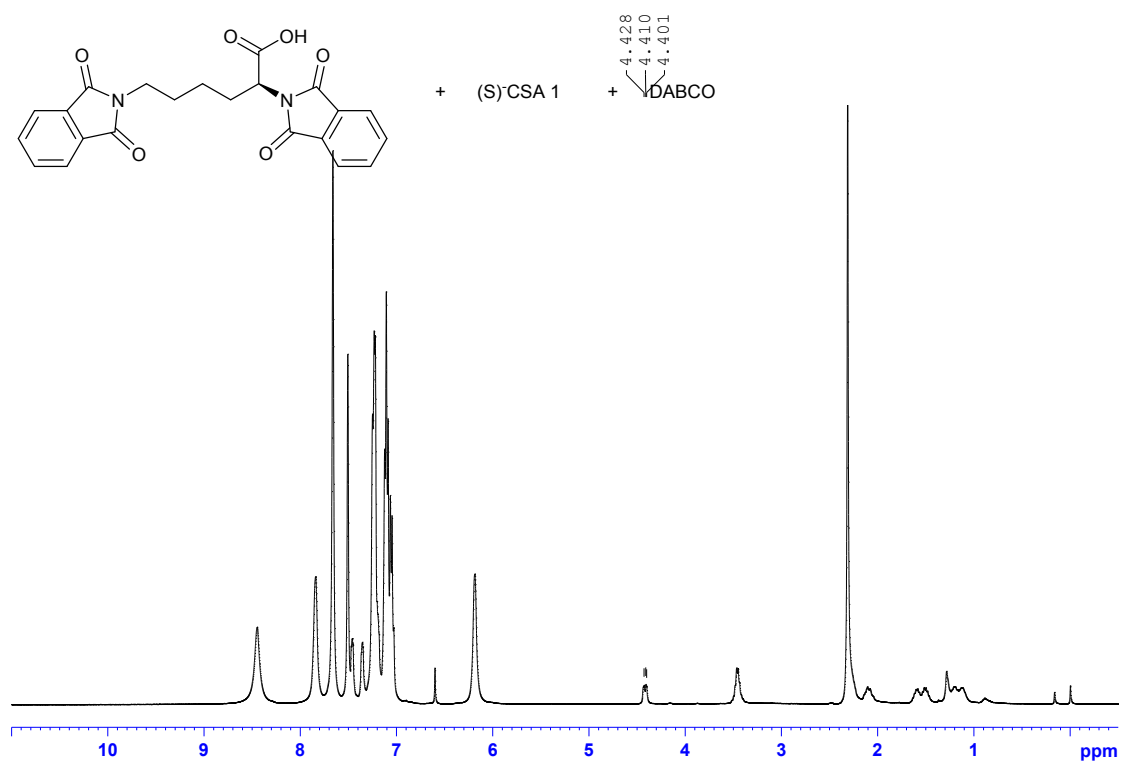


Figure S31. ¹H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 16

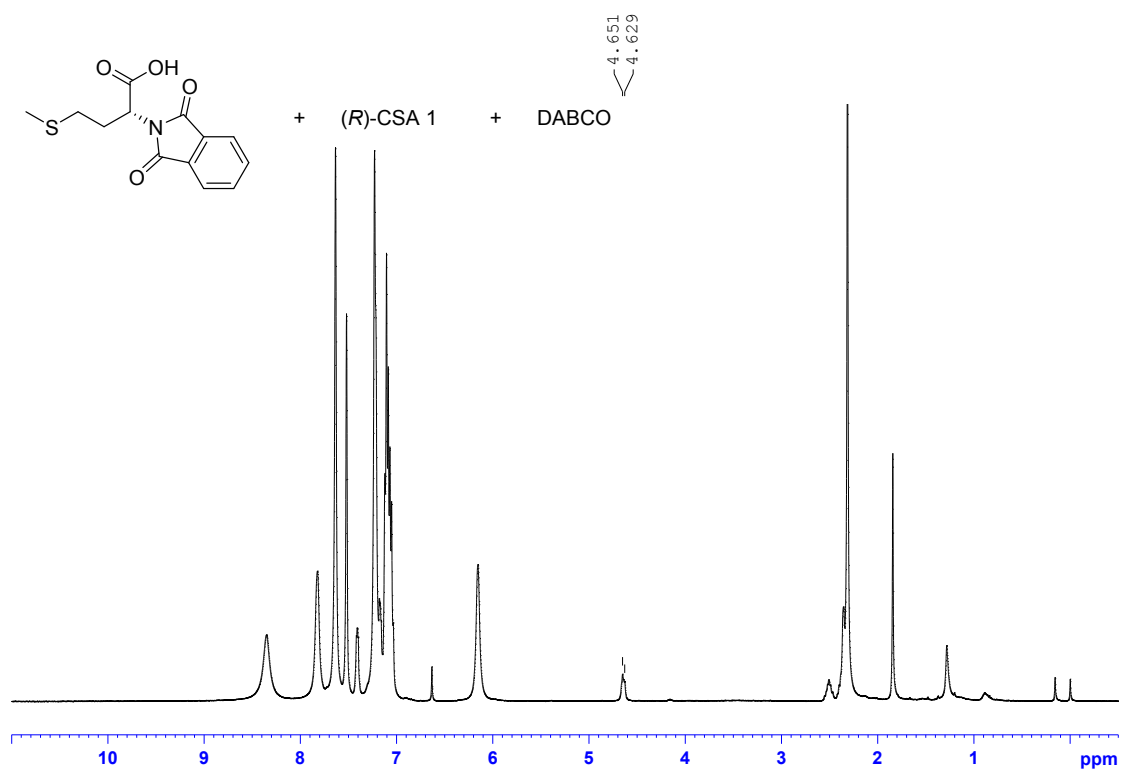


Figure S32. ¹H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 16

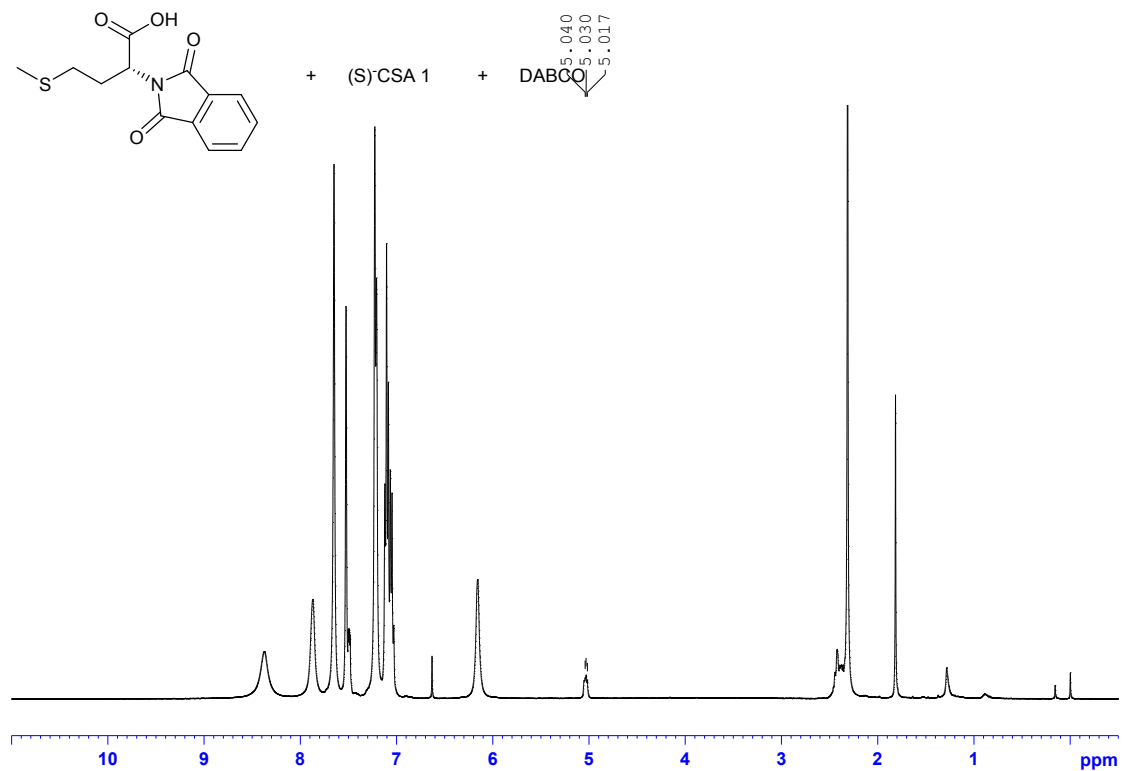


Figure S33. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 17

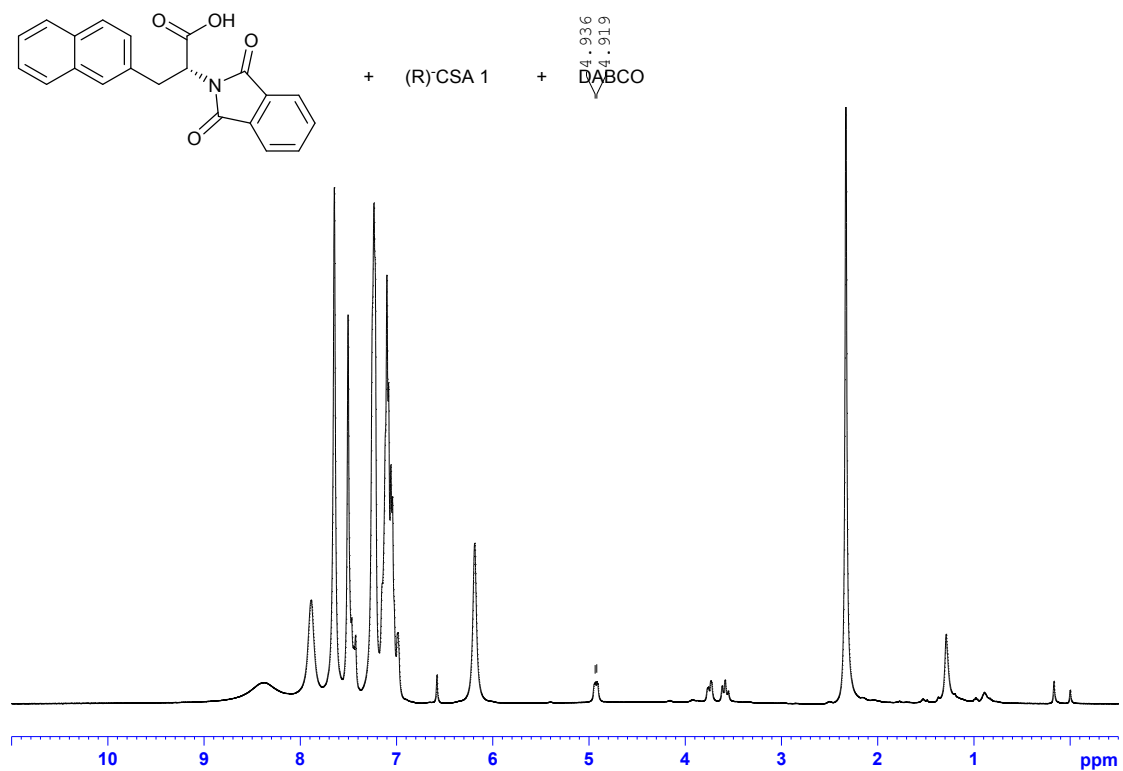


Figure S34. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 17

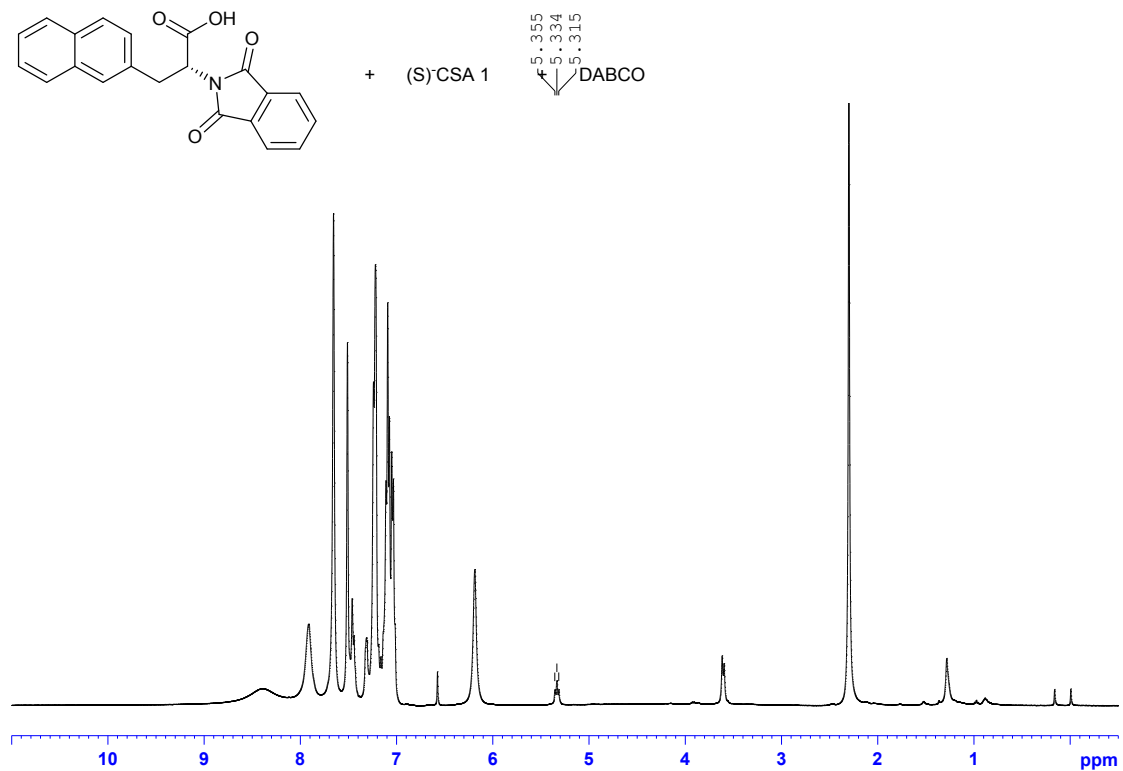


Figure S35. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 18

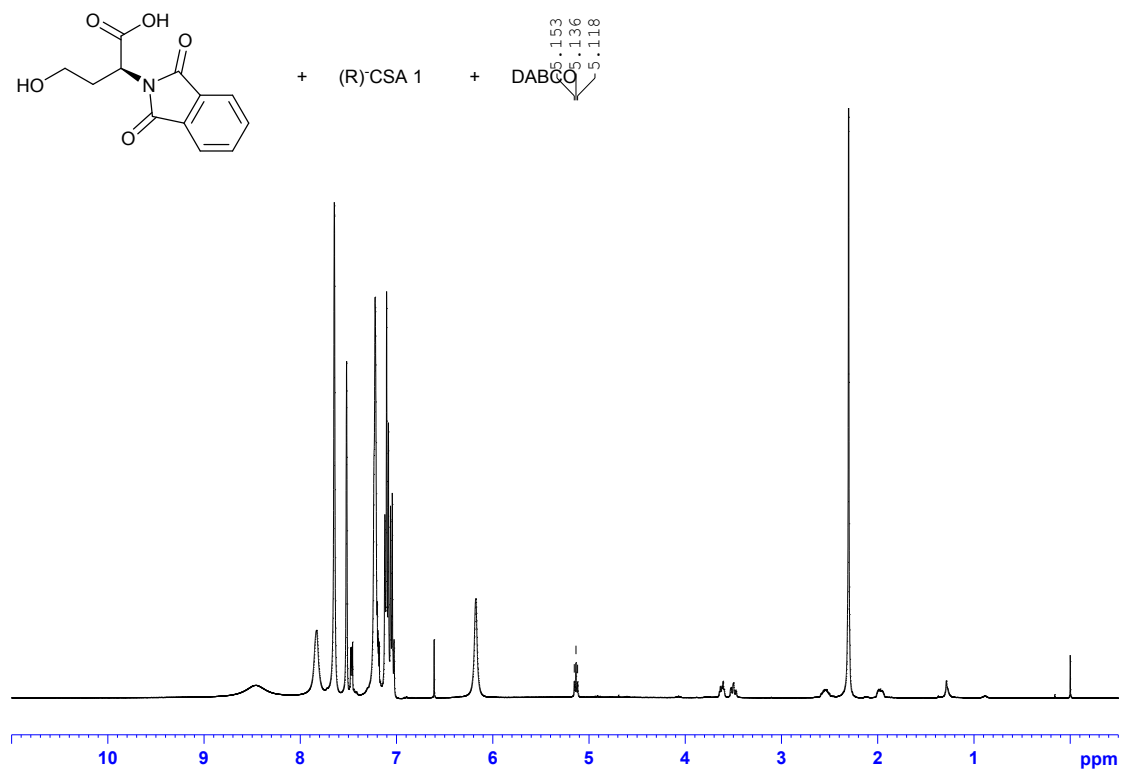


Figure S36. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 18

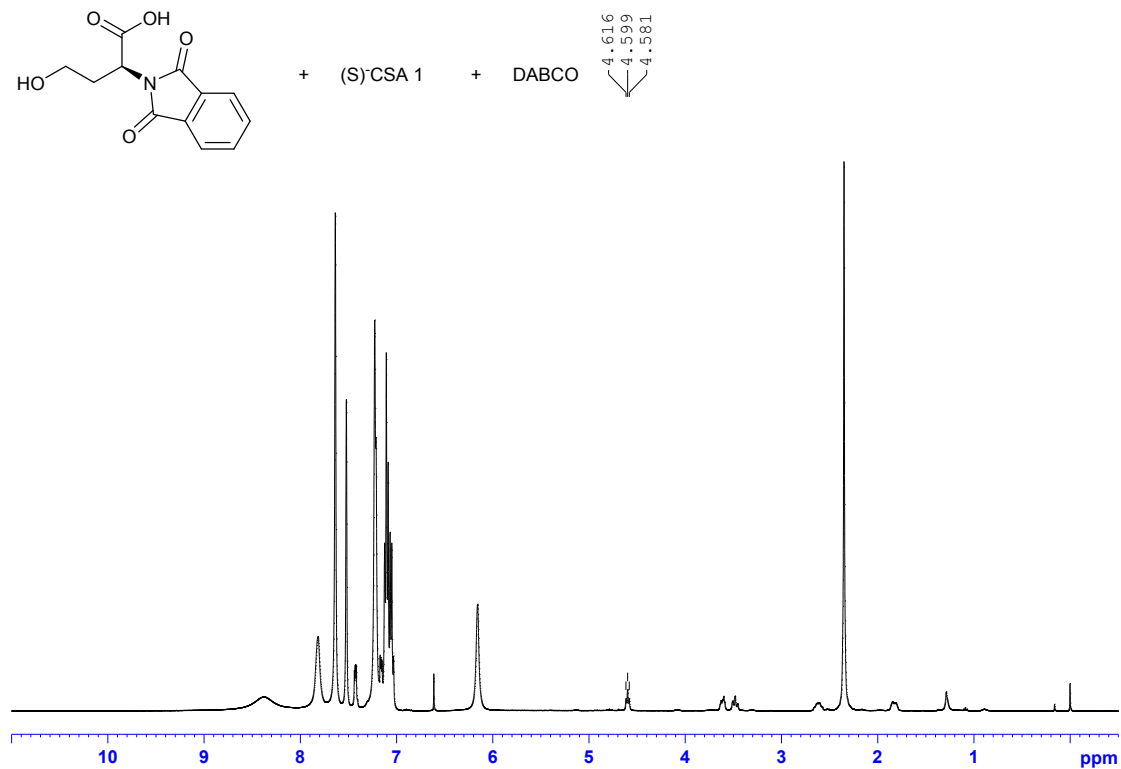


Figure S37. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 19

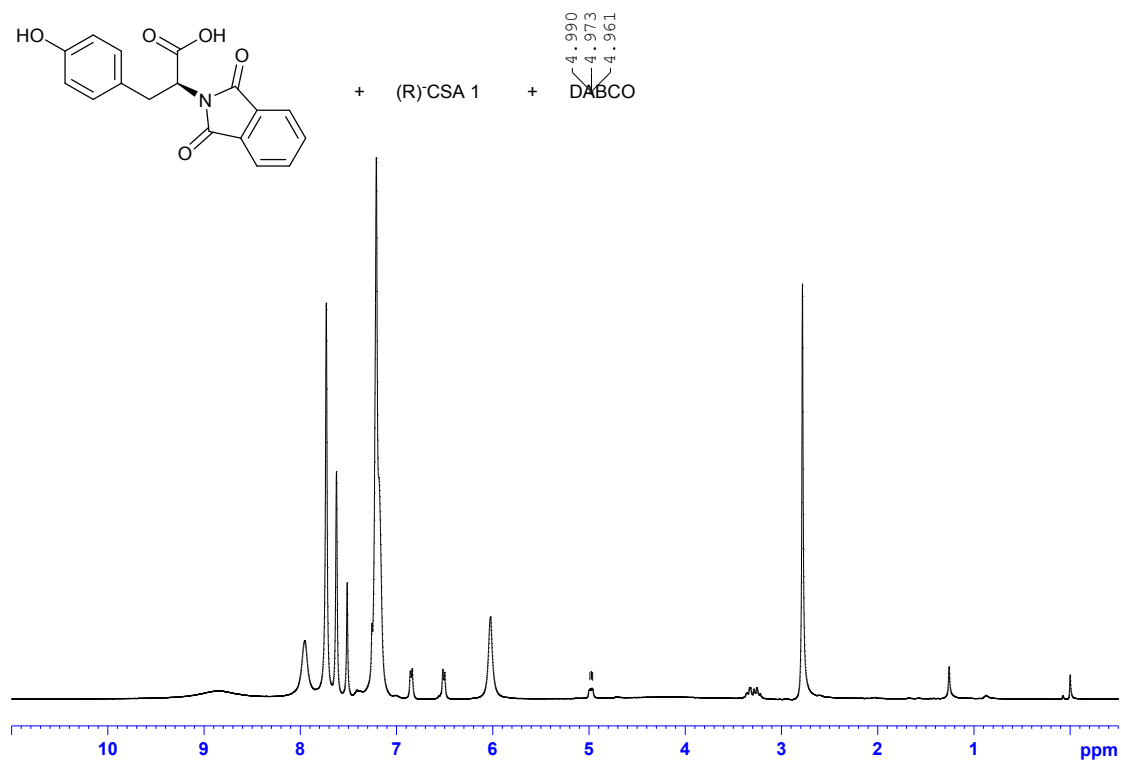


Figure S38. ¹H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 19

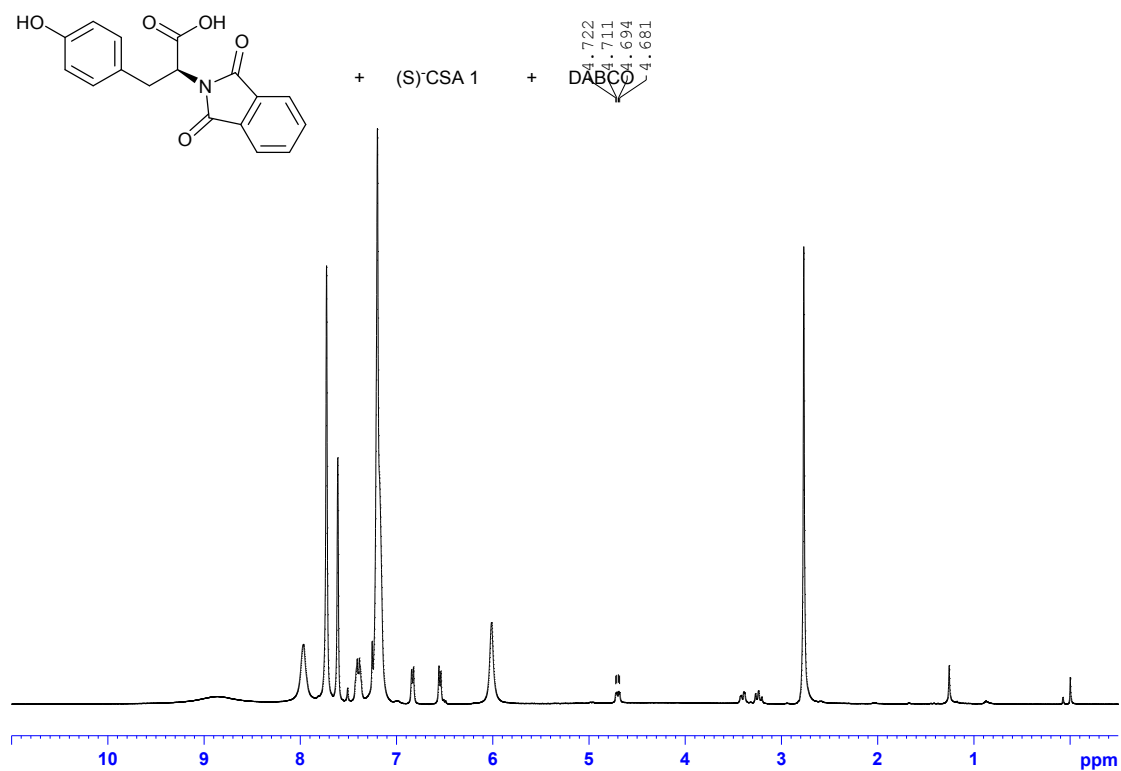


Figure S39. ¹H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 20

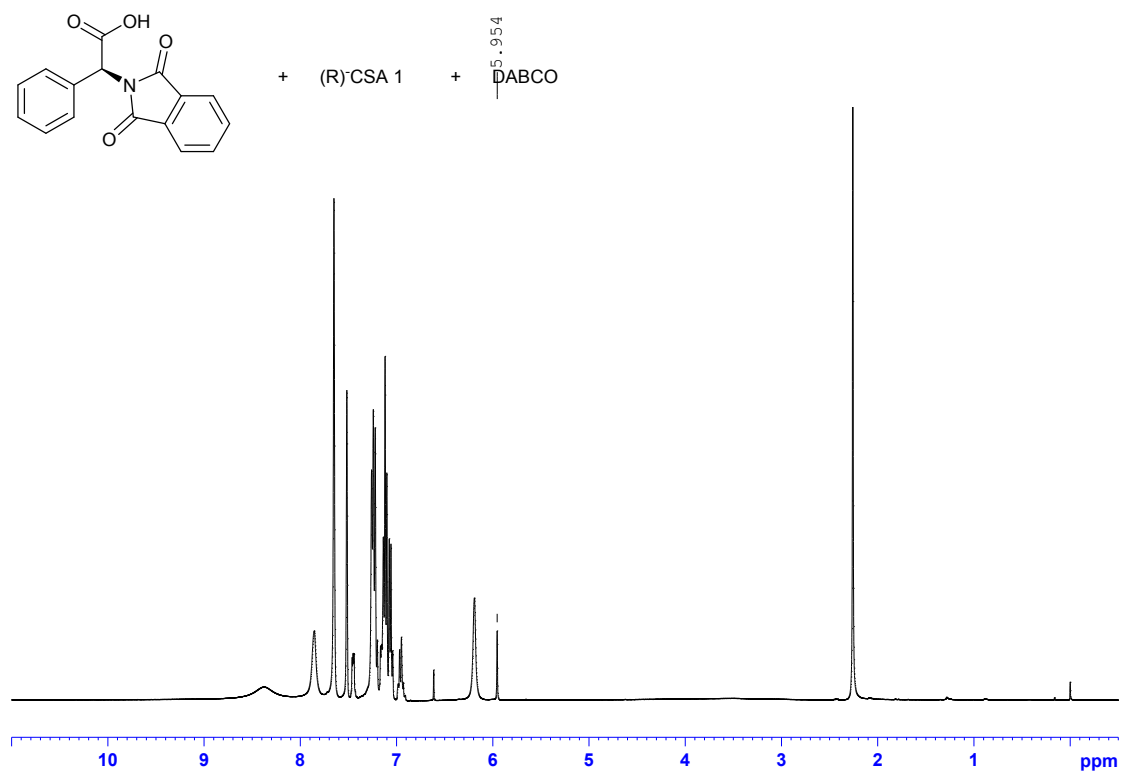


Figure S40. ^1H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 20

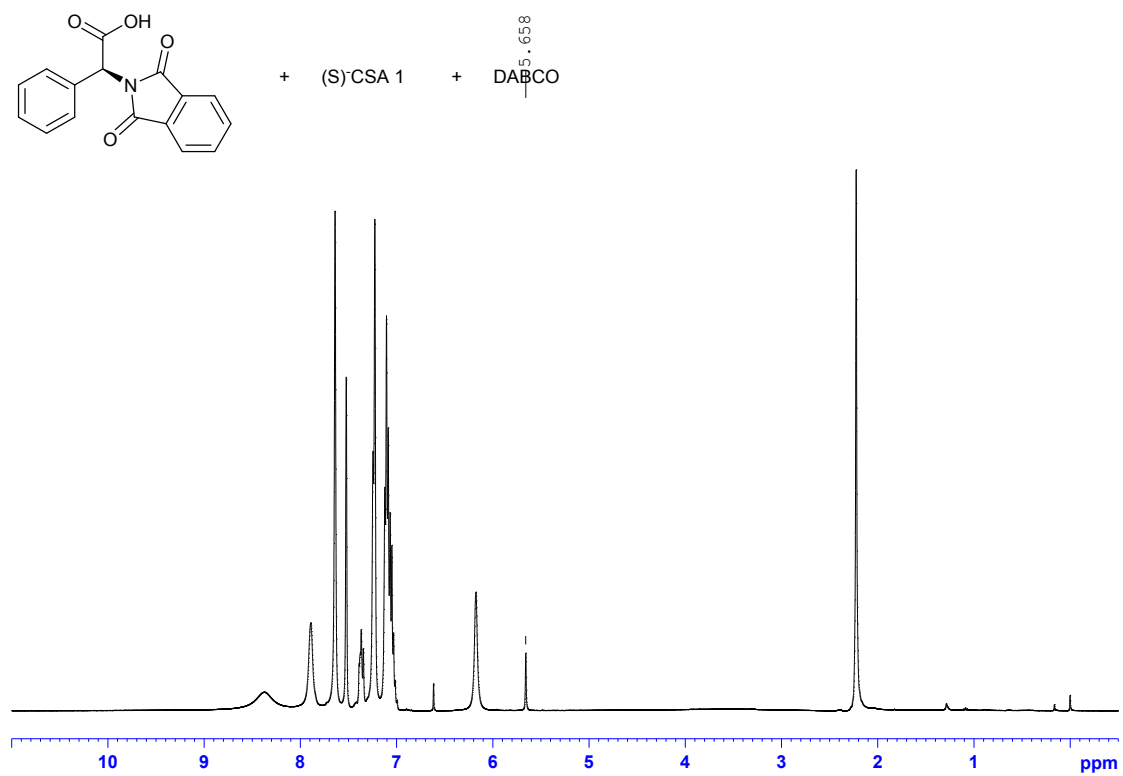


Figure S41. ^1H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 21

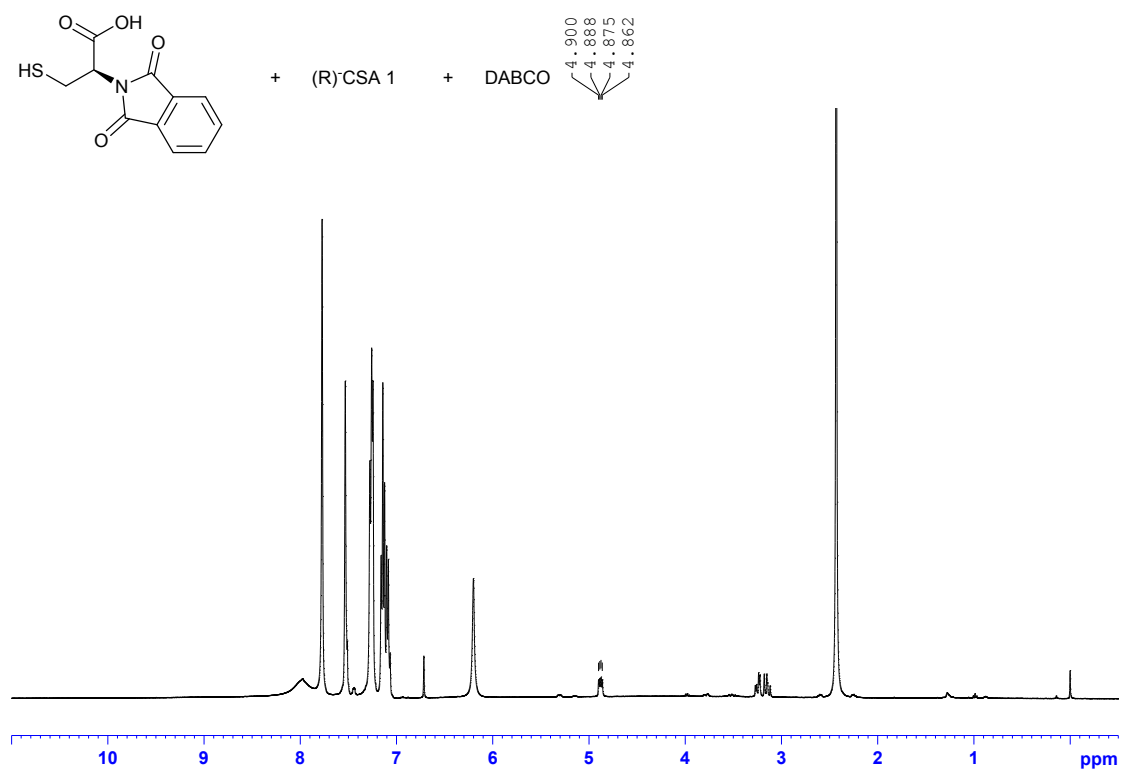


Figure S42. ^1H NMR (400 MHz, TMS) of (*S*)-CSA 1, DABCO and N-Pht- α -amino acid 21

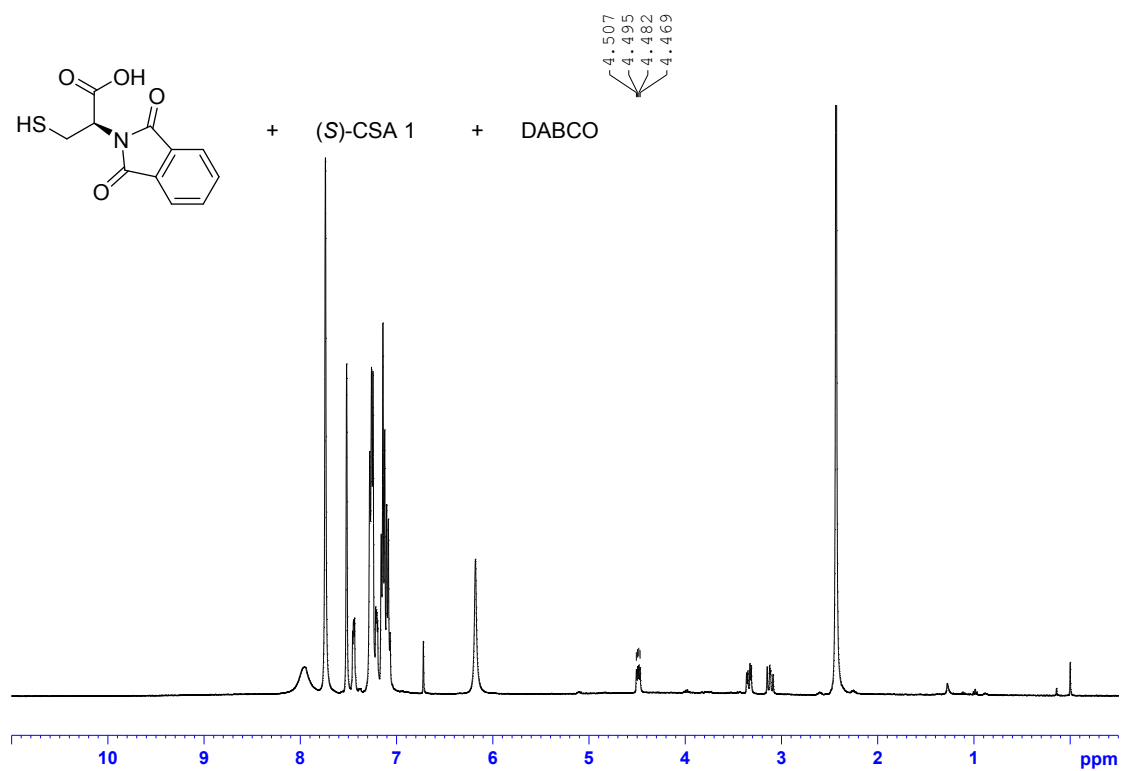


Figure S43. ^1H NMR (400 MHz, TMS) of (*R*)-CSA 1, DABCO and N-Pht- α -amino acid 22

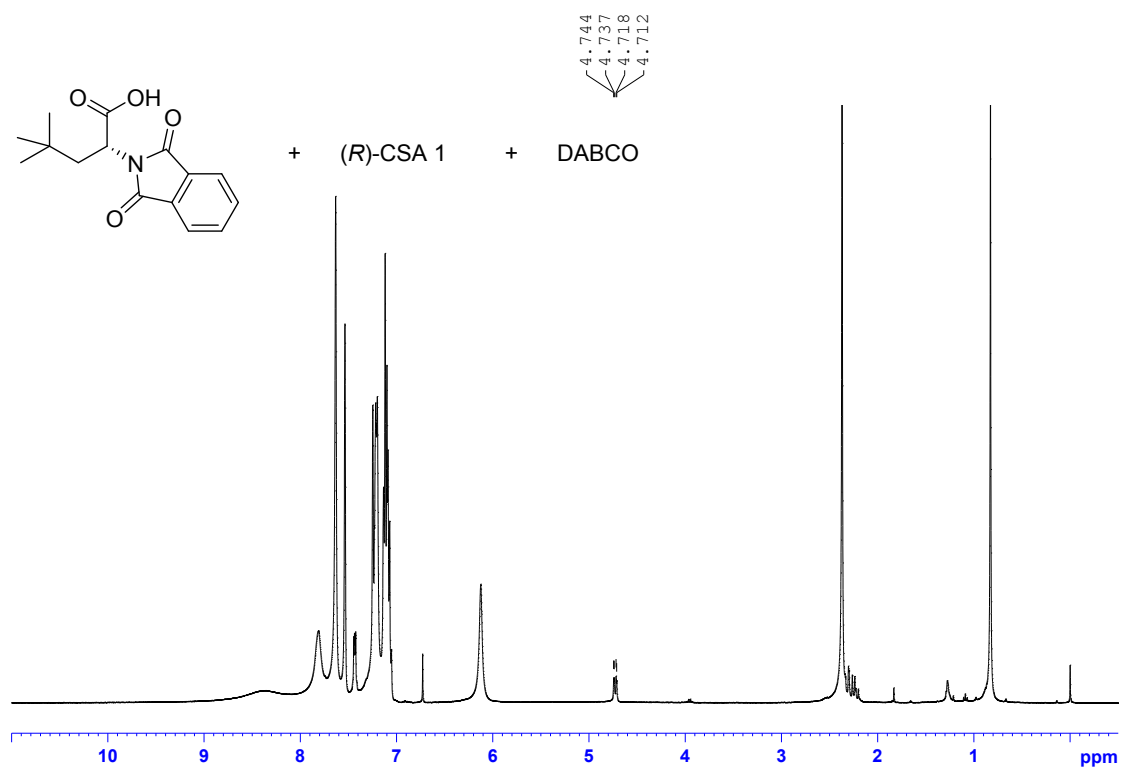


Figure S44. ^1H NMR (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 22

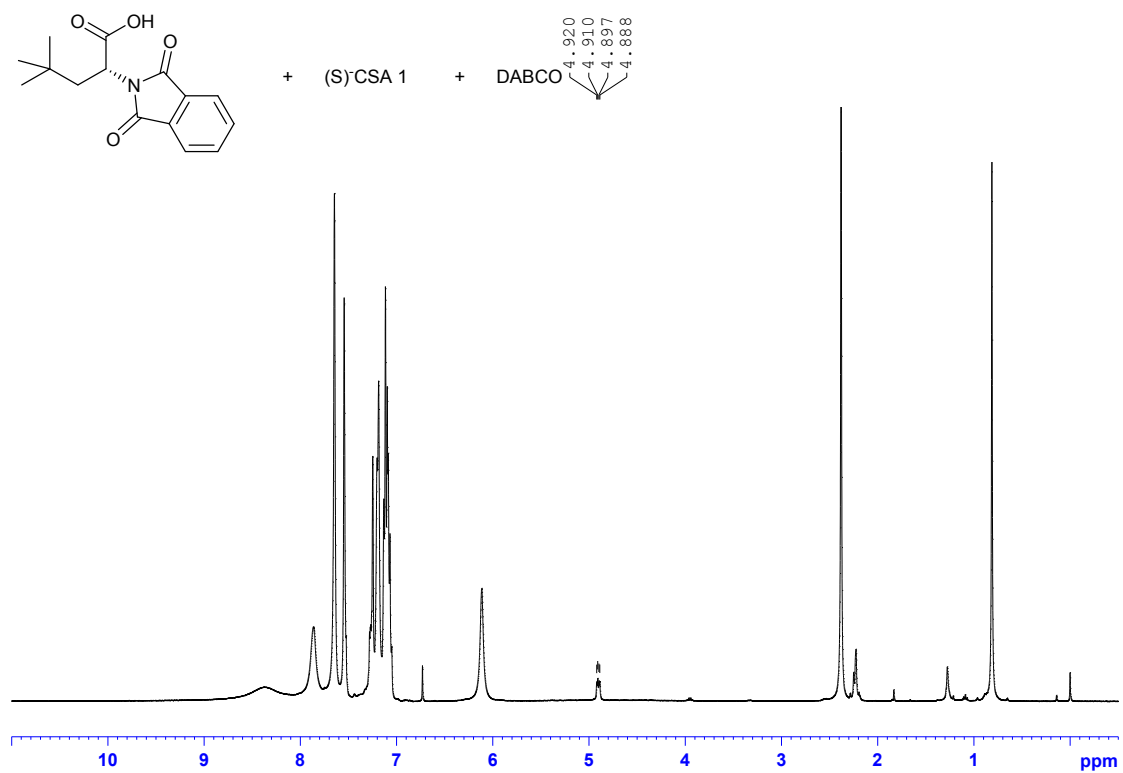


Figure S45. ^1H NMR (400 MHz, TMS) of (R)-CSA 1, DABCO and N-Pht- α -amino acid 23

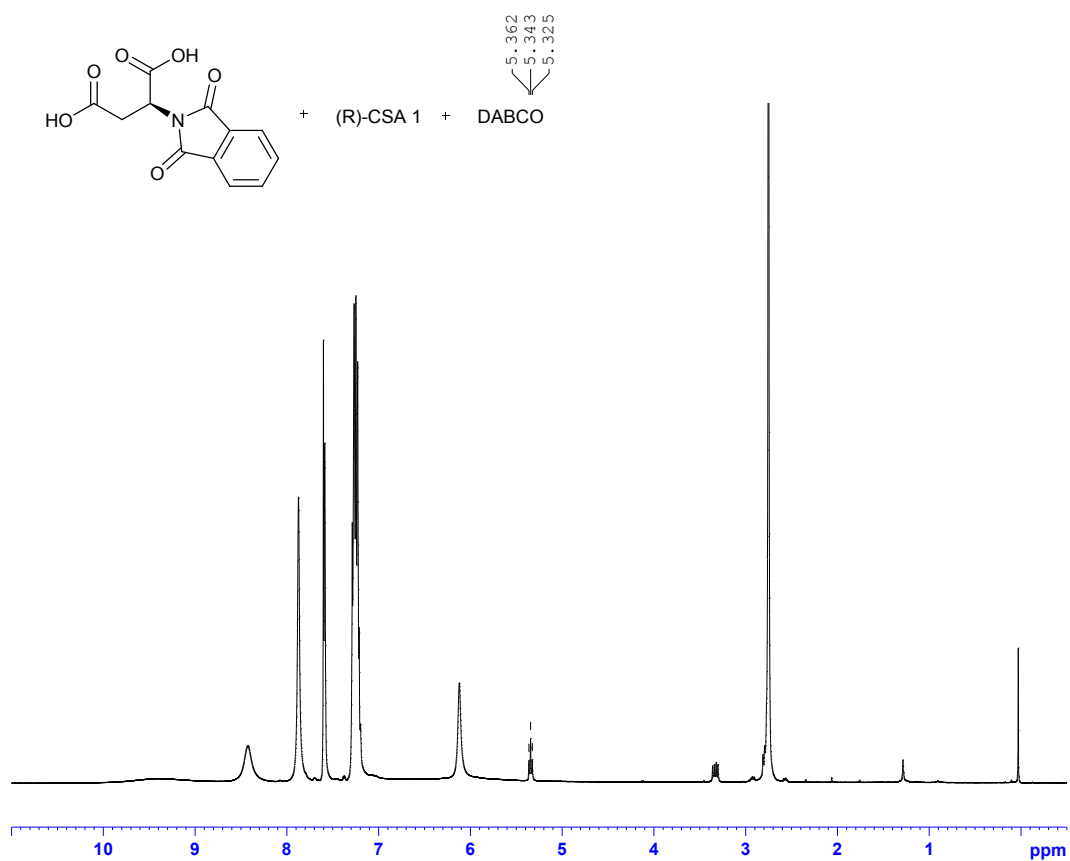


Figure S46. $^1\text{H NMR}$ (400 MHz, TMS) of (S)-CSA 1, DABCO and N-Pht- α -amino acid 23

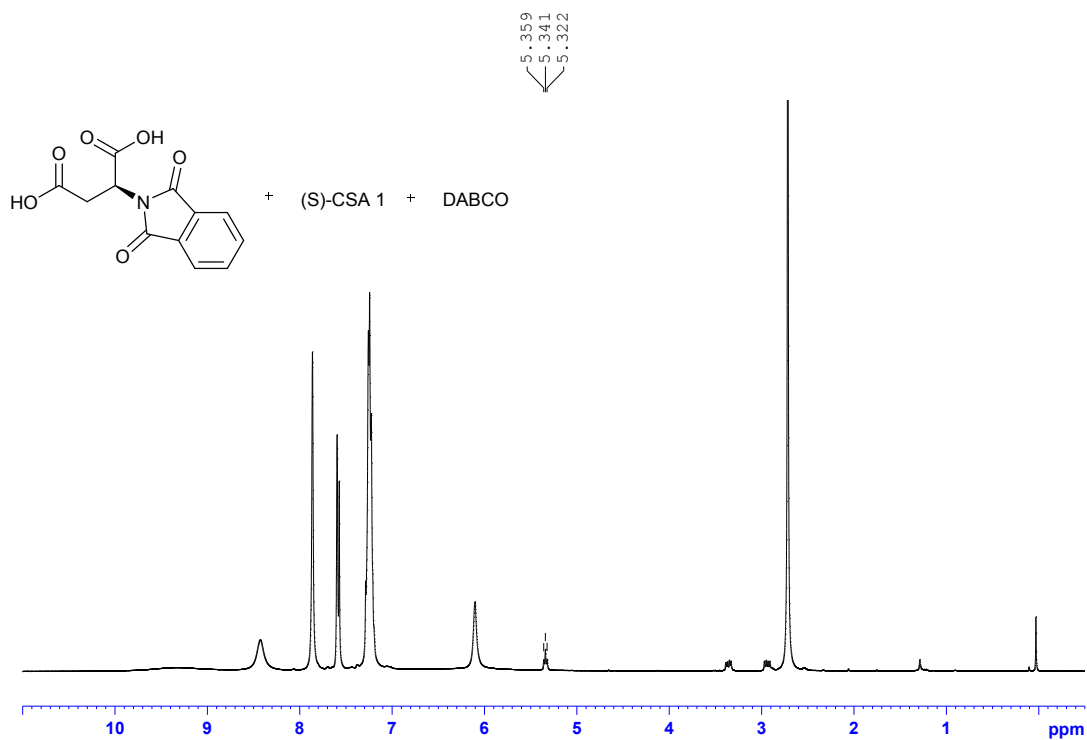


Figure S47. $^1\text{H NMR}$ (400 MHz, CDCl_3 , TMS) N-Pht- α -amino acid 10

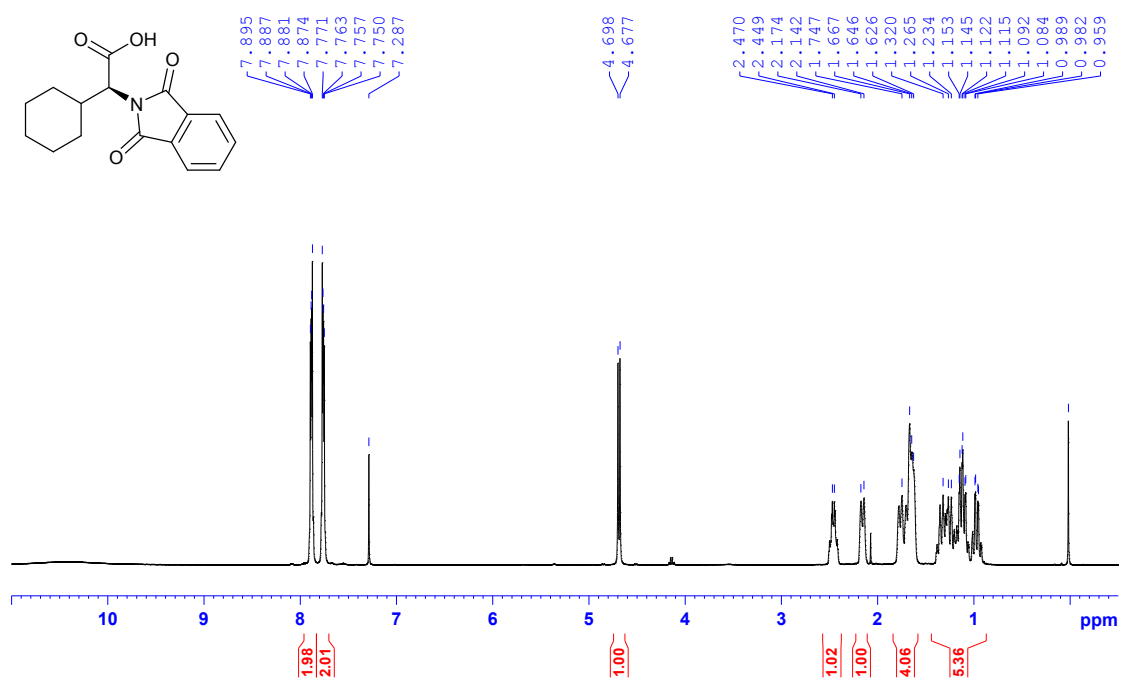


Figure S48. ^{13}C NMR (100 MHz, CDCl_3 , TMS) N-Pht- α -amino acid 10

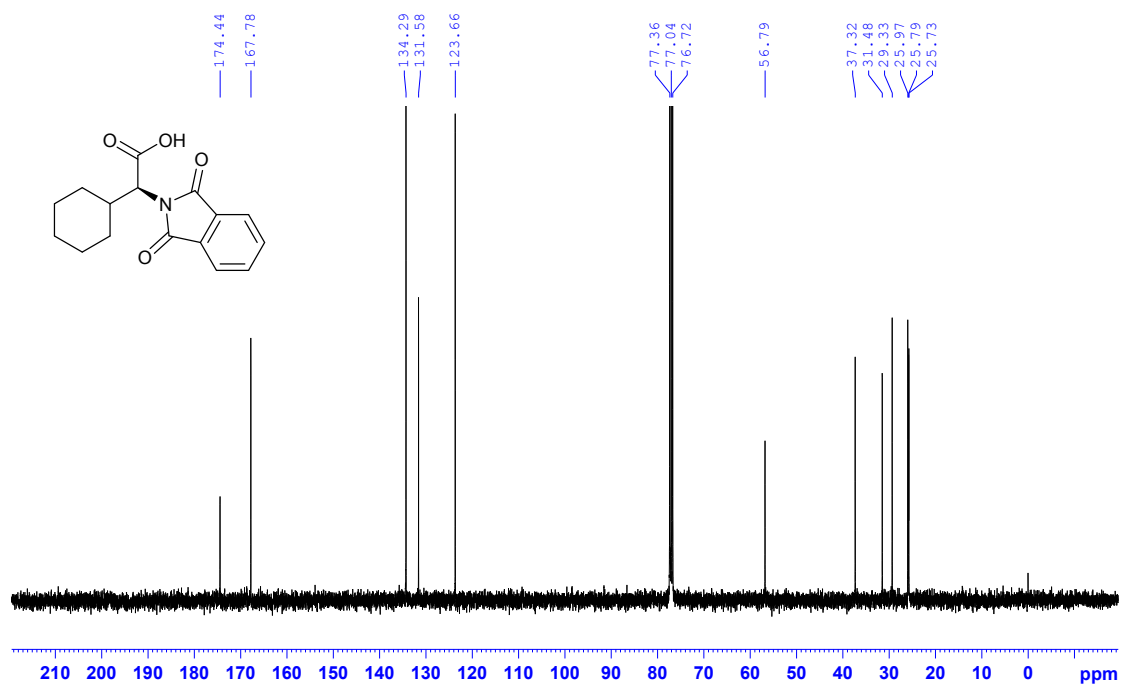


Figure S49. ^{13}C NMR (400 MHz, CDCl_3 , TMS) N-Pht- α -amino acid 22

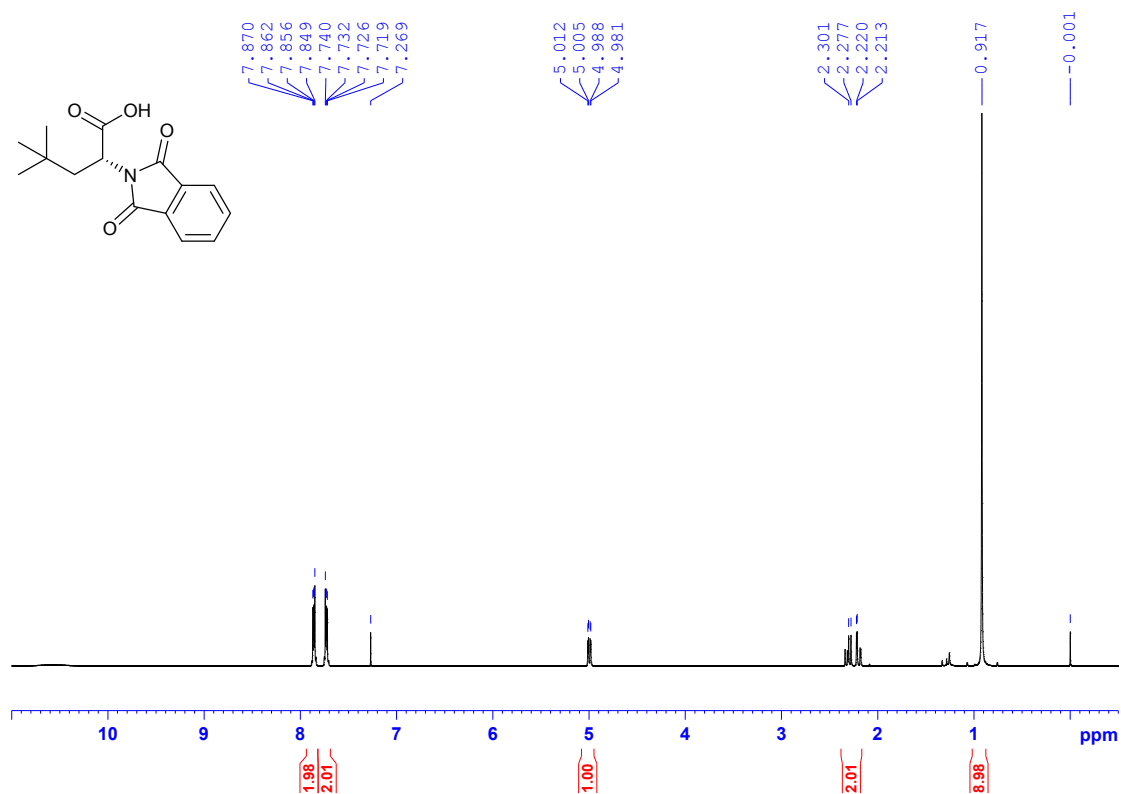


Figure S50. ^{13}C NMR (100 MHz, CDCl_3 , TMS) N-Pht- α -amino acid 22

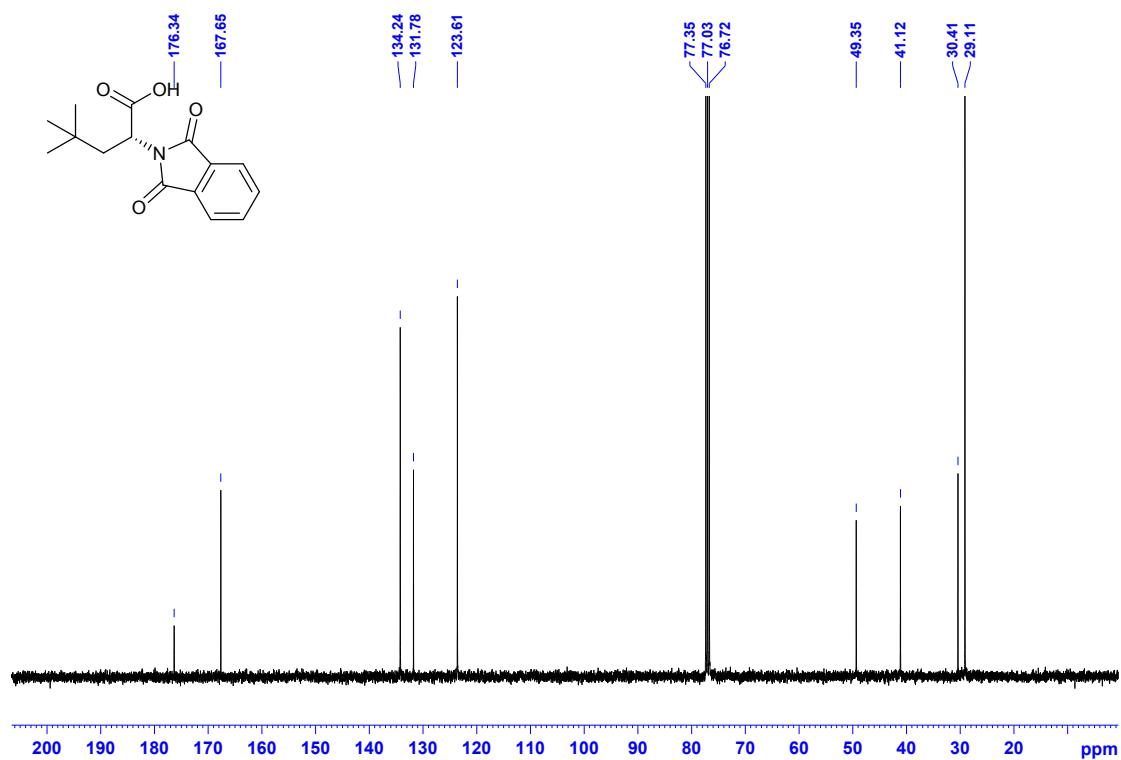


Figure S51. ^1H NMR (500 MHz, TMS) of 50 mM (R)-CSA 1/50 mM L-Pht-Ala /50 mM DABCO

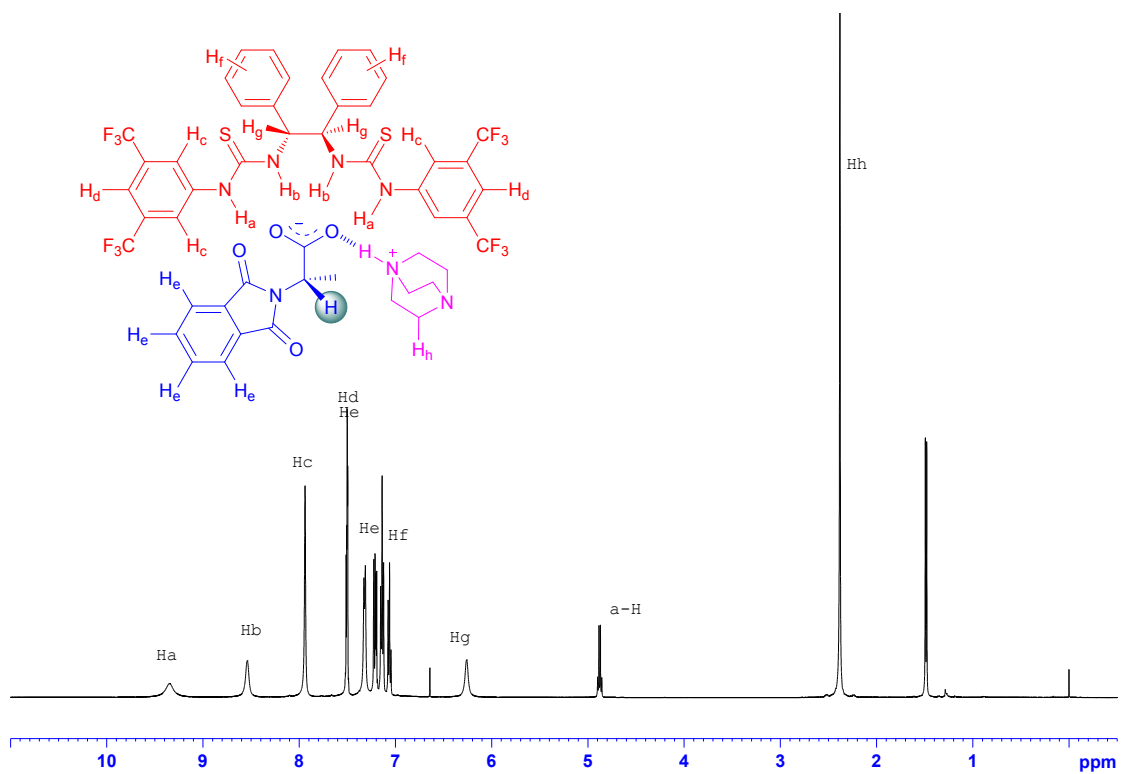


Figure S52. 1D NOESY (500 MHz, TMS) of 50 mM (*R*)-CSA 1/50 mM L-Pht-Ala /50 mM DABCO

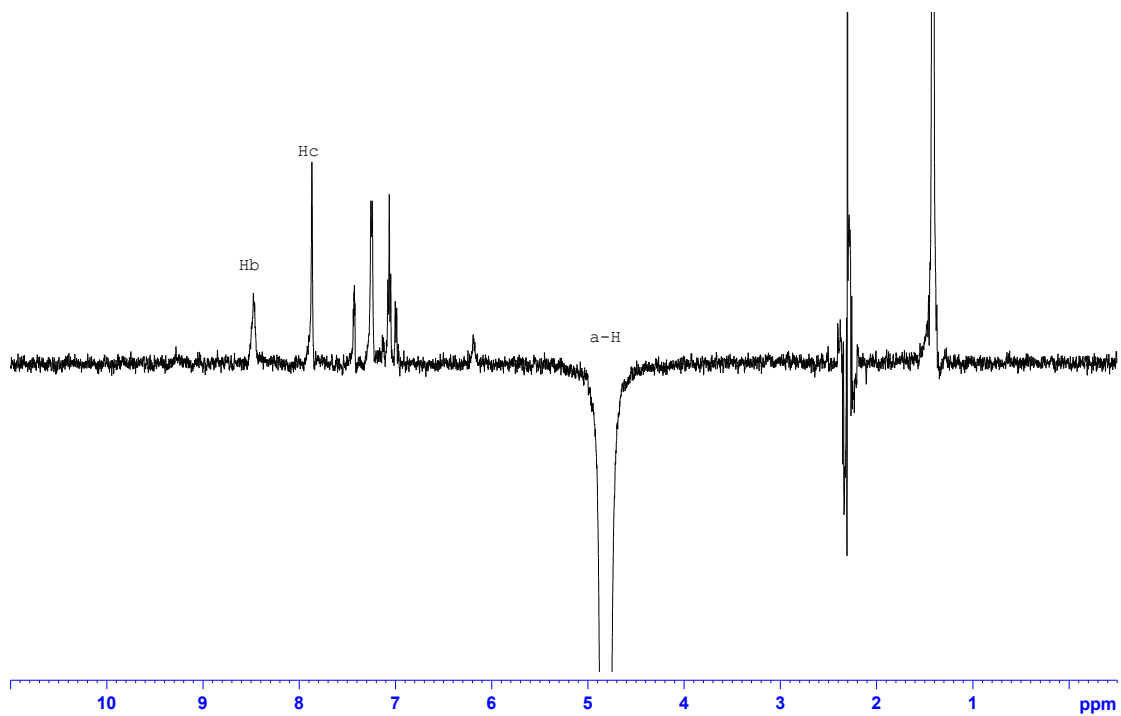


Figure S53. ¹H NMR (500 MHz, TMS) of 50 mM (*S*)-CSA 1/50 mM L-Pht-Ala/50 mM DABCO

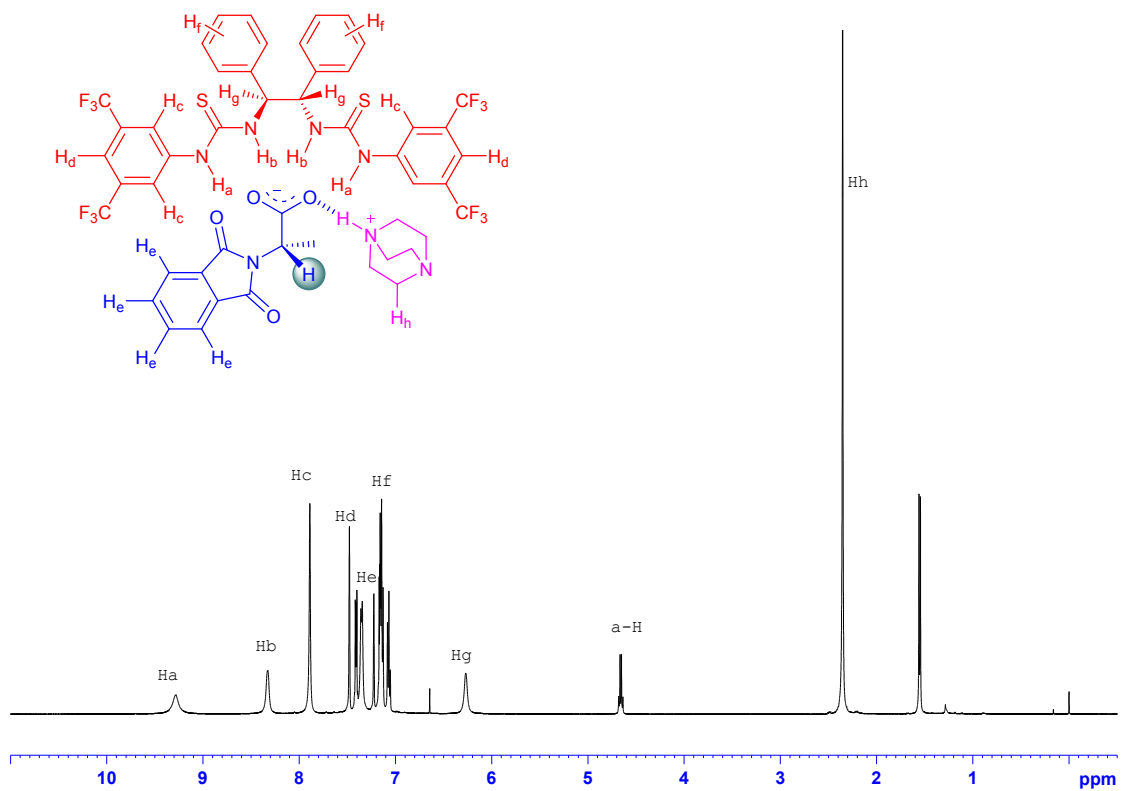


Figure S54. 1D NOESY (500 MHz, TMS) of 50 mM (*S*)-CSA 1/50 mM L-Pht-Ala /50 mM DABCO

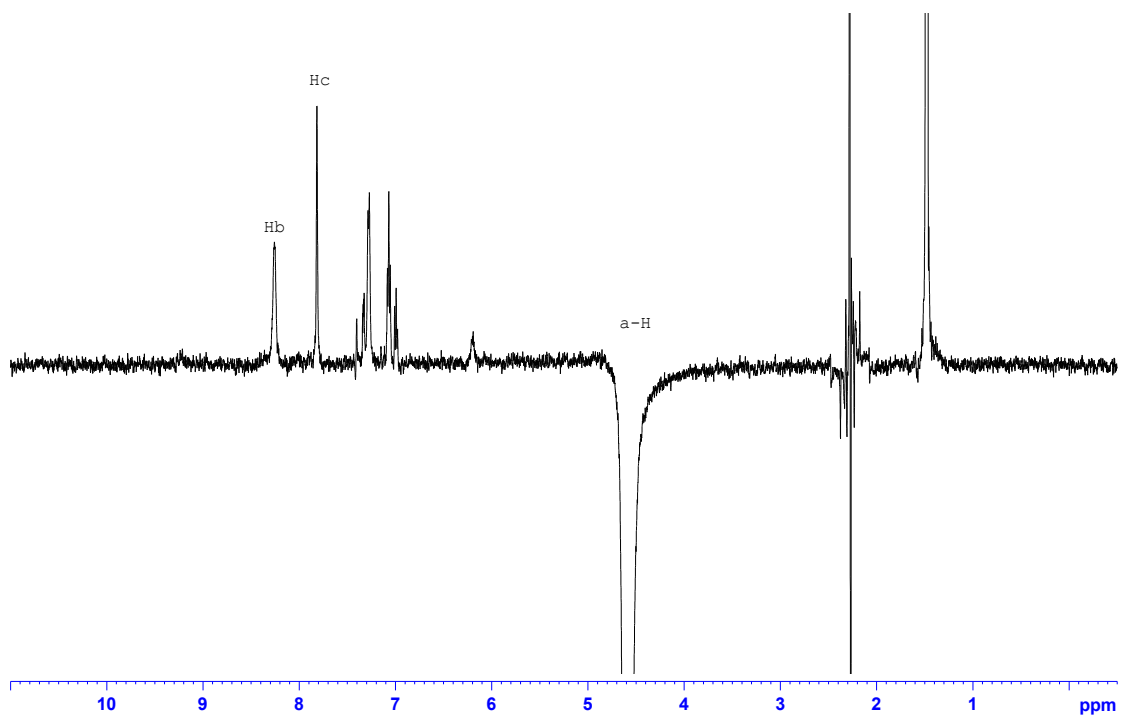
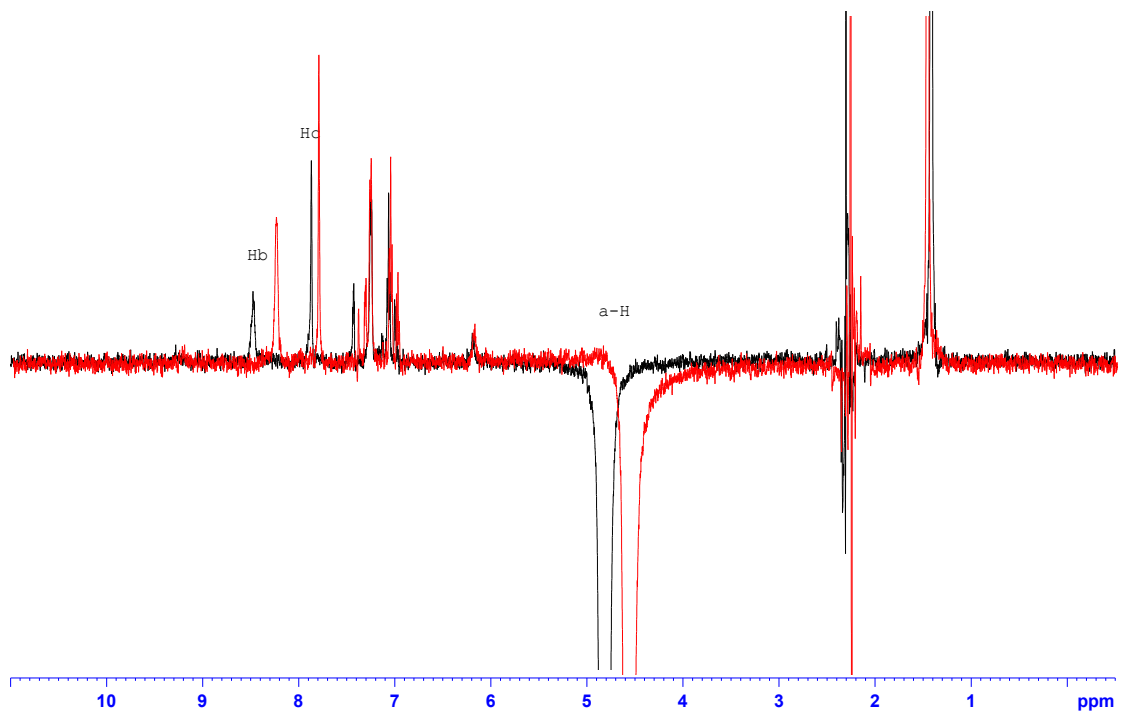


Figure S55. Contrasted 1D NOESY spectra

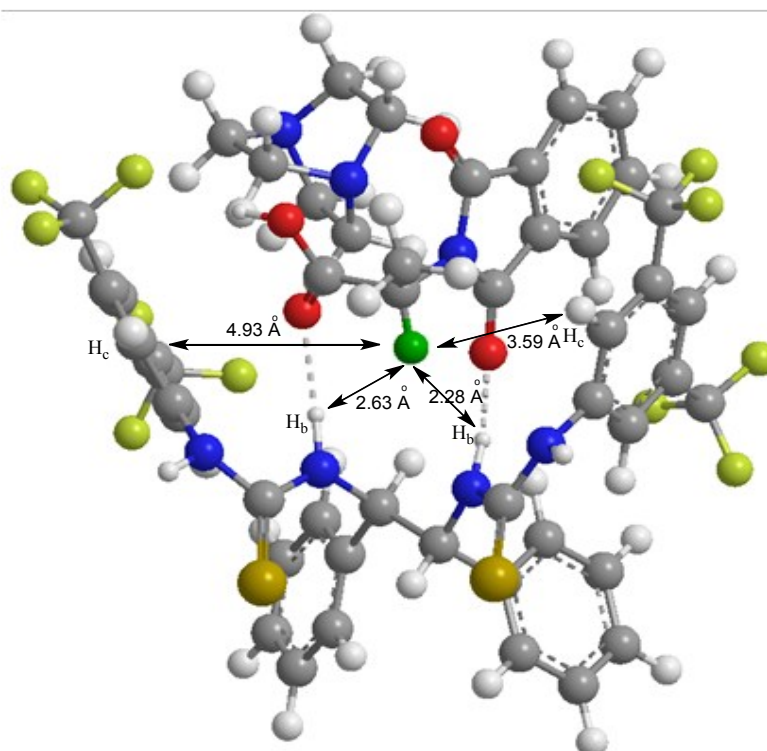
(*S*)-CSA 1/L-Pht-Ala/DABCO
 (*R*)-CSA 1/L-Pht-Ala/DABCO



Computational models of complexes.

Ball-cylinder model for (*R*)-CSA 1/*L*-Pht-Ala/DABCO complex and cartesian coordinates

(Gaussian 09).



The distances between α -H of L-Pht-Ala and Ar-Hs and N-Hs of CSA 1 have been marked.

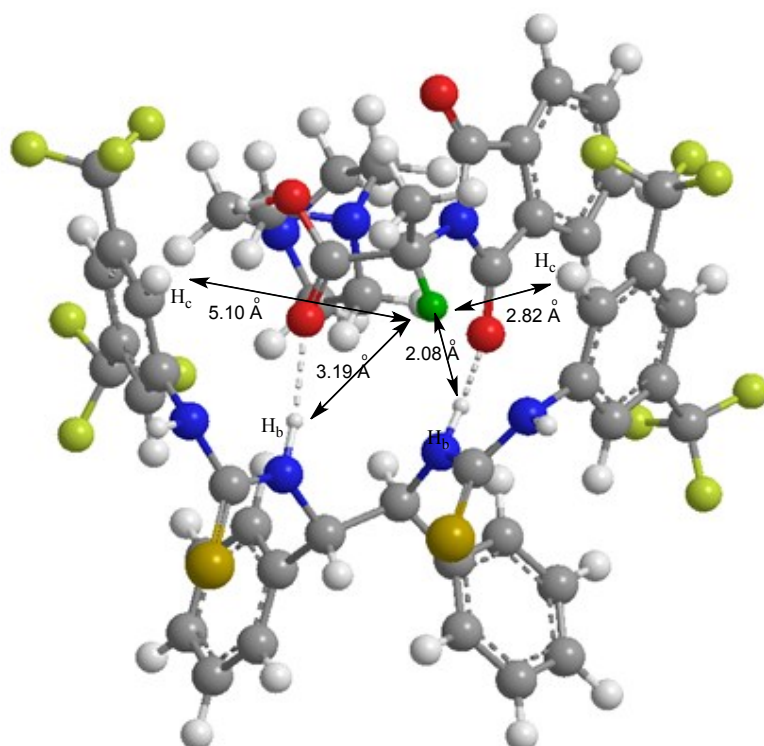
C	0.171534000	-1.312610000	-2.043635000
C	-1.308569000	-1.354826000	-1.675182000
O	-1.799885000	-0.604777000	-0.858186000
O	-1.984188000	-2.306956000	-2.299634000
N	0.868676000	-2.046029000	-0.992756000
H	0.050377000	-1.135948000	-4.181412000
H	0.480766000	-0.263155000	-1.927763000
C	1.322134000	-1.430924000	0.169520000
C	-0.142129000	2.842862000	-0.018100000
C	1.163356000	3.339840000	-0.666208000
N	1.768192000	2.202390000	-1.350715000
C	2.622916000	2.321530000	-2.385373000
N	3.305952000	1.145698000	-2.691988000
C	3.821865000	0.257347000	-1.725428000
C	3.969118000	-1.090967000	-2.060015000
C	4.463902000	-1.995892000	-1.124274000
C	4.809962000	-1.584845000	0.158143000
C	4.981179000	0.237144000	1.872274000
F	3.850065000	0.473995000	2.575749000
F	5.678726000	-0.670092000	2.567839000
F	5.673483000	1.378766000	1.870646000
C	4.568905000	-3.442130000	-1.520606000

F	5.513521000	-3.641152000	-2.447228000
F	3.410388000	-3.877372000	-2.053395000
F	4.850558000	-4.232846000	-0.478659000
S	2.852624000	3.689838000	-3.308463000
C	4.664447000	-0.237666000	0.481499000
C	4.202382000	0.688717000	-0.446754000
N	-1.071491000	2.243652000	-0.979981000
C	-1.776455000	2.882526000	-1.937004000
N	-2.851238000	2.137451000	-2.423367000
C	-3.706985000	1.350330000	-1.633841000
C	-4.381597000	0.278292000	-2.229191000
C	-5.172506000	-0.558745000	-1.451583000
C	-5.321974000	-0.354053000	-0.081213000
C	-4.787365000	0.996222000	1.968339000
F	-5.581838000	0.106910000	2.578270000
F	-5.269126000	2.217377000	2.219372000
F	-3.584831000	0.926689000	2.576827000
C	-5.764355000	-1.787279000	-2.074813000
F	-6.843897000	-2.226310000	-1.428795000
F	-6.082928000	-1.613703000	-3.358524000
F	-4.859410000	-2.807876000	-2.041322000
S	-1.454768000	4.375858000	-2.600091000
C	-4.664732000	0.728149000	0.493019000
C	-3.881635000	1.592470000	-0.266759000
H	0.134430000	1.991926000	0.623942000
H	0.949245000	4.097166000	-1.428229000
C	2.128839000	3.894548000	0.366638000
C	-0.854340000	3.843952000	0.876078000
H	1.729842000	1.313206000	-0.849837000
H	3.832007000	1.225847000	-3.557740000
H	-1.323433000	1.271796000	-0.794925000
H	-3.242703000	2.530762000	-3.274093000
H	3.684426000	-1.428854000	-3.057589000
H	5.170666000	-2.301213000	0.894282000
H	4.131633000	1.744644000	-0.177388000
H	-4.248558000	0.079852000	-3.294201000
H	-5.941130000	-1.019267000	0.518839000
H	-3.397914000	2.449259000	0.206804000
N	-1.587786000	-2.924819000	1.215659000
C	-2.953502000	-3.135511000	0.708977000
N	-3.217513000	-3.370919000	3.162572000
C	-3.945543000	-3.315968000	1.894207000
C	-2.523742000	-2.094263000	3.359310000
C	-1.616467000	-1.776095000	2.136165000

C	-2.222897000	-4.441784000	3.078694000
C	-1.181625000	-4.120214000	1.970985000
H	-3.226916000	-2.252440000	0.112308000
H	-2.938002000	-4.017585000	0.048618000
H	-4.650285000	-2.471878000	1.956074000
H	-4.537510000	-4.237880000	1.790460000
H	-3.278217000	-1.309169000	3.510310000
H	-1.935675000	-2.171716000	4.286468000
H	-0.581775000	-1.555629000	2.446130000
H	-1.987497000	-0.908942000	1.569128000
H	-1.739691000	-4.546353000	4.061853000
H	-2.755829000	-5.382122000	2.870698000
H	-1.065494000	-4.953432000	1.259377000
H	-0.193117000	-3.917153000	2.410974000
C	1.810895000	-2.523762000	1.059076000
O	1.333070000	-0.232973000	0.375407000
C	0.883288000	-3.454911000	-0.871297000
C	1.601203000	-3.731492000	0.406167000
O	0.399497000	-4.230742000	-1.649191000
H	2.962667000	-5.817813000	2.672755000
C	2.006272000	-4.937809000	0.951460000
H	1.845280000	-5.874480000	0.417437000
H	3.290804000	-3.679243000	3.856813000
H	2.570693000	-1.510110000	2.811709000
C	2.409932000	-2.463898000	2.308626000
H	-2.896724000	-2.327281000	-1.954188000
C	2.811921000	-3.678053000	2.876752000
C	0.487716000	-1.819985000	-3.441865000
C	2.623505000	-4.892872000	2.205145000
H	0.086721000	-2.827148000	-3.592436000
H	1.574949000	-1.843149000	-3.586644000
C	-0.839948000	5.222687000	0.654394000
C	-1.580847000	6.071593000	1.476438000
C	-2.352405000	5.554285000	2.515680000
C	-2.372136000	4.178751000	2.744079000
C	-1.615983000	3.335142000	1.933661000
C	2.660902000	5.175781000	0.215043000
C	3.574379000	5.674496000	1.143793000
C	3.971563000	4.890165000	2.224402000
C	3.457904000	3.601218000	2.372793000
C	2.540011000	3.105706000	1.448744000
H	-0.256593000	5.635946000	-0.168006000
H	-1.559834000	7.146821000	1.295372000
H	-2.937330000	6.222438000	3.149128000

H	-2.971381000	3.758808000	3.553144000
H	-1.623660000	2.258317000	2.120072000
H	2.361452000	5.778030000	-0.645118000
H	3.983591000	6.677521000	1.016566000
H	4.688809000	5.279103000	2.948192000
H	3.777935000	2.972819000	3.204250000
H	2.159635000	2.085517000	1.562810000

Ball-cylinder model for (S)-CSA 1/L-Pht-Ala/DABCO complex and cartesian coordinates (Gaussian 09).



The distances between α -H of L-Pht-Ala and Ar-Hs and N-Hs of CSA 1 have been marked.

C	0.635641000	-1.422848000	-1.846760000
C	-0.742265000	-1.577653000	-1.213262000
O	-1.328056000	-0.690480000	-0.628991000
O	-1.213189000	-2.809793000	-1.350317000
N	1.607568000	-1.954654000	-0.898159000
H	0.125702000	-1.470106000	-3.933091000
H	0.823868000	-0.342697000	-1.903361000
C	2.074073000	-1.189270000	0.165285000
C	1.247456000	6.174876000	1.004668000
C	-3.615242000	2.801386000	2.758581000
C	-1.659381000	3.219415000	-0.492198000
C	-0.251969000	2.798970000	-0.033271000

C	-3.921108000	5.061535000	1.970817000
N	0.562494000	2.165641000	-1.073524000
C	1.010087000	2.728232000	-2.216978000
N	2.080707000	2.039886000	-2.783254000
C	3.119615000	1.456650000	-2.015692000
C	3.646643000	0.227704000	-2.414579000
C	4.626111000	-0.393859000	-1.642456000
C	5.092008000	0.194009000	-0.471825000
C	2.190042000	5.761950000	1.943681000
C	5.012982000	2.039656000	1.209993000
F	4.167439000	1.719965000	2.214687000
F	6.223677000	1.600428000	1.579332000
F	5.057431000	3.372151000	1.151667000
C	5.151613000	-1.736143000	-2.070564000
F	6.025988000	-1.637506000	-3.077766000
F	4.152696000	-2.530386000	-2.502687000
F	5.761794000	-2.375221000	-1.065326000
S	0.357769000	4.043146000	-3.003983000
C	4.567532000	1.426149000	-0.088075000
C	3.601473000	2.071592000	-0.852058000
N	-2.229199000	2.134154000	-1.274878000
C	-3.233684000	2.306605000	-2.149473000
N	-3.745974000	1.104163000	-2.650626000
C	-4.062324000	0.009638000	-1.825898000
C	-4.120561000	-1.272808000	-2.386497000
C	-4.403142000	-2.368702000	-1.579279000
C	-4.606739000	-2.226456000	-0.206102000
C	-4.730196000	-0.745568000	1.812897000
F	-5.261561000	-1.820624000	2.410274000
F	-5.499670000	0.306620000	2.096748000
F	-3.535726000	-0.523506000	2.410630000
C	-4.435866000	-3.758276000	-2.152023000
F	-5.606441000	-4.364779000	-1.929139000
F	-4.207214000	-3.775938000	-3.467070000
F	-3.490786000	-4.525726000	-1.566922000
S	-3.846271000	3.767109000	-2.661582000
C	-4.556332000	-0.945843000	0.334157000
C	-4.318522000	0.170715000	-0.459029000
C	-4.175429000	4.069769000	2.915786000
C	-2.531518000	3.529911000	0.713760000
C	0.542443000	3.884770000	0.673040000
C	1.493412000	3.476408000	1.616565000
C	0.428677000	5.242642000	0.366448000
C	2.315569000	4.406411000	2.247878000

C	-3.106919000	4.790821000	0.871211000
C	-2.795968000	2.536569000	1.663806000
H	-0.388641000	1.981893000	0.692838000
H	-1.610430000	4.092698000	-1.151274000
H	1.069875000	1.354866000	-0.716950000
H	2.331590000	2.401760000	-3.699178000
H	-1.860141000	1.193023000	-1.128789000
H	-4.362553000	1.255544000	-3.444268000
H	1.149147000	7.233005000	0.758948000
H	-3.819867000	2.014048000	3.484785000
H	-4.367496000	6.050406000	2.083366000
H	3.258362000	-0.251589000	-3.314765000
H	5.841151000	-0.307695000	0.139225000
H	2.829201000	6.495526000	2.436803000
H	3.201991000	3.038635000	-0.536672000
H	-3.922775000	-1.409827000	-3.449836000
H	-4.817610000	-3.091675000	0.423278000
H	-4.325059000	1.168478000	-0.016118000
H	-4.816661000	4.282008000	3.772292000
H	1.598748000	2.411408000	1.844069000
H	-0.288260000	5.579681000	-0.382025000
H	3.055550000	4.068292000	2.973766000
H	-2.928312000	5.556930000	0.114467000
H	-2.372163000	1.535466000	1.538806000
N	-0.104255000	-2.684839000	1.894859000
C	-1.501722000	-3.115509000	1.719744000
N	-1.239622000	-3.048856000	4.180831000
C	-2.154660000	-3.418003000	3.099740000
C	-0.858983000	-1.642159000	4.018984000
C	-0.111211000	-1.433720000	2.670428000
C	-0.039287000	-3.878881000	4.073587000
C	0.604718000	-3.718677000	2.667894000
H	-2.029782000	-2.290753000	1.213477000
H	-1.510328000	-4.002261000	1.065343000
H	-3.091863000	-2.859147000	3.230444000
H	-2.386610000	-4.488674000	3.205703000
H	-1.775895000	-1.037926000	4.063124000
H	-0.229186000	-1.356233000	4.874661000
H	0.936209000	-1.131665000	2.830083000
H	-0.587882000	-0.659209000	2.048975000
H	0.657935000	-3.568843000	4.866815000
H	-0.321288000	-4.924122000	4.271509000
H	0.564394000	-4.654186000	2.087604000
H	1.661989000	-3.427336000	2.752550000

C	3.003326000	-2.055998000	0.935587000
O	1.779474000	-0.031982000	0.385958000
C	2.008657000	-3.304981000	-0.772684000
C	2.970846000	-3.323781000	0.371316000
O	1.641333000	-4.219967000	-1.457121000
H	5.161759000	-4.864910000	2.414279000
C	3.732580000	-4.363324000	0.878253000
H	3.694884000	-5.355923000	0.429209000
H	5.224680000	-2.609427000	3.405364000
H	3.822651000	-0.747228000	2.447572000
C	3.801011000	-1.754816000	2.028590000
H	-2.052096000	-2.875530000	-0.858918000
C	4.577903000	-2.796362000	2.547292000
C	0.741109000	-2.050507000	-3.232161000
C	4.542470000	-4.077637000	1.982848000
H	0.407941000	-3.092561000	-3.221231000
H	1.786335000	-2.025813000	-3.568476000