Universitat de Girona

NEW CARBOCYCLISATIONS OF POLYUNSATURATED HYDRAZONES CATALYSED BY RHODIUM(I)

Supplementary data

Òscar Torres Antón

Figure S1: ^{1}H NMR spectrum (300 MHz) of **4a** in CDCl$_3$.
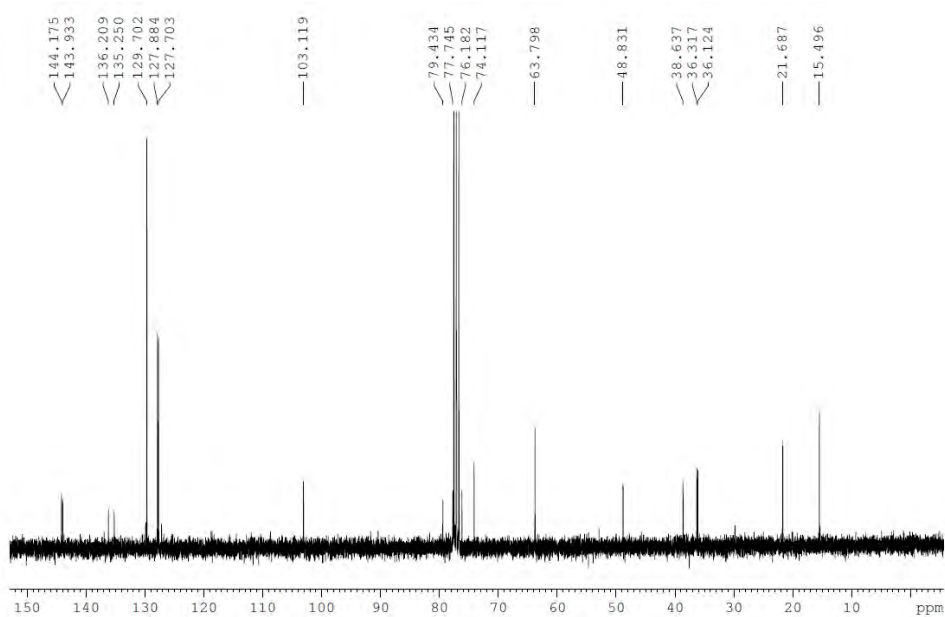
Figure S2: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **4a** in CDCl$_3$.
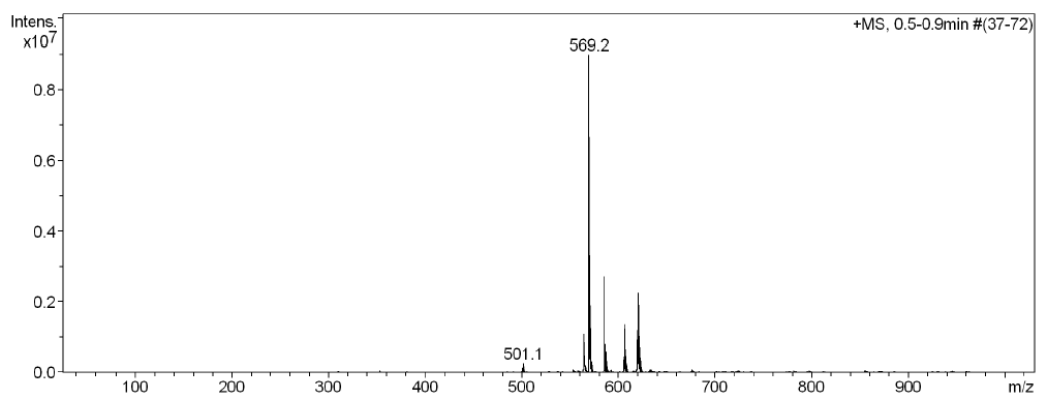
Figure S3: ESI-MS spectrum of **4a**.
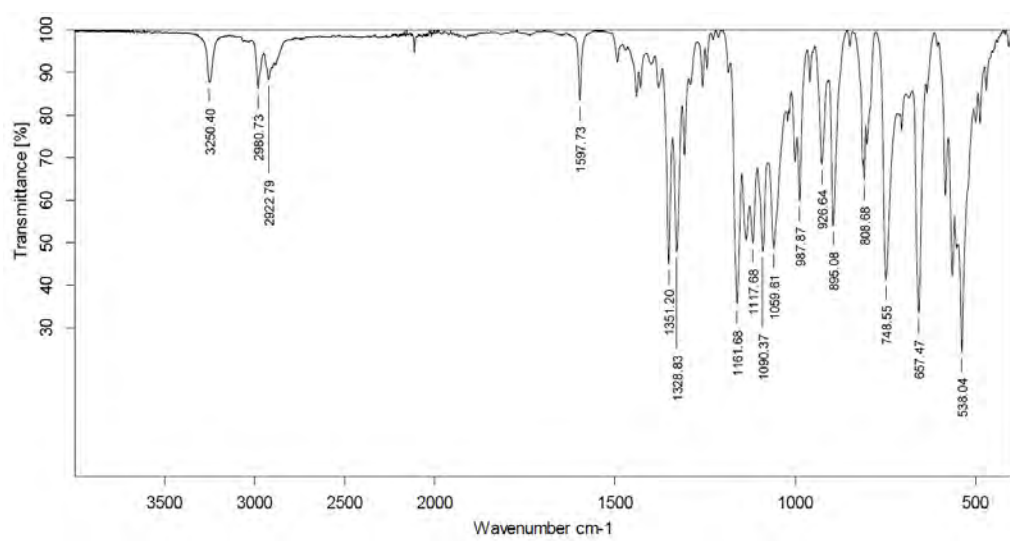
Figure S4: IR spectrum of **4a**.

Figure S5: ^{1}H NMR spectrum (400 MHz) of **4b** in CDCl$_3$.
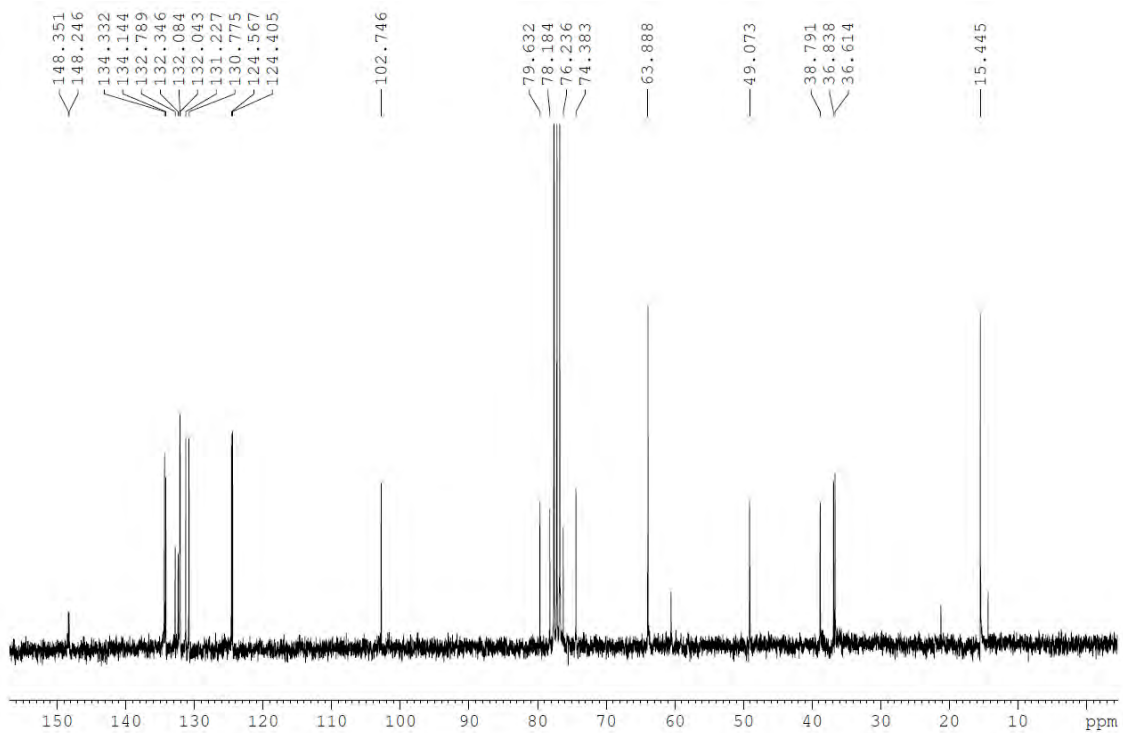
Figure S6: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **4b** in CDCl$_3$.

Figure S7: ESI-MS spectrum of **4b**.
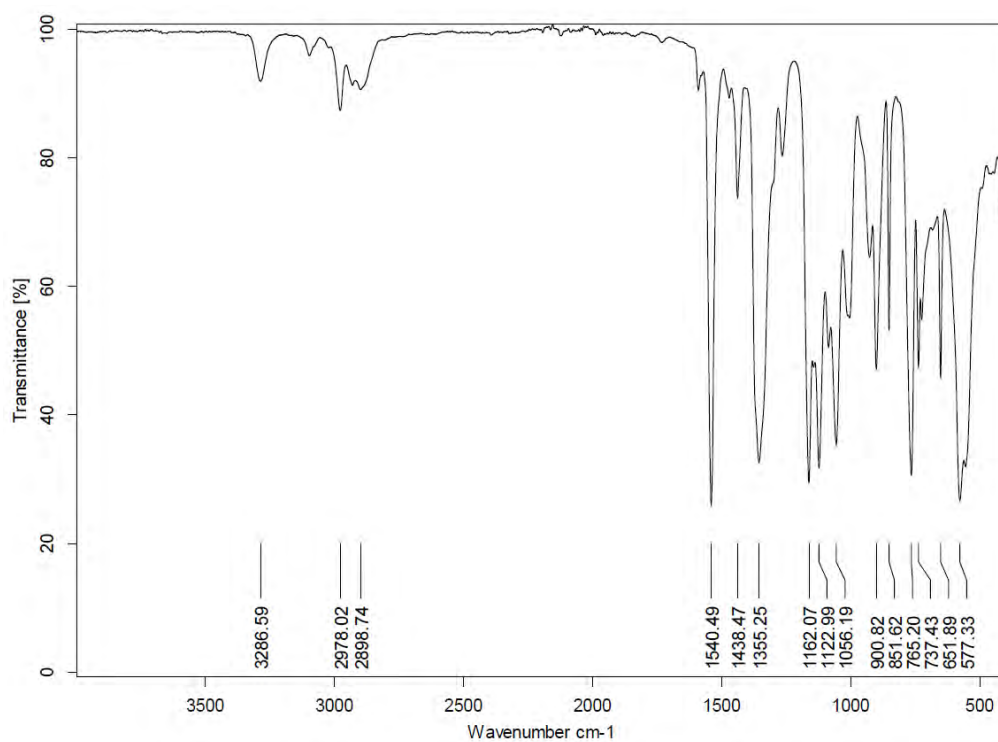
Figure S8: IR spectrum of **4b**.
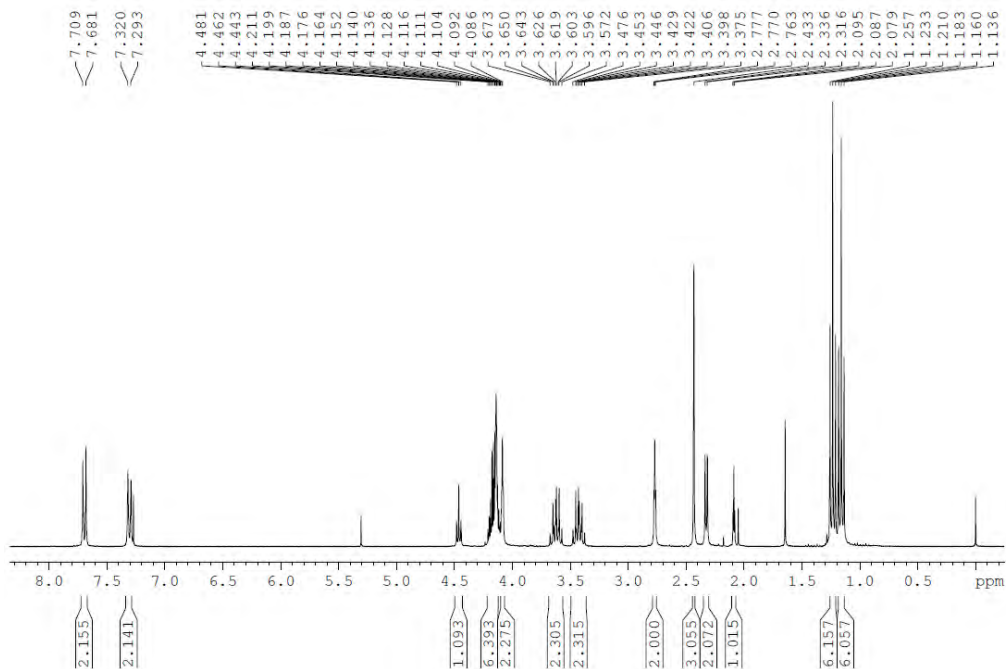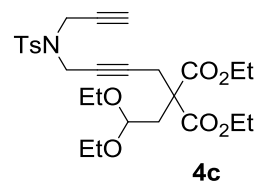
Figure S9: ^{1}H NMR spectrum (300 MHz) of **4c** in CDCl$_3$.
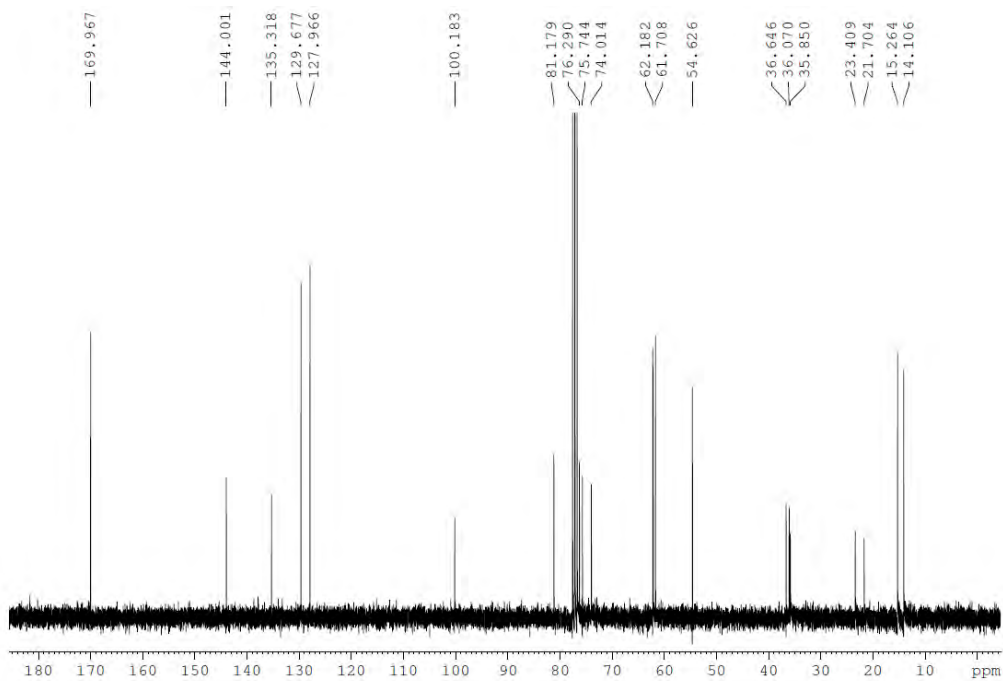
Figure S10: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **4c** in CDCl$_3$.
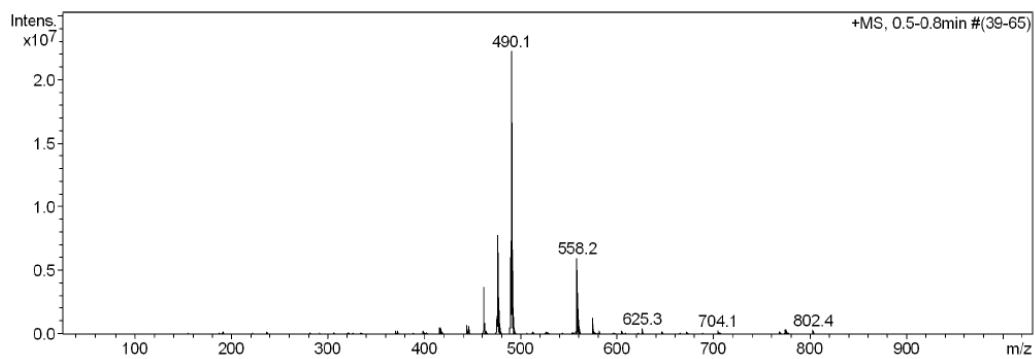
Figure S11: ESI-MS spectrum of **4c**.
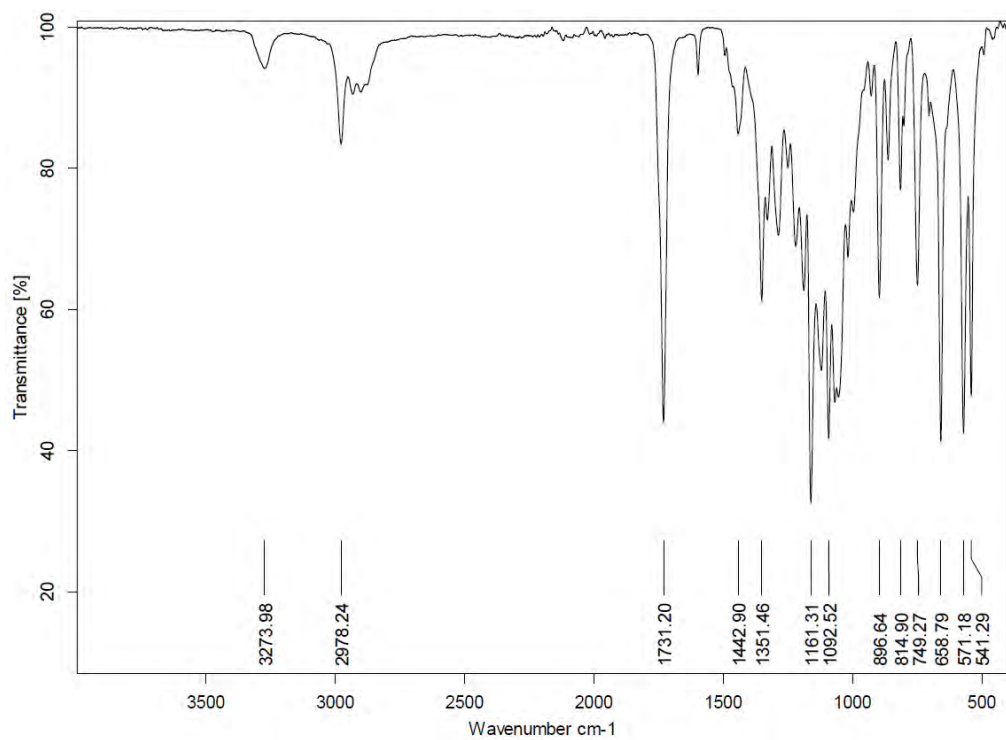
Figure S12: IR spectrum of **4c**.

Figure S13: ^{1}H NMR spectrum (300 MHz) of **4d** in CDCl$_3$.
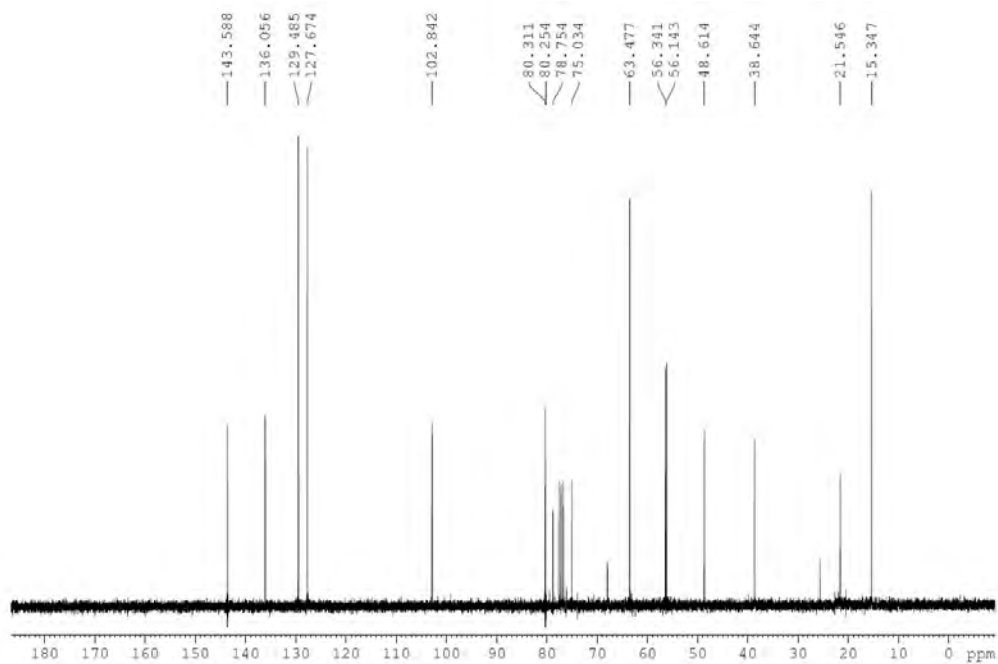
Figure S14: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **4d** in CDCl$_3$.
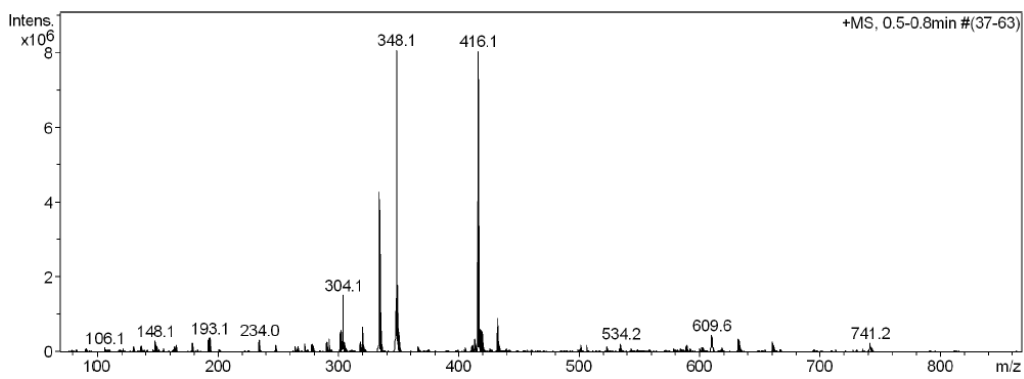
Figure S15: ESI-MS spectrum of **4d**.
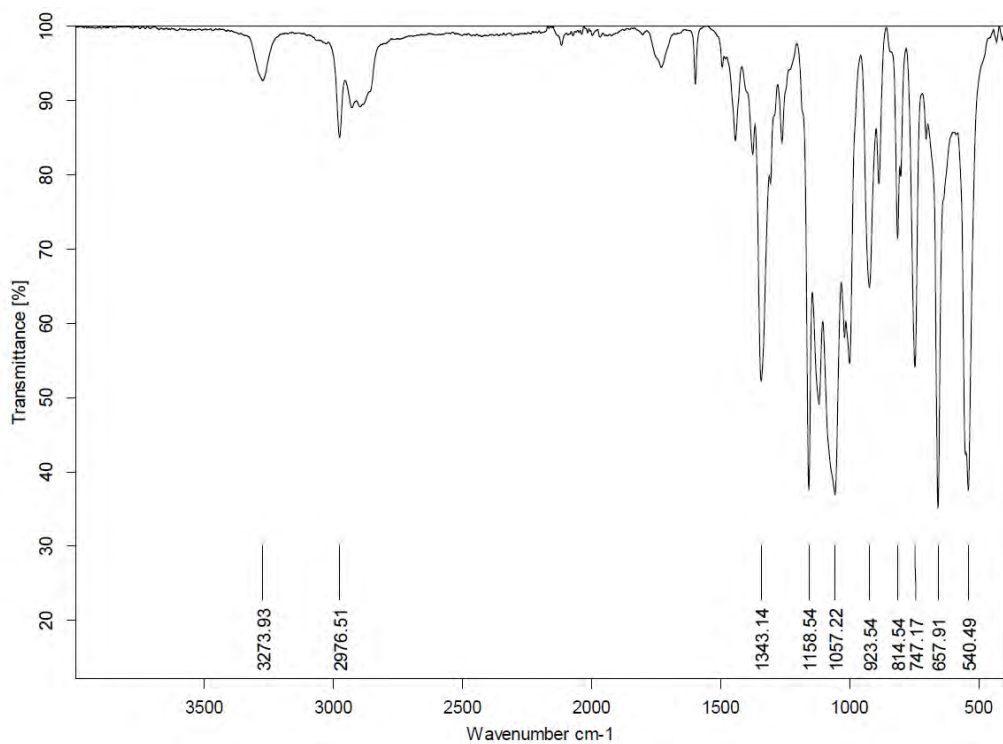
Figure S16: IR spectrum of **4d**.
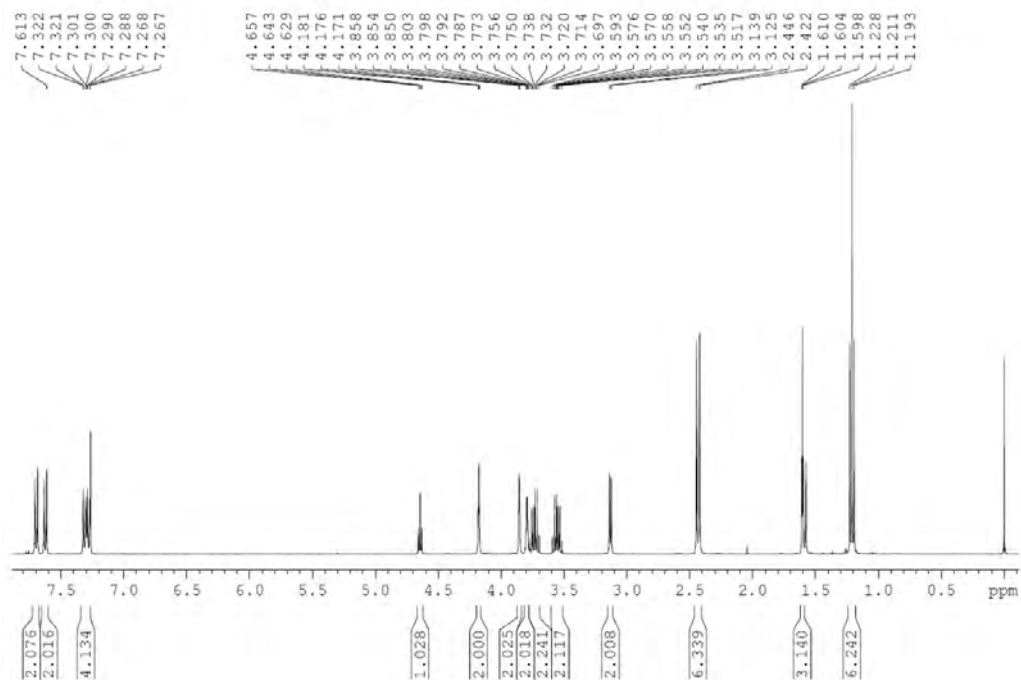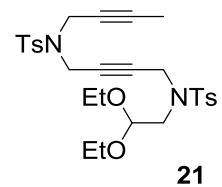
Figure S17: ^{1}H NMR spectrum (400 MHz) of **21** in CDCl$_3$.
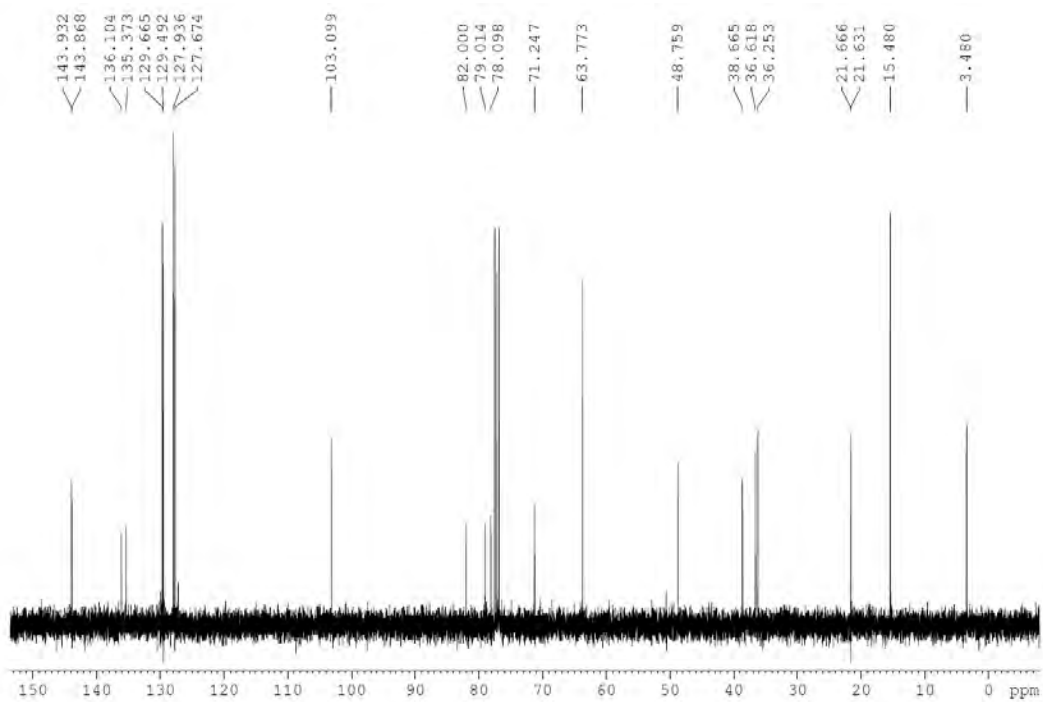
Figure S18: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **21** in CDCl$_3$.
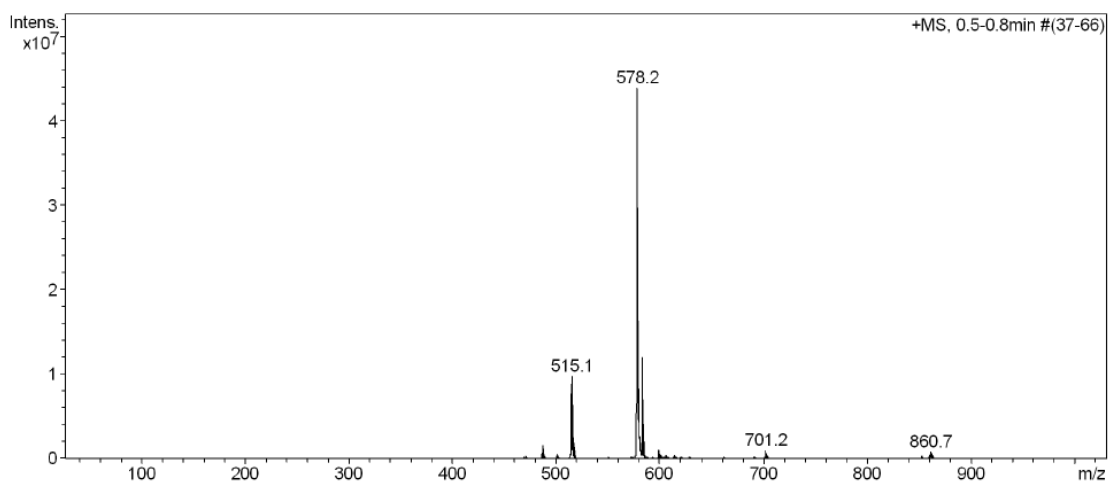
Figure S19: ESI-MS spectrum of **21**.
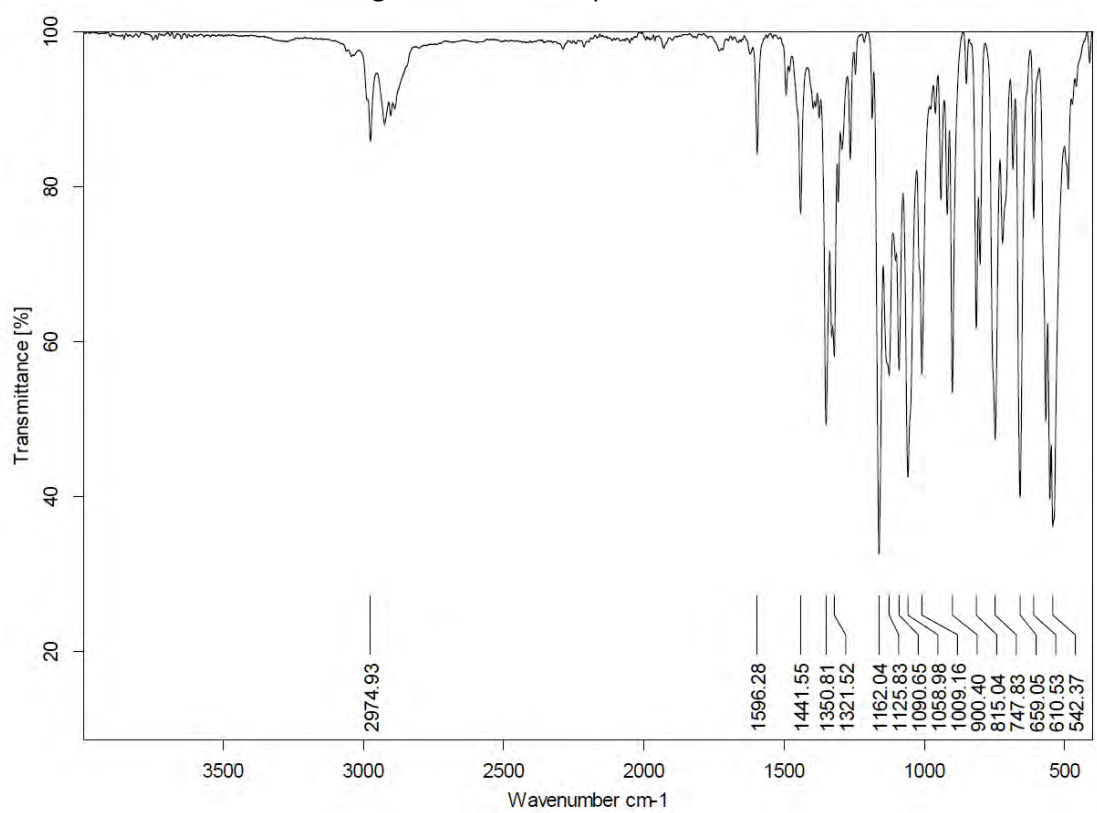
Figure S20: IR spectrum of **21**.
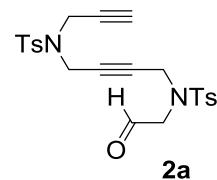
Figure S21: ^{1}H NMR spectrum (300 MHz) of **2a** in CDCl$_3$.
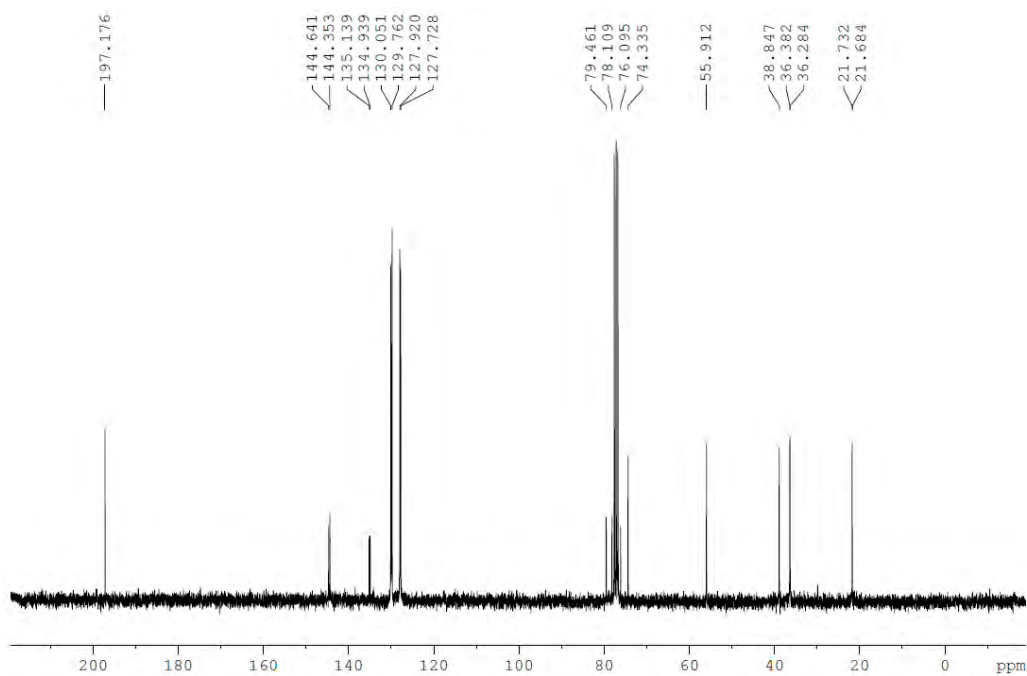
Figure S22: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **2a** in CDCl$_3$.
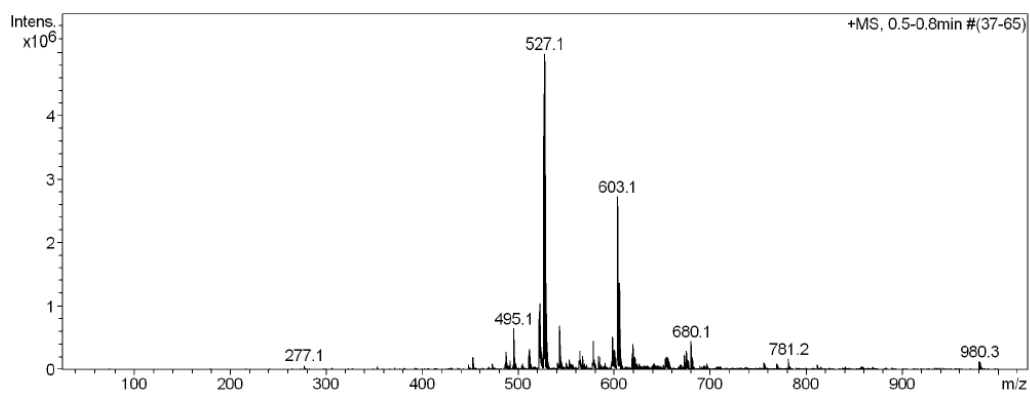
Figure S23: ESI-MS spectrum of **2a**.
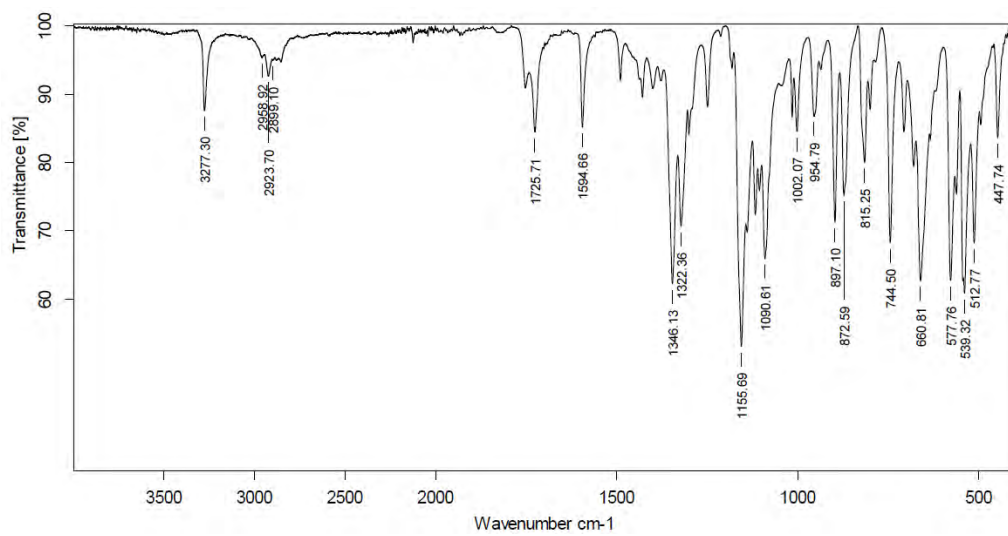
Figure S24: IR spectrum of **2a**.
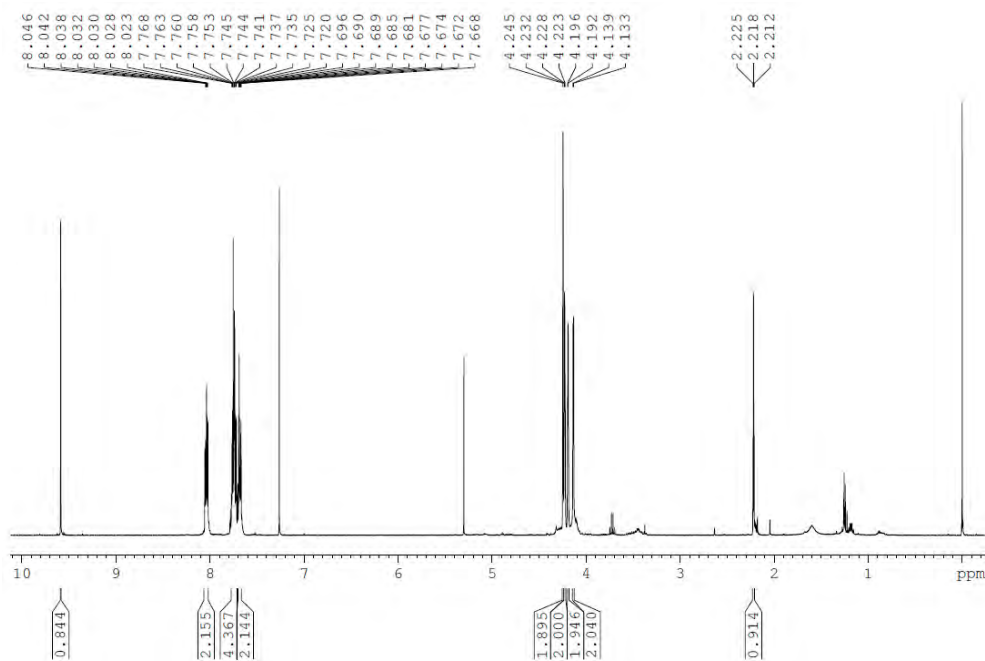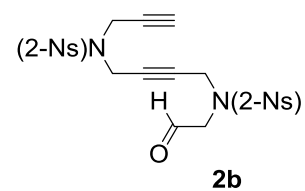
Figure S25: ^{1}H NMR spectrum (400 MHz) of **2b** in CDCl$_3$.
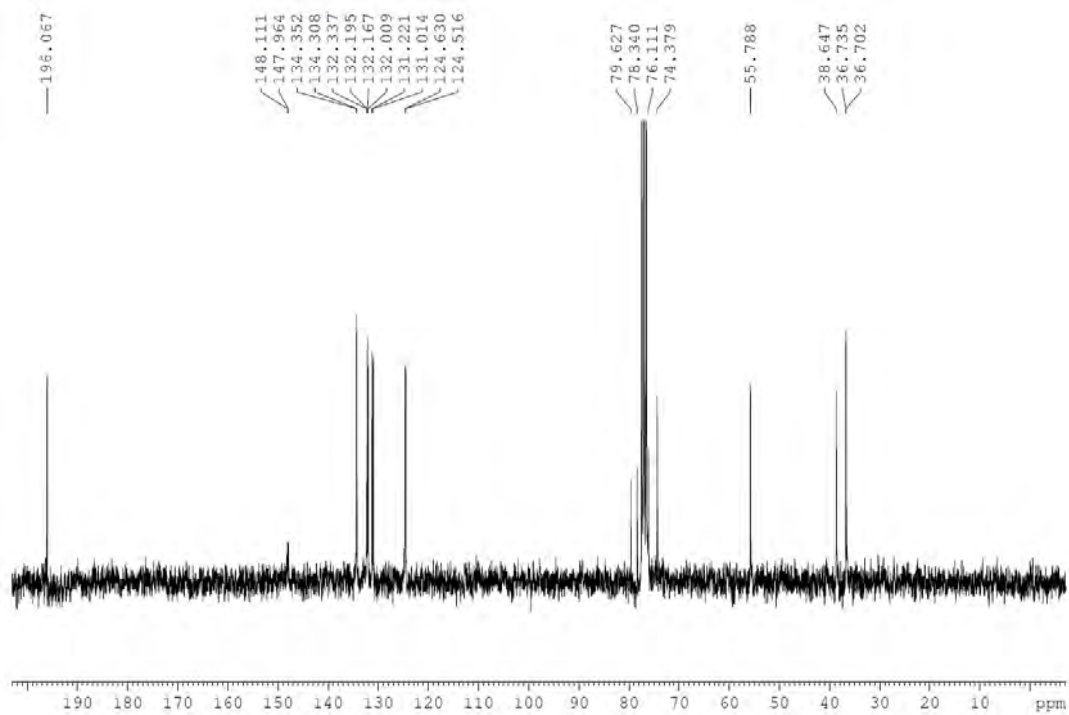
Figure S26: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **2b** in CDCl$_3$.
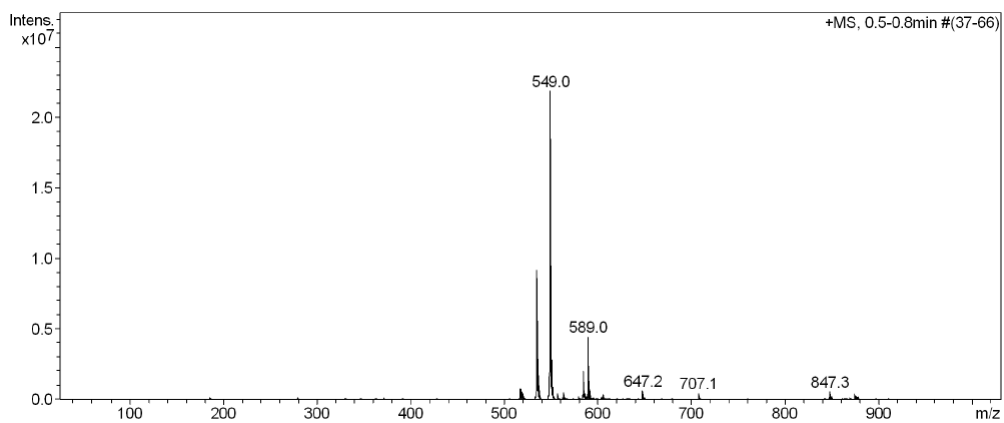
Figure S27: ESI-MS spectrum of **2b**.
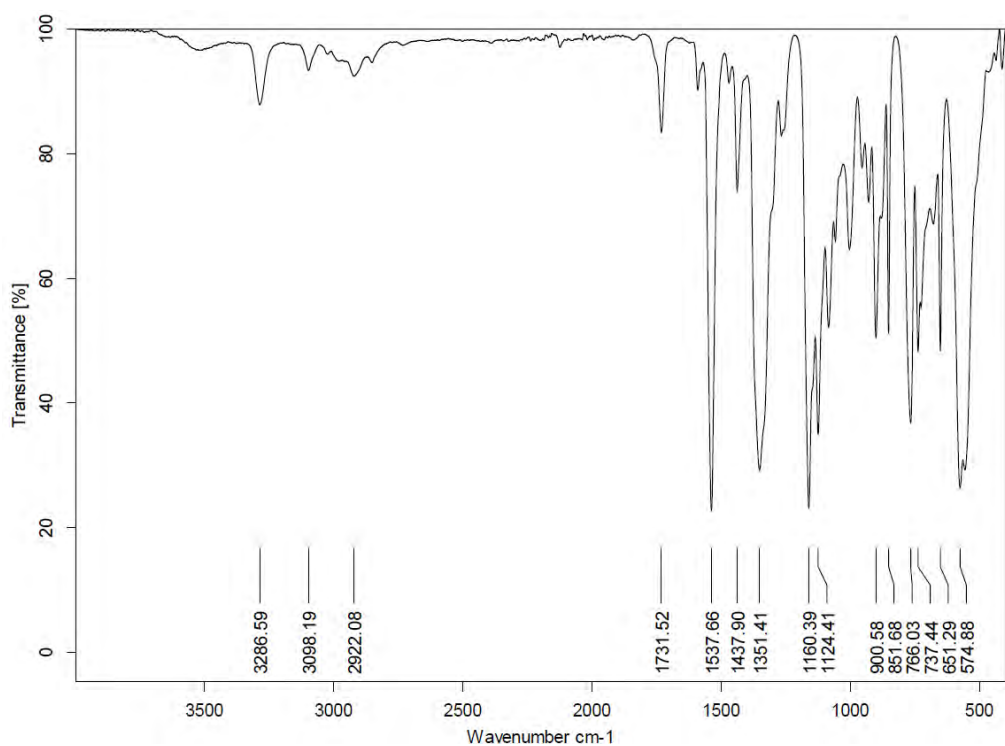
Figure S28: IR spectrum of **2b**.
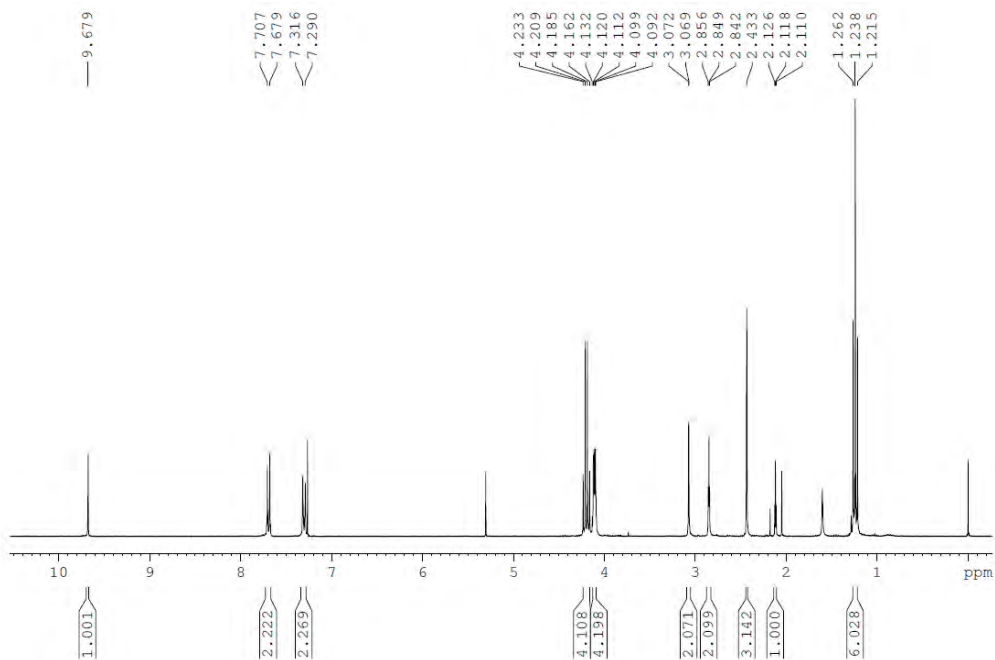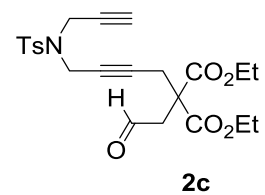
Figure S29: ^{1}H NMR spectrum (300 MHz) of **2c** in CDCl$_3$.
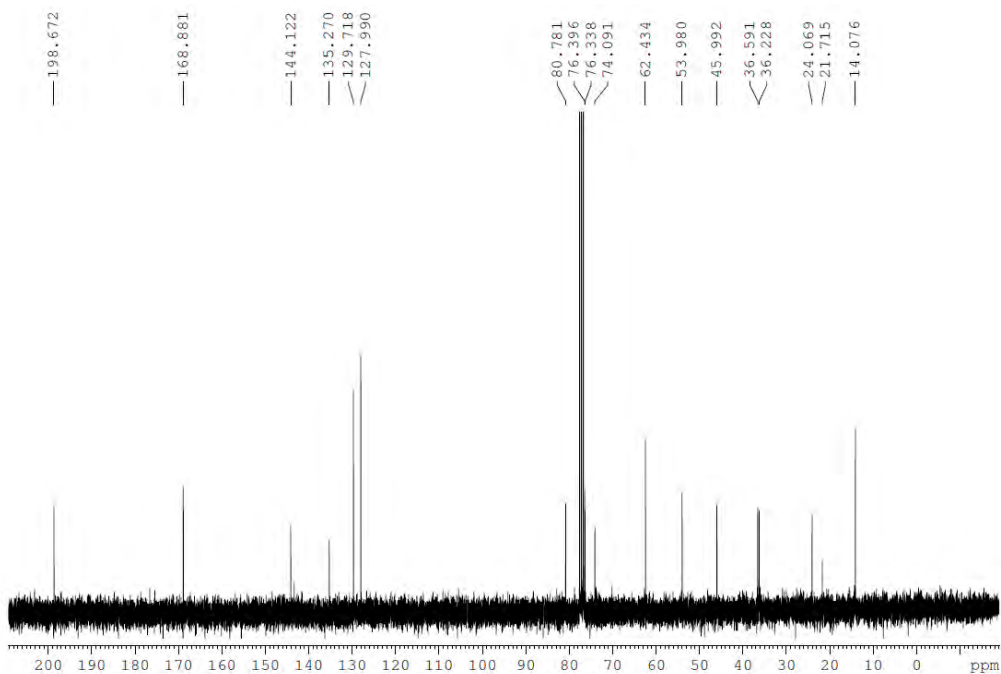
Figure S30: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **2c** in CDCl$_3$.
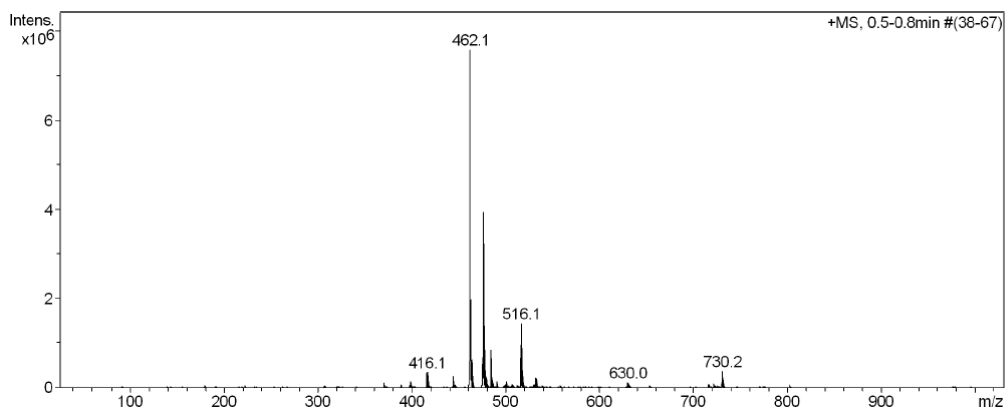
Figure S31: ESI-MS spectrum of **2c**.

Figure S32: IR spectrum of **2c**.

Figure S33: ^{1}H NMR spectrum (400 MHz) of **2d** in CDCl$_3$.

Figure S34: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **2d** in CDCl$_3$.
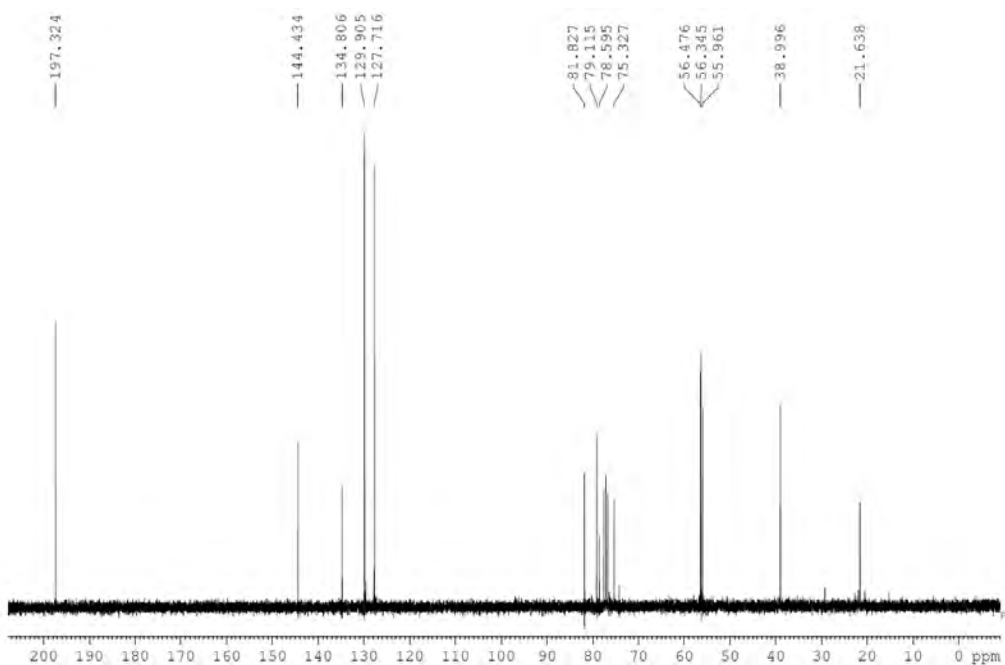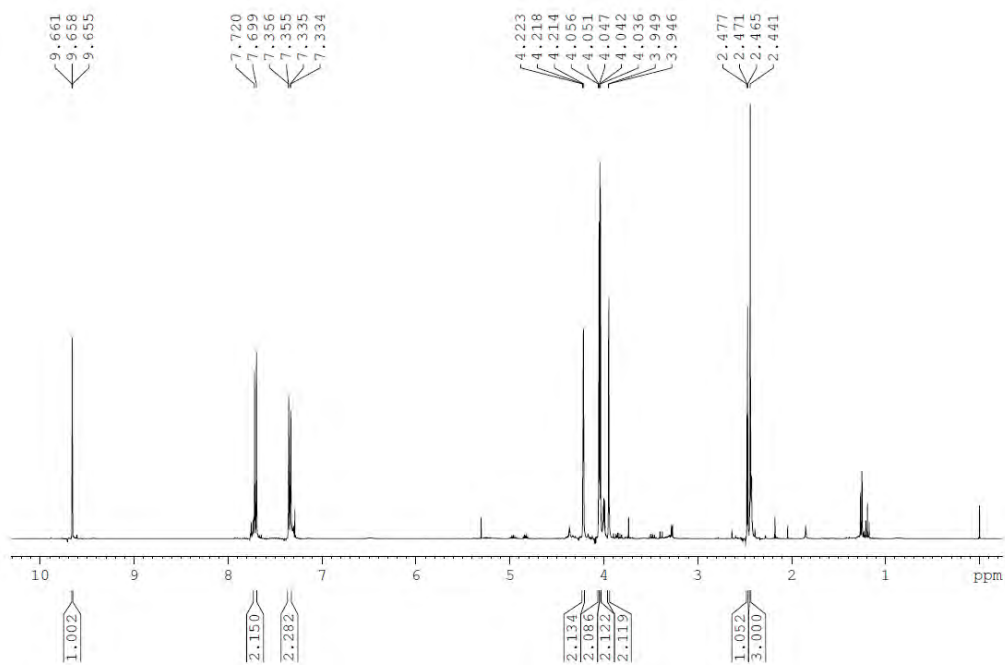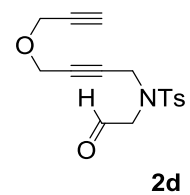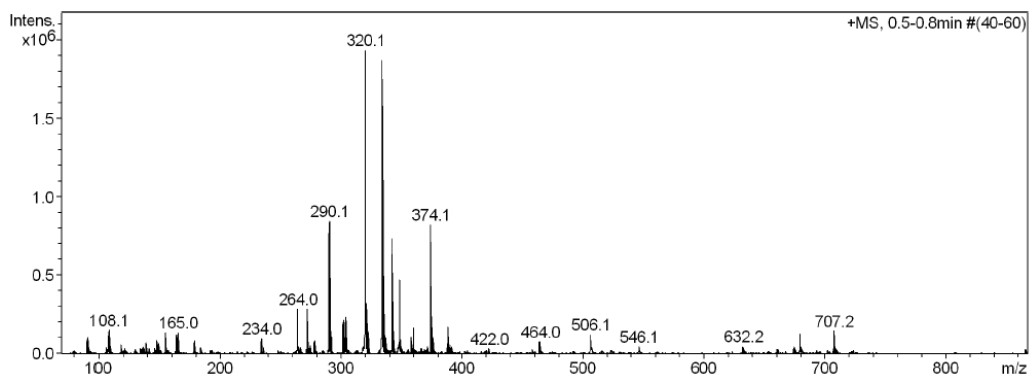
Figure S35: ESI-MS spectrum of **2d**.
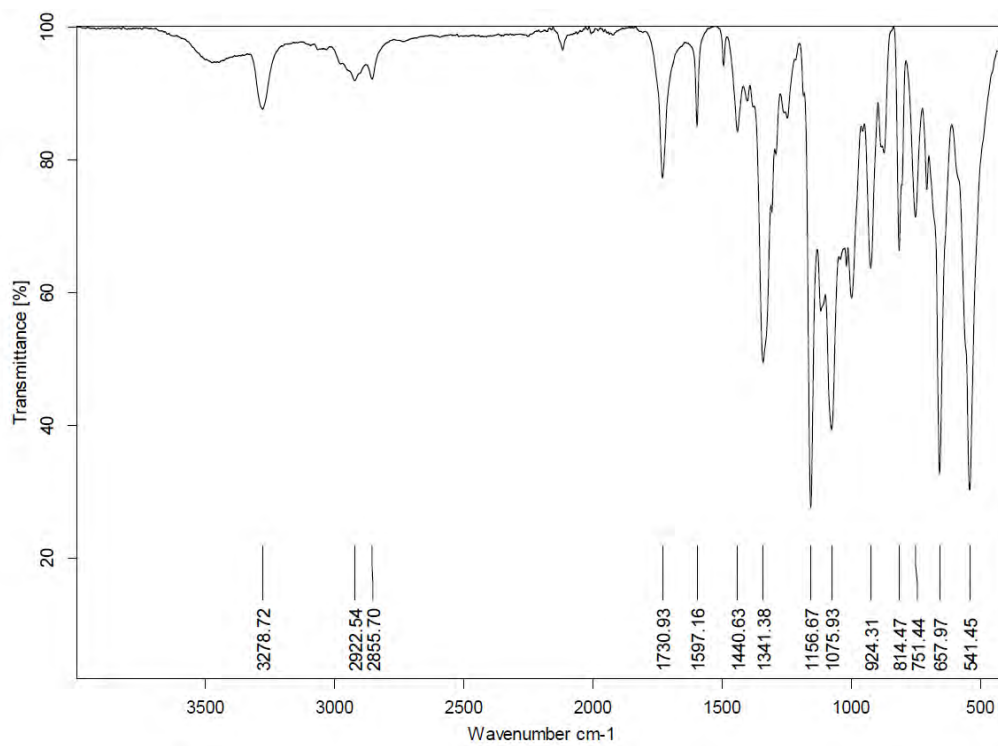
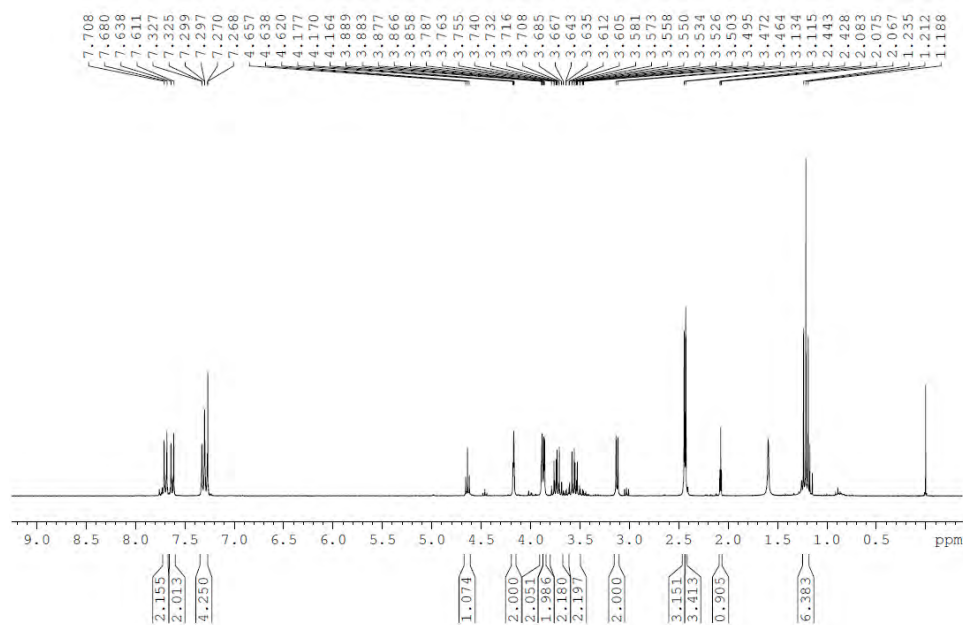**Figure S36**: IR spectrum of **2d**.
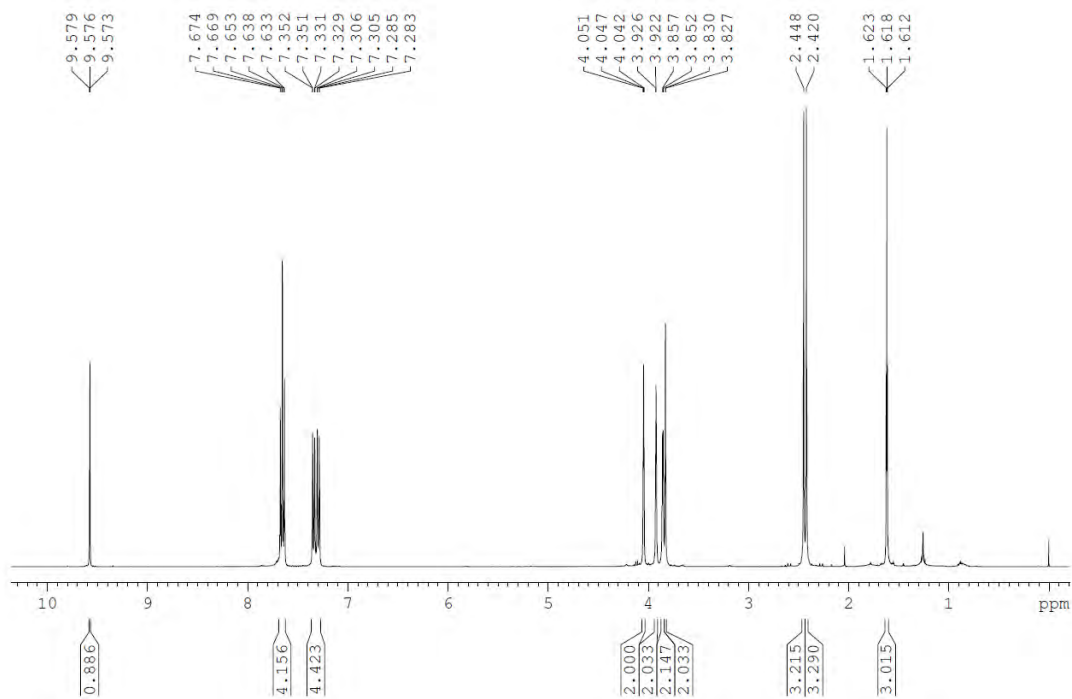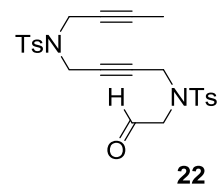
Figure S37: ^{1}H NMR spectrum (400 MHz) of **22** in CDCl$_3$.
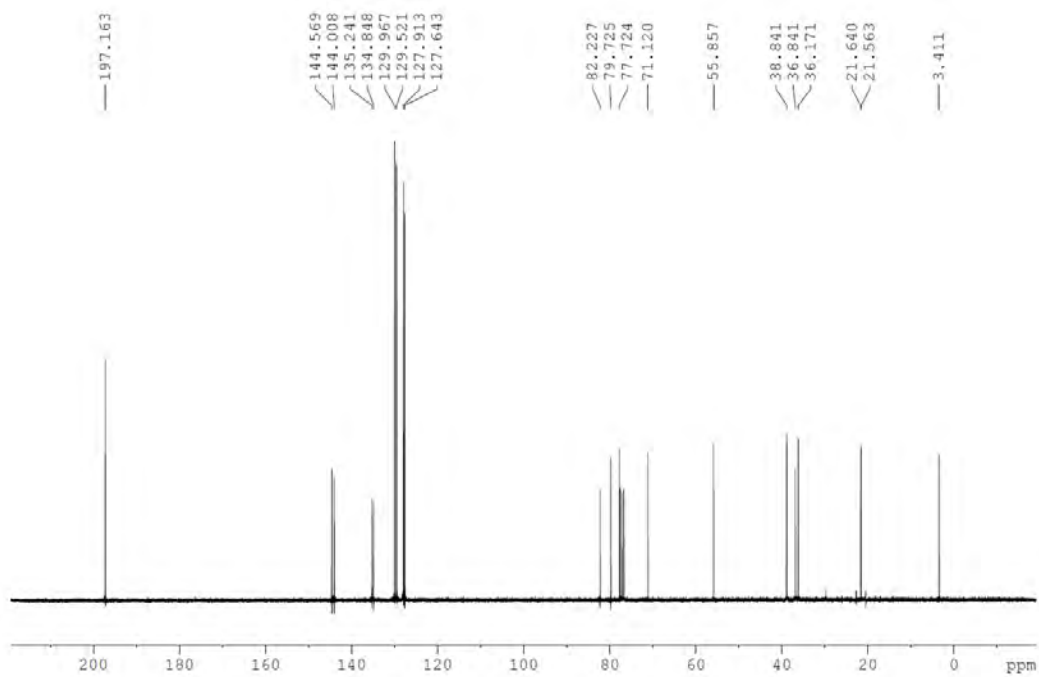
Figure S38: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **22** in CDCl$_3$.
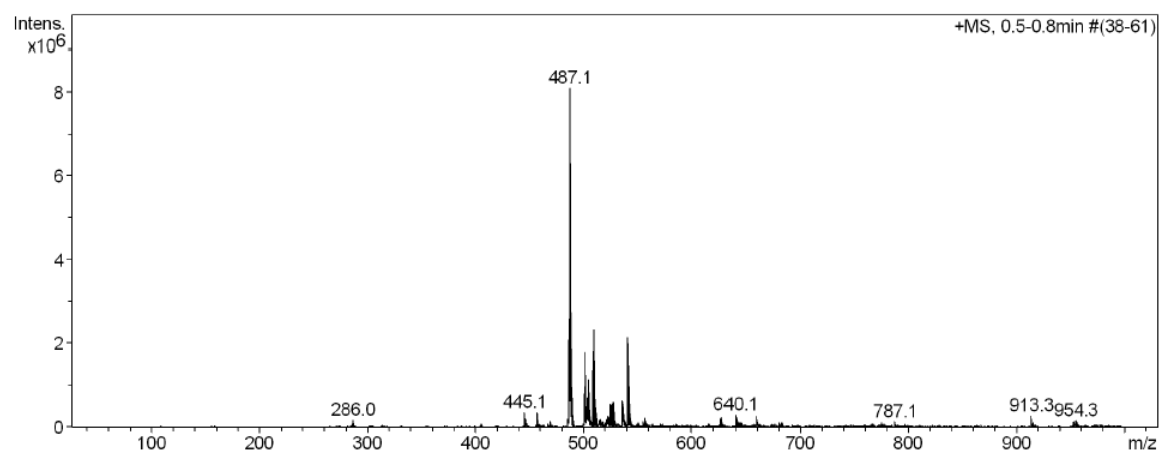
Figure S39: ESI-MS spectrum of **22**.
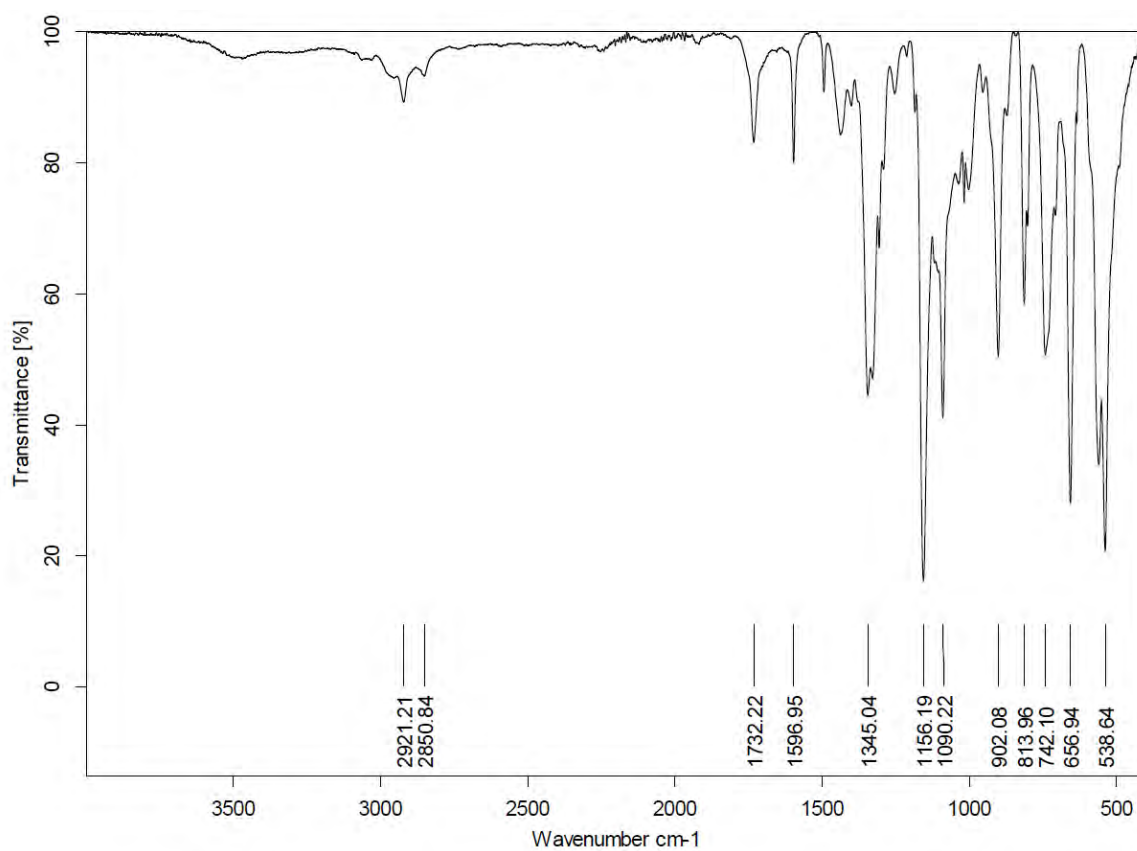
Figure S40: IR spectrum of **22**.
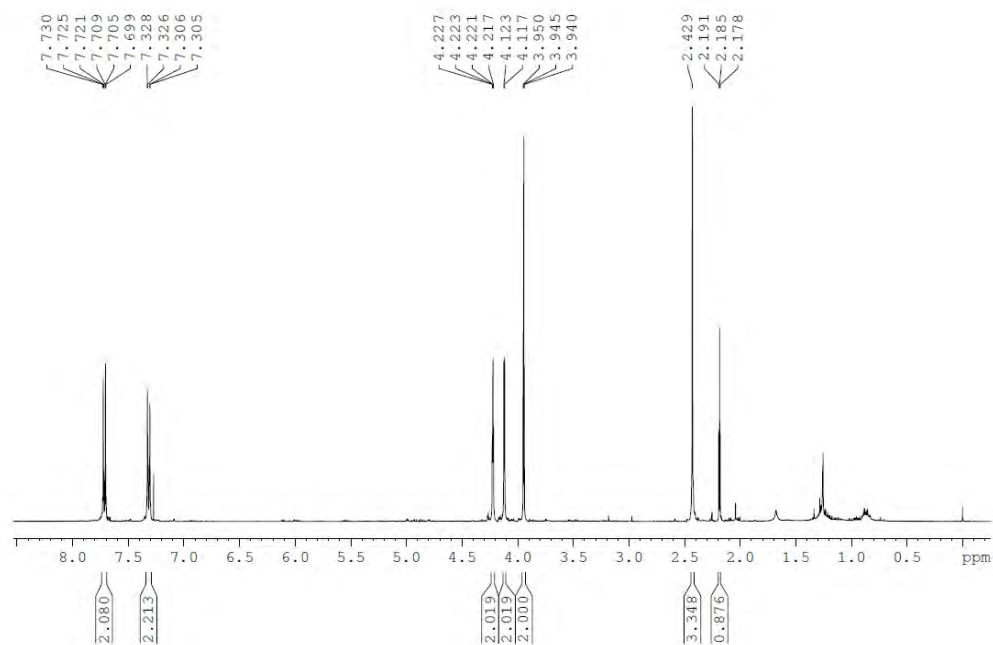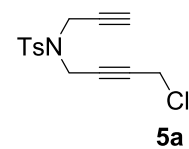
Figure S41: ^{1}H NMR spectrum (400 MHz) of **5a** in CDCl$_3$.
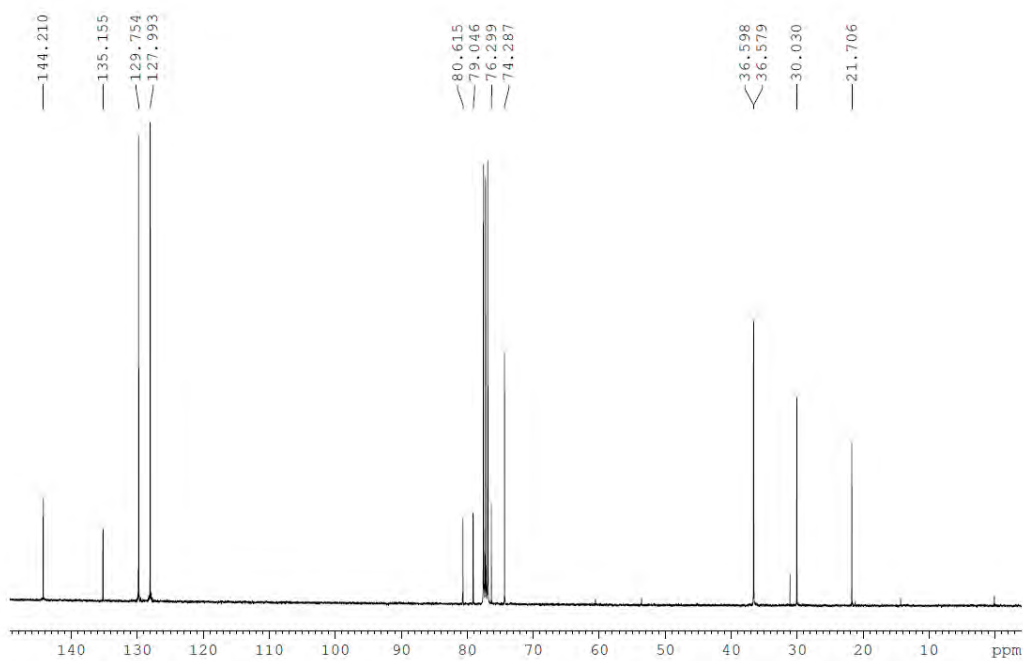
Figure S42: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **5a** in CDCl$_3$.
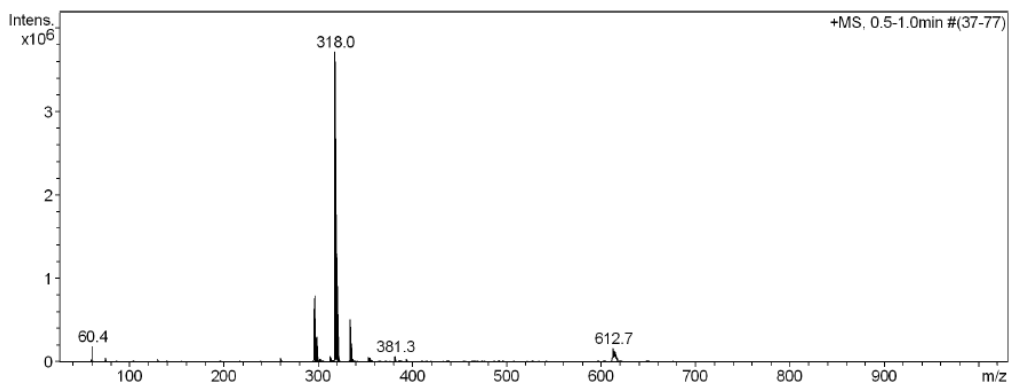
Figure S43: ESI-MS spectrum of **5a**.
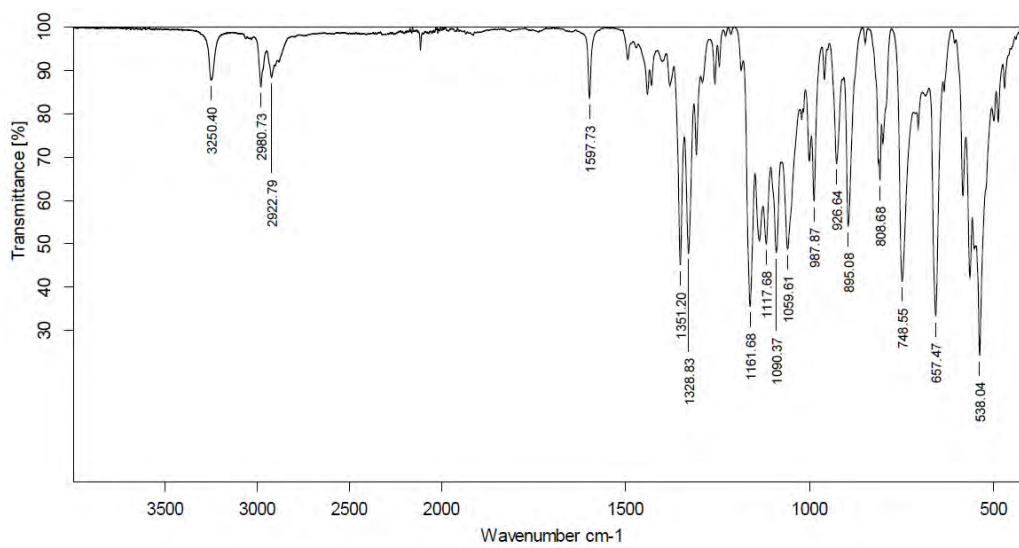
Figure S44: IR spectrum of **5a**.

EtO   NHTs

EtO

6a
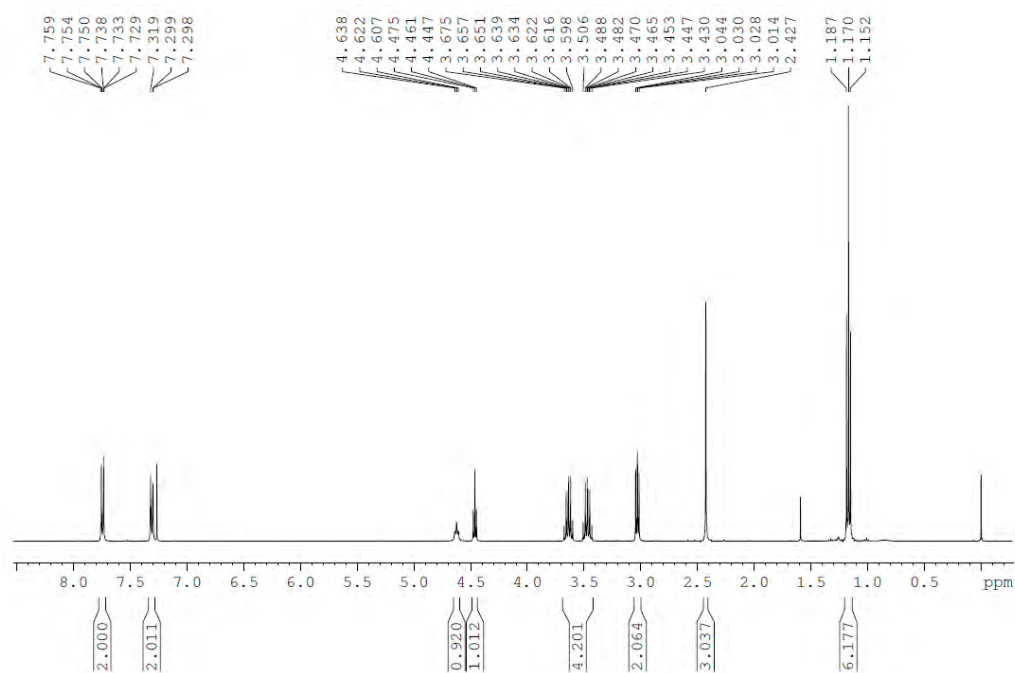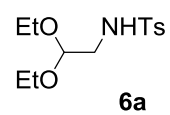
Figure S45: ^{1}H NMR spectrum (400 MHz) of **6a** in CDCl$_3$.
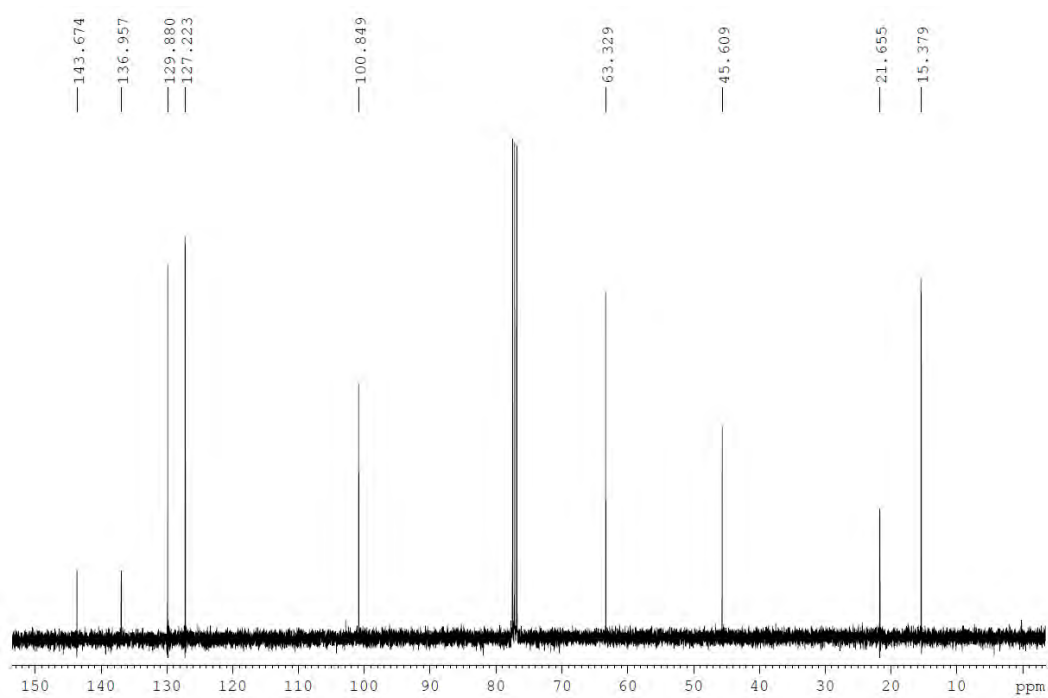
Figure S46: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **6a** in CDCl$_3$.
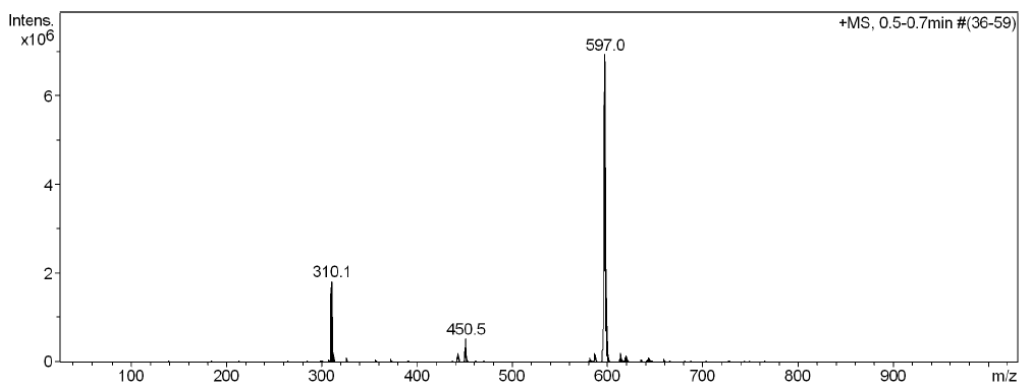
Figure S47: ESI-MS spectrum of **6a**.
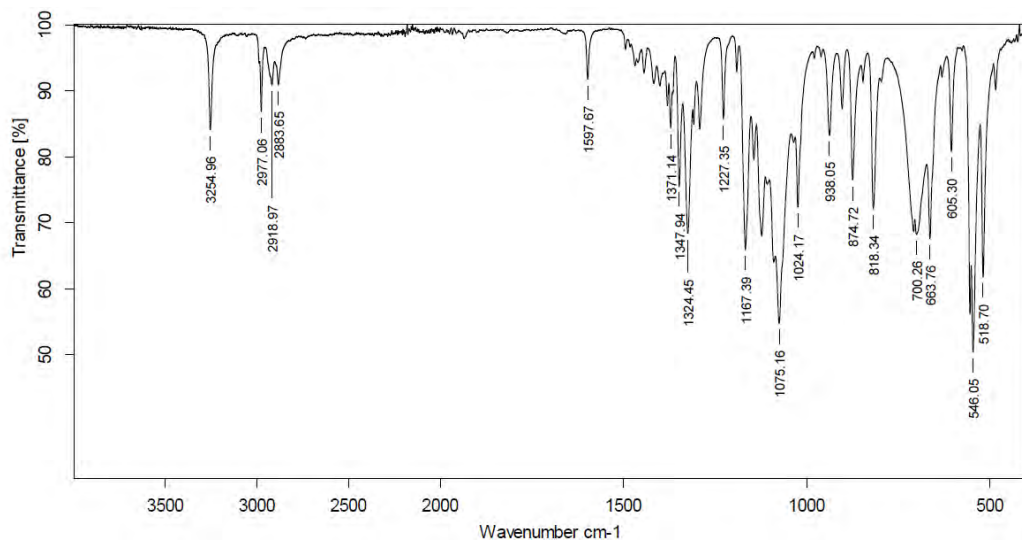
Figure S48: IR spectrum of **6a**.
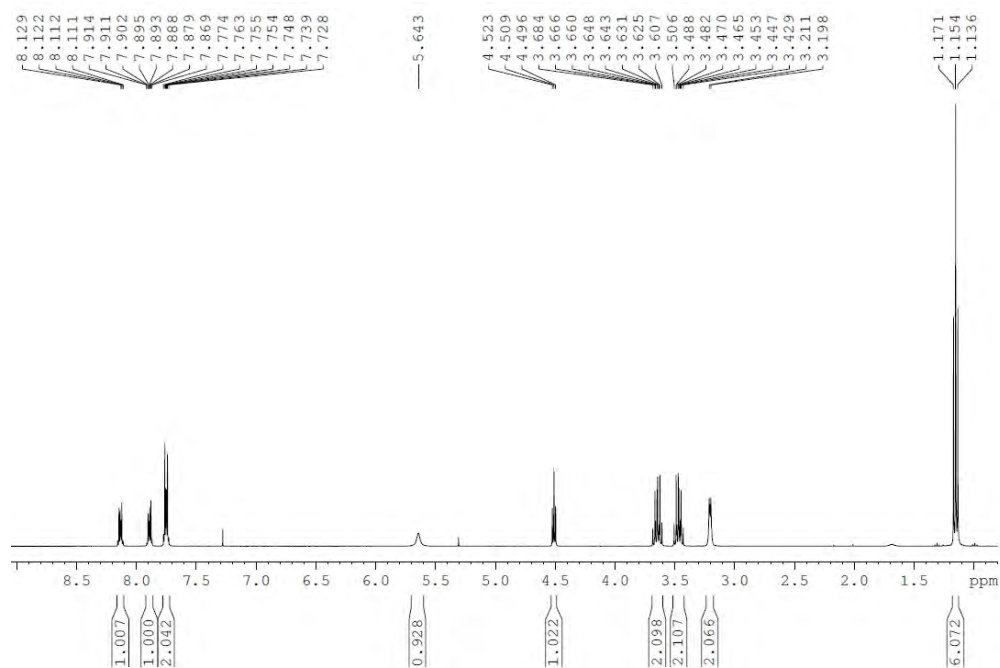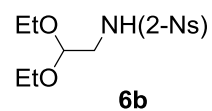
Figure S49: ^{1}H NMR spectrum (400 MHz) of **6b** in CDCl$_3$.
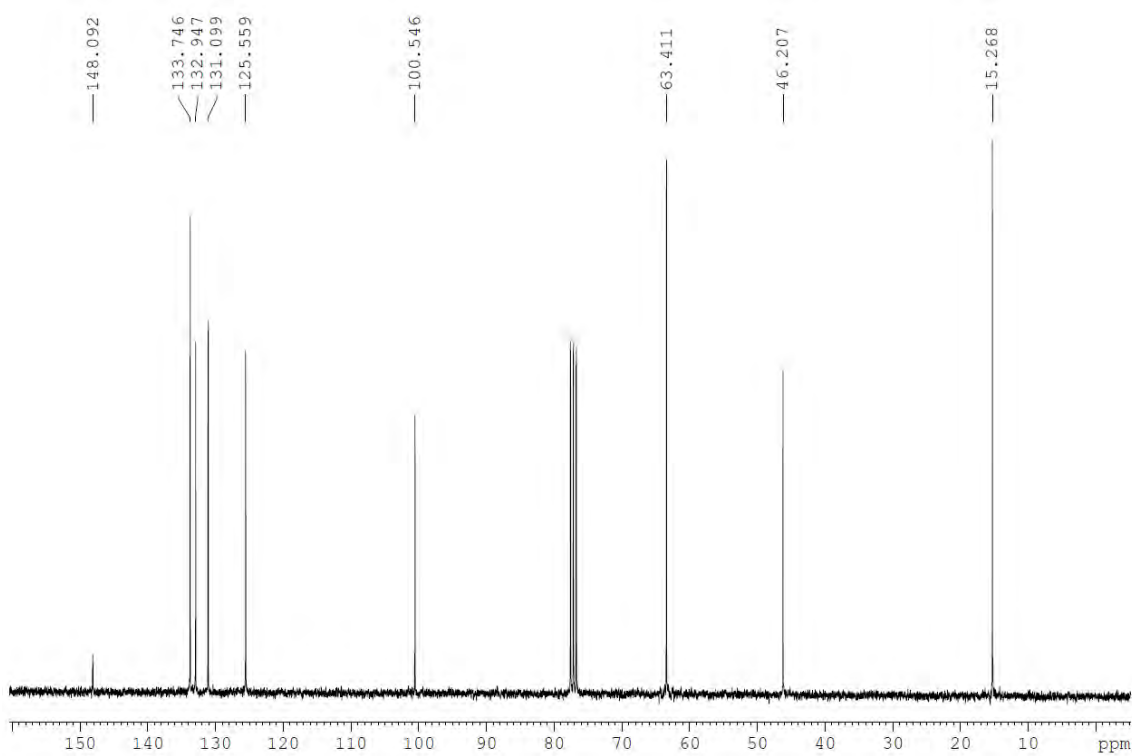
Figure S50: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **6b** in CDCl$_3$.
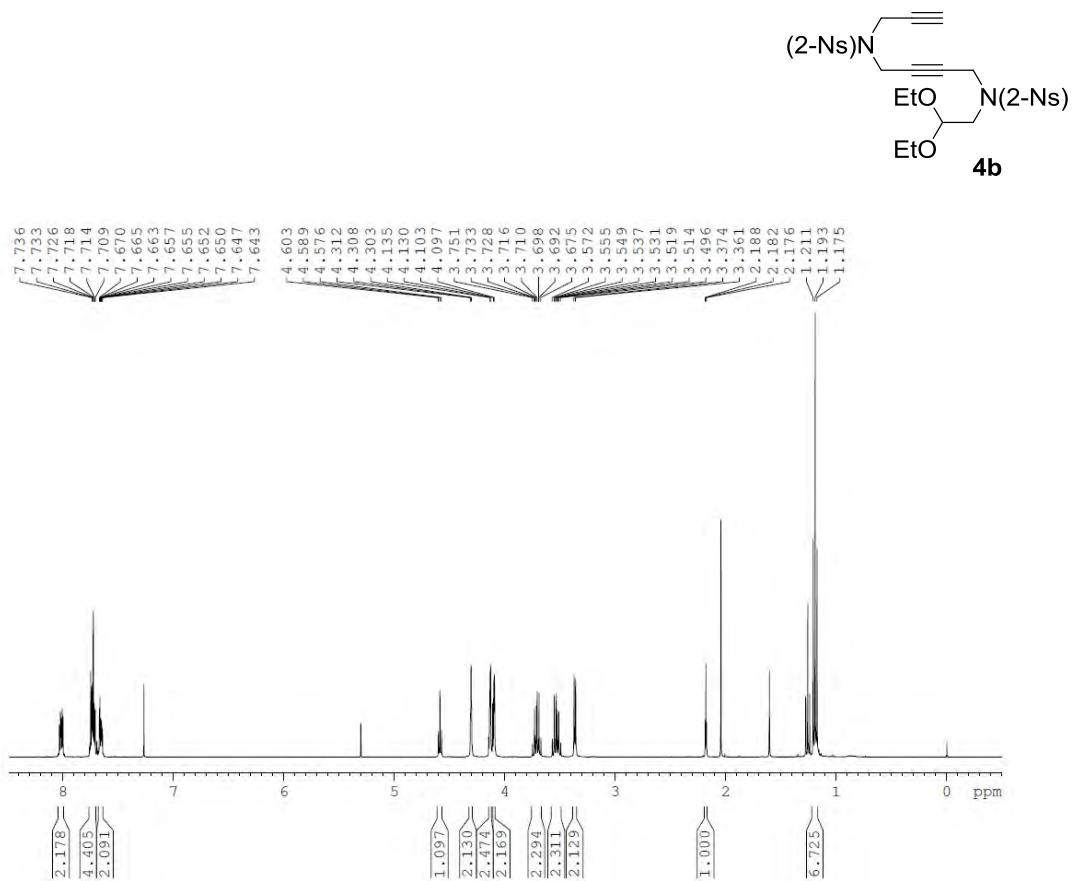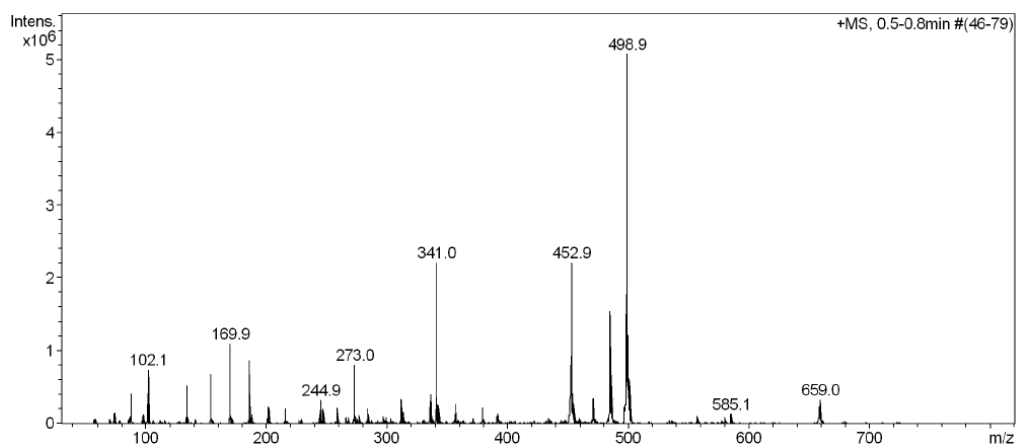
Figure S51: ESI-MS spectrum of **6b**.
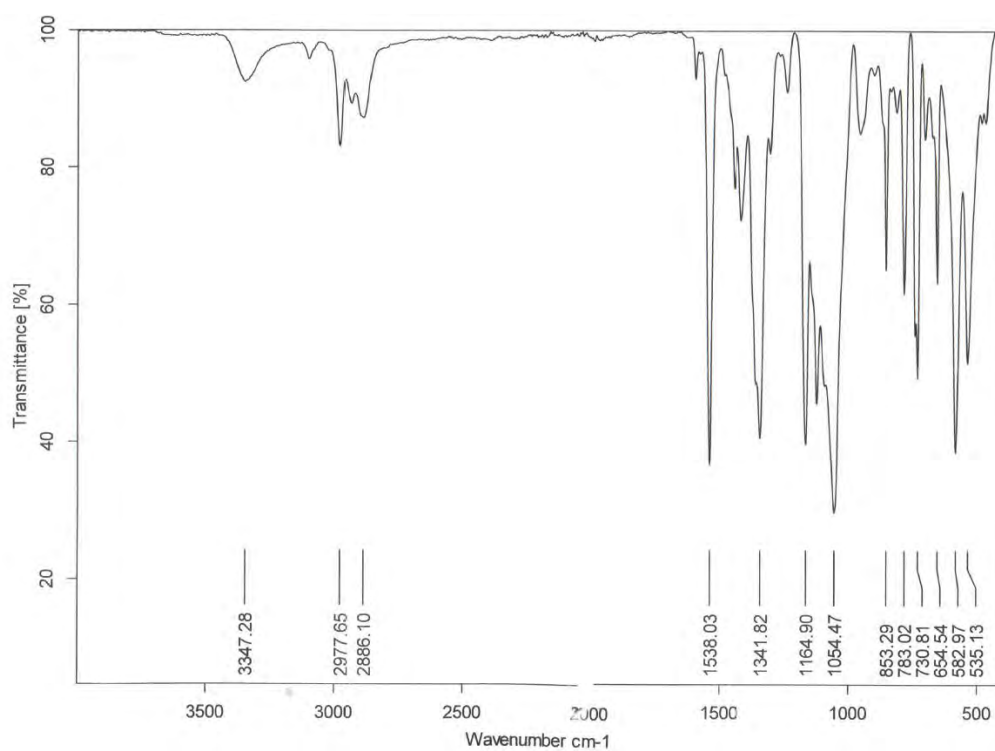
Figure S52: IR spectrum of **6b**.

(2-Ns)HN

9b
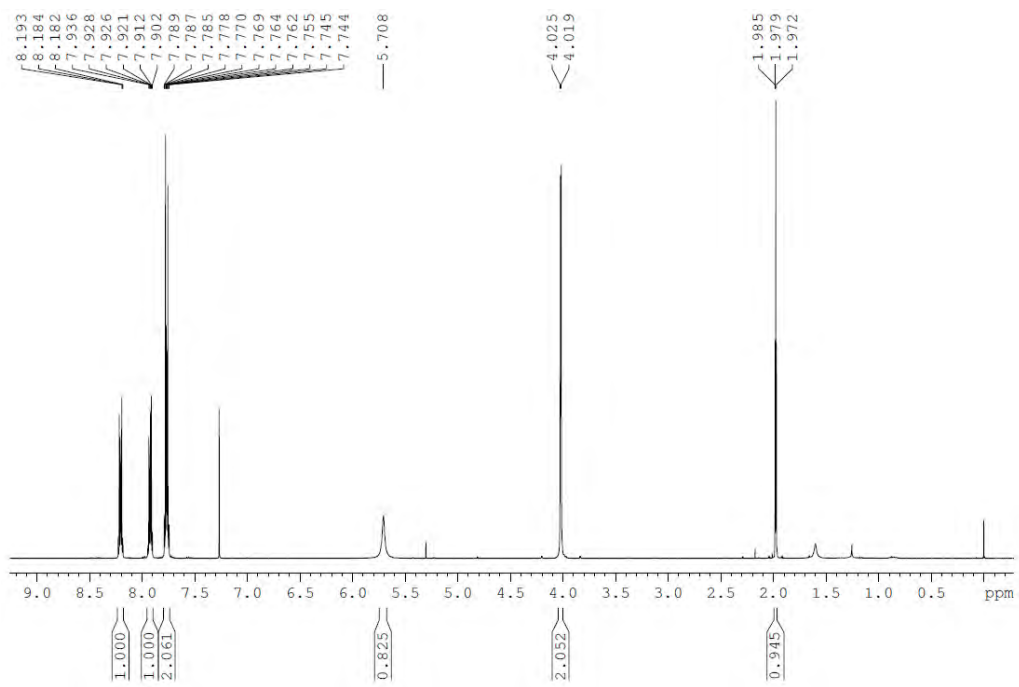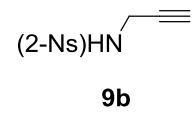
Figure S53: ^{1}H NMR spectrum (400 MHz) of **9b** in CDCl$_3$.
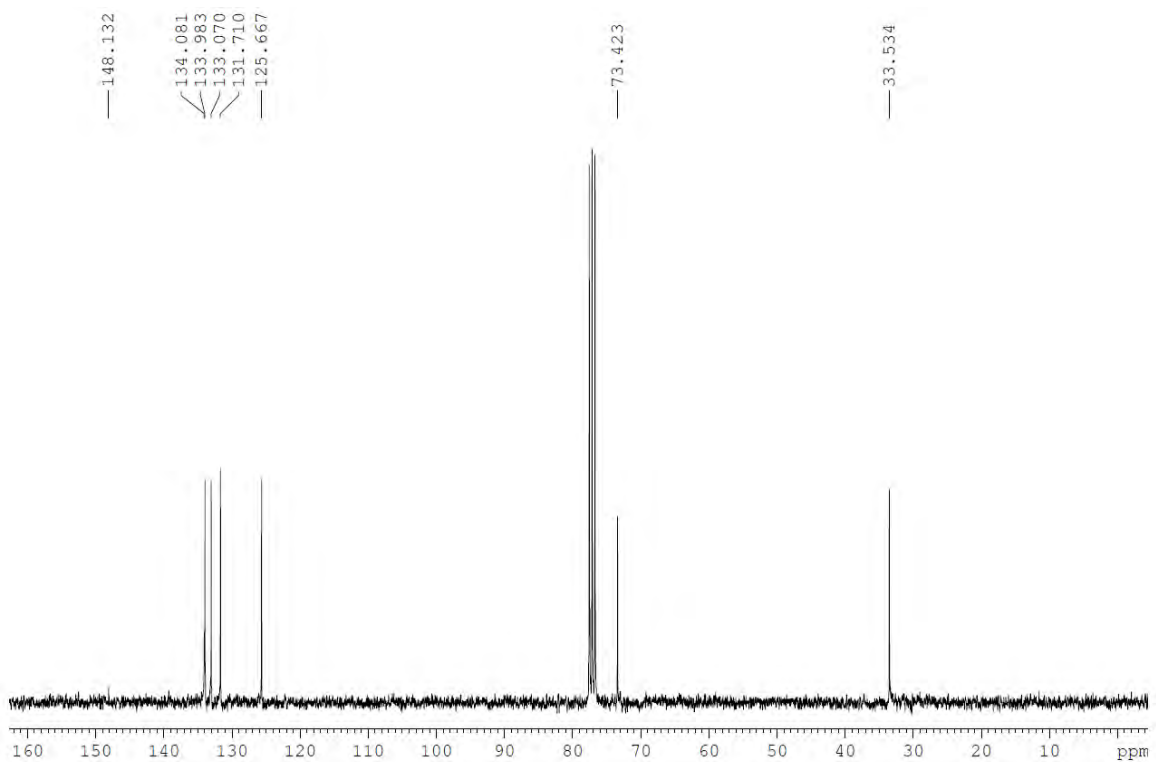
Figure S54: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **9b** in CDCl$_3$.
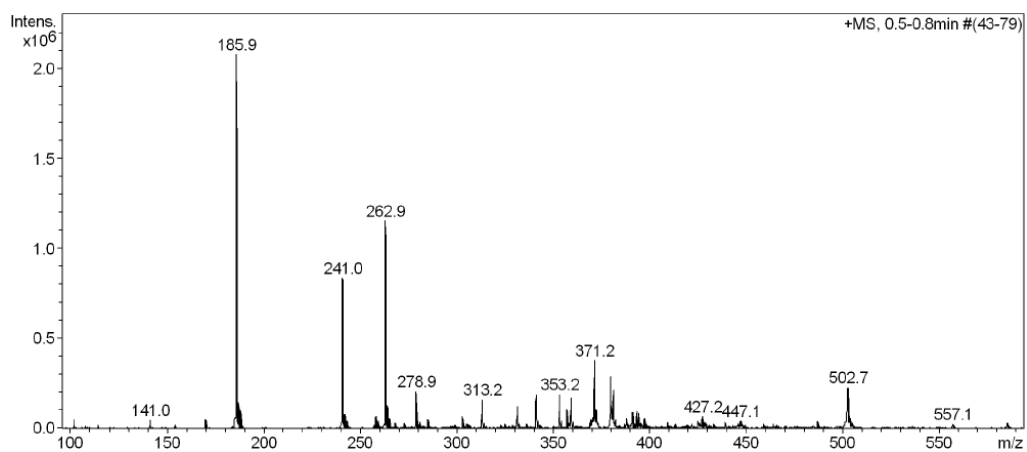
Figure S55: ESI-MS spectrum of **9b**.
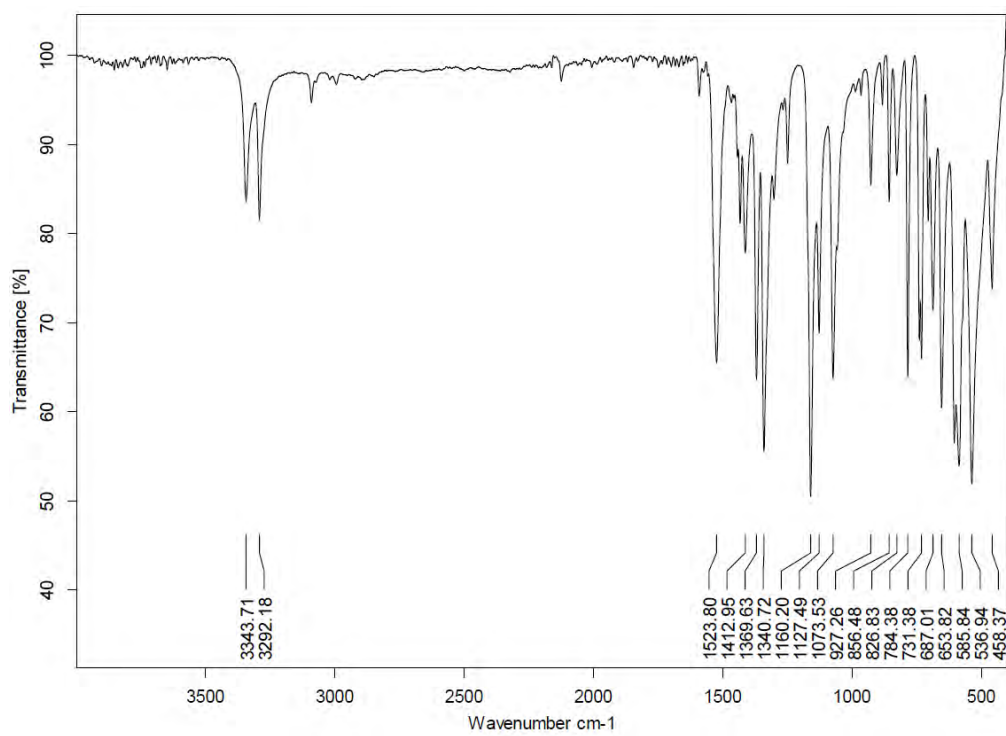
Figure S56: IR spectrum of **9b**.
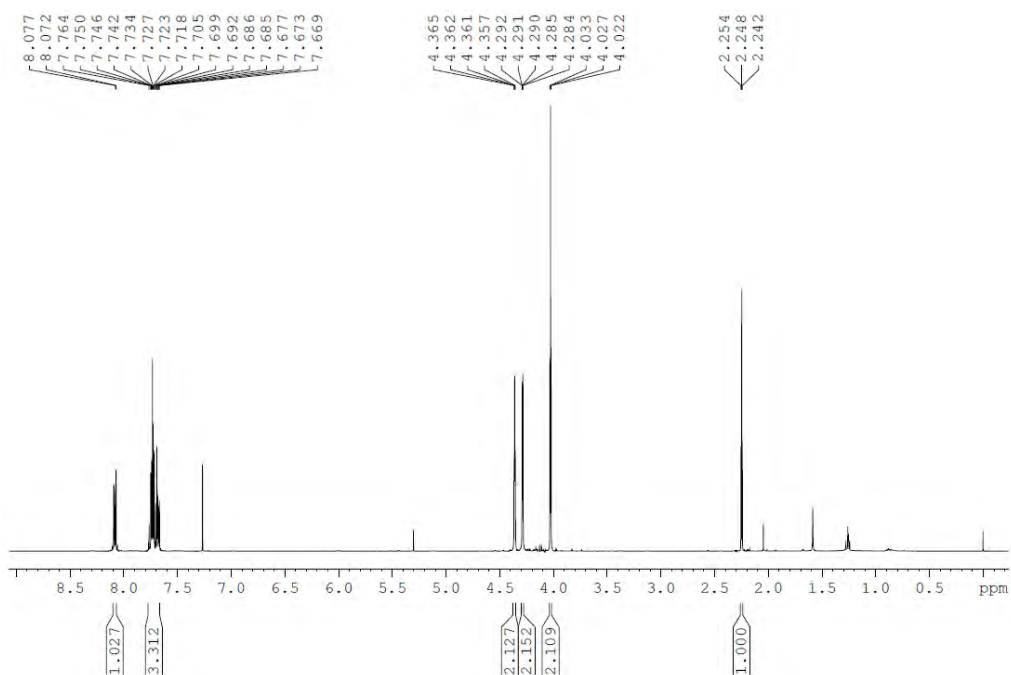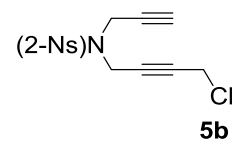
Figure S57: ^{1}H NMR spectrum (400 MHz) of **5b** in CDCl$_3$.
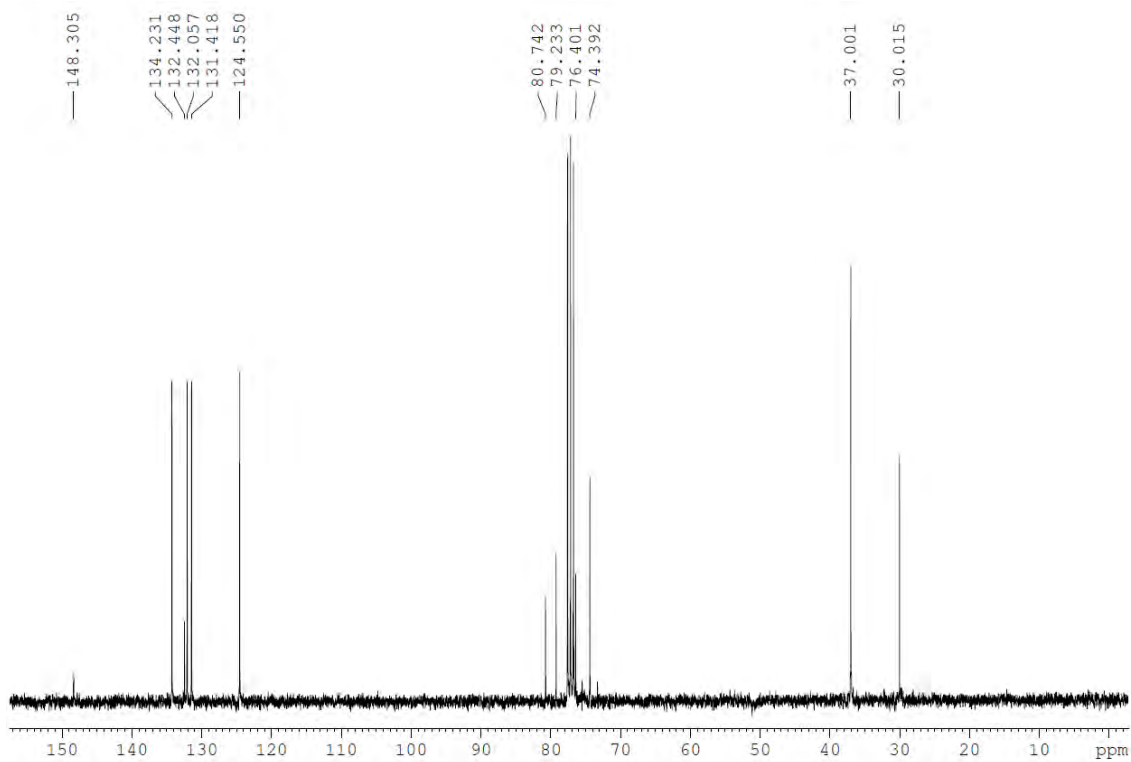
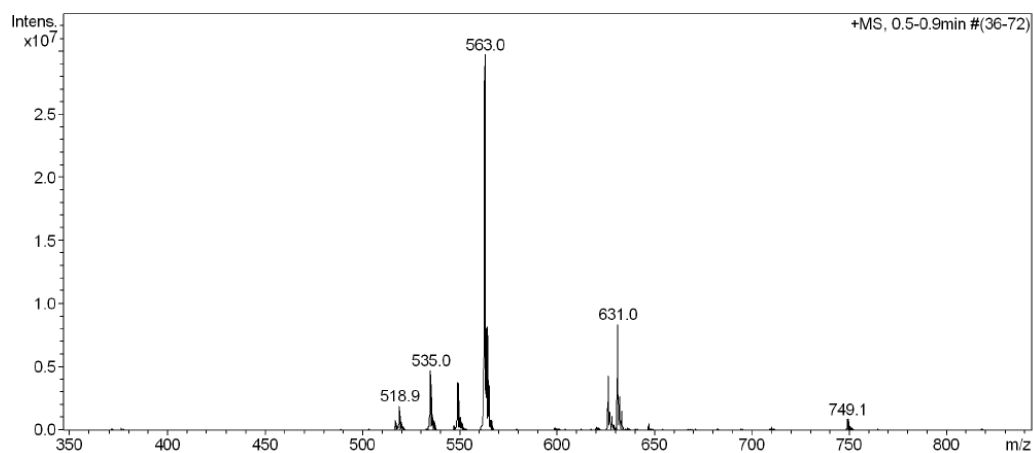**Figure S58**: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **5b** in CDCl$_3$.
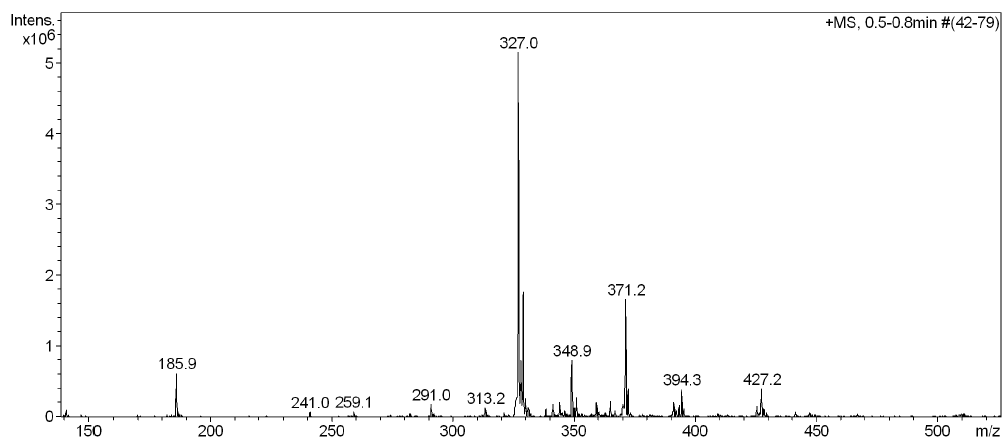
Figure S59: ESI-MS spectrum of **5b**.
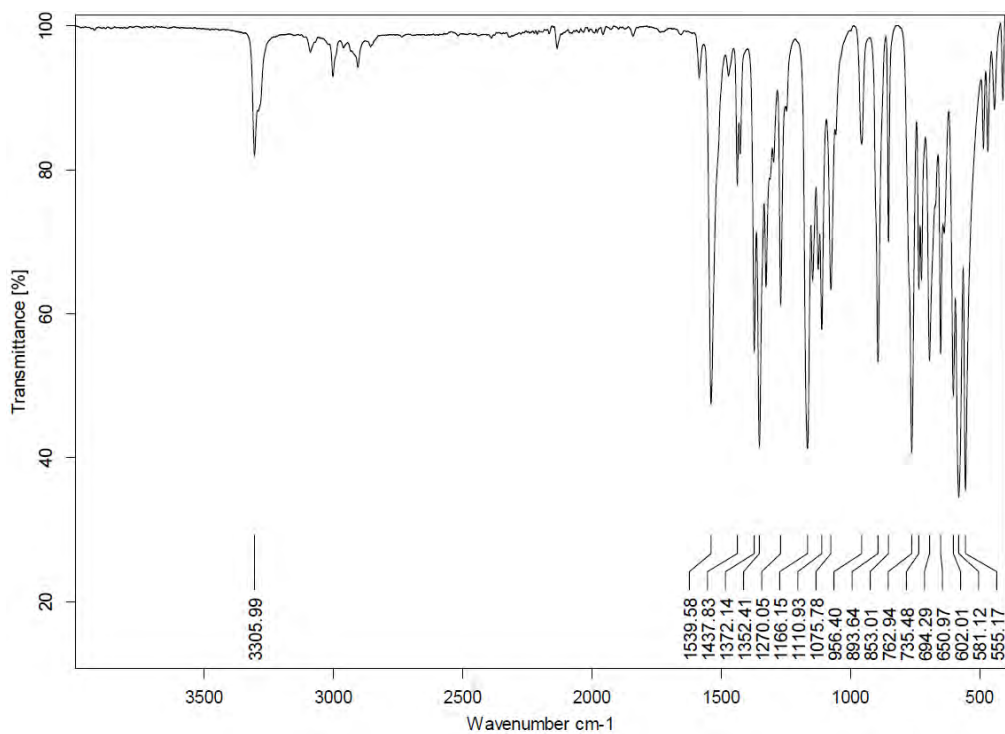
Figure S60: IR spectrum of **5b**.
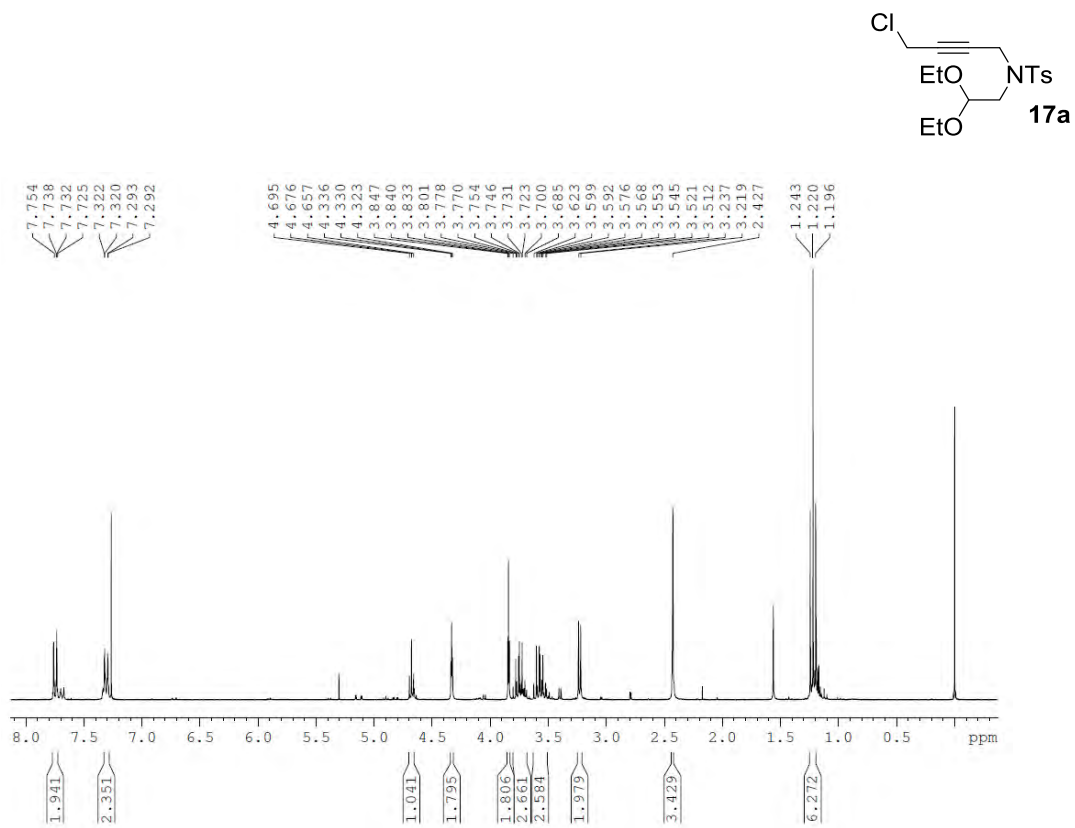
Figure S61: ^{1}H NMR spectrum (300 MHz) of **17a** in CDCl$_3$.
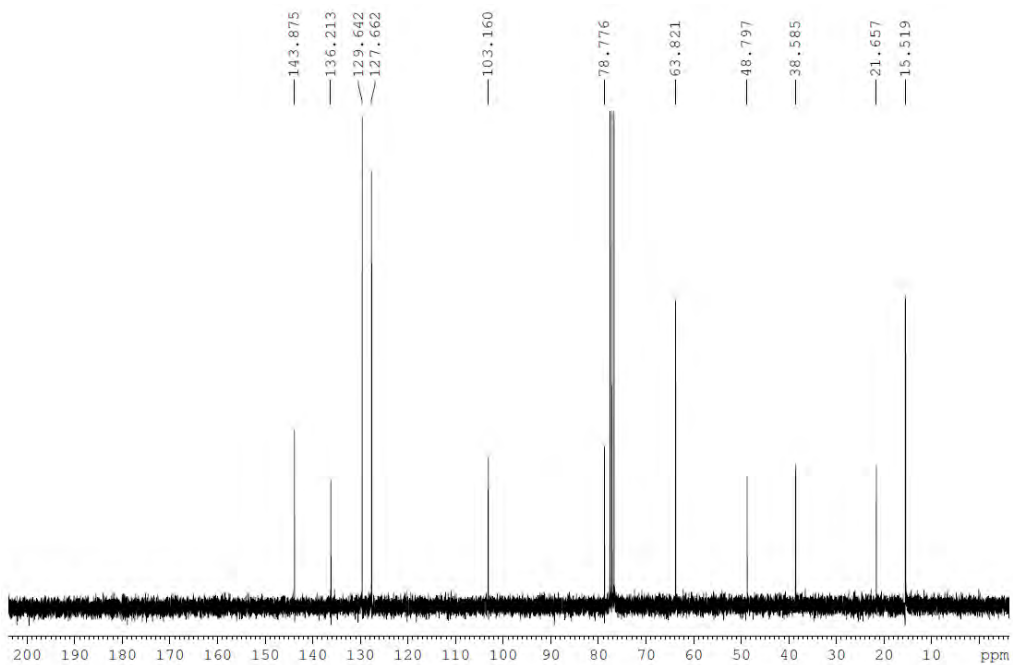
Figure S62: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **17a** in CDCl$_3$.
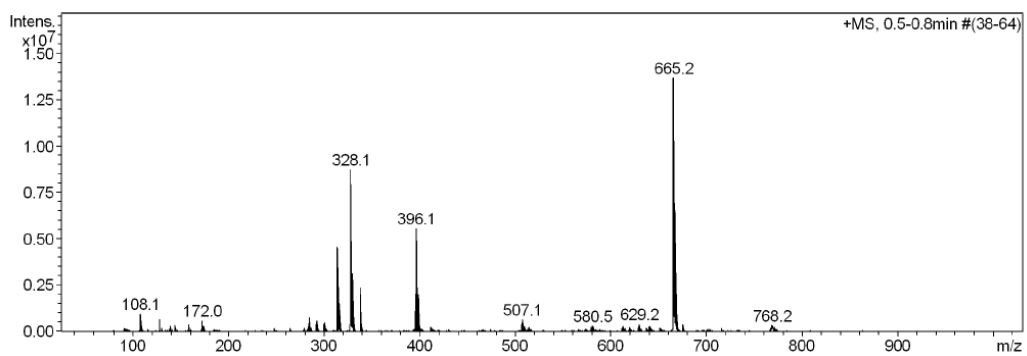
Figure S63: ESI-MS spectrum of **17a**.
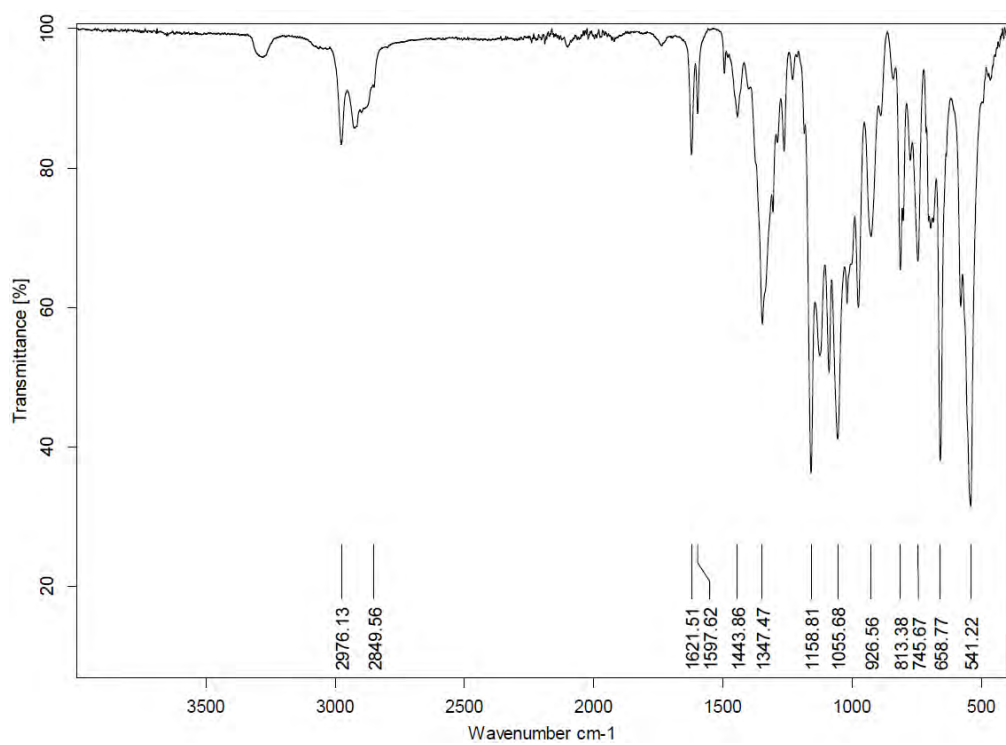
Figure S64: IR spectrum of **17a**.
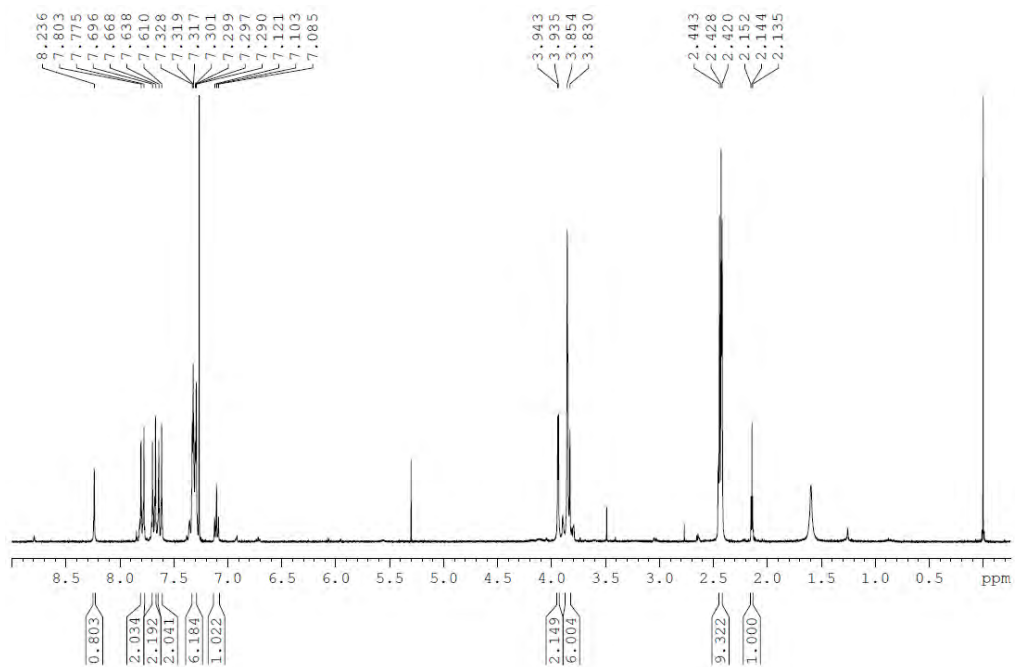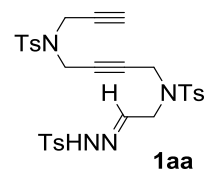
Figure S65: ^{1}H NMR spectrum (300 MHz) of **1aa** in CDCl$_3$.
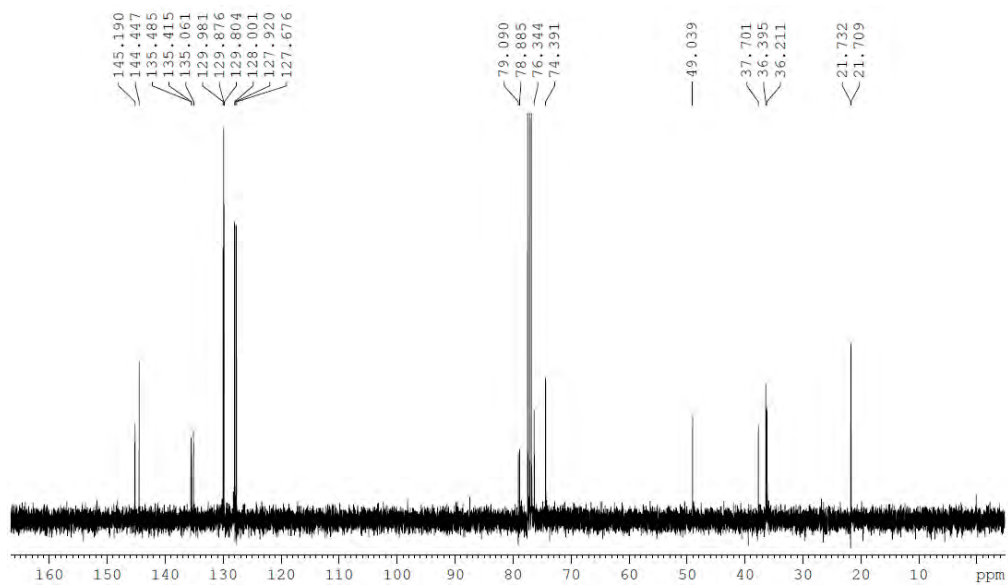
Figure S66: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **1aa** in CDCl$_3$.
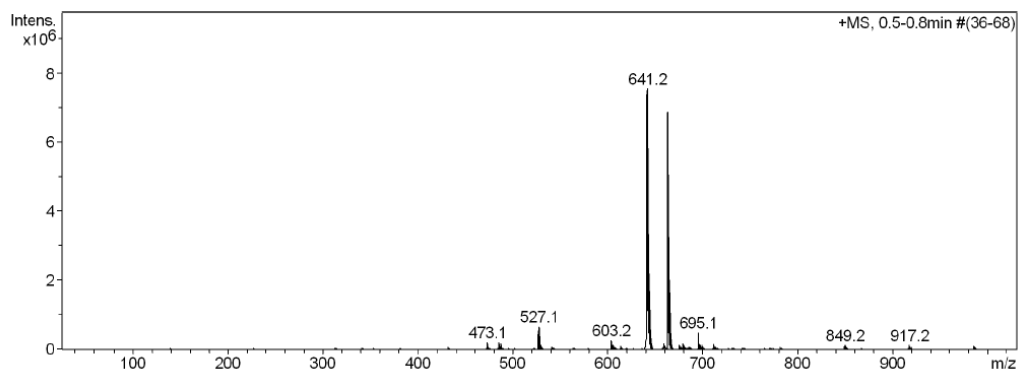
Figure S67: ESI-MS spectrum of **1aa**.
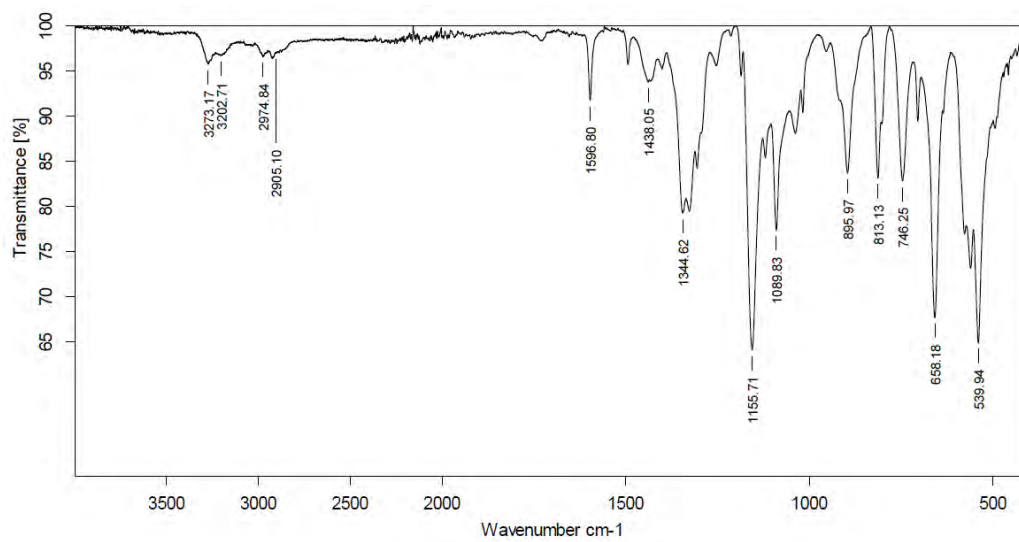
Figure S68: IR spectrum of **1aa**.
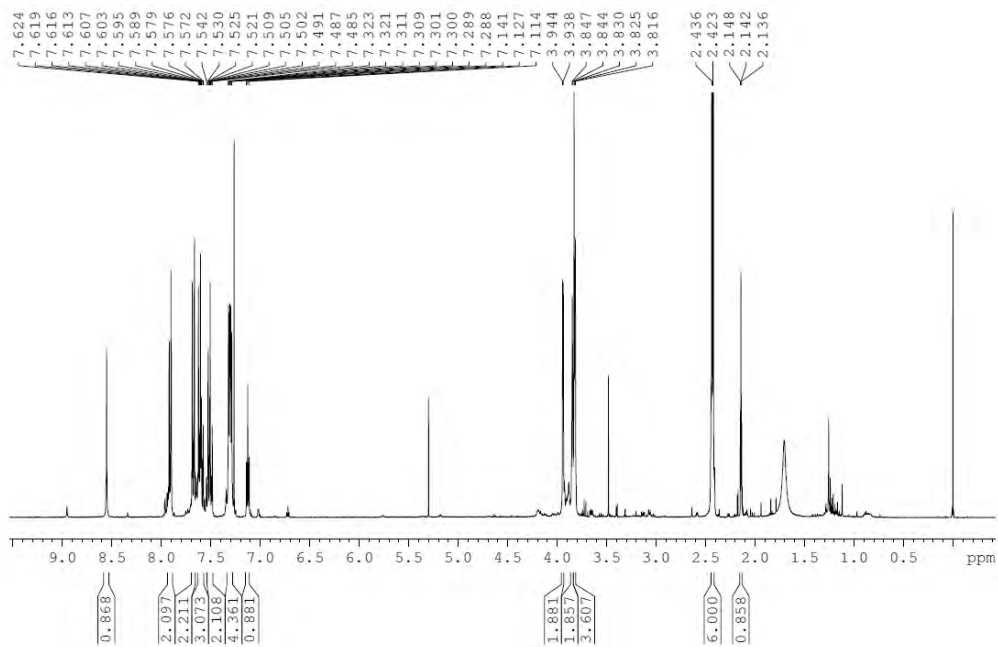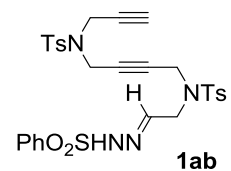
Figure S69: ^{1}H NMR spectrum (400 MHz) of **1ab** in CDCl$_3$.
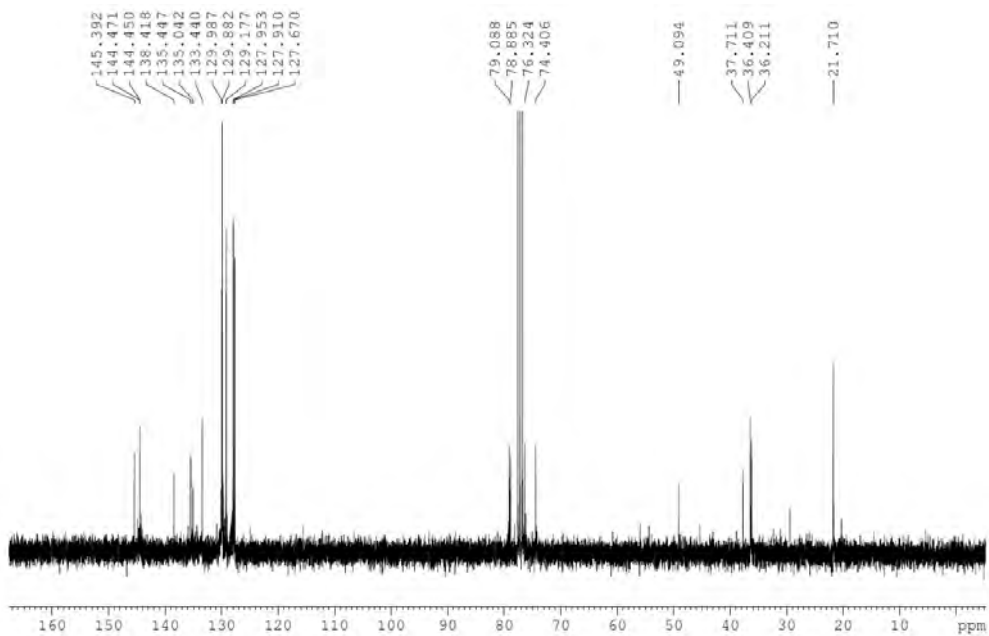
Figure S70: ESI-MS spectrum of **1ab**.
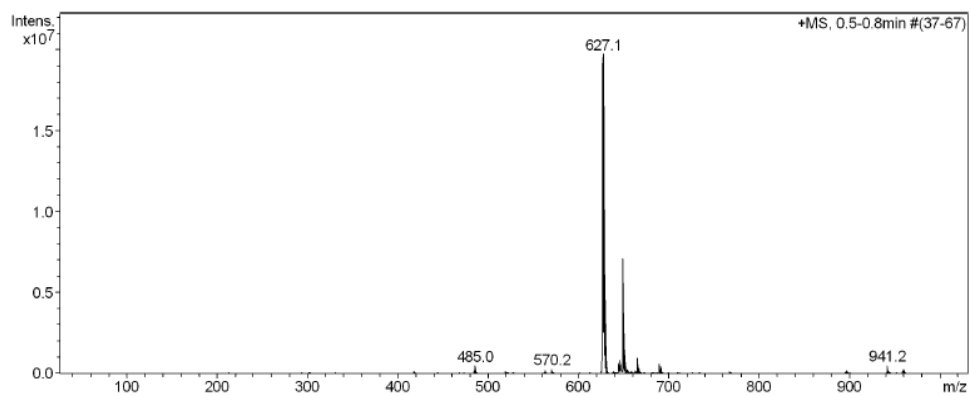
Figure S71: ESI-MS spectrum of **1ab**.
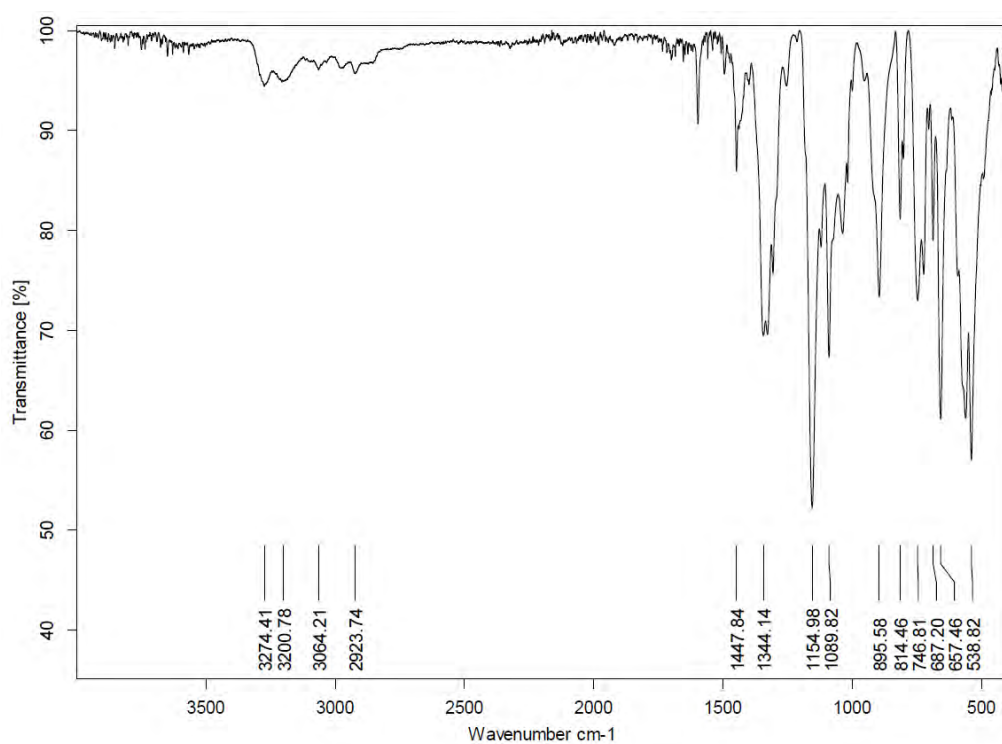
Figure S72: IR spectrum of **1ab**.
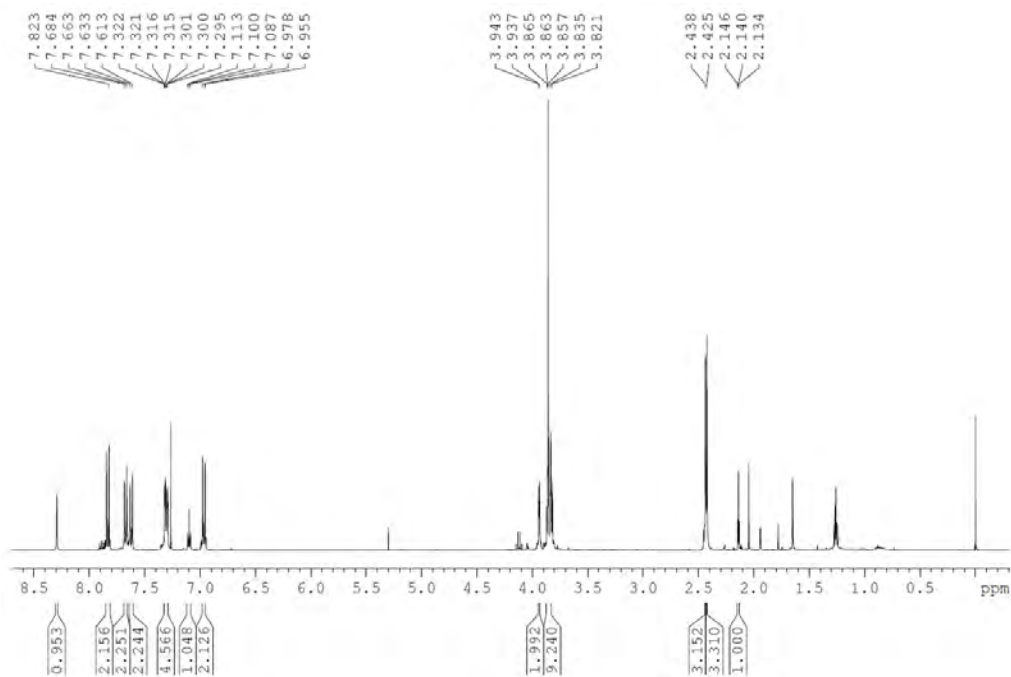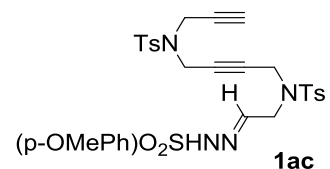
Figure S73: ^{1}H NMR spectrum (400 MHz) of **1ac** in CDCl$_3$.
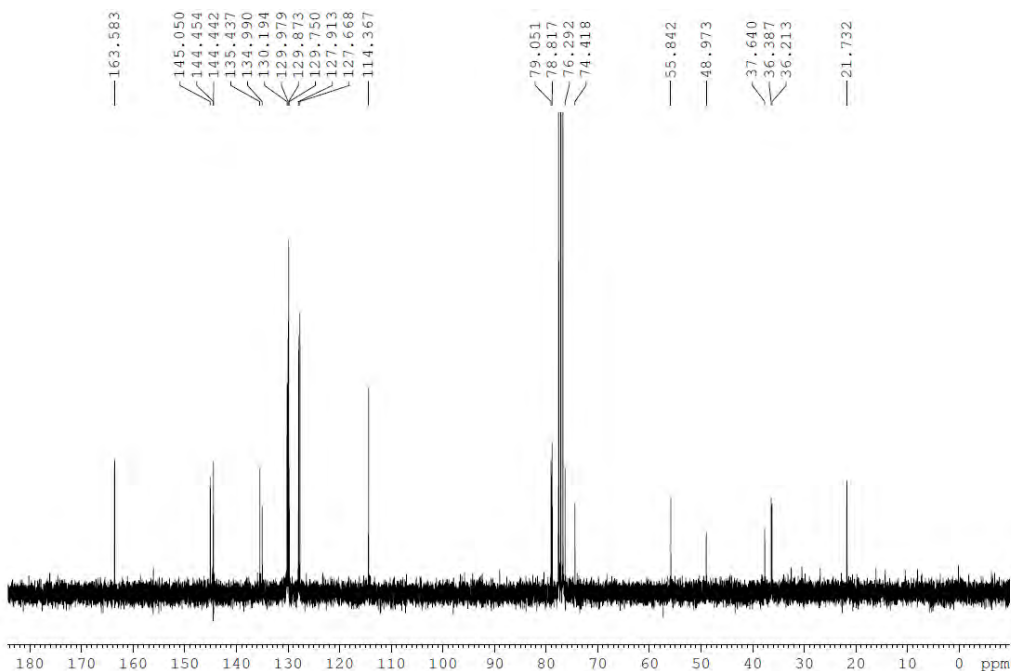
Figure S74: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **1ac** in CDCl$_3$.
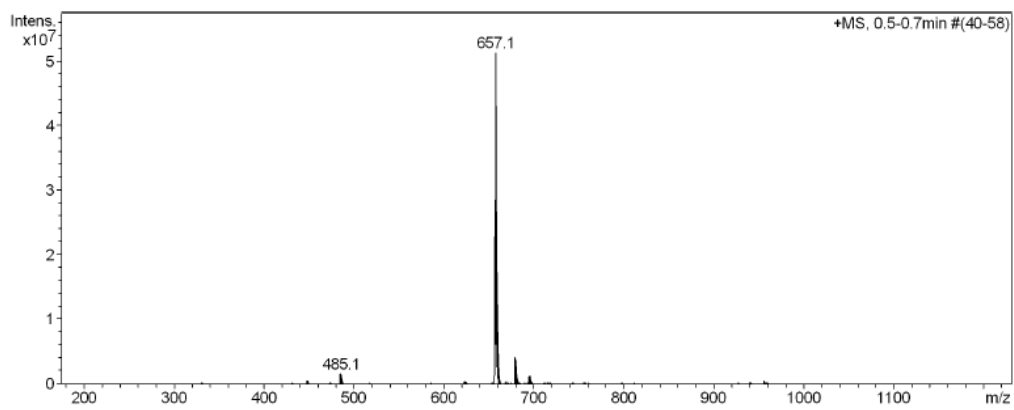
Figure S75: ESI-MS spectrum of **1ac**.
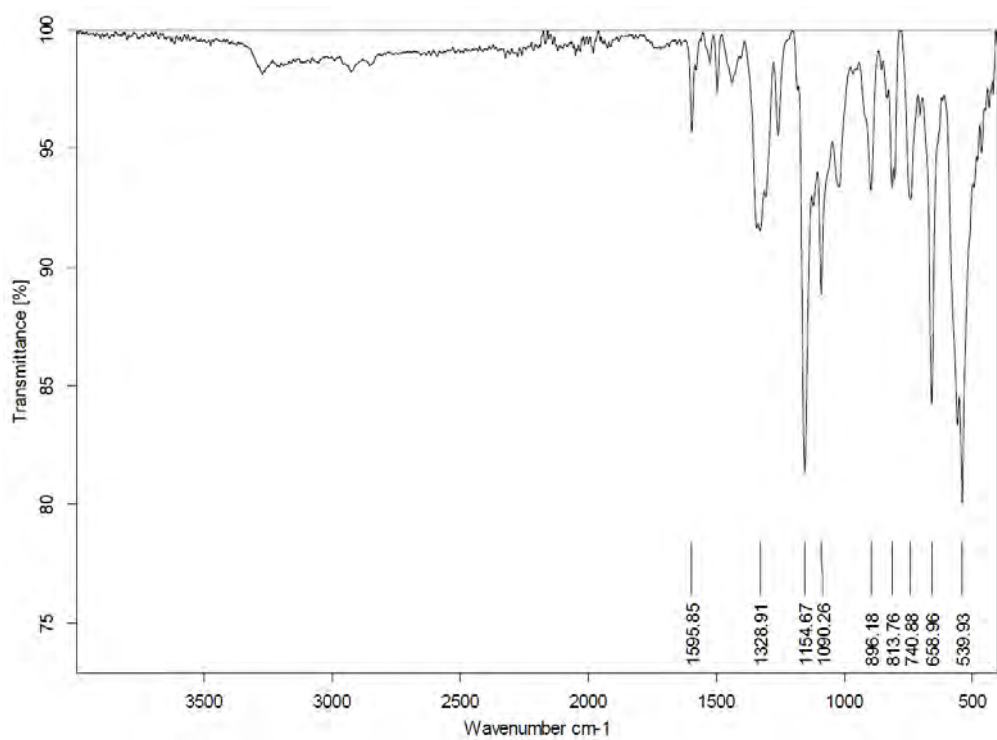
Figure S76: IR spectrum of **1ac**.
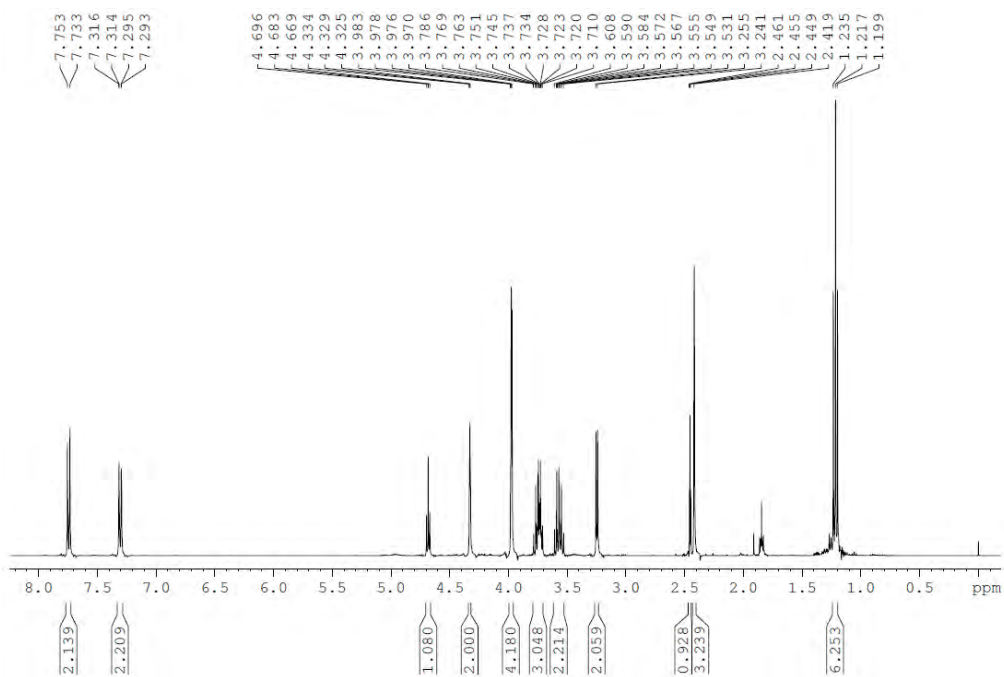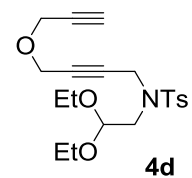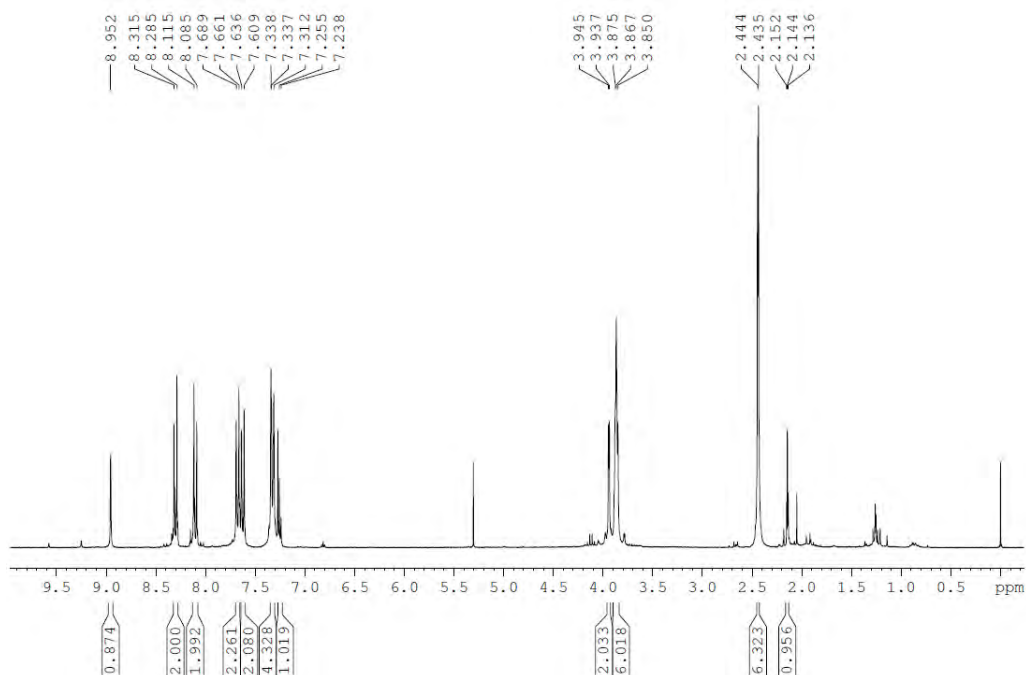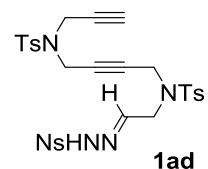
Figure S77: ^{1}H NMR spectrum (300 MHz) of **1ad** in CDCl$_3$.
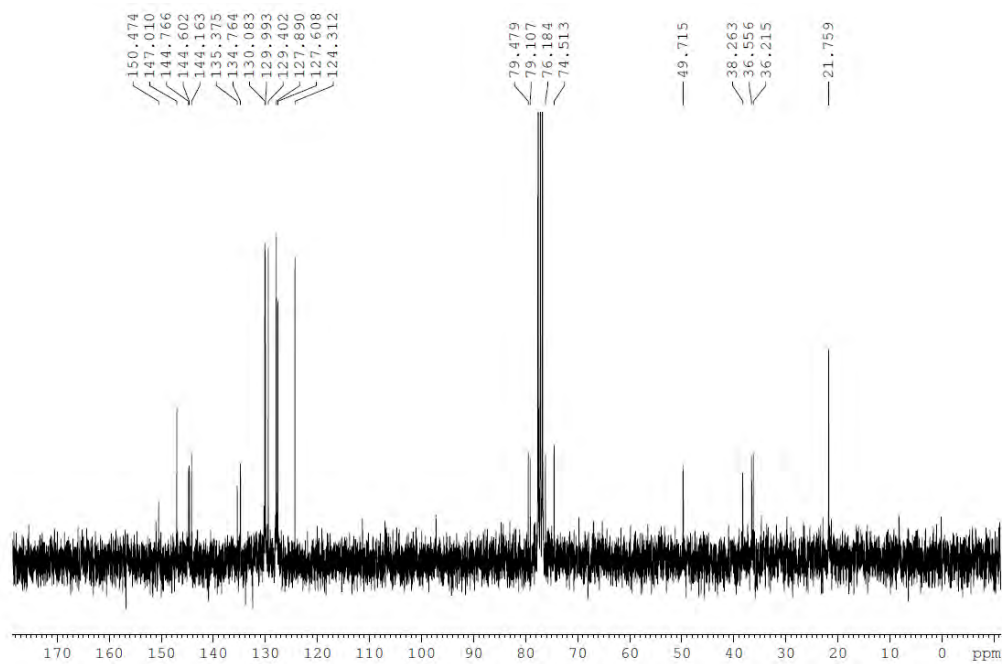
Figure S78: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **1ad** in CDCl$_3$.
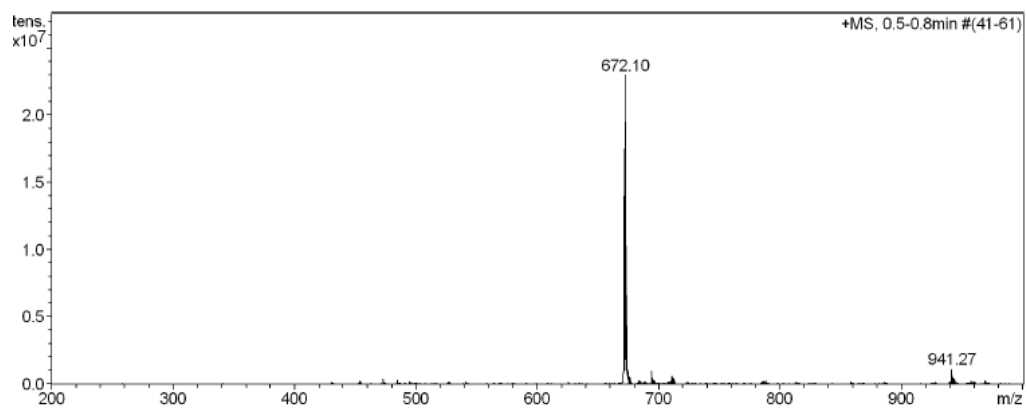
Figure S79: ESI-MS spectrum of **1ad**.
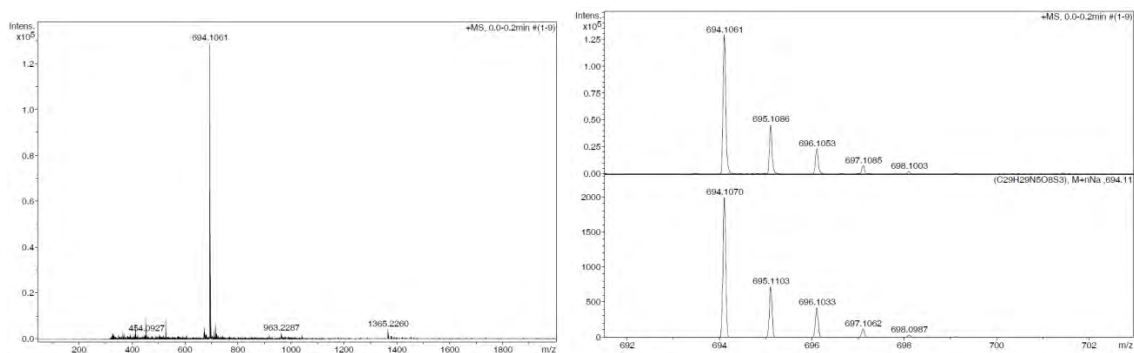
Figure S80: ESI-HRMS spectrum of **1ad**.
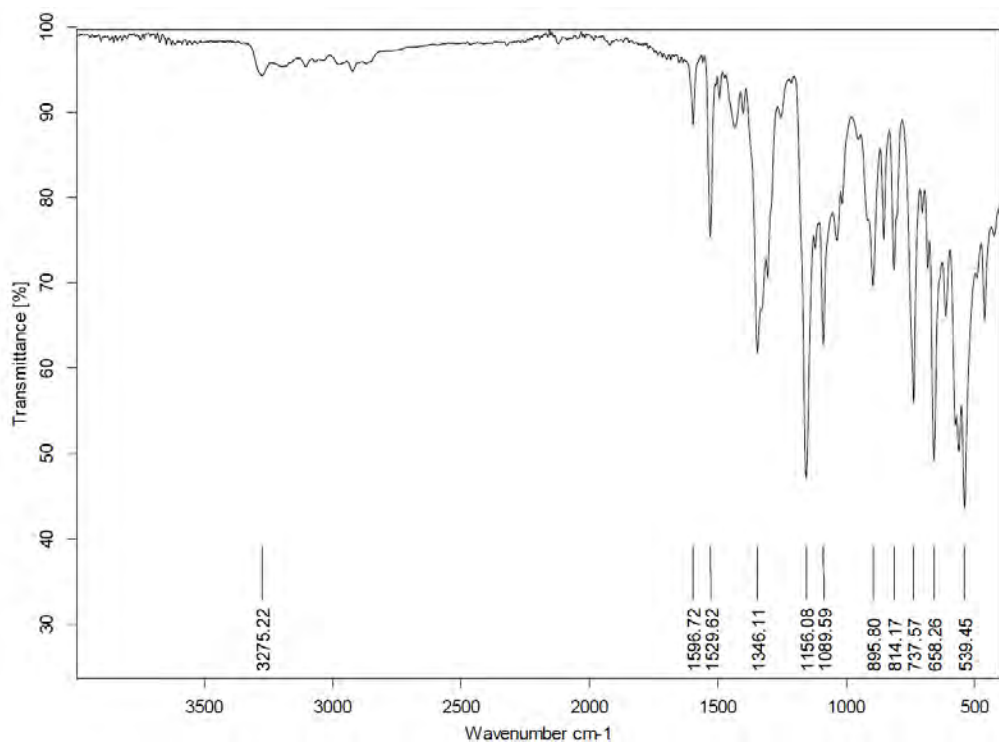
Figure S81: IR spectrum of **1ad**.
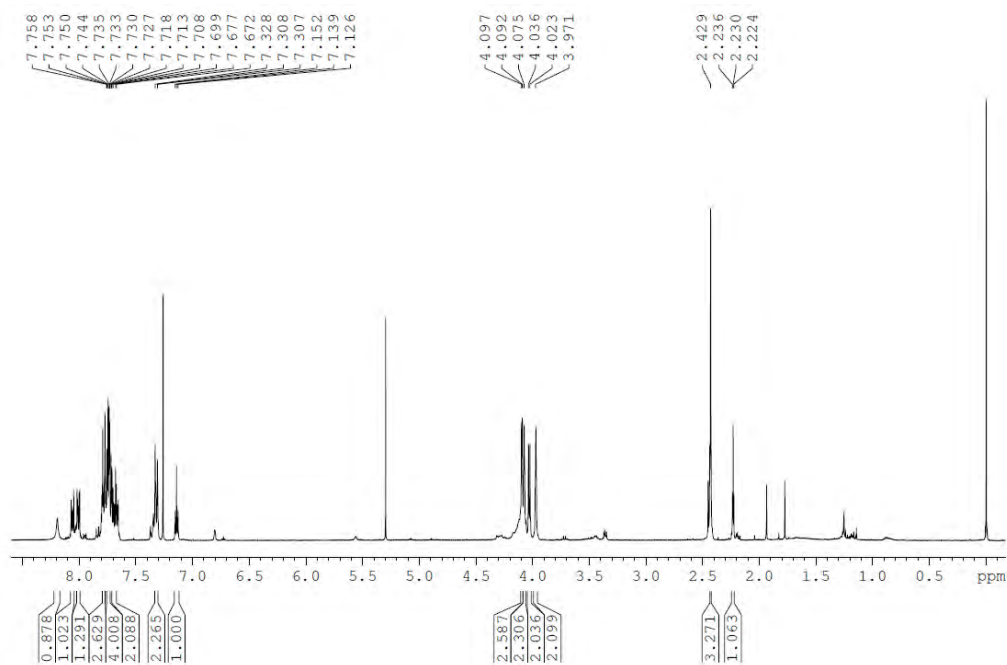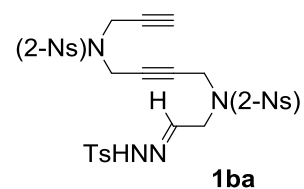
Figure S82: ^{1}H NMR spectrum (400 MHz) of **1ba** in CDCl$_3$.
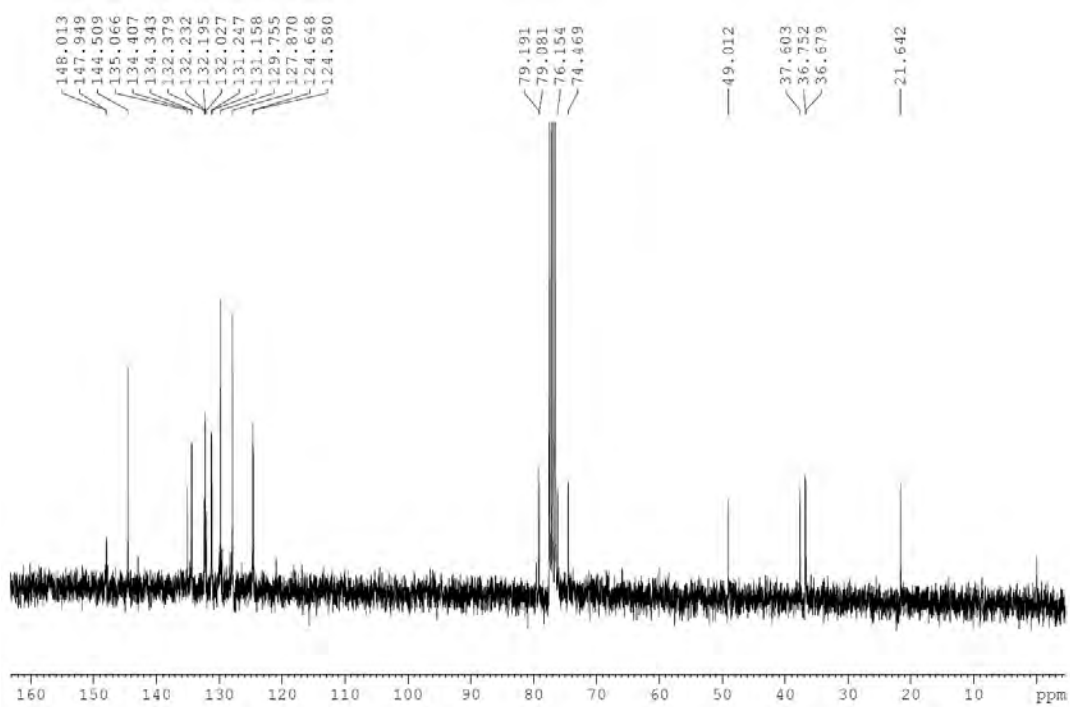
Figure S83: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **1ba** in CDCl$_3$.
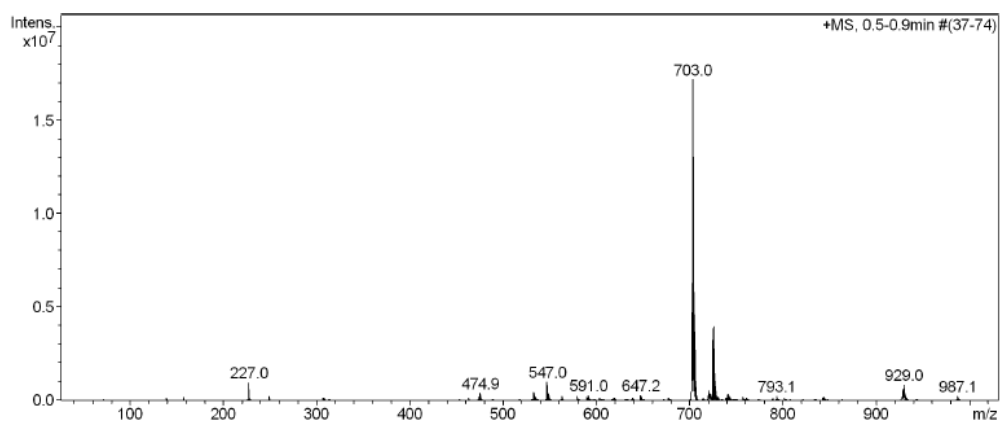
Figure S84: ESI-MS spectrum of **1ba**.
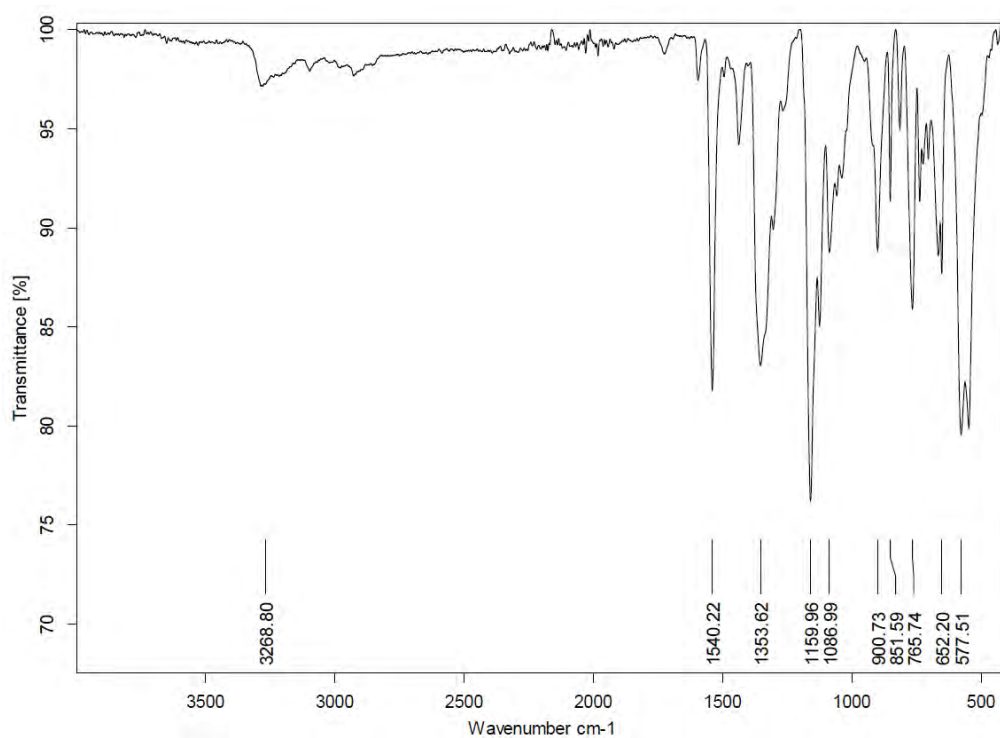
Figure S85: IR spectrum of **1ba**.
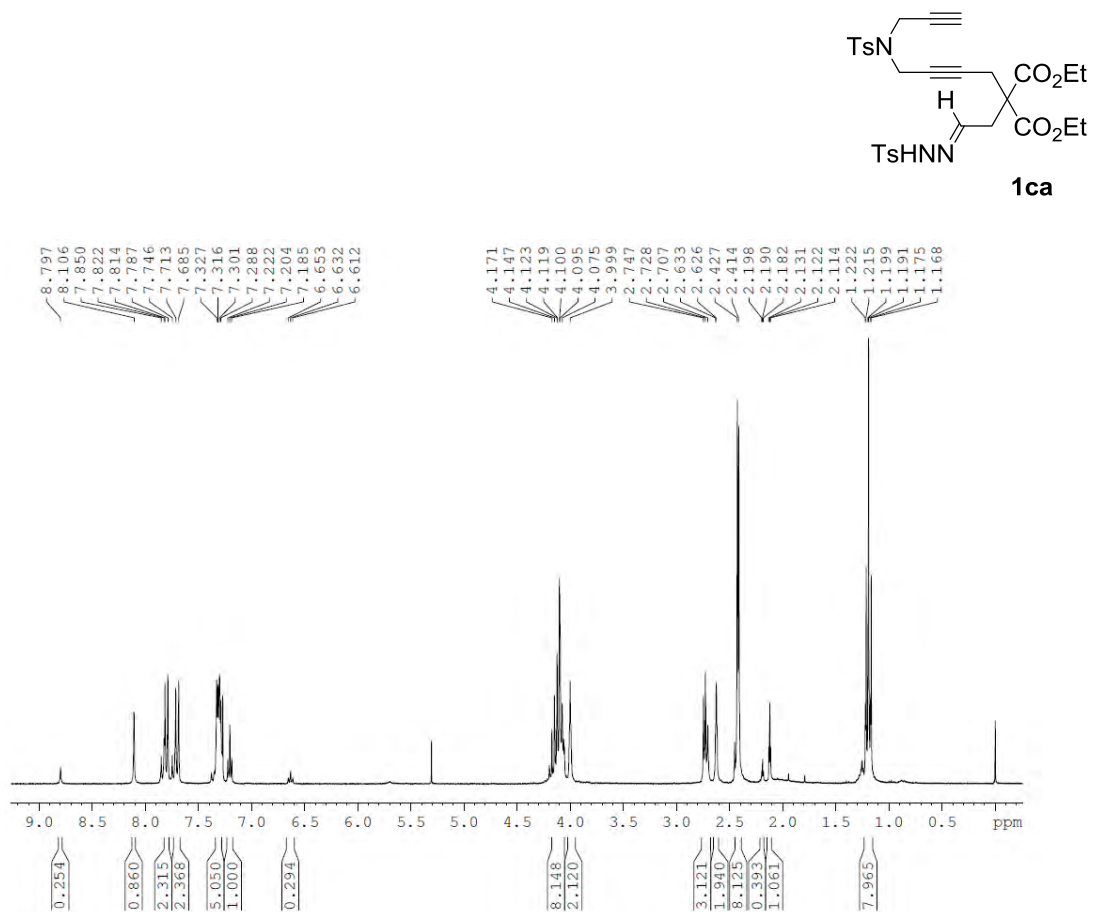
Figure S86: ^{1}H NMR spectrum (300 MHz) of **1ca** in CDCl$_3$.
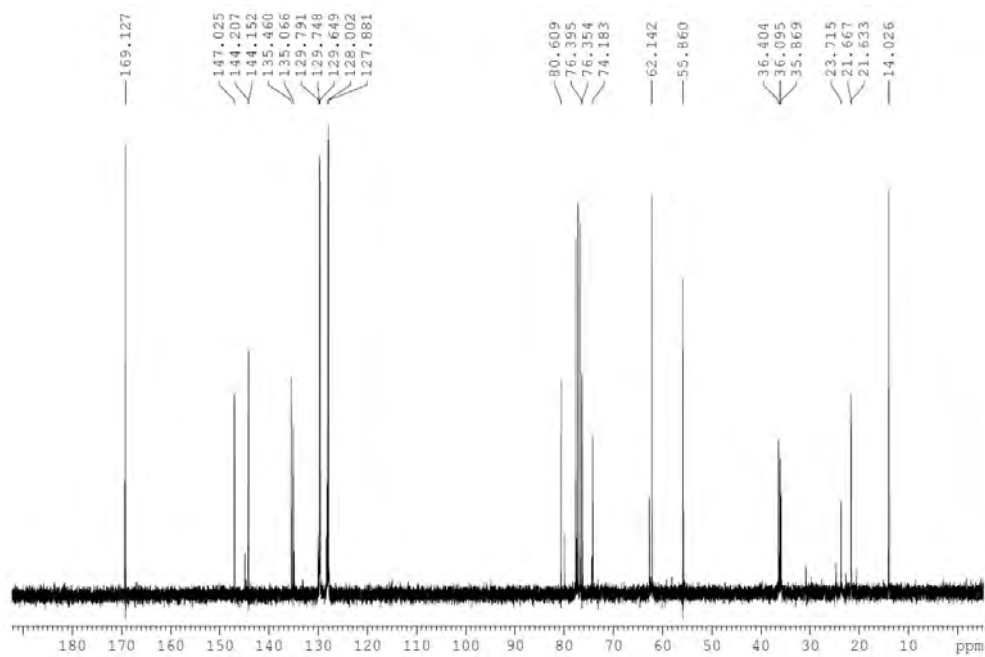
Figure S87: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **1ca** in CDCl$_3$.
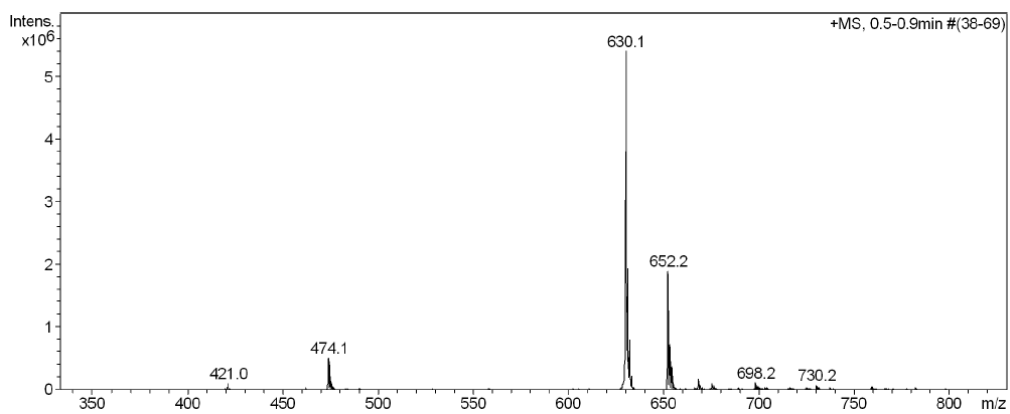
Figure S88: ESI-MS spectrum of **1ca**.
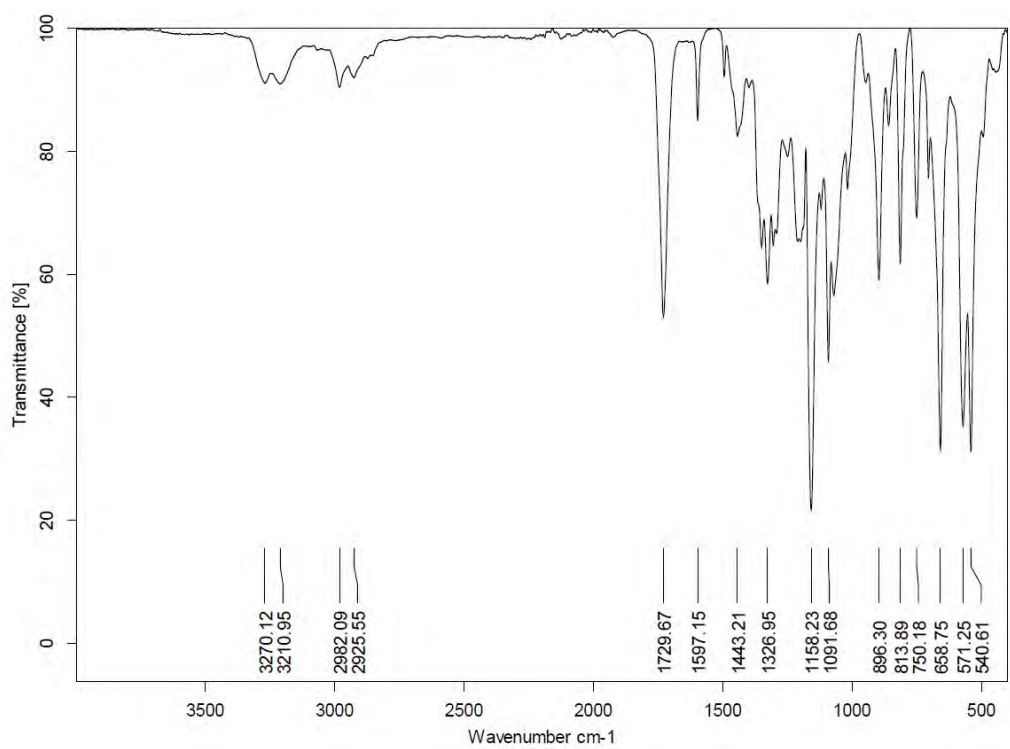
Figure S89: IR spectrum of **1ca**.
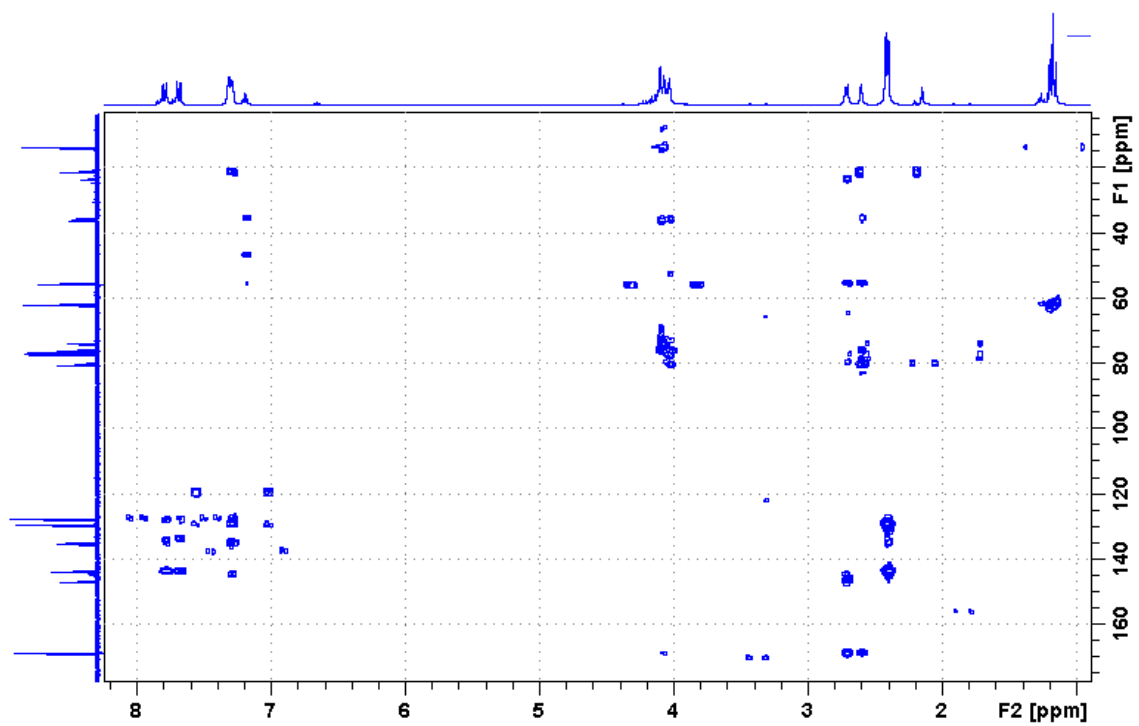
Figure S90: 2D ^{1}H-^{13}C HMBC correlation of **1ca** in CDCl$_3$.
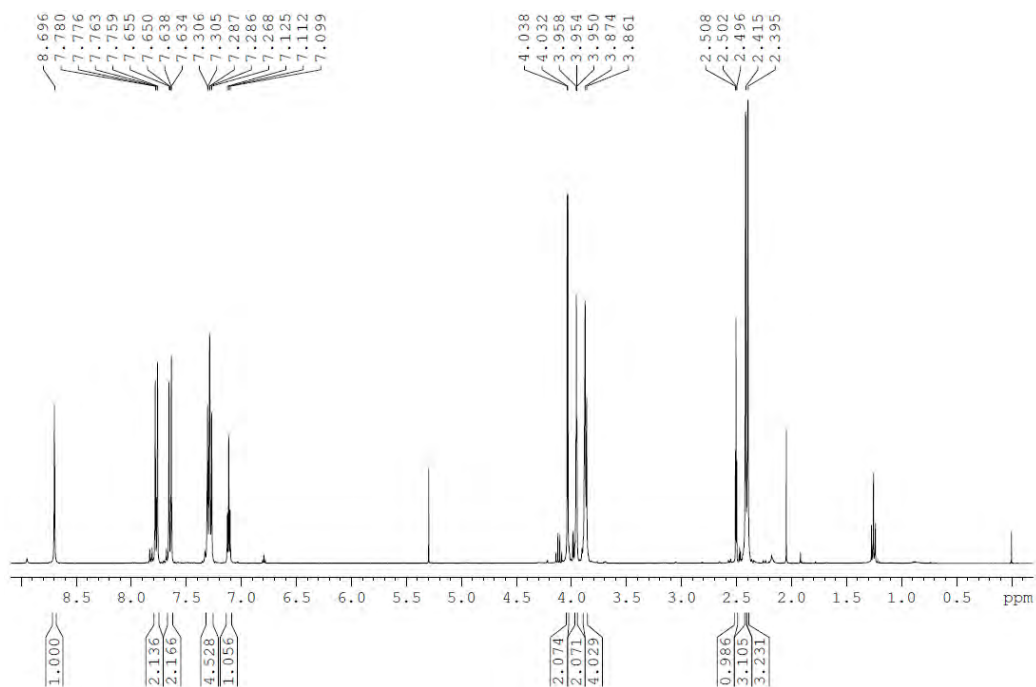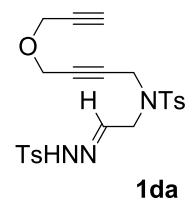
Figure S91: ^{1}H NMR spectrum (400 MHz) of **1da** in CDCl$_3$.
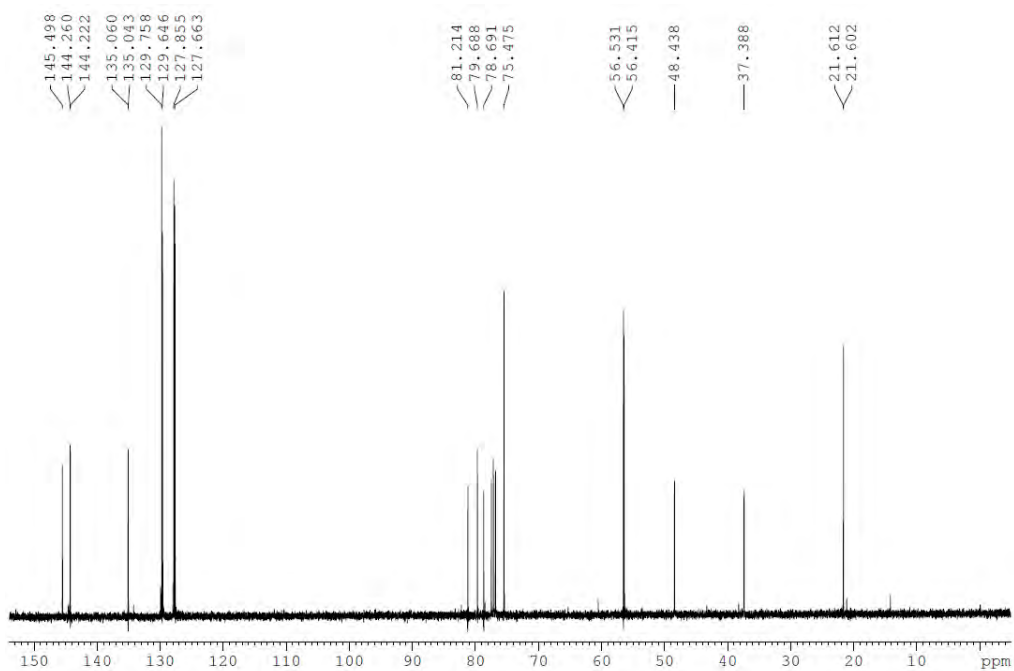
Figure S92: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **1da** in CDCl$_3$.
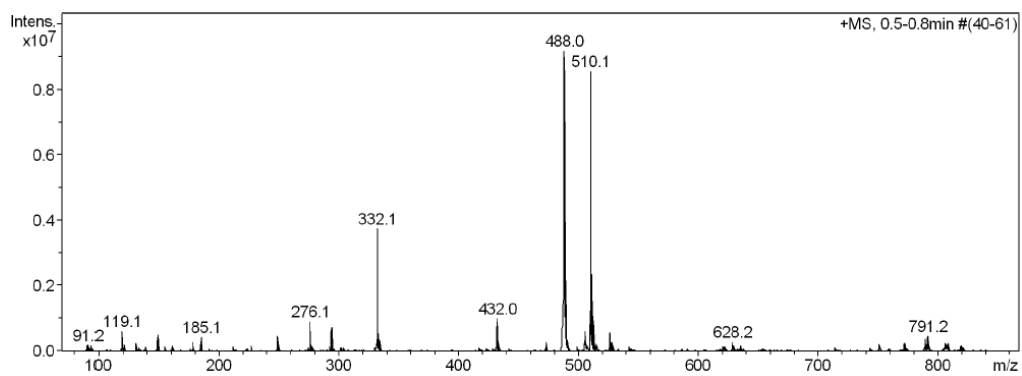
Figure S93: ESI-MS spectrum of **1da**.
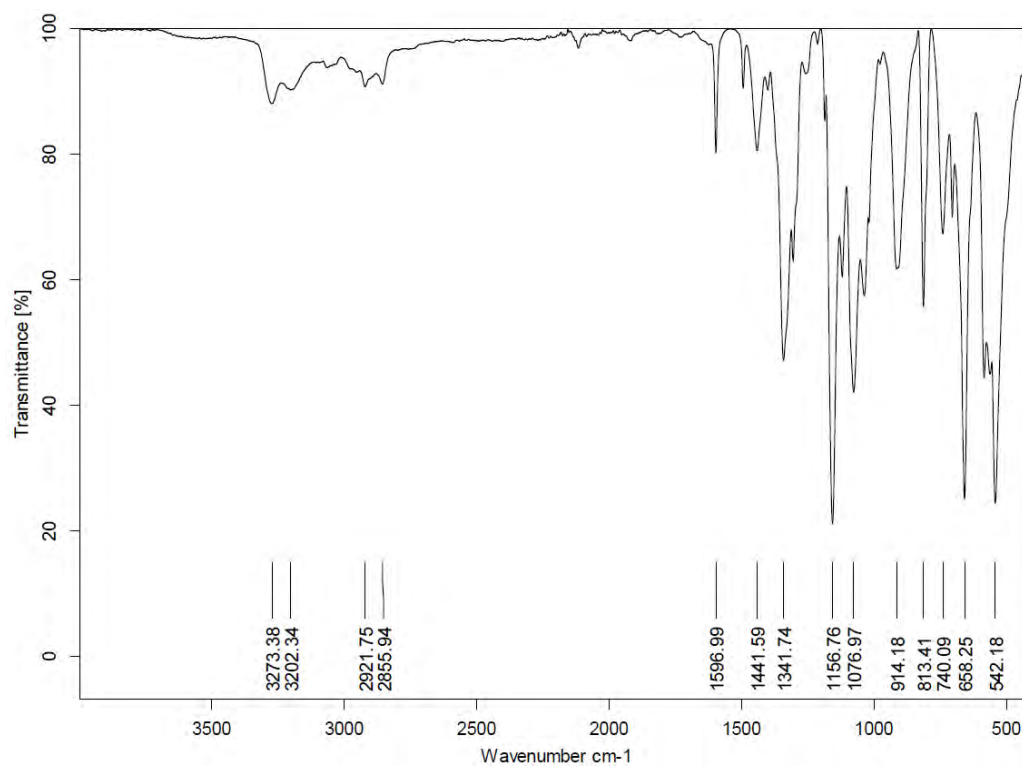
Figure S94: IR spectrum of **1da**.
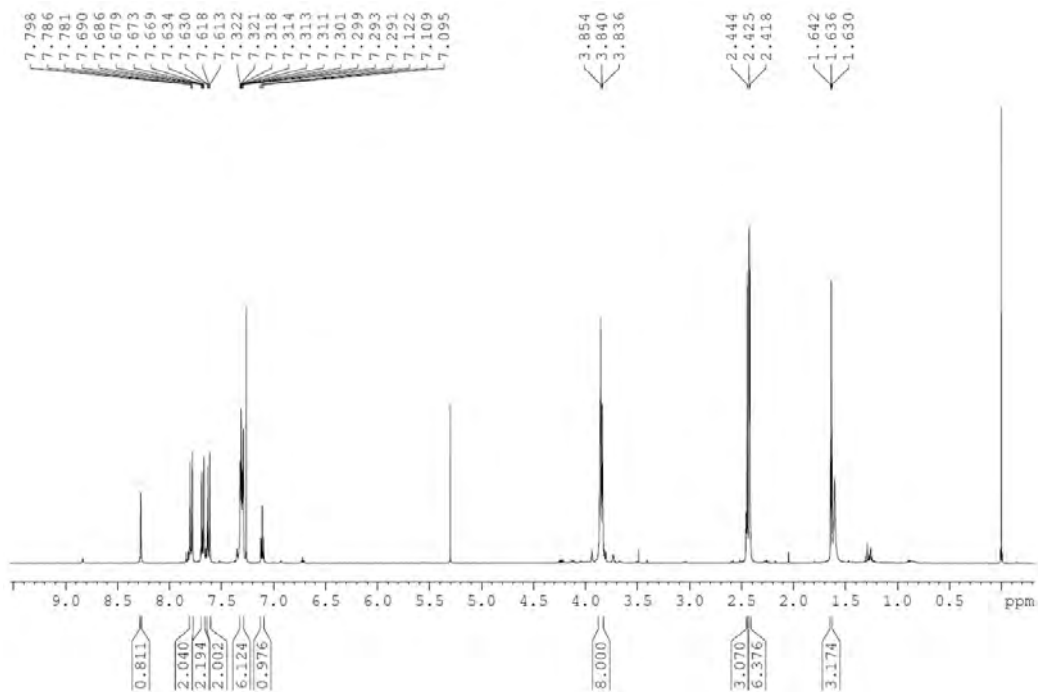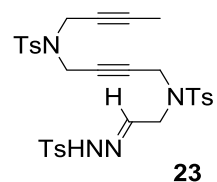
Figure S95: ^{1}H NMR spectrum (400 MHz) of **23** in CDCl$_3$.
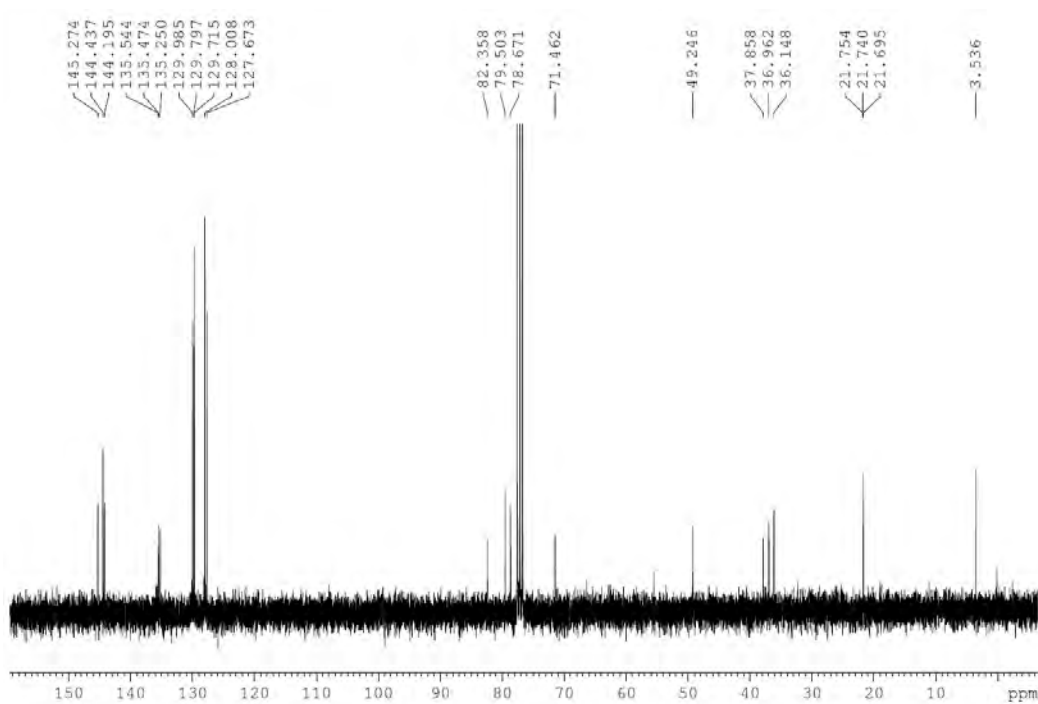
Figure S96: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **23** in CDCl$_3$.
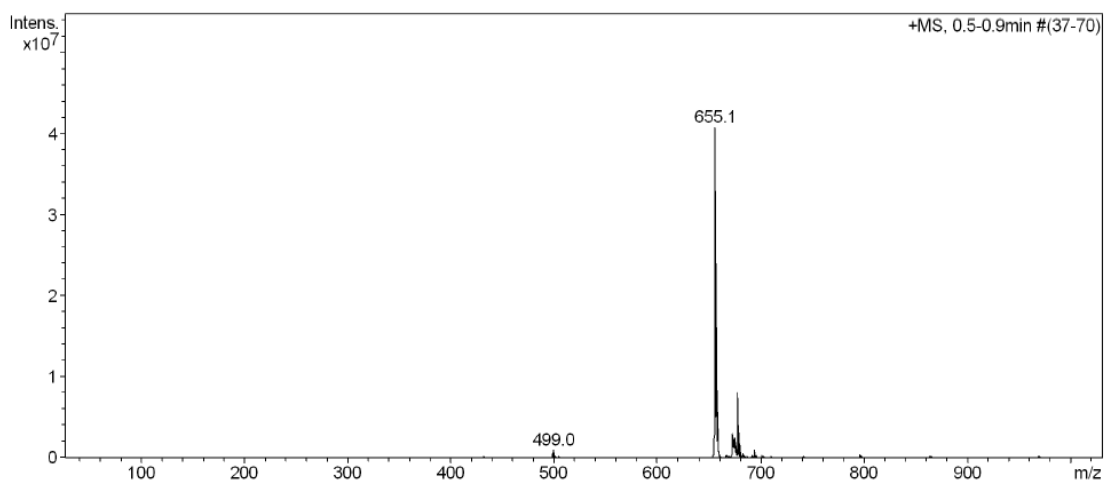
Figure S97: ESI-MS spectrum of **23**.
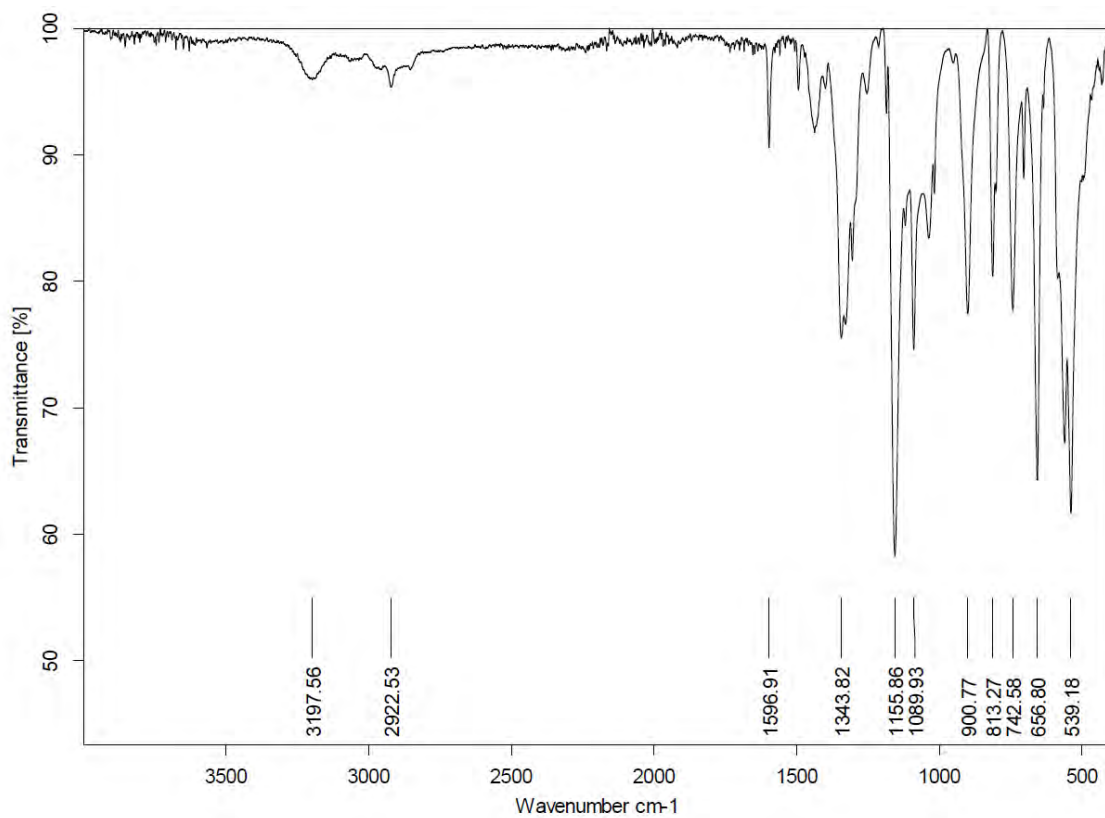
Figure S98: IR spectrum of **23**.
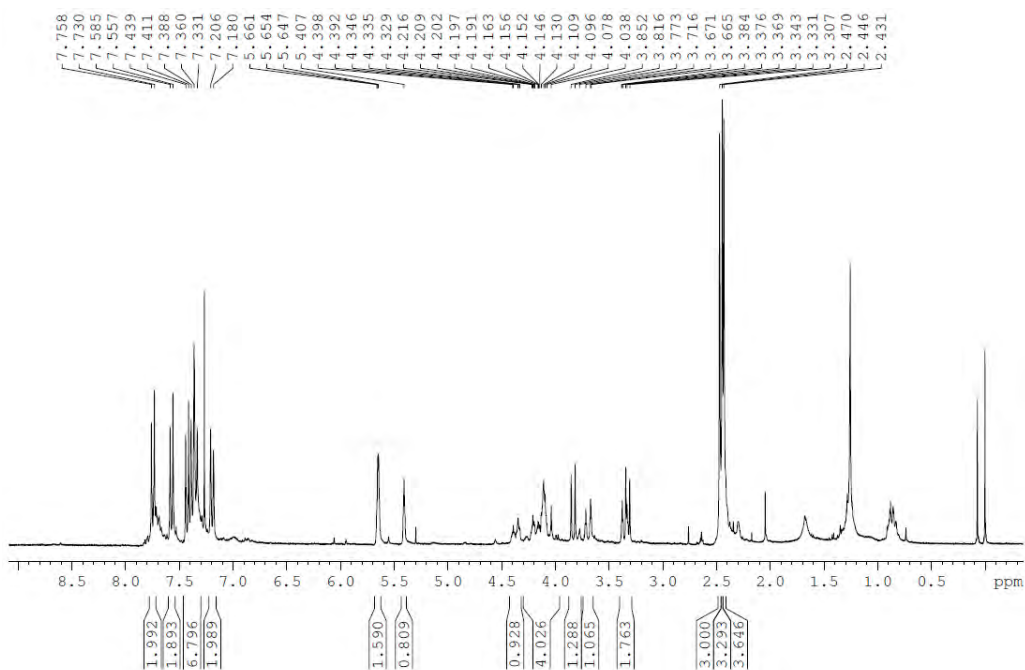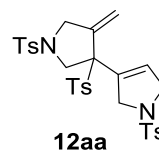
Figure S99: ^{1}H NMR spectrum (400 MHz) of **12aa** in CDCl$_3$.
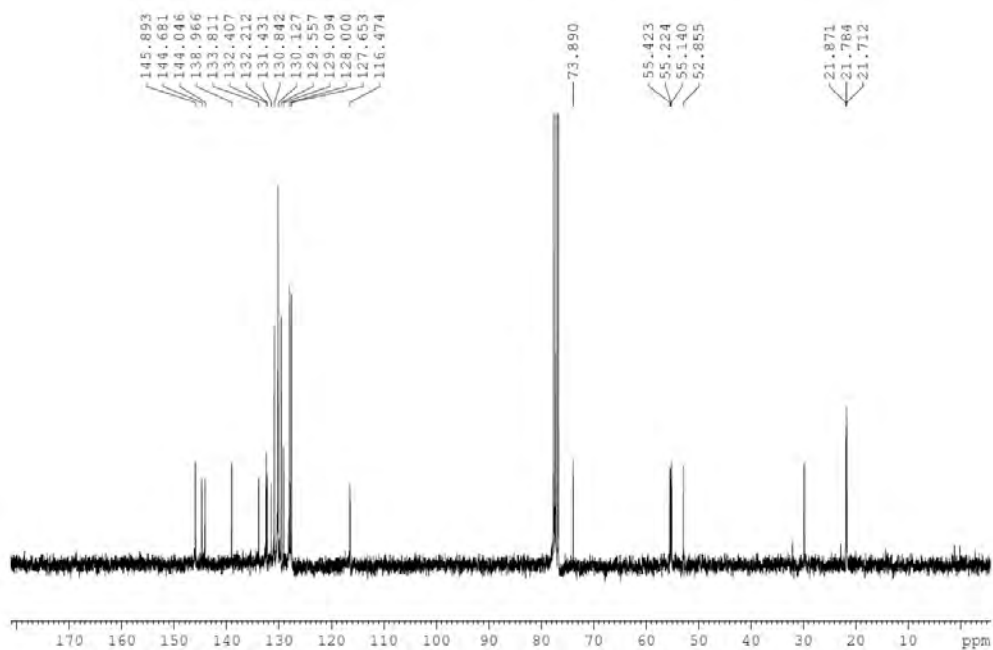
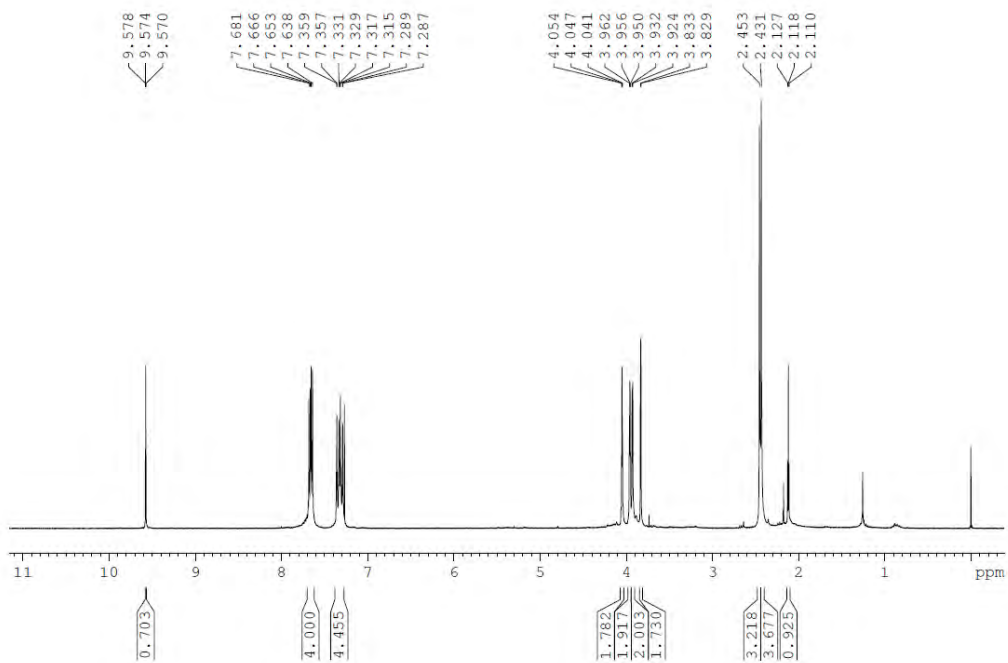**Figure S100**: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **12aa** in CDCl$_3$.
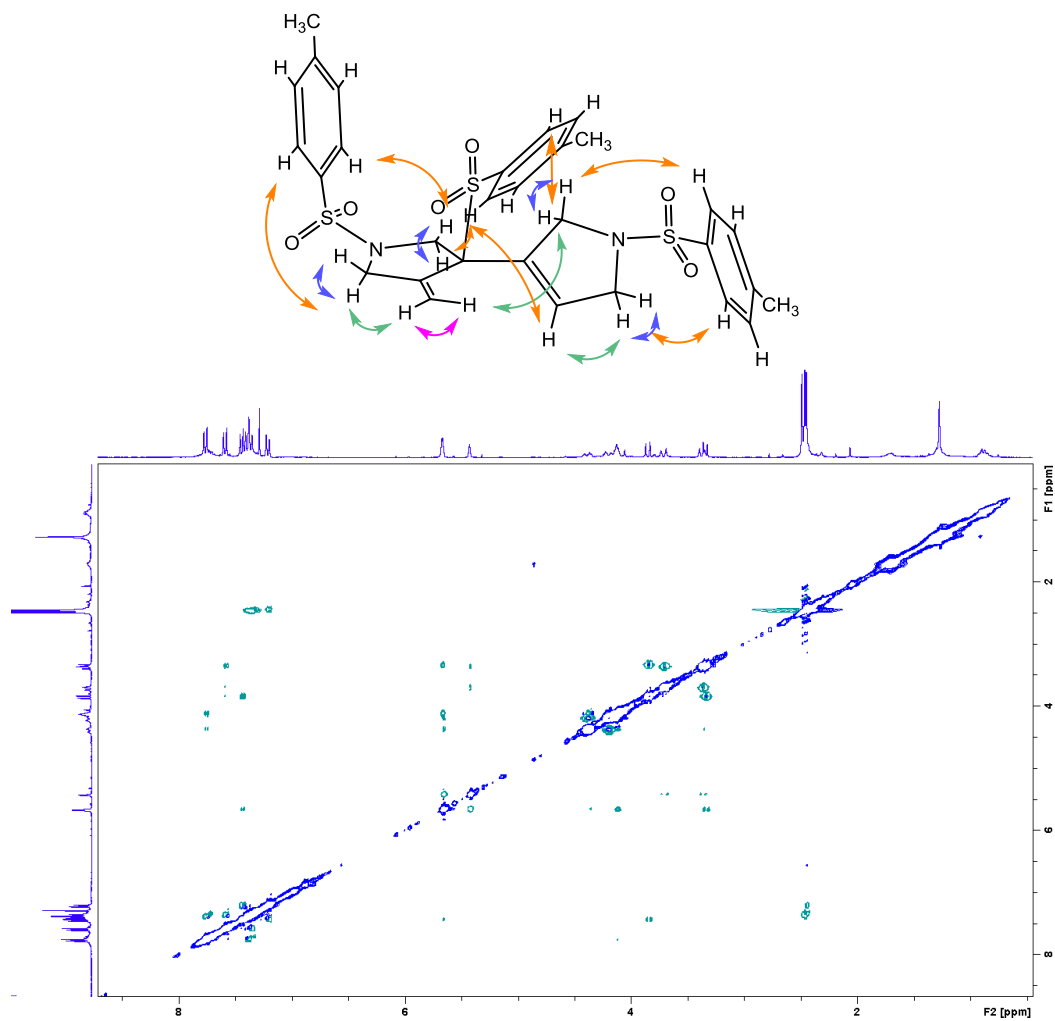
Figure S101: 2D [1]H-^{1}H NOESY correlation of **2aa** in CDCl₃.
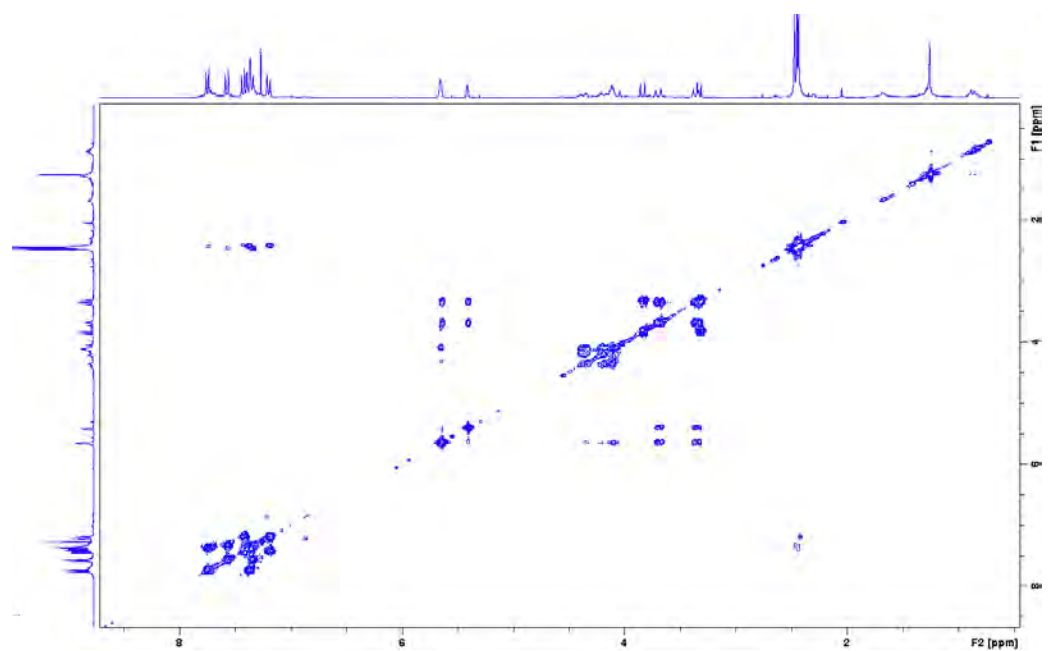
Figure S102: 2D ^{1}H-^{1}H COSY correlation of **12aa** in CDCl₃.
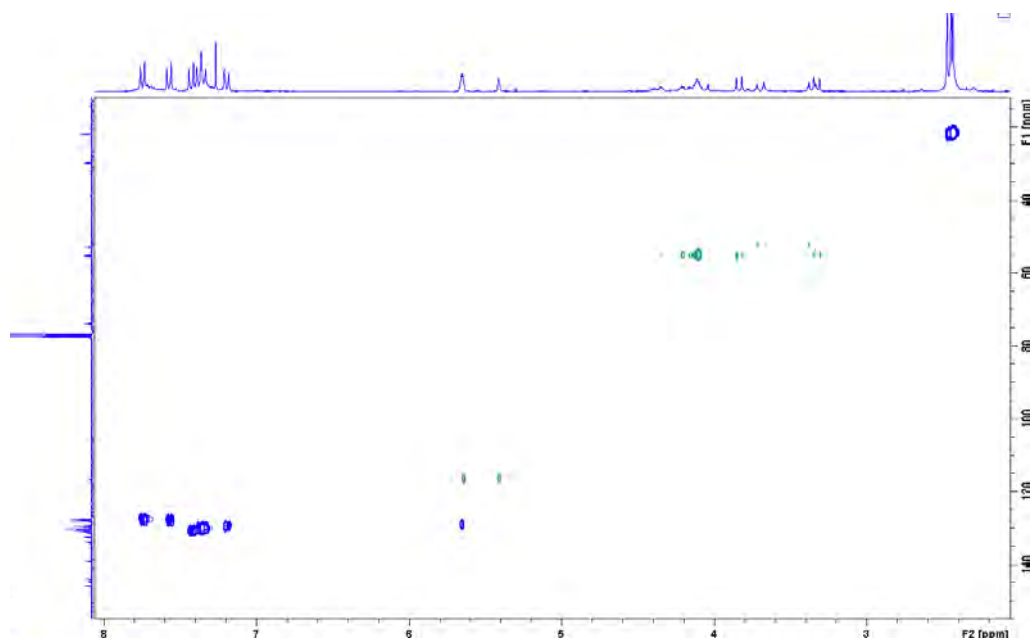
Figure S103: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **12aa** in CDCl$_3$.
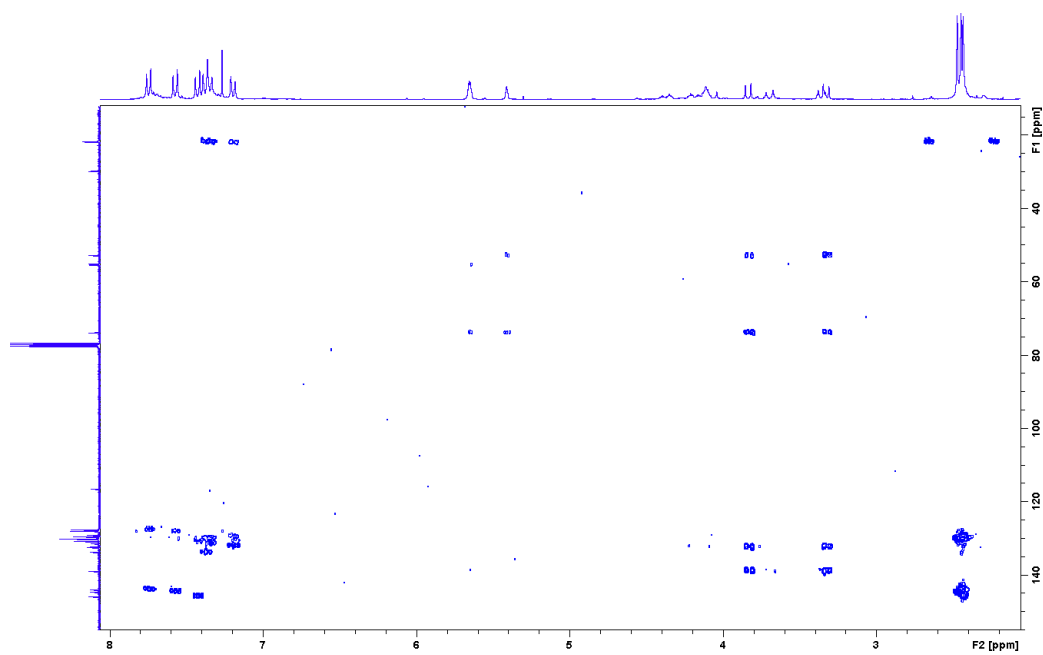
Figure S104: 2D ^{1}H-^{13}C HMBC correlation of **12aa** in CDCl$_3$.
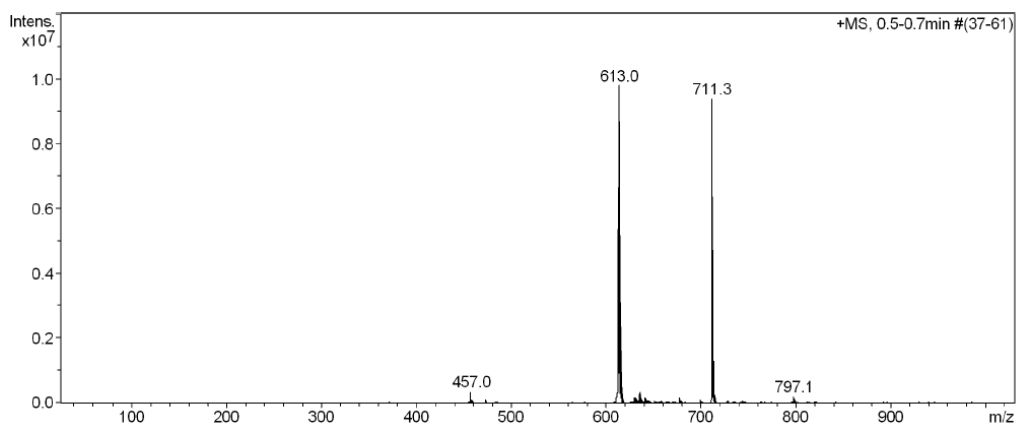
Figure S105: ESI-MS spectrum of **12aa**.
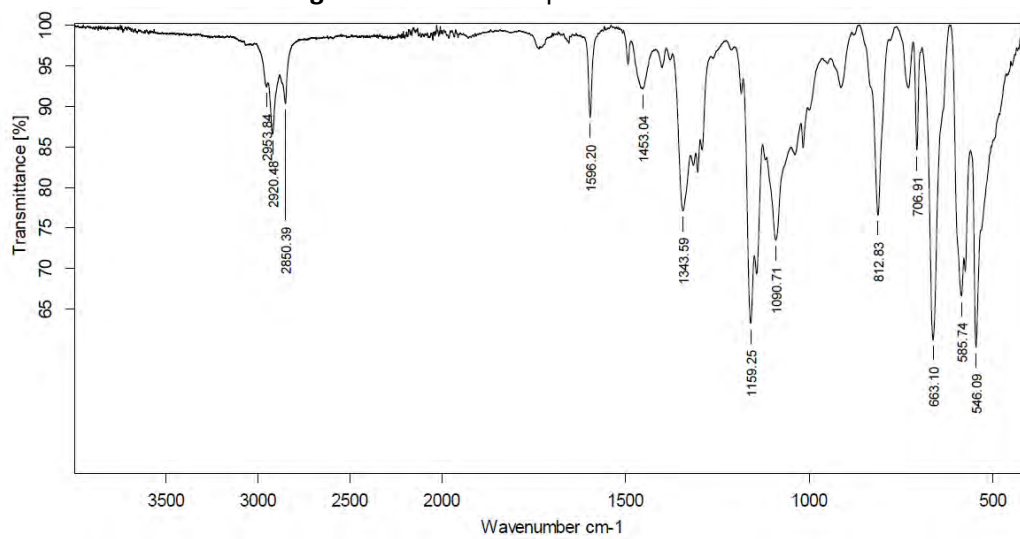
Figure S106: IR spectrum of **12aa**.
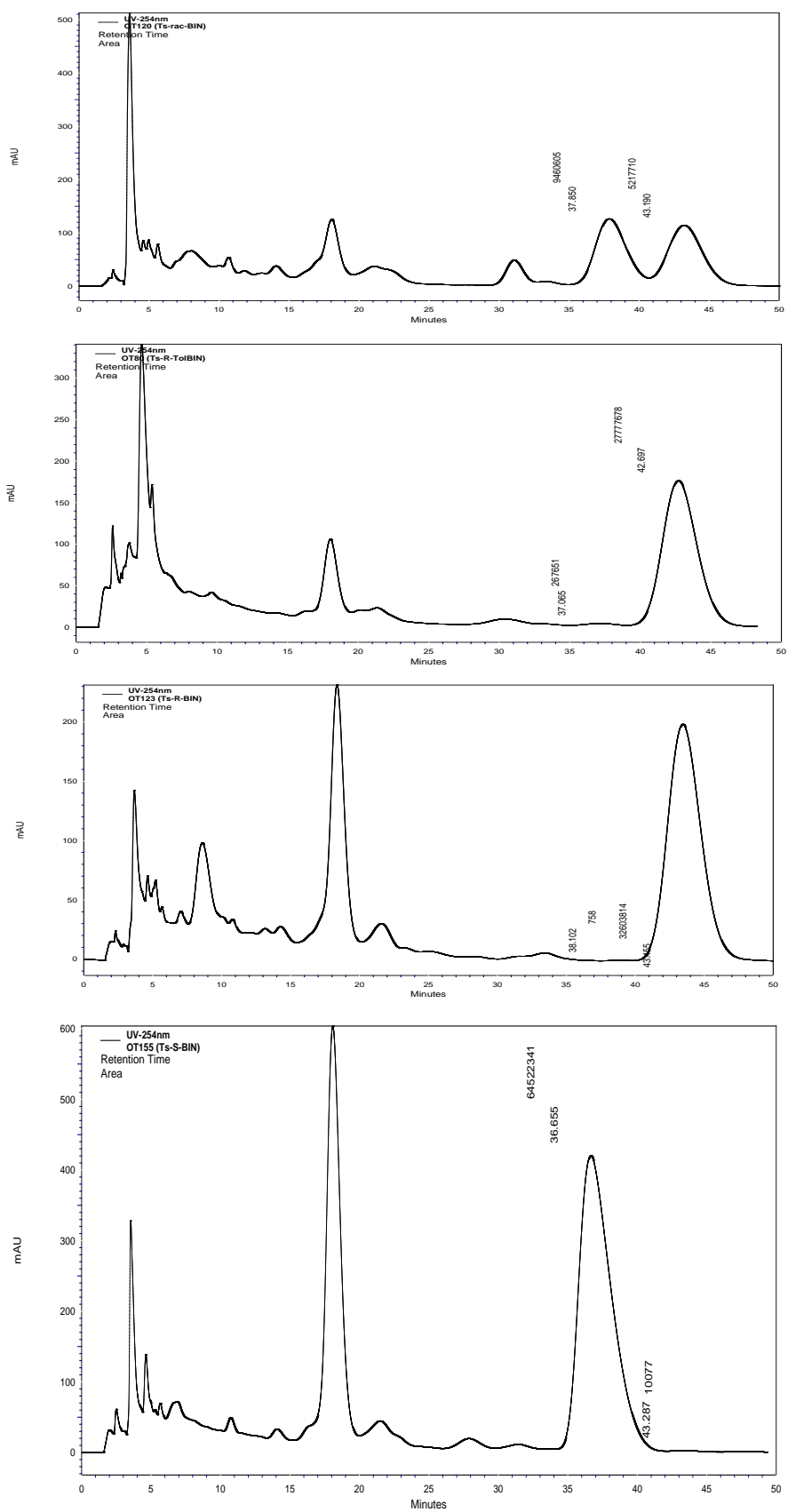
Figure S107: HPLC chromatograms with *rac*-BINAP, Tol-BINAP, *(R)-(+)*-BINAP and *(S)-(-)*-BINAP for **12aa**.
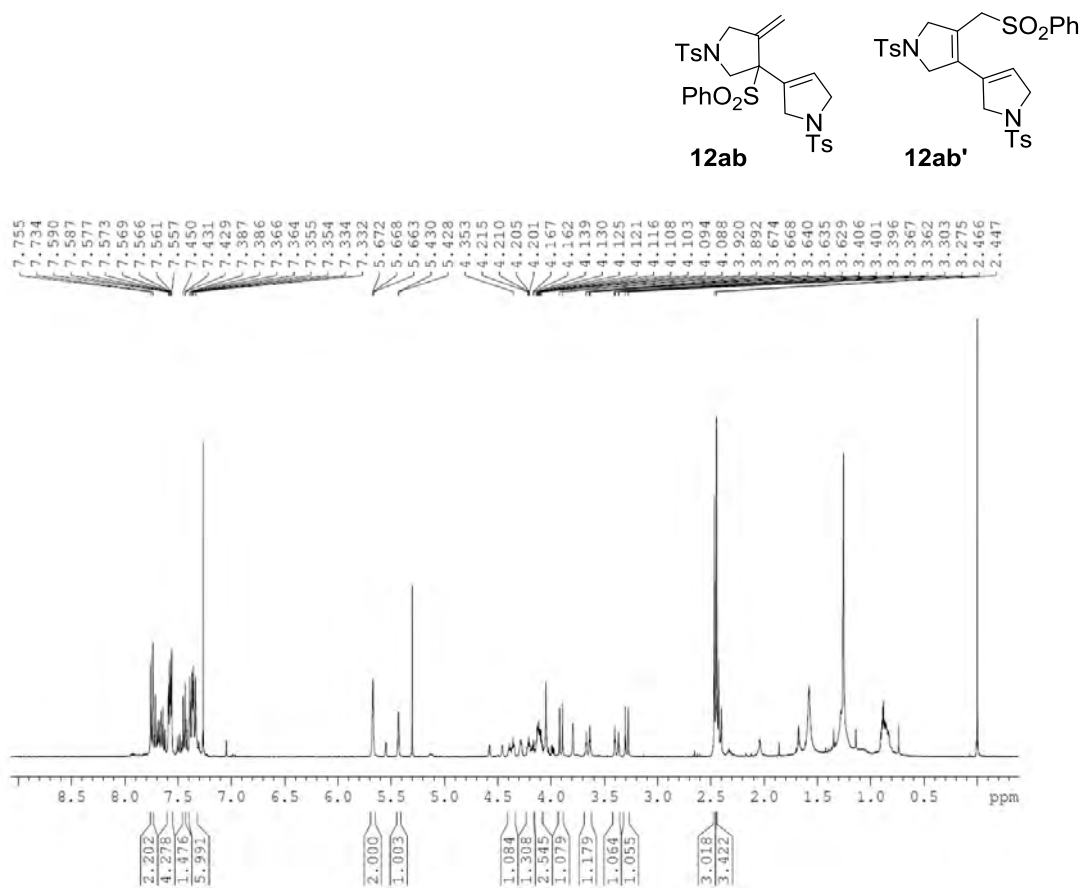
Figure S108: ^{1}H NMR spectrum (400 MHz) of **12ab** and **12ab'** in CDCl$_3$.
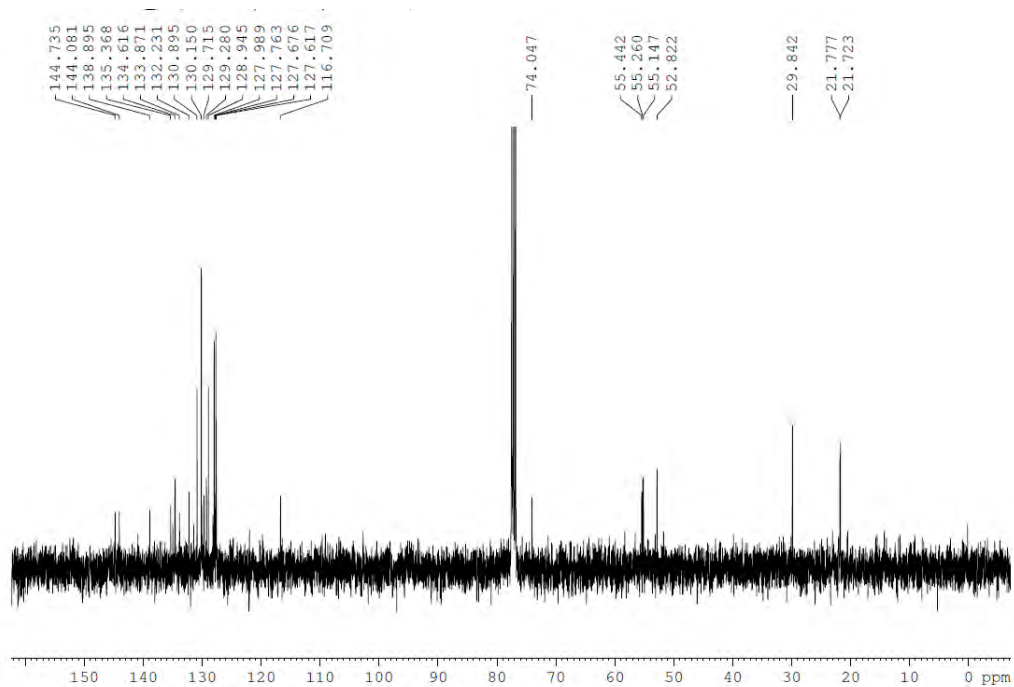
Figure S109: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **12ab** and **12ab'** in CDCl$_3$.
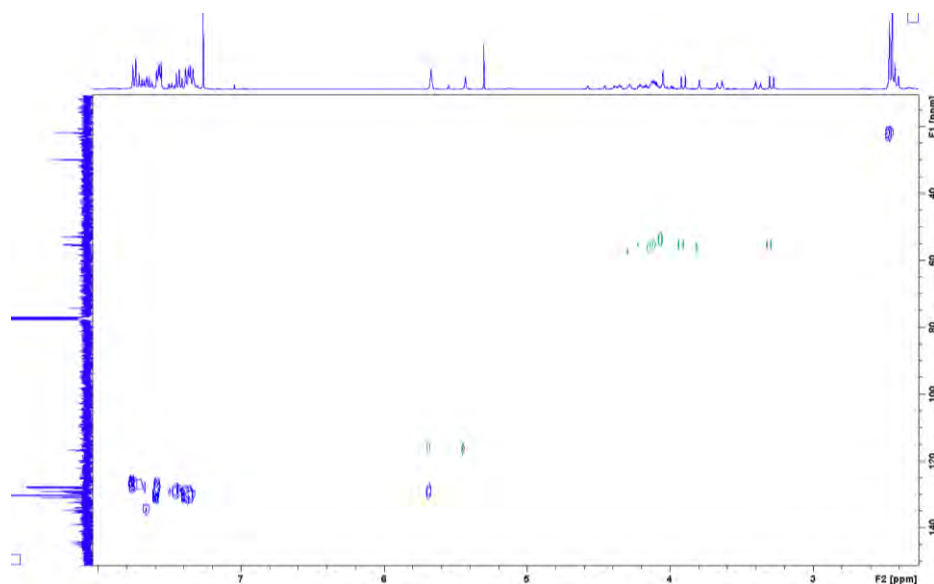
Figure S110: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **12ab** and **12ab'** in CDCl$_3$.
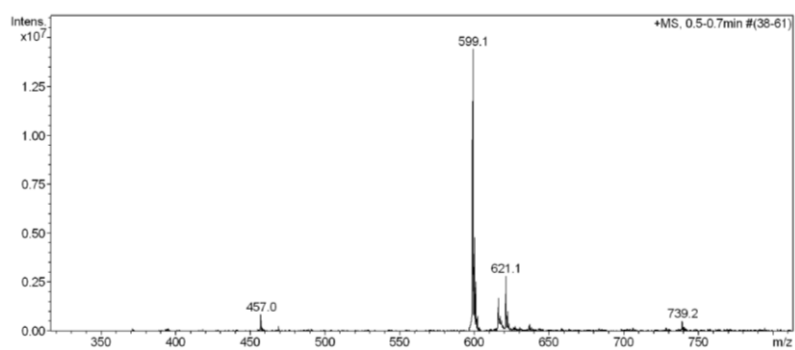
Figure S111: ESI-MS spectrum of **12ab** and **12ab'**.
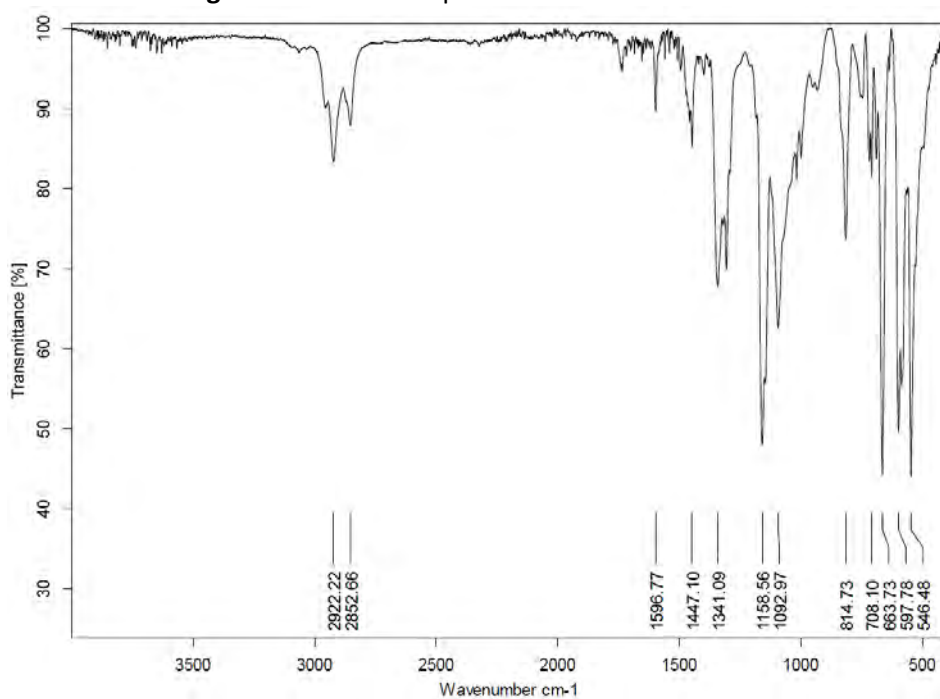
Figure S112: IR spectrum of **12ab** and **12ab'**.
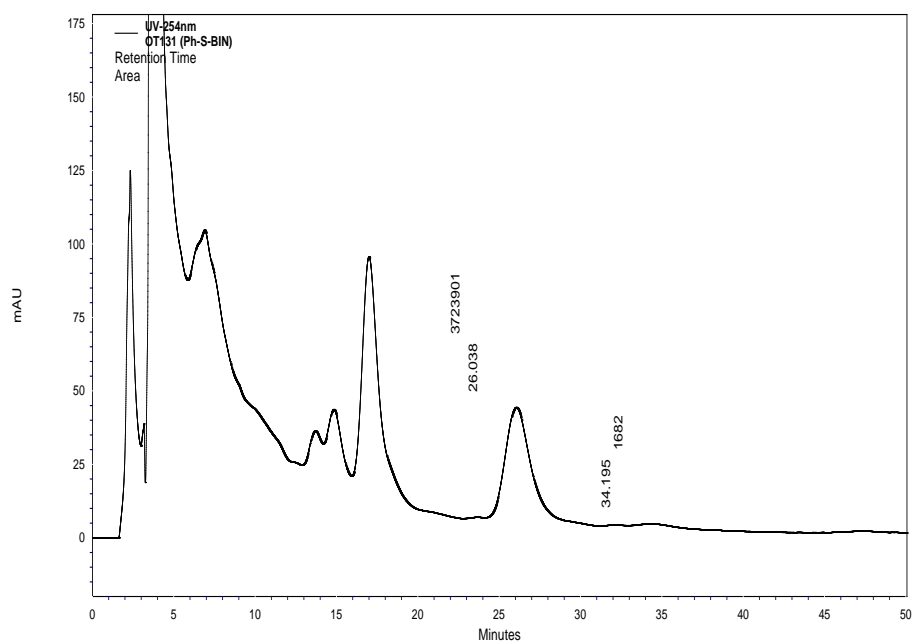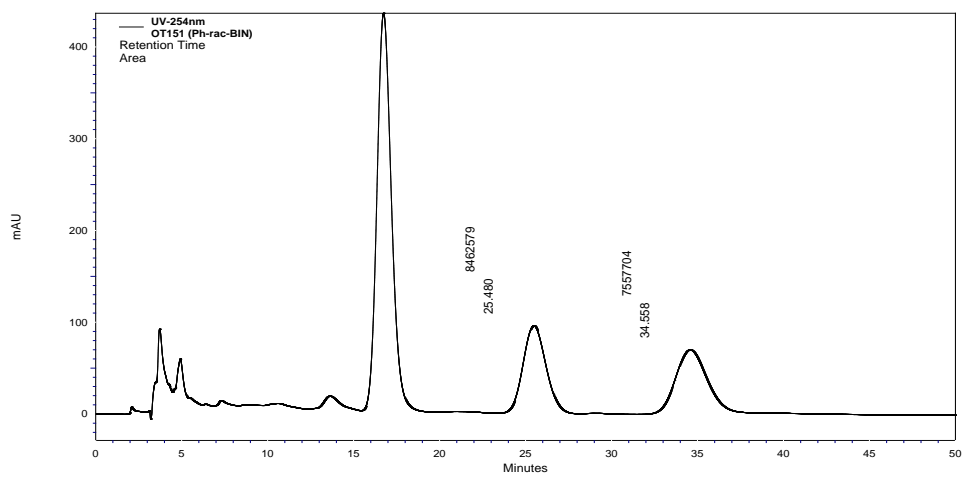
Figure S113: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **12ab** and **12ab'**.
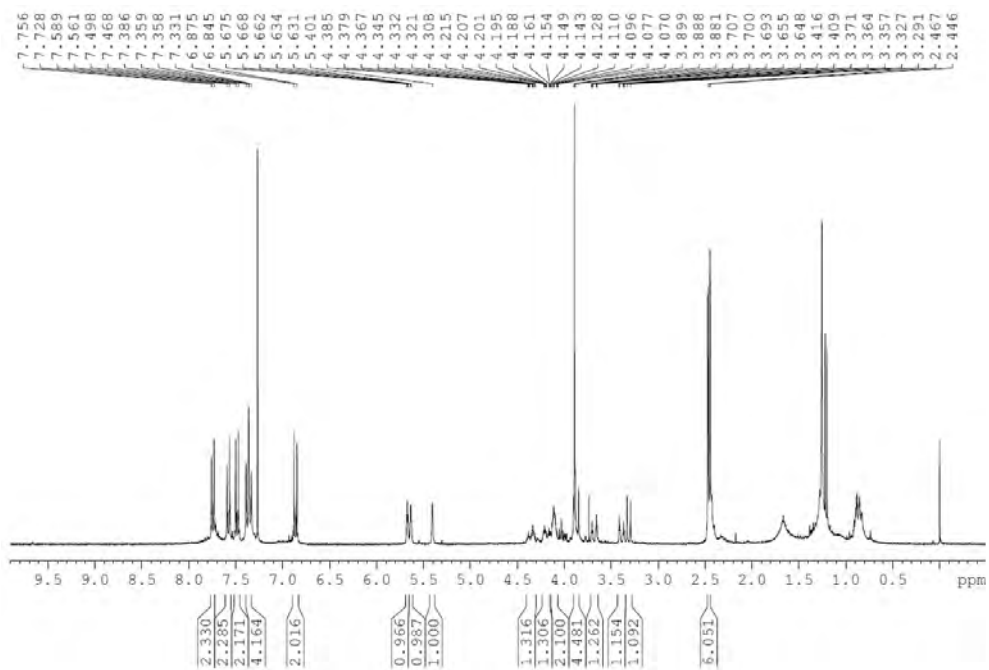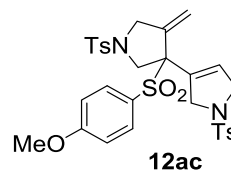
Figure S114. ^{1}H NMR spectrum (300 MHz) of **12ac** in CDCl$_3$.
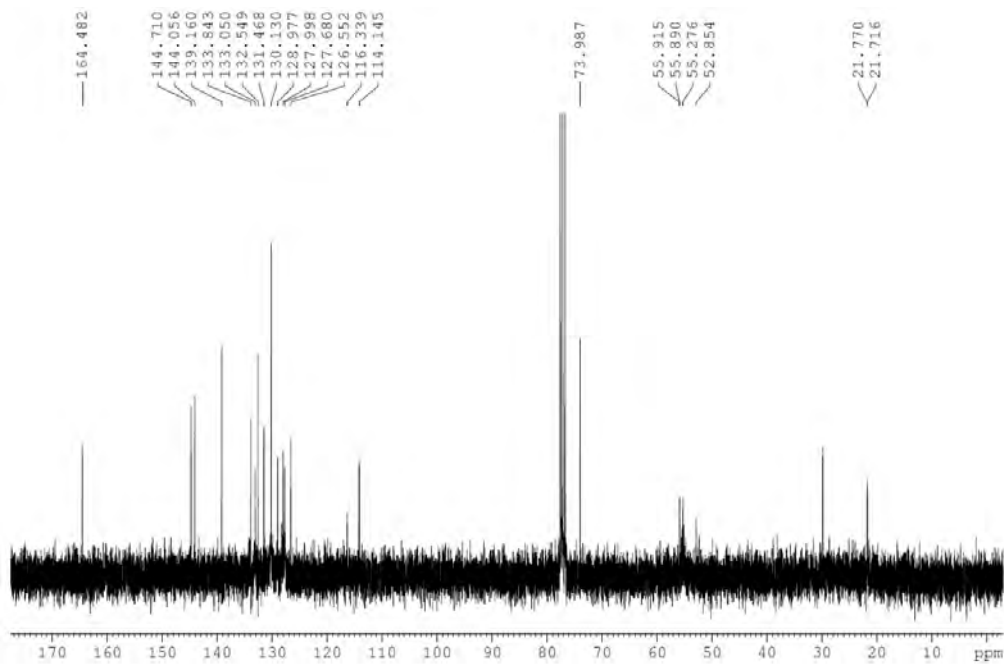
Figure S115: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **12ac** in CDCl$_3$.
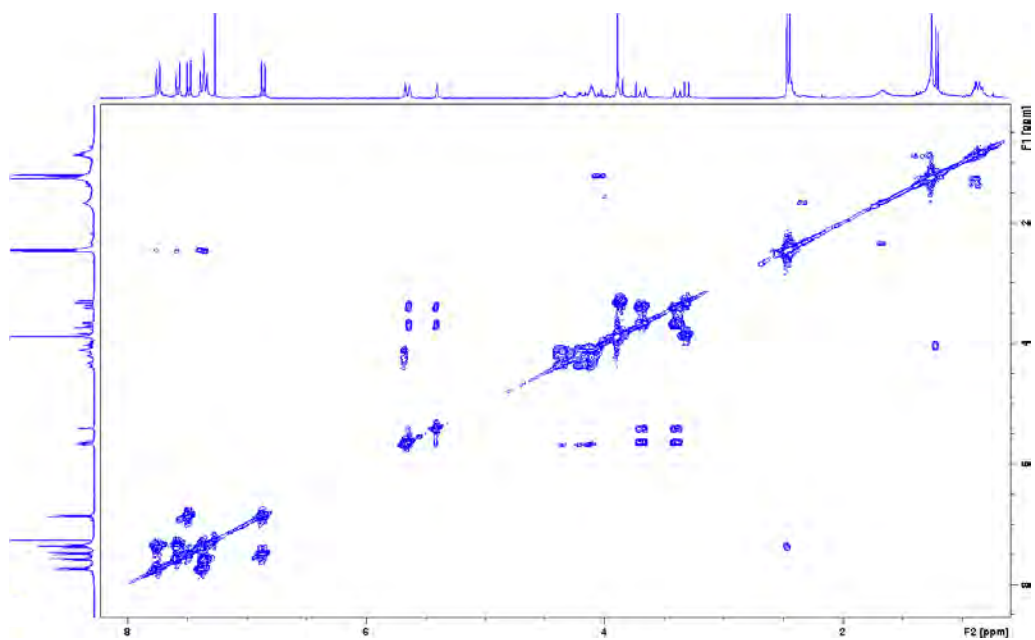
Figure S116: 2D ^{1}H-^{1}H COSY correlation of **12ac** in CDCl$_3$.
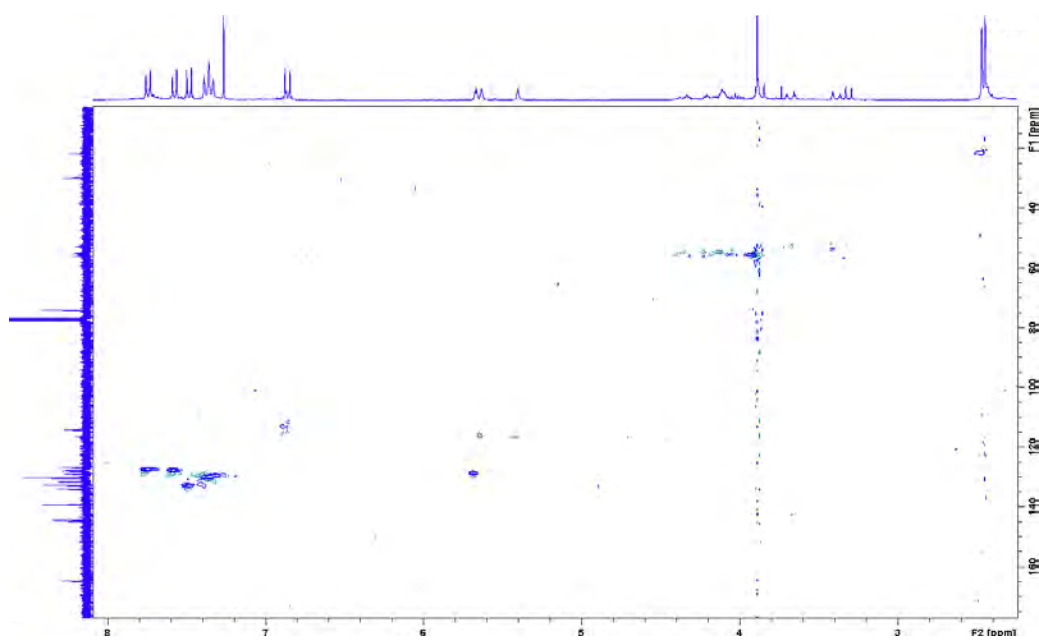
Figure S117: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **12ac** in CDCl$_3$.
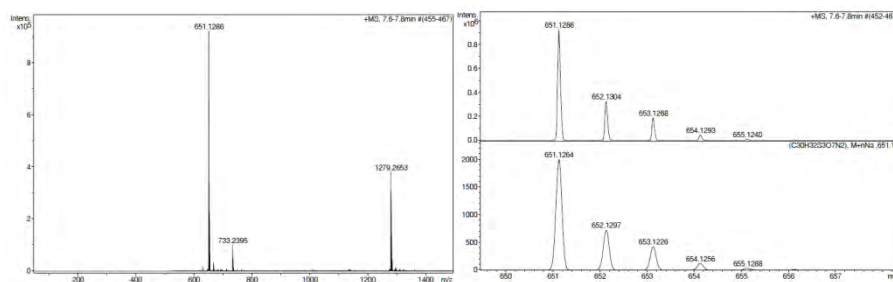
Figure S118: ESI-HRMS spectrum of **12ac**.
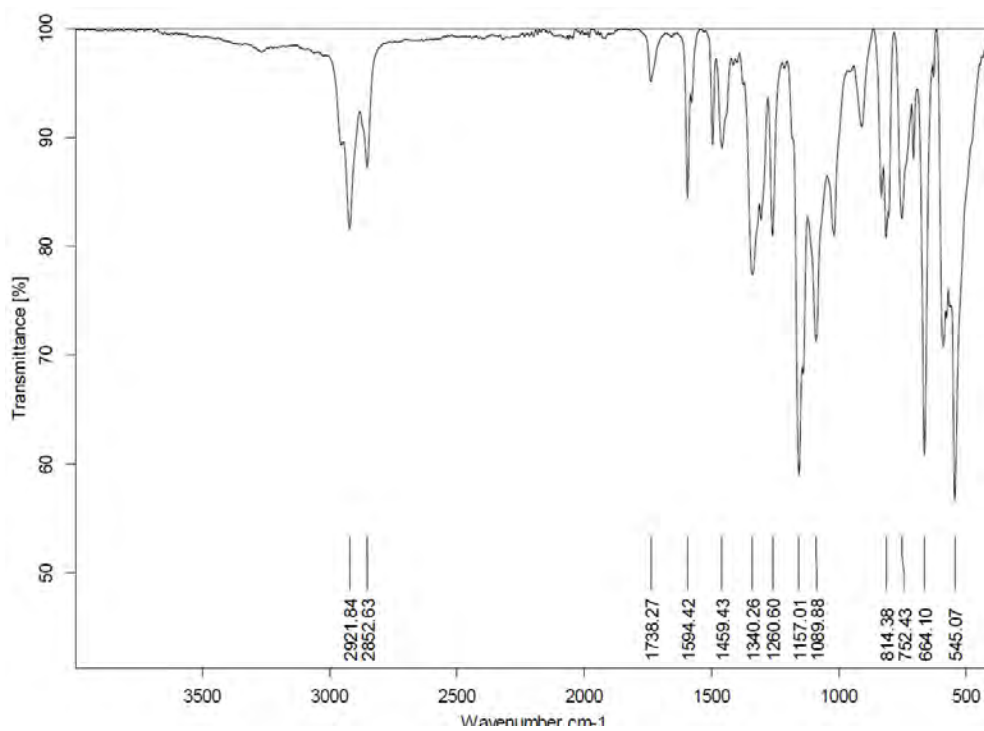
Figure S119: IR spectrum of **12ac**.
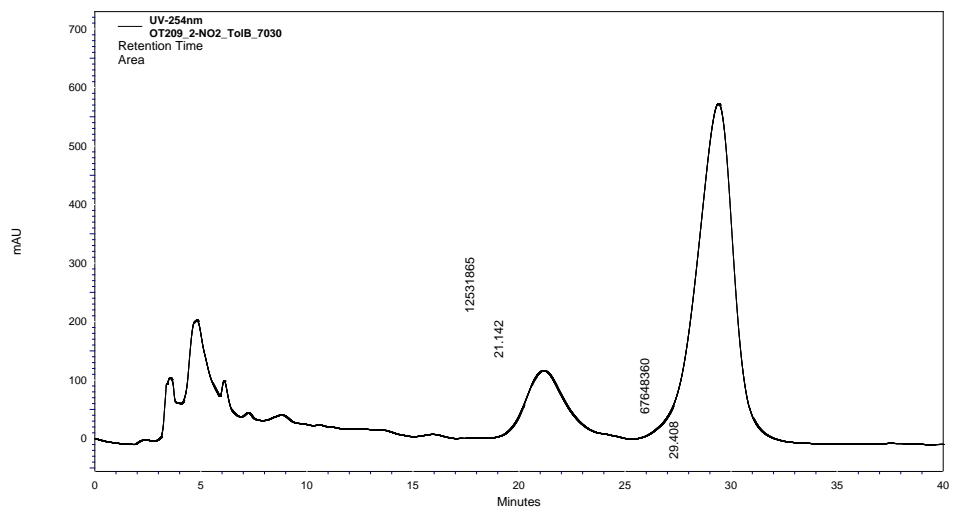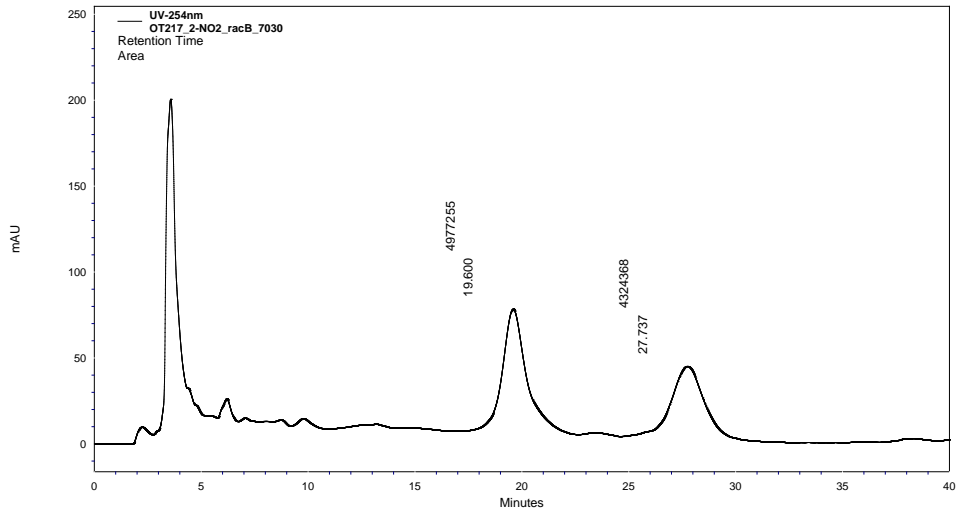
Figure S120: HPLC chromatograms with *rac*-BINAP and *(R)-(+)*-BINAP for **12ac**.
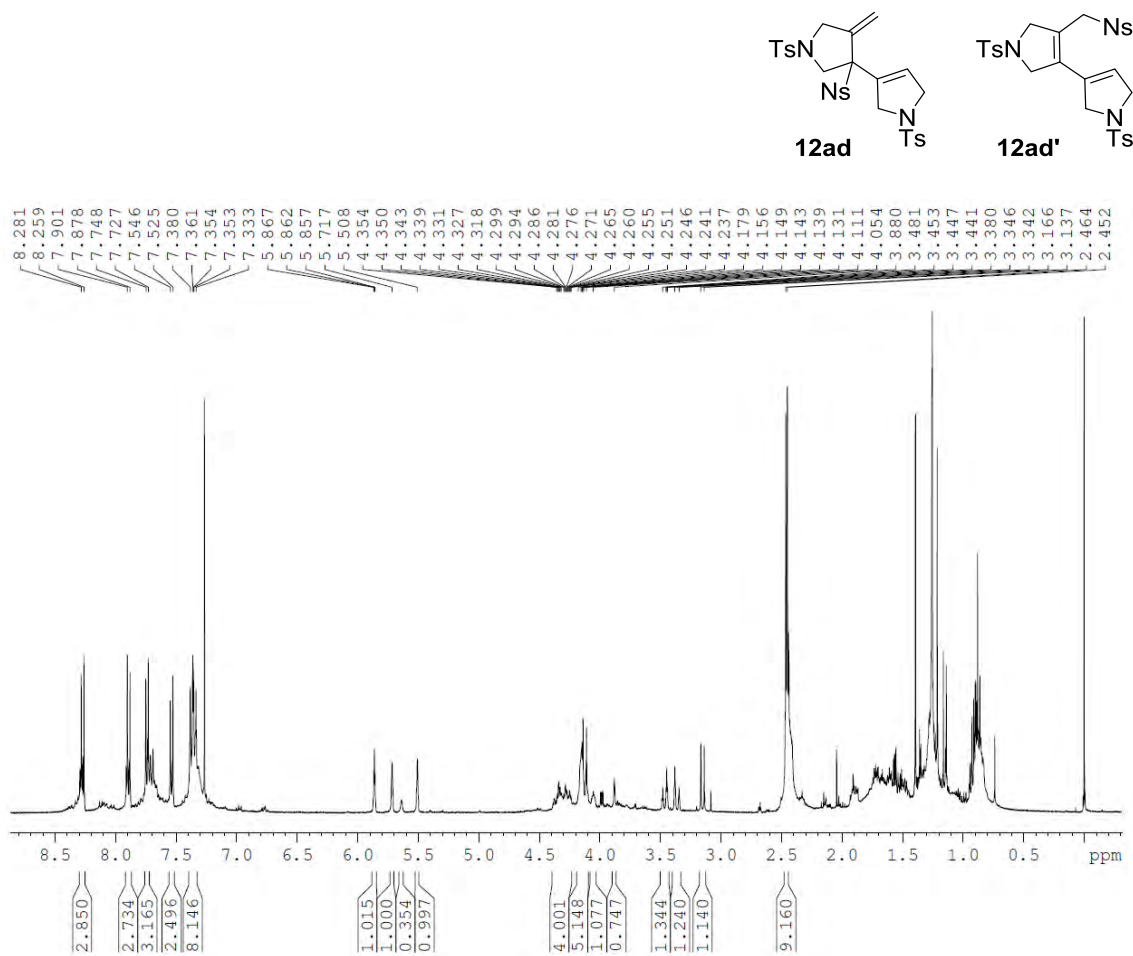
Figure S121: ^{1}H NMR spectrum (300 MHz) of **12ad** and **12ad'** in CDCl$_3$.
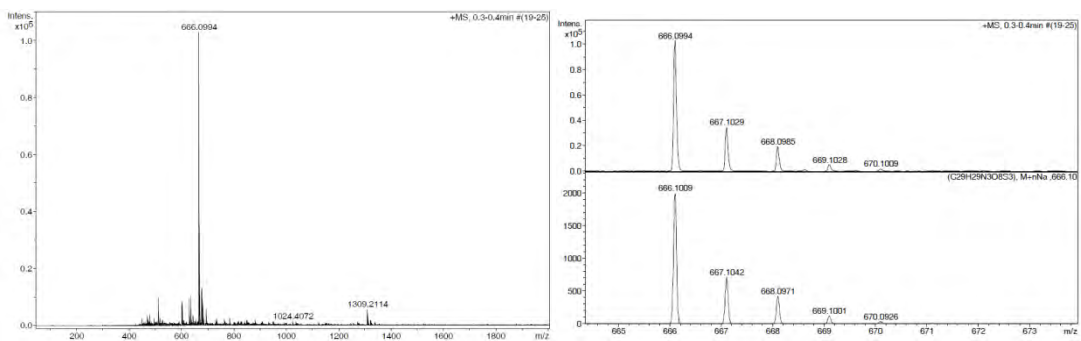
Figure S122: ESI-HRMS spectrum of **12ad** and **12ad'**.
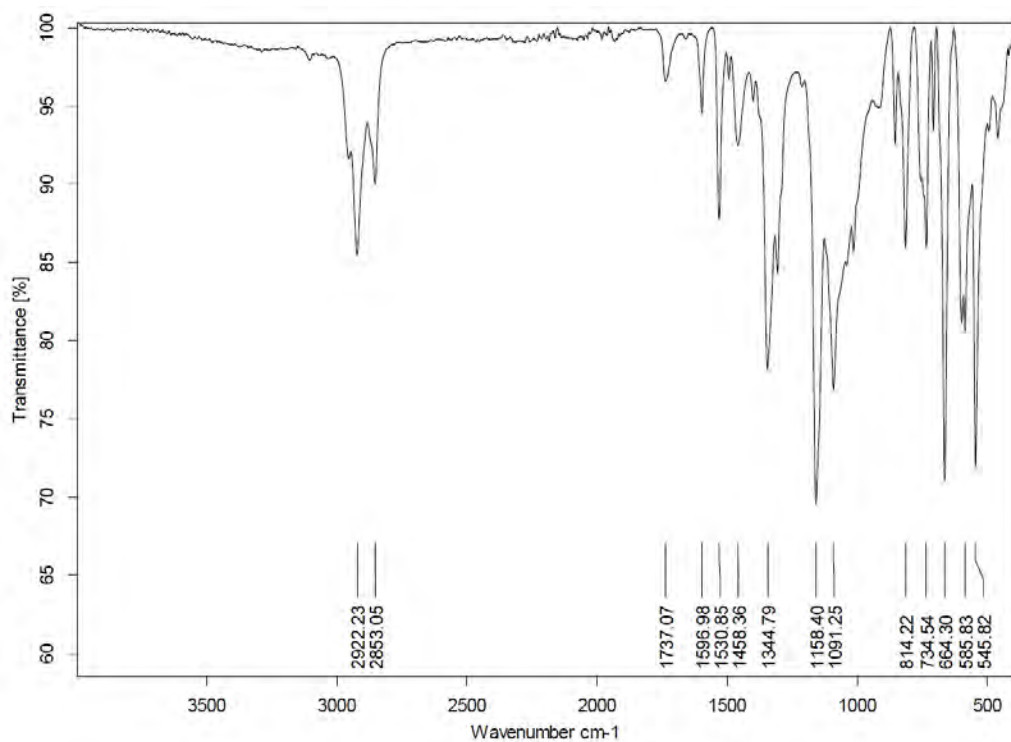
Figure S123: IR spectrum of **12ad** and **12ad'**.
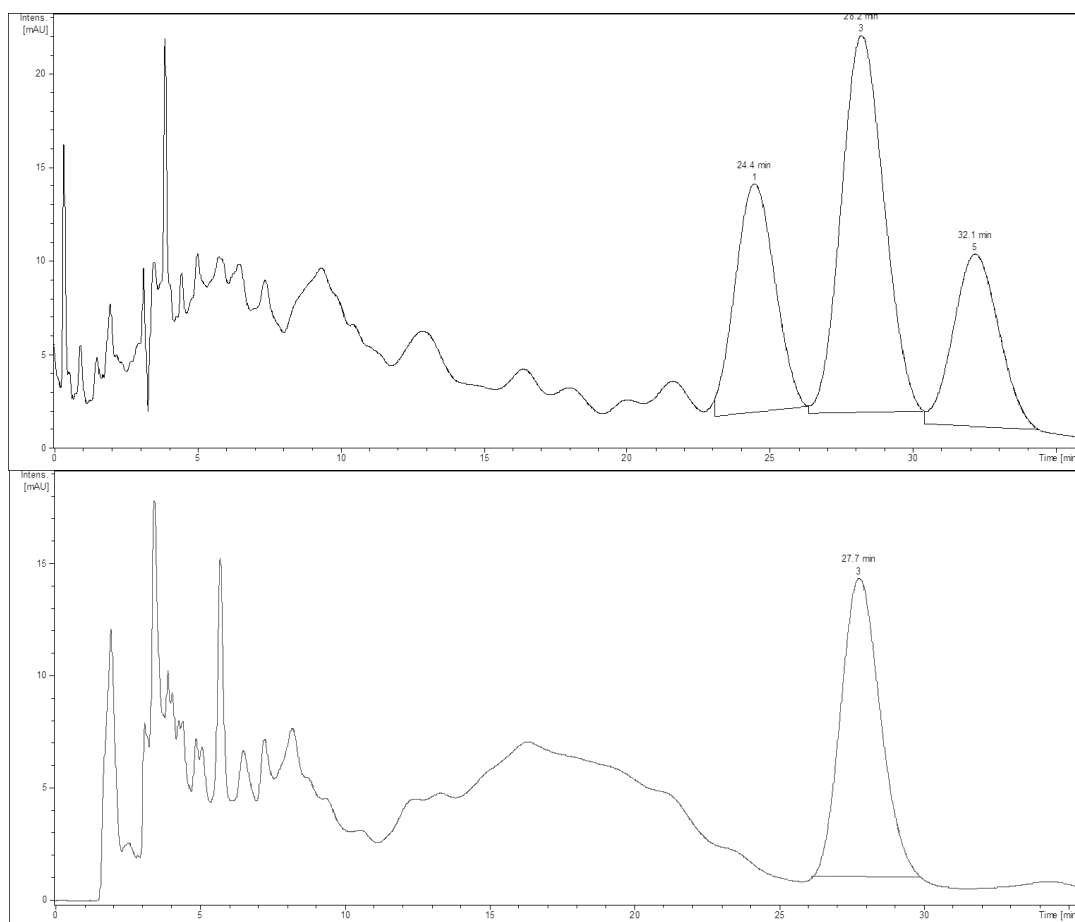
Figure S124: HPLC chromatograms with *rac*-BINAP (mixture of **2ad** and **2ad'**) and *(R)-(+)*-BINAP for **2ad.**
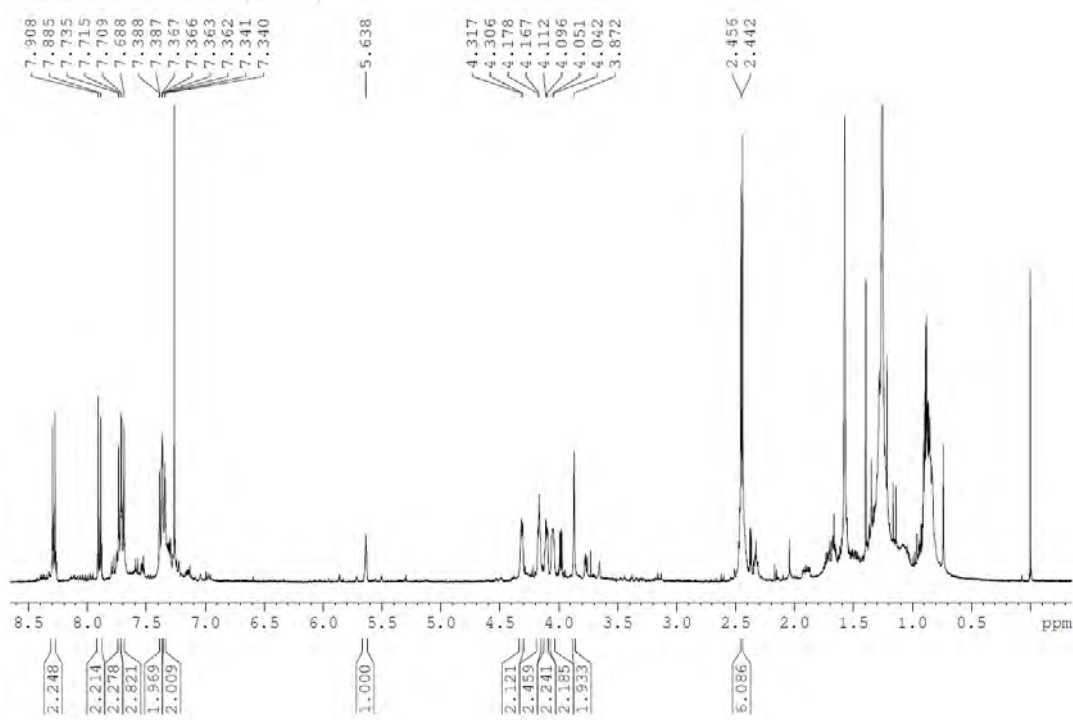
Figure S125: ^{1}H NMR spectrum (300 MHz) of **12ad'** in CDCl$_3$.
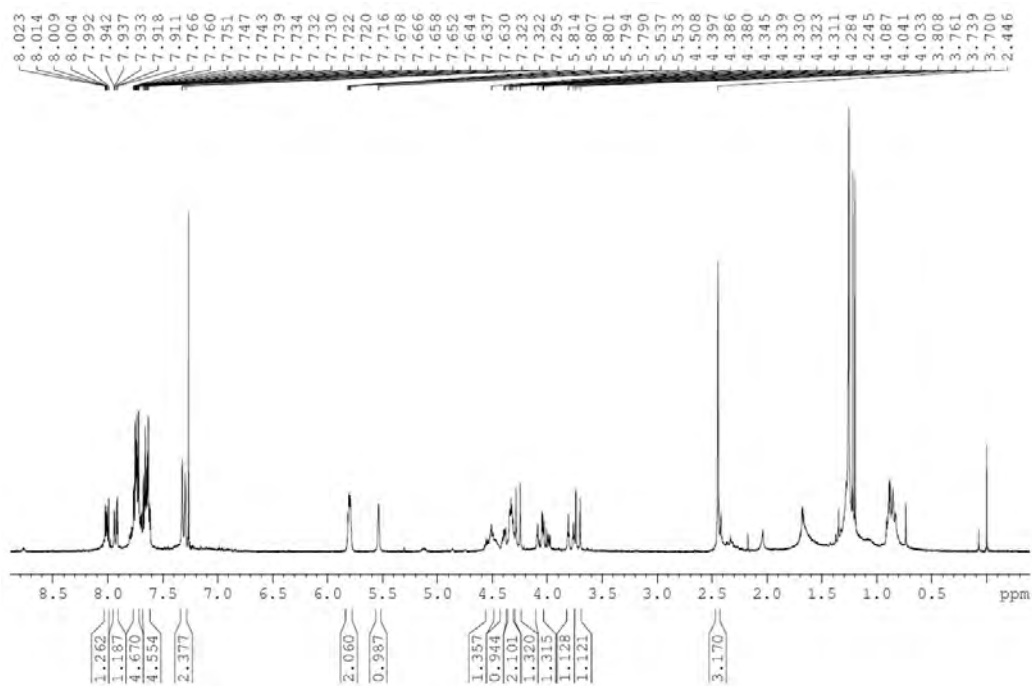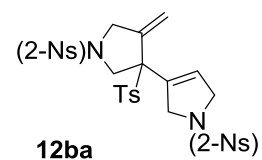
Figure S126: ^{1}H NMR spectrum (300 MHz) of **12ba** in CDCl$_3$.
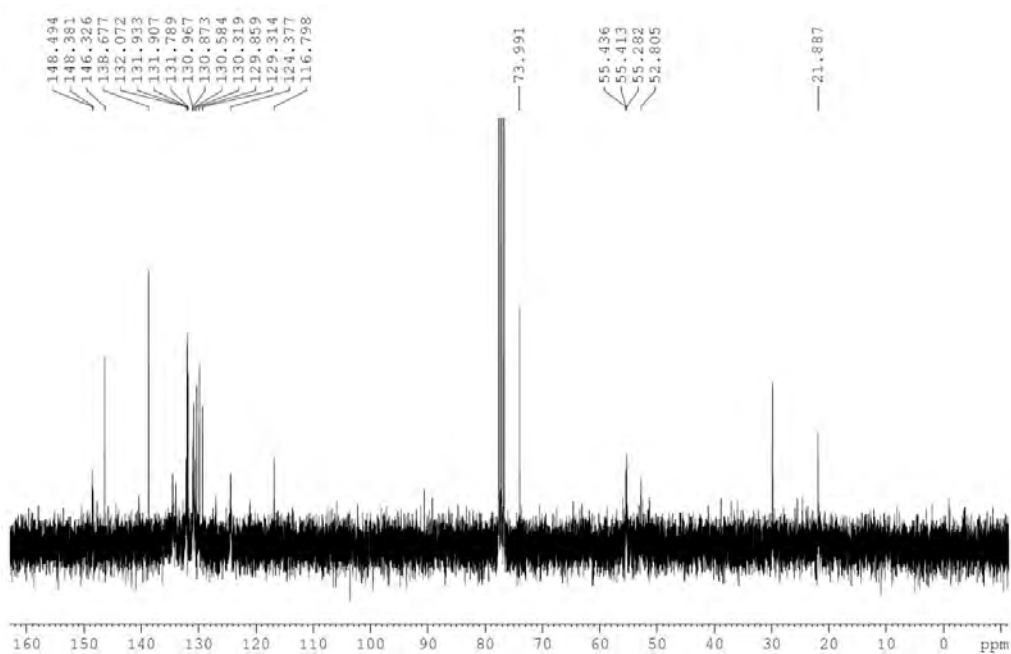
Figure S127: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **12ba** in CDCl$_3$.
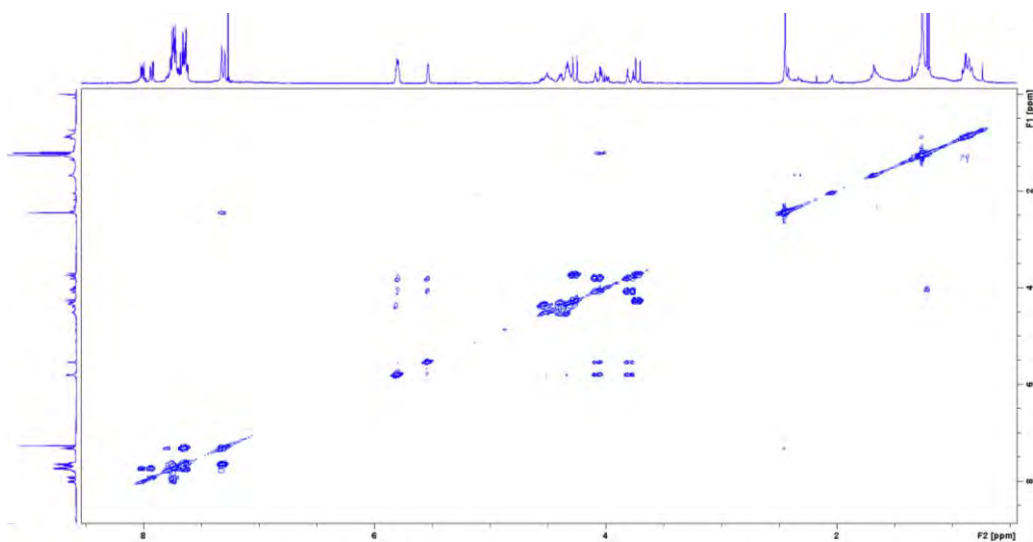
Figure S128: 2D ^{1}H-^{1}H COSY correlation of **12ba** in CDCl$_3$.
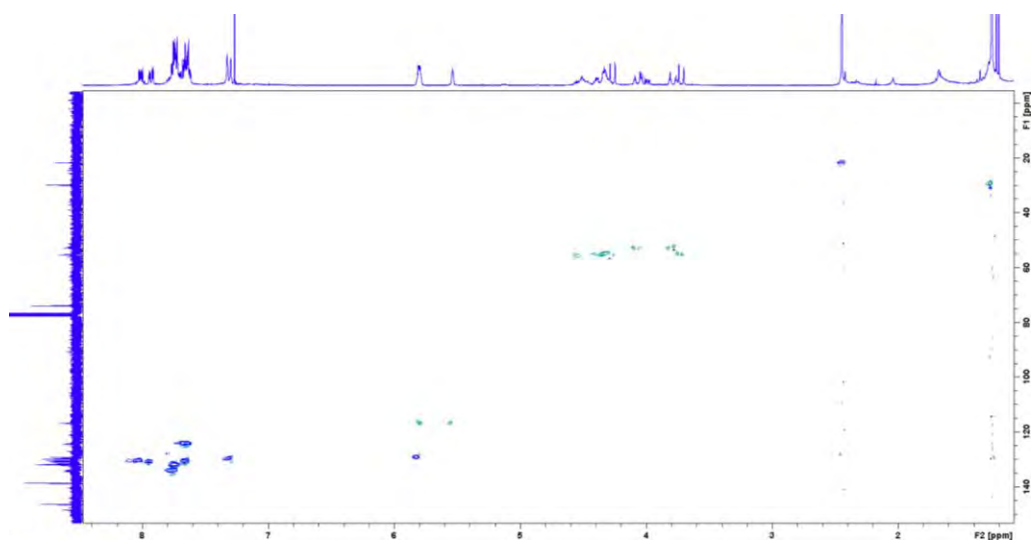
**Figure S129**: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **12ba** in CDCl$_3$.
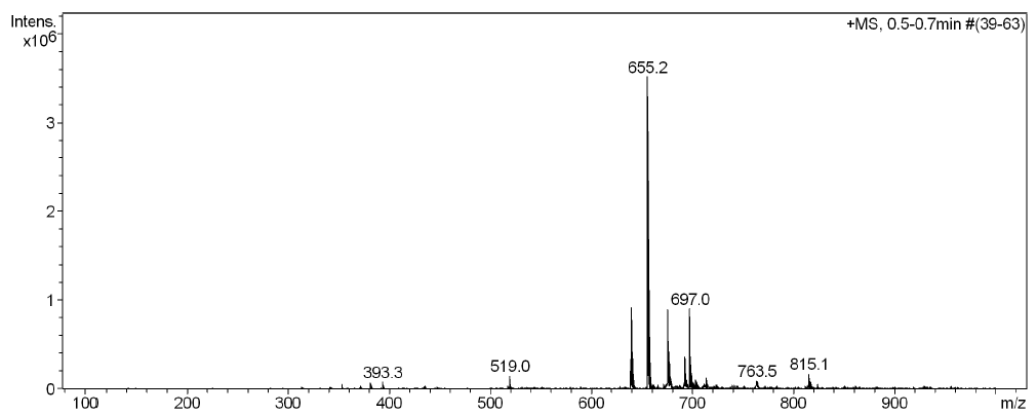
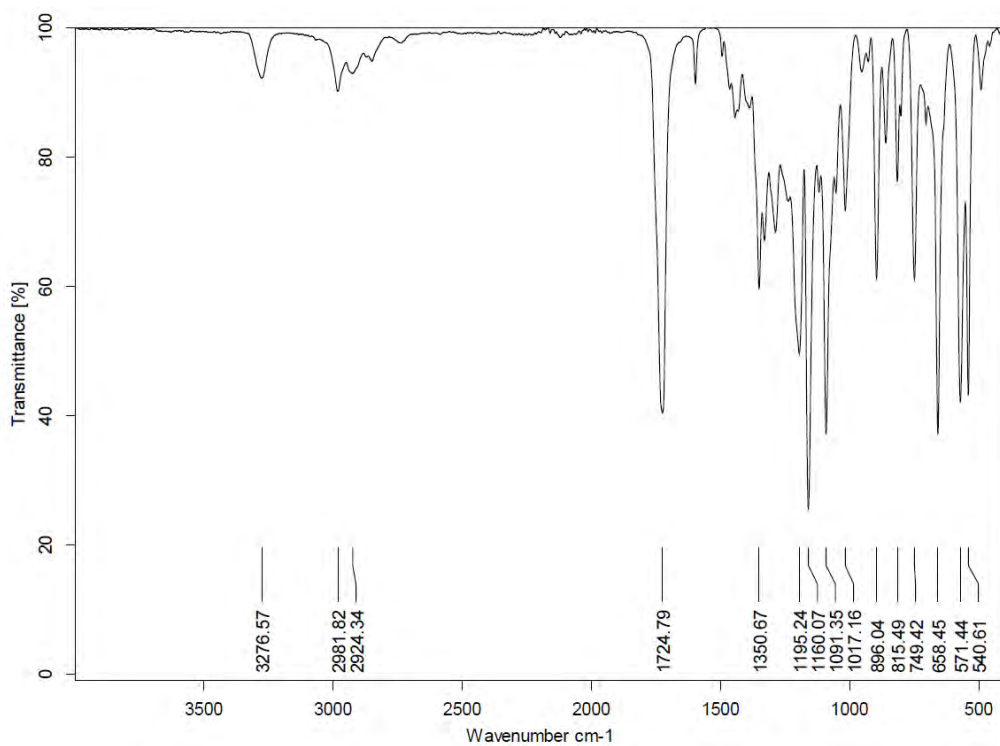**Figure S130:** ESI-MS spectrum of **12ba**.
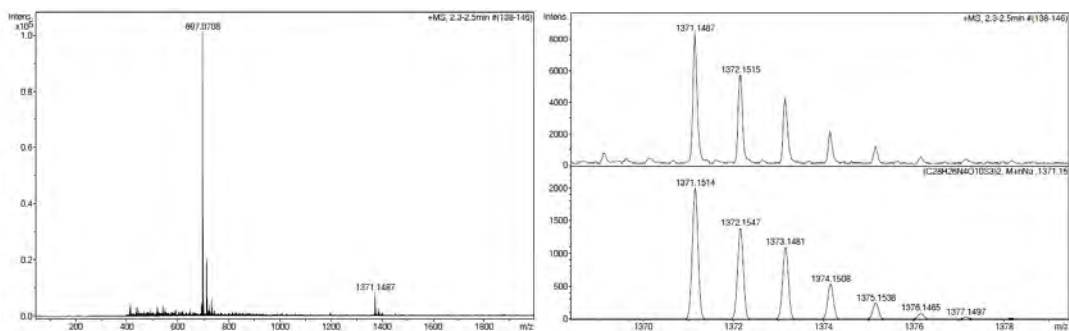
Figure S131: ESI-HRMS spectrum of **12ba**.
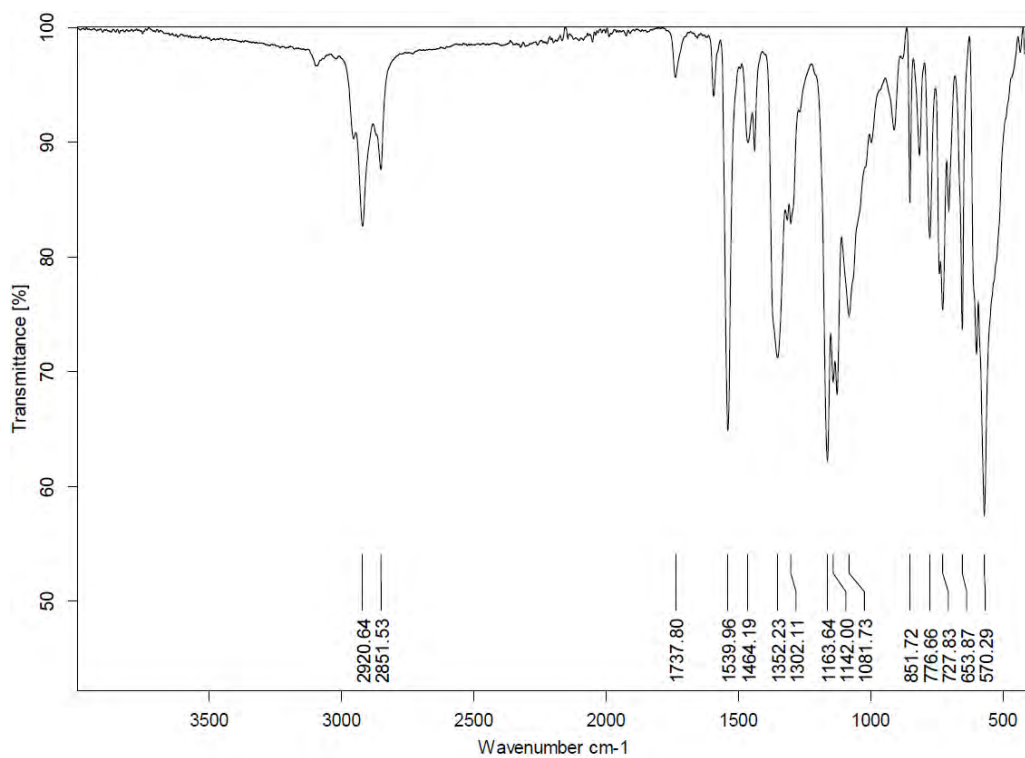
Figure S132: IR spectrum of **12ba**.
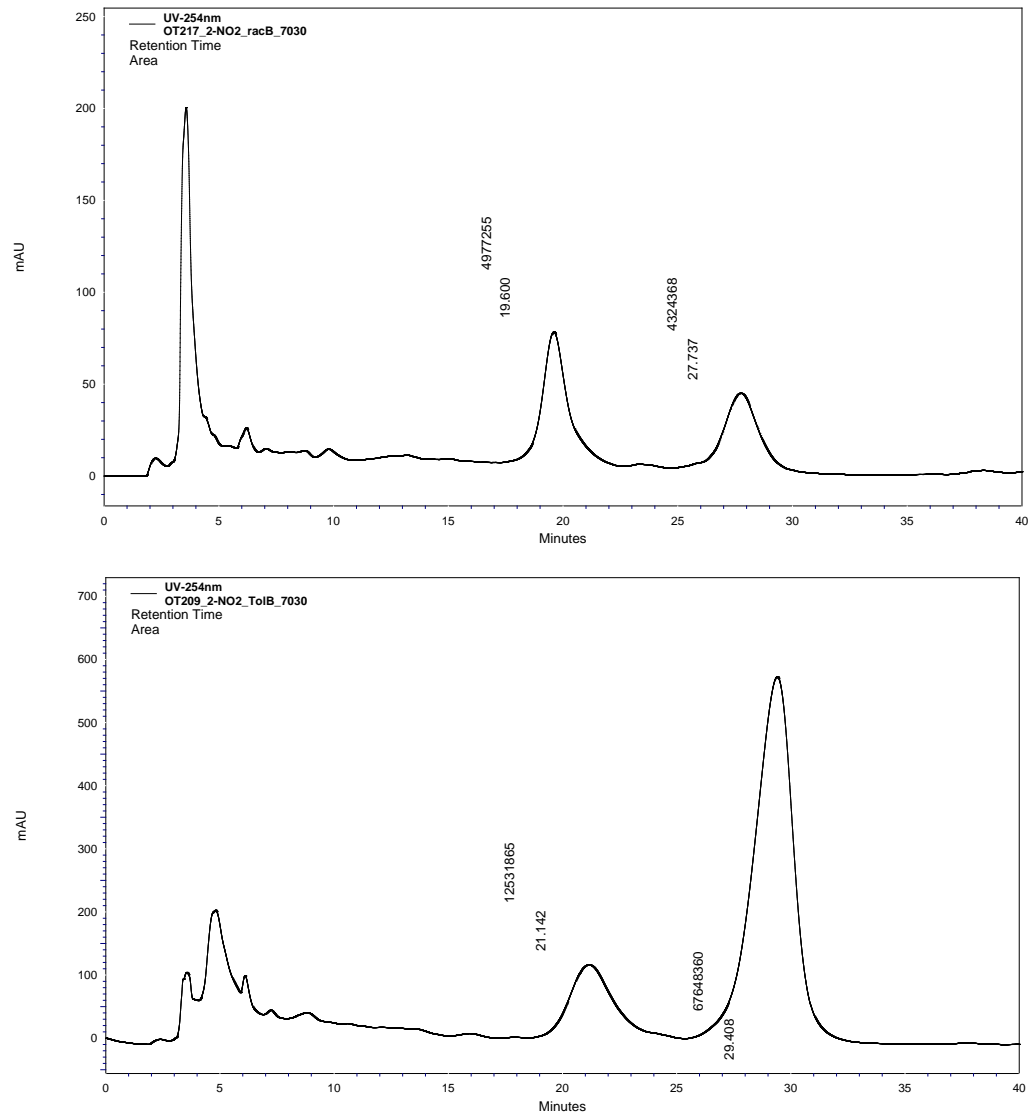
Figure S133: HPLC chromatograms with *rac*-BINAP and *(R)-(+)*-BINAP for **12ba**.
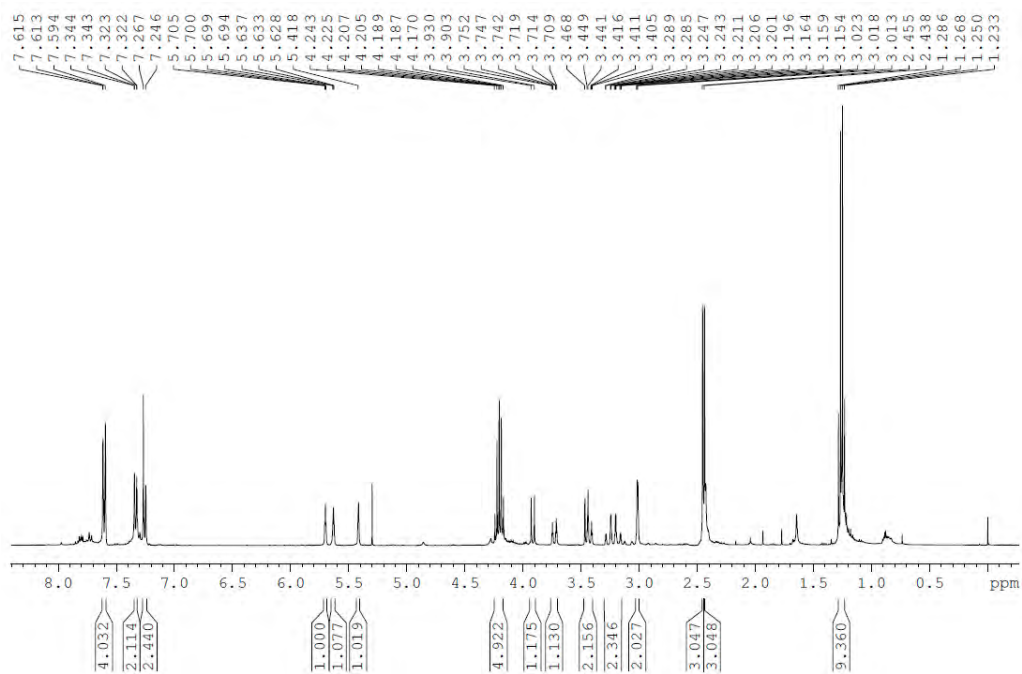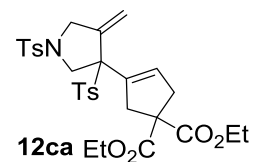
Figure S134: ^{1}H NMR spectrum (400 MHz) of **12ca** in CDCl$_3$.
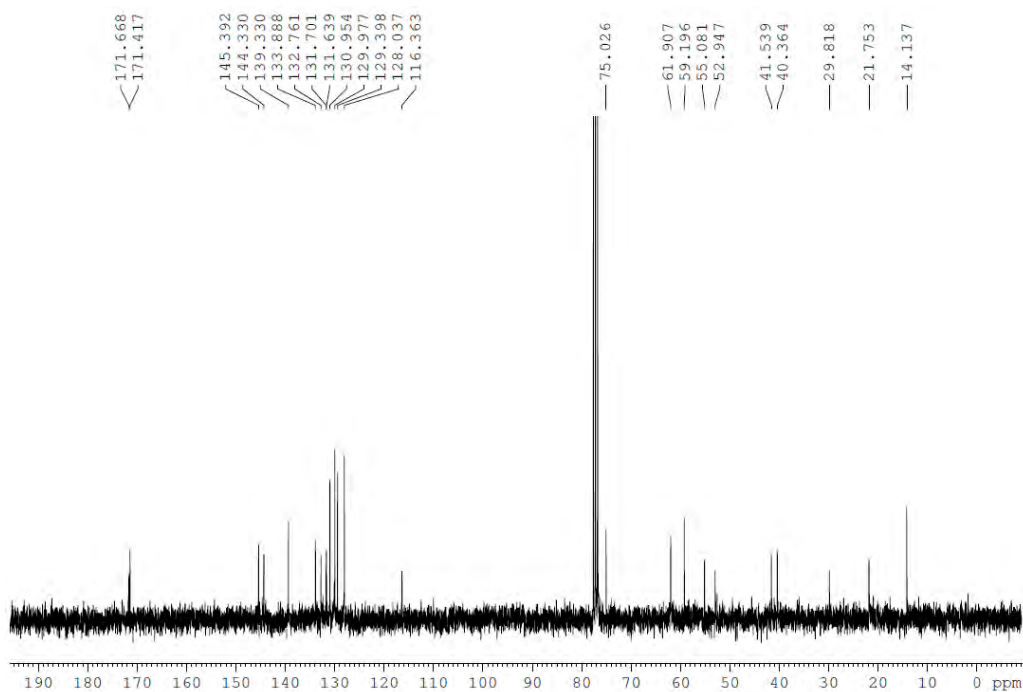
Figure S135: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **12ca** in CDCl$_3$.
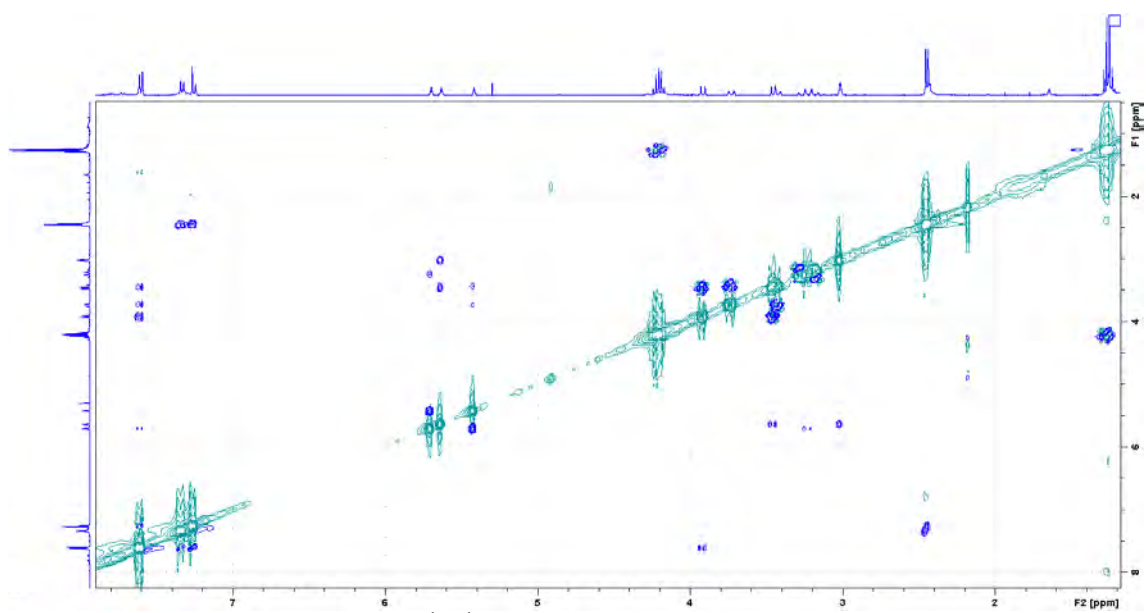
Figure S136: 2D [1]H-^{1}H NOESY correlation of **12ca** in CDCl$_3$.
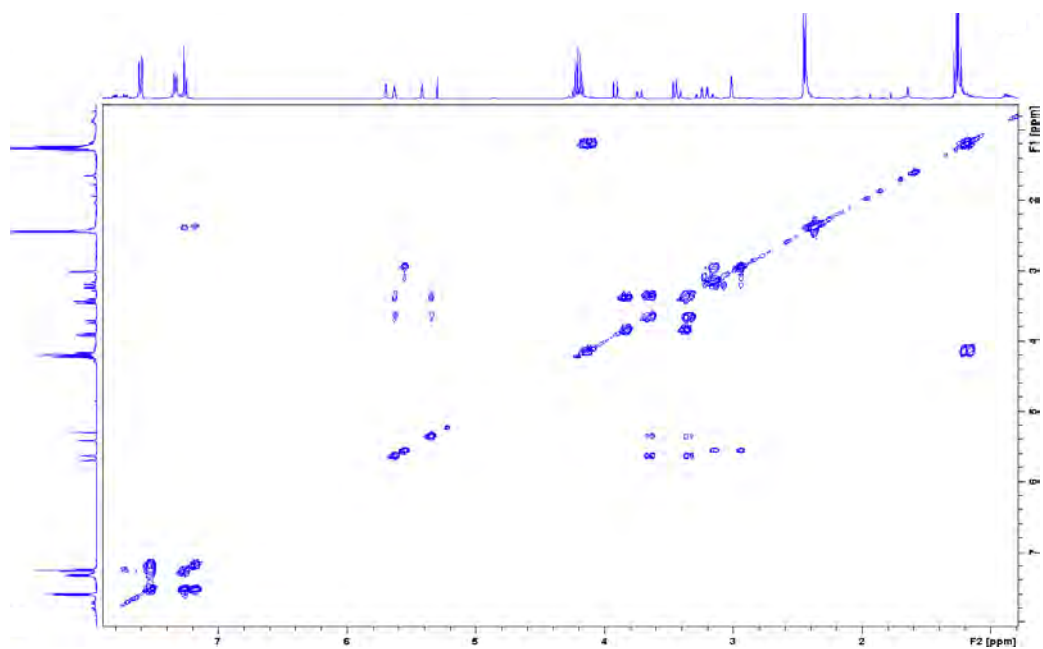
Figure S137: 2D ^{1}H-^{1}H COSY correlation of **12ca** in CDCl$_3$.
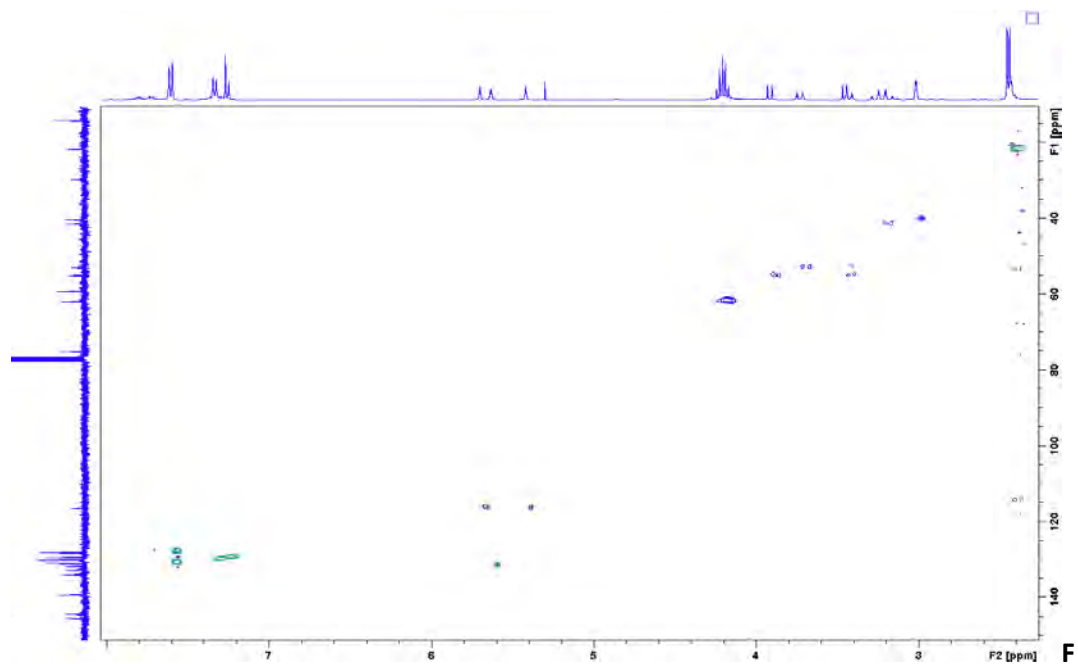
Figure S138: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **12ca** in CDCl$_3$.
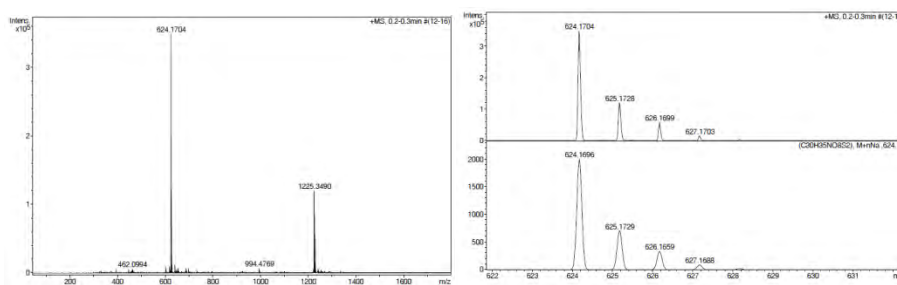
Figure S139: ESI-HRMS spectrum of **12ca**.
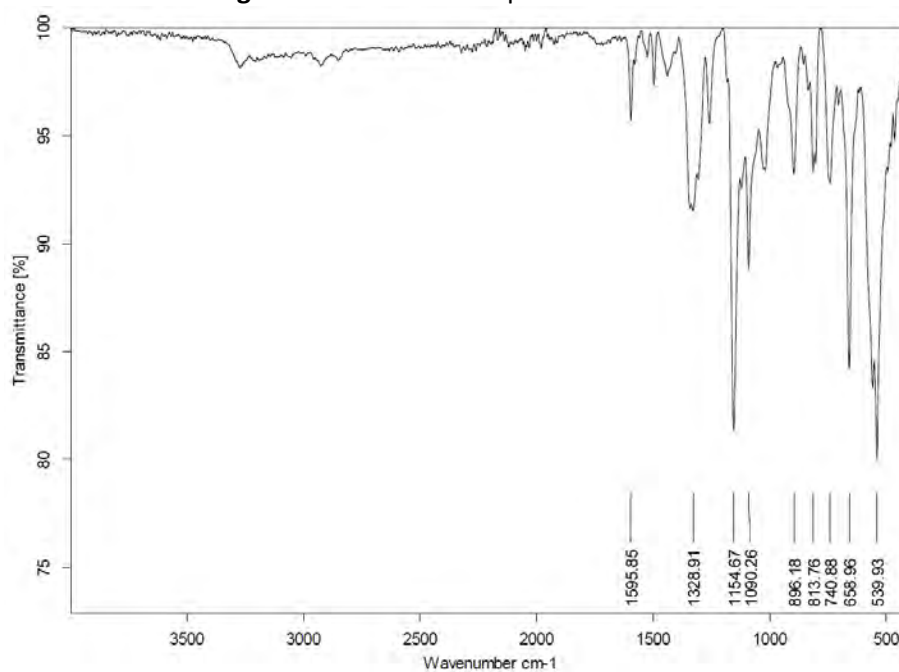
Figure S140: IR spectrum of **12ca**.
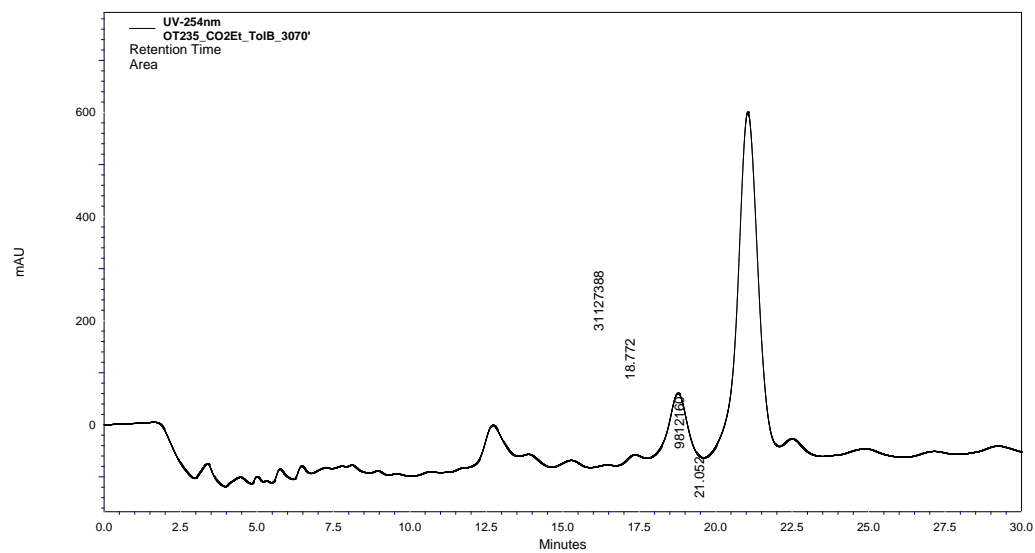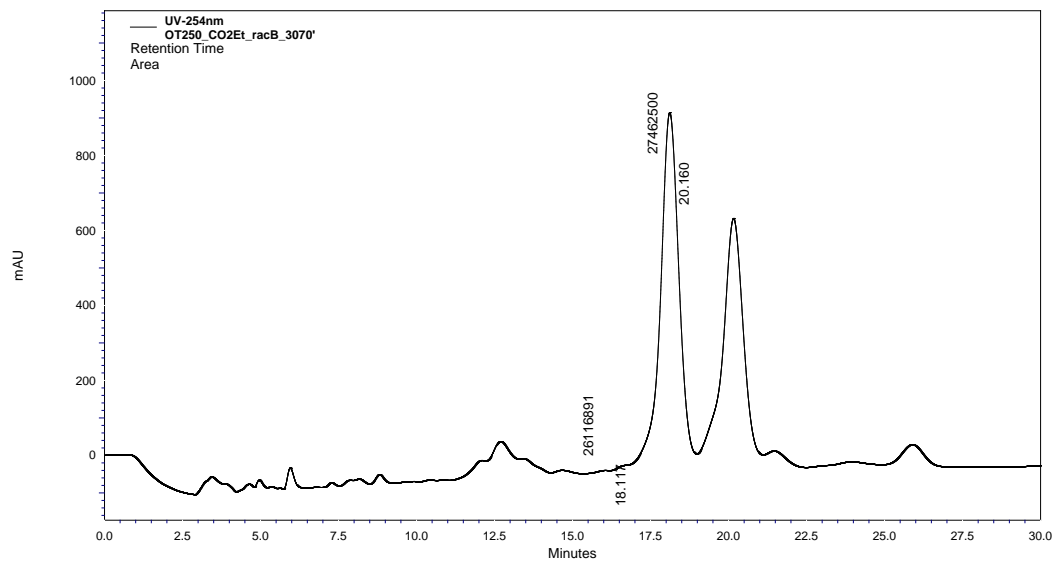
Figure S141: HPLC chromatograms with *rac*-BINAP and *(R)-(+)*-BINAP for **12ca**.
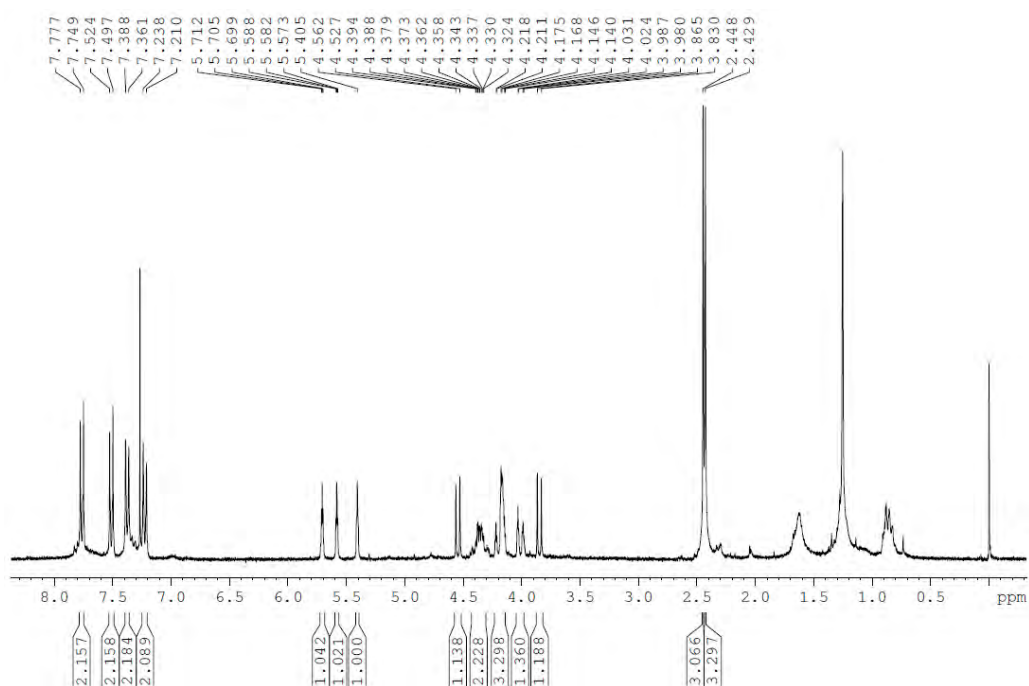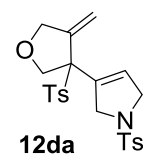
Figure S142: ^{1}H NMR spectrum (300 MHz) of **12da** in CDCl$_3$.
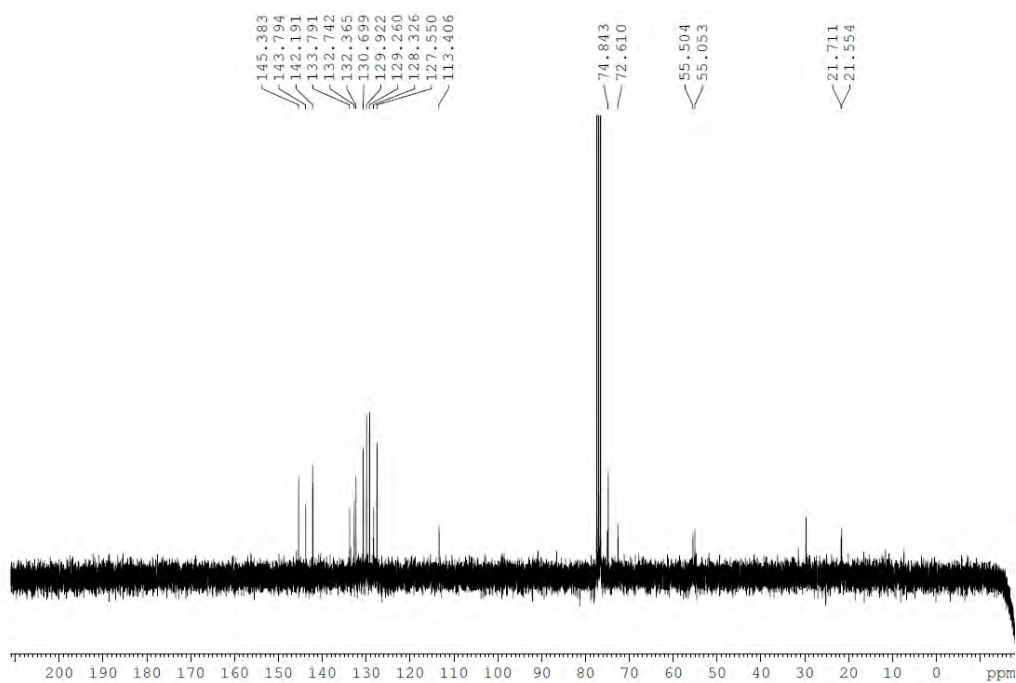
Figure S143: ^{1}H NMR spectrum (75 MHz) of **12da** in CDCl$_3$.
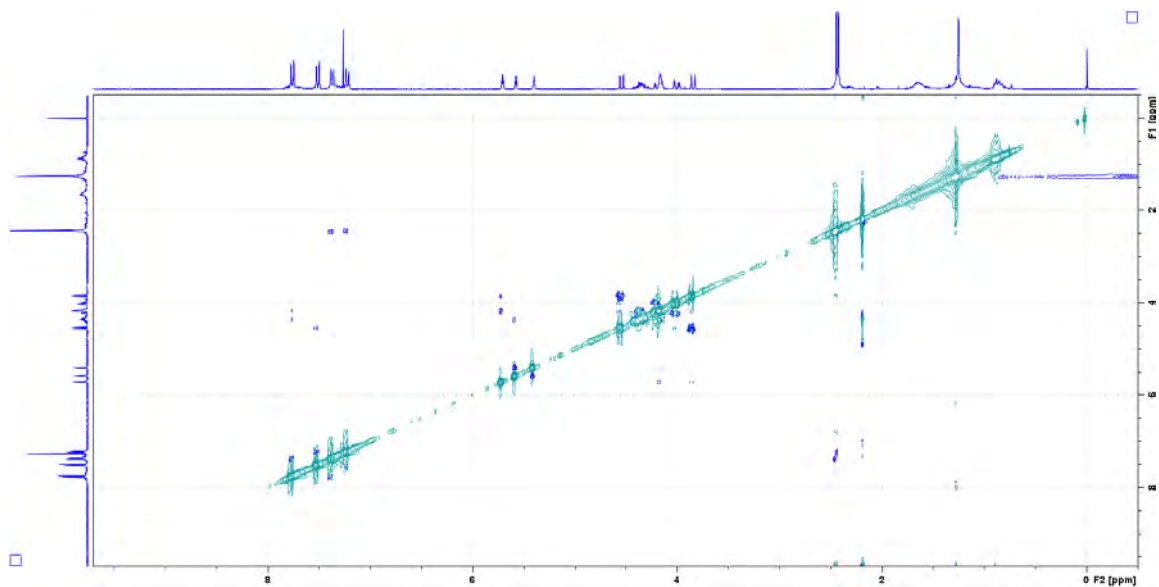
Figure S144: 2D ^{1}H-^{1}H NOESY correlation of **12da** in CDCl$_3$.
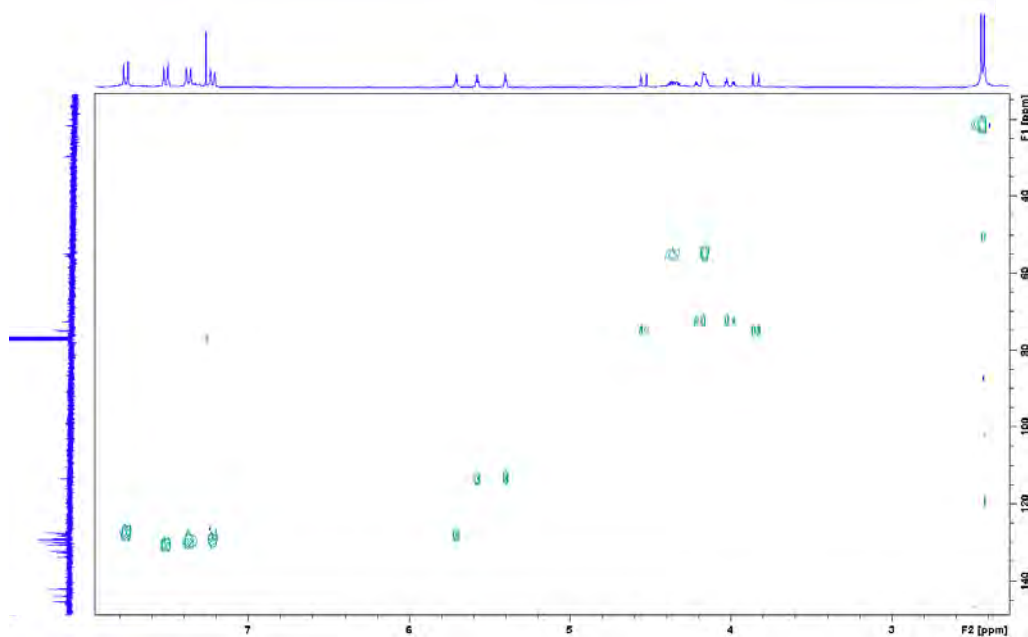
Figure S145: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **12da** in CDCl$_3$.
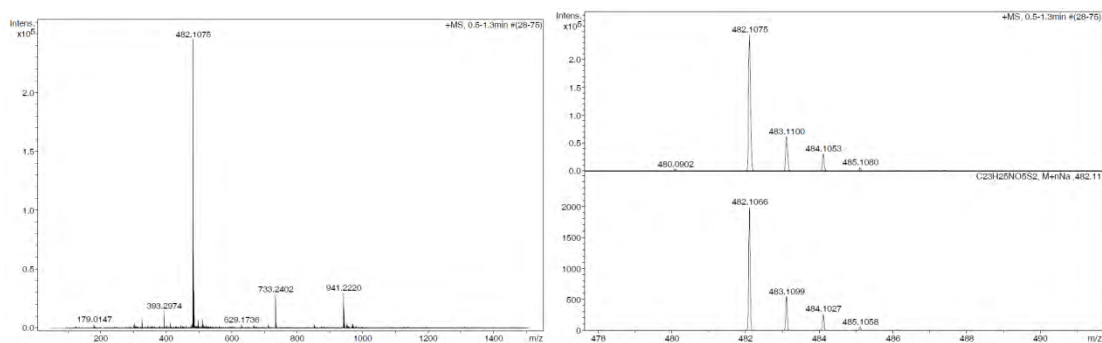
Figure S146: ESI-HRMS spectrum of **12da**.
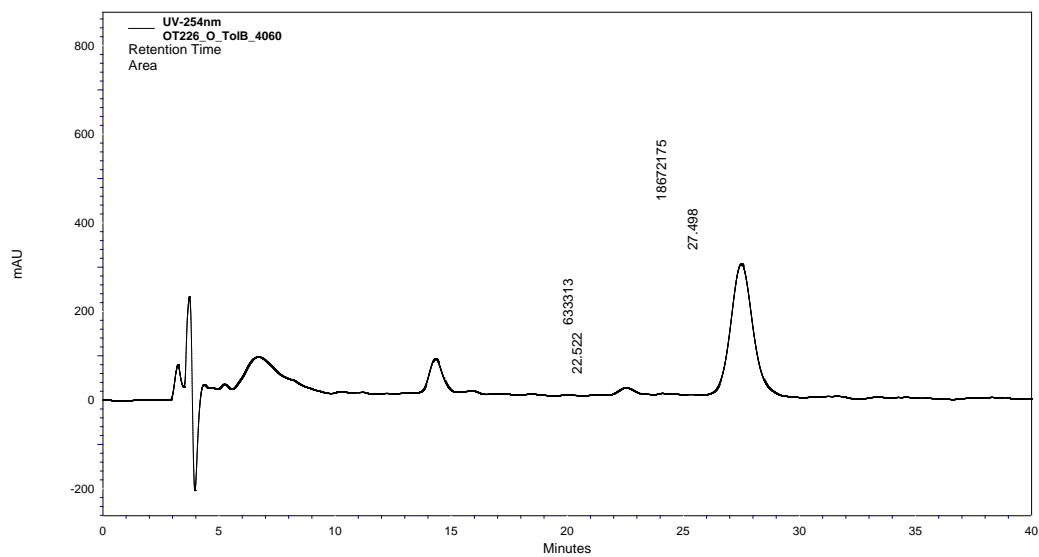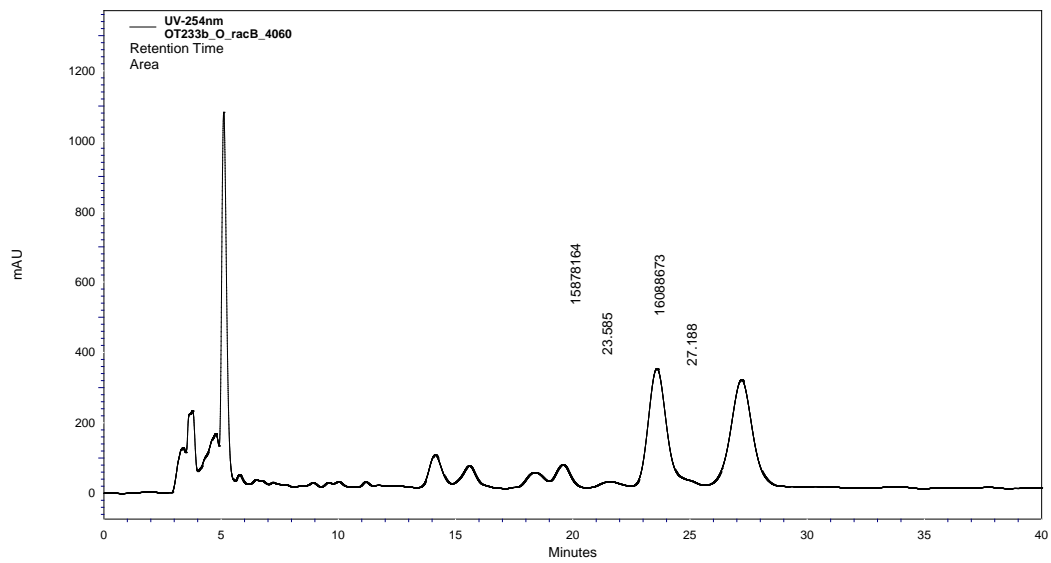
Figure S147: HPLC chromatograms with *rac*-BINAP and *(R)-(+)*-BINAP for **12da**.
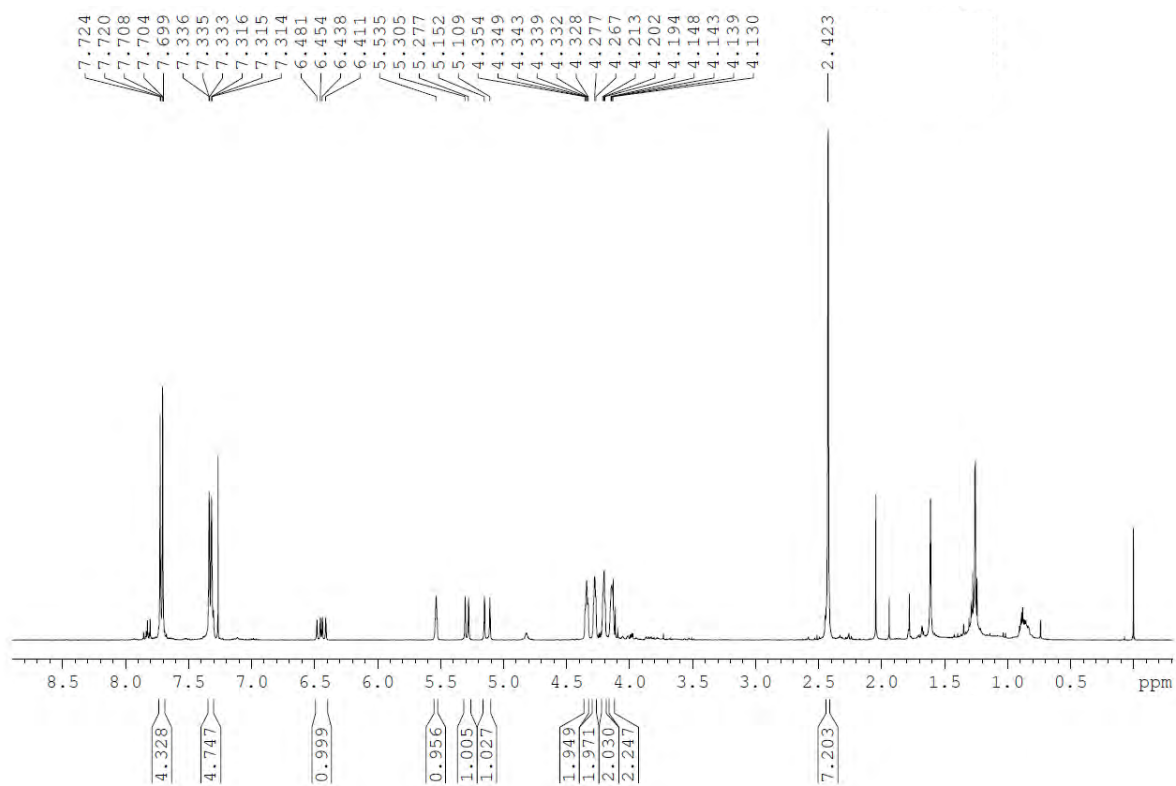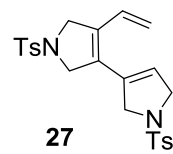
Figure S148: ^{1}H NMR spectrum (400 MHz) of **27** in CDCl$_3$.
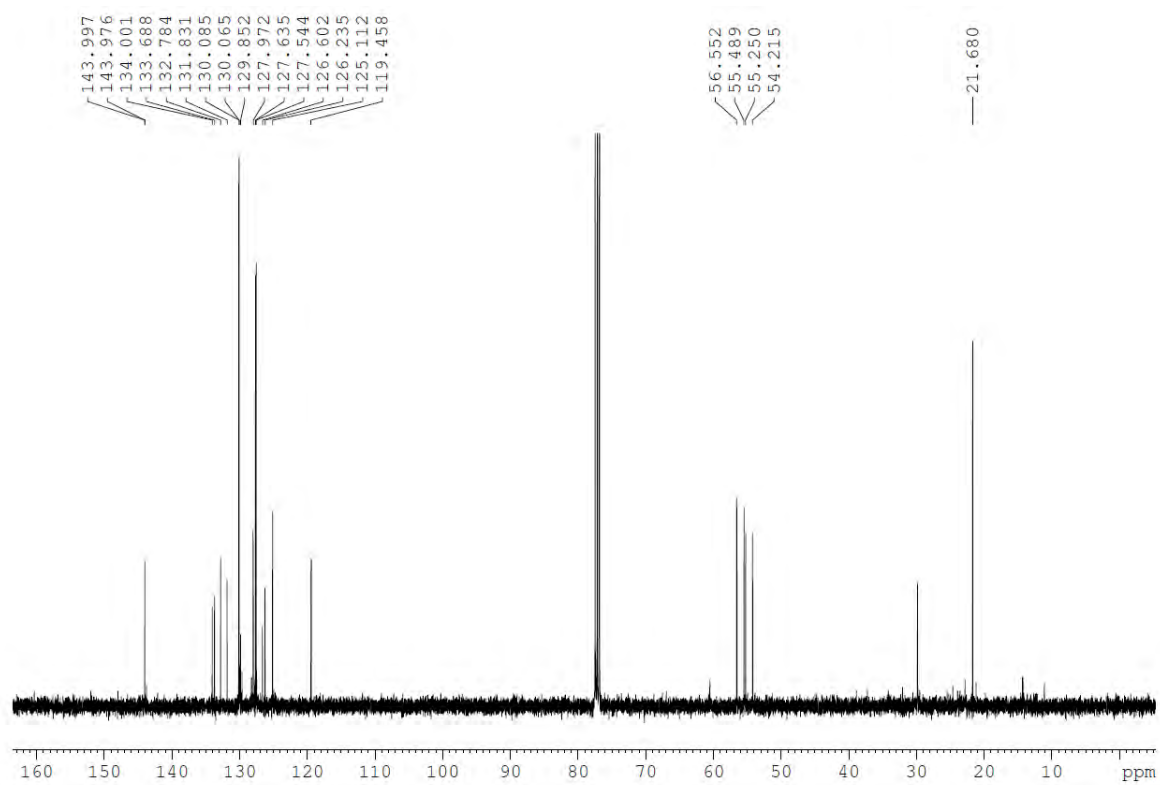
Figure S149: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **27** in CDCl$_3$.
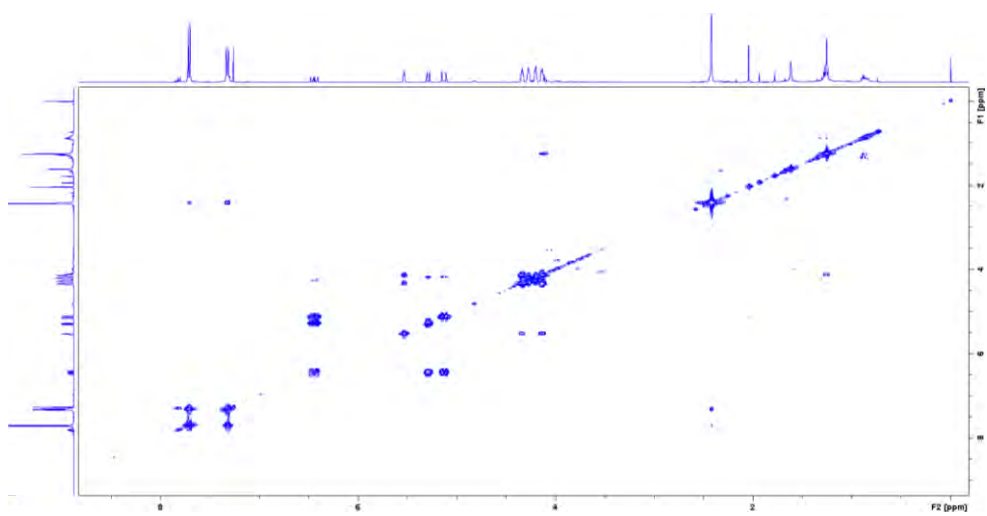
Figure S150: 2D ^{1}H-^{1}H COSY correlation of **27** in CDCl$_3$.
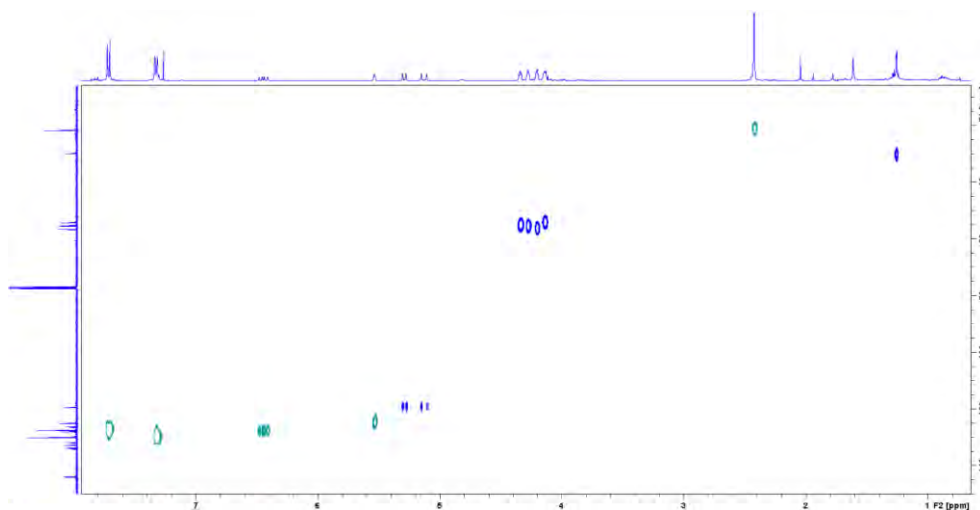
Figure S151: 2D ^{1}H-^{13}C HSQC$_{ed}$ correlation of **27** in CDCl$_3$.
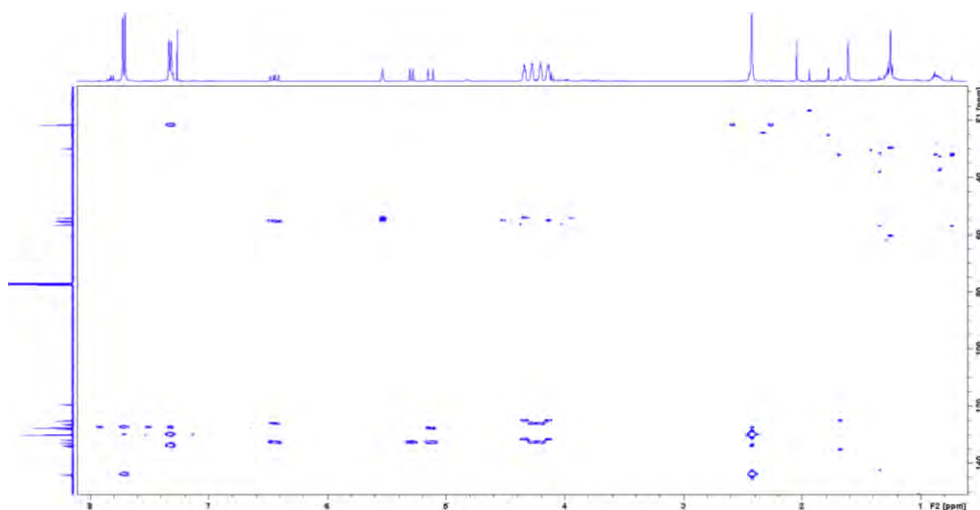
Figure S152: 2D ^{1}H-^{13}C HMBC correlation of **27** in CDCl$_3$.
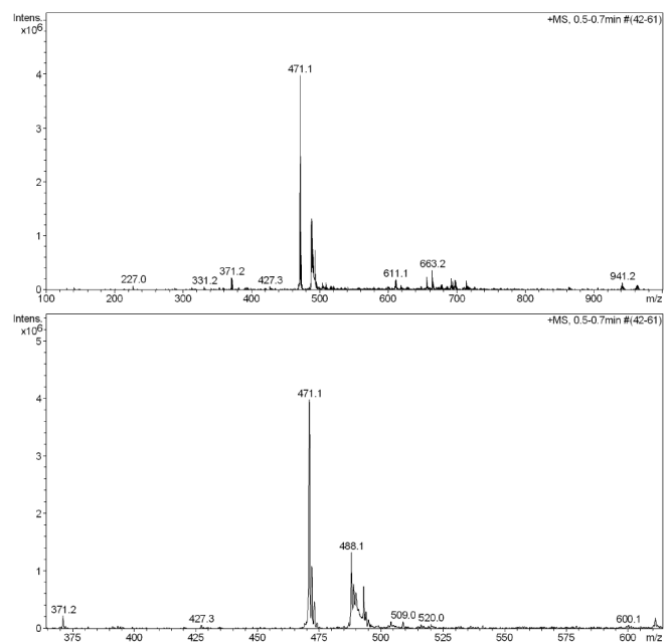
Figure S153: ESI-MS spectrum of **27**.
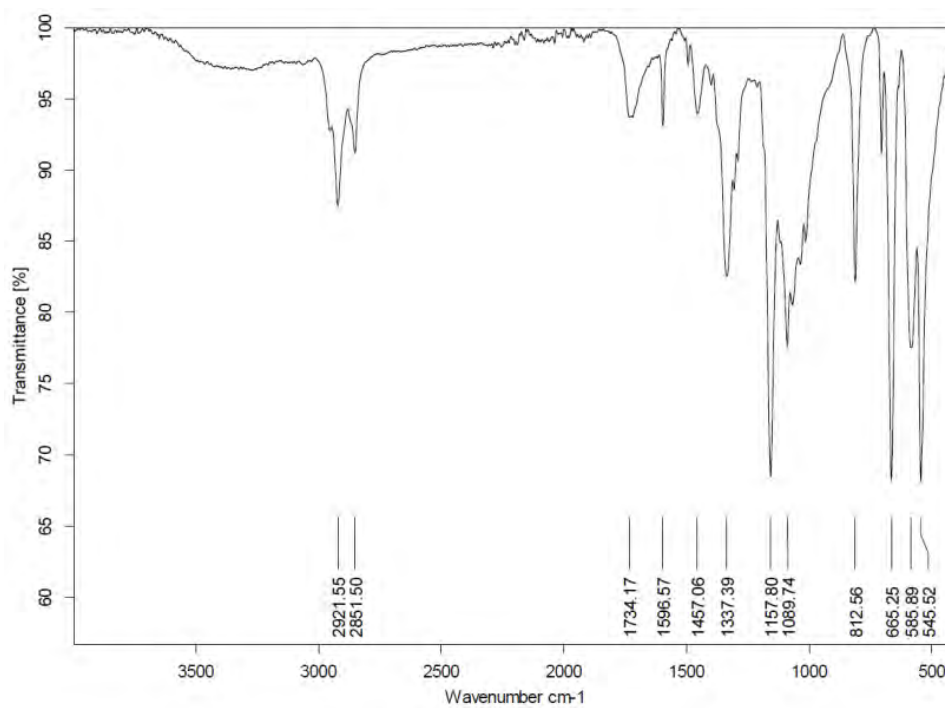
Figure S154: IR spectrum of **27**.
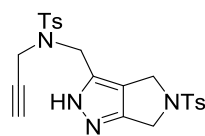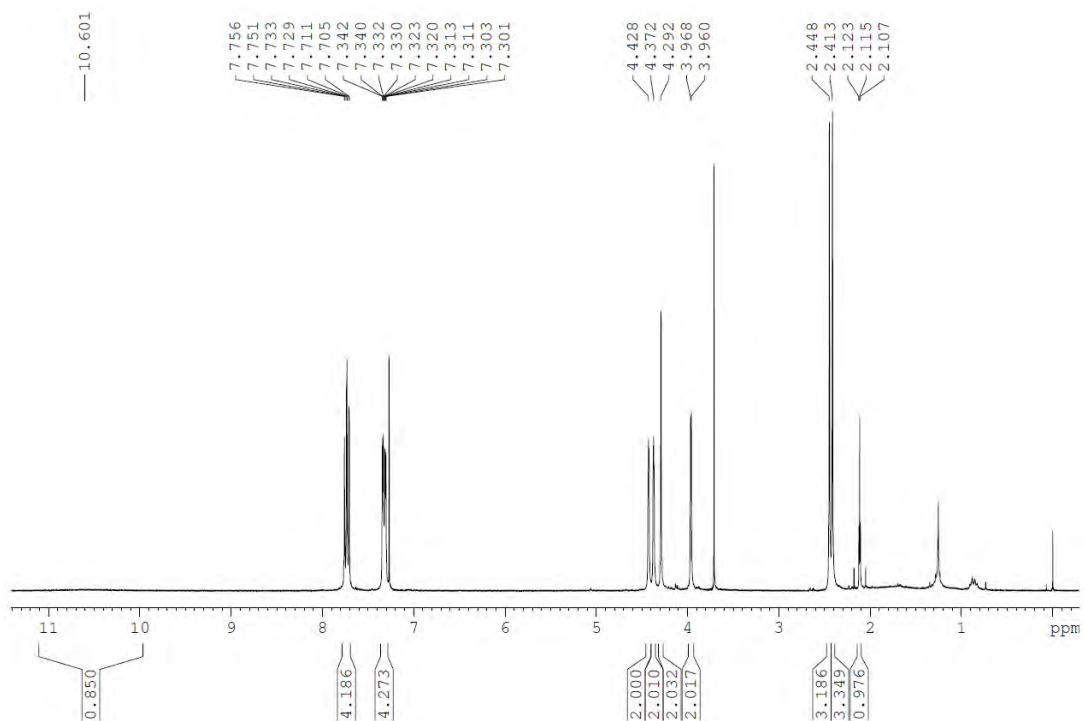
Figure S155: ^{1}H NMR spectrum (300 MHz) of **13** in CDCl$_3$.
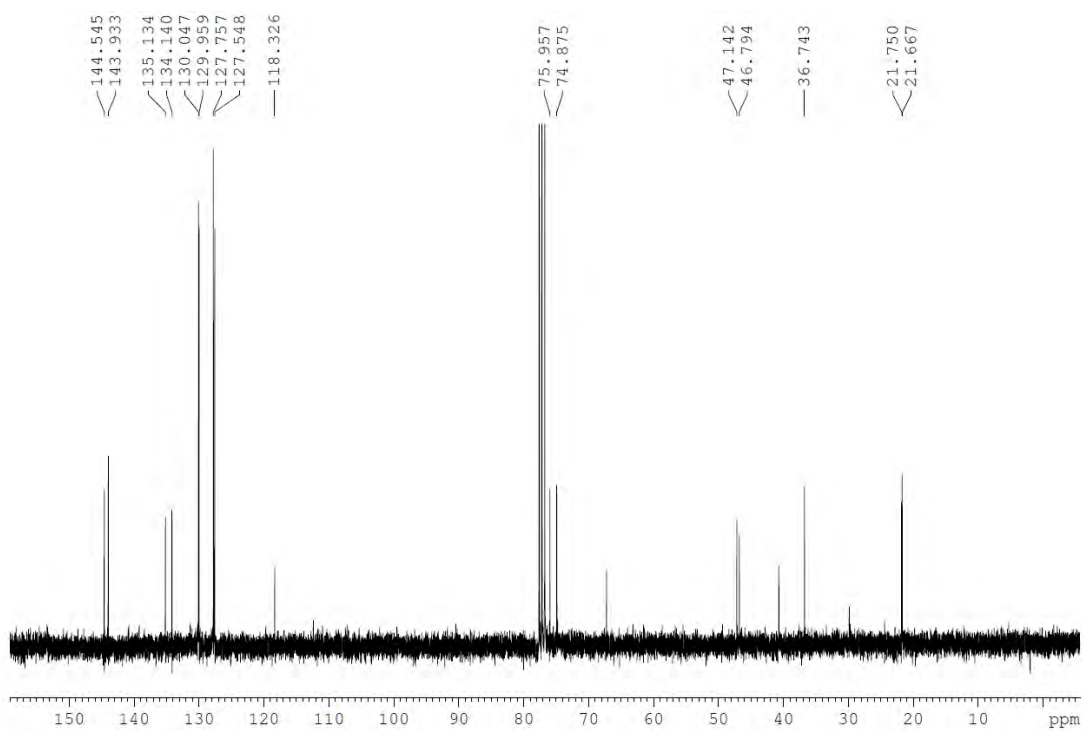
Figure S156: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **13** in CDCl$_3$.

Table S1. Cartesian coordinates of all optimized stationary points (Å).

RhBINAP (nimag=0)   **E(au)=** − 1414.6121   **G(au)=** −1414.3445

```
45       2.255926000      -0.003327000       0.000062000
15       0.736338000       1.212589000       1.059987000
15       0.732718000      -1.214482000      -1.060122000
6       -0.759962000       1.662125000       0.077575000
6       -1.768738000       0.714056000      -0.235968000
6       -0.875332000       2.975846000      -0.410933000
6       -2.866414000       1.136503000      -1.007145000
6       -1.968759000       3.368742000      -1.185213000
1       -0.108335000       3.716575000      -0.186114000
6       -2.971083000       2.445092000      -1.481444000
1       -3.645758000       0.411345000      -1.249565000
1       -2.033920000       4.395699000      -1.549057000
1       -3.833485000       2.738038000      -2.083196000
6       -0.764671000      -1.660133000      -0.077606000
6       -0.883625000      -2.973591000       0.410751000
6       -1.770692000      -0.709266000       0.236257000
6       -1.977987000      -3.363489000       1.185229000
1       -0.118728000      -3.716431000       0.185738000
6       -2.869395000      -1.128701000       1.007614000
6       -2.977637000      -2.437047000       1.481788000
1       -2.045951000      -4.390293000       1.548992000
1       -3.646653000      -0.401386000       1.250267000
1       -3.840733000      -2.727633000       2.083688000
6        1.535214000       2.801672000       1.561149000
1        1.936570000       3.337632000       0.690521000
1        0.818962000       3.443294000       2.097832000
1        2.367343000       2.560245000       2.240292000
6        0.140452000       0.542466000       2.673927000
1        1.006684000       0.443141000       3.344854000
1       -0.591587000       1.236956000       3.115372000
1       -0.320818000      -0.443374000       2.540913000
6        0.138309000      -0.541779000      -2.673521000
1        1.004645000      -0.444451000      -3.344610000
1       -0.595769000      -1.233976000      -3.115180000
1       -0.320202000       0.445251000      -2.539771000
6        1.526962000      -2.805564000      -1.562297000
1        0.808769000      -3.444875000      -2.099145000
1        2.359603000      -2.566129000      -2.241519000
1        1.927018000      -3.343105000      -0.692047000
```

N2 (nimag=0) E(au)= −109.5334   **G(au)=** −109.5462

```
7        0.000000000       0.000000000       0.552224000
7        0.000000000       0.000000000      -0.552224000
```

Ts (nimag=0) E(au)= −819.6170   **G(au)=** −819.5308

```
16       2.261209000      -0.001037000      -0.346217000
8        2.631446000      -1.305724000       0.398389000
8        2.632179000       1.306465000       0.393058000
6        0.366826000      -0.000005000      -0.137276000
6       -0.334149000       1.205679000      -0.081673000
6       -0.335874000      -1.205662000      -0.083806000
6       -1.731074000       1.206030000       0.002385000
6       -1.732023000      -1.204954000       0.000146000
6       -2.453288000       0.001231000       0.034148000
1        0.247970000       2.132515000      -0.067253000
1        0.245310000      -2.133106000      -0.070913000
1       -2.276754000       2.156154000       0.058401000
1       -2.278410000      -2.154857000       0.054544000
6       -3.964989000      -0.000104000       0.088473000
```

```
1      -4.354897000      0.930767000      0.532678000
1      -4.414182000     -0.089562000     -0.918984000
1      -4.349952000     -0.844532000      0.685041000
```

1 (nimag=0)   E(au)= -2564.2300   **G(au)=** -2564.6139

```
6       4.020744000      1.749564000      0.913109000
6       3.577677000     -1.329264000      0.381708000
6       2.394197000     -1.447062000      0.141860000
6       5.013062000     -1.222244000      0.684641000
6       5.407090000      1.267417000      0.970849000
1       5.536553000     -2.072830000      0.224491000
1       5.167070000     -1.305629000      1.774329000
1       6.074635000      2.040071000      0.563653000
1       5.697913000      1.112953000      2.024781000
6       0.978418000     -1.507192000     -0.235353000
1       0.730693000     -0.611925000     -0.830988000
1       0.818746000     -2.382619000     -0.883802000
6      -1.048179000     -2.633440000      0.758450000
1      -1.633152000     -2.641906000      1.685190000
6       2.878145000      2.153353000      0.890779000
1       1.836387000      2.414866000      0.850389000
7       5.695468000      0.010524000      0.258456000
16      6.121639000      0.128493000     -1.405025000
7       0.054352000     -1.658139000      0.912484000
16     -0.317092000     -0.208304000      1.767963000
6       0.956057000     -0.185200000      3.046189000
1       0.845336000     -1.098097000      3.643662000
1       0.760547000      0.711268000      3.650539000
1       1.935396000     -0.126096000      2.556028000
6       7.915112000     -0.111741000     -1.345340000
1       8.269284000     -0.049352000     -2.383638000
1       8.123188000     -1.102742000     -0.922793000
1       8.357125000      0.687265000     -0.736811000
8      -0.098949000      0.968556000      0.882242000
8      -1.625067000     -0.408490000      2.440131000
8       5.879451000      1.519685000     -1.847825000
8       5.543672000     -1.043978000     -2.100288000
6      -1.992180000     -2.388882000     -0.392560000
1      -1.607002000     -2.452332000     -1.427469000
1      -0.563688000     -3.619003000      0.646390000
7      -3.224686000     -2.147966000     -0.145821000
7      -4.090087000     -2.008111000     -1.181873000
16     -5.500966000     -1.033128000     -0.848433000
8      -6.215990000     -1.045599000     -2.143891000
8      -6.076943000     -1.556441000      0.400620000
6      -4.840617000      0.616130000     -0.574101000
6      -4.092015000      0.881413000      0.578938000
6      -5.072988000      1.599520000     -1.537259000
6      -3.549193000      2.153609000      0.741959000
6      -4.538632000      2.875142000     -1.338830000
6      -3.766500000      3.169931000     -0.205296000
1      -3.902275000      0.103162000      1.317397000
1      -5.665335000      1.361596000     -2.421382000
1      -2.931813000      2.351741000      1.620557000
1      -4.721542000      3.653384000     -2.084120000
1      -3.704276000     -1.786021000     -2.111004000
6      -3.167118000      4.539112000     -0.000151000
1      -3.537704000      4.999262000      0.931114000
1      -2.069455000      4.477836000      0.085216000
1      -3.407149000      5.217155000     -0.832015000
```

A (nimag=0)   E(au)= -3050.2300   **G(au)=** -3049.7202

```
6      -6.660079000      2.106099000     -1.612635000
6      -5.889278000     -1.026601000     -1.211725000
6      -4.767295000     -1.218625000     -1.631343000
```

```
45      2.051020000    -1.003941000    -0.756078000
6      -7.244861000    -0.831317000    -0.670403000
6      -7.709891000     1.661430000    -0.687090000
1      -7.491390000    -1.676720000    -0.013327000
1      -7.971709000    -0.838593000    -1.498334000
1      -7.917148000     2.466579000     0.034329000
1      -8.645121000     1.509005000    -1.251484000
6      -3.432338000    -1.396079000    -2.187584000
1      -3.242083000    -2.455004000    -2.436872000
1      -3.325582000    -0.805347000    -3.110882000
6      -0.992505000    -0.639694000    -1.814538000
1      -0.850520000     0.445453000    -1.919063000
6      -5.878019000     2.539695000    -2.429824000
1      -5.188461000     2.931821000    -3.151990000
7      -7.467886000     0.419593000     0.074047000
16     -6.618641000     0.572167000     1.552984000
7      -2.373256000    -0.867317000    -1.272509000
16     -2.275632000    -1.549440000     0.256069000
6      -3.136190000    -0.566153000     1.470260000
1      -3.079282000     0.488993000     1.178224000
1      -2.635804000    -0.781757000     2.425524000
1      -4.183850000    -0.918496000     1.486447000
6      -7.917887000     1.021535000     2.717324000
1      -7.421871000     1.142239000     3.690017000
1      -8.650810000     0.206218000     2.739098000
1      -8.370563000     1.969340000     2.399202000
8      -2.572367000    -2.982389000     0.364145000
8      -0.693557000    -1.120348000     0.480830000
8      -5.623236000     1.672537000     1.489488000
8      -6.150616000    -0.806766000     1.886666000
6      -0.011356000    -1.279623000    -0.836839000
1       0.009384000    -2.380715000    -1.025775000
1      -0.905120000    -1.108192000    -2.805966000
15      4.448567000    -1.254975000    -0.863674000
15      2.168474000     0.990544000     0.267941000
6       5.236611000    -0.777963000     0.737503000
6       5.333650000     0.580957000     1.137882000
6       5.691425000    -1.784420000     1.608568000
6       5.908707000     0.875146000     2.386423000
6       6.243055000    -1.469529000     2.853318000
1       5.634661000    -2.833786000     1.319355000
6       6.353501000    -0.134750000     3.242855000
1       6.000399000     1.919529000     2.691876000
1       6.594613000    -2.269308000     3.507490000
1       6.790217000     0.125007000     4.208876000
6       3.622546000     2.010165000    -0.188203000
6       3.393874000     3.117781000    -1.029861000
6       4.941137000     1.735907000     0.266341000
6       4.433328000     3.969724000    -1.402086000
1       2.392322000     3.338168000    -1.397797000
6       5.965441000     2.624041000    -0.107658000
6       5.723796000     3.726546000    -0.929168000
1       4.229724000     4.823544000    -2.050352000
1       6.979768000     2.427830000     0.244609000
1       6.546332000     4.389877000    -1.203221000
6       4.840959000    -3.042009000    -1.120923000
1       4.345046000    -3.675971000    -0.372039000
1       5.927676000    -3.214090000    -1.082606000
1       4.474128000    -3.327913000    -2.118671000
6       5.373503000    -0.439350000    -2.234991000
1       5.018137000    -0.868349000    -3.184231000
1       6.451144000    -0.634207000    -2.127613000
1       5.194223000     0.642630000    -2.244247000
6       2.164944000     0.673100000     2.081903000
1       1.210825000     0.193785000     2.346393000
1       2.248480000     1.639502000     2.604261000
1       3.001130000     0.029114000     2.379243000
6       0.683741000     2.038782000     0.014112000
```

1	0.798847000	2.983510000	0.566620000
1	-0.178430000	1.484302000	0.407690000
1	0.520381000	2.252589000	-1.049963000
1	2.030240000	-0.259379000	-2.079677000

B (nimag=0)   E(au)= -3050.2554   G(au)= -3049.

6	3.637469000	-2.714808000	2.745708000
6	0.143667000	-2.702974000	0.708757000
45	-0.376446000	-0.671487000	-0.418986000
6	1.495675000	-3.307425000	0.713218000
6	3.865971000	-2.723142000	1.303995000
1	1.516043000	-4.122036000	-0.035140000
1	1.635513000	-3.781435000	1.698462000
1	4.625233000	-1.973421000	1.037278000
1	4.242626000	-3.716498000	0.995569000
6	3.486381000	-2.742829000	3.947616000
7	2.618097000	-2.364387000	0.561180000
16	2.885548000	-1.703274000	-0.987348000
16	-4.277400000	-0.928669000	-0.094065000
6	-5.940846000	-1.594821000	0.065288000
1	-6.185666000	-2.132243000	-0.858967000
1	-6.598672000	-0.725474000	0.205318000
1	-5.968185000	-2.251272000	0.944118000
6	3.610187000	-2.955538000	-2.069291000
1	3.704850000	-2.477362000	-3.054189000
1	2.947458000	-3.828766000	-2.121158000
1	4.602625000	-3.209496000	-1.674008000
8	-3.881504000	-0.310787000	1.196823000
8	-4.181666000	-0.175855000	-1.371778000
8	3.830460000	-0.585850000	-0.837826000
8	1.497655000	-1.448283000	-1.542135000
15	0.531530000	0.626359000	1.534091000
15	-0.434230000	1.347463000	-1.645446000
6	-0.269091000	2.293804000	1.655990000
6	0.132174000	3.374279000	0.831054000
6	-1.295843000	2.496791000	2.594856000
6	-0.469495000	4.630731000	1.016849000
6	-1.901110000	3.747323000	2.745688000
1	-1.638066000	1.680471000	3.229685000
6	-1.477173000	4.822246000	1.963923000
1	-0.150982000	5.465552000	0.389187000
1	-2.694452000	3.877780000	3.483790000
1	-1.931777000	5.807283000	2.084216000
6	1.058935000	2.379860000	-1.345461000
6	2.105063000	2.312896000	-2.285788000
6	1.178648000	3.248247000	-0.229499000
6	3.243023000	3.109431000	-2.155106000
1	2.038702000	1.643711000	-3.142780000
6	2.324082000	4.055753000	-0.132238000
6	3.347070000	3.993305000	-1.080255000
1	4.038556000	3.044413000	-2.899116000
1	2.413985000	4.735952000	0.716980000
1	4.225831000	4.632178000	-0.974415000
6	0.074732000	-0.220294000	3.108208000
1	-0.994834000	-0.469133000	3.128040000
1	0.323418000	0.417194000	3.969360000
1	0.656036000	-1.150751000	3.175132000
6	2.339865000	0.927333000	1.772709000
1	2.794108000	-0.013888000	2.110896000
1	2.476674000	1.696710000	2.546892000
1	2.822774000	1.240636000	0.840117000
6	-1.956337000	2.347436000	-1.420473000
1	-2.805398000	1.747147000	-1.778455000
1	-0.304298000	1.926127000	-4.016459000
1	-1.415664000	0.560044000	-3.707082000
6	-1.085332000	-2.590676000	0.776012000
6	-1.365647000	-1.626956000	-1.767506000

6	-2.547431000	-2.834861000	0.847300000
6	-2.607369000	-2.419131000	-1.607275000
7	-3.296238000	-2.361486000	-0.325769000
1	-2.965361000	-2.360098000	1.745438000
1	-2.679648000	-3.926880000	0.949157000
1	-3.300492000	-2.143656000	-2.423148000
1	-2.343748000	-3.476085000	-1.837546000
1	-0.954484000	-1.743670000	-2.789564000
1	-1.655274000	-0.166107000	0.246489000
1	0.356436000	0.281133000	-3.721763000
1	3.376741000	-2.769051000	5.017074000
1	-1.860631000	3.271662000	-2.009900000
1	-2.118020000	2.593186000	-0.365318000
6	-0.436320000	0.991377000	-3.451853000

B (nimag=0) E(au)= -3050.2226   G(au)= -3049.7072

6	-4.682145000	1.511742000	1.367415000
6	-2.325747000	0.954614000	-0.711451000
45	0.296566000	0.682880000	-0.837654000
6	-3.324355000	-0.057213000	-1.094519000
6	-5.196170000	0.439684000	0.509733000
1	-2.821347000	-0.937610000	-1.515282000
1	-3.938669000	0.397028000	-1.896471000
1	-5.917646000	-0.147479000	1.095919000
1	-5.736436000	0.880904000	-0.347873000
6	-4.332235000	2.416212000	2.095176000
7	-4.146650000	-0.495123000	0.040921000
16	-4.622383000	-2.156640000	0.013617000
16	1.243955000	3.550569000	0.241192000
6	1.144300000	4.710136000	1.602451000
1	1.230733000	5.712840000	1.168131000
1	2.006698000	4.468852000	2.238438000
1	0.204991000	4.571762000	2.149319000
6	-5.944422000	-2.333049000	-1.203946000
1	-6.211231000	-3.398530000	-1.195543000
1	-5.559328000	-2.038069000	-2.188154000
1	-6.801013000	-1.720353000	-0.896731000
8	1.057776000	2.145668000	0.802545000
8	2.447798000	3.811137000	-0.577215000
8	-5.172438000	-2.436365000	1.357979000
8	-3.437373000	-2.893189000	-0.499398000
15	0.140698000	-0.940474000	1.030553000
15	2.406337000	-0.171913000	-1.392465000
6	1.767739000	-1.052360000	1.912822000
6	2.855200000	-1.804948000	1.401242000
6	1.930876000	-0.357591000	3.124388000
6	4.046430000	-1.867912000	2.144589000
6	3.130987000	-0.413754000	3.837011000
1	1.112600000	0.233423000	3.533229000
6	4.191173000	-1.178862000	3.349524000
1	4.878459000	-2.456722000	1.753968000
1	3.227741000	0.134434000	4.775930000
1	5.131262000	-1.238745000	3.900993000
6	2.567849000	-1.991149000	-1.148453000
6	2.481833000	-2.814909000	-2.285738000
6	2.792897000	-2.578016000	0.121747000
6	2.642969000	-4.197929000	-2.187643000
1	2.296903000	-2.384171000	-3.269076000
6	2.979698000	-3.969646000	0.191615000
6	2.906198000	-4.775946000	-0.944805000
1	2.572235000	-4.815068000	-3.084825000
1	3.161880000	-4.424055000	1.167081000
1	3.045446000	-5.854834000	-0.855300000
6	-1.056882000	-0.378985000	2.312114000
1	-0.872471000	0.670029000	2.579458000
1	-0.985414000	-1.014871000	3.206418000
1	-2.066895000	-0.462178000	1.886772000

```
6       -0.385212000      -2.671102000       0.689262000
1       -1.450947000      -2.667327000       0.419811000
1       -0.232433000      -3.280140000       1.592457000
1        0.187938000      -3.096369000      -0.142528000
6        3.773623000       0.657675000      -0.485527000
1        3.837611000       1.692296000      -0.849122000
1        4.708939000       0.121113000      -0.703866000
1        3.588116000       0.667545000       0.593479000
6        2.837228000       0.135922000      -3.151418000
1        3.799560000      -0.342250000      -3.383668000
1        2.939015000       1.223236000      -3.282703000
6       -1.666693000       1.960494000      -0.444718000
6        0.323210000       1.964638000      -2.294734000
6       -1.396671000       3.399666000      -0.191381000
6        0.102856000       3.419817000      -2.130386000
7       -0.122210000       3.893742000      -0.752424000
1       -1.441798000       3.601344000       0.886659000
1       -2.203565000       3.984368000      -0.658440000
1        0.979233000       3.935781000      -2.568383000
1       -0.747098000       3.753567000      -2.756085000
1        0.444393000       1.698126000      -3.358073000
1       -0.175565000      -0.358186000      -1.862783000
1        2.061228000      -0.239103000      -3.830844000
1       -4.020558000       3.211075000       2.746866000
```

B (nimag=0)   E(au)= -3049.9594   G(au)= -3049.4548

```
6       -5.145430000       0.103820000      -1.418830000
6       -2.028260000      -0.339310000      -0.529290000
45       0.054450000       0.409080000      -0.781920000
6       -2.531060000      -1.639970000      -1.041660000
6       -5.011000000      -1.359830000      -1.424140000
1       -1.869040000      -2.450620000      -0.709570000
1       -2.494530000      -1.634670000      -2.142830000
1       -5.955190000      -1.793510000      -1.057410000
1       -4.903520000      -1.704040000      -2.466710000
6       -5.360900000       1.292740000      -1.513780000
7       -3.909730000      -1.974240000      -0.660370000
16      -4.181390000      -2.204170000       1.031510000
16      -0.174380000       3.736360000       0.658040000
6       -0.742290000       5.329110000       1.287270000
1       -1.014070000       5.958840000       0.431990000
1        0.103360000       5.755560000       1.843170000
1       -1.597850000       5.154380000       1.951100000
6       -5.098930000      -3.755830000       1.060330000
1       -5.310200000      -3.957580000       2.119560000
1       -4.464670000      -4.537310000       0.624820000
1       -6.038500000      -3.635440000       0.504500000
8        0.090490000       2.857730000       1.826370000
8        0.877160000       3.997390000      -0.362830000
8       -5.045930000      -1.128040000       1.560000000
8       -2.831500000      -2.464970000       1.610540000
15       0.782700000      -0.975090000       1.204520000
15       2.299450000       0.517850000      -1.513450000
6        2.534280000      -0.695900000       1.763240000
6        3.645830000      -1.120760000       0.993760000
6        2.771190000      -0.021420000       2.974740000
6        4.942070000      -0.903480000       1.490830000
6        4.068320000       0.210170000       3.440380000
1        1.934840000       0.334660000       3.575440000
6        5.159760000      -0.243520000       2.701310000
1        5.794760000      -1.244450000       0.899210000
1        4.217770000       0.737510000       4.384250000
1        6.179160000      -0.081050000       3.058230000
6        3.026760000      -1.189620000      -1.501150000
6        3.004900000      -1.922680000      -2.700040000
6        3.529910000      -1.812580000      -0.333750000
6        3.478240000      -3.229830000      -2.772090000
```

```
1        2.612030000      -1.463740000      -3.611260000
6        4.020160000      -3.127160000      -0.425420000
6        3.993910000      -3.836920000      -1.626170000
1        3.450400000      -3.766510000      -3.719640000
1        4.422000000      -3.600050000       0.475440000
1        4.377030000      -4.859710000      -1.663670000
6       -0.239820000      -0.528880000       2.669000000
1       -0.216660000       0.561150000       2.814790000
1        0.113030000      -1.043590000       3.578640000
1       -1.267080000      -0.851670000       2.458560000
6        0.605320000      -2.817390000       1.157480000
1       -0.479950000      -3.047630000       1.142350000
1        1.039090000      -3.261950000       2.071300000
1        1.096190000      -3.244790000       0.278880000
6        3.430510000       1.672350000      -0.621360000
1        3.044950000       2.687040000      -0.802030000
1        4.456010000       1.575490000      -1.009390000
1        3.421640000       1.490240000       0.458950000
6        2.539120000       1.093550000      -3.257010000
1        3.582470000       0.934840000      -3.574830000
1        2.323670000       2.170870000      -3.283000000
6       -1.986070000       0.762050000       0.050120000
6       -0.438140000       1.762390000      -1.971550000
6       -2.349500000       2.124000000       0.500880000
6       -1.332360000       2.925750000      -1.625040000
7       -1.584970000       3.172120000      -0.196670000
1       -2.206830000       2.230120000       1.583420000
1       -3.423380000       2.268000000       0.285540000
1       -0.958050000       3.854640000      -2.082960000
1       -2.316720000       2.734040000      -2.105440000
1       -0.101090000       1.876130000      -3.031250000
1        1.861840000       0.582160000      -3.952090000
1       -5.581240000       2.340860000      -1.582100000
```

TS_BC (nimag=1) (-278.69i) E(au)= -3050.2443   G(au)= -3049.7287

```
6        3.748580000      -2.792616000       2.685970000
6        0.283022000      -2.730550000       0.505464000
45      -0.282370000      -0.605276000      -0.324282000
6        1.633463000      -3.308442000       0.573074000
6        3.975545000      -2.759679000       1.242246000
1        1.708870000      -4.111236000      -0.183246000
1        1.704709000      -3.806500000       1.556162000
1        4.757016000      -2.024442000       1.005496000
1        4.321855000      -3.748649000       0.893234000
6        3.567944000      -2.845802000       3.883316000
7        2.739351000      -2.338388000       0.522131000
16       3.020294000      -1.532765000      -0.958370000
16      -4.292877000      -1.149363000      -0.123888000
6       -5.884844000      -1.945696000       0.118781000
1       -6.127085000      -2.499565000      -0.795808000
1       -6.604824000      -1.136960000       0.301756000
1       -5.805183000      -2.607205000       0.990066000
6        3.742413000      -2.676431000      -2.147772000
1        3.906236000      -2.085477000      -3.059115000
1        3.042187000      -3.499844000      -2.331163000
1        4.696561000      -3.027310000      -1.734623000
8       -3.912865000      -0.465143000       1.141690000
8       -4.320750000      -0.404024000      -1.410719000
8        3.975043000      -0.443833000      -0.681299000
8        1.640935000      -1.200158000      -1.483482000
15       0.525106000       0.700909000       1.573477000
15      -0.568760000       1.304153000      -1.621722000
6       -0.323664000       2.344303000       1.702287000
6       -0.024175000       3.410010000       0.816956000
6       -1.301049000       2.537588000       2.693753000
6       -0.684021000       4.639566000       0.986967000
6       -1.963978000       3.759870000       2.831441000
```

```
1      -1.558045000       1.731079000       3.379144000
6      -1.647378000       4.819276000       1.980870000
1      -0.445470000       5.461301000       0.309028000
1      -2.719887000       3.879264000       3.609791000
1      -2.150624000       5.782522000       2.083362000
6       0.854001000       2.460572000      -1.408390000
6       1.856486000       2.461734000      -2.395816000
6       0.984776000       3.318278000      -0.286748000
6       2.964133000       3.305684000      -2.301083000
1       1.780764000       1.802673000      -3.259369000
6       2.099048000       4.172592000      -0.222055000
6       3.082402000       4.170326000      -1.212623000
1       3.726262000       3.287184000      -3.082012000
1       2.195769000       4.840696000       0.635751000
1       3.939798000       4.840732000      -1.129011000
6       0.103914000      -0.176633000       3.140764000
1      -0.960005000      -0.446136000       3.170650000
1       0.355953000       0.446887000       4.010960000
1       0.702958000      -1.098222000       3.180337000
6       2.319461000       1.060526000       1.817051000
1       2.831684000       0.104391000       1.989841000
1       2.440319000       1.711219000       2.695602000
1       2.753418000       1.538229000       0.931354000
6      -2.142774000       2.218532000      -1.395944000
1      -2.959588000       1.527848000      -1.651806000
1      -0.549964000       1.758748000      -4.026692000
1      -1.528300000       0.321691000      -3.598017000
6      -0.968570000      -2.650428000       0.472185000
6      -1.111104000      -1.988640000      -1.498472000
6      -2.404448000      -2.935646000       0.759227000
6      -2.487954000      -2.571833000      -1.615561000
7      -3.235866000      -2.498519000      -0.367107000
1      -2.716870000      -2.437869000       1.686240000
1      -2.490769000      -4.027034000       0.896381000
1      -2.997294000      -1.990056000      -2.406926000
1      -2.456256000      -3.620410000      -1.957817000
1      -0.394221000      -2.471487000      -2.187589000
1      -1.621435000      -0.202967000       0.290200000
1       0.256870000       0.193735000      -3.647567000
1       3.404310000      -2.880177000       4.944785000
1      -2.147885000       3.089921000      -2.067039000
1      -2.262633000       2.544481000      -0.356786000
6      -0.586175000       0.853222000      -3.403844000
```

TS_BC (nimag=1) (−451.92*i*) **E(au)=** −3050.2392   **G(au)=** −3049.7230

```
6      -4.129426000       1.114847000       1.625941000
6      -2.178782000       0.775691000      -0.935741000
45      0.024307000       0.585499000      -0.757716000
6      -3.375348000      -0.093629000      -1.099492000
6      -4.734251000      -0.056806000       0.991192000
1      -3.093071000      -0.843952000      -1.859097000
1      -4.190100000       0.523986000      -1.515502000
1      -5.054419000      -0.758478000       1.775401000
1      -5.632137000       0.260912000       0.429430000
6      -3.701249000       2.105767000       2.179518000
7      -3.785963000      -0.783089000       0.115951000
16     -4.053726000      -2.487646000      -0.012906000
16      0.748121000       3.624525000       0.327533000
6       0.306211000       4.724830000       1.669779000
1       0.394250000       5.746887000       1.282709000
1       1.046441000       4.525377000       2.456230000
1      -0.707523000       4.496814000       2.018189000
6      -5.718278000      -2.743139000      -0.662353000
1      -5.845373000      -3.832697000      -0.715061000
1      -5.777912000      -2.293823000      -1.661139000
1      -6.443419000      -2.304888000       0.034265000
8       0.536114000       2.196171000       0.818787000
```

8	2.075432000	3.976023000	-0.218833000
8	-4.002221000	-2.993100000	1.377959000
8	-3.074168000	-2.948812000	-1.031441000
15	0.141143000	-1.023662000	1.055757000
15	2.190825000	-0.026940000	-1.448516000
6	1.798534000	-0.878506000	1.877181000
6	2.971781000	-1.482389000	1.357900000
6	1.891187000	-0.120403000	3.058634000
6	4.178301000	-1.343189000	2.066830000
6	3.103847000	0.026554000	3.735326000
1	1.006287000	0.361630000	3.471964000
6	4.251674000	-0.595578000	3.242572000
1	5.077811000	-1.817663000	1.670010000
1	3.143458000	0.620095000	4.650593000
1	5.204130000	-0.497446000	3.766733000
6	2.650317000	-1.791341000	-1.173204000
6	2.671284000	-2.651932000	-2.285626000
6	2.997102000	-2.298043000	0.104296000
6	3.050446000	-3.989365000	-2.156188000
1	2.395296000	-2.285876000	-3.273713000
6	3.402202000	-3.640040000	0.205933000
6	3.429316000	-4.481946000	-0.906647000
1	3.056312000	-4.636636000	-3.034765000
1	3.676249000	-4.031458000	1.187211000
1	3.737637000	-5.522845000	-0.792974000
6	-1.064712000	-0.713929000	2.410852000
1	-1.118258000	0.355177000	2.652721000
1	-0.788823000	-1.294328000	3.303261000
1	-2.047196000	-1.044227000	2.050278000
6	-0.113966000	-2.811829000	0.691971000
1	-1.164547000	-2.958474000	0.409589000
1	0.119398000	-3.402553000	1.589832000
1	0.517026000	-3.139129000	-0.141249000
6	3.506409000	1.012396000	-0.689403000
1	3.345425000	2.051844000	-1.004984000
1	4.482391000	0.650075000	-1.045714000
1	3.464735000	0.963349000	0.404127000
6	2.424144000	0.261949000	-3.249207000
1	3.417547000	-0.092982000	-3.559178000
1	2.362509000	1.345631000	-3.421517000
6	-1.739479000	1.975900000	-1.154368000
6	-0.212819000	1.972881000	-2.285428000
6	-1.747735000	3.405110000	-0.674310000
6	0.037543000	3.466777000	-2.225833000
7	-0.410073000	3.981807000	-0.914314000
1	-2.054549000	3.474188000	0.376003000
1	-2.474819000	3.968071000	-1.281447000
1	1.105415000	3.689026000	-2.379741000
1	-0.527733000	4.014053000	-2.996658000
1	-0.475562000	1.580412000	-3.276646000
1	-0.288340000	-0.513646000	-1.786288000
1	1.644581000	-0.238979000	-3.837176000
1	-3.331261000	2.966942000	2.704887000

TS_BC (nimag=1) (-297.20*i*) E(au)= -3049.9434   **G(au)=** -3049.4410

6	3.724788000	-1.112072000	3.143688000
6	0.828763000	-2.347728000	0.582032000
45	-0.269463000	-0.735693000	-0.393249000
6	2.237357000	-2.573409000	1.009275000
6	4.230755000	-1.252697000	1.778944000
1	2.584184000	-3.510705000	0.533243000
1	2.239841000	-2.750847000	2.097024000
1	4.768789000	-0.336762000	1.490004000
1	4.958439000	-2.088698000	1.771703000
6	3.360023000	-1.040942000	4.297233000
1	3.047239000	-0.959543000	5.321259000
7	3.150348000	-1.445059000	0.781244000

16	3.680298000	-1.195453000	-0.843572000
16	-3.693015000	-1.914972000	-0.121956000
6	-5.258271000	-2.807434000	-0.209256000
1	-5.372679000	-3.204890000	-1.225131000
1	-6.041864000	-2.071274000	0.016092000
1	-5.241871000	-3.607970000	0.540239000
6	5.178400000	-2.195041000	-1.077276000
1	5.441460000	-2.061903000	-2.135382000
1	4.947079000	-3.248606000	-0.872152000
1	5.983835000	-1.815509000	-0.436895000
8	-3.486444000	-1.508374000	1.293499000
8	-3.677615000	-0.923522000	-1.227020000
8	4.067301000	0.228114000	-0.944125000
8	2.639673000	-1.782117000	-1.723967000
15	-0.213675000	0.708441000	1.539336000
15	-0.191352000	1.140153000	-1.814506000
6	-1.485158000	2.042416000	1.281783000
6	-1.226707000	3.195350000	0.496535000
6	-2.765273000	1.875931000	1.839197000
6	-2.240845000	4.157622000	0.348393000
6	-3.765097000	2.835810000	1.665609000
1	-3.001699000	0.977760000	2.407719000
6	-3.499913000	3.988180000	0.926080000
1	-2.033380000	5.048648000	-0.248109000
1	-4.748505000	2.678504000	2.113183000
1	-4.269711000	4.750430000	0.789940000
6	0.664204000	2.650060000	-1.162780000
6	1.935167000	2.975800000	-1.667853000
6	0.093393000	3.471669000	-0.156926000
6	2.623500000	4.109088000	-1.228942000
1	2.413061000	2.335707000	-2.407611000
6	0.790625000	4.621914000	0.250301000
6	2.041710000	4.945903000	-0.277185000
1	3.610373000	4.333406000	-1.638058000
1	0.343291000	5.259564000	1.015650000
1	2.562036000	5.842717000	0.065152000
6	-0.776768000	-0.161331000	3.071380000
1	-1.695854000	-0.726566000	2.868422000
1	-0.941854000	0.548255000	3.896189000
1	0.016463000	-0.868056000	3.358307000
6	1.300622000	1.576000000	2.157867000
1	1.940098000	0.818525000	2.632635000
1	1.031873000	2.342742000	2.900173000
1	1.854927000	2.036896000	1.331875000
6	-1.834703000	1.713925000	-2.434666000
1	-2.293773000	0.883263000	-2.989739000
1	-1.707014000	2.586689000	-3.092869000
1	-2.493570000	1.967441000	-1.595846000
6	0.702785000	0.737422000	-3.379201000
1	0.816557000	1.624459000	-4.020126000
1	0.097545000	-0.015349000	-3.905595000
6	-0.367780000	-2.756764000	0.510847000
6	-0.595064000	-2.150448000	-1.661129000
6	-1.622206000	-3.549329000	0.587140000
6	-1.822022000	-3.029630000	-1.765596000
7	-2.554046000	-3.176413000	-0.499866000
1	-2.120140000	-3.398670000	1.553499000
1	-1.396653000	-4.624453000	0.478389000
1	-2.480066000	-2.577170000	-2.528282000
1	-1.575807000	-4.048531000	-2.113587000
1	0.249664000	-2.552271000	-2.254203000
1	1.681227000	0.292742000	-3.154653000

C (nimag=0)   **E(au)=** -3050.2741   **G(au)=** -3049.7559

6	-3.737138000	0.182877000	2.120587000
6	-2.025921000	0.489232000	-0.680270000
45	-0.056247000	0.338313000	-0.496000000

```
6      -3.368989000     -0.105981000     -0.797307000
6      -4.469610000     -0.798537000      1.319072000
1      -3.317801000     -0.503737000     -1.838083000
1      -4.153011000      0.673051000     -0.820355000
1      -4.643150000     -1.711417000      1.907277000
1      -5.454309000     -0.376540000      1.043805000
6      -3.148033000      1.026705000      2.762865000
7      -3.692946000     -1.184858000      0.118166000
16     -4.026439000     -2.724576000     -0.568725000
16      0.095973000      4.327063000      0.574644000
6      -0.290032000      6.012258000      1.060050000
1      -0.134662000      6.655044000      0.185546000
1       0.406886000      6.262399000      1.870951000
1      -1.329926000      6.037232000      1.406706000
6      -5.737457000     -2.729316000     -1.139993000
1      -5.906700000     -3.728887000     -1.562407000
1      -5.853601000     -1.955180000     -1.908302000
1      -6.395379000     -2.557666000     -0.278499000
8      -0.201033000      3.413176000      1.713862000
8       1.446682000      4.305373000     -0.051505000
8      -3.896146000     -3.687823000      0.548927000
8      -3.129181000     -2.800831000     -1.753997000
15      0.294978000     -1.628390000      0.716897000
15      2.343426000      0.686578000     -0.744735000
6       1.872941000     -1.668359000      1.681649000
6       3.148026000     -1.860124000      1.094746000
6       1.781866000     -1.505150000      3.077240000
6       4.272420000     -1.946665000      1.933971000
6       2.915256000     -1.563916000      3.890051000
1       0.817035000     -1.336483000      3.552870000
6       4.165164000     -1.802212000      3.317537000
1       5.251860000     -2.107252000      1.479944000
1       2.812648000     -1.434257000      4.968735000
1       5.057912000     -1.865604000      3.942344000
6       3.120620000     -0.907790000     -1.278372000
6       3.399745000     -1.089382000     -2.646078000
6       3.382967000     -1.969506000     -0.377317000
6       3.939383000     -2.286550000     -3.122202000
1       3.207736000     -0.288767000     -3.359600000
6       3.946948000     -3.157285000     -0.872100000
6       4.218879000     -3.323391000     -2.231149000
1       4.147431000     -2.398891000     -4.187699000
1       4.159805000     -3.968343000     -0.173112000
1       4.647154000     -4.261209000     -2.589659000
6      -0.985626000     -2.073737000      1.951105000
1      -1.196771000     -1.233215000      2.623281000
1      -0.639945000     -2.946450000      2.523582000
1      -1.901995000     -2.332964000      1.410862000
6       0.270282000     -3.036634000     -0.472817000
1      -0.757863000     -3.125677000     -0.855495000
1       0.552922000     -3.960272000      0.054389000
1       0.959728000     -2.862531000     -1.307329000
6       3.236937000      1.366426000      0.715669000
1       2.897433000      2.407384000      0.820206000
1       3.880040000      1.859580000     -2.238625000
1       2.521331000      2.889506000     -1.683466000
6      -1.708903000      1.809133000     -1.094998000
6      -0.767409000      2.139254000     -2.048684000
6      -2.134292000      3.089450000     -0.346430000
6      -0.530802000      3.637285000     -2.001447000
7      -1.085075000      4.048958000     -0.693690000
1      -2.238580000      2.962299000      0.735403000
1      -3.100876000      3.411205000     -0.772364000
1       0.519137000      3.932852000     -2.103555000
1      -1.102450000      4.127788000     -2.808672000
1      -0.485753000      1.523623000     -2.905131000
1      -0.033187000      1.041415000      0.848425000
1       2.260377000      1.697159000     -2.998948000
```

```
1        -2.621255000        1.760907000        3.344861000
1         4.320130000        1.340594000        0.527923000
1         2.999680000        0.811181000        1.629362000
6         2.795120000        1.894841000       -2.060700000
```

C (nimag=0)   E(au)= -3050.3026   G(au)= -3049.7844

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6        -4.388889000        0.476607000        2.790167000
6        -1.860898000        1.351463000       -0.148016000
45       -0.072892000        0.658610000       -0.299276000
6        -3.307063000        1.094165000        0.064925000
6        -4.748017000       -0.277638000        1.592031000
1        -3.870824000        1.402377000       -0.838069000
1        -3.586761000        1.835785000        0.846022000
1        -4.893277000       -1.338759000        1.844978000
1        -5.708239000        0.112242000        1.202144000
6        -4.151876000        1.128955000        3.783971000
1        -3.965222000        1.686561000        4.683845000
7        -3.670876000       -0.225302000        0.563900000
16       -3.794973000       -1.461610000       -0.651663000
16        1.753303000        3.465572000       -0.128343000
6         2.192692000        4.764539000        1.027658000
1         2.464056000        5.641607000        0.426337000
1         3.054126000        4.382598000        1.592641000
1         1.341707000        4.966724000        1.689758000
6        -5.436006000       -1.353194000       -1.404757000
1        -5.440273000       -2.126357000       -2.186134000
1        -5.570135000       -0.358464000       -1.849302000
1        -6.195431000       -1.579722000       -0.645714000
8         1.309310000        2.261192000        0.702327000
8         2.824494000        3.269046000       -1.124052000
8        -3.693561000       -2.741199000        0.074525000
8        -2.798883000       -1.060620000       -1.686162000
15        0.182458000       -0.813467000        1.503880000
15        1.605224000       -0.529626000       -1.626419000
6         1.982646000       -1.103350000        1.772535000
6         2.726933000       -2.047181000        1.015938000
6         2.627869000       -0.368608000        2.786374000
6         4.078634000       -2.249441000        1.344993000
6         3.976326000       -0.573556000        3.080289000
1         2.075507000        0.364628000        3.372900000
6         4.702460000       -1.525459000        2.362479000
1         4.651823000       -2.983824000        0.775762000
1         4.451258000       -0.000058000        3.878220000
1         5.754684000       -1.705274000        2.590755000
6         1.611547000       -2.342855000       -1.284299000
6         1.071405000       -3.216283000       -2.245604000
6         2.149236000       -2.879256000       -0.086166000
6         1.078496000       -4.599400000       -2.051658000
1         0.643203000       -2.828679000       -3.169422000
6         2.170755000       -4.275656000        0.075386000
6         1.641064000       -5.132028000       -0.891428000
1         0.655463000       -5.254872000       -2.814796000
1         2.595767000       -4.692185000        0.990801000
1         1.665556000       -6.211842000       -0.734008000
6        -0.452180000       -0.024069000        3.035874000
1        -0.050271000        0.991982000        3.143001000
1        -0.182666000       -0.629657000        3.914361000
1        -1.546881000        0.031809000        2.951262000
6        -0.674262000       -2.433402000        1.452985000
1        -1.757349000       -2.260482000        1.495950000
1        -0.351325000       -3.023177000        2.324365000
1        -0.444884000       -2.980158000        0.532028000
6         3.349075000        0.052075000       -1.478395000
1         3.401592000        1.091594000       -1.829012000
1         3.991228000       -0.594980000       -2.095204000
1         3.682748000        0.015458000       -0.434671000
6         1.273725000       -0.367861000       -3.431811000
```

1	1.964756000	-1.002791000	-4.005939000
1	1.446171000	0.681122000	-3.712722000
6	-1.308872000	2.463650000	-0.869345000
6	-0.648193000	2.302118000	-2.077172000
6	-0.897718000	3.813991000	-0.266375000
6	0.228006000	3.522318000	-2.316768000
7	0.370173000	4.130668000	-0.963489000
1	-0.791553000	3.813019000	0.825019000
1	-1.640474000	4.580351000	-0.545589000
1	1.211652000	3.316667000	-2.755779000
1	-0.282742000	4.255936000	-2.965257000
1	-0.927360000	1.585075000	-2.847738000
1	-0.898011000	-0.468130000	-0.931837000
1	0.236706000	-0.639351000	-3.672230000

C (nimag=0) E(au)= -3050.0234   G(au)= -3049.5435

6	2.634813000	-2.621241000	3.119976000
6	0.408278000	-2.172116000	-0.273120000
45	-0.581835000	-0.591858000	-0.469600000
6	1.600841000	-2.873860000	0.286443000
6	3.459105000	-2.472443000	1.920811000
1	1.958735000	-3.617953000	-0.452508000
1	1.259591000	-3.455626000	1.163232000
1	4.245376000	-1.724992000	2.106318000
1	3.956001000	-3.442386000	1.717218000
6	1.980863000	-2.797932000	4.124951000
1	1.416713000	-2.946777000	5.026433000
7	2.676574000	-1.993721000	0.756875000
16	3.656909000	-1.283401000	-0.474772000
16	-3.663584000	-1.521538000	0.104626000
6	-5.418126000	-1.490648000	-0.290384000
1	-5.540342000	-1.275499000	-1.359096000
1	-5.852258000	-0.689285000	0.322199000
1	-5.829636000	-2.471282000	-0.023417000
6	4.899999000	-2.521017000	-0.940408000
1	5.478582000	-2.057044000	-1.750678000
1	4.393096000	-3.424745000	-1.303478000
1	5.550627000	-2.728575000	-0.081905000
8	-3.480164000	-1.975473000	1.504610000
8	-3.102742000	-0.177992000	-0.299594000
8	4.360093000	-0.149220000	0.160247000
8	2.774966000	-1.099179000	-1.653746000
15	-0.129385000	0.598786000	1.534009000
15	-0.119738000	1.287578000	-1.840511000
6	-1.043694000	2.213514000	1.428459000
6	-0.551826000	3.316041000	0.683644000
6	-2.290828000	2.329068000	2.067564000
6	-1.309500000	4.500049000	0.646301000
6	-3.036374000	3.507954000	2.004277000
1	-2.693365000	1.488560000	2.632011000
6	-2.540754000	4.602421000	1.295336000
1	-0.920641000	5.351638000	0.083910000
1	-3.998646000	3.568910000	2.516607000
1	-3.108038000	5.533960000	1.244762000
6	1.098331000	2.482902000	-1.114804000
6	2.394765000	2.544237000	-1.655675000
6	0.774838000	3.317926000	-0.014747000
6	3.351042000	3.430711000	-1.156770000
1	2.678279000	1.884929000	-2.474199000
6	1.743217000	4.222953000	0.453647000
6	3.019786000	4.285611000	-0.106408000
1	4.351174000	3.448702000	-1.593440000
1	1.487179000	4.873958000	1.292241000
1	3.753769000	4.991799000	0.286769000
6	-0.836621000	-0.231234000	3.025340000
1	-1.860419000	-0.576427000	2.828611000
1	-0.811398000	0.430731000	3.904584000

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1        -0.209575000      -1.114079000       3.218440000
6         1.578969000       1.004667000       2.112233000
1         1.977832000       0.095830000       2.583117000
1         1.541275000       1.815200000       2.855082000
1         2.237075000       1.281122000       1.280757000
6        -1.567015000       2.314768000      -2.368237000
1        -2.228949000       1.677032000      -2.973517000
1        -1.231825000       3.174201000      -2.968663000
1        -2.127098000       2.668777000      -1.493999000
6         0.619849000       0.804860000      -3.459484000
1         0.926991000       1.689095000      -4.037621000
1        -0.147782000       0.259299000      -4.027158000
6        -0.740809000      -2.697499000      -0.923132000
6        -1.167003000      -1.971628000      -2.081112000
6        -1.918998000      -3.515627000      -0.392715000
6        -2.650177000      -2.262849000      -2.270209000
7        -3.102040000      -2.793171000      -0.949475000
1        -1.992113000      -3.595186000       0.697576000
1        -1.932188000      -4.527780000      -0.831054000
1        -3.250764000      -1.393890000      -2.570450000
1        -2.816286000      -3.060819000      -3.015466000
1        -0.508896000      -1.829290000      -2.937929000
1         1.477385000       0.140662000      -3.287999000
```

D (nimag=0)   E(au)= -3050.3086   G(au)= -3049.7908

```
6        -1.481409000       1.261092000      -1.880608000
6        -1.617769000       1.192186000       0.798961000
45       -0.259728000       0.149336000      -0.201063000
6        -1.936423000       2.650899000       0.612060000
6        -1.551423000       2.743427000      -1.836479000
1        -1.630251000       3.156823000       1.546963000
1        -3.025288000       2.819868000       0.523204000
1        -0.846055000       3.162663000      -2.566863000
1        -2.569420000       3.028758000      -2.154853000
6        -1.703755000       0.059807000      -2.047289000
1        -2.083831000      -0.909376000      -2.326748000
7        -1.287151000       3.319424000      -0.512901000
16        0.306875000       3.950018000      -0.249206000
16       -4.615236000      -1.634913000      -0.274212000
6        -6.038307000      -2.726415000      -0.156568000
1        -5.874876000      -3.432202000       0.667619000
1        -6.091437000      -3.253608000      -1.119176000
1        -6.922722000      -2.099271000       0.008810000
6         0.169903000       5.665475000      -0.773743000
1         1.170294000       6.099436000      -0.636806000
1        -0.570469000       6.155803000      -0.129918000
1        -0.121353000       5.690299000      -1.831578000
8        -4.878467000      -0.553016000      -1.253269000
8        -3.367770000      -2.447756000      -0.419511000
8         1.248173000       3.245307000      -1.166186000
8         0.519205000       3.903460000       1.219959000
15        1.237281000      -1.241086000      -1.627076000
15        1.337899000      -0.061063000       1.535372000
6         2.237827000      -2.520648000      -0.739024000
6         3.352060000      -2.189416000       0.073817000
6         1.861458000      -3.871665000      -0.864385000
6         4.073405000      -3.229297000       0.686092000
6         2.577355000      -4.887044000      -0.225420000
1         1.006629000      -4.155181000      -1.477698000
6         3.695485000      -4.565586000       0.544541000
1         4.941058000      -2.975905000       1.298800000
1         2.266250000      -5.926280000      -0.345635000
1         4.273406000      -5.350268000       1.036205000
6         3.050804000       0.221262000       0.917091000
6         3.586836000       1.513649000       1.073684000
6         3.829478000      -0.789715000       0.299279000
6         4.885970000       1.807437000       0.656692000
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1	2.995175000	2.308343000	1.527052000
6	5.141345000	-0.472848000	-0.094490000
6	5.669569000	0.807517000	0.079043000
1	5.283135000	2.814578000	0.793474000
1	5.750453000	-1.249941000	-0.560417000
1	6.690874000	1.021737000	-0.241264000
6	0.362643000	-2.188207000	-2.951879000
1	-0.447010000	-2.809845000	-2.544337000
1	1.079891000	-2.826885000	-3.488035000
1	-0.061837000	-1.467975000	-3.665300000
6	2.397620000	-0.202916000	-2.619545000
1	1.790912000	0.425659000	-3.288912000
1	3.056643000	-0.848446000	-3.218905000
1	2.998814000	0.449242000	-1.975150000
6	1.301206000	-1.680714000	2.430657000
1	0.483174000	-1.653030000	3.165905000
1	2.248860000	-1.797677000	2.977103000
1	1.166493000	-2.531967000	1.753565000
6	1.103195000	1.141333000	2.907560000
1	1.927607000	1.041370000	3.629185000
1	0.153266000	0.903889000	3.409109000
6	-2.608705000	0.355199000	1.400829000
6	-2.396261000	-0.839765000	2.029678000
6	-4.146601000	0.516075000	1.255555000
6	-3.701149000	-1.542804000	2.272006000
7	-4.634311000	-0.872257000	1.333777000
1	-4.468659000	0.983981000	0.318482000
1	-4.563950000	1.085965000	2.103477000
1	-3.634487000	-2.627716000	2.110638000
1	-4.058773000	-1.381561000	3.306784000
1	-1.432647000	-1.234736000	2.348115000
1	1.053840000	2.168194000	2.524280000
1	0.655116000	1.301635000	-0.561848000

D (nimag=0) E(au)= -3050.3052   G(au)= -3049.7866

6	1.363786000	0.280603000	2.307696000
6	1.704193000	0.111798000	-0.616835000
45	-0.003248000	-0.292954000	0.354951000
6	1.990548000	1.550057000	-0.295737000
6	1.399180000	1.739300000	2.124401000
1	1.859052000	2.159747000	-1.207596000
1	3.025782000	1.695281000	0.069616000
1	0.671527000	2.227361000	2.789467000
1	2.408928000	2.130285000	2.342574000
6	1.374356000	-0.941995000	2.349043000
1	1.488493000	-1.994600000	2.543145000
7	0.982502000	1.972976000	0.716812000
16	0.096972000	3.470107000	0.410316000
16	5.680803000	-0.921356000	0.118086000
6	7.440249000	-0.848193000	-0.237835000
1	7.739210000	-1.813085000	-0.665712000
1	7.935899000	-0.671036000	0.726814000
1	7.615342000	-0.019543000	-0.934774000
6	1.230298000	4.836016000	0.742002000
1	0.652940000	5.746487000	0.524189000
1	2.092366000	4.757629000	0.067135000
1	1.517827000	4.813125000	1.801162000
8	5.214012000	0.420959000	0.570493000
8	5.378009000	-2.122920000	0.932794000
8	-0.976418000	3.464368000	1.420964000
8	-0.169529000	3.414503000	-1.045587000
15	-2.042417000	-0.691501000	1.688371000
15	-1.322039000	-0.239433000	-1.578271000
6	-3.223707000	-1.859004000	0.868677000
6	-4.045365000	-1.467362000	-0.218269000
6	-3.283776000	-3.188908000	1.324173000
6	-4.920567000	-2.413533000	-0.780643000

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6      -4.144770000    -4.119566000     0.737311000
1      -2.666516000    -3.517332000     2.159973000
6      -4.972284000    -3.728527000    -0.315737000
1      -5.563569000    -2.107874000    -1.608539000
1      -4.174978000    -5.142725000     1.116140000
1      -5.658898000    -4.442266000    -0.774563000
6      -2.953827000     0.580989000    -1.339826000
6      -3.081835000     1.914620000    -1.777010000
6      -4.074014000    -0.076728000    -0.767238000
6      -4.303308000     2.584189000    -1.693782000
1      -2.225353000     2.451321000    -2.179987000
6      -5.297158000     0.613551000    -0.716246000
6      -5.419046000     1.926360000    -1.174847000
1      -4.378795000     3.615387000    -2.042674000
1      -6.164671000     0.109032000    -0.286660000
1      -6.383105000     2.435067000    -1.116037000
6      -1.690593000    -1.463434000     3.329428000
1      -1.106655000    -2.388260000     3.231448000
1      -2.635350000    -1.682992000     3.848677000
1      -1.111767000    -0.747331000     3.929398000
6      -2.995087000     0.808262000     2.196581000
1      -2.363059000     1.400394000     2.874744000
1      -3.910162000     0.499013000     2.723642000
1      -3.253395000     1.434459000     1.335520000
6      -1.595391000    -1.911401000    -2.299356000
1      -0.624382000    -2.284881000    -2.657623000
1      -2.287959000    -1.826687000    -3.150307000
1      -2.004349000    -2.608134000    -1.559300000
6      -0.523119000     0.660191000    -2.971498000
1      -1.206822000     0.677416000    -3.833325000
1       0.390826000     0.114891000    -3.248017000
6       2.708340000    -0.623116000    -1.290104000
6       2.793685000    -1.992575000    -1.225918000
6       4.041321000    -0.117281000    -1.860031000
6       4.183873000    -2.435384000    -1.557175000
7       4.996188000    -1.193118000    -1.517817000
1       4.380970000     0.846781000    -1.471214000
1       3.979760000    -0.046840000    -2.959981000
1       4.562277000    -3.199225000    -0.862728000
1       4.216730000    -2.868131000    -2.578117000
1       1.991286000    -2.662068000    -0.910258000
1      -0.268871000     1.687102000    -2.681402000
1      -0.027275000    -1.798697000     0.096799000
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D (nimag=0)   E(au)= -3050.0253   G(au)= -3049.5165

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6      -0.199514000     1.680630000    -1.968226000
6      -1.317972000     1.614427000     0.420746000
45     -0.182435000     0.318374000    -0.350026000
6      -1.470636000     3.079428000     0.104723000
6       0.047364000     3.141837000    -1.905012000
1      -1.637260000     3.634169000     1.040723000
1      -2.389627000     3.211460000    -0.502630000
1       1.117377000     3.347396000    -2.052054000
1      -0.516941000     3.630200000    -2.720161000
6      -0.758272000     0.648622000    -2.427824000
1      -1.284705000     0.080808000    -3.182005000
7      -0.362124000     3.712217000    -0.610557000
16      0.841130000     4.493952000     0.326667000
16     -4.596865000    -1.392889000    -0.293908000
6      -6.360962000    -1.752456000    -0.349749000
1      -6.664435000    -2.134924000     0.632547000
1      -6.493744000    -2.514663000    -1.129534000
1      -6.889289000    -0.825740000    -0.604236000
6       0.759468000     6.203573000    -0.243366000
1       1.527385000     6.750414000     0.320695000
1      -0.243466000     6.590028000    -0.025010000
1       0.980282000     6.226291000    -1.318206000
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8	-4.205023000	-0.747975000	-1.575198000
8	-3.887209000	-2.617471000	0.168702000
8	2.180314000	3.967566000	-0.055688000
8	0.379516000	4.444682000	1.734993000
15	0.502788000	-1.915592000	-1.290797000
15	1.520476000	0.070161000	1.280631000
6	1.365812000	-3.125287000	-0.172315000
6	2.668593000	-2.874149000	0.330816000
6	0.706547000	-4.305081000	0.217266000
6	3.271594000	-3.831304000	1.164099000
6	1.313764000	-5.233350000	1.067656000
1	-0.298427000	-4.519215000	-0.144641000
6	2.606095000	-5.000458000	1.536829000
1	4.278828000	-3.638131000	1.539587000
1	0.775170000	-6.139667000	1.351454000
1	3.096408000	-5.721736000	2.193596000
6	3.078480000	-0.333815000	0.358308000
6	3.882679000	0.751559000	-0.039118000
6	3.461843000	-1.648195000	-0.006124000
6	5.068888000	0.549923000	-0.746770000
1	3.580755000	1.773430000	0.192239000
6	4.671001000	-1.827892000	-0.702346000
6	5.472881000	-0.746459000	-1.069037000
1	5.675523000	1.409303000	-1.038793000
1	4.972778000	-2.842495000	-0.970978000
1	6.404471000	-0.918434000	-1.611856000
6	-1.001917000	-2.824689000	-1.859076000
1	-1.724569000	-2.956748000	-1.041044000
1	-0.732747000	-3.800156000	-2.291321000
1	-1.493770000	-2.216439000	-2.630696000
6	1.548768000	-1.896915000	-2.818775000
1	1.034595000	-1.300068000	-3.586236000
1	1.702384000	-2.921702000	-3.188830000
1	2.520463000	-1.432381000	-2.606570000
6	1.306009000	-1.188350000	2.627041000
1	0.645746000	-0.735095000	3.382883000
1	2.275749000	-1.408478000	3.097636000
1	0.854378000	-2.117842000	2.263403000
6	1.972238000	1.535944000	2.301936000
1	2.822276000	1.278010000	2.952347000
1	1.102291000	1.809401000	2.915643000
6	-2.443602000	0.925038000	1.017458000
6	-2.412417000	-0.035142000	1.974228000
6	-3.900122000	1.080464000	0.549330000
6	-3.781534000	-0.628362000	2.177923000
7	-4.546871000	-0.177788000	0.984065000
1	-4.004594000	1.214961000	-0.533992000
1	-4.394259000	1.924584000	1.062528000
1	-3.769173000	-1.724229000	2.250774000
1	-4.273253000	-0.229944000	3.084808000
1	-1.539220000	-0.314074000	2.560990000
1	2.226744000	2.396661000	1.675709000

TS_DE (nimag=1) (−431.56*i*)   **E(au)=** −3050.2825   **G(au)=** −3049.7630

6	-1.625141000	1.707284000	-1.308591000
6	-1.529607000	1.614624000	0.642897000
45	-0.255662000	0.309416000	-0.251628000
6	-1.632886000	3.112594000	0.860353000
6	-1.546042000	3.214004000	-1.495296000
1	-1.081246000	3.349799000	1.786832000
1	-2.680644000	3.429146000	1.011562000
1	-0.889541000	3.446988000	-2.342940000
1	-2.567888000	3.561299000	-1.727328000
6	-1.670429000	0.584909000	-1.910342000
1	-2.083925000	-0.074901000	-2.662530000
7	-1.075624000	3.841778000	-0.270325000
16	0.641264000	4.207355000	-0.209519000

16	-4.184218000	-1.788656000	-0.253292000
6	-5.746501000	-2.676937000	-0.277527000
1	-5.866612000	-3.187676000	0.686270000
1	-5.668944000	-3.400129000	-1.101083000
1	-6.544952000	-1.946572000	-0.456185000
6	0.667173000	5.956048000	-0.623898000
1	1.725819000	6.250685000	-0.603944000
1	0.088795000	6.490693000	0.139395000
1	0.245425000	6.085188000	-1.628681000
8	-4.070346000	-0.957066000	-1.485333000
8	-3.075818000	-2.727783000	0.078849000
8	1.326517000	3.439643000	-1.283587000
8	1.036080000	4.038704000	1.211833000
15	0.808793000	-1.495340000	-1.523647000
15	1.367060000	-0.057560000	1.465124000
6	1.707760000	-2.797165000	-0.563510000
6	2.947820000	-2.549895000	0.080259000
6	1.138034000	-4.082046000	-0.483315000
6	3.594518000	-3.617872000	0.726216000
6	1.786570000	-5.121398000	0.188017000
1	0.178011000	-4.293771000	-0.952382000
6	3.027252000	-4.892160000	0.783080000
1	4.555614000	-3.433395000	1.210492000
1	1.323900000	-6.108937000	0.230761000
1	3.552408000	-5.699459000	1.296882000
6	3.045862000	-0.062742000	0.706586000
6	3.757095000	1.152162000	0.701651000
6	3.621606000	-1.214590000	0.113848000
6	5.035555000	1.232122000	0.147414000
1	3.320165000	2.052646000	1.133106000
6	4.917397000	-1.111760000	-0.422185000
6	5.621134000	0.093868000	-0.409085000
1	5.572489000	2.182026000	0.160516000
1	5.372361000	-1.998172000	-0.868605000
1	6.624494000	0.141769000	-0.836269000
6	-0.417872000	-2.433624000	-2.534440000
1	-1.271425000	-2.753804000	-1.919827000
1	0.064203000	-3.304415000	-3.001421000
1	-0.776288000	-1.774786000	-3.337656000
6	1.985832000	-0.851820000	-2.788895000
1	1.429716000	-0.197204000	-3.477015000
1	2.421497000	-1.691120000	-3.351376000
1	2.786062000	-0.270173000	-2.314960000
6	1.161118000	-1.582395000	2.493491000
1	0.420558000	-1.366498000	3.277531000
1	2.121748000	-1.807694000	2.979809000
1	0.836273000	-2.449017000	1.907733000
6	1.401042000	1.251613000	2.756292000
1	2.243761000	1.067090000	3.439461000
1	0.459408000	1.189262000	3.322319000
6	-2.531077000	0.723539000	1.216184000
6	-2.358354000	-0.272823000	2.115149000
6	-4.019881000	0.697414000	0.775718000
6	-3.646364000	-1.042784000	2.298944000
7	-4.442422000	-0.671721000	1.103529000
1	-4.181383000	0.918828000	-0.284623000
1	-4.606333000	1.405396000	1.386992000
1	-3.485442000	-2.126689000	2.367787000
1	-4.191607000	-0.717554000	3.203212000
1	-1.452481000	-0.490341000	2.676836000
1	1.478741000	2.250427000	2.310325000
1	0.826686000	1.222244000	-0.795523000

TS_DE (nimag=1) (-423.99*i*)   E(au)= -3050.2995   G(au)= -3049.7779

6	-1.959098000	0.877238000	-1.174482000
6	-1.759732000	0.961161000	0.759271000
45	-0.079776000	0.128331000	-0.229413000

6	-2.010535000	2.468484000	0.858721000
6	-2.179794000	2.337014000	-1.483688000
1	-1.439297000	2.877690000	1.706314000
1	-3.070216000	2.716315000	1.029749000
1	-1.749602000	2.604569000	-2.457028000
1	-3.265258000	2.523676000	-1.529666000
6	-1.699888000	-0.283508000	-1.631346000
1	-1.961109000	-1.174555000	-2.188529000
7	-1.619824000	3.145641000	-0.388296000
16	0.096323000	3.380920000	-0.474879000
16	-5.001129000	-1.389748000	-0.311390000
6	-6.493742000	-2.390127000	-0.284477000
1	-6.355275000	-3.215667000	0.425209000
1	-6.617712000	-2.770612000	-1.307676000
1	-7.324280000	-1.735296000	0.005530000
6	0.288282000	4.719658000	-1.653063000
1	1.371450000	4.887755000	-1.731138000
1	-0.222686000	5.592510000	-1.227184000
1	-0.132776000	4.423370000	-2.621764000
8	-5.225032000	-0.164160000	-1.118381000
8	-3.823545000	-2.257206000	-0.636034000
8	0.727330000	2.135168000	-1.082299000
8	0.545604000	3.800265000	0.868325000
15	1.530025000	-1.024867000	-1.636515000
15	1.458609000	0.004294000	1.567097000
6	2.617217000	-2.255986000	-0.788096000
6	3.678478000	-1.869374000	0.070891000
6	2.370272000	-3.625933000	-0.995580000
6	4.473205000	-2.873025000	0.652800000
6	3.158694000	-4.606444000	-0.388515000
1	1.560635000	-3.950935000	-1.648322000
6	4.220862000	-4.228017000	0.432773000
1	5.296860000	-2.577232000	1.305666000
1	2.946607000	-5.661339000	-0.571297000
1	4.852745000	-4.983179000	0.903833000
6	3.160628000	0.462480000	1.032370000
6	3.592502000	1.780508000	1.277691000
6	4.031986000	-0.448123000	0.380498000
6	4.876640000	2.194884000	0.921399000
1	2.929047000	2.500381000	1.755459000
6	5.325433000	-0.010152000	0.045583000
6	5.749514000	1.293137000	0.310460000
1	5.194121000	3.217493000	1.132898000
1	6.005462000	-0.709619000	-0.444498000
1	6.760095000	1.601744000	0.036295000
6	0.733496000	-1.965145000	-3.010157000
1	0.007004000	-2.697042000	-2.631733000
1	1.494348000	-2.483440000	-3.612120000
1	0.209326000	-1.243863000	-3.654579000
6	2.632105000	0.129866000	-2.562992000
1	2.006531000	0.719725000	-3.248598000
1	3.366876000	-0.450283000	-3.140984000
1	3.149510000	0.813617000	-1.880658000
6	1.519048000	-1.617996000	2.439428000
1	0.579789000	-1.729745000	3.001870000
1	2.359338000	-1.614259000	3.149686000
1	1.630065000	-2.455553000	1.742231000
6	1.037689000	1.157787000	2.939386000
1	1.811783000	1.104210000	3.719647000
1	0.074108000	0.836436000	3.360987000
6	-2.760517000	0.137825000	1.398705000
6	-2.623818000	-1.125422000	1.884431000
6	-4.272926000	0.468330000	1.450049000
6	-3.973089000	-1.728245000	2.162934000
7	-4.904621000	-0.866968000	1.387537000
1	-4.635952000	1.095977000	0.629288000
1	-4.560101000	0.935658000	2.407402000
1	-4.027986000	-2.786344000	1.871251000

1	-4.246384000	-1.662223000	3.232598000
1	-1.685781000	-1.658713000	2.030119000
1	0.945743000	2.188218000	2.574656000
1	-0.540940000	-1.232967000	0.302697000

TS_DE (nimag=1) (-272.85*i*)   E(au)= -3050.0091   G(au)= -3049.5005

6	-1.667225000	0.679244000	-1.408126000
6	-1.611706000	0.461122000	0.782853000
45	0.106231000	0.066236000	-0.183407000
6	-2.009260000	1.924416000	1.032250000
6	-2.379000000	1.984687000	-1.357222000
1	-1.340362000	2.347921000	1.795268000
1	-3.042115000	2.014832000	1.403456000
1	-2.187487000	2.558827000	-2.272960000
1	-3.465439000	1.821605000	-1.262824000
6	-1.060689000	-0.332798000	-1.873406000
1	-0.902703000	-1.005371000	-2.707301000
7	-1.926257000	2.756536000	-0.183139000
16	-0.414363000	3.602163000	-0.401678000
16	-5.695317000	-1.427840000	-0.258465000
6	-7.385607000	-1.582103000	0.343444000
1	-7.478010000	-2.550115000	0.850752000
1	-8.032726000	-1.535384000	-0.543081000
1	-7.588390000	-0.746591000	1.024597000
6	-0.931726000	5.316398000	-0.189898000
1	-0.025197000	5.925700000	-0.306321000
1	-1.355620000	5.426821000	0.815668000
1	-1.668407000	5.550108000	-0.968052000
8	-5.534358000	-0.066446000	-0.839840000
8	-5.366029000	-2.634960000	-1.054406000
8	0.025029000	3.427023000	-1.811802000
8	0.492538000	3.256186000	0.726688000
15	2.041976000	0.105093000	-1.603323000
15	1.425160000	-0.841882000	1.527764000
6	3.208333000	-1.334399000	-1.468433000
6	4.050777000	-1.533355000	-0.344470000
6	3.195757000	-2.310490000	-2.481848000
6	4.857568000	-2.685013000	-0.296937000
6	3.991725000	-3.455607000	-2.408507000
1	2.559376000	-2.181702000	-3.357325000
6	4.830338000	-3.643840000	-1.310094000
1	5.511425000	-2.829386000	0.565763000
1	3.958628000	-4.191198000	-3.214597000
1	5.463397000	-4.530490000	-1.239830000
6	3.157813000	-0.195005000	1.679934000
6	3.431386000	0.740015000	2.695313000
6	4.196219000	-0.554238000	0.782517000
6	4.699459000	1.302668000	2.849875000
1	2.647281000	1.045052000	3.387083000
6	5.470943000	0.010732000	0.968402000
6	5.728350000	0.930274000	1.985514000
1	4.877417000	2.025477000	3.648306000
1	6.270818000	-0.271403000	0.280863000
1	6.727589000	1.356027000	2.095660000
6	1.698995000	0.245531000	-3.415362000
1	1.128103000	-0.610202000	-3.799792000
1	2.636433000	0.339334000	-3.983482000
1	1.094880000	1.154764000	-3.551321000
6	3.051401000	1.637411000	-1.358006000
1	2.432400000	2.477417000	-1.705298000
1	3.977466000	1.580574000	-1.949603000
1	3.291872000	1.794482000	-0.300522000
6	1.565624000	-2.686081000	1.467607000
1	0.567044000	-3.107456000	1.657416000
1	2.258573000	-3.037414000	2.247226000
1	1.914068000	-3.024119000	0.484677000
6	0.706322000	-0.590379000	3.213497000

1	1.356200000	-1.014906000	3.993358000
1	-0.269491000	-1.096160000	3.231661000
6	-2.623196000	-0.516338000	1.131677000
6	-2.469738000	-1.865360000	1.047517000
6	-4.072807000	-0.242288000	1.553129000
6	-3.766845000	-2.580647000	1.271075000
7	-4.790663000	-1.503985000	1.255123000
1	-4.547161000	0.588957000	1.020145000
1	-4.142498000	-0.042705000	2.637548000
1	-3.977613000	-3.333482000	0.496340000
1	-3.785262000	-3.097104000	2.250525000
1	-1.536059000	-2.368153000	0.795197000
1	0.540739000	0.477872000	3.407011000

E (nimag=0) E(au)= -3050.3698   **G(au)=** -3049.8453

6	-2.683203000	-0.169119000	1.688750000
6	-3.462145000	0.517511000	0.763702000
45	-0.031936000	0.226798000	0.513328000
6	-4.703978000	-0.304147000	0.479426000
6	-3.492065000	-1.415131000	2.126291000
1	-4.982741000	-0.303821000	-0.581734000
1	-5.562741000	0.081849000	1.058680000
1	-2.872091000	-2.290493000	2.342013000
1	-4.122431000	-1.190886000	3.004260000
6	-1.310828000	-0.014140000	2.002234000
1	-1.043612000	-0.522383000	2.944107000
7	-4.371253000	-1.658366000	0.969163000
16	-3.559291000	-2.636820000	-0.278117000
16	-0.377282000	3.393580000	-0.834440000
6	0.471766000	4.968421000	-0.698972000
1	-0.030822000	5.663225000	-1.384570000
1	1.511879000	4.792222000	-1.004415000
1	0.399657000	5.307804000	0.341457000
6	-4.798732000	-3.901036000	-0.591077000
1	-4.377593000	-4.551158000	-1.370257000
1	-5.714398000	-3.407724000	-0.940200000
1	-4.962486000	-4.450706000	0.343866000
8	0.252361000	2.483063000	0.215297000
8	-0.374012000	2.923316000	-2.240222000
8	-2.361198000	-3.257077000	0.344551000
8	-3.393734000	-1.792426000	-1.496363000
15	1.798393000	-0.039304000	1.817924000
15	1.108178000	-0.453114000	-1.533544000
6	3.361797000	0.325182000	0.930634000
6	3.950717000	-0.571558000	-0.002744000
6	4.013578000	1.537269000	1.237412000
6	5.204924000	-0.232714000	-0.539952000
6	5.247975000	1.856418000	0.672349000
1	3.570304000	2.240568000	1.941098000
6	5.852353000	0.959646000	-0.210452000
1	5.670171000	-0.919927000	-1.248996000
1	5.739079000	2.794961000	0.934826000
1	6.824994000	1.188533000	-0.650178000
6	2.129444000	-1.950327000	-1.182542000
6	1.665686000	-3.209106000	-1.600318000
6	3.344097000	-1.865816000	-0.454576000
6	2.387024000	-4.373403000	-1.323119000
1	0.730674000	-3.295713000	-2.153877000
6	4.064393000	-3.047249000	-0.203850000
6	3.593163000	-4.291971000	-0.626805000
1	2.007243000	-5.338918000	-1.661791000
1	5.007652000	-2.984838000	0.342949000
1	4.170893000	-5.193132000	-0.413473000
6	1.700108000	1.120427000	3.239277000
1	1.525726000	2.145295000	2.886509000
1	2.627939000	1.073565000	3.828949000
1	0.855876000	0.815438000	3.872672000

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6      1.924629000    -1.703800000     2.578674000
1      1.035767000    -1.879839000     3.201553000
1      2.826622000    -1.733186000     3.209363000
1      1.987583000    -2.478657000     1.805413000
6      2.162537000     0.726175000    -2.484750000
1      1.516014000     1.544882000    -2.830040000
1      2.599859000     0.203593000    -3.349185000
1      2.966368000     1.133712000    -1.859565000
6     -0.167773000    -0.942169000    -2.769064000
1      0.302657000    -1.437244000    -3.632295000
1     -0.647130000    -0.013200000    -3.113240000
6     -3.209948000     1.809482000     0.174193000
6     -3.605300000     2.218758000    -1.055623000
6     -2.432619000     2.948455000     0.833464000
6     -3.017871000     3.566976000    -1.374569000
7     -1.985897000     3.782203000    -0.312297000
1     -1.595782000     2.651491000     1.469063000
1     -3.121675000     3.561252000     1.440191000
1     -2.582619000     3.628236000    -2.380882000
1     -3.773139000     4.369582000    -1.284291000
1     -4.219679000     1.659887000    -1.762116000
1     -0.940484000    -1.589604000    -2.331487000
1     -0.129466000    -1.302500000     0.588969000
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E (nimag=0)   E(au)= -3050.3556   G(au)= -3049.8328

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6      2.309374000     1.422930000     1.742020000
6      3.148245000     1.163864000     0.655157000
45     0.130280000     0.180468000     0.690648000
6      3.572149000     2.502281000     0.064345000
6      2.349490000     2.966530000     1.981809000
1      3.566917000     2.520473000    -1.032615000
1      4.573663000     2.812459000     0.409069000
1      1.436768000     3.377751000     2.425603000
1      3.208891000     3.250388000     2.611282000
6      1.201092000     0.733364000     2.253290000
1      0.921363000     0.947308000     3.297227000
7      2.588103000     3.466766000     0.620111000
16     1.103037000     3.512671000    -0.335284000
16     2.475641000    -3.281282000    -0.687058000
6      3.120428000    -4.938703000    -0.948972000
1      3.940254000    -4.884402000    -1.676863000
1      2.285164000    -5.529524000    -1.349022000
1      3.460137000    -5.322196000     0.020488000
6      0.576594000     5.212689000    -0.104776000
1     -0.363174000     5.314618000    -0.664367000
1      1.366843000     5.850014000    -0.521178000
1      0.422424000     5.398228000     0.965582000
8      1.482992000    -3.311866000     0.423872000
8      2.063379000    -2.703692000    -2.001097000
8      0.037339000     2.623900000     0.280335000
8      1.483666000     3.265377000    -1.743055000
15    -1.734937000    -0.305282000     1.872216000
15    -0.909585000    -0.292460000    -1.464829000
6     -2.937971000    -1.422427000     1.055993000
6     -3.733401000    -1.028621000    -0.054190000
6     -3.089482000    -2.715566000     1.596258000
6     -4.697766000    -1.935863000    -0.527944000
6     -4.037448000    -3.603738000     1.088741000
1     -2.473733000    -3.044967000     2.432072000
6     -4.855895000    -3.205058000     0.030942000
1     -5.319954000    -1.640019000    -1.374569000
1     -4.139277000    -4.597225000     1.528440000
1     -5.611002000    -3.884129000    -0.369532000
6     -2.477786000     0.682551000    -1.504852000
6     -2.508802000     1.888489000    -2.227733000
6     -3.629027000     0.279039000    -0.779067000
6     -3.655193000     2.685514000    -2.254833000
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1	-1.633762000	2.210178000	-2.792956000
6	-4.775730000	1.092238000	-0.829094000
6	-4.793002000	2.286788000	-1.551468000
1	-3.661222000	3.608504000	-2.837800000
1	-5.669588000	0.777327000	-0.286543000
1	-5.697774000	2.897141000	-1.570831000
6	-1.367986000	-1.040686000	3.514952000
1	-0.770648000	-1.956261000	3.412899000
1	-2.309040000	-1.260889000	4.040214000
1	-0.798892000	-0.309564000	4.105023000
6	-2.590518000	1.275119000	2.267790000
1	-1.918393000	1.897990000	2.875471000
1	-3.500114000	1.043529000	2.844049000
1	-2.860932000	1.814563000	1.352285000
6	-1.267766000	-2.035066000	-1.944651000
1	-0.295252000	-2.507125000	-2.146472000
1	-1.885457000	-2.042353000	-2.855081000
1	-1.776854000	-2.582796000	-1.144036000
6	0.122389000	0.288794000	-2.875302000
1	-0.451432000	0.233964000	-3.813113000
1	0.977185000	-0.402065000	-2.938720000
6	3.644221000	-0.102269000	0.195800000
6	4.343488000	-0.303535000	-0.953609000
6	3.546776000	-1.430014000	0.944487000
6	4.669904000	-1.756043000	-1.130686000
7	3.886831000	-2.450763000	-0.074762000
1	2.575558000	-1.654575000	1.395158000
1	4.306343000	-1.458350000	1.746043000
1	4.414384000	-2.121278000	-2.137037000
1	5.751275000	-1.936987000	-0.977639000
1	4.642359000	0.457295000	-1.676202000
1	0.491193000	1.310597000	-2.717255000
1	0.360365000	-1.322131000	0.864101000

E' (nimag=0) E(au)= -3050.3849   G(au)= -3049.8574

6	-2.401248000	-0.478580000	1.436039000
6	-2.895435000	0.730120000	0.990639000
45	0.052799000	0.570538000	0.378359000
6	-4.397271000	0.748657000	1.177210000
6	-3.573494000	-1.342487000	1.888766000
1	-4.939301000	1.277519000	0.384999000
1	-4.670900000	1.190439000	2.152756000
1	-3.481299000	-2.396436000	1.607059000
1	-3.736467000	-1.274605000	2.977548000
6	-1.026815000	-0.734584000	1.273703000
1	-0.638995000	-1.700634000	1.628575000
7	-4.727763000	-0.701198000	1.204708000
16	-4.908624000	-1.337808000	-0.465454000
16	0.596960000	3.630849000	-0.298459000
6	1.305333000	4.775684000	-1.483363000
1	1.137381000	4.401119000	-2.500560000
1	2.377782000	4.823384000	-1.250090000
1	0.815691000	5.743322000	-1.314833000
6	-6.591105000	-1.965990000	-0.426301000
1	-6.781961000	-2.377635000	-1.427187000
1	-7.262705000	-1.127315000	-0.205122000
1	-6.643479000	-2.746527000	0.342742000
8	0.679130000	4.170486000	1.071548000
8	1.239803000	2.263394000	-0.567513000
8	-3.954069000	-2.468006000	-0.623248000
8	-4.821009000	-0.176555000	-1.392363000
15	2.021205000	0.068465000	1.601722000
15	0.723897000	-1.057225000	-1.404211000
6	3.491051000	-0.141556000	0.514395000
6	3.749121000	-1.335446000	-0.207900000
6	4.393550000	0.934835000	0.416657000
6	4.931021000	-1.415639000	-0.964254000

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6        5.551614000      0.837278000     -0.356467000
1        4.208515000      1.861621000      0.958771000
6        5.825571000     -0.346512000     -1.042978000
1        5.141750000     -2.337083000     -1.510678000
1        6.241772000      1.681163000     -0.408517000
1        6.733855000     -0.440861000     -1.641102000
6        1.531684000     -2.555220000     -0.676724000
6        0.784706000     -3.746236000     -0.596828000
6        2.860156000     -2.540690000     -0.180158000
6        1.334129000     -4.912533000     -0.058028000
1       -0.237673000     -3.785573000     -0.973171000
6        3.401530000     -3.732896000      0.332940000
6        2.652200000     -4.908809000      0.399379000
1        0.734341000     -5.823424000     -0.014760000
1        4.430486000     -3.727284000      0.698465000
1        3.099638000     -5.817389000      0.806490000
6        2.415062000      1.452993000      2.746751000
1        2.381860000      2.419258000      2.227903000
1        3.401432000      1.295509000      3.207435000
1        1.642916000      1.459520000      3.529595000
6        1.921521000     -1.378260000      2.736845000
1        1.177093000     -1.153794000      3.515536000
1        2.904312000     -1.521820000      3.210840000
1        1.642092000     -2.296493000      2.207126000
6        1.855285000     -0.381798000     -2.697941000
1        1.278321000      0.321383000     -3.317309000
1        2.228275000     -1.197909000     -3.334418000
1        2.698361000      0.153133000     -2.245567000
6       -0.667219000     -1.732386000     -2.418228000
1       -0.309152000     -2.564943000     -3.041797000
1       -1.023110000     -0.934947000     -3.087118000
6       -2.025825000      1.639921000      0.253317000
6       -1.640199000      1.265905000     -1.043053000
6       -1.958821000      3.169255000      0.352049000
6       -1.297688000      2.522615000     -1.820381000
7       -1.066528000      3.551045000     -0.771813000
1       -1.592048000      3.569025000      1.303563000
1       -2.955820000      3.598621000      0.149732000
1       -0.440067000      2.422193000     -2.497625000
1       -2.167705000      2.836599000     -2.423247000
1       -2.033469000      0.379334000     -1.536955000
1       -1.511953000     -2.071243000     -1.799639000
1       -0.176892000      1.501948000      1.640172000
```

E (nimag=0)   E(au)= -3050.0091   G(au)= -3049.5005

```
6       -1.176838000      2.137499000     -1.568807000
6       -1.761161000      1.915151000     -0.262739000
45       0.162848000      0.748818000     -0.561250000
6       -1.558697000      3.219687000      0.516409000
6       -0.757668000      3.605573000     -1.673120000
1       -1.253494000      3.078258000      1.561502000
1       -2.479172000      3.828539000      0.513547000
1        0.133994000      3.801108000     -2.278007000
1       -1.585643000      4.238220000     -2.032928000
6       -0.648075000      1.016230000     -2.232162000
1       -0.469094000      0.810368000     -3.290295000
7       -0.528457000      3.979623000     -0.245183000
16       1.085780000      3.616854000      0.296465000
16      -4.424668000     -2.141064000      0.102364000
6       -6.066435000     -2.841233000     -0.136435000
1       -6.765814000     -2.330834000      0.537952000
1       -5.984859000     -3.905560000      0.122212000
1       -6.342501000     -2.701760000     -1.188193000
6        1.340876000      4.878588000      1.549969000
1        2.341058000      4.695610000      1.964855000
1        0.569748000      4.775973000      2.323324000
```

```
1        1.283900000       5.850246000       1.044855000
8       -3.515547000      -2.691284000      -0.938905000
8       -4.057805000      -2.296972000       1.539392000
8        2.015126000       3.839511000      -0.836274000
8        1.139378000       2.282838000       1.026276000
15       2.244169000      -0.019696000      -1.436149000
15       0.121095000      -1.000765000       1.056166000
6        2.584933000      -1.838517000      -1.344813000
6        2.829030000      -2.501622000      -0.114593000
6        2.561671000      -2.595105000      -2.530478000
6        3.076820000      -3.885973000      -0.132411000
6        2.786165000      -3.973286000      -2.523064000
1        2.370982000      -2.110260000      -3.487545000
6        3.052557000      -4.621862000      -1.317534000
1        3.273096000      -4.393310000       0.814330000
1        2.759892000      -4.531580000      -3.460785000
1        3.237775000      -5.697498000      -1.295439000
6        1.792391000      -1.169871000       1.844602000
6        1.985461000      -0.576110000       3.106099000
6        2.889359000      -1.817731000       1.219116000
6        3.216481000      -0.630585000       3.760847000
1        1.158799000      -0.063925000       3.597750000
6        4.116005000      -1.878853000       1.906222000
6        4.287498000      -1.293258000       3.160544000
1        3.331091000      -0.164005000       4.741219000
1        4.955444000      -2.388857000       1.429167000
1        5.254936000      -1.354045000       3.662884000
6        2.523038000       0.415865000      -3.210046000
1        1.740854000      -0.005003000      -3.856459000
1        3.508116000       0.068140000      -3.555472000
1        2.480834000       1.512899000      -3.279606000
6        3.701905000       0.802570000      -0.647590000
1        3.634385000       1.877308000      -0.870159000
1        4.634109000       0.387436000      -1.059429000
1        3.683603000       0.665654000       0.440010000
6       -0.358471000      -2.657715000       0.407001000
1       -1.415372000      -2.620237000       0.106229000
1       -0.229766000      -3.409707000       1.200501000
1        0.245091000      -2.934817000      -0.463821000
6       -1.039630000      -0.799247000       2.475256000
1       -0.812106000      -1.539727000       3.256754000
1       -2.059422000      -0.982060000       2.107566000
6       -2.974931000       1.133747000      -0.019645000
6       -3.806191000       1.253703000       1.034845000
6       -3.572369000       0.160433000      -1.020796000
6       -5.018782000       0.375076000       0.885172000
7       -4.703082000      -0.477830000      -0.295798000
1       -2.874934000      -0.599586000      -1.395195000
1       -3.966881000       0.703275000      -1.899228000
1       -5.213800000      -0.242510000       1.775037000
1       -5.931690000       0.963246000       0.675680000
1       -3.674801000       1.917682000       1.890174000
1       -0.981364000       0.214549000       2.893595000
```

TS_EF (nimag=1) (−866.95*i*)   E(au)= −3050.3449   **G(au)=** −3049.8240

```
6       -2.142523000       1.702426000      -1.357084000
6       -3.270338000       1.699722000      -0.512757000
45       0.583409000       0.751462000      -0.693302000
6       -3.342553000       3.088188000       0.110391000
6       -1.742163000       3.146161000      -1.606312000
1       -3.446962000       3.060432000       1.203591000
1       -4.225526000       3.628298000      -0.278404000
1       -0.686768000       3.320468000      -1.848530000
1       -2.343908000       3.575480000      -2.423982000
6       -1.289665000       0.597103000      -1.300811000
1       -1.738380000      -0.404692000      -1.238288000
7       -2.134406000       3.831177000      -0.341407000
```

16	-0.724944000	3.782054000	0.679878000
16	-3.896573000	-2.854707000	0.221677000
6	-4.751066000	-4.314069000	-0.386514000
1	-5.696781000	-4.401457000	0.163074000
1	-4.092679000	-5.167776000	-0.174803000
1	-4.917405000	-4.192854000	-1.463886000
6	-1.297775000	4.409673000	2.264756000
1	-0.377899000	4.594049000	2.836741000
1	-1.925681000	3.666722000	2.770446000
1	-1.823684000	5.353370000	2.067945000
8	-2.673825000	-2.641252000	-0.619592000
8	-3.762816000	-2.931329000	1.693779000
8	0.254920000	4.702459000	0.077703000
8	-0.260061000	2.341009000	0.874825000
15	1.352919000	-1.264923000	-1.426639000
15	2.685083000	1.091686000	0.557596000
6	1.707463000	-2.210838000	0.109432000
6	2.943281000	-2.142045000	0.803466000
6	0.647189000	-2.970329000	0.644856000
6	3.080380000	-2.885530000	1.988814000
6	0.806209000	-3.684170000	1.833391000
1	-0.320341000	-3.010562000	0.143497000
6	2.030130000	-3.649619000	2.502750000
1	4.033530000	-2.851525000	2.520207000
1	-0.028159000	-4.265804000	2.229081000
1	2.170785000	-4.212124000	3.427705000
6	4.162182000	0.043365000	0.188560000
6	5.346547000	0.665068000	-0.247167000
6	4.135851000	-1.368712000	0.329751000
6	6.493730000	-0.079665000	-0.534474000
1	5.395361000	1.746994000	-0.361890000
6	5.304665000	-2.095799000	0.048686000
6	6.473807000	-1.465463000	-0.383236000
1	7.399119000	0.429784000	-0.868917000
1	5.287424000	-3.181819000	0.160451000
1	7.363928000	-2.058928000	-0.599938000
6	0.128122000	-2.250675000	-2.382991000
1	-0.815911000	-2.397962000	-1.843969000
1	0.571534000	-3.233171000	-2.606798000
1	-0.065462000	-1.724373000	-3.330034000
6	2.781492000	-1.245811000	-2.586935000
1	2.399052000	-0.898060000	-3.558510000
1	3.171414000	-2.269350000	-2.694917000
1	3.583249000	-0.579372000	-2.254473000
6	2.416009000	0.954758000	2.379260000
1	1.587341000	1.619964000	2.658986000
1	3.334302000	1.249357000	2.909326000
1	2.156421000	-0.078842000	2.645903000
6	3.222369000	2.834204000	0.300642000
1	4.067041000	3.084158000	0.959988000
1	2.375296000	3.497617000	0.519996000
6	-4.150111000	0.620849000	-0.185783000
6	-4.847277000	0.472123000	0.973743000
6	-4.485510000	-0.560727000	-1.097406000
6	-5.559942000	-0.846124000	0.997846000
7	-5.040422000	-1.579186000	-0.184118000
1	-3.653287000	-0.970920000	-1.675291000
1	-5.270934000	-0.251619000	-1.809603000
1	-5.377821000	-1.406883000	1.927833000
1	-6.654465000	-0.703486000	0.905568000
1	-4.883963000	1.173010000	1.809410000
1	3.511051000	2.990346000	-0.748241000
1	0.015029000	0.901339000	-2.174212000

TS_EF (nimag=1) (−762.87*i*)   E(au)= −3050.3727   G(au)= −3049.8476

| 6 | -2.545560000 | -0.036118000 | 1.540493000 |
| 6 | -3.028070000 | 1.007225000 | 0.809788000 |

45	0.053991000	0.557690000	0.416600000
6	−4.545064000	0.934985000	0.786388000
6	−3.720246000	−0.890299000	2.017151000
1	−4.987485000	1.246472000	−0.166692000
1	−4.992272000	1.535568000	1.598526000
1	−3.528449000	−1.967706000	1.976883000
1	−4.038646000	−0.619163000	3.038195000
6	−1.137884000	−0.243488000	1.669360000
1	−0.820769000	−0.904047000	2.487996000
7	−4.798563000	−0.501304000	1.073083000
16	−4.695885000	−1.464574000	−0.436085000
16	0.779791000	3.596006000	−0.277903000
6	1.624145000	4.742717000	−1.369310000
1	1.473679000	4.432158000	−2.410607000
1	2.685884000	4.696841000	−1.091543000
1	1.200455000	5.735451000	−1.171482000
6	−6.346353000	−2.170381000	−0.514379000
1	−6.371796000	−2.778758000	−1.429029000
1	−7.066800000	−1.344627000	−0.564895000
1	−6.493980000	−2.786883000	0.380855000
8	0.837848000	4.060864000	1.122281000
8	1.336756000	2.202754000	−0.587752000
8	−3.694763000	−2.545939000	−0.222333000
8	−4.500202000	−0.518653000	−1.570510000
15	1.976180000	−0.054702000	1.597534000
15	0.657006000	−0.992064000	−1.377459000
6	3.440105000	−0.295936000	0.510642000
6	3.657724000	−1.490882000	−0.222787000
6	4.386466000	0.743851000	0.438216000
6	4.844732000	−1.613521000	−0.964302000
6	5.550269000	0.605123000	−0.319956000
1	4.232218000	1.671162000	0.988764000
6	5.784176000	−0.581827000	−1.016459000
1	5.022563000	−2.535274000	−1.521706000
1	6.276390000	1.419233000	−0.352894000
1	6.696215000	−0.706844000	−1.603154000
6	1.364304000	−2.548492000	−0.670572000
6	0.528176000	−3.677454000	−0.577112000
6	2.704275000	−2.642328000	−0.217537000
6	1.008379000	−4.892019000	−0.081361000
1	−0.512240000	−3.628445000	−0.898575000
6	3.174164000	−3.881780000	0.251347000
6	2.340829000	−4.999514000	0.319910000
1	0.341250000	−5.754060000	−0.025755000
1	4.211034000	−3.959164000	0.584783000
1	2.731909000	−5.948462000	0.691440000
6	2.410180000	1.301203000	2.762543000
1	2.426431000	2.273353000	2.253873000
1	3.382936000	1.094347000	3.233070000
1	1.631689000	1.334796000	3.538356000
6	1.826124000	−1.518616000	2.705545000
1	1.179136000	−1.250228000	3.553928000
1	2.825362000	−1.767381000	3.093563000
1	1.412067000	−2.387852000	2.181136000
1	1.281619000	0.367490000	−3.278483000
1	2.146810000	−1.201957000	−3.306709000
1	2.694408000	0.117154000	−2.213841000
6	−0.771235000	−1.575608000	−2.394294000
1	−0.446831000	−2.424574000	−3.014682000
1	−1.080590000	−0.761674000	−3.064981000
6	−2.129122000	1.873650000	0.036879000
6	−1.705745000	1.507400000	−1.213862000
6	−1.838503000	3.362894000	0.248944000
6	−1.132021000	2.714498000	−1.923535000
7	−0.859216000	3.679417000	−0.823547000
1	−1.448947000	3.638063000	1.235815000
1	−2.754721000	3.951133000	0.063356000
1	−0.237472000	2.516781000	−2.527329000

```
1      -1.894793000      3.154680000      -2.590232000
1      -2.063057000      0.613976000      -1.722766000
1      -1.629303000      -1.876681000     -1.776553000
1      -0.385638000      1.270806000      1.848326000
```

F (nimag=0)   E(au)= -3050.4274   G(au)= -3049.8951

```
45     -0.161292000      0.440519000      -0.681607000
15      0.498951000      -0.942090000      1.156870000
15      2.092168000      0.662909000      -1.334952000
6       2.135074000      -0.479172000      1.875301000
6       3.361968000      -0.827878000      1.254845000
6       2.160151000      0.198240000      3.108977000
6       4.563752000      -0.525339000      1.917911000
6       3.366792000      0.505096000      3.741881000
1       1.232492000      0.481096000      3.603305000
6       4.573668000      0.132733000      3.149242000
1       5.508799000      -0.800219000      1.445368000
1       3.357199000      1.020830000      4.703767000
1       5.523112000      0.354700000      3.639989000
6       2.979026000      -0.952742000      -1.278730000
6       3.161679000      -1.654315000      -2.486244000
6       3.462052000      -1.514301000      -0.069710000
6       3.817093000      -2.886728000      -2.513845000
1       2.807237000      -1.239549000      -3.429679000
6       4.131847000      -2.749534000      -0.124542000
6       4.306914000      -3.435253000      -1.327469000
1       3.953171000      -3.406776000      -3.463659000
1       4.514714000      -3.179794000      0.802940000
1       4.828854000      -4.393877000      -1.336568000
6       -0.721189000      -0.658433000     2.501058000
1       -0.786009000      0.409744000      2.745008000
1       -0.427147000      -1.234426000     3.391875000
1       -1.712018000      -0.995748000     2.172576000
6       0.517882000      -2.767464000      0.919967000
1       -0.523386000      -3.122453000     0.912204000
1       1.037971000      -3.223389000      1.776021000
1       1.037190000      -3.049494000      -0.004913000
6       3.068496000      1.921677000      -0.408199000
1       2.708358000      2.914685000      -0.713311000
1       4.128051000      1.819839000      -0.686817000
1       2.951965000      1.813107000      0.674474000
6       2.292013000      1.263266000      -3.068653000
1       1.729877000      0.658187000      -3.791437000
1       3.358429000      1.246622000      -3.339743000
1       1.931708000      2.300426000      -3.118495000
6       -2.090839000      1.469793000      -1.557829000
6       -2.528594000      0.113561000      -1.446330000
6       -1.738125000      -1.014792000     -1.739841000
6       -0.391765000      -0.961014000     -2.245753000
6       -2.527745000      -2.256534000     -1.411191000
6       -3.873210000      -0.336416000     -0.906483000
1       -1.981120000      -3.013706000     -0.834774000
1       -2.803713000      -2.722878000     -2.377843000
1       -4.166851000      0.158015000      0.030652000
1       -4.654545000      -0.132633000     -1.661868000
6       -2.772434000      2.593839000      -0.789529000
6       -0.803650000      3.442591000      -1.763578000
6       -0.934965000      1.980423000      -2.185910000
1       0.224797000      3.757866000      -1.541884000
1       -1.197391000      4.125779000      -2.535602000
1       -3.249458000      2.311628000      0.156176000
1       -3.534672000      3.067718000      -1.433008000
1       -0.571079000      1.647793000      -3.156334000
7       -3.730902000      -1.792454000     -0.702412000
7       -1.686374000      3.578089000      -0.567293000
16      -0.910086000      3.230433000      0.942133000
16      -3.899311000      -2.350764000     0.945934000
```

8	-4.040079000	-1.152212000	1.812699000
8	-2.791752000	-3.314409000	1.184317000
8	0.176922000	2.165646000	0.730635000
8	-1.950650000	2.919090000	1.937454000
6	-0.070680000	4.764007000	1.344105000
1	0.459632000	4.574198000	2.287268000
1	-0.855726000	5.520340000	1.472840000
1	0.627299000	5.029757000	0.540969000
6	-5.456454000	-3.245120000	0.911150000
1	-6.249351000	-2.541832000	0.627566000
1	-5.609324000	-3.621381000	1.932345000
1	-5.359839000	-4.069105000	0.193657000
1	-0.234812000	-0.442233000	-3.196642000
1	0.170140000	-1.898696000	-2.188461000

F (nimag=0)   E(au)= -3050.4077   G(au)= -3049.8783

6	-2.436180000	-0.139343000	1.441215000
6	-2.879827000	0.973538000	0.834459000
45	0.185803000	0.618775000	0.360805000
6	-4.408706000	0.977886000	0.817384000
6	-3.638952000	-0.972927000	1.873487000
1	-4.841452000	1.355648000	-0.116101000
1	-4.825138000	1.555954000	1.660805000
1	-3.507713000	-2.051796000	1.732116000
1	-3.895914000	-0.789846000	2.931872000
6	-1.004026000	-0.500058000	1.629362000
1	-0.848284000	-1.589542000	1.604589000
7	-4.748573000	-0.452022000	1.033553000
16	-4.823049000	-1.319540000	-0.517381000
16	0.908041000	3.670568000	-0.174282000
6	1.694325000	4.944447000	-1.160801000
1	1.467890000	4.770850000	-2.220260000
1	2.771926000	4.858972000	-0.966176000
1	1.295864000	5.904621000	-0.808903000
6	-6.550126000	-1.812935000	-0.565926000
1	-6.685704000	-2.357791000	-1.510199000
1	-7.163502000	-0.903722000	-0.540168000
1	-6.741725000	-2.456789000	0.301078000
8	1.060210000	3.937074000	1.274070000
8	1.434168000	2.316613000	-0.660377000
8	-3.969336000	-2.538551000	-0.400832000
8	-4.549287000	-0.361106000	-1.626268000
15	2.112546000	-0.064637000	1.474349000
15	0.417079000	-1.097111000	-1.130677000
6	3.492458000	-0.410050000	0.313756000
6	3.577376000	-1.632528000	-0.401428000
6	4.476260000	0.576820000	0.125610000
6	4.671715000	-1.828775000	-1.260497000
6	5.549288000	0.362679000	-0.741989000
1	4.421081000	1.520079000	0.667888000
6	5.648100000	-0.845214000	-1.434382000
1	4.749633000	-2.768920000	-1.810054000
1	6.309523000	1.135782000	-0.866084000
1	6.485716000	-1.026162000	-2.110535000
6	1.198020000	-2.622505000	-0.469196000
6	0.352050000	-3.722207000	-0.217025000
6	2.593948000	-2.746653000	-0.238007000
6	0.869030000	-4.942016000	0.221922000
1	-0.723538000	-3.645305000	-0.376264000
6	3.090675000	-3.993872000	0.179324000
6	2.245738000	-5.082002000	0.406505000
1	0.195299000	-5.780875000	0.404285000
1	4.163389000	-4.100559000	0.351097000
1	2.664453000	-6.034830000	0.735800000
6	2.625871000	1.332994000	2.556130000
1	2.729217000	2.271848000	2.001129000
1	3.572884000	1.070149000	3.052631000

1	1.849056000	1.471861000	3.323020000
6	1.980876000	-1.456692000	2.673386000
1	1.358686000	-1.127214000	3.517959000
1	2.991848000	-1.688218000	3.041408000
1	1.541209000	-2.354315000	2.225612000
6	1.416075000	-0.465739000	-2.541555000
1	0.797381000	0.252242000	-3.098810000
1	1.668866000	-1.313466000	-3.197050000
1	2.329878000	0.031252000	-2.199202000
6	-1.140225000	-1.662442000	-1.920356000
1	-0.889527000	-2.524571000	-2.558146000
1	-1.528443000	-0.862484000	-2.563169000
6	-2.010188000	1.910081000	0.101864000
6	-1.669971000	1.737117000	-1.210212000
6	-1.656761000	3.343644000	0.508897000
6	-1.106958000	3.013630000	-1.784767000
7	-0.756019000	3.821916000	-0.581022000
1	-1.189684000	3.468306000	1.494214000
1	-2.569420000	3.965922000	0.498597000
1	-0.250677000	2.888352000	-2.460320000
1	-1.894779000	3.549304000	-2.344244000
1	-2.058409000	0.923268000	-1.819448000
1	-1.922991000	-1.951472000	-1.204781000
1	-0.645503000	-0.144388000	2.617661000

G (nimag=0) E(au)= -3870.2778   G(au)= -3869.6363

45	-1.179303000	-0.861898000	0.461553000
15	-2.100336000	0.543890000	-1.248763000
15	-2.881284000	-0.071620000	1.922526000
6	-2.653095000	2.208272000	-0.659854000
6	-3.862221000	2.428009000	0.050535000
6	-1.813245000	3.303054000	-0.932582000
6	-4.189021000	3.742331000	0.429731000
6	-2.145062000	4.596288000	-0.524232000
1	-0.869544000	3.162307000	-1.453428000
6	-3.343305000	4.818507000	0.153622000
1	-5.122381000	3.913795000	0.969970000
1	-1.452778000	5.411685000	-0.739420000
1	-3.621903000	5.824415000	0.473968000
6	-4.552632000	0.219565000	1.179537000
6	-5.556025000	-0.742075000	1.400989000
6	-4.848243000	1.353098000	0.381538000
6	-6.839587000	-0.589218000	0.873702000
1	-5.347984000	-1.628823000	1.998579000
6	-6.154229000	1.497602000	-0.120317000
6	-7.143087000	0.542647000	0.116950000
1	-7.598177000	-1.350452000	1.064839000
1	-6.385119000	2.374468000	-0.728389000
1	-8.144611000	0.681818000	-0.294555000
6	-1.137930000	0.871311000	-2.787372000
1	-0.242870000	1.475077000	-2.608670000
1	-1.805356000	1.396529000	-3.487687000
1	-0.863373000	-0.103107000	-3.215183000
6	-3.576841000	-0.289253000	-1.993659000
1	-3.193401000	-1.028486000	-2.709181000
1	-4.168654000	0.468442000	-2.527735000
1	-4.199178000	-0.793268000	-1.248462000
6	-2.429133000	1.471150000	2.832568000
1	-1.555526000	1.248475000	3.463432000
1	-3.268780000	1.783810000	3.471162000
1	-2.172761000	2.282309000	2.141616000
6	-3.234391000	-1.213640000	3.334617000
1	-3.454485000	-2.229617000	2.981456000
1	-4.081299000	-0.834180000	3.925365000
1	-2.341247000	-1.249933000	3.973479000
6	1.055715000	-0.444111000	0.059941000
6	0.852244000	-1.826889000	-0.008725000

```
6      0.218427000    -2.621637000    1.020745000
6     -0.310890000    -2.218748000    2.233545000
6      0.020753000    -4.008106000    0.433763000
6      1.123926000    -2.733782000   -1.189450000
1     -0.904799000    -4.503491000    0.750728000
1      0.872088000    -4.639623000    0.739969000
1      1.048006000    -2.262041000   -2.173831000
1      2.134357000    -3.160413000   -1.076611000
6      1.653213000     0.393855000   -1.019334000
6      0.818655000     1.811422000    0.759068000
6      0.501565000     0.375931000    1.107424000
1      0.000042000     2.526370000    0.918133000
1      1.671467000     2.095620000    1.402088000
1      1.350222000     0.112892000   -2.036647000
1      2.742244000     0.228609000   -0.929207000
1      0.656558000     0.128059000    2.153960000
7      0.115726000    -3.832347000   -1.035734000
7      1.185050000     1.749097000   -0.671477000
16     2.107255000     3.051271000   -1.311198000
16    -1.432749000    -3.383191000   -1.676263000
8     -1.223689000    -2.624832000   -2.930601000
8     -2.292231000    -2.740820000   -0.591246000
8      1.391837000     4.268312000   -0.850121000
8      2.227584000     2.725283000   -2.752299000
6      3.748143000     2.974401000   -0.527440000
1      4.476494000     2.951579000   -1.347246000
1      3.808767000     2.063618000    0.098451000
1      3.846598000     3.885456000    0.074857000
6     -2.168325000    -4.981651000   -2.038004000
1     -1.539732000    -5.454538000   -2.802454000
1     -3.177641000    -4.772646000   -2.416745000
1     -2.208824000    -5.577568000   -1.117993000
1      0.127774000    -1.434082000    2.842256000
1     -0.933003000    -2.939397000    2.768659000
16     4.102014000    -1.043186000    1.198669000
8      3.684874000    -1.703157000   -0.158266000
8      3.373149000     0.347675000    1.368651000
6      5.826405000    -0.503670000    0.852215000
6      6.535910000    -1.097037000   -0.190329000
6      6.434192000     0.450865000    1.674945000
1      6.031121000    -1.829259000   -0.822875000
1      5.863259000     0.917276000    2.480789000
6      7.864435000    -0.721559000   -0.417324000
6      7.760760000     0.812793000    1.439705000
1      8.418956000    -1.178828000   -1.241554000
1      8.235221000     1.564063000    2.077701000
6      8.499154000     0.231384000    0.392683000
6      9.939180000     0.622010000    0.162249000
1     10.055773000     1.716965000    0.111845000
1     10.583531000     0.267924000    0.985190000
1     10.329404000     0.195590000   -0.773434000
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TS_GH (nimag=1) (−84.19*i*) E(au)= −3870.2675   **G(au)=** −3869.6260

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45     0.655171000    -0.765426000   -0.158466000
15     2.440613000     0.339573000    0.951621000
15     2.170835000    -1.251116000   -1.937067000
6      3.484036000     1.405841000   -0.143092000
6      4.478407000     0.896200000   -1.017821000
6      3.248053000     2.791974000   -0.111901000
6      5.210951000     1.803749000   -1.804091000
6      3.971165000     3.673008000   -0.918505000
1      2.483616000     3.212906000    0.537067000
6      4.962652000     3.177042000   -1.764704000
1      5.981906000     1.413209000   -2.471581000
1      3.745488000     4.739648000   -0.872606000
1      5.542851000     3.852659000   -2.396386000
6      3.945432000    -1.576496000   -1.511677000
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6        4.402465000     -2.907590000     -1.541673000
6        4.843439000     -0.551893000     -1.119318000
6        5.720948000     -3.234263000     -1.219961000
1        3.728125000     -3.715123000     -1.824401000
6        6.173004000     -0.900971000     -0.821115000
6        6.614760000     -2.223339000     -0.866777000
1        6.045116000     -4.276028000     -1.255223000
1        6.865829000     -0.110399000     -0.526197000
1        7.651453000     -2.460531000     -0.620281000
6        2.081081000      1.371258000      2.437057000
1        1.482975000      2.258972000      2.212648000
1        3.044386000      1.674654000      2.874793000
1        1.546718000      0.729527000      3.152102000
6        3.559103000     -0.908582000      1.741345000
1        3.068116000     -1.220368000      2.672831000
1        4.517428000     -0.422806000      1.976656000
1        3.728217000     -1.786946000      1.111964000
6        2.180132000      0.084176000     -3.217284000
1        1.163784000      0.157982000     -3.633122000
1        2.885482000     -0.170142000     -4.022689000
1        2.456884000      1.050821000     -2.780822000
6        1.717899000     -2.711720000     -2.980654000
1        1.568955000     -3.609785000     -2.366340000
1        2.498581000     -2.902241000     -3.731942000
1        0.776457000     -2.480115000     -3.497411000
6       -1.081884000      0.614847000      0.407014000
6       -1.651611000     -0.638519000      0.749764000
6       -1.456700000     -1.816274000     -0.070335000
6       -1.037559000     -1.922639000     -1.383447000
6       -1.680815000     -3.013353000      0.837827000
6       -1.914925000     -1.097811000      2.178683000
1       -1.072004000     -3.888733000      0.583768000
1       -2.743885000     -3.302150000      0.777204000
1       -1.402165000     -0.503656000      2.942762000
1       -2.993296000     -1.071004000      2.407516000
6       -1.074060000      1.824365000      1.303170000
6       -0.169726000      2.398978000     -0.875344000
6       -0.516577000      0.927498000     -0.872806000
1        0.808096000      2.646640000     -1.309255000
1       -0.950824000      2.917704000     -1.464874000
1       -0.681601000      1.651295000      2.313595000
1       -2.120495000      2.167545000      1.391982000
1       -0.973219000      0.580030000     -1.796568000
7       -1.437528000     -2.516055000      2.212420000
7       -0.207367000      2.756758000      0.555684000
16      -0.229666000      4.400002000      1.002698000
16       0.248287000     -2.639722000      2.604768000
8        0.588396000     -1.587981000      3.591765000
8        1.075304000     -2.720332000      1.333578000
8        0.786993000      5.049157000      0.139487000
8       -0.113739000      4.391622000      2.478531000
6       -1.855622000      5.059936000      0.560209000
1       -1.866115000      6.091538000      0.937506000
1       -2.634591000      4.460219000      1.048193000
1       -1.958671000      5.046039000     -0.531854000
6        0.325697000     -4.254305000      3.391212000
1       -0.292942000     -4.199973000      4.295219000
1        1.382835000     -4.424903000      3.634620000
1       -0.044220000     -5.012999000      2.690578000
1       -1.253748000     -1.169956000     -2.135965000
1       -0.840671000     -2.927251000     -1.761358000
16      -4.042135000      0.291752000      0.219303000
8       -4.407978000      0.559166000      1.682276000
8       -3.462212000      1.479726000     -0.572261000
6       -5.614279000     -0.099899000     -0.625881000
6       -6.662480000     -0.641019000      0.119639000
6       -5.731962000      0.098143000     -2.004040000
1       -6.551707000     -0.760518000      1.198513000
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1	-4.907694000	0.549171000	-2.558617000
6	-7.848892000	-0.985525000	-0.532739000
6	-6.923746000	-0.253670000	-2.638127000
1	-8.678157000	-1.398759000	0.047388000
1	-7.027085000	-0.090848000	-3.714442000
6	-7.999607000	-0.801359000	-1.916692000
6	-9.292955000	-1.149286000	-2.611597000
1	-9.112133000	-1.592012000	-3.603477000
1	-9.891910000	-1.858781000	-2.021975000
1	-9.909110000	-0.246558000	-2.766956000

H (nimag=0) E(au)= -3870.2883   G(au)= -3869.6405

45	0.439228000	-0.642544000	-0.115927000
15	2.342648000	0.180835000	1.041925000
15	1.994123000	-1.939226000	-1.491756000
6	3.715941000	0.763274000	-0.057234000
6	4.630221000	-0.103536000	-0.710717000
6	3.817877000	2.149740000	-0.273386000
6	5.610939000	0.463293000	-1.546270000
6	4.789779000	2.688418000	-1.118779000
1	3.131834000	2.841188000	0.211810000
6	5.692284000	1.840035000	-1.759460000
1	6.317902000	-0.202175000	-2.046137000
1	4.827715000	3.769377000	-1.264262000
1	6.460948000	2.243308000	-2.421867000
6	3.637279000	-2.490324000	-0.817672000
6	3.822802000	-3.859951000	-0.549903000
6	4.686584000	-1.587788000	-0.509859000
6	5.015819000	-4.349022000	-0.014824000
1	3.027099000	-4.573400000	-0.761625000
6	5.888816000	-2.105101000	0.007960000
6	6.060451000	-3.466412000	0.257666000
1	5.125203000	-5.417880000	0.178746000
1	6.697888000	-1.409100000	0.238296000
1	7.003651000	-3.831194000	0.668946000
6	2.162601000	1.493005000	2.327685000
1	1.818334000	2.449784000	1.927387000
1	3.138046000	1.622286000	2.820808000
1	1.426384000	1.128378000	3.057982000
6	3.054710000	-1.144122000	2.128480000
1	2.434941000	-1.177950000	3.032943000
1	4.084423000	-0.867030000	2.397112000
1	3.046586000	-2.132832000	1.661016000
6	2.407762000	-0.942816000	-2.999983000
1	1.470625000	-0.760403000	-3.547780000
1	3.108975000	-1.490904000	-3.647237000
1	2.844803000	0.023276000	-2.721479000
6	1.374595000	-3.486915000	-2.312014000
1	0.975676000	-4.203028000	-1.579863000
1	2.178737000	-3.964874000	-2.890565000
1	0.567347000	-3.207025000	-3.002960000
6	-0.989443000	1.025362000	0.001893000
6	-2.247792000	0.197650000	0.092384000
6	-1.826318000	-1.218484000	-0.276090000
6	-1.238176000	-1.666614000	-1.433225000
6	-2.309950000	-2.135968000	0.826811000
6	-2.829673000	0.047987000	1.531317000
1	-1.680904000	-3.018752000	0.985417000
1	-3.331939000	-2.475824000	0.583242000
1	-2.503099000	0.835082000	2.217317000
1	-3.928236000	0.039168000	1.516522000
6	-0.832970000	2.333434000	0.763277000
6	0.477235000	2.422245000	-1.280463000
6	-0.209582000	1.078831000	-1.201771000
1	1.534552000	2.396164000	-1.575065000
1	-0.063947000	3.026435000	-2.038124000

1	-0.633917000	2.229507000	1.837845000
1	-1.763597000	2.918800000	0.634722000
1	-0.581562000	0.714135000	-2.157421000
7	-2.405122000	-1.285699000	2.030209000
7	0.326866000	2.953453000	0.086626000
16	0.651777000	4.595469000	0.377506000
16	-0.947460000	-1.300798000	2.959817000
8	-0.724632000	0.051008000	3.526049000
8	0.140303000	-1.959623000	2.150996000
8	1.906556000	4.884849000	-0.359059000
8	0.546661000	4.761218000	1.844705000
6	-0.673647000	5.560090000	-0.393051000
1	-0.451812000	6.608385000	-0.151150000
1	-1.636801000	5.261675000	0.040166000
1	-0.645486000	5.404122000	-1.478832000
6	-1.373562000	-2.431311000	4.293106000
1	-2.207617000	-1.984898000	4.847932000
1	-0.477073000	-2.519442000	4.921412000
1	-1.646855000	-3.400624000	3.858265000
1	-1.241752000	-1.081875000	-2.350481000
1	-1.081666000	-2.740541000	-1.534970000
16	-3.564721000	0.964466000	-1.077952000
8	-3.849253000	2.309930000	-0.492408000
8	-3.014456000	0.828282000	-2.460835000
6	-5.070487000	-0.022401000	-0.979594000
6	-6.101098000	0.391562000	-0.127331000
6	-5.215016000	-1.143700000	-1.802705000
1	-5.985168000	1.300485000	0.464786000
1	-4.424615000	-1.415678000	-2.502995000
6	-7.277899000	-0.354555000	-0.081811000
6	-6.400034000	-1.879012000	-1.737263000
1	-8.088451000	-0.033006000	0.576789000
1	-6.522638000	-2.753758000	-2.380369000
6	-7.447017000	-1.500807000	-0.879523000
6	-8.738361000	-2.277203000	-0.837685000
1	-8.637507000	-3.261754000	-1.316031000
1	-9.082438000	-2.427466000	0.197430000
1	-9.536626000	-1.728918000	-1.366654000

2 (nimag=0) E(au)= -2455.6047 **G(au)=** -2455.2568

6	1.282407000	0.123561000	0.219196000
6	-0.215436000	0.300330000	0.133104000
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```

31a

Figure S1: ^{1}H NMR spectrum (300 MHz) of **31a** in CDCl$_3$.

Figure S2: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **31a** in CDCl$_3$.
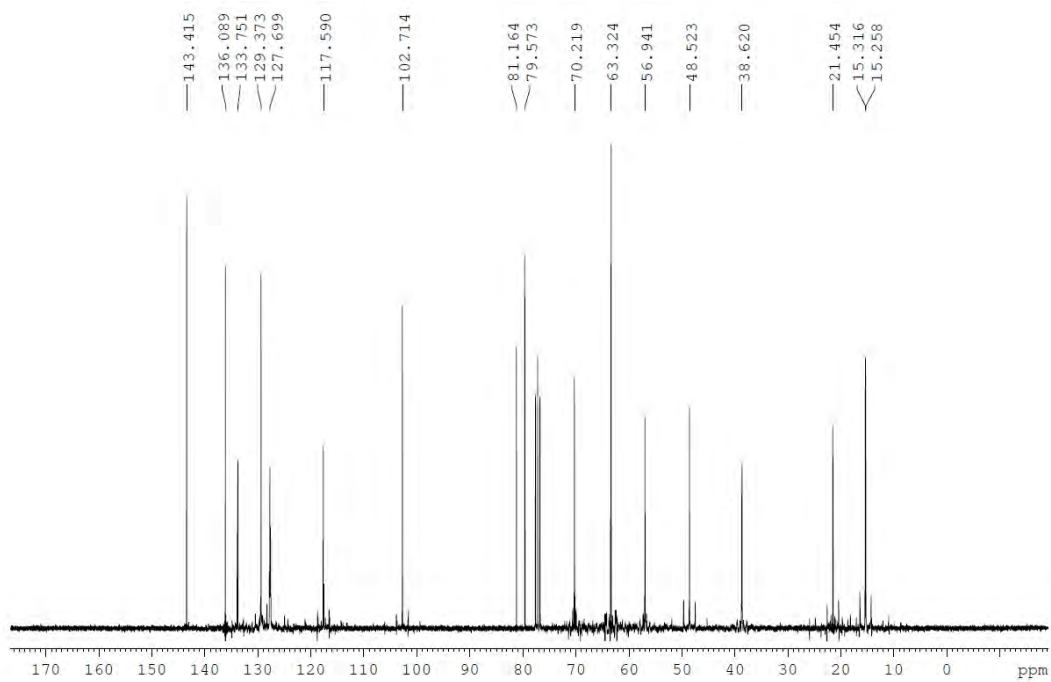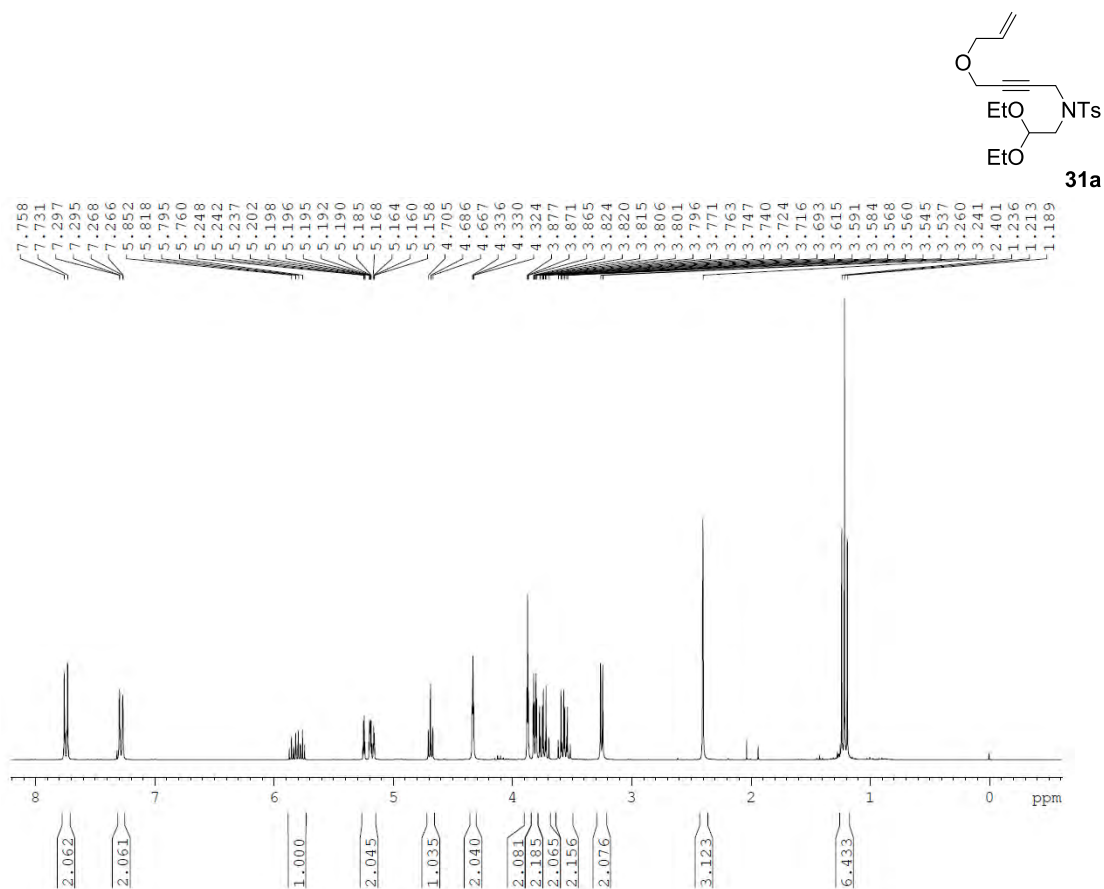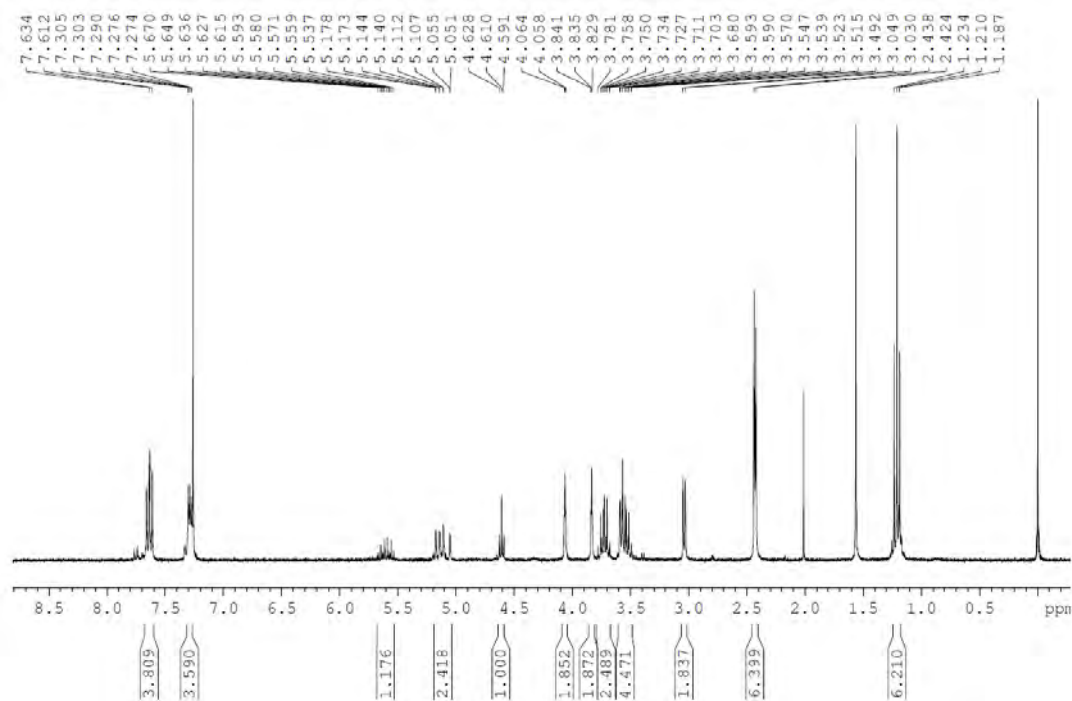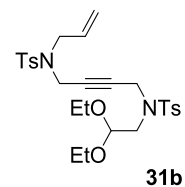
Figure S3: ^{1}H NMR spectrum (400 MHz) of **31b** in CDCl$_3$.
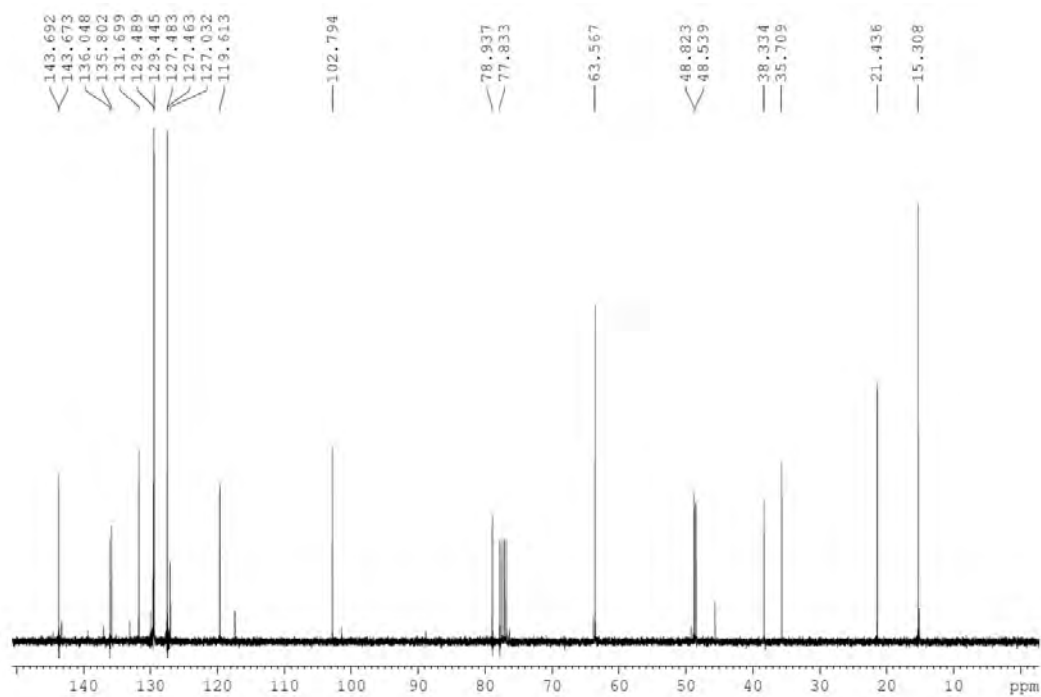
Figure S4: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31b** in CDCl$_3$.

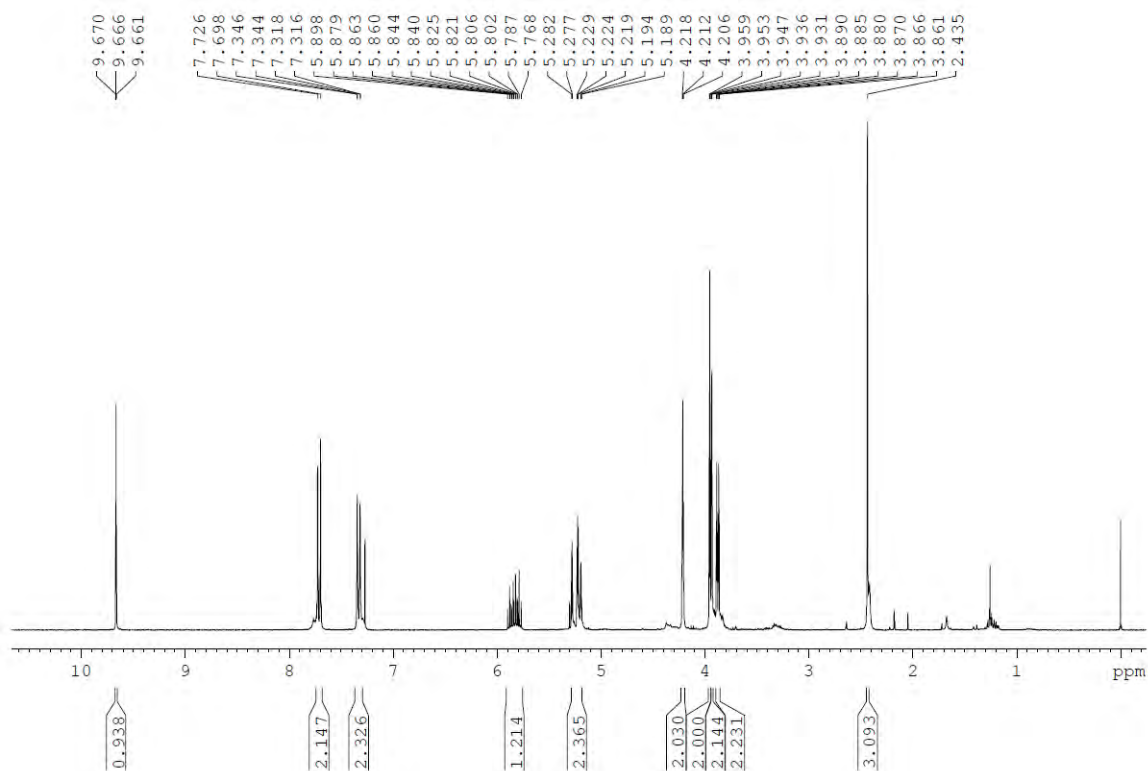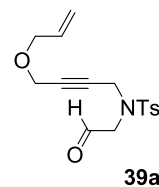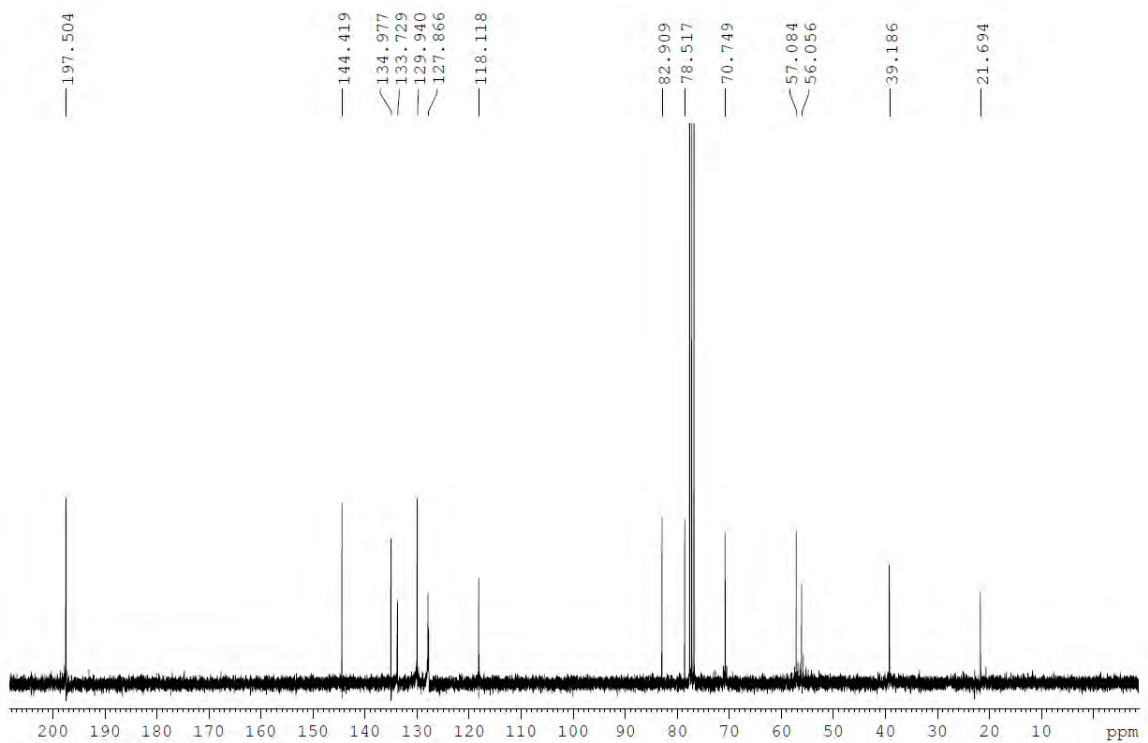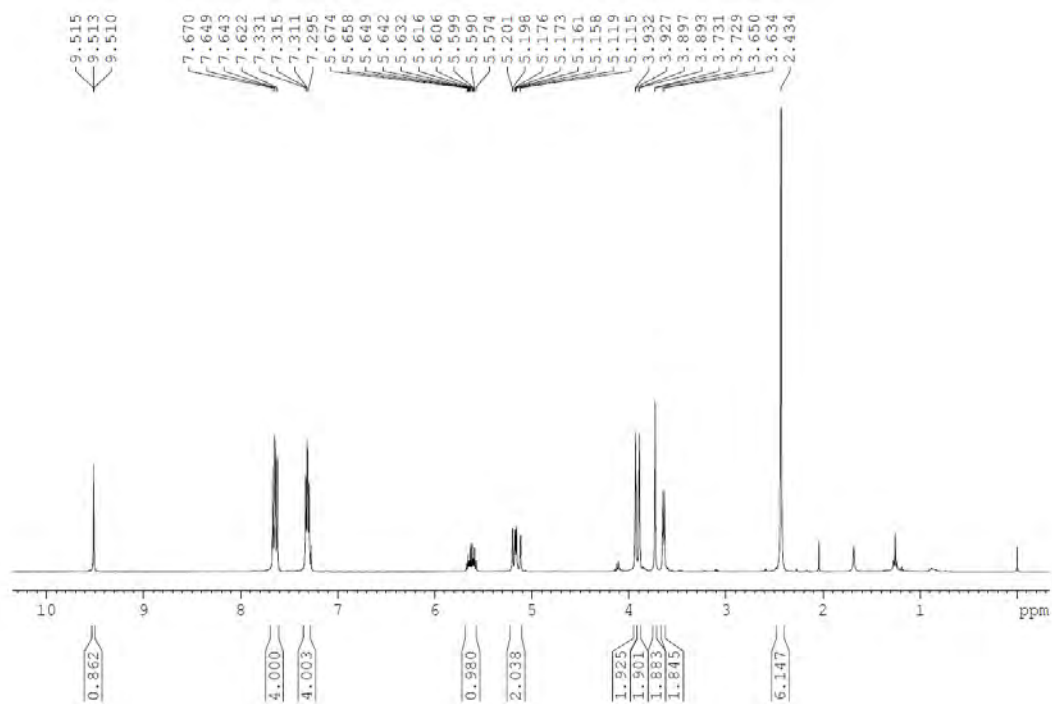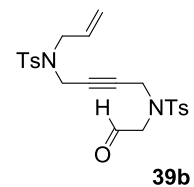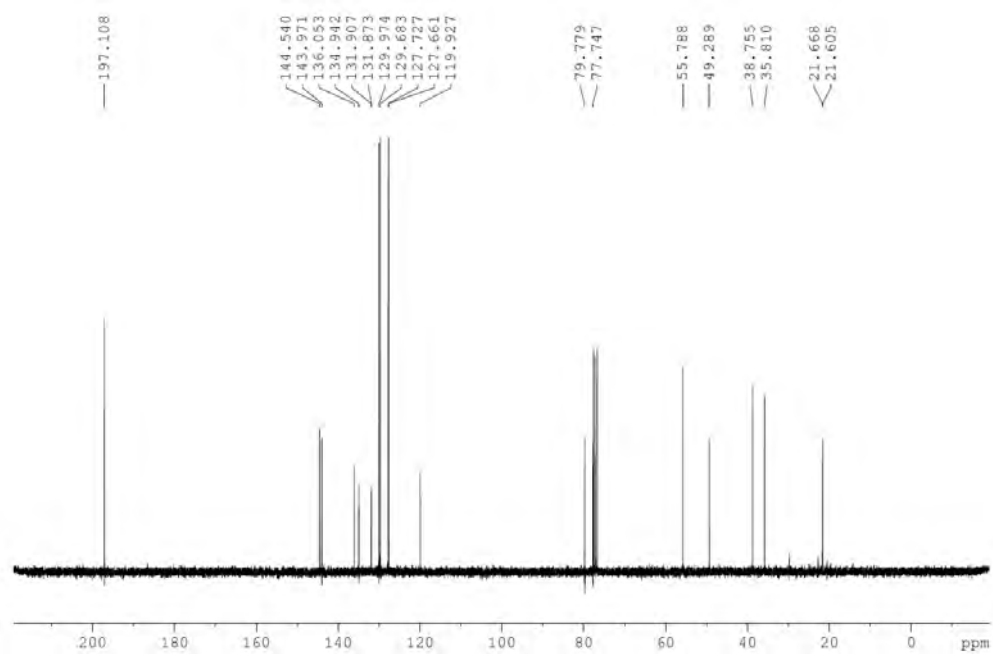**Figure S5**: ^{1}H NMR spectrum (300 MHz) of **31c** in CDCl$_3$.

Figure S6: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **31c** in CDCl$_3$.
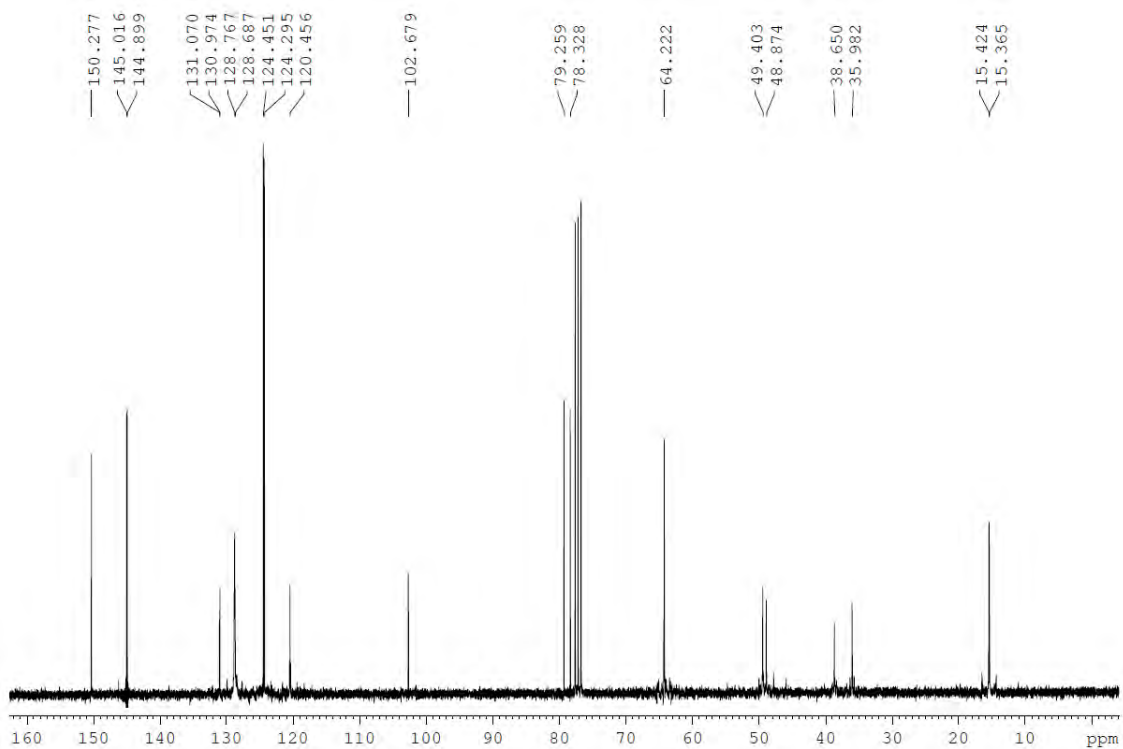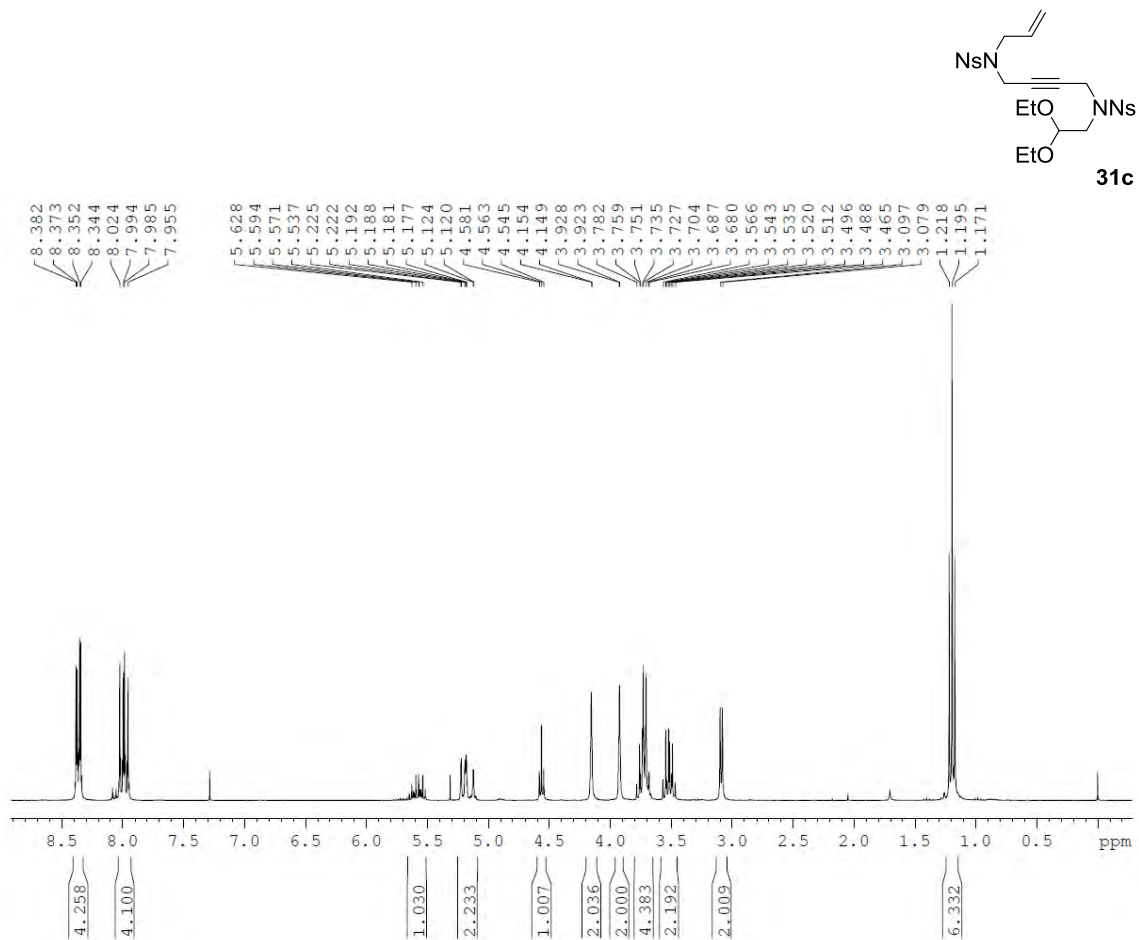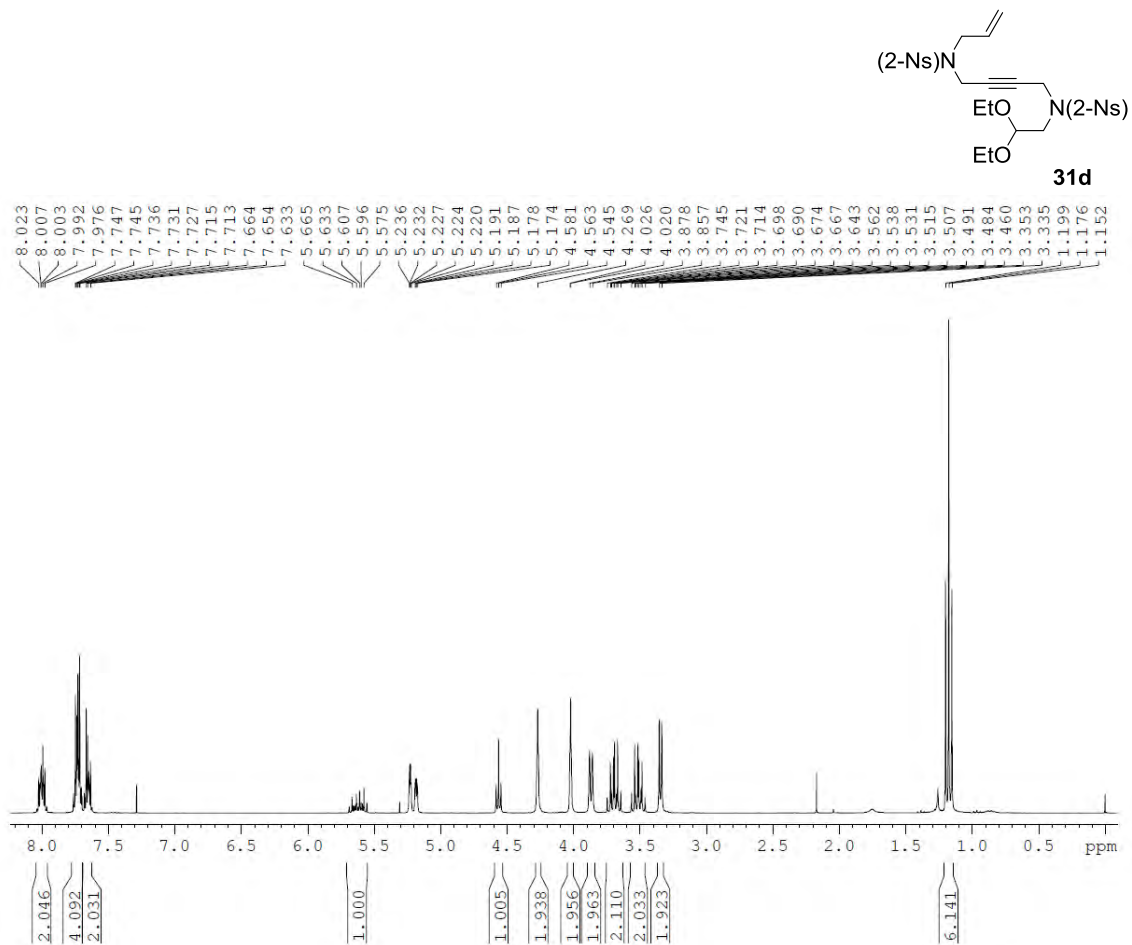
Figure S7: ^{1}H NMR spectrum (300 MHz) of **31d** in CDCl$_3$.
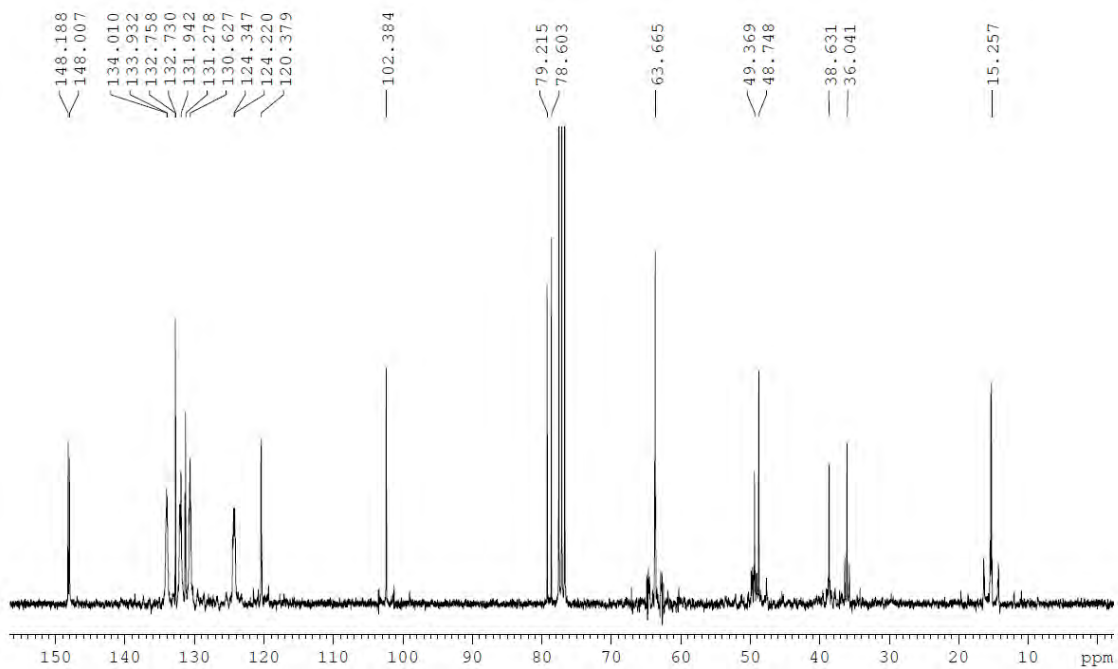
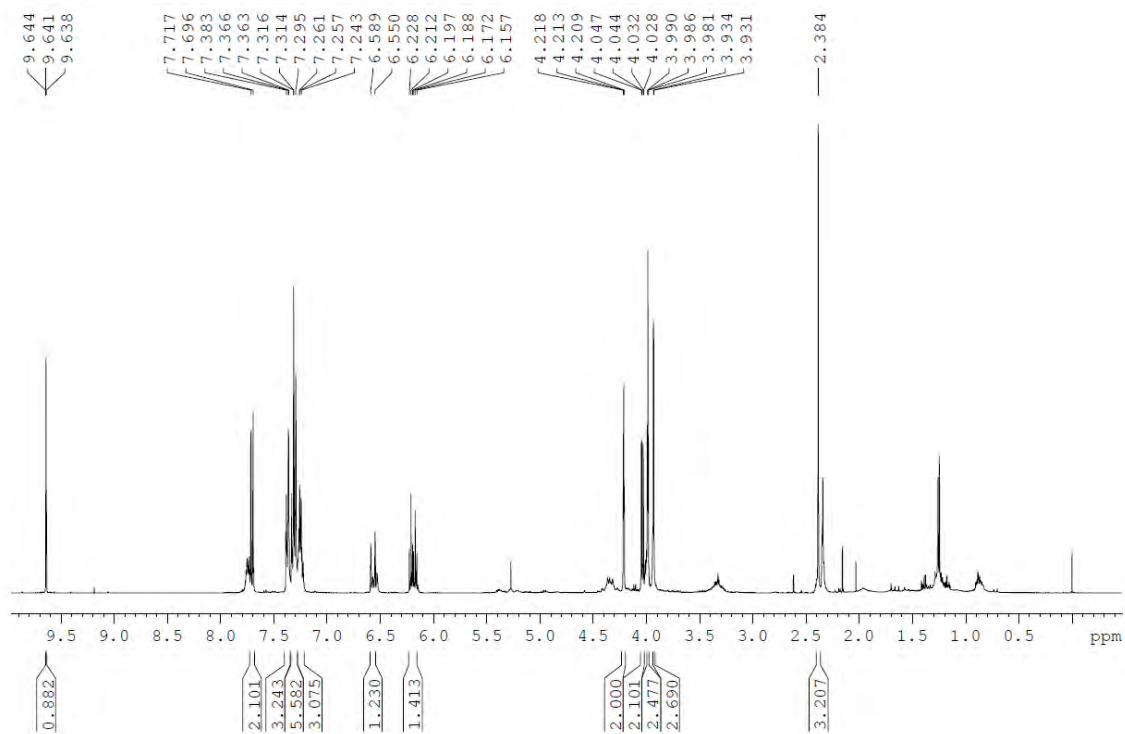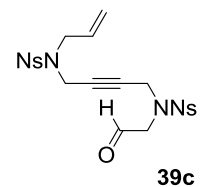**Figure S8**: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **31d** in CDCl$_3$.
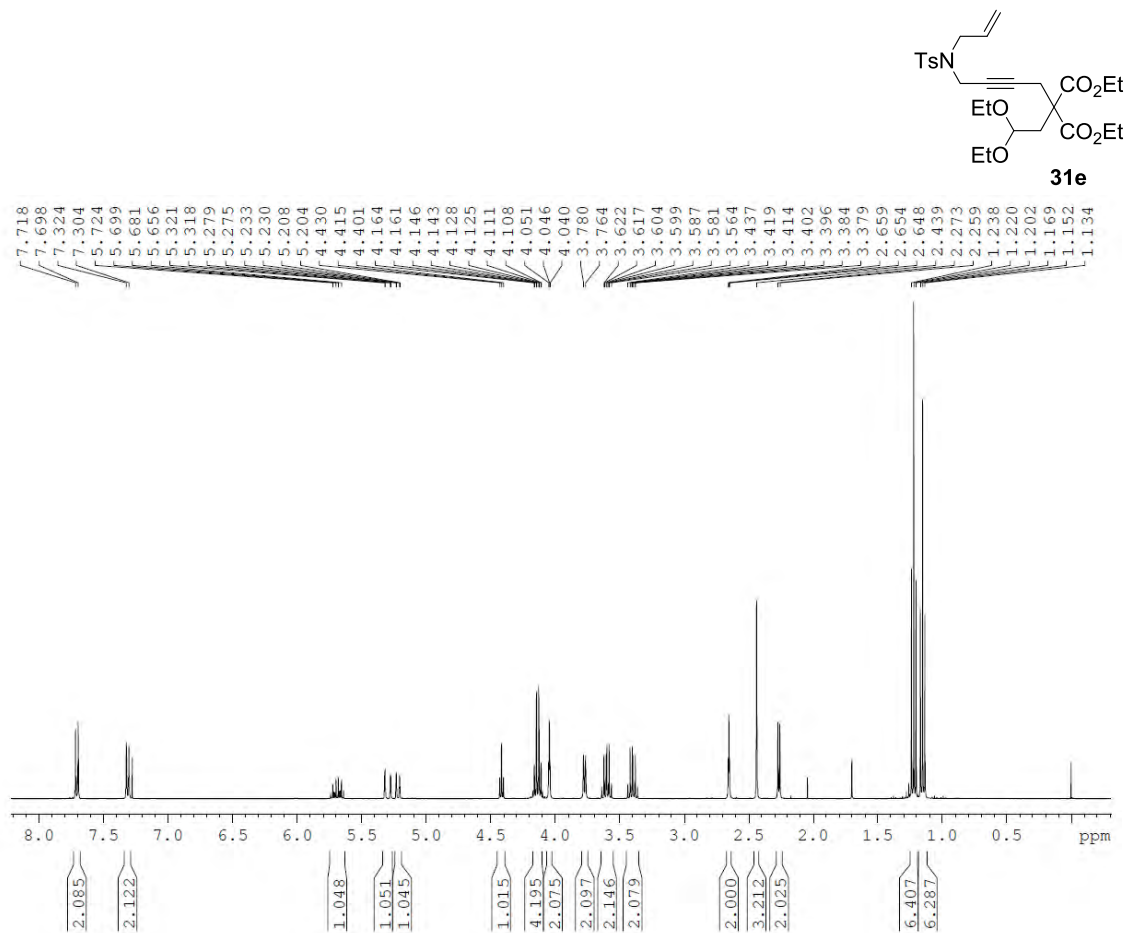
Figure S9: ^{1}H NMR spectrum (400 MHz) of **31e** in CDCl$_3$.
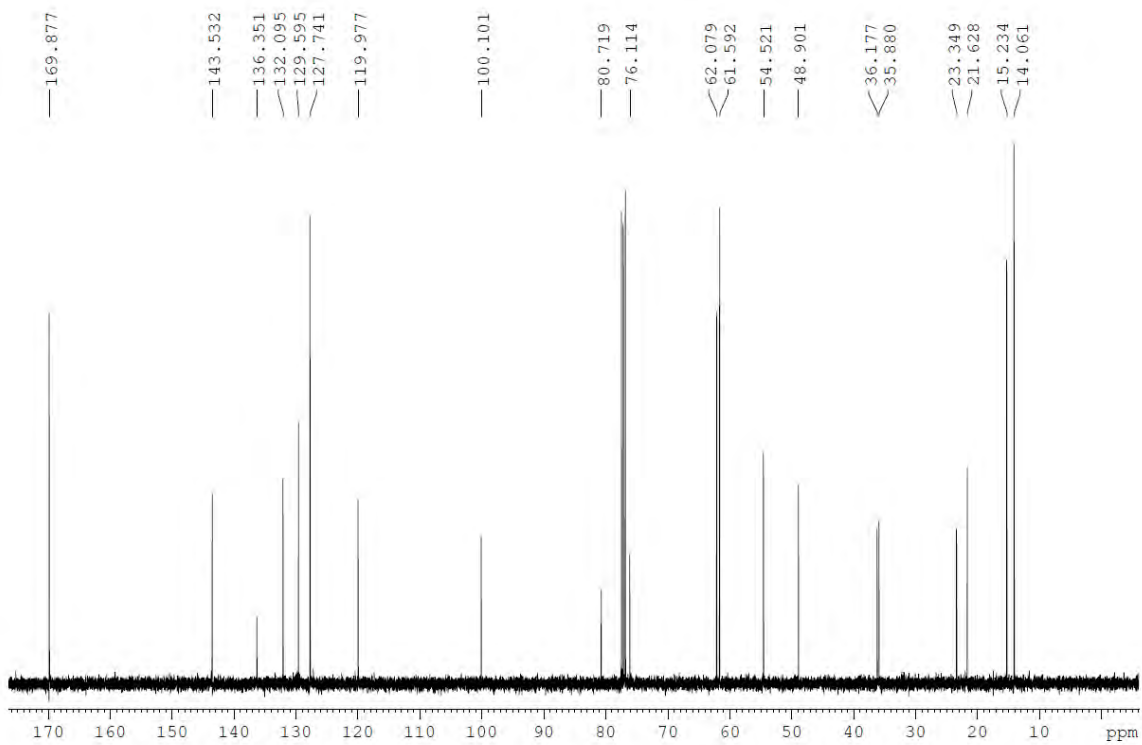
Figure S10: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31e** in CDCl$_3$.
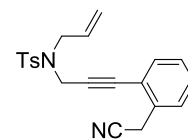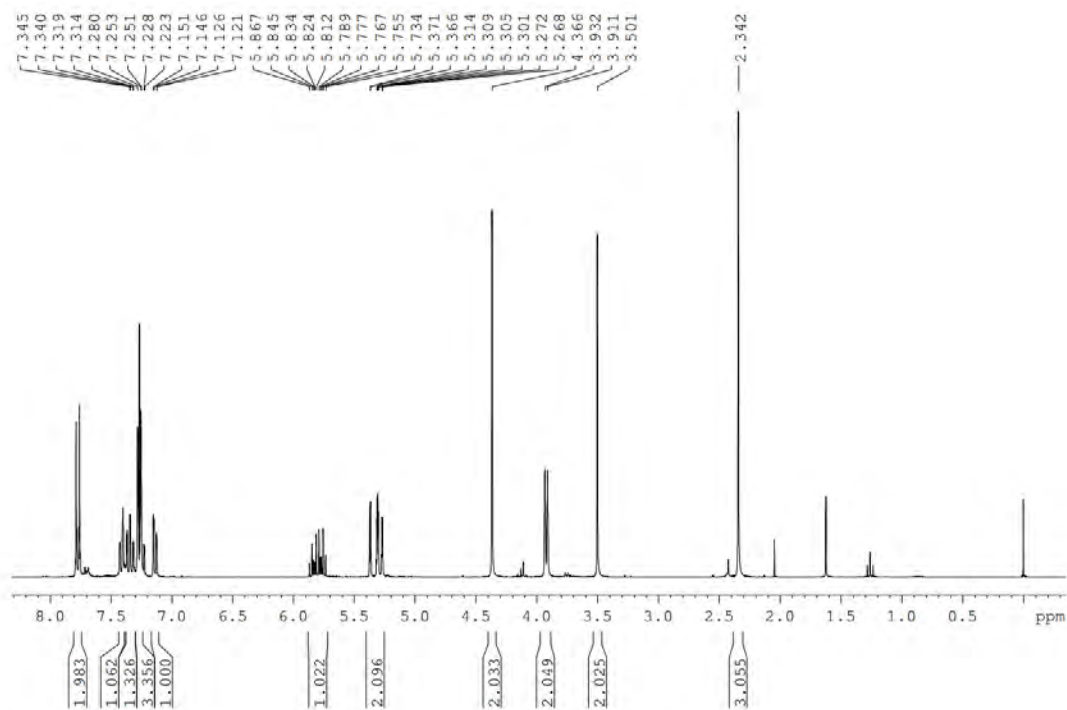
Figure S11: ^{1}H NMR spectrum (300 MHz) of **41a** in CDCl$_3$.
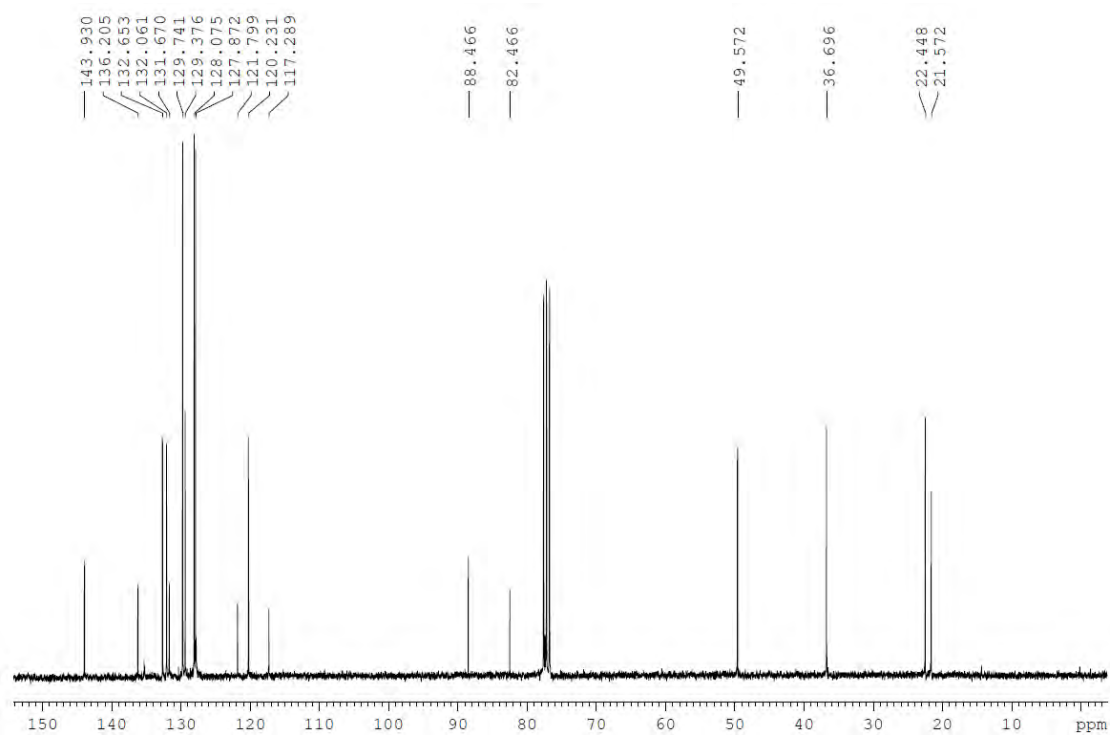
Figure S12: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **41a** in CDCl$_3$.
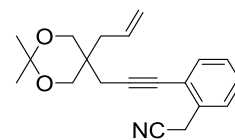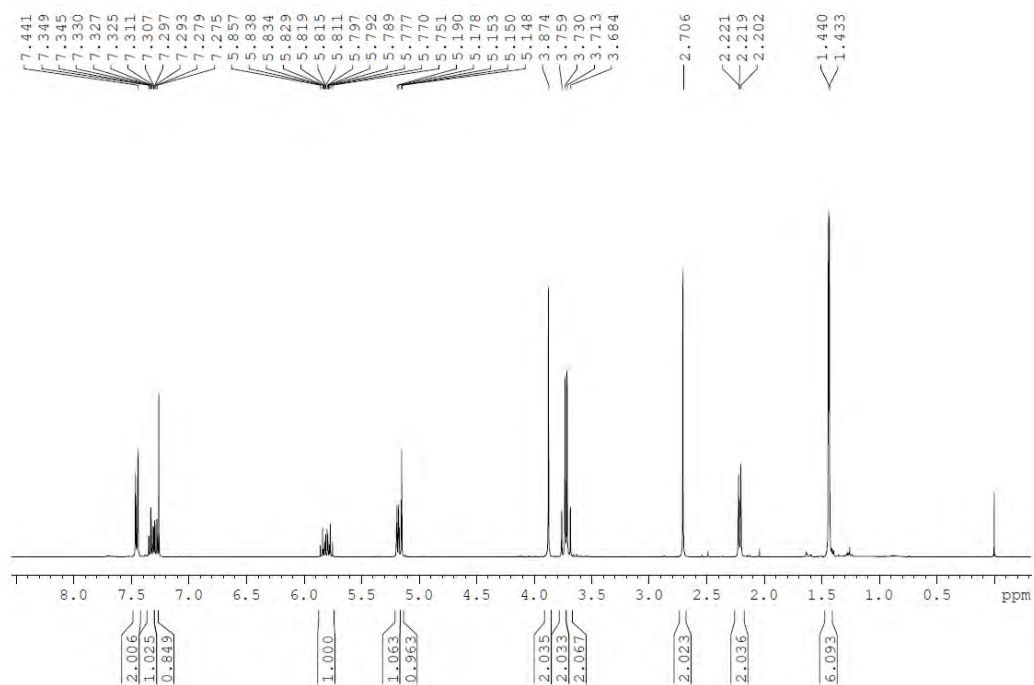
Figure S13: ^{1}H NMR spectrum (400 MHz) of **41b** in CDCl$_3$.
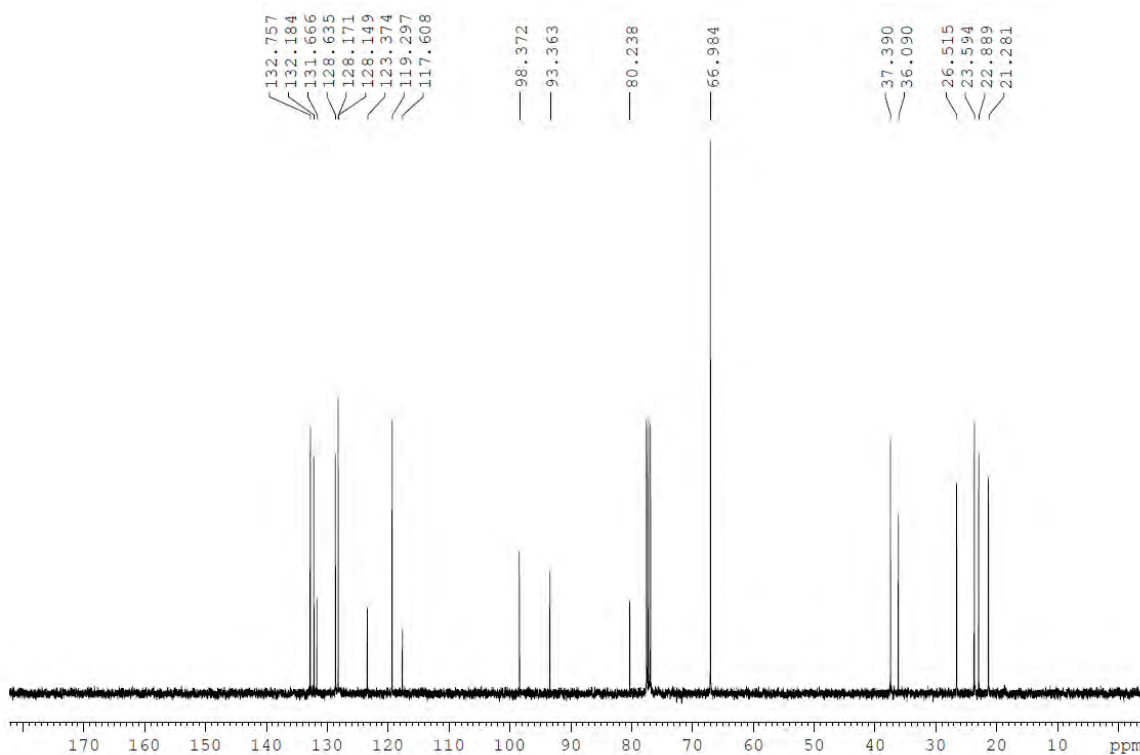
Figure S14: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **41b** in CDCl$_3$.
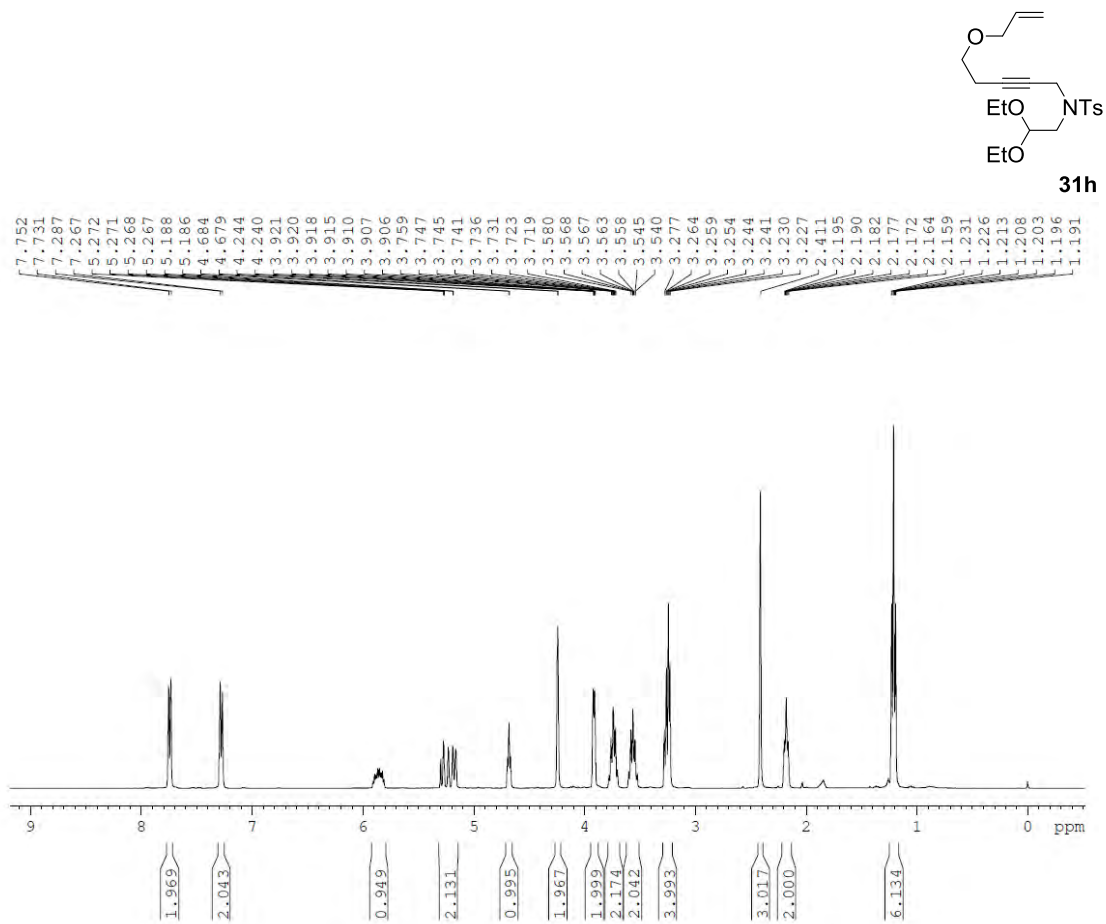
Figure S15: ^{1}H NMR spectrum (400 MHz) of **31h** in CDCl$_3$.
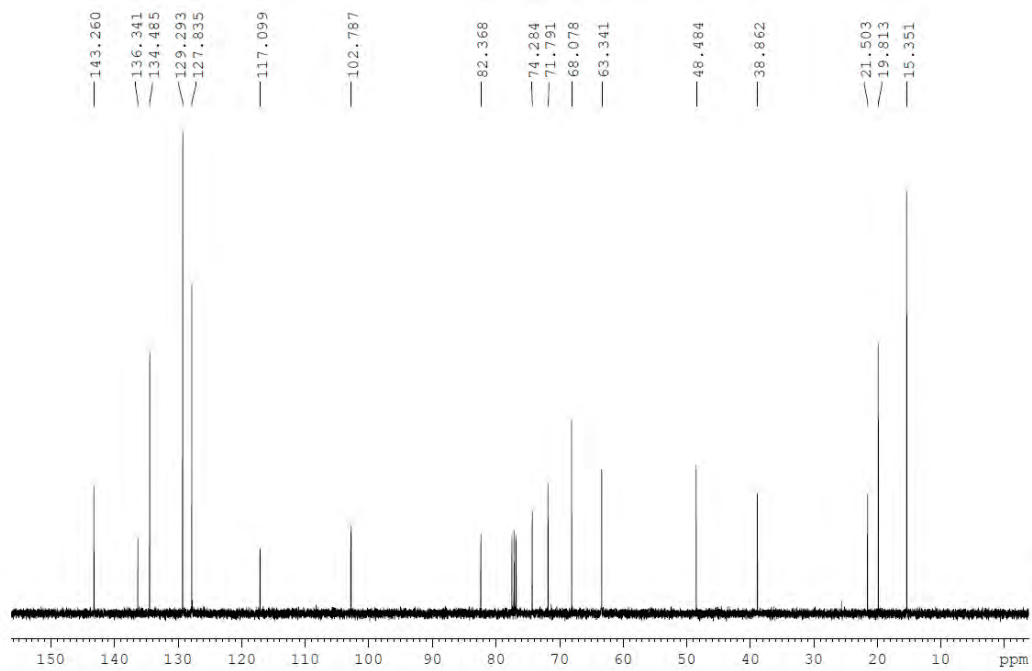
Figure S16: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31h** in CDCl$_3$.
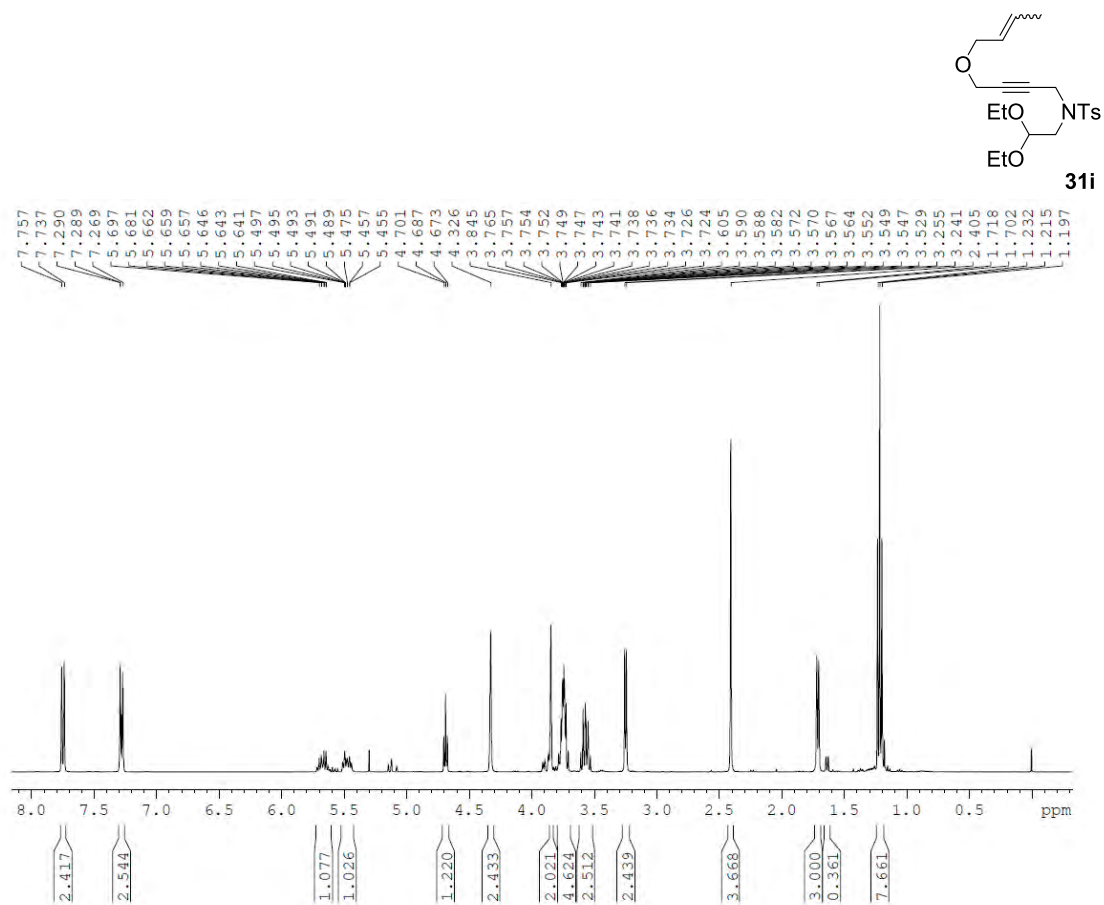
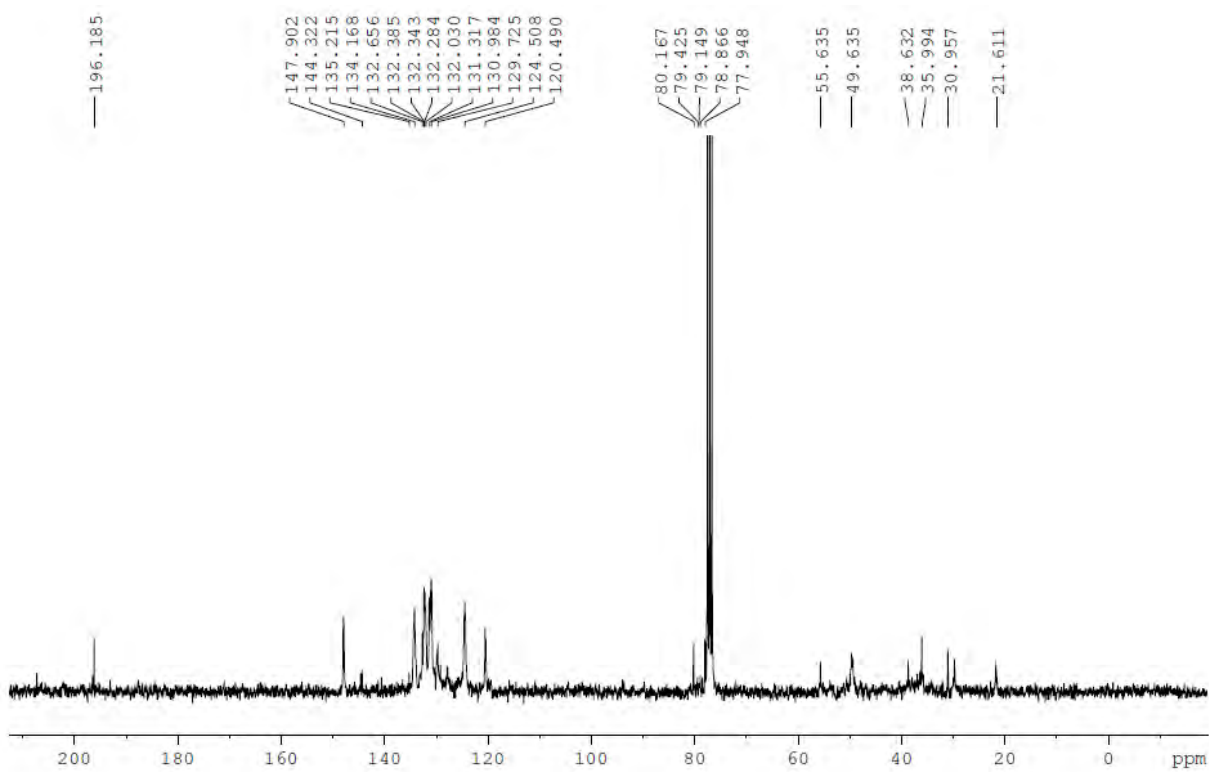**Figure S17**: ^{1}H NMR spectrum (400 MHz) of **31i** in CDCl$_3$.
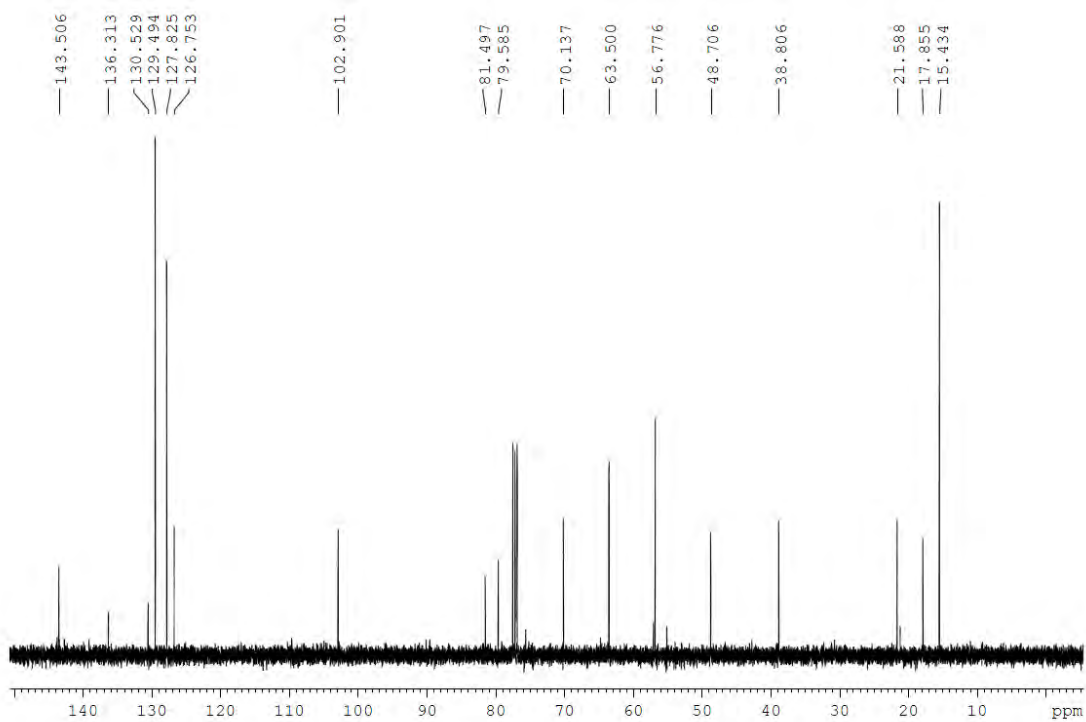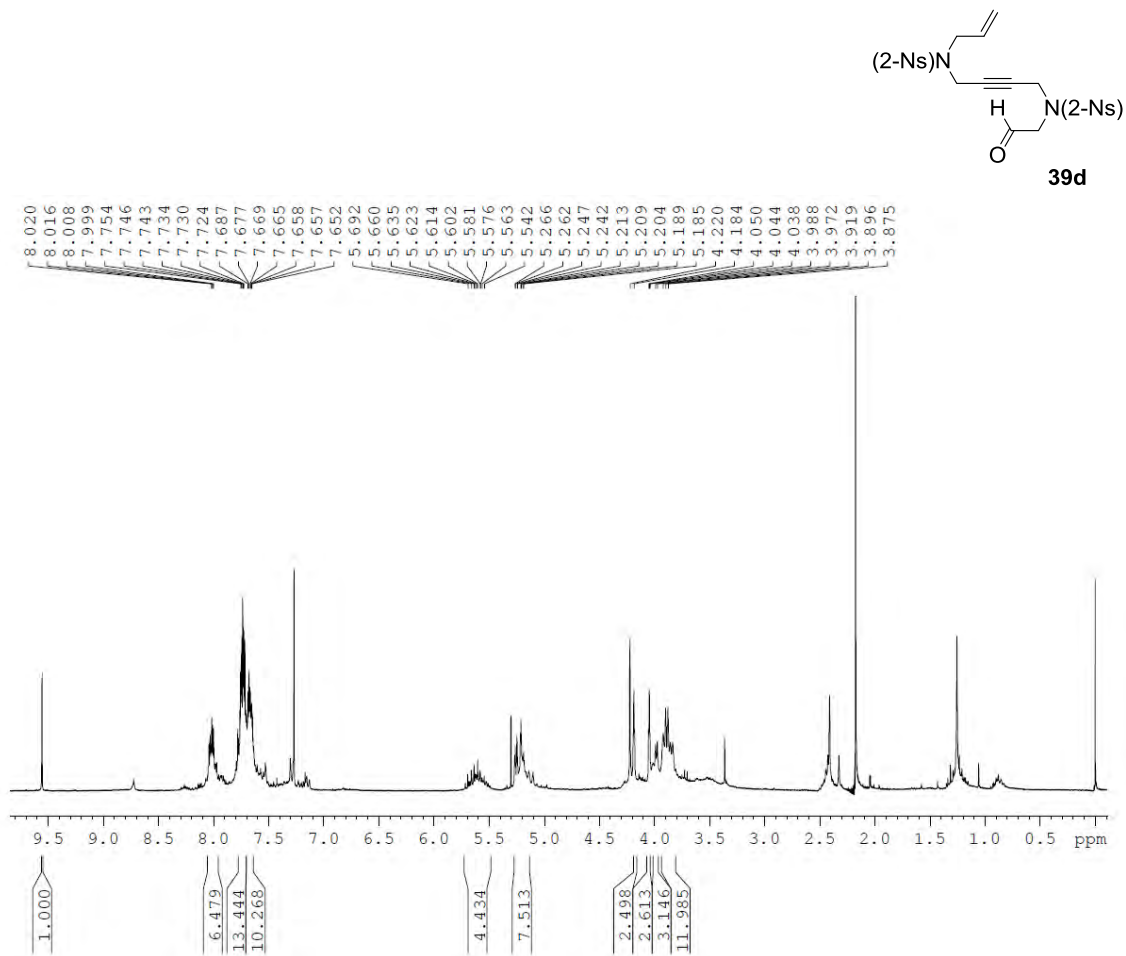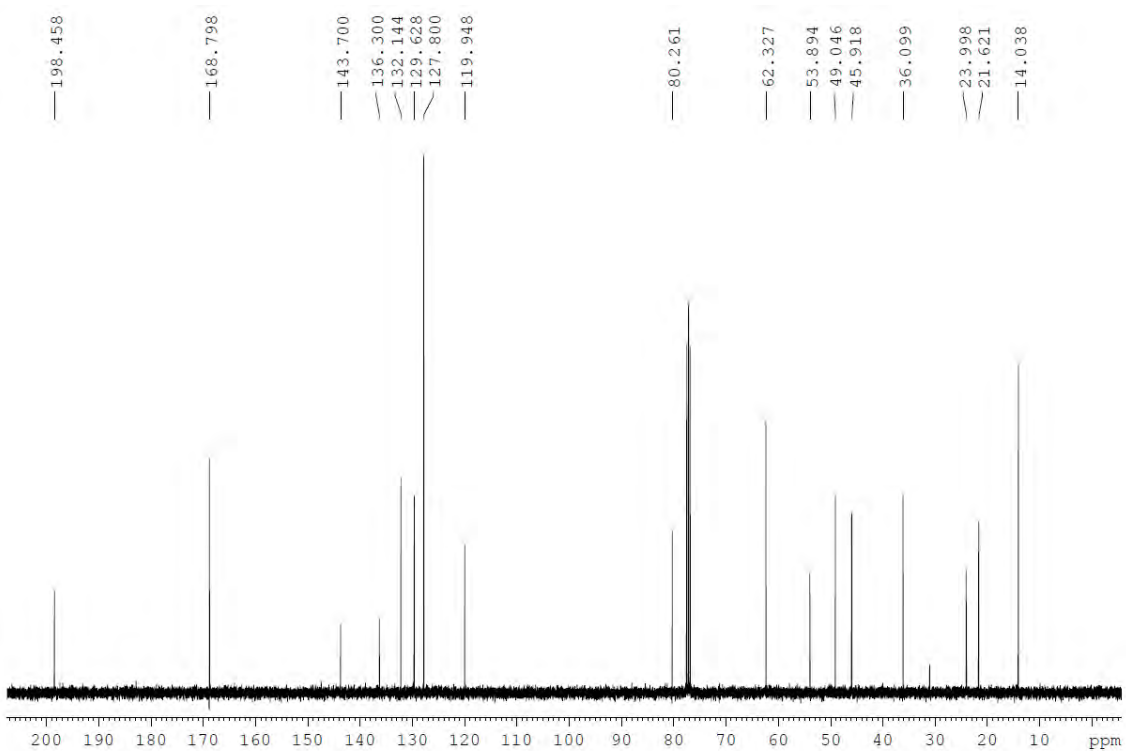

Figure S18: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31i** in CDCl$_3$.

Figure S19: ^{1}H NMR spectrum (400 MHz) of **31j** in CDCl$_3$.

Figure S20: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31j** in CDCl$_3$.
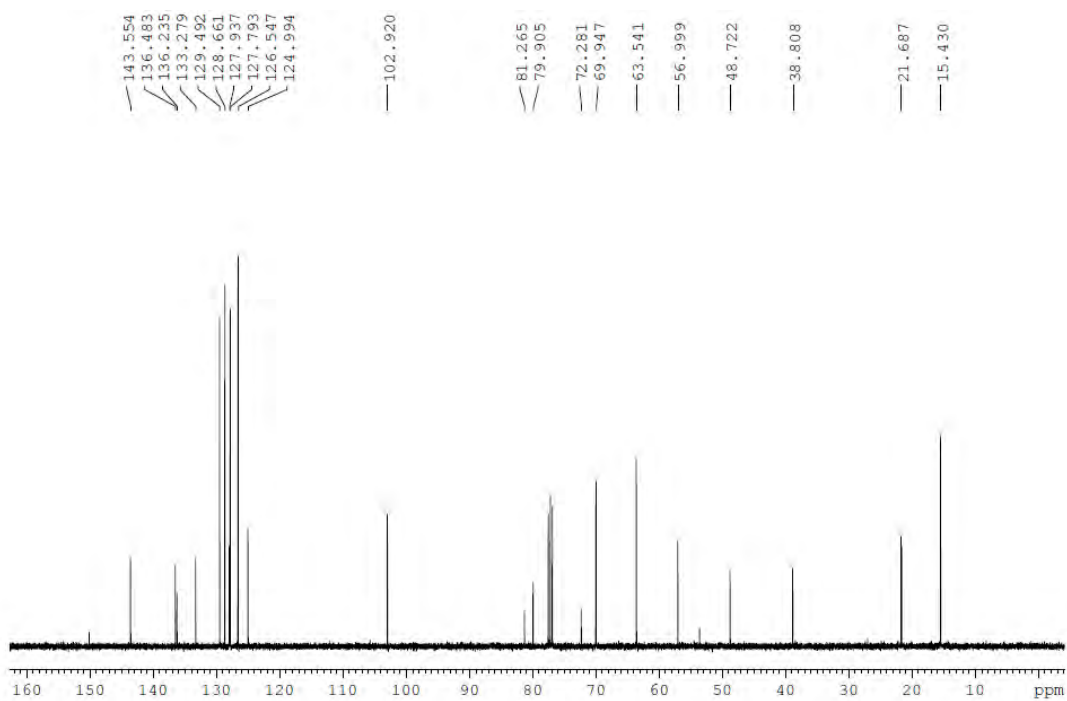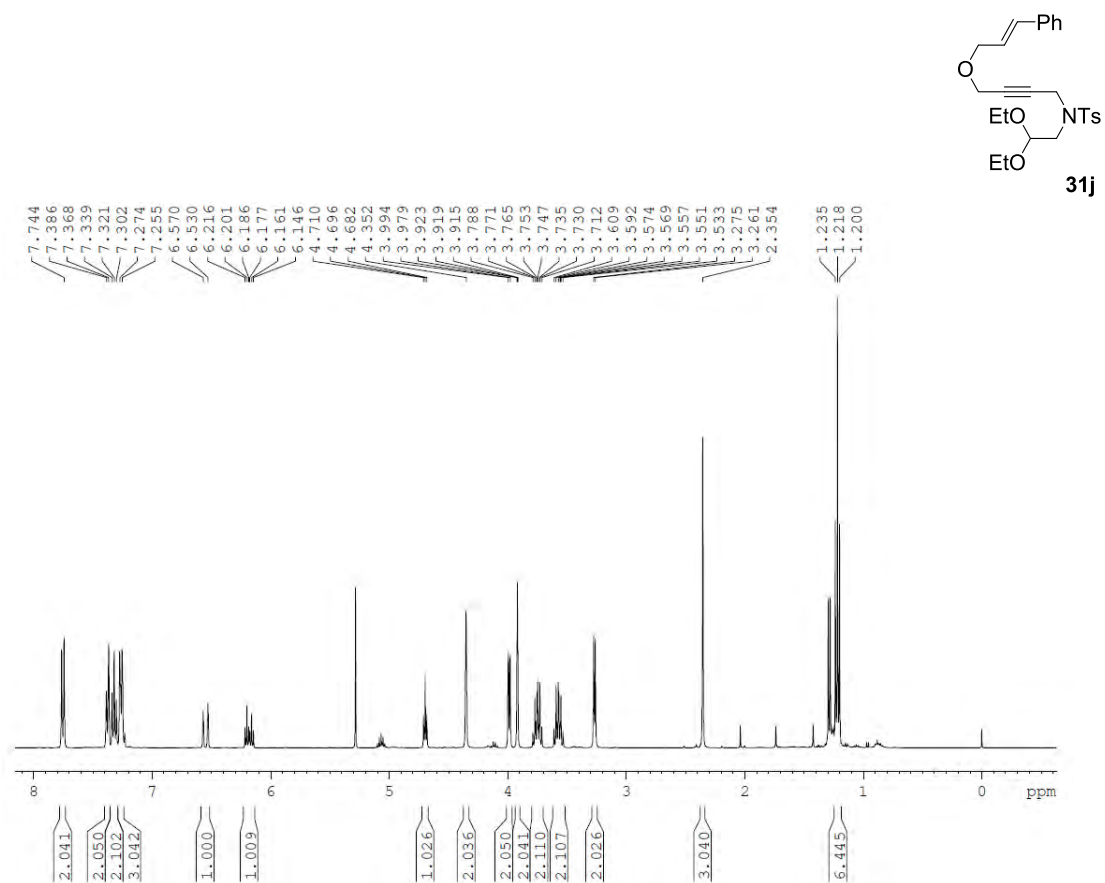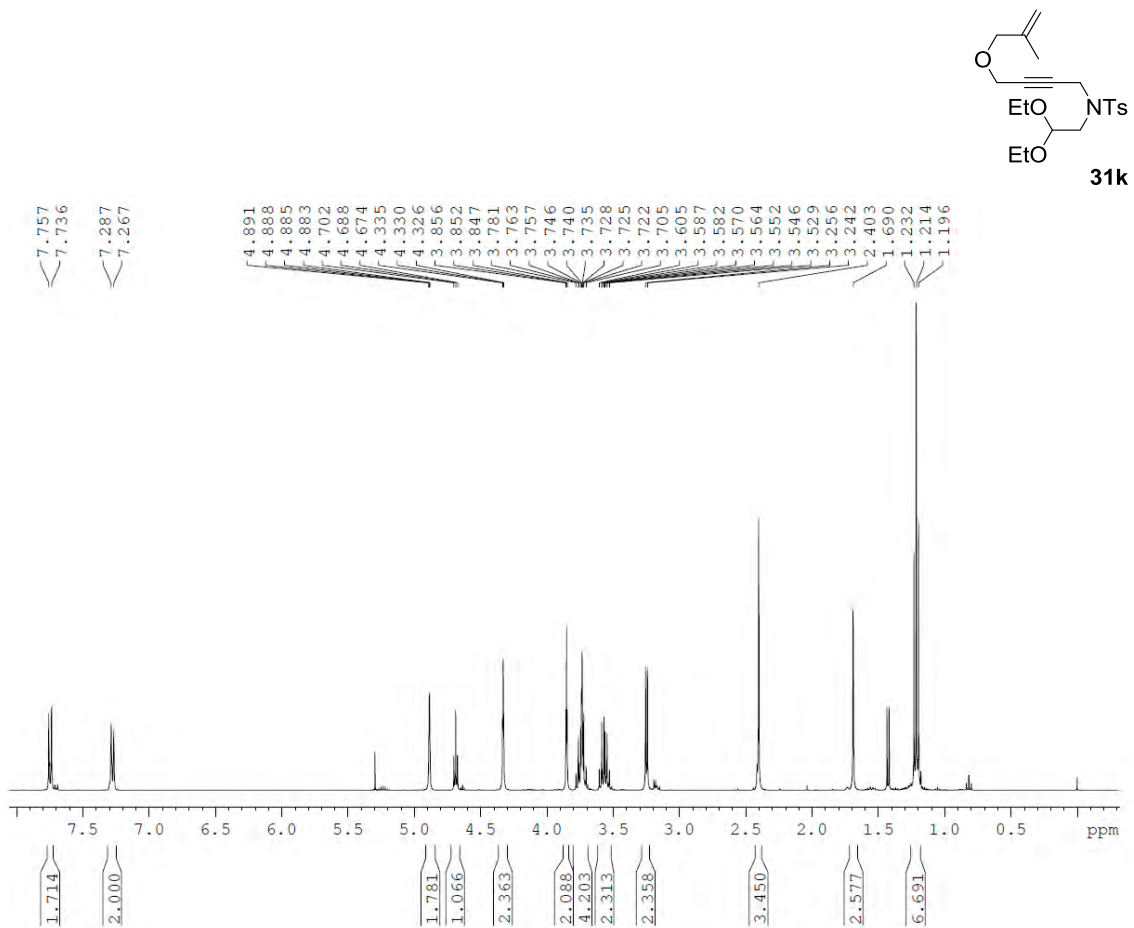
Figure S21: ^{1}H NMR spectrum (400 MHz) of **31k** in CDCl$_3$.
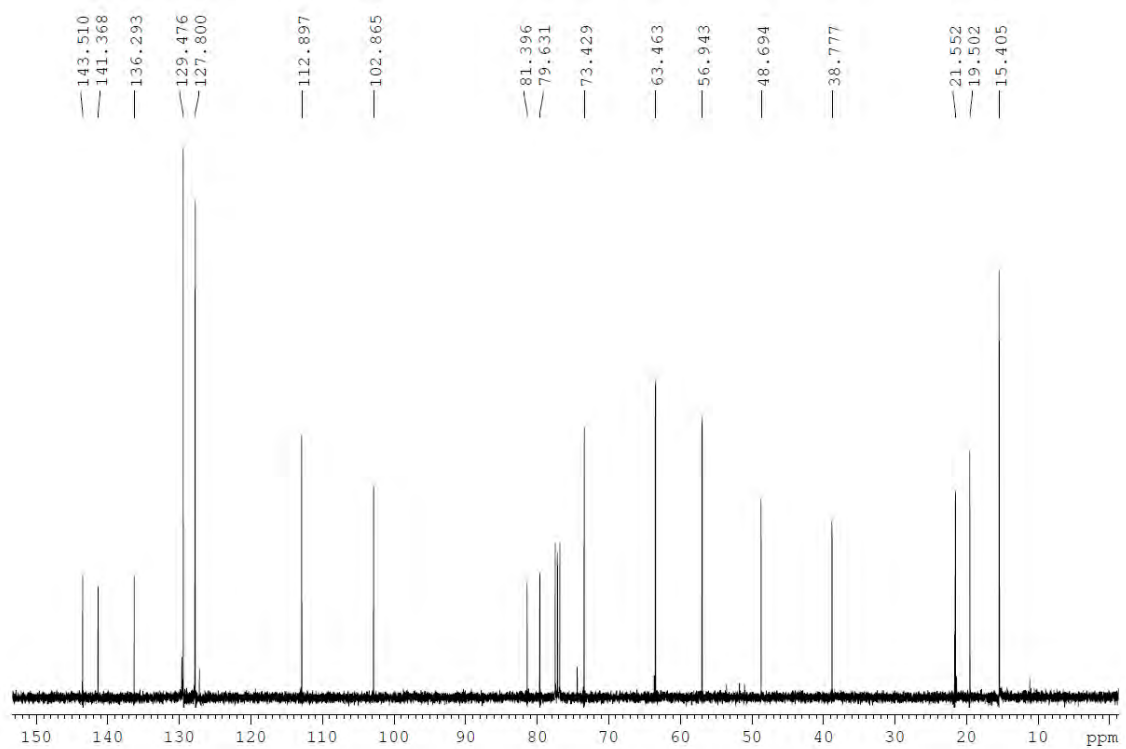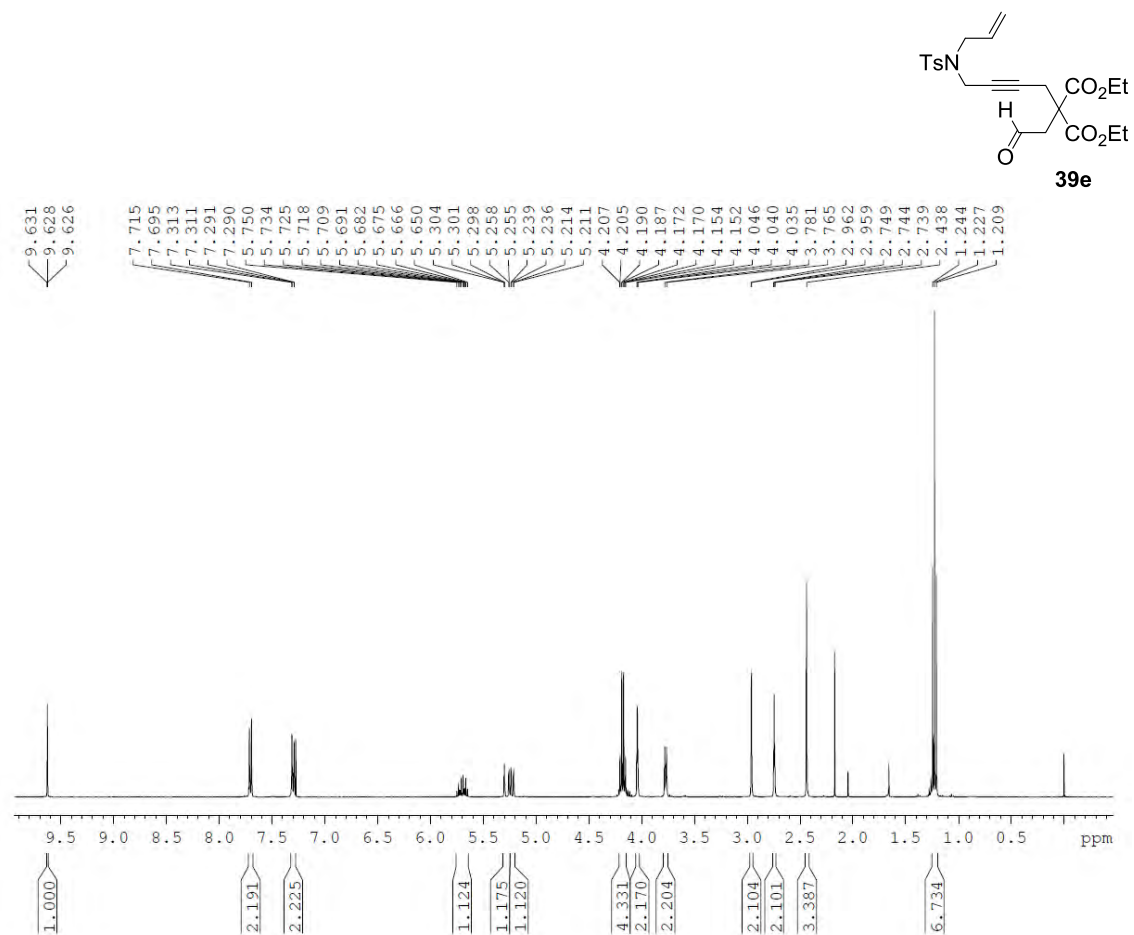

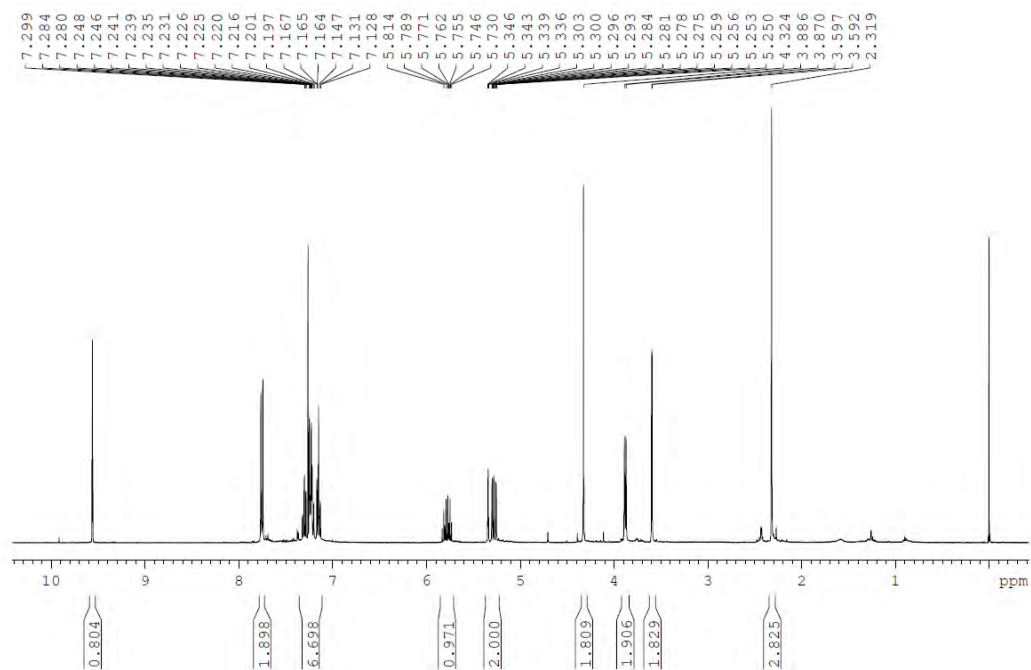**Figure S22**: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31k** in CDCl$_3$.

Figure S23: ^{1}H NMR spectrum (300 MHz) of **39a** in CDCl$_3$.

Figure S24: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **39a** in CDCl$_3$.

Figure S25: ^{1}H NMR spectrum (400 MHz) of **39b** in CDCl$_3$.

Figure S26: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **39b** in CDCl$_3$.

Figure S27: ^{1}H NMR spectrum (400 MHz) of **39c** in CDCl$_3$.
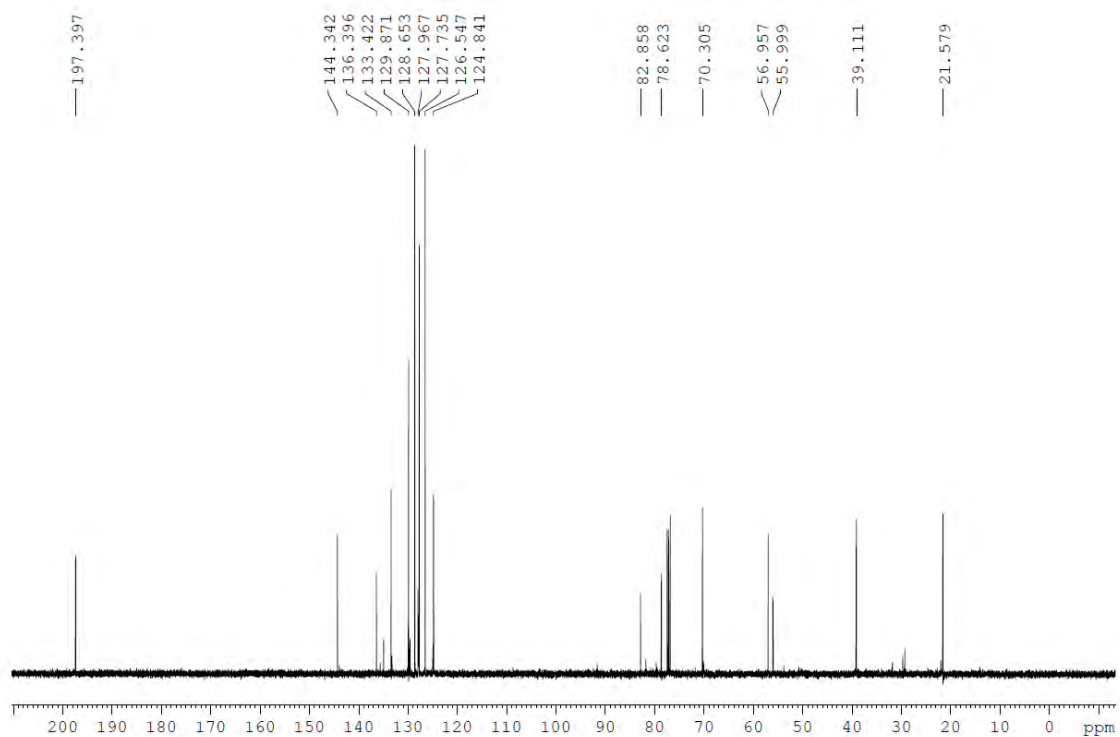
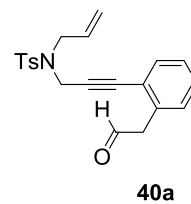**Figure S28**: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **39c** in CDCl$_3$.

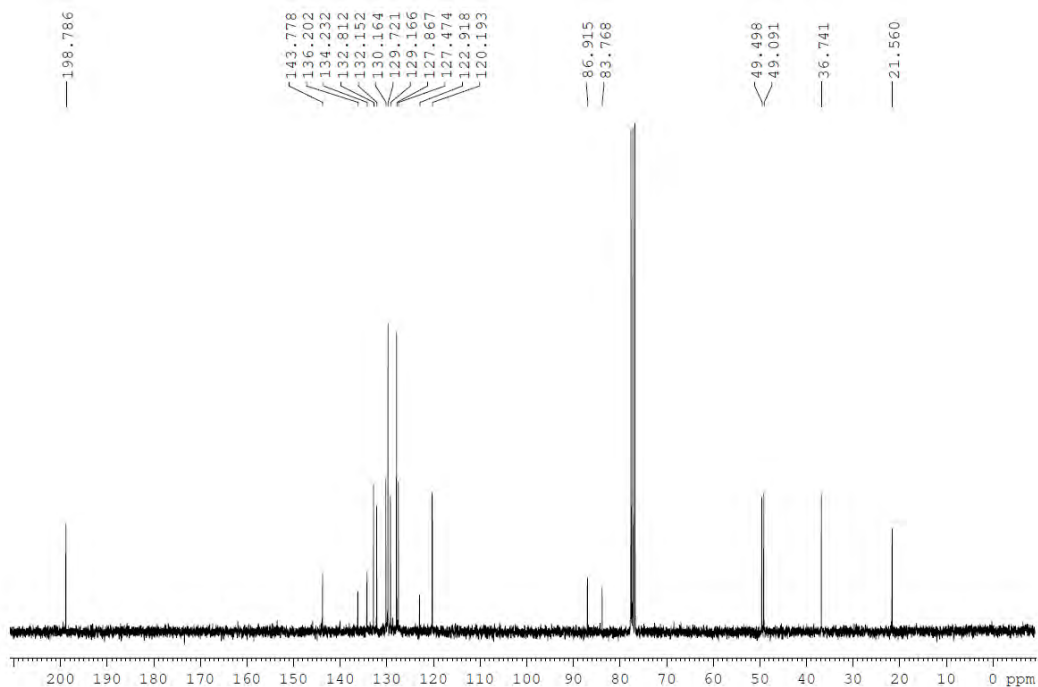**Figure S29**: ^1H NMR spectrum (300 MHz) of **39d** in CDCl$_3$.

Figure S30: ^1H-decoupled^{13}C NMR spectrum (75 MHz) of **39d** in CDCl$_3$.

Figure S31: ^{1}H NMR spectrum (400 MHz) of **39e** in CDCl$_3$.

Figure S32: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **39e** in CDCl$_3$.

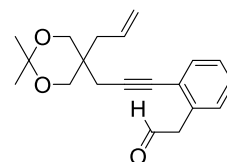**Figure S33**: ^{1}H NMR spectrum (300 MHz) of **40a** in CDCl$_3$.

Figure S34: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **40a** in CDCl$_3$.
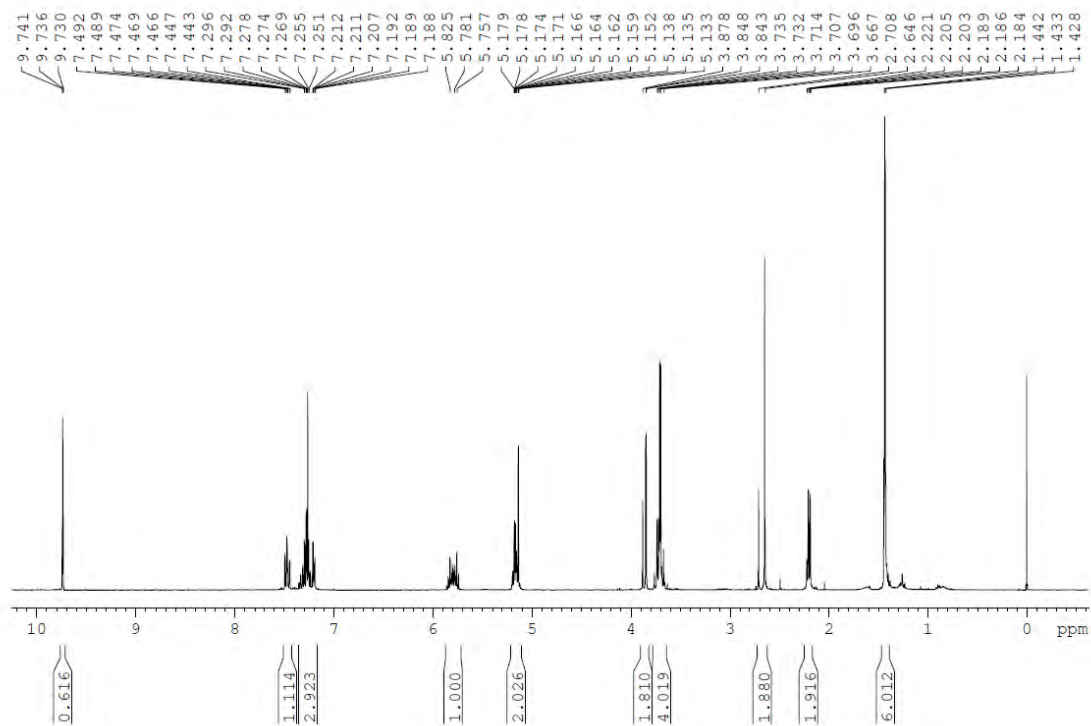
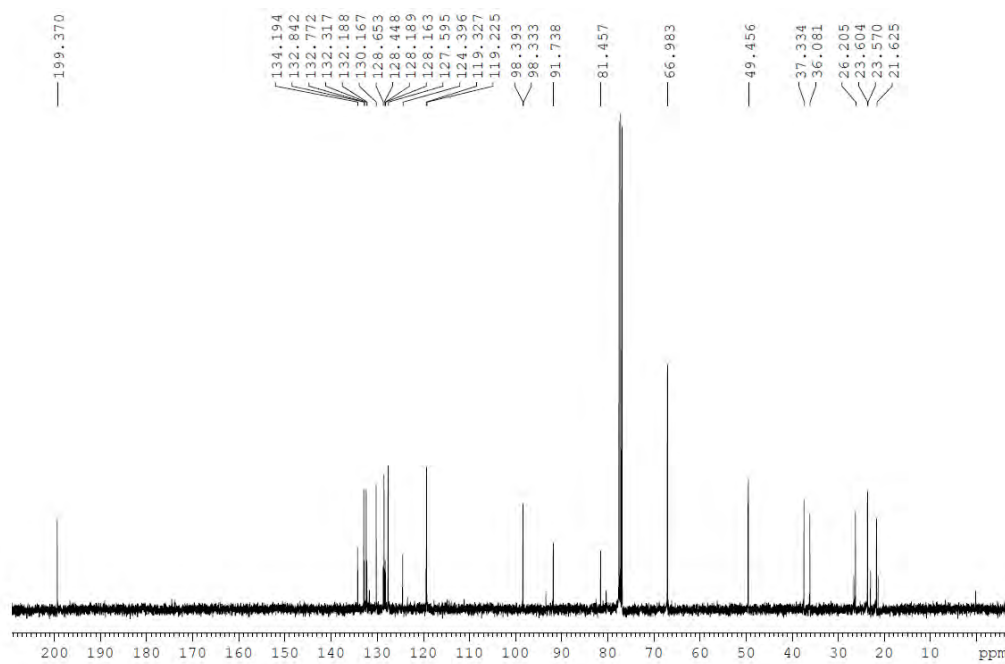**Figure S35**: ^{1}H NMR spectrum (400 MHz) of **40b** in CDCl$_3$.

Figure S36: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **40b** in CDCl$_3$.
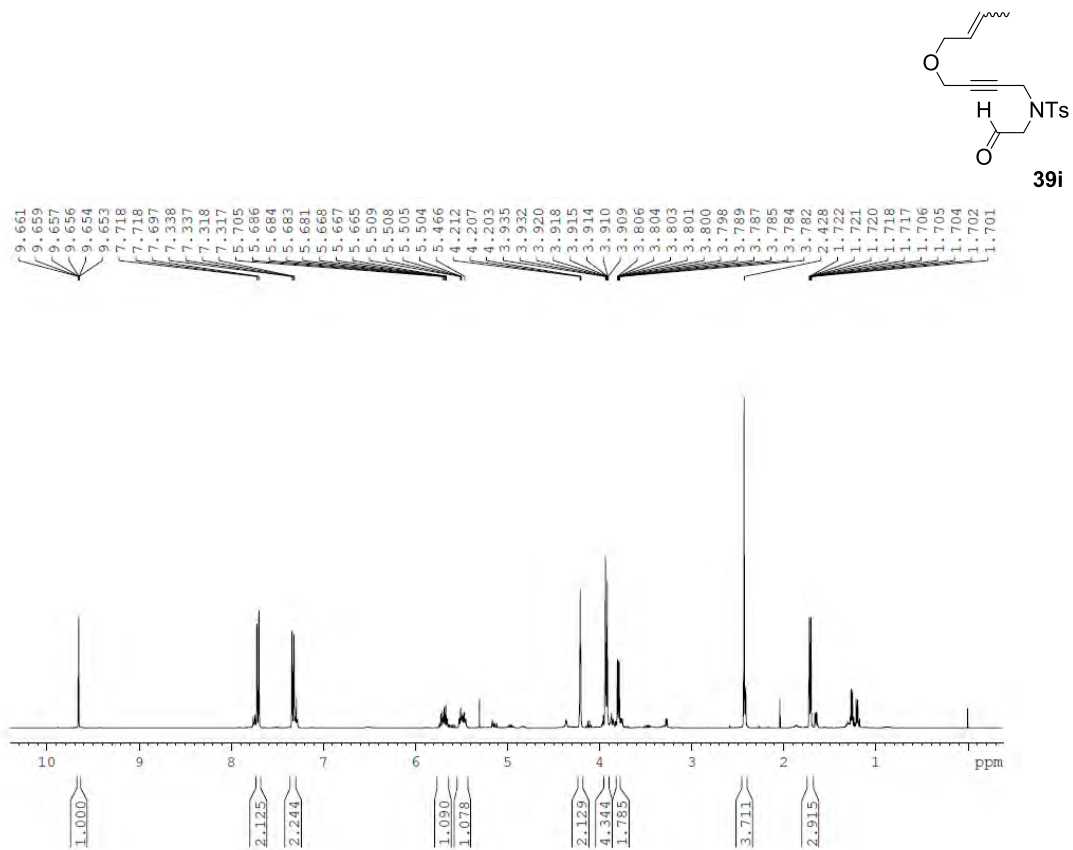
Figure S37: ^{1}H NMR spectrum (400 MHz) of **39i** in CDCl$_3$.
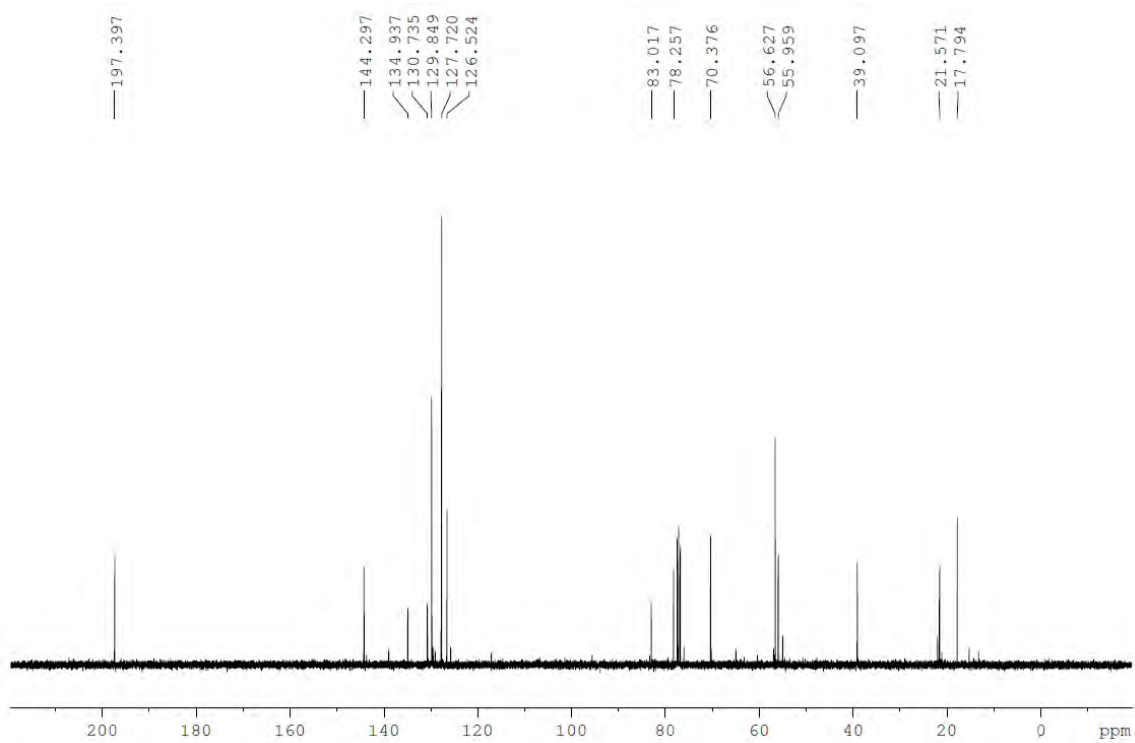

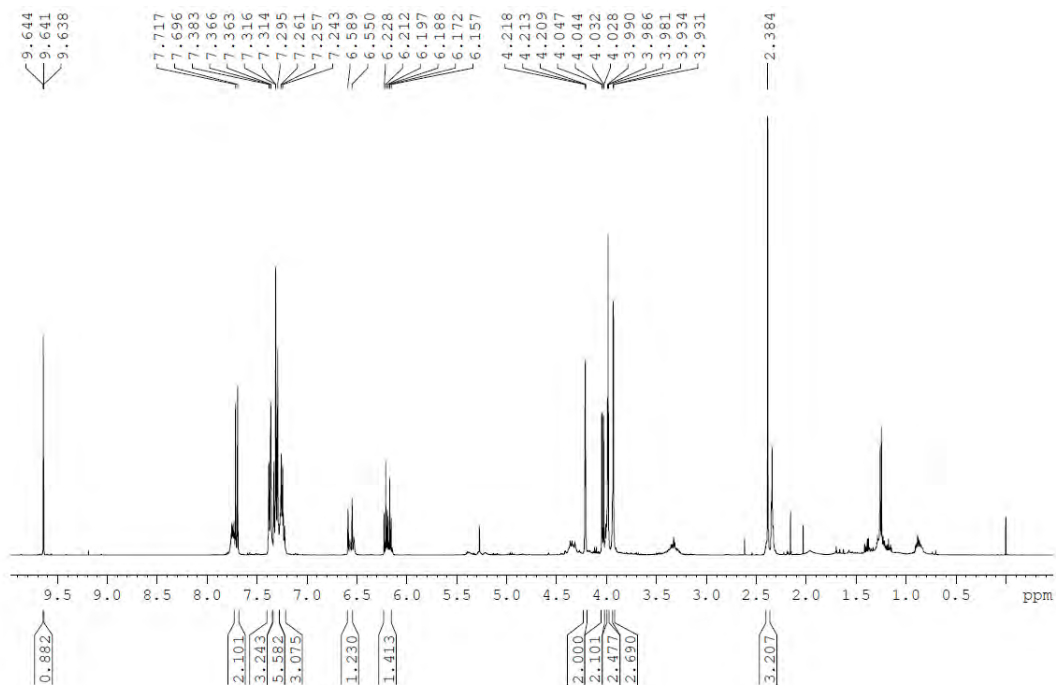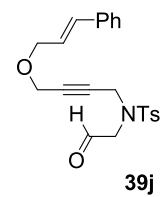**Figure S38**: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **39i** in CDCl$_3$.

Figure S39: ^{1}H NMR spectrum (400 MHz) of **39j** in CDCl$_3$.

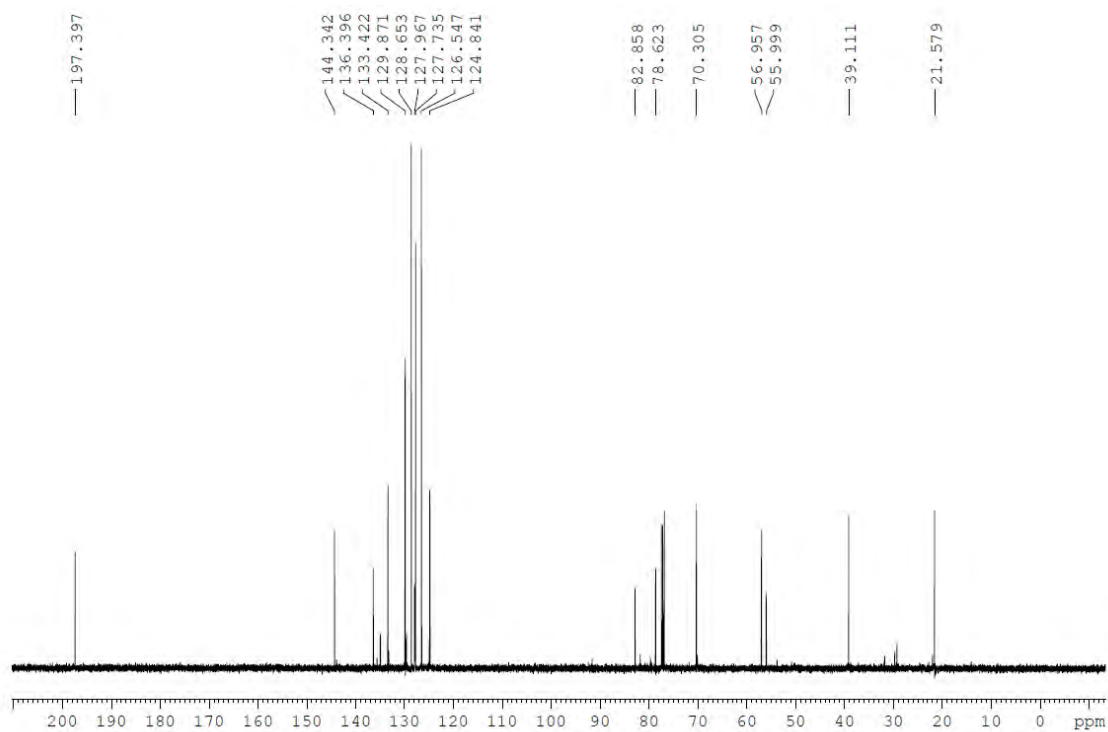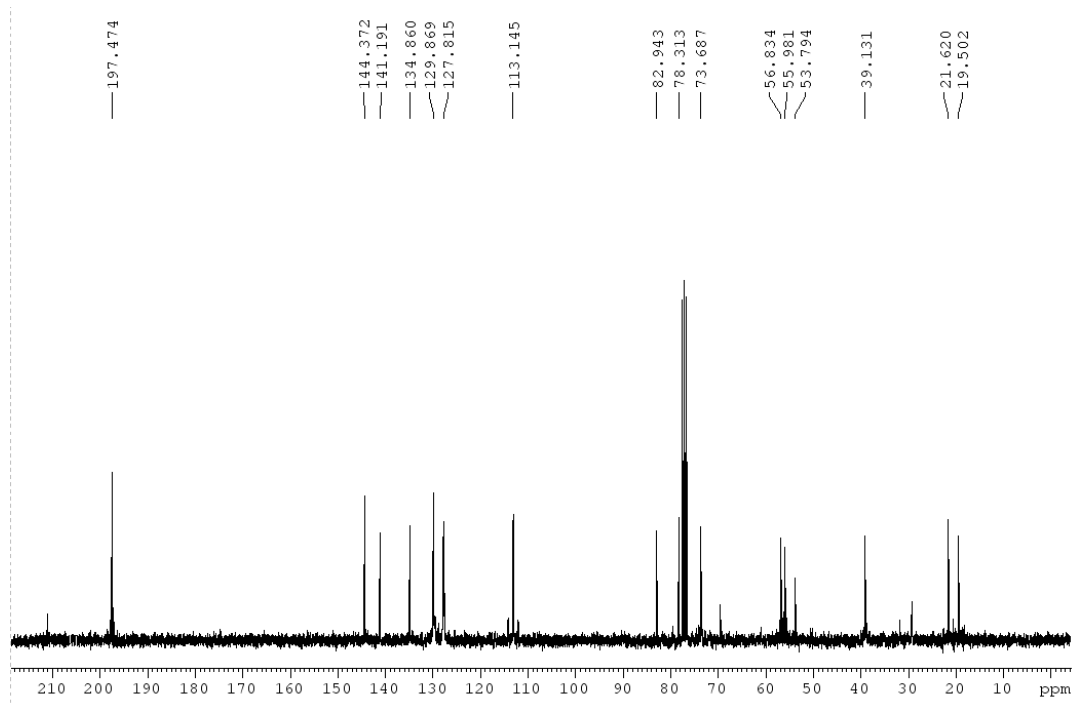

Figure S40: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **39j** in CDCl$_3$.

Figure S41: ^{1}H NMR spectrum (300 MHz) of **39k** in CDCl$_3$.

Figure S42: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **39k** in CDCl$_3$.

NsHN
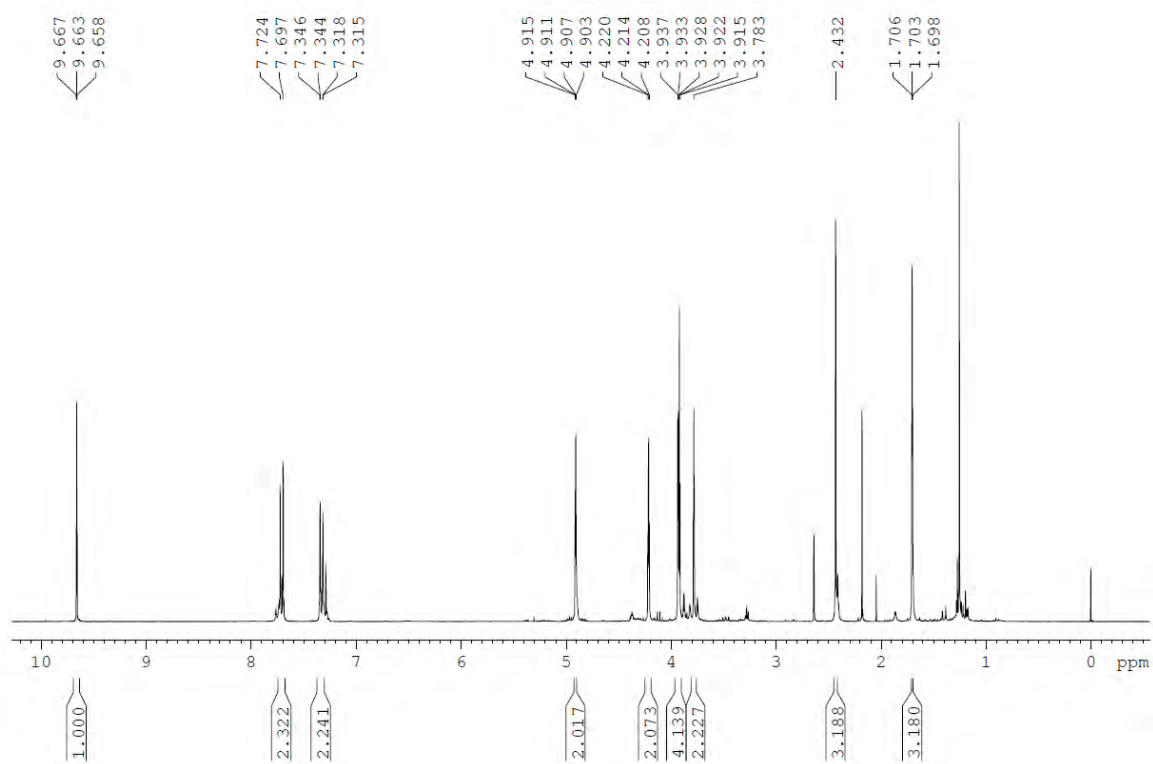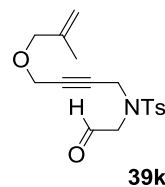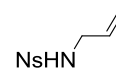
33d

Figure S43: ^{1}H NMR spectrum (300 MHz) of **33d** in CDCl$_3$.
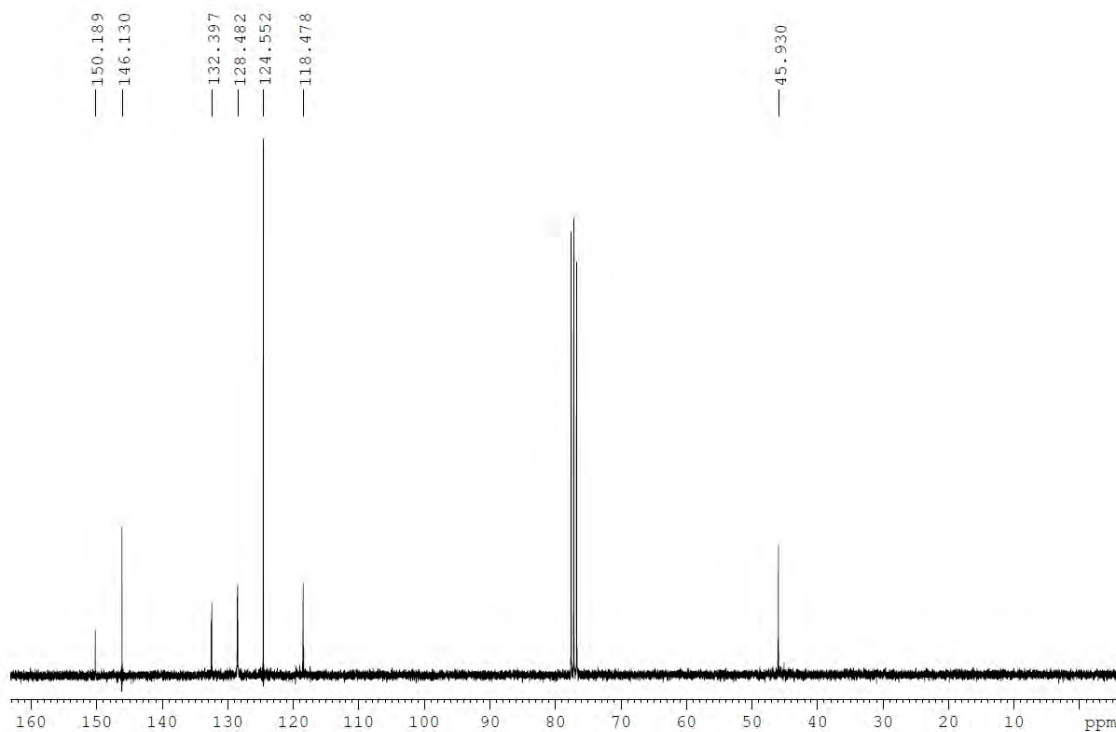
Figure S44: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **33d** in CDCl$_3$.

(2-Ns)HN
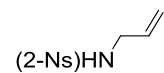
33b

Figure S45: ^{1}H NMR spectrum (300 MHz) of **33b** in CDCl$_3$.
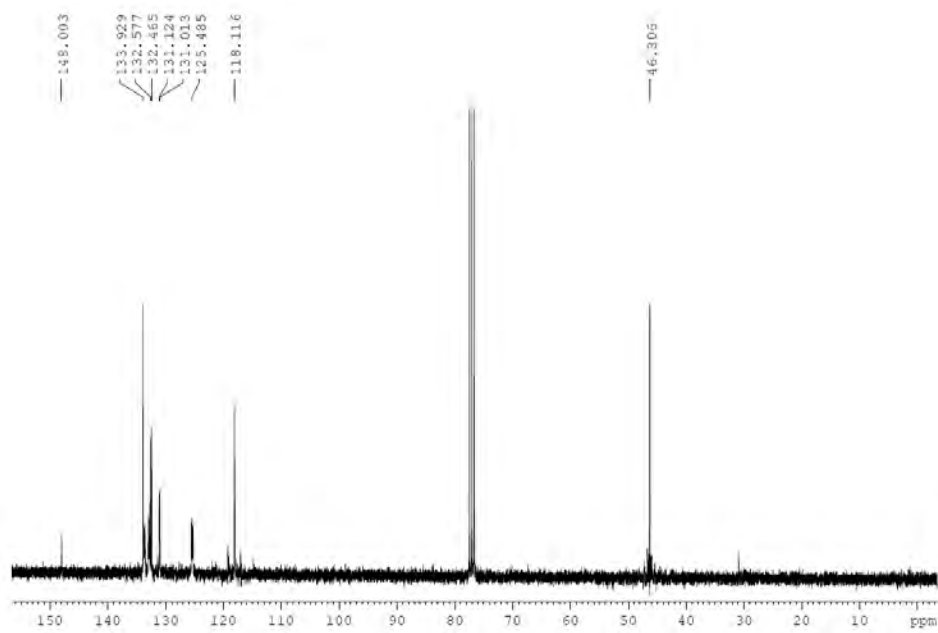
Figure S46: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **33b** in CDCl$_3$.
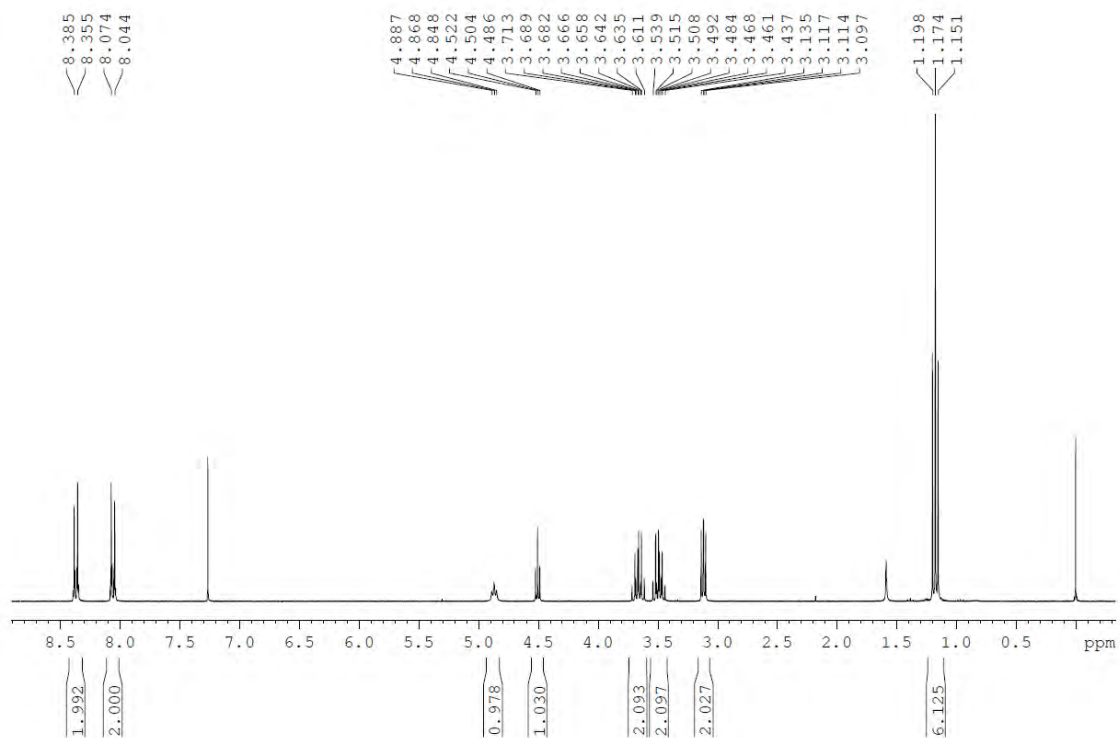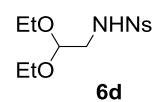
Figure S47: ^{1}H NMR spectrum (300 MHz) of **6d** in CDCl$_3$.
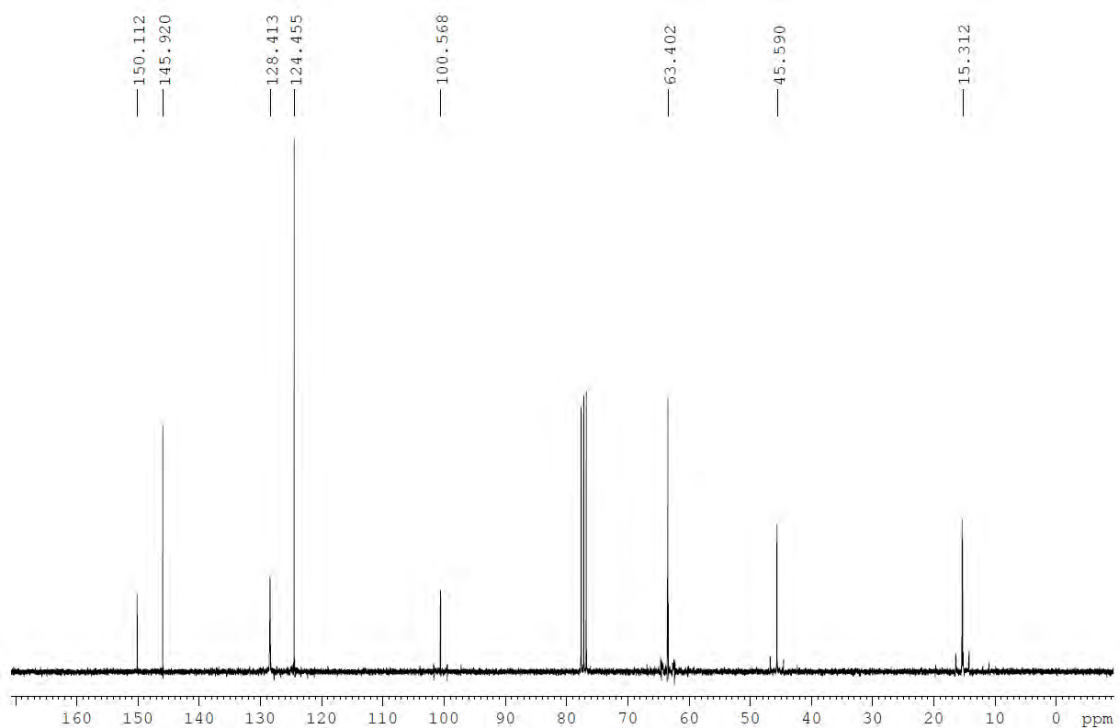
Figure S48: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **6d** in CDCl$_3$.
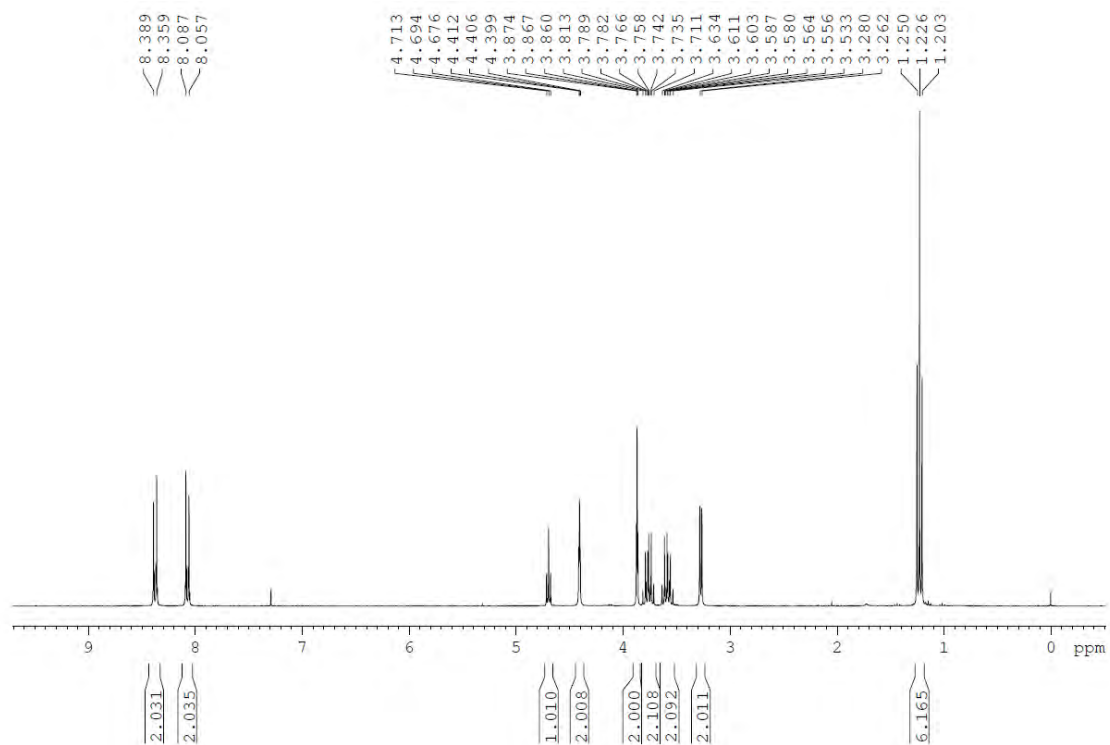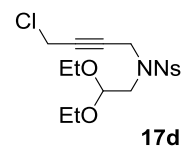
Figure S49: ^{1}H NMR spectrum (300 MHz) of **17d** in CDCl$_3$.
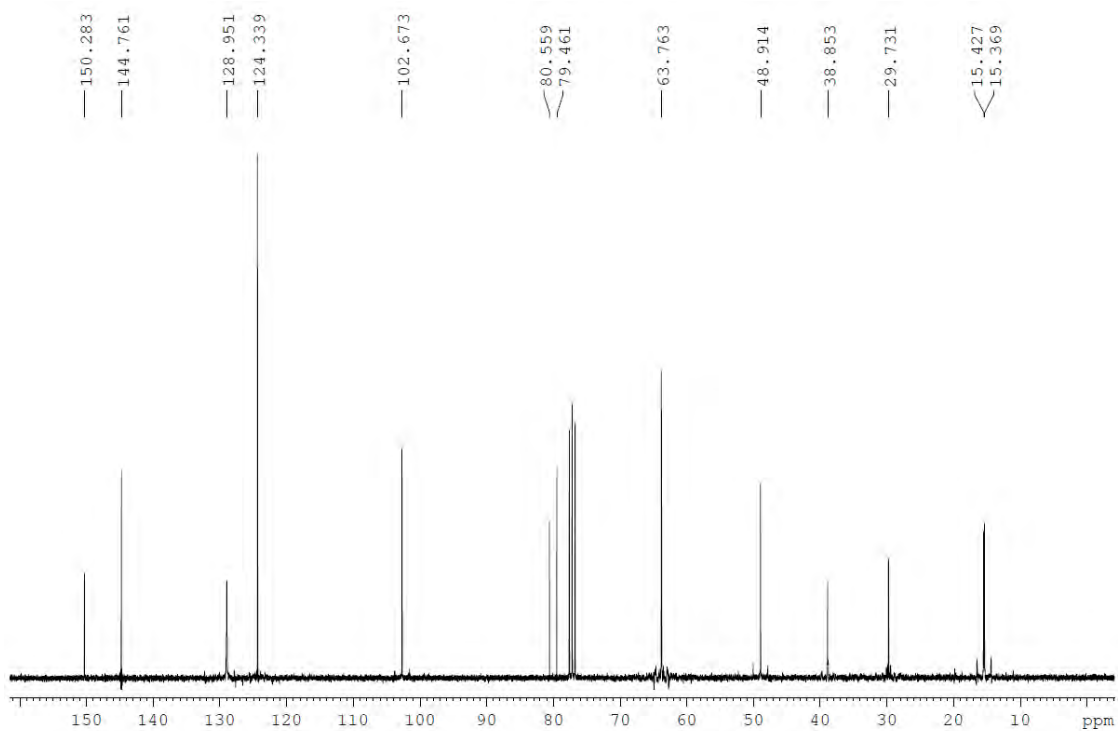
Figure S50: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **17d** in CDCl$_3$.
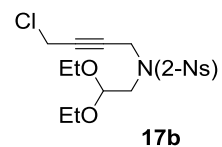
Figure S51: ^{1}H NMR spectrum (300 MHz) of **17b** in CDCl$_3$.
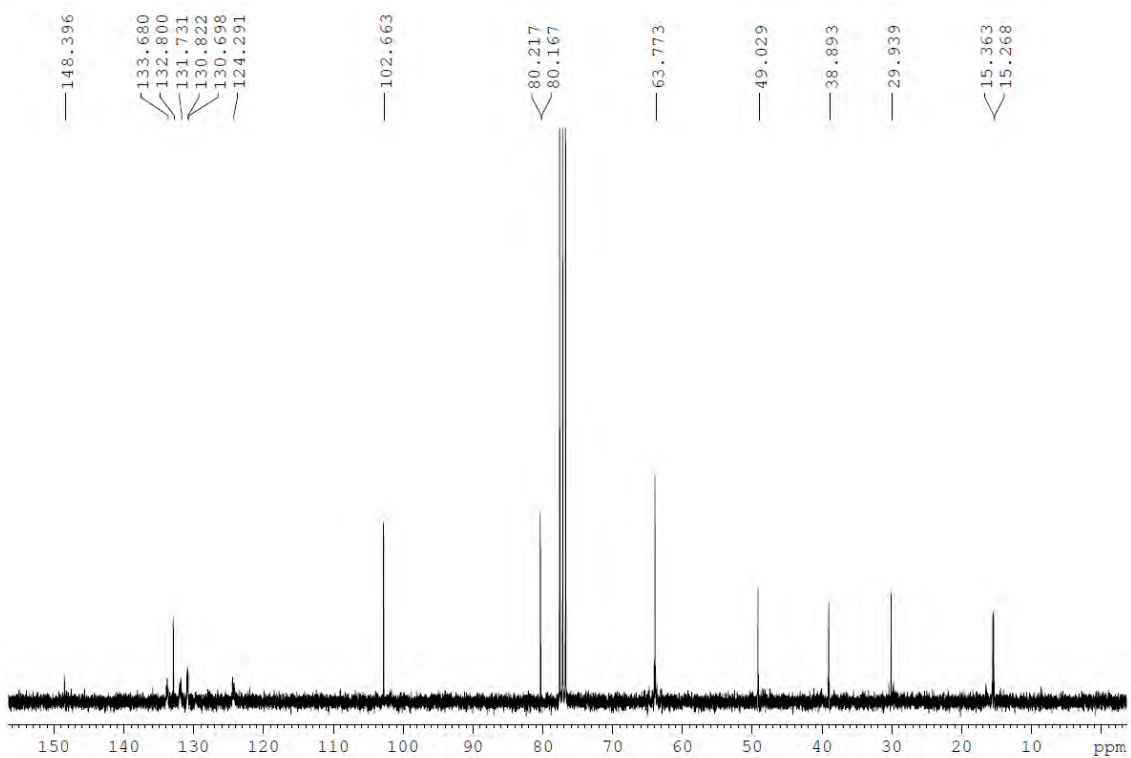
Figure S52: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **17b** in CDCl$_3$.

OTBDMS

EtO   NTs

EtO
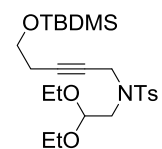
37
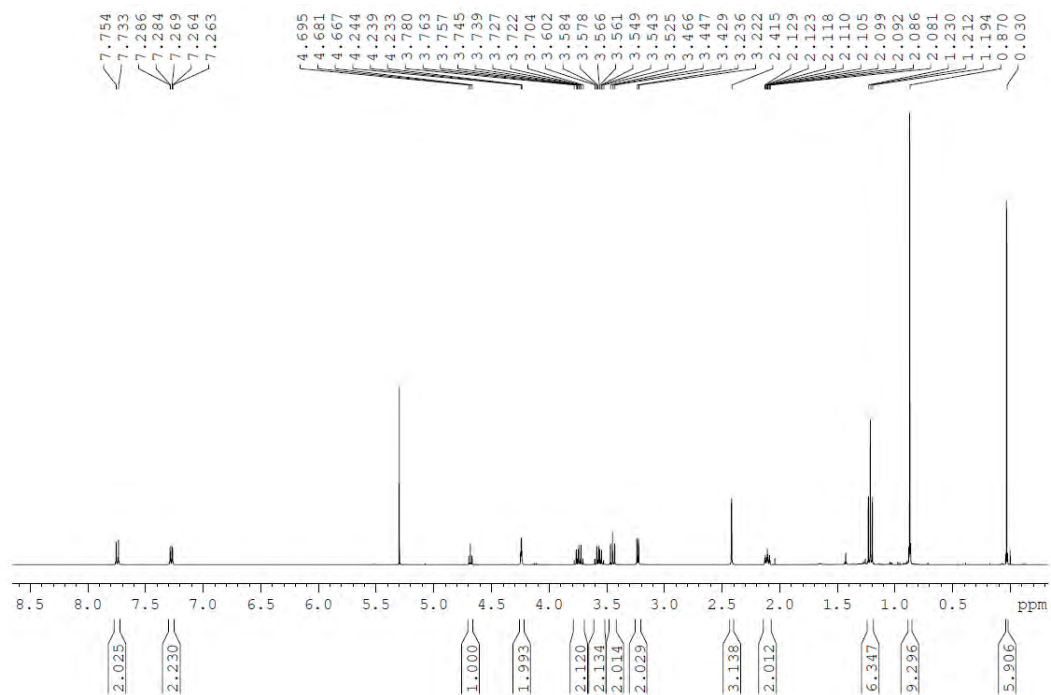
Figure S53: ^{1}H NMR spectrum (400 MHz) of **37** in CDCl$_3$.
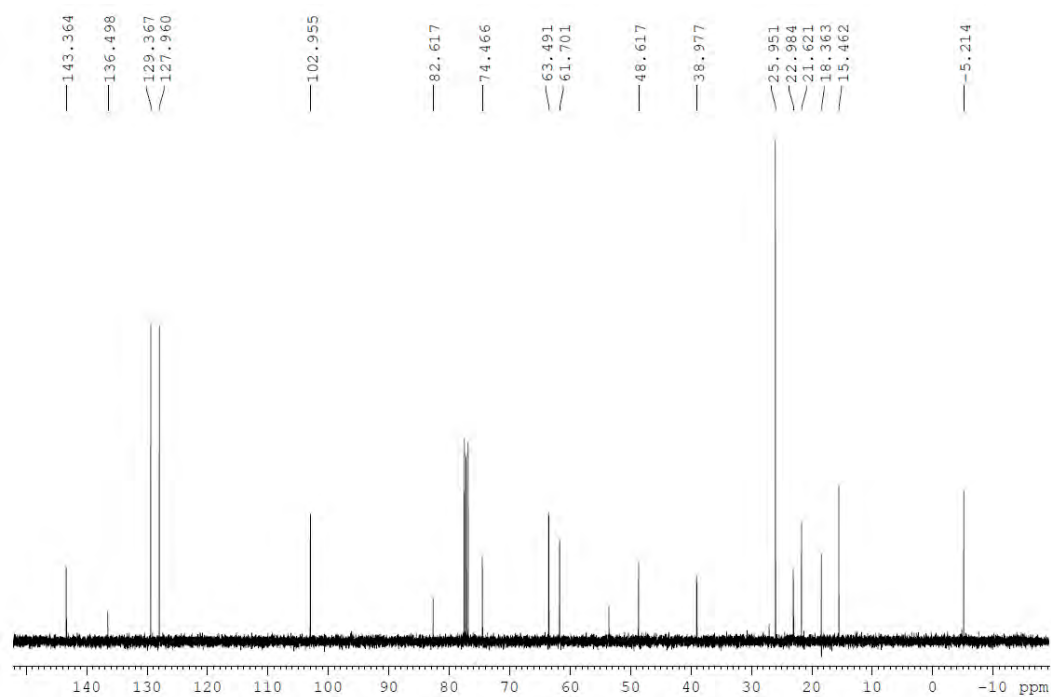
Figure S54: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **37** in CDCl$_3$.
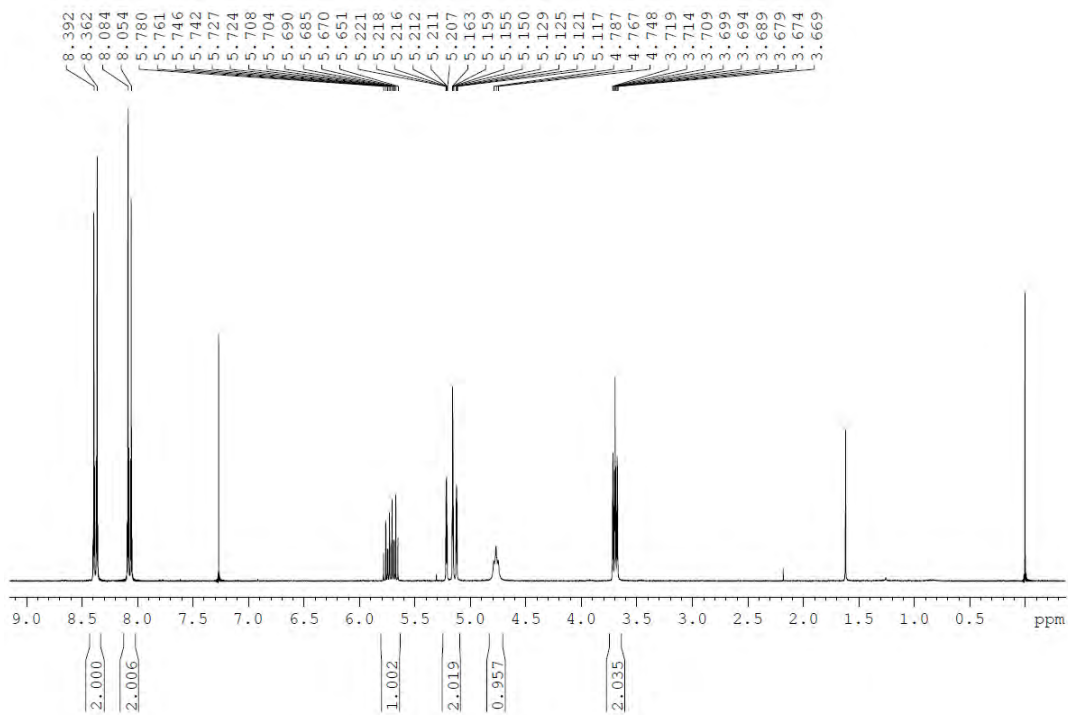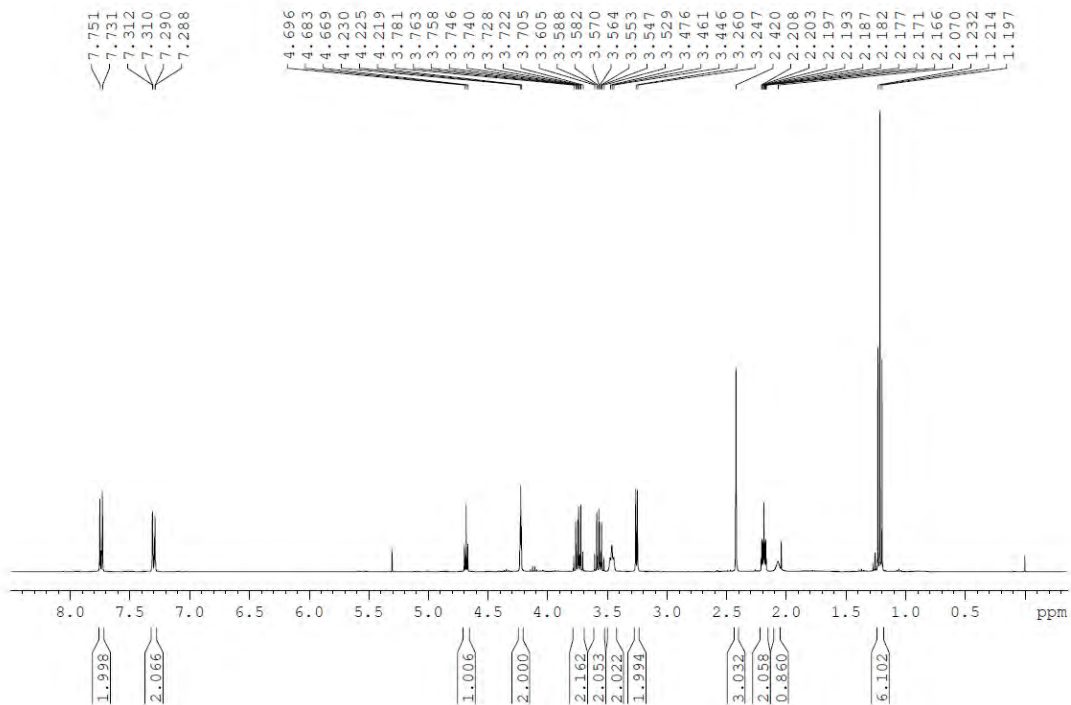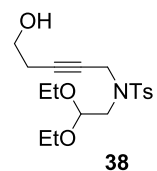
Figure S55: ^{1}H NMR spectrum (400 MHz) of **38** in CDCl$_3$.
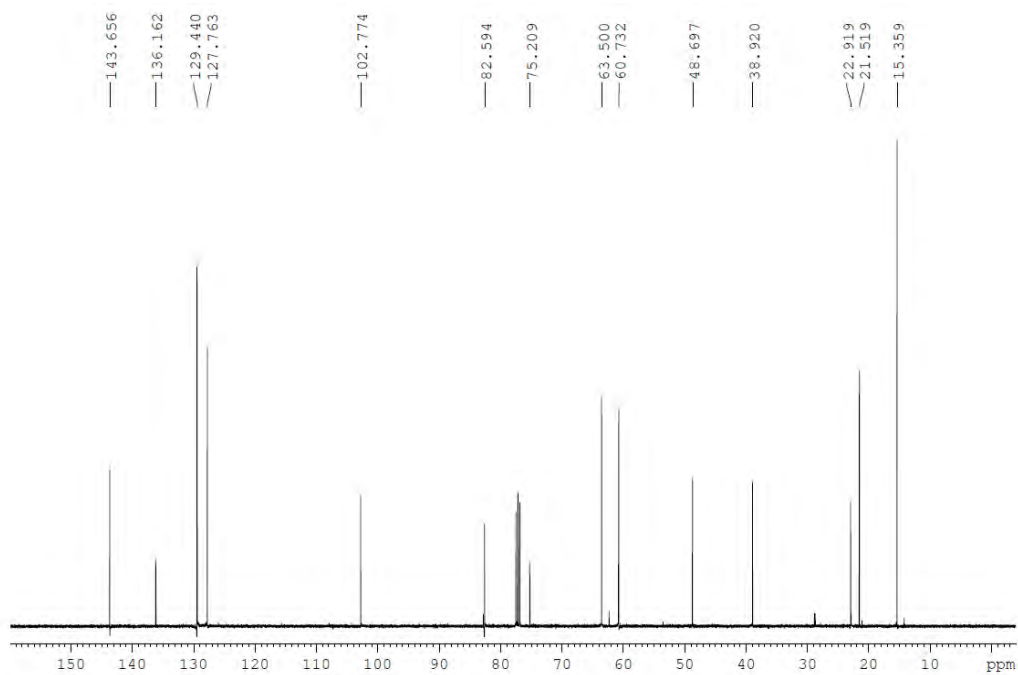
Figure S56: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **38** in CDCl$_3$.
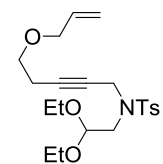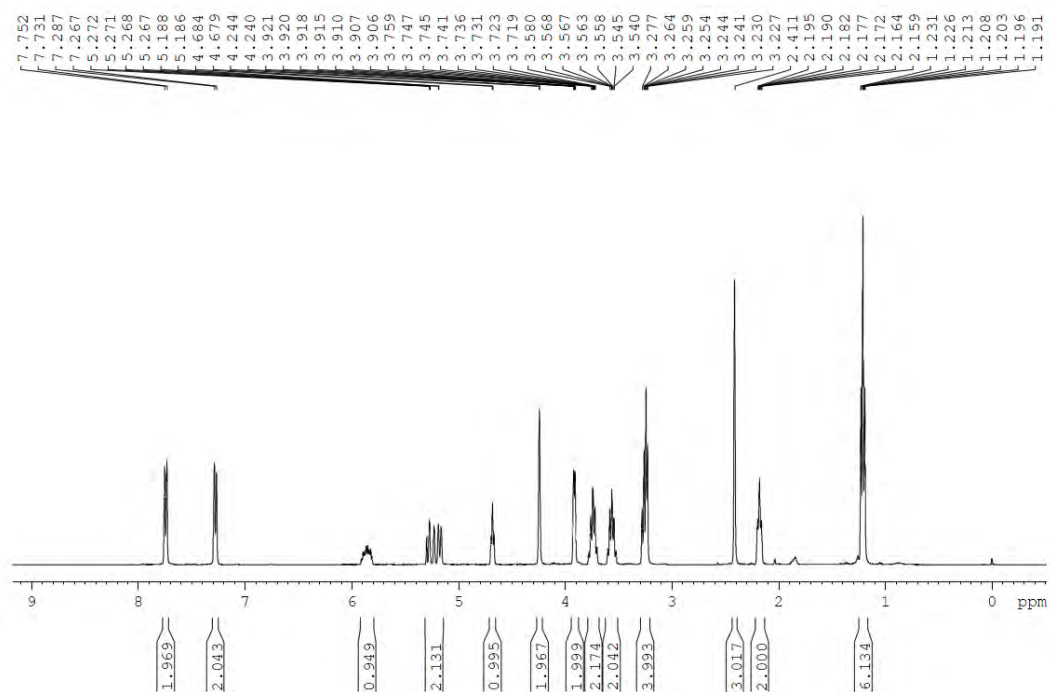
Figure S57: ^{1}H NMR spectrum (400 MHz) of **31h** in CDCl$_3$.
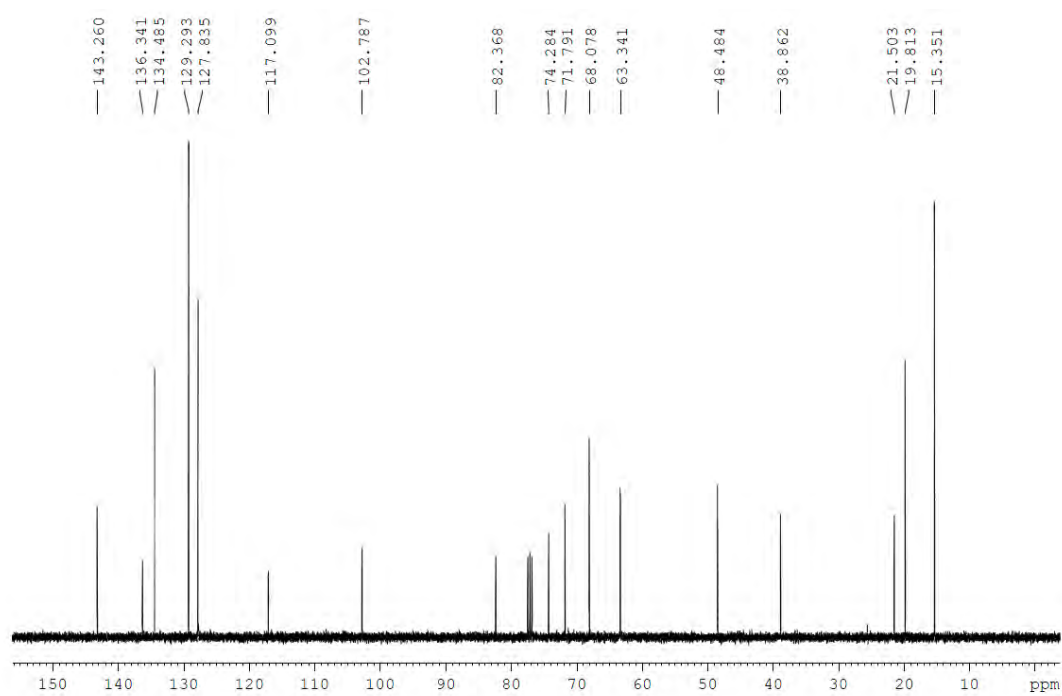
Figure S58: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **31h** in CDCl$_3$.
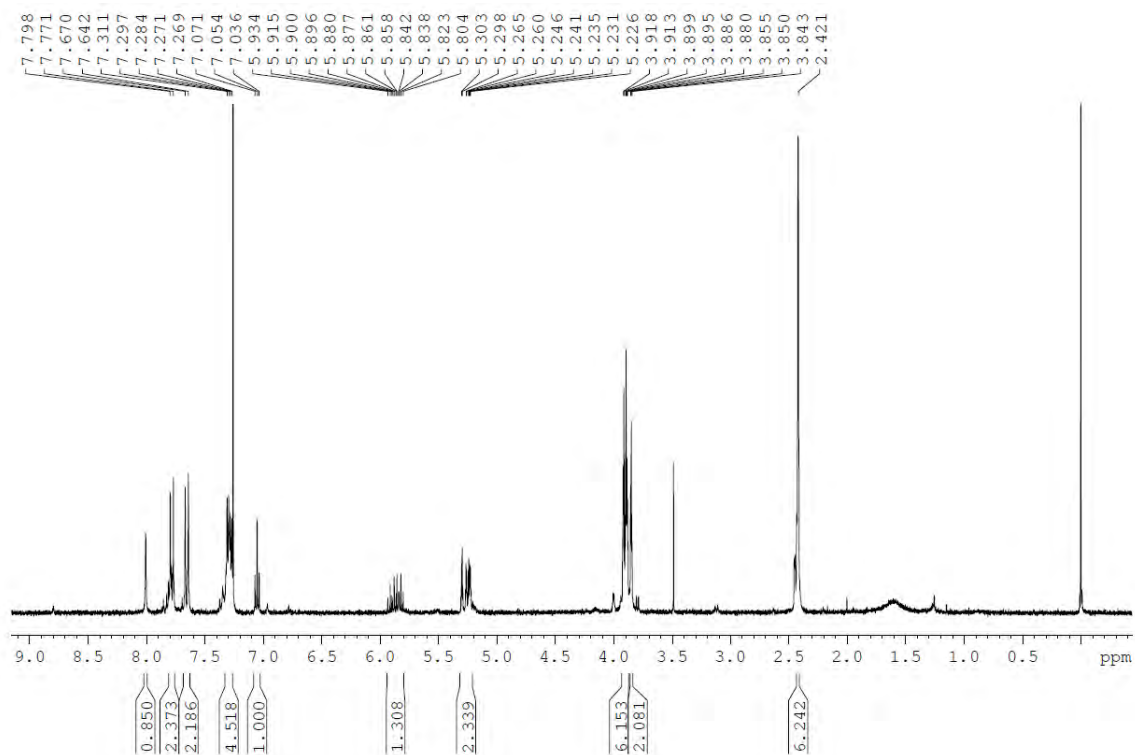
Figure S59: ^{1}H NMR spectrum (400 MHz) of **28a** in CDCl$_3$.
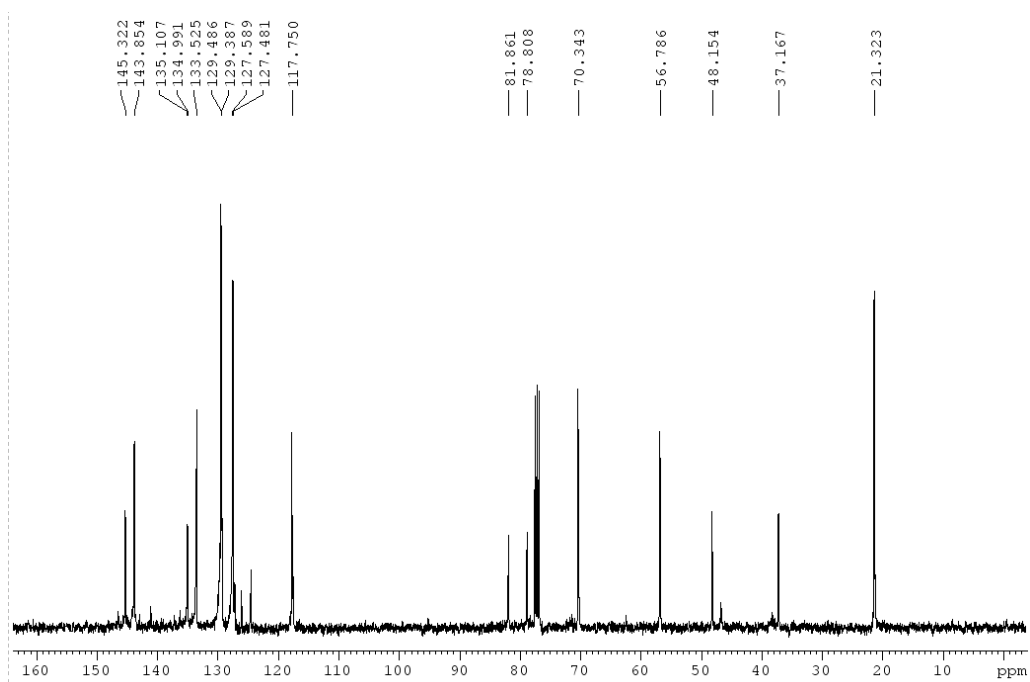
Figure S60: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **28a** in CDCl$_3$.
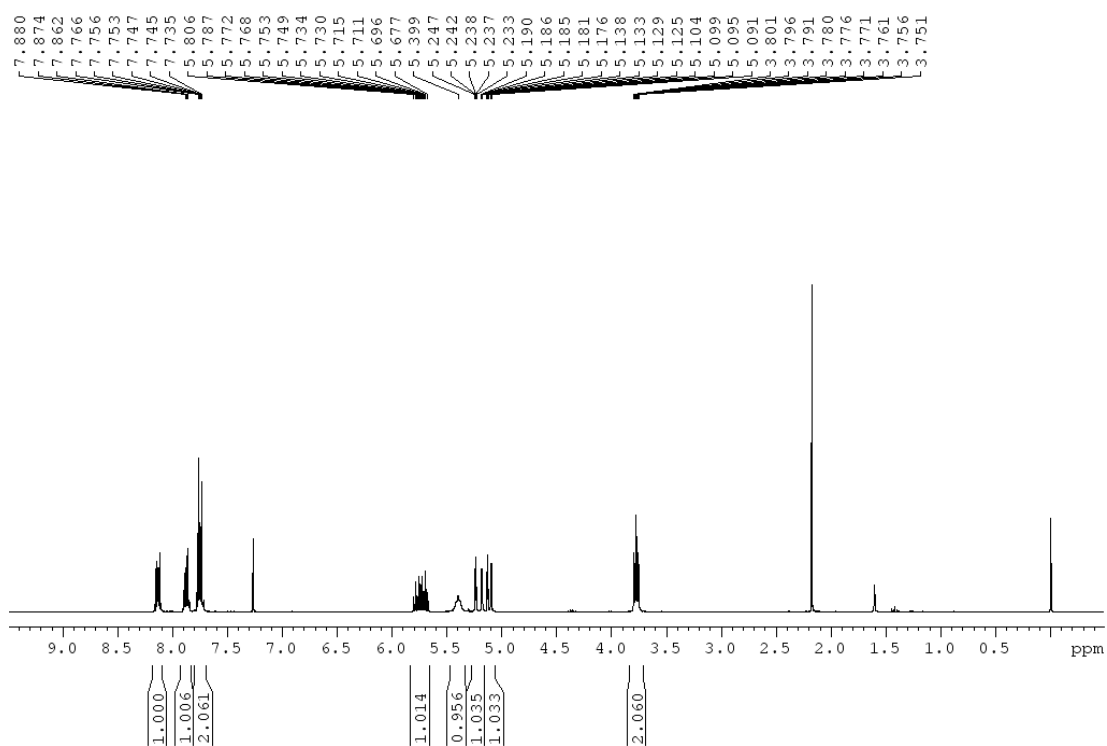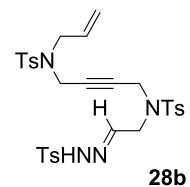
Figure S61: ^{1}H NMR spectrum (400 MHz) of **28b** in CDCl$_3$.
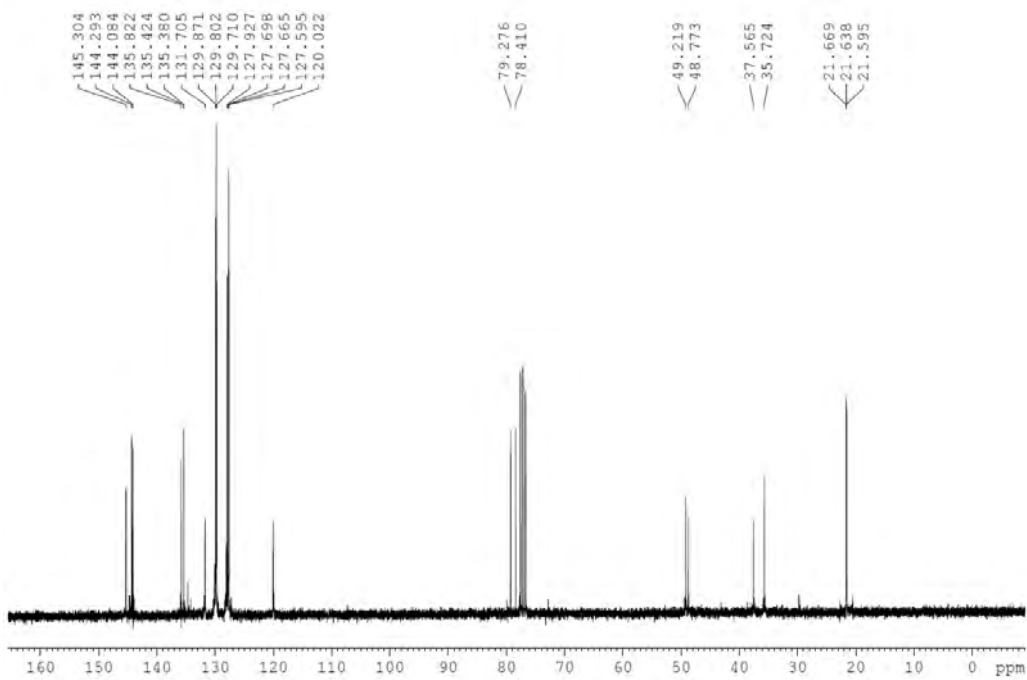
Figure S62: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **28b** in CDCl$_3$.

Figure S63: ^{1}H NMR spectrum (300 MHz) of **28c** in CDCl$_3$.

Figure S64: ^{1}H-decoupled ^{13}C NMR spectrum (75 MHz) of **28c** in CDCl$_3$.
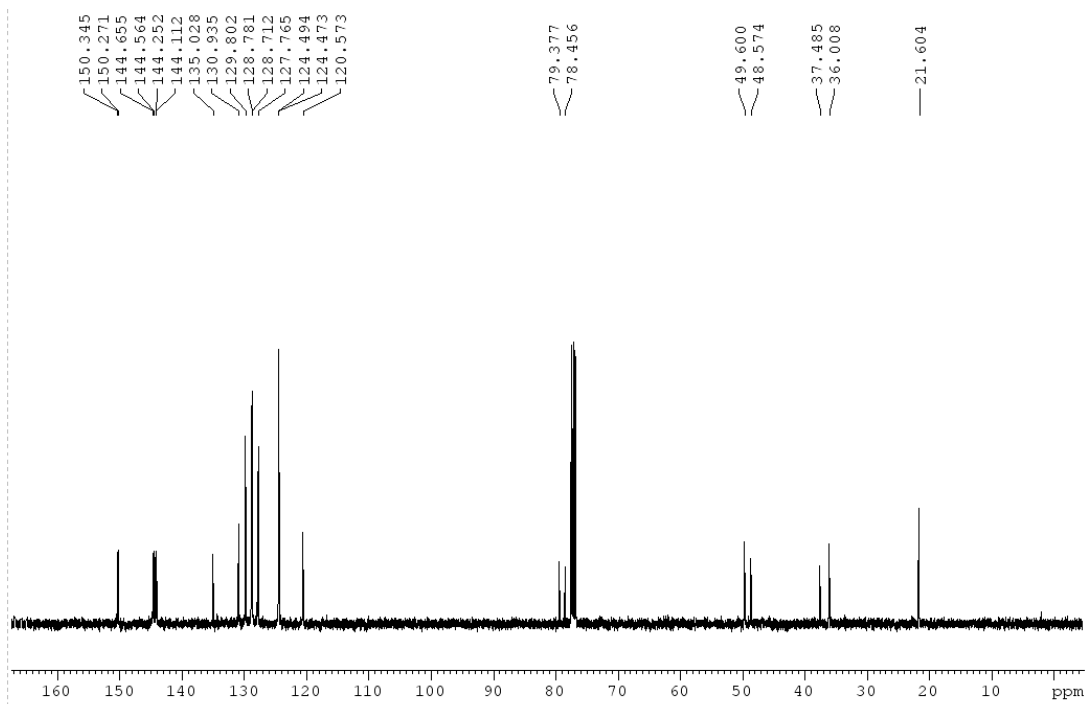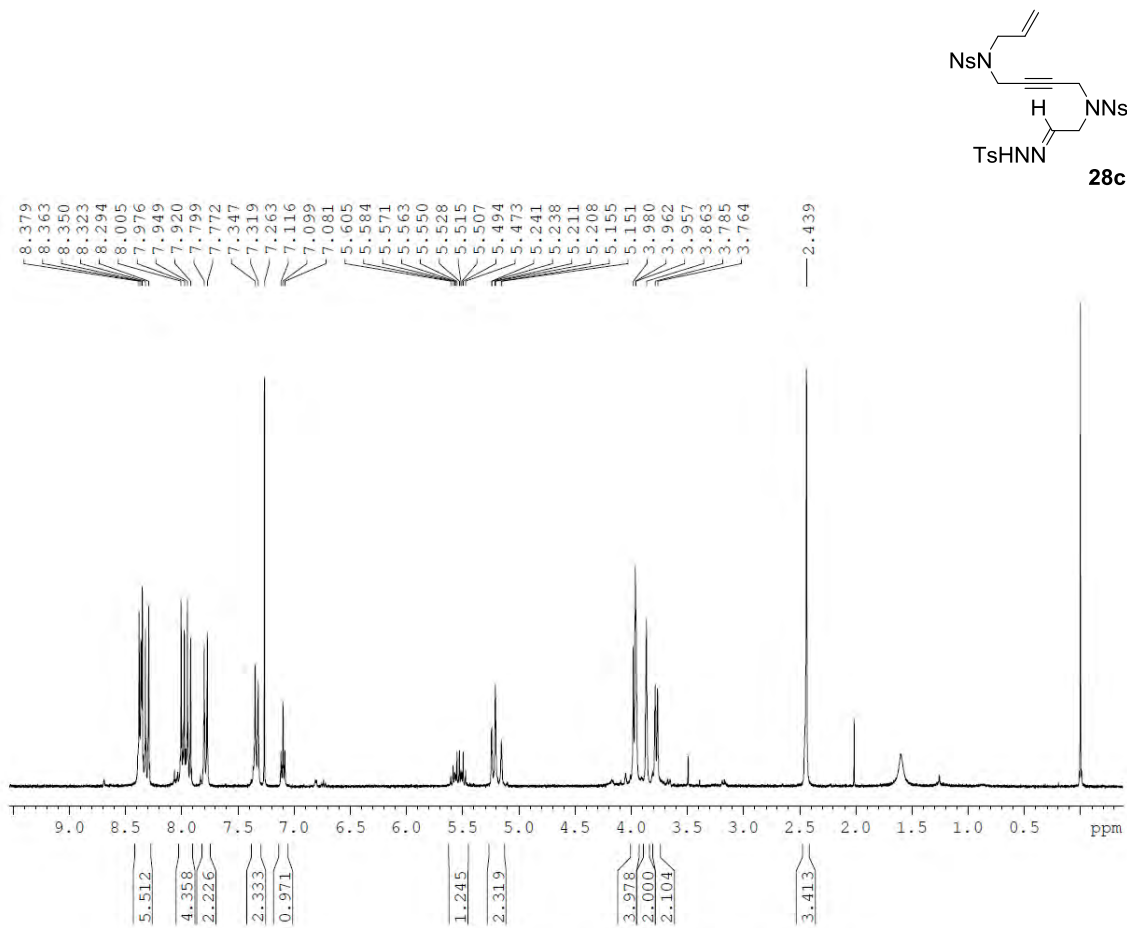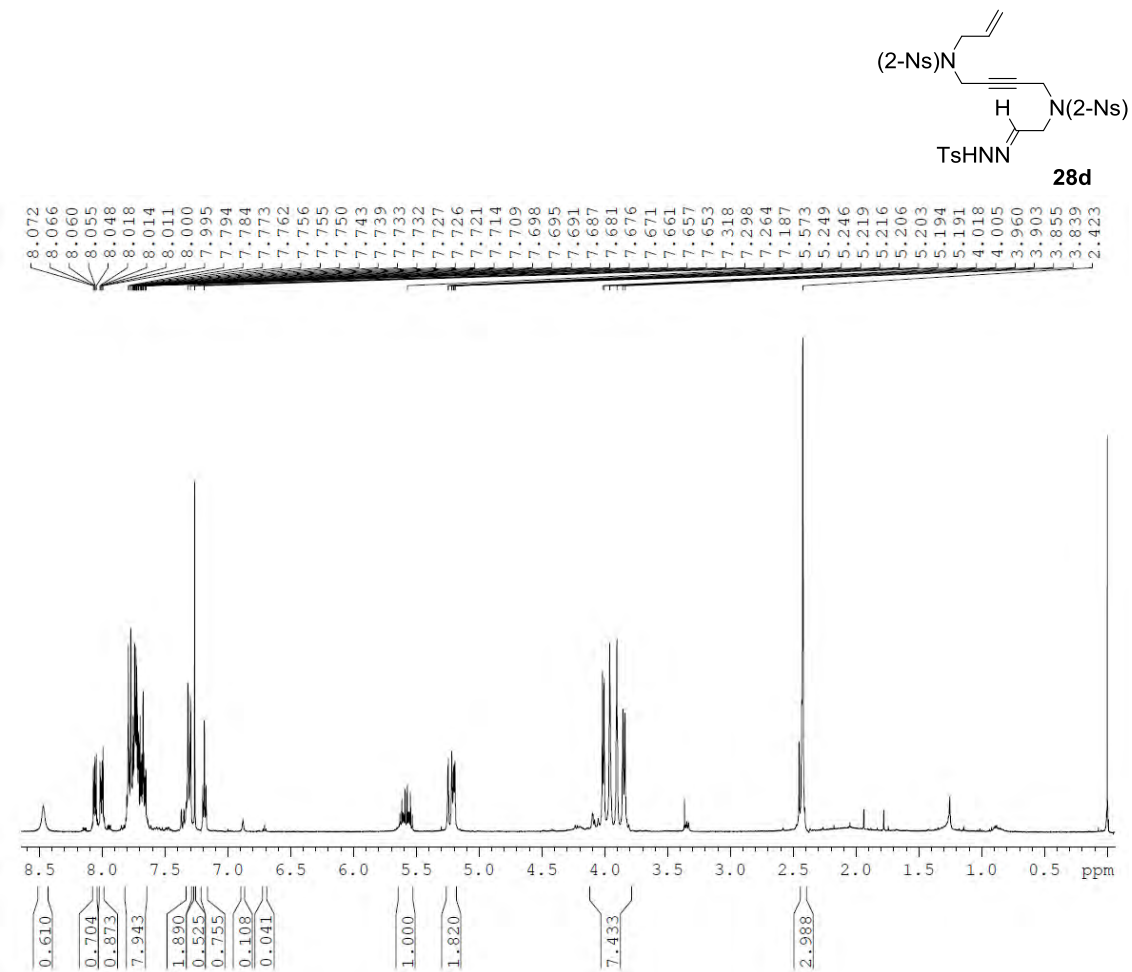
Figure S65: ^{1}H NMR spectrum (400 MHz) of **28d** in CDCl$_3$.
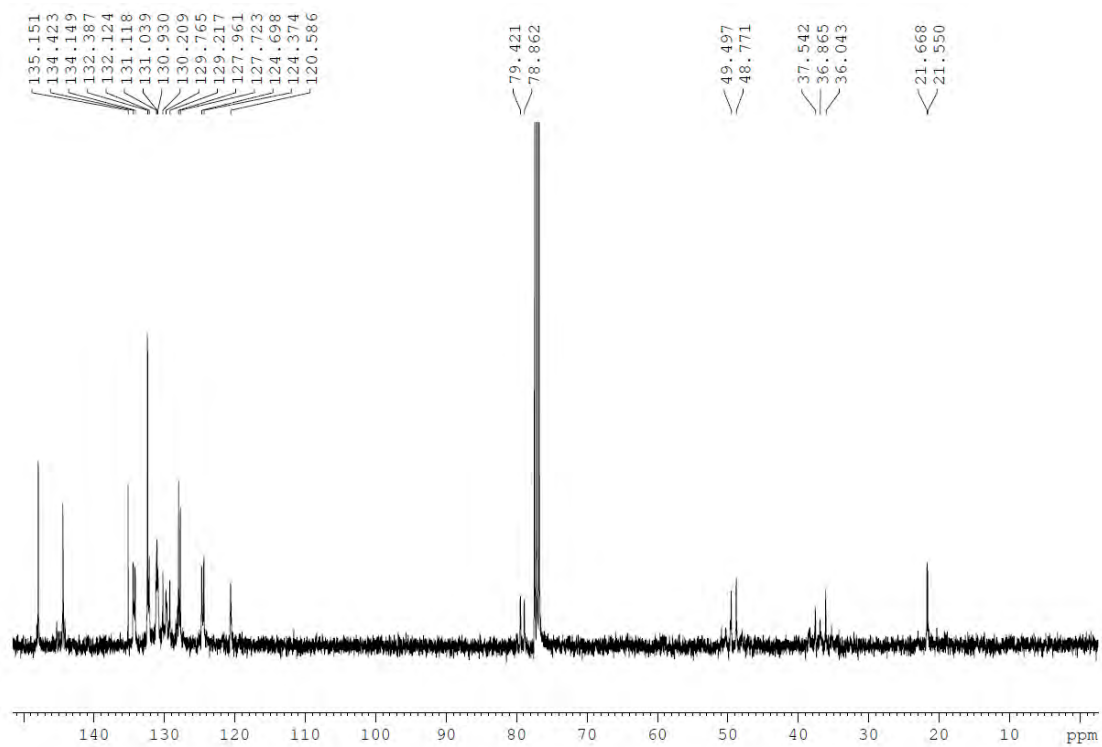
Figure S66: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **28d** in CDCl$_3$.
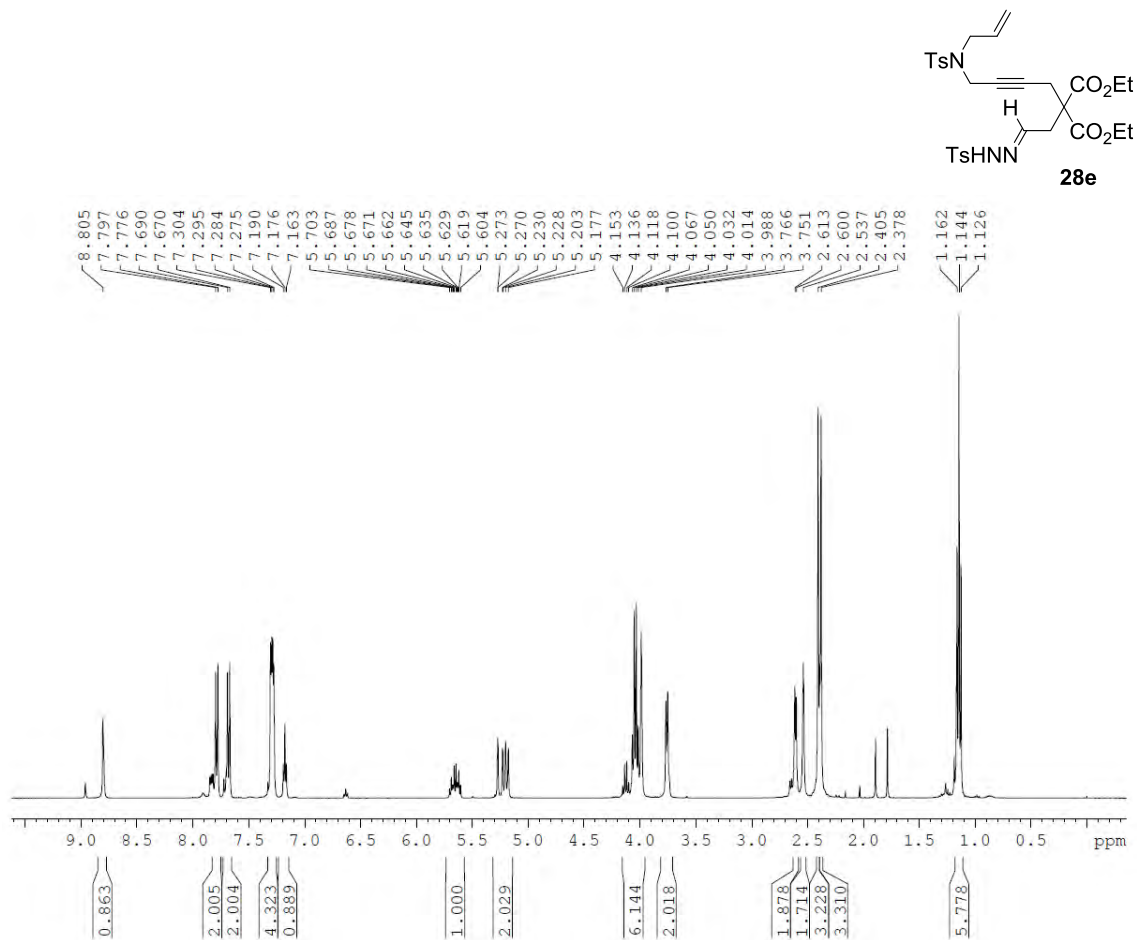
Figure S67: ^{1}H NMR spectrum (400 MHz) of **28e** in CDCl$_3$.
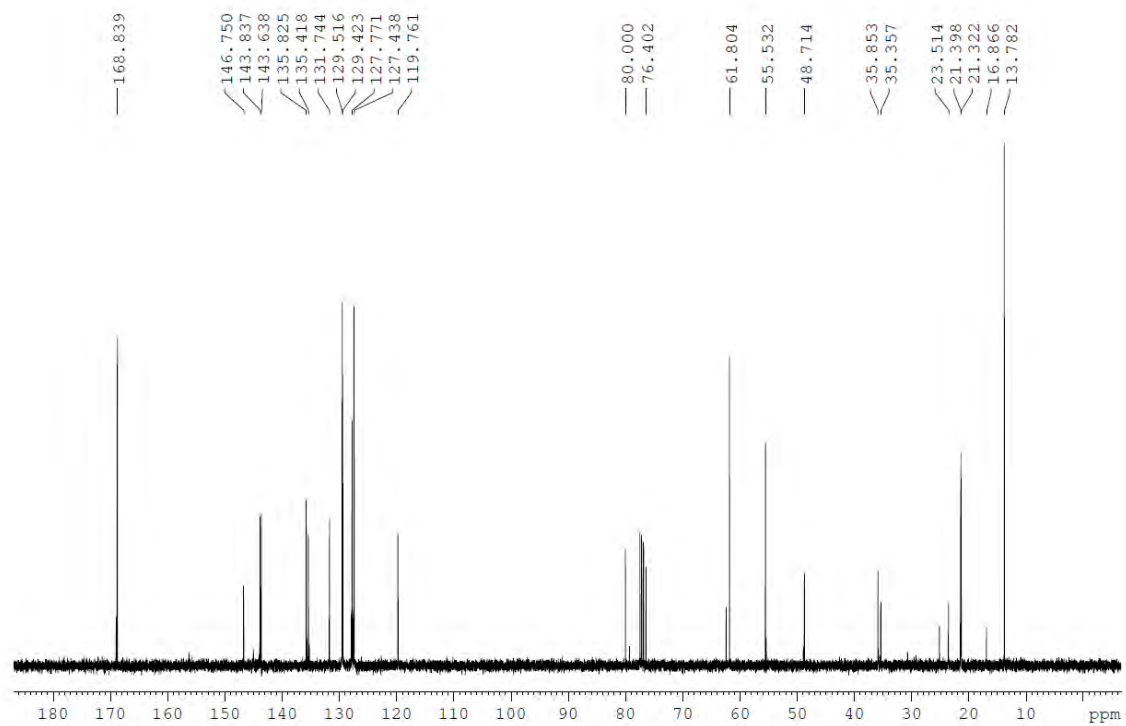
Figure S68: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **28e** in CDCl$_3$.
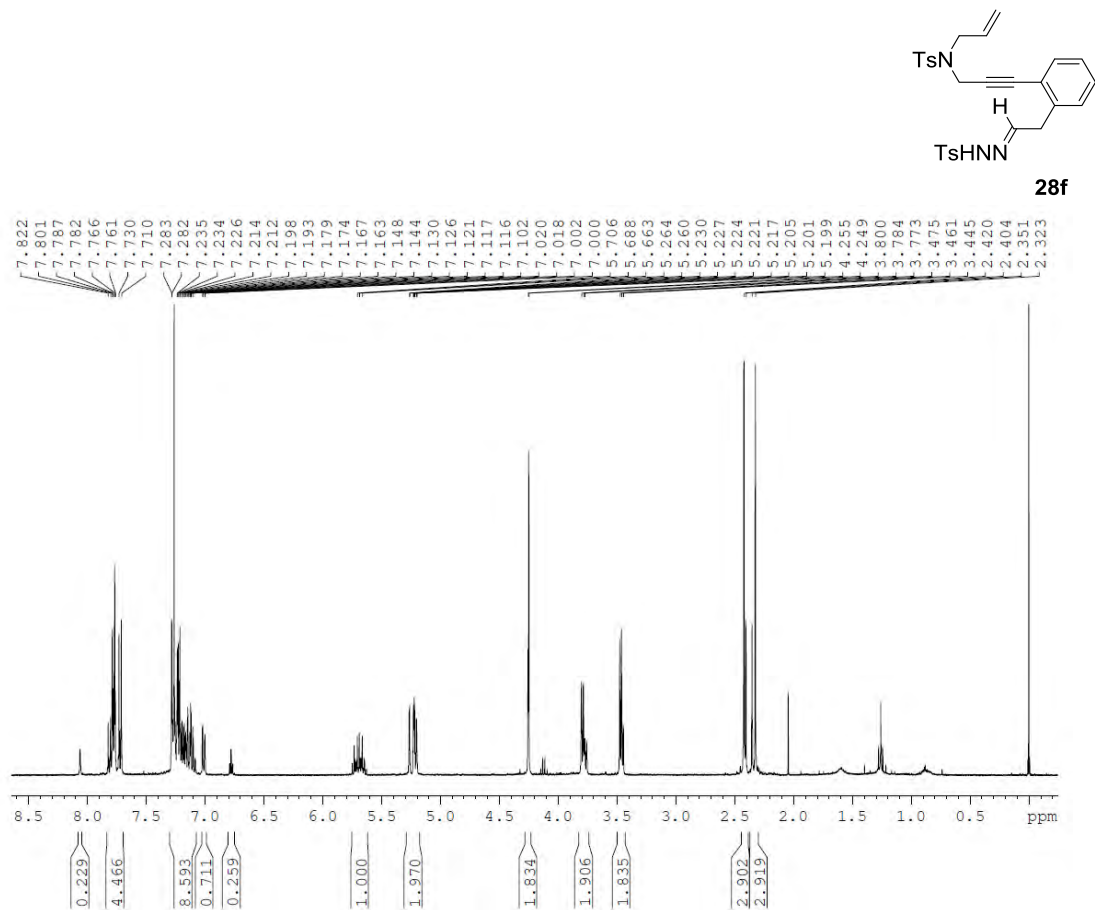
Figure S69: ^{1}H NMR spectrum (400 MHz) of **28f** in CDCl$_3$.
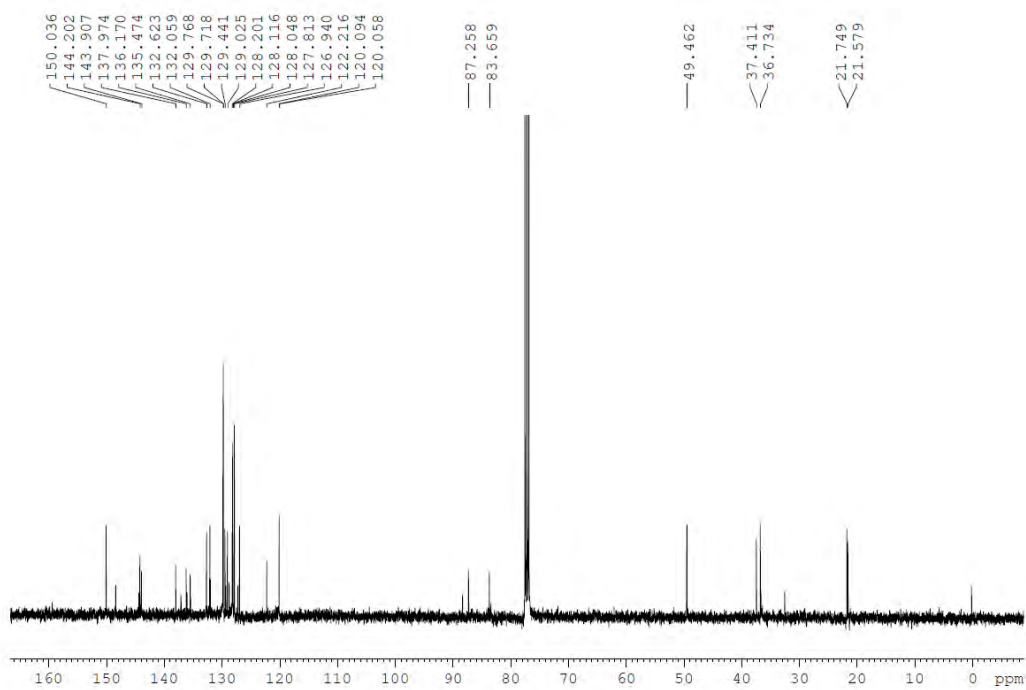
Figure S70: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **28f** in CDCl$_3$.
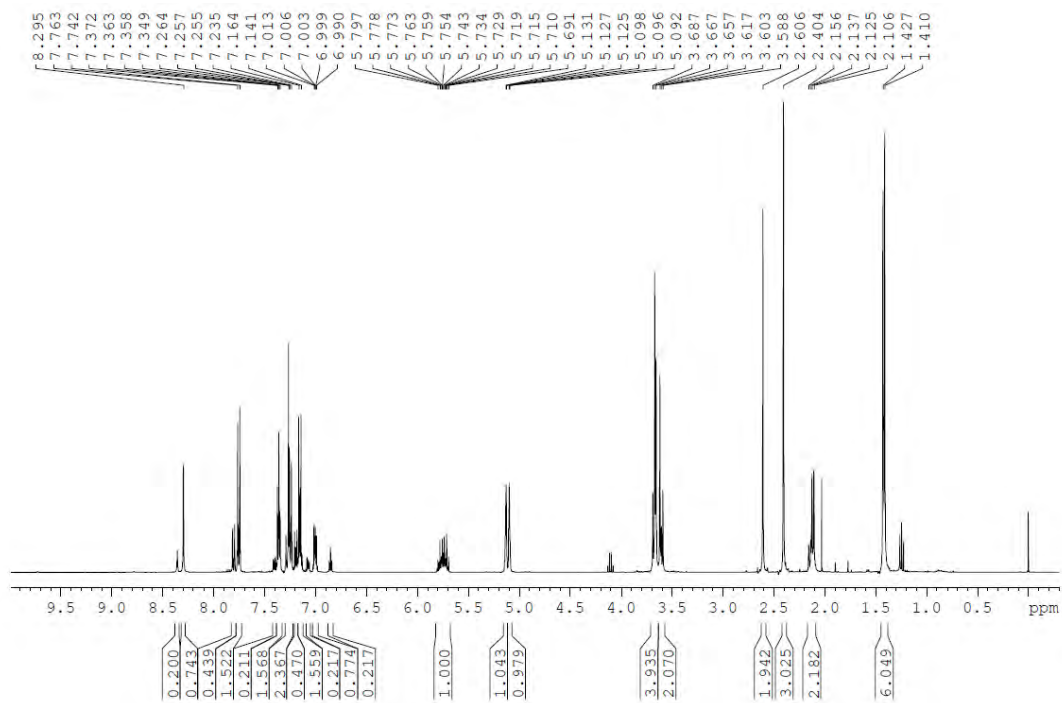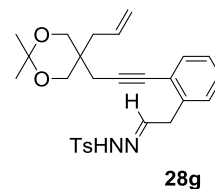
Figure S71: ^{1}H NMR spectrum (400 MHz) of **28g** in CDCl$_3$.
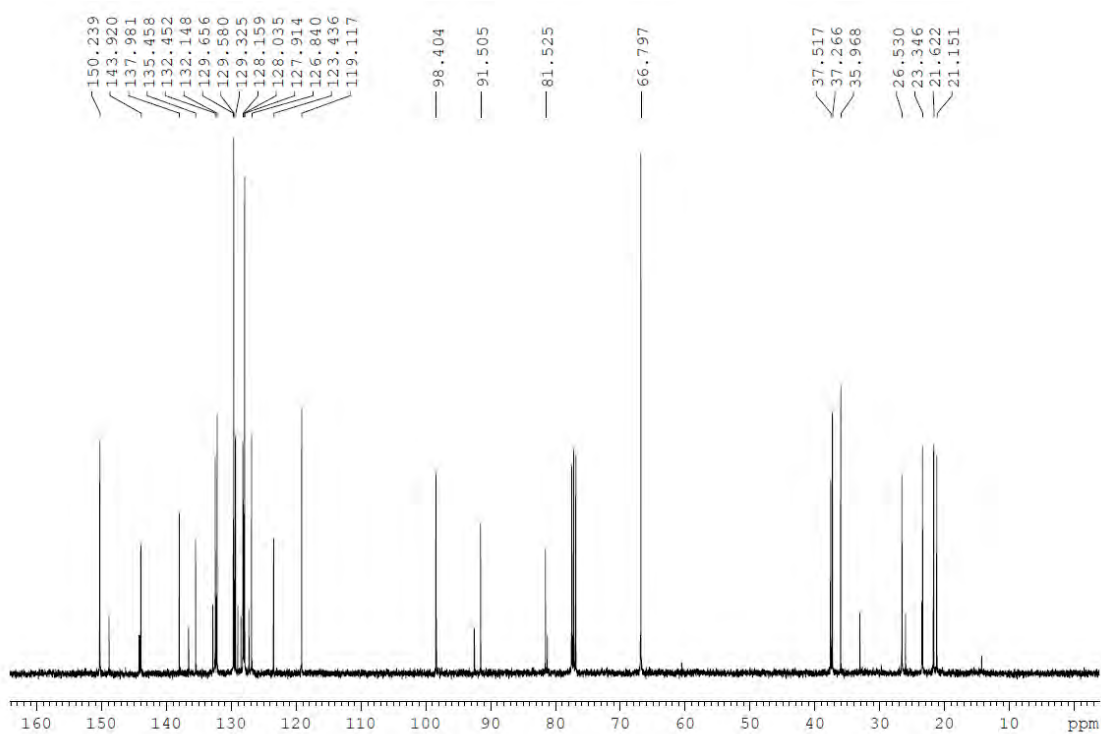
Figure S72: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **28g** in CDCl$_3$
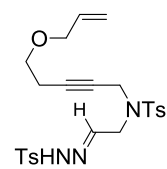
Figure S73: ^{1}H NMR spectrum (400 MHz) of **28h** in CDCl$_3$.
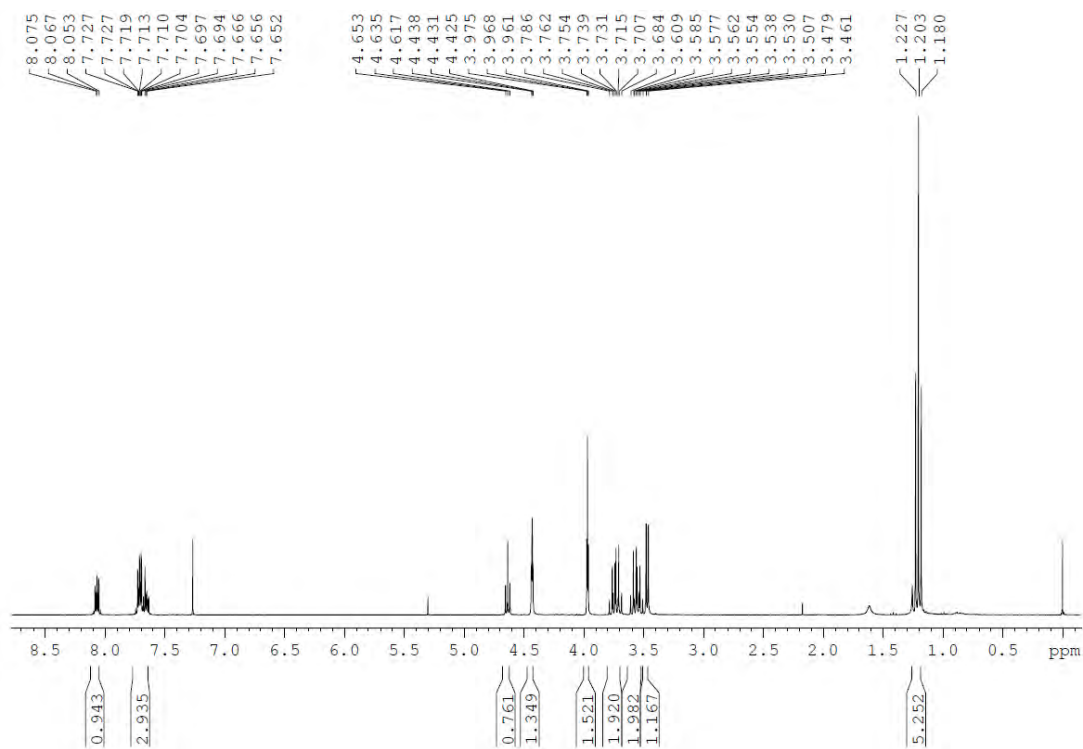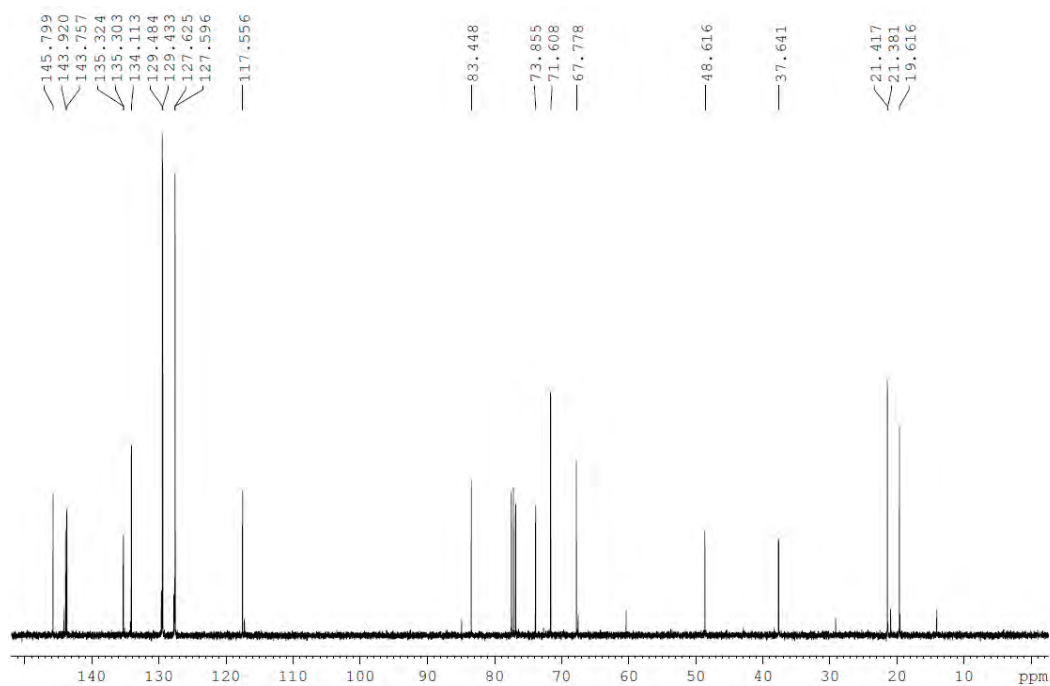

Figure S74: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **28h** in CDCl$_3$

Figure S75: ^{1}H NMR spectrum (400 MHz) of **28i** in CDCl$_3$.
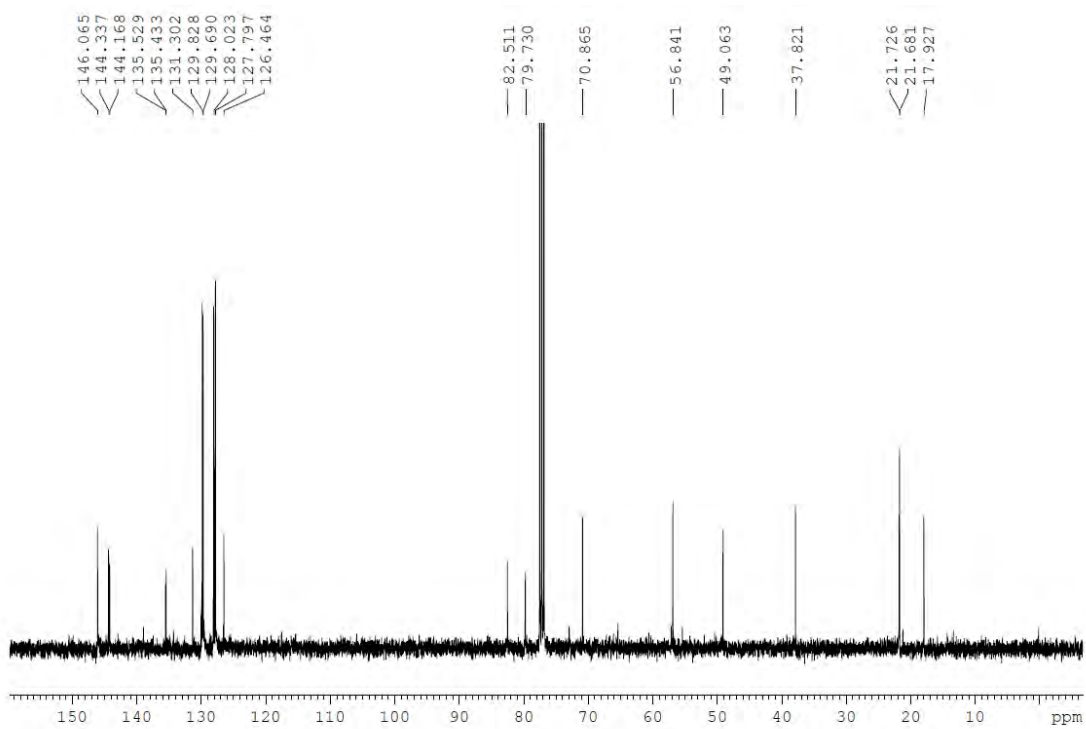
Figure S76: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **28i** in CDCl$_3$.

Figure S77: [1]H NMR spectrum (400 MHz) of **28k** in CDCl$_3$.
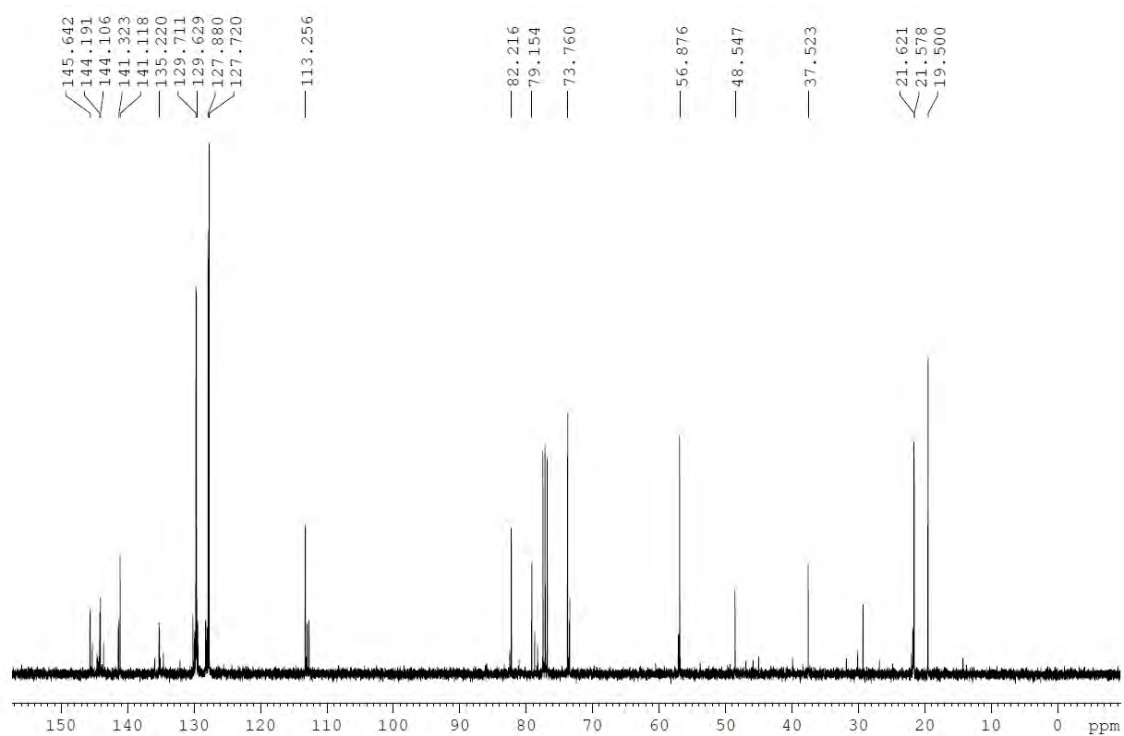
Figure S78: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **28k** in CDCl$_3$.
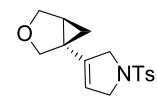
Figure S79: ^{1}H NMR spectrum (300 MHz) of **48a** in CDCl$_3$.
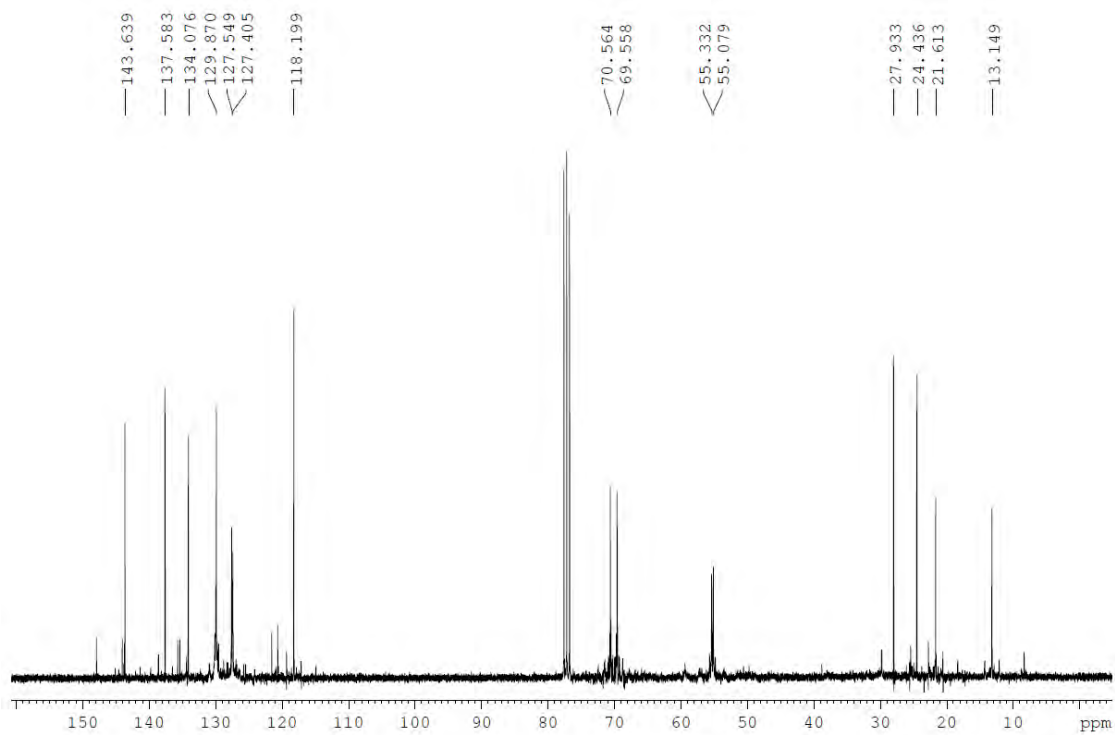
Figure S80: ^{1}H-decoupled^{13}C NMR spectrum (75 MHz) of **48a** in CDCl$_3$.

DAD1 F, Sig=220,16 Ref=360,100 (OSCAR\OT443RACB_9901.D)
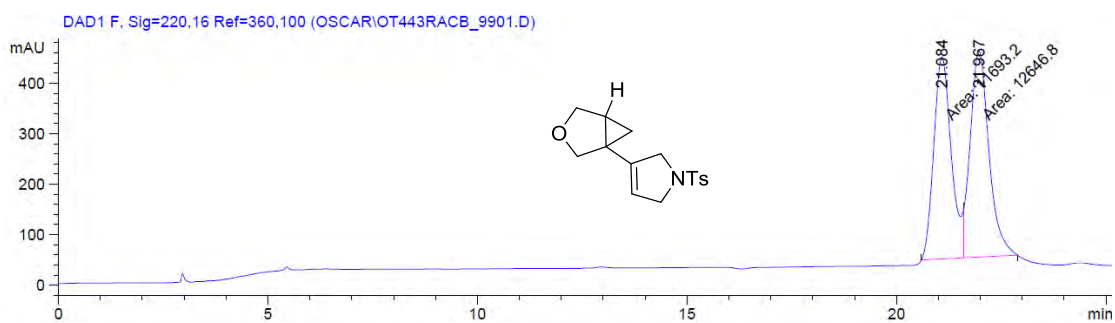
Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	21.084	1	MF	1.16932e4	399.54666	48.0410
2	21.967	1	FM	1.26468e4	408.73270	51.9590

DAD1 F, Sig=220,16 Ref=360,100 (OSCAR\OT443SB_9901.D)
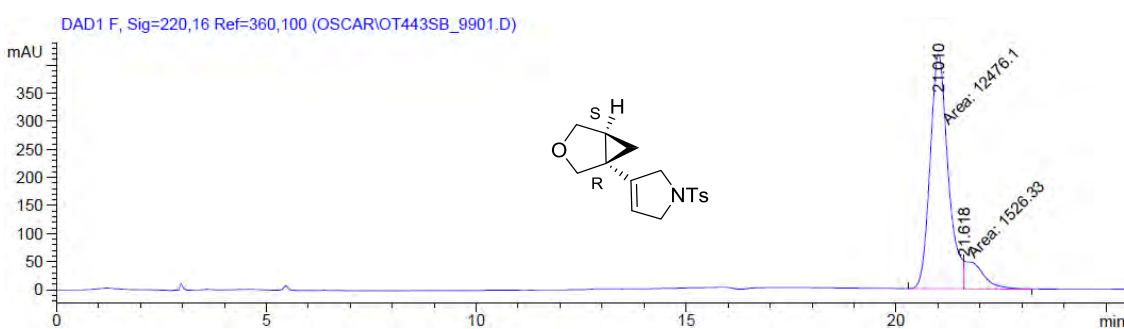
Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	21.010	1	MF	1.24761e4	417.57892	89.0996
2	21.618	1	FM	1526.33105	49.76136	10.9004

DAD1 F, Sig=220,16 Ref=360,100 (OSCAR\OT443RB_9901.D)
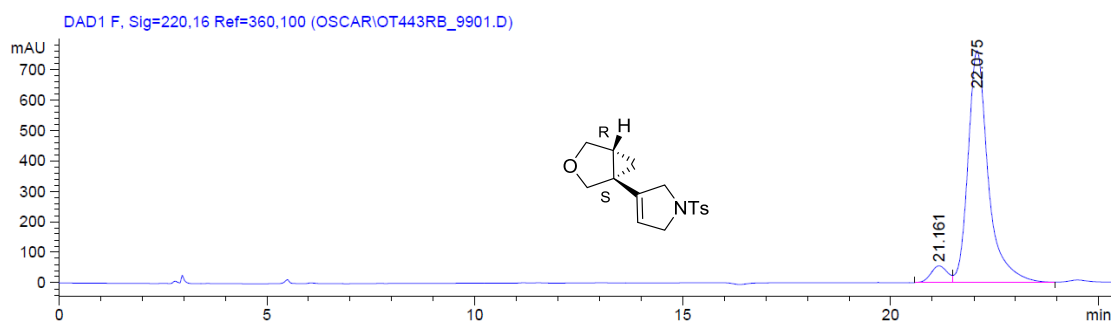
Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	21.161	1	BV	1497.24731	54.77953	5.5005
2	22.075	1	VV	2.57228e4	760.16022	94.4995

Figure S81: HPLC chromatograms with *rac*-BINAP, *(R)-(+)*-BINAP, and *(S)-(-)*-BINAP for **48a**.
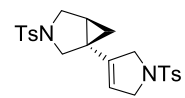
Figure S82: ^{1}H NMR spectrum (400 MHz) of **48b** in CDCl$_3$.
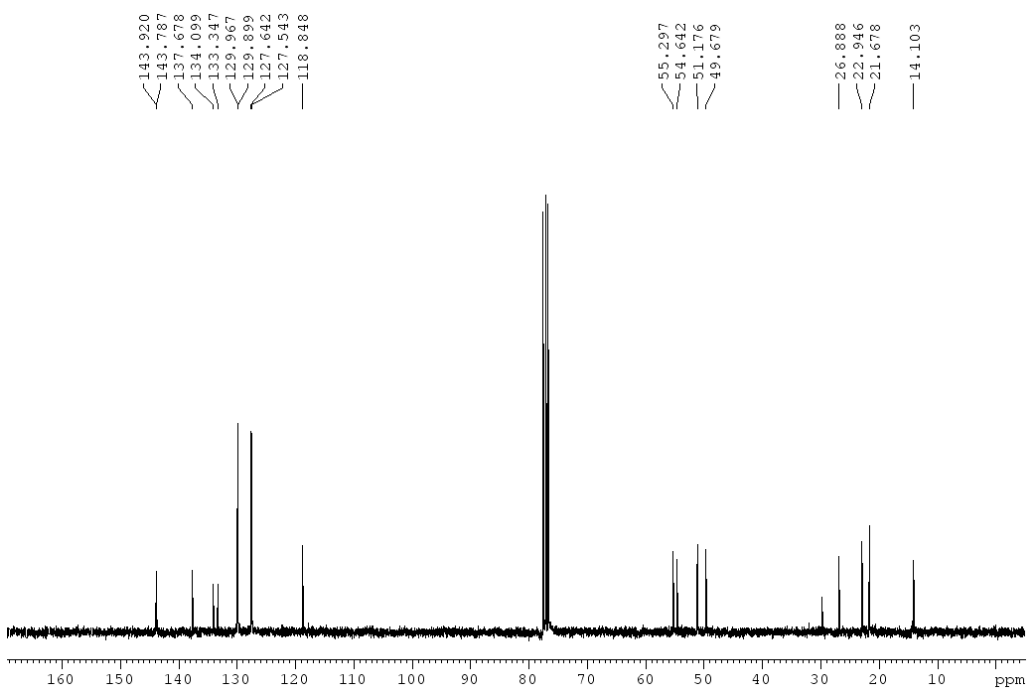
Figure S83: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **48b** in CDCl$_3$.

#	Time	Area	Height	Width	Area%	Symmetry
1	35.198	1614.7	18.1	1.4275	48.529	0.971
2	40.654	1712.6	17.6	1.5703	51.471	1.15

#	Time	Area	Height	Width	Area%	Symmetry
1	34.54	713.8	6.4	1.4551	11.982	0.641
2	40.014	5243.4	39.3	1.8544	88.018	0.737

Figure S84: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **48b**.
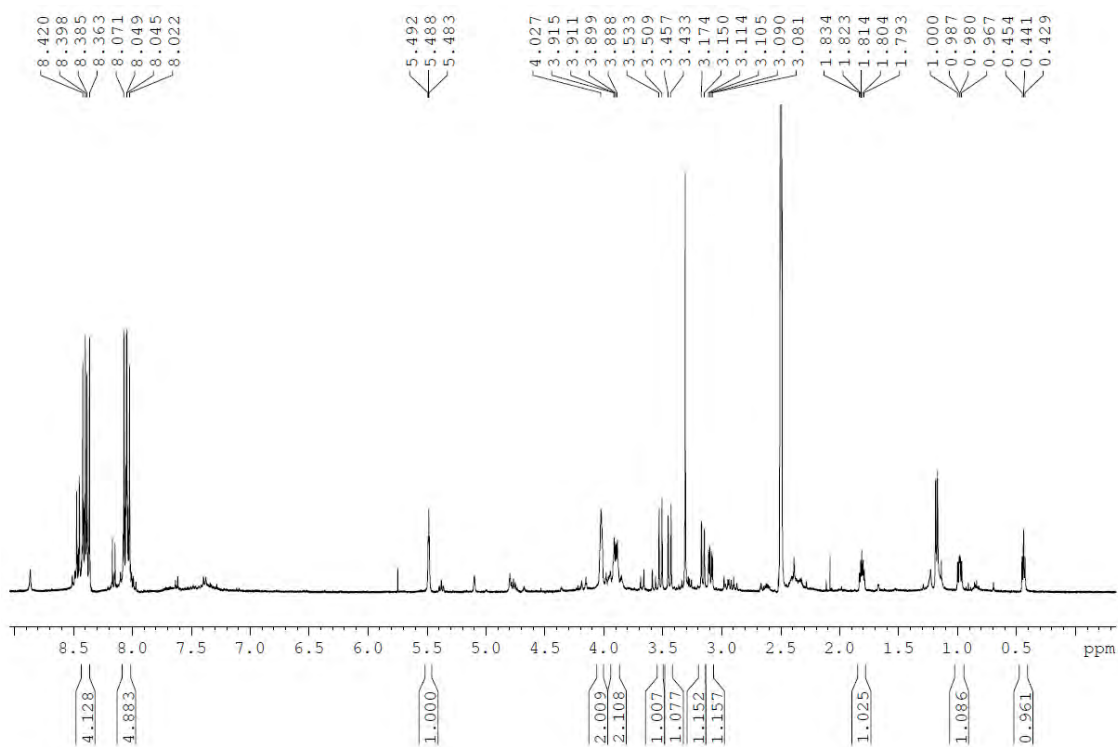
Figure S85: [1]H NMR spectrum (400 MHz) of **48c** in DMSO-d6.
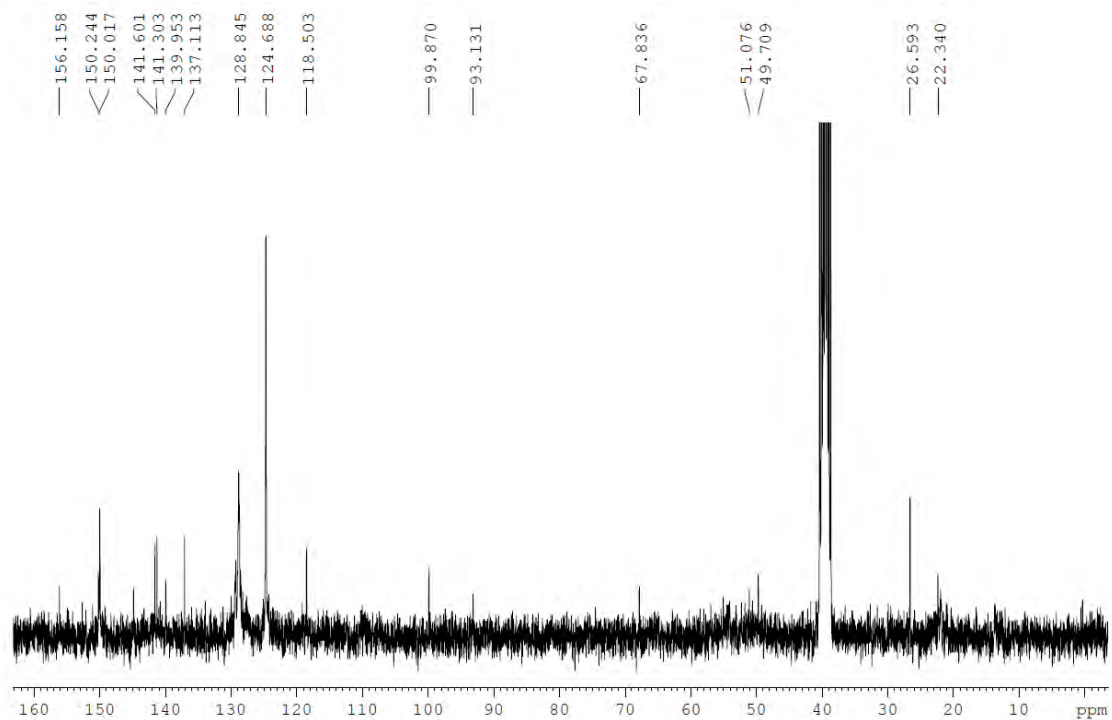
Figure S86: [1]H-decoupled [13]C NMR spectrum (100 MHz) of **48c** in DMSO-d6.
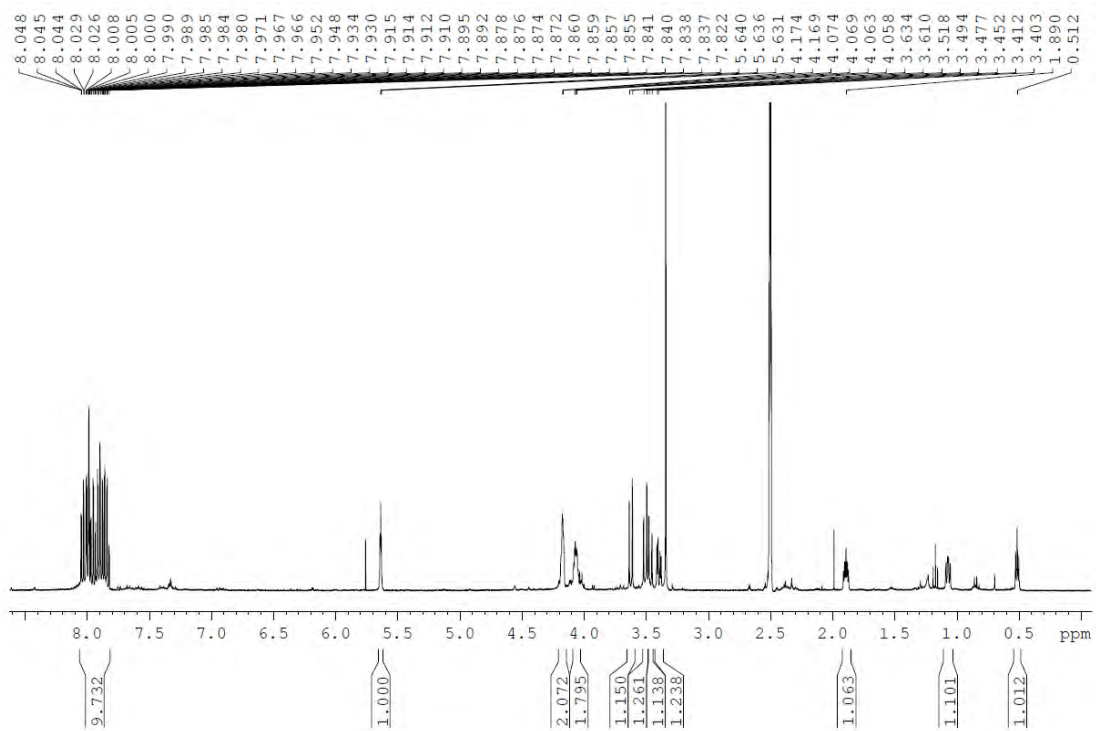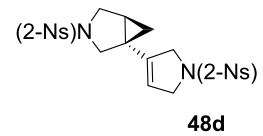
Figure S87: [1]H NMR spectrum (400 MHz) of **48d** in DMSO-d6.
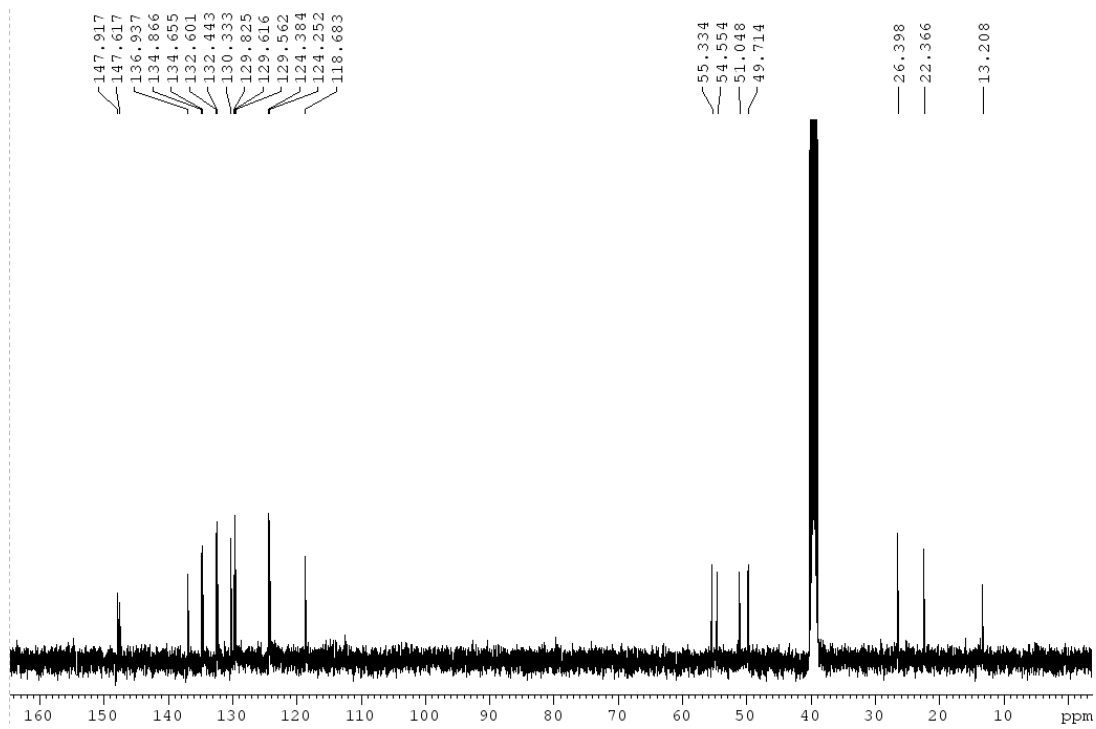
Figure S88: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **48d** in DMSO-d6.
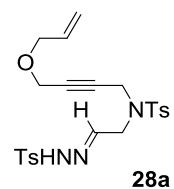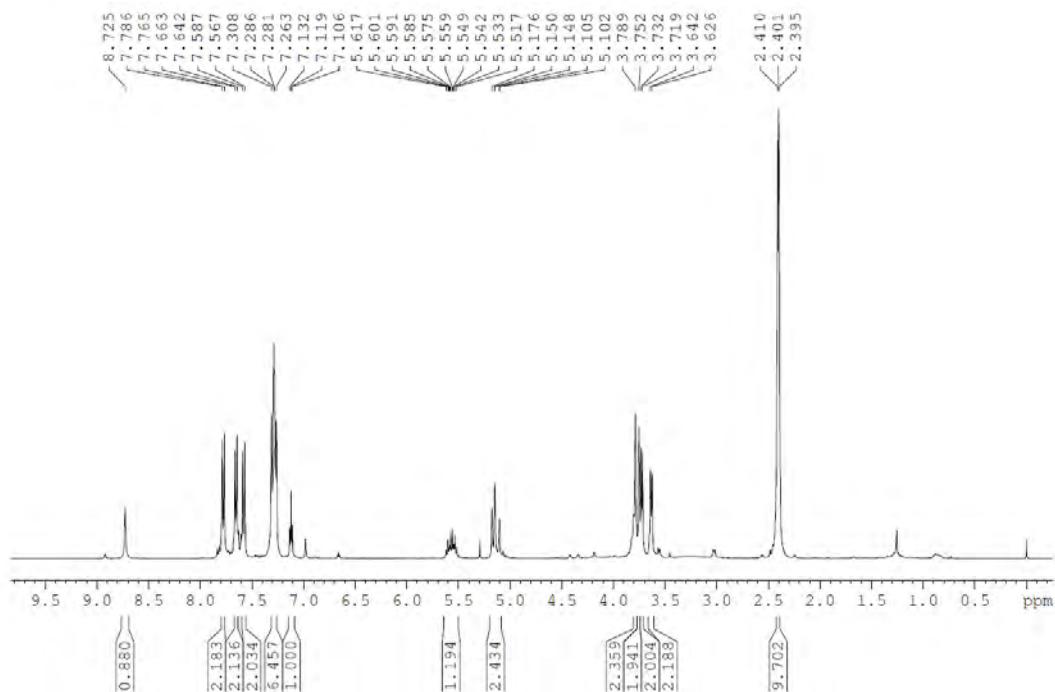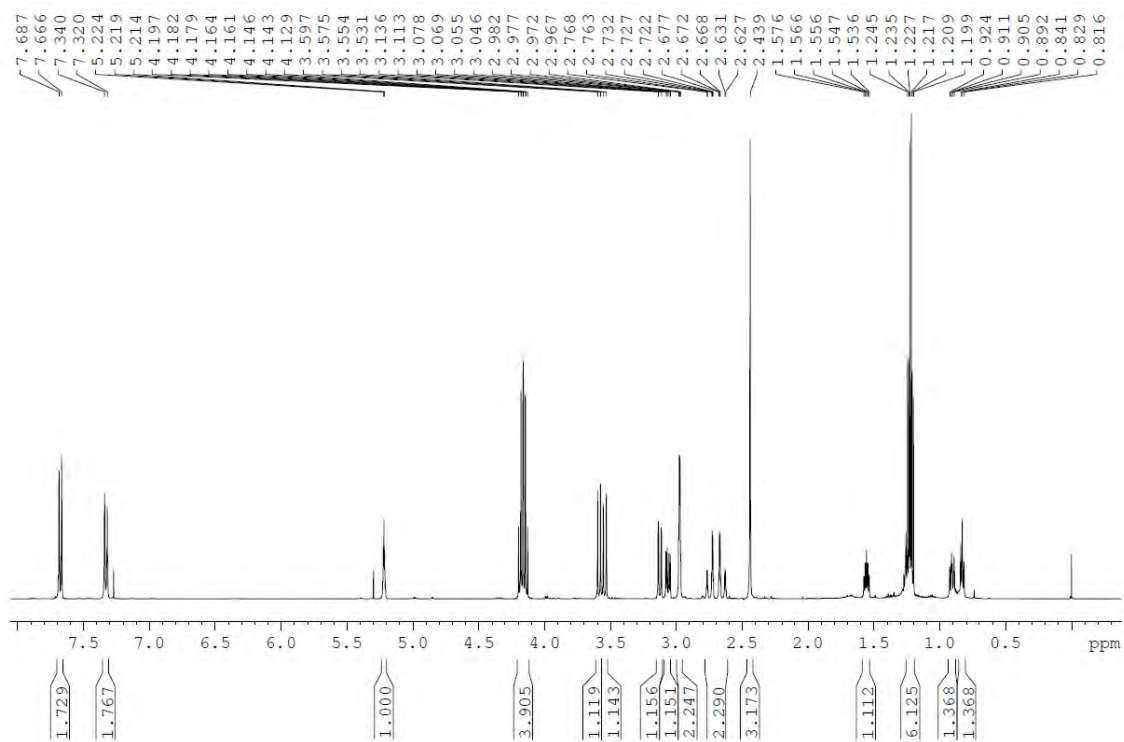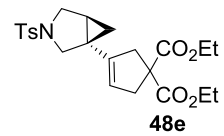
Figure S89: ^{1}H NMR spectrum (400 MHz) of **48e** in CDCl$_3$.
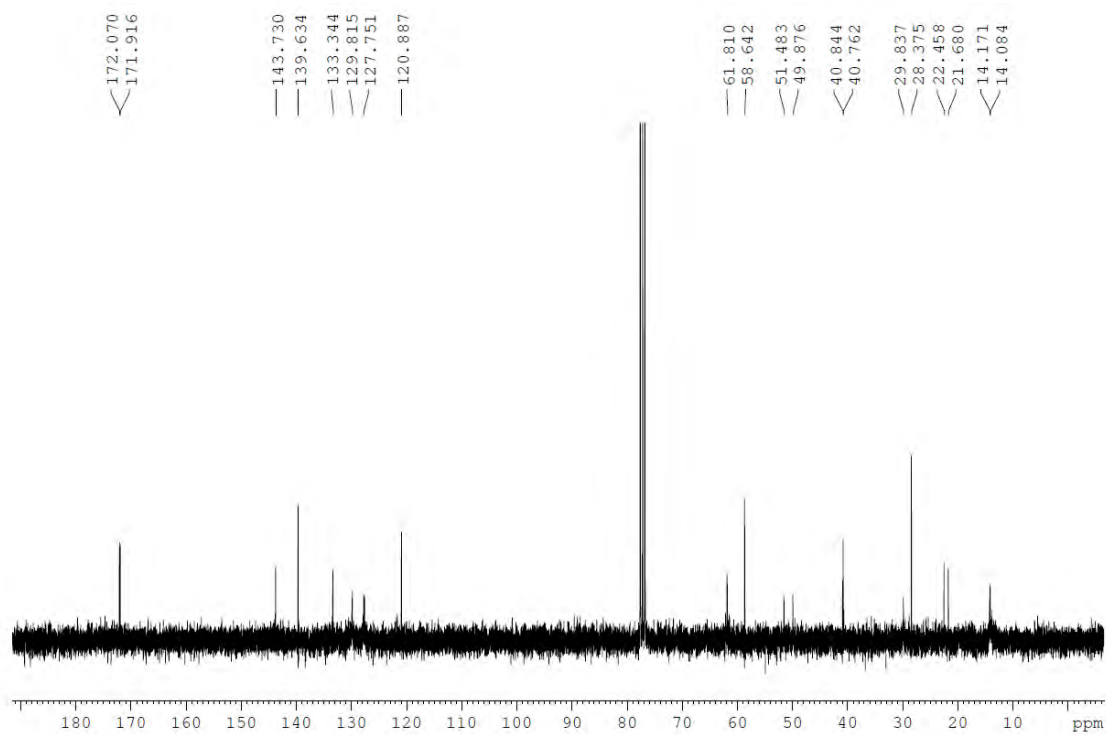
Figure S90: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **48e** in CDCl$_3$.

DAD1 F, Sig=220,16 Ref=360,100 (OSCAR\OT450RACB_9901.D)
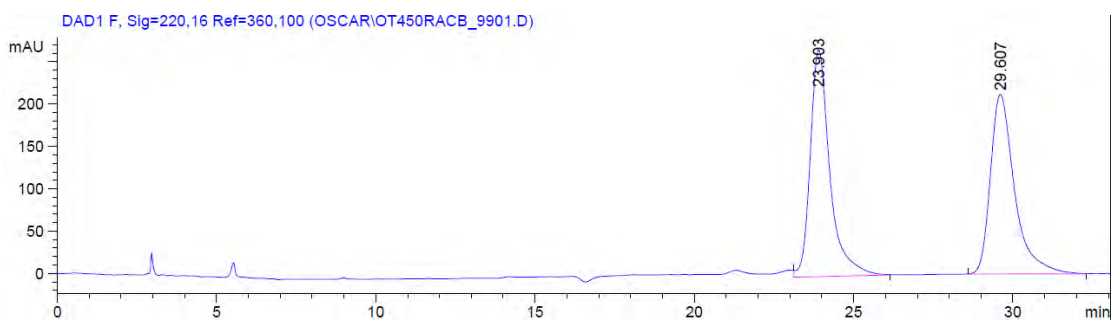
Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	23.903	1	VB	1.14859e4	268.02643	50.6684
2	29.607	1	BB	1.11829e4	211.83099	49.3316

DAD1 F, Sig=220,16 Ref=360,100 (OSCAR\OT450RB_9901.D)
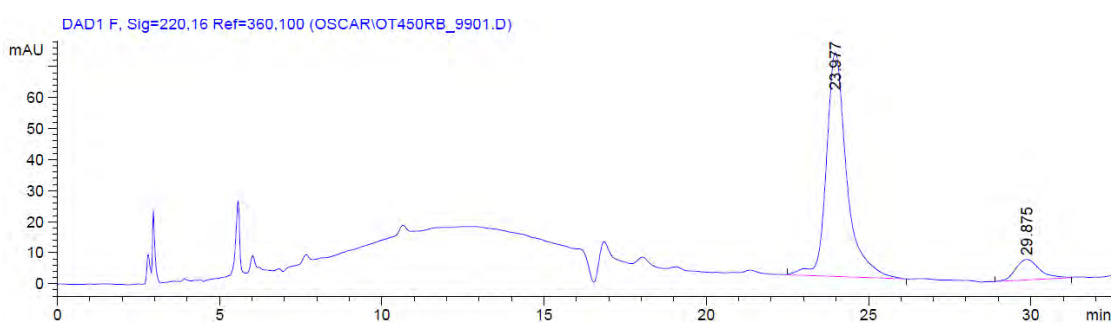
Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	23.977	1	BB	3152.80762	72.06113	90.3673
2	29.875	1	BB	336.07483	6.58009	9.6327

Figure S91: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **48e**.
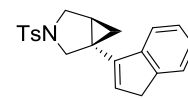
48f
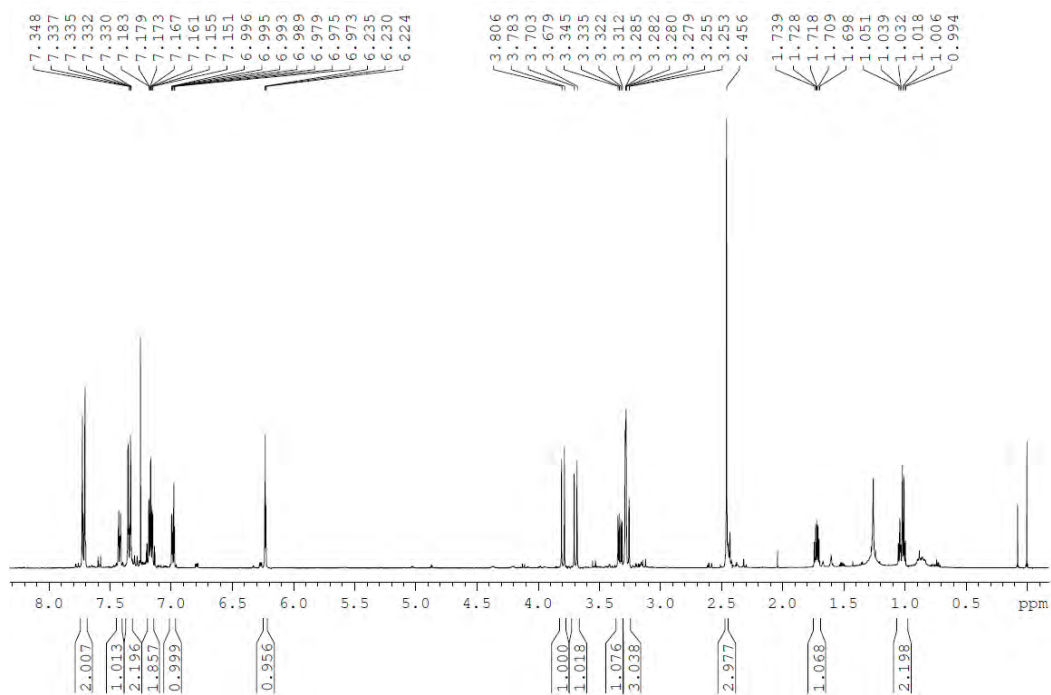
Figure S92: [1]H NMR spectrum (400 MHz) of **48f** in CDCl$_3$.
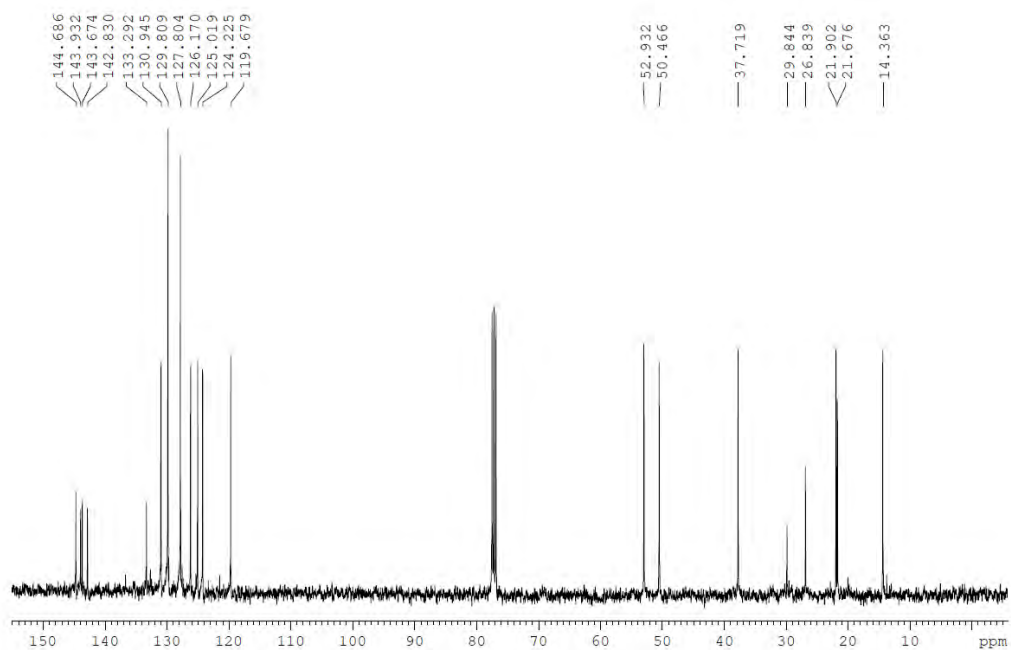
Figure S93: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **48f** in CDCl$_3$.

VWD1 A, Wavelength=240 nm (OSCAR\OT665racB 2016-03-11 13-01-20.D)
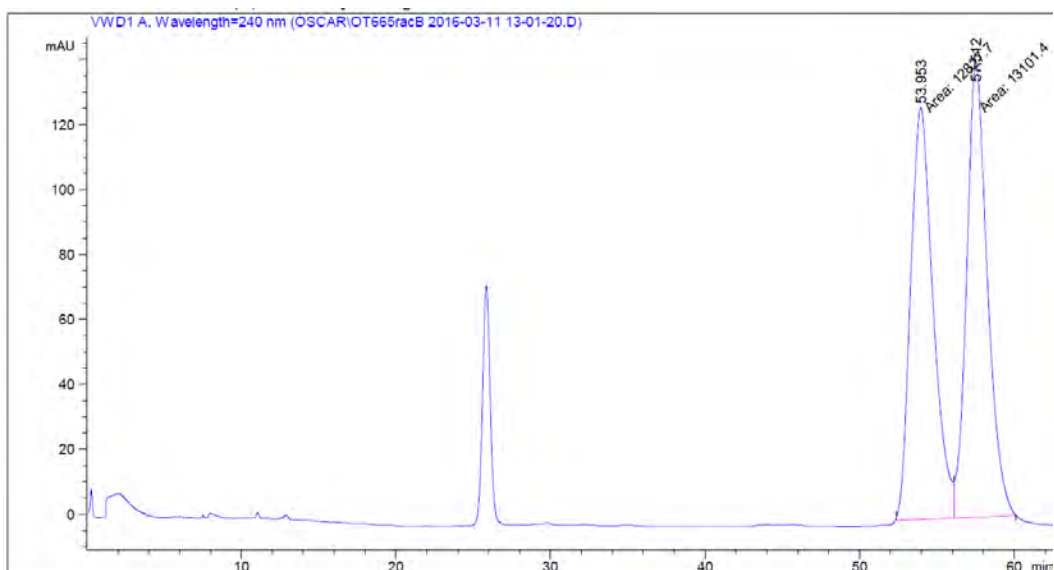
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	53.953	MF	1.6851	1.28277e4	126.87060	49.4722
2	57.512	FM	1.5556	1.31014e4	140.36919	50.5278

VWD1 A, Wavelength=240 nm (ÖSCAR\OT665SBINAP 2016-03-11 14-06-10.D)
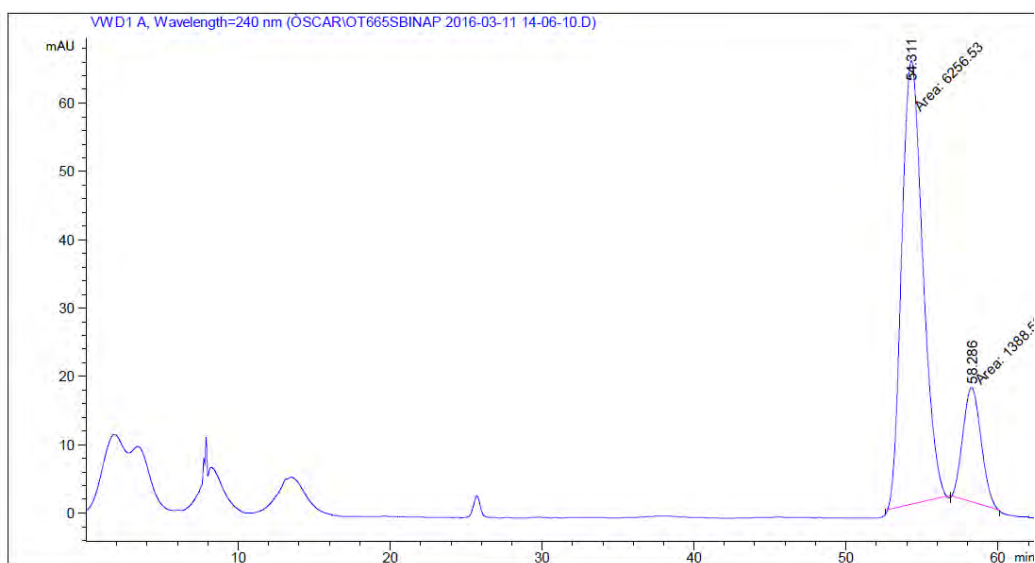
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	54.311	MM	1.6073	6256.52686	64.87655	81.8369
2	58.286	MM	1.3820	1388.59131	16.74557	18.1631

Figure S94: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **48f**.
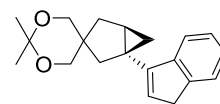
48g
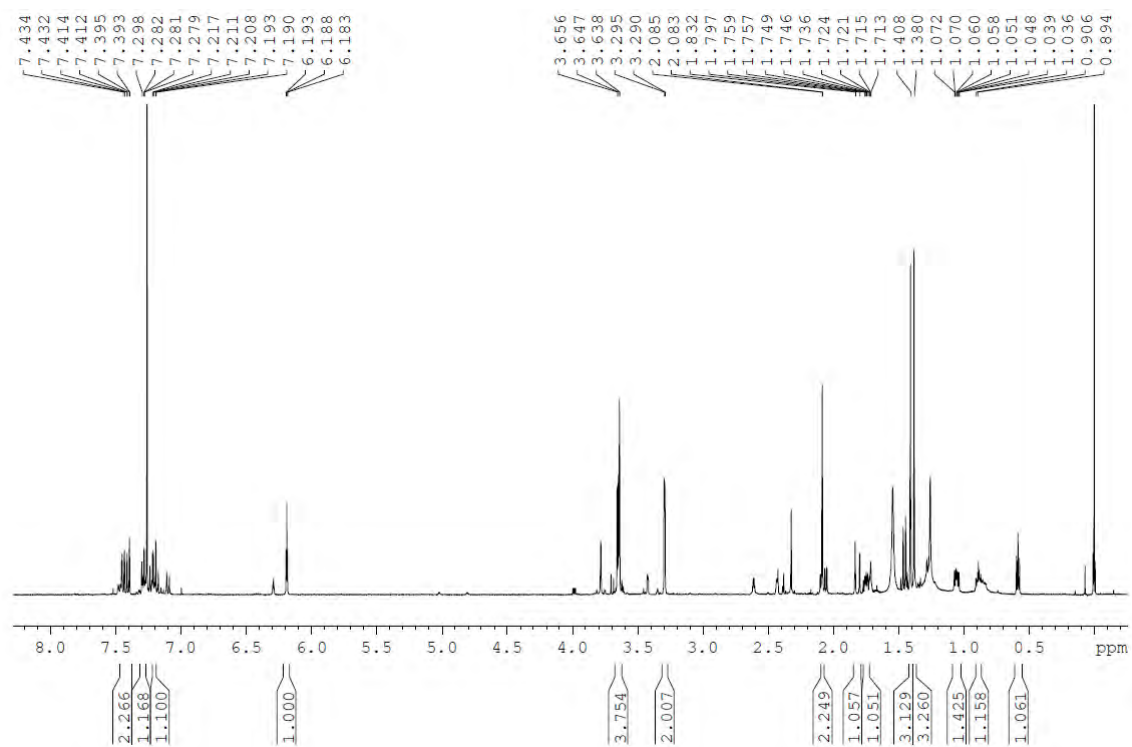
Figure S95: ¹H NMR spectrum (400 MHz) of **48g** in CDCl₃
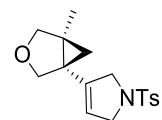
48k
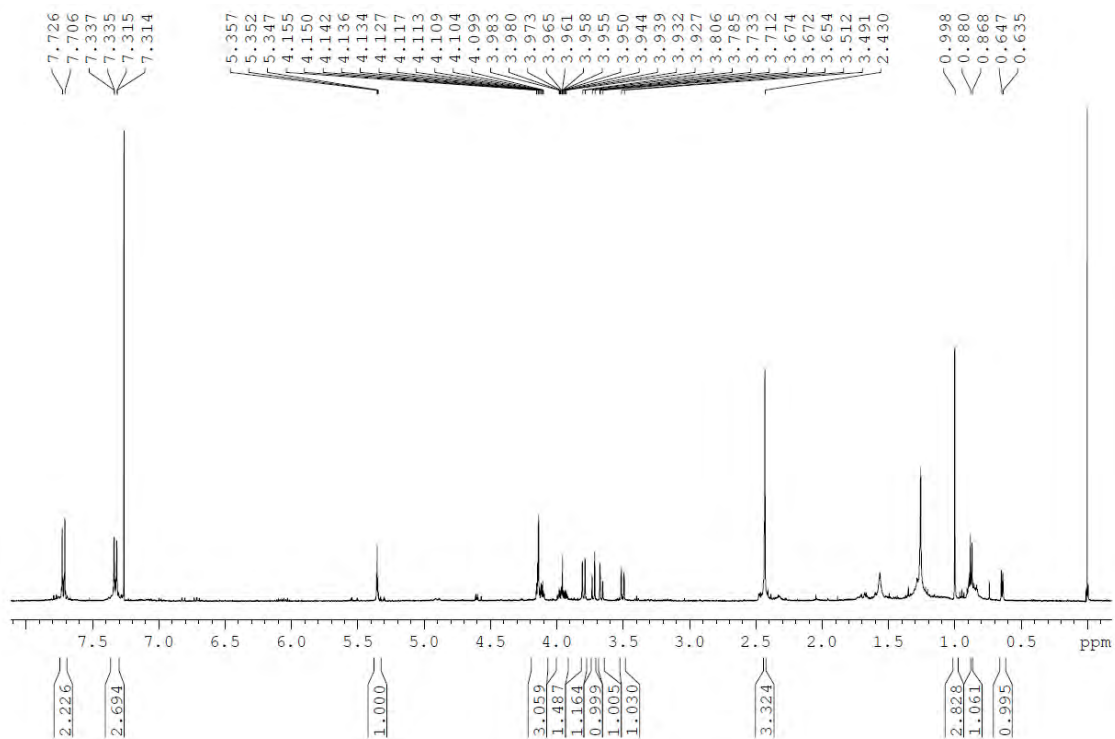
Figure S96: ^{1}H NMR spectrum (400 MHz) of **48k** in CDCl$_3$.
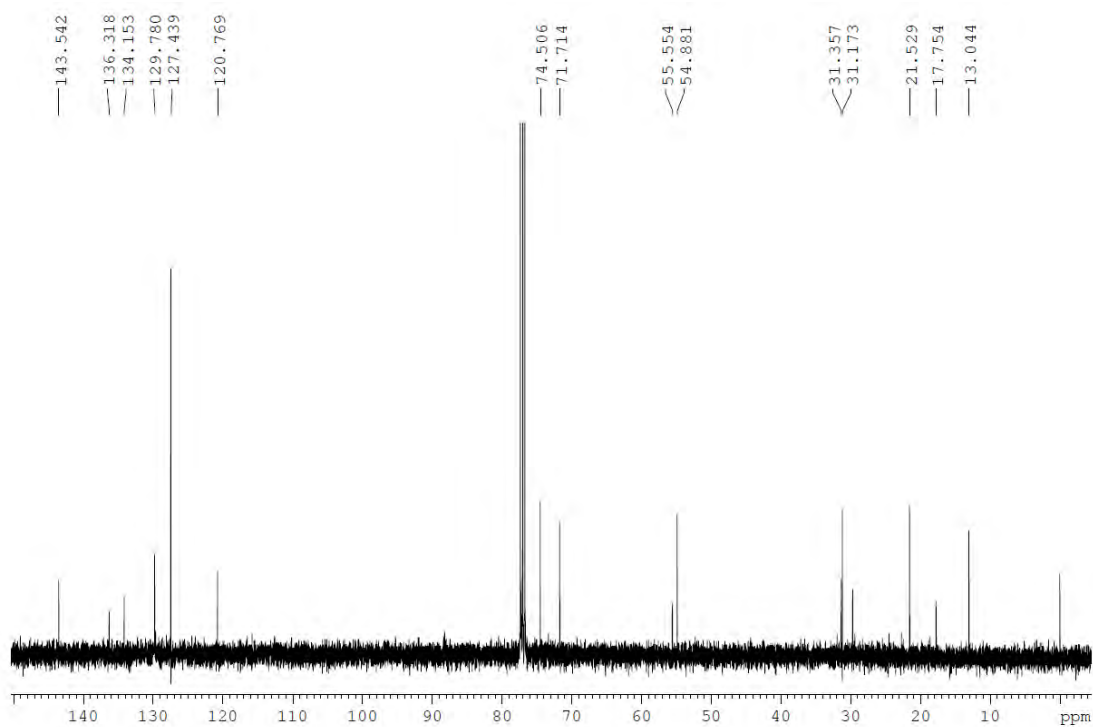
Figure S97: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **48k** in CDCl$_3$.
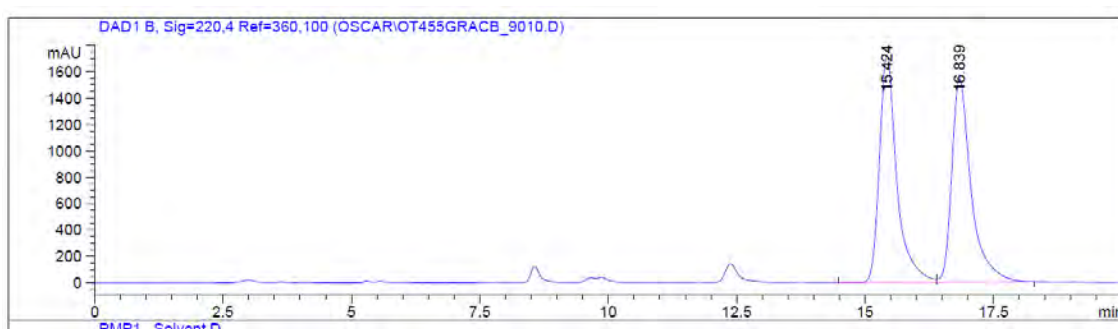
```
Peak RetTime Sig Type    Area      Height    Area
 #    [min]            [mAU*s]     [mAU]       %
----|-------|---|----|----------|----------|--------|
  1  15.424  1  BV   4.04547e4  1717.51904  50.0348
  2  16.839  1  VB   4.03985e4  1539.20007  49.9652
```
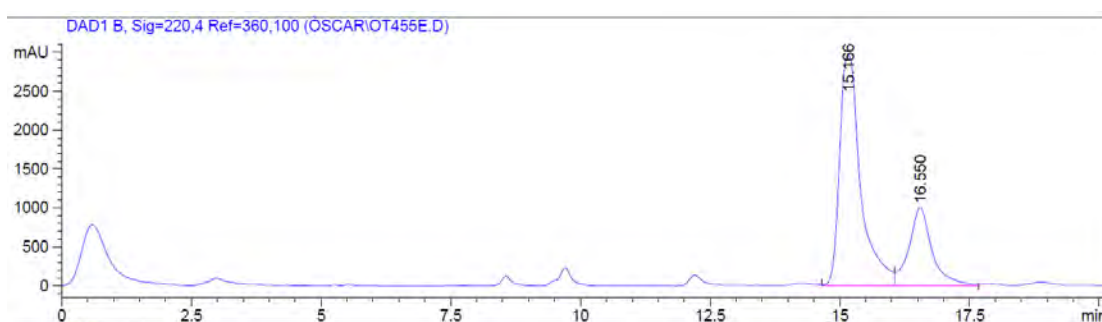


```
Peak RetTime Sig Type    Area      Height    Area
 #    [min]            [mAU*s]     [mAU]       %
----|-------|---|----|----------|----------|--------|
  1  15.166  1  VV   8.36357e4  2961.88379  72.7747
  2  16.550  1  VV   3.12884e4  1006.34058  27.2253
```

Figure S98: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **48k**.

Crystallographic data for compound 48a

Colourless crystals of **48a** ($C_{16}H_{19}NO_3S$) were grown from slow diffusion of pentane in a dichloroethane solution of the compound, and used for room temperature (298(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo $K\alpha$ radiation (λ = 0.71073 Å) from an x-Ray Tube. The measurements were made in the range 2.220 to 28.245° for θ. Hemi-sphere data collection was carried out with ω and φ scans. A total of 4750 reflections were collected of which 3037 [R(int) = 0.0449] were unique. Programs used: data collection, Smart[1]; data reduction, Saint+[2]; absorption correction, SADABS[3]. Structure solution and refinement was done using SHELXTL[4]. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached.

Table 1. Crystal data for **48a**.

Empirical formula	$C_{16}H_{19}NO_3S$
Formula weight	305.38
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 9.450(4) Å
	$\alpha = 90^o$
	b = 6.141(2) Å
	$\beta = 103.880(7)^o$
	c = 13.667(5) Å
	$\gamma = 90^o$
Volume	770.0(5) A^3
Z, Calculated density	2, 1.317 Mg/m^3
Absorption coefficient	0.219 mm^{-1}
F(000)	324
Crystal size	0.25 x 0.20 x 0.15 mm
Theta range for data collection	2.220^o to 28.245^o
Limiting indices	-12<=h<=11
	-8<=k<=7
	-15<=l<=17
Reflections collected / unique	4750 / 3037
	[R(int) = 0.0449]
Completeness to theta = 25.242	99.1 %
Absorption correction	Empirical
Max. and min. transmission	1.0 and 0.483867
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3037 / 1 / 191
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1180

[1] Bruker Advanced X-ray Solutions. SMART: Version 5.631, 1997-2002.

[2] Bruker Advanced X-ray Solutions. SAINT +, Version 6.36A, 2001.

[3] G. M. Sheldrick, *Empirical Absorption Correction Program*, Universität Göttingen, 1996.
Bruker Advanced X-ray Solutions. SADABS Version 2.10, 2001.

[4] G. M. Sheldrick, *Program for Crystal Structure Refinement*, Universität Göttingen, 1997.
Bruker Advanced X-ray Solutions. SHELXTL Version 6.14, 2000-2003. SHELXL-2013 (Sheldrick, 2013).

R indices (all data)	R1 = 0.0917, wR2 = 0.1379
Absolute structure parameter	-0.01(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.229 and -0.201 e.A^{-3}

52a
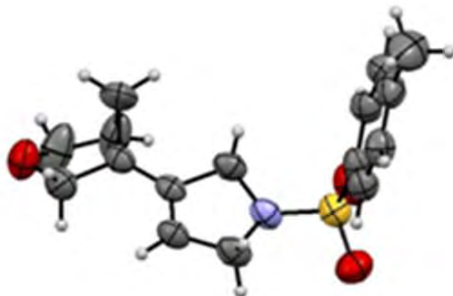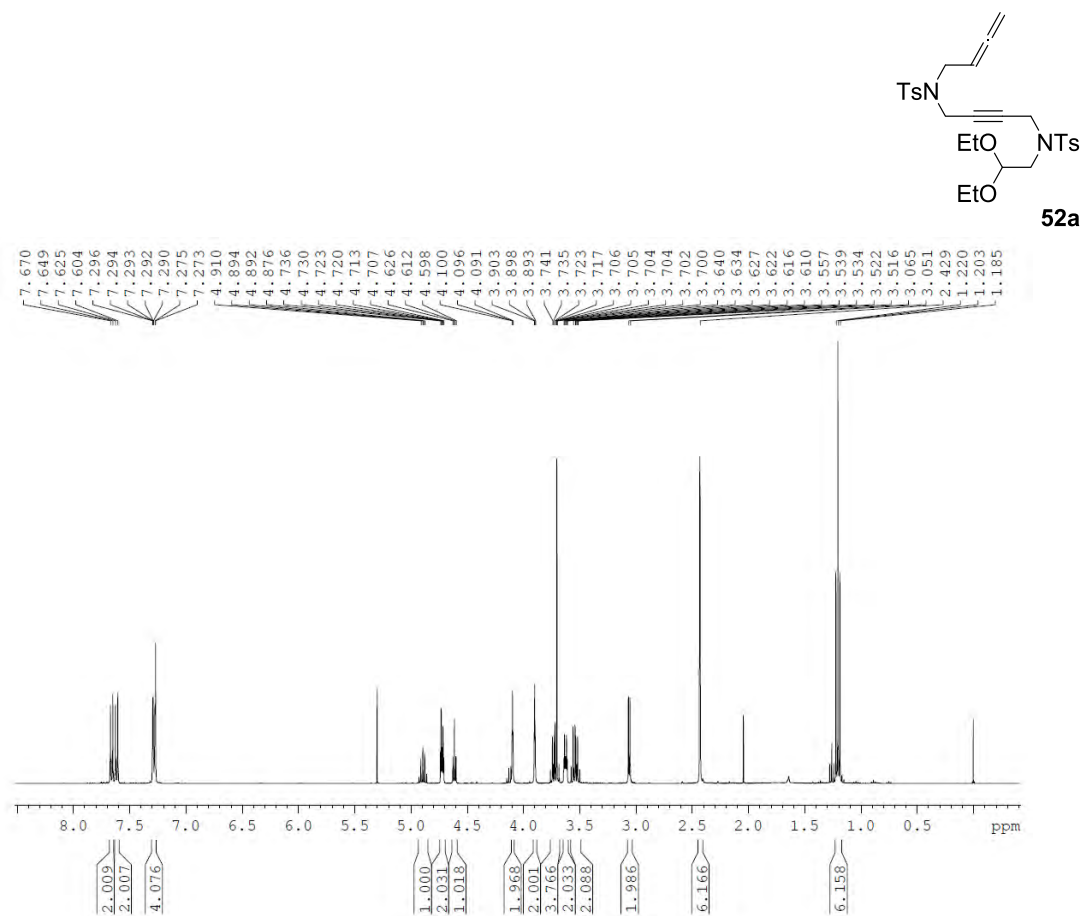
Figure S1: ^{1}H NMR spectrum (400 MHz) of **52a** in CDCl$_3$.
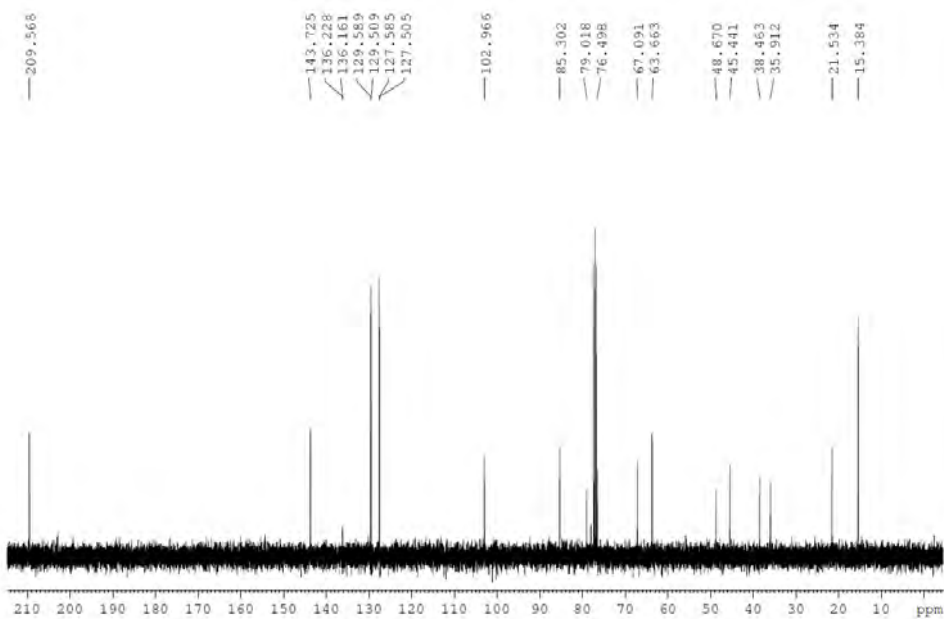
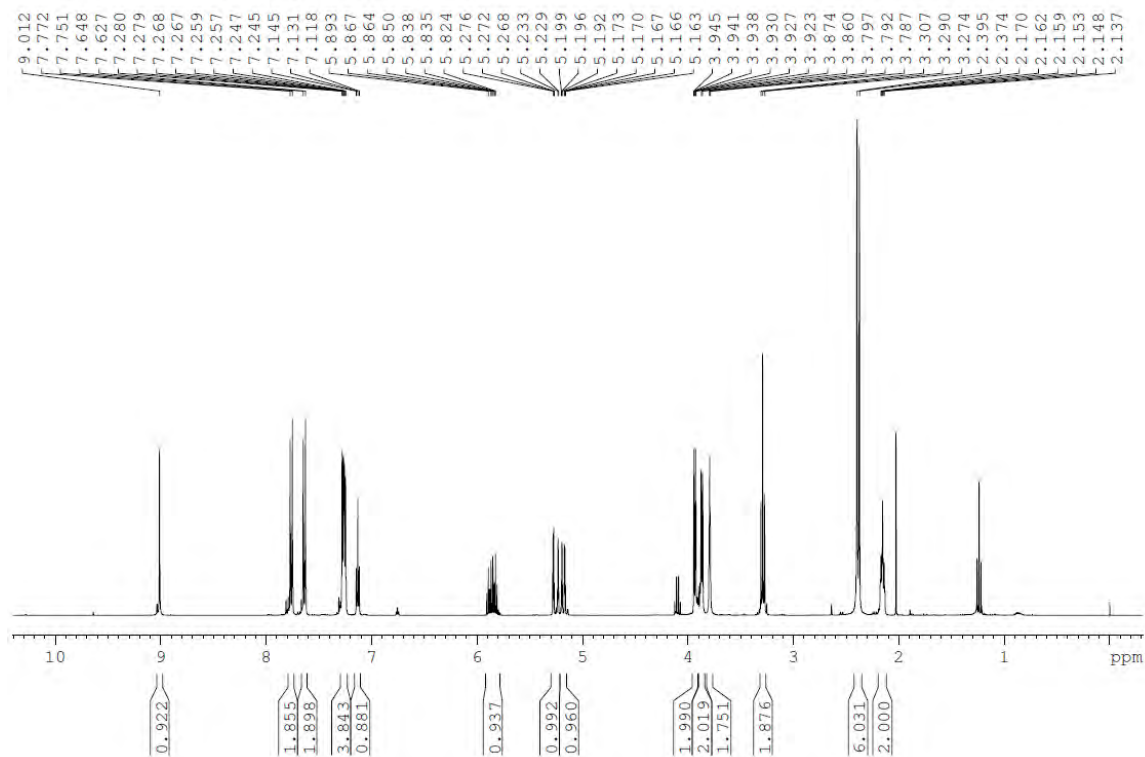**Figure S2**: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **52a** in CDCl$_3$.

52b
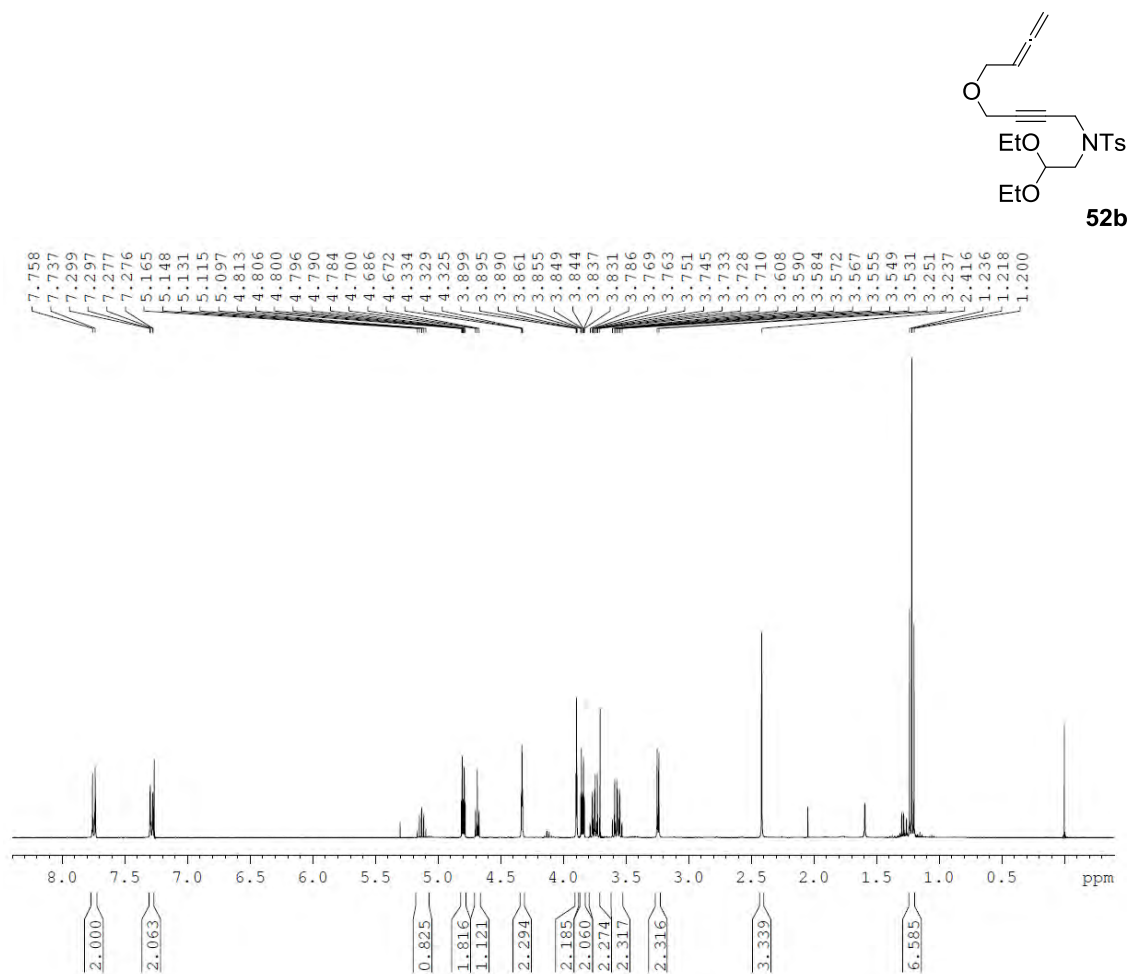
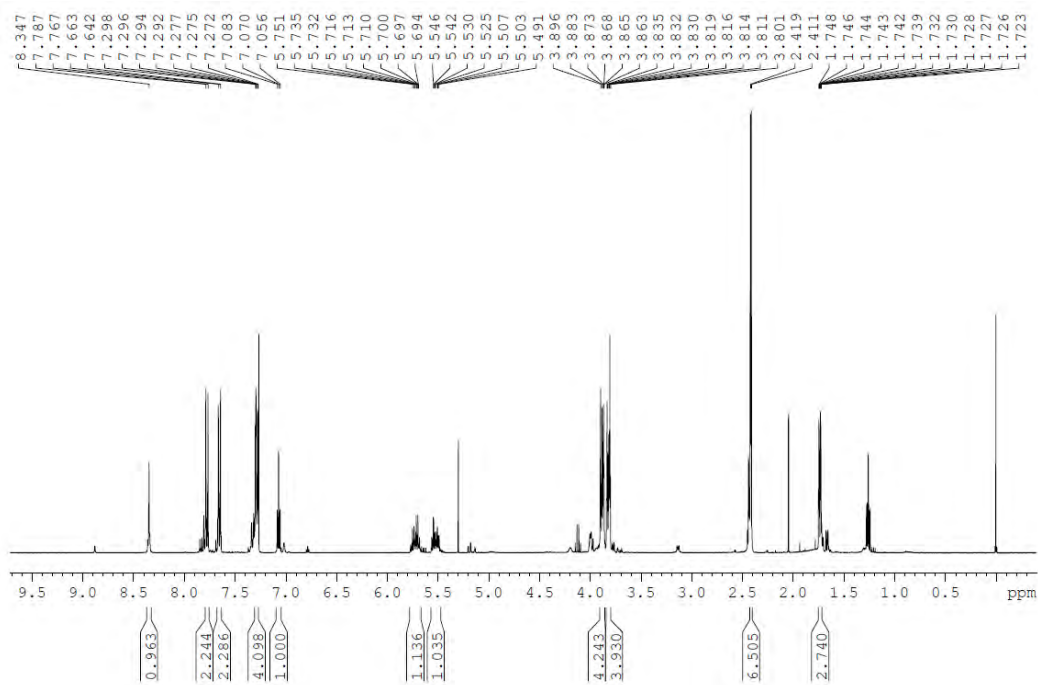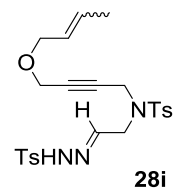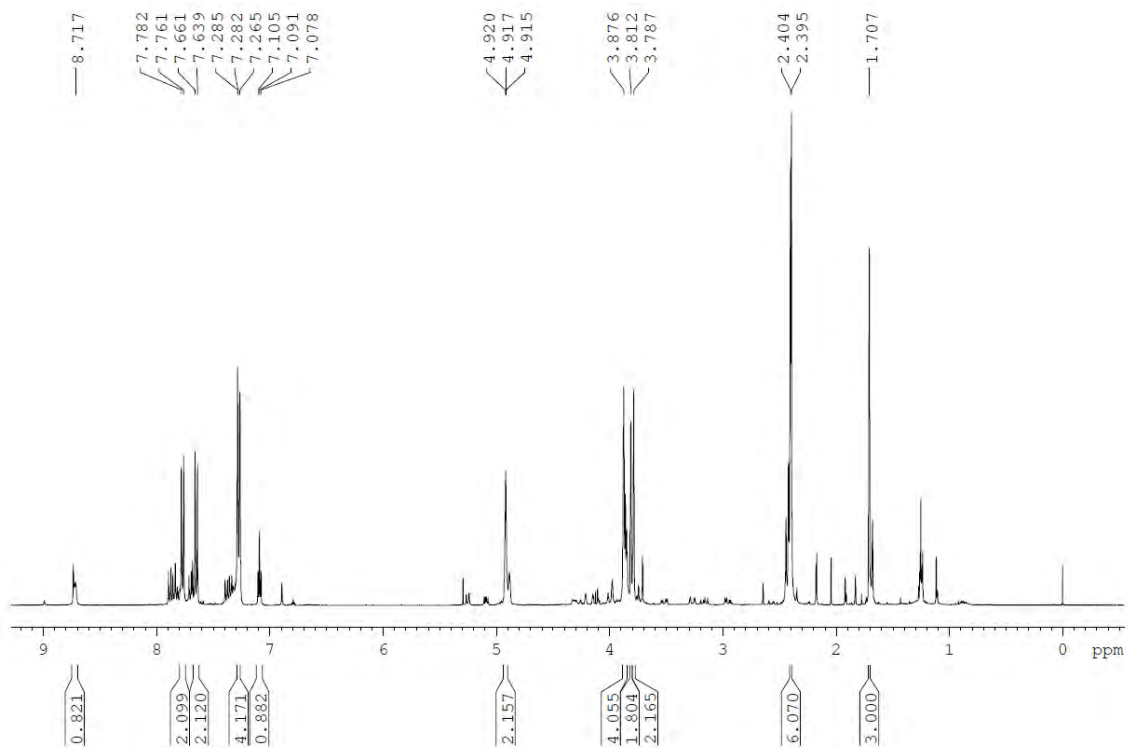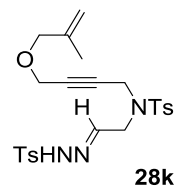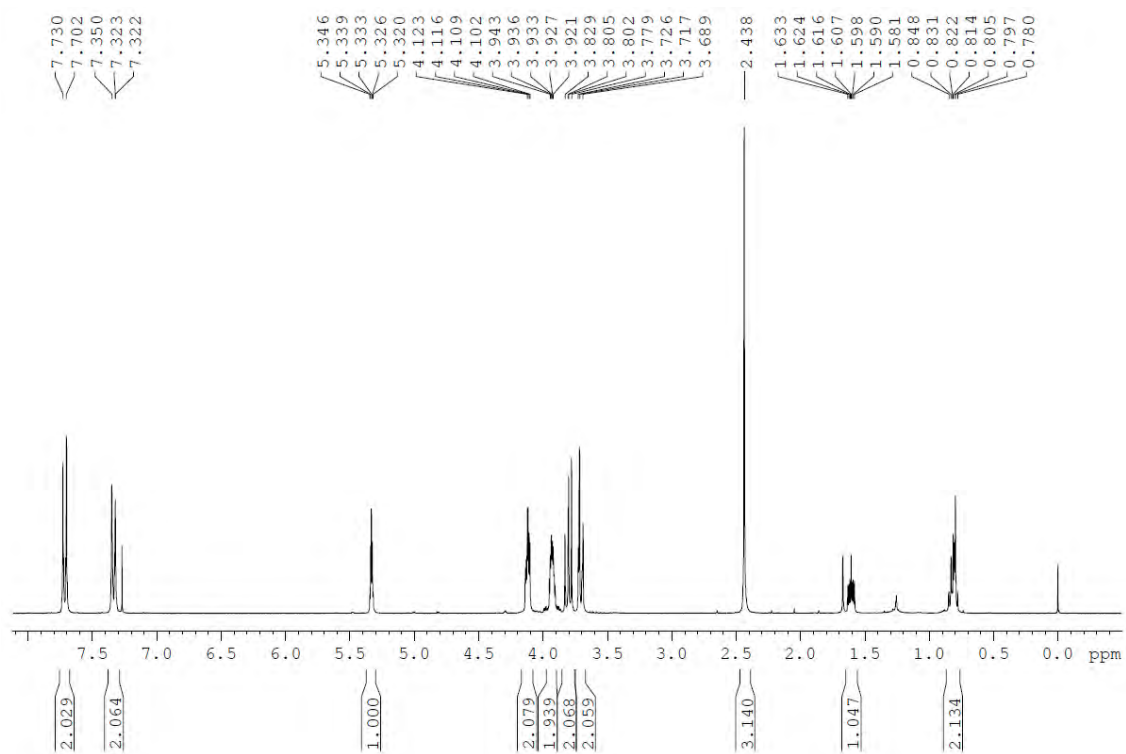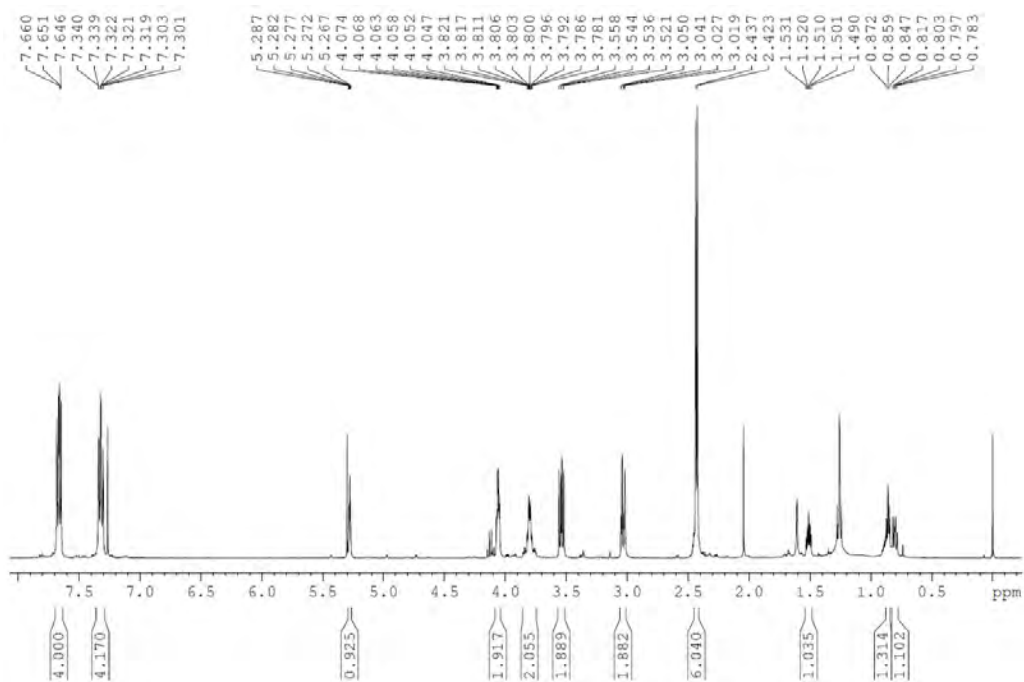**Figure S5**: ^{1}H NMR spectrum (400 MHz) of **52b** in CDCl$_3$.
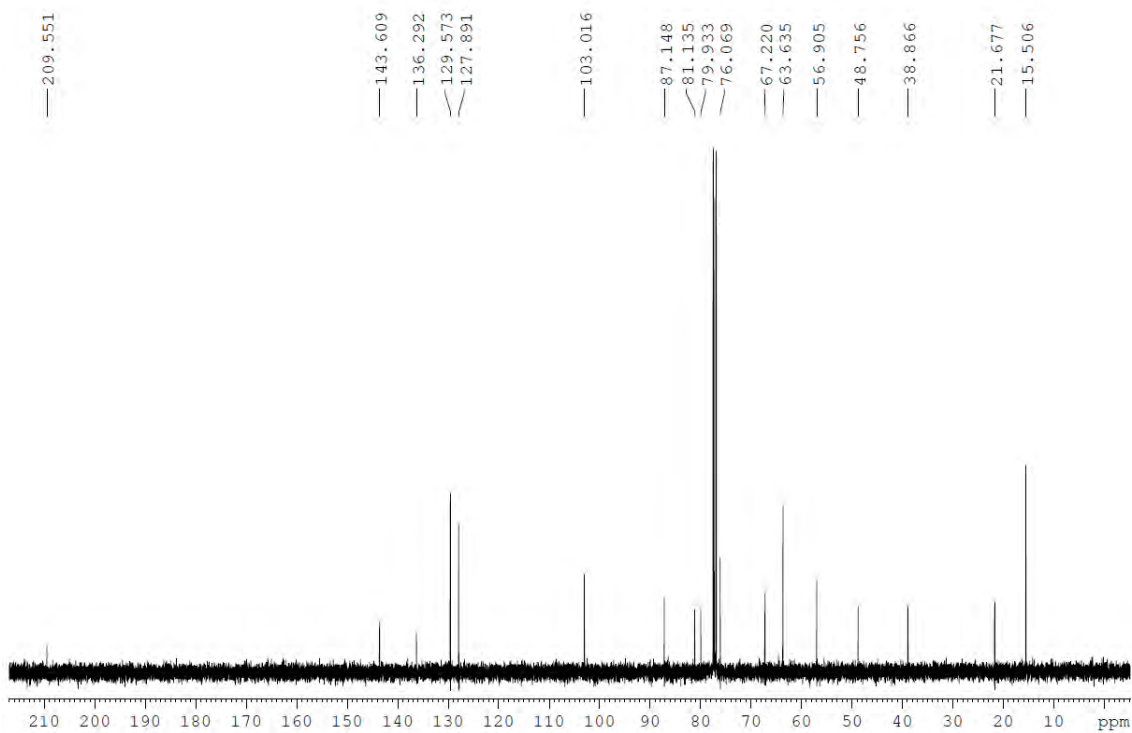
Figure S6: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **52b** in CDCl$_3$.
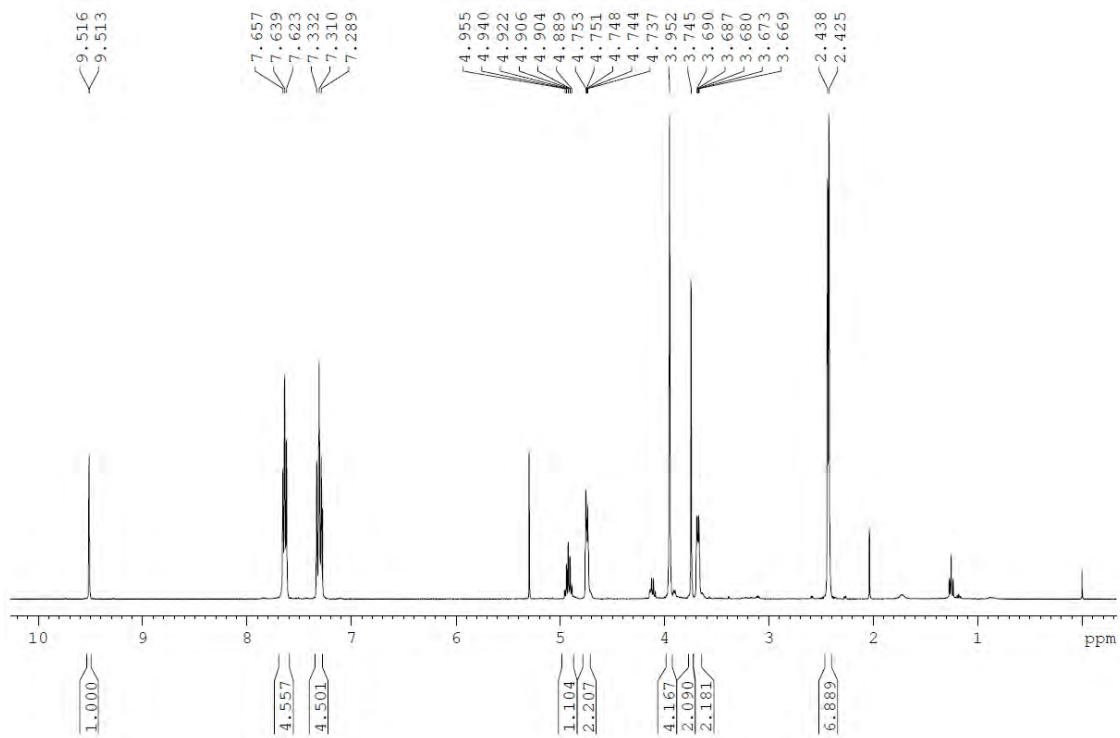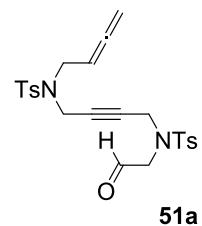
Figure S9: ^{1}H NMR spectrum (400 MHz) of **51a** in CDCl$_3$.
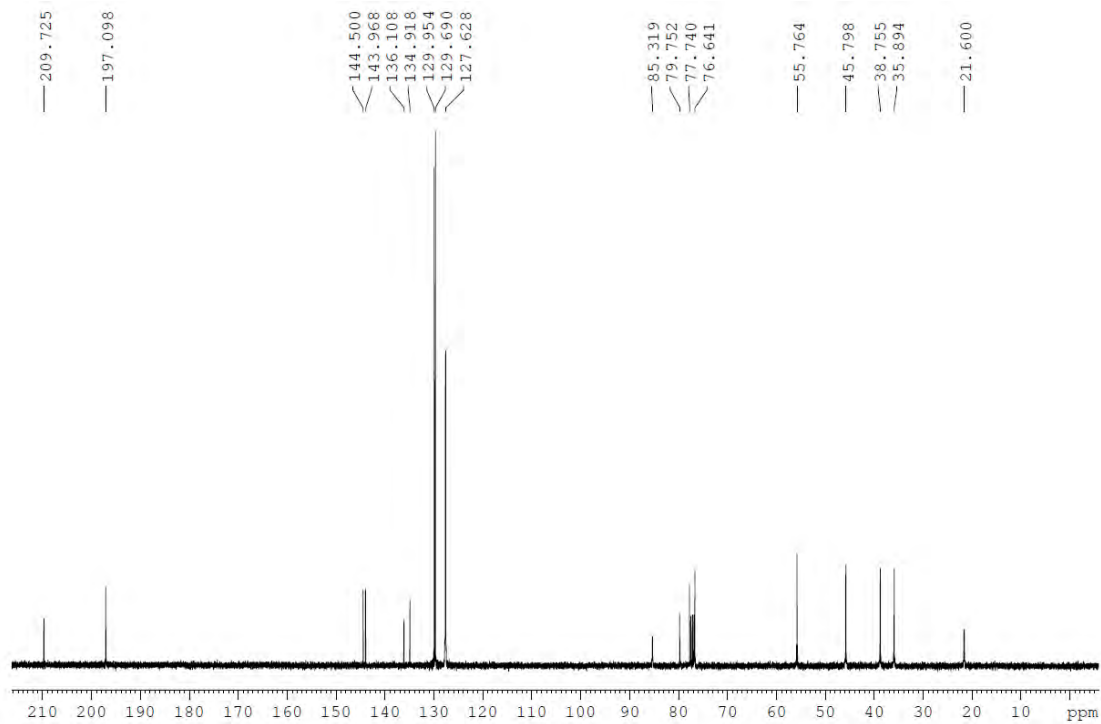
Figure S10: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **51a** in CDCl$_3$.
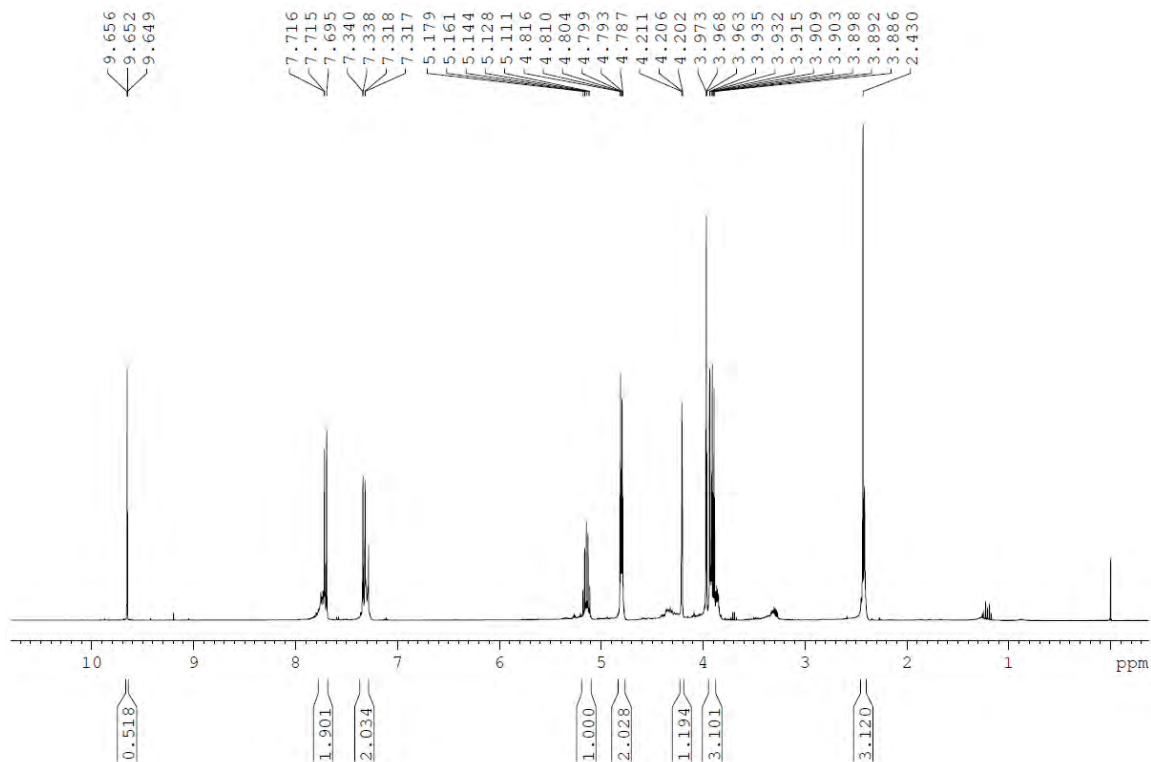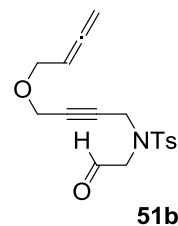
Figure S13: ^{1}H NMR spectrum (400 MHz) of **51b** in CDCl$_3$.
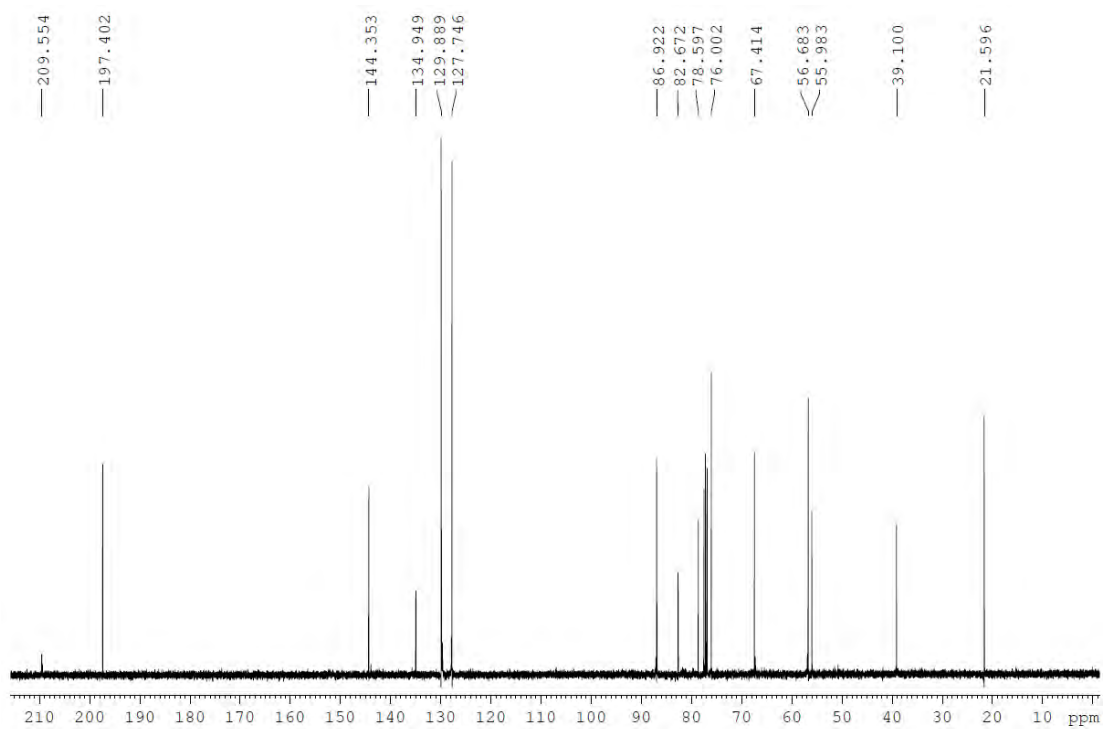
Figure S14: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **51b** in CDCl$_3$.

Figure S17: ^{1}H NMR spectrum (400 MHz) of **49** in CDCl$_3$.
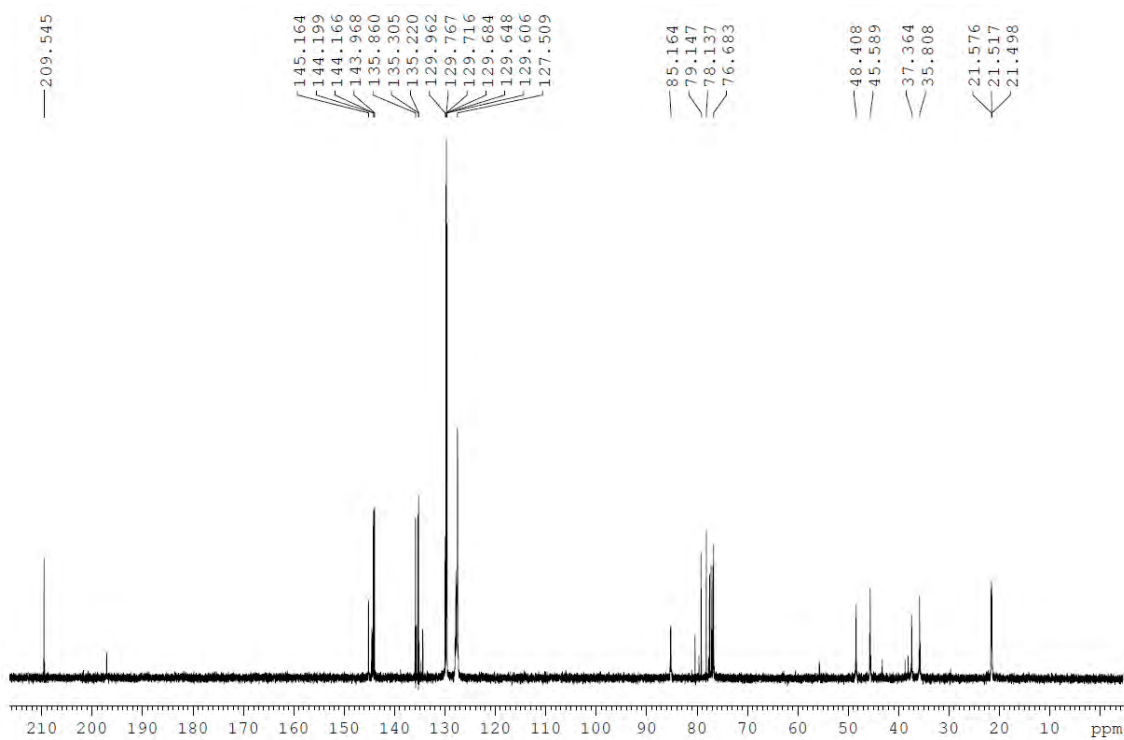
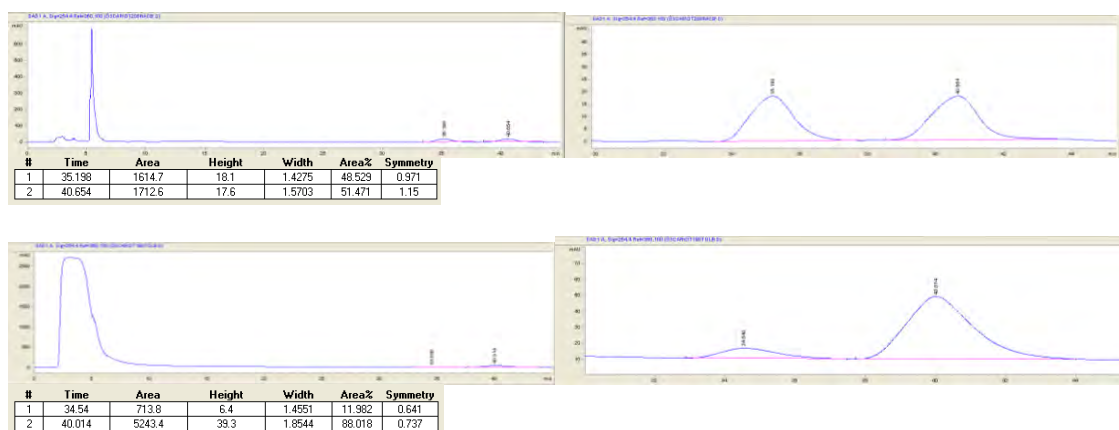**Figure S18**: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **49** in CDCl$_3$.

Figure S21: ^{1}H NMR spectrum (400 MHz) of **50a** in CDCl$_3$.
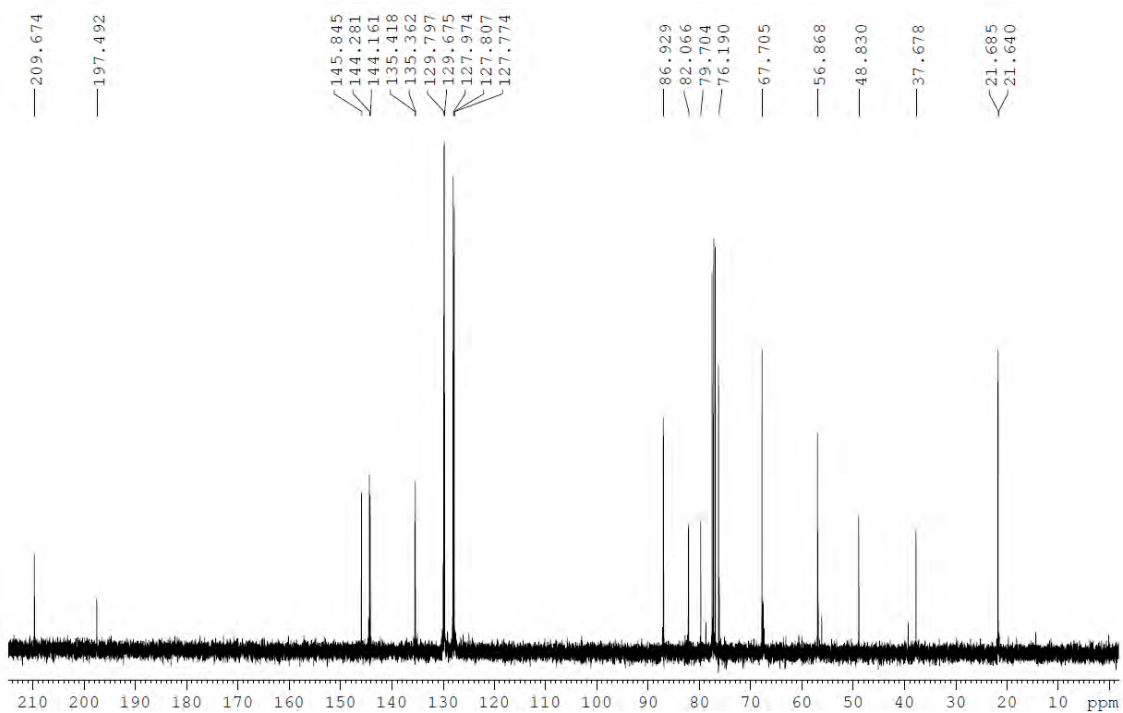
Figure S22: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50a** in CDCl$_3$.
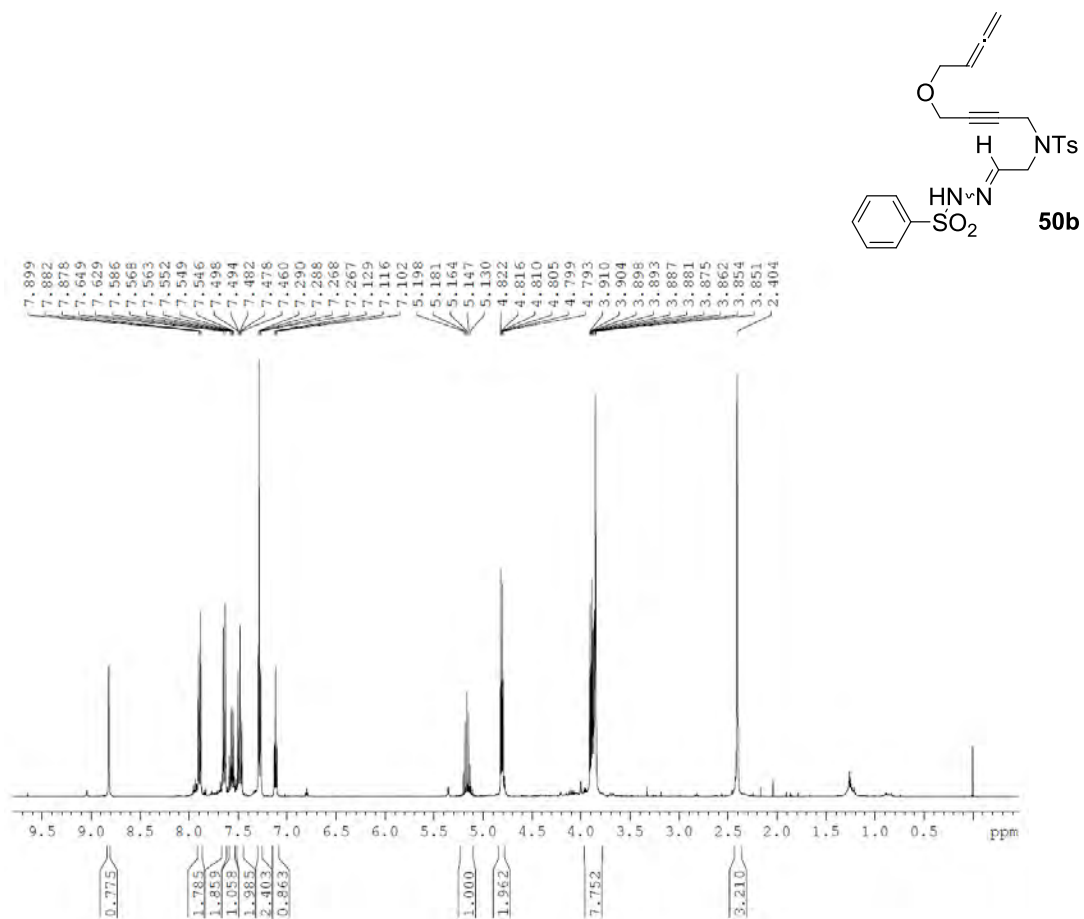
Figure S25: ^{1}H NMR spectrum (400 MHz) of **50b** in CDCl$_3$.
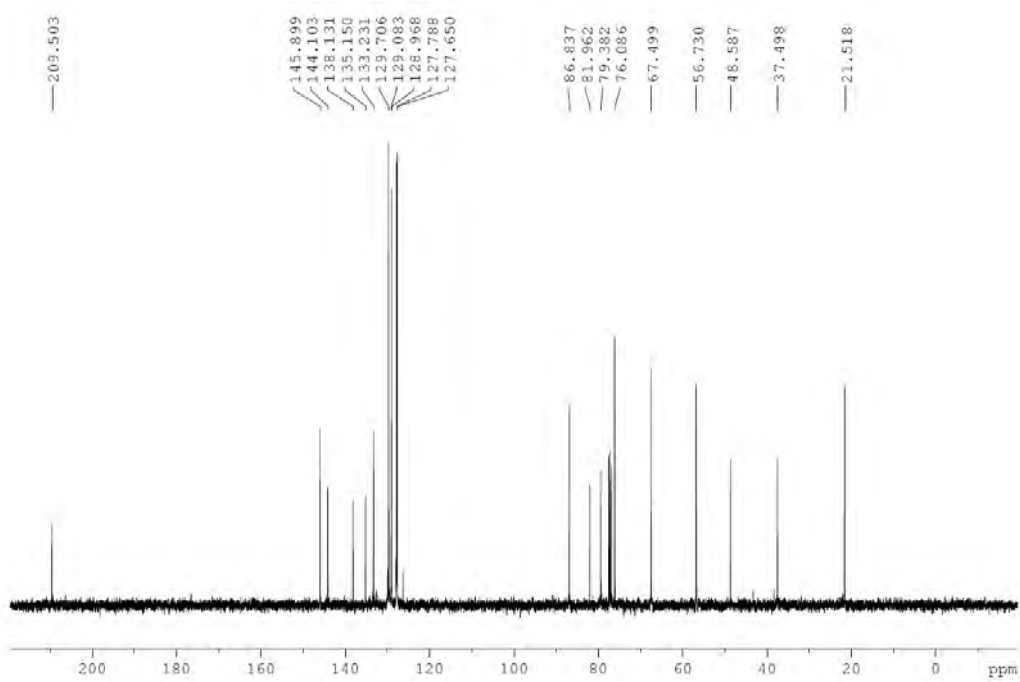
Figure S26: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50b** in CDCl$_3$.
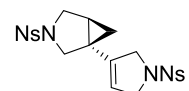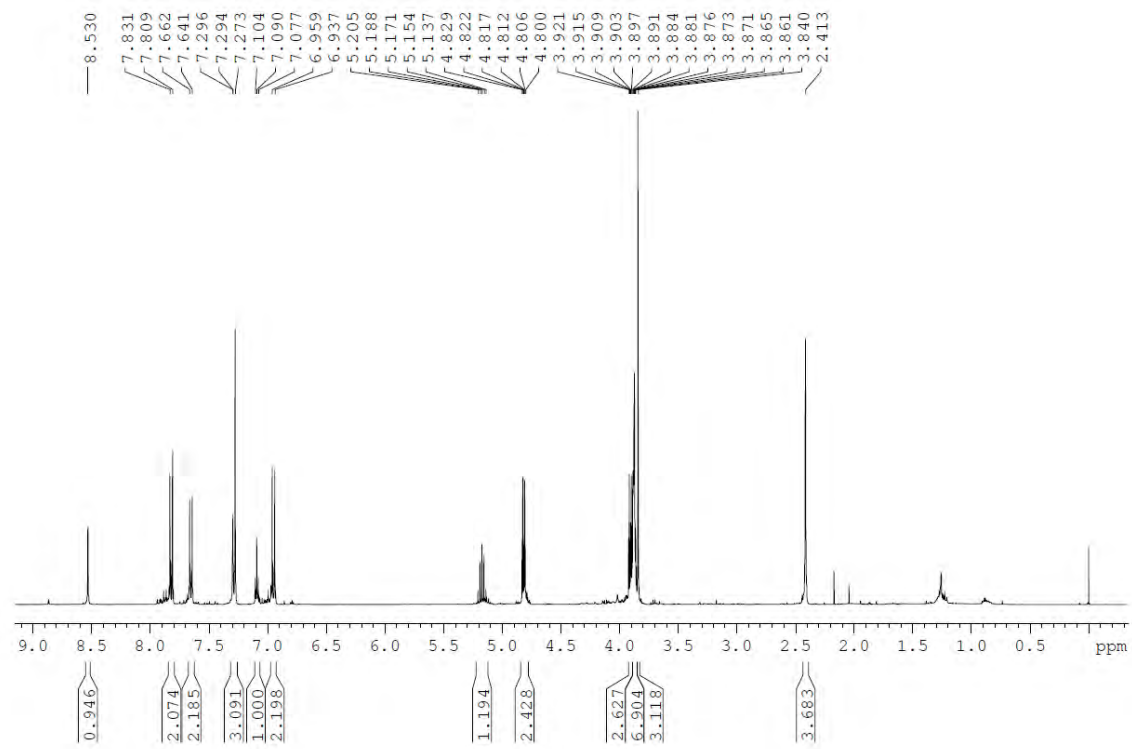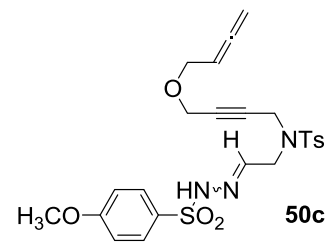
Figure S29: ^{1}H NMR spectrum (400 MHz) of **50c** in CDCl$_3$.
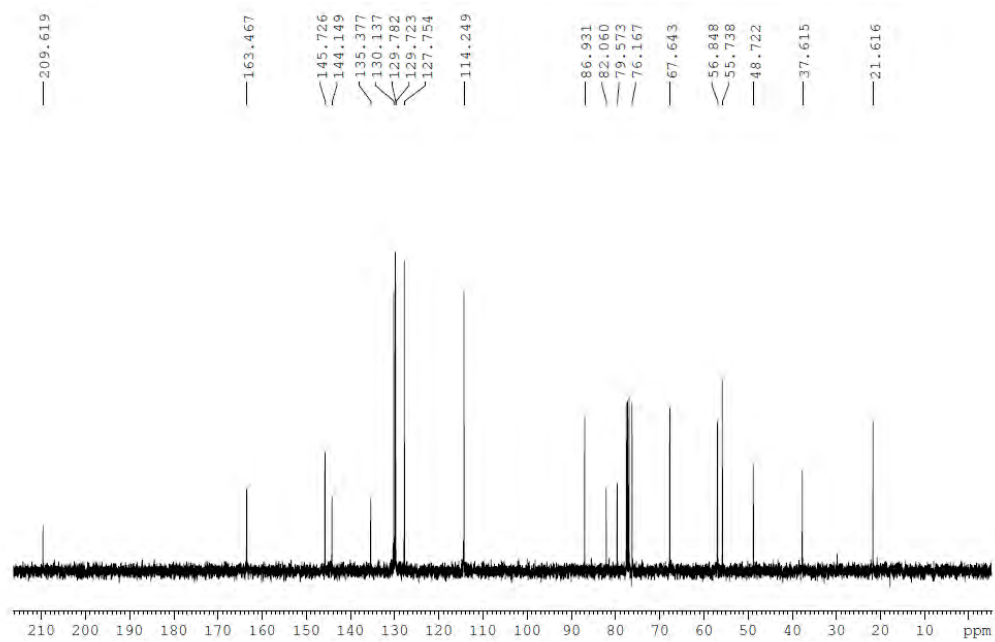
Figure S30: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50c** in CDCl$_3$.
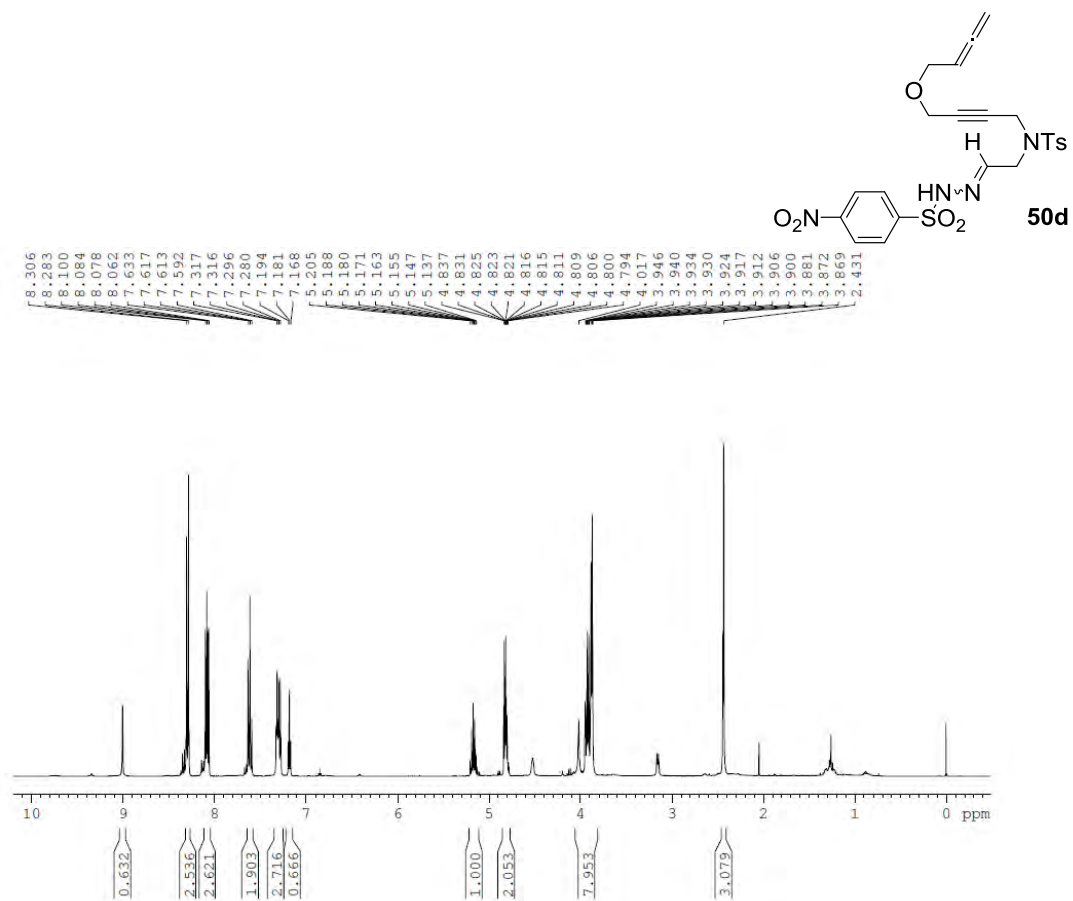
Figure S33: ^{1}H NMR spectrum (400 MHz) of **50d** in CDCl$_3$.
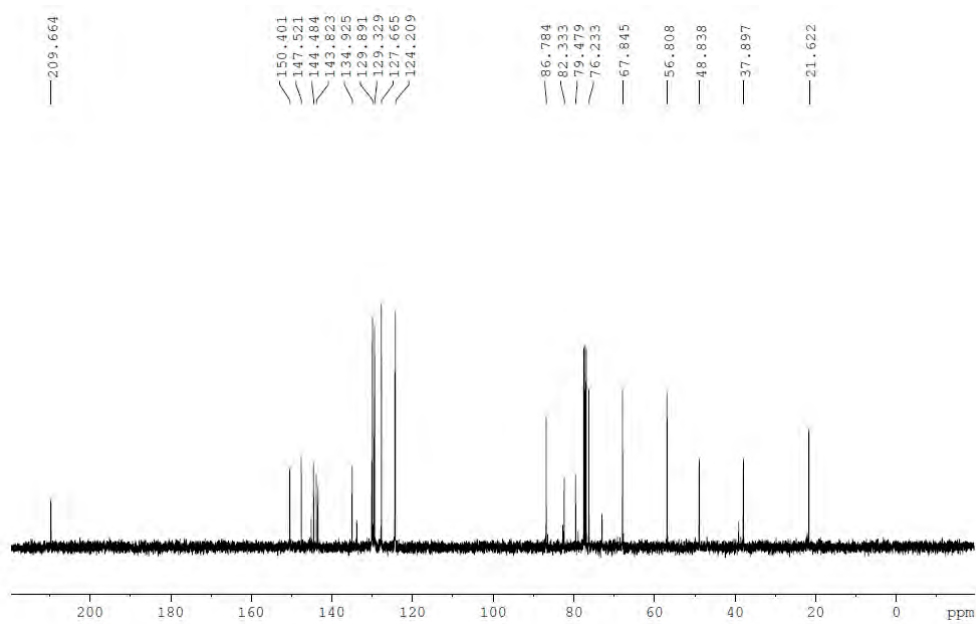
Figure S34: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50d** in CDCl$_3$.
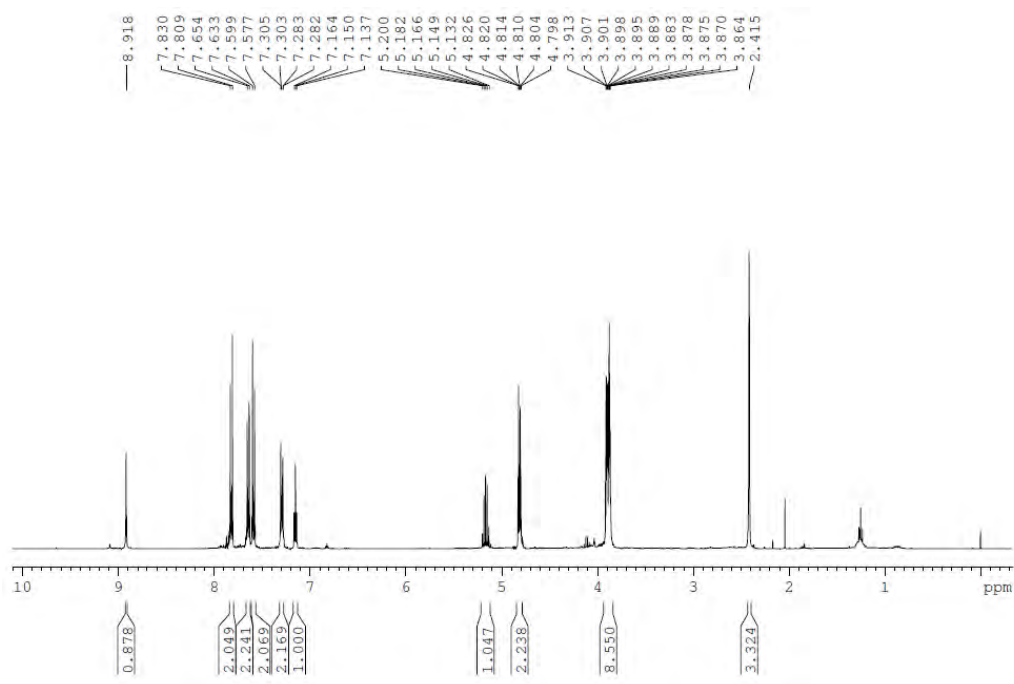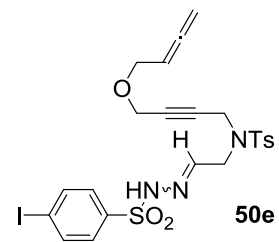
Figure S37: ^{1}H NMR spectrum (400 MHz) of **50e** in CDCl$_3$.
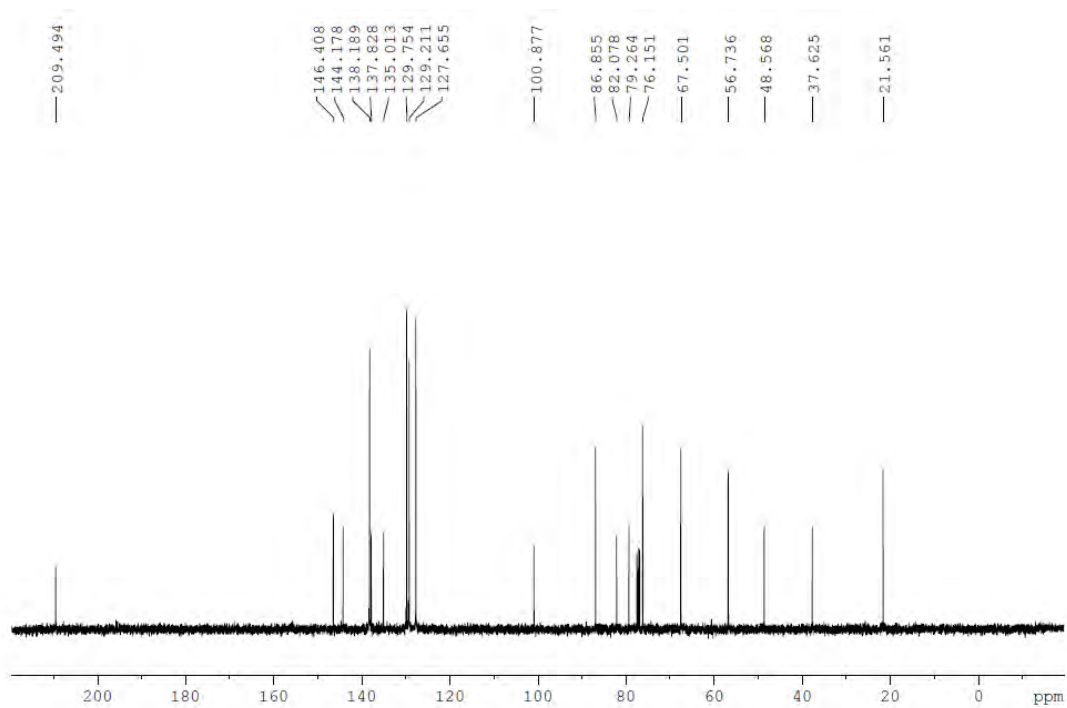
Figure S38: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50e** in CDCl$_3$.

Figure S41: ^{1}H NMR spectrum (400 MHz) of **50f** in CDCl$_3$.

Figure S42: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50f** in CDCl$_3$.
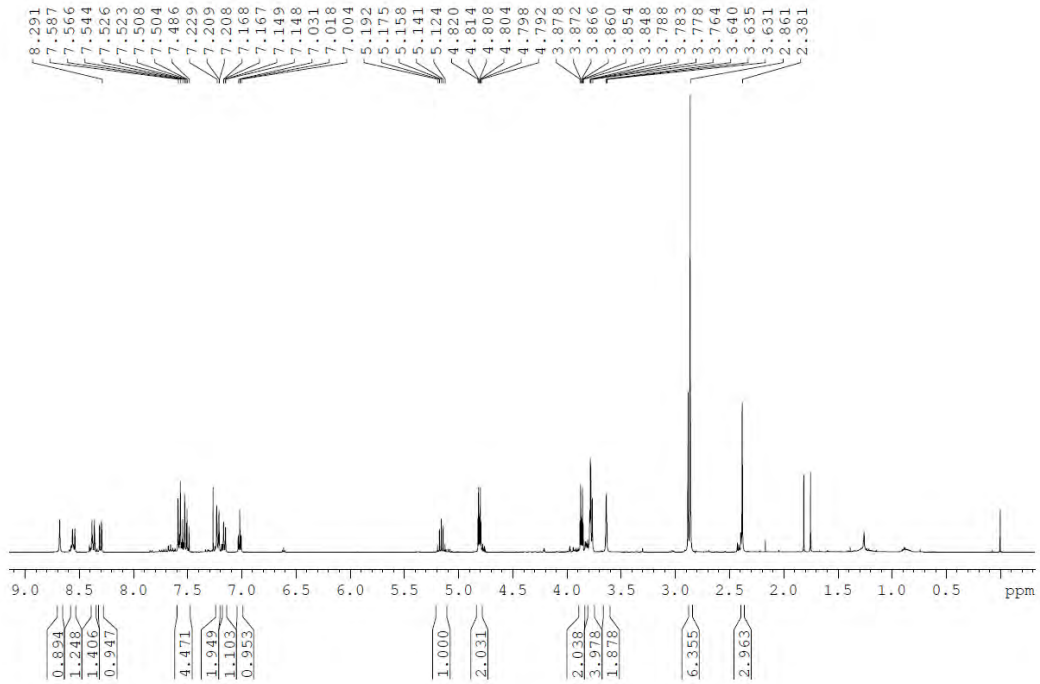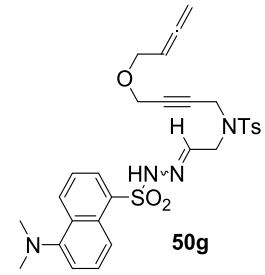
Figure S45: ^{1}H NMR spectrum (400 MHz) of **50g** in CDCl$_3$.
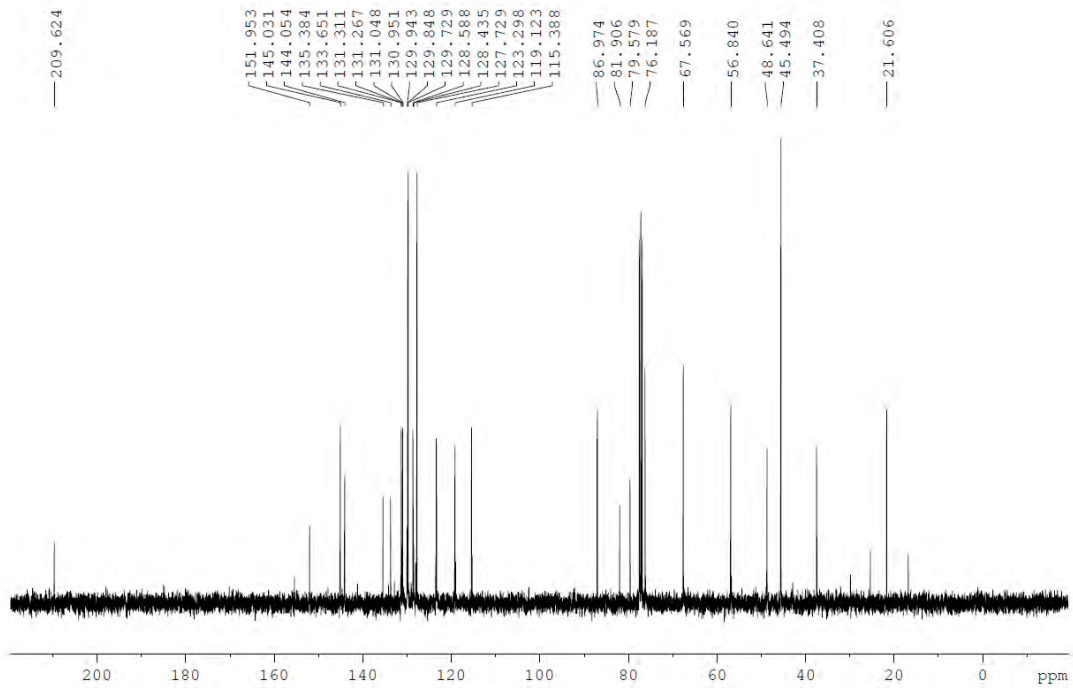
Figure S46: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50g** in CDCl$_3$.
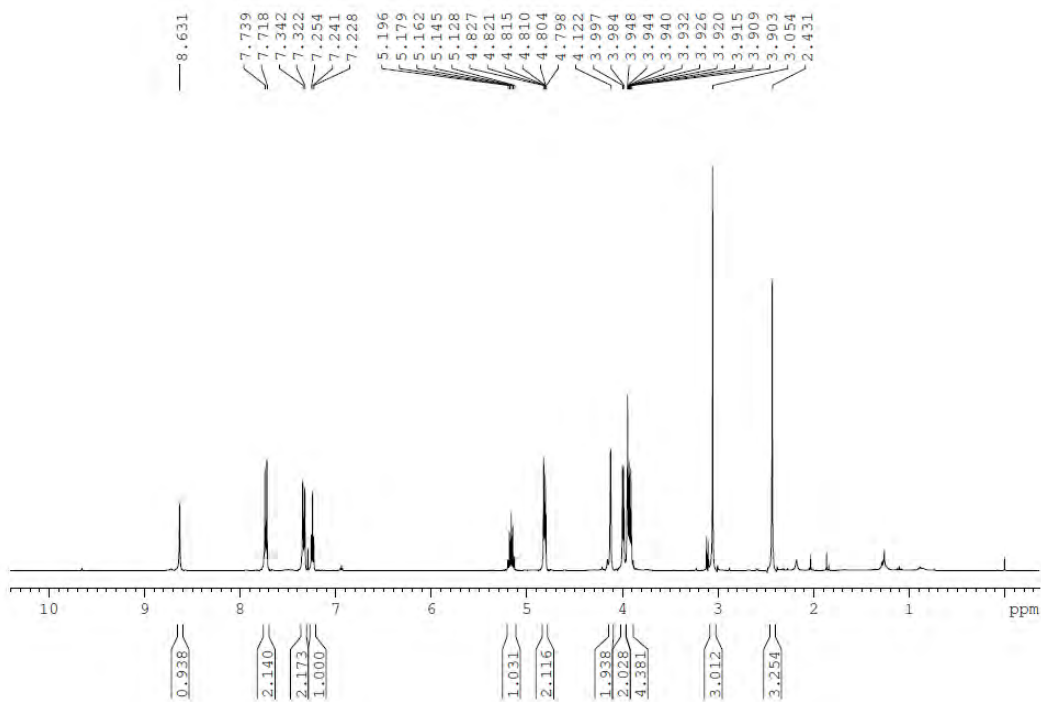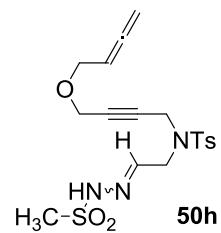
Figure S48: ^{1}H NMR spectrum (400 MHz) of **50h** in CDCl$_3$.
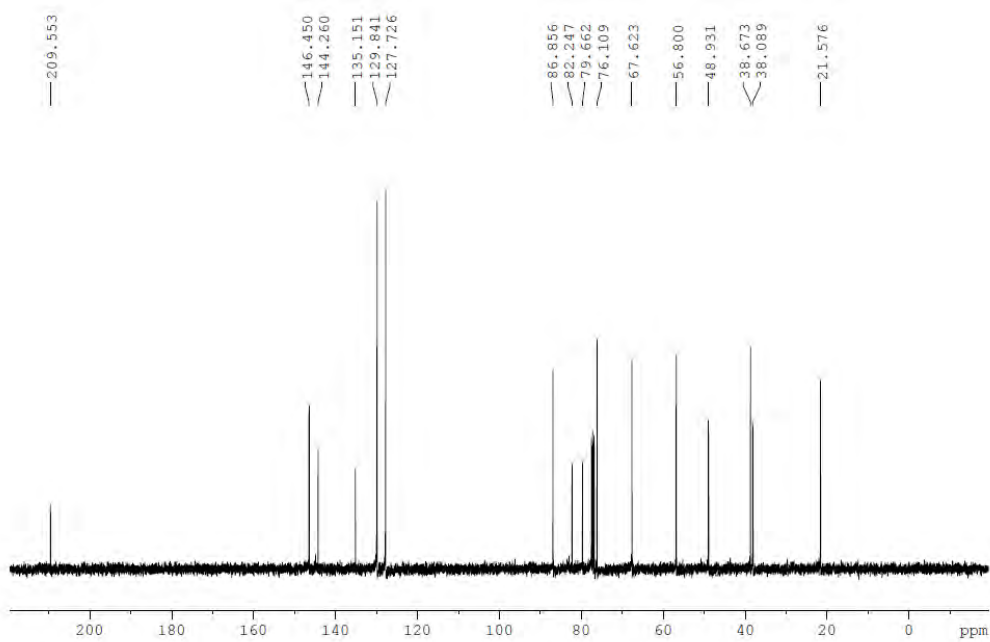
Figure S49: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50h** in CDCl$_3$.
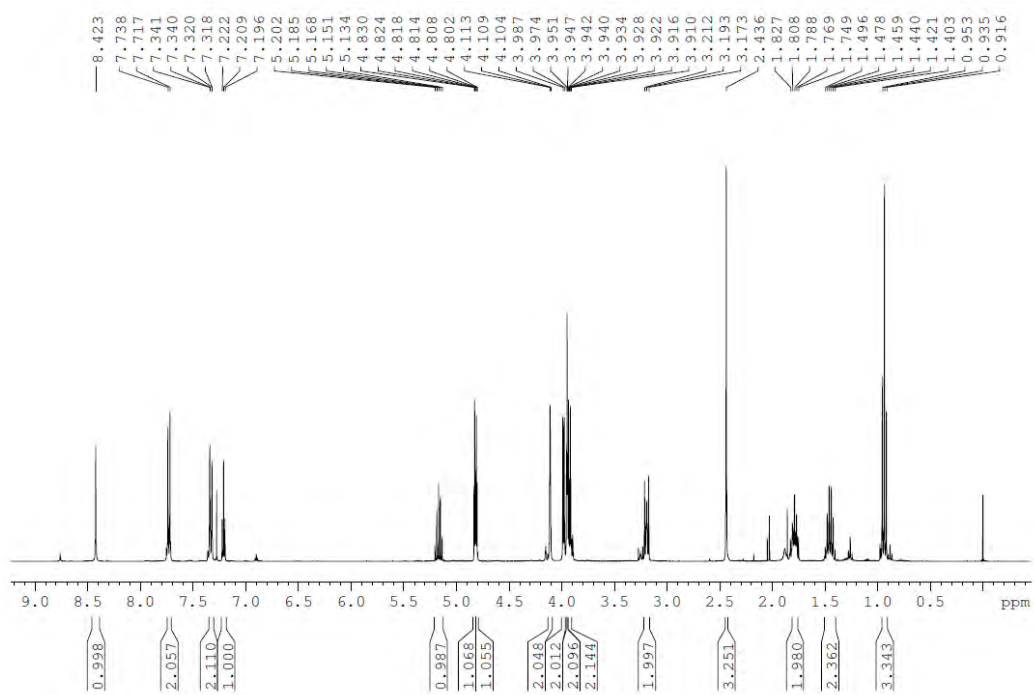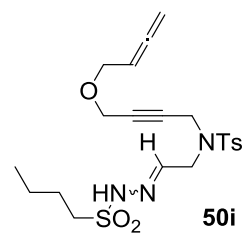
Figure S51: ^{1}H NMR spectrum (400 MHz) of **50i** in CDCl$_3$.
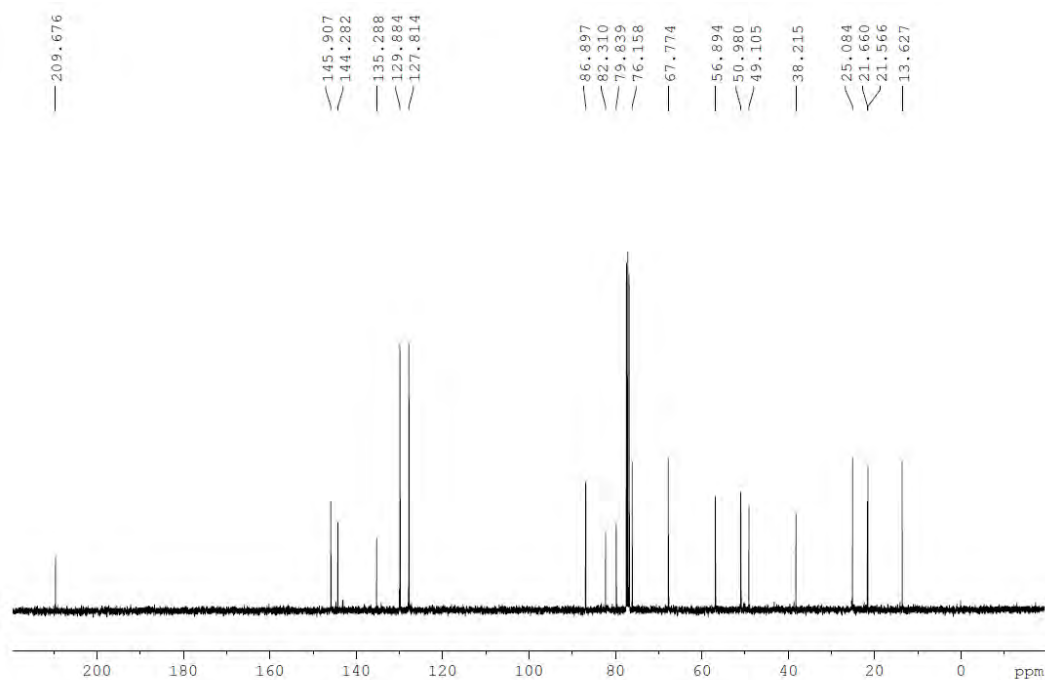
Figure S52: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50i** in CDCl$_3$.
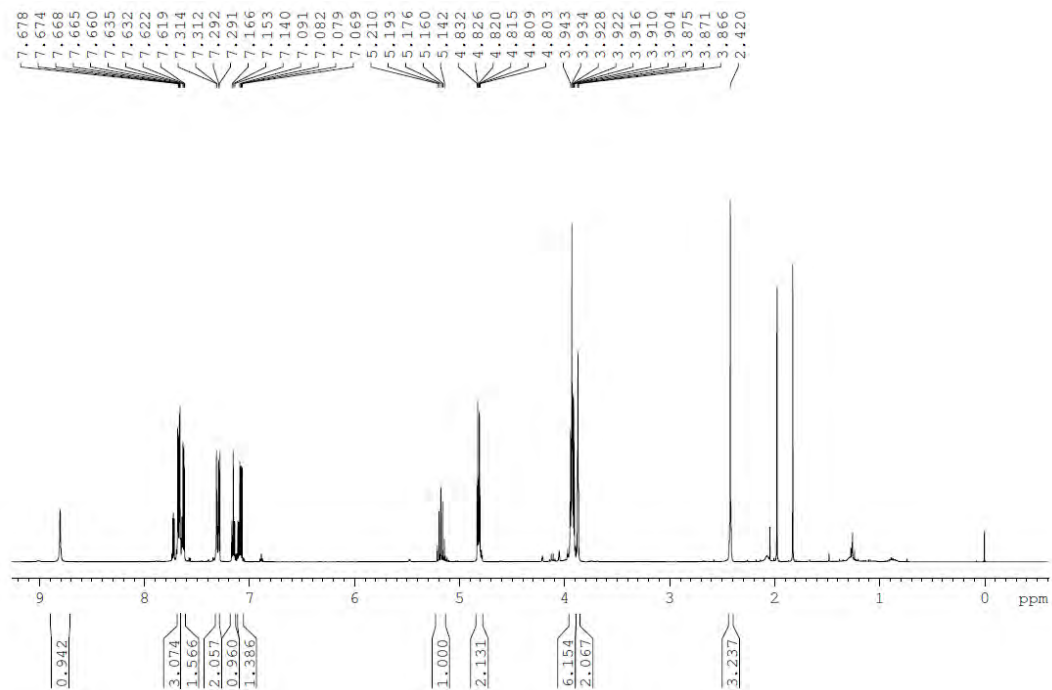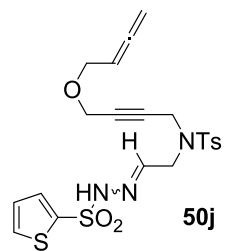
Figure S53: ^{1}H NMR spectrum (400 MHz) of **50j** in CDCl$_3$.
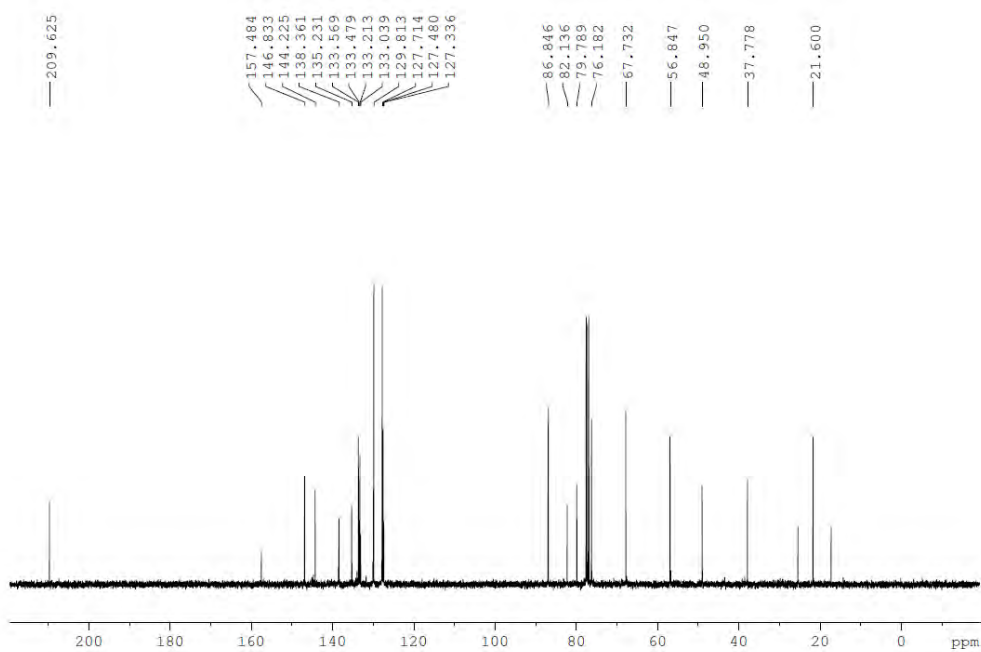
Figure S54: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **50j** in CDCl$_3$.
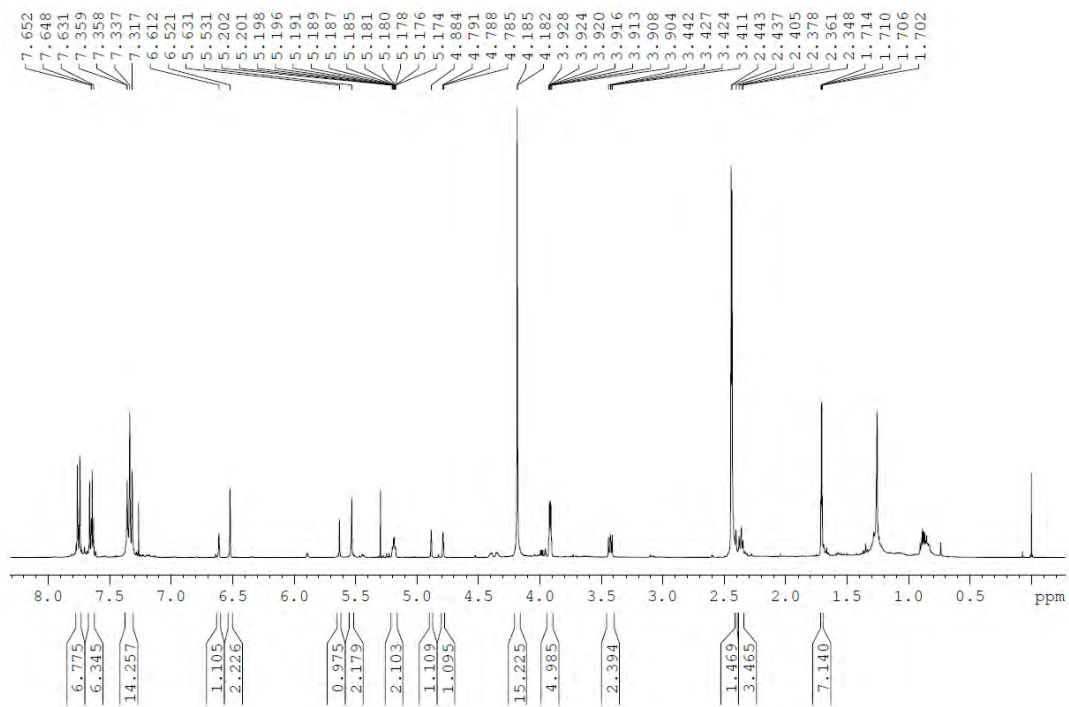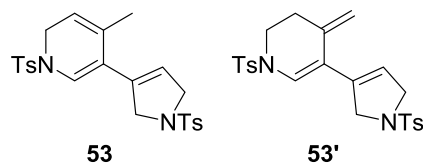
Figure S55: ^{1}H NMR spectrum (400 MHz) of **53** and **53'** in CDCl$_3$.
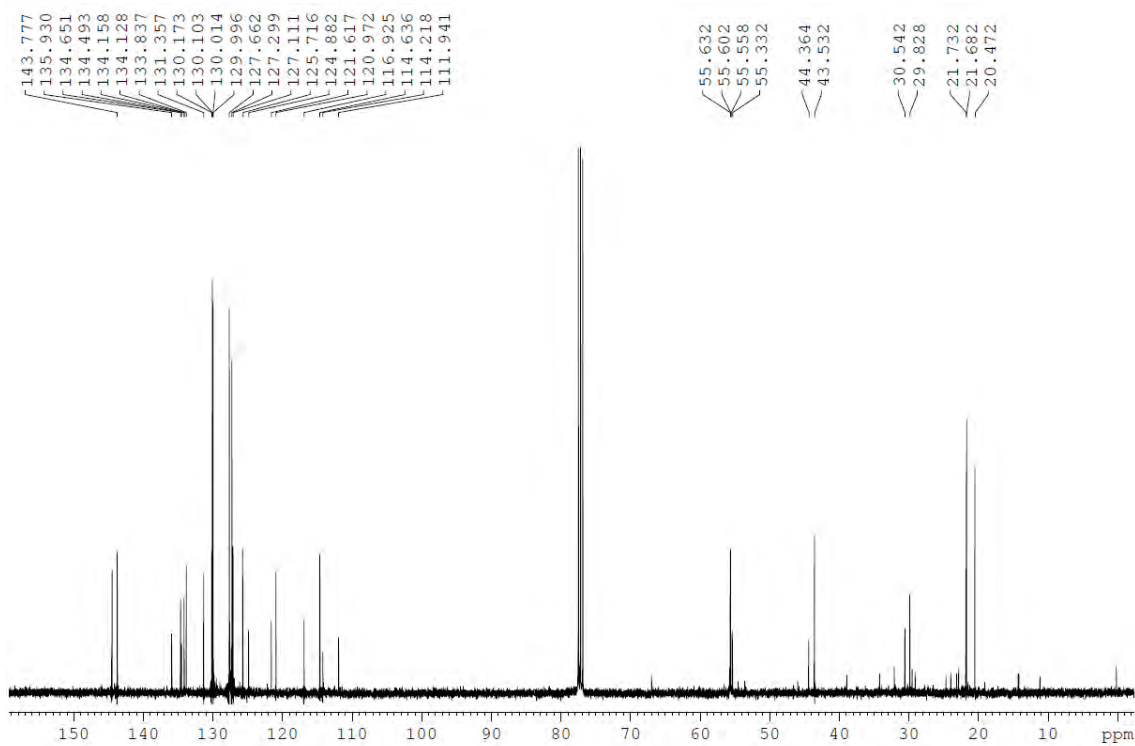
Figure S56: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **53** and **53'** in CDCl$_3$.
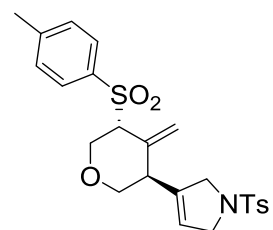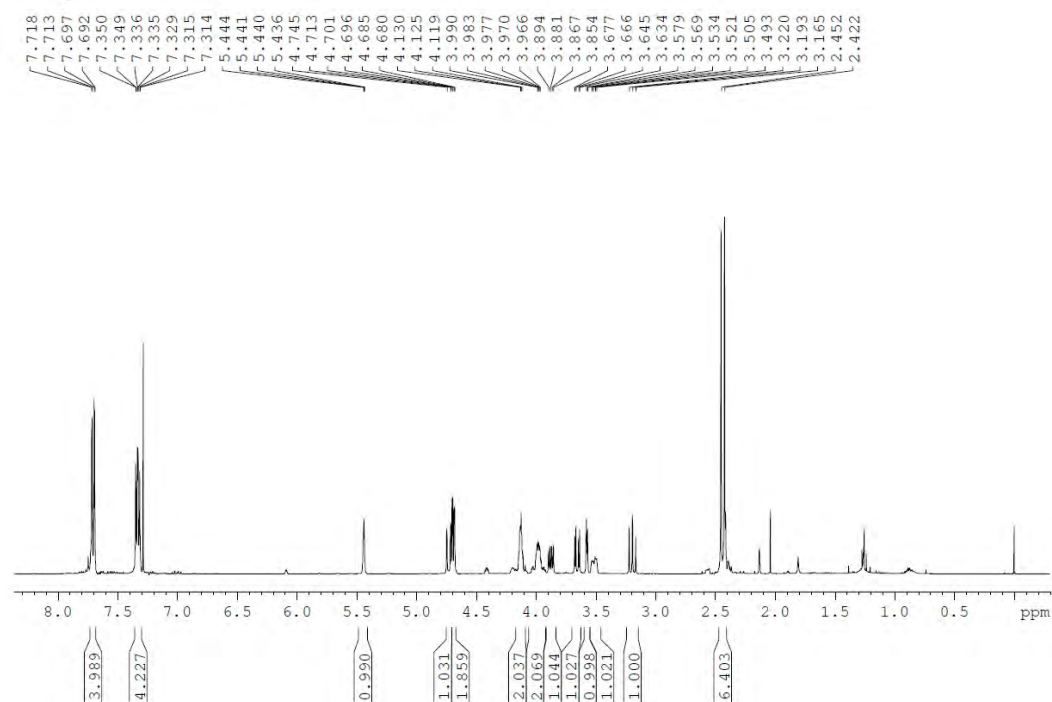
Figure S57: ^{1}H NMR spectrum (400 MHz) of **54a** in CDCl$_3$.
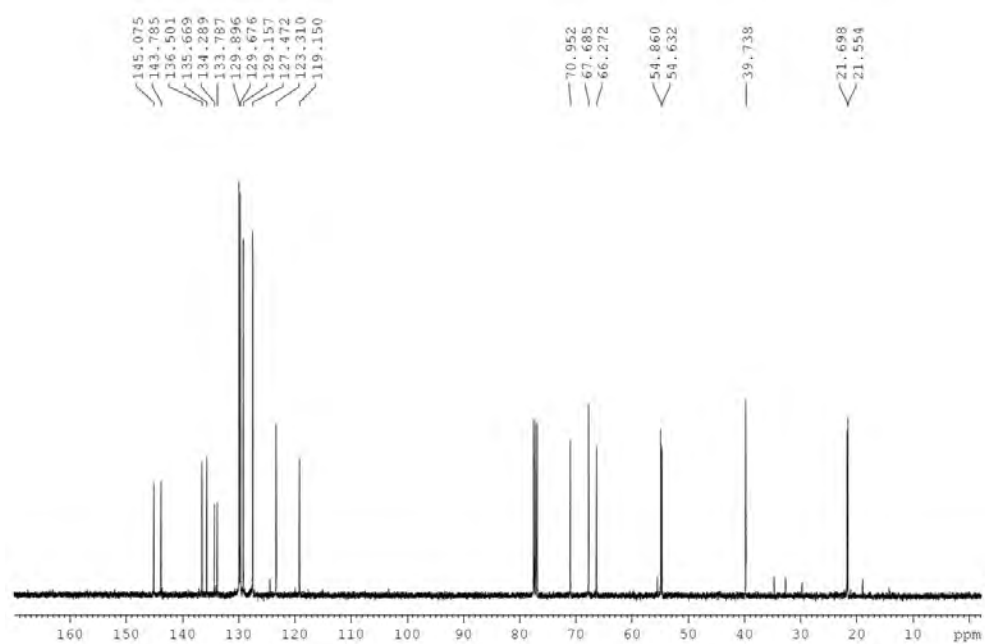
Figure S58: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54a** in CDCl$_3$.

Figure S59: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54a**.
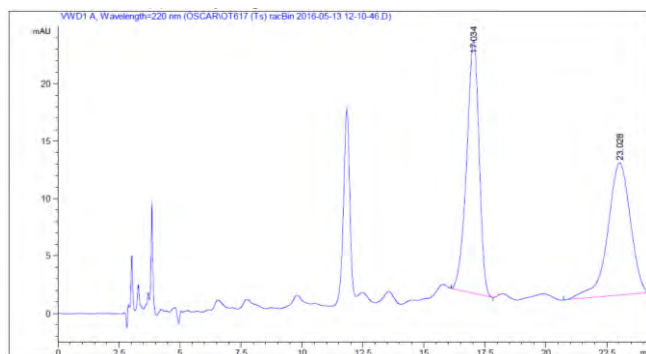
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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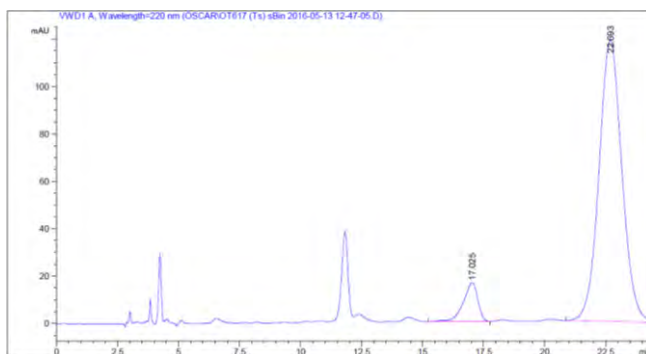
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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2	22.693	BB	1.0041	7752.93604	118.52721	91.8866
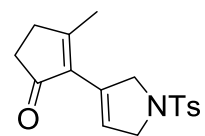
55
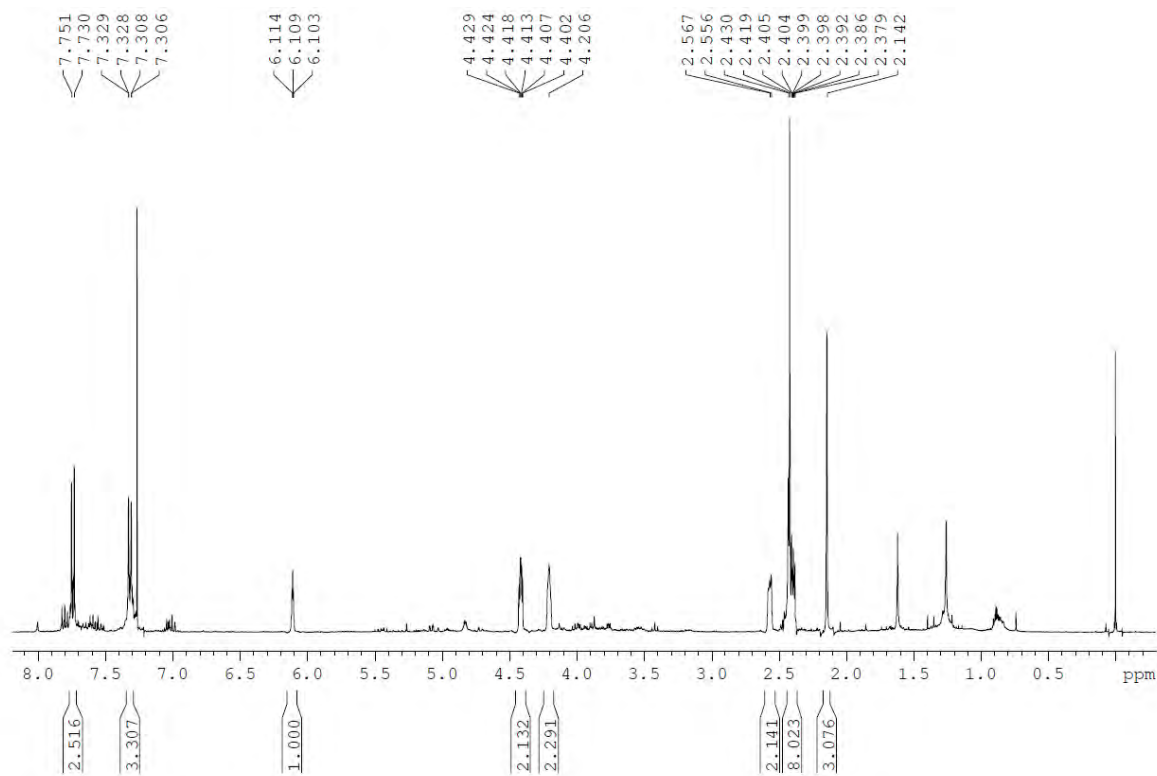
Figure S60: ^{1}H NMR spectrum (400 MHz) of **55** in CDCl$_3$.
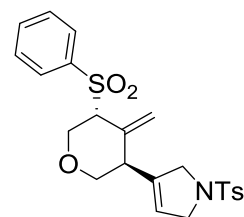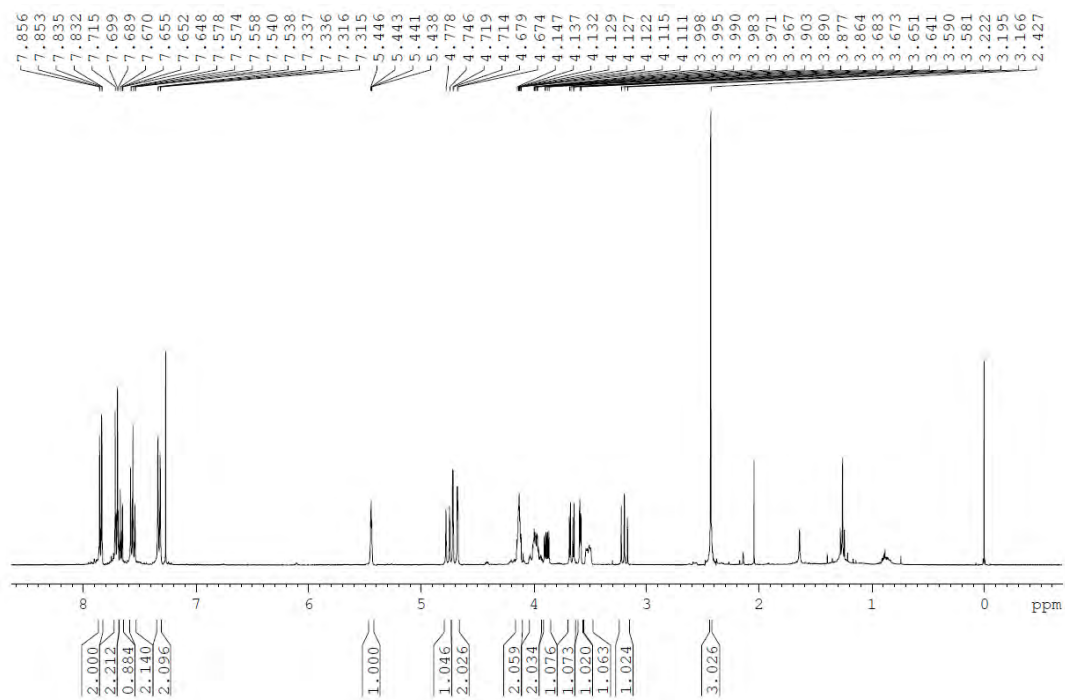
Figure S61: ^{1}H NMR spectrum (400 MHz) of **54b** in CDCl$_3$.
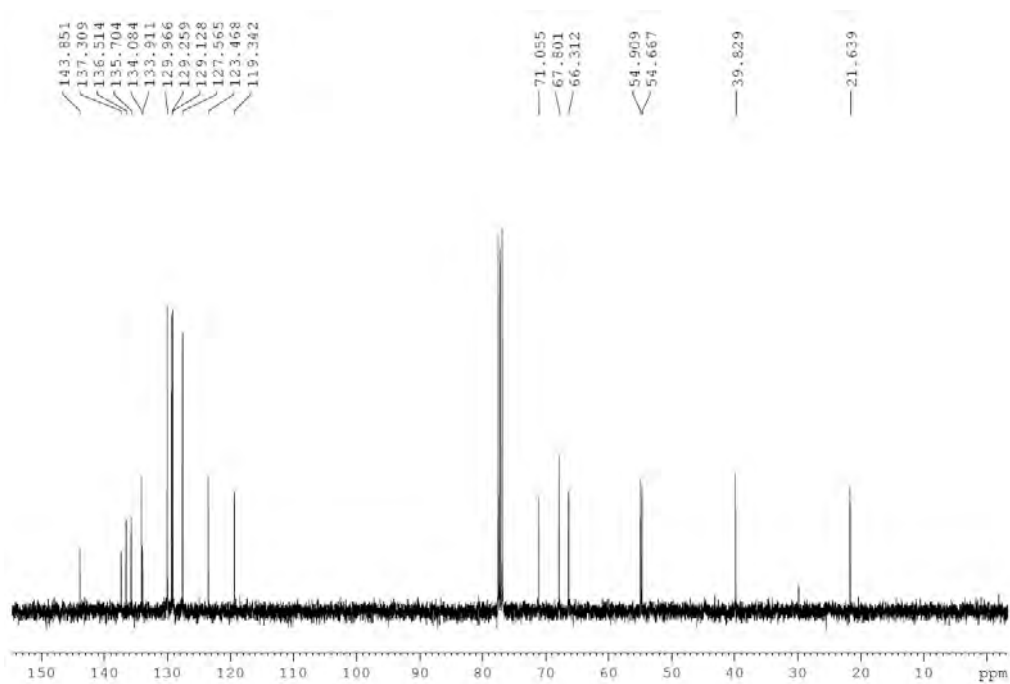
Figure S62: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54b** in CDCl$_3$.

Figure S64: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54b**.
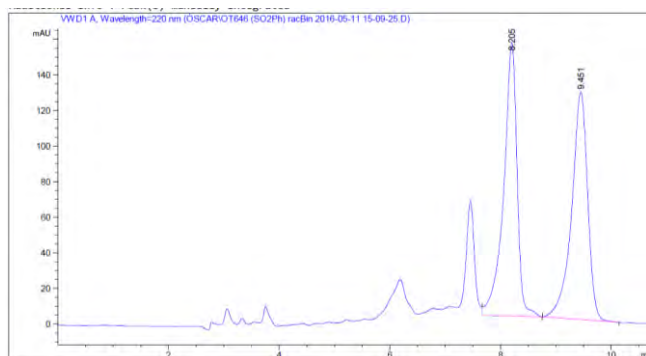

```
Peak RetTime Type  Width     Area      Height    Area
 #    [min]        [min]    [mAU*s]    [mAU]      %
----|-------|----|-------|----------|----------|--------|
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 2    9.451  BB   0.2996 2572.07935 127.89095  49.8142
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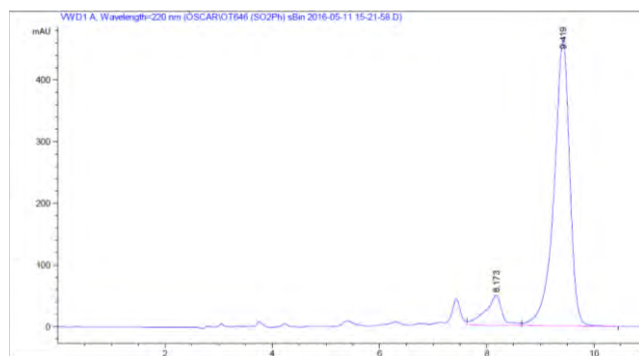


```
Peak RetTime Type  Width     Area      Height    Area
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```
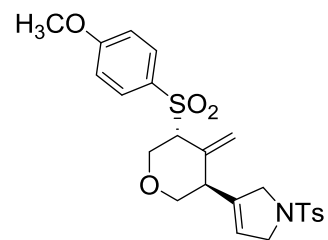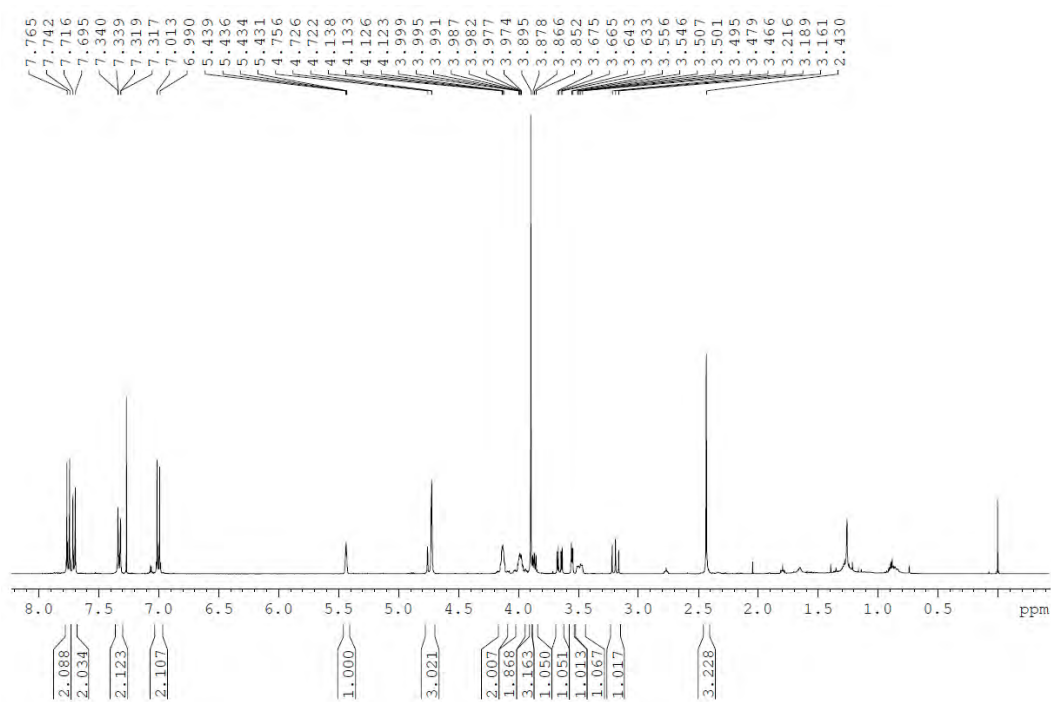
Figure S65: ^{1}H NMR spectrum (400 MHz) of **54c** in CDCl$_3$.
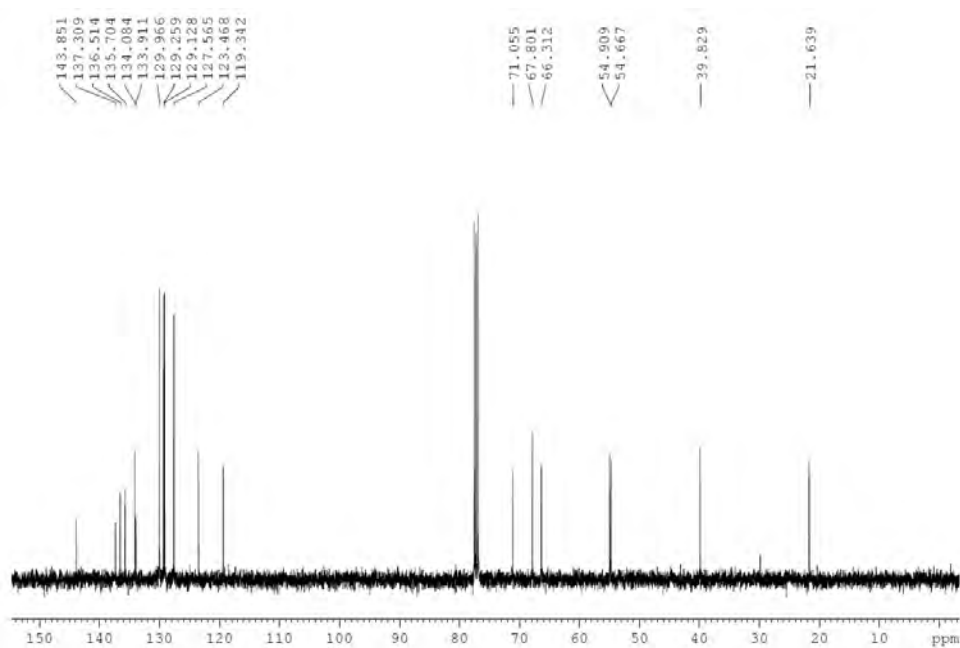
Figure S66: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54c** in CDCl$_3$.

Figure S67: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54c**.
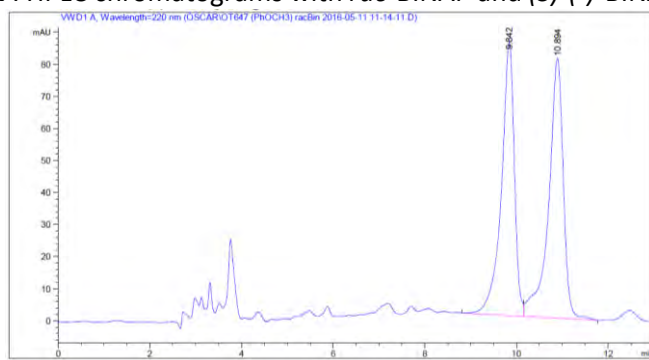

```
Peak RetTime Type  Width     Area      Height     Area
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 2  10.894 VB    0.3255 1802.29626   81.04118  51.7102
```
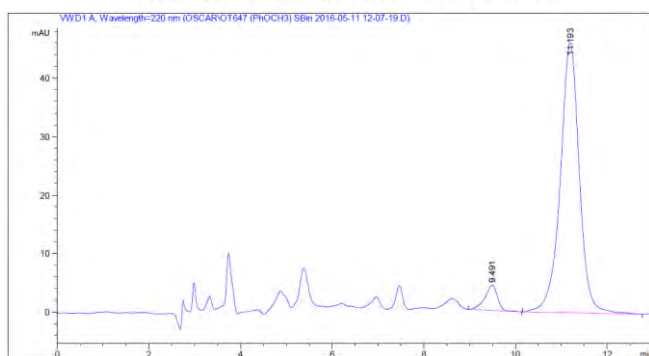


```
Peak RetTime Type  Width     Area      Height     Area
 #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
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 2  11.193 BB    0.4334 1332.61035   46.21558  94.1840
```
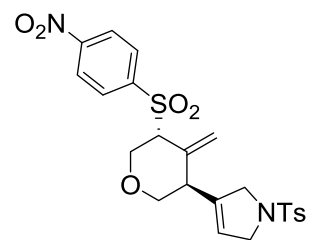
54d
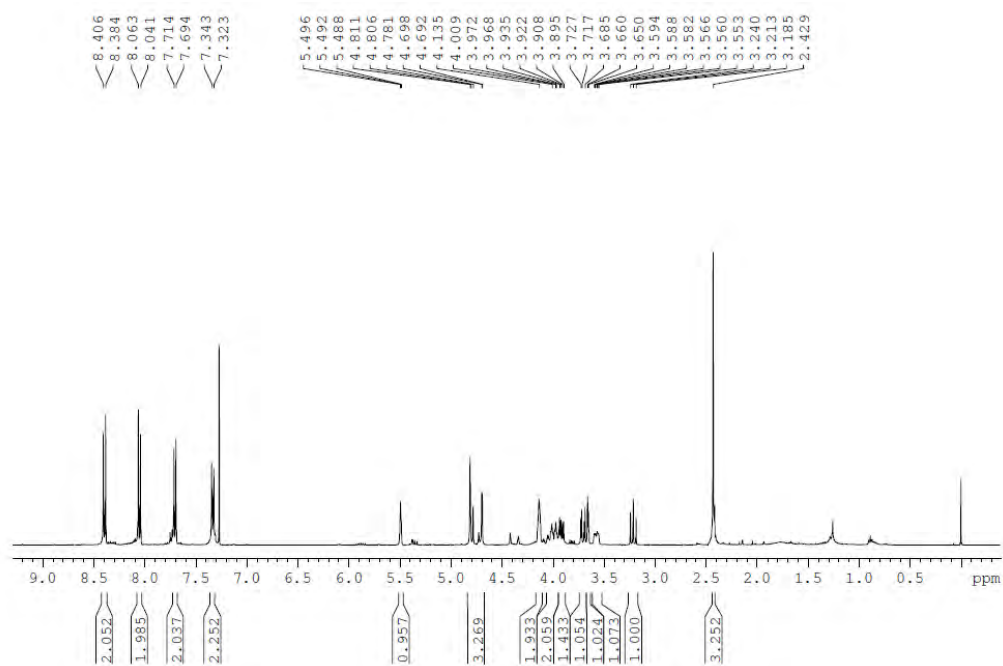
Figure S68: ^{1}H NMR spectrum (400 MHz) of **54d** in CDCl$_3$.
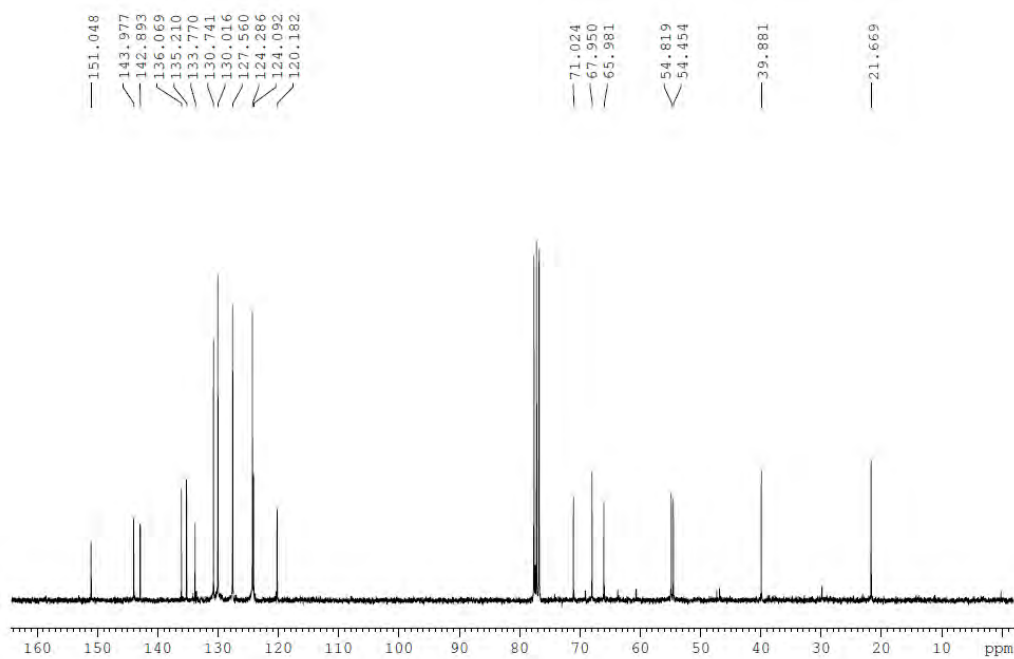
Figure S69: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4d** in CDCl$_3$.

Figure S70: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54d**.
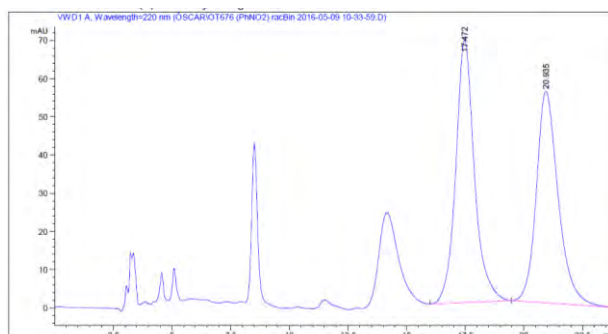

```
Peak  RetTime Type  Width     Area      Height    Area
 #     [min]        [min]   [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
  1   17.472 BB   0.8236 3798.95630  68.64777  51.4397
  2   20.935 BBA  0.9719 3586.30005  55.35153  48.5603
```
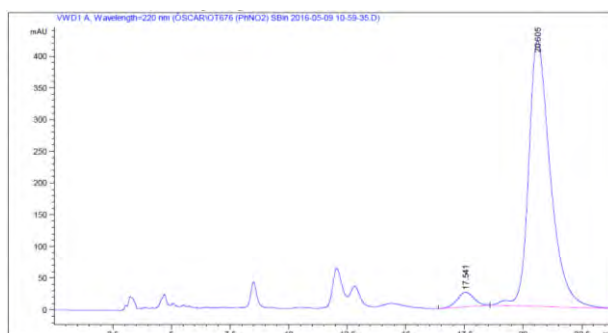


```
Peak  RetTime Type  Width     Area      Height    Area
 #     [min]        [min]   [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
  1   17.541 BB   0.7489 1128.23279  23.05537   4.0254
  2   20.605 VBAR 0.9587 2.68995e4  418.88434  95.9746
```

54e
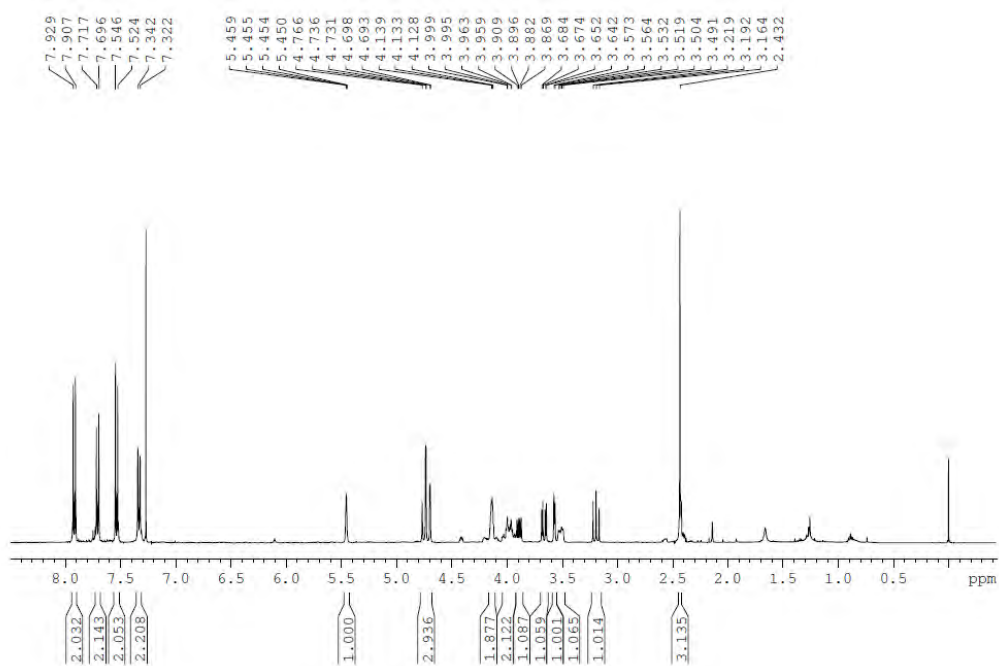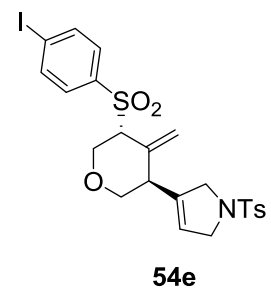
Figure S71: ^{1}H NMR spectrum (400 MHz) of **54e** in CDCl$_3$.
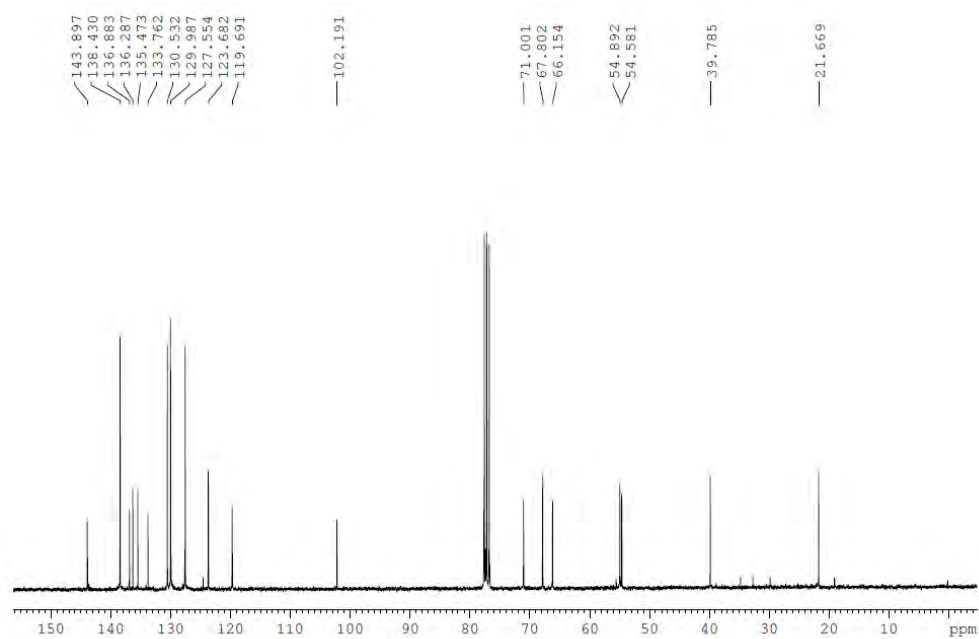
Figure S72: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54e** in CDCl$_3$.

Figure S73: HPLC chromatograms with *rc*-BINAP and *(S)-(-)*-BINAP for **54e**.
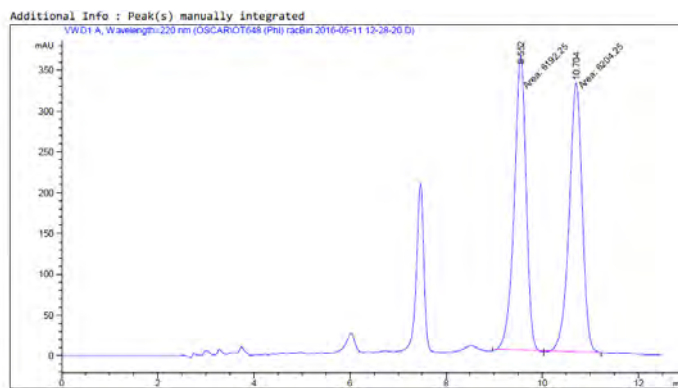
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.552	MF	0.2865	6192.24512	360.18045	49.9516
2	10.704	FM	0.3137	6204.24951	329.65921	50.0484
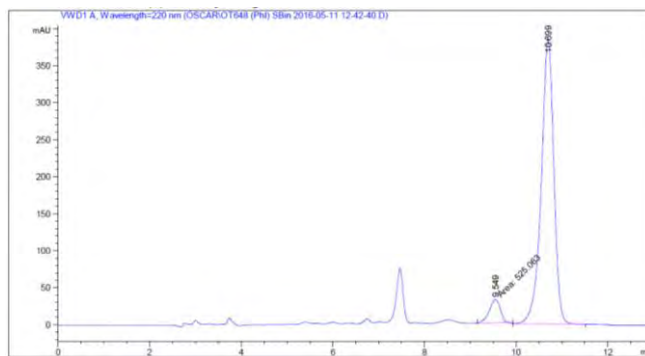
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.549	MM	0.2778	525.06299	31.50030	6.6903
2	10.699	VB	0.2886	7323.03467	383.81519	93.3097
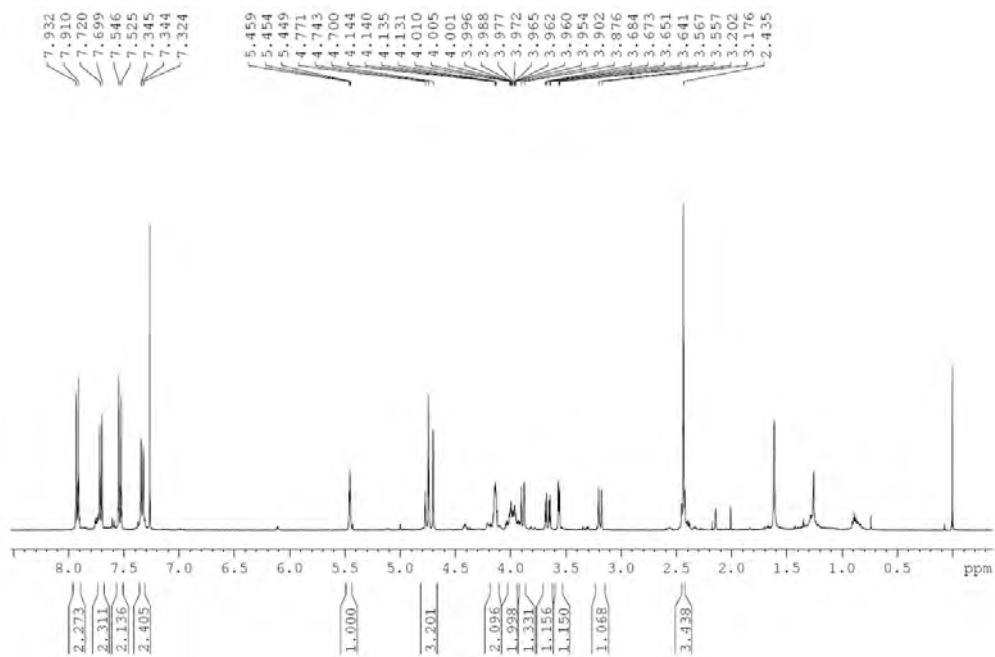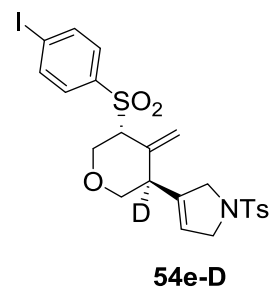
Figure S74: ^{1}H NMR spectrum (400 MHz) of **54e-D** in CDCl$_3$.
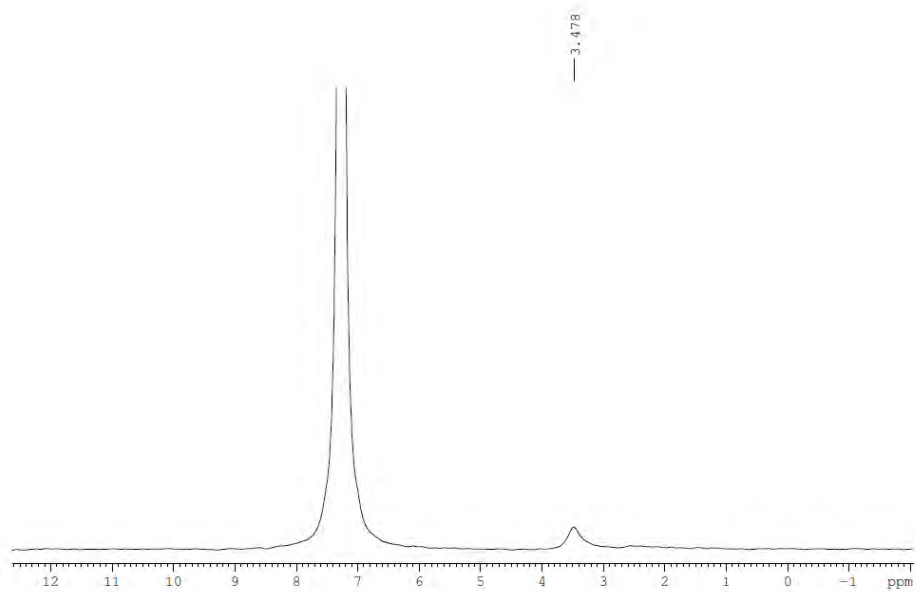
Figure S75: ^{2}H NMR spectrum (61 MHz) of **54e-D** in CHCl$_3$.
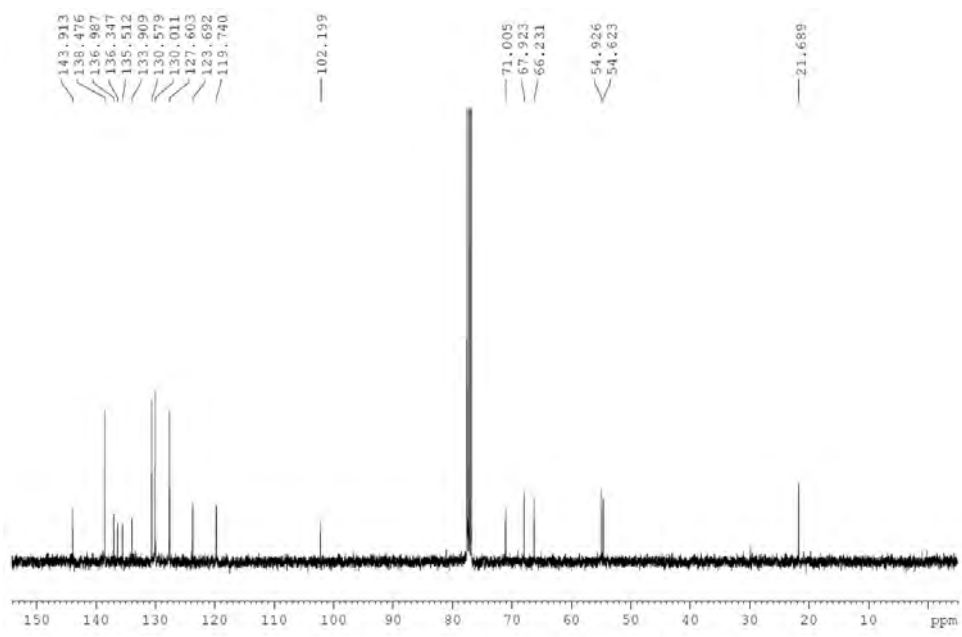
Figure S76: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **54e-D** in CDCl$_3$.
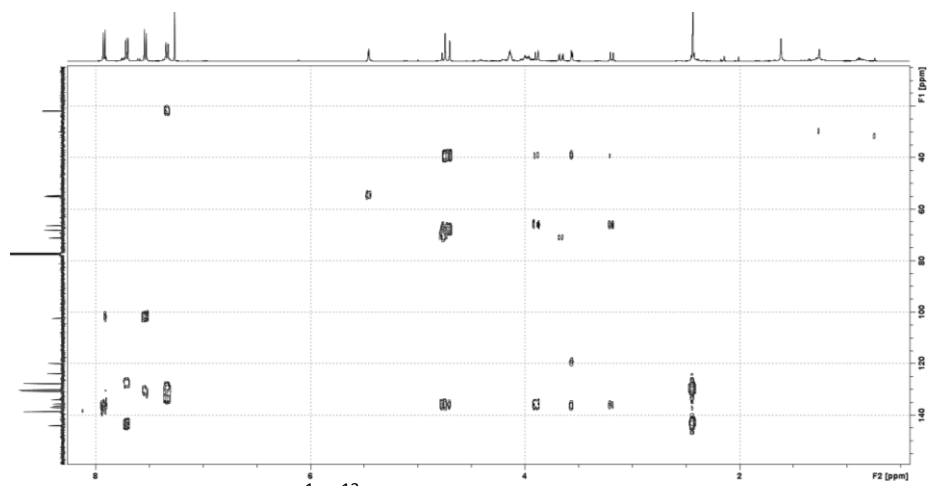
Figure S77: 2D ^{1}H-^{13}C HMBC correlation of **54e-D** in CDCl$_3$.

54f   **55**
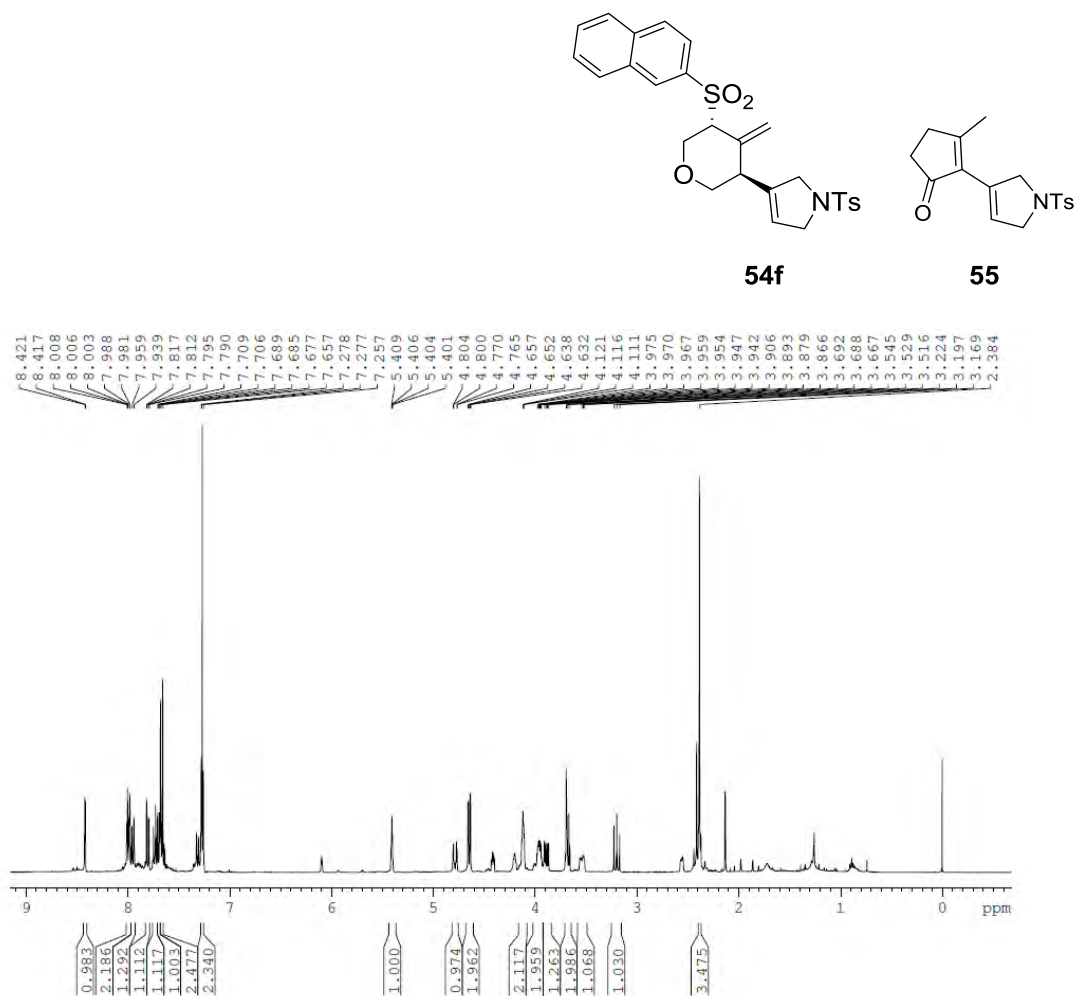
Figure S78: ^{1}H NMR spectrum (400 MHz) of **54f** and **55** in CDCl$_3$.
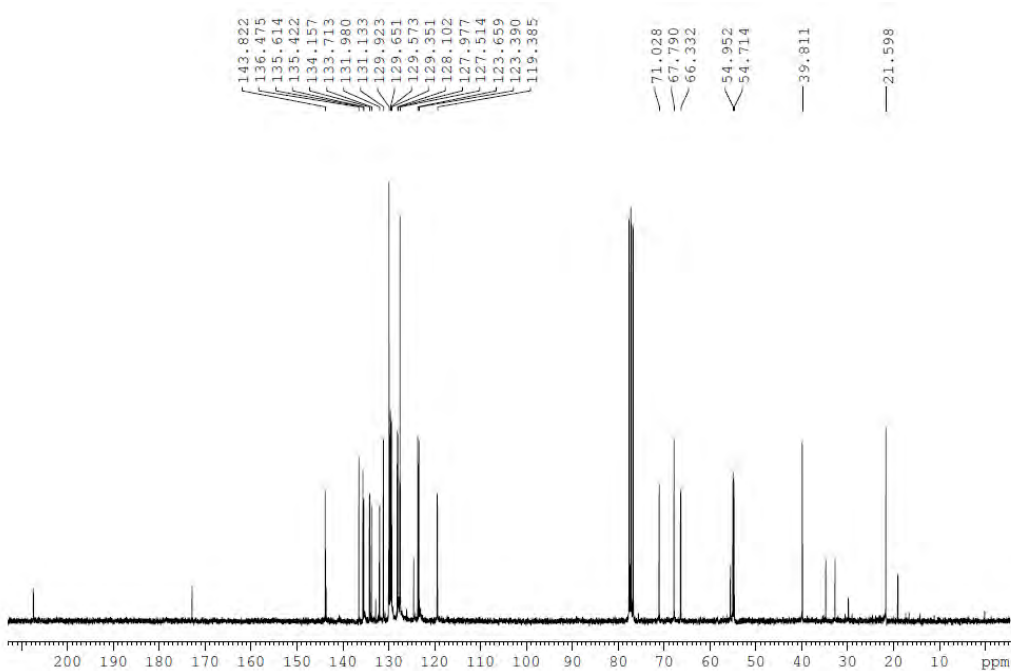
Figure S79: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54f** and **55** in CDCl$_3$.

Figure S80: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54f** and **55**.
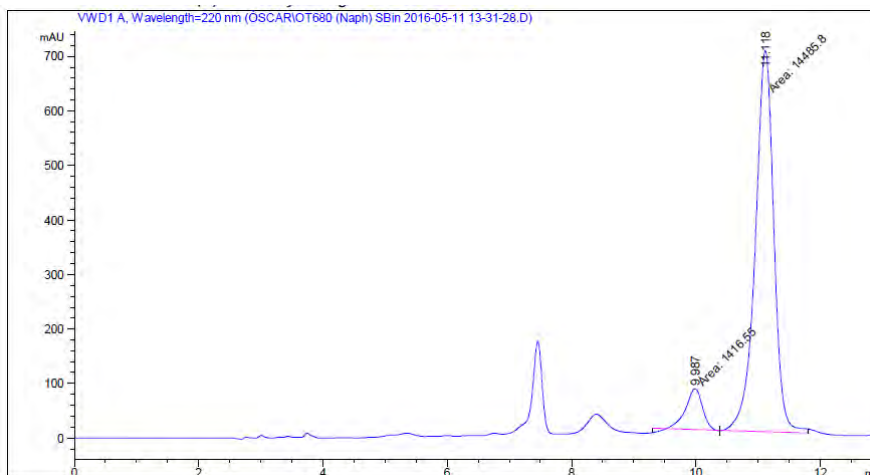
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.987	MF	0.3154	1416.54834	74.85448	8.9078
2	11.118	FM	0.3456	1.44858e4	698.62634	91.0922
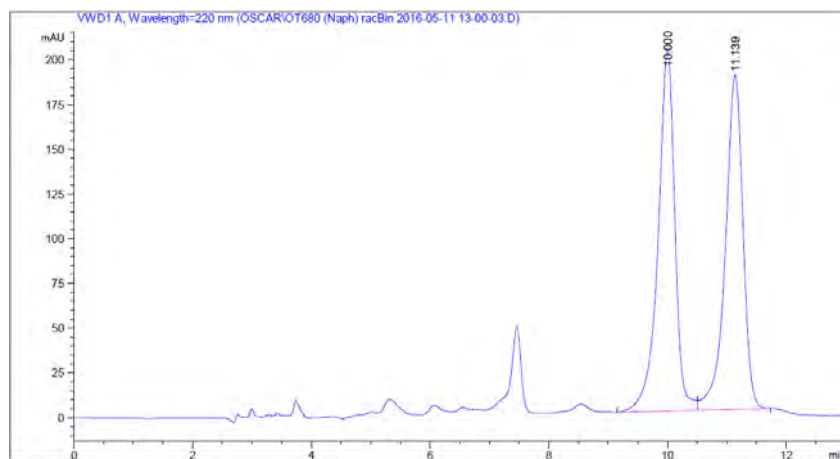
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.000	BV	0.2948	3995.48901	201.93044	50.8017
2	11.139	VB	0.3124	3869.38843	187.04228	49.1983
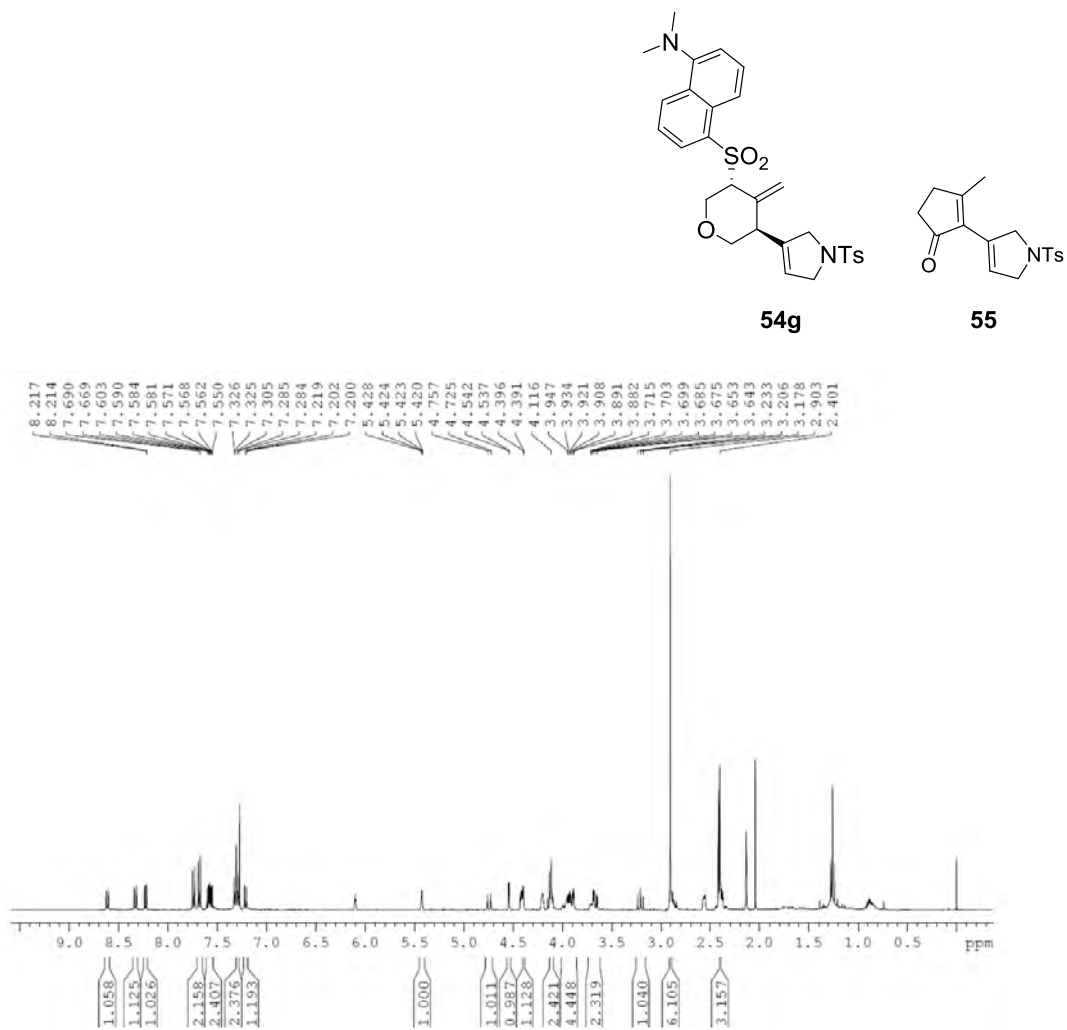
Figure S81: ^{1}H NMR spectrum (400 MHz) of **54g** and **55** in CDCl$_3$.
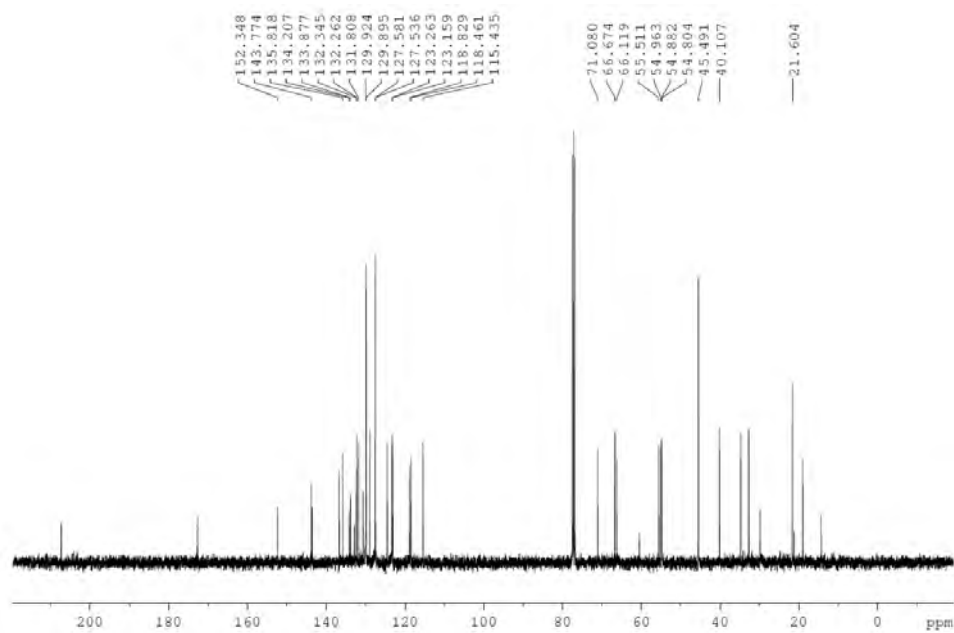
Figure S82: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54g** and **55** in CDCl$_3$.

Figure S83: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54g** and **55**.
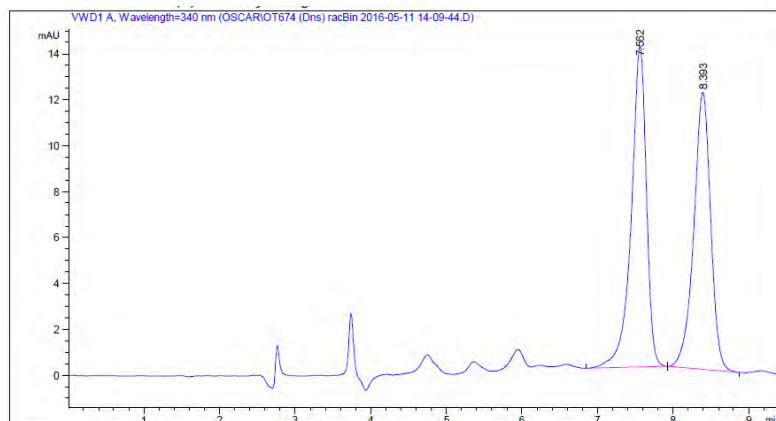

```
Peak RetTime Type  Width     Area      Height    Area
  #   [min]        [min]   [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
  1   7.562 BB    0.2074  194.30940  13.95584  50.9750
  2   8.393 BB    0.2347  186.87616  12.06372  49.0250
```
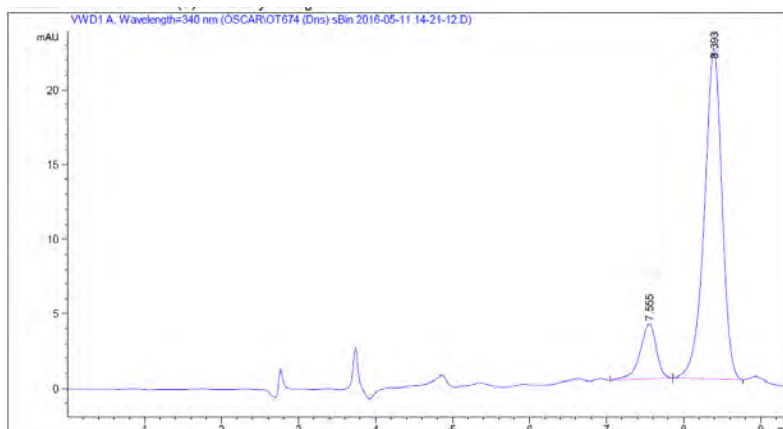


```
Peak RetTime Type  Width     Area      Height    Area
  #   [min]        [min]   [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
  1   7.555 BB    0.2245   53.87198   3.68561  13.2600
  2   8.393 BB    0.2420  352.40271  22.10864  86.7400
```
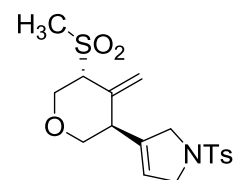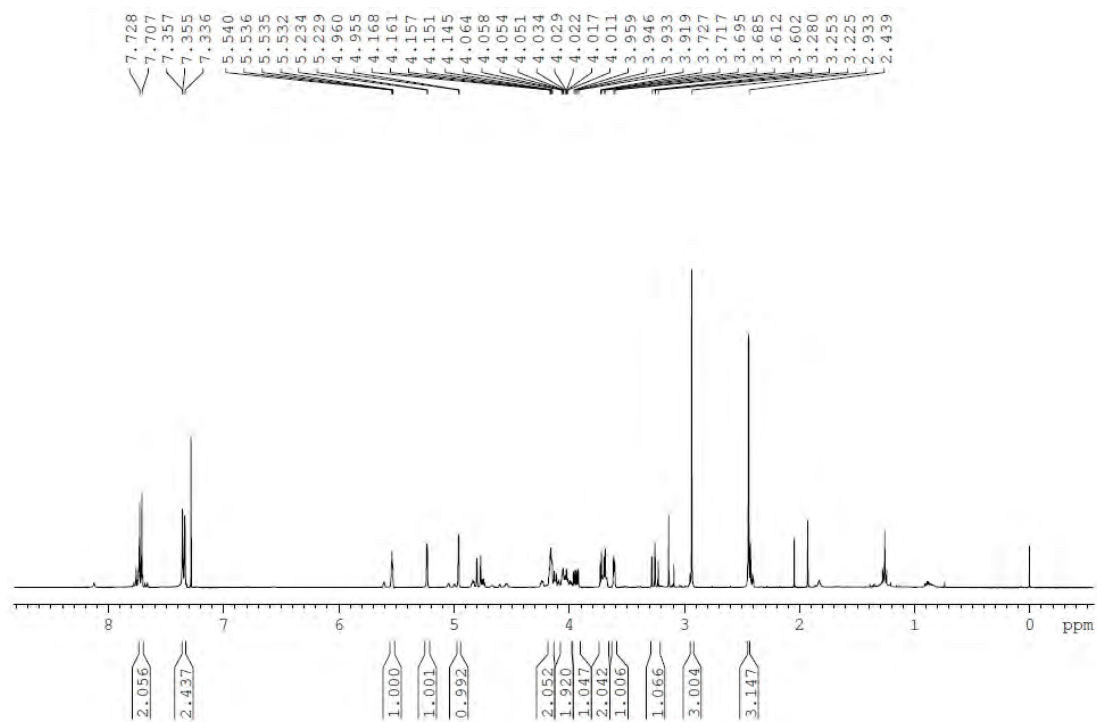
Figure S84: ^{1}H NMR spectrum (400 MHz) of **54h** in CDCl$_3$.
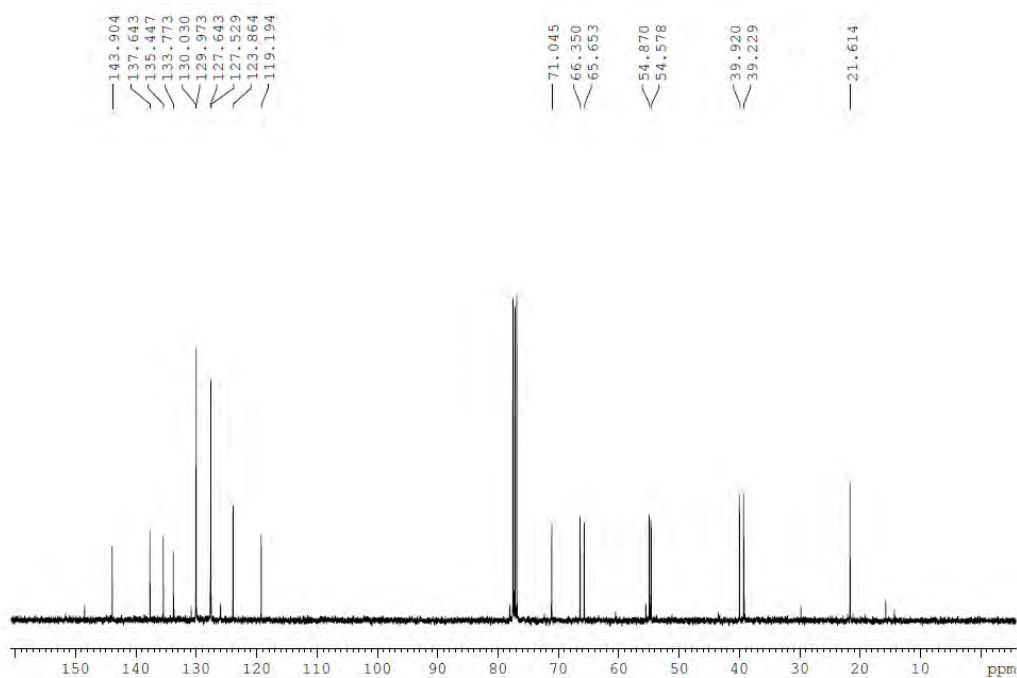
Figure S85: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54h** in CDCl$_3$.

Figure S86: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54h**.

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.963	BV	0.6549	1.29495e4	283.50995	47.7959
2	19.775	VB	0.6569	1.41439e4	314.37537	52.2041

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.830	MF	0.8716	900.24341	17.21378	6.8634
2	19.510	FM	0.7974	1.22164e4	255.34004	93.1366
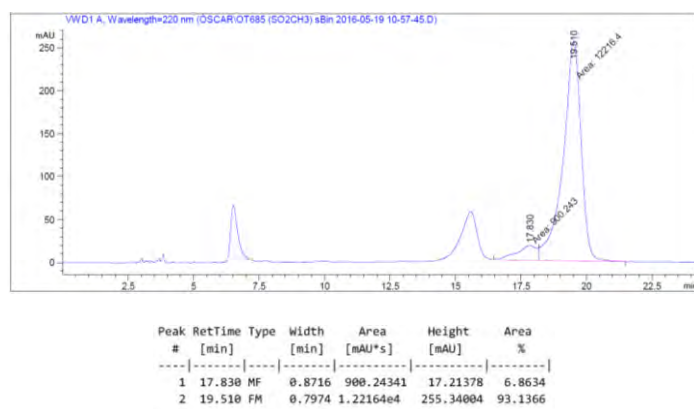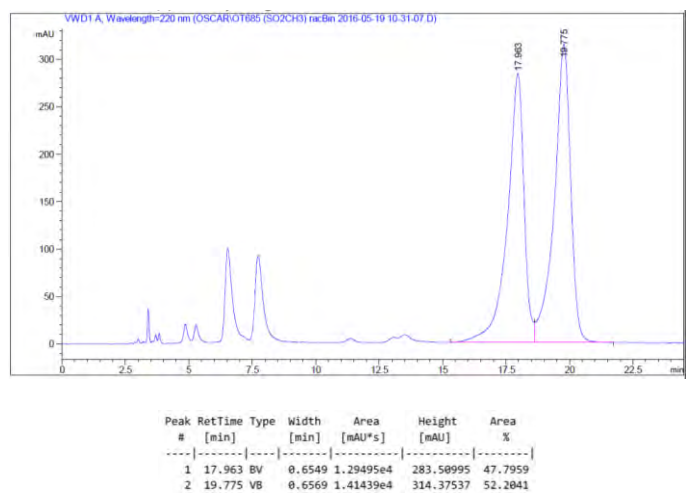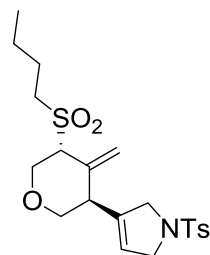
54i
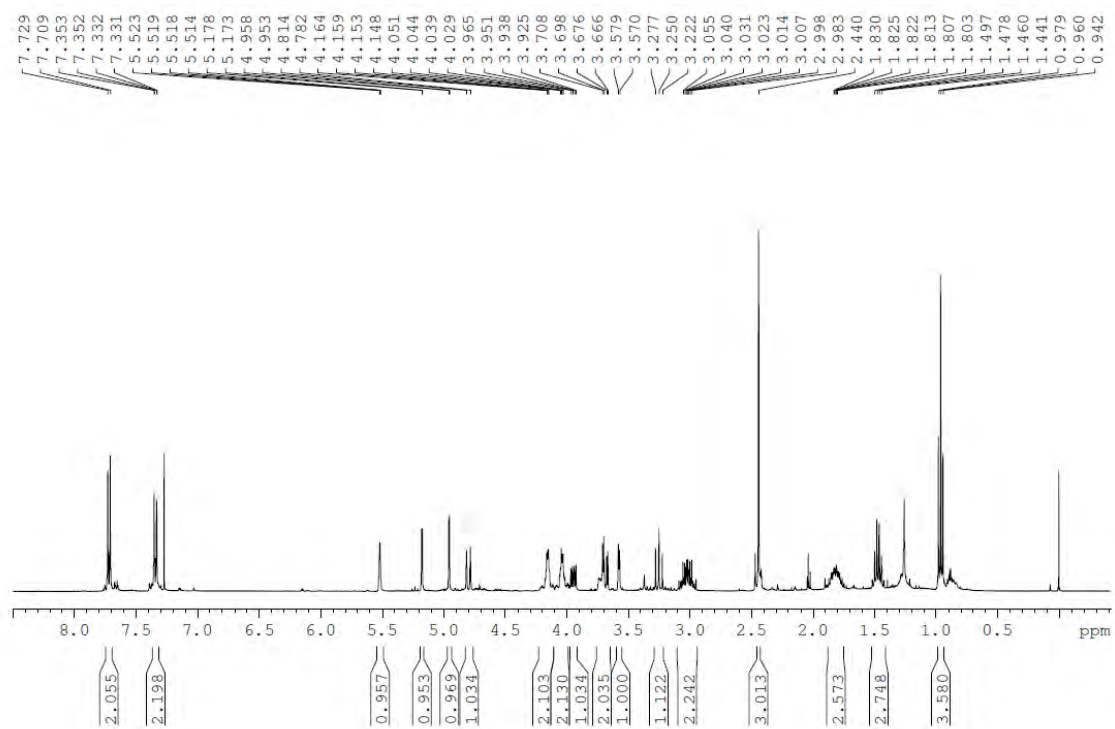
Figure S87: ^{1}H NMR spectrum (400 MHz) of **54i** in CDCl$_3$.
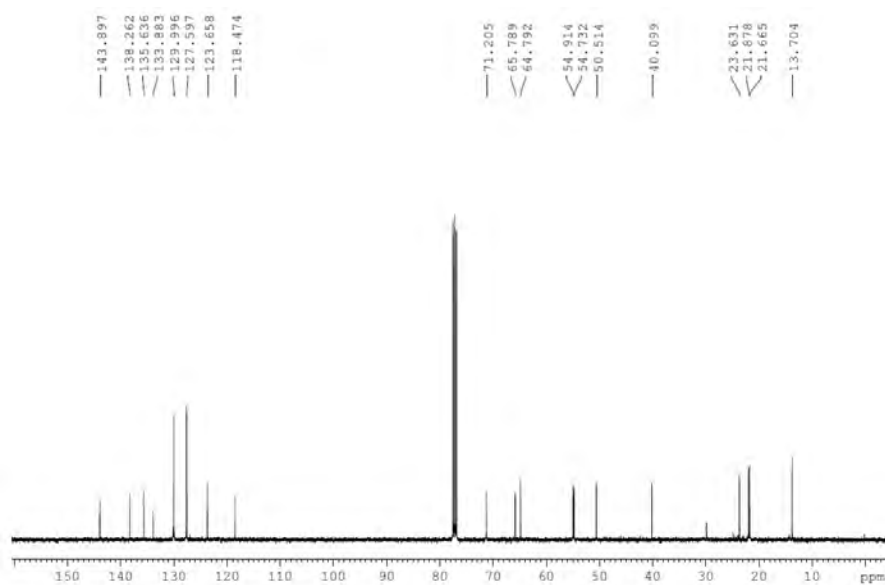
Figure S88: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54i** in CDCl$_3$.

Figure S89: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54i**.
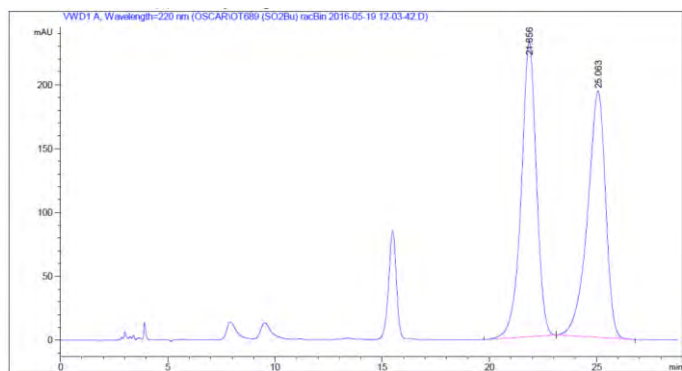

```
Peak RetTime Type  Width     Area      Height    Area
 #   [min]        [min]   [mAU*s]    [mAU]      %
----|-------|----|-------|----------|----------|--------|
 1   21.856 BB   0.7386 1.13577e4   230.61523  50.1925
 2   25.063 BB   0.8750 1.12706e4   192.79381  49.8075
```
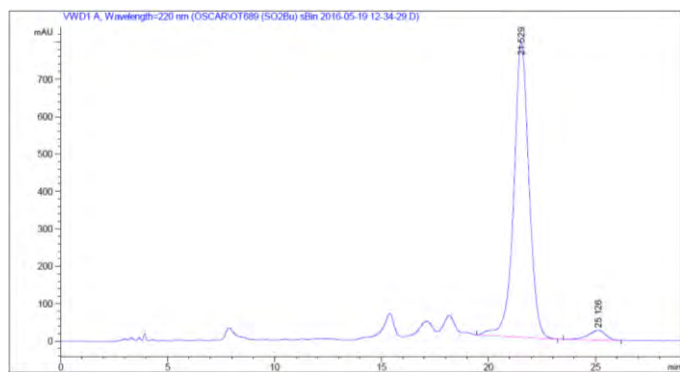


```
Peak RetTime Type  Width     Area       Height    Area
 #   [min]        [min]   [mAU*s]     [mAU]      %
----|-------|----|-------|-----------|----------|--------|
 1   21.529 VB R 0.7370 3.89881e4    788.88440  96.4638
 2   25.126 BB   0.8204 1429.22351    25.91453   3.5362
```
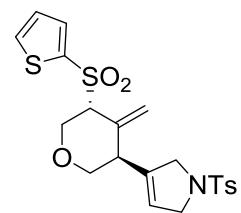
54j
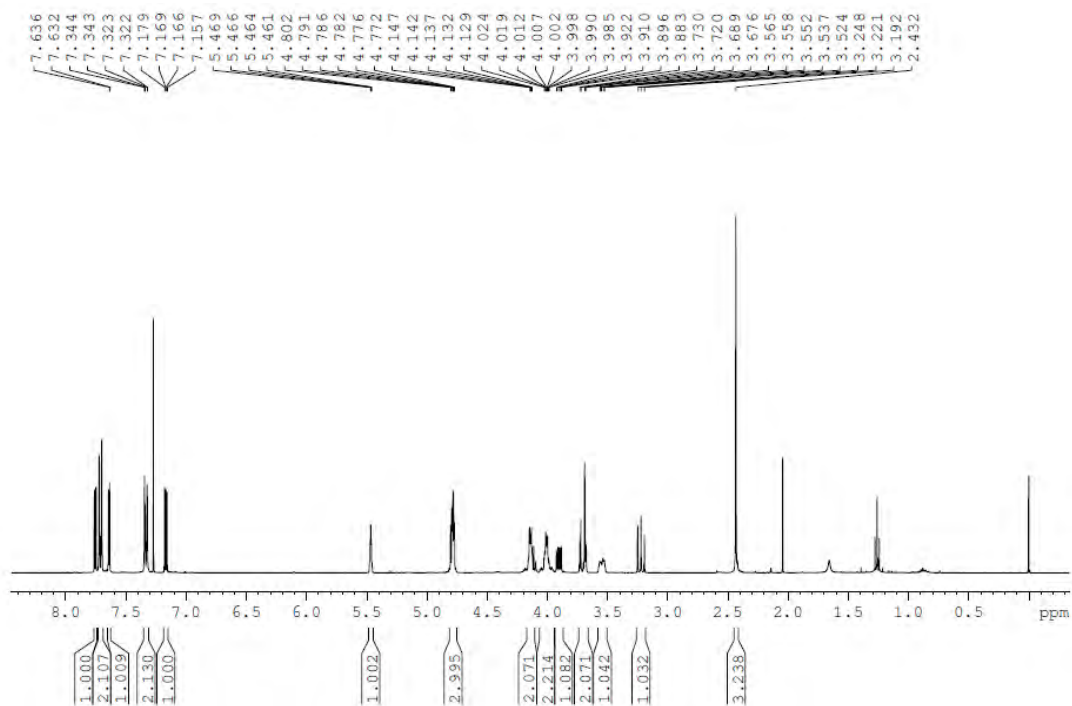
Figure S90: ^{1}H NMR spectrum (400 MHz) of **54j** in CDCl$_3$.

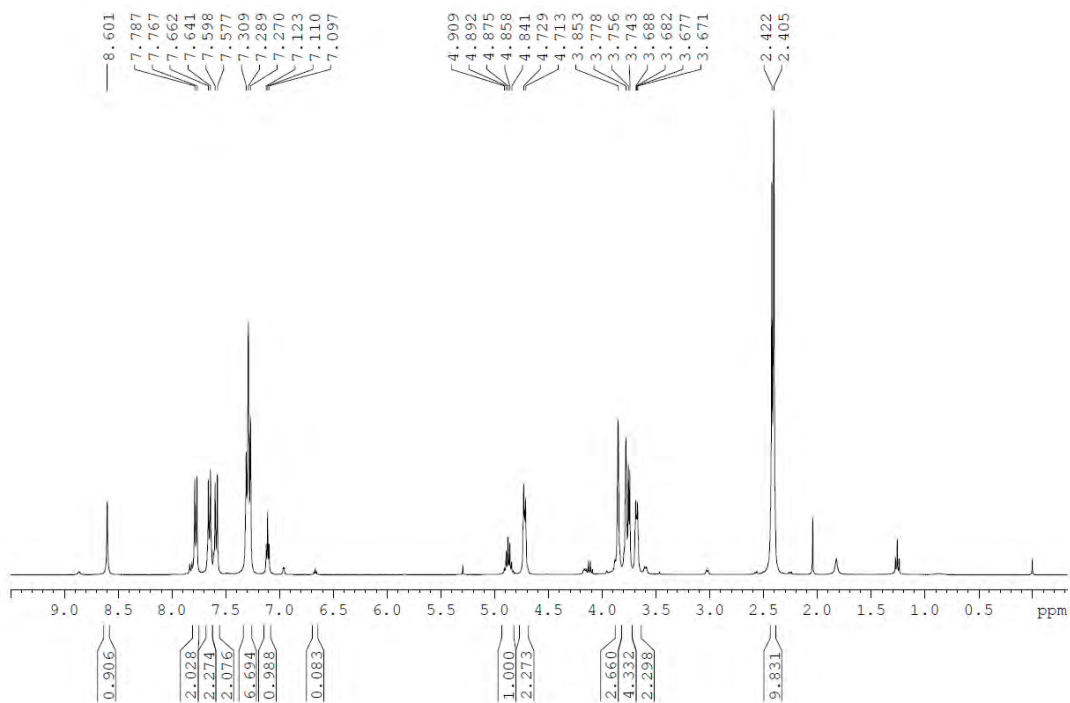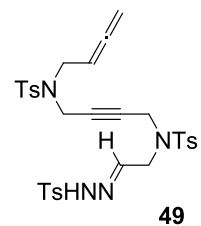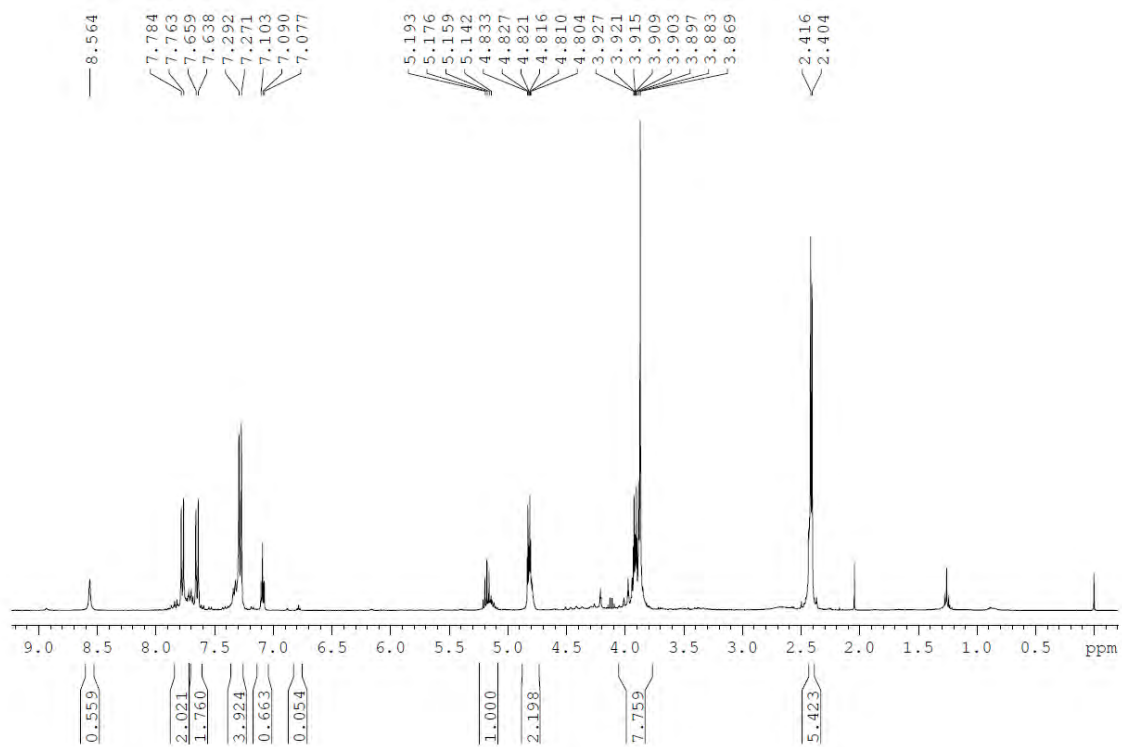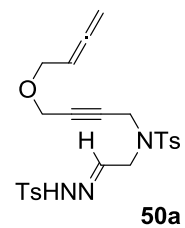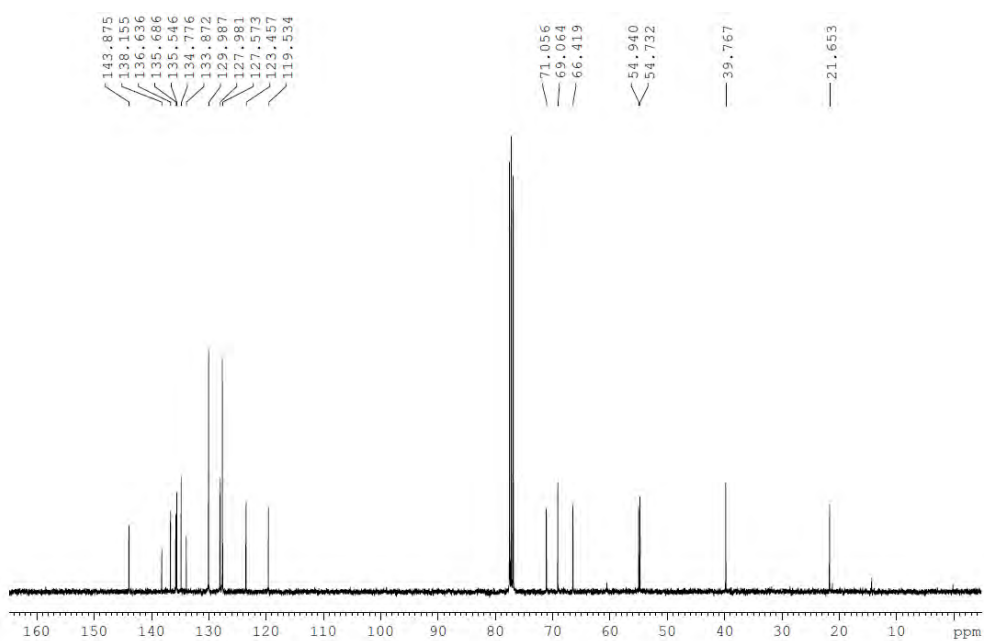**Figure S91**: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **54j** in CDCl$_3$.

Figure S92: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **54j**.

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.866	BB	0.9187	7209.38281	116.69721	51.0275
2	28.728	BB	0.9342	6919.04736	111.77527	48.9725

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.846	BB	0.8000	1523.73608	28.62833	4.1525
2	28.791	MM	1.1038	3.51709e4	531.07910	95.8475
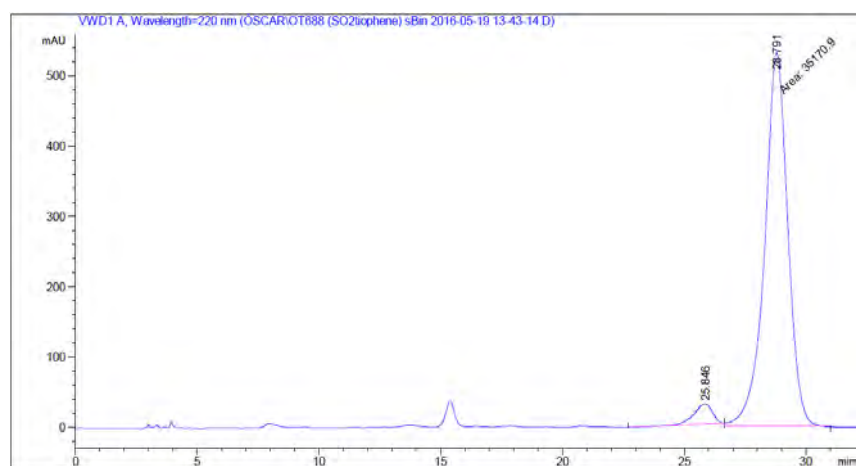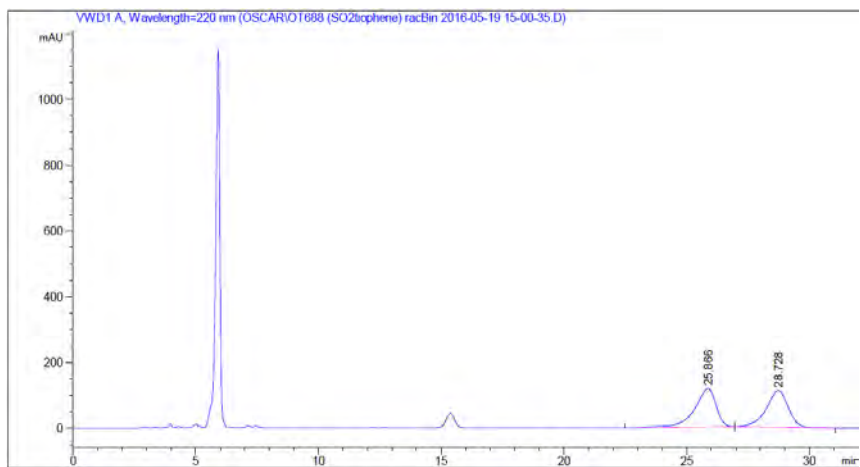
Crystallographic data for compounds 54a and 55

Colorless crystals of **54a** ($C_{24}H_{27}NO_5S_2$), were grown from from slow diffusion of pentane in a CH_2Cl_2 solution of the compound, and used for low temperature (293(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo $K\alpha$ radiation (λ = 0.71073 Å) from an x-Ray Tube. The measurements were made in the range 1.3 to 27.5° for θ. Hemi-sphere data collection was carried out with ω and φ scans. A total of 7368 reflections were collected of which 4812 [R(int) = 0.029] were unique. Programs used: data collection, Smart[1]; data reduction, Saint+[2]; absorption correction, SADABS[3]. Structure solution and refinement was done using SHELXTL[4]. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached.

Table 1. Crystal data for **54a**.

Empirical formula	$C_{24}H_{27}NO_5S_2$
Formula weight	473.58
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21
Unit cell dimensions	a = 10.607(4) Å
	$\alpha = 90^o$
	b = 7.076(3) Å
	$\beta = 91(10)^o$
	c = 15.851(8) Å
	$\gamma = 90^o$
Volume	1189.3(9) A^3
Z, Calculated density	2, 1.322 Mg/m^3
Absorption coefficient	0.259 mm^{-1}
F(000)	500
Crystal size	0.08 x 0.20 x 0.20 mm
Theta range for data collection	1.3^o to 27.5^o
Limiting indices	-13<=h<=12
	-9<=k<=9
	-20<=l<=20
Reflections collected / unique	7368 / 4812
	[R(int) = 0.0289]
Completeness to theta = 27.50	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.950 and 0.0979
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4812 / 1 / 291
Goodness-of-fit on F^2	1.146

[1] Bruker Advanced X-ray Solutions. SMART: Version 5.631, 1997-2002.

[2] Bruker Advanced X-ray Solutions. SAINT +, Version 6.36A, 2001.

[3] G. M. Sheldrick, *Empirical Absorption Correction Program*, Universität Göttingen, 1996 Bruker Advanced X-ray Solutions. SADABS Version 2.10, 2001

[4] G. M. Sheldrick, *Program for Crystal Structure Refinement*, Universität Göttingen, 1997 Bruker Advanced X-ray Solutions. SHELXTL Version 6.14, 2000-2003. SHELXL-2013 (Sheldrick, 2013)

Final R indices [I>2sigma(I)]	R1 = 0.0764, wR2 = 0.1654
R indices (all data)	R1 = 0.1229, wR2 = 0.1912
Extinction coefficient	n/a
Largest diff. peak and hole	0.612 and -0.185 e.A^{-3}
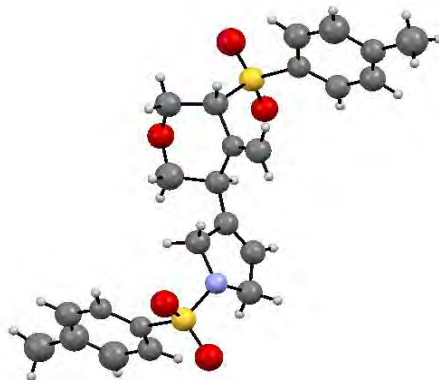
Colorless crystals of **55** ($C_{17}H_{19}NO_3S$), were grown from slow diffusion of pentane in a CH_2Cl_2 solution of the compound, and used for room temperature (293(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo $K\alpha$ radiation (λ = 0.71073 Å) from an x-Ray Tube. The measurements were made in the range 2.526 to 28.642° for θ. Full-sphere data collection was carried out with ω and ϕ scans. A total of 12558 reflections were collected of which 3921 [R(int) = 0.0470] were unique. Programs used: data collection, Smart[5]; data reduction, Saint+[6]; absorption correction, SADABS[7]. Structure solution and refinement was done using SHELXTL[8]. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached.

Table 2. Crystal data for **55**

Empirical formula	$C_{17}H_{19}NO_3S$
Formula weight	317.39
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 7.965(9) Å
	α = 80°
	b = 8.677(10) Å
	β = 90(17)°
	c = 12.496(14) Å

[5] Bruker Advanced X-ray Solutions. SMART: Version 5.631, 1997-2002.

[6] Bruker Advanced X-ray Solutions. SAINT +, Version 6.36A, 2001.

[7] G. M. Sheldrick, *Empirical Absorption Correction Program*, Universität Göttingen, 1996.
Bruker Advanced X-ray Solutions. SADABS Version 2.10, 2001.

[8] G. M. Sheldrick, *Program for Crystal Structure Refinement*, Universität Göttingen, 1997.
Bruker Advanced X-ray Solutions. SHELXTL Version 6.14, 2000-2003. SHELXL-2014/7 (Sheldrick, 2014).

	$\gamma = 68^{\circ}$
Volume	798.1(16) A^3
Z, Calculated density	2, 1.321 Mg/m^3
Absorption coefficient	0.215 mm^{-1}
F(000)	336
Crystal size	0.30 x 0.25 x 0.10 mm
Theta range for data collection	2.526° to 28.642°
Limiting indices	-10<=h<=10
	-11<=k<=11
	-16<=l<=16
Reflections collected / unique	4750 / 3037
	[R(int) = 0.0470]
Completeness to theta = 25.242	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0 and 0.793027
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3921 / 0 / 201
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0508, wR2 = 0.1357
R indices (all data)	R1 = 0.0648, wR2 = 0.1473
Extinction coefficient	n/a
Largest diff. peak and hole	0.382 and -0.295 e.A^{-3}
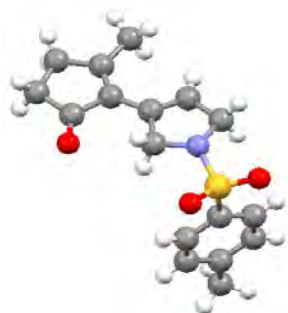
Computational details

Table S3. Cartesian coordinates of all optimized stationary points (Å).

RhBINAP (nimag=0)   E(au)= - 1414.6121   G(au)= -1414.3445

45	2.255926000	-0.003327000	0.000062000
15	0.736338000	1.212589000	1.059987000
15	0.732718000	-1.214482000	-1.060122000
6	-0.759962000	1.662125000	0.077575000
6	-1.768738000	0.714056000	-0.235968000
6	-0.875332000	2.975846000	-0.410933000
6	-2.866414000	1.136503000	-1.007145000
6	-1.968759000	3.368742000	-1.185213000
1	-0.108335000	3.716575000	-0.186114000
6	-2.971083000	2.445092000	-1.481444000
1	-3.645758000	0.411345000	-1.249565000
1	-2.033920000	4.395699000	-1.549057000
1	-3.833485000	2.738038000	-2.083196000
6	-0.764671000	-1.660133000	-0.077606000
6	-0.883625000	-2.973591000	0.410751000
6	-1.770692000	-0.709266000	0.236257000
6	-1.977987000	-3.363489000	1.185229000
1	-0.118728000	-3.716431000	0.185738000
6	-2.869395000	-1.128701000	1.007614000
6	-2.977637000	-2.437047000	1.481788000
1	-2.045951000	-4.390293000	1.548992000
1	-3.646653000	-0.401386000	1.250267000
1	-3.840733000	-2.727633000	2.083688000
6	1.535214000	2.801672000	1.561149000
1	1.936570000	3.337632000	0.690521000
1	0.818962000	3.443294000	2.097832000
1	2.367343000	2.560245000	2.240292000
6	0.140452000	0.542466000	2.673927000
1	1.006684000	0.443141000	3.344854000
1	-0.591587000	1.236956000	3.115372000
1	-0.320818000	-0.443374000	2.540913000
6	0.138309000	-0.541779000	-2.673521000
1	1.004645000	-0.444451000	-3.344610000
1	-0.595769000	-1.233976000	-3.115180000
1	-0.320202000	0.445251000	-2.539771000
6	1.526962000	-2.805564000	-1.562297000
1	0.808769000	-3.444875000	-2.099145000
1	2.359603000	-2.566129000	-2.241519000
1	1.927018000	-3.343105000	-0.692047000

N$_2$ (nimag=0) E(au)= -109.5334   G(au)= -109.5462

7	0.000000000	0.000000000	0.552224000
7	0.000000000	0.000000000	-0.552224000

Ts (nimag=0) E(au)= -819.6170   G(au)= -819.5308

16	2.261209000	-0.001037000	-0.346217000
8	2.631446000	-1.305724000	0.398389000
8	2.632179000	1.306465000	0.393058000
6	0.366826000	-0.000005000	-0.137276000
6	-0.334149000	1.205679000	-0.081673000
6	-0.335874000	-1.205662000	-0.083806000
6	-1.731074000	1.206030000	0.002385000
6	-1.732023000	-1.204954000	0.000146000
6	-2.453288000	0.001231000	0.034148000

```
1        0.247970000      2.132515000     -0.067253000
1        0.245310000     -2.133106000     -0.070913000
1       -2.276754000      2.156154000      0.058401000
1       -2.278410000     -2.154857000      0.054544000
6       -3.964989000     -0.000104000      0.088473000
1       -4.354897000      0.930767000      0.532678000
1       -4.414182000     -0.089562000     -0.918984000
1       -4.349952000     -0.844532000      0.685041000
```

A (nimag=0)   E(au)= -2035.8287   **G(au)=** -2035.9254

```
6        4.426160000      1.531010000      0.019140000
6        4.151770000     -1.596060000     -1.104940000
6        2.954550000     -1.798770000     -1.143500000
6        5.599420000     -1.331890000     -1.063860000
6        5.778150000      0.848960000     -0.044030000
1        6.085350000     -1.858960000     -1.900260000
1        6.017890000     -1.749550000     -0.127170000
1        6.571950000      1.608820000     -0.082520000
1        5.933080000      0.234820000      0.863860000
6        1.505350000     -1.988260000     -1.237350000
1        1.055070000     -1.076450000     -1.666840000
1        1.297120000     -2.814300000     -1.935880000
6       -0.392130000     -3.149380000     -0.073650000
1       -0.772500000     -3.338690000      0.935870000
6        4.283220000      2.832360000     -0.086110000
8        5.959380000      0.033990000     -1.209000000
7        0.863890000     -2.373880000      0.041520000
16       0.926310000     -1.190520000      1.292720000
6        2.306020000     -1.763170000      2.298740000
1        2.043450000     -2.751680000      2.694370000
1        2.423220000     -1.028580000      3.106890000
1        3.197510000     -1.804710000      1.661920000
8        1.287970000      0.127450000      0.697670000
8       -0.311290000     -1.310400000      2.110480000
6       -1.487310000     -2.508260000     -0.891810000
1       -1.360660000     -2.430240000     -1.985450000
1       -0.113580000     -4.115620000     -0.525880000
7       -2.549080000     -2.102430000     -0.303180000
7       -3.565570000     -1.604960000     -1.074710000
16      -4.558160000     -0.424760000     -0.281730000
8       -5.609060000     -0.130170000     -1.285390000
8       -4.886940000     -0.990680000      1.043870000
6       -3.522790000      1.028490000     -0.084480000
6       -2.443090000      0.996850000      0.807880000
6       -3.809250000      2.164000000     -0.845590000
6       -1.634500000      2.126750000      0.914390000
6       -2.995850000      3.291250000     -0.705530000
6       -1.898280000      3.291210000      0.169530000
1       -2.209170000      0.100790000      1.383340000
1       -4.656120000      2.161380000     -1.531910000
1       -0.768850000      2.093710000      1.579060000
1       -3.217660000      4.185030000     -1.293440000
1       -3.330710000     -1.298920000     -2.030660000
6       -1.015020000      4.504730000      0.316550000
1       -1.112780000      4.940290000      1.325320000
1        0.046370000      4.240010000      0.183420000
1       -1.272240000      5.283950000     -0.414940000
6        4.153430000      4.134250000     -0.184540000
1        3.535810000      0.908560000      0.168850000
1        4.191270000      4.779250000      0.699530000
1        4.001550000      4.618540000     -1.154820000
```

B (nimag=0)   E(au)= -2520.9860   **G(au)=** -2521.0953

```
1       -7.568330000     -2.571830000     -0.014030000
1       -8.668250000     -1.160660000      0.267760000
```

1	-7.438360000	-1.606800000	1.519100000
8	-6.540090000	0.838210000	0.350000000
8	-6.701560000	-0.543430000	-1.818750000
15	2.477860000	1.327830000	-0.943590000
15	1.102380000	-1.354140000	0.604840000
6	3.560730000	-0.065930000	-1.509970000
6	4.127860000	-1.002110000	-0.609780000
6	3.798500000	-0.218010000	-2.887850000
6	4.941210000	-2.029000000	-1.119770000
6	-0.685740000	3.616700000	0.453420000
6	-1.602830000	0.285250000	0.539160000
45	0.192410000	0.663350000	-0.225790000
6	-1.593960000	1.061060000	1.808450000
6	-0.334640000	3.138390000	1.837640000
1	-1.722000000	0.406980000	2.690980000
1	-2.412320000	1.803420000	1.846050000
1	0.667200000	3.479970000	2.137820000
1	-1.056390000	3.517770000	2.579910000
6	-0.634330000	2.843930000	-0.609370000
8	-0.294020000	1.697910000	1.889610000
16	-6.499610000	-0.474830000	-0.346520000
6	-7.670160000	-1.581960000	0.447430000
6	4.591290000	-1.258600000	-3.377530000
1	3.371730000	0.484230000	-3.602840000
6	5.171830000	-2.164360000	-2.489340000
1	5.383520000	-2.743240000	-0.422930000
1	4.758160000	-1.349340000	-4.452340000
1	5.800280000	-2.977080000	-2.857940000
6	2.683780000	-1.071250000	1.516490000
6	2.616080000	-0.969770000	2.918910000
6	3.939540000	-0.938910000	0.872740000
6	3.764490000	-0.767660000	3.685830000
1	1.660920000	-1.057110000	3.434850000
6	5.085880000	-0.761610000	1.667110000
6	5.007140000	-0.673870000	3.057280000
1	3.683090000	-0.693770000	4.771500000
1	6.054850000	-0.671350000	1.172790000
1	5.914960000	-0.525970000	3.644950000
6	2.551780000	2.544960000	-2.329870000
1	2.063390000	2.164700000	-3.236330000
1	3.601110000	2.783200000	-2.557060000
1	2.041190000	3.462910000	-2.005250000
6	3.406210000	2.237770000	0.371180000
1	2.923630000	3.218980000	0.492110000
1	4.451430000	2.382640000	0.062160000
1	3.371380000	1.702210000	1.327050000
6	1.356020000	-2.643250000	-0.683270000
1	0.356610000	-2.963400000	-1.012230000
1	1.888020000	-3.497180000	-0.239790000
1	1.913710000	-2.257290000	-1.542880000
6	0.023270000	-2.240230000	1.804790000
1	0.555370000	-3.125730000	2.181740000
1	-0.881990000	-2.559880000	1.270080000
6	-2.766310000	-0.420370000	0.153320000
6	-2.878480000	-1.135980000	-1.009540000
6	-4.075080000	-0.506750000	0.929060000
6	-4.223360000	-1.730750000	-1.157720000
7	-4.982620000	-1.239320000	0.012660000
1	-4.492100000	0.480320000	1.177830000
1	-3.942230000	-1.068940000	1.869230000
1	-4.704990000	-1.440690000	-2.108920000
1	-4.152130000	-2.836870000	-1.172390000
1	-2.082740000	-1.271520000	-1.743490000
1	-0.264000000	-1.601990000	2.649250000
1	0.067950000	-0.145270000	-1.513590000
6	-0.759670000	2.189960000	-1.776620000
1	-0.006830000	2.258960000	-2.561200000
1	-1.728360000	1.773750000	-2.068020000

| 1 | −1.018290000 | 4.654690000 | 0.333630000 |

TS_BC (nimag=1) (−227.96i) E**(au)=** −2520.9677   **G(au)=** −2521.0717

6	−1.797710000	−2.206310000	2.311880000
6	−1.573300000	−1.043070000	−0.152480000
45	0.182880000	−0.287470000	0.585490000
6	−1.757720000	−2.504340000	−0.464560000
6	−1.538340000	−3.501340000	1.610920000
1	−1.452930000	−2.647640000	−1.514580000
1	−2.816960000	−2.815470000	−0.401760000
1	−0.847850000	−4.109640000	2.219500000
1	−2.489400000	−4.066200000	1.541010000
6	−1.377070000	−0.986040000	1.947770000
8	−0.951400000	−3.350670000	0.331480000
16	−6.149490000	0.915020000	−0.216990000
6	−7.498550000	0.819200000	−1.400050000
1	−7.354450000	1.612530000	−2.143470000
1	−8.424830000	0.971650000	−0.829930000
1	−7.475600000	−0.176140000	−1.860120000
8	−6.270480000	−0.223150000	0.733400000
8	−6.069260000	2.306900000	0.301410000
15	2.192800000	0.586900000	1.699140000
15	1.440750000	−0.452310000	−1.437280000
6	3.170430000	1.757870000	0.644980000
6	4.001920000	1.324180000	−0.417360000
6	3.039650000	3.138210000	0.886740000
6	4.699550000	2.285280000	−1.169330000
6	3.722950000	4.078940000	0.112820000
1	2.406510000	3.499930000	1.695980000
6	4.562690000	3.650700000	−0.915910000
1	5.348820000	1.946770000	−1.978930000
1	3.602730000	5.142620000	0.325840000
1	5.109690000	4.374600000	−1.522650000
6	3.196420000	−0.984900000	−1.209840000
6	3.508560000	−2.331380000	−1.475860000
6	4.219680000	−0.115470000	−0.758910000
6	4.808860000	−2.816420000	−1.324980000
1	2.737120000	−3.022610000	−1.812410000
6	5.526990000	−0.618630000	−0.638640000
6	5.825490000	−1.953230000	−0.914070000
1	5.021520000	−3.865390000	−1.537990000
1	6.316720000	0.054400000	−0.300180000
1	6.848500000	−2.316590000	−0.800910000
6	1.891660000	1.538630000	3.251460000
1	1.149960000	2.333520000	3.100170000
1	2.835360000	1.974180000	3.610530000
1	1.514510000	0.839920000	4.011400000
6	3.323060000	−0.743330000	2.298620000
1	2.794310000	−1.270250000	3.107280000
1	4.250440000	−0.302750000	2.692340000
1	3.557710000	−1.459040000	1.502940000
6	1.403080000	1.152770000	−2.345020000
1	0.373650000	1.293260000	−2.706360000
1	2.087320000	1.100490000	−3.204270000
1	1.680220000	1.992710000	−1.698800000
6	0.777040000	−1.609200000	−2.705290000
1	1.462500000	−1.629160000	−3.564890000
1	−0.200120000	−1.230820000	−3.037200000
6	−2.632800000	−0.166690000	−0.592320000
6	−2.531670000	1.178370000	−0.784560000

6	-4.031770000	-0.621010000	-1.005300000
6	-3.799010000	1.757230000	-1.312450000
7	-4.768430000	0.640680000	-1.238240000
1	-4.531190000	-1.218370000	-0.229680000
1	-3.997490000	-1.217330000	-1.932830000
1	-4.141180000	2.626800000	-0.729000000
1	-3.663740000	2.100310000	-2.356110000
1	-1.642550000	1.793240000	-0.640660000
1	0.660170000	-2.624730000	-2.307790000
1	0.717060000	-1.678150000	0.824830000
6	-1.057110000	0.284600000	2.355060000
1	-0.544600000	0.418720000	3.307750000
1	-1.553370000	1.163860000	1.926750000
1	-2.469030000	-2.249440000	3.178420000

C (nimag=0)   E(au)= -2521.0154   G(au)= -2521.1223

6	-0.532930000	-2.599590000	0.725030000
6	-2.269290000	-1.046760000	0.020050000
45	0.819720000	-0.702890000	0.661170000
6	-2.190660000	-1.653950000	-1.350550000
6	-0.836070000	-3.357910000	-0.532070000
1	-2.223120000	-0.852270000	-2.108570000
1	-3.123340000	-2.247700000	-1.498030000
1	0.000990000	-4.001520000	-0.824110000
1	-1.720500000	-4.015430000	-0.397720000
6	-1.261310000	-1.401160000	1.013160000
8	-1.054340000	-2.435090000	-1.598070000
16	-7.089430000	0.475850000	-0.417560000
6	-7.669540000	2.009480000	-1.149930000
1	-7.626810000	2.791180000	-0.382060000
1	-8.702870000	1.826450000	-1.474010000
1	-7.023190000	2.241670000	-2.005150000
8	-7.030350000	-0.563880000	-1.477530000
8	-7.843070000	0.224080000	0.838720000
15	1.961790000	1.173450000	1.447940000
15	2.553030000	-1.365010000	-0.827210000
6	2.512520000	2.116290000	-0.041600000
6	3.645120000	1.742310000	-0.810800000
6	1.726540000	3.207720000	-0.459980000
6	3.963640000	2.504810000	-1.948130000
6	2.052140000	3.938720000	-1.603220000
1	0.853630000	3.509650000	0.118150000
6	3.178500000	3.587460000	-2.348960000
1	4.844040000	2.230630000	-2.532350000
1	1.430500000	4.785240000	-1.900160000
1	3.449670000	4.153970000	-3.241760000
6	4.244320000	-0.739240000	-0.397700000
6	5.220120000	-1.668050000	0.008170000
6	4.584380000	0.637790000	-0.431900000
6	6.511850000	-1.265820000	0.355310000
1	4.983630000	-2.729950000	0.055020000
6	5.898590000	1.018600000	-0.105540000
6	6.856640000	0.084040000	0.288420000
1	7.244220000	-2.012310000	0.667980000
1	6.160270000	2.077780000	-0.141170000
1	7.864360000	0.413770000	0.547940000
6	0.936700000	2.348850000	2.428730000
1	0.009560000	2.612650000	1.903890000
1	1.512980000	3.258970000	2.652050000
1	0.674900000	1.843690000	3.369270000
6	3.387260000	0.897590000	2.579290000
1	2.969600000	0.538630000	3.531750000
1	3.914640000	1.848300000	2.744730000
1	4.080140000	0.146480000	2.185850000

6	2.208620000	-0.792890000	-2.550950000
1	1.261600000	-1.254800000	-2.867520000
1	3.021940000	-1.114480000	-3.218660000
1	2.112410000	0.299360000	-2.589960000
6	2.781590000	-3.178010000	-1.062820000
1	3.653220000	-3.378510000	-1.702240000
1	1.885960000	-3.562110000	-1.569190000
6	-3.411300000	-0.260970000	0.305440000
6	-3.888080000	0.055580000	1.556490000
6	-4.381040000	0.251240000	-0.747930000
6	-5.163370000	0.788730000	1.477810000
7	-5.461730000	0.889490000	0.037860000
1	-4.785660000	-0.552970000	-1.381960000
1	-3.890350000	0.988670000	-1.406340000
1	-5.968630000	0.272730000	2.034550000
1	-5.059400000	1.782690000	1.959530000
1	-3.436760000	-0.226360000	2.506710000
1	2.892580000	-3.690790000	-0.097840000
1	1.555690000	-1.448670000	1.754110000
6	-0.841500000	-0.547270000	2.082950000
1	-0.493260000	-0.999520000	3.013520000
1	-1.319360000	0.426440000	2.190000000
1	-0.108460000	-3.164310000	1.558460000

TS_CD (nimag=1) (-73.7*i*) E(au)= -2521.6009   **G(au)=** -2521.1013

6	-0.489800000	-3.112740000	0.568900000
6	-1.601510000	-1.082360000	-0.179210000
45	0.622900000	-1.071940000	0.729080000
6	-1.677020000	-1.750480000	-1.565590000
6	-0.644410000	-3.713470000	-0.800030000
1	-1.623930000	-0.990770000	-2.355770000
1	-2.689900000	-2.205120000	-1.600640000
1	0.198230000	-4.371670000	-1.039830000
1	-1.570510000	-4.321510000	-0.843300000
6	-1.255670000	-1.985150000	0.961860000
8	-0.677150000	-2.700030000	-1.806450000
16	-6.192620000	0.481820000	-0.264400000
6	-7.376140000	1.210610000	0.874870000
1	-7.240030000	2.298730000	0.855100000
1	-7.189730000	0.795450000	1.872520000
1	-8.372230000	0.928970000	0.507590000
8	-6.267300000	-0.999450000	-0.145210000
8	-6.359490000	1.126010000	-1.594140000
15	1.343040000	1.103730000	1.460960000
15	2.259320000	-1.170740000	-1.033740000
6	1.965800000	2.171050000	0.089470000
6	3.204230000	1.932400000	-0.559110000
6	1.152630000	3.230510000	-0.351780000
6	3.600820000	2.797430000	-1.593340000
6	1.554220000	4.061250000	-1.400560000
1	0.191080000	3.425260000	0.122320000
6	2.787950000	3.849770000	-2.017440000
1	4.560190000	2.622900000	-2.083850000
1	0.904250000	4.876290000	-1.723630000
1	3.118080000	4.497760000	-2.831420000
6	3.856830000	-0.549800000	-0.338710000
6	4.809210000	-1.501380000	0.075020000
6	4.145270000	0.830590000	-0.178400000
6	6.038490000	-1.110830000	0.608980000
1	4.601860000	-2.566340000	-0.025530000
6	5.400630000	1.200740000	0.333030000
6	6.340700000	0.246530000	0.726710000
1	6.758910000	-1.869580000	0.919200000
1	5.630460000	2.262520000	0.438700000
1	7.303320000	0.566510000	1.129630000
6	0.048590000	2.093950000	2.317150000
1	-0.861930000	2.172250000	1.710290000

```
1      0.428470000      3.098870000      2.553260000
1     -0.198180000      1.571770000      3.252340000
6      2.658470000      0.985110000      2.750110000
1      2.204270000      0.538780000      3.647210000
1      3.025660000      1.994400000      2.989290000
1      3.493910000      0.358600000      2.417890000
6      1.871970000     -0.240200000     -2.573750000
1      1.084710000     -0.805330000     -3.093620000
1      2.767830000     -0.193050000     -3.209680000
1      1.512490000      0.772320000     -2.358270000
6      2.643360000     -2.849750000     -1.686040000
1      3.532660000     -2.799770000     -2.331360000
1      1.778910000     -3.169390000     -2.282660000
6     -2.590700000      0.006320000     -0.019120000
6     -2.651980000      1.131010000     -0.759970000
6     -3.794870000     -0.064390000      0.918160000
6     -3.878670000      1.927450000     -0.431150000
7     -4.677700000      1.011290000      0.421750000
1     -3.519630000      0.137430000      1.966210000
1     -4.307950000     -1.035590000      0.883410000
1     -3.626810000      2.851470000      0.120540000
1     -4.441730000      2.218620000     -1.330040000
1     -1.912650000      1.461040000     -1.491380000
1      2.810210000     -3.570550000     -0.875590000
1     -0.392260000     -0.355560000     -0.329550000
6     -1.026770000     -1.370580000      2.221530000
1     -1.552840000     -0.459750000      2.497310000
1     -0.670030000     -1.991840000      3.046950000
1     -0.093400000     -3.763360000      1.354330000
```

D (nimag=0)   E(au)= -2521.0149   G(au)= -2521.1203

```
6       0.680980000     -2.527900000     -0.768580000
6       2.285130000     -1.237730000      0.567780000
45     -0.590230000     -0.614030000     -0.501650000
6       2.102330000     -2.304510000      1.625590000
6       0.749170000     -3.608920000      0.262220000
1       2.158260000     -1.875680000      2.634620000
1       2.974130000     -2.988470000      1.514690000
1      -0.165520000     -4.212100000      0.278350000
1       1.594280000     -4.295820000      0.039060000
6       1.480670000     -1.351110000     -0.649320000
8       0.904070000     -3.028980000      1.550960000
16      6.703030000      0.588050000     -0.492970000
6       7.357990000      2.164890000     -1.050840000
1       7.521730000      2.795470000     -0.168660000
1       6.631230000      2.610820000     -1.740570000
1       8.304510000      1.942610000     -1.561870000
8       6.347310000     -0.230170000     -1.681540000
8       7.607610000      0.037930000      0.551350000
15     -1.529980000      1.466650000     -0.990650000
15     -2.522130000     -1.370460000      0.700090000
6      -2.651580000      2.137140000      0.314720000
6      -3.936140000      1.598780000      0.579590000
6      -2.178230000      3.202250000      1.103180000
6      -4.709810000      2.180950000      1.599730000
6      -2.955060000      3.750060000      2.125570000
1      -1.190430000      3.623820000      0.921450000
6      -4.231100000      3.241200000      2.370290000
1      -5.703300000      1.774510000      1.797700000
1      -2.562200000      4.577090000      2.719580000
1      -4.854120000      3.663380000      3.160970000
6      -4.073930000     -0.862450000     -0.180970000
6      -4.763110000     -1.838560000     -0.924550000
6      -4.558840000      0.470500000     -0.186020000
6      -5.914590000     -1.525180000     -1.649940000
1      -4.409500000     -2.868950000     -0.938400000
6      -5.731900000      0.760470000     -0.905840000
```

6	-6.405550000	-0.219430000	-1.636120000
1	-6.426830000	-2.306190000	-2.214830000
1	-6.110180000	1.784490000	-0.898900000
1	-7.308440000	0.040130000	-2.191990000
6	-0.306290000	2.802580000	-1.316720000
1	0.404440000	2.900330000	-0.485570000
1	-0.820520000	3.759450000	-1.488100000
1	0.248170000	2.524390000	-2.223880000
6	-2.464300000	1.382660000	-2.579680000
1	-1.737790000	1.172090000	-3.378670000
1	-2.952450000	2.350030000	-2.771460000
1	-3.217010000	0.586060000	-2.556500000
6	-2.646740000	-0.777000000	2.444190000
1	-1.838320000	-1.265840000	3.008450000
1	-3.618250000	-1.063920000	2.872630000
1	-2.519540000	0.309520000	2.507160000
6	-2.703790000	-3.190840000	0.934790000
1	-3.678590000	-3.421220000	1.389100000
1	-1.905650000	-3.510340000	1.619520000
6	3.346860000	-0.308680000	0.719690000
6	4.036780000	-0.136010000	1.900580000
6	3.967260000	0.615270000	-0.330190000
6	5.163250000	0.805660000	1.742280000
7	5.225250000	1.080080000	0.294440000
1	3.322090000	1.486800000	-0.522060000
1	4.172750000	0.109920000	-1.282460000
1	4.978670000	1.726150000	2.332940000
1	6.109020000	0.378610000	2.121280000
1	3.800940000	-0.590440000	2.863040000
1	-2.600880000	-3.734070000	-0.013790000
1	-0.206510000	0.116790000	0.774950000
6	1.249670000	-0.288470000	-1.586760000
1	1.772910000	0.657050000	-1.485600000
1	1.004850000	-0.567990000	-2.617100000
1	0.338520000	-2.813290000	-1.770000000

TS_DE (nimag=1) (−188.30*i*)   E(au)= −2520.9901   G(au)= −2521.0895

6	-0.489800000	-3.112740000	0.568900000
6	-1.601510000	-1.082360000	-0.179210000
45	0.622900000	-1.071940000	0.729080000
6	-1.677020000	-1.750480000	-1.565590000
6	-0.644410000	-3.713470000	-0.800030000
1	-1.623930000	-0.990770000	-2.355770000
1	-2.689900000	-2.205120000	-1.600640000
1	0.198230000	-4.371670000	-1.039830000
1	-1.570510000	-4.321510000	-0.843300000
6	-1.255670000	-1.985150000	0.961860000
8	-0.677150000	-2.700030000	-1.806450000
16	-6.192620000	0.481820000	-0.264400000
6	-7.376140000	1.210610000	0.874870000
1	-7.240030000	2.298730000	0.855100000
1	-7.189730000	0.795450000	1.872520000
1	-8.372230000	0.928970000	0.507590000
8	-6.267300000	-0.999450000	-0.145210000
8	-6.359490000	1.126010000	-1.594140000
15	1.343040000	1.103730000	1.460960000
15	2.259320000	-1.170740000	-1.033740000
6	1.965800000	2.171050000	0.089470000
6	3.204230000	1.932400000	-0.559110000
6	1.152630000	3.230510000	-0.351780000
6	3.600820000	2.797430000	-1.593340000
6	1.554220000	4.061250000	-1.400560000
1	0.191080000	3.425260000	0.122320000
6	2.787950000	3.849770000	-2.017440000
1	4.560190000	2.622900000	-2.083850000
1	0.904250000	4.876290000	-1.723630000
1	3.118080000	4.497760000	-2.831420000
6	3.856830000	-0.549800000	-0.338710000

```
6       4.809210000    -1.501380000     0.075020000
6       4.145270000     0.830590000    -0.178400000
6       6.038490000    -1.110830000     0.608980000
1       4.601860000    -2.566340000    -0.025530000
6       5.400630000     1.200740000     0.333030000
6       6.340700000     0.246530000     0.726710000
1       6.758910000    -1.869580000     0.919200000
1       5.630460000     2.262520000     0.438700000
1       7.303320000     0.566510000     1.129630000
6       0.048590000     2.093950000     2.317150000
1      -0.861930000     2.172250000     1.710290000
1       0.428470000     3.098870000     2.553260000
1      -0.198180000     1.571770000     3.252340000
6       2.658470000     0.985110000     2.750110000
1       2.204270000     0.538780000     3.647210000
1       3.025660000     1.994400000     2.989290000
1       3.493910000     0.358600000     2.417890000
6       1.871970000    -0.240200000    -2.573750000
1       1.084710000    -0.805330000    -3.093620000
1       2.767830000    -0.193050000    -3.209680000
1       1.512490000     0.772320000    -2.358270000
6       2.643360000    -2.849750000    -1.686040000
1       3.532660000    -2.799770000    -2.331360000
1       1.778910000    -3.169390000    -2.282660000
6      -2.590700000     0.006320000    -0.019120000
6      -2.651980000     1.131010000    -0.759970000
6      -3.794870000    -0.064390000     0.918160000
6      -3.878670000     1.927450000    -0.431150000
7      -4.677700000     1.011290000     0.421750000
1      -3.519630000     0.137430000     1.966210000
1      -4.307950000    -1.035590000     0.883410000
1      -3.626810000     2.851470000     0.120540000
1      -4.441730000     2.218620000    -1.330040000
1      -1.912650000     1.461040000    -1.491380000
1       2.810210000    -3.570550000    -0.875590000
1      -0.392260000    -0.355560000    -0.329550000
6      -1.026770000    -1.370580000     2.221530000
1      -1.552840000    -0.459750000     2.497310000
1      -0.670030000    -1.991840000     3.046950000
1      -0.093400000    -3.763360000     1.354330000
```

E (nimag=0)   E(au)= -2520.9974   G(au)= -2521.1019

```
6      -0.450810000    -2.568350000     0.480980000
6      -1.698130000    -0.654140000    -0.454900000
45      0.717420000    -0.558640000     0.113750000
6      -2.059540000    -1.621780000    -1.613520000
6      -0.821900000    -3.395530000    -0.721970000
1      -2.206080000    -1.048140000    -2.536790000
1      -3.019320000    -2.105360000    -1.345200000
1      -0.023600000    -4.096980000    -0.992000000
1      -1.722260000    -4.000590000    -0.487630000
6      -1.132100000    -1.362800000     0.766500000
8      -1.059880000    -2.580350000    -1.863520000
16     -6.478140000     0.439460000     0.085790000
6      -7.422890000     0.880600000     1.551130000
1      -7.450290000     1.974520000     1.621290000
1      -6.928230000     0.432720000     2.422030000
1      -8.429780000     0.464390000     1.412810000
8      -6.377780000    -1.045830000     0.031220000
8      -7.030150000     1.182580000    -1.078060000
15      1.345060000     1.730780000     0.457020000
15      2.319130000    -1.218750000    -1.402320000
6       3.047640000     2.082870000    -0.145560000
6       4.072760000     1.153220000     0.145440000
6       3.363160000     3.263660000    -0.834900000
6       5.395630000     1.449040000    -0.224440000
```

6	4.678390000	3.529860000	-1.225620000
1	2.587440000	3.992550000	-1.068050000
6	5.695730000	2.624960000	-0.914460000
1	6.188640000	0.735290000	0.005890000
1	4.905320000	4.451200000	-1.764730000
1	6.725490000	2.829520000	-1.212380000
6	3.010470000	-1.197950000	0.312660000
6	2.866330000	-2.396650000	1.082650000
6	3.807650000	-0.123850000	0.865800000
6	3.452870000	-2.536680000	2.333740000
1	2.319380000	-3.240140000	0.667420000
6	4.413370000	-0.314230000	2.108310000
6	4.236550000	-1.496830000	2.839780000
1	3.317810000	-3.459150000	2.898690000
1	5.023000000	0.488830000	2.524400000
1	4.716840000	-1.599130000	3.814730000
6	0.244190000	2.959620000	-0.347870000
1	0.252070000	2.821510000	-1.437930000
1	0.554530000	3.984240000	-0.096870000
1	-0.775710000	2.800490000	0.029580000
6	1.392050000	2.251420000	2.226800000
1	0.373930000	2.220630000	2.638390000
1	1.787890000	3.275420000	2.295100000
1	2.033000000	1.568700000	2.801020000
6	3.185090000	-0.199060000	-2.652060000
1	2.684250000	-0.425240000	-3.606400000
1	4.239510000	-0.502900000	-2.718710000
1	3.102920000	0.871630000	-2.446080000
6	2.419510000	-2.908300000	-2.105800000
1	3.449110000	-3.098650000	-2.442980000
1	1.734230000	-2.943210000	-2.965230000
6	-2.802050000	0.336820000	-0.226350000
6	-3.087750000	1.411140000	-0.976940000
6	-3.879380000	0.128240000	0.827010000
6	-4.369700000	2.060580000	-0.541670000
7	-4.925460000	1.110870000	0.460000000
1	-3.507790000	0.335580000	1.844840000
1	-4.286790000	-0.893690000	0.820910000
1	-4.190930000	3.046380000	-0.075320000
1	-5.076990000	2.211960000	-1.369780000
1	-2.489540000	1.794120000	-1.804970000
1	2.118210000	-3.673720000	-1.383390000
1	-0.778930000	-0.029750000	-0.901660000
6	-0.741060000	-0.562990000	1.864960000
1	-1.228910000	0.395360000	2.039040000
1	-0.277510000	-1.037460000	2.732480000
1	0.006750000	-3.098800000	1.320270000

TS_EF (nimag=1) (-18.9i) E(au)= -2521.6066   G(au)= -2521.1393

6	-0.444290000	-2.526940000	0.423280000
6	-1.751450000	-0.681580000	-0.627100000
45	0.787540000	-0.539570000	0.044030000
6	-2.098550000	-1.738600000	-1.707210000
6	-0.771570000	-3.410980000	-0.752520000
1	-2.296270000	-1.236200000	-2.661860000
1	-3.018440000	-2.267380000	-1.391340000
1	0.057620000	-4.086240000	-0.995600000
1	-1.643470000	-4.047950000	-0.495010000
6	-1.130930000	-1.311400000	0.623160000
8	-1.046020000	-2.653040000	-1.923010000
16	-6.651720000	0.462430000	0.194630000
6	-7.440380000	1.186560000	1.640170000
1	-7.312370000	2.274750000	1.588990000
1	-6.964730000	0.765690000	2.534440000
1	-8.502610000	0.911550000	1.590230000
8	-6.701910000	-1.018840000	0.332500000
8	-7.221560000	1.112140000	-1.016580000
15	1.371780000	1.753760000	0.317730000

15	2.492650000	-1.337030000	-1.280820000
6	3.099850000	2.079750000	-0.219230000
6	4.114060000	1.184420000	0.195030000
6	3.445390000	3.213790000	-0.969020000
6	5.455240000	1.471440000	-0.113490000
6	4.779760000	3.468820000	-1.297710000
1	2.679450000	3.916420000	-1.296270000
6	5.784940000	2.600650000	-0.864520000
1	6.238890000	0.784810000	0.211440000
1	5.031350000	4.354690000	-1.883260000
1	6.828700000	2.797970000	-1.114550000
6	3.001240000	-1.134940000	0.485770000
6	2.799470000	-2.268820000	1.342040000
6	3.812450000	-0.038510000	0.985330000
6	3.340700000	-2.329540000	2.616510000
1	2.233570000	-3.119940000	0.972310000
6	4.383100000	-0.158050000	2.252400000
6	4.145870000	-1.276650000	3.063530000
1	3.157380000	-3.198830000	3.248070000
1	5.002300000	0.656420000	2.629990000
1	4.593150000	-1.317760000	4.058590000
6	0.307650000	2.914050000	-0.625460000
1	0.370180000	2.699110000	-1.701280000
1	0.605200000	3.954780000	-0.430030000
1	-0.728980000	2.777170000	-0.287060000
6	1.318480000	2.391030000	2.047000000
1	0.279330000	2.375430000	2.403300000
1	1.701750000	3.421920000	2.065160000
1	1.931980000	1.756220000	2.699880000
6	3.471460000	-0.423570000	-2.530170000
1	3.088670000	-0.764950000	-3.504860000
1	4.534300000	-0.693870000	-2.449060000
1	3.338060000	0.659260000	-2.451800000
6	2.680450000	-3.085630000	-1.800230000
1	3.743570000	-3.287210000	-1.999170000
1	2.102970000	-3.214480000	-2.727760000
6	-2.910440000	0.244660000	-0.379050000
6	-3.198240000	1.375730000	-1.037770000
6	-4.011720000	-0.096420000	0.607300000
6	-4.507030000	1.962870000	-0.599110000
7	-5.018890000	0.967590000	0.379750000
1	-3.656570000	-0.074100000	1.652170000
1	-4.446510000	-1.093120000	0.431700000
1	-4.374900000	2.950310000	-0.120540000
1	-5.212280000	2.093800000	-1.434450000
1	-2.584720000	1.840760000	-1.810800000
1	2.306110000	-3.786300000	-1.046290000
1	-0.910820000	-0.056080000	-1.109620000
6	-0.777400000	-0.450220000	1.688040000
1	-1.290380000	0.506130000	1.792820000
1	-0.338230000	-0.867420000	2.596860000
1	-0.022060000	-3.021440000	1.302290000

F (nimag=0)   E(au)= -2521.031891   **G(au)=** -2521.1393

6	0.400660000	0.979800000	1.608720000
6	2.370720000	1.545700000	0.015820000
45	-0.372570000	-0.609880000	0.460840000
6	1.972510000	2.985600000	0.391460000
6	0.001040000	2.438010000	1.545010000
1	2.338830000	3.692990000	-0.363150000
1	2.400760000	3.265430000	1.371360000
1	-1.088700000	2.565330000	1.499630000
1	0.345940000	2.918660000	2.483870000
6	1.607350000	0.559180000	0.907370000
8	0.550400000	3.114010000	0.425940000
16	6.069850000	-1.363860000	-0.488930000
6	7.070390000	-1.716260000	-1.941470000

```
1        8.035070000     -1.211650000     -1.812290000
1        6.540120000     -1.349010000     -2.828870000
1        7.189620000     -2.807290000     -1.979130000
8        4.732810000     -2.007470000     -0.687880000
8        6.855260000     -1.701380000      0.727670000
15      -1.485250000      0.365900000     -1.281520000
15      -2.434690000     -1.040300000      1.429210000
6       -3.001550000      1.329680000     -0.892390000
6       -4.248080000      0.726800000     -0.579380000
6       -2.893230000      2.733290000     -0.900650000
6       -5.346740000      1.564580000     -0.322290000
6       -3.997200000      3.543110000     -0.626960000
1       -1.941990000      3.214500000     -1.123980000
6       -5.230080000      2.955730000     -0.344050000
1       -6.308920000      1.107840000     -0.084710000
1       -3.887010000      4.628430000     -0.641200000
1       -6.103200000      3.575810000     -0.133590000
6       -3.782780000     -1.633990000      0.328980000
6       -4.092250000     -3.005110000      0.318160000
6       -4.485500000     -0.750330000     -0.529780000
6       -5.091330000     -3.509580000     -0.517850000
1       -3.562240000     -3.697370000      0.971050000
6       -5.492830000     -1.279270000     -1.353140000
6       -5.794660000     -2.643010000     -1.354120000
1       -5.316120000     -4.577260000     -0.507090000
1       -6.037380000     -0.605760000     -2.016950000
1       -6.577980000     -3.024050000     -2.011630000
6       -0.395010000      1.474680000     -2.248450000
1       -0.045300000      2.307000000     -1.627710000
1       -0.956800000      1.844480000     -3.119190000
1        0.460930000      0.878880000     -2.595810000
6       -1.889100000     -0.968860000     -2.482320000
1       -0.939980000     -1.375260000     -2.860640000
1       -2.449790000     -0.519420000     -3.316130000
1       -2.480510000     -1.772510000     -2.031240000
6       -3.133330000      0.245670000      2.540720000
1       -2.404320000      0.457430000      3.336040000
1       -4.056570000     -0.153930000      2.986330000
1       -3.363380000      1.166660000      1.992200000
6       -1.985230000     -2.423880000      2.551940000
1       -2.866800000     -2.740280000      3.130160000
1       -1.213650000     -2.061340000      3.245810000
6        3.862090000      1.307030000      0.075570000
6        4.698140000      1.464540000      1.110170000
6        4.638610000      0.822290000     -1.135070000
6        6.101300000      1.057800000      0.733520000
7        5.941260000      0.369590000     -0.582580000
1        4.816750000      1.649640000     -1.846250000
1        4.138540000      0.013010000     -1.683610000
1        6.762650000      1.932700000      0.597710000
1        6.581580000      0.388910000      1.459860000
1        4.443710000      1.835370000      2.104310000
1       -1.582750000     -3.275880000      1.988120000
1        2.051880000      1.380330000     -1.022940000
6        1.873790000     -0.797480000      0.930420000
1        2.659740000     -1.253500000      0.320960000
1        1.491210000     -1.419520000      1.755800000
1        0.250530000      0.539960000      2.604960000
```

G (nimag=0)   E(au)= -3341.6060   G(au)= -3340.9884

```
6       -0.499540000     -3.024370000      1.602030000
6       -1.557180000     -2.630000000     -0.601900000
45       1.004470000      0.117330000      0.306340000
6       -0.998400000     -4.032740000     -0.887880000
6       -0.535090000     -4.507090000      1.386120000
1        0.082470000     -3.953180000     -1.110350000
1       -1.503390000     -4.490770000     -1.749220000
```

1	0.511010000	-4.884760000	1.372910000
1	-1.038180000	-5.009680000	2.229540000
6	-0.940030000	-2.116930000	0.702990000
8	-1.219610000	-4.913890000	0.210490000
16	-6.379760000	-0.634640000	-0.318730000
6	-7.626330000	-0.633280000	-1.618320000
1	-8.048690000	-1.643360000	-1.692510000
1	-7.142370000	-0.330420000	-2.554640000
1	-8.396480000	0.089210000	-1.316230000
8	-5.692240000	0.686950000	-0.331190000
8	-7.034490000	-1.107220000	0.933100000
15	0.144910000	1.364540000	-1.411990000
15	0.886690000	1.871970000	1.768210000
6	1.129150000	2.928590000	-1.515840000
6	0.880280000	4.038810000	-0.668080000
6	2.188360000	2.994230000	-2.438790000
6	1.685740000	5.183140000	-0.806550000
6	2.987500000	4.134410000	-2.546760000
1	2.396940000	2.148840000	-3.093650000
6	2.730920000	5.236480000	-1.730400000
1	1.492190000	6.041200000	-0.160120000
1	3.802010000	4.157770000	-3.273040000
1	3.343100000	6.137110000	-1.806700000
6	-0.331340000	3.224830000	1.458900000
6	-1.413080000	3.374970000	2.344680000
6	-0.225720000	4.094380000	0.342180000
6	-2.375800000	4.368560000	2.152540000
1	-1.515070000	2.716520000	3.206490000
6	-1.194430000	5.100370000	0.180200000
6	-2.262330000	5.238990000	1.068480000
1	-3.206200000	4.459820000	2.854910000
1	-1.113190000	5.773220000	-0.675560000
1	-3.004440000	6.023340000	0.907940000
6	0.437800000	0.482440000	-3.001080000
1	1.473110000	0.123090000	-3.056280000
1	0.207770000	1.133500000	-3.857240000
1	-0.226400000	-0.393240000	-3.018190000
6	-1.631430000	1.844400000	-1.539860000
1	-2.205590000	0.954030000	-1.829940000
1	-1.739810000	2.610000000	-2.321840000
1	-2.019790000	2.231040000	-0.590660000
6	2.555480000	2.653620000	1.862030000
1	3.258850000	1.883540000	2.212190000
1	2.534580000	3.490700000	2.575860000
1	2.876360000	3.014850000	0.877630000
6	0.622100000	1.317680000	3.501960000
1	0.764790000	2.158170000	4.196530000
1	1.370780000	0.538190000	3.704800000
6	-3.077010000	-2.600340000	-0.567820000
6	-3.918230000	-3.574780000	-0.195220000
6	-3.848340000	-1.376090000	-1.004050000
6	-5.358310000	-3.169590000	-0.320870000
7	-5.266210000	-1.793180000	-0.877310000
1	-3.617750000	-1.102240000	-2.050800000
1	-3.635590000	-0.491120000	-0.383010000
1	-5.922780000	-3.828910000	-1.005650000
1	-5.885660000	-3.173320000	0.648140000
1	-3.619390000	-4.558690000	0.163280000
1	-0.377590000	0.887120000	3.642910000
1	-1.221570000	-1.974840000	-1.423710000
6	-0.839320000	-0.661000000	0.978180000
1	-1.648230000	-0.076370000	0.525020000
1	-0.813640000	-0.478130000	2.059420000
1	-0.036530000	-2.689400000	2.535660000
16	2.469230000	-2.261060000	0.453320000
8	2.310810000	-1.077350000	1.529570000
8	1.833020000	-1.540680000	-0.833980000
6	4.239420000	-2.277470000	0.111440000

```
6      4.867980000    -3.524610000     0.026370000
6      4.963450000    -1.093020000    -0.060290000
1      4.294410000    -4.443160000     0.170630000
1      4.467380000    -0.124680000     0.026390000
6      6.236140000    -3.582200000    -0.243590000
6      6.329690000    -1.168330000    -0.327920000
1      6.729430000    -4.554850000    -0.310420000
1      6.901850000    -0.247010000    -0.460140000
6      6.987440000    -2.408690000    -0.425400000
6      8.465020000    -2.485700000    -0.716330000
1      8.993140000    -3.048230000     0.070770000
1      8.651020000    -3.012960000    -1.666740000
1      8.916880000    -1.486260000    -0.786380000
```

G′ (nimag=0) E(au)= -3341.6060   G(au)= -3340.9884

```
6       0.071980000     0.362690000     0.945000000
6      -1.671750000    -1.526820000     0.566520000
45      1.212200000    -0.001650000    -0.806770000
6      -1.403100000    -1.774820000     2.072480000
6       0.349770000    -0.233580000     2.298210000
1      -1.663660000    -2.803890000     2.351900000
1      -2.017180000    -1.082050000     2.677860000
1       1.414770000    -0.170950000     2.559450000
1      -0.207180000     0.361360000     3.052170000
6      -0.928480000    -0.274880000     0.108150000
8      -0.025540000    -1.603290000     2.389840000
16     -6.328560000    -3.160250000    -1.007090000
6      -7.735790000    -3.604220000     0.024000000
1      -8.216540000    -2.678450000     0.364490000
1      -7.365500000    -4.198930000     0.867850000
1      -8.418110000    -4.190210000    -0.606440000
8      -5.584790000    -4.405840000    -1.341680000
8      -6.828990000    -2.285980000    -2.103890000
15      2.370650000    -1.916760000    -0.382640000
15      3.219150000     1.179640000    -0.593160000
6       3.533420000    -1.832870000     1.048490000
6       4.805620000    -1.208470000     0.987550000
6       3.094250000    -2.381720000     2.268240000
6       5.588250000    -1.170160000     2.155310000
6       3.889890000    -2.329220000     3.414360000
1       2.110640000    -2.840650000     2.343730000
6       5.142480000    -1.719280000     3.358270000
1       6.566930000    -0.689240000     2.112190000
1       3.522050000    -2.762900000     4.345800000
1       5.774580000    -1.666620000     4.246620000
6       4.846660000     0.411740000    -1.016350000
6       5.535470000     0.884700000    -2.148280000
6       5.415290000    -0.639950000    -0.255030000
6       6.762850000     0.339530000    -2.532950000
1       5.124620000     1.697440000    -2.744000000
6       6.653710000    -1.170170000    -0.656370000
6       7.324140000    -0.693930000    -1.784260000
1       7.273190000     0.729160000    -3.415470000
1       7.088870000    -1.984100000    -0.073900000
1       8.281030000    -1.132550000    -2.073280000
6       1.297120000    -3.373590000    -0.072190000
1       0.703990000    -3.236870000     0.836700000
1       1.940460000    -4.261470000     0.023430000
1       0.633240000    -3.497990000    -0.939300000
6       3.265680000    -2.448790000    -1.904330000
1       2.502080000    -2.732200000    -2.643530000
1       3.878380000    -3.329330000    -1.659480000
1       3.901220000    -1.660060000    -2.319570000
6       3.381800000     1.999990000     1.041540000
1       2.463370000     2.592680000     1.198510000
1       4.267140000     2.653760000     1.019640000
```

1	3.498490000	1.252440000	1.837390000
6	2.972200000	2.539400000	-1.799090000
1	3.738600000	3.315430000	-1.650970000
1	1.960050000	2.948880000	-1.636990000
6	-3.161180000	-1.457310000	0.307360000
6	-3.939600000	-0.389880000	0.090430000
6	-3.982920000	-2.727250000	0.320670000
6	-5.382110000	-0.767630000	-0.085280000
7	-5.362670000	-2.247150000	0.062490000
1	-3.932810000	-3.246570000	1.295170000
1	-3.652650000	-3.446720000	-0.446080000
1	-6.027710000	-0.307360000	0.684840000
1	-5.780100000	-0.471400000	-1.069480000
1	-3.610430000	0.647640000	0.030030000
1	3.027180000	2.150660000	-2.825180000
1	-1.284930000	-2.391220000	0.004380000
6	-1.005390000	0.221390000	-1.184880000
1	-1.569430000	-0.310820000	-1.955060000
1	-0.735630000	1.283080000	-1.373880000
1	0.147160000	1.471430000	0.917920000
16	-0.190570000	4.108640000	-0.107560000
8	0.362170000	3.383200000	1.165300000
8	-0.109470000	3.166980000	-1.366440000
6	-2.007070000	4.128790000	0.219610000
6	-2.475550000	4.176340000	1.533430000
6	-2.907540000	4.192890000	-0.850070000
1	-1.760060000	4.120720000	2.356200000
1	-2.531610000	4.149510000	-1.874390000
6	-3.850820000	4.271750000	1.776670000
6	-4.277260000	4.289550000	-0.596600000
1	-4.214690000	4.299030000	2.807750000
1	-4.978140000	4.331550000	-1.435530000
6	-4.772590000	4.333480000	0.719910000
6	-6.255870000	4.451820000	0.977270000
1	-6.815900000	3.649250000	0.469360000
1	-6.484650000	4.399970000	2.051740000
1	-6.650790000	5.408090000	0.594160000

TS_GH (nimag=1) (-181.82*i*)   **E(au)=** -3341.5599   **G(au)=** -3340.9363

6	1.845825000	1.769401000	0.088508000
6	2.273740000	-0.095299000	-1.522228000
45	-1.033542000	0.157151000	-0.237572000
6	2.427239000	1.060342000	-2.517617000
6	3.020657000	2.427291000	-0.591876000
1	1.427921000	1.392054000	-2.843769000
1	2.998080000	0.735852000	-3.399806000
1	3.005083000	3.519105000	-0.447049000
1	3.922195000	2.046316000	-0.068215000
6	1.531287000	0.409985000	-0.274324000
8	3.141300000	2.185497000	-1.986174000
16	5.681980000	-3.042832000	1.101932000
6	6.419807000	-4.588436000	0.545739000
1	7.216474000	-4.350282000	-0.170205000
1	5.632417000	-5.195707000	0.083029000
1	6.830314000	-5.082102000	1.436950000
8	4.505951000	-3.371077000	1.954918000
8	6.775098000	-2.195130000	1.654455000
15	-1.504867000	-1.804178000	-1.307496000
15	-2.757480000	-0.160937000	1.225393000
6	-3.331576000	-2.073404000	-1.523408000
6	-4.161077000	-2.539278000	-0.471872000
6	-3.917544000	-1.771851000	-2.765973000
6	-5.532440000	-2.725008000	-0.719888000
6	-5.286796000	-1.941324000	-2.986409000
1	-3.306465000	-1.401693000	-3.588271000
6	-6.097465000	-2.429773000	-1.961587000

1	-6.166600000	-3.089736000	0.090481000
1	-5.711015000	-1.696882000	-3.962094000
1	-7.167474000	-2.575363000	-2.121870000
6	-3.041614000	-1.912837000	1.749022000
6	-2.599048000	-2.318839000	3.020685000
6	-3.655930000	-2.866260000	0.898536000
6	-2.769945000	-3.632673000	3.463739000
1	-2.116709000	-1.606131000	3.688333000
6	-3.835954000	-4.178045000	1.369759000
6	-3.398308000	-4.565114000	2.637633000
1	-2.416140000	-3.918512000	4.456083000
1	-4.314952000	-4.909227000	0.715696000
1	-3.544688000	-5.593483000	2.973624000
6	-0.861175000	-1.754047000	-3.038821000
1	-1.121540000	-0.805025000	-3.526756000
1	-1.255112000	-2.598229000	-3.623501000
1	0.233109000	-1.837574000	-2.998603000
6	-0.831976000	-3.413749000	-0.697485000
1	0.257246000	-3.410336000	-0.850036000
1	-1.272806000	-4.243818000	-1.268798000
1	-1.042193000	-3.546259000	0.370511000
6	-4.401532000	0.537746000	0.752245000
1	-4.268407000	1.622000000	0.621875000
1	-5.135058000	0.348663000	1.550645000
1	-4.757151000	0.104603000	-0.190034000
6	-2.385882000	0.759247000	2.777300000
1	-3.184275000	0.604513000	3.518019000
1	-2.323609000	1.821983000	2.508249000
6	3.600331000	-0.745970000	-1.166798000
6	4.840041000	-0.322091000	-1.451025000
6	3.649153000	-2.069863000	-0.437407000
6	5.896161000	-1.272874000	-0.967663000
7	5.100692000	-2.366685000	-0.349649000
1	3.124717000	-2.863593000	-1.002620000
1	3.191418000	-2.027604000	0.562745000
1	6.516690000	-1.661852000	-1.795843000
1	6.578355000	-0.813771000	-0.233491000
1	5.091118000	0.602726000	-1.969988000
1	-1.418976000	0.450426000	3.196262000
1	1.664550000	-0.865266000	-2.019851000
6	0.815415000	-0.436860000	0.625615000
1	0.951360000	-1.517075000	0.535314000
1	0.734070000	-0.099474000	1.666520000
1	1.766501000	2.024125000	1.151390000
16	0.076302000	2.993208000	-0.420489000
8	-0.974141000	2.197079000	0.429550000
8	-0.222141000	2.999476000	-1.899841000
6	-0.053787000	4.686656000	0.186510000
6	-0.172071000	4.937448000	1.560277000
6	0.040492000	5.728432000	-0.739488000
1	-0.247698000	4.115119000	2.272880000
1	0.130961000	5.505910000	-1.803090000
6	-0.211202000	6.259473000	1.998147000
6	-0.001089000	7.045793000	-0.276914000
1	-0.313754000	6.463861000	3.066681000
1	0.062314000	7.865346000	-0.996407000
6	-0.125591000	7.333631000	1.091497000
6	-0.171002000	8.755616000	1.590072000
1	-1.122340000	8.959493000	2.108806000
1	0.636767000	8.944809000	2.315917000
1	-0.068848000	9.476272000	0.766744000

TS_G'H' (nimag=1) (-56.3*i*)   **E(au)=** -3341.4941   **G(au)=** -3340.8769

6	-0.350684916	0.437802923	0.670881276
6	-1.081110872	-2.015792310	0.833724705

```
45        1.303320412      -0.043962622      -0.740476379
 6       -0.700872612      -1.825003971       2.325093990
 6       -0.012665063       0.389752855       2.136833041
 1       -0.402641673      -2.781211814       2.774984430
 1       -1.565787187      -1.429298249       2.881858763
 1        0.825091405       1.062438719       2.362537933
 1       -0.890603456       0.705234553       2.739141723
 6       -0.721164598      -0.780249377       0.000724840
 8        0.390950602      -0.927773088       2.497103781
16       -5.844530426      -2.491544597      -1.392478432
 6       -6.432280477      -4.088724948      -1.986475472
 1       -6.767460849      -4.674527145      -1.121196664
 1       -5.606825907      -4.584844144      -2.511712086
 1       -7.269419628      -3.885476905      -2.668047819
 8       -5.257522926      -1.761471125      -2.550074479
 8       -6.946635201      -1.876362256      -0.603686891
15        2.755040328      -1.746871456      -0.349835108
15        3.066142618       1.513668887      -0.403759741
 6        4.063065759      -1.413903652       0.912527233
 6        5.219477638      -0.632899385       0.657681269
 6        3.873484571      -1.959528364       2.195936079
 6        6.165943639      -0.480795022       1.686600056
 6        4.816584804      -1.777266522       3.208547812
 1        2.975928352      -2.532034538       2.422628504
 6        5.975451093      -1.044988555       2.948598785
 1        7.059537099       0.114445284       1.490399561
 1        4.641565498      -2.212012976       4.194111957
 1        6.726311944      -0.900497786       3.727631411
 6        4.674990510       1.055981461      -1.193006270
 6        5.048721603       1.673165306      -2.399296008
 6        5.510715662       0.052033305      -0.641560289
 6        6.230766926       1.319767821      -3.055963095
 1        4.422568128       2.447328580      -2.841864473
 6        6.702066142      -0.277389472      -1.309317508
 6        7.061730962       0.342558132      -2.507744951
 1        6.498004944       1.815715917      -3.990842914
 1        7.348492462      -1.046320868      -0.882184552
 1        7.989235531       0.059704403      -3.009042511
 6        2.046895054      -3.372239808       0.137023721
 1        1.509942231      -3.314128283       1.089649072
 1        2.868986380      -4.098531836       0.223783463
 1        1.358466304      -3.698400451      -0.654898126
 6        3.568566830      -2.169779743      -1.954139722
 1        2.801265614      -2.629451185      -2.594034299
 1        4.377814086      -2.893279318      -1.771869620
 1        3.970565962      -1.281440024      -2.453150084
 6        3.445457335       2.065438643       1.315005884
 1        2.564792997       2.602634642       1.695091947
 1        4.308404398       2.747127096       1.298897262
 1        3.657221372       1.210786250       1.968149852
 6        2.528948537       3.074146576      -1.224178258
 1        3.317689015       3.839263085      -1.167265351
 1        1.636959167       3.436121426      -0.691750205
 6       -2.558570098      -2.346970396       0.676303539
 6       -3.447615678      -2.591458295       1.647497552
 6       -3.214664548      -2.456874631      -0.681065029
 6       -4.821276662      -2.853213927       1.110221086
 7       -4.576017961      -2.939400340      -0.350195506
 1       -2.699598760      -3.177684503      -1.341921504
 1       -3.245156724      -1.482520809      -1.190853222
 1       -5.264406538      -3.790212203       1.490524151
 1       -5.503673685      -2.023543986       1.362330400
 1       -3.266953507      -2.569496926       2.720997582
 1        2.259789927       2.889890484      -2.273208735
 1       -0.524331731      -2.866645859       0.411623538
 6       -0.647456294      -0.814971574      -1.396911822
 1       -0.774844034      -1.758823582      -1.930093024
 1       -0.842736783       0.089271363      -1.988031086
```

1	-0.454019941	1.404801726	0.161483721
16	-3.032036811	1.247633735	1.123265146
8	-3.070556440	1.233492311	2.660232654
8	-4.151362563	0.488260024	0.405207738
6	-3.324000563	3.008533761	0.674675669
6	-2.872200334	4.025908334	1.517321494
6	-3.950863726	3.308929956	-0.538443107
1	-2.405120793	3.774353579	2.470966295
1	-4.315652718	2.497916946	-1.170849887
6	-3.054065131	5.359278294	1.136702447
6	-4.125456571	4.644938651	-0.904083333
1	-2.709482111	6.157786685	1.799292661
1	-4.624259785	4.881591206	-1.848102314
6	-3.679722293	5.691218819	-0.076250740
6	-3.894108957	7.130823579	-0.476470899
1	-4.954826311	7.415510795	-0.366820091
1	-3.299566124	7.816220810	0.145023362
1	-3.624739606	7.298434830	-1.531454397

H (nimag=0) E(au)= -3341.5730   G(au)= -3340.9491

6	-2.012380000	1.313460000	0.204570000
6	-1.897800000	-0.923630000	1.414710000
45	0.931610000	0.135830000	-0.051150000
6	-2.060320000	-0.029470000	2.647170000
6	-3.221030000	1.463830000	1.130740000
1	-1.081130000	0.407500000	2.905160000
1	-2.418710000	-0.614670000	3.506480000
1	-3.540690000	2.516240000	1.183350000
1	-4.044200000	0.894740000	0.662110000
6	-1.364150000	-0.072010000	0.244150000
8	-3.008230000	1.032920000	2.463980000
16	-5.382780000	-3.644270000	-1.369880000
6	-5.779410000	-5.392400000	-1.201410000
1	-6.421580000	-5.516900000	-0.320420000
1	-4.838940000	-5.946460000	-1.095030000
1	-6.311750000	-5.684630000	-2.116690000
8	-4.394040000	-3.497770000	-2.473950000
8	-6.667890000	-2.893730000	-1.432300000
15	1.819010000	-1.908940000	0.422930000
15	3.045390000	0.840850000	-0.868520000
6	3.384260000	-1.662310000	1.401230000
6	4.649540000	-1.400270000	0.819680000
6	3.276240000	-1.674960000	2.804810000
6	5.758490000	-1.206840000	1.664040000
6	4.384290000	-1.460890000	3.626890000
1	2.312560000	-1.857430000	3.279490000
6	5.636130000	-1.234610000	3.053510000
1	6.732870000	-1.014300000	1.210590000
1	4.264070000	-1.478060000	4.711780000
1	6.514340000	-1.073640000	3.681740000
6	4.276700000	-0.390090000	-1.507380000
6	4.581310000	-0.412120000	-2.880040000
6	4.893120000	-1.340570000	-0.655700000
6	5.479510000	-1.341530000	-3.411810000
1	4.118800000	0.304030000	-3.557670000
6	5.807600000	-2.255120000	-1.204900000
6	6.099500000	-2.265040000	-2.570080000
1	5.693040000	-1.334720000	-4.482430000
1	6.282420000	-2.983250000	-0.544230000
1	6.805790000	-2.994570000	-2.971250000
6	0.895380000	-3.117570000	1.481820000
1	0.543490000	-2.667990000	2.418200000
1	1.558180000	-3.964420000	1.713920000
1	0.029870000	-3.493430000	0.919190000
6	2.193890000	-3.023170000	-1.007780000
1	1.226100000	-3.384570000	-1.388230000

1	2.793540000	-3.883910000	-0.676570000
1	2.712820000	-2.494900000	-1.814380000
6	3.987170000	1.903560000	0.319500000
1	3.332760000	2.740160000	0.605910000
1	4.899790000	2.291870000	-0.157220000
1	4.253080000	1.333610000	1.218870000
6	2.769530000	1.995150000	-2.281130000
1	3.723510000	2.395270000	-2.654750000
1	2.144090000	2.814890000	-1.904790000
6	-3.168430000	-1.697360000	1.087030000
6	-4.356260000	-1.626800000	1.705010000
6	-3.201060000	-2.761300000	0.011220000
6	-5.351660000	-2.606020000	1.156260000
7	-4.579850000	-3.304480000	0.095500000
1	-2.462470000	-3.562270000	0.203310000
1	-2.993830000	-2.365190000	-0.994040000
1	-5.697520000	-3.322900000	1.923500000
1	-6.245500000	-2.113660000	0.739480000
1	-4.613950000	-0.939930000	2.510770000
1	2.228540000	1.488680000	-3.092310000
1	-1.135940000	-1.670580000	1.670450000
6	-0.847320000	-0.621710000	-0.950790000
1	-0.804770000	-1.705220000	-1.080380000
1	-0.947430000	-0.067350000	-1.890700000
1	-2.307720000	1.595570000	-0.817640000
16	-0.732310000	2.621480000	0.586340000
8	0.408170000	2.228910000	-0.370130000
8	-0.410450000	2.697580000	2.038980000
6	-1.336140000	4.208890000	0.025910000
6	-1.407780000	4.490600000	-1.345270000
6	-1.719100000	5.144190000	0.990410000
1	-1.085560000	3.757630000	-2.085780000
1	-1.638610000	4.903500000	2.050580000
6	-1.882940000	5.737230000	-1.743020000
6	-2.190350000	6.387940000	0.565550000
1	-1.939360000	5.969670000	-2.808810000
1	-2.487860000	7.127170000	1.312130000
6	-2.282320000	6.703750000	-0.799190000
6	-2.791900000	8.045720000	-1.257140000
1	-2.038130000	8.560710000	-1.874830000
1	-3.693010000	7.929300000	-1.881470000
1	-3.043710000	8.695010000	-0.407420000

H' (nimag=0) E(au)= -3341.6113   G(au)= -3340.9861

6	-1.306270000	0.887330000	0.309320000
6	-1.057720000	-1.548140000	1.111810000
45	1.339950000	0.120380000	-0.190280000
6	-0.628390000	-0.999380000	2.494400000
6	-1.635330000	1.051560000	1.805550000
1	0.405030000	-1.305560000	2.705500000
1	-1.271900000	-1.397650000	3.296310000
1	-1.644160000	2.110660000	2.090410000
1	-2.622770000	0.617430000	2.036140000
6	-0.757650000	-0.507990000	0.024380000
8	-0.606810000	0.433880000	2.560070000
16	-5.533170000	-3.074960000	-1.080680000
6	-6.212180000	-4.743480000	-1.098450000
1	-6.617200000	-4.962580000	-0.102390000
1	-5.405740000	-5.436900000	-1.365620000
1	-7.010490000	-4.751660000	-1.852850000
8	-4.834170000	-2.844690000	-2.374000000
8	-6.624110000	-2.154250000	-0.654900000
15	2.710650000	-1.648270000	-0.322330000
15	3.216410000	1.562530000	-0.039160000
6	4.128630000	-1.550790000	0.872740000
6	5.305660000	-0.795820000	0.637700000

```
6        3.993690000     -2.234860000      2.095560000
6        6.318290000     -0.802480000      1.614380000
6        5.001760000     -2.211080000      3.061100000
1        3.089430000     -2.804170000      2.309290000
6        6.176940000     -1.500350000      2.814190000
1        7.226940000     -0.226800000      1.428060000
1        4.866050000     -2.753720000      3.998440000
1        6.978970000     -1.479130000      3.554490000
6        4.743570000      1.110360000     -0.982540000
6        5.075860000      1.833140000     -2.140930000
6        5.556020000      0.014750000     -0.596280000
6        6.192810000      1.495420000     -2.910160000
1        4.463460000      2.676580000     -2.458170000
6        6.683750000     -0.298710000     -1.373550000
6        7.001900000      0.426810000     -2.523420000
1        6.426330000      2.073100000     -3.806500000
1        7.311540000     -1.140330000     -1.074200000
1        7.878580000      0.153720000     -3.113950000
6        1.991120000     -3.318930000      0.008590000
1        1.507010000     -3.378520000      0.990880000
1        2.792410000     -4.070840000     -0.048260000
1        1.245790000     -3.534520000     -0.769130000
6        3.407350000     -1.931710000     -2.011500000
1        2.570150000     -2.246640000     -2.652000000
1        4.162820000     -2.731260000     -1.976270000
1        3.847640000     -1.019350000     -2.427400000
6        3.767770000      1.986440000      1.674520000
1        2.920550000      2.464510000      2.188560000
1        4.617460000      2.684470000      1.637990000
1        4.052560000      1.081310000      2.224590000
6        2.698200000      3.206710000     -0.697710000
1        3.519740000      3.936830000     -0.642700000
1        1.865050000      3.556790000     -0.070670000
6       -2.486880000     -2.058740000      1.036750000
6       -3.446300000     -2.058490000      1.970920000
6       -2.966870000     -2.750820000     -0.218140000
6       -4.708110000     -2.714670000      1.492520000
7       -4.341570000     -3.187260000      0.133180000
1       -2.334900000     -3.623930000     -0.465890000
1       -2.968660000     -2.080640000     -1.089340000
1       -5.009010000     -3.562860000      2.134530000
1       -5.555270000     -2.009280000      1.455620000
1       -3.380880000     -1.638500000      2.974510000
1        2.341940000      3.116840000     -1.732990000
1       -0.425690000     -2.421340000      0.890720000
6       -0.304970000     -0.851750000     -1.254670000
1       -0.152120000     -1.904250000     -1.500780000
1       -0.473280000     -0.186210000     -2.103670000
1       -0.601410000      1.687740000      0.003930000
16      -2.767950000      1.313730000     -0.806200000
8       -3.853090000      0.316160000     -0.568990000
8       -2.202570000      1.495100000     -2.179330000
6       -3.340300000      2.919280000     -0.221610000
6       -4.418950000      2.976170000      0.663980000
6       -2.718900000      4.082360000     -0.691950000
1       -4.910380000      2.059190000      0.990070000
1       -1.903940000      4.019820000     -1.413960000
6       -4.864110000      4.225430000      1.102600000
6       -3.177110000      5.317930000     -0.238960000
1       -5.709720000      4.278050000      1.791940000
1       -2.698410000      6.230450000     -0.602310000
6       -4.251750000      5.411000000      0.665630000
6       -4.736130000      6.759100000      1.135340000
1       -5.120870000      7.352560000      0.289390000
1       -5.539700000      6.664290000      1.878910000
1       -3.914100000      7.338660000      1.585960000
```

I (nimag=0) E(au)= -1926.8872   **G(au)=** -1926.5540

6	1.406570000	1.767120000	0.173780000
6	2.200430000	0.003710000	-1.517380000
6	2.242140000	1.223550000	-2.443920000
6	2.611880000	2.504510000	-0.407700000
1	1.221290000	1.424700000	-2.804190000
1	2.895280000	1.027610000	-3.307240000
1	2.581200000	3.575440000	-0.162320000
1	3.501410000	2.078450000	0.093780000
6	1.340150000	0.326230000	-0.291840000
8	2.751280000	2.414240000	-1.819240000
16	5.781420000	-2.729960000	1.107530000
6	6.416920000	-4.309860000	0.520150000
1	7.201310000	-4.107860000	-0.219870000
1	5.583850000	-4.871130000	0.079070000
1	6.825540000	-4.834020000	1.394740000
8	4.638700000	-3.011670000	2.020140000
8	6.938170000	-1.931190000	1.599130000
6	3.570640000	-0.519180000	-1.134320000
6	4.770490000	0.038370000	-1.344950000
6	3.717740000	-1.862700000	-0.459250000
6	5.896390000	-0.822930000	-0.850980000
7	5.186140000	-2.013910000	-0.313920000
1	3.299550000	-2.675740000	-1.082230000
1	3.210120000	-1.904830000	0.517000000
1	6.587390000	-1.113800000	-1.663700000
1	6.499860000	-0.331150000	-0.070960000
1	4.946640000	1.008510000	-1.810420000
1	1.690310000	-0.802760000	-2.073540000
6	0.575600000	-0.583050000	0.327010000
1	0.516050000	-1.612180000	-0.036840000
1	-0.024990000	-0.321280000	1.199470000
1	1.436110000	1.835870000	1.271170000
16	-0.241720000	2.610610000	-0.198690000
8	-1.237410000	2.013010000	0.744810000
8	-0.515430000	2.561380000	-1.669080000
6	-0.008320000	4.338490000	0.264690000
6	-0.278760000	4.736930000	1.578150000
6	0.401210000	5.257650000	-0.704440000
1	-0.625260000	4.007630000	2.311180000
1	0.592140000	4.926800000	-1.725890000
6	-0.115640000	6.078220000	1.921720000
6	0.558000000	6.596870000	-0.339920000
1	-0.326360000	6.396840000	2.945560000
1	0.878980000	7.320870000	-1.092360000
6	0.305480000	7.027940000	0.972700000
6	0.464540000	8.475920000	1.362960000
1	-0.511350000	8.921520000	1.619300000
1	1.107260000	8.577870000	2.252170000
1	0.904470000	9.068860000	0.548720000

I' (nimag=0) E(au)= -1926.8848   **G(au)=** -1926.5502

6	-0.107580000	-2.118620000	-0.331820000
6	2.127040000	-1.044030000	0.599060000
6	2.066060000	-2.239680000	1.575980000
6	0.112920000	-3.183080000	0.763870000
1	2.566250000	-1.986990000	2.520550000
1	2.570690000	-3.122730000	1.143530000
1	-0.849100000	-3.595920000	1.088970000
1	0.735000000	-4.018520000	0.391660000
6	0.859870000	-0.947400000	-0.275720000
8	0.729000000	-2.596310000	1.896800000
16	5.670790000	0.181210000	-3.077340000
6	6.676940000	1.664840000	-2.896140000

```
1      7.522920000      1.426190000     -2.240020000
1      6.046730000      2.455280000     -2.469880000
1      7.021300000      1.937050000     -3.902980000
8      4.477430000      0.547790000     -3.892360000
8      6.565110000     -0.918890000     -3.537350000
6      3.443330000     -1.002920000     -0.155300000
6      4.492360000     -1.828790000     -0.027980000
6      3.786130000      0.135220000     -1.093340000
6      5.674830000     -1.399250000     -0.845190000
7      5.185670000     -0.154170000     -1.488070000
1      3.718290000      1.114250000     -0.582420000
1      3.126310000      0.176540000     -1.972630000
1      6.561020000     -1.194630000     -0.216370000
1      5.971990000     -2.152210000     -1.591970000
1      4.547910000     -2.716780000      0.600430000
6      0.521910000      0.203360000     -0.876310000
1      1.147110000      1.095640000     -0.800290000
1     -0.391700000      0.284060000     -1.468090000
1      2.106150000     -0.123990000      1.211170000
1     -1.130750000     -1.720760000     -0.254790000
16    -0.276750000     -2.924890000     -2.010660000
8     -1.001130000     -4.212960000     -1.765880000
8     -0.881820000     -1.901100000     -2.917900000
6      1.364340000     -3.311850000     -2.639450000
6      1.925640000     -4.566660000     -2.385620000
6      2.022550000     -2.370180000     -3.437600000
1      1.377360000     -5.305440000     -1.800290000
1      1.551520000     -1.411410000     -3.652210000
6      3.184080000     -4.862160000     -2.915570000
6      3.276460000     -2.683900000     -3.958370000
1      3.630020000     -5.839980000     -2.718610000
1      3.798920000     -1.939800000     -4.561470000
6      3.878610000     -3.929610000     -3.704470000
6      5.232540000     -4.246120000     -4.288010000
1      5.900820000     -3.374790000     -4.209060000
1      5.700730000     -5.104450000     -3.784480000
1      5.144480000     -4.495010000     -5.359880000
```