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ELECTRONIC SUPPLEMENTARY INFORMATION

Unusual reactivity of rhodium carbenes with allenes: an efficient asymmetric synthesis of methylenetetrahydropyran scaffolds

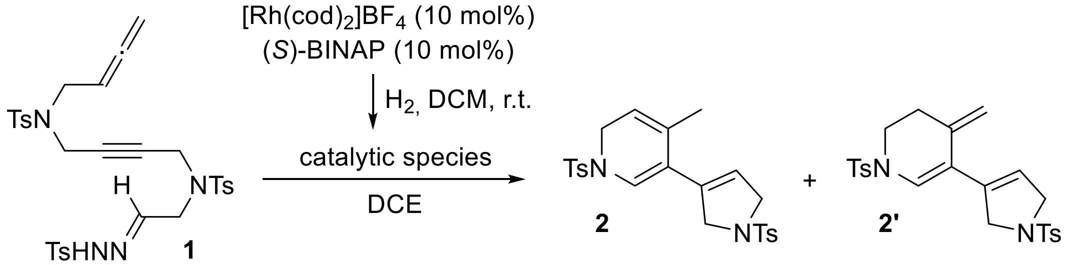
Òscar Torres, Miquel Solà, Anna Roglans and Anna Pla-Quintana*

Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química, Universitat de Girona, Facultat de Ciències, C/ Maria Aurèlia Capmany, 69, E-17003-Girona, Catalunya, Spain.

Content

S.1. Optimization for the cyclization of 1 and 3a

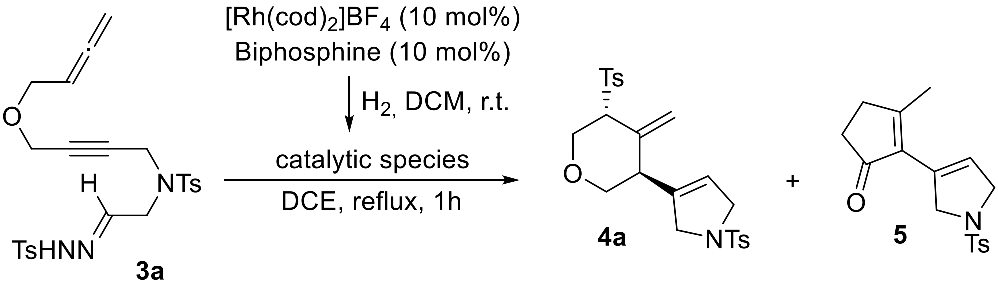
Table S1. Optimization of the cyclization of NTs-tethered substrate **1**[a]



Entry	Temperature (ºC)	Reaction time (h)	Base (equiv.)	Yield (%)[b]	**2**:**2'** ratio[c]
1	Reflux	1	-	28	2:1
2	50	14	-	-[d]	n.d.
3	Reflux	1	LiO^{t}Bu[1] (3)	< 5	2:1
4	Reflux	1	K_2CO_3[2] (3)	< 5	2:1

[a] The reaction was performed with 0.12 mmol of substrate **1** in dichloroethane (DCE) (3 mL, 40 mM). The mixture of $[Rh(cod)_2]BF_4$ and (*S*)-BINAP was treated with hydrogen in dichloromethane (DCM) solution for catalyst activation prior to the reaction. [b] Combined yield for the two isomers that could not be separated. [c] Ratio of isomers determined by NMR. [d] Starting material recovered.

Table S2. Optimization of the cyclization of O-tethered substrate **3a**[a]



Entry	Biphosphine	Concentration (mM) / base (equiv.)	Yield of **4a** (%)[b]	ee of **4a** (%)[c]	Yield of **5** (%)[b]
1	(*S*)-BINAP	40 / -	21[d]	89	21[d]
2	(*S*)-BINAP	3 / -	60	89	2
3	BINAP	3 / -	59	-	4
4	(*R*)-TolBINAP	3 / -	53	92[e]	5
5	(*R*)-H_8BINAP	3 / -	42	75[e]	5
6	(*R*)-DTBM-SegPhos	3 / -	< 5	n.d.	-
7	(*S*)-BINAP	3 / LiO^{t}Bu[1] (3)	-	-	-
8	(*S*)-BINAP	3 / K_2CO_3[2] (3)	61	87	-
9	(*S*)-BINAP	3 / -	64[d]	84	11[d]

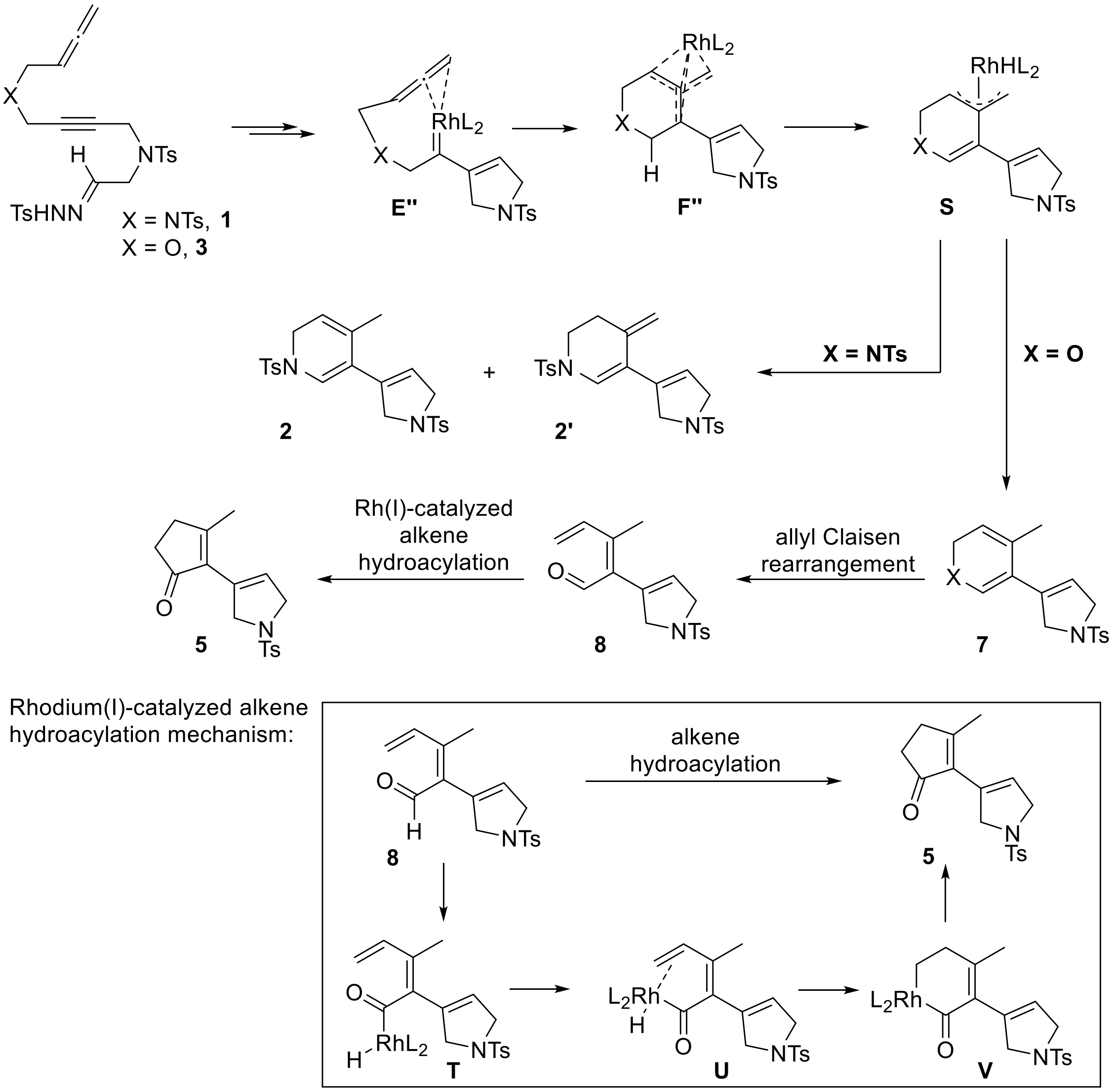
[1] Xia, J.; Liu, Z.; Xiao, Q.; Qu, P.; Ge, R.; Zhang. Y.; Wang, J. *Angew. Chem. Int. Ed.* **2012**, *51*, 5714-5717.
[2] Feng, X.-W.; Wang, J.; Zhang, J.; Yang, J.; Wang, N.; Yu, X.-Q. *Org. Lett.* **2010**, *12*, 4408-4411.

[a] The reaction was performed with 0.25 mmol of substrate **3a** in dichloroethane (DCE) at the concentration indicated in the table. The mixture of $[Rh(cod)_2]BF_4$ and biphosphine was treated with hydrogen in dichloromethane (DCM) solution for catalyst activation prior to the reaction. [b] Yield determined by NMR using *p*-methylanisole as internal standard unless otherwise noted. [c] Enantiomeric excess determined by chiral HPLC chromatography. [d] Isolated yield. [e] The reaction forms the opposite enantiomer to the one obtained with (*S*)-BINAP.

S.2. Mechanistic proposal for the formation of 2, 2', and 5

The tosylhydrazone moiety of substrate **1** or **3** is decomposed in a process assisted by the rhodium to initally form the rhodium-carbene intermediate that subsequently suffers a carbene-alkyne metathesis to deliver **E''** where the rhodium atom is already coordinated to the allene. Ring-closure through a [2+2] cycloaddition of the double bond of the external allene and the rhodium-carbene bond to form intermediate **F''** that has an electronic structure resembling that of the trimethylenemethane. This part is analogous to the formation of **4** but from here it diverges. Instead of a reverse β-H-elimination that would lead to intermediate **H** and continue to the formation of **4**, a β-H-elimination takes place forming intermediate **S**. Intermediate **S**, which has a rhodium-π-allyl substructure, suffers a reductive elimination furnishing product **7** or **2**. In this point it is important to highlight that product **2'** is obtained when the reductive elimination places the hydrogen on the other extreme of the rhodium-π-allyl substructure. From this point, the 2H-pyran framework undergoes an electrocyclic ring-opening (allyl Claisen rearrangement) to form 1-oxatriene **8** in a thermally induced process. Compound **8** that features 1-oxatriene or 2,4-dienal substructure can be subsequently involved in an intramolecular alkene hydroacylation[3] to afford the cyclopentenone ring in **5**. The catalytic system that we have in the reaction media is an efficient catalyst in alkene hydroacylation reactions.[4] This transformation is postulated to take place through oxidative addition of the rhodium catalyst across the aldehyde C-H bond to generate an acyl metal hydride **T**, subsequent addition across the alkene to form **V**, followed by reductive elimination to generate cyclopentenone product **5** and regenerate the catalyst.

[3] M. C. Willis, *Chem. Rev.* 2010, **110**, 725.
[4] a) R. Okamoto, K. Tanaka, *Org. Lett.* 2013, **15**, 2112; b) K. F. Johnson, A. C. Schmidt, L. M. Stanley, *Org. Lett.* 2015, **17**, 4654; c) S. Y. Y. Yip, C. Aïssa, *Angew. Chem. Int. Ed.* 2015, **54**, 6870; d) J.-W. Park, K. G. M. Kou, D. K. Kim, V. M. Dong, *Chem. Sci.* 2015, **6**, 4479.



Scheme S1. Detailed mechanistic proposal for the formation of **2**, **2'** and **5**.

S.3. General methods and materials

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. CH_2Cl_2 was dried under nitrogen by passing through solvent purification columns (MBraun, SPS-800). Solvents were removed under reduced pressure with a rotary evaporator. When necessary, reaction mixtures were chromatographed on silica gel (230-400 mesh) using a gradient solvent system as the eluent. All cyclization reactions were carried out using Schlenk techniques.

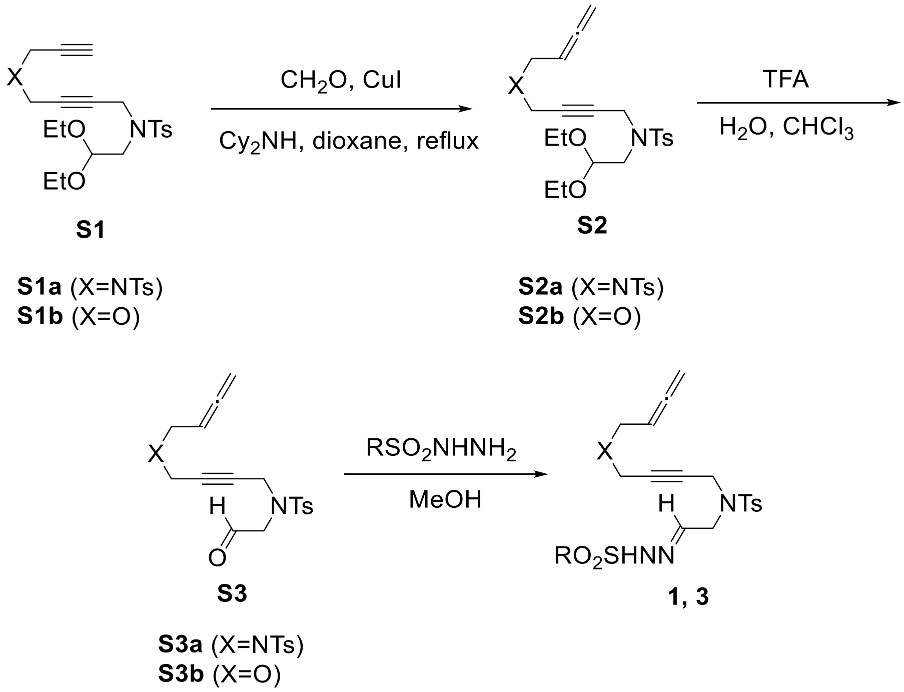
All ^{1}H and ^{13}C NMR spectra were recorded using Bruker Ultrashield AVANCE III400 (400 MHz) and Bruker Ultrashield DPX300 (300 MHz) spectrometers at 298K with $CDCl_3$ as a deuterated solvent. Chemical shifts (δ) for ^{1}H and ^{13}C NMR were referenced to internal solvent resonances and reported relative to $SiMe_4$.

Electrospray mass spectrometry analyses were recorded on an Esquire 6000 Ion Trap Mass Spectrometer (Bruker) equipped with an electrospray ion source. The instrument was operated in the positive ESI(+) ion mode. HPLC analysis were recorded with a CHIRALPAK IC, 4.6 x 250 mm, 5 µm column in a Spectra System Thermo (Shimadzu) apparatus equipped with an SN4000 connector, SCM1000 degaser, P2000 pump and UV6000LP detector with a 20 µL loop. Infrared spectra were recorded on a Bruker Alpha FT-IR spectrometer with a DTGS detector and an ATR adapter. Elemental analyses were recorded on a Perkin Elmer EA2400 series II. Optical rotations were recorded on a JASCO P-2000 polarimeter at the sodium K line at room temperature (concentration in g/100 mL).

N-Sulfonylhidrazines (RSO_2NHNH_2) were prepared following a published procedure.[5] Compounds **S1a**[6] and **S1b**[6] have been previously synthesized and characterized by our group.

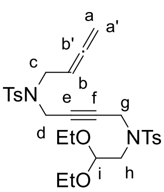
[5] (a) Backes, G. L.; Jursic, B. S.; Neumann, D. M. *Bioorg. Med. Chem.* **2015**, *23*, 3397. (b) Ozdemir, U. O.; Ilbiz, F.; Gunduzalp, A. B.; Ozbek, N.; Genç´, Z. K.; Hamurcu, F.; Tekin, S. *J. Mol. Struct.* **2015**, *1100*, 464.
[6] Torres, Ò.; Parella, T.; Solà, M.; Roglans, A.; Pla-Quintana, A. *Chem. Eur. J.* **2015**, *21*, 16240.

S.4. Experimental procedure for the synthesis of *N*-sulfonylhydrazones



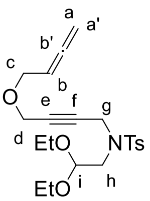
X	R	*N*-Sulfonylhydrazone
NTs	*p*-CH_3Ph	**1**
O	*p*-CH_3Ph	**3a**
O	Ph	**3b**
O	*p*-OCH_3Ph	**3c**
O	*p*-NO_2Ph	**3d**
O	*p*-IPh	**3e**
O	Naphthalene	**3f**
O	Dansyl	**3g**
O	CH_3	**3h**
O	$CH_3CH_2CH_2CH_2$	**3i**
O	2-thiophene	**3j**

S.4.1. Synthesis of allene derivatives S2



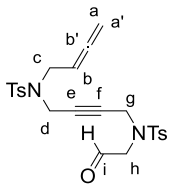
S2a

*General procedure for **S2**.* In a 250 mL 2-necked round bottom flask, a mixture of **S1a**[6] (3.01 g, 5.51 mmols), formaldehyde (0.41 g, 13.67 mmols) and copper(I) iodide (0.36 g, 2.76 mmols) in dioxane (100 mL) was heated to reflux. Dicyclohexylamine (1.4 mL, 10.00 mmols) was then added slowly to the reaction mixture. The mixture was stirred for 15 hours until completion (TLC monitoring). The insoluble salts were filtered off and the solvent was removed under reduced pressure. The reaction crude was purified by column chromatography on silica gel (hexane/ethyl acetate, 9:1 to 6:4) to afford **S2a** as a dark brown waxy solid (2.46 g, 80% yield). **MW**: 560.72 g/mol; **IR (ATR) ν (cm^{-1})**: 2975, 2929, 1331, 1158; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 1.20 (t, ^3J = 7.2 Hz, 6$H_{OCH2\mathit{CH3}}$), 2.43 (s, 6H_{Ts}), 3.06 (d, ^3J = 5.6 Hz, 2H_h), 3.54 (dq, ^2J = 9.4 Hz / ^3J = 7.2 Hz, 2$H_{O\mathit{CH2}CH3}$), 3.62 (dt, ^3J = 6.8 Hz / ^5J = 2.4 Hz, 2H_c), 3.72 (dq, ^2J = 9.4 Hz / ^3J = 7.2 Hz, 2$H_{O\mathit{CH2}CH3}$), 3.90 (t, ^5J = 2.0 Hz, 2$H_{d/g}$), 4.10 (t, ^5J = 2.0 Hz, 2$H_{d/g}$), 4.61 (t, ^3J = 5.6 Hz, H_i), 4.72 (dt, ^4J = 6.8 Hz / ^5J = 2.4 Hz, 2$H_{a,a'}$), 4.89 (tt, ^3J = 6.8 Hz, ^4J = 6.8 Hz, H_b),7.27-7.30 (m, 4H_{Ts}), 7.61 (d, ^3J = 8.4 Hz, 2H_{Ts}), 7.66 (d, ^3J = 8.4 Hz, 2H_{Ts}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 15.4 (2$C_{OCH2\mathit{CH3}}$), 21.5 (2$C_{Ts,CH3}$), 35.9 ($C_{g,CH2}$), 38.5 ($C_{d,CH2}$), 45.4 ($C_{c,CH2}$), 48.7 ($C_{h,CH2}$), 63.7 (2$C_{CO2\mathit{CH2}CH3}$), 67.1 ($C_{a,CH2}$), 76.5 ($C_{e/f,C}$), 79.0 ($C_{e/f,C}$), 85.3 ($C_{b,CH}$), 103.0 ($C_{i,CH}$), 127.5 (2$C_{Ts,CH}$), 127.6 (2$C_{Ts,CH}$), 129.5 (2$C_{Ts,CH}$), 129.6 (2$C_{Ts,CH}$), 136.2 ($C_{Ts,C}$), 136.2 ($C_{Ts,C}$), 143.7 (2$C_{Ts,C}$), 209.6 ($C_{b',C}$); **ESI-MS (m/z)**: 583.2 [M+Na]$^+$; **EA:** calculated for $C_{28}H_{36}N_2O_6S_2$: C, 59.98; H, 6.47; N, 5.00; found: C, 60.08 and 60.11; H, 6.62 and 6.54; N, 5.15 and 5.03.



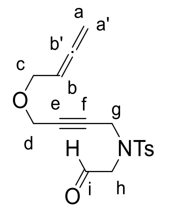
S2b Using the same experimental procedure as for compound **S2a**, **S2b** was obtained as a pale orange oil (1.85 g, 71% yield) after 15 hours. **MW**: 407.52 g/mol; **IR (ATR) ν (cm^{-1})**: 2976, 2931, 1346, 1159; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 1.22 (t, ^3J = 7.2 Hz, 6$H_{OCH2\mathit{CH3}}$), 2.42 (s, 3H_{Ts}), 3.24 (d, ^3J = 5.6 Hz, 2H_h), 3.57 (dq, ^2J = 9.4 Hz / ^3J = 7.2 Hz, 2$H_{O\mathit{CH2}CH3}$), 3.75 (dq, ^2J = 9.4 Hz / ^3J = 7.2 Hz, 2$H_{O\mathit{CH2}CH3}$), 3.85 (dt, ^3J = 6.6 Hz, ^5J = 2.4 Hz, 2H_c), 3.90 (t, ^5J = 2.0 Hz, 2H_g), 4.33 (t, ^5J = 2.0 Hz, 2H_d), 4.69 (t, ^3J = 5.6 Hz, H_i), 4.80 (dt, ^4J = 6.6 Hz / ^5J = 2.4 Hz, 2$H_{a,a'}$), 5.13 (tt, ^3J = 6.6 Hz, ^4J = 6.6 Hz, 1H_b), 7.28 (d, ^3J = 8.4 Hz, 2H_{Ts}), 7.74 (d, ^3J = 8.4 Hz, 2H_{Ts}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 15.5 (2$C_{OCH2\mathit{CH3}}$), 21.7 ($C_{Ts,CH3}$), 38.9 ($C_{g,CH2}$), 48.8 ($C_{h,CH2}$), 56.9 ($C_{d,CH2}$), 63.6 (2$C_{CO2\mathit{CH2}CH3}$), 67.2 ($C_{c,CH2}$), 76.1 ($C_{a,CH2}$), 79.9 ($C_{e/f,C}$), 81.1 ($C_{e/f,C}$), 87.1 ($C_{b,CH}$), 103.0 ($C_{i,CH}$), 127.9 (2$C_{Ts,CH}$), 129.6 (2$C_{Ts,CH}$), 136.3 ($C_{Ts,C}$), 143.6 ($C_{,C}$), 209.5 ($C_{b',C}$); **ESI-MS (m/z)**: 430.1 [M+Na]$^+$, 446.1 [M+K]$^+$; **EA:** calculated for $C_{21}H_{29}NO_5S$: C, 61.89; H, 7.17; N, 3.44; found: C, 61.81; H, 6.93; N, 3.68.

S.4.2. Synthesis of aldehyde derivatives S3



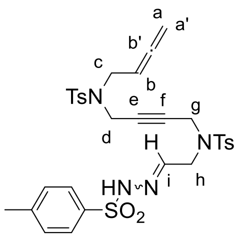
S3a *General procedure for **S3**.* A solution of **S2a** (2.09 g, 3.73 mmol) in trifluoroacetic acid (5 mL, 65.3 mmol), $CHCl_3$ (10 mL) and H_2O (5 mL) was stirred at room temperature for 24 hours (TLC monitoring). The mixture was diluted with CH_2Cl_2 and washed successively with 5% aqueous $Na_2S_2O_3$ (3 x 50 mL), H_2O (3 x 50 mL) and brine (3 x 50 mL). The organic layer was dried (Na_2SO_4), concentrated *in vacuo* and purified by column chromatography on silica gel (hexane/ethyl acetate 8:2 to 5:5) to afford **S3a** (1.31 g, 73%) as a pale orange waxy solid. **MW**: 486.60 g/mol; **IR (ATR) ν (cm^{-1})**: 2922, 1342, 1156; **^{1}H-NMR (400**

MHz, $CDCl_3$) δ (ppm): 2.43 (s, $3H_{Ts}$), 2.44 (s, $3H_{Ts}$), 3.70-3.69 (m, $2H_{d/g}$), 3.75 (s, $2H_{d/g}$), 3.95 (s, $4H_{c,h}$), 4.74-4.75 (m, $2H_{a,a'}$), 4.93 (m, H_b), 7.29-7.33 (m, $4H_{Ts}$), 7.62-7.66 (m, $4H_{Ts}$), 9.52 (t, ^3J = 1.2 Hz, H_i); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($2C_{Ts,CH3}$), 35.9 ($C_{g,CH2}$), 38.5 ($C_{d,CH2}$), 45.8 ($C_{c,CH2}$), 55.8 ($C_{h,CH2}$), 76.6 ($C_{a,CH2}$), 77.7 ($C_{e/f,C}$), 79.8 ($C_{e/f,C}$), 85.3 ($C_{b,CH}$), 127.6 ($4C_{Ts,CH}$), 129.7 ($2C_{Ts,CH}$), 130.0 ($2C_{Ts,C}$), 134.9 ($C_{Ts,C}$), 136.1 ($C_{Ts,C}$), 144.0 ($C_{Ts,C}$), 144.5 ($2C_{Ts,C}$), 197.1 ($C_{i,CH}$), 209.7 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 509.1175; experimental: 509.1162.



S3b Using the same experimental procedure as for compound **S3a**, **S3b** was obtained as a colorless oil (1.26 g, 85% yield) after 24 hours. **MW**: 333.40 g/mol; **IR (ATR) ν (cm^{-1})**: 2926, 1344, 1157; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.44 (s, $3H_{Ts}$), 3.89-3.98 (m, $6H_{CH2}$), 4.20-4.21 (m, $2H_{CH2}$), 4.79-4.82 (m, $2H_{a,a'}$), 5.14 (m, H_b), 7.33 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 7.71 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 9.66 (t, ^3J = 1.2 Hz, H_i); **^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 39.1 ($C_{g,CH2}$), 56.0 ($C_{d,CH2}$), 56.7 ($C_{h,CH2}$), 67.4 ($C_{c,CH2}$), 76.0 ($C_{a/a',CH2}$), 78.6 ($C_{e/f,C}$), 82.7 ($C_{e/f,C}$), 87.0 ($C_{b,CH}$), 127.7 ($2C_{Ts,CH}$), 129.9 ($2C_{Ts,CH}$), 135.0 ($C_{Ts,C}$), 144.4 ($C_{Ts,C}$), 197.4 ($C_{i,CH}$), 209.6 ($C_{b',C}$); **ESI-MS (m/z)**: 334.1 $[M+H]^+$; **EA:** calculated for $C_{17}H_{19}NO_4S$: C, 61.24; H, 5.74; N, 4.20; found: C, 61.01; H, 6.00; N, 4.28.

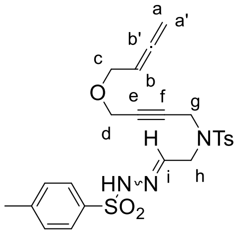
S.4.3. Synthesis of *N*-sulfonylhydrazones 1 and 3



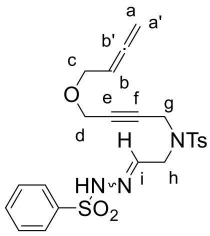
1 *General procedure for **1**.* A solution of *p*-toluensulfonyl hydrazide (0.47 g, 2.53 mmol) in methanol (15 mL) was prepared. A solution of **S3a** (1.23 g, 2.53 mmol) in methanol (15 mL) and the minimum amount of acetonitrile to completely dissolve the product was added dropwise to this mixture whilst it was being rapidly stirred. The mixture was then stirred at room temperature for 1 hour until completion (TLC monitoring). The solvent was removed under reduced pressure and the reaction crude was purified by column chromatography on silica gel (hexane/ethyl acetate, 9:1 to 6:4) to afford **1** (1.65 g, 73%, *Z/E*:8/92)[7] as a colourless solid. **MW**: 654.82 g/mol; **IR (ATR) ν (cm^{-1})**: 3197, 2922, 1342, 1155; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.41-2.42 (m, $9H_{Ts}$), 3.67-3.69 (m, $2H_c$), 3.75 (d, ^3J = 5.2 Hz, $2H_h$), 3.77 (s, $2H_{d/g}$), 3.85 (s, $2H_{d/g}$), 4.71-4.73 (m, $2H_{a,a'}$), 4.86 (tt, ^3J = 6.8 Hz, ^4J = 6.8 Hz, H_b), 7.11 (t, ^3J = 5.2 Hz, H_i), 7.27-7.31 (m, $6H_{Ts}$), 7.59 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.65 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.77 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 8.60 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.5 ($C_{Ts,CH3}$), 21.5

[7] Hydrazone derivatives **1** were obtained as a mixture of *E*/*Z* isomers. Only the *E* isomer, which is the major product obtained, is described but the ratio of isomers as determined by ^{1}H-NMR integration is given for completeness.

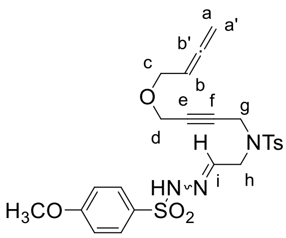
($C_{Ts,CH3}$), 21.6 ($C_{Ts,CH3}$), 35.8 ($C_{d/g,CH2}$), 37.4 ($C_{d/g,CH2}$), 45.6 ($C_{c,CH2}$), 48.4 ($C_{h,CH2}$), 76.7 ($C_{a/a',CH2}$), 78.1 ($C_{e/f,C}$), 79.1 ($C_{e/f,C}$), 85.2 ($C_{b,CH}$), 127.5 ($6C_{Ts,CH}$), 129.8 ($2C_{Ts,CH}$), 130.0 ($2C_{Ts,C}$), 135.2 ($C_{Ts,C}$), 135.3 ($C_{Ts,C}$), 135.9 ($2C_{Ts,C}$), 144.0 ($C_{Ts,C}$), 144.2 ($C_{Ts,C}$), 144.3 ($C_{Ts,C}$), 145.2 ($C_{i,CH}$), 209.6 ($C_{b',C}$); **ESI-MS (m/z)**: 655.1 $[M+H]^+$, 677.2 $[M+Na]^+$; **EA:** calculated for $C_{31}H_{34}N_4O_6S_3.0.5H_2O$: C, 56.09; H, 5.31; N, 8.44; found: C, 56.03 and 55.96; H, 5.36 and 5.24; N, 8.42 and 8.21.



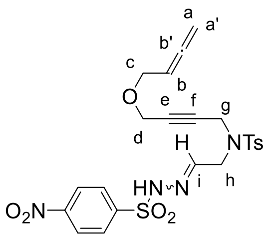
3a Using the same experimental procedure as for compound **1a**, **3a** was obtained as a pale orange waxy solid (1.48 g, 85% yield, *Z*/*E*:6/94)[7] after 1 hour. **MW**: 501.62 g/mol; **IR (ATR) ν (cm^{-1})**: 3200, 2921, 1345, 1158; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.41 (s, $3H_{Ts}$), 2.42 (s, $3H_{Ts}$), 3.87-3.87 (m, $4H_{d,g}$), 3.89 (d, ^3J = 5.2 Hz, $2H_h$), 3.92 (dt, ^3J = 6.8 Hz, ^5J = 2.2 Hz, $2H_c$), 4.82 (dt, ^4J = 6.8 Hz, ^5J = 2.2 Hz, $2H_{a/a'}$), 5.19 (tt, ^3J = 6.8 Hz, ^4J = 6.8 Hz, H_b), 7.07 (t, ^3J = 5.2 Hz, H_i), 7.28-7.30 (m, $4H_{Ts}$), 7.65 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.78 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 8.30 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.5 ($C_{Ts,CH3}$), 21.6 ($C_{Ts,CH3}$), 37.4 ($C_{g,CH2}$), 48.5 ($C_{h,CH2}$), 56.7 ($C_{d,CH2}$), 67.4 ($C_{c,CH2}$), 76.1 ($C_{a,CH2}$), 79.2 ($C_{e/f,C}$), 81.9 ($C_{e/f,CH2}$), 86.9 ($C_{b,CH}$), 127.7 ($4C_{Ts,CH}$), 129.7 ($4C_{Ts,CH}$), 135.1 ($C_{Ts,C}$), 135.2 ($C_{Ts,C}$), 144.1 ($C_{Ts,C}$), 144.6 ($C_{Ts,C}$), 145.6 ($C_{i,CH}$), 209.5 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 524.1284 and $[M+K]^+$: 540.1024; experimental: 524.1282 and 540.1017.



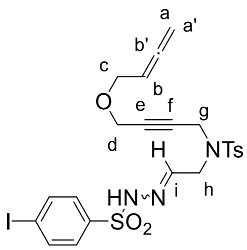
3b Using the same experimental procedure as for compound **1**, **3b** was obtained as a colorless waxy solid (0.10 g, 45% yield, *Z*/*E*:6/94)[7] after 1 hour. **MW**: 487.59 g/mol; **IR (ATR) ν (cm^{-1})**: 3195, 2861, 1346, 1161; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.40 (s, $3H_{Ts}$), 3.86-3.88 (m, $4H_{d,g}$), 3.87 (d, ^3J = 5.2 Hz, $2H_h$), 3.91 (dt, ^3J = 6.8 Hz, ^5J = 2.4 Hz, $2H_c$), 4.80 (dt, ^4J = 6.8 Hz, ^5J = 2.4 Hz, $2H_{a/a'}$), 5.16 (tt, ^3J = 6.8 Hz, ^4J = 6.8 Hz, H_b), 7.12 (t, ^3J = 5.2 Hz, H_i), 7.28 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.48 (m, $2H_{Ph}$), 7.56 (m, H_{Ph}), 7.64 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.89 (m, $2H_{Ph}$), 8.82 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.5 ($C_{Ts,CH3}$), 37.5 ($C_{g,CH2}$), 48.6 ($C_{h,CH2}$), 56.7 ($C_{d,CH2}$), 67.5 ($C_{c,CH2}$), 76.1 ($C_{a,CH2}$), 79.4 ($C_{e/f,C}$), 82.0 ($C_{e/f,C}$), 86.8 ($C_{b,CH}$), 127.7 ($2C_{Ph,CH}$), 127.8 ($2C_{Ph,CH}$), 129.0 ($2C_{Ts,CH}$), 129.7 ($2C_{Ts,CH}$), 133.2 ($C_{Ph,CH}$), 135.2 ($C_{Ts,C}$), 138.1 ($C_{Ph,C}$), 144.1 ($C_{Ts,C}$), 145.9 ($C_{i,CH}$), 209.5 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 510.1128; experimental: 510.1130.



3c Using the same experimental procedure as for compound **1**, **3c** was obtained as a colorless waxy solid (0.34 g, 63% yield, *Z*/*E*:7/93)[7] after 1 hour. **MW**: 517.61 g/mol; **IR (ATR) ν (cm^{-1})**: 3191, 2928, 1344, 1155; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.41 (s, $3H_{Ts}$), 3.84 (s, $3H_{OCH3}$), 3.86-3.88 (m, $6H_{d,g,h}$), 3.91 (dt, ^{3}J = 6.8 Hz, ^{5}J = 2.4 Hz, $2H_c$), 4.81 (dt, ^{4}J = 6.8 Hz, ^{5}J = 2.4 Hz, $2H_{a/a'}$), 5.17 (tt, ^{3}J = 6.8 Hz, ^{4}J = 6.8 Hz, H_b), 6.95 (d, ^{3}J = 8.8 Hz, $2H_{p\text{-OCH3Ph}}$), 7.10 (t, ^{3}J = 5.6 Hz, H_i), 7.27-7.10 (m, $2H_{Ts}$), 7.65 (d, ^{3}J = 9.2 Hz, $2H_{Ts}$), 7.82 (d, ^{3}J = 8.8 Hz, $2H_{p\text{-OCH3Ph}}$), 8.53 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 37.6 ($C_{g,CH2}$), 48.7 ($C_{h,CH2}$), 55.7 (C_{OCH3}), 56.8 ($C_{h,CH2}$), 67.6 ($C_{c,CH2}$), 76.2 ($C_{a,CH2}$), 79.6 ($C_{e/f,C}$), 82.1 ($C_{e/f,C}$), 86.9 ($C_{b,CH}$), 114.2 ($2C_{p\text{-OCH3Ph,CH}}$), 127.7 ($2C_{Ts,CH}$), 129.7 ($2C_{Ts,CH}$), 129.8 ($2C_{p\text{-OCH3Ph,CH}}$), 130.1 ($C_{p\text{-OCH3Ph,C}}$), 135.4 ($C_{Ts,C}$), 144.1 ($C_{Ts,C}$), 145.8 ($C_{i,CH}$), 163.5 ($C_{p\text{-OCH3Ph,C}}$), 209.6 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 540.1233; experimental: 540.1234.

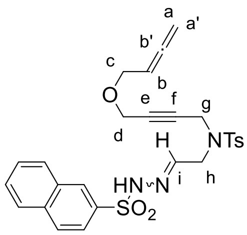


3d Using the same experimental procedure as for compound **1**, **3d** was obtained as a colorless solid (0.28 g, 81% yield, *Z*/*E*:4/96)[7] after 1 hour. **MW**: 532.59 g/mol; **IR (ATR) ν (cm^{-1})**: 3238, 2862, 1529, 1346, 1307, 1158; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.40 (s, $3H_{Ts}$), 3.87-4.02 (m, $8H_{c,d,g,h}$), 4.79-4.84 (m, $2H_{a,a'}$), 5.17 (m, H_b), 7.18 (t, ^{3}J = 6.2 Hz, H_i), 7.28-7.32 (m, $2H_{Ts}$), 7.60-7.63 (m, $2H_{Ts}$), 8.06-8.11 (m, $2H_{p\text{-NO2Ph}}$), 8.29 (d, ^{3}J = 9.2 Hz, $2H_{p\text{-NO2Ph}}$), 9.00 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 37.9 ($C_{g,CH2}$), 48.8 ($C_{h,CH2}$), 56.8 ($C_{d,CH2}$), 67.8 ($C_{c,CH2}$), 76.2 ($C_{a,CH2}$), 79.5 ($C_{e/f,C}$), 82.3 ($C_{e/f,C}$), 86.8 ($C_{b,CH}$), 124.2 ($2C_{p\text{-NO2Ph,CH}}$), 127.7 ($2C_{Ts,CH}$), 129.3 ($2C_{p\text{-NO2Ph,CH}}$), 129.9 ($2C_{Ts,CH}$), 134.9 ($C_{Ts,C}$), 143.8 ($C_{Ts,C}$), 144.5 ($C_{i,CH}$), 147.5 ($C_{p\text{-NO2Ph,C}}$), 150.4 ($C_{p\text{-NO2Ph,C}}$), 209.7 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 555.0979; experimental: 555.0975.

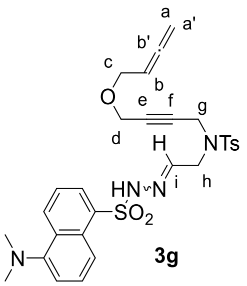


3e Using the same experimental procedure as for compound **1**, **3e** was obtained as a pale orange waxy solid (0.38 g, 85% yield, *Z*/*E*:7/93)[7] after 1 hour. **MW**: 613.49 g/mol; **IR (ATR) ν (cm^{-1})**: 3192, 2924, 1345, 1158; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.42 (s, $3H_{Ts}$), 3.86-3.91 (m, $8H_{c,d,g,h}$), 4.80 (dt, ^{4}J = 6.8 Hz, ^{5}J = 2.4 Hz, $2H_{a/a'}$), 5.17 (tt, ^{3}J = 6.8 Hz, ^{4}J = 6.8 Hz, H_b), 7.15 (t, ^{3}J = 5.6 Hz, H_i), 7.29 (d, ^{3}J = 8.6 Hz, $2H_{Ts}$), 7.58 (d, ^{3}J = 8.6 Hz, $2H_{p\text{-IPh}}$), 7.64 (d, ^{3}J =

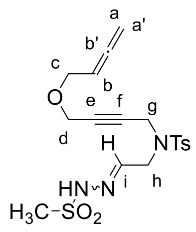
8.6 Hz, $2H_{Ts}$), 7.82 (d, ^3J = 8.6 Hz, $2H_{p\text{-IPh}}$), 8.92 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 37.6 ($C_{g,CH2}$), 48.6 ($C_{h,CH2}$), 56.7 ($C_{d,CH2}$), 67.5 ($C_{c,CH2}$), 76.2 ($C_{a,CH2}$), 79.3 ($C_{e/f,C}$), 82.1 ($C_{e/f,C}$), 86.9 ($C_{b,CH}$), 100.9 ($C_{p\text{-IPh},C}$), 127.7 ($2C_{Ts,CH}$), 129.2 ($2C_{p\text{-IPh},CH}$), 129.8 ($2C_{Ts,CH}$), 135.0 ($C_{Ts,C}$), 137.8 ($C_{p\text{-IPh},C}$), 138.2 ($2C_{p\text{-IPh},CH}$), 144.2 ($C_{Ts,C}$), 146.4 ($C_{i,CH}$), 209.5 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 636.0094; experimental: 636.0108.



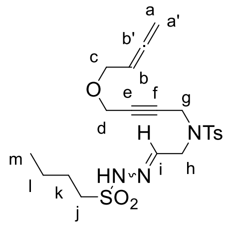
3f Using the same experimental procedure as for compound **1**, **3f** was obtained as a colorless waxy solid (0.25 g, 73% yield, *Z*/*E*:6/94)[7] after 1 hour. **MW**: 537.65 g/mol; **IR (ATR) ν (cm^{-1})**: 3211, 2923, 1343, 1157; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.35 (s, $3H_{Ts}$), 3.82-3.87 (m, $8H_{c,d,g,h}$), 4.78 (dt, ^4J = 6.8 Hz, ^5J = 2.4 Hz, $2H_{a/a'}$), 5.15 (tt, ^3J = 6.8 Hz, ^4J = 6.8 Hz, H_b), 7.14 (t, ^3J = 5.2 Hz, H_i), 7.18 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.55-7.62 (m, $4H_{Naph}$), 7.83-7.86 (m, $2H_{Ts}$+$2H_{Naph}$), 8.48 (s, H_{Naph}), 8.99 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.5 ($C_{Ts,CH3}$), 37.5 ($C_{g,CH2}$), 48.6 ($C_{h,CH2}$), 56.7 ($C_{d,CH2}$), 67.5 ($C_{c,CH2}$), 76.1 ($C_{a,CH2}$), 79.3 ($C_{e/f,C}$), 81.9 ($C_{e/f,C}$), 86.9 ($C_{b,CH}$), 122.7 ($C_{Naph,CH}$), 127.5 ($C_{Naph,CH}$), 127.6 ($2C_{Ts,CH}$), 127.9 ($C_{Naph,CH}$), 129.0 ($C_{Naph,CH}$), 129.3 ($C_{Naph,CH}$), 129.4 ($C_{Naph,CH}$), 129.5 ($C_{Naph,CH}$), 129.7 ($2C_{Ts,CH}$), 132.0 ($C_{Naph,C}$), 135.0 ($C_{Naph,C}$), 135.1 ($C_{Naph,C}$), 135.2 ($C_{Ts,C}$), 144.0 ($C_{Ts,C}$), 146.0 ($C_{i,CH}$), 209.6 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 560.1284; experimental: 560.1276.



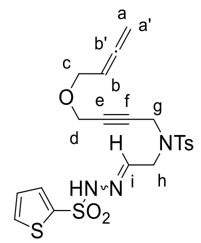
3g Using the same experimental procedure as for compound **1**, **3g** was obtained as a yellow fluorescent waxy solid (0.29 g, 86% yield, *Z*/*E*:9/91)[7] after 1 hour. **MW**: 580.72 g/mol; **IR (ATR) ν (cm^{-1})**: 3203, 2922, 2853, 1345, 1159; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.38 (s, $3H_{Ts}$), 3.87 (s, $6H_{N(CH3)2}$), 3.64 (t, ^5J = 1.6 Hz, $2H_g$), 3.76-3.79 (m, $4H_{d/h}$), 3.87 (dt, ^3J = 6.8 Hz, ^5J = 2.4 Hz, $2H_c$), 4.80 (dt, ^4J = 6.8 Hz, ^5J = 2.4 Hz, $2H_{a/a'}$), 5.16 (tt, ^3J = 6.8 Hz, ^4J = 6.8 Hz, H_b), 7.02 (t, ^3J = 5.6 Hz, H_i), 7.15 (m, H_{Dns}), 7.17 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.49-7.54 (m, $2H_{Dns}$), 7.58 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 8.29 (m, H_{Dns}), 8.37 (m, H_{Dns}), 8.55 (m, H_{Dns}), 8.68 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 37.4 ($C_{g,CH2}$), 45.5 ($2C_{N(CH3)2}$), 48.6 ($C_{h,CH2}$), 56.8 ($C_{d,CH2}$), 67.6 ($C_{c,CH2}$), 76.2 ($C_{a,CH2}$), 79.6 ($C_{e/f,C}$), 81.9 ($C_{e/f,C}$), 87.0 ($C_{b,CH}$), 115.4 ($C_{Dns,CH}$), 119.1 ($C_{Dns,CH}$), 123.3 ($C_{Dns,CH}$), 128.4 ($2C_{Ts,CH}$), 128.6 ($C_{Dns,CH}$), 129.7 ($2C_{Ts,CH}$), 129.8 ($C_{Dns,CH}$), 129.9 ($C_{Dns,CH}$), 130.9 ($C_{Dns,C}$), 131.3 ($C_{Dns,C}$), 133.7 ($C_{Dns,C}$), 135.4 ($C_{Ts,C}$), 144.0 ($C_{Ts,C}$), 145.0 ($C_{i,CH}$), 152.0 ($C_{Dns,C}$), 209.6 ($C_{b',C}$); **EA:** calculated for $C_{29}H_{32}N_4O_5S_2$: C, 59.94; H, 5.55; N, 9.65; found: C, 59.94 and 59.98; H, 5.62 and 5.78; N, 9.43 and 9.49.



3h Using the same experimental procedure as for compound **1**, **3h** was obtained as a colorless waxy solid (0.11 g, 27% yield, *Z*/*E*:6/94)[7] after 1 hour. **MW**: 425.52 g/mol; **IR (ATR) ν (cm^{-1})**: 3205, 2926, 1343, 1158; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.43 (s, $3H_{Ts}$), 3.05 (s, $3H_{SO2CH3}$), 3.90-3.95 (m, $4H_{d/g, c}$), 3.99 (d, ^{3}J = 5.2 Hz, $2H_h$), 4.12 (s, $2H_{d/g}$), 4.80 (dt, ^{4}J = 6.8 Hz, ^{5}J = 2.4 Hz, $2H_{a/a'}$), 5.19 (tt, ^{3}J = 6.8 Hz, ^{4}J = 6.8 Hz, H_b), 7.24 (t, ^{3}J = 5.2 Hz, H_i), 7.33 (d, ^{3}J = 8.2 Hz, $2H_{Ts}$), 7.73 (d, ^{3}J = 8.2 Hz, $2H_{Ts}$), 8.63 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 38.1 ($C_{,CH2}$), 38.7 (C_{SO2CH3}), 48.9 ($C_{h,CH2}$), 56.8 ($C_{d,CH2}$), 67.6 ($C_{c,CH2}$), 76.1 ($C_{a,CH2}$), 79.7 ($C_{e/f,C}$), 82.2 ($C_{e/f,C}$), 86.9 ($C_{b,CH}$), 127.7 ($2C_{Ts,CH}$), 129.8 ($2C_{Ts,CH}$), 135.2 ($C_{Ts,C}$), 144.3 ($C_{Ts,C}$), 146.5 ($C_{i,CH}$), 209.6 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 448.0971; experimental: 448.0979.



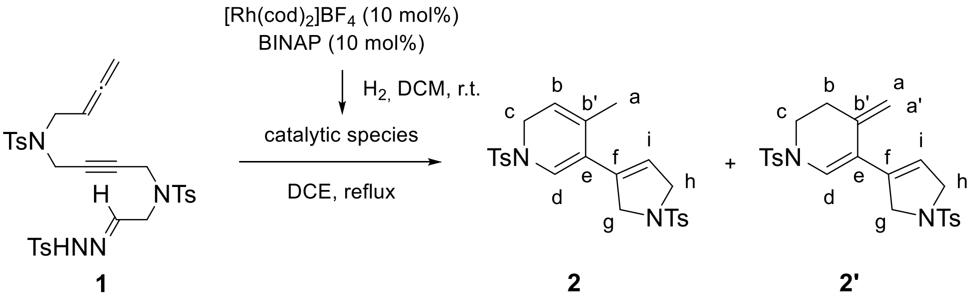
3i Using the same experimental procedure as for compound **1**, **3i** was obtained as a colorless waxy solid (0.32 g, 20% yield, *Z*/*E*:7/93)[7] after 1 hour. **MW**: 467.60 g/mol; **IR (ATR) ν (cm^{-1})**: 3201, 2962, 1343, 1154; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 0.94 (t, ^{3}J = 7.4 Hz, $3H_m$), 1.46 (tt, ^{3}J = 7.2 Hz / ^{3}J = 7.2 Hz, $2H_l$), 1.75-1.83 (m, $2H_k$), 2.44 (s, $3H_{Ts}$), 3.17-3.21 (m, $2H_j$), 3.93 (dt, ^{3}J = 6.8 Hz / ^{5}J = 2.4 Hz, $2H_c$), 3.95 (t, ^{5}J = 1.6 Hz, $2H_{d/g}$), 3.98 (d, ^{3}J = 5.2 Hz, $2H_h$), 4.11 (t, ^{5}J = 1.6 Hz, $2H_{d/g}$), 4.82 (dt, ^{4}J = 7.2 Hz, ^{5}J = 2.4 Hz, $2H_{a/a'}$), 5.17 (tt, ^{3}J = 6.8 Hz, ^{4}J = 6.8 Hz, H_b), 7.21 (t, ^{3}J = 5.2 Hz, H_i), 7.21 (d, ^{3}J = 8.4 Hz, $2H_{Ts}$), 7.73 (d, ^{3}J = 8.4 Hz, $2H_{Ts}$), 8.42 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 13.6 ($C_{m,CH3}$), 21.6 ($C_{Ts,CH3}$), 21.7 ($C_{l,CH2}$), 25.1 ($C_{k,CH2}$), 38.2 ($C_{g,CH2}$), 49.1 ($C_{h,CH2}$), 51.0 ($C_{j,CH2}$), 56.9 ($C_{d,CH2}$), 67.8 ($C_{c,CH2}$), 76.2 ($C_{a,CH2}$), 79.8 ($C_{e/f,C}$), 82.3 ($C_{e/f,C}$), 86.9 ($C_{b,CH}$), 127.8 ($2C_{Ts,CH}$), 129.9 ($2C_{Ts,CH}$), 135.3 ($C_{Ts,C}$), 144.3 ($C_{Ts,C}$), 145.9 ($C_{i,CH}$), 209.7 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 490.1441; experimental: 490.1430.



3j Using the same experimental procedure as for compound **1**, **3j** was obtained as a pale yellow oil (0.10 g, 18% yield, *Z*/*E*:6/94)[7] after 1 hour. **MW**: 493.61 g/mol; **IR (ATR) ν (cm^{-1})**: 3200, 3102, 1342, 1159; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.42 (s, $3H_{Ts}$), 3.87 (t, ^{5}J = 1.6 Hz, $2H_{d/g}$), 3.90-3.94 (m, $6H_{c/d,g,h}$), 4.81 (dt, ^{4}J = 6.8 Hz / ^{5}J = 2.4 Hz, $H_{a/a'}$), 7.08 (dd, ^{4}J = 3.6 Hz / ^{3}J = 4.8 Hz, $H_{thiophene}$), 7.15 (t, ^{3}J = 5.2 Hz, H_i), 7.62-7.64 (m, $2H_{Ts}$), 7.66-7.68 (m, $3H_{Ts,thiophene}$), 8.80 (s, H_{NH}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 37.8 ($C_{g,CH2}$), 49.0 ($C_{h,CH2}$), 56.8

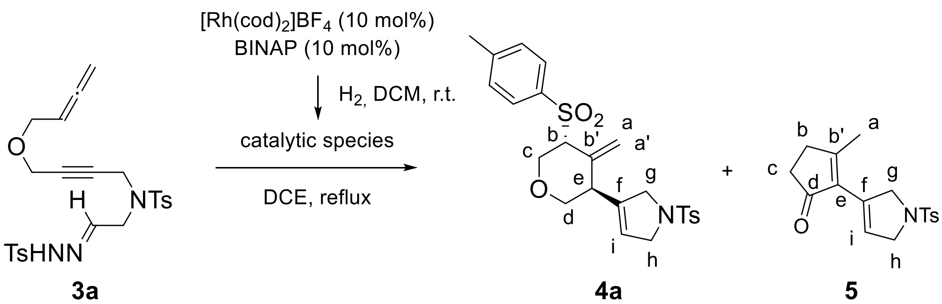
($C_{d,CH2}$), 67.7 ($C_{c,CH2}$), 76.2 ($C_{a,CH2}$), 79.8 ($C_{e/f,C}$), 82.1 ($C_{e/f,C}$), 86.8 ($C_{b,CH}$), 127.3 ($C_{thiophene,C}$), 127.7 (2$C_{Ts,CH}$), 129.8 (2$C_{Ts,CH}$), 133.0 ($C_{thiophene,CH}$), 133.6 ($C_{thiophene,CH}$), 135.2 ($C_{thiophene,CH}$), 138.4 ($C_{Ts,C}$), 144.2 ($C_{Ts,C}$), 146.8 ($C_{i,CH}$), 209.6 ($C_{b',C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 516.0692; experimental: 516.0680.

S.5. Experimental procedure for the rhodium(I)-catalyzed cyclization of *N*-sulfonylhydrazone derivative 1



*General procedure for **2** and **2'**.* A mixture of $[Rh(COD)_2]BF_4$ (0.0052 g, 0.01 mmol) and BINAP (0.0079 g, 0.01 mmol) was dissolved in dichloromethane (4 mL) under nitrogen. Hydrogen gas was bubbled to the stirred catalytic solution for 30 minutes and the resulting mixture was concentrated to dryness. The mixture was dissolved in 1,2-dichloroethane (1.5 mL) and a solution of **1** (0.0818 g, 0.12 mmol) in dichloroethane (1.5 mL) was added. The reaction mixture was heated at reflux for 2 hours until completion (TLC monitoring). The solvent was evaporated and the residue was purified by column chromatography on silica gel (hexane/ethyl acetate, 7:3) to afford a mixture of compounds which was identified by spectroscopy data as **2** and **2'** (ratio 2:1) as a colourless solid (0.0164 g, 28% yield). **MW**: 470.60 g/mol; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 1.70-1.71 (m, $3H_a$, **2**), 2.34-2.41 (m, $2H_b$, **2'**), 2.44-2.44 (m, $12H_{Ts}$, **2/2'**), 3.43 (m, $2H_c$, **2'**), 3.90-3.93 (m, $2H_c$, **2**), 4.18-4.19 (m, $8H_{g,h}$, **2/2'**), 4.79 (m, $H_{a/a'}$, **2'**), 4.88 (m, $H_{a/a'}$, **2'**), 5.19 (m, H_b, **2**), 5.53 (s, H_i, **2**), 5.63 (s, H_i, **2'**), 6.52 (s, H_d, **2**), 6.61 (s, H_d, **2'**), 7.31-7.36 (m, $8H_{Ts}$, **2/2'**), 7.63-7.65 (m, $4H_{Ts}$, **2/2'**), 7.74-7.76 (m, $4H_{Ts}$, **2/2'**); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 20.5 ($C_{a,CH3}$, **2**), 21.7 ($2C_{Ts,CH3,}$ **2** and **2'**), 21.8 ($2C_{Ts,CH3,}$ **2** and **2'**), 30.5 ($C_{b,CH2,}$ **2'**), 43.5 ($C_{c,CH2,}$ **2**), 44.4 ($C_{c,CH2,}$ **2'**), 55.3 ($C_{g/h,CH2,}$ **2'**), 55.6 ($C_{g/h,CH2,}$ **2'**), 55.7 ($C_{g/h,CH2,}$ **2**), 55.8 ($C_{g/h,CH2,}$ **2'**), 111.9 ($C_{a/a',CH2,}$ **2'**), 114.2 ($C_{f,C,}$ **2'**), 114.6 ($C_{d,CH,}$ **2**), 116.9 ($C_{f,CH,}$ **2**), 121.0 ($C_{i,CH,}$ **2**), 121.6 ($C_{i,CH,}$ **2'**), 124.9 ($C_{d,C,}$ **2'**), 125.7 ($C_{b,CH,}$ **2**), 127.1 ($2C_{Ts,CH,}$ **2'**), 127.3 ($2C_{Ts,CH,}$ **2'**), 127.7 ($4C_{Ts,CH,}$ **2** and **2'**), 130.0 ($2C_{Ts,C,}$ **2**), 130.1 ($2C_{Ts,C,}$ **2'**), 130.2 ($2C_{Ts,C}$, **2**), 130.3 ($2C_{Ts,C}$, **2'**), 131.4 ($C_{b',C,}$ **2**), 133.8 ($C_{e,C,}$ **2**), 134.1 ($C_{Ts,C,}$ **2**), 134.2 ($C_{Ts,C,}$ **2'**), 134.5 ($C_{Ts,C,}$ **2'**), 134.7 ($C_{e,C,}$ **2'**), 134.8 ($C_{Ts,C,}$ **2'**), 135.9 ($C_{b',C,}$ **2'**), 143.7 ($2C_{Ts,C,}$ **2** and **2'**), 144.5 ($C_{Ts,C,}$ **2**), 144.6 ($C_{Ts,C,}$ **2'**); **ESI-MS (m/z)**: 471.1 $[M+H]^+$, 493.1 $[M+Na]^+$.

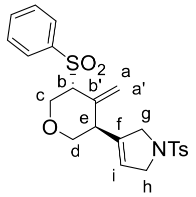
S.6. Experimental procedure for the rhodium(I)-catalyzed cyclization of *N*-sulfonylhydrazone derivatives 3



*General procedure for **4a** and **5**.* A mixture of $[Rh(COD)_2]BF_4$ (0.0101 g, 0.02 mmol) and BINAP (0.0156 g, 0.01 mmol) was dissolved in dichloromethane (4 mL) under nitrogen. Hydrogen gas was bubbled to the stirred catalytic solution for 30 minutes and the resulting mixture was concentrated to dryness. The mixture was dissolved in 1,2-dichloroethane (35 mL) and a solution of **1** (0.1253 g, 0.25 mmol) in dichloroethane (35 mL) was added. The reaction mixture was heated at reflux for 2 hours until completion (TLC monitoring). The solvent was evaporated and the residue was purified by column chromatography on silica gel (hexane/ethyl acetate, 8:2) to afford a mixture of compounds, which were identified by spectroscopy data as **4a** and **5**.

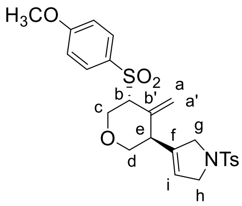
Compound **4a** was obtained as a colourless solid (0.0759 g, 64% yield, ee=84%). **MW**: 473.60 g/mol; **m.p.**: 132-133 °C; **[α]**$^{20}_{D}$ +69.86 (c 0.12 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2922, 2852, 1335, 1160; **^{1}H-NMR (400 MHz, CDCl$_3$) δ (ppm)**: 2.42 (s, $3H_{Ts}$), 2.45 (s, $3H_{Ts}$), 3.19 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, H_d), 3.51 (m, H_e), 3.57 (d, ^3J = 4.2 Hz, H_b), 3.65 (dd, ^2J = 12.8 Hz / ^3J = 4.2 Hz, H_c), 3.87 (dd, ^2J = 10.8 Hz / ^3J = 5.4 Hz, H_d), 3.97-3.99 (m, $2H_g$), 4.12-4.13 (m, $2H_h$), 4.68 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.69 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.73 (d, ^2J = 12.8 Hz, H_c), 5.44 (m, H_i), 7.31-7.35 (m, $4H_{Ts}$), 7.69-7.72 (m, $4H_{Ts}$); **^{13}C-NMR (100 MHz, CDCl$_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 21.7 ($C_{Ts,CH3}$), 39.8 ($C_{e,CH}$), 54.6 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 66.3 ($C_{c,CH2}$), 67.7 ($C_{b,CH}$), 71.0 ($C_{d,CH2}$), 119.2 ($C_{a/a',CH2}$), 123.3 ($C_{i,CH}$), 127.4 ($2C_{Ts,CH}$), 129.2 ($2C_{Ts,CH}$), 129.7 ($2C_{Ts,CH}$), 129.9 ($2C_{Ts,CH}$), 133.8 ($C_{Ts,C}$), 134.3 ($C_{Ts,C}$), 135.7 ($C_{f,C}$), 136.5 ($C_{b',C}$), 143.8 ($C_{Ts,C}$), 145.1 ($C_{Ts,C}$); **ESI-MS (m/z)**: 474.2 $[M+H]^+$; **AE:** calculated for $C_{24}H_{27}NO_5S_2$: C, 60.87; H, 5.75; N, 2.96; found: C, 60.63; H, 5.58; N, 3.25. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 76 % hexane / 20 % 2-PrOH / 6 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 22.7 min and for the minor isomer is 17.0 min.

Compound **5** was obtained as a colourless solid (0.0088 g, 11 % yield). **MW**: 317.40 g/mol; **IR (ATR) ν (cm^{-1})**: 2922, 2849, 1686, 1337, 1159; **^{1}H-NMR (400 MHz, CDCl$_3$) δ (ppm)**: 2.14 (s, $3H_a$), 2.38-2.38-2.41 (m, $2H_b$), 2.42 (s, $3H_{Ts}$), 2.56-2.57 (m, $2H_c$), 4.21-4.22 (m, $2H_g$), 4.40-4.43 (m, $2H_h$), 6.10 (m, H_i), 7.31 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.40 (d, ^3J = 8.4 Hz, $2H_{Ts}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 340.0978; experimental: 340.0976.

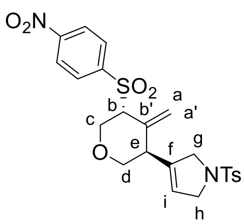


4b Using the same experimental procedure as for compound **4a**, **4b** was obtained as a colourless solid (0.0479 g, 50% yield, ee=80%) after 1 hour. **MW**: 459.57 g/mol; **m.p.**: 82-84 °C; **[α]**$^{20}_{D}$ +58.33 (c 0.10 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2921, 2852, 1594, 1130; **^{1}H-NMR (400 MHz, CDCl$_3$) δ (ppm)**: 2.42 (s, $3H_{Ts}$), 3.20 (dd, ^2J = 10.6 Hz / ^3J = 10.6 Hz, H_d), 3.53 (m, H_e), 3.59 (d, ^3J = 3.6 Hz, H_b), 3.66 (dd, ^2J = 12.8 Hz / ^3J = 4.0 Hz, H_c), 3.89 (dd, ^2J = 10.6 Hz / ^3J = 5.2 Hz, H_d), 3.97-4.00 (m, $2H_g$), 4.11-4.15 (m, $2H_h$), 4.67 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.70 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.76 (d, ^2J = 12.8 Hz, H_c), 5.44 (m, H_i), 7.32 (d, ^3J = 7.4 Hz, $2H_{Ts}$), 7.54-7.58 (m, $2H_{Ph}$), 7.66

(m, H_{Ph}), 7.70 (d, ^3J = 7.4 Hz, $2H_{Ts}$), 7.83-7.86 (m, $2H_{Ph}$); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 39.8 ($C_{e,CH}$), 54.7 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 66.3 ($C_{c,CH2}$), 67.8 ($C_{b,CH}$), 71.1 ($C_{d,CH2}$), 119.3 ($C_{a/a',CH2}$), 123.5 ($C_{i,CH}$), 127.6 ($2C_{Ph,CH}$), 129.1 ($2C_{Ts,CH}$), 129.3 ($2C_{Ph,CH}$), 130.0 ($2C_{Ts,CH}$), 133.9 ($C_{Ph,C}$), 134.1 ($C_{Ts,C}$), 135.7 ($C_{f,C}$), 136.5 ($C_{b',CH}$), 137.3 ($C_{Ph,C}$), 143.9 ($C_{Ts,C}$); **ESI-MS (m/z)**: 460.1 $[M+H]^+$; **AE:** calculated for $C_{23}H_{25}NO_5S_2$: C, 60.11; H, 5.48; N, 3.05; found: C, 59.67; H, 5.44; N, 3.33. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 μm) with 70 % hexane / 20 % 2-PrOH / 10 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 9.4 min and for the minor isomer is 8.2 min.

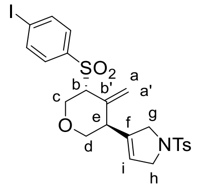


4c Using the same experimental procedure as for compound **4a**, **4c** was obtained as a colourless solid (0.0238 g, 55% yield, ee=88%) after 1 hour. **MW**: 489.60 g/mol; **m.p.**: 86-87 °C; **[α]$^{20}_D$** +112.92 (c 0.04 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2920, 2851, 1339, 1304, 1159; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.43 (s, $3H_{Ts}$), 3.20 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, $1H_d$), 3.50 (m, H_e), 3.55 (d, ^3J = 4.0 Hz, H_b), 3.65 (dd, ^2J = 12.8 Hz / ^3J = 4.0 Hz, H_c), 3.87 (dd, ^2J = 10.4 Hz / ^3J = 5.6 Hz, H_d), 3.90 (s, $3H_{OCH3}$), 3.97-4.00 (m, $2H_g$), 4.12-4.14 (m, $2H_h$), 4.72-4.76 (m, $3H_{a,a',c}$), 5.43 (m, H_i), 7.00 (d, ^3J = 9.2 Hz, $2H_{p\text{-}OCH3Ph}$), 7.32 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.70 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.75 (d, ^3J = 9.2 Hz, $2H_{p\text{-}OCH3Ph}$); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.7 ($C_{Ts,CH3}$), 39.8 ($C_{e,CH}$), 54.7 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 55.8 (C_{OCH3}), 66.5 ($C_{c,CH2}$), 68.0 ($C_{b,CH}$), 71.0 ($C_{d,CH2}$), 114.3 ($2C_{p\text{-}OCH3Ph,CH}$), 119.2 ($C_{a/a',CH2}$), 123.4 ($C_{i,CH}$), 127.6 ($2C_{Ts,CH}$), 128.9 ($C_{p\text{-}OCH3Ph,C}$), 130.0 ($2C_{Ts}$), 131.4 ($2C_{p\text{-}OCH3Ph,CH}$), 134.0 ($C_{p\text{-}OCH3Ph,C}$), 135.8 ($C_{Ts,C}$), 135.9 ($C_{f,C}$), 136.7 ($C_{b',C}$), 143.9 ($C_{Ts,C}$), 164.0 ($C_{p\text{-}OCH3Ph,C}$); **ESI-MS (m/z)**: 490.1 $[M+H]^+$; **AE:** calculated for $C_{24}H_{27}NO_6S_2$: C, 58.88; H, 5.56; N, 2.86; found: C, 58.79 and 58.99; H, 5.58 and 5.82; N, 3.18 and 3.31. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 μm) with 70 % hexane / 20 % 2-PrOH / 10 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 10.9 min and for the minor isomer is 9.8 min. min.

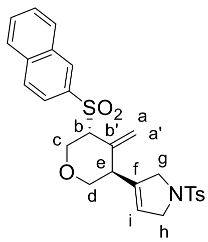


4d Using the same experimental procedure as for compound **4a**, **4d** was obtained as a colourless solid (0.0451 g, 43% yield, ee=92%) after 24 hours. **MW**: 504.57 g/mol; **m.p.**: 122-124 °C; **[α]$^{20}_D$** +89.79 (c 0.28 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2922, 1530, 1347, 1303, 1158, 1105; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.43 (s, $3H_{Ts}$), 3.21 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, $1H_d$), 3.57 (m, H_e), 3.66 (d, ^3J = 4.0 Hz, H_b), 3.72 (dd, ^2J = 12.8 Hz / ^3J = 4.0 Hz, H_c), 3.91 (dd, ^2J = 10.8 Hz / ^3J = 5.2 Hz, H_d), 3.97-4.01 (m, $2H_g$), 4.13-4.14 (m, $2H_h$), 4.70-4.81

(m, $3H_{a,a',c}$), 5.50 (m, H_i), 7.33 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 7.70 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 8.05 (d, ^3J = 8.6 Hz, $2H_{p\text{-NO2Ph}}$), 8.39 (d, ^3J = 8.6 Hz, $2H_{p\text{-NO2Ph}}$); **^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm)**: 21.7 ($C_{Ts,CH3}$), 39.9 ($C_{e,CH}$), 54.5 ($C_{h/g,CH2}$), 54.8 ($C_{h/g,CH2}$), 66.0 ($C_{c,CH2}$), 68.0 ($C_{b,CH}$), 71.0 ($C_{d,CH2}$), 120.2 ($C_{a/a',CH2}$), 124.1 ($C_{i,CH}$), 124.3 ($2C_{p\text{-NO2Ph,CH}}$), 127.6 ($2C_{Ts,CH}$), 130.0 ($2C_{Ts,CH}$), 130.7 ($2C_{p\text{-NO2Ph,CH}}$), 133.7 ($C_{Ts,C}$), 135.2 ($C_{f,C}$), 136.1 ($C_{b',C}$), 142.9 ($C_{p\text{-NO2Ph,C}}$), 143.9 ($C_{Ts,C}$), 151.0 ($C_{p\text{-NO2Ph,C}}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 527.0917; experimental: 527.0915. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 50 % hexane / 50 % 2-PrOH mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 20.6 min and for the minor isomer is 17.5 min.

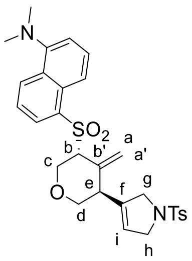


4e Using the same experimental procedure as for compound **4a**, **4e** was obtained as a colourless solid (0.0436 g, 41% yield, ee=86%) after 24 hours. **MW**: 585.47 g/mol; **m.p.**: 168-170°C; **[α]**$^{20}_D$ +64.19 (c 0.16 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2918, 2850, 1336, 1307, 1142, 1099; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.43 (s, $3H_{Ts}$), 3.20 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, $1H_d$), 3.51 (m, H_e), 3.57 (d, ^3J = 4.2 Hz, H_b), 3.66 (dd, ^2J = 12.8 Hz / ^3J = 4.2 Hz, H_c), 3.89 (dd, ^2J = 10.8 Hz / ^3J = 5.2 Hz, H_d), 3.96-4.00 (m, $2H_g$), 4.13-4.14 (m, $2H_h$), 4.69-4.77 (m, $3H_{a,a',c}$), 5.45 (m, H_i), 7.33 (d, ^3J = 8.2 Hz, $2H_{Ts}$), 7.53 (d, ^3J = 8.6 Hz, $2H_{p\text{-IPh}}$), 7.70 (d, ^3J = 8.2 Hz, $2H_{Ts}$), 7.91 (d, ^3J = 8.6 Hz, $2H_{p\text{-IPh}}$); **^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm)**: 21.7 ($C_{Ts,CH3}$), 39.8 ($C_{e,CH}$), 54.6 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 66.2 ($C_{c,CH2}$), 67.8 ($C_{b,CH}$), 71.0 ($C_{d,CH2}$), 102.2 ($C_{p\text{-IPh,C}}$), 119.7 ($C_{a/a',CH2}$), 123.7 ($C_{i,CH}$), 127.6 ($2C_{Ts,CH}$), 130.0 ($2C_{Ts,CH}$), 130.5 ($2C_{p\text{-IPh,CH}}$), 133.8 ($C_{Ts,C}$), 135.5 ($C_{f,C}$), 136.3 ($C_{b',C}$), 136.9 ($C_{p\text{-IPh,C}}$), 138.4 ($2C_{p\text{-IPh,CH}}$), 143.9 ($C_{Ts,C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 608.0033; experimental: 608.0023. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 70 % hexane / 20 % 2-PrOH / 10 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 10.7 min and for the minor isomer is 9.6 min.

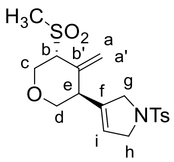


4f Using the same experimental procedure as for compound **4a**, **4f** was obtained as a colourless solid (0.0443 g, 47% yield, ee=82%) after 1 hour together with traces of compound **5** which could not be separated. **MW**: 509.63 g/mol; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.39 (s, $3H_{Ts}$), 3.20 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, H_d), 3.53 (m, H_e), 3.67-3.69 (m, $2H_{b,c}$), 3.88 (dd, ^2J = 10.8 Hz / ^3J = 5.2 Hz, H_d), 3.94-3.98 (m, $2H_g$), 4.11-4.12 (m, $2H_h$), 4.64 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.65 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.79 (dd, ^2J = 13.6 Hz / ^3J = 1.6 Hz, H_c), 5.40 (m, H_i), 7.26 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 7.66 (d, ^3J = 8.0 Hz, $2H_{Ts}$), 7.69-7.71 (m, $2H_{Naph}$), 7.80-7.82 (m, H_{Naph}), 7.98-8.00

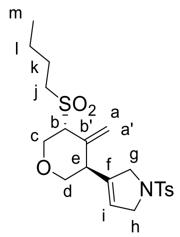
(m, $2H_{Naph}$), 8.42 (m, H_{Naph}); **^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 39.8 ($C_{e,CH}$), 54.7 ($C_{h/g,CH2}$), 55.0 ($C_{h/g,CH2}$), 66.3 ($C_{c,CH2}$), 67.8 ($C_{b,CH}$), 71.0 ($C_{d,CH2}$), 119.4 ($C_{a,CH2}$), 123.4 ($C_{i,CH}$), 123.7 ($2C_{Ts,CH}$), 127.5 ($C_{Naph,CH}$), 128.0 ($C_{Naph,CH}$), 128.1 ($C_{Naph,CH}$), 129.4 ($C_{Naph,CH}$), 129.6 ($C_{Naph,CH}$), 129.7 ($C_{Naph,CH}$), 129.9 ($2C_{Ts,CH}$), 131.1 ($C_{Naph,CH}$), 132.0 ($C_{Naph,C}$), 133.7 ($C_{Ts,C}$), 134.1 ($C_{Naph,C}$), 135.4 ($C_{Naph,C}$), 135.6 ($C_{f,C}$), 136.5 ($C_{b',C}$), 143.8 ($C_{Ts,C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 532.1123; experimental: 532.1227. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 70 % hexane / 20 % 2-PrOH / 10 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 11.1 min and for the minor isomer is 10.0 min.



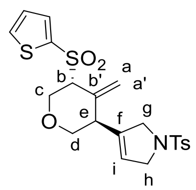
4g Using the same experimental procedure as for compound **4a**, **4g** was obtained as a orange waxy solid (0.0268 g, 25% yield, ee=73%) after 24 hours together with traces of compound **5** which could not be separated.. **MW**: 552.70 g/mol; **IR (ATR) ν (cm^{-1})**: 2943, 2863, 1340, 1305, 1160, 1134; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.40 (s, $3H_{Ts}$), 2.90 (s, $6H_{N(CH3)2}$), 3.21 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, $1H_d$), 3.64-3.72 (m, $2H_{c,e}$), 3.88-3.95 (m, $4H_{g,d,b}$), 4.11-4.11 (m, $2H_h$), 4.39 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.54 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 4.74 (d, ^2J = 12.8 Hz, H_c), 5.42 (m, H_i), 7.21 (d, ^3J = 6.8 Hz, H_{Dns}), 7.29-7.33 (m, $2H_{Ts}$), 7.55-7.60 (m, $2H_{Dns}$), 7.68 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 8.22 (dd, ^3J = 1.2 Hz, ^3J = 7.2 Hz, H_{Dns}), 8.32 (d, ^3J = 8.4 Hz, H_{Dns}), 8.61 (d, ^3J = 8.4 Hz, H_{Dns}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 40.1 ($C_{e,CH}$), 45.5 ($2C_{Dns,CH3}$), 54.8 ($C_{h/g,CH2}$), 55.5 ($C_{h/g,CH2}$), 66.1 ($C_{c,CH2}$), 66.7 ($C_{b,CH}$), 71.1 ($C_{d,CH2}$), 115.4 ($C_{Dns,CH}$), 118.5 ($C_{Dns,CH}$), 118.8 ($C_{Dns,CH}$), 123.2 ($C_{Dns,CH}$), 123.3 ($C_{Dns,CH}$), 127.5 ($2C_{Ts,CH}$), 127.6 ($C_{Dns,CH}$), 129.9 ($2C_{Ts,CH}$), 131.8 ($C_{Dns,C}$), 132.3 ($C_{Dns,C}$), 132.4 ($C_{Dns,C}$), 133.9 ($C_{Ts,C}$), 135.8 ($C_{f,C}$), 136.7 ($C_{b',C}$), 143.8 ($C_{Ts,C}$), 152.3 ($C_{Dns,C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 575.1645; experimental: 575.1658. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 70 % hexane / 20 % 2-PrOH / 10 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 340 nm. The retention time for the major isomer is 8.4 min and for the minor isomer is 7.6 min.



4h Using the same experimental procedure as for compound **4a**, **4h** was obtained as a pale orange solid (0.0496 g, 72% yield, ee=87%) after 2.5 hours. **MW**: 397.50 g/mol; **m.p.**: 52-53°C; **[α]**$^{20}_{D}$ +51.46 (c 0.18 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2928, 2856, 1336, 1299, 1159, 1107; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.44 (s, $3H_{Ts}$), 2.93 (s, $3H_{SO2CH3}$), 3.25 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, H_d), 3.61 (d, ^3J = 4.0 Hz, H_b), 3.69-3.73 (m, $2H_{c,e}$), 3.93 (dd, ^2J = 10.4 Hz / ^3J = 5.2 Hz, H_d), 4.01-4.07 (m, $2H_g$), 4.15-4.17 (m, $2H_h$), 4.78 (d, ^2J = 12.8 Hz, H_c), 4.96 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 5.23 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 5.53 (m, H_i), 7.36 (d, ^3J = 8.4 Hz, $2H_{Ts}$), 7.71 (d, ^3J = 8.4 Hz, 2H$_{Ts}$); **^{13}C-NMR (100 MHz, CDCl$_3$) δ (ppm)**: 21.6 ($C_{Ts,CH3}$), 39.2 ($C_{e/SO2CH3,CH/CH3}$), 39.9 ($C_{e/SO2CH3,CH/CH3}$), 54.6 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 65.6 ($C_{c,CH2}$), 66.4 ($C_{b,CH}$), 71.0 ($C_{d,CH2}$), 119.2 ($C_{a/a',CH2}$), 123.9 ($C_{i,CH}$), 127.5 (2$C_{Ts,CH}$), 130.0 (2$C_{Ts,CH}$), 133.7 ($C_{Ts,C}$), 135.4 ($C_{f,C}$), 137.6 ($C_{b',C}$), 143.9 ($C_{Ts,C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 420.0910; experimental: 420.0918. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 76 % hexane / 20 % 2-PrOH / 4 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 19.8 min and for the minor isomer is 18.0 min.



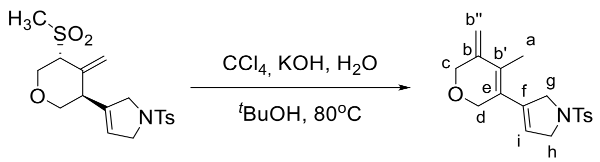
4i Using the same experimental procedure as for compound **4a**, **4i** was obtained as a colorless solid (0.0437 g, 85% yield, ee=93%) after 2 hours. **MW**: 439.58 g/mol; **m.p.**: 56-58^{o}C; **[α]$^{20}_D$** +80.54 (c 0.25 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2960, 2871, 1339, 1295, 1159, 1106; **^{1}H-NMR (400 MHz, CDCl$_3$) δ (ppm)**: 0.96 (t, ^3J = 7.6 Hz, 3H_m), 1.47 (tq, ^3J = 7.6 Hz / ^3J = 7.6 Hz, 2H_l), 1.80-1.83 (m, 2H_k), 2.44 (s, 3H_{Ts}), 2.98-3.06 (m, 2H_j), 3.25 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, 1H_d), 3.57 (d, ^3J = 3.6 Hz, H_b), 3.67-3.71 (m, 2$H_{c,e}$), 3.94 (dd, ^2J = 10.8 Hz / ^3J = 5.6 Hz, H_d), 4.03-4.05 (m, 2H_g), 4.15-4.16 (m, 2H_h), 4.79 (d, ^2J = 12.8 Hz, H_c), 4.95 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 5.17 (d, ^2J = 2.0 Hz, $H_{a/a'}$), 5.52 (m, H_i), 7.34 (d, ^3J = 8.0 Hz, 2H_{Ts}), 7.72 (d, ^3J = 8.0 Hz, 2H_{Ts}); **^{13}C-NMR (100 MHz, CDCl$_3$) δ (ppm)**: 13.7 ($C_{m,CH3}$), 21.7 ($C_{Ts,CH3}$), 21.9 ($C_{l,CH2}$), 23.6 ($C_{k,CH2}$), 40.1 ($C_{e,CH}$), 50.5 ($C_{j,CH2}$), 54.7 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 64.8 ($C_{c,CH2}$), 65.8 ($C_{b,CH}$), 71.2 ($C_{d,CH2}$), 118.5 ($C_{a/a',CH2}$), 123.7 ($C_{i,CH}$), 127.6 (2$C_{Ts,CH}$), 130.0 (2$C_{Ts,CH}$), 133.9 ($C_{Ts,C}$), 135.6 ($C_{f,C}$), 138.3 ($C_{b',C}$), 143.9 ($C_{Ts,C}$); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 462.1379; experimental: 462.1373. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 78 % hexane / 20 % 2-PrOH / 2 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 21.9 min and for the minor isomer is 25.1 min.



4j Using the same experimental procedure as for compound **4a**, **4j** was obtained as a colorless solid (0.0437 g, 40% yield, ee=92%) after 24 hours. **MW**: 465.60 g/mol; **m.p.**: 74-76^{o}C; **[α]$^{20}_D$** +86.47 (c 0.09 g / 100 mL, CH_3CN); **IR (ATR) ν (cm^{-1})**: 2959, 2860, 1307, 1159, 1141, 1106; **^{1}H-NMR (400 MHz, CDCl$_3$) δ (ppm)**: 2.43 (s, 3H_{Ts}), 3.22 (dd, ^2J = 10.8 Hz / ^3J = 10.8 Hz, H_d), 3.55 (m, H_e), 3.68-3.73 (m, 2$H_{c,b}$), 3.90 (dd, ^2J = 10.4 Hz / ^3J = 4.8 Hz, H_d), 4.00-4.02 (m, 2H_g), 4.13-4.15 (m, 2H_h), 4.77-4.80 (m, 3$H_{a,a',c}$), 5.46 (m, H_i), 7.17 (dd, ^3J = 5.2 Hz / ^3J = 3.8 Hz, $H_{thiophene}$), 7.33 (d, ^3J = 8.4 Hz, 2H_{Ts}), 7.64 (dd, ^3J = 3.8 Hz / ^4J = 1.4 Hz, $H_{thiophene}$), 7.71 (d, ^3J = 8.4 Hz, 2H_{Ts}) 7.75 (dd, ^3J = 5.2 Hz / ^4J = 1.4 Hz, $H_{thiophene}$); **^{13}C-NMR (100 MHz, CDCl$_3$) δ (ppm)**: 21.7

($C_{Ts,CH3}$), 39.8 ($C_{e,CH}$), 54.7 ($C_{h/g,CH2}$), 54.9 ($C_{h/g,CH2}$), 66.4 ($C_{c,CH2}$), 69.1 ($C_{b,CH}$), 71.1 ($C_{d,CH2}$), 119.5 ($C_{a/a',CH2}$), 123.5 ($C_{i,CH}$), 127.6 (2$C_{Ts,CH}$), 128.0 ($C_{thiophene,C}$), 130.0 (2$C_{Ts,CH}$), 133.9 ($C_{Ts,C}$), 134.8 ($C_{thiophene,C}$), 135.5 ($C_{f,C}$), 135.7 ($C_{thiophene,C}$), 136.6 ($C_{b',C}$), 138.2 ($C_{thiophene,C}$), 143.9 ($C_{Ts,C}$); **ESI-MS (m/z)**: 466.1 $[M+H]^+$; **AE:** calculated for $C_{21}H_{23}NO_5S_3$: C, 54.17; H, 4.98; N, 3.01; found: C, 54.39 and 54.21; H, 5.09 and 4.97; N, 3.35 and 3.29. The enantiomeric excess has been determined by **HPLC** analysis using a CHIRALPAK IA column (4.6 x 250 mm, 5 µm) with 78 % hexane / 20 % 2-PrOH / 2 % acetonitrile mobile phase at a 1.0 mL/min flow rate, using a UV detector set up at λ = 220 nm. The retention time for the major isomer is 28.8 min and for the minor isomer is 25.9 min.

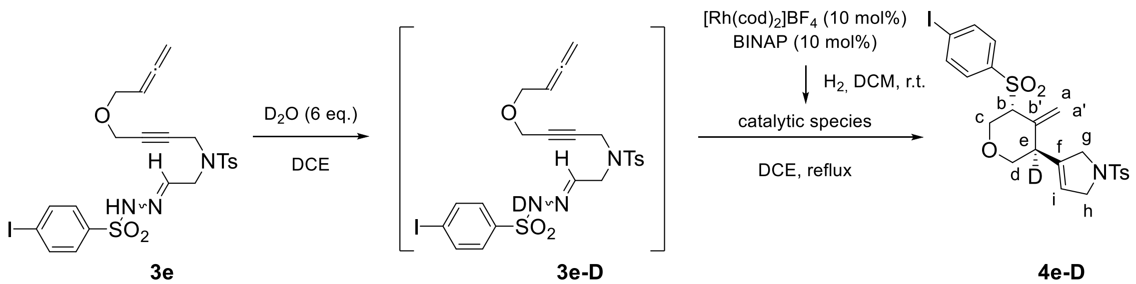
S.7. Experimental procedure for the Ramberg-Bäcklund rearrangement of 4h



4h **6**

To a stirred solution of **4h** (0.0180 g, 0.04 mmol) in carbon tetrachloride (0.3 mL), *tert*-butanol (0.3 mL) and water (0.05 mL), was added powdered potassium hydroxide (0.0559 g, 1.00 mmol). The mixture was stirred for 14 hours until completion (TLC monitoring). The mixture was diluted with AcOEt and washed successively with H_2O (3 x 20 mL) and brine (3 x 20 mL). The organic layer was dried (Na_2SO_4), concentrated *in vacuo* and purified by column chromatography on silica gel (hexane/ethyl acetate, 9.5:0.5 to 8:2) to afford **6** as a yellow oil (0.0103 g, 69% yield)**. MW**: 331.43 g/mol; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 1.78 (t, ^4J = 2.0 Hz, H_a), 2.44 (s, 3H_{Ts}), 4.08-4.09 (m, 2H_c), 4.19-4.21 (m, 6$H_{d,g,h}$), 4.89 (s, $H_{b''}$), 5.07 (s, $H_{b''}$), 5.52 (t, ^3J = 1.6 Hz, H_i), 7.33 (d, ^3J = 8.4 Hz, 2H_{Ts}), 7.73 (d, ^3J = 8.4 Hz, 2H_{Ts}); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 14.4 (C_a), 21.5 (C_{Ts}), 55.0 ($C_{g/h}$), 56.0 ($C_{h/g}$), 68.3 ($C_{c/d}$), 69.8 ($C_{c/d}$), 108.8 ($C_{b''}$), 123.9 (C_i), 127.5 (2C_{Ts}), 128.7 ($C_{b/b'}$), 128.8 ($C_{b/b'}$), 129.8 (2C_{Ts}), 1341 (C_{Ts}), 135.5 (C_f), 140.3 (C_e), 143.7 (C_{Ts}); **ESI-MS (*m/z*):** calculated for $[M+H]^+$: 332.1; experimental: 332.1. **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 354.1134; experimental: 354.1132.

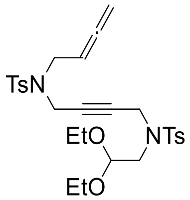
S.8. Deuterium labelling experiment



3e **3e-D** **4e-D**

Compound **4e-D** was obtained following the same procedure as for compound **4a** but stirring D_2O (6 eq.) in DCE before adding the catalytic system. The compound **4e-D** was obtained as a colourless solid (0.0169 g, 31% yield). **MW**: 586.48 g/mol; **^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)**: 2.45 (s, 3H_{Ts}), 3.19 (d, ^{2}J = 10.4 Hz, H_d), 3.56 (d, ^{3}J = 4.0 Hz, H_b), 3.66 (dd, ^{2}J = 13.2 Hz / ^{3}J = 4.4 Hz, H_c), 3.89 (d, ^{2}J = 10.4 Hz, H_d), 3.95-4.01 (m, 2H_g), 4.13-4.14 (m, 2H_h), 4.70-4.77 (m, 3$H_{a,a',c}$), 5.45 (m, H_i), 7.34 (d, ^{3}J = 8.4 Hz, 2H_{Ts}), 7.53 (d, ^{3}J = 8.6 Hz, 2$H_{p\text{-IPh}}$), 7.71 (d, ^{3}J = 8.4 Hz, 2H_{Ts}), 7.92 (d, ^{3}J = 8.6 Hz, 2$H_{p\text{-IPh}}$); **^{2}H-NMR (400 MHz, $CHCl_3$) δ (ppm)**: 3.48 (s, D_e); **^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)**: 21.7 (C_{Ts}), 39.3 (C_e), 54.6 ($C_{h/g}$), 54.9 ($C_{h/g}$), 66.2 (C_c), 67.9 (C_b), 71.0 (C_d), 102.2 ($C_{p\text{-IPh}}$), 119.7 ($C_{a/a'}$), 123.7 (C_i), 127.6 (2C_{Ts}), 130.0 (2C_{Ts}), 130.6 (2$C_{p\text{-IPh}}$), 133.9 (C_{Ts}), 135.5 (C_f), 136.3 ($C_{b'}$), 137.0 ($C_{p\text{-IPh}}$), 138.5 ($C_{p\text{-IPh}}$), 143.9 (C_{Ts}); **ESI-HRMS (*m/z*):** calculated for $[M+Na]^+$: 609.0096; experimental: 609.0094.

S.9. Spectra



S2a

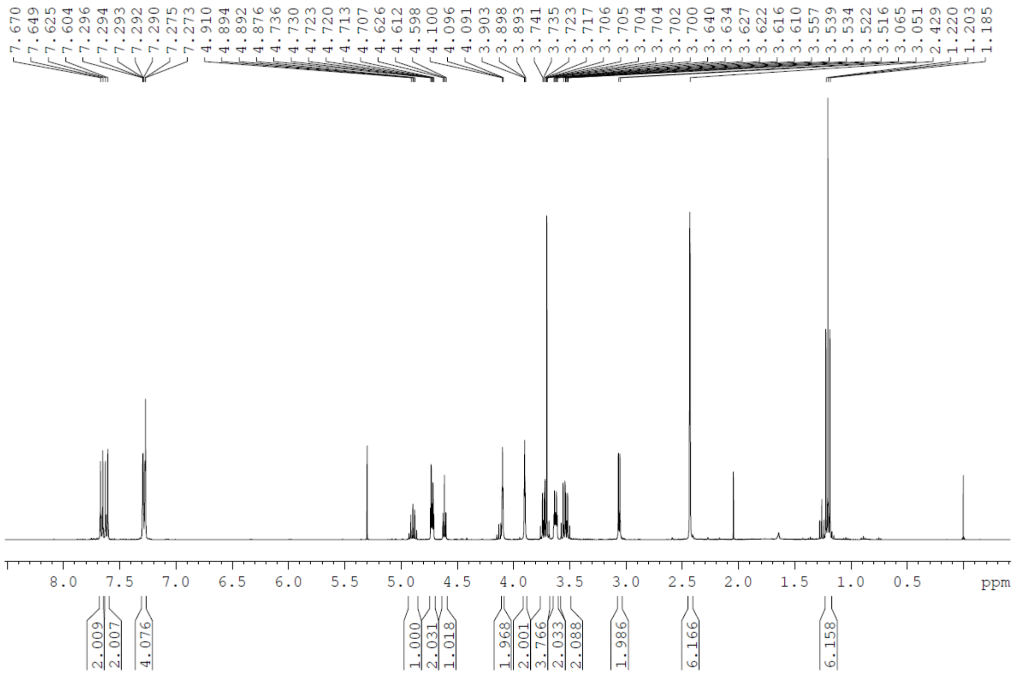


Figure S1: ^{1}H NMR spectrum (400 MHz) of **S2a** in $CDCl_3$.

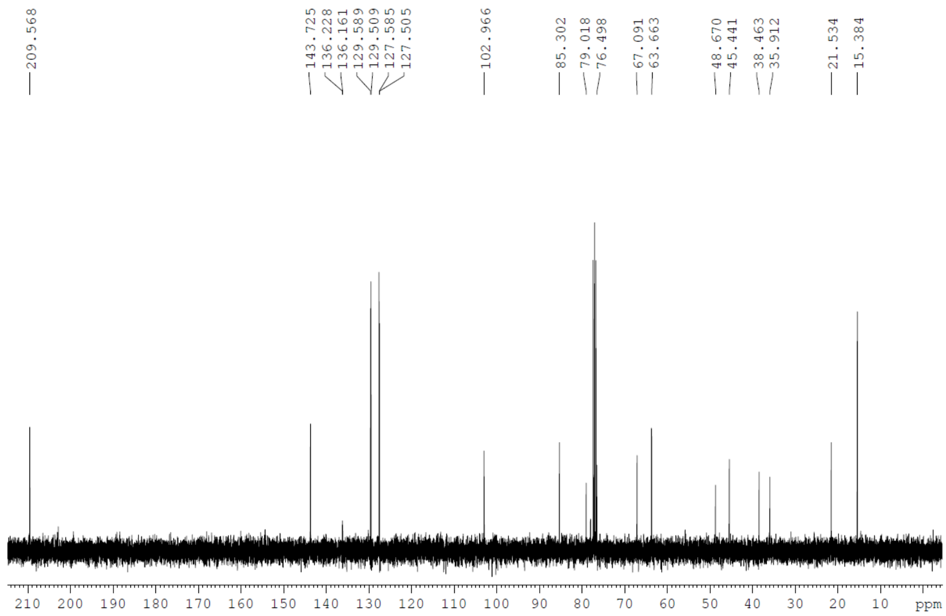
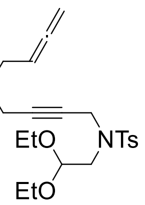


Figure S2: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **S2a** in $CDCl_3$.



S2b

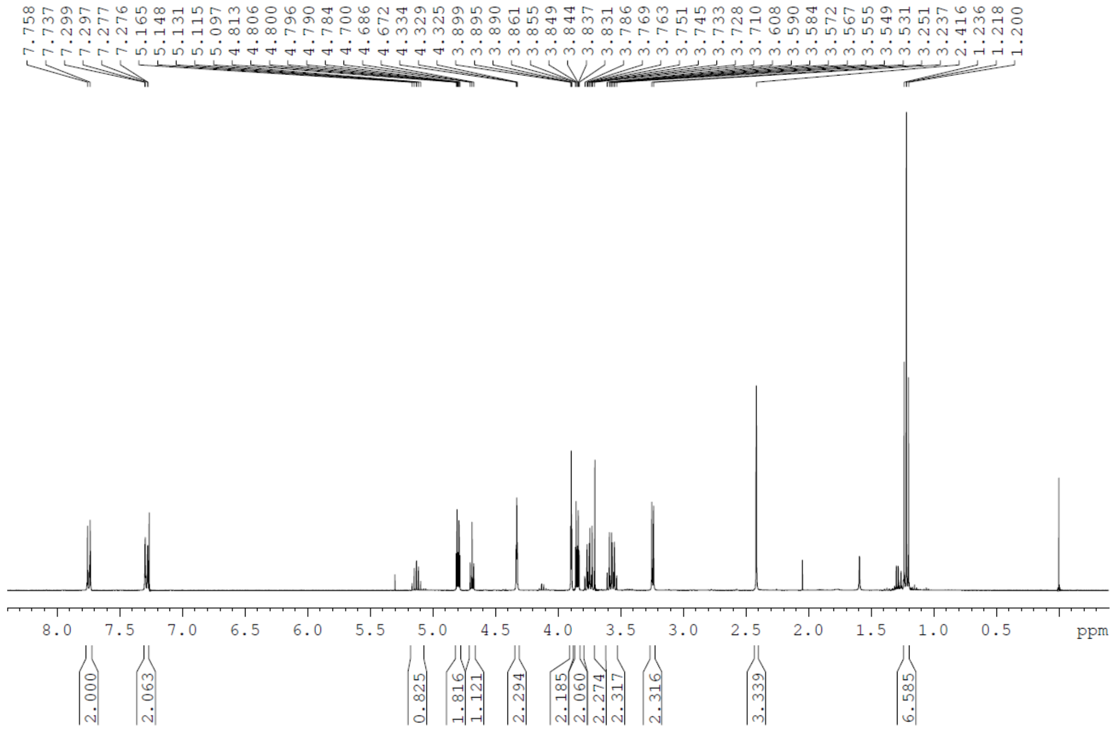


Figure S3: ^{1}H NMR spectrum (400 MHz) of **S2b** in $CDCl_3$.

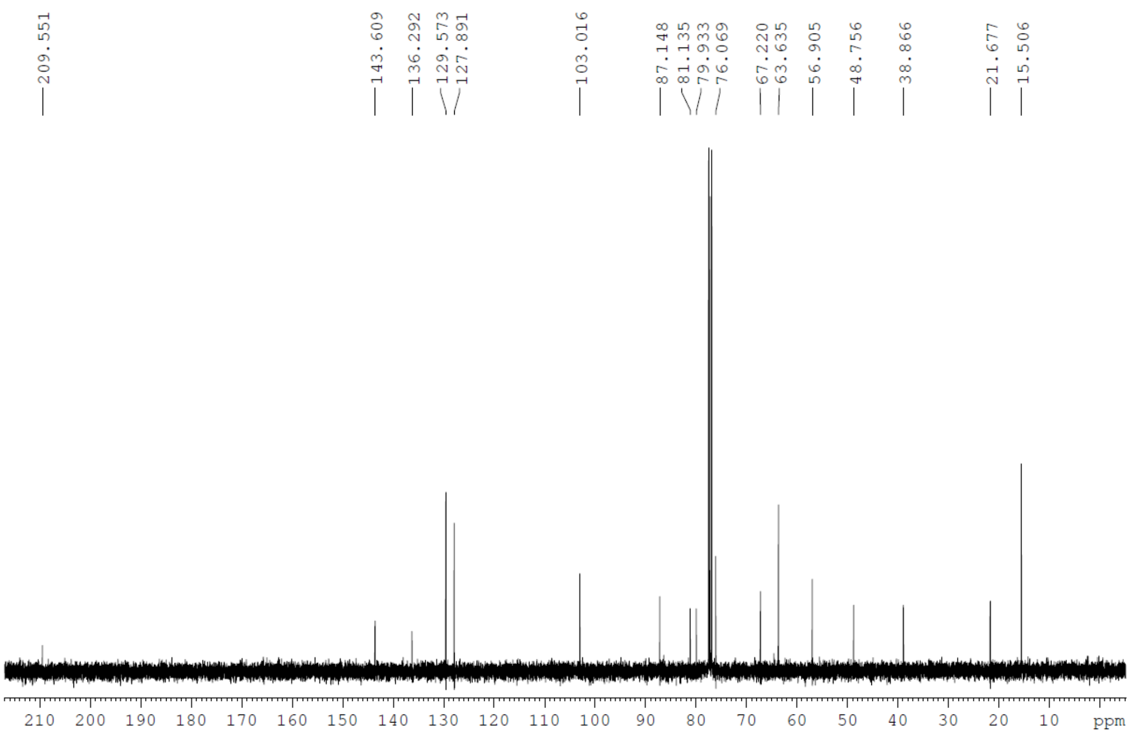
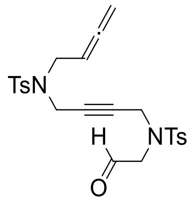


Figure S4: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **S2b** in $CDCl_3$.



S3a

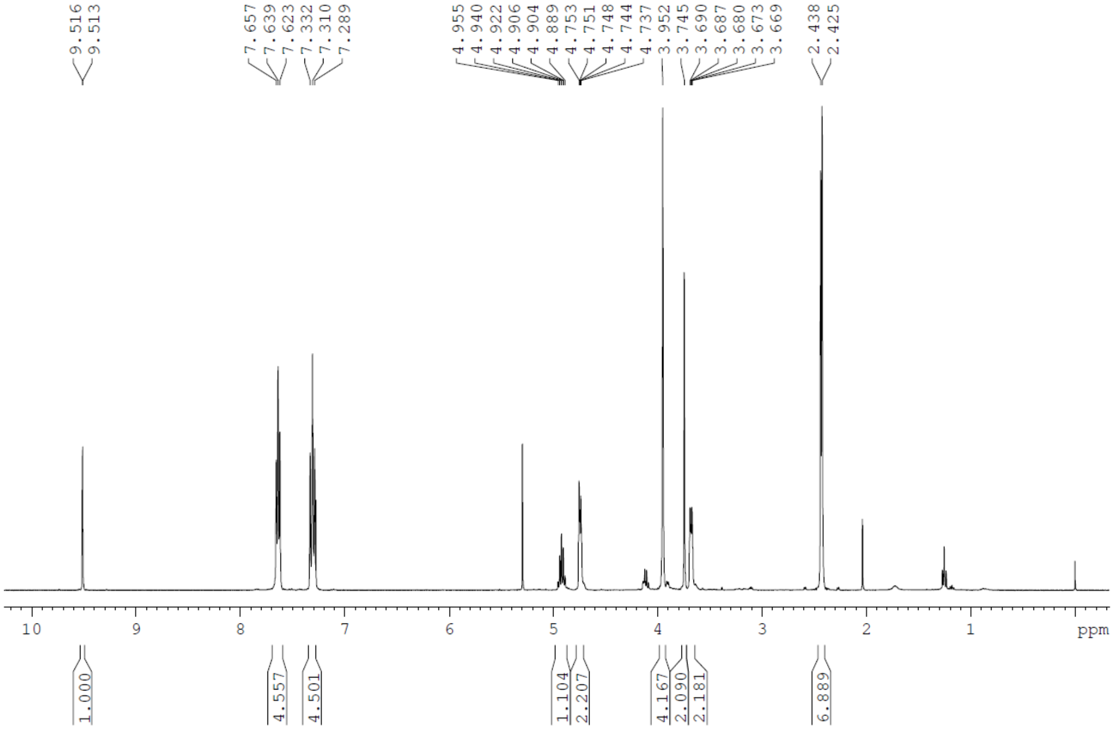


Figure S5: ^{1}H NMR spectrum (400 MHz) of **S3a** in $CDCl_3$.

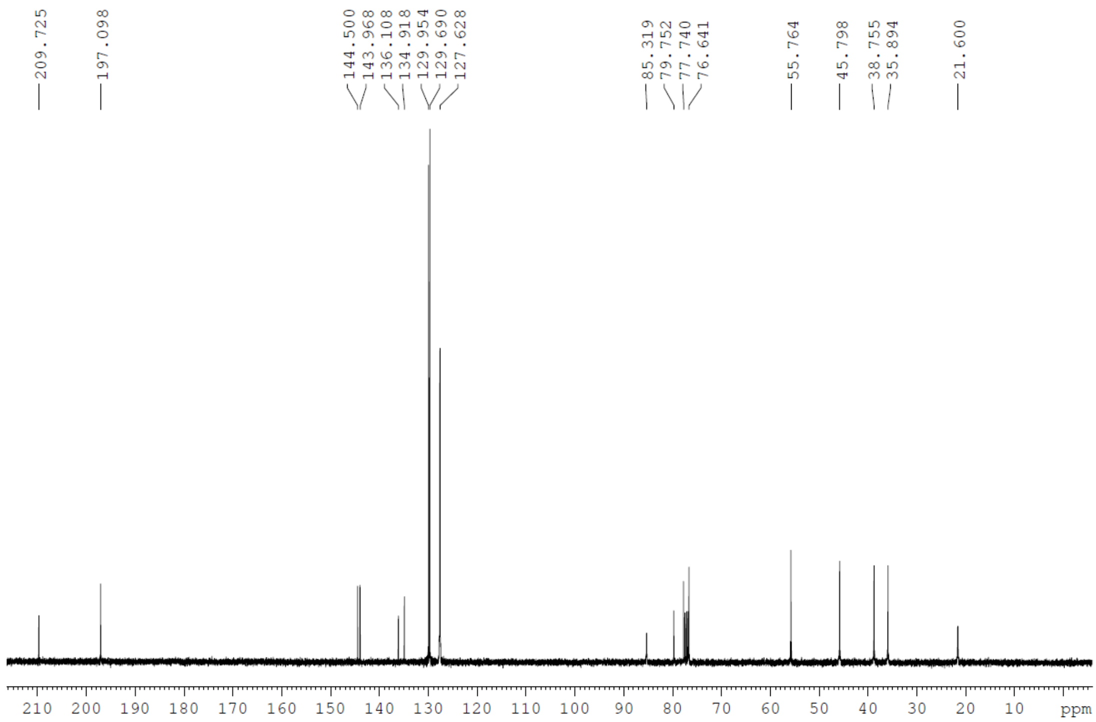
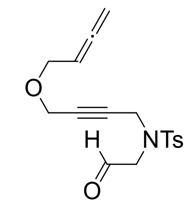


Figure S6: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **S3a** in $CDCl_3$.



S3b

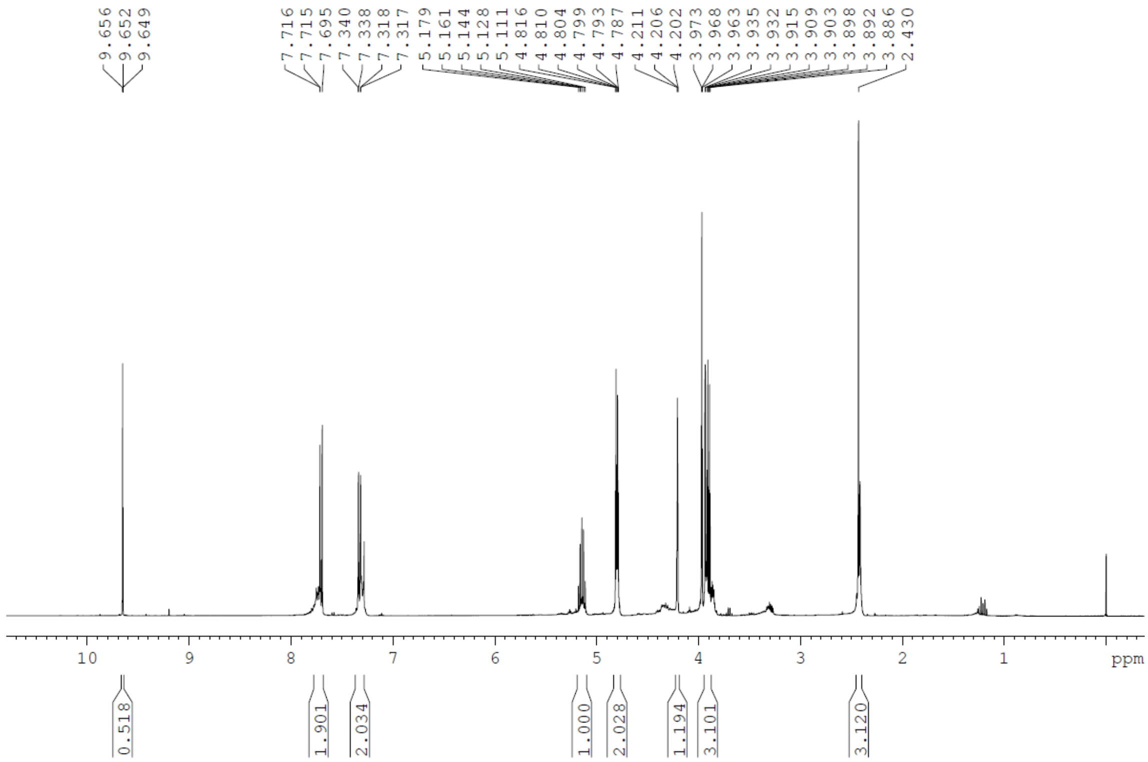


Figure S7: ^{1}H NMR spectrum (400 MHz) of **S3b** in $CDCl_3$.

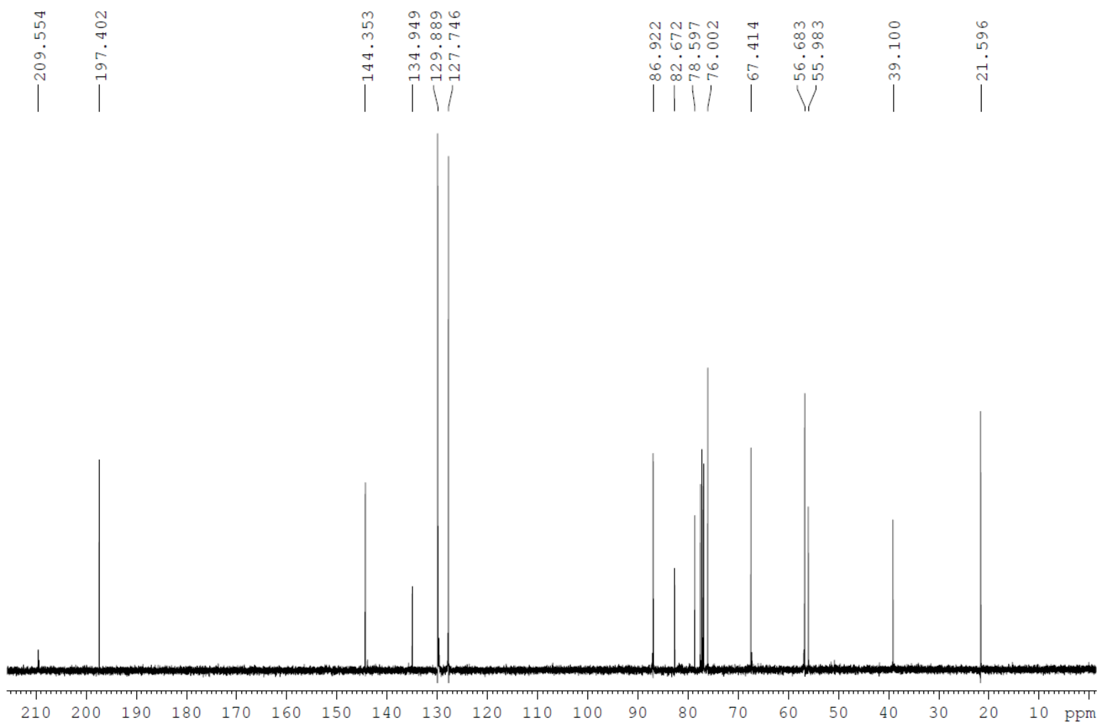
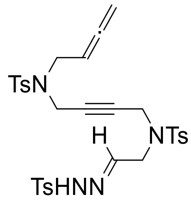


Figure S8: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **S3b** in $CDCl_3$.



1

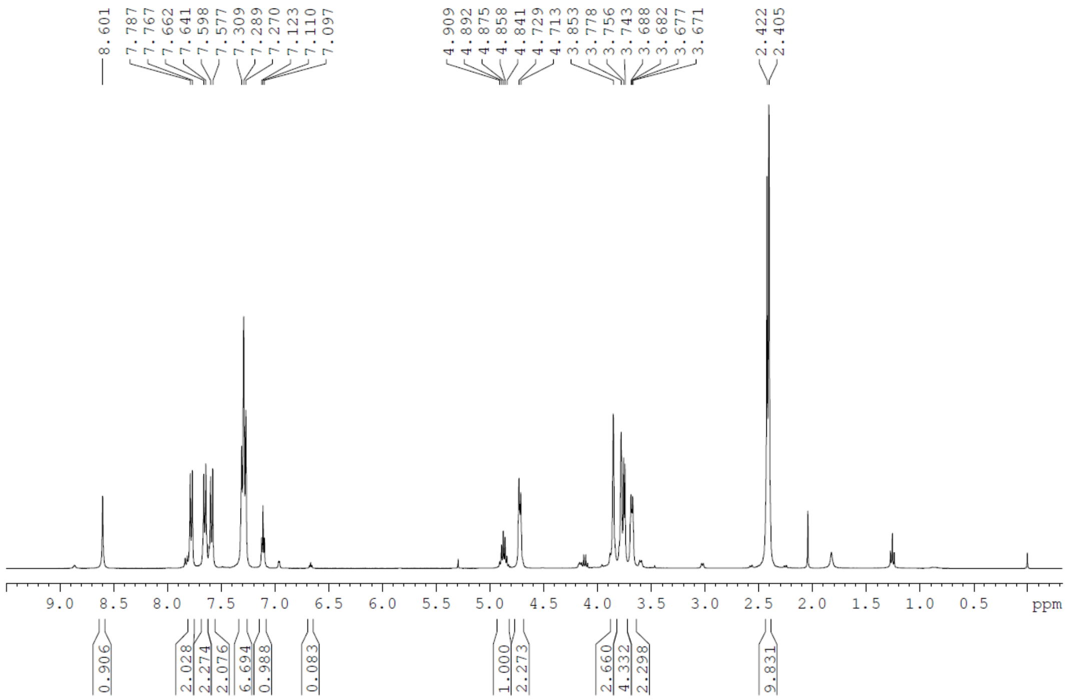


Figure S9: ^{1}H NMR spectrum (400 MHz) of **1** in $CDCl_3$.

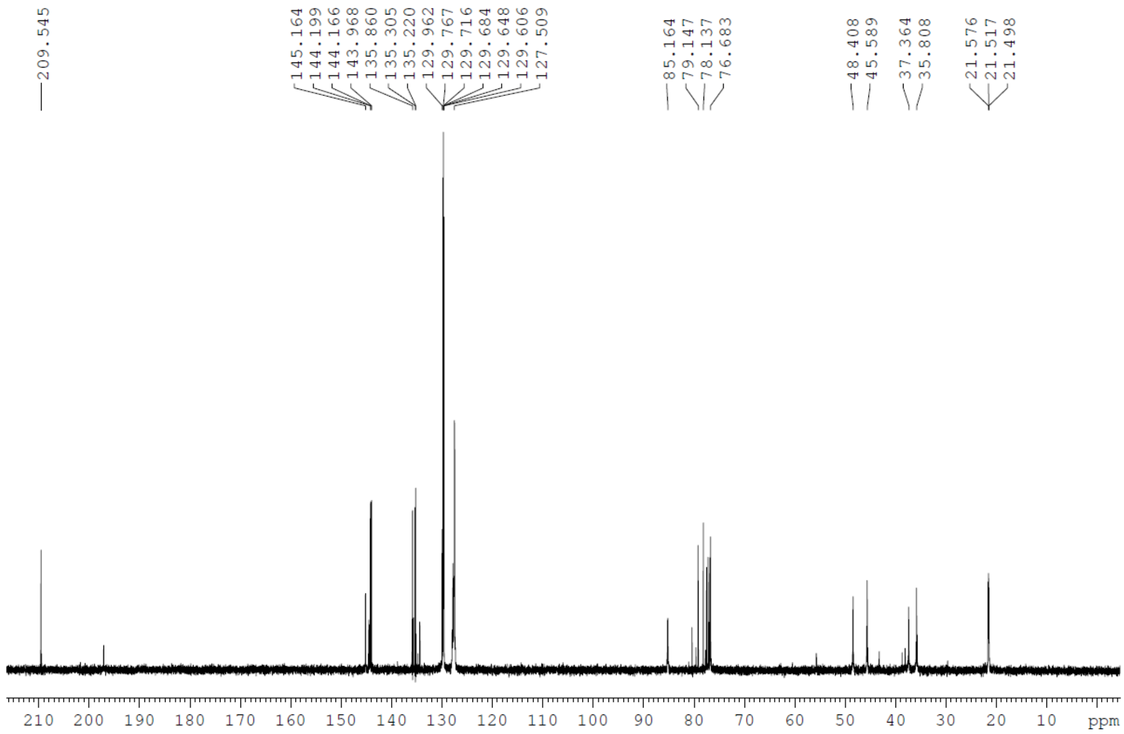
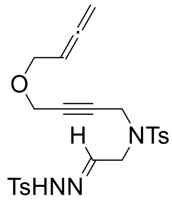


Figure S10: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **1** in $CDCl_3$.



3a

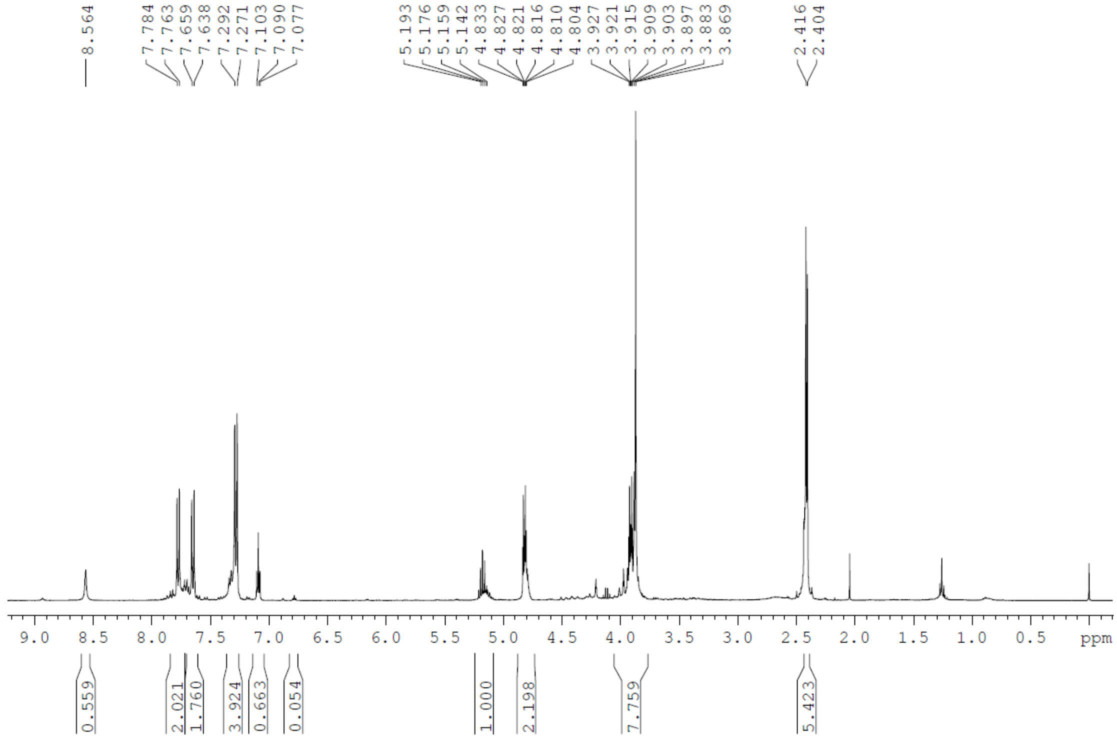


Figure S11: ^{1}H NMR spectrum (400 MHz) of **3a** in $CDCl_3$.

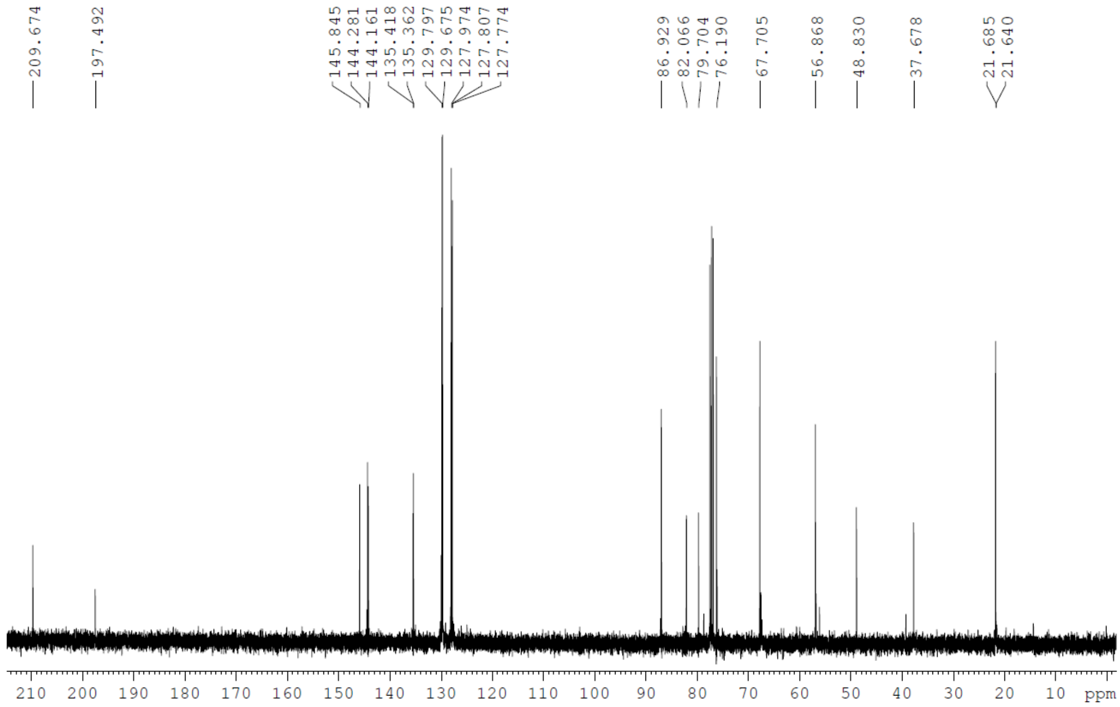
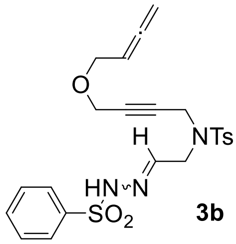


Figure S12: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **3a** in $CDCl_3$.



3b

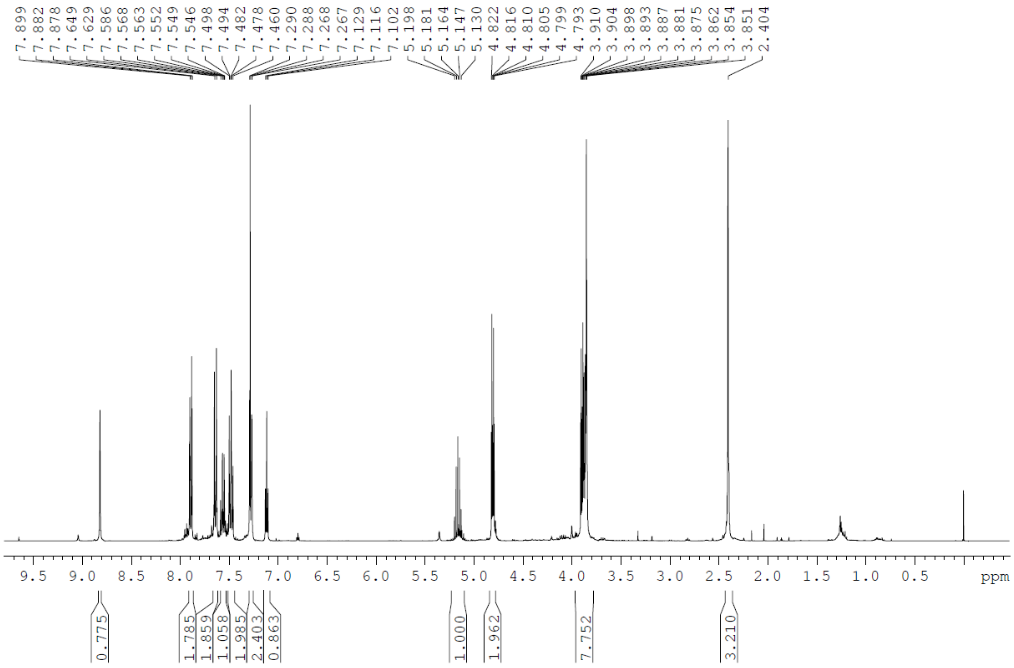


Figure S13: ^{1}H NMR spectrum (400 MHz) of **3b** in $CDCl_3$.

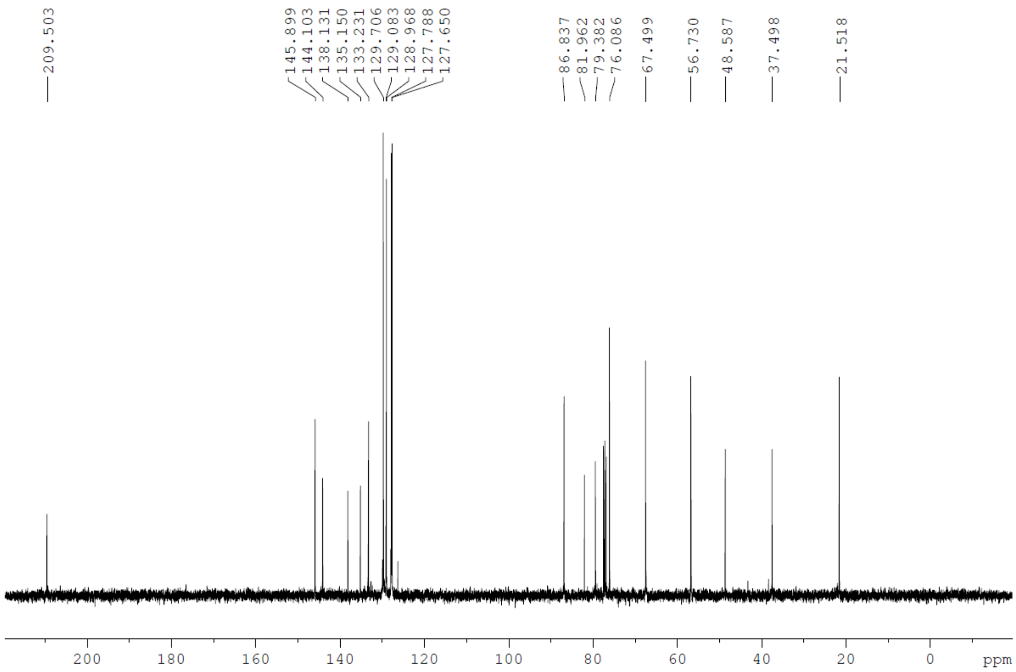
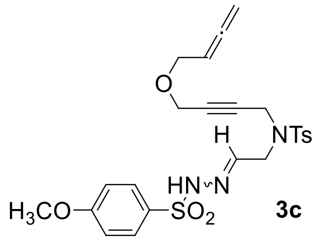


Figure S14: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **3b** in $CDCl_3$.



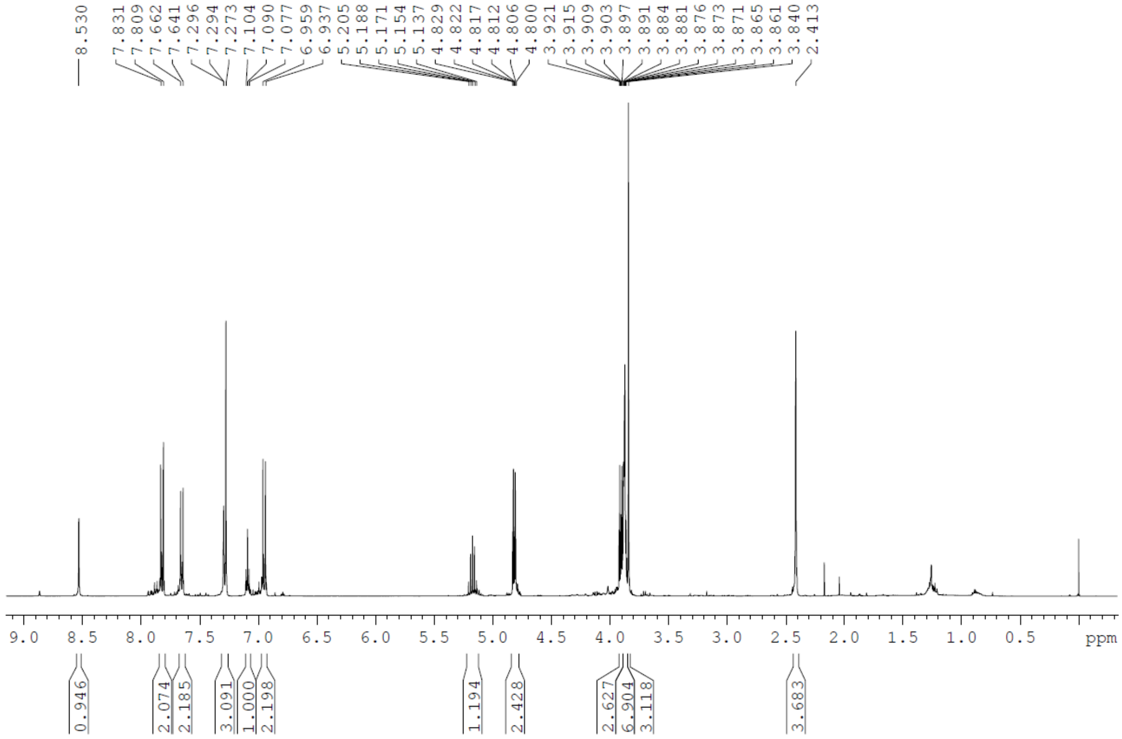


Figure S15: [1]H NMR spectrum (400 MHz) of **3c** in $CDCl_3$.

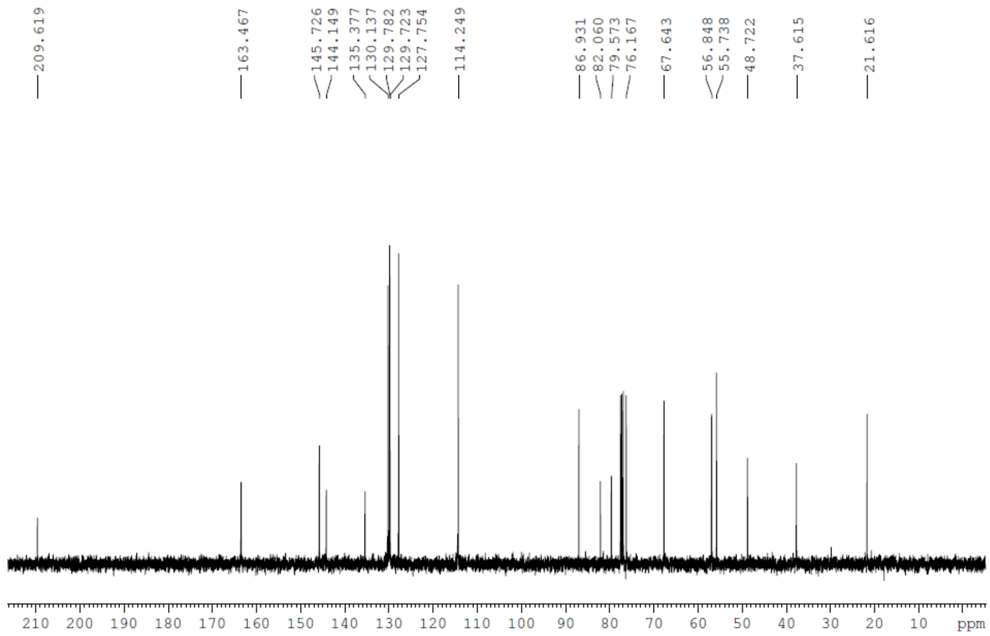
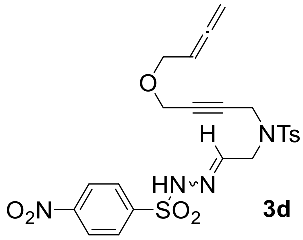


Figure S16: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **3c** in $CDCl_3$.



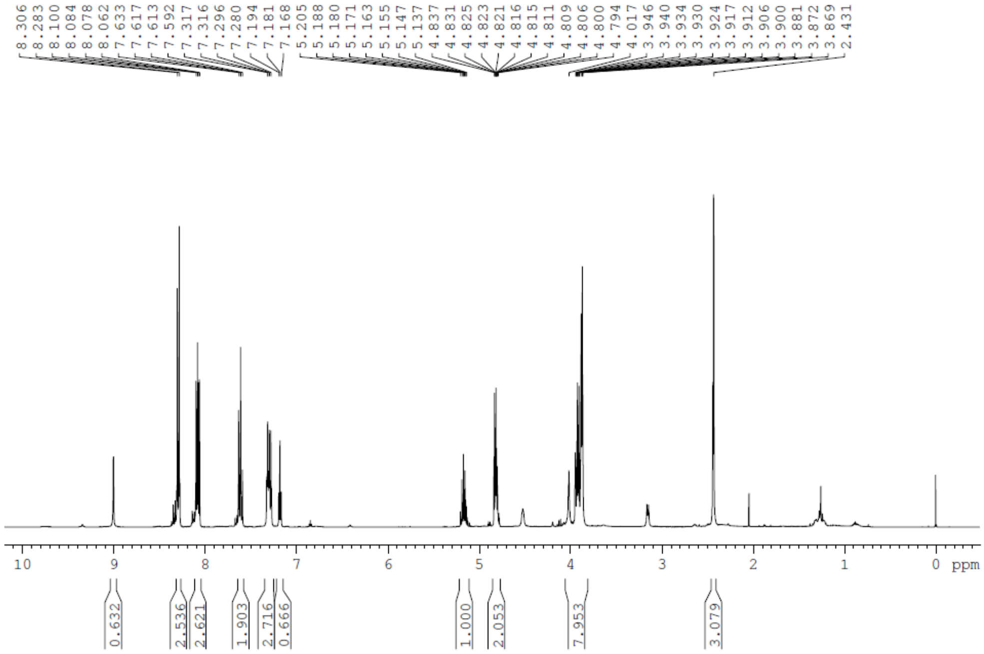


Figure S17: [1]H NMR spectrum (400 MHz) of **3d** in $CDCl_3$.

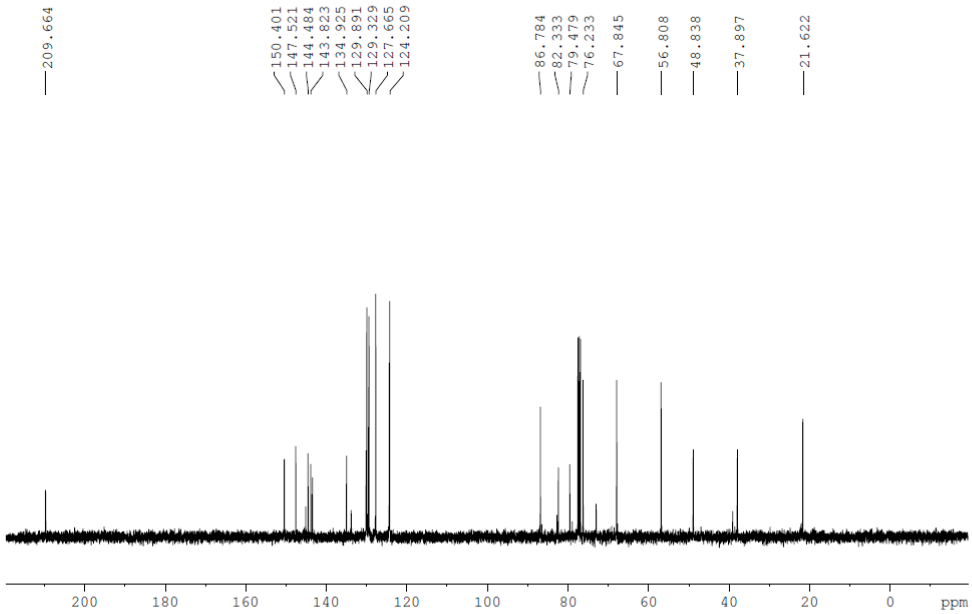
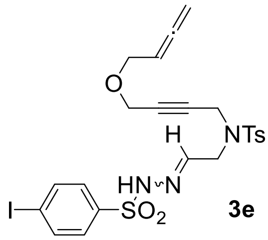


Figure S18: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **3d** in $CDCl_3$.



3e

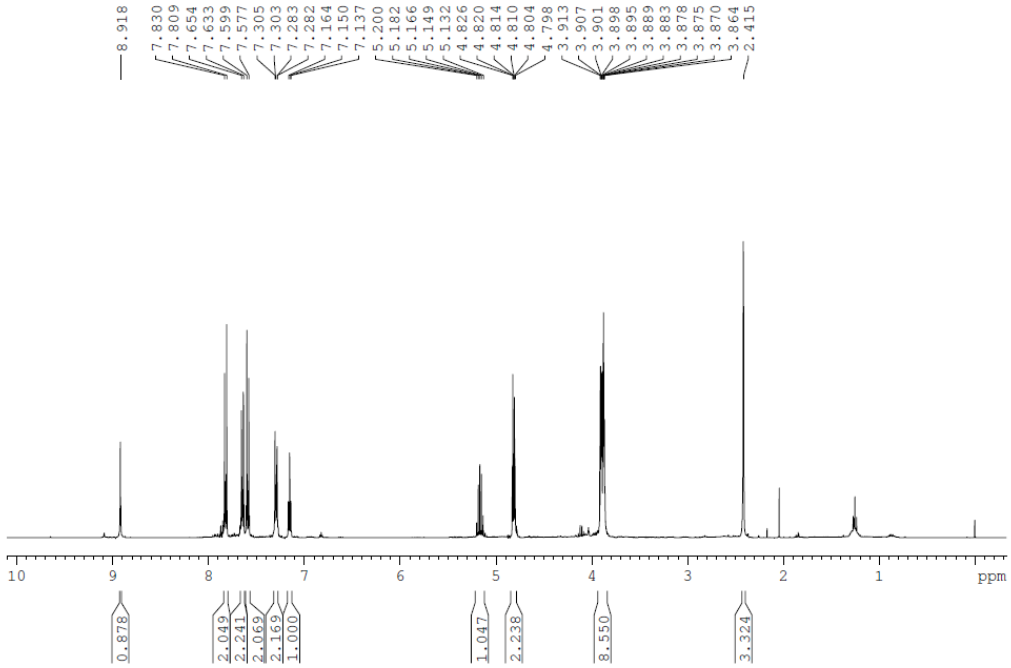


Figure S19: ^{1}H NMR spectrum (400 MHz) of **3e** in $CDCl_3$.

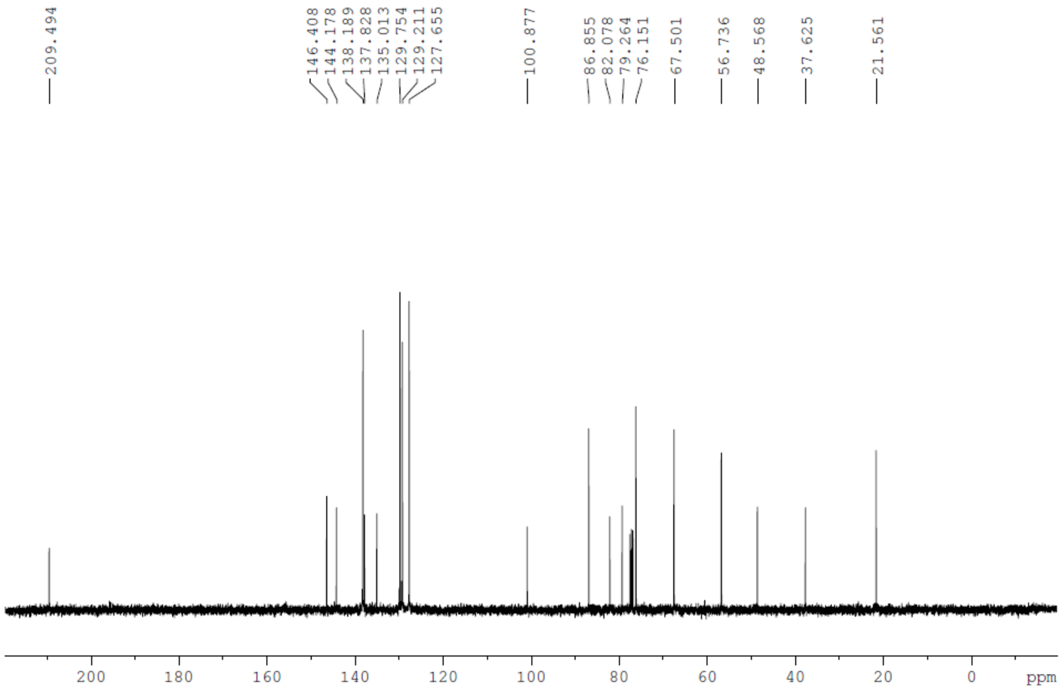
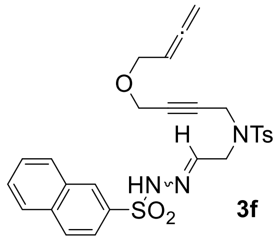


Figure S20: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **3e** in $CDCl_3$.



3f

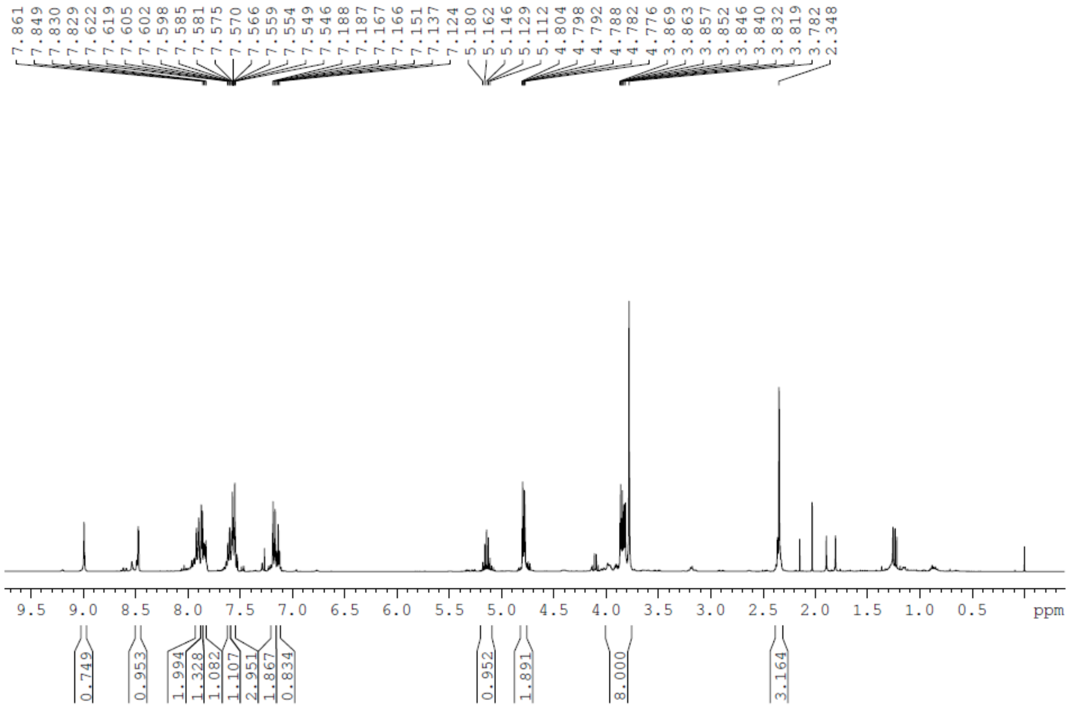


Figure S21: [1]H NMR spectrum (400 MHz) of **3f** in $CDCl_3$.

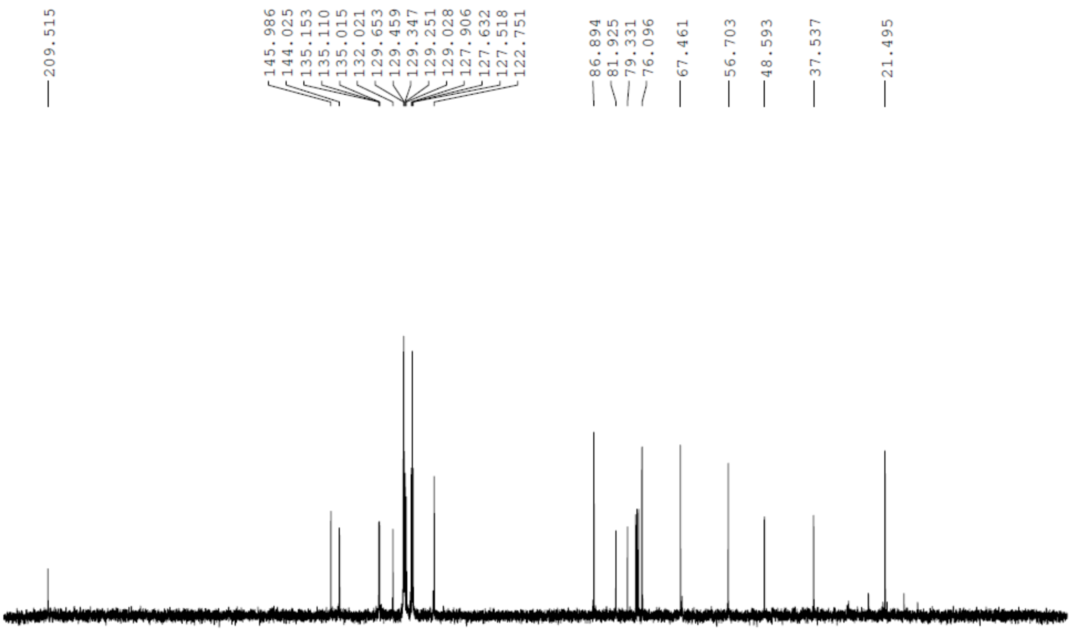
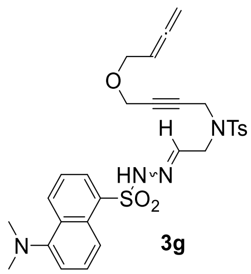


Figure S22: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **3f** in $CDCl_3$.



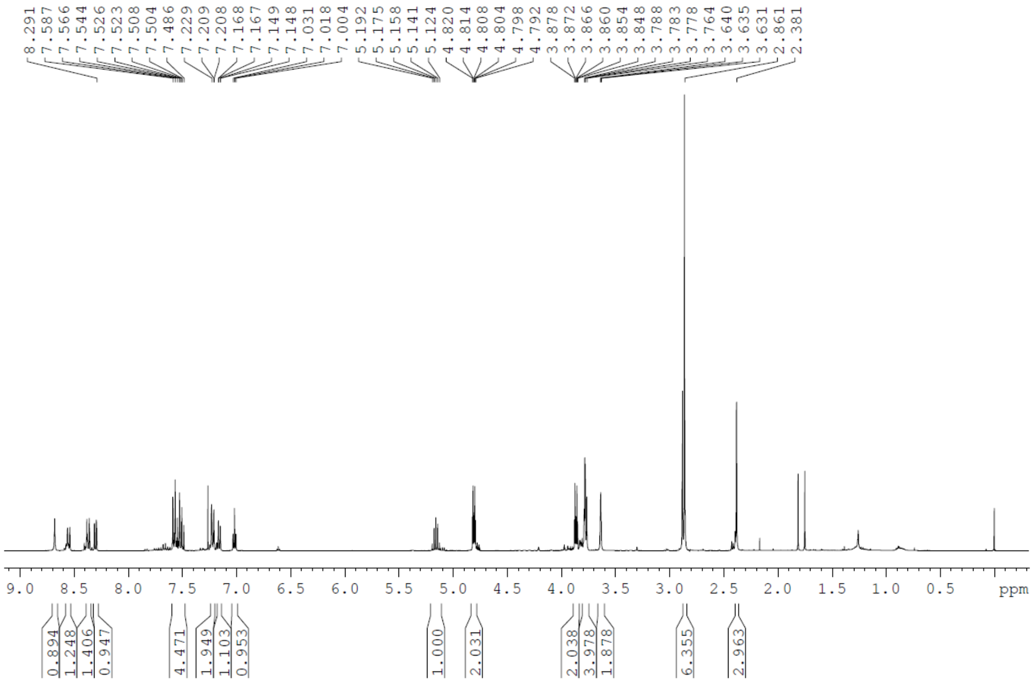


Figure S23: ^{1}H NMR spectrum (400 MHz) of **3g** in $CDCl_3$.

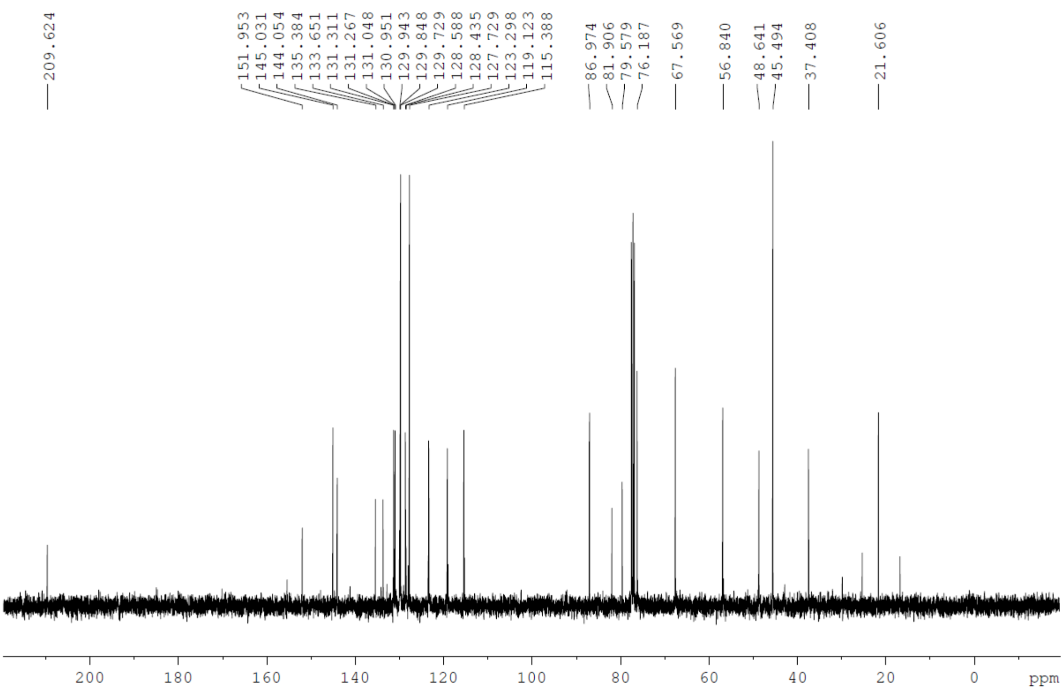
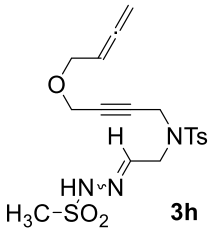


Figure S24: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **3g** in $CDCl_3$.



3h

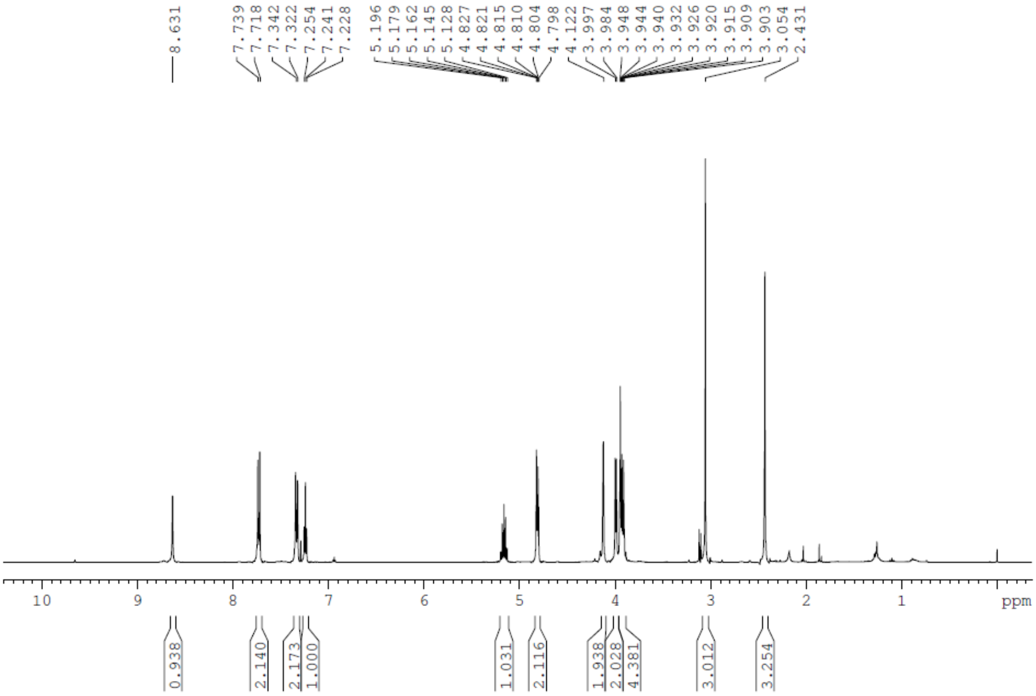


Figure S25: ^{1}H NMR spectrum (400 MHz) of **3h** in $CDCl_3$.

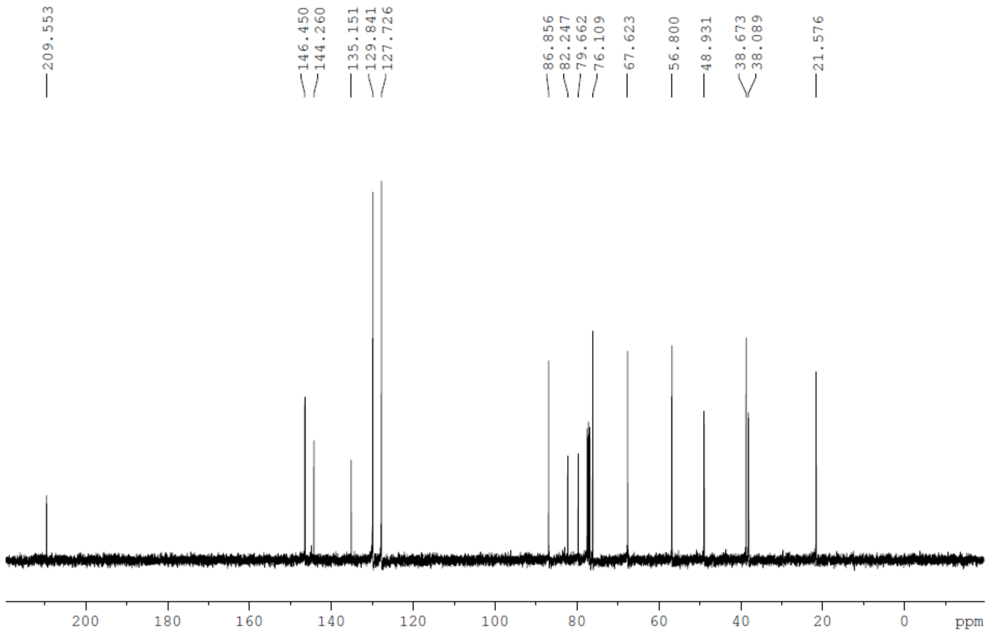
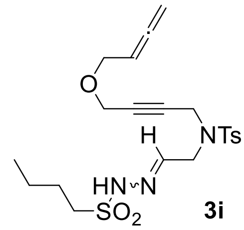


Figure S26: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **3h** in $CDCl_3$.



3i

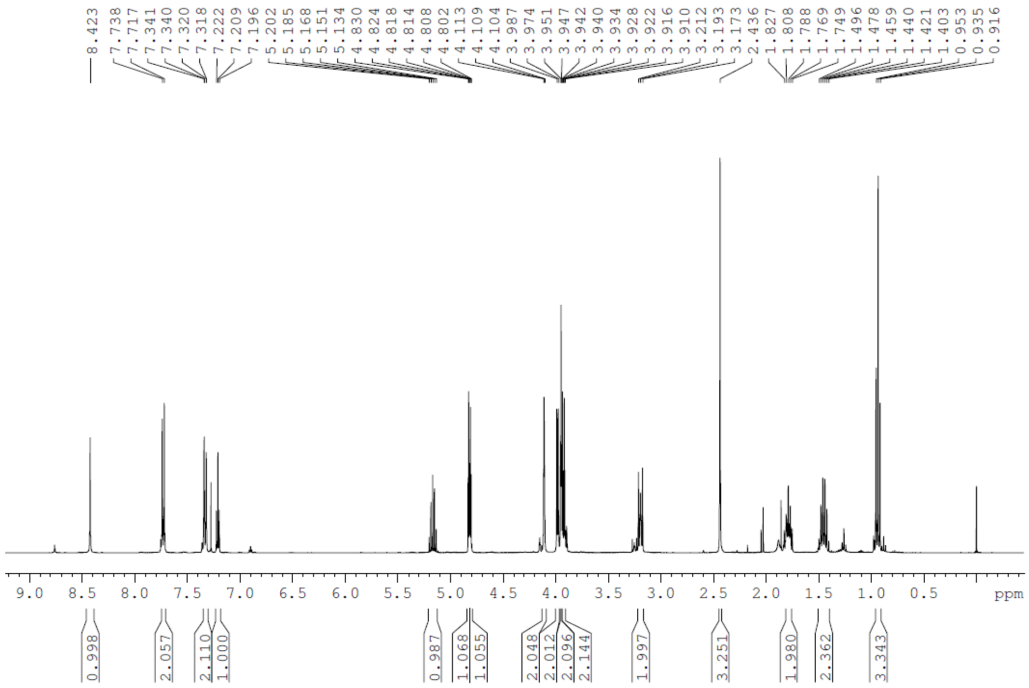


Figure S27: ^{1}H NMR spectrum (400 MHz) of **3i** in $CDCl_3$.

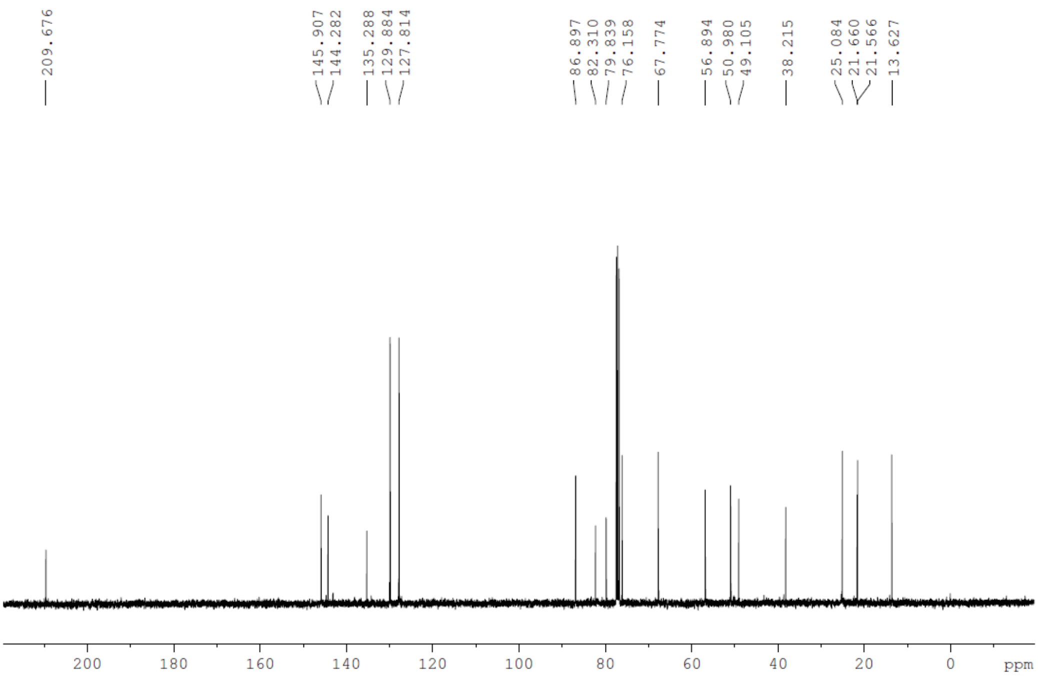
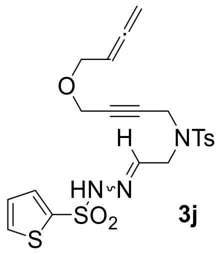


Figure S28: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **3i** in $CDCl_3$.



3j

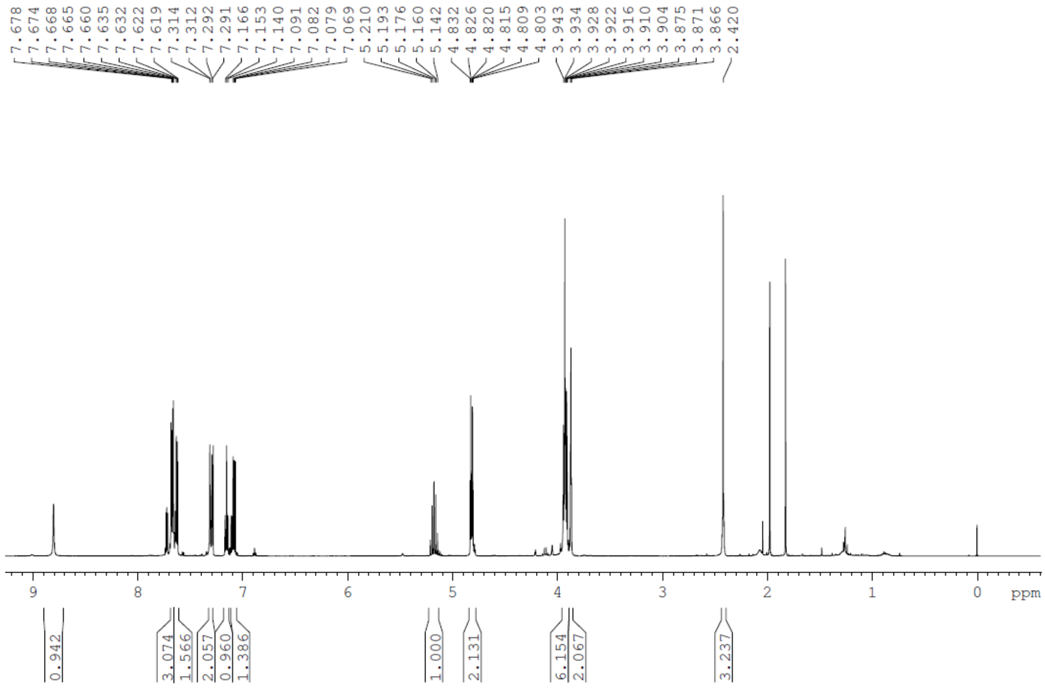


Figure S29: ¹H NMR spectrum (400 MHz) of **3j** in $CDCl_3$.

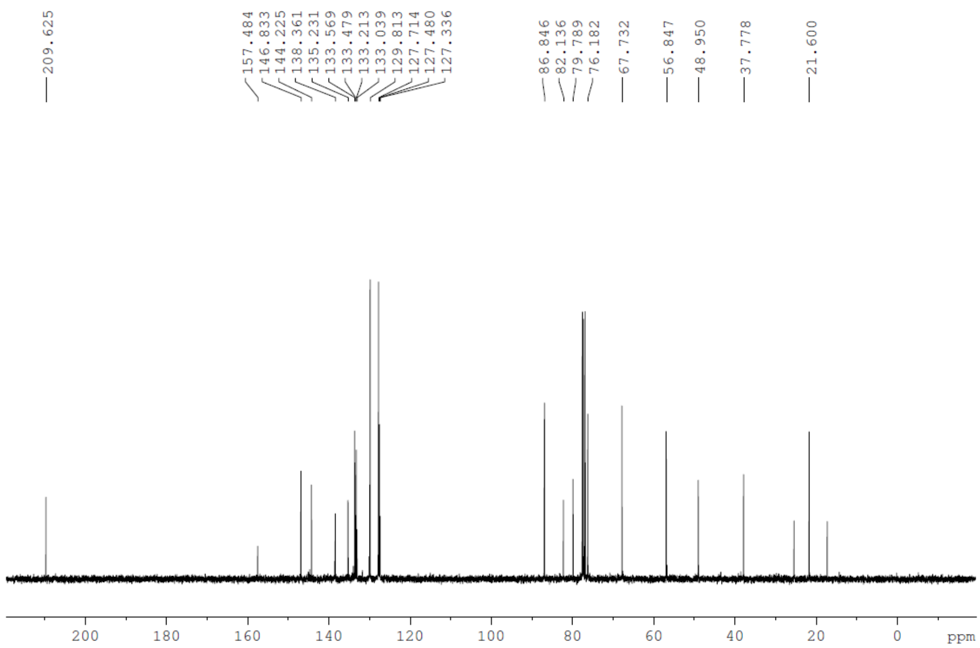
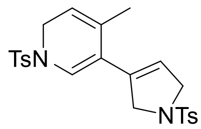
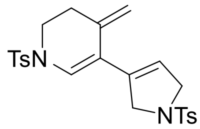


Figure S30: ¹H-decoupled¹³C NMR spectrum (100 MHz) of **3j** in $CDCl_3$.



2



2'

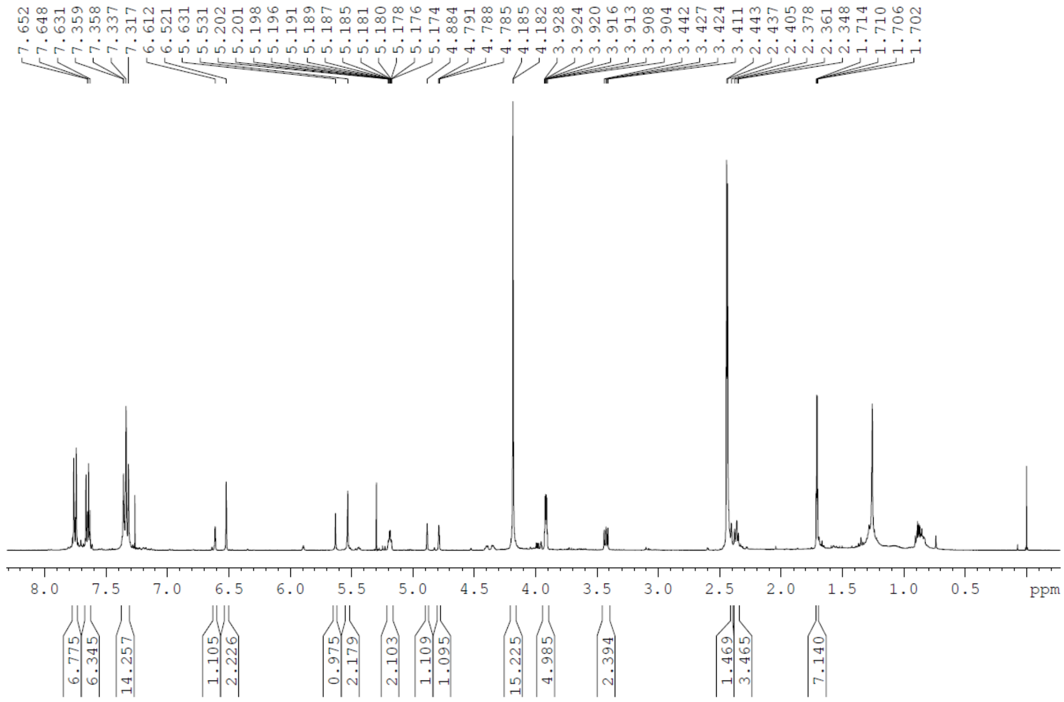


Figure S31: ^{1}H NMR spectrum (400 MHz) of **2** and **2'** in $CDCl_3$.

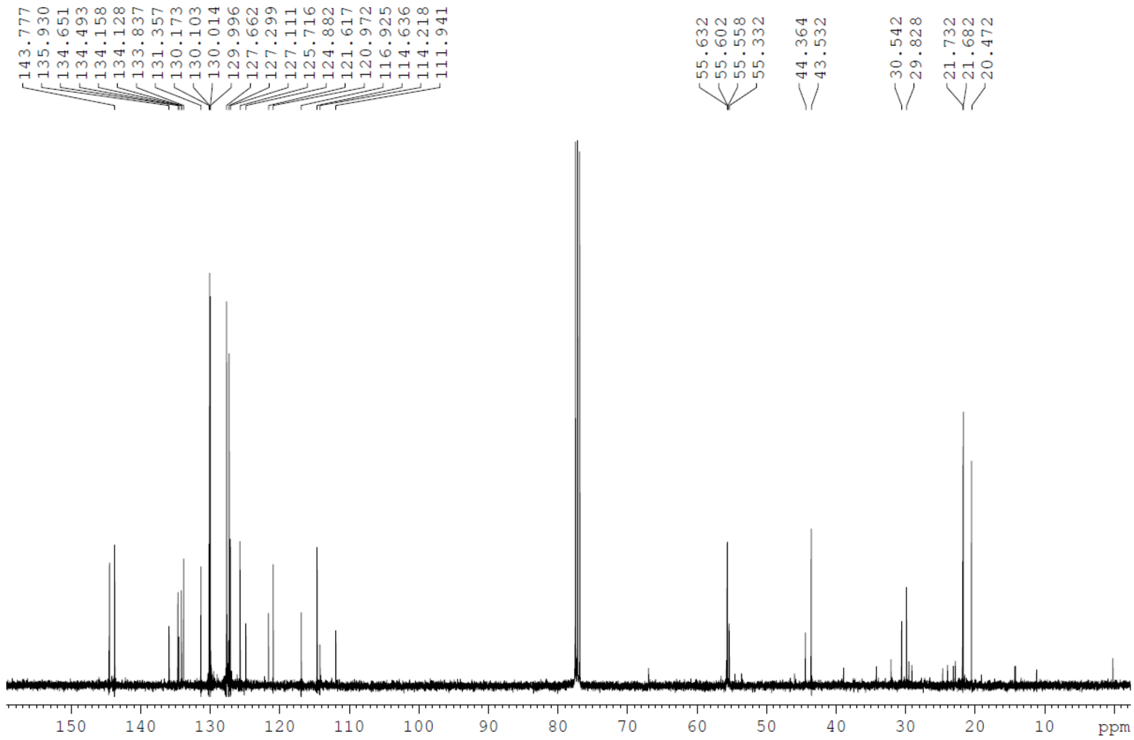
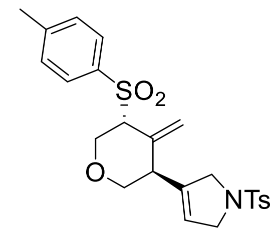


Figure S32: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **2** and **2'** in $CDCl_3$.



4a

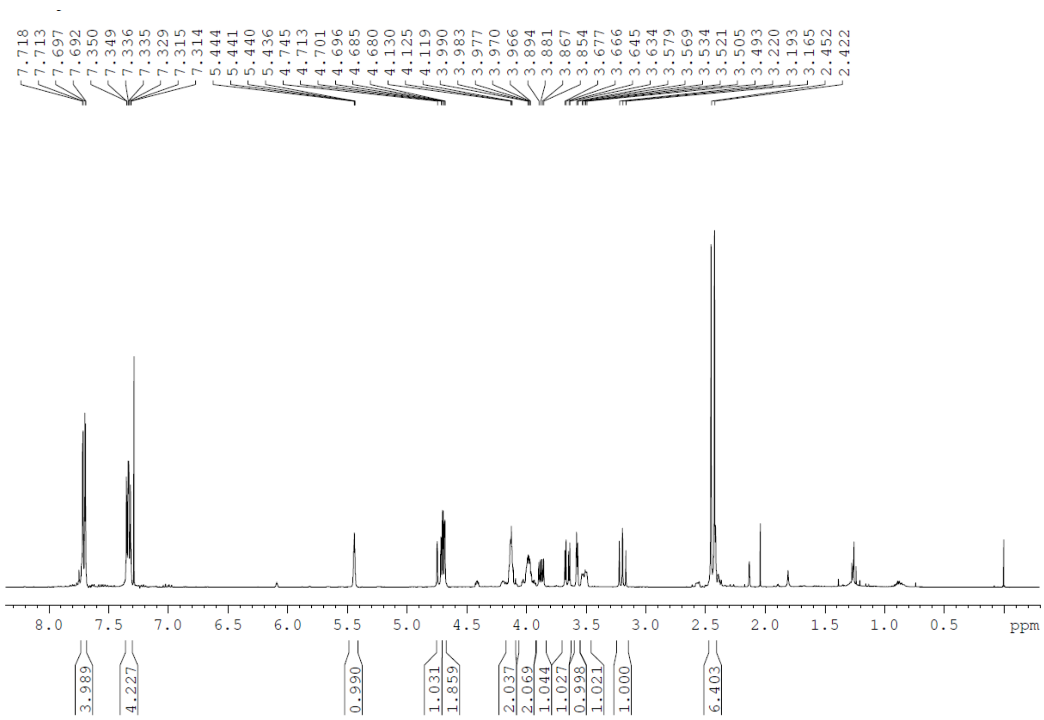


Figure S33: ^{1}H NMR spectrum (400 MHz) of **4a** in $CDCl_3$.

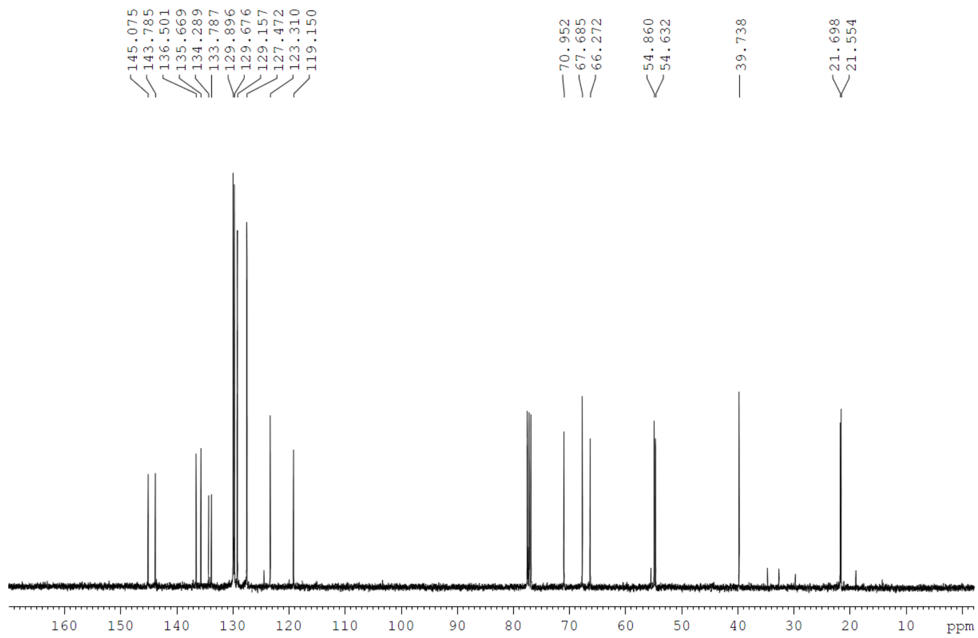
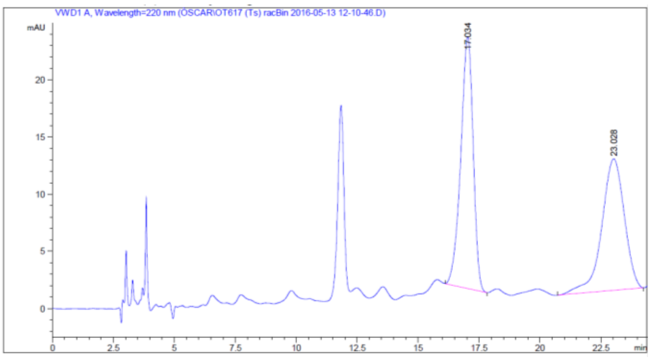


Figure S34: ^{1}H-decoupled ^{13}C NMR spectrum (100 MHz) of **4a** in $CDCl_3$.

Figure S35: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4a**.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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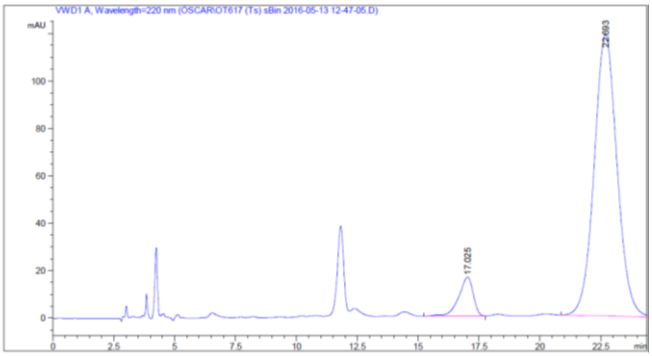
2	23.028	BB	0.9748	741.54004	11.52347	48.7377



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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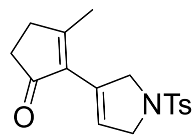
2	22.693	BB	1.0041	7752.93604	118.52721	91.8866



5

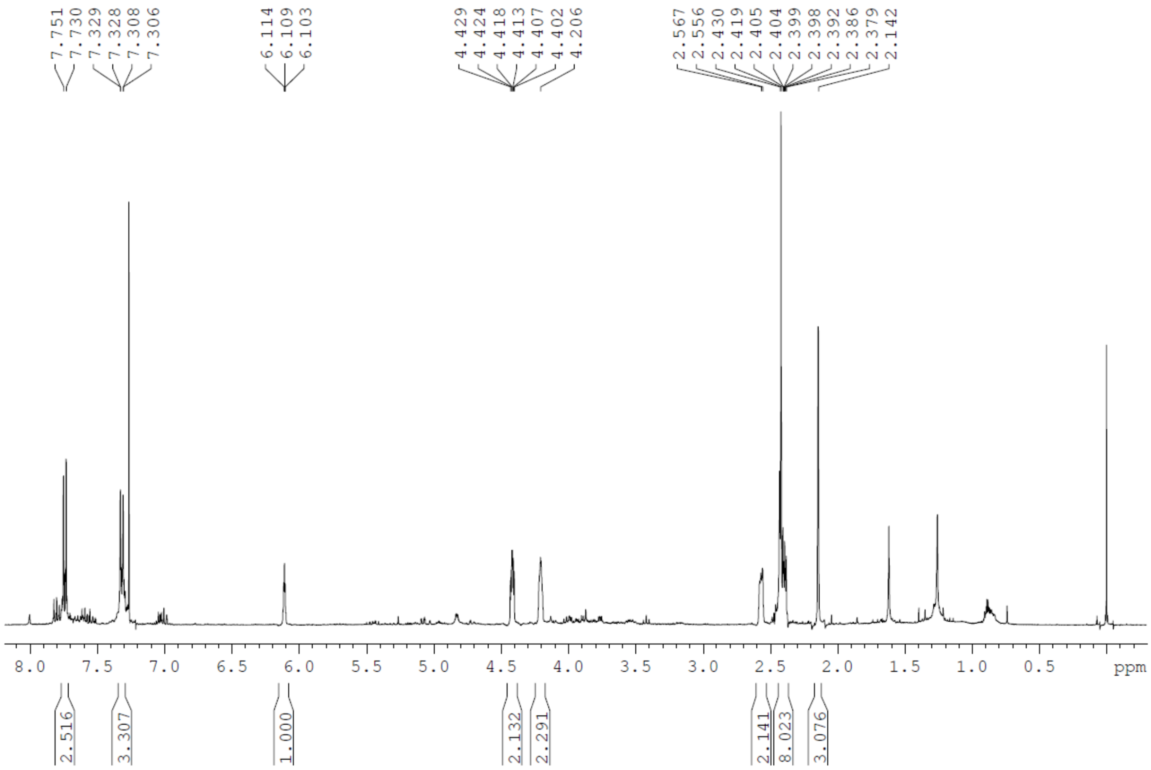
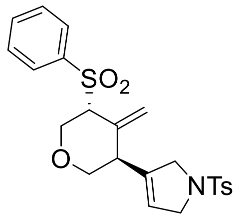


Figure S36: ^{1}H NMR spectrum (400 MHz) of **5** in $CDCl_3$.



4b

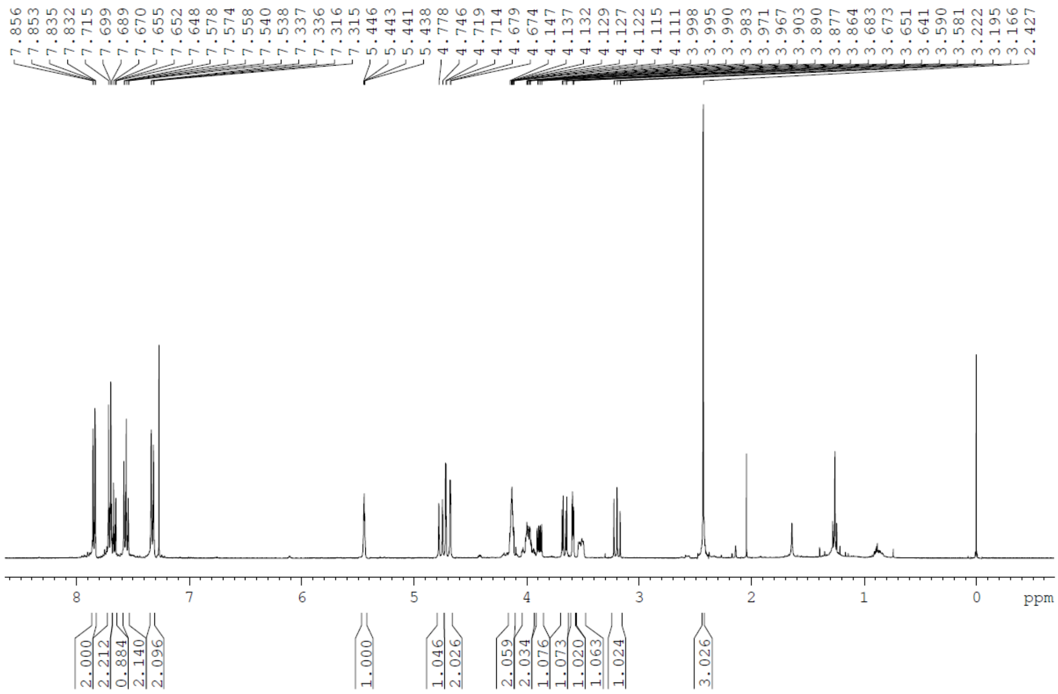


Figure S37: ^{1}H NMR spectrum (400 MHz) of **4b** in $CDCl_3$.

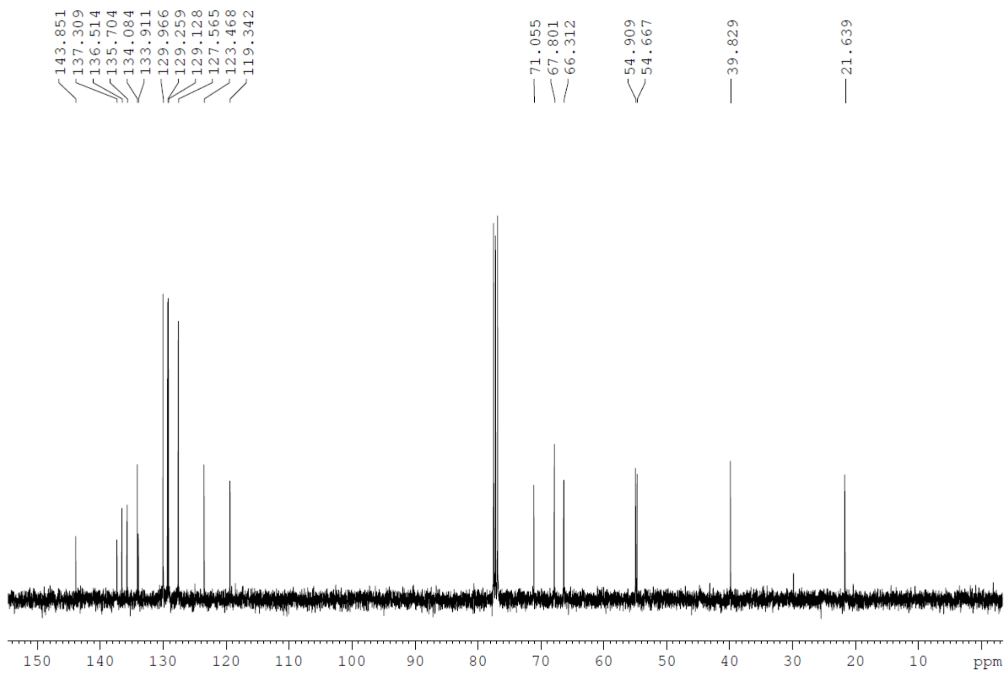
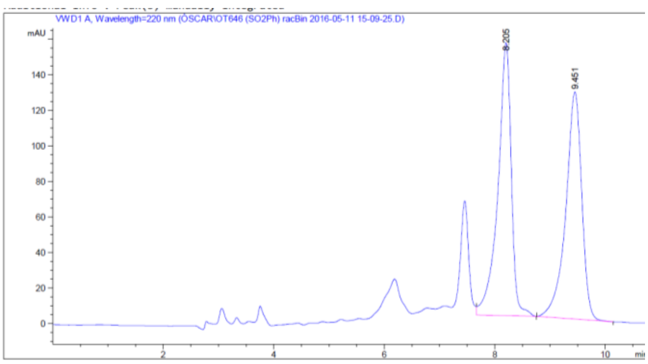
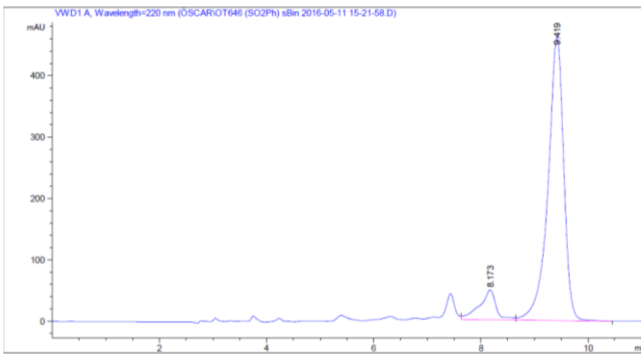


Figure S38: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4b** in $CDCl_3$.

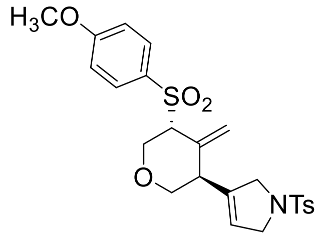
Figure S39: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4b**.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.205	VB	0.2458	2591.26440	153.61497	50.1858
2	9.451	BB	0.2996	2572.07935	127.89095	49.8142



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.173	VV R	0.2879	1043.57056	48.35429	9.9397
2	9.419	VB	0.3047	9455.40234	462.21680	90.0603



4c

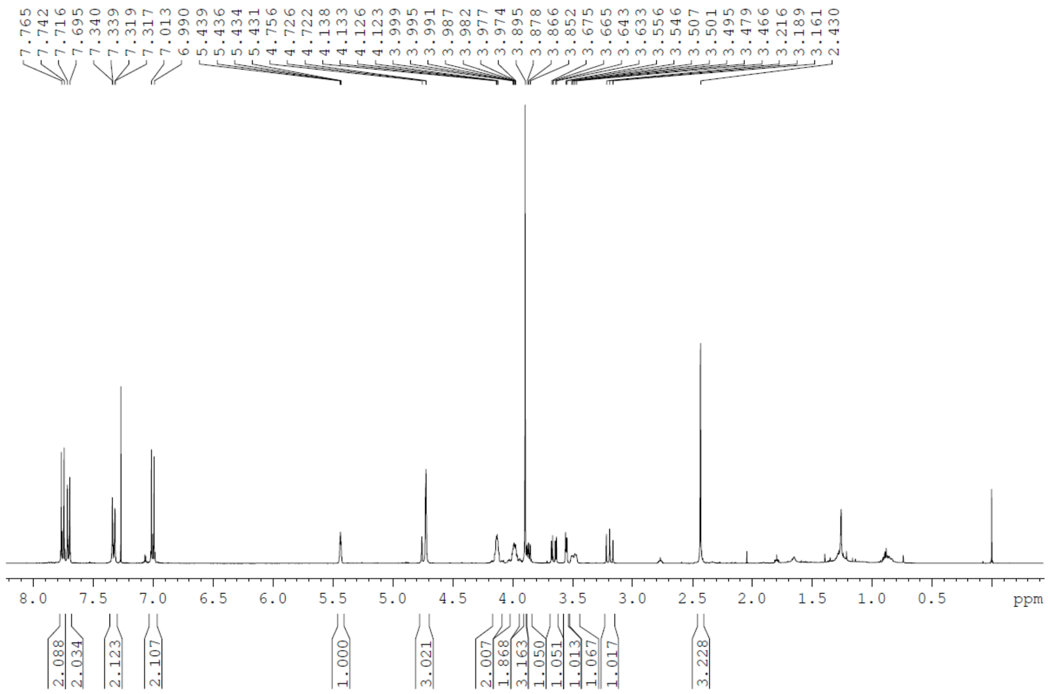


Figure S40: [1]H NMR spectrum (400 MHz) of **4c** in $CDCl_3$.

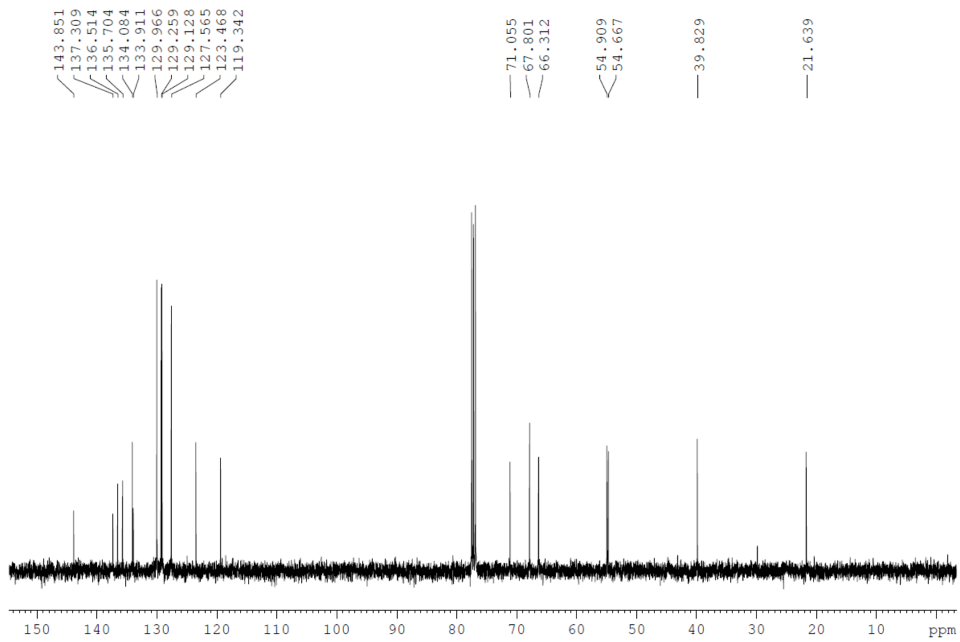
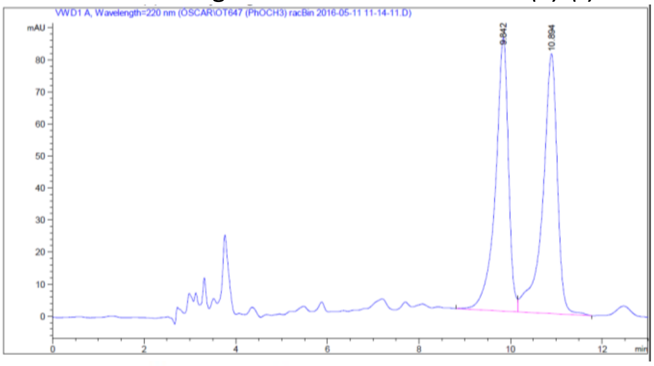
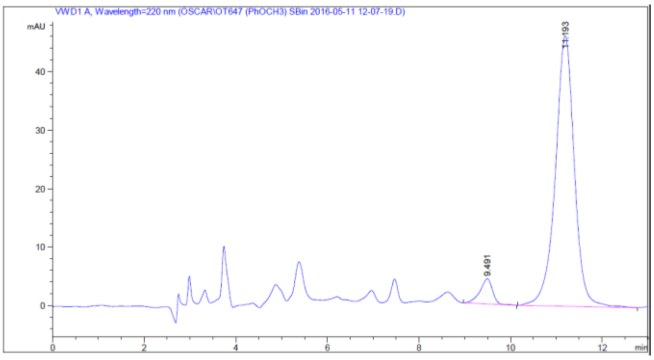


Figure S41: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **4c** in $CDCl_3$.

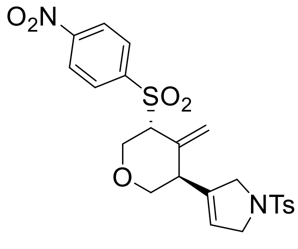
Figure S42: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4c**.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.842	BV	0.2889	1683.08215	85.42197	48.2898
2	10.894	VB	0.3255	1802.29626	81.04118	51.7102



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.491	BB	0.2838	82.29128	4.30832	5.8160
2	11.193	BB	0.4334	1332.61035	46.21558	94.1840



4d

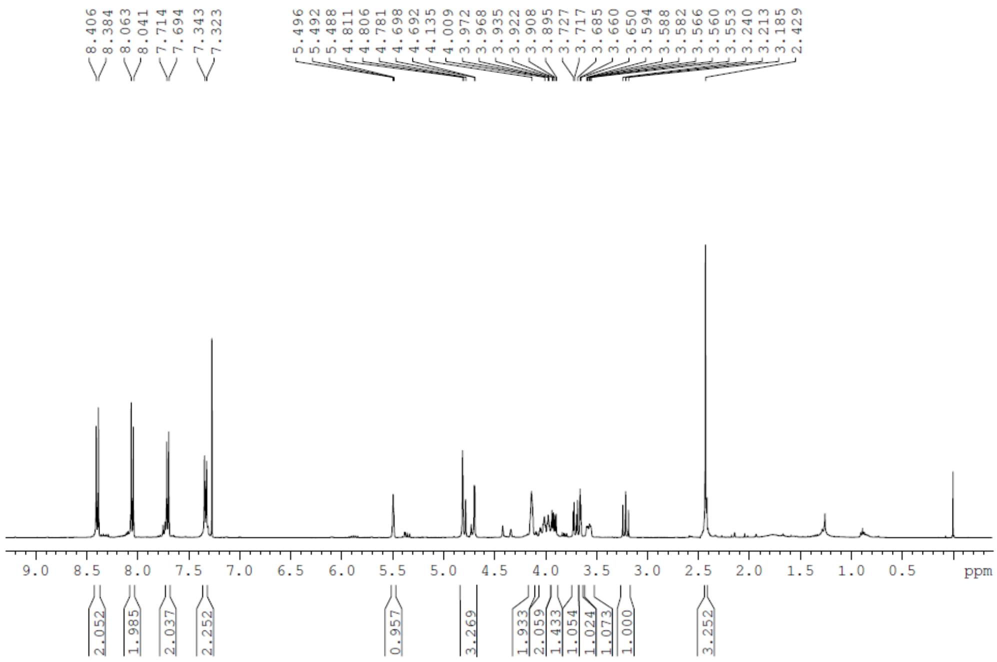


Figure S43: [1]H NMR spectrum (400 MHz) of **4d** in $CDCl_3$.

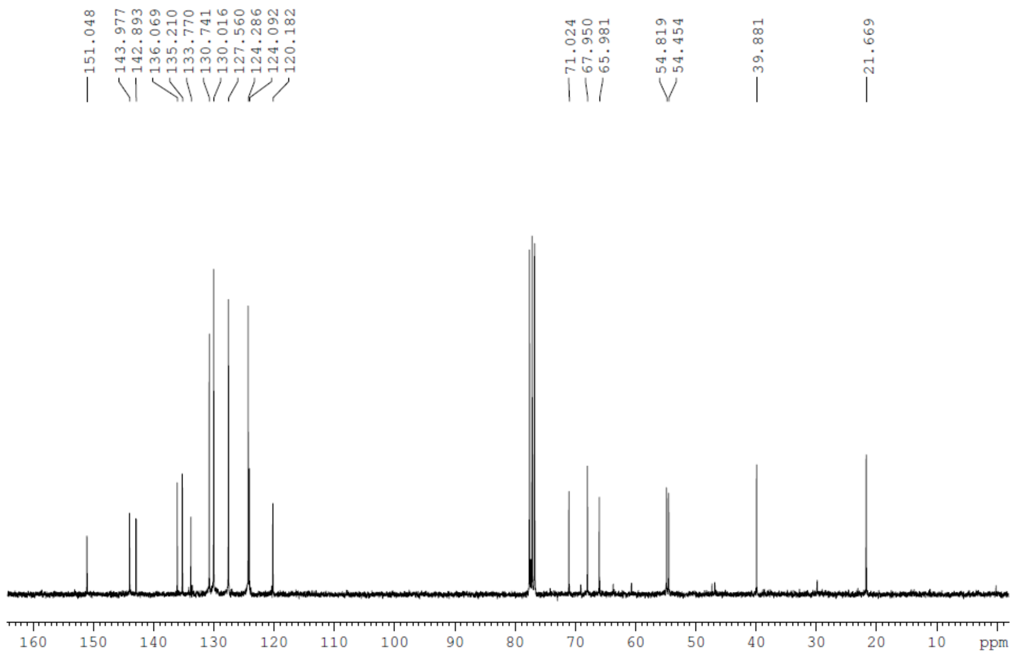
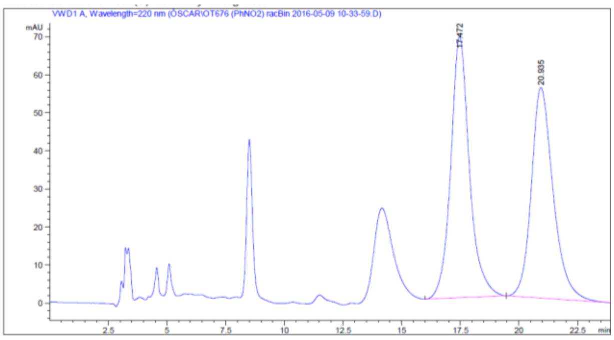
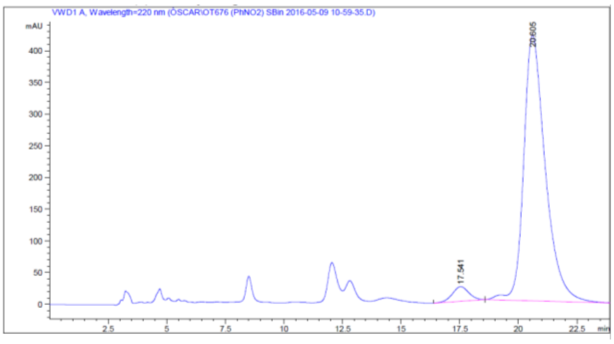


Figure S44: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **4d** in $CDCl_3$.

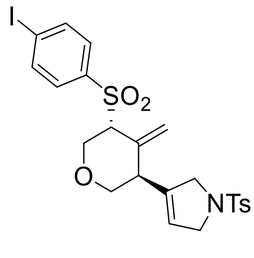
Figure S45: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4d**.



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



4e

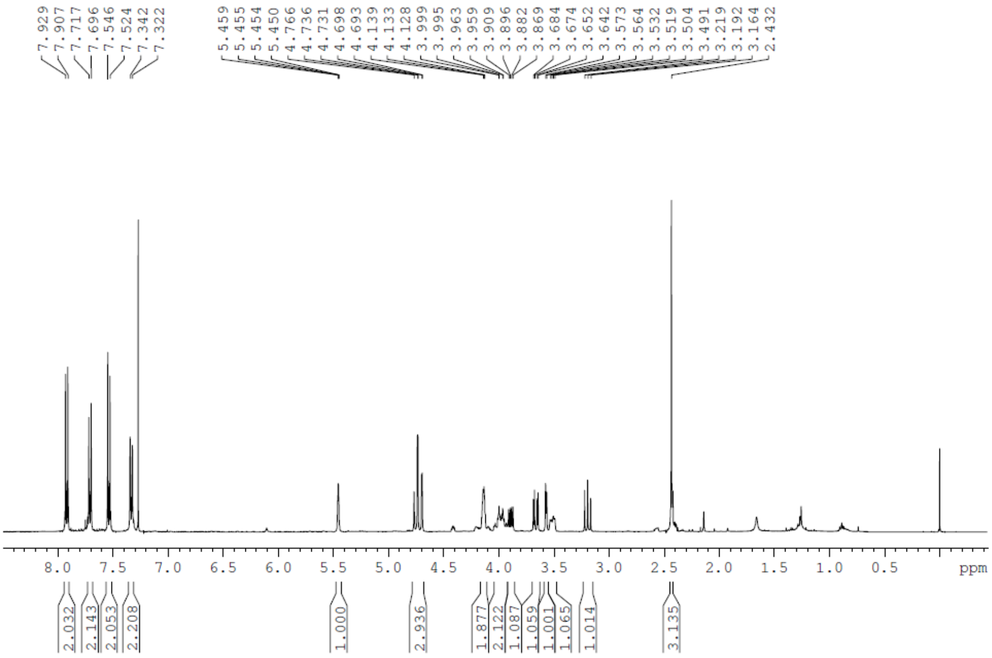


Figure S46: ^{1}H NMR spectrum (400 MHz) of **4e** in $CDCl_3$.

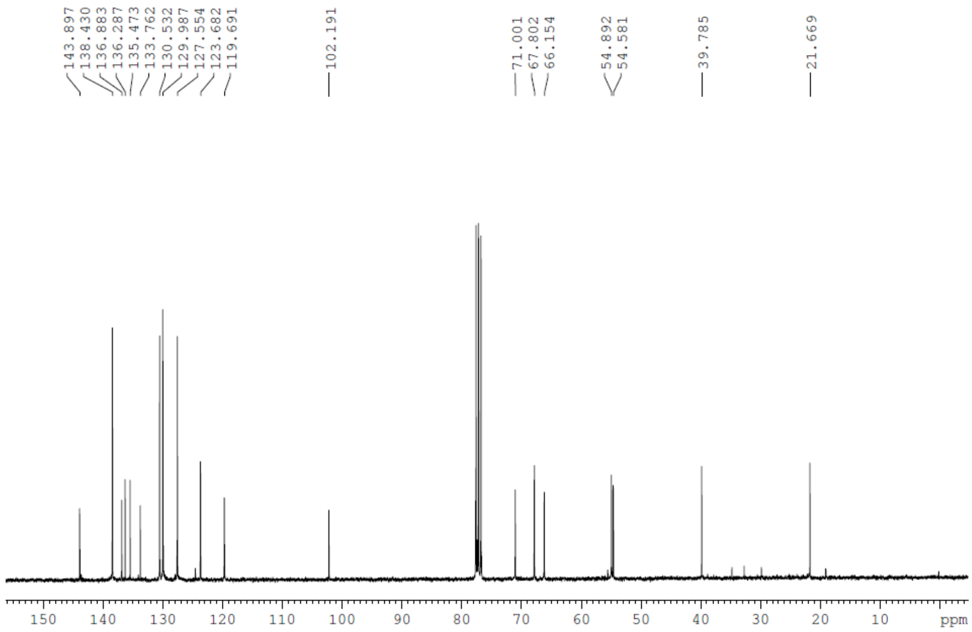
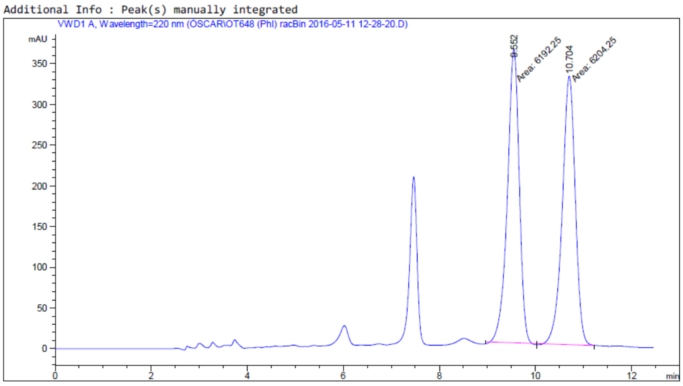
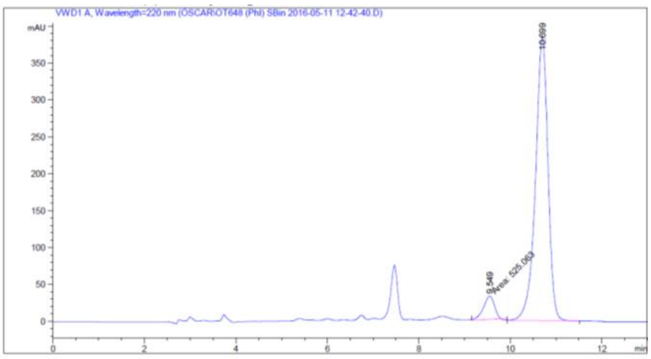


Figure S47: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4e** in $CDCl_3$.

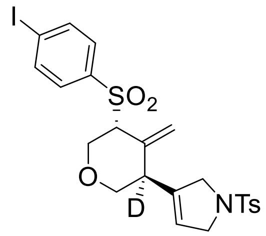
Figure S48: HPLC chromatograms with *rc*-BINAP and *(S)-(-)*-BINAP for **4e**.



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



4e-D

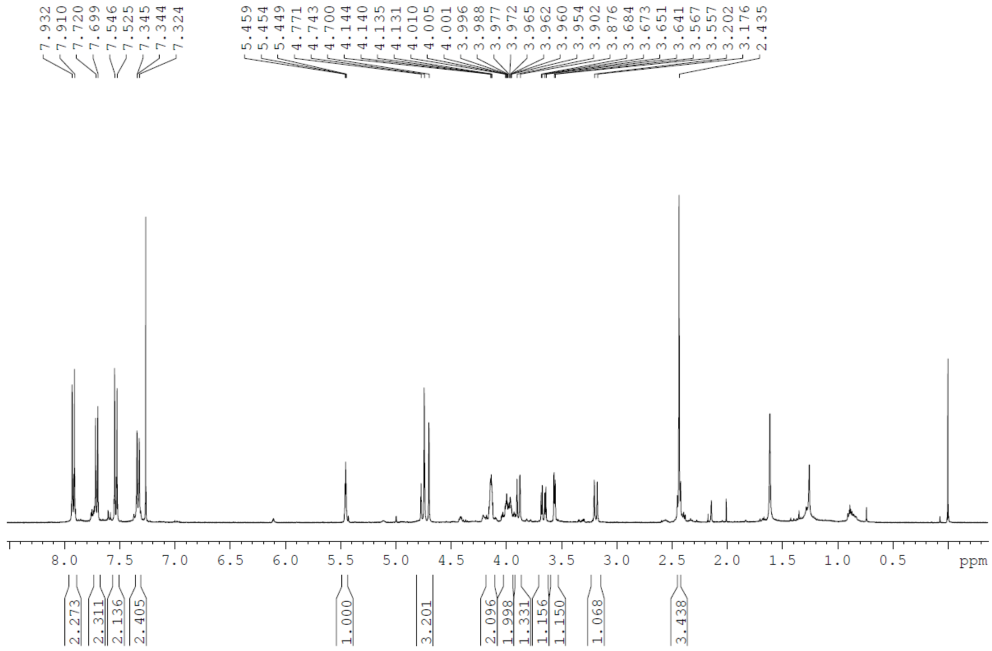


Figure S49: ^{1}H NMR spectrum (400 MHz) of **4e-D** in $CDCl_3$.

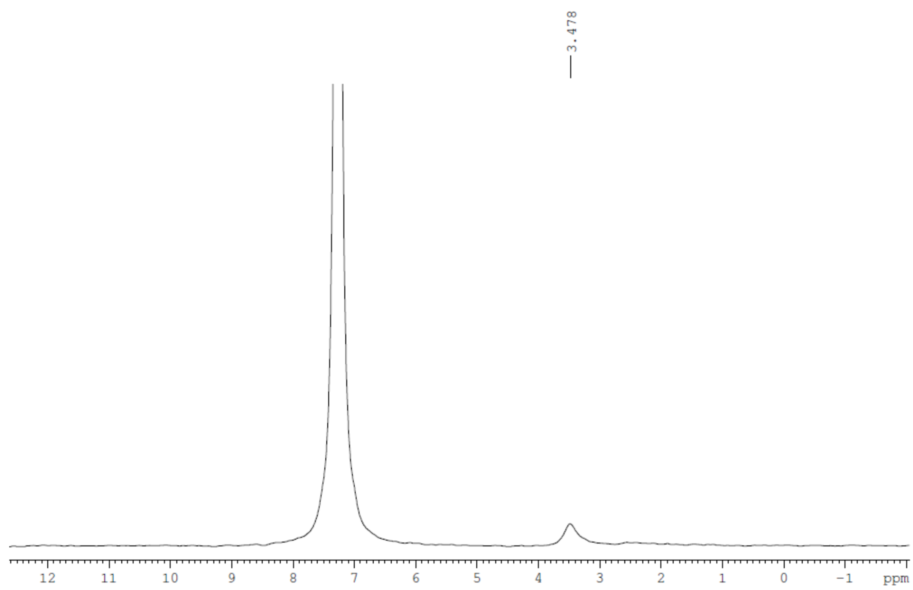


Figure S50: ^{2}H NMR spectrum (61 MHz) of **4e-D** in $CHCl_3$.

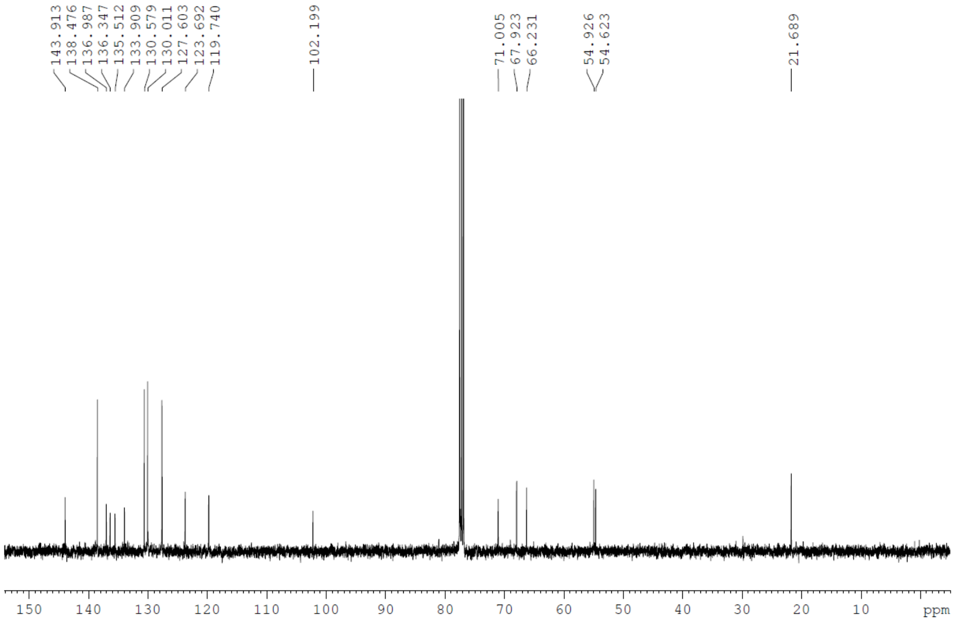


Figure S51: [1]H-decoupled[13]C NMR spectrum (100 MHz) of **4e-D** in $CDCl_3$.

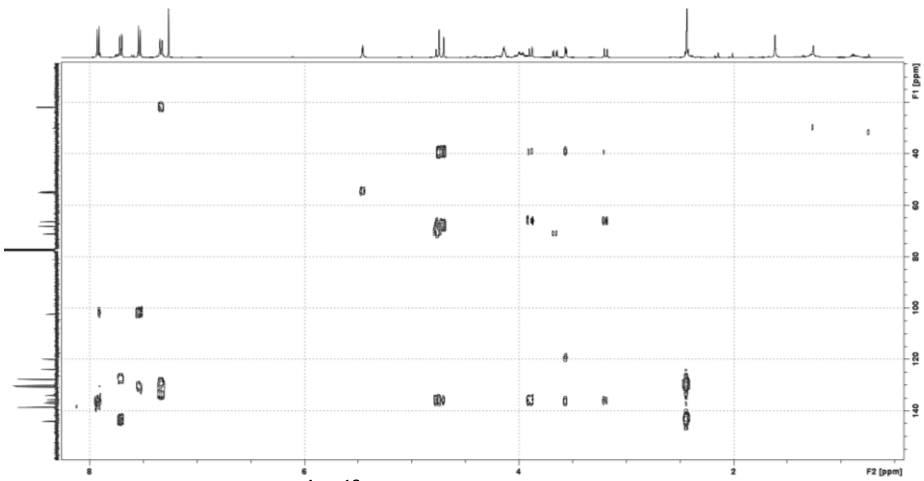
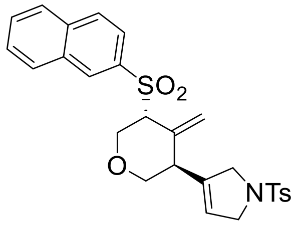
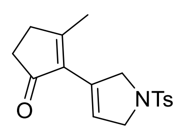


Figure S52: 2D [1]H-[13]C HMBC correlation of **4e-D** in $CDCl_3$.





4f **5**

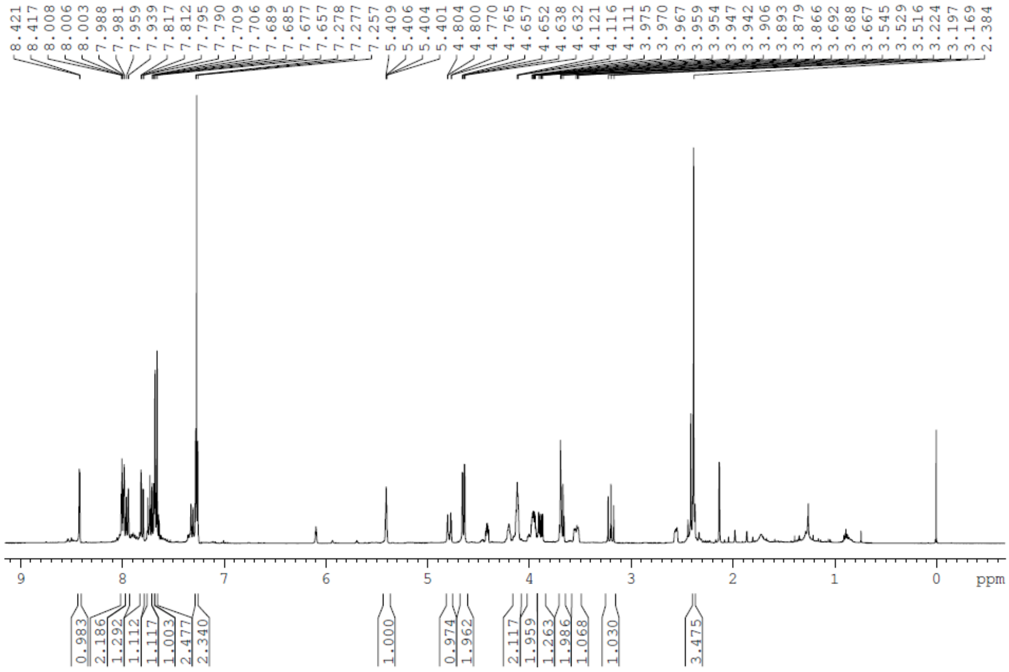


Figure S53: ^{1}H NMR spectrum (400 MHz) of **4f** and **5** in $CDCl_3$.

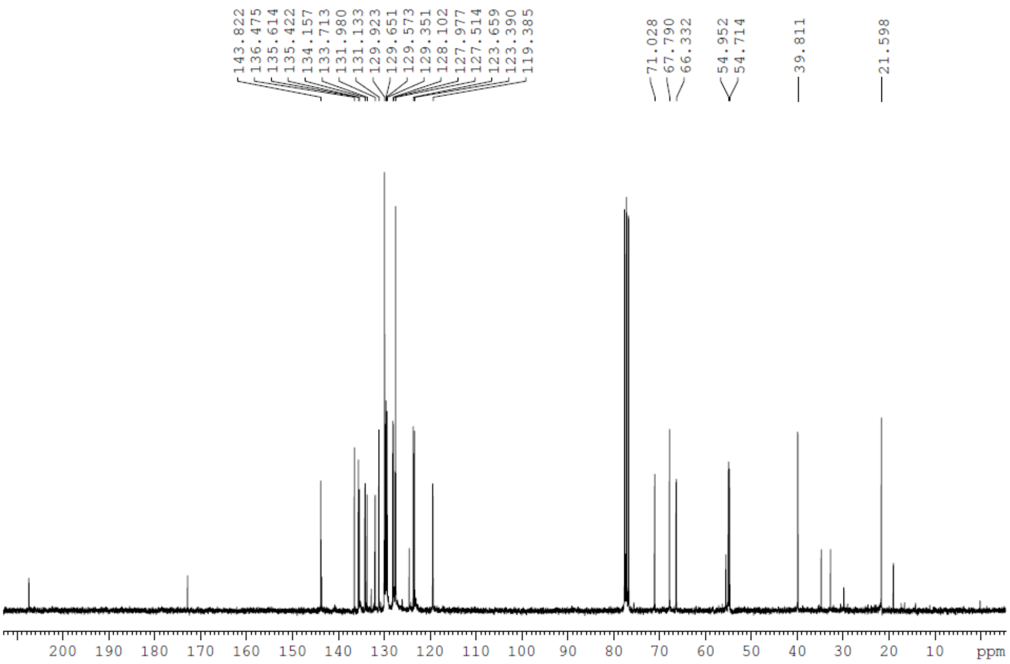
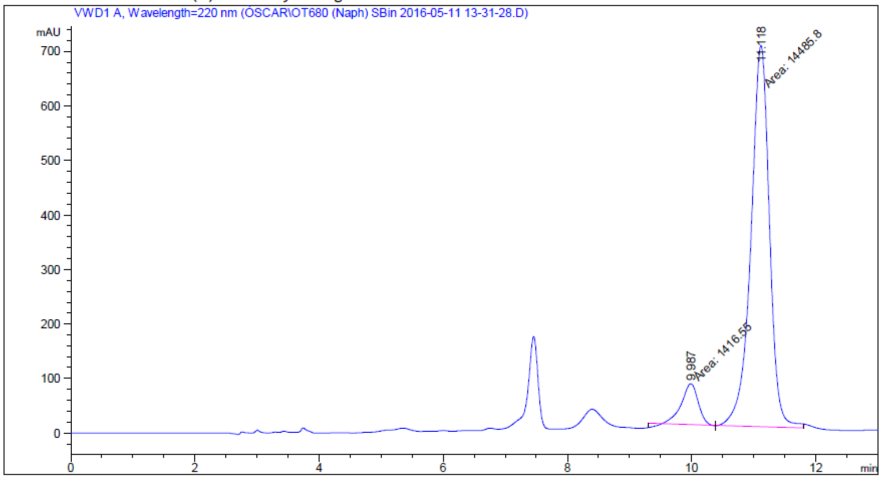
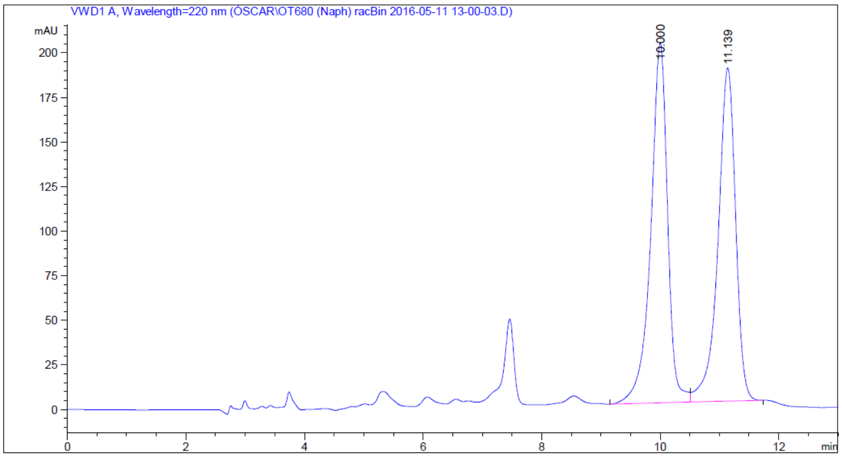


Figure S54: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4f** and **5** in $CDCl_3$.

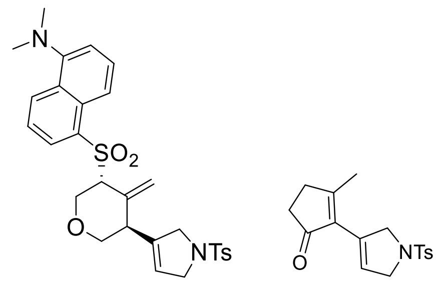
Figure S55: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4f** and **5**.



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



4g **5**

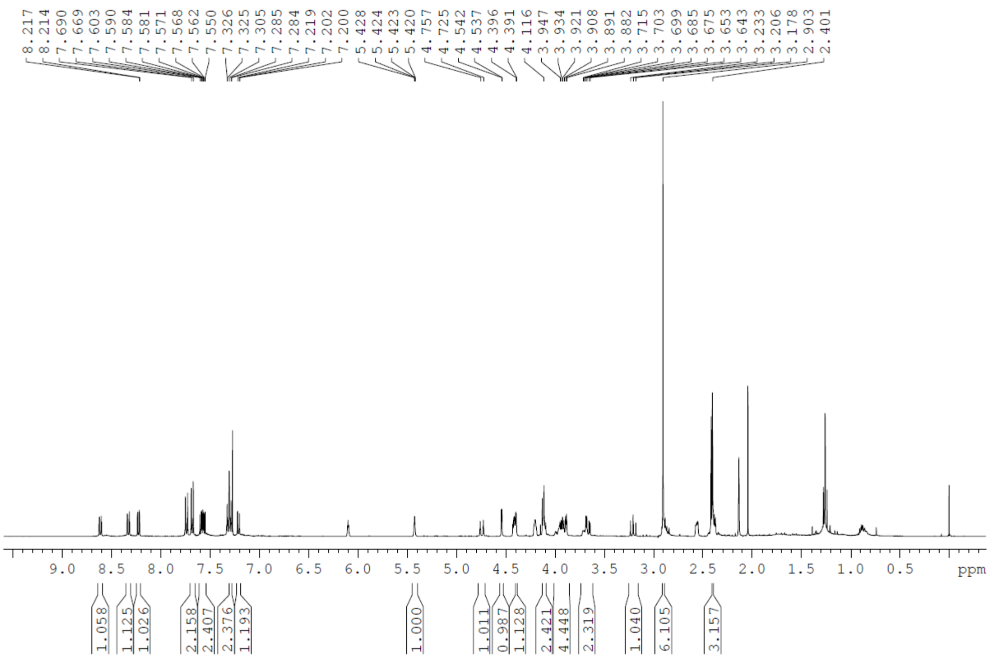


Figure S56: ^{1}H NMR spectrum (400 MHz) of **4g** and **5** in $CDCl_3$.

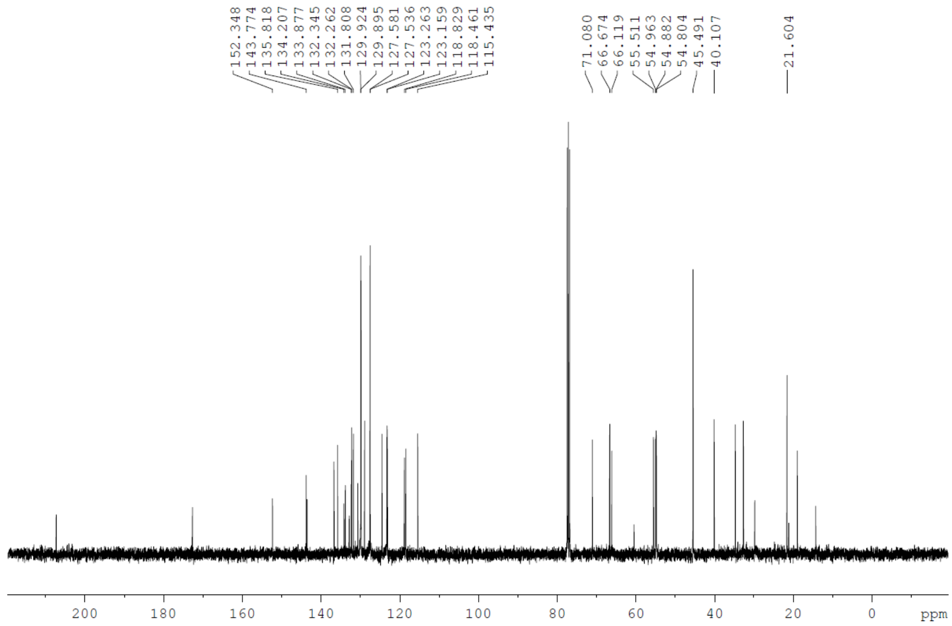
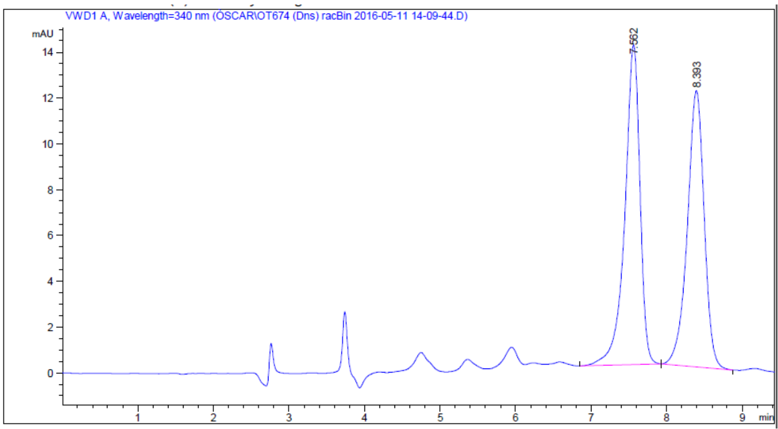
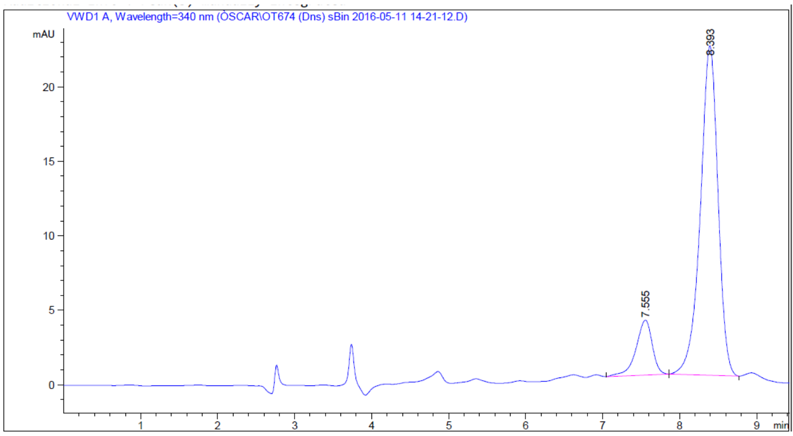


Figure S57: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4g** and **5** in $CDCl_3$.

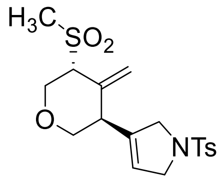
Figure S58: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4g** and **5**.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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 [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.555	BB	0.2245	53.87198	3.68561	13.2600
2	8.393	BB	0.2420	352.40271	22.10864	86.7400



4h

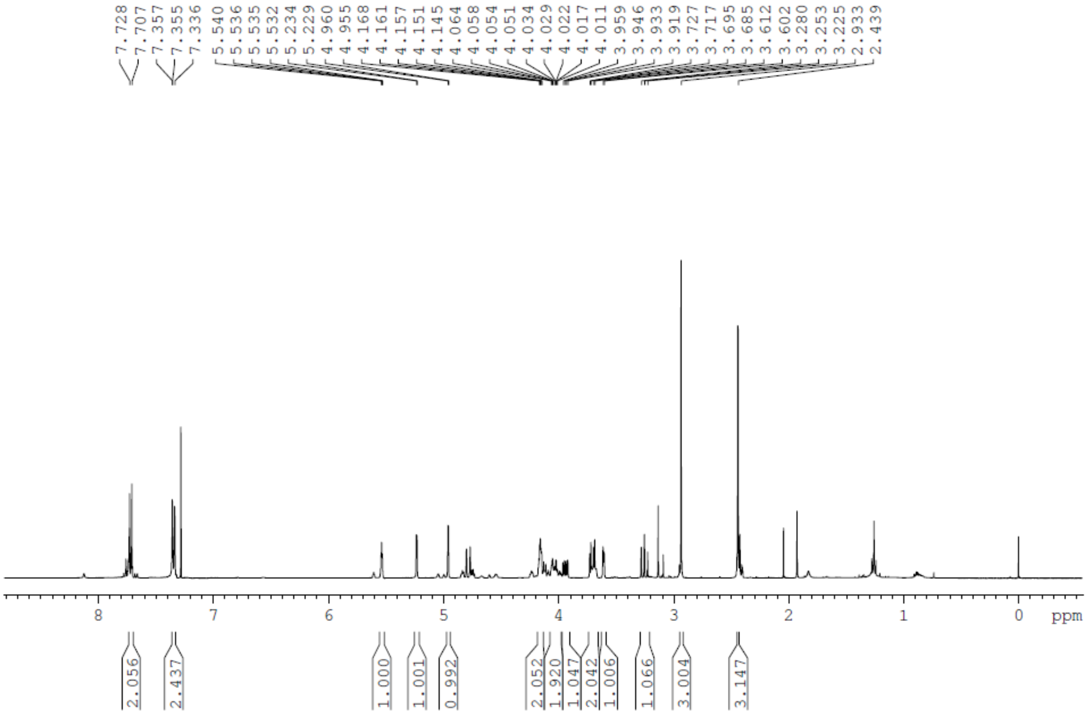


Figure S59: ^{1}H NMR spectrum (400 MHz) of **4h** in $CDCl_3$.

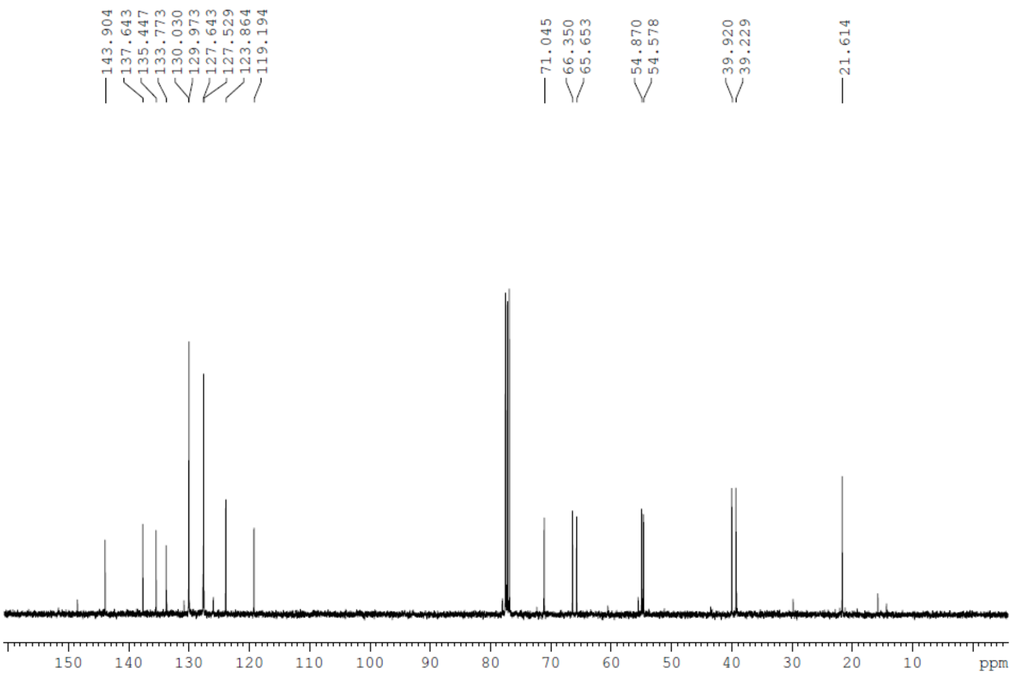
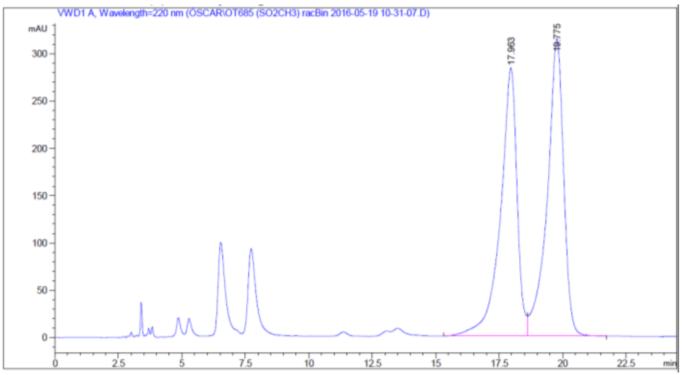
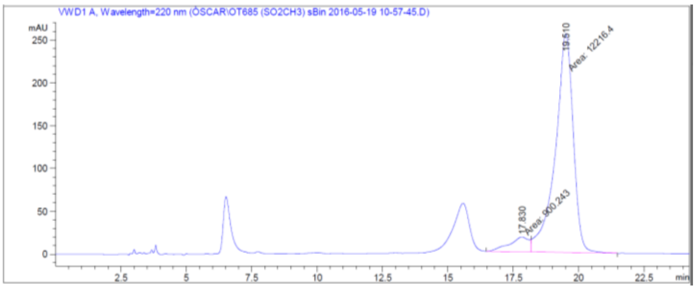


Figure S60: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4h** in $CDCl_3$.

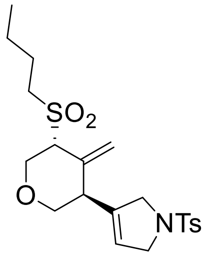
Figure S61: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4h**.



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



4i

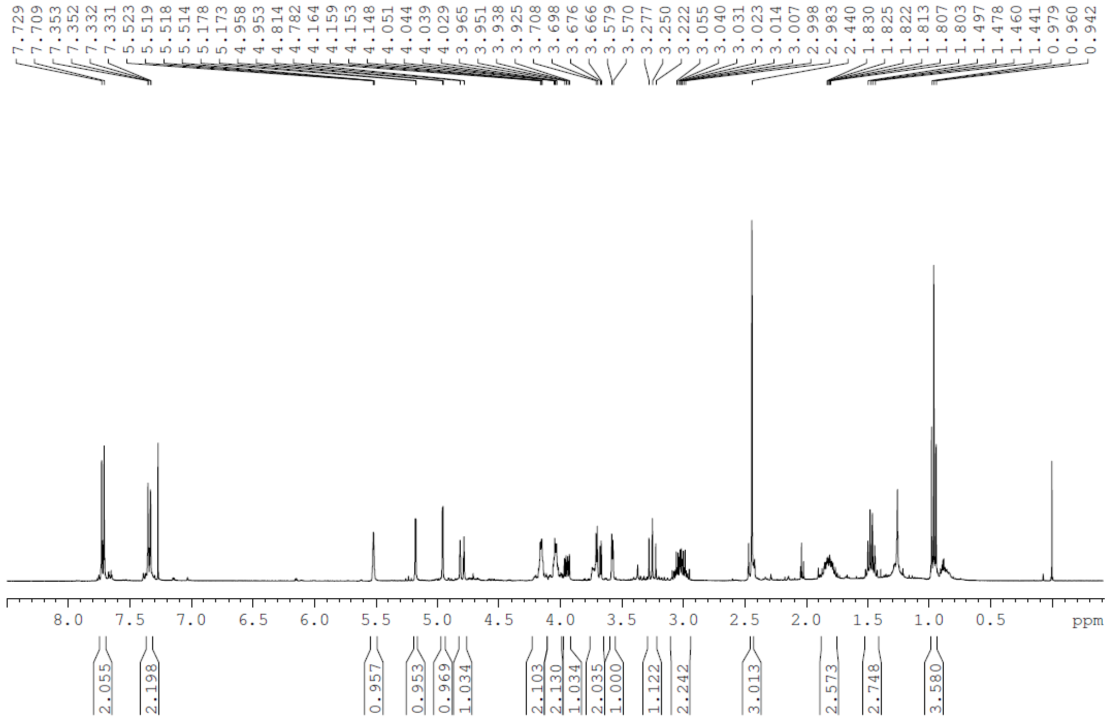


Figure S62: ^{1}H NMR spectrum (400 MHz) of **4i** in $CDCl_3$.

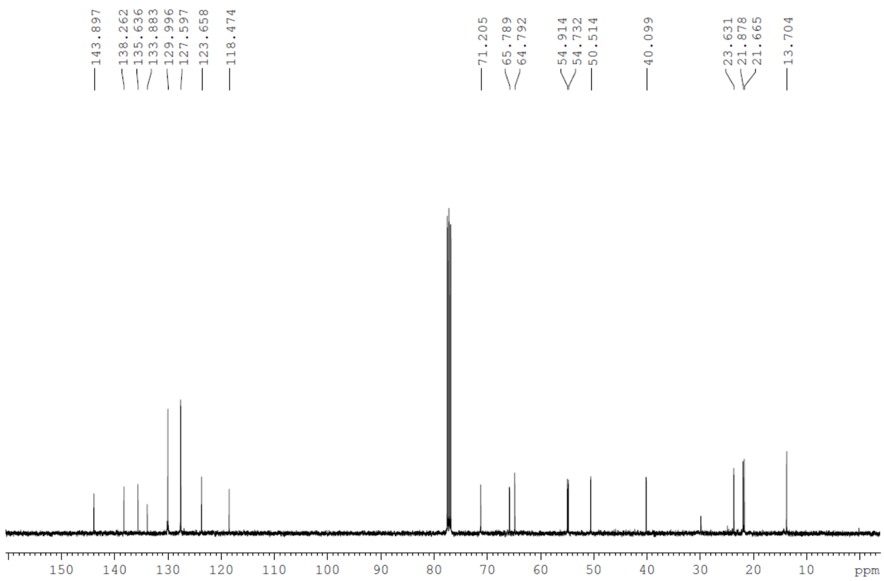
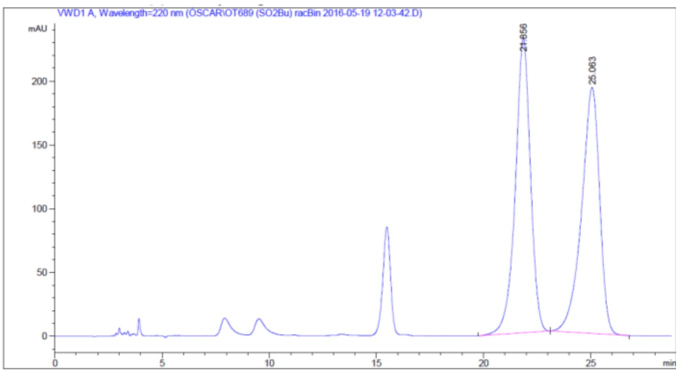
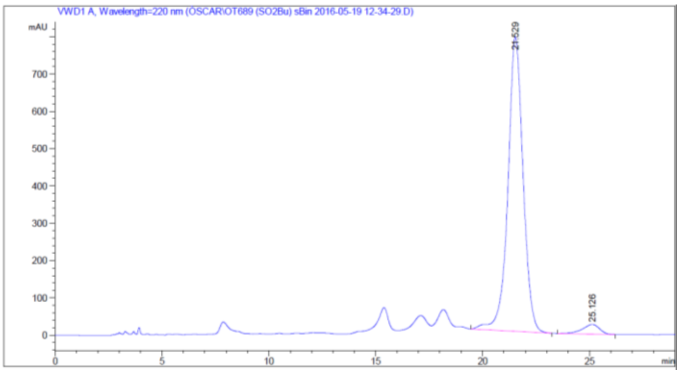


Figure S63: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4i** in $CDCl_3$.

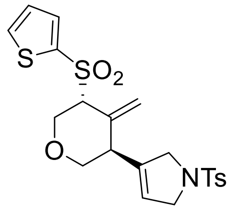
Figure S64: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4i**.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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 [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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



4j

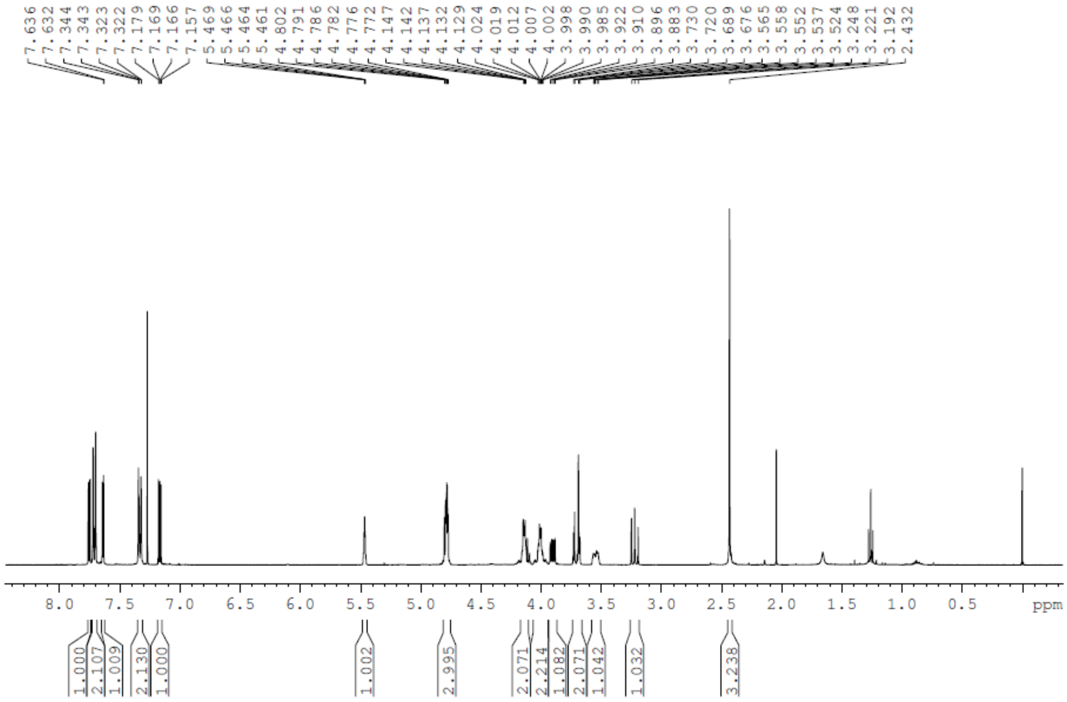


Figure S65: ^{1}H NMR spectrum (400 MHz) of **4j** in $CDCl_3$.

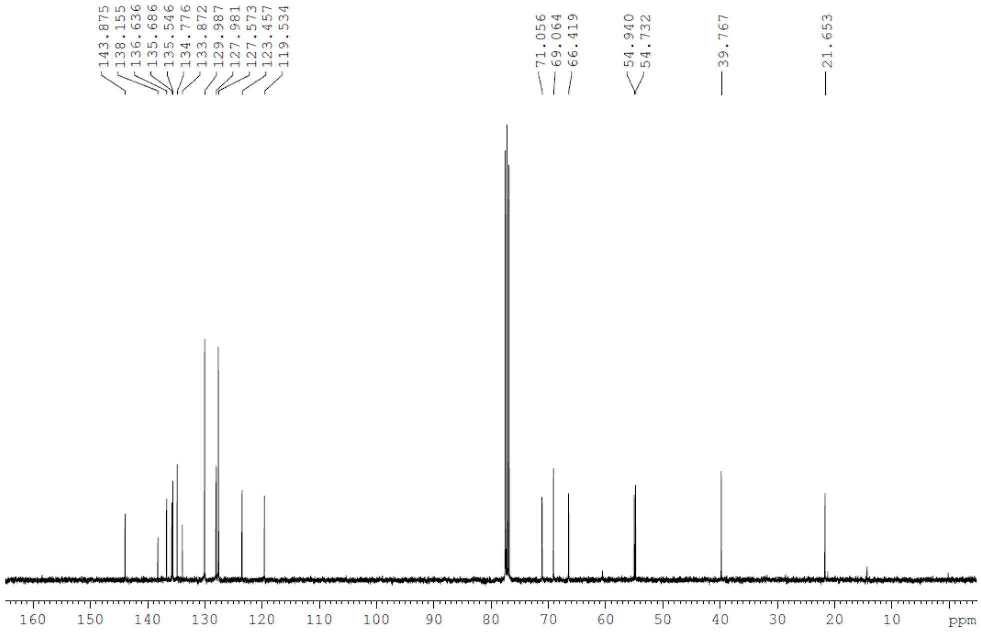
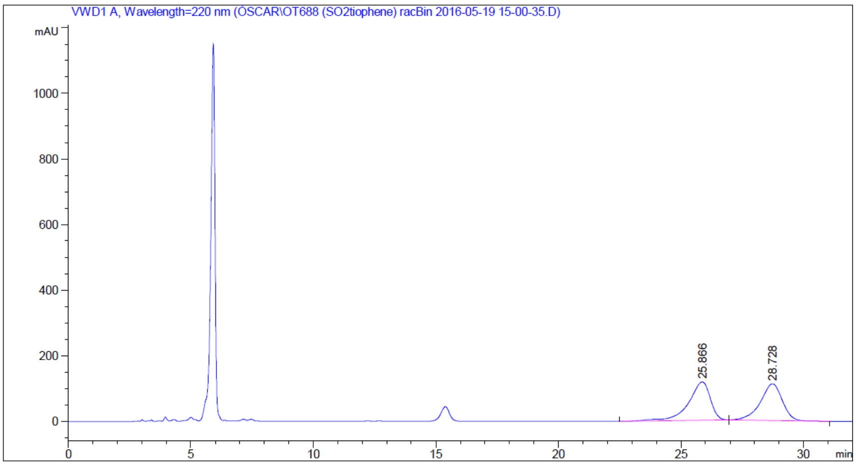
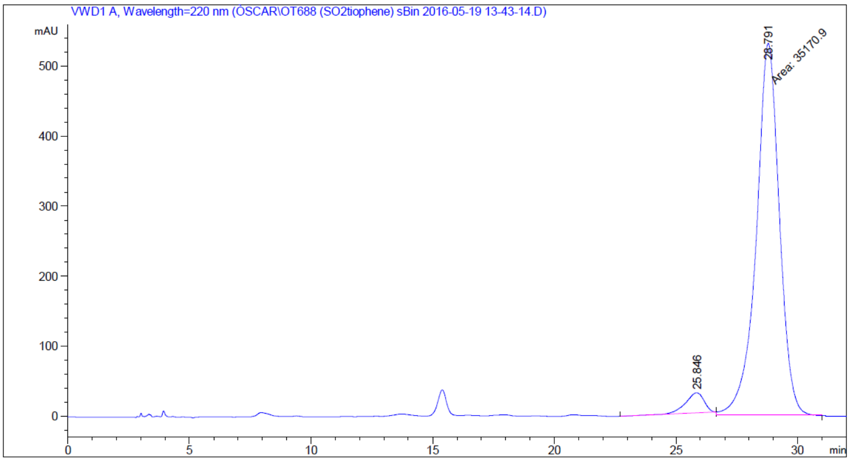


Figure S66: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4j** in $CDCl_3$.

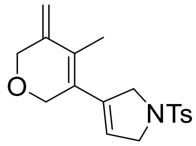
Figure S67: HPLC chromatograms with *rac*-BINAP and *(S)-(-)*-BINAP for **4j**.



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



6

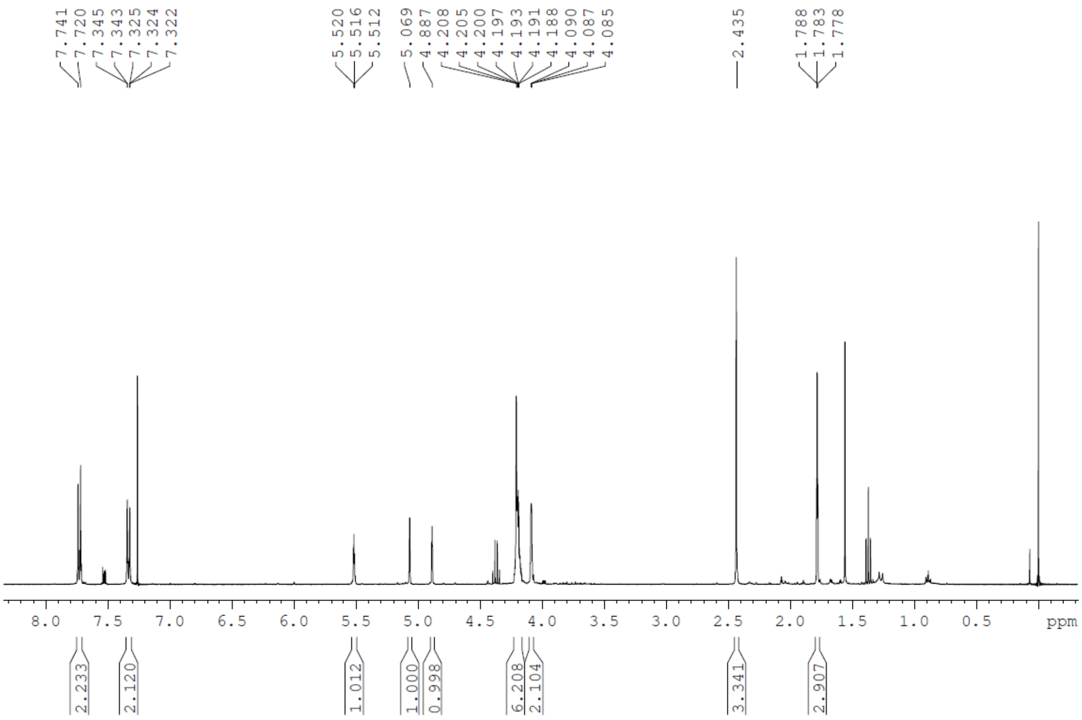


Figure S68: ^{1}H NMR spectrum (400 MHz) of **6** in $CDCl_3$.

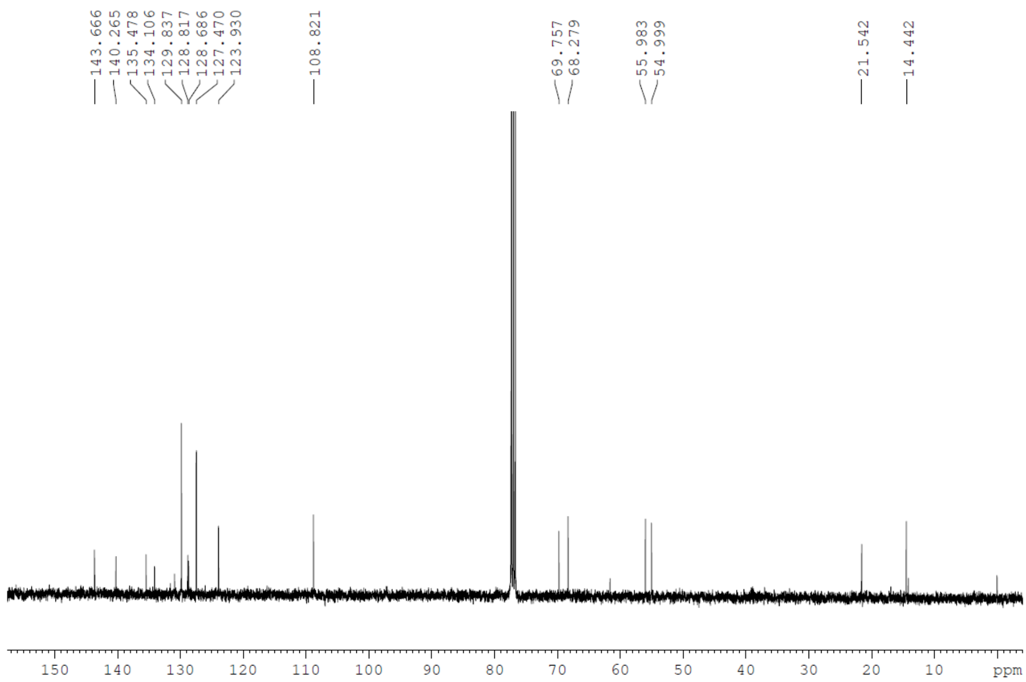


Figure S69: ^{1}H-decoupled^{13}C NMR spectrum (100 MHz) of **4h** in $CDCl_3$.

S.10. Crystallographic data for compounds 4a and 5

Colorless crystals of **4a** ($C_{24}H_{27}NO_5S_2$), 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[8]; data reduction, Saint+[9]; absorption correction, SADABS[10]. Structure solution and refinement was done using SHELXTL[11]. 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 **4a**.

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
	α = 90°
	b = 7.076(3) Å
	β = 91(10)°
	c = 15.851(8) Å
	γ = 90°
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 ° to 27.5 °
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

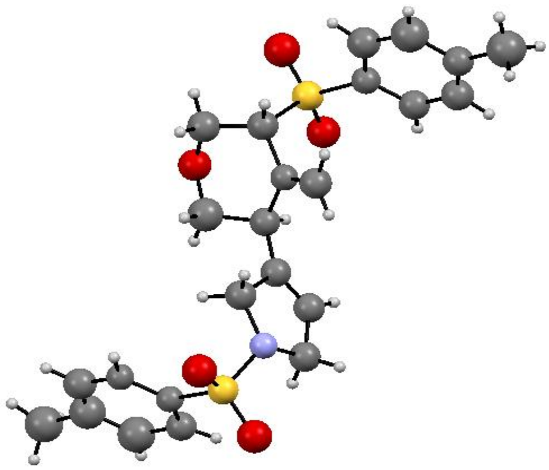
[8] Bruker Advanced X-ray Solutions. SMART: Version 5.631, 1997-2002.

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

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

[11] 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 **5** ($C_{17}H_{19}NO_3S$), 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[12]; data reduction, Saint+[13]; absorption correction, SADABS[14]. Structure solution and refinement was done using SHELXTL[15]. 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 **5**

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^o
	b = 8.677(10) Å

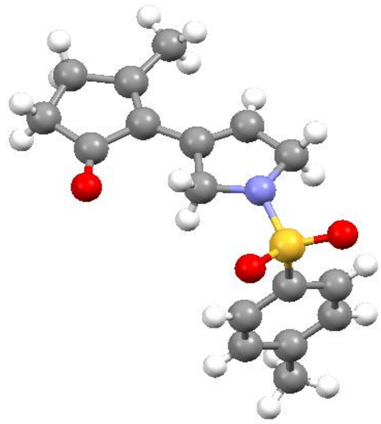
[12] Bruker Advanced X-ray Solutions. SMART: Version 5.631, 1997-2002.

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

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

[15] 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).

	β = 90(17)^{o}
	c = 12.496(14) Å
	γ = 68^{o}
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^{o} to 28.642^{o}
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}



S.11. Computational details

Computational details. All geometry optimizations have been performed using the hybrid DFT B3LYP[16] method with the Gaussian09[17] program package. These geometry optimizations were performed without symmetry constraints using the cc-pVDZ basis set for P, O, N, C, S, and H atoms[18] and the cc-pVDZ-PP basis set[19] containing an effective core relativistic pseudopotential for Rh. Analytical Hessians were computed to determine the nature of stationary points (one or zero imaginary frequencies for transition states and minima, respectively) and to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects using the standard statistical-mechanics relationships for an ideal gas.[20] These two latter terms were computed at 298.15 K and 1 atm to provide the reported relative Gibbs free energies (ΔG_{298}). Furthermore, the connectivity between stationary points was established by intrinsic reaction paths[21] calculations. All calculations were performed in dichloroethane solution using the Polarizable Continuum Method.[22] Single point energy calculations at the B3LYP/cc-pVDZ-PP geometries were carried out with the all-electron aug-cc-pVDZ basis set (for P, O, N, C, S, and H atoms[18]), and the aug-cc-pVDZ-PP basis set[19] containing an effective core relativistic pseudopotential for Rh. B3LYP/aug-cc-pVDZ-PP electronic energies were corrected with ZPEs, thermal energies, entropy effects, and solvent effects calculated at the B3LYP/cc-pVDZ-PP level. We also applied a concentration correction of 1.89 kcal/mol to the Gibbs energy values to account for the condition change from 1 atm to 1 M concentration when going from gas phase to solution.[23] Relative energies were computed taking into account the total number of molecules present. The Ar group of the Ts = SO_2-Ar moiety present in the experimental tether was substituted by a CH_3 to yield Ms = SO_2-CH_3 group in order to reduce the computational cost of the calculations. The migrating Ts group was included in the calculations without any simplification. The four Ph groups of the diphenylphosphino groups in the BINAP catalysts were substituted by methyl groups and the binaphthyl core by a biphenyl one.

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[16] a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; c) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623-11627.

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S.12. Optimized molecular structures of selected transition states

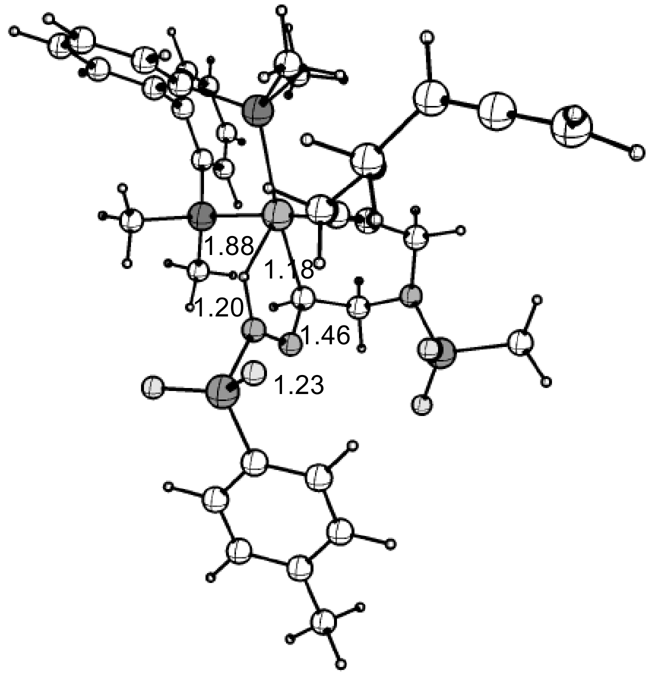


Figure S70. Optimized structure (B3LYP/cc-pVDZ) for **TS_BC.** Distances in Å.

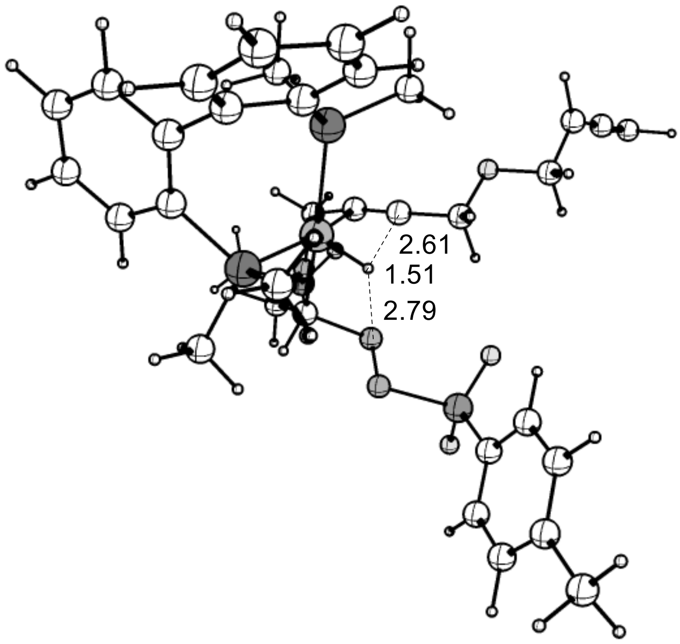


Figure S71. Optimized structure (B3LYP/cc-pVDZ) for **TS_CD.** Distances in Å.

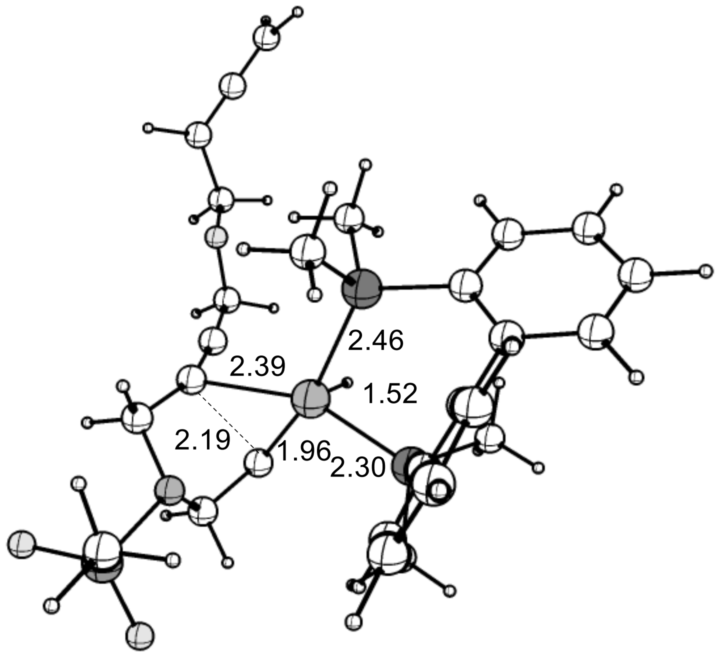


Figure S72. Optimized structure (B3LYP/cc-pVDZ) for **TS_DE.** Distances in Å.

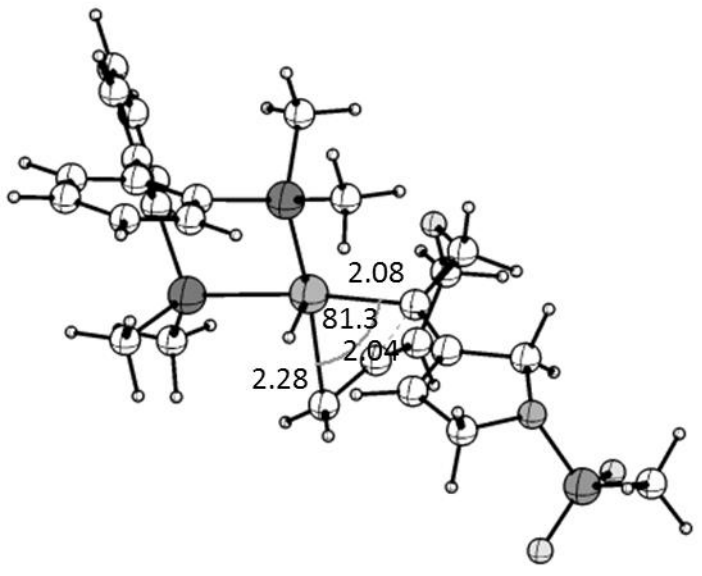


Figure S73. Optimized structure (B3LYP/cc-pVDZ) for **TS_EF.** Distances in Å and angles in degrees.

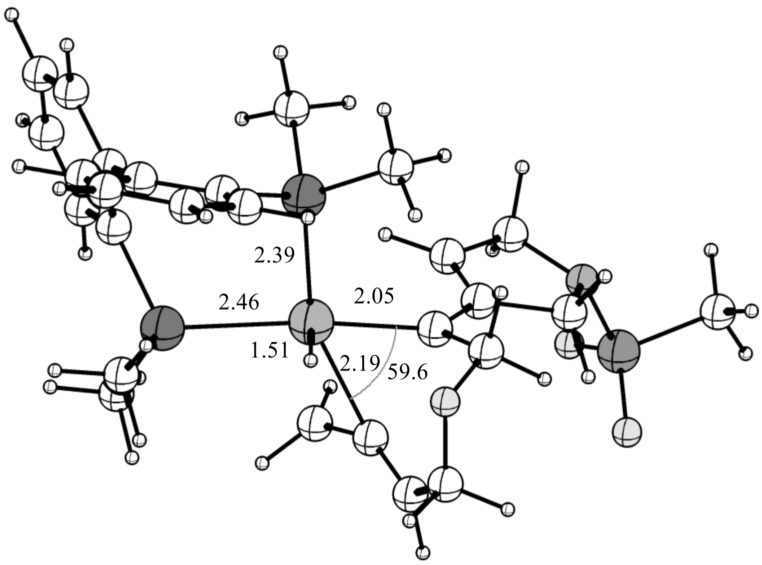


Figure S74. Optimized structure (B3LYP/cc-pVDZ) for **TS_E'F'.** Distances in Å and angles in degrees.

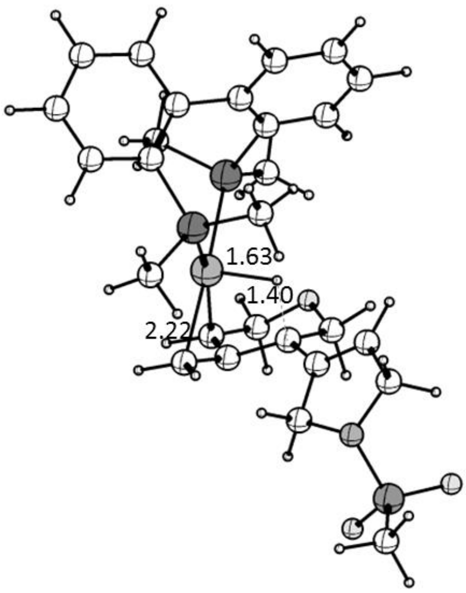


Figure S75. Optimized structure (B3LYP/cc-pVDZ) for **TS_FG.** Distances in Å.

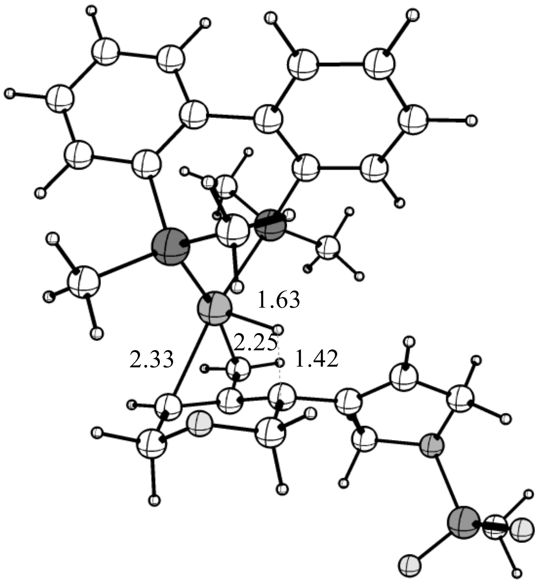


Figure S76. Optimized structure (B3LYP/cc-pVDZ) for **TS_F'G'.** Distances in Å.

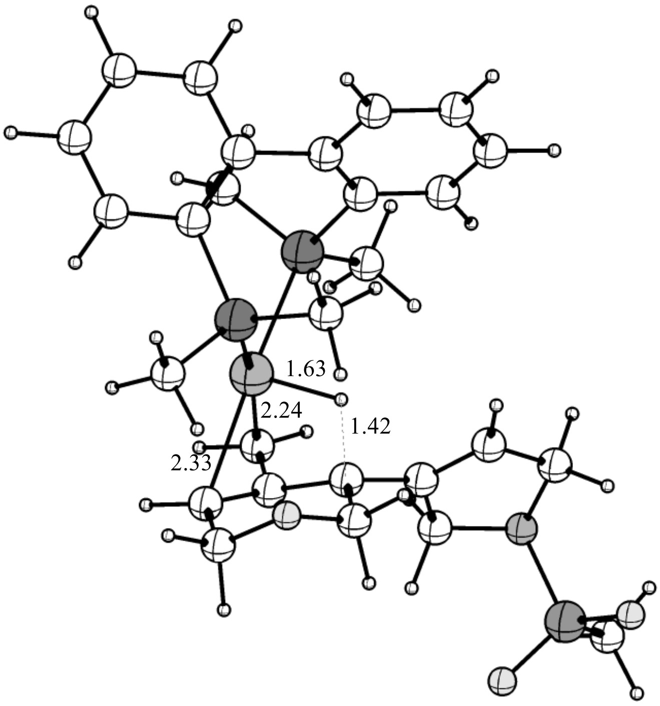


Figure S77. Optimized structure (B3LYP/cc-pVDZ) for **TS_G'H'.** Distances in Å.

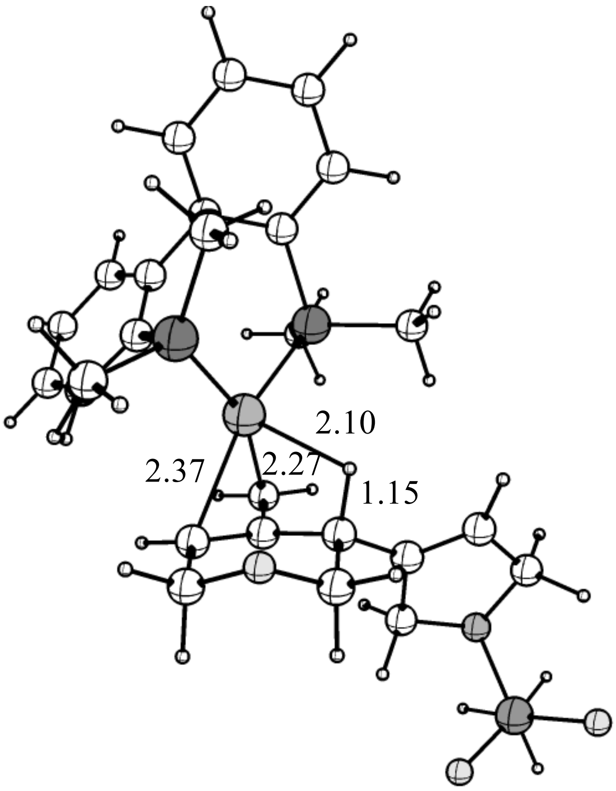


Figure S78. Optimized structure (B3LYP/cc-pVDZ) for **TS_H''I'.** Distances in Å.

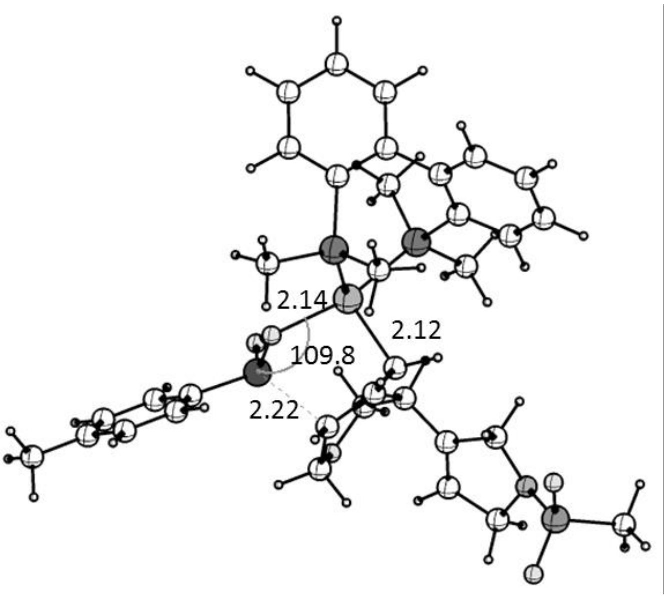


Figure S79. Optimized structure (B3LYP/cc-pVDZ) for **TS_HI.** Distances in Å.

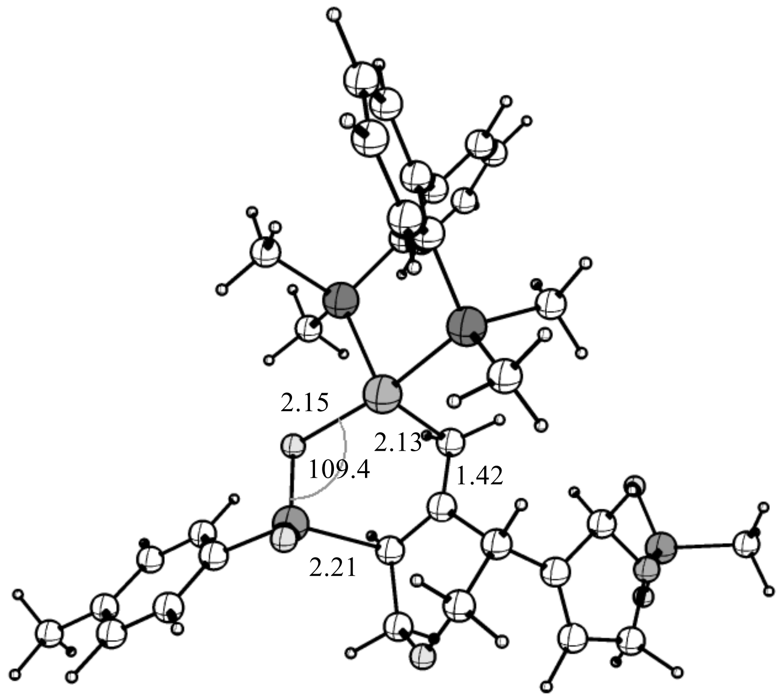


Figure S80. Optimized structure (B3LYP/cc-pVDZ) for **TS_J'K.** Distances in Å and angles in degrees.

S.13. Cartesian coordinates of all optimized molecular structures

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)= -3450.9813 **G(au)=** -3450.3587

45	0.970030000	-0.272970000	0.268460000
15	2.087170000	-2.324910000	-0.165330000
15	2.942340000	0.749420000	0.678880000
6	3.698910000	-2.664930000	0.691470000
6	4.875870000	-1.921360000	0.418820000
6	3.739420000	-3.655800000	1.688950000
6	6.047770000	-2.222830000	1.135330000
6	4.909350000	-3.927420000	2.403030000
1	2.847650000	-4.237060000	1.920460000
6	6.072040000	-3.210300000	2.121460000
1	6.953590000	-1.652570000	0.920010000
1	4.906320000	-4.702980000	3.171430000
1	6.995820000	-3.413290000	2.666800000
6	4.239430000	0.365150000	-0.593790000
6	4.437530000	1.303240000	-1.624280000
6	4.973560000	-0.847530000	-0.623290000
6	5.344530000	1.072000000	-2.660150000
1	3.878260000	2.238760000	-1.627850000
6	5.894800000	-1.054180000	-1.667190000
6	6.081710000	-0.112670000	-2.679730000
1	5.473630000	1.820770000	-3.444100000
1	6.463500000	-1.985970000	-1.685280000
1	6.797850000	-0.308080000	-3.480260000
6	1.059550000	-3.817130000	0.195310000
1	0.748870000	-3.838080000	1.248730000
1	1.607260000	-4.738310000	-0.051700000
1	0.157870000	-3.745820000	-0.427660000
6	2.433480000	-2.549740000	-1.970630000
1	1.469890000	-2.548430000	-2.501670000
1	2.944140000	-3.509720000	-2.140140000
1	3.052110000	-1.728730000	-2.353100000
6	3.656450000	0.359100000	2.342060000
1	3.008130000	0.845530000	3.086390000
1	4.673910000	0.771090000	2.420810000
1	3.676110000	-0.718350000	2.537320000
6	2.934100000	2.593120000	0.773380000
1	3.955190000	2.960100000	0.953940000
1	2.288140000	2.878690000	1.615430000
1	2.535440000	3.055060000	-0.137100000
6	-1.093740000	1.394380000	2.263680000
1	-0.542460000	0.873150000	3.063330000
1	-1.192090000	2.448040000	2.561090000
6	-2.755090000	-0.562600000	1.863410000
1	-3.005300000	-1.105670000	2.792330000
7	-2.465320000	0.864950000	2.135920000
16	-3.760230000	1.851550000	2.589500000
8	-4.981270000	1.262410000	1.980310000
8	-3.367590000	3.255220000	2.311120000
6	-1.518150000	-1.193650000	1.288620000
1	-0.749360000	-1.466820000	2.018760000
1	-3.611530000	-0.627000000	1.186860000
7	-1.110190000	-1.354040000	0.074010000
7	-1.808720000	-1.268520000	-1.086120000
16	-3.121420000	-0.194420000	-1.656990000
8	-3.235420000	1.002080000	-0.797350000
8	-2.738990000	-0.094370000	-3.089640000
6	-4.609510000	-1.178000000	-1.508010000

6	-4.770880000	-2.293690000	-2.340040000
6	-5.606800000	-0.768390000	-0.620440000
6	-5.954290000	-3.020640000	-2.256210000
6	-6.787100000	-1.515700000	-0.558620000
6	-6.981200000	-2.645330000	-1.367170000
1	-3.988950000	-2.582690000	-3.042900000
1	-5.467650000	0.110850000	0.010990000
1	-6.090360000	-3.893730000	-2.898590000
1	-7.574060000	-1.205750000	0.132430000
6	-8.259060000	-3.441960000	-1.304440000
1	-8.791130000	-3.402040000	-2.269450000
1	-8.051810000	-4.504280000	-1.096520000
1	-8.935180000	-3.062540000	-0.525720000
1	-1.166320000	-1.316100000	-1.879710000
6	-0.334680000	1.342800000	0.983470000
6	-0.044860000	1.575400000	-0.214110000
6	-3.924110000	1.672510000	4.380300000
1	-3.003040000	2.035050000	4.853790000
1	-4.782330000	2.290000000	4.678140000
1	-4.108930000	0.615990000	4.612690000
6	-0.083260000	2.277940000	-1.526880000
1	0.943160000	2.490100000	-1.878960000
1	-0.547700000	1.616980000	-2.273300000
6	-0.249730000	4.605780000	-0.947360000
1	0.239390000	4.381490000	0.016340000
1	-1.077580000	5.305140000	-0.751650000
6	0.726500000	5.236740000	-1.917190000
1	0.341200000	5.428570000	-2.926960000
6	1.954130000	5.595910000	-1.618200000
6	3.172770000	5.971520000	-1.311190000
1	4.028660000	5.303860000	-1.453570000
1	3.374160000	6.968990000	-0.906880000
8	-0.882880000	3.448480000	-1.495410000

TS_BC (nimag=1) (-582.44i) E**(au)=** -3450.9439 **G(au)=** -3450.3308

45	0.936370000	-0.181040000	0.539510000
15	2.221450000	-2.039390000	-0.172030000
15	2.903850000	1.196440000	0.275840000
6	3.889760000	-2.127320000	0.644530000
6	5.000320000	-1.342870000	0.245610000
6	4.023300000	-2.967600000	1.766400000
6	6.207900000	-1.466000000	0.957580000
6	5.223840000	-3.059900000	2.473250000
1	3.180260000	-3.570690000	2.102960000
6	6.326690000	-2.310390000	2.061510000
1	7.064350000	-0.867650000	0.640530000
1	5.292940000	-3.722550000	3.338150000
1	7.275100000	-2.376560000	2.598240000
6	4.164510000	0.741040000	-1.015140000
6	4.252360000	1.542040000	-2.169460000
6	4.990270000	-0.408070000	-0.924500000
6	5.135660000	1.239220000	-3.207950000
1	3.625810000	2.427280000	-2.270940000
6	5.888430000	-0.685500000	-1.971110000
6	5.964330000	0.121440000	-3.106600000
1	5.175550000	1.883400000	-4.088550000
1	6.525990000	-1.568340000	-1.892160000
1	6.664100000	-0.126600000	-3.907070000
6	1.540680000	-3.739540000	0.110440000
1	1.266750000	-3.907410000	1.160360000
1	2.278520000	-4.494540000	-0.198370000
1	0.639140000	-3.850760000	-0.509970000
6	2.487260000	-2.123630000	-2.003270000
1	1.508180000	-2.347640000	-2.454300000
1	3.196330000	-2.927480000	-2.250270000
1	2.849810000	-1.171050000	-2.404300000
6	3.799880000	1.198510000	1.901130000
1	3.151140000	1.721310000	2.620760000
1	4.756330000	1.735460000	1.815750000
1	3.977610000	0.178600000	2.261580000
6	2.701000000	3.019620000	0.036880000
1	3.678260000	3.518940000	0.111660000
1	2.030750000	3.394100000	0.821990000
1	2.243640000	3.255920000	-0.931190000
6	-0.877030000	0.955180000	2.984180000
1	-0.073660000	0.679360000	3.683960000

1	-1.335900000	1.875440000	3.375070000
6	-1.365790000	-1.432110000	2.490130000
1	-0.573210000	-1.758160000	3.182870000
7	-1.858770000	-0.140610000	3.010290000
16	-3.477300000	0.274570000	2.587280000
8	-4.223990000	-1.007210000	2.496400000
8	-3.530170000	1.223830000	1.436930000
6	-0.768900000	-1.430210000	1.075180000
1	-0.422700000	-2.464460000	0.905550000
1	-2.197270000	-2.145630000	2.572590000
7	-1.821290000	-1.325230000	0.071460000
7	-1.401610000	-0.855570000	-0.987230000
16	-2.583270000	-0.676930000	-2.456170000
8	-2.795390000	0.786890000	-2.490630000
8	-1.870400000	-1.380270000	-3.542780000
6	-4.045540000	-1.542900000	-1.953110000
6	-4.302960000	-2.795830000	-2.518760000
6	-4.904180000	-0.951060000	-1.016290000
6	-5.468600000	-3.462770000	-2.143120000
6	-6.051940000	-1.646900000	-0.651440000
6	-6.357690000	-2.903440000	-1.209370000
1	-3.612980000	-3.228050000	-3.243290000
1	-4.663940000	0.009620000	-0.560270000
1	-5.690570000	-4.436610000	-2.584320000
1	-6.722240000	-1.209140000	0.091020000
6	-7.617360000	-3.624280000	-0.806500000
1	-7.658870000	-4.637320000	-1.229790000
1	-7.693370000	-3.699810000	0.290010000
1	-8.507250000	-3.072000000	-1.152350000
1	-0.262410000	-0.482260000	-0.871580000
6	-0.332080000	1.230610000	1.634320000
6	-0.257090000	1.690420000	0.478240000
6	-4.028750000	1.150960000	4.063640000
1	-3.427920000	2.057330000	4.204050000
1	-5.075910000	1.417160000	3.867980000
1	-3.941630000	0.466010000	4.914700000
6	-0.527390000	2.607720000	-0.646420000
1	0.211600000	2.475250000	-1.458960000
1	-1.515960000	2.343750000	-1.071800000
6	-0.902120000	4.880920000	-1.166580000
1	-0.251740000	4.752060000	-2.055810000
1	-1.946500000	4.706710000	-1.483700000
6	-0.736620000	6.268540000	-0.609240000
1	0.267250000	6.542780000	-0.262100000
6	-1.709990000	7.147260000	-0.538500000
6	-2.683500000	8.022750000	-0.481640000
1	-3.320810000	8.106500000	0.404660000
1	-2.889750000	8.699520000	-1.317230000
8	-0.517810000	3.941890000	-0.158020000

C (nimag=0) **E(au)=** -3450.9700 **G(au)=** -3450.3524

45	1.103060000	-0.277240000	0.312080000
15	2.234230000	-2.092540000	-0.617310000
15	3.140320000	1.066570000	0.158190000
6	3.833650000	-2.334670000	0.290880000
6	5.016100000	-1.603580000	0.014200000
6	3.839030000	-3.266700000	1.346700000
6	6.166330000	-1.868050000	0.779600000
6	4.985750000	-3.497750000	2.108520000
1	2.940020000	-3.836200000	1.581210000
6	6.158850000	-2.799790000	1.818040000
1	7.079950000	-1.313370000	0.557480000
1	4.958990000	-4.228660000	2.918720000
1	7.066660000	-2.975320000	2.398340000
6	4.401960000	0.618540000	-1.125630000
6	4.601130000	1.492520000	-2.210510000
6	5.139020000	-0.591510000	-1.081870000
6	5.512440000	1.197590000	-3.227280000
1	4.044500000	2.426160000	-2.275810000
6	6.068180000	-0.859820000	-2.102270000
6	6.255320000	0.018370000	-3.170480000
1	5.641090000	1.896460000	-4.055930000
1	6.638310000	-1.789880000	-2.060170000
1	6.975070000	-0.222800000	-3.955000000
6	1.437890000	-3.756400000	-0.551720000
1	1.100740000	-4.021850000	0.457840000

1	2.158940000	-4.506680000	-0.908100000
1	0.567650000	-3.744740000	-1.222400000
6	2.562580000	-1.952800000	-2.426080000
1	1.590580000	-2.073010000	-2.927440000
1	3.242870000	-2.754450000	-2.747540000
1	2.980600000	-0.976090000	-2.689470000
6	4.019450000	1.032280000	1.787130000
1	3.349780000	1.491810000	2.530200000
1	4.952630000	1.611760000	1.729780000
1	4.241520000	0.003180000	2.094910000
6	2.890620000	2.877330000	-0.081600000
1	3.856920000	3.401070000	-0.039650000
1	2.236270000	3.246000000	0.718620000
1	2.399310000	3.083900000	-1.040760000
6	-0.264140000	0.562950000	3.030640000
1	0.652830000	0.139990000	3.469170000
1	-0.606090000	1.357590000	3.708760000
6	-0.963380000	-1.672970000	2.130800000
1	-0.079360000	-2.158870000	2.578930000
7	-1.269640000	-0.497840000	2.959760000
16	-2.910760000	0.006140000	3.088940000
8	-3.743390000	-0.980730000	2.350550000
8	-3.001220000	1.456570000	2.785890000
6	-0.690930000	-1.457770000	0.624980000
1	-0.582770000	-2.449010000	0.162970000
1	-1.802540000	-2.373280000	2.250990000
7	-1.758250000	-0.735450000	-0.003160000
7	-2.135900000	-1.178880000	-1.092600000
16	-3.399220000	-0.040510000	-1.827250000
8	-3.554650000	1.178800000	-0.982030000
8	-2.985080000	0.084530000	-3.253730000
6	-4.884900000	-1.040810000	-1.720880000
6	-5.395400000	-1.615820000	-2.885210000
6	-5.504470000	-1.218300000	-0.476730000
6	-6.560400000	-2.382930000	-2.801020000
6	-6.661050000	-1.992860000	-0.418170000
6	-7.210140000	-2.582700000	-1.573140000
1	-4.890410000	-1.456450000	-3.838220000
1	-5.078060000	-0.784220000	0.429090000
1	-6.971010000	-2.832440000	-3.708090000
1	-7.151600000	-2.143860000	0.546750000
6	-8.468660000	-3.408240000	-1.479760000
1	-8.749440000	-3.831190000	-2.454590000
1	-8.343440000	-4.239410000	-0.766500000
1	-9.311930000	-2.798100000	-1.115680000
1	0.699390000	0.014620000	-1.115400000
6	0.001220000	1.176080000	1.708520000
6	-0.114890000	1.762540000	0.631530000
6	-3.235280000	-0.220660000	4.848370000
1	-2.544000000	0.411340000	5.419600000
1	-4.274660000	0.094060000	5.012660000
1	-3.100110000	-1.282930000	5.084430000
6	-0.506860000	2.673410000	-0.457550000
1	0.031910000	2.438550000	-1.394370000
1	-1.584870000	2.498520000	-0.647130000
6	-0.790040000	4.964770000	-0.951900000
1	-0.380530000	4.772930000	-1.964140000
1	-1.889600000	4.873900000	-1.006980000
6	-0.387750000	6.337070000	-0.486400000
1	0.688050000	6.539330000	-0.416020000
6	-1.247050000	7.282620000	-0.182240000
6	-2.110080000	8.224820000	0.108090000
1	-2.488720000	8.352730000	1.127350000
1	-2.479800000	8.913740000	-0.658290000
8	-0.253160000	4.003950000	-0.034150000

TS_CD (nimag=1) (-56.72i) E**(au)=** -3450.9494 **G(au)=** -3450.3337

45	0.915250000	-0.334370000	-0.181850000
15	2.129750000	1.087970000	-1.561020000
15	2.469560000	0.149920000	1.682520000
6	3.882290000	0.492210000	-1.504030000
6	4.805470000	0.851550000	-0.490290000
6	4.275100000	-0.434250000	-2.490060000
6	6.096470000	0.293600000	-0.528870000
6	5.555530000	-0.989460000	-2.498340000
1	3.580020000	-0.727430000	-3.276750000

6	6.473510000	-0.619320000	-1.514440000
1	6.811530000	0.579350000	0.244840000
1	5.831550000	-1.701970000	-3.277740000
1	7.481140000	-1.039210000	-1.510180000
6	3.553060000	1.656930000	1.613030000
6	3.389280000	2.663780000	2.582190000
6	4.521590000	1.845120000	0.594240000
6	4.160280000	3.828820000	2.563580000
1	2.653330000	2.549600000	3.376230000
6	5.301660000	3.014730000	0.604290000
6	5.125340000	4.004350000	1.572250000
1	4.005590000	4.590480000	3.330180000
1	6.049400000	3.152130000	-0.179250000
1	5.738740000	4.907010000	1.547110000
6	1.719700000	1.131440000	-3.359450000
1	1.678960000	0.131400000	-3.807570000
1	2.475620000	1.736780000	-3.880790000
1	0.735790000	1.607780000	-3.473720000
6	2.040880000	2.883280000	-1.155810000
1	1.038140000	3.218440000	-1.460910000
1	2.800790000	3.433580000	-1.729010000
1	2.169620000	3.069160000	-0.084930000
6	3.639520000	-1.276300000	1.862310000
1	3.041530000	-2.176030000	2.072790000
1	4.333940000	-1.094880000	2.696120000
1	4.210100000	-1.432360000	0.937710000
6	1.708300000	0.220980000	3.361710000
1	2.487550000	0.287880000	4.134860000
1	1.118230000	-0.692360000	3.516920000
1	1.030840000	1.081290000	3.445800000
6	0.239450000	-3.403610000	0.023980000
1	1.321700000	-3.495940000	-0.180820000
1	-0.068540000	-4.275120000	0.619270000
6	-0.241640000	-2.372400000	-2.227300000
1	0.788760000	-2.511430000	-2.618240000
7	-0.553770000	-3.375990000	-1.203620000
16	-1.334220000	-4.809970000	-1.678290000
8	-2.356320000	-4.423070000	-2.679980000
8	-1.719330000	-5.502380000	-0.423190000
6	-0.346340000	-0.918030000	-1.764230000
1	-0.288240000	-0.284280000	-2.656870000
1	-0.935860000	-2.547500000	-3.061860000
7	-1.942430000	-0.666750000	-1.235680000
7	-2.488360000	0.173050000	-1.896500000
16	-4.324640000	0.499740000	-1.095090000
8	-5.322050000	-0.122040000	-2.018780000
8	-4.279600000	0.105960000	0.349150000
6	-4.448010000	2.287010000	-1.219620000
6	-4.050900000	3.083000000	-0.142790000
6	-4.913620000	2.850160000	-2.413110000
6	-4.124460000	4.472050000	-0.270860000
6	-4.976570000	4.238090000	-2.520330000
6	-4.583600000	5.070610000	-1.455590000
1	-3.708620000	2.621380000	0.783930000
1	-5.231300000	2.207050000	-3.234400000
1	-3.825320000	5.102780000	0.569540000
1	-5.344150000	4.686000000	-3.446870000
6	-4.667470000	6.569940000	-1.591460000
1	-4.284750000	7.079810000	-0.696250000
1	-4.089650000	6.920220000	-2.462330000
1	-5.710370000	6.891670000	-1.748710000
1	0.011870000	0.860040000	0.042510000
6	-0.051940000	-2.185330000	0.801930000
6	-0.589850000	-1.268100000	1.422460000
6	-0.098090000	-5.828080000	-2.515050000
1	0.702580000	-6.064910000	-1.802700000
1	-0.615090000	-6.743290000	-2.834100000
1	0.281450000	-5.277470000	-3.385140000
6	-1.456710000	-0.453210000	2.290750000
1	-1.108670000	0.595190000	2.333630000
1	-2.465420000	-0.441770000	1.830690000
8	-1.468160000	-1.043590000	3.580450000
6	-2.407060000	-0.398640000	4.451200000
1	-3.433720000	-0.507840000	4.058970000
1	-2.173510000	0.684090000	4.500580000
6	-2.286150000	-1.014230000	5.818020000
1	-1.307830000	-0.940880000	6.308190000

6	-3.281150000	-1.597470000	6.441030000
6	-4.283300000	-2.166470000	7.064440000
1	-4.974350000	-1.584540000	7.682710000
1	-4.475300000	-3.239700000	6.965880000

D (nimag=0) E(au)= -2521.6907 **G(au)=** -2521.1973

1	-3.183880000	-0.835530000	1.995070000
6	-2.748070000	-2.143700000	-1.124620000
1	-2.658030000	-3.230240000	-1.369400000
7	-3.257540000	-1.958560000	0.227820000
16	-5.009000000	-1.859030000	0.327250000
8	-5.516020000	-1.823180000	-1.068210000
8	-5.332860000	-0.771380000	1.281410000
6	-1.464430000	-1.594010000	-1.543510000
1	-1.305320000	-1.888470000	-2.593690000
1	-3.501320000	-1.810630000	-1.875770000
1	-0.013250000	0.253250000	-1.975080000
6	-2.116550000	0.172700000	0.484420000
6	-2.061780000	1.216610000	-0.162460000
6	-5.436130000	-3.438800000	1.068290000
1	-4.956780000	-3.491710000	2.053470000
1	-6.530740000	-3.444760000	1.159830000
1	-5.092130000	-4.236350000	0.398910000
6	-2.245690000	2.509250000	-0.838510000
1	-1.548210000	2.605840000	-1.690840000
1	-3.272910000	2.512220000	-1.255470000
8	-2.072830000	3.548830000	0.106180000
6	-2.375630000	4.840830000	-0.453570000
1	-3.404600000	4.817750000	-0.861050000
1	-1.680930000	5.072700000	-1.280090000
6	-2.271160000	5.861010000	0.643700000
1	-2.942530000	5.733510000	1.501300000
6	-1.443900000	6.881090000	0.608100000
6	-0.628750000	7.905300000	0.560400000
1	-0.933270000	8.852750000	0.104200000
1	0.380930000	7.847700000	0.979560000
45	-0.146330000	-0.465900000	-0.644650000
15	1.619150000	-1.815430000	-1.322680000
15	1.456200000	1.155550000	0.387600000
6	2.380670000	-2.266520000	0.293240000
6	3.335350000	-1.460200000	0.963810000
6	1.903880000	-3.438080000	0.915620000
6	3.788660000	-1.875620000	2.228090000
6	2.360870000	-3.822640000	2.176100000
1	1.175650000	-4.073840000	0.413560000
6	3.306930000	-3.036360000	2.835580000
1	4.531690000	-1.264350000	2.743260000
1	1.980720000	-4.737590000	2.633250000
1	3.674970000	-3.325420000	3.821660000
6	3.269850000	0.953160000	0.057030000
6	3.981700000	2.023790000	-0.514120000
6	3.966560000	-0.241820000	0.366490000
6	5.353050000	1.934500000	-0.765380000
1	3.473680000	2.952060000	-0.768590000
6	5.349840000	-0.304960000	0.124540000
6	6.042690000	0.767470000	-0.438510000
1	5.875730000	2.783280000	-1.209790000
1	5.883400000	-1.225200000	0.369300000
1	7.115230000	0.685540000	-0.623480000
6	1.121550000	-3.389060000	-2.129230000
1	0.329190000	-3.905930000	-1.574300000
1	2.001420000	-4.044090000	-2.212640000
1	0.758270000	-3.149950000	-3.139150000
6	2.820510000	-1.137500000	-2.532780000
1	2.305200000	-1.129210000	-3.504570000
1	3.690670000	-1.807780000	-2.584070000
1	3.139790000	-0.121980000	-2.281930000
6	1.285920000	1.074160000	2.226970000
1	0.245850000	1.317820000	2.489720000
1	1.964990000	1.801280000	2.696100000
1	1.525270000	0.064990000	2.587740000
6	1.106180000	2.915020000	-0.004560000
1	1.809450000	3.569240000	0.530690000
1	0.083910000	3.153410000	0.320220000
1	1.186060000	3.085900000	-1.087230000
6	-2.527550000	-1.084900000	1.150270000

1	-1.660340000	-1.626430000	1.565310000

TS_DE (nimag=1) (-105.36i) E**(au)=** -2521.6860 **G(au)=** -2521.1910

45	-0.059860000	-0.360130000	0.810390000
15	-1.284240000	1.419200000	1.616020000
15	1.318030000	1.114280000	-0.591200000
6	-2.021330000	2.138810000	0.090900000
6	-1.326570000	3.040250000	-0.756030000
6	-3.301950000	1.682700000	-0.281840000
6	-1.956770000	3.459190000	-1.941060000
6	-3.902270000	2.109350000	-1.467060000
1	-3.852230000	0.995840000	0.360100000
6	-3.224860000	2.999940000	-2.301360000
1	-1.430790000	4.159670000	-2.592000000
1	-4.899140000	1.750430000	-1.728150000
1	-3.682310000	3.343400000	-3.230950000
6	1.221810000	2.946900000	-0.334900000
6	2.399220000	3.655700000	-0.034190000
6	-0.001060000	3.658590000	-0.427980000
6	2.385050000	5.037780000	0.169040000
1	3.352590000	3.135820000	0.039880000
6	0.009190000	5.051370000	-0.237500000
6	1.184860000	5.740000000	0.064160000
1	3.315730000	5.558280000	0.401620000
1	-0.932690000	5.597870000	-0.312850000
1	1.158160000	6.820410000	0.216750000
6	-2.674880000	0.916190000	2.702410000
1	-3.307690000	0.157810000	2.225600000
1	-3.282160000	1.797880000	2.954400000
1	-2.242270000	0.494420000	3.621260000
6	-0.401780000	2.665280000	2.632600000
1	-0.214590000	2.199530000	3.611210000
1	-1.050350000	3.544460000	2.759530000
1	0.550090000	2.962530000	2.182030000
6	0.956450000	0.849490000	-2.384490000
1	1.076350000	-0.221770000	-2.606920000
1	1.658540000	1.435200000	-2.995980000
1	-0.072740000	1.154700000	-2.616660000
6	3.103640000	0.701890000	-0.450420000
1	3.691200000	1.270720000	-1.185490000
1	3.227390000	-0.374080000	-0.638820000
1	3.465210000	0.918570000	0.564890000
6	-0.858940000	-3.109230000	-0.712090000
6	-1.983610000	-2.704440000	1.353320000
1	-2.886290000	-2.297890000	1.852120000
7	-2.097090000	-2.563310000	-0.103880000
16	-3.584040000	-3.235410000	-0.754270000
8	-4.604630000	-2.944270000	0.281280000
8	-3.339500000	-4.626780000	-1.207030000
6	-0.857660000	-1.852920000	1.806990000
1	-0.443670000	-2.175990000	2.776700000
1	-1.890100000	-3.753410000	1.695730000
1	0.854380000	-0.123460000	1.997030000
6	0.280720000	-2.607810000	0.094300000
6	1.419680000	-2.562430000	0.580330000
6	-3.857720000	-2.186820000	-2.186530000
1	-3.026040000	-2.319370000	-2.889170000
1	-4.793600000	-2.546210000	-2.635320000
1	-3.951980000	-1.150530000	-1.842850000
6	2.777880000	-2.705600000	1.116600000
1	2.943940000	-1.987140000	1.942400000
1	2.853410000	-3.723740000	1.549730000
8	3.681670000	-2.525880000	0.046080000
6	5.044730000	-2.803340000	0.431410000
1	5.074690000	-3.790560000	0.930520000
1	5.402540000	-2.040740000	1.144030000
6	5.883220000	-2.823120000	-0.813320000
1	5.616360000	-3.565500000	-1.575010000
6	6.907730000	-2.024310000	-1.010890000
6	7.936800000	-1.235990000	-1.197110000
1	8.939280000	-1.523640000	-0.864230000
1	7.827930000	-0.268000000	-1.696530000

E (nimag=0) E(au)= -2520.5953 **G(au)=** -2521.0949

15	-2.548920000	-0.971410000	1.245670000
15	-1.055220000	1.158190000	-0.927950000
6	-3.818070000	-0.796850000	-0.094040000
6	-4.236720000	0.464780000	-0.585030000
6	-4.358980000	-1.963160000	-0.665430000
6	-5.210030000	0.510700000	-1.597990000
45	-0.245410000	-0.610940000	0.414610000
6	-5.307320000	-1.897120000	-1.688870000
1	-4.052460000	-2.945580000	-0.309010000
6	-5.741500000	-0.654640000	-2.151980000
1	-5.539190000	1.484340000	-1.965810000
1	-5.710080000	-2.819270000	-2.111580000
1	-6.489470000	-0.588790000	-2.944200000
6	-2.371500000	2.170630000	-0.116860000
6	-1.993700000	3.403230000	0.447140000
6	-3.727160000	1.764940000	-0.049480000
6	-2.933590000	4.240400000	1.050740000
1	-0.955760000	3.732280000	0.415410000
6	-4.660700000	2.635640000	0.539790000
6	-4.275760000	3.859700000	1.087150000
1	-2.612720000	5.190870000	1.480350000
1	-5.706690000	2.327390000	0.584260000
1	-5.023140000	4.509240000	1.546350000
6	-2.833900000	-2.668200000	1.913960000
1	-2.538720000	-3.438790000	1.191040000
1	-3.894640000	-2.790690000	2.177010000
1	-2.228100000	-2.793170000	2.822510000
6	-3.089750000	0.086150000	2.659800000
1	-2.498700000	-0.204860000	3.540850000
1	-4.156490000	-0.080910000	2.867900000
1	-2.912760000	1.147280000	2.451550000
6	-1.689210000	0.589590000	-2.563320000
1	-0.821850000	0.316370000	-3.180810000
1	-2.227150000	1.420330000	-3.043490000
1	-2.351000000	-0.277560000	-2.462610000
6	0.236710000	2.373210000	-1.411160000
1	-0.227250000	3.195380000	-1.974350000
1	0.964320000	1.858760000	-2.053980000
1	0.762180000	2.772370000	-0.534990000
1	7.484870000	2.408440000	-0.836390000
1	8.630960000	1.014360000	-0.984170000
1	7.260980000	1.180250000	-2.155360000
8	6.627490000	-1.048720000	-0.483360000
8	6.914910000	0.711780000	1.377390000
6	0.572000000	-3.650190000	0.599450000
6	1.570320000	-0.533980000	-0.402470000
6	1.515470000	-1.603620000	-1.434100000
6	0.230860000	-3.578730000	-0.865040000
1	1.618760000	-1.184330000	-2.452890000
1	2.319940000	-2.351720000	-1.314390000
1	-0.775870000	-3.980290000	-1.054940000
1	0.945630000	-4.161870000	-1.468990000
6	0.513280000	-2.611200000	1.402690000
8	0.205180000	-2.213660000	-1.324660000
16	6.576350000	0.365570000	-0.028820000
6	7.597090000	1.356640000	-1.126230000
6	2.769070000	0.191210000	-0.208610000
6	2.955910000	1.110010000	0.789680000
6	4.043850000	0.066920000	-1.032560000
6	4.322670000	1.668850000	0.774330000
7	4.991820000	0.981850000	-0.350470000
1	4.439700000	-0.959720000	-1.055250000
1	3.875710000	0.389910000	-2.073960000
1	4.848370000	1.504560000	1.732950000
1	4.284080000	2.767040000	0.630380000
1	2.200720000	1.409130000	1.517820000
1	-0.088340000	0.531620000	1.415450000
6	0.577640000	-1.676040000	2.366160000
1	-0.217400000	-1.561910000	3.105990000
1	1.525930000	-1.183080000	2.595810000
1	0.884260000	-4.617290000	1.011550000

E′ (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_EF (nimag=1) (-291.44i) E**(au)=** -2520.5761 **G(au)=** -2521.07311

45	-0.279130000	-0.583580000	0.251880000
15	-2.306430000	-0.734170000	1.570790000
15	-1.361630000	0.949010000	-1.226590000
6	-3.771780000	-0.945850000	0.460890000
6	-4.373030000	0.138170000	-0.226290000
6	-4.271950000	-2.245630000	0.257110000

6	-5.478370000	-0.115740000	-1.056520000
6	-5.355600000	-2.480000000	-0.591900000
1	-3.825240000	-3.096390000	0.770330000
6	-5.967010000	-1.409460000	-1.245580000
1	-5.948440000	0.721960000	-1.575010000
1	-5.722840000	-3.498490000	-0.729750000
1	-6.820700000	-1.577700000	-1.904570000
6	-2.645220000	2.032800000	-0.454090000
6	-2.325320000	3.385990000	-0.239430000
6	-3.926490000	1.558170000	-0.075570000
6	-3.251410000	4.269610000	0.318800000
1	-1.345750000	3.773300000	-0.515480000
6	-4.851310000	2.470650000	0.460970000
6	-4.524210000	3.812270000	0.661050000
1	-2.975410000	5.314040000	0.473300000
1	-5.840430000	2.106310000	0.744290000
1	-5.261630000	4.493970000	1.088620000
6	-2.347870000	-2.216620000	2.669930000
1	-2.022870000	-3.121190000	2.138960000
1	-3.363260000	-2.361910000	3.066630000
1	-1.664950000	-2.035810000	3.511750000
6	-2.639080000	0.631820000	2.762420000
1	-1.865390000	0.569280000	3.542360000
1	-3.630910000	0.497540000	3.217840000
1	-2.579420000	1.613380000	2.279680000
6	-2.154230000	0.092930000	-2.656650000
1	-1.372550000	-0.407490000	-3.245280000
1	-2.660020000	0.843520000	-3.282320000
1	-2.879630000	-0.654460000	-2.316500000
6	-0.185850000	2.109490000	-2.036060000
1	-0.733770000	2.795240000	-2.698130000
1	0.522050000	1.521310000	-2.635630000
1	0.381550000	2.682890000	-1.291900000
1	0.049700000	0.687650000	0.993750000
6	1.571980000	-3.171880000	0.254870000
6	1.575230000	-0.630260000	-0.683610000
6	1.681190000	-1.456600000	-1.939150000
6	1.257460000	-3.585980000	-1.142940000
1	1.435000000	-0.805700000	-2.795440000
1	2.701340000	-1.842610000	-2.123900000
1	0.495510000	-4.384030000	-1.121030000
1	2.163640000	-4.021650000	-1.609960000
6	1.269840000	-1.981810000	0.812490000
8	0.746220000	-2.526430000	-1.933360000
16	6.364280000	0.501270000	0.357880000
6	7.623330000	1.425520000	-0.531100000
1	7.453630000	2.493390000	-0.346370000
1	8.592300000	1.103380000	-0.126410000
1	7.535870000	1.179870000	-1.596330000
8	6.491550000	-0.937580000	0.003980000
8	6.396790000	0.918250000	1.785910000
6	2.704500000	0.219570000	-0.387430000
6	2.729730000	1.260440000	0.490620000
6	4.064300000	0.118920000	-1.074180000
6	4.053440000	1.937610000	0.517570000
7	4.906880000	1.105150000	-0.359150000
1	4.505560000	-0.885910000	-1.005570000
1	3.993600000	0.386920000	-2.142590000
1	4.465580000	2.002920000	1.538280000
1	3.971330000	2.973900000	0.137210000
1	1.891180000	1.614810000	1.089710000
6	0.970300000	-1.354680000	1.999780000
1	0.417890000	-1.912800000	2.757280000
1	1.507740000	-0.466390000	2.335800000
1	2.163070000	-3.871510000	0.858510000

TS_E'F' (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

F (nimag=0) **E(au)=** -2521.6288 **G(au)=** -2521.1253

45	0.729950000	0.171750000	-0.685330000
1	-1.854180000	-2.011250000	-3.351010000
15	1.885100000	1.552620000	0.805780000
15	2.406580000	-1.529670000	-0.672200000
6	3.594370000	1.731120000	0.121020000
6	4.590360000	0.733770000	0.280890000
6	3.882610000	2.870100000	-0.654400000
6	5.846710000	0.935930000	-0.316680000
6	5.131520000	3.040770000	-1.255190000
1	3.131630000	3.647980000	-0.790210000
6	6.119740000	2.070830000	-1.082220000

1	6.618120000	0.175200000	-0.182900000
1	5.328650000	3.935250000	-1.848790000
1	7.102730000	2.193630000	-1.540740000
6	3.511510000	-1.550250000	0.816910000
6	3.427120000	-2.643880000	1.697940000
6	4.412750000	-0.497290000	1.117540000
6	4.222080000	-2.720570000	2.843830000
1	2.735840000	-3.460280000	1.494390000
6	5.222990000	-0.606500000	2.261660000
6	5.132230000	-1.700980000	3.122570000
1	4.131470000	-3.582420000	3.507530000
1	5.923620000	0.200210000	2.485240000
1	5.767440000	-1.750590000	4.008940000
6	1.230430000	3.269210000	0.946840000
1	1.068550000	3.721240000	-0.039800000
1	1.919990000	3.892400000	1.535440000
1	0.262940000	3.209700000	1.466120000
6	1.977300000	1.045080000	2.574840000
1	0.986310000	1.239340000	3.011050000
1	2.732110000	1.650430000	3.097210000
1	2.212040000	-0.019490000	2.677650000
6	3.511030000	-1.345610000	-2.143200000
1	2.894210000	-1.487640000	-3.043780000
1	4.307500000	-2.104240000	-2.118220000
1	3.958250000	-0.343840000	-2.167130000
6	1.816930000	-3.267200000	-0.824610000
1	2.661820000	-3.967720000	-0.759130000
1	1.341620000	-3.375580000	-1.807450000
1	1.068610000	-3.494900000	-0.055440000
1	0.205130000	-0.485020000	0.579820000
6	-0.603870000	-0.512250000	-2.417390000
6	-2.407850000	-0.425160000	-0.773990000
6	-2.428050000	-1.924000000	-0.796320000
6	-0.999740000	-1.941190000	-2.646120000
1	-2.506500000	-2.301580000	0.238010000
1	-3.381450000	-2.216020000	-1.298010000
1	-0.172830000	-2.519060000	-3.076790000
6	-1.334920000	0.276460000	-1.473480000
8	-1.330940000	-2.548500000	-1.397840000
16	-7.222580000	0.053450000	0.632660000
6	-7.904970000	0.005870000	2.293000000
1	-7.820640000	1.010980000	2.723210000
1	-8.955930000	-0.295210000	2.186900000
1	-7.338890000	-0.734900000	2.871020000
8	-7.199770000	-1.328130000	0.085440000
8	-7.878340000	1.148850000	-0.129050000
6	-3.518270000	0.219300000	-0.183380000
6	-3.916680000	1.518800000	-0.401990000
6	-4.538150000	-0.473690000	0.708260000
6	-5.180460000	1.817120000	0.293750000
7	-5.580420000	0.552500000	0.935740000
1	-4.977530000	-1.371120000	0.246040000
1	-4.074100000	-0.773680000	1.663300000
1	-5.956460000	2.195820000	-0.397450000
1	-5.015050000	2.631970000	1.029580000
1	-3.419500000	2.248300000	-1.039360000
6	-0.858570000	1.580570000	-1.131830000
1	-0.422950000	2.197120000	-1.925440000
1	-1.320820000	2.129810000	-0.313140000
1	-0.096720000	0.003510000	-3.240950000

F′ (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_FG (nimag=1) (-88.3*i*) **E(au)=** -2521.5952 **G(au)=** -2521.0908

45	-0.518870000	0.652200000	-1.118510000
15	-1.313150000	-1.585250000	-0.640660000
15	-2.325840000	1.645970000	0.134250000
6	-3.155030000	-1.679410000	-0.754150000
6	-4.007830000	-1.181860000	0.264250000
6	-3.724620000	-2.241160000	-1.912670000
6	-5.397660000	-1.309620000	0.099100000
6	-5.109240000	-2.336280000	-2.065470000
1	-3.088380000	-2.623230000	-2.710250000
6	-5.949590000	-1.875750000	-1.051170000
1	-6.054420000	-0.938770000	0.888100000
1	-5.523670000	-2.779170000	-2.972740000
1	-7.033680000	-1.951590000	-1.152980000
6	-2.814560000	0.658600000	1.618710000
6	-2.424610000	1.143930000	2.880910000
6	-3.522910000	-0.567310000	1.541450000
6	-2.730290000	0.449360000	4.052800000

1	-1.878480000	2.083000000	2.963930000
6	-3.839920000	-1.239020000	2.735900000
6	-3.446910000	-0.745870000	3.980540000
1	-2.414700000	0.851540000	5.017140000
1	-4.394140000	-2.177560000	2.676720000
1	-3.700070000	-1.296260000	4.888510000
6	-0.692260000	-2.847220000	-1.831130000
1	-0.869970000	-2.540320000	-2.869670000
1	-1.172870000	-3.817910000	-1.639360000
1	0.390990000	-2.945490000	-1.674460000
6	-0.806910000	-2.304680000	0.980530000
1	0.275460000	-2.495090000	0.932040000
1	-1.338110000	-3.254590000	1.138610000
1	-1.016890000	-1.619730000	1.809600000
6	-3.805690000	1.825630000	-0.956890000
1	-4.050450000	0.893070000	-1.477650000
1	-3.573150000	2.603960000	-1.699020000
1	-4.664770000	2.147770000	-0.349930000
6	-2.127050000	3.365090000	0.757570000
1	-3.025170000	3.651130000	1.323940000
1	-2.026690000	4.021230000	-0.118370000
6	0.678730000	2.429430000	-1.962480000
6	1.718180000	1.047730000	-0.246840000
6	1.864400000	2.352900000	0.563290000
6	0.871570000	3.658400000	-1.119730000
1	1.808970000	2.150140000	1.639530000
1	2.896480000	2.693230000	0.334450000
1	0.041940000	4.363680000	-1.250430000
1	1.804860000	4.176900000	-1.421030000
6	1.408920000	1.235830000	-1.697990000
8	0.916770000	3.334820000	0.268190000
16	6.171640000	-0.742730000	0.379150000
6	7.131120000	-2.233310000	0.084080000
1	6.930840000	-2.934750000	0.903140000
1	6.828390000	-2.645290000	-0.885880000
1	8.185640000	-1.926370000	0.075610000
8	6.307130000	0.153900000	-0.799510000
8	6.495790000	-0.233910000	1.738470000
6	2.614200000	-0.022020000	0.231600000
6	2.752000000	-0.383740000	1.528310000
6	3.631430000	-0.784310000	-0.616070000
6	3.864560000	-1.368850000	1.700490000
7	4.545730000	-1.374930000	0.383230000
1	3.161180000	-1.598920000	-1.190480000
1	4.180550000	-0.141500000	-1.317070000
1	3.473460000	-2.374290000	1.943180000
1	4.556450000	-1.078360000	2.505260000
1	2.140430000	-0.045740000	2.366230000
1	0.436480000	0.640790000	0.209280000
6	1.150180000	0.074400000	-2.471470000
1	1.629540000	-0.873480000	-2.245860000
1	0.808750000	0.204300000	-3.501970000
1	0.329420000	2.591890000	-2.987010000
1	-1.225790000	3.470660000	1.370570000

TS_F′G′ (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

G (nimag=0) E(au)= -2521.6480 **G(au)=** -2521.1369

45	-0.444200000	-0.077800000	0.858270000
15	-1.325780000	0.554480000	-1.144840000
15	-2.619990000	-0.482180000	1.655570000
6	-2.562610000	1.863300000	-0.759330000
6	-3.917260000	1.584020000	-0.439820000
6	-2.114550000	3.198710000	-0.769220000
6	-4.779800000	2.664040000	-0.190180000
6	-2.987080000	4.253600000	-0.497600000
1	-1.076130000	3.432910000	-1.001340000
6	-4.327150000	3.985030000	-0.217570000
1	-5.824640000	2.455920000	0.046310000
1	-2.616450000	5.279600000	-0.515350000
1	-5.023330000	4.800400000	-0.013580000
6	-4.020520000	-0.797230000	0.507680000
6	-4.619140000	-2.068580000	0.497840000
6	-4.493670000	0.205100000	-0.376920000
6	-5.683410000	-2.353860000	-0.361380000
1	-4.269910000	-2.852060000	1.169100000
6	-5.575070000	-0.098430000	-1.219370000
6	-6.165570000	-1.364340000	-1.218110000
1	-6.133060000	-3.348040000	-0.351550000
1	-5.944380000	0.670210000	-1.900540000
1	-6.998850000	-1.574480000	-1.890920000

6	-0.027810000	1.374260000	-2.158640000
1	0.653770000	1.971400000	-1.538810000
1	-0.518090000	2.013430000	-2.907190000
1	0.539570000	0.595950000	-2.684330000
6	-2.033680000	-0.691080000	-2.285820000
1	-1.215570000	-1.364530000	-2.578470000
1	-2.421130000	-0.150380000	-3.163190000
1	-2.839670000	-1.266300000	-1.820080000
6	-3.111730000	0.899540000	2.773150000
1	-2.327250000	1.025530000	3.533790000
1	-4.060710000	0.634710000	3.263660000
1	-3.234780000	1.834350000	2.212850000
6	-2.505840000	-1.927000000	2.785050000
1	-3.458990000	-2.064990000	3.316390000
1	-1.718100000	-1.709670000	3.521290000
1	-2.243990000	-2.842250000	2.238010000
6	0.378240000	-1.982730000	0.596510000
6	2.265810000	-1.273390000	-1.036970000
6	1.848870000	-2.580810000	-1.736590000
6	-0.042150000	-3.021150000	-0.418910000
1	2.158560000	-2.564720000	-2.789000000
1	2.320160000	-3.452580000	-1.247050000
1	-1.136030000	-3.119370000	-0.476960000
1	0.356730000	-4.001150000	-0.083290000
6	1.551580000	-1.163010000	0.316770000
8	0.429420000	-2.726020000	-1.722870000
16	6.016150000	1.198500000	0.529360000
6	7.052030000	2.414260000	-0.297040000
1	7.999990000	1.926670000	-0.553290000
1	6.525350000	2.765090000	-1.193110000
1	7.202320000	3.234450000	0.417600000
8	4.702050000	1.848980000	0.829480000
8	6.788090000	0.588700000	1.644470000
6	3.762890000	-1.139070000	-0.868930000
6	4.615530000	-1.968970000	-0.253670000
6	4.519010000	0.062610000	-1.404000000
6	6.013970000	-1.403420000	-0.256110000
7	5.836700000	0.004170000	-0.721830000
1	4.672010000	-0.021180000	-2.495540000
1	4.016310000	1.019500000	-1.210270000
1	6.674180000	-1.933930000	-0.965960000
1	6.501100000	-1.423660000	0.727990000
1	4.374980000	-2.929470000	0.204260000
1	1.929590000	-0.442110000	-1.671350000
6	1.856610000	-0.180340000	1.241470000
1	2.613640000	0.583830000	1.041950000
1	1.570730000	-0.289390000	2.297790000
1	0.271040000	-2.322270000	1.637990000

G′ (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_G'H' (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

H (nimag=0) E(au)= -3341.6174 **G(au)=** -3340.9966

1	1.607770000	0.535070000	-3.120790000
1	0.363250000	-0.685700000	-2.673080000
6	-0.821900000	2.099900000	-2.459380000
1	-1.445690000	1.338560000	-2.951410000
1	-0.183730000	2.590830000	-3.209310000
1	-1.471640000	2.843290000	-1.982960000
6	0.410550000	2.396580000	2.812370000
1	0.380800000	1.648700000	3.617230000
1	0.322070000	3.401520000	3.249590000
1	1.362250000	2.309130000	2.275010000
45	-1.103580000	0.237320000	0.351280000
15	0.235530000	1.225810000	-1.222750000
15	-1.026250000	2.102520000	1.691450000
6	1.520120000	2.412210000	-0.630980000
6	1.194820000	3.685420000	-0.095050000
6	2.866260000	2.005870000	-0.666660000
6	2.239620000	4.507920000	0.361960000
6	3.885540000	2.828330000	-0.179820000
1	3.152170000	1.044080000	-1.091080000
6	3.571140000	4.087130000	0.332120000
1	1.992970000	5.491300000	0.767000000
1	4.915570000	2.467850000	-0.209640000
1	4.356410000	4.744750000	0.710250000
6	-1.250360000	3.661790000	0.724660000
6	-2.517860000	4.270780000	0.712700000
6	-0.196840000	4.239270000	-0.029740000
6	-2.753930000	5.439970000	-0.014230000
1	-3.339690000	3.838810000	1.283000000
6	-0.452380000	5.425770000	-0.739590000
6	-1.714150000	6.023180000	-0.739010000
1	-3.747480000	5.891850000	-0.004800000
1	0.357370000	5.874720000	-1.317850000

1	-1.881590000	6.939420000	-1.308440000
6	1.117200000	0.014050000	-2.285590000
1	1.870030000	-0.543730000	-1.718880000
6	-2.442110000	2.019260000	2.863230000
1	-2.506720000	2.937610000	3.464820000
1	-2.265120000	1.157290000	3.522210000
1	-3.382370000	1.846990000	2.323630000
6	-0.087260000	-2.854030000	2.358890000
6	1.237240000	-2.804890000	0.265540000
6	0.793680000	-4.282300000	0.198250000
6	-0.019530000	-4.351780000	2.400360000
1	-0.246990000	-4.329030000	-0.177800000
1	1.430240000	-4.862880000	-0.484210000
1	-1.039880000	-4.766870000	2.240280000
1	0.305090000	-4.691980000	3.397720000
6	0.493150000	-2.106500000	1.395790000
8	0.895850000	-4.906990000	1.469520000
16	5.612360000	-1.062220000	-1.181860000
6	6.962500000	-1.787810000	-2.124470000
1	7.681860000	-2.208140000	-1.411470000
1	6.544670000	-2.562770000	-2.778770000
1	7.409300000	-0.973300000	-2.710130000
8	4.597980000	-0.559660000	-2.158980000
8	6.191430000	-0.103290000	-0.198420000
6	2.737650000	-2.659530000	0.384630000
6	3.467300000	-2.343970000	1.462860000
6	3.658230000	-2.909440000	-0.795770000
6	4.938860000	-2.301630000	1.150300000
7	4.990270000	-2.429870000	-0.335960000
1	3.725200000	-3.986060000	-1.035760000
1	3.353020000	-2.387350000	-1.713010000
1	5.485190000	-3.147490000	1.606760000
1	5.433740000	-1.375570000	1.474090000
1	3.076400000	-2.149900000	2.461920000
1	0.922170000	-2.348020000	-0.687570000
6	0.465100000	-0.621780000	1.460960000
1	1.404790000	-0.170800000	1.116200000
1	0.259180000	-0.300010000	2.489280000
1	-0.655840000	-2.371950000	3.160700000
16	-2.702240000	-2.062710000	0.335470000
8	-2.727300000	-0.813280000	1.338580000
8	-1.736230000	-1.467370000	-0.807620000
6	-4.337720000	-2.021840000	-0.424350000
6	-5.004300000	-3.240300000	-0.592970000
6	-4.921300000	-0.819190000	-0.835500000
1	-4.542650000	-4.173010000	-0.260640000
1	-4.399010000	0.127380000	-0.684650000
6	-6.266140000	-3.250880000	-1.189690000
6	-6.182990000	-0.846910000	-1.427980000
1	-6.788750000	-4.201180000	-1.322690000
1	-6.645620000	0.089410000	-1.749010000
6	-6.874340000	-2.058270000	-1.616610000
6	-8.237100000	-2.084740000	-2.261630000
1	-8.972760000	-2.584030000	-1.610350000
1	-8.211950000	-2.649270000	-3.208630000
1	-8.602140000	-1.071180000	-2.479180000

H' (nimag=0) E(au)= -3341.5799 **G(au)=** -3340.9589

45	-1.077820000	0.367430000	-0.059460000
15	-1.668200000	-1.821310000	-0.541110000
15	-3.306860000	0.868650000	0.624480000
6	-2.915710000	-1.466820000	-1.869710000
6	-4.292080000	-1.238320000	-1.614290000
6	-2.436540000	-1.352190000	-3.189900000
6	-5.139830000	-0.952410000	-2.698570000
6	-3.292530000	-1.044560000	-4.248940000
1	-1.380560000	-1.513330000	-3.407060000
6	-4.652680000	-0.852760000	-4.003140000
1	-6.201730000	-0.790380000	-2.503850000
1	-2.893300000	-0.964460000	-5.261540000
1	-5.336170000	-0.621000000	-4.822130000
6	-4.559920000	-0.482910000	0.825020000
6	-5.196390000	-0.662060000	2.065620000
6	-4.910920000	-1.332130000	-0.254660000

6	-6.167710000	-1.650510000	2.247430000
1	-4.946770000	-0.022710000	2.910950000
6	-5.903970000	-2.306190000	-0.058600000
6	-6.527670000	-2.472330000	1.179470000
1	-6.642650000	-1.767550000	3.223280000
1	-6.173040000	-2.957260000	-0.892540000
1	-7.288130000	-3.245190000	1.306580000
6	-0.423530000	-2.878810000	-1.408530000
1	0.257400000	-2.288670000	-2.034970000
1	-0.956700000	-3.612190000	-2.030470000
1	0.157080000	-3.426990000	-0.655450000
6	-2.356790000	-3.026630000	0.667250000
1	-1.523150000	-3.313630000	1.321980000
1	-2.742590000	-3.902860000	0.125590000
1	-3.147790000	-2.587440000	1.281920000
6	-4.117020000	2.044540000	-0.544440000
1	-3.479450000	2.933250000	-0.629410000
1	-5.110620000	2.312410000	-0.156130000
1	-4.220750000	1.579430000	-1.533580000
6	-3.311070000	1.768850000	2.227990000
1	-4.303360000	2.204610000	2.415070000
1	-2.547480000	2.558640000	2.180350000
6	0.036640000	0.360970000	1.729560000
6	1.716800000	-1.489730000	1.029910000
6	1.325740000	-2.083030000	2.406060000
6	-0.318390000	-0.511180000	2.910200000
1	1.504830000	-3.166000000	2.426890000
1	1.937340000	-1.613370000	3.199840000
1	-1.382300000	-0.425770000	3.168390000
1	0.260620000	-0.156890000	3.789770000
6	1.030750000	-0.142750000	0.793570000
8	-0.053490000	-1.887380000	2.683190000
16	6.405090000	-2.737080000	-0.645810000
6	7.764250000	-3.530150000	0.227770000
1	8.272950000	-2.769470000	0.832960000
1	7.347480000	-4.329130000	0.852880000
1	8.437970000	-3.936310000	-0.538880000
8	5.631500000	-3.794220000	-1.353940000
8	6.967610000	-1.596690000	-1.421080000
6	3.224740000	-1.388140000	0.921680000
6	4.019320000	-0.314970000	1.016760000
6	4.046770000	-2.643250000	0.723460000
6	5.471890000	-0.674430000	0.885400000
7	5.441210000	-2.141520000	0.637310000
1	3.945390000	-3.344600000	1.572070000
1	3.763860000	-3.193260000	-0.187840000
1	6.038720000	-0.450120000	1.807650000
1	5.968170000	-0.145910000	0.056380000
1	3.696890000	0.716080000	1.163110000
1	1.393120000	-2.193710000	0.251890000
6	1.220550000	0.536670000	-0.400520000
1	1.782590000	0.048240000	-1.200470000
1	1.074980000	1.610100000	-0.490330000
1	0.018010000	1.437670000	1.942020000
16	-0.652960000	3.839160000	0.410440000
8	-0.538150000	3.554820000	1.920080000
8	-1.017830000	2.472350000	-0.384580000
6	1.086300000	4.133490000	-0.110620000
6	2.074980000	4.317980000	0.855020000
6	1.382460000	4.281480000	-1.471920000
1	1.813720000	4.221700000	1.910330000
1	0.601580000	4.154530000	-2.225640000
6	3.380610000	4.621230000	0.451790000
6	2.687250000	4.585500000	-1.859400000
1	4.157070000	4.761100000	1.208540000
1	2.919700000	4.695270000	-2.922070000
6	3.708470000	4.758910000	-0.905820000
6	5.114090000	5.088940000	-1.344800000
1	5.544480000	4.269290000	-1.944500000
1	5.776010000	5.263160000	-0.484440000
1	5.130620000	5.991120000	-1.978000000
1	-3.049160000	1.089620000	3.050830000

H'' (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_HI (nimag=1) (-181.2*i*) E(au)= -3341.5564 **G(au)=** -3340.9353

45	-1.005960000	-0.122340000	0.248120000
15	-0.964170000	-2.155620000	1.306390000
15	-2.636880000	-0.899560000	-1.165260000
6	-1.242890000	-3.674530000	0.272400000

6	-2.507120000	-4.036030000	-0.259300000
6	-0.125980000	-4.472780000	-0.037900000
6	-2.601760000	-5.195500000	-1.050650000
6	-0.237430000	-5.608890000	-0.842380000
1	0.857800000	-4.217830000	0.353900000
6	-1.484590000	-5.976550000	-1.347260000
1	-3.576730000	-5.472570000	-1.456080000
1	0.650830000	-6.203240000	-1.064460000
1	-1.590810000	-6.864020000	-1.974070000
6	-3.974450000	-1.929440000	-0.408160000
6	-5.215820000	-1.320190000	-0.147580000
6	-3.775000000	-3.277430000	-0.017700000
6	-6.254040000	-2.020240000	0.470210000
1	-5.387910000	-0.282600000	-0.431320000
6	-4.838660000	-3.969440000	0.588540000
6	-6.066230000	-3.353650000	0.836480000
1	-7.206550000	-1.520960000	0.657410000
1	-4.686480000	-5.009320000	0.883960000
1	-6.869530000	-3.915060000	1.317450000
6	0.534000000	-2.589220000	2.297990000
1	1.446570000	-2.608160000	1.690060000
1	0.390420000	-3.572510000	2.769670000
1	0.644650000	-1.829870000	3.084850000
6	-2.240130000	-2.160870000	2.646720000
1	-1.935900000	-1.400790000	3.382690000
1	-2.275120000	-3.146860000	3.133860000
1	-3.232030000	-1.902280000	2.259540000
6	-1.952830000	-1.835900000	-2.602460000
1	-1.352250000	-1.125940000	-3.190450000
1	-2.774920000	-2.222270000	-3.223610000
1	-1.309630000	-2.661100000	-2.277550000
6	-3.519970000	0.476200000	-2.015650000
1	-4.282750000	0.067090000	-2.694510000
1	-2.769250000	1.034810000	-2.590320000
6	1.351590000	2.175580000	-0.147150000
6	2.277910000	0.517460000	1.472340000
6	2.139380000	1.689970000	2.450130000
6	2.331840000	3.125330000	0.494710000
1	1.092770000	1.754080000	2.789350000
1	2.788270000	1.540260000	3.325310000
1	2.037060000	4.173650000	0.329340000
1	3.293160000	2.973580000	-0.039270000
6	1.404870000	0.788390000	0.235320000
8	2.526490000	2.954020000	1.891010000
16	6.310790000	-1.334580000	-1.253640000
6	7.548800000	-2.541440000	-0.750900000
1	8.241520000	-2.054050000	-0.053170000
1	7.030170000	-3.384590000	-0.278900000
1	8.072770000	-2.855650000	-1.663690000
8	5.274270000	-2.034480000	-2.061910000
8	7.029310000	-0.168070000	-1.839050000
6	3.725010000	0.239450000	1.095810000
6	4.811500000	0.967160000	1.391410000
6	4.117460000	-1.007030000	0.333960000
6	6.077680000	0.338730000	0.887820000
7	5.595860000	-0.907210000	0.233940000
1	3.831820000	-1.926010000	0.880250000
1	3.653790000	-1.067690000	-0.662410000
1	6.780210000	0.100990000	1.707710000
1	6.613340000	0.981720000	0.170100000
1	4.813430000	1.914990000	1.928910000
1	1.902330000	-0.373910000	1.994680000
6	0.918130000	-0.231130000	-0.641820000
1	1.333600000	-1.237000000	-0.537540000
1	0.742110000	0.052600000	-1.686890000
1	1.167290000	2.387950000	-1.206230000
16	-0.663910000	2.905110000	0.433910000
8	-1.486030000	1.860190000	-0.398850000
8	-0.913160000	2.818190000	1.920870000
6	-1.276630000	4.504920000	-0.135970000
6	-1.509470000	4.732530000	-1.499070000
6	-1.440440000	5.519100000	0.810730000
1	-1.380330000	3.932330000	-2.229040000
1	-1.251700000	5.315250000	1.865090000
6	-1.930280000	5.997690000	-1.903570000
6	-1.863090000	6.779320000	0.381600000
1	-2.124400000	6.180670000	-2.963240000

1	-2.003180000	7.573800000	1.118170000
6	-2.113280000	7.040360000	-0.974870000
6	-2.569920000	8.400630000	-1.437480000
1	-3.559720000	8.339860000	-1.919450000
1	-1.874500000	8.816780000	-2.184680000
1	-2.639990000	9.109730000	-0.600810000
1	-3.973490000	1.164890000	-1.293060000

TS_H'I' (nimag=1) (-21.9*i*) **E(au)=** -3341.5017 **G(au)=** -3340.8861

45	1.099420000	-0.037890000	0.794750000
15	2.050100000	-1.928350000	-0.035530000
15	3.148810000	1.122810000	0.595030000
6	3.673070000	-2.238550000	0.788770000
6	4.881600000	-1.597030000	0.407730000
6	3.686290000	-3.134380000	1.875770000
6	6.058480000	-1.919160000	1.106000000
6	4.864190000	-3.422840000	2.566270000
1	2.769120000	-3.627830000	2.193680000
6	6.058730000	-2.818940000	2.173200000
1	6.989890000	-1.433090000	0.810520000
1	4.842070000	-4.122700000	3.403290000
1	6.990200000	-3.038840000	2.698020000
6	4.329270000	0.638090000	-0.736920000
6	4.539470000	1.511340000	-1.817900000
6	5.006050000	-0.607810000	-0.710670000
6	5.404580000	1.173820000	-2.862050000
1	4.031840000	2.474460000	-1.857760000
6	5.884380000	-0.920000000	-1.762140000
6	6.081600000	-0.045210000	-2.832550000
1	5.547840000	1.869360000	-3.690800000
1	6.408440000	-1.877300000	-1.742410000
1	6.762530000	-0.319950000	-3.640220000
6	1.038430000	-3.421000000	0.342220000
1	0.736010000	-3.441300000	1.396910000
1	1.617160000	-4.323460000	0.095990000
1	0.136780000	-3.400010000	-0.282070000
6	2.261580000	-1.991330000	-1.857840000
1	1.291650000	-1.757250000	-2.318140000
1	2.596100000	-3.000560000	-2.141150000
1	2.992690000	-1.249460000	-2.195180000
6	4.106870000	1.134900000	2.174370000
1	3.477380000	1.594080000	2.950720000
1	5.022520000	1.730920000	2.044410000
1	4.371670000	0.115890000	2.480950000
6	2.786690000	2.911410000	0.343400000
1	3.718650000	3.495840000	0.336580000
1	2.162650000	3.242800000	1.186460000
1	2.233650000	3.081400000	-0.589410000
6	-0.322410000	1.042780000	-0.455000000
6	-1.601290000	-1.112030000	-1.034530000
6	-1.621330000	-0.431540000	-2.419820000
6	-0.112750000	1.286660000	-1.929340000
1	-1.838120000	-1.168050000	-3.204900000
1	-2.385250000	0.365480000	-2.447810000
1	0.917040000	1.614700000	-2.130260000
1	-0.810020000	2.081830000	-2.259240000
6	-1.036180000	-0.129480000	0.000500000
8	-0.332260000	0.112900000	-2.701190000
16	-5.106940000	-4.658680000	0.350180000
6	-6.428770000	-5.364150000	-0.648010000
1	-7.245310000	-4.633320000	-0.703480000
1	-6.022380000	-5.589130000	-1.641580000
1	-6.757450000	-6.278850000	-0.136230000
8	-3.943590000	-5.587780000	0.301180000
8	-5.688010000	-4.283480000	1.669660000
6	-2.960140000	-1.673230000	-0.674370000
6	-4.018980000	-1.036410000	-0.157160000
6	-3.282600000	-3.120250000	-0.970050000
6	-5.200460000	-1.951720000	-0.014020000
7	-4.691300000	-3.255040000	-0.524010000
1	-3.193610000	-3.352510000	-2.047820000
1	-2.623160000	-3.822610000	-0.434570000
1	-6.062480000	-1.610150000	-0.615860000
1	-5.543800000	-2.043100000	1.029290000
1	-4.057730000	0.019120000	0.129660000
1	-0.906520000	-1.960240000	-1.120410000

6	-1.037230000	-0.391520000	1.370030000
1	-1.439080000	-1.332710000	1.748860000
1	-0.985920000	0.429780000	2.094410000
1	-0.216030000	1.901190000	0.225040000
16	-2.652320000	2.717080000	-0.383400000
8	-2.951210000	2.795880000	-1.895770000
8	-3.779380000	2.130370000	0.486740000
6	-2.591080000	4.486450000	0.130650000
6	-2.202690000	5.463820000	-0.791080000
6	-2.887390000	4.830940000	1.450430000
1	-2.000520000	5.178790000	-1.824860000
1	-3.214020000	4.058780000	2.149270000
6	-2.114180000	6.795060000	-0.380700000
6	-2.793840000	6.168990000	1.847860000
1	-1.823030000	7.561610000	-1.104510000
1	-3.037450000	6.441080000	2.878390000
6	-2.403910000	7.170260000	0.944000000
6	-2.303400000	8.615430000	1.368660000
1	-2.567380000	8.745300000	2.428170000
1	-2.975800000	9.252360000	0.770080000
1	-1.281490000	9.003300000	1.221880000

TS_H''I' (nimag=1) (-18.9*i*) **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

I (nimag=0) E(au)= -3341.5750 **G(au)=** -3340.9513

45	0.932810000	0.134550000	0.320780000
15	1.868750000	-1.915900000	-0.075930000
15	3.116180000	1.094560000	0.338170000
6	3.361450000	-2.210170000	1.002860000
6	4.660000000	-1.725130000	0.707650000
6	3.165730000	-2.927440000	2.198230000
6	5.714120000	-2.024070000	1.590900000
6	4.219460000	-3.194050000	3.074540000
1	2.174190000	-3.295120000	2.460540000
6	5.505570000	-2.750690000	2.763060000
1	6.714050000	-1.655020000	1.354370000
1	4.030910000	-3.753940000	3.992580000
1	6.342780000	-2.959580000	3.431900000
6	4.411360000	0.355860000	-0.765280000
6	4.790420000	1.049090000	-1.928600000
6	4.992440000	-0.909770000	-0.502440000
6	5.735260000	0.522540000	-2.813350000
1	4.349280000	2.018190000	-2.159410000
6	5.956210000	-1.413530000	-1.392600000
6	6.326690000	-0.711370000	-2.540880000
1	6.008390000	1.083880000	-3.709020000
1	6.407270000	-2.385610000	-1.183240000
1	7.070900000	-1.131620000	-3.220250000
6	0.885880000	-3.461120000	0.224750000
1	0.421820000	-3.475720000	1.219070000
1	1.544540000	-4.335390000	0.118300000
1	0.093480000	-3.529640000	-0.532860000
6	2.395740000	-2.236190000	-1.823620000
1	1.479470000	-2.379220000	-2.416310000
1	3.006470000	-3.149570000	-1.879720000
1	2.952580000	-1.389040000	-2.238690000
6	3.871980000	1.200140000	2.024260000
1	3.205140000	1.819080000	2.642810000
1	4.862940000	1.674630000	1.963360000
1	3.963530000	0.208030000	2.481410000
6	3.067180000	2.875720000	-0.143460000
1	4.082640000	3.297600000	-0.155490000
1	2.458000000	3.392420000	0.609430000
6	-2.001790000	1.200930000	-0.268340000
6	-1.560120000	-1.051090000	-1.382090000
6	-1.452390000	-0.184750000	-2.640090000
6	-2.960070000	1.302360000	-1.459620000
1	-0.442700000	0.260300000	-2.675740000
1	-1.596810000	-0.792470000	-3.545120000
1	-3.285600000	2.343830000	-1.605040000
1	-3.855390000	0.715140000	-1.189860000
6	-1.295290000	-0.161280000	-0.153660000
8	-2.428540000	0.864190000	-2.697690000
16	-5.632960000	-3.444570000	0.749010000
6	-5.939190000	-5.214710000	0.866230000
1	-6.337280000	-5.558230000	-0.096660000
1	-4.990370000	-5.709130000	1.108160000
1	-6.675840000	-5.356180000	1.668730000
8	-4.972190000	-3.008930000	2.010990000
8	-6.900280000	-2.790080000	0.320980000
6	-2.865020000	-1.830450000	-1.305180000

6	-3.866400000	-1.843020000	-2.195870000
6	-3.149390000	-2.805300000	-0.182750000
6	-4.955380000	-2.804280000	-1.819130000
7	-4.488310000	-3.351070000	-0.517380000
1	-2.401500000	-3.619810000	-0.150760000
1	-3.158510000	-2.332780000	0.810420000
1	-5.068680000	-3.614890000	-2.562500000
1	-5.937130000	-2.317160000	-1.711750000
1	-3.926620000	-1.232810000	-3.096910000
1	-0.751980000	-1.794420000	-1.444510000
6	-0.939140000	-0.646610000	1.109990000
1	-0.849970000	-1.717090000	1.290310000
1	-1.146700000	-0.045790000	2.000270000
1	-2.557880000	1.430250000	0.653370000
16	-0.752220000	2.576470000	-0.302540000
8	0.229080000	2.149680000	0.800640000
8	-0.210570000	2.807620000	-1.670990000
6	-1.552140000	4.066250000	0.280080000
6	-1.863590000	4.211230000	1.638810000
6	-1.834500000	5.068710000	-0.651250000
1	-1.617080000	3.429020000	2.357680000
1	-1.564870000	4.936470000	-1.699180000
6	-2.479720000	5.387630000	2.056810000
6	-2.451720000	6.239270000	-0.206240000
1	-2.722650000	5.513910000	3.114180000
1	-2.672750000	7.030420000	-0.925620000
6	-2.786090000	6.417250000	1.145690000
6	-3.465750000	7.675250000	1.620660000
1	-2.958490000	8.089180000	2.506330000
1	-4.507610000	7.464400000	1.915770000
1	-3.484810000	8.445580000	0.837330000
1	2.583060000	3.006980000	-1.120010000

I′ (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

J′ (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

J’’ (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_J'K (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_J''K'' (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

K (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

K′ (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

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

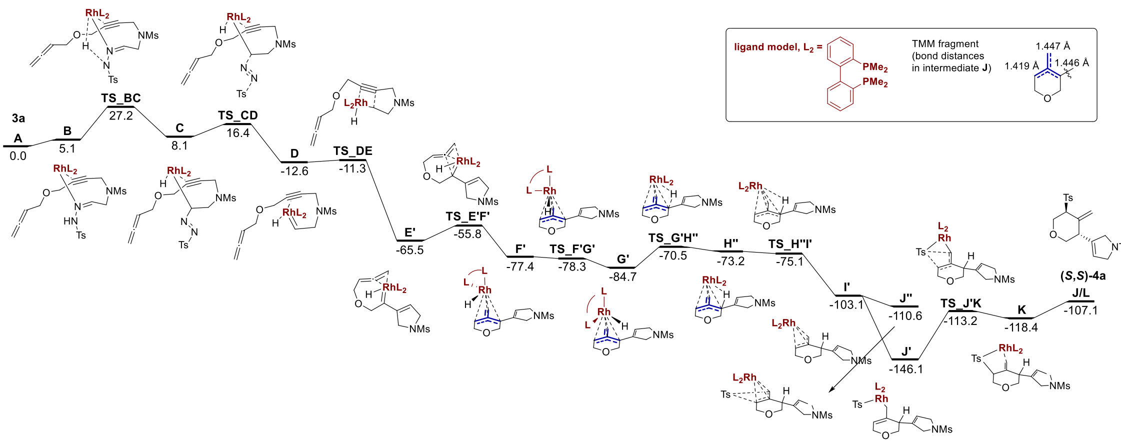
6	1.406570000	1.767120000	0.173780000
6	2.200430000	0.003710000	-1.517380000
6	2.242140000	1.223550000	-2.443920000
6	2.611880000	2.504510000	-0.407700000
1	1.221290000	1.424700000	-2.804190000
1	2.895280000	1.027610000	-3.307240000
1	2.581200000	3.575440000	-0.162320000
1	3.501410000	2.078450000	0.093780000
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

L (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

S.14. Reaction mechanism for the formation of (*S*,*S*)-4a (Scheme S2)

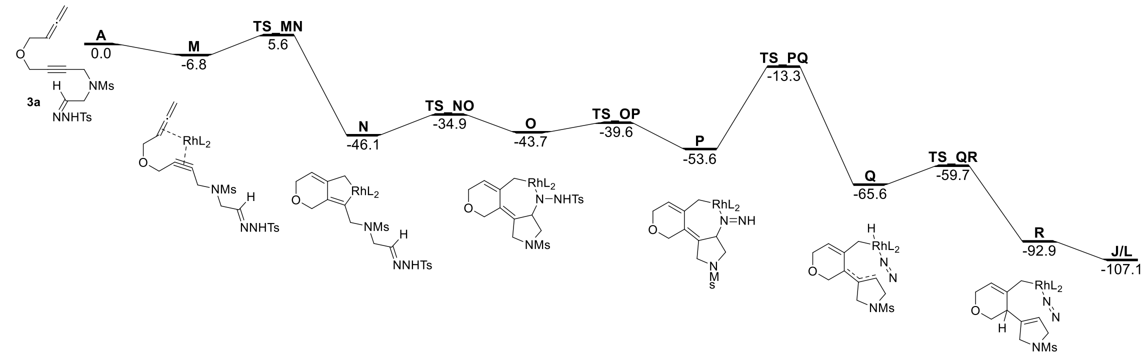


Scheme S2. Gibbs energy profile (kcal/mol) for the Rh^{I}/BINAP catalyzed transformation of **3a** into **L.** Intermediates and TS from **B** to **TS_CD** and from **J'** and **J''** to **K** have +1 charge. Intermediates and TS from **D** to **I'** have +2 charge.

Scheme S2 represents the Gibbs energy profile for the transformation of reactant **3a** to product (*S*,*S*)-**4a** (enantiomer of the experimentally obtained (*R*,*R*)-**4a**) by an alternative diastereomeric route. The first steps of this path are shared by the pathway already discussed in the manuscript (Scheme 4). The differences start in intermediate **E'**. The relative Gibbs energy of **E'** with respect to our model of **3a** and Rh^{I}/BINAP is -65.5 kcal/mol in dichloroethane. **E'** is a rhodium(I) species in an square pyramidal coordination geometry in which the π-system of the external double bond of the allene group interacts with the *d* orbitals of the metal in a basal position and the hydride occupies the apical position. Ring closure through a [2+2] cycloaddition of the double bond of the external allene and the rhodium-carbene double bond develops a strained rhodacyclobutane that is not stable and which rearranges to form intermediate **F'** in an exergonic process (11.9 kcal/mol) that takes place through a barrier of 9.7 kcal/mol. Like **F**, intermediate **F'** had an electronic structure resembling that of trimethylenemethane (fragment in blue in Scheme 4 and Scheme S2). The rhodium-bound trimethylenemethane **F'** does not evolve through a formal [3+2] cycloaddition but transforms into **G'** by a rotation of the 4-methylenetrihydropyran ring to locate the hydride in front of the C atom attached to the 2,5-dihydropyrrole ring. This process is exergonic by 7.3 kcal/mol and has a small Gibbs energy barrier of 0.9 kcal/mol. This is not surprising taking into account that similar rotations of tetracyanoethylene and benzene in ML_3 complexes are known to take place with very low barriers.

After this, there is a reverse β-H-elimination via **TS_G'H''** that transfers the H atom from Rh to the C atom attached to the 2,5-dihydropyrrole substituent to yield **H''**. This process is endergonic by 11.5 kcal/mol and has to surpass a barrier of 14.2 kcal/mol. In **H''**, there is an agostic interaction between the new formed C–H bond and the metal ($d_{C–H}$ = 1.198 Å) that helps to stabilize the complex. Rotation of the 4-methylenetrihydropyran ring by about 90º leads to **I'**, which is 29.9 kcal/mol more stable than **H''**. In the next step, the Ts^{-} group coordinates to Rh to yield intermediate **J',** which has a square pyramid geometry with the diphosphine ligand and the Ts^{-} group, coordinating in a bidentate fashion, occupying the basal positions. This process is exergonic by 43.0 kcal/mol. An alternative pathway through **J''** (Scheme S2) in which the Ts^- group directly attacks the other side of the 4-methylenetrihydropyran ring of intermediate **I'** without prior coordination to Rh is also possible, although this alternative is energetically less favourable. From **J'**, an intramolecular nucleophilic attack of the Ts^- group to C5 of the dihydropyran ring takes place to yield **K**, in which the final *trans*-disubstituted product (*S*,*S*)-**4a** coordinated to the metal has already been formed. This attack is endergonic by 27.7 kcal/mol and has to surmount a barrier of 32.9 kcal/mol (see Fig. S80 for the molecular structure of this TS). This step, therefore, is the rate determining step of the reaction mechanism for the formation of (*S*,*S*)-**4a**. Final release of (*S*,*S*)-**4a** costs an additional 11.3 kcal/mol. However, it is likely that release of (*S*,*S*)-**4a** would be assisted by the addition of **3a** to reduce or even remove this energetic cost.

S.15. Alternative reaction mechanism (Scheme S3)



Scheme S3. Gibbs energy profile (kcal/mol) for the Rh^I/BINAP catalyzed transformation of **3a** into **L**.

An alternative mechanism for the conversion of **3a** into **L** catalyzed by Rh^I/BINAP involving an oxidative addition of the alkyne and allene groups and an insertion of the C=N unit into a Rh–C bond (similar steps to those found in the [2+2+2] cycloadditions) was also studied (Scheme S3). In the first step, there is the coordination of the Rh^I/BINAP catalyst with the alkyne and allene groups of **3a**. Oxidative addition leads to intermediate **N**, with a Gibbs energy barrier of 12.4 kcal/mol. Subsequent insertion of the N=C bond into the Rh–C bond yields **O** with a relatively small energy barrier (11.2 kcal/mol). Release of the Ts- group generates **P** in an exergonic process by 9.9 kcal/mol. Next step corresponds to the breaking of the N–C bond prior to N_2 release. This step, which forms intermediate **Q**, has a high Gibbs energy barrier of 40.3 kcal/mol. All attempts to break the Rh–N bond failed leading to intermediate **O**. Hydrogen transfer in **Q** produces **R** that after N_2 release yields **J**. These final transformations are exergonic and involve low energy barriers. Since the Gibbs energy barrier for TS_PQ was higher than 40 kcal/mol, this alternative mechanism was ruled out.