Supporting Information

Controlled Cyclopolymerization of 1,5-Hexadiynes to Give Narrow Band Gap Conjugated Polyacetylenes Containing Highly Strained Cyclobutenes

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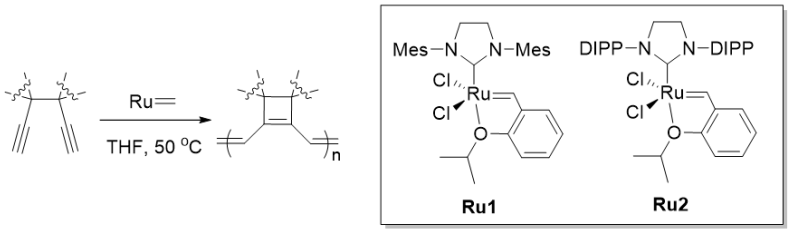
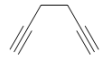
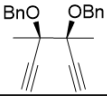
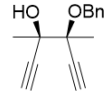
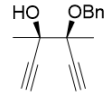
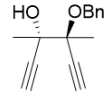
1. Supporting Figures

Table S1. Polymerization of simple 1,5-hexadiyne and tetra-substituted benzyl-containing monomers with different stereochemistry



monomer	cat	M/I	conc	time	conv[a]	yield[b]
	**Ru1**	20	0.5 M	3	10%	-
	**Ru1**	20	0.5 M	24	0%	-
	**Ru2**	30	0.5 M	3	54%	-
	**Ru2**	30	1 M	3	69%	35%
	**Ru2**	30	0.5 M	3	0%	-

[a]Calculated from crude ^{1}H NMR. [b]Isolated yield.

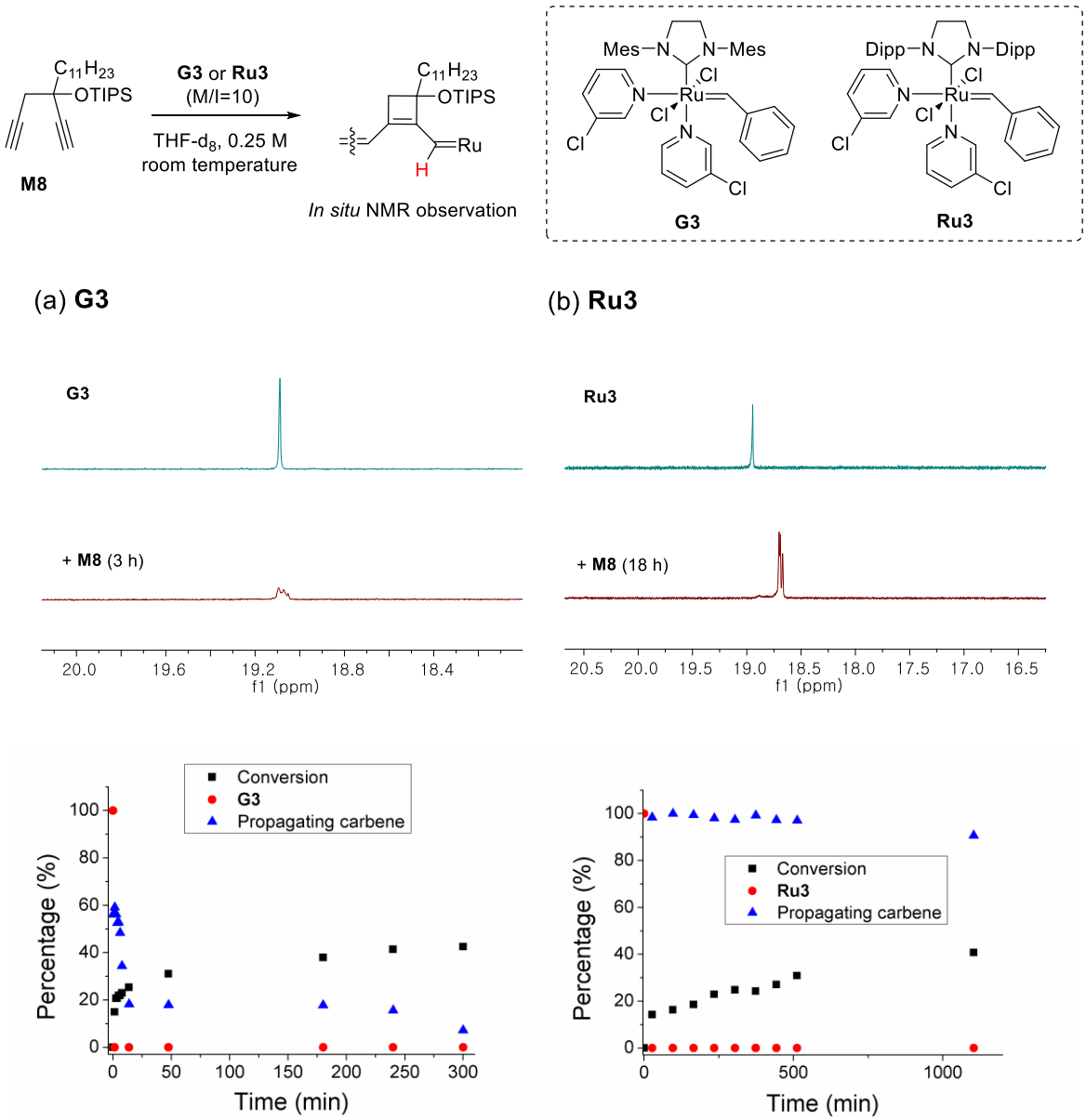
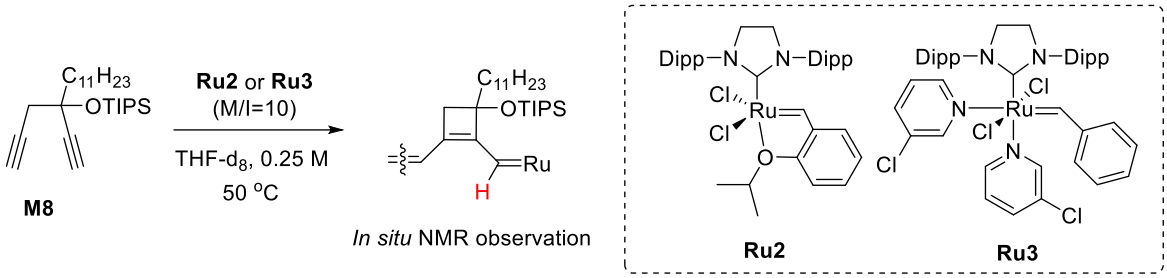
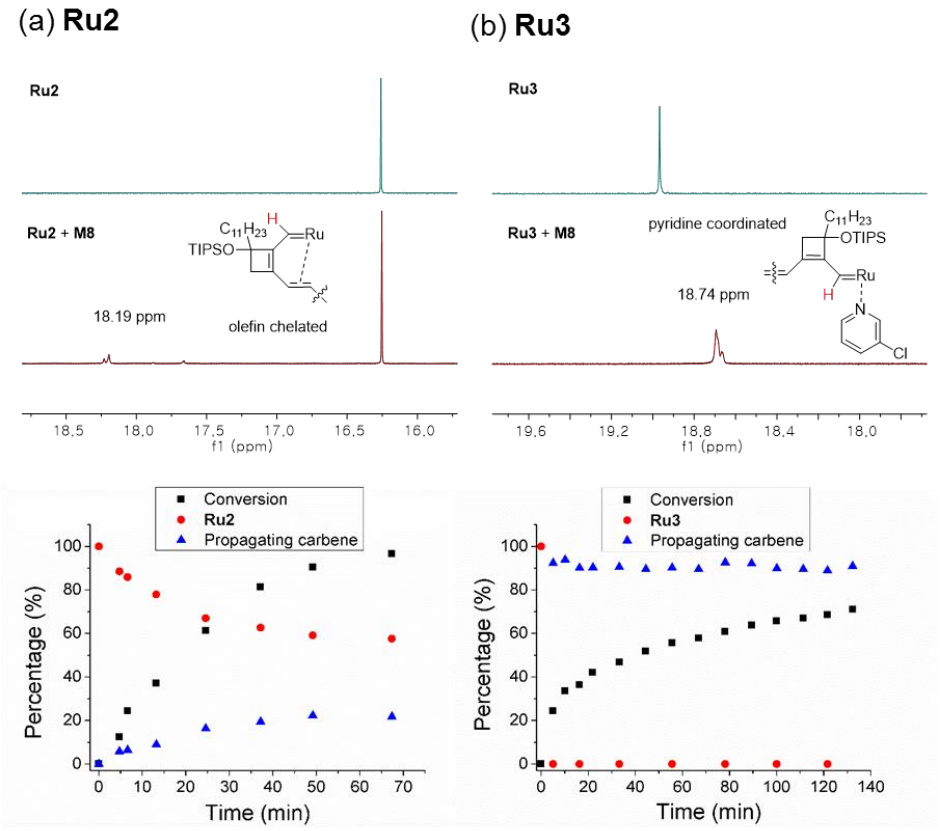


Figure S1. Carbene, conversion, and propagating carbene changes for the polymerization of **M8** (M/I = 10) using (a) **G3** or (b) **Ru3**. The reaction was conducted in THF-d_8 (0.25 M for monomer) at room temperature and monitored by *in situ* ^{1}H NMR analysis. The propagating carbene from **G3** decomposed severely during polymerization, while the propagating carbene from **Ru3** maintained high throughout the reaction.





	k_i (min^{-1} M^{-1})	k_p (min^{-1} M^{-1})	k_i/k_p
(a)	0.056	2.04	0.027
(b)	> 1.18	0.27	> 4.4

Figure S2. Carbene, conversion, and propagating carbene changes for the polymerization of **M8** (M/I = 10) using (a) **Ru2** or (b) **Ru3**. The reaction was conducted in THF-d_8 (0.25 M for monomer) at 50°C and monitored by *in situ* ^{1}H NMR analysis. The propagating carbene from **Ru2** was shown at 18.19 ppm which is putatively assigned as olefin chelated complex, while that from **Ru3** (pyridine bound complex) was shown at more downfield region of 18.74 ppm. All of the k_i and k_p values were calculated based on the equations; -d[I]/dt = k_i[M][I] and -d[M]/dt = k_p[M][I]. The exact k_i from **Ru3** could not be obtained due to too fast initiation.

Detailed Characterization of the Polymer Structures (^{1}H, ^{13}C, HSQC, and HMBC NMR analyses)

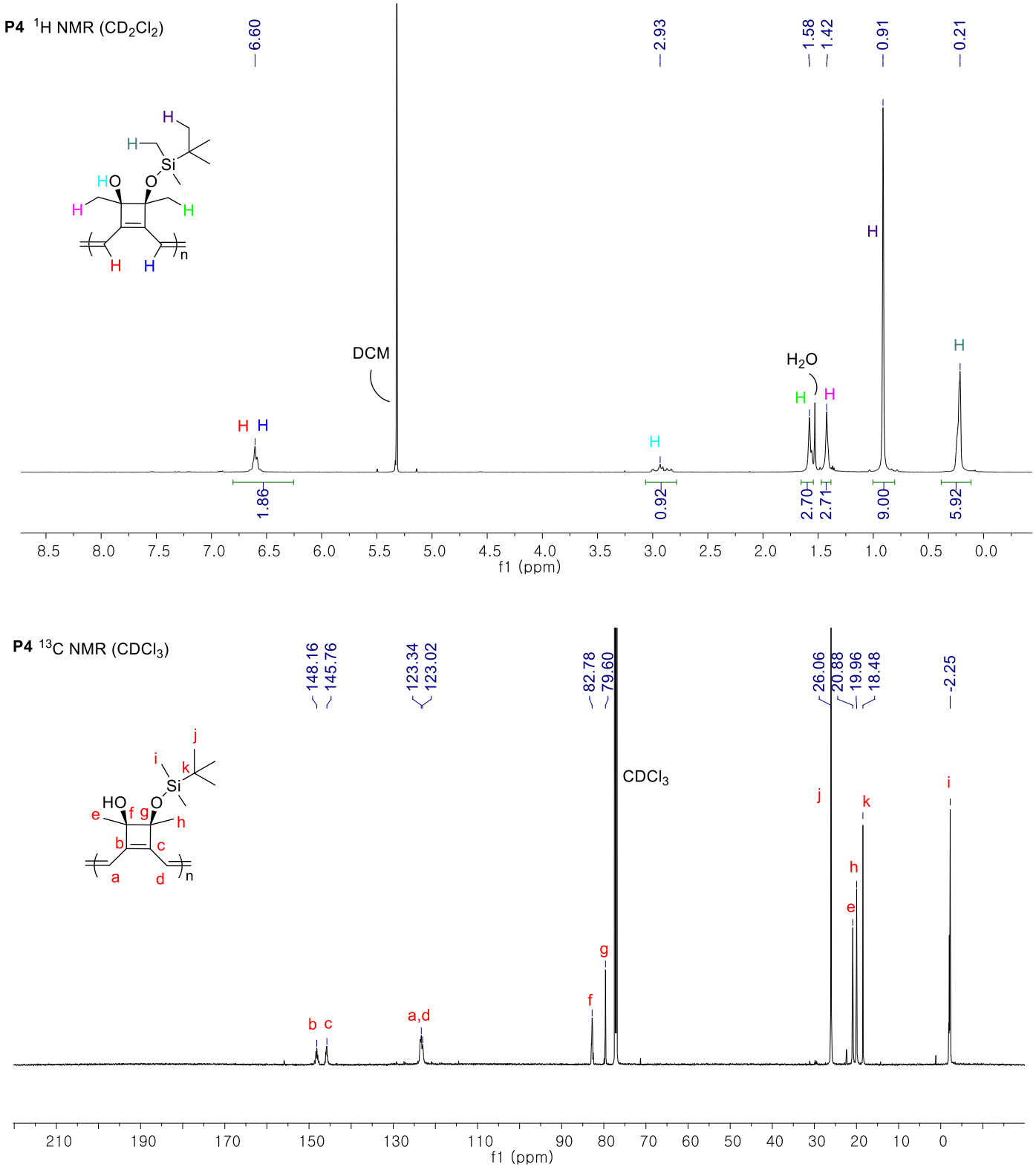


Figure S3. ^{1}H (up) and ^{13}C (down) NMR spectra of **P4**.

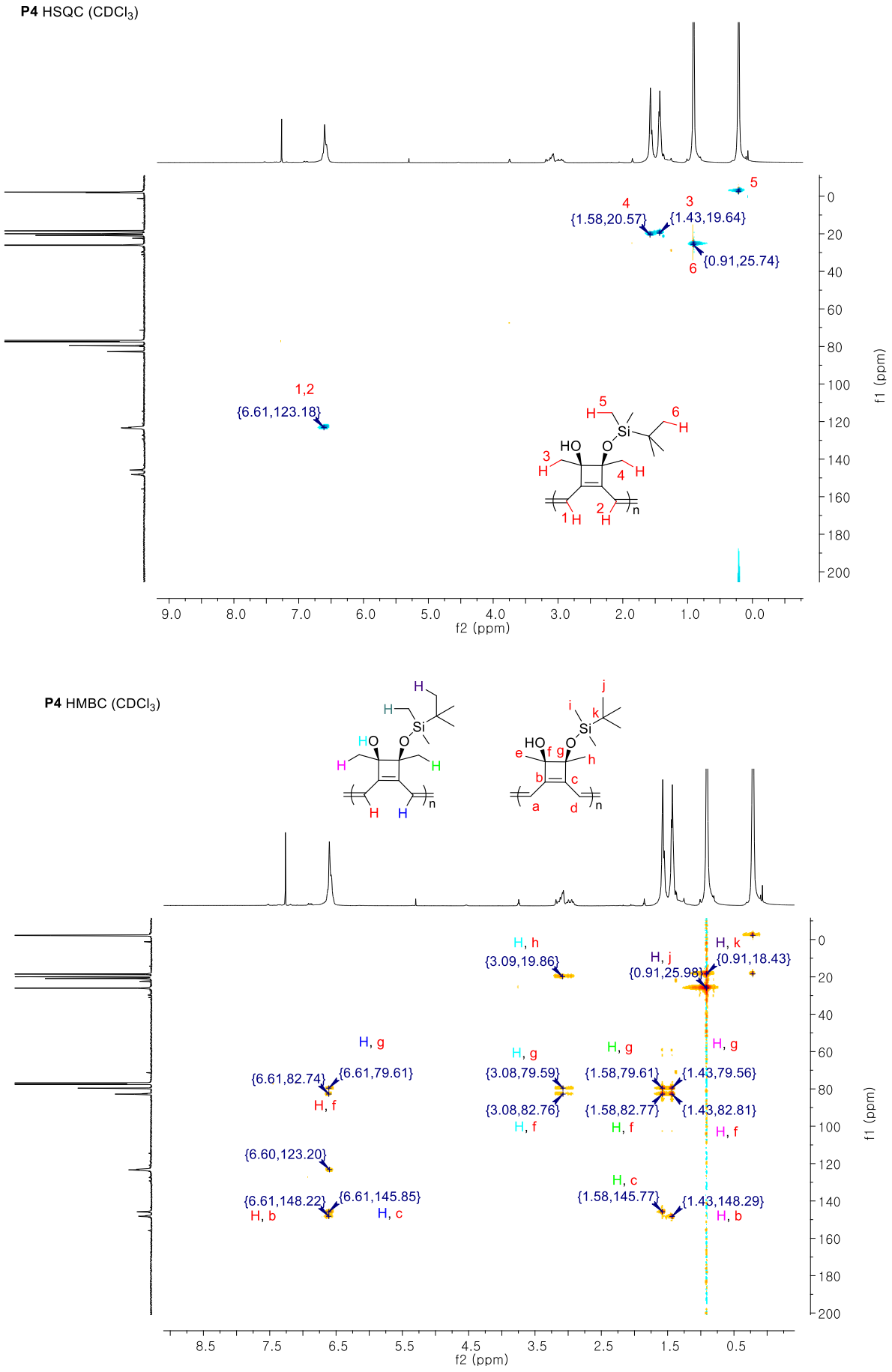


Figure S4. ^{1}H – ^{13}C HSQC (Heteronuclear Single Quantum Coherence) NMR (up) and ^{1}H – ^{13}C HMBC (Heteronuclear Multiple Bond Correlation) NMR (down) spectra of **P4**.

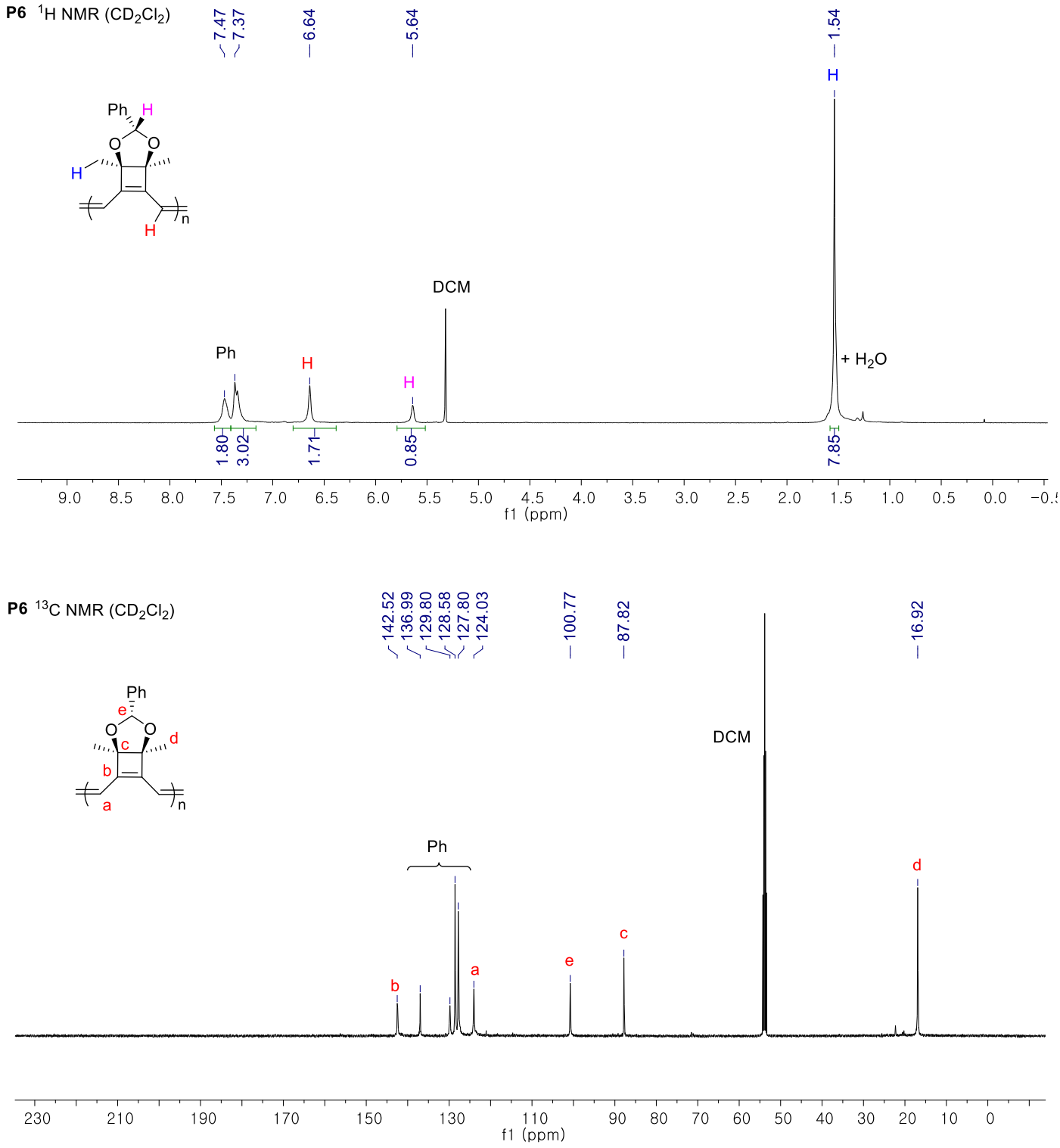


Figure S5. ^{1}H (up) and ^{13}C (down) NMR spectra of **P6**.

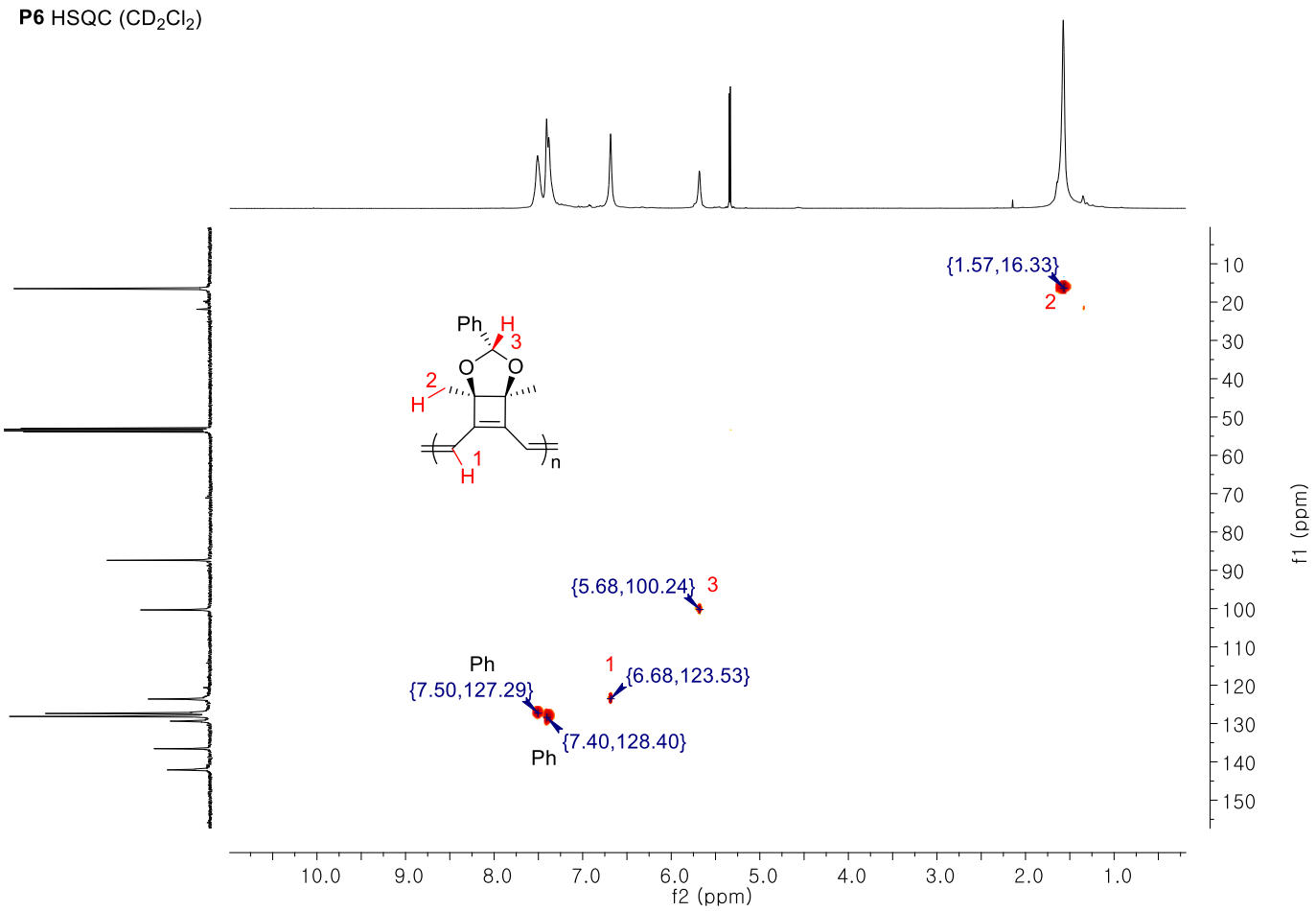


Figure S6. ^{1}H – ^{13}C HSQC NMR spectrum of **P6**.

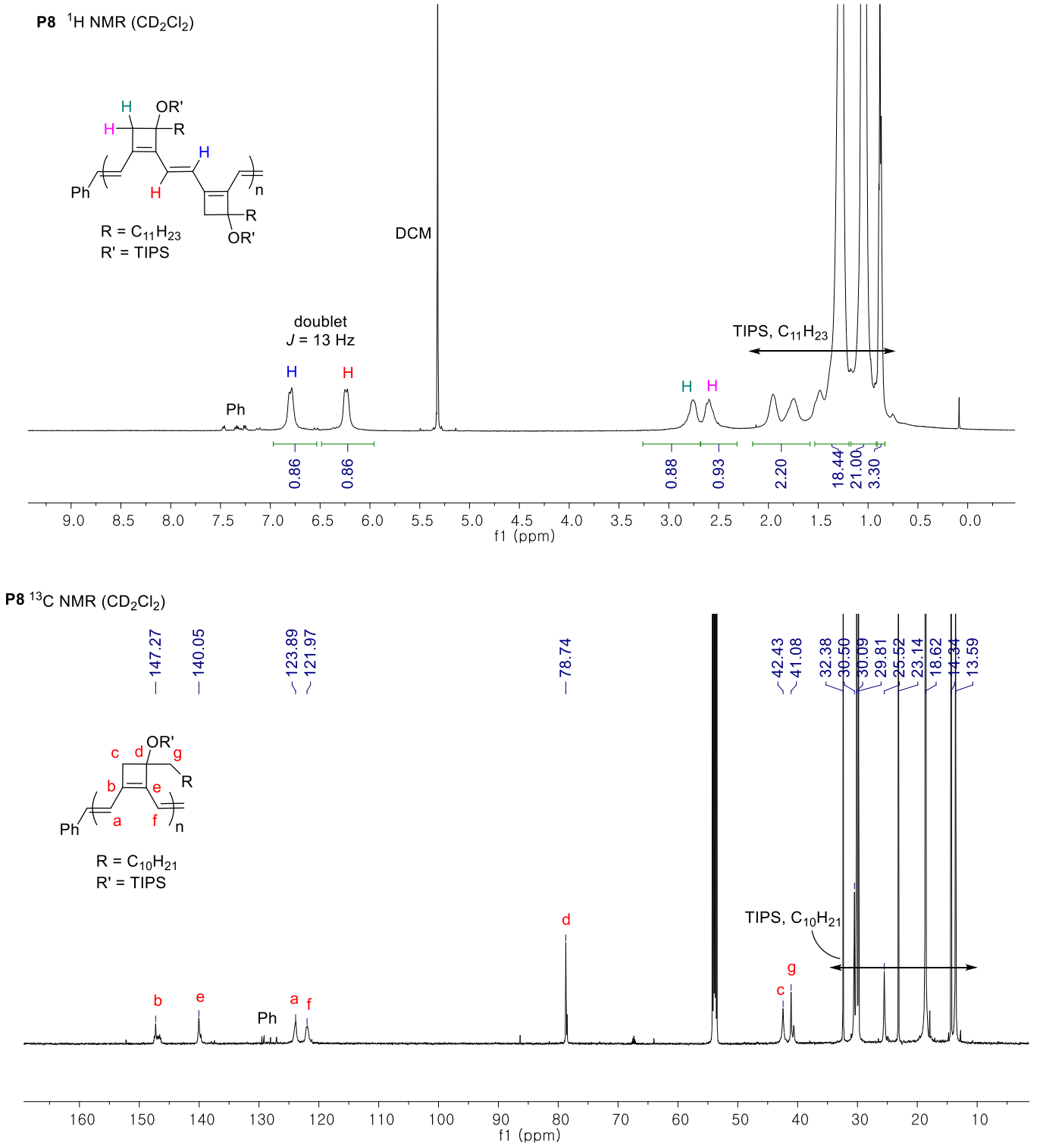


Figure S7. ^{1}H (up) and ^{13}C (down) NMR spectra of **P8**.

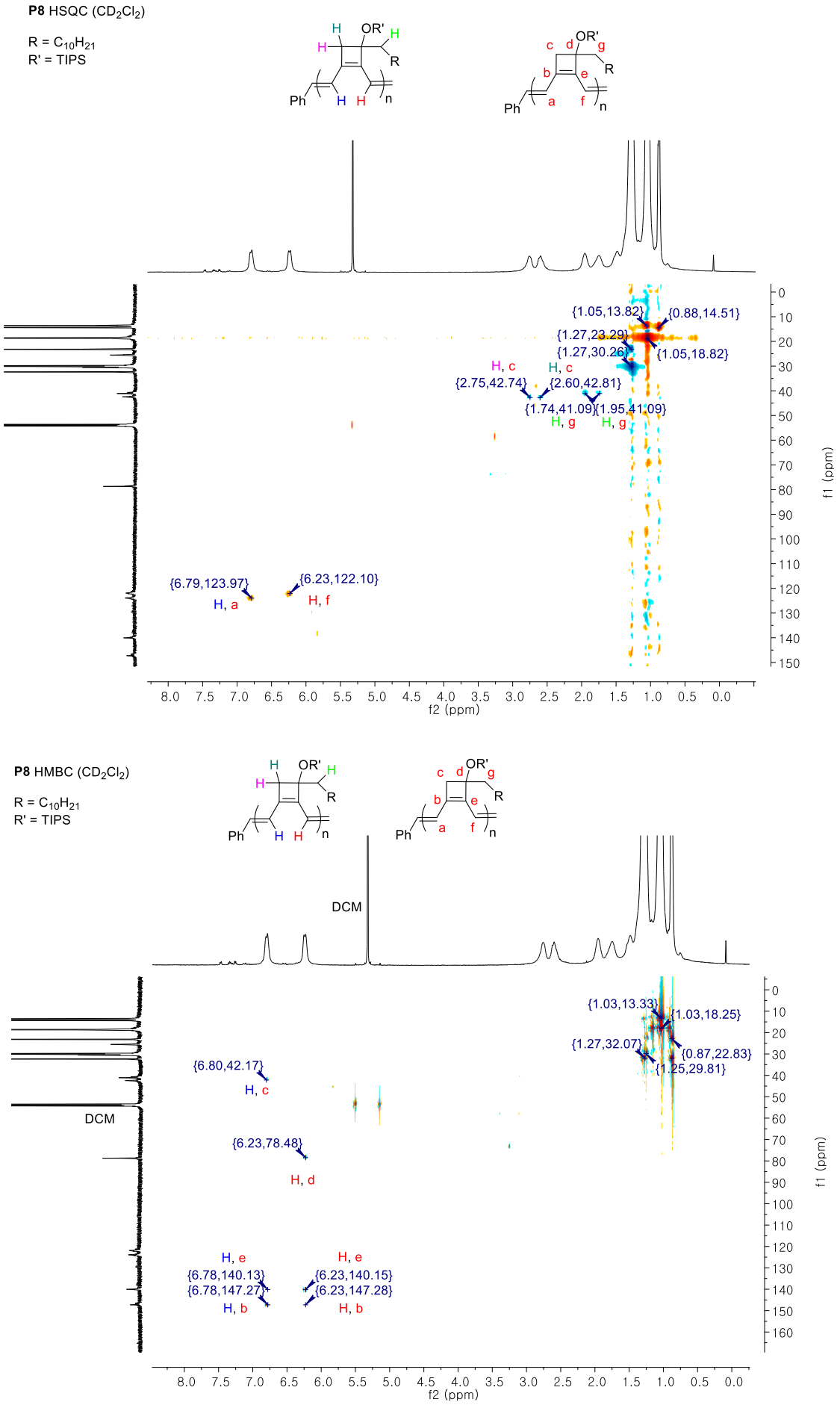


Figure S8. ^{1}H – ^{13}C HSQC NMR (up) and ^{1}H – ^{13}C HMBC NMR (down) spectra of **P8**.

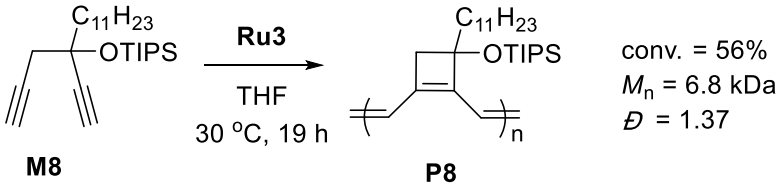


Figure S9. Polymerization of **M8** using **Ru3** at 30 °C. The conversion was as low as 56% even after 19 h, giving an M_n of 6.8 kDa and a relatively broad dispersity of 1.37.

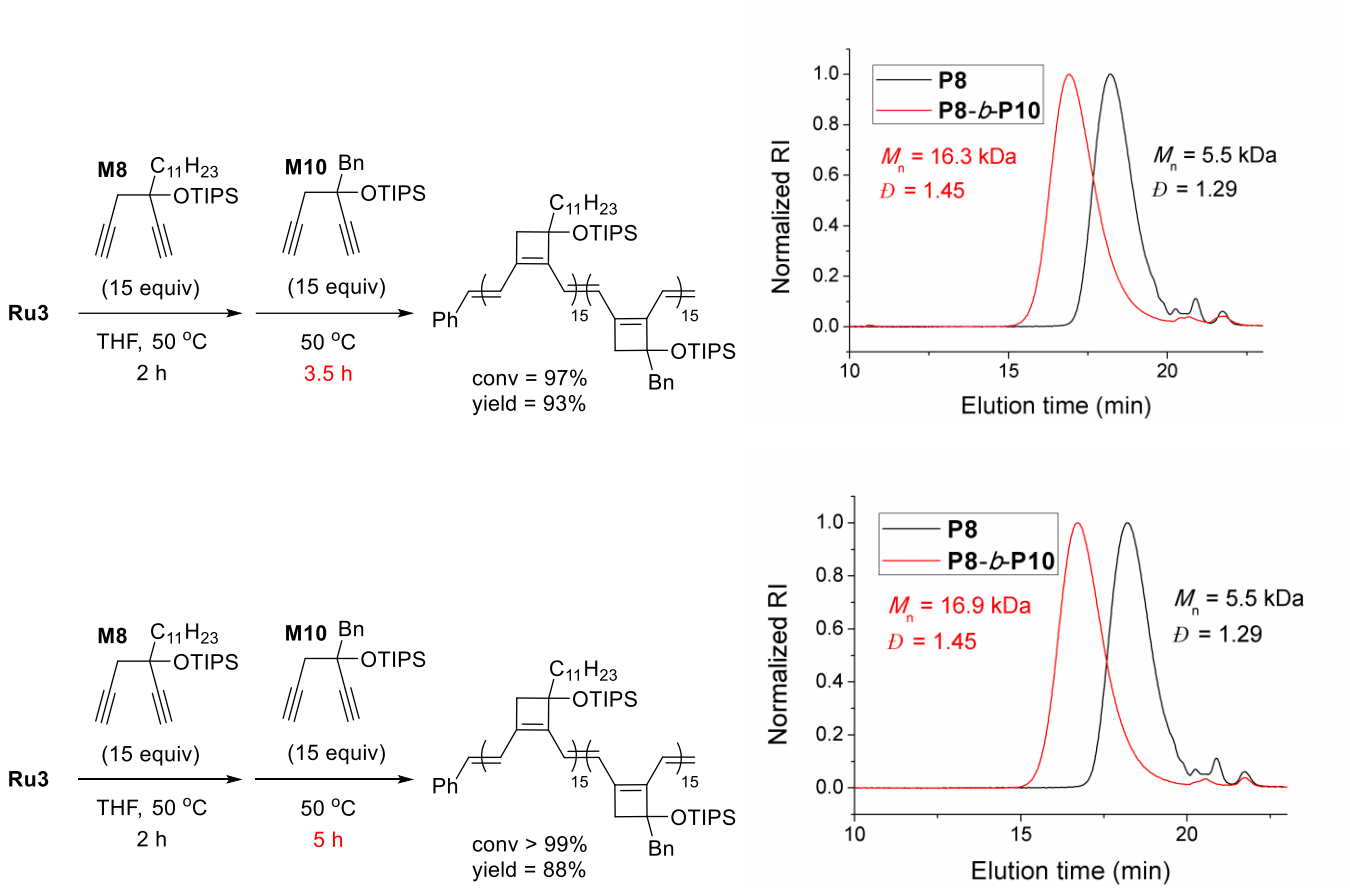


Figure S10. Block copolymerization by sequential addition of **M8** and **M10**. The longer reaction time for the second block propagation (3.5 vs 5 h) did not broaden the dispersity of the resulting polymer, implying that the chain transfer reaction did not occur under the reaction condition.

Table S2. Optical and Physical Properties of **P3** – **P10**

	Solution		Film		E_{HOMO} (eV)	T_d (°C)
	λ_{abs} (nm)	E_g^{opt} (eV)	λ_{abs} (nm)	E_g^{opt} (eV)		
P3	552, 595	1.96	544	1.94	-5.12	177
P4	550, 592	1.97	538	1.92	-5.17	175
P6	556, 600	1.95	551	1.90	-5.23	284
P7	582	1.81	569	1.77	-5.26	328
P8	597, 646	1.80	602, 652	1.74	-5.34	348
P9	603, 652	1.77	598	1.75	-5.15	334
P10	605, 656	1.77	603, 655	1.75	-5.20	340

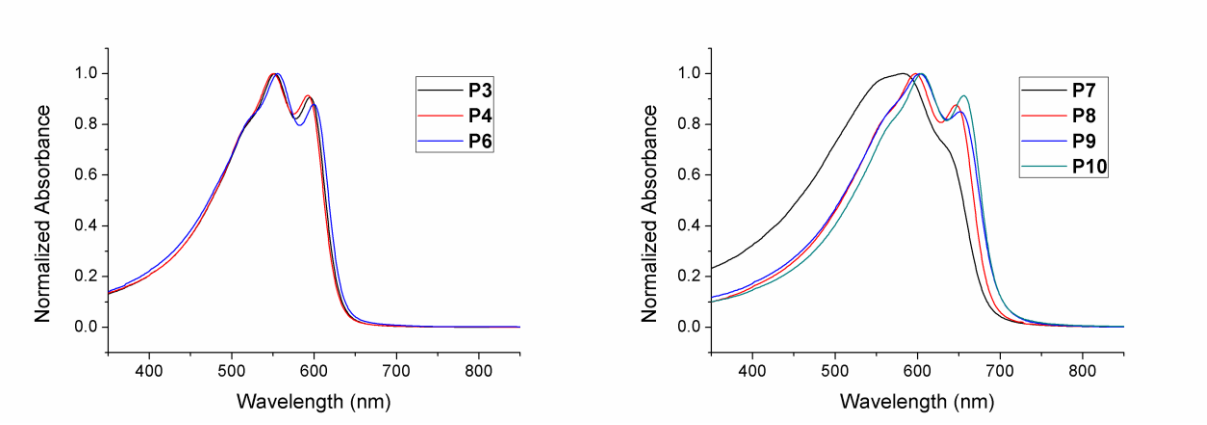


Figure S11. UV-Vis spectra of **P3** – **P10** in THF solution (ca. 0.01 g/L).

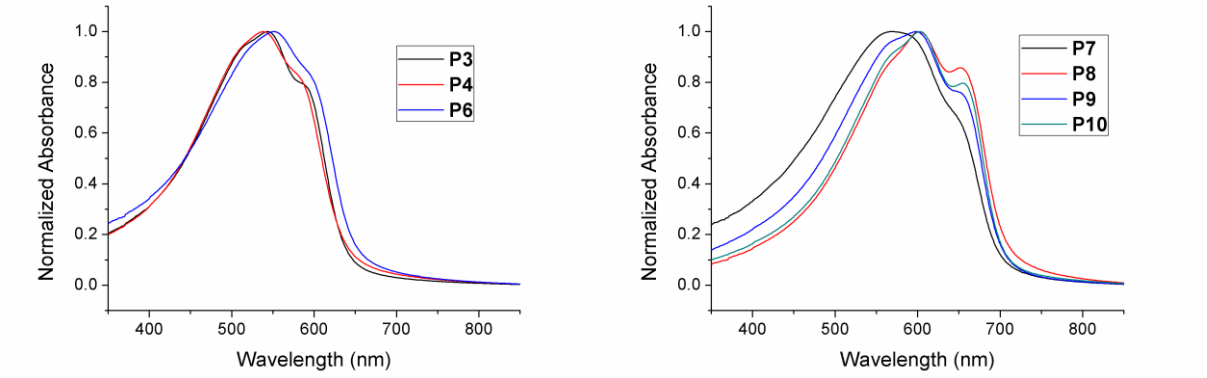


Figure S12. UV-Vis spectra of **P3** – **P10** in film state.

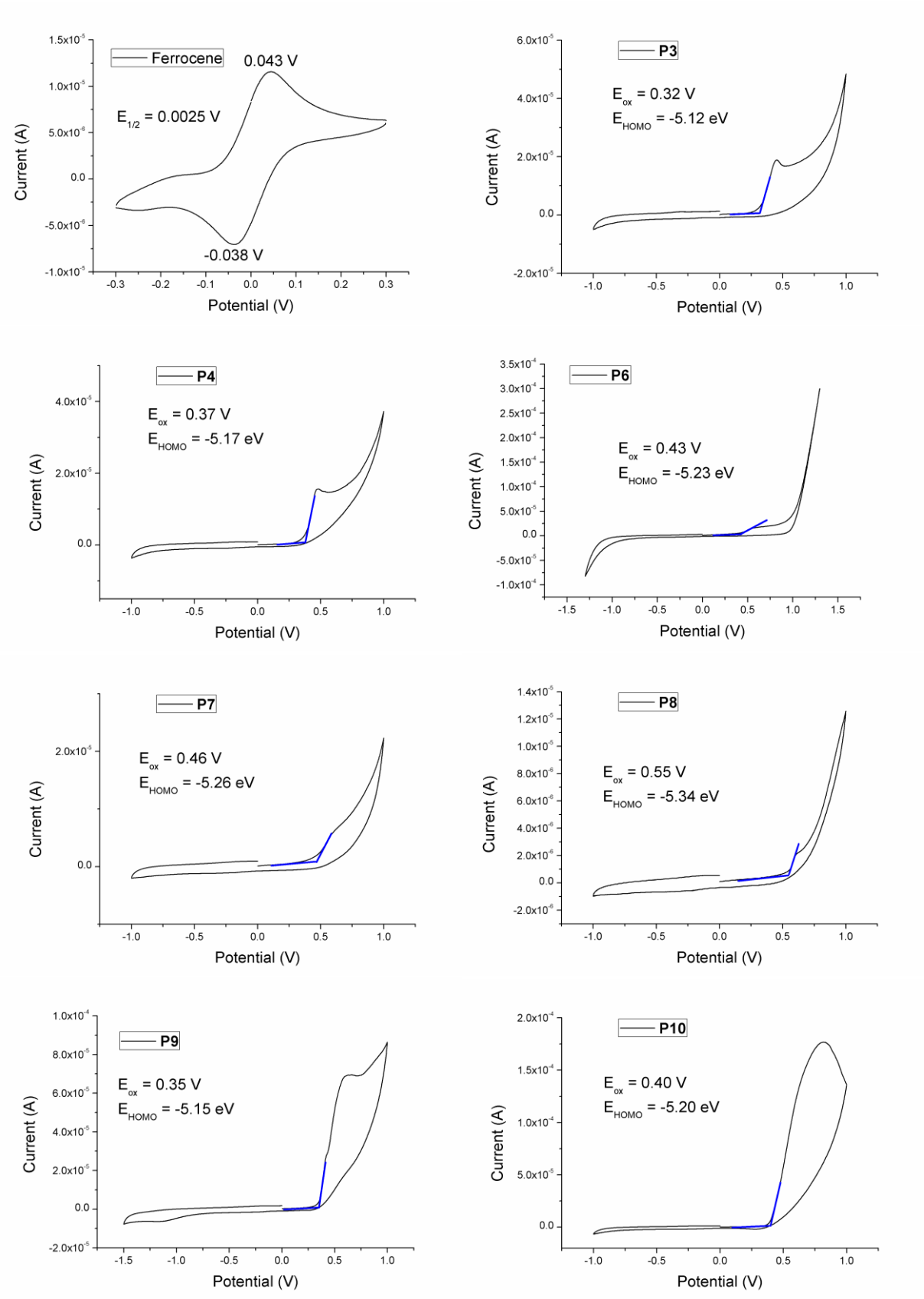


Figure S13. Cyclic voltammograms of ferrocene (measured in DMSO) and **P3** – **P10**. Polymer samples were prepared as film deposited on a working electrode, using a reference electrode of Ag/Ag^+ (0.1 M $AgNO_3$ in acetonitrile) with a platinum wire counter electrode. All the polymers were measured using NBu_4PF_6 electrolyte in DMSO solution (0.1 M). The absolute energy level was obtained using ferrocene/ferrocenium as an internal standard. The oxidation potential of ferrocene was regarded as -4.8 eV.

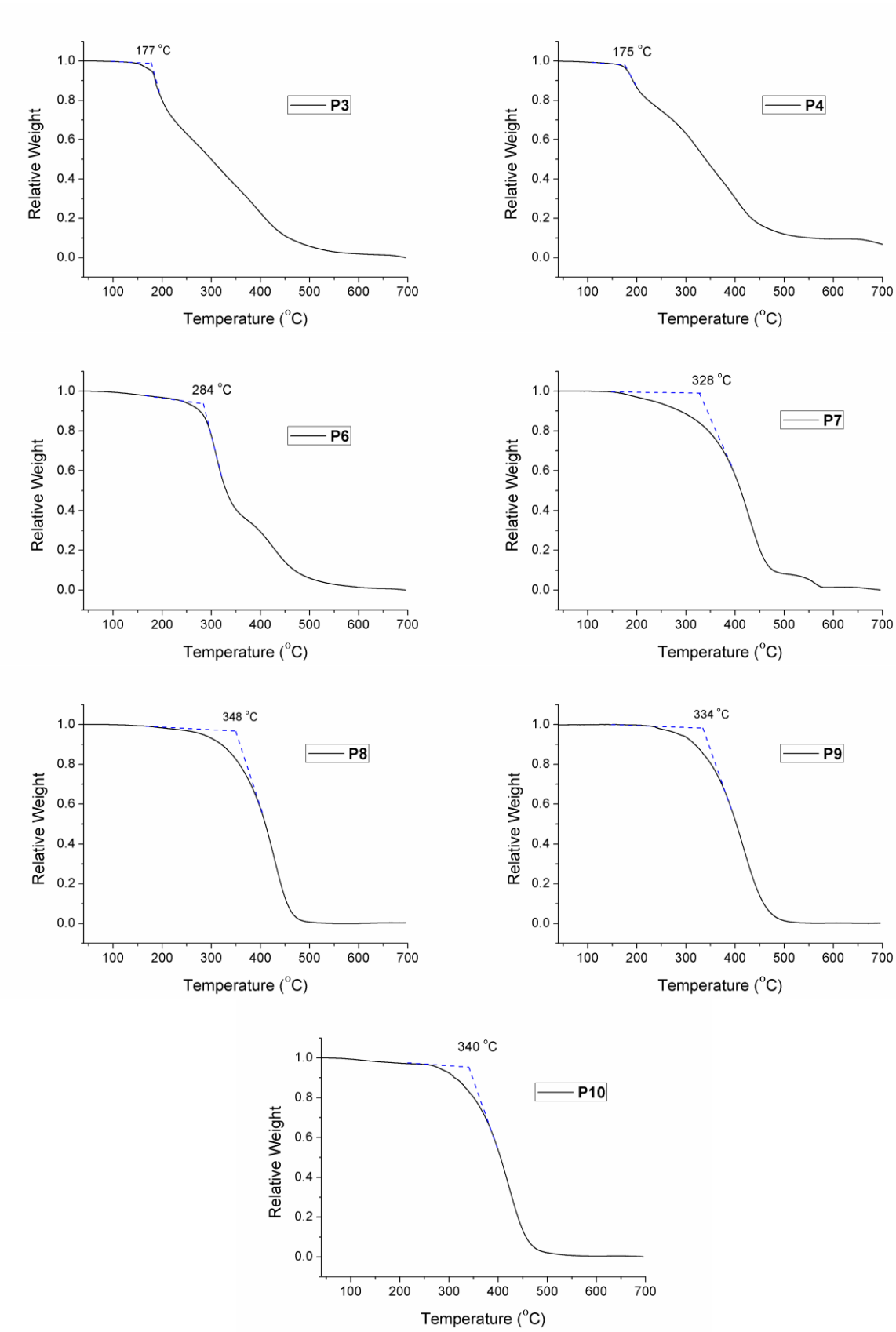


Figure S14. TGA curves of **P3 – P10**. The samples were equilibrated at 30 ºC, then heated at 10 ºC/min to 700 ºC. The onset points were reported as the thermal decomposition temperatures (T_d).

2. General Experimental

Characterization

^{1}H NMR and ^{13}C NMR were recorded by Varian/Oxford As-500 (500 MHz for ^{1}H, 125 MHz for ^{13}C), Agilent 400-MR (400 MHz for ^{1}H and 100 MHz for ^{13}C), and Bruker AVANCE 600 (600 MHz for ^{1}H and 150 MHz for ^{13}C). *In situ* NMR experiments at 50 °C were conducted by using Bruker AVANCE III 500 (500 MHz for ^{1}H). Size exclusion chromatography (SEC) analyses were carried out with Waters system (1515 pump and 2707 autosampler) and Shodex GPC LF-804 column eluted with THF (HPLC grade, TEDIA) and filtered through a 0.2 μm PTFE filter (Whatman®) before injection. The flow rate was 1.0 mL/min and temperature of the column was maintained at 35 °C. Wyatt OptiLab T-rEx refractive index detector was used for molecular weight measurement. High-resolution mass spectroscopy (HRMS) analyses were performed by ultra high resolution ESI Q-TOF mass spectrometer (Bruker) and FAB mass spectrometer JMS-700(JEOL). Elemental analysis was carried out by Flash2000 (Thermo Fisher Scientific). UV/Vis spectra were obtained by UV-vis Spectrometer V-650 (Jasco Inc.). Cyclic voltammetry (CV) measurements were carried out by CHI 660 Electrochemical Analyzer (CH Instruments, Insc.) Thermogravimetric analysis (TGA) was carried out under N_2 gas at a scan rate of 10 °C/min with Q50 model device (TA Instruments).

Materials

All reagents which are commercially available from Sigma-Aldrich®, Tokyo Chemical Industry Co. Ltd., Acros Organics, Alfa Aesar®, and Umicore (**Ru2**) were used without further purification. **Ru3** was prepared from dichloro[1,3-bis(2,6-isopropylphenyl)-2-imidazolidinylidene](benzylidene)(tricyclohexylphosphine)ruthenium(II) purchased from BOC Sciences, by following the modified procedure from the literature method (details below).[1] Tetrahydrofuran for the polymerization were purified by distillation and degassed further by Ar bubbling for 10 minutes before performing reactions. THF-d_8 (99.50% D, 0.75mL) was purchased from Deutero GmbH and used without further purification.

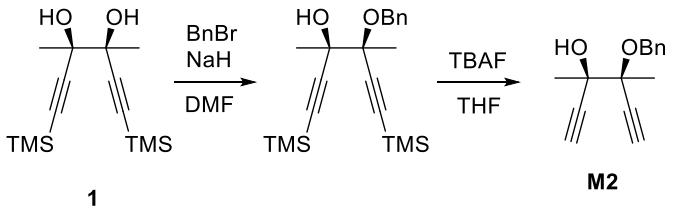
Computational Method

All the theoretical calculations were performed with the Gaussian 09 program.[2] The geometries of the singlet ground states of model oligomer structures were optimized by the density functional theory (DFT) method with B3LYP hybrid function. The 6-31G(d) basis sets were employed for all atoms. Vibrational frequencies were calculated with the optimized geometries at the same level of theory optimizations. All the structures were confirmed by observing no or only one imaginary frequency.

3. Experimental procedures for the preparation of monomers and Ru3

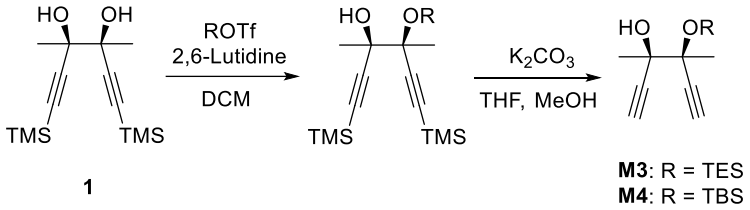
Compounds **M1**,[3] **1**,[3] **2**,[4] and **3**[5] were prepared by literature methods. Schlenk line techniques were used for all the synthesis using Ar gas for the inert condition.

Synthesis of M2



Compound **1** (139 mg, 1.01 mmol) was dissolved in DMF (3 ml), and NaH (60% dispersion in mineral oil, 44 mg, 1.1 mmol) was slowly added to the solution at 0 °C. Then, benzyl bromide (0.13 ml, 1.1 mmol) was added and the reaction mixture was stirred at room temperature for 2.5 h. After quenching with a saturated NH_4Cl aqueous solution, the organic layer was washed with brine and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. Purification with flash column chromatography afforded a mixture of the desired product and its TMS-deprotected derivatives. This mixture was dissolved in THF (3 ml), then tetrabutylammonium fluoride solution (1.0 M in THF, 0.77 ml, 0.77 mmol) was added. After stirring for 40 min, the reaction mixture was quenched with NH_4Cl aqueous solution. The organic layer was washed with water and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. The product was purified by flash column chromatography on silica gel to afford **M2** as white powder (46 mg, 0.20 mmol, 20% via two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.27 (m, 5H), 4.89 (d, J = 11.3 Hz, 1H), 4.66 (d, J = 11.3 Hz, 1H), 2.85 (s, 1H), 2.65 (s, 1H), 2.50 (s, 1H), 1.63 (s, 3H), 1.60 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.69, 128.44, 127.63, 127.56, 85.76, 82.34, 79.11, 76.41, 73.61, 72.60, 67.46, 24.48, 21.18. HRMS (FAB): m/z for $C_{15}H_{17}O_2$ $[M+H]^+$, calcd: 229.1223, found: 229.1223.

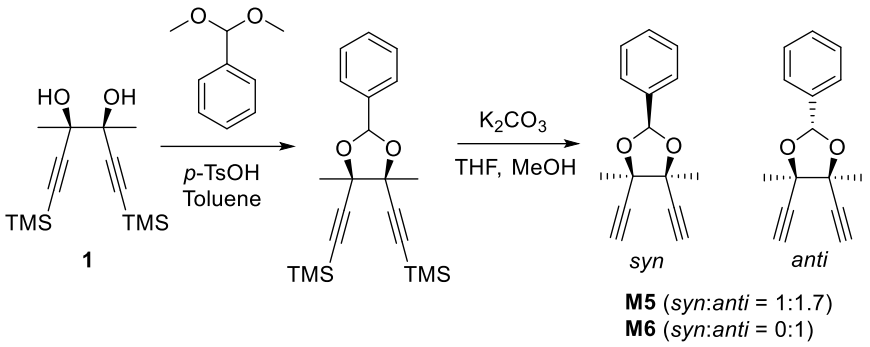
Synthesis of M3 and M4



Compound **1** (720 mg, 2.5 mmol) was dissolved in DCM. Then, 2,6-lutidine (90 µl, 0.77mmol) and triethylsilyl trifluoromethanesulfonate (0.16 ml, 0.77 mmol) was added sequentially at 0 °C. After stirring 1 h, the reaction was quenched by saturated NH_4Cl aqueous solution. The organic layer was washed with brine and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. This product was mixed with K_2CO_3 (67 mg), and dissolved in THF (0.6 ml) and methanol (0.6 ml). After 4 h, the reaction was quenched by saturated NH_4Cl aqueous solution. The organic layer was washed with brine and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. The product was purified by flash column chromatography on silica gel to afford **M3** as colorless liquid (88 mg, 0.35 mmol, 45% via two steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.74 (br, 1H), 2.54 (s, 1H), 2.41 (s, 1H), 1.54 (d, J = 1.6 Hz, 6H), 0.98 (t, J = 7.9 Hz, 9H), 0.81 – 0.67 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 86.12, 85.40, 74.60, 74.58, 74.23, 72.13, 25.34, 24.05, 7.11, 6.04. HRMS (ESI): m/z for $C_{14}H_{24}NaO_2Si$ $[M+Na]^+$, calcd: 275.1438, found: 275.1440.

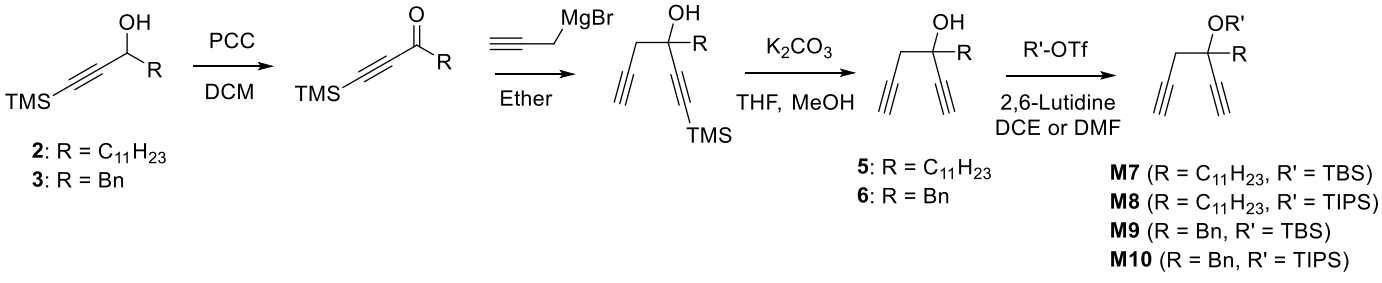
Following the same procedure, compound **1** (2.07 g, 7.34 mmol) was reacted with *tert*-butyldimethylsilyl trifluoromethanesulfonate (0.51 ml, 2.20 mmol) to afford **M4** as colorless liquid (333 mg, 1.32 mmol, 60% via two steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.71 (br, 1H), 2.55 (s, 1H), 2.41 (s, 1H), 1.55 (s, 3H), 1.54 (s, 3H), 0.90 (s, 9H), 0.24 (s, 3H), 0.23 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 86.02, 85.18, 74.90, 74.70, 74.22, 72.15, 25.82, 25.23, 24.07, 18.28, -2.97, -3.27. HRMS (ESI): m/z for $C_{14}H_{24}NaO_2Si$ $[M+Na]^+$, calcd: 275.1438, found 275.1439.

Synthesis of M5 and M6



To a dried round-bottom flask containing a stirring bar, compound **1** (412 mg, 1.46 mmol) and *p*-toluenesulfonic acid (56 mg, 0.29 mmol) was added and purged with Ar gas. The mixture was dissolved in toluene (1.5 ml), then benzaldehyde dimethyl acetal (0.26 ml, 1.75 mmol) was added. After stirring for 6 h at 70 °C, the organic layer was washed with brine and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. This crude mixture was dissolved in THF (2 ml) and methanol (2 ml), then K_2CO_3 (508 mg, 3.63 mmol) was added. After vigorous stirring for 3 h, the reaction was quenched by saturated NH_4Cl aqueous solution. The organic layer was washed with brine and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. The product was purified by flash column chromatography on silica gel to afford **M5** (*syn*:*anti* = 1:1.7) as colorless liquid (264 mg, 1.17 mmol, 80% via two steps). Further purification by recrystallization afforded **M6** (*syn*:*anti* = 0:1) as white solid (90 mg). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.45 (m, 2H), 7.42 – 7.35 (m, 3H), 6.27 (s, 1H), 2.70 (s, 2H), 1.62 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 129.58, 128.52, 126.76, 102.29, 82.64, 80.32, 75.51, 23.87. HRMS (ESI): m/z for $C_{15}H_{14}NaO_2$ $[M+Na]^+$, calcd: 249.0886, found: 249.0887.

Synthesis of M7-10



Compound **2** (5.25 g, 18.6 mmol) was dissolved in DCM (62 ml), and pyridinium chlorochromate (6.01 g, 27.9 mmol) was added. After strring for 5 h, the crude mixture was filtered with silica. Further purification with flash column chromatography afforded a mixture of the desired oxidized product and its TMS-deprotected derivative. A portion of this product (2.21 g) was dissolved in degassed diethyl ether (30 ml), then propargyl magnesium bromide solution (30 ml)* was added at -30 °C. After checking the complete consumption of the starting materials by thin layer chromatography, the reaction was quenched by saturated NH_4Cl

aqueous solution. The organic layer was washed with brine and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. This crude mixture was dissolved in THF (10 ml) and methanol (10 ml), then K_2CO_3 (5.9 g, 43 mmol) was added. After vigorous stirring for 2 h, the reaction was quenched by saturated NH_4Cl aqueous solution. The organic layer was washed with water and extracted by ethyl acetate, dried with $MgSO_4$, and concentrated. The product was purified by flash column chromatography on silica gel to afford **5** as colorless liquid (1.74 g, 7.0 mmol, ca. 70% via three steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.62 (ddd, J = 40.5, 16.6, 2.6 Hz, 2H), 2.50 (s, 1H), 2.38 (br, 1H), 2.16 (t, J = 2.6 Hz, 1H), 1.80 – 1.70 (m, 2H), 1.55 – 1.49 (m, 2H), 1.38 – 1.23 (m, 16H), 0.88 (t, J = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 85.52, 79.40, 72.82, 72.06, 69.70, 40.97, 33.33, 32.07, 29.79, 29.77, 29.75, 29.71, 29.65, 29.50, 24.41, 22.84, 14.28. HRMS (ESI): m/z for $C_{17}H_{28}NaO$ $[M+Na]^+$, calcd: 271.2032, found: 271.2031.

* Preparation of propargyl magnesium bromide (Grignard reagent)

To a two-neck round-bottom flask with a reflux condenser, magnesium turnings (2.2 g, 90 mmol) and mercury (II) chloride (610 mg, 2.3 mmol) was added. After drying it in *vacuo* using a torch, diethyl ether (30 ml) was added. Propargyl bromide solution (80% in toluene, 5.0 ml, 45 mmol) was slowly added, then the reaction mixture is warmed over a water bath for 1 h. After seeing bubbling stopped, the reagent was directly used for the Grignard reaction.

Following the same procedure, compound **3** was used to afford **6** as colorless liquid: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.27 (m, 5H), 3.11 (q, J = 13.4 Hz, 2H), 2.64 (d, J = 2.6 Hz, 2H), 2.54 (s, 1H), 2.42 (s, 1H), 2.22 (t, J = 2.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 135.41, 130.89, 128.36, 127.37, 85.12, 79.41, 74.18, 72.33, 69.72, 46.58, 32.63. HRMS (ESI): m/z for $C_{13}H_{12}NaO$ $[M+Na]^+$, calcd: 207.0780, found: 207.0783.

Compound **5** (150 mg, 0.61 mmol) was dissolved in DCE (3 ml). Then, 2,6-lutidine (0.35 ml, 3.0 mmol) and tert-butyldimethylsilyl trifluoromethanesulfonate (0.42 ml, 1.8 mmol) was added. After stirring for 5 h at 50 °C, the reaction was quenched by saturated $NaHCO_3$ aqueous solution. The organic layer was washed with water and extracted by dichloromethane, dried with $MgSO_4$, and concentrated. The product was purified by flash column chromatography on silica gel to afford **M7** as colorless liquid (188 mg, 0.518 mmol, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.56 (dd, J = 2.5, 1.5 Hz, 2H), 2.50 (s, 1H), 2.04 (t, J = 2.6 Hz, 1H), 1.81 – 1.71 (m, 2H), 1.51 – 1.39 (m, 2H), 1.37 – 1.19 (m, 17H), 0.91 – 0.85 (m, 12H), 0.19 (d, J = 8.9 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 86.41, 80.37, 73.70, 70.99, 70.77, 42.14, 33.80, 32.08, 29.80, 29.76, 29.73, 29.69, 29.51, 25.84, 24.14, 22.85, 18.33, 14.28, -2.84, -2.95. HRMS (ESI): m/z for $C_{23}H_{42}NaOSi$ $[M+Na]^+$, calcd: 385.2897, found: 385.2899.

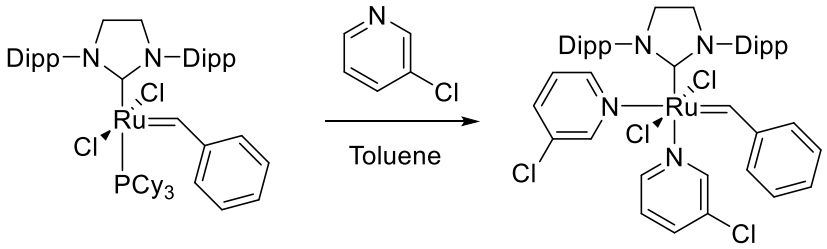
Following the similar procedure with different reaction times, **M8-M10** were obtained from compounds **5** and **6**.

From the reaction of compound **5** (550 mg, 2.2 mmol) with triisopropylsilyl trifluoromethanesulfonate (1.8 ml, 6.6 mmol), **M8** was obtained as colorless liquid (818 mg, 2.02 mmol, 91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.64 (d, J = 2.7 Hz, 2H), 2.47 (s, 1H), 2.03 (t, J = 2.7 Hz, 1H), 1.93 – 1.81 (m, 2H), 1.49 – 1.42 (m, 2H), 1.40 – 1.21 (m, 18H), 1.21 – 1.14 (m, 3H), 1.08 (dd, J = 7.3, 2.4 Hz, 18H), 0.88 (t, J = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 86.85, 80.31, 73.22, 70.89, 70.79, 42.01, 33.11, 32.08, 29.80, 29.79, 29.71, 29.67, 29.51, 24.09, 22.85, 18.51, 14.28, 13.18. HRMS (ESI): m/z for $C_{26}H_{48}NaOSi$ $[M+Na]^+$, calcd: 427.3367, found: 427.3369.

From the reaction of compound **6** (109 mg, 0.59 mmol) with tert-butyldimethylsilyl trifluoromethanesulfonate (0.54 ml, 2.4 mmol), **M9** was obtained as colorless liquid (138 mg, 0.46 mmol, 78%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, J = 6.9 Hz, 2H), 7.33 – 7.24 (m, 3H), 3.10 (qd, J = 13.2, 2.3 Hz, 2H), 2.58 (d, J = 2.9 Hz, 1H), 2.56 (s, 2H), 2.16 (q, J = 2.6 Hz, 1H), 0.88 (d, J = 2.8 Hz, 9H), 0.17 (d, J = 2.6 Hz, 3H), -0.06 (d, J = 2.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.34, 131.35, 127.75, 126.83, 85.75, 80.38, 75.45, 71.53, 71.28, 47.76, 33.68, 25.96, 18.37, -2.80, -3.35. HRMS (ESI): m/z for $C_{19}H_{26}NaOSi$ $[M+Na]^+$, calcd: 321.1645, found: 321.1648.

From the reaction of compound **6** (150 mg, 0.83 mmol) with triisopropylsilyl trifluoromethanesulfonate (0.90 ml, 3.3 mmol) in DMF (80 °C, 40 h), **M10** was obtained as colorless liquid (143 mg, 0.42 mmol, 51%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 6.8 Hz, 2H), 7.32 – 7.22 (m, 3H), 3.20 (dd, *J* = 40.7, 13.2 Hz, 2H), 2.57 – 2.52 (m, 3H), 2.17 (t, *J* = 2.6 Hz, 1H), 1.25 – 1.16 (m, 3H), 1.07 (dd, *J* = 7.4, 4.4 Hz, 18H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.28, 131.21, 127.90, 126.89, 86.23, 80.52, 74.95, 71.77, 71.26, 47.39, 32.75, 18.53, 18.49, 13.20. HRMS (ESI): m/z for $C_{22}H_{32}NaOSi$ $[M+Na]^+$, calcd: 363.2115, found: 363.2117.

Preparation of Ru3



Ru3

Under argon atmosphere, 3-chloropyridine (0.4 ml, 4.2 mmol) was added to a solution of dichloro[1,3-bis(2,6-isopropylphenyl)-2-imidazolidinylidene](benzylidene)(tricyclohexylphosphine)ruthenium(II) (59.4 mg, 0.0636 mmol) in toluene (0.33 ml). After stirring for 2 min, the solution was mixed with degassed n-pentane (ca. 8 ml). A small amount of green precipitate formed immediately, and the vial was stored at - 24 °C for 2 days. Dark green crystals formed and were isolated by filtration, washed with pentane, and then dried *in vacuo* (34 mg, 61%). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 19.00 (s, 1H), 8.56 (br d, *J* = 45.3 Hz, 2H), 7.99 (br d, *J* = 28.4 Hz, 2H), 7.76 (br s, 1H), 7.55 (br s, 1H), 7.52 – 7.42 (m, 3H), 7.41 – 7.13 (m, 7H), 7.09 – 6.90 (m, 3H), 4.61 – 3.07 (m, 8H), 1.87 – 0.93 (m, 28H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 218.73, 152.10, 151.55, 149.19, 148.04, 137.00, 136.08, 130.39, 129.35, 128.37, 124.73, 55.09, 29.23, 28.51, 27.49, 26.62, 23.58. Anal. Calcd. for $C_{44}H_{52}Cl_4N_4Ru$: C, 60.07; H, 5.96; Cl, 16.12; N, 6.37; Ru, 11.49. Found: C, 60.07; H, 6.06; N, 6.39.

4. General Procedure for Polymerization

A 4-mL sized screw-cap vial with septum was flame dried and charged with monomer (ca. 20 mg). The vial was purged with Ar three times, and degassed anhydrous solvent was added. A mixture of initiator and additive in another 4-mL vial was dissolved in solvent under Ar atmosphere. The initiator solution was rapidly injected to the monomer solution at experimental temperature under vigorous stirring. The reaction was quenched by excess ethyl vinyl ether (ca. 50 – 100 μl) after desired reaction time, and resulting polymer was precipitated in methanol, remaining small amount of crude mixture (c.a. 2 mg). Obtained solid was filtered and dried *in vacuo*. Monomer conversion was calculated from the ^{1}H NMR spectrum of the remained crude mixture.

5. ^{1}H and ^{13}C NMR characterization of polymers

P3: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 6.83 – 6.27 (m, 2H), 3.12 – 2.89 (m, 1H), 1.58 (s, 3H), 1.43 (s, 3H), 1.06 – 0.93 (m, 9H), 0.79 – 0.64 (m, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.45, 145.75, 123.57, 122.94, 82.71, 79.18, 20.91, 19.91, 7.20, 6.72.

P4: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 6.79 – 6.29 (m, 2H), 3.06 – 2.79 (m, 1H), 1.58 (br, 3H), 1.42 (s, 3H), 0.91 (s, 9H), 0.38 – 0.12 (m, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.16, 145.76, 123.34, 123.02, 82.78, 79.60, 26.06, 20.88, 19.96, 18.48, -2.25.

P6: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.47 (br, 2H), 7.36 (d, J = 12.1 Hz, 3H), 6.64 (s, 2H), 5.64 (s, 1H), 1.54 (s, 6H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 142.52, 136.99, 129.80, 128.58, 127.80, 124.03, 100.77, 87.82, 16.92.

P7: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 6.74 (d, J = 13.7 Hz, 1H), 6.25 (d, J = 15.5 Hz, 1H), 3.06 – 2.26 (m, 2H), 1.96 (br, 1H), 1.73 – 1.08 (m, 19H), 1.08 – 0.61 (m, 12H), 0.38 – -0.41 (m, 6H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 146.73, 140.06, 124.17, 121.99, 79.10, 41.99, 40.66, 32.38, 30.44, 30.11, 29.81, 26.26, 26.19, 23.14, 18.67, 14.35, -2.51, -3.36.

P8: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 6.80 (d, J = 12.7 Hz, 1H), 6.24 (d, J = 12.7 Hz, 1H), 2.76 (s, 1H), 2.60 (s, 1H), 1.95 (s, J = 84.6 Hz, 1H), 1.75 (s, 1H), 1.65 – 1.12 (m, 18H), 1.05 (s, 18H), 0.88 (t, J = 6.1 Hz, 3H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 147.26, 140.04, 123.97, 121.88, 78.74, 42.44, 41.10, 40.68, 32.39, 30.51, 30.10, 29.81, 25.54, 23.15, 18.64, 14.35, 13.61.

P9: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.48 – 6.89 (m, 5H), 6.54 – 6.11 (m, 1H), 6.11 – 5.84 (m, 1H), 3.44 – 2.94 (m, 2H), 2.94 – 2.27 (m, 2H), 1.12 – 0.56 (m, 9H), 0.28 – -0.33 (m, 6H). ^{13}C NMR (150 MHz, CD_2Cl_2) δ 146.53, 140.20, 138.96, 131.30, 127.95, 126.64, 124.43, 122.14, 79.30, 47.32, 41.83, 26.34, 18.69, -2.59, -3.44.

P10: ^{1}H NMR (500 MHz, THF-d_8) δ 7.60 – 6.76 (m, 5H), 6.37 (br, 1H), 6.03 (br, 1H), 3.45 – 2.98 (m, 2H), 2.97 – 2.53 (m, 2H), 1.24 (br, 21H). ^{13}C NMR (125 MHz, THF-d_8) δ 146.72, 140.32, 138.73, 131.53, 128.12, 126.94, 124.39, 122.43, 79.35, 54.69, 47.65, 42.53, 18.82, 13.99.

6. General procedure for *In situ* NMR Experiment

An NMR tube was filled with monomer (0.125 mmol, 10 eq), purged with argon, and THF-d_8 (300 μL) was added. A 4-mL vial containing initiator (0.0156 mmol, 1.25 eq) was argon-purged, and hexamethyldisilane was added as an internal standard. The total amount of initiator was 5/4 of the amount used for the reaction; after dissolving those using THF-d_8 (250 μL), 1/5 (50 μL) of it was diluted in another NMR tube and used for checking the ratio between initial carbene and the internal standard. Then, the remaining 200 μL of initiator solution was added to the monomer solution and ^{1}H NMR was recorded over time.

7. SEC Traces of Polymers

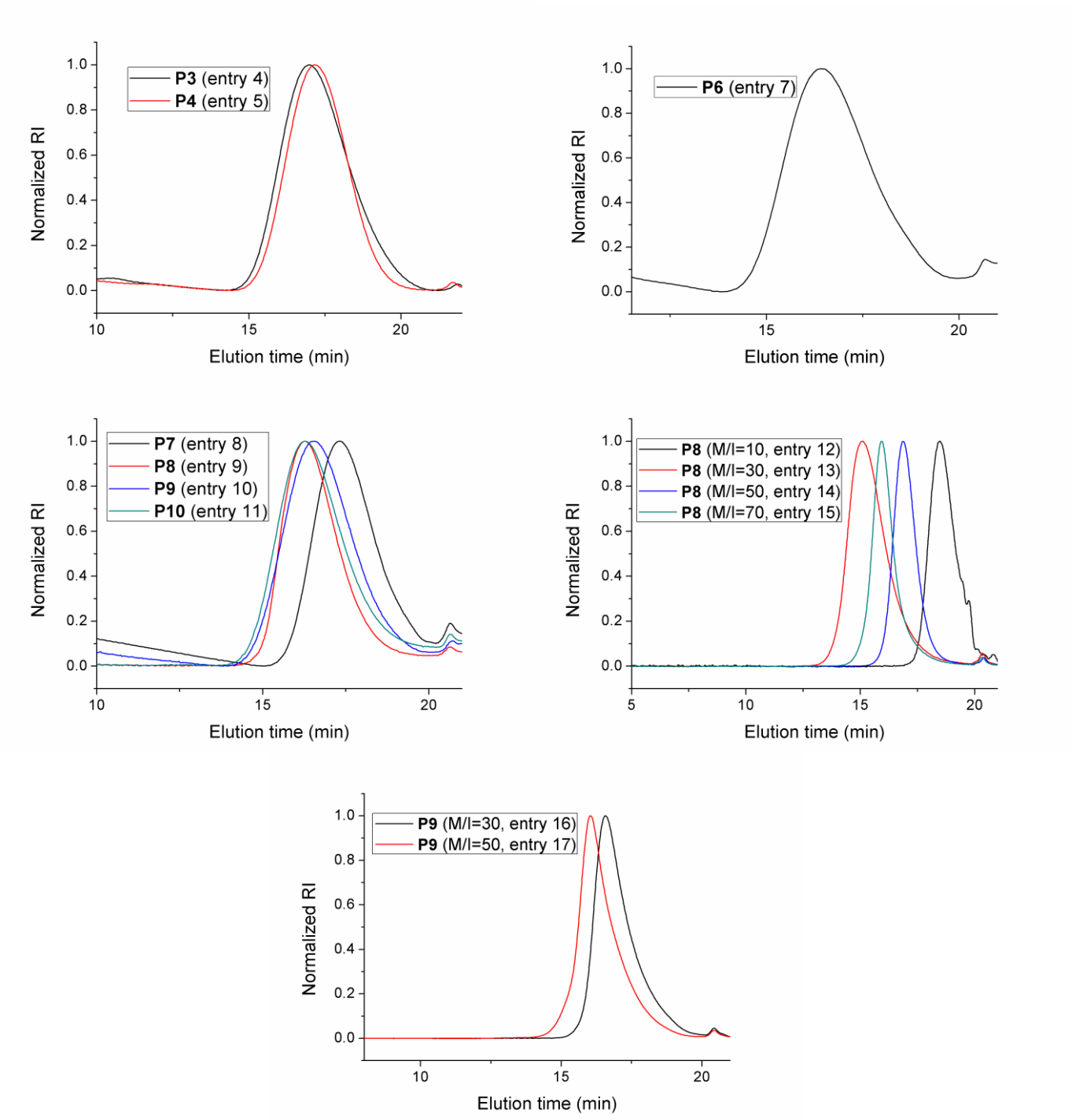
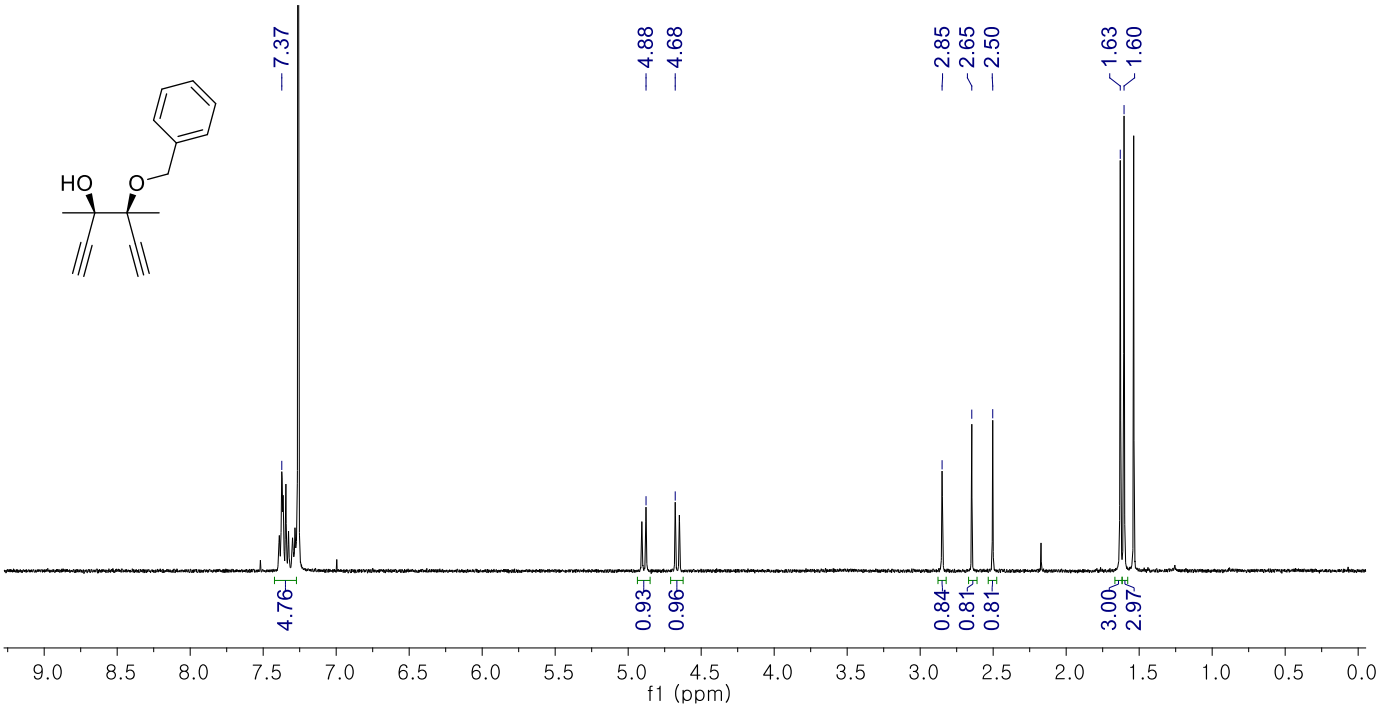


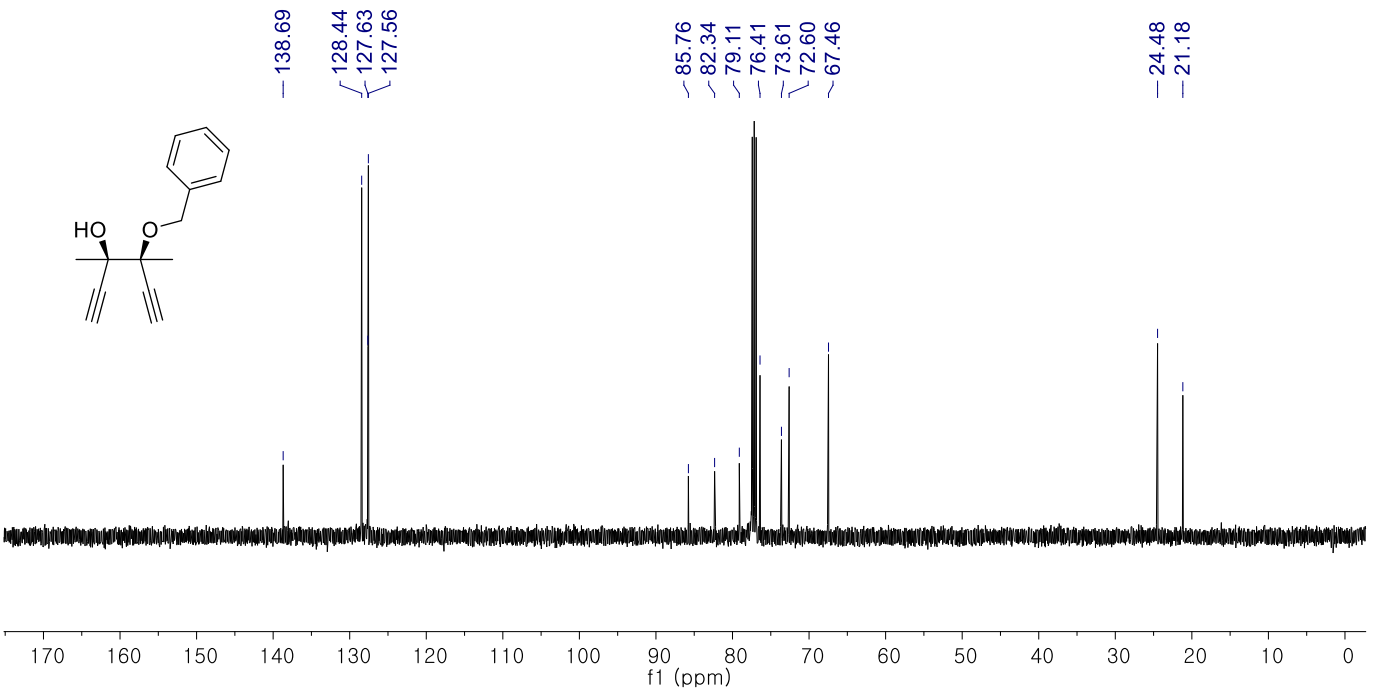
Figure S15. SEC traces of **P3 – P10** from **Table 1**.

8. ^{1}H and ^{13}C NMR Spectra of New Compounds

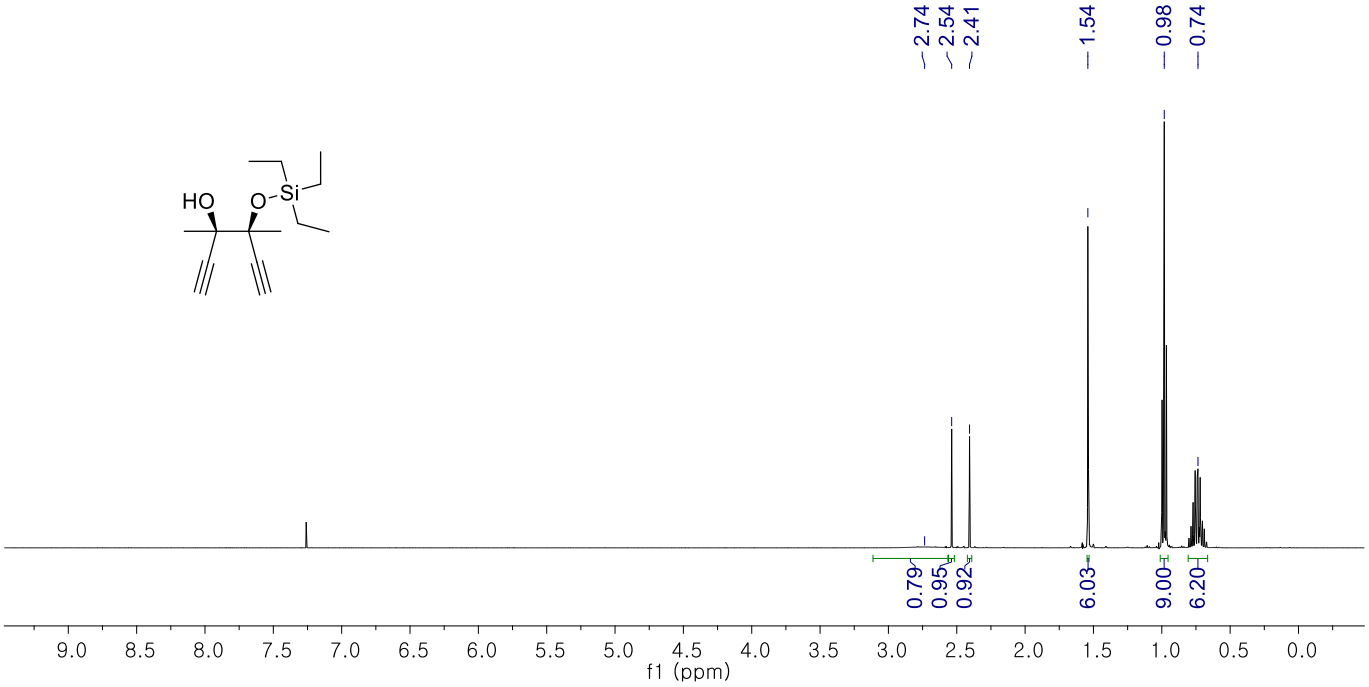
M2 ^{1}H NMR (400 MHz, $CDCl_3$)



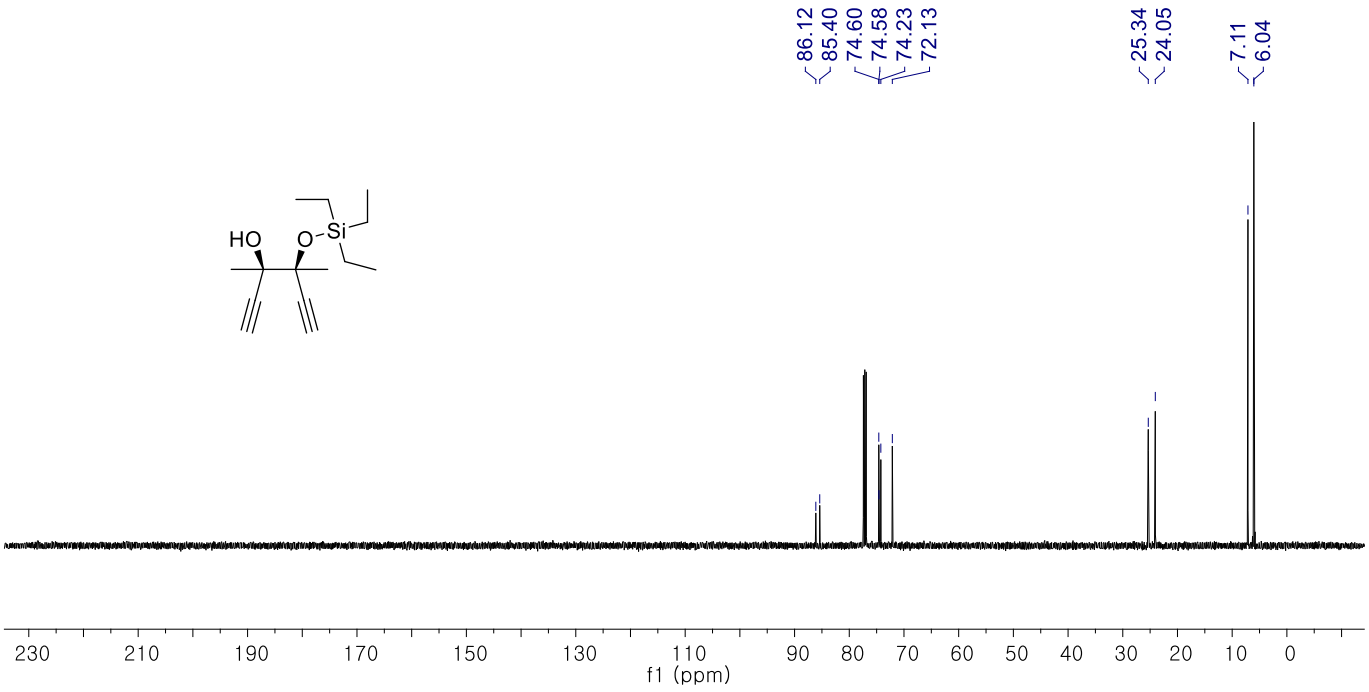
M2 ^{13}C NMR (125 MHz, $CDCl_3$)



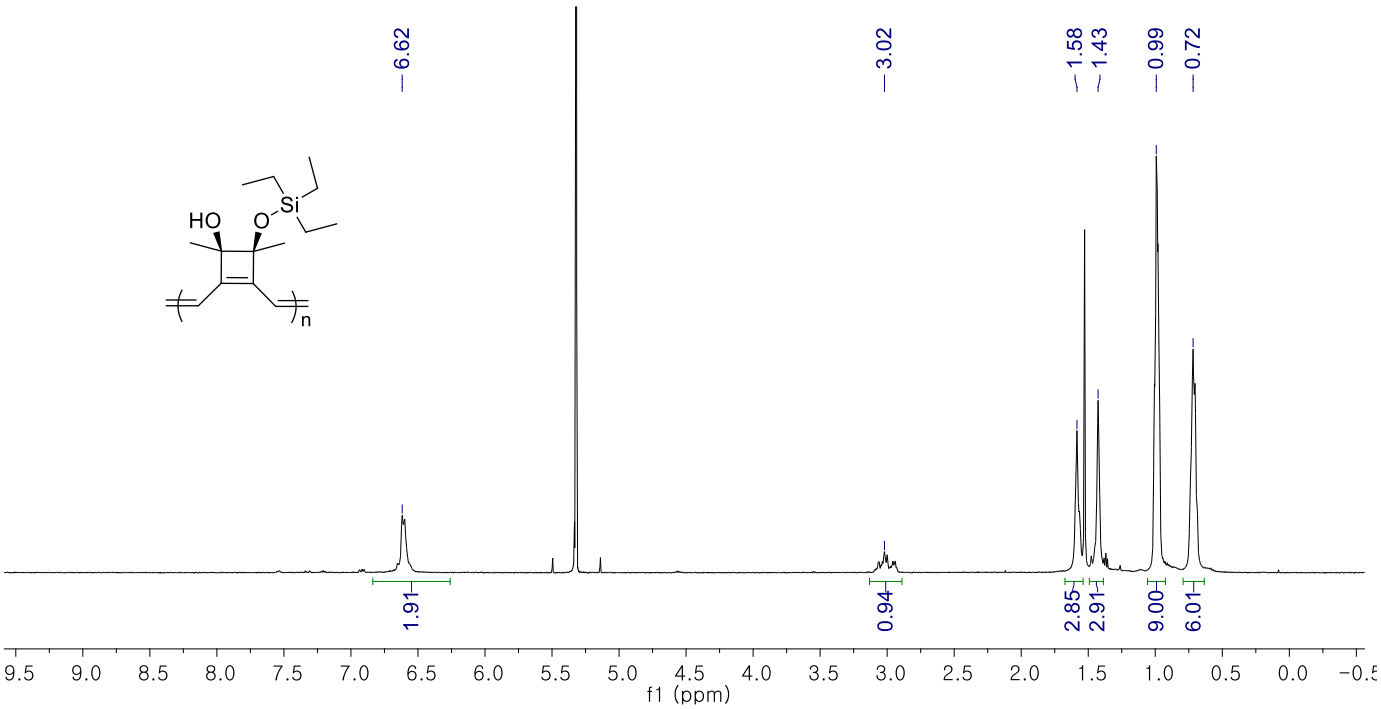
M3 ^{1}H NMR (500 MHz, $CDCl_3$)



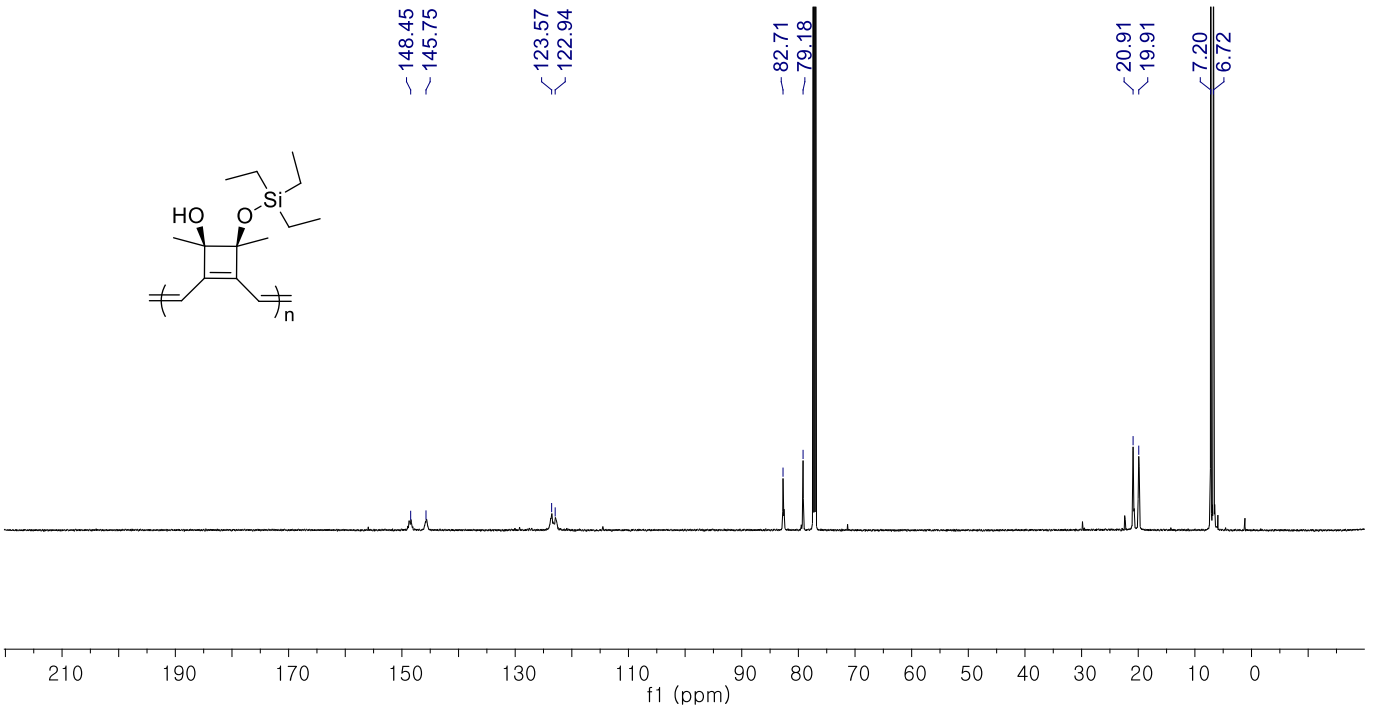
M3 ^{13}C NMR (125 MHz, $CDCl_3$)



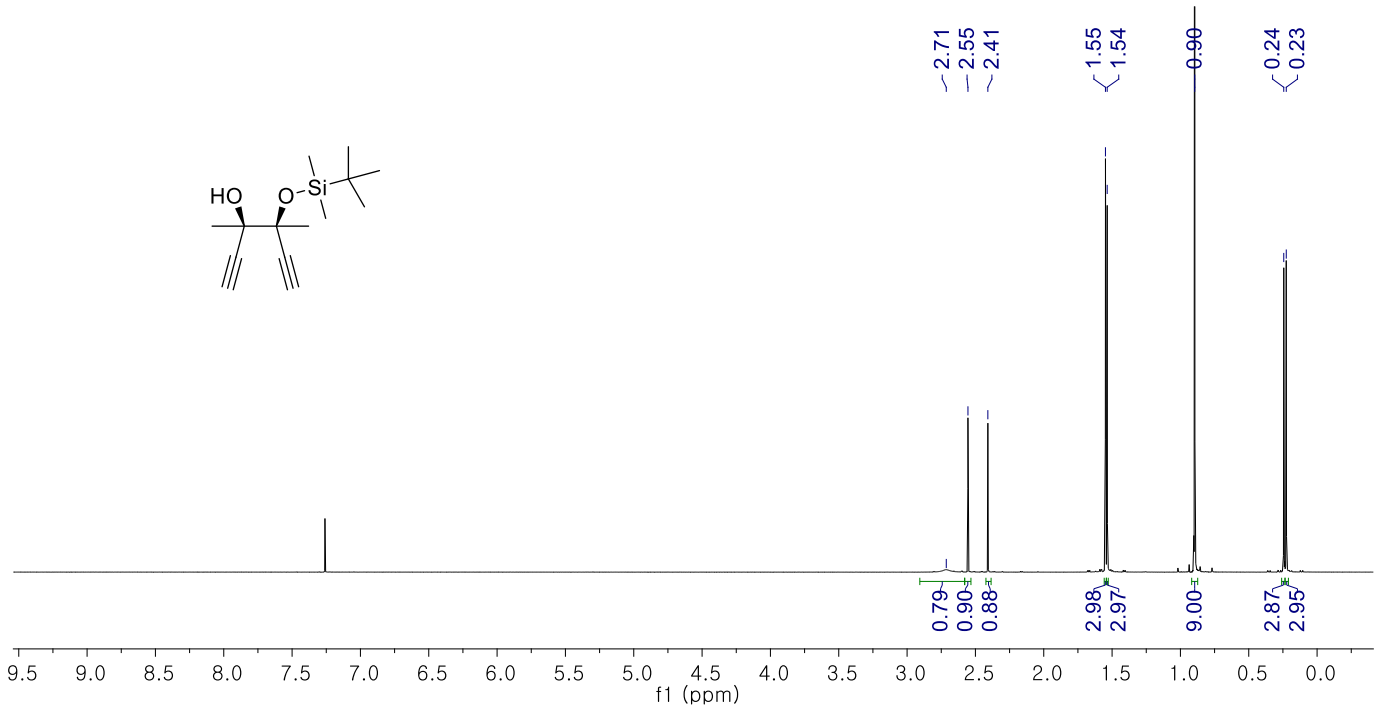
P3 ^{1}H NMR (500 MHz, CD_2Cl_2)



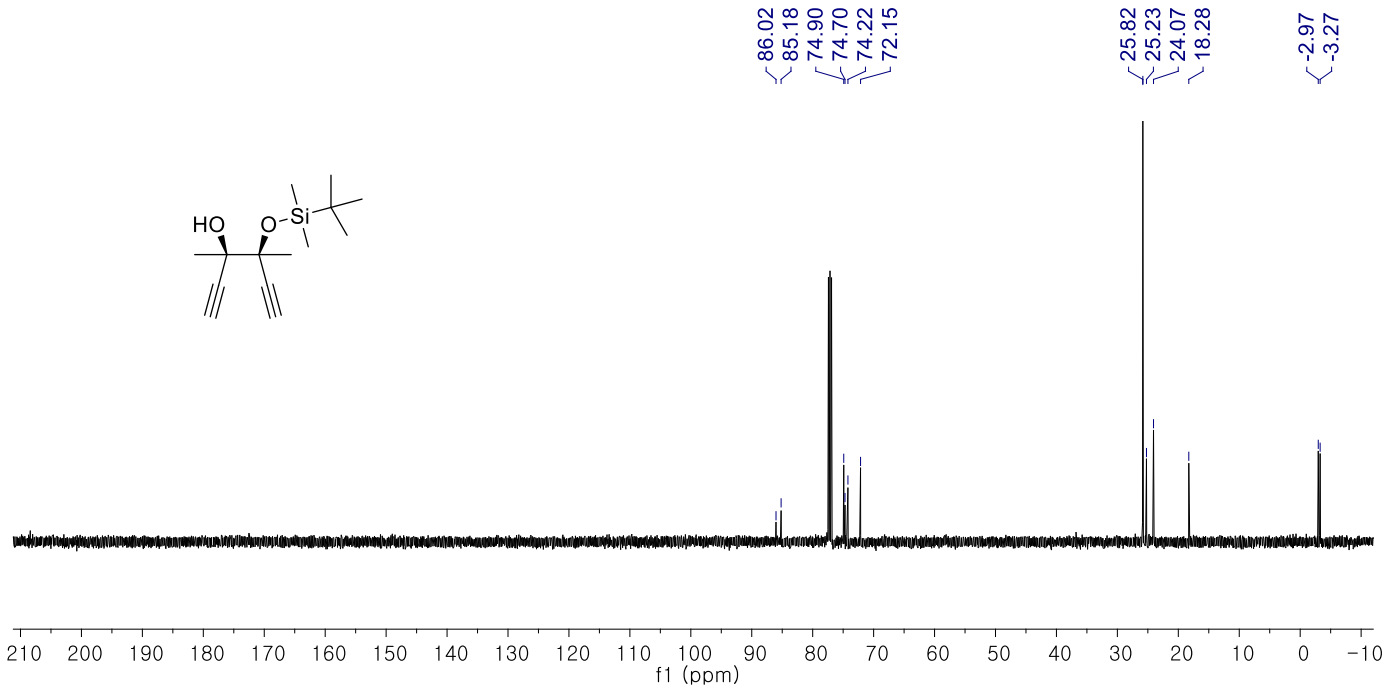
P3 ^{13}C NMR (150 MHz, $CDCl_3$)



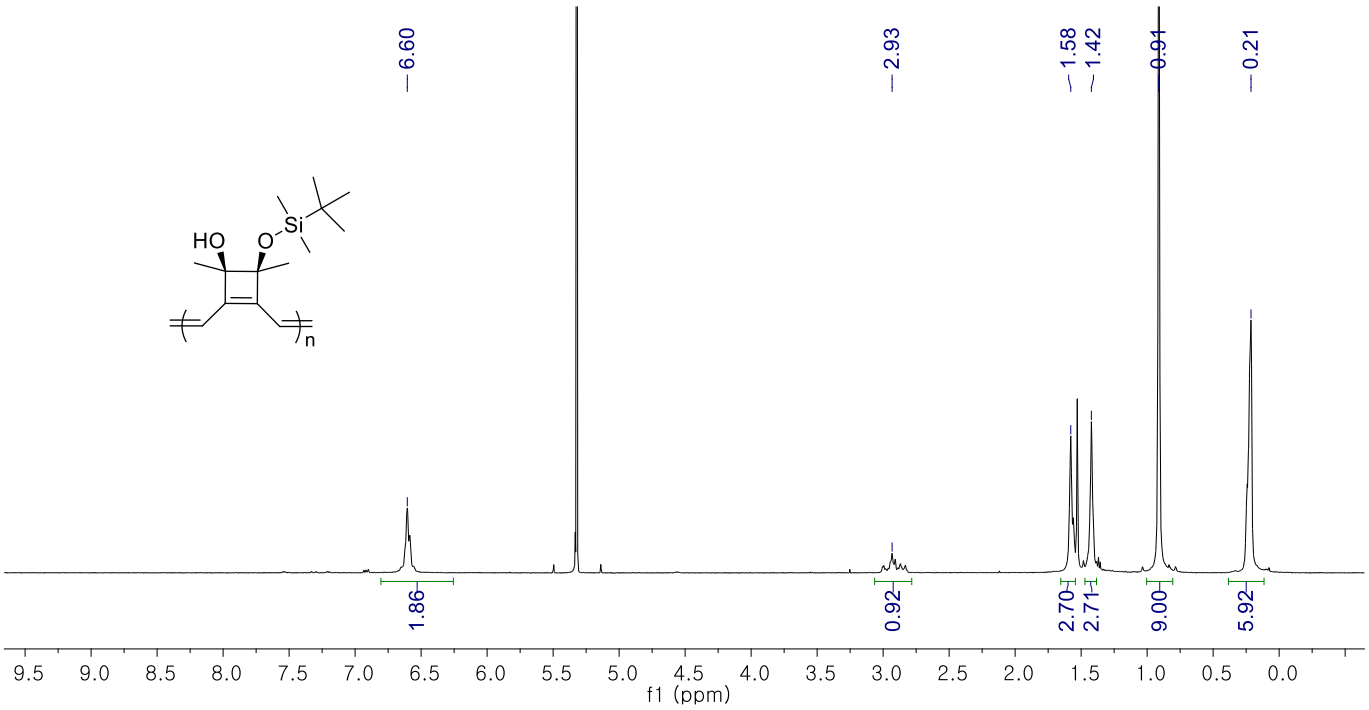
M4 ^{1}H NMR (500 MHz, $CDCl_3$)



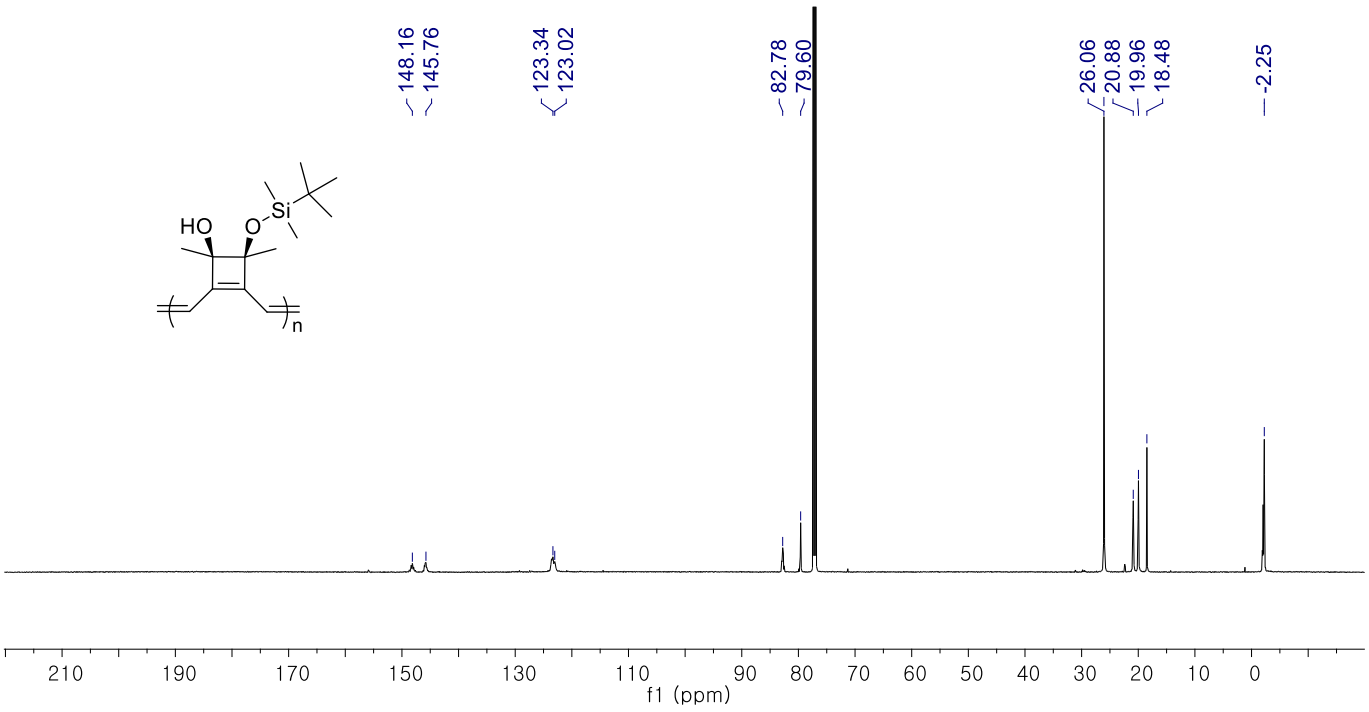
M4 ^{13}C NMR (125 MHz, $CDCl_3$)



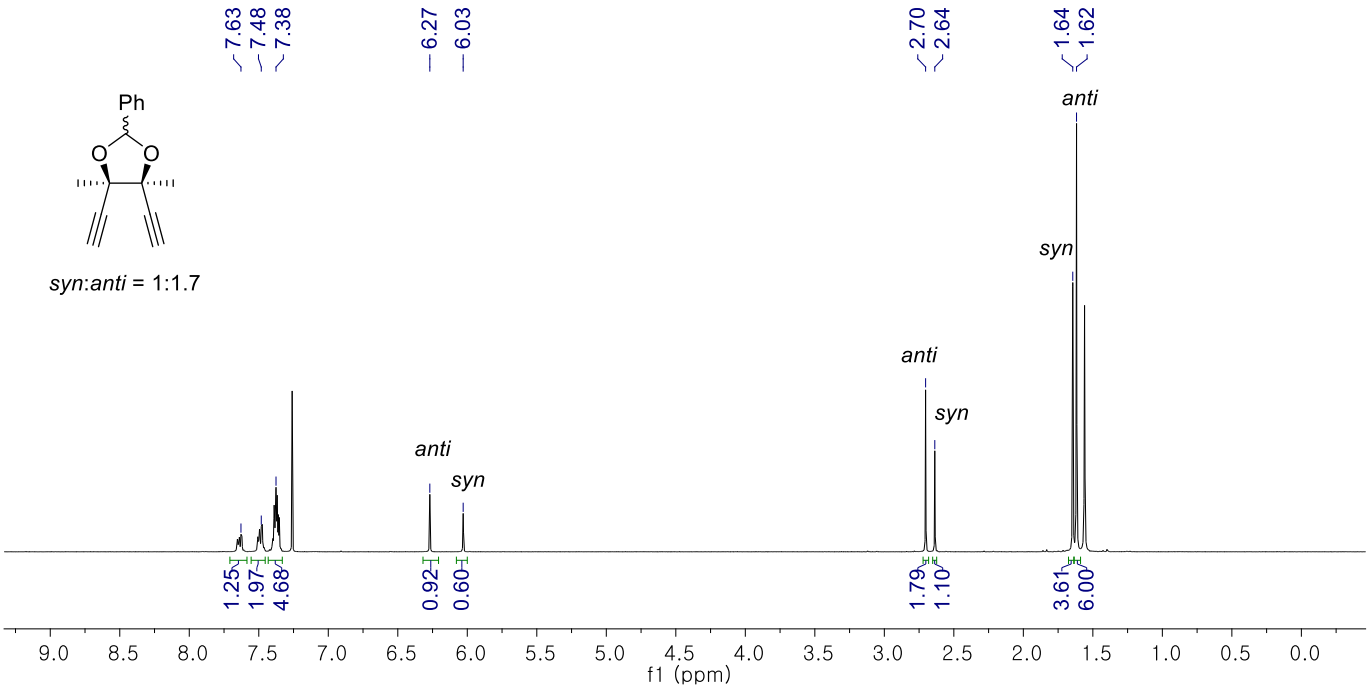
P4 ^{1}H NMR (500 MHz, CD_2Cl_2)



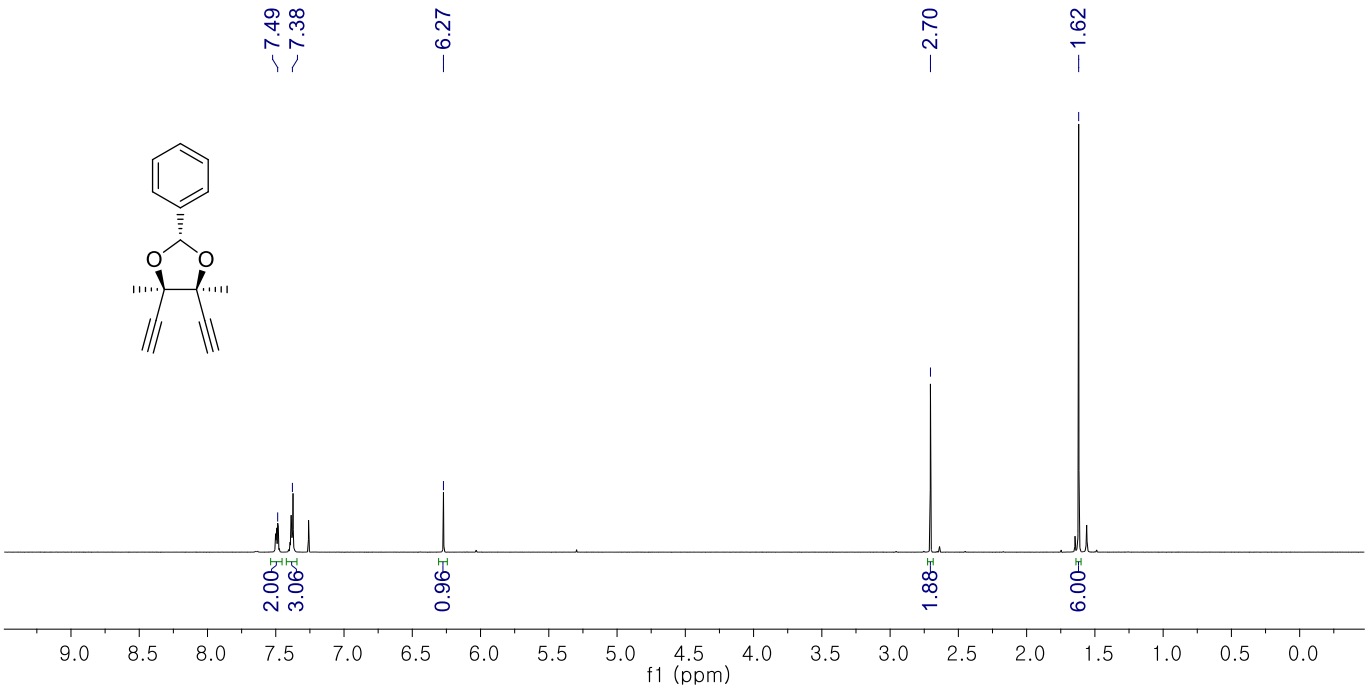
P4 ^{13}C NMR (150 MHz, $CDCl_3$)



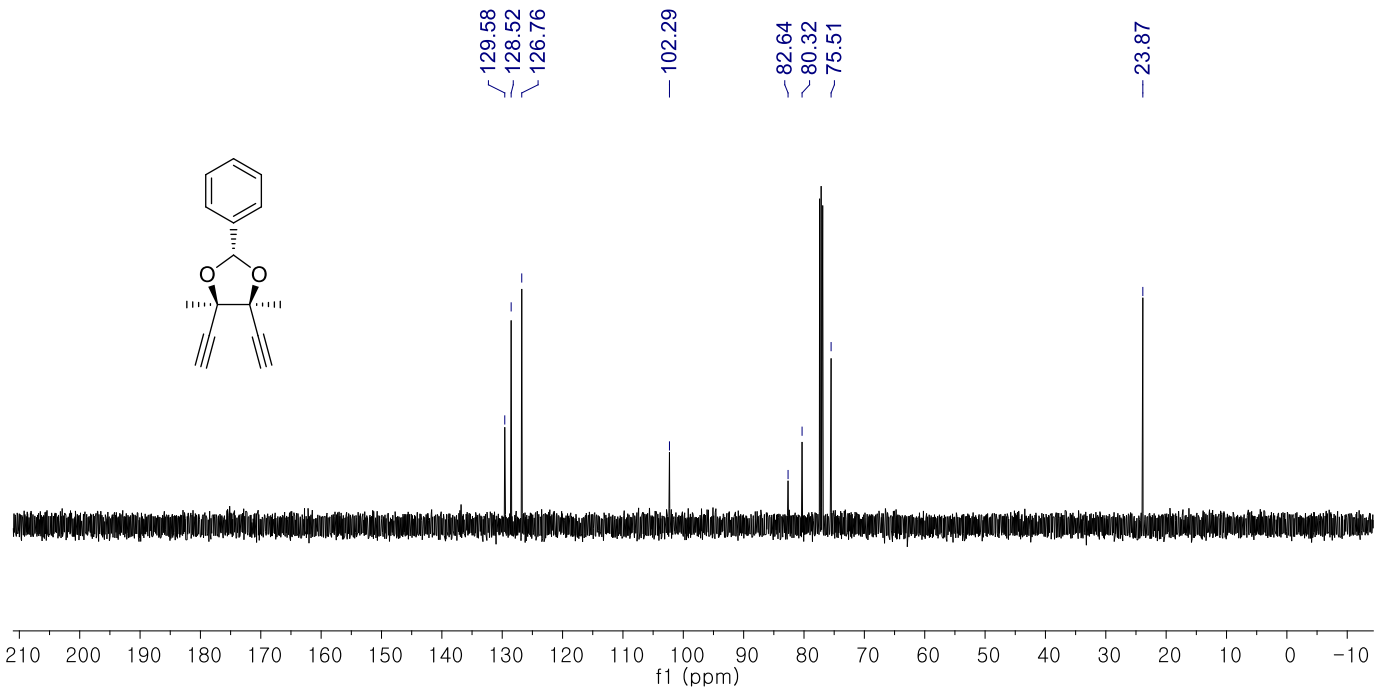
M5 ^{1}H NMR (500 MHz, $CDCl_3$)



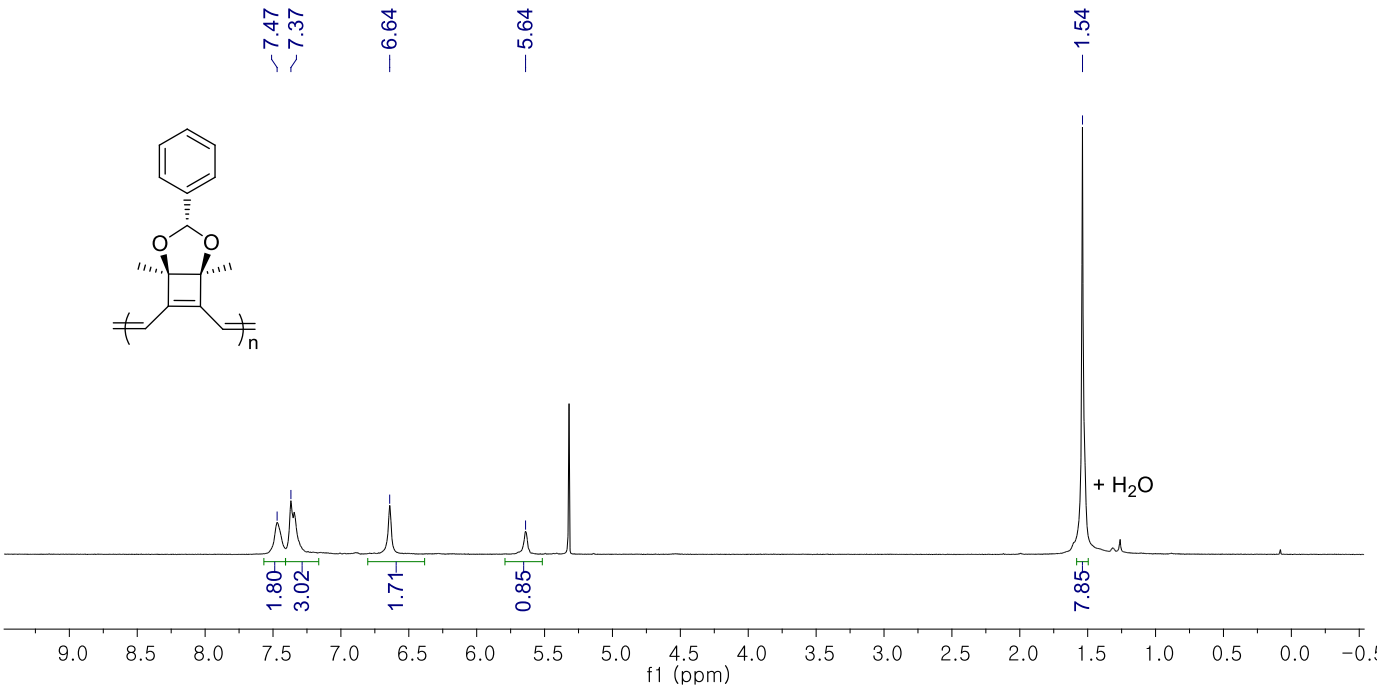
M6 ^{1}H NMR (500 MHz, $CDCl_3$)



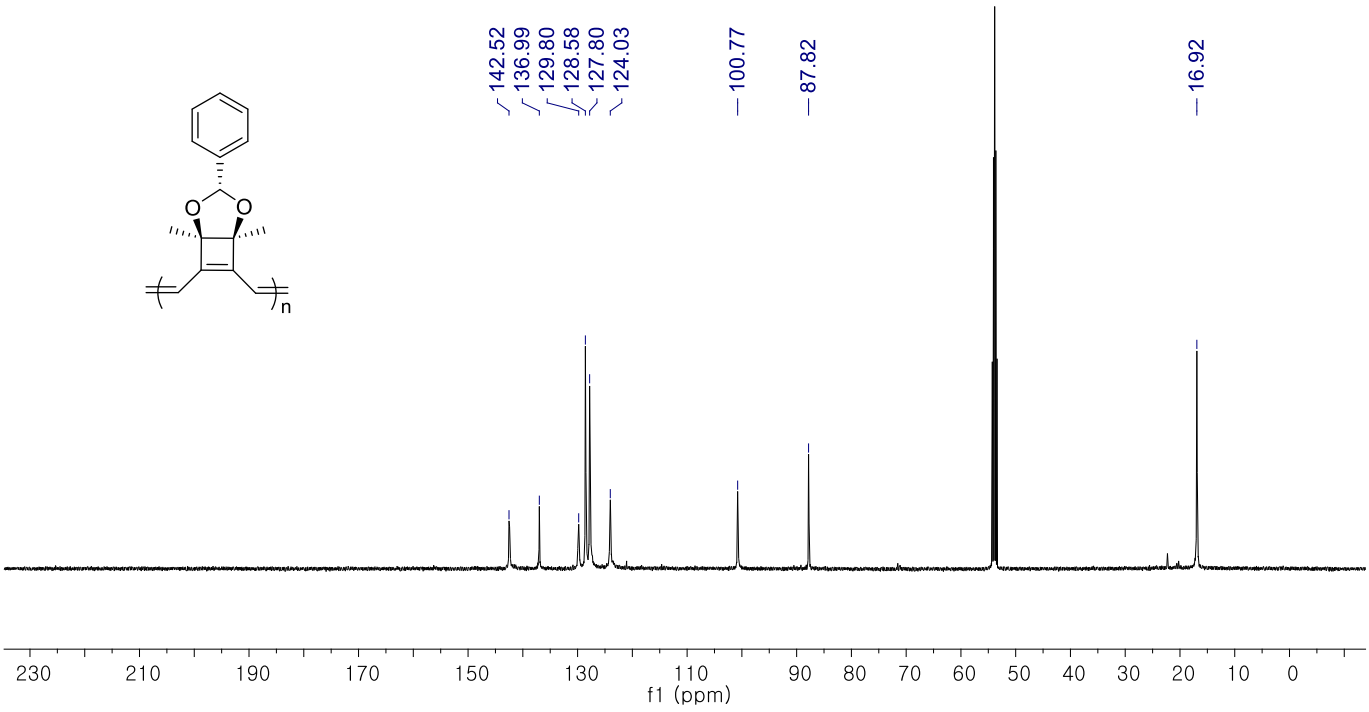
M6 ^{13}C NMR (125 MHz, $CDCl_3$)



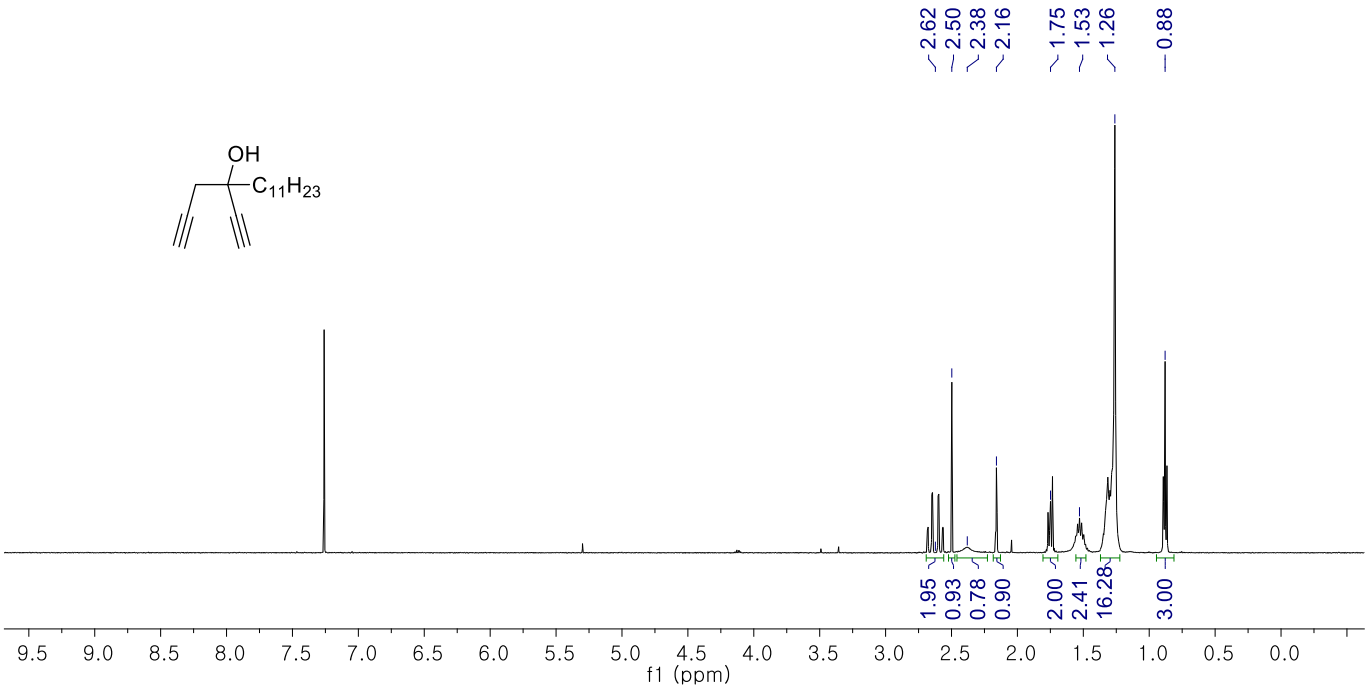
P6 ^{1}H NMR (500 MHz, CD_2Cl_2)



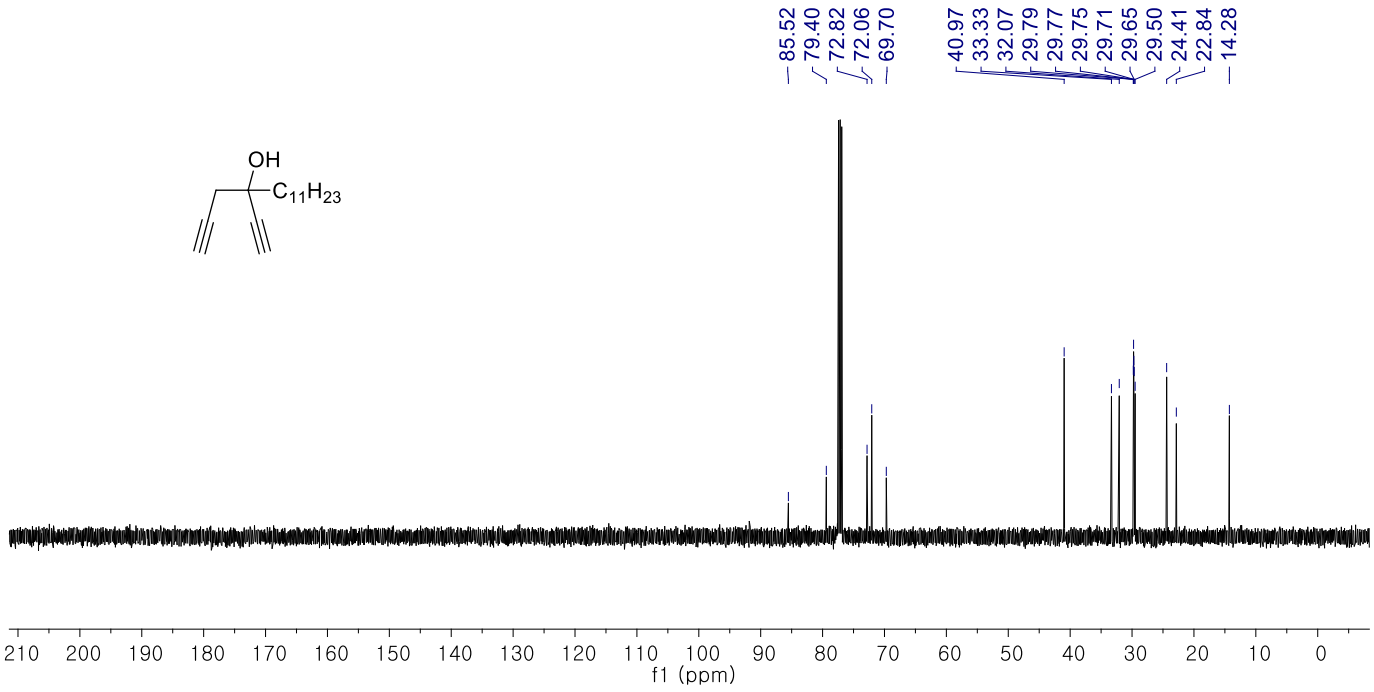
P6 ^{13}C NMR (125 MHz, CD_2Cl_2)



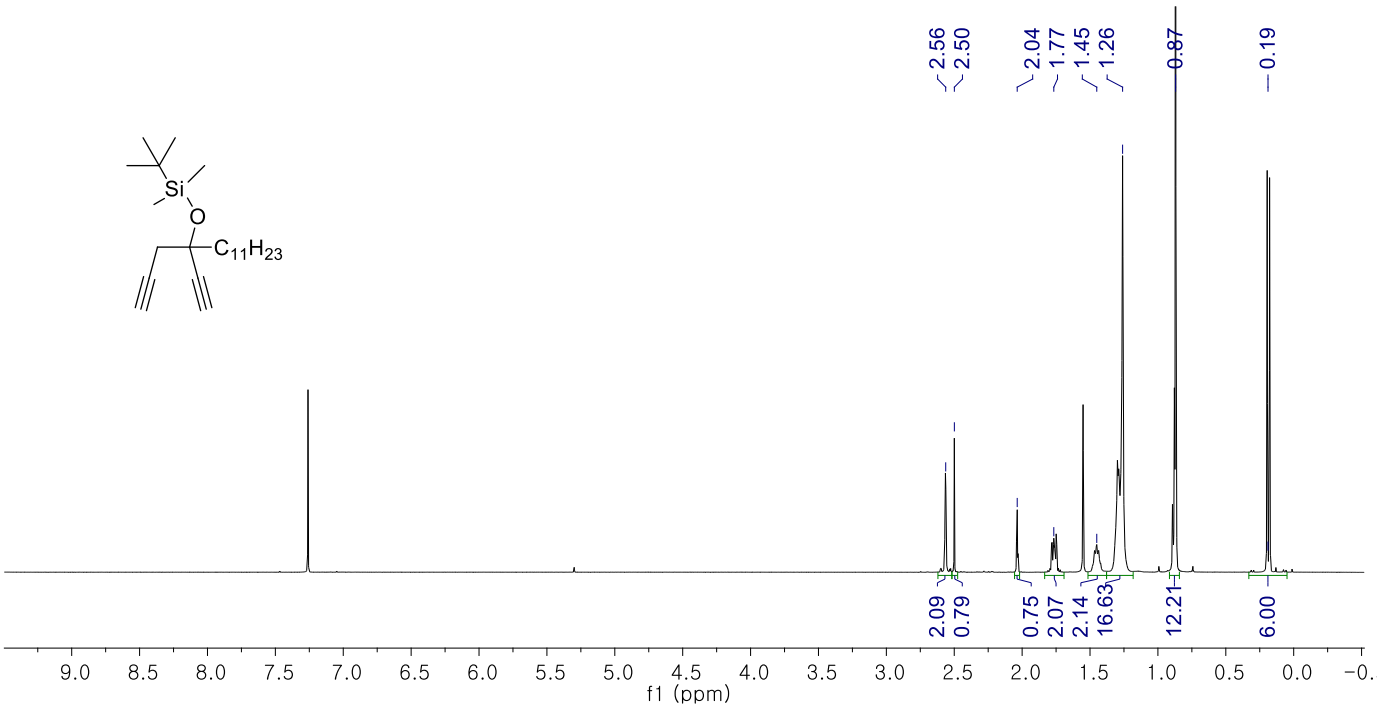
5 ^{1}H NMR (500 MHz, $CDCl_3$)



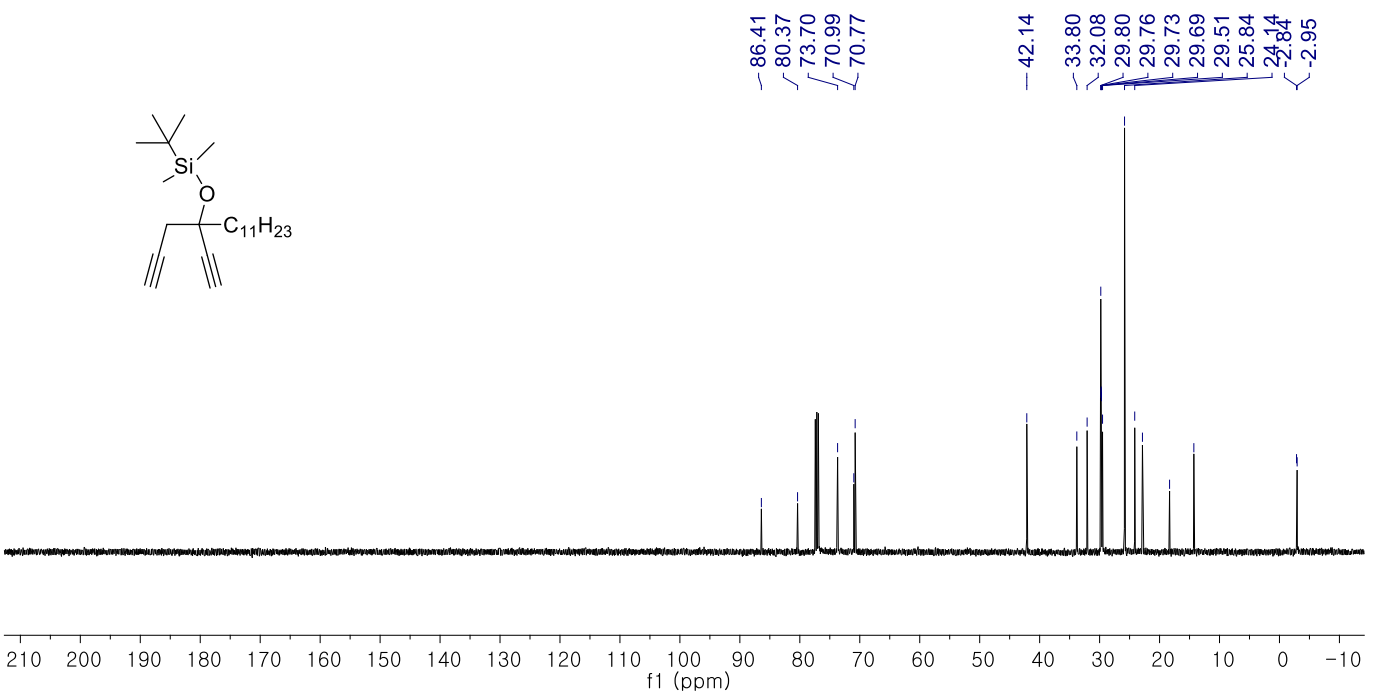
5 ^{13}C NMR (125 MHz, $CDCl_3$)



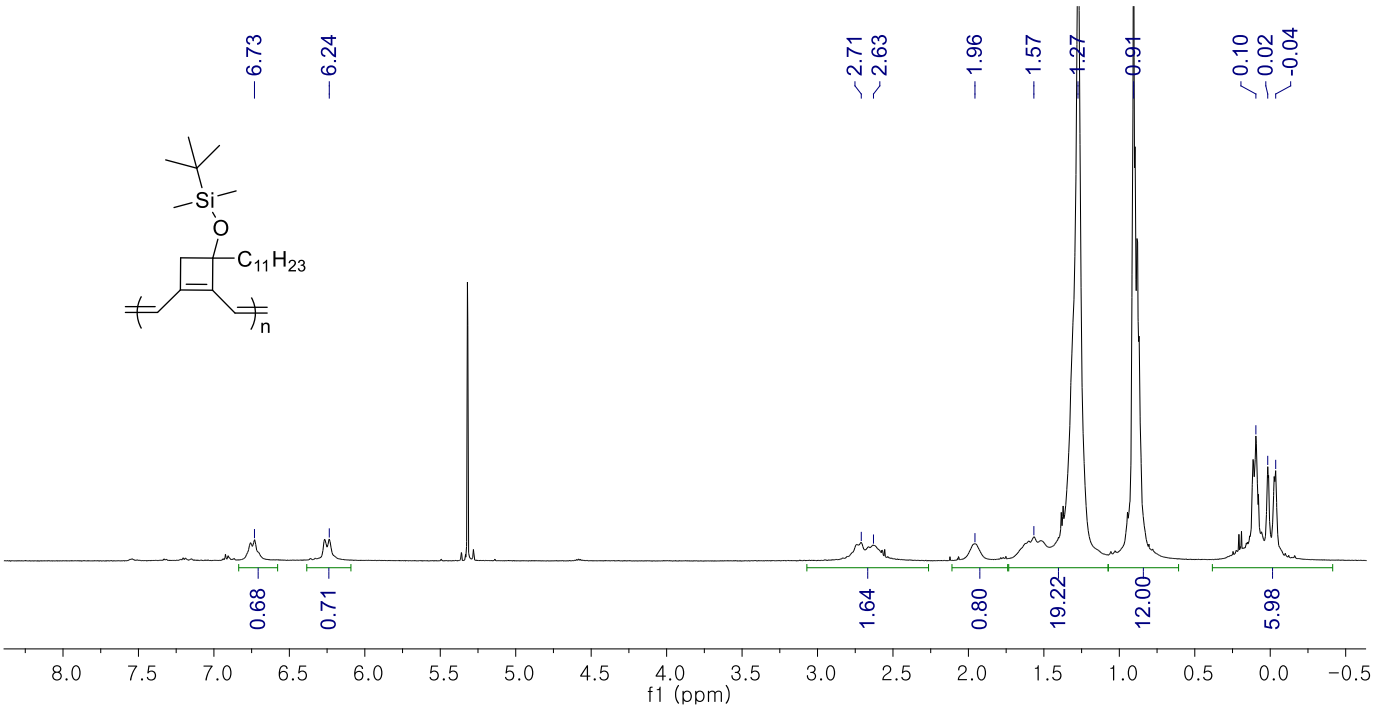
M7 ^{1}H NMR (500 MHz, $CDCl_3$)



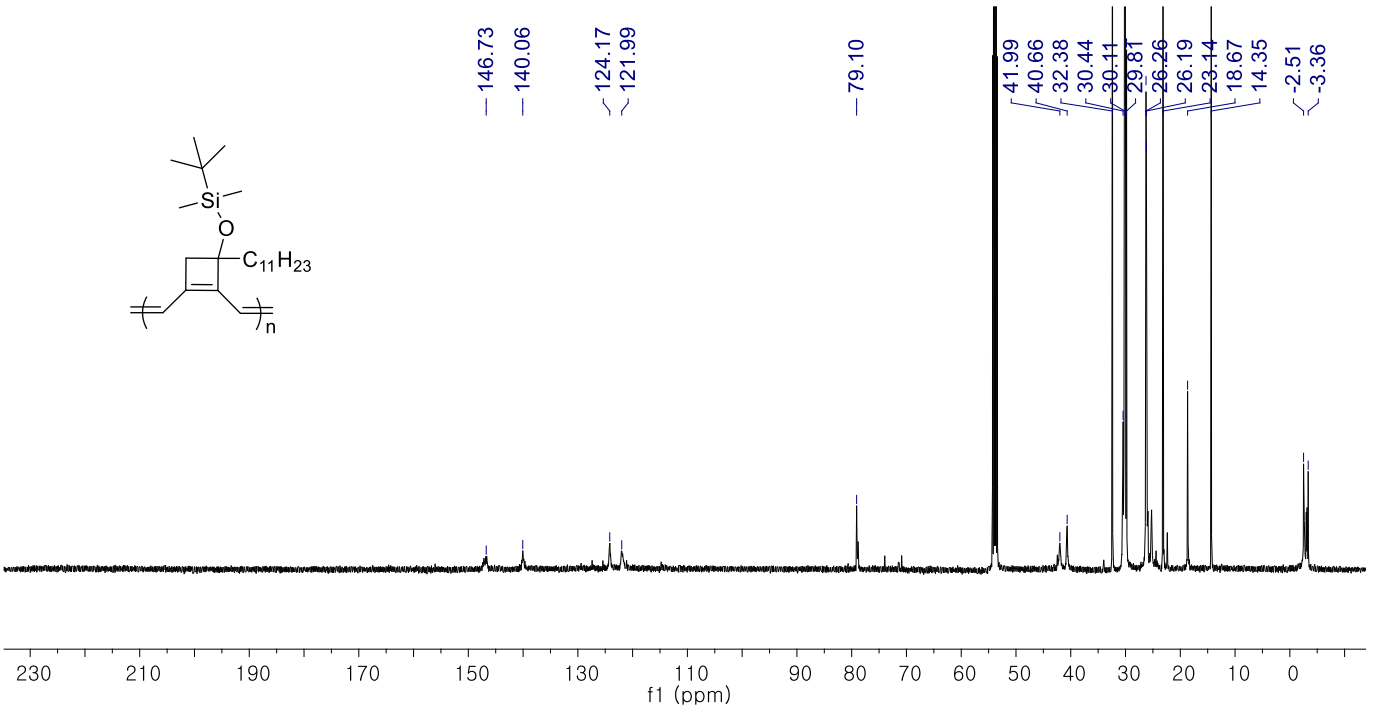
M7 ^{13}C NMR (125 MHz, $CDCl_3$)



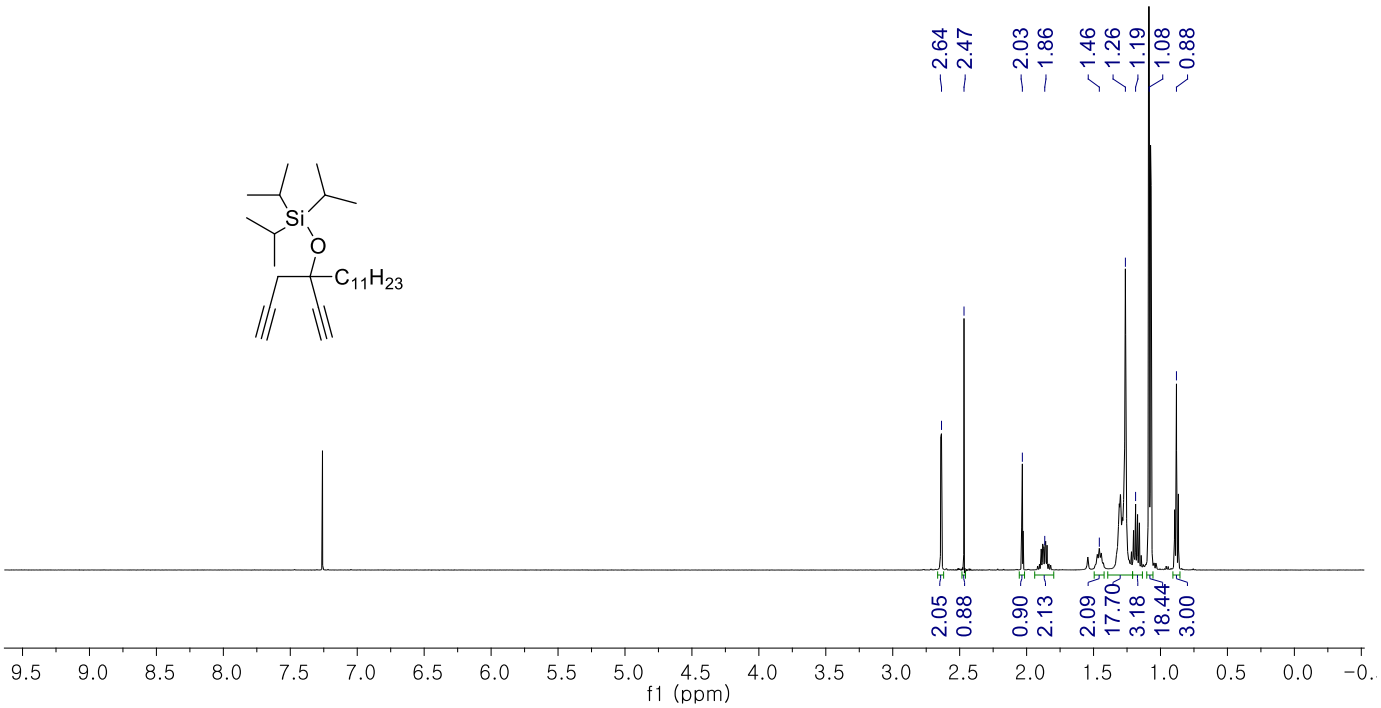
P7 ^{1}H NMR (500 MHz, CD_2Cl_2)



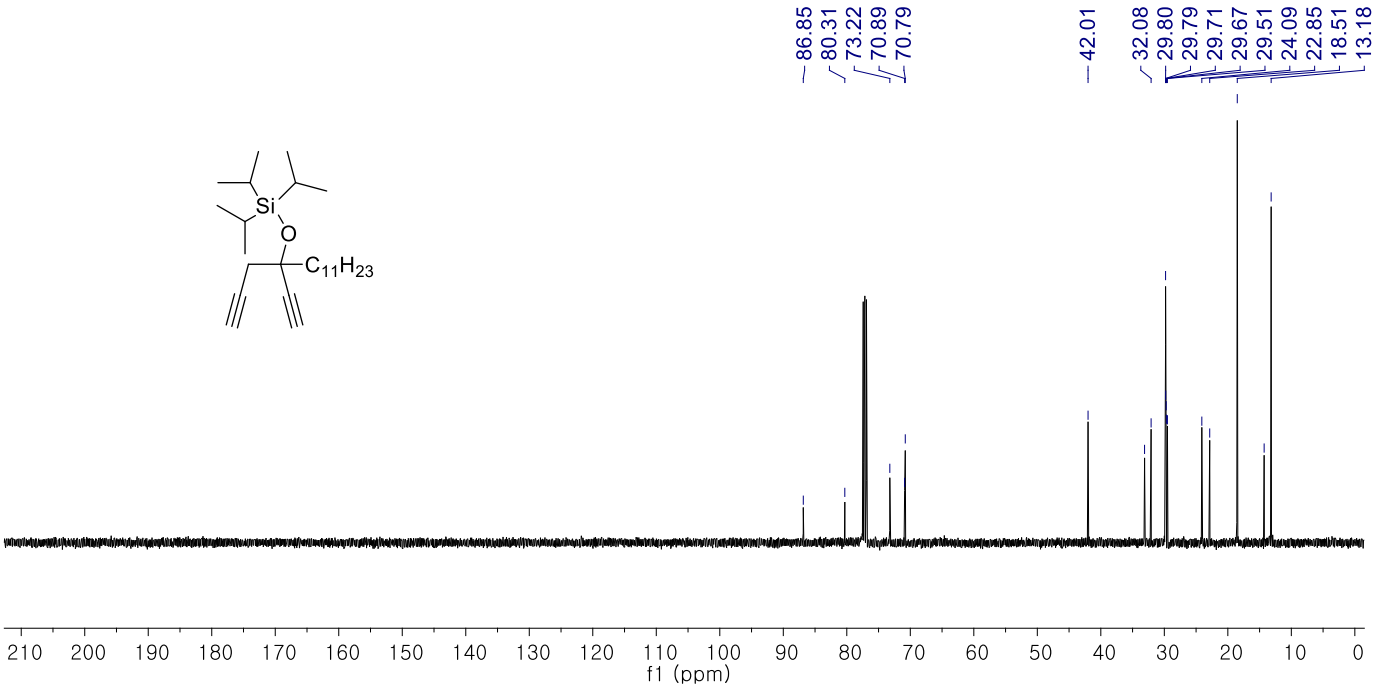
P7 ^{13}C NMR (125 MHz, CD_2Cl_2)



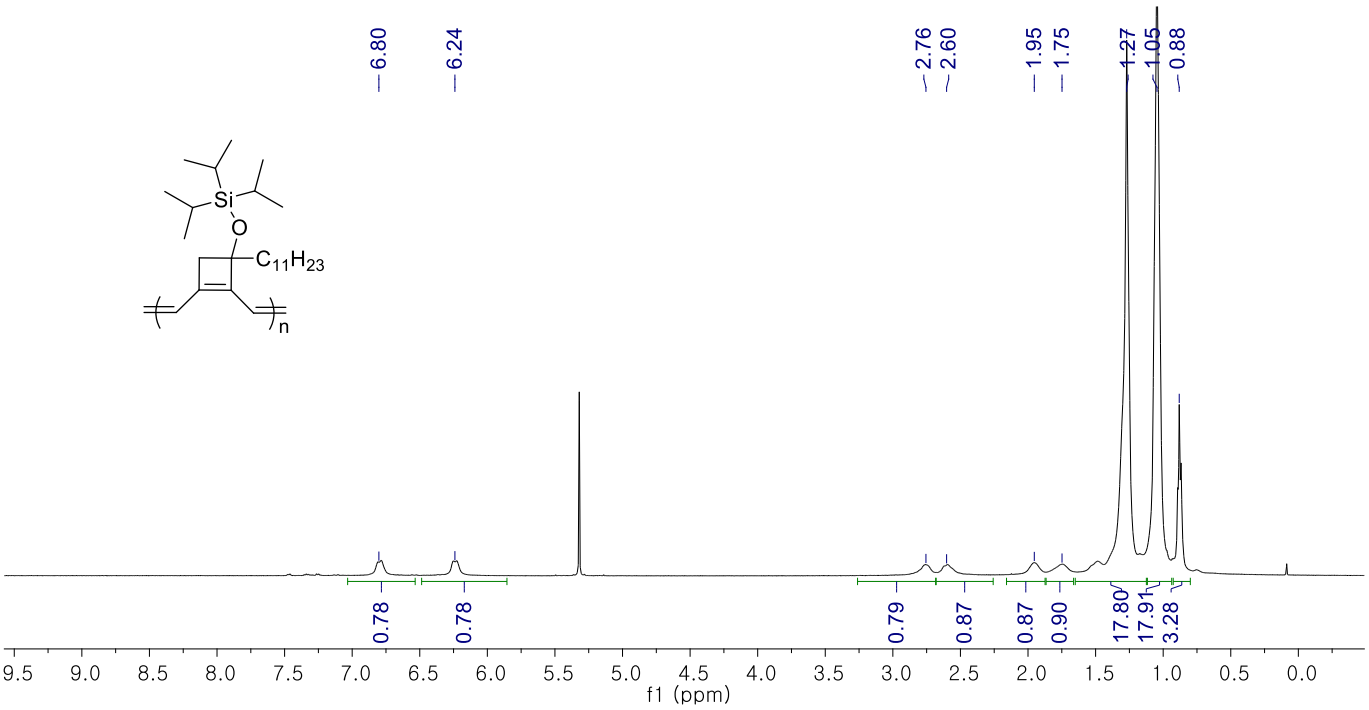
M8 ^{1}H NMR (500 MHz, $CDCl_3$)



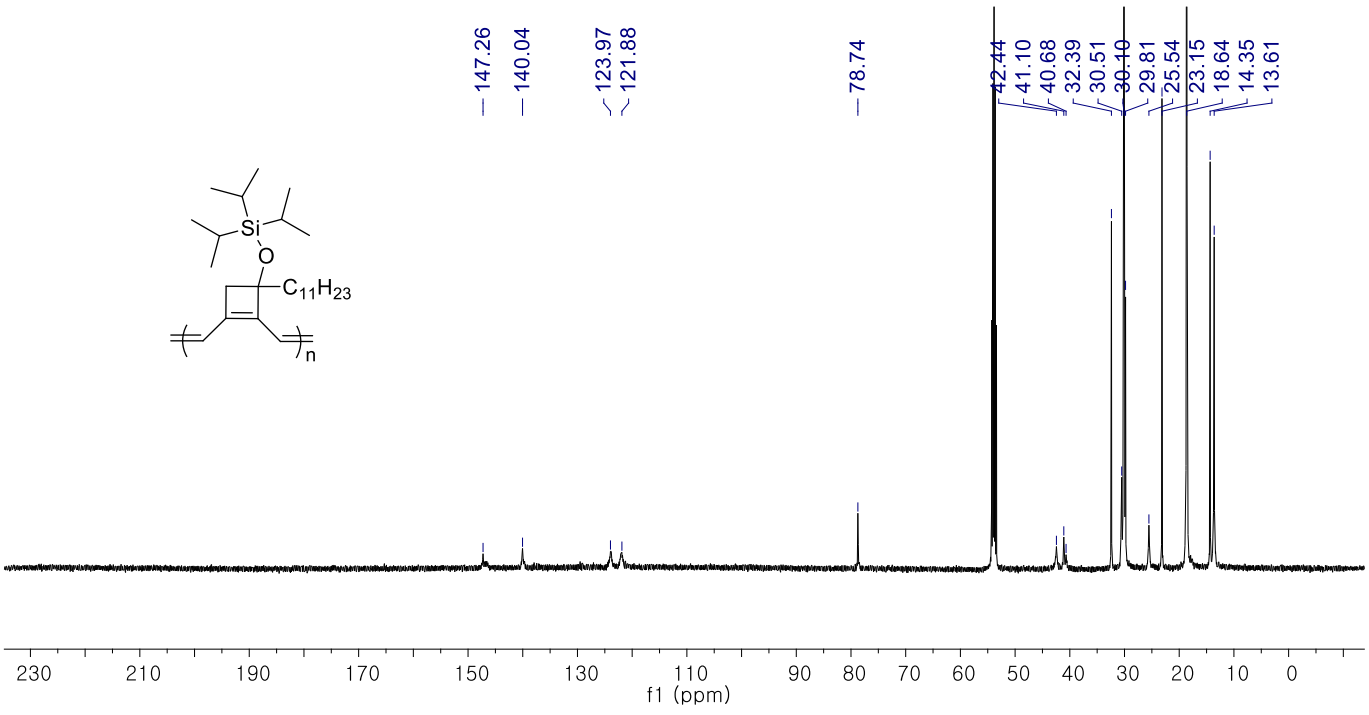
M8 ^{13}C NMR (125 MHz, $CDCl_3$)



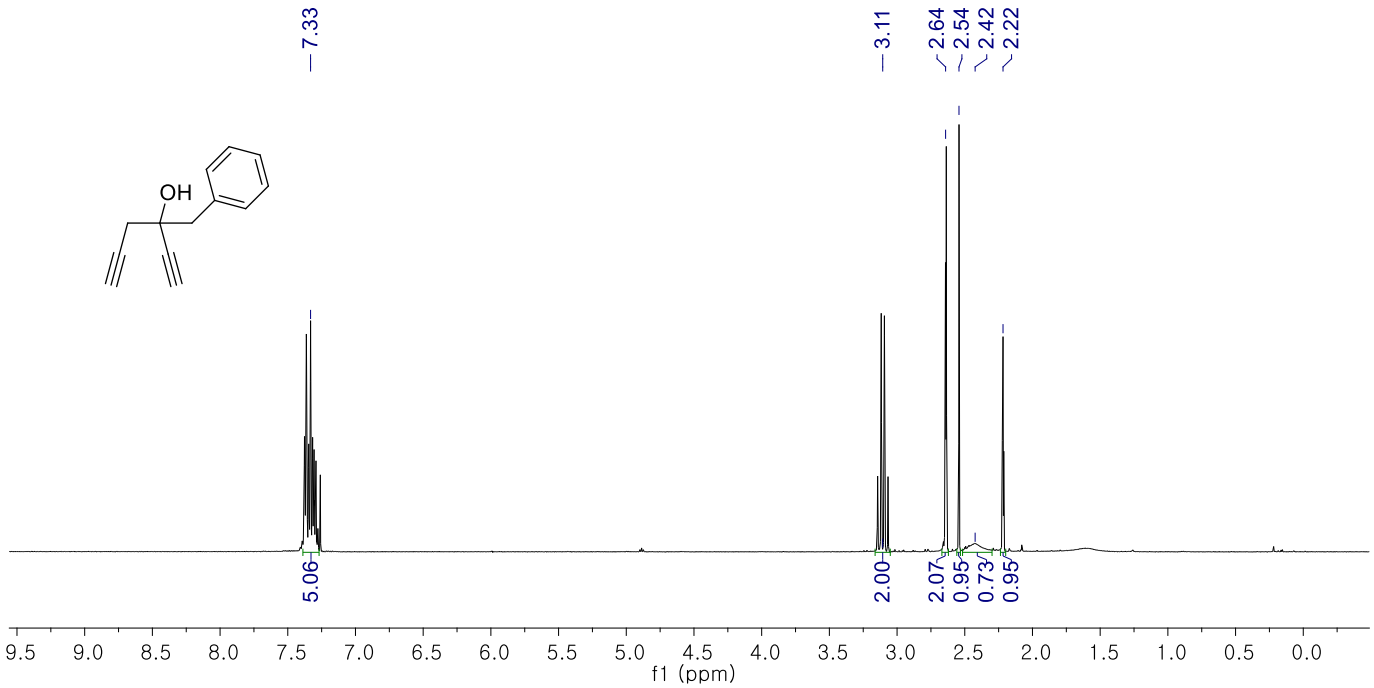
P8 ^{1}H NMR (500 MHz, CD_2Cl_2)



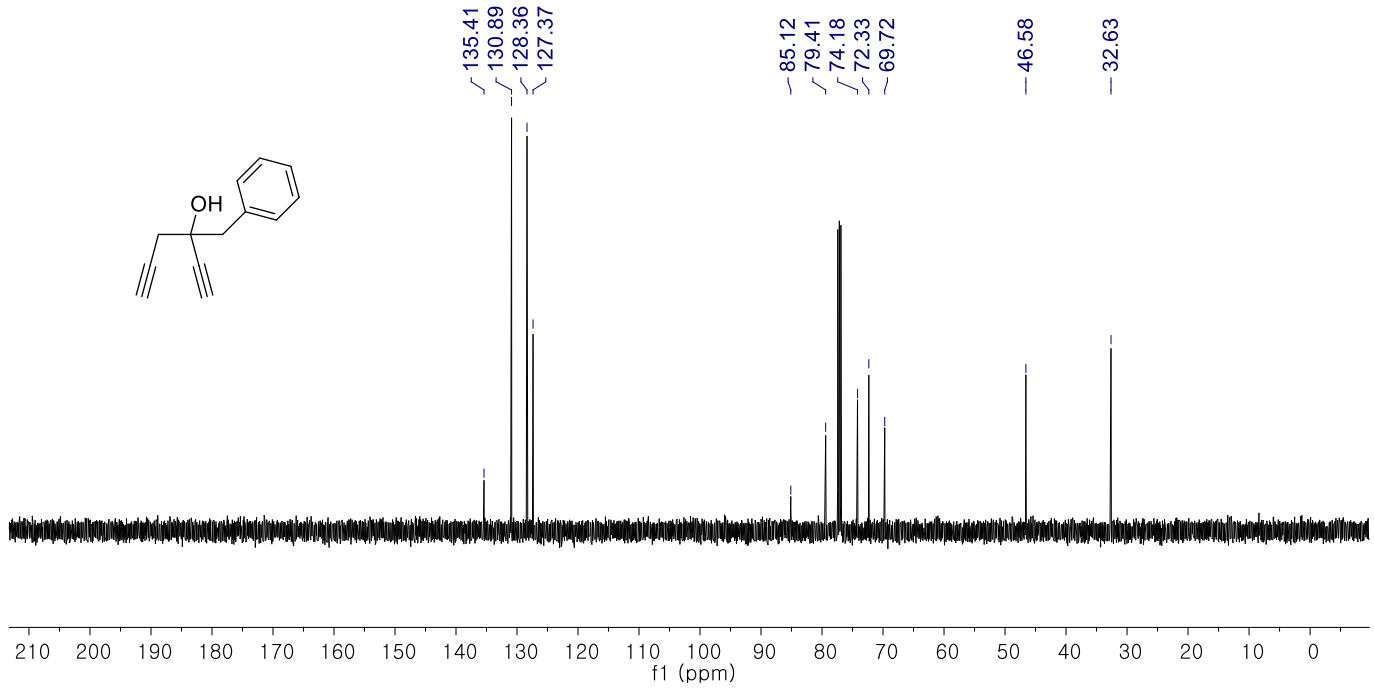
P8 ^{13}C NMR (125 MHz, CD_2Cl_2)



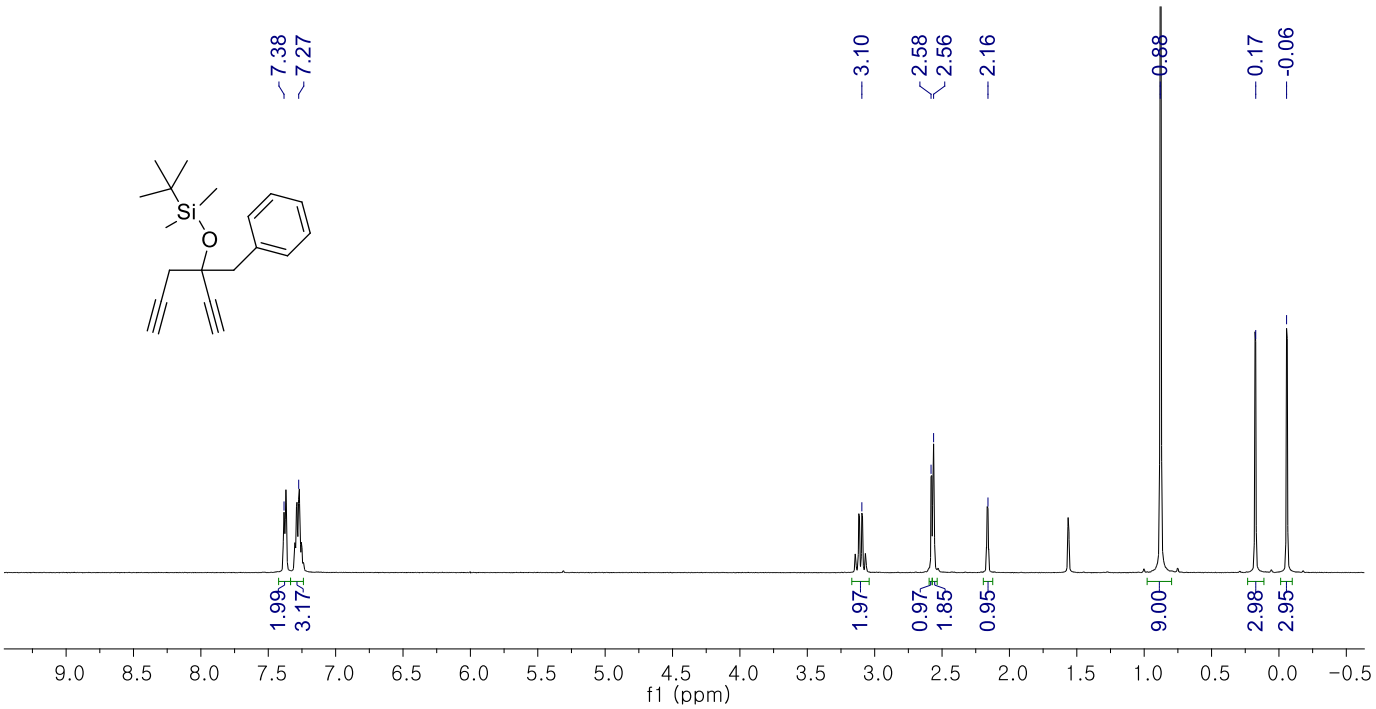
6 ^{1}H NMR (500 MHz, $CDCl_3$)



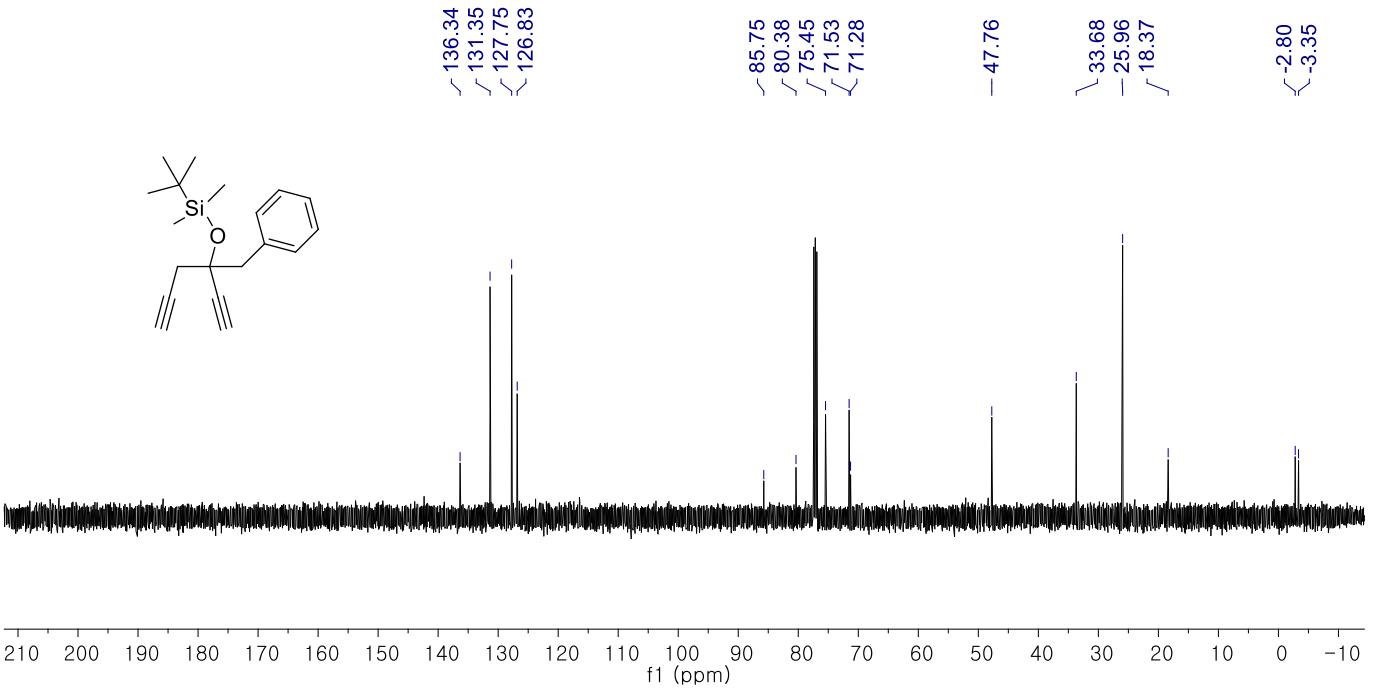
6 ^{13}C NMR (125 MHz, $CDCl_3$)



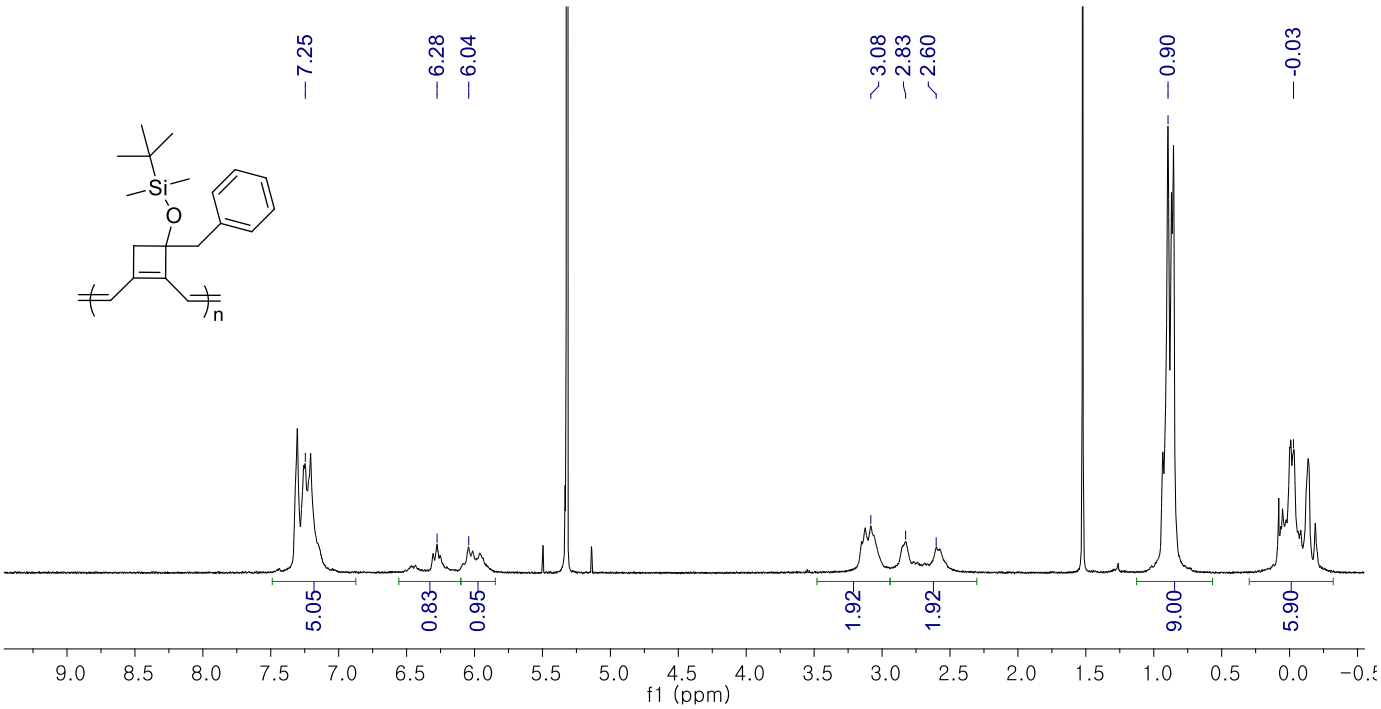
M9 ^{1}H NMR (500 MHz, $CDCl_3$)



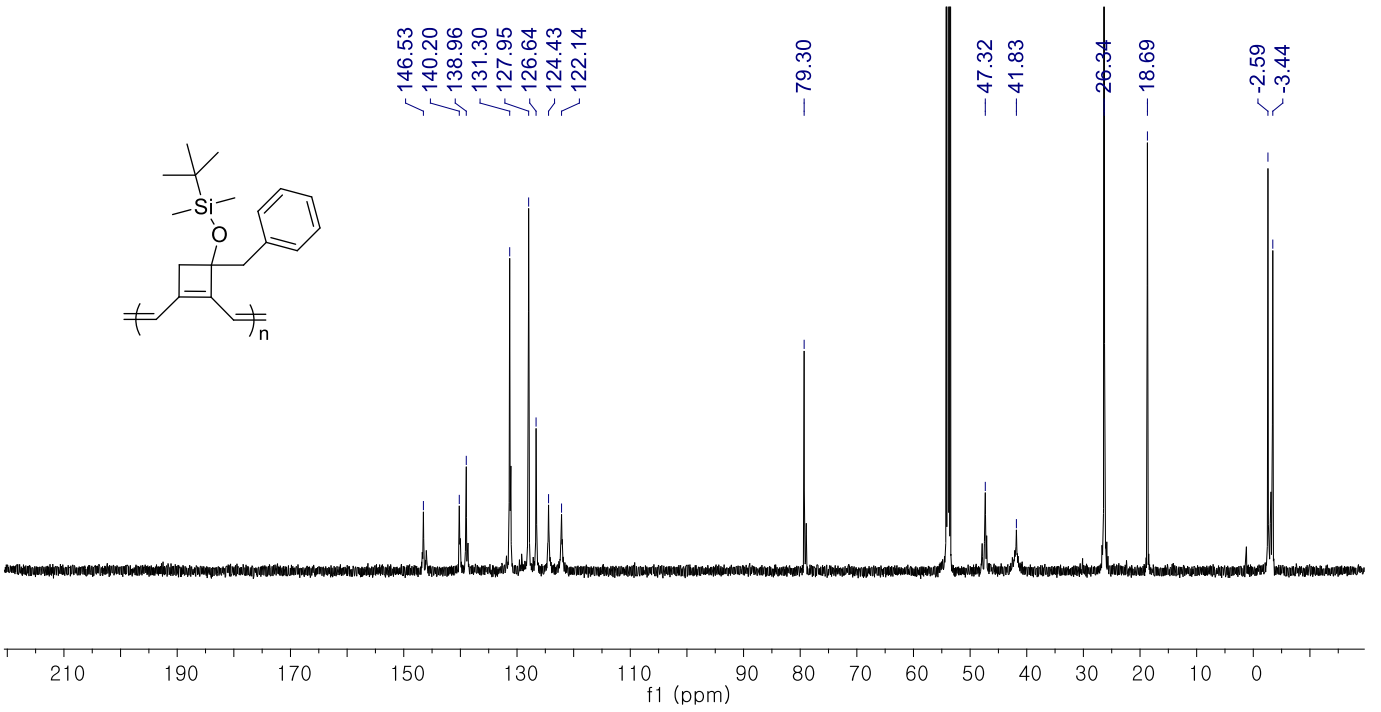
M9 ^{13}C NMR (125 MHz, $CDCl_3$)



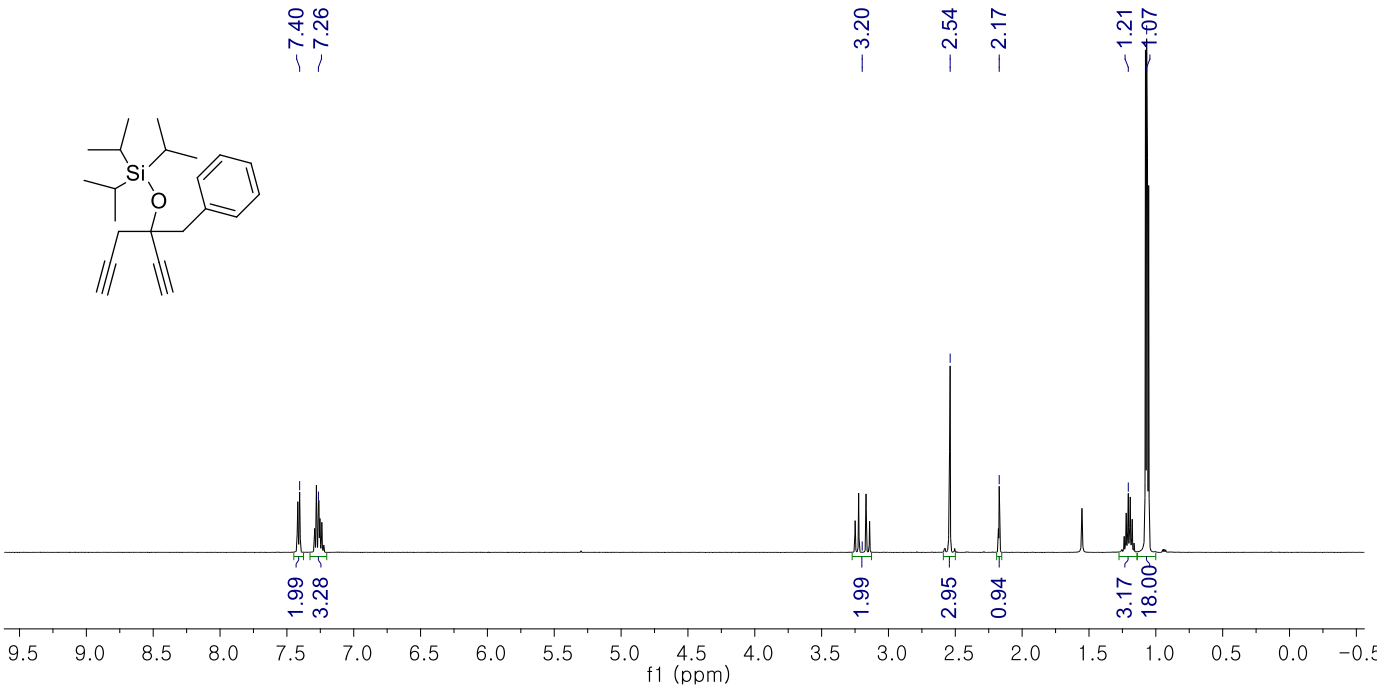
P9 ^{1}H NMR (500 MHz, CD_2Cl_2)



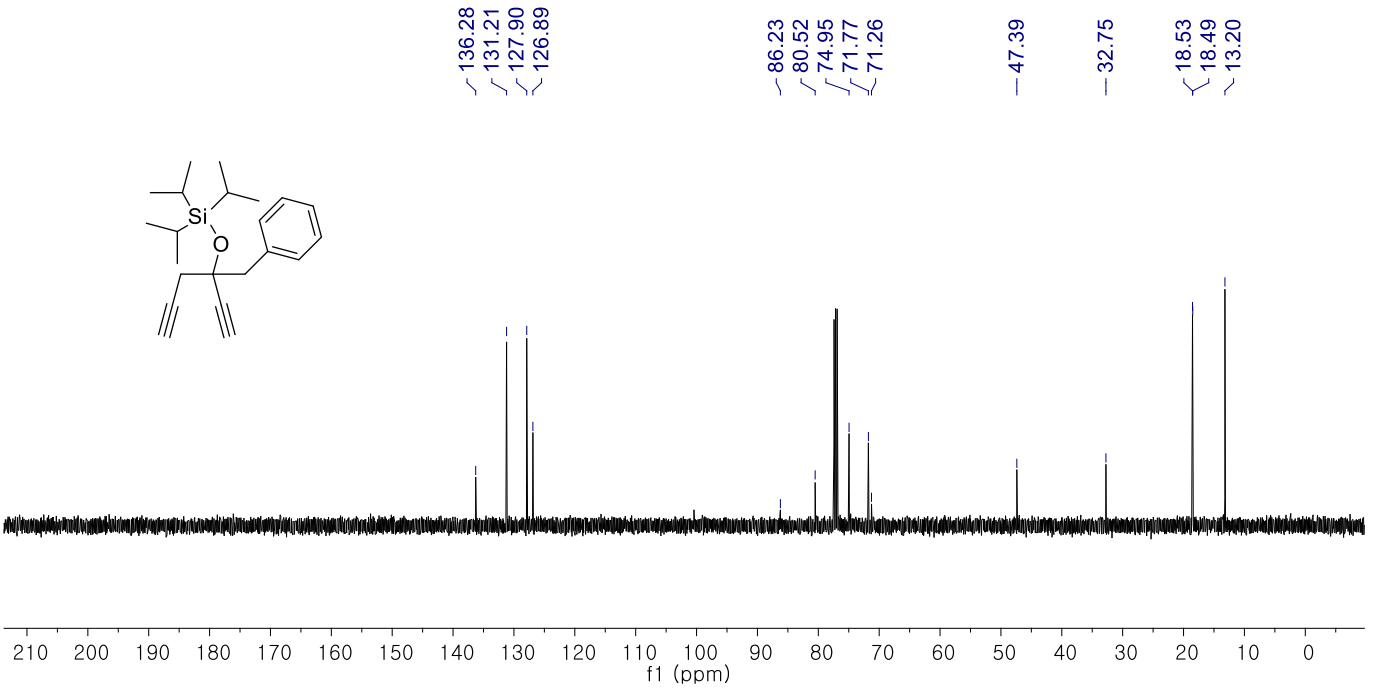
P9 ^{13}C NMR (150 MHz, CD_2Cl_2)



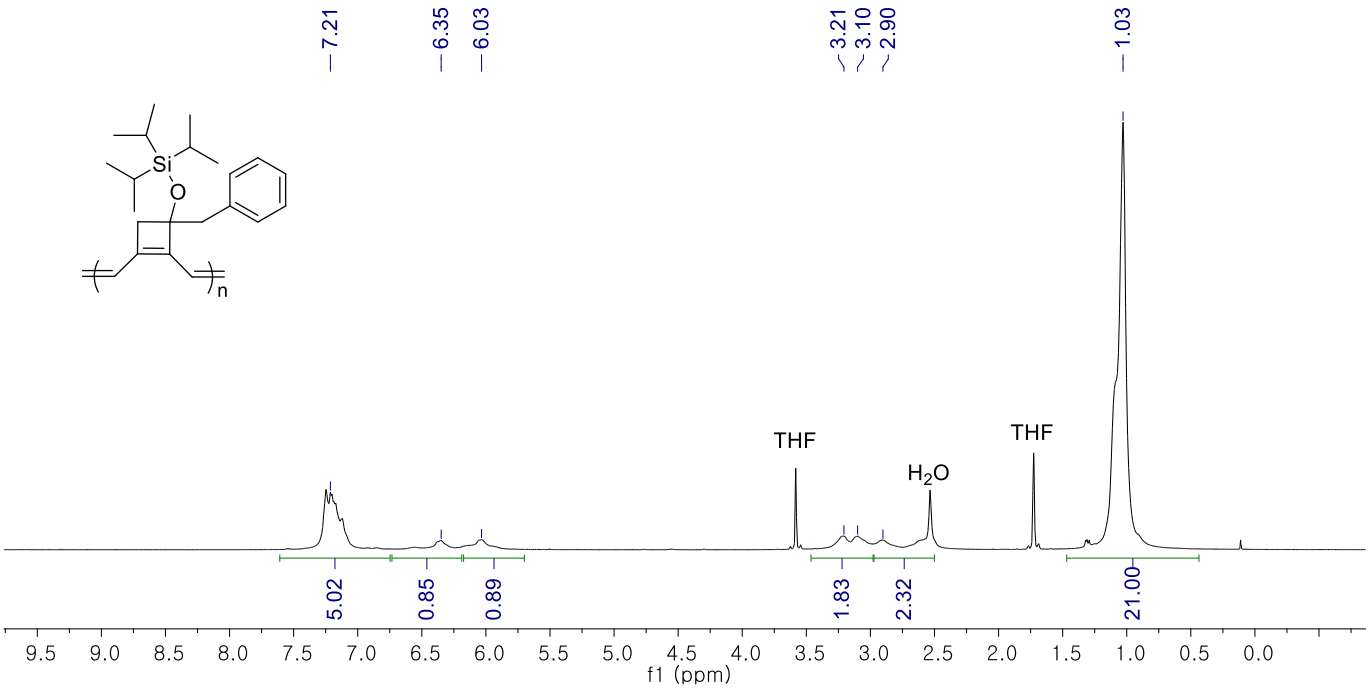
M10 ^{1}H NMR (500 MHz, $CDCl_3$)



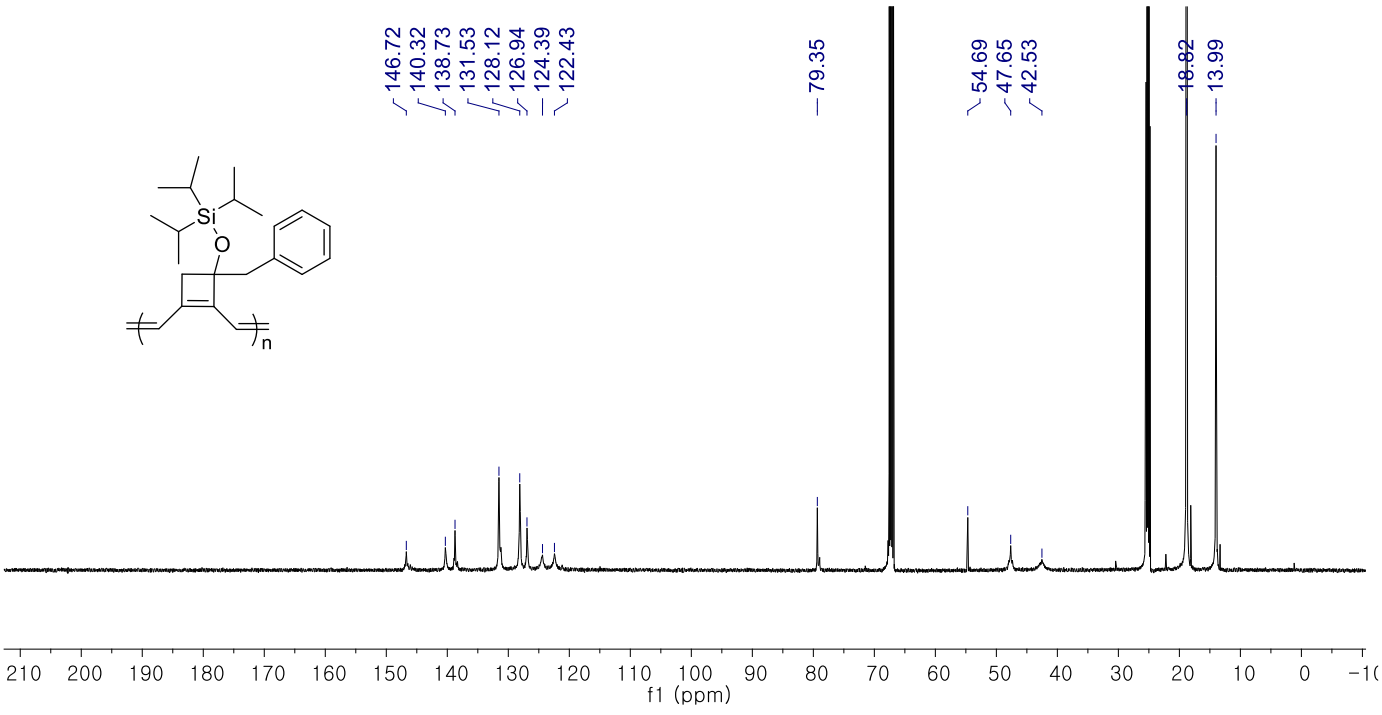
M10 ^{13}C NMR (125 MHz, $CDCl_3$)



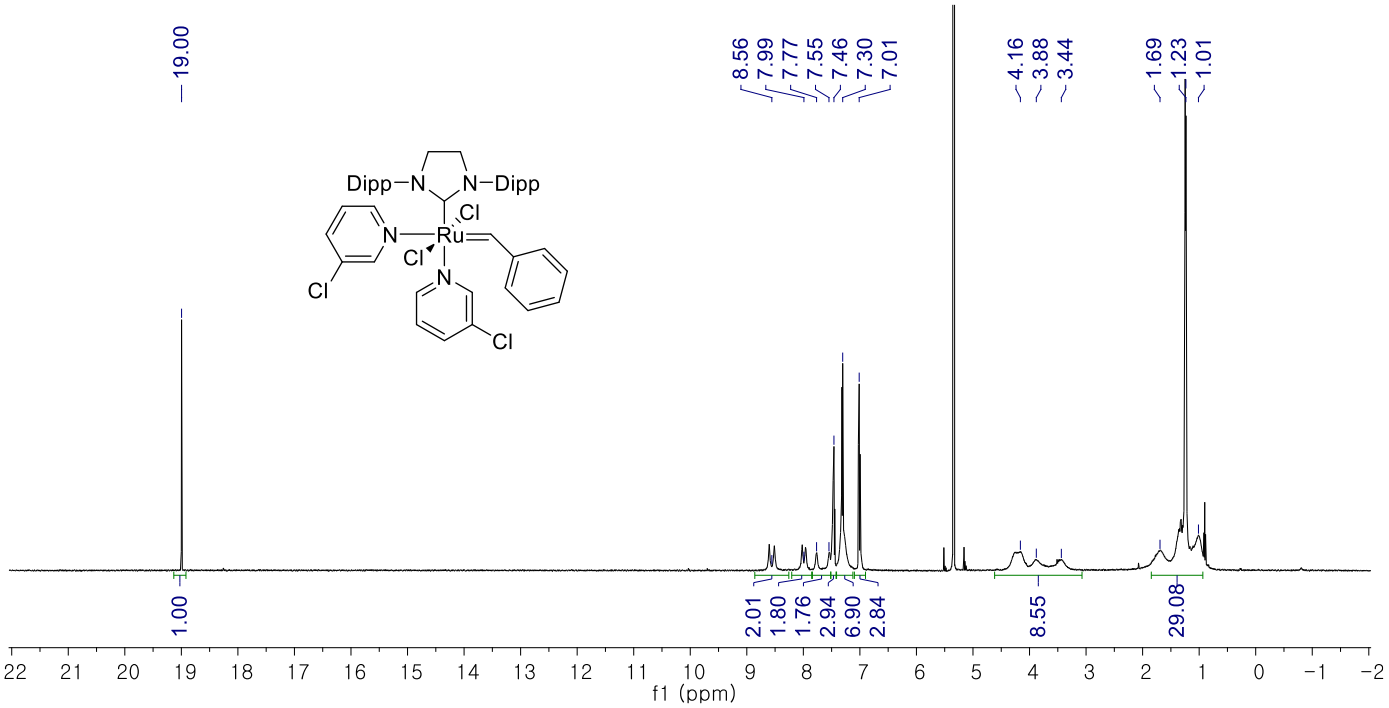
P10 ^{1}H NMR (500 MHz, THF-d_8)



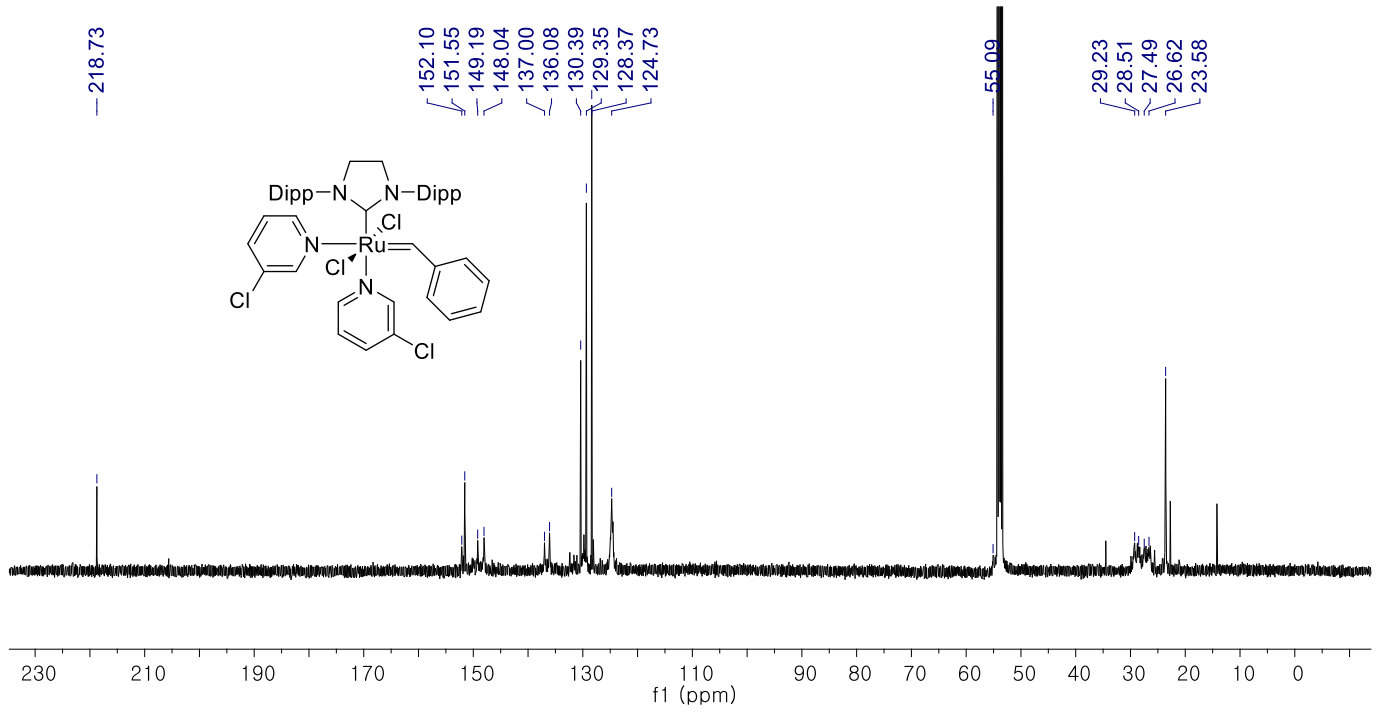
P10 ^{13}C NMR (125 MHz, THF-d_8)



Ru3 ^{1}H NMR (500 MHz, CD_2Cl_2)



Ru3 ^{13}C NMR (125 MHz, CD_2Cl_2)



9. References

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Appendix A. Cartesian Coordinates of the Optimized Geometries

A (DP = 1)

C	1.690129	-0.984768	-0.000259
H	1.333402	-2.014964	0.000065
C	0.682705	0.049584	-0.000022
C	0.784364	1.56672	-0.000076
C	-0.784364	1.56672	0.000076
H	1.246001	2.011905	-0.890099
H	1.246129	2.011951	0.889816
H	-1.246129	2.011951	-0.889816
H	-1.246001	2.011905	0.890099
C	-0.682705	0.049584	0.000022
C	-1.690129	-0.984768	0.000259
H	-1.333402	-2.014964	-0.000065
C	-3.013173	-0.75001	-0.000033
H	-3.410958	0.261802	-0.00034
H	-3.736269	-1.55985	-0.000391
C	3.013173	-0.75001	0.000033
H	3.736269	-1.55985	0.000391
H	3.410958	0.261802	0.00034

A (DP = 3)

C	-0.000027	7.725832	0.230463
H	-0.000021	8.12148	-0.782137
C	-0.000012	6.401755	0.468367
H	-0.00002	6.048626	1.499865
C	0.000012	5.39294	-0.55984
C	0.000011	5.487434	-2.076405
C	0.000072	3.919152	-2.072488
H	0.88958	5.948207	-2.523978
H	-0.889586	5.948145	-2.523989
H	0.890073	3.457055	-2.51686
H	-0.889869	3.456992	-2.516913
C	0.000016	4.021138	-0.553471
C	0.000004	3.026783	0.474104
H	-0.000025	3.376036	1.506724
C	0.000027	1.683643	0.239039
H	0.000052	1.335758	-0.79414
C	-0.000074	0.784018	2.780853
C	0.000011	0.688659	1.262325
C	-0.000011	-0.688659	1.262325
C	0.000074	-0.784018	2.780853
H	0.889539	1.245139	3.22748
H	-0.889803	1.244986	3.227411
H	0.889803	-1.244986	3.227411
H	-0.889539	-1.245139	3.22748
C	-0.000027	-1.683643	0.239039
H	-0.000052	-1.335758	-0.79414
C	-0.000004	-3.026783	0.474104
H	0.000025	-3.376036	1.506724
C	-0.000016	-4.021138	-0.553471
C	-0.000072	-3.919152	-2.072488
C	-0.000011	-5.487434	-2.076405
H	0.889869	-3.456992	-2.516913
H	-0.890073	-3.457055	-2.51686
H	0.889586	-5.948145	-2.523989
H	-0.88958	-5.948207	-2.523978
C	-0.000012	-5.39294	-0.55984
C	0.000012	-6.401755	0.468367
H	0.00002	-6.048626	1.499865
C	0.000027	-7.725832	0.230463
H	0.000047	-8.450419	1.038855
H	0.000021	-8.12148	-0.782137
H	-0.000047	8.450419	1.038855

A (DP = 5)

C	-12.439764	0.08603	0.000025
H	-12.833443	-0.927336	-0.000011
C	-11.116013	0.326534	0.000032
H	-10.765021	1.358768	0.000068
C	-10.105241	-0.699374	-0.000008
C	-10.196436	-2.216072	-0.000086
C	-8.628182	-2.208986	-0.000037
H	-10.656247	-2.664607	-0.88969
H	-10.656292	-2.664686	0.889452
H	-8.165178	-2.652438	-0.890009
H	-8.165223	-2.652466	0.889947
C	-8.732976	-0.690081	-0.000026
C	-5.501376	2.648253	0.000024
C	-5.404323	1.129958	0.000009
C	-4.0249	1.131958	0.000006

C	-3.933405	2.65108	0.000022
H	-5.963238	3.094252	-0.889569
H	-5.963228	3.094227	0.889635
H	-3.47332	3.098538	-0.889648
H	-3.47331	3.098526	0.889693
C	-6.396676	0.10627	-0.000009
H	-6.0474	-0.926457	-0.000026
C	-3.030174	0.112901	0.000003
H	-3.374933	-0.921294	0.000004
C	-7.741181	0.338916	-0.000007
H	-8.092165	1.370938	0.000013
C	-1.683922	0.351345	0.000004
H	-1.338908	1.385468	0.000003
C	-0.690335	-0.668035	0.000011
C	-0.783931	-2.186884	0.000036
C	0.783931	-2.186884	0.00003
H	-1.244878	-2.633679	-0.889572
H	-1.244883	-2.63366	0.889651
H	1.244883	-2.633681	-0.889575
H	1.244878	-2.633658	0.889649
C	0.690335	-0.668035	0.00002
C	1.683922	0.351345	0.000003
H	1.338908	1.385468	-0.00002
C	3.030174	0.112901	0.000008
H	3.374933	-0.921294	0.000029
C	3.933405	2.65108	-0.000081
C	4.0249	1.131958	-0.000021
C	5.404323	1.129958	-0.000034
C	5.501376	2.648253	-0.000066
H	3.473318	3.098503	-0.889768
H	3.473313	3.098562	0.889573
H	5.963236	3.094214	-0.889679
H	5.963231	3.094265	0.889524
C	6.396676	0.10627	-0.000002
H	6.0474	-0.926457	0.000035
C	7.741181	0.338916	-0.00001
H	8.092165	1.370938	-0.000047
C	8.732976	-0.690081	0.000026
C	8.628182	-2.208986	0.000077
C	10.196436	-2.216072	0.000098
H	8.16521	-2.652485	-0.889889
H	8.165191	-2.652419	0.890067
H	10.656279	-2.664692	-0.889445
H	10.656261	-2.664601	0.889696
C	10.105241	-0.699374	0.000016
C	11.116013	0.326534	-0.000036
H	10.765021	1.358768	-0.000082
C	12.439764	0.08603	-0.000029
H	13.165892	0.893032	-0.00007
H	12.833443	-0.927336	0.000015
H	-13.165892	0.893032	0.000055

A (DP = 10)

C	-18.183054	-0.13353	0.000504
H	-17.849479	0.904405	0.000847
C	-17.175367	-1.141761	-0.000018
C	-17.249108	-2.661339	-0.000566
C	-15.681315	-2.640331	-0.000765
H	-17.70425	-3.114039	-0.890256
H	-17.704015	-3.114694	0.888911
H	-15.214587	-3.080418	-0.890653
H	-15.214353	-3.081057	0.888684
C	-15.795718	-1.122686	-0.00021
C	-12.601884	2.241672	0.000458
C	-12.487818	0.724243	-0.000005
C	-11.10626	0.743137	-0.000118
C	-11.034195	2.263302	0.00026
H	-13.069094	2.682421	-0.888926
H	-13.068864	2.6819	0.890221
H	-10.57962	2.716689	-0.889275
H	-10.579392	2.716223	0.889915
C	-13.466503	-0.308326	-0.000213
H	-13.107051	-1.337519	-0.000574
C	-10.10013	-0.26185	-0.000455
H	-10.43127	-1.300514	-0.000655
C	-14.816585	-0.089285	0.000014
H	-15.176252	0.9398	0.000391
C	-8.755625	-0.005841	-0.000525
H	-8.424715	1.03291	-0.000329
C	-7.74934	-1.010212	-0.000799
C	-7.820412	-2.530342	-0.000971
C	-6.252741	-2.507999	-0.001269
H	-8.275064	-2.983665	-0.890522

H	-8.274758	-2.983927	0.888606	C	10.10013	0.261853	-0.000328
H	-5.785651	-2.948039	-0.891036	H	10.431271	1.300516	-0.00056
H	-5.785343	-2.948473	0.888117	C	11.106259	-0.743135	0.000016
C	-6.367145	-0.990433	-0.000843	C	11.034193	-2.2633	0.000459
C	-5.389815	0.041862	-0.0007	C	12.601882	-2.241671	0.000566
H	-5.749516	1.070953	-0.000514	H	10.579572	-2.716715	-0.889038
C	-4.03831	-0.176502	-0.000802	H	10.579436	-2.716192	0.890153
H	-3.678613	-1.205597	-0.000969	H	13.069045	-2.68242	-0.888843
C	-3.175562	2.373273	-0.000486	H	13.068908	-2.681899	0.890305
C	-3.061075	0.855739	-0.000697	C	12.487818	-0.724242	0.00012
C	-1.678662	0.87561	-0.000671	C	13.466504	0.308327	-0.000114
C	-1.607906	2.395811	-0.000648	H	13.107052	1.337519	-0.000477
H	-3.642954	2.813606	-0.889954	C	14.816585	0.089284	0.000083
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H	-1.153563	2.849345	-0.890241	C	15.681318	2.640329	-0.00072
H	-1.153394	2.849282	0.888889	C	15.79572	1.122685	-0.00017
C	-0.672416	-0.128278	-0.000701	C	17.175369	1.141758	0
H	-1.002902	-1.167158	-0.000704	C	17.24911	2.661336	-0.00059
C	0.672416	0.128284	-0.000714	H	15.214553	3.080413	-0.89059
H	1.002902	1.167165	-0.000726	H	15.214392	3.081059	0.888747
C	1.678662	-0.875604	-0.000685	H	17.704217	3.114016	-0.890309
C	1.607906	-2.395805	-0.000569	H	17.704055	3.114709	0.888859
C	3.175562	-2.373268	-0.000614	C	18.183054	0.133525	0.000518
H	1.15346	-2.849368	-0.890092	H	17.849478	-0.904408	0.000886
H	1.153496	-2.849246	0.889037	C	19.523983	0.386695	0.000584
H	3.642851	-2.813538	-0.890169	H	19.859142	1.423991	0.000212
H	3.642885	-2.813455	0.888963	C	20.531577	-0.626631	0.001121
C	3.061075	-0.855733	-0.00067	C	20.450871	-2.147018	0.001751
C	4.03831	0.176507	-0.000735	C	22.019057	-2.129301	0.001923
H	3.678614	1.205603	-0.00085	H	19.995087	-2.598148	-0.888094
C	6.252742	2.508004	-0.001004	H	19.994879	-2.597398	0.891869
C	6.367145	0.990438	-0.000768	H	22.486036	-2.570953	-0.887405
C	7.749341	1.010217	-0.000658	H	22.485828	-2.570215	0.891726
C	7.820413	2.530346	-0.000985	C	21.903912	-0.614225	0.001288
H	5.785514	2.948116	-0.89066	C	22.898215	0.427601	0.00098
H	5.785483	2.948406	0.888493	H	22.530821	1.454122	0.000514
H	8.27493	2.983613	-0.890636	C	24.225654	0.208205	0.001227
H	8.274896	2.983986	0.888492	H	24.938875	1.026644	0.000976
C	5.389815	-0.041857	-0.00067	H	24.635378	-0.798771	0.001689
H	5.749516	-1.070947	-0.000534	C	-22.898215	-0.427611	0.001117
C	8.755625	0.005844	-0.000363	H	-22.53082	-1.454131	0.00067
H	8.424714	-1.032907	-0.000141	C	-22.019059	2.129292	0.001949

C	-21.903913	0.614216	0.001369
C	-20.531577	0.626624	0.001155
C	-20.450874	2.147011	0.001771
H	-22.486044	2.570915	-0.887391
H	-22.485825	2.570236	0.89174
H	-19.995095	2.598131	-0.888082
H	-19.994876	2.597404	0.891881
C	-19.523982	-0.386701	0.000608
C	-24.225654	-0.208216	0.001392
H	-24.938874	-1.026655	0.001182
H	-24.635379	0.798759	0.001836
H	-19.85914	-1.423997	0.000264

A (DP = 15)

C	-6.403668	0.917644	-0.431364
H	-6.088407	1.954329	-0.311867
C	-5.386196	-0.063935	-0.577122
C	-5.445921	-1.573129	-0.764407
C	-3.87905	-1.536217	-0.788852
H	-5.913789	-1.917172	-1.695141
H	-5.880166	-2.137701	0.070018
H	-3.424856	-1.858399	-1.734079
H	-3.39267	-2.079141	0.031052
C	-4.003921	-0.031402	-0.598526
C	-0.784083	3.298957	-0.214022
C	-0.691369	1.791475	-0.40056
C	0.691403	1.791452	-0.400599
C	0.784177	3.298934	-0.214087
H	-1.244951	3.852089	-1.041759
H	-1.244733	3.633148	0.723867
H	1.244982	3.852033	-1.041881
H	1.244922	3.633137	0.723751
C	-1.678083	0.776168	-0.52149
H	-1.324978	-0.247162	-0.65045
C	1.678083	0.77612	-0.521589
H	1.324947	-0.247199	-0.650552
C	-3.029022	0.99635	-0.482758
H	-3.387588	2.017474	-0.352077
C	3.029028	0.996267	-0.482908
H	3.387625	2.01738	-0.352223
C	4.003899	-0.031505	-0.598729
C	3.878992	-1.536316	-0.789069
C	5.445861	-1.573267	-0.764627
H	3.424803	-1.85846	-1.734311
H	3.392585	-2.079251	0.030812
H	5.913735	-1.917347	-1.695344
H	5.880078	-2.137832	0.069818
C	5.386176	-0.06407	-0.577352
C	6.403665	0.917496	-0.431632
H	6.088417	1.954188	-0.312157
C	7.743675	0.635998	-0.429619
H	8.053996	-0.402409	-0.547704
C	8.739739	3.116408	-0.094329
C	8.770957	1.606172	-0.279247
C	10.151766	1.545033	-0.239699
C	10.305702	3.046967	-0.048967
H	8.328234	3.68886	-0.934832
H	8.267173	3.471265	0.829931
H	10.814574	3.578768	-0.862439
H	10.753345	3.36069	0.902205
C	11.09753	0.488681	-0.335514
H	10.70594	-0.519021	-0.47605
C	12.454662	0.654231	-0.261397
H	12.849717	1.660384	-0.119893
C	13.392586	-0.40968	-0.354668
C	13.218471	-1.909155	-0.548094
C	14.782308	-2.001593	-0.489552
H	12.774049	-2.215546	-1.503164
H	12.695172	-2.433956	0.260772
H	15.257755	-2.362683	-1.409924
H	15.178085	-2.580513	0.354097
C	14.771885	-0.491161	-0.303425
C	15.818067	0.45676	-0.138172
H	15.532769	1.502731	-0.024078
C	18.203845	2.588173	0.23953
C	18.199697	1.077615	0.054392
C	19.577418	0.981629	0.114246
C	19.766578	2.479121	0.307924
H	17.819338	3.170733	-0.606782
H	17.726756	2.954797	1.156841
H	20.300646	2.997829	-0.497818
H	20.208042	2.781432	1.265672
C	17.148632	0.135546	-0.11309

H	17.431377	-0.911217	-0.226563
C	20.49958	-0.09714	0.030549
H	20.087099	-1.09564	-0.115828
C	21.858361	0.039123	0.12205
H	22.272494	1.036833	0.26888
C	22.776953	-1.043344	0.039591
C	22.578443	-2.539591	-0.155282
C	24.139924	-2.65903	-0.080516
H	22.13881	-2.838644	-1.114872
H	22.037758	-3.054814	0.648261
H	24.618535	-3.028679	-0.995855
H	24.517049	-3.24425	0.767329
C	24.15307	-1.148708	0.105029
C	25.21315	-0.216166	0.279728
H	24.941445	0.833757	0.390941
C	26.537681	-0.554997	0.316244
H	26.808824	-1.60509	0.205476
C	27.616846	1.887207	0.67609
C	27.599646	0.376505	0.492129
C	28.973253	0.266925	0.562586
C	29.1778	1.76196	0.756405
H	27.244765	2.472712	-0.173696
H	27.136655	2.25929	1.589537
H	29.723393	2.274246	-0.045795
H	29.615333	2.060538	1.71719
C	29.888027	-0.823617	0.486419
H	29.466417	-1.818044	0.338102
C	31.243199	-0.699158	0.587006
H	31.666457	0.2944	0.735532
C	32.157075	-1.795121	0.511365
C	31.944795	-3.290212	0.317133
C	33.505502	-3.420054	0.401221
H	31.50887	-3.586445	-0.644817
H	31.396011	-3.799441	1.118755
H	33.987839	-3.793882	-0.510716
H	33.87471	-4.006338	1.252088
C	33.522552	-1.911748	0.584185
C	34.600969	-0.974738	0.765328
H	34.323586	0.074247	0.8723
C	35.902078	-1.314398	0.808473
H	36.680878	-0.570869	0.946993
H	36.224195	-2.347776	0.706483
C	-11.097525	0.488853	-0.335212
H	-10.705931	-0.518848	-0.475741
C	-10.305691	3.047134	-0.048601
C	-10.151762	1.545206	-0.239382
C	-8.770952	1.60634	-0.278937
C	-8.739729	3.116574	-0.094007
H	-10.814595	3.578971	-0.862029
H	-10.753296	3.360816	0.902603
H	-8.328258	3.689023	-0.934528
H	-8.267128	3.471437	0.830233
C	-7.74368	0.636161	-0.429343
H	-8.054014	-0.402239	-0.547454
C	-33.522538	-1.911886	0.584058
C	-33.505466	-3.420199	0.401154
C	-31.944759	-3.290342	0.317098
H	-33.987776	-3.794069	-0.51078
H	-33.874688	-4.006453	1.252035
H	-31.508807	-3.586616	-0.644828
H	-31.395986	-3.799523	1.118758
C	-32.157062	-1.795242	0.511244
C	-29.177855	1.761901	0.756143
C	-28.973276	0.26686	0.562404
C	-27.59967	0.376461	0.491978
C	-27.6169	1.88717	0.675881
H	-29.72342	2.274131	-0.046112
H	-29.615439	2.060526	1.716891
H	-27.24479	2.472655	-0.173906
H	-27.136754	2.259286	1.589338
C	-29.888029	-0.823703	0.486281
H	-29.466399	-1.818131	0.338027
C	-26.537683	-0.555025	0.316143
H	-26.808803	-1.605124	0.205374
C	-31.243205	-0.699262	0.586837
H	-31.666482	0.294299	0.735296
C	-25.213156	-0.216171	0.279671
H	-24.941474	0.833759	0.390881
C	-24.153053	-1.148696	0.105021
C	-24.139873	-2.659024	-0.080476
C	-22.578392	-2.539558	-0.155201
H	-24.618447	-3.028703	-0.995823
H	-24.517017	-3.244233	0.767369
H	-22.138721	-2.83863	-1.114767

H	-22.037726	-3.054749	0.648375
C	-22.776934	-1.043311	0.039641
C	-21.858365	0.039175	0.122101
H	-22.27252	1.036882	0.268883
C	-20.49958	-0.097068	0.030648
H	-20.087077	-1.095566	-0.115688
C	-19.766625	2.479206	0.308026
C	-19.577437	0.981718	0.114342
C	-18.199718	1.077726	0.054513
C	-18.203894	2.588286	0.239627
H	-20.300714	2.99792	-0.497699
H	-20.208081	2.781489	1.265786
H	-17.819407	3.170827	-0.606709
H	-17.726804	2.954951	1.156921
C	-17.148635	0.135672	-0.112953
H	-17.431365	-0.91109	-0.226468
C	-15.818072	0.456902	-0.137979
H	-15.532791	1.502874	-0.02385
C	-14.771876	-0.491006	-0.303221
C	-14.782283	-2.001436	-0.489364
C	-13.218443	-1.908986	-0.547857
H	-15.257695	-2.362521	-1.409755
H	-15.178083	-2.580366	0.354267
H	-12.773991	-2.21536	-1.502917
H	-12.695165	-2.433793	0.261019
C	-13.392576	-0.409514	-0.354418
C	-12.45466	0.654401	-0.261124
H	-12.849719	1.660554	-0.11963
C	-34.600967	-0.974881	0.765151
H	-34.323597	0.074114	0.87207
C	-35.902072	-1.314553	0.808312
H	-36.224176	-2.347941	0.706376
H	-36.680881	-0.571027	0.946795

B (DP = 1)

C	-1.548219	-1.264314	-0.046431
H	-1.062475	-2.234476	-0.135927
C	-0.682454	-0.098962	-0.000133
C	-1.224822	1.313583	0.114637
C	0.682454	-0.098962	-0.000133
C	0	2.202424	-0.195871
H	-1.608541	1.489207	1.131379
H	-2.062731	1.500826	-0.567992
C	1.224822	1.313583	0.114637
H	0	2.461723	-1.26082
H	0	3.140914	0.367345
H	2.062731	1.500826	-0.567992
H	1.608541	1.489207	1.131379
C	1.548219	-1.264314	-0.046431
H	1.062475	-2.234476	-0.135927
C	-2.890176	-1.235005	0.01767
H	-3.446991	-0.307018	0.112273
H	-3.475342	-2.148939	-0.019843
C	2.890176	-1.235005	0.01767
H	3.475342	-2.148939	-0.019843
H	3.446991	-0.307018	0.112273

B (DP = 3)

C	5.99332	0.509697	-0.040942
C	5.127104	-0.651591	0.005555
C	5.666088	-2.064791	0.115164
C	3.756131	-0.647495	0.01009
C	4.440884	-2.949807	-0.201582
H	6.04723	-2.24728	1.132034
H	6.505441	-2.251168	-0.566101
C	3.218171	-2.064169	0.123616
H	4.437149	-3.196371	-1.269602
H	4.442012	-3.894816	0.3507
H	2.375153	-2.252646	-0.552069
H	2.845863	-2.245732	1.143437
H	5.509171	1.481231	-0.125404
C	2.902836	0.512576	-0.032658
H	3.391775	1.479977	-0.119324
C	1.541928	0.483264	0.028231
H	1.054307	-0.484965	0.114401
C	0.688195	1.640037	-0.014633
C	1.223182	3.057161	-0.124188
C	-0.688191	1.64004	-0.014658
C	0.000003	3.939163	0.206371
H	1.592846	3.244428	-1.144214
H	2.067554	3.245075	0.550061
C	-1.223169	3.057165	-0.124227

H	-0.000014	4.173993	1.277072
H	0.000013	4.889995	-0.335834
H	-2.067561	3.245082	0.549996
H	-1.592803	3.244434	-1.144263
C	-1.541929	0.483267	0.02817
H	-1.054309	-0.484965	0.114304
C	-2.902837	0.512588	-0.032713
H	-3.391772	1.479991	-0.119367
C	-3.756135	-0.647486	0.009997
C	-5.127105	-0.651586	0.005634
C	-3.218156	-2.064174	0.123274
C	-5.666092	-2.064799	0.115019
C	-4.440901	-2.949783	-0.201893
H	-2.845712	-2.245872	1.143023
H	-6.047242	-2.24745	1.131854
H	-6.505447	-2.251058	-0.566278
H	-4.44199	-3.894825	0.35033
H	-4.437256	-3.196288	-1.269926
C	-5.993318	0.509727	-0.040504
H	-5.509168	1.481282	-0.124679
C	-7.336899	0.479712	0.017038
H	-7.922043	1.393595	-0.020712
H	-7.893829	-0.448724	0.105987
H	-2.375225	-2.252543	-0.552546
C	7.336892	0.479729	0.01683
H	7.922012	1.393622	-0.021059
H	7.89383	-0.448659	0.106224

B (DP = 5)

C	11.755616	0.27504	-0.510573
H	12.308625	-0.659294	-0.546136
C	10.425189	0.316466	-0.315775
C	9.569499	-0.838673	-0.131178
C	10.106752	-2.256729	-0.12575
C	8.205182	-0.830167	0.007076
C	8.928858	-3.093036	0.420223
H	11.013466	-2.363043	0.482493
H	10.382654	-2.561605	-1.147285
C	7.67108	-2.248252	0.121041
H	8.88116	-4.097193	-0.012731
H	6.904946	-2.350619	0.899085
H	9.038377	-3.210469	1.504482
H	7.195912	-2.549813	-0.824911
C	7.350704	0.329123	-0.001126
H	7.836713	1.298057	-0.086447
C	5.990133	0.297052	0.076856
H	5.504689	-0.673375	0.149756
C	5.135143	1.452141	0.05648
C	5.667234	2.871307	-0.038559
C	3.757256	1.450262	0.065974
C	4.445709	3.746905	0.313787
H	6.027955	3.073119	-1.059083
H	6.517038	3.051519	0.630983
C	3.221522	2.868936	-0.022978
H	4.452352	3.964637	1.388098
H	4.441446	4.706261	-0.213226
H	2.379811	3.048002	0.656901
H	2.848239	3.069412	-1.039148
C	2.906016	0.294318	0.101365
H	3.394017	-0.674624	0.176613
C	1.542157	0.323605	0.045465
C	0.689919	-0.831006	0.079905
C	1.222831	-2.249327	0.186597
C	-0.689019	-0.831125	0.070945
C	0.00204	-3.128953	-0.158086
H	1.583833	-2.442165	1.208696
H	2.072456	-2.434894	-0.481622
C	-1.222938	-2.249501	0.171805
H	0.008523	-3.355492	-1.230587
H	-0.001108	-4.083962	0.3768
H	-2.064577	-2.435455	-0.506335
H	-1.595871	-2.442117	1.189653
H	1.054998	1.292837	-0.031457
C	-1.540989	0.32323	0.023298
H	-1.053188	1.292267	-0.052105
C	-2.905376	0.293726	0.064238
H	-3.393722	-0.675096	0.138659
C	-3.756738	1.449018	0.01352
C	-3.220846	2.867175	-0.082277
C	-5.134524	1.450135	-0.007184
C	-4.448181	3.747353	0.236857
H	-2.838925	3.05954	-1.09679
H	-2.38506	3.052183	0.60331

C	-5.666428	2.868216	-0.118112
H	-4.463849	3.97419	1.30919
H	-4.439922	4.7022	-0.298237
H	-6.521599	3.053514	0.543144
H	-6.01916	3.061464	-1.143069
C	-5.988889	0.294656	0.017228
H	-5.503258	-0.674315	0.10649
C	-7.34926	0.324828	-0.064871
H	-7.83625	1.29289	-0.154917
C	-8.203352	-0.83459	-0.040696
C	-9.574377	-0.838151	-0.067687
C	-7.668037	-2.252101	0.075733
C	-10.115477	-2.251539	0.027741
C	-8.88569	-3.135761	-0.272934
H	-7.31237	-2.438062	1.100674
H	-10.512775	-2.438005	1.037689
H	-10.94394	-2.434997	-0.667528
H	-8.8961	-4.083138	0.275203
H	-8.864814	-3.377792	-1.341796
C	-10.439135	0.323579	-0.124137
H	-9.953184	1.295204	-0.196572
C	-11.783596	0.294218	-0.089406
H	-12.367464	1.208625	-0.133673
H	-12.342526	-0.634152	-0.01327
H	-6.814284	-2.438259	-0.586979
H	12.332988	1.184813	-0.644497
H	9.943844	1.29293	-0.298337

B (DP = 10)

C	1.567215	-1.072482	-1.270489
C	1.070132	-2.506154	-1.338926
C	2.946065	-1.039628	-1.225545
C	2.325604	-3.313381	-1.732193
H	0.249213	-2.636281	-2.054446
H	0.679849	-2.819442	-0.35817
C	3.513944	-2.447977	-1.26128
H	2.33609	-4.321637	-1.306227
H	4.383472	-2.538195	-1.923547
H	2.36276	-3.419256	-2.822592
H	3.856251	-2.744163	-0.257578
C	3.766729	0.130629	-1.105321
H	3.25659	1.090963	-1.089749
C	5.12845	0.125845	-0.993287
H	5.63731	-0.83525	-0.995084
C	5.947887	1.295093	-0.855429
C	5.381218	2.704186	-0.835424
C	7.3154	1.320527	-0.672455
C	6.622577	3.604384	-1.013231
H	4.877154	2.8964	0.124402
H	4.630453	2.870334	-1.617477
C	7.805066	2.749165	-0.509982
H	6.761403	3.826186	-2.077707
H	6.534604	4.561578	-0.489632
H	8.729007	2.946744	-1.066832
H	8.030338	2.954728	0.547986
C	8.184872	0.182719	-0.588852
H	7.731546	-0.795182	-0.732394
C	9.527304	0.236963	-0.341183
C	10.395927	-0.901761	-0.256341
C	9.908768	-2.328188	-0.444511
C	11.759313	-0.879134	-0.047004
C	11.08277	-3.190852	0.065903
H	9.698979	-2.519617	-1.508236
H	8.976609	-2.532881	0.095813
C	12.326851	-2.287681	-0.07409
H	10.924826	-3.430437	1.123826
H	11.180849	-4.139235	-0.471717
H	13.06066	-2.46447	0.721577
H	12.851768	-2.466721	-1.025231
H	9.980236	1.214704	-0.195032
C	12.575375	0.288203	0.129085
H	12.066286	1.249185	0.134353
C	13.93139	0.279998	0.290332
H	14.440218	-0.681042	0.285891
C	14.747735	1.447322	0.470333
C	14.18109	2.856435	0.494306
C	16.107985	1.468712	0.690836
C	15.427442	3.758623	0.367358
H	13.647665	3.034147	1.44088
H	13.454773	3.034812	-0.307835
C	16.596207	2.893379	0.88576
H	15.594884	4.000714	-0.688517
H	15.325657	4.705734	0.906493

H	17.533202	3.097091	0.353314
H	16.798011	3.082791	1.951466
C	16.975032	0.326404	0.783305
H	16.522499	-0.64908	0.621948
C	18.30948	0.375814	1.05772
H	18.763883	1.350177	1.219962
C	19.175189	-0.771482	1.149707
C	20.527924	-0.757181	1.374467
C	18.682118	-2.194796	0.948306
C	21.097702	-2.16215	1.350217
C	19.850625	-3.066746	1.457933
H	18.475417	-2.37567	-0.117598
H	21.645363	-2.33358	0.410376
H	21.815132	-2.340828	2.160654
H	19.954686	-4.005354	0.904612
H	19.679333	-3.325713	2.509115
C	21.359054	0.415186	1.562788
H	20.854633	1.380057	1.568563
C	22.694454	0.403067	1.724996
H	23.253166	1.324423	1.85885
H	23.27086	-0.517693	1.726657
H	17.746841	-2.398466	1.483595
C	-18.309285	-0.400044	1.05008
H	-18.764232	-1.377309	1.192251
C	-16.982384	-0.347114	0.741827
C	-16.124059	-1.489197	0.586146
C	-16.614464	-2.917839	0.74257
C	-14.770407	-1.465884	0.328421
C	-15.465727	-3.768809	0.159701
H	-17.567319	-3.09751	0.230004
H	-16.787037	-3.145276	1.805972
C	-14.211244	-2.877388	0.283066
H	-15.353581	-4.735215	0.661248
H	-13.509822	-3.029035	-0.546272
H	-15.664803	-3.97203	-0.898868
H	-13.651159	-3.092367	1.206214
C	-13.952475	-0.296472	0.171025
H	-14.453534	0.666741	0.230646
C	-12.60221	-0.304774	-0.033143
H	-12.098689	-1.267466	-0.081795
C	-11.783972	0.865623	-0.175205
C	-12.343079	2.276618	-0.114942
C	-10.413201	0.893925	-0.327905
C	-11.188926	3.154284	-0.644409
H	-12.604512	2.536265	0.922593
H	-13.260545	2.395194	-0.704017
C	-9.91248	2.327036	-0.381736
H	-11.31035	3.302547	-1.72369
H	-11.158853	4.145342	-0.18067
H	-9.149526	2.480941	-1.154348
H	-9.444179	2.600944	0.576306
C	-9.538006	-0.241506	-0.385508
H	-10.002664	-1.224165	-0.353822
C	-8.17636	-0.177658	-0.476393
C	-7.299006	-1.310801	-0.539408
C	-7.797762	-2.745369	-0.524626
C	-5.925475	-1.276506	-0.668414
C	-6.523308	-3.57706	-0.265538
H	-8.254324	-2.997459	-1.49423
H	-8.569695	-2.91854	0.234948
C	-5.363342	-2.684815	-0.756807
H	-6.416117	-3.752435	0.81119
H	-6.545521	-4.556161	-0.754446
H	-4.453913	-2.817263	-0.158433
H	-5.087496	-2.917708	-1.796934
H	-7.712993	0.805675	-0.505236
C	-5.10761	-0.10136	-0.755472
H	-5.61356	0.857769	-0.673918
C	-3.752045	-0.097861	-0.927042
H	-3.24474	-1.056431	-1.007033
C	-2.93509	1.078679	-1.003066
C	-3.500373	2.485397	-0.908177
C	-1.56	1.116299	-1.112929
C	-2.334303	3.384027	-1.372139
H	-3.792057	2.70687	0.130138
H	-4.401053	2.623041	-1.518583
C	-1.063445	2.551798	-1.098676
H	-2.423415	3.568392	-2.449029
H	-2.322088	4.358872	-0.874436
H	-0.276351	2.735831	-1.839857
H	-0.628018	2.792224	-0.116402
H	-16.52973	0.631423	0.600469
C	0.685427	0.057172	-1.211691
H	1.146671	1.041393	-1.178209

C	-0.678793	-0.013364	-1.181105
H	-1.139495	-0.998296	-1.198796
C	-19.166474	0.747526	1.200778
C	-20.513213	0.732314	1.458872
C	-18.671277	2.174186	1.030537
H	-17.722158	2.357359	1.548609
H	-18.489679	2.386321	-0.034181
C	-21.07634	2.139799	1.490729
H	-21.772945	2.297144	2.323438
H	-21.645813	2.341548	0.570062
C	-19.822537	3.035471	1.594614
H	-19.935463	3.990577	1.072106
H	-19.624236	3.262399	2.648448
C	-21.345687	-0.441354	1.6325
H	-20.846279	-1.408223	1.598724
C	-22.676919	-0.427709	1.82595
H	-23.248088	0.495396	1.867229
H	-23.237387	-1.349882	1.946123

B (DP = 15)

C	9.588421	1.310985	-1.157265
C	10.112313	2.725835	-0.981025
C	8.210507	1.31123	-1.234932
C	8.909134	3.614692	-1.361558
H	10.994688	2.931724	-1.598896
H	10.419759	2.888448	0.063632
C	7.670848	2.726277	-1.117075
H	8.878105	4.554666	-0.801482
H	6.862218	2.933077	-1.828456
H	8.968455	3.87036	-2.425864
H	7.250201	2.888502	-0.112576
C	7.36362	0.16026	-1.358043
H	7.854511	-0.806967	-1.436989
C	5.997542	0.189357	-1.37247
H	5.506759	1.155518	-1.281768
C	5.149802	-0.961973	-1.485099
C	5.688843	-2.376445	-1.610424
C	3.770171	-0.970617	-1.44874
C	4.458796	-3.204059	-2.040421
H	6.087237	-2.717583	-0.642369
H	6.514155	-2.453339	-2.328596
C	3.24343	-2.392125	-1.543822
H	4.429326	-3.269723	-3.134213
H	4.475889	-4.227583	-1.652821
H	2.380984	-2.480652	-2.215468
H	2.90352	-2.737588	-0.55519
C	2.915058	0.170738	-1.29692
H	3.397021	1.144368	-1.248427
C	1.552172	0.124974	-1.209495
C	0.697481	1.267316	-1.062187
C	1.224284	2.690256	-0.991042
C	-0.681792	1.258545	-1.01436
C	0.011585	3.509577	-0.500174
H	1.559059	3.020692	-1.98651
H	2.090249	2.789154	-0.325362
C	-1.220571	2.674841	-0.909639
H	0.047355	3.592622	0.592248
H	-0.00809	4.526817	-0.903864
H	-2.041998	2.763492	-0.188424
H	-1.624107	2.999891	-1.881095
H	1.070077	-0.848709	-1.256705
C	-1.529769	0.104594	-1.093721
H	-1.039261	-0.863986	-1.155688
C	-2.895909	0.133291	-1.095277
H	-3.385908	1.102199	-1.034268
C	-3.744802	-1.020557	-1.165811
C	-3.20762	-2.43927	-1.241178
C	-5.124328	-1.026358	-1.124808
C	-4.440257	-3.280968	-1.634826
H	-2.805362	-2.74464	-0.262866
H	-2.385354	-2.54363	-1.959425
C	-5.652542	-2.449998	-1.162838
H	-4.474958	-3.386825	-2.725312
H	-4.422222	-4.289553	-1.209898
H	-6.518891	-2.563409	-1.825641
H	-5.986747	-2.757323	-0.159771
C	-5.97775	0.121199	-1.016612
H	-5.494668	1.095499	-1.013863
C	-7.34015	0.080681	-0.919787
H	-7.823269	-0.893648	-0.920967
C	-8.19345	1.229232	-0.820552
C	-9.572435	1.223477	-0.764968
C	-7.666035	2.653739	-0.820795

C	-10.110168	2.643544	-0.727532	H	21.090817	1.101564	0.326624
C	-8.87601	3.496075	-0.363382	C	19.254264	0.103148	0.055653
H	-7.336974	2.935516	-1.832972	C	18.398201	1.253972	0.072024
H	-10.515998	2.92125	-1.712634	C	18.918284	2.668989	0.257681
H	-10.929506	2.767921	-0.009221	C	17.031501	1.261735	-0.11907
H	-8.897153	4.493166	-0.814501	C	17.647264	3.492793	0.554785
H	-8.835228	3.630549	0.723741	H	19.4162	3.013143	-0.661995
C	-10.420836	0.067211	-0.782504	H	19.662336	2.745773	1.059731
H	-9.930442	-0.903347	-0.795595	C	16.496521	2.682924	-0.07966
C	-11.78694	0.096021	-0.781229	H	17.496565	3.550129	1.639049
H	-12.276818	1.066857	-0.769267	H	17.705357	4.519137	0.178748
H	-6.79624	2.784336	-0.165646	H	15.562747	2.769422	0.488972
C	29.348005	0.058321	1.837666	H	16.272625	3.031753	-1.099663
H	29.815531	1.020041	2.034167	H	18.776439	-0.864438	-0.078135
C	28.027173	0.04273	1.500246	C	16.200108	0.120943	-0.373793
C	27.191535	1.205986	1.382722	H	16.685534	-0.852245	-0.375999
C	27.700234	2.615639	1.628211	C	14.855762	0.1676	-0.61375
C	25.844934	1.219977	1.089578	H	14.370693	1.140956	-0.611515
C	26.580703	3.515849	1.063068	C	14.023929	-0.972346	-0.870242
H	28.668841	2.806357	1.150318	C	14.557742	-2.393847	-0.91219
H	27.848412	2.783091	2.706334	C	12.657356	-0.96291	-1.063174
C	25.309408	2.641341	1.109646	C	13.407281	-3.201077	-1.55056
H	26.472021	4.45702	1.611196	H	14.779711	-2.745425	0.107296
H	24.629745	2.850238	0.274715	H	15.492344	-2.47982	-1.479551
H	26.809354	3.769436	0.021454	C	12.136438	-2.377037	-1.253222
H	24.7323	2.815662	2.030876	H	13.559635	-3.255618	-2.63474
C	25.013788	0.076002	0.840804	H	13.347728	-4.228384	-1.177383
H	25.499028	-0.897146	0.849525	H	11.3935	-2.451223	-2.056542
C	23.669341	0.120137	0.605357	H	11.636951	-2.723071	-0.335118
H	23.182275	1.092467	0.608433	H	27.561432	-0.919992	1.303606
C	22.836959	-1.02318	0.361821	C	10.443326	0.15975	-1.183728
C	23.373044	-2.443902	0.326325	H	9.963942	-0.807355	-1.315638
C	21.469744	-1.016858	0.177308	C	11.802448	0.188449	-1.04499
C	22.219964	-3.257432	-0.299283	H	12.280211	1.154494	-0.900192
H	23.602047	-2.788096	1.346798	C	30.183262	-1.109142	1.953831
H	24.304205	-2.532136	-0.246349	C	31.524965	-1.127677	2.237072
C	20.949643	-2.432825	-0.001128	C	29.668468	-2.518841	1.714616
H	22.366288	-3.320192	-1.383837	H	28.705559	-2.706761	2.204778
H	22.163916	-4.281899	0.082136	H	29.5067	-2.684491	0.63849
H	20.203088	-2.513036	-0.800502	C	32.063986	-2.544874	2.22093
H	20.454661	-2.773303	0.92145	H	32.74305	-2.748031	3.058202
C	20.613162	0.133828	0.193481	H	32.645942	-2.71922	1.302492

C	30.79348	-3.421572	2.266631
H	30.900238	-4.358023	1.710162
H	30.570718	-3.684515	3.307144
C	32.372895	0.023506	2.474495
H	31.890144	0.999384	2.470184
C	33.699577	-0.020358	2.693001
H	34.25509	-0.953752	2.708078
H	34.27216	0.886706	2.861409
C	-17.081857	1.206334	-0.526702
C	-16.554178	2.62863	-0.603114
C	-18.451503	1.206594	-0.358203
C	-17.817247	3.477363	-0.861809
H	-15.796974	2.758481	-1.38575
H	-16.070063	2.904726	0.346433
C	-18.981996	2.629072	-0.308171
H	-17.762632	4.473383	-0.411114
H	-19.903977	2.758899	-0.887701
H	-17.948265	3.614326	-1.941462
H	-19.225586	2.906102	0.729204
C	-19.290386	0.054399	-0.19539
H	-18.806045	-0.918279	-0.239472
C	-20.638771	0.090337	0.021667
H	-21.12082	1.06356	0.076355
C	-21.476516	-1.061002	0.197716
C	-20.944565	-2.483246	0.162565
C	-22.829773	-1.056361	0.465885
C	-22.216331	-3.351748	0.055304
H	-20.383004	-2.700365	1.084349
H	-20.251335	-2.656376	-0.669428
C	-23.344231	-2.474756	0.639955
H	-22.427086	-3.559088	-1.000225
H	-22.118723	-4.316303	0.563452
H	-24.304602	-2.642138	0.137425
H	-23.511091	-2.689307	1.706917
C	-23.665134	0.100897	0.615211
H	-23.196317	1.070072	0.462623
C	-24.993528	0.074264	0.930894
C	-25.829232	1.232854	1.074949
C	-25.315011	2.649902	0.887672
C	-27.181075	1.239782	1.342868
C	-26.445037	3.5325	1.459803
H	-25.144956	2.852895	-0.180965
H	-24.356247	2.822965	1.391324
C	-27.71556	2.660994	1.361813
H	-26.236168	3.753394	2.512939
H	-26.543167	4.490456	0.939464
H	-28.409309	2.842001	2.191763
H	-28.277531	2.867148	0.437685
H	-25.462799	-0.894615	1.083872
C	-28.018806	0.087849	1.534539
H	-27.532296	-0.884391	1.508322
C	-29.365379	0.125081	1.74391
H	-29.853366	1.096441	1.769734
C	-30.202783	-1.030711	1.936824
C	-29.663663	-2.451404	1.924604
C	-31.548907	-1.028115	2.198735
C	-30.932376	-3.327936	1.837113
H	-29.096911	-2.64814	2.847458
H	-28.973234	-2.634918	1.092547
C	-32.067967	-2.439791	2.390971
H	-31.137145	-3.567173	0.787243
H	-30.832546	-4.276924	2.373255
H	-33.022108	-2.612287	1.877793
H	-32.252913	-2.634217	3.458967
C	-32.399045	0.13747	2.33744
H	-31.932455	1.108377	2.179589
C	-12.63618	-1.059754	-0.789684
C	-12.099786	-2.480784	-0.794062
C	-14.015496	-1.062964	-0.743733
C	-13.333746	-3.340411	-1.14205
H	-11.696494	-2.736269	0.198027
H	-11.278648	-2.622162	-1.507238
C	-14.544117	-2.486501	-0.707666
H	-13.37189	-3.499969	-2.225879
H	-13.31471	-4.326817	-0.66792
H	-15.413405	-2.633046	-1.360036
H	-14.873707	-2.742545	0.31121
C	-16.230011	0.053618	-0.5816
H	-16.712788	-0.919248	-0.526029
C	-14.868367	0.088881	-0.689614
H	-14.384833	1.062032	-0.732206
C	-33.707666	0.112155	2.648376
H	-34.282301	1.029086	2.737926
H	-34.244701	-0.815361	2.825284

C (DP = 1)

C	2.820644	-1.620516	-0.087413
H	3.471248	-0.752737	-0.047091
C	1.479593	-1.540374	-0.059378
H	0.938316	-2.479286	-0.120681
C	0.685135	-0.309329	0.003299
C	-0.685165	-0.309292	-0.003269
C	1.478662	0.987006	0.047509
H	2.294879	0.875804	0.772463
H	1.969937	1.135366	-0.92689
C	-1.478599	0.987118	-0.047376
H	-1.969614	1.135612	0.927134
H	-2.294985	0.875949	-0.772135
C	0.649955	2.22516	0.399912
H	0.415455	2.220971	1.473693
H	1.236408	3.131832	0.207663
C	-0.649811	2.225136	-0.400047
H	-1.236173	3.131902	-0.207968
H	-0.41533	2.220701	-1.473832
C	-2.820748	-1.620364	0.087483
H	-3.471315	-0.752541	0.047445
C	-1.479695	-1.540284	0.059273
H	-0.938493	-2.479261	0.120302
H	-3.314887	-2.584858	0.158561
H	3.314736	-2.585026	-0.158621

C (DP = 3)

C	-5.786483	0.56602	0.037171
H	-5.256554	1.509629	-0.04878
C	-4.985123	-0.658778	0.002894
C	-3.612348	-0.647963	-0.089516
C	-2.830971	0.578959	-0.005986
H	-3.383906	1.498888	0.134311
C	-5.770436	-1.95957	0.046509
H	-6.531377	-1.885282	0.833943
H	-6.332797	-2.067188	-0.894465
C	-2.827907	-1.942872	-0.255195
H	-2.270782	-2.143412	0.673327
H	-2.065199	-1.797038	-1.030423
C	-4.917654	-3.209022	0.280111
H	-4.604217	-3.25379	1.33262
H	-5.51516	-4.108579	0.088613
C	-3.681343	-3.16262	-0.612455
H	-3.082118	-4.075939	-0.513717
H	-3.994868	-3.100762	-1.664051
C	-1.47311	0.660946	-0.048159
C	-0.689994	1.885163	0.024347
C	0.689994	1.885153	-0.024433
H	-0.921433	-0.260002	-0.188505
C	1.473077	0.660913	0.04796
H	0.921361	-0.260066	0.187945
C	2.830953	0.578946	0.006053
H	3.38387	1.498944	-0.13387
C	3.612335	-0.647969	0.089468
C	4.985113	-0.658777	-0.00294
C	2.827906	-1.942902	0.255051
H	2.06501	-1.797051	1.030083
H	2.271019	-2.143568	-0.673591
C	5.770421	-1.959555	-0.04654
H	6.332913	-2.067086	0.894369
H	6.531283	-1.885305	-0.834066
C	3.681339	-3.162568	0.612585
H	3.994816	-3.1005	1.664184
H	3.082138	-4.075917	0.513988
C	4.917676	-3.209074	-0.27994
H	5.51524	-4.108561	-0.088295
H	4.60425	-3.254041	-1.332444
C	7.126699	0.640987	-0.119653
H	7.77009	-0.229874	-0.194044
C	5.786466	0.566034	-0.037285
H	5.256485	1.509644	0.048313
C	1.474164	3.186295	-0.12166
H	2.019495	3.346377	0.821656
H	2.247773	3.075172	-0.892258
C	-1.474139	3.18631	0.121661
H	-2.247788	3.075169	0.892214
H	-2.019426	3.346473	-0.821669
C	0.625324	4.420609	-0.436367
H	0.329472	4.409382	-1.49483
H	1.220624	5.328885	-0.283146
C	-0.625277	4.420568	0.436516
H	-1.220556	5.328878	0.283414

H	-0.329425	4.40919	1.494977
C	-7.126701	0.641008	0.119765
H	-7.770073	-0.229847	0.194439
H	-7.627043	1.604862	0.110591
H	7.627007	1.60487	-0.110584

C (DP = 5)

C	-10.093127	0.336866	0.068528
H	-9.563083	1.27894	-0.032337
C	-9.293748	-0.889142	0.036127
C	-7.922001	-0.880972	-0.073033
C	-7.138321	0.345392	-0.010367
H	-7.688509	1.267308	0.127618
C	-10.079974	-2.188442	0.101606
H	-10.831778	-2.105539	0.896933
H	-10.653187	-2.304809	-0.831765
C	-7.141273	-2.178559	-0.23594
H	-6.572738	-2.370738	0.687395
H	-6.388277	-2.041332	-1.02214
C	-9.225861	-3.436442	0.337767
H	-8.899613	-3.470652	1.386772
H	-9.826602	-4.337228	0.162899
C	-8.000595	-3.400766	-0.570279
H	-7.401289	-4.31383	-0.46963
H	-8.326957	-3.349188	-1.618526
C	-5.78056	0.425188	-0.06848
C	-4.995201	1.648114	-0.015463
C	-3.614675	1.645354	-0.077707
H	-5.231846	-0.49805	-0.2054
C	-2.832964	0.422336	-0.004413
H	-3.384172	-0.498665	0.1371
C	-1.473095	0.340372	-0.046546
H	-0.921826	1.261533	-0.187017
C	-0.690862	-0.881965	0.025566
C	0.690824	-0.881986	-0.025291
C	-1.473963	-2.183816	0.125326
H	-2.246133	-2.07281	0.89736
H	-2.02099	-2.345151	-0.816854
C	1.473904	-2.183864	-0.124851
H	2.021016	-2.344995	0.817314
H	2.246006	-2.073023	-0.896978
C	-0.624002	-3.417659	0.438707
H	-0.324947	-3.405549	1.496278
H	-1.219512	-4.326263	0.287974
C	0.62392	-3.417779	-0.437903
H	1.219422	-4.32635	-0.286936
H	0.32486	-3.405945	-1.495476
C	2.832955	0.42229	0.004499
C	3.614673	1.64531	0.077717
C	4.995195	1.64808	0.015388
H	3.384151	-0.49872	-0.13699
C	5.780578	0.425162	0.068354
H	5.231887	-0.498087	0.205295
C	7.138336	0.345389	0.010185
H	7.688508	1.267314	-0.127797
C	7.922031	-0.880968	0.072815
C	9.293785	-0.889119	-0.036294
C	7.141293	-2.178555	0.235656
H	6.388315	-2.041369	1.021883
H	6.572732	-2.370641	-0.687681
C	10.080013	-2.188423	-0.101743
H	10.653081	-2.304852	0.83171
H	10.831929	-2.105491	-0.896957
C	8.000592	-3.40081	0.569881
H	8.326901	-3.349373	1.618152
H	7.40128	-4.313855	0.469089
C	9.225908	-3.436388	-0.338099
H	9.826632	-4.3372	-0.163301
H	8.899727	-3.470467	-1.387129
C	1.473087	0.340343	0.046692
H	0.921838	1.261523	0.187124
C	10.093152	0.336894	-0.068606
H	9.563092	1.278957	0.032271
C	11.432263	0.414528	-0.166222
H	11.931418	1.378967	-0.154048
H	12.075866	-0.454694	-0.256433
C	5.776563	2.951216	-0.077935
H	6.541803	2.848913	-0.85805
H	6.332137	3.102665	0.860853
C	2.830774	2.94556	0.192849
H	2.279775	3.115354	-0.745516
H	2.062109	2.826586	0.967103
C	4.923418	4.187974	-0.370792

H	5.519317	5.095166	-0.213461
H	4.617164	4.188051	-1.426365
C	3.681397	4.176852	0.514048
H	3.987298	4.153419	1.569459
H	3.083946	5.08637	0.377157
C	-2.830774	2.945606	-0.192784
H	-2.279782	3.115359	0.745591
H	-2.062099	2.826656	-0.967034
C	-5.776578	2.951244	0.077852
H	-6.541882	2.848903	0.857901
H	-6.332078	3.10274	-0.860973
C	-3.681384	4.176916	-0.513951
H	-3.987237	4.153546	-1.569378
H	-3.083941	5.086425	-0.37698
C	-4.923451	4.187986	0.370828
H	-5.519343	5.095186	0.213519
H	-4.617251	4.188002	1.426417
C	-11.432232	0.414483	0.166218
H	-12.075839	-0.454733	0.256439
H	-11.931404	1.378914	0.15409

C (DP = 10)

C	20.708136	-0.827081	1.179713
C	20.019184	0.451914	0.999091
C	18.654663	0.546447	0.848606
H	20.092062	-1.719641	1.232297
C	17.802917	-0.624793	0.692505
H	18.30149	-1.585386	0.669301
C	16.451075	-0.613309	0.532267
H	15.951569	0.347111	0.558417
C	15.601871	-1.784368	0.382878
C	14.230352	-1.691174	0.241863
C	13.550391	-0.422241	0.040749
H	14.178004	0.455614	-0.050645
C	22.031751	-1.006661	1.336335
H	22.43892	-2.001315	1.492355
H	22.750854	-0.193961	1.321063
C	16.299031	-3.136746	0.427463
H	17.178955	-3.101826	-0.227632
H	16.694194	-3.301712	1.442186
C	13.353211	-2.935484	0.257885
H	12.931245	-3.08739	-0.747946
H	12.491917	-2.752552	0.912703
C	15.419477	-4.322705	0.024209
H	15.275289	-4.326047	-1.065433
H	15.924008	-5.262371	0.279964
C	14.062561	-4.213384	0.712355
H	13.432116	-5.084209	0.495131
H	14.208426	-4.190955	1.801536
C	12.204314	-0.250589	-0.087516
C	11.518162	1.014914	-0.282097
C	10.142282	1.098688	-0.391207
H	11.577625	-1.128054	0.010156
C	9.303279	-0.079268	-0.528465
H	9.818135	-1.02457	-0.644374
C	7.940758	-0.099345	-0.568085
H	7.421328	0.842635	-0.443264
C	7.117389	-1.288935	-0.69954
C	5.735637	-1.245049	-0.66395
C	7.857777	-2.612107	-0.841778
H	8.651399	-2.493116	-1.59042
H	8.376088	-2.836508	0.103907
C	4.909698	-2.524067	-0.631229
H	4.365652	-2.621644	-1.583773
H	4.135217	-2.424343	0.139838
C	6.973466	-3.799463	-1.229121
H	6.691487	-3.724182	-2.28876
H	7.536414	-4.733939	-1.116042
C	5.713455	-3.800467	-0.370302
H	5.089608	-4.679171	-0.574445
H	5.997331	-3.852049	0.690288
C	3.634977	0.122137	-0.630811
C	2.884698	1.365284	-0.651018
C	1.504856	1.399829	-0.55882
H	3.060063	-0.788613	-0.523351
C	0.690358	0.19875	-0.61776
H	1.213821	-0.73354	-0.78654
C	-0.66874	0.144308	-0.522966
H	-1.196169	1.07408	-0.350483
C	-1.474272	-1.0634	-0.575279
C	-2.851116	-1.044584	-0.44502
C	-3.617803	0.189157	-0.441134
H	-3.062457	1.10677	-0.589338

C	-0.719324	-2.374883	-0.745908
H	0.012368	-2.258259	-1.555497
H	-0.126198	-2.567038	0.161995
C	-3.647348	-2.337585	-0.331387
H	-4.249036	-2.467796	-1.244556
H	-4.37253	-2.235093	0.485878
C	-1.604596	-3.588165	-1.040706
H	-1.961429	-3.545508	-2.079406
H	-1.01597	-4.508661	-0.945073
C	-2.80148	-3.59131	-0.095934
H	-3.419349	-4.486828	-0.234604
H	-2.443836	-3.609788	0.943202
C	-4.97225	0.285817	-0.317225
C	-5.743393	1.516448	-0.315517
C	-7.118951	1.529609	-0.17006
H	-5.525084	-0.63266	-0.167077
C	-7.916635	0.316015	-0.19522
H	-7.384988	-0.610199	-0.372403
C	-9.271837	0.245564	-0.063137
H	-9.805153	1.170778	0.115107
C	-10.065958	-0.970692	-0.085697
C	-11.440314	-0.96312	0.068155
C	-9.301423	-2.276837	-0.253443
H	-8.585481	-2.163752	-1.077434
H	-8.690399	-2.451252	0.646059
C	-12.222728	-2.261629	0.20955
H	-12.837091	-2.408438	-0.69261
H	-12.936234	-2.155905	1.036656
C	-10.179863	-3.502202	-0.517392
H	-10.553983	-3.476737	-1.550562
H	-9.580945	-4.415793	-0.419455
C	-11.361327	-3.50441	0.446785
H	-11.972771	-4.407343	0.329359
H	-10.986901	-3.50638	1.480153
C	4.992241	0.003097	-0.683247
H	5.571091	0.912947	-0.783002
C	-13.570724	0.351975	0.211926
C	-14.349754	1.578759	0.212099
C	-15.72229	1.586409	0.374791
H	-14.115386	-0.568902	0.376848
C	-16.514763	0.367009	0.375393
H	-15.97971	-0.559564	0.210384
C	-17.866665	0.293665	0.51831
H	-18.403972	1.218833	0.68301
C	-18.657925	-0.929458	0.515675
C	-20.022367	-0.928003	0.694735
C	-17.892481	-2.2339	0.336674
H	-17.183982	-2.117086	-0.492935
H	-17.27433	-2.409338	1.230861
C	-20.809723	-2.221454	0.826756
H	-21.429489	-2.354431	-0.074048
H	-21.520262	-2.118322	1.656918
C	-18.773073	-3.458929	0.075414
H	-19.153461	-3.429222	-0.955327
H	-18.172811	-4.372492	0.16527
C	-19.94971	-3.468306	1.04635
H	-20.562258	-4.36966	0.922939
H	-19.569857	-3.480911	2.077651
C	-12.217759	0.264198	0.070892
H	-11.671995	1.184658	-0.093575
C	-20.813262	0.30296	0.741126
H	-20.284722	1.238988	0.588863
C	-22.144942	0.390794	0.907605
H	-22.63951	1.357634	0.899014
H	-22.786978	-0.472227	1.052388
C	-16.489226	2.892196	0.53058
H	-17.201526	2.78711	1.358795
H	-17.10453	3.054495	-0.368306
C	-13.569737	2.877139	0.05601
H	-12.953764	3.033694	0.955399
H	-12.85798	2.764262	-0.771559
C	-15.612474	4.122465	0.776678
H	-16.213611	5.033569	0.669922
H	-15.23489	4.110017	1.808818
C	-14.434099	4.115955	-0.191347
H	-14.811766	4.10626	-1.223488
H	-13.823728	5.021061	-0.08561
C	-7.879755	2.838427	-0.007564
H	-8.484368	3.014422	-0.911114
H	-8.601535	2.728427	0.811757
C	-4.954516	2.811836	-0.448485
H	-4.232878	2.703406	-1.268133
H	-4.349003	2.956176	0.460071
C	-6.998457	4.060746	0.261447

H	-6.632321	4.035046	1.297466
H	-7.593023	4.976559	0.157931
C	-5.809401	4.057649	-0.693481
H	-5.195657	4.958466	-0.571846
H	-6.175551	4.060153	-1.729814
C	0.758749	2.719757	-0.420015
H	0.189605	2.906221	-1.344283
H	0.006136	2.619054	0.372357
C	3.698801	2.648248	-0.744452
H	4.454901	2.529878	-1.531062
H	4.265052	2.781856	0.190788
C	1.647916	3.928373	-0.116255
H	1.972653	3.897277	0.933327
H	1.072138	4.853268	-0.242663
C	2.873937	3.907093	-1.023115
H	3.495898	4.798456	-0.876171
H	2.549821	3.915239	-2.073323
C	9.433977	2.445732	-0.407813
H	8.99729	2.605602	-1.406026
H	8.580674	2.405391	0.281411
C	12.387088	2.26351	-0.317299
H	13.238348	2.083275	-0.986236
H	12.825411	2.423555	0.680346
C	10.31947	3.639201	-0.038789
H	10.494692	3.651526	1.046248
H	9.802775	4.574431	-0.28651
C	11.658108	3.533169	-0.763307
H	12.287743	4.410084	-0.569589
H	11.483343	3.50094	-1.847972
C	17.962776	1.902022	0.803132
H	17.584514	2.073894	-0.216605
H	17.073234	1.866424	1.444618
C	20.905475	1.686289	1.01898
H	21.306103	1.821019	2.036157
H	21.78107	1.501689	0.383322
C	18.841793	3.081235	1.22884
H	18.966095	3.076313	2.320891
H	18.345801	4.024907	0.970984
C	20.211874	2.973128	0.565633
H	20.840778	3.839213	0.80501
H	20.087279	2.963108	-0.526353

C (DP = 15)

C	31.549682	0.106223	-0.714764
C	30.737704	-1.101837	-0.871037
C	29.363765	-1.089393	-0.796319
H	31.022009	1.044025	-0.570292
C	28.612524	0.093324	-0.397667
H	29.191458	0.969974	-0.136577
C	27.258325	0.176835	-0.286127
H	26.68014	-0.699703	-0.549951
C	26.506674	1.358595	0.105421
C	25.126911	1.366649	0.182812
C	24.331903	0.155383	0.067643
H	24.877122	-0.774898	-0.031501
C	32.891001	0.180349	-0.77945
H	33.396588	1.136009	-0.676779
H	33.529603	-0.682922	-0.937435
C	27.318914	2.612904	0.395298
H	28.158167	2.346513	1.050499
H	27.77782	2.966154	-0.541528
C	24.361768	2.659276	0.430882
H	23.908004	2.618168	1.433477
H	23.519428	2.711939	-0.270483
C	26.52507	3.754072	1.035835
H	26.326802	3.522529	2.091858
H	27.120422	4.675041	1.019429
C	25.200022	3.933438	0.301873
H	24.637023	4.788849	0.694619
H	25.397928	4.143179	-0.75873
C	22.971701	0.084463	0.121525
C	22.177248	-1.126434	0.007196
C	20.794952	-1.113509	0.04856
H	22.42657	1.014967	0.218
C	20.036003	0.076869	0.390914
H	20.607647	0.955866	0.660905
C	18.67697	0.171368	0.444008
H	18.102708	-0.70471	0.169978
C	17.91821	1.365601	0.77188
C	16.535803	1.377751	0.798302
C	18.720801	2.629591	1.045124
H	19.532255	2.388836	1.743905
H	19.217741	2.946725	0.114872
C	15.763524	2.680601	0.950085

H	15.256855	2.682669	1.927732	C	1.462333	2.695496	0.22106
H	14.959252	2.7044	0.203531	H	2.183	2.586138	1.041446
C	17.902684	3.793747	1.608687	H	2.068581	2.856165	-0.684236
H	17.657435	3.600834	2.66259	C	-1.462312	2.69548	-0.221928
H	18.500174	4.7132	1.585101	H	-2.068546	2.85616	0.683375
C	16.611588	3.947523	0.810307	H	-2.182991	2.586108	-1.042302
H	16.034617	4.818291	1.144737	C	0.593978	3.929589	0.477648
H	16.857504	4.116803	-0.247505	H	0.226615	3.917751	1.513488
C	14.386425	0.087926	0.678008	H	1.198335	4.838003	0.365903
C	13.601671	-1.132886	0.62038	C	-0.593969	3.929575	-0.478544
C	12.223544	-1.127972	0.499927	H	-1.198335	4.837985	-0.366818
H	13.839326	1.021568	0.649937	H	-0.226608	3.917715	-1.514384
C	11.436845	0.091282	0.567425	C	15.747191	0.159848	0.721645
H	11.980063	1.013532	0.729024	H	16.297451	-0.77279	0.741994
C	10.078694	0.172111	0.478177	C	-2.828353	0.090927	-0.185759
H	9.533937	-0.748249	0.310484	C	-3.614372	-1.130331	-0.169856
C	9.293631	1.392966	0.531693	C	-4.990219	-1.129916	-0.313359
C	7.915562	1.394806	0.41292	H	-3.368981	1.014131	-0.351347
C	7.130872	0.172518	0.420574	C	-5.77469	0.092346	-0.304288
H	7.674006	-0.751791	0.571513	H	-5.231995	1.016517	-0.151504
C	10.070544	2.692937	0.689697	C	-7.130854	0.172516	-0.421068
H	10.807921	2.568146	1.49298	H	-7.674005	-0.751786	-0.572003
H	10.65823	2.87169	-0.22444	C	-7.915541	1.394805	-0.413307
C	7.138206	2.699214	0.300383	C	-9.293618	1.392963	-0.532009
H	6.546335	2.842379	1.218019	C	-7.138185	2.699212	-0.300765
H	6.404587	2.604584	-0.51029	H	-6.404575	2.60457	0.509918
C	9.206552	3.920944	0.986936	H	-6.546301	2.84238	-1.218391
H	8.858185	3.888118	2.028865	C	-10.070534	2.692933	-0.690008
H	9.80824	4.831961	0.882206	H	-10.658191	2.871713	0.224142
C	8.001528	3.93865	0.052524	H	-10.807936	2.568121	-1.493265
H	7.398983	4.844301	0.192768	C	-8.001503	3.938652	-0.052907
H	8.350428	3.947335	-0.989706	H	-8.350392	3.947355	0.989326
C	5.774721	0.092354	0.30366	H	-7.398961	4.8443	-0.193172
C	4.990245	-1.129907	0.312602	C	-9.206544	3.920928	-0.987303
C	3.614411	-1.130309	0.168983	H	-9.808224	4.831951	-0.882589
H	5.23204	1.016531	0.150862	H	-8.858193	3.888068	-2.029236
C	2.82839	0.090949	0.184903	C	-1.47312	0.17127	-0.058649
H	3.369018	1.014148	0.350522	H	-0.932065	-0.7516	0.107612
C	1.473159	0.171289	0.05778	C	-10.078671	0.172109	-0.4784
H	0.932113	-0.751583	-0.108501	H	-9.533887	-0.74824	-0.31073
C	0.687837	1.39302	0.07204	C	-11.436831	0.091273	-0.567517
C	-0.687806	1.393012	-0.072902	H	-11.980061	1.013522	-0.729081

C	-5.765889	-2.432445	-0.455766	C	20.795913	-3.528669	-0.833211
H	-6.489718	-2.32493	-1.273576	H	21.020529	-3.320201	-1.888768
H	-6.36858	-2.590592	0.452387	H	20.198371	-4.448168	-0.811863
C	-2.84032	-2.432923	-0.019207	C	22.102486	-3.694594	-0.063774
H	-2.235581	-2.595628	-0.925156	H	22.673204	-4.558833	-0.424848
H	-2.118285	-2.322236	0.79977	H	21.87906	-3.881607	0.996027
C	-4.898859	-3.667484	-0.712079	C	28.550805	-2.340793	-1.09994
H	-5.503381	-4.575386	-0.597081	H	28.097879	-2.705963	-0.165029
H	-4.534051	-3.657813	-1.748843	H	27.708321	-2.066555	-1.747258
C	-3.708682	-3.666223	0.241309	C	31.508067	-2.380809	-1.154988
H	-4.073695	-3.65248	1.277958	H	31.949432	-2.314718	-2.162041
H	-3.10492	-4.575065	0.129797	H	32.3608	-2.439051	-0.466415
C	2.840371	-2.432895	0.01821	C	29.343332	-3.4721	-1.76069
H	2.235575	-2.595659	0.92411	H	29.531616	-3.226119	-2.815267
H	2.118383	-2.322162	-0.800804	H	28.749768	-4.394389	-1.751817
C	5.765897	-2.432443	0.455023	C	30.676236	-3.660477	-1.042348
H	6.489635	-2.324969	1.272923	H	31.237107	-4.506972	-1.456795
H	6.368694	-2.590539	-0.453067	H	30.48946	-3.890391	0.016079
C	3.708755	-3.666175	-0.242323	C	-12.22352	-1.127981	-0.499935
H	4.073857	-3.652355	-1.278939	C	-13.601662	-1.132898	-0.620243
H	3.104985	-4.575026	-0.130925	C	-14.386425	0.08791	-0.677776
C	4.898847	-3.667502	0.711171	H	-13.839335	1.021557	-0.649688
H	5.503381	-4.575393	0.596155	C	-15.747192	0.159827	-0.721344
H	4.533943	-3.657914	1.747902	H	-16.297457	-0.772808	-0.741727
C	11.446399	-2.424335	0.311926	C	-16.535798	1.377742	-0.797892
H	10.86454	-2.626063	1.225123	C	-17.918207	1.365608	-0.771415
H	10.703919	-2.279511	-0.482949	C	-18.676975	0.17137	-0.443577
C	14.381251	-2.440088	0.672243	H	-18.102719	-0.704717	-0.169567
H	15.133351	-2.371121	1.468087	C	-15.763511	2.680589	-0.949631
H	14.951044	-2.554724	-0.263489	H	-14.95921	2.704324	-0.203104
C	12.306944	-3.645312	-0.022418	H	-15.256876	2.682717	-1.927296
H	12.643985	-3.588137	-1.067035	C	-18.72079	2.629621	-1.044579
H	11.705449	-4.558147	0.066849	H	-19.217718	2.946713	-0.114306
C	13.52239	-3.686582	0.897391	H	-19.532255	2.3889	-1.743361
H	14.123872	-4.587584	0.725842	C	-16.611556	3.947512	-0.809741
H	13.186334	-3.72303	1.943242	H	-16.857436	4.116722	0.248091
C	19.988491	-2.372902	-0.237416	H	-16.034582	4.818295	-1.144129
H	19.50428	-2.705486	0.694184	C	-17.902676	3.793801	-1.608094
H	19.167706	-2.119841	-0.920374	H	-18.500151	4.713262	-1.584437
C	22.945406	-2.424363	-0.199914	H	-17.657457	3.600949	-2.662015
H	23.77348	-2.463758	0.519162	C	-20.036008	0.076871	-0.390512
H	23.419221	-2.404234	-1.19397	C	-20.794961	-1.113516	-0.048201

C	-22.177257	-1.126456	-0.006859
H	-20.607643	0.955878	-0.660488
C	-22.971728	0.084424	-0.12125
H	-22.426615	1.014925	-0.217853
C	-24.331926	0.155349	-0.067295
H	-24.877146	-0.774919	0.031963
C	-25.126936	1.366608	-0.182523
C	-26.506699	1.358563	-0.105112
C	-24.361798	2.659222	-0.430677
H	-23.519429	2.711905	0.270653
H	-23.908072	2.61808	-1.433288
C	-27.318944	2.612856	-0.395042
H	-27.777863	2.966133	0.541766
H	-28.158188	2.346426	-1.05024
C	-25.200046	3.933389	-0.301681
H	-25.397928	4.143151	0.758922
H	-24.637053	4.788791	-0.694456
C	-26.525107	3.754012	-1.035613
H	-27.120458	4.674981	-1.019213
H	-26.326861	3.522449	-2.091637
C	-28.612555	0.09333	0.39804
C	-29.363809	-1.089367	0.796729
C	-30.737749	-1.101795	0.871426
H	-29.191482	0.969973	0.136912
C	-31.549706	0.106274	0.715114
H	-31.022012	1.044063	0.570627
C	-32.891023	0.180432	0.779791
H	-33.529647	-0.682819	0.937792
C	-27.258356	0.176826	0.286498
H	-26.680177	-0.699705	0.550357
C	-31.508135	-2.380752	1.155381
H	-32.360845	-2.438998	0.46678
H	-31.949535	-2.314629	2.162416
C	-28.55087	-2.340768	1.100396
H	-28.097936	-2.705969	0.1655
H	-27.708393	-2.066531	1.747722
C	-30.676316	-3.660431	1.042798
H	-31.237206	-4.506908	1.457257
H	-30.489516	-3.890381	-0.015617
C	-29.343424	-3.472051	1.761163
H	-29.531723	-3.226038	2.815731
H	-28.749868	-4.394344	1.752325
C	-22.945398	-2.424386	0.200323
H	-23.41916	-2.404223	1.194405
H	-23.773508	-2.463821	-0.518706
C	-19.988488	-2.372902	0.23777
H	-19.167686	-2.119847	0.920709
H	-19.5043	-2.705479	-0.693844
C	-22.102479	-3.694616	0.064185
H	-21.879079	-3.881648	-0.995619
H	-22.673184	-4.55885	0.42529
C	-20.795886	-3.528675	0.833585
H	-20.198336	-4.448169	0.812222
H	-21.020478	-3.320207	1.889147
C	-14.38125	-2.440098	-0.672015
H	-14.950949	-2.554716	0.263777
H	-15.133427	-2.371142	-1.467784
C	-11.446355	-2.424346	-0.312015
H	-10.703782	-2.279524	0.48277
H	-10.864607	-2.626082	-1.225283
C	-13.522415	-3.686599	-0.897233
H	-13.186473	-3.723064	-1.943121
H	-14.12388	-4.587597	-0.725607
C	-12.306866	-3.645316	0.022441
H	-11.705384	-4.558155	-0.066873
H	-12.643792	-3.588119	1.067094
H	-33.396587	1.136102	0.677095

Appendix B. Vibrational Frequencies (in cm^{-1}) of the Optimized Structures

A (DP = 1)

100.7524	132.7443	160.5307
175.559	225.1347	285.442
377.4055	438.3976	590.0505
623.386	671.2238	724.0516
743.0399	830.0584	922.2296
922.4425	925.7066	979.2832
1022.7341	1028.159	1030.9572
1053.785	1063.16	1102.63
1184.0692	1228.273	1233.2283
1287.3021	1327.484	1335.247
1379.6207	1450.355	1481.8049
1498.8418	1516.14	1641.1861
1695.7849	1710.7	3046.9622
3052.1342	3083.522	3098.2682
3149.4827	3155.441	3168.8312
3169.0457	3250.699	3250.8658

A (DP = 3)

18.1705	23.6707	26.2059
63.0111	65.8129	77.242
98.8802	116.2131	137.2212
160.6695	165.9367	171.7718
202.2611	203.4697	203.5918
207.1931	233.143	240.8237
320.6197	325.4926	326.3928
381.4932	384.3177	477.8127
525.3224	538.4173	567.785
582.0572	593.499	642.4892
655.08	702.6922	707.6147
709.84	764.4549	808.7188
811.2224	822.2438	823.5377
835.4374	882.9099	887.5963
916.7888	916.8139	930.4692
931.0708	936.302	982.6529
986.2968	987.5612	990.1916
995.7841	1023.4119	1023.4736
1041.6708	1042.1925	1057.5275
1060.3757	1061.0335	1098.997
1101.2526	1102.8615	1185.4919
1185.7312	1187.4861	1221.4827
1227.2615	1228.0486	1235.0973
1235.6237	1237.9526	1259.3958
1288.06	1290.8567	1309.9858
1317.9059	1321.9186	1323.6539
1330.9842	1332.2936	1387.393
1389.7596	1404.2223	1464.805
1472.1198	1497.5071	1498.05
1498.0997	1511.2696	1514.6284
1514.8959	1584.6596	1620.3696
1630.5814	1665.1619	1668.2253
1691.314	1698.0589	3045.0972
3045.2655	3045.8542	3050.5833
3051.4802	3051.9694	3081.5358
3081.5465	3081.8447	3096.7235
3097.5117	3097.6455	3149.0852
3149.9198	3151.7125	3154.3964
3158.4845	3160.4319	3169.2628
3169.2787	3251.5683	3251.5743

A (DP = 5)

6.8313	9.944	12.6801
20.3777	26.3365	26.4394
41.6445	64.292	72.2609
74.8439	77.5984	78.7601
86.9955	120.9548	130.2815
143.2283	157.0752	157.7808
163.7819	166.9111	183.141
202.32	202.6482	202.7628
203.136	206.16	208.7332
224.1996	240.8	241.2341
257.4216	300.2232	326.5764
326.6148	356.3196	359.1646
377.7035	388.4127	410.2801
485.2195	504.5428	533.3072
541.8821	549.3403	550.0527
576.1826	579.0317	586.1224
611.9355	646.9948	649.4371
692.6206	695.7176	708.2957
708.3607	724.8091	771.7681
796.6929	806.408	811.5061

815.913	821.9732	822.6067
822.6697	834.927	839.6356
881.3609	883.5835	886.5155
889.037	916.317	916.3251
930.8422	930.8432	936.2341
936.5509	937.3236	981.8207
981.9556	984.6519	985.2917
987.731	988.6632	990.2191
996.439	1000.4748	1023.2785
1023.2839	1041.8998	1041.9749
1056.0129	1057.3504	1058.6278
1060.5552	1060.6263	1098.4083
1099.5023	1100.9645	1102.2534
1102.9777	1185.7244	1185.7367
1187.6616	1188.0778	1188.7086
1215.0413	1223.0808	1226.2551
1227.6807	1227.7287	1235.465
1235.48	1238.3901	1238.6569
1239.0053	1249.3231	1267.8379
1285.2007	1287.5051	1291.4299
1309.8894	1311.8736	1315.0227
1316.0225	1316.6983	1319.5392
1320.1981	1330.1503	1331.21
1335.4	1388.5948	1388.8364
1400.7124	1402.7882	1420.4866
1466.9134	1470.0427	1497.121
1497.2646	1497.3024	1497.9883
1498.0141	1504.3184	1512.0445
1513.702	1514.6359	1514.6615
1555.5491	1583.9949	1595.6121
1625.4228	1625.9656	1649.8417
1657.9965	1670.3464	1670.3496
1693.3104	1694.528	3044.9586
3045.0371	3045.7036	3045.8443
3045.8589	3050.3938	3050.4081
3050.8198	3051.6943	3051.9086
3081.3825	3081.3838	3081.7386
3081.7398	3081.7584	3096.6197
3096.6986	3096.8802	3097.5954
3097.6208	3148.8956	3149.2954
3150.0197	3151.0843	3152.6379
3154.0823	3157.0746	3158.729
3159.9727	3160.7579	3169.2833
3169.2886	3251.6165	3251.6187

A (DP = 10)

-5.4134	2.0322	2.2362
5.0137	7.5194	10.0105
12.6034	14.9353	16.1646
19.2105	23.6904	24.2736
25.2137	31.8053	33.36
43.4632	47.2093	64.423
65.8409	68.9795	72.4951
75.9012	76.3217	78.175
79.9922	87.144	88.7828
92.498	111.0417	124.0798
125.5961	135.8156	143.879
154.6846	155.1461	158.1855
161.6648	162.0517	162.9983
164.9589	167.2389	167.2879
184.5236	197.4927	199.2695
202.5284	202.53	202.6745
202.7182	205.0186	205.6721
205.9659	207.2678	213.5943
217.7165	221.4326	228.0282
233.7759	236.9666	246.3596
254.8117	261.4404	264.4731
266.1525	298.0518	326.6137
326.6144	330.5899	357.6196
359.1769	359.2588	363.6509
371.189	380.5874	382.091
392.0281	396.5086	413.0638
429.0169	490.0567	493.4815
515.3692	529.6113	531.151
535.005	536.7594	540.0474
546.8916	551.6708	554.3066
559.0942	561.6109	572.3027
577.8728	578.324	588.313
601.7198	611.8107	617.7083
648.0459	648.0511	688.4965
688.7393	692.7335	693.6721
696.2283	708.1816	708.1828
709.4688	728.1982	748.8668

777.5277	786.5	803.8012	1310.5099	1311.5218	1313.0238
804.2217	805.8073	807.9427	1313.126	1313.4134	1313.4773
810.2627	812.5577	814.441	1314.8789	1315.43	1315.9412
815.8378	816.1998	816.4957	1316.204	1316.4712	1319.0457
822.5717	822.5745	825.481	1319.6576	1326.0907	1330.4109
832.0989	836.6449	838.9026	1331.1769	1335.0057	1339.2207
839.2988	839.9479	880.7035	1388.7692	1388.7808	1401.3276
881.3221	882.3126	883.5928	1401.5347	1402.341	1402.8557
885.2179	886.5601	887.9428	1404.6454	1410.9963	1421.7915
889.0652	889.8206	915.8953	1435.6522	1467.3774	1468.4375
915.8986	930.8168	930.8186	1485.8736	1496.8844	1496.9407
936.2755	936.3376	936.675	1496.9931	1497.0218	1497.0697
936.8316	937.1869	937.4719	1497.1092	1497.2664	1497.2711
937.5186	937.5616	979.031	1497.9826	1497.9839	1502.7425
980.0362	981.1756	981.2874	1509.2473	1511.7278	1512.8332
982.2181	982.8941	983.8001	1513.3912	1513.6835	1513.7917
984.9887	985.2857	985.6964	1514.6063	1514.6087	1529.8353
988.1616	988.1767	988.3007	1549.1501	1564.1211	1574.4143
991.8563	995.3816	998.1551	1578.3345	1595.7855	1597.2744
1000.0217	1000.9574	1001.2199	1613.4293	1618.7145	1628.4459
1022.8773	1022.8795	1041.6542	1638.4078	1641.83	1651.657
1041.6737	1055.174	1055.6182	1655.2546	1660.1611	1665.5291
1056.1755	1056.797	1057.4576	1668.9141	1670.9955	1674.3387
1058.0653	1058.5712	1058.8463	1693.5297	1693.5303	3044.9086
1060.5422	1060.5427	1098.2384	3044.9311	3045.6113	3045.6149
1098.5262	1099.0297	1099.6873	3045.6958	3045.7241	3045.8192
1100.4551	1101.1772	1101.8875	3045.8272	3045.9134	3045.9179
1102.4729	1102.8907	1103.1274	3050.2291	3050.2321	3050.3233
1185.7538	1185.7552	1187.9701	3050.338	3050.4652	3050.5043
1187.9886	1188.3675	1188.612	3050.654	3051.0293	3051.6943
1188.8988	1189.1632	1189.3922	3051.7652	3081.2853	3081.2909
1189.5637	1210.3925	1214.6077	3081.6125	3081.6174	3081.6413
1219.2416	1222.7489	1224.9316	3081.6424	3081.6593	3081.6602
1225.9344	1226.115	1226.602	3081.6787	3081.6811	3096.5454
1227.7009	1227.7093	1235.5216	3096.5474	3096.5689	3096.577
1235.5321	1238.6708	1238.6794	3096.6323	3096.7123	3096.8178
1239.2444	1239.2494	1239.384	3096.9388	3097.5224	3097.5294
1239.5957	1239.6572	1239.7688	3148.7019	3148.852	3149.0636
1245.7178	1249.7351	1257.4586	3149.3604	3149.7576	3150.381
1267.4079	1268.868	1281.3115	3150.9263	3151.6335	3152.4225
1283.0785	1289.4017	1290.9734	3153.294	3153.7981	3155.9263
1292.1707	1309.926	1309.9631	3156.809	3157.6511	3158.4587

3159.0325	3159.7432	3160.2563
3160.6347	3160.8585	3169.1664
3169.1721	3251.5509	3251.5568

A (DP = 15)

2.3451	2.7833	4.6973
4.9785	6.4011	8.0394
8.3294	11.6125	12.7372
13.7306	15.5966	16.0999
18.1393	19.6661	19.9238
22.5249	22.8125	22.8183
24.0837	27.9464	27.9617
30.6566	36.8674	40.7705
43.1387	48.554	49.1012
67.0117	68.3388	68.9272
71.3349	73.4648	75.8517
77.9267	78.0658	79.7262
80.9458	86.0226	86.8086
90.6691	92.7802	94.6916
97.0502	105.2027	116.9166
125.6095	125.9232	133.9751
139.7526	147.3212	153.0561
154.9344	157.2526	159.6156
161.3673	162.0398	164.3124
166.7406	166.7514	169.0024
169.7366	170.4875	170.9383
171.1942	186.3984	195.5861
198.6566	200.3654	201.3613
202.9186	203.3149	204.141
204.1673	205.3144	205.8357
206.0878	206.4793	206.6422
207.6683	210.0691	217.4636
219.4648	220.821	222.7868
225.7974	230.2419	231.4271
235.2545	241.4134	247.6286
252.6052	253.0375	257.4937
261.2319	264.2407	266.0955
274.0342	297.9744	320.4997
327.1147	327.118	341.8126
357.1201	357.7496	359.0435
360.6972	361.6862	364.8518
369.7799	376.0007	376.6387
383.9918	387.9865	393.2363
393.8917	403.6093	414.6478
425.4194	434.1846	491.5837
492.3742	506.6286	518.3525
527.3233	530.9949	531.2885
533.2274	534.3707	537.974
542.2281	543.7709	543.9337
550.9109	551.0437	556.2238
558.19	559.0123	564.2417
564.2492	568.0964	578.7859
578.8056	579.3837	589.3972
598.4627	606.1024	612.234
616.6603	619.0437	648.1966
648.2047	686.9311	687.307
689.8893	690.01	692.6812
693.4689	693.8186	696.2037
704.6927	708.5121	708.5135
716.2532	729.4239	743.3158
756.6831	779.6669	783.5391
796.3238	804.4209	805.7601
805.9521	806.8239	808.2221
809.5442	811.3361	812.4756
814.166	814.2599	815.3116
816.3857	816.8715	818.0514
818.0729	821.1058	824.761
824.7615	826.7631	831.2428
834.6506	837.0895	838.0277
838.8376	839.2943	839.8073
839.9051	880.0256	880.6354
881.0787	881.7041	882.4261
883.3462	884.3861	885.4588
886.3492	887.2158	888.0899
888.7576	889.3849	889.5895
916.4962	916.4973	931.1599
931.1608	935.8074	936.3142
936.4871	936.618	936.6815
937.159	937.2408	937.3064
937.4423	937.6987	937.8871
938.0464	938.23	977.2411
978.0312	978.5776	979.3986
980.0328	980.7665	981.5552

981.624 982.1801 982.8823
983.1117 983.5692 984.2781
984.5742 984.6184 986.131
987.6799 987.6928 988.2849
990.7216 993.2108 995.7401
997.4342 999.2965 1000.3359
1001.0861 1001.3639 1001.5858
1001.6703 1023.1149 1023.1155
1042.299 1042.3056 1055.8008
1056.1729 1056.4647 1056.7948
1057.1682 1057.5656 1058.0124
1058.3708 1058.7447 1059.1253
1059.3284 1059.734 1059.7516
1061.5645 1061.5646 1100.7266
1101.1499 1101.3445 1101.6084
1101.9736 1102.42 1102.8081
1103.4263 1103.8551 1104.3171
1104.7133 1105.1475 1105.3085
1105.7605 1105.7794 1188.4699
1188.4703 1190.1454 1190.6921
1190.7389 1190.804 1190.8779
1191.2848 1191.3095 1191.6217
1191.6543 1191.9115 1191.9135
1192.1817 1192.1827 1209.984
1212.4543 1215.5983 1219.102
1222.2252 1224.6714 1226.4197
1227.1963 1227.63 1228.3895
1228.6097 1228.9039 1229.0143
1230.146 1230.1475 1238.165
1238.1687 1241.4671 1241.4676
1241.765 1241.8336 1241.9783
1242.0871 1242.1353 1242.1464
1242.297 1242.3576 1242.3836
1242.566 1242.5725 1246.2977
1247.9801 1250.7349 1255.1614
1259.5218 1261.3957 1269.271
1271.6106 1278.4024 1281.999
1285.4115 1288.7533 1290.7905
1292.406 1292.6652 1308.9846
1309.4458 1309.6432 1309.8661
1309.899 1310.3285 1311.4506
1312.4957 1312.7475 1312.787
1312.8659 1313.584 1313.9131
1314.6788 1315.0138 1315.0292
1315.2363 1315.2854 1315.836
1316.03 1316.7917 1319.2751
1319.6838 1321.9477 1327.8483
1331.2247 1331.7877 1333.6843
1336.8007 1338.843 1388.9548
1388.9582 1401.283 1401.3034
1402.0839 1402.2458 1402.6401
1402.9789 1403.4129 1405.2461
1409.1431 1414.8403 1422.3081
1431.0154 1439.5154 1468.0163
1468.6495 1477.2531 1492.0397
1497.6152 1497.8132 1497.8201
1497.9038 1497.9467 1498.0394
1498.0513 1498.1453 1498.156
1498.2796 1498.2849 1498.4922
1498.4941 1499.2944 1499.2948
1502.7132 1508.2355 1510.944
1512.4481 1513.1755 1513.8233
1514.0923 1514.344 1514.3948
1514.6953 1514.6962 1515.6724
1515.6731 1525.682 1533.4099
1547.1765 1559.6422 1564.173
1566.9088 1575.6146 1581.7609
1587.4204 1596.1611 1600.9465
1607.814 1615.6268 1619.8199
1628.885 1630.0926 1638.0157
1642.3375 1645.9949 1652.7586
1652.7851 1658.3131 1660.6711
1662.2781 1666.538 1669.0738
1670.8624 1673.4218 1675.1608
1693.8482 1693.8491 3045.1142
3045.1236 3045.4783 3045.6127
3045.7237 3045.732 3045.7487
3045.7773 3045.843 3045.8878
3045.9043 3045.9706 3046.002
3046.0542 3046.0653 3050.1451
3050.283 3050.3807 3050.4411
3050.4565 3050.4741 3050.5405
3050.5959 3050.6358 3050.6552
3050.7905 3051.0148 3051.2803

3051.8597	3051.8893	3081.358
3081.3829	3081.423	3081.4233
3081.5715	3081.5726	3081.6758
3081.676	3081.7028	3081.7028
3081.7479	3081.7851	3081.7875
3081.8075	3081.81	3096.4379
3096.4854	3096.6159	3096.6177
3096.6679	3096.6682	3096.7762
3096.7873	3096.8193	3096.8889
3096.9411	3097.0294	3097.0692
3097.643	3097.6441	3148.8417
3148.8621	3149.0094	3149.1101
3149.2825	3149.4645	3149.6066
3150.7119	3150.8343	3151.2121
3151.6085	3152.0786	3152.5855
3153.1187	3153.5422	3153.8276
3155.9989	3156.4188	3157.0073
3157.5257	3158.0632	3158.5725
3158.8292	3159.2161	3160.0902
3160.2926	3160.6278	3160.8256
3161.015	3161.3102	3169.0717
3169.0728	3250.9882	3250.9889

B (DP = 1)

106.4217	140.678	146.3001
162.9512	184.5578	250.201
300.4331	402.7884	462.1849
546.8683	578.8831	602.585
677.1477	728.3269	746.843
866.4944	909.6433	918.6054
920.6598	936.8824	980.5863
1016.8262	1021.1218	1028.284
1036.7372	1064.5251	1072.409
1165.7355	1232.834	1240.268
1256.7177	1296.4836	1331.453
1343.8551	1353.9175	1366.37
1403.2018	1462.8663	1484.638
1514.615	1517.1902	1538.116
1632.3751	1696.0578	1696.324
3017.618	3017.7344	3057.826
3070.2865	3077.057	3111.618
3157.7661	3169.0524	3173.857
3176.9368	3251.131	3251.506

B (DP = 3)

17.4817	20.2983	30.4483
61.8116	62.5145	76.9978
118.0947	121.9632	126.3778
134.0831	140.2491	149.7433
150.4381	171.6044	194.1995
198.1569	202.3214	209.5806
220.5225	227.3961	263.1227
329.8619	333.1533	340.3864
398.832	420.4752	491.082
504.6283	533.5861	533.8505
547.9002	590.1584	591.6823
594.8179	623.1835	638.4337
641.0223	682.3478	714.7931
721.935	745.7204	788.6098
803.7131	867.0304	867.4382
870.9721	875.2381	884.0718
908.6351	909.0635	912.426
915.6887	915.9391	939.2283
939.5378	942.4635	972.7297
974.3071	984.4341	985.9456
996.8335	1020.435	1020.534
1026.5933	1027.968	1043.388
1055.3196	1055.542	1068.066
1070.9317	1072.738	1163.683
1164.678	1165.043	1221.448
1226.1704	1233.625	1235.789
1244.0174	1246.522	1253.735
1259.4579	1265.198	1299.687
1299.9672	1303.123	1312.962
1327.2926	1335.962	1337.203
1342.5789	1344.472	1355.207
1356.0872	1356.688	1361.644
1367.3521	1369.596	1409.245
1409.7334	1418.131	1473.607
1476.6524	1513.168	1514.228
1514.644	1515.797	1516.26
1516.5379	1537.061	1537.543

1537.6334	1577.257	1616.656
1628.2528	1638.387	1660.935
1688.9573	1689.51	3013.22
3013.3593	3015.046	3015.17
3018.1203	3018.454	3057.277
3057.3346	3057.488	3069.649
3069.8233	3070.483	3076.699
3076.8371	3077.008	3111.105
3111.1329	3111.223	3160.542
3160.5804	3171.019	3173.644
3173.8784	3180.545	3184.214
3188.9858	3251.506	3251.515

B (DP = 5)

6.9463	10.0508	14.5669
18.1715	20.466	33.3287
45.9527	58.5578	59.4202
66.8401	71.871	87.8876
94.6594	122.8846	124.5337
130.021	135.4477	139.0572
139.3383	147.1334	149.2517
167.654	170.2199	173.8744
174.33	191.283	198.2467
201.061	203.715	215.9856
217.8629	227.9176	228.2037
228.8516	234.9562	261.7251
310.4777	336.4232	336.7229
366.8574	370.5009	393.0925
426.2181	429.755	478.8153
505.9474	516.1446	518.5197
522.1233	541.61	545.5934
560.0531	586.7393	592.3016
595.2465	604.4003	617.9171
621.1078	630.4369	636.7816
645.4594	653.3956	677.5561
706.0891	716.9242	724.2856
748.8726	778.586	795.4549
803.3228	805.251	864.235
867.0872	867.8322	868.914
872.5211	875.1809	877.288
882.4662	887.0462	907.0674
908.4593	910.9569	911.9273
912.311	915.4807	916.9465
939.4114	939.6362	942.1585
942.3429	943.3197	968.0301
969.8988	975.0507	977.576
982.442	985.5918	986.9282
994.968	1000.9753	1020.267
1020.6876	1027.2482	1027.3355
1041.3086	1042.4702	1045.7566
1055.4052	1055.5362	1067.1745
1068.5415	1070.2266	1071.8207
1072.668	1163.0968	1163.7962
1164.4105	1164.9116	1165.3822
1220.8489	1222.5159	1225.3311
1226.7067	1230.1281	1233.9597
1240.4691	1244.8685	1247.58
1248.1869	1253.7385	1255.1641
1260.4096	1264.3806	1266.5991
1299.8543	1300.0417	1302.7644
1303.4718	1304.8619	1308.5788
1314.1724	1326.939	1328.9584
1333.5239	1339.0774	1340.6974
1341.5513	1343.8238	1344.5921
1355.2777	1355.5291	1356.7555
1357.0549	1357.5429	1359.1481
1364.3553	1365.2209	1366.7604
1374.407	1409.5949	1409.7448
1417.4211	1418.5894	1425.6753
1474.7572	1475.4482	1511.2553
1513.2392	1513.8411	1514.2599
1514.5726	1515.2141	1515.4682
1515.5376	1515.6702	1516.2031
1535.5033	1536.7278	1536.8835
1537.1013	1537.4788	1553.9918
1583.3872	1605.4174	1609.4302
1627.3255	1633.1391	1636.0778
1653.2319	1663.4366	1688.7295
1688.8191	3012.9048	3013.0502
3014.1882	3014.3225	3014.7669
3014.8135	3015.198	3015.4924
3018.4151	3018.4216	3057.2222
3057.3003	3057.3427	3057.4021

3057.4455	3069.6115	3069.7169
3070.5153	3070.6948	3070.7253
3076.6169	3076.6908	3076.709
3076.9716	3076.9862	3110.6786
3110.7982	3110.9048	3111.052
3111.1327	3160.4385	3160.9233
3169.3879	3171.4149	3173.4824
3173.8808	3174.3555	3181.2
3182.7454	3185.758	3188.681
3190.3696	3251.4771	3251.7933

B (DP = 10)

-5.4134	2.0322	2.2362
5.0137	7.5194	10.0105
12.6034	14.9353	16.1646
19.2105	23.6904	24.2736
25.2137	31.8053	33.36
43.4632	47.2093	64.423
65.8409	68.9795	72.4951
75.9012	76.3217	78.175
79.9922	87.144	88.7828
92.498	111.0417	124.0798
125.5961	135.8156	143.879
154.6846	155.1461	158.1855
161.6648	162.0517	162.9983
164.9589	167.2389	167.2879
184.5236	197.4927	199.2695
202.5284	202.53	202.6745
202.7182	205.0186	205.6721
205.9659	207.2678	213.5943
217.7165	221.4326	228.0282
233.7759	236.9666	246.3596
254.8117	261.4404	264.4731
266.1525	298.0518	326.6137
326.6144	330.5899	357.6196
359.1769	359.2588	363.6509
371.189	380.5874	382.091
392.0281	396.5086	413.0638
429.0169	490.0567	493.4815
515.3692	529.6113	531.151
535.005	536.7594	540.0474
546.8916	551.6708	554.3066
559.0942	561.6109	572.3027
577.8728	578.324	588.313
601.7198	611.8107	617.7083
648.0459	648.0511	688.4965
688.7393	692.7335	693.6721
696.2283	708.1816	708.1828
709.4688	728.1982	748.8668
777.5277	786.5	803.8012
804.2217	805.8073	807.9427
810.2627	812.5577	814.441
815.8378	816.1998	816.4957
822.5717	822.5745	825.481
832.0989	836.6449	838.9026
839.2988	839.9479	880.7035
881.3221	882.3126	883.5928
885.2179	886.5601	887.9428
889.0652	889.8206	915.8953
915.8986	930.8168	930.8186
936.2755	936.3376	936.675
936.8316	937.1869	937.4719
937.5186	937.5616	979.031
980.0362	981.1756	981.2874
982.2181	982.8941	983.8001
984.9887	985.2857	985.6964
988.1616	988.1767	988.3007
991.8563	995.3816	998.1551
1000.0217	1000.9574	1001.2199
1022.8773	1022.8795	1041.6542
1041.6737	1055.174	1055.6182
1056.1755	1056.797	1057.4576
1058.0653	1058.5712	1058.8463
1060.5422	1060.5427	1098.2384
1098.5262	1099.0297	1099.6873
1100.4551	1101.1772	1101.8875
1102.4729	1102.8907	1103.1274
1185.7538	1185.7552	1187.9701
1187.9886	1188.3675	1188.612
1188.8988	1189.1632	1189.3922
1189.5637	1210.3925	1214.6077
1219.2416	1222.7489	1224.9316
1225.9344	1226.115	1226.602

1227.7009	1227.7093	1235.5216
1235.5321	1238.6708	1238.6794
1239.2444	1239.2494	1239.384
1239.5957	1239.6572	1239.7688
1245.7178	1249.7351	1257.4586
1267.4079	1268.868	1281.3115
1283.0785	1289.4017	1290.9734
1292.1707	1309.926	1309.9631
1310.5099	1311.5218	1313.0238
1313.126	1313.4134	1313.4773
1314.8789	1315.43	1315.9412
1316.204	1316.4712	1319.0457
1319.6576	1326.0907	1330.4109
1331.1769	1335.0057	1339.2207
1388.7692	1388.7808	1401.3276
1401.5347	1402.341	1402.8557
1404.6454	1410.9963	1421.7915
1435.6522	1467.3774	1468.4375
1485.8736	1496.8844	1496.9407
1496.9931	1497.0218	1497.0697
1497.1092	1497.2664	1497.2711
1497.9826	1497.9839	1502.7425
1509.2473	1511.7278	1512.8332
1513.3912	1513.6835	1513.7917
1514.6063	1514.6087	1529.8353
1549.1501	1564.1211	1574.4143
1578.3345	1595.7855	1597.2744
1613.4293	1618.7145	1628.4459
1638.4078	1641.83	1651.657
1655.2546	1660.1611	1665.5291
1668.9141	1670.9955	1674.3387
1693.5297	1693.5303	3044.9086
3044.9311	3045.6113	3045.6149
3045.6958	3045.7241	3045.8192
3045.8272	3045.9134	3045.9179
3050.2291	3050.2321	3050.3233
3050.338	3050.4652	3050.5043
3050.654	3051.0293	3051.6943
3051.7652	3081.2853	3081.2909
3081.6125	3081.6174	3081.6413
3081.6424	3081.6593	3081.6602
3081.6787	3081.6811	3096.5454
3096.5474	3096.5689	3096.577
3096.6323	3096.7123	3096.8178
3096.9388	3097.5224	3097.5294
3148.7019	3148.852	3149.0636
3149.3604	3149.7576	3150.381
3150.9263	3151.6335	3152.4225
3153.294	3153.7981	3155.9263
3156.809	3157.6511	3158.4587
3159.0325	3159.7432	3160.2563
3160.6347	3160.8585	3169.1664
3169.1721	3251.5509	3251.5568

B (DP = 15)

-0.4414	1.5155	2.9247
4.6754	5.3443	6.2738
7.3495	7.9965	10.2498
10.4683	11.4534	13.0489
13.2578	14.85	15.1787
16.5779	21.358	21.489
22.4124	23.7724	29.9676
36.8413	40.2442	44.2033
48.4669	52.1586	52.931
57.2523	58.1416	59.2772
60.6526	61.3813	63.9271
64.2652	66.3388	68.0764
68.37	69.8409	72.4568
76.6739	78.9841	90.4647
90.6939	113.6362	123.7204
124.3204	126.8226	127.2352
128.2471	129.5693	130.2061
132.462	133.9713	135.3735
136.1451	137.011	137.368
137.7644	137.8721	138.7991
139.9379	145.723	148.617
149.9909	166.1677	167.5932
168.3287	169.115	169.8267
170.2163	171.0163	171.893
172.6559	173.5643	173.8325
174.7544	175.5381	176.056
188.8439	190.2306	192.5123
195.2799	195.5317	198.6579

201.2439 203.0705 204.6576
208.2619 212.1706 216.0656
217.2014 224.9723 225.1135
225.9518 227.716 228.2987
229.2201 229.8302 230.5208
230.9504 231.6013 233.2112
234.326 235.0792 236.1526
237.4948 238.4939 238.7957
239.4452 243.1219 261.888
283.3218 306.1836 329.8106
336.4136 336.5996 353.5163
357.2491 360.4672 363.304
367.2975 372.8408 376.9911
379.9225 388.5211 397.8234
399.3322 408.1337 418.6773
420.7427 429.0447 438.3989
441.3564 444.9504 458.9146
476.2459 491.6268 504.3367
510.2704 510.815 514.1725
515.0408 518.1028 520.9986
523.3733 528.0246 529.5624
530.735 534.31 534.8165
537.2661 543.8683 544.8747
548.4892 557.5179 567.123
575.885 585.1685 591.8546
592.5395 593.2965 597.1878
603.9494 606.8199 612.9787
613.3239 614.5781 615.2931
616.3007 620.0548 620.4633
620.7317 624.5757 625.7418
628.5642 631.4986 634.4885
637.6525 638.5714 640.7564
641.9139 644.0614 645.1645
650.8947 653.0475 655.0862
661.201 670.6884 680.6622
691.5239 703.6358 713.3857
718.6446 723.1545 732.6198
742.87 751.702 765.657
774.5276 781.5972 787.9008
792.7566 796.8713 799.9091
801.9617 803.4504 804.0234
804.4401 805.7529 805.947
806.2604 864.584 864.8787
866.1882 867.0555 867.2729
867.5189 867.6128 867.9064
868.1352 868.6455 868.7084
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872.3612 873.1192 873.9888
876.5183 876.7675 878.0622
879.8481 880.6461 881.6899
882.675 883.7073 884.8055
885.6155 886.9749 887.3997
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912.256 912.6511 912.9331
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942.5708 942.6299 942.8276
942.9886 943.0551 943.2013
943.4586 943.736 944.1035
944.1851 944.3996 963.7164
965.936 966.8277 968.5683
969.3297 970.5408 970.9326
972.5347 974.0613 974.7642
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980.4002 981.7112 982.6296
983.7921 984.7975 985.6514
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992.3859 995.4051 997.9701
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1003.0949 1020.191 1021.059
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1072.2684 1072.788 1163.466

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1164.2124 1164.368 1164.634
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1216.9446 1220.21 1220.889
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1248.8819 1249.387 1249.642
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1475.4397 1505.739 1508.275
1510.1362 1511.34 1512.038
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1513.6711 1513.786 1513.851
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1514.3876 1514.422 1514.488
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1515.0881 1515.117 1515.204
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1516.5283 1527.886 1531.52
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1537.9266 1539.924 1542.627
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1593.7326 1598.692 1600.913
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1618.0438 1621.24 1626.048
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1633.9689 1635.745 1642.815
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1661.161 1663.288 1663.697
1688.1515 1688.875 3012.961
3013.5761 3013.785 3013.928
3013.9325 3013.984 3014.09
3014.1784 3014.196 3014.265
3014.3026 3014.419 3014.488
3014.5405 3014.551 3014.571
3014.6487 3014.697 3014.854
3014.8754 3015.042 3015.077
3015.1945 3015.23 3015.323

3015.3612	3015.402	3015.863
3017.7968	3018.917	3057.216
3057.2659	3057.282	3057.286
3057.29	3057.302	3057.32
3057.3243	3057.339	3057.346
3057.3733	3057.402	3057.413
3057.4338	3057.494	3069.37
3069.8184	3070.229	3070.331
3070.6153	3070.648	3070.709
3070.736	3070.807	3070.851
3070.8737	3070.939	3070.997
3071.0584	3071.079	3076.508
3076.5641	3076.575	3076.648
3076.6655	3076.741	3076.751
3076.7901	3076.826	3076.848
3076.9321	3077.004	3077.036
3077.0849	3077.159	3110.422
3110.4357	3110.548	3110.587
3110.5938	3110.676	3110.685
3110.699	3110.827	3110.88
3110.908	3110.954	3110.987
3111.3037	3111.311	3162.451
3162.7062	3169.792	3170.353
3171.1027	3171.595	3172.595
3173.2144	3173.546	3174.374
3174.8916	3175.129	3175.334
3175.8757	3176.377	3177.54
3177.585	3182.841	3183.78
3184.2572	3184.8	3185.625
3186.6968	3187.438	3188.255
3189.4105	3190.459	3190.906
3191.3315	3191.674	3192.917
3193.114	3252.552	3252.718

C (DP = 1)

90.0612	98.337	108.787
118.4895	233.3177	267.7862
306.5525	325.7956	412.4362
423.3795	458.3008	509.1598
550.9565	586.5005	676.882
684.3565	743.16	858.9693
873.528	894.2746	917.2297
919.4837	934.0569	964.0026
1004.6451	1019.5078	1028.6729
1064.6791	1092.7011	1105.2527
1114.9161	1171.6729	1197.7439
1219.352	1284.9644	1291.8808
1319.7725	1335.8465	1391.2038
1391.2742	1400.9128	1410.3747
1418.6927	1469.8407	1478.5982
1504.346	1513.4408	1522.1314
1534.6223	1630.3784	1689.7812
1692.0879	3010.5551	3010.9537
3030.8577	3036.0891	3062.9513
3063.5483	3079.1139	3083.218
3173.7627	3176.1191	3189.5554
3212.5371	3253.0875	3254.2995

C (DP = 3)

16.8935	17.6566	29.8666
46.8887	57.8455	76.5579
81.5238	98.7188	106.9362
111.8028	118.3987	119.746
132.8332	155.0556	168.207
170.8541	188.6885	190.9155
232.2136	246.2003	284.2112
308.9146	311.7863	313.8862
328.2298	350.6605	361.6938
409.2103	419.531	421.6556
464.2412	477.9547	483.6667
489.9676	496.2046	527.5555
528.6572	535.0831	546.5041
549.3558	606.7506	617.7047
623.5499	658.4265	695.8272
710.7034	719.5298	762.7081
785.033	838.0927	840.1441
857.9817	867.2794	875.434
880.1437	888.1976	896.2545
902.7498	909.3411	909.5155
913.4605	913.6679	932.9438
935.7113	937.8274	969.9977
972.9118	978.4271	986.697

997.3204	1018.1656	1019.3156
1045.8614	1046.5103	1081.7847
1082.863	1091.4365	1099.1539
1105.1968	1107.4432	1112.2921
1113.5639	1113.7433	1171.8181
1172.1562	1173.0698	1179.9078
1199.8668	1205.3926	1216.699
1220.7792	1225.0973	1280.3167
1285.0134	1293.1409	1293.4348
1294.861	1298.101	1322.4698
1322.6418	1325.7343	1333.7829
1337.4195	1349.4707	1370.698
1390.0184	1391.4171	1391.7759
1391.8023	1392.1974	1396.3175
1401.7465	1408.1569	1411.9468
1413.1418	1415.7757	1419.6038
1426.844	1428.6191	1474.7398
1475.1808	1503.1743	1503.7848
1504.3065	1512.0416	1512.9057
1512.9409	1521.691	1521.8239
1521.8336	1533.619	1533.6506
1533.7498	1584.9466	1613.1941
1625.2441	1635.1784	1655.6603
1685.5611	1685.7806	3007.997
3008.1059	3008.6443	3009.0662
3009.6563	3009.9973	3030.4358
3030.6891	3030.8246	3035.402
3035.6091	3035.6286	3058.2798
3058.4702	3060.2106	3060.3088
3062.2062	3062.3077	3078.6036
3078.85	3079.3779	3082.9596
3083.0145	3083.2384	3175.7702
3175.8157	3194.9757	3195.0019
3218.6908	3237.6026	3241.6999
3248.1638	3254.8381	3254.9714

C (DP = 5)

5.9876	6.9131	15.8152
17.3273	17.7561	33.4974
43.6347	49.678	49.9926
56.0506	64.4259	80.4351
84.5342	92.1274	97.8896
102.0534	109.1859	112.2707
115.492	119.4214	119.7622
154.1922	156.5467	156.8707
166.3646	166.6126	176.6254
181.9612	189.1569	189.2855
193.0234	203.6234	228.741
245.6095	252.7344	281.4067
307.3694	310.6211	311.7039
312.8072	315.4553	319.9626
351.2591	355.759	361.2559
384.726	405.8809	417.6806
420.4493	426.1018	463.4345
466.177	475.2775	482.4803
486.2228	489.3347	493.9902
494.8549	498.7303	525.0228
527.8189	530.6279	537.5572
538.603	541.7091	545.5494
575.836	606.2279	618.1414
619.8126	631.1345	631.462
651.7692	679.5212	699.9993
712.6662	717.7053	750.9388
769.8465	782.5726	789.3841
837.6852	838.093	839.6512
842.9633	857.5815	862.4905
870.4933	872.9899	878.9609
881.3981	887.5282	889.9921
895.3865	901.0586	905.2657
908.5781	909.1259	911.5811
912.6066	913.115	913.1281
932.0151	933.7681	935.5024
937.1962	938.159	966.2858
971.5842	974.6277	976.6159
984.4192	985.713	995.8174
997.1481	1002.601	1018.826
1018.8852	1046.418	1046.434
1078.7643	1080.614	1082.642
1085.3966	1094.713	1097.604
1099.3612	1102.128	1106.879
1106.9002	1111.779	1112.298
1112.3238	1113.556	1113.564
1167.9793	1171.634	1171.918

1172.1714	1172.998	1173.054
1187.3201	1199.951	1204.726
1205.5404	1215.943	1217.578
1221.2143	1225.063	1225.238
1281.3301	1281.584	1286.092
1292.3598	1293.328	1293.376
1294.4275	1294.7	1295.318
1300.303	1322.596	1322.679
1325.065	1325.605	1326.731
1333.0039	1334.278	1337.468
1344.403	1357.761	1362.601
1377.4486	1388.262	1391.204
1391.3094	1391.413	1391.526
1391.6434	1391.743	1393.651
1396.1094	1396.688	1400.219
1406.8716	1408.349	1411.65
1412.2763	1413.032	1413.76
1415.6735	1420.057	1424.16
1424.9832	1429.319	1430.544
1474.9911	1475.04	1502.331
1502.9362	1503.445	1503.885
1504.1795	1511.577	1512.172
1512.5586	1512.78	1512.81
1521.6502	1521.661	1521.677
1521.7085	1521.715	1533.388
1533.3935	1533.494	1533.508
1533.5554	1569.642	1587.556
1604.8311	1619.468	1619.723
1623.0826	1636.561	1650.164
1656.6794	1685.434	1685.475
3007.5983	3007.723	3007.821
3007.9621	3008.036	3008.35
3008.4288	3008.555	3010.013
3010.0267	3030.199	3030.288
3030.3959	3030.657	3030.713
3035.0688	3035.202	3035.21
3035.4933	3035.498	3057.968
3058.0158	3058.059	3058.296
3058.9487	3059.042	3060.125
3060.1599	3062.038	3062.054
3078.5212	3078.591	3078.823
3078.8388	3079.139	3082.707
3082.8866	3082.893	3082.962
3082.9766	3175.915	3175.924
3195.3619	3195.367	3216.958
3219.0354	3221.275	3238.258
3239.5319	3243.469	3247.417
3249.7885	3255.01	3255.025

C (DP = 10)

2.8821	5.2998	6.9336
7.0335	7.7617	9.7201
9.8204	10.5075	13.6524
17.0313	17.2572	22.1984
29.5828	33.6553	39.3803
46.907	48.3298	51.4143
52.1984	52.5976	54.1963
54.6196	57.4128	62.1075
65.6277	69.0444	80.6621
82.0455	86.6983	91.9474
95.1039	97.128	101.623
106.2624	109.7198	110.5193
111.207	112.2519	113.3796
118.6956	120.4048	124.5995
148.0615	154.0126	155.1921
156.5122	157.0991	157.7129
158.204	161.9836	162.7821
166.8441	168.6625	174.5938
175.8472	176.7109	178.1569
181.1075	182.8636	186.514
189.6625	190.3356	197.9056
202.2106	202.6579	208.2132
210.1257	230.7292	236.4788
245.3755	248.6472	251.6288
269.9596	287.9572	305.6698
308.7654	310.2588	310.7673
312.0802	312.743	313.0122
313.9587	315.0829	316.3726
317.7369	337.4485	351.279
353.482	360.8819	365.8405
380.9656	386.0504	387.8954
397.3596	407.9222	416.0355
418.8278	420.4539	423.9404

424.8354 462.6373 463.9208
465.96 470.1304 470.9805
474.9057 478.8555 482.1091
484.3845 487.952 489.2114
492.666 493.4651 493.623
494.2452 494.6288 495.9975
498.4164 502.3336 522.8376
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537.3521 538.8115 541.3043
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858.3457 861.6741 865.8616
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875.8716 879.0503 880.8479
882.997 885.4778 887.6209
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1112.753 1113.218 1113.504
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1334.0019 1336.233 1338.105
1338.9268 1343.774 1350.696
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1384.5926 1388.659 1390.276
1390.4083 1390.763 1390.947
1391.0017 1391.112 1391.245
1391.3489 1391.366 1391.532

1391.943	1392.182	1393.619
1394.9746	1395.526	1395.737
1396.0437	1396.724	1398.411
1401.1144	1404.677	1407.249
1408.1109	1408.817	1411.736
1411.9464	1412.149	1412.599
1413.1137	1413.423	1414.211
1414.8151	1415.899	1416.168
1420.6718	1421.019	1423.023
1423.9943	1426.869	1427.18
1429.6767	1429.888	1431.659
1432.4743	1475.394	1476.491
1501.2084	1501.434	1501.701
1502.0943	1502.475	1502.809
1502.9828	1503.181	1503.567
1503.8422	1509.704	1510.412
1510.6868	1510.761	1510.952
1511.0907	1511.554	1511.875
1511.9188	1512.631	1521.47
1521.5745	1521.61	1521.638
1521.7354	1521.752	1522.41
1522.4302	1523.095	1523.106
1532.3726	1532.429	1532.467
1532.5025	1532.787	1533.186
1533.7455	1534.28	1534.617
1534.691	1560.882	1567.435
1575.7914	1585.013	1594.097
1602.5201	1609.881	1611.83
1615.5531	1617.754	1621.429
1621.9978	1625.486	1633.503
1641.4593	1647.622	1652.259
1655.3519	1656.584	1685.634
1686.3915	3005.3	3006.737
3006.9911	3007.201	3007.338
3007.4433	3007.514	3007.582
3007.6683	3007.707	3007.936
3007.9918	3008.166	3008.206
3008.3461	3008.43	3008.946
3009.0123	3010.629	3010.833
3030.0126	3030.106	3030.127
3030.1881	3030.214	3030.274
3030.3546	3030.434	3030.511
3030.7972	3034.836	3034.845
3034.8702	3034.88	3034.997
3035.0061	3035.18	3035.197
3035.2446	3035.54	3057.375
3058.481	3058.625	3058.72
3058.8967	3058.924	3059.038
3059.1031	3059.259	3059.358
3059.4353	3059.463	3059.502
3059.5224	3059.705	3060.054
3060.1407	3061.376	3062.261
3062.3726	3078.127	3078.158
3078.1795	3078.255	3078.307
3078.3818	3078.451	3078.498
3078.587	3078.748	3082.345
3082.418	3082.505	3082.519
3082.5506	3082.59	3082.643
3082.6652	3082.786	3082.791
3175.7551	3175.993	3192.744
3195.8223	3213.05	3214.439
3217.6481	3218.349	3219.564
3221.6368	3222.592	3224.268
3234.6892	3238.439	3238.936
3241.4352	3242.617	3244.427
3245.8231	3248.779	3250.431
3251.8523	3254.987	3255.103

C (DP = 15)

2.5164	3.1877	4.0342
4.5955	6.097	7.6474
8.1007	8.132	9.1204
9.1597	10.058	10.3744
11.388	11.43	12.6257
17.3504	18.7407	19.1798
22.0226	24.5954	30.7592
36.7104	38.228	43.2921
45.9683	49.8306	49.8426
51.4081	51.4883	51.8456
52.1987	53.7571	54.3727
55.6658	55.8646	59.1115
61.3172	63.8113	66.9815
68.9085	70.2458	80.4162

81.1849	82.9676	85.6204
91.6678	93.9578	95.3974
99.2618	101.1401	104.2036
108.1878	109.4309	110.4704
110.5619	111.9374	112.2382
112.8871	113.7924	114.8218
119.9893	120.2954	127.4966
145.4042	152.7731	153.1313
155.8133	156.5752	156.8265
156.8352	157.0547	158.1263
158.3339	158.5799	161.3259
162.0656	162.9471	164.111
166.8725	168.1849	171.682
173.9896	175.9502	176.4073
177.709	178.9714	180.0207
180.2304	180.8158	183.3184
183.5754	189.9152	190.5742
191.1725	198.0144	199.693
203.1505	204.8358	206.2794
206.6915	211.8376	213.4438
234.6845	236.0272	240.6808
244.4552	246.8099	250.6439
253.1559	260.1668	277.2633
290.6043	304.4743	308.8572
309.0426	310.5074	311.0344
311.2031	311.8353	312.1761
312.872	312.8944	313.336
314.3945	314.9321	315.1927
315.9256	316.1674	329.9177
345.3551	352.2481	354.6206
360.5692	364.6408	365.1882
380.7071	382.185	384.9865
387.9679	390.6867	394.5186
400.6699	408.4733	415.4647
418.1349	419.7784	421.8259
422.2013	424.3046	424.3573
462.4249	462.8925	464.5138
465.9298	468.2341	468.8289
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477.4494	479.8965	481.7774
483.3625	484.6258	488.2814
488.406	491.8004	492.5975
493.1745	493.3254	493.6184
493.8148	494.4262	494.78
495.2228	496.5659	498.5324
501.2973	504.3549	521.9286
522.8208	524.7968	525.9814
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533.6009	534.2826	536.0571
536.1686	539.0257	539.7755
541.9724	542.4118	545.0755
545.1799	552.0983	558.4391
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596.1746	604.7586	613.0201
617.2964	618.4776	621.8852
624.1114	625.9173	626.6262
628.3401	629.9693	632.067
633.8083	635.6495	637.8463
638.8161	645.4009	653.9831
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715.1021	715.894	738.0407
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765.8461	771.1367	775.6197
779.9019	783.4487	786.0218
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791.2493	836.0652	836.1841
836.6245	837.5212	837.5562
837.6543	838.6788	838.9181
839.5713	840.7948	841.9494
843.3193	844.7274	845.8878
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861.7392	864.6458	867.8439
870.5162	872.8975	873.972
874.4952	876.5444	877.2277
879.2146	879.7916	882.2521
882.3935	885.7054	886.3915
887.8242	889.3269	890.0944
890.2577	890.9021	893.8627
896.79	899.3039	901.7887
904.022	905.8861	907.8832
908.556	908.6421	908.9763
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910.322	910.9872	911.5629

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3220.349	3221.086	3221.259	3243.217	3244.976	3245.789
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3224.877	3237.945	3237.948	3249.192	3250.318	3251.625
3239.823	3239.867	3241.775	3252.417	3253.694	3253.695