Supplementary Information

Asymmetric hydrogenation of an α-unsaturated carboxylic acid catalyzed by intact chiral transition metal carbonyl clusters – diastereomeric control of enantioselectivity

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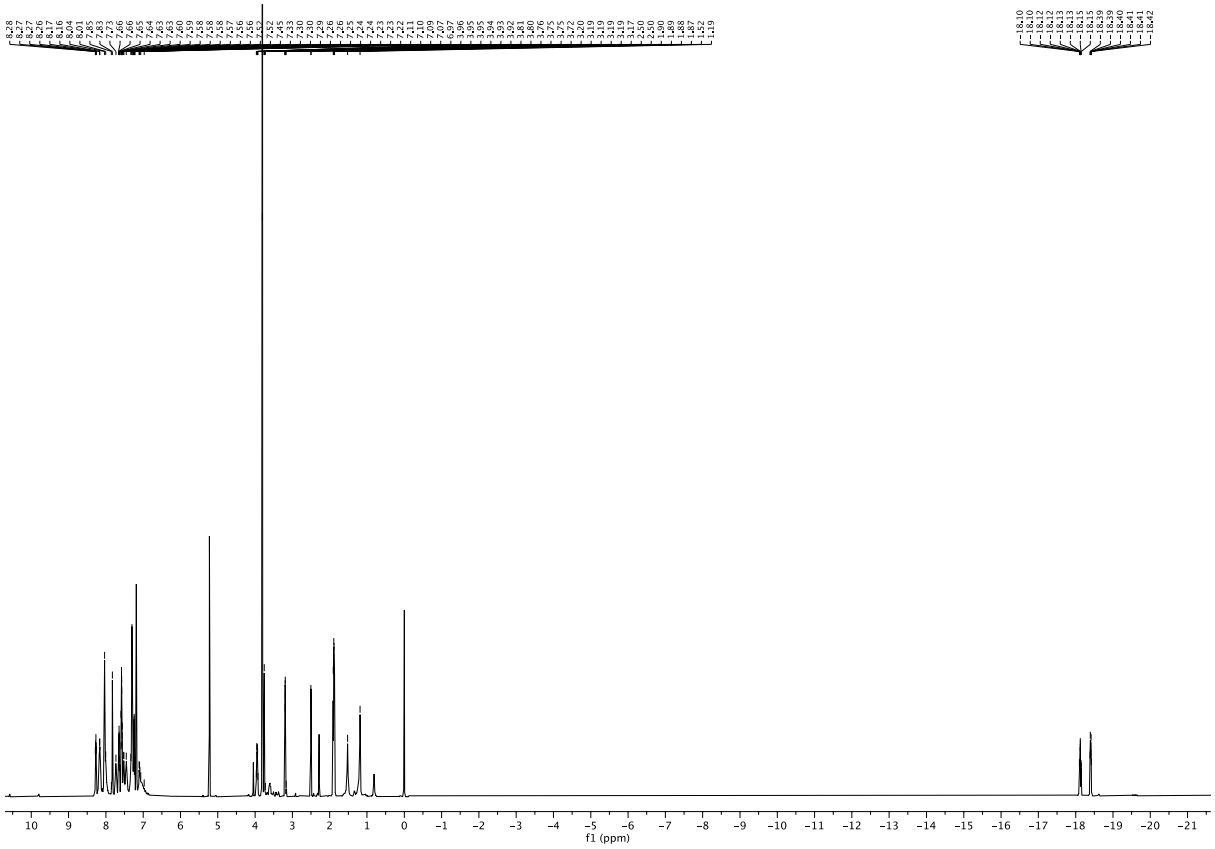

Figure S1. ^{1}H NMR of **3**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 7.7, 5.0 Hz, 1H), 8.16 (m, 1H), 8.02 (d, *J* = 15.0 Hz, 3H), 7.83 (s, 1H), 7.73 (s, 1H), 7.64 (m, 1H), 7.57 (m, 2H), 7.47 (m, 1H), 7.30 (m, 5H), 7.05 (m, 2H), 3.95 (m, 1H), 3.78 (m, 6H), 3.19 (m, 1H), 2.50 (d, *J* = 2.7 Hz, 1H), 1.89 (dd, *J* = 10.3, 7.2 Hz, 3H), 1.52 (s, 1H), 1.19 (s, 1H), –18.13 (ddd, *J* = 12.4, 11.2, 2.9 Hz, 1H), –18.40 (dt, *J* = 9.8, 2.9 Hz, 1H).

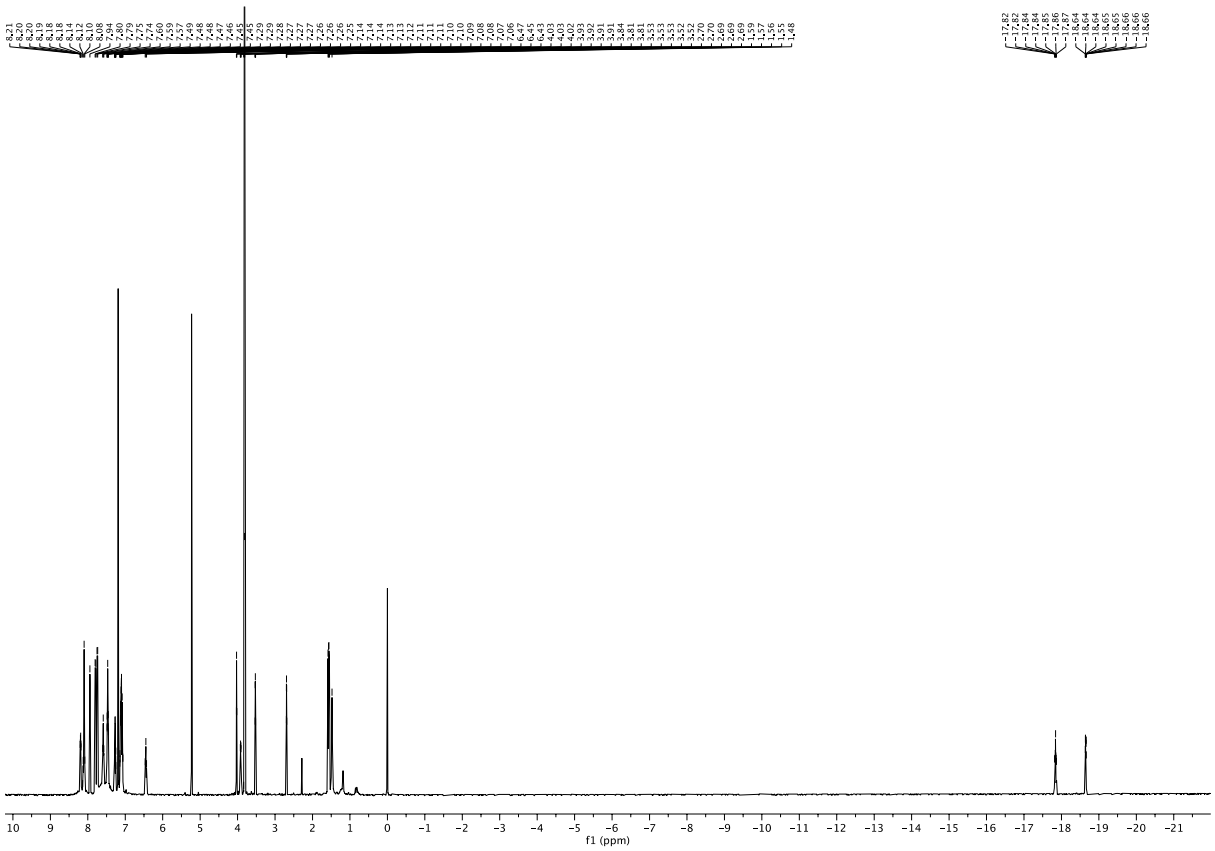

Figure S2. ^{1}H NMR of **4**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (td, *J* = 4.9, 2.4 Hz, 1H), 8.11 (d, *J* = 11.0 Hz, 3H), 7.94 (s, 1H), 7.77 (dd, *J* = 25.5, 8.9 Hz, 4H), 7.58 (m, 1H), 7.47 (m, 3H), 7.27 (tt, *J* = 7.3, 1.4 Hz, 1H), 7.10 (m, 3H), 6.45 (t, *J* = 8.5 Hz, 1H), 4.03 (t, *J* = 2.7 Hz, 1H), 3.92 (dd, *J* = 7.1, 2.8 Hz, 1H), 3.81 (s, 5H), 3.53 (dt, *J* = 2.6, 1.2 Hz, 1H), 2.69 (dt, *J* = 2.5, 1.1 Hz, 1H), 1.57 (dd, *J* = 12.1, 7.1 Hz, 3H), 1.48 (s, 2H), –17.82 (ddd, *J* = 12.2, 8.8, 3.5 Hz, 1H), –18.63 (ddd, *J* = 7.5, 3.5, 2.2 Hz, 1H).

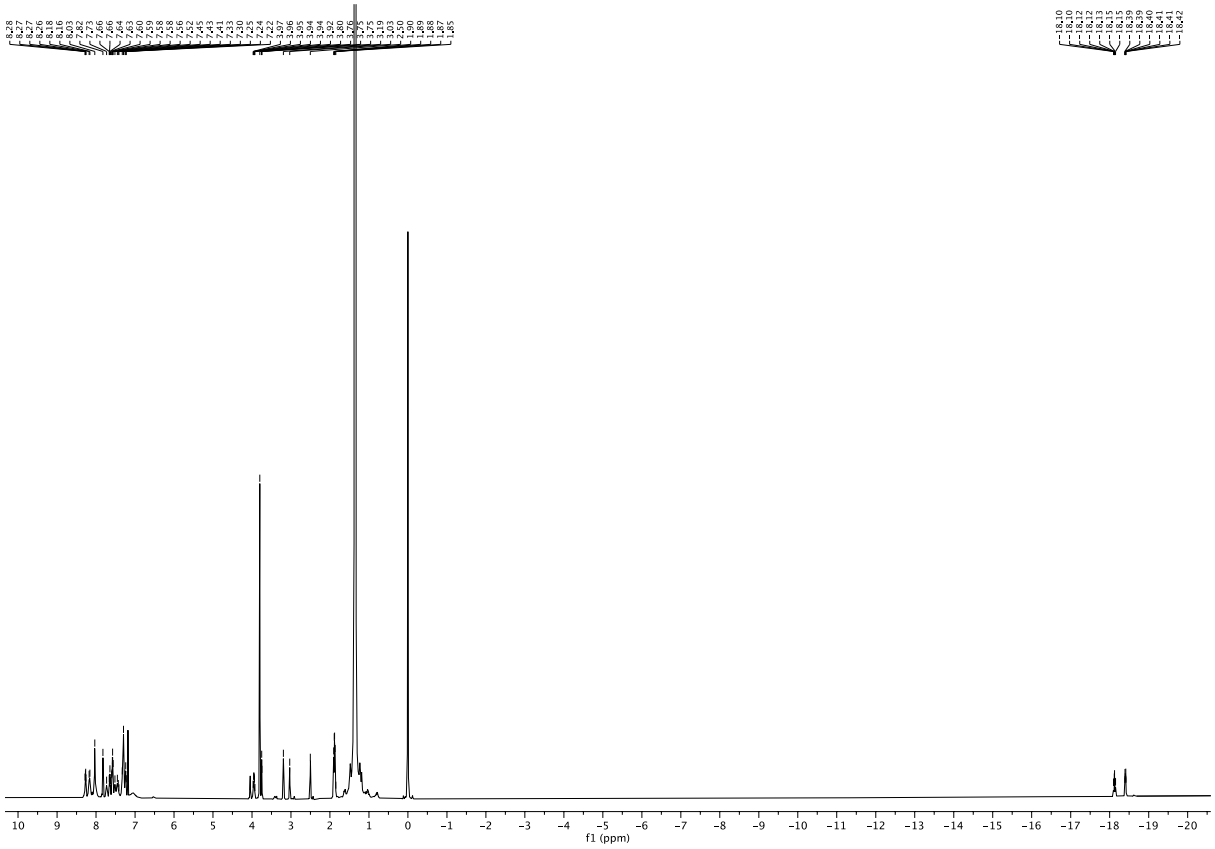

Figure S3. ^{1}H NMR of **5**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 7.8, 4.9 Hz, 1H), 8.17 (d, *J* = 9.4 Hz, 2H), 8.03 (s, 2H), 7.82 (s, 2H), 7.73 (s, 1H), 7.65 (m, 2H), 7.50 (m, 3H), 7.29 (m, 5H), 3.95 (m, 1H), 3.80 (s, 6H), 3.19 (s, 1H), 3.03 (s, 1H), 2.50 (s, 1H), 1.89 (dd, *J* = 10.3, 7.2 Hz, 4H), –18.12 (ddd, *J* = 12.6, 11.1, 3.0 Hz, 1H), –18.40 (dt, *J* = 9.6, 3.1, 3.0 Hz, 1H).

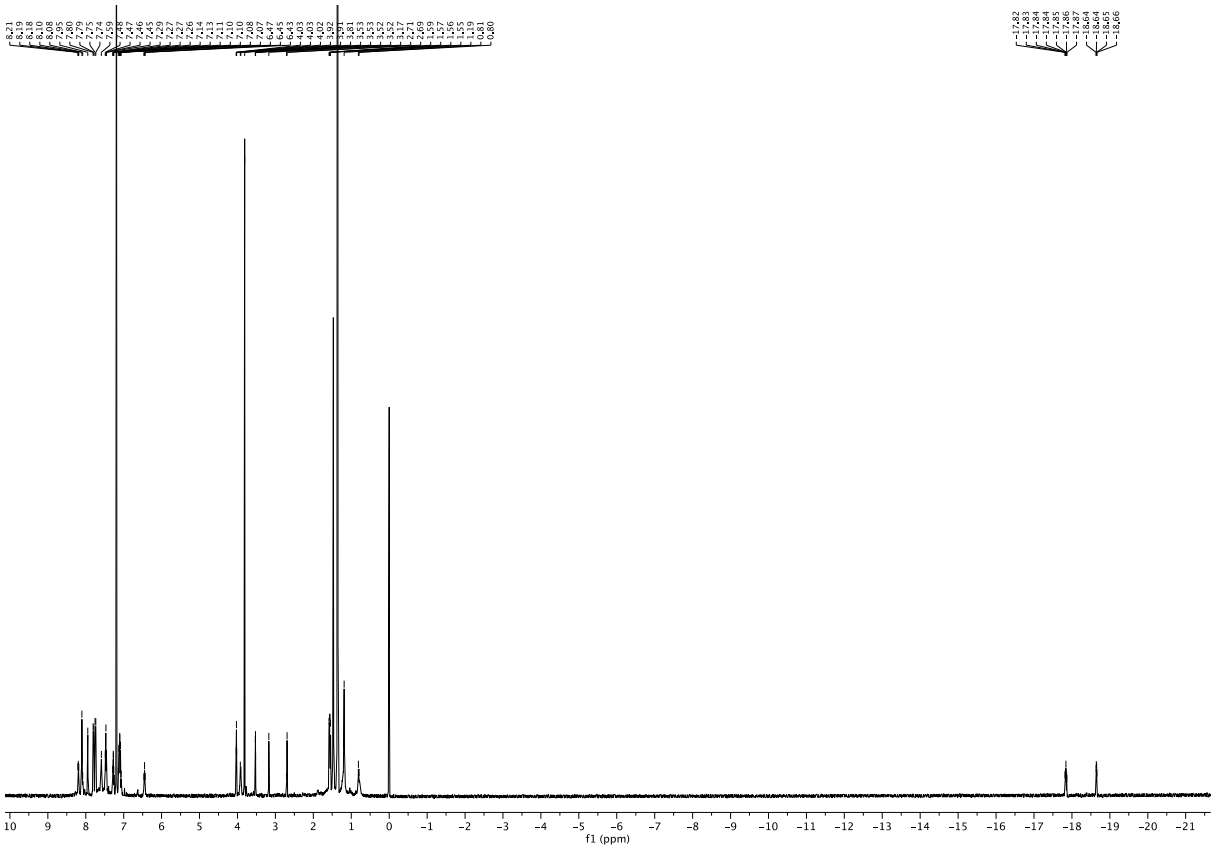

Figure S4. ^{1}H NMR of **6**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (m, 1H), 8.10 (s, 2H), 7.95 (s, 1H), 7.77 (dd, *J* = 25.5, 8.9 Hz, 4H), 7.59 (s, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 7.11 (m, 3H), 6.45 (t, *J* = 8.5 Hz, 1H), 4.03 (t, *J* = 2.7 Hz, 1H), 3.92 (d, *J* = 7.0 Hz, 1H), 3.81 (s, 5H), 3.53 (dd, *J* = 2.5, 1.4 Hz, 1H), 2.70 (d, *J* = 6.4 Hz, 1H), 1.57 (dd, *J* = 12.2, 7.0 Hz, 2H), 1.19 (s, 3H), 0.79 (m, 2H), –17.84 (ddd, *J* = 12.4, 9.1, 3.0 Hz, 1H), –18.65 (ddd, *J* = 7.1, 3.2, 3.0 Hz, 1H).

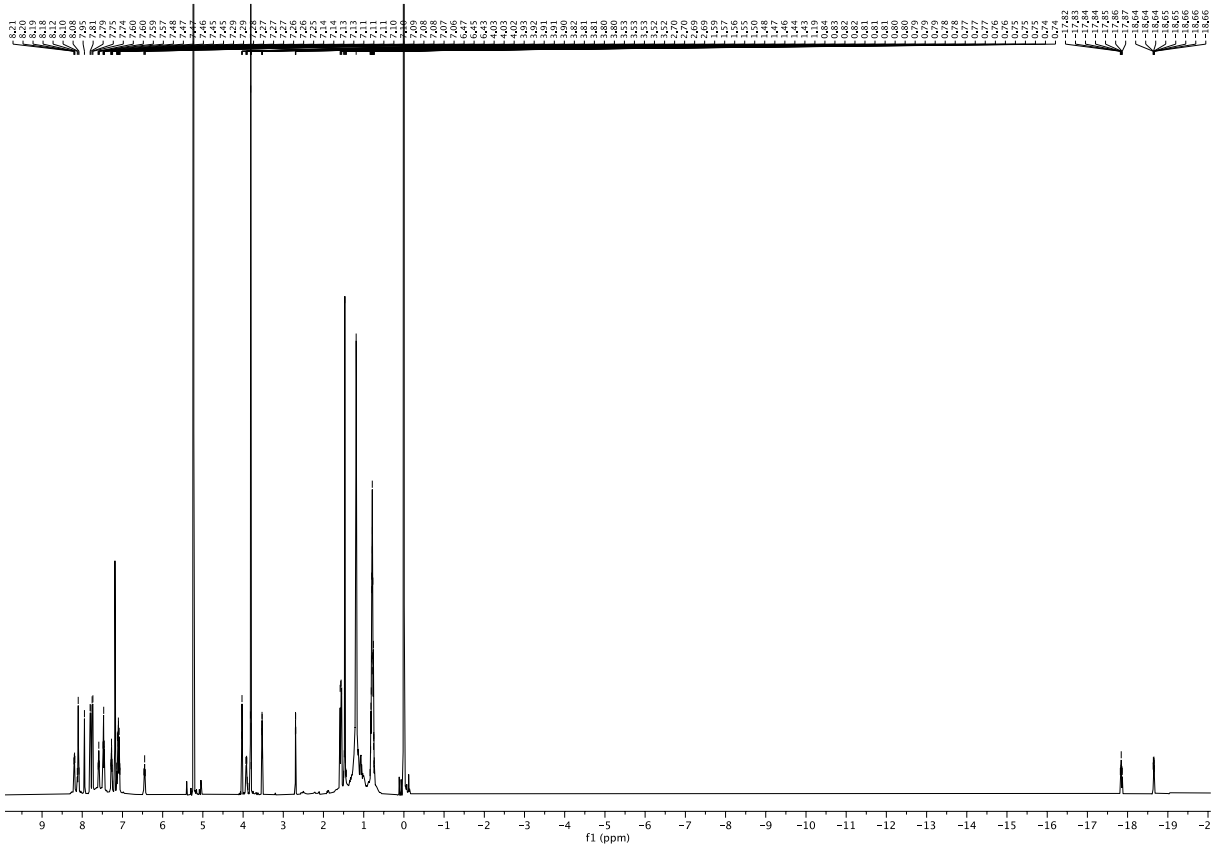

Figure S5. ^{1}H NMR of **7**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 7.8, 4.5 Hz, 1H), 7.95 (s, 1H), 7.77 (dd, *J* = 25.5, 8.9 Hz, 4H), 7.59 (t, 1H), 7.46 (m, 2H), 7.27 (ddd, *J* = 8.9, 6.9, 1.6 Hz, 1H), 7.10 (m, 3H), 6.45 (t, *J* = 8.6 Hz, 1H), 4.03 (t, *J* = 2.7 Hz, 1H), 3.91 (dt, *J* = 8.5, 4.3 Hz, 1H), 3.81 (d, *J* = 0.9 Hz, 5H), 3.53 (dt, *J* = 2.3, 1.2 Hz, 1H), 2.69 (dd, *J* = 2.6, 1.3 Hz, 1H), 1.57 (dd, *J* =

12.1, 7.1 Hz, 3H), 1.11 (m, 22H), –18.51(ddd, *J* = 11.0, 9.7, 3.0 Hz, 1H), –18.64 (dt, *J* = 11.8, 3.0 Hz, 1H).

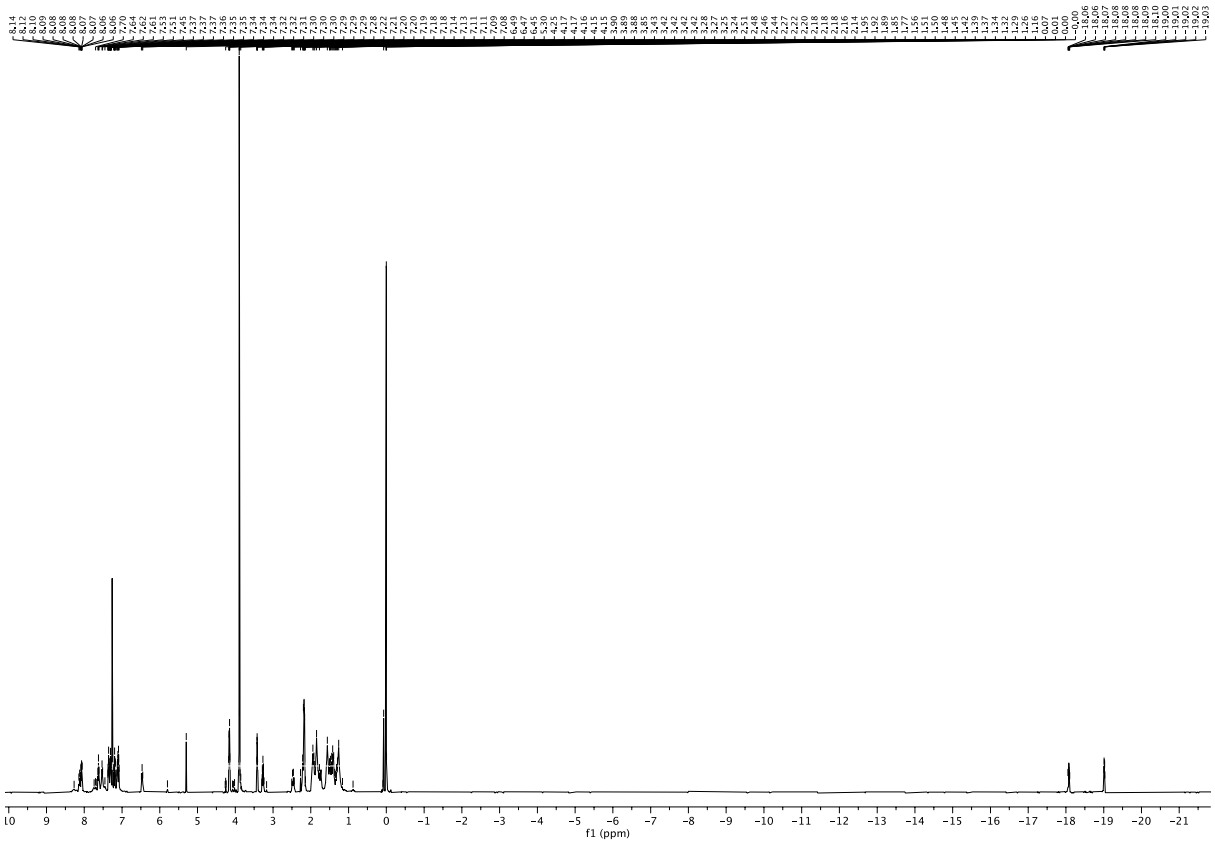

Figure S6. ^{1}H NMR of **8**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (m, 1H), 7.64 (m, 2H), 7.33 (m, 6H), 7.20 (ddd, *J* = 9.6, 8.0, 1.4 Hz, 5H), 7.11 (m, 1H), 6.47 (t, *J* = 8.6 Hz, 1H), 4.16 (dt, *J* = 8.7, 2.7 Hz, 1H), 3.90 (s, 5H), 3.42 (dt, *J* = 2.6, 1.2 Hz, 1H), 3.27 (p, *J* = 7.2 Hz, 1H), 2.52 – 2.42 (m, 1H), 2.19 (m, 1H), 1.48 (m, 22H), –18.08 (ddd, *J* = 10.3, 9.0, 3.0 Hz, 1H), –19.02 ('m', ddd, *J* = not resolved 1H).

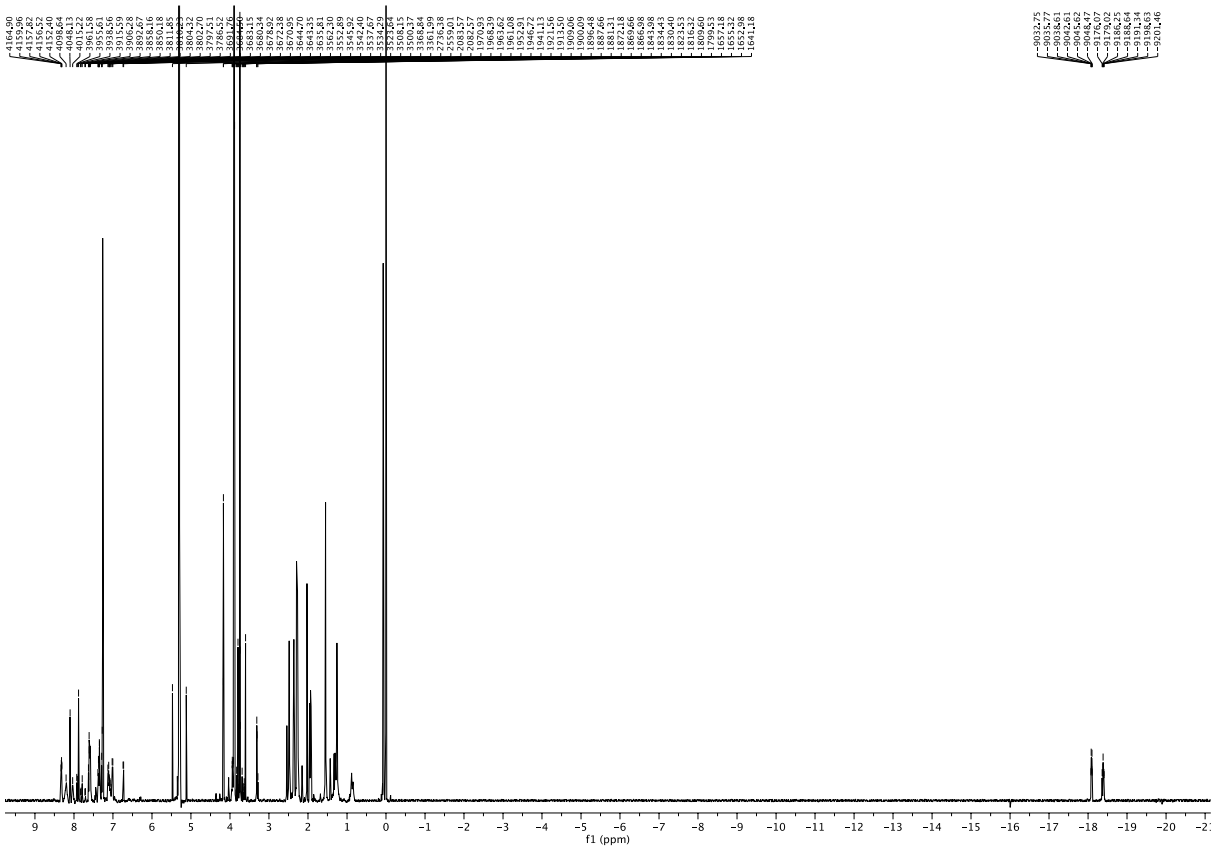

Figure S7. ^{1}H NMR of **9**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (m, 1H), 8.20 (s, 1H), 8.10 (s, 1H), 7.98 (m, 1H), 7.88 (s, 1H), 7.76 (m, 1H), 7.60 (m, 3H), 7.35 (m, 1H), 7.28 (d, *J* = 7.5 Hz, 1H), 7.06 (m, 2H), 6.73 (d, *J* = 6.9 Hz, 2H), 5.48 (s, 5H), 5.12 (s, 2H), 4.17 (d, *J* = 1.0 Hz, 1H), 3.89 (d, *J* = 5.6 Hz, 10H), 3.71 (m, 7H), 3.29 (m, 4H), –18.09 (dt, *J* = 9.6, 2.8 Hz, 1H), –18.39 (ddd, *J* = 12.8, 10.2, 2.9 Hz, 1H).

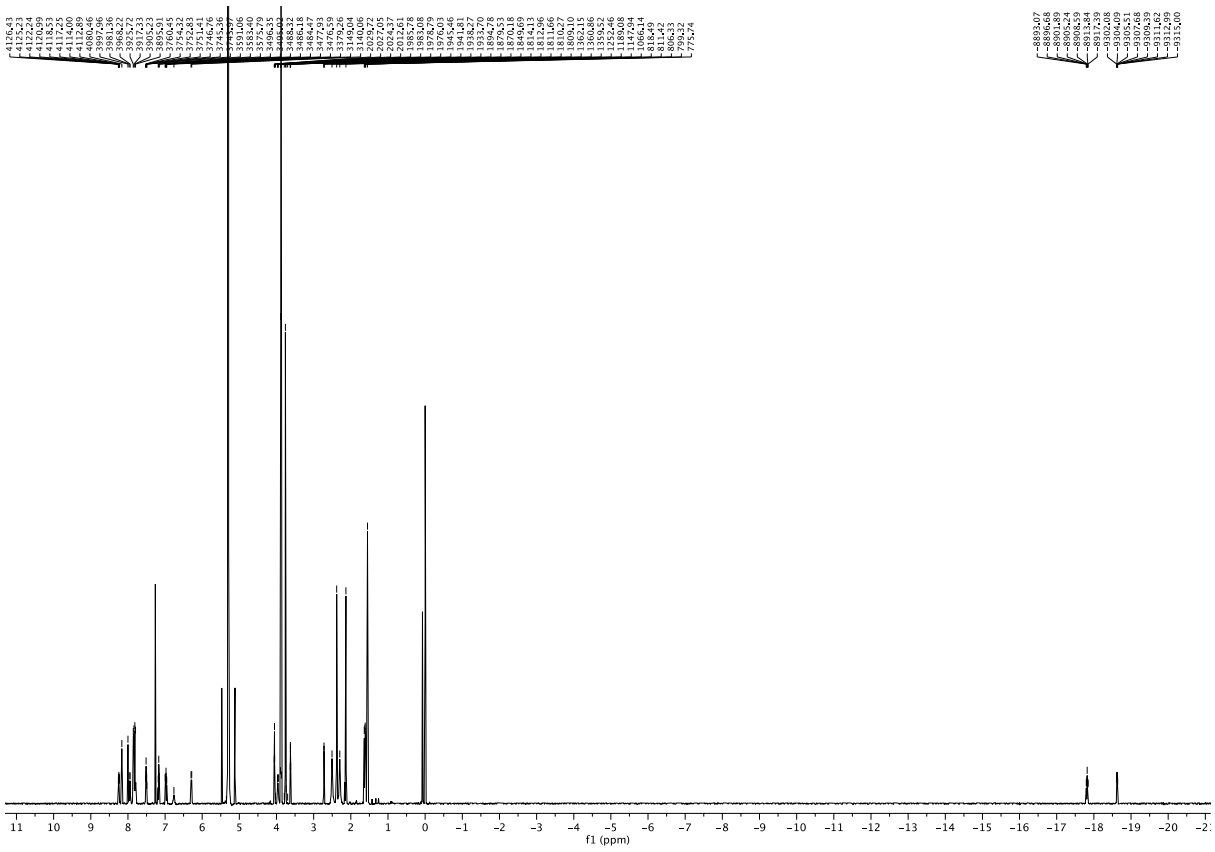

Figure S8. ^{1}H NMR of **10**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (m, 1H), 8.16 (s, 1H), 7.97 (m, 2H), 7.83 (dd, *J* = 21.0, 8.9 Hz, 5H), 7.50 (m, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.98 (ddd, *J* = 9.6, 8.0, 1.3 Hz, 1H), 6.76 (s, 1H), 6.29 (d, *J* = 9.0 Hz, 1H), 4.06 (t, *J* = 2.7 Hz, 1H), 3.88 (d, *J* = 3.5 Hz, 10H), 3.76 (s, 3H), 3.62 (dt, *J* = 2.6, 1.2 Hz, 1H), 2.72 (d, *J* = 2.6 Hz, 2H), 2.40 (m, 4H), 2.13 (s, 3H), 1.62 (dd, *J* = 12.1, 7.0 Hz, 3H), 1.55 (s, 3H), –17.82 (ddd, *J* = 12.2, 8.8, 3.4 Hz, 1H), –18.63 (ddd, *J* = 7.3, 3.4, 2.0 Hz, 1H).

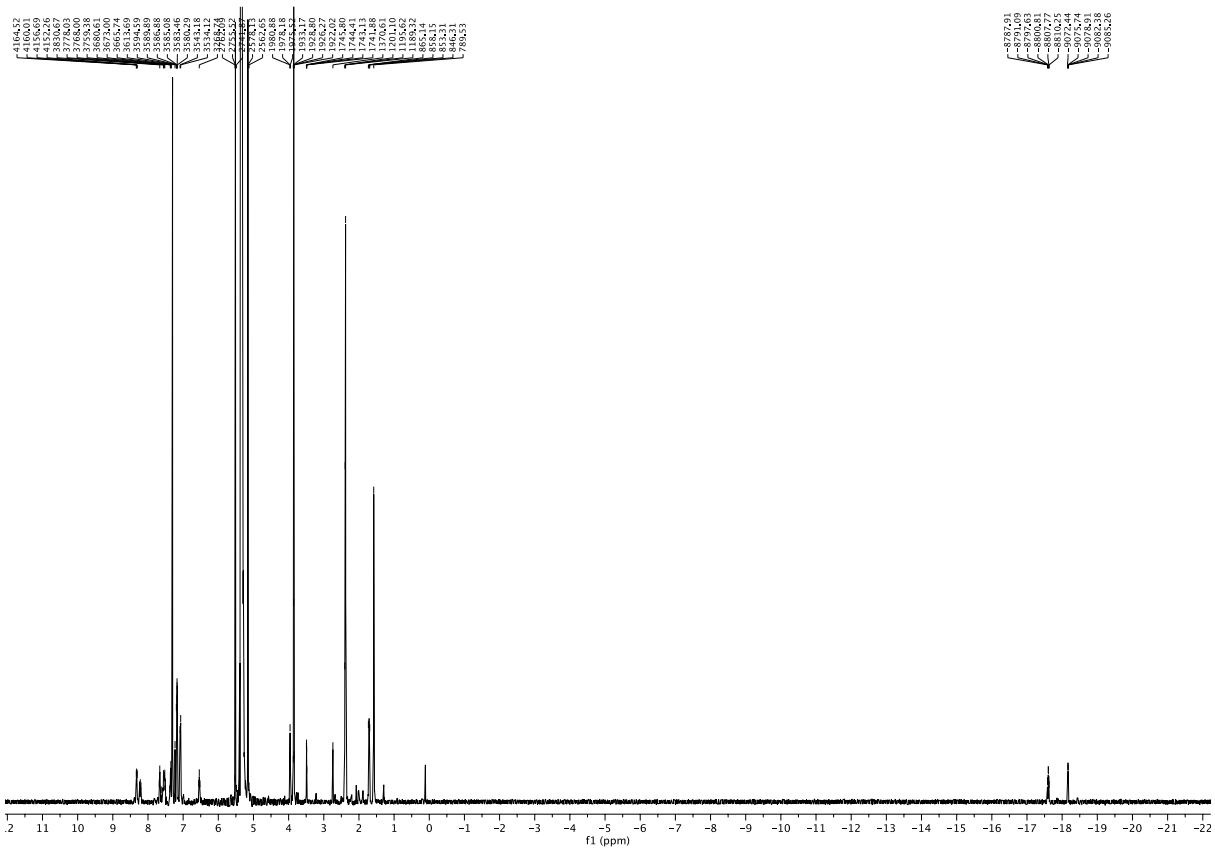

Figure S9. ^{1}H NMR of **11**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (m, 2H), 7.59 (m, 2H), 7.36 (q, *J* = 7.2 Hz, 2H), 7.23 (s, 1H), 7.17 (m, 3H), 7.08 (d, *J* = 9.1 Hz, 2H), 6.54 (t, *J* = 8.4 Hz, 2H), 5.51 (s, 3H), 5.16 (s, 2H), 3.96 (t, *J* = 2.7 Hz, 2H), 3.86 (d, *J* = 2.5 Hz, 4H), 3.49 (dd, *J* = 2.6, 1.3 Hz, 1H), 2.74 (s, 1H), 2.39 (d, *J* = 6.3 Hz, 12H), 1.71 (dd, *J* = 11.8, 7.0 Hz, 2H), 1.58 (s, 3H), –17.61 (td, *J* = 9.8, 3.0 Hz, 1H), –18.17 ('m', ddd, *J* = not resolved 1H).

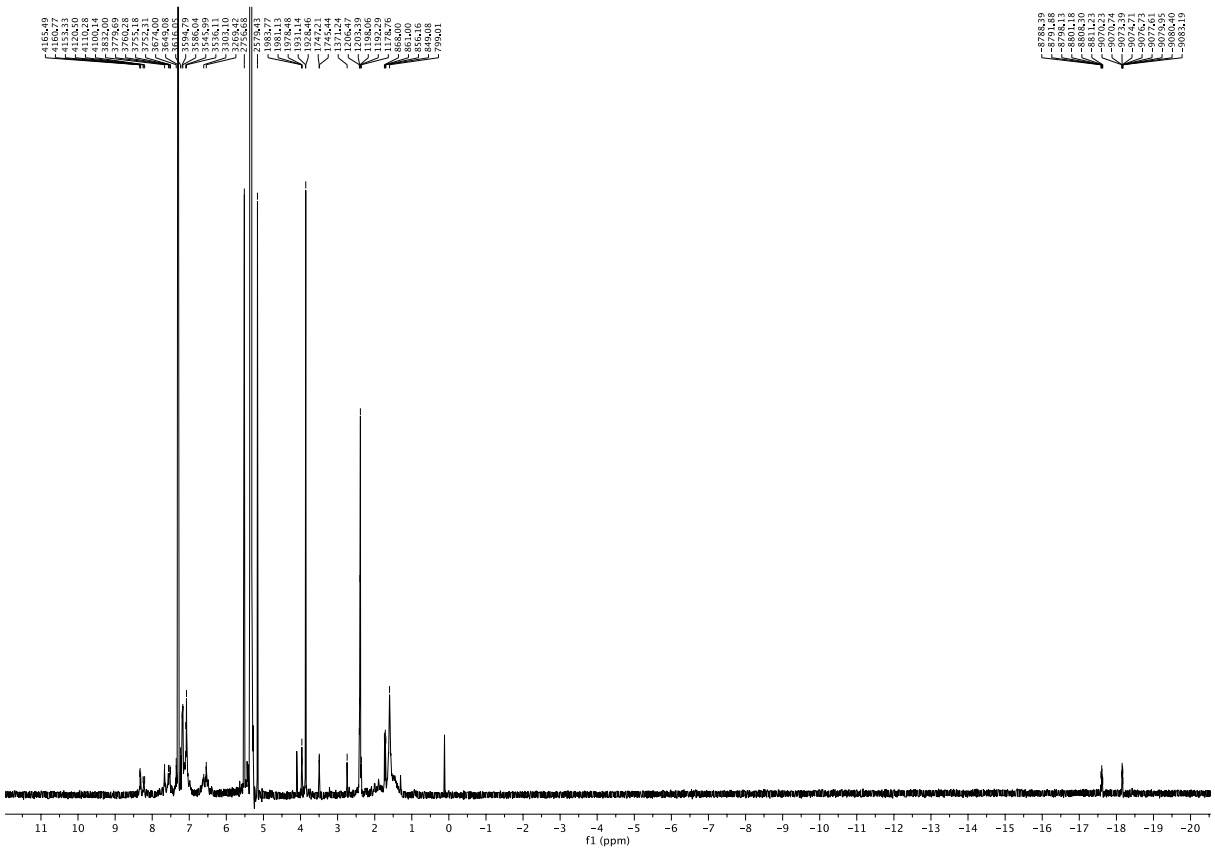

Figure S10. ^{1}H NMR of **12**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.3(m, 2H), 7.61 (m, 2H), 7.30 (s, 4H), 7.06 (m, 4H), 6.58 (d, *J* = 33.7 Hz, 2H), 5.52 (s, 3H), 5.16 (s, 2H), 3.96 (t, *J* = 2.6 Hz, 2H), 3.86 (d, *J* = 2.7 Hz, 4H), 3.49 (d, *J* = 1.8 Hz, 1H), 2.74 (s, 1H), 2.39 (m, 9H), 1.59 (m, 8H), –17.61 (ddd, *J* = 10.0, 3.0 Hz, 1H), –18.16 (m, ddd, *J* = not resolved 1H).

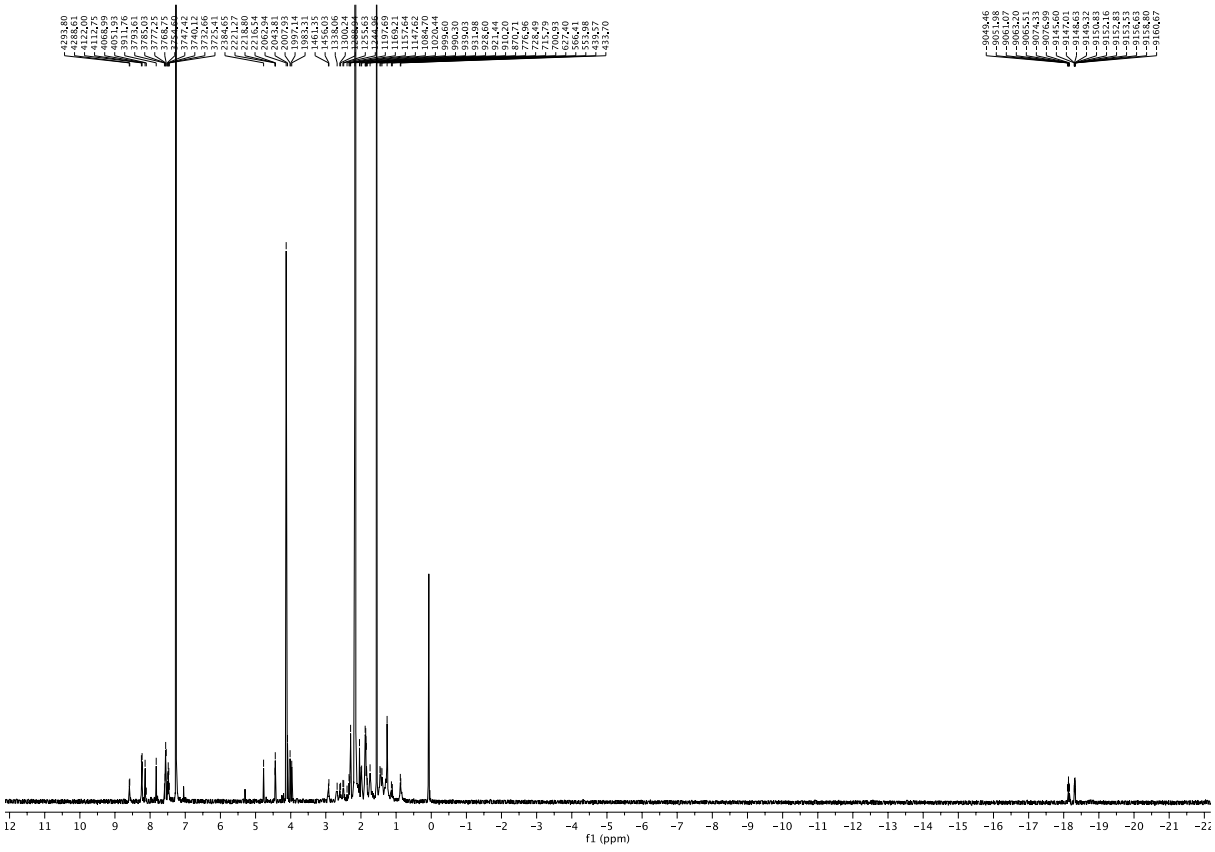

Figure S11. ^{1}H NMR of **13**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.2 Hz, 1H), 8.24 (d, *J* = 9.3 Hz, 2H), 8.12 (d, *J* = 17.1 Hz, 1H), 7.83 (s, 1H), 7.53 (ddd, *J* = 36.1, 15.6, 8.0 Hz, 5H), 4.77 (s, 1H), 4.44 (t, *J* = 2.4 Hz, 1H), 4.13 (s, 5H), 3.99 (d, *J* = 24.6 Hz, 1H), 2.59 (m, 2H), 2.32 (d, *J* = 21.6 Hz, 2H), 1.99 (d, *J* = 9.3 Hz, 2H), 1.86 (dd, *J* = 10.5, 7.1 Hz, 4H), 1.74 (s, 3H), 1.55 (s, 13H), –18.14 (ddd, *J* = 13.8, 4.5, 2.5 Hz, 1H), –18.31 ('m', ddd, *J* = not resolved 1H).

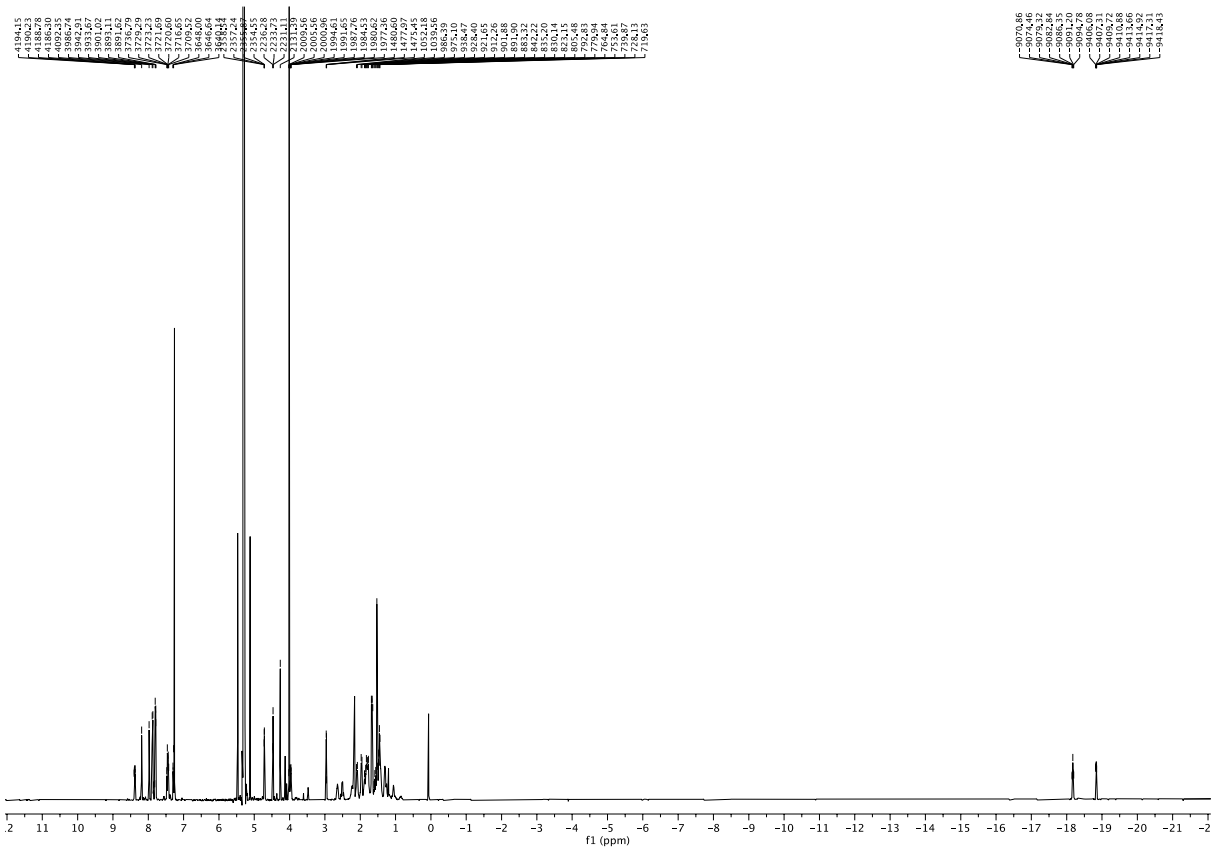

Figure S12. ^{1}H NMR of **14**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (ddd, *J* = 8.0, 3.9, 1.5 Hz, 1H), 8.19 (s, 1H), 7.98 (s, 1H), 7.88 (d, *J* = 9.2 Hz, 2H), 7.80 (m, 3H), 7.45 (dt, *J* = 12.2, 7.3 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 1H), 4.72 (dd, *J* = 2.7, 1.3 Hz, 1H), 4.47 (t, *J* = 2.6 Hz, 1H), 4.26 (s, 1H), 4.01 (s, 6H), 2.96 (d, *J* = 2.6 Hz, 1H), 1.94(m, 12H), 1.67 (dd, *J* = 12.1, 7.0 Hz, 3H), 1.50 (m, 8H), –18.17 (ddd, *J* = 11.9, 7.0, 3.6 Hz, 1H), –18.83 (ddd, *J* = 4.8, 3.6, 1.2 Hz, 1H).

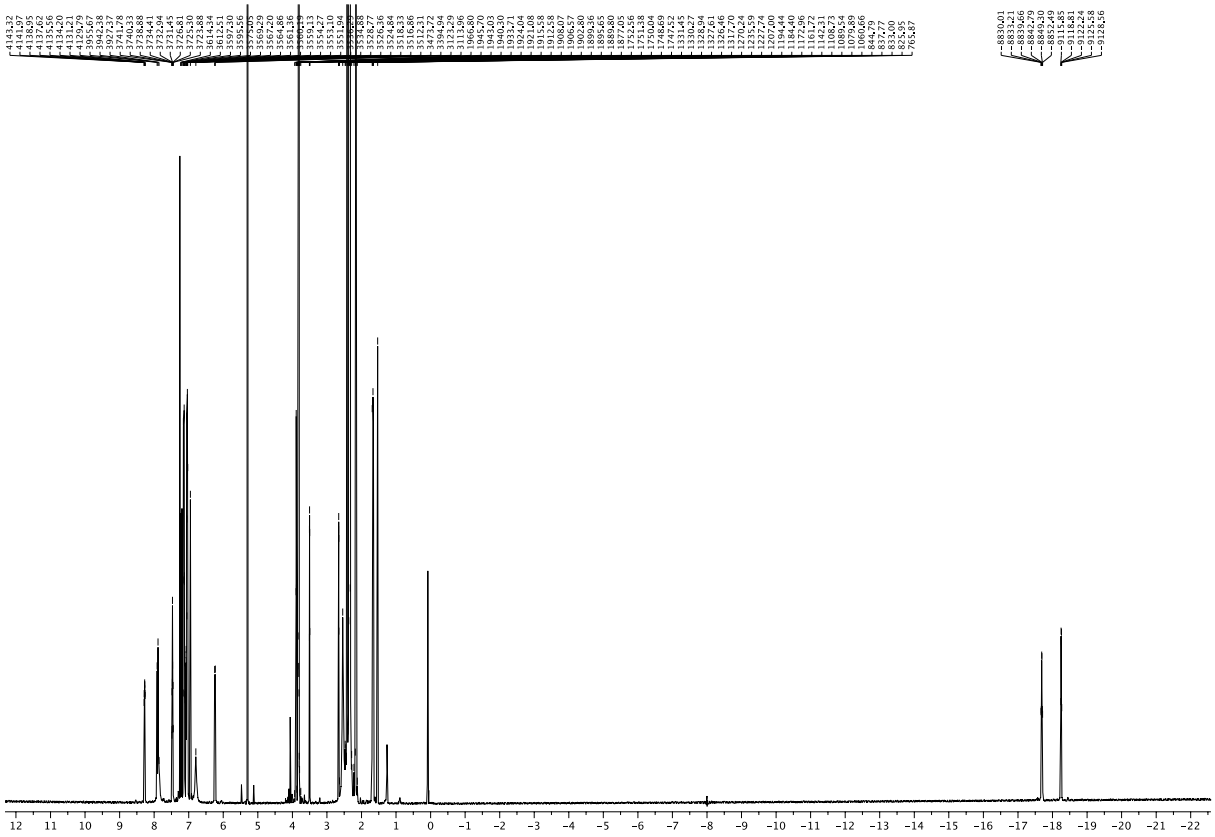

Figure S13. ^{1}H NMR of **15**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (ddd, *J* = 7.8, 4.4, 1.4 Hz, 1H), 7.89 (t, *J* = 14.2 Hz, 2H), 7.47 (tt, *J* = 7.6, 1.4 Hz, 1H), 7.21 (m, 2H), 7.13 (m, 3H), 7.04 (m, 4H), 6.95 (s, 1H), 6.79 (s, 1H), 6.24 (d, *J* = 9.3 Hz, 1H), 3.83 (s, 7H), 3.50 (dt, *J* = 2.5, 1.2 Hz, 1H), 2.66 (dt, *J* = 2.5, 1.2 Hz, 1H), 2.38 (d, *J* = 34.0 Hz, 21H), 2.16 (s, 3H), 1.67 (dd, *J* = 11.8, 7.0 Hz, 3H), –17.69 (td, *J* = 9.7, 3.0 Hz, 1H), –18.25 (dt, *J* = 6.4, 3.0 Hz, 1H).

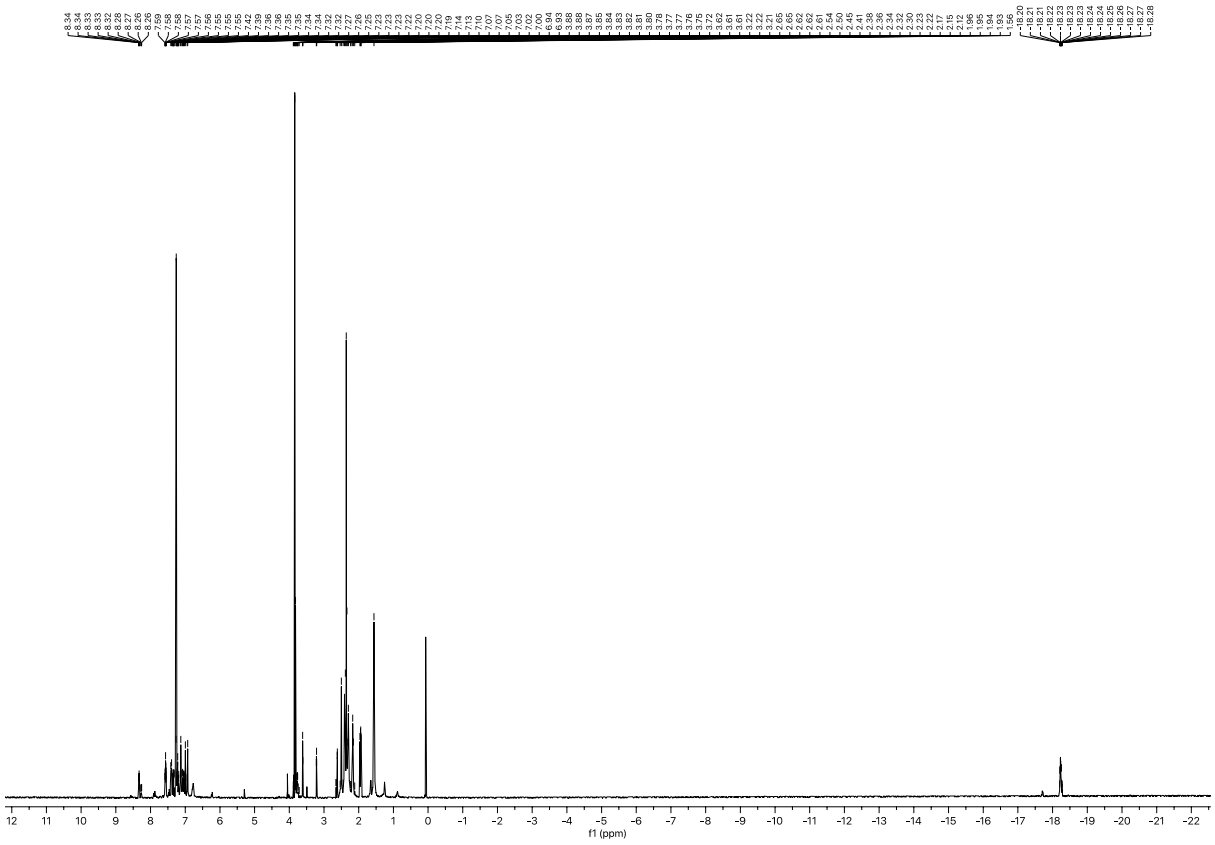

Figure S14. ^{1}H NMR of **16**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (ddd, *J* = 31.7, 7.4, 4.3 Hz, 1H), 7.57 (tt, *J* = 6.5, 2.0 Hz, 1H), 7.41 (d, *J* = 11.4 Hz, 2H), 7.34 (ddd, *J* = 11.9, 8.0, 1.4 Hz, 1H), 7.20 (m, 2H), 7.07 (m, 4H), 6.94 (d, *J* = 7.6 Hz, 1H), 3.83 (d, *J* = 11.5 Hz, 6H), 3.61 (t, *J* = 2.7 Hz, 1H), 3.22 (t, *J* = 2.1 Hz, 1H), 2.56 (m, 1H), 2.46 (d, *J* = 44.8 Hz, 7H), 2.33 (m, 18H), 1.95 (dd, *J* = 10.3, 7.2 Hz, 3H), 1.56 (s, 3H), –18.16 (m, 2H).

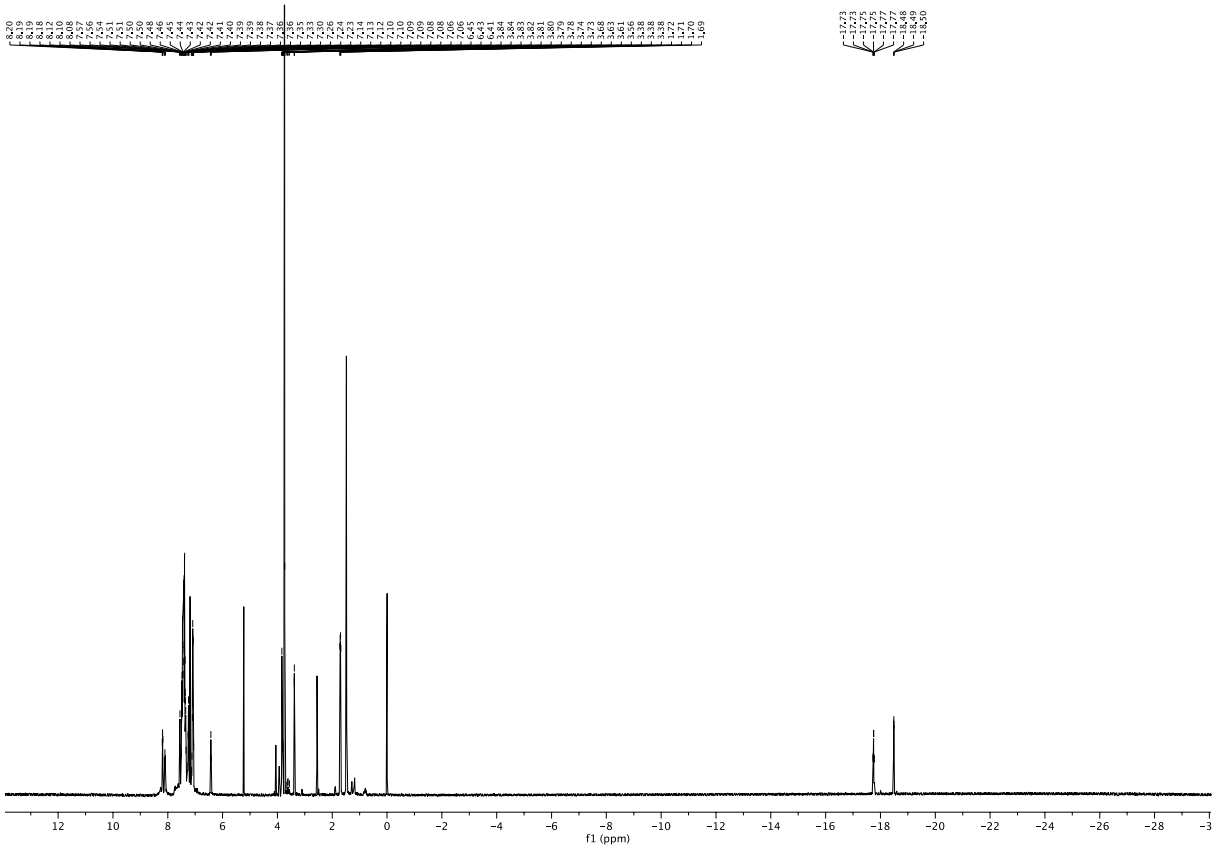

Figure S15. ^{1}H NMR of **17**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 7.8, 4.5 Hz, 1H), 8.10 (m, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.41 (m, 14H), 7.24 (t, *J* = 7.4 Hz, 1H), 7.09 (qd, *J* = 9.5, 8.9, 4.2 Hz, 4H), 6.43 (t, *J* = 8.5 Hz, 1H), 3.82 (m, 1H), 3.74 (s, 6H), 3.62 (dd, *J* = 33.4, 25.7 Hz, 1H), 3.38 (m, 1H), 1.70 (dd, *J* = 11.9, 7.0 Hz, 4H), –17.75 (ddd, *J* = 10.1, 9.1, 3.0 Hz, 1H), –18.47 (dt, *J* = 6.1, 3.0 Hz, 1H).

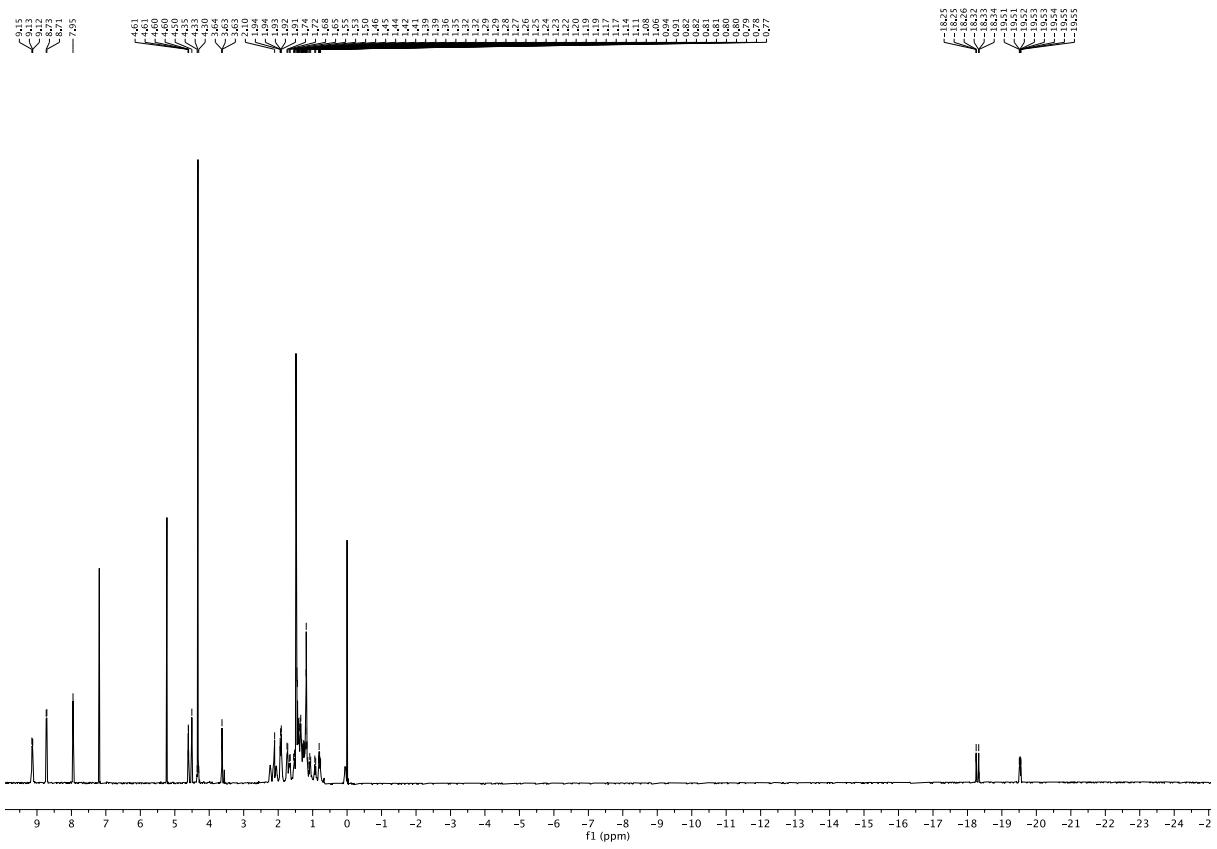

Figure S16. ^{1}H NMR of **18**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.15 (d, *J* = 9.9 Hz, 2H), 8.72 (d, *J* = 10.4 Hz, 2H), 7.95 (s, 2H), 4.61 (q, *J* = 2.3 Hz, 1H), 4.50 (s, 1H), 4.33 (s, 5H), 3.63 (d, *J* = 2.9 Hz, 1H), 2.05 (m, 4H), 1.66 (m, 5H), 1.38 (m, 6H), 1.01 (m, 11H), –18.29 (dt, *J* = 36.5, 2.5 Hz, 1H), –19.46 (ddd, *J* = 13.3, 7.1, 2.5 Hz, 1H).

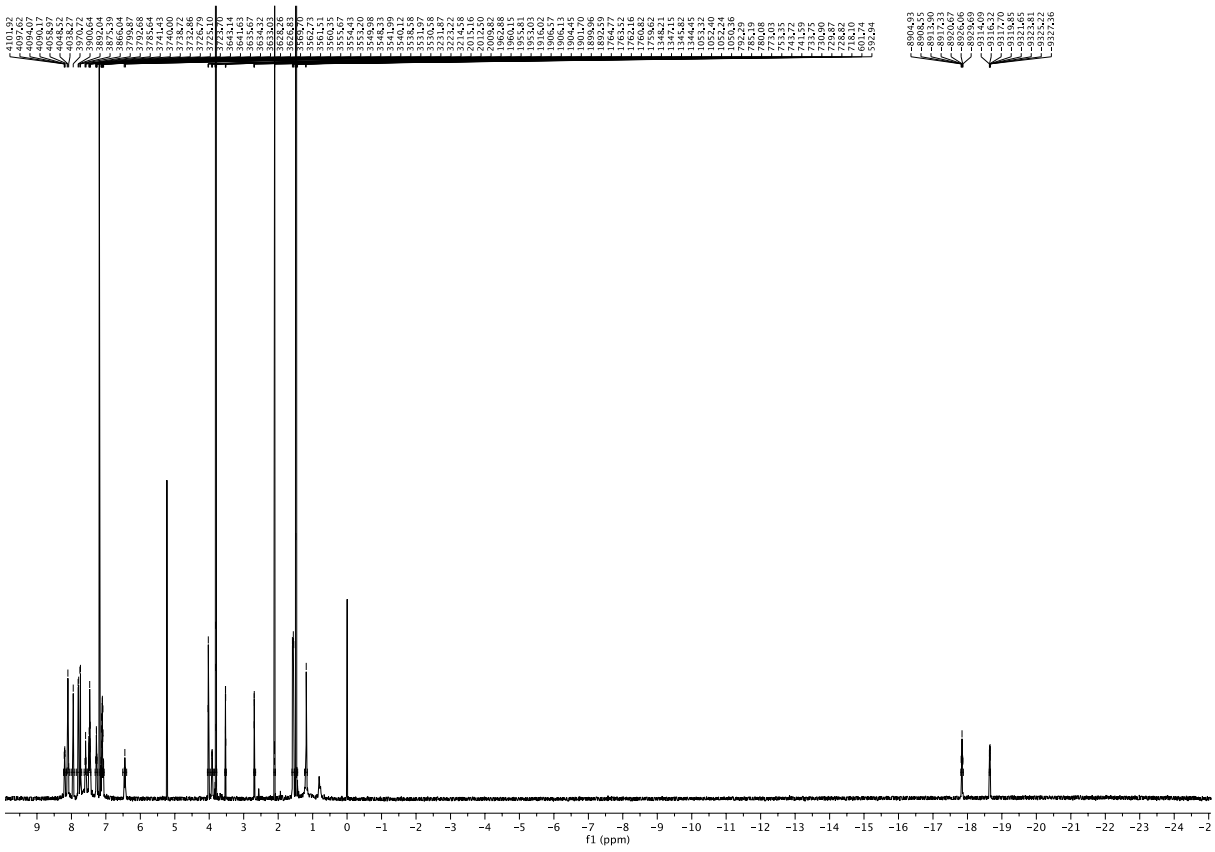

Figure S17. ^{1}H NMR of **19**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 7.7, 4.1 Hz, 1H), 8.09 (d, *J* = 10.2 Hz, 2H), 7.95 (s, 1H), 7.77 (dd, *J* = 25.6, 9.0 Hz, 4H), 7.59 (t, *J* = 7.1 Hz, 1H), 7.48 (m, 2H), 7.27 (td, *J* = 7.5, 1.5 Hz, 1H), 7.11 (m, 3H), 6.45 (t, *J* = 8.6 Hz, 1H), 4.03 (t, *J* = 2.7 Hz, 1H), 3.92 (dd, *J* = 7.1, 2.8 Hz, 1H), 3.81 (s, 5H), 3.53 (dt, *J* = 2.5, 1.2 Hz, 1H), 2.69 (dd, *J* = 2.5, 1.2 Hz, 1H), 2.10 (s, 2H), 1.57 (dd, *J* = 12.2, 7.1 Hz, 3H), 1.48 (s, 11H), –17.84 (ddd, *J* = 12.7, 9.0, 3.6 Hz, 1H), –18.65 (ddd, *J* = 7.5, 3.6, 2.2 Hz, 1H).

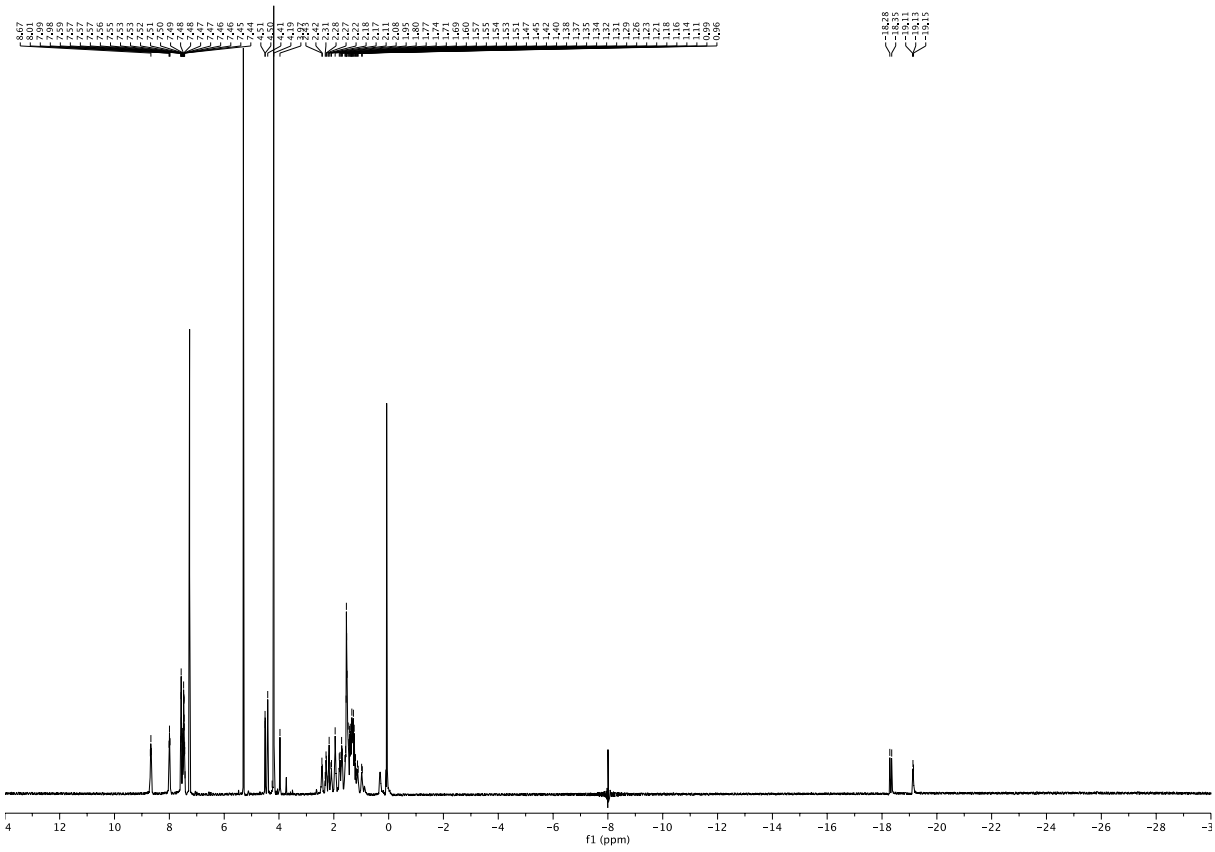

Figure S18. ^{1}H NMR of **20**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (t, *J* = 9.6 Hz, 2H), 7.99 (m, 2H), 7.51 (m, 7H), 4.45 (m, 3H), 4.19 (s, 6H), 3.97 (s, 1H), 1.69 (m, 23H), –18.32 (d, *J* = 34.2 Hz, 1H), –19.13 ('t', ddd, *J* = not resolved 1H).

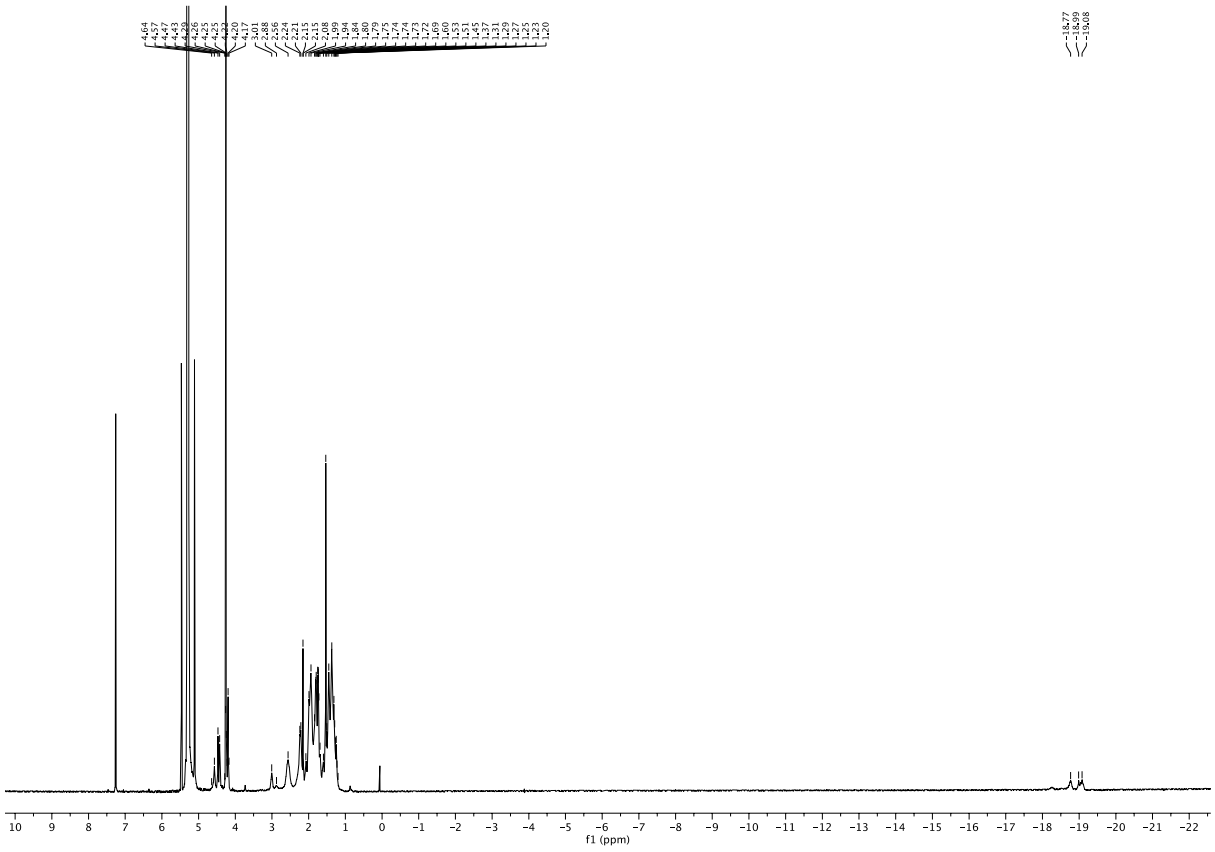

Figure S19. ^{1}H NMR of **21**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.57 (s, 1H), 4.45 (d, *J* = 22.8 Hz, 2H), 4.25 (s, 5H), 2.11 (m, 24H), –18.77 (br, 1H), –19.09 (m, 1H).

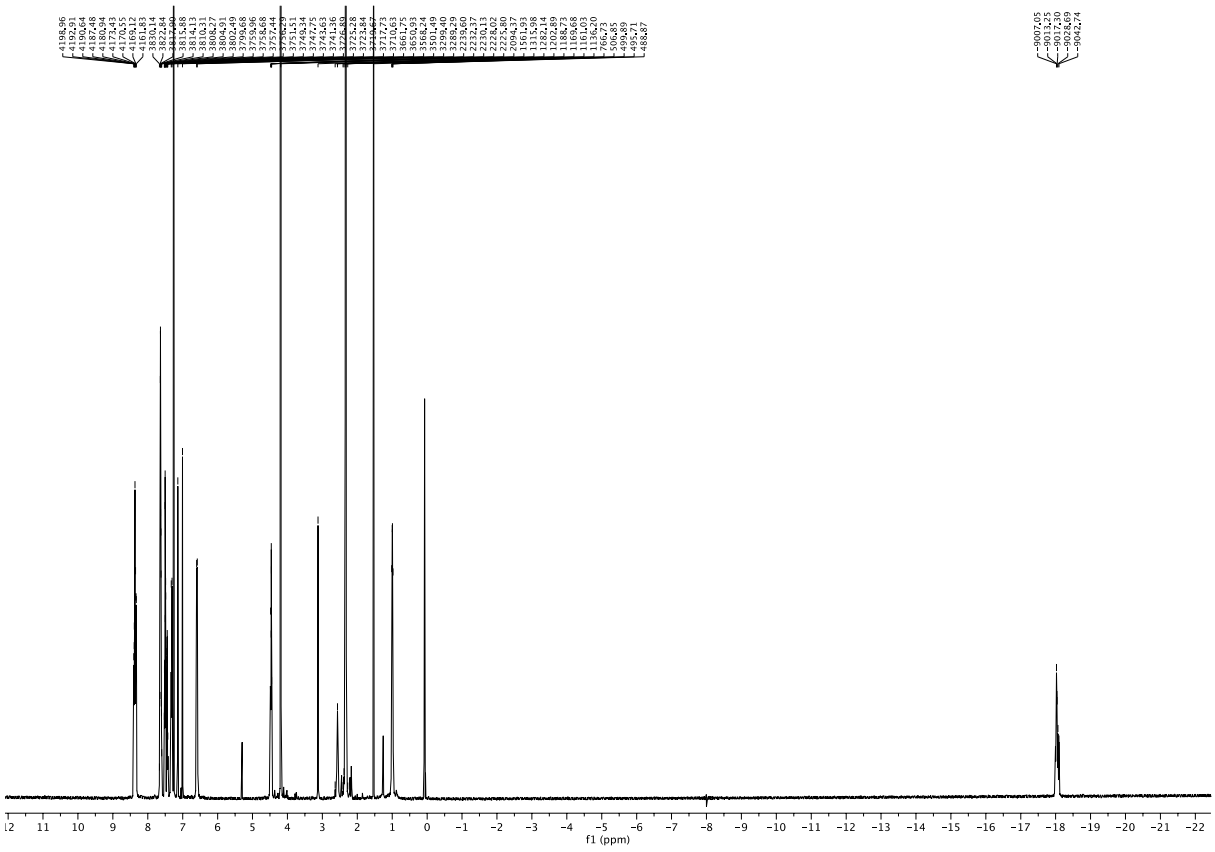

Figure S20. ^{1}H NMR of **22**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (m, 4H), 7.63 (h, *J* = 5.8, 5.4 Hz, 3H), 7.51 (m, 2H), 7.44 (m, 1H), 7.32 (d, *J* = 10.8 Hz, 2H), 7.14 (s, 1H), 7.01 (s, 1H), 6.59 (d, *J* = 10.1 Hz, 2H), 4.47 (m, 2H), 4.19 (s, 5H), 3.13 (s, 1H), 2.57 (s, 1H), 2.33 (d, *J* = 8.6 Hz, 11H), 1.53 (s, 1H), 1.00 (dd, *J* = 11.1, 6.9 Hz, 3H), –17.93 (ddd, *J* = 11.8, 2.0 Hz, 1H), –18.10 (m, ddd, *J* = 23.4, 10.4, 2.0 Hz, 1H).

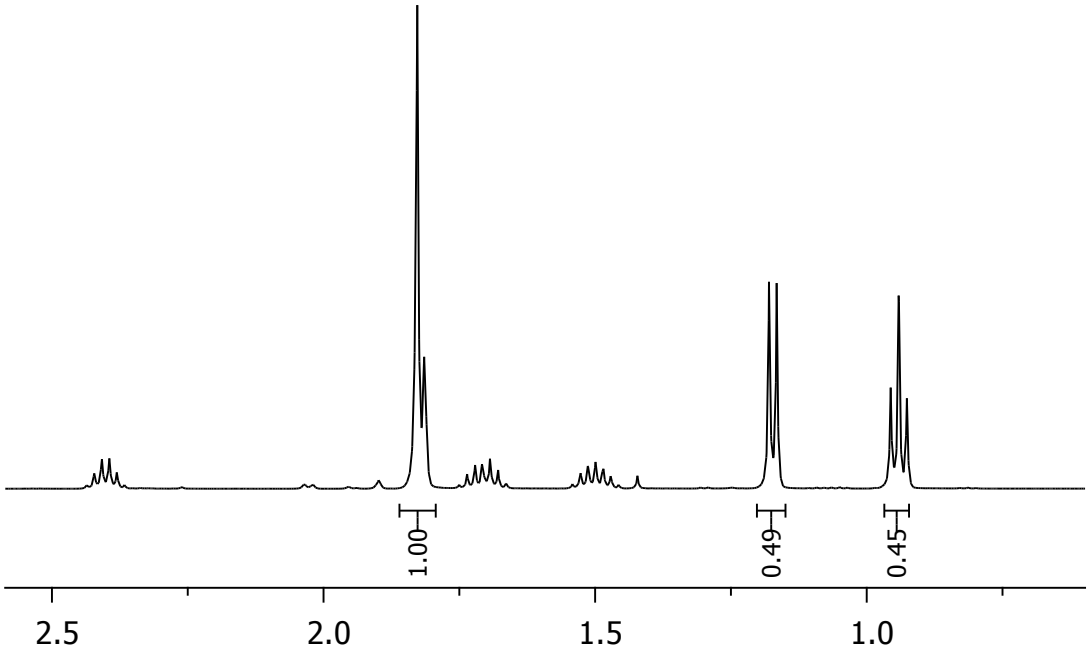

Figure S21. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1a})]$ **3**.

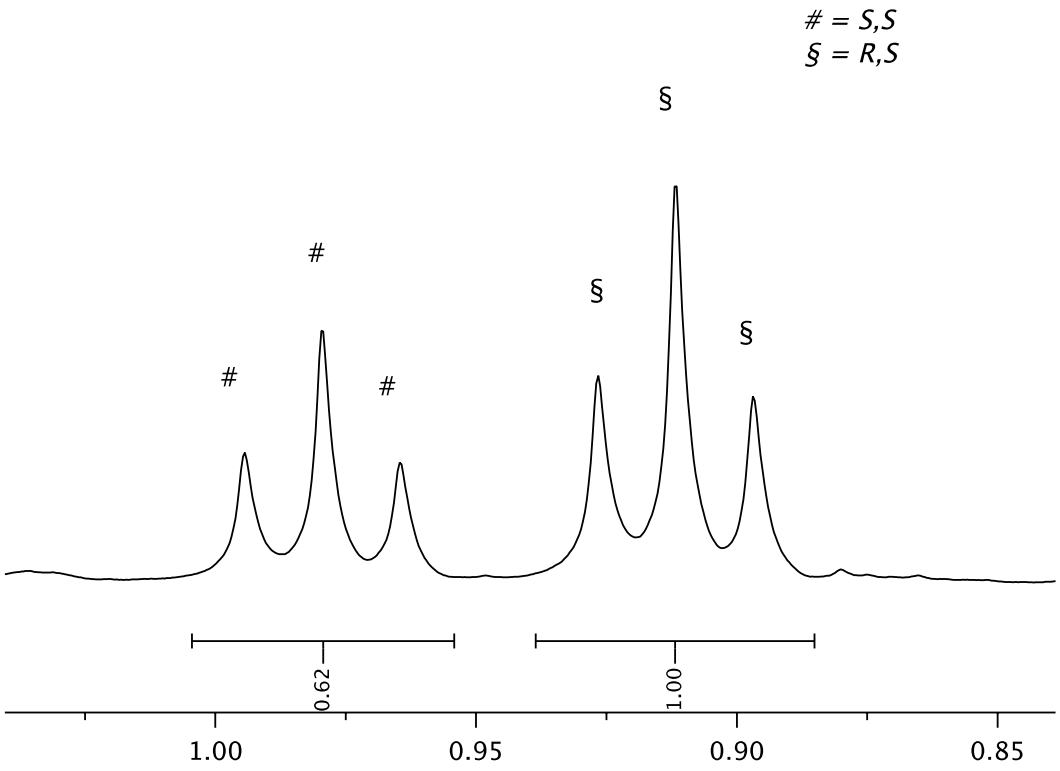

***Figure S22*.** Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1a**)] **3**.

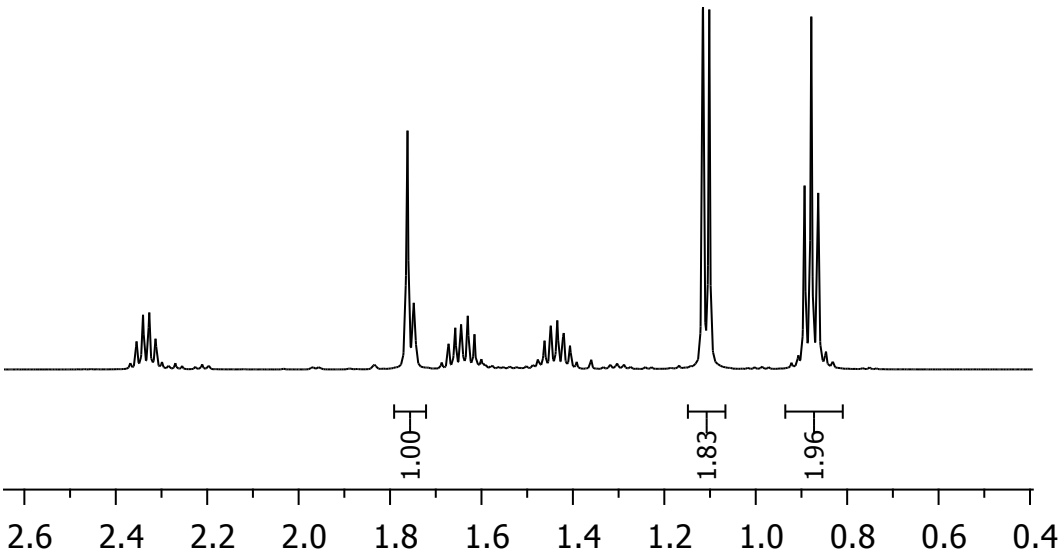

Figure S23. Determination of catalytic asymetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1a**)] **4**.

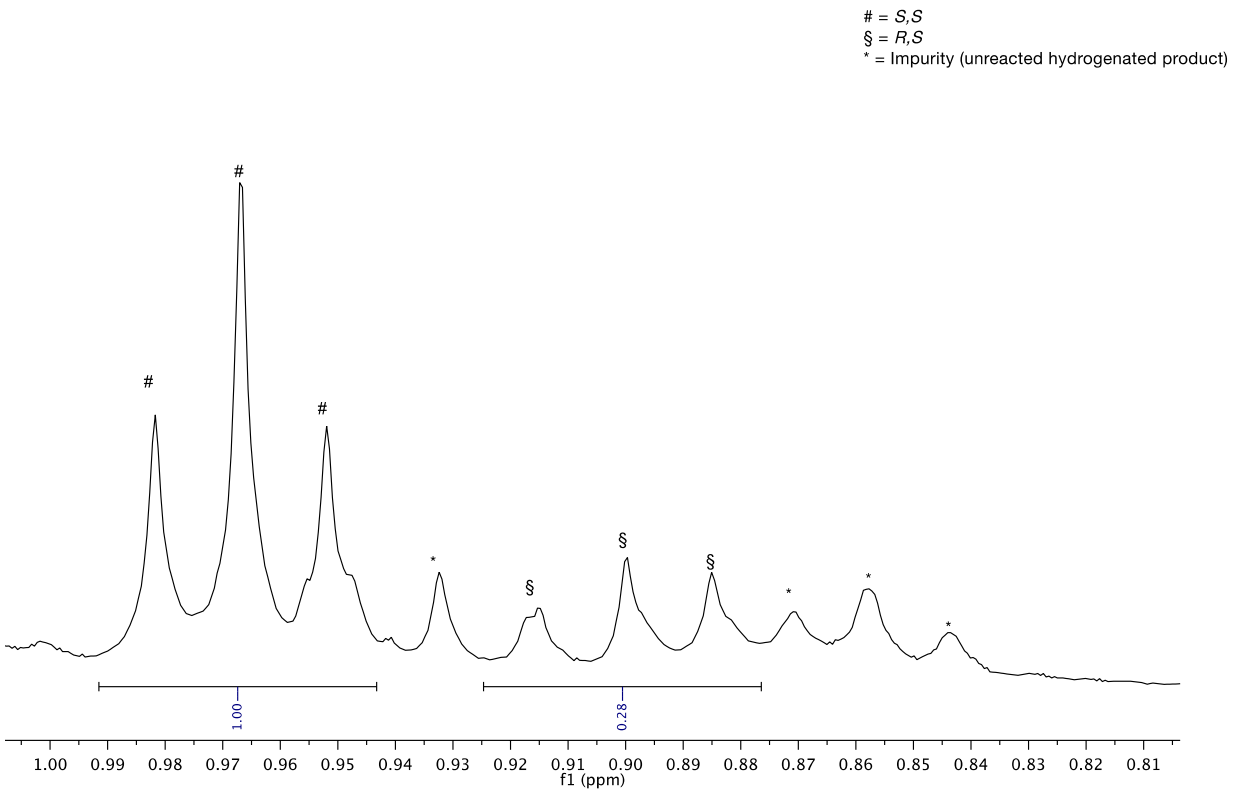

***Figure S24*.** Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1a**)] **4**.

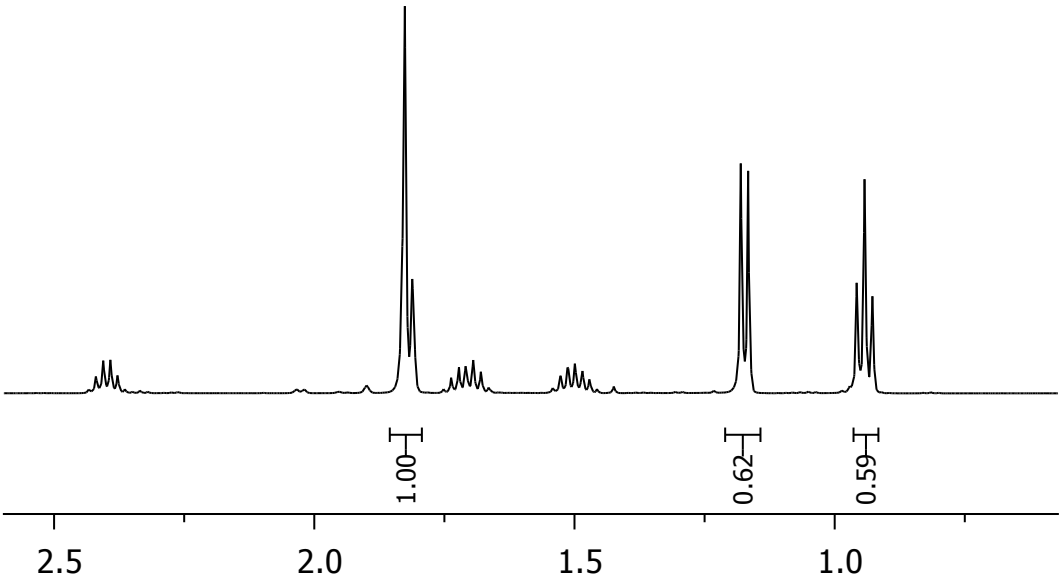

Figure S25*.** Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis ofproducts from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-S,S*-1b**)] **5**.

= *S,S*
§ = *R,S*
* = Impurity (unreacted hydrogenated Product)

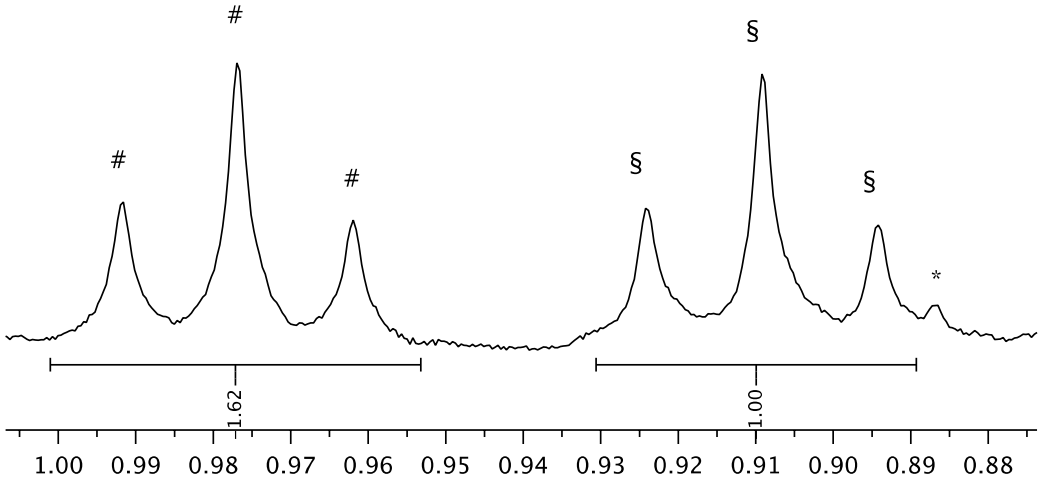

Figure S26*.** Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-S,S***-**1b**)] **5**.

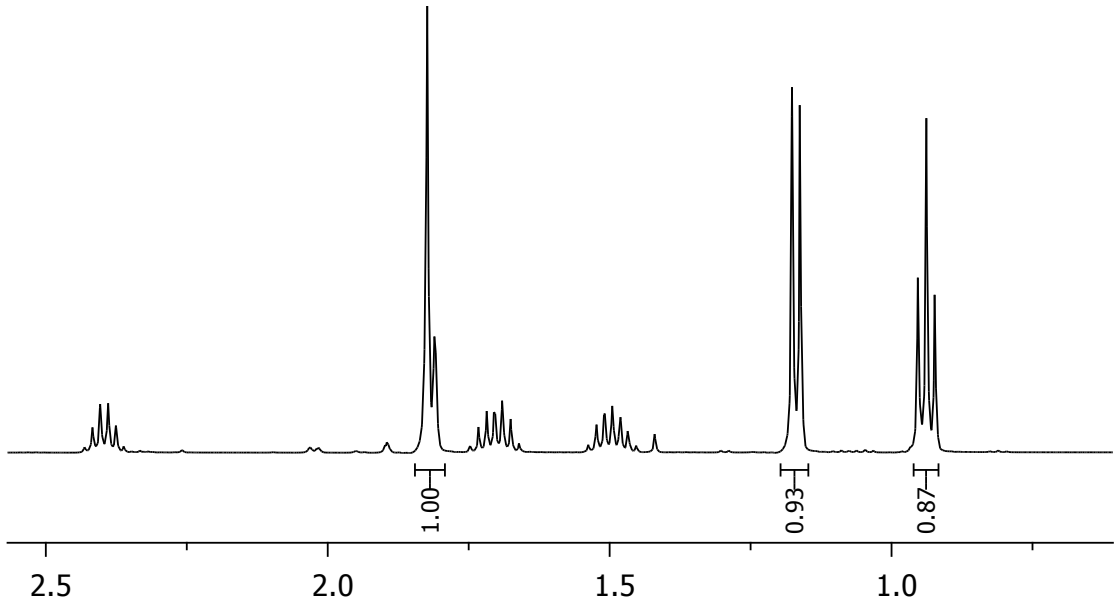

***Figure S27*.** Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}\boldsymbol{S,S}\text{-}\mathbf{1b})]$ **6**.

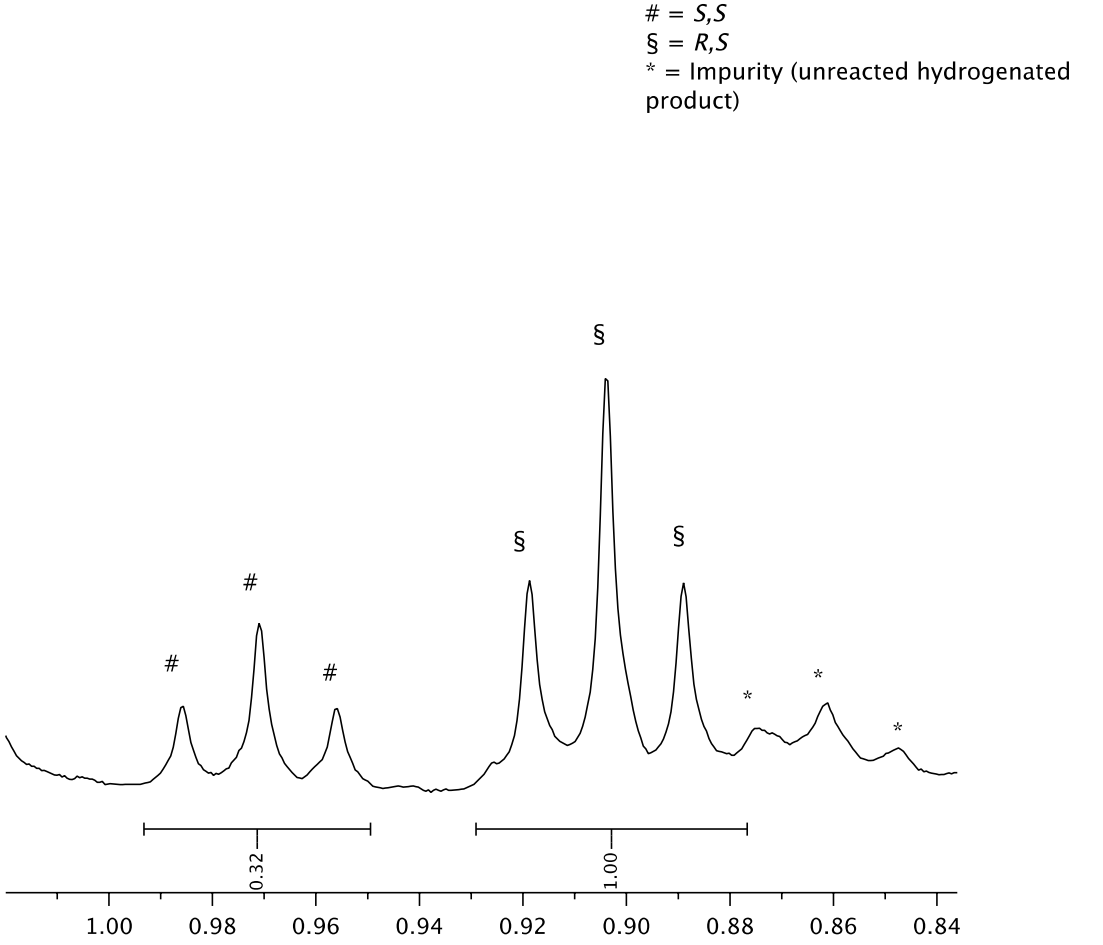

Figure S28. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}\boldsymbol{S,S}\text{-}\mathbf{1b})]$ **6**.

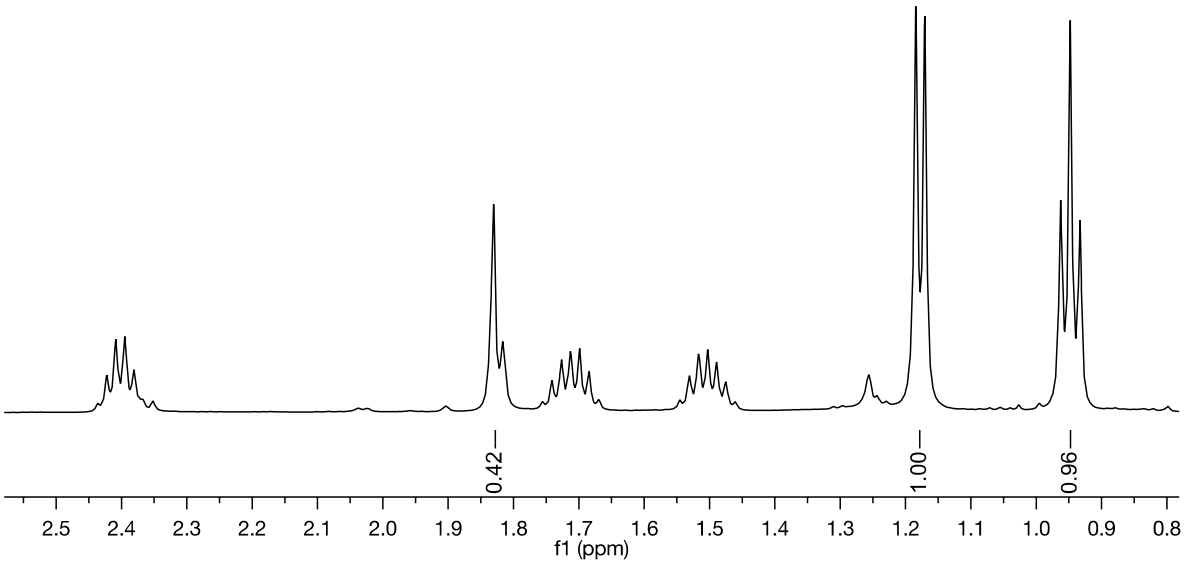

Figure S29. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1c})]$ **7**.

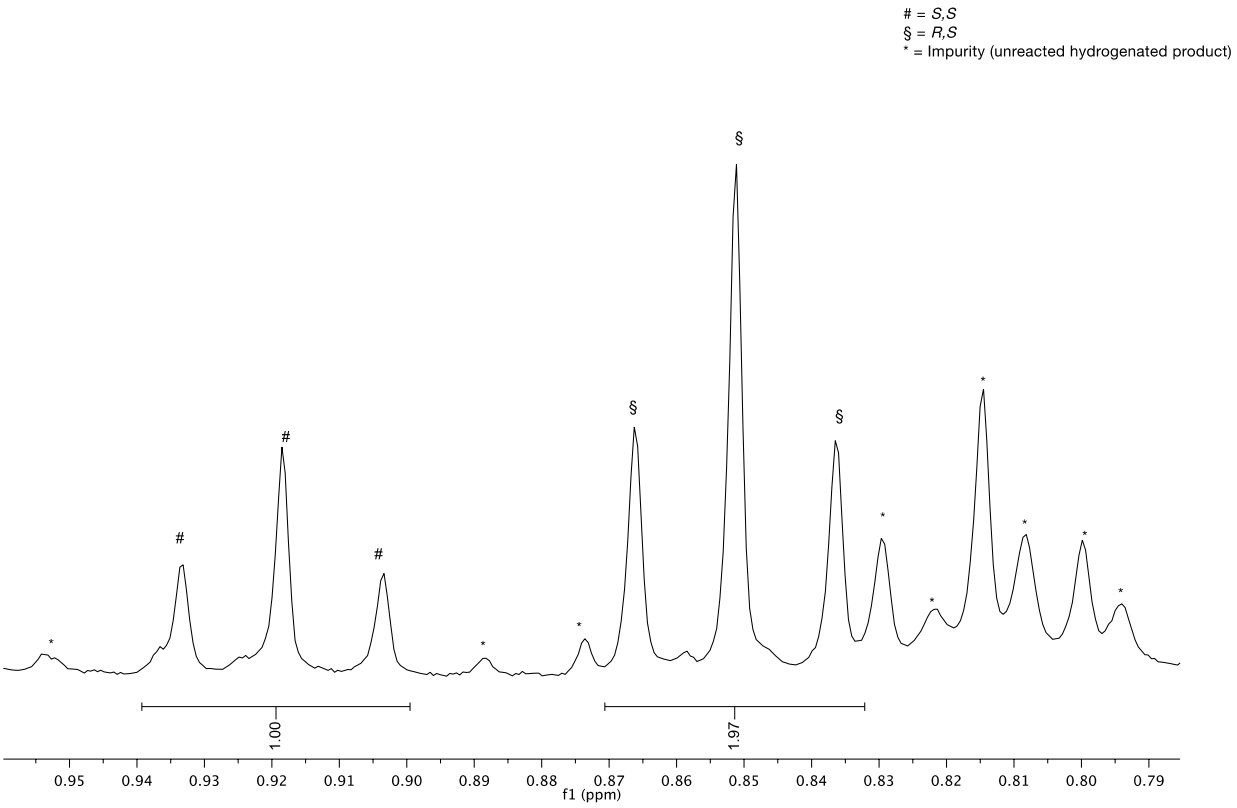

Figure S30. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1c**)] **7**.

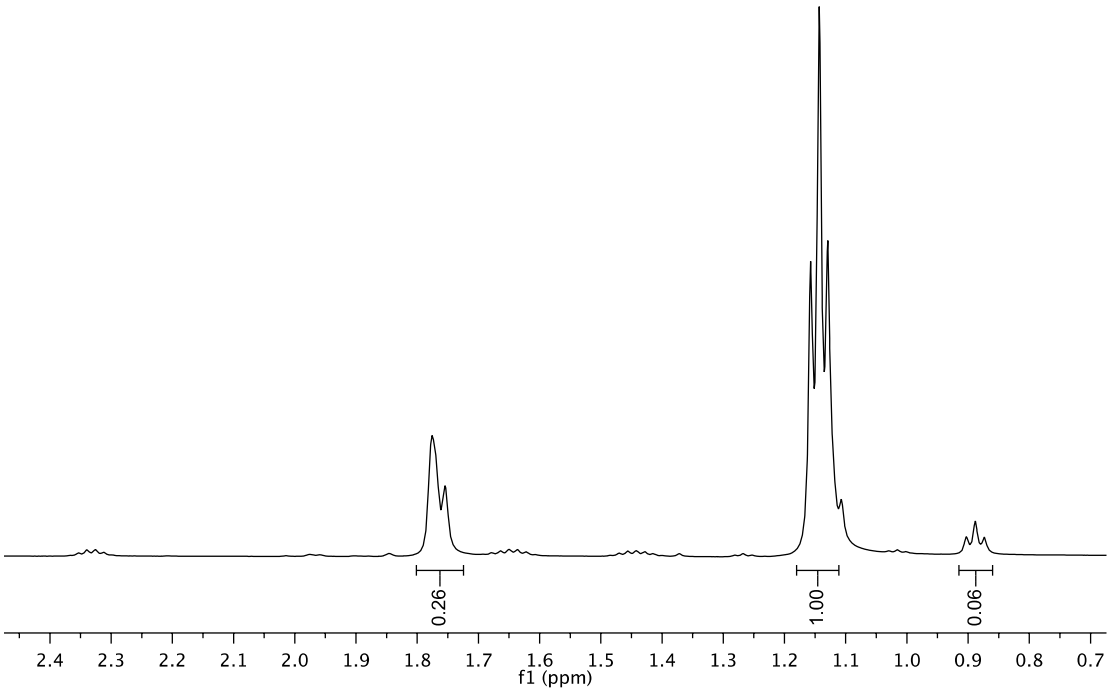

Figure S31. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1c})]$ **8**.

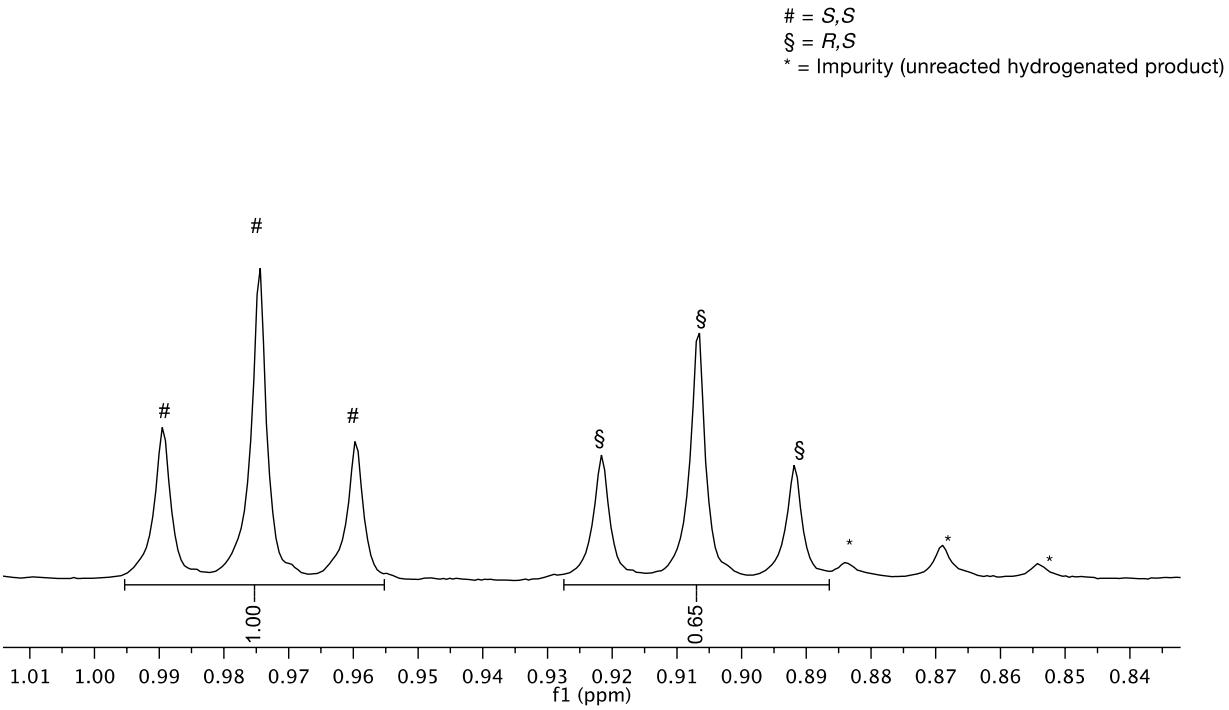

Figure S32. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1c**)] **8**.

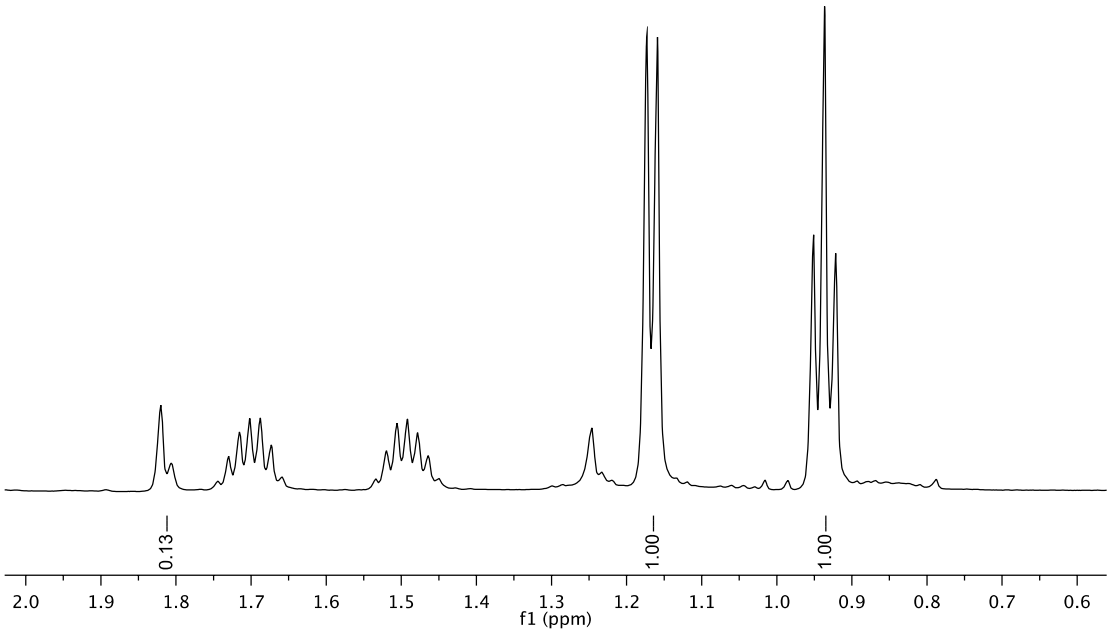

Figure S33. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1d})]$ **9**.

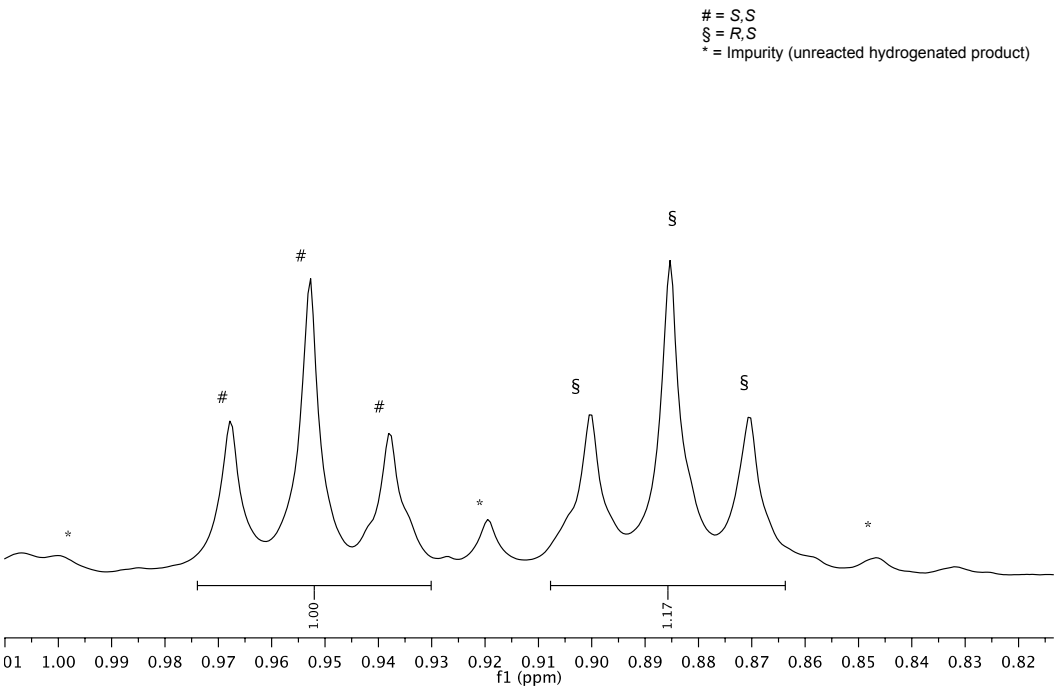

Figure S34. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1d**)] **9**.

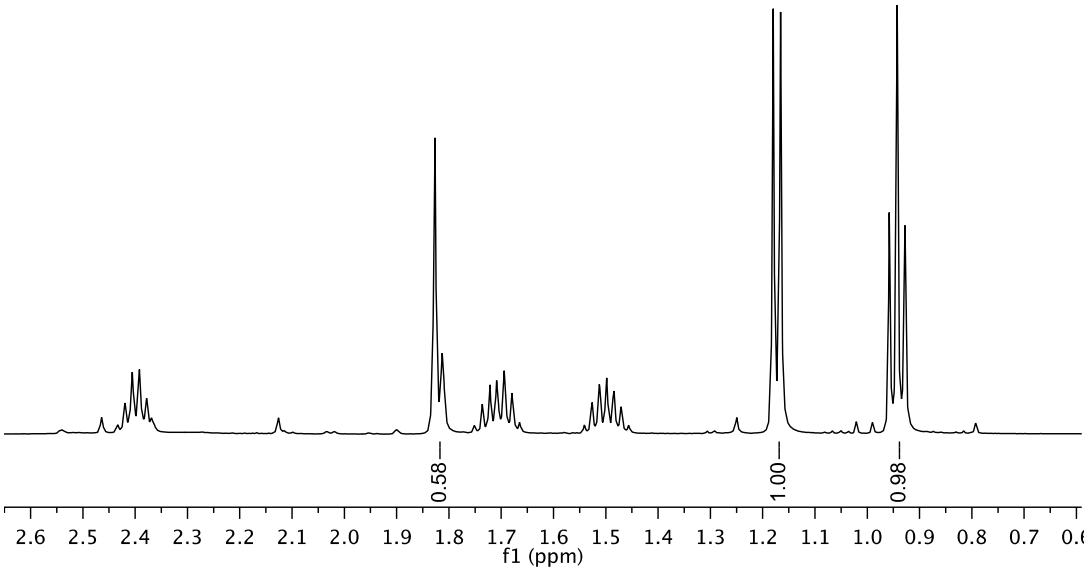

Figure S35. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}$**1d**$)]$ **10**.

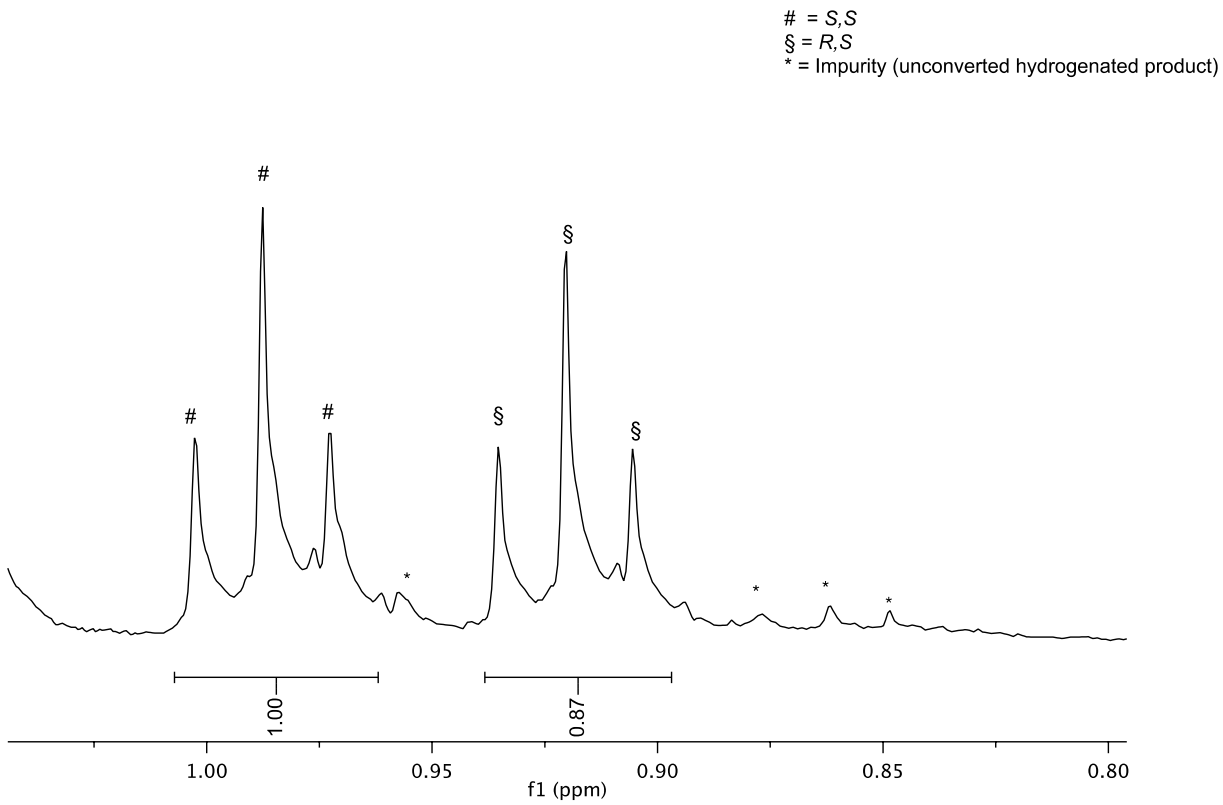

Figure S36. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1d**)] **10**.

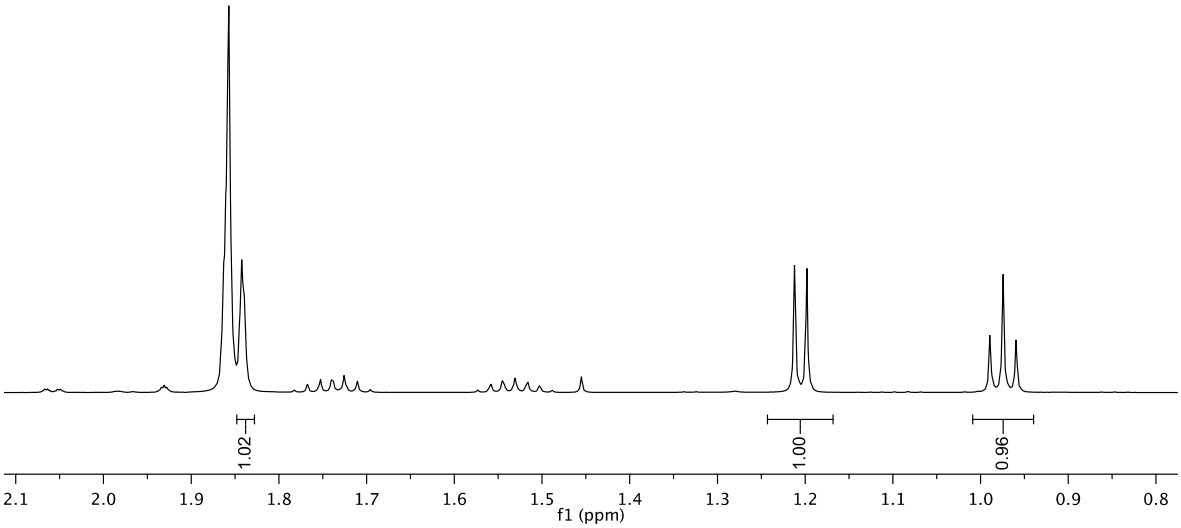

Figure S37. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1e})]$ **11**.

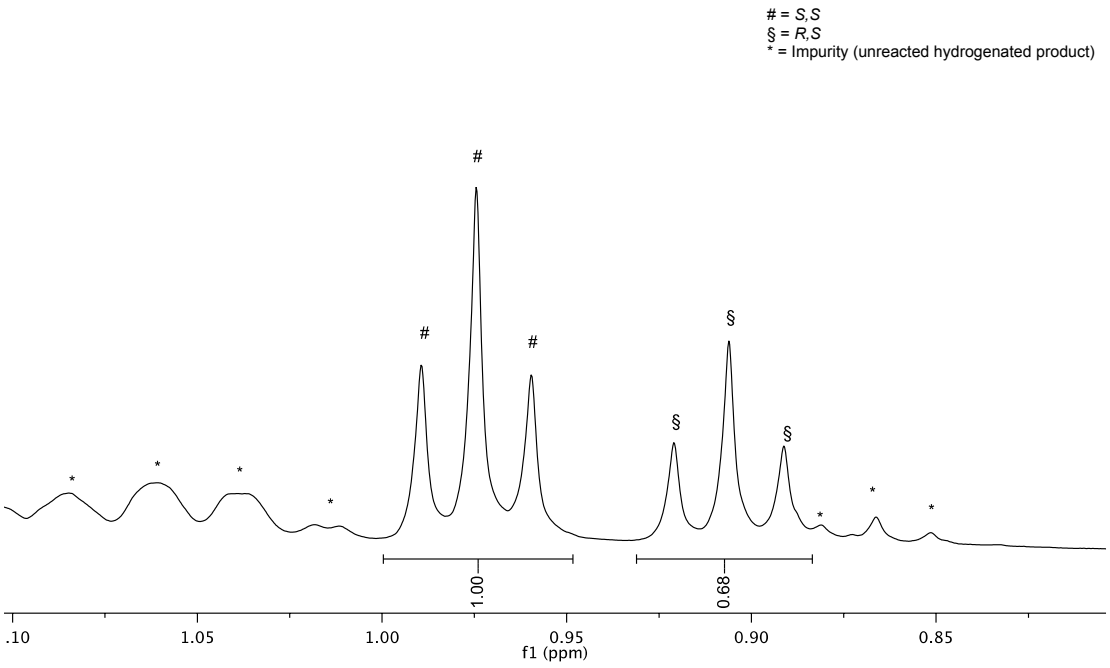

Figure S38. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1e**)] **11**.

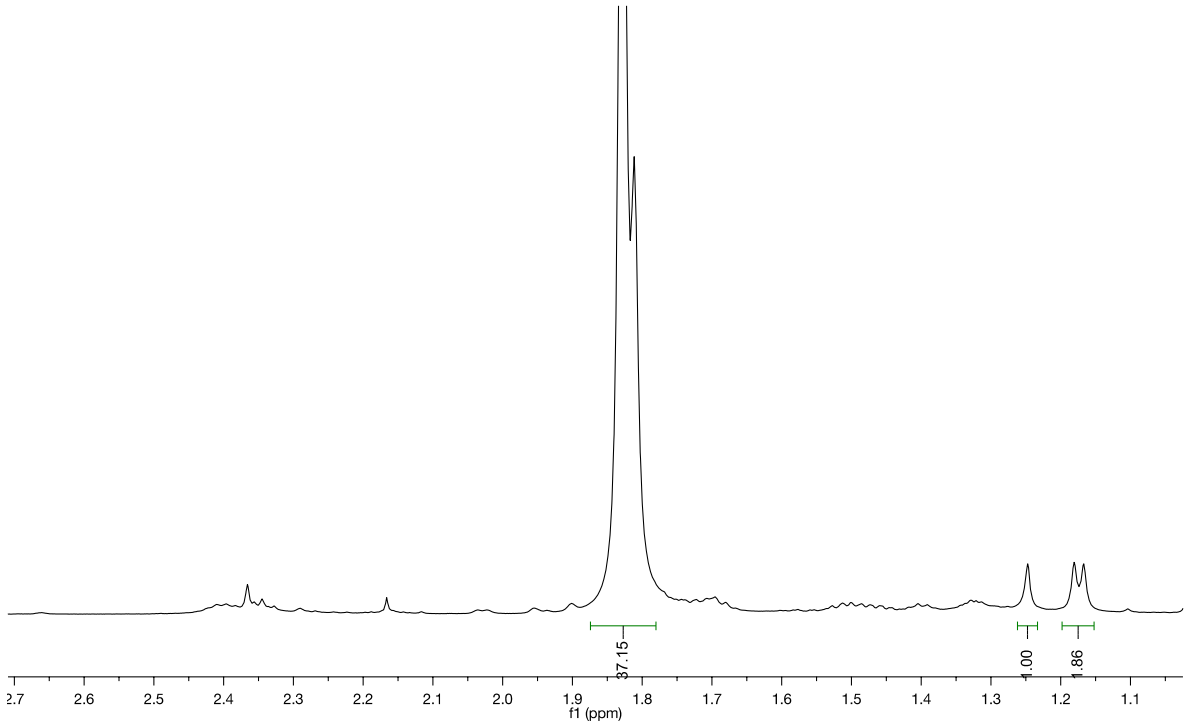

Figure S39. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1e})]$ **12**.

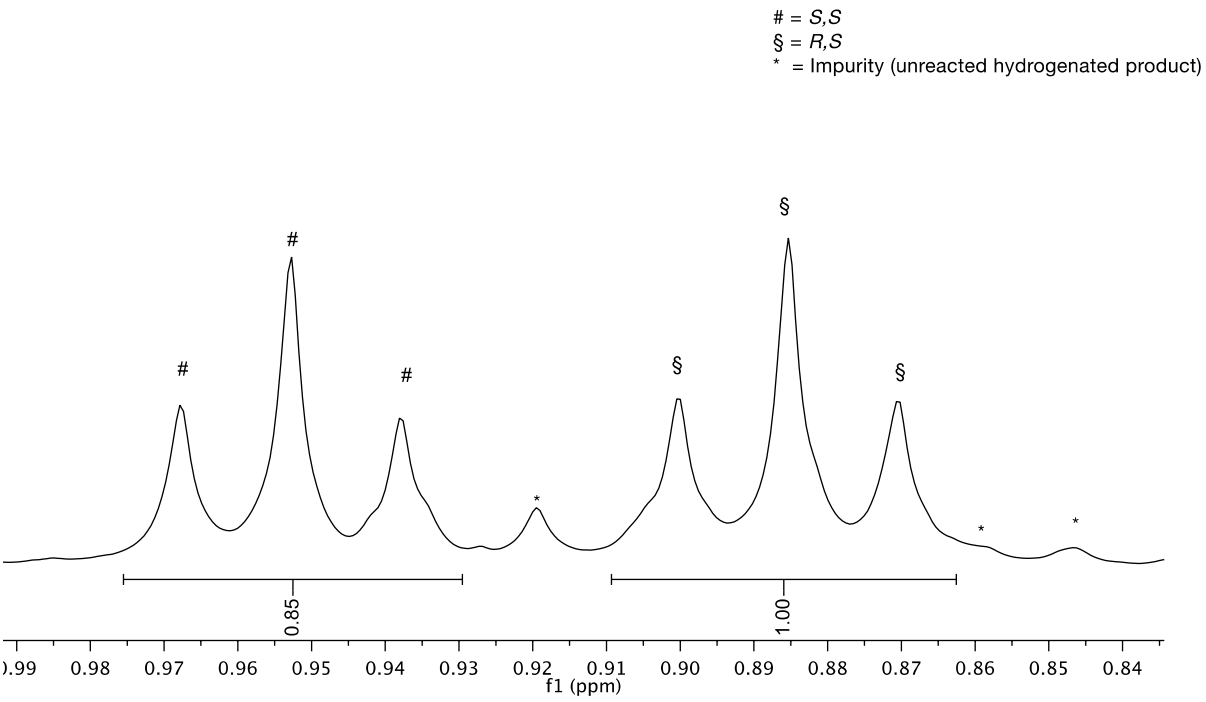

Figure S40. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1e**)] **12**.

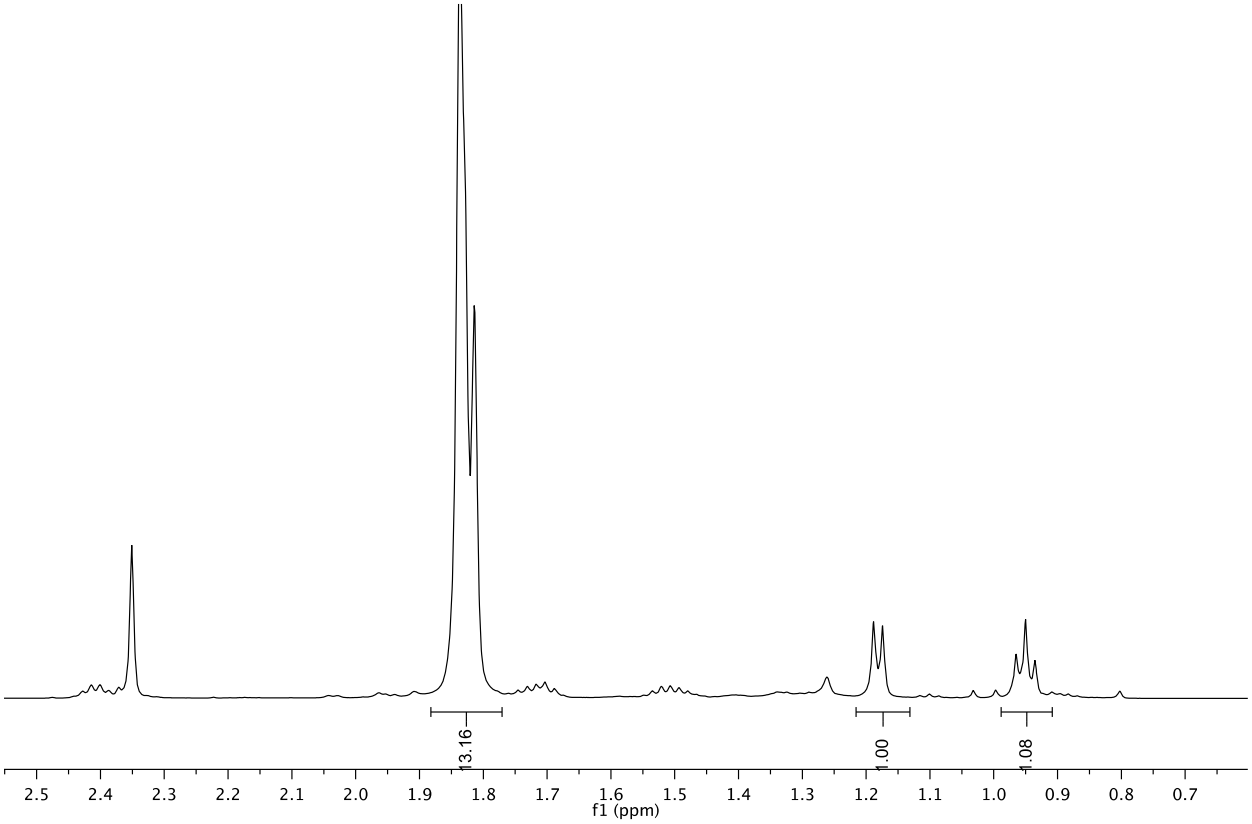

Figure S41. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1f})]$ **13**.

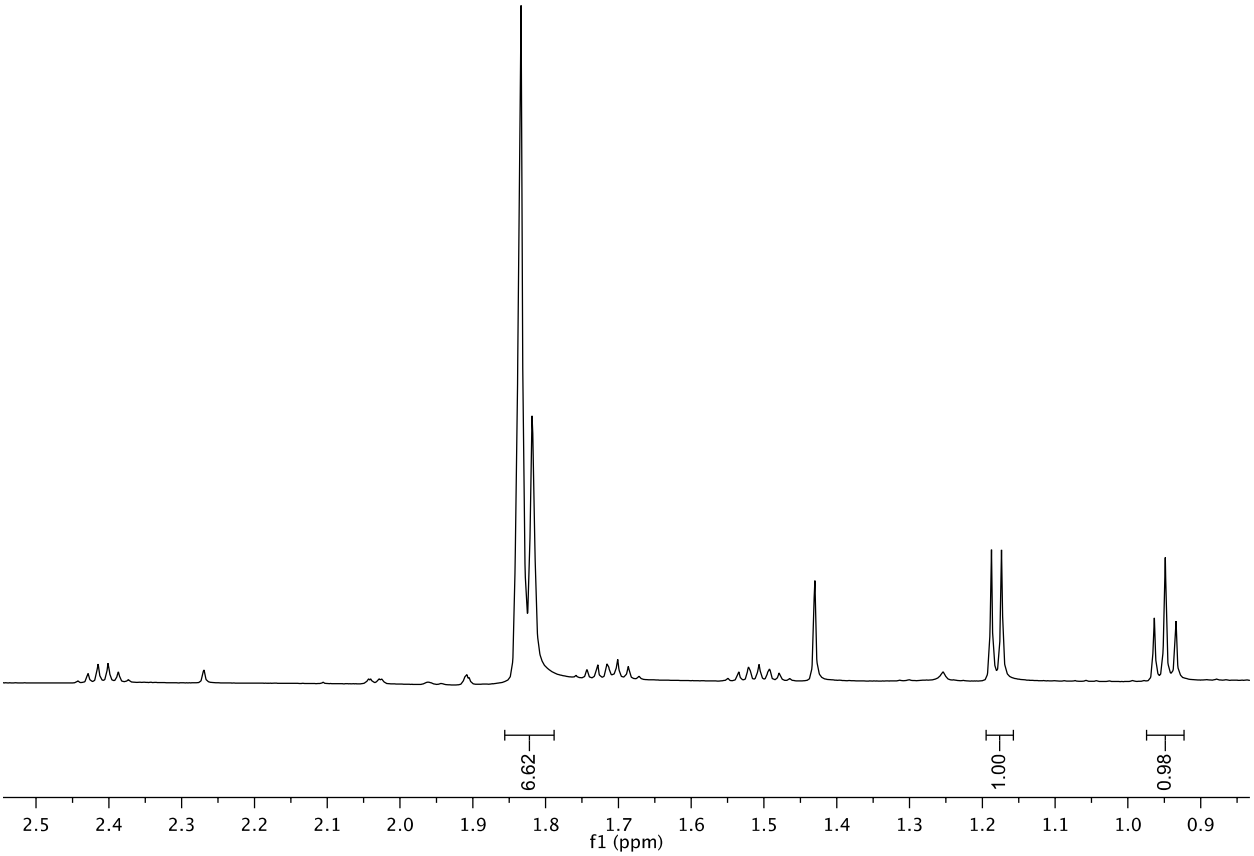

Figure S42. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1f})]$ **14**.

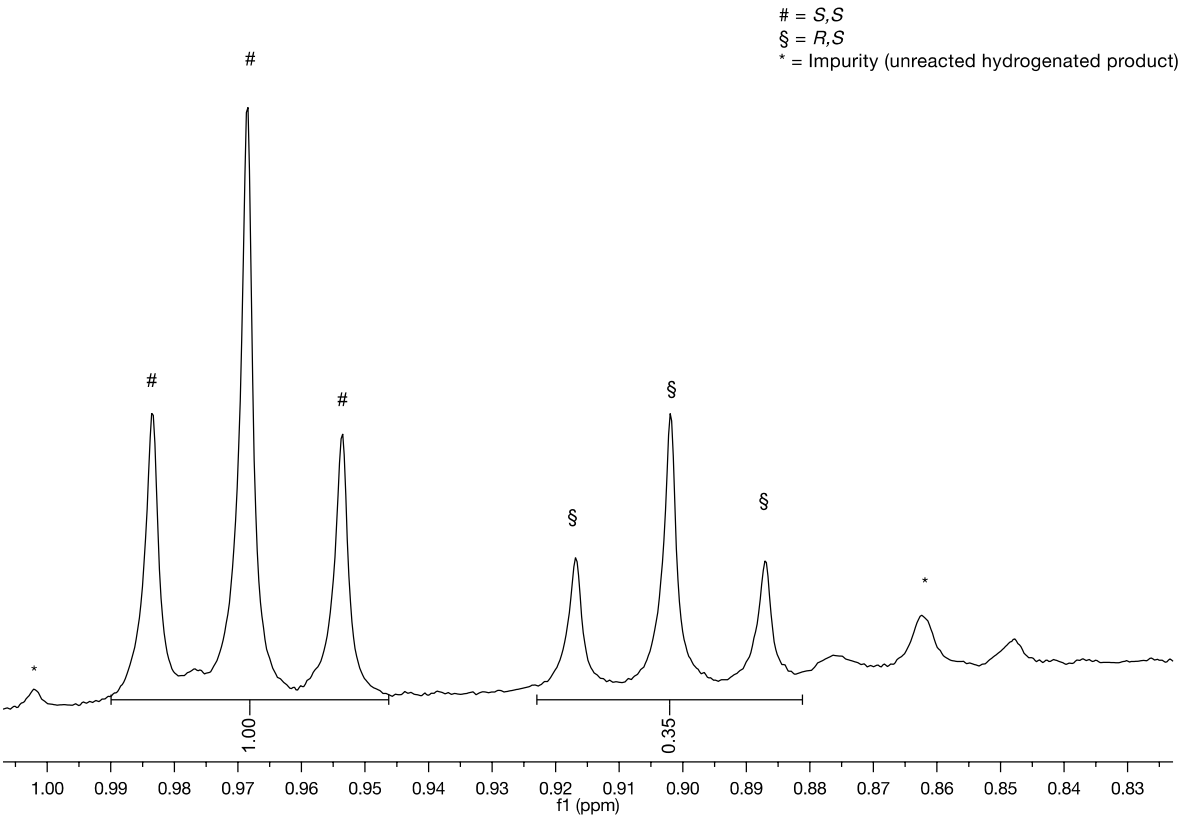

Figure S43. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1f**)] **14**.

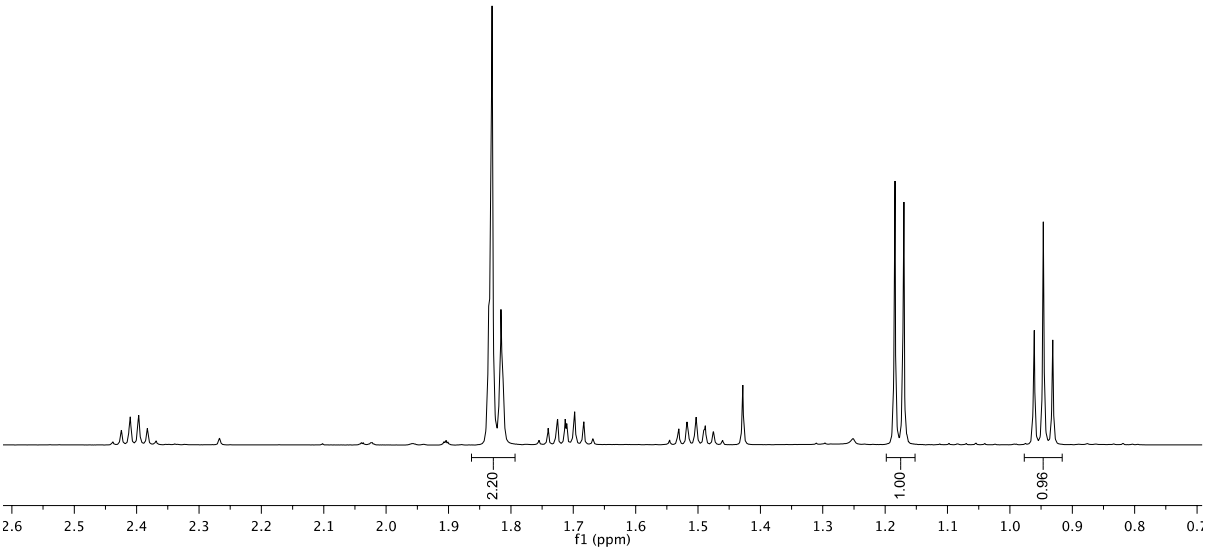

Figure S44. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1g})]$ **15**.

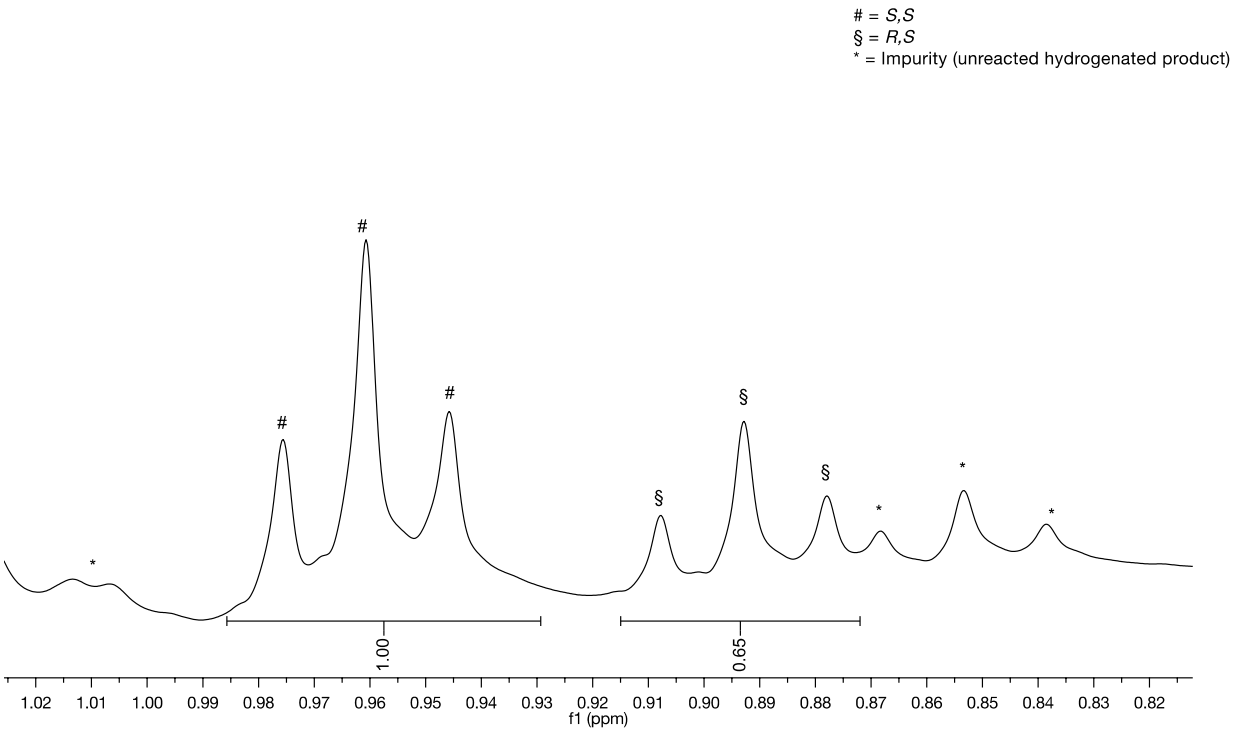

Figure S45. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1g**)] **15**.

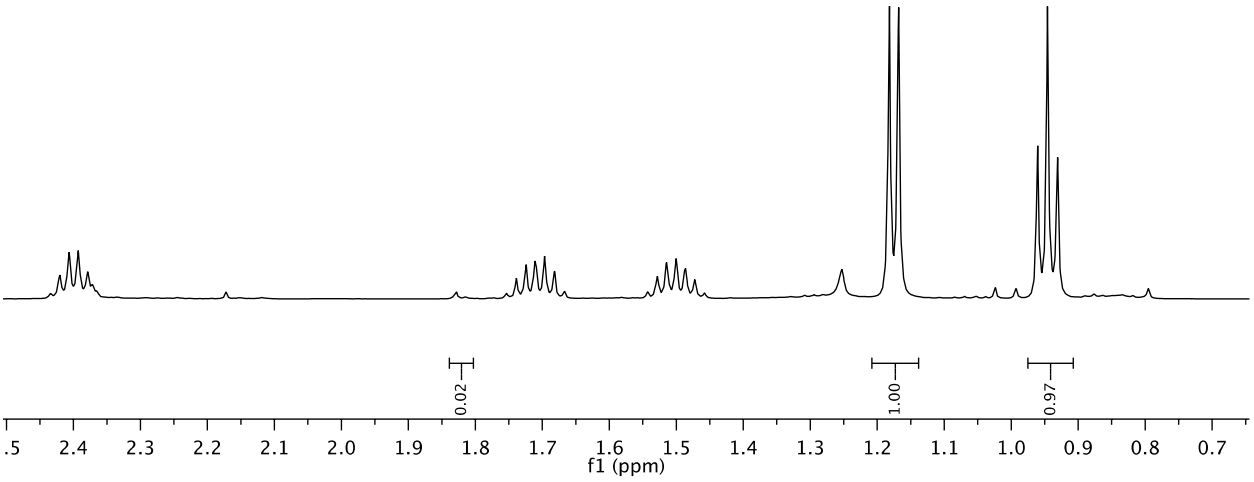

Figure S46. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1g})]$ **16**.

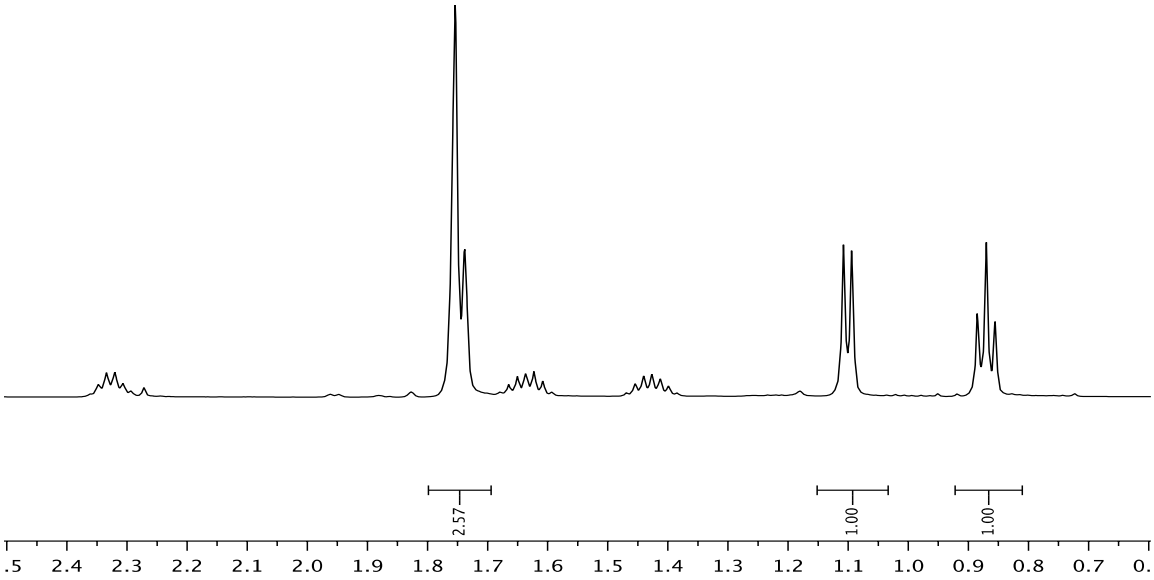

Figure S47. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{1h})]$ **17**.

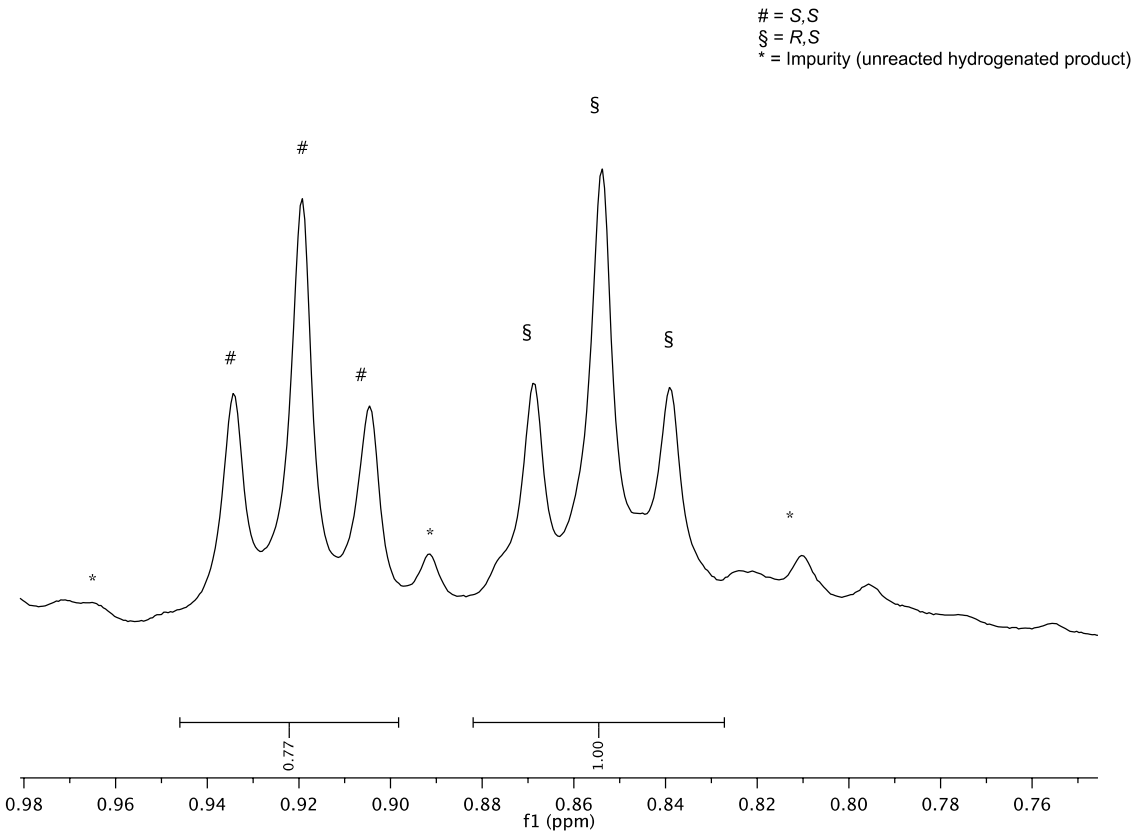

Figure S48. Determination of enantioeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**1h**)] **17**.

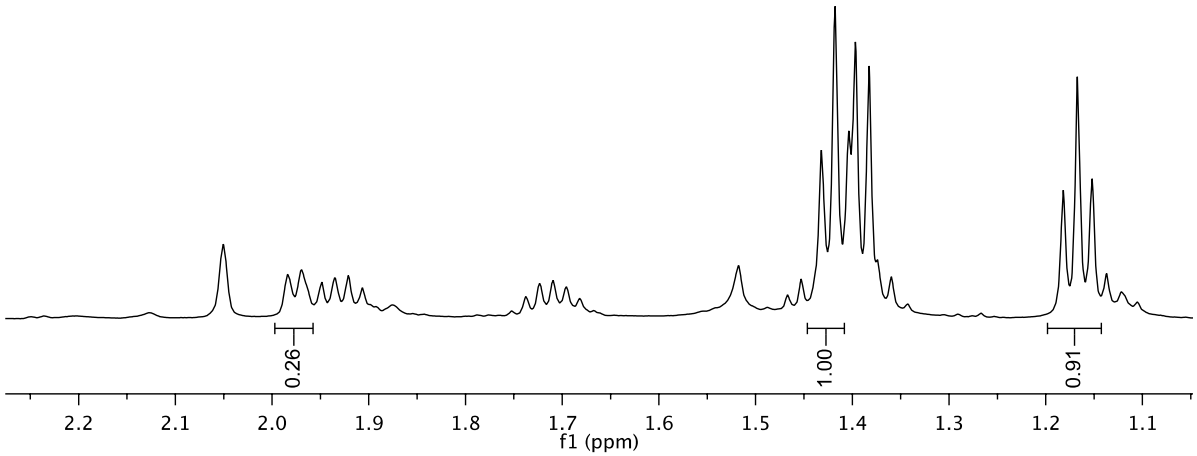

Figure S49. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{2a})]$ **18**.

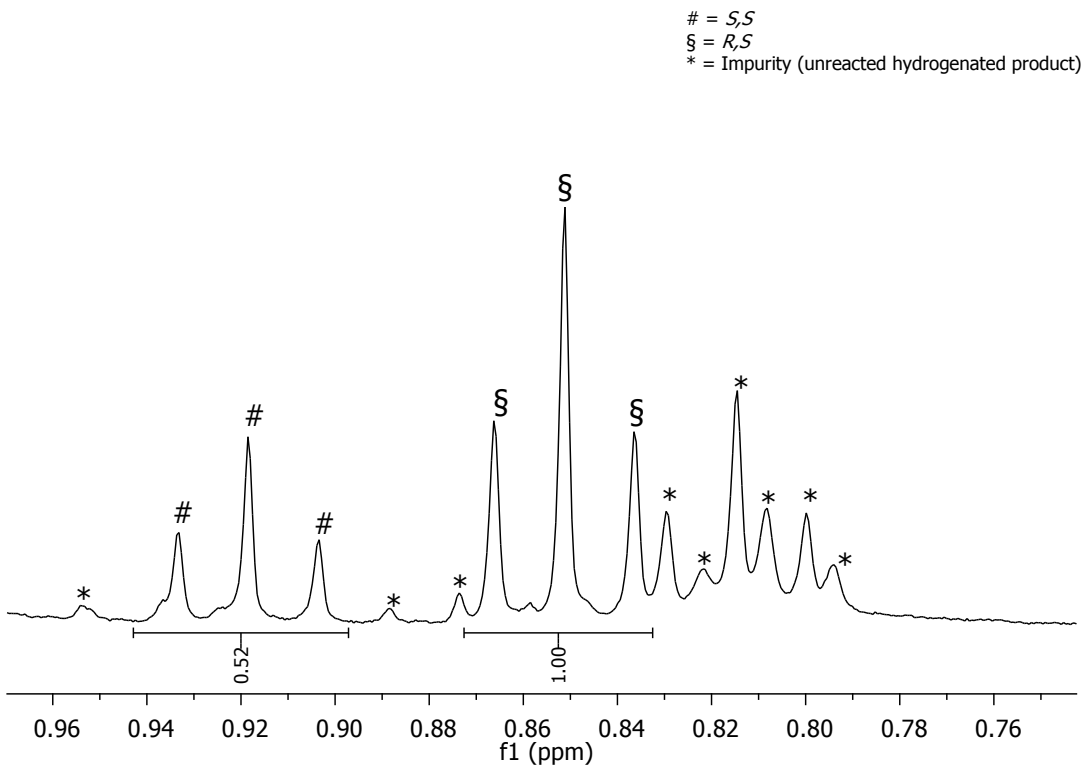

Figure S50. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{2a})]$ **18**.

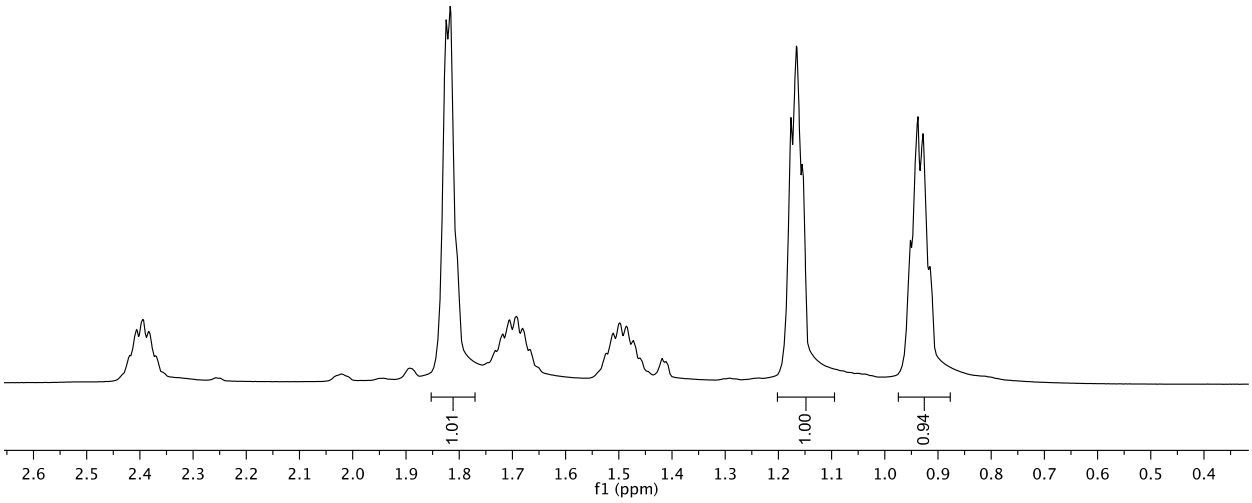

Figure S51. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{2a})]$ **19**.

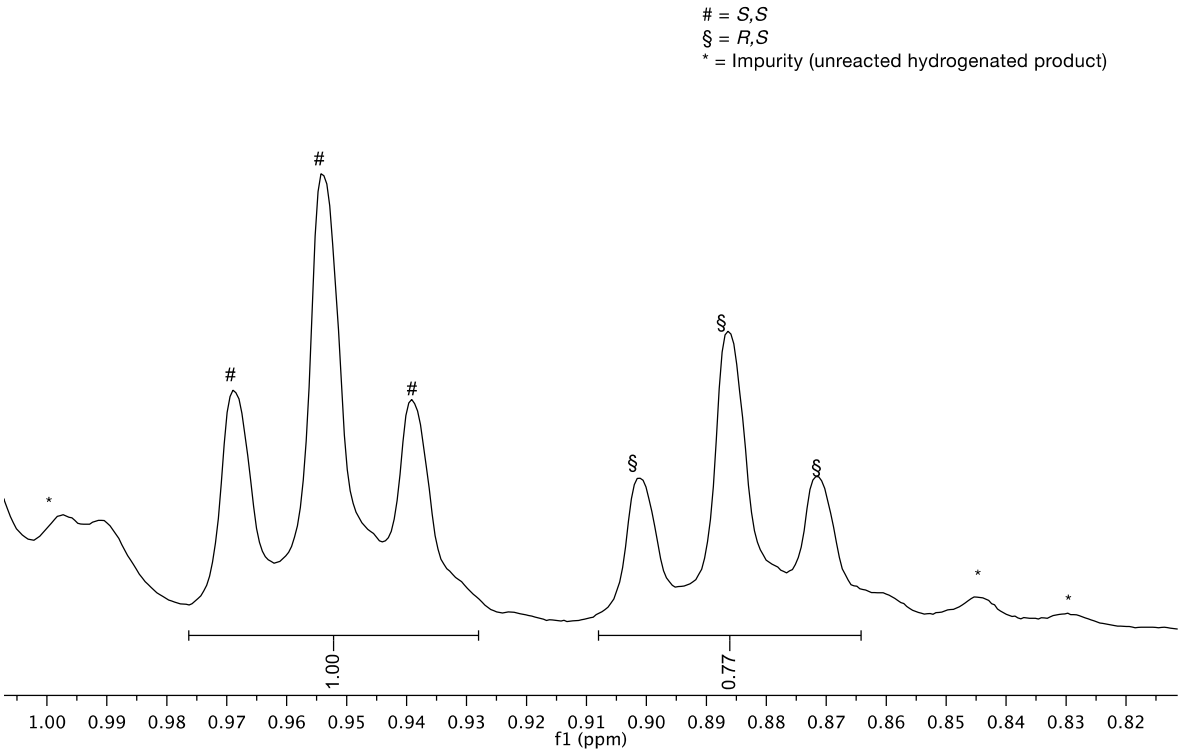

Figure S52. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**2a**)] **19**.

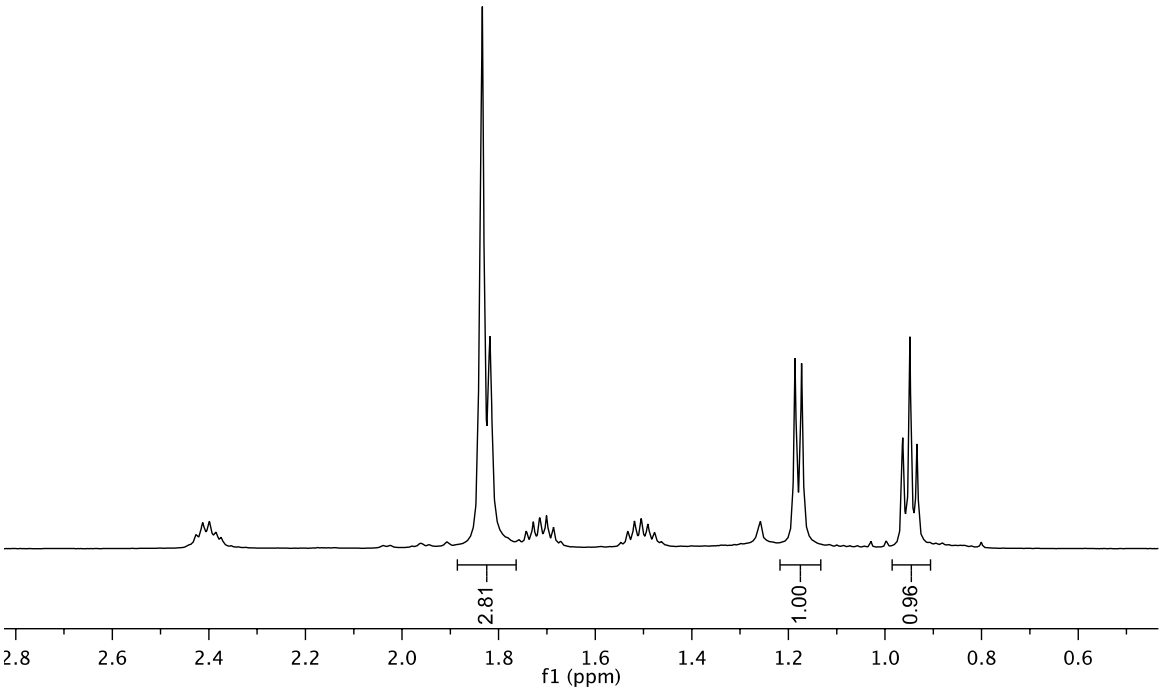

Figure S53. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{2b})]$ **20**.

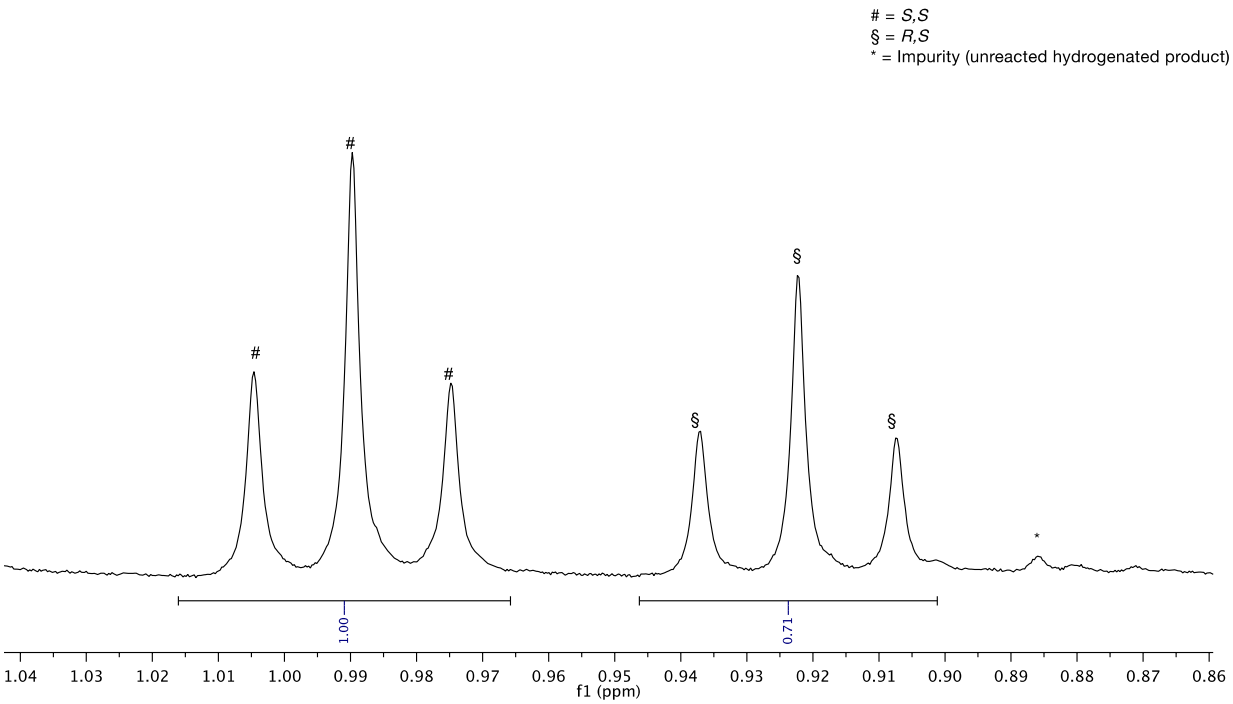

Figure S54. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**2b**)] **20**.

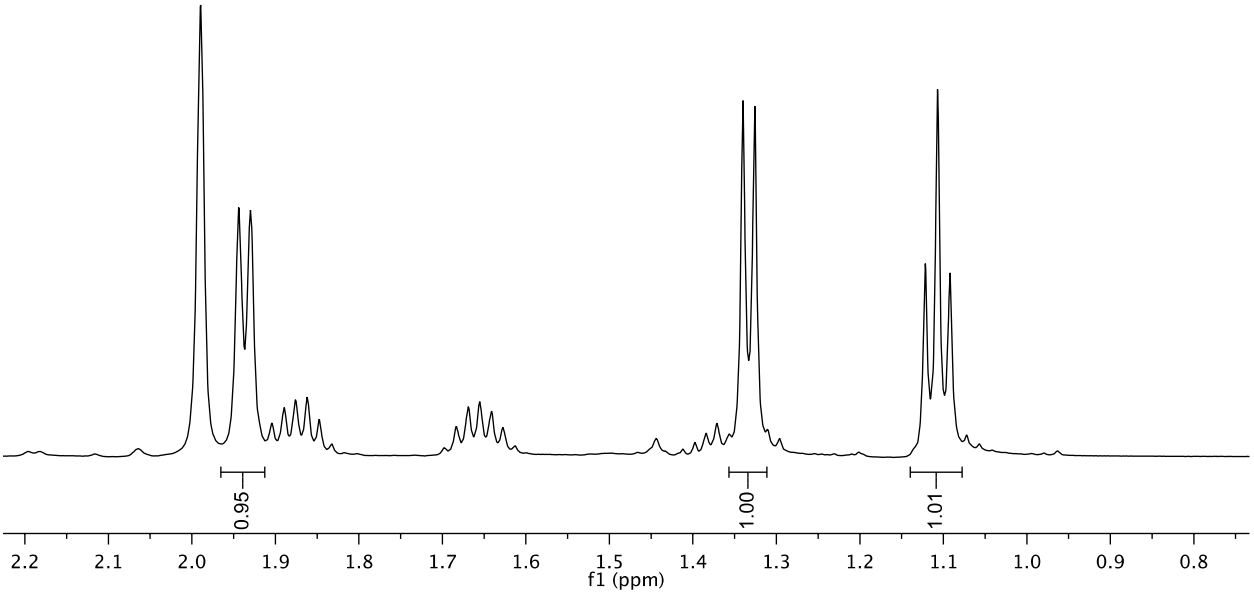

Figure S55. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}\mathbf{2c})]$ **21**.

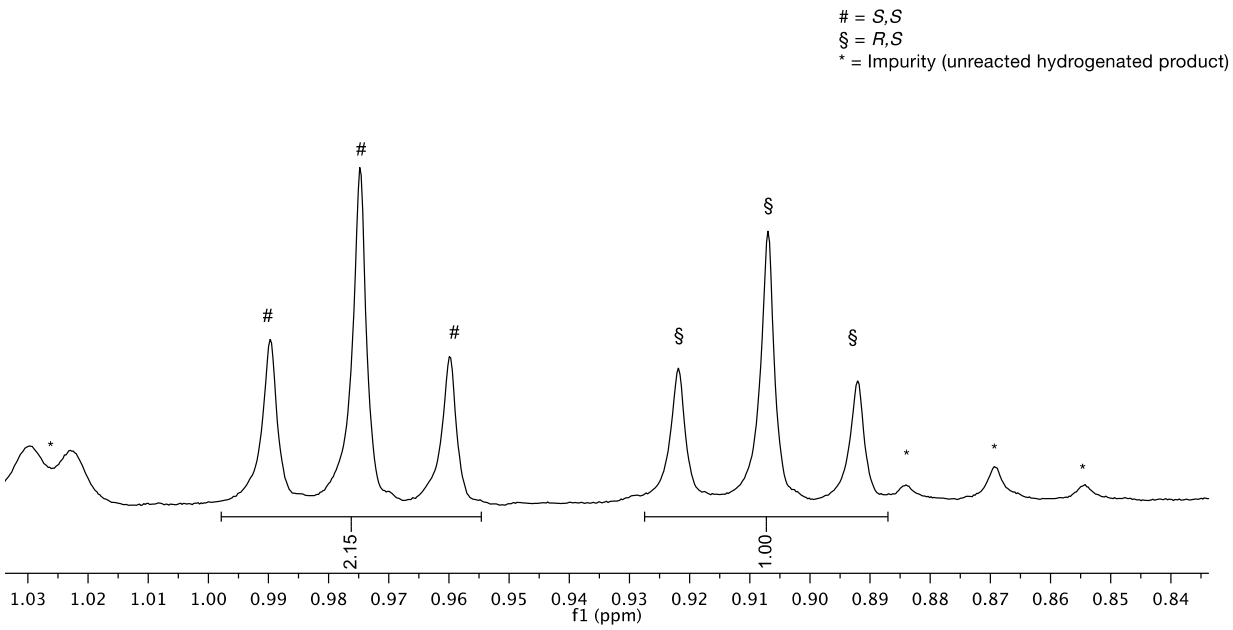

Figure S56. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using [(μ-H)$_2$Ru$_3$(μ$_3$-S)(CO)$_7$(μ-1,2-**2c**)] **21**.

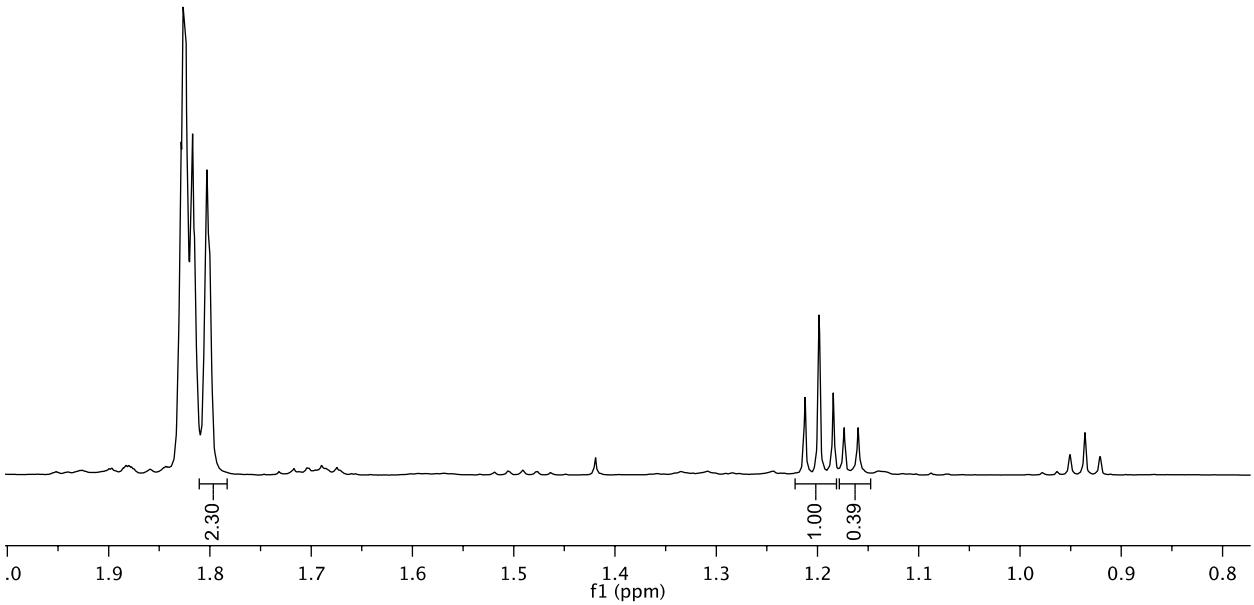

Figure S57. Determination of catalytic asymmetric hydrogenation conversion percentage by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}$**2d**$)]$ **22**.

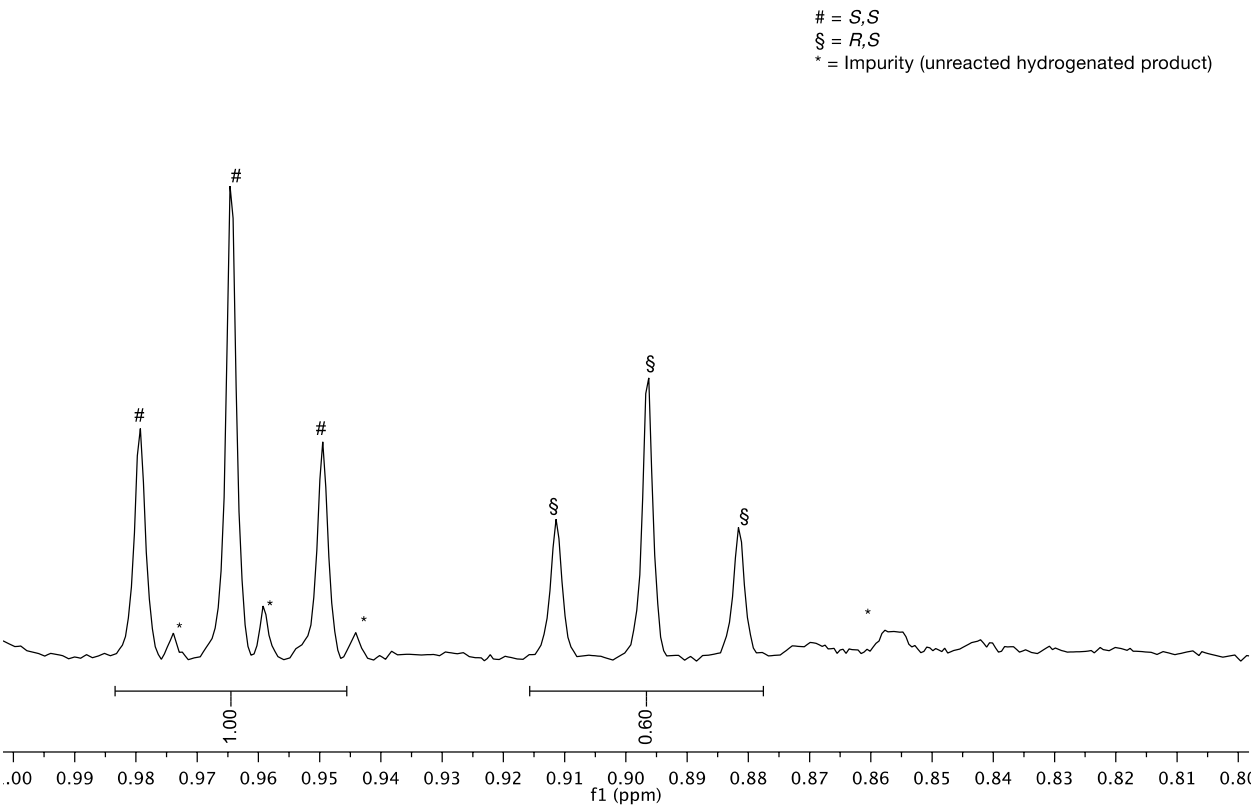

Figure S58. Determination of enantiomeric excess by using ^{1}H NMR spectroscopy. Analysis of products from hydrogenation of tiglic acid using $[(\mu\text{-}H)_2Ru_3(\mu_3\text{-}S)(CO)_7(\mu\text{-}1,2\text{-}$**2d**$)]$ **22**.

2. Computational Details

4.1. B3LYP geometries and energies for all optimized minima and transition structures (S2-S39)

Species A
HF energy = -2294.624983562325
No imaginary frequency
Zero-point correction = 0.711046 (Hartree/Particle)
Thermal correction to Energy = 0.789816
Thermal correction to Enthalpy = 0.790760
Thermal correction to Gibbs Free Energy = 0.582051
Sum of electronic and zero-point Energies = -2293.913937
Sum of electronic and thermal Energies = -2293.835168
Sum of electronic and thermal Enthalpies = -2293.834223
Sum of electronic and thermal Free Energies = -2294.042933

Coordinates: **A**

Ru	13.72080000	10.34560000	18.30760000
H	12.16870000	10.61720000	17.33010000
Ru	12.06370000	9.50820000	15.93120000
H	13.30050000	10.54100000	15.16260000
Ru	14.99220000	10.11560000	15.79950000
Fe	8.86720000	13.68250000	18.93140000
S	13.88500000	8.33640000	16.98990000
P	12.37760000	9.94550000	20.18590000
P	10.29840000	10.92050000	15.19410000
F	6.66330000	6.60450000	14.97810000
F	5.47710000	6.95580000	13.26370000
F	5.37440000	8.28430000	14.90360000
F	9.09420000	8.19450000	9.67890000
F	7.79400000	9.86600000	9.58490000
F	9.87180000	10.15430000	9.84200000
F	7.91960000	13.71810000	10.97480000
F	7.11470000	14.75890000	12.63470000
F	8.38000000	15.76010000	11.26940000
F	12.73100000	16.68140000	13.40640000
F	13.29820000	15.54160000	15.08840000
F	13.91640000	14.94900000	13.14520000
O	16.24630000	9.95470000	19.93750000
O	13.82220000	13.38390000	18.48710000
O	10.01390000	7.72200000	17.31860000
O	12.08040000	7.81200000	13.39320000
O	15.73190000	8.90410000	13.04060000
O	17.77050000	9.65600000	16.96010000
O	15.51710000	13.09200000	15.28130000

C	15.29090000	10.10490000	19.30800000
C	13.77010000	12.23040000	18.44980000
C	10.77820000	8.41300000	16.80930000
C	12.05980000	8.44560000	14.35040000
C	15.43400000	9.33250000	14.06440000
C	16.71580000	9.83480000	16.53820000
C	15.32830000	11.97370000	15.47620000
C	12.44950000	11.22270000	21.53830000
C	13.64370000	11.92310000	21.73590000
C	13.75530000	12.84110000	22.78750000
C	12.67160000	13.06170000	23.64260000
C	11.47690000	12.36310000	23.44360000
C	11.36430000	11.44240000	22.39510000
C	12.90600000	8.47770000	21.19750000
C	12.75120000	8.43020000	22.58770000
C	13.16550000	7.29850000	23.29960000
C	13.73440000	6.21190000	22.62810000
C	13.89310000	6.26090000	21.24020000
C	13.48410000	7.39400000	20.52670000
C	10.53260000	9.68880000	20.07860000
C	10.04930000	8.47040000	20.58340000
C	8.68410000	8.17810000	20.60900000
C	7.76920000	9.10810000	20.10930000
C	8.23640000	10.30930000	19.58500000
C	9.61480000	10.62570000	19.56230000
C	9.92680000	11.92620000	18.94840000
C	9.55180000	12.31180000	17.55450000
C	10.09750000	13.65860000	17.31130000
C	10.80310000	14.10430000	18.51780000
C	10.69520000	13.04280000	19.52600000
C	6.82890000	13.50550000	18.94690000
C	7.24630000	14.77860000	18.34490000
C	8.04940000	15.50560000	19.33760000
C	8.12640000	14.68050000	20.55290000
C	7.37700000	13.44270000	20.30920000
C	8.96730000	11.40600000	16.52260000
C	7.70380000	12.01440000	15.91760000
C	9.21470000	9.95070000	14.01370000
C	8.18920000	9.13560000	14.49780000
C	7.36850000	8.42740000	13.60180000
C	6.25000000	7.58520000	14.15960000
C	7.58690000	8.51280000	12.22310000
C	8.63970000	9.30900000	11.74470000
C	8.85450000	9.38310000	10.25330000
C	9.45810000	10.01670000	12.63500000
C	10.42350000	12.51830000	14.24210000

C	9.35200000	12.95040000	13.45250000
C	9.42330000	14.17700000	12.77370000
C	8.24970000	14.60200000	11.93080000
C	10.56130000	14.98470000	12.88870000
C	11.62730000	14.55270000	13.68750000
C	12.85840000	15.41290000	13.82680000
C	11.56770000	13.31340000	14.35160000
H	11.19750000	13.05480000	20.48510000
H	10.08580000	14.19030000	16.37110000
H	6.92300000	12.08160000	16.69650000
H	7.84840000	13.05110000	15.57760000
H	7.26280000	11.43860000	15.09750000
H	8.68170000	10.43350000	17.02080000
H	6.87740000	15.18680000	17.41650000
H	6.08120000	12.84130000	18.54260000
H	7.11700000	12.71070000	21.05930000
H	8.51890000	15.00280000	21.50560000
H	8.37060000	16.53330000	19.25580000
H	11.44450000	14.97420000	18.58810000
H	12.75850000	13.77570000	24.46180000
H	14.68930000	13.38230000	22.93910000
H	14.51240000	11.77510000	21.08920000
H	12.31470000	9.25610000	23.15400000
H	13.04710000	7.26700000	24.38200000
H	14.05660000	5.33190000	23.18490000
H	14.34060000	5.41980000	20.71030000
H	13.63250000	7.40250000	19.43780000
H	6.70090000	8.89250000	20.12580000
H	8.33770000	7.22600000	21.00950000
H	7.52440000	11.04110000	19.18640000
H	12.42890000	12.98620000	14.95070000
H	10.28430000	10.61910000	12.23540000
H	7.99820000	9.03040000	15.57400000
H	6.95070000	7.96540000	11.51690000
H	8.43900000	12.34970000	13.34120000
H	10.61720000	15.94220000	12.35720000
H	10.71990000	7.69320000	20.96940000
H	10.41290000	10.91600000	22.26950000
H	10.62960000	12.53410000	24.10690000

Species B

HF energy = -2181.261546472092

no imaginary frequency

Zero-point correction = 0.703305 (Hartree/Particle)

Thermal correction to Energy = 0.779532
Thermal correction to Enthalpy = 0.780477
Thermal correction to Gibbs Free Energy = 0.577492
Sum of electronic and zero-point Energies = -2180.558242
Sum of electronic and thermal Energies = -2180.482014
Sum of electronic and thermal Enthalpies = -2180.481070
Sum of electronic and thermal Free Energies = -2180.684055

Coordinates: **B**

Ru	13.72790000	10.44320000	18.23330000
H	12.17780000	10.73000000	17.25230000
Ru	12.06400000	9.63900000	15.83890000
H	13.22440000	10.71040000	15.06840000
Ru	14.95250000	10.34900000	15.74660000
Fe	8.80430000	13.66790000	18.97380000
S	13.92650000	8.46730000	16.84870000
P	12.40380000	9.99160000	20.12390000
P	10.26010000	11.01890000	15.15620000
F	6.70510000	6.63790000	14.89230000
F	5.49430000	7.00080000	13.19770000
F	5.38560000	8.29460000	14.86450000
F	9.06200000	8.37300000	9.60450000
F	7.71890000	10.01190000	9.55090000
F	9.79080000	10.34930000	9.79360000
F	7.80190000	13.84970000	11.00380000
F	6.97150000	14.83610000	12.68400000
F	8.21200000	15.89580000	11.34040000
F	12.45220000	16.92950000	13.67520000
F	13.21470000	15.62220000	15.14250000
F	13.70090000	15.32110000	13.09750000
O	16.27600000	10.00810000	19.82370000
O	13.76560000	13.46610000	18.55480000
O	10.10460000	7.74090000	17.23330000
O	12.12230000	8.01590000	13.25490000
O	17.80910000	9.96210000	16.64000000
O	15.48970000	13.24100000	14.99810000
C	15.31370000	10.17080000	19.21260000
C	13.72730000	12.31580000	18.47760000
C	10.83110000	8.47230000	16.72550000
C	12.08150000	8.62070000	14.23100000
C	16.71130000	10.11320000	16.31090000
C	15.30640000	12.12580000	15.24470000
C	12.47550000	11.23410000	21.49600000
C	13.66750000	11.93430000	21.71110000
C	13.77610000	12.82220000	22.78780000
C	12.69260000	13.01200000	23.65120000

C	11.50160000	12.31240000	23.43550000
C	11.39100000	11.42140000	22.36120000
C	12.98730000	8.51200000	21.06880000
C	12.87940000	8.43220000	22.46240000
C	13.32690000	7.28850000	23.13350000
C	13.88180000	6.22270000	22.41810000
C	13.99270000	6.30410000	21.02710000
C	13.55040000	7.44870000	20.35340000
C	10.57540000	9.69890000	20.01690000
C	10.12460000	8.46070000	20.50600000
C	8.76730000	8.13700000	20.53810000
C	7.82700000	9.05350000	20.05980000
C	8.26160000	10.27360000	19.55230000
C	9.63190000	10.62380000	19.52480000
C	9.90920000	11.94110000	18.93310000
C	9.50220000	12.34830000	17.55420000
C	10.01120000	13.71340000	17.33610000
C	10.72230000	14.15030000	18.54310000
C	10.65680000	13.06400000	19.52730000
C	6.77100000	13.43890000	19.01010000
C	7.14850000	14.73580000	18.43330000
C	7.94610000	15.45970000	19.43270000
C	8.05900000	14.60920000	20.62750000
C	7.33800000	13.35880000	20.36390000
C	8.92930000	11.45150000	16.50790000
C	7.64890000	12.04670000	15.92560000
C	9.18150000	10.05260000	13.96810000
C	8.17760000	9.20800000	14.44630000
C	7.36220000	8.50040000	13.54480000
C	6.26590000	7.62670000	14.09720000
C	7.56630000	8.61520000	12.16610000
C	8.59880000	9.44050000	11.69300000
C	8.79810000	9.54540000	10.20130000
C	9.41190000	10.14760000	12.58880000
C	10.33720000	12.64240000	14.24180000
C	9.25490000	13.06430000	13.46230000
C	9.29330000	14.30900000	12.81370000
C	8.11050000	14.72140000	11.97780000
C	10.40730000	15.14520000	12.95300000
C	11.48250000	14.72510000	13.74660000
C	12.68050000	15.62690000	13.91100000
C	11.46000000	13.46520000	14.37210000
H	11.16960000	13.06840000	20.48020000
H	9.97330000	14.26590000	16.40800000
H	6.87360000	12.08670000	16.71120000
H	7.77160000	13.09050000	15.59900000

H	7.21180000	11.47590000	15.09960000
H	8.66840000	10.46270000	16.98600000
H	6.75760000	15.15590000	17.51880000
H	6.03450000	12.76600000	18.59950000
H	7.10390000	12.60440000	21.10010000
H	8.45430000	14.92020000	21.58260000
H	8.23950000	16.49730000	19.37100000
H	11.34090000	15.03590000	18.62410000
H	12.77740000	13.70380000	24.49010000
H	14.70750000	13.36500000	22.95290000
H	14.53620000	11.80870000	21.05910000
H	12.45540000	9.24110000	23.06230000
H	13.24560000	7.23110000	24.21850000
H	14.23050000	5.33300000	22.94370000
H	14.42920000	5.47890000	20.46270000
H	13.66150000	7.48150000	19.25920000
H	6.76400000	8.81160000	20.07940000
H	8.44590000	7.17010000	20.92440000
H	7.52980000	10.99520000	19.16990000
H	12.33260000	13.14120000	14.95690000
H	10.22450000	10.77150000	12.19330000
H	8.00010000	9.07830000	15.52180000
H	6.93470000	8.06800000	11.45570000
H	8.35860000	12.44230000	13.33510000
H	10.43940000	16.11620000	12.44450000
H	10.81560000	7.69150000	20.87240000
H	10.44190000	10.89310000	22.22360000
H	10.65470000	12.45950000	24.10570000

Species CO

HF energy = -113.307959585
No imaginary frequency
Zero-point correction = 0.005033 (Hartree/Particle)
Thermal correction to Energy = 0.007394
Thermal correction to Enthalpy = 0.008338
Thermal correction to Gibbs Free Energy = -0.014099
Sum of electronic and zero-point Energies = -113.302926
Sum of electronic and thermal Energies = -113.300566
Sum of electronic and thermal Enthalpies = -113.299621
Sum of electronic and thermal Free Energies = -113.322058

Coordinates: **CO**

C	-0.000000289	-0.000005840	-0.000000214
O	0.000000289	0.000005840	0.000000214

Species C
HF energy = -345.788827461
No imaginary frequency
Zero-point correction = 0.124101 (Hartree/Particle)
Thermal correction to Energy = 0.132046
Thermal correction to Enthalpy = 0.132990
Thermal correction to Gibbs Free Energy = 0.091776
Sum of electronic and zero-point Energies = -345.664726
Sum of electronic and thermal Energies = -345.656781
Sum of electronic and thermal Enthalpies = -345.655837
Sum of electronic and thermal Free Energies = -345.697051

Coordinates: **C**

C	-2.53660000	1.26390000	0.05650000
H	-3.62460000	1.33420000	0.06220000
C	-1.87280000	2.43200000	-0.04110000
C	-1.97150000	-0.11900000	0.15860000
H	-2.31680000	-0.60380000	1.08360000
H	-2.33950000	-0.74270000	-0.66930000
H	-0.87790000	-0.14900000	0.14680000
C	-0.37500000	2.61020000	-0.07020000
H	-0.05570000	3.10990000	-0.99360000
H	-0.03770000	3.24580000	0.75840000
H	0.15150000	1.65380000	-0.00140000
C	-2.72530000	3.65470000	-0.12750000
O	-1.98380000	4.79120000	-0.22350000
H	-2.62350000	5.52100000	-0.27390000
O	-3.93820000	3.69290000	-0.11800000

Species D
HF energy = -2527.066253703269
No imaginary frequency
Zero-point correction = 0.829494 (Hartree/Particle)
Thermal correction to Energy = 0.914558
Thermal correction to Enthalpy = 0.915502
Thermal correction to Gibbs Free Energy = 0.695013
Sum of electronic and zero-point Energies = -2526.236760
Sum of electronic and thermal Energies = -2526.151696
Sum of electronic and thermal Enthalpies = -2526.150751
Sum of electronic and thermal Free Energies = -2526.371241

Coordinates: **D**

Ru	9.20980000	12.71780000	17.48030000

H	7.77630000	12.63080000	18.64190000
Ru	6.79100000	11.16310000	18.38380000
H	6.12400000	11.98310000	16.96900000
Ru	7.34040000	11.98060000	15.52100000
Fe	7.52570000	15.79770000	22.24900000
S	8.58680000	10.46020000	16.92980000
P	10.67170000	12.73910000	19.32200000
P	5.25480000	12.23250000	19.84110000
F	5.15530000	7.75390000	23.26650000
F	3.16290000	7.61500000	23.95930000
F	4.34990000	9.27730000	24.49840000
F	0.69560000	9.18550000	18.59290000
F	-0.16680000	8.64400000	20.44560000
F	-0.12790000	10.67340000	19.85710000
F	0.02000000	13.92700000	20.95700000
F	1.15570000	15.30760000	22.09240000
F	-0.03950000	15.98710000	20.48740000
F	3.60370000	17.58500000	17.10740000
F	4.55780000	16.04740000	16.01270000
F	2.45500000	16.25360000	15.92440000
O	11.60090000	12.89060000	15.62180000
O	8.62740000	15.70560000	17.41080000
O	8.07210000	9.69800000	20.74020000
O	4.81320000	8.87040000	17.97330000
O	9.35390000	12.44050000	13.31070000
O	6.12230000	14.72500000	15.03790000
C	10.67790000	12.82540000	16.31100000
C	8.87480000	14.57870000	17.46800000
C	7.59590000	10.27510000	19.86700000
C	5.58720000	9.71060000	18.07990000
C	8.59150000	12.25140000	14.15710000
C	6.57150000	13.66860000	15.17650000
C	11.60130000	14.32160000	19.61240000
C	11.92790000	15.12660000	18.51620000
C	12.68910000	16.28760000	18.69780000
C	13.12450000	16.64710000	19.97670000
C	12.79680000	15.84340000	21.07270000
C	12.03850000	14.68030000	20.89340000
C	12.12920000	11.61170000	19.11440000
C	13.39580000	11.92740000	19.61920000
C	14.46070000	11.03640000	19.44210000
C	14.26580000	9.83000000	18.76250000
C	13.00170000	9.51700000	18.25440000
C	11.93610000	10.40840000	18.42540000
C	10.13490000	12.35390000	21.05980000
C	10.79670000	11.28600000	21.68850000

C	10.52620000	10.93650000	23.01290000
C	9.56440000	11.64940000	23.73330000
C	8.88570000	12.69480000	23.11490000
C	9.15780000	13.07120000	21.77930000
C	8.33070000	14.17930000	21.27800000
C	6.83890000	14.15230000	21.21700000
C	6.40510000	15.41520000	20.59510000
C	7.59410000	16.21230000	20.27050000
C	8.77840000	15.45610000	20.69470000
C	6.99580000	15.50480000	24.20380000
C	6.21410000	16.59150000	23.59950000
C	7.15600000	17.60820000	23.11140000
C	8.51950000	17.14860000	23.41650000
C	8.42040000	15.84700000	24.08650000
C	5.97840000	12.96430000	21.49130000
C	4.91290000	13.29790000	22.53360000
C	4.09360000	10.95510000	20.57010000
C	4.48330000	10.20120000	21.68100000
C	3.60500000	9.25310000	22.23260000
C	4.04610000	8.48680000	23.45300000
C	2.34600000	9.03210000	21.66050000
C	1.97390000	9.76880000	20.52880000
C	0.62860000	9.56250000	19.87890000
C	2.84770000	10.72050000	19.97800000
C	4.01020000	13.55060000	19.40130000
C	2.89470000	13.76610000	20.21640000
C	1.98850000	14.79690000	19.91710000
C	0.80810000	15.00650000	20.82830000
C	2.19160000	15.61110000	18.79790000
C	3.30700000	15.38450000	17.97750000
C	3.48870000	16.28610000	16.78210000
C	4.21360000	14.35350000	18.27360000
H	9.80040000	15.75590000	20.50150000
H	5.39420000	15.67220000	20.31300000
H	5.39940000	13.47140000	23.50990000
H	4.38190000	14.23680000	22.31380000
H	4.17040000	12.51160000	22.70390000
H	6.62810000	12.14130000	21.91090000
H	5.14330000	16.71000000	23.66740000
H	6.59090000	14.71040000	24.81100000
H	9.23390000	15.33110000	24.57420000
H	9.41690000	17.74040000	23.31810000
H	6.89020000	18.59350000	22.75850000
H	7.60550000	17.10750000	19.66090000
H	13.71750000	17.55110000	20.11810000
H	12.94280000	16.91030000	17.83930000

H	11.60800000	14.87740000	17.50110000
H	13.59600000	12.85920000	20.15320000
H	15.44640000	11.28730000	19.83250000
H	15.09730000	9.13830000	18.62540000
H	12.84330000	8.58080000	17.71800000
H	10.95800000	10.13450000	18.00300000
H	9.34430000	11.38490000	24.76780000
H	11.05610000	10.10480000	23.47640000
H	8.12410000	13.25360000	23.67120000
H	5.07680000	14.18440000	17.61410000
H	2.52920000	11.26680000	19.08000000
H	5.46960000	10.33150000	22.14500000
H	1.66280000	8.29010000	22.08970000
H	2.69630000	13.14230000	21.09860000
H	1.48950000	16.41880000	18.55700000
H	11.54350000	10.67460000	21.16740000
H	11.80080000	14.07820000	21.77620000
H	13.13260000	16.12150000	22.07150000
C	5.33360000	10.90230000	14.52920000
H	4.97440000	10.42530000	15.43660000
C	6.39170000	10.27060000	13.90220000
C	4.36280000	11.85140000	13.87460000
H	3.54780000	11.26980000	13.41440000
H	3.90620000	12.52280000	14.60930000
H	4.81730000	12.46390000	13.09060000
C	6.77670000	10.51770000	12.45710000
H	7.84120000	10.35010000	12.28220000
H	6.22680000	9.81800000	11.81020000
H	6.52790000	11.53370000	12.13750000
C	6.88960000	9.00290000	14.53000000
O	7.97220000	8.49930000	13.88690000
H	8.22310000	7.69940000	14.37790000
O	6.38380000	8.42370000	15.46950000

Species TSDE
HF energy = -2527.031281279194
Imaginary frequency: 846*i*
Zero-point correction = 0.827784 (Hartree/Particle)
Thermal correction to Energy = 0.912524
Thermal correction to Enthalpy = 0.913468
Thermal correction to Gibbs Free Energy = 0.694254
Sum of electronic and zero-point Energies = -2526.203497
Sum of electronic and thermal Energies = -2526.118757
Sum of electronic and thermal Enthalpies = -2526.117813

Sum of electronic and thermal Free Energies = -2526.337027

Coordinates: **TSDE**

Ru	9.27840000	12.60910000	17.51680000
H	7.84360000	12.62400000	18.62980000
Ru	6.88170000	11.11540000	18.45150000
H	5.87480000	10.97700000	16.28690000
Ru	7.27540000	11.80230000	15.61940000
Fe	7.57580000	15.87390000	22.16150000
S	8.63600000	10.33630000	17.00860000
P	10.69550000	12.67000000	19.35370000
P	5.27340000	12.28490000	19.79790000
F	5.05220000	7.96570000	23.44220000
F	3.02240000	7.82840000	24.01710000
F	4.14890000	9.53810000	24.53740000
F	0.90690000	9.08020000	18.39760000
F	-0.05150000	8.53570000	20.20110000
F	-0.06430000	10.55330000	19.57030000
F	-0.07620000	13.81330000	20.60080000
F	0.93190000	15.15780000	21.88960000
F	-0.15320000	15.89290000	20.23180000
F	3.71590000	17.76730000	17.28260000
F	4.81230000	16.33030000	16.18810000
F	2.72090000	16.49480000	15.91170000
O	11.75090000	12.56480000	15.74420000
O	8.77280000	15.60760000	17.33590000
O	8.03980000	9.81140000	20.94240000
O	5.04020000	8.71200000	18.09510000
O	9.31030000	12.95790000	13.65570000
O	5.59970000	14.33290000	15.40480000
C	10.80270000	12.58980000	16.39860000
C	8.99050000	14.47940000	17.44470000
C	7.60820000	10.35760000	20.02320000
C	5.72910000	9.62930000	18.20840000
C	8.60000000	12.51950000	14.45090000
C	6.23100000	13.36150000	15.43930000
C	11.64750000	14.24580000	19.59200000
C	12.00030000	15.00850000	18.47360000
C	12.77810000	16.16250000	18.62550000
C	13.20570000	16.55710000	19.89690000
C	12.85390000	15.79490000	21.01470000
C	12.07840000	14.63890000	20.86500000
C	12.12320000	11.50100000	19.19860000
C	13.41450000	11.84210000	19.61650000
C	14.45740000	10.91660000	19.49050000
C	14.21580000	9.65080000	18.94850000

C	12.92680000	9.31180000	18.52610000
C	11.88320000	10.23650000	18.64610000
C	10.12710000	12.36340000	21.09320000
C	10.78150000	11.32380000	21.77710000
C	10.48610000	11.02230000	23.10750000
C	9.50470000	11.75500000	23.78050000
C	8.83940000	12.77700000	23.11150000
C	9.14150000	13.10960000	21.77020000
C	8.33970000	14.21540000	21.22540000
C	6.84810000	14.22510000	21.15990000
C	6.44960000	15.48650000	20.51240000
C	7.65950000	16.24570000	20.17440000
C	8.82250000	15.46780000	20.61670000
C	7.03710000	15.63380000	24.12140000
C	6.28010000	16.72420000	23.49330000
C	7.24460000	17.70940000	22.98550000
C	8.59760000	17.22700000	23.30240000
C	8.46920000	15.94200000	23.99870000
C	5.95410000	13.06530000	21.44770000
C	4.85230000	13.45970000	22.42880000
C	4.10660000	11.01030000	20.52370000
C	4.43840000	10.32350000	21.69490000
C	3.54810000	9.37890000	22.23400000
C	3.92320000	8.68760000	23.51980000
C	2.33840000	9.09220000	21.58990000
C	2.02700000	9.75970000	20.39830000
C	0.73740000	9.47930000	19.66830000
C	2.91000000	10.71080000	19.86210000
C	4.02360000	13.59740000	19.33700000
C	2.84620000	13.74920000	20.07580000
C	1.94370000	14.77970000	19.76350000
C	0.69130000	14.91520000	20.58870000
C	2.21600000	15.66380000	18.71400000
C	3.40030000	15.50970000	17.97850000
C	3.66790000	16.48980000	16.86370000
C	4.29980000	14.47540000	18.28410000
H	9.85260000	15.73600000	20.42100000
H	5.44520000	15.76750000	20.22960000
H	5.30560000	13.71970000	23.40200000
H	4.30800000	14.36540000	22.12200000
H	4.12080000	12.67210000	22.63730000
H	6.56940000	12.24700000	21.92360000
H	5.21190000	16.86670000	23.55600000
H	6.61490000	14.86200000	24.74590000
H	9.27030000	15.41840000	24.49870000
H	9.50770000	17.79690000	23.19290000

H	7.00070000	18.69280000	22.61190000
H	7.69470000	17.12920000	19.54920000
H	13.81160000	17.45600000	20.01510000
H	13.05110000	16.75260000	17.75010000
H	11.68850000	14.73100000	17.46320000
H	13.65190000	12.82010000	20.04220000
H	15.46220000	11.18720000	19.81340000
H	15.03000000	8.93200000	18.85110000
H	12.73160000	8.32850000	18.09610000
H	10.88480000	9.93920000	18.29390000
H	9.26050000	11.52420000	24.81770000
H	11.01000000	10.21120000	23.61230000
H	8.06500000	13.35330000	23.63160000
H	5.21800000	14.36960000	17.69040000
H	2.63770000	11.20840000	18.92190000
H	5.38840000	10.50310000	22.21550000
H	1.64610000	8.35320000	22.00970000
H	2.59720000	13.08010000	20.91040000
H	1.51660000	16.47080000	18.46390000
H	11.54310000	10.69750000	21.29690000
H	11.82340000	14.06920000	21.76460000
H	13.18420000	16.09980000	22.00760000
C	5.55370000	10.28270000	15.03600000
H	5.71440000	9.30220000	15.48700000
C	6.47780000	10.53650000	13.95510000
C	4.08900000	10.68350000	14.94210000
H	3.58840000	10.04230000	14.20350000
H	3.58160000	10.54240000	15.90320000
H	3.95510000	11.72470000	14.63400000
C	6.05140000	11.29680000	12.70510000
H	6.91400000	11.69160000	12.16280000
H	5.50970000	10.62930000	12.01630000
H	5.39060000	12.13390000	12.94790000
C	7.46730000	9.42700000	13.73000000
O	8.31580000	9.69310000	12.70170000
H	8.90950000	8.92610000	12.64260000
O	7.52460000	8.37850000	14.33860000

Species E

HF energy = -2527.038102460158
No imaginary frequency
Zero-point correction = 0.831038 (Hartree/Particle)
Thermal correction to Energy = 0.916231
Thermal correction to Enthalpy = 0.917175
Thermal correction to Gibbs Free Energy = 0.695325

Sum of electronic and zero-point Energies = -2526.207065
Sum of electronic and thermal Energies = -2526.121872
Sum of electronic and thermal Enthalpies = -2526.120927
Sum of electronic and thermal Free Energies = -2526.342777

Coordinates: **E**

Ru	9.07640000	12.62030000	17.55110000
H	7.76670000	12.60610000	18.77900000
Ru	6.77050000	11.10140000	18.60230000
H	5.90930000	9.93240000	15.84760000
Ru	6.98650000	11.51220000	15.76350000
Fe	7.60300000	15.82710000	22.32960000
S	8.54920000	10.31650000	17.18340000
P	10.59960000	12.71110000	19.28690000
P	5.20240000	12.33880000	19.89510000
F	4.61570000	7.88520000	23.34910000
F	2.60720000	7.97920000	24.00150000
F	3.95540000	9.51630000	24.52870000
F	0.51010000	9.57350000	18.48900000
F	-0.47240000	9.13790000	20.30890000
F	-0.26770000	11.14430000	19.67910000
F	0.01240000	14.38700000	20.68260000
F	1.15360000	15.63670000	21.95580000
F	0.14450000	16.45980000	20.29180000
F	4.14940000	17.91090000	17.30480000
F	5.13170000	16.36610000	16.25420000
F	3.06810000	16.70380000	15.94090000
O	11.40100000	12.59670000	15.56860000
O	8.49340000	15.61540000	17.47940000
O	7.83540000	9.69910000	21.09890000
O	4.73570000	8.89990000	18.08570000
O	8.37070000	13.66680000	14.15700000
O	4.42600000	13.15770000	15.64930000
C	10.51870000	12.61570000	16.30520000
C	8.75220000	14.49480000	17.54180000
C	7.44290000	10.29130000	20.18820000
C	5.50980000	9.74420000	18.25040000
C	7.91090000	12.85170000	14.83940000
C	5.40680000	12.54200000	15.66920000
C	11.51950000	14.30170000	19.47470000
C	11.78320000	15.08650000	18.34690000
C	12.54830000	16.25230000	18.46620000
C	13.05300000	16.63460000	19.71330000
C	12.79140000	15.84890000	20.83960000
C	12.02760000	14.68130000	20.72340000
C	12.03070000	11.57540000	19.02930000

C	13.34660000	11.97640000	19.29030000
C	14.40320000	11.07770000	19.10250000
C	14.15280000	9.77750000	18.65380000
C	12.83970000	9.37730000	18.38910000
C	11.78180000	10.27440000	18.57280000
C	10.10550000	12.37390000	21.03150000
C	10.80360000	11.33050000	21.66720000
C	10.55100000	10.98130000	22.99390000
C	9.56780000	11.66680000	23.71330000
C	8.86720000	12.69750000	23.09660000
C	9.12920000	13.08340000	21.76070000
C	8.30720000	14.20660000	21.28560000
C	6.81420000	14.22980000	21.28830000
C	6.40140000	15.52290000	20.71570000
C	7.60120000	16.28890000	20.35970000
C	8.77450000	15.48310000	20.71370000
C	7.13460000	15.50480000	24.29620000
C	6.37400000	16.63510000	23.74870000
C	7.33570000	17.62730000	23.24920000
C	8.69100000	17.10950000	23.49120000
C	8.56630000	15.79610000	24.13240000
C	5.91390000	13.07020000	21.55950000
C	4.83510000	13.45050000	22.57120000
C	3.92650000	11.15780000	20.58910000
C	4.22090000	10.38950000	21.71980000
C	3.25500000	9.51580000	22.24760000
C	3.58970000	8.73780000	23.49400000
C	2.00810000	9.37410000	21.62600000
C	1.73530000	10.11600000	20.46980000
C	0.41030000	9.98680000	19.76250000
C	2.69400000	10.99920000	19.94620000
C	4.07180000	13.75420000	19.42000000
C	2.91640000	14.02690000	20.15730000
C	2.11820000	15.13730000	19.83310000
C	0.88710000	15.40520000	20.65760000
C	2.47250000	15.97680000	18.77180000
C	3.63490000	15.69980000	18.03690000
C	3.99270000	16.63470000	16.91070000
C	4.42860000	14.58510000	18.35300000
H	9.79620000	15.75490000	20.48670000
H	5.38800000	15.82350000	20.49020000
H	5.30830000	13.66790000	23.54510000
H	4.30100000	14.37420000	22.30500000
H	4.09280000	12.66950000	22.76590000
H	6.52790000	12.23120000	21.99950000
H	5.31130000	16.79110000	23.85830000

H	6.72270000	14.71080000	24.89960000
H	9.37600000	15.23730000	24.57760000
H	9.60590000	17.66970000	23.37330000
H	7.09500000	18.63070000	22.93130000
H	7.61630000	17.20030000	19.77560000
H	13.64940000	17.54330000	19.80590000
H	12.75140000	16.86200000	17.58500000
H	11.40950000	14.81630000	17.35530000
H	13.59520000	12.98230000	19.63800000
H	15.42560000	11.39580000	19.30420000
H	14.97790000	9.07960000	18.50700000
H	12.63500000	8.36650000	18.03200000
H	10.76360000	9.92250000	18.34880000
H	9.34990000	11.39180000	24.74590000
H	11.10510000	10.16660000	23.45920000
H	8.09280000	13.23810000	23.65440000
H	5.32610000	14.37230000	17.75730000
H	2.45170000	11.55270000	19.02900000
H	5.20020000	10.44820000	22.21340000
H	1.25790000	8.68810000	22.03540000
H	2.60530000	13.39250000	20.99820000
H	1.85350000	16.84360000	18.51110000
H	11.56940000	10.73950000	21.15050000
H	11.84220000	14.09200000	21.62800000
H	13.18260000	16.14470000	21.81330000
C	6.09940000	9.42960000	14.79450000
H	6.66190000	8.54090000	15.09790000
C	6.95930000	10.30750000	13.93470000
C	4.68100000	9.08610000	14.32560000
H	4.72730000	8.50310000	13.39720000
H	4.16770000	8.48260000	15.08260000
H	4.07660000	9.97940000	14.13680000
C	6.34140000	10.96450000	12.70210000
H	6.99900000	11.73650000	12.29550000
H	6.17130000	10.22390000	11.90390000
H	5.37820000	11.42870000	12.93570000
C	8.32630000	9.73410000	13.69910000
O	9.07630000	10.50370000	12.86180000
H	9.93380000	10.05290000	12.78750000
O	8.76770000	8.69690000	14.15360000

Species H_2

HF energy = -1.17548238770

No imaginary frequency

Zero-point correction = 0.010145 (Hartree/Particle)

Thermal correction to Energy = 0.012505
Thermal correction to Enthalpy = 0.013450
Thermal correction to Gibbs Free Energy = -0.001342
Sum of electronic and zero-point Energies = -1.165337
Sum of electronic and thermal Energies = -1.162977
Sum of electronic and thermal Enthalpies = -1.162033
Sum of electronic and thermal Free Energies = -1.176825

Coordinates: **H_2**

H	0.000000300	0.000000000	0.000000000
H	-0.000000300	0.000000000	0.000000000

Species F

HF energy = -2528.232971369584
No imaginary frequency
Zero-point correction = 0.848970 (Hartree/Particle)
Thermal correction to Energy = 0.934244
Thermal correction to Enthalpy = 0.935188
Thermal correction to Gibbs Free Energy = 0.713730
Sum of electronic and zero-point Energies = -2527.384001
Sum of electronic and thermal Energies = -2527.298727
Sum of electronic and thermal Enthalpies = -2527.297783
Sum of electronic and thermal Free Energies = -2527.519241

Coordinates: **F**

Ru	8.86210000	12.39040000	17.56700000
H	7.52910000	12.54380000	18.81540000
Ru	6.44080000	11.09670000	18.83950000
H	8.31890000	8.56430000	14.88510000
Ru	6.69620000	11.22390000	15.81790000
Fe	7.70260000	15.94300000	22.17670000
S	8.13800000	10.13240000	17.42510000
P	10.41530000	12.43150000	19.28930000
P	5.00960000	12.41050000	20.19320000
F	4.60090000	8.28060000	24.02320000
F	2.62620000	8.40830000	24.76740000
F	3.98450000	9.98860000	25.11410000
F	0.20020000	9.62170000	19.30390000
F	-0.67600000	9.37280000	21.21190000
F	-0.47020000	11.31090000	20.39470000
F	-0.05100000	14.64610000	21.16630000
F	1.20980000	16.00360000	22.19250000
F	0.07300000	16.66030000	20.53630000
F	3.89360000	17.65530000	17.08150000
F	4.63550000	15.94680000	16.08180000

F	2.57330000	16.40520000	15.99240000
O	11.22520000	12.13750000	15.65050000
O	8.67950000	15.43820000	17.41790000
O	7.62230000	9.81920000	21.36340000
O	4.41420000	8.84690000	18.50910000
O	7.25740000	14.09270000	14.84700000
O	3.95570000	11.71550000	14.62100000
C	10.30220000	12.22690000	16.32240000
C	8.77320000	14.29390000	17.48960000
C	7.21250000	10.33540000	20.42020000
C	5.18090000	9.69090000	18.64430000
C	7.20410000	13.04740000	15.34010000
C	5.02330000	11.54110000	15.01540000
C	11.45360000	13.96140000	19.38300000
C	11.82350000	14.61500000	18.20220000
C	12.67950000	15.72150000	18.24830000
C	13.17100000	16.17700000	19.47560000
C	12.80520000	15.52220000	20.65520000
C	11.95110000	14.41370000	20.61160000
C	11.77660000	11.19780000	19.09200000
C	13.09010000	11.49160000	19.48070000
C	14.09750000	10.53230000	19.32980000
C	13.80090000	9.27590000	18.79230000
C	12.49110000	8.98170000	18.40350000
C	11.48260000	9.94130000	18.54960000
C	9.93200000	12.22860000	21.06360000
C	10.55950000	11.16540000	21.73790000
C	10.35020000	10.93340000	23.09780000
C	9.48230000	11.76240000	23.81390000
C	8.83860000	12.80470000	23.15540000
C	9.05230000	13.06580000	21.78130000
C	8.27540000	14.19970000	21.25790000
C	6.78660000	14.30670000	21.32600000
C	6.41000000	15.56110000	20.65100000
C	7.62820000	16.22500000	20.17390000
C	8.77600000	15.39210000	20.55030000
C	7.31920000	15.82530000	24.18330000
C	6.58730000	16.94020000	23.56850000
C	7.56930000	17.83110000	22.93540000
C	8.90840000	17.26640000	23.16210000
C	8.75330000	16.02500000	23.92820000
C	5.84360000	13.22960000	21.74750000
C	4.84320000	13.75290000	22.77570000
C	3.76530000	11.30950000	21.05420000
C	4.11500000	10.63300000	22.22650000
C	3.17290000	9.81810000	22.87700000

C	3.57420000	9.13480000	24.15890000
C	1.88880000	9.65040000	22.34410000
C	1.55620000	10.30400000	21.15080000
C	0.18660000	10.14740000	20.53850000
C	2.49370000	11.12360000	20.50090000
C	3.87980000	13.79010000	19.65370000
C	2.79270000	14.16800000	20.44730000
C	1.98350000	15.25140000	20.06670000
C	0.83020000	15.63690000	20.95510000
C	2.25690000	15.95670000	18.89000000
C	3.34540000	15.56900000	18.09420000
C	3.61270000	16.36320000	16.84050000
C	4.15300000	14.48310000	18.46930000
H	9.79720000	15.58800000	20.25080000
H	5.40290000	15.88880000	20.43530000
H	5.37960000	14.02450000	23.70230000
H	4.34520000	14.68100000	22.45820000
H	4.07360000	13.03270000	23.07290000
H	6.43680000	12.39940000	22.23060000
H	5.54060000	17.16220000	23.71300000
H	6.90080000	15.11320000	24.87740000
H	9.55670000	15.46790000	24.38650000
H	9.84230000	17.76490000	22.95080000
H	7.36170000	18.81310000	22.53660000
H	7.66290000	17.07630000	19.50470000
H	13.83790000	17.03940000	19.51110000
H	12.96330000	16.22690000	17.32390000
H	11.46690000	14.28740000	17.22130000
H	13.37330000	12.45910000	19.90320000
H	15.11850000	10.76850000	19.62860000
H	14.58840000	8.53090000	18.67300000
H	12.25140000	8.00610000	17.97830000
H	10.46640000	9.67270000	18.22560000
H	9.30760000	11.58930000	24.87630000
H	10.85140000	10.10230000	23.59340000
H	8.15140000	13.45540000	23.70990000
H	4.99490000	14.18480000	17.82860000
H	2.20320000	11.60730000	19.55850000
H	5.11900000	10.72110000	22.66170000
H	1.15520000	9.01290000	22.85130000
H	2.54380000	13.63560000	21.37530000
H	1.63080000	16.80470000	18.58580000
H	11.23090000	10.46470000	21.22620000
H	11.68990000	13.92840000	21.55790000
H	13.18600000	15.87400000	21.61410000
C	8.72660000	9.37320000	14.26700000

H	9.46890000	9.89460000	14.87810000
C	7.57290000	10.34100000	13.91040000
C	9.46190000	8.76360000	13.05630000
H	9.88810000	9.54700000	12.41850000
H	10.28960000	8.13060000	13.40250000
H	8.80590000	8.13610000	12.44100000
C	6.49100000	9.61270000	13.09000000
H	5.63290000	10.24960000	12.86290000
H	6.89030000	9.26840000	12.12490000
H	6.12920000	8.73370000	13.63620000
C	8.11540000	11.53410000	13.18960000
O	7.22170000	12.12140000	12.33910000
H	7.66780000	12.91960000	12.00950000
O	9.23290000	12.01030000	13.31310000
H	5.76090000	11.76450000	17.36490000
H	6.03690000	9.72600000	15.76910000

Species TSFBG
HF energy = -2528.216870846642
Imaginary frequency: 718*i*
Zero-point correction = 0.846815 (Hartree/Particle)
Thermal correction to Energy = 0.932260
Thermal correction to Enthalpy = 0.933204
Thermal correction to Gibbs Free Energy = 0.711261
Sum of electronic and zero-point Energies = -2527.370056
Sum of electronic and thermal Energies = -2527.284611
Sum of electronic and thermal Enthalpies = -2527.283667
Sum of electronic and thermal Free Energies = -2527.505610

Coordinates: **TSFBG**

Ru	9.11230000	12.69960000	17.56030000
H	7.75340000	12.70180000	18.79840000
Ru	6.70170000	11.24300000	18.65000000
H	5.89100000	8.38930000	15.13560000
Ru	7.05920000	11.73530000	15.70380000
Fe	7.63780000	15.97540000	22.30500000
S	8.44810000	10.42640000	17.19830000
P	10.59630000	12.73360000	19.36270000
P	5.19350000	12.41730000	20.05250000
F	4.89520000	8.11580000	23.69720000
F	2.88820000	8.08750000	24.36120000
F	4.12760000	9.73300000	24.82980000
F	0.22180000	10.49020000	19.03480000
F	0.27180000	8.53670000	19.84230000

F	-0.53570000	10.13570000	20.97570000
F	-0.04510000	14.24320000	20.84940000
F	1.03160000	15.61450000	22.05220000
F	-0.04100000	16.30100000	20.36510000
F	3.81960000	17.86120000	17.30070000
F	4.95320000	16.36480000	16.33570000
F	2.87460000	16.51460000	15.96490000
O	11.51560000	12.63570000	15.69400000
O	8.64890000	15.71290000	17.42640000
O	7.88730000	9.81030000	21.08240000
O	4.74060000	8.98520000	18.07020000
O	8.81860000	13.56620000	13.98040000
O	4.74310000	13.42200000	14.69620000
C	10.59100000	12.66120000	16.37730000
C	8.85990000	14.58260000	17.50690000
C	7.46190000	10.37700000	20.17610000
C	5.48300000	9.83170000	18.30260000
C	8.25910000	12.87920000	14.72470000
C	5.64780000	12.78760000	15.02950000
C	11.55680000	14.30260000	19.57350000
C	11.90910000	15.04380000	18.44040000
C	12.70740000	16.18660000	18.56770000
C	13.15600000	16.59110000	19.82880000
C	12.80390000	15.85070000	20.96120000
C	12.00760000	14.70600000	20.83650000
C	12.02460000	11.57830000	19.15730000
C	13.28080000	11.86280000	19.70910000
C	14.34040000	10.96590000	19.53730000
C	14.15350000	9.78240000	18.81510000
C	12.90160000	9.49860000	18.26340000
C	11.84000000	10.39590000	18.43180000
C	10.06270000	12.41160000	21.10440000
C	10.69420000	11.32740000	21.73950000
C	10.44650000	11.01760000	23.07740000
C	9.53440000	11.78540000	23.80650000
C	8.88070000	12.84250000	23.18180000
C	9.13040000	13.18060000	21.83110000
C	8.32710000	14.30660000	21.33130000
C	6.83340000	14.34180000	21.34230000
C	6.42380000	15.60970000	20.71350000
C	7.62700000	16.34950000	20.31600000
C	8.79750000	15.55250000	20.69920000
C	7.18500000	15.74370000	24.28720000
C	6.42520000	16.85280000	23.69590000
C	7.38760000	17.81660000	23.14470000
C	8.74230000	17.30260000	23.39830000

C	8.61670000	16.01990000	24.09910000
C	5.92910000	13.20190000	21.67330000
C	4.86100000	13.62930000	22.67760000
C	3.98720000	11.20820000	20.81830000
C	4.33310000	10.50540000	21.97480000
C	3.41780000	9.60940000	22.55550000
C	3.81120000	8.89740000	23.82410000
C	2.16850000	9.39230000	21.96560000
C	1.84130000	10.07540000	20.78370000
C	0.48900000	9.82080000	20.16590000
C	2.75000000	10.97160000	20.20460000
C	4.01140000	13.76730000	19.54920000
C	2.85700000	14.01840000	20.29640000
C	2.00260000	15.07600000	19.94210000
C	0.76620000	15.31050000	20.76920000
C	2.30740000	15.89370000	18.84880000
C	3.47300000	15.64370000	18.10880000
C	3.77960000	16.56290000	16.95330000
C	4.31580000	14.57220000	18.44550000
H	9.81910000	15.80910000	20.45210000
H	5.41110000	15.90410000	20.47730000
H	5.34530000	13.90090000	23.63250000
H	4.31870000	14.53590000	22.37090000
H	4.12630000	12.85490000	22.92170000
H	6.54210000	12.37920000	22.14380000
H	5.36460000	17.02020000	23.80870000
H	6.77450000	14.98090000	24.93030000
H	9.42760000	15.47830000	24.56280000
H	9.65910000	17.85240000	23.24810000
H	7.14940000	18.80650000	22.78420000
H	7.64570000	17.23380000	19.69090000
H	13.77890000	17.48100000	19.92770000
H	12.98050000	16.76000000	17.68090000
H	11.58190000	14.75770000	17.43690000
H	13.47590000	12.77470000	20.27820000
H	15.31680000	11.19330000	19.96400000
H	14.98240000	9.08660000	18.67970000
H	12.74740000	8.58130000	17.69210000
H	10.87260000	10.13750000	17.97510000
H	9.33210000	11.55270000	24.85260000
H	10.95250000	10.17300000	23.54480000
H	8.15540000	13.44220000	23.74510000
H	5.21070000	14.37340000	17.83880000
H	2.47620000	11.47910000	19.27050000
H	5.31280000	10.63370000	22.45350000
H	1.44840000	8.69560000	22.41180000

H	2.58920000	13.40570000	21.16780000
H	1.64670000	16.72280000	18.56680000
H	11.39650000	10.67020000	21.21150000
H	11.75140000	14.15440000	21.74720000
H	13.15040000	16.16400000	21.94610000
C	6.86180000	8.52930000	14.63990000
H	7.63020000	8.43310000	15.41180000
C	6.92040000	9.96180000	14.05550000
C	7.05910000	7.41460000	13.59690000
H	8.03250000	7.50180000	13.10120000
H	7.02590000	6.43640000	14.09330000
H	6.27620000	7.41980000	12.82880000
C	5.79230000	10.23710000	13.05420000
H	5.80210000	11.26800000	12.69440000
H	5.89180000	9.58650000	12.17480000
H	4.81590000	10.03880000	13.51340000
C	8.29480000	10.21360000	13.48930000
O	8.27960000	11.01740000	12.38660000
H	9.21120000	11.13940000	12.13850000
O	9.33650000	9.72260000	13.88260000
H	6.07020000	12.07820000	17.23120000
H	6.07880000	10.47200000	15.41740000

Species G

HF energy = -347.012290858
No imaginary frequency
Zero-point correction = 0.147777 (Hartree/Particle)
Thermal correction to Energy = 0.156144
Thermal correction to Enthalpy = 0.157088
Thermal correction to Gibbs Free Energy = 0.114323
Sum of electronic and zero-point Energies = -346.864514
Sum of electronic and thermal Energies = -346.856147
Sum of electronic and thermal Enthalpies = -346.855203
Sum of electronic and thermal Free Energies = -346.897968

Coordinates: **G**

H	14.25080000	12.10450000	10.31550000
C	15.86580000	12.84060000	11.56360000
H	16.25400000	13.81360000	11.89300000
C	14.63330000	13.07290000	10.67160000
C	16.97740000	12.02780000	10.88920000
H	17.40220000	12.54540000	10.02010000
H	17.79920000	11.84280000	11.59200000
H	16.60870000	11.05080000	10.54710000
C	14.92520000	13.94570000	9.43110000

H	14.01820000	14.09870000	8.83680000
H	15.31250000	14.92890000	9.72960000
H	15.67410000	13.46790000	8.79000000
C	13.50990000	13.70860000	11.47610000
O	12.32120000	13.63700000	10.82190000
H	11.67040000	14.08360000	11.38990000
O	13.61210000	14.23710000	12.55860000
H	15.54290000	12.32650000	12.47830000

Species D'

HF energy = -2527.064042007192
No imaginary frequency
Zero-point correction = 0.829282 (Hartree/Particle)
Thermal correction to Energy = 0.914329
Thermal correction to Enthalpy = 0.915273
Thermal correction to Gibbs Free Energy = 0.693825
Sum of electronic and zero-point Energies = -2526.234760
Sum of electronic and thermal Energies = -2526.149713
Sum of electronic and thermal Enthalpies = -2526.148769
Sum of electronic and thermal Free Energies = -2526.370217

Coordinates: **D'**

Ru	13.97820000	10.89120000	16.51200000
H	12.32790000	11.35190000	15.84080000
Ru	12.13270000	10.85750000	14.12390000
H	13.07140000	12.28290000	13.63460000
Ru	14.89270000	12.15200000	14.15630000
Fe	8.87590000	12.59100000	18.94460000
S	14.30010000	9.81640000	14.38420000
P	12.99870000	9.42590000	18.05980000
P	10.07700000	12.06460000	14.25660000
F	7.10910000	7.61180000	12.46240000
F	5.63930000	8.39520000	11.16050000
F	5.58850000	8.87930000	13.21650000
F	7.35300000	12.07450000	8.32600000
F	7.82600000	13.81030000	9.43560000
F	9.37470000	12.55960000	8.70930000
F	6.58980000	15.78530000	11.95840000
F	5.93650000	15.81900000	13.97270000
F	6.76320000	17.55660000	13.09830000
F	12.68130000	17.16010000	14.03530000
F	11.24850000	18.45780000	14.88660000
F	12.10780000	16.93690000	16.07000000
O	16.70550000	10.14510000	17.61600000
O	13.70110000	13.39850000	18.21930000

O	10.69910000	8.26460000	14.87300000
O	11.59090000	10.13310000	11.21540000
O	17.69270000	12.17680000	15.30220000
O	14.30480000	14.91200000	15.30140000
C	15.67850000	10.44500000	17.18700000
C	13.78700000	12.43210000	17.59290000
C	11.22920000	9.25620000	14.63440000
C	11.84370000	10.43010000	12.29760000
C	16.64260000	12.15290000	14.83000000
C	14.57270000	13.87390000	14.87240000
C	13.12040000	9.93320000	19.84530000
C	14.23590000	10.66360000	20.26850000
C	14.38760000	10.99900000	21.61930000
C	13.42300000	10.60540000	22.55160000
C	12.30800000	9.87540000	22.12940000
C	12.15630000	9.53590000	20.77960000
C	13.87570000	7.79710000	18.18660000
C	14.01180000	7.11480000	19.40100000
C	14.67550000	5.88300000	19.43960000
C	15.20410000	5.32960000	18.26930000
C	15.07250000	6.01390000	17.05740000
C	14.41400000	7.24850000	17.01650000
C	11.21560000	8.89450000	18.00280000
C	10.98450000	7.50970000	17.94820000
C	9.69170000	6.98250000	17.95980000
C	8.59390000	7.84540000	18.01010000
C	8.80830000	9.21960000	18.04490000
C	10.11150000	9.76900000	18.05180000
C	10.15150000	11.23890000	18.07740000
C	9.52230000	12.11700000	17.04660000
C	9.84060000	13.50950000	17.40640000
C	10.65290000	13.50510000	18.62890000
C	10.84110000	12.11000000	19.04520000
C	6.90350000	12.05140000	19.02530000
C	7.05500000	13.51220000	19.04650000
C	7.89420000	13.86250000	20.20070000
C	8.25900000	12.61680000	20.89250000
C	7.65140000	11.49800000	20.16330000
C	8.91720000	11.65550000	15.76320000
C	7.49970000	12.20160000	15.60480000
C	8.96380000	11.48730000	12.86210000
C	8.15520000	10.35790000	13.01560000
C	7.31980000	9.94090000	11.96510000
C	6.43620000	8.73920000	12.18170000
C	7.30810000	10.63250000	10.74770000
C	8.14290000	11.74650000	10.58980000

C	8.16710000	12.51820000	9.29410000
C	8.97430000	12.16890000	11.63950000
C	9.79140000	13.90480000	14.11380000
C	8.54570000	14.38160000	13.68890000
C	8.29580000	15.76140000	13.63260000
C	6.93930000	16.23030000	13.17630000
C	9.28870000	16.67560000	14.00500000
C	10.53290000	16.19550000	14.43110000
C	11.61150000	17.16560000	14.84490000
C	10.79100000	14.81210000	14.47580000
H	11.47480000	11.79240000	19.86360000
H	9.61910000	14.38660000	16.81580000
H	6.84940000	11.75920000	16.38050000
H	7.43920000	13.28750000	15.77480000
H	7.02290000	11.97380000	14.64590000
H	8.85510000	10.52780000	15.78270000
H	6.50160000	14.21140000	18.43840000
H	6.19830000	11.50790000	18.41640000
H	7.60350000	10.47700000	20.51130000
H	8.74270000	12.55350000	21.85560000
H	8.06120000	14.86100000	20.57660000
H	11.17570000	14.35960000	19.04160000
H	13.54080000	10.86680000	23.60350000
H	15.26020000	11.56710000	21.94300000
H	15.01340000	10.98680000	19.57140000
H	13.61770000	7.51080000	20.34000000
H	14.78380000	5.35640000	20.38710000
H	15.72130000	4.37040000	18.30250000
H	15.48820000	5.59170000	16.14200000
H	14.33950000	7.76540000	16.04860000
H	7.57980000	7.44540000	18.01740000
H	9.54230000	5.90410000	17.91910000
H	7.95200000	9.90300000	18.07880000
H	11.78430000	14.46780000	14.79820000
H	9.62430000	13.03900000	11.47650000
H	8.15050000	9.77840000	13.94820000
H	6.65760000	10.30520000	9.92820000
H	7.73780000	13.69930000	13.39060000
H	9.09260000	17.75350000	13.96150000
H	11.80390000	6.78370000	17.88210000
H	11.26940000	8.96360000	20.48960000
H	11.55310000	9.56760000	22.85250000
C	15.50760000	13.34350000	12.21700000
H	16.44770000	13.79790000	12.52250000
C	15.58400000	11.99220000	11.85040000
C	14.47920000	14.31910000	11.69200000

H	14.42000000	15.20760000	12.33010000
H	14.77740000	14.65880000	10.68730000
H	13.47690000	13.88800000	11.61510000
C	14.60660000	11.33340000	10.90060000
H	15.01490000	11.35470000	9.87900000
H	14.43550000	10.28500000	11.15400000
H	13.64980000	11.85730000	10.88200000
C	16.93990000	11.36600000	11.92140000
O	16.94310000	10.08030000	11.48140000
H	17.86230000	9.77680000	11.56590000
O	17.96780000	11.90830000	12.27800000

Species TSD'E'
HF energy = -2527.027983157663
Imaginary frequency: 857*i*
Zero-point correction = 0.828381 (Hartree/Particle)
Thermal correction to Energy = 0.912907
Thermal correction to Enthalpy = 0.913851
Thermal correction to Gibbs Free Energy = 0.695266
Sum of electronic and zero-point Energies = -2526.199602
Sum of electronic and thermal Energies = -2526.115076
Sum of electronic and thermal Enthalpies = -2526.114132
Sum of electronic and thermal Free Energies = -2526.332717

Coordinates: **TSD'E'**

Ru	13.87140000	10.80910000	16.34560000
H	12.21930000	11.28310000	15.80040000
Ru	11.94550000	10.80840000	14.08160000
H	13.54210000	11.85790000	12.44290000
Ru	14.58550000	12.01610000	13.80880000
Fe	8.91410000	12.62110000	19.05160000
S	14.05790000	9.66290000	14.22900000
P	12.93730000	9.39410000	17.92990000
P	9.97670000	12.19080000	14.30350000
F	6.74260000	7.92940000	12.46700000
F	5.25320000	8.84010000	11.27480000
F	5.32950000	9.23850000	13.34800000
F	8.10840000	12.08210000	8.31470000
F	6.68160000	13.40670000	9.15230000
F	8.74390000	13.85030000	9.28390000
F	6.73750000	16.18440000	12.07370000
F	6.00310000	16.16740000	14.06000000
F	6.95410000	17.89380000	13.29760000
F	12.89290000	16.92390000	14.73490000

F	11.50940000	18.47390000	15.12100000
F	11.87440000	17.00290000	16.59370000
O	16.61050000	9.88600000	17.31020000
O	13.70280000	13.36310000	17.99740000
O	10.30640000	8.34500000	14.78290000
O	11.24810000	10.33980000	11.15790000
O	16.96690000	12.68730000	15.61460000
O	13.67210000	14.90890000	13.97620000
C	15.58430000	10.25660000	16.94220000
C	13.74360000	12.37020000	17.41220000
C	10.90520000	9.30760000	14.56860000
C	11.56780000	10.53390000	12.25070000
C	16.03850000	12.36600000	15.00750000
C	14.06480000	13.82500000	13.88780000
C	13.15760000	9.90830000	19.69770000
C	14.28920000	10.64500000	20.06340000
C	14.50700000	10.98080000	21.40480000
C	13.59350000	10.58030000	22.38480000
C	12.46320000	9.84300000	22.01990000
C	12.24450000	9.50370000	20.67930000
C	13.78130000	7.74890000	18.00570000
C	14.05850000	7.11070000	19.21990000
C	14.68350000	5.85780000	19.22510000
C	15.03330000	5.23900000	18.02150000
C	14.76120000	5.87880000	16.80820000
C	14.14120000	7.13310000	16.80000000
C	11.14700000	8.91930000	17.93990000
C	10.87840000	7.53970000	17.89090000
C	9.57440000	7.04530000	17.93760000
C	8.50020000	7.93600000	18.01740000
C	8.75100000	9.30330000	18.05600000
C	10.06770000	9.82060000	18.03460000
C	10.14290000	11.28790000	18.09110000
C	9.48660000	12.20520000	17.11360000
C	9.83160000	13.58090000	17.50960000
C	10.68840000	13.52860000	18.70020000
C	10.87670000	12.11920000	19.06250000
C	6.93950000	12.09790000	19.18740000
C	7.10700000	13.55550000	19.24730000
C	7.99070000	13.86230000	20.38030000
C	8.36710000	12.59270000	21.02070000
C	7.72250000	11.50280000	20.28000000
C	8.83470000	11.79700000	15.83500000
C	7.44280000	12.41490000	15.71760000
C	8.79960000	11.70280000	12.92760000
C	7.94510000	10.60850000	13.07950000

C	7.04970000	10.26410000	12.05100000
C	6.11710000	9.10030000	12.26620000
C	7.02770000	10.99340000	10.85810000
C	7.91360000	12.07070000	10.69770000
C	7.87310000	12.83710000	9.39920000
C	8.80350000	12.41910000	11.72240000
C	9.74980000	14.04520000	14.24430000
C	8.54680000	14.60530000	13.80020000
C	8.36860000	15.99780000	13.81140000
C	7.05880000	16.55790000	13.32330000
C	9.38560000	16.84110000	14.27710000
C	10.58210000	16.27610000	14.73260000
C	11.68660000	17.15190000	15.26960000
C	10.76690000	14.88120000	14.71110000
H	11.53390000	11.76860000	19.84740000
H	9.58990000	14.48110000	16.96250000
H	6.79810000	12.01940000	16.52260000
H	7.44200000	13.50500000	15.86660000
H	6.92230000	12.19650000	14.77930000
H	8.72130000	10.67410000	15.83100000
H	6.54040000	14.27840000	18.67990000
H	6.20630000	11.57980000	18.58910000
H	7.67530000	10.47210000	20.59850000
H	8.88380000	12.49570000	21.96350000
H	8.18120000	14.84740000	20.77990000
H	11.23170000	14.36550000	19.12170000
H	13.76320000	10.84230000	23.42970000
H	15.39110000	11.55500000	21.68450000
H	15.02810000	10.97350000	19.32750000
H	13.80790000	7.55640000	20.18580000
H	14.90110000	5.36630000	20.17290000
H	15.52050000	4.26340000	18.02830000
H	15.03730000	5.40520000	15.86550000
H	13.95190000	7.61150000	15.82810000
H	7.47640000	7.56190000	18.04490000
H	9.39610000	5.97110000	17.89820000
H	7.91330000	10.00860000	18.11490000
H	11.72030000	14.47000000	15.07050000
H	9.49730000	13.25550000	11.56510000
H	7.94990000	9.99860000	13.99270000
H	6.33330000	10.73180000	10.05060000
H	7.71690000	13.98210000	13.44140000
H	9.24430000	17.92810000	14.28610000
H	11.67600000	6.79200000	17.80470000
H	11.34720000	8.92630000	20.43340000
H	11.74820000	9.53010000	22.78070000

C	14.81270000	11.84740000	11.44260000
H	14.44550000	12.76290000	10.98010000
C	16.06900000	12.01390000	12.11470000
C	14.50710000	10.57860000	10.66800000
H	13.51060000	10.61240000	10.22260000
H	15.23590000	10.49010000	9.84930000
H	14.58170000	9.67790000	11.28390000
C	17.08060000	10.87530000	12.17940000
H	17.64800000	10.81700000	11.23710000
H	17.80310000	11.02750000	12.98460000
H	16.58760000	9.91350000	12.34030000
C	16.63180000	13.40160000	12.02740000
O	17.90780000	13.47360000	12.48550000
H	18.16800000	14.40620000	12.39980000
O	16.06650000	14.38140000	11.58360000

Species E'

HF energy = -2527.038633265699
No imaginary frequency
Zero-point correction = 0.831531 (Hartree/Particle)
Thermal correction to Energy = 0.916458
Thermal correction to Enthalpy = 0.917402
Thermal correction to Gibbs Free Energy = 0.697565
Sum of electronic and zero-point Energies = -2526.207102
Sum of electronic and thermal Energies = -2526.122176
Sum of electronic and thermal Enthalpies = -2526.121231
Sum of electronic and thermal Free Energies = -2526.341068

Coordinates: **E'**

Ru	13.80450000	10.89350000	16.33260000
H	12.12450000	11.27260000	15.83540000
Ru	11.87990000	10.84610000	14.09060000
H	13.90510000	11.59870000	11.88680000
Ru	14.49970000	12.01150000	13.67210000
Fe	8.80930000	12.56050000	19.05610000
S	13.99980000	9.70520000	14.25520000
P	12.94300000	9.46780000	17.93310000
P	9.93040000	12.19170000	14.32150000
F	6.83980000	7.96060000	12.15430000
F	5.26070000	8.93130000	11.13810000
F	5.43040000	9.11550000	13.23460000
F	7.94430000	12.49790000	8.37390000
F	6.47310000	13.67680000	9.34110000
F	8.51290000	14.21080000	9.47480000
F	6.63360000	16.35410000	12.45340000

F	6.05260000	16.26020000	14.48780000
F	6.98510000	17.99940000	13.73290000
F	13.03340000	16.71850000	14.64070000
F	11.77940000	18.39340000	14.93220000
F	12.09710000	17.02900000	16.51630000
O	16.61130000	10.10060000	17.24530000
O	13.53010000	13.44100000	17.98460000
O	10.25030000	8.30310000	14.56730000
O	11.44690000	10.74040000	11.08150000
O	16.57260000	13.08700000	15.59070000
O	13.51170000	14.87620000	13.32460000
C	15.56130000	10.41660000	16.90030000
C	13.61270000	12.44910000	17.40490000
C	10.83620000	9.29120000	14.44500000
C	11.65060000	10.79310000	12.21990000
C	15.75080000	12.61790000	14.92260000
C	13.90960000	13.79760000	13.43020000
C	13.15670000	10.00330000	19.68870000
C	14.26140000	10.78430000	20.04550000
C	14.47370000	11.13100000	21.38460000
C	13.58250000	10.69590000	22.37080000
C	12.48020000	9.91360000	22.01470000
C	12.26620000	9.56360000	20.67600000
C	13.85280000	7.86400000	18.00270000
C	14.20950000	7.26890000	19.21830000
C	14.87910000	6.03930000	19.22570000
C	15.19400000	5.40020000	18.02310000
C	14.84150000	5.99620000	16.80830000
C	14.17670000	7.22720000	16.79720000
C	11.17600000	8.94100000	17.93550000
C	10.95430000	7.55300000	17.87190000
C	9.66790000	7.01460000	17.90380000
C	8.56340000	7.86790000	17.98350000
C	8.76760000	9.24230000	18.03900000
C	10.06580000	9.80460000	18.03100000
C	10.08960000	11.27310000	18.10020000
C	9.41100000	12.17350000	17.12170000
C	9.71060000	13.55730000	17.52720000
C	10.55580000	13.52670000	18.72690000
C	10.78620000	12.12240000	19.08390000
C	6.85020000	11.97710000	19.16440000
C	6.97290000	13.43850000	19.23890000
C	7.83420000	13.76190000	20.38440000
C	8.24120000	12.49870000	21.01860000
C	7.63810000	11.39650000	20.26150000
C	8.78400000	11.75090000	15.83510000

C	7.36890000	12.31200000	15.71350000
C	8.75200000	11.77790000	12.92540000
C	7.95240000	10.63450000	13.00360000
C	7.04500000	10.33710000	11.97120000
C	6.16690000	9.12060000	12.10850000
C	6.96330000	11.15910000	10.84250000
C	7.79920000	12.28280000	10.75140000
C	7.69570000	13.14830000	9.52130000
C	8.69920000	12.58630000	11.78250000
C	9.73670000	14.05210000	14.32880000
C	8.52090000	14.65510000	13.99190000
C	8.38760000	16.05200000	14.04890000
C	7.05850000	16.66170000	13.68970000
C	9.46910000	16.85440000	14.43480000
C	10.68500000	16.24520000	14.76700000
C	11.86540000	17.08060000	15.19230000
C	10.81750000	14.84540000	14.71910000
H	11.44530000	11.78930000	19.87390000
H	9.45250000	14.45110000	16.97690000
H	6.72640000	11.85330000	16.48560000
H	7.31770000	13.39330000	15.90900000
H	6.87660000	12.11130000	14.75610000
H	8.71570000	10.62350000	15.82050000
H	6.39150000	14.14890000	18.67060000
H	6.14120000	11.44230000	18.55160000
H	7.61770000	10.36230000	20.57090000
H	8.74930000	12.40910000	21.96650000
H	7.99010000	14.74860000	20.79440000
H	11.06710000	14.37820000	19.15800000
H	13.74800000	10.96680000	23.41450000
H	15.33570000	11.74060000	21.65840000
H	14.98190000	11.13920000	19.30330000
H	13.98880000	7.73070000	20.18410000
H	15.15790000	5.58150000	20.17440000
H	15.71580000	4.44240000	18.03170000
H	15.08820000	5.50610000	15.86560000
H	13.92110000	7.66920000	15.82270000
H	7.55250000	7.45910000	17.99620000
H	9.52590000	5.93550000	17.84980000
H	7.90590000	9.91830000	18.09660000
H	11.77990000	14.39040000	14.99040000
H	9.35690000	13.45870000	11.67590000
H	8.01390000	9.94870000	13.85950000
H	6.26110000	10.93300000	10.03130000
H	7.65110000	14.06210000	13.67890000
H	9.36480000	17.94470000	14.47590000

H	11.77670000	6.83280000	17.78620000
H	11.39060000	8.95070000	20.43580000
H	11.78290000	9.57370000	22.78070000
C	14.92280000	11.49420000	11.29470000
H	14.79610000	12.32340000	10.59090000
C	16.09630000	11.76360000	12.19330000
C	14.82500000	10.12940000	10.60620000
H	13.91040000	10.07170000	10.00660000
H	15.68270000	9.99200000	9.93590000
H	14.81400000	9.30350000	11.32450000
C	17.09420000	10.63980000	12.46520000
H	17.72310000	10.45270000	11.57950000
H	17.76500000	10.90220000	13.28710000
H	16.58760000	9.70710000	12.72490000
C	16.71820000	13.10220000	11.93010000
O	17.93030000	13.24830000	12.52730000
H	18.21510000	14.15570000	12.32630000
O	16.23990000	14.00020000	11.26260000

Species F'

HF energy = -2528.229692793709
No imaginary frequency
Zero-point correction = 0.848836 (Hartree/Particle)
Thermal correction to Energy = 0.934170
Thermal correction to Enthalpy = 0.935114
Thermal correction to Gibbs Free Energy = 0.712826
Sum of electronic and zero-point Energies = -2527.380857
Sum of electronic and thermal Energies = -2527.295523
Sum of electronic and thermal Enthalpies = -2527.294578
Sum of electronic and thermal Free Energies = -2527.516867

Coordinates: **F'**

Ru	13.82430000	10.92640000	16.40540000
H	12.10700000	11.31940000	15.89320000
Ru	11.81340000	10.89080000	14.17000000
H	16.35980000	11.65370000	10.89080000
Ru	14.62420000	11.89820000	13.66830000
Fe	8.76480000	12.53880000	19.10200000
S	13.90660000	9.69510000	14.36890000
P	12.93220000	9.47550000	17.98280000
P	9.85230000	12.19830000	14.37020000
F	6.72350000	8.01660000	12.23540000
F	5.19890000	8.97300000	11.12610000
F	5.28250000	9.21450000	13.22320000

F	7.94530000	12.51940000	8.40540000
F	6.47340000	13.71830000	9.34840000
F	8.51760000	14.22900000	9.51080000
F	6.65020000	16.41820000	12.52990000
F	6.08470000	16.34550000	14.56970000
F	7.04990000	18.06080000	13.79950000
F	13.02570000	16.45560000	15.50820000
F	12.21990000	18.02070000	14.33640000
F	11.62780000	17.79340000	16.35880000
O	16.59400000	10.21310000	17.45230000
O	13.48750000	13.42010000	18.14310000
O	10.17810000	8.36950000	14.77170000
O	11.48840000	10.54140000	11.15880000
O	15.82970000	13.83000000	15.74840000
O	14.37450000	14.33490000	11.87690000
C	15.56310000	10.48730000	17.02650000
C	13.61300000	12.46040000	17.52170000
C	10.79680000	9.32140000	14.58410000
C	11.60950000	10.66570000	12.29360000
C	15.33360000	13.00080000	15.11170000
C	14.55690000	13.43020000	12.56170000
C	13.10920000	10.00740000	19.74630000
C	14.21550000	10.77210000	20.13230000
C	14.40140000	11.11220000	21.47720000
C	13.48250000	10.68640000	22.44140000
C	12.37880000	9.91940000	22.05700000
C	12.19150000	9.57620000	20.71270000
C	13.84290000	7.87190000	18.08120000
C	14.11950000	7.25650000	19.30830000
C	14.79830000	6.03280000	19.34190000
C	15.20300000	5.41740000	18.15360000
C	14.92950000	6.03190000	16.92810000
C	14.25530000	7.25760000	16.89210000
C	11.16060000	8.94650000	17.95780000
C	10.94860000	7.55760000	17.88660000
C	9.66620000	7.00900000	17.91360000
C	8.55560000	7.85370000	17.99660000
C	8.74980000	9.22950000	18.05560000
C	10.04350000	9.80260000	18.05160000
C	10.05020000	11.27150000	18.12520000
C	9.34960000	12.17250000	17.16140000
C	9.64040000	13.55740000	17.57180000
C	10.49790000	13.52760000	18.76190000
C	10.74680000	12.12340000	19.10660000
C	6.81270000	11.93630000	19.22620000
C	6.92290000	13.39820000	19.31300000

C	7.79400000	13.71890000	20.45200000
C	8.21950000	12.45350000	21.06970000
C	7.61800000	11.35280000	20.30900000
C	8.70470000	11.76380000	15.87920000
C	7.29880000	12.34920000	15.76640000
C	8.67910000	11.80070000	12.96810000
C	7.85670000	10.67370000	13.04240000
C	6.96200000	10.38380000	11.99710000
C	6.06390000	9.18100000	12.12860000
C	6.90880000	11.20190000	10.86380000
C	7.76290000	12.31260000	10.78030000
C	7.68710000	13.17680000	9.54630000
C	8.65380000	12.60580000	11.82190000
C	9.72170000	14.05570000	14.37320000
C	8.51480000	14.68390000	14.05220000
C	8.40990000	16.08360000	14.11150000
C	7.09170000	16.72200000	13.76130000
C	9.51010000	16.85800000	14.49490000
C	10.71900000	16.22200000	14.81530000
C	11.87620000	17.09060000	15.24020000
C	10.83020000	14.82390000	14.74550000
H	11.41890000	11.79520000	19.88820000
H	9.37050000	14.45110000	17.02690000
H	6.65650000	11.91180000	16.55150000
H	7.26710000	13.43320000	15.95020000
H	6.79330000	12.14590000	14.81640000
H	8.61560000	10.63860000	15.86250000
H	6.32770000	14.10860000	18.75910000
H	6.10040000	11.40060000	18.61820000
H	7.60990000	10.31570000	20.60950000
H	8.73860000	12.36000000	22.01150000
H	7.94490000	14.70320000	20.87010000
H	11.00650000	14.38060000	19.19440000
H	13.62750000	10.95190000	23.48950000
H	15.26540000	11.70960000	21.77190000
H	14.95980000	11.12010000	19.41050000
H	13.82820000	7.69820000	20.26470000
H	15.01520000	5.56100000	20.30000000
H	15.73330000	4.46470000	18.18250000
H	15.24650000	5.56140000	15.99640000
H	14.06510000	7.71250000	15.90870000
H	7.54770000	7.43740000	18.01040000
H	9.53270000	5.92900000	17.85660000
H	7.88250000	9.89830000	18.11860000
H	11.78930000	14.34230000	14.98330000
H	9.32500000	13.46890000	11.72170000

H	7.88700000	9.99670000	13.90610000
H	6.21420000	10.98320000	10.04370000
H	7.62940000	14.10960000	13.74780000
H	9.43610000	17.95140000	14.54620000
H	11.77710000	6.84420000	17.79780000
H	11.31430000	8.97440000	20.45210000
H	11.65990000	9.58590000	22.80570000
C	16.80290000	10.88280000	11.52890000
H	17.87350000	10.85650000	11.25620000
C	16.72920000	11.33670000	13.01250000
C	16.20860000	9.51340000	11.18050000
H	16.32640000	9.32100000	10.10600000
H	16.70880000	8.69750000	11.71630000
H	15.13890000	9.46010000	11.41570000
C	17.32440000	10.26290000	13.93580000
H	18.34400000	10.00050000	13.60620000
H	17.40500000	10.60350000	14.96910000
H	16.72660000	9.34700000	13.91800000
C	17.48600000	12.63330000	13.10660000
O	18.22190000	12.76830000	14.24990000
H	18.59520000	13.66490000	14.20830000
O	17.49240000	13.52530000	12.27740000
H	12.79390000	12.31300000	13.83270000
H	14.37660000	11.28150000	12.18280000

Species TSF'BG
HF energy = -2528.215830924713
Imaginary frequency: 635*i*
Zero-point correction = 0.846886 (Hartree/Particle)
Thermal correction to Energy = 0.932323
Thermal correction to Enthalpy = 0.933267
Thermal correction to Gibbs Free Energy = 0.711550
Sum of electronic and zero-point Energies = -2527.368945
Sum of electronic and thermal Energies = -2527.283508
Sum of electronic and thermal Enthalpies = -2527.282564
Sum of electronic and thermal Free Energies = -2527.504281

Coordinates: **TSF'BG**

Ru	13.91000000	10.86470000	16.69750000
H	12.21920000	11.23290000	16.08250000
Ru	12.01230000	10.75360000	14.35570000
H	16.78030000	13.32840000	11.81680000
Ru	14.77970000	11.90900000	14.10570000
Fe	8.77860000	12.68030000	19.09130000

S	14.13250000	9.63120000	14.65250000
P	12.90280000	9.48690000	18.28960000
P	10.01940000	12.03510000	14.42580000
F	6.87880000	7.72370000	12.57310000
F	5.44530000	8.59280000	11.28490000
F	5.42330000	9.05430000	13.34640000
F	8.43160000	11.75750000	8.36590000
F	6.96200000	13.09910000	9.09650000
F	9.01410000	13.55590000	9.31310000
F	6.98530000	16.05490000	11.97620000
F	6.21410000	16.14310000	13.94690000
F	7.24770000	17.80060000	13.13910000
F	12.92010000	16.41140000	15.79600000
F	12.43550000	17.76680000	14.24280000
F	11.45270000	17.89390000	16.11600000
O	16.60900000	10.02250000	17.82010000
O	13.63590000	13.47580000	18.25270000
O	10.42700000	8.20860000	14.98030000
O	11.87590000	10.29850000	11.34650000
O	17.00730000	12.77990000	16.03690000
O	14.58010000	14.84980000	13.38080000
C	15.60010000	10.36590000	17.38530000
C	13.72480000	12.46540000	17.70550000
C	11.02210000	9.17200000	14.77760000
C	11.91340000	10.46280000	12.48370000
C	16.12960000	12.36900000	15.40900000
C	14.71080000	13.73810000	13.66190000
C	13.01750000	10.07980000	20.03980000
C	14.13090000	10.82830000	20.43690000
C	14.27500000	11.21970000	21.77300000
C	13.30620000	10.86300000	22.71610000
C	12.19420000	10.11420000	22.31980000
C	12.04860000	9.71920000	20.98450000
C	13.76970000	7.86650000	18.48970000
C	13.90780000	7.25300000	19.74070000
C	14.55880000	6.01860000	19.84660000
C	15.07360000	5.39220000	18.70750000
C	14.93900000	6.00600000	17.45870000
C	14.29230000	7.24230000	17.35020000
C	11.12410000	8.98180000	18.21340000
C	10.88700000	7.59590000	18.18140000
C	9.59290000	7.07410000	18.18740000
C	8.49800000	7.94260000	18.20780000
C	8.71810000	9.31580000	18.21980000
C	10.02300000	9.86230000	18.23220000
C	10.06270000	11.33220000	18.23180000

C	9.41610000	12.19170000	17.19500000
C	9.72470000	13.59120000	17.53660000
C	10.54480000	13.61020000	18.75320000
C	10.74990000	12.22290000	19.18440000
C	6.80890000	12.13280000	19.18230000
C	6.95430000	13.59420000	19.19710000
C	7.79700000	13.95280000	20.34620000
C	8.16980000	12.71160000	21.04200000
C	7.56390000	11.58760000	20.31980000
C	8.81010000	11.72020000	15.91570000
C	7.42750000	12.33510000	15.70900000
C	8.90460000	11.51530000	13.01470000
C	8.04600000	10.42320000	13.15970000
C	7.20060000	10.04550000	12.10120000
C	6.26090000	8.88550000	12.30740000
C	7.23300000	10.73910000	10.88730000
C	8.12380000	11.81360000	10.73630000
C	8.14210000	12.54200000	9.41550000
C	8.96450000	12.19490000	11.79060000
C	9.87170000	13.88730000	14.28270000
C	8.69740000	14.47310000	13.80120000
C	8.57480000	15.87190000	13.75110000
C	7.29720000	16.46380000	13.21690000
C	9.61830000	16.68840000	14.19960000
C	10.78880000	16.09510000	14.69640000
C	11.87900000	17.00840000	15.19810000
C	10.92570000	14.69770000	14.71980000
H	11.38890000	11.92500000	20.00510000
H	9.48790000	14.45860000	16.93690000
H	6.74880000	11.98540000	16.50740000
H	7.42440000	13.43130000	15.79920000
H	6.94490000	12.06650000	14.76340000
H	8.69090000	10.59880000	15.96380000
H	6.39560000	14.28880000	18.58800000
H	6.10250000	11.58350000	18.57970000
H	7.51940000	10.56820000	20.67320000
H	8.65650000	12.65490000	22.00390000
H	7.96020000	14.95380000	20.71760000
H	11.05750000	14.47580000	19.15440000
H	13.41870000	11.16810000	23.75730000
H	15.14530000	11.80280000	22.07760000
H	14.91170000	11.12340000	19.73030000
H	13.52590000	7.70490000	20.65950000
H	14.66810000	5.54680000	20.82280000
H	15.58200000	4.43100000	18.79310000
H	15.34370000	5.52710000	16.56590000

H	14.21400000	7.69830000	16.35220000
H	7.48190000	7.54660000	18.20880000
H	9.43910000	5.99550000	18.16330000
H	7.86340000	10.00320000	18.23010000
H	11.86160000	14.25030000	15.08310000
H	9.66360000	13.02790000	11.64060000
H	8.00880000	9.84130000	14.09000000
H	6.57700000	10.45170000	10.05660000
H	7.84980000	13.86660000	13.45460000
H	9.52960000	17.78130000	14.16600000
H	11.70340000	6.86450000	18.13940000
H	11.16320000	9.13480000	20.71310000
H	11.43620000	9.83540000	23.05200000
C	16.54350000	12.39570000	11.29570000
H	17.46390000	12.12870000	10.75060000
C	16.31280000	11.28170000	12.33650000
C	15.42690000	12.63460000	10.27430000
H	15.71320000	13.44840000	9.59640000
H	15.22830000	11.74910000	9.65860000
H	14.48420000	12.92510000	10.75620000
C	15.99770000	9.92330000	11.69000000
H	16.83150000	9.63360000	11.03040000
H	15.86930000	9.13870000	12.43620000
H	15.08880000	9.96660000	11.08110000
C	17.53300000	11.20000000	13.21790000
O	17.68260000	9.99930000	13.85350000
H	18.49550000	10.09000000	14.37800000
O	18.37960000	12.06460000	13.33420000
H	12.95600000	12.20800000	14.04220000
H	14.63740000	11.62590000	12.51600000

Crystallographic refinement

The crystal of **6** was found to be twinned and was solved using the JANA2006 program.[S1] It was refined as an inversion twin, yielding the absolute configuration and the absolute structure, x(u)=0.05(3). Two large non-solvent hydrogen atoms with large thermal displacment parameters, due to disorder on the cyclopentadienyl rings. The structure contains voids of 259 Å3. This is due to the packing of the molecules in the solid state. There is no rest electron density to account for any solvent molecules.
The other structures were solved by a charge flipping (Superflip)[S2] method or by direct methods using SHELXS-97[S3] software. Structures were refined with SHELXL-2017[S3] programs. The low-quality crystal of **4** was solved as a racemic twin. The BASF value was refined to 0.039. The chiral space group $P2_12_12_1$ gave the best results. Also, some CF_3 moieties were slightly disordered. To avoid using a series of additional strong constraints and restraints, no disorder model was used for the final refinement. However, the anisotropic displacement parameters were constrained on series of atoms to avoid non positive definite U-values. The crystal of **5** was found to be twinned (twin matrix [-1.000 0.000 0.000 0.000 -1.000 0.000 0.000 0.000 -1.000]). The BASF value was refined to 0.024. The fluorines in one of the CF_3 groups were disordered over two sites with occupancy ratio of 0.52/0.48. Fluorine atoms F4 - F7 were restrained so that their U_{ij} components approximate to isotropic behavior. The crystal of compound **8** contained ca. ¼ disordered and partially lost hexane of crystallization per Ru cluster. However, no stable model could be obtained for the disordered solvent and therefore it was omitted from the final model. The contribution of the missing solvent to the calculated structure factors were taken into account by using the SQUEEZE routine of PLATON.[S4] In compound **17** one of the phenyl rings was disordered over two sites with occupancy ratio of 0.49/0.51. The five carbon atoms of the disordered groups were fitted to a regular hexagon (C-C = 1.39 Å) and the anisotropic displacement parameters were set to be equal. Hexane of crystallization was disordered forming a chain-like string. Because of that disorder the atoms in hexane was refined with occupancies of 0.25. Furthermore, all carbon atoms in the hexane molecule were restrained with effective standard deviation 0.01 so that their U_{ij} components approximate to isotropic behaviour. The hydride hydrogens is compounds **3**, **5** and **20** were located from the difference Fourier map and refined isotropically. In compounds **8** and **17** the hydride hydrogens were located from the difference Fourier map but constrained to ride on one of the related Ru atoms with U_{iso}=1.2-1.5 U_{eq}(Ru atom). In **4**, the hydride hydrogens could not be located from the difference Fourier map and they were placed on the most likely positions and constrained to ride on one of the parent Ru atoms with U_{iso}=1.5 U_{eq}(Ru atom).

S1. (a) V. Petricek, M. Dusek, L. Palatinus, (2014). *Z. Kristallogr*. **229**, 345-352. (b) V. Petricek, M. Dusek, J. Plasil, (2016). *Z. Kristallogr*. **231**, 583-599.

S2. L. Palatinus, G. Chapuis, *J. Appl. Cryst.* **2007**, *40*, 786-790.

S3. G.M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3-8.

S4. A.L. Spek, *Acta Cryst.* **2009**, *D65*, 148-155.

Table S1 Crystallographic data for clusters $[(\mu\text{-H})_2Ru_3(\mu_3\text{-S})(CO)_7(\mu\text{-P-P*})]$ **3**-**6**, **8**, **17** and **20**, where (P-P*= **1a**, **1a**, **1b**, **1b**, **1c**, **1h** and **2b**, respectively).

	3	**4**	**5**	**6**	**8**	**17**	**20**
empirical formula	$C_{53}H_{34}F_{12}FeO_7P_2Ru_3S$	$C_{53}H_{34}F_{12}FeO_7P_2Ru_3S$	$C_{53}H_{34}F_{12}FeO_7P_2Ru_3S$	$C_{106}H_{68}F_{24}Fe_2O_{14}P_4Ru_6S_2$	$C_{49}H_{50}FeO_7P_2Ru_3S$	$C_{101}H_{83}Fe_2O_{14}P_4Ru_6S_2$	$C_{43}H_{46}FeO_7P_2Ru_3S$
fw	1463.86	1463.86	1463.86	2928	1203.95	2426.79	1127.86
temp (K)	170(2)	170(2)	100(2)	293	170(2)	170(2)	170(2)
λ(Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
cryst syst	Orthorhombic	Orthorhombic	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
space group	$P2_12_12_1$	$P2_12_12_1$	Cc	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12$
a (Å)	10.9799(5)	11.9655(4)	14.9044(2)	17.9576(9)	10.4751(2)	a = 12.11044(17)	a = 15.06019(16)
b (Å)	14.7027(5)	20.1151(5)	24.9178(4)	59.4487(11)	17.5460(4)	b = 20.7626(4)	b = 18.1823(2)
c (Å)	35.1126(9)	49.045(3)	14.7954(2)	10.978(5)	30.9412(8)	c = 21.0868(4)	c = 15.73196(19)
α (deg)	90	90	90	90	90	90	
β (deg)	90	90	99.8870(10)	90	90	90	90
γ (deg)	90	90	90	90	90	90	
V (Å^3)	5668.4(3)	11804.5(8)	5413.18(14)	11720(6)	5686.9(2)	5302.14(16)	4307.87(8)
Z	4	8	4	4	4	2	4
ρ_{calc} (Mg/m^3)	1.715	1.647	1.796	1.6589	1.406	1.520	1.739
μ(Mo Kα) (mm^{-1})	1.216	1.168	1.274	1.177	1.166	1.252	1.533
No. reflns.	31467	42539	50958	249874	16529	25373	115230
Unique reflns.	12988	26879	20611	23804	12194	14236	17855
GOOF (F^2)	1.008	1.073	1.027	1.94	1.008	1.045	1.077
R_{int}	0.0541	0.0800	0.0227	0.0497	0.0222	0.0555	0.0583
R1[a] ($I \geq 2\sigma$)	0.0521	0.1029	0.0218	0.0675 ($I \geq 3\sigma$)	0.0322	0.0503	0.0300
wR2[b] ($I \geq 2\sigma$)	0.0781	0.1685	0.0511	0.1872 ($I \geq 3\sigma$)	0.0629	0.1054	0.0608

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$. [c] $w=1/(\sigma^2(I)+0.0049\ I^2)$