

*Supporting Information for*

Intramolecular rhodium-catalysed [2+2+2]  
cycloaddition of linear chiral *N*-bridged triynes:  
Straightforward access to fused  
tetrahydroisoquinoline core

Alberto Llobat, Jorge Escorihuela, Carmen Ramírez de Arellano, Santos Fustero  
and Mercedes Medio-Simón\*

Departamento de Química Orgánica, Universitat de València, 46100 Burjassot,  
València, Spain.

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## I. X-ray structure of compound (*R,R*)-9e.

### Single crystal X-ray diffraction discussion

Crystals of (*R,R*)-9e suitable for single crystal X-ray diffraction were grown from  $\text{Cl}_2\text{CH}_2$  / *n*-hexane solution and its absolute structure unambiguously determined (Figure 1).

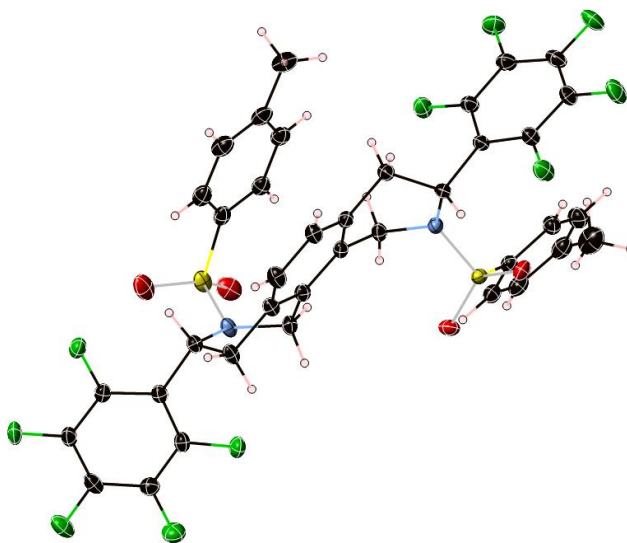


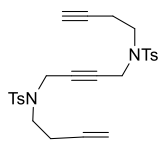
Figure 1. X-ray thermal ellipsoid plot for (*R,R*)-9e (40% probability level).

### Single crystal X-ray diffraction experimental data for compound $[(R,R)\text{-}9\text{e}]_4 \cdot \text{CH}_2\text{Cl}_2$

$[\text{C}_{38}\text{H}_{26}\text{F}_{10}\text{N}_2\text{O}_4\text{S}_2]_4 \cdot [\text{CH}_2\text{Cl}_2]$ , (CCDC 2100190)  $M = 3399.83$ , orthorhombic,  $a = 7.7647(5)$ ,  $b = 12.5408(11)$ ,  $c = 38.014(3)$  Å,  $V = 3701.6(5)$  Å<sup>3</sup>, space group  $P_{2(1)2(1)2(1)}$ ,  $Z = 1$ ,  $T = 120(2)$  K,  $\lambda = 0.71073$  Å,  $D_{\text{calc}} = 1.525$  g·cm<sup>-3</sup>,  $\mu = 0.275$  cm<sup>-1</sup>, 127114 reflections measured, 10449 unique ( $R_{\text{int}} = 0.0451$ ), colorless crystals obtained by  $\text{CH}_2\text{Cl}_2$ /*n*-hexane diffusion, crystal structure solved by dual methods and all non hydrogen atoms refined anisotropically on  $F^2$  using the programs SHELXT-2018 and SHELXL-2018<sup>[5]</sup>, methyl group hydrogen atoms were included as *riding* and others using a *riding* model, the dichloromethane molecule is disordered over two sites and was refined with restrained bond lengths and angles, absolute structure was determined with Flack  $x = 0.033(19)$ , GOF = 1.144,  $R$  ( $F_o, I > 2\sigma(I)$ ) = 0.0523,  $R_w$  ( $F_o^2$ , all data) = 0.1371.

## II. Cartesian coordinates of optimized structures.

6



Zero-point correction= 0.484475 (Hartree/Particle)  
 Thermal correction to Energy= 0.521304  
 Thermal correction to Enthalpy= 0.522248  
 Thermal correction to Gibbs Free Energy= 0.411342  
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 Sum of electronic and thermal Energies= -2213.340339  
 Sum of electronic and thermal Enthalpies= -2213.339395  
 Sum of electronic and thermal Free Energies= -2213.450301

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RhCl(Ph<sub>3</sub>)<sub>3</sub>

Zero-point correction= 0.834166 (Hartree/Particle)  
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A

Zero-point correction= 0.764965 (Hartree/Particle)  
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Sum of electronic and thermal Free Energies= -3820.446851

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**B**

Zero-point correction= 0.764561 (Hartree/Particle)  
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6	-1.078771000	-1.495858000	-0.115533000	1	-5.570127000	4.722126000	3.572642000
1	-1.061114000	-2.404985000	0.489402000	1	-4.345949000	4.500013000	4.819883000
1	-1.032381000	-1.796177000	-1.163208000	1	5.823693000	2.008859000	1.892719000
7	-2.343025000	-0.780058000	0.116591000	6	-0.659698000	2.327402000	-0.179747000
7	2.565118000	1.156838000	2.489705000	6	5.573891000	-0.274943000	4.148165000
6	3.747511000	1.519869000	1.681255000	1	-1.642617000	0.166265000	-2.527341000
1	3.919000000	0.680445000	1.012103000	1	5.811735000	-1.104846000	4.764487000
1	3.556032000	2.380611000	1.046720000	1	-0.557987000	3.066790000	0.583691000
6	4.984332000	1.787449000	2.559708000	1	-3.897966000	5.204439000	3.271587000
1	4.804784000	2.686318000	3.151593000	1	-2.773656000	1.493373000	-2.365709000
6	5.321801000	0.662131000	3.430469000	15	1.569648000	2.745145000	-2.426983000
6	-3.094752000	-0.087948000	-0.929938000	6	2.864977000	3.818810000	-1.586116000
1	-3.828025000	0.554277000	-0.440001000	6	2.601017000	4.261573000	-0.279942000
1	-3.639967000	-0.784667000	-1.575229000	6	4.087390000	4.132458000	-2.189309000
6	-2.155569000	0.792971000	-1.795730000	6	3.544086000	5.026419000	0.410510000
6	-1.164885000	1.534386000	-0.994741000	6	5.032052000	4.894441000	-1.493783000
45	0.940929000	1.020151000	-0.849795000	6	4.761774000	5.344962000	-0.198838000
17	3.031111000	-0.143223000	-1.263984000	1	1.680059000	3.986801000	0.215772000
16	1.635502000	2.534080000	3.228329000	1	4.312556000	3.774533000	-3.183193000
16	-3.239189000	-1.180799000	1.627395000	1	3.335077000	5.318318000	1.429390000
8	0.159555000	2.859332000	2.574566000	1	5.978878000	5.126198000	-1.963212000
8	2.695446000	3.786879000	3.306826000	1	5.498870000	5.926977000	0.338003000
8	-2.120956000	-1.924233000	2.571558000	6	0.184805000	3.946336000	-2.879123000
8	-4.677497000	-1.901775000	1.311333000	6	-0.816184000	3.475238000	-3.740553000
6	-3.634686000	0.537133000	2.269839000	6	0.091649000	5.238293000	-2.356572000
6	-4.961450000	0.849201000	2.523388000	6	-1.899246000	4.288308000	-4.074006000
6	-2.584614000	1.420505000	2.465396000	6	-0.997619000	6.052416000	-2.689882000
6	-5.245143000	2.131918000	3.000507000	6	-1.994448000	5.580622000	-3.545236000
1	-5.734033000	0.115783000	2.343666000	1	-0.744174000	2.478480000	-4.156214000
6	-2.892608000	2.698302000	2.933894000	1	0.859247000	5.617235000	-1.698017000
1	-1.565050000	1.156028000	2.231294000	1	-2.663424000	3.917664000	-4.744575000
6	-4.220262000	3.068926000	3.211563000	1	-1.059846000	7.052600000	-2.282115000
1	-6.272198000	2.405595000	3.203183000	1	-2.834843000	6.211586000	-3.801677000
1	-2.083691000	3.403748000	3.064989000	6	2.248516000	2.360318000	-4.137197000
6	1.281085000	1.781553000	4.912226000	6	2.594002000	1.050142000	-4.485093000
6	2.353823000	1.299496000	5.649411000	6	2.387267000	3.393007000	-5.078030000
6	-0.032635000	1.738763000	5.351480000	6	3.079534000	0.777150000	-5.768793000
6	2.080410000	0.740975000	6.897852000	6	2.875095000	3.115277000	-6.355669000
1	3.358054000	1.319178000	5.253198000	6	3.222642000	1.805095000	-6.702756000
6	-0.281028000	1.171663000	6.603399000	1	2.503384000	0.257912000	-3.758350000
1	-0.829395000	2.114543000	4.729256000	1	2.102945000	4.403632000	-4.818228000
6	0.766098000	0.671193000	7.393198000	1	3.346994000	-0.237624000	-6.030588000
1	2.896900000	0.346924000	7.488215000	1	2.979829000	3.915608000	-7.076098000
1	-1.300139000	1.109147000	6.960458000	1	3.599283000	1.589871000	-7.693933000

C

Zero-point correction= 0.485617 (Hartree/Particle)  
Thermal correction to Energy= 0.525070  
Thermal correction to Enthalpy= 0.526014  
Thermal correction to Gibbs Free Energy= 0.407581  
Sum of electronic and zero-point Energies= -2784.245166  
Sum of electronic and thermal Energies= -2784.205714  
Sum of electronic and thermal Enthalpies= -2784.204769  
Sum of electronic and thermal Free Energies= -2784.323202

6	0.962964000	0.596539000	2.378148000	1	-0.424840000	-2.726886000	0.117887000
1	1.020373000	-0.173733000	3.153362000	1	-0.152918000	-2.065052000	-1.497528000
1	0.110837000	1.237646000	2.635486000	7	-1.895298000	-1.339055000	-0.459549000
6	0.716762000	-0.011772000	1.058358000	7	2.192436000	1.395497000	2.416185000
6	0.327586000	-0.747913000	0.126617000	6	2.229049000	2.838423000	2.169205000
6	-0.482428000	-1.817938000	-0.486034000	1	1.197780000	3.188123000	2.096982000

1	2.694741000	3.338555000	3.019323000	1	-3.972983000	0.059392000	4.197072000
6	3.024641000	3.232729000	0.898048000	6	4.599275000	-0.244936000	2.374811000
1	3.944594000	2.646156000	0.875491000	6	5.666081000	0.401029000	1.772995000
6	2.339185000	3.070186000	-0.388209000	6	4.246285000	-1.558533000	2.115181000
6	-2.482299000	-0.682756000	-1.650503000	6	6.414311000	-0.319858000	0.843609000
1	-3.417408000	-0.224559000	-1.326948000	1	5.909992000	1.420089000	2.035243000
1	-2.716696000	-1.404780000	-2.439213000	6	5.010306000	-2.258092000	1.182915000
6	-1.560494000	0.405542000	-2.249072000	1	3.414297000	-2.018214000	2.627112000
6	-0.963597000	1.336401000	-1.272148000	6	6.087284000	-1.646773000	0.522771000
45	1.120073000	1.075392000	-0.727151000	1	7.249230000	0.159597000	0.350538000
17	3.251905000	0.054100000	-0.971735000	1	4.751172000	-3.281922000	0.949666000
16	3.508152000	0.743192000	3.522739000	6	6.846966000	-2.386470000	-0.550368000
16	-3.092440000	-2.655696000	0.161779000	1	6.363945000	-2.235770000	-1.519931000
8	2.777583000	-0.306217000	4.552377000	1	7.874718000	-2.031465000	-0.634615000
8	4.344474000	2.059283000	4.031705000	1	6.872893000	-3.459784000	-0.358351000
8	-2.182847000	-3.667053000	1.076149000	6	-6.561591000	0.838829000	3.835547000
8	-4.043927000	-3.206994000	-1.057665000	1	-7.408341000	1.276691000	3.307066000
6	-4.154401000	-1.594558000	1.273891000	1	-6.960897000	0.235586000	4.655567000
6	-5.452391000	-1.318387000	0.878276000	1	3.314453000	4.285960000	0.989205000
6	-3.591580000	-1.121337000	2.450555000	6	-0.752212000	2.210087000	-0.414490000
6	-6.228325000	-0.512116000	1.716621000	6	1.922873000	3.074036000	-1.544776000
1	-5.839233000	-1.731234000	-0.042181000	1	-0.766067000	-0.072158000	-2.825654000
6	-4.384190000	-0.320937000	3.271312000	1	1.700455000	3.335131000	-2.552689000
1	-2.577113000	-1.377670000	2.718239000	1	-0.918243000	3.058187000	0.210337000
6	-5.709300000	-0.004913000	2.917739000	1	-5.984603000	1.650712000	4.280885000
1	-7.246545000	-0.281095000	1.433582000	1	-2.160501000	0.970728000	-2.969679000

## TS1

Frequency -330.1960

Zero-point correction= 0.486237 (Hartree/Particle)  
 Thermal correction to Energy= 0.524299  
 Thermal correction to Enthalpy= 0.525243  
 Thermal correction to Gibbs Free Energy= 0.412223  
 Sum of electronic and zero-point Energies= -2784.230055  
 Sum of electronic and thermal Energies= -2784.191993  
 Sum of electronic and thermal Enthalpies= -2784.191049  
 Sum of electronic and thermal Free Energies= -2784.304069

6	1.489810000	2.337028000	1.923402000	16	-1.461794000	-2.557175000	0.186948000
1	1.028726000	1.703536000	2.687319000	8	2.402630000	1.243503000	4.711748000
1	1.034662000	3.327849000	2.029065000	8	5.054519000	1.730002000	3.778615000
6	1.208958000	1.805088000	0.573149000	8	-0.235351000	-3.088771000	1.141230000
6	0.749614000	0.850929000	-0.163358000	8	-1.970246000	-3.415898000	-1.118393000
6	0.490542000	-0.600017000	-0.252677000	6	-2.950145000	-2.217009000	1.262074000
1	0.859744000	-1.089868000	0.646316000	6	-4.207162000	-2.500112000	0.754587000
1	1.021282000	-1.036534000	-1.103824000	6	-2.731708000	-1.685834000	2.525420000
7	-0.988145000	-0.793186000	-0.308199000	6	-5.311032000	-2.226656000	1.567687000
7	2.940652000	2.431157000	2.154001000	1	-4.312813000	-2.932455000	-0.229817000
6	3.640521000	3.715086000	2.061452000	6	-3.847257000	-1.421891000	3.318013000
1	3.001754000	4.531174000	2.416769000	1	-1.728606000	-1.498837000	2.879320000
1	4.518647000	3.661715000	2.705922000	6	-5.148805000	-1.686005000	2.852525000
6	4.137046000	3.999350000	0.622456000	1	-6.305071000	-2.440340000	1.198414000
1	4.726948000	3.151972000	0.276257000	1	-3.707208000	-1.008499000	4.308017000
6	3.072089000	4.281815000	-0.344728000	6	3.354740000	-0.337223000	2.574768000
6	-1.694297000	-0.404299000	-1.563778000	6	4.001620000	-0.464354000	1.357745000
1	-2.610930000	0.107522000	-1.272619000	6	2.570601000	-1.334421000	3.143306000
1	-1.960758000	-1.290017000	-2.146911000	6	3.841012000	-1.666101000	0.664099000
6	-0.843341000	0.514749000	-2.464387000	1	4.559399000	0.349909000	0.924228000
6	-0.278443000	1.714465000	-1.794805000	6	2.428919000	-2.525743000	2.432711000
45	1.659379000	2.541561000	-1.208048000	1	2.080946000	-1.167923000	4.091384000
17	3.786184000	1.350689000	-1.582682000	6	3.059890000	-2.708338000	1.187317000
16	3.506018000	1.287474000	3.493650000	1	4.305997000	-1.768350000	-0.306121000



1	1.790597000	-3.305620000	2.821588000	1	4.798924000	4.872210000	0.656505000
6	2.848022000	-3.990379000	0.423082000	6	-0.276400000	3.000052000	-1.649948000
1	3.331422000	-3.960798000	-0.553187000	6	2.232880000	4.739939000	-1.119262000
1	3.252059000	-4.845015000	0.971534000	1	-0.034621000	-0.059620000	-2.920351000
1	1.780154000	-4.164579000	0.282476000	1	1.653459000	5.428363000	-1.688417000
6	-6.341824000	-1.416474000	3.738245000	1	-0.889885000	3.865406000	-1.827078000
1	-7.268864000	-1.389413000	3.165915000	1	-6.240684000	-0.464805000	4.262454000
1	-6.444832000	-2.196589000	4.497455000	1	-1.482998000	0.853678000	-3.284541000

#### D

Zero-point correction= 0.490473 (Hartree/Particle)  
Thermal correction to Energy= 0.528040  
Thermal correction to Enthalpy= 0.528984  
Thermal correction to Gibbs Free Energy= 0.417933  
Sum of electronic and zero-point Energies= -2784.308498  
Sum of electronic and thermal Energies= -2784.270932  
Sum of electronic and thermal Enthalpies= -2784.269987  
Sum of electronic and thermal Free Energies= -2784.381039

6	2.317549000	3.065470000	2.225929000	6	-5.192154000	-2.954639000	0.510769000
1	2.155584000	2.671902000	3.234158000	1	-3.326338000	-3.305193000	-0.551586000
1	2.396761000	4.152167000	2.317621000	6	-4.969315000	-1.862097000	2.658365000
6	1.179990000	2.721281000	1.325189000	1	-2.946784000	-1.365558000	3.253390000
6	0.491360000	1.445441000	0.941226000	6	-5.789814000	-2.439323000	1.671780000
6	0.434611000	-0.015387000	1.223315000	1	-5.809853000	-3.404387000	-0.254977000
1	0.609742000	-0.242679000	2.270812000	1	-5.416979000	-1.464359000	3.559537000
1	1.156654000	-0.566762000	0.619174000	6	3.752196000	-0.361038000	2.111911000
7	-0.980471000	-0.400144000	0.893572000	6	3.941086000	-0.601783000	0.759044000
7	3.580964000	2.519091000	1.679702000	6	3.143842000	-1.261559000	2.975872000
6	4.558645000	3.428487000	1.056701000	6	3.481745000	-1.814772000	0.247399000
1	4.348968000	4.458999000	1.356665000	1	4.380138000	0.135650000	0.107060000
1	5.555074000	3.169941000	1.420672000	6	2.693182000	-2.469346000	2.439716000
6	4.575624000	3.311046000	-0.484406000	1	3.010843000	-1.014790000	4.018800000
1	4.777829000	2.276431000	-0.763861000	6	2.856560000	-2.765055000	1.075611000
6	3.343991000	3.755169000	-1.143807000	1	3.577447000	-2.000550000	-0.812742000
6	-1.461447000	0.055539000	-0.448261000	1	2.172047000	-3.168738000	3.075596000
1	-2.389861000	-0.463502000	-0.677443000	6	2.318924000	-4.046233000	0.492053000
1	-0.727751000	-0.165886000	-1.227381000	1	1.353627000	-3.868268000	0.011443000
6	-1.725036000	1.579649000	-0.354577000	1	2.997738000	-4.453517000	-0.259024000
6	-0.516168000	2.193432000	0.256058000	1	2.164479000	-4.800311000	1.263221000
45	1.437703000	2.412684000	-0.710134000	6	-7.283024000	-2.529148000	1.878742000
17	2.298301000	0.696811000	-2.146555000	1	-7.812785000	-2.645817000	0.933336000
16	4.370535000	1.249700000	2.833999000	1	-7.535185000	-3.388936000	2.505715000
16	-1.194862000	-2.238971000	1.099683000	1	5.407312000	3.915060000	-0.864564000
8	3.699248000	1.403677000	4.326589000	6	0.145926000	3.472579000	0.599702000
8	5.986507000	1.411811000	2.612832000	6	2.417200000	4.256872000	-1.768627000
8	-0.430895000	-2.589042000	2.507585000	1	-1.949586000	1.984539000	-1.343264000
8	-0.837228000	-3.072115000	-0.271672000	1	1.780296000	4.836156000	-2.393466000
6	-3.047900000	-2.317637000	1.328872000	1	-0.125132000	4.511218000	0.534084000
6	-3.807638000	-2.900860000	0.327327000	1	-7.671047000	-1.639122000	2.376169000
6	-3.585864000	-1.797192000	2.497497000	1	-2.592859000	1.755468000	0.287928000

#### E

Zero-point correction= 0.491197 (Hartree/Particle)  
Thermal correction to Energy= 0.528086  
Thermal correction to Enthalpy= 0.529030  
Thermal correction to Gibbs Free Energy= 0.418775  
Sum of electronic and zero-point Energies= -2784.343376  
Sum of electronic and thermal Energies= -2784.306487  
Sum of electronic and thermal Enthalpies= -2784.305543

Sum of electronic and thermal Free Energies= -2784.415798

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6	1.542666000	2.130688000	1.703355000	6	-6.030059000	-2.379663000	-0.552660000
1	0.571030000	2.217237000	2.198803000	1	-5.424782000	-3.243887000	-2.430997000
1	2.050651000	3.085366000	1.856091000	1	-6.303689000	-1.387183000	1.342884000
6	1.377022000	1.853146000	0.245085000	6	4.388975000	2.979553000	3.182114000
6	0.235464000	1.875572000	-0.474055000	6	4.282120000	3.078763000	4.563140000
6	-1.151787000	2.017407000	0.096066000	6	4.695926000	4.041707000	2.346351000
1	-1.536929000	3.039195000	0.012881000	6	4.493051000	4.332908000	5.133969000
1	-1.206207000	1.722301000	1.139702000	1	4.054611000	2.212280000	5.166292000
7	-2.136223000	1.197683000	-0.661956000	6	4.898654000	5.287328000	2.946482000
7	2.268471000	1.097977000	2.502403000	1	4.758659000	3.906634000	1.275564000
6	1.849136000	-0.321507000	2.322749000	6	4.803138000	5.450806000	4.337326000
1	0.784988000	-0.282640000	2.085826000	1	4.417591000	4.444857000	6.207413000
6	-2.168822000	1.542912000	-2.110949000	1	5.130021000	6.136812000	2.318470000
1	-2.630935000	2.533523000	-2.119616000	6	5.058228000	6.795980000	4.974075000
1	-2.865529000	0.864024000	-2.601332000	1	6.107270000	6.890428000	5.268832000
6	-0.802329000	1.565366000	-2.846905000	1	4.837106000	7.611871000	4.285784000
6	0.397752000	1.713850000	-1.921975000	1	4.453304000	6.935541000	5.870869000
45	3.021569000	1.491216000	-0.809267000	6	-7.423889000	-2.960725000	-0.581480000
17	3.561818000	3.788113000	-1.086562000	1	-7.707180000	-3.273848000	-1.586286000
16	4.102951000	1.303803000	2.412594000	1	-7.492299000	-3.837154000	0.068929000
16	-1.730801000	-0.648197000	-0.405661000	6	1.683631000	1.605435000	-2.312238000
8	4.593183000	1.446321000	0.809908000	6	2.634554000	-0.582184000	-1.364856000
8	4.744355000	0.113699000	3.333255000	1	-0.690906000	0.624976000	-3.385697000
8	-1.170303000	-0.752663000	1.139923000	1	1.998151000	1.506078000	-3.348975000
8	-0.909695000	-1.336774000	-1.652259000	1	-8.163419000	-2.238326000	-0.232223000
6	-3.463918000	-1.346370000	-0.461781000	1	-0.823313000	2.368369000	-3.588479000
6	-3.821140000	-2.120632000	-1.553561000	1	2.484018000	-0.904764000	-2.369040000
6	-4.322985000	-1.065505000	0.591203000	6	2.609489000	-0.599894000	-0.125013000
6	-5.120292000	-2.635701000	-1.589707000	1	1.984143000	-0.824386000	3.277009000
1	-3.100860000	-2.320963000	-2.333391000	6	2.578857000	-1.146752000	1.240187000
6	-5.613004000	-1.590465000	0.535049000	1	3.602965000	-1.337420000	1.570743000
1	-3.991339000	-0.467056000	1.426399000	1	2.077293000	-2.117839000	1.191252000

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## TS2

Frequency -329.1158

Zero-point correction= 0.489711 (Hartree/Particle)  
Thermal correction to Energy= 0.526040  
Thermal correction to Enthalpy= 0.526984  
Thermal correction to Gibbs Free Energy= 0.417517  
Sum of electronic and zero-point Energies= -2784.326472  
Sum of electronic and thermal Energies= -2784.290142  
Sum of electronic and thermal Enthalpies= -2784.289198  
Sum of electronic and thermal Free Energies= -2784.398665

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6	1.735244000	1.936294000	1.712861000	6	-0.644005000	1.014921000	-2.745411000
1	0.775458000	1.865169000	2.235381000	6	0.538554000	1.393393000	-1.873756000
1	2.052572000	2.979556000	1.785406000	45	3.191458000	1.796712000	-0.957657000
6	1.608020000	1.543029000	0.261189000	17	3.260369000	4.197944000	-1.084979000
6	0.423154000	1.441916000	-0.435461000	16	4.464617000	1.529619000	2.192357000
6	-0.943654000	1.494206000	0.205437000	16	-1.875614000	-1.059135000	-0.350013000
1	-1.293509000	2.528557000	0.295287000	8	4.811298000	1.872504000	0.593010000
1	-0.954050000	1.059516000	1.202232000	8	5.321396000	0.369979000	2.962534000
7	-1.998931000	0.816529000	-0.586696000	8	-1.421509000	-1.229515000	1.225163000
7	2.659501000	1.120841000	2.540761000	8	-1.049880000	-1.865377000	-1.521539000
6	2.401262000	-0.331712000	2.632321000	6	-3.678568000	-1.505198000	-0.549138000
1	1.645402000	-0.448555000	3.411900000	6	-4.030003000	-2.330513000	-1.605037000
6	-1.996885000	1.193177000	-2.029148000	6	-4.590017000	-1.007866000	0.371928000
1	-2.298195000	2.244369000	-2.024358000	6	-5.379278000	-2.667601000	-1.745576000
1	-2.787609000	0.631430000	-2.526430000	1	-3.271168000	-2.696892000	-2.281170000

6	-5.929734000	-1.357640000	0.212166000	1	4.467560000	7.732698000	4.514786000
1	-4.264846000	-0.370672000	1.180360000	1	4.399749000	6.896862000	6.068497000
6	-6.343080000	-2.190056000	-0.844433000	6	-7.795661000	-2.579193000	-0.983176000
1	-5.681298000	-3.309163000	-2.562488000	1	-8.018056000	-2.949218000	-1.983880000
1	-6.662678000	-0.981886000	0.913893000	1	-8.054229000	-3.370173000	-0.273740000
6	4.599597000	3.173900000	3.069654000	6	1.802456000	1.649712000	-2.327455000
6	4.663939000	3.161250000	4.456358000	6	3.357507000	-0.281142000	-0.803097000
6	4.620455000	4.326430000	2.300486000	1	-0.543984000	-0.033141000	-3.032303000
6	4.752878000	4.390970000	5.106576000	1	2.019423000	1.779635000	-3.388149000
1	4.655692000	2.230250000	5.003699000	1	-8.455215000	-1.733594000	-0.781686000
6	4.702692000	5.545347000	2.980022000	1	-0.649578000	1.608362000	-3.662907000
1	4.563225000	4.280105000	1.221538000	1	4.063677000	-0.852165000	-1.378156000
6	4.772798000	5.596480000	4.380609000	6	2.525347000	-0.455741000	0.130489000
1	4.807664000	4.415633000	6.186884000	1	3.318269000	-0.795540000	2.992995000
1	4.710614000	6.461620000	2.405518000	6	1.907230000	-1.029821000	1.327370000
6	4.898337000	6.919076000	5.098575000	1	2.198841000	-2.085964000	1.371681000
1	5.949484000	7.163554000	5.276443000	1	0.820438000	-1.012417000	1.260128000

F

Zero-point correction= 0.493676 (Hartree/Particle)  
Thermal correction to Energy= 0.530417  
Thermal correction to Enthalpy= 0.531361  
Thermal correction to Gibbs Free Energy= 0.418091  
Sum of electronic and zero-point Energies= -2784.325944  
Sum of electronic and thermal Energies= -2784.289202  
Sum of electronic and thermal Enthalpies= -2784.288258  
Sum of electronic and thermal Free Energies= -2784.401528

6	1.900559000	0.131536000	1.741123000	1	-2.870527000	-3.082474000	-4.739080000
1	2.043159000	-0.614798000	0.966879000	1	-5.642907000	-4.913747000	-2.013179000
1	1.427335000	-0.363802000	2.601547000	6	4.244276000	-1.971246000	1.331044000
6	0.970287000	1.229853000	1.209604000	6	5.216190000	-1.717490000	0.376374000
6	-0.257625000	0.712172000	0.697253000	6	3.247570000	-2.927109000	1.182187000
6	-0.298868000	-0.823038000	0.639944000	6	5.175315000	-2.470754000	-0.799279000
1	-0.178419000	-1.242069000	1.648181000	1	5.971048000	-0.963877000	0.546970000
1	0.522913000	-1.193339000	0.032214000	6	3.213132000	-3.652043000	-0.008721000
7	-1.532933000	-1.337900000	0.023752000	1	2.517898000	-3.088436000	1.961940000
7	3.242724000	0.603651000	2.111864000	6	4.172778000	-3.432885000	-1.012095000
6	1.419714000	2.569032000	1.373965000	1	5.920867000	-2.296802000	-1.563706000
6	0.944917000	3.707713000	0.731088000	1	2.410053000	-4.357728000	-0.165060000
1	1.568348000	4.604990000	0.849705000	6	4.124063000	-4.233647000	-2.291166000
6	-1.460830000	1.384589000	0.337282000	1	4.565780000	-5.223509000	-2.145998000
6	-1.601646000	2.704138000	-0.072030000	1	3.094698000	-4.382099000	-2.620388000
1	-2.607248000	2.986113000	-0.413443000	1	4.672511000	-3.742335000	-3.095105000
45	-0.432868000	4.105052000	-0.458628000	6	-5.303566000	-4.309939000	-4.662514000
17	0.186485000	4.151858000	-2.680753000	1	-5.352564000	-3.463624000	-5.349448000
16	4.177230000	-0.877231000	2.844959000	1	-4.961107000	-5.175414000	-5.236372000
16	-1.456629000	-3.220058000	-0.001228000	1	-6.314903000	-4.523253000	-4.317146000
8	3.216540000	-1.608340000	3.962021000	6	-2.802450000	0.621616000	0.334660000
8	5.650552000	-0.284684000	3.224043000	1	-3.215617000	0.666424000	-0.674467000
8	-2.112191000	-3.862720000	1.358704000	1	-3.500409000	1.142097000	0.996155000
8	0.091006000	-3.563674000	-0.432897000	6	2.631518000	2.876350000	2.278373000
6	-2.627344000	-3.548378000	-1.417153000	1	2.367762000	3.694826000	2.952833000
6	-2.249069000	-3.144219000	-2.690207000	1	3.444809000	3.230004000	1.641104000
6	-3.826800000	-4.182932000	-1.136624000	6	3.149558000	1.699941000	3.097111000
6	-3.136407000	-3.390135000	-3.736512000	1	4.139091000	1.909273000	3.496296000
1	-1.300555000	-2.655832000	-2.856210000	6	-2.721234000	-0.847084000	0.744500000
6	-4.699445000	-4.419807000	-2.202558000	1	-3.609377000	-1.381802000	0.412553000
1	-4.058311000	-4.485092000	-0.125367000	1	-2.619345000	-0.981490000	1.826321000
6	-4.369492000	-4.029599000	-3.509768000	1	2.474020000	1.444633000	3.922566000

TS3

Frequency -249.4168

Zero-point correction= 0.492621 (Hartree/Particle)  
 Thermal correction to Energy= 0.528839  
 Thermal correction to Enthalpy= 0.529783  
 Thermal correction to Gibbs Free Energy= 0.418223  
 Sum of electronic and zero-point Energies= -2784.306637  
 Sum of electronic and thermal Energies= -2784.270419  
 Sum of electronic and thermal Enthalpies= -2784.269474  
 Sum of electronic and thermal Free Energies= -2784.381035

6	2.091559000	0.113409000	1.797236000	1	-2.637264000	-2.878670000	-4.878404000
1	2.221406000	-0.688735000	1.079156000	1	-5.498535000	-4.839138000	-2.340511000
1	1.722986000	-0.335781000	2.732797000	6	4.370323000	-1.868200000	1.374780000
6	1.065372000	1.099844000	1.265460000	6	4.887564000	-1.613281000	0.114938000
6	-0.140464000	0.519032000	0.780885000	6	3.541810000	-2.946113000	1.665204000
6	-0.162003000	-1.004815000	0.700481000	6	4.525586000	-2.483467000	-0.918157000
1	-0.095051000	-1.441328000	1.707728000	1	5.530140000	-0.762390000	-0.057690000
1	0.690973000	-1.367381000	0.131226000	6	3.184195000	-3.790800000	0.616605000
7	-1.367341000	-1.478421000	-0.001799000	1	3.169719000	-3.088069000	2.669446000
7	3.411847000	0.732717000	1.996745000	6	3.654202000	-3.561361000	-0.689446000
6	1.309999000	2.477086000	1.404350000	1	4.905258000	-2.305272000	-1.915223000
6	0.498010000	3.505810000	0.905737000	1	2.494618000	-4.602506000	0.796497000
1	0.526633000	4.457309000	1.446117000	6	3.190040000	-4.453303000	-1.813303000
6	-1.312288000	1.233943000	0.493998000	1	3.529998000	-5.481276000	-1.665019000
6	-1.421818000	2.634908000	0.372014000	1	2.098926000	-4.470264000	-1.845199000
1	-2.331790000	3.120860000	0.737738000	1	3.562534000	-4.112967000	-2.779367000
45	-0.375872000	3.689486000	-0.818886000	6	-5.089528000	-4.066310000	-4.936306000
17	-0.239059000	4.407094000	-3.021746000	1	-5.133901000	-3.163955000	-5.548262000
16	4.585598000	-0.574634000	2.707728000	1	-4.729074000	-4.875928000	-5.576641000
16	-1.334066000	-3.346536000	-0.131134000	1	-6.104775000	-4.315982000	-4.629227000
8	3.940119000	-1.172893000	4.097442000	6	-2.645833000	0.507017000	0.265600000
8	6.055546000	0.132449000	2.682995000	1	-2.915610000	0.592287000	-0.788155000
8	-2.028922000	-4.060366000	1.172505000	1	-3.432103000	1.002018000	0.842573000
8	0.213930000	-3.695221000	-0.552978000	6	2.587407000	2.973414000	2.101868000
6	-2.478587000	-3.563366000	-1.589446000	1	2.342973000	3.811640000	2.759363000
6	-2.064199000	-3.084178000	-2.824948000	1	3.270685000	3.350556000	1.338758000
6	-3.692939000	-4.196101000	-1.377611000	6	3.320106000	1.896723000	2.904855000
6	-2.930759000	-3.246579000	-3.904284000	1	4.325312000	2.226496000	3.157766000
1	-1.105226000	-2.600927000	-2.937388000	6	-2.604401000	-0.980203000	0.627392000
6	-4.543964000	-4.348953000	-2.476019000	1	-3.466608000	-1.490932000	0.201786000
1	-3.952349000	-4.559517000	-0.393620000	1	-2.600764000	-1.143928000	1.709868000
6	-4.178243000	-3.879423000	-3.747141000	1	2.781980000	1.644804000	3.826282000

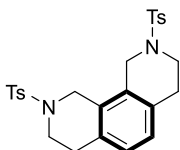
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Zero-point correction= 0.496168 (Hartree/Particle)  
 Thermal correction to Energy= 0.532440  
 Thermal correction to Enthalpy= 0.533385  
 Thermal correction to Gibbs Free Energy= 0.419963  
 Sum of electronic and zero-point Energies= -2784.385414  
 Sum of electronic and thermal Energies= -2784.349142  
 Sum of electronic and thermal Enthalpies= -2784.348198  
 Sum of electronic and thermal Free Energies= -2784.46161

6	2.247433000	0.547838000	1.535248000	1	0.501283000	-1.381282000	0.614228000
1	2.349683000	-0.379444000	0.976952000	7	-1.524192000	-1.238921000	0.104697000
1	2.257522000	0.295613000	2.607651000	7	3.393131000	1.420508000	1.190377000
6	0.960483000	1.264912000	1.202559000	6	0.906489000	2.750145000	1.265449000
6	-0.213769000	0.633172000	0.955968000	6	-0.282840000	3.363573000	1.845098000
6	-0.384229000	-0.867188000	0.978643000	1	-0.237905000	4.310887000	2.361088000
1	-0.562223000	-1.199634000	2.013491000	6	-1.405731000	1.500689000	0.781977000

6	-1.505977000	2.691443000	1.586952000	6	6.669161000	2.169703000	-1.876704000
1	-2.462037000	3.108297000	1.867090000	1	5.067353000	0.791567000	-1.408529000
45	-0.526411000	3.230549000	-0.251175000	6	7.698475000	2.984298000	-1.368416000
17	0.591967000	4.240877000	-2.029910000	1	8.691465000	3.650262000	0.423670000
16	5.009584000	0.521251000	1.490104000	1	6.500945000	2.125317000	-2.944545000
16	-1.702673000	-3.110424000	0.042782000	6	8.569213000	3.778848000	-2.312292000
8	4.750500000	-0.984856000	0.906213000	1	9.185008000	3.116181000	-2.925669000
8	5.550778000	0.768972000	3.020853000	1	7.964488000	4.381714000	-2.992849000
8	-2.743387000	-3.629919000	1.202028000	1	9.238036000	4.449533000	-1.773660000
8	-0.167965000	-3.666618000	-0.056828000	6	-4.516333000	-3.643072000	-5.392007000
6	-2.562990000	-3.272116000	-1.607016000	1	-4.246006000	-2.826958000	-6.064128000
6	-1.824667000	-3.024274000	-2.755835000	1	-4.219977000	-4.576514000	-5.878201000
6	-3.900268000	-3.634285000	-1.616869000	1	-5.601594000	-3.653091000	-5.293049000
6	-2.477603000	-3.139714000	-3.981824000	6	-2.656726000	0.885931000	0.183034000
1	-0.779575000	-2.759742000	-2.692645000	1	-2.609629000	0.965924000	-0.905624000
6	-4.533779000	-3.744130000	-2.858192000	1	-3.546216000	1.425329000	0.514474000
1	-4.414837000	-3.836010000	-0.688382000	6	2.217747000	3.517856000	1.256384000
6	-3.836547000	-3.498987000	-4.051264000	1	2.100810000	4.476583000	1.764976000
1	-1.927585000	-2.951181000	-4.894253000	1	2.498523000	3.727962000	0.225497000
1	-5.577232000	-4.026836000	-2.896266000	6	3.360625000	2.717232000	1.899943000
6	6.098584000	1.509095000	0.337224000	1	4.303201000	3.237727000	1.739467000
6	7.099288000	2.290092000	0.891453000	6	-2.794095000	-0.607197000	0.523929000
6	5.858435000	1.419668000	-1.027305000	1	-3.614721000	-1.039343000	-0.046122000
6	7.901767000	3.031700000	0.018952000	1	-2.992337000	-0.766623000	1.589183000
1	7.244523000	2.306128000	1.962044000	1	3.219584000	2.582686000	2.978124000

9



Zero-point correction= 0.495029 (Hartree/Particle)  
 Thermal correction to Energy= 0.527693  
 Thermal correction to Enthalpy= 0.528637  
 Thermal correction to Gibbs Free Energy= 0.425269  
 Sum of electronic and zero-point Energies= -2213.569087  
 Sum of electronic and thermal Energies= -2213.536422  
 Sum of electronic and thermal Enthalpies= -2213.535478  
 Sum of electronic and thermal Free Energies= -2213.638846

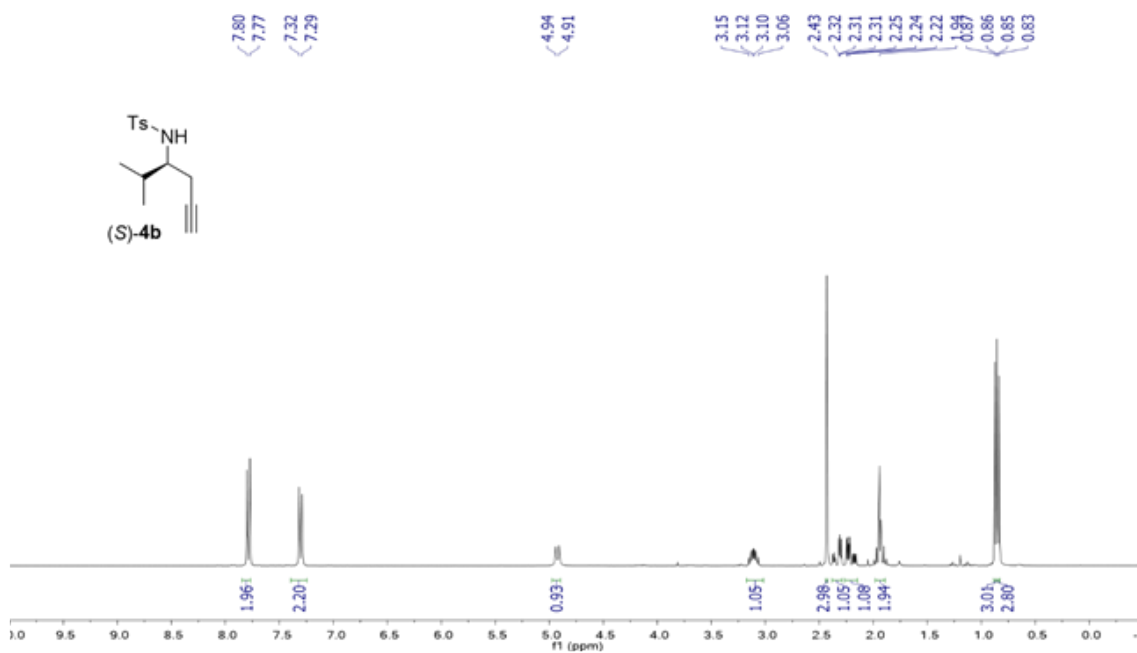
6	2.285661000	0.562771000	1.039017000	8	-2.131259000	-3.804845000	1.097472000
1	2.396854000	-0.182103000	0.255253000	8	0.033413000	-3.554070000	-0.766439000
1	2.252786000	0.026457000	1.999088000	6	-2.696496000	-3.374658000	-1.645479000
6	1.010220000	1.372972000	0.872042000	6	-2.294155000	-3.049509000	-2.932945000
6	-0.201085000	0.700683000	0.594732000	6	-3.956474000	-3.861717000	-1.337062000
6	-0.195708000	-0.814498000	0.471017000	6	-3.218398000	-3.217296000	-3.963304000
1	-0.065795000	-1.260338000	1.468407000	1	-1.293651000	-2.688841000	-3.120323000
1	0.623669000	-1.166353000	-0.150496000	6	-4.866814000	-4.021761000	-2.385535000
7	-1.453269000	-1.277123000	-0.163415000	1	-4.202300000	-4.117703000	-0.316439000
7	3.467847000	1.454293000	0.963321000	6	-4.513317000	-3.703401000	-3.706101000
6	1.016219000	2.765248000	1.056851000	1	-2.931830000	-2.971846000	-4.977468000
6	-0.187811000	3.472909000	0.951907000	1	-5.857480000	-4.401224000	-2.173225000
1	-0.185832000	4.546285000	1.096705000	6	6.263491000	1.602018000	0.413430000
6	-1.402093000	1.423055000	0.503015000	6	7.153582000	2.294916000	1.217956000
6	-1.378181000	2.812244000	0.679312000	6	6.240071000	1.705246000	-0.970133000
1	-2.303620000	3.370891000	0.611652000	6	8.067190000	3.148370000	0.592803000
16	5.033057000	0.458263000	1.232373000	1	7.135824000	2.154927000	2.289274000
16	-1.467548000	-3.149718000	-0.255564000	6	7.160176000	2.562326000	-1.572318000
8	4.831704000	-0.888464000	0.325130000	1	5.535003000	1.129624000	-1.551278000
8	5.420701000	0.381387000	2.827444000	6	8.083410000	3.294061000	-0.803067000

1	8.774410000	3.700892000	1.196966000	1	-2.954965000	0.842342000	-0.858488000
1	7.164761000	2.662566000	-2.649752000	1	-3.525426000	1.187955000	0.770996000
6	9.092178000	4.194013000	-1.476782000	6	2.303541000	3.511111000	1.351637000
1	9.928210000	3.610605000	-1.872470000	1	2.115646000	4.318668000	2.063628000
1	8.647526000	4.733980000	-2.314242000	1	2.678078000	3.969458000	0.432158000
1	9.502582000	4.927125000	-0.782332000	6	3.395436000	2.591473000	1.906338000
6	-5.489978000	-3.908055000	-4.839965000	1	4.353835000	3.108073000	1.919898000
1	-5.414124000	-3.110178000	-5.580272000	6	-2.664592000	-0.771936000	0.518520000
1	-5.291567000	-4.851533000	-5.356159000	1	-3.541121000	-1.273829000	0.111871000
1	-6.519138000	-3.939736000	-4.482058000	1	-2.627141000	-0.958833000	1.596640000
6	-2.714923000	0.725689000	0.201981000	1	3.167482000	2.256947000	2.923605000

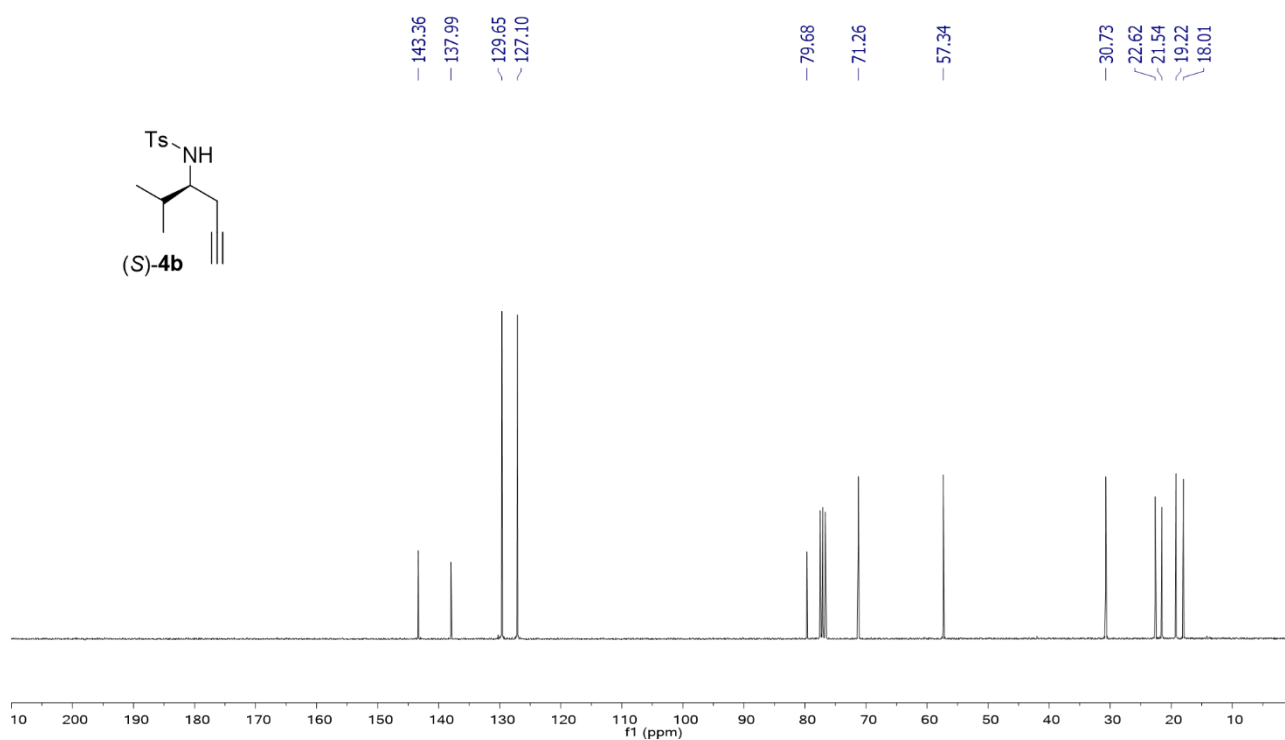
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### III. $^1\text{H}$ , $^{13}\text{C}$ and $^{19}\text{F}$ NMR spectra of new compounds.

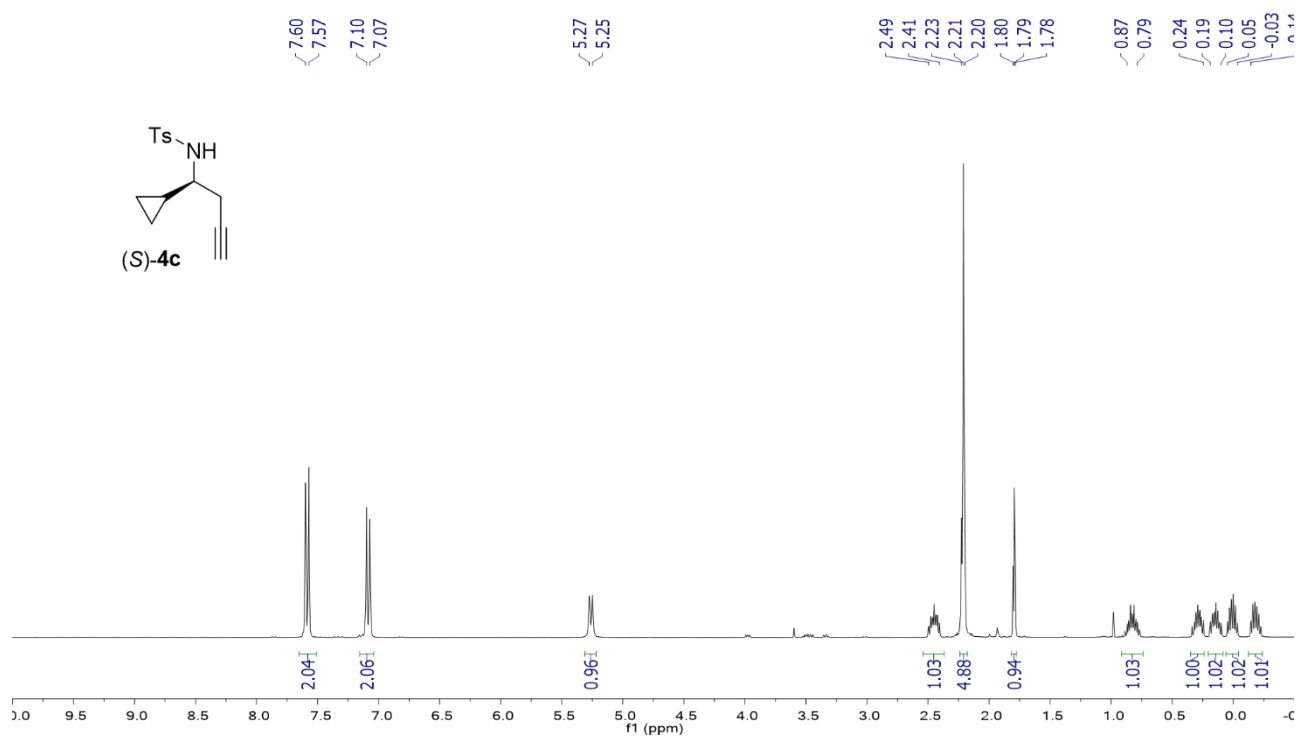
$^1\text{H}$  NMR spectrum of compound (*S*)-**4b** (300 MHz,  $\text{CDCl}_3$ )



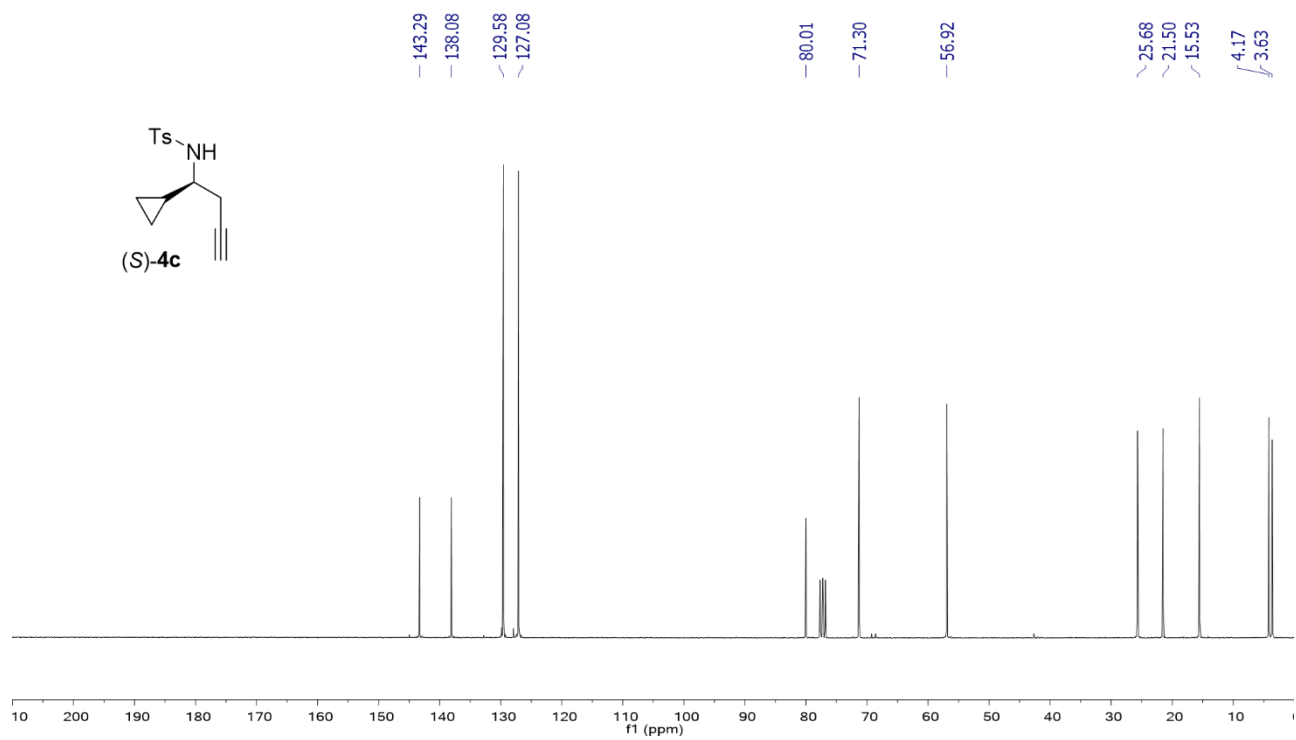
$^{13}\text{C}$  NMR spectrum of compound (*S*)-**4b** (75 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR spectrum of compound (S)-4c (300 MHz, CDCl<sub>3</sub>)

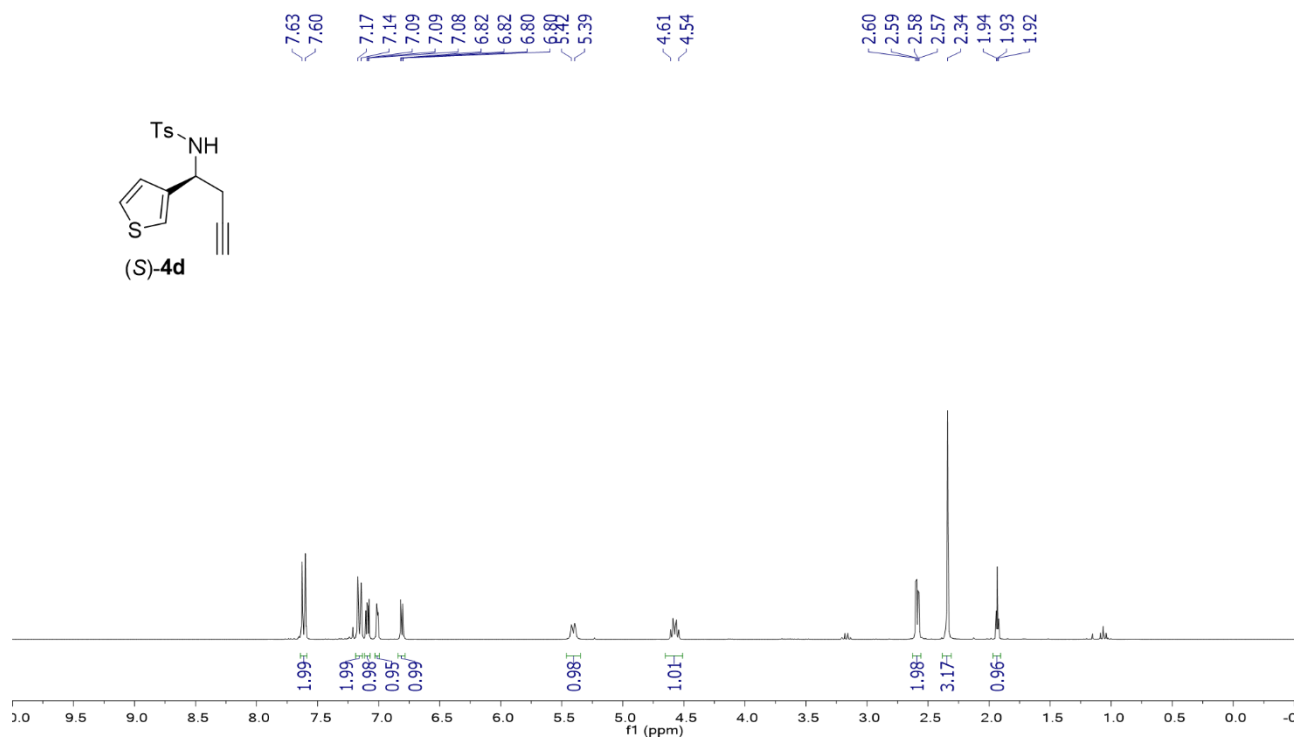


<sup>13</sup>C NMR spectrum of compound (S)-4c (75 MHz, CDCl<sub>3</sub>)

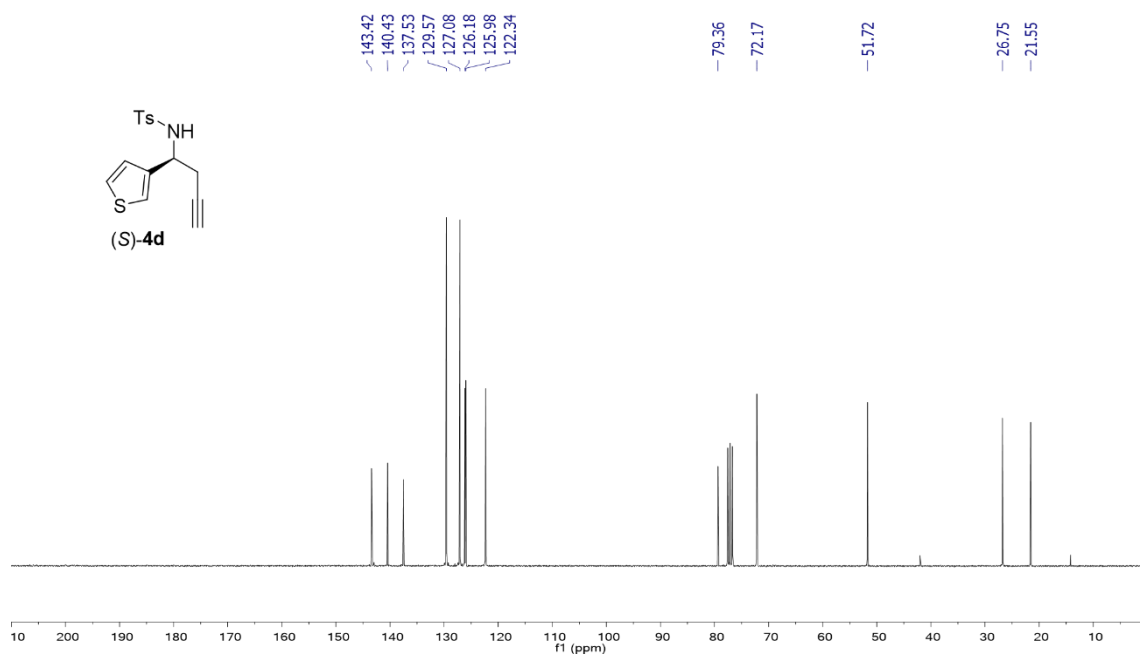




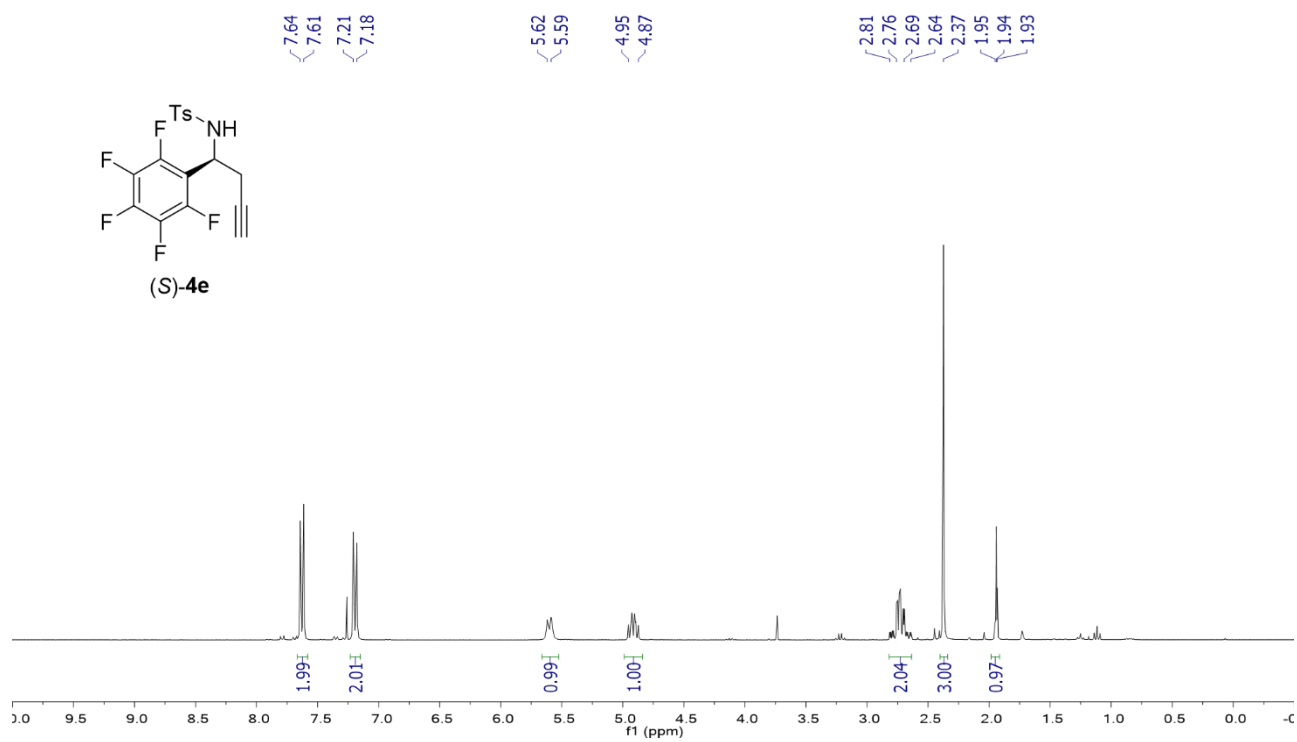
$^1\text{H}$  NMR spectrum of compound (*S*)-**4d** (300 MHz,  $\text{CDCl}_3$ )



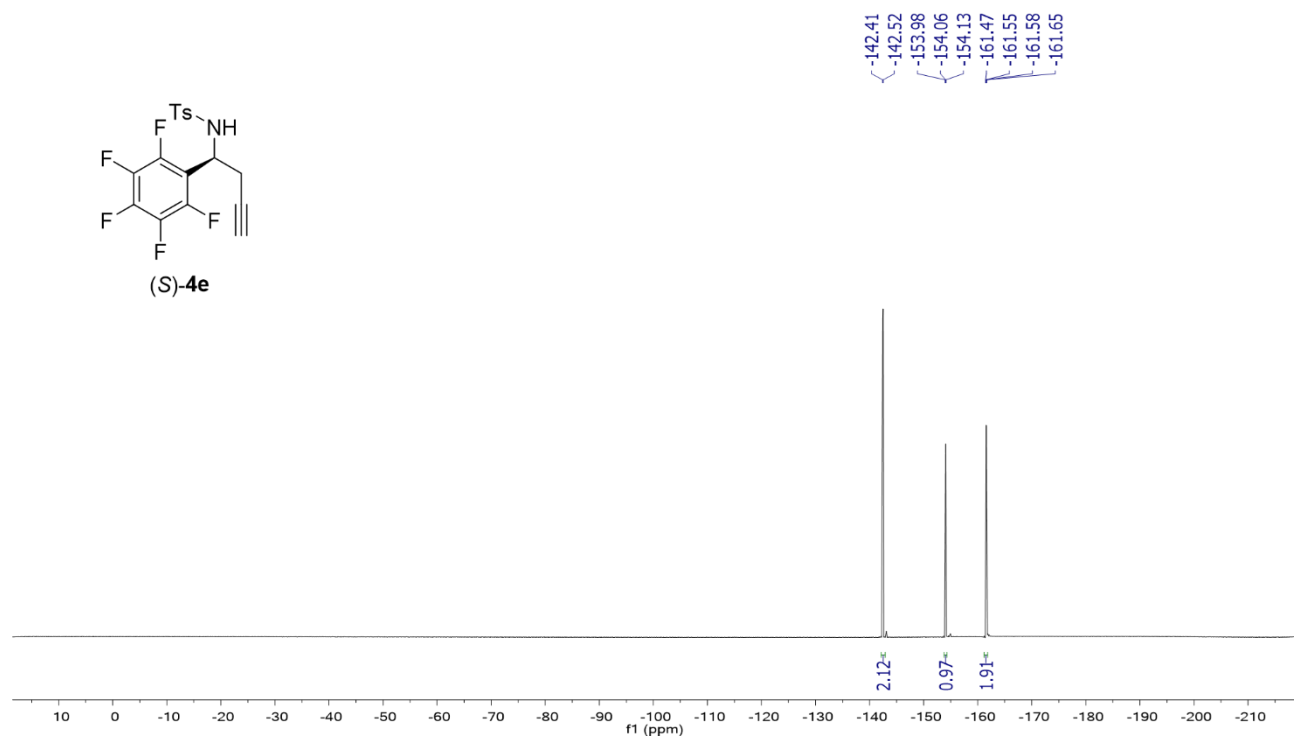
$^{13}\text{C}$  NMR spectrum of compound (*S*)-**4d** (75 MHz,  $\text{CDCl}_3$ )



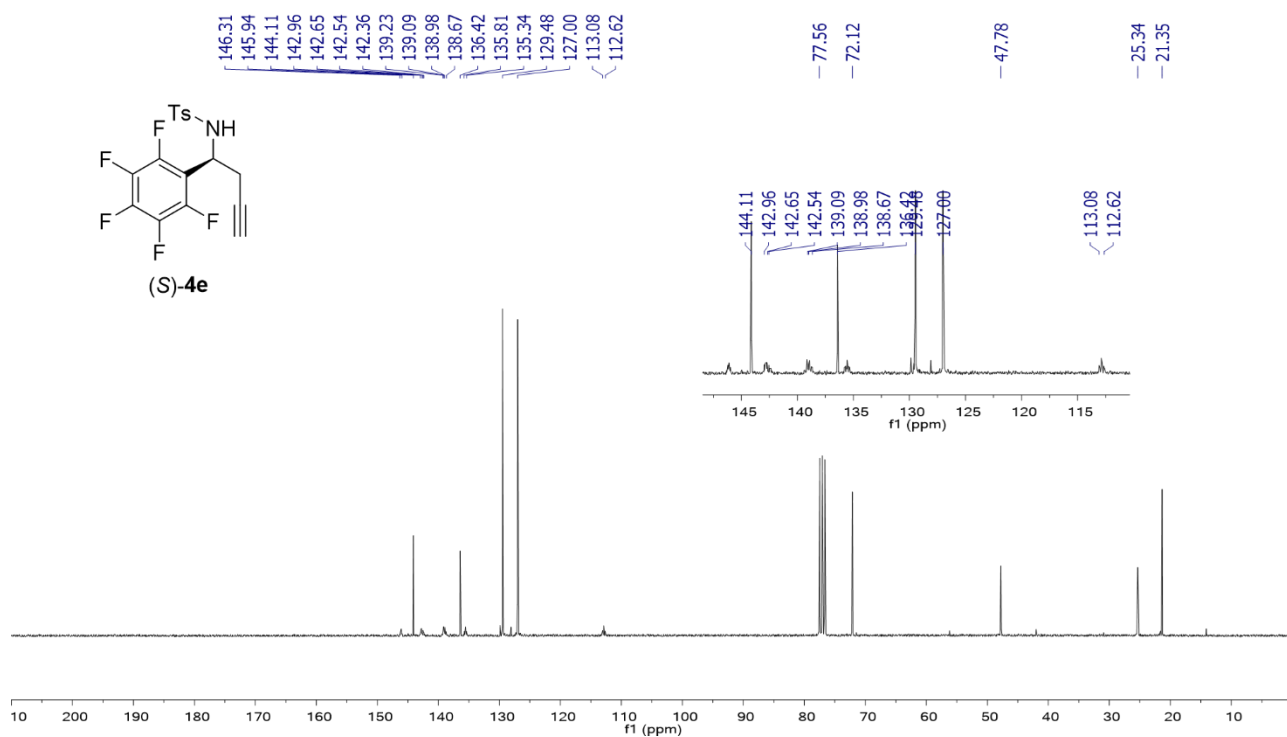
$^1\text{H}$  NMR spectrum of compound (*S*)-**4e** (300 MHz,  $\text{CDCl}_3$ )



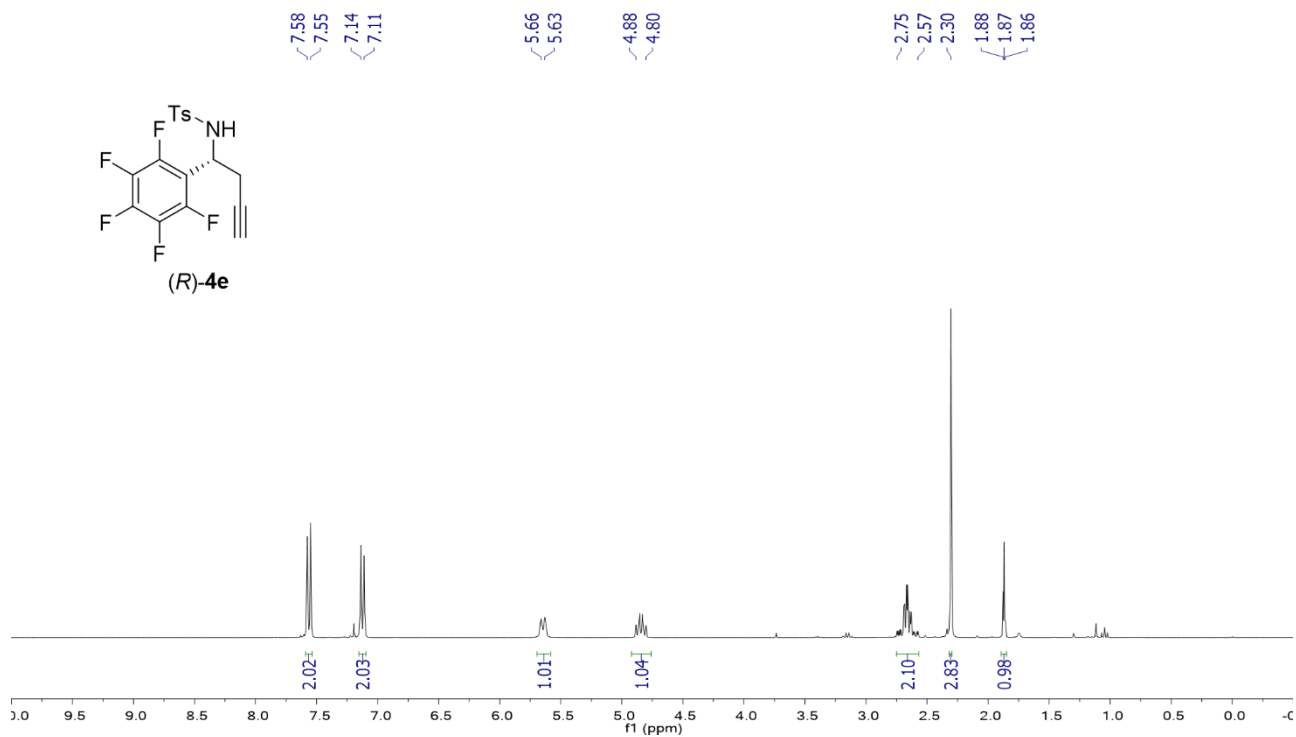
$^{19}\text{F}$  NMR spectrum of compound (*S*)-**4e** (282 MHz,  $\text{CDCl}_3$ )



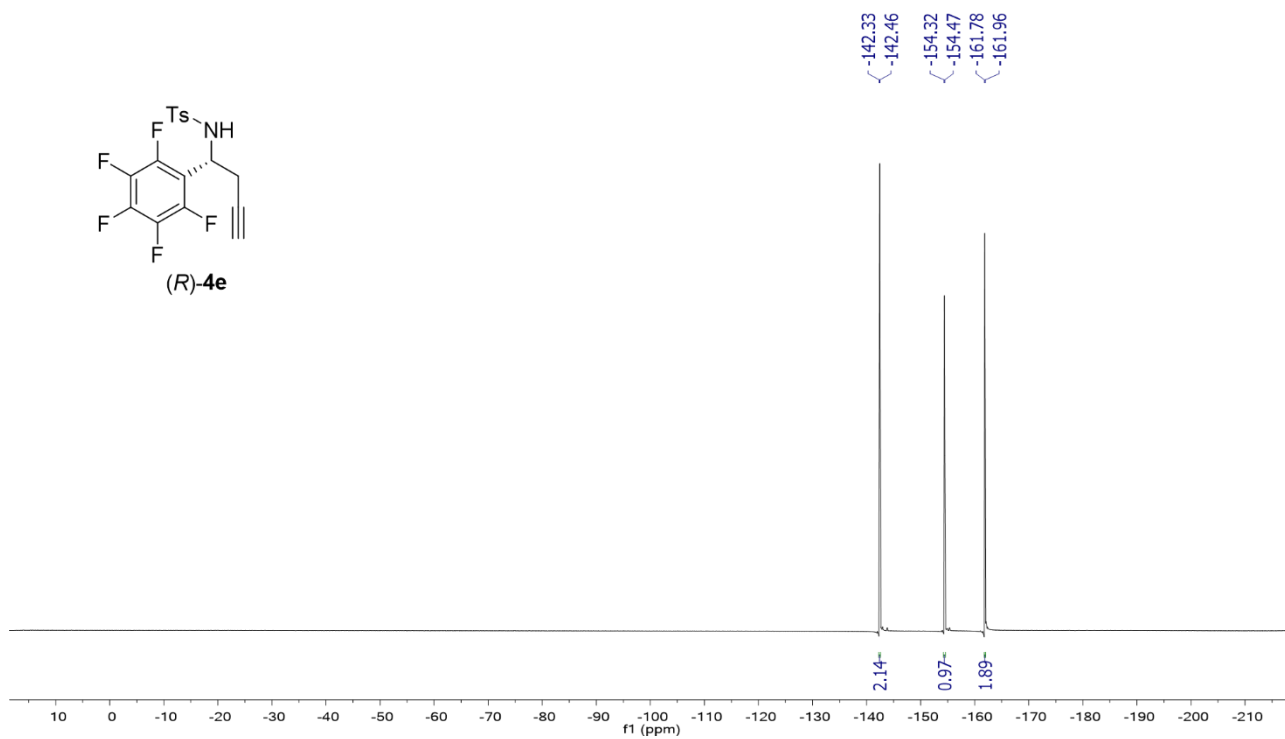
$^{13}\text{C}$  NMR spectrum of compound (*S*)-**4e** (75 MHz,  $\text{CDCl}_3$ )



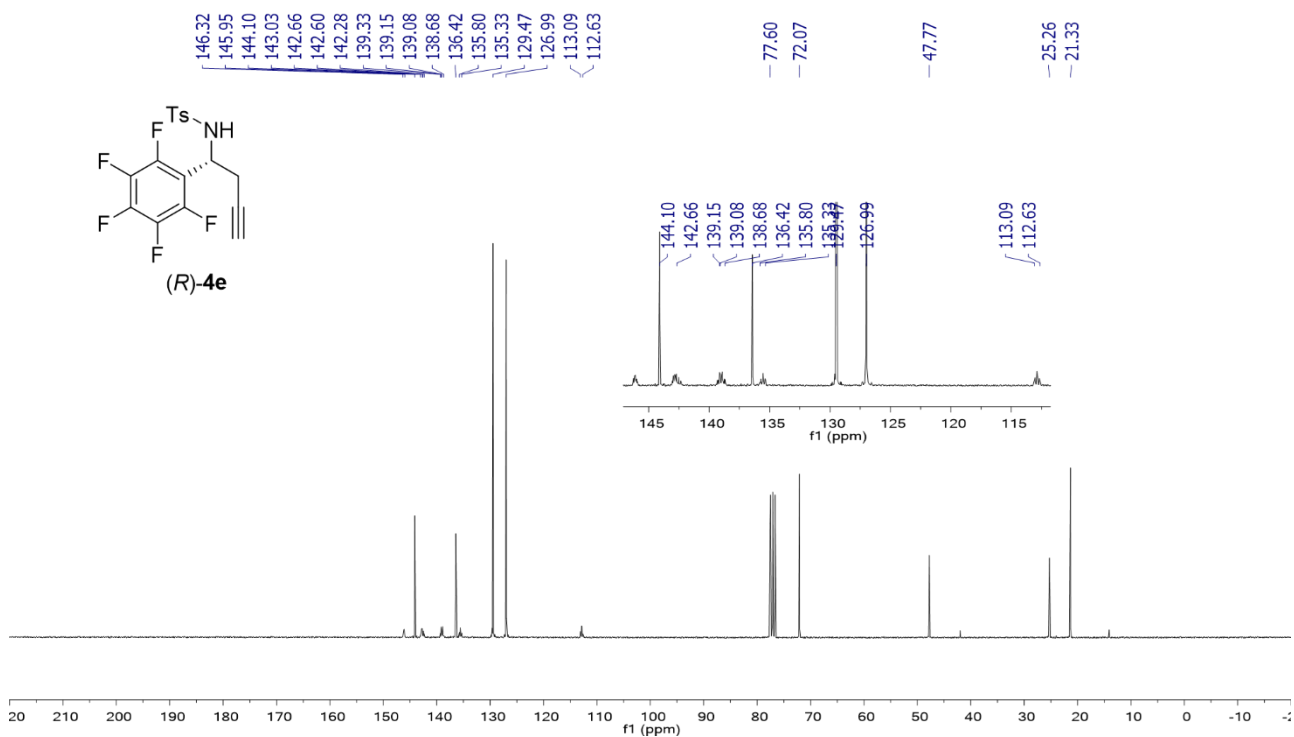
$^1\text{H}$  NMR spectrum of compound (*R*)-**4e** (300 MHz,  $\text{CDCl}_3$ )



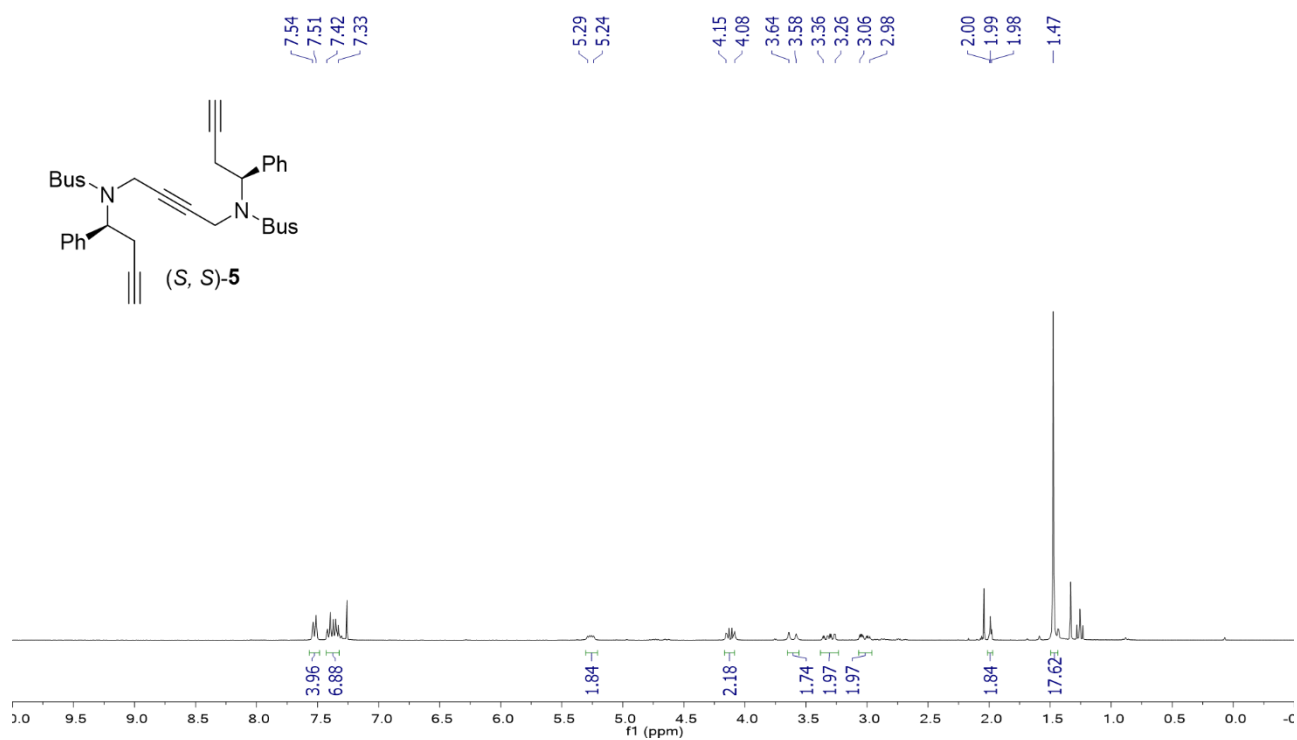
$^{19}\text{F}$  NMR spectrum of compound (*R*)-**4e** (282 MHz,  $\text{CDCl}_3$ )



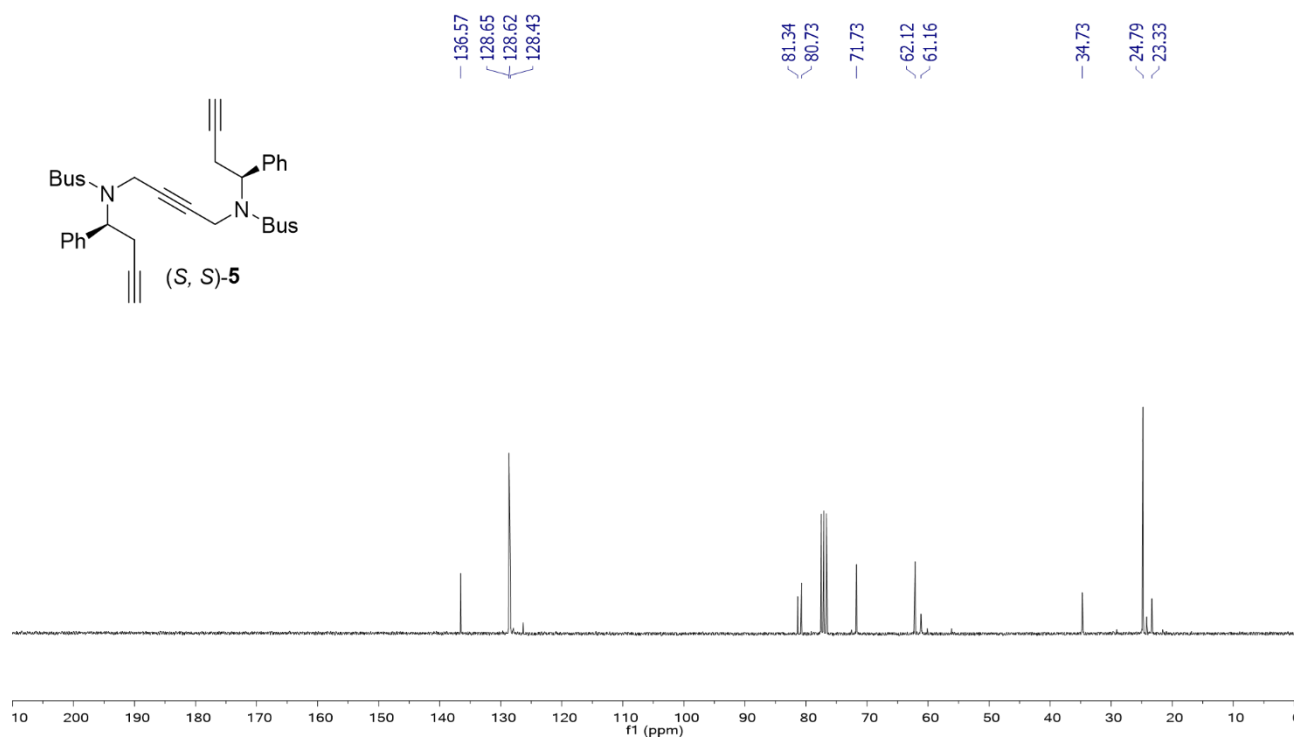
$^{13}\text{C}$  NMR spectrum of compound (*R*)-**4e** (75 MHz,  $\text{CDCl}_3$ )



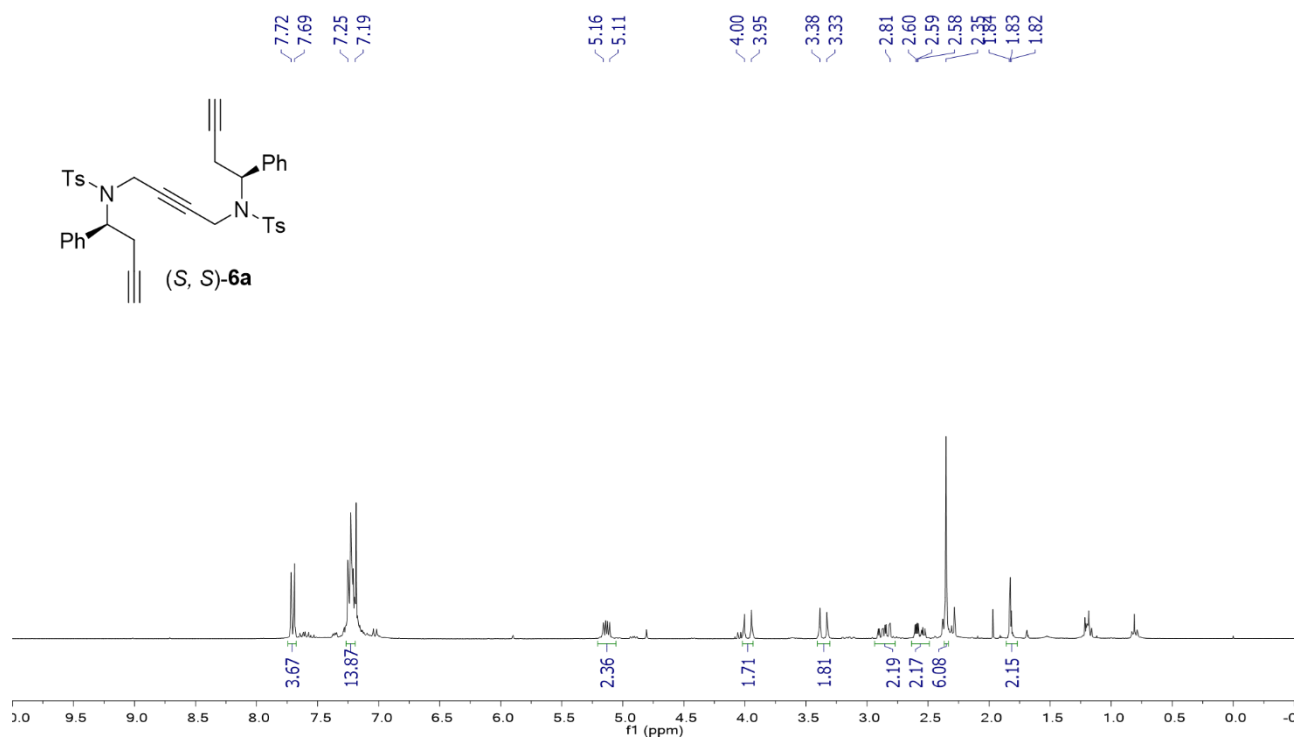
<sup>1</sup>H NMR spectrum of compound (S,S)-5 (300 MHz, CDCl<sub>3</sub>)



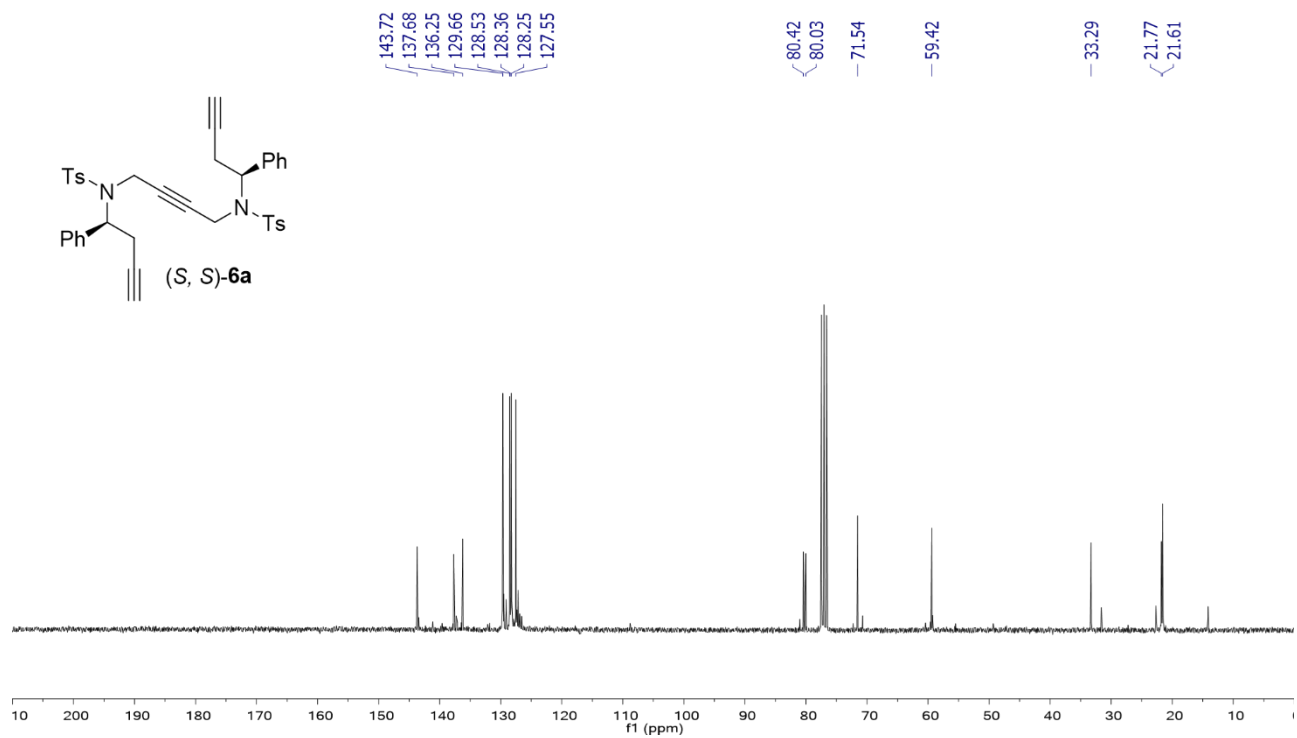
<sup>13</sup>C NMR spectrum of compound (S,S)-5 (75 MHz, CDCl<sub>3</sub>)



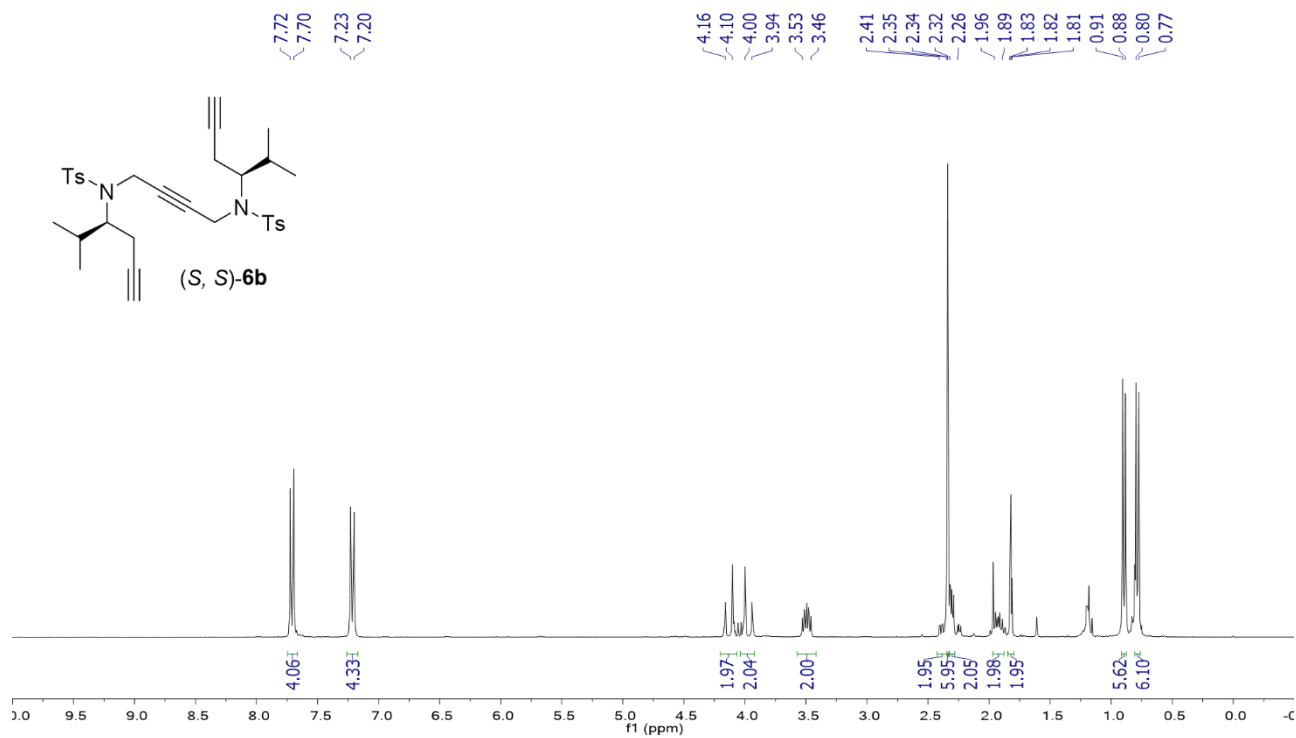
<sup>1</sup>H NMR spectrum of compound (S,S)-6a (300 MHz, CDCl<sub>3</sub>)



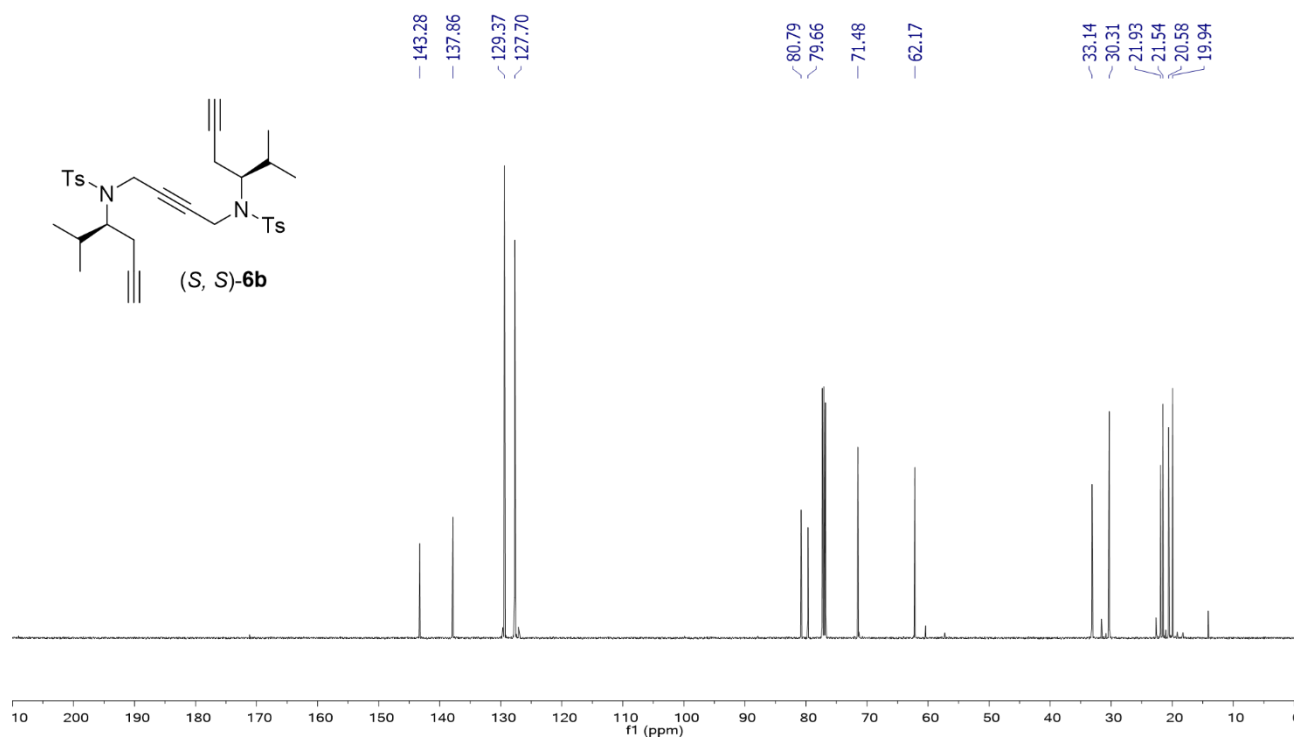
<sup>13</sup>C NMR spectrum of compound (S,S)-6a (75 MHz, CDCl<sub>3</sub>)



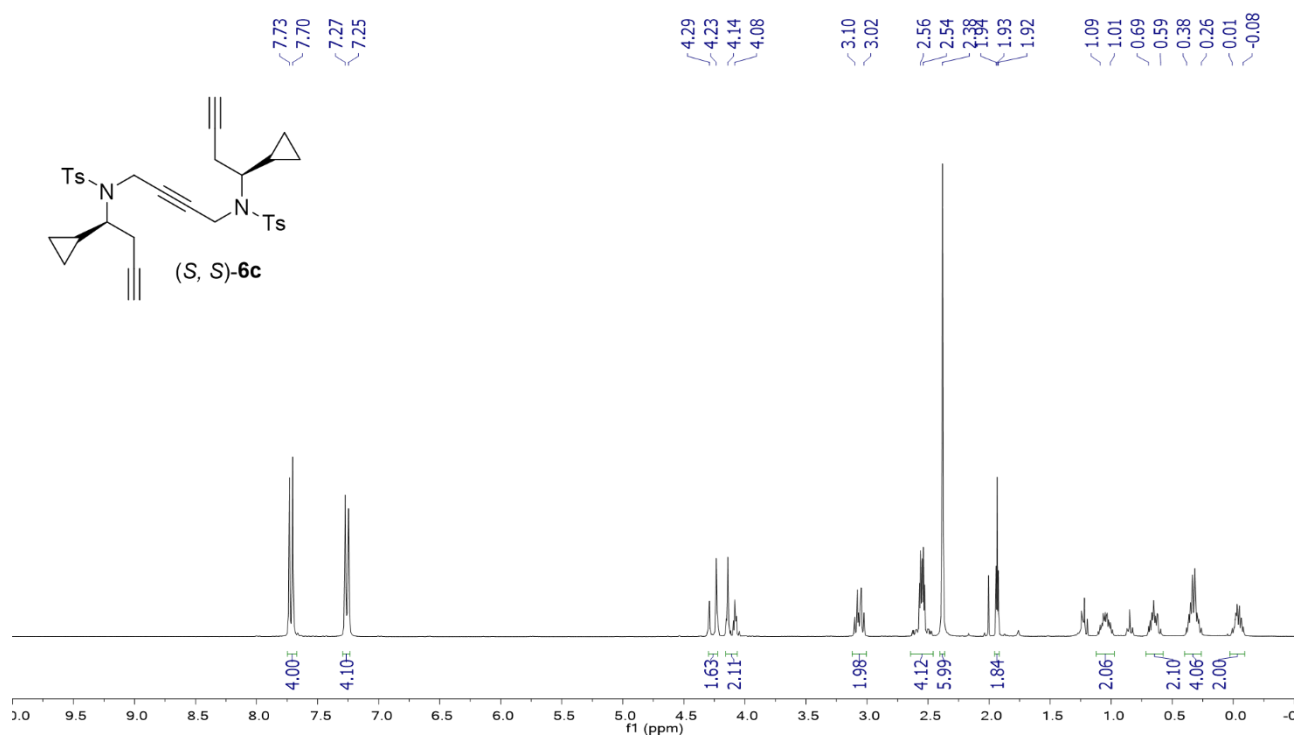
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**6b** (300 MHz,  $\text{CDCl}_3$ )



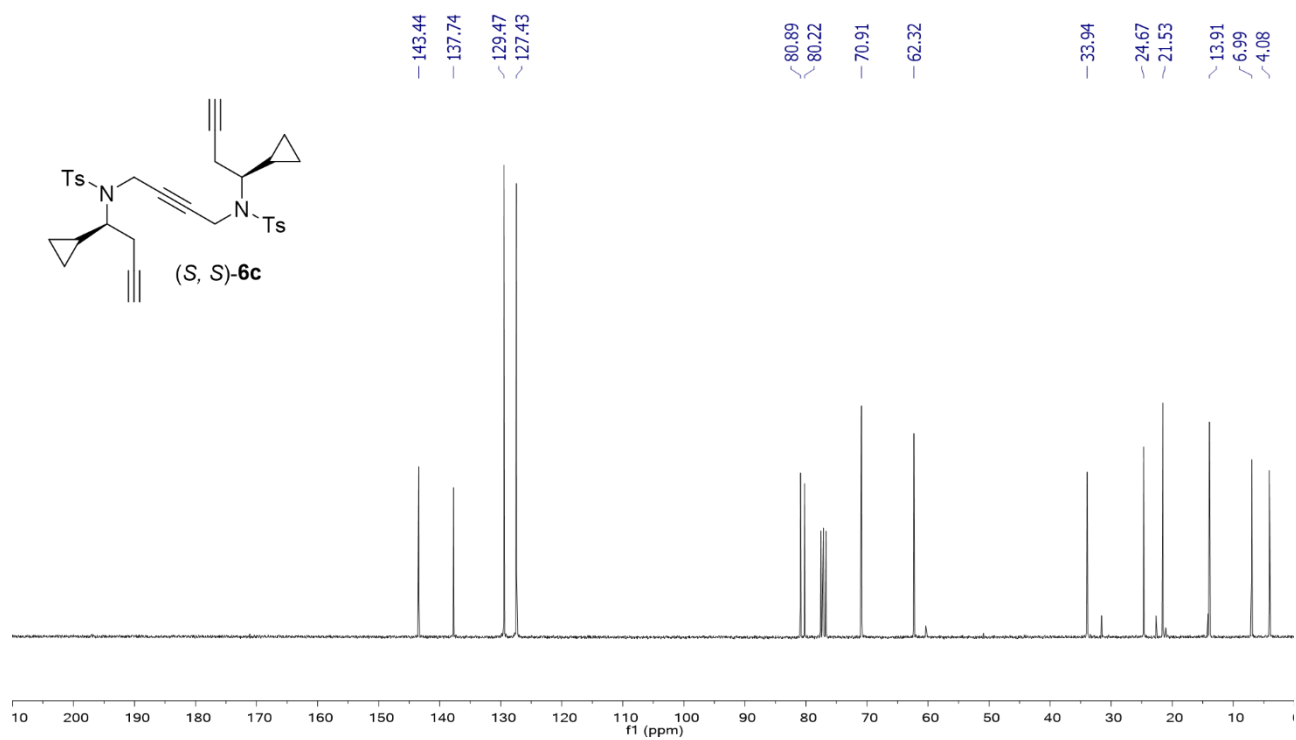
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**6b** (75 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR spectrum of compound (S,S)-6c (300 MHz, CDCl<sub>3</sub>)

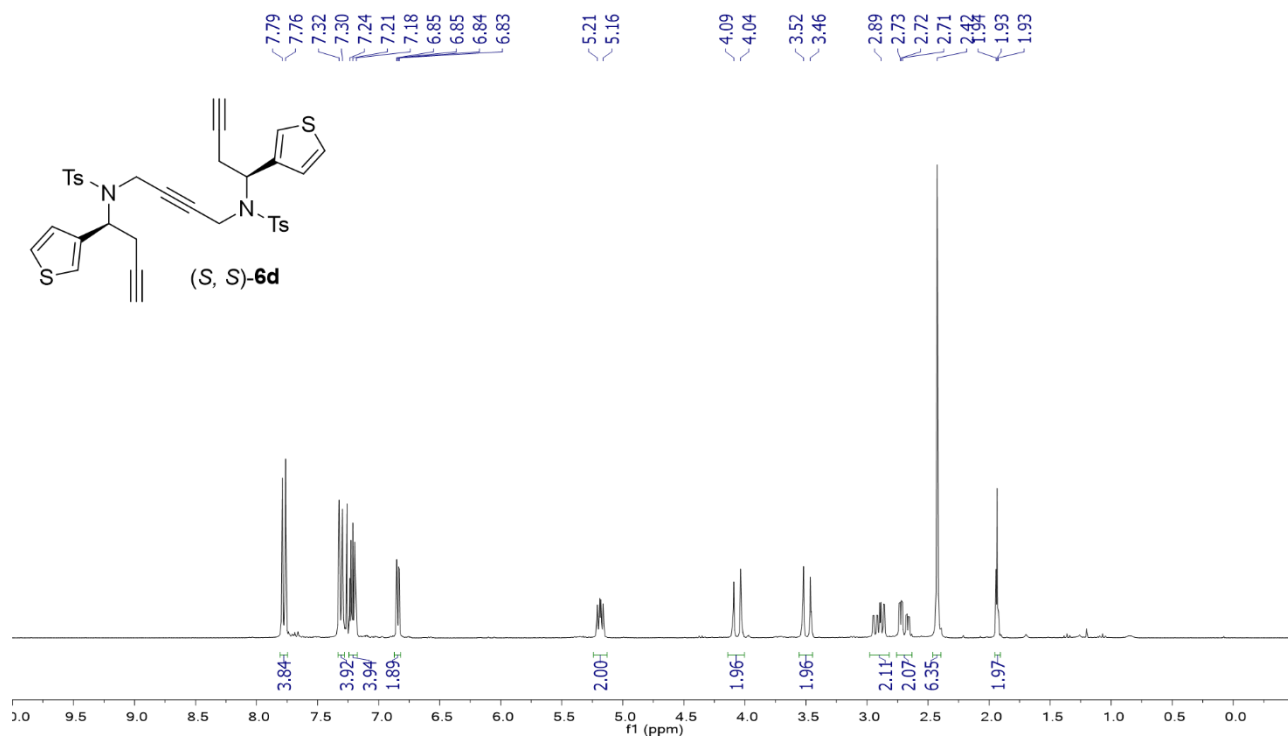


<sup>13</sup>C NMR spectrum of compound (S,S)-6c (75 MHz, CDCl<sub>3</sub>)

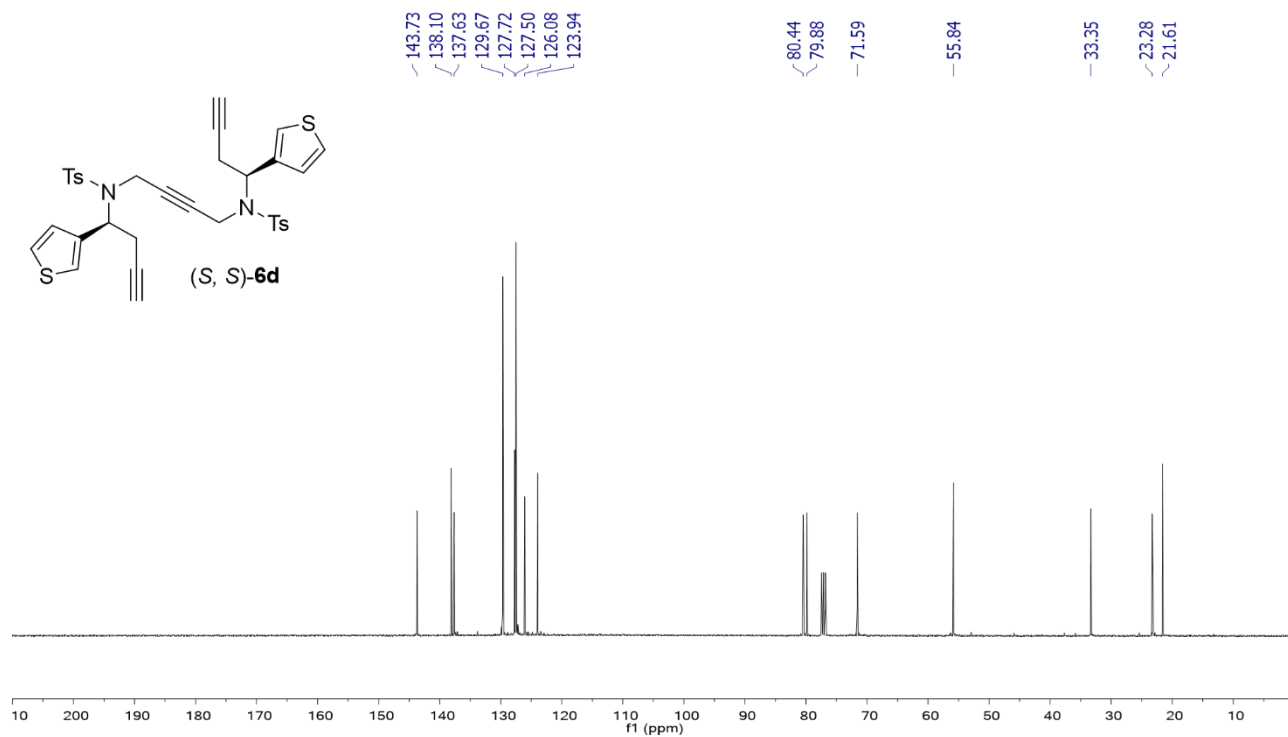




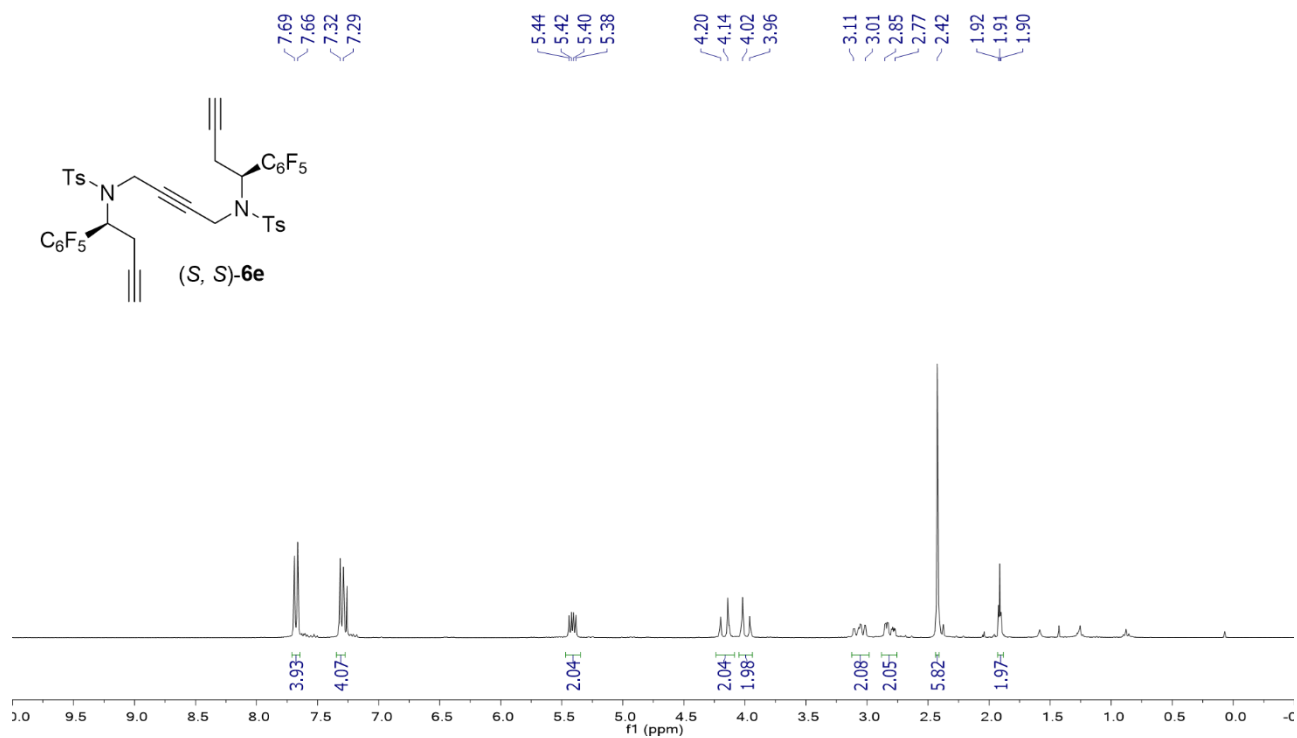
<sup>1</sup>H NMR spectrum of compound (S,S)-6d (300 MHz, CDCl<sub>3</sub>)



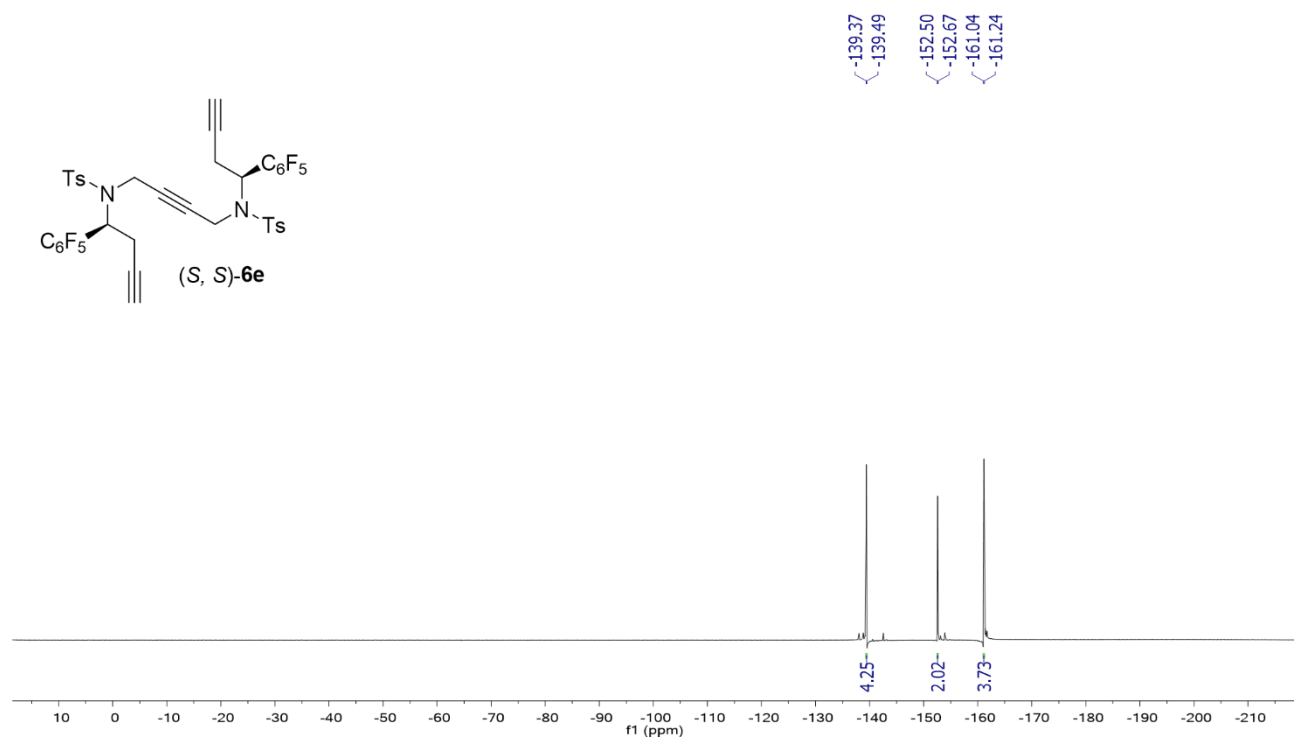
<sup>13</sup>C NMR spectrum of compound (S,S)-6d (75 MHz, CDCl<sub>3</sub>)



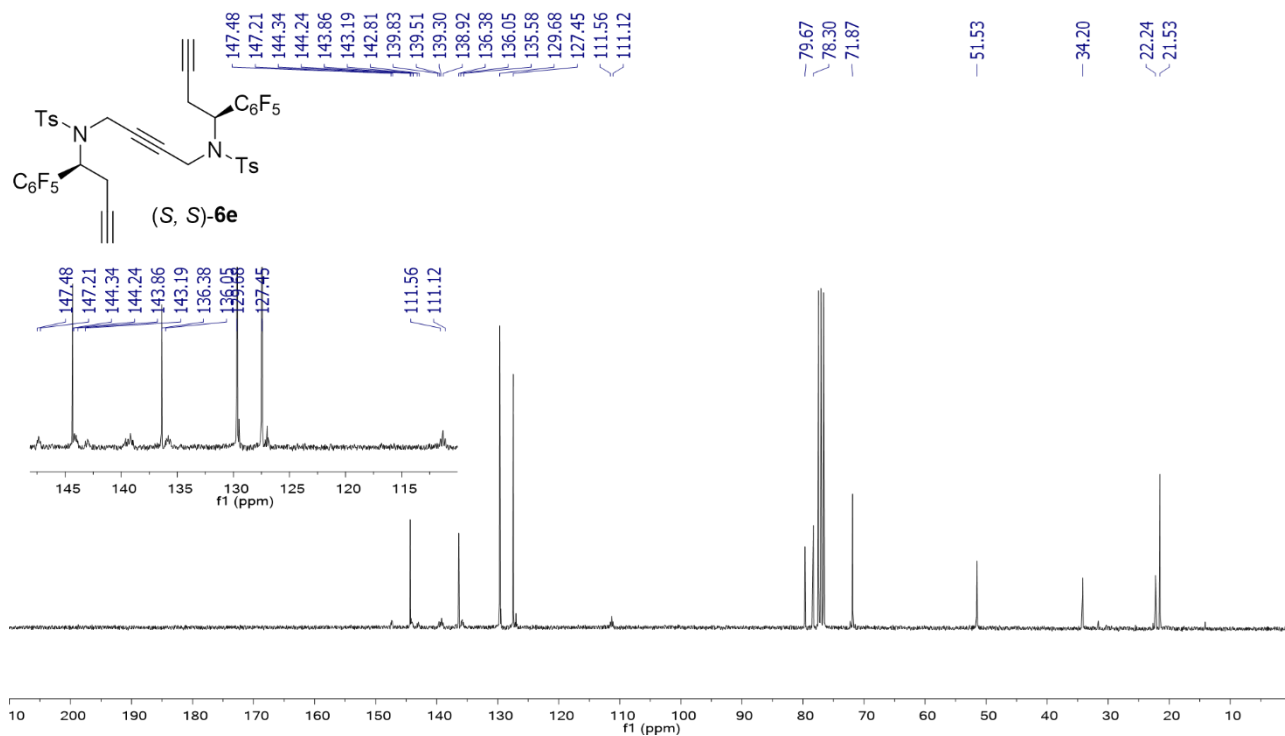
<sup>1</sup>H NMR spectrum of compound (S,S)-6e (300 MHz, CDCl<sub>3</sub>)



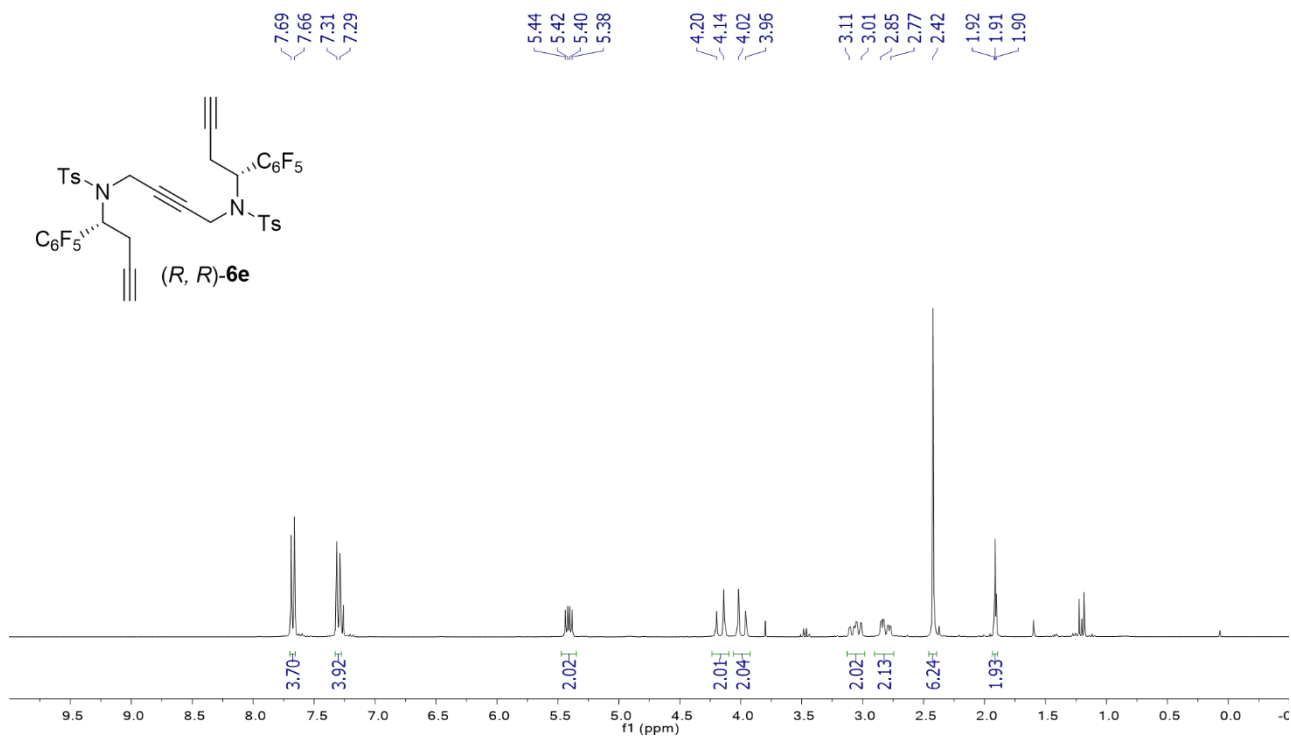
<sup>19</sup>F NMR spectrum of compound (S,S)-6e (282 MHz, CDCl<sub>3</sub>)



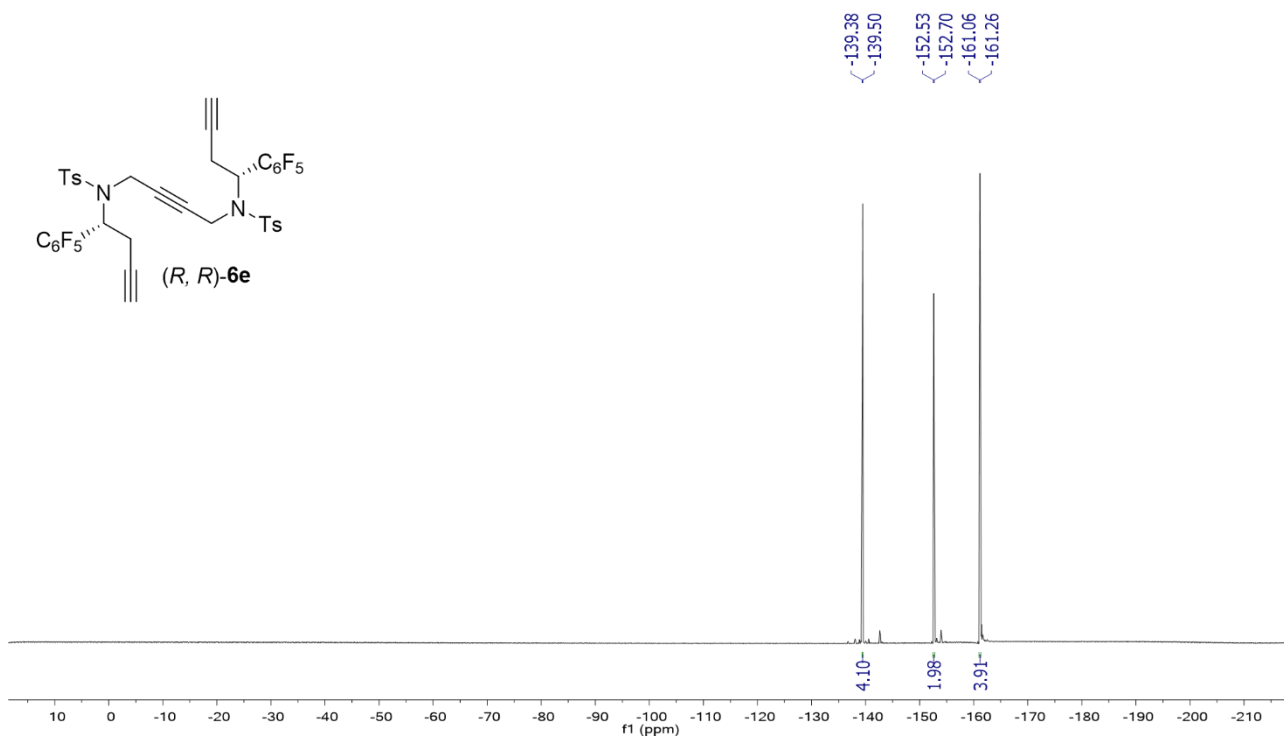
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**6e** (75 MHz,  $\text{CDCl}_3$ )



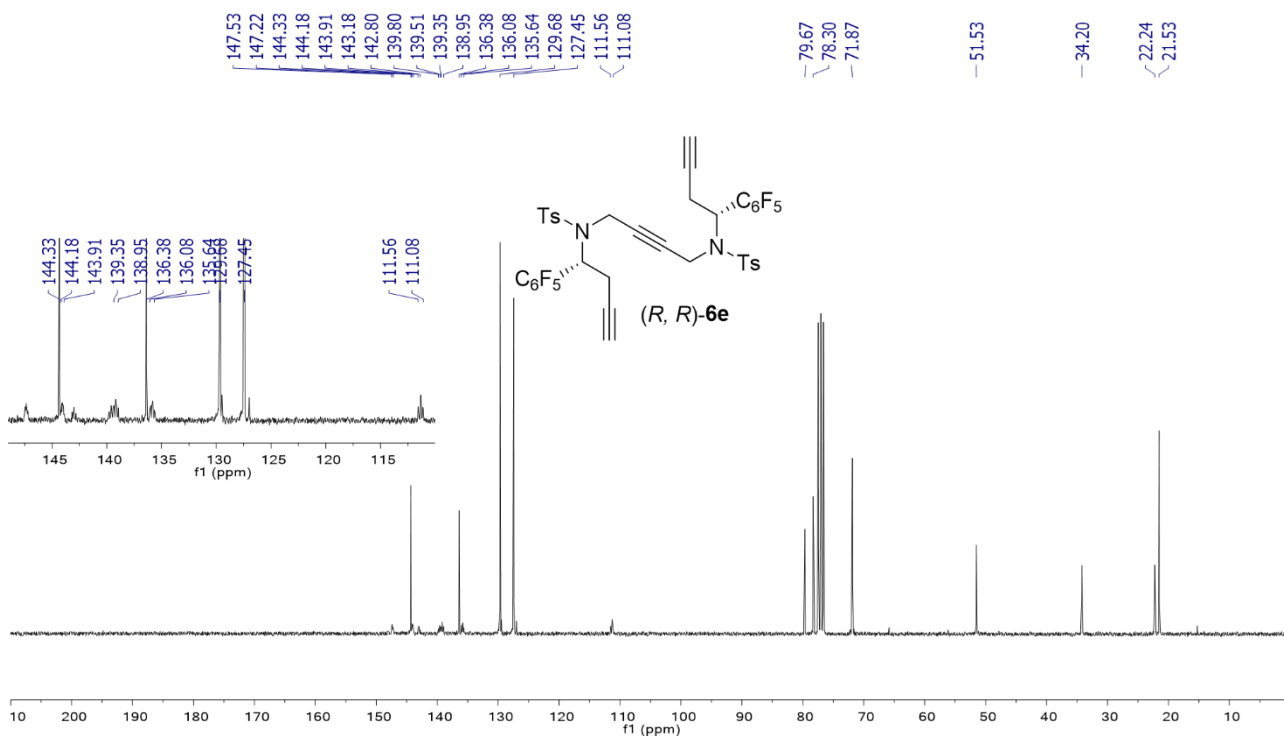
$^1\text{H}$  NMR spectrum of compound (*R,R*)-**6e** (300 MHz,  $\text{CDCl}_3$ )



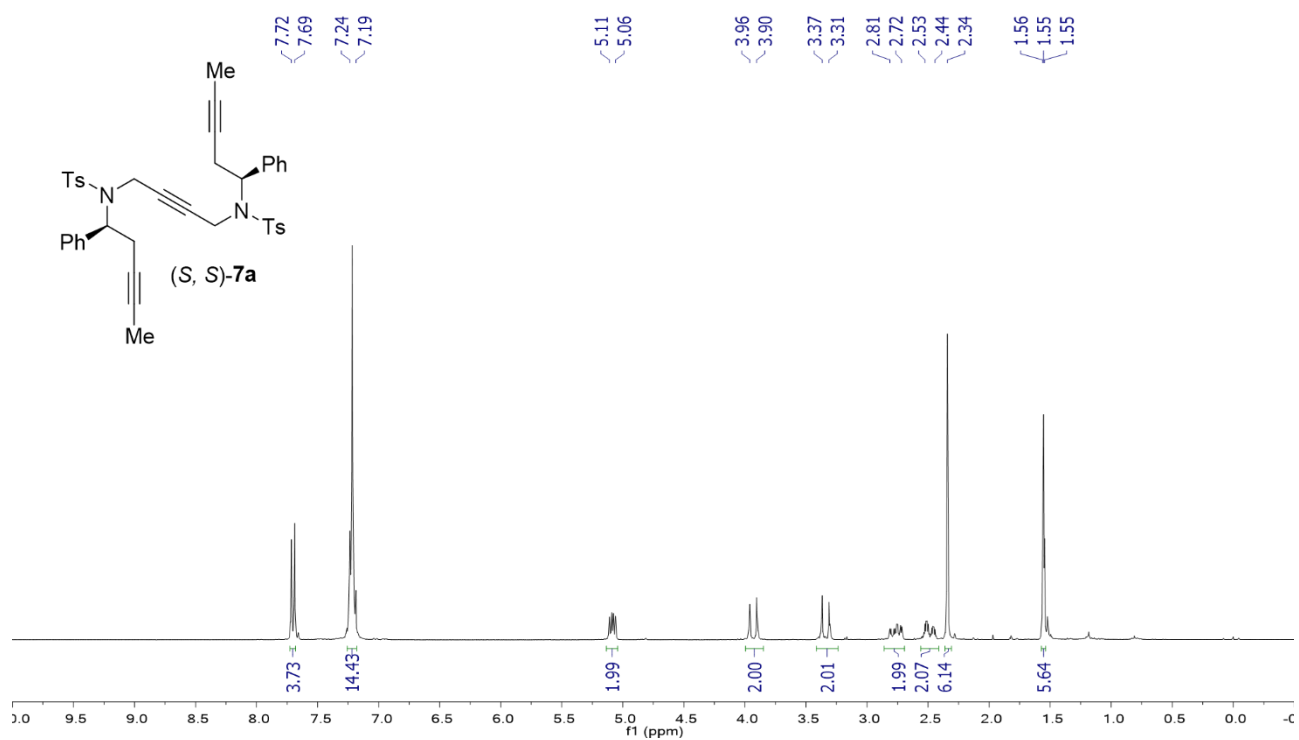
$^{19}\text{F}$  NMR spectrum of compound (*R,R*)-**6e** (282 MHz,  $\text{CDCl}_3$ )



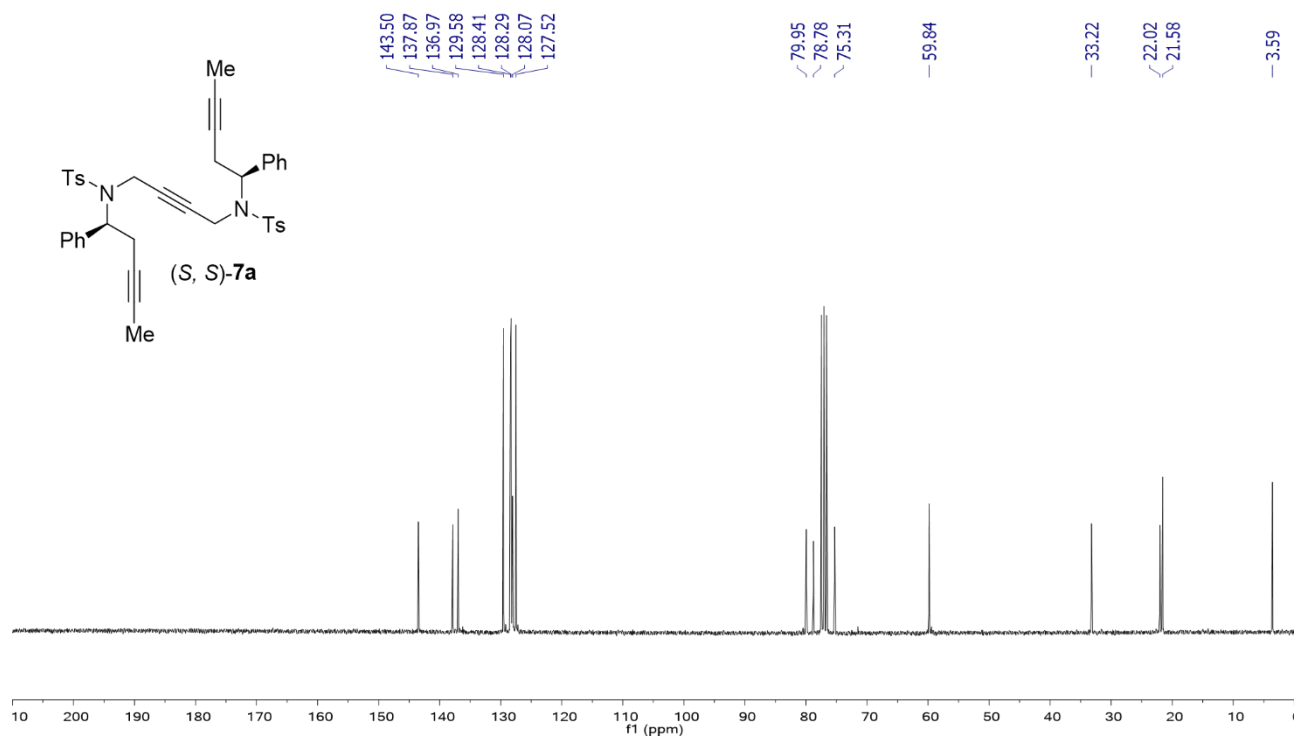
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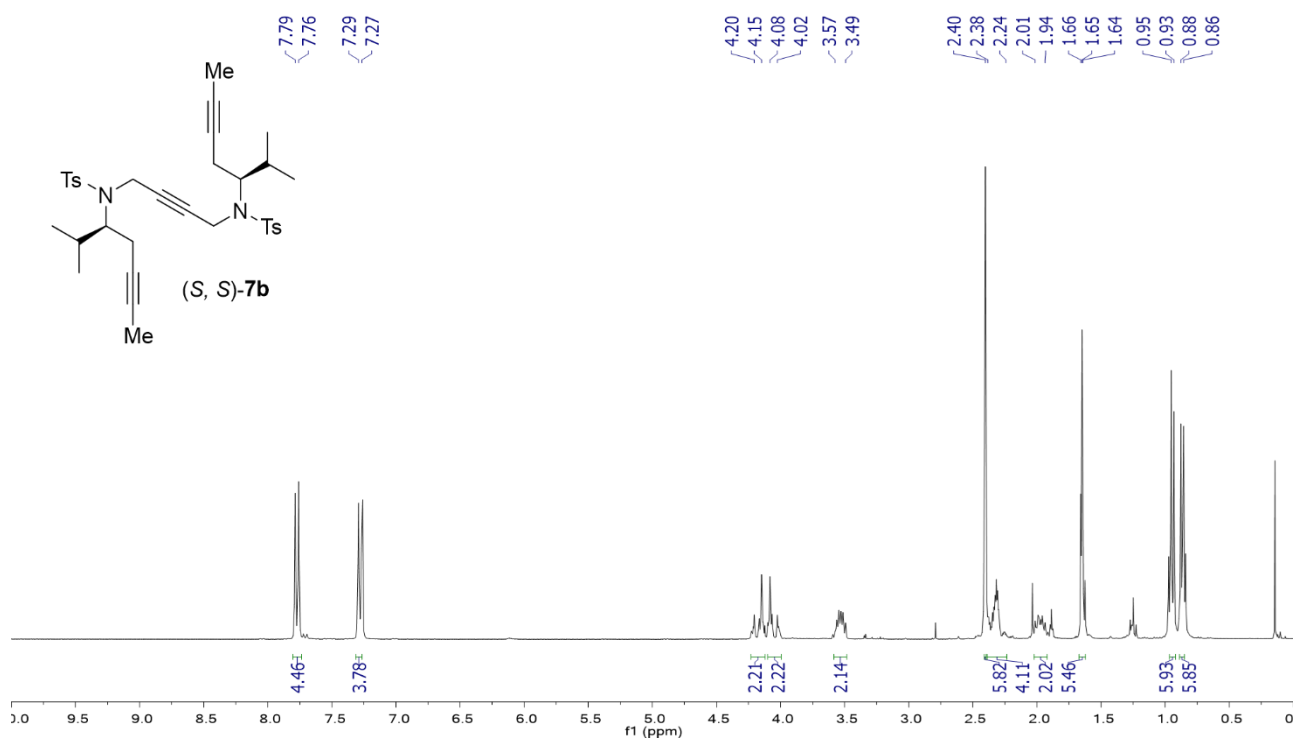
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**7a** (300 MHz,  $\text{CDCl}_3$ )



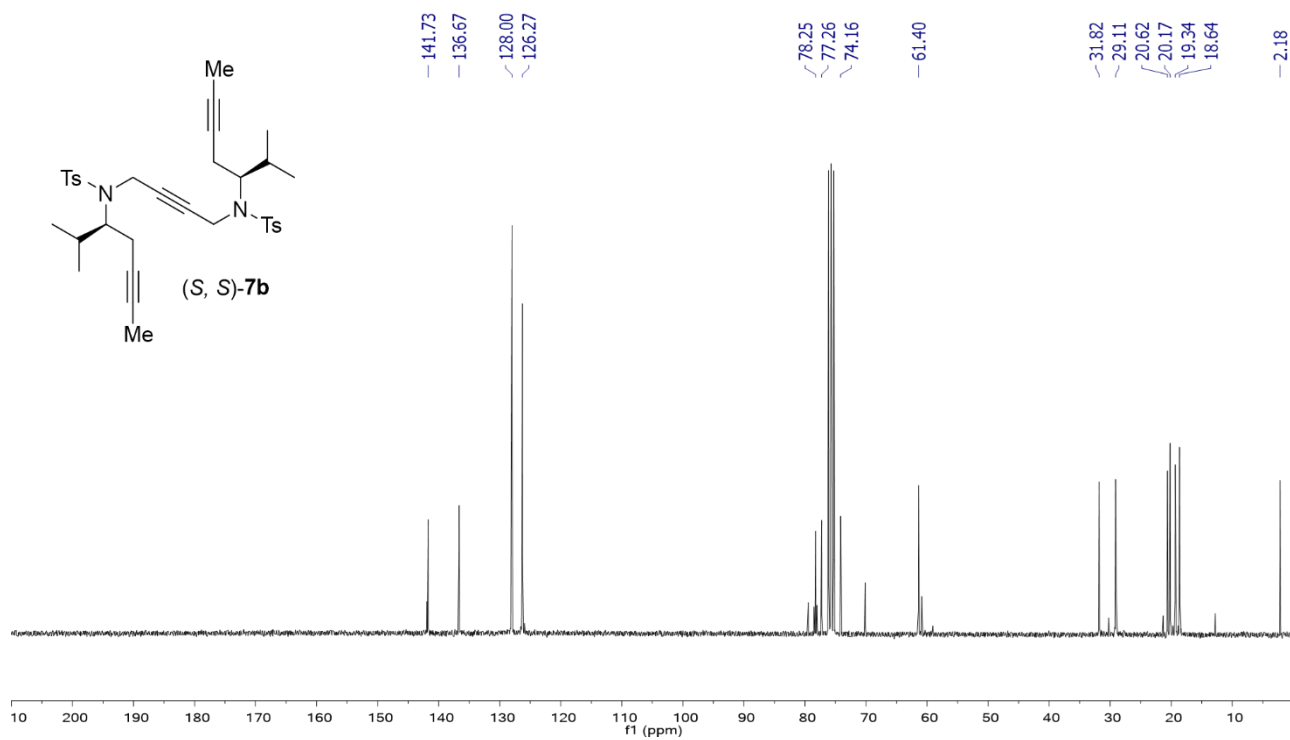
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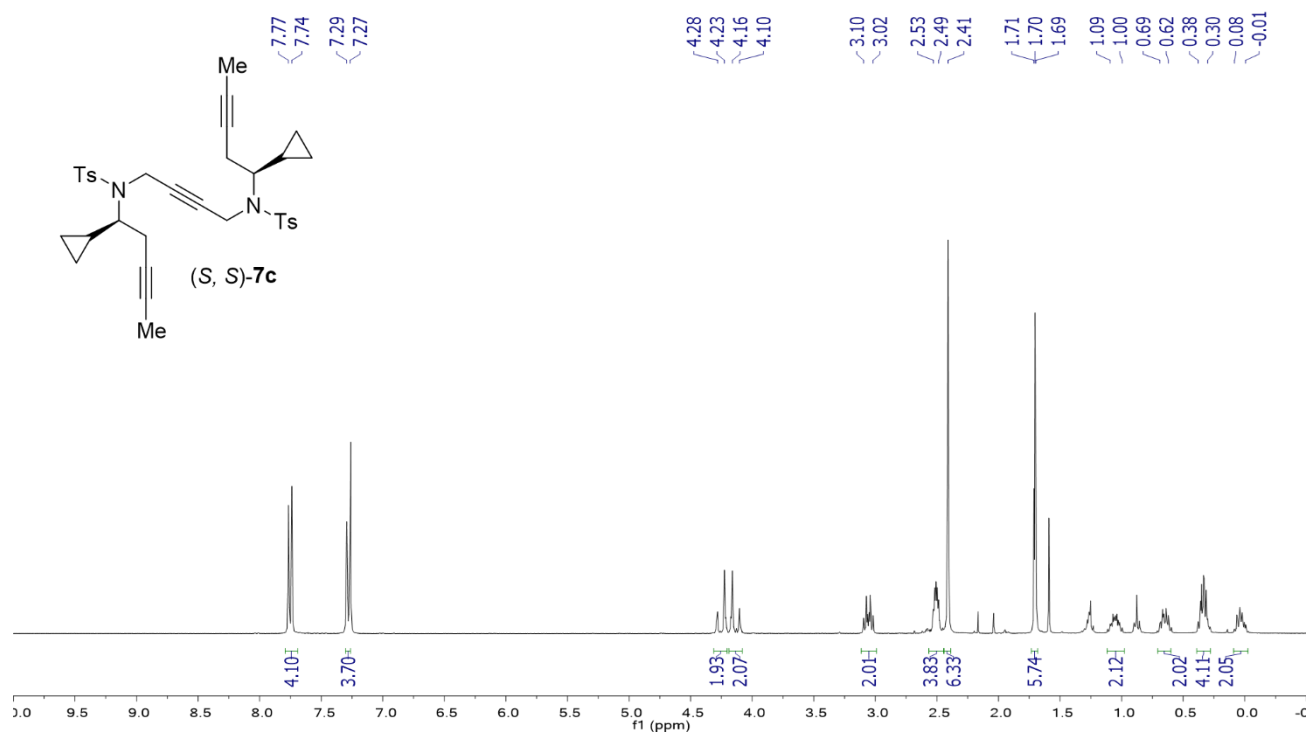
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**7b** (300 MHz,  $\text{CDCl}_3$ )



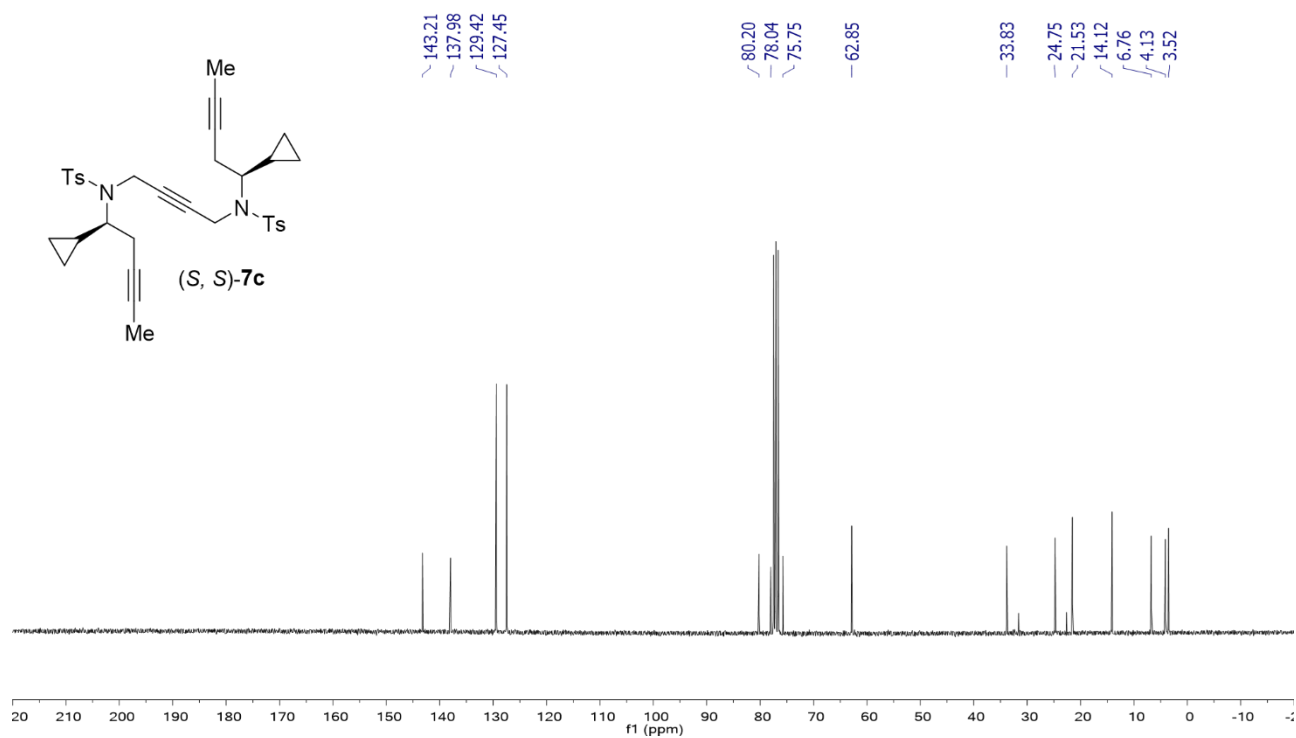
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**7b** (75 MHz,  $\text{CDCl}_3$ )



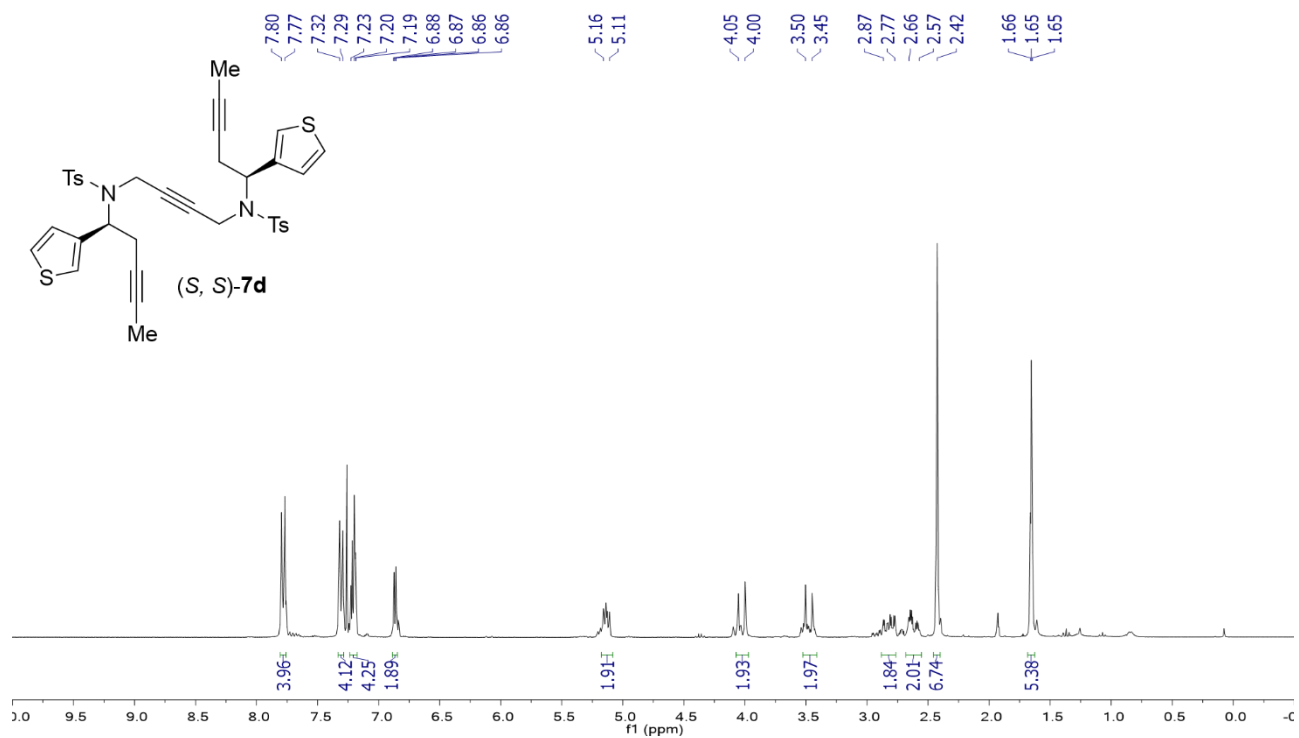
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**7c** (300 MHz,  $\text{CDCl}_3$ )



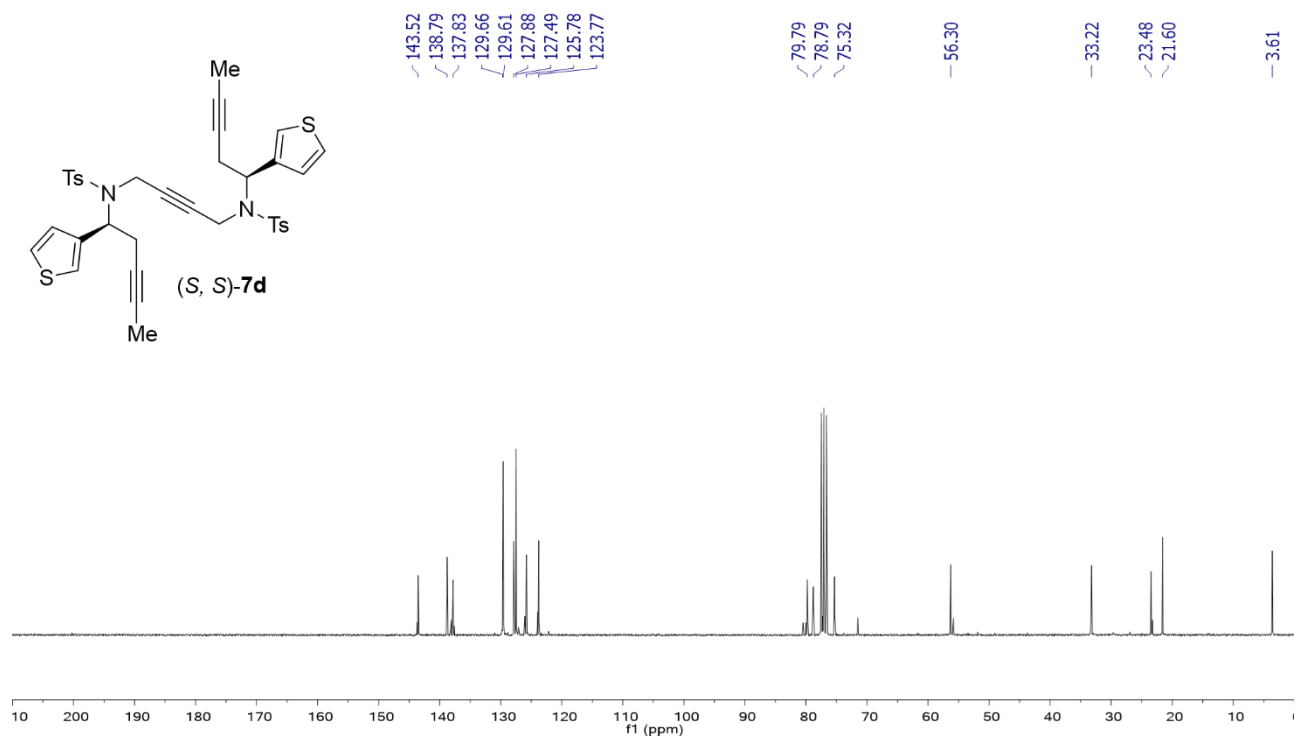
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**7c** (75 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR spectrum of compound (S,S)-7d (300 MHz, CDCl<sub>3</sub>)

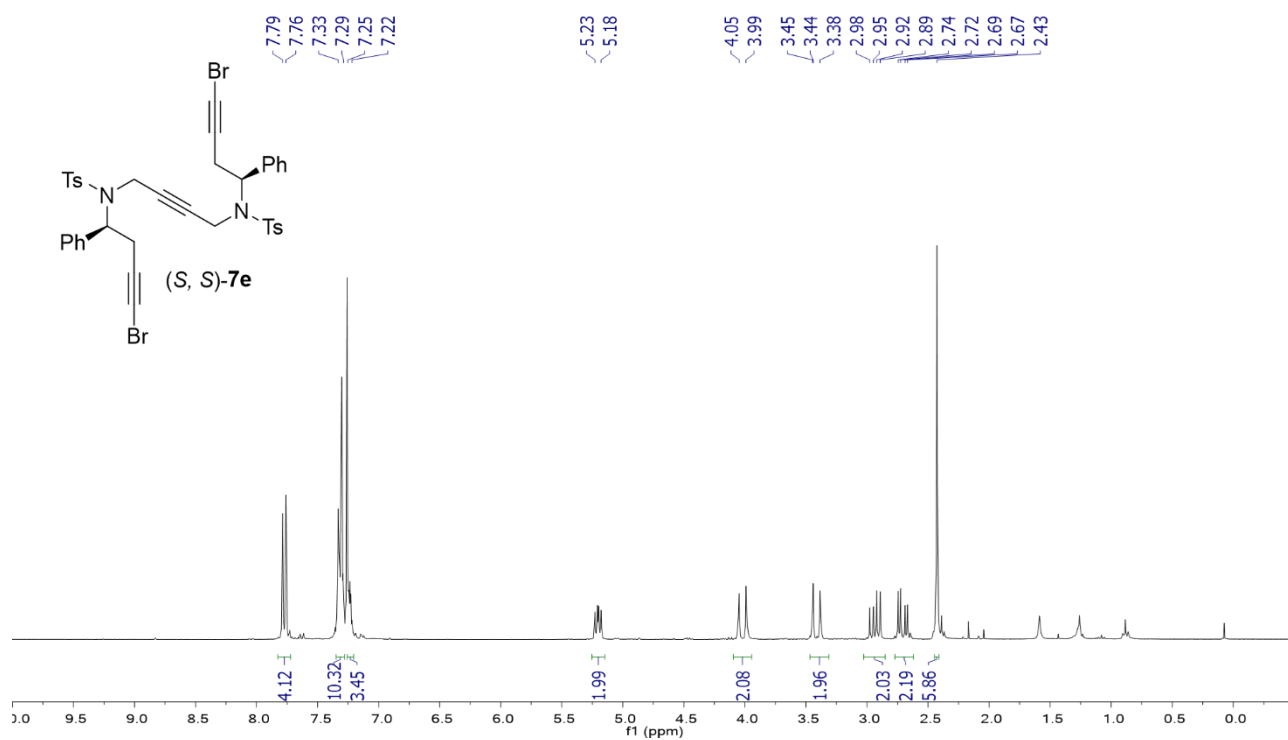


<sup>13</sup>C NMR spectrum of compound (S,S)-7d (75 MHz, CDCl<sub>3</sub>)

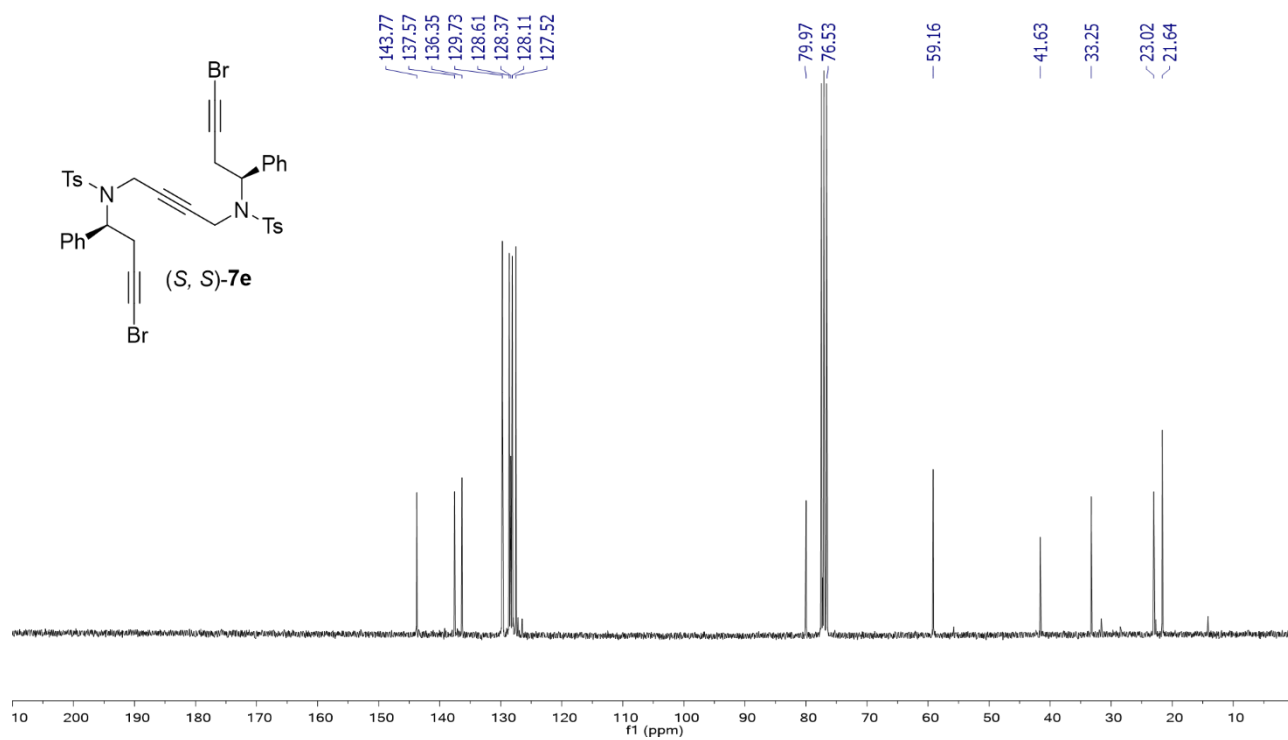




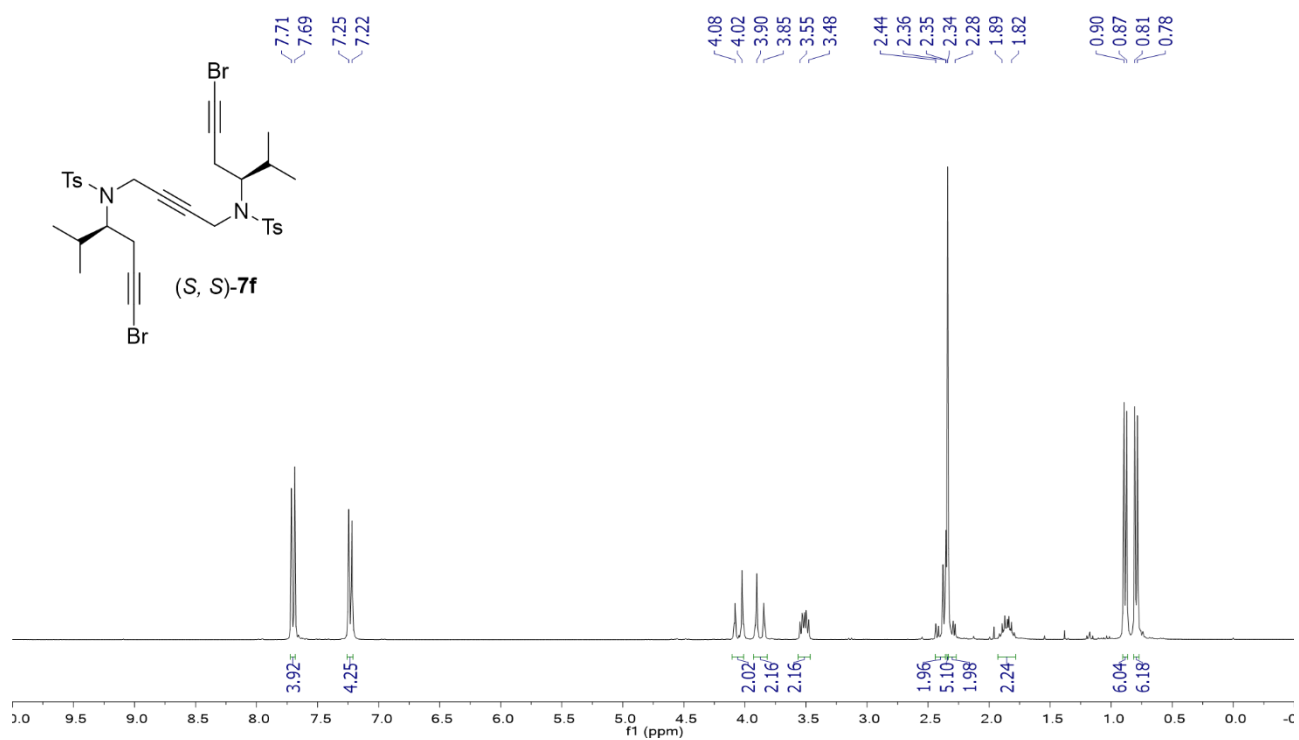
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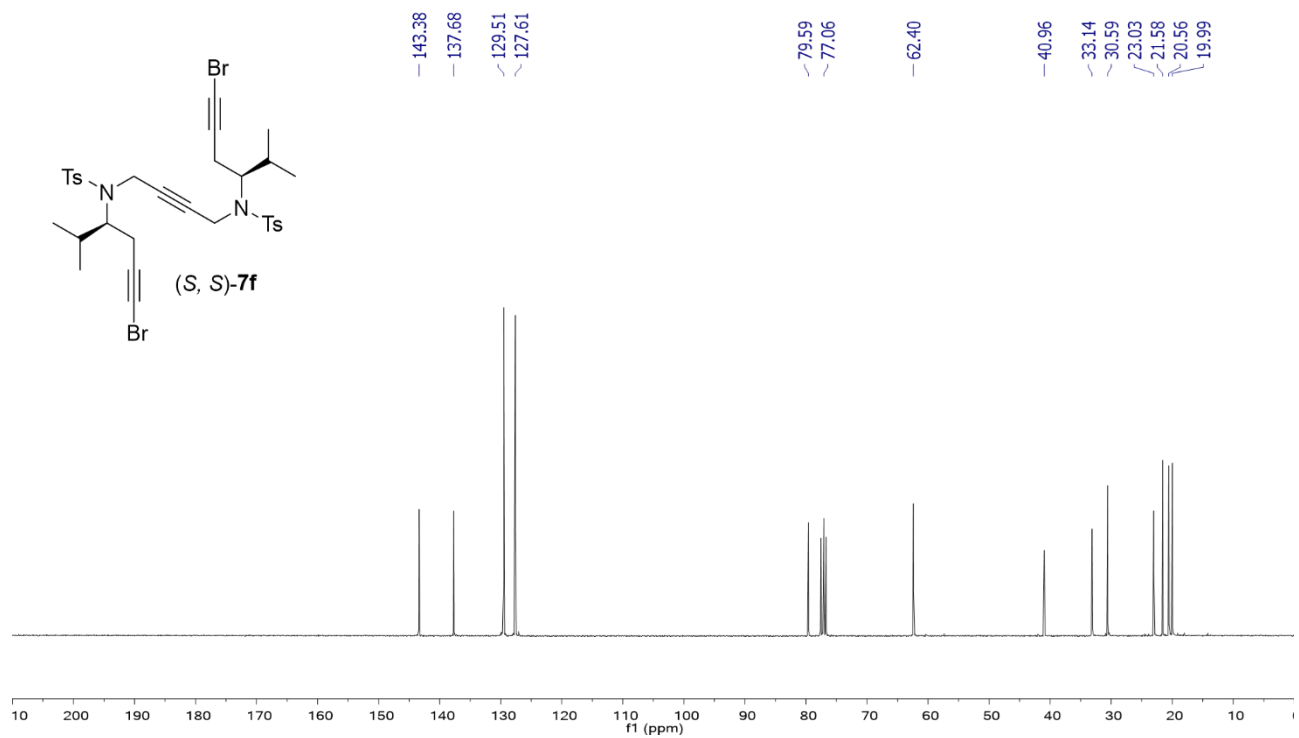
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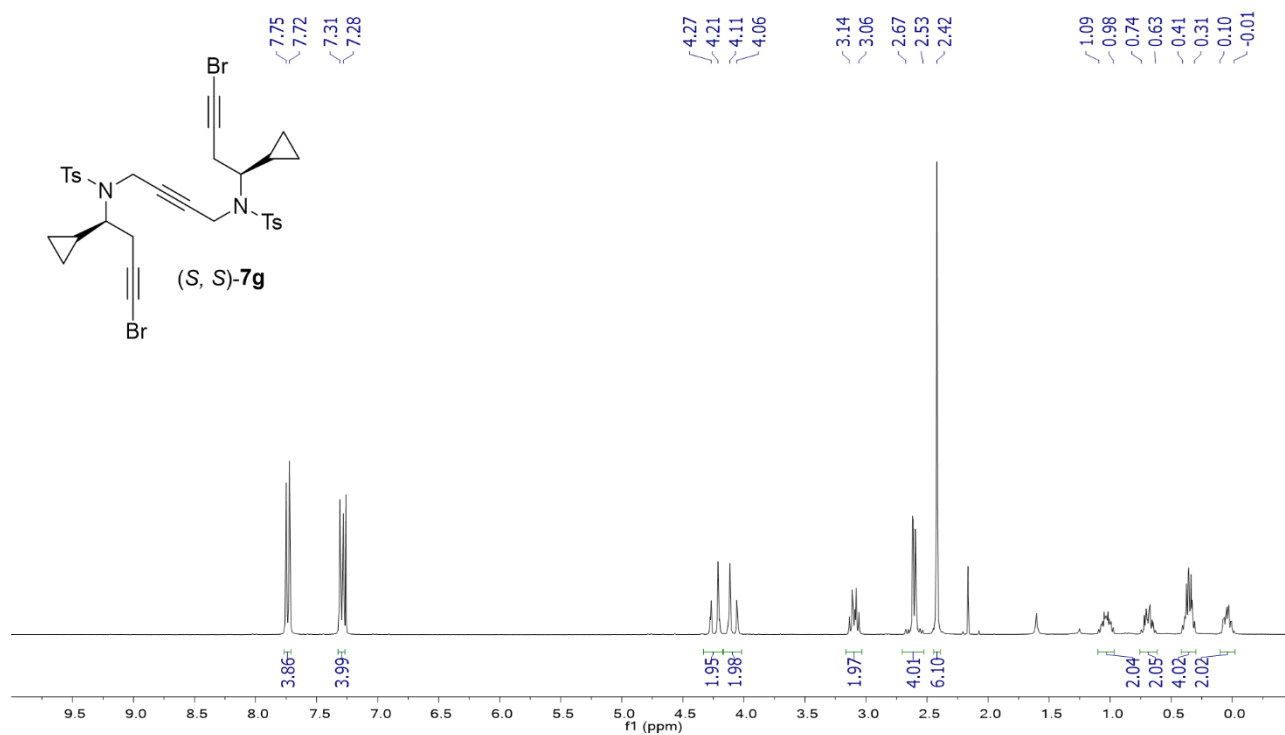
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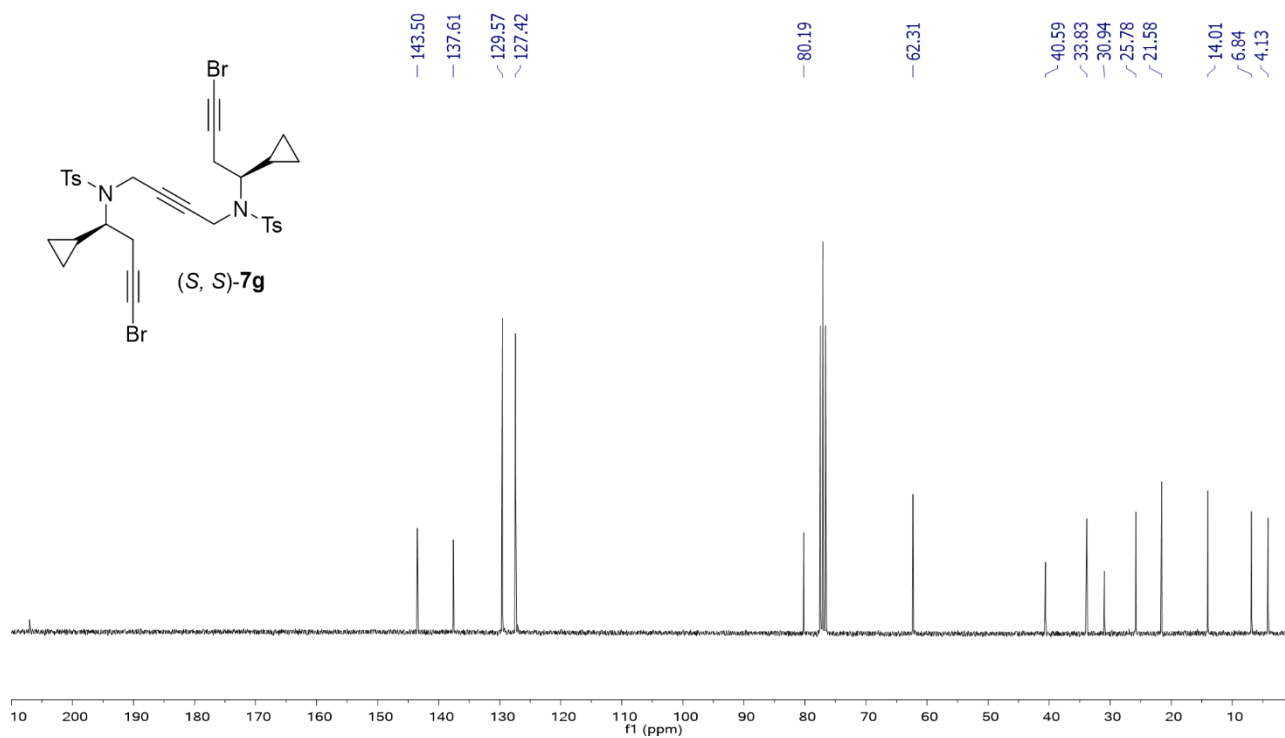
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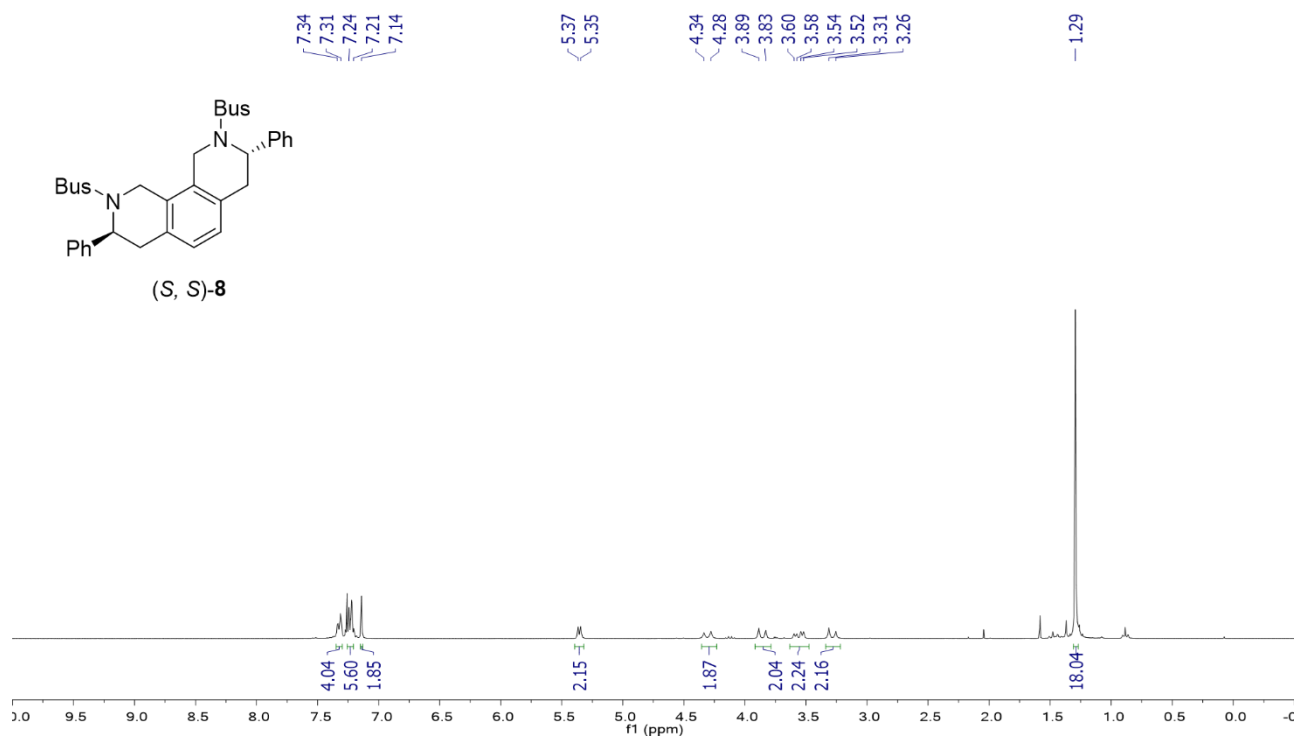
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**7g** (300 MHz,  $\text{CDCl}_3$ )



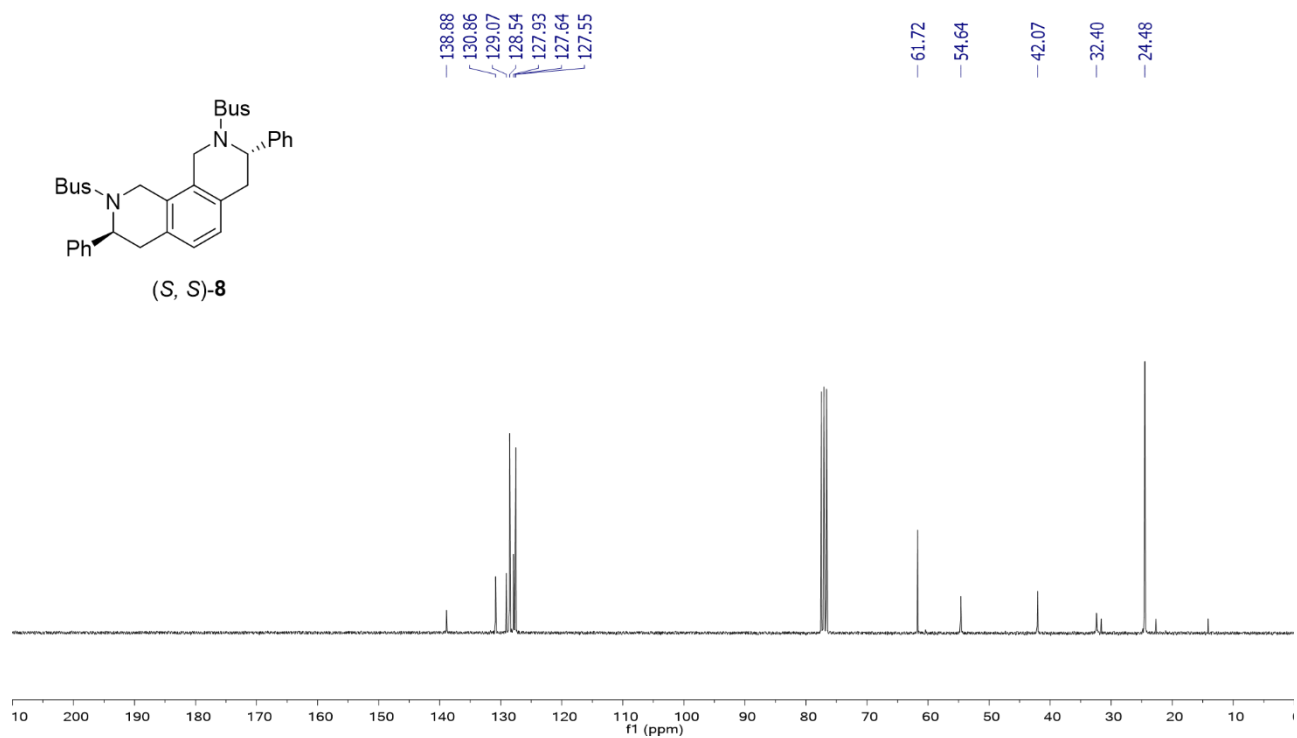
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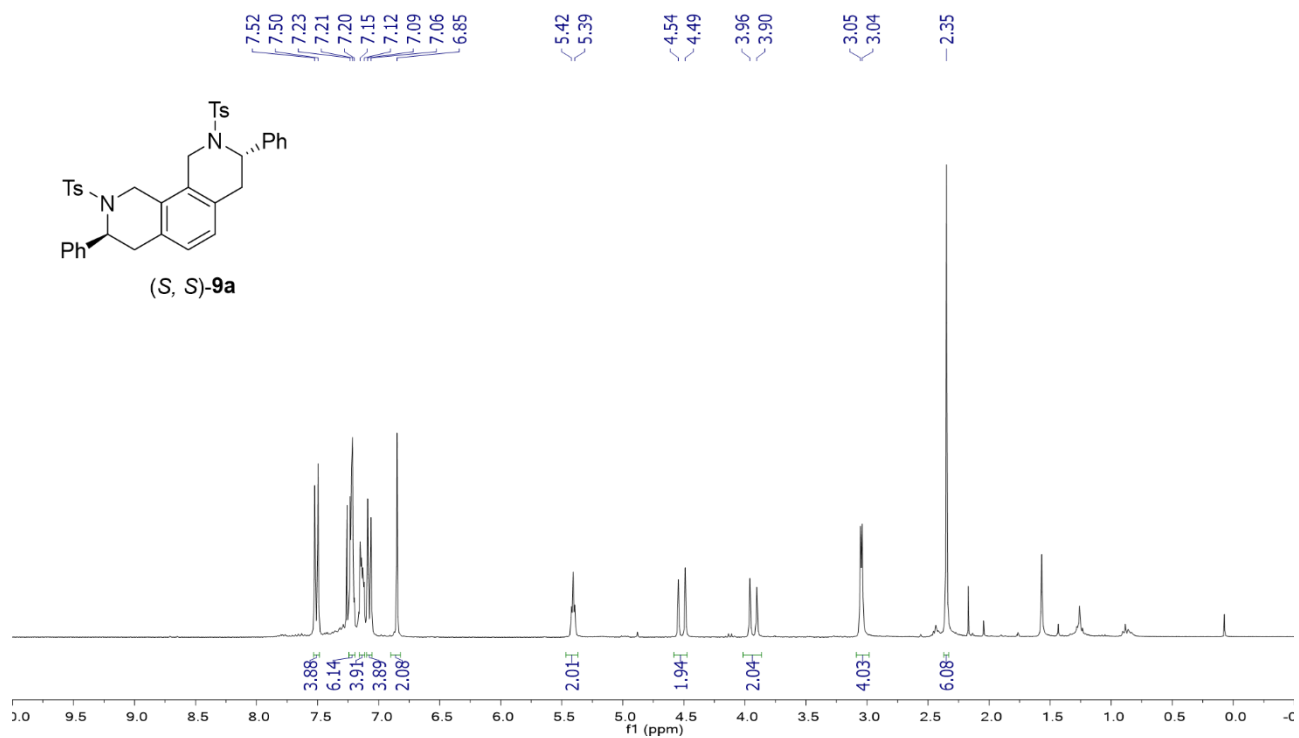
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**8** (300 MHz,  $\text{CDCl}_3$ )



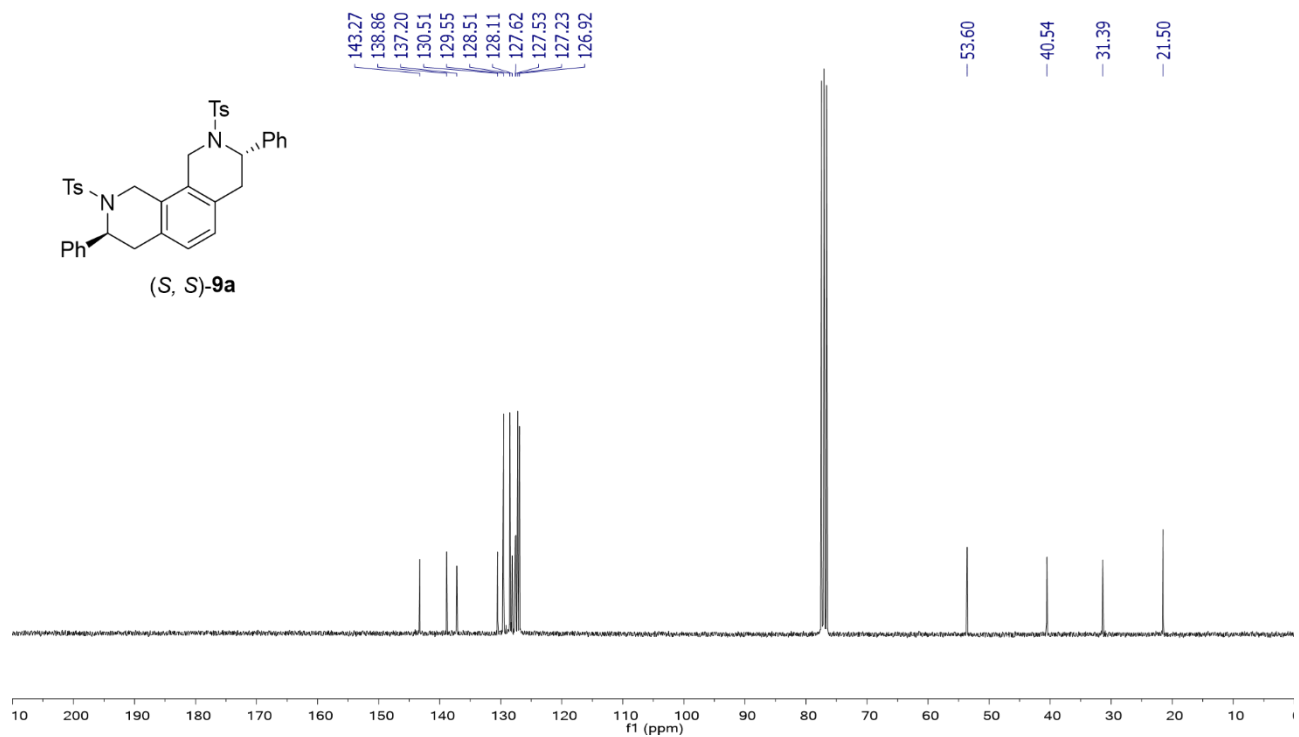
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**8** (75 MHz,  $\text{CDCl}_3$ )



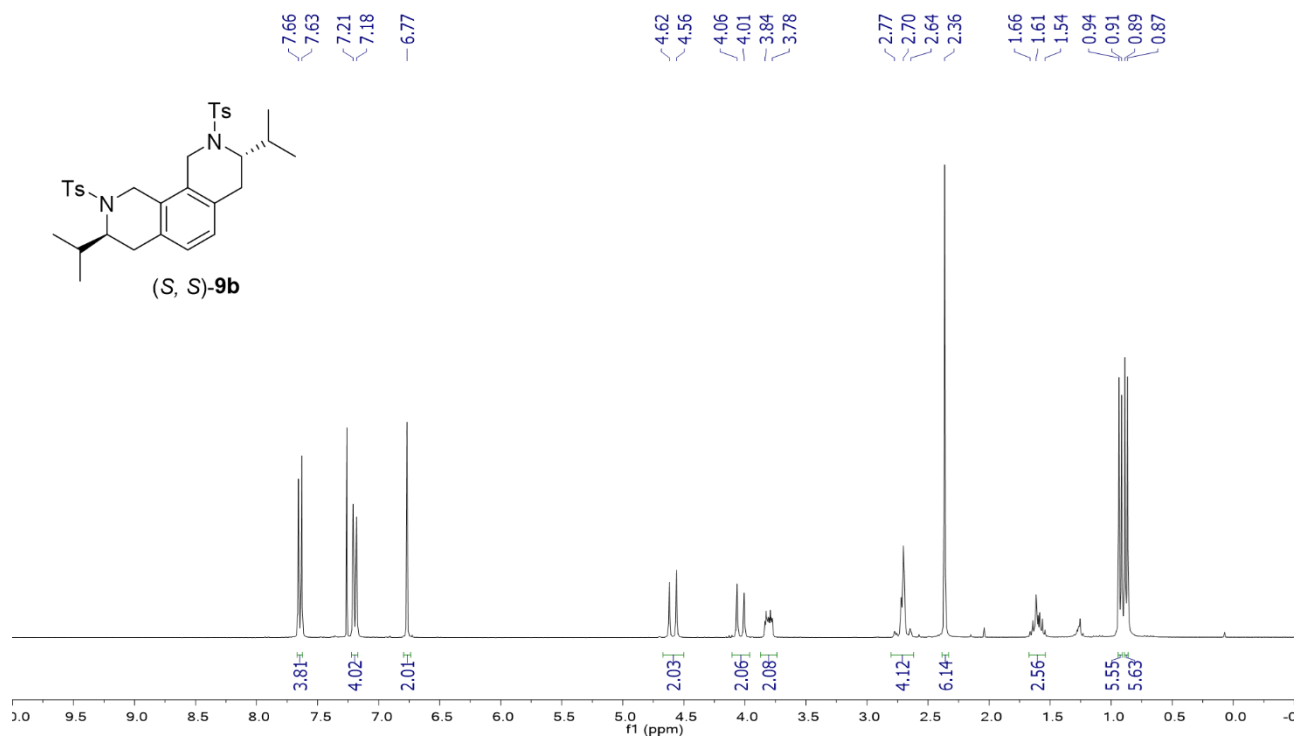
<sup>1</sup>H NMR spectrum of compound (*S,S*)-**9a** (300 MHz, CDCl<sub>3</sub>)



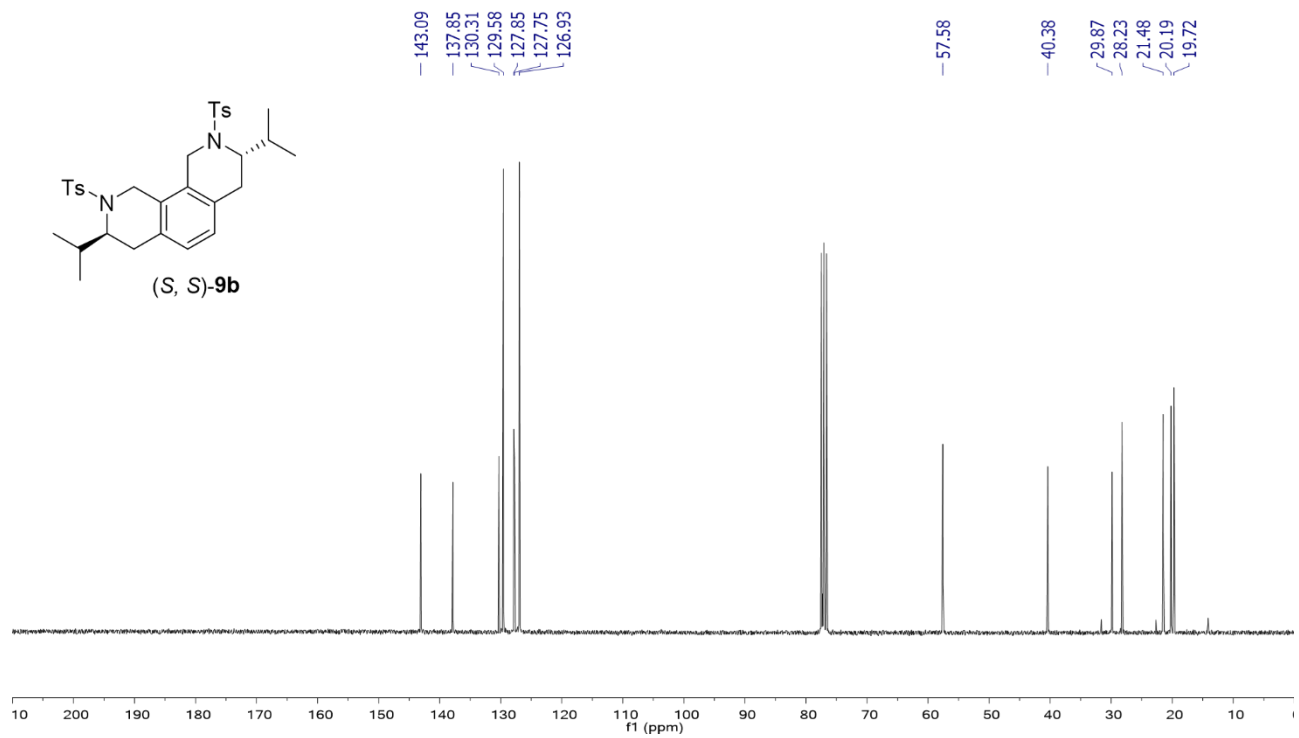
<sup>13</sup>C NMR spectrum of compound (*S,S*)-**9a** (75 MHz, CDCl<sub>3</sub>)



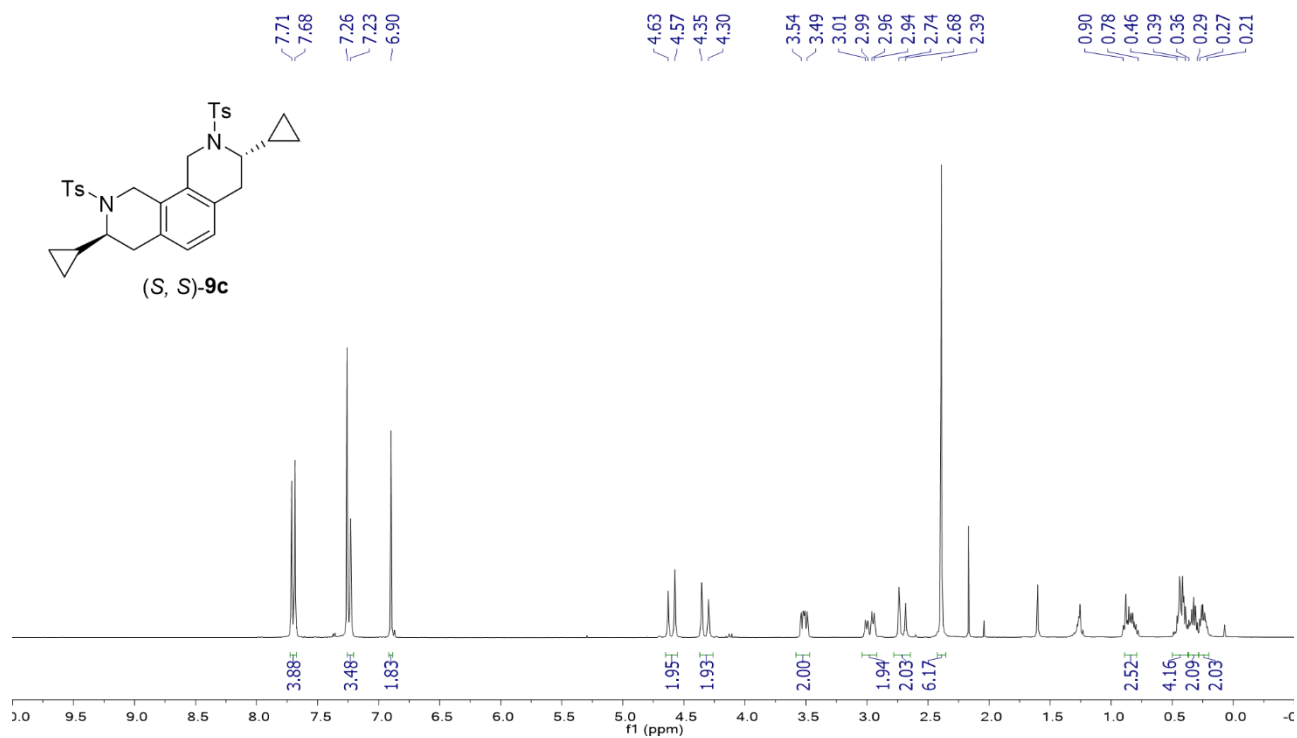
<sup>1</sup>H NMR spectrum of compound (S,S)-**9b** (300 MHz, CDCl<sub>3</sub>)



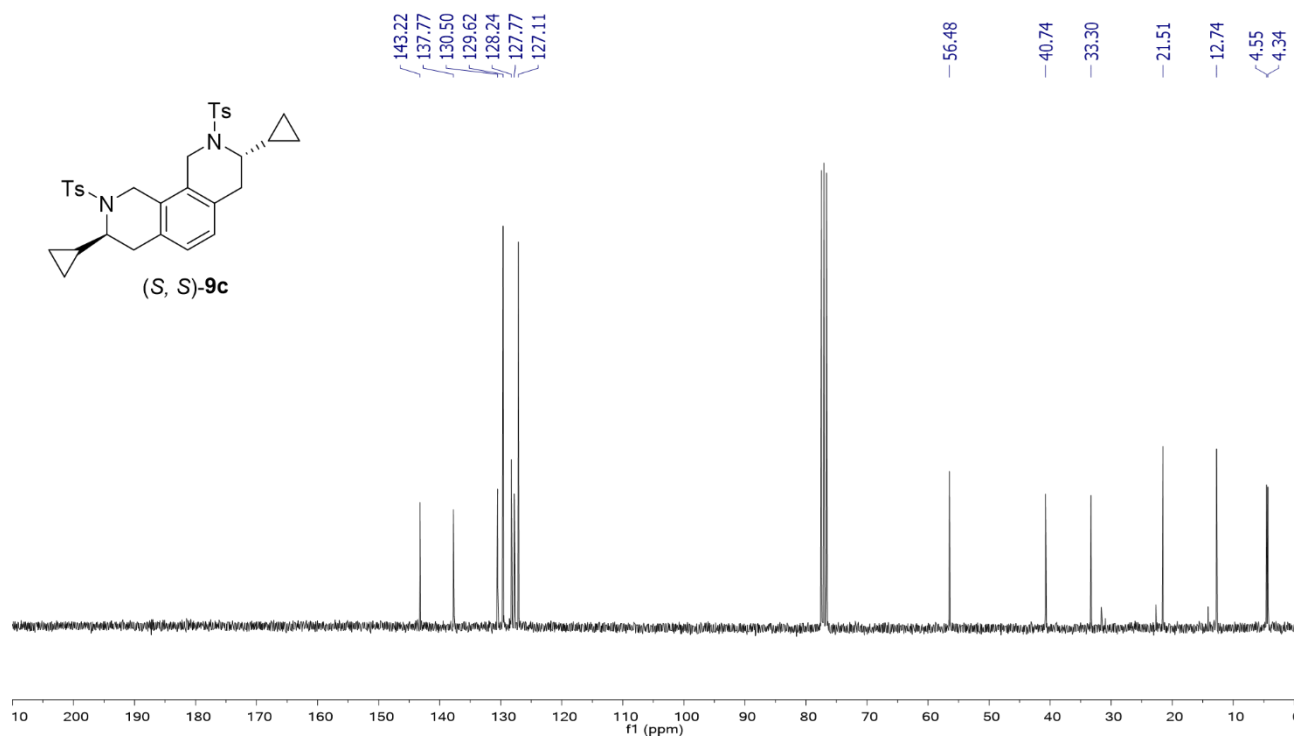
<sup>13</sup>C NMR spectrum of compound (S,S)-**9b** (75 MHz, CDCl<sub>3</sub>)



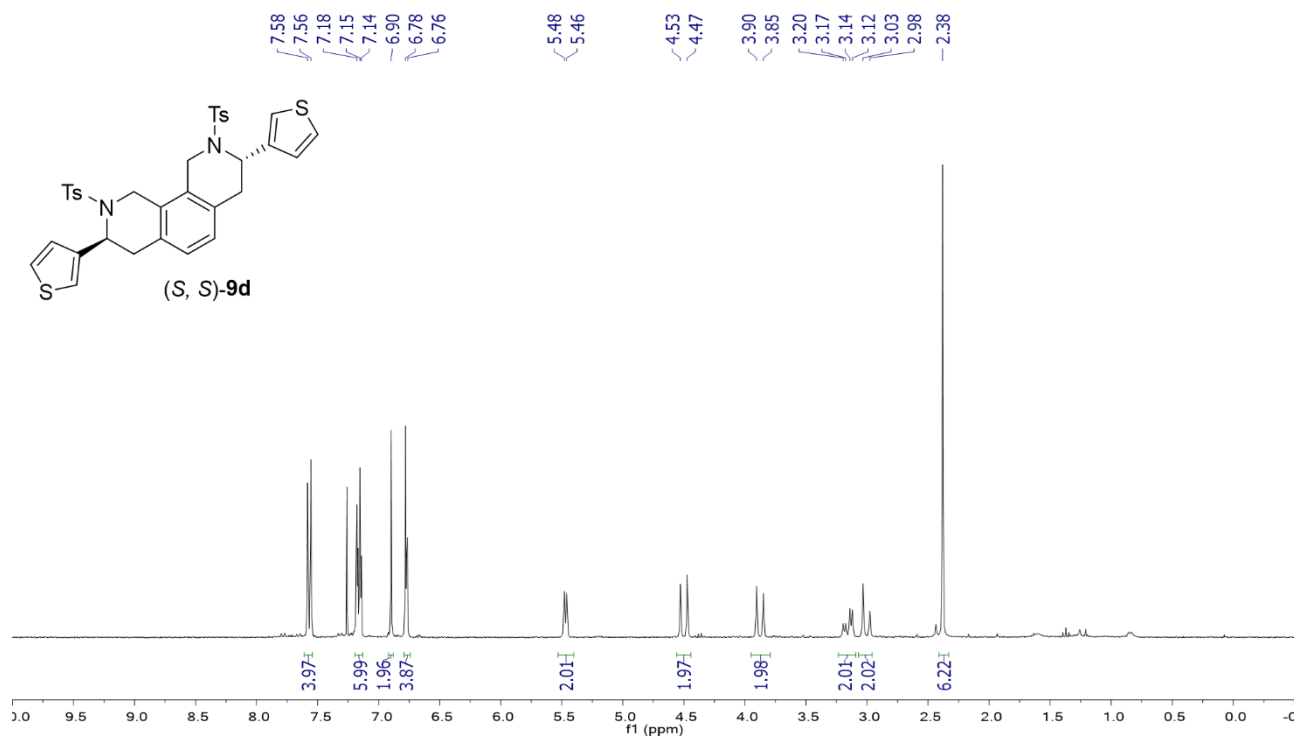
<sup>1</sup>H NMR spectrum of compound (S,S)-9c (300 MHz, CDCl<sub>3</sub>)



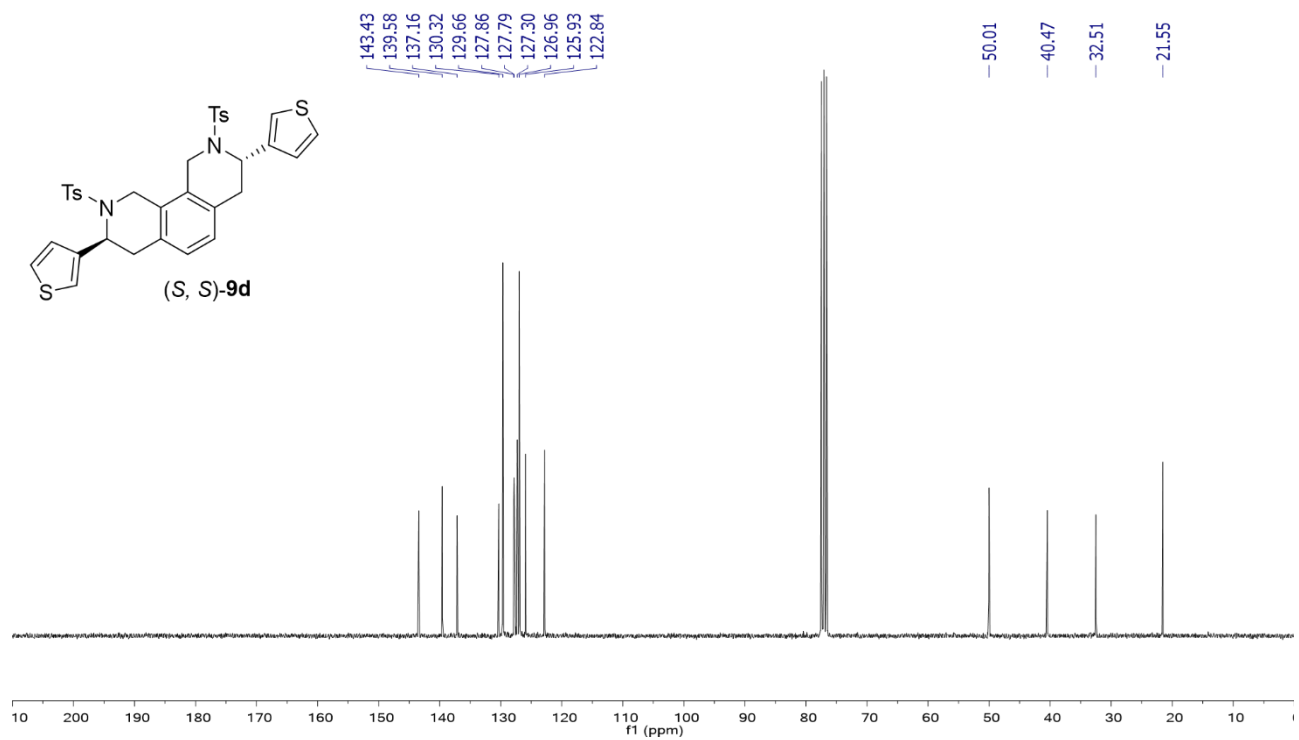
<sup>13</sup>C NMR spectrum of compound (S,S)-9c (75 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR spectrum of compound (S,S)-9d (300 MHz, CDCl<sub>3</sub>)

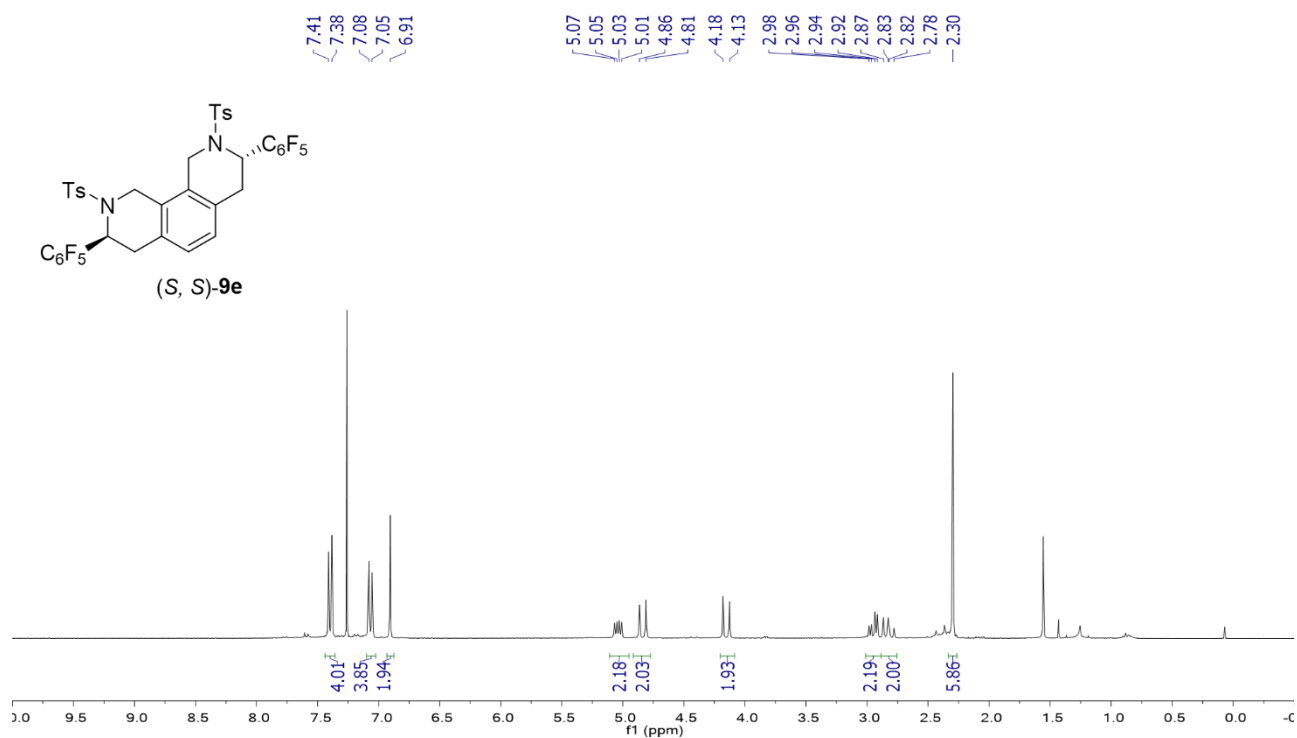


<sup>13</sup>C NMR spectrum of compound (S,S)-9d (75 MHz, CDCl<sub>3</sub>)

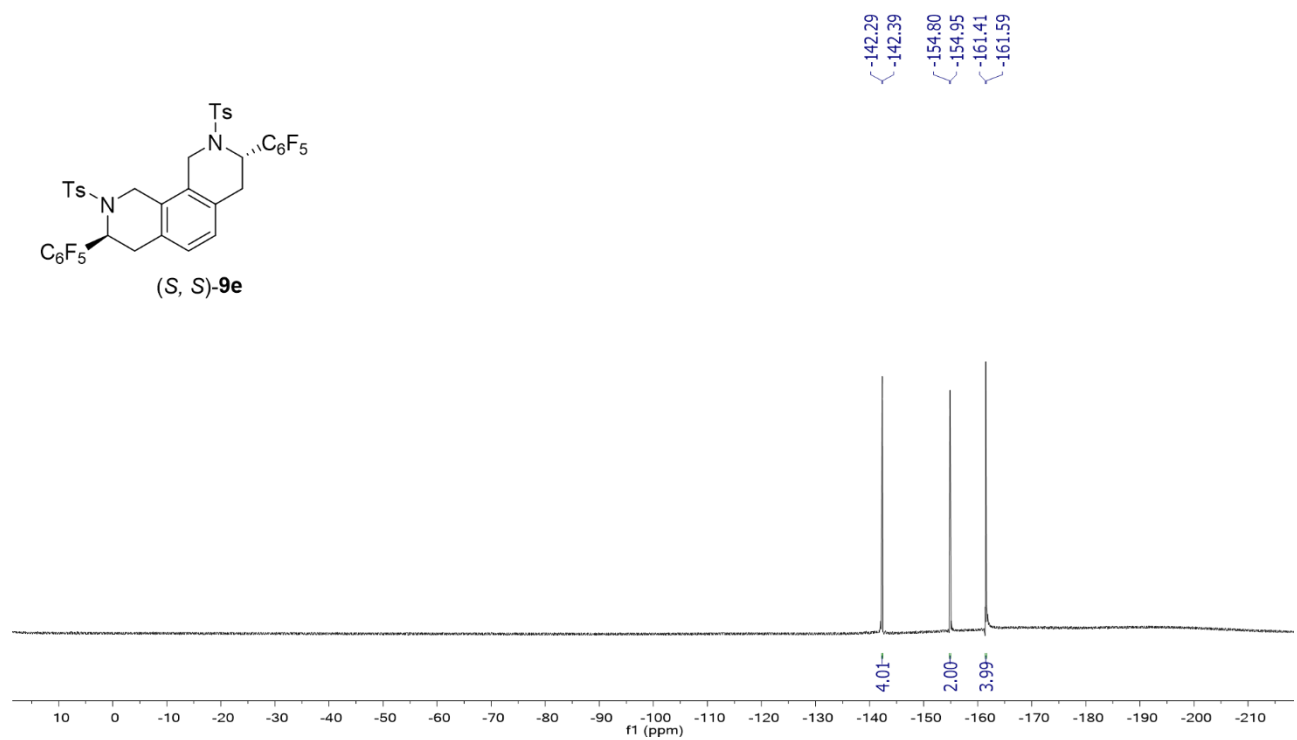




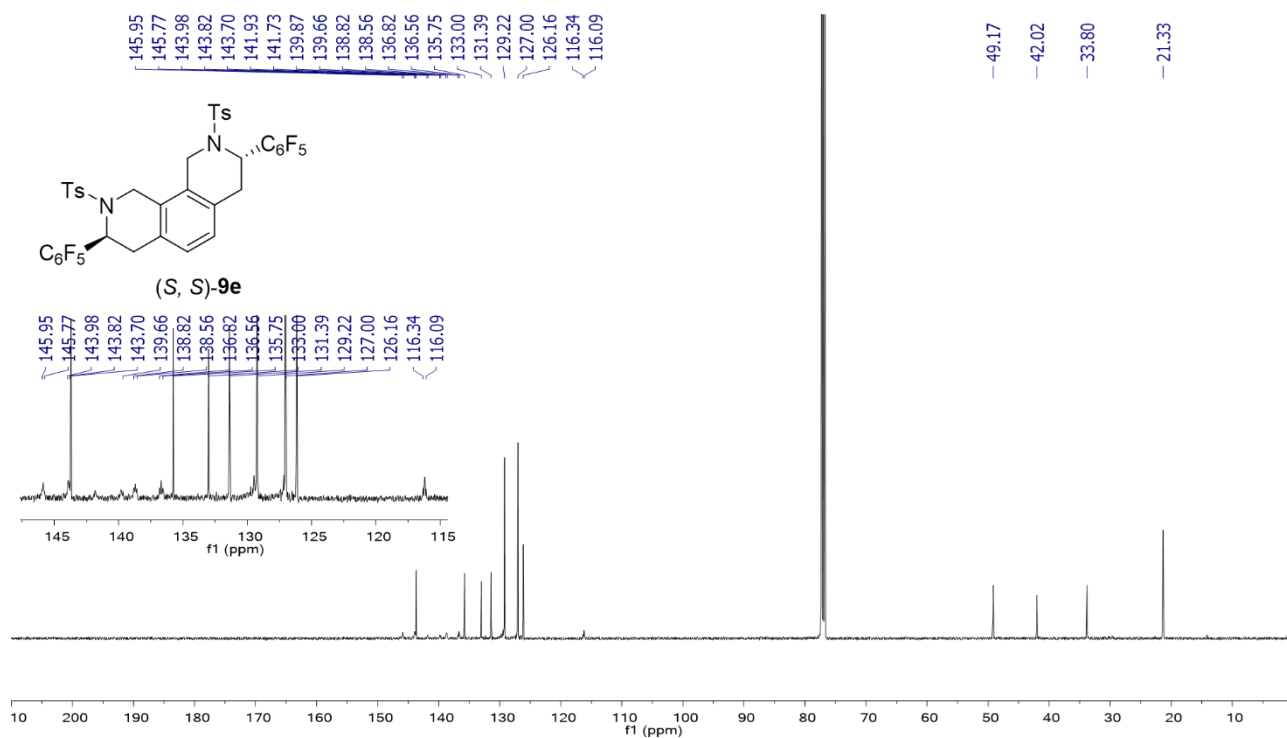
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**9e** (300 MHz,  $\text{CDCl}_3$ )



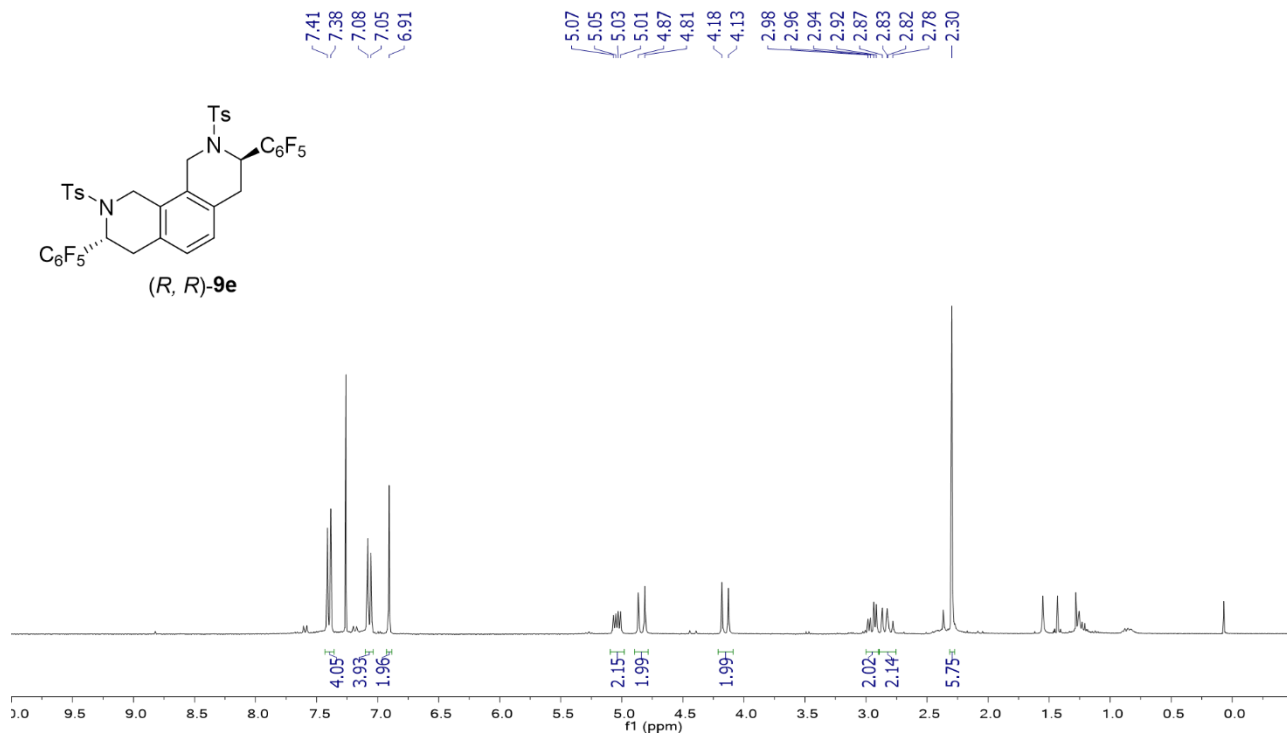
$^{19}\text{F}$  NMR spectrum of compound (*S,S*)-**9e** (282 MHz,  $\text{CDCl}_3$ )



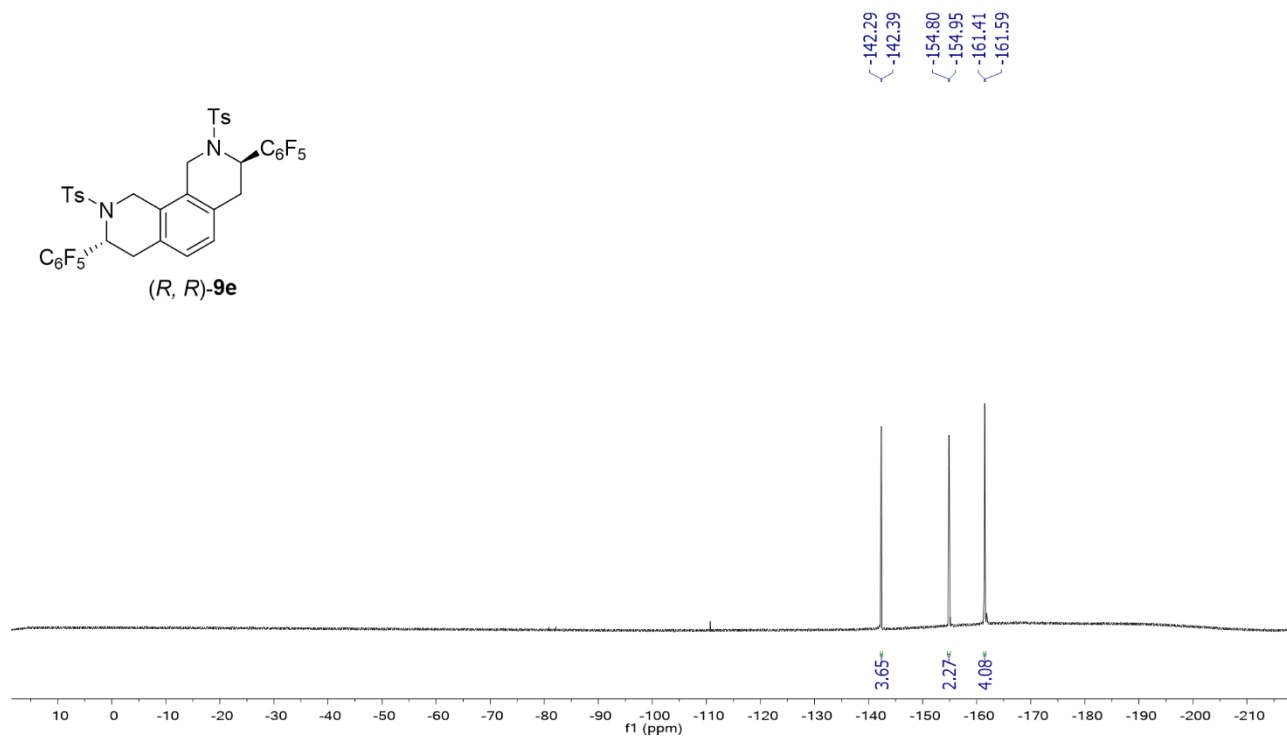
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**9e** (75 MHz,  $\text{CDCl}_3$ )



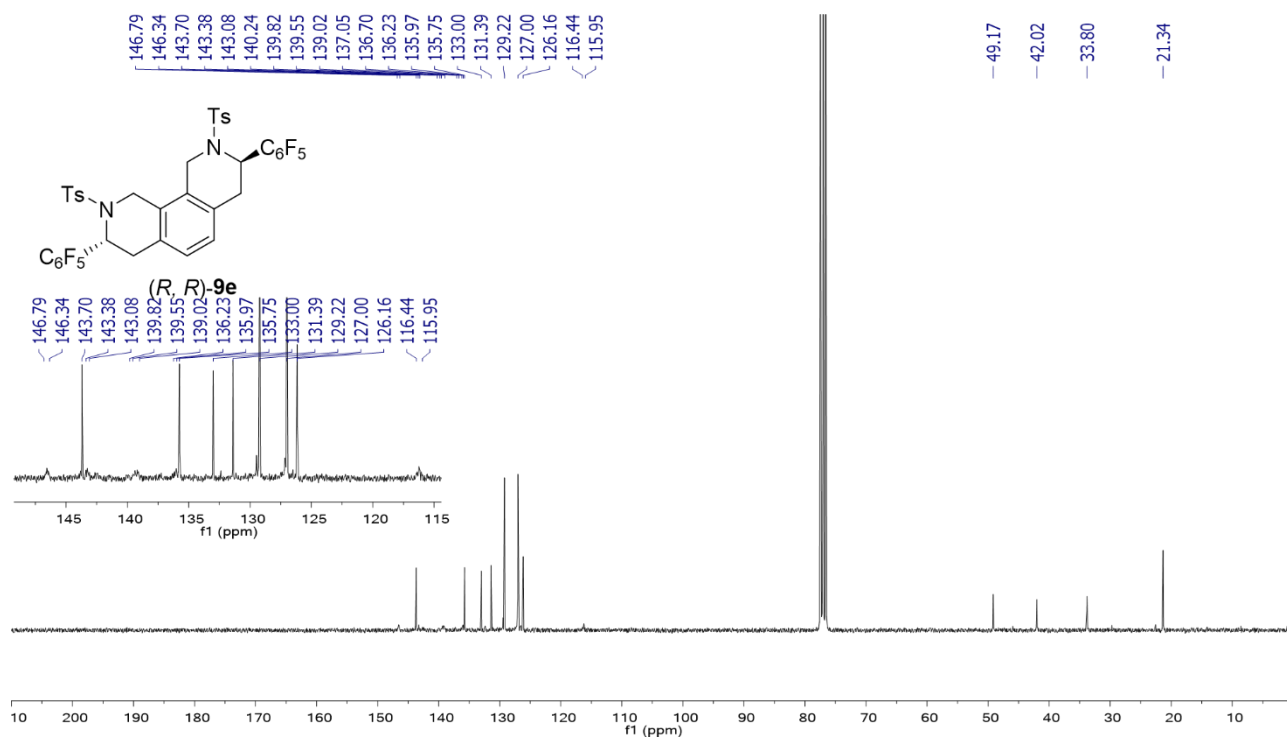
$^1\text{H}$  NMR spectrum of compound (*R,R*)-**9e** (300 MHz,  $\text{CDCl}_3$ )



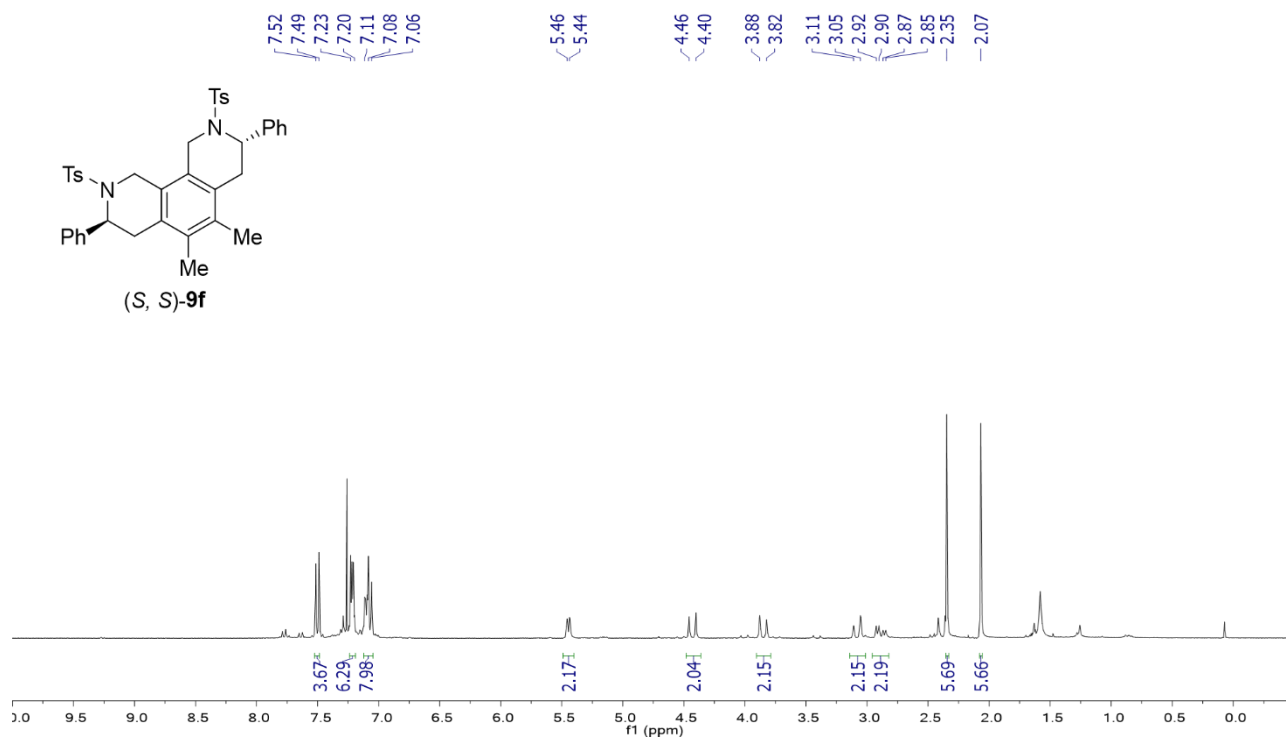
$^{19}\text{F}$  NMR spectrum of compound (*R,R*)-**9e** (282 MHz,  $\text{CDCl}_3$ )



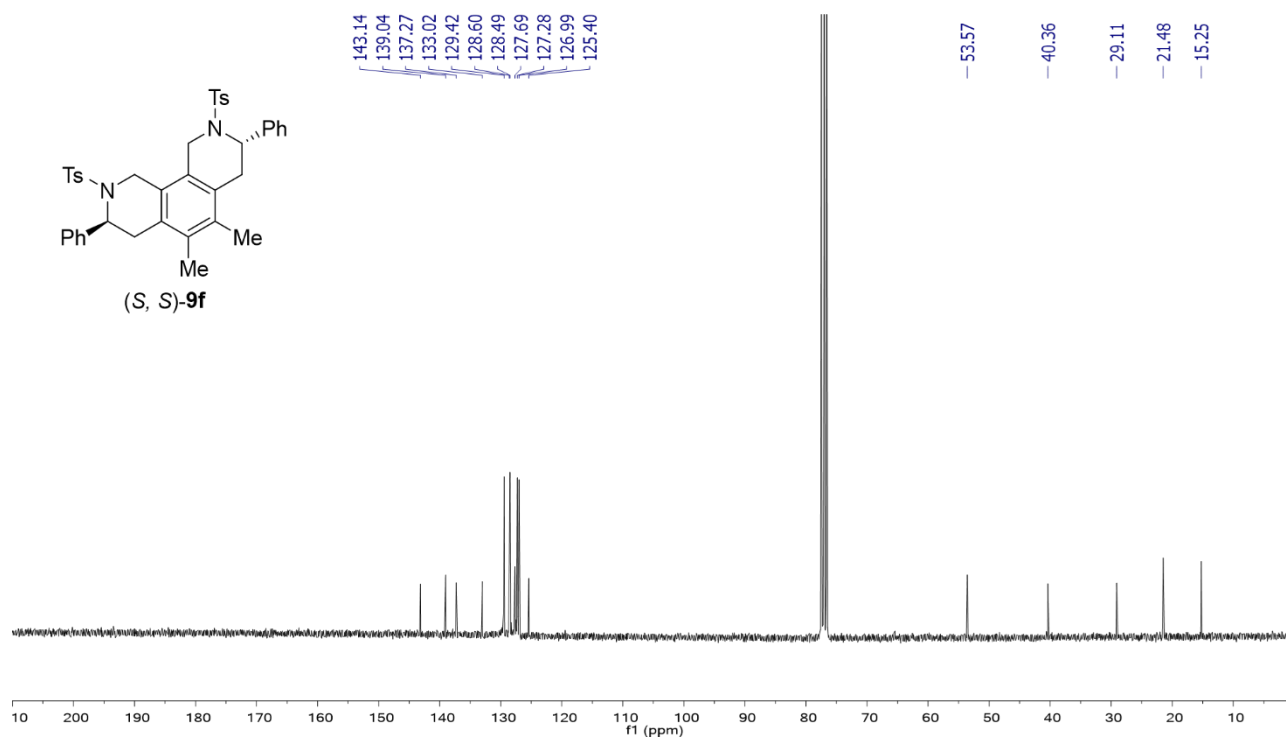
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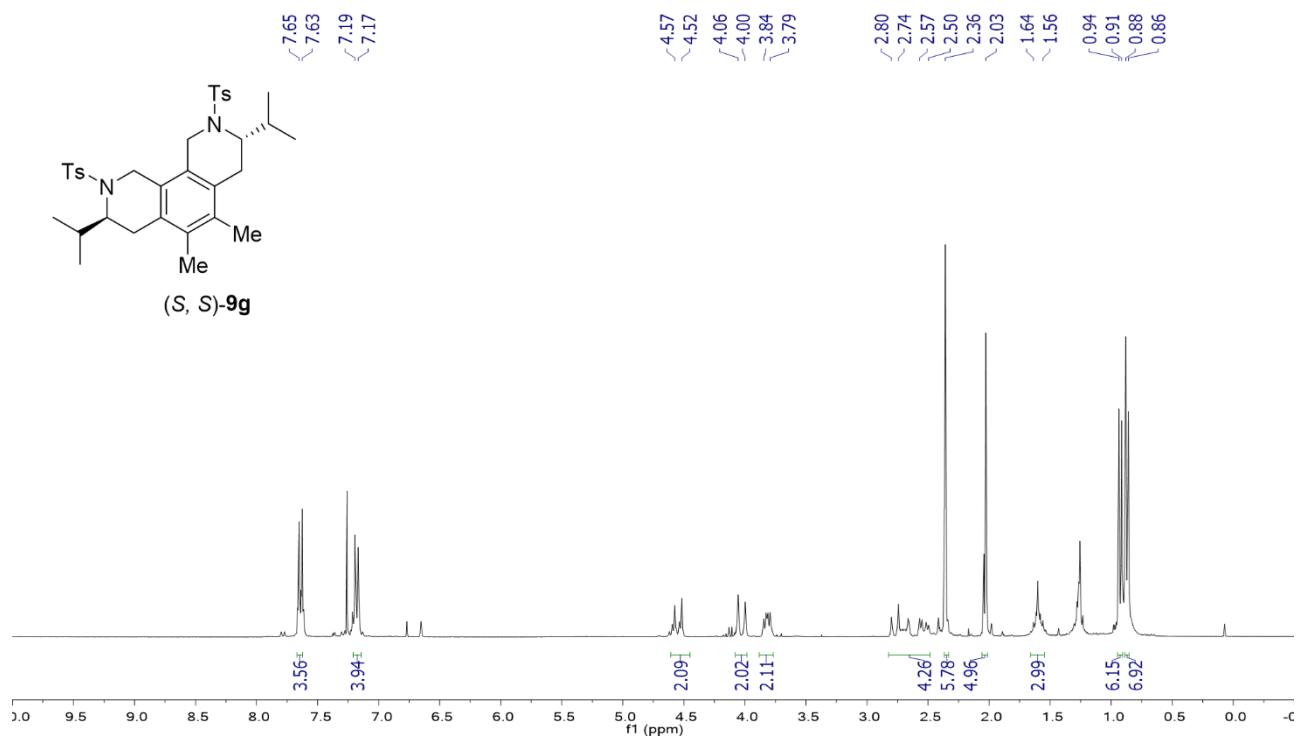
$^1\text{H}$  NMR spectrum of compound (*S,S*)-**9f** (300 MHz,  $\text{CDCl}_3$ )



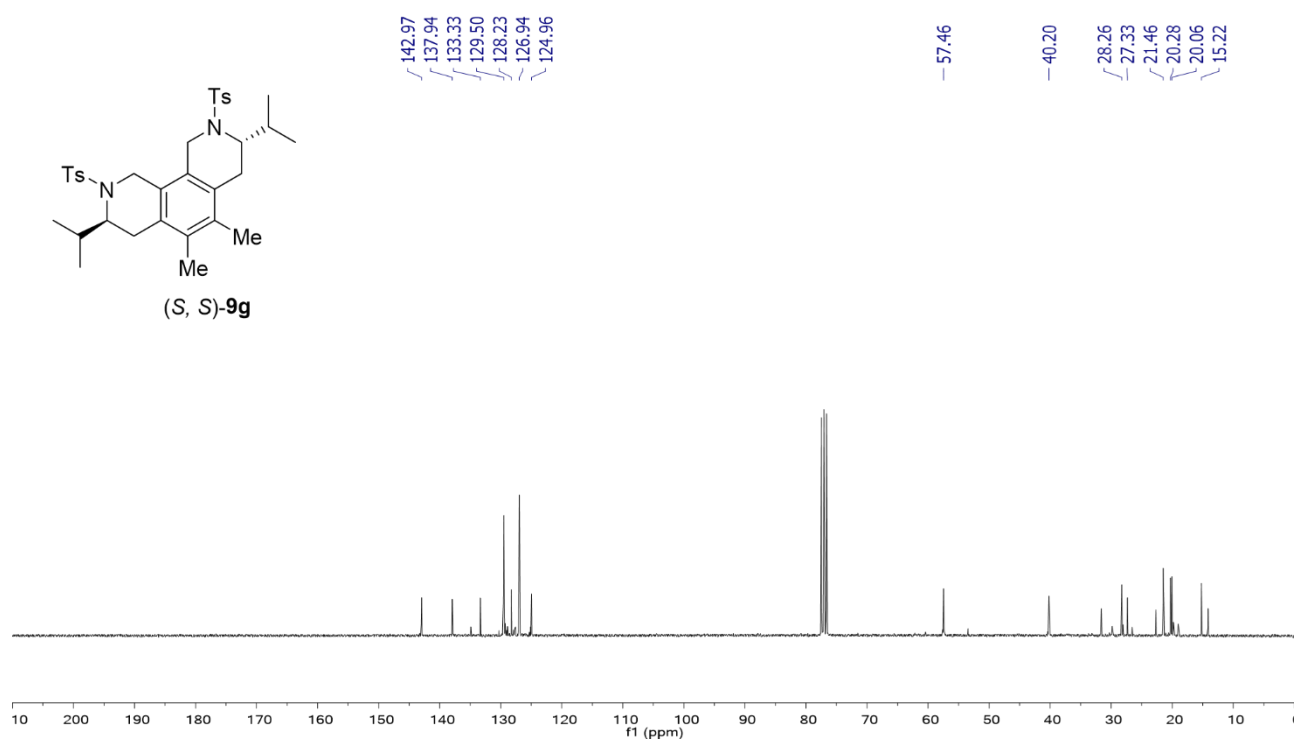
$^{13}\text{C}$  NMR spectrum of compound (*S,S*)-**9f** (75 MHz,  $\text{CDCl}_3$ )



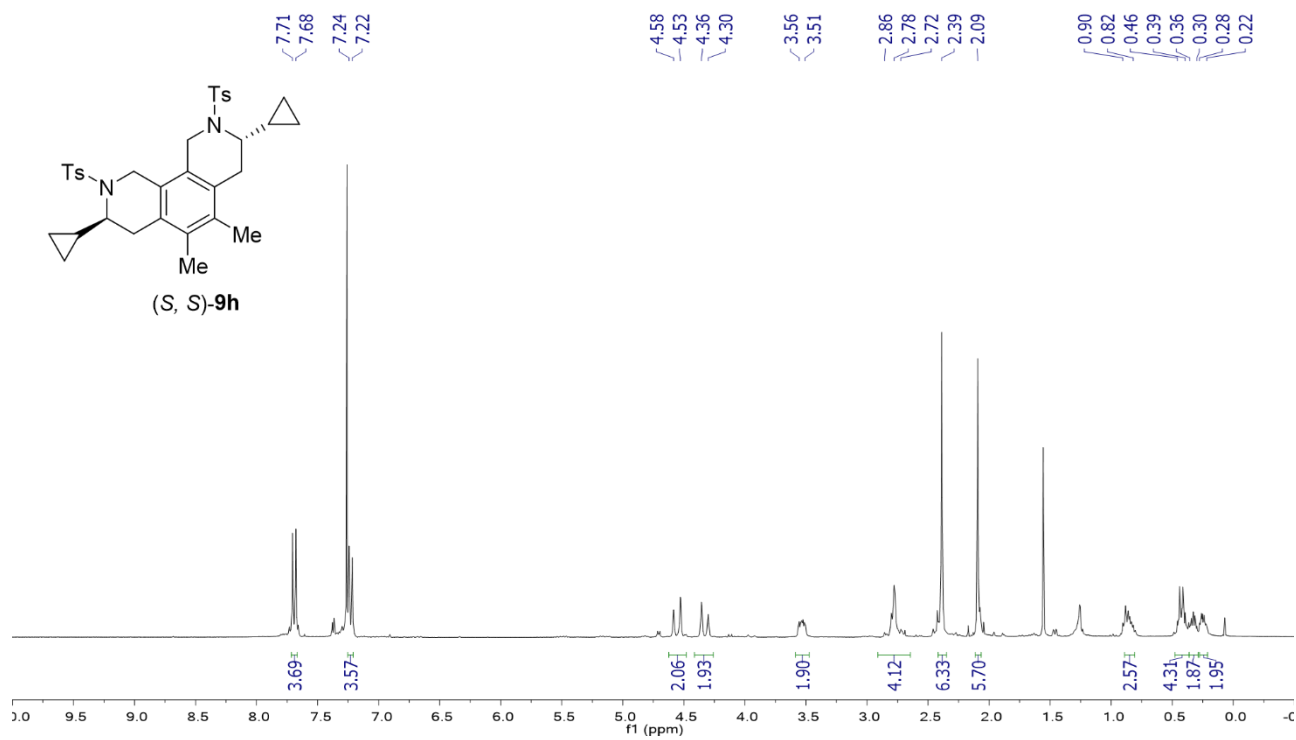
<sup>1</sup>H NMR spectrum of compound (S,S)-9g (300 MHz, CDCl<sub>3</sub>)



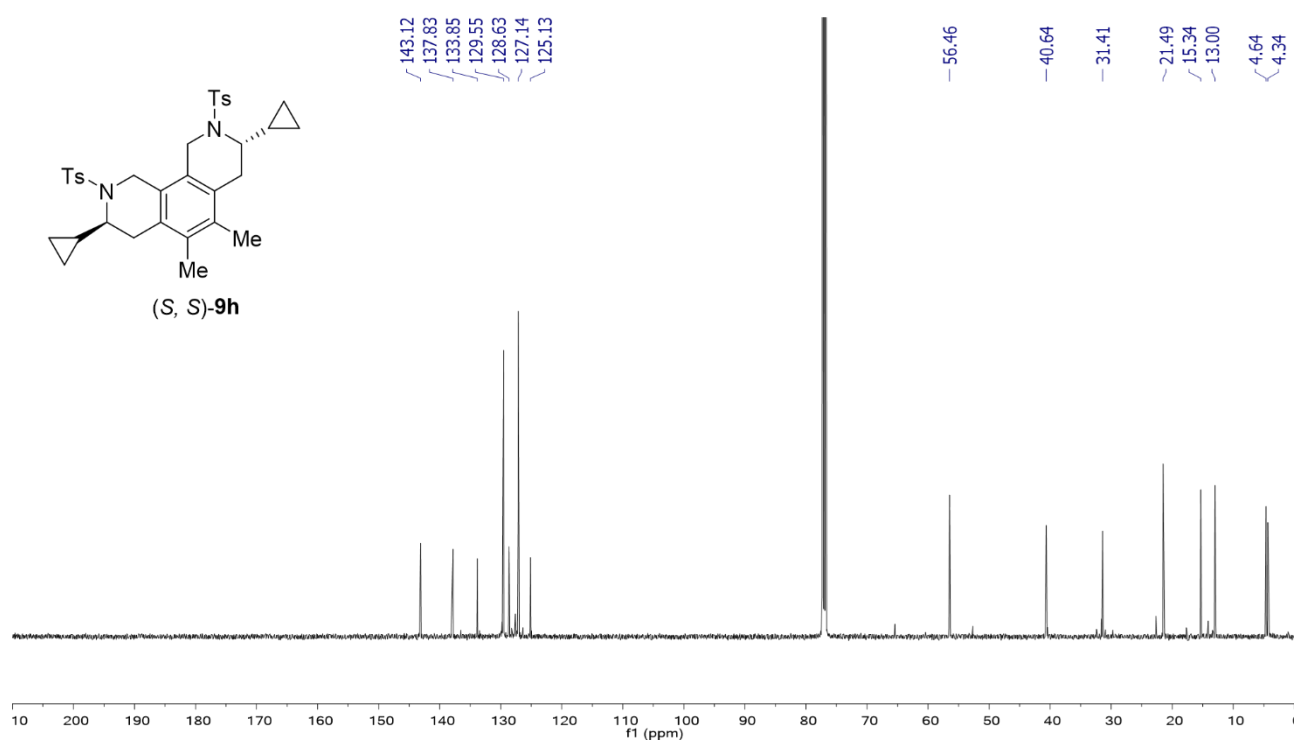
<sup>13</sup>C NMR spectrum of compound (S,S)-9g (75 MHz, CDCl<sub>3</sub>)



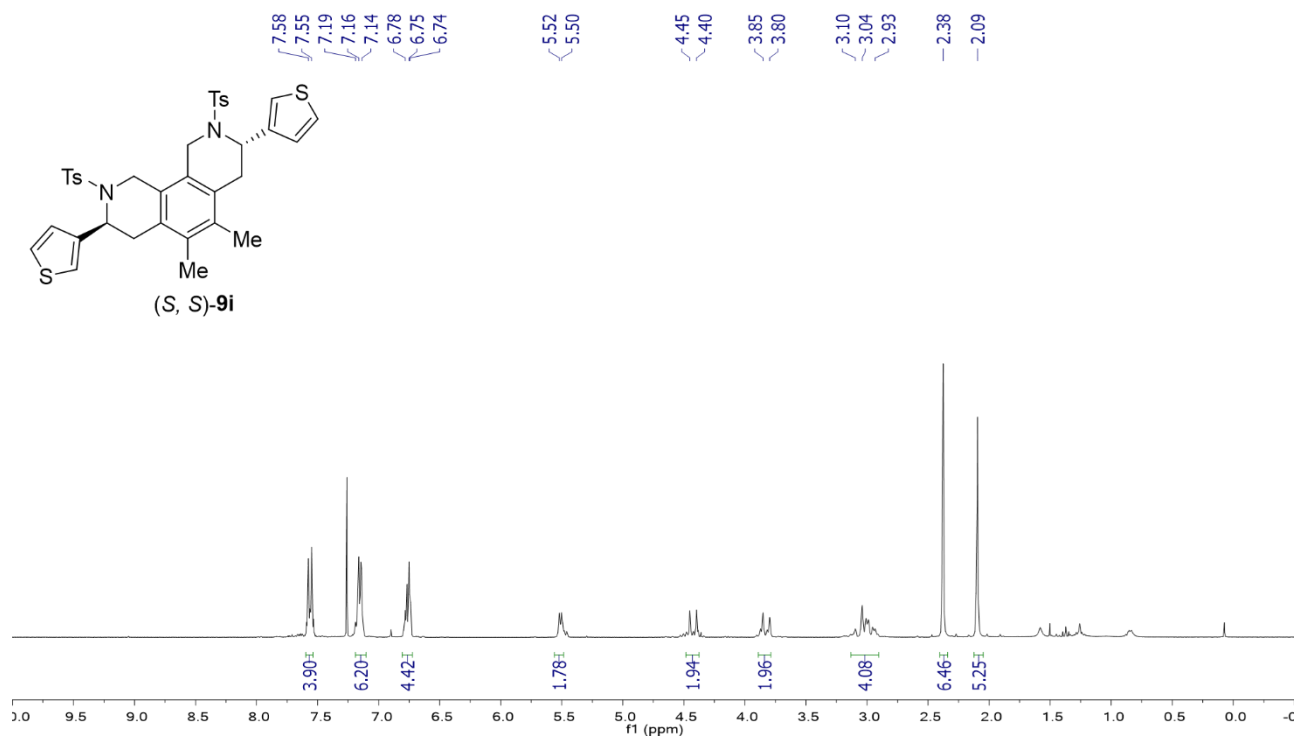
<sup>1</sup>H NMR spectrum of compound (S,S)-9h (300 MHz, CDCl<sub>3</sub>)



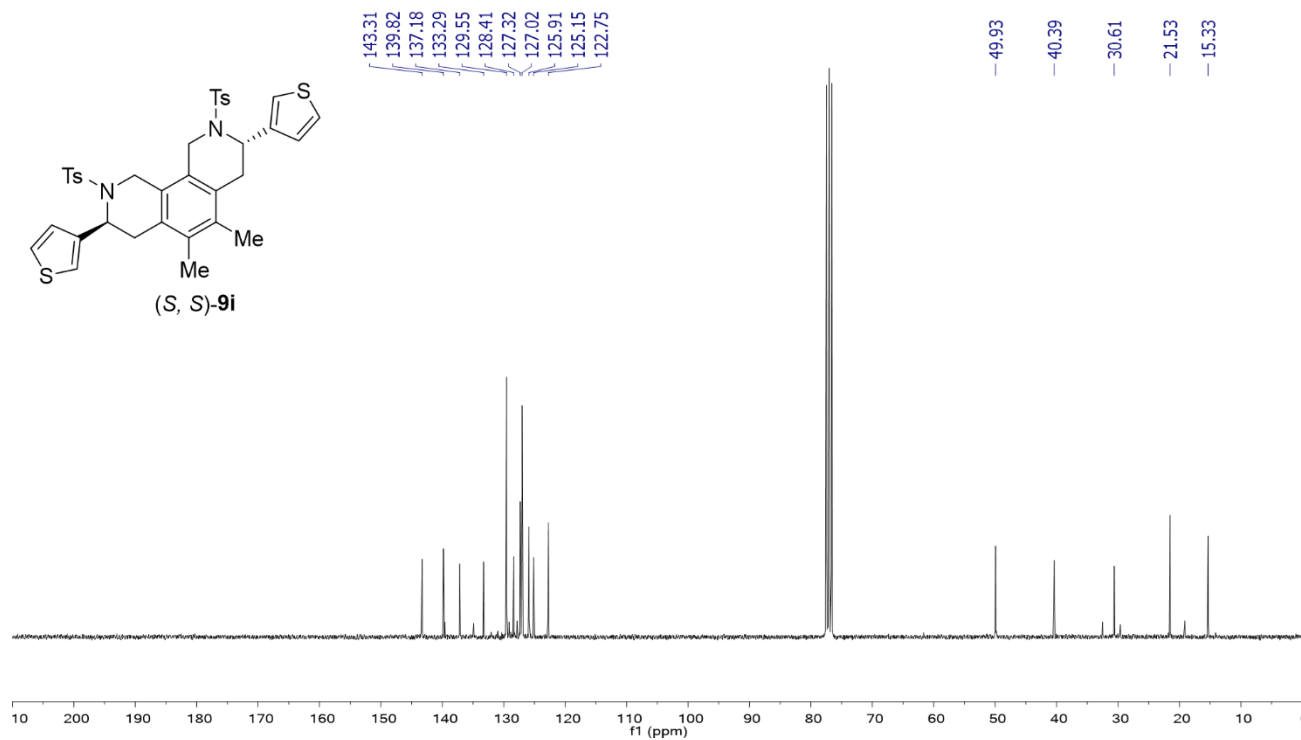
<sup>13</sup>C NMR spectrum of compound (S,S)-9h (75 MHz, CDCl<sub>3</sub>)



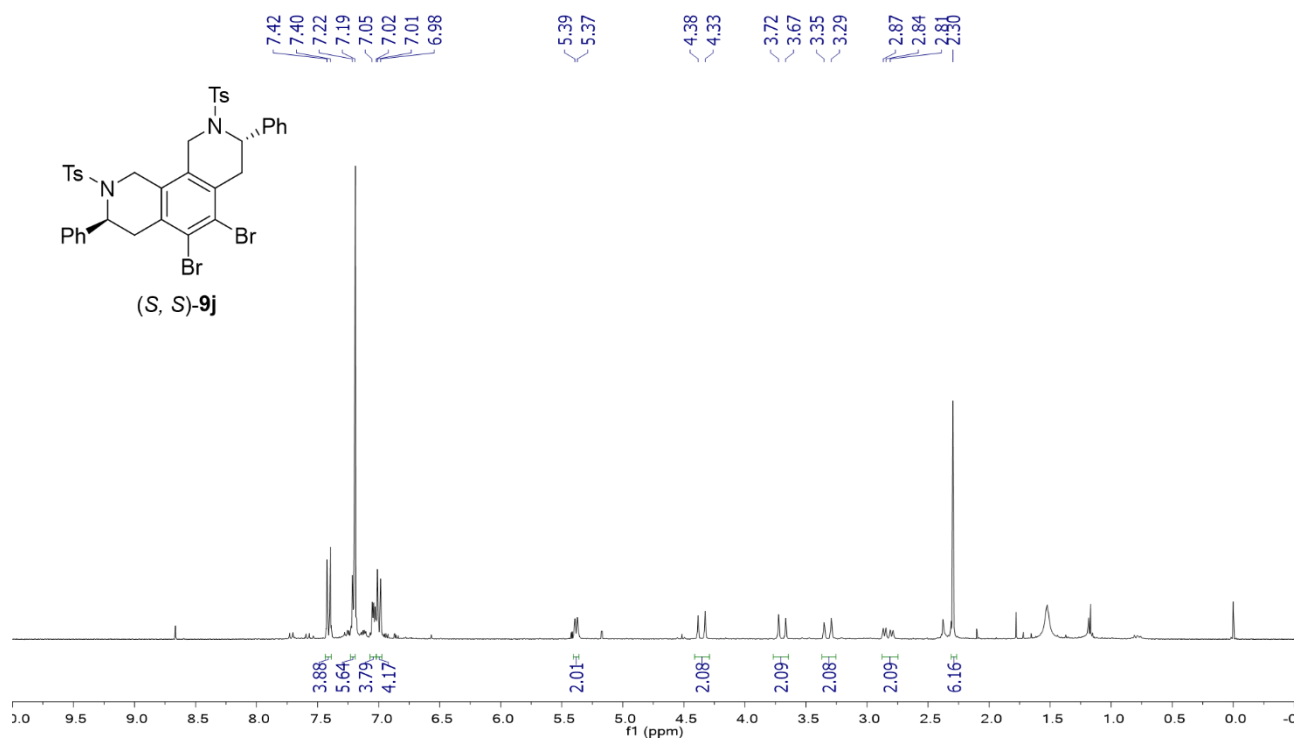
<sup>1</sup>H NMR spectrum of compound (S,S)-9i (300 MHz, CDCl<sub>3</sub>)



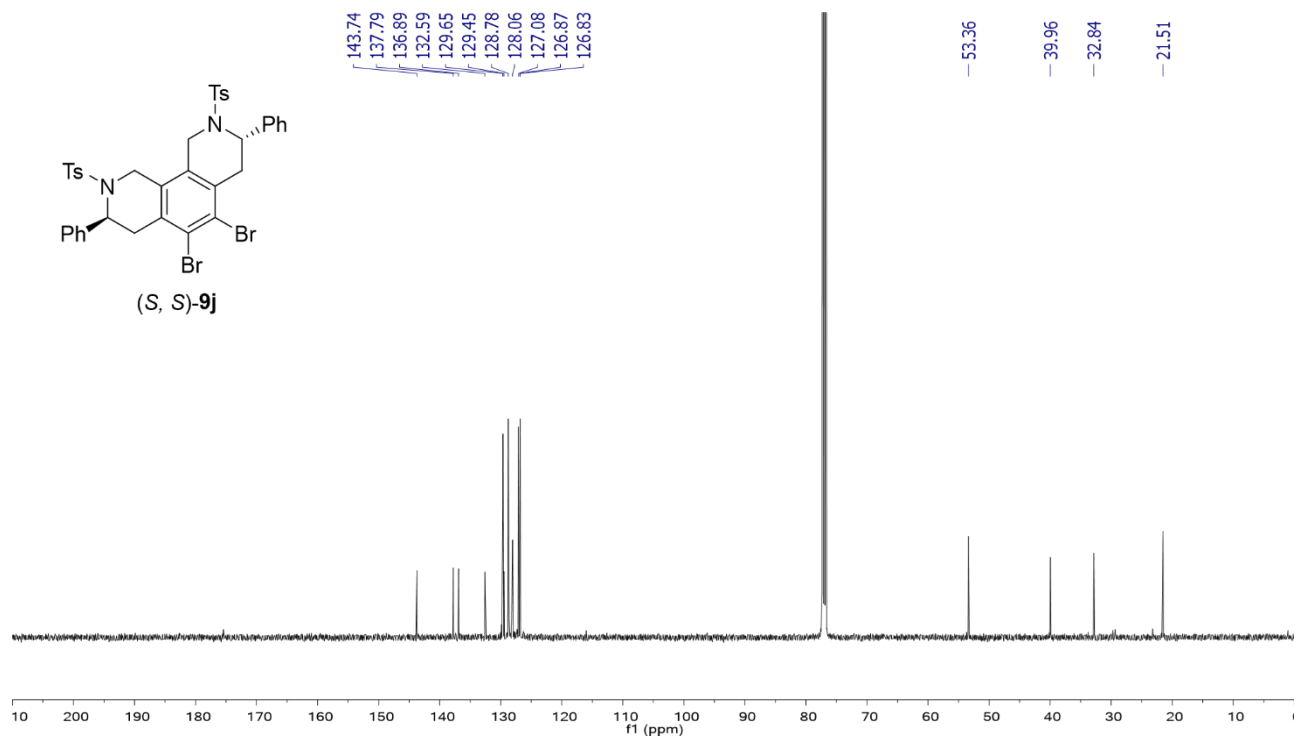
<sup>13</sup>C NMR spectrum of compound (S,S)-9i (75 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR spectrum of compound (*S,S*)-**9j** (300 MHz, CDCl<sub>3</sub>)

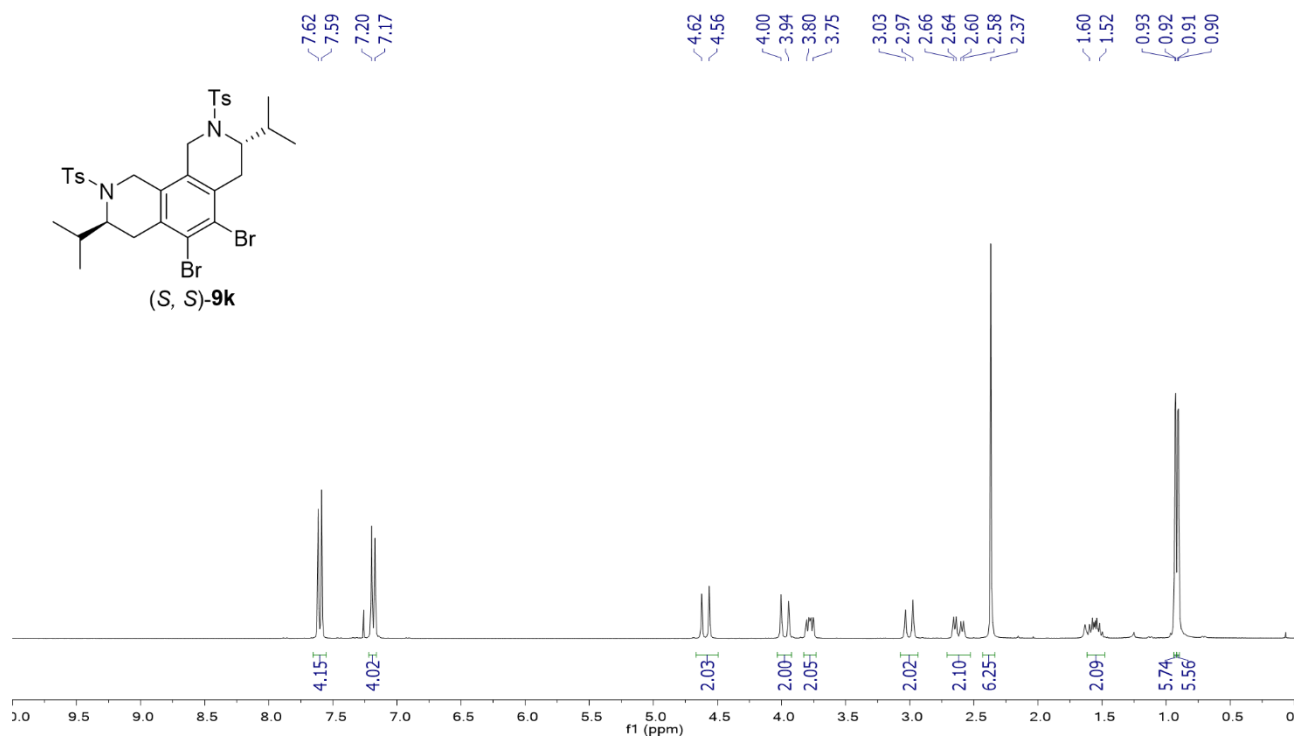


<sup>13</sup>C NMR spectrum of compound (*S,S*)-**9j** (75 MHz, CDCl<sub>3</sub>)

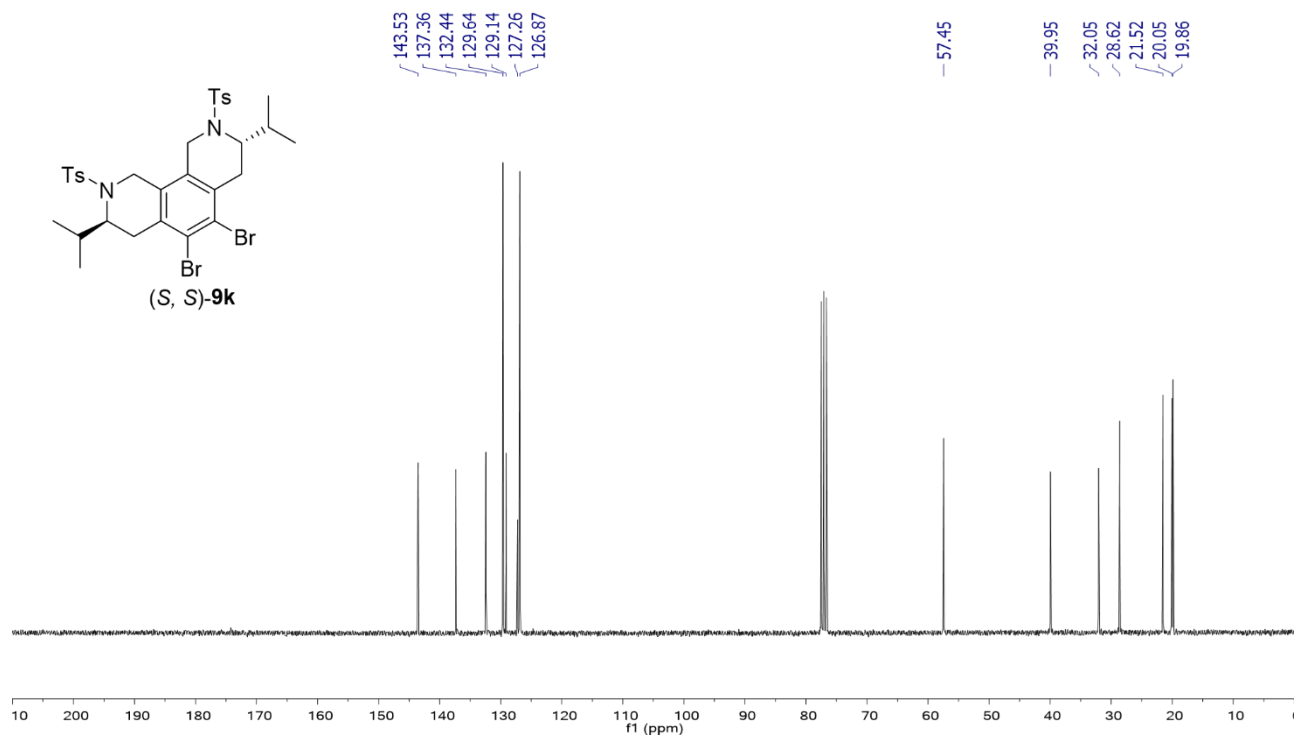




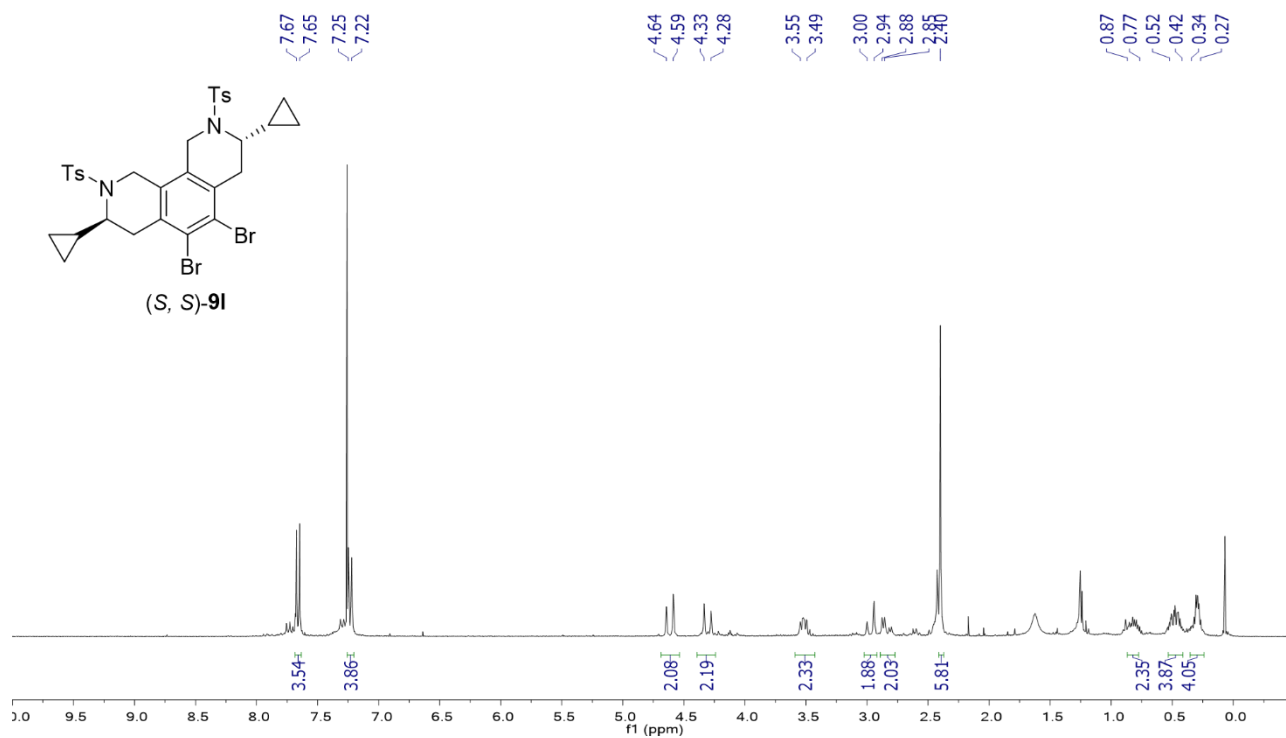
<sup>1</sup>H NMR spectrum of compound (S,S)-9k (300 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound (S,S)-9k (75 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR spectrum of compound (S,S)-9I (300 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound (S,S)-9I (75 MHz, CDCl<sub>3</sub>)

