Efficient *Z*-Selective Olefin-Acrylamide Cross-Metathesis Enabled by Sterically Demanding Cyclometalated Ruthenium Catalysts

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1. General consideration

All reactions were carried out in dry glassware under an argon atmosphere using standard Schlenk techniques or in a Vacuum Atmospheres Glovebox under a nitrogen atmosphere, unless otherwise specified. All solvents were purified by passing through solvent purification columns and further degassed by bubbling nitrogen. NMR solvents were dried over pre-baked 3 Å or 4 Å molecule sieves and subsequently degassed with bubbling nitrogen. CDCl$_3$ was used as received. Liquid olefin substrates purchased from commercial sources were filtered through a plug of neutral alumina prior to use. The retention factor (R$_f$) of thin-layer chromatography (TLC) was recorded by using E. Merck silica gel 60 F254 precoated plates (0.25 mm) and visualized by UV fluorescence quenching or potassium permanganate staining. ^{1}H and ^{13}C NMR spectra were recorded on either a Bruker Ascend 400 spectrometer (400 MHz and 101 MHz, respectively) or a Varian Inova 500 MHz (500 MHz and 126 MHz, respectively). For CDCl$_3$ solutions, the chemical shifts are reported as parts per million (ppm) referenced to residual protium or carbon of the solvents; CHCl$_3$ δ H (7.26 ppm) and CDCl$_3$ δ C (77.16 ppm). For C$_6$D$_6$ solutions, the chemical shifts are reported as parts per million (ppm) referenced to residual protium or carbon of the solvents; C$_6$D$_5$H δ H (7.16 ppm) and C$_6$D$_6$ δ C (128.06 ppm). Coupling constants are reported in Hertz (Hz). Data for ^{1}H NMR spectra are reported as follows: chemical shift (ppm, referenced to protium: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet (quintet), h = heptet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, the coupling constant (Hz), and integration). High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High-Resolution Mass Spectrometer. Infrared (IR) spectra were recorded on a Perkin Elmer Paragon 1000 spectrometer using neat samples on ATR diamond, and are reported in frequency of absorption (cm^{-1}).

2. Catalyst synthesis
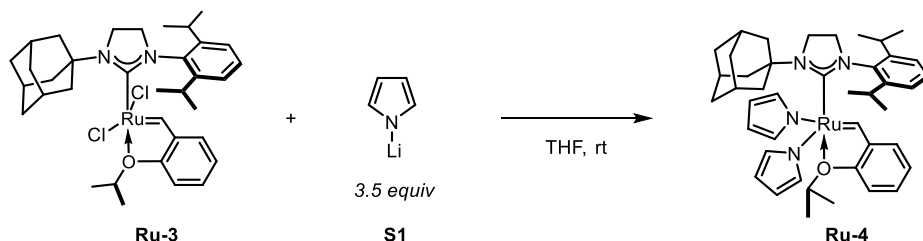
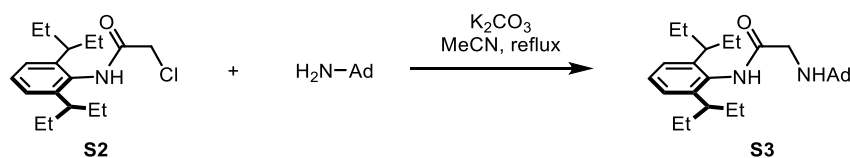**Ru-3** was synthesized according to the literature procedure.[1]

S1 was prepared according to the following procedure: An oven-dried flask was fitted with a stir bar and a rubber septum and cycled under an argon atmosphere. To this flask was added dry hexanes (6 mL) and pyrrole (248 mg, 3.7 mmol, 1.0 equiv) through the septum. The solution was cooled to −78 °C with a dry ice/acetone bath, and *n*-BuLi (1.5 mL, 2.45 M in hexane, 3.6 mmol, 0.98 equiv) was added dropwise. The reaction was left to stir for 15 minutes and the cold bath was removed. After stirring for additional 4 hours, the solution was transferred into a glass centrifuge tube in a glovebox, and pentane (10 mL) was added. The tube was centrifuged and the supernatant was removed. This rinse was repeated three more times and the residual solvent was removed using a high vacuum to yield an off-white powder in > 90% yield.

Ru-4: A 8 mL vial was charged with **Ru-3** (130 mg, 0.19 mmol, 1 equiv) in THF (2.5 mL, *solution A*). A 4 mL vial was charged with lithium pyrrolide (50 mg, 0.68 mmol, 3.5 equiv) in THF (2.25 mL, *solution B*). *Solution A* was chilled in a glovebox freezer for 2~3 minutes. *Solution A* was then taken out of the freezer, and *Solution B* was transferred into *solution A* using a syringe over one minute. The resulting mixture was stirred for 24 hours at room temperature and monitored by NMR to ensure full conversion. Over a period of

3 minutes and with vigorous stirring, the reaction solution was dropwise added to a 60 mL vial pre-charged with pentane (40 mL), which led to the generation of a large amount of precipitate. The reaction vessel (the 8 mL vial) was rinsed with benzene (2 mL), and the resulting solution was transferred to the 60 mL vial as well. The precipitate was then collected in a glass funnel through filtration. Benzene (6 mL + 6 mL + 2 mL) was added to the glass funnel, and the resulting suspension was filtered to give a clear dark-green solution. Removal of the solvent furnished **Ru-4** as a dark green solid (124 mg, 88% yield). ^{1}H NMR (400 MHz, THF-d_8) δ 16.04 (s, 1H), 7.55 (ddd, J = 8.7, 7.4, 1.7 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.32 – 7.25 (m, 1H), 7.20 (d, J = 7.8 Hz, 2H), 6.87 (t, J = 7.4 Hz, 1H), 6.59 (dd, J = 7.5, 1.7 Hz, 1H), 6.22 (t, J = 1.9 Hz, 4H), 5.72 (t, J = 1.8 Hz, 4H), 5.17 (hept, J = 6.0 Hz, 1H), 4.19 (dd, J = 10.8, 8.4 Hz, 2H), 3.94 (dd, J = 10.6, 8.5 Hz, 2H), 3.58 – 2.18 (m, 8H), 2.13 (br, 3H), 1.65 (br, 6H), 1.53 (d, J = 6.0 Hz, 6H), 1.08 (d, J = 6.7 Hz, 6H), 0.12 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, THF-d_8) δ 296.3, 214.1, 153.4, 149.3, 144.3, 140.9, 130.4, 130.0, 129.9, 125.8, 124.4, 124.0, 114.7, 107.1, 76.2, 68.0, 67.8, 67.6, 67.4, 67.1, 59.1, 56.3, 45.5, 40.3, 37.0, 31.0, 29.8, 25.9, 25.9, 25.7, 25.5, 25.3, 25.1, 23.5, 23.0. HRMS: *Chemical fomular* ([M]): $C_{43}H_{56}N_4ORu$, calcd. [M]$^+$ 746.3498 Found: 746.3496.

**Ru-4** → (HOPiv, benzene; then THF, NH$_4$NO$_3$; rt) → **Ru-2**
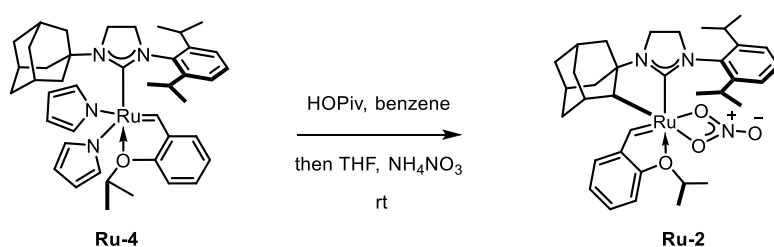
A 8 mL vial was charged with **Ru-4** (36 mg, 0.048 mmol, 1 equiv), pivalic acid (22 mg, 0.218 mmol, 4.5 equiv) and benzene (2 mL), and stirred at room temperature for 12 hours. Upon solvent removal, THF (1.4 mL) was added to dissolve the residue, and the solution was stirred at room temperature for 3 hours. To this was added NH$_4$NO$_3$ (52 mg, 0.65 mmol, 13.5 equiv), and the resulting suspension was stirred at room temperature for additional 3 hours. The reaction mixture was then concentrated *in vacuo*, triturated with pentane (2 mL), and stirred at room temperature for 5 minutes. The suspension was transferred onto a short Celite column. The column was flushed with pentane (1 mL × 3) to remove a yellow band and then benzene (2 mL) to obtain the product as a purple solution. Removal of the solvent furnished **Ru-2** as a purple solid (22.2 mg, 68% yield). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 15.21 (s, 1H), 7.45 (dd, J = 7.5, 1.7 Hz, 1H), 7.22 – 7.17 (m, 3H), 7.00 (dd, J = 6.6, 2.7 Hz, 1H), 6.85 (td, J = 7.4, 0.9 Hz, 1H), 6.48 (d, J = 8.4 Hz, 1H), 4.54 (hept, J = 6.3 Hz, 1H), 4.10 (s, 1H), 3.87 – 3.72 (m, 2H), 3.59 (ddd, J = 11.6, 10.1, 8.1 Hz, 1H), 3.37 (ddd, J = 10.9, 9.6, 8.0 Hz, 1H), 3.29 – 3.14 (m, 2H), 2.26 (q, J = 2.9 Hz, 1H), 2.06 (p, J = 3.1 Hz, 1H), 1.98 – 1.90 (m, 2H), 1.82 – 1.72 (m, 5H), 1.67 – 1.61 (m, 1H), 1.49 (d, J = 7.6 Hz, 2H), 1.45 – 1.40 (m, 4H), 1.20 (d, J = 6.9 Hz, 3H), 1.18 – 1.09 (m, 8H), 0.97 (d, J = 6.2 Hz, 3H), 0.58 (d, J = 11.7 Hz, 1H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 267.4, 211.9, 154.8, 147.5, 147.4, 143.4, 135.6, 129.2, 126.9, 124.8, 124.2, 123.4, 123.4, 113.2, 74.5, 66.4, 63.2, 54.1, 43.0, 41.6, 40.3, 38.0, 37.8, 37.8, 33.3, 30.9, 29.8, 29.0, 28.7, 27.9, 26.8, 23.6, 23.1, 21.1, 20.3. The spectra match reported literature.[2]

S2 + H$_2$N−Ad → (K$_2$CO$_3$, MeCN, reflux) → **S3**

S2 was synthesized according to the literature procedure.[3]

S3: A 100 mL round bottom flask equipped with a reflux condenser was charged with **S2** (3.1 g, 10 mmol, 1 equiv), 1-adamantylamine (3.1 g, 20 mmol, 2 equiv), K$_2$CO$_3$ (2.8 g, 20 mmol, 2 equiv), and MeCN (60 mL).

The flask was placed into an oil bath pre-heated to 100 °C and stirred overnight. After cooled to room temperature, the reaction mixture was filtered and concentrated in *vacuo*. The residue was further purified by column chromatography over silica gel (hexane/acetone, 6:1 to 4:1) to give **S3** as an off-white solid (3.4 g, 80% yield). R_f = 0.4 (hexane/acetone = 3:1). ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.92 (br, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.05 (d, *J* = 7.7 Hz, 2H), 3.43 (br, 2H), 2.57 (ddd, *J* = 14.3, 8.4, 6.0 Hz, 2H), 2.11 (s, 3H), 1.79 – 1.42 (m, 21H), 0.77 (t, *J* = 7.4 Hz, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 171.4, 143.2, 134.6, 127.6, 124.0, 51.3, 44.1, 43.1, 43.0, 36.6, 29.6, 29.0, 12.3. IR: 3305, 2958, 2904, 2849, 1677, 1499, 1461, 1143, 1097 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{28}H_{44}N_2O$, calcd. [M+H]$^+$ 425.3532 Found: 425.3519.
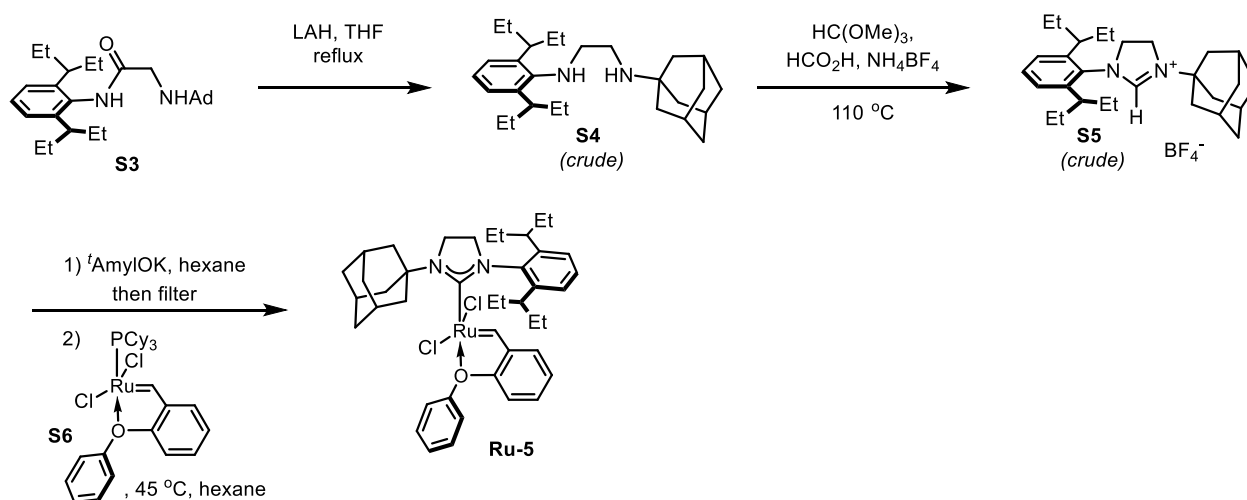

S4: A 100 mL round bottom flask equipped with a reflux condenser and a nitrogen bubbler was charged with **S3** (2.55 g, 6 mmol, 1 equiv), lithium aluminum hydride (1.9 g, 50 mmol) under a nitrogen atmosphere. To this was added THF (53 mL). The flask was placed in an oil bath and the bath temperature was then set to 95 °C (to ensure reflux). The reaction mixture was stirred at this temperature for 6 days and monitored by TLC until full conversion. The reaction mixture was then cooled with an ice bath, and sequentially charged with H$_2$O (1 mL), NaOH (aq., 3M, 2 mL), H$_2$O (2 mL), and Et$_2$O (30 mL). The resulting suspension was filtered, dried over Na$_2$SO$_4$, and concentrated *in vacuo*. The residue was further purified by column chromatography over silica gel (DCM/MeOH, 40:1, with 0.5% v/v NEt$_3$) to give crude **S4** as a colorless oil (1.8 g, 73% yield, mixed with a small amount of Et$_2$O and other minor impurities). R_f = 0.5 (DCM/MeOH = 10:1, with 0.5% v/v NEt$_3$). Crude **S4** was directly used in the next step without further purification (*in our hands, this compound appears to slowly decompose during storage and is recommended to be used immediately after preparation*). A crude spectrum of **S4** was recorded: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.02 (dd, *J* = 8.6, 6.4 Hz, 1H), 6.99 – 6.90 (m, 2H), 3.01 – 3.80 (m, 6H), 2.09 (s, 3H), 1.82 – 1.56 (m, 17H), 1.50 (ddt, *J* = 13.5, 8.6, 7.3 Hz, 4H), 0.81 (t, *J* = 7.4 Hz, 12H).

S5: A 20 mL vial that was charged with crude **S4** (740 mg, 1.8 mmol, 1 equiv), NH$_4$BF$_4$ (198 mg, 1.9 mmol, 1.05 equiv), trimethyl orthoformate (10 mL), and a small drop of formic acid under air atmosphere. The vial was sealed and stirred at 110 °C for 4.5 hours and monitored by TLC to ensure full conversion. After cooled to room temperature, the reaction mixture was filtered through a short plug of Celite and concentrated *in vacuo*. The orange-brown residue was then purified by flash column chromatography (DCM/MeOH, 50:1) to give the crude NHC salt as a yellow oil. The crude product was then triturated with Et$_2$O. After filtration and Et$_2$O wash, **S5** was collected as an off-white solid (350 mg, 38% yield, ca. 92~95% purity). R_f = 0.35 (DCM/Acetone = 5:1). A crude spectrum of **S5** was recorded: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.46 (t, *J* = 7.8 Hz, 1H), 7.39 (s, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 4.48 (dd, *J* = 12.7, 9.2 Hz, 2H), 4.28 (dd, *J* = 12.5, 9.2 Hz, 2H), 2.47 – 2.31 (m, 2H), 2.26 (s, 3H), 2.00 (br, 6H), 1.85 – 1.45 (m, 15H), 0.85 – 0.66 (m, 12H).

S6 was prepared according to the following procedure: Grubbs first generation catalyst M1a (C823) (1.5 g, 1.82 mmol, 1 equiv), phenoxylvinylbenzene (0.376 g, 1.91 mmol, 1.05 equiv), Amberlyst-15 (1.5 g), and DCM (15 mL) were added to a 20 mL vial in a glovebox and stirred vigorously at room temperature for 18 hours. The reaction was filtered and the filtrate concentrated *in vacuo*. The residue was triturated with pentane (10 mL) until it solidified. The resulting powder was filtered and rinsed until the eluent was clear to yield **S6** (941 mg, 82% yield). ^1H NMR (400 MHz, C_6D_6) δ 17.41 (d, J = 4.6 Hz, 1H), 7.79 (d, J = 7.9 Hz, 2H), 7.41 (d, J = 7.6 Hz, 1H), 7.00 (t, J = 7.8 Hz, 3H), 6.86 (t, J = 7.4 Hz, 1H), 6.73 (t, J = 7.5 Hz, 1H), 6.57 (d, J = 8.3 Hz, 1H), 2.40 (q, J = 12.1 Hz, 3H), 2.17 (d, J = 12.4 Hz, 6H), 1.88 (q, J = 12.6 Hz, 6H), 1.67 (d, J = 11.9 Hz, 6H), 1.53 (d, J = 10.8 Hz, 3H), 1.28 – 1.01 (m, 9H). ^{13}C NMR (101 MHz, C_6D_6) δ 271.2, 155.4, 153.6, 142.9, 130.1, 129.2, 127.0, 124.2, 124.1, 122.4, 114.4, 36.3, 36.1, 30.4, 28.1, 28.0, 26.5. HRMS: *Chemical fomular* ([M]): $C_{31}H_{43}Cl_2OPRu$, calcd. $[M]^+$ 634.1473 Found: 634.1460.

Ru-5: A 20 mL vial was charged with **S5** (244 mg, 0.48 mmol, 1 equiv) and hexane (9 mL) in a N_2 glovebox. To this was added potassium *tert*-pentoxide (0.9 M solution in cyclohexane, 0.55 mL, 0.50 mmol, 1.03 equiv). The vial was sealed and stirred at room temperature for 1 hour. The reaction mixture was then filtered through a short plug of Celite into a 40 mL vial containing **S6** (290 mg, 0.46 mmol, 0.95 equiv). The 40 mL vial was sealed and stirred at 45 °C for 4 hours. After cooled to room temperature, the reaction mixture was concentrated *in vacuo*. The residue was further purified by flash column chromatography over silica in a glovebox (hexane/benzene/Et₂O, 6:3:0.5 to 6:3:1) to give **Ru-5** as a green solid (230 mg, 62% yield, containing ca. 2% unknown impurity). ^1H NMR (400 MHz, C_6D_6) δ 17.14 (s, 1H), 7.74 (d, J = 7.4 Hz, 2H), 7.44 (t, J = 7.7 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.21 (dd, J = 7.6, 1.6 Hz, 1H), 7.04 – 6.85 (m, 4H), 6.66 (td, J = 7.4, 1.0 Hz, 1H), 6.43 (d, J = 8.3 Hz, 1H), 3.68 (dd, J = 10.6, 8.4 Hz, 2H), 3.36 (dd, J = 10.6, 8.4 Hz, 2H), 3.16 (dq, J = 8.2, 6.2 Hz, 2H), 2.82 (br, 6H), 2.01 (br, 3H), 1.86 – 1.17 (m, 18H), 1.02 (t, J = 7.2 Hz, 6H), 0.97 – 0.71 (m, 8H). ^{13}C NMR (101 MHz, C_6D_6) δ 303.5, 211.9, 155.0, 154.6, 146. 8, 144.0, 142.0, 129.8, 129.7, 128.5, 126.6, 126.3, 124.2, 123.5, 123.2, 114.0, 57.2, 54.9, 44.2, 42.0, 40.9, 36.3, 30.5, 28.7, 28.3, 12.6, 11.9. HRMS: *Chemical fomular* ([M]): $C_{42}H_{54}Cl_2N_2ORu$, calcd. $[M]^+$ 774.2657 Found 774.2682.
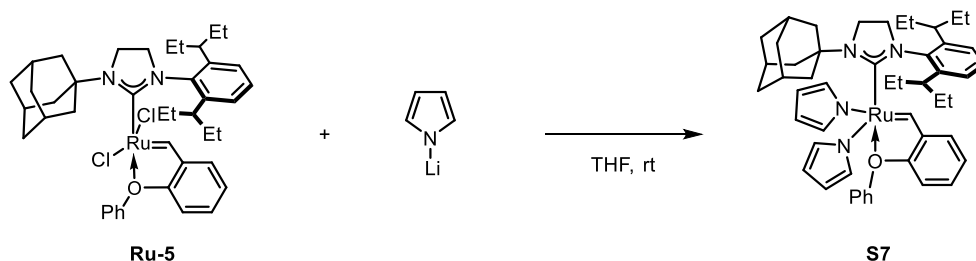
A 40 mL vial was charged with **Ru-5** (565 mg, 0.73 mmol, 1 equiv) in THF (11 mL, *solution A*). A 20 mL vial was charged with lithium pyrrolate (270 mg, 3.78 mmol, 5 equiv) in THF (9 mL, *solution B*). *Solution A* was chilled in a glovebox freezer for 2~3 minutes. *Solution A* was then taken out of the freezer, and *Solution B* was transferred into *solution A* using a syringe over two minutes. The resulting mixture was stirred for 6 hours at room temperature, monitored by NMR to ensure full conversion, and then concentrated *in vacuo*. Benzene (6~7 mL) was added to the residue to dissolve most of the solid, resulting in a green suspension. Over a period of 3 minutes and with vigorous stirring, the suspension was dropwise added to a 100 mL flask pre-charged with pentane (50 mL), which led to a green solution and the generation of white precipitate. The white solid was removed through filtration and the filtrate was concentrated *in vacuo*. The residue was transferred onto a short Celite column. The column was flushed with hexamethyldisiloxane (3 mL × 3) and a hexamethyldisiloxane/pentane solution (1:1, 2 mL) to remove the impurity as a brown band. The Celite column was then flushed with a benzene/pentane solution (2:3, 3 mL × 5) to generate a green solution. Removal of the solvent furnished **S7** as a green solid (550 mg, 90% yield). ^1H NMR (400 MHz, C_6D_6) δ 16.74 (s, 1H), 7.58 (d, J = 8.0 Hz, 2H), 7.32 (t, J = 7.7 Hz, 1H), 7.13 (d, J = 7.7 Hz, 2H), 7.01 – 6.91 (m,

2H), 6.86 (dt, J = 8.3, 6.8 Hz, 3H), 6.80 – 6.75 (m, 1H), 6.72 (br, 4H), 6.66 (d, J = 7.3 Hz, 1H), 6.49 (br, 4H), 3.64 (dd, J = 10.0, 8.4 Hz, 2H), 3.39 (dd, J = 10.0, 8.4 Hz, 2H), 3.21 (dp, J = 9.6, 4.9 Hz, 2H), 3.10 – 1.94 (m, 4H), 1.91 (br, 3H), 1.75 – 1.19 (m, 16H), 1.01 (t, J = 7.4 Hz, 6H), 0.12 (t, J = 7.3 Hz, 6H). ^{13}C NMR (101 MHz, C_6D_6) carbon signals were observed at δ 295.5, 214.8, 154.2, 153.5, 145.8, 142.7, 141.8, 130.1, 129.7, 129.0, 126.5, 126.5, 125.0, 124.4, 122.7, 113.4, 108.0, 58.4, 56.4, 44.4, 40.1, 36.2, 31.2, 30.0, 26.4, 12.0, 11.0. HRMS: *Chemical fomular* ([M]): $C_{50}H_{62}N_4ORu$, calcd. [M]$^+$ 836.3968 Found: 836.3992.
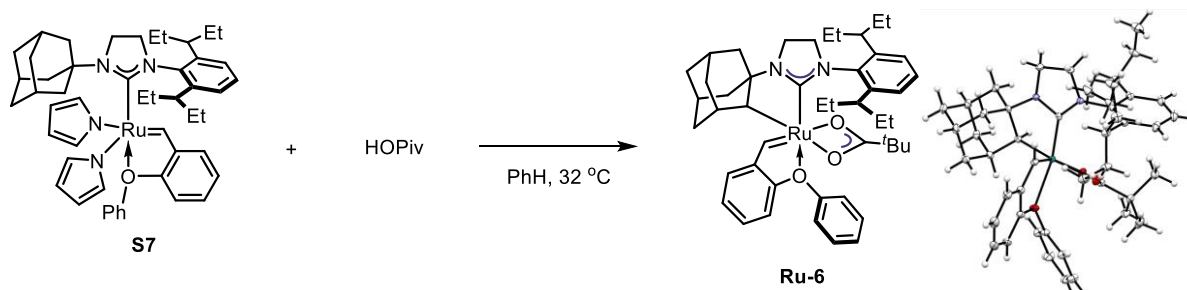
A 40 mL vial was charged with **S7** (580 mg, 0.693 mmol, 1 equiv). To this, a benzene (20 mL) solution of pivalic acid (290 mg, 2.84 mmol, 4 equiv.) was added at room temperature. The reaction mixture was stirred at 32 °C for 24 hours, monitored by NMR to ensure full conversion, and then concentrated *in vacuo*. Hexamethyldisiloxane (5 mL) was added to the residue, and the resulting mixture was stirred at room temperature for 5 minutes before concentrated *in vacuo* (*During this process, formation of a purple precipitate is expected --- if not, such a "trituration" procedure should be repeated*). The residue was transferred onto a short Celite column. The column was flushed with hexamethyldisiloxane (3 mL × 3) and a hexamethyldisiloxane/pentane solution (1:1, 3mL × 2) to remove the impurity as a brown band. The Celite column was then flushed with benzene (5 mL) to generate a purple solution. Removal of the solvent furnished **Ru-6** as a purple solid (390 mg, 70% yield). ^{1}H NMR (400 MHz, C_6D_6) δ 14.84 (s, 1H), 7.53 (dd, J = 7.5, 1.6 Hz, 1H), 7.25 (d, J = 7.6 Hz, 2H), 7.14 (d, J = 7.7 Hz, 1H), 7.05 (dd, J = 7.8, 1.6 Hz, 1H), 7.00 (ddd, J = 8.2, 7.3, 1.6 Hz, 1H), 6.98 – 6.91 (m, 3H), 6.87 (td, J = 7.4, 1.1 Hz, 1H), 6.84 – 6.76 (m, 1H), 6.60 (dt, J = 8.2, 0.9 Hz, 1H), 4.11 (s, 1H), 3.99 (dt, J = 11.7, 10.3 Hz, 1H), 3.63 (td, J = 10.5, 4.8 Hz, 1H), 3.59 – 3.43 (m, 2H), 3.24 (ddd, J = 12.1, 9.6, 4.8 Hz, 1H), 2.79 (q, J = 2.9 Hz, 1H), 2.31 – 2.13 (m, 5H), 2.10 (d, J = 12.1 Hz, 1H), 2.04 – 1.77 (m, 4H), 1.74 – 1.64 (m, 1H), 1.64 – 1.31 (m, 7H), 1.30 – 1.20 (m, 4H), 1.12 – 1.01 (m, 4H), 0.80 (td, J = 7.4, 6.2 Hz, 6H), 0.70 (s, 9H), 0.68 – 0.63 (m, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 256.8, 213.9, 188.3, 157.1, 154.7, 147.2, 145.3, 142.9, 140.5, 129.6, 128.6, 125.7, 125.0, 124.9, 124.6, 124.4, 123.4, 122.2, 115.5, 68.4, 63.0, 55.7, 43.9, 43.5, 42.6, 41.1, 40.9, 39.6, 38.3, 38.2, 36.4, 33.8, 31.4, 31.1, 30.1, 28.1, 28.0, 28.0, 26.4, 14.2, 13.2, 13.1, 12.6. HRMS: *Chemical fomular* ([M]): $C_{47}H_{62}N_2O_3Ru$, calcd. [M-H]$^+$ 803.3726 Found: 803.3737. A single-crystal of **Ru-6** for X-ray diffraction analysis was prepared through slow evaporation of a benzene solution in a glovebox (see Section 6).
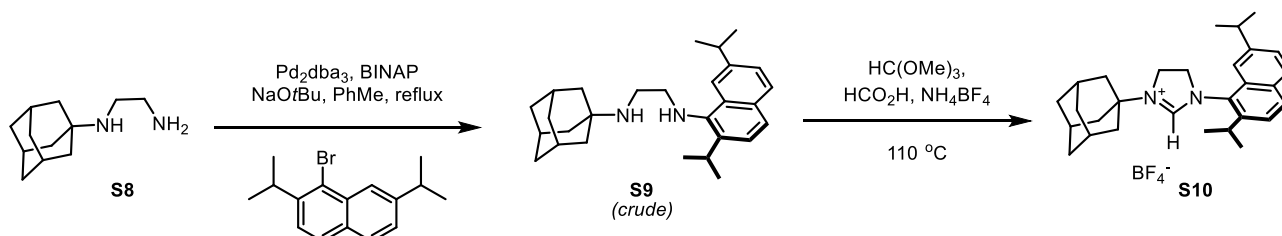
**S8** was prepared according to the literature procedure.[4]

S9: A 20 mL vial was first charged with Pd$_2$(dba)$_3$ (23 mg, 0.025 mmol, 0.04 equiv), BINAP (37 mg, 0.06 mmol, 0.10 equiv), 1-bromo-2,7-diisopropylnaphthalene[5] (174 mg, 0.6 mmol, 1 equiv) and **S8** (116 mg, 0.6

mmol, 1 equiv) under air atmosphere, and then with NaO^{t}Bu (87 mg, 0.9 mmol, 1.5 equiv) and toluene (6 mL) in a N$_2$ glovebox. The vial was sealed and stirred at 110 °C for 18 hours. After cooled to room temperature, the reaction mixture was filtered through a short plug of Celite and concentrated *in vacuo*. The residue was purified by flash column chromatography (DCM/MeOH, 40:1 to 20:1, with 0.5% v/v NEt$_3$) to give the crude coupling products **S9** as a yellowish oil (160 mg, ca. 90% purity). R$_f$ = 0.2 (DCM/MeOH = 12:1). A crude NMR spectrum is recorded for **S9**: ^{1}H NMR (400 MHz, CDCl$_3$, crude) δ 8.02 (d, J = 1.6 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 8.5 Hz, 1H), 7.35 – 7.28 (m, 2H), 3.54 (p, J = 6.8 Hz, 1H), 3.33 (br, 2H), 3.10 (hept, J = 7.0 Hz, 1H), 2.97 (t, J = 5.7 Hz, 2H), 2.09 (s, 3H), 1.80 (br, 6H), 1.73 – 1.55 (m, 7H), 1.34 (d, J = 7.0 Hz, 6H), 1.29 (d, J = 6.9 Hz, 6H). The crude **S9** was directly carried out to the next step without further purification.

S10: A 4 mL vial that was charged with crude **S9** (160 mg), NH$_4$BF$_4$ (37 mg, 0.35 mmol), trimethyl orthoformate (2 mL), and a small drop of formic acid under air atmosphere. The vial was sealed and heated at 110 °C with stirring for 3 hours and followed by TLC to ensure full conversion. After cooled to room temperature, the reaction mixture was filtered through a short plug of Celite and concentrated *in vacuo*. The orange-brown residue was then purified by flash column chromatography (DCM/MeOH, 40:1) to give the crude NHC salt as a yellowish solid. We also noticed that the crude NHC salt sometimes remains a thick oil instead of a solid. In such cases, the following procedure could be applied to further purify the NHC salt: To an 8 mL vial containing 160 mg of crude NHC was added toluene (0.6 mL) and hexane (1.2 mL). After stirring for 1 minute, a small amount of DCM (0.3 – 0.5 mL) was then added, during which process the solid particles of the NHC salt were usually observed. More hexane (0.8 mL) was added dropwise in order to precipitate most of the NHC salt, which was collected through filtration as a white solid (120 mg, 40% yield over two steps). R$_f$ = 0.35 (DCM/MeOH = 12:1). ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.87 (s, 1H), 7.86 (d, J = 8.8 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.43 (dd, J = 8.5, 1.6 Hz, 1H), 7.39 (d, J = 8.7 Hz, 1H), 7.37 (s, 1H), 4.53 – 4.18 (m, 4H), 3.24 – 3.06 (m, 2H), 2.22 (s, 3H), 2.05 (d, J = 2.9 Hz, 6H), 1.70 (t, J = 3.1 Hz, 6H), 1.33 – 1.24 (m, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.3, 149.9, 145.1, 131.6, 131.0, 130.1, 129.0, 127.3, 126.3, 123.4, 117.4, 58.4, 52.8, 45.5, 41.1, 35.5, 34.6, 29.3, 28.9, 24.3, 24.1, 24.0, 23.9. IR: 2970, 2913, 2855, 1624, 1263, 1048, 910 cm^{-1}. HRMS: *Chemical fomular of the cation* ([M$^+$]): C$_{29}$H$_{39}$N$_2^+$, calcd. [M$^+$] 415.3113 Found: 415.3108.
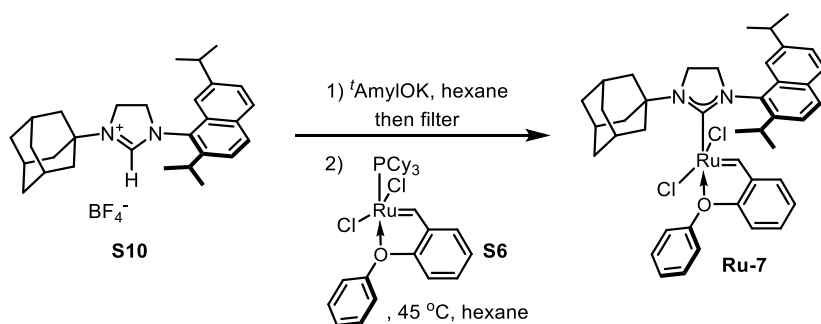
Ru-7: A 20 mL vial was charged with the NHC salt **S10** (364 mg, 0.72 mmol, 1.14 equiv) and hexane (18 mL) in a N$_2$ glovebox. To this was added potassium *tert*-pentoxide (0.9 M solution in cyclohexane, 0.8 mL, 0.72 mmol, 1.14 equiv). The vial was sealed and stirred at room temperature for 1 hour. The reaction mixture was then filtered through a short plug of Celite into a 40 mL vial pre-charged with **S6** (400 mg, 0.63 mmol, 1 equiv). The 40 mL vial was sealed and stirred at 45 °C for 2 hours. After cooled to room temperature, **Ru-7**, as a green solid, was collected through filtration and further purified by pentane wash (2 mL × 3) (386 mg, 80% yield). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 16.84 (d, J = 1.0 Hz, 1H), 8.07 (dd, J = 1.7, 0.8 Hz, 1H), 7.95 (d, J = 8.6 Hz, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.74 – 7.70 (m, 1H), 7.70 (dd, J = 2.1, 0.9 Hz, 1H), 7.52 (d, J = 8.6 Hz, 1H), 7.31 (dd, J = 8.4, 1.7 Hz, 1H), 7.03 – 6.98 (m, 2H), 6.93 – 6.87 (m, 1H), 6.83 (ddd, J = 8.7, 7.4, 1.6 Hz, 1H), 6.78 (dd, J = 7.6, 1.6 Hz, 1H), 6.39 (td, J = 7.4, 0.9 Hz, 1H), 6.34 (d, J = 8.3 Hz, 1H), 3.78

(hept, $J = 6.8$ Hz, 1H), 3.67 – 3.46 (m, 2H), 3.45 – 3.23 (m, 2H), 3.15 (hept, $J = 7.0$ Hz, 1H), 2.89 (br, 6H), 2.01 (s, 3H), 1.72 (d, $J = 12.3$ Hz, 3H), 1.53 (d, $J = 12.4$ Hz, 3H), 1.39 (t, $J = 6.9$ Hz, 6H), 1.30 (d, $J = 6.6$ Hz, 3H), 1.25 (d, $J = 6.9$ Hz, 3H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 305.5, 211.6, 154.6, 154.6, 148.0, 145.5, 144.5, 137.0, 132.5, 131.8, 129.8, 129.4, 129.2, 126.6, 126.5, 124.1, 123.9, 123.5, 122.9, 122.2, 113.6, 57.1, 53.7, 44.3, 41.7, 36.3, 35.1, 30.4, 28.5, 24.9, 24.2, 23.9, 23.8. HRMS: *Chemical fomular* ([M]): C$_{42}$H$_{48}$Cl$_2$N$_2$ORu, calcd. [M]$^+$ 768.2188 Found: 768.2177.
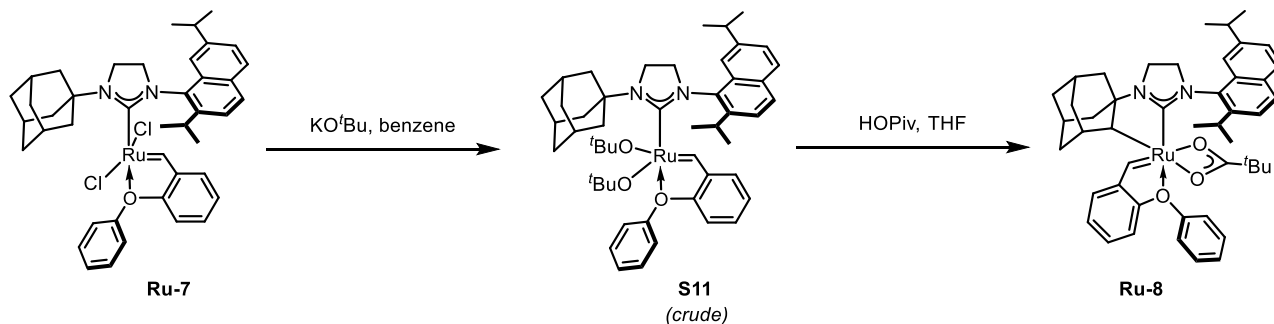
S11: A 20 mL vial was charged with **Ru-7** (347 mg, 0.46 mmol, 1 equiv), potassium *tert*-butoxide (157 mg, 1.4 mmol, 3 equiv), and benzene (13 mL) in a N$_2$ glovebox. The vial was sealed and stirred at room temperature for 18 hours. The reaction mixture was then filtered through a short plug of Celite and concentrated *in vacuo*. The residue was transferred onto a short Celite column. The column was flushed with pentane (3 mL) to remove the dark brown band and then a pentane/benzene solution (8:1, 20 mL) to generate a brown solution. Removal of the solvent furnished crude **S11** as a brown solid (310 mg). A ^{1}H NMR spectrum was recorded: ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 16.16 (s, 1H), 7.94 – 7.55 (m, 5H), 7.54 (d, $J = 8.6$ Hz, 1H), 7.30 (dd, $J = 8.5, 1.7$ Hz, 1H), 7.12 (dd, $J = 8.6, 7.3$ Hz, 3H), 6.94 – 6.89 (m, 1H), 6.84 (ddd, $J = 8.6,$ 7.3, 1.6 Hz, 1H), 6.70 (d, $J = 8.2$ Hz, 1H), 6.65 (t, $J = 7.4$ Hz, 1H), 4.20 – 4.04 (m, 1H), 3.49 – 3.31 (m, 3H), 3.31 – 3.23 (m, 1H), 3.19 (p, $J = 6.9$ Hz, 1H), 3.12 – 2.98 (m, 6H), 2.33 (s, 3H), 1.97 (d, $J = 12.1$ Hz, 2H), 1.74 (d, $J = 12.3$ Hz, 2H), 1.51 (d, $J = 6.6$ Hz, 3H), 1.35 – 1.32 (m, 6H), 1.24 (d, $J = 6.8$ Hz, 3H), 1.11 (s, 9H), 0.84 (s, 9H).

Ru-8: A 20 mL vial was charged with **S11** (280 mg, 0.33 mmol, 1 equiv) in THF (5 mL, *solution A*). A 8 mL vial was charged with PivOH (86 mg, 0.84 mmol, 2.5 equiv) in THF (5 mL, *solution B*). Both vials were put in the glovebox freezer (−20 ℃) for 10 minutes. *Solution B* was quickly transferred into *solution A* by using a 6 mL syringe, and the resulting mixture was put back into the freezer and sat without stirring for 20 minutes. The mixture was then taken out of the freezer and stirred for 30 minutes at room temperature before it was concentrated *in vacuo*. The residue was transferred onto a short Celite column. The Celite column was flushed with pentane (3.5 mL × 2) to remove the brown band and then benzene (7 mL) to generate a purple solution. Removal of the solvent furnished **Ru-8** as a purple solid (195 mg, 75% yield). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 14.87 (s, 1H), 7.72 – 7.59 (m, 3H), 7.52 (dd, $J = 7.5, 1.7$ Hz, 1H), 7.34 (d, $J = 8.6$ Hz, 1H), 7.24 – 7.18 (m, 3H), 7.06 – 6.98 (m, 1H), 6.90 (t, $J = 7.7$ Hz, 3H), 6.77 (t, $J = 7.4$ Hz, 1H), 6.61 (d, $J = 8.1$ Hz, 1H), 4.45 – 4.26 (m, 2H), 3.75 (q, $J = 9.6, 8.6$ Hz, 1H), 3.56 – 3.38 (m, 2H), 3.31 (dt, $J = 11.3, 8.6$ Hz, 1H), 3.00 (hept, $J = 6.9$ Hz, 1H), 2.66 (s, 1H), 2.25 – 2.01 (m, 4H), 1.81 (d, $J = 12.1$ Hz, 1H), 1.71 (s, 1H), 1.64 – 1.47 (m, 3H), 1.47 – 1.40 (m, 6H), 1.40 – 1.32 (m, 6H), 1.24 – 1.14 (m, 2H), 0.71 (d, $J = 12.2$ Hz, 1H), 0.30 (br, 9H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 257.5, 216.9, 156.7, 154.6, 147.0, 144.8, 143.3, 135.0, 132.7, 132.4, 129.6, 128.8, 128.6, 125.6, 125.4, 125.1, 124.9, 123.9, 123.0, 122.3, 120.7, 115.2, 69.0, 62.7, 54.2, 43.8, 41.4, 40.6, 39.0, 38.3, 38.1, 37.0, 34.6, 33.7, 31.2, 30.1, 28.8, 27.2, 25.2, 24.3, 24.1, 23.6. HRMS: *Chemical fomular* ([M]): C$_{47}$H$_{56}$N$_2$O$_3$Ru, calcd. [M-H]$^+$ 797.3257 Found: 797.3243.
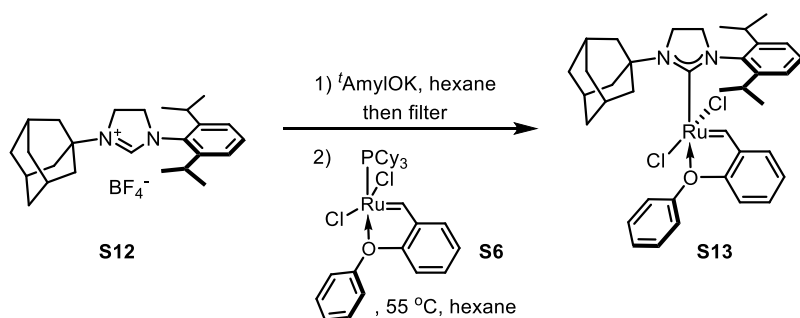
S12 was synthesized according to the literature procedure.[1]

S13: A 40 mL vial was charged with **S12** (452 mg, 1 mmol, 1.47 equiv) and hexane (25 mL) in a N_2 glovebox. To this was added potassium *tert*-pentoxide (0.9 M solution in cyclohexane, 1.1 mL, 1 mmol, 1.47 equiv). The vial was sealed and stirred at room temperature for 1 hour. The reaction mixture was then filtered through a short plug of Celite into a 40 mL vial containing **S6** (431 mg, 0.68 mmol, 1 equiv). The 40 mL vial was sealed and stirred at 55 °C for 1 hour. After cooled to room temperature, **S13**, as a green solid, was collected through filtration and further purified by pentane wash (3 mL × 3) (422 mg, 86% yield). ^{1}H NMR (400 MHz, C_6D_6) δ 17.09 (d, J = 1.0 Hz, 1H), 7.88 – 7.70 (m, 2H), 7.44 (dd, J = 8.3, 7.1 Hz, 1H), 7.32 (d, J = 7.6 Hz, 2H), 7.21 – 7.18 (m, 1H), 7.04 – 6.95 (m, 3H), 6.94 – 6.82 (m, 1H), 6.64 (t, J = 7.4 Hz, 1H), 6.45 (d, J = 8.3 Hz, 1H), 3.76 – 3.41 (m, 4H), 3.34 (dd, J = 11.1, 8.3 Hz, 2H), 2.83 (br, 6H), 1.99 (br, 3H), 1.70 (d, J = 12.4 Hz, 3H), 1.51 (d, J = 12.4 Hz, 3H), 1.24 (d, J = 6.7 Hz, 6H), 1.19 (d, J = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 303.7, 210.7, 154.9, 154.6, 149.0, 144.7, 139.9, 129.9, 129.7, 129.6, 126.6, 125.2, 124.3, 123.5, 123.0, 114.0, 57.1, 54.3, 44.1, 41.8, 36.3, 30.4, 28.3, 26.1, 24.6. HRMS: *Chemical fomular* ([M]): $C_{38}H_{46}Cl_2N_2ORu$, calcd. [M]$^+$ 718.2031 Found: 718.2017.
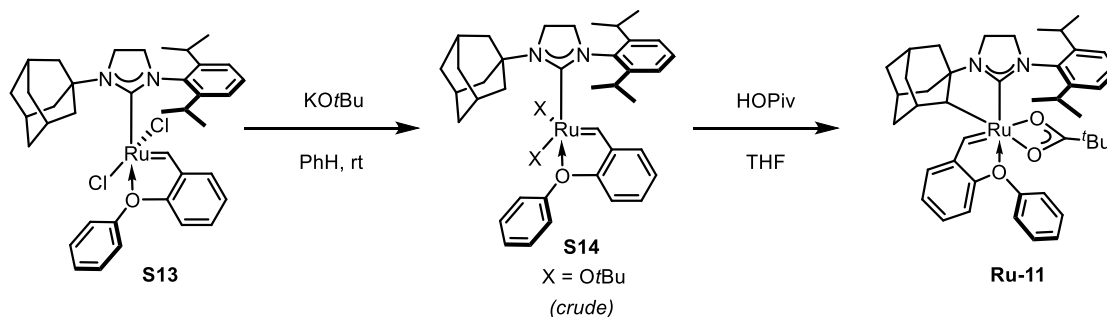

S14: A 20 mL vial was charged with **S13** (360 mg, 0.5 mmol, 1 equiv), potassium *tert*-butoxide (170 mg, 1.5 mmol, 3 equiv), and benzene (10 mL) in a N_2 glovebox. The vial was sealed and stirred at room temperature for 15 hours. The reaction mixture was then filtered through a short plug of Celite and concentrated *in vacuo*. The residue was transferred onto a short Celite column. The Celite column was flushed with a small amount of pentane (4 mL) to remove the impurity and then a large amount of pentane (120 mL) to obtain the product as a brown solution. Removal of the solvent furnished crude **S14** as a brown-red solid (355 mg, ca. 90% purity). A crude NMR spectrum was recorded for **S14**: ^{1}H NMR (500 MHz, C_6D_6) δ 16.28 (s, 1H), 7.66 (br, 2H), 7.29 (br, 3H), 7.15 – 7.08 (m, 3H), 6.95 – 6.86 (m, 2H), 6.76 (t, J = 6.7 Hz, 2H), 3.73 (br, 2H), 3.45 (dd, J = 10.7, 8.2 Hz, 2H), 3.22 (dd, J = 10.7, 8.2 Hz, 2H), 2.99 (s, 6H), 2.31 (s, 3H), 1.97 (d, J = 12.2 Hz, 3H), 1.73 (d, J = 12.2 Hz, 3H), 1.36 (d, J = 6.6 Hz, 6H), 1.14 (d, J = 6.8 Hz, 6H), 1.09 (s, 18H). The crude **S14** was directly carried out to the next step without further purification.

Ru-11: A 20 mL vial was charged with **S14** (320 mg, 0.4 mmol, 1 equiv) in THF (6.5 mL, *solution A*). A 8 mL vial was charged with PivOH (82 mg, 0.8 mmol, 2 equiv) in THF (6.5 mL, *solution B*). Both vials were put in the glovebox freezer (−20 °C) for 10 minutes. *Solution B* was quickly transferred into *solution A* by

using a 12 mL syringe, and the resulting mixture was put back into the freezer and sat without stirring for 2.5 hours. The mixture was then taken out of the freezer and stirred for 10 minutes at room temperature before it was concentrated *in vacuo*. The residue was transferred onto a short Celite column. The column was flushed with pentane (1.5 mL × 2) to remove the brown band and then benzene (3.5 mL) to obtain the product as a purple solution. Removal of the solvent furnished **Ru-11** as a purple solid (200 mg, 59% yield over two steps). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 14.95 (s, 1H), 7.52 (dd, J = 7.5, 1.6 Hz, 1H), 7.28 (d, J = 7.6 Hz, 2H), 7.15 – 7.09 (m, 2H), 7.05 – 6.94 (m, 4H), 6.88 (td, J = 7.4, 1.0 Hz, 1H), 6.81 (t, J = 7.4 Hz, 1H), 6.67 (d, J = 8.2 Hz, 1H), 4.23 – 4.04 (m, 2H), 3.75 (dt, J = 11.8, 9.6 Hz, 1H), 3.53 (td, J = 10.5, 6.1 Hz, 1H), 3.48 – 3.35 (m, 1H), 3.18 (ddd, J = 12.1, 9.6, 6.1 Hz, 1H), 2.95 (p, J = 6.9 Hz, 1H), 2.48 (s, 1H), 2.13 – 2.00 (m, 2H), 1.96 (d, J = 12.3 Hz, 1H), 1.88 (d, J = 10.8 Hz, 1H), 1.74 (dd, J = 12.1, 2.3 Hz, 1H), 1.66 (br, 1H), 1.60 – 1.45 (m, 5H), 1.45 – 1.30 (m, 7H), 1.21 (d, J = 6.9 Hz, 3H), 1.16 (d, J = 9.7 Hz, 1H), 1.10 (d, J = 11.3 Hz, 1H), 0.78 (s, 9H), 0.66 (d, J = 12.4 Hz, 1H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 258.2, 213.3, 187.1, 156.1, 155.0, 148.9, 146.8, 143.5, 137.7, 129.6, 128.6, 125.4, 125.3, 125.1, 124.7, 124.1, 122.6, 122.3, 115.8, 68.4, 63.0, 55.0, 43.7, 41.1, 40.6, 39.4, 38.3, 37.6, 36.6, 33.8, 31.0, 30.1, 28.9, 28.8, 28.0, 26.6, 25.2, 23.5. HRMS: *Chemical fomular* ([M]): C$_{43}$H$_{54}$N$_2$O$_3$Ru, calcd. [M-H]$^+$ 747.3100 Found: 747.3109.
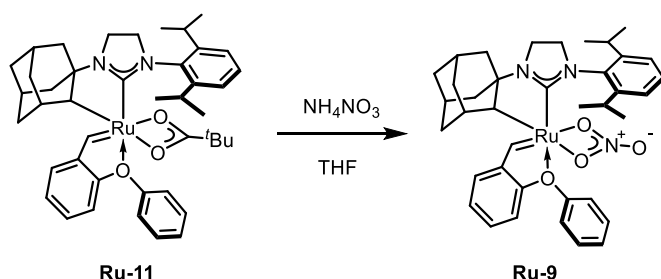
Ru-9: An 8 mL vial was charged with **Ru-11** (80 mg, 0.11 mmol, 1 equiv), NH$_4$NO$_3$ (104 mg), and THF (3 mL) in a N$_2$ glovebox. The vial was sealed and stirred at room temperature for 2.5 hours. The reaction mixture was then filtered through a short plug of Celite and concentrated *in vacuo*. The residue was transferred onto a short Celite column. The column was flushed with pentane (3 mL) to remove the impurity and then a benzene/DCM solution (5:2 v/v, 2 mL) to obtain the product as a purple solution. Removal of the solvent furnished **Ru-9** as a purple solid (53 mg, 70% yield). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 15.06 (s, 1H), 7.46 (d, J = 7.4 Hz, 1H), 7.20 (t, J = 7.7 Hz, 1H), 7.12 (dd, J = 7.8, 1.7 Hz, 1H), 7.06 (d, J = 7.3 Hz, 3H), 6.97 (td, J = 7.8, 1.6 Hz, 1H), 6.90 (t, J = 7.8 Hz, 2H), 6.83 (t, J = 7.4 Hz, 1H), 6.78 (t, J = 7.4 Hz, 1H), 6.41 (d, J = 8.2 Hz, 1H), 4.26 (s, 1H), 3.84 (p, J = 6.9 Hz, 1H), 3.74 (td, J = 10.5, 8.3 Hz, 1H), 3.63 (td, J = 10.8, 10.3, 7.6 Hz, 1H), 3.36 (td, J = 10.3, 7.7 Hz, 1H), 3.25 (dt, J = 11.1, 8.6 Hz, 1H), 3.08 (hept, J = 6.6 Hz, 1H), 2.55 (d, J = 3.5 Hz, 1H), 2.03 (s, 1H), 2.00 – 1.86 (m, 2H), 1.76 (t, J = 10.1 Hz, 2H), 1.70 (s, 1H), 1.61 – 1.47 (m, 5H), 1.45 (d, J = 11.9 Hz, 1H), 1.27 (t, J = 3.3 Hz, 6H), 1.24 – 1.13 (m, 2H), 1.07 (d, J = 6.8 Hz, 3H), 0.76 (d, J = 12.2 Hz, 1H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 264.2, 213.0, 157.3, 154.1, 147.8, 147.3, 142.7, 135.8, 130.4, 129.2, 126.6, 126.6, 125.1, 124.7, 124.2, 122.7, 122.1, 115.0, 67.3, 63.1, 54.1, 42.9, 41.7, 40.2, 38.1, 37.8, 37.5, 33.4, 30.9, 30.0, 28.9, 28.7, 27.5, 26.7, 23.8, 22.9. HRMS: *Chemical fomular* ([M]): C$_{38}$H$_{45}$N$_3$O$_4$Ru, calcd. [M-H]$^+$ 708.2376 Found: 708.2364.
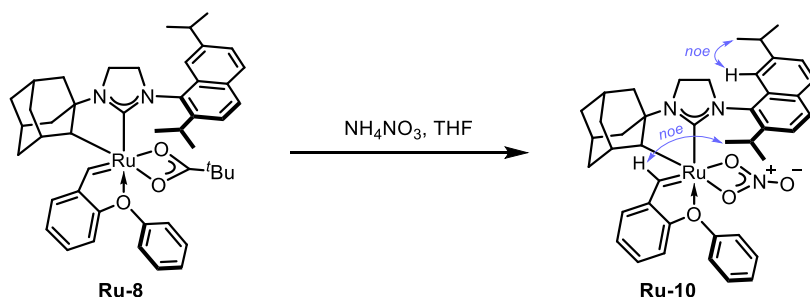
Ru-10: A 20 mL vial was charged with **Ru-8** (80 mg, 0.1 mmol, 1 equiv)**,** NH$_4$NO$_3$ (320 mg) and THF (3 mL, *solution A*). After stirring overnight at room temperature, all the salts were removed through filtration, and a new batch of NH$_4$NO$_3$ (640 mg) was re-added. The resulting suspension was stirred overnight at room temperature, filtered, and concentrated *in vacuo*. The residue was transferred onto a short Celite column. The column was flushed with a pentane/benzene solution to remove the impurity and then a benzene/DCM solution to obtain the product as a purple solution. Removal of the solvent furnished **Ru-10** as a purple solid (60 mg, 79% yield). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 14.99 (s, 1H), 7.68 (dd, J = 8.5, 6.5 Hz, 2H), 7.57 (dd, J = 1.7, 0.9 Hz, 1H), 7.47 (dd, J = 7.5, 1.6 Hz, 1H), 7.32 (dd, J = 8.4, 1.7 Hz, 1H), 7.22 (d, J = 8.7 Hz, 1H), 6.99 – 6.87 (m, 3H), 6.87 – 6.75 (m, 3H), 6.72 – 6.65 (m, 1H), 6.37 (dd, J = 8.2, 1.0 Hz, 1H), 4.36 (s, 1H), 4.06 (hept, J = 6.8 Hz, 1H), 3.72 (td, J = 11.4, 10.1 Hz, 1H), 3.52 (ddd, J = 9.9, 8.5, 6.2 Hz, 1H), 3.37 – 3.23 (m, 2H), 3.11 (hept, J = 6.8 Hz, 1H), 2.55 (d, J = 3.0 Hz, 1H), 2.16 – 2.05 (m, 2H), 2.04 – 1.92 (m, 2H), 1.87 – 1.77 (m, 1H), 1.73 (s, 1H), 1.58 (d, J = 12.5 Hz, 1H), 1.54 – 1.46 (m, 8H), 1.35 (d, J = 2.8 Hz, 3H), 1.34 (d, J = 2.8 Hz, 3H), 1.26 (d, J = 12.4 Hz, 1H), 1.16 (d, J = 11.3 Hz, 1H), 0.77 (d, J = 12.3 Hz, 1H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 263.1, 217.6, 157.3, 154.0, 147.7, 143.3, 142.6, 133.5, 133.0, 132.4, 130.2, 129.1, 128.8, 128.6, 126.5, 126.4, 125.7, 125.0, 122.8, 122.5, 122.0, 119.0, 114.9, 67.9, 62.9, 53.8, 43.4, 42.0, 40.3, 38.0, 37.8, 37.5, 35.1, 33.6, 31.0, 30.0, 28.7, 25.2, 24.1, 24.0, 23.6. HRMS: *Chemical fomular* ([M]): C$_{42}$H$_{47}$N$_3$O$_4$Ru, calcd. [M-H]$^+$ 758.2573 Found: 758.2546. The stereochemistry of the side-arm with respect to the metal center was further determined through 2D NMR analysis.

3. Catalyst screening

[Ru] catalyst tested: **Ru-2**, **Ru-6**, **Ru-8**, **Ru-9**, **Ru-10**, and **Ru-11**
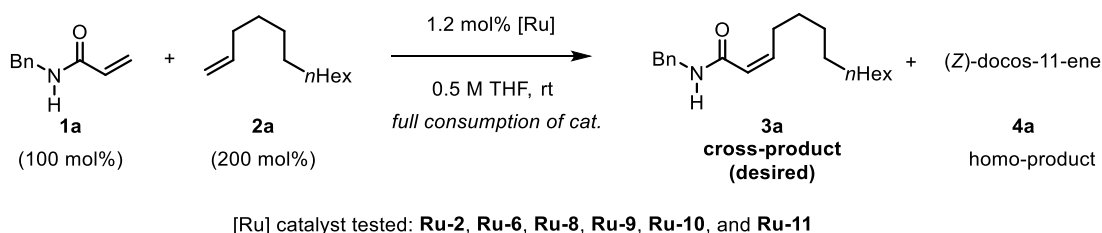
The general procedure for catalyst screening: A 4 mL vial was charged with a stir bar, **1a** (0.25 mmol, 1 equiv, 40.3 mg), **2a** (0.5 mmol, 2 equiv, 84 mg), and anthracene (*as the internal standard*) in a nitrogen glovebox. To this was added a stock solution of the ruthenium catalyst (0.003 mmol, 0.012 equiv) in d_8-THF (0.4 mL). The vial was loosely capped with a screw thread hole cap, and a 20-gauge needle was used to puncture the cap and left on (Figure S1). The reaction mixture was allowed to stir at room temperature in the glovebox for 4 – 48 hours until its color changed from purple to bright yellow (*which indicated the complete consumption of the catalyst*). The reaction can also be monitored by ^{1}H NMR to determine the quantity of the remaining ruthenium catalyst. Upon full consumption of the catalyst, the reaction was transferred to an NMR tube and removed from the glovebox. The yields and the *Z/E* ratio of the metathesis products were further determined by ^{1}H NMR analysis of the crude reaction mixture.

Note 1: After 24 hours of reaction, a small amount of d_8-THF (0.15 mL) was added to compensate for the loss of the solvent (*due to slow evaporation*) if the reaction hadn't reached full catalyst consumption.

Note 2: In the model reaction where **1a** and **2a** has an initial feed ratio of 1:2, we noticed that the ratio between **3a** (*cross-product*) and **4a** (*homo-product*) changes along the course of the reaction. Especially for catalysts **Ru-6**, **Ru-8**, and **Ru-11** that favor cross-metathesis over homo-dimerization, the ratio between **3a** and **4a** decreases as the conversion increases. This can be easily explained: At a high conversion, the real-time ratio between the unreacted **2a** and **1a** would be much larger than 2:1, as most of the **1a** has already been consumed at that point. Because of this, and given the fact that the conversion of each reaction varies

drastically from 23% to 80% in the model study, we decided to simply report the NMR yields of cross-product **3a** and homo-product **4a** in Scheme 3 of the manuscript, instead of a formal "selectivity ratio" that is calculated based on the final distribution of the products for a certain catalyst.

Figure S1 | Reaction setup

When **Ru-6** was used as the catalyst, the reaction was further purified by flash column chromatography over silica gel, furnishing pure *Z*-product **3a** in 75% isolated yield as a colorless oil (56.2 mg). *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.5 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.42 – 7.25 (m, 5H), 6.01 (dt, *J* = 11.4, 7.5 Hz, 1H), 5.81 (br, 1H), 5.69 (dt, *J* = 11.4, 1.8 Hz, 1H), 4.47 (d, *J* = 5.5 Hz, 2H), 2.67 (qd, *J* = 7.4, 1.7 Hz, 2H), 1.42 (p, *J* = 7.4 Hz, 2H), 1.35 – 1.23 (m, 14H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) carbon signals were observed at δ 166.5, 146.5, 138.5, 128.8, 128.0, 127.6, 121.9, 43.5, 32.0, 29.7, 29.6, 29.5, 29.5, 29.5, 29.0, 22.8, 14.3. IR: 3292, 2919, 2852, 1657, 1631, 1538, 1454, 1237 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{20}$H$_{31}$NO, calcd. [M+H]$^+$ 302.2484 Found: 302.2492.

4. Substrate scope study

4.1 Substrate synthesis

As shown in Figure S2, **2d**,[6] **2e**,[7] **2p**,[8] **1t**,[9] and **1v**[10] were synthesized according to the literature procedure.

2n, **1u**, and **1w** were synthesized according to the following procedure (*vide infra*).

Other substrates were commercially available.
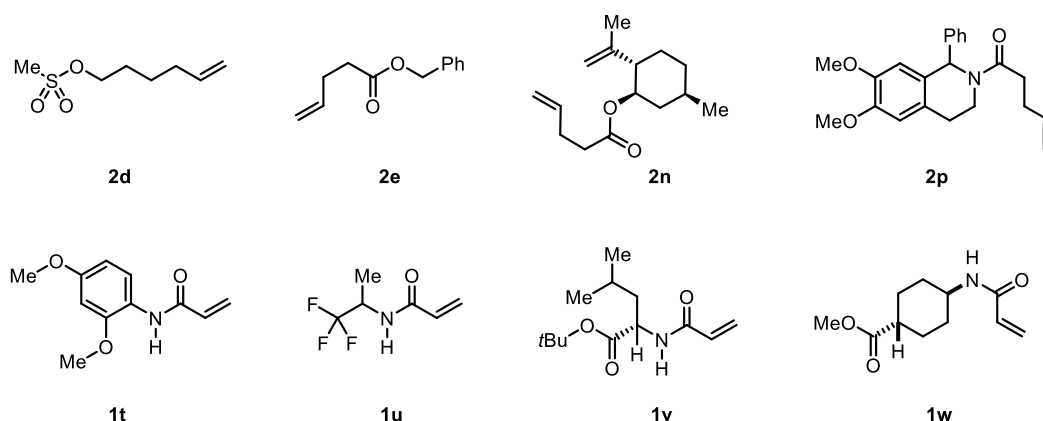
Figure S2 | Substrates synthesized for this study
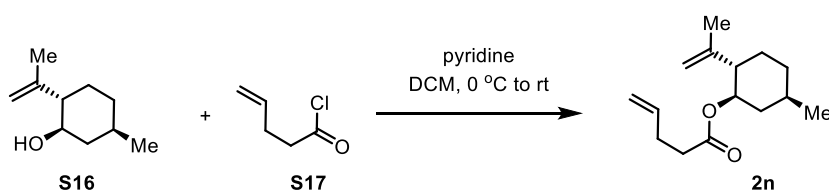
2n: A 50 mL round bottom flask was charged with (−)-*isopulegol* (**S16**) (1.46 g, 9.5 mmol, 1.05 equiv), pyridine (1.45 mL), and DCM (10 mL). The flask was placed into an ice bath. To this was added a DCM (5 mL) solution of pent-4-enoyl chloride (**S17**) (1.06 g, 9 mmol, 1 equiv) over 5 minutes. The reaction was then stirred overnight at room temperature. Upon full conversion, the reaction mixture was washed with 1 M HCl and then saturated aqueous NaHCO$_3$, dried over Na$_2$SO$_4$, and concentrated in *vacuo*. The residue was further purified by column chromatography over silica gel (hexane/ethyl acetate, 40:1 to 20:1) to give **2n** as a colorless oil (1.9 g, 90% yield). R$_f$ = 0.5 (hexane/ethyl acetate = 20:1). ^{1}H NMR (400 MHz, CDCl$_3$) δ 5.90 − 5.68 (m, 1H), 5.03 (dd, J = 16.9, 1.7 Hz, 1H), 4.98 (dd, J = 10.0, 1.7 Hz, 1H), 4.80 (td, J = 10.9, 4.4 Hz, 1H), 4.72 (t, J = 1.4 Hz, 2H), 2.42 − 2.30 (m, 4H), 2.10 (ddd, J = 12.5, 10.7, 3.7 Hz, 1H), 2.02 − 1.94 (m, 1H), 1.75 − 1.63 (m, 5H), 1.62 − 1.48 (m, 1H), 1.46 − 1.31 (m, 1H), 1.06 − 0.87 (m, 5H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 172.6, 146.4, 137.0, 115.4, 111.9, 73.6, 50.9, 40.6, 34.3, 33.9, 31.5, 30.6, 29.2, 22.2, 19.6. IR: 3076, 2954, 2925, 1733, 1453, 1252, 1170, 1129 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{15}$H$_{24}$O$_2$, calcd. [M+H]$^+$ 237.1855 Found: 237.1836.
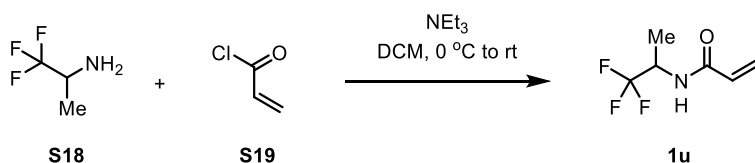
1u: To a 40 mL vial under an argon atmosphere was added 1,1,1-trifluoropropan-2-amine (**S18**) (800 mg, 7.1 mmol, 1.0 equiv), triethylamine (790 mg, 7.8 mmol, 1.1 equiv), and DCM (15 mL). The solution was cooled to 0 °C and a solution of acryloyl chloride (706 mg, 7.8 mmol, 1.1 equiv) in DCM (15 mL) was added dropwise with stirring. The solution was stirred for 5 min further and then removed from the ice bath and allowed to warm to room temperature, where it was stirred for 48 h and monitored by TLC analysis. The reaction was filtered, rinsed with DCM (5 mL) and the filtrate was concentrated under reduced pressure. The residue was further purified by column chromatography over silica gel (dichloromethane/ethyl acetate = 20:1) to give **1u** as a white solid (785 mg, 67%). ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.36 (dd, J = 17.0, 1.2 Hz, 1H), 6.12 (dd, J = 17.0, 10.3 Hz, 1H), 5.85 − 5.65 (m, 2H), 4.80 (dhept, J = 9.4, 7.1 Hz, 1H), 1.35 (d, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.0, 129.9, 128.4, 125.4 (q, J = 280.9 Hz), 46.5 (q, J = 31.7 Hz),

14.6 (q, J = 2.1 Hz). ^{19}F NMR (282 MHz, CDCl$_3$) δ -77.51 (d, J = 7.4 Hz, 3F). IR: 3274, 3066, 3000, 1663, 1544, 1274, 1159, 1139 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_6$H$_8$F$_3$NO, calcd. [M+H]$^+$ 168.0636 Found: 168.0655.
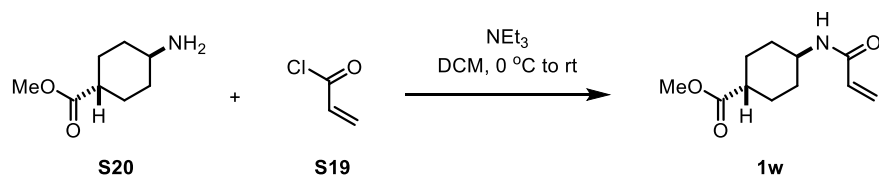
1w: A 100 mL round bottom flask was charged with **S20** (1.05 g, 6.7 mmol, 1 equiv), triethylamine (0.81 g, 8 mmol, 1.2 equiv) and DCM (20 mL). The flask was placed into an ice bath. To this was added a DCM (10 mL) solution of acryloyl chloride (1.36 g, 15 mmol, 2.4 equiv) over 5 minutes. The reaction was then stirred overnight at room temperature. Upon full conversion, the reaction mixture was filtered through a short pad of Na$_2$SO$_4$ and concentrated in *vacuo*. The residue was further purified by column chromatography over silica gel (hexane/acetone, 4:1 to 2:1) to give **1w** as a white solid (1.05 g, 74% yield). R$_f$ = 0.3 (hexane/acetone = 3:2). ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.25 (dd, J = 16.9, 1.5 Hz, 1H), 6.05 (dd, J = 17.0, 10.2 Hz, 1H), 5.72 – 5.47 (m, 2H), 3.82 (dtd, J = 11.7, 7.8, 4.0 Hz, 1H), 3.65 (s, 3H), 2.23 (tt, J = 12.1, 3.5 Hz, 1H), 2.12 – 1.95 (m, 4H), 1.55 (qd, J = 13.1, 3.0 Hz, 2H), 1.26 – 1.09 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 175.8, 164.8, 131.1, 126.5, 51.8, 47.9, 42.5, 32.2, 27.8. IR: 3249, 3067, 2930, 2860, 1724, 1617, 1560, 1433, 1253, 1196, 1149 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{11}$H$_{17}$NO$_3$, calcd. [M+H]$^+$ 212.1287 Found: 212.1265.

4.2 General procedure
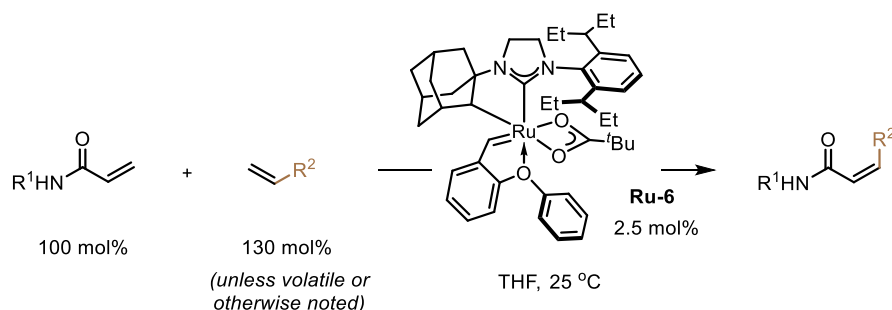
A 4 mL vial was charged with a stir bar, an acrylamide substrate (0.25 mmol, 1 equiv), and an olefin substrate (0.325 mmol, 1.3 equiv) in a nitrogen glovebox. To this was added a stock solution of **Ru-6** (5.0 mg, 0.00625 mmol, 0.025 equiv) in THF (0.4 mL). The vial was loosely capped with a screw thread hole cap, and a 20-gauge needle was used to puncture the cap and left on (see Figure S1). The reaction mixture was allowed to stir at room temperature in the glovebox for 12 – 40 hours until its color changed from purple to bright yellow (*which indicates the complete consumption of the catalyst*). The reaction was then removed from the glovebox, concentrated, and further purified by flash column chromatography over silica. The reported yield was the isolated yield of the *Z*-metathesis product. Unless otherwise noted, the *Z/E* ratio of the metathesis product was determined by ^{1}H NMR analysis of the crude reaction mixture using d_8-THF or CDCl$_3$ as the NMR solvent.

<u>Note</u>: In some cases, the metathesis reaction was also conducted in d_8-THF (instead of THF). No difference in the reaction outcome was observed.

4.3 Product characterization

3b
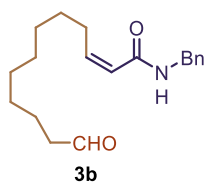
3b: White solid (53.3 mg, 71% yield). M.p. = 54 – 56 °C. Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.3 (hexane/ethyl acetate/dichloromethane = 5:1:2). Chromatography condition: hexane/ethyl acetate/dichloromethane, 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 9.73 (t, *J* = 1.9 Hz, 1H), 7.35 – 7.25 (m, 5H), 6.00 (dt, *J* = 11.5, 7.4 Hz, 1H), 5.89 (br, 1H), 5.69 (dt, *J* = 11.5, 1.7 Hz, 1H), 4.45 (d, *J* = 5.6 Hz, 2H), 2.66 (qd, *J* = 7.4, 1.7 Hz, 2H), 2.40 (td, *J* = 7.4, 1.9 Hz, 2H), 1.60 (p, *J* = 7.0 Hz, 2H), 1.47 – 1.36 (m, 2H), 1.36 – 1.23 (m, 8H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 203.2, 166.5, 146.4, 138.5, 128.8, 128.0, 127.6, 122.0, 44.0, 43.4, 29.4, 29.4, 29.3, 29.3, 29.2, 28.9, 22.2. IR: 3296, 2924, 2853, 1721, 1657, 1631, 1533, 1454, 1234 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{19}$H$_{27}$NO$_2$, calcd. [M+H]$^+$ 302.2120 Found: 302.2106.

3c
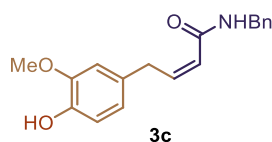
3c: Colorless oil (55.5 mg, 75% yield). Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by chromatography isolation of the crude reaction mixture). R_f = 0.25 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 5:1:2 to 3:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.37 – 7.27 (m, 5H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 1.9 Hz, 1H), 6.71 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.15 (dt, *J* = 11.3, 7.6 Hz, 1H), 5.92 (br, 1H), 5.76 (dt, *J* = 11.3, 1.7 Hz, 1H), 4.50 (d, *J* = 5.6 Hz, 2H), 3.99 (dd, *J* = 7.6, 1.7 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.3, 146.7, 144.8, 144.1, 138.3, 132.0, 128.8, 128.0, 127.7, 121.8, 121.2, 114.5, 111.4, 56.0, 43.5, 34.7. IR: 3296, 3029, 2935, 1656, 1514, 1268, 1232, 1150 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{18}$H$_{19}$NO$_3$, calcd. [M+H]$^+$ 298.1443 Found: 298.1427.

3d
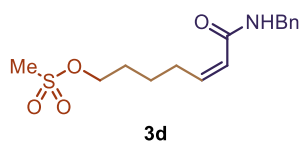
3d: White solid (60.3 mg, 78% yield). Reaction time = 15 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.15 (hexane/ethyl acetate/dichloromethane = 2:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 3:1:1 to 2:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.36 – 7.24 (m, 5H), 6.17 – 5.81 (m, 2H), 5.73 (dt, *J* = 11.4, 1.6 Hz, 1H), 4.44 (d, *J* = 5.4 Hz, 2H), 4.22 (t, *J* = 6.4 Hz, 2H), 2.97 (s, 3H), 2.74 (qd, *J* = 7.5, 1.6 Hz, 2H), 1.78 (dq, *J* = 8.3, 6.3 Hz, 2H), 1.56 (p, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.2, 145.3, 138.4, 128.8, 127.9, 127.6, 122.7, 70.1, 43.4, 37.3, 28.6, 27.8, 25.0. IR: 3304, 3028, 2935, 1660, 1632, 1526, 1347, 1176, 972 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{15}$H$_{21}$NO$_4$S, calcd. [M+H]$^+$ 312.1270 Found: 312.1290.

3e

3e: Colorless oil (57 mg, 71% yield). Reaction time = 15 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.3 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 10:1:3 to 3:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.41 – 7.23 (m, 10H), 6.52 (br, 1H), 5.94 (dt, *J* = 11.5, 7.6 Hz, 1H), 5.77 (dt, *J* = 11.5, 1.5 Hz, 1H), 5.10 (s, 2H), 4.48 (d, *J* = 5.7 Hz, 2H), 2.91 (qd, *J* = 7.1, 1.5 Hz, 2H), 2.55 (t, *J* = 6.9 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.2, 166.2, 141.6, 138.4, 135.9, 128.8, 128.7, 128.4, 128.0, 127.5, 124.1, 66.6, 43.5, 33.4, 24.2. The spectra match the reported literature.[11]

3f

3f: Colorless oil (52.1 mg, 73% yield). Reaction time = 20 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.35 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 10:1:3 to 3:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.37 – 7.22 (m, 5H), 6.00 (dt, *J* = 11.5, 7.5 Hz, 1H), 5.87 (br, 1H), 5.69 (dt, *J* = 11.5, 1.7 Hz, 1H), 4.45 (d, *J* = 5.7 Hz, 2H), 2.88 (qd, *J* = 5.4, 3.3 Hz, 1H), 2.72 (dd, *J* = 5.0, 4.0 Hz, 1H), 2.67 (td, *J* = 7.5, 1.7 Hz, 2H), 2.44 (dd, *J* = 5.0, 2.8 Hz, 1H), 1.56 – 1.25 (m, 10H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.5, 146.4, 138.5, 128.8, 128.0, 127.6, 122.0, 52.5, 47.2, 43.4, 32.5, 29.3, 29.3, 29.3, 28.8, 26.0. IR: 3301, 3029, 2925, 28540, 1658, 1632, 1533, 1236 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{18}$H$_{25}$NO$_2$, calcd. [M+H]$^+$ 288.1964 Found: 288.1957.

3g

3g: Following a modified *General procedure*, the reaction was conducted with the use of 1.6 equivalent (*instead of 1.3 equiv.*) of allylcyclohexane (b.p. = 150 °C, 50 mg). The titled compound was isolated as a white soild (57.7 mg, 90% yield). M.p. = 77 – 79 °C. Reaction time = 36 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.3 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.37 – 7.26 (m, 5H), 6.04 (dt, *J* = 11.5, 7.6 Hz, 1H), 5.83 (br, 1H), 5.73 (dt, *J* = 11.5, 1.7 Hz, 1H), 4.46 (d, *J* = 5.5 Hz, 2H), 2.57 (td, *J* = 7.3, 1.7 Hz, 2H), 1.75 – 1.57 (m, 5H), 1.38 (tdq, *J* = 14.2, 6.9, 3.5 Hz, 1H), 1.32 – 1.08 (m, 3H), 1.08 – 0.89 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.6, 145.1, 138.5, 128.8, 128.0, 127.6, 122.6, 43.4, 38.3, 36.4, 33.2, 26.6, 26.4. IR: 3294, 2920, 2849, 1653, 1625, 1536, 1447, 1239 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{17}$H$_{23}$NO, calcd. [M+H]$^+$ 258.1858 Found: 258.1834.

3h

3h: Colorless oil (49 mg, 60% yield). Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.4 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/acetone/dichloromethane, 10:1:3. ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 7.13 – 6.99 (m, 5H), 5.83 (dt, *J* = 11.4, 7.5 Hz, 1H), 5.57 – 4.99 (m, 2H), 4.26 (d, *J* = 6.0 Hz, 2H), 2.98 (qd, *J* = 7.5, 1.7 Hz, 2H), 1.72 (p, *J* = 7.7 Hz, 2H), 1.07 (s, 12H), 0.99 (d, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ

165.8, 145.9, 139.7, 128.7, 128.1, 127.2, 122.8, 82.9, 43.2, 31.4, 25.0, 24.5, 11.34. IR: 3296, 2977, 2928, 1657, 1537, 1371, 1315, 1142 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{19}H_{28}BNO_3$, calcd. [M+H]$^+$ 330.2241 Found: 330.2253.

3i: Following a modified *General procedure*, the reaction was conducted with the use of 1.6 equivalent (*instead of 1.3 equiv.*) of pent-4-en-1-ol (b.p. = 133 °C, 34.5 mg). The titled compound was isolated as a colorless oil (43.6 mg, 80% yield). Reaction time = 15 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.15 (hexane/ethyl acetate/dichloromethane = 3:2:2). Chromatography condition: hexane/ethyl acetate/dichloromethane, 3:1:1 to 3:2:2. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.38 – 7.26 (m, 5H), 6.21 (br, 1H), 5.99 (dt, J = 11.5, 8.6 Hz, 1H), 5.84 (d, J = 11.5 Hz, 1H), 4.47 (d, J = 5.5 Hz, 2H), 3.58 (t, J = 5.6 Hz, 2H), 3.16 (br, 1H), 2.73 (q, J = 7.8 Hz, 2H), 1.76 – 1.59 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.0, 144.9, 138.0, 128.9, 128.1, 127.7, 123.5, 60.0, 43.7, 30.5, 24.7. The spectra match the reported literature.[11]

3j: Colorless oil (48 mg, 70% yield). Reaction time = 15 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.6 (hexane/acetone/dichloromethane = 3:1:1). Chromatography condition: hexane/acetone/dichloromethane, 10:1:3 to 5:1:2. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.36 – 7.24 (m, 5H), 5.99 (dt, J = 11.5, 7.5 Hz, 1H), 5.91 (br, 1H), 5.71 (dt, J = 11.4, 1.7 Hz, 1H), 4.45 (d, J = 5.7 Hz, 2H), 4.05 (t, J = 6.6 Hz, 2H), 2.72 (qd, J = 7.5, 1.7 Hz, 2H), 2.02 (s, 3H), 1.71 – 1.59 (m, 2H), 1.55 – 1.44 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 171.3, 166.3, 145.7, 138.4, 128.8, 128.0, 127.6, 122.4, 64.5, 43.4, 28.4, 28.4, 25.8, 21.1. IR: 3304, 2935, 1735, 1659, 1532, 1249, 1030 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{16}H_{21}NO_3$, calcd. [M+H]$^+$ 276.1600 Found: 276.1629.
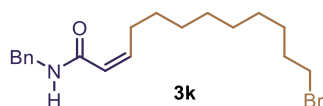
3k: Colorless oil (73 mg, 80% yield). Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.3 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.39 – 7.20 (m, 5H), 6.00 (dt, J = 11.4, 7.5 Hz, 1H), 5.94 (br, 1H), 5.69 (dt, J = 11.5, 1.7 Hz, 1H), 4.44 (d, J = 5.7 Hz, 2H), 3.39 (t, J = 6.9 Hz, 2H), 2.66 (qd, J = 7.4, 1.7 Hz, 2H), 1.92 – 1.76 (m, 2H), 1.50 – 1.36 (m, 4H), 1.36 – 1.24 (m, 8H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.5, 146.4, 138.5, 128.7, 127.9, 127.5, 121.9, 43.3, 34.2, 32.9, 29.4, 29.4, 29.4, 29.3, 28.9, 28.8, 28.2. IR: 3293, 3032, 2923, 2852, 1656, 1631, 1538, 1454, 1240 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{19}H_{28}BrNO$, calcd. [M+H]$^+$ 366.1432 Found: 366.1431.
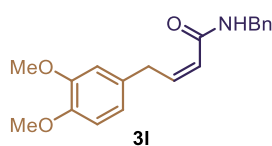
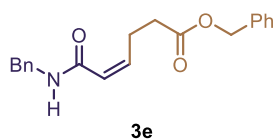**3l**: White solid (55 mg, 71% yield). M.p. = 77 – 79 °C. Reaction time = 20 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.25 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 5:1:2. ^{1}H NMR (400 MHz, CDCl₃) δ 7.38 – 7.27 (m, 5H), 6.85 – 6.71 (m, 3H), 6.17 (dt, *J* = 11.3, 7.6 Hz, 1H), 5.85 (br, 1H), 5.76 (dt, *J* = 11.3, 1.8 Hz, 1H), 4.51 (d, *J* = 5.7 Hz, 2H), 4.01 (dd, *J* = 7.6, 1.8 Hz, 2H), 3.85 (s, 6H). ^{13}C NMR (101 MHz, CDCl₃) δ 166.2, 149.1, 147.6, 144.7, 138.3, 132.7, 128.9, 128.0, 127.7, 121.9, 120.5, 112.1, 111.4, 56.1, 56.0, 43.6, 34.6. The spectra match the reported literature.[11]

3m
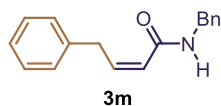
3m: White solid (42.4 mg, 68% yield). M.p. = 74 – 75 °C. Reaction time = 20 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.3 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl₃) δ 7.32 – 7.11 (m, 10H), 6.09 (dt, *J* = 11.3, 7.6 Hz, 1H), 5.86 (br, 1H), 5.70 (dt, *J* = 11.3, 1.7 Hz, 1H), 4.41 (d, *J* = 5.0 Hz, 2H), 3.99 (dd, *J* = 7.5, 1.7 Hz, 2H). ^{13}C NMR (101 MHz, CDCl₃) δ 166.2, 144.3, 140.1, 138.3, 128.8, 128.7, 128.7, 128.0, 127.7, 126.3, 122.2, 43.5, 35.0. IR: 3291, 3067, 3028, 1654, 1625, 1545, 1494, 1261, 1236, 1029 cm⁻¹. HRMS: *Chemical fomular* ([M]): $C_{17}H_{17}NO$, calcd. [M+H]⁺ 252.1388 Found: 252.1379.

3n
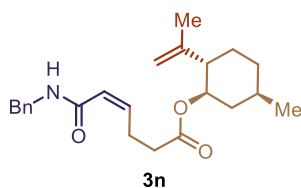
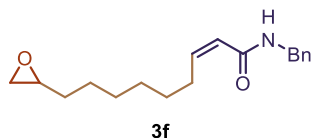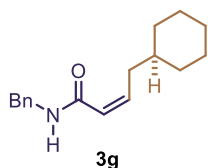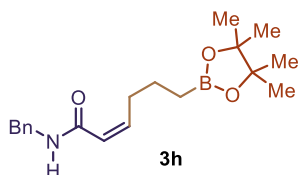**3n**: Colorless oil (57.8 mg, 63% yield). Reaction time = 40 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.0.4 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 10:1:3 to 5:1:2. ^{1}H NMR (400 MHz, CDCl₃) δ 7.35 – 7.23 (m, 5H), 6.74 (br, 1H), 5.88 (dt, *J* = 11.6, 7.5 Hz, 1H), 5.76 (dt, *J* = 11.5, 1.4 Hz, 1H), 4.79 (td, *J* = 10.9, 4.4 Hz, 1H), 4.72 – 4.63 (m, 2H), 4.48 (d, *J* = 5.7 Hz, 2H), 2.92 – 2.72 (m, 2H), 2.40 (dd, *J* = 7.2, 6.5 Hz, 2H), 2.08 (ddd, *J* = 12.5, 10.7, 3.7 Hz, 1H), 1.94 (dddd, *J* = 10.4, 3.5, 2.6, 1.6 Hz, 1H), 1.73 – 1.64 (m, 2H), 1.62 (t, *J* = 1.2 Hz, 3H), 1.58 – 1.46 (m, 1H), 1.42 – 1.29 (m, 1H), 1.06 – 0.97 (m, 1H), 0.97 – 0.86 (m, 4H). ^{13}C NMR (101 MHz, CDCl₃) δ 172.9, 166.4, 146.2, 141.4, 138.5, 128.7, 128.0, 127.4, 124.0, 112.0, 73.9, 50.8, 43.4, 40.5, 34.1, 33.5, 31.5, 30.4, 24.3, 22.1, 19.6. IR: 3304, 2950, 2925, 2868, 1727, 1660, 1537, 1454, 1236, 1164 cm⁻¹. HRMS: *Chemical fomular* ([M]): $C_{23}H_{31}NO_3$, calcd. [M+H]⁺ 370.2382 Found: 370.2402.

3o

3o: White solid (85.8 mg, 74% yield). M.p. = 145 – 147 °C. Reaction time = 20 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.65 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl₃) δ 7.27 – 7.15 (m, 5H), 7.00 – 6.86 (m, 2H), 6.81 (ddd, *J* = 8.6, 4.2,

1.9 Hz, 1H), 5.92 (dt, J = 11.5, 7.4 Hz, 1H), 5.84 (t, J = 5.4 Hz, 1H), 5.61 (dt, J = 11.4, 1.7 Hz, 1H), 4.37 (d, J = 5.7 Hz, 2H), 2.62 (qd, J = 7.6, 1.7 Hz, 2H), 2.39 – 2.23 (m, 1H), 1.87 – 1.68 (m, 6H), 1.65 (d, J = 10.3 Hz, 2H), 1.34 – 1.17 (m, 4H), 1.15 – 0.73 (m, 9H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.5, 150.6 (dd, J = 166.7, 12.6 Hz), 148.2 (dd, J = 165.0, 12.6 Hz), 146.8, 145.0 (dd, J = 4.9, 3.8 Hz), 138.5, 128.8, 127.9, 127.5, 122.6 (dd, J = 5.9, 3.3 Hz), 121.8, 116.8 (d, J = 16.6 Hz), 115.5 (d, J = 16.6 Hz), 43.9 (d, J = 1.3 Hz), 43.4, 43.3, 42.8, 37.8, 37.0, 34.7, 33.5, 30.3, 30.1, 26.6. ^{19}F NMR (282 MHz, CDCl$_3$) δ -138.76 (ddd, J = 20.7, 12.0, 8.2 Hz, 1F), -142.67 (dddd, J = 21.9, 11.7, 7.9, 4.2 Hz, 1F). IR: 2919, 2850, 1657, 1515, 1450, 1212, 905 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{30}$H$_{37}$F$_2$NO, calcd. [M+H]$^+$ 466.2922 Found: 466.2938.
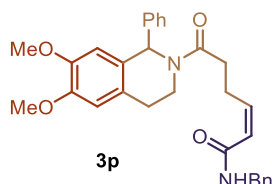
3p: Colorless wax (86 mg, 71% yield). Reaction time = 40 hours. *Z:E* ratio > 20:1 (determined by chromatography isolation of the crude reaction mixture). R$_f$ = 0.15 (hexane/acetone/dichloromethane = 3:1:1). Chromatography condition: hexane/acetone/dichloromethane, 6:1:2 to 3:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) (*mixture of amide rotamers, ca. 5:1*) δ 8.04 (s, 0.83H), 7.82 (s, 0.17H), 7.42 – 7.27 (m, 5H), 7.26 – 7.22 (m, 3H), 7.18 – 7.13 (m, 2H), 6.81 (s, 0.83H), 6.66 (s, 0.17H), 6.65 (s, 1H), 6.50 (s, 0.83H), 6.02 (s, 0.17H), 5.93 – 5.76 (m, 2H), 4.61 – 4.42 (m, 2H), 4.27 (dt, J = 13.0, 5.3 Hz, 0.17H), 3.88 (s, 3H), 3.82 – 3.72 (m, 3.83H), 3.35 (ddd, J = 13.8, 11.6, 4.4 Hz, 0.83H), 3.18 (ddd, J = 13.7, 9.4, 5.1 Hz, 0.17H), 2.97 – 2.51 (m, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) *major rotamer:* δ 170.7, 166.8, 148.2, 147.8, 142.4, 140.0, 138.7, 128.8, 128.6, 128.4, 128.0, 127.5, 127.3, 126.9, 126.4, 124.9, 111.3, 111.1, 56.1, 56.0, 54.9, 43.5, 39.4, 32.3, 28.6, 24.7. *for the minor rotamer, carbon signals were observed at:* δ 171.4, 166.7, 148.5, 147.5, 141.4, 140.3, 138.7, 128.7, 128.6, 127.9, 127.8, 127.5, 127.3, 126.9, 124.8, 111.5, 111.1, 59.4, 56.1, 43.3, 37.6, 32.8, 27.4, 24.9. IR: 3293, 3028, 2935, 1622, 1514, 1452, 1249, 1117 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{30}$H$_{32}$N$_2$O$_4$, calcd. [M+H]$^+$ 485.2440 Found: 485.2453.
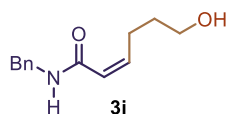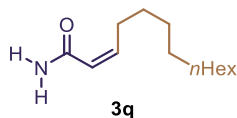

3q: Following a modified *General procedure*, the reaction was conducted with the use of 2.0 equivalent (*instead of 1.3 equiv.*) of 1-dodecene (84 mg). The titled compound was isolated as a white solid (41.1 mg, 78% yield). M.p. = 62 – 64 °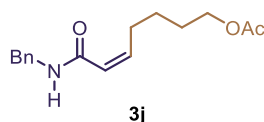C. Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.2 (hexane/ethyl acetate/dichloromethane = 3:2:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 3:1:1 to 3:2:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.05 (dt, J = 11.5, 7.4 Hz, 1H), 5.91 (br, 1H), 5.73 (dt, J = 11.5, 1.7 Hz, 1H), 5.63 (br, 1H), 2.62 (qd, J = 7.4, 1.8 Hz, 2H), 1.41 (p, J = 7.3 Hz, 2H), 1.36 – 1.08 (m, 14H), 0.92 – 0.80 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 169.0, 147.5, 121.2, 32.0, 29.7, 29.7, 29.6, 29.5, 29.4, 29.4, 29.0, 22.8, 14.2. IR: 3330, 3183, 2924, 2854, 1669, 1631, 1312 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{13}$H$_{25}$NO, calcd. [M+H]$^+$ 212.2014 Found: 212.2024.
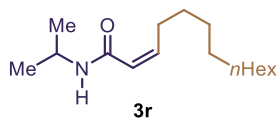
3r: White solid (46.7 mg, 74% yield). M.p. = 45 – 47 °C. Reaction time = 18 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.5 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane,

20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 5.93 (dt, J = 11.5, 7.4 Hz, 1H), 5.62 (dt, J = 11.5, 1.7 Hz, 1H), 5.37 (br, 1H), 4.10 (h, J = 6.6 Hz, 1H), 2.61 (qd, J = 7.4, 1.7 Hz, 2H), 1.40 (p, J = 6.7 Hz, 2H), 1.35 – 1.20 (m, 14H), 1.15 (d, J = 6.6 Hz, 6H), 0.86 (d, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.9, 145.4, 122.6, 41.1, 32.0, 29.7, 29.7, 29.6, 29.5, 29.5, 29.5, 28.9, 23.0, 22.8, 14.2. IR: 3258, 2960, 2917, 2850, 1653, 1624, 1546, 1466, 1242 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{16}$H$_{31}$NO, calcd. [M+H]$^+$ 254.2484 Found: 254.2454.
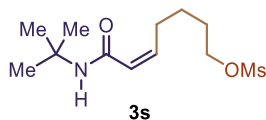
3s: White solid (50.0 mg, 72% yield). M.p. = 50 – 53 °C. Reaction time = 20 hours. *Z:E* ratio = 15:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.15 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 5:1:2 to 3:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 5.86 (dt, J = 11.4, 7.5 Hz, 1H), 5.62 (dt, J = 11.5, 1.7 Hz, 1H), 5.34 (br, 1H), 4.23 (t, J = 6.4 Hz, 2H), 2.99 (s, 3H), 2.69 (qd, J = 7.5, 1.7 Hz, 2H), 1.77 (dq, J = 8.3, 6.5 Hz, 2H), 1.54 (tt, J = 9.6, 6.5 Hz, 2H), 1.35 (s, 9H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.0, 143.7, 124.2, 70.1, 51.3, 37.4, 28.9, 28.6, 27.6, 25.1. IR: 2968, 1661, 1525, 1350, 1171, 909 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{12}$H$_{23}$NO$_4$S, calcd. [M+H]$^+$ 278.1426 Found: 278.1419.
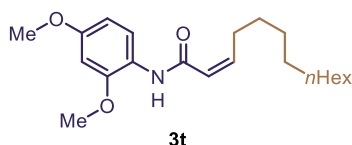
3t: Following a modified *General procedure*, the reaction was conducted with the use of 2.0 equivalent (*instead of 1.3 equiv.*) of 1-dodecene (84 mg). The titled compound was isolated as a colorless oil (34.4 mg, 40% yield). Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by chromatography isolation of the crude reaction mixture). R$_f$ = 0.4 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5 to 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.32 (d, J = 9.6 Hz, 1H), 7.58 (br, 1H), 6.53 – 6.40 (m, 2H), 6.08 (dt, J = 11.4, 7.4 Hz, 1H), 5.84 (d, J = 11.5 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 2.71 (qd, J = 7.4, 1.6 Hz, 2H), 1.45 (p, J = 7.4 Hz, 2H), 1.40 – 1.22 (m, 14H), 0.87 (t, J = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) carbon signals were observed at δ 164.4, 156.4, 149.2, 146.9, 123.0, 121.5, 120.6, 103.8, 98.7, 55.8, 55.7, 32.1, 29.8, 29.7, 29.6, 29.5, 29.5, 29.0, 22.8, 14.3. IR: 2923, 2853, 1674, 1521, 1463, 1299, 1280, 1207, 1035 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{21}$H$_{33}$NO$_3$, calcd. [M+H]$^+$ 348.2539 Found: 348.2547.
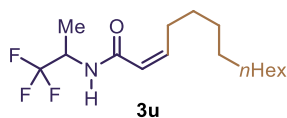
3u: Following a modified *General procedure*, the reaction was conducted with the use of 2.0 equivalent (*instead of 1.3 equiv.*) of 1-dodecene (84 mg). The titled compound was isolated as a white solid (65 mg, 85% yield). M.p. = 47 – 49 °C. Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R$_f$ = 0.5 (hexane/ethyl acetate/dichloromethane = 10:1:3). Chromatography condition: hexane/ethyl acetate/dichloromethane, 20:1:5. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.08 (dt, J = 11.4, 7.5 Hz, 1H), 5.74 (d, J = 9.8 Hz, 1H), 5.69 (dt, J = 11.5, 1.7 Hz, 1H), 4.74 (qq, J = 9.6, 7.2 Hz, 1H), 2.62 (qd, J = 7.5, 1.8 Hz, 2H), 1.41 (p, J = 7.4 Hz, 2H), 1.36 – 1.14 (m, 17H), 0.86 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.9, 148.1, 125.5 (q, J = 281.0 Hz), 121.1, 45.9 (q, J = 31.5 Hz), 32.0, 29.7, 29.6, 29.5, 29.5, 29.3, 29.1, 22.8, 14.5 (q, J = 2.0 Hz), 14.2. ^{19}F NMR (282 MHz, CDCl$_3$) δ -77.53 (d, J = 7.4 Hz,

3F). IR: 3284, 2924, 2854, 1660, 1540, 1459, 1230, 1137 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{16}H_{28}F_3NO$, calcd. $[M+H]^+$ 308.2201 Found: 308.2213.
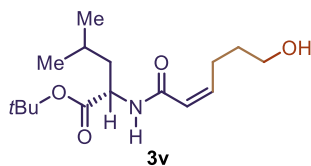

3v: Following a modified *General procedure*, the reaction was conducted with the use of 1.8 equivalent (*instead of 1.3 equiv.*) of pent-4-en-1-ol (b.p. = 133 °C, 38.8 mg). The titled compound was isolated as a colorless oil (64 mg, 86% yield). Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.15 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 3:1:1 to 2:1:1. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.42 (d, *J* = 8.4 Hz, 1H), 5.96 (dt, *J* = 11.4, 8.4 Hz, 1H), 5.84 (d, *J* = 11.5 Hz, 1H), 4.53 (td, *J* = 8.5, 5.3 Hz, 1H), 3.70 (br, 1H), 3.55 (t, *J* = 5.6 Hz, 2H), 2.69 (qp, *J* = 13.8, 7.0, 6.1 Hz, 2H), 1.73 – 1.49 (m, 5H), 1.49 – 1.38 (m, 9H), 0.92 (d, *J* = 6.3 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 172.6, 166.8, 144.6, 123.6, 82.2, 60.0, 51.3, 42.0, 30.5, 28.1, 25.1, 24.7, 22.9, 22.2. IR: 3285, 2957, 2871, 1732, 1658, 1537, 1368, 1249, 1149 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{16}H_{29}NO_4$, calcd. $[M+H]^+$ 300.2175 Found: 300.2195.
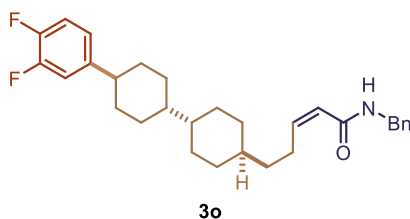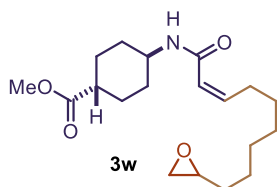

3w: White solid (51.2 mg, 61% yield). M.p. = 40 – 41 °C. Reaction time = 24 hours. *Z:E* ratio > 20:1 (determined by ^{1}H NMR analysis of the crude reaction mixture). R_f = 0.15 (hexane/ethyl acetate/dichloromethane = 3:1:1). Chromatography condition: hexane/ethyl acetate/dichloromethane, 3:1:1 to 2:1:2. ^{1}H NMR (400 MHz, CDCl$_3$) δ 5.94 (dt, *J* = 11.5, 7.5 Hz, 1H), 5.61 (dt, *J* = 11.5, 1.7 Hz, 1H), 5.42 (d, *J* = 8.2 Hz, 1H), 3.77 (tdq, *J* = 12.0, 8.1, 4.0 Hz, 1H), 3.64 (s, 3H), 2.87 (tdd, *J* = 5.3, 3.9, 2.7 Hz, 1H), 2.71 (dd, *J* = 5.0, 4.0 Hz, 1H), 2.61 (qd, *J* = 7.4, 1.7 Hz, 2H), 2.43 (dd, *J* = 5.0, 2.7 Hz, 1H), 2.21 (tt, *J* = 12.1, 3.5 Hz, 1H), 2.10 – 1.93 (m, 4H), 1.62 – 1.30 (m, 12H), 1.19 – 1.06 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 175.8, 165.9, 145.8, 122.4, 52.5, 51.8, 47.5, 47.2, 42.5, 32.5, 32.3, 29.3, 29.3, 28.7, 27.9, 26.0. IR: 3294, 2930, 2856, 1733, 1657, 1628, 1532, 1453, 1254, 1174 cm^{-1}. HRMS: *Chemical fomular* ([M]): $C_{19}H_{31}NO_4$, calcd. $[M+H]^+$ 338.2331 Found: 338.2338.
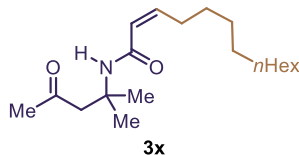
3x: Following a modified *General procedure*, the reaction was conducted with the use of 2.0 equivalent (*instead of 1.3 equiv.*) of 1-dodecene (84 mg). The titled compound was isolated as a white solid (46.1 mg, 60% yield). M.p. = 49 – 50 °C. Reaction time = 24 hours. *Z:E* ratio = 17:1 (determined by chromatography isolation of the crude reaction mixture; *trans*-product: 2.7 mg). R_f = 0.35 (hexane/ethyl acetate/dichloromethane = 5:1:2). Chromatography condition: hexane/ethyl acetate/dichloromethane, 10:1:3. ^{1}H NMR (400 MHz, CDCl$_3$) δ 5.89 (dt, *J* = 11.5, 7.4 Hz, 1H), 5.77 (br, 1H), 5.60 (dt, *J* = 11.5, 1.7 Hz, 1H), 2.96 (s, 2H), 2.57 (qd, *J* = 7.3, 1.7 Hz, 2H), 2.11 (s, 3H), 1.50 – 1.35 (m, 8H), 1.34 – 1.18 (m, 14H), 0.86 (t, *J* = 6.9, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) carbon signals were observed at δ 208.1, 166.7, 145.2, 123.2,

52.3, 51.2, 32.0, 31.9, 29.7, 29.6, 29.5, 29.5, 29.4, 28.7, 27.7, 22.8, 14.3. IR: 3319, 2923, 2853, 1708, 1658, 1532, 1456, 1361 cm^{-1}. HRMS: *Chemical fomular* ([M]): C$_{19}$H$_{35}$NO$_2$, calcd. [M+H]$^+$ 310.2746 Found: 310.2718.

5. Computational study

5.1 Detailed energy profiles for "olefin-first" and "acrylamide-first" mechanisms

Scheme S1 | Calculated energies (kcal/mol) for "olefin-first" pathways with both [Ru]-OPiv (top) and [Ru]-NO₃ (bottom).

■ **A.** Free energy profile of "olefin-first" pathway using [Ru]-OPiv
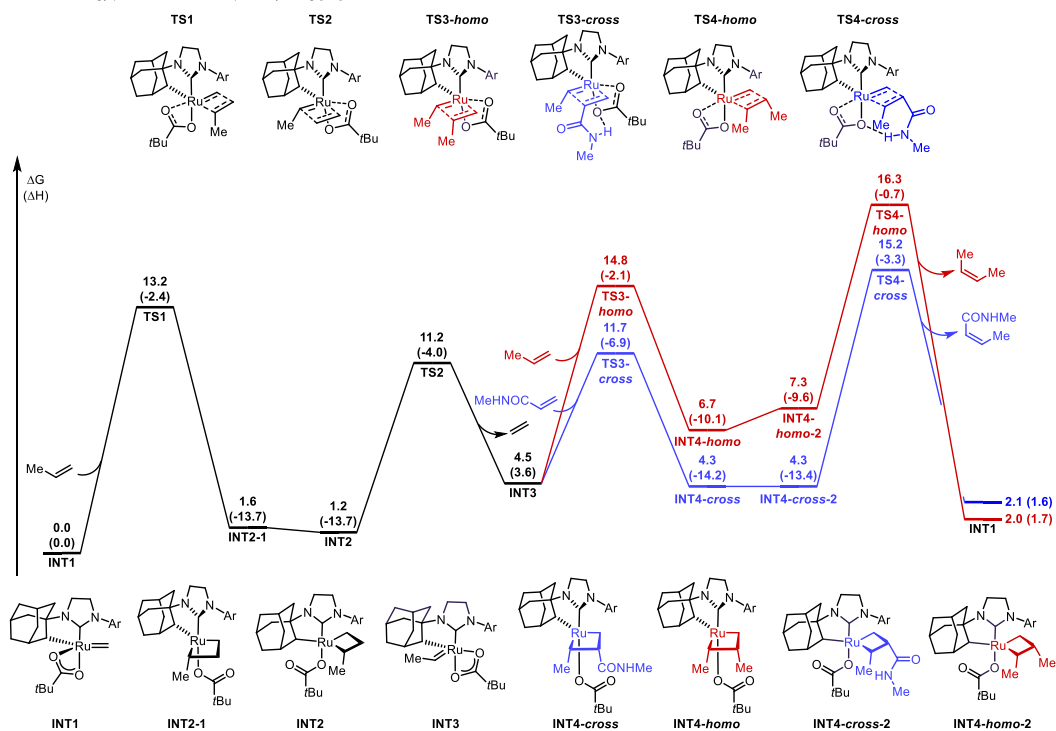
■ **B.** Free energy profile of "olefin-first" pathway using [Ru]-NO₃
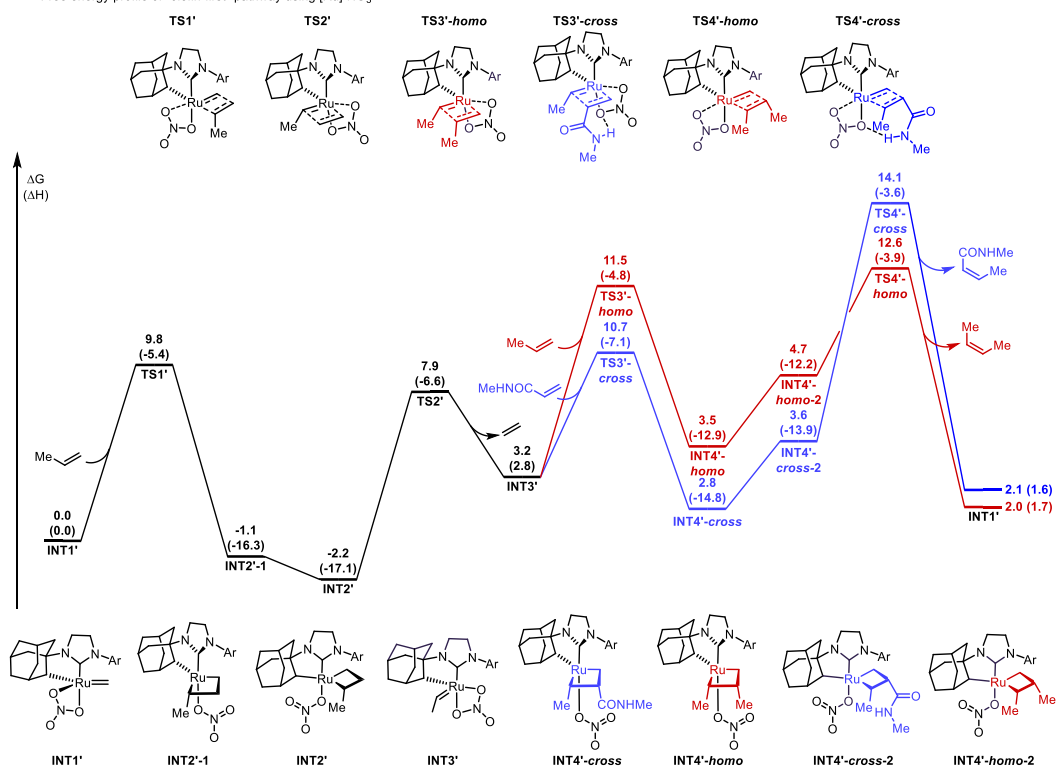
Scheme S2 | Calculated energies (kcal/mol) for "acrylamide-first" pathways with both [Ru]-OPiv (top) and [Ru]-NO₃ (bottom). No barrier could be located for the extrusion of ethylene.
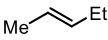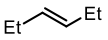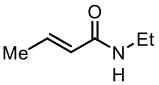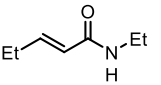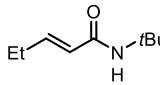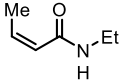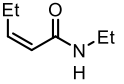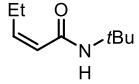
■ **A.** Free energy profile of "acrylamide-first" pathway using [Ru]-OPiv
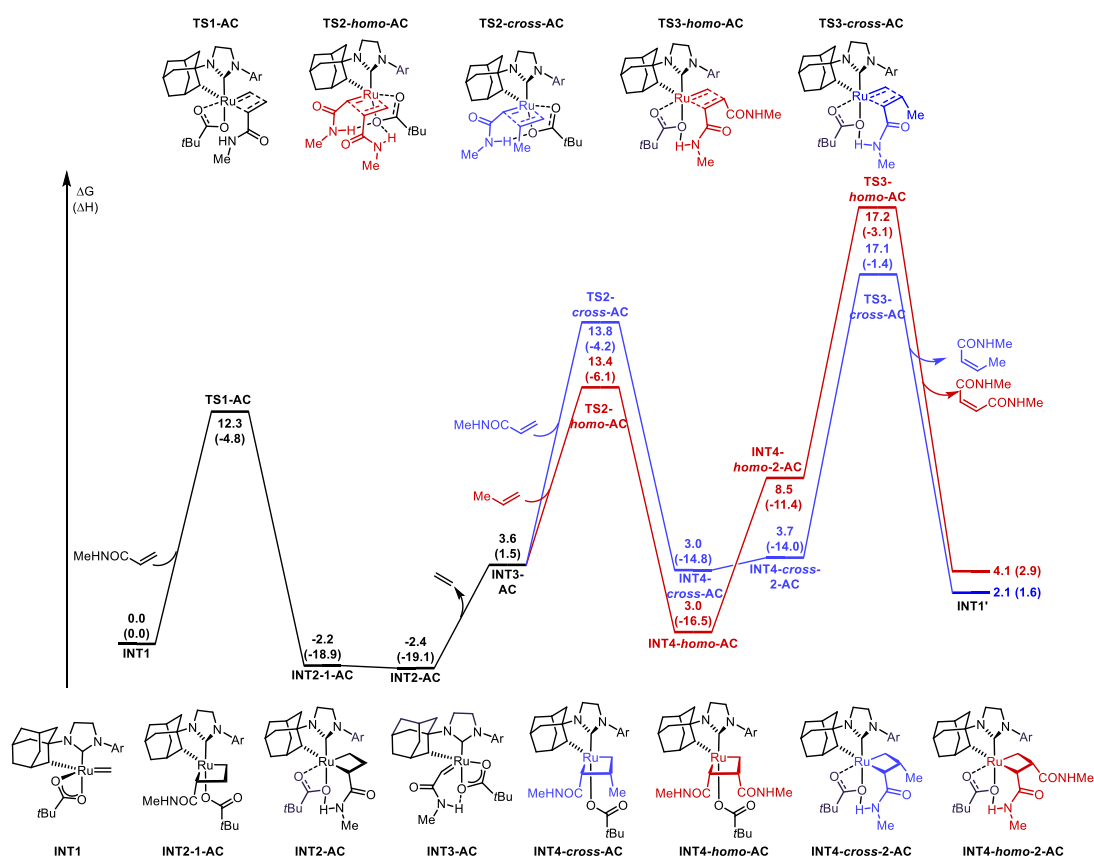
■ **B.** Free energy profile of "acrylamide-first" pathway using [Ru]-NO₃
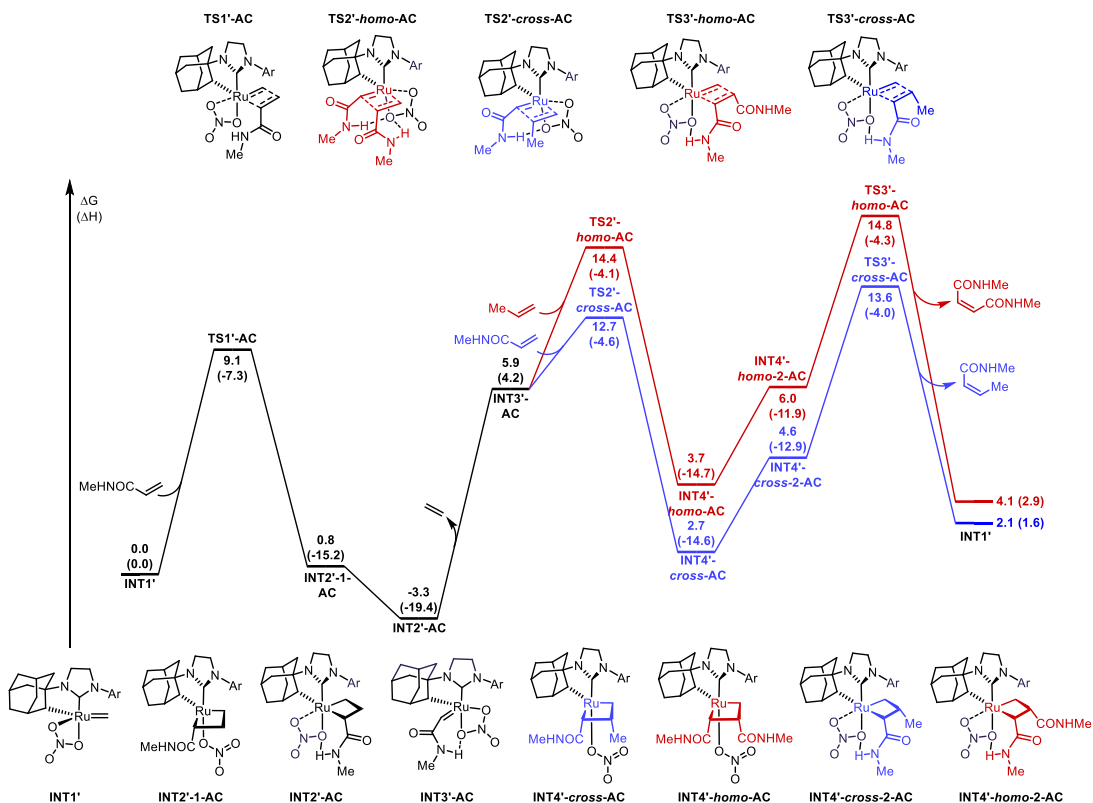
5.2 Relative stabilities of olefin isomers

E-olefin	S21-*E*	S22-*E*	S23-*E*	S24-*E*	S25-*E*
Z-olefin	S21-*Z*	S22-*Z*	S23-*Z*	S24-*Z*	S25-*Z*
$\Delta\Delta G_{Z-E}$ (kcal mol^{-1})	1.1	1.2	2.5	3.6	4.1

5.3 Computational methods

All calculations were carried out with the Gaussian 16[12] software package. Ground state and transition state geometries were optimized in the gas phase using the B3LYP[13] functional with the D3 version of Grimme's empirical dispersion correction.[14] The SDD[15] basis set was used for Ru and the 6-31G(d) basis set for all other atoms. Frequency calculations were carried out at the same level of theory to ensure that stationary points were truly minima or saddle points on the potential energy surface. Thermal corrections to free energies were calculated using Grimme's quasi-rigid rotor-harmonic oscillator approximation at 298 K.[16] Intrinsic reaction coordinate calculations were also carried out at this level of theory in order to confirm that all transition states connected reactants and products. Single-point and CM5 charge calculations were performed at with the M06[17] functional with the SDD basis set for Ru and 6-311++G(d,p) basis set for all other atoms. Solvation effects were incorporated with the SMD[18] model in THF. Conformational searches were carried out using the CREST conformer-rotamer ensemble sampling tool[19], version 2.7.1 with XTB version 6.2 RC2 (SAW190805)[20]. Images of molecular structures were rendered in CYLview.[21]

5.4 Computed energies

Structure	E(THF)	ΔG	G(THF)	ΔH	H(THF)	Imaginary Frequency
N-methylacrylamide	-286.5029417	0.076517	-286.4264247	0.115155	-286.3877867	
propene	-117.8372324	0.055064	-117.7821684	0.085077	-117.7521554	
ethylene	-78.53966431	0.029686	-78.50997831	0.055199	-78.48446531	
INT1	-1563.215087	0.657167	-1562.55792	0.75511	-1562.459977	
TS1	-1681.059482	0.740378	-1680.319104	0.843491	-1680.215991	-174.207
INT2-1	-1681.079695	0.742179	-1680.337516	0.84571	-1680.233985	
INT2	-1681.079033	0.740798	-1680.338235	0.845062	-1680.233971	
TS2	-1681.061332	0.739102	-1680.32223	0.84287	-1680.218462	-85.457
INT3	-1602.506962	0.684052	-1601.82291	0.784983	-1601.721979	
TS3-*cross*	-1889.029597	0.791762	-1888.237835	0.903199	-1888.126398	-147.311
TS3-*homo*	-1720.355847	0.767109	-1719.588738	0.872675	-1719.483172	-189.132
INT4-*cross*	-1889.04313	0.793492	-1888.249638	0.905073	-1888.138057	
INT4-*homo*	-1720.370612	0.769052	-1719.60156	0.874649	-1719.495963	
INT4-*cross*-2	-1889.0423	0.792681	-1888.249619	0.905431	-1888.136869	
INT4-*homo*-2	-1720.370631	0.77001	-1719.600621	0.875445	-1719.495186	
TS4-*cross*	-1889.024016	0.791649	-1888.232367	0.90332	-1888.120696	-181.9
TS4-*homo*	-1720.35421	0.767919	-1719.586291	0.87322	-1719.48099	-196.89
INT1'	-1497.16598	0.542247	-1496.623733	0.630328	-1496.535652	
TS1'	-1615.014866	0.62452	-1614.390346	0.718401	-1614.296465	-167.841

INT2'-1	-1615.034662	0.627023	-1614.407639	0.720923	-1614.313739	
INT2'	-1615.035252	0.625916	-1614.409336	0.720198	-1614.315054	
TS2'	-1615.016256	0.622985	-1614.393271	0.717906	-1614.29835	-91.457
INT3'	-1536.458818	0.56799	-1535.890828	0.659983	-1535.798835	
TS3'-*cross*	-1822.980355	0.675067	-1822.305288	0.777969	-1822.202386	-152.524
TS3'-*homo*	-1654.310846	0.651076	-1653.65977	0.747735	-1653.563111	-193.156
INT4'-*cross*	-1822.994489	0.676607	-1822.317882	0.779774	-1822.214715	
INT4'-*homo*	-1654.325969	0.653467	-1653.672502	0.749885	-1653.576084	
INT4'-*cross*-2	-1822.993675	0.677142	-1822.316533	0.780356	-1822.213319	
INT4'-*homo*-2	-1654.325656	0.654999	-1653.670657	0.750786	-1653.57487	
TS4'-*cross*	-1822.975001	0.675057	-1822.299944	0.778108	-1822.196893	-178.016
TS4'-*homo*	-1654.309904	0.651854	-1653.65805	0.748135	-1653.561769	-197.958
TS1-AC	-1849.728742	0.764052	-1848.96469	0.873292	-1848.85545	-109.727
INT2-1-AC	-1849.753786	0.765973	-1848.987813	0.875834	-1848.877952	
INT2-AC	-1849.753605	0.765486	-1848.988119	0.875438	-1848.878167	
INT3-AC	-1771.176444	0.707834	-1770.46861	0.81555	-1770.360894	
TS2-*cross*-AC	-1889.025347	0.790829	-1888.234518	0.903156	-1888.122191	-179.59
TS2-*homo*-AC	-2057.694046	0.814589	-2056.879457	0.933198	-2056.760848	-150.201
INT4-*cross*-AC	-1889.043843	0.792153	-1888.25169	0.904831	-1888.139012	
INT4-*homo*-AC	-2057.712369	0.816402	-2056.895967	0.935022	-2056.777347	
INT4-*cross*-2-AC	-1889.042731	0.79206	-1888.250671	0.904937	-1888.137794	
INT4-*homo*-2-AC	-2057.705122	0.817953	-2056.887169	0.935899	-2056.769223	
TS3-*cross*-AC	-1889.021096	0.791815	-1888.229281	0.90346	-1888.117636	-156.865
TS3-*homo*-AC	-2057.689438	0.816072	-2056.873366	0.933423	-2056.756015	-84.641
TS1'-AC	-1783.68323	0.647618	-1783.035612	0.748128	-1782.935102	-81.634
INT2'-1-AC	-1783.698131	0.649233	-1783.048898	0.750412	-1782.947719	
INT2'-AC	-1783.704869	0.649457	-1783.055412	0.750426	-1782.954443	
INT3'-AC	-1705.122935	0.592093	-1704.530842	0.690661	-1704.432274	
TS2'-*cross*-AC	-1822.97652	0.67449	-1822.30203	0.778099	-1822.198421	-193.455
TS2'-*homo*-AC	-1991.641265	0.697577	-1990.943688	0.807933	-1990.833332	-149.366
INT4'-*cross*-AC	-1822.994286	0.676219	-1822.318067	0.779844	-1822.214442	
INT4'-*homo*-AC	-1991.659687	0.699018	-1990.960669	0.809532	-1990.850155	
INT4'-*cross*-2-AC	-1822.991274	0.676254	-1822.31502	0.779626	-1822.211648	
INT4'-*homo*-2-AC	-1991.65532	0.698319	-1990.957001	0.809569	-1990.845751	
TS3'-*cross*-AC	-1822.975344	0.674714	-1822.30063	0.777818	-1822.197526	-152.852
TS3'-*homo*-AC	-1991.641411	0.69835	-1990.943061	0.807794	-1990.833617	-121.789
(Z)-*N*-methyl-2-butenamide	-325.7975671	0.102234	-325.6953331	0.144666	-325.6529011	
N,N'-Dimethyl-ethen-1,2-dicarboxamid	-494.4613585	0.12496	-494.3363985	0.174849	-494.2865095	
(Z)-2-butene	-157.1319831	0.080762	-157.0512211	0.114879	-157.0171041	
S21-*E*	-196.424489	0.107505	-196.316984	0.144717	-196.279772	
S21-*Z*	-196.422758	0.107487	-196.315271	0.144729	-196.278029	
S22-*E*	-235.715458	0.134067	-235.581391	0.174548	-235.54091	
S22-*Z*	-235.713605	0.134183	-235.579422	0.174563	-235.539042	
S23-*E*	-365.095935	0.130053	-364.965882	0.174649	-364.921286	
S23-*Z*	-365.0917	0.129873	-364.961827	0.174556	-364.917144	
S24-*E*	-404.386657	0.156721	-404.229936	0.204412	-404.182245	
S24-*Z*	-404.381303	0.157094	-404.224209	0.204532	-404.176771	
S25-*E*	-482.974531	0.210501	-482.76403	0.263149	-482.711382	
S25-*Z*	-482.969167	0.21161	-482.757557	0.263453	-482.705714	

5.5. Cartesian coordinates of computed structuresV. Cartesian Coordinates of Computed Structure

N-methylacrylamide

C	-2.517904	-0.043126	0.000097
H	-3.454615	-0.592425	0.000147
H	-2.558802	1.042565	0.000107
C	-1.335767	-0.660517	0.000007
H	-1.272177	-1.748439	-0.000026
C	-0.064791	0.130285	-0.000076
O	-0.044861	1.357833	-0.000051
N	1.073416	-0.634077	-0.000305
H	0.984267	-1.639803	0.000412
C	2.404950	-0.058672	0.000155
H	2.967278	-0.359298	0.892675

H	2.968517	-0.360944	-0.891002
H	2.291583	1.026397	-0.000868

Propene

C	-1.282937	-0.220582	0.000002
H	-1.303362	-1.309002	-0.000005
H	-2.245988	0.283216	-0.000011
C	-0.134056	0.456138	0.000004
H	-0.163130	1.546985	-0.000007
C	1.234870	-0.163109	-0.000001
H	1.182098	-1.257324	-0.000014
H	1.811568	0.150733	-0.880727
H	1.811557	0.150710	0.880740

Ethene

C	0.000000	0.665588	0.000000
H	0.923860	1.239753	0.000000
H	-0.923823	1.239796	-0.000000
C	-0.000000	-0.665588	-0.000000
H	-0.923860	-1.239753	0.000000
H	0.923823	-1.239796	-0.000000

INT1

Ru	-0.385355	0.792580	0.343963
O	1.506087	1.559478	-0.278968
O	0.167899	3.022861	0.689998
N	-1.636626	-1.622570	-0.593293
N	0.482044	-2.065546	-0.197060
C	-0.458679	-1.087363	-0.174227
C	-1.580459	-3.082368	-0.684200
H	-2.099520	-3.454052	-1.572192
H	-2.037804	-3.543459	0.202172
C	-0.057597	-3.330289	-0.730143
H	0.261160	-4.177274	-0.115978
H	0.298707	-3.492538	-1.755150
C	-2.832843	-0.808085	-0.371400
C	-3.485973	-1.160197	0.986923
H	-2.728753	-1.096490	1.773850
H	-3.856124	-2.194975	0.959884
C	-4.646659	-0.192479	1.278297
H	-5.099030	-0.449934	2.245062
C	-5.700283	-0.323619	0.160114
H	-6.105212	-1.345401	0.141650
H	-6.543200	0.353656	0.352611
C	-5.054033	0.019173	-1.198478
H	-5.801344	-0.075192	-1.996962
C	-3.890814	-0.963798	-1.482801
H	-3.432850	-0.749469	-2.457445
H	-4.274480	-1.994385	-1.518133
C	-4.532140	1.472663	-1.145558
H	-4.099436	1.756058	-2.114772
H	-5.370898	2.156927	-0.955222
C	-3.462521	1.608358	-0.030169
H	-3.083605	2.637120	-0.001709
C	-2.312999	0.650581	-0.369122
H	-1.986925	0.877192	-1.412822
C	-4.096532	1.247954	1.326426
H	-3.344237	1.335933	2.119194
H	-4.907765	1.951279	1.559068
C	1.894085	-1.804067	-0.165174

C	2.588441	-1.974780	1.046854
C	3.966644	-1.729263	1.057110
H	4.524926	-1.856730	1.980254
C	4.630381	-1.322194	-0.096983
C	3.922985	-1.152516	1.284534
H	4.448002	-0.828833	-2.178767
C	2.544892	-1.385135	-1.344389
C	1.884219	-2.418831	2.320425
H	0.809164	-2.423758	2.116818
C	1.807104	-1.199393	-2.666032
H	0.734223	-1.312345	-2.482618
C	-0.602293	0.428654	2.107347
H	-0.576765	-0.545366	2.608643
H	-0.705651	1.294798	2.778538
H	5.700866	-1.135258	-0.071001
C	2.295868	-3.851998	2.707512
H	3.369919	-3.908844	2.921607
H	1.756005	-4.181711	3.603427
H	2.081526	-4.560044	1.898081
C	2.129742	-1.437231	3.480200
H	1.532843	-1.724277	4.354416
H	3.182301	-1.430482	3.786633
H	1.851931	-0.418852	3.190916
C	2.227326	-2.279081	-3.683369
H	2.066260	-3.290488	-3.292059
H	1.656539	-2.175651	-4.614014
H	3.291764	-2.188266	-3.930226
C	2.007453	0.210801	-3.251227
H	3.052311	0.380589	-3.537661
H	1.395401	0.333442	-4.153373
H	1.728687	0.972745	-2.520018
C	1.284336	2.753013	0.171813
C	2.420168	3.769104	0.073378
C	1.961944	5.141115	0.585785
H	1.124204	5.523164	-0.006329
H	2.788723	5.858817	0.522221
H	1.630451	5.081192	1.626641
C	3.588656	3.231520	0.930982
H	4.444143	3.914805	0.866239
H	3.898870	2.241034	0.584824
H	3.296687	3.152065	1.984940
C	2.865678	3.861233	-1.401223
H	3.701606	4.564717	-1.495259
H	2.048671	4.220350	-2.038824
H	3.186940	2.883902	-1.772123

TS1

Ru	0.480811	0.317323	-0.643165
O	2.122507	1.650040	-1.320335
O	1.559528	1.854263	0.801482
N	-0.186842	-2.135336	0.722171
N	-2.114782	-1.151458	0.384623
C	-0.756068	-1.006634	0.215329
C	-1.151990	-3.182837	1.041648
H	-0.888765	-3.708900	1.963157
H	-1.211077	-3.919101	0.226837
C	-2.440026	-2.365366	1.163539
H	-3.316545	-2.869871	0.751885
H	-2.653481	-2.092329	2.205956
C	1.233483	-2.363628	0.463743

C	1.431620	-3.176197	-0.839336
H	0.888720	-2.689801	-1.655374
H	1.010501	-4.184532	-0.715231
C	2.931483	-3.267020	-1.171461
H	3.064362	-3.829659	-2.105344
C	3.653301	-3.996179	-0.019877
H	3.262768	-5.018919	0.081693
H	4.726288	-4.081064	-0.238983
C	3.448378	-3.212823	1.293764
H	3.954056	-3.734699	2.116862
C	1.935445	-3.123729	1.612015
H	1.770333	-2.590333	2.557217
H	1.523500	-4.137850	1.726756
C	4.046703	-1.799294	1.124230
H	3.950829	-1.230695	2.059012
H	5.121037	-1.880903	0.904035
C	3.313587	-1.053930	-0.020106
H	3.741460	-0.057139	-0.136835
C	1.831763	-0.945851	0.369575
H	1.777904	-0.513083	1.378810
C	3.495307	-1.839721	-1.332338
H	2.979063	-1.317475	-2.146974
H	4.560976	-1.888896	-1.596567
C	-3.067601	-0.080823	0.413930
C	-4.056945	-0.024405	-0.592245
C	-4.989595	1.018149	-0.544768
H	-5.756841	1.085760	-1.310338
C	-4.952729	1.967294	0.473993
C	-3.994698	1.872616	1.479714
H	-3.986941	2.604829	2.282011
C	-3.041878	0.845695	1.480976
C	-4.163913	-1.100266	-1.668203
H	-3.223769	-1.662411	-1.663130
C	-2.053880	0.744866	2.640984
H	-1.366304	-0.081810	2.445574
C	0.150404	-0.388469	-2.345708
H	-0.616479	-1.093010	-2.695714
C	-0.913658	2.114302	-0.925658
H	-1.620045	1.981745	-0.115335
C	-1.144246	1.344300	-2.081129
H	-2.023220	0.715786	-2.120722
H	0.829961	-0.070871	-3.149988
C	-4.369909	-0.540788	-3.087864
H	-4.356050	-1.359427	-3.816582
H	-5.335788	-0.032599	-3.187241
H	-3.588865	0.172863	-3.367341
C	-5.309716	-2.076689	-1.326550
H	-5.349884	-2.897700	-2.052316
H	-5.192769	-2.508031	-0.326864
H	-6.275420	-1.557324	-1.348176
C	-2.805273	0.426593	3.950184
H	-3.472264	1.249149	4.234314
H	-3.418142	-0.477630	3.855192
H	-2.093398	0.274604	4.769814
C	-1.186875	2.007931	2.800296
H	-0.545313	2.166752	1.931302
H	-1.802730	2.901352	2.959551
H	-0.530270	1.897958	3.671199
H	-5.681305	2.773532	0.491795
H	-0.790699	1.731074	-3.035516

C	-0.303896	3.492730	-1.012195
H	-1.098220	4.225924	-1.212632
H	0.174514	3.772246	-0.070352
H	0.436644	3.557789	-1.812723
C	3.406569	3.236571	0.003793
C	3.441374	4.167822	-1.222500
H	4.267384	4.883502	-1.128384
H	3.575838	3.593105	-2.142687
H	2.509953	4.738596	-1.310785
C	3.168375	4.050575	1.285271
H	3.131318	3.399791	2.162944
H	3.974778	4.781898	1.421044
H	2.218618	4.594749	1.235839
C	4.750244	2.481446	0.108478
H	4.938013	1.893119	-0.795732
H	5.573345	3.196073	0.232485
H	4.755971	1.804206	0.970223
C	2.294165	2.190523	-0.177375

INT2-1

Ru	-0.494493	-0.410849	-0.392762
O	-2.154144	-1.630092	-1.038576
O	-2.210766	-1.743466	1.179239
N	0.406400	2.211894	0.407658
N	2.260183	1.099105	0.082358
C	0.893308	0.976249	0.110399
C	1.413312	3.268807	0.338665
H	1.284752	4.003804	1.137571
H	1.360522	3.792788	-0.626385
C	2.703818	2.453971	0.472248
H	3.508156	2.801436	-0.180802
H	3.077786	2.442261	1.505090
C	-1.027981	2.420891	0.235784
C	-1.354594	2.849026	-1.220030
H	-0.920513	2.119765	-1.915089
H	-0.892082	3.823638	-1.432051
C	-2.880147	2.935464	-1.409888
H	-3.100510	3.235864	-2.442761
C	-3.445928	3.985843	-0.431848
H	-3.019527	4.974995	-0.651765
H	-4.533852	4.068954	-0.556616
C	-3.116599	3.574039	1.018543
H	-3.517888	4.321717	1.715038
C	-1.584105	3.490821	1.198732
H	-1.329858	3.219298	2.231661
H	-1.130805	4.471803	0.991769
C	-3.748496	2.197157	1.305151
H	-3.548341	1.894046	2.341451
H	-4.840158	2.259783	1.191862
C	-3.178626	1.136484	0.328016
H	-3.636705	0.174902	0.556300
C	-1.660959	1.051608	0.556249
H	-1.466175	0.808059	1.610931
C	-3.501949	1.554358	-1.119382
H	-3.113280	0.800403	-1.814122
H	-4.590531	1.597734	-1.262583
C	3.190967	0.023720	0.255948
C	4.015951	-0.345949	-0.826479
C	4.899375	-1.417141	-0.644179
H	5.540891	-1.727106	-1.463930

C	4.975239	-2.084310	0.576311	C	0.657288	-2.476631	-0.065331
C	4.191870	-1.667039	1.650055	C	0.087022	-1.698984	-1.308571
H	4.275784	-2.178127	2.604993	H	0.849059	-1.361530	-2.008612
C	3.295635	-0.599507	1.519738	H	-0.753570	-2.192338	-1.792274
C	4.022645	0.443154	-2.130981	H	0.078597	-3.392446	0.072733
H	3.147285	1.100478	-2.121541	H	1.712864	-2.687980	-0.255411
C	2.492441	-0.137053	2.734237	C	0.954714	0.892015	-0.271714
H	1.866267	0.708298	2.438253	N	0.518991	2.167039	-0.441112
C	0.246367	-0.506419	-2.227009	C	-0.914023	2.435772	-0.342612
H	1.034498	0.162238	-2.579133	C	-1.490617	1.285869	0.502480
C	0.663224	-2.055436	-0.088025	C	-3.018159	1.422045	0.596281
H	1.598362	-1.844299	0.418257	C	-3.676354	1.458868	-0.797771
C	0.811227	-1.874707	-1.642515	C	-3.097913	2.631761	-1.610105
H	1.885517	-1.887237	-1.839129	C	-1.575530	2.435229	-1.744617
H	-0.523171	-0.677932	-2.985913	H	-1.357551	1.480864	-2.241231
C	3.931063	-0.436161	-3.390017	H	-1.143043	3.239435	-2.356677
H	3.907095	0.195391	-4.285623	C	-3.381421	3.965285	-0.890373
H	4.795416	-1.103417	-3.483690	C	-2.733606	3.942446	0.509683
H	3.027086	-1.051518	-3.389475	C	-3.311882	2.762565	1.322657
C	5.283944	1.330599	-2.196110	H	-4.396640	2.892596	1.440364
H	5.267250	1.962461	-3.092091	H	-2.877360	2.751898	2.332157
H	5.365968	1.981127	-1.318265	C	-1.204152	3.782699	0.354434
H	6.189886	0.713729	-2.233521	H	-0.708050	3.797765	1.334075
C	3.440680	0.358996	3.844449	H	-0.801935	4.620812	-0.233698
H	4.060648	-0.456443	4.234767	H	-2.941516	4.886506	1.029941
H	4.115220	1.140604	3.475287	H	-4.465098	4.116386	-0.798165
H	2.864253	0.769501	4.681608	H	-2.986472	4.808938	-1.474618
C	1.536095	-1.220131	3.268434	H	-3.546849	2.647506	-2.611462
H	0.759720	-1.458129	2.537692	H	-3.505666	0.514304	-1.318888
H	2.072190	-2.142716	3.520541	H	-4.762794	1.583389	-0.685527
H	1.039197	-0.863147	4.178145	H	-3.420713	0.586843	1.177011
H	5.660509	-2.919168	0.696636	H	-1.069654	1.354728	1.530506
H	0.306701	-2.704784	-2.141473	C	1.479799	3.033737	-1.122180
C	0.106045	-3.390499	0.362267	C	2.779636	2.229441	-0.970485
H	0.895014	-4.154901	0.286056	N	2.288519	0.884242	-0.598915
H	-0.224584	-3.344112	1.402826	C	3.245051	-0.056340	-0.085846
H	-0.739233	-3.712340	-0.248123	C	3.623463	0.019540	1.275538
C	-3.974478	-2.878134	-0.068310	C	4.543705	-0.919772	1.755435
C	-3.611904	-4.182107	-0.809305	C	5.092896	-1.884545	0.914368
H	-4.508036	-4.798257	-0.954939	C	4.754624	-1.904041	-0.436028
H	-3.176169	-3.961798	-1.788601	C	3.836269	-0.987490	-0.964674
H	-2.888990	-4.773367	-0.234266	C	3.564191	-0.959587	-2.463395
C	-4.544501	-3.200435	1.319775	C	3.289964	-2.350628	-3.061779
H	-4.798833	-2.283999	1.861879	H	4.180128	-2.989084	-3.025742
H	-5.450769	-3.811742	1.224041	H	3.000025	-2.254877	-4.114250
H	-3.815441	-3.746785	1.925570	H	2.482798	-2.866781	-2.533927
C	-5.007577	-2.090246	-0.899698	H	2.675900	-0.340822	-2.625049
H	-4.598359	-1.830907	-1.880050	C	4.744798	-0.289060	-3.197315
H	-5.915665	-2.689456	-1.042535	H	4.943394	0.716019	-2.808835
H	-5.295966	-1.160474	-0.394900	H	5.661922	-0.877512	-3.073620
C	-2.695306	-2.028261	0.061648	H	4.536131	-0.207513	-4.270592
				H	5.216654	-2.635961	-1.091560
INT2				H	5.802139	-2.607979	1.307557
Ru	-0.478446	-0.470758	0.153708	H	4.839801	-0.890262	2.800194
C	0.625002	-1.670276	1.310403	C	3.125184	1.121954	2.210733
C	-0.014669	-2.395940	2.481770	C	2.458882	0.589181	3.492515
H	-1.028794	-2.723414	2.248879	H	1.565389	0.004258	3.263749
H	-0.054996	-1.740800	3.360800	H	3.140949	-0.041149	4.074278
H	0.592787	-3.271686	2.758073	H	2.158580	1.428142	4.131220
H	1.623222	-1.319985	1.557813	C	4.290093	2.068593	2.570450

H	5.053553	1.544795	3.157462
H	3.927749	2.913505	3.167742
H	4.780917	2.466228	1.674942
H	2.366334	1.709415	1.687699
H	3.420231	2.630335	-0.176128
H	3.367042	2.183827	-1.891353
H	1.531208	4.022252	-0.657105
H	1.201156	3.163673	-2.176278
O	-2.171287	-1.716957	0.542187
C	-3.067286	-1.980356	-0.357622
O	-3.026099	-1.611501	-1.540981
C	-4.262198	-2.814905	0.169507
C	-5.249869	-3.099391	-0.970244
H	-4.766971	-3.660578	-1.776192
H	-5.624744	-2.167067	-1.403041
H	-6.102154	-3.682738	-0.598517
C	-4.960390	-2.006404	1.282169
H	-4.262666	-1.787342	2.096151
H	-5.810969	-2.567962	1.689584
H	-5.341884	-1.054312	0.892381
C	-3.729147	-4.138719	0.751239
H	-3.028251	-3.950384	1.569714
H	-3.208258	-4.723114	-0.017783
H	-4.555955	-4.750333	1.134896

TS2

Ru	0.337267	-0.576449	-0.690959
O	1.753137	-1.341141	1.033538
O	1.906216	-2.127760	-1.020865
N	-0.242179	2.210864	-0.221568
N	-2.157976	1.172167	0.005124
C	-0.819287	0.978699	-0.224555
C	-1.129819	3.277895	0.238090
H	-1.051972	4.162771	-0.399286
H	-0.884258	3.575535	1.267117
C	-2.506600	2.600201	0.143716
H	-3.124969	2.758765	1.032427
H	-3.073101	2.936102	-0.733777
C	1.218800	2.282837	-0.166547
C	1.695357	2.253786	1.308200
H	1.303873	1.347674	1.785558
H	1.296269	3.124265	1.849089
C	3.235086	2.261603	1.365026
H	3.558184	2.264180	2.414684
C	3.775880	3.515699	0.651652
H	3.420888	4.426834	1.154842
H	4.873254	3.528325	0.698016
C	3.309958	3.507205	-0.818852
H	3.704508	4.391479	-1.336727
C	1.764872	3.553424	-0.850141
H	1.396301	3.596090	-1.883854
H	1.415619	4.462848	-0.337437
C	3.828447	2.225173	-1.511995
H	3.536118	2.226262	-2.571076
H	4.927689	2.214515	-1.481718
C	3.257385	0.968630	-0.798838
H	3.621927	0.064852	-1.300048
C	1.719415	1.038538	-0.924265
H	1.523219	1.234722	-1.988484
C	3.754518	0.994097	0.662519

H	3.404454	0.114249	1.200720
H	4.854508	0.985219	0.676799
C	-3.064660	0.180018	0.489492
C	-2.982131	-0.205081	1.846409
C	-3.861887	-1.195956	2.299476
H	-3.804111	-1.528465	3.332179
C	-4.809084	-1.760531	1.447746
C	-4.915180	-1.320795	0.129847
H	-5.682369	-1.741273	-0.513826
C	-4.053149	-0.337962	-0.371761
C	-2.000653	0.442102	2.821048
H	-1.464531	1.234533	2.292123
C	-4.245054	0.222952	-1.775935
H	-3.346455	0.797515	-2.023639
C	-0.836690	-2.310652	0.212485
H	-1.546834	-1.950049	0.942004
C	-0.449737	-0.625862	-2.395200
H	-1.416909	-0.172011	-2.658241
C	-1.208863	-2.401778	-1.125977
H	-2.207404	-2.100649	-1.421463
H	-0.050414	-2.953486	0.590523
C	-5.444019	1.194770	-1.785254
H	-5.556332	1.664019	-2.770015
H	-6.374712	0.662678	-1.554106
H	-5.322153	1.987242	-1.038766
C	-4.423916	-0.851394	-2.861580
H	-5.327600	-1.449680	-2.699581
H	-4.518237	-0.376608	-3.845059
H	-3.570281	-1.535001	-2.901093
C	-2.757576	1.106477	3.988263
H	-3.513479	1.812826	3.624882
H	-3.269145	0.363662	4.611170
H	-2.057670	1.652627	4.631297
C	-0.932586	-0.539983	3.339847
H	-0.308865	-0.046053	4.094580
H	-1.393810	-1.416931	3.810598
H	-0.273247	-0.879183	2.536939
H	-5.479632	-2.531701	1.817530
H	-0.689239	-3.089131	-1.787376
C	0.231088	-1.242826	-3.584562
H	-0.450175	-1.868436	-4.180544
H	0.552920	-0.417016	-4.240483
H	1.115362	-1.821323	-3.304584
C	2.314066	-2.103542	0.188500
C	3.478957	-3.016860	0.592419
C	3.081255	-4.468820	0.253284
H	2.849958	-4.567699	-0.811097
H	3.900970	-5.154130	0.501485
H	2.198212	-4.778627	0.826460
C	3.781782	-2.887558	2.092175
H	4.604916	-3.558942	2.366478
H	4.070216	-1.864478	2.351284
H	2.906018	-3.146767	2.695430
C	4.715658	-2.612644	-0.237873
H	5.023029	-1.585895	-0.009588
H	5.557278	-3.278073	-0.009214
H	4.498889	-2.675598	-1.308385

INT3

Ru	-0.502902	0.233337	-0.797113

C	0.341379	-0.158742	-2.357829
C	0.034474	0.542028	-3.654418
H	-0.778457	1.267283	-3.559737
H	-0.244370	-0.203625	-4.416639
H	0.926130	1.064266	-4.034979
H	1.153137	-0.893939	-2.430372
C	0.397461	-1.210926	0.158770
N	1.663529	-1.424756	0.601988
C	2.753310	-0.499998	0.490759
C	2.816309	0.588741	1.392428
C	3.909517	1.455516	1.287747
C	4.909578	1.249060	0.339137
C	4.828427	0.171799	-0.536371
C	3.746115	-0.715735	-0.485084
C	3.684484	-1.891422	-1.451942
C	4.685442	-2.989321	-1.038732
H	4.513174	-3.326743	-0.010767
H	5.713763	-2.612247	-1.093443
H	4.607628	-3.857919	-1.703738
C	3.926452	-1.469040	-2.912892
H	3.750446	-2.317558	-3.584469
H	3.259442	-0.652747	-3.207224
H	4.957698	-1.134097	-3.071846
H	2.675472	-2.314283	-1.401025
H	5.611635	0.019388	-1.273229
H	5.752589	1.932971	0.283135
H	3.985277	2.305030	1.957633
C	1.761957	0.796054	2.476921
C	2.078155	-0.065725	3.716613
H	2.120963	-1.132188	3.476845
H	3.045805	0.218449	4.147845
H	1.309581	0.074761	4.486431
C	1.588218	2.264694	2.893097
H	1.421709	2.895466	2.018029
H	2.453312	2.640499	3.453416
H	0.713612	2.356758	3.547432
H	0.800470	0.472172	2.071520
C	1.788793	-2.750110	1.241252
H	2.440183	-2.705605	2.116102
C	0.323050	-3.076696	1.571265
N	-0.363397	-2.277200	0.556732
C	-1.809786	-2.054425	0.453232
C	-2.631096	-3.353800	0.398554
C	-4.118679	-2.985519	0.171161
C	-4.623499	-2.128580	1.351074
C	-3.797638	-0.828602	1.435784
C	-2.317318	-1.195194	1.643533
H	-2.189860	-1.749347	2.584590
H	-1.707994	-0.283339	1.727260
C	-3.939462	-0.026468	0.125542
C	-3.442232	-0.875958	-1.062527
C	-1.969293	-1.284449	-0.884639
H	-1.715092	-1.990060	-1.682362
H	-3.553993	-0.305735	-1.992553
C	-4.282646	-2.177201	-1.136369
H	-3.962561	-2.780130	-1.996746
H	-5.345285	-1.938517	-1.286999
H	-4.990670	0.254003	-0.027658
H	-3.365918	0.907844	0.182670
H	-4.145747	-0.223459	2.283326

H	-5.686541	-1.890918	1.211174
H	-4.539630	-2.690333	2.292183
H	-4.707869	-3.909628	0.109321
H	-2.260366	-3.986647	-0.418193
H	-2.528976	-3.925553	1.333529
H	0.092403	-4.140634	1.476060
H	0.054031	-2.745620	2.586299
H	2.206028	-3.476504	0.531767
O	-0.154055	2.098086	0.241199
C	-0.996755	2.761172	-0.480072
O	-1.598904	2.179389	-1.422918
C	-1.236249	4.232909	-0.144484
C	0.103985	4.982227	-0.308170
H	-0.024407	6.039635	-0.047345
H	0.459501	4.928674	-1.344054
H	0.873931	4.553173	0.339381
C	-2.299125	4.829739	-1.077536
H	-1.987559	4.760626	-2.124161
H	-3.250911	4.298161	-0.980803
H	-2.462441	5.885707	-0.830583
C	-1.702080	4.316515	1.325256
H	-0.956218	3.881184	1.996060
H	-1.862151	5.363699	1.608608
H	-2.647971	3.779406	1.467612

TS3-*cross*
Ru	-0.358285	0.424118	-0.398666
O	-1.819454	0.677933	1.483214
O	-1.845149	2.101176	-0.200040
N	0.050865	-2.380053	-0.918618
N	2.018643	-1.606804	-0.328867
C	0.698584	-1.268846	-0.479962
C	0.870610	-3.591050	-0.887514
H	0.755051	-4.171984	-1.806244
H	0.590035	-4.231196	-0.039728
C	2.282965	-3.004375	-0.732890
H	2.879177	-3.514752	0.028755
H	2.840450	-3.020243	-1.676827
C	-1.412306	-2.382636	-0.883044
C	-1.905615	-2.874132	0.501923
H	-1.467140	-2.234130	1.276785
H	-1.564448	-3.904344	0.678375
C	-3.443576	-2.812166	0.566717
H	-3.779110	-3.184897	1.543629
C	-4.046174	-3.679415	-0.555545
H	-3.750919	-4.730869	-0.428100
H	-5.142835	-3.644319	-0.507074
C	-3.561616	-3.155063	-1.922999
H	-3.999380	-3.760427	-2.727484
C	-2.021612	-3.274029	-1.985068
H	-1.644074	-2.950148	-2.964170
H	-1.728903	-4.326328	-1.850124
C	-3.996415	-1.680191	-2.088103
H	-3.689374	-1.305519	-3.074131
H	-5.093257	-1.616100	-2.046756
C	-3.365558	-0.812298	-0.964409
H	-3.670367	0.231758	-1.095157
C	-1.834989	-0.921831	-1.114972
H	-1.619144	-0.699131	-2.173158
C	-3.880678	-1.346827	0.389302

H	-3.488657	-0.746507	1.210502
H	-4.978320	-1.280664	0.415919
C	2.944268	-0.951692	0.546557
C	2.770980	-1.099507	1.941482
C	3.666971	-0.431877	2.785654
H	3.542758	-0.508900	3.862253
C	4.716085	0.323643	2.266992
C	4.905992	0.404157	0.889285
H	5.741394	0.975482	0.496968
C	4.030979	-0.235115	0.002844
C	1.684115	-1.986800	2.546064
H	1.133654	-2.463548	1.731218
C	4.291423	-0.206851	-1.499114
H	3.364892	-0.515134	-1.995826
C	0.833414	1.579886	1.008443
H	1.409109	0.929260	1.652742
C	0.569563	1.024167	-1.940096
H	1.517085	0.606016	-2.301311
H	0.178192	2.269475	1.533350
C	5.379415	-1.243255	-1.853339
H	5.533859	-1.286384	-2.938068
H	6.333673	-0.972556	-1.385598
H	5.112715	-2.246761	-1.503469
C	4.682154	1.179249	-2.045449
H	5.656202	1.501668	-1.659270
H	4.770702	1.129430	-3.137150
H	3.952788	1.958829	-1.802593
C	2.317028	-3.116031	3.383685
H	3.045979	-3.688004	2.797376
H	2.836331	-2.720693	4.264162
H	1.542156	-3.806416	3.736958
C	0.649396	-1.198131	3.371231
H	-0.057707	-1.891685	3.842175
H	1.132025	-0.621660	4.169739
H	0.072010	-0.512812	2.745441
H	5.397595	0.838575	2.938799
C	-0.025505	1.998723	-2.918514
H	0.691042	2.778288	-3.211148
H	-0.267253	1.423240	-3.826487
H	-0.945179	2.460792	-2.551546
C	1.438599	2.011658	-0.205458
H	2.404885	1.584753	-0.432463
C	1.340427	3.422055	-0.729257
O	2.309147	3.911171	-1.316096
N	0.180852	4.091100	-0.504049
H	-0.642986	3.538194	-0.267433
C	-0.027401	5.407316	-1.080106
H	-0.861340	5.893133	-0.566120
H	0.877077	6.005676	-0.952930
H	-0.252325	5.355655	-2.154995
C	-2.294702	1.710239	0.938752
C	-3.410660	2.526301	1.601949
C	-3.673930	2.018948	3.027202
H	-4.475898	2.605492	3.491530
H	-3.971642	0.966456	3.021151
H	-2.776796	2.105183	3.648920
C	-2.980032	4.007442	1.632953
H	-2.825221	4.390216	0.619581
H	-3.754087	4.615139	2.116328
H	-2.047638	4.138929	2.195878

C	-4.683780	2.377472	0.740586
H	-5.020397	1.335324	0.713730
H	-5.494012	2.985796	1.160596
H	-4.497262	2.705409	-0.286783

TS3-*homo*

Ru	0.355749	-0.587501	-0.571758
O	1.825822	-1.142846	1.232311
O	1.922662	-2.163318	-0.721388
N	-0.213655	2.241506	-0.499407
N	-2.140137	1.259213	-0.144163
C	-0.799149	1.026326	-0.326876
C	-1.099794	3.372613	-0.230140
H	-1.009073	4.141237	-1.002384
H	-0.863059	3.832898	0.739184
C	-2.479340	2.694551	-0.230156
H	-3.102603	2.991109	0.618796
H	-3.037934	2.893772	-1.153028
C	1.246011	2.317839	-0.441490
C	1.707295	2.528763	1.023410
H	1.304391	1.714338	1.637144
H	1.307956	3.477574	1.410385
C	3.246410	2.538975	1.095113
H	3.558308	2.711937	2.133832
C	3.800481	3.658888	0.193083
H	3.445308	4.640820	0.538087
H	4.897362	3.675113	0.248246
C	3.349295	3.413952	-1.261628
H	3.753239	4.201360	-1.911663
C	1.805196	3.457544	-1.318476
H	1.448951	3.330003	-2.349554
H	1.452682	4.439049	-0.966291
C	3.866738	2.034964	-1.732560
H	3.581768	1.864477	-2.779911
H	4.965590	2.024245	-1.692087
C	3.285077	0.913200	-0.828947
H	3.648579	-0.059981	-1.175832
C	1.750458	0.964949	-0.969848
H	1.545472	0.956179	-2.054308
C	3.767132	1.172222	0.614437
H	3.406350	0.388375	1.280305
H	4.866823	1.162486	0.642273
C	-3.049023	0.372573	0.512673
C	-2.940879	0.208849	1.912297
C	-3.820037	-0.685027	2.535646
H	-3.741900	-0.849588	3.606708
C	-4.793711	-1.363283	1.805342
C	-4.926639	-1.135884	0.437227
H	-5.713830	-1.641123	-0.114777
C	-4.064267	-0.259774	-0.233296
C	-1.935584	0.993945	2.752984
H	-1.400780	1.683001	2.094301
C	-4.280359	0.067722	-1.706224
H	-3.381092	0.581285	-2.061955
C	-0.788032	-2.053293	0.545356
H	-1.480517	-1.582314	1.227977
C	-0.525603	-0.936531	-2.207090
H	-1.497577	-0.516440	-2.497027
C	-1.248928	-2.397771	-0.758159
H	-2.259473	-2.073191	-0.986395

H	-0.074861	-2.726285	1.015820
C	-5.468340	1.042007	-1.851529
H	-5.597856	1.343362	-2.897930
H	-6.399422	0.569348	-1.516260
H	-5.320548	1.945345	-1.249558
C	-4.493782	-1.167721	-2.597299
H	-5.403271	-1.715050	-2.324963
H	-4.598930	-0.859462	-3.643943
H	-3.651206	-1.863320	-2.536098
C	-2.667758	1.850234	3.805558
H	-3.422349	2.496367	3.341338
H	-3.176929	1.226091	4.548965
H	-1.952650	2.486124	4.340303
C	-0.867943	0.099011	3.411714
H	-0.229439	0.703961	4.066720
H	-1.329051	-0.683840	4.026287
H	-0.223184	-0.375076	2.667353
H	-5.464229	-2.055562	2.307622
C	0.179914	-1.606868	-3.355137
H	0.536836	-0.800831	-4.017344
H	1.051022	-2.182540	-3.032727
H	-0.481597	-2.243119	-3.959769
C	-0.822886	-3.714551	-1.374282
H	-1.319604	-4.531436	-0.833948
H	-1.102659	-3.798481	-2.428021
H	0.257932	-3.848444	-1.282254
C	3.520106	-2.880989	0.950548
C	4.751265	-2.565799	0.074869
H	5.066776	-1.524034	0.202946
H	5.591487	-3.211968	0.357749
H	4.524432	-2.728054	-0.983173
C	3.837593	-2.605262	2.427304
H	2.967418	-2.802477	3.061416
H	4.663292	-3.246889	2.759250
H	4.127450	-1.561421	2.580379
C	3.113789	-4.356860	0.759298
H	2.879147	-4.560729	-0.289418
H	3.930137	-5.019236	1.072445
H	2.230323	-4.602497	1.361993
C	2.355675	-2.003207	0.470905

INT4-*cross*

Ru	-0.397995	0.359910	-0.412648
O	-2.014479	0.753575	1.499936
O	-1.852977	2.042023	-0.291337
N	0.090814	-2.430709	-0.914072
N	2.041240	-1.608309	-0.331759
C	0.716888	-1.300453	-0.484829
C	0.940562	-3.621386	-0.888776
H	0.838056	-4.202983	-1.808838
H	0.679725	-4.270041	-0.041585
C	2.338347	-2.999395	-0.734966
H	2.946604	-3.494536	0.027075
H	2.895805	-3.002389	-1.678873
C	-1.367329	-2.468771	-0.839066
C	-1.824756	-3.039113	0.529150
H	-1.374371	-2.436310	1.326821
H	-1.468024	-4.072316	0.641209
C	-3.361907	-3.000187	0.629272
H	-3.669717	-3.426691	1.592850

C	-3.974856	-3.821149	-0.522687
H	-3.661880	-4.872633	-0.452267
H	-5.070497	-3.805598	-0.450927
C	-3.527708	-3.225905	-1.873942
H	-3.972221	-3.799859	-2.697186
C	-1.989156	-3.306187	-1.977309
H	-1.641735	-2.917882	-2.943876
H	-1.663922	-4.354529	-1.906653
C	-3.983089	-1.752776	-1.962731
H	-3.692535	-1.325615	-2.932317
H	-5.078914	-1.698517	-1.901867
C	-3.353038	-0.931661	-0.803554
H	-3.671834	0.111096	-0.883968
C	-1.831314	-1.013677	-0.960826
H	-1.567220	-0.641546	-1.982932
C	-3.825434	-1.535254	0.535217
H	-3.421031	-0.953406	1.365299
H	-4.922420	-1.486173	0.590477
C	2.952158	-0.930674	0.544469
C	2.769529	-1.070045	1.939008
C	3.645944	-0.379548	2.784785
H	3.512577	-0.448238	3.860771
C	4.684082	0.392578	2.268663
C	4.884019	0.465163	0.892133
H	5.710600	1.050304	0.501762
C	4.029730	-0.199071	0.003544
C	1.686795	-1.961406	2.543776
H	1.155971	-2.461468	1.729707
C	4.307520	-0.178881	-1.494954
H	3.393598	-0.507382	-2.001063
C	0.722361	1.450850	0.876431
H	1.447078	0.975719	1.528329
C	0.781871	1.180410	-1.782411
H	1.604776	0.597082	-2.200999
H	0.134955	2.197396	1.410269
C	5.418624	-1.197652	-1.827919
H	5.590184	-1.242673	-2.910019
H	6.360885	-0.908656	-1.347041
H	5.164136	-2.204335	-1.477706
C	4.680163	1.210496	-2.045773
H	5.654898	1.541484	-1.668613
H	4.758305	1.162141	-3.138204
H	3.947175	1.982592	-1.791645
C	2.319517	-3.066826	3.412547
H	3.063447	-3.641987	2.848526
H	2.820912	-2.649041	4.292956
H	1.546944	-3.758810	3.767927
C	0.630528	-1.168849	3.337422
H	1.094025	-0.583667	4.140776
H	0.068088	-0.488849	2.692553
H	-0.084733	-1.860337	3.799432
H	5.348925	0.927377	2.941602
C	0.130380	2.028689	-2.866389
H	0.828029	2.788223	-3.247487
H	-0.145262	1.378604	-3.706313
H	-0.773955	2.535251	-2.519849
C	1.351696	1.945605	-0.456239
H	2.398149	1.656933	-0.419358
C	1.331890	3.458944	-0.680160
O	2.357735	4.020965	-1.063660

N	0.158551	4.099844	-0.455909
H	-0.677517	3.530440	-0.327360
C	0.000948	5.501784	-0.797185
H	-0.850902	5.910718	-0.247252
H	0.908353	6.043126	-0.521088
H	-0.167178	5.646447	-1.873721
C	-2.380030	1.761963	0.853601
C	-3.490815	2.685956	1.378237
C	-3.703027	2.456470	2.882266
H	-4.515453	3.095041	3.250057
H	-3.955916	1.412646	3.086339
H	-2.795436	2.693582	3.448098
C	-3.111935	4.154728	1.110372
H	-2.997289	4.339921	0.038305
H	-3.891686	4.823037	1.494807
H	-2.168994	4.416134	1.606370
C	-4.781720	2.334865	0.605367
H	-5.076608	1.295082	0.787654
H	-5.604235	2.983345	0.931063
H	-4.640020	2.470608	-0.472101

INT4-*homo*

Ru	0.403892	-0.562873	-0.525656
O	2.045562	-1.108261	1.318132
O	1.955574	-2.116991	-0.650519
N	-0.278077	2.234592	-0.658599
N	-2.170941	1.215643	-0.228436
C	-0.826816	1.013960	-0.398374
C	-1.205021	3.352551	-0.486352
H	-1.142199	4.054500	-1.322533
H	-0.987852	3.902875	0.439051
C	-2.559581	2.627522	-0.423426
H	-3.188196	2.967023	0.405136
H	-3.129383	2.735252	-1.354162
C	1.171793	2.360984	-0.546756
C	1.570125	2.769565	0.896032
H	1.152887	2.033679	1.594006
H	1.139358	3.751009	1.138381
C	3.104459	2.822746	1.025459
H	3.368200	3.135374	2.044309
C	3.673423	3.831879	0.008210
H	3.286504	4.840750	0.211481
H	4.766436	3.880934	0.102167
C	3.287475	3.396086	-1.420602
H	3.701944	4.104945	-2.149130
C	1.748659	3.385556	-1.547275
H	1.442155	3.109513	-2.564963
H	1.349482	4.390134	-1.343435
C	3.844749	1.982382	-1.695792
H	3.596916	1.671800	-2.720110
H	4.940882	1.993801	-1.618791
C	3.259179	0.971673	-0.670893
H	3.651560	-0.026730	-0.882735
C	1.737057	0.970630	-0.850963
H	1.510762	0.716831	-1.918502
C	3.670401	1.419131	0.746905
H	3.296188	0.702450	1.479765
H	4.767313	1.436719	0.819640
C	-3.048664	0.352426	0.501410
C	-2.907615	0.279765	1.905634

C	-3.752042	-0.592867	2.602357
H	-3.647525	-0.688523	3.679470
C	-4.724157	-1.337066	1.937358
C	-4.891694	-1.197342	0.561389
H	-5.677644	-1.753567	0.059099
C	-4.064530	-0.346004	-0.181553
C	-1.907906	1.139587	2.676377
H	-1.397348	1.794422	1.965463
C	-4.320110	-0.120230	-1.666978
H	-3.442133	0.389023	-2.077501
C	-0.642500	-1.882145	0.591745
H	-1.428658	-1.552446	1.261626
C	-0.711579	-1.316924	-1.993838
H	-1.583603	-0.749976	-2.330351
C	-1.164029	-2.330647	-0.812010
H	-2.248124	-2.204667	-0.763294
H	0.008065	-2.618281	1.066865
C	-5.535668	0.813243	-1.847772
H	-5.695897	1.040765	-2.908475
H	-6.446633	0.341284	-1.460383
H	-5.399051	1.758261	-1.310317
C	-4.519394	-1.417652	-2.468708
H	-5.415000	-1.961403	-2.147222
H	-4.643777	-1.183446	-3.532249
H	-3.661673	-2.089132	-2.369449
C	-2.644631	2.050280	3.679221
H	-3.417950	2.649011	3.183258
H	-3.131895	1.467189	4.469097
H	-1.936311	2.734397	4.161026
C	-0.813432	0.313634	3.379159
H	-0.173267	0.976058	3.974540
H	-1.249845	-0.427245	4.059990
H	-0.177009	-0.207340	2.659524
H	-5.367009	-2.012074	2.496128
C	0.035285	-1.905433	-3.182950
H	-0.595898	-2.597981	-3.759847
H	0.326793	-1.094207	-3.862861
H	0.942161	-2.435967	-2.881668
C	-0.800828	-3.793302	-1.094958
H	-1.195914	-4.127099	-2.061010
H	0.284365	-3.923502	-1.095591
H	-1.223665	-4.437008	-0.315151
C	3.620686	-2.924392	0.902566
C	4.726480	-2.823337	-0.167182
H	5.153967	-1.813430	-0.194726
H	5.538561	-3.525774	0.058192
H	4.327299	-3.052287	-1.159325
C	4.182393	-2.554191	2.282353
H	3.405922	-2.610070	3.051030
H	4.995944	-3.238222	2.554561
H	4.573919	-1.531688	2.284111
C	3.052112	-4.358954	0.924567
H	2.646868	-4.629763	-0.055123
H	3.838597	-5.076685	1.189056
H	2.247958	-4.450525	1.665197
C	2.473461	-1.976808	0.516297

INT4-*cross*-2

Ru	0.498044	0.146672	-0.167850
O	2.172791	1.551013	-0.329389

O	2.068946	0.915480	1.790432	
N	-0.366952	-2.590245	-0.290058	
N	-2.237467	-1.451443	-0.189112	
C	-0.869710	-1.337670	-0.142895	
C	-1.366041	-3.576964	-0.692651	
H	-1.219349	-4.532944	-0.183076	
H	-1.322408	-3.751321	-1.776995	
C	-2.661034	-2.867548	-0.280180	
H	-3.468478	-2.984080	-1.005585	
H	-3.022357	-3.210202	0.698569	
C	1.073285	-2.718053	-0.493913	
C	1.428956	-2.644966	-2.002304	
H	0.990885	-1.737147	-2.433468	
H	0.988405	-3.504880	-2.526817	
C	2.958717	-2.643700	-2.177956	
H	3.200813	-2.585363	-3.247216	
C	3.529976	-3.948834	-1.586459	
H	3.125914	-4.816523	-2.126950	
H	4.621028	-3.972447	-1.709031	
C	3.170713	-4.038924	-0.088406	
H	3.573810	-4.968920	0.332942	
C	1.633521	-4.038256	0.077244	
H	1.358192	-4.123873	1.136574	
H	1.202489	-4.902832	-0.449120	
C	3.776554	-2.825397	0.645764	
H	3.557749	-2.881716	1.720423	
H	4.870449	-2.835993	0.537554	
C	3.200269	-1.510148	0.060530	
H	3.637245	-0.668466	0.596640	
C	1.680238	-1.526517	0.277719	
H	1.469515	-1.657922	1.348817	
C	3.549177	-1.425592	-1.438063	
H	3.153333	-0.491822	-1.855499	
H	4.640117	-1.404047	-1.567597	
C	-3.154855	-0.537581	0.436426	
C	-4.040131	0.212476	-0.367802	
C	-4.909312	1.105676	0.270450	
H	-5.587890	1.707573	-0.325263	
C	-4.911080	1.241227	1.656251	
C	-4.057242	0.463919	2.434547	
H	-4.073428	0.569098	3.515623	
C	-3.171417	-0.447134	1.847385	
C	-4.100078	0.036235	-1.881506	
H	-3.164918	-0.442221	-2.191609	
C	-2.268752	-1.292833	2.744281	
H	-1.679172	-1.966767	2.118315	
C	-0.222963	0.731790	-1.909863	
H	-0.959758	0.161408	-2.479407	
C	-0.713587	1.599692	0.590332	
H	-1.625092	1.208232	1.027954	
H	0.529431	1.185635	-2.561570	
C	-4.241473	1.359237	-2.660284	
H	-4.140169	1.163761	-3.734123	
H	-5.230150	1.807961	-2.508162	
H	-3.492892	2.106710	-2.379030	
C	-5.262219	-0.909531	-2.254340	
H	-5.277680	-1.095437	-3.334823	
H	-5.187558	-1.874338	-1.741300	
H	-6.223401	-0.462236	-1.973705	
C	-3.110044	-2.171400	3.691271	

H	-3.682581	-1.563515	4.401136	
H	-3.823324	-2.790586	3.134410	
H	-2.458863	-2.835048	4.272026	
C	-1.258797	-0.437601	3.533913	
H	-0.563104	0.076467	2.865932	
H	-1.766502	0.312326	4.151960	
H	-0.667760	-1.076428	4.200897	
H	-5.585220	1.949104	2.130910	
C	-0.228651	2.766232	1.427662	
H	-1.029978	3.517491	1.486792	
H	-0.005722	2.420891	2.440331	
H	0.658604	3.258004	1.032485	
C	-0.943125	1.808167	-0.962059	
H	-2.005937	1.624187	-1.088038	
C	-0.689310	3.241443	-1.438730	
O	-1.651030	3.955163	-1.721428	
N	0.606112	3.626881	-1.540730	
H	1.326487	2.995804	-1.187229	
C	0.971235	4.984139	-1.900423	
H	1.127202	5.613060	-1.013143	
H	1.894207	4.976035	-2.488200	
H	0.163767	5.417474	-2.493348	
C	2.604853	1.593785	0.889600	
C	3.822390	2.492924	1.172671	
C	3.971172	2.715928	2.684790	
H	4.069743	1.762926	3.211152	
H	4.857458	3.328353	2.891427	
H	3.094093	3.229460	3.093489	
C	5.073690	1.777543	0.616705	
H	4.952905	1.550454	-0.447617	
H	5.957246	2.416190	0.738450	
H	5.261930	0.839419	1.150960	
C	3.650446	3.843508	0.450826	
H	2.744996	4.363488	0.785966	
H	4.506738	4.494919	0.663017	
H	3.585280	3.705847	-0.632238	

INT4-*homo*-2

Ru	-0.503614	-0.369980	-0.323111	
O	-2.161462	-1.647028	-0.879669	
O	-2.167077	-1.569623	1.337426	
N	0.370730	2.314305	0.273376	
N	2.236128	1.194618	0.055181	
C	0.869170	1.061725	0.083923	
C	1.368924	3.370409	0.121896	
H	1.227519	4.169867	0.853956	
H	1.320002	3.809330	-0.884926	
C	2.664258	2.581508	0.334848	
H	3.472325	2.880760	-0.337056	
H	3.027703	2.658882	1.368720	
C	-1.064306	2.497042	0.080293	
C	-1.390760	2.804393	-1.405819	
H	-0.948352	2.026545	-2.039960	
H	-0.936690	3.763416	-1.693705	
C	-2.916695	2.861342	-1.604392	
H	-3.137474	3.075217	-2.658491	
C	-3.494108	3.982049	-0.715277	
H	-3.075989	4.954049	-1.013556	
H	-4.582461	4.045013	-0.848044	

C	-3.164535	3.691519	0.764129
H	-3.574014	4.489299	1.397431
C	-1.631869	3.636522	0.952870
H	-1.377586	3.451539	2.004749
H	-1.186609	4.601568	0.668144
C	-3.785145	2.336699	1.159865
H	-3.585072	2.120211	2.217701
H	-4.877051	2.380169	1.039820
C	-3.203073	1.205778	0.272713
H	-3.654247	0.261885	0.576665
C	-1.685417	1.153492	0.511232
H	-1.492932	1.001123	1.582782
C	-3.526900	1.502587	-1.204149
H	-3.130633	0.698664	-1.835559
H	-4.615599	1.525052	-1.351610
C	3.176307	0.149950	0.334405
C	4.029378	-0.294235	-0.697409
C	4.921846	-1.334516	-0.410463
H	5.584350	-1.701189	-1.189086
C	4.978557	-1.900436	0.861149
C	4.167807	-1.408050	1.881452
H	4.237378	-1.839100	2.876202
C	3.263082	-0.365739	1.647059
C	4.053056	0.385151	-2.062339
H	3.168886	1.027617	-2.124386
C	2.432516	0.186214	2.804335
H	1.812681	1.005093	2.430815
C	0.262865	-0.564684	-2.133140
H	1.037500	0.095787	-2.530094
C	0.680940	-1.976765	0.089412
H	1.603715	-1.707850	0.591168
C	0.876696	-1.894216	-1.478145
H	1.957128	-1.771821	-1.583289
H	-0.495115	-0.805465	-2.886676
C	3.999921	-0.594815	-3.247393
H	3.988138	-0.037921	-4.191463
H	4.874255	-1.255276	-3.268287
H	3.103971	-1.221081	-3.216155
C	5.303946	1.282558	-2.175175
H	5.297352	1.839529	-3.119657
H	5.360404	2.003064	-1.351667
H	6.218160	0.677593	-2.145207
C	3.354281	0.768986	3.894494
H	3.964819	-0.011798	4.362659
H	4.037175	1.520785	3.481361
H	2.757756	1.242566	4.682861
C	1.465005	-0.855442	3.397122
H	0.703288	-1.145936	2.670061
H	1.995694	-1.756750	3.726082
H	0.950175	-0.433622	4.268346
H	5.670565	-2.713834	1.062630
C	0.141230	-3.265553	0.674509
H	0.929159	-4.034424	0.650692
H	-0.149393	-3.111708	1.716457
H	-0.725027	-3.653035	0.140179
C	0.386709	-3.129512	-2.240905
H	-0.701750	-3.207833	-2.175727
H	0.663627	-3.046257	-3.298183
H	0.830596	-4.048931	-1.843495
C	-3.943475	-2.830298	0.234889

C	-3.576315	-4.190546	-0.394663
H	-4.465995	-4.828594	-0.465961
H	-3.164463	-4.053909	-1.399365
H	-2.833419	-4.719289	0.214611
C	-4.480179	-3.034388	1.658155
H	-4.736367	-2.076213	2.121497
H	-5.379455	-3.662811	1.636932
H	-3.731245	-3.515373	2.294351
C	-5.004733	-2.134233	-0.641792
H	-5.905620	-2.756701	-0.711760
H	-5.297902	-1.167215	-0.216145
H	-4.618750	-1.957944	-1.649653
C	-2.674951	-1.956635	0.260182

TS4-*cross*

Ru	0.515593	0.277210	-0.119294
O	2.301534	1.597838	-0.061494
O	1.729135	0.795698	1.913278
N	-0.341949	-2.440775	-0.517034
N	-2.216593	-1.319901	-0.339113
C	-0.851987	-1.213716	-0.230172
C	-1.326218	-3.386790	-1.038443
H	-1.211709	-4.375936	-0.585810
H	-1.217092	-3.492847	-2.125876
C	-2.644784	-2.700924	-0.660587
H	-3.374667	-2.695773	-1.472999
H	-3.114533	-3.160561	0.218003
C	1.101955	-2.582445	-0.700852
C	1.485988	-2.483856	-2.198421
H	1.061425	-1.568781	-2.623702
H	1.057576	-3.333573	-2.748693
C	3.018501	-2.483787	-2.342483
H	3.282405	-2.394113	-3.404600
C	3.569356	-3.810789	-1.781411
H	3.170259	-4.657692	-2.357558
H	4.662698	-3.839556	-1.881722
C	3.177198	-3.943138	-0.294899
H	3.560362	-4.891003	0.105068
C	1.635404	-3.929806	-0.160745
H	1.338039	-4.044329	0.889803
H	1.208820	-4.775528	-0.720476
C	3.788770	-2.760560	0.485427
H	3.554851	-2.848079	1.554900
H	4.883897	-2.785361	0.390768
C	3.231380	-1.423685	-0.065435
H	3.675591	-0.598199	0.496353
C	1.707733	-1.434013	0.129298
H	1.500611	-1.655904	1.187786
C	3.600471	-1.291163	-1.554386
H	3.206830	-0.344902	-1.944087
H	4.692881	-1.266901	-1.671606
C	-3.154065	-0.517568	0.394350
C	-4.018583	0.351618	-0.305972
C	-4.927455	1.110607	0.441991
H	-5.595104	1.798445	-0.067220
C	-5.000275	0.985427	1.827729
C	-4.178497	0.078475	2.492274
H	-4.252643	-0.019962	3.571401
C	-3.245651	-0.697383	1.793143
C	-4.056267	0.385225	-1.831527

H	-3.119464	-0.053117	-2.192815
C	-2.379082	-1.699258	2.555885
H	-1.827706	-2.308284	1.835991
C	0.116528	0.601177	-1.921637
H	-0.759079	0.280204	-2.500361
C	-0.420002	2.205124	0.620974
H	0.448793	2.825749	0.822125
H	0.834485	1.164682	-2.530667
C	-4.190431	1.790700	-2.446489
H	-4.214456	1.705625	-3.539125
H	-5.125023	2.276212	-2.142318
H	-3.359525	2.455772	-2.195802
C	-5.219752	-0.504304	-2.325456
H	-5.211813	-0.578244	-3.419312
H	-5.167758	-1.516884	-1.911319
H	-6.182549	-0.075755	-2.021807
C	-3.245746	-2.663842	3.388528
H	-3.766468	-2.144591	4.200981
H	-4.004184	-3.156740	2.768896
H	-2.616852	-3.438083	3.843056
C	-1.317987	-1.007602	3.432307
H	-0.597037	-0.459947	2.820100
H	-1.780152	-0.306417	4.137429
H	-0.765489	-1.755841	4.013378
H	-5.709118	1.587939	2.389475
C	-1.365681	2.150944	1.789765
H	-2.270479	1.593351	1.571705
H	-0.874400	1.721177	2.665458
H	-1.656631	3.180343	2.047745
C	-0.851414	2.194331	-0.725356
H	-1.873412	1.893774	-0.917085
C	-0.374163	3.248970	-1.702902
O	-1.184647	3.744047	-2.486056
N	0.925694	3.639617	-1.609572
H	1.568484	3.059686	-1.070579
C	1.476655	4.612168	-2.536088
H	2.349288	5.089643	-2.081345
H	1.780630	4.151679	-3.486883
H	0.719751	5.368712	-2.752343
C	2.502877	1.494200	1.204712
C	3.654919	2.291385	1.827047
C	3.170862	3.757092	1.920835
H	2.283437	3.836666	2.560100
H	3.957079	4.388763	2.351218
H	2.917048	4.151356	0.930548
C	3.981321	1.753932	3.228148
H	4.306101	0.708822	3.179706
H	4.787578	2.344863	3.679405
H	3.104779	1.797957	3.880067
C	4.894977	2.212613	0.917587
H	4.666632	2.573915	-0.088628
H	5.706932	2.820185	1.335145
H	5.254632	1.180748	0.830826

TS4-*homo*

Ru	-0.500899	-0.447340	-0.550968
O	-2.206874	-1.799912	-0.960108
O	-1.565784	-1.734324	1.151857
N	0.165243	2.269104	0.101799
N	2.117540	1.277580	-0.032068

C	0.755947	1.055722	-0.061145
C	1.087517	3.397331	0.025054
H	0.870405	4.149127	0.789207
H	1.023398	3.880473	-0.959624
C	2.436230	2.700618	0.235217
H	3.213750	3.056467	-0.443977
H	2.801743	2.814825	1.263653
C	-1.286079	2.377894	-0.037693
C	-1.679121	2.817736	-1.469262
H	-1.203870	2.153257	-2.197275
H	-1.309312	3.836020	-1.658254
C	-3.210131	2.773776	-1.622034
H	-3.481201	3.066770	-2.645189
C	-3.838956	3.760013	-0.616701
H	-3.501927	4.784078	-0.832385
H	-4.933058	3.753642	-0.713443
C	-3.438960	3.356790	0.818018
H	-3.876463	4.063390	1.535573
C	-1.897619	3.393957	0.955714
H	-1.594572	3.131251	1.977726
H	-1.535265	4.413156	0.753451
C	-3.965779	1.933155	1.097041
H	-3.727257	1.633397	2.126360
H	-5.061334	1.922993	1.002815
C	-3.328635	0.933771	0.099191
H	-3.715068	-0.067722	0.305048
C	-1.806416	0.967551	0.307806
H	-1.606867	0.805813	1.377820
C	-3.703489	1.338909	-1.338434
H	-3.252849	0.631518	-2.044255
H	-4.793309	1.289146	-1.471986
C	3.068433	0.324216	0.467866
C	4.067970	-0.172222	-0.396500
C	5.005222	-1.071291	0.126766
H	5.779380	-1.475057	-0.518451
C	4.963751	-1.453232	1.465832
C	3.993165	-0.923672	2.311569
H	3.973375	-1.222186	3.355748
C	3.034933	-0.018375	1.839097
C	4.177925	0.298327	-1.842535
H	3.205499	0.717470	-2.123723
C	2.016908	0.564442	2.818690
H	1.419384	1.318721	2.302877
C	-0.132654	-0.054921	-2.341471
H	0.684307	0.538638	-2.776892
C	0.570379	-2.424185	-0.627468
H	-0.255299	-3.127661	-0.729407
C	1.010786	-1.868770	-1.852701
H	1.991272	-1.403109	-1.839122
H	-0.829388	-0.432235	-3.101423
C	4.520014	-0.827105	-2.836561
H	4.444105	-0.453073	-3.863939
H	5.545109	-1.189854	-2.698875
H	3.848834	-1.685450	-2.736459
C	5.232361	1.420021	-1.957823
H	5.274030	1.809982	-2.981935
H	5.016614	2.253845	-1.282543
H	6.226994	1.036921	-1.699309
C	2.724495	1.273956	3.990252
H	3.280676	0.566722	4.616050

H	3.434031	2.029783	3.632739
H	1.986654	1.771318	4.630455
C	1.022626	-0.495353	3.329329
H	0.399092	-0.878828	2.518450
H	1.544309	-1.338069	3.798936
H	0.357548	-0.051886	4.080308
H	5.694491	-2.159056	1.851737
C	1.498201	-2.769320	0.508532
H	0.978625	-2.719908	1.467794
H	1.843519	-3.806474	0.375557
H	2.376249	-2.130917	0.540035
C	0.625752	-2.551623	-3.156705
H	-0.433515	-2.826261	-3.152995
H	0.829395	-1.935676	-4.037977
H	1.214110	-3.475331	-3.250756
C	-3.477953	-3.137277	0.632078
C	-4.104054	-2.709647	1.972165
H	-3.342803	-2.648600	2.754111
H	-4.578901	-1.724982	1.886791
H	-4.871694	-3.431140	2.278062
C	-4.548916	-3.183391	-0.468291
H	-5.007627	-2.198464	-0.609526
H	-4.116759	-3.486323	-1.425890
H	-5.337939	-3.895446	-0.196232
C	-2.815620	-4.524764	0.787303
H	-3.564839	-5.274436	1.070107
H	-2.354095	-4.845366	-0.154766
H	-2.040601	-4.499088	1.560621
C	-2.359858	-2.155712	0.256984

INT1'

Ru	-0.426987	1.057751	0.447116
O	1.146322	2.460593	0.022000
O	-0.628526	3.230209	1.021614
N	-0.982422	-1.488826	-0.777283
N	1.175454	-1.410190	-0.369463
C	0.015959	-0.717744	-0.271672
C	-0.547872	-2.864159	-1.031356
H	-0.951275	-3.248888	-1.972000
H	-0.872056	-3.527821	-0.218083
C	0.985727	-2.702247	-1.055994
H	1.514940	-3.501122	-0.529345
H	1.374812	-2.644235	-2.080125
C	-2.351832	-1.050738	-0.502576
C	-2.885027	-1.713589	0.790736
H	-2.171083	-1.541714	-1.602036
H	-2.965532	-2.799368	0.640625
C	-4.261643	-1.127699	1.152260
H	-4.626992	-1.602875	2.071973
C	-5.243629	-1.407149	-0.003293
H	-5.361400	-2.490822	-0.144098
H	-6.236179	-1.003806	0.237667
C	-4.714468	-0.754853	-1.297612
H	-5.410550	-0.953380	-2.122566
C	-3.331790	-1.355439	-1.654206
H	-2.949178	-0.919577	-2.586448
H	-3.425744	-2.440094	-1.811436
C	-4.598275	0.769364	-1.072824
H	-4.258080	1.264394	-1.992512
H	-5.587925	1.182059	-0.832764

C	-3.602663	1.057795	0.081548
H	-3.512118	2.140401	0.231039
C	-2.241453	0.481624	-0.327336
H	-1.983689	0.904991	-1.328622
C	-4.115818	0.392090	1.372340
H	-3.414535	0.587164	2.192449
H	-5.084621	0.824896	1.655850
C	2.478565	-0.822612	-0.234414
C	3.178679	-0.999724	0.973881
C	4.461280	-0.448798	1.077259
H	5.023150	-0.572710	1.998631
C	5.024851	0.257683	0.018296
C	4.312456	0.425820	-1.166347
H	4.758816	0.983314	-1.984594
C	3.027960	-0.107337	-1.319176
C	2.584218	-1.772667	2.142266
H	1.544842	-2.004958	1.889984
C	2.287933	0.073601	-2.640191
H	1.268208	-0.305817	-2.520262
C	-0.530883	0.438011	2.148824
H	-0.233586	-0.547743	2.522709
H	-0.879436	1.138941	2.922187
H	6.020616	0.681612	0.117114
C	3.324076	-3.107308	2.354621
H	4.376187	-2.937139	2.612334
H	2.865713	-3.678791	3.170678
H	3.300886	-3.724457	1.448521
C	2.569910	-0.934792	3.433394
H	2.050168	-1.476459	4.232968
H	3.585506	-0.720466	3.785575
H	2.058866	0.019778	3.272750
C	2.964867	-0.742562	-3.759859
H	3.039529	-1.805054	-3.500170
H	2.400095	-0.656076	-4.695772
H	3.981910	-0.377952	-3.946058
C	2.166384	1.554659	-3.044687
H	3.147241	1.991160	-3.265936
H	1.553861	1.646208	-3.949996
H	1.710594	2.143827	-2.245048
N	0.527060	3.498098	0.540934
O	1.025925	4.598021	0.544518

TS1'

Ru	0.570893	0.821147	-0.615844
O	1.772924	2.536465	-1.264404
O	1.210373	2.563064	0.832058
N	0.638935	-1.761782	0.658741
N	-1.491356	-1.356846	0.349907
C	-0.233543	-0.827458	0.197407
C	0.015568	-3.052250	0.939939
H	0.421024	-3.508347	1.846809
H	0.170439	-3.747779	0.102567
C	-1.454083	-2.643453	1.078358
H	-2.148817	-3.361254	0.637687
H	-1.737161	-2.483507	2.127452
C	2.067158	-1.553719	0.420731
C	2.512615	-2.217115	-0.904792
H	1.860062	-1.880877	-1.716543
H	2.408213	-3.309000	-0.826368
C	3.976405	-1.844106	-1.202708

H	4.281350	-2.302622	-2.152792
C	4.867414	-2.374810	-0.061247
H	4.796436	-3.470539	-0.006191
H	5.919705	-2.129320	-0.257354
C	4.423045	-1.741809	1.273831
H	5.049819	-2.123959	2.090080
C	2.948234	-2.117443	1.558570
H	2.620486	-1.695556	2.517617
H	2.852996	-3.211557	1.627136
C	4.577070	-0.208931	1.171238
H	4.304203	0.266663	2.122489
H	5.629400	0.041171	0.975827
C	3.674047	0.336332	0.034748
H	3.796416	1.421722	-0.030106
C	2.220935	-0.020432	0.387546
H	2.024166	0.335632	1.409779
C	4.096460	-0.308098	-1.299674
H	3.461903	0.071678	-2.109649
H	5.132243	-0.031162	-1.538660
C	-2.707154	-0.599086	0.403249
C	-3.672861	-0.794191	-0.608217
C	-4.860289	-0.056396	-0.538551
H	-5.616629	-0.184961	-1.307115
C	-5.089913	0.835691	0.506270
C	-4.142942	0.985079	1.516025
H	-4.340695	1.666570	2.338343
C	-2.940294	0.267015	1.495562
C	-3.474993	-1.827355	-1.712773
H	-2.416777	-2.110504	-1.710947
C	-1.962412	0.411916	2.659628
H	-1.066210	-0.173863	2.439990
C	0.432212	0.080047	-2.328127
H	-0.127341	-0.798153	-2.677128
C	-1.263352	2.191986	-0.847413
H	-1.903458	1.846231	-0.044173
C	-1.291749	1.434271	-2.029135
H	-1.969804	0.594503	-2.094830
H	0.988735	0.572618	-3.138692
N	1.863703	3.124490	-0.118551
O	2.521125	4.137523	0.038026
C	-3.818566	-1.306022	-3.120148
H	-3.586027	-2.072411	-3.868363
H	-4.884207	-1.069418	-3.216271
H	-3.253693	-0.404210	-3.375530
C	-4.310534	-3.089553	-1.409749
H	-4.119121	-3.870164	-2.155550
H	-4.085424	-3.498586	-0.419123
H	-5.381637	-2.855264	-1.431427
C	-2.586458	-0.158040	3.950168
H	-3.463828	0.424038	4.255805
H	-2.909538	-1.197322	3.817758
H	-1.860375	-0.125727	4.770699
C	-1.497113	1.864236	2.874979
H	-0.814736	1.912444	3.731198
H	-0.956471	2.247209	2.006859
H	-2.341463	2.531194	3.085596
H	-6.015266	1.404426	0.541205
H	-1.041355	1.925099	-2.967877
C	-1.009227	3.681251	-0.866865
H	-1.956969	4.202710	-1.060840

H	-0.630818	4.034284	0.095499
H	-0.297505	3.964608	-1.646912

INT2'-1

Ru	0.619307	0.845551	-0.490721
O	1.861489	2.458482	-1.227508
O	1.739126	2.624231	0.940157
N	0.540591	-1.837577	0.550609
N	-1.562761	-1.342676	0.213929
C	-0.292349	-0.832004	0.171369
C	-0.116203	-3.141383	0.622590
H	0.235293	-3.724597	1.477581
H	0.070605	-3.720087	-0.293106
C	-1.585886	-2.723464	0.741622
H	-2.265497	-3.349298	0.158415
H	-1.929375	-2.717823	1.784881
C	1.971673	-1.636187	0.338062
C	2.388107	-2.080641	-1.088657
H	1.747722	-1.578913	-1.824253
H	2.231872	-3.163268	-1.198359
C	3.867497	-1.730665	-1.332367
H	4.152266	-2.044986	-2.344909
C	4.734467	-2.472960	-0.294639
H	4.618204	-3.559629	-0.413166
H	5.795674	-2.242603	-0.457094
C	4.318964	-2.044385	1.128403
H	4.933998	-2.573146	1.867944
C	2.833742	-2.402537	1.363378
H	2.524258	-2.126482	2.379859
H	2.690527	-3.487994	1.255351
C	4.520712	-0.522023	1.273471
H	4.258231	-0.196776	2.288774
H	5.579527	-0.272445	1.118432
C	3.646242	0.232052	0.236982
H	3.813455	1.303925	0.358521
C	2.178102	-0.120141	0.529033
H	1.943535	0.133081	1.572510
C	4.054405	-0.206967	-1.183739
H	3.450353	0.329915	-1.925152
H	5.103655	0.059937	-1.368040
C	-2.763971	-0.568532	0.319551
C	-3.670423	-0.567124	-0.760885
C	-4.824861	0.217512	-0.648407
H	-5.536722	0.242976	-1.468235
C	-5.079329	0.957673	0.504050
C	-4.198388	0.898029	1.581575
H	-4.418475	1.459520	2.485093
C	-3.031821	0.126354	1.520122
C	-3.459938	-1.456651	-1.981240
H	-2.430886	-1.828521	-1.943625
C	-2.117134	0.043408	2.740829
H	-1.271335	-0.606116	2.501206
C	-0.109824	0.532412	-2.306989
H	-0.666599	-0.368475	-2.572737
C	-0.968511	2.118470	-0.328317
H	-1.795716	1.704230	0.237271
C	-1.061544	1.727464	-1.843329
H	-2.089106	1.393259	-2.000683
H	0.567241	0.845970	-3.108003
N	2.220645	3.077726	-0.139129

O	2.979128	4.033201	-0.192187
C	-3.641392	-0.725957	-3.322831
H	-3.444856	-1.414723	-4.152498
H	-4.663055	-0.349233	-3.445956
H	-2.955091	0.119933	-3.420220
C	-4.408648	-2.672237	-1.908691
H	-4.216934	-3.363098	-2.738213
H	-4.290045	-3.222448	-0.968618
H	-5.455153	-2.350549	-1.970782
C	-2.866831	-0.596167	3.926929
H	-3.697925	0.035343	4.261605
H	-3.281823	-1.574612	3.657531
H	-2.188304	-0.732561	4.776924
C	-1.520039	1.407100	3.136549
H	-0.927513	1.303293	4.052971
H	-0.859360	1.792042	2.356174
H	-2.302875	2.150398	3.327693
H	-5.976380	1.567492	0.569935
H	-0.835246	2.608703	-2.447737
C	-0.814956	3.599121	-0.045353
H	-1.774043	4.101932	-0.243267
H	-0.557405	3.772323	1.002710
H	-0.054628	4.072853	-0.670974

INT2'

Ru	-0.491024	1.150985	-0.054075
O	-1.855898	1.452297	2.023887
O	-1.608306	2.957798	0.470733
N	-0.520089	-1.529386	-1.110911
N	1.586285	-1.124626	-0.659393
C	0.323828	-0.606698	-0.574539
C	0.117922	-2.809282	-1.419685
H	-0.162145	-3.162459	-2.415887
H	-0.172870	-3.576702	-0.690164
C	1.609723	-2.447634	-1.317478
H	2.182284	-3.160242	-0.716582
H	2.084925	-2.367986	-2.302297
C	-1.949139	-1.372770	-0.855971
C	-2.354694	-2.139039	0.430097
H	-1.729954	-1.784601	1.259450
H	-2.164968	-3.213320	0.298968
C	-3.844963	-1.900554	0.738677
H	-4.120732	-2.467108	1.637467
C	-4.700192	-2.369827	-0.455164
H	-4.562751	-3.447266	-0.625181
H	-5.764377	-2.211018	-0.236817
C	-4.298773	-1.579850	-1.718126
H	-4.914424	-1.901460	-2.567925
C	-2.814216	-1.860714	-2.037995
H	-2.505378	-1.338127	-2.953025
H	-2.664602	-2.937367	-2.206100
C	-4.507167	-0.069835	-1.468725
H	-4.249849	0.501426	-2.371067
H	-5.565878	0.128383	-1.253169
C	-3.634567	0.396853	-0.269487
H	-3.785985	1.468758	-0.108770
C	-2.173281	0.128197	-0.647585
H	-1.956928	0.657900	-1.610275
C	-4.063239	-0.396886	0.982574
H	-3.491178	-0.061934	1.849816

H	-5.124008	-0.200861	1.189991
C	2.695342	-0.735777	0.158375
C	2.680069	-1.092427	1.525656
C	3.756472	-0.680051	2.320084
H	3.759164	-0.919349	3.379740
C	4.823623	0.029031	1.772875
C	4.850148	0.309793	0.408585
H	5.705914	0.827757	-0.014046
C	3.793684	-0.074512	-0.426565
C	1.565840	-1.935883	2.141808
H	0.847895	-2.186060	1.356314
C	3.884120	0.134957	-1.933435
H	2.885490	-0.032501	-2.350058
C	0.900097	1.791728	1.275146
H	1.631681	1.109078	1.691819
C	0.693615	2.081108	-1.357047
H	1.384615	1.477021	-1.948872
C	1.394625	2.550713	0.010315
H	2.461322	2.342670	-0.100309
H	0.467897	2.441039	2.037086
C	4.832622	-0.916905	-2.546614
H	4.860602	-0.823714	-3.638808
H	5.853279	-0.784496	-2.168251
H	4.517210	-1.935962	-2.296387
C	4.324754	1.551592	-2.338999
H	5.343873	1.772516	-2.002158
H	4.313772	1.647971	-3.430721
H	3.659174	2.315488	-1.926740
C	2.134646	-3.265935	2.675822
H	2.682881	-3.808358	1.896326
H	2.823808	-3.100266	3.511761
H	1.323118	-3.908824	3.036183
C	0.778837	-1.191752	3.236885
H	0.033578	-1.862410	3.681089
H	1.439732	-0.849313	4.041928
H	0.250362	-0.325463	2.831268
H	5.647181	0.344948	2.407567
H	1.213721	3.622327	0.125928
N	-2.141722	2.616339	1.608405
O	-2.871695	3.386036	2.211391
C	0.101031	3.213927	-2.180694
H	0.890435	3.891338	-2.542147
H	-0.416146	2.814101	-3.062152
H	-0.615410	3.806343	-1.603047

TS2'

Ru	-0.445840	1.163954	-0.020871
O	-1.566418	1.126775	1.997932
O	-1.635385	2.880417	0.719970
N	-0.552211	-1.527306	-1.048448
N	1.568623	-1.137609	-0.660143
C	0.311969	-0.602191	-0.557541
C	0.061432	-2.829312	-1.308663
H	-0.254690	-3.231244	-2.274837
H	-0.215504	-3.553168	-0.529933
C	1.559098	-2.481349	-1.273813
H	2.147857	-3.179992	-0.672038
H	1.997805	-2.437921	-2.278216
C	-1.985390	-1.325344	-0.824969
C	-2.406869	-1.950556	0.529263

H	-1.794254	-1.512814	1.326369
H	-2.220772	-3.034351	0.515200
C	-3.900572	-1.677576	0.794815
H	-4.189420	-2.147714	1.744009
C	-4.746113	-2.262358	-0.353275
H	-4.611924	-3.352172	-0.413547
H	-5.811918	-2.078734	-0.162820
C	-4.326251	-1.603301	-1.683234
H	-4.936674	-2.003451	-2.503477
C	-2.841053	-1.936473	-1.953820
H	-2.517180	-1.523785	-2.918744
H	-2.713543	-3.028665	-2.002129
C	-4.529808	-0.072965	-1.584436
H	-4.268362	0.403133	-2.539462
H	-5.591586	0.141966	-1.398232
C	-3.655552	0.506789	-0.437215
H	-3.801464	1.591792	-0.378272
C	-2.185265	0.200785	-0.803558
H	-2.066089	0.537473	-1.843651
C	-4.119326	-0.155555	0.879175
H	-3.581092	0.246496	1.737177
H	-5.186456	0.056706	1.034181
C	2.710510	-0.719064	0.090855
C	2.781482	-1.064041	1.459214
C	3.898127	-0.631467	2.185165
H	3.968722	-0.864790	3.243907
C	4.920205	0.088904	1.570549
C	4.859056	0.364901	0.206166
H	5.679565	0.894400	-0.269207
C	3.759886	-0.040249	-0.561036
C	1.716655	-1.919286	2.143161
H	0.956004	-2.179390	1.402353
C	3.747806	0.164495	-2.071437
H	2.726748	-0.024520	-2.419213
C	1.116391	1.930373	1.430342
H	1.724368	1.115368	1.795384
C	0.286181	1.942983	-1.569216
H	1.100620	1.508960	-2.166551
C	1.491506	2.597599	0.263184
H	2.382861	2.278617	-0.264559
H	0.531134	2.458489	2.176169
C	4.673374	-0.872197	-2.742528
H	4.625579	-0.786023	-3.834619
H	5.714469	-0.717645	-2.434641
H	4.395150	-1.895051	-2.465905
C	4.134465	1.586253	-2.512631
H	5.163693	1.835172	-2.230995
H	4.064380	1.671362	-3.603155
H	3.474362	2.341765	-2.075268
C	2.334381	-3.239519	2.646275
H	2.844303	-3.776632	1.837679
H	3.068551	-3.061058	3.440366
H	1.554482	-3.892692	3.054481
C	0.985947	-1.182157	3.281462
H	0.289086	-1.865785	3.780417
H	1.689505	-0.813788	4.037661
H	0.405111	-0.336484	2.904657
H	5.776447	0.419140	2.152521
H	1.171974	3.623481	0.102269
N	-2.038292	2.305845	1.804147

O	-2.812675	2.839270	2.577043
C	-0.252794	3.207280	-2.177780
H	0.544536	3.903515	-2.476981
H	-0.784438	2.922781	-3.100537
H	-0.962865	3.722676	-1.524766
INT3'			
Ru	0.522053	0.753103	0.759543
O	-0.232309	2.524832	-0.219775
O	1.254311	2.832045	1.337338
N	0.760822	-1.790758	-0.528180
N	-1.368597	-1.247890	-0.593661
C	-0.150393	-0.843265	-0.158948
C	0.202348	-2.715787	-1.515851
H	0.583206	-3.731162	-1.382582
H	0.430592	-2.383729	-2.540079
C	-1.298091	-2.592544	-1.202057
H	-1.940886	-2.660350	-2.081442
H	-1.616373	-3.352496	-0.477033
C	2.159095	-1.355596	-0.432702
C	2.538579	-0.469009	-1.649596
H	1.803222	0.342503	-1.758709
H	2.492806	-1.062751	-2.573596
C	3.949733	0.114366	-1.457637
H	4.207854	0.736707	-2.324212
C	4.954981	-1.049426	-1.334232
H	4.955086	-1.646493	-2.257012
H	5.971852	-0.655731	-1.205075
C	4.577525	-1.932662	-0.126754
H	5.294209	-2.759033	-0.037022
C	3.159867	-2.519885	-0.338973
H	2.882723	-3.174093	0.497759
H	3.143584	-3.128830	-1.255512
C	4.619259	-1.068694	1.154334
H	4.388160	-1.684092	2.034076
H	5.635061	-0.672933	1.295146
C	3.599090	0.094127	1.041317
H	3.626510	0.702048	1.953898
C	2.201189	-0.529757	0.879967
H	2.054081	-1.241388	1.699094
C	3.970880	0.969035	-0.173584
H	3.269200	1.809565	-0.262055
H	4.969142	1.404342	-0.031386
C	-2.584264	-0.492983	-0.492143
C	-2.814510	0.552031	-1.417775
C	-4.022962	1.250137	-1.319994
H	-4.227957	2.063743	-2.006908
C	-4.973007	0.921067	-0.354975
C	-4.726023	-0.110533	0.544277
H	-5.471694	-0.358291	1.294008
C	-3.524904	-0.829482	0.500920
C	-1.813496	0.885889	-2.521406
H	-0.809744	0.698322	-2.129726
C	-3.282091	-1.957899	1.495356
H	-2.223408	-2.233450	1.439402
C	-0.237212	0.256090	2.333472
H	-0.886575	-0.623832	2.424257
C	-4.118859	-3.199514	1.126335
H	-3.908375	-4.029095	1.811981
H	-5.190024	-2.973199	1.187645

H	-3.912182	-3.536770	0.104644	C	3.363283	-1.878147	2.292558
C	-3.564605	-1.534462	2.948818	H	3.317367	-2.149207	3.343640
H	-4.631371	-1.347701	3.115349	C	4.551467	-1.380395	1.762275
H	-3.259373	-2.329332	3.639424	C	4.634459	-1.061101	0.408826
H	-3.020429	-0.621739	3.211182	H	5.572801	-0.698039	0.001534
C	-2.026776	-0.033329	-3.742104	C	3.523728	-1.196224	-0.432847
H	-1.924322	-1.091820	-3.484656	C	0.968057	-2.671079	2.084518
H	-3.029444	0.111887	-4.161961	H	0.213087	-2.745207	1.297686
H	-1.294642	0.195002	-4.526045	C	3.645618	-0.921638	-1.927523
C	-1.847962	2.357532	-2.964397	H	2.629228	-0.827834	-2.325570
H	-1.008343	2.552884	-3.641284	C	1.186254	1.234688	1.380219
H	-2.766717	2.597924	-3.513266	H	1.566512	0.315032	1.804233
H	-1.754912	3.029614	-2.108773	C	0.553217	1.461579	-1.549482
H	-5.906840	1.474765	-0.303803	H	1.278829	0.863028	-2.112293
N	0.495997	3.376000	0.463362	H	0.833853	1.955639	2.114373
O	0.442157	4.566402	0.257000	C	4.308954	-2.130550	-2.621647
C	-0.067404	1.017967	3.619055	H	5.336411	-2.263175	-2.262149
H	-1.044987	1.351786	3.999732	H	3.766006	-3.061067	-2.421592
H	0.358543	0.350319	4.385143	H	4.346447	-1.980207	-3.707080
H	0.581677	1.892159	3.518024	C	4.409397	0.371364	-2.269805
				H	5.465578	0.299241	-1.985310
TS3'-cross				H	4.379890	0.537068	-3.353173
Ru	-0.411906	0.839161	-0.038489	H	3.993867	1.259171	-1.782153
O	-1.561766	1.065638	2.005540	C	1.263795	-4.106253	2.564600
O	-1.263938	2.766323	0.688288	H	1.694609	-4.715534	1.761242
N	-1.000346	-1.766408	-1.115662	H	1.972501	-4.110855	3.400544
N	1.152480	-1.789611	-0.690771	H	0.341702	-4.590371	2.906758
C	0.014210	-1.037198	-0.586878	C	0.343523	-1.829161	3.213050
C	-0.631895	-3.147923	-1.427556	H	-0.515259	-2.358679	3.642283
H	-1.001475	-3.443214	-2.412868	H	1.060955	-1.647838	4.022094
H	-1.049418	-3.839335	-0.683142	H	-0.014362	-0.864461	2.844245
C	0.903127	-3.081142	-1.367028	H	5.420719	-1.256108	2.402367
H	1.346328	-3.900978	-0.794936	N	-1.769449	2.305250	1.796211
H	1.355572	-3.071648	-2.365444	O	-2.392574	3.019589	2.558986
C	-2.374222	-1.318618	-0.878596	C	0.244416	2.764299	-2.233672
C	-2.906673	-1.923442	0.445670	H	1.155652	3.324128	-2.483360
H	-2.225283	-1.645339	1.258904	H	-0.251881	2.508627	-3.183390
H	-2.920654	-3.020608	0.377508	H	-0.432016	3.402083	-1.658624
C	-4.325860	-1.396438	0.733765	C	1.813452	1.720920	0.196624
H	-4.698025	-1.852053	1.660633	H	2.569706	1.079988	-0.233986
C	-5.260263	-1.760529	-0.436593	C	2.148863	3.171929	-0.040167
H	-5.326391	-2.852187	-0.549862	O	3.163243	3.451957	-0.683123
H	-6.275304	-1.395608	-0.231174	N	1.315235	4.105915	0.484666
C	-4.724049	-1.125136	-1.735961	H	0.390573	3.809762	0.784996
H	-5.394278	-1.367941	-2.570742	C	1.517425	5.515626	0.194380
C	-3.322399	-1.706155	-2.032293	H	0.945594	6.112216	0.909302
H	-2.926322	-1.309610	-2.976729	H	2.578949	5.754005	0.285751
H	-3.391909	-2.799379	-2.136476	H	1.196744	5.773368	-0.824560
C	-4.647507	0.409726	-1.562620				
H	-4.300513	0.877023	-2.494321	**TS3'-homo**			
H	-5.652574	0.805163	-1.359443	Ru	-0.454391	1.085089	-0.046200
C	-3.687203	0.764925	-0.392974	O	-1.633808	1.189216	1.982766
H	-3.633804	1.854333	-0.283281	O	-1.592677	2.865829	0.604207
C	-2.298310	0.213468	-0.776275	N	-0.627099	-1.614132	-1.047866
H	-2.092792	0.586354	-1.793477	N	1.504367	-1.280926	-0.663295
C	-4.261616	0.133584	0.894210	C	0.261195	-0.713025	-0.556291
H	-3.651174	0.389130	1.761086	C	-0.048033	-2.927471	-1.328604
H	-5.270277	0.530766	1.073803	H	-0.372782	-3.303880	-2.302225
C	2.315392	-1.651102	0.135060	H	-0.346852	-3.656625	-0.563241
C	2.226853	-2.041011	1.490672	C	1.458146	-2.620698	-1.285505

H	2.024535	-3.338914	-0.685353
H	1.902270	-2.583774	-2.287604
C	-2.053544	-1.381843	-0.817335
C	-2.484045	-2.019568	0.528429
H	-1.855523	-1.609170	1.328129
H	-2.323956	-3.107003	0.495851
C	-3.968929	-1.714411	0.806206
H	-4.264808	-2.193109	1.748945
C	-4.833447	-2.259763	-0.347345
H	-4.726400	-3.351438	-0.425304
H	-5.893541	-2.053067	-0.149034
C	-4.403836	-1.590330	-1.669094
H	-5.027271	-1.963029	-2.492405
C	-2.928130	-1.952334	-1.953121
H	-2.599489	-1.529065	-2.911831
H	-2.824727	-3.045894	-2.021816
C	-4.569317	-0.057630	-1.545885
H	-4.298585	0.427001	-2.494023
H	-5.624515	0.181492	-1.352352
C	-3.678165	0.482053	-0.392400
H	-3.797528	1.569014	-0.317405
C	-2.218163	0.144895	-0.760952
H	-2.070112	0.516434	-1.789583
C	-4.148007	-0.189092	0.916808
H	-3.586260	0.189461	1.771259
H	-5.207370	0.048692	1.086801
C	2.649540	-0.918271	0.113026
C	2.676285	-1.270185	1.481550
C	3.794122	-0.887648	2.232920
H	3.830665	-1.124955	3.292466
C	4.860459	-0.212384	1.642700
C	4.842261	0.066353	0.277785
H	5.695708	0.559093	-0.178659
C	3.743023	-0.287684	-0.514273
C	1.561490	-2.080528	2.140638
H	0.808285	-2.310934	1.382775
C	3.774214	-0.077777	-2.023698
H	2.753855	-0.219646	-2.394999
C	1.071154	1.738113	1.345121
H	1.655432	0.908492	1.716726
C	0.407955	1.831857	-1.555401
H	1.222742	1.348982	-2.108928
C	1.544898	2.437785	0.195463
H	2.429579	2.009113	-0.265424
H	0.578101	2.326897	2.116858
C	4.667078	-1.152750	-2.678573
H	4.648755	-1.059774	-3.770993
H	5.706686	-1.047233	-2.345955
H	4.336169	-2.163071	-2.414003
C	4.234070	1.327114	-2.449266
H	4.187676	1.420873	-3.540340
H	3.602266	2.110074	-2.018521
H	5.268682	1.525915	-2.148000
C	2.112545	-3.424706	2.657662
H	2.619152	-3.982560	1.861116
H	2.834021	-3.276465	3.469348
H	1.296843	-4.045107	3.046621
C	0.834850	-1.313700	3.261919
H	0.097960	-1.967858	3.742641
H	1.534927	-0.975922	4.035365

H	0.300471	-0.443265	2.872951
H	5.717314	0.079019	2.244222
N	-2.037721	2.373774	1.715234
O	-2.789766	2.998014	2.442587
C	-0.157381	3.022252	-2.282193
H	-0.836358	3.615726	-1.664207
H	0.614600	3.676981	-2.709731
H	-0.740780	2.624047	-3.128441
C	1.445025	3.948962	0.152408
H	1.685694	4.361215	-0.831130
H	0.444191	4.281989	0.440233
H	2.162804	4.366325	0.870792

INT4'-*cross*

Ru	-0.435307	0.833422	-0.105771
C	0.894381	1.416019	-1.461177
C	0.561099	2.633104	-2.312534
H	-0.039000	3.375717	-1.780404
H	-0.005812	2.306608	-3.193116
H	1.477827	3.124639	-2.668068
H	1.397643	0.657399	-2.063537
C	1.782594	1.646174	-0.114876
C	2.346919	3.069840	-0.102962
O	3.481775	3.260899	-0.538773
N	1.548305	4.054675	0.374621
H	0.568545	3.841689	0.543970
C	1.948134	5.448648	0.282790
H	1.780613	5.856232	-0.723638
H	3.013065	5.530851	0.509570
H	1.373342	6.034697	1.004345
H	2.634418	0.985327	-0.247421
C	1.079510	1.178662	1.193417
H	1.603357	0.360100	1.675198
H	0.851812	1.976448	1.901296
C	-0.044470	-1.075614	-0.577818
N	-1.079329	-1.787377	-1.098893
C	-2.434838	-1.304374	-0.845093
C	-2.312352	0.212122	-0.663611
C	-3.671115	0.813311	-0.289176
C	-4.259235	0.159097	0.978789
C	-4.391996	-1.358765	0.761247
C	-2.997754	-1.937364	0.454202
H	-3.060461	-3.028229	0.340202
H	-2.304648	-1.724202	1.277431
C	-5.338699	-1.640899	-0.422336
C	-4.774890	-0.985534	-1.700091
C	-4.634674	0.536545	-1.477523
H	-5.619690	0.972888	-1.263267
H	-4.260046	1.019564	-2.390217
C	-3.394595	-1.601899	-2.017354
H	-3.494572	-2.686837	-2.167100
H	-2.980112	-1.178467	-2.941784
H	-5.452029	-1.173440	-2.543021
H	-6.337363	-1.239785	-0.205382
H	-5.451524	-2.723990	-0.572403
H	-4.784423	-1.831499	1.670739
H	-3.619074	0.366969	1.838612
H	-5.245220	0.595690	1.187914
H	-3.572257	1.894346	-0.148024
H	-1.986470	0.660479	-1.637316

C	-0.749183	-3.185272	-1.380960	C	-4.816290	-2.321844	-0.406220
C	0.786545	-3.163987	-1.297026	H	-4.714739	-3.405928	-0.558135
N	1.067098	-1.866201	-0.645528	H	-5.873996	-2.124572	-0.187757
C	2.222213	-1.746085	0.196896	C	-4.393442	-1.567047	-1.683621
C	3.460128	-1.367956	-0.362961	H	-5.022089	-1.882675	-2.526120
C	4.557796	-1.242691	0.497322	C	-2.919912	-1.901033	-2.002914
C	4.433656	-1.499384	1.860710	H	-2.597399	-1.403741	-2.927270
C	3.215060	-1.925049	2.384328	H	-2.805505	-2.984517	-2.153617
C	2.089505	-2.074129	1.565100	C	-4.551390	-0.047153	-1.459340
C	0.791037	-2.613582	2.161516	H	-4.277974	0.500140	-2.371753
C	0.178623	-1.673241	3.216549	H	-5.602289	0.189682	-1.244557
H	0.880072	-1.484252	4.037689	C	-3.660386	0.410890	-0.270294
H	-0.721882	-2.128565	3.646069	H	-3.775796	1.489708	-0.128076
H	-0.107316	-0.712966	2.779801	C	-2.210119	0.087765	-0.646023
H	0.054011	-2.706664	1.359660	H	-1.974953	0.597989	-1.616067
C	1.008224	-4.026562	2.738886	C	-4.110187	-0.346902	0.996496
H	0.056201	-4.446159	3.084533	H	-3.523513	-0.016541	1.855842
H	1.430645	-4.704544	1.987807	H	-5.162992	-0.112384	1.204428
H	1.693752	-4.009871	3.593671	C	2.630681	-0.934408	0.167857
H	3.135353	-2.146421	3.444896	C	2.600606	-1.265005	1.541378
H	5.293665	-1.382246	2.514432	C	3.695020	-0.886623	2.328161
H	5.518238	-0.935188	0.096208	H	3.687808	-1.106572	3.391988
C	3.629136	-1.164202	-1.864004	C	4.793323	-0.237938	1.767845
C	4.462693	0.075919	-2.238197	C	4.831470	0.016120	0.398623
H	5.512550	-0.046343	-1.947313	H	5.708918	0.487898	-0.033506
H	4.445143	0.214253	-3.325537	C	3.757266	-0.333572	-0.428897
H	4.095726	0.995813	-1.772244	C	1.452794	-2.051020	2.171780
C	4.250335	-2.430950	-2.490759	H	0.722198	-2.280231	1.391621
H	5.260319	-2.597784	-2.097666	C	3.851297	-0.145666	-1.938467
H	4.323483	-2.326921	-3.579820	H	2.844770	-0.275065	-2.349605
H	3.657844	-3.325869	-2.269533	C	0.921140	1.679086	1.224361
H	2.628863	-1.039069	-2.292292	H	1.615793	0.977300	1.672495
H	1.254039	-3.191360	-2.287886	C	0.716576	1.933821	-1.403904
H	1.194612	-3.983910	-0.699596	H	1.375700	1.292986	-1.994416
H	-1.112570	-3.487653	-2.366636	C	1.486072	2.386801	-0.052394
H	-1.196603	-3.850576	-0.630689	H	2.491488	1.978571	-0.176467
O	-1.680092	1.497341	2.007112	H	0.519559	2.375729	1.963130
N	-1.679546	2.683020	1.579045	C	4.752857	-1.242735	-2.542891
O	-2.156596	3.629620	2.182845	H	4.780305	-1.163313	-3.636182
O	-1.118708	2.866180	0.407480	H	5.779669	-1.148223	-2.169813
				H	4.396905	-2.245038	-2.279737
INT4'-*homo*				C	4.349067	1.247002	-2.361549
Ru	-0.493817	1.066022	-0.080730	H	5.377821	1.428909	-2.030643
O	-1.841188	1.457881	2.000392	H	4.337900	1.331078	-3.454300
O	-1.562600	2.914120	0.406337	H	3.717803	2.042821	-1.955715
N	-0.613249	-1.629578	-1.087901	C	1.966061	-3.397527	2.720823
N	1.506423	-1.291278	-0.643803	H	2.487426	-3.972834	1.946469
C	0.263001	-0.727165	-0.567170	H	2.665085	-3.250949	3.552138
C	-0.020629	-2.936160	-1.373987	H	1.129114	-4.000369	3.092163
H	-0.316293	-3.298682	-2.362266	C	0.702134	-1.260640	3.259865
H	-0.334343	-3.679109	-0.628753	H	-0.069869	-1.893331	3.714008
C	1.482422	-2.623439	-1.283371	H	1.379548	-0.937544	4.059187
H	2.033880	-3.346367	-0.675213	H	0.210014	-0.377316	2.845366
H	1.954903	-2.573169	-2.271433	H	5.631196	0.051263	2.396532
C	-2.035471	-1.422051	-0.831560	N	-2.091459	2.619821	1.559136
C	-2.461688	-2.153059	0.468491	O	-2.784507	3.431387	2.151708
H	-1.822889	-1.805181	1.289839	C	0.109930	3.024560	-2.275403
H	-2.307531	-3.234977	0.355041	H	0.885190	3.667478	-2.717978
C	-3.942250	-1.860787	0.777174	H	-0.436895	2.560608	-3.106364
H	-4.233353	-2.402939	1.686121	H	-0.588300	3.662761	-1.727357

C	1.537656	3.907918	0.135875
H	1.967199	4.406541	-0.740074
H	0.536664	4.311048	0.311153
H	2.160513	4.151092	1.003919

INT4'-*cross*-2

Ru	0.614649	0.630755	0.073479
O	1.612457	2.545641	0.310344
O	1.662879	1.595175	2.271257
N	0.901681	-2.159049	-0.523826
N	-1.268551	-1.850484	-0.492790
C	-0.062427	-1.238781	-0.273732
C	0.395836	-3.373492	-1.160772
H	0.875675	-4.270059	-0.759932
H	0.570432	-3.341357	-2.245203
C	-1.096934	-3.285093	-0.818843
H	-1.748224	-3.573943	-1.645838
H	-1.354784	-3.896831	0.055544
C	2.286501	-1.694590	-0.570295
C	2.669734	-1.239963	-2.003098
H	1.936370	-0.505993	-2.358356
H	2.630722	-2.101367	-2.684861
C	4.083880	-0.631044	-1.996271
H	4.344259	-0.308927	-3.012787
C	5.086600	-1.700601	-1.516843
H	5.087260	-2.554676	-2.208743
H	6.104098	-1.288073	-1.513275
C	4.706434	-2.165894	-0.095512
H	5.417661	-2.928710	0.246226
C	3.286796	-2.778105	-0.114400
H	3.006153	-3.137876	0.884124
H	3.262386	-3.640011	-0.797452
C	4.744243	-0.952890	0.856872
H	4.504911	-1.264627	1.882140
H	5.757986	-0.529590	0.876839
C	3.732732	0.124750	0.384901
H	3.779940	0.971863	1.072267
C	2.333222	-0.509431	0.418489
H	2.131144	-0.892006	1.430351
C	4.105564	0.579320	-1.040631
H	3.402707	1.350012	-1.379809
H	5.105582	1.033229	-1.036504
C	-2.507418	-1.459001	0.124140
C	-3.555110	-0.964265	-0.682209
C	-4.742336	-0.576646	-0.049084
H	-5.557242	-0.175531	-0.642795
C	-4.891376	-0.688793	1.330839
C	-3.859988	-1.215521	2.103988
H	-3.990251	-1.309866	3.178278
C	-2.653357	-1.620403	1.521047
C	-3.437936	-0.891285	-2.200945
H	-2.371673	-0.929125	-2.448647
C	-1.559412	-2.214522	2.406914
H	-0.707430	-2.490162	1.780688
C	-0.180851	1.226688	-1.632221
H	-0.600511	0.534399	-2.364562
C	-1.090308	1.386765	0.895824
H	-1.801931	0.617235	1.175581
H	0.366769	2.042128	-2.113890
N	1.947293	2.604193	1.578252

O	2.496282	3.605449	2.010856
C	-4.025448	0.396388	-2.811917
H	-3.780562	0.439351	-3.879449
H	-5.118774	0.412287	-2.733104
H	-3.647975	1.308506	-2.338987
C	-4.115472	-2.123068	-2.839468
H	-3.984035	-2.115273	-3.927925
H	-3.708603	-3.063079	-2.451474
H	-5.191487	-2.119272	-2.628032
C	-2.055693	-3.501921	3.094559
H	-2.874605	-3.293548	3.792487
H	-2.422277	-4.230853	2.362186
H	-1.242678	-3.966351	3.664583
C	-1.028813	-1.204835	3.442825
H	-0.554509	-0.348453	2.956766
H	-1.831905	-0.833743	4.090068
H	-0.277758	-1.682977	4.082558
H	-5.816954	-0.371723	1.803552
C	-1.114720	2.489189	1.936667
H	-2.133624	2.899817	1.991030
H	-0.866087	2.072608	2.916392
H	-0.438181	3.319766	1.737732
C	-1.312286	1.756568	-0.627029
H	-2.209838	1.207501	-0.895992
C	-1.625057	3.238901	-0.865454
O	-2.773772	3.559274	-1.165848
N	-0.595792	4.113285	-0.755965
H	0.298131	3.775735	-0.405531
C	-0.800519	5.545723	-0.887098
H	-1.068744	6.007978	0.072330
H	0.116478	6.011192	-1.258592
H	-1.614237	5.722345	-1.593097

INT4'-*homo*-2

Ru	0.623999	0.849877	-0.280458
O	1.832465	2.602735	-0.696818
O	1.704182	2.321928	1.456984
N	0.609668	-1.984832	0.217314
N	-1.508107	-1.476613	0.018349
C	-0.247002	-0.941055	0.058284
C	-0.022780	-3.290187	0.039351
H	0.356236	-4.024438	0.754861
H	0.154558	-3.671101	-0.976489
C	-1.496180	-2.934406	0.264848
H	-2.177913	-3.448060	-0.417021
H	-1.816216	-3.140102	1.295352
C	2.034167	-1.715682	0.040120
C	2.448767	-1.861193	-1.447802
H	1.792423	-1.240136	-2.069074
H	2.315531	-2.904695	-1.767160
C	3.918556	-1.435897	-1.622023
H	4.201993	-1.536956	-2.677771
C	4.809785	-2.348901	-0.755160
H	4.716176	-3.392963	-1.086230
H	5.864450	-2.066798	-0.872446
C	4.396185	-2.220074	0.725900
H	5.027823	-2.871029	1.344043
C	2.920660	-2.650793	0.890000
H	2.613376	-2.588880	1.942136
H	2.799917	-3.696215	0.569231

C	4.566669	-0.752546	1.169186	O	1.284392	1.218548	2.375402
H	4.305084	-0.640907	2.229675	N	0.913935	-2.134840	-0.506977
H	5.618755	-0.453694	1.063161	N	-1.256500	-1.831326	-0.471660
C	3.668174	0.172020	0.305643	C	-0.052907	-1.218293	-0.242934
H	3.813919	1.202112	0.636474	C	0.403335	-3.350936	-1.137264
C	2.210486	-0.263966	0.527933	H	0.890658	-4.245735	-0.741348
H	1.980842	-0.229722	1.601924	H	0.566104	-3.319065	-2.223613
C	4.074272	0.032061	-1.175226	C	-1.085114	-3.267968	-0.780986
H	3.453518	0.691522	-1.793657	H	-1.744211	-3.570449	-1.596700
H	5.116312	0.353099	-1.306731	H	-1.330107	-3.869163	0.104771
C	-2.718268	-0.764891	0.305998	C	2.301395	-1.675343	-0.581312
C	-3.659632	-0.575729	-0.727282	C	2.681875	-1.292756	-2.032449
C	-4.821459	0.148226	-0.432592	H	1.943253	-0.588293	-2.428356
H	-5.559592	0.315837	-1.211402	H	2.660050	-2.187828	-2.670331
C	-5.048745	0.649379	0.847231	C	4.087307	-0.664725	-2.050586
C	-4.132747	0.402264	1.867317	H	4.343957	-0.380573	-3.079602
H	-4.331436	0.776053	2.867745	C	5.102659	-1.702431	-1.530100
C	-2.958176	-0.320210	1.625325	H	5.111511	-2.583146	-2.187827
C	-3.474106	-1.208162	-2.102413	H	6.116150	-1.279880	-1.543615
H	-2.438200	-1.556602	-2.166759	C	4.726382	-2.112806	-0.091117
C	-2.004944	-0.618604	2.781080	H	5.442619	-2.857395	0.279606
H	-1.164976	-1.204857	2.399866	C	3.309071	-2.736287	-0.084263
C	-0.122543	0.843541	-2.109762	H	3.032652	-3.056358	0.928787
H	-0.655592	-0.008688	-2.538087	H	3.294157	-3.627305	-0.729502
C	-0.994966	2.037027	0.114332	C	4.766416	-0.858284	0.808176
H	-1.799512	1.498599	0.602904	H	4.539579	-1.126508	1.848441
C	-1.128057	1.914202	-1.452460	H	5.779531	-0.432346	0.798456
H	-2.115776	1.466468	-1.582810	C	3.738866	0.186150	0.300355
H	0.533913	1.320392	-2.846400	H	3.779248	1.070344	0.944193
N	2.173954	2.999143	0.495054	C	2.348057	-0.463510	0.369573
O	2.903852	3.966842	0.642728	H	2.206482	-0.855887	1.388349
C	-3.711180	-0.237627	-3.272615	C	4.093560	0.585279	-1.145086
H	-3.531922	-0.750683	-4.224461	H	3.369291	1.322910	-1.512318
H	-4.742032	0.133770	-3.290541	H	5.084456	1.058460	-1.171389
H	-3.041844	0.626109	-3.226289	C	-2.512076	-1.413733	0.085346
C	-4.399977	-2.435771	-2.238850	C	-3.518181	-0.926741	-0.777760
H	-4.223424	-2.950420	-3.190745	C	-4.730314	-0.520182	-0.207320
H	-4.242999	-3.153227	-1.425769	H	-5.515734	-0.128169	-0.845460
H	-5.452974	-2.131125	-2.208770	C	-4.943676	-0.607338	1.166336
C	-2.712795	-1.473621	3.851359	C	-3.952433	-1.125089	1.995963
H	-3.533505	-0.922988	4.325346	H	-4.133539	-1.201375	3.064328
H	-3.133899	-2.388663	3.418322	C	-2.722138	-1.546801	1.476615
H	-2.005303	-1.759422	4.638296	C	-3.331873	-0.892376	-2.291783
C	-1.400464	0.654805	3.401926	H	-2.256150	-0.958265	-2.490541
H	-0.763369	1.179637	2.686405	C	-1.674587	-2.136301	2.419025
H	-2.179931	1.344709	3.745974	H	-0.788889	-2.405267	1.837764
H	-0.781702	0.391208	4.267624	C	0.276545	1.102879	-1.626560
H	-5.951721	1.217233	1.054882	H	-0.288264	0.561189	-2.395338
C	-0.866150	3.421940	0.715510	C	-1.352530	1.582723	0.938892
H	-0.620129	3.349064	1.777754	H	-1.916320	0.710936	1.247726
H	-0.111179	4.044525	0.233580	H	0.726040	2.026650	-2.013433
H	-1.832079	3.943196	0.633262	N	1.744283	2.327212	1.950843
C	-1.023546	3.248555	-2.199400	O	2.295563	3.146655	2.661453
H	-0.015026	3.662009	-2.110225	C	-3.862076	0.389723	-2.963167
H	-1.238463	3.095158	-3.262929	H	-3.605776	0.374657	-4.028914
H	-1.736681	3.982932	-1.809640	H	-4.954595	0.452481	-2.897907
				H	-3.450033	1.308024	-2.532962
TS4'-*cross*				C	-4.008177	-2.126212	-2.928310
Ru	0.576938	0.647039	0.165375	H	-3.820856	-2.155247	-4.008140
O	1.582730	2.535284	0.676006	H	-3.647814	-3.063889	-2.491884

H	-5.093173	-2.088409	-2.773642
C	-2.202892	-3.427241	3.075719
H	-3.061599	-3.222283	3.725353
H	-2.523861	-4.157293	2.323318
H	-1.421693	-3.888394	3.691011
C	-1.207220	-1.126554	3.484545
H	-0.714344	-0.264286	3.029022
H	-2.045489	-0.767449	4.093034
H	-0.484405	-1.600633	4.158614
H	-5.889082	-0.279055	1.589769
C	-1.276809	2.639657	2.019397
H	-2.289475	3.030602	2.190751
H	-0.924286	2.203067	2.956133
H	-0.639094	3.487150	1.770298
C	-1.437321	1.853031	-0.449822
H	-2.071781	1.184052	-1.012950
C	-1.457004	3.241731	-1.051161
O	-2.387515	3.534115	-1.803326
N	-0.467806	4.104171	-0.711261
H	0.328074	3.760271	-0.181297
C	-0.422320	5.447118	-1.264712
H	0.208745	6.072434	-0.628369
H	-0.018113	5.454584	-2.285677
H	-1.432807	5.860763	-1.297504

TS4'-*homo*

Ru	0.573385	0.854310	-0.361078
O	1.718802	2.678582	-0.767894
O	1.285675	2.346331	1.333355
N	0.710898	-1.913542	0.444810
N	-1.427931	-1.511824	0.207445
C	-0.186108	-0.929870	0.165148
C	0.119623	-3.249640	0.470755
H	0.533676	-3.858940	1.278407
H	0.296848	-3.769470	-0.481488
C	-1.362185	-2.914527	0.668273
H	-2.033274	-3.547906	0.084013
H	-1.660488	-2.973872	1.723921
C	2.128334	-1.638014	0.207544
C	2.537455	-2.042803	-1.229722
H	1.852681	-1.577048	-1.945632
H	2.451930	-3.132630	-1.347969
C	3.985226	-1.594514	-1.500633
H	4.264104	-1.869642	-2.526527
C	4.921291	-2.303786	-0.500970
H	4.866998	-3.392840	-0.641472
H	5.962979	-2.006892	-0.682126
C	4.513947	-1.929270	0.939333
H	5.173570	-2.438896	1.653725
C	3.054867	-2.378784	1.197716
H	2.754178	-2.141575	2.226528
H	2.976346	-3.469203	1.071921
C	4.642541	-0.400087	1.109337
H	4.394475	-0.108104	2.138282
H	5.684097	-0.097801	0.930436
C	3.694550	0.321801	0.116967
H	3.799305	1.403272	0.245876
C	2.258975	-0.121441	0.443146
H	2.087857	0.045517	1.516810
C	4.081427	-0.064173	-1.323896

H	3.415292	0.442215	-2.033005
H	5.105019	0.270921	-1.540089
C	-2.663730	-0.808345	0.378472
C	-3.595393	-0.802603	-0.681849
C	-4.794095	-0.102562	-0.500831
H	-5.526214	-0.077433	-1.302566
C	-5.066043	0.556101	0.696364
C	-4.153122	0.501044	1.746688
H	-4.383291	1.001112	2.683144
C	-2.941187	-0.188948	1.617492
C	-3.352482	-1.597996	-1.960579
H	-2.292010	-1.871112	-1.979860
C	-1.989186	-0.267396	2.809025
H	-1.105013	-0.837983	2.513705
C	0.310358	0.422272	-2.164429
H	-0.276099	-0.391008	-2.612510
C	-1.266068	2.167702	-0.252438
H	-1.923485	1.603835	0.396552
C	-1.303628	1.792424	-1.621050
H	-1.996575	0.991546	-1.851964
H	0.840944	1.021194	-2.916451
N	1.868926	3.071692	0.455243
O	2.517203	4.064283	0.736238
C	-3.657239	-0.816650	-3.251287
H	-4.717657	-0.550560	-3.325327
H	-3.075600	0.107659	-3.320150
H	-3.413371	-1.431858	-4.124987
C	-4.182216	-2.899516	-1.932280
H	-3.959216	-3.521353	-2.807384
H	-3.981087	-3.489344	-1.031600
H	-5.254974	-2.672061	-1.942279
C	-2.655776	-1.020895	3.977669
H	-3.521986	-0.471522	4.364409
H	-3.004027	-2.013511	3.668368
H	-1.945379	-1.147419	4.802732
C	-1.484860	1.116322	3.260342
H	-0.884101	1.594878	2.483652
H	-2.315616	1.782451	3.521788
H	-0.850286	1.010653	4.147799
H	-5.999001	1.100353	0.816239
C	-1.092494	3.611652	0.165344
H	-2.043389	4.143143	0.010232
H	-0.836674	3.685138	1.224171
H	-0.326142	4.135534	-0.408894
C	-1.084043	2.819431	-2.714950
H	-0.127382	3.333993	-2.589876
H	-1.105664	2.362416	-3.708490
H	-1.880360	3.575128	-2.668944

TS1-AC

Ru	0.470884	0.086930	-0.587622
O	2.169145	1.480210	-1.022746
O	1.432537	1.421194	1.054028
N	-0.187779	-2.457093	0.598491
N	-2.108613	-1.423106	0.414341
C	-0.762644	-1.294702	0.186736
C	-1.155437	-3.504886	0.910673
H	-0.856003	-4.083637	1.788215
H	-1.268723	-4.194501	0.061363
C	-2.418130	-2.672104	1.143089

H	-3.325635	-3.135879	0.751545
H	-2.569744	-2.449668	2.207068
C	1.221453	-2.684260	0.286991
C	1.375678	-3.411292	-1.070534
H	0.816947	-2.868365	-1.838591
H	0.944629	-4.420475	-1.000434
C	2.865110	-3.495168	-1.448617
H	2.966754	-3.996529	-2.420390
C	3.609734	-4.303983	-0.367030
H	3.210763	-5.327297	-0.320815
H	4.675244	-4.384556	-0.620963
C	3.448841	-3.605085	0.999226
H	3.970351	-4.183589	1.772862
C	1.945686	-3.524469	1.363817
H	1.810756	-3.053877	2.346299
H	1.527147	-4.540459	1.421936
C	4.059984	-2.189540	0.905171
H	3.997577	-1.681121	1.876449
H	5.126551	-2.268440	0.649677
C	3.304994	-1.363978	-0.167834
H	3.738961	-0.363198	-0.234845
C	1.836283	-1.271527	0.275712
H	1.819641	-0.916404	1.315224
C	3.441003	-2.065901	-1.532143
H	2.909950	-1.488114	-2.298529
H	4.498335	-2.108035	-1.828306
C	-3.065428	-0.356898	0.495186
C	-4.082672	-0.292319	-0.482304
C	-5.028128	0.734916	-0.385144
H	-5.817004	0.808915	-1.127985
C	-4.974997	1.660973	0.653478
C	-3.985907	1.560291	1.627613
H	-3.960252	2.281080	2.438718
C	-3.017232	0.549782	1.579259
C	-4.204038	-1.339688	-1.584980
H	-3.272395	-1.915848	-1.596337
C	-1.991203	0.441330	2.705138
H	-1.234205	-0.293934	2.418819
C	0.179774	-0.504443	-2.342123
H	-0.572216	-1.191577	-2.753923
C	-0.923097	1.886874	-0.742309
H	-1.598318	1.743551	0.088882
C	-1.191767	1.171656	-1.924579
H	-2.057385	0.524181	-1.950912
H	0.847643	-0.108135	-3.122441
C	-4.397344	-0.736809	-2.988836
H	-4.408264	-1.534833	-3.740279
H	-5.347691	-0.197564	-3.070649
H	-3.596746	-0.037983	-3.250609
C	-5.363528	-2.308941	-1.271728
H	-5.413862	-3.109578	-2.019322
H	-5.253669	-2.768432	-0.283583
H	-6.322293	-1.776795	-1.280111
C	-2.678870	-0.062330	3.992094
H	-3.416619	0.666454	4.348624
H	-3.204748	-1.010961	3.832628
H	-1.938993	-0.209289	4.787596
C	-1.247805	1.762376	2.980425
H	-0.721089	2.130615	2.099171
H	-1.932040	2.544715	3.328267

H	-0.500081	1.601237	3.765318
H	-5.711169	2.458236	0.708821
H	-0.891894	1.608781	-2.873931
C	-0.412423	3.300930	-0.780196
O	-0.889342	4.135453	-0.012860
N	0.477945	3.629819	-1.770034
H	1.151265	2.908022	-2.009368
C	0.898866	5.014910	-1.910258
H	1.511660	5.362067	-1.068740
H	1.473832	5.116401	-2.834840
H	0.015315	5.655609	-1.962296
C	3.356234	2.825369	0.652696
C	2.696702	3.946813	1.483110
H	3.454148	4.673051	1.801916
H	1.927898	4.474386	0.909158
H	2.210817	3.530953	2.369774
C	4.330545	2.031308	1.552314
H	4.840534	1.241862	0.988238
H	5.095309	2.703907	1.959245
H	3.794276	1.567380	2.385735
C	4.113457	3.404850	-0.550716
H	3.447688	3.977857	-1.202932
H	4.909611	4.074649	-0.204304
H	4.563505	2.609195	-1.151985
C	2.257214	1.860751	0.198982

INT2-1-AC

Ru	0.634559	0.599723	-0.301608
C	1.281422	0.077412	-2.288515
H	1.424029	-0.996035	-2.440209
H	2.190630	0.618704	-2.551984
C	0.021875	0.622814	-2.941948
C	-0.929706	0.459978	-1.777255
C	-2.004797	1.506137	-1.641169
O	-1.896607	2.657610	-2.076184
N	-3.147327	1.069219	-1.027934
H	-3.102265	0.180266	-0.556437
C	-4.225957	1.960138	-0.655490
H	-5.179209	1.423002	-0.698124
H	-4.245127	2.791193	-1.362476
H	-4.093061	2.366164	0.356660
H	-1.347395	-0.542020	-1.717580
H	0.124890	1.687017	-3.170479
H	-0.285284	0.102124	-3.865553
C	0.365657	-1.246090	0.385743
N	1.484769	-1.892193	0.847012
C	2.796894	-1.351592	0.532162
C	2.556249	0.077824	0.044822
C	3.864040	0.719815	-0.420903
C	4.596866	-0.131354	-1.482002
C	4.858726	-1.542716	-0.927631
C	3.510814	-2.190282	-0.557481
H	3.678989	-3.208415	-0.181400
H	2.862935	-2.265851	-1.437311
C	5.751713	-1.453046	0.325392
C	5.044581	-0.599664	1.397623
C	4.779109	0.814759	0.833938
H	4.308276	1.447276	1.598220
H	5.730169	1.292394	0.562356
C	3.711943	-1.279697	1.782643

H	3.197079	-0.717907	2.572411
H	3.904952	-2.290369	2.170375
H	5.678579	-0.525458	2.290262
H	6.718614	-1.003307	0.064157
H	5.958735	-2.458204	0.718513
H	5.353152	-2.155687	-1.692001
H	5.548006	0.354743	-1.737889
H	4.012179	-0.195921	-2.403221
H	3.653880	1.722391	-0.808738
H	2.182600	0.696585	0.935405
C	1.247884	-3.284913	1.215782
C	-0.268848	-3.280498	1.402536
N	-0.680275	-2.098963	0.617318
C	-2.090038	-1.869312	0.498391
C	-2.769823	-2.450787	-0.598107
C	-4.164600	-2.343466	-0.644749
C	-4.869027	-1.691904	0.365163
C	-4.184035	-1.127011	1.437514
C	-2.786776	-1.202215	1.530797
C	-2.086980	-0.599976	2.742952
C	-2.490557	0.868001	2.976119
H	-1.910151	1.282144	3.809210
H	-3.551231	0.955834	3.240739
H	-2.285447	1.473343	2.091883
C	-2.371094	-1.441695	4.004530
H	-2.088534	-2.492408	3.873611
H	-1.817541	-1.042339	4.862405
H	-3.438901	-1.418109	4.253478
H	-1.008941	-0.610966	2.555573
H	-4.740700	-0.617152	2.217586
H	-5.951918	-1.618861	0.312764
H	-4.705450	-2.775309	-1.481176
C	-2.031195	-3.201352	-1.701186
C	-2.248769	-4.722186	-1.563926
H	-1.940760	-5.093043	-0.580124
H	-3.307937	-4.974899	-1.693680
H	-1.676697	-5.263464	-2.326685
C	-2.435854	-2.735791	-3.113175
H	-3.475045	-2.998067	-3.342705
H	-2.327878	-1.653575	-3.228698
H	-1.801880	-3.224538	-3.861867
H	-0.962377	-2.998587	-1.579578
H	-0.756336	-4.184036	1.031038
H	-0.549716	-3.140842	2.454045
H	1.790194	-3.564610	2.123623
H	1.554276	-3.961669	0.405600
O	0.930509	2.758903	-0.675085
C	-0.014938	3.035359	0.121133
O	-0.610673	2.061147	0.722771
C	-0.405700	4.477785	0.417658
C	-1.909860	4.561921	0.726502
H	-2.182143	5.597615	0.963965
H	-2.485175	4.234644	-0.142995
H	-2.176072	3.928247	1.577980
C	-0.065460	5.356326	-0.798007
H	1.003871	5.318183	-1.024141
H	-0.345068	6.397218	-0.593778
H	-0.612666	5.005192	-1.677714
C	0.417523	4.917503	1.650905
H	0.186915	4.291275	2.520584

H	1.492958	4.851446	1.448748
H	0.180736	5.957748	1.904719

INT2-AC

Ru	0.381653	-0.547533	-0.085859
O	1.928001	-0.233516	1.819699
O	2.018286	-1.944298	0.430728
N	-0.436024	1.980354	-1.201252
N	-2.286605	1.060385	-0.478334
C	-0.932185	0.901619	-0.542140
C	-1.426989	3.020269	-1.476567
H	-1.372289	3.353890	-2.516416
H	-1.268454	3.891943	-0.827867
C	-2.743881	2.289343	-1.159475
H	-3.403795	2.863309	-0.502062
H	-3.301813	2.028847	-2.066067
C	1.002757	2.211270	-1.156583
C	1.365381	3.139940	0.031483
H	0.977675	2.692575	0.954914
H	0.882742	4.118093	-0.101081
C	2.894170	3.312934	0.117471
H	3.132901	3.990738	0.947283
C	3.423512	3.902283	-1.205164
H	2.985587	4.894454	-1.384786
H	4.511700	4.036443	-1.144901
C	3.073961	2.952034	-2.369263
H	3.460863	3.361221	-3.311239
C	1.539003	2.821079	-2.470510
H	1.255034	2.175088	-3.311376
H	1.089914	3.809530	-2.645977
C	3.702347	1.565401	-2.109990
H	3.480148	0.887596	-2.945199
H	4.795621	1.657454	-2.050614
C	3.156122	0.976061	-0.778960
H	3.597822	-0.010772	-0.611970
C	1.639479	0.836598	-0.940299
H	1.437277	0.200330	-1.839374
C	3.531129	1.934916	0.370257
H	3.185460	1.525874	1.320941
H	4.625017	2.031556	0.420570
C	-3.151252	0.426431	0.469998
C	-3.085376	0.843301	1.818620
C	-3.906409	0.189169	2.744685
H	-3.857944	0.470825	3.792810
C	-4.784274	-0.815260	2.342229
C	-4.883320	-1.159799	0.996016
H	-5.600209	-1.915171	0.688456
C	-4.078276	-0.540279	0.031553
C	-2.188658	1.990607	2.280294
H	-1.687387	2.410364	1.403749
C	-4.278498	-0.840164	-1.449558
H	-3.422822	-0.425563	-1.991795
C	-0.635199	-1.469970	1.415322
H	-1.472963	-0.979747	1.896685
C	-0.710244	-1.810084	-1.200256
H	-1.602762	-1.425614	-1.686863
C	-1.041529	-2.410421	0.249120
H	-2.128000	-2.523875	0.280014
H	0.036947	-1.930639	2.139288
C	-5.547632	-0.120412	-1.953423

H	-5.672336	-0.269378	-3.032371
H	-6.440217	-0.511955	-1.450755
H	-5.504185	0.956988	-1.757431
C	-4.350035	-2.340893	-1.779179
H	-5.221695	-2.817422	-1.315918
H	-4.434512	-2.479365	-2.862424
H	-3.453510	-2.872440	-1.448721
C	-3.036779	3.120073	2.898775
H	-3.822626	3.453123	2.210473
H	-3.523100	2.795974	3.825950
H	-2.403101	3.981447	3.140296
C	-1.078873	1.538521	3.249025
H	-0.517509	2.411107	3.604753
H	-1.499628	1.033145	4.126743
H	-0.371422	0.861376	2.763921
H	-5.409377	-1.315474	3.077161
H	-0.551240	-3.380871	0.346687
C	-0.007131	-2.690736	-2.203381
O	-0.377189	-2.690575	-3.380357
N	1.031080	-3.467128	-1.764017
H	1.479272	-3.200422	-0.891751
C	1.835663	-4.198007	-2.727639
H	2.503919	-3.536984	-3.298653
H	2.438667	-4.942662	-2.200139
H	1.177603	-4.701313	-3.439046
C	2.458190	-1.315199	1.463414
C	3.629567	-1.933766	2.236356
C	3.161782	-3.299192	2.783322
H	2.850338	-3.958795	1.967762
H	3.975533	-3.785159	3.335101
H	2.314132	-3.177686	3.468929
C	4.804536	-2.141737	1.258665
H	5.157823	-1.183036	0.860114
H	5.644671	-2.622011	1.774641
H	4.503748	-2.771962	0.416674
C	4.055979	-1.015682	3.390611
H	3.227455	-0.844537	4.084378
H	4.887663	-1.469279	3.943387
H	4.380471	-0.039363	3.016588

INT3-AC

Ru	0.518297	0.217089	0.394889
C	-0.524196	0.253286	1.893772
C	-0.350110	1.019732	3.174153
O	-1.080872	0.734148	4.132199
N	0.603275	1.984242	3.247286
H	1.189517	2.155442	2.437068
C	0.839177	2.709515	4.480328
H	-0.116095	2.983743	4.937166
H	1.397352	2.106530	5.209208
H	1.411156	3.614574	4.258575
H	-1.450101	-0.320668	1.952769
C	-0.517719	-1.289784	-0.310249
N	-1.801313	-1.476993	-0.698439
C	-2.832491	-0.477960	-0.653860
C	-2.858993	0.508264	-1.667664
C	-3.870047	1.473476	-1.608437
C	-4.825946	1.456580	-0.594614
C	-4.786146	0.471743	0.386182
C	-3.786877	-0.509743	0.384102

C	-3.796116	-1.596789	1.455126
C	-4.886715	-2.640374	1.131255
H	-5.881001	-2.180784	1.182506
H	-4.859103	-3.466594	1.851610
H	-4.769881	-3.056127	0.124028
C	-3.988686	-1.055233	2.885014
H	-4.966921	-0.576006	3.006049
H	-3.945957	-1.887519	3.597476
H	-3.213882	-0.336981	3.169947
H	-2.823798	-2.101735	1.434386
H	-5.536079	0.467152	1.170963
H	-5.604030	2.215180	-0.571127
H	-3.915532	2.249747	-2.364403
C	-1.857244	0.501267	-2.820116
C	-2.311714	-0.474416	-3.925106
H	-1.581985	-0.494654	-4.743782
H	-3.278713	-0.164704	-4.339661
H	-2.423328	-1.495833	-3.549029
C	-1.600904	1.890707	-3.423054
H	-1.338933	2.609663	-2.644039
H	-2.467772	2.264756	-3.981452
H	-0.761195	1.834523	-4.125041
H	-0.898716	0.151175	-2.430033
C	-2.030214	-2.876733	-1.117180
H	-2.669367	-2.921196	-2.000905
H	-2.510809	-3.440935	-0.309399
C	-0.594420	-3.374686	-1.364094
N	0.158850	-2.453769	-0.513636
C	1.613719	-2.363996	-0.362134
C	2.278510	-3.709918	-0.024398
C	3.786244	-3.463320	0.229958
C	4.436242	-2.894841	-1.048713
C	3.769547	-1.552645	-1.414264
C	2.266558	-1.791032	-1.648391
H	2.114460	-2.489006	-2.484106
H	1.770050	-0.849528	-1.926368
C	3.946879	-0.545030	-0.259388
C	3.302863	-1.104510	1.026403
C	1.804050	-1.386431	0.830606
H	1.426349	-1.894188	1.723350
C	3.982979	-2.452343	1.382979
H	3.557654	-2.850914	2.313473
H	5.057755	-2.301755	1.557517
H	3.436839	-0.390032	1.847364
H	5.015911	-0.357220	-0.089973
H	3.491692	0.419419	-0.517752
H	4.221633	-1.151968	-2.330982
H	5.512361	-2.748177	-0.886600
H	4.329278	-3.607496	-1.878578
H	4.262055	-4.416878	0.492172
H	1.800959	-4.140465	0.865121
H	2.153516	-4.427811	-0.848973
H	-0.449225	-4.415402	-1.064533
H	-0.300227	-3.266029	-2.419124
O	1.855751	2.120270	0.666120
C	1.358787	2.544466	-0.417662
O	0.495784	1.816876	-1.038194
C	1.733983	3.901313	-1.005704
C	2.936405	4.495207	-0.257676
H	3.812950	3.844140	-0.339871

H	2.716163	4.622697	0.806182
H	3.190917	5.474002	-0.680656
C	2.060063	3.722677	-2.502475
H	2.928364	3.066811	-2.639668
H	1.212962	3.285178	-3.037269
H	2.296368	4.694769	-2.950734
C	0.498705	4.818202	-0.845701
H	0.236258	4.944049	0.211253
H	-0.368353	4.402189	-1.367242
H	0.715412	5.808342	-1.263479

TS2-*cross*-AC

Ru	-0.348122	0.501833	-0.097843
O	-1.785566	0.174709	1.793709
O	-1.983747	1.922475	0.466496
N	0.309229	-2.076594	-1.210396
N	2.213552	-1.250147	-0.513942
C	0.864826	-1.023819	-0.560940
C	1.240987	-3.172663	-1.474218
H	1.153463	-3.526807	-2.504795
H	1.045506	-4.020345	-0.803392
C	2.598418	-2.505055	-1.192095
H	3.243930	-3.105228	-0.543796
H	3.150106	-2.279132	-2.112475
C	-1.145424	-2.220103	-1.187701
C	-1.576531	-3.051385	0.046990
H	-1.187957	-2.564205	0.949384
H	-1.141444	-4.059619	-0.009842
C	-3.113496	-3.143868	0.108874
H	-3.404032	-3.754108	0.974279
C	-3.648302	-3.788025	-1.184909
H	-3.258479	-4.810333	-1.293880
H	-4.743069	-3.863590	-1.139864
C	-3.227999	-2.929309	-2.395473
H	-3.618358	-3.375717	-3.319336
C	-1.684582	-2.892439	-2.468054
H	-1.348099	-2.324561	-3.345541
H	-1.297133	-3.917508	-2.569011
C	-3.793902	-1.499735	-2.231119
H	-3.530759	-0.887798	-3.104511
H	-4.891611	-1.543966	-2.187158
C	-3.232336	-0.853213	-0.934743
H	-3.631364	0.161920	-0.832663
C	-1.700514	-0.789173	-1.092288
H	-1.513419	-0.312319	-2.068031
C	-3.682822	-1.721236	0.259805
H	-3.337106	-1.287811	1.198094
H	-4.781580	-1.761553	0.290022
C	3.121183	-0.652063	0.415432
C	3.076872	-1.076494	1.762954
C	3.940415	-0.454144	2.672325
H	3.909877	-0.741404	3.719676
C	4.840249	0.523976	2.253146
C	4.917740	0.872984	0.906670
H	5.652073	1.605609	0.585157
C	4.068620	0.286796	-0.040917
C	2.161305	-2.205482	2.235406
H	1.637896	-2.610350	1.365057
C	4.243832	0.586482	-1.526239
H	3.377655	0.171835	-2.052056

C	0.772742	1.421513	1.560525
H	1.464521	0.700395	1.970011
C	1.239002	2.313961	0.566836
H	2.245636	2.140329	0.201556
C	0.755209	3.745205	0.523875
H	1.244285	4.294170	1.340297
H	1.012603	4.241781	-0.415042
H	-0.325775	3.794999	0.677664
H	0.026964	1.793732	2.258090
C	5.499813	-0.144866	-2.046625
H	5.604861	-0.007384	-3.129135
H	6.404536	0.245969	-1.565613
H	5.452480	-1.220056	-1.838763
C	4.315238	2.085843	-1.865782
H	5.145240	2.581152	-1.349106
H	4.474402	2.213140	-2.942198
H	3.387888	2.610447	-1.619683
C	2.994252	-3.355027	2.837275
H	3.766163	-3.697961	2.138275
H	3.496344	-3.047101	3.761571
H	2.346682	-4.205741	3.079393
C	1.074094	-1.736529	3.222050
H	0.515027	-2.601935	3.597759
H	1.515037	-1.224092	4.085757
H	0.358108	-1.062231	2.744980
H	5.499716	0.998693	2.974850
C	0.559088	1.506599	-1.416774
H	1.538583	1.241888	-1.822661
C	0.073046	2.714586	-2.177677
O	0.852730	3.318427	-2.925119
N	-1.225939	3.081112	-2.021732
H	-1.749238	2.665393	-1.256325
C	-1.719931	4.303016	-2.628220
H	-2.811137	4.315909	-2.567368
H	-1.322212	5.197411	-2.128056
H	-1.412462	4.343158	-3.676121
C	-2.375418	1.245275	1.483257
C	-3.552916	1.783246	2.304629
C	-3.192272	3.208635	2.773481
H	-2.989712	3.859663	1.918094
H	-4.019397	3.636801	3.352372
H	-2.301963	3.198416	3.414526
C	-4.794633	1.837303	1.389467
H	-5.075464	0.834261	1.048959
H	-5.646136	2.261297	1.935305
H	-4.601253	2.457273	0.508692
C	-3.826703	0.879635	3.515442
H	-2.947176	0.811182	4.163234
H	-4.661080	1.283117	4.101939
H	-4.084920	-0.135771	3.200330

TS2-*homo*-AC

Ru	-0.344078	0.265813	-0.114925
O	-1.736689	-0.018787	1.813357
O	-1.972578	1.723179	0.487982
N	0.284054	-2.326788	-1.198366
N	2.199249	-1.509512	-0.511757
C	0.853992	-1.275660	-0.559960
C	1.208010	-3.431128	-1.458127
H	1.106321	-3.798222	-2.482571

H	1.016975	-4.267758	-0.772433	
C	2.569806	-2.763354	-1.202377	
H	3.230621	-3.363547	-0.570564	
H	3.097314	-2.531553	-2.134621	
C	-1.170697	-2.466962	-1.145741	
C	-1.575799	-3.284862	0.106812	
H	-1.164948	-2.791460	0.995954	
H	-1.145034	-4.294641	0.049899	
C	-3.110743	-3.372927	0.204836	
H	-3.382751	-3.973702	1.082684	
C	-3.676265	-4.028419	-1.070069	
H	-3.291287	-5.052591	-1.177089	
H	-4.769821	-4.100928	-0.999515	
C	-3.281389	-3.182932	-2.298338	
H	-3.693555	-3.637207	-3.208554	
C	-1.739633	-3.150391	-2.406944	
H	-1.421710	-2.592387	-3.297363	
H	-1.356535	-4.177097	-2.505720	
C	-3.841757	-1.750891	-2.135242	
H	-3.598545	-1.147843	-3.020382	
H	-4.938053	-1.792944	-2.064818	
C	-3.249141	-1.092291	-0.858604	
H	-3.643776	-0.075069	-0.757823	
C	-1.722048	-1.034576	-1.055188	
H	-1.558720	-0.571830	-2.041727	
C	-3.672920	-1.947493	0.354876	
H	-3.306002	-1.506476	1.281962	
H	-4.770663	-1.984827	0.410705	
C	3.110052	-0.937449	0.434222	
C	3.035941	-1.367932	1.778447	
C	3.907250	-0.776937	2.701587	
H	3.856303	-1.069976	3.746543	
C	4.841318	0.175375	2.298986	
C	4.941987	0.534328	0.956721	
H	5.691373	1.257371	0.650497	
C	4.085922	-0.018281	-0.003996	
C	2.083668	-2.472175	2.235985	
H	1.551748	-2.853950	1.360432	
C	4.257280	0.319024	-1.481007	
H	3.348119	-0.003202	-1.999416	
C	0.802744	1.226608	1.501949	
H	1.449062	0.493517	1.964200	
H	0.094158	1.698201	2.176263	
C	5.435937	-0.492787	-2.059988	
H	5.533130	-0.313891	-3.137114	
H	6.377576	-0.199020	-1.580692	
H	5.305040	-1.569109	-1.899880	
C	4.454524	1.819523	-1.767114	
H	5.406323	2.182218	-1.361229	
H	4.478788	1.983544	-2.850079	
H	3.656047	2.445532	-1.356655	
C	2.875841	-3.652983	2.832068	
H	3.637918	-4.016185	2.132597	
H	3.385418	-3.368132	3.759560	
H	2.199810	-4.483589	3.066337	
C	1.008278	-1.975170	3.221322	
H	0.410220	-2.822121	3.578802	
H	1.462363	-1.495128	4.096654	
H	0.324596	-1.264539	2.749604	
H	5.505272	0.626647	3.031393	

C	0.514223	1.223450	-1.508794
H	1.500002	0.989420	-1.915658
C	-0.125764	2.224268	-2.441076
O	0.392815	2.400242	-3.546597
N	-1.284508	2.825841	-2.066899
H	-1.740636	2.525773	-1.212487
C	-1.980354	3.714274	-2.978568
H	-2.716867	4.294959	-2.416709
H	-1.261963	4.392228	-3.447460
H	-2.493056	3.163292	-3.778238
C	1.325819	1.980028	0.425439
H	2.310599	1.707143	0.075387
C	1.058768	3.447442	0.196058
O	1.924959	4.132586	-0.345875
N	-0.119370	3.946317	0.659566
H	-0.867069	3.278666	0.828872
C	-0.506628	5.305358	0.321798
H	-0.804870	5.390847	-0.731968
H	-1.342050	5.606526	0.959992
H	0.339065	5.974489	0.491371
C	-3.495467	1.582417	2.369099
C	-3.664391	0.739992	3.641821
H	-4.496480	1.129749	4.240081
H	-3.872679	-0.305562	3.397170
H	-2.756885	0.762532	4.253694
C	-3.190489	3.050235	2.735563
H	-3.108164	3.669508	1.836995
H	-3.994534	3.456538	3.360019
H	-2.252287	3.133906	3.297791
C	-4.780270	1.520289	1.514279
H	-5.028804	0.486440	1.251379
H	-5.623192	1.940565	2.075640
H	-4.659757	2.091341	0.588309
C	-2.337282	1.046154	1.522253

INT4-*cross*-AC

Ru	0.399384	-0.455334	-0.089480
O	2.000701	-0.212066	1.820720
O	2.012756	-1.886902	0.382619
N	-0.359457	2.093527	-1.198765
N	-2.233296	1.219308	-0.479678
C	-0.882984	1.026573	-0.539821
C	-1.323554	3.159139	-1.471821
H	-1.259365	3.495128	-2.510410
H	-1.143809	4.024537	-0.820187
C	-2.658744	2.461013	-1.158178
H	-3.304259	3.049855	-0.499638
H	-3.223397	2.217276	-2.065430
C	1.084755	2.288798	-1.154379
C	1.471506	3.202029	0.038093
H	1.075576	2.758218	0.959753
H	1.011090	4.191761	-0.087543
C	3.004005	3.339243	0.121424
H	3.260286	4.006099	0.954842
C	3.543818	3.924597	-1.198733
H	3.128486	4.927674	-1.371354
H	4.634939	4.033236	-1.140252
C	3.169911	2.989899	-2.367849
H	3.563731	3.396236	-3.308257
C	1.632285	2.894633	-2.465567

H	1.331965	2.260850	-3.310234
H	1.205586	3.894133	-2.634172
C	3.766504	1.587546	-2.118855
H	3.526470	0.920253	-2.957718
H	4.861803	1.653915	-2.062087
C	3.210120	1.002621	-0.790388
H	3.630673	0.005430	-0.630819
C	1.689619	0.897827	-0.946649
H	1.469999	0.270185	-1.847675
C	3.609875	1.945425	0.363842
H	3.258090	1.537602	1.312756
H	4.705828	2.016925	0.411659
C	-3.118394	0.604954	0.462995
C	-3.044710	1.015210	1.813307
C	-3.884369	0.379233	2.735195
H	-3.830966	0.655481	3.784555
C	-4.789400	-0.598097	2.325996
C	-4.897041	-0.931807	0.977764
H	-5.634910	-1.664506	0.665189
C	-4.072464	-0.332111	0.017081
C	-2.128223	2.146126	2.278314
H	-1.611285	2.551971	1.404378
C	-4.281511	-0.620671	-1.466039
H	-3.424842	-0.209360	-2.009764
C	-0.626960	-1.332689	1.427821
H	-1.415984	-0.795767	1.941354
C	-1.139918	-2.258963	0.289569
H	-2.227836	-2.165955	0.296013
C	-0.730150	-3.720786	0.503318
H	-1.158467	-4.086242	1.443623
H	-1.094546	-4.354720	-0.312503
H	0.356849	-3.816056	0.563873
H	0.042976	-1.834012	2.128384
C	-5.545508	0.119357	-1.954140
H	-5.675822	-0.012810	-3.034575
H	-6.440436	-0.270519	-1.454407
H	-5.490408	1.193500	-1.742408
C	-4.368795	-2.117602	-1.811925
H	-5.204449	-2.605243	-1.296918
H	-4.529643	-2.237722	-2.888795
H	-3.446942	-2.650875	-1.566627
C	-2.961852	3.294162	2.882717
H	-3.735638	3.636653	2.185440
H	-3.462242	2.983574	3.807014
H	-2.315569	4.145890	3.125150
C	-1.035036	1.681751	3.259905
H	-0.467812	2.548117	3.621434
H	-1.470622	1.181395	4.133181
H	-0.330131	0.996299	2.782688
H	-5.429793	-1.084102	3.057307
C	-0.736435	-1.682862	-1.178606
H	-1.624371	-1.273807	-1.655255
C	-0.185899	-2.707167	-2.154514
O	-0.929297	-3.172786	-3.023188
N	1.119498	-3.072874	-2.044131
H	1.648793	-2.754386	-1.238159
C	1.655021	-4.146564	-2.860378
H	2.746719	-4.128916	-2.801674
H	1.295700	-5.131435	-2.530554
H	1.343837	-4.009362	-3.898999

C	2.491747	-1.294976	1.421247
C	3.653070	-1.976608	2.156495
C	3.116429	-3.301876	2.739175
H	2.734255	-3.949716	1.944260
H	3.915397	-3.833720	3.269933
H	2.302658	-3.116203	3.450735
C	4.777112	-2.273316	1.143552
H	5.174348	-1.345379	0.714461
H	5.604133	-2.796045	1.639071
H	4.409117	-2.898076	0.324603
C	4.177373	-1.073954	3.282176
H	3.386233	-0.842147	4.001120
H	4.998481	-1.572042	3.812013
H	4.548912	-0.124580	2.882703

INT4-*homo*-AC

Ru	-0.389081	0.210787	-0.131386
O	-1.959536	0.095949	1.799566
O	-1.957313	1.744675	0.332969
N	0.262383	-2.414372	-1.115341
N	2.168041	-1.581579	-0.425536
C	0.827933	-1.342161	-0.503668
C	1.186039	-3.528178	-1.332649
H	1.103117	-3.918663	-2.350334
H	0.979549	-4.347730	-0.631422
C	2.545764	-2.859704	-1.065209
H	3.185704	-3.442515	-0.396663
H	3.099072	-2.662757	-1.990324
C	-1.188872	-2.548956	-1.068120
C	-1.615952	-3.392837	0.160936
H	-1.202270	-2.928525	1.064469
H	-1.199099	-4.405994	0.078848
C	-3.153326	-3.460340	0.244433
H	-3.439446	-4.078683	1.105003
C	-3.715537	-4.078516	-1.051150
H	-3.343018	-5.104759	-1.178355
H	-4.810339	-4.138230	-0.991870
C	-3.299869	-3.212104	-2.258096
H	-3.708772	-3.641527	-3.181480
C	-1.759182	-3.186478	-2.354432
H	-1.430239	-2.602922	-3.224093
H	-1.375260	-4.209463	-2.478242
C	-3.837722	-1.776578	-2.072099
H	-3.568616	-1.156867	-2.938121
H	-4.934862	-1.794202	-2.015901
C	-3.258735	-1.158614	-0.768398
H	-3.635730	-0.138264	-0.654400
C	-1.736030	-1.127031	-0.923582
H	-1.488996	-0.551909	-1.852029
C	-3.700342	-2.032619	0.424150
H	-3.333888	-1.601412	1.357346
H	-4.798421	-2.055936	0.471001
C	3.073135	-0.973168	0.504644
C	2.972511	-1.338164	1.866237
C	3.831389	-0.709040	2.775099
H	3.758768	-0.949535	3.832055
C	4.777337	0.218889	2.344069
C	4.905423	0.510024	0.987997
H	5.665105	1.212528	0.660202
C	4.064692	-0.085353	0.038806

C	1.998516	-2.406125	2.361373		Ru	0.487045	0.105534	-0.249178
H	1.482047	-2.830238	1.495666		O	2.215582	1.227943	-0.821666
C	4.278008	0.173542	-1.448439		O	3.105490	1.558701	1.213621
H	3.388045	-0.180743	-1.978221		N	-0.586180	-2.493753	0.414623
C	0.687320	1.132754	1.324383		N	-2.367284	-1.313754	-0.045741
H	1.457392	0.594074	1.864480		C	-1.006114	-1.244303	0.083297
H	0.061157	1.711263	2.002848		C	-1.621866	-3.517431	0.279448
C	5.477650	-0.660152	-1.947684		H	-1.588900	-4.235762	1.102609
H	5.609554	-0.533032	-3.028485		H	-1.500652	-4.066702	-0.664403
H	6.402486	-0.339971	-1.452950		C	-2.889969	-2.658399	0.281210
H	5.344139	-1.728244	-1.740016		H	-3.629706	-2.972417	-0.458959
C	4.475638	1.658619	-1.806041		H	-3.373154	-2.641369	1.265572
H	5.421104	2.043022	-1.405294		C	0.845565	-2.765153	0.356508
H	4.511777	1.769946	-2.895073		C	1.251214	-3.227298	-1.069535
H	3.670397	2.299640	-1.435713		H	0.907690	-2.480377	-1.797414
C	2.763023	-3.561134	3.038617		H	0.748394	-4.175300	-1.306984
H	3.535044	-3.971474	2.377040		C	2.777385	-3.402853	-1.153510
H	3.256487	-3.231266	3.959830		H	3.049401	-3.733244	-2.164558
H	2.071848	-4.369692	3.304066		C	3.217098	-4.464013	-0.123862
C	0.908367	-1.842927	3.293409		H	2.753711	-5.432899	-0.358236
H	0.286326	-2.660928	3.676981		H	4.304679	-4.606784	-0.173240
H	1.350404	-1.328341	4.155058		C	2.813736	-4.008982	1.294527
H	0.253004	-1.142209	2.769863		H	3.127833	-4.763042	2.027670
H	5.429691	0.703109	3.065765		C	1.279182	-3.845825	1.368888
C	0.781410	1.303659	-1.323842		H	0.969306	-3.545740	2.378494
H	1.644098	0.835626	-1.789402		H	0.790949	-4.805317	1.143213
C	0.184121	2.190709	-2.401799		C	3.494095	-2.660817	1.603143
O	0.736709	2.250906	-3.500828		H	3.240664	-2.329027	2.618895
N	-0.970972	2.865709	-2.138840		H	4.586111	-2.778573	1.566749
H	-1.498812	2.637482	-1.305190		C	3.051335	-1.588381	0.573479
C	-1.602691	3.660949	-3.175727		H	3.539845	-0.647503	0.820595
H	-2.381848	4.280006	-2.722239		C	1.527289	-1.423810	0.691701
H	-0.857560	4.305012	-3.649724		H	1.269922	-1.134011	1.728859
H	-2.052079	3.036344	-3.959779		C	3.448915	-2.052057	-0.841663
C	1.252487	1.921441	0.113213		H	3.148282	-1.295965	-1.576237
H	2.324214	1.737779	0.107398		H	4.540715	-2.151487	-0.909371
C	1.094680	3.445275	0.129960		C	-3.300100	-0.222459	0.008467
O	2.006738	4.138488	-0.311478		C	-3.950285	0.180398	-1.176447
N	-0.055319	3.953586	0.647962		C	-4.855641	1.246502	-1.100295
H	-0.833345	3.309830	0.756821		H	-5.361566	1.583381	-2.000027
C	-0.372087	5.359314	0.462462		C	-5.120103	1.878567	0.111240
H	-0.684555	5.569492	-0.569996		C	-4.507335	1.432101	1.279105
H	-1.176706	5.639132	1.147851		H	-4.734114	1.920610	2.221854
H	0.514961	5.958089	0.677252		C	-3.597473	0.369544	1.258335
C	-3.589806	1.878608	2.123751		C	-3.748962	-0.556101	-2.495714
C	-3.779386	1.270395	3.521357		H	-2.869354	-1.198512	-2.384878
H	-4.623469	1.752182	4.029111		C	-2.998457	-0.131145	2.572224
H	-3.974983	0.196495	3.457895		H	-2.255443	-0.901524	2.346484
H	-2.882950	1.407886	4.135341		C	-0.130967	0.495171	-2.086740
C	-3.294356	3.387269	2.231840		H	-0.883708	-0.136247	-2.558811
H	-3.196941	3.840482	1.240733		C	-0.735944	1.781418	-1.377659
H	-4.108749	3.894033	2.762550		H	-1.809679	1.731897	-1.573180
H	-2.365931	3.570844	2.786606		C	-0.129541	3.068731	-1.944128
C	-4.862496	1.659528	1.275247		H	-0.262311	3.093919	-3.031717
H	-5.101859	0.593114	1.194867		H	-0.616818	3.941778	-1.504422
H	-5.716274	2.164741	1.742414		H	0.940202	3.109558	-1.727294
H	-4.732811	2.062081	0.265074		H	0.695003	0.744910	-2.758683
C	-2.430691	1.183140	1.397677		C	-3.501680	0.381748	-3.691038
					H	-3.279378	-0.206814	-4.588630
INT4-*cross*-2-AC					H	-4.382781	0.994315	-3.912787

H	-2.660723	1.057617	-3.512064
C	-4.963646	-1.464325	-2.781984
H	-4.804034	-2.047955	-3.696424
H	-5.151344	-2.161839	-1.958197
H	-5.871128	-0.863825	-2.917030
C	-4.101411	-0.778755	3.436235
H	-4.843775	-0.033544	3.744993
H	-4.634397	-1.566665	2.891551
H	-3.669913	-1.218660	4.342919
C	-2.269500	0.965180	3.372813
H	-1.405098	1.358856	2.833960
H	-2.931511	1.805764	3.606974
H	-1.910374	0.550365	4.322122
H	-5.814198	2.713473	0.148271
C	-0.668580	1.686779	0.218518
H	-1.652364	1.427793	0.589943
C	-0.308172	2.970534	0.955490
O	-1.112342	3.906961	0.897474
N	0.803048	2.997998	1.712730
H	1.518152	2.272083	1.605822
C	1.176733	4.210981	2.419930
H	2.122370	4.028908	2.935030
H	1.295195	5.054722	1.729151
H	0.407458	4.484753	3.149699
C	3.147992	1.636729	-0.031939
C	4.380021	2.250686	-0.733297
C	5.373842	2.778114	0.311137
H	6.251143	3.210026	-0.186457
H	4.913127	3.549861	0.935854
H	5.707272	1.975858	0.975966
C	5.045455	1.155436	-1.591092
H	4.344676	0.768450	-2.336779
H	5.922130	1.560623	-2.111723
H	5.380093	0.316547	-0.969180
C	3.908413	3.401712	-1.643926
H	4.767723	3.870153	-2.139824
H	3.221892	3.033840	-2.411479
H	3.390442	4.175936	-1.064370

INT4-*homo*-2-AC

Ru	-0.483880	0.108095	-0.233847
O	-2.224007	-1.064844	-0.725749
O	-2.506679	-0.847232	1.470034
N	0.660888	2.724514	0.085517
N	2.407301	1.414177	0.015725
C	1.041168	1.428157	0.041067
C	1.758710	3.690047	0.062895
H	1.801249	4.249180	1.005500
H	1.634898	4.409050	-0.753291
C	2.976746	2.773606	-0.147185
H	3.401088	2.880772	-1.150824
H	3.777225	2.943662	0.576635
C	-0.749807	3.038763	-0.106816
C	-1.043396	3.267351	-1.614154
H	-0.687839	2.398273	-2.182125
H	-0.480940	4.143549	-1.967776
C	-2.552687	3.474531	-1.831874
H	-2.747180	3.636008	-2.900048
C	-3.007063	4.710081	-1.027588
H	-2.486821	5.608128	-1.389608

H	-4.081994	4.879829	-1.173483
C	-2.712628	4.490839	0.471416
H	-3.036558	5.369481	1.043846
C	-1.193957	4.289779	0.679555
H	-0.965131	4.154390	1.744845
H	-0.646753	5.178874	0.332955
C	-3.475307	3.240380	0.954173
H	-3.303054	3.078339	2.026616
H	-4.555693	3.390878	0.820381
C	-3.016456	1.993430	0.153430
H	-3.561171	1.124177	0.518472
C	-1.514305	1.803664	0.410769
H	-1.342219	1.704205	1.494604
C	-3.302761	2.218380	-1.343690
H	-2.990025	1.335812	-1.915185
H	-4.382626	2.341712	-1.502444
C	3.290462	0.328403	0.331531
C	4.103552	-0.216972	-0.684498
C	5.017876	-1.219726	-0.335045
H	5.647036	-1.657687	-1.103577
C	5.119964	-1.671174	0.974594
C	4.305760	-1.126063	1.966215
H	4.391424	-1.500370	2.980048
C	3.381780	-0.117168	1.675031
C	4.032846	0.255308	-2.132222
H	3.142522	0.884512	-2.234154
C	2.500351	0.468829	2.779879
H	1.515231	0.671389	2.344969
C	0.300972	-0.406391	-1.964075
H	1.130530	0.138237	-2.415950
H	-0.448130	-0.706516	-2.699988
C	3.898006	-0.907131	-3.137183
H	3.710034	-0.508271	-4.140826
H	4.820406	-1.496398	-3.189775
H	3.087125	-1.595965	-2.883227
C	5.267531	1.111880	-2.482359
H	5.190835	1.500767	-3.504606
H	5.385144	1.960060	-1.798963
H	6.181805	0.510102	-2.418937
C	3.059925	1.807051	3.302741
H	4.070273	1.670079	3.705963
H	3.109418	2.566816	2.519116
H	2.423569	2.198283	4.105346
C	2.282577	-0.492309	3.961741
H	1.975068	-1.488322	3.628633
H	3.188701	-0.600426	4.569332
H	1.501911	-0.093377	4.620052
H	5.828243	-2.455597	1.226316
C	0.513157	-1.532569	0.439949
H	1.423534	-1.321799	0.993929
C	-0.270194	-2.603519	1.168111
O	-0.789808	-3.585463	0.645771
N	-0.280196	-2.396513	2.526818
H	-0.158001	-1.428691	2.797046
C	-1.191752	-3.157848	3.368410
H	-1.222873	-4.184589	3.001310
H	-0.824741	-3.152806	4.399306
H	-2.201842	-2.734474	3.332021
C	0.841312	-1.644268	-1.089326
H	1.924995	-1.554221	-1.119553

C	0.516924	-2.985237	-1.777525
O	1.449670	-3.748412	-2.009859
N	-0.764691	-3.183156	-2.171165
H	-1.458754	-2.602815	-1.702159
C	-1.183457	-4.516622	-2.569084
H	-1.313550	-5.164161	-1.692092
H	-2.128700	-4.452102	-3.114532
H	-0.418642	-4.951366	-3.215152
C	-4.209811	-2.058863	0.214437
C	-5.226767	-1.112713	-0.461799
H	-4.841577	-0.748160	-1.419509
H	-6.169518	-1.642865	-0.644954
H	-5.447071	-0.246622	0.173762
C	-3.983827	-3.296877	-0.673865
H	-3.177709	-3.919277	-0.272285
H	-4.900614	-3.897352	-0.721867
H	-3.719003	-3.003011	-1.693933
C	-4.732873	-2.493149	1.590896
H	-5.712607	-2.975324	1.486365
H	-4.048665	-3.209219	2.057037
H	-4.831778	-1.635586	2.262201
C	-2.888622	-1.282037	0.365387

TS3-*cross*-AC

Ru	0.488469	0.072508	-0.531608
O	2.136451	1.543317	-1.002287
O	1.494672	1.404900	1.103117
N	-0.059611	-2.495083	0.664243
N	-2.020889	-1.538153	0.501251
C	-0.683242	-1.351986	0.267618
C	-0.983481	-3.584100	0.970401
H	-0.655614	-4.159510	1.839930
H	-1.073854	-4.268399	0.114272
C	-2.277384	-2.805918	1.217165
H	-3.167483	-3.300496	0.822947
H	-2.434921	-2.601191	2.284177
C	1.344375	-2.674708	0.302167
C	1.469747	-3.371850	-1.074697
H	0.869241	-2.829303	-1.810873
H	1.070335	-4.394197	-1.009167
C	2.945873	-3.407069	-1.506876
H	3.026261	-3.887676	-2.491067
C	3.751448	-4.213669	-0.468180
H	3.383197	-5.248687	-0.427541
H	4.808978	-4.259060	-0.761273
C	3.620624	-3.544915	0.916378
H	4.185744	-4.122367	1.659586
C	2.129971	-3.513479	1.335987
H	2.017802	-3.065289	2.331668
H	1.741548	-4.541697	1.388930
C	4.188193	-2.111063	0.827522
H	4.147888	-1.622200	1.809948
H	5.246303	-2.154502	0.531461
C	3.371029	-1.288391	-0.201117
H	3.775031	-0.276262	-0.266014
C	1.918060	-1.244583	0.298799
H	1.926467	-0.908819	1.343762
C	3.476471	-1.960465	-1.583393
H	2.900619	-1.384108	-2.317965
H	4.523143	-1.965325	-1.918127

C	-3.024663	-0.517373	0.591492
C	-4.028519	-0.470429	-0.400409
C	-5.009697	0.522167	-0.297721
H	-5.789842	0.584257	-1.050847
C	-5.002782	1.429303	0.759252
C	-4.026778	1.342543	1.747711
H	-4.034839	2.050261	2.570598
C	-3.024618	0.366056	1.694622
C	-4.096598	-1.502498	-1.522118
H	-3.143104	-2.041695	-1.531609
C	-2.005174	0.273020	2.827504
H	-1.247173	-0.466952	2.555774
C	0.039861	-0.474883	-2.279339
H	-0.711897	-1.196228	-2.625965
C	-1.217383	1.121308	-1.859388
H	-2.087369	0.476458	-1.809298
C	-1.082889	1.848293	-3.190928
H	-1.367237	1.191235	-4.018627
H	-1.753697	2.716336	-3.191632
H	-0.072321	2.215351	-3.372290
H	0.656620	-0.092981	-3.104235
C	-4.297131	-0.885933	-2.918925
H	-4.276638	-1.673379	-3.681294
H	-5.263138	-0.375461	-3.001952
H	-3.515905	-0.159800	-3.164196
C	-5.220126	-2.521366	-1.236746
H	-5.231731	-3.311039	-1.997508
H	-5.101130	-2.992324	-0.255024
H	-6.198990	-2.027150	-1.246081
C	-2.698345	-0.215122	4.116968
H	-3.437036	0.516866	4.464550
H	-3.223323	-1.165633	3.963910
H	-1.961521	-0.354293	4.916678
C	-1.260599	1.597359	3.081868
H	-0.699569	1.925134	2.206134
H	-1.949605	2.399569	3.368348
H	-0.545236	1.460551	3.901291
H	-5.764965	2.201540	0.816865
C	-0.944663	1.755295	-0.595029
H	-1.654805	1.519138	0.183462
C	-0.602231	3.220182	-0.478867
O	-1.279815	3.923495	0.272114
N	0.362623	3.745587	-1.288013
H	1.087294	3.113942	-1.613034
C	0.618382	5.175100	-1.280428
H	1.245129	5.426817	-2.140490
H	-0.331007	5.711374	-1.353667
H	1.120287	5.511660	-0.364572
C	2.273409	1.882263	0.228781
C	3.389208	2.839854	0.667315
C	4.486171	1.993851	1.354338
H	5.255395	2.653173	1.774477
H	4.061730	1.394123	2.165834
H	4.973976	1.318012	0.643492
C	3.988431	3.582105	-0.536369
H	3.245230	4.223005	-1.021374
H	4.817356	4.220205	-0.207287
H	4.364089	2.878153	-1.284428
C	2.806121	3.834302	1.691197
H	3.580407	4.542278	2.010621

H	1.972763	4.401941	1.265318
H	2.426712	3.304945	2.568918

TS3-*homo*-AC

Ru	0.527833	0.016619	-0.352518
O	1.919325	1.703142	-0.605390
O	1.339494	1.297609	1.477329
N	0.260804	-2.814884	0.133123
N	-1.803566	-2.079693	0.031042
C	-0.483892	-1.687144	0.001181
C	-0.517856	-4.047157	0.036519
H	-0.188540	-4.790613	0.767511
H	-0.424647	-4.484775	-0.967057
C	-1.936327	-3.528539	0.303415
H	-2.689206	-3.978762	-0.346505
H	-2.241177	-3.686960	1.346136
C	1.707309	-2.722021	-0.064963
C	2.085547	-3.057290	-1.527624
H	1.487639	-2.443253	-2.208592
H	1.847924	-4.109607	-1.739829
C	3.586273	-2.797735	-1.749044
H	3.843344	-3.021315	-2.792882
C	4.393324	-3.715045	-0.807678
H	4.189385	-4.769304	-1.043148
H	5.469864	-3.554515	-0.954017
C	4.013806	-3.411021	0.656764
H	4.580435	-4.068681	1.328763
C	2.500612	-3.669892	0.863377
H	2.215574	-3.481734	1.906811
H	2.273514	-4.723560	0.642116
C	4.354667	-1.935519	0.959424
H	4.131464	-1.699737	2.008586
H	5.431978	-1.771612	0.813801
C	3.535692	-1.006451	0.027689
H	3.778773	0.034832	0.247577
C	2.048916	-1.265597	0.308752
H	1.889017	-1.167942	1.393769
C	3.891079	-1.317071	-1.438225
H	3.314453	-0.662178	-2.102608
H	4.955324	-1.111498	-1.618327
C	-2.874826	-1.222519	0.454044
C	-3.853080	-0.823879	-0.483518
C	-4.856174	0.053228	-0.052232
H	-5.607991	0.393325	-0.756577
C	-4.900995	0.504572	1.264383
C	-3.952380	0.065509	2.186083
H	-4.011070	0.402289	3.217868
C	-2.925035	-0.808275	1.806074
C	-3.858581	-1.360477	-1.911323
H	-2.841780	-1.703982	-2.134063
C	-1.915628	-1.271946	2.854511
H	-1.178658	-1.918250	2.372781
C	0.359676	-0.285699	-2.187726
H	-0.322207	-0.954018	-2.732142
H	0.999616	0.301630	-2.858315
C	-4.260040	-0.323436	-2.978530
H	-4.139148	-0.763466	-3.974999
H	-5.313651	-0.036482	-2.882051
H	-3.660002	0.591486	-2.943675
C	-4.800019	-2.581802	-2.001722

H	-4.761009	-3.025534	-3.003408
H	-4.539343	-3.356150	-1.272824
H	-5.835728	-2.279824	-1.804580
C	-2.615471	-2.102798	3.948408
H	-3.332203	-1.495356	4.513320
H	-3.164853	-2.949781	3.520872
H	-1.877926	-2.494679	4.658333
C	-1.125482	-0.101602	3.469805
H	-0.550968	0.442460	2.715942
H	-1.789857	0.601940	3.988093
H	-0.414158	-0.482392	4.212015
H	-5.682937	1.192184	1.575069
C	-1.239064	1.496080	-0.146865
H	-1.961937	0.893950	0.381296
C	-0.961380	2.807749	0.524552
O	-0.256611	3.710351	0.071451
N	-1.638806	2.926476	1.704779
H	-2.151186	2.125341	2.044583
C	-1.506542	4.078153	2.574176
H	-2.477801	4.330510	3.012570
H	-0.784498	3.895986	3.380288
H	-1.153852	4.918192	1.973637
C	-1.209339	1.287312	-1.534496
H	-1.918997	0.560215	-1.903425
C	-0.941552	2.351502	-2.579728
O	-1.890127	2.627232	-3.318184
N	0.286917	2.900360	-2.645660
H	0.922856	2.706345	-1.872143
C	0.529138	4.089992	-3.440801
H	0.296125	4.998932	-2.870360
H	1.580213	4.118220	-3.741873
H	-0.105933	4.060549	-4.328175
C	2.892248	3.142517	1.100888
C	4.258565	2.524804	1.477220
H	4.737592	2.065055	0.605497
H	4.927683	3.305900	1.858119
H	4.144421	1.760336	2.253870
C	3.071127	4.163341	-0.035635
H	2.102594	4.582182	-0.324082
H	3.723136	4.980751	0.296109
H	3.522332	3.696082	-0.916105
C	2.274208	3.826349	2.332330
H	2.947642	4.608446	2.703826
H	1.319972	4.286468	2.063629
H	2.098082	3.103532	3.134160
C	1.986739	1.995996	0.640674

TS1'-AC

Ru	0.569363	0.598168	-0.515087
O	1.664899	2.480624	-0.852382
O	0.988834	2.154039	1.185512
N	0.833361	-2.102613	0.455204
N	-1.327074	-1.807453	0.238327
C	-0.108159	-1.188523	0.110565
C	0.302310	-3.453046	0.622076
H	0.757149	-3.963560	1.474768
H	0.485589	-4.053659	-0.280155
C	-1.187924	-3.159815	0.823005
H	-1.843054	-3.871284	0.316656
H	-1.459285	-3.131973	1.886282

C	2.242795	-1.771043	0.246785
C	2.732388	-2.267917	-1.134192
H	2.059172	-1.902015	-1.915002
H	2.703292	-3.366754	-1.162867
C	4.165979	-1.766671	-1.385847
H	4.500313	-2.106441	-2.374940
C	5.093835	-2.343889	-0.297687
H	5.100235	-3.441865	-0.351645
H	6.125856	-2.006981	-0.462681
C	4.607676	-1.878657	1.090700
H	5.259976	-2.295319	1.869042
C	3.163035	-2.383057	1.328038
H	2.807570	-2.083872	2.322707
H	3.145409	-3.482331	1.285931
C	4.655354	-0.336127	1.140521
H	4.352877	0.023511	2.132881
H	5.687306	0.003844	0.975252
C	3.714192	0.254797	0.058979
H	3.758815	1.347271	0.100192
C	2.291092	-0.235424	0.372859
H	2.081038	-0.003715	1.427665
C	4.176324	-0.224134	-1.330423
H	3.514066	0.186784	-2.102228
H	5.188493	0.148609	-1.537334
C	-2.587711	-1.140920	0.402490
C	-3.581684	-1.317860	-0.585576
C	-4.808020	-0.666308	-0.413402
H	-5.584405	-0.780066	-1.163872
C	-5.048621	0.125217	0.706844
C	-4.074564	0.249016	1.693751
H	-4.284719	0.840653	2.579939
C	-2.833743	-0.390691	1.574552
C	-3.365590	-2.235505	-1.785071
H	-2.293666	-2.455419	-1.842108
C	-1.843590	-0.321527	2.734959
H	-0.905039	-0.788947	2.425705
C	0.573880	0.034059	-2.293692
H	0.132754	-0.858159	-2.758405
C	-1.346585	1.866611	-0.714885
H	-1.885778	1.560297	0.175724
C	-1.399332	1.057378	-1.848809
H	-1.960255	0.136853	-1.834980
H	1.060475	0.694651	-3.025799
N	1.647186	2.898078	0.361012
O	2.208967	3.920774	0.712156
C	-3.787723	-1.608360	-3.127016
H	-3.530630	-2.283788	-3.950926
H	-4.869125	-1.437460	-3.171141
H	-3.292864	-0.649573	-3.308919
C	-4.118002	-3.566655	-1.573945
H	-3.911158	-4.263303	-2.394897
H	-3.834897	-4.050546	-0.633028
H	-5.200394	-3.394380	-1.540493
C	-2.390316	-1.117222	3.938937
H	-3.307596	-0.659381	4.327458
H	-2.628955	-2.151752	3.666531
H	-1.653504	-1.136568	4.750324
C	-1.502232	1.119245	3.152372
H	-1.032998	1.664967	2.332348
H	-2.391356	1.668619	3.482491

H	-0.789314	1.109119	3.984358
H	-6.003200	0.631922	0.819280
H	-1.250628	1.546968	-2.808148
C	-1.114373	3.341993	-0.928359
O	-1.037198	3.832888	-2.051846
N	-1.060585	4.083209	0.218633
H	-0.859519	3.581268	1.073835
C	-0.692970	5.491746	0.176315
H	-1.083542	5.994424	1.065769
H	0.395704	5.618116	0.136968
H	-1.132768	5.936416	-0.717549

INT2'-1-AC

Ru	0.606755	0.521973	-0.544877
O	1.739775	2.244649	-1.238195
O	1.516976	2.333931	0.925579
N	0.729046	-2.113006	0.582028
N	-1.412159	-1.768604	0.291970
C	-0.180404	-1.185238	0.190237
C	0.161656	-3.451598	0.737580
H	0.571051	-3.965025	1.611240
H	0.366083	-4.063124	-0.152451
C	-1.331329	-3.125093	0.875562
H	-1.978721	-3.818725	0.334774
H	-1.652697	-3.097564	1.925478
C	2.141523	-1.815904	0.349245
C	2.584951	-2.278556	-1.062484
H	1.908138	-1.855894	-1.813802
H	2.511079	-3.373288	-1.130714
C	4.033255	-1.825620	-1.325319
H	4.336160	-2.148313	-2.329756
C	4.957362	-2.469549	-0.271567
H	4.920729	-3.564896	-0.355861
H	5.998026	-2.167324	-0.447935
C	4.517482	-2.027981	1.139956
H	5.170231	-2.489279	1.892079
C	3.062044	-2.483546	1.394202
H	2.737019	-2.198385	2.403261
H	2.996900	-3.579244	1.320954
C	4.612370	-0.491464	1.237713
H	4.333287	-0.154277	2.244669
H	5.649943	-0.173145	1.066763
C	3.680044	0.165291	0.185916
H	3.769777	1.250369	0.271079
C	2.244239	-0.281571	0.500511
H	2.001606	-0.027274	1.540522
C	4.107588	-0.287916	-1.224583
H	3.459269	0.178930	-1.976020
H	5.132515	0.049407	-1.428411
C	-2.647969	-1.050035	0.396681
C	-3.592908	-1.162112	-0.645094
C	-4.771227	-0.413525	-0.543977
H	-5.511962	-0.471117	-1.335765
C	-5.007670	0.406465	0.557561
C	-4.088400	0.455740	1.602675
H	-4.296327	1.076037	2.469805
C	-2.900470	-0.284769	1.556101
C	-3.384618	-2.124853	-1.809608
H	-2.331260	-2.425052	-1.803394
C	-1.957824	-0.274265	2.758713

H	-1.124486	-0.952420	2.556677
C	-0.028144	0.039372	-2.350309
H	-0.445171	-0.939707	-2.597954
C	-1.059134	1.735673	-0.557612
H	-1.823264	1.418070	0.146638
C	-1.183822	1.080782	-1.950505
H	-2.121828	0.530148	-1.962563
H	0.608575	0.430982	-3.149921
N	1.979426	2.875322	-0.134030
O	2.616422	3.915858	-0.123851
C	-3.684170	-1.514850	-3.190280
H	-4.735972	-1.223323	-3.286918
H	-3.070425	-0.631781	-3.389352
H	-3.476694	-2.251919	-3.974424
C	-4.245189	-3.388908	-1.596641
H	-4.048687	-4.128534	-2.381764
H	-4.047471	-3.856667	-0.625821
H	-5.312050	-3.137353	-1.627595
C	-2.683551	-0.805738	4.011152
H	-3.494183	-0.136175	4.320146
H	-3.120580	-1.794511	3.829038
H	-1.982384	-0.888291	4.849606
C	-1.336877	1.109690	3.023789
H	-0.653805	1.385718	2.217555
H	-2.103412	1.887772	3.114347
H	-0.760229	1.092183	3.955904
H	-5.920199	0.993847	0.610049
H	-1.172841	1.896073	-2.676464
C	-0.982695	3.258176	-0.620972
O	-1.135843	3.877589	-1.671425
N	-0.837551	3.879566	0.588131
H	-0.394479	3.322861	1.307113
C	-0.566611	5.311479	0.639284
H	-0.791562	5.683549	1.642877
H	0.481537	5.528417	0.397477
H	-1.205460	5.814828	-0.087707

INT2'-AC

Ru	0.506885	0.716326	-0.473783
O	1.758654	0.009247	-2.459452
O	1.730936	2.050022	-1.717409
N	0.401171	-1.358193	1.521450
N	-1.687820	-1.005735	0.968878
C	-0.401672	-0.653807	0.685871
C	-0.302908	-2.357540	2.325395
H	-0.023243	-2.283575	3.379795
H	-0.068047	-3.372057	1.978302
C	-1.774903	-1.980702	2.076638
H	-2.390315	-2.835048	1.779342
H	-2.236638	-1.510972	2.952105
C	1.832218	-1.389038	1.243258
C	2.185267	-2.618901	0.367482
H	1.571358	-2.589315	-0.541419
H	1.940747	-3.542367	0.909977
C	3.683266	-2.597277	0.008038
H	3.921484	-3.485037	-0.591630
C	4.524476	-2.599961	1.300216
H	4.333440	-3.514430	1.879438
H	5.593239	-2.594768	1.049278
C	4.175944	-1.356746	2.144556

H	4.782131	-1.347364	3.059186
C	2.682449	-1.412296	2.532868
H	2.408266	-0.556238	3.162794
H	2.478690	-2.326508	3.108942
C	4.459072	-0.079550	1.323740
H	4.238876	0.813177	1.924209
H	5.523843	-0.035595	1.057995
C	3.600294	-0.080922	0.026348
H	3.801858	0.833305	-0.541020
C	2.134799	-0.104842	0.469277
H	1.951411	0.773245	1.141053
C	3.976478	-1.324718	-0.806435
H	3.415037	-1.333921	-1.742765
H	5.043966	-1.279573	-1.060894
C	-2.804957	-0.854007	0.085664
C	-2.878191	-1.691080	-1.050414
C	-3.956322	-1.510995	-1.924922
H	-4.025701	-2.123757	-2.819267
C	-4.941604	-0.560970	-1.663825
C	-4.885419	0.203933	-0.500806
H	-5.680257	0.912254	-0.287528
C	-3.823859	0.066603	0.402699
C	-1.858604	-2.795206	-1.324084
H	-1.128044	-2.800505	-0.510370
C	-3.834084	0.823001	1.726172
H	-2.835463	0.738052	2.166537
C	-0.896592	0.922672	-1.932047
H	-1.680669	0.184401	-2.050543
C	-0.627122	2.123615	0.399490
H	-1.325602	1.806193	1.169039
C	-1.305959	2.134980	-1.049107
H	-2.381887	2.064325	-0.873108
H	-0.455418	1.202848	-2.889531
C	-4.833012	0.154480	2.694603
H	-4.805610	0.644288	3.674946
H	-5.856045	0.227455	2.306564
H	-4.608236	-0.908941	2.834610
C	-4.150483	2.321753	1.585179
H	-3.449384	2.823591	0.912543
H	-5.165587	2.488557	1.207011
H	-4.077942	2.810263	2.562833
C	-2.549856	-4.173660	-1.320668
H	-3.104538	-4.340649	-0.389711
H	-3.259150	-4.268150	-2.150782
H	-1.806220	-4.972174	-1.426077
C	-1.066264	-2.578368	-2.627209
H	-0.398025	-3.429818	-2.803305
H	-1.734868	-2.496186	-3.492286
H	-0.452093	-1.675710	-2.578305
H	-5.767796	-0.432106	-2.357872
H	-1.064558	3.075169	-1.549132
N	2.151179	1.205150	-2.617761
O	2.873735	1.566920	-3.528399
C	0.060339	3.363799	0.911664
O	-0.012319	3.644642	2.110145
N	0.752068	4.141987	0.022331
H	1.025090	3.728076	-0.861018
C	1.574260	5.237201	0.511360
H	2.502669	4.880152	0.979103
H	1.826769	5.896087	-0.323705

H   1.012946   5.797125   1.261733

INT3'-AC

Ru	-0.560941	0.666504	0.316241
O	-0.207580	0.834218	2.434003
O	-1.525752	2.330036	1.570001
N	-0.665603	-1.921637	-0.849823
N	1.450676	-1.563116	-0.382963
C	0.213512	-1.020050	-0.341688
C	-0.074007	-3.254863	-0.960761
H	-0.420199	-3.778922	-1.854769
H	-0.316322	-3.865115	-0.078000
C	1.423823	-2.898853	-1.019335
H	2.061957	-3.600193	-0.478754
H	1.775761	-2.832875	-2.054799
C	-2.082740	-1.575202	-0.710417
C	-2.608426	-1.948368	0.700952
H	-1.952315	-1.510702	1.468605
H	-2.568007	-3.038579	0.835444
C	-4.049948	-1.436184	0.877486
H	-4.412811	-1.709803	1.876413
C	-4.945560	-2.084182	-0.198252
H	-4.954301	-3.176130	-0.074525
H	-5.981148	-1.738484	-0.082233
C	-4.421634	-1.710264	-1.600529
H	-5.059912	-2.167999	-2.366781
C	-2.977880	-2.243517	-1.768812
H	-2.593629	-2.012881	-2.770714
H	-2.970053	-3.337650	-1.653402
C	-4.450986	-0.172298	-1.753945
H	-4.112747	0.115475	-2.758051
H	-5.483913	0.186781	-1.645607
C	-3.541808	0.483792	-0.681615
H	-3.559504	1.574332	-0.796206
C	-2.113490	-0.034869	-0.915722
H	-1.839420	0.155658	-1.957692
C	-4.063869	0.098171	0.718326
H	-3.447675	0.569225	1.494691
H	-5.085621	0.477467	0.852666
C	2.658441	-0.900508	0.027568
C	2.958524	-0.841206	1.408010
C	4.137339	-0.190727	1.789063
H	4.393829	-0.118543	2.840211
C	4.992246	0.367397	0.841004
C	4.680594	0.290306	-0.512129
H	5.353788	0.728812	-1.242058
C	3.505960	-0.335093	-0.948658
C	2.065593	-1.504897	2.453431
H	1.031078	-1.435331	2.106780
C	3.214338	-0.428929	-2.444312
H	2.165018	-0.719683	-2.569004
C	4.097667	-1.523000	-3.081931
H	3.847492	-1.655053	-4.141248
H	5.155801	-1.242949	-3.017369
H	3.984089	-2.488843	-2.576839
C	3.400095	0.903245	-3.197131
H	4.440856	1.244522	-3.161875
H	3.141209	0.762537	-4.253128
H	2.761969	1.701190	-2.805600
C	2.419968	-3.000327	2.589036

H	2.318575	-3.533110	1.638251
H	3.455622	-3.120920	2.928891
H	1.763359	-3.486197	3.320799
C	2.116585	-0.825916	3.831130
H	1.342043	-1.252823	4.477533
H	3.080550	-0.983793	4.329834
H	1.929565	0.247580	3.751291
H	5.903981	0.865236	1.160521
N	-0.946285	1.896024	2.630297
O	-1.070502	2.398466	3.720410
C	0.418925	1.618438	-0.894176
H	1.231825	1.146211	-1.447173
C	0.304362	3.050208	-1.335065
O	0.819913	3.361094	-2.416005
N	-0.358321	3.941854	-0.554397
H	-0.804513	3.613220	0.292889
C	-0.547019	5.318087	-0.974988
H	-0.735218	5.940523	-0.096291
H	0.355003	5.666303	-1.484209
H	-1.390167	5.420628	-1.671407

TS2'-cross-AC

Ru	-0.474581	0.683943	0.399004
O	-1.644295	0.025812	2.332760
O	-1.687568	2.077475	1.627752
N	-0.538728	-1.543367	-1.430599
N	1.580305	-1.243137	-0.967028
C	0.316491	-0.812851	-0.676898
C	0.097058	-2.649167	-2.147583
H	-0.222229	-2.677396	-3.192627
H	-0.160581	-3.611080	-1.684504
C	1.589512	-2.305729	-1.994468
H	2.191478	-3.154493	-1.656962
H	2.026178	-1.922130	-2.924073
C	-1.972321	-1.453228	-1.155258
C	-2.381695	-2.521691	-0.110401
H	-1.771638	-2.383806	0.790587
H	-2.178987	-3.527373	-0.505765
C	-3.878365	-2.380127	0.229947
H	-4.158789	-3.158490	0.951424
C	-4.718671	-2.532823	-1.053068
H	-4.570074	-3.529241	-1.493440
H	-5.786213	-2.442526	-0.812535
C	-4.311257	-1.441545	-2.064338
H	-4.917408	-1.534994	-2.974689
C	-2.822275	-1.634700	-2.430768
H	-2.506429	-0.901587	-3.184816
H	-2.676845	-2.636444	-2.862061
C	-4.535175	-0.047033	-1.434477
H	-4.279932	0.738517	-2.158617
H	-5.598702	0.076259	-1.186656
C	-3.668694	0.101165	-0.152329
H	-3.831760	1.094282	0.282811
C	-2.197720	-0.039888	-0.594639
H	-2.059885	0.659619	-1.435476
C	-4.116500	-0.989087	0.845990
H	-3.575342	-0.903602	1.788665
H	-5.184795	-0.859359	1.067791
C	2.730939	-1.065949	-0.134920
C	2.830305	-1.839209	1.044223

C	3.943736	-1.634763	1.867766	H	1.640507	-3.841063	-1.388354
H	4.035529	-2.199811	2.791148	H	1.577259	-2.731724	-2.774126
C	4.937585	-0.722992	1.517326	C	-2.255427	-1.566061	-0.982495
C	4.853592	-0.023897	0.315334	C	-2.746483	-2.447463	0.193692
H	5.655011	0.652155	0.032830	H	-2.084129	-2.288610	1.053515
C	3.756562	-0.187731	-0.540593	H	-2.687912	-3.509004	-0.085564
C	1.804969	-2.912446	1.408464	C	-4.197367	-2.077993	0.559776
H	1.032995	-2.929839	0.634481	H	-4.539125	-2.727043	1.376327
C	3.738473	0.487062	-1.908444	C	-5.106471	-2.266261	-0.670455
H	2.731092	0.372217	-2.322116	H	-5.101915	-3.316958	-0.993833
C	1.032394	0.897240	1.973111	H	-6.142846	-2.013537	-0.410467
H	1.626806	-0.002346	2.039630	C	-4.612659	-1.357997	-1.815303
C	1.515882	1.963192	1.170025	H	-5.265770	-1.475369	-2.689479
H	2.409486	1.753421	0.590926	C	-3.176915	-1.780763	-2.201627
C	1.330147	3.398871	1.606048	H	-2.806756	-1.185078	-3.046367
H	2.025918	3.594446	2.433170	H	-3.175854	-2.835377	-2.514792
H	1.553669	4.106569	0.804305	C	-4.635345	0.116110	-1.347832
H	0.313666	3.570612	1.970267	H	-4.318439	0.776119	-2.166520
H	0.495553	1.162747	2.881629	H	-5.663358	0.400720	-1.083835
C	4.715013	-0.249640	-2.850285	C	-3.700479	0.297216	-0.118621
H	4.663760	0.169124	-3.862042	H	-3.718208	1.346287	0.200295
H	5.747359	-0.150575	-2.494071	C	-2.281395	-0.080599	-0.589084
H	4.486114	-1.320020	-2.908166	H	-2.100768	0.493647	-1.511678
C	4.056846	1.992552	-1.874828	C	-4.233969	-0.607141	1.014247
H	3.313703	2.562466	-1.310165	H	-3.646227	-0.487862	1.925051
H	5.046875	2.188684	-1.447820	H	-5.266806	-0.317382	1.251558
H	4.053750	2.392728	-2.894667	C	2.481350	-1.708559	-0.087451
C	2.474228	-4.301998	1.416260	C	2.489659	-2.350881	1.171503
H	2.978734	-4.508267	0.464918	C	3.639218	-2.223939	1.960750
H	3.223734	-4.379663	2.212190	H	3.666641	-2.688877	2.942293
H	1.725485	-5.084563	1.585362	C	4.749551	-1.517403	1.502892
C	1.082457	-2.643325	2.742264	C	4.742737	-0.948537	0.231311
H	0.422751	-3.484810	2.984319	H	5.623272	-0.423546	-0.125323
H	1.793667	-2.529937	3.568925	C	3.614336	-1.038375	-0.593499
H	0.464252	-1.743183	2.691260	C	1.325140	-3.210169	1.662524
H	5.792178	-0.574596	2.171987	H	0.548461	-3.213218	0.893000
N	-2.117689	1.201095	2.484287	C	3.647671	-0.483944	-2.013327
O	-2.912819	1.495536	3.356498	H	2.614873	-0.441226	-2.374921
C	0.420316	1.879687	-0.762905	C	1.153589	0.759568	1.760074
H	1.253755	1.591214	-1.406552	H	1.589340	-0.206430	1.974738
C	0.088809	3.316961	-1.076113	H	0.727264	1.267752	2.621298
O	0.893975	4.004174	-1.715245	C	4.419347	-1.458678	-2.928491
N	-1.108465	3.799744	-0.651875	H	4.399450	-1.107419	-3.966623
H	-1.654161	3.241823	-0.006578	H	5.467648	-1.532877	-2.615315
C	-1.440754	5.204078	-0.814919	H	3.992617	-2.467834	-2.897726
H	-1.215261	5.516157	-1.837553	C	4.243420	0.932419	-2.121160
H	-2.505754	5.343714	-0.615405	H	5.312264	0.935459	-1.877058
H	-0.860787	5.839630	-0.132210	H	4.142593	1.293311	-3.150534
				H	3.750452	1.659026	-1.467874
TS2'-*homo*-AC				C	1.782968	-4.670704	1.850437
Ru	-0.440721	0.524642	0.258459	H	2.239864	-5.066694	0.935879
O	-1.571708	0.219329	2.298639	H	2.522317	-4.757834	2.654685
O	-1.425339	2.186346	1.395460	H	0.929279	-5.306706	2.111956
N	-0.856505	-1.869446	-1.285191	C	0.668117	-2.669880	2.946890
N	1.298534	-1.806948	-0.889792	H	-0.105981	-3.365603	3.291519
C	0.113092	-1.181158	-0.639055	H	1.399917	-2.559025	3.755704
C	-0.393105	-3.126007	-1.876096	H	0.189238	-1.701656	2.778078
H	-0.752180	-3.234485	-2.902567	H	5.630271	-1.424994	2.132594
H	-0.752972	-3.984173	-1.293009	N	-1.897408	1.446783	2.361988
C	1.134913	-2.962351	-1.798426	O	-2.590590	1.918750	3.241099

C	0.494293	1.453287	-1.106174
H	1.285290	1.019185	-1.719632
C	0.124762	2.775043	-1.736617
O	0.565504	3.025719	-2.860033
N	-0.737810	3.601330	-1.087635
H	-1.191074	3.282950	-0.241969
C	-1.185990	4.834734	-1.709483
H	-1.666055	5.459399	-0.952164
H	-0.326456	5.364039	-2.129581
H	-1.896693	4.646349	-2.524437
C	1.746659	1.531785	0.733560
H	2.539976	1.060518	0.171210
C	1.930218	3.029667	0.771641
O	2.871479	3.527581	0.156393
N	1.063457	3.751555	1.531400
H	0.189473	3.311658	1.798467
C	1.093869	5.204333	1.475907
H	0.495497	5.604608	2.298085
H	2.125422	5.547307	1.575604
H	0.699624	5.578516	0.521808

INT4'-*cross*-AC

Ru	-0.516671	0.679948	0.405221
O	-1.854588	0.213702	2.453236
O	-1.653269	2.172923	1.536545
N	-0.554243	-1.512734	-1.463741
N	1.556959	-1.262674	-0.942109
C	0.298366	-0.813531	-0.673043
C	0.078297	-2.604762	-2.204614
H	-0.207215	-2.583649	-3.259840
H	-0.214963	-3.577780	-1.789526
C	1.572825	-2.304831	-1.990274
H	2.138415	-3.176099	-1.647059
H	2.053630	-1.917144	-2.895398
C	-1.983261	-1.431212	-1.184532
C	-2.413739	-2.576051	-0.231414
H	-1.798055	-2.526028	0.675383
H	-2.229486	-3.546962	-0.711385
C	-3.906886	-2.435006	0.121309
H	-4.200813	-3.264268	0.777328
C	-4.748195	-2.468888	-1.170181
H	-4.616832	-3.429633	-1.687847
H	-5.814125	-2.378916	-0.923324
C	-4.321874	-1.308609	-2.093235
H	-4.927300	-1.320677	-3.008406
C	-2.835557	-1.485227	-2.471800
H	-2.508340	-0.691949	-3.156594
H	-2.691856	-2.446361	-2.986324
C	-4.520768	0.035237	-1.358871
H	-4.244038	0.870413	-2.016359
H	-5.580285	0.165357	-1.100323
C	-3.662290	0.064107	-0.062061
H	-3.807076	1.024247	0.443418
C	-2.199656	-0.081929	-0.494658
H	-1.961791	0.736954	-1.221390
C	-4.117281	-1.095493	0.849303
H	-3.557214	-1.078722	1.786182
H	-5.179529	-0.965487	1.096422
C	2.693931	-1.126558	-0.081496
C	2.730119	-1.895982	1.103368

C	3.828846	-1.731831	1.954886
H	3.872632	-2.293712	2.883638
C	4.868363	-0.864415	1.625434
C	4.845455	-0.171877	0.416995
H	5.680842	0.468947	0.151904
C	3.765348	-0.295153	-0.466665
C	1.654959	-2.926248	1.445901
H	0.898932	-2.912859	0.656053
C	3.812433	0.374902	-1.836208
H	2.811776	0.308354	-2.275909
C	0.885779	0.847961	1.862822
H	1.586342	0.042199	2.048539
C	1.446044	1.958149	0.926099
H	2.470301	1.660478	0.692049
C	1.429094	3.340055	1.589739
H	2.048395	3.318903	2.493306
H	1.828999	4.103795	0.914005
H	0.414408	3.624731	1.880104
H	0.458817	1.235983	2.789881
C	4.778520	-0.408108	-2.751311
H	4.772689	0.010362	-3.764460
H	5.804567	-0.354260	-2.368225
H	4.504744	-1.467705	-2.814144
C	4.198900	1.864063	-1.796704
H	3.476198	2.463255	-1.237269
H	5.193069	2.013383	-1.360221
H	4.222537	2.265004	-2.815774
C	2.267143	-4.341832	1.465254
H	2.778836	-4.569407	0.522566
H	2.999593	-4.448551	2.273554
H	1.484821	-5.093597	1.622317
C	0.918088	-2.627830	2.765105
H	0.209159	-3.434664	2.986100
H	1.615617	-2.559026	3.608097
H	0.353780	-1.693687	2.706656
H	5.710658	-0.746226	2.301822
N	-2.171197	1.438548	2.483869
O	-2.906489	1.932264	3.320277
C	0.720353	1.934803	-0.529508
H	1.405112	1.512928	-1.261045
C	0.326765	3.292770	-1.083595
O	1.066898	3.840311	-1.904866
N	-0.835116	3.864406	-0.666847
H	-1.345430	3.445557	0.100482
C	-1.173757	5.219381	-1.067862
H	-1.050589	5.324789	-2.148618
H	-2.213367	5.419836	-0.797232
H	-0.526452	5.961439	-0.581700

INT4'-*homo*-AC

Ru	-0.461124	0.567993	0.225743
O	-1.726751	0.699025	2.364644
O	-1.184311	2.432359	1.171124
N	-1.066017	-1.823248	-1.257704
N	1.076247	-1.959768	-0.820045
C	-0.044006	-1.216858	-0.604984
C	-0.715007	-3.124337	-1.829439
H	-1.053079	-3.203879	-2.865934
H	-1.174531	-3.938310	-1.253741
C	0.819399	-3.114827	-1.706926

H	1.219076	-4.029417	-1.259776
H	1.311709	-2.957503	-2.672845
C	-2.428587	-1.395940	-0.960305
C	-3.033930	-2.269406	0.168973
H	-2.369569	-2.226376	1.041135
H	-3.088188	-3.315668	-0.161321
C	-4.439886	-1.756570	0.534994
H	-4.862726	-2.397089	1.319362
C	-5.344438	-1.794226	-0.712825
H	-5.449617	-2.825476	-1.078135
H	-6.350822	-1.439562	-0.454845
C	-4.738190	-0.901762	-1.815514
H	-5.385156	-0.915219	-2.701609
C	-3.347014	-1.450189	-2.201460
H	-2.900655	-0.855529	-3.009000
H	-3.439571	-2.484007	-2.564166
C	-4.607686	0.545751	-1.293046
H	-4.201801	1.196964	-2.078771
H	-5.599164	0.937623	-1.029156
C	-3.686403	0.576555	-0.039992
H	-3.593806	1.608626	0.313937
C	-2.317713	0.054511	-0.485273
H	-1.958064	0.685316	-1.339020
C	-4.318850	-0.311974	1.052347
H	-3.712690	-0.283286	1.960118
H	-5.312670	0.080380	1.306446
C	2.254443	-1.954434	-0.002780
C	2.173616	-2.533837	1.283662
C	3.316008	-2.489805	2.091448
H	3.276468	-2.904819	3.094618
C	4.501839	-1.924443	1.626902
C	4.577356	-1.422832	0.329700
H	5.514444	-1.011779	-0.032141
C	3.460907	-1.435671	-0.516382
C	0.914122	-3.232199	1.793849
H	0.160559	-3.209486	1.001524
C	3.587465	-0.968368	-1.962121
H	2.576135	-0.841559	-2.361564
C	1.046508	0.674571	1.582853
H	1.581678	-0.218185	1.885741
H	0.792402	1.291406	2.445519
C	4.281154	-2.065666	-2.797670
H	4.327695	-1.771830	-3.852661
H	5.306668	-2.228555	-2.445219
H	3.752075	-3.023389	-2.729465
C	4.326843	0.373117	-2.125162
H	5.386923	0.278325	-1.861750
H	4.275880	0.693109	-3.171360
H	3.901738	1.174620	-1.514145
C	1.207232	-4.715784	2.094719
H	1.640363	-5.221846	1.223905
H	1.912624	-4.824522	2.926287
H	0.283657	-5.237333	2.371913
C	0.289790	-2.534329	3.017030
H	-0.571093	-3.110219	3.377424
H	1.007735	-2.457535	3.842077
H	-0.060040	-1.528618	2.770181
H	5.375807	-1.891882	2.271754
N	-1.764187	1.954028	2.247132
O	-2.285475	2.706073	3.050520

C	0.927522	1.346637	-0.979856
H	1.454280	0.677038	-1.652743
C	0.643640	2.586623	-1.808077
O	1.003705	2.607333	-2.985256
N	-0.033551	3.629007	-1.249245
H	-0.473183	3.518468	-0.346970
C	-0.370436	4.793835	-2.049504
H	-0.757462	5.574564	-1.389761
H	0.523264	5.159983	-2.561543
H	-1.123744	4.561181	-2.813378
C	1.756317	1.423295	0.420419
H	2.650003	0.845472	0.195570
C	2.248483	2.851089	0.683330
O	3.294265	3.216278	0.154463
N	1.504446	3.644079	1.498304
H	0.561521	3.343961	1.717797
C	1.801671	5.063849	1.601229
H	1.291333	5.474759	2.475858
H	2.879594	5.196016	1.710813
H	1.480408	5.607874	0.702461

INT4'-*cross*-2-AC

Ru	0.487667	0.782591	0.349214
C	1.063396	1.618068	-1.541777
H	1.877583	1.187974	-2.119833
H	1.320694	2.654466	-1.283945
C	-0.304091	1.484577	-2.190288
C	-0.675605	2.550502	-3.226858
H	-1.704195	2.408223	-3.578605
H	-0.002238	2.497438	-4.091609
H	-0.603478	3.555394	-2.797771
H	-0.356594	0.499320	-2.674396
C	-1.128979	1.402224	-0.901619
C	-1.948682	2.631696	-0.561370
O	-3.169521	2.605414	-0.738507
N	-1.306319	3.768269	-0.160807
H	-0.351137	3.683228	0.157534
C	-2.052166	4.946590	0.252350
H	-2.405817	4.862007	1.288621
H	-2.919700	5.060143	-0.399903
H	-1.411413	5.828862	0.166943
H	-1.844495	0.587929	-0.888975
C	0.249022	-1.061672	-0.311616
N	1.366053	-1.776180	-0.620092
C	2.675212	-1.165952	-0.448502
C	2.422539	0.199243	0.208478
C	3.718517	1.006576	0.296626
C	4.442229	1.132248	-1.061001
C	4.728765	-0.270946	-1.633388
C	3.400147	-1.030006	-1.810004
H	3.589854	-2.035747	-2.210550
H	2.745312	-0.520602	-2.522207
C	5.631854	-1.055457	-0.660765
C	4.920300	-1.191715	0.701103
C	4.644656	0.218650	1.269008
H	4.179149	0.148743	2.261021
H	5.592057	0.759180	1.396246
C	3.596298	-1.969319	0.509777
H	3.086735	-2.116771	1.471089
H	3.805329	-2.964313	0.092369

H	5.558789	-1.748205	1.398628	H	-1.529423	-4.069217	-1.183989
H	6.589560	-0.534671	-0.531332	H	-1.395934	-4.062140	0.583663
H	5.857483	-2.049143	-1.071647	C	2.368636	-2.006974	-0.019789
H	5.224816	-0.178853	-2.607672	C	3.015230	-2.038213	-1.428129
H	5.386713	1.673175	-0.914538	H	2.413041	-1.423974	-2.110634
H	3.845847	1.720515	-1.764257	H	3.009463	-3.067503	-1.812757
H	3.504331	1.998047	0.710968	C	4.458947	-1.504111	-1.356950
H	2.087371	0.009343	1.287209	H	4.907157	-1.548161	-2.357478
C	1.103644	-3.199469	-0.831570	C	5.278820	-2.369362	-0.379215
C	-0.416892	-3.184803	-1.053676	H	5.323956	-3.409084	-0.732919
N	-0.817892	-1.894075	-0.454012	H	6.311538	-2.000340	-0.330672
C	-2.139930	-1.702285	0.077159	C	4.634634	-2.314277	1.021620
C	-3.212934	-1.492251	-0.812709	H	5.219673	-2.922456	1.723068
C	-4.500601	-1.375119	-0.277416	C	3.201235	-2.885888	0.940292
C	-4.712879	-1.444763	1.094625	H	2.725733	-2.892844	1.929981
C	-3.638442	-1.641130	1.959438	H	3.237027	-3.924809	0.582234
C	-2.333394	-1.783273	1.476176	C	4.596372	-0.850106	1.512821
C	-1.184611	-2.077072	2.439081	H	4.162683	-0.800853	2.521115
C	-1.377738	-1.468854	3.837979	H	5.619250	-0.455948	1.582150
H	-2.170517	-1.977966	4.398977	C	3.766294	0.017354	0.527824
H	-0.453165	-1.580919	4.416745	H	3.732515	1.053706	0.880219
H	-1.617410	-0.404964	3.773912	C	2.345991	-0.562168	0.506044
C	-0.948509	-3.597432	2.552505	H	1.943207	-0.562702	1.546388
H	-1.840202	-4.095066	2.952004	C	4.424522	-0.045493	-0.865405
H	-0.110845	-3.808307	3.228740	H	3.870492	0.581037	-1.567651
H	-0.721556	-4.051941	1.583005	H	5.446106	0.353322	-0.805417
H	-0.274909	-1.629169	2.028300	C	-2.518321	-1.666945	-0.066876
H	-3.821635	-1.684173	3.027396	C	-3.353420	-1.354348	-1.161052
H	-5.717173	-1.336686	1.495294	C	-4.655794	-0.914460	-0.893612
H	-5.341137	-1.205650	-0.942928	H	-5.309419	-0.651445	-1.718919
C	-3.006339	-1.382935	-2.318855	C	-5.120364	-0.795950	0.412030
C	-3.736384	-0.169161	-2.928688	C	-4.293956	-1.137884	1.478354
H	-3.408839	-0.022699	-3.965059	H	-4.667865	-1.047420	2.493117
H	-3.546818	0.748108	-2.362997	C	-2.985966	-1.588624	1.267992
H	-4.820951	-0.328649	-2.951647	C	-2.894157	-1.503758	-2.605759
C	-3.441967	-2.682413	-3.025637	H	-1.804263	-1.608265	-2.598127
H	-3.251472	-2.619704	-4.103857	C	-2.145150	-2.010769	2.472122
H	-4.515707	-2.852956	-2.882735	H	-1.103866	-2.111673	2.148299
H	-2.915479	-3.560052	-2.633601	C	-0.344846	1.000100	-1.723187
H	-1.934238	-1.240690	-2.495844	H	-0.771347	0.249083	-2.383395
H	-0.666295	-3.193039	-2.121417	H	0.129092	1.812929	-2.272341
H	-0.937467	-4.014048	-0.571163	N	2.264417	2.932722	-1.057231
H	1.390579	-3.783314	0.054181	O	2.567534	4.115522	-0.922270
H	1.651214	-3.586922	-1.695357	C	-3.256662	-0.282829	-3.475809
O	0.677641	2.629050	1.606252	H	-2.739934	-0.344463	-4.440426
N	-0.318746	2.282346	2.352688	H	-4.331662	-0.250410	-3.686215
O	-0.712363	2.945115	3.284342	H	-2.990414	0.665525	-2.999010
O	-0.866534	1.155485	2.014588	C	-3.479941	-2.788704	-3.226976
				H	-3.122153	-2.917757	-4.255274
INT4'-*homo*-2-AC				H	-3.204027	-3.681116	-2.653933
Ru	0.660688	0.418239	-0.111830	H	-4.574942	-2.739089	-3.252773
O	1.607477	2.373758	-0.047055	C	-2.620656	-3.381794	3.001766
O	2.506362	2.248835	-2.057784	H	-3.648215	-3.307929	3.376464
N	0.971861	-2.430861	-0.075664	H	-2.612556	-4.156262	2.227476
N	-1.187599	-2.158725	-0.321918	H	-1.982988	-3.716465	3.828461
C	-0.008268	-1.497049	-0.147749	C	-2.172792	-0.988616	3.628119
C	0.526381	-3.777956	-0.431825	H	-1.974643	0.034281	3.300039
H	0.924358	-4.527991	0.256803	H	-3.147745	-0.983547	4.128704
H	0.854757	-4.033104	-1.447915	H	-1.425079	-1.265323	4.380571
C	-0.998219	-3.627337	-0.337915	H	-6.128523	-0.437631	0.599684

C	-0.917196	1.141298	0.881369
H	-1.598550	0.385955	1.255304
C	-0.943946	2.243854	1.941714
O	-2.016102	2.444036	2.513886
N	0.199605	2.890644	2.278074
H	0.992206	2.827790	1.645975
C	0.157197	3.989616	3.230210
H	1.176964	4.228979	3.541126
H	-0.306457	4.884631	2.794727
H	-0.432836	3.693805	4.100517
C	-1.373139	1.486982	-0.615334
H	-2.280619	0.906058	-0.760965
C	-1.766123	2.950439	-0.887062
O	-2.875705	3.174856	-1.358834
N	-0.831726	3.897246	-0.644006
H	0.063227	3.618307	-0.262141
C	-1.072308	5.306415	-0.903716
H	-1.524288	5.804657	-0.036619
H	-0.119656	5.787359	-1.139677
H	-1.755945	5.402087	-1.750140

TS3'-*cross*-AC

Ru	0.590105	0.647008	-0.575606
O	1.560913	2.571926	-0.889178
O	0.828685	2.227295	1.121935
N	1.035174	-2.092369	0.178407
N	-1.142691	-1.951881	-0.033491
C	0.027502	-1.226862	-0.083375
C	0.625901	-3.492983	0.204125
H	1.095554	-4.035271	1.029189
H	0.899693	-3.991424	-0.735920
C	-0.894802	-3.357769	0.364647
H	-1.457839	-4.044707	-0.270971
H	-1.211575	-3.511457	1.403828
C	2.413585	-1.604893	0.137058
C	3.066476	-1.877045	-1.238346
H	2.421725	-1.486320	-2.031185
H	3.160251	-2.961812	-1.393140
C	4.451355	-1.206510	-1.292892
H	4.901915	-1.385275	-2.278045
C	5.344600	-1.819105	-0.195079
H	5.476940	-2.895727	-0.373825
H	6.343072	-1.362849	-0.221073
C	4.697420	-1.581204	1.185258
H	5.325103	-2.024912	1.968945
C	3.302795	-2.252377	1.224212
H	2.835458	-2.115352	2.208382
H	3.410316	-3.334146	1.055043
C	4.569514	-0.060350	1.417405
H	4.147313	0.140435	2.410981
H	5.567540	0.399069	1.392564
C	3.663098	0.566030	0.326082
H	3.587887	1.642940	0.501501
C	2.281355	-0.097623	0.441611
H	1.950446	-0.011769	1.487361
C	4.288095	0.311119	-1.059432
H	3.651934	0.750778	-1.836886
H	5.267876	0.803237	-1.123697
C	-2.407567	-1.387022	0.344427
C	-3.465267	-1.391661	-0.589189

C	-4.688635	-0.828293	-0.205928
H	-5.514604	-0.810366	-0.909954
C	-4.859202	-0.278605	1.061769
C	-3.813296	-0.311796	1.981867
H	-3.964715	0.095742	2.977769
C	-2.573155	-0.875706	1.653103
C	-3.298293	-2.000507	-1.975025
H	-2.222458	-2.082154	-2.165038
C	-1.485157	-0.951343	2.723211
H	-0.582910	-1.378623	2.280227
C	0.640728	0.142441	-2.388945
H	0.227137	-0.751040	-2.875368
C	-1.088447	1.373066	-2.180719
H	-1.605771	0.548931	-2.666976
C	-0.751694	2.540186	-3.087865
H	-0.533545	2.186826	-4.100448
H	-1.609695	3.221069	-3.123957
H	0.089658	3.115993	-2.703499
H	1.217097	0.768347	-3.081704
N	1.463314	3.009166	0.320650
O	1.959255	4.057802	0.676551
C	-3.915285	-1.139962	-3.092654
H	-3.627024	-1.535015	-4.073377
H	-5.010472	-1.145129	-3.050441
H	-3.588003	-0.097395	-3.031066
C	-3.899454	-3.420980	-2.014048
H	-3.734338	-3.884955	-2.993623
H	-3.459904	-4.069890	-1.249309
H	-4.980639	-3.384898	-1.833650
C	-1.926554	-1.885469	3.868574
H	-2.796855	-1.480437	4.397884
H	-2.199843	-2.880144	3.497287
H	-1.116265	-2.001650	4.597553
C	-1.087473	0.432272	3.269026
H	-0.689244	1.077448	2.483361
H	-1.937665	0.938789	3.742724
H	-0.307565	0.322110	4.031227
H	-5.810836	0.167455	1.337242
C	-1.448517	1.521209	-0.803982
H	-2.149372	0.786079	-0.433069
C	-1.589794	2.865274	-0.153506
O	-1.128999	3.910150	-0.606203
N	-2.327057	2.824229	1.001449
H	-2.543861	1.913231	1.381536
C	-2.324774	3.950035	1.919377
H	-1.428075	3.949080	2.553501
H	-2.330415	4.872400	1.336698
H	-3.218410	3.911632	2.549544

TS3'-*homo*-AC

Ru	0.584658	0.570779	-0.115605
O	1.385617	2.592399	0.095691
O	0.937486	1.587025	1.965304
N	1.292500	-2.220307	-0.250324
N	-0.897339	-2.209197	-0.343894
C	0.208479	-1.409381	-0.195557
C	0.980336	-3.589263	-0.656201
H	1.540549	-4.321176	-0.068382
H	1.222128	-3.739689	-1.717173
C	-0.532062	-3.642261	-0.399927

H	-1.086013	-4.152369	-1.190508
H	-0.770618	-4.124488	0.557032
C	2.621877	-1.610061	-0.293518
C	3.108219	-1.435469	-1.752179
H	2.345359	-0.905972	-2.331466
H	3.247449	-2.422442	-2.216138
C	4.432340	-0.650057	-1.764977
H	4.761840	-0.513424	-2.803226
C	5.493658	-1.451978	-0.984561
H	5.665308	-2.422783	-1.470837
H	6.451728	-0.915530	-0.988684
C	5.016400	-1.657847	0.468146
H	5.765145	-2.236345	1.024534
C	3.680517	-2.440504	0.467941
H	3.336081	-2.617640	1.495298
H	3.827387	-3.421974	-0.006862
C	4.828029	-0.275551	1.128883
H	4.524833	-0.391431	2.177864
H	5.784767	0.265050	1.127889
C	3.753730	0.535568	0.358924
H	3.636811	1.513151	0.835148
C	2.440319	-0.259749	0.429321
H	2.238527	-0.489272	1.486532
C	4.209950	0.725365	-1.100518
H	3.453630	1.297054	-1.651923
H	5.141557	1.306259	-1.128551
C	-2.198223	-1.861104	0.151752
C	-3.252122	-1.658446	-0.765472
C	-4.491170	-1.247937	-0.257334
H	-5.314271	-1.064922	-0.940350
C	-4.685251	-1.070881	1.110440
C	-3.650003	-1.338886	2.004432
H	-3.824307	-1.236524	3.072254
C	-2.390638	-1.749474	1.548873
C	-3.083809	-1.956552	-2.252573
H	-2.008529	-1.965512	-2.465302
C	-1.299826	-2.086728	2.563944
H	-0.384684	-2.344199	2.025777
C	0.467517	0.639989	-1.992017
H	0.071124	-0.095929	-2.701681
H	0.862856	1.535133	-2.487238
N	1.423615	2.628470	1.383226
O	1.897790	3.562790	1.997117
C	-3.743469	-0.932248	-3.194650
H	-3.554373	-1.225024	-4.233864
H	-4.831361	-0.905663	-3.062858
H	-3.357288	0.083591	-3.068325
C	-3.639594	-3.367831	-2.548686
H	-3.449370	-3.645683	-3.591861
H	-3.192046	-4.130122	-1.901617
H	-4.723477	-3.393163	-2.383751
C	-1.709129	-3.318205	3.396902
H	-2.595791	-3.108826	4.006530
H	-1.943913	-4.176072	2.756111
H	-0.897356	-3.606913	4.074548
C	-0.943339	-0.899764	3.476588
H	-0.558103	-0.053317	2.903109
H	-1.809541	-0.569730	4.064584
H	-0.162964	-1.193529	4.187861
H	-5.651589	-0.741441	1.482335

C	-1.511720	1.320452	0.221120
H	-2.045475	0.467075	0.616585
C	-1.590010	2.513163	1.122749
O	-1.181056	3.648697	0.859417
N	-2.172552	2.239932	2.323195
H	-2.354667	1.273527	2.551799
C	-2.071574	3.196600	3.415310
H	-2.447825	4.168051	3.087150
H	-2.673194	2.839849	4.254751
H	-1.028776	3.320359	3.732436
C	-1.440423	1.321767	-1.201022
H	-1.908318	0.452736	-1.643313
C	-1.539769	2.479805	-2.184154
O	-2.145292	2.266561	-3.238784
N	-0.929323	3.639171	-1.874839
H	-0.660080	3.779135	-0.898626
C	-1.032607	4.787810	-2.756828
H	-0.230545	5.489662	-2.515651
H	-0.933154	4.458564	-3.794075
H	-1.998875	5.299323	-2.653641

(Z)-N-methyl-2-butenamide

C	2.025221	0.702964	0.000033
H	2.700276	1.560604	0.000103
C	0.711929	0.981133	0.000205
H	0.416565	2.030348	0.000348
C	-0.399528	-0.013422	0.000112
O	-0.250446	-1.235219	0.000273
N	-1.646670	0.564680	-0.000253
H	-1.717629	1.571512	-0.000068
C	-2.871151	-0.211520	-0.000087
H	-3.474704	-0.002686	0.891956
H	-3.475282	-0.001915	-0.891540
H	-2.589634	-1.265545	-0.000593
C	2.698478	-0.636275	-0.000240
H	1.977784	-1.451981	-0.000788
H	3.351969	-0.723962	-0.879348
H	3.351212	-0.724660	0.879373

N,N'-Dimethyl-ethen-1,2-dicarboxamid

C	0.619599	1.348230	0.061719
H	1.185501	2.279378	0.092100
C	-0.719764	1.485360	0.048633
H	-1.096086	2.505575	0.064175
C	-1.896383	0.545535	-0.011435
O	-3.019706	1.047124	-0.114669
N	-1.682730	-0.785232	0.059211
H	-0.721502	-1.126132	0.100586
C	-2.804431	-1.701721	-0.011297
H	-3.542604	-1.467384	0.763449
H	-3.312786	-1.635619	-0.981156
H	-2.436164	-2.719931	0.133790
C	1.463263	0.121161	0.036122
N	2.802054	0.376526	-0.007362
H	3.120022	1.327954	-0.118262
C	3.778753	-0.697336	-0.081599
H	4.751804	-0.320768	0.242978
H	3.464193	-1.510921	0.575353
H	3.867532	-1.096084	-1.100101
O	1.049531	-1.044936	0.066082

(Z)-2-butene

C	-1.282937	-0.220582	0.000002
H	-1.303362	-1.309002	-0.000005
H	-2.245988	0.283216	-0.000011
C	-0.134056	0.456138	0.000004
H	-0.163130	1.546985	-0.000007
C	1.234870	-0.163109	-0.000001
H	1.182098	-1.257324	-0.000014
H	1.811568	0.150733	-0.880727
H	1.811557	0.150710	0.880740

S21-*E*

C	-1.168882	0.334453	0.244000
C	-0.063653	-0.025321	-0.413308
C	1.304201	0.568265	-0.211702
C	2.331105	-0.472023	0.267988
H	3.326503	-0.025981	0.376903
H	2.411835	-1.302644	-0.443906
H	2.035460	-0.892136	1.235915
H	1.658613	1.003820	-1.158245
H	1.248410	1.394482	0.509061
H	-0.127474	-0.828894	-1.151519
C	-2.530208	-0.271750	0.051263
H	-2.910720	-0.702849	0.987532
H	-2.514893	-1.065144	-0.704327
H	-3.262292	0.483730	-0.265892
H	-1.100818	1.133875	0.985022

S21-*Z*

C	0.012459	0.833264	0.124045
C	1.301149	0.611713	-0.160689
C	2.056371	-0.685658	-0.070189
H	1.430957	-1.521937	0.254329
H	2.491506	-0.950690	-1.043430
H	2.895014	-0.601455	0.634554
H	1.894944	1.461903	-0.499346
C	-1.020668	-0.158601	0.588955
H	-0.570382	-1.139190	0.777864
C	-2.173144	-0.308289	-0.419952
H	-2.940291	-0.996452	-0.046350
H	-1.803854	-0.693107	-1.377163
H	-2.654398	0.657958	-0.614480
H	-1.434268	0.179906	1.550747
H	-0.366228	1.848499	-0.009743

S22-*E*

C	-0.575503	-0.484719	-0.338471
C	0.575506	-0.484728	0.338467
C	1.949686	-0.465741	-0.274142
C	2.748572	0.789246	0.118038
H	3.756521	0.768613	-0.312323
H	2.243756	1.696198	-0.233275
H	2.850376	0.866554	1.207476
H	1.870314	-0.528734	-1.367242
H	2.509042	-1.356372	0.049968
H	0.543874	-0.478941	1.431056
C	-1.949684	-0.465742	0.274139
C	-2.748577	0.789243	-0.118033
H	-3.756524	0.768603	0.312330

H	-2.243764	1.696196	0.233283
H	-2.850383	0.866555	-1.207470
H	-1.870310	-0.528741	1.367239
H	-2.509035	-1.356374	-0.049976
H	-0.543872	-0.478909	-1.431059

S22-*Z*

C	0.669066	-0.946666	-0.283409
C	-0.669280	-0.946879	-0.283441
C	-1.598226	-0.121978	0.567708
C	-2.443777	0.847479	-0.277382
H	-3.023429	0.307086	-1.035673
H	-3.148377	1.407720	0.348188
H	-1.802635	1.565972	-0.800407
H	-1.043527	0.442650	1.324885
H	-2.273662	-0.794161	1.117564
H	-1.174509	-1.600835	-0.997062
C	1.597727	-0.121564	0.567849
C	2.444381	0.846877	-0.277288
H	1.803991	1.565251	-0.801399
H	3.148702	1.407300	0.348432
H	3.024436	0.305654	-1.034680
H	2.272432	-0.793643	1.118742
H	1.042689	0.443888	1.324162
H	1.174541	-1.600493	-0.996977

S23-*E*

C	-2.352470	0.283430	0.082723
C	-1.260854	-0.475534	-0.060130
C	0.078437	0.147965	-0.264309
O	0.252634	1.363328	-0.340540
N	1.115241	-0.743113	-0.385509
H	0.947507	-1.713317	-0.157821
C	2.497381	-0.285598	-0.466545
C	3.087300	0.085907	0.897523
H	4.122078	0.431834	0.790062
H	3.082762	-0.773331	1.578744
H	2.496846	0.890243	1.345970
H	3.085341	-1.075444	-0.947265
H	2.505679	0.587416	-1.124480
H	-1.332473	-1.563191	-0.031518
C	-3.744310	-0.225382	0.291732
H	-3.784452	-1.319544	0.317871
H	-4.161910	0.157767	1.232681
H	-4.410623	0.124866	-0.508168
H	-2.211417	1.363138	0.040847

S23-*Z*

C	-2.495667	0.569197	0.268669
C	-1.229077	0.991372	0.127632
C	-0.053925	0.146108	-0.228843
O	-0.101173	-1.054503	-0.500541
N	1.135631	0.833753	-0.256089
H	1.164334	1.771540	0.118509
C	2.400881	0.143275	-0.474647
C	2.927323	-0.556783	0.782256
H	3.873863	-1.068344	0.571775
H	2.198969	-1.299169	1.121238
H	3.098992	0.161048	1.593109
H	2.231432	-0.592418	-1.265388

H	3.123593	0.877793	-0.847118
H	-1.025485	2.050063	0.287321
C	-3.042201	-0.817008	0.105232
H	-3.802380	-0.825240	-0.688408
H	-2.260898	-1.534415	-0.139405
H	-3.554687	-1.127072	1.026405
H	-3.231769	1.329005	0.537125

S24-*E*

C	-1.789831	0.182804	-0.342881
C	-0.694761	-0.530908	-0.061007
C	0.614075	0.142636	0.178882
O	0.757321	1.364372	0.162929
N	1.658252	-0.707152	0.444668
H	1.526158	-1.697745	0.295060
C	3.020984	-0.207866	0.584824
C	3.700252	0.066973	-0.760460
H	4.717043	0.448175	-0.609454
H	3.127022	0.815958	-1.314631
H	3.762983	-0.844694	-1.366476
H	2.963672	0.715796	1.166873
H	3.588879	-0.940015	1.169731
H	-0.741335	-1.618721	-0.001279
C	-3.160203	-0.374323	-0.585324
C	-4.185918	0.151946	0.435300
H	-3.912941	-0.149338	1.452495
H	-5.186983	-0.237030	0.218734
H	-4.236137	1.246785	0.413465
H	-3.488562	-0.087460	-1.595502
H	-3.134917	-1.471210	-0.560889
H	-1.678804	1.267016	-0.380240

S24-*Z*

C	1.943198	-0.895310	0.186412
C	0.832925	-1.555241	-0.172513
C	-0.580692	-1.062264	-0.133038
O	-1.485501	-1.765985	0.309867
N	-0.811463	0.187384	-0.640746
H	-0.047522	0.690591	-1.065913
C	-2.147075	0.775111	-0.637619
C	-2.521388	1.377711	0.719263
H	-2.488368	0.598903	1.486588
H	-3.534750	1.794984	0.690519
H	-1.826355	2.177320	1.000582
H	-2.179013	1.534215	-1.426411
H	-2.857795	-0.015007	-0.900041
H	0.899835	-2.607403	-0.438963
C	2.070142	0.521966	0.681674
H	1.090463	0.928504	0.951061
C	2.759555	1.441141	-0.343871
H	3.747119	1.054559	-0.621256
H	2.892613	2.450611	0.060574
H	2.172356	1.520819	-1.267482
H	2.670439	0.513070	1.601908
H	2.885229	-1.443665	0.133270

S25-*E*

C	2.511895	-0.171117	-0.354416
C	1.361345	0.501358	-0.247543
C	0.059476	-0.224224	-0.140459

O	-0.015195	-1.454208	-0.142349
N	-1.032751	0.593204	-0.040084
H	-0.872895	1.590648	-0.048728
C	-2.436144	0.142382	0.078511
C	-2.609897	-0.696900	1.357797
H	-3.652910	-1.018852	1.458484
H	-1.968217	-1.579262	1.319608
H	-2.343304	-0.106794	2.242018
C	-2.829079	-0.678890	-1.163356
H	-2.718199	-0.076075	-2.071899
H	-3.874245	-1.000615	-1.087218
H	-2.191593	-1.560961	-1.248775
C	-3.299056	1.410112	0.162690
H	-3.030844	2.014708	1.038210
H	-3.185631	2.027353	-0.737413
H	-4.355542	1.139096	0.252817
H	1.357139	1.591899	-0.237867
C	3.877692	0.439389	-0.450517
C	4.786854	0.006839	0.714241
H	4.884838	-1.084341	0.752257
H	5.790356	0.432958	0.605680
H	4.375004	0.338314	1.673720
H	3.804061	1.533925	-0.482993
H	4.343131	0.125470	-1.396778
H	2.451150	-1.259923	-0.353430

S25-*Z*

C	-2.579449	-0.792073	-0.096697
C	-1.509482	-1.532470	-0.421080
C	-0.071496	-1.273610	-0.083693
O	0.651442	-2.192031	0.299475
N	0.358165	0.015862	-0.244220
H	-0.264366	0.639634	-0.737982
C	1.740663	0.493380	-0.020817
C	2.714408	-0.234788	-0.965947
H	3.736729	0.129198	-0.811071
H	2.440308	-0.056082	-2.012193
H	2.688923	-1.309878	-0.776144
C	1.733658	1.998639	-0.325429
H	1.031347	2.529684	0.328485
H	2.731391	2.419146	-0.165552
H	1.453015	2.191741	-1.368953
C	2.135948	0.258542	1.447697
H	3.149677	0.634375	1.627634
H	2.105778	-0.806892	1.682968
H	1.447205	0.785826	2.117536
H	-1.654302	-2.495874	-0.904220
C	-2.623568	0.513447	0.654409
H	-3.381360	0.429880	1.445561
C	-2.993201	1.700593	-0.254574
H	-3.948956	1.528976	-0.763253
H	-2.235471	1.859315	-1.032120
H	-3.079640	2.626071	0.325389
H	-1.667871	0.706818	1.150405
H	-3.555995	-1.176689	-0.395971

6. Crystallographic data for Ru-6
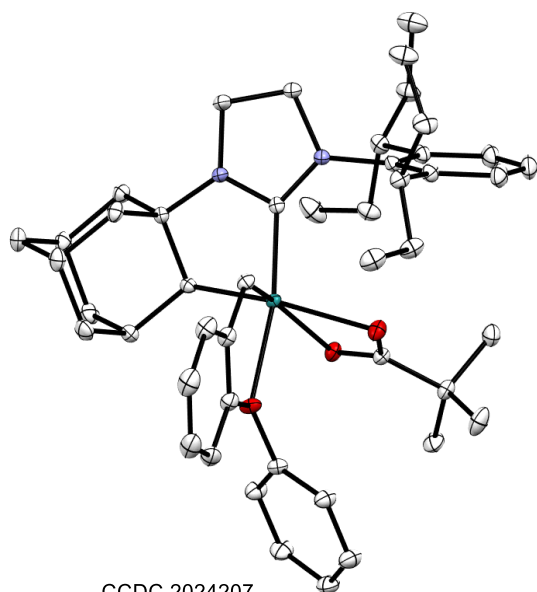
CCDC 2024207

all hydrogen atoms are omitted for clarity

Table S1 | Crystal data and structure refinement for Ru-6.

Identification code	yx-531
Empirical formula	$C_{53}H_{68}N_2O_3Ru$
Formula weight	882.16
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	11.506(8)
b/Å	12.614(6)
c/Å	17.118(16)
α/°	75.681(17)
β/°	71.28(3)
γ/°	88.660(15)
Volume/Å^3	2276(3)
Z	2
ρ_{calc}g/cm^3	1.287
μ/mm^{-1}	0.389
F(000)	936.0
Crystal size/mm^3	0.28 × 0.27 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.338 to 72.28
Index ranges	−19 ≤ h ≤ 19, −20 ≤ k ≤ 20, −28 ≤ l ≤ 28

Reflections collected	210134
Independent reflections	20832 [R_{int} = 0.0507, R_{sigma} = 0.0345]
Data/restraints/parameters	20832/21/539
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0338, wR_2 = 0.0724
Final R indexes [all data]	R_1 = 0.0472, wR_2 = 0.0769
Largest diff. peak/hole / e Å^{-3}	1.30/-1.17

7. Further study

7.1 Further lowering the equivalent of the regular olefin:

Scheme S3 | Further lowering the equivalent of the regular olefin.
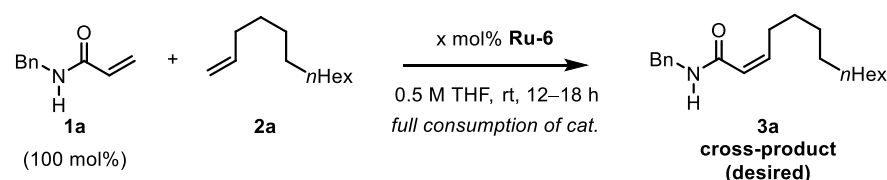
entry	equiv. of **2a**	loading of **Ru-6**	yield of **3a**
1	2 equiv.	1.2 mol% cat.	80% yield (75% isolated)
2	1.3 equiv.	2.5 mol% cat.	79% yield (75% isolated)
3	1 equiv.	2.5 mol% cat.	65% yield

The experiment in *entry 1* was conducted as described in *Section 3*. The experiment in *entry 2* was conducted as described in *Section 4.2*. The experiment in *entry 3* was conducted as follows:

A 4 mL vial was charged with a stir bar, **1a** (0.25 mmol, 1 equiv, 40.3 mg), **2a** (0.25 mmol, 1 equiv, 42 mg), and anthracene (*as the internal standard*) in a nitrogen glovebox. To this was added a stock solution of the ruthenium catalyst **Ru-6** (0.00625 mmol, 0.025 equiv, 5.0 mg) in d_8-THF (0.4 mL). The vial was loosely capped with a screw thread hole cap, and a 20-gauge needle was used to puncture the cap and left on (see Figure S1). The reaction mixture was allowed to stir at room temperature in the glovebox for 22 hours. The reaction was then transferred to an NMR tube and removed from the glovebox. The yield of the metathesis product **3a** was determined by ^{1}H NMR analysis of the crude reaction mixture.

7.2 Kinetic preference between cross- and homo-metathesis using acrylate S21
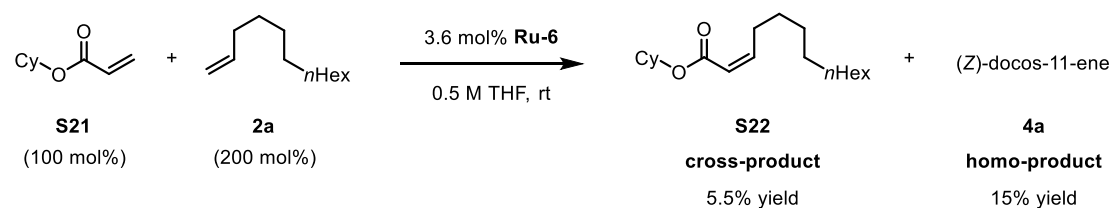
A 4 mL vial was charged with a stir bar, **S21** (0.25 mmol, 1 equiv, 38.6 mg), **2a** (0.5 mmol, 2 equiv, 84 mg), and anthracene (*as the internal standard*) in a nitrogen glovebox. To this was added a stock solution of the ruthenium catalyst **Ru-6** (0.009 mmol, 0.036 equiv, 7.2 mg) in d_8-THF (0.4 mL). The vial was loosely capped with a screw thread hole cap, and a 20-gauge needle was used to puncture the cap and left on (see Figure S1). The reaction mixture was stir at room temperature, and then removed from the glovebox when the yield of **S22** reached ~5%. The yields of the metathesis products were determined by ^{1}H NMR analysis of the crude reaction mixture: **S22**, 5.5% yield; **4a**, 15% yield. This result indicates that the reaction with acrylate **S21** favors *homo-metathesis* over *cross-metathesis* kinetically.

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9. Spectra

Figure S3 | ¹H NMR (400 MHz, THF-d_8) spectrum of **Ru-4**.
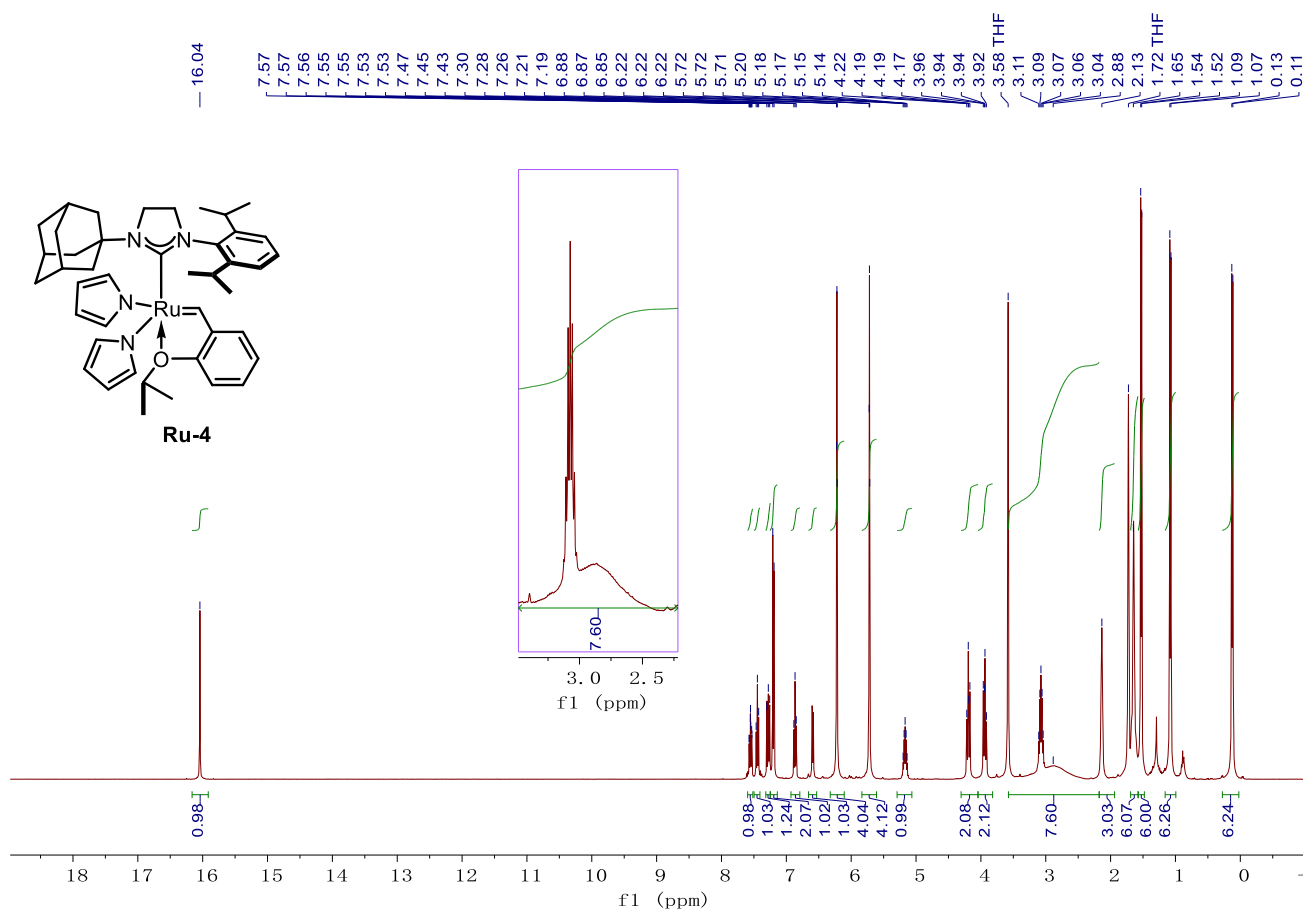
Figure S4 | ¹³C NMR (101 MHz, THF-d_8) spectrum of **Ru-4**.
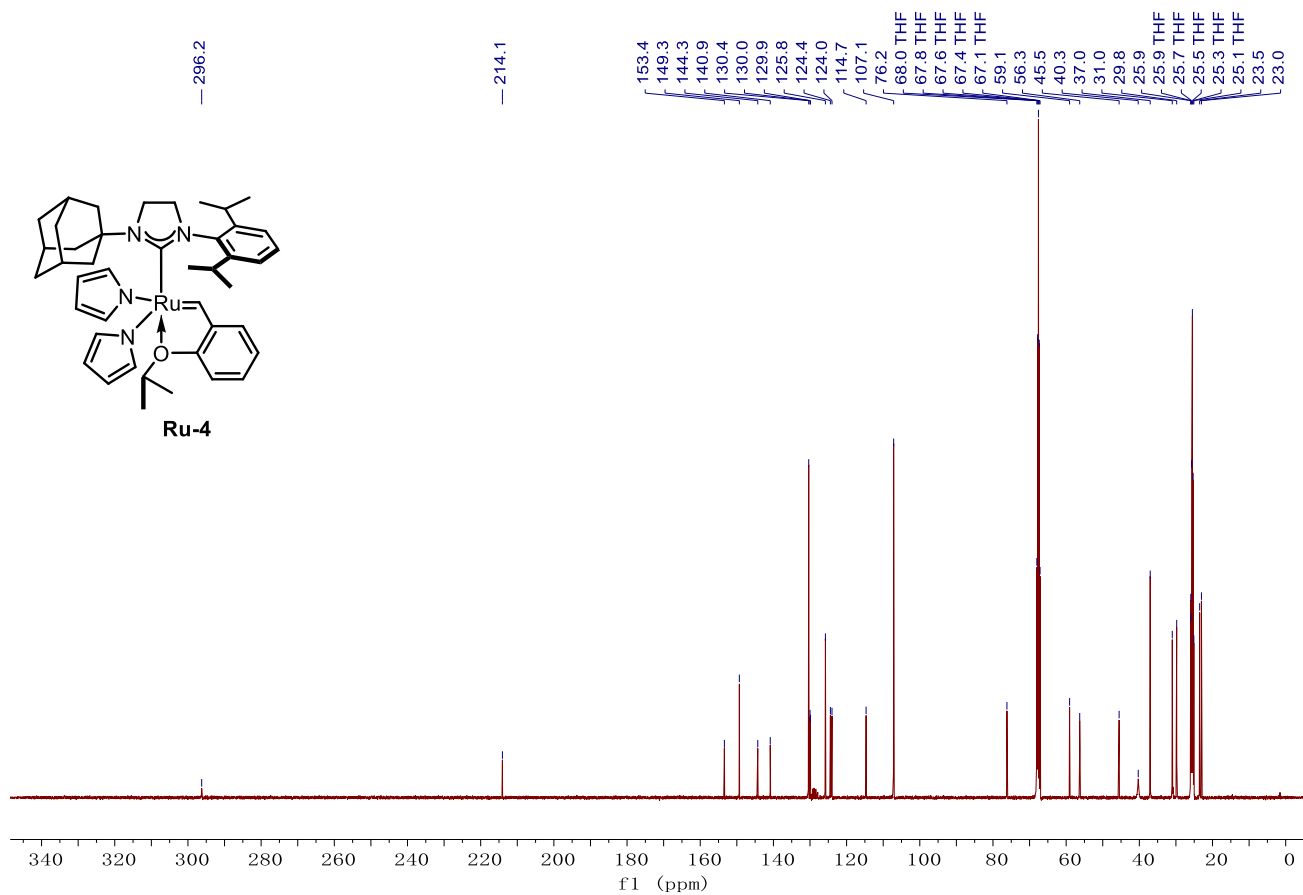
Figure S5 | ¹H NMR (400 MHz, C₆D₆) spectrum of **Ru-2**.
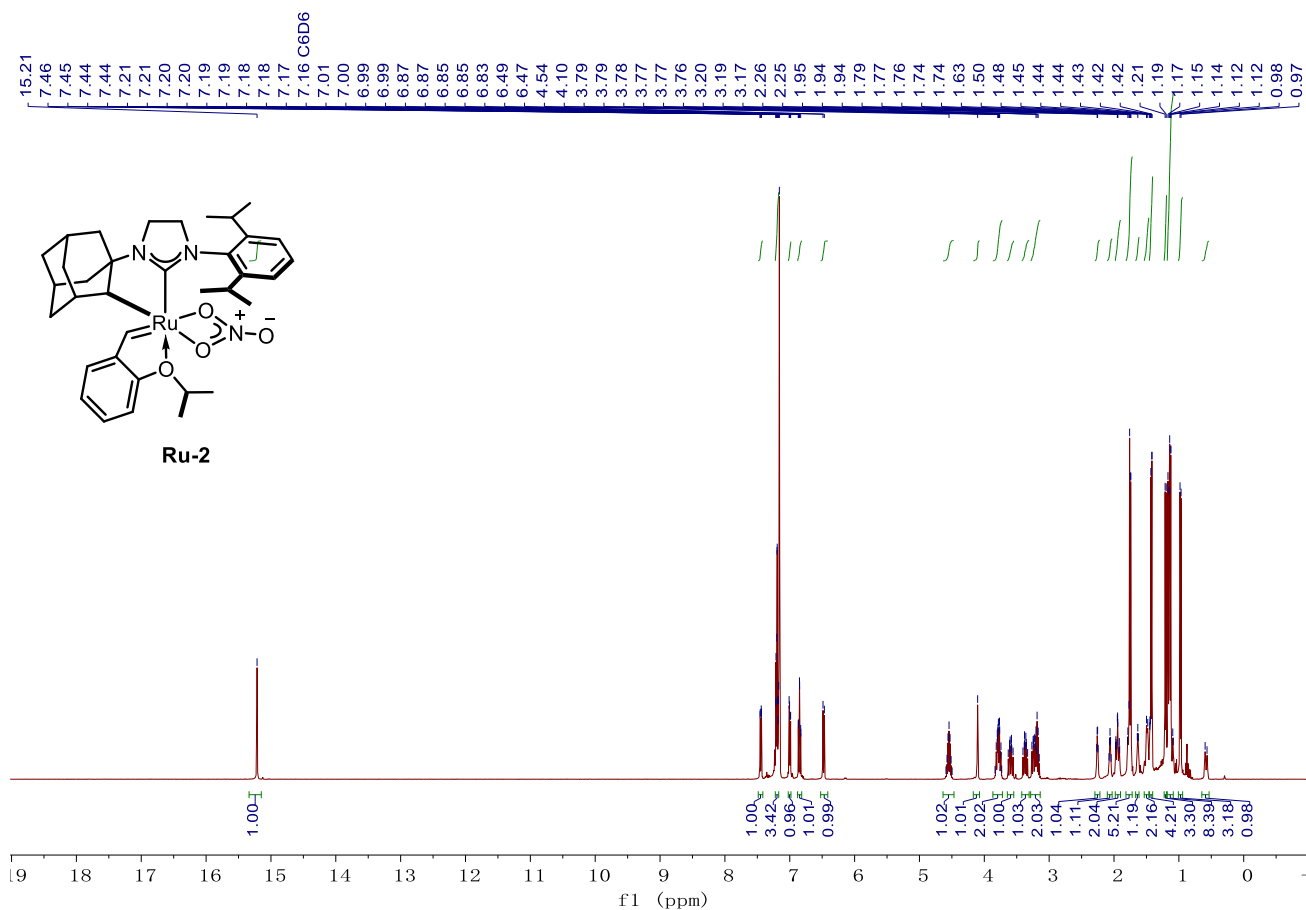
Figure S6 | ¹³C NMR (101 MHz, C₆D₆) spectrum of **Ru-2**.
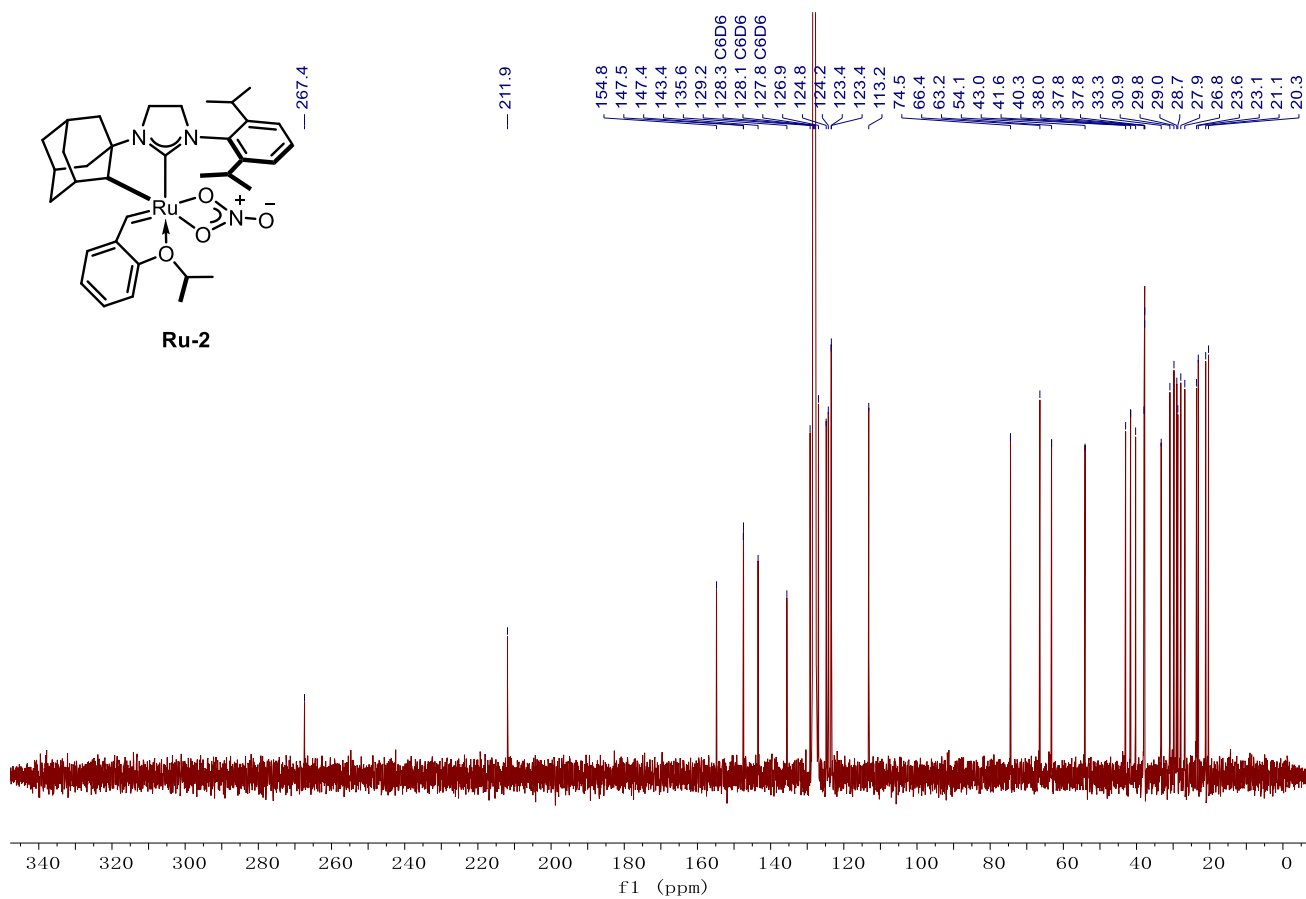
Figure S7 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **S3**.
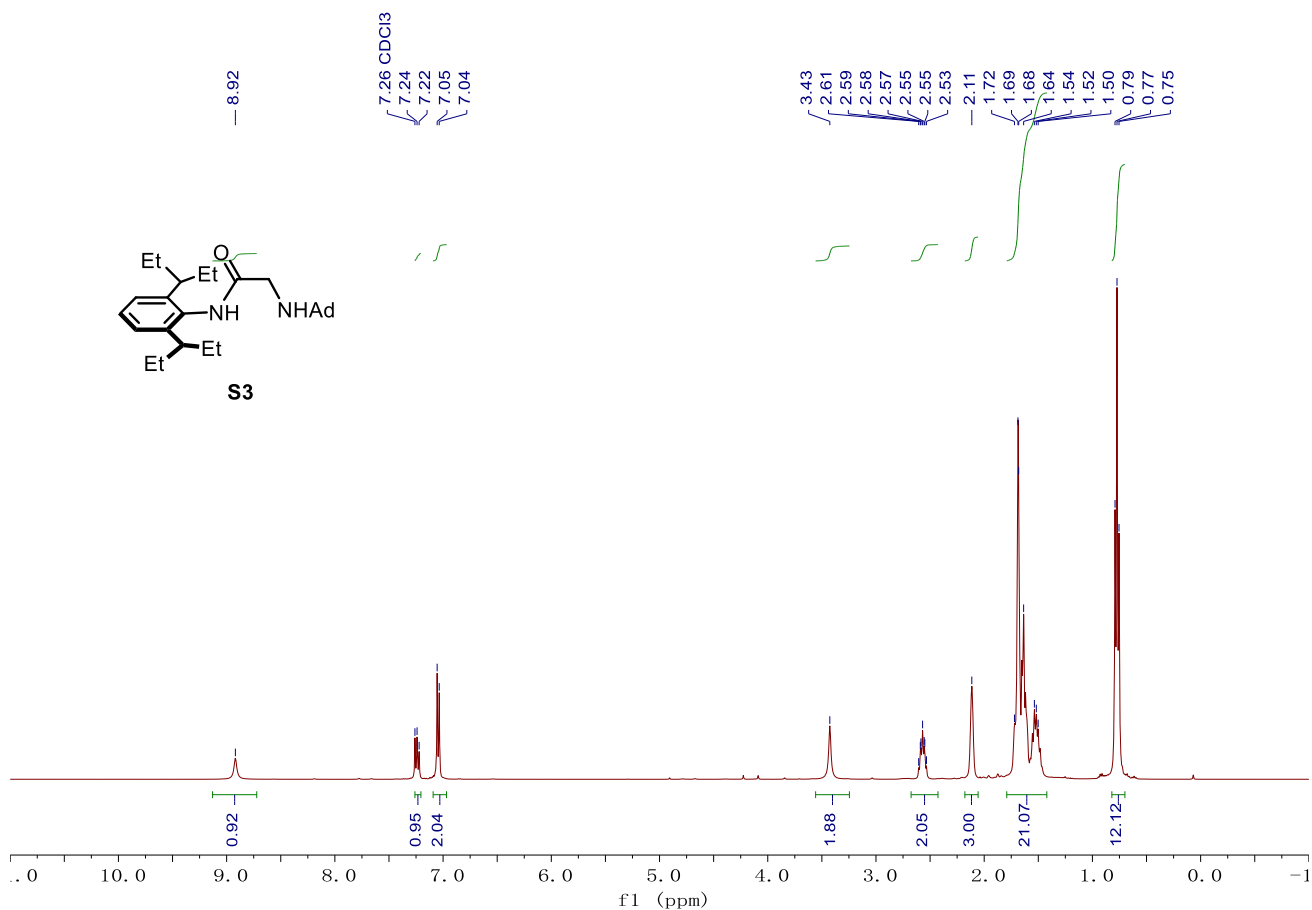
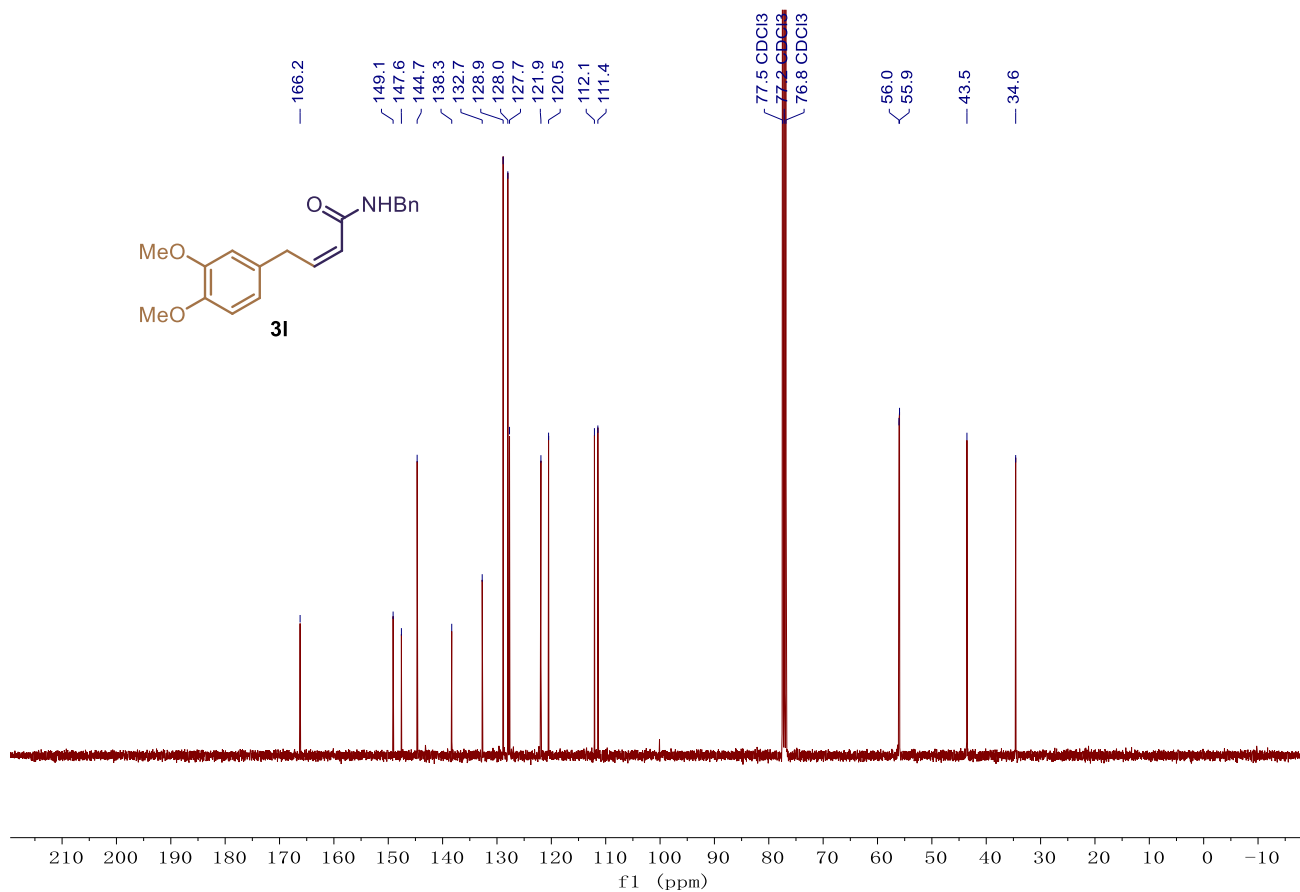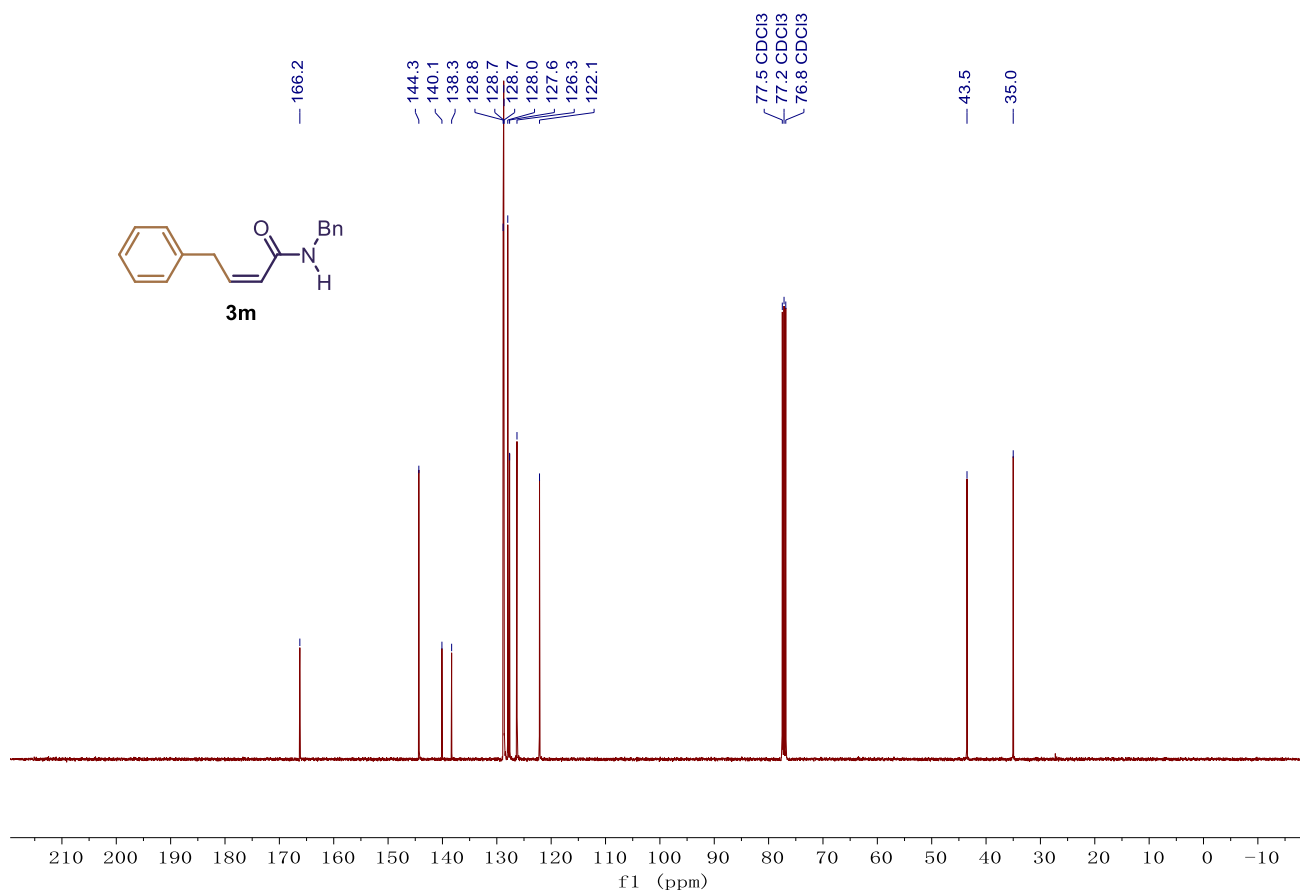**Figure S8 |** ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **S3**.
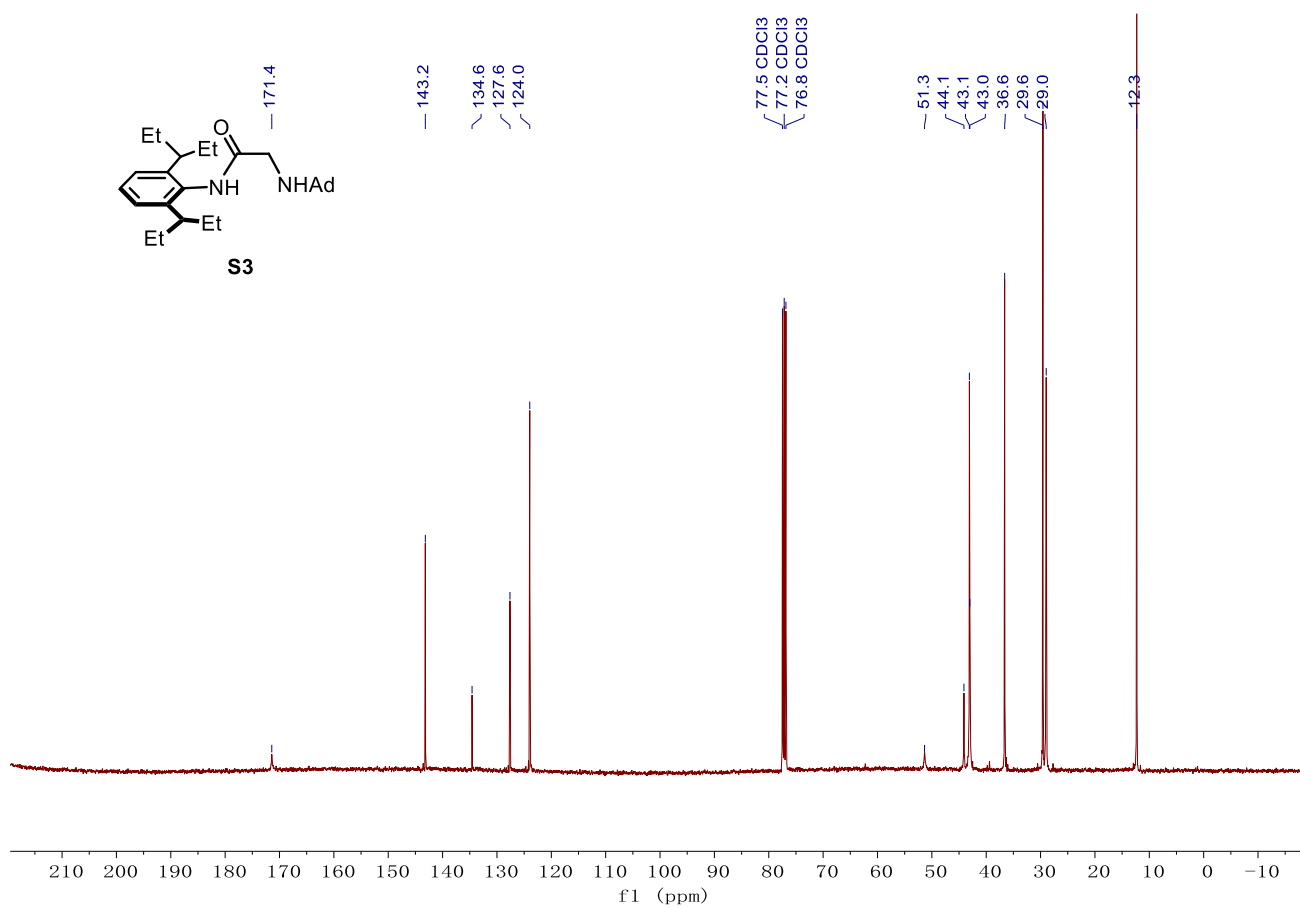
Figure S9 | Crude ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **S4**.
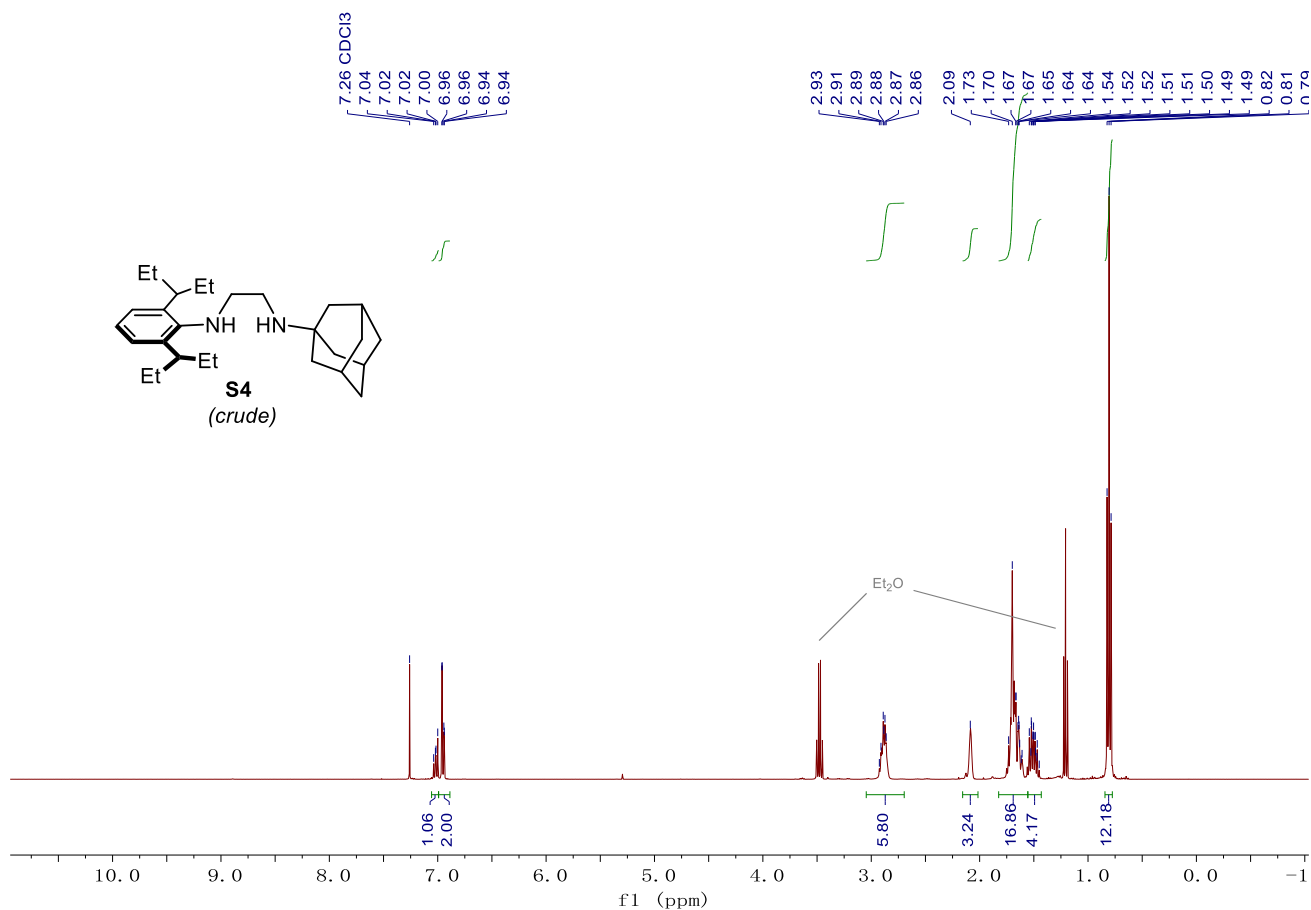
Figure S10 | Crude ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **S4**.
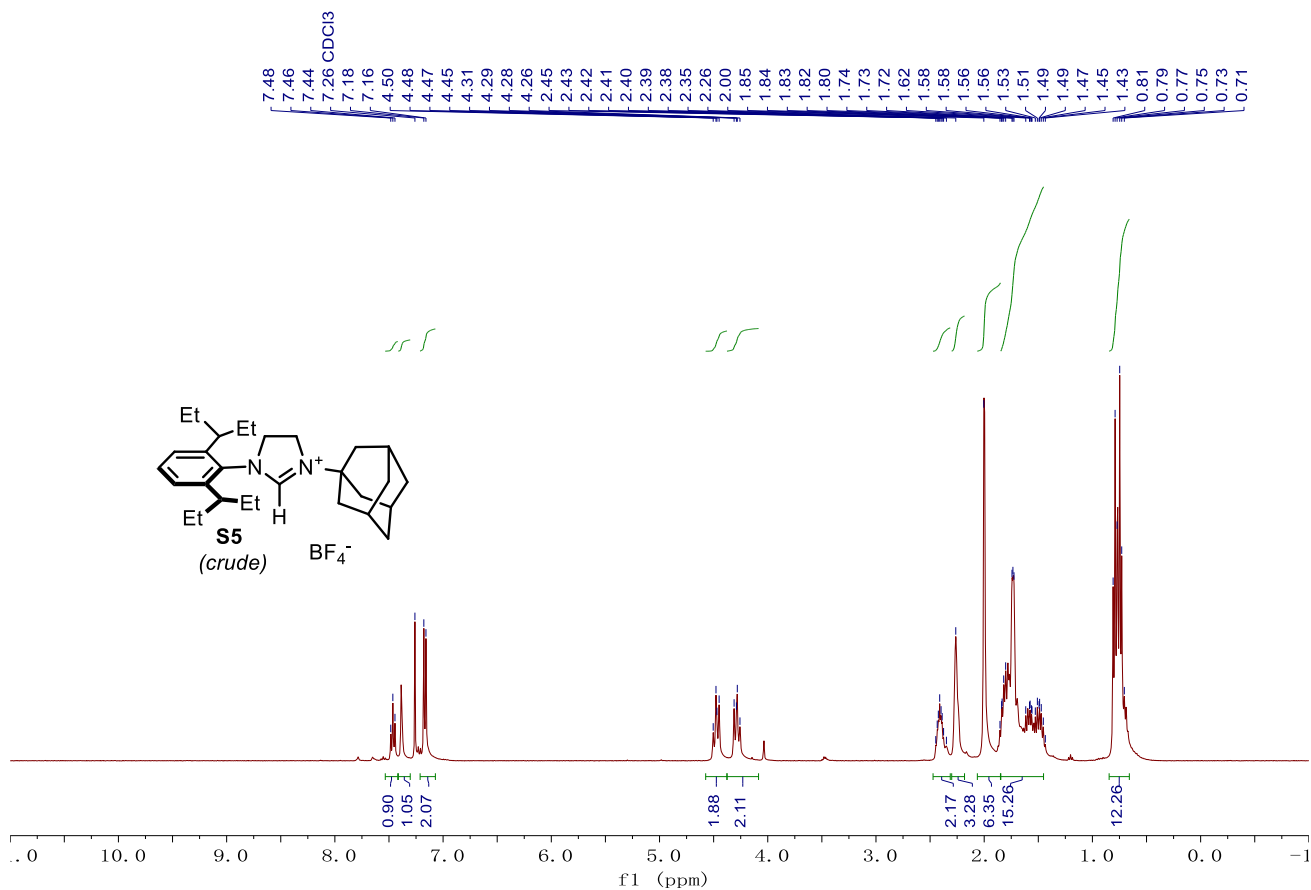
Figure S11 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **S6**.
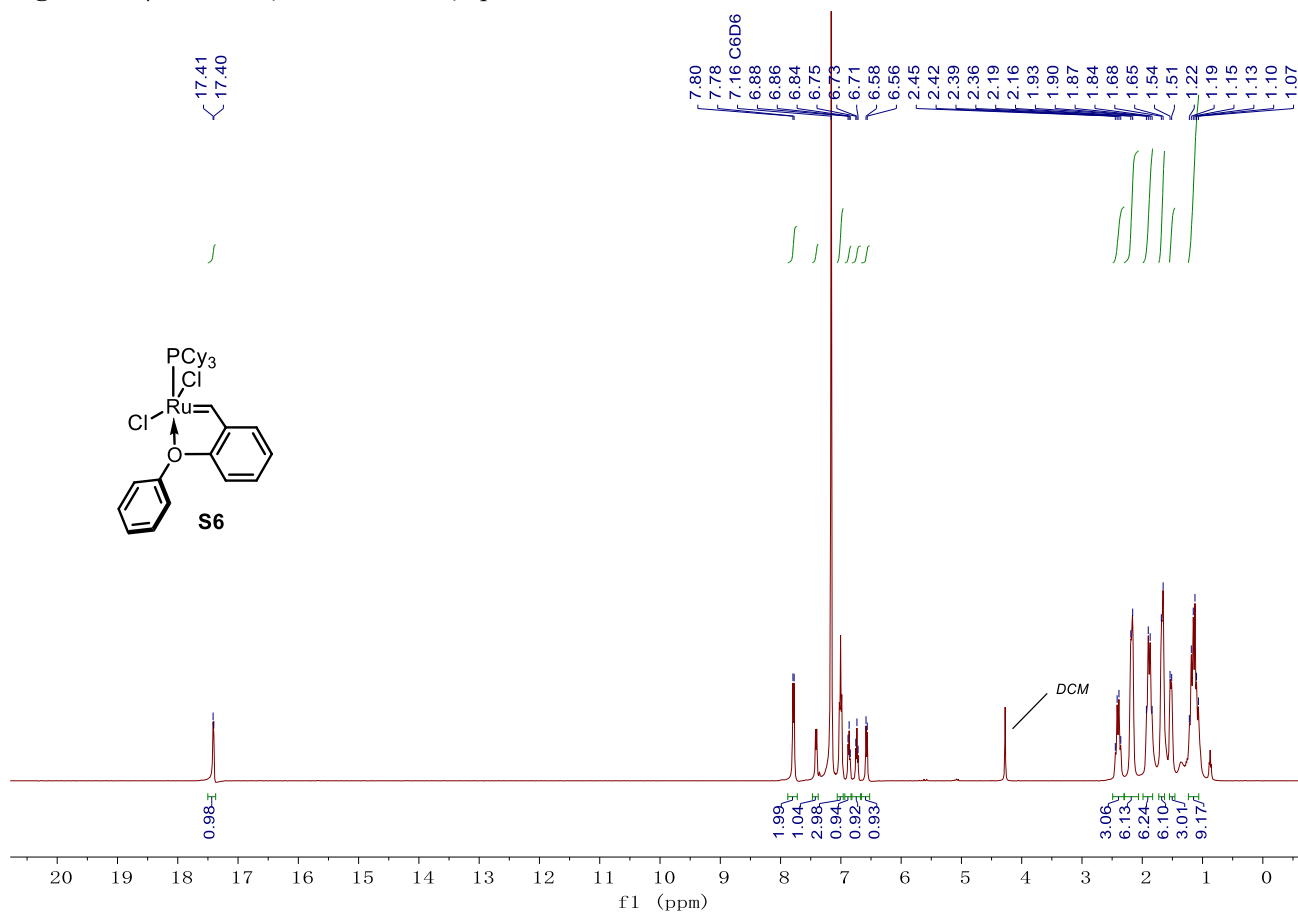
Figure S12 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **S6**.
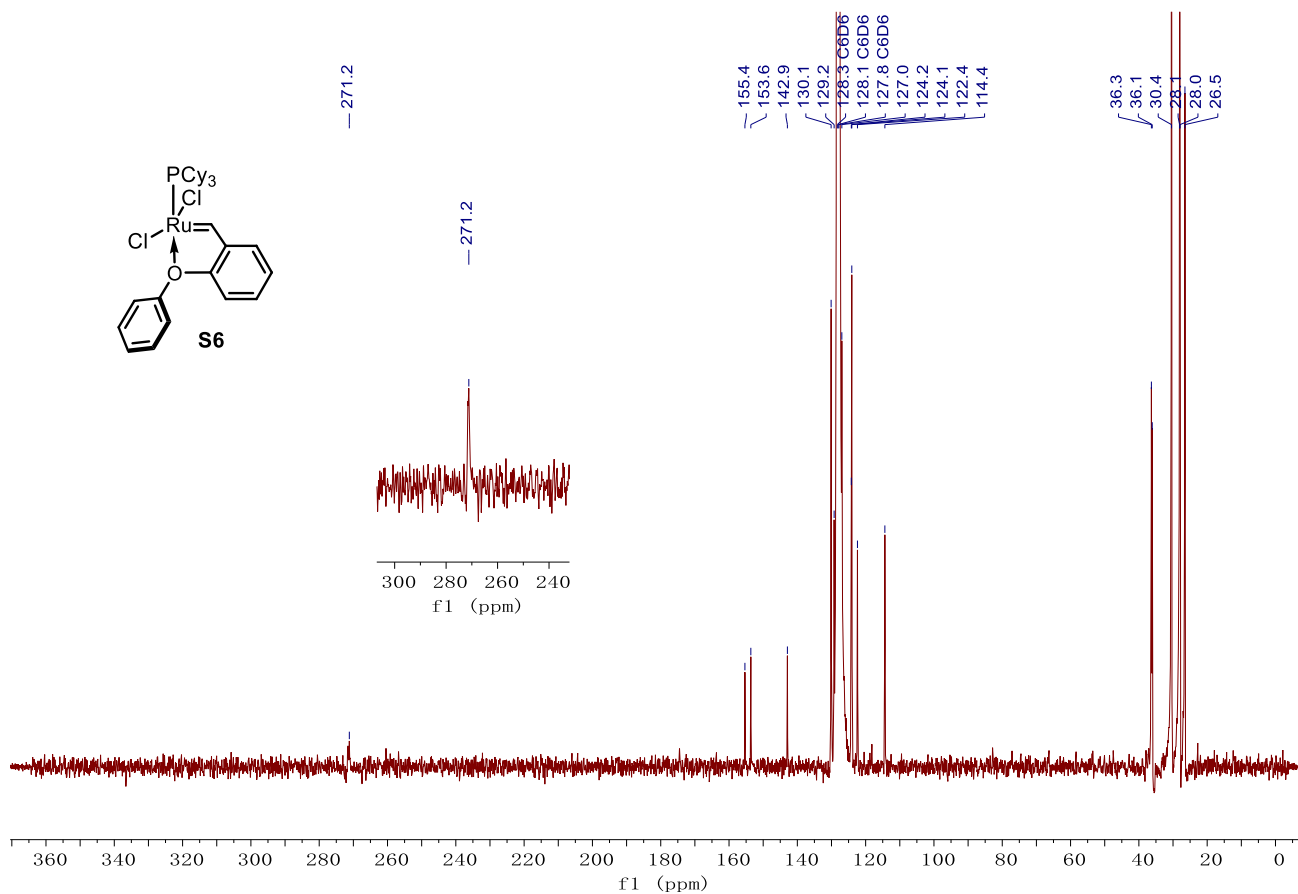
Figure S13 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **Ru-5**.
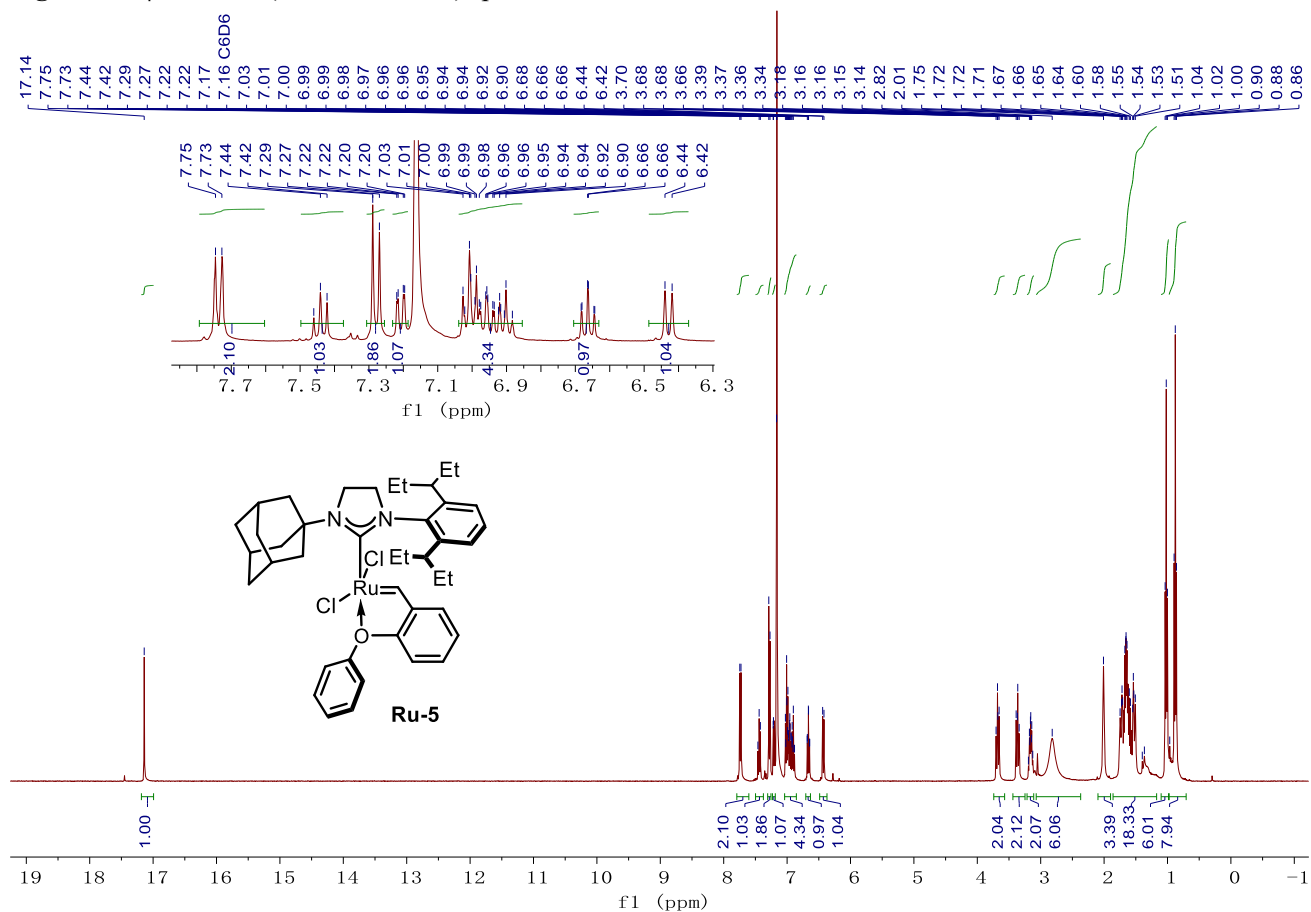
Figure S14 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **Ru-5**.
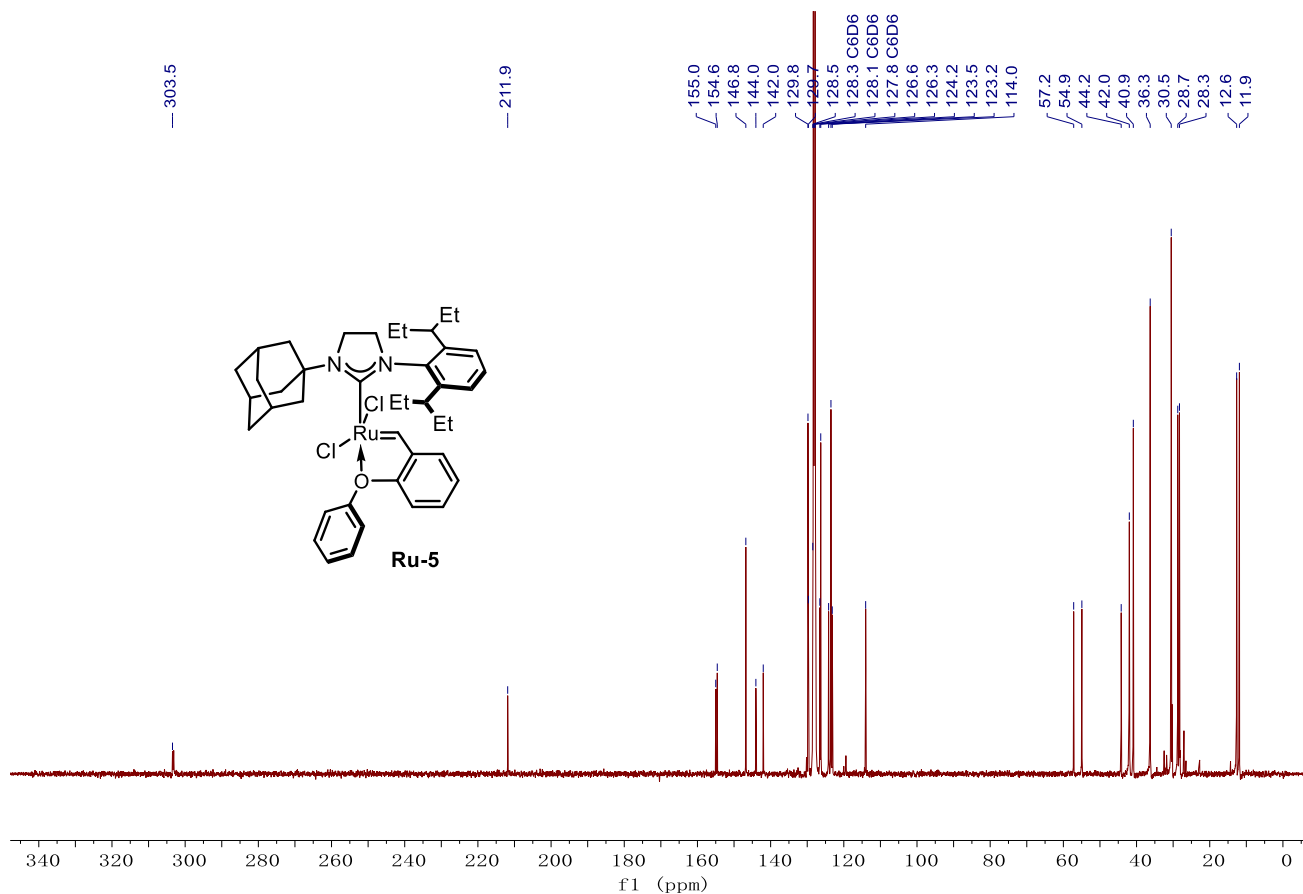
Figure S15 | ^{1}H NMR (400 MHz, C_6D_6) spectrum of **S7**.
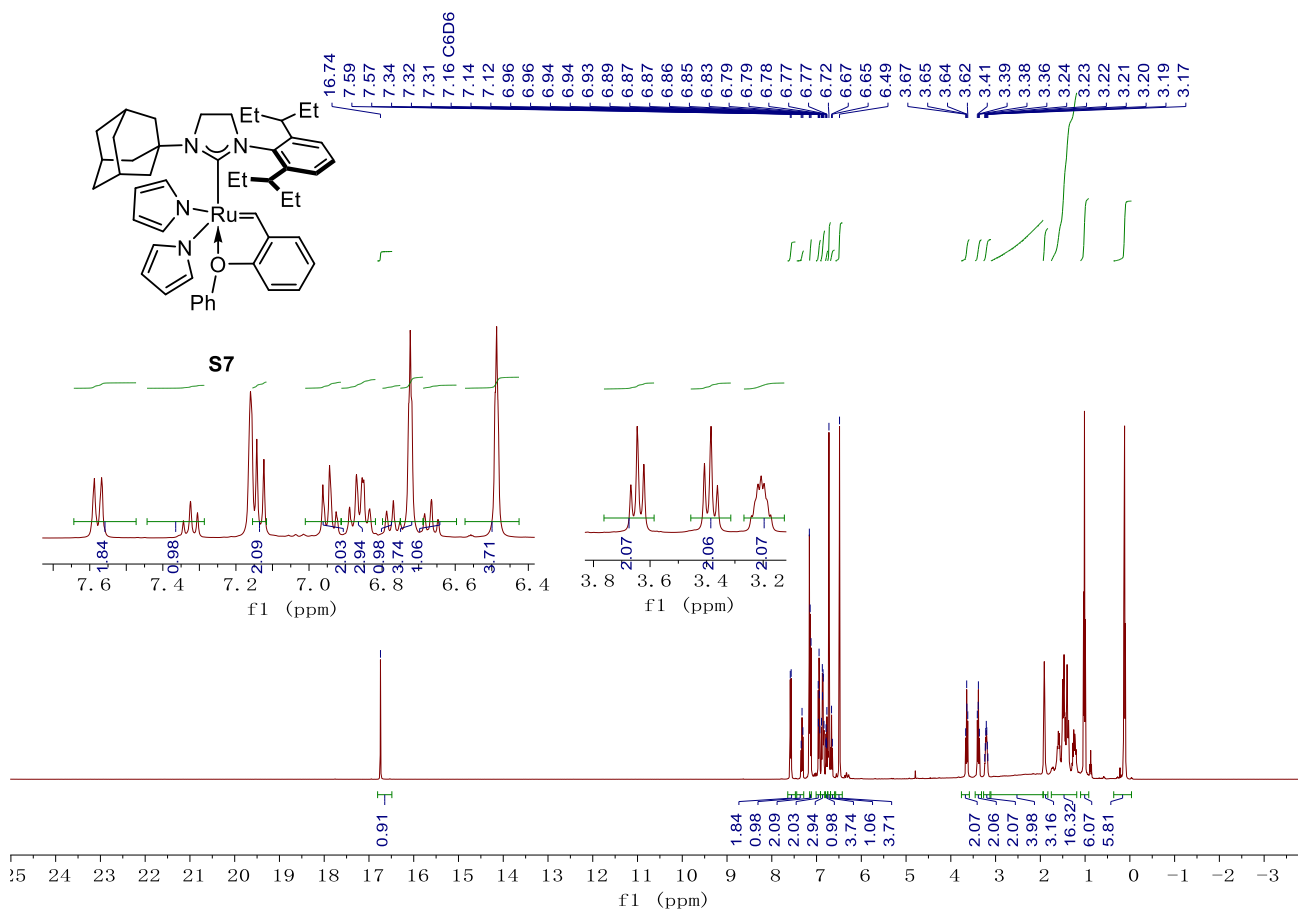
Figure S16 | ^{13}C NMR (101 MHz, C_6D_6) spectrum of **S7**.
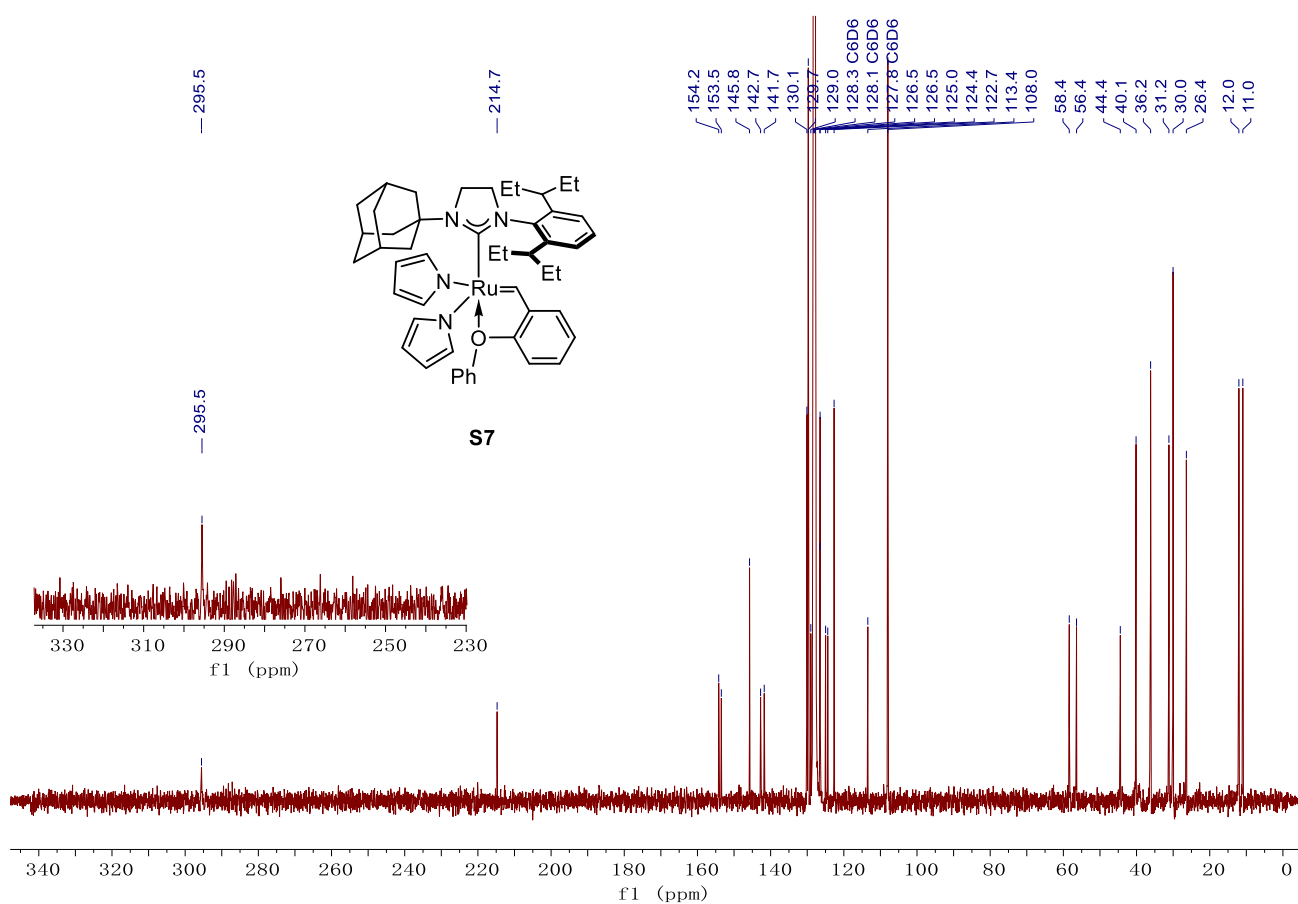
Figure S17 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **Ru-6**.
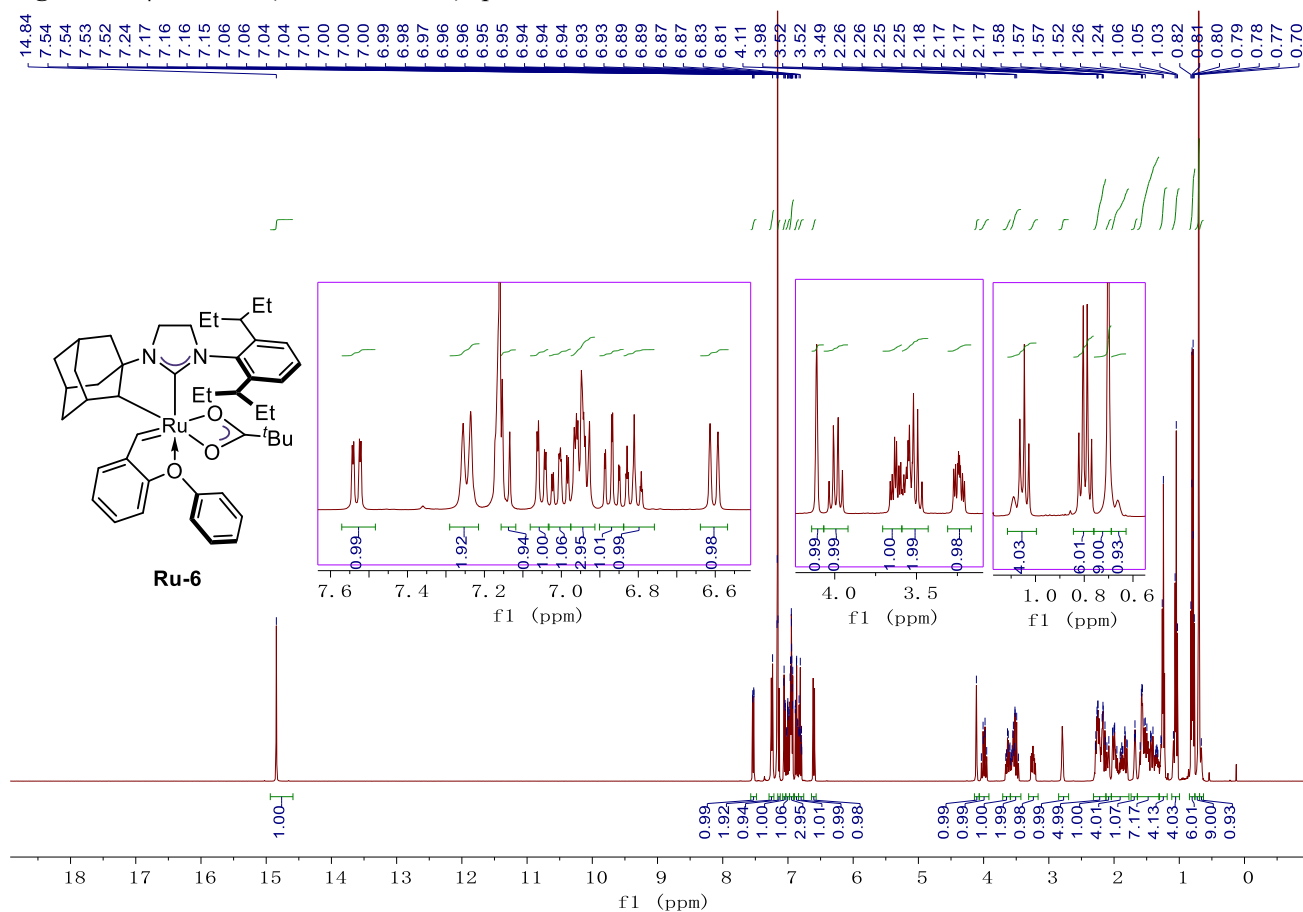
Figure S18 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **Ru-6**.
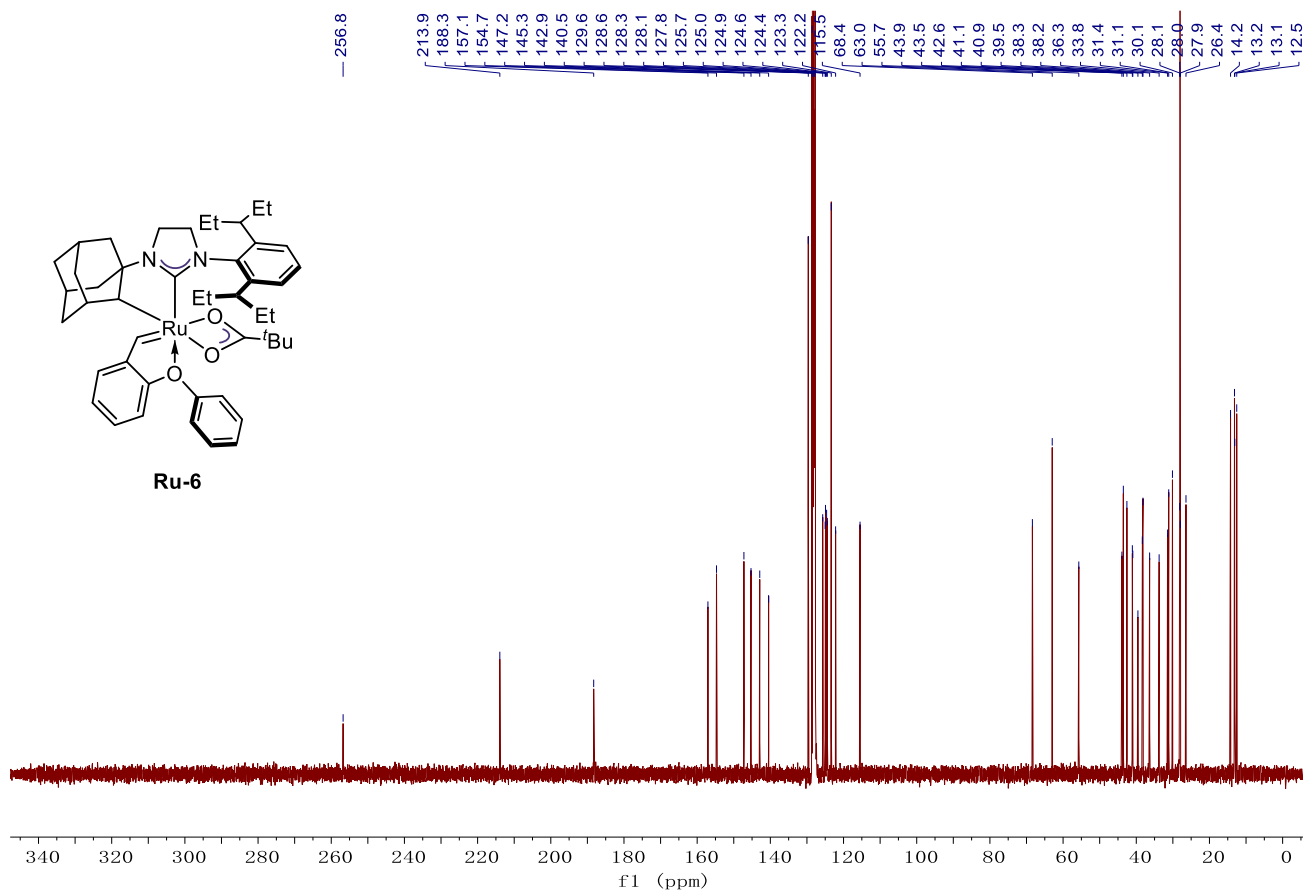
Figure S19 | Crude ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **S9**.
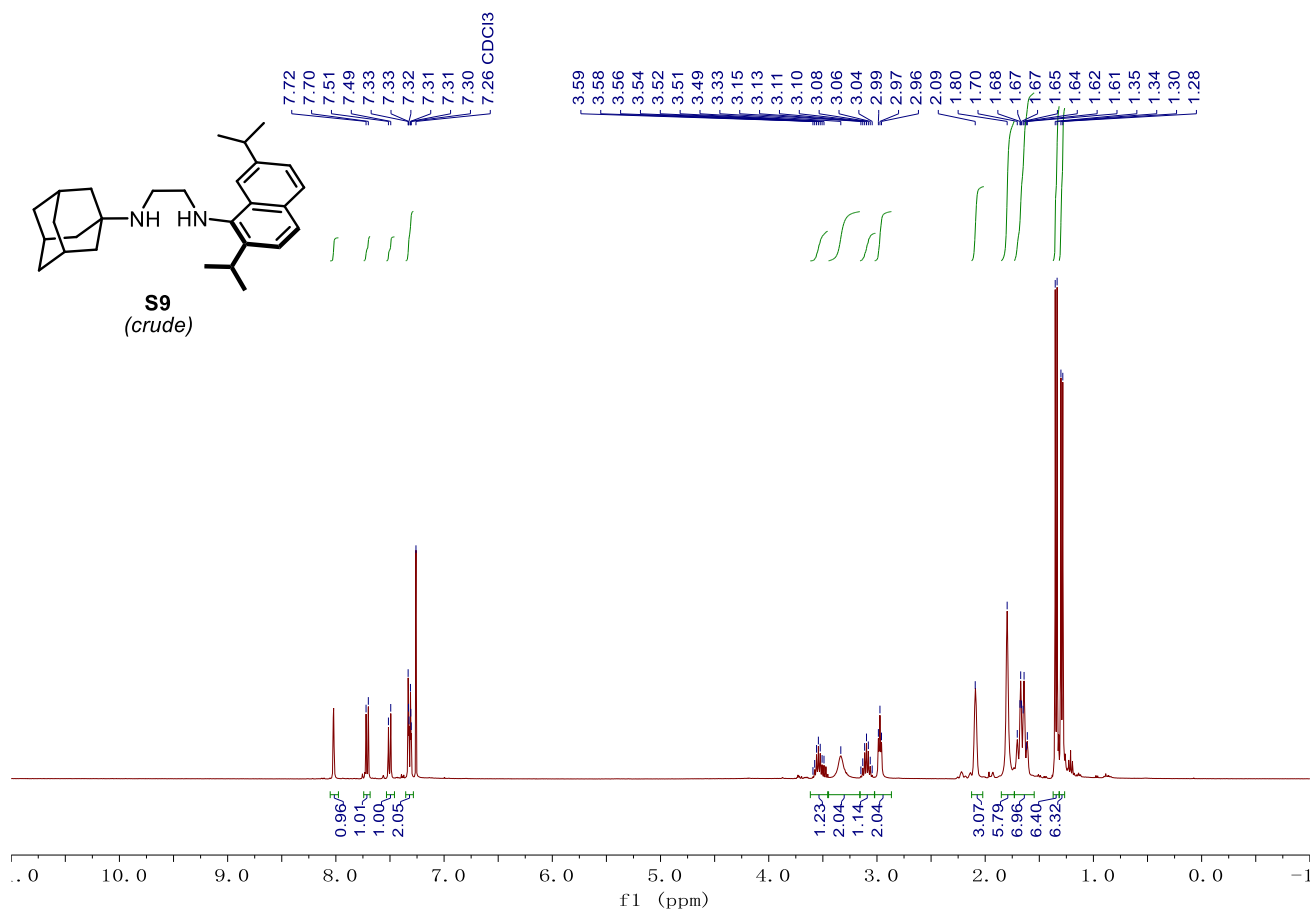
Figure S20 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **S10**.
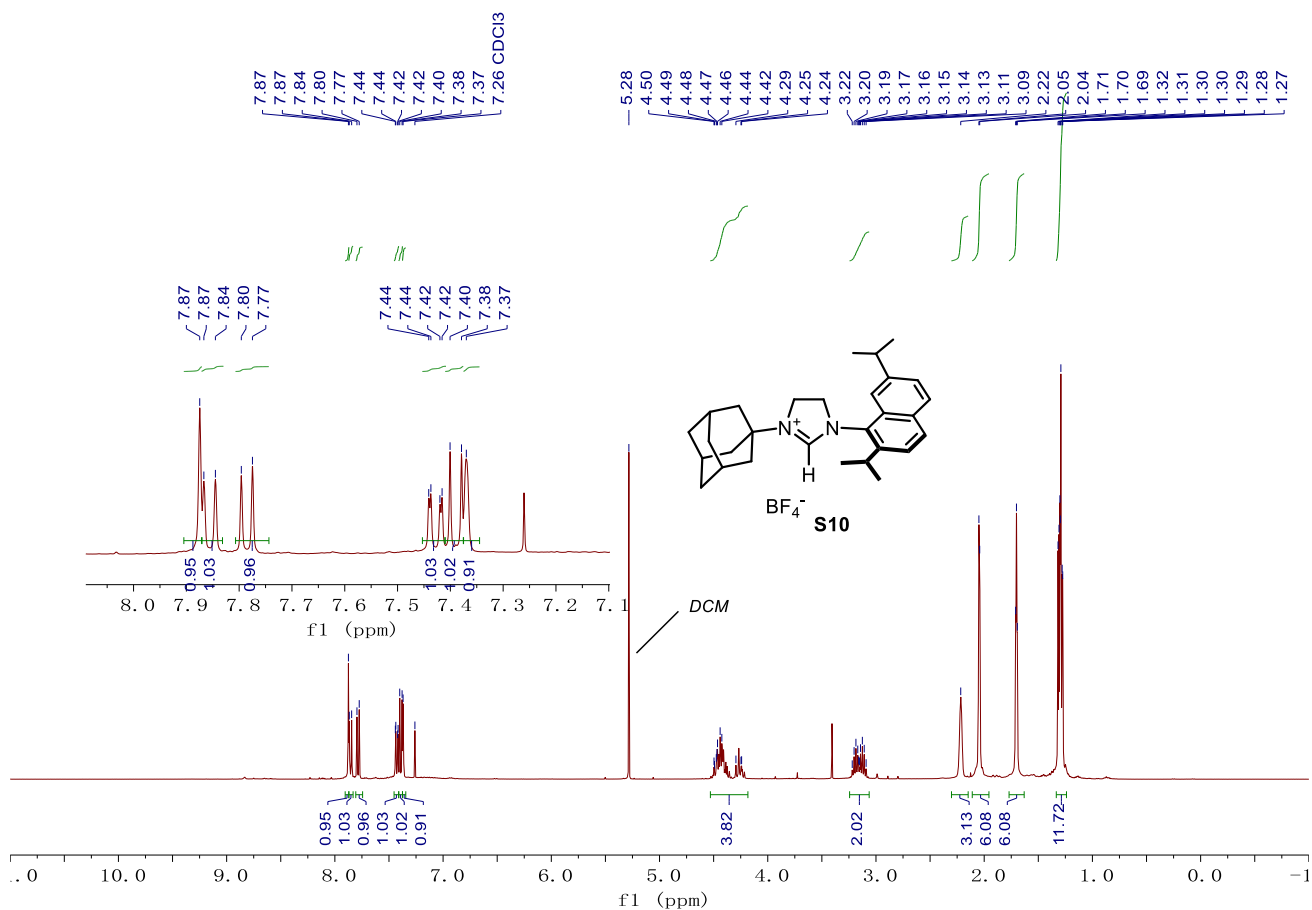
Figure S21 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **S10**.
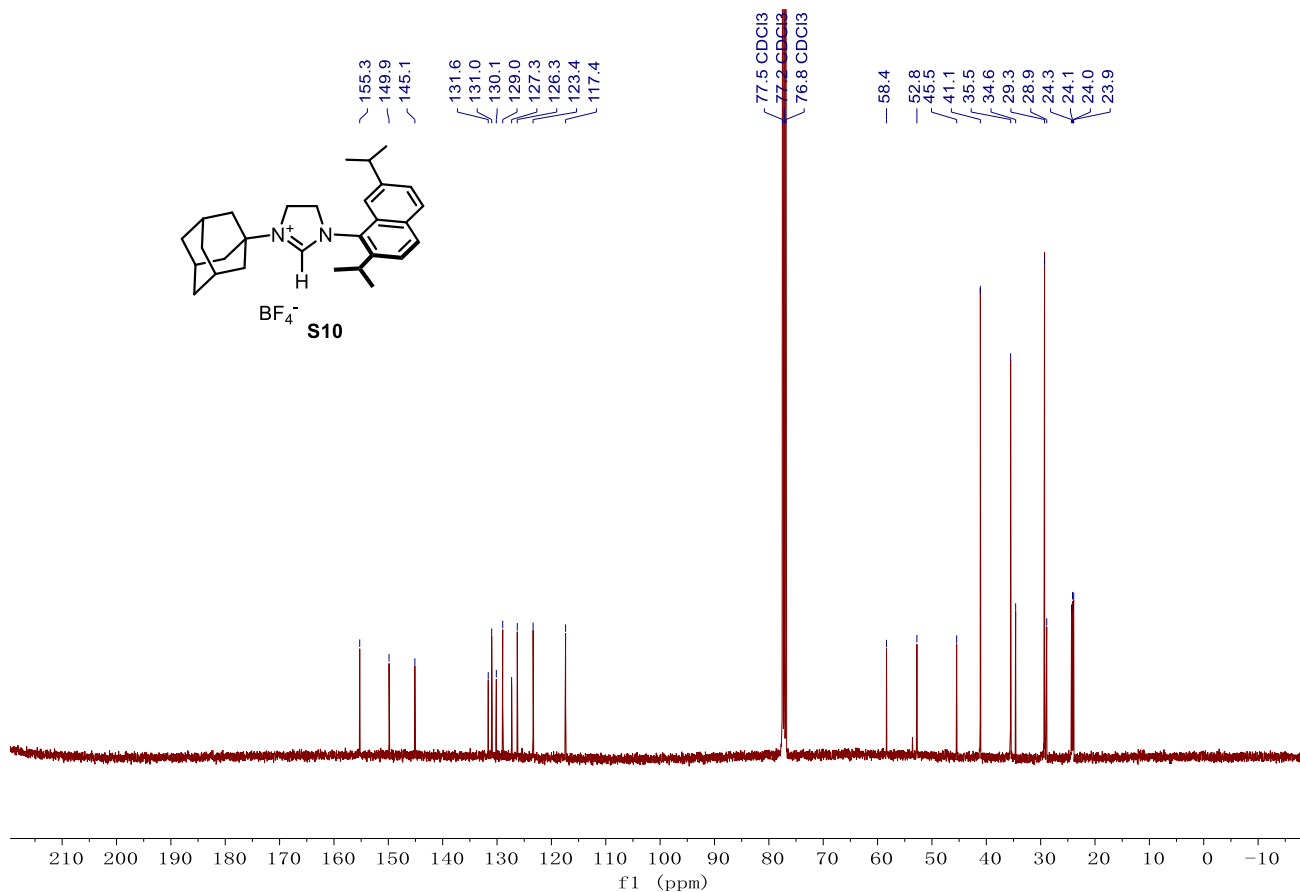
Figure S22 | [^1]H NMR (400 MHz, C_6D_6) spectrum of **Ru-7**.
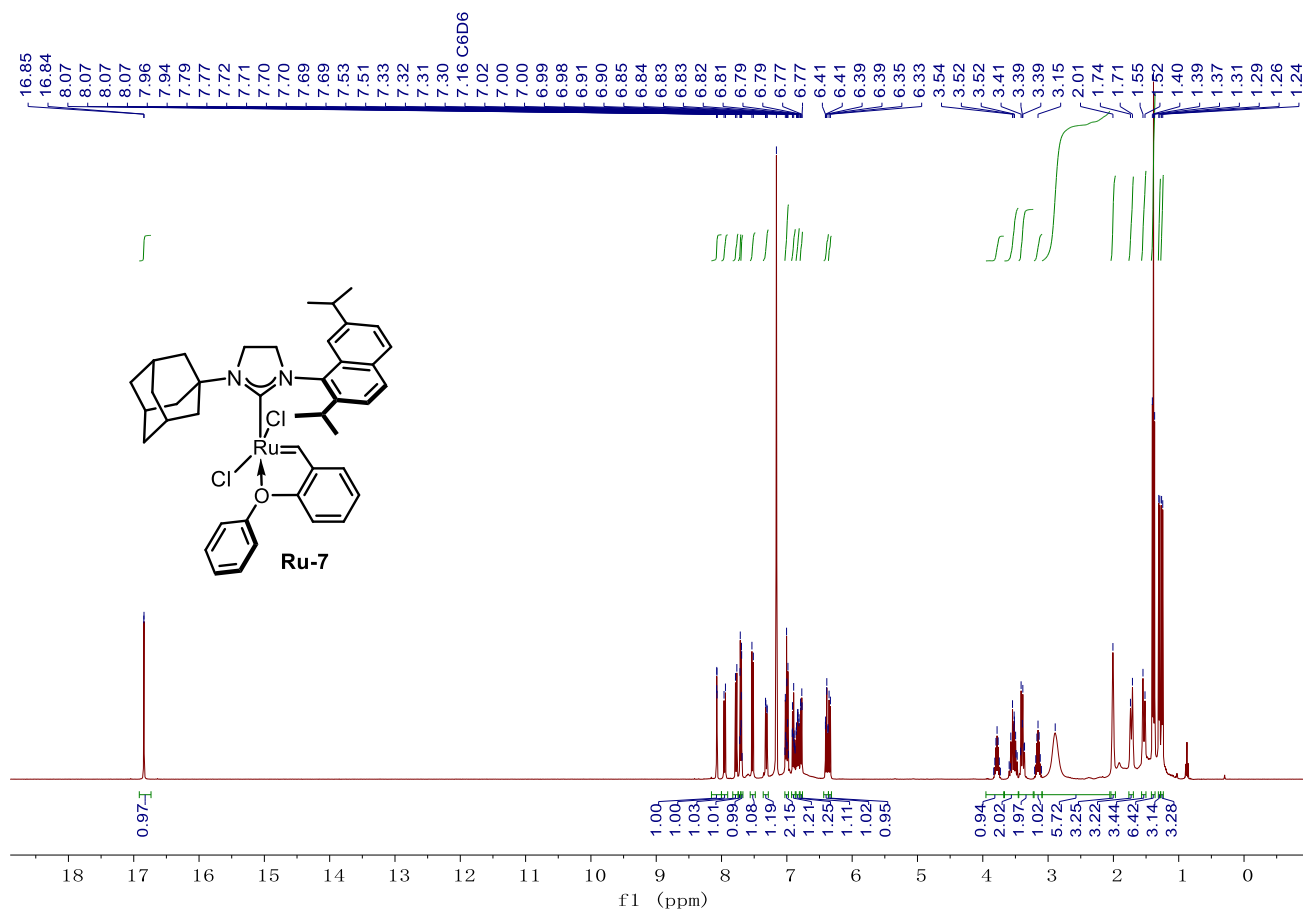
Figure S23 | [^13]C NMR (101 MHz, C_6D_6) spectrum of **Ru-7**.
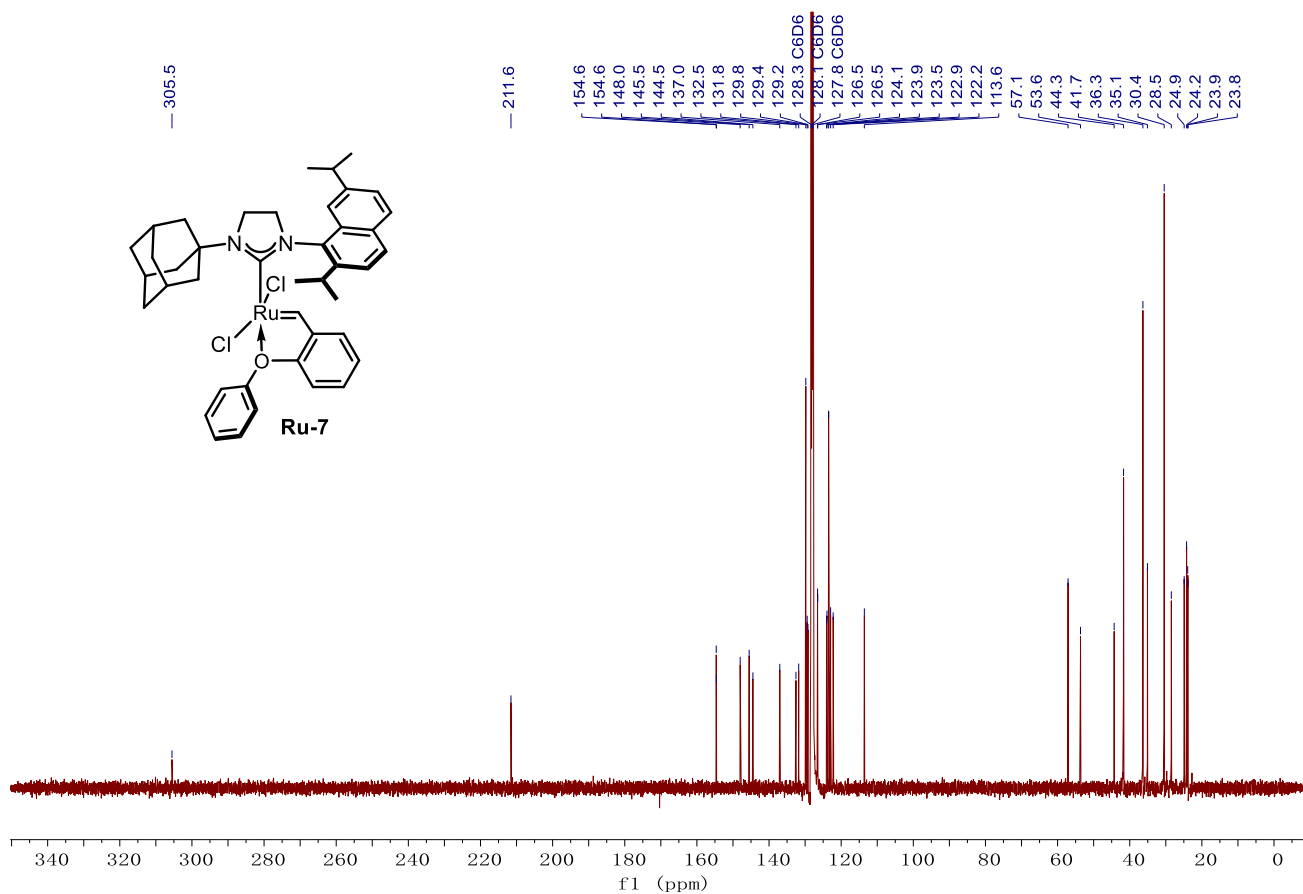
Figure S24 | Crude ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **S11**.
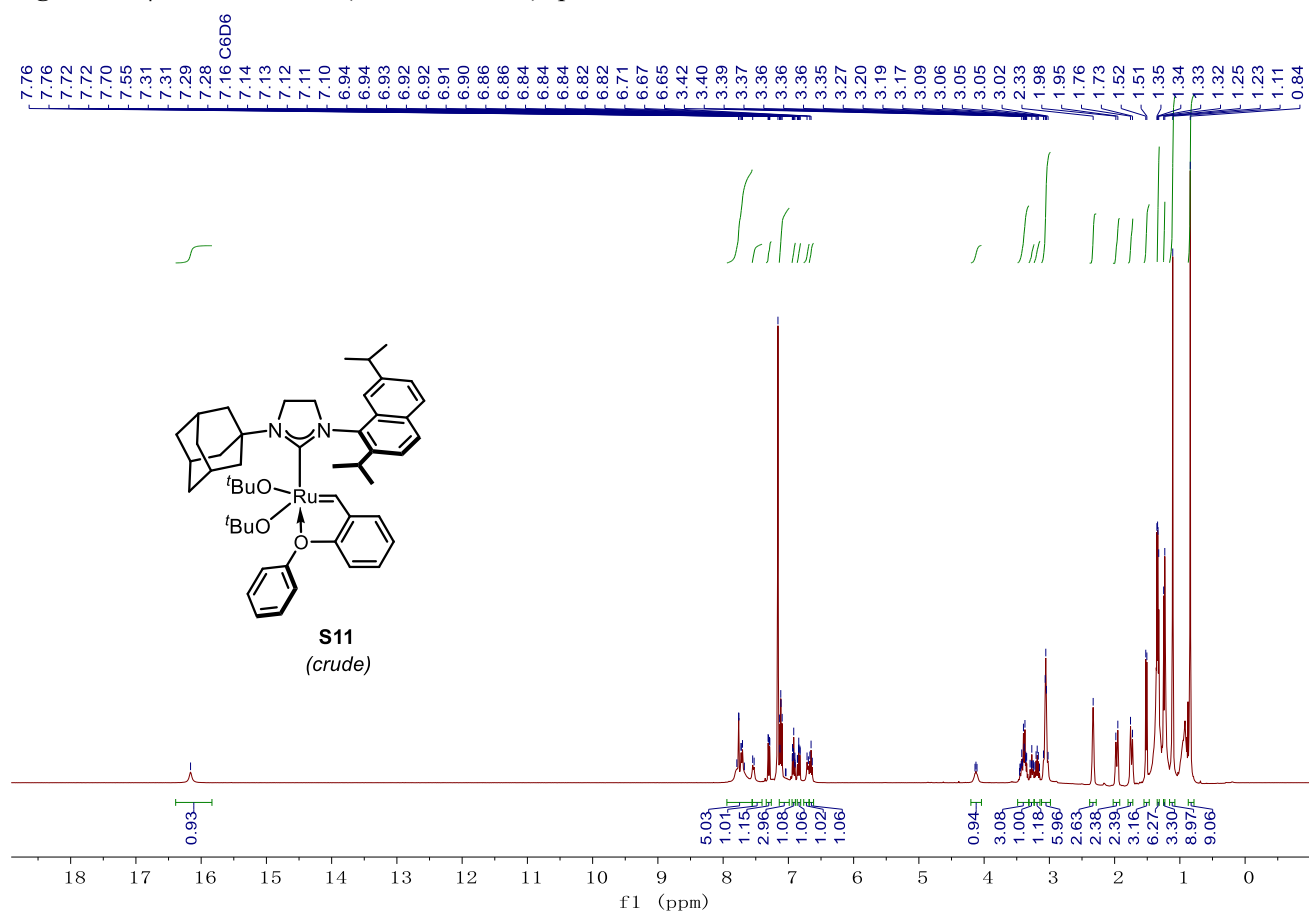
Figure S25 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **Ru-8**.
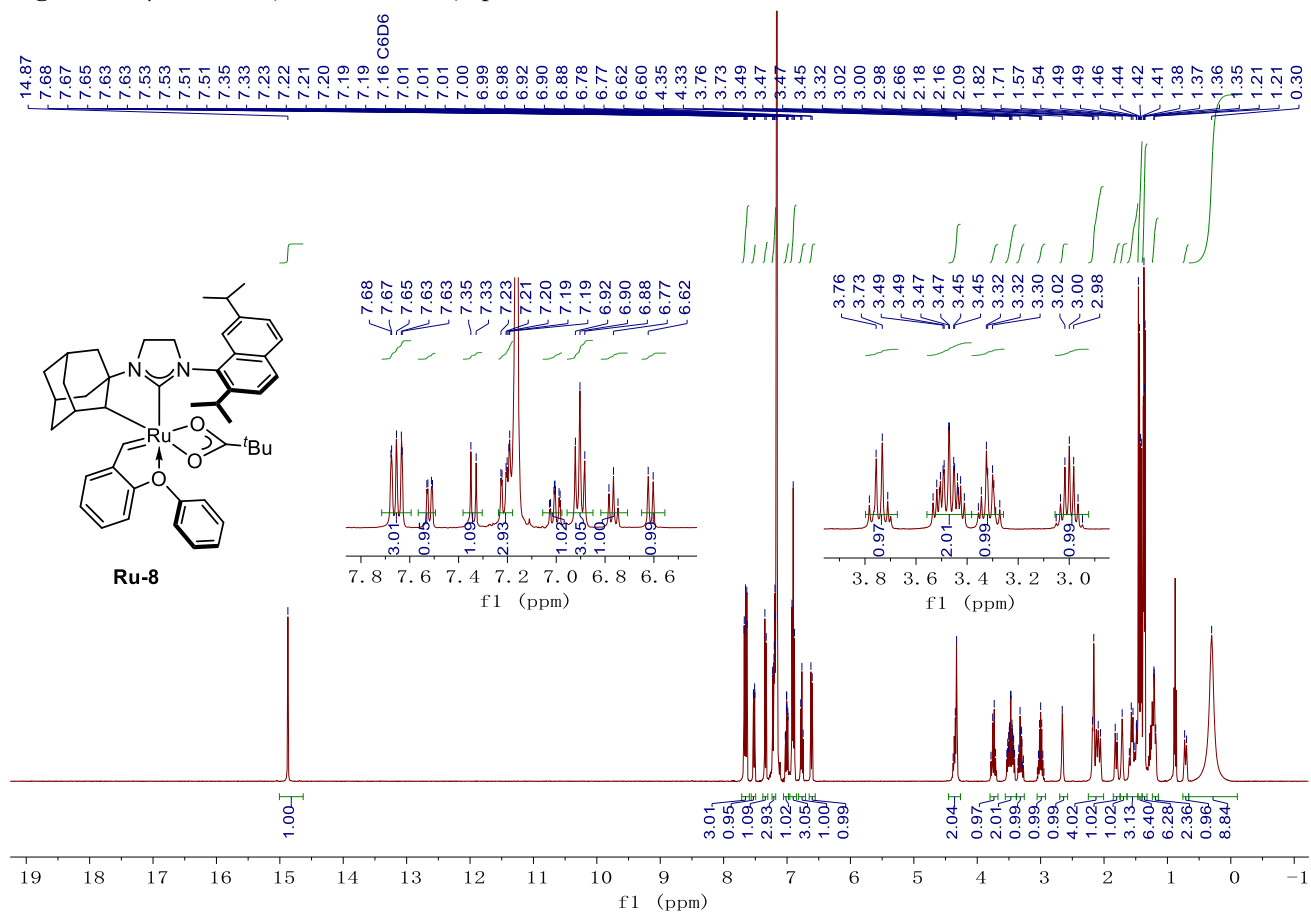
Figure S26 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **Ru-8**.
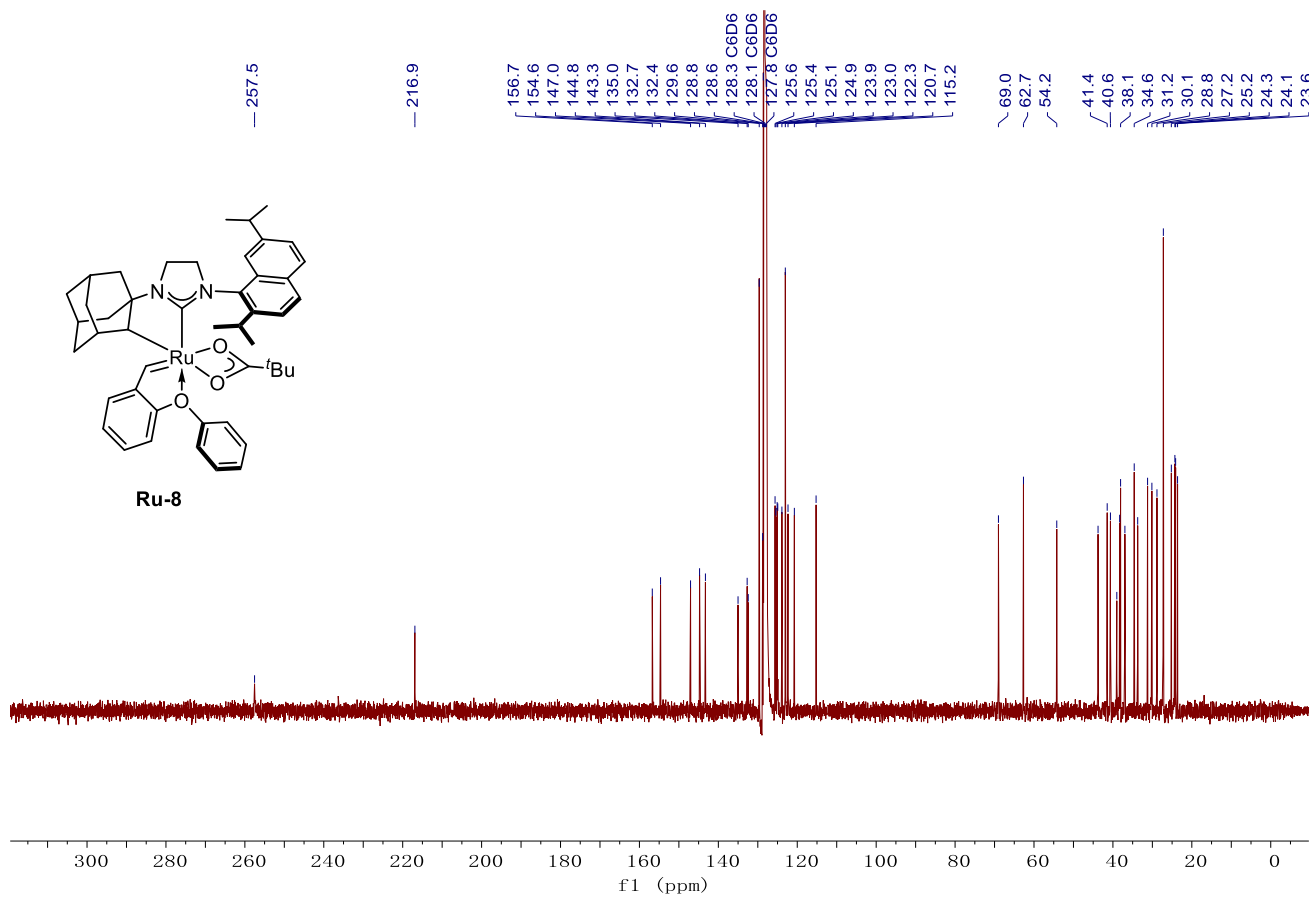
Figure S27 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **S13**.
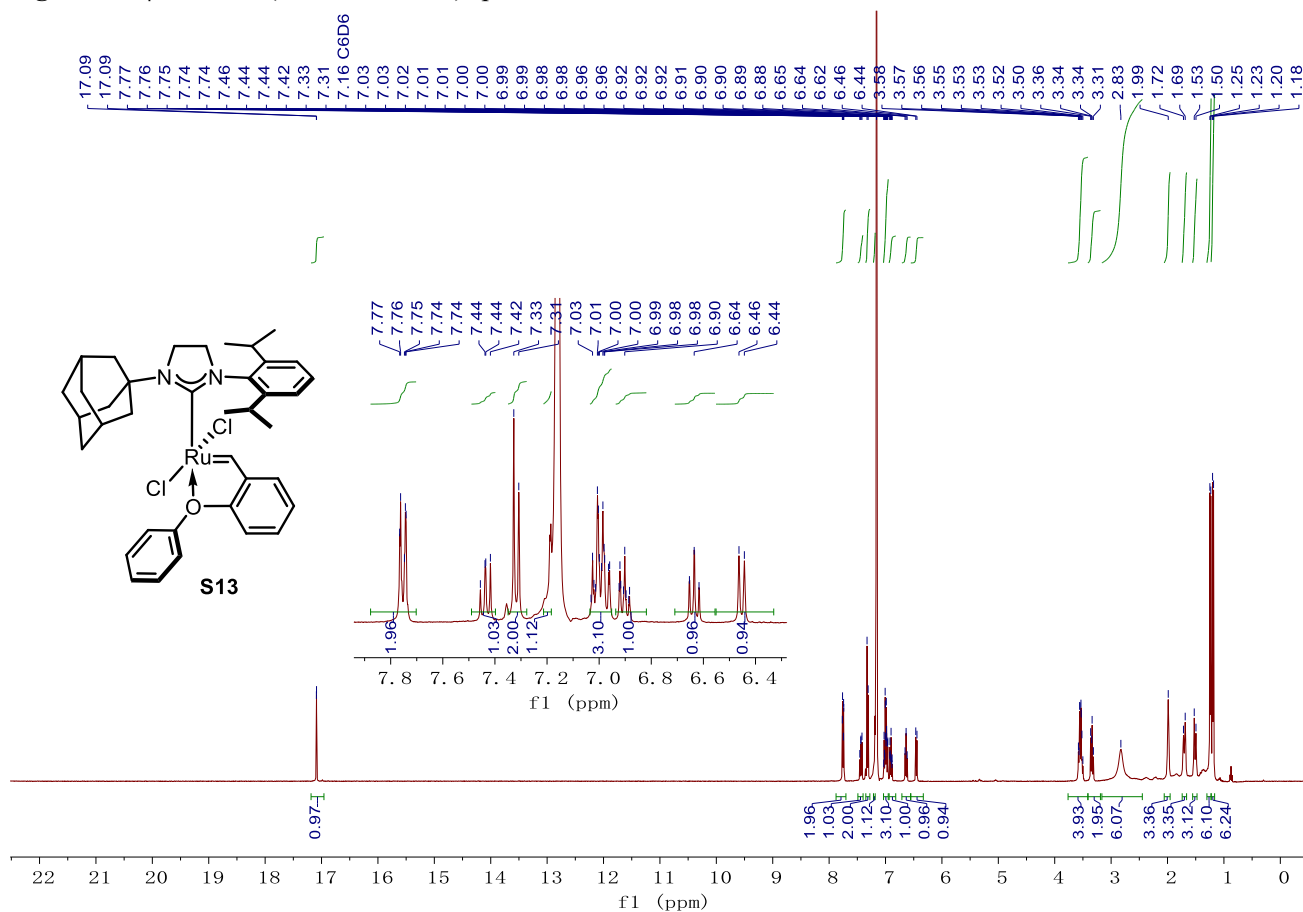
Figure S28 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **S13**.
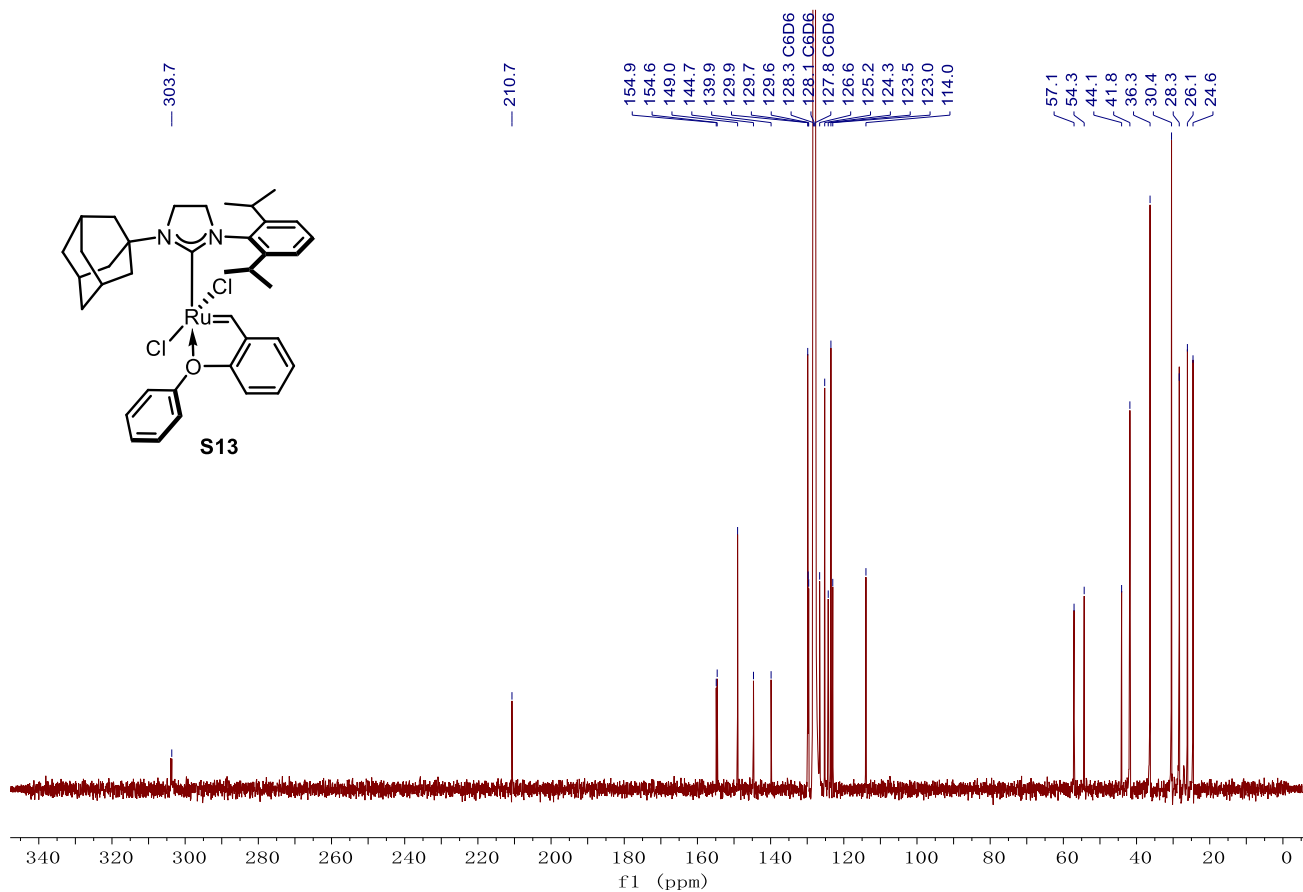
Figure S29 | Crude ^{1}H NMR (500 MHz, C$_6$D$_6$) spectrum of **S14**.

S14

X = OtBu

(crude)
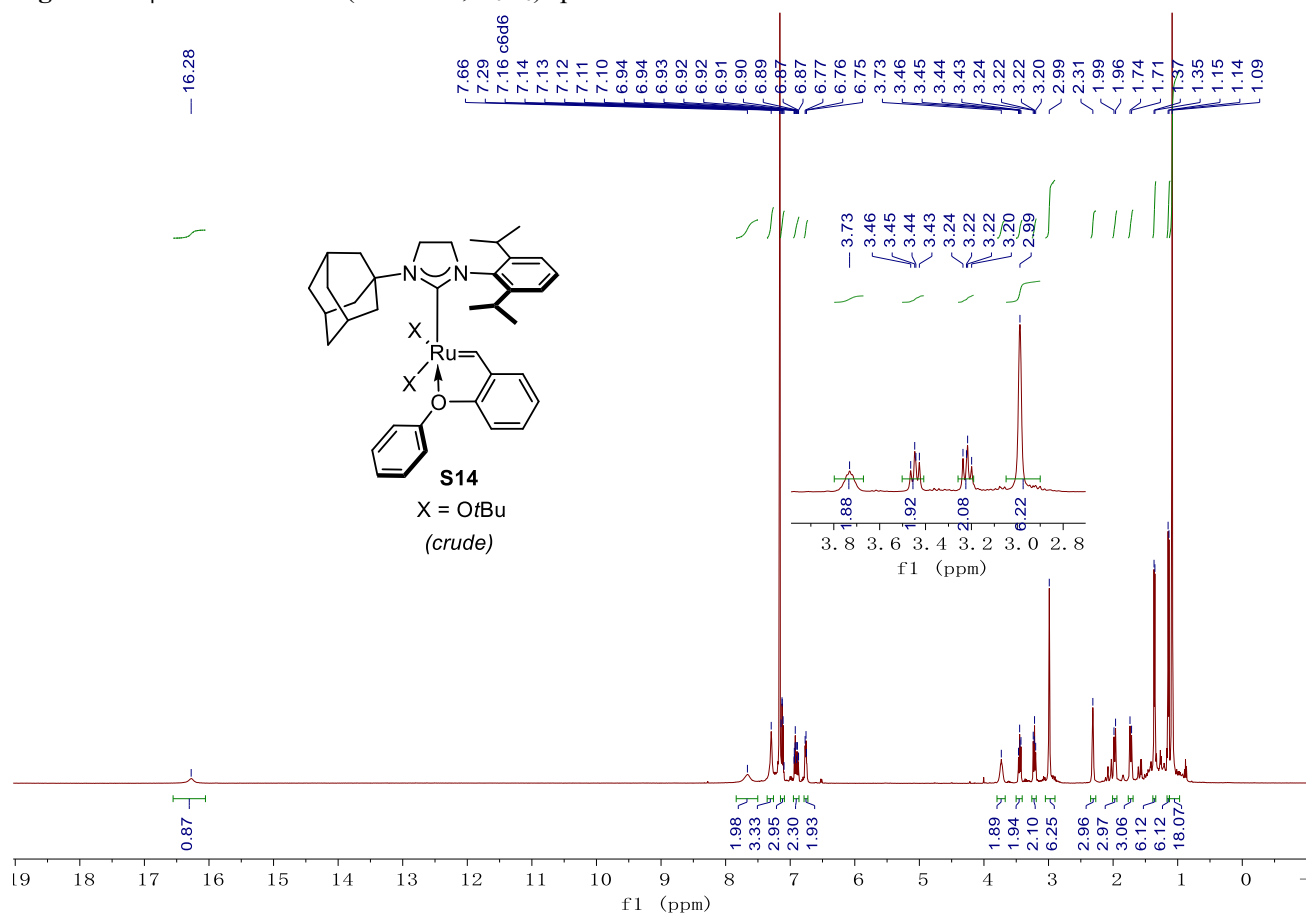
Figure S30 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **Ru-11**.
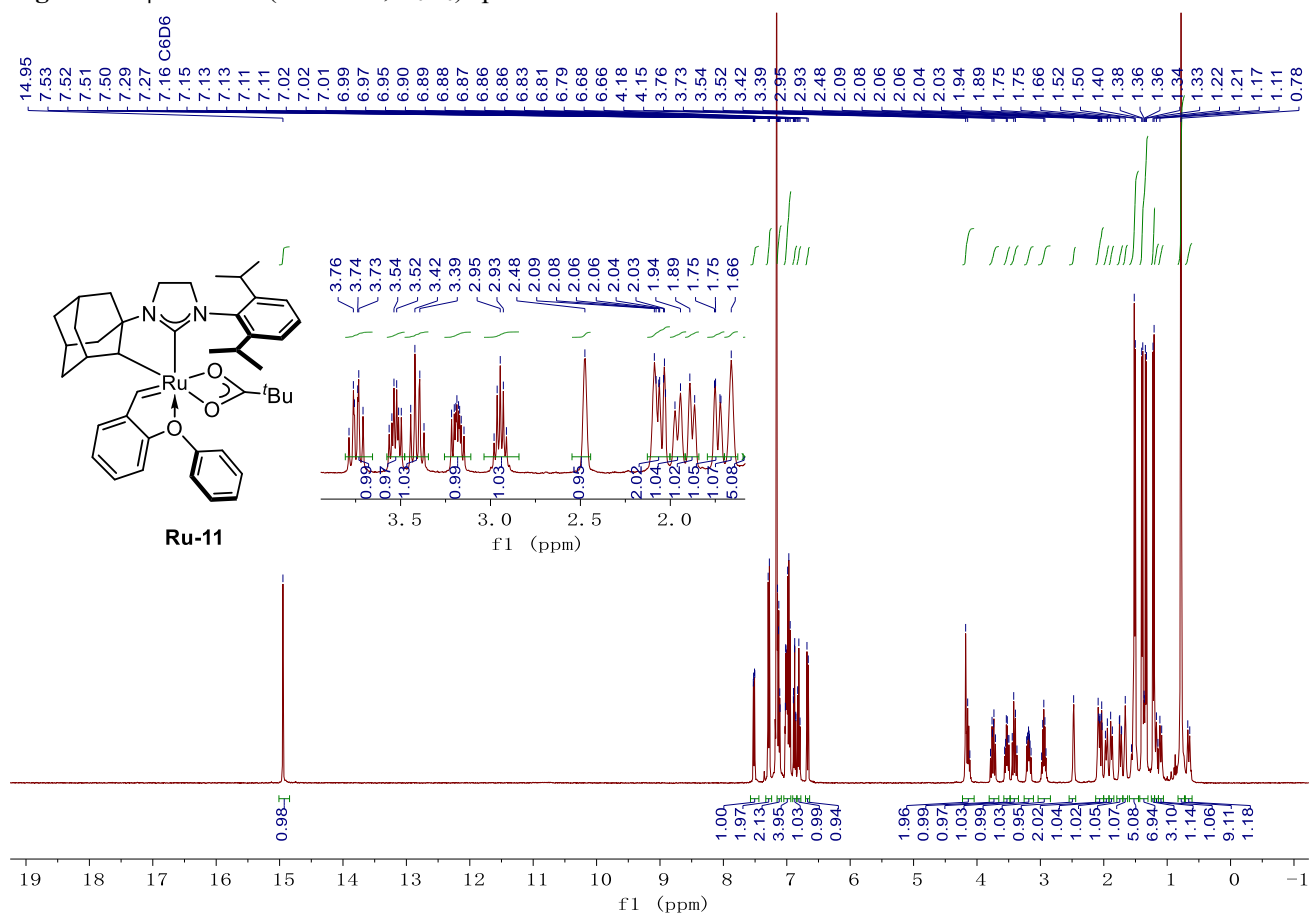
Figure S31 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **Ru-11**.

Figure S32 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **Ru-9**.

Figure S33 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **Ru-9**.

Figure S34 | ^{1}H NMR (400 MHz, C$_6$D$_6$) spectrum of **Ru-10**.
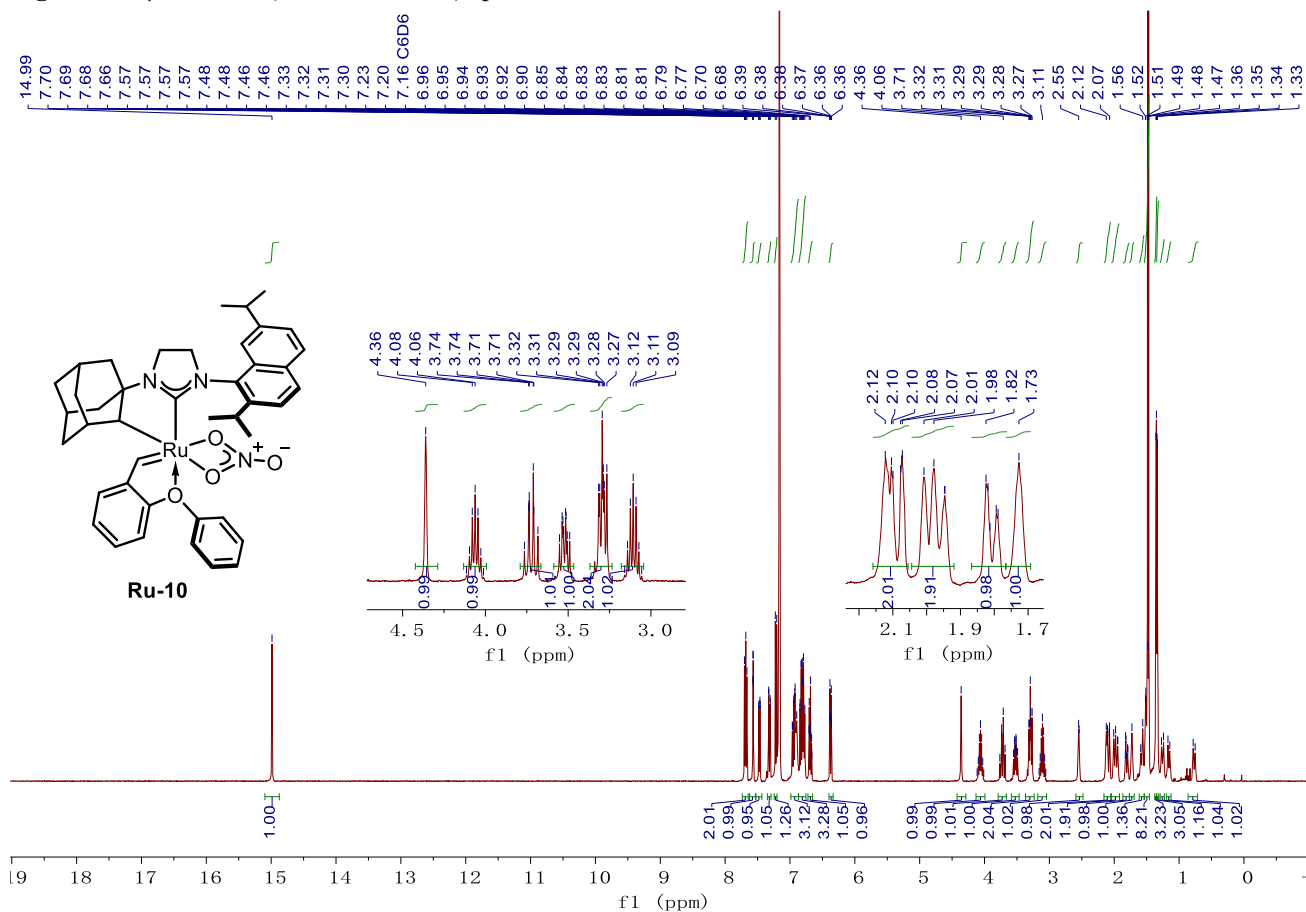
Figure S35 | ^{13}C NMR (101 MHz, C$_6$D$_6$) spectrum of **Ru-10**.
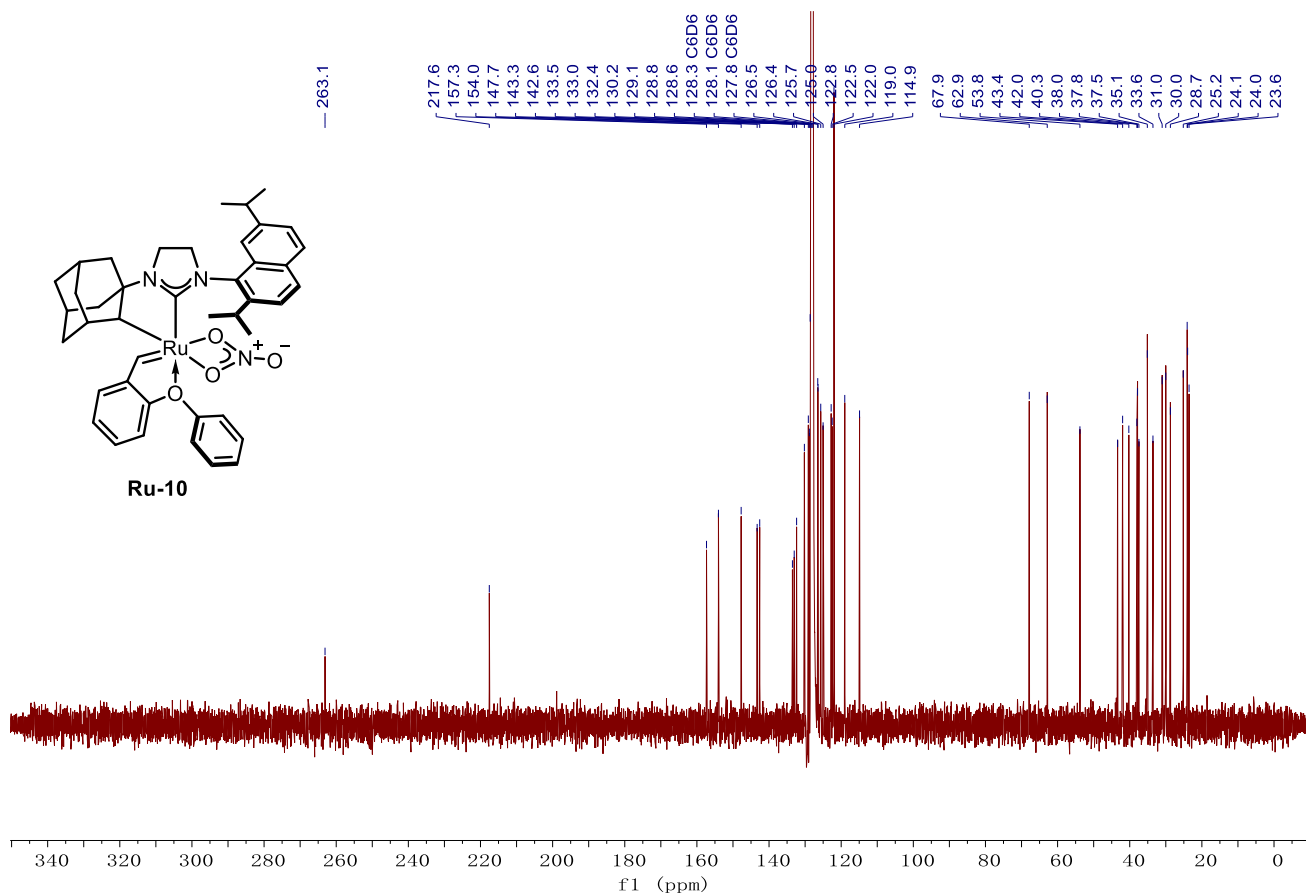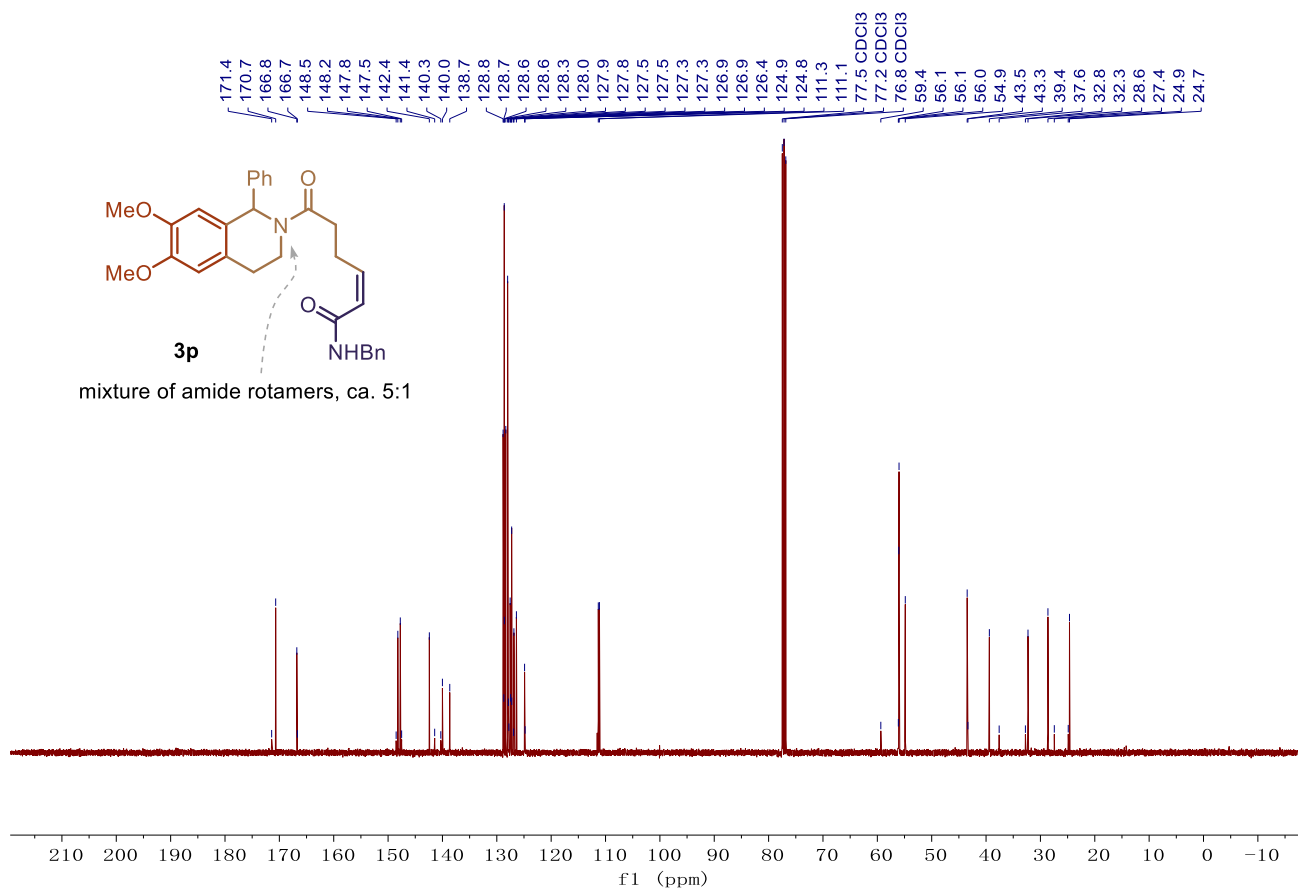
Figure S36 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **2n**.
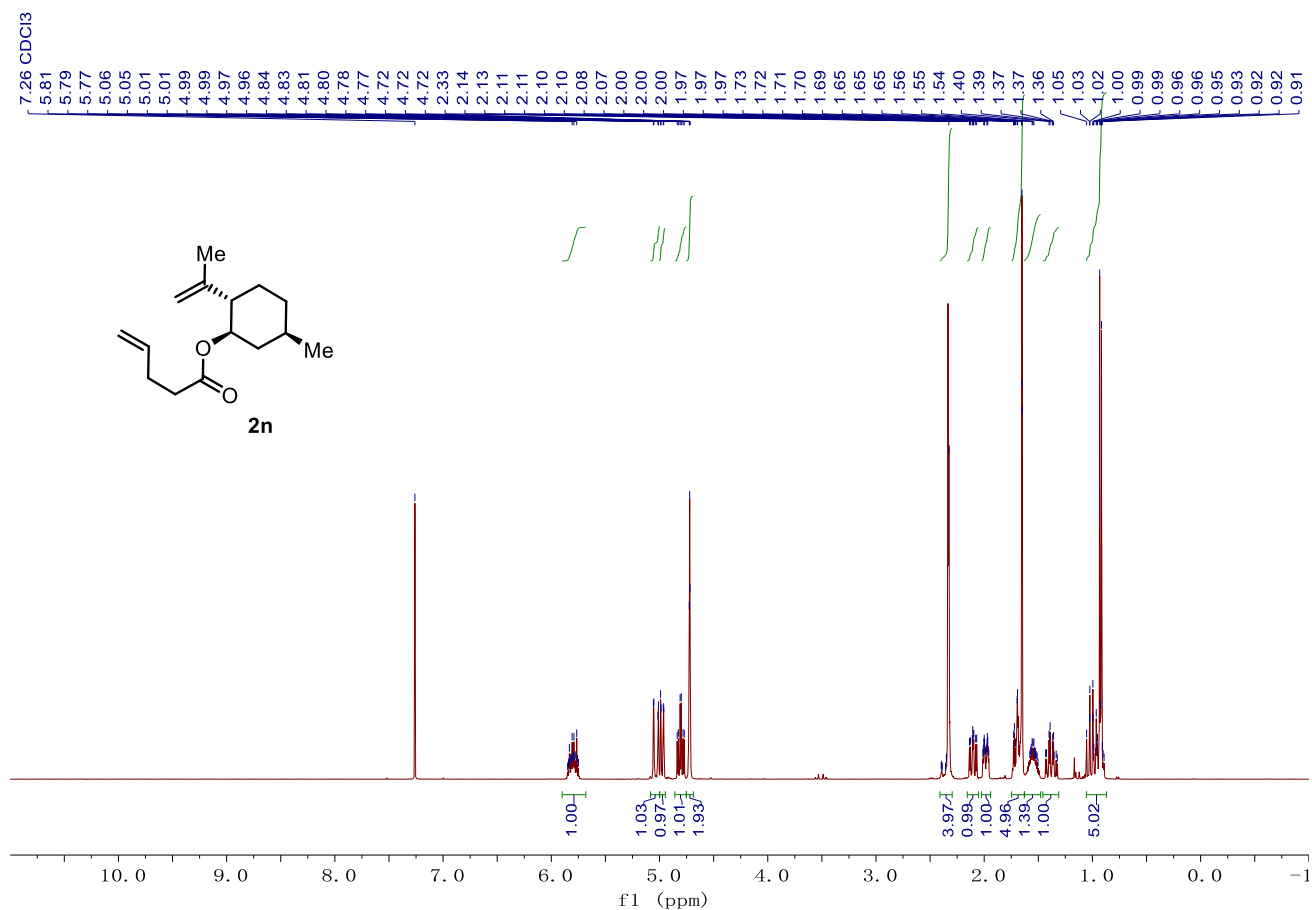
Figure S37 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **2n**.
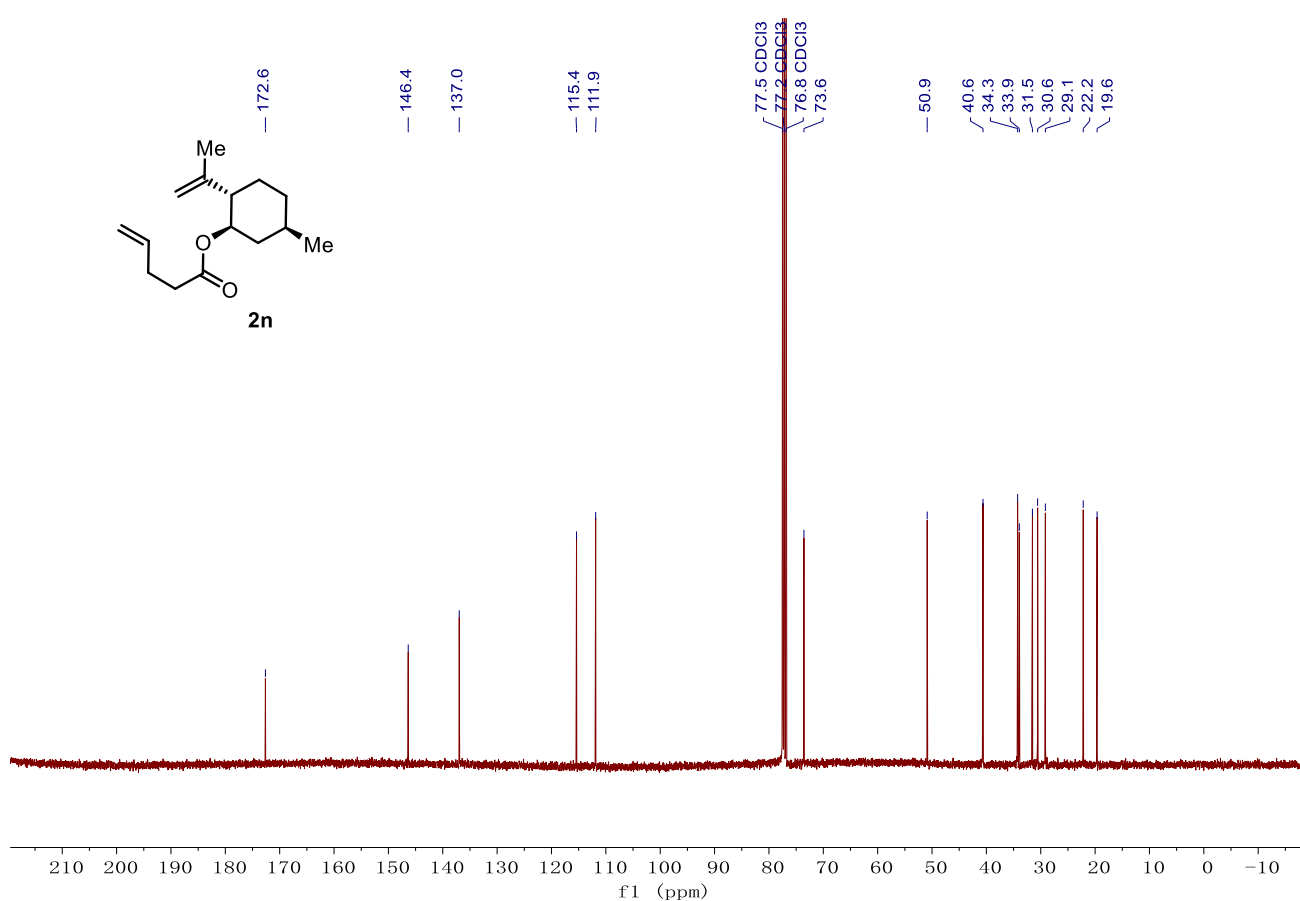
Figure S38 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **1u**.
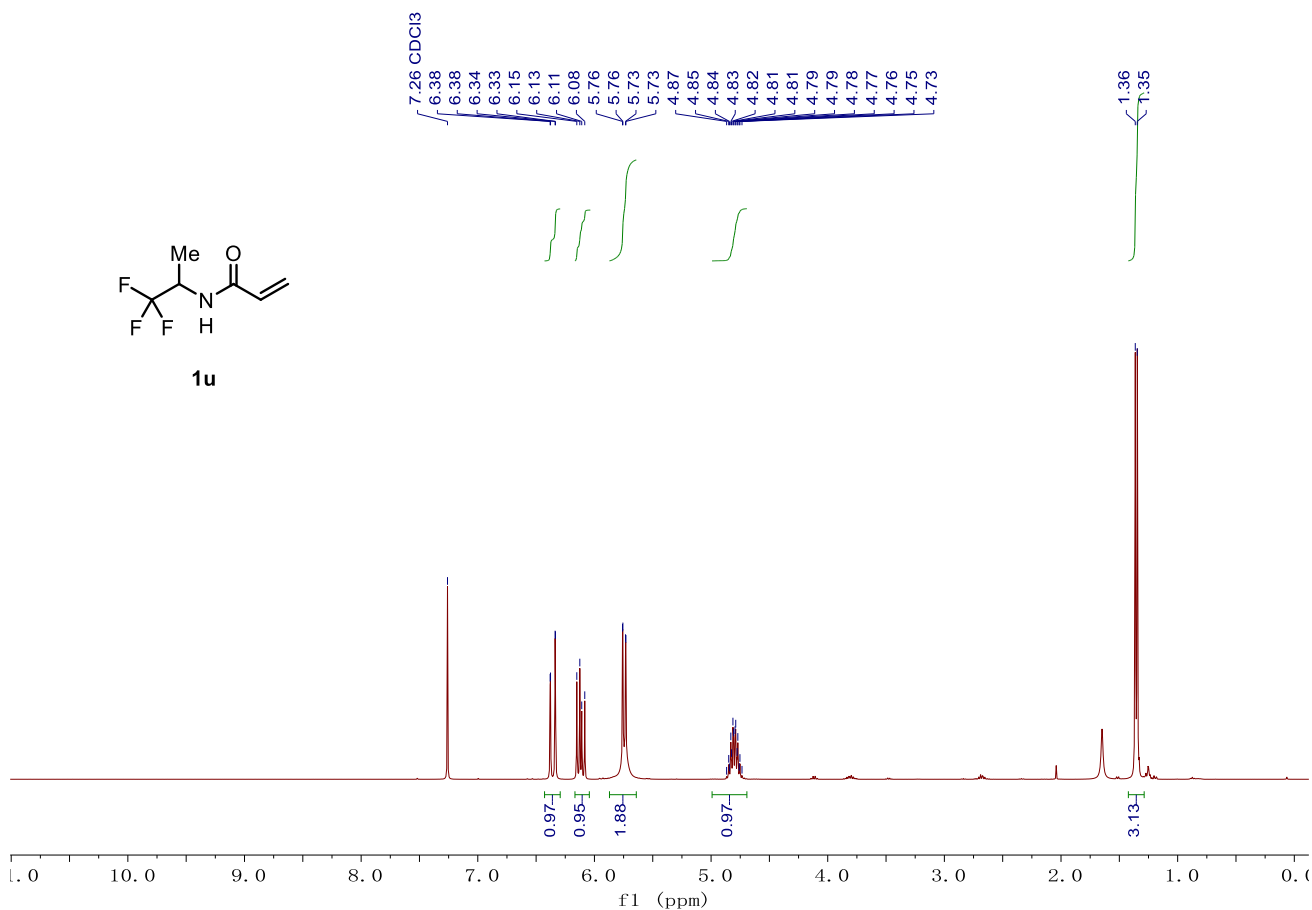
Figure S39 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **1u**.
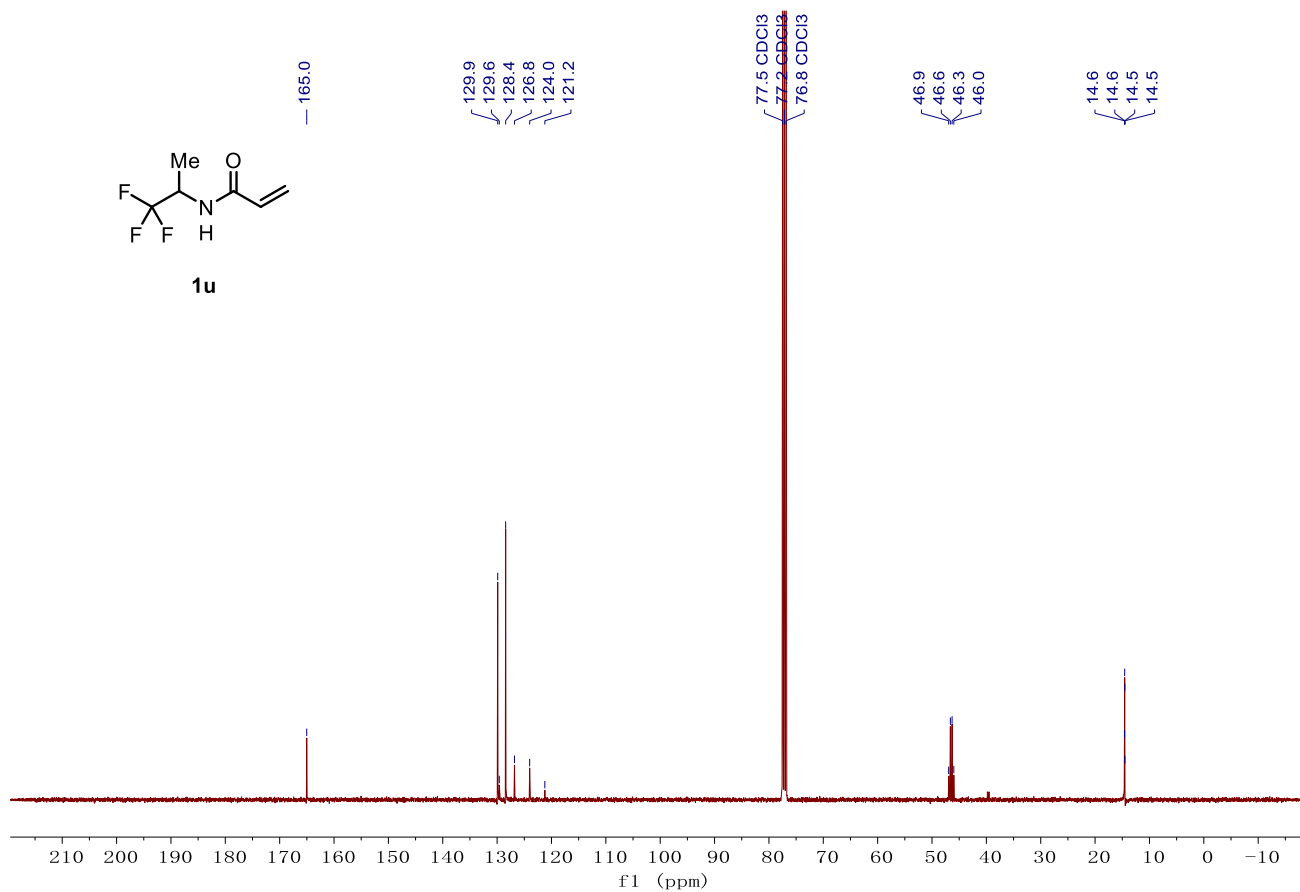
Figure S40 | ^{19}F NMR (282 MHz, CDCl$_3$) spectrum of **1u**.

-77.50
-77.53

1u

3.00

f1 (ppm)

20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190
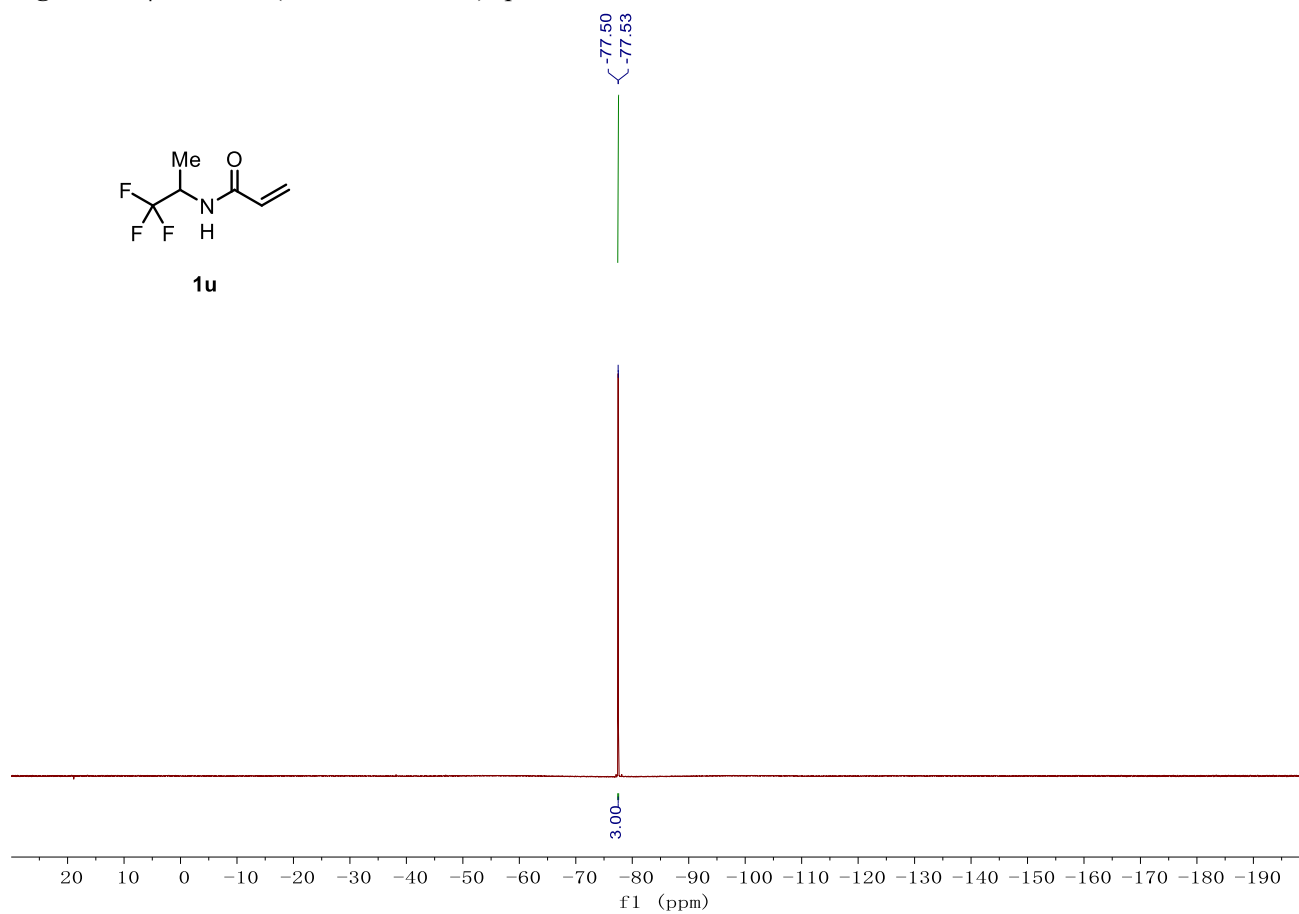
Figure S41 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **1w**.
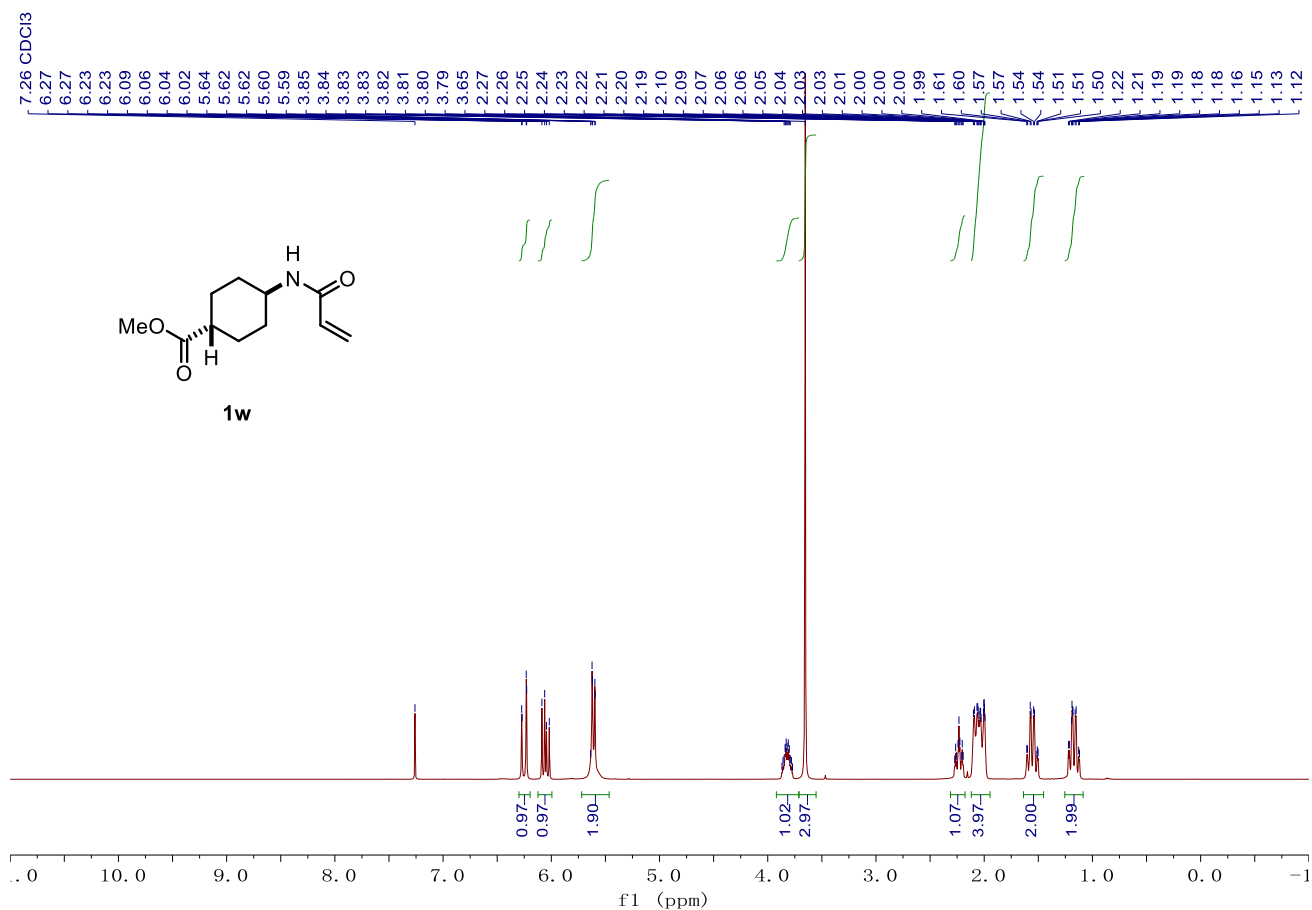
Figure S42 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **1w**.
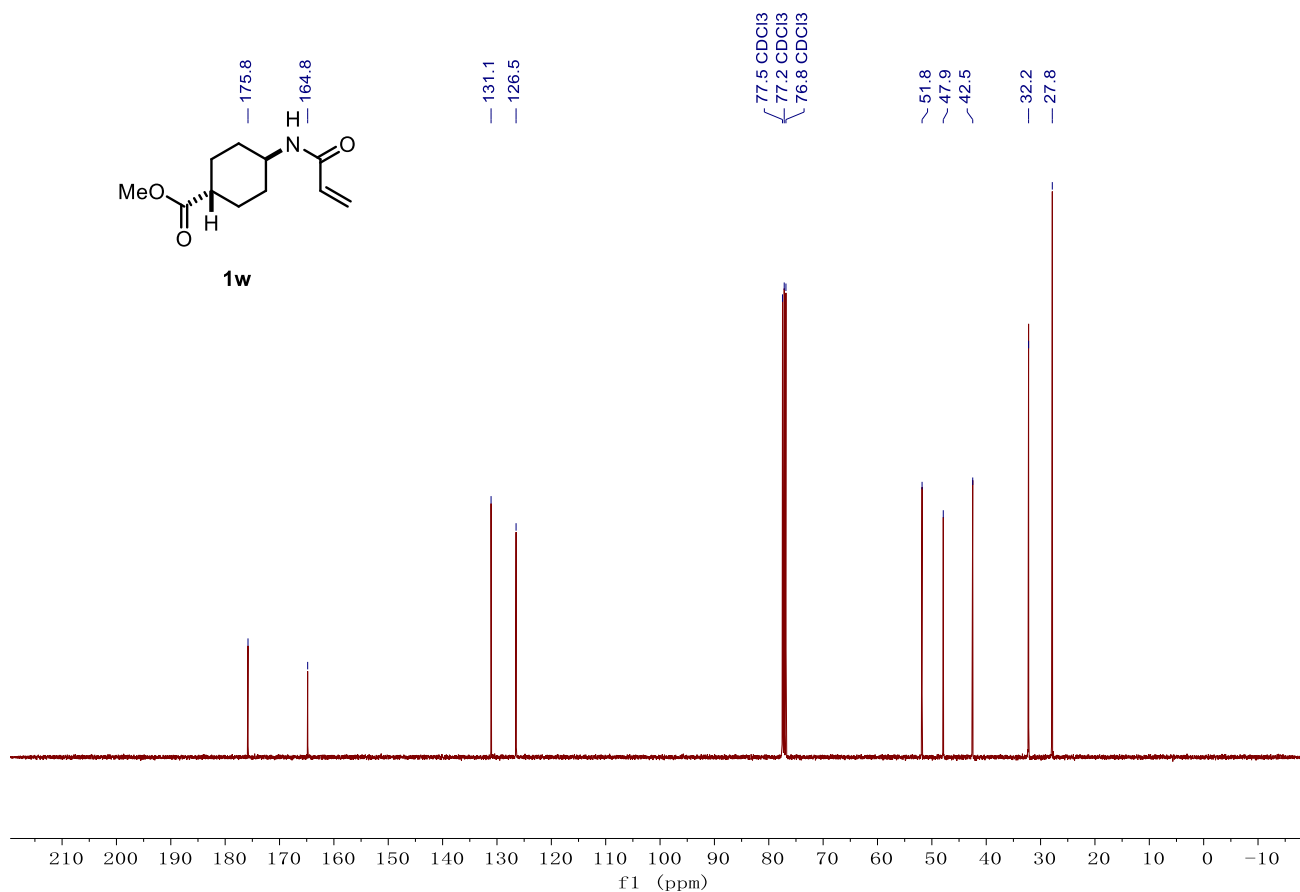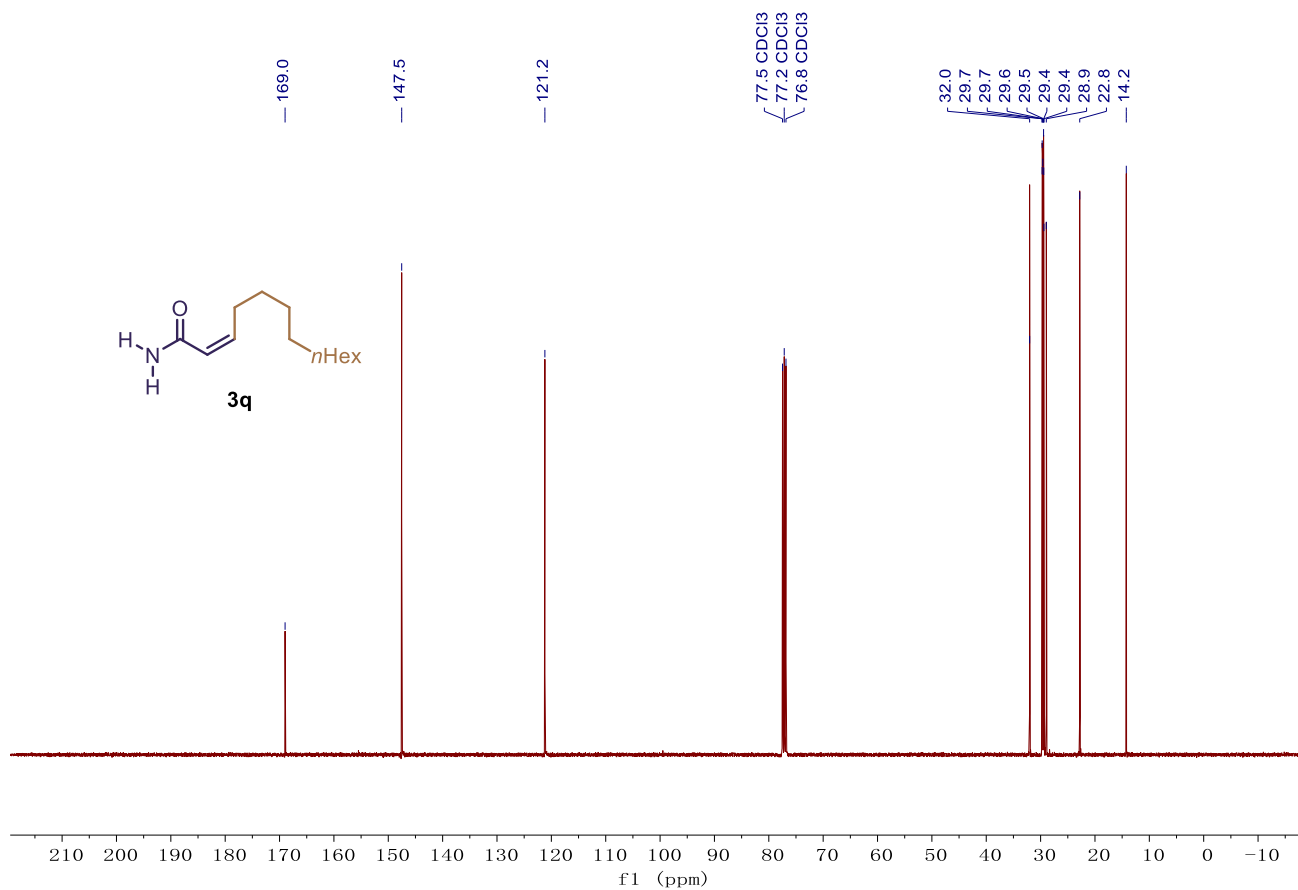
Figure S43 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3a**.
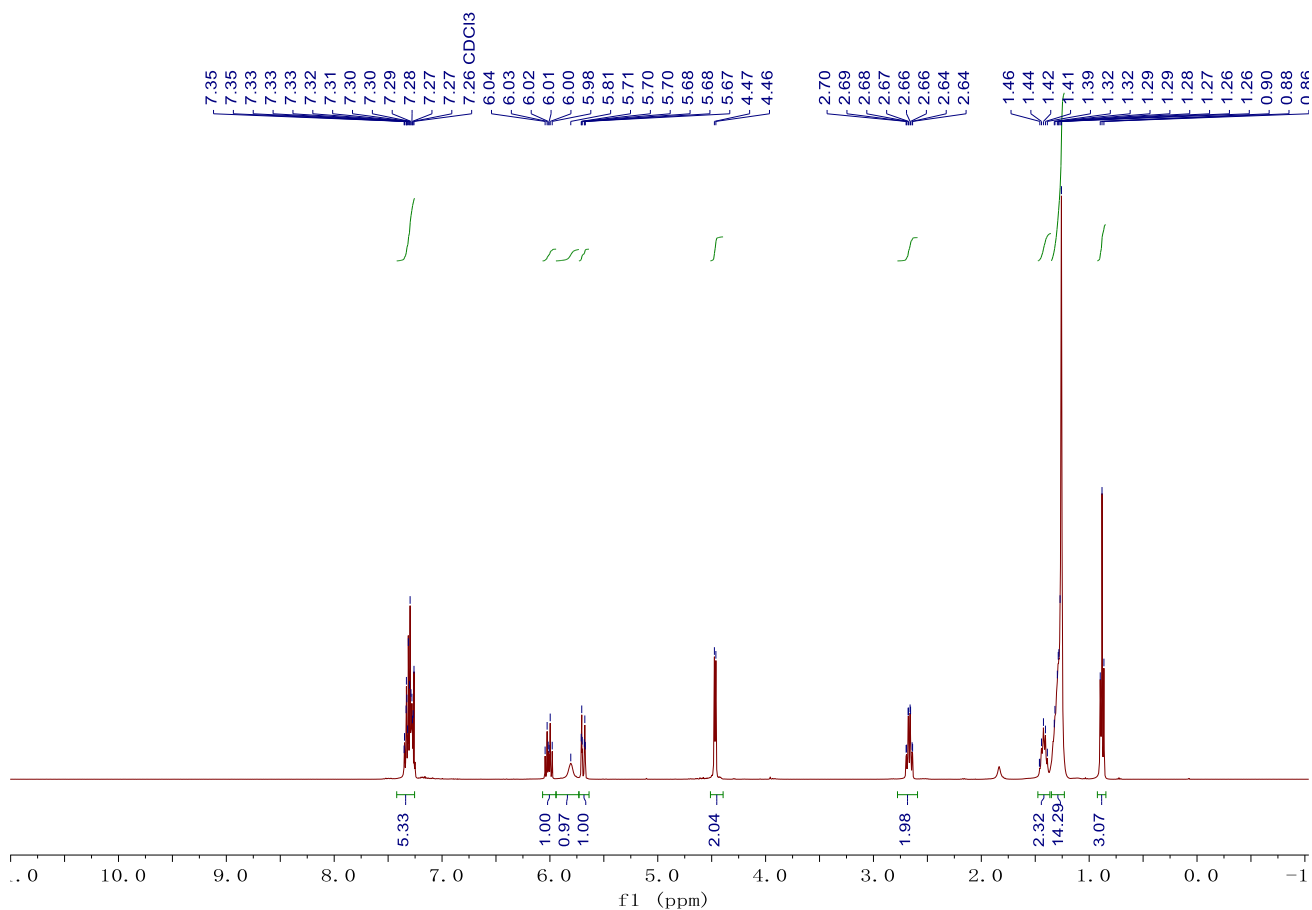
Figure S44 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3a**.
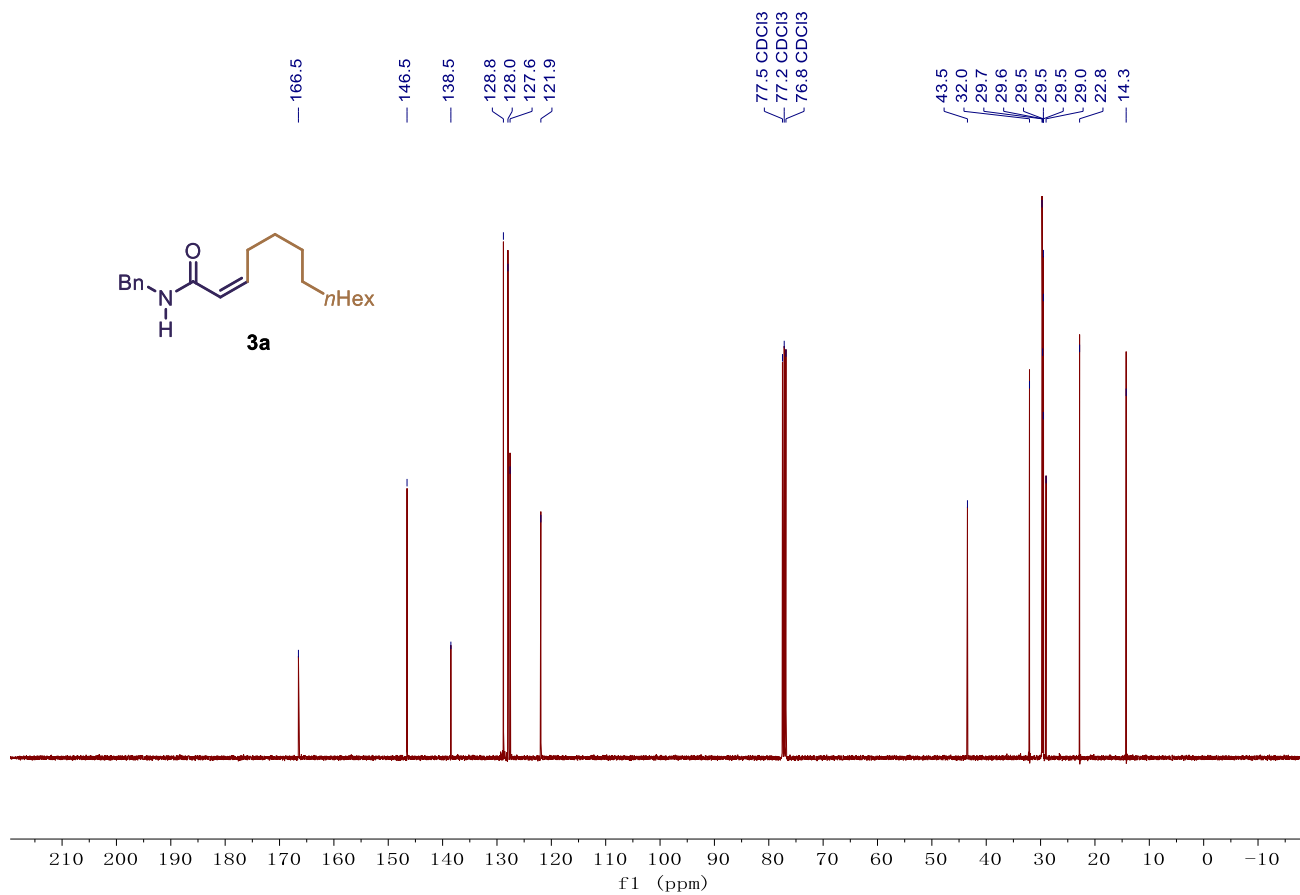
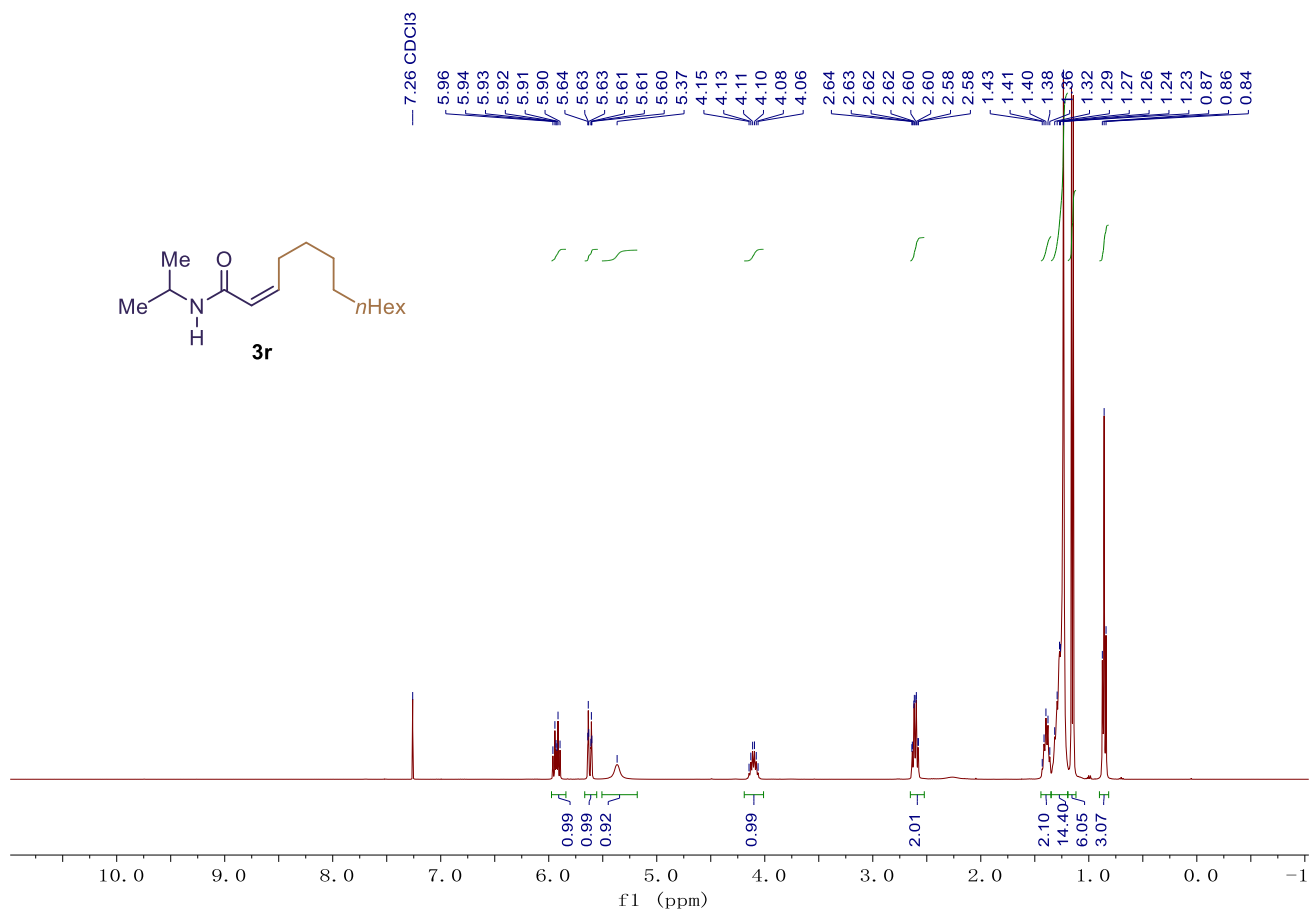**Figure S45 |** ¹H NMR (400 MHz, CDCl₃) spectrum of **3b**.
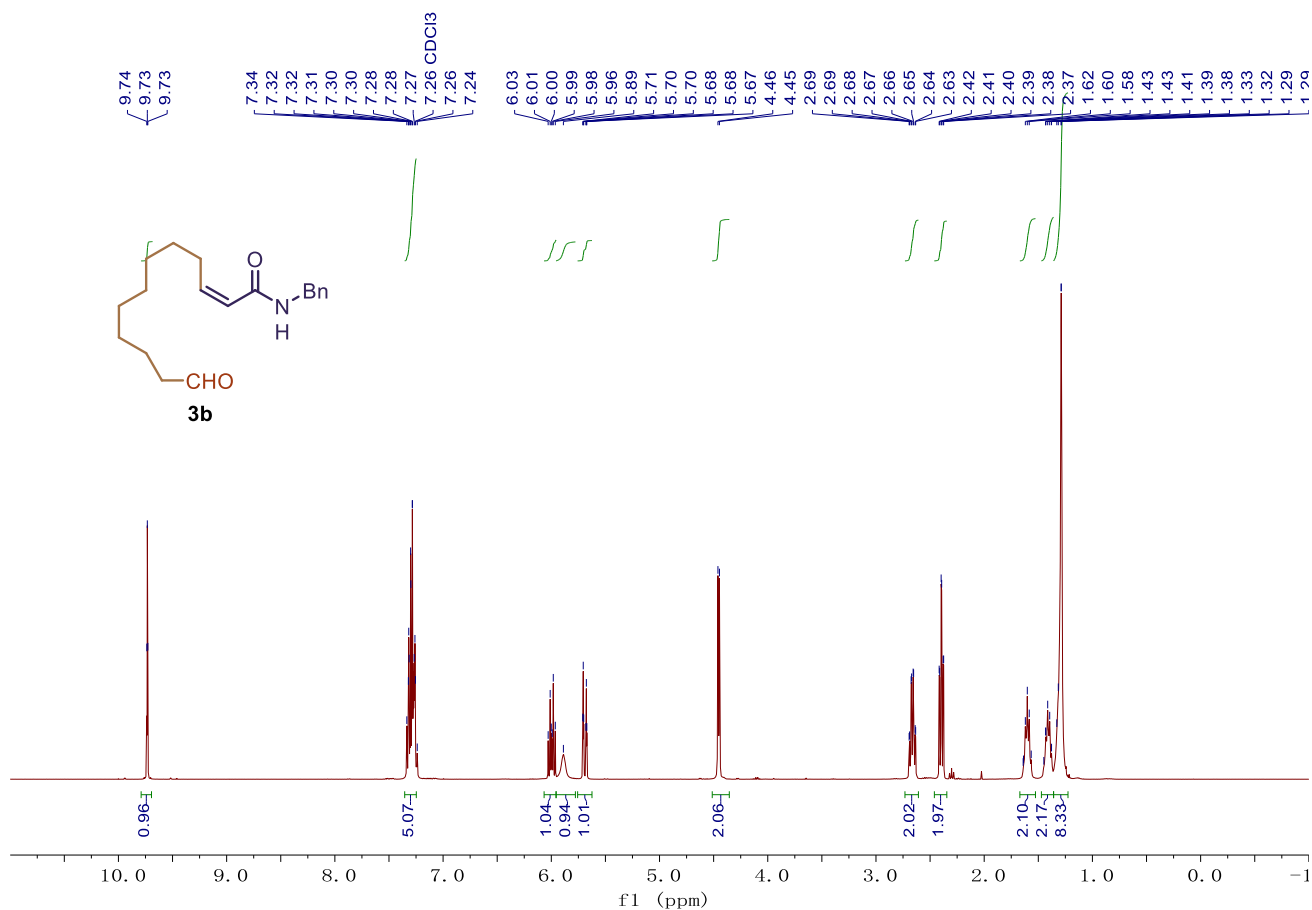
Figure S46 | ¹³C NMR (101 MHz, CDCl₃) spectrum of **3b**.
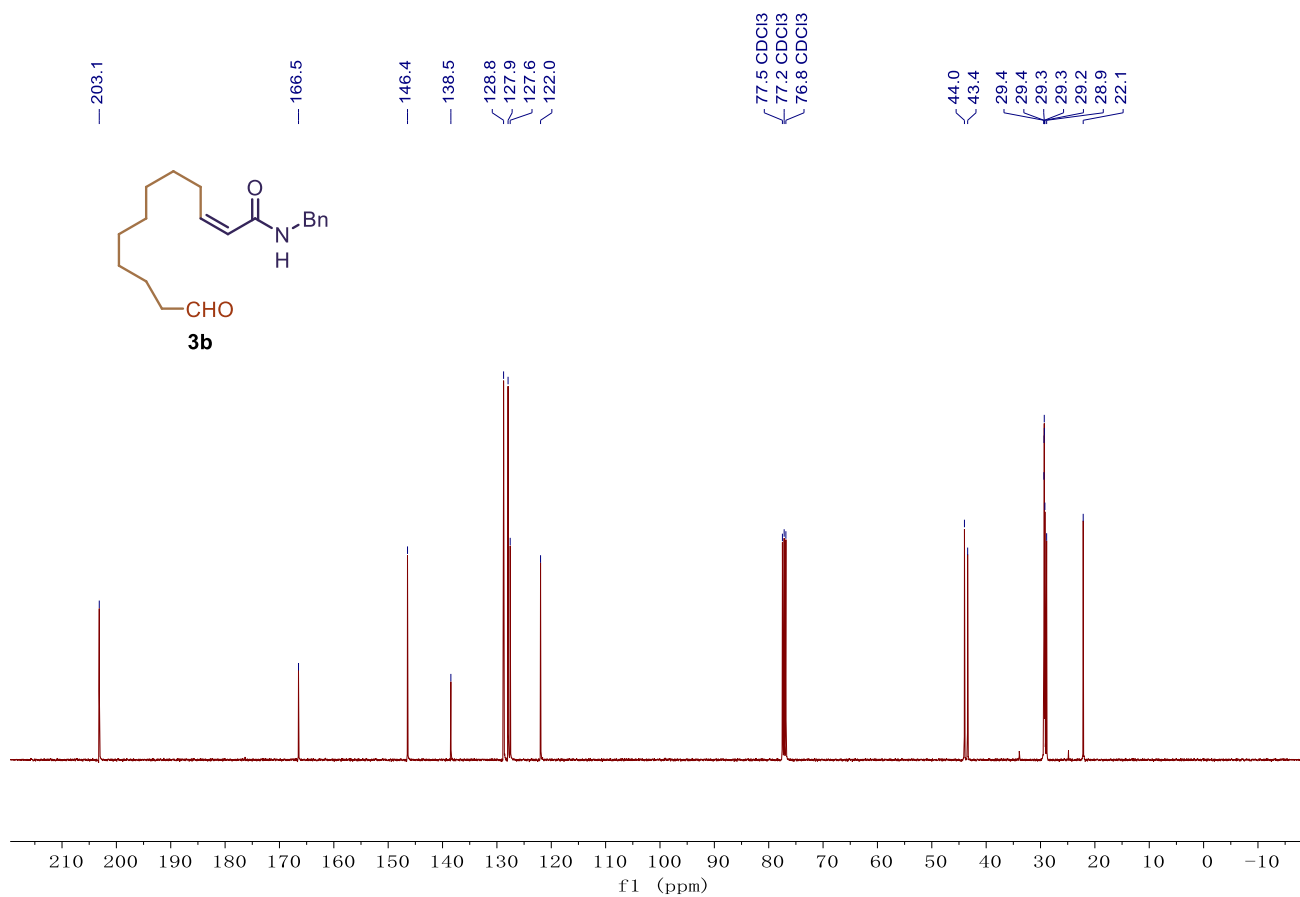
Figure S47 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3c**.
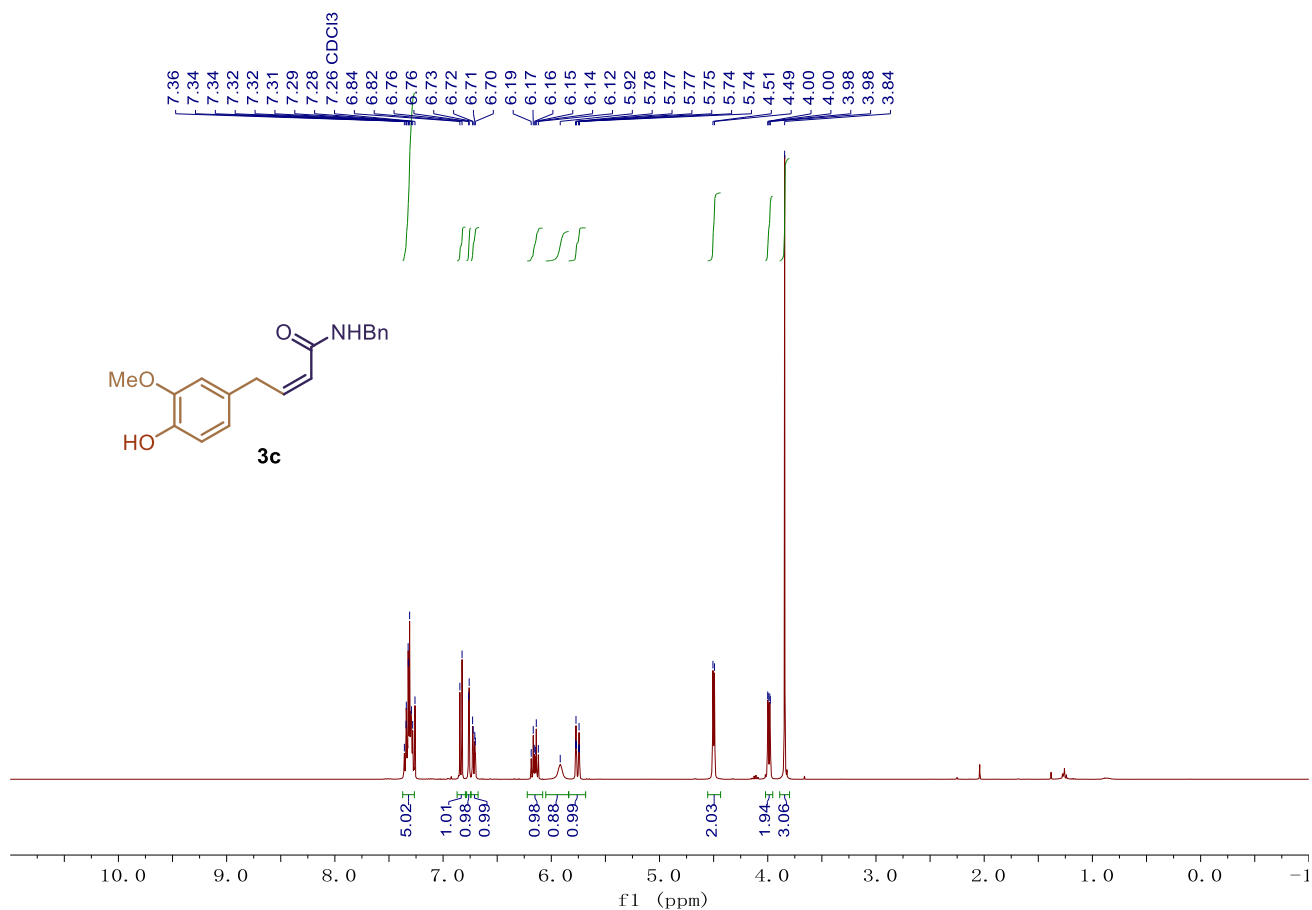
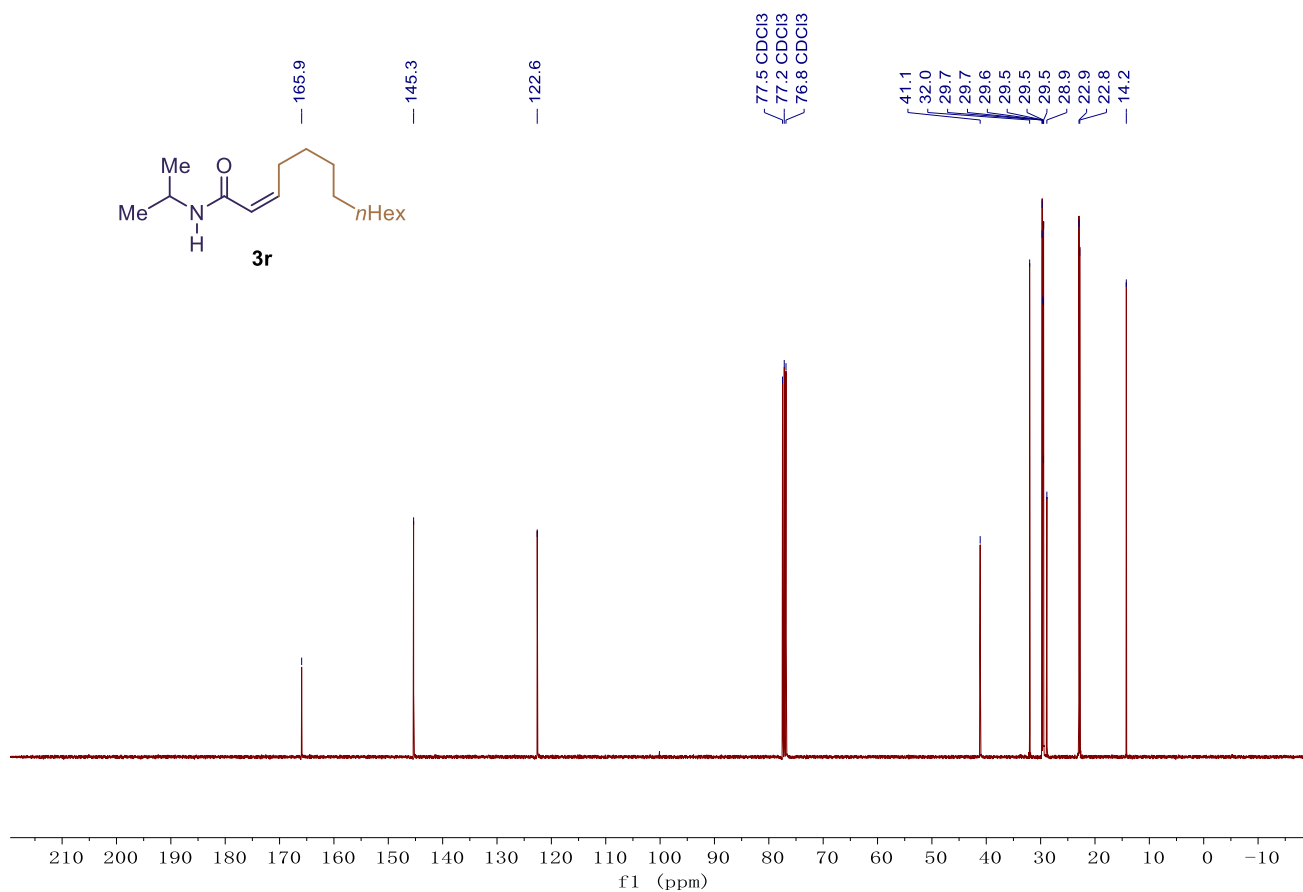**Figure S48 |** ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3c**.
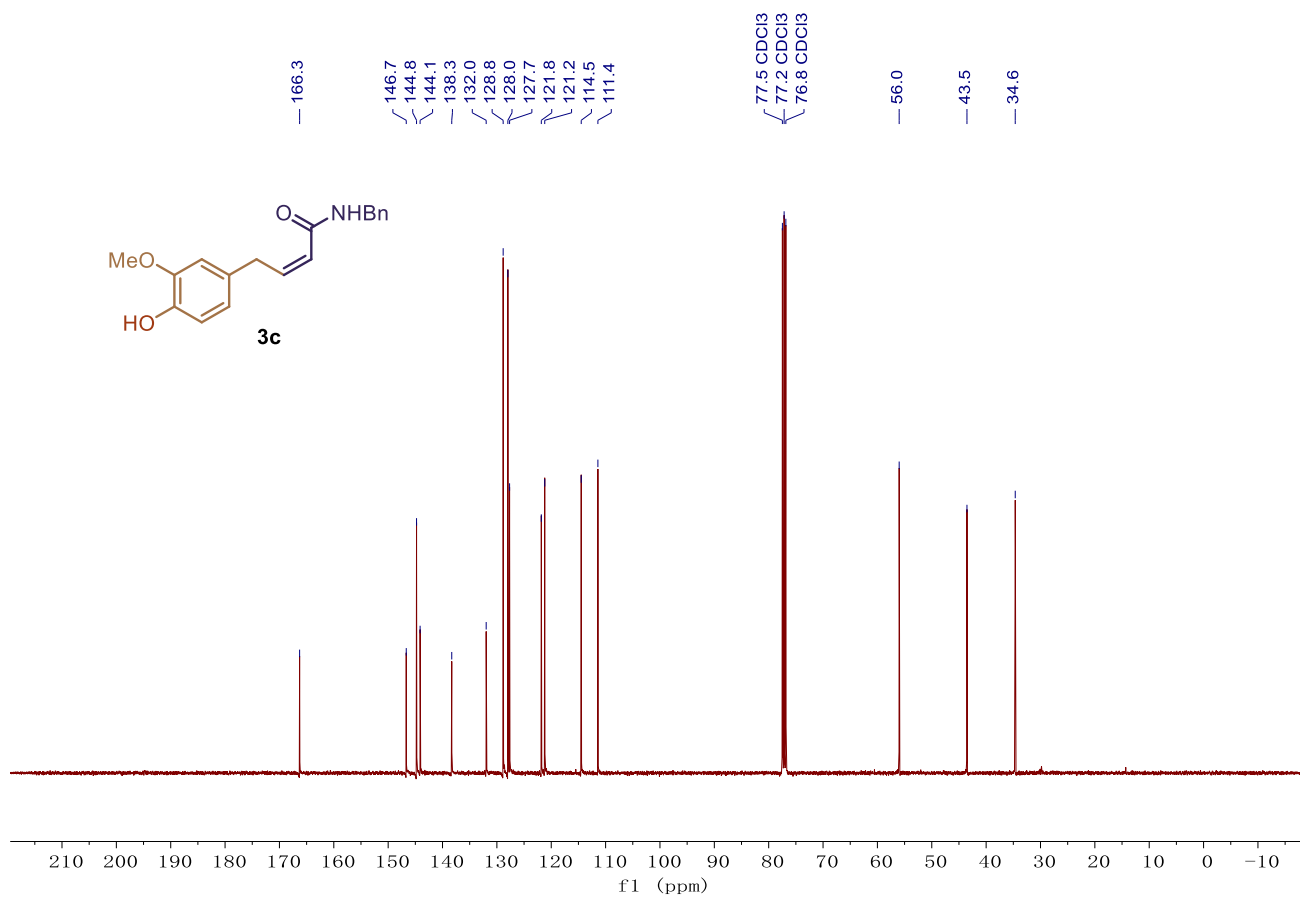
Figure S49 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3d**.
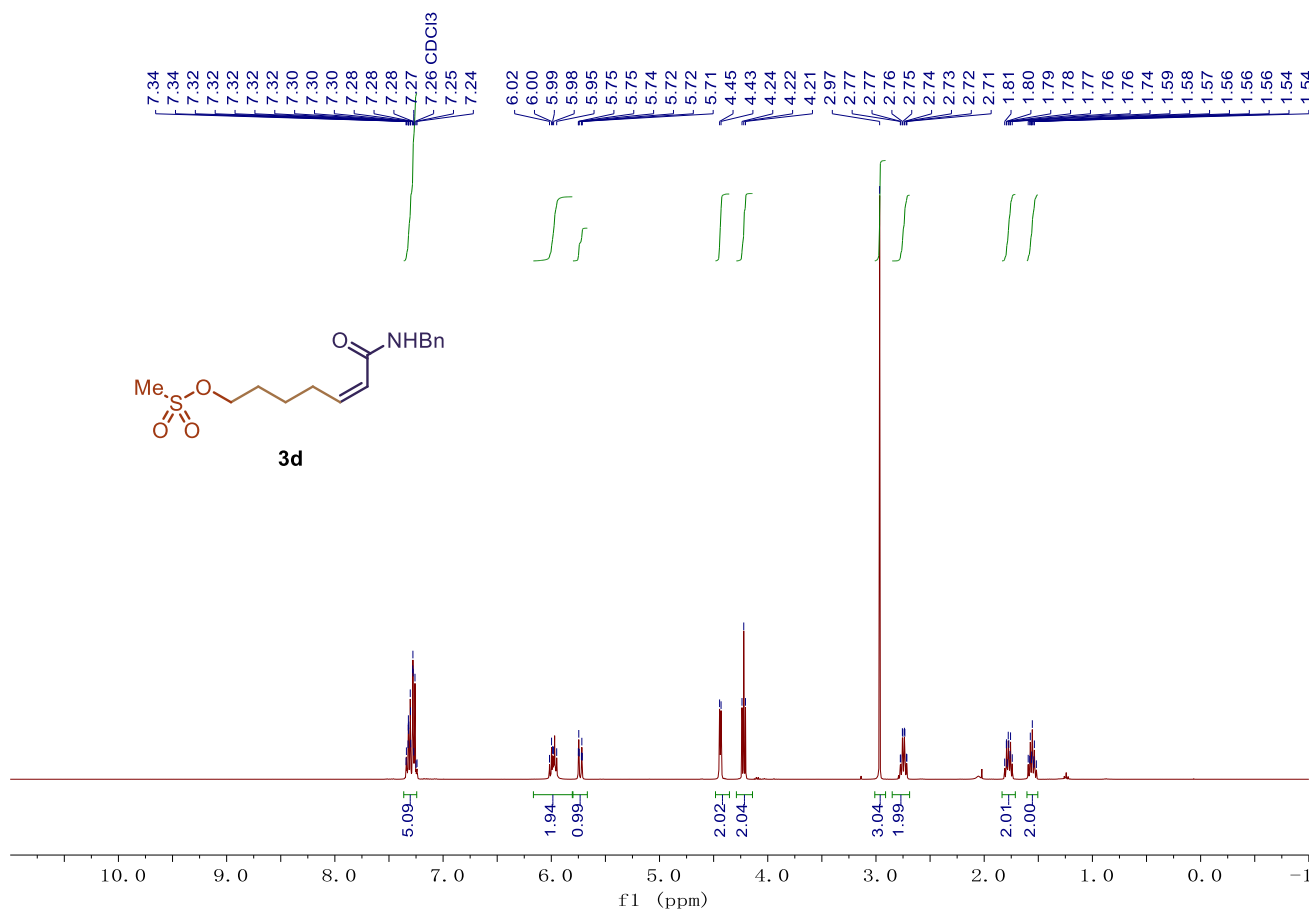
Figure S50 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3d**.
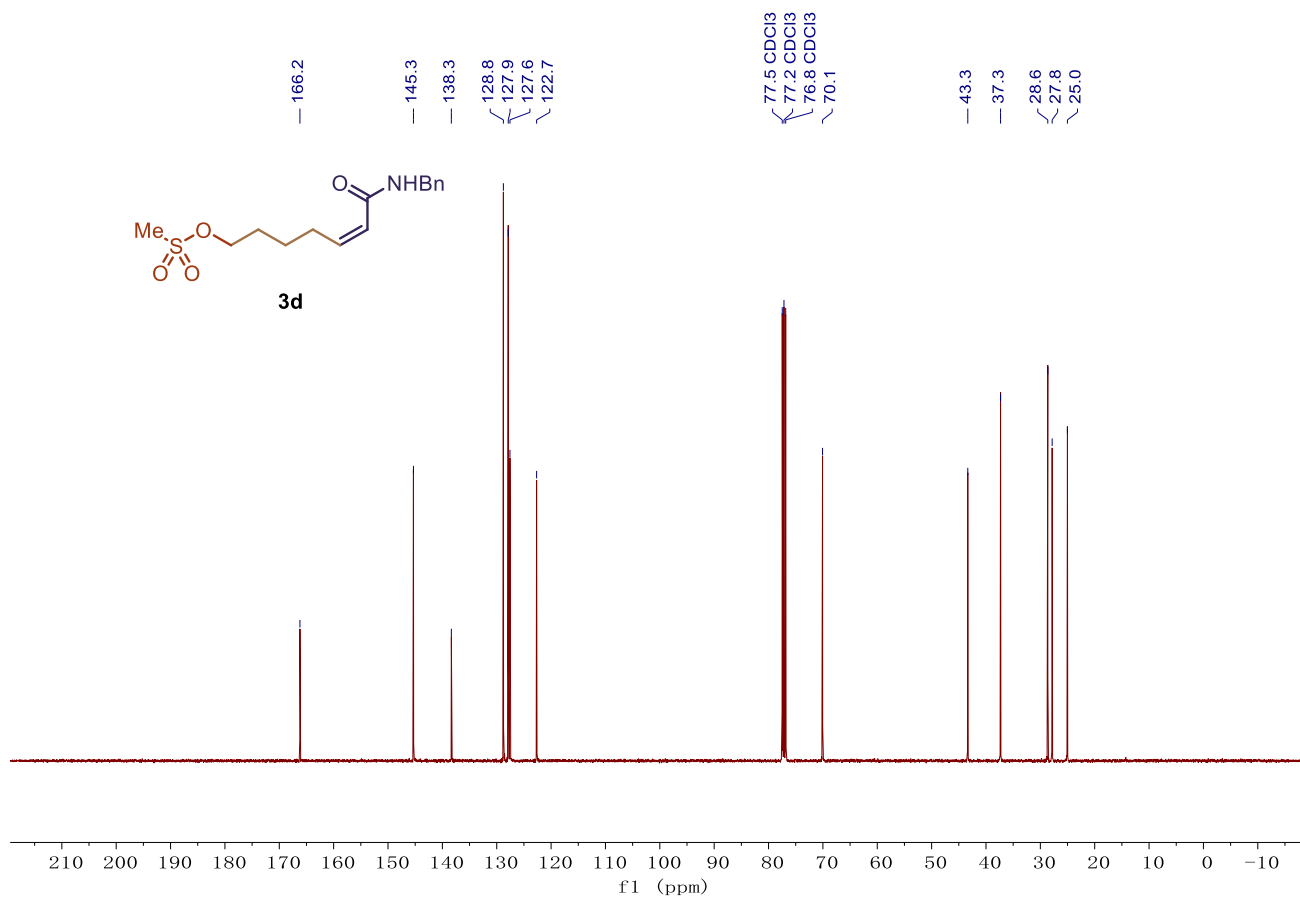
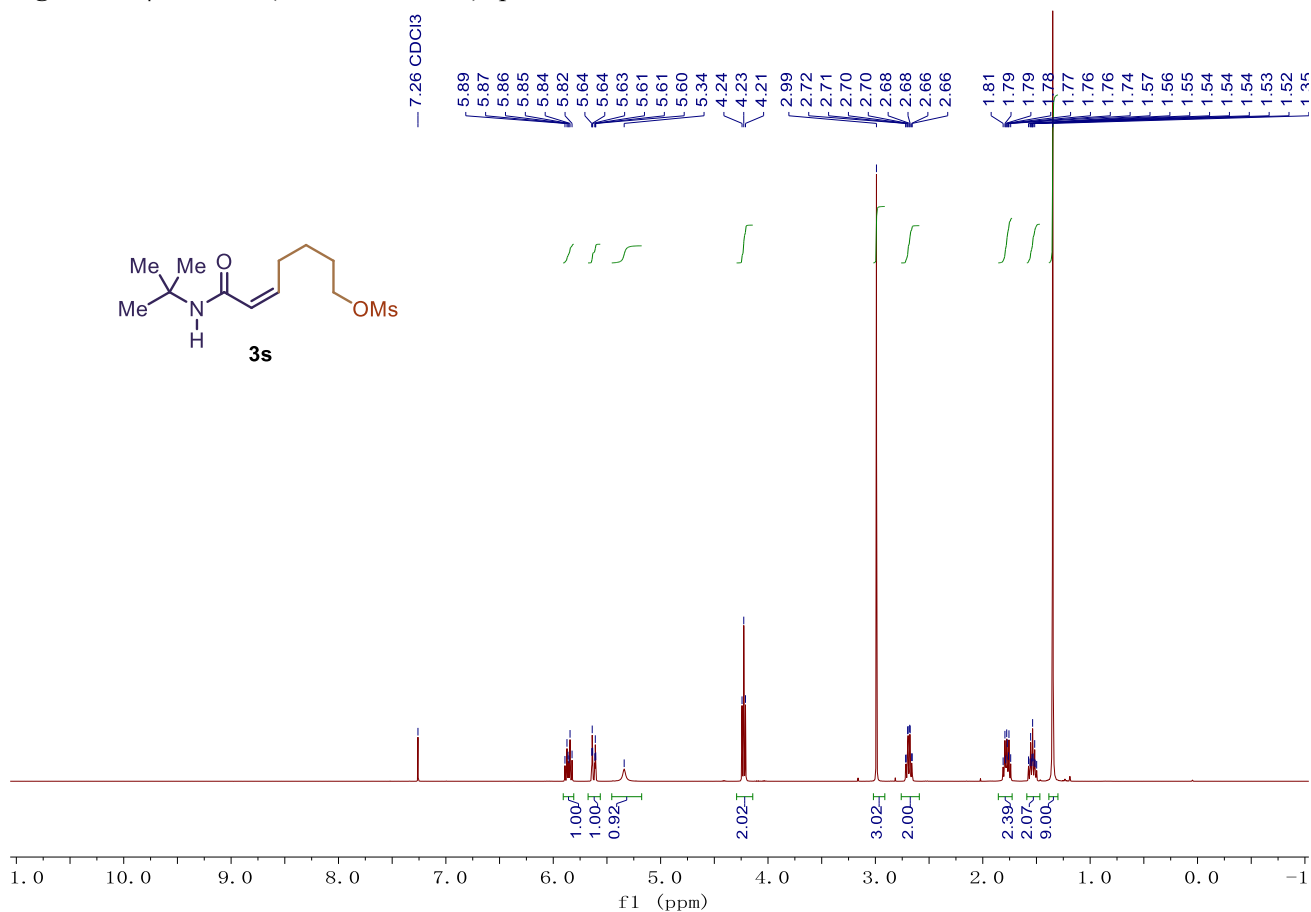**Figure S51 | ¹H NMR (400 MHz, CDCl₃) spectrum of 3e.**
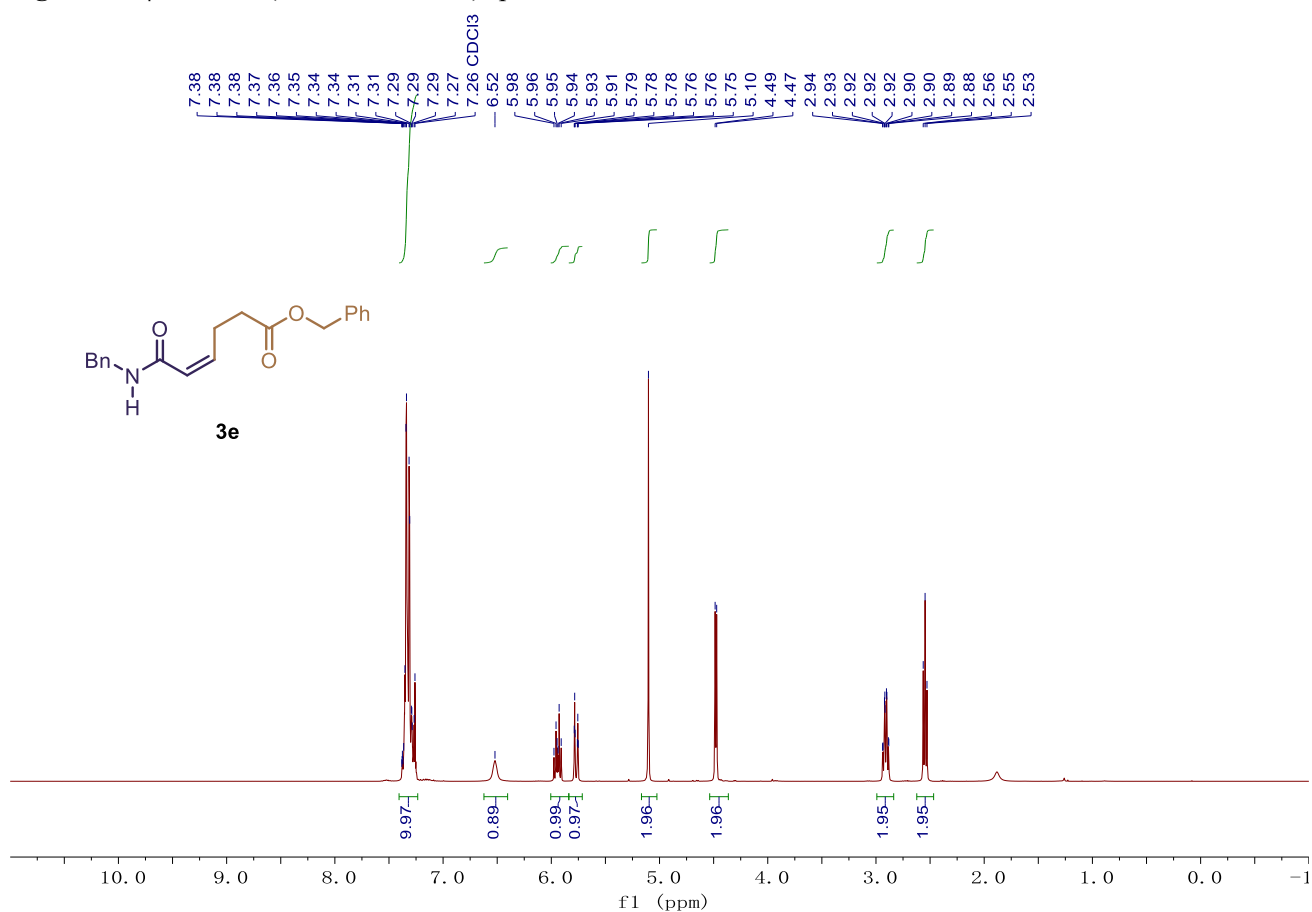
Figure S52 | ¹³C NMR (101 MHz, CDCl₃) spectrum of 3e.
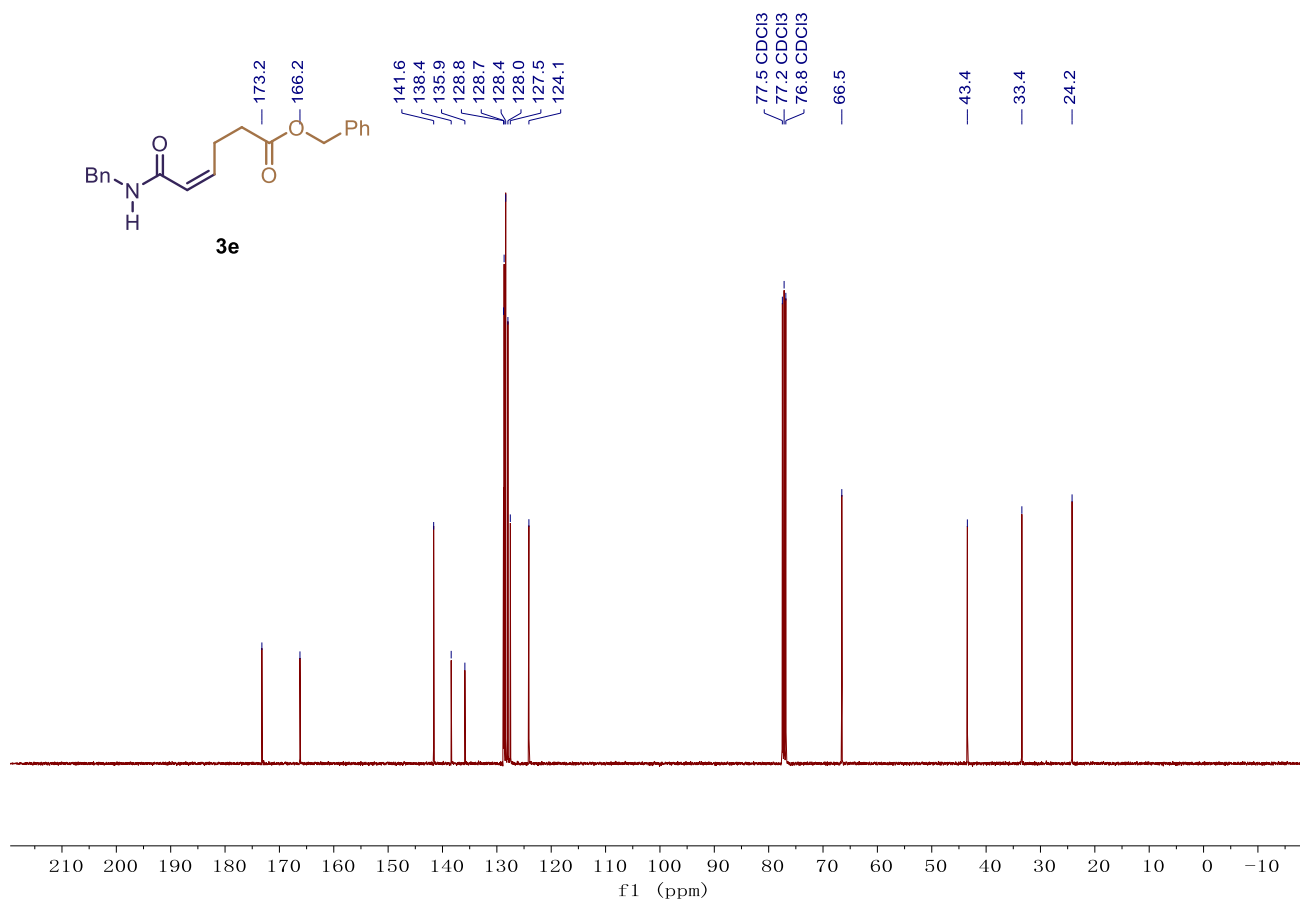
Figure S53 | ¹H NMR (400 MHz, CDCl₃) spectrum of **3f**.
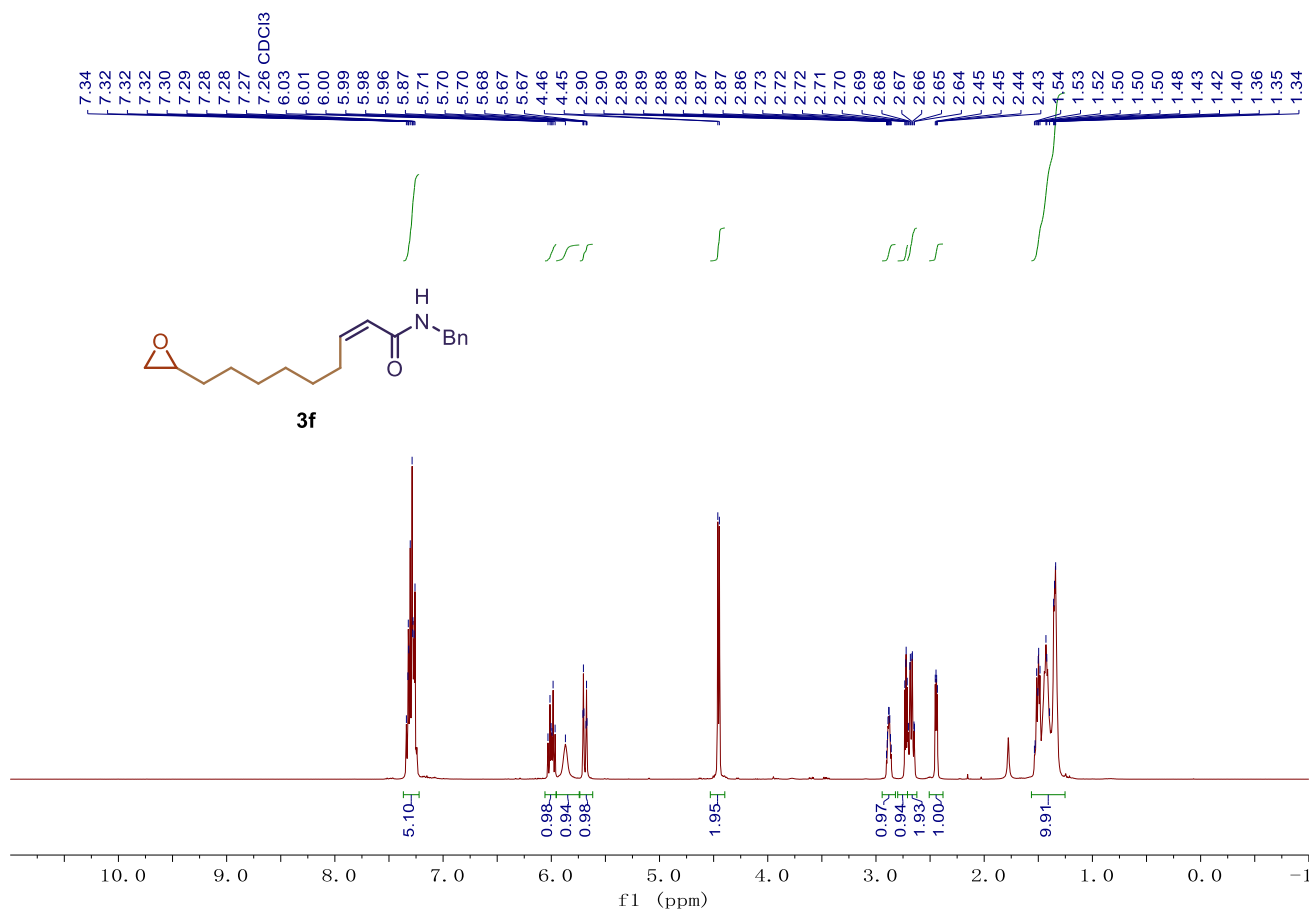
Figure S54 | ¹³C NMR (101 MHz, CDCl₃) spectrum of **3f**.
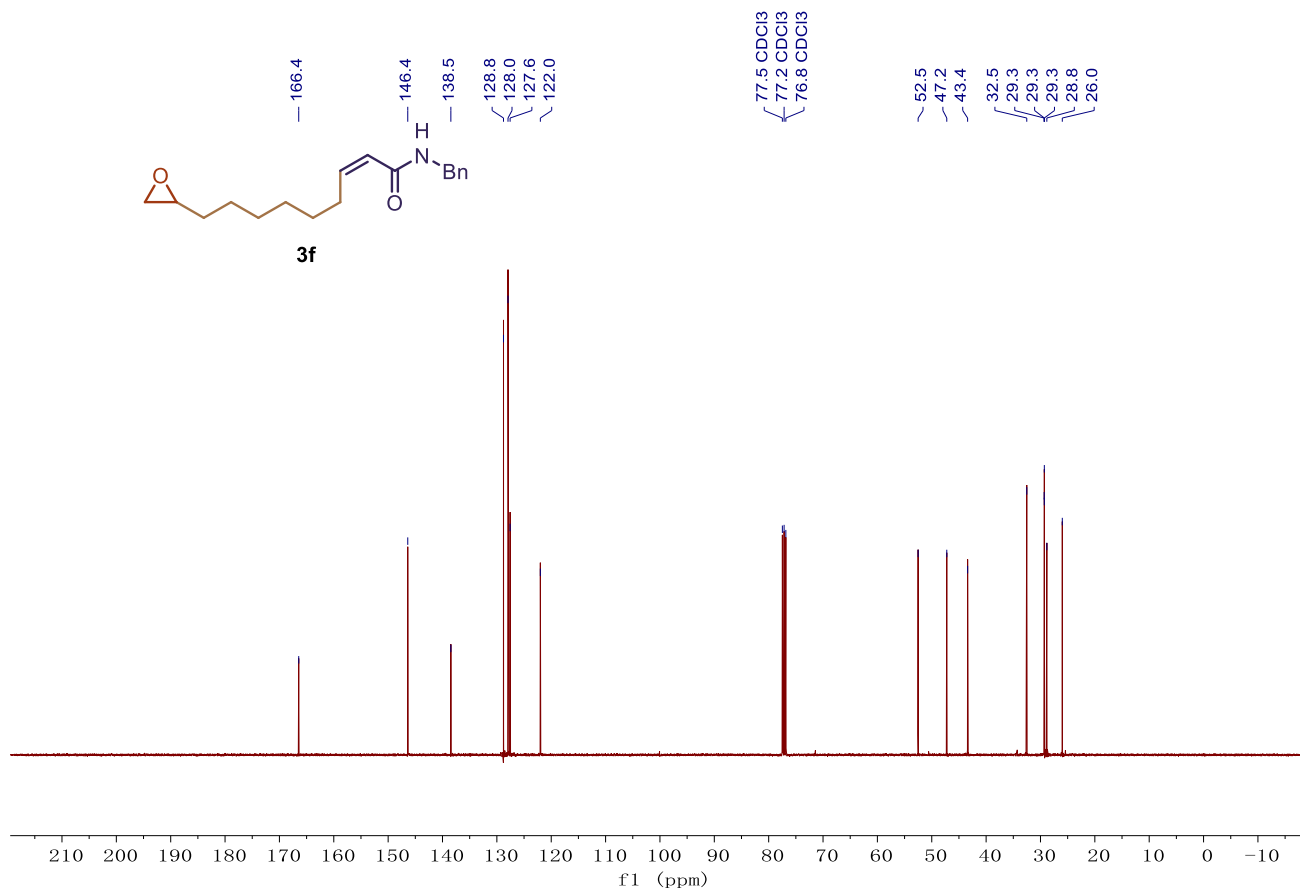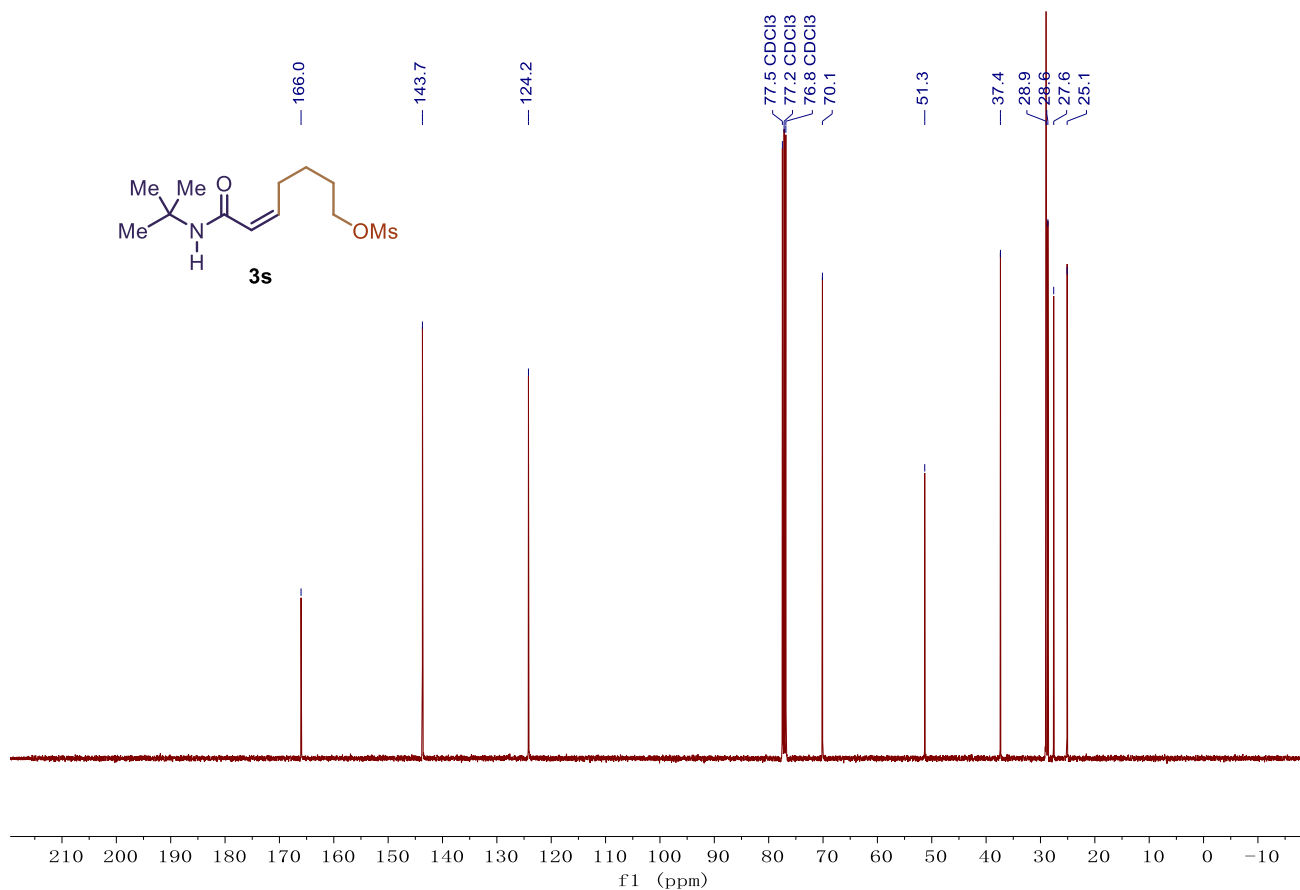
Figure S55 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3g**.
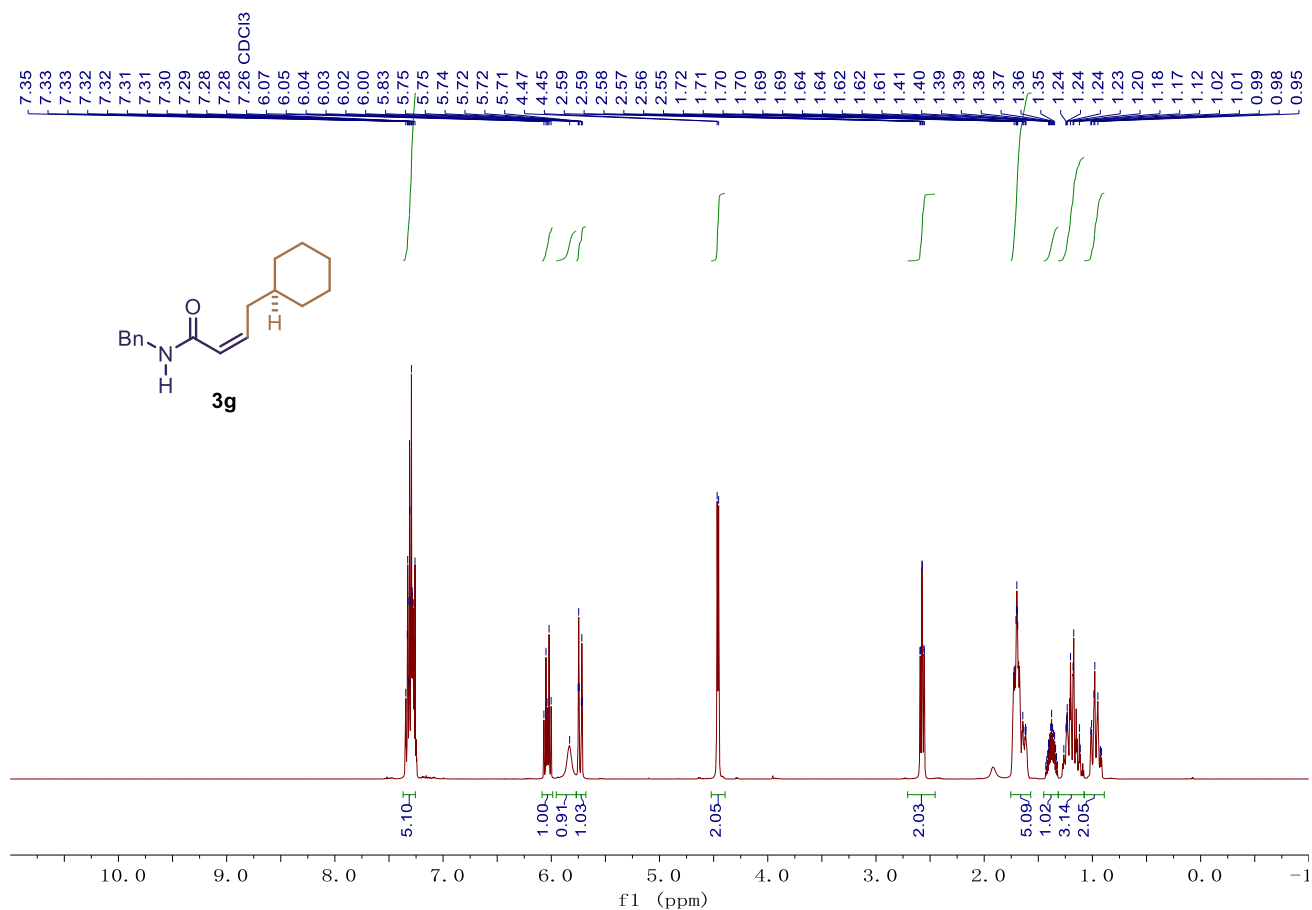
Figure S56 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3g**.
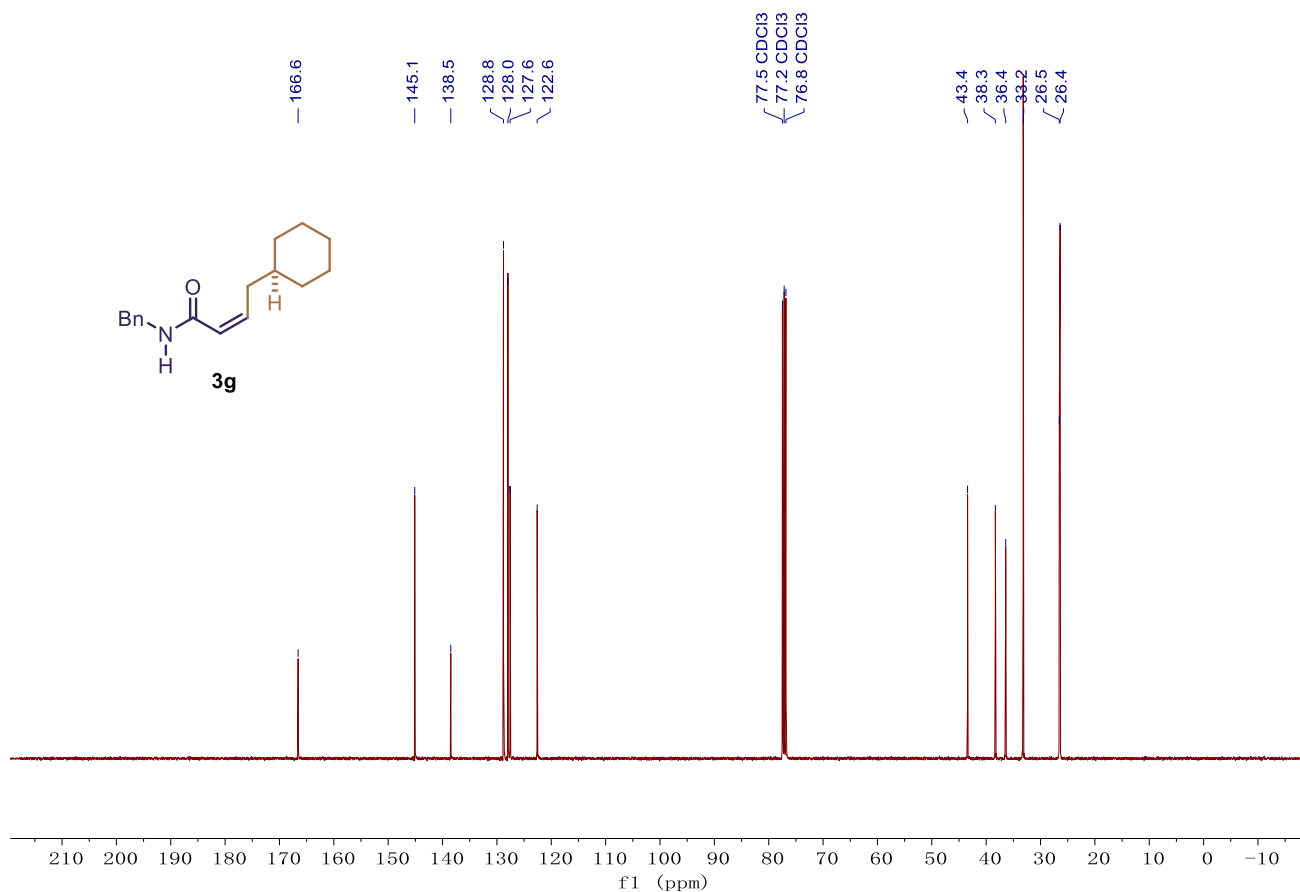
Figure S57 | ^{1}H NMR (400 MHz, C6D6) spectrum of **3h**.
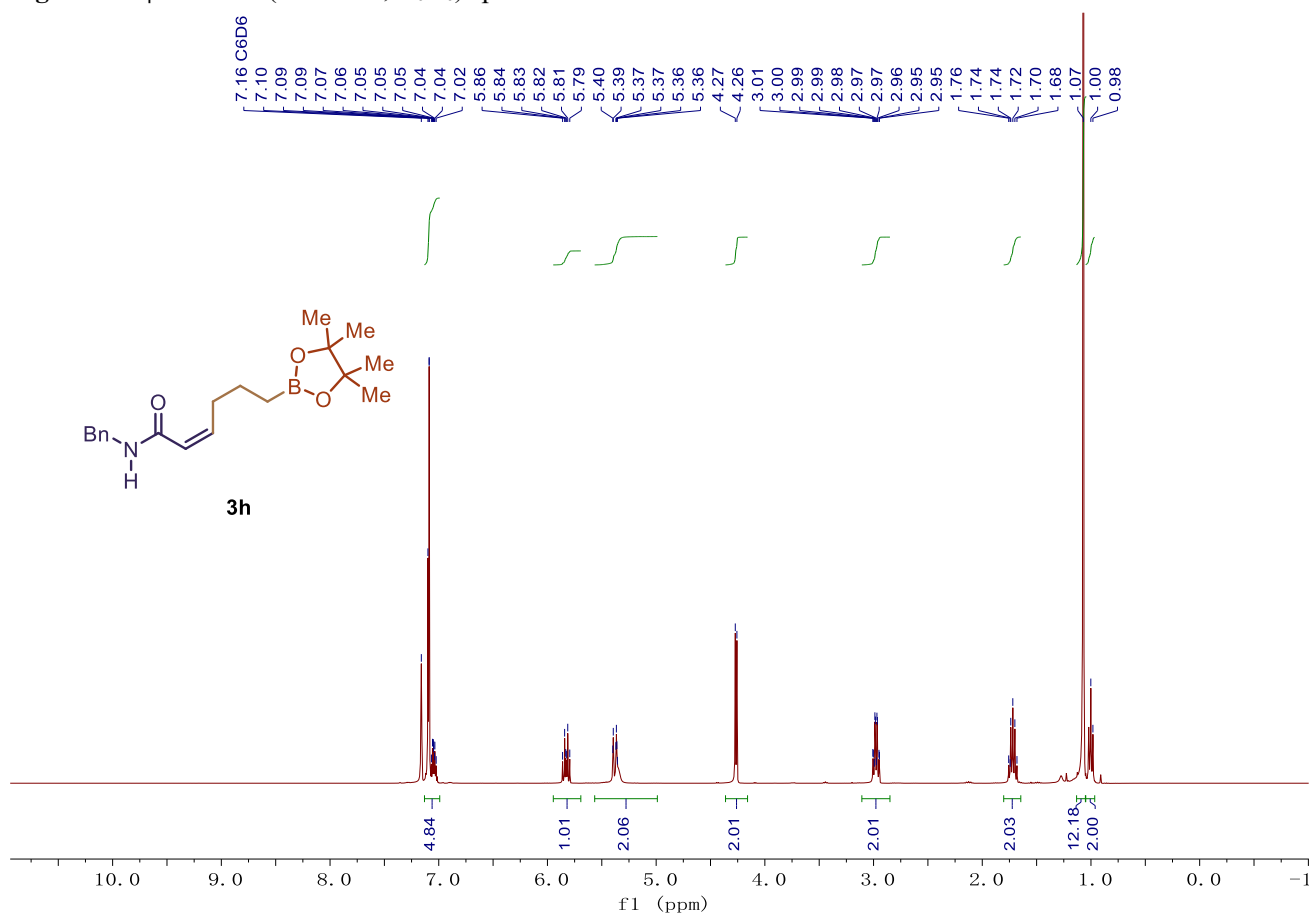
Figure S58 | ^{13}C NMR (101 MHz, C6D6) spectrum of **3h**.
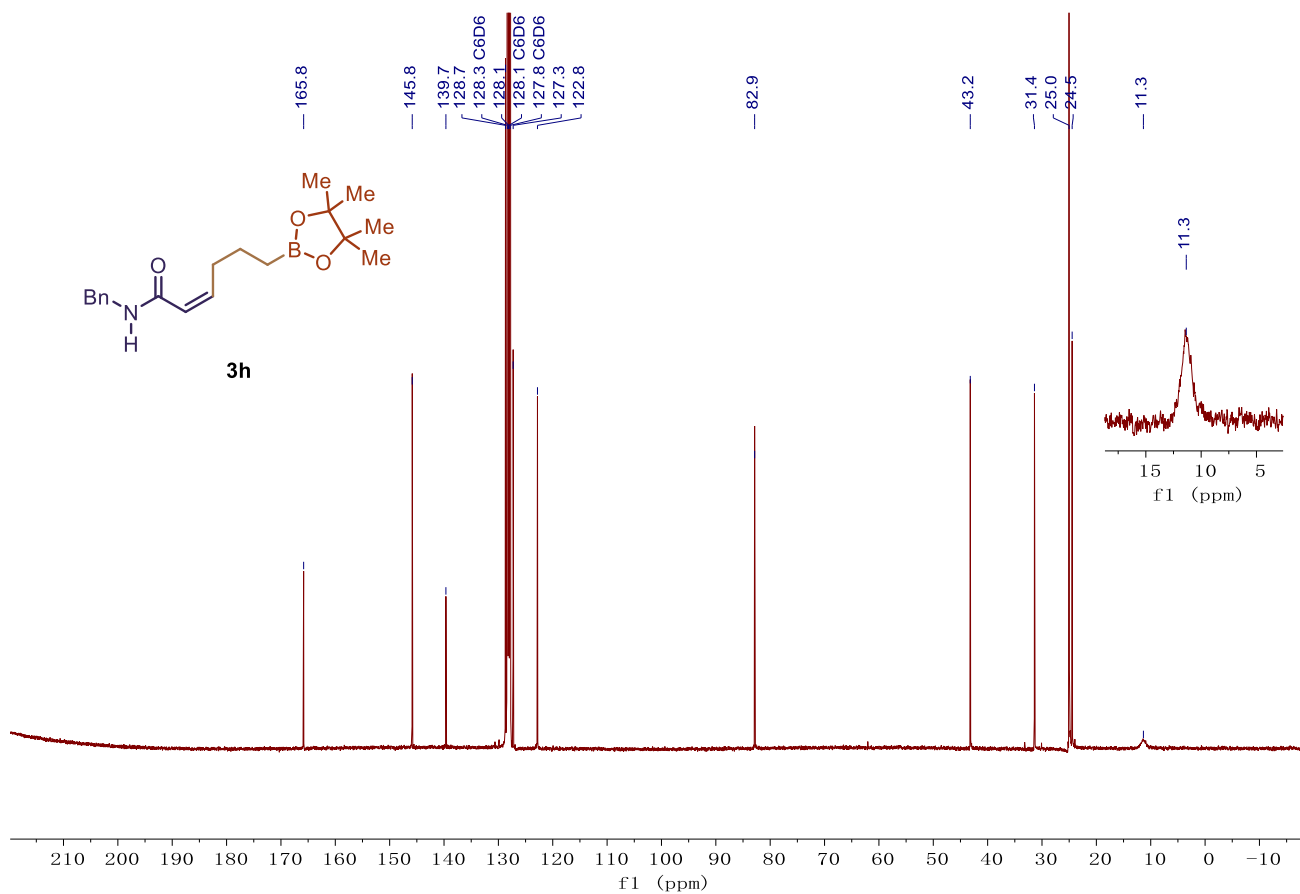
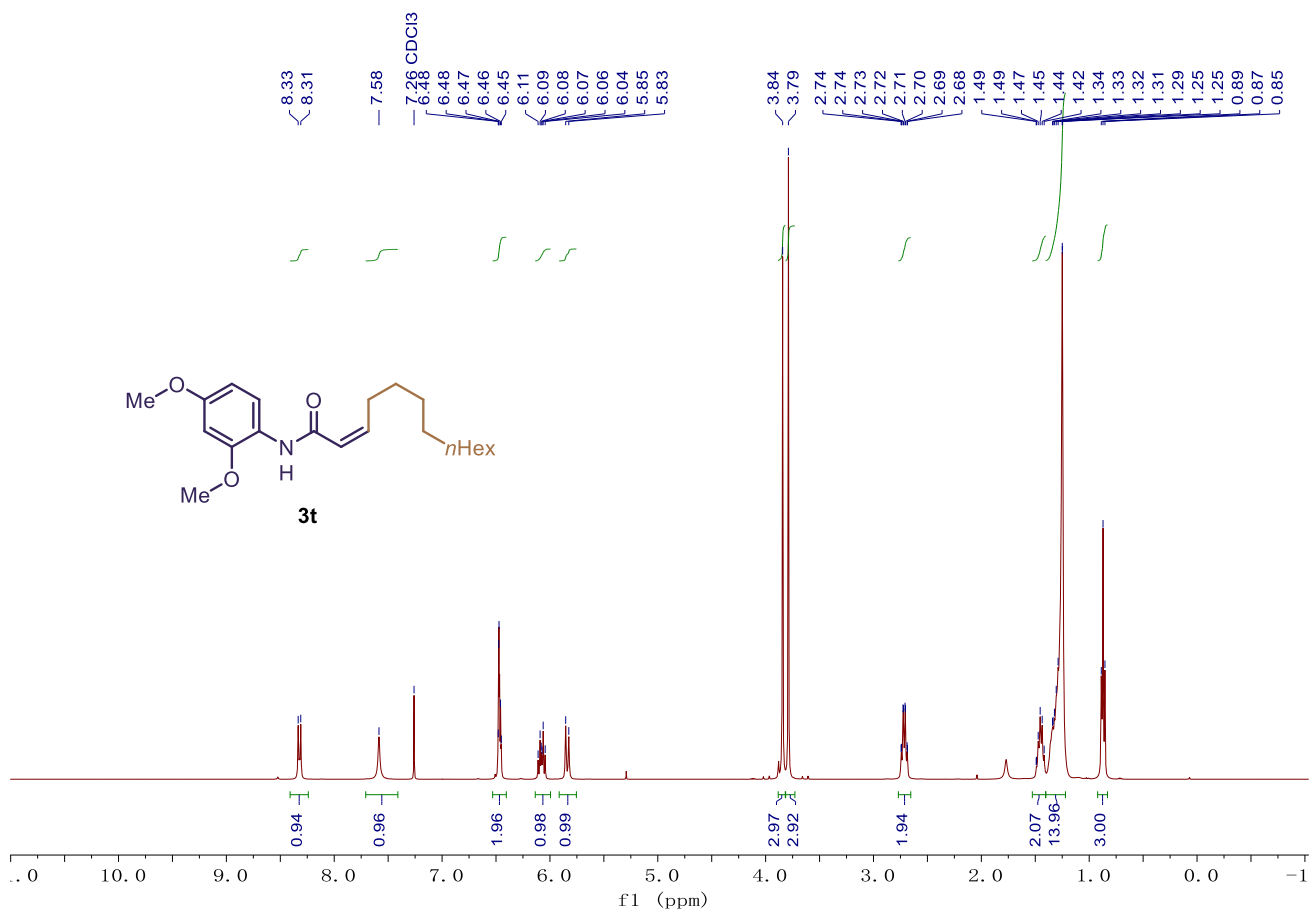**Figure S59 |** ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3i**.
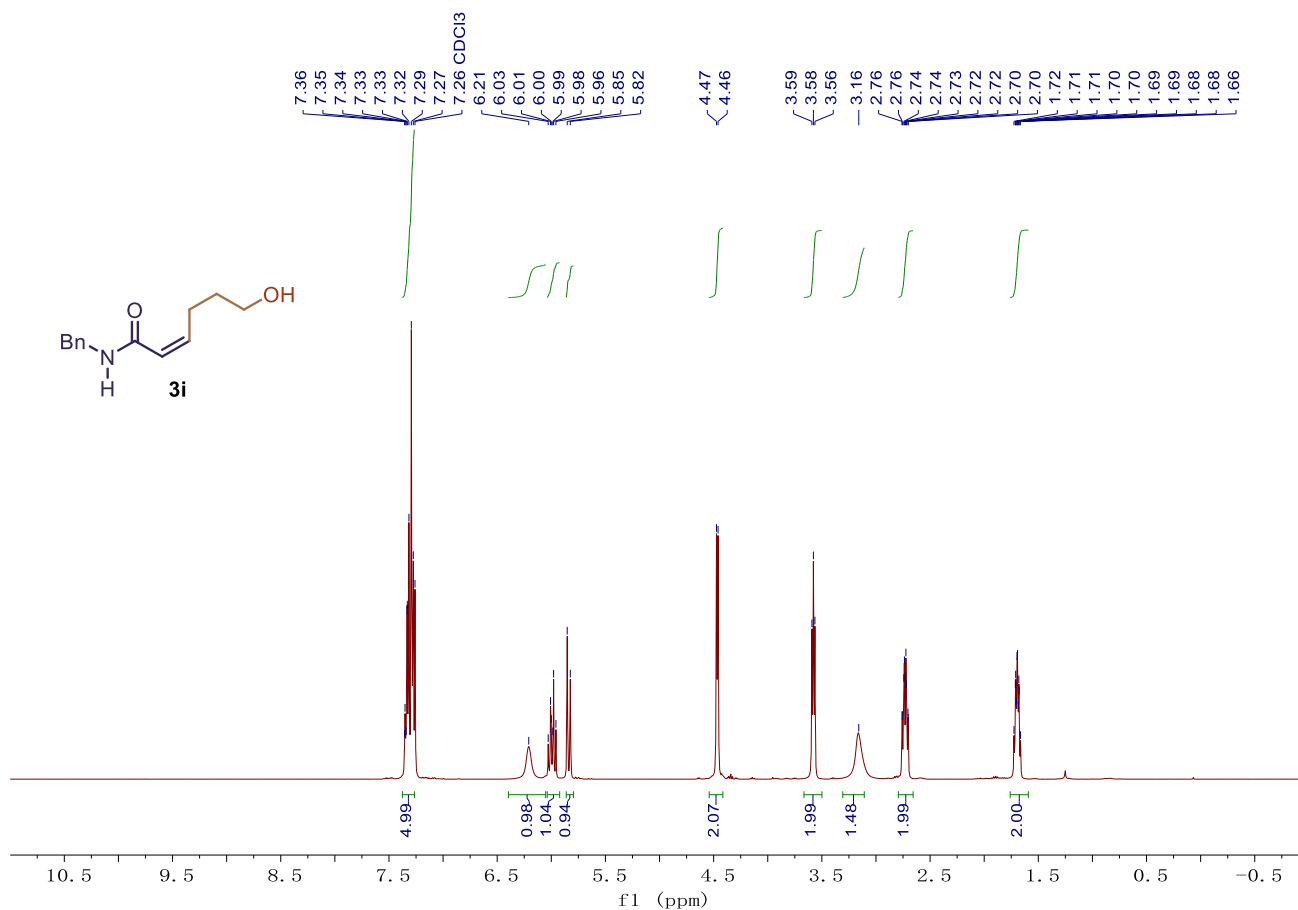
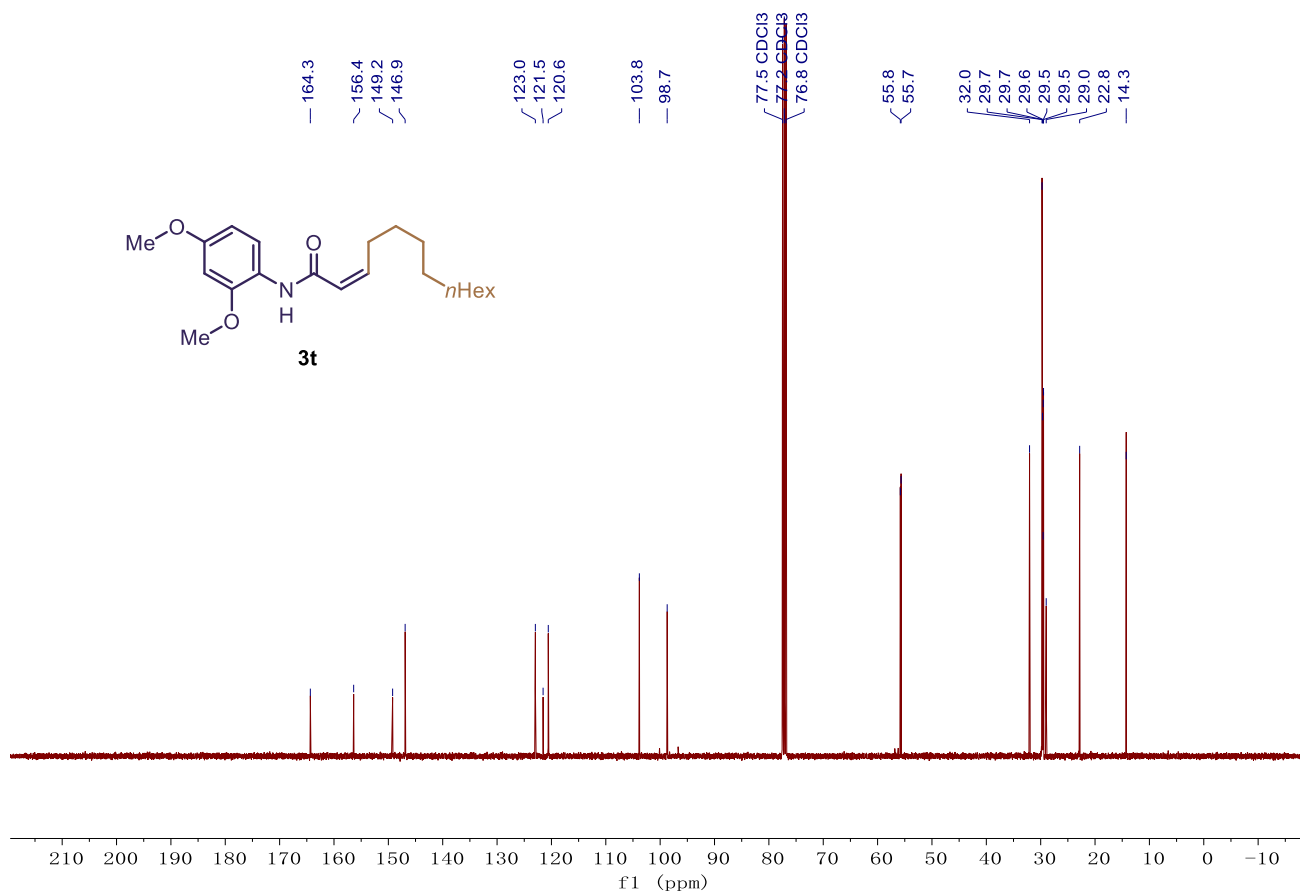**Figure S60 |** ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3i**.
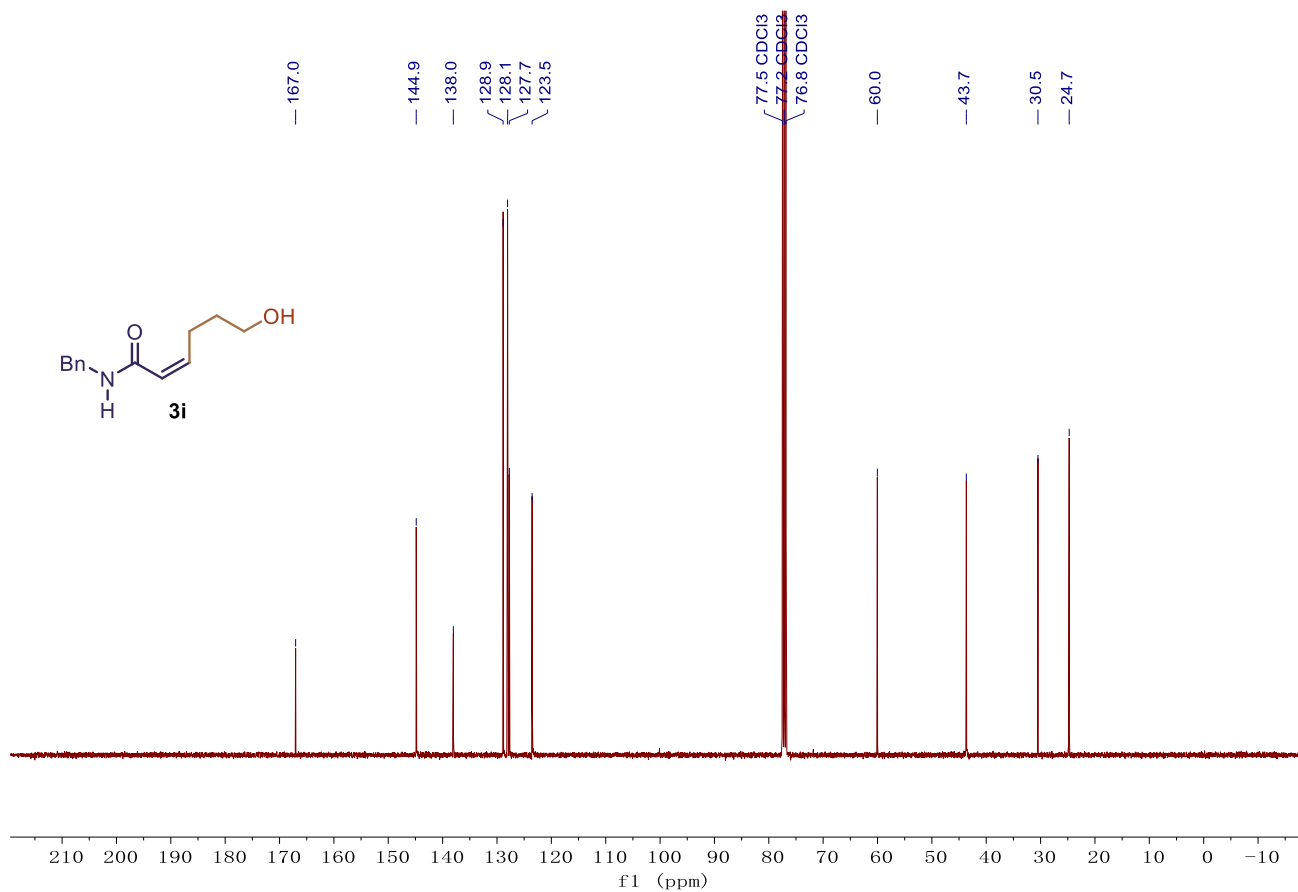
Figure S61 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3j**.
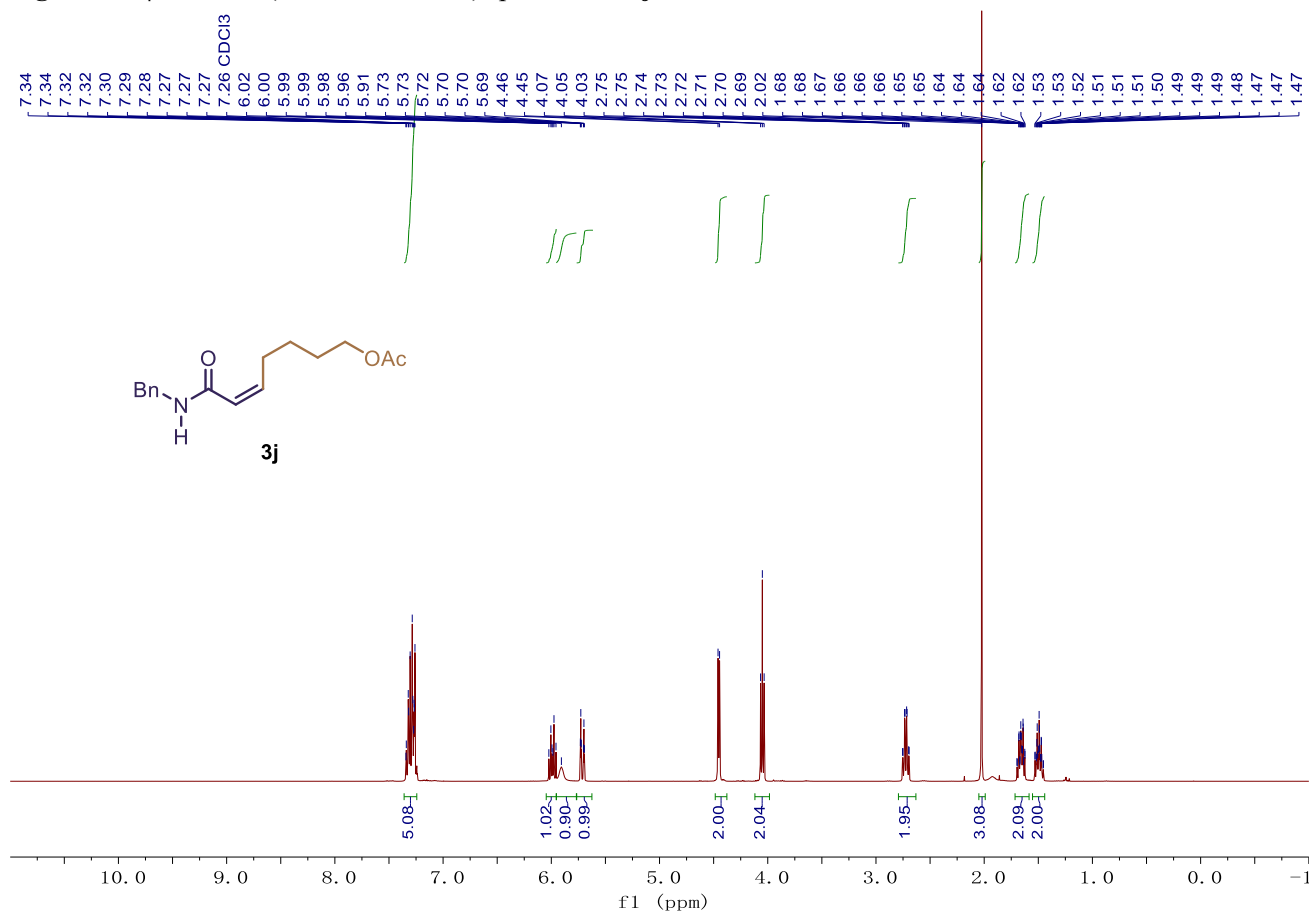
Figure S62 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3j**.
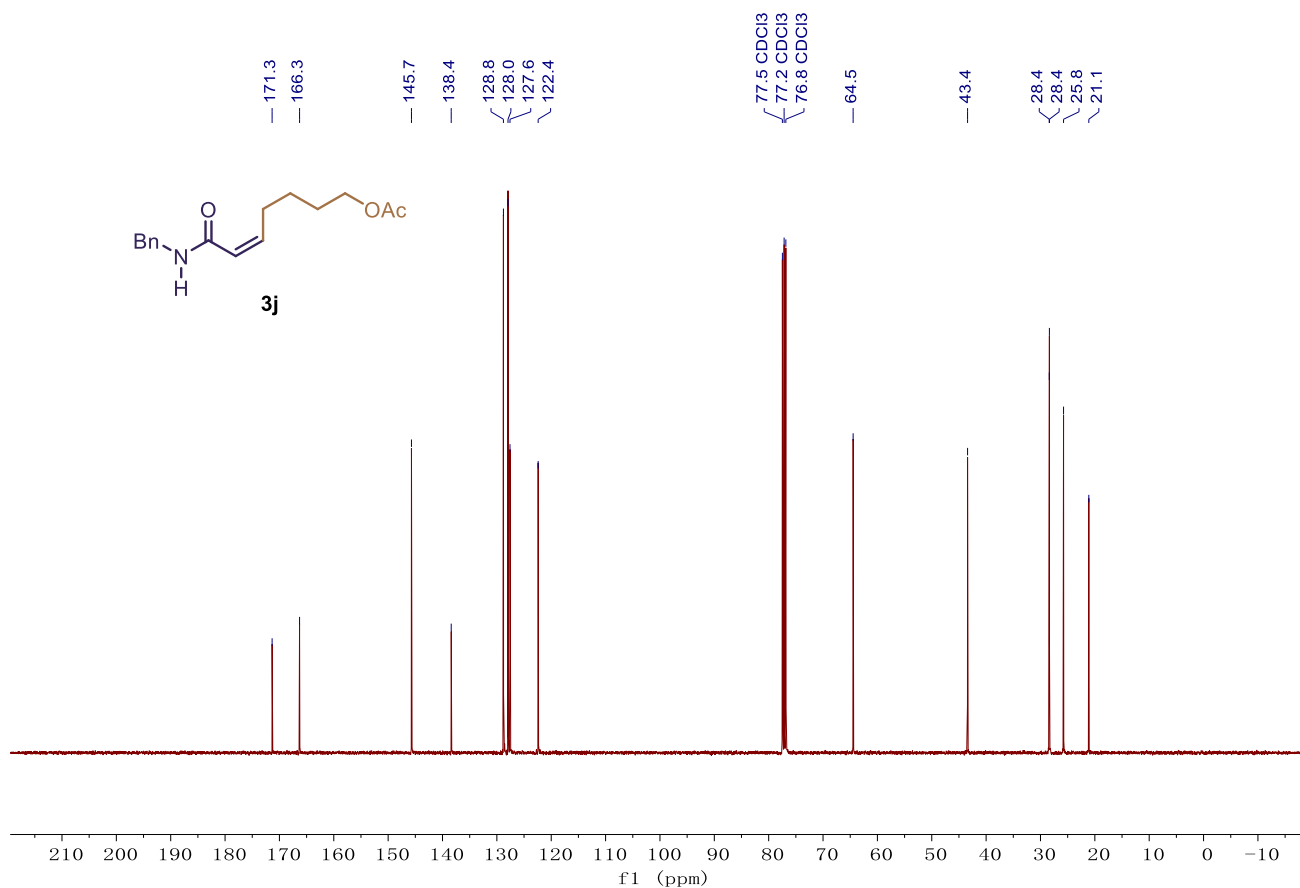
Figure S63 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3k**.
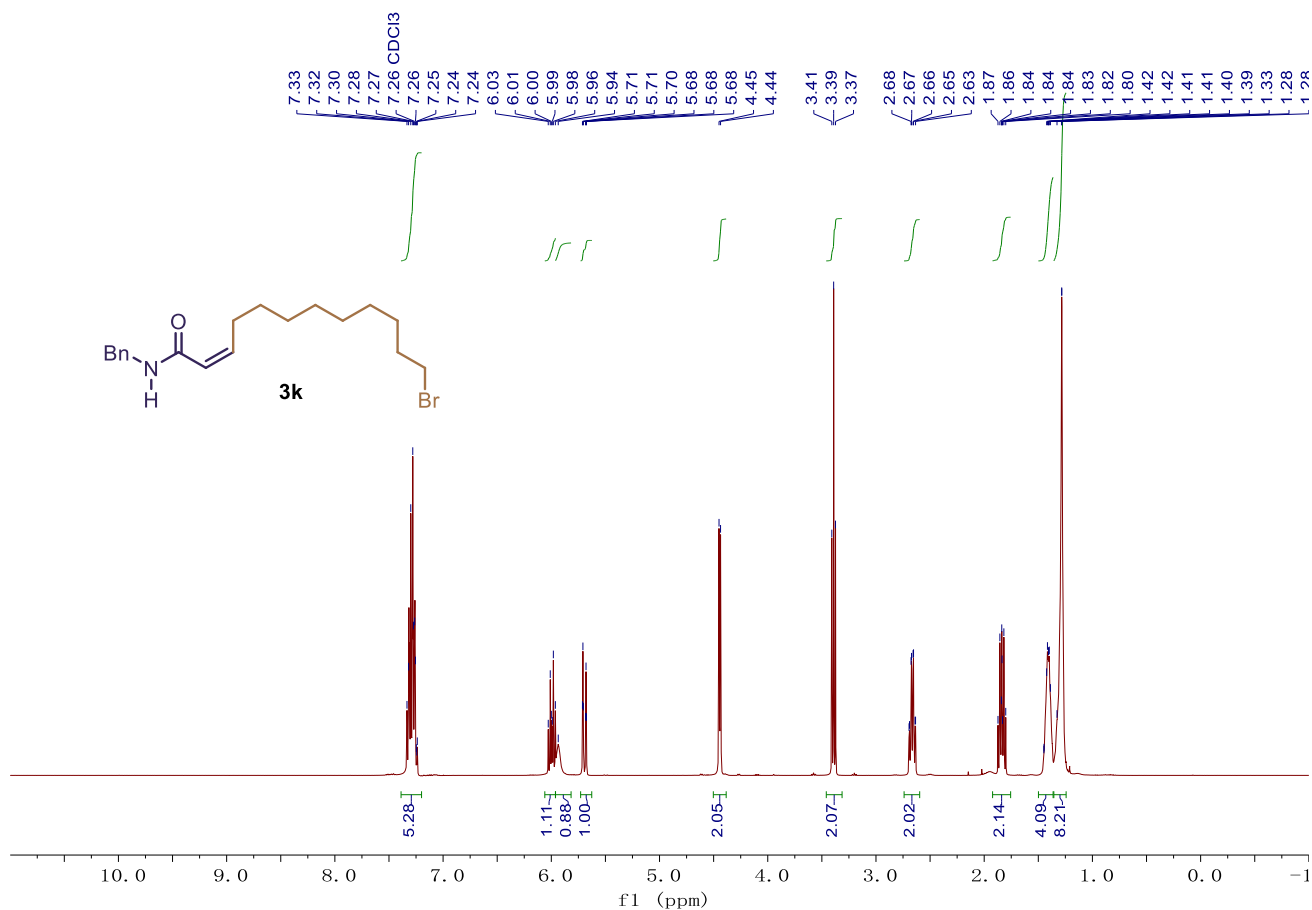
Figure S64 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3k**.
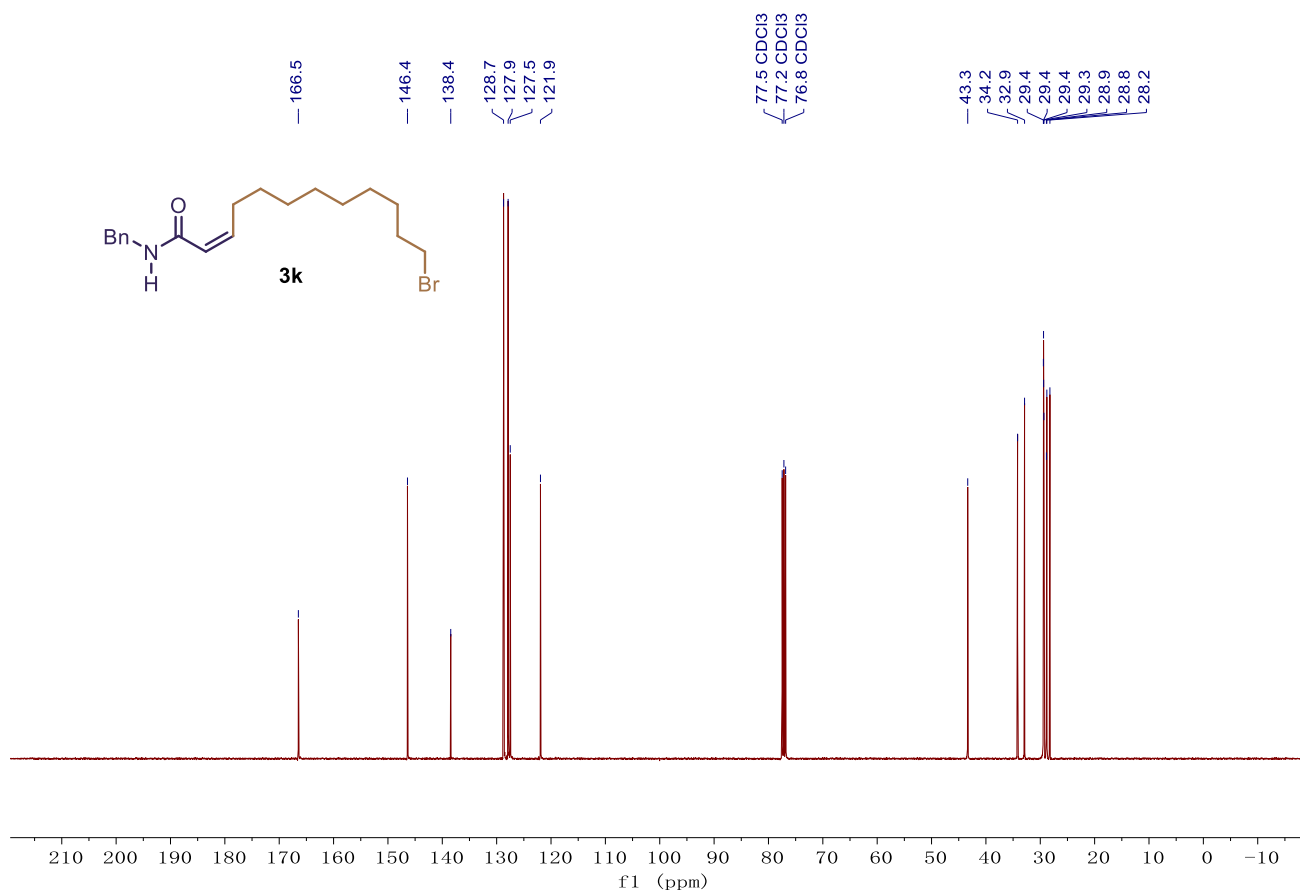
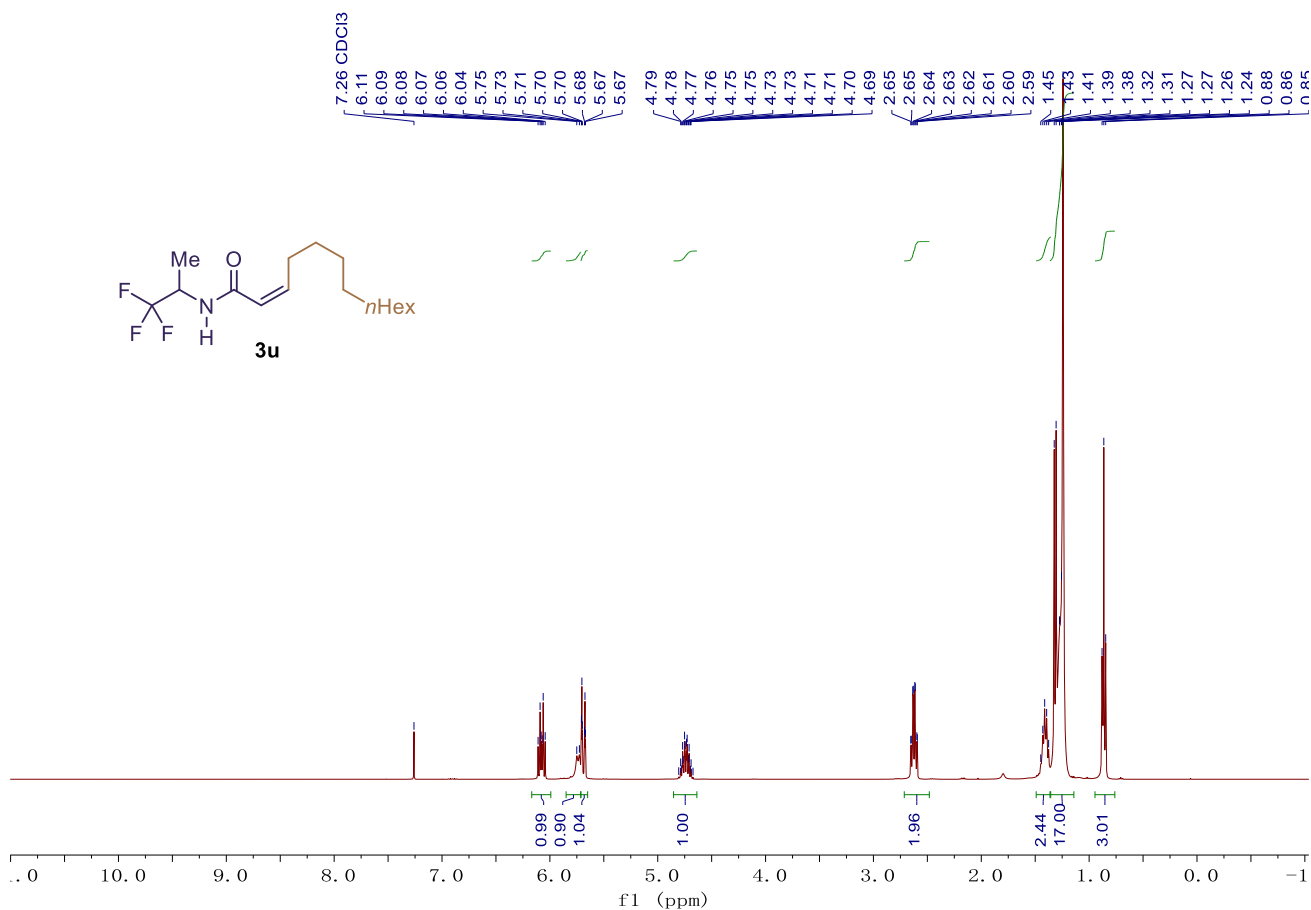**Figure S65** | ¹H NMR (400 MHz, CDCl₃) spectrum of **3l**.
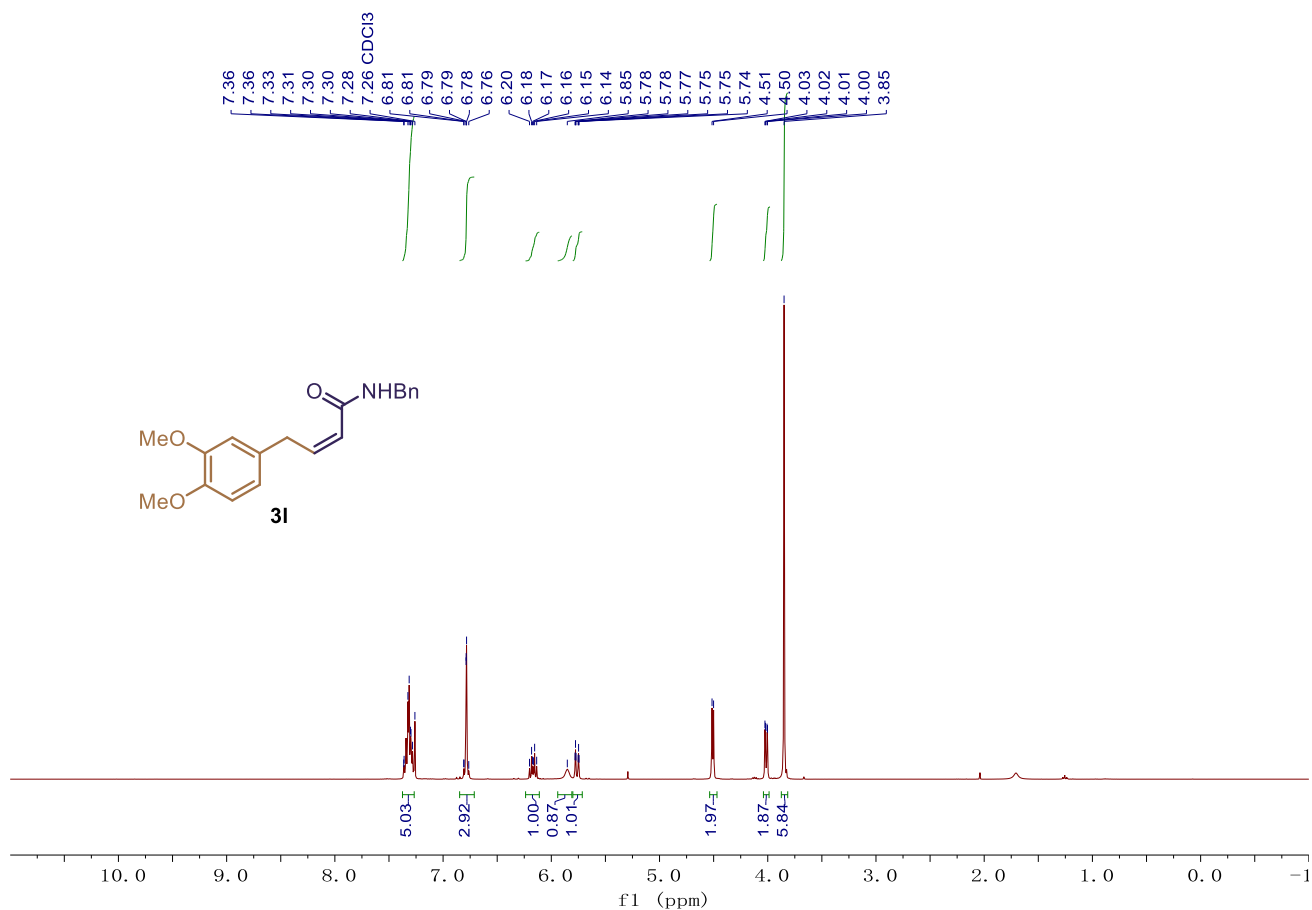
Figure S66 | ¹³C NMR (101 MHz, CDCl₃) spectrum of **3l**.

Figure S67 | ¹H NMR (400 MHz, CDCl₃) spectrum of **3m**.
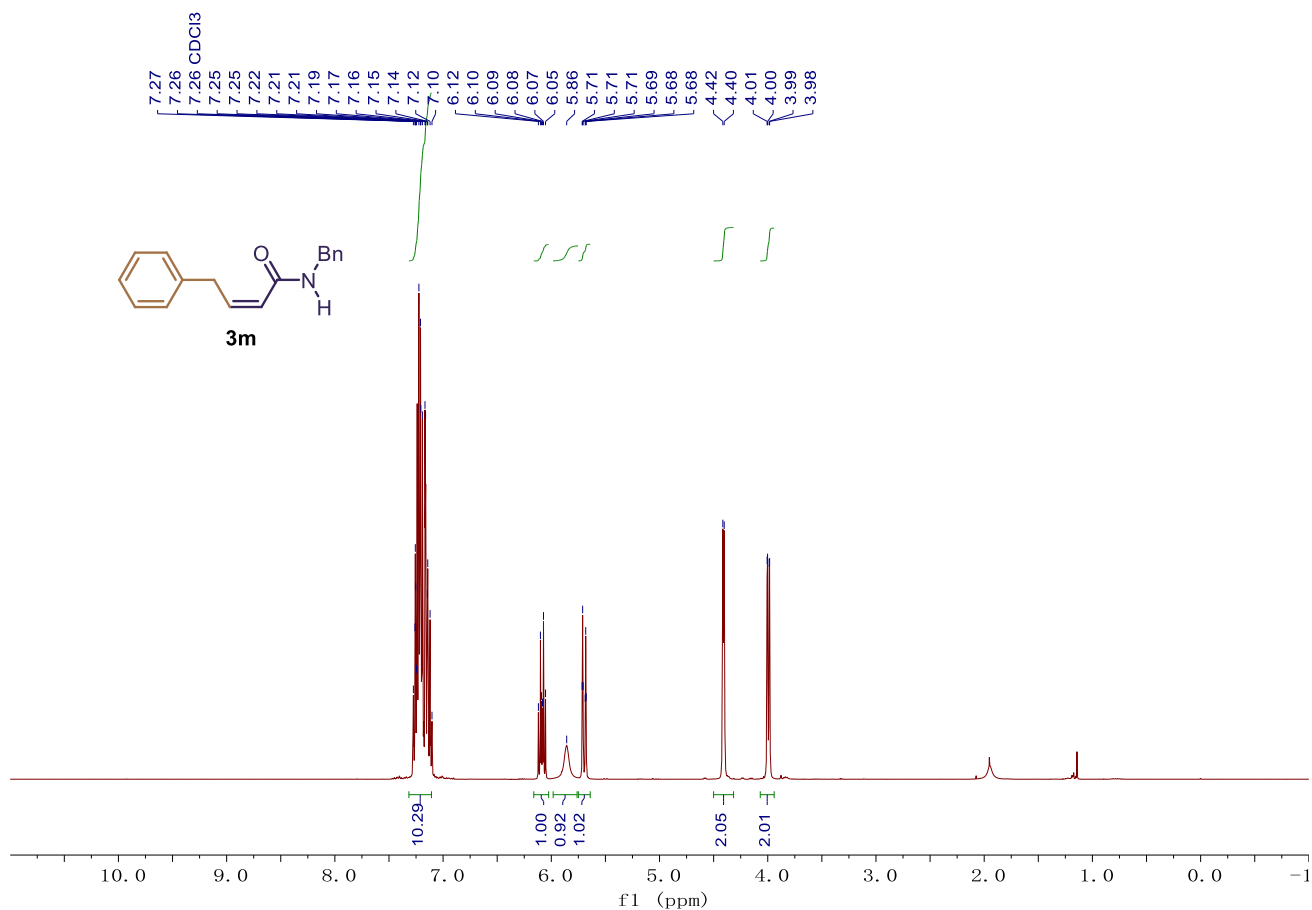
Figure S68 | ¹³C NMR (101 MHz, CDCl₃) spectrum of **3m**.

Figure S69 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3n**.
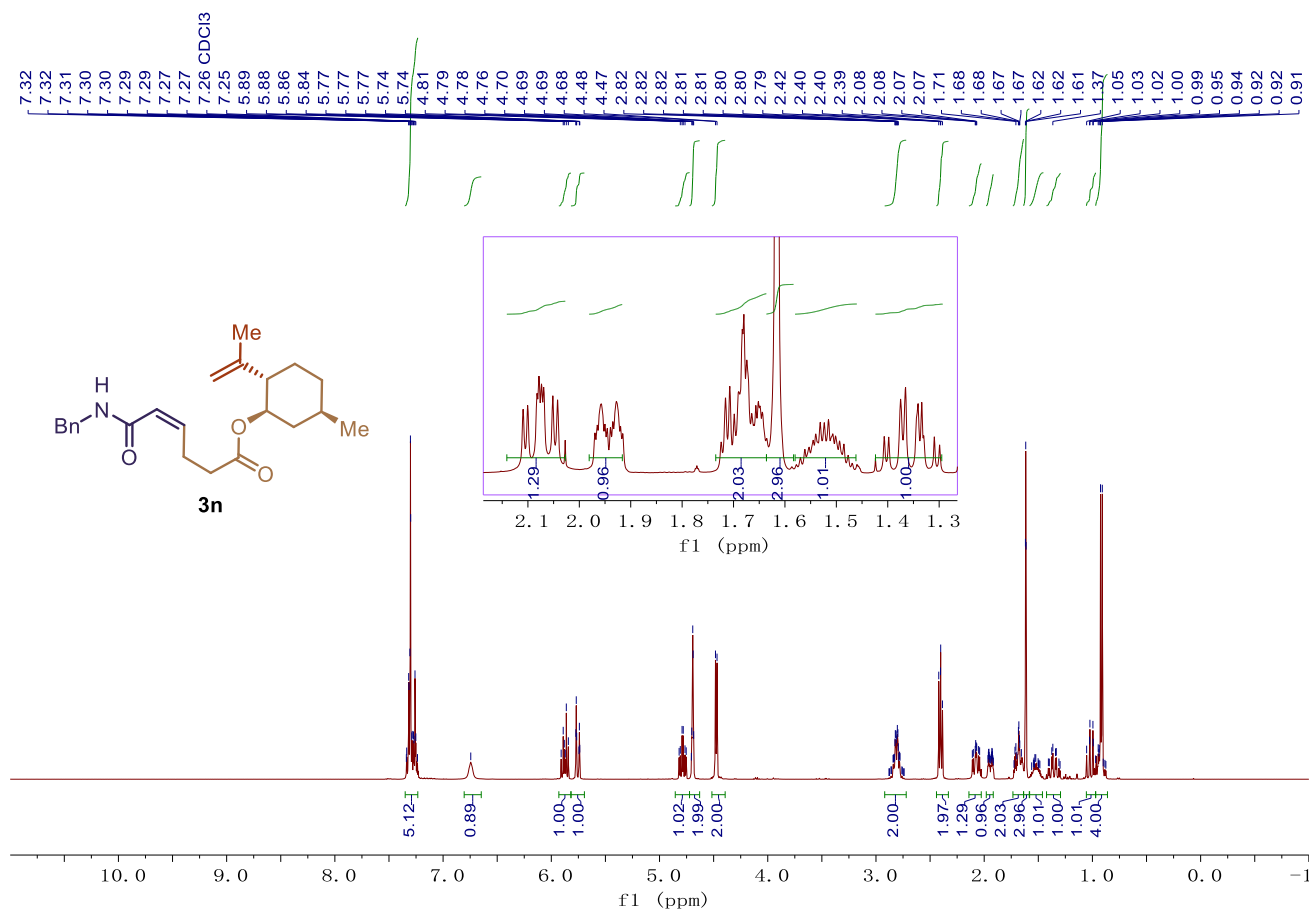
Figure S70 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3n**.
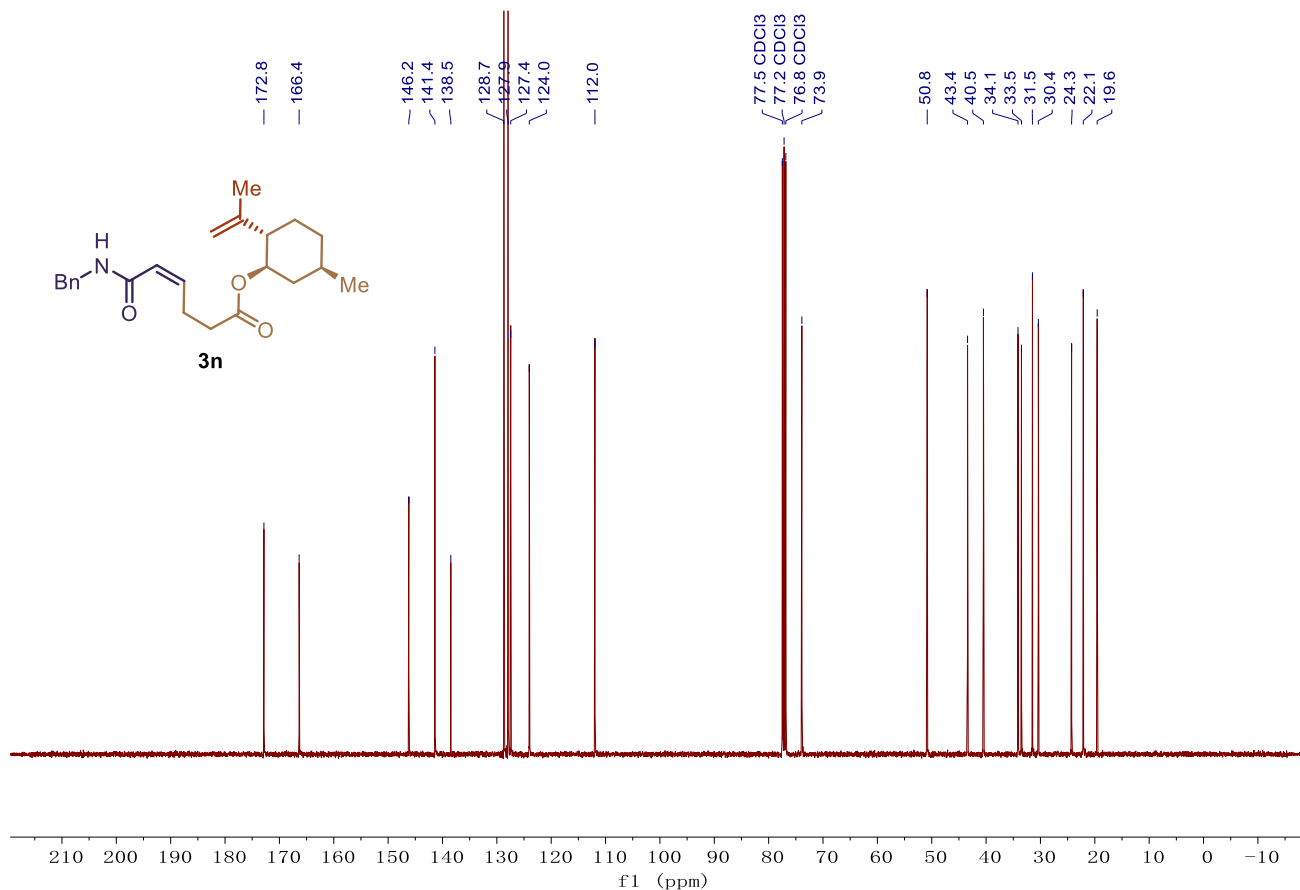
Figure S71 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3o**.
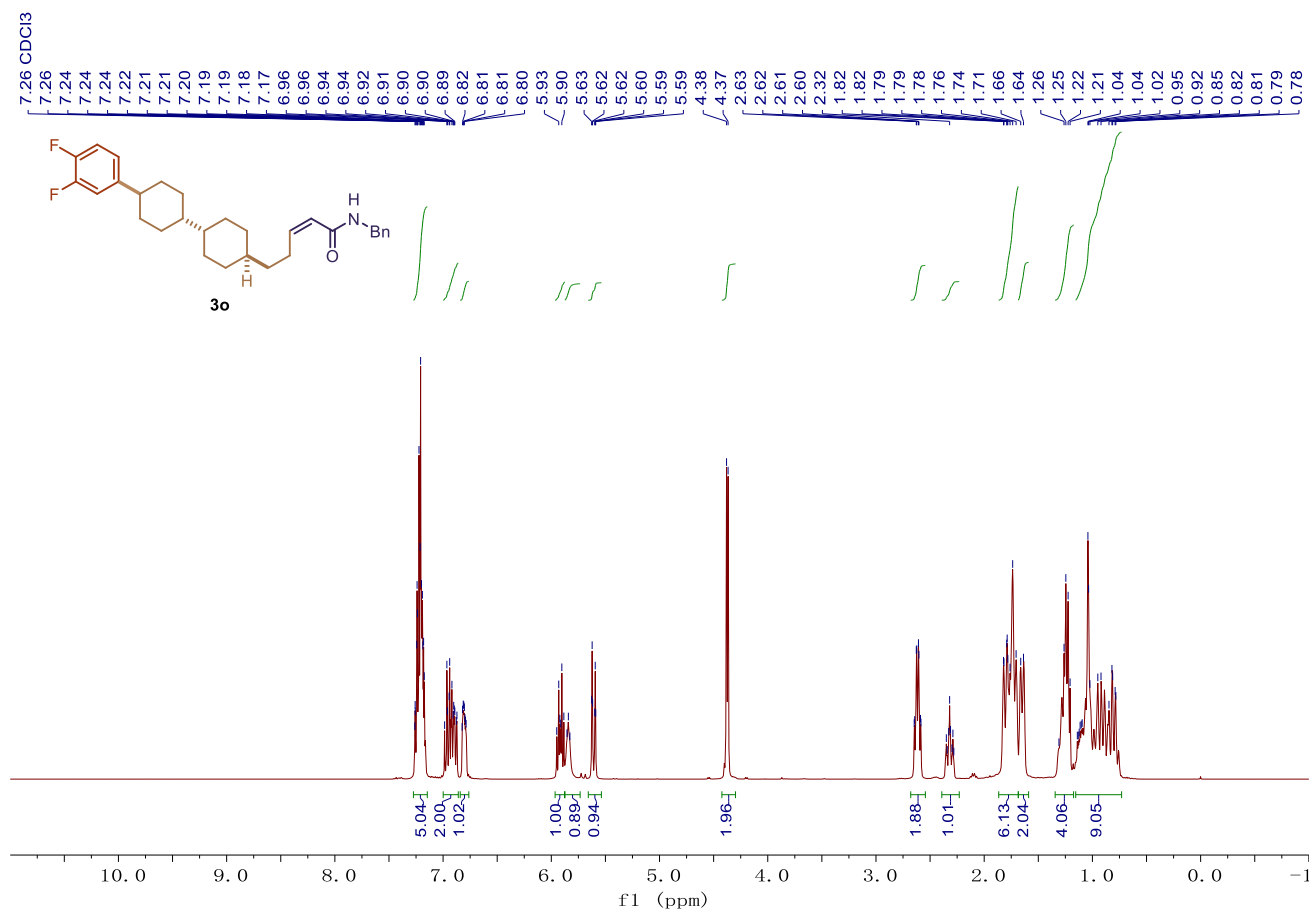
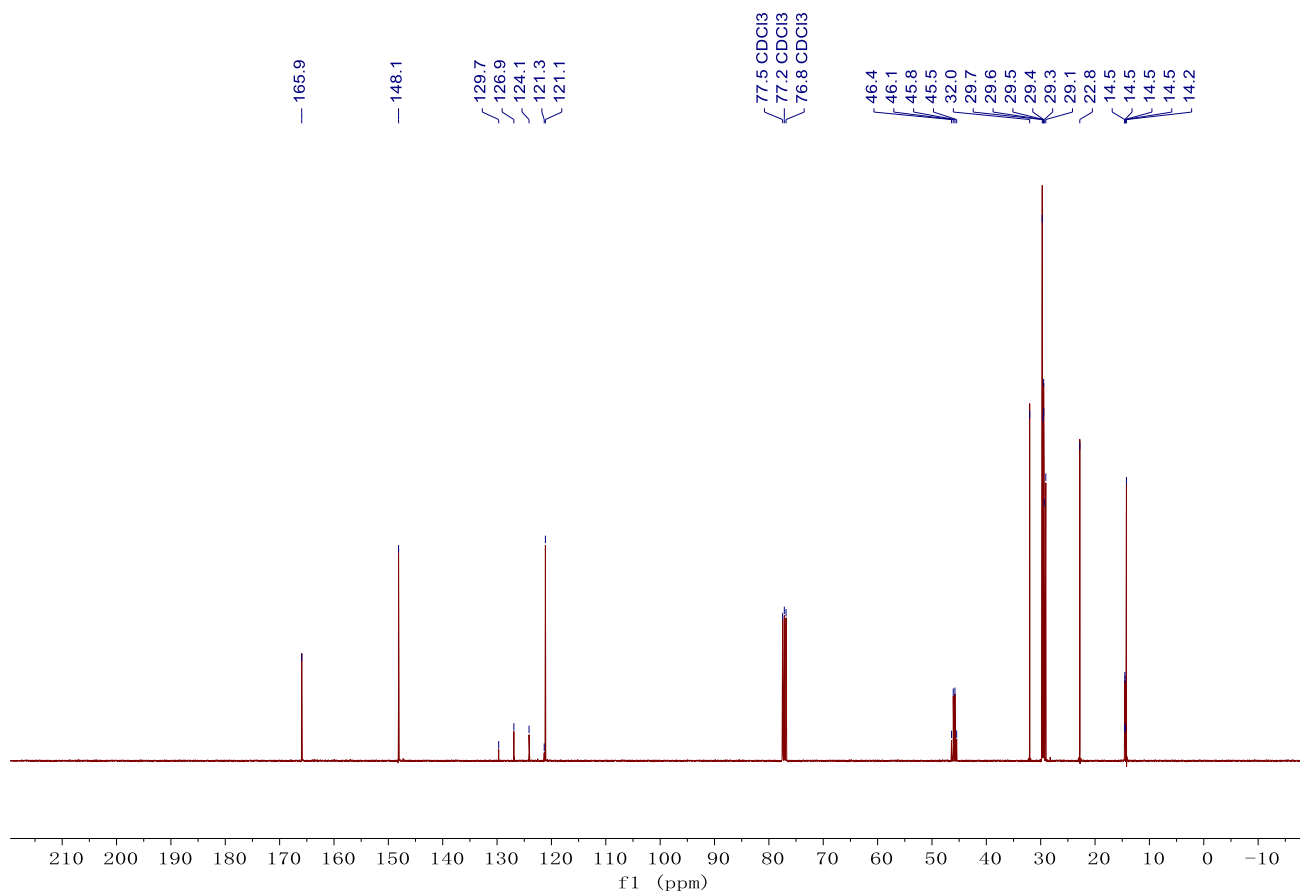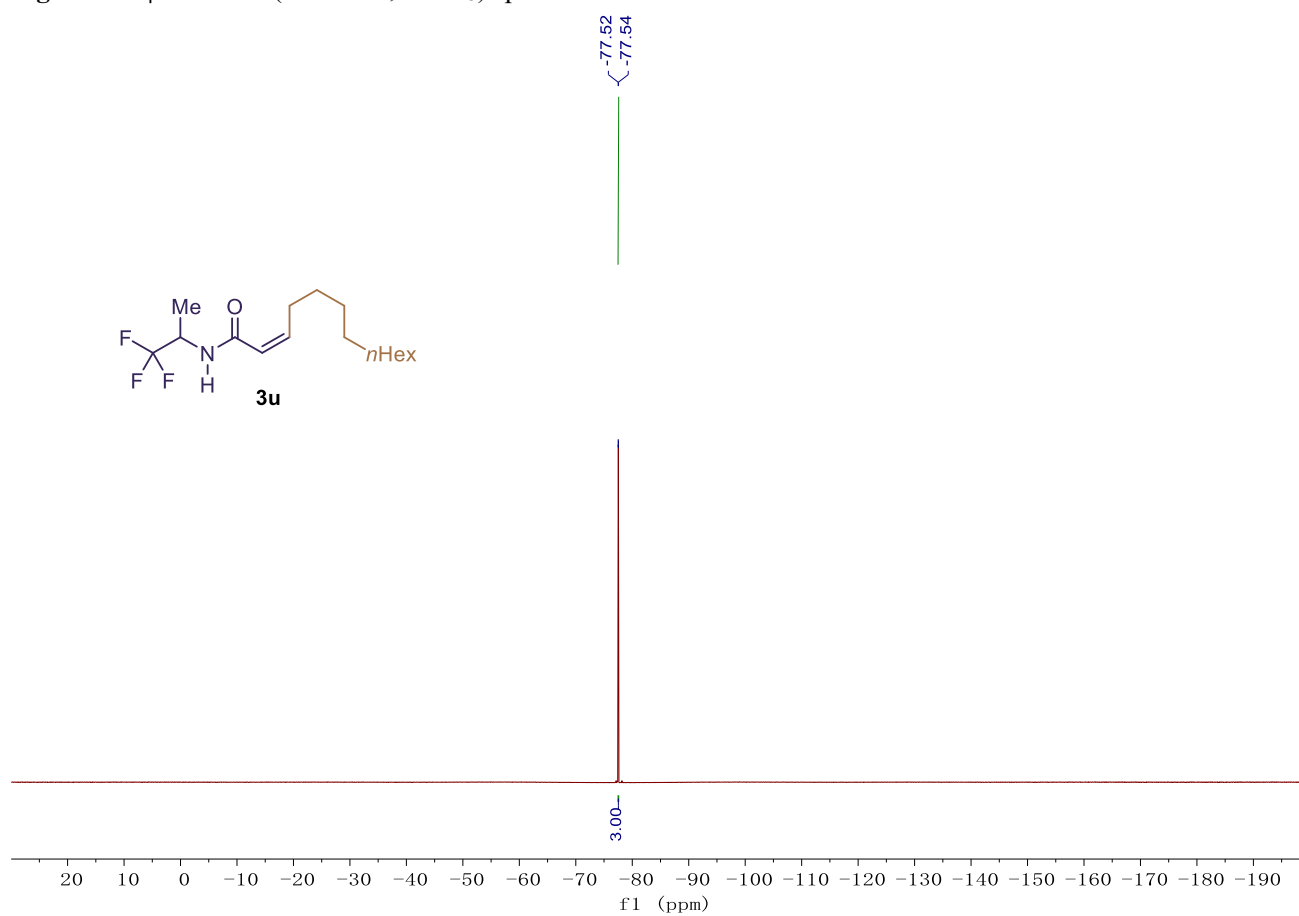**Figure S72 |** ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3o**.
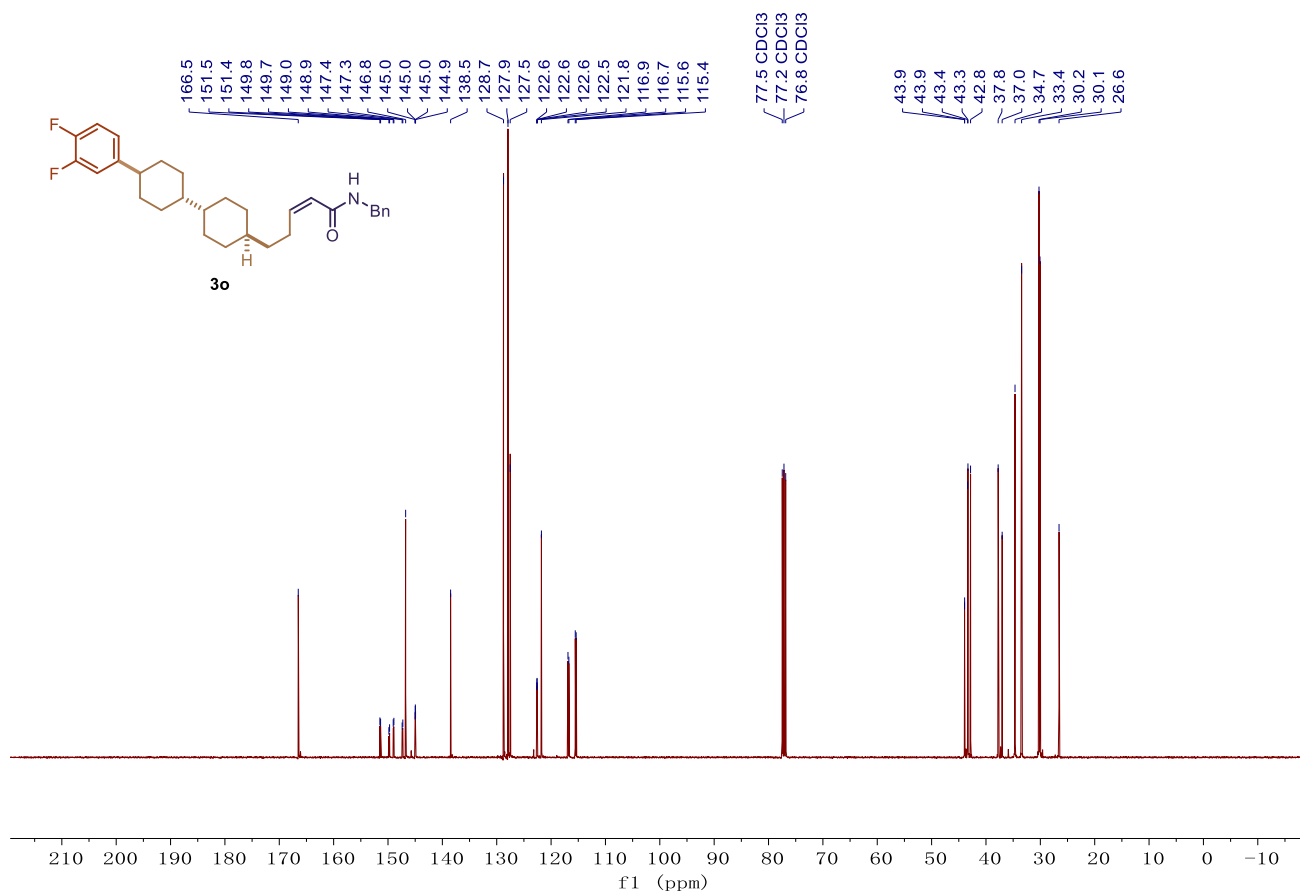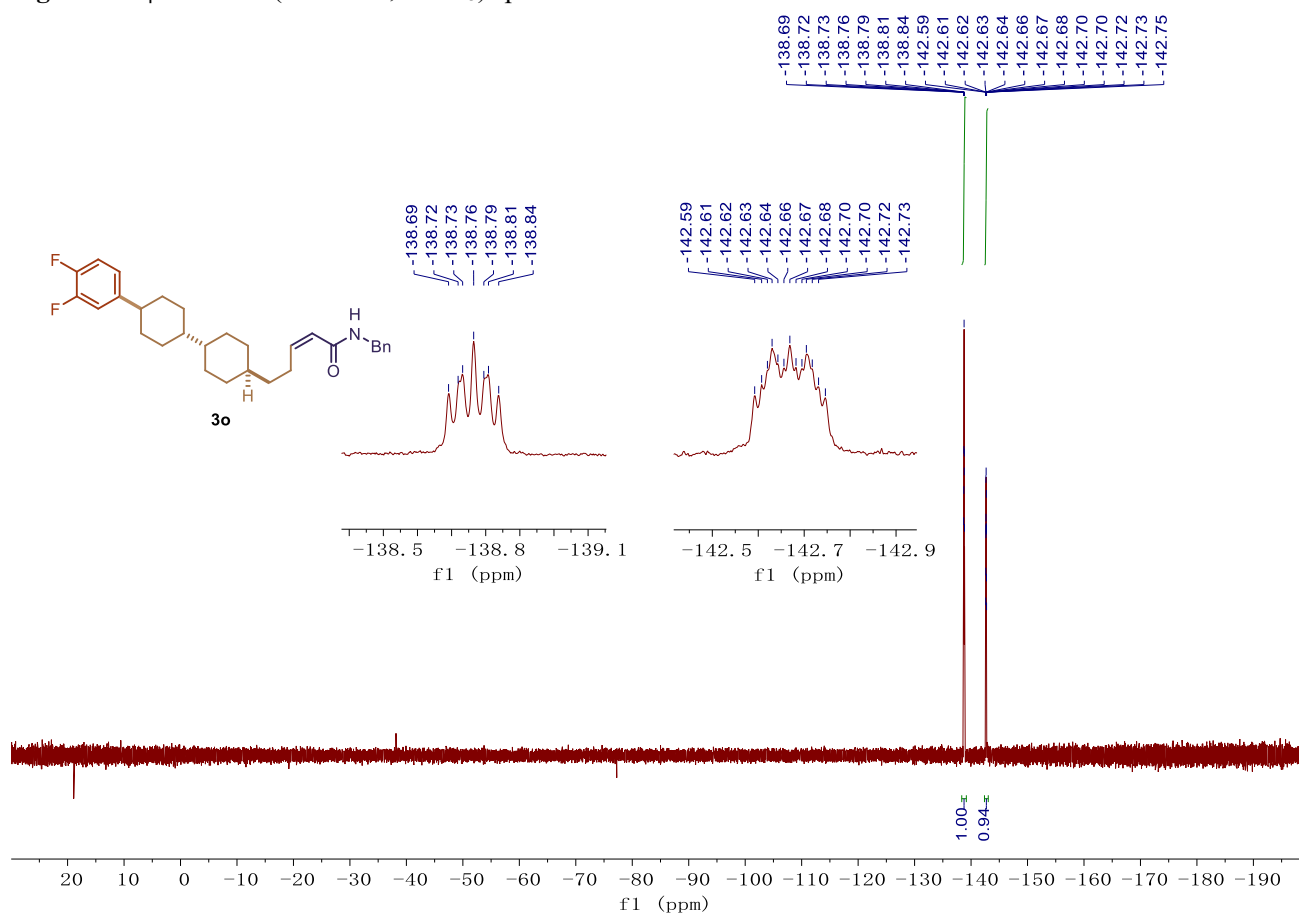
Figure S74 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3p**.

3p

mixture of amide rotamers, ca. 5:1
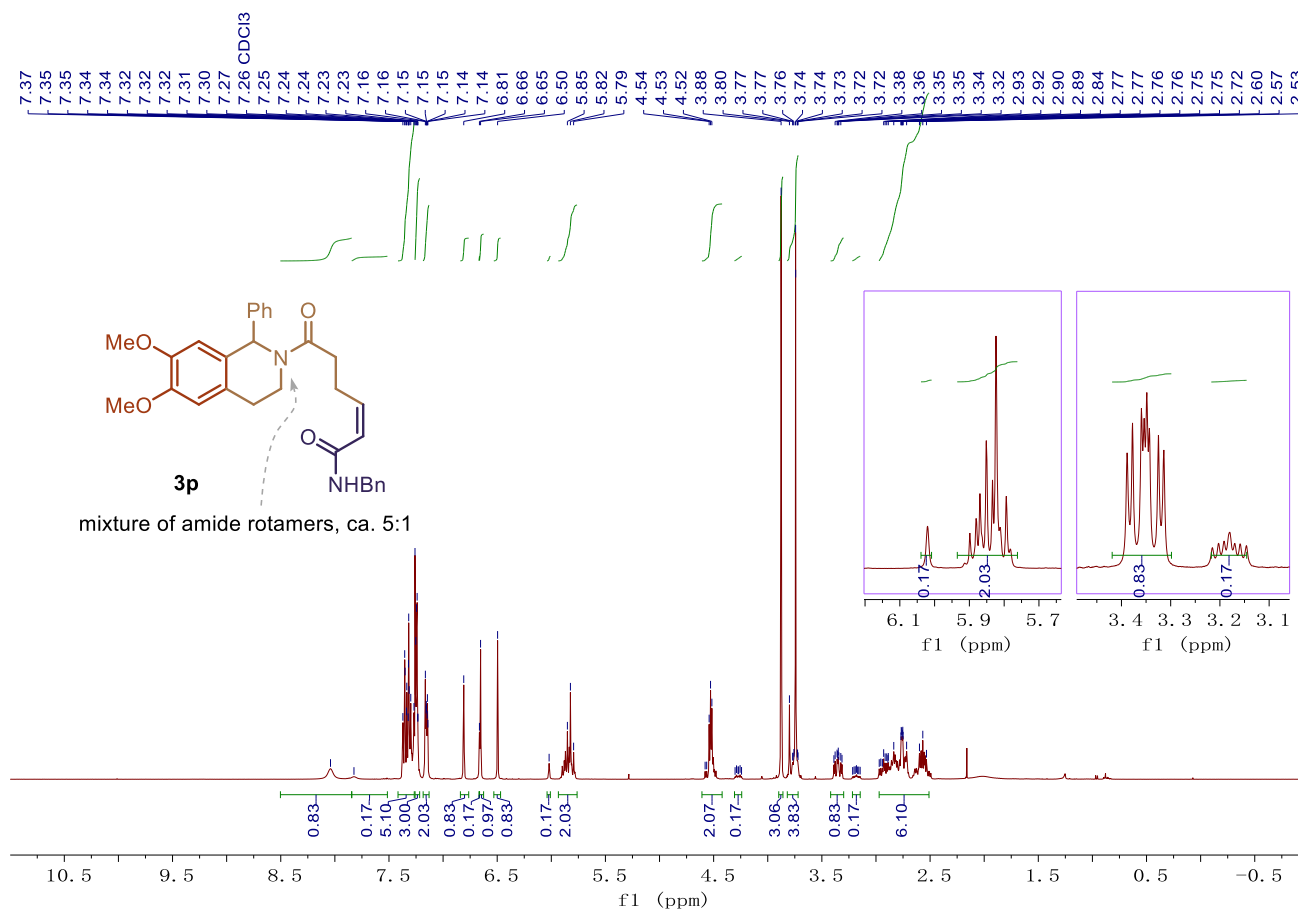
Figure S75 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3p**.

3p

mixture of amide rotamers, ca. 5:1

Figure S76 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3q**.
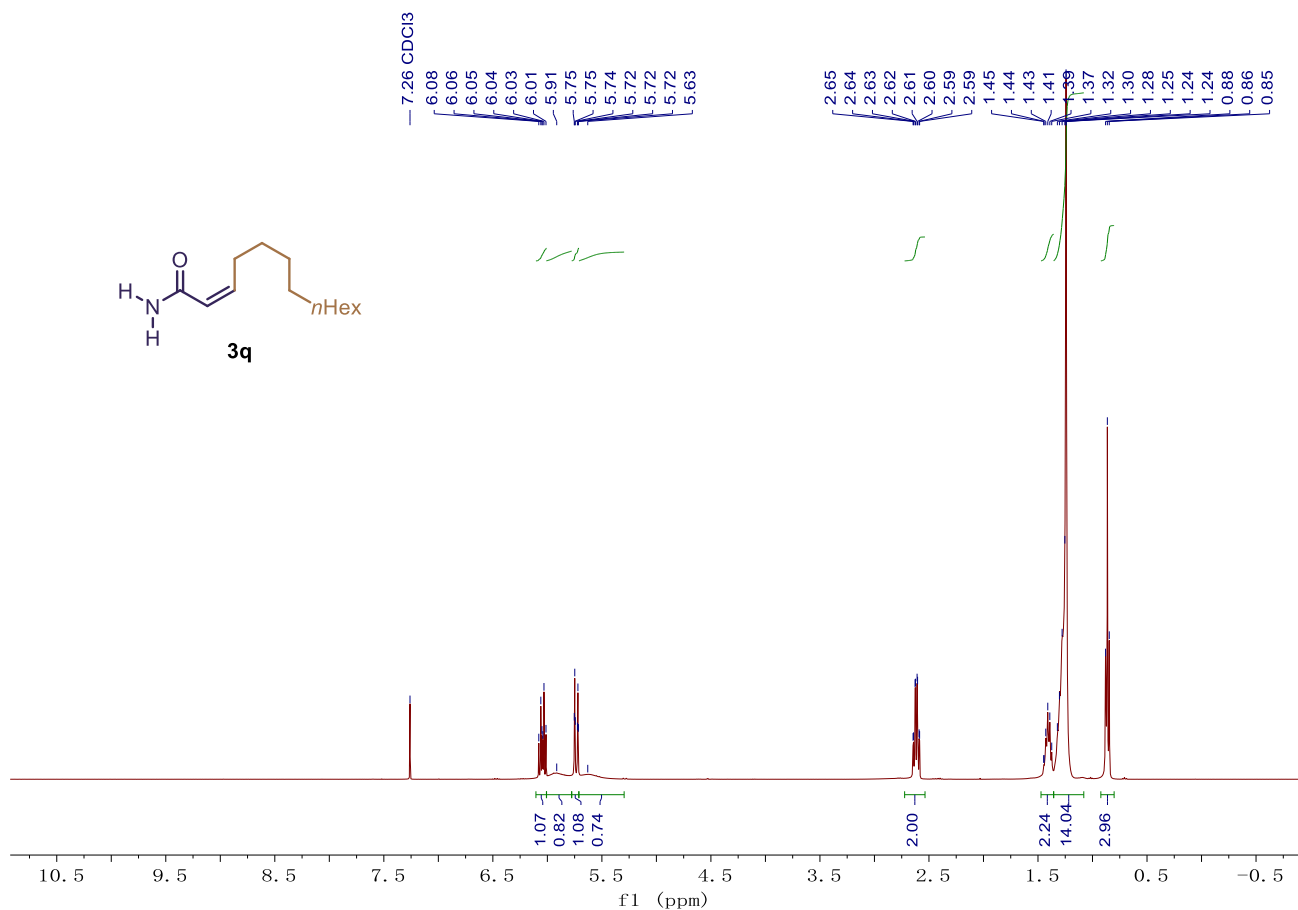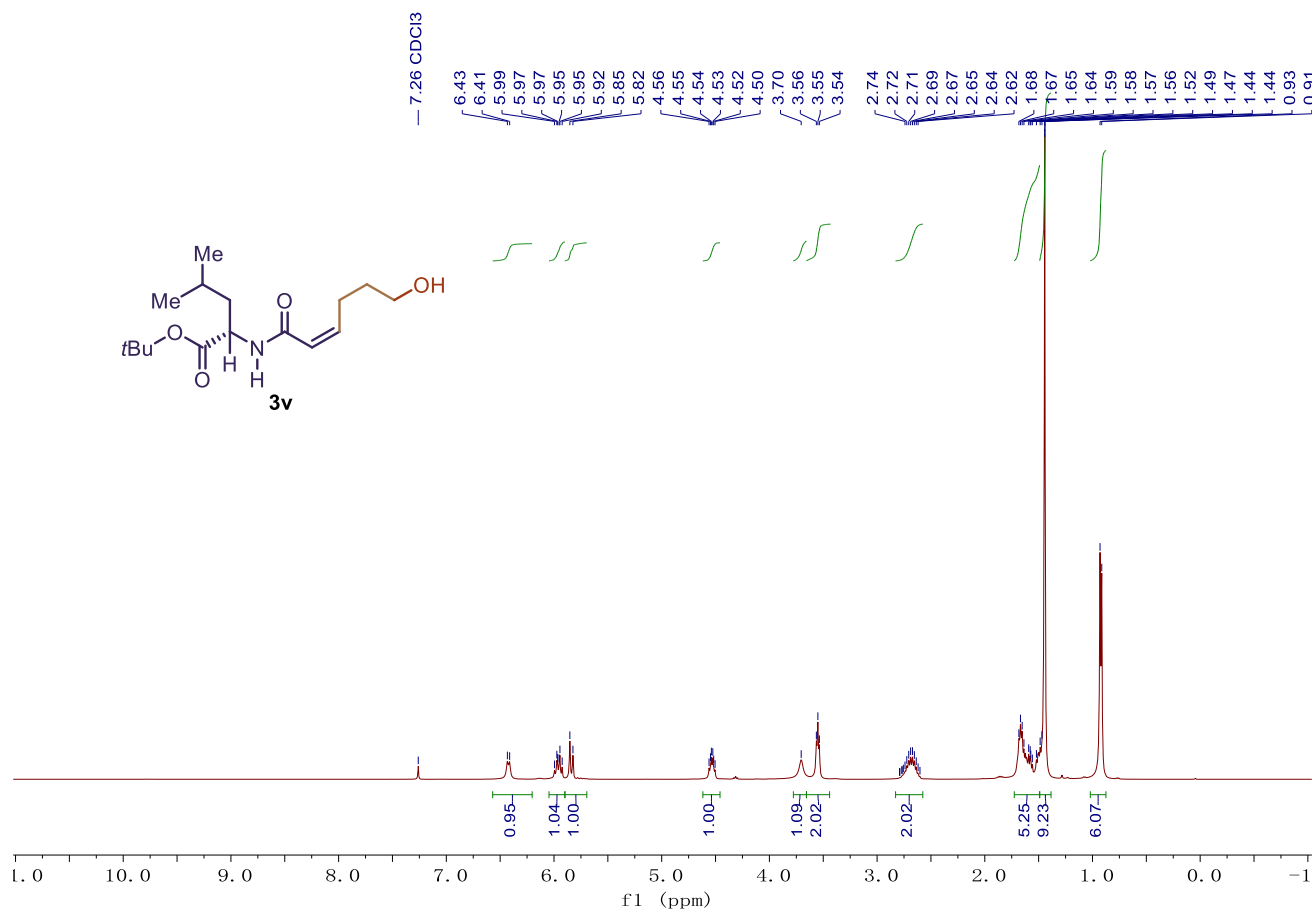

Figure S77 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3q**.

Figure S78 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3r**.

Figure S79 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3r**.

Figure S80 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3s**.

Figure S81 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3s**.

Figure S82 | ¹H NMR (400 MHz, CDCl₃) spectrum of **3t**.

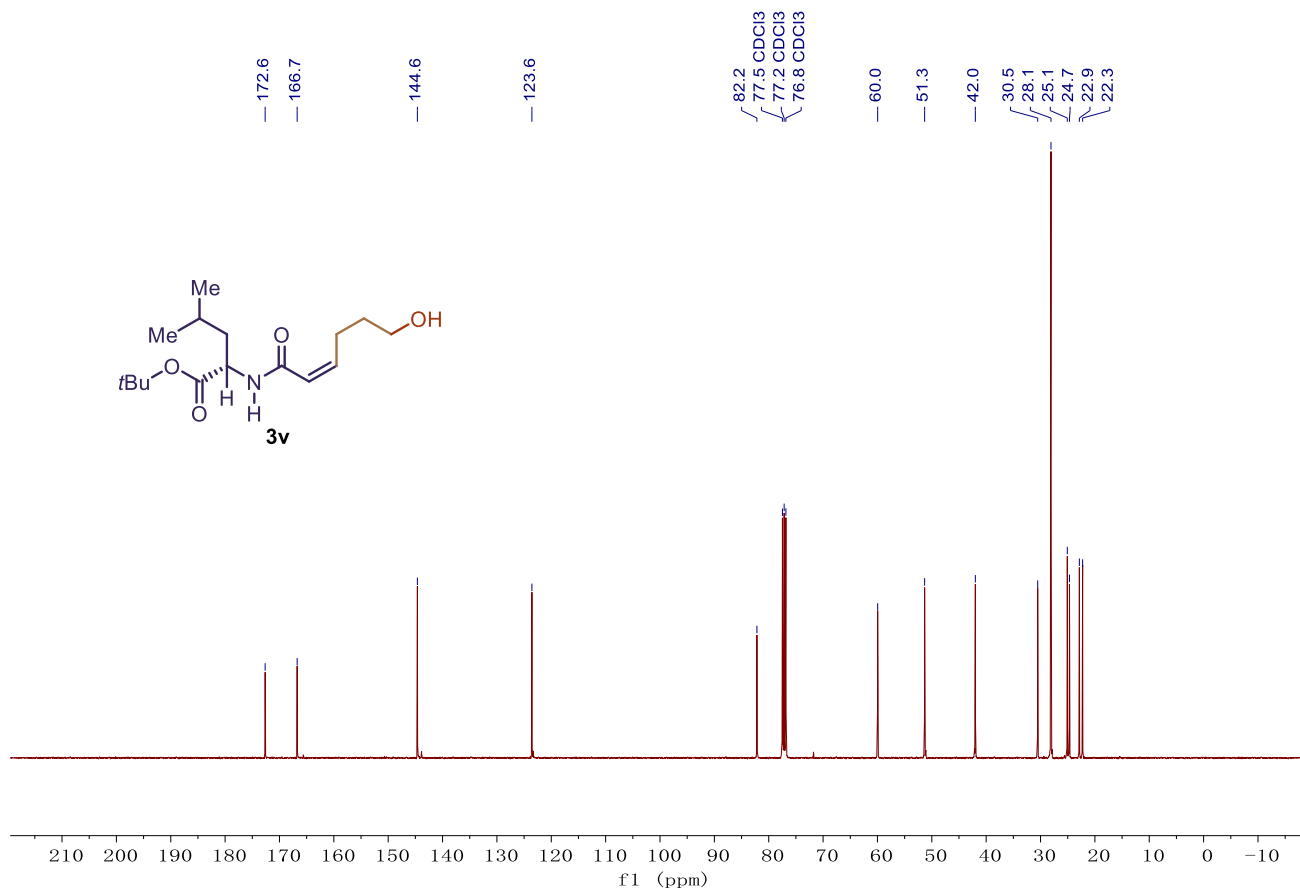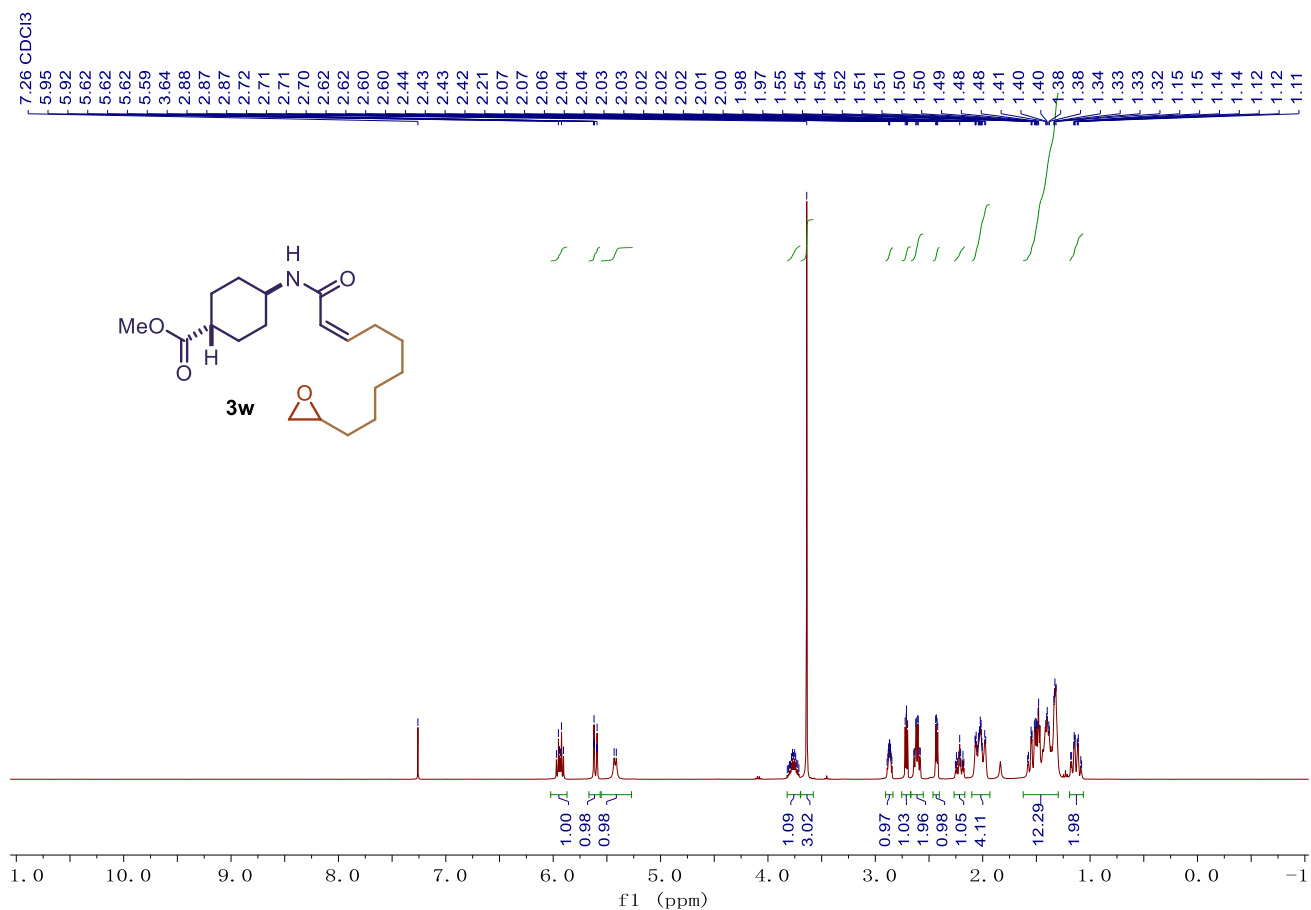**Figure S83 |** ¹³C NMR (101 MHz, CDCl₃) spectrum of **3t**.

Figure S84 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3u**.

Figure S85 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3u**.

Figure S86 | ^{19}F NMR (282 MHz, CDCl$_3$) spectrum of **3u**.

Figure S87 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3v**.

Figure S88 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3v**.

Figure S89 | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3w**.

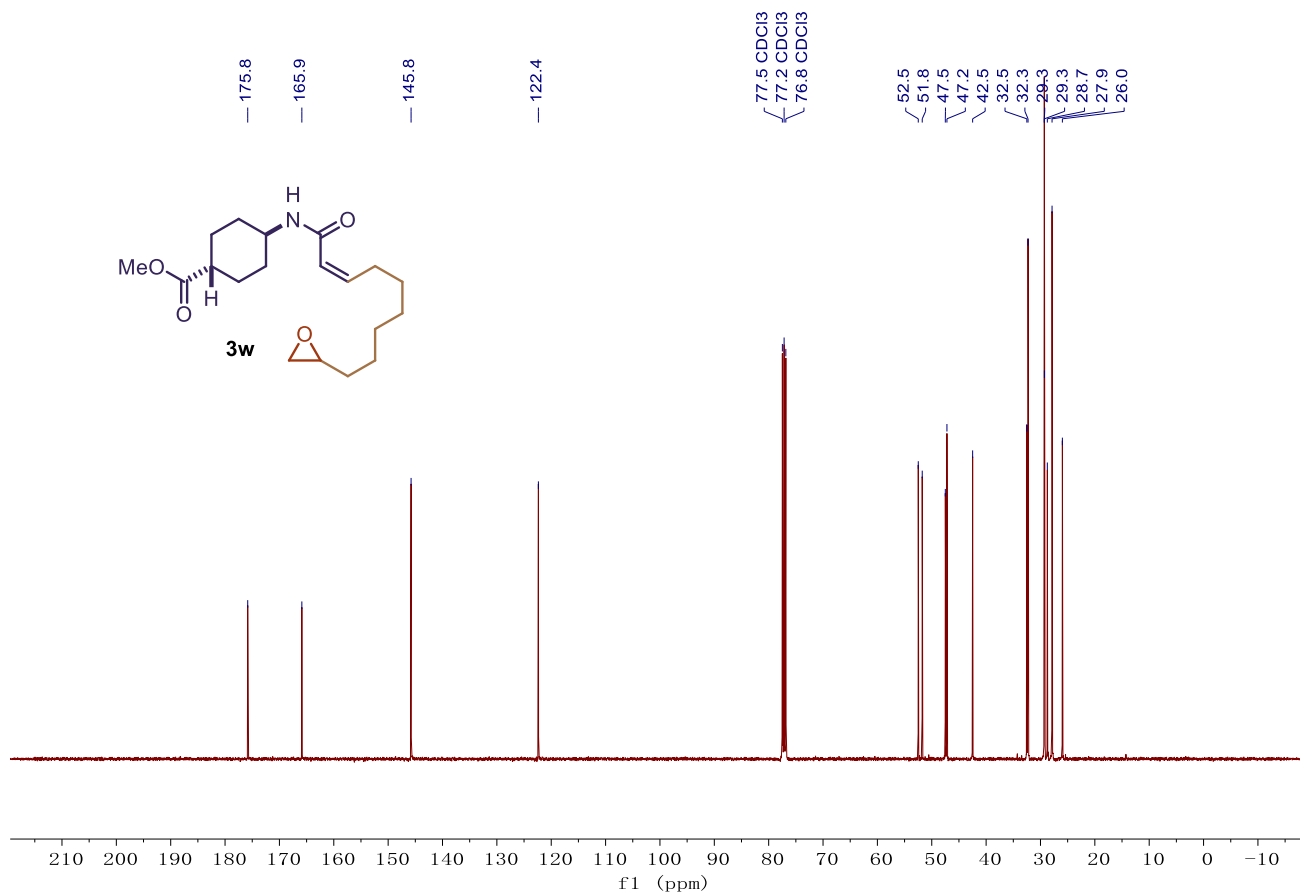**Figure S90 |** ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3w**.

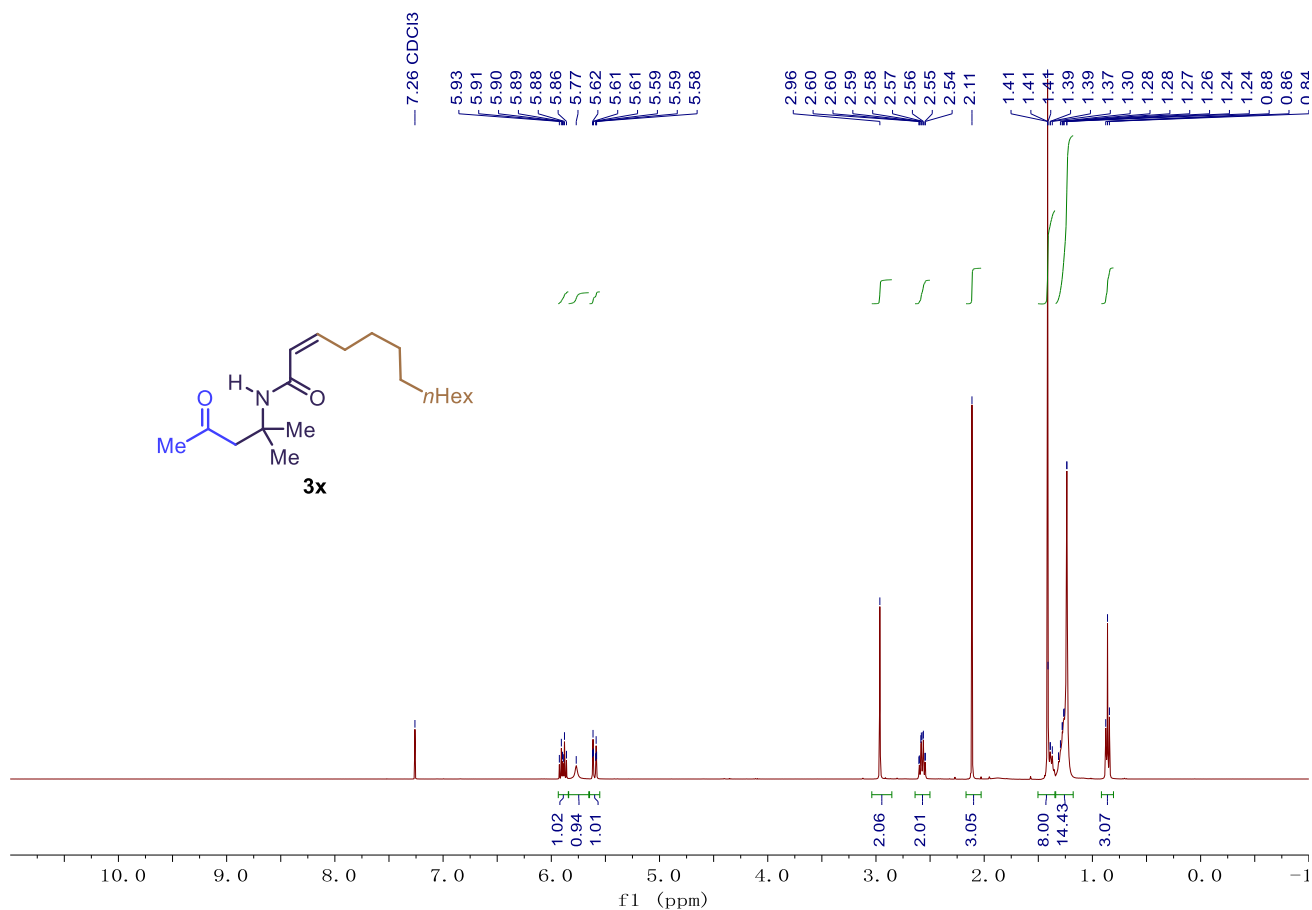**Figure S91** | ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of **3x**.

Figure S92 | ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of **3x**.