Supplementary Information (SI) for ChemComm.

Supporting Information

Design, synthesis and reactivity of *N*-adamantyl cyclometalated cyclic(alkyl)(amino)carbene ruthenium complexes in *Z*-selective olefin metathesis

Clément Casalta,[a] Fanny Morvan,[a] Sophie Colombel-Rouen,[a] Thierry Roisnel,[a] Rodolphe Jazzar*[a,b], Angelino Doppiu*[c] and Marc Mauduit*[a]

[a] Univ Rennes, Ecole Nationale Supérieure de Chimie de Rennes, CNRS, ISCR UMR 6226, 35000 Rennes, France.

[b] Department of Chemistry and Biochemistry, San Diego State University 5500 Campanile Drive, San Diego, California 92182, United States.

[c] Umicore AG & Co. KG, Rodenbacher Chaussee 4, D-63457 Hanau-Wolfgang, Germany.

*marc.mauduit@ensc-rennes.fr

*rjazzar@ucsd.edu

*Angelino.Doppiu@eu.umicore.com

1. General information

All commercial reagents were used as purchased and without further purification, unless otherwise mentioned. For the synthesis of iminium salts, all reactions were performed under an atmosphere of argon using standard Schlenk techniques; all solvents and substrates were dried and degassed using standard procedures. Toluene, dichloromethane, pentane used for complex synthesis and catalysis, were either purified using MBraun Solvent Purification Systems or freshly distilled and degassed prior use, unless differently mentioned. All commercial chemicals were used as received unless otherwise noted. 1-dodecene, allylbenzene, 1-decene, 4-penten-1-ol, allyl acetate, styrene and 1,3,5-trimethoxybenzene were used as received. 1-dec-9-en-1-yl acetate[1], methyl dec-9-enoate[2], but-3-en-1-yl acetate[3] were prepared following described procedures. Reactions at elevated temperature were maintained by thermostatically controlled oil-baths. Reactions were monitored by thin-layer chromatography (TLC) carried out on aluminum backed silica gel 60 (F254) plates from MERCK (grain-size distribution 60/20 µm); visualized using 254 nm UV light and $KMnO_4$ in water for staining. Columns chromatography were performed with silica gel (spherical, particle size 40 µm, neutral) purchased from Sigma-Aldrich. The eluents employed are reported as volume (volume percentages). The required amounts of [Ru] were taken prior each reaction from freshly prepared stock solutions. All the reactions were quenched with ethylvinyl ether (EVE). NMR: Multinuclear NMR spectra were recorded on a Bruker ARX400 (^1H: 400 MHz, ^{13}C: 101 MHz) spectrometer with complete proton decoupling for nucleus other than ^1H. Chemical shifts are reported in parts per million with the solvent resonance as the internal standard ($CDCl_3$, ^1H: δ 7.26 ppm, ^{13}C: δ 77.16 ppm). Coupling constants (*J*) are reported in Hertz (Hz). Multiplicities in ^1H NMR are reported using following abbreviations: s = singlet, brs = broad singlet, d = doublet, dd = double doublet, ddd = double double doublet, dt = double triplet, ddt = double double triplet; t = triplet, tt = triple triplet, dq = double quartet; q = quartet, qd = quartet doublet; quint = quintet, sept = septet, m = multiplet. GC spectra have been performed on Rtx-5 column (30 m x 0.25 mm ID; 0.25 µm thickness) (Restek) or DB-23 column (60 m x 0.25 mm ID; 0.25 µm thickness) (Agilent). GC-MS spectra have been performed on SH-Rxi-5ms column (30.0 m x 0.25 mm ID; 0.25 µm thickness) (Shimadzu). HRMS were recorded on a Waters QTof-I spectrometer using ESI at the Centre Régional de Mesures Physiques de l'Ouest (CRMPO), Université de Rennes 1. X-Ray crystallography: Intensity data were collected on a D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector using MoKα radiation (0.71073 Å) at T = 150 K. Data reduction was performed using the SHELXT program. The structures were resolved using the software SHELXS-97 by the direct methods and refined using

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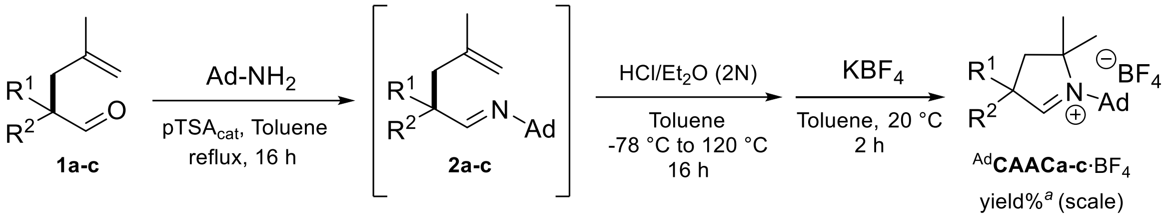
[1] A. Gilbert, P. Langowski, M. Delgado, L. Chabaud, M. Pucheault and J.-F. Paquin, *Beilstein J. Org. Chem.* 2020, ***16***, 3069.

[2] A. Brandolese, D. H. Lamparelli, I. Grimaldi, S. Impemba, P. Baglioni and A. W. Kleij, *Macromolecules* 2024, **57**, 3816.

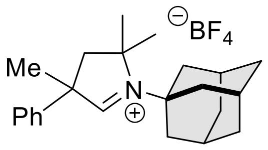
[3] D. Gärtner, A. L. Stein, S. Grupe, J. Arp and A. Jacobi von Wangelin, *Angew. Chem., Int. Ed.* 2015, **54**, 10545.

SHELXL-2013-4. The CIF file of complex **Ru8c** and **Ru7** have been deposited with CCDC numbers 2442418 and 2442417 respectively.

2. Synthesis of Iminium salts



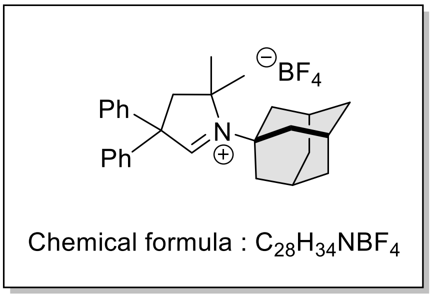
The iminium salts ^{Ad}**CAACa-c.BF4** were prepared as follow. To a mixture of 1-adamantylamine in dry toluene (0.8 M) was added aldehyde **1a-c** (1.1 equiv) and pTSA (catalytic amount). The mixture was heated to reflux overnight with a Dean-Stark apparatus. The reaction vessel was cooled to room temperature and the reaction mixture was filtered over an alumina column. The solvent and volatiles were evaporated at the vacuum ramp. In a Schlenk tube under argon containing the obtained imine and dry toluene (0.4 M) at -78 °C HCl (2 M in dry diethyl ether, 2.0 equiv) was added then the mixture was heated overnight at 120 °C. The mixture was cooled to room temperature and the supernatant was removed then the residue was washed with pentane. The obtained residue was dissolved with a mixture of CH_2Cl_2/H_2O (0.1 M) and KBF_4 (2.1 equiv) was added. The mixture was stirred vigorously for 2 hours. After decantation and separation of the two layers, the aqueous phase was extracted with CH_2Cl_2. Organic layers were reunited, dried over $MgSO_4$ and evaporated under vacuum. The obtained solid was dissolved in the smallest quantity of CH_2Cl_2, then precipitated in a mixture of pentane/ether. The precipitate was filtrate over a sintered glass filter and wash several times with pentane and ether to obtain the ^{Ad}**CAACa-c.BF4** as a powder.



Chemical formula : $C_{23}H_{32}NBF_4$

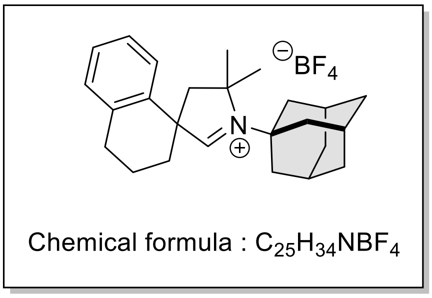
The product was obtained following the general procedure for the synthesis of iminium salts using 1-adamantylamine (0.738 g, 4.9 mmol), aldehyde **1a** (1.019 g, 5.4 mmol), APTS (catalytic amount), toluene (6.0 mL), HCl (2 M in dry diethyl ether, 4.9 mL, 9.8 mmol), KBF_4 (1.296 g, 10.3 mmol), CH_2Cl_2/H_2O (1:1, 49 mL). The desired product was isolated as a white solid (0.934 g, 47% yield). **^{1}H**

NMR (400 MHz, CDCl$_3$) δ 9.25 (s, 1H), 7.40-7.37 (m, 2H), 7.30-7.26 (m, 3H), 2.76 (d, *J* = 13.5 Hz, 1H), 2.47 (d, *J* = 13.6 Hz, 1H), 2.36-2.27 (m, 9H), 1.88 (s, 3H), 1.79-1.68 (m, 7H), 1.77 (s, 3H), 1.52 (s, 3H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ (ppm) 183.8, 141.7, 129.8, 128.2, 125.5, 82.7, 77.4, 70.8, 52.6, 52.2, 42.5, 35.0, 30.2, 30.1, 29.4, 27.7. **^{11}B NMR (128 MHz, CDCl$_3$)** δ (ppm) -0.9. **^{19}F NMR (376 MHz, CDCl$_3$)** δ (ppm) -150.6, -150.6. **HRMS (ESI)** calcd. for $C_{23}H_{32}N$ [M^+]: *m/z* 322.2529, found : 322.2527 (1 ppm). The data were consistent with reported literature[4].



Chemical formula : $C_{28}H_{34}NBF_4$

The product was obtained following the general procedure for the synthesis of iminium salts using 1-adamantylamine (0.295 g, 2.4 mmol), aldehyde **1b** (0.512 g, 2.0 mmol), APTS (catalytic amount), toluene (2.5 mL), HCl (2 M in dry diethyl ether, 2.0 mL, 4.1 mmol), KBF_4 (0.539 g, 4.3 mmol), CH_2Cl_2/H_2O (1:1, 20 mL). The desired product was isolated as a white solid (0.525 g, 54% yield). **^{1}H NMR (400 MHz, CD$_2$Cl$_2$)** δ 9.49 (s, 1H), 7.46-7.41 (m, 4H), 7.37-7.33 (m, 2H), 7.30-7.27 (m, 4H), 3.09 (s, 2H), 2.34 (s, 9H), 1.78 (s, 6H), 1.72 (s, 6H). **^{13}C NMR (101 MHz, CD$_2$Cl$_2$)** δ (ppm) 180.8, 140.4, 129.8, 128.5, 126.8, 82.9, 71.6, 60.1, 52.0, 42.8, 34.7, 30.1, 29.0. **^{11}B NMR (128 MHz, CD$_2$Cl$_2$)** δ (ppm) -1.1. **^{19}F NMR (376 MHz, CD$_2$Cl$_2$)** δ (ppm) -151.3, -151.4. **HRMS (ESI)** calcd. for $C_{28}H_{34}N$ [M^+]: *m/z* 384.2685, found : 384.2684 (0 ppm). The data were consistent with reported literature[4].



Chemical formula : $C_{25}H_{34}NBF_4$

The product was obtained following the general procedure for the synthesis of iminium salts using 1-adamantylamine (1.180 g, 7.8 mmol), aldehyde **1c** (1.839 g, 8.6 mmol), APTS (catalytic amount), toluene (10.0 mL), HCl (2 M in dry diethyl ether, 7.8 mL, 7.8 mmol), KBF_4 (2.062 g, 16.4 mmol), CH_2Cl_2/H_2O (1:1, 78 mL). The desired product was isolated as a white solid (1.447 g, 43% yield). **^{1}H**

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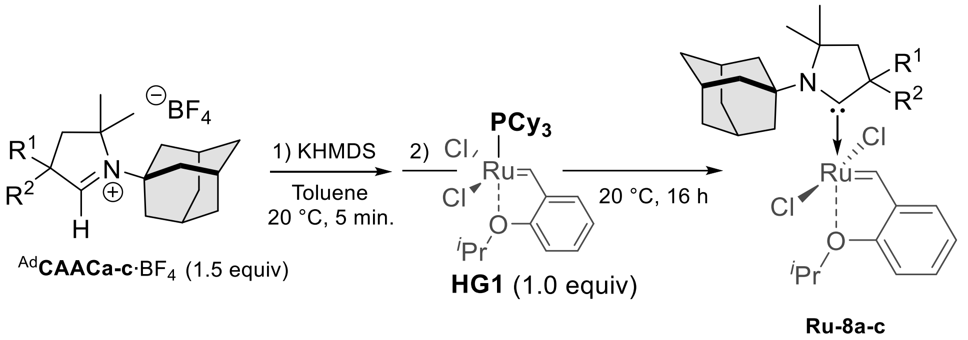
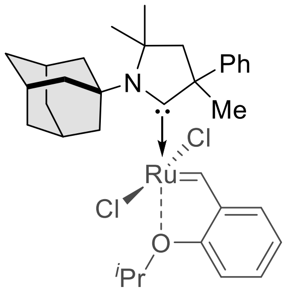
[4] V. Farkas, D. Csókás, Á. Erdélyi, G. Turczel, A. Bényei, T. Nagy, S. Kéki, I. Pápai and R. Tuba, *Adv. Sci.* 2024, **11**, 2400118

NMR (400 MHz, CDCl$_3$) δ (ppm) 8.55 (s, 1H), 7.22-7.17 (m, 2H), 7.15-7.12 (m, 1H), 6.67-6.63 (m, 1H), 2.83-2.76 (m, 2H), 2.58 (d, *J* = 14.0 Hz, 1H), 2.39-2.32 (m, 6H), 2.30-2.26 (m, 4H), 2.09-1.96 (m, 2H), 1.90 (s, 3H), 1.86 (s, 3H), 1.80-1.68 (m, 7H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ (ppm) 181.4, 137.0, 134.9, 130.5, 128.5, 127.4, 127.4, 82.6, 70.7, 55.5, 52.3, 42.5, 34.8, 31.7, 31.6, 30.8, 30.0, 28.6, 18.7. **^{11}B NMR (128 MHz, CDCl$_3$)** δ (ppm) -1.0. **^{19}F NMR (376 MHz, CDCl$_3$)** δ (ppm) -151.2, -151.3. **HRMS (ESI)** calcd. for $C_{25}H_{34}N$ [M$^+$]: *m/z* 348.2685, found : 348.2685 (0 ppm).

3. Synthesis of ruthenium-CAAC complex Ru8a-c



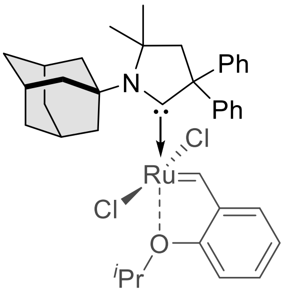
The ruthenium-CAAC complexes **Ru8a-c** were prepared as follow. The **^{Ad}CAACa-c.BF4** were dried overnight at 90 °C under high vacuum then introduced to Ar-filled glovebox. The **^{Ad}CAACa-c.BF4** (1.5 equiv) was dissolved in dry and degassed toluene (10 mL/mmol Ru). KHMDS (1.6 equiv) was added. The mixture was allowed to stirred 5 minutes at room temperature. Then, HG1 complex (1 equiv) was added and the reaction was stirred at room temperature overnight. The solvent was removed under vacuum and the product was purified by column chromatography (eluent: toluene/CH_2Cl_2 (1/1)) to obtain the ruthenium-CAAC complex **Ru8a-c** as a green powder.



Chemical formula : $C_{33}H_{43}NCl_2ORu$

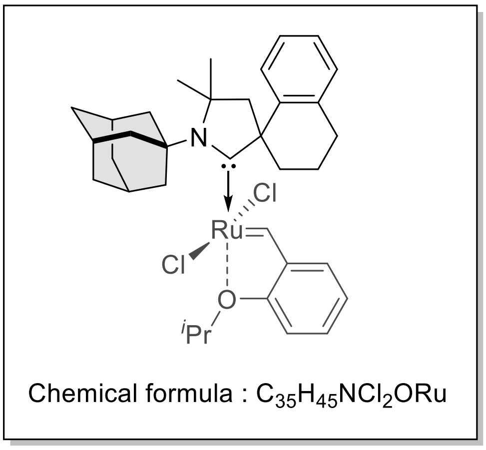
The product was obtained following the general procedure for the synthesis of ruthenium-CAAC complexes using **^{Ad}CAACa.BF4** (0.153 g, 0.38 mmol), KHMDS (0.080 g, 0.40 mmol), toluene (2.5 mL), M700 complex (0.150 g, 0.25 mmol). The desired product was isolated as a green powder (0.111

g, 69% yield). **^{1}H NMR (400 MHz, CDCl$_3$)** : δ 17.92 (s, 1H), 7.58-7.53 (m, 1H), 7.32 (brs, 3H), 7.22-7.18 (m, 1H), 6.96-6.93 (m, 2H), 6.89-6.85 (m, 1H), 5.12-5.06 (m, 1H), 3.32 (brs, 3H), 3.05 (brs, 2H), 2.47 (brs, 3H), 2.23 (dd, *J* = 24.1, 13.2 Hz, 1H), 2.17 (s, 1H), 2.03 (brd, 3H), 1.94 (s, 3H), 1.83 (brd, 3H), 1.76 (s, 3H), 1.71 (s, 3H), 1.67 (d, *J* = 6.1 Hbz, 3H), 1.62 (d, *J* = 6.1 Hz, 3H), 1.56 (brs, 2H). **^{13}C NMR (101 MHz, CDCl$_3$) :** δ 264.7, 153.6, 151.2, 144.8, 132.1, 128.4, 126.4, 124.7, 122.3, 113.4, 75.5, 74.0, 65.1, 63.2, 62.9, 43.2, 35.8, 33.4, 33.1, 30.9, 26.5, 22.7, 22.6. **HRMS (ESI)** calcd. for $C_{33}H_{43}NCl_2ORuNa$ [M+Na$^+$]: *m/z* 664.1657, found : 664.1654 (0 ppm). The data were consistent with reported literature[4].



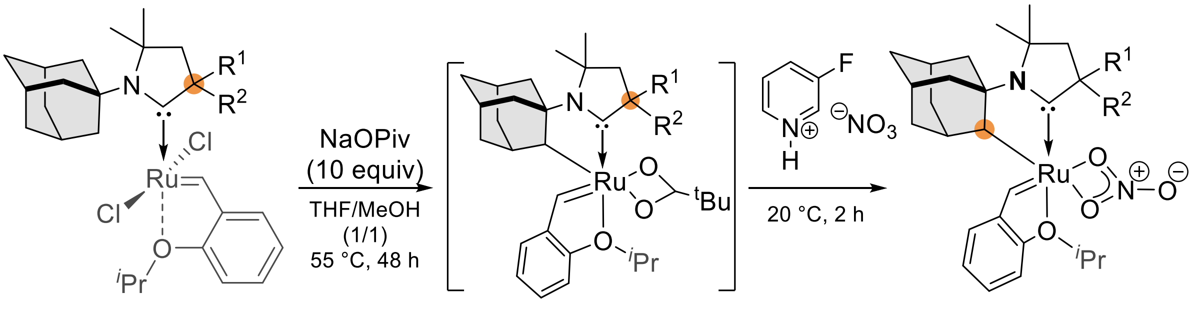
Chemical formula : $C_{38}H_{45}NCl_2ORu$

The product was obtained following the general procedure for the synthesis of ruthenium-CAAC complexes using **^{Ad}CAACb.BF4** (0.177 g, 0.38 mmol), KHMDS (0.080 g, 0.40 mmol), toluene (2.5 mL), M700 complex (0.150 g, 0.25 mmol). The desired product was isolated as a green powder (0.098 g, 56% yield). **^{1}H NMR (400 MHz, CDCl$_3$)** : δ (ppm) 17.97 (s, 1H), 7.71-7.68 (m, 4H), 7.52-7.48 (m, 1H), 7.29-7.19 (m, 6H), 6.93 (d, *J* = 8.5 Hz, 1H), 6.80 (td, *J* = 7.4 , 0.8 Hz, 1H), 6.74 (dd, *J* = 7.5 , 1.8 Hz, 1H), 5.10-5.04 (m, 1H), 3.11 (brs, 4H), 2.77 (s, 2H), 2.45 (brs, 3H), 2.04 (d, *J* = 12.4 Hz, 3H), 1.79 (d, *J* = 12.4 Hz, 3H), 1.69 (d, *J* = 6.1 Hz, 6H), 1.45 (s, 6H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ (ppm) 268.2, 153.8, 146.3, 143.9, 132.2, 130.1, 127.8, 126.7, 124.4, 121.9, 113.4, 74.5, 74.2, 72.1, 66.0, 60.7, 43.7, 35.7, 31.9, 31.0, 22.6. **HRMS (ESI)** calcd. for $C_{38}H_{45}NCl_2ORu$ [M$^+$]: *m/z* 703.1916, found : 703.1921 (1 ppm). The data were consistent with reported literature[4]



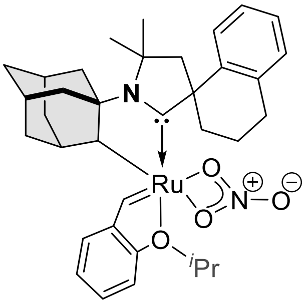
The product was obtained following the general procedure for the synthesis of ruthenium-CAAC complexes using **^{Ad}CAACc.BF4** (0.632 g, 1.45 mmol), KHMDS (0.328 g, 1.64 mmol), toluene (10.0 mL), M700 complex (0.612 g, 1.02 mmol). The desired product was isolated as a green powder (0.588 g, 86% yield. **^{1}H NMR (400 MHz, CDCl$_3$)** : δ 17.96 (s, 1H), 7.59-7.54 (m, 1H), 7.18-7.16 (m, 1H), 7.11-7.07 (m, 1H), 7.03-6.98 (m, 2H), 6.95-6.87 (m, 2H), 6.81-6.79 (m, 1H), 5.12-5.06 (m, 1H), 3.31 (brs, 3H), 3.22-3.13 (m, 2H), 3.08-3.03 (m, 1H), 2.72 (t, *J* = 13.9 Hz, 1H), 2.52 (d, *J* = 13.3 Hz, 1H), 2.47 (brs, 3H), 2.18-1.81 (m, 12H), 1.79 (s, 3H), 1.71 (s, 3H), 1.66 (d, *J* = 6.1 Hbz, 3H), 1.62 (d, *J* = 6.1 Hz, 3H). **^{13}C NMR (101 MHz, CDCl$_3$) :** δ 265.2, 153.5, 145.3, 134.6, 132.0, 130.8, 128.1, 126.8, 126.5, 124.6, 122.4, 113.5, 77.4, 75.3, 73.9, 65.3, 64.0, 60.7, 43.2, 35.8, 34.3, 33.9, 33.5, 30.9, 30.0, 22.7, 22.6, 20.5. **HRMS (ESI)** calcd. for $C_{35}H_{45}NCl_2ORu$ [M$^+$]: *m/z* 667.1916, found : 667.1922 (1 ppm). Single-crystals of Ru8c were obtained by slow diffusion between chloroform and pentane. CCDC 2442418.

4. Synthesis of cyclometalated ruthenium-CAAC complexes



Ru8a-c

The cyclometalation of ruthenium-CAAC complexes was attempted as follow. The **Ru8a-c** were dried overnight at 90 °C under high vacuum then introduced to Ar-filled glovebox. The **Ru8a-c** (1.0 equiv) was dissolved in a mixture of dry and degassed THF and methanol (0.04 M). NaOPiv (10.0 equiv) was added. The mixture was allowed to stirred 48 hours at 55 °C. The mixture was concentrated under reduced pressure then taken up in dry and degassed THF and filtered through celite. The mixture was reduced under reduced pressure then solubilized in dry and degassed THF (0.08 M). 3-fluoropyridinium nitrate (1.1 equiv) was added and the mixture was allowed to stirred 2 hours at room temperature. HMDSO (13 mL/mmol Ru) was poured into the reaction which was then concentrated under vacuum. The residue was solubilized in THF and filtered through celite then concentrated under reduced pressure. Benzene was added on the residue and filtered on Buchner. For compound **7** the product was obtained as a pink powder.

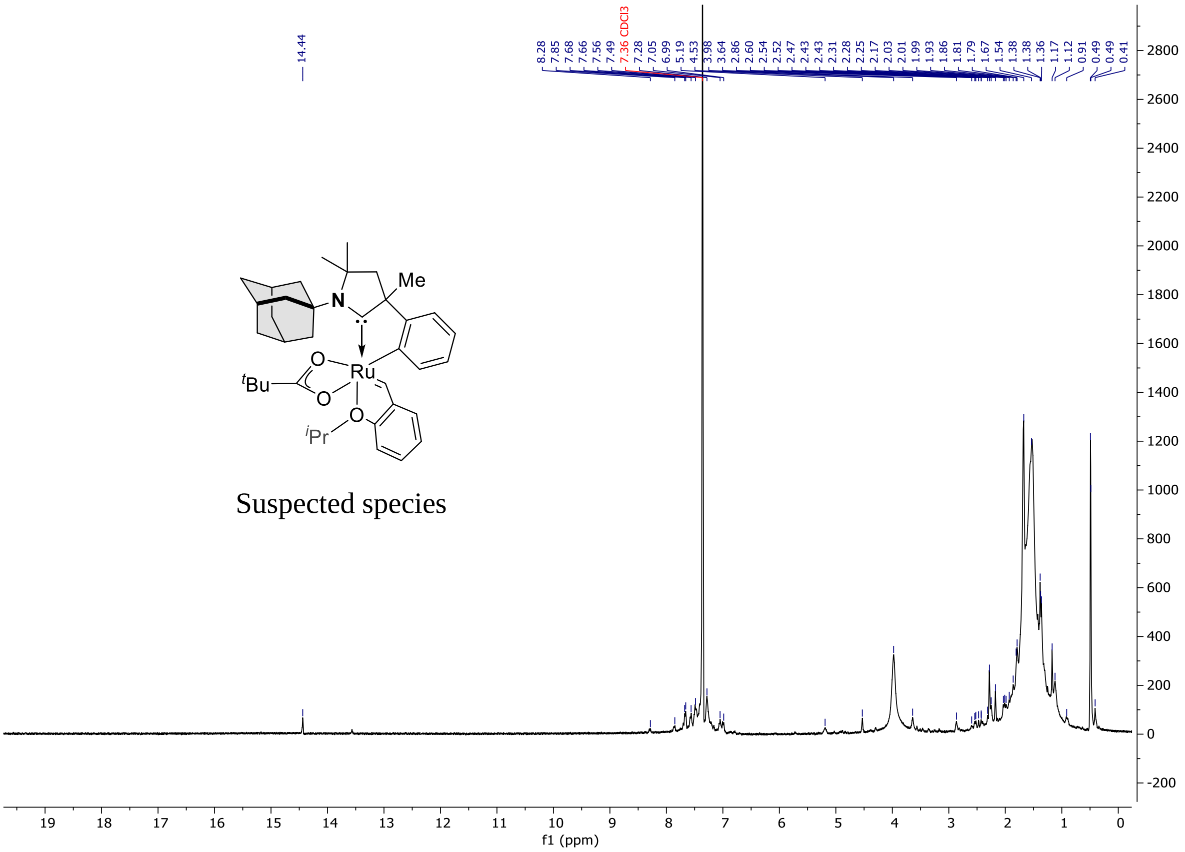


Chemical formula : $C_{36}H_{48}NO_4Ru$

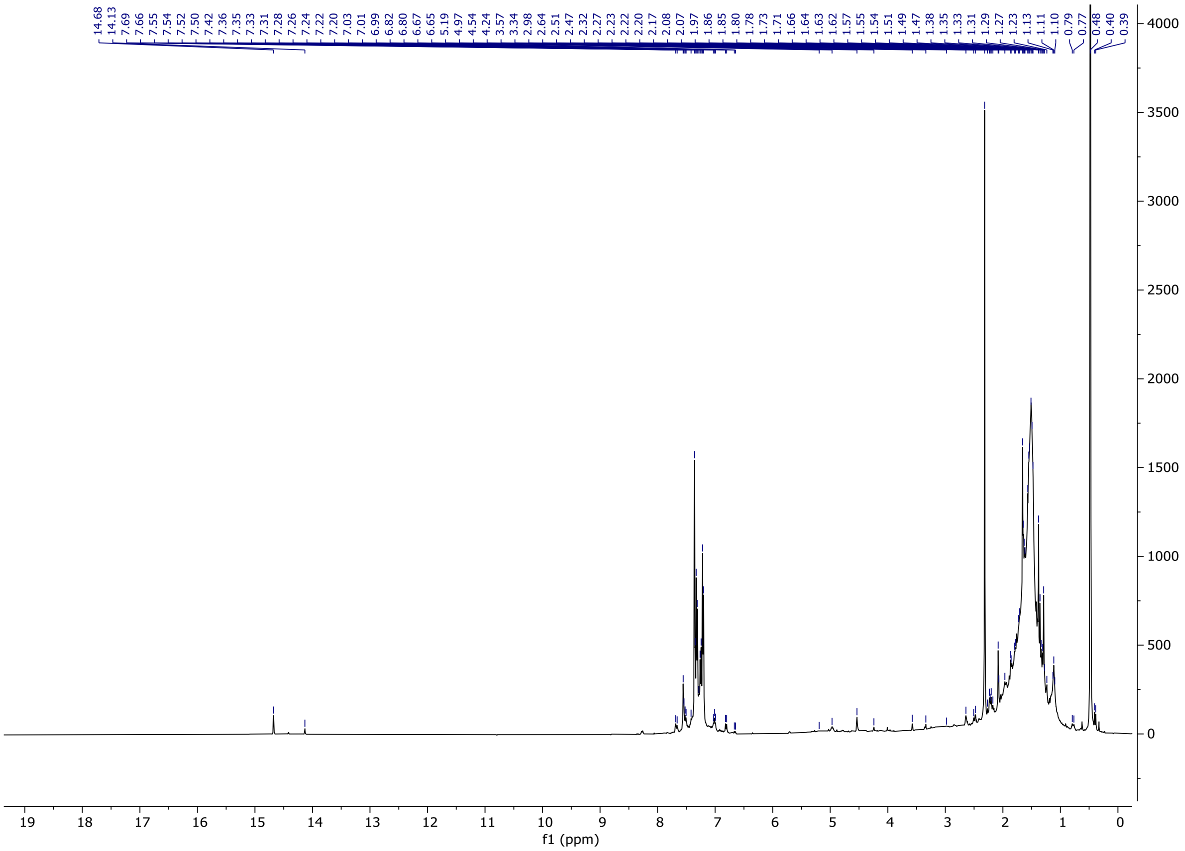
The product was obtained following the general procedure for the synthesis of cyclometalated ruthenium-CAAC complexes using **Ru8c** (1.0 g, 1.5 mmol), NaOPiv (1.861 g, 15.0 mmol), a mixture of THF/MeOH (40.0 mL), 3-fluoropyridinium nitrate (0.264 g, 1.65 mmol) and HMDSO (20 mL). The desired product was isolated as a pink powder (0.343 g, 35% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** as conformer mixture (86/14) : δ (ppm) 14.62 (s, 0.16H, conf. 1), 14.54 (s, 0.84H, conf. 2), 7.55-7.49 (m, 1H), 7.46-7.41 (m, 1H), 7.23-7.21 (m, 1H), 7.04-6.91 (m, 4H), 6.86-6.83 (m, 1H), 5.35-5.29 (m, 0.84H, conf. 2), 5.27-5.22 (m, 0.16H, conf. 1), 4.11 (s, 0.84H, conf. 2), 3.91 (s, 0.16H, conf. 1), 3.62 (s, 2H), 2.82-2.72 (m, 2H), 2.55-2.49 (m, 1H), 2.35-2.20 (m, 5H), 2.07-1.96 (m, 4H), 1.81-1.74 (m, 6H), 1.69 (s, 3H), 1.67 (s, 3H), 1.63-1.55 (m, 3H), 1.52 (d, J = 6.6 Hz, 3H), 1.24 (d, J = 6.4 Hz, 3H), 1.00-0.93 (m, 1H), 0.47-0.44 (m, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** as conformer mixture (84/16) : δ (ppm) 256.7, 153.9, 143.0, 138.8, 134.6, 128.7, 128.0, 127.6, 126.8, 125.5, 125.5, 123.2, 122.7, 112.8, 73.7, 71.7, 71.2, 67.6, 60.4, 58.7, 44.5, 40.0, 39.6, 38.1, 37.8, 32.1, 31.2, 30.4, 30.2, 29.2, 20.3, 19.6, 19.5. Single-crystals of Ru7 were obtained by slow diffusion between tetrahydrofuran and pentane. CCDC 2442417.

Due to the rapid decomposition of the catalyst in solution the HRMS analysis failed despite several attempts.

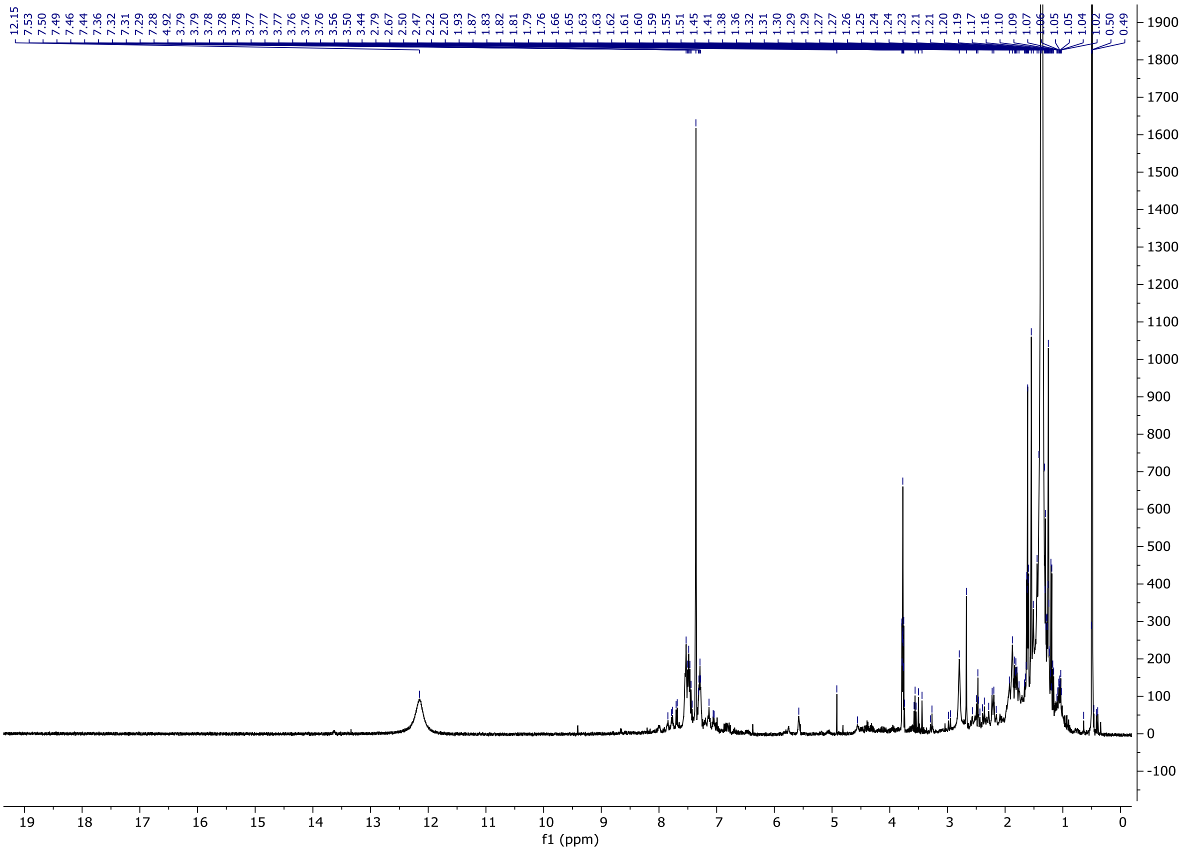
NMR spectra of Ru8a after treatment with NaOPiv



NMR spectra of Ru8a after treatment with 3-fluoropyridinium nitrate



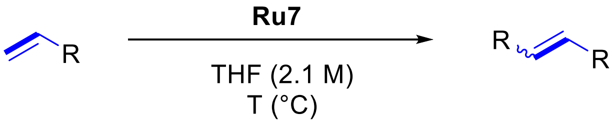
NMR spectra of Ru8b after treatment with NaOPiv



5. Catalytic performance of Ru-complexes

5.1. Self-Metathesis

5.1.1. General procedure for Self-Metathesis



Inside a glovebox, the terminal olefin (0.45 mmol, 1.0 equiv.), 1,3,5- trimethoxybenzene as internal standard (0.13 mmol, 0.33 equiv.) and a solution of ruthenium-CAAC complex **Ru7** (1.0 mol% or 1.5 mol%) in THF (216 μL) were sequentially loaded into an oven-dried vial. The reaction was stirred at 25 °C for 28 or 32 hours or at 35 °C for 16 hours then quenched with EVE. The final conversions and yields were measured by ^{1}H-NMR. The *Z/E* ratio was monitored by GC. For compounds **P1a** and **P1b** :

Column Information: Rtx-5 (30 m x 0.25 mm ID; 0.25 μm thickness) (Restek)

Carrier gas: Helium

Linear velocity: constant = 40.0 cm/s

Temperature protocol:

Rate (°C/min)	Temperature (°C)	Hold time (min)
-	175	35
15	280	10

For compounds **P1c** and **P1d** :

Column Information: DB-23 (60 m x 0.25 mm ID; 0.25 µm thickness) (Agilent)

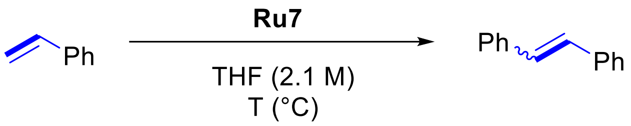
Carrier gas: Helium

Linear velocity: constant = 40.0 cm/s

Temperature protocol:

Rate (°C/min)	Temperature (°C)	Hold time (min)
-	205	35
10	240	8

5.1.2. Study of self-metathesis of allylbenzene

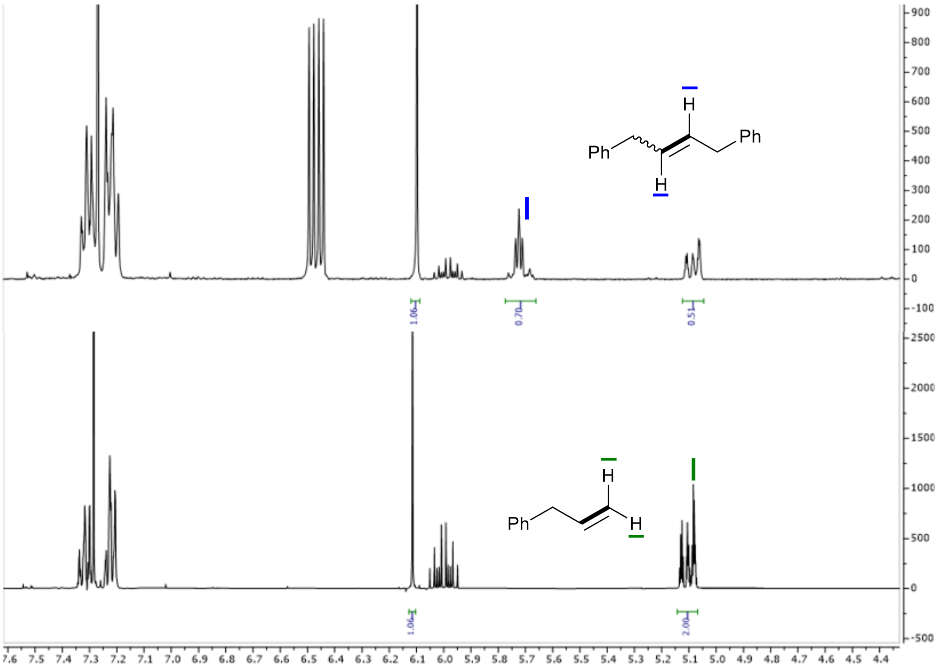


The reaction was performed following the general procedure, stirring a solution of allylbenzene (0.45 mmol, 60 µL, 1.0 equiv.) and **Ru7** (0.0045 mmol, 2.96 mg, 1.0 mol% or 0.0067, 4.44 mg, 1.5 mol%) in THF (216 µL) and stirred at 25 °C or 35 °C. Aliquots were taken over time, quenched with EVE and analyzed by ^{1}H NMR to determine conversion and yield and by GC chromatography to determine *Z/E* ratio.

Entry	**Ru7** (mol%)	Temp. (° C)	Time (h)	Conv.(Yield)(%)	*Z/E* ratio
1	1	25	3.5	5 (2)	97:3
2			6.5	19 (14)	97:3
3			21	65 (60)	95:5
4			24	69 (64)	95:5
5			28	76 (68)	95:5
6	1.5	25	3.5	12 (8)	96:4
7			6.5	32 (30)	96:4
8			21	69 (68)	95:5
9			24	74 (72)	94:6
10			28	79 (74)	94:6
11	1	35	16	74 (66)	87:13
12	1.5	35	16	74 (70)	82:18

- Reaction performed at 35 °C for 16 hours

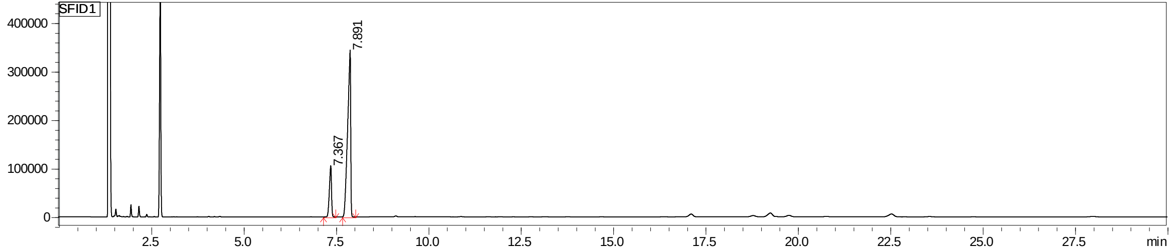
^{1}H NMR to determine conversion and yield



Ru7 (1.5 mol%)
16 h, 35 °C
74% conv., 70% yield

t0

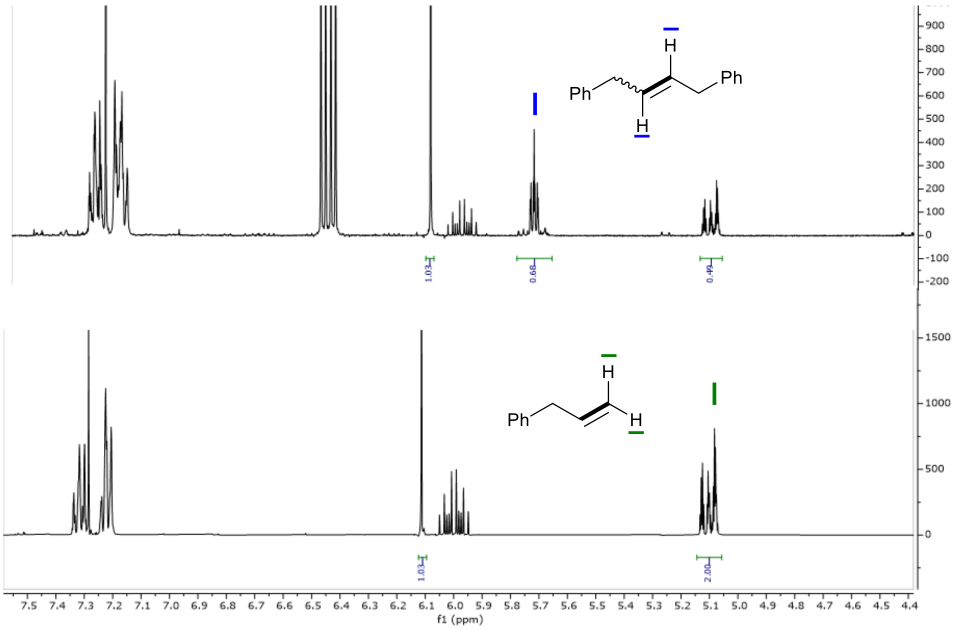
GC analysis to determine *Z/E* ratio



Peak	**Retention time [min]**	**Area**	**Area [%]**
1	7.367	419268	17.684
2	7.891	1951612	82.316

- Reaction performed at 25 °C for 28 hours

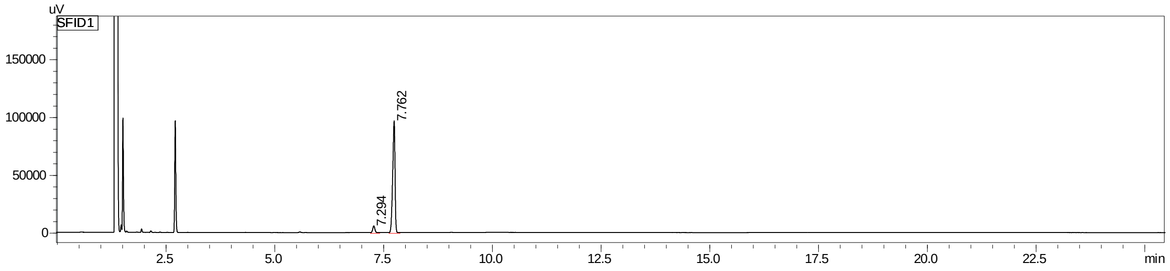
^{1}H NMR to determine conversion and yield



Ru7 (1.0 mol%)
28 h, 25 °C
76% conv., 68% yield

t0

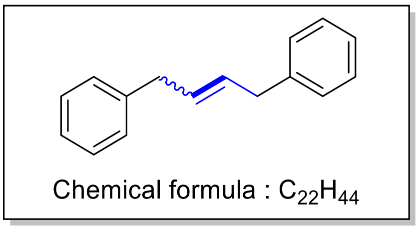
GC analysis to determine *Z/E* ratio



Peak	**Retention time [min]**	**Area**	**Area [%]**
1	7.294	19400	5.160
2	7.762	356558	94.840

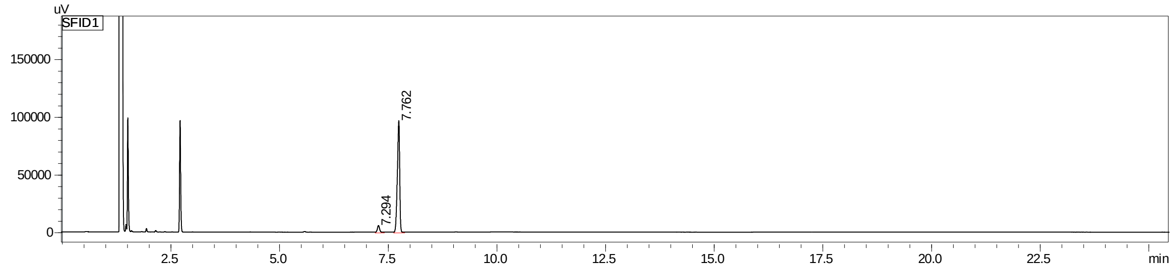
5.1.3. Self-Metathesis: Substrate Scope

1,4-diphenylbut-2-ene (P1a)



The reaction was performed following the general procedure, stirring a solution of allylbenzene (0.45 mmol, 60 µL, 1.0 equiv.) and **Ru7** (0.0045 mmol, 2.96 mg, 1.0 mol%) in THF (216 µL) at 25 °C for 28 hours or at 35 °C for 16 hours. At a temperature of 25 °C, compound **P1a** was obtained with a conversion of 76% and yield of 68% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 95/5 measured by GC analysis. At a temperature of 35 °C, compound **P1a** was obtained with a conversion of 74% and yield of 64% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 87/13 measured by GC analysis. The data were consistent with reported literature[5]. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.38-7.33 (m, 4H), 7.29-7.24 (m, 6H), 5.82-5.73 (m, 2H), 3.58 (d, *J* = 5.6 Hz, 3.69H, *Z* isomer), 3.43 (d, *J* = 5.2 Hz, 3.24 H, *E* isomer).

GC analysis for reaction performed at 25 °C



Peak	Retention time [min]	Area	Area [%]
1	7.418	1418389	80.124
2	7.812	351849	19.876

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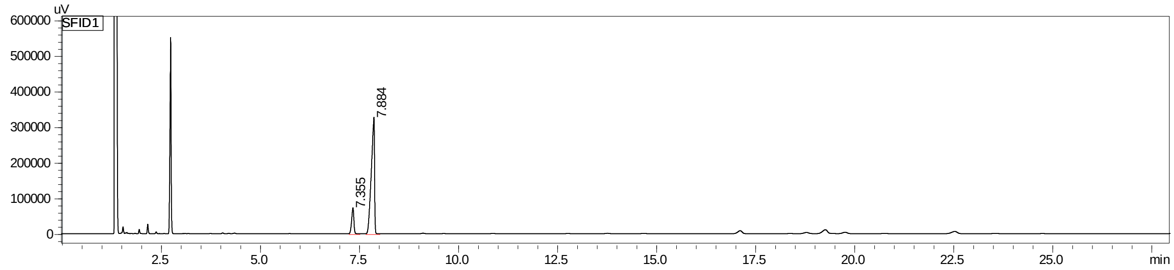
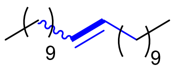
[5] J. J. Van Veldhuizen, D. G. Gillingham, S. B. Garber, O. Kataoka and A. H. Hoveyda, *J. Am. Chem. Soc.*, 2003, **125**, 12502.

GC analysis for reaction performed at 35 °C



Peak	Retention time [min]	Area	Area [%]
1	7.355	278347	13.165
2	7.884	1835944	86.835

Docos-11-ene (P1b)



Chemical formula : $C_{22}H_{44}$

The reaction was performed following the general procedure, stirring a solution of 1-dodecene (0.45 mmol, 100 μL, 1.0 equiv.) and **Ru7** (0.0045 mmol, 2.96 mg, 1.0 mol%) in THF (216 μL) at 25 °C for 28 hours or at 35 °C for 16 hours. At a temperature of 25 °C, compound **P1b** was obtained with a conversion of 53% and yield of 52% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 93/7 measured by GC analysis. At a temperature of 35 °C, compound **P1b** was obtained with a conversion of 56% and yield of 56% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 91/9 measured by GC analysis. The data were consistent with reported literature[6]. **^{1}H NMR (400 MHz, CDCl$_3$)** δ 5.40-5.31 (m, 2H), 2.04-1.96 (m, 4H), 1.35-1.27 (m, 32H), 0.89 (t, *J* = 6.8 Hz, 6H).

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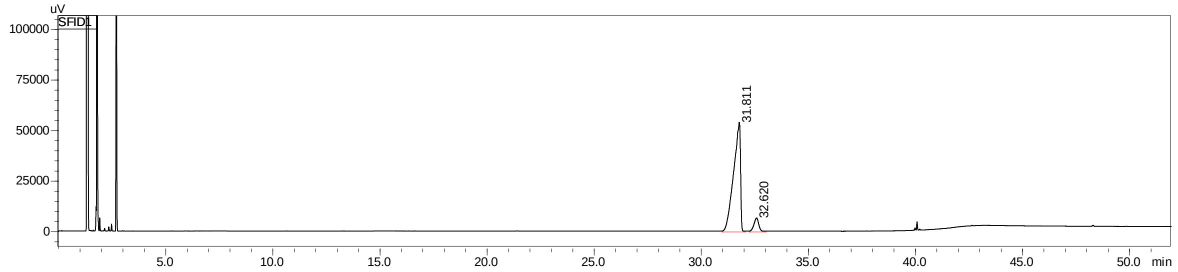
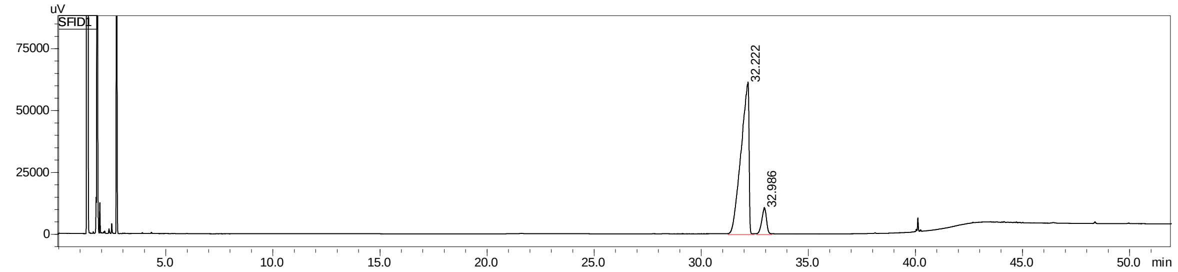
[6] A. Dumas, R. Tarrieu, T. Vives, T. Roisnel, V. Dorcet, O. Baslé and M. Mauduit, *ACS Catal*. 2018, **8**, 3257.

GC analysis for reaction performed at 25 °C



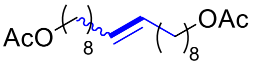
Peak	Retention time [min]	Area	Area [%]
1	31.811	1206818	92.527
2	32.620	97469	7.473

GC analysis for reaction performed at 35 °C



Peak	Retention time [min]	Area	Area [%]
1	32.222	1574418	91.060
2	32.986	154581	8.940

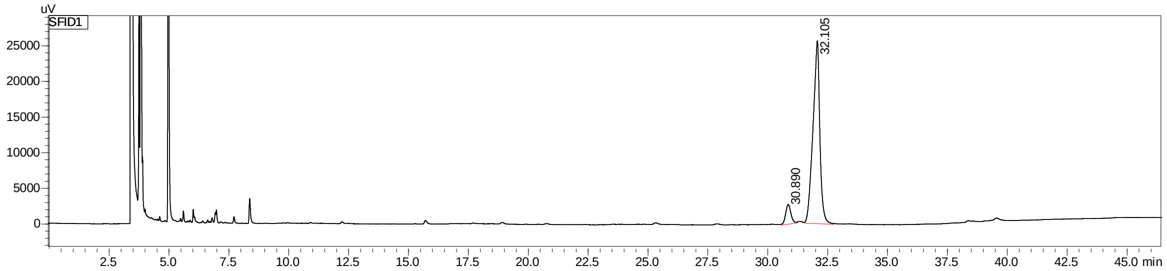
Octadec-9-ene-1,18-diyl diacetate (P1c)



Chemical formula : $C_{22}H_{40}O_4$

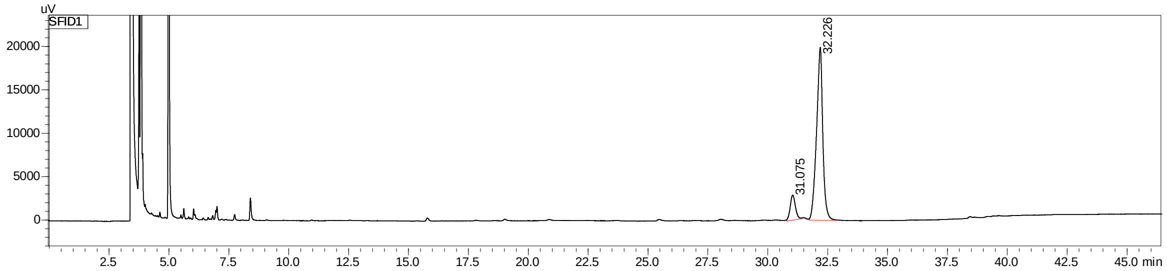
The reaction was performed following the general procedure, stirring a solution of 1-dec-9-en-1-yl acetate (0.45 mmol, 101 µL, 1.0 equiv.) and **Ru7** (0.0045 mmol, 2.96 mg, 1.0 mol%) in THF (216 µL) at 25 °C for 32 hours or at 35 °C for 16 hours. At a temperature of 25 °C, compound **P1c** was obtained with a conversion of 53% and yield of 52% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 93/7 measured by GC analysis. At a temperature of 35 °C, compound **P1c** was obtained with a conversion of 54% and yield of 54% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 90/10 measured by GC analysis. **^{1}H NMR (400 MHz, CDCl$_3$)** δ 5.37-5.29 (m, 2H), 4.03 (t, *J* = 6.8 Hz, 4H), 2.03 (s, 6H), 2.04-1.95 (m, 4H), 1.63-1.56 (m, 4H), 1.35-1.24 (m, 20H).

GC analysis for reaction performed at 25 °C



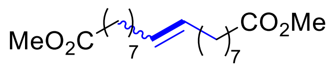
Peak	Retention time [min]	Area	Area [%]
1	30.890	38086	7.061
2	32.105	501334	92.939

GC analysis for reaction performed at 35 °C



Peak	Retention time [min]	Area	Area [%]
1	31.075	40113	10.135
2	32.226	355664	89.865

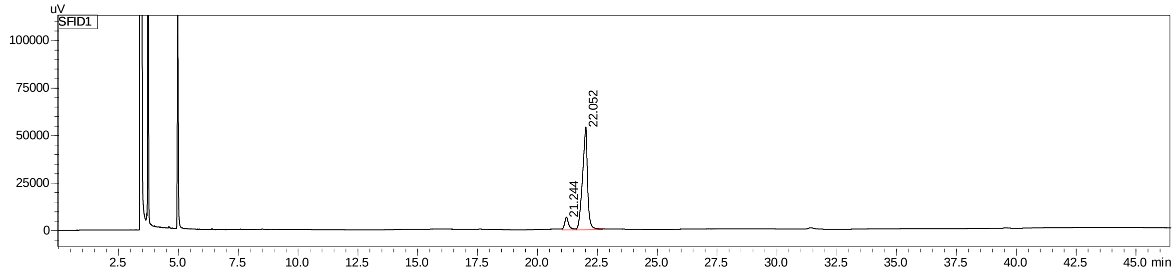
Dimethyl octadec-9-enedioate (P1d)



Chemical formula : $C_{20}H_{36}O_4$

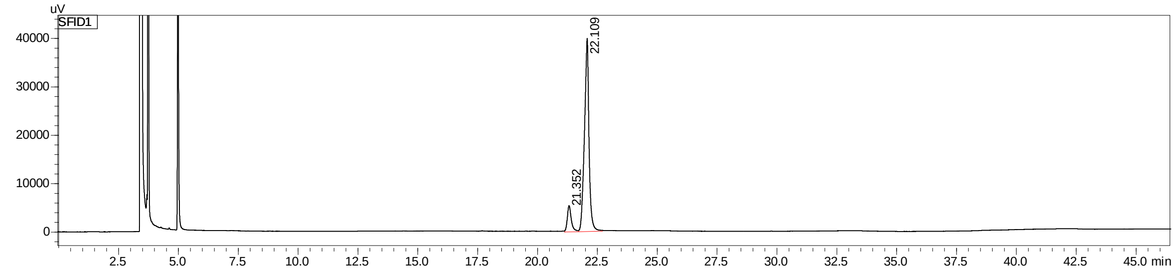
The reaction was performed following the general procedure, stirring a solution of methyl dec-9-enoate (0.45 mmol, 92 µL, 1.0 equiv.) and **Ru7** (0.0045 mmol, 2.96 mg, 1.0 mol%) in THF (216 µL) at 25 °C for 32 hours or at 35 °C for 16 hours. At a temperature of 25 °C, compound **P1d** was obtained with a conversion of 65% and yield of 65% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 92/8 measured by GC analysis. At a temperature of 35 °C, compound **P1d** was obtained with a conversion of 56% and yield of 56% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 90/10 measured by GC analysis. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 5.35-5.27 (m, 2H), 3.63 (s, 6H), 2.27 (t, *J* = 7.6 Hz, 4H), 2.00-1.92 (m, 4H), 1.63-1.55 (m, 4H), 1.34-1.27 (m, 16H).

GC analysis for reaction performed at 25 °C



Peak	Retention time [min]	Area	Area [%]
1	21.244	66667	8.038
2	22.052	762713	91.962

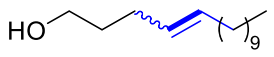
GC analysis for reaction performed at 35 °C



Peak	Retention time [min]	Area	Area [%]
1	21.352	57732	10.088
2	22.109	514528	89.912

5.2.Cross-Metathesis

Hexadec-4-en-1-ol (P2a)



Chemical formula : $C_{15}H_{30}O$

Inside a glovebox, 4-penten-1-ol (0.2 mmol, 23 µL, 1.0 equiv.), dodec-1-ene (0.5 mmol, 113 µL, 2.5 equiv.), 1,3,5-trimethoxybenzene as internal standard (0.2 mmol, 1.0 equiv.) and a solution of ruthenium-CAAC complex **Ru7** (0.006 mmol, 3.94 mg, 3 mol% or 0.004 mmol, 2.63 mg, 2 mol%) in THF (0.2 mL) were sequentially loaded into an oven-dried vial. The reaction was stirred at 25 °C for 28 hours then quenched with EVE. At a catalytic loading of 3 mol%, compound **P2a** was obtained with a conversion of 48% and yield of 41% measured by ^{1}H-NMR (IS: 0.15 mmol, 25.2 mg, 0.33 equiv.) and *Z/E* ratio of 92/8 measured by ^{13}C-NMR. At a catalytic loading of 2 mol%, compound **P1d** was obtained with a conversion of 36% and yield of 31% measured by ^{1}H-NMR (IS: 0.067 mmol, 11.3 mg, 0.33 equiv.) and *Z/E* ratio of 93/7 measured by ^{13}C-NMR. The data were consistent with reported literature[7].
^{1}H NMR (400 MHz, CDCl$_3$) δ 5.49-5.33 (m, 2H), 3.65 (td, *J* = 6.5, 2.6 Hz, 2H), 2.15-1.94 (m, 4H), 1.69-1.59 (m, 2 H), 1.37-1.26 (m, 17H), 0.88 (t, *J* = 6.8 Hz, 3H).

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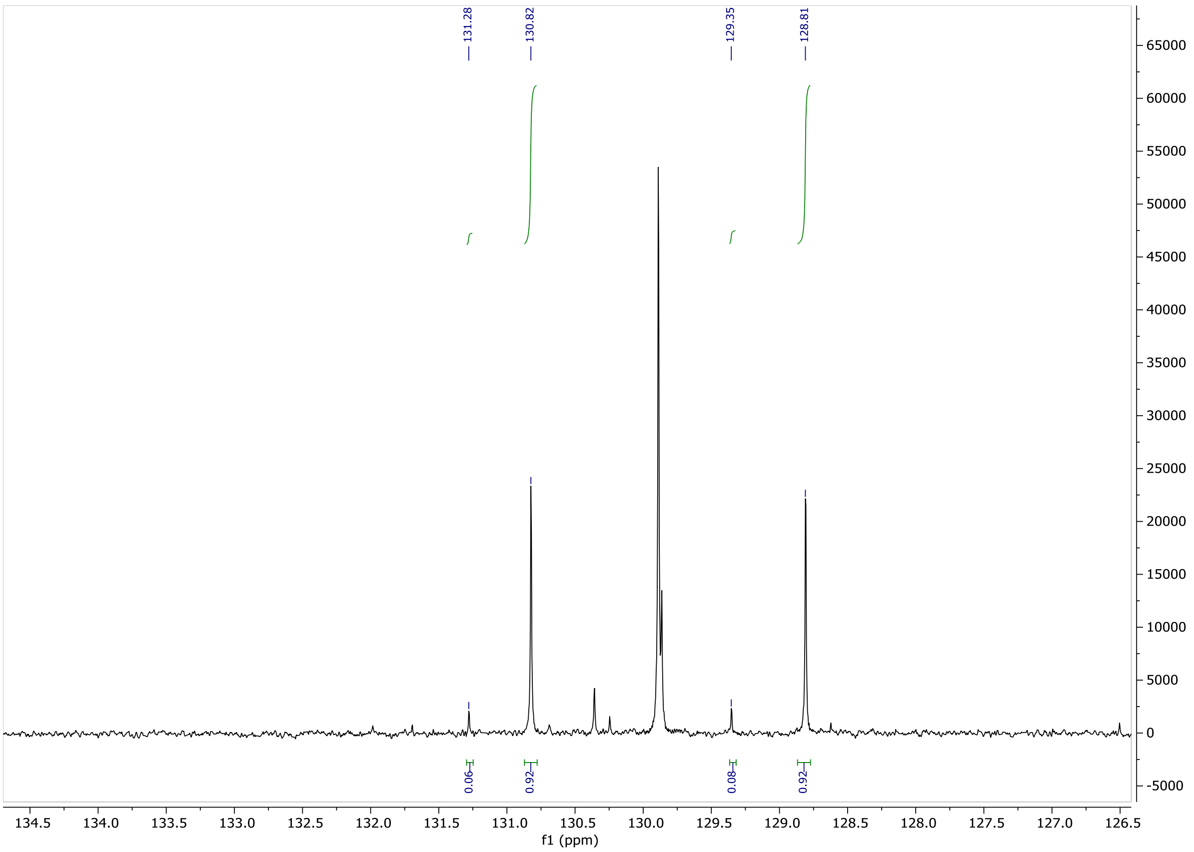
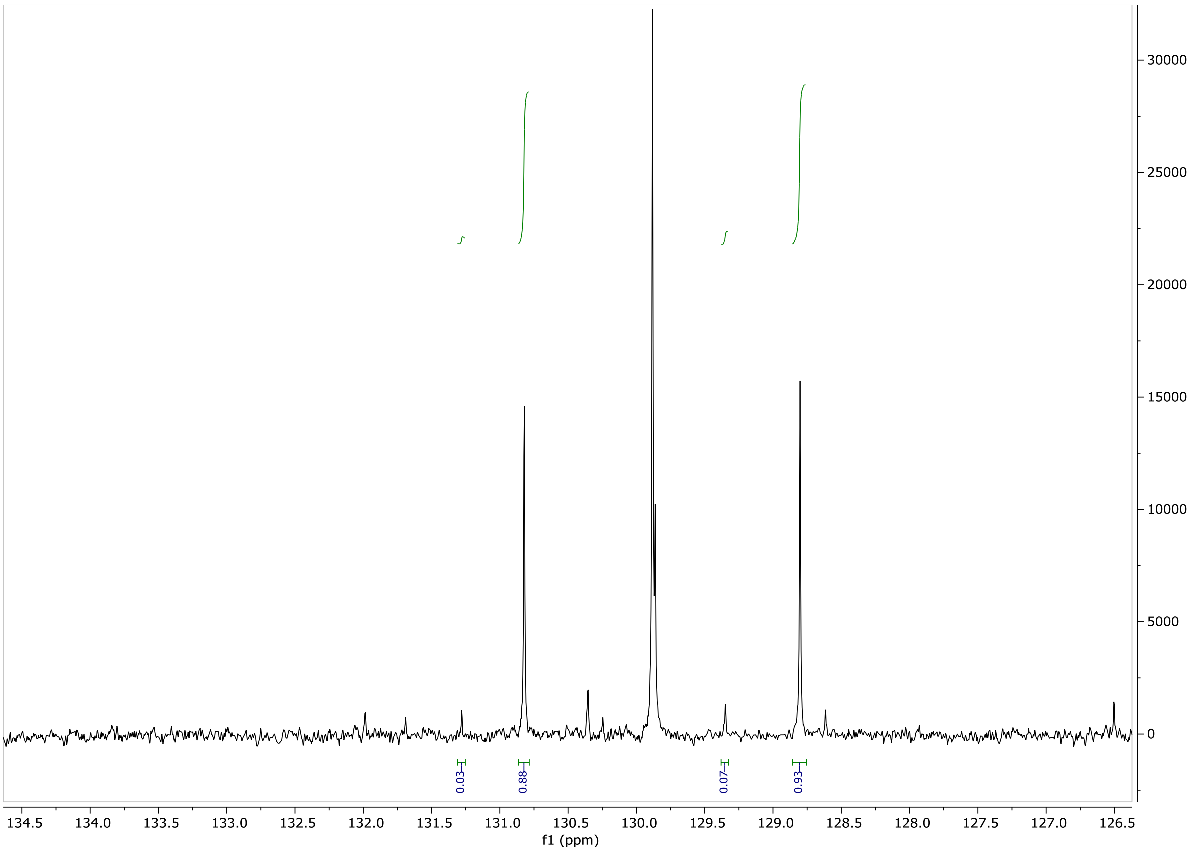
[7] U. Grünanger and B. Breit, *Angew. Chem., Int. Ed.* 2010, **49**, 967.

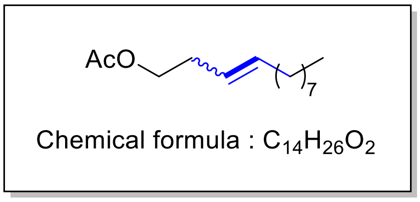
^{13}C-NMR for reaction performed at a catalytic loading of 3 mol%



^{13}C-NMR for reaction performed at a catalytic loading of 2 mol%



Dodec-3-en-1-yl acetate (P2b)



Inside a glovebox, but-3-en-1-yl acetate (0.2 mmol, 25 μL, 1.0 equiv.), 1-decene (0.6 mmol, 114 μL, 3.0 equiv.), 1,3,5-trimethoxybenzene as internal standard (0.2 mmol, 1.0 equiv.) and a solution of ruthenium-CAAC complex **Ru7** (0.006 mmol, 3.94 mg, 3 mol% or 0.004 mmol, 2.63 mg, 2 mol%) in THF (0.2 mL) were sequentially loaded into an oven-dried vial. The reaction was stirred at 25 °C for 48 hours then quenched with EVE. At a catalytic loading of 3 mol%, compound **P2b** was obtained with a conversion of 82% and yield of 50% measured by ^{1}H-NMR and *Z/E* ratio of 94/6 measured by GC analysis. At a catalytic loading of 2 mol%, compound **P2b** was obtained with a conversion of 81% and yield of 46% measured by ^{1}H-NMR and *Z/E* ratio of 94/6 measured by GC analysis. The data were consistent with reported literature[8]. **^{1}H NMR (400 MHz, CDCl$_3$)** δ 5.54-5.47 (m, 1 H), 5.37-5.30 (m, 1 H), 4.06 (t, *J* = 7.0 Hz, 2 H), 2.40-2.30 (m, 2 H), 2.06-1.97 (m, 5 H), 1.36-1.25 (m, 12 H), 0.88 (t, J = 6.9 Hz, 3 H).

Column Information: DB-23 (60 m x 0.25 mm ID; 0.25 μm thickness) (Agilent)
Carrier gas: Helium
Linear velocity: constant = 40.0 cm/s
Temperature protocol:

Rate (°C/min)	Temperature (°C)	Hold time (min)
-	80	2
1	125	2
10	240	0

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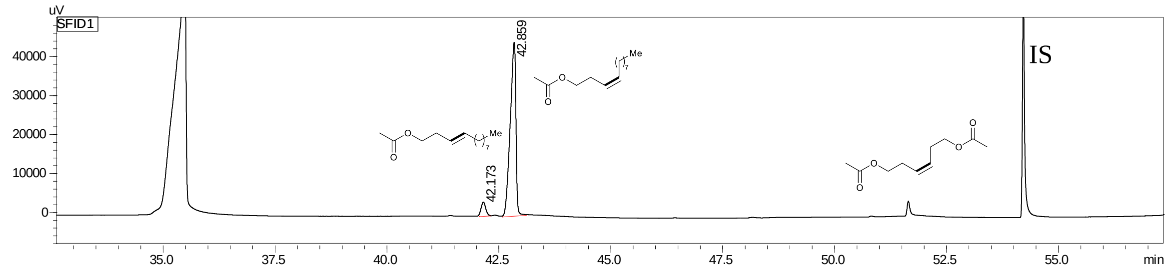
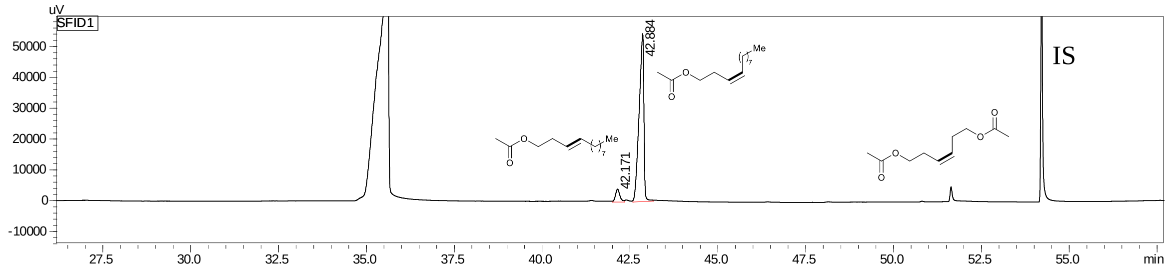
[8] J. Morvan, T. McBride, I. Curbet, S. Colombel-Rouen, T. Roisnel, C. Crévisy, D. L. Browne and M. Mauduit, *Angew. Chem. Int. Ed*. 2021, **60**, 19685.

GC analysis for reaction performed at a catalytic loading of 3 mol%



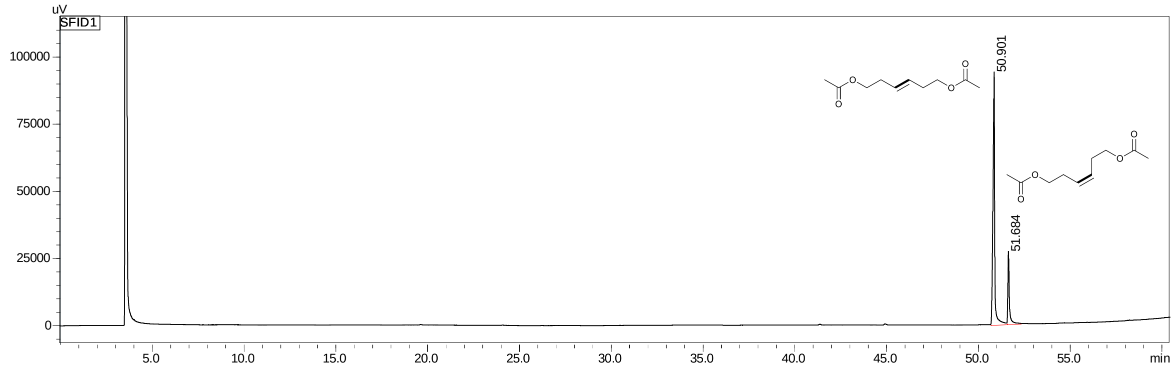
Peak	Retention time [min]	Area	Area [%]
1	42.173	23589	5.741
2	42.859	387296	94.259

GC analysis for reaction performed at a catalytic loading of 2 mol%

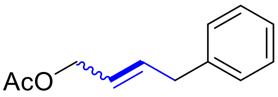


Peak	Retention time [min]	Area	Area [%]
1	42.171	31299	5.884
2	42.884	500656	94.116

GC analysis of but-3-en-1-yl acetate self-metathesis product



4-phenylbut-2-en-1-yl acetate (P2c)



Chemical formula : $C_{12}H_{14}O_2$

Inside a glovebox, allyl acetate (0.2 mmol, 22 μL, 1.0 equiv.), allylbenzene (0.5 mmol, 68 μL, 3.0 equiv.), 1,3,5-trimethoxybenzene as internal standard (0.2 mmol, 1.0 equiv.) and a solution of ruthenium-CAAC complex **Ru7** (0.006 mmol, 3.94 mg, 3 mol% or 0.004 mmol, 2.63 mg, 2 mol%) in THF (0.2 mL) were sequentially loaded into an oven-dried vial. The reaction was stirred at 25 °C and aliquots were taken at 21 hours and 48 hours then quenched with EVE. At a catalytic loading of 3 mol%, after 21 hours of reaction compound **P2c** was obtained with a conversion of 65% and yield of 29% for the *Z* isomer measured by ^{1}H-NMR and *Z/E* ratio of 92/8 measured by GC analysis. After 48 hours of reaction compound **P2c** was obtained with a conversion of 90% and yield of 39% for the *Z* isomer measured by ^{1}H-NMR and *Z/E* ratio of 85/15 measured by GC analysis. At a catalytic loading of 2 mol%, after 21 hours of reaction compound **P2c** was obtained with a conversion of 65% and yield of 22% for the *Z* isomer measured by ^{1}H-NMR and *Z/E* ratio of 92/8 measured by GC analysis. After 48 hours of reaction compound **P2c** was obtained with a conversion of 94% and yield of 29% for the *Z* isomer measured by ^{1}H-NMR and *Z/E* ratio of 88/12 measured by GC analysis. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.32-7.28 (m, 2H), 7.23-7.18 (m, 3H), 5.97-5.80 (m, 1H), 5.72-5.64 (m, 1H), 4.75 (d, *J* = 6.9, 1.75H, *Z* isomer), 4.56 (d, *J* = 6.4, 0.25H, *E* isomer), 3.48 (d, *J* = 7.5 Hz, 1.75H, *Z* isomer), 3.41 (d, *J* = 6.7, 0.25H, *E* isomer), 2.09 (s, 2.52H, *Z* isomer), 2.07 (s, 0.35H, *E* isomer).

Column Information: DB-23 (60 m x 0.25 mm ID; 0.25 μm thickness) (Agilent)

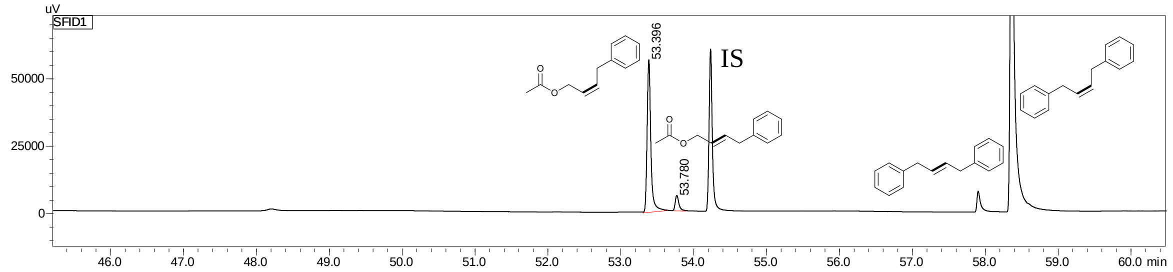
Carrier gas: Helium

Linear velocity: constant = 40.0 cm/s

Temperature protocol:

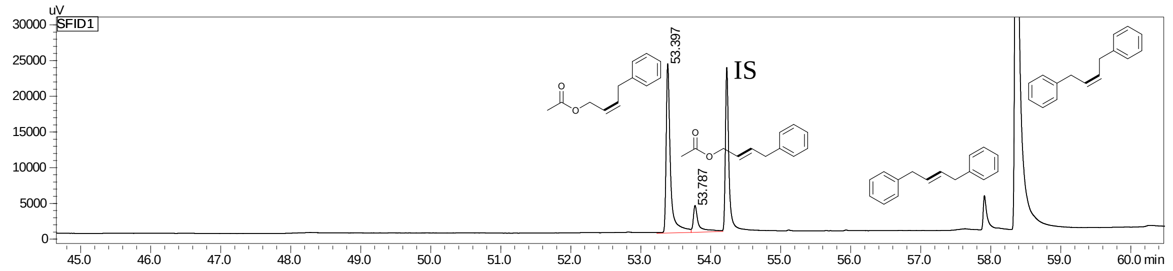
Rate (°C/min)	Temperature (°C)	Hold time (min)
-	80	2
1	125	2
10	240	0

GC analysis for reaction performed at a catalytic loading of 3 mol% and a reaction time of 21 hours



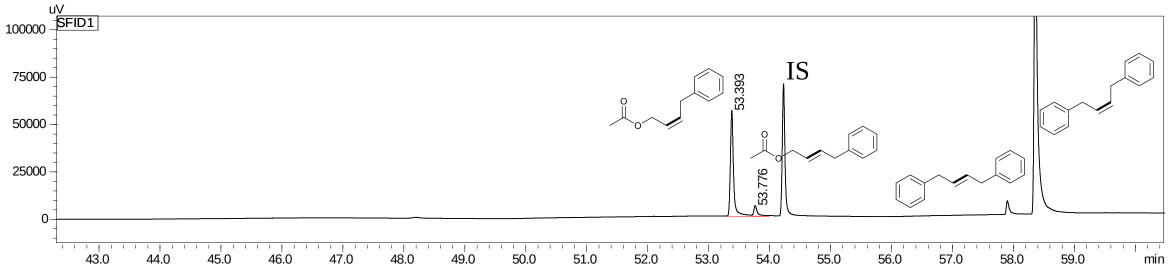
Peak	Retention time [min]	Area	Area [%]
1	53.396	196624	91.751
2	53.780	17677	8.249

GC analysis for reaction performed at a catalytic loading of 3 mol% and a reaction time of 48 hours



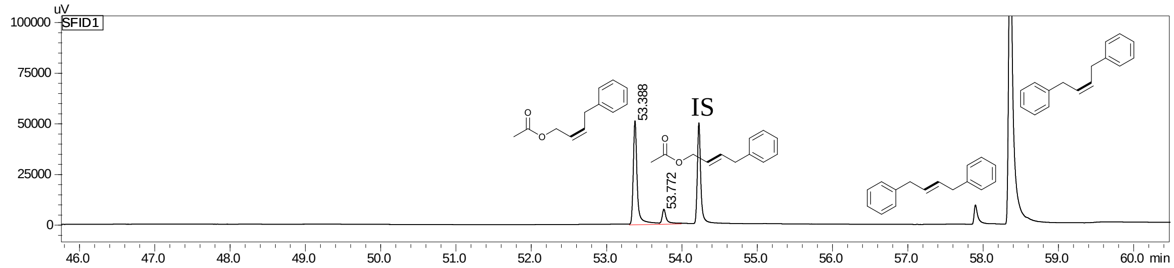
Peak	Retention time [min]	Area	Area [%]
1	53.397	98481	84.942
2	53.787	17459	15.058

GC analysis for reaction performed at a catalytic loading of 2 mol% and a reaction time of 21 hours



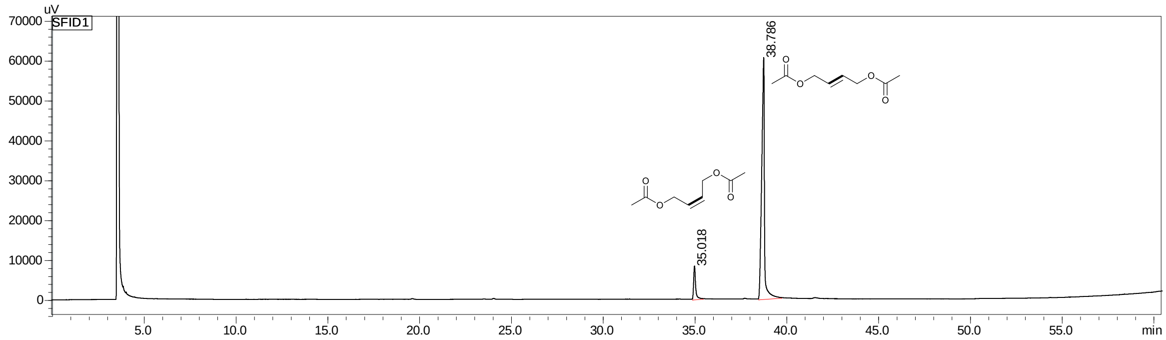
Peak	Retention time [min]	Area	Area [%]
1	53.393	200097	92.093
2	53.776	17180	7.907

GC analysis for reaction performed at a catalytic loading of 2 mol% and a reaction time of 48 hours

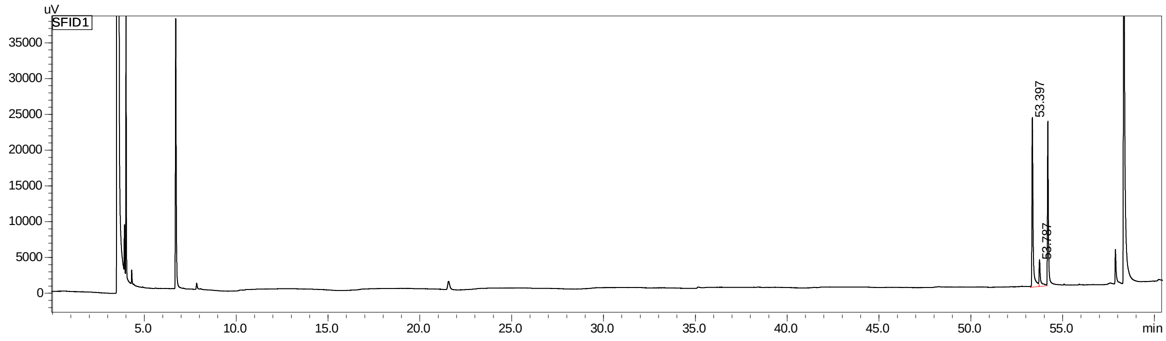


Peak	Retention time [min]	Area	Area [%]
1	53.388	181896	87.869
2	53.772	25111	12.131

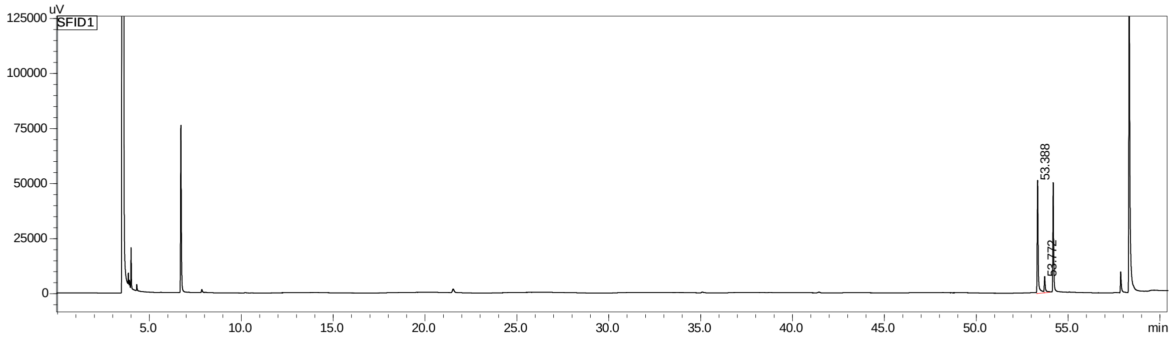
GC analysis of allyl acetate self-metathesis product



Full spectrum for the reaction performed at a catalytic loading of 3 mol% and a reaction time of 48 hours

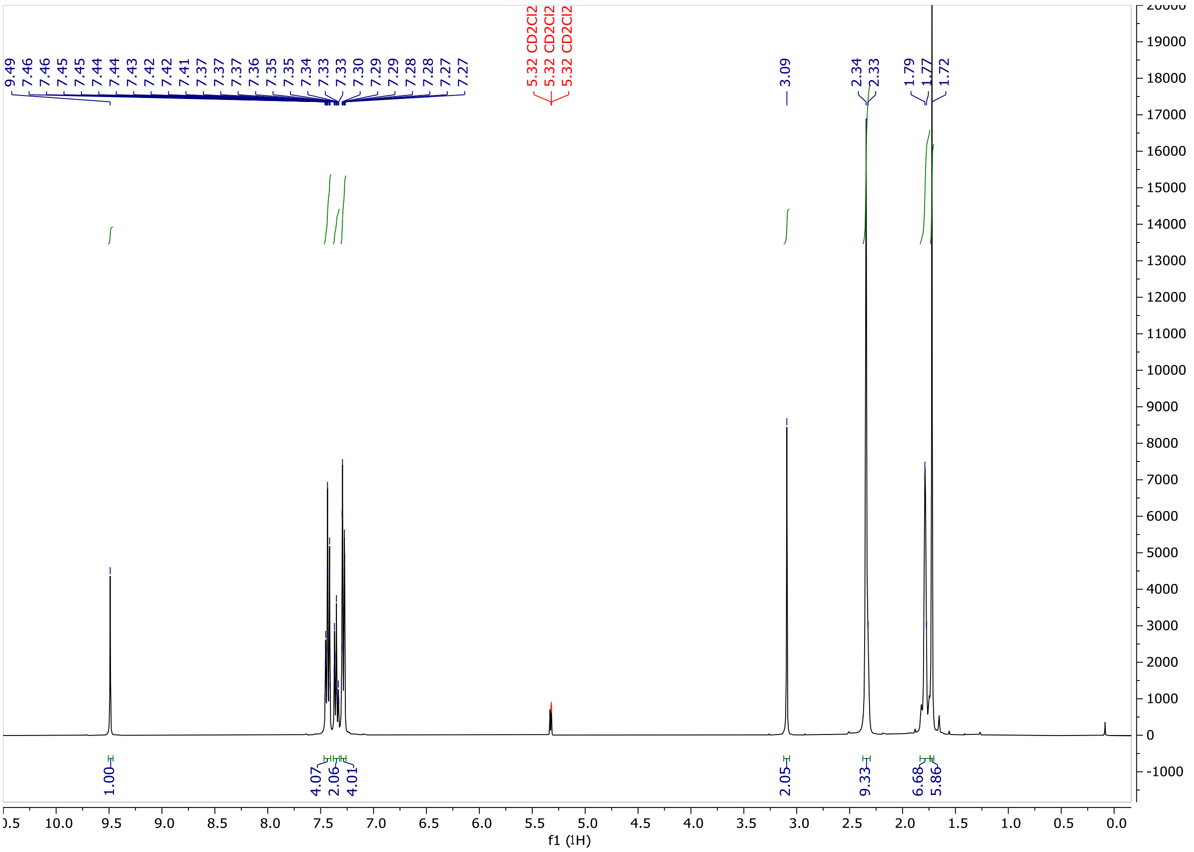


Full spectrum for the reaction performed at a catalytic loading of 2 mol% and a reaction time of 48 hours

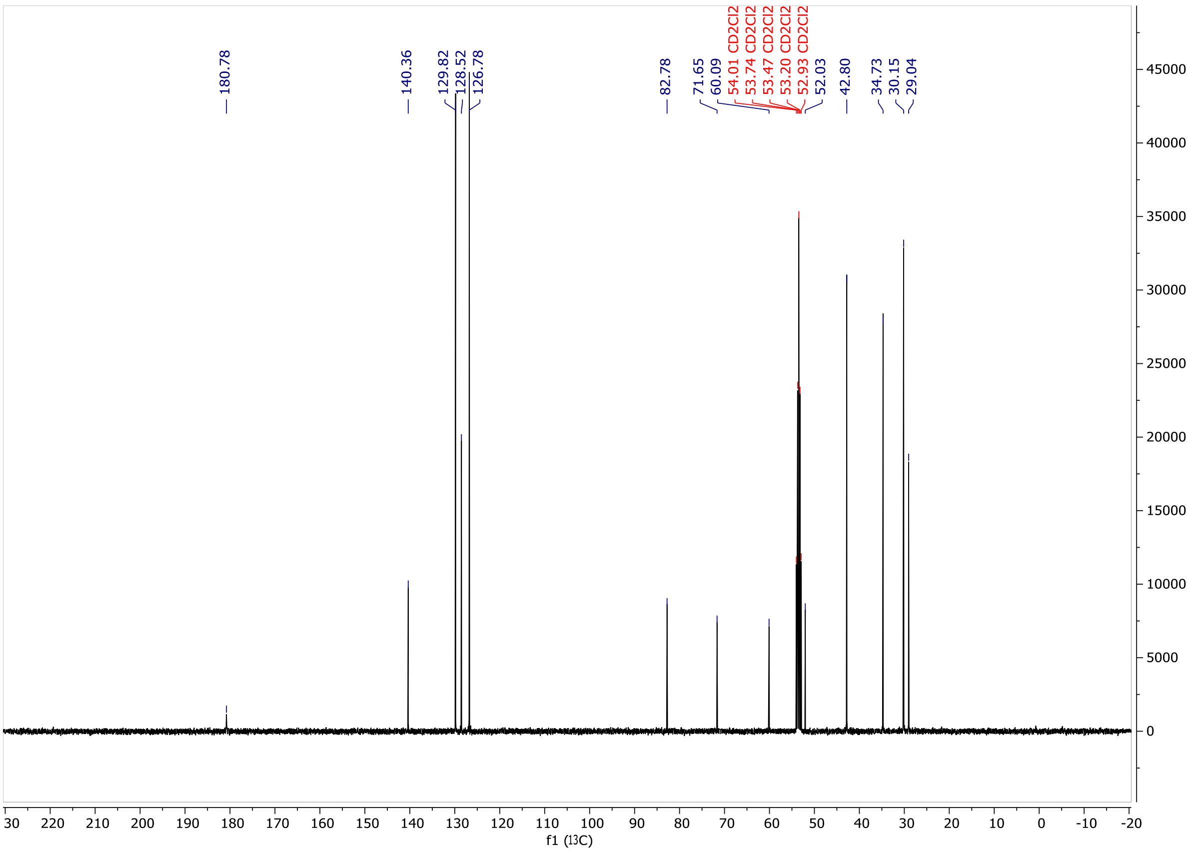


6. NMR Spectra

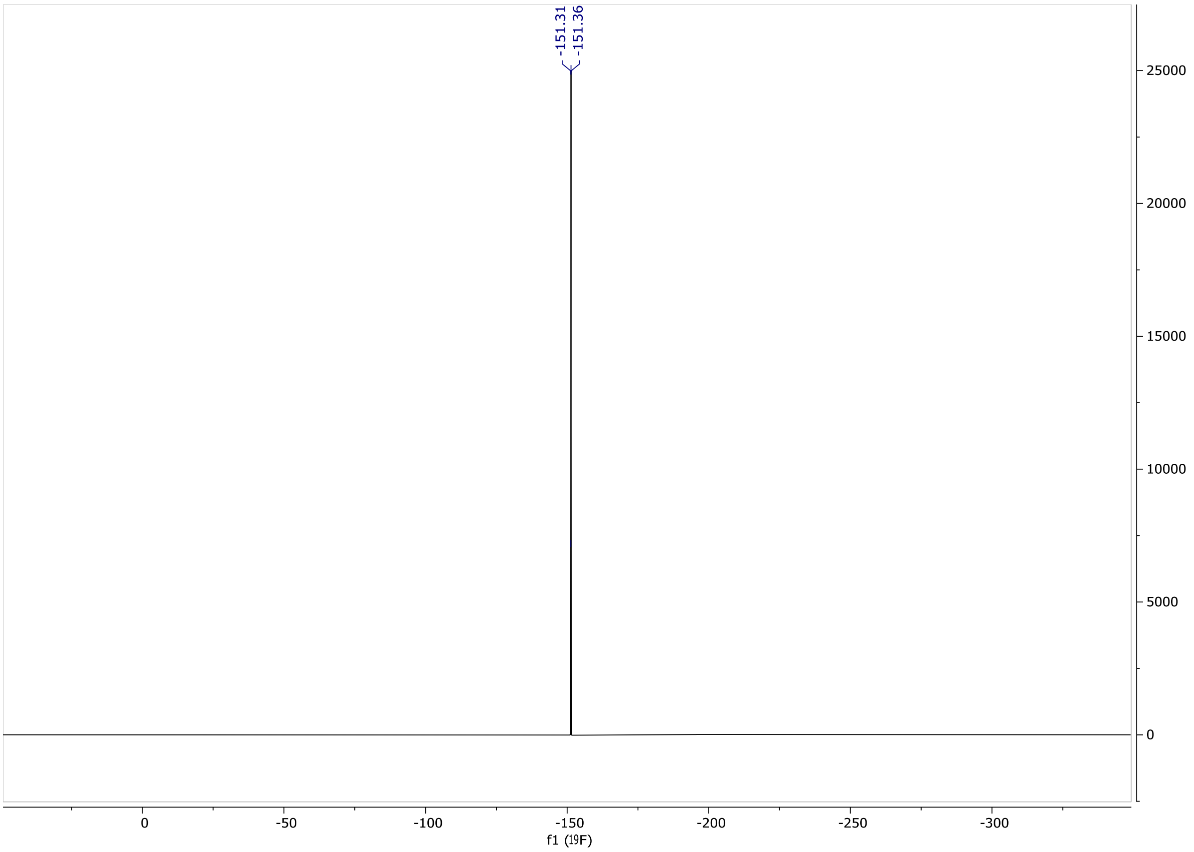
^{1}H NMR (400 MHz, CDCl$_3$) (^{Ad}CAAC-1a.BF$_4$)



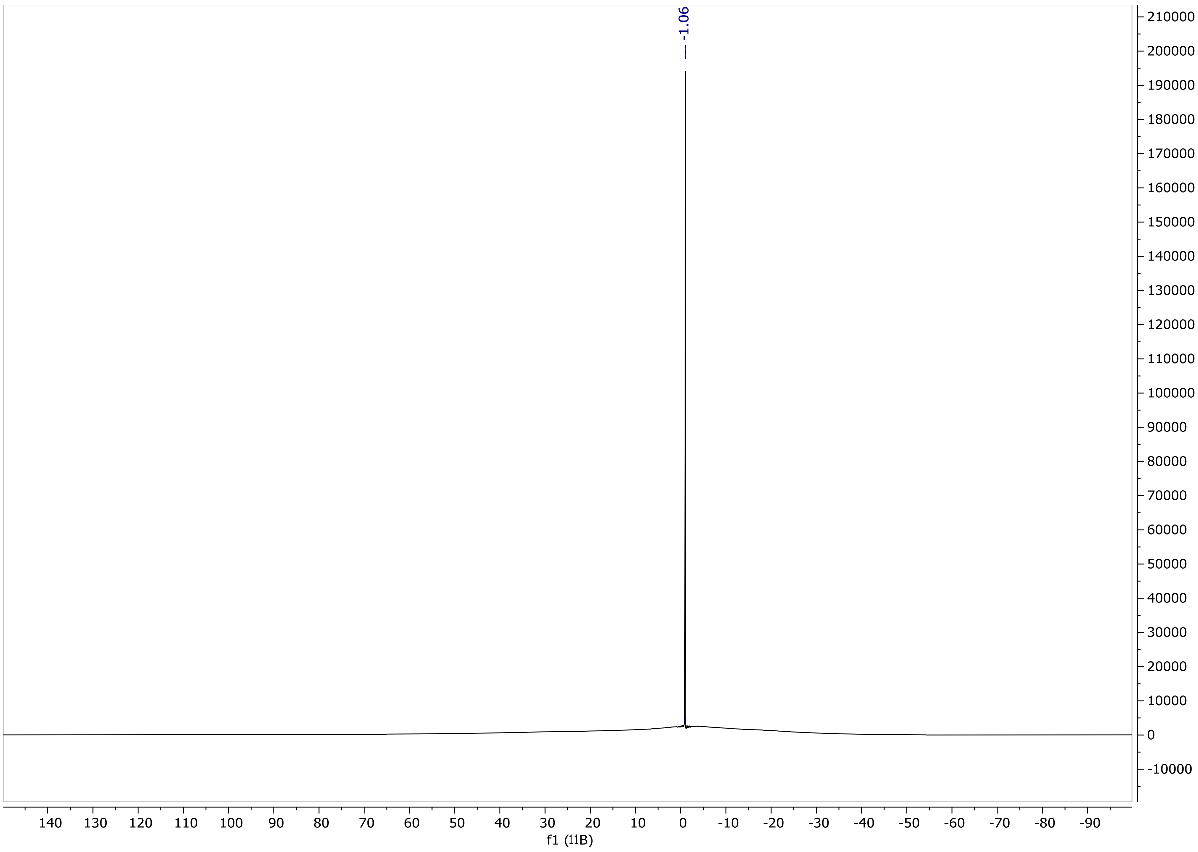
^{13}C NMR (101 MHz, CDCl$_3$) (^{Ad}CAAC-1a.BF$_4$)



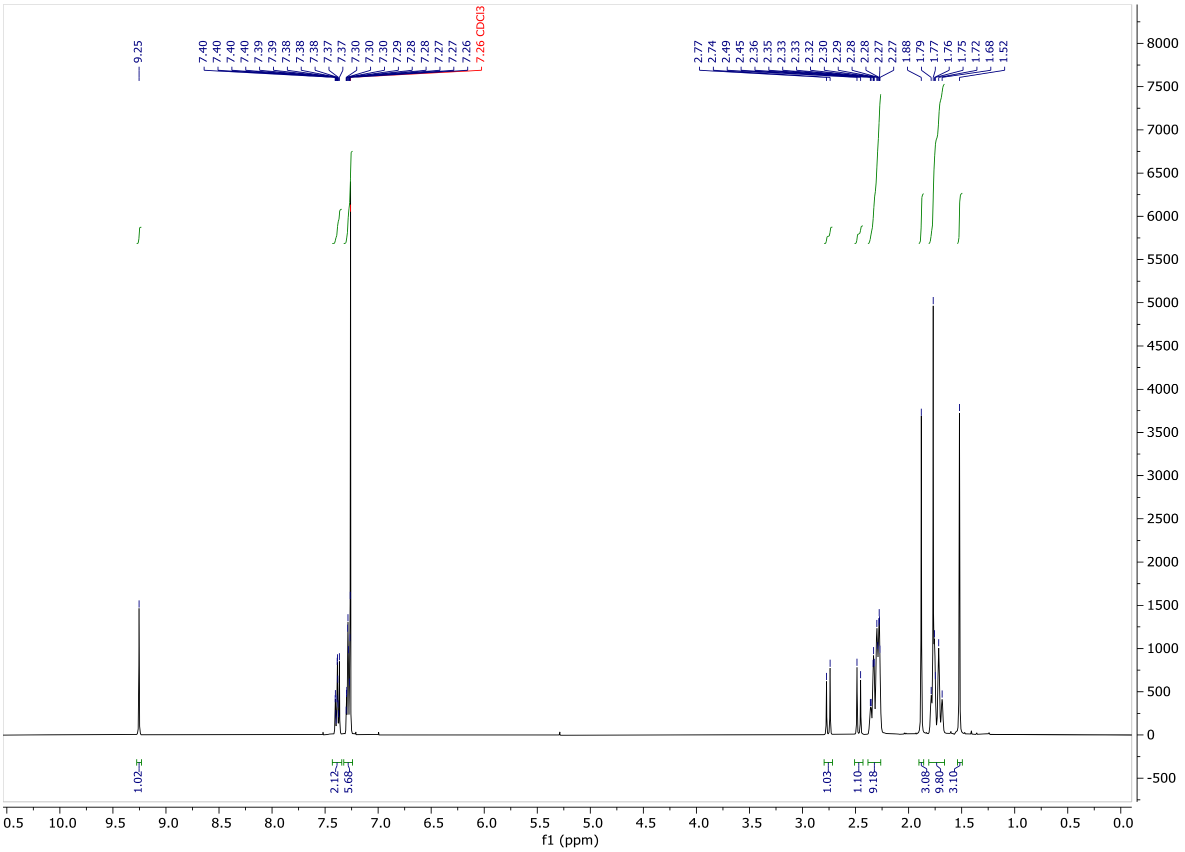
^{19}F NMR (376 MHz, CDCl$_3$) (^{Ad}CAAC-1a.BF$_4$)



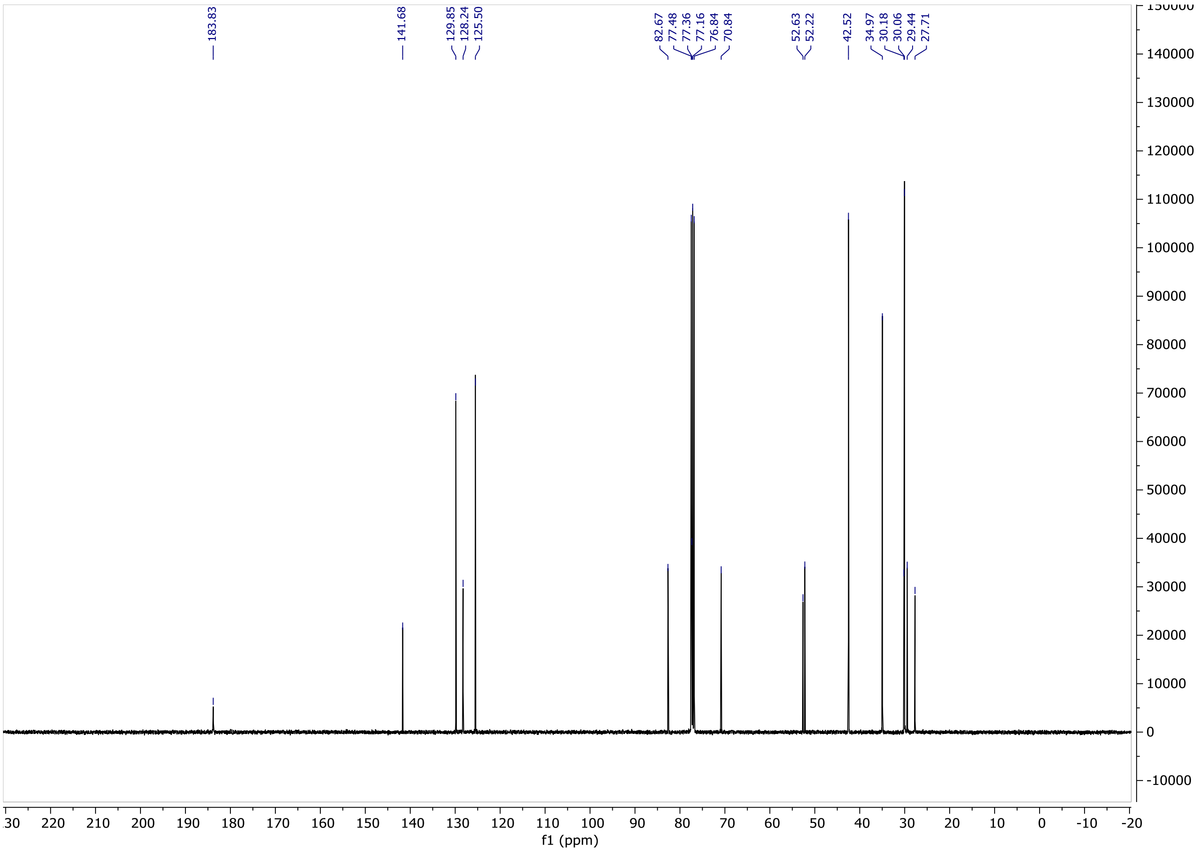
^{11}B NMR (128 MHz, CDCl$_3$) (^{Ad}CAAC-1a.BF$_4$)



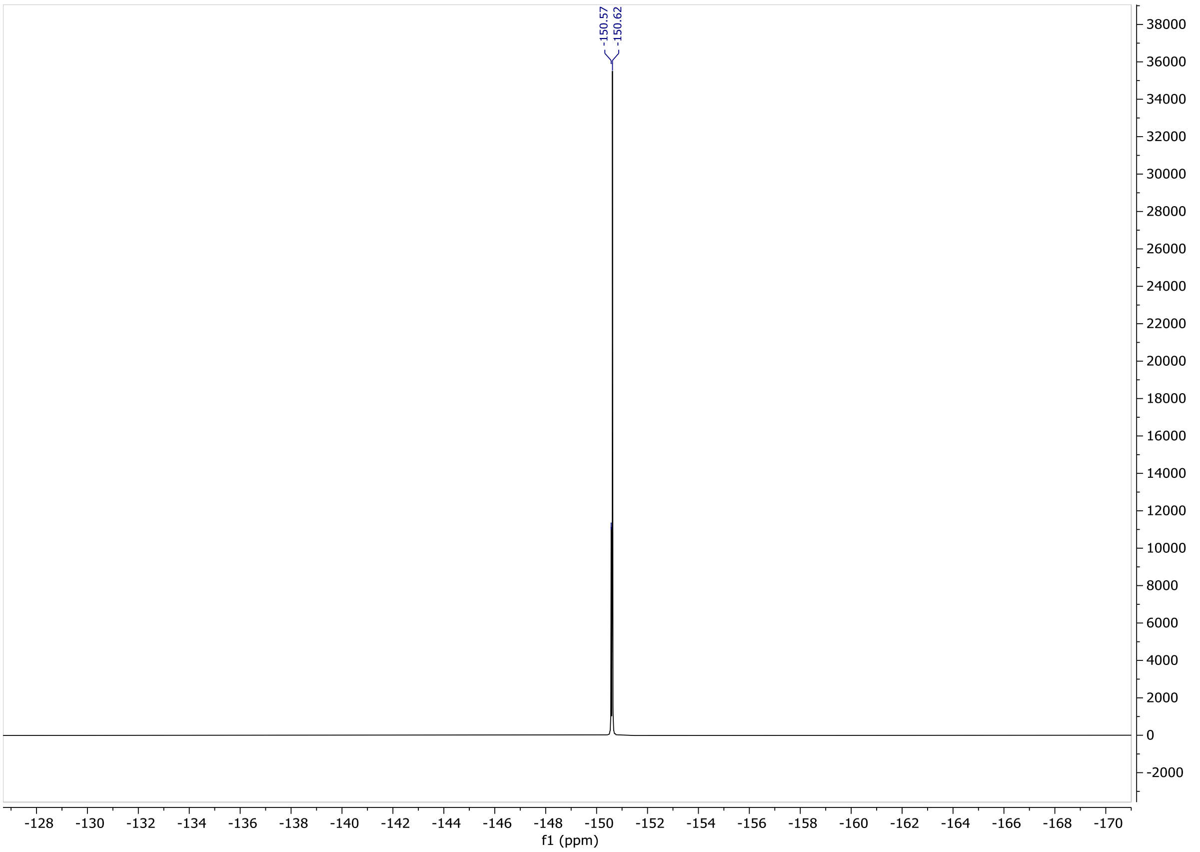
^{1}H NMR (400 MHz, CDCl$_3$) (^{Ad}CAAC-1b.BF$_4$)



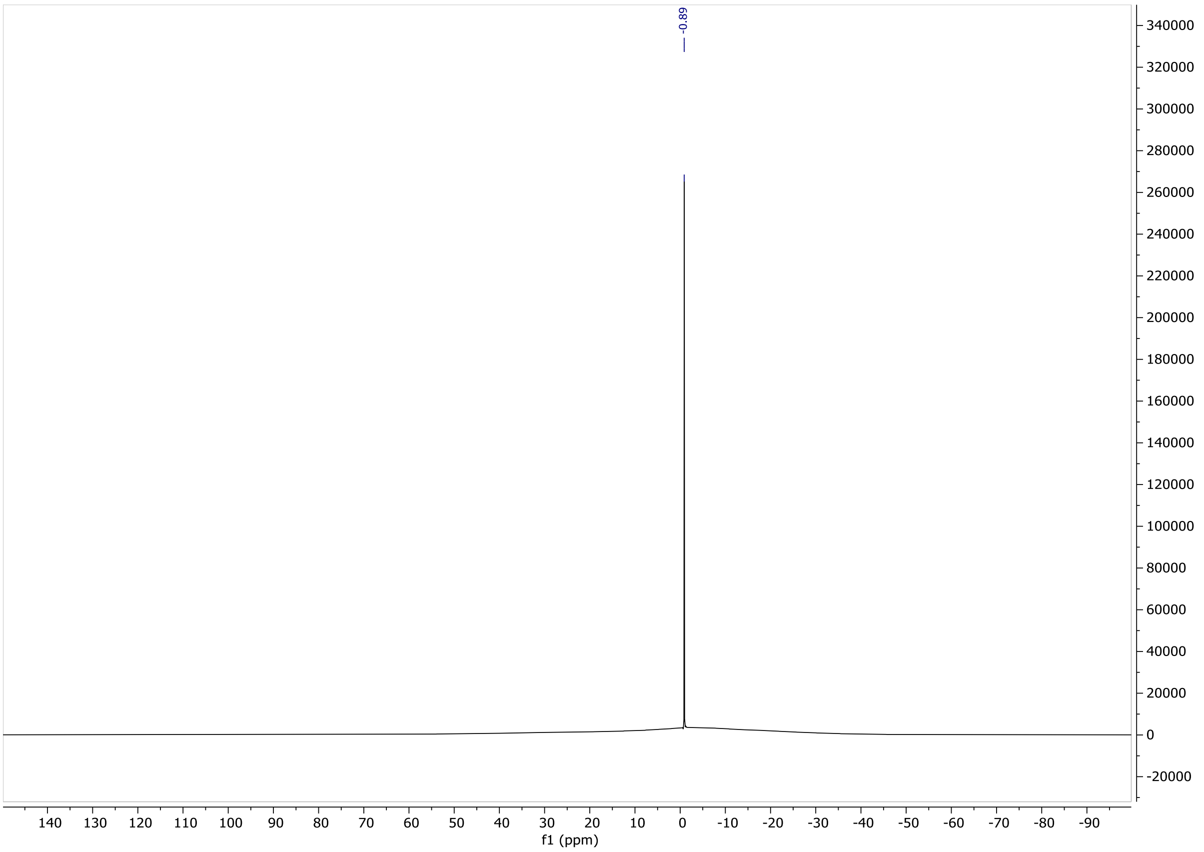
^{13}C NMR (101 MHz, CDCl$_3$) (CAAC-1b.BF$_4$)



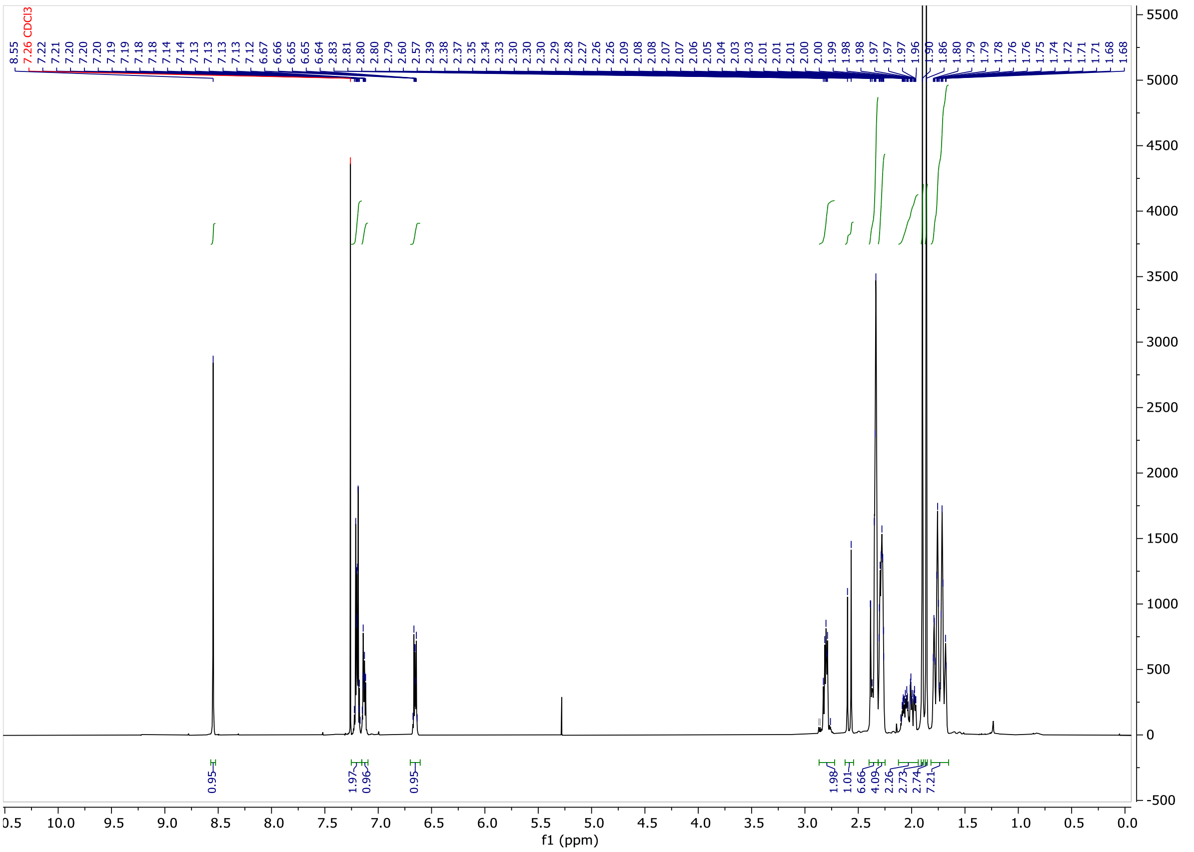
^{19}F NMR (376 MHz, $CDCl_3$) (CAAC-1b.BF_4)



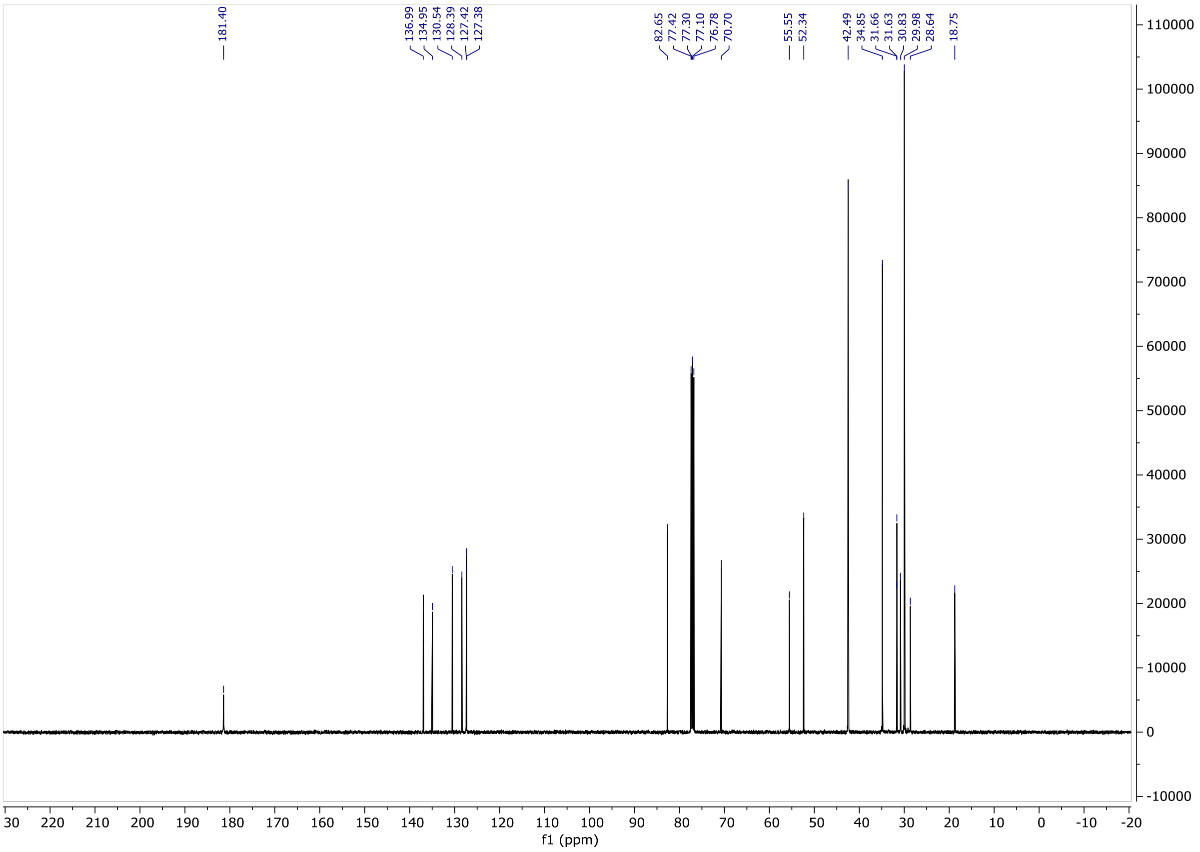
^{11}B NMR (128 MHz, $CDCl_3$) (CAAC-1b.BF_4)



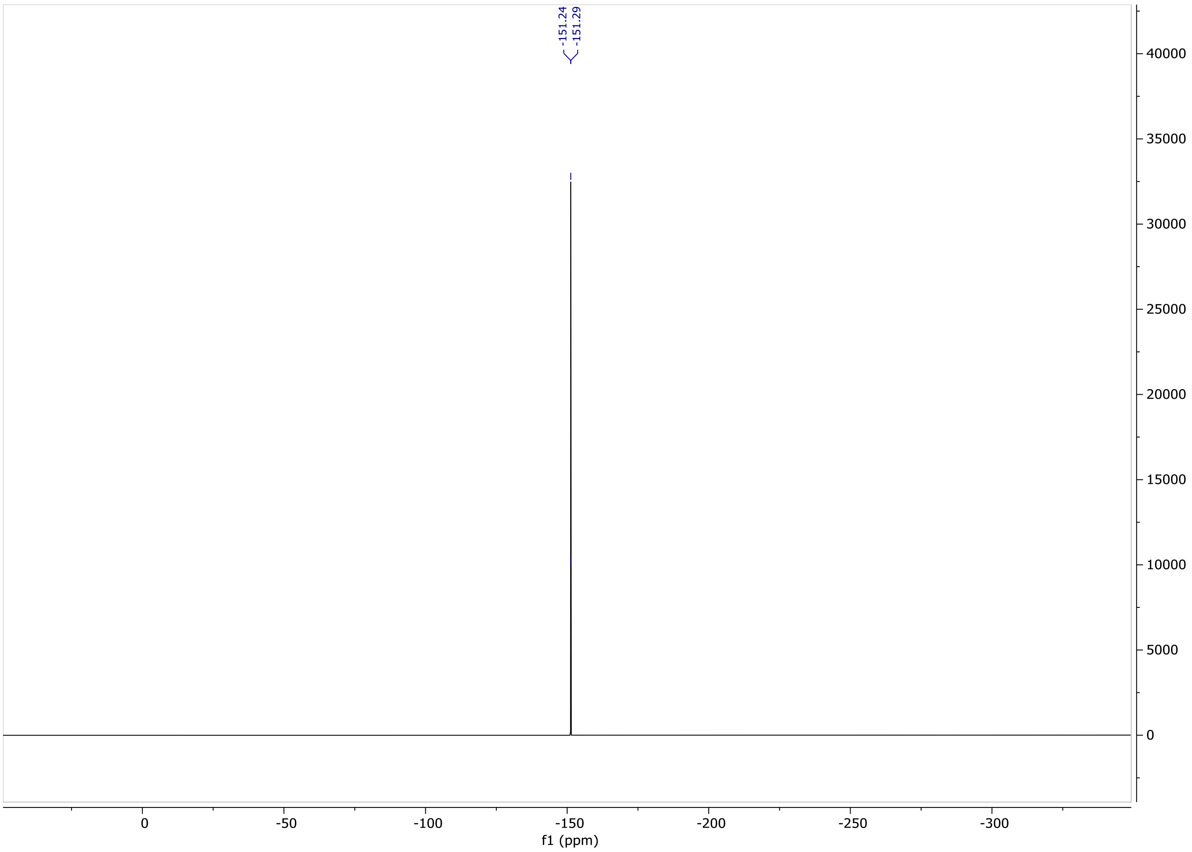
^{1}H NMR (400 MHz, CDCl$_3$) (^{Ad}CAAC-1c.BF$_4$)



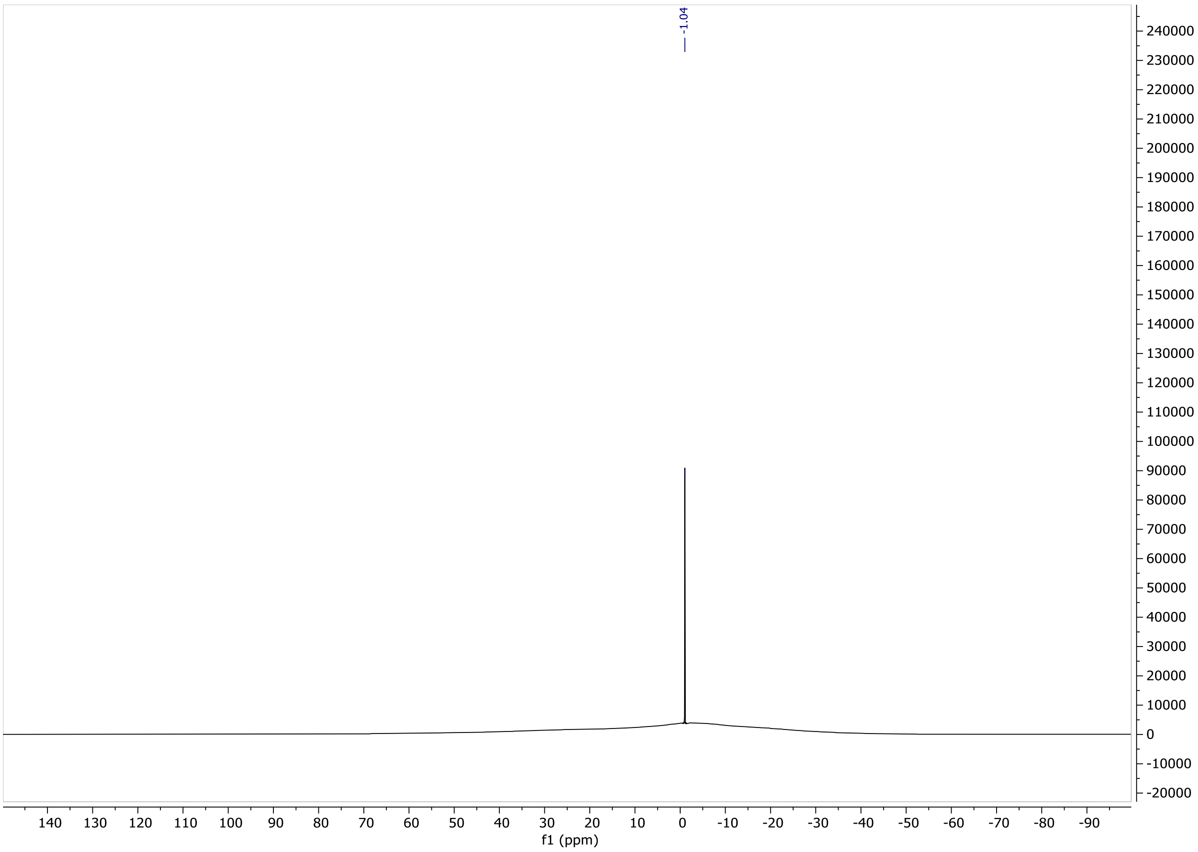
^{13}C NMR (101 MHz, CDCl$_3$) (CAAC-1c.BF$_4$)



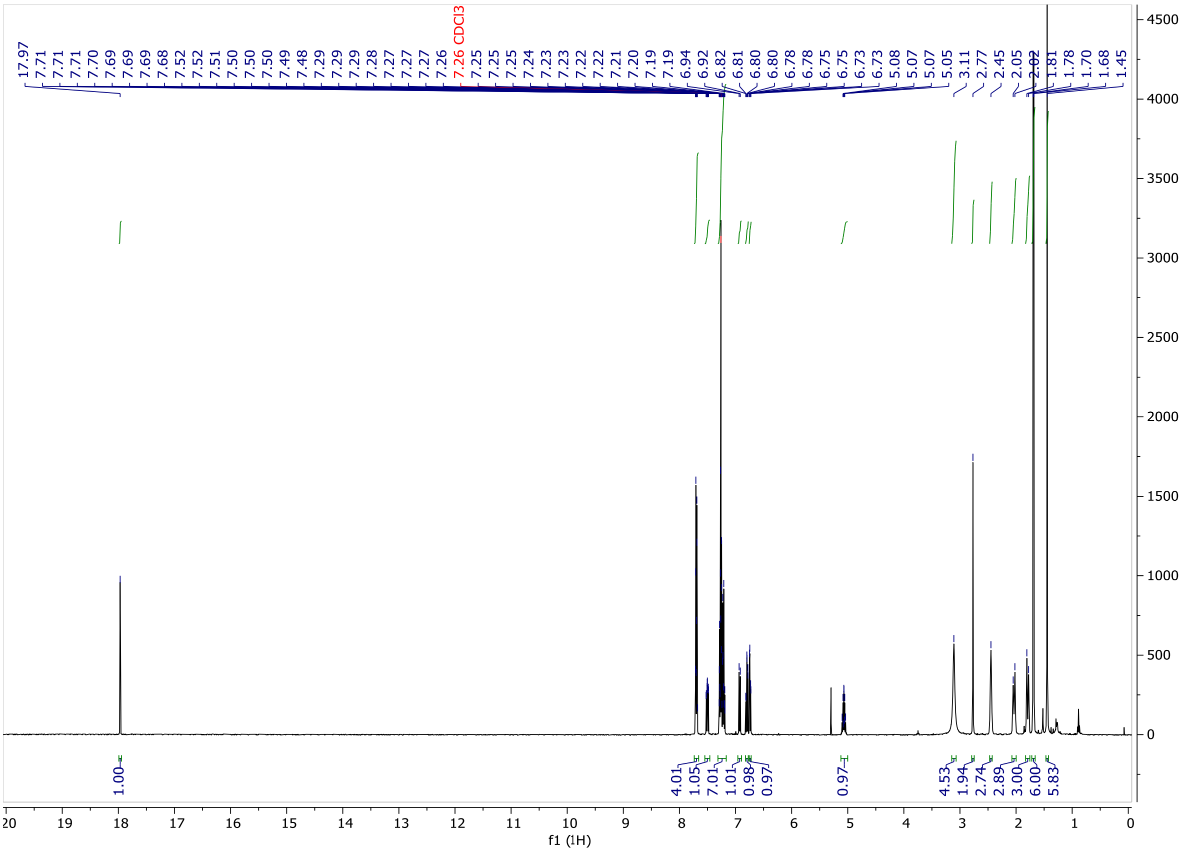
^{19}F NMR (376 MHz, $CDCl_3$) (CAAC-1c.BF_4)



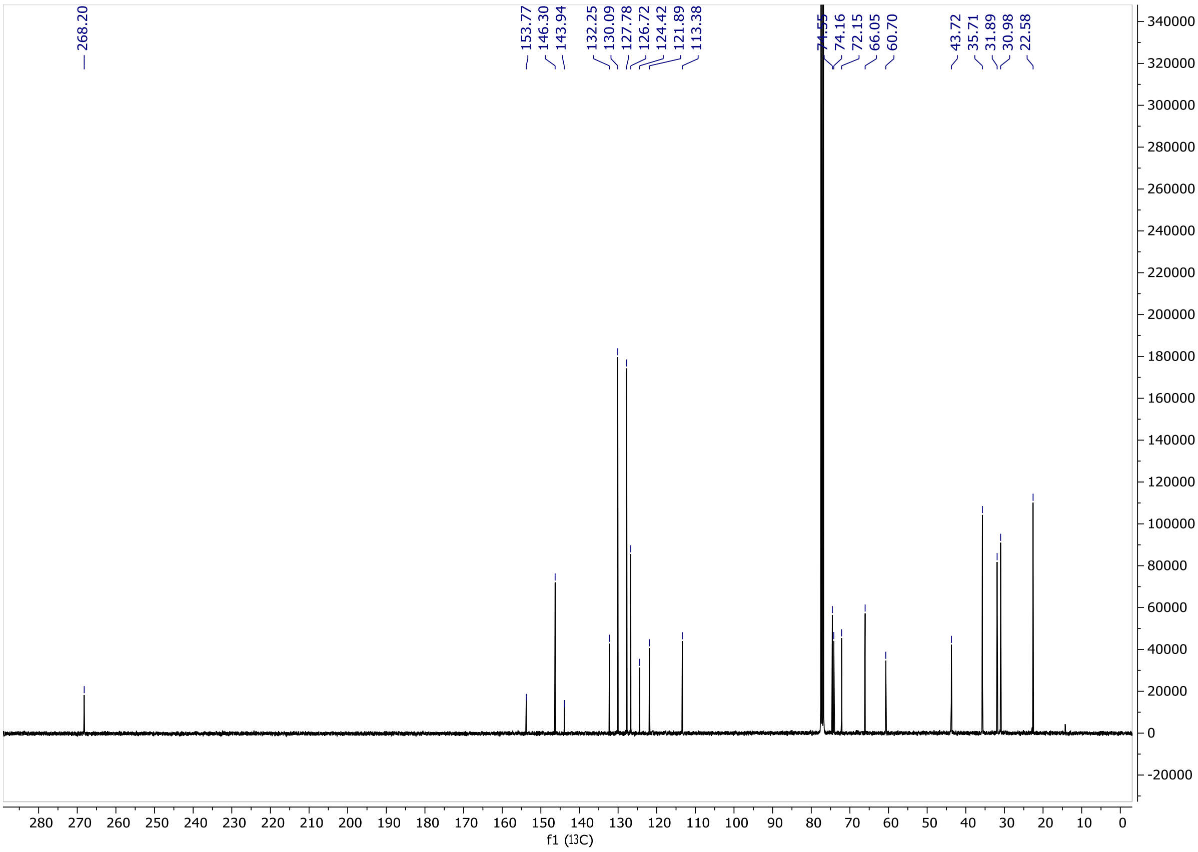
^{11}B NMR (128 MHz, $CDCl_3$) (CAAC-1c.BF_4)



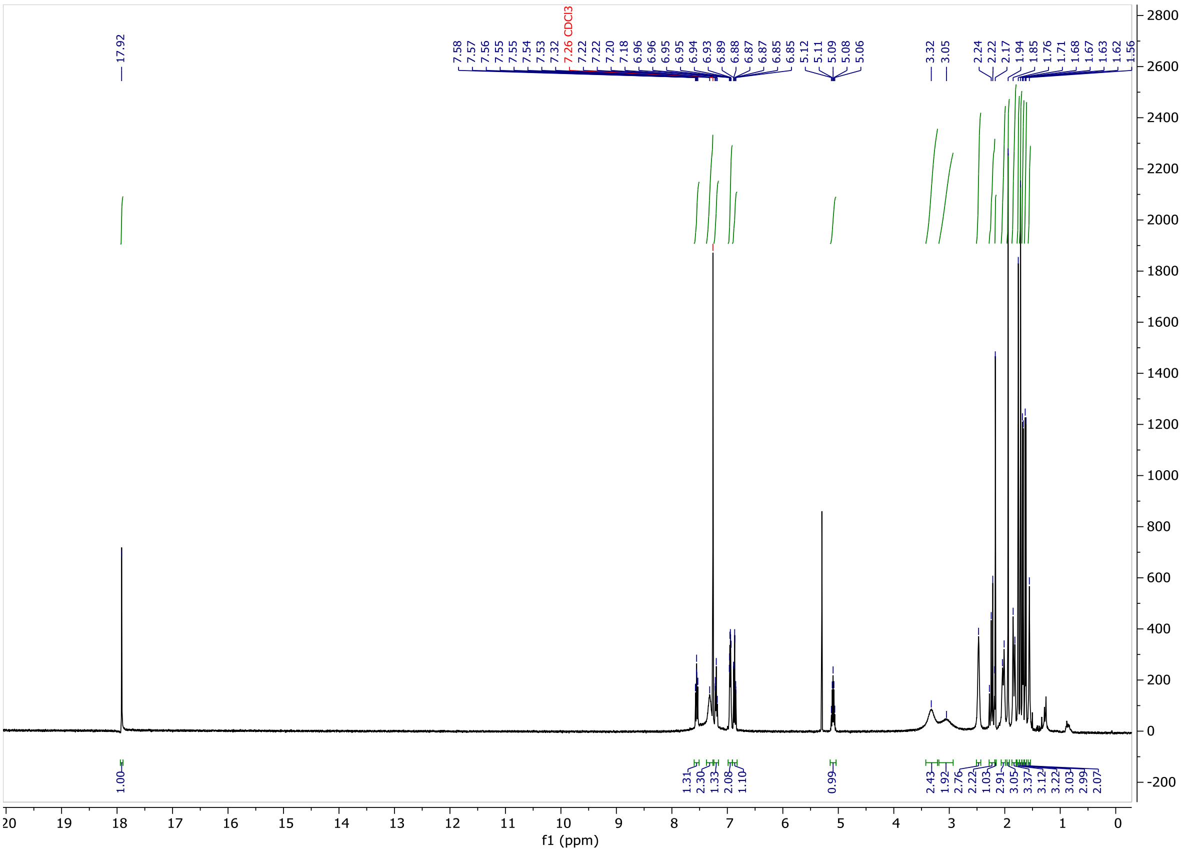
^{1}H NMR (400 MHz, CDCl$_3$) (Ru8a)



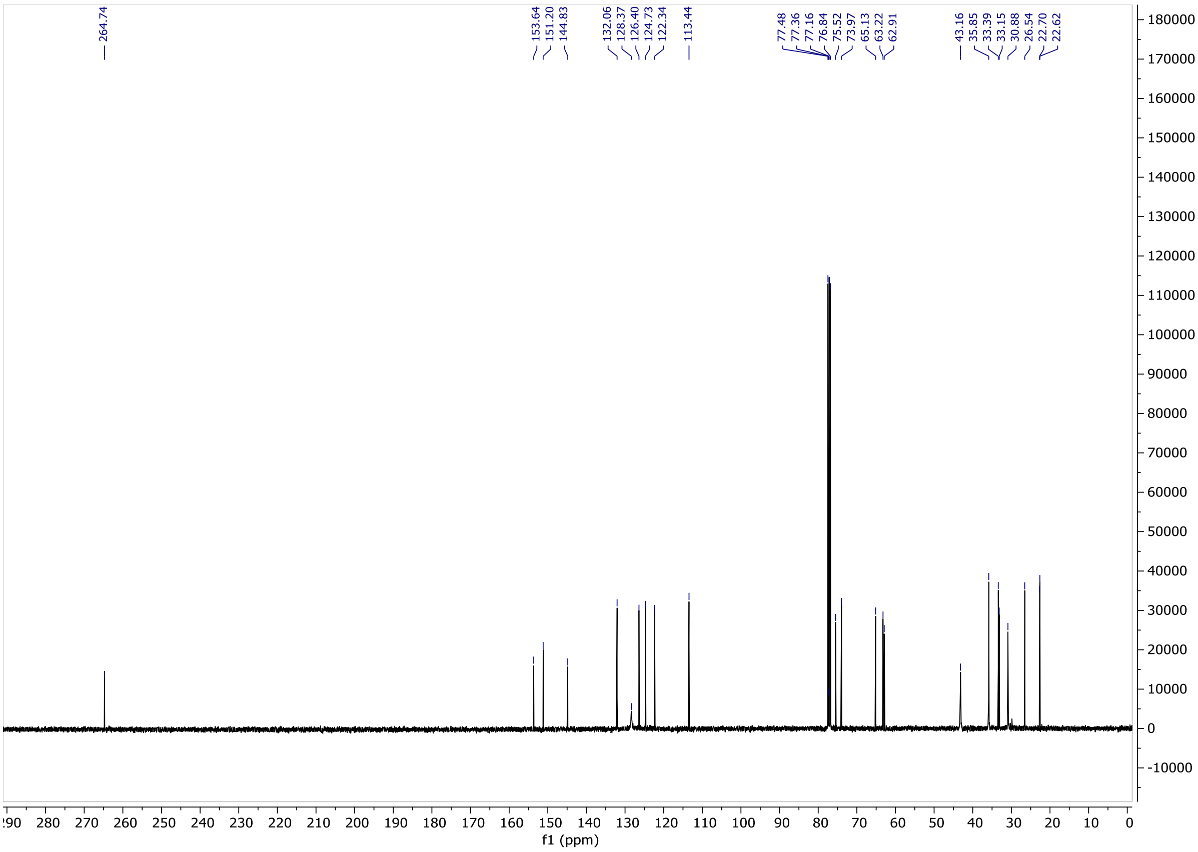
^{13}C NMR (101 MHz, CDCl$_3$) (Ru8a)



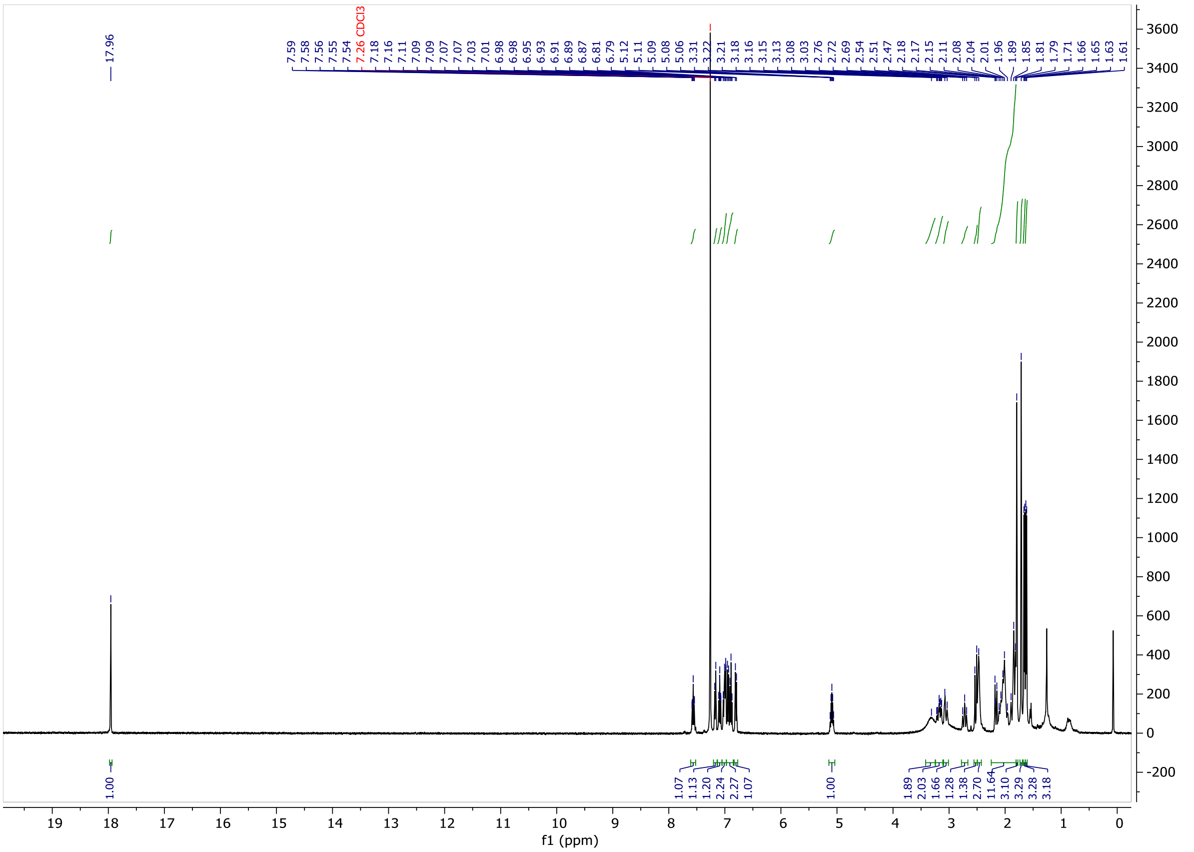
^{1}H NMR (400 MHz, CDCl$_3$) (Ru8b)



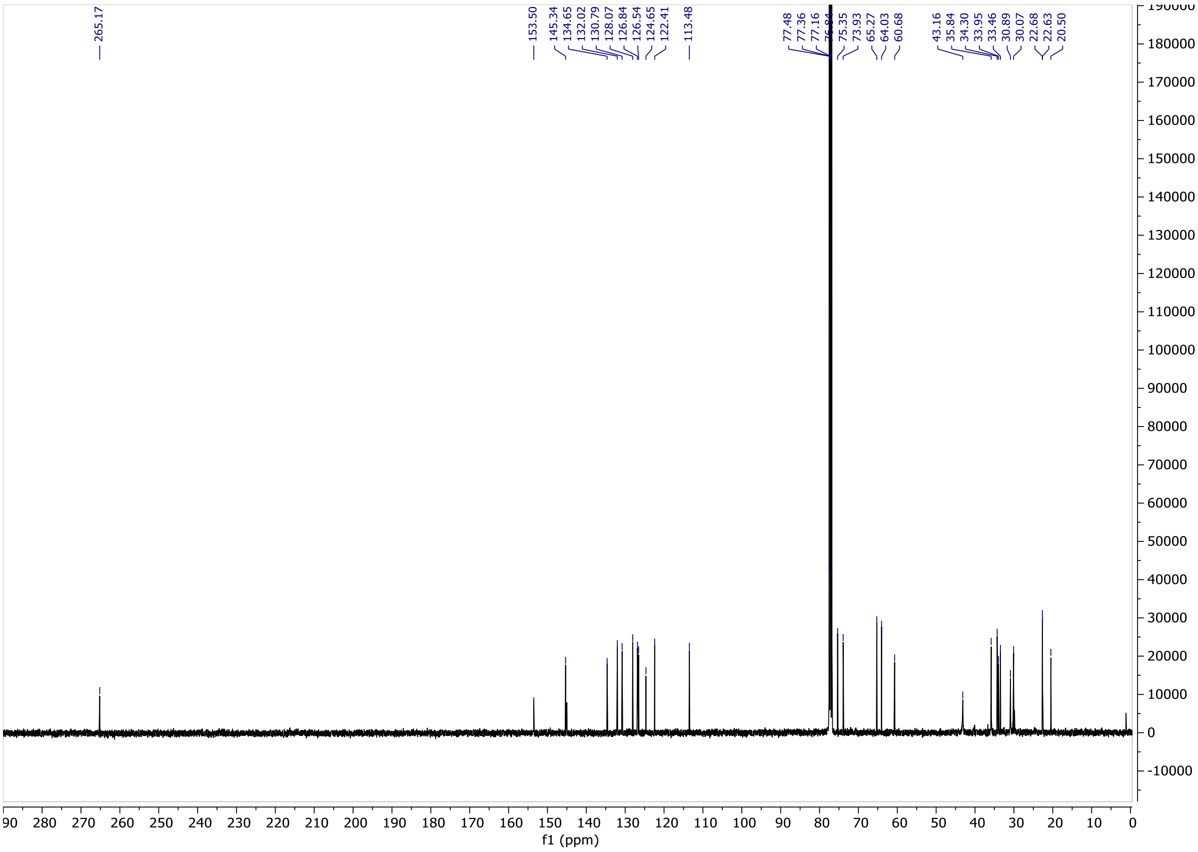
^{13}C NMR (101 MHz, CDCl$_3$) (Ru8b)



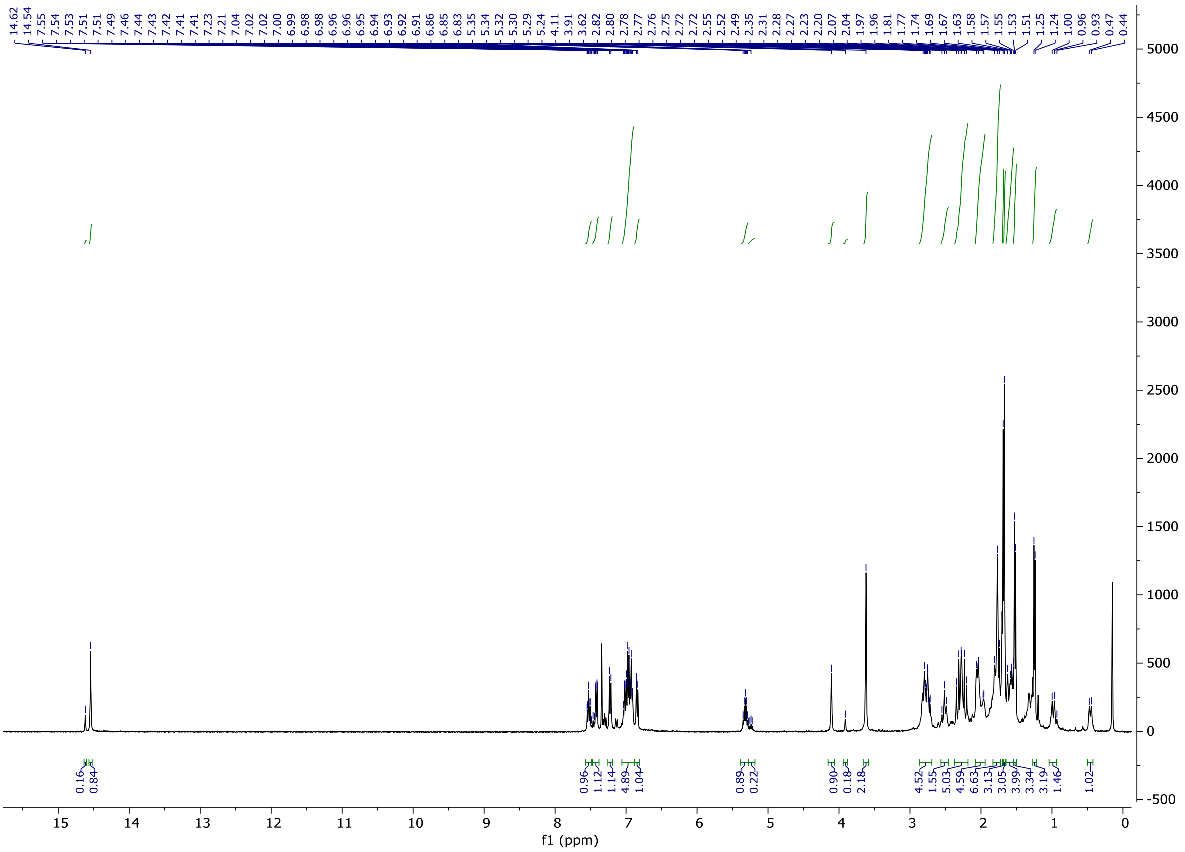
^{1}H NMR (400 MHz, CDCl$_3$) (Ru8c)



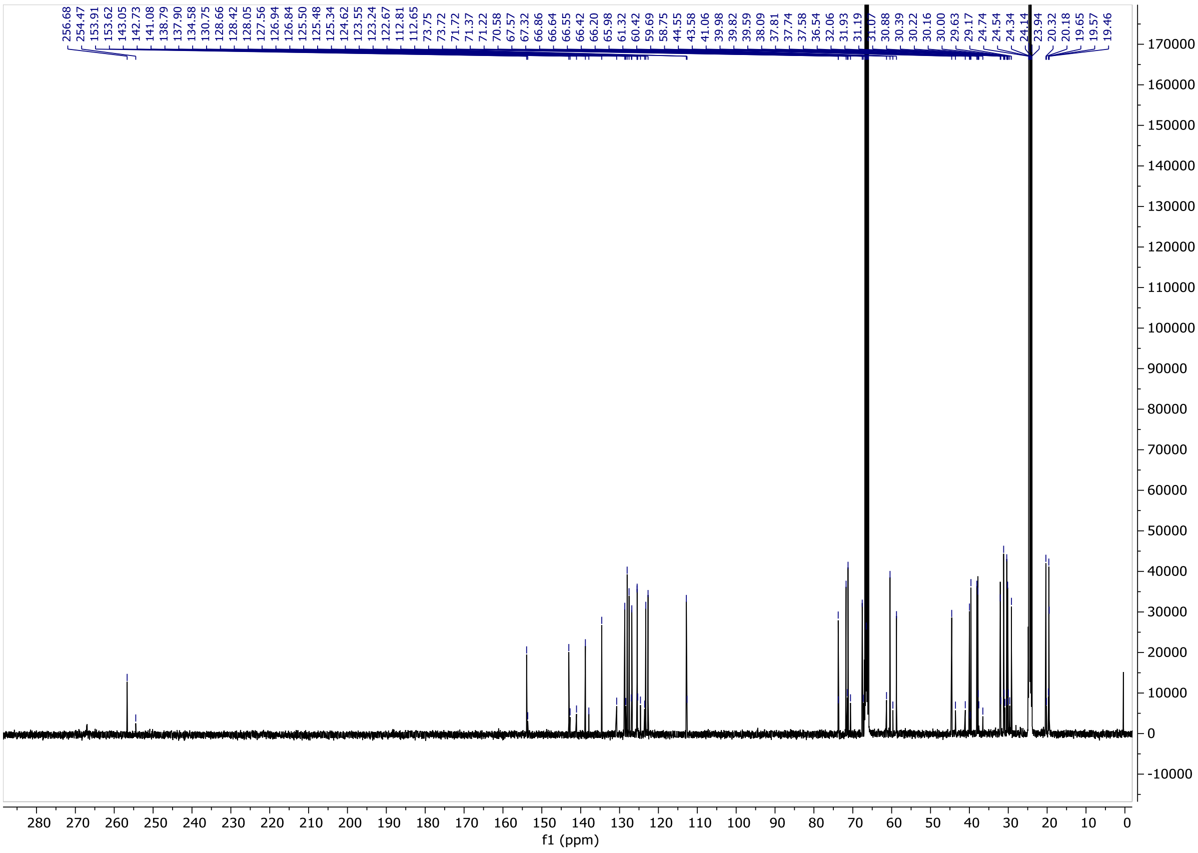
^{13}C NMR (101 MHz, CDCl$_3$) (Ru8c)



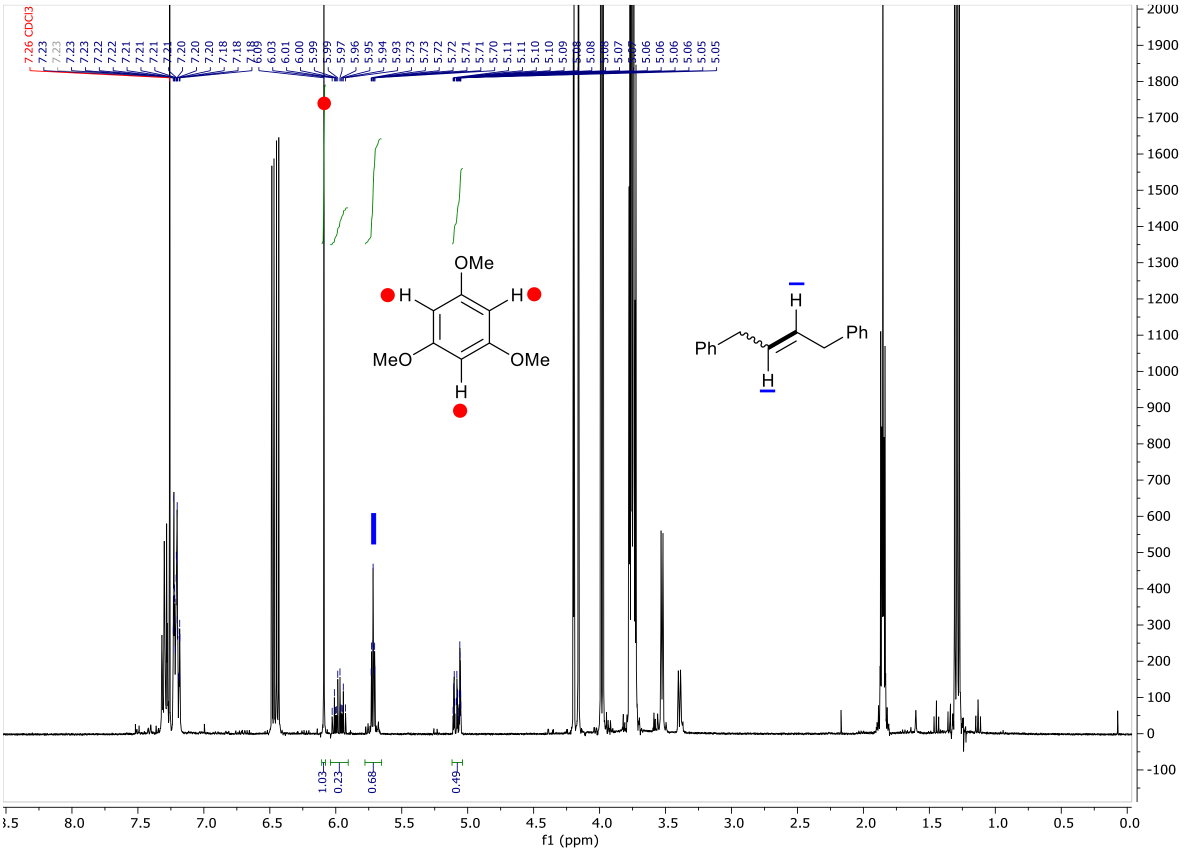
^{1}H NMR (400 MHz, $CDCl_3$) (Ru7)



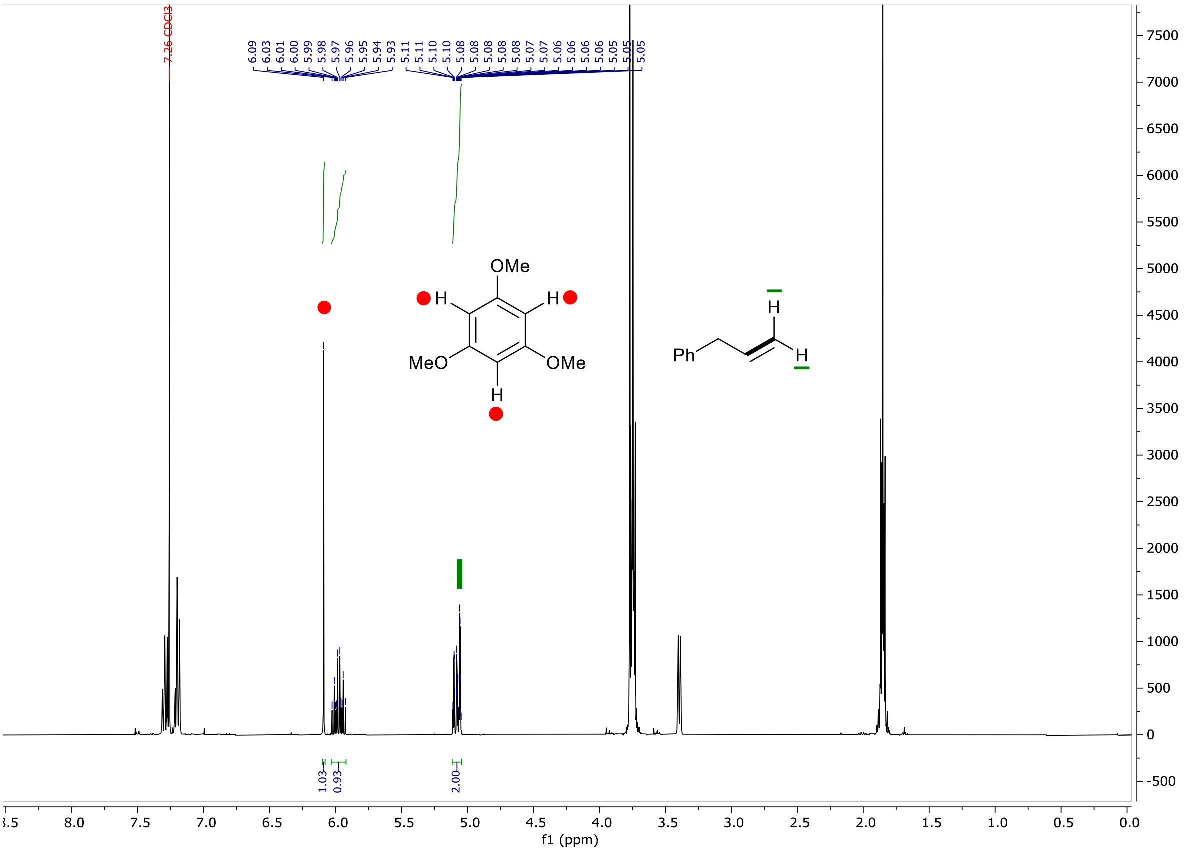
^{13}C NMR (101 MHz, $CDCl_3$) (Ru7)



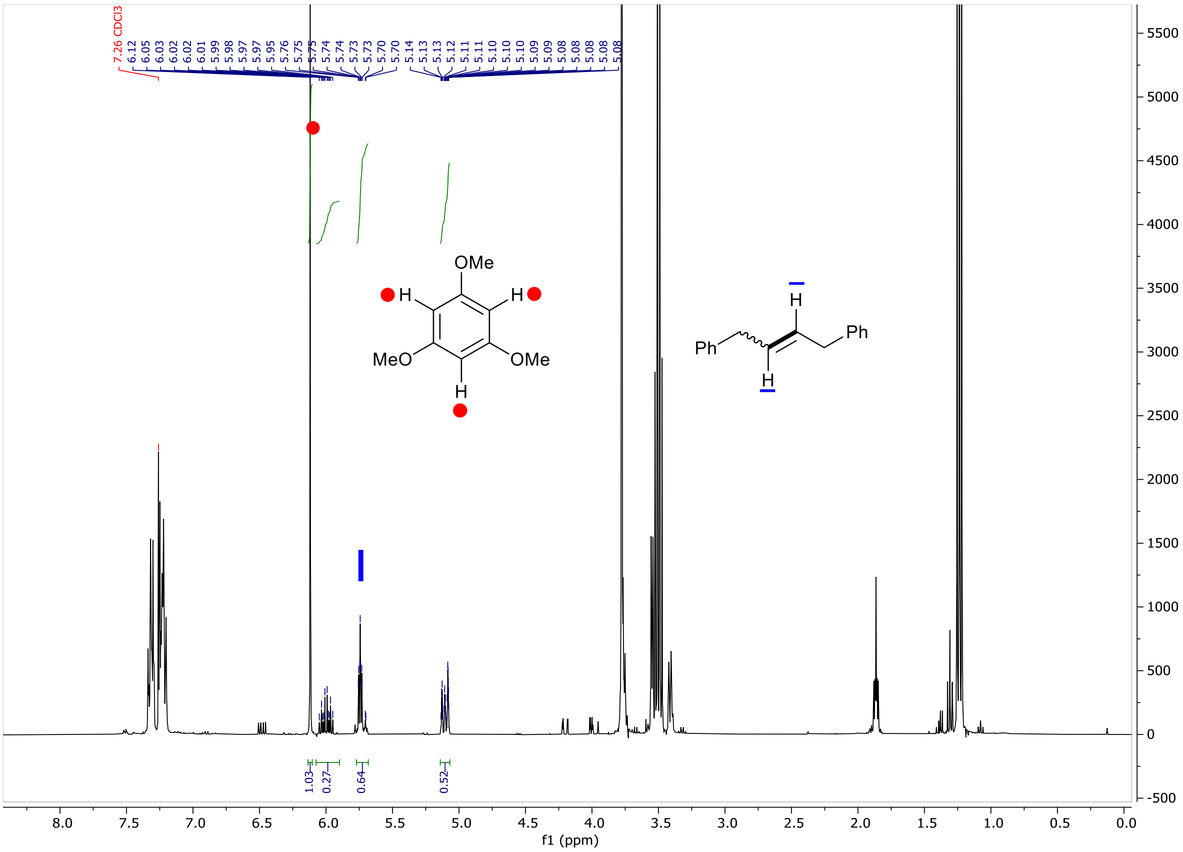
^{1}H NMR (400 MHz, CDCl$_3$) (P1a, 25 °C, 1 mol%, 28 h)



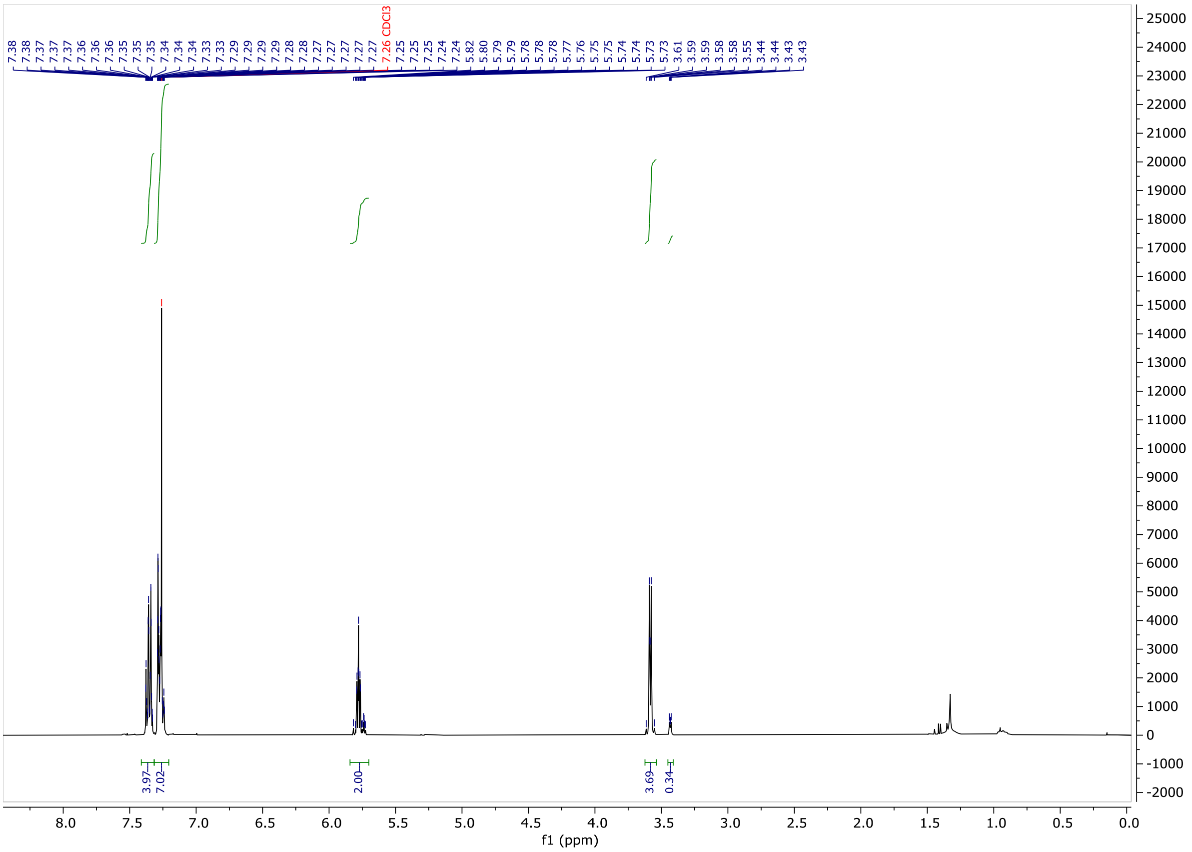
^{1}H NMR (400 MHz, CDCl$_3$) (P1a, 35 °C, 1 mol%, t0)



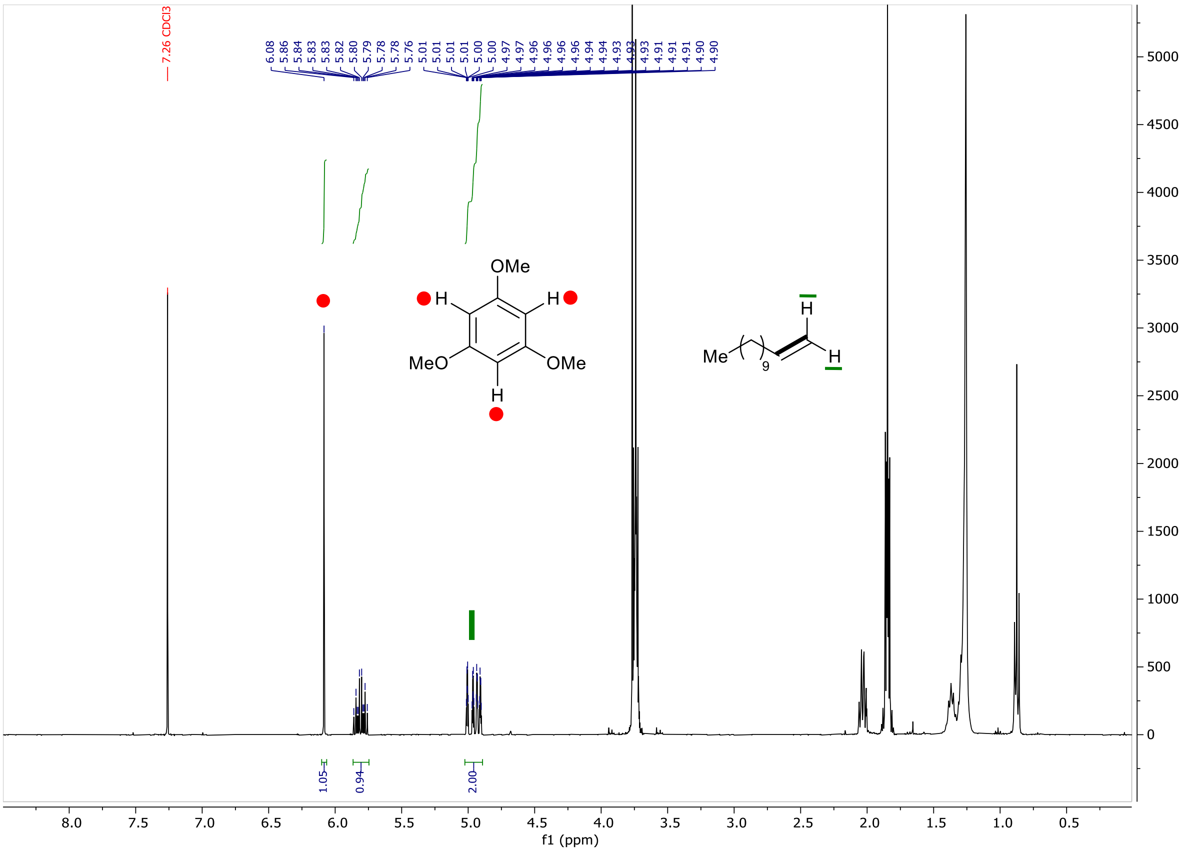
^{1}H NMR (400 MHz, $CDCl_3$) (P1a, 35 °C, 1 mol%, 16 h)



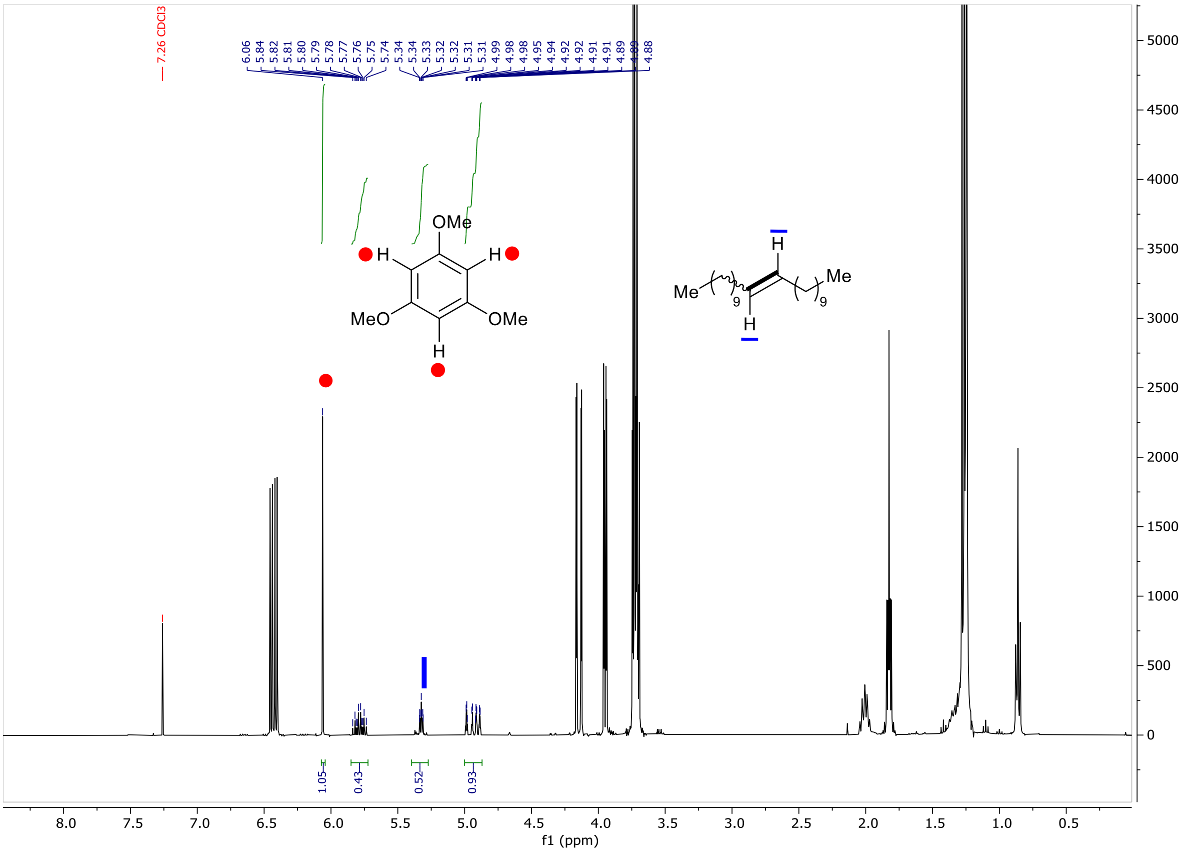
^{1}H NMR (400 MHz, $CDCl_3$) (P2a)



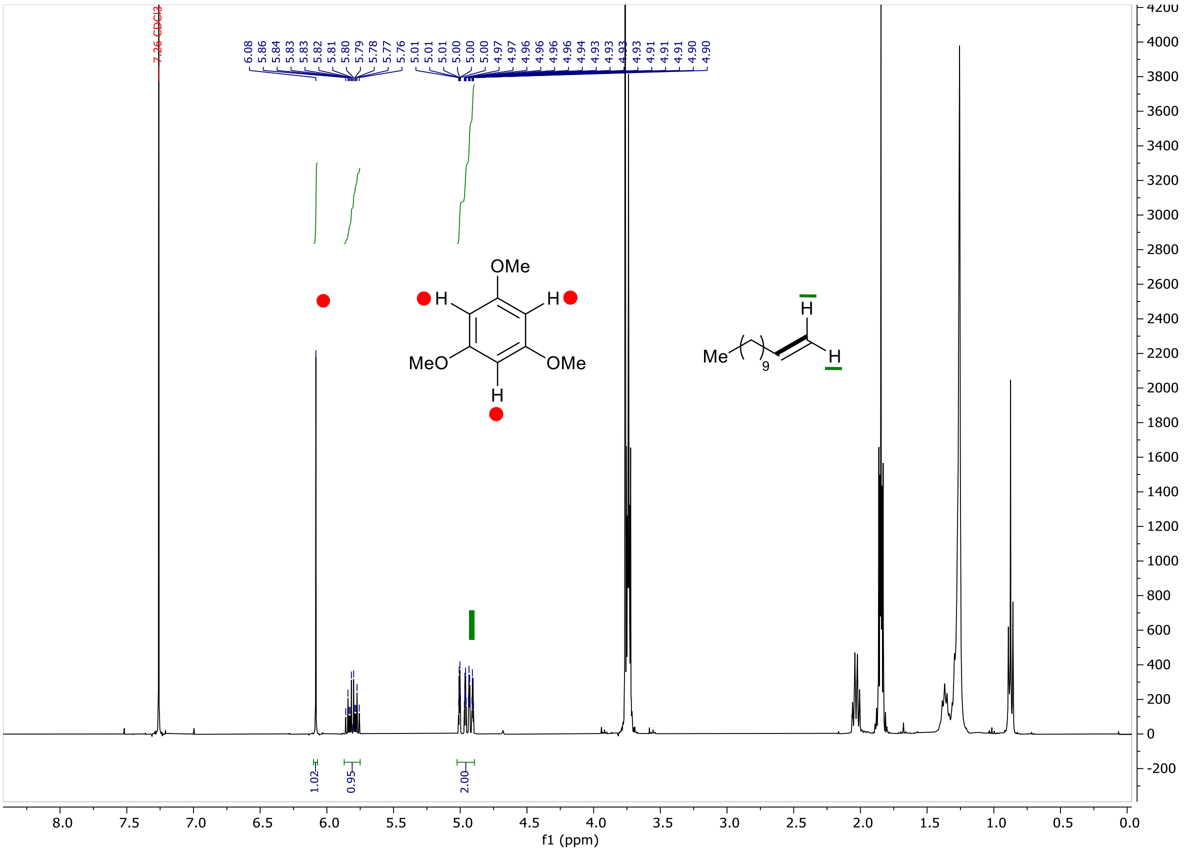
^{1}H NMR (400 MHz, CDCl$_3$) (P1b, 25 °C, 1 mol%, t0)



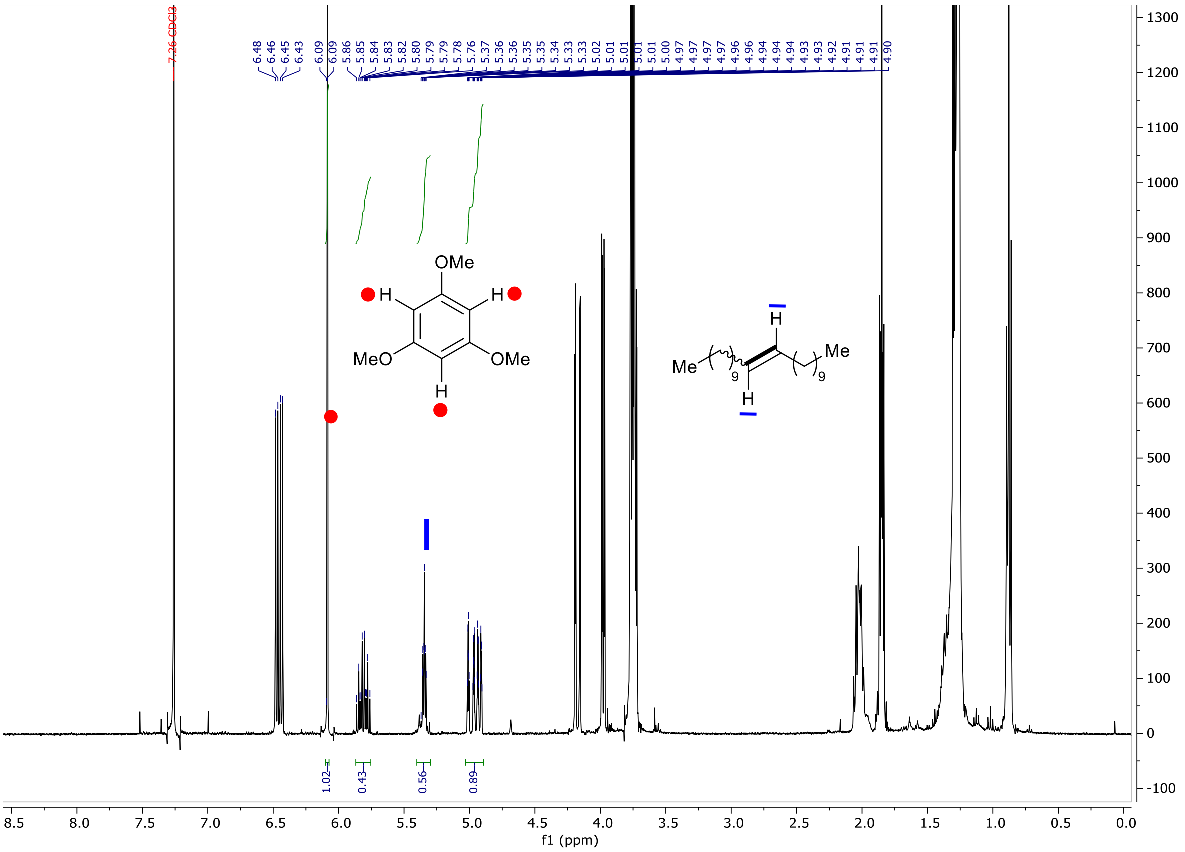
^{1}H NMR (400 MHz, CDCl$_3$) (P1b, 25 °C, 1 mol%, 28 h)



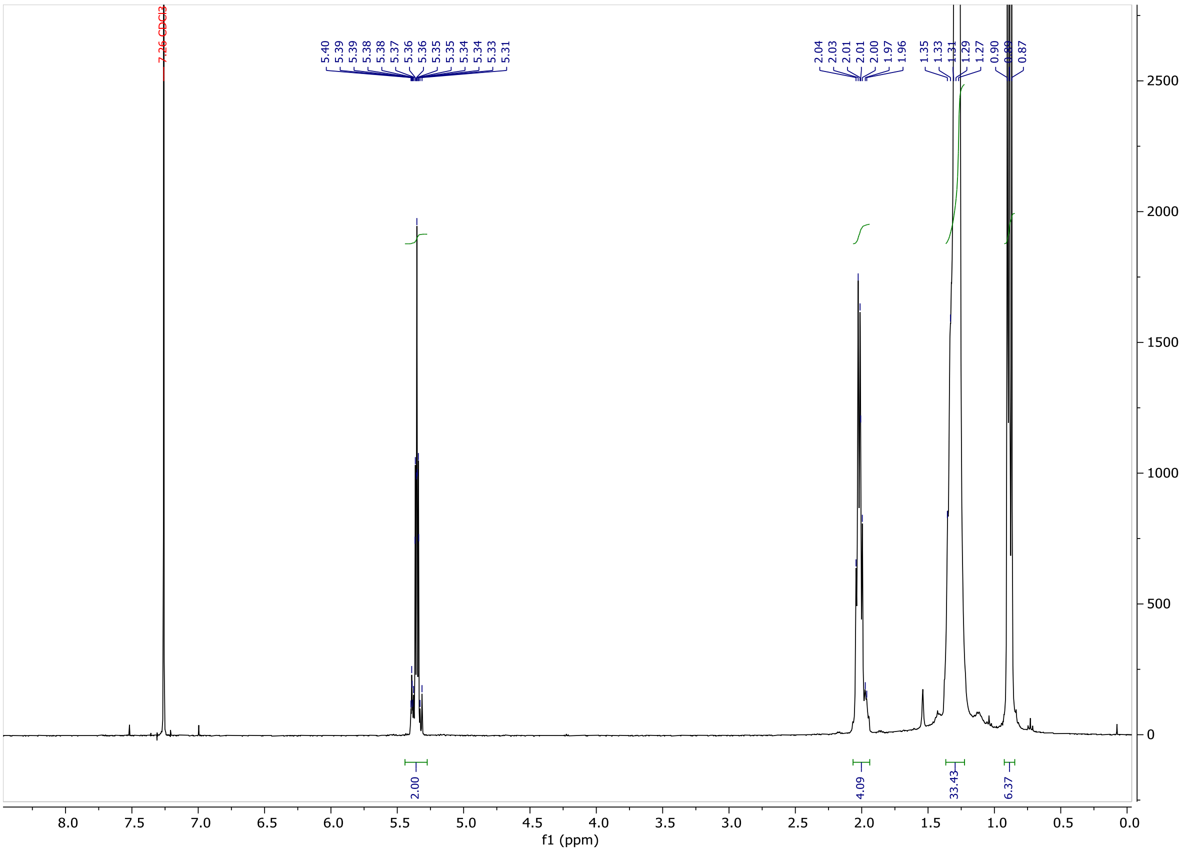
^{1}H NMR (400 MHz, CDCl$_3$) (P1b, 35 °C, 1 mol%, t0)



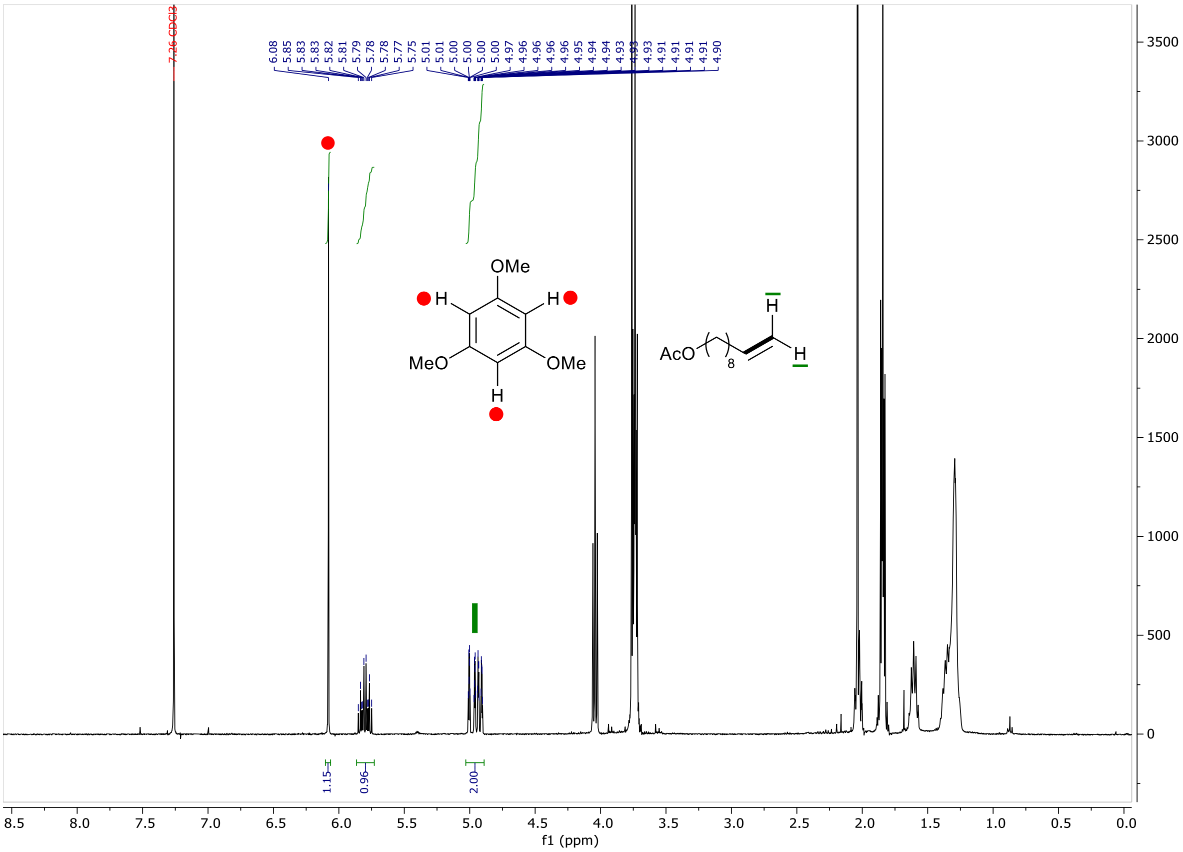
^{1}H NMR (400 MHz, CDCl$_3$) (P1b, 35 °C, 1 mol%, 16 h)



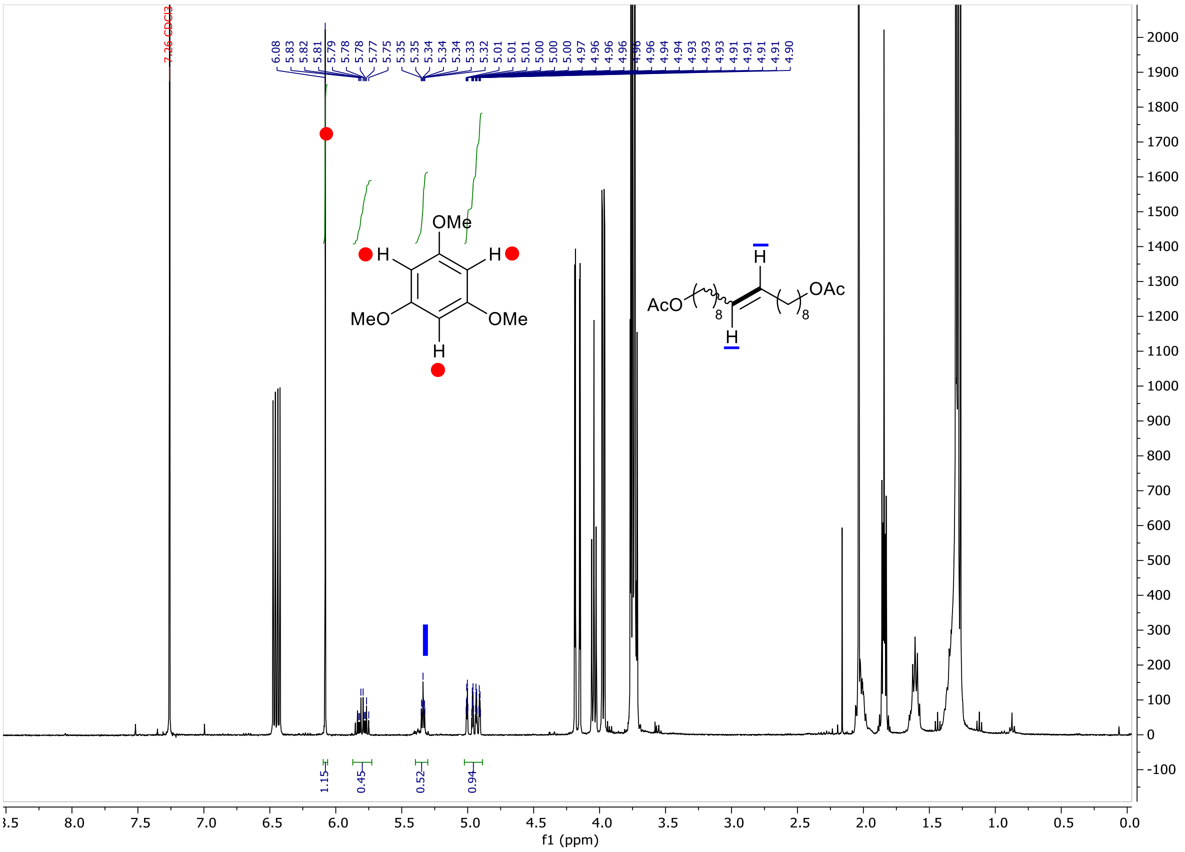
^{1}H NMR (400 MHz, CDCl$_3$) (P1b)



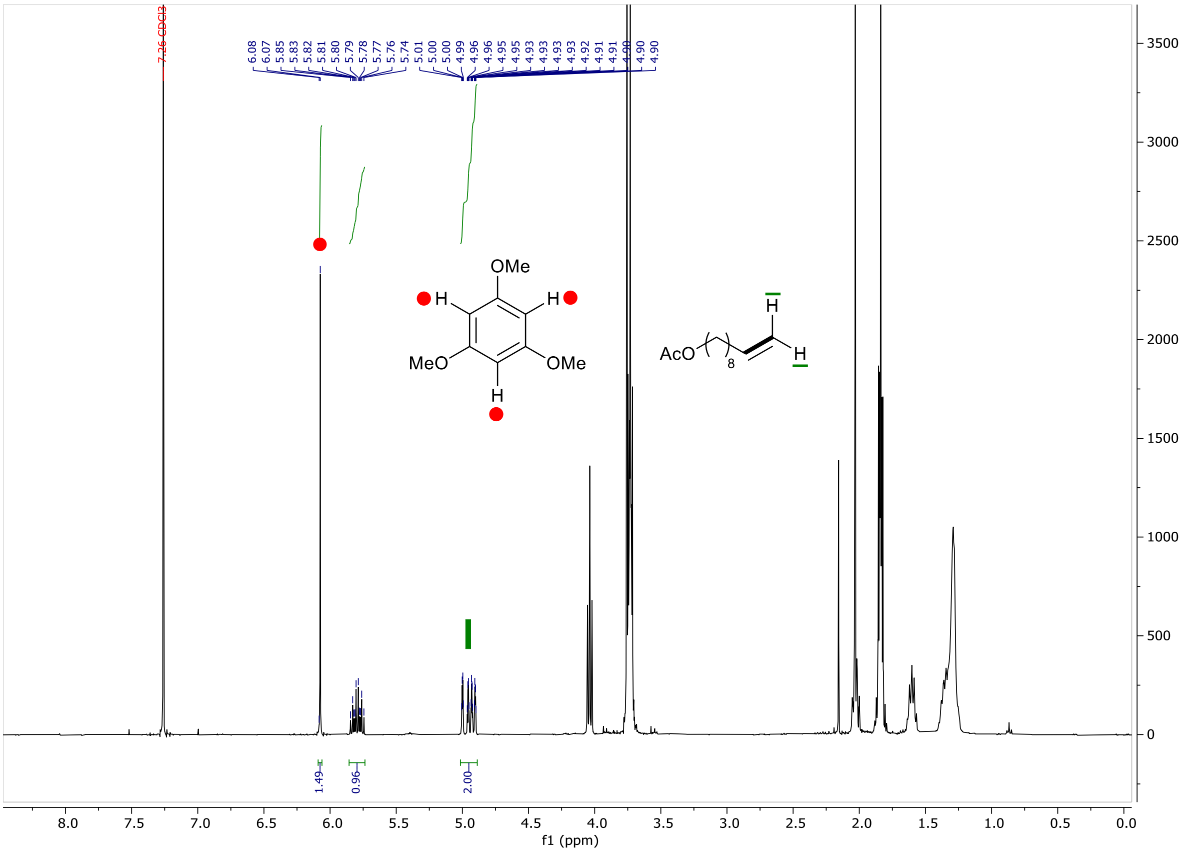
^{1}H NMR (400 MHz, CDCl$_3$) (P1c, 25 °C, 1 mol%, t0)



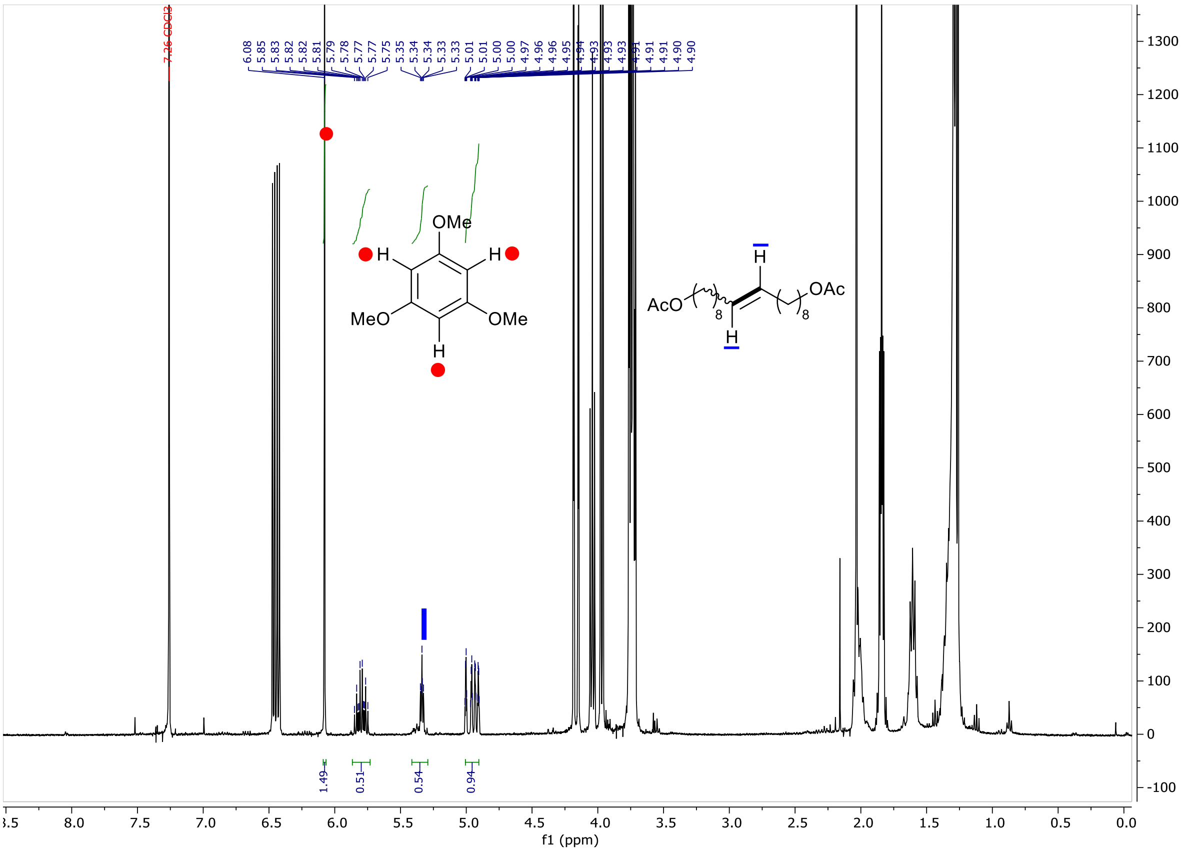
^{1}H NMR (400 MHz, CDCl$_3$) (P1c, 25 °C, 1 mol%, 32 h)



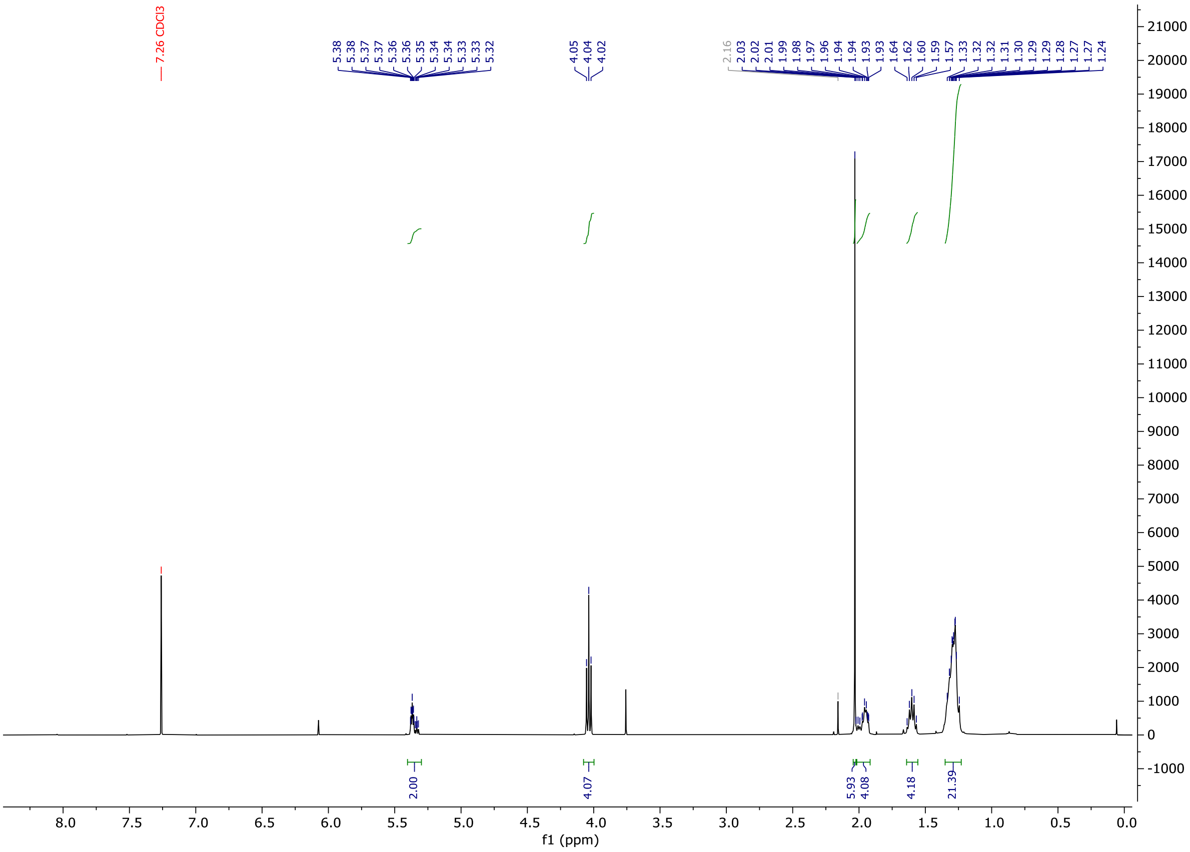
^{1}H NMR (400 MHz, CDCl$_3$) (P1c, 35 °C, 1 mol%, t0)



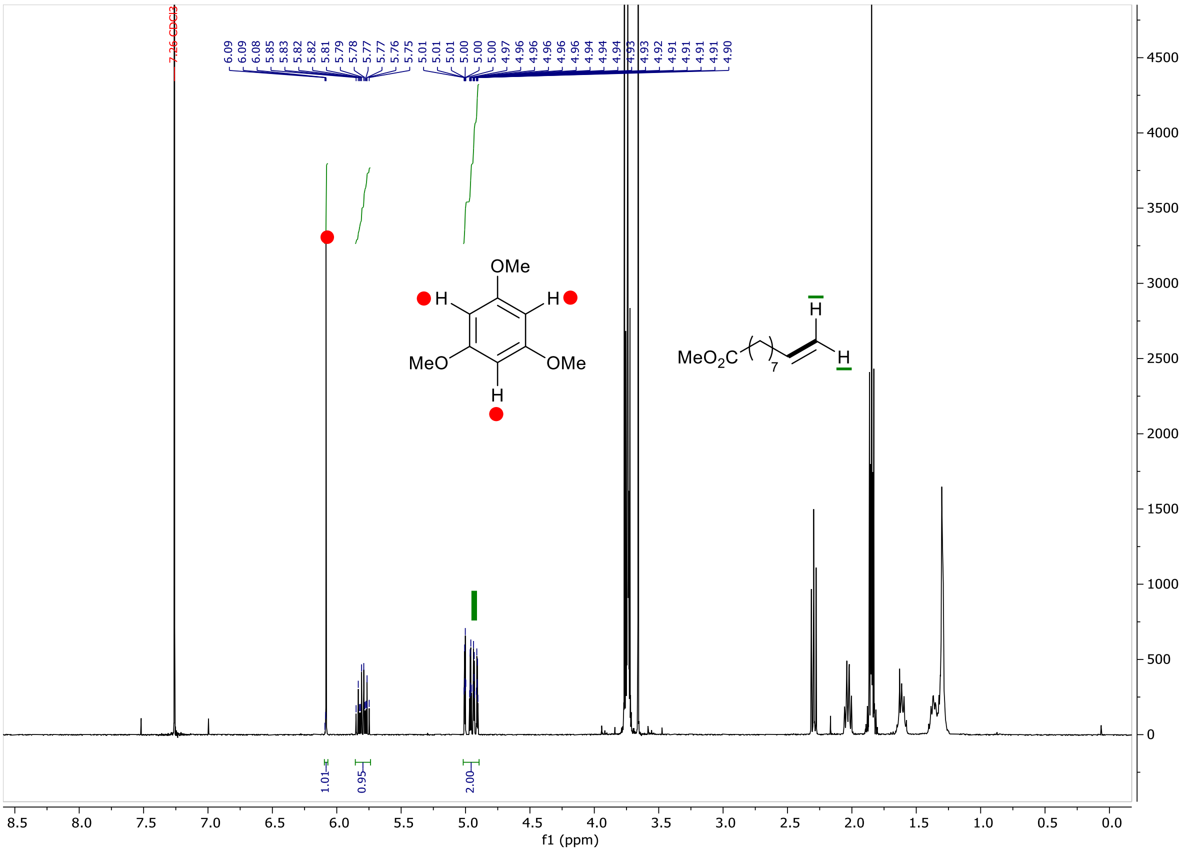
^{1}H NMR (400 MHz, CDCl$_3$) (P1c, 35 °C, 1 mol%, 16 h)



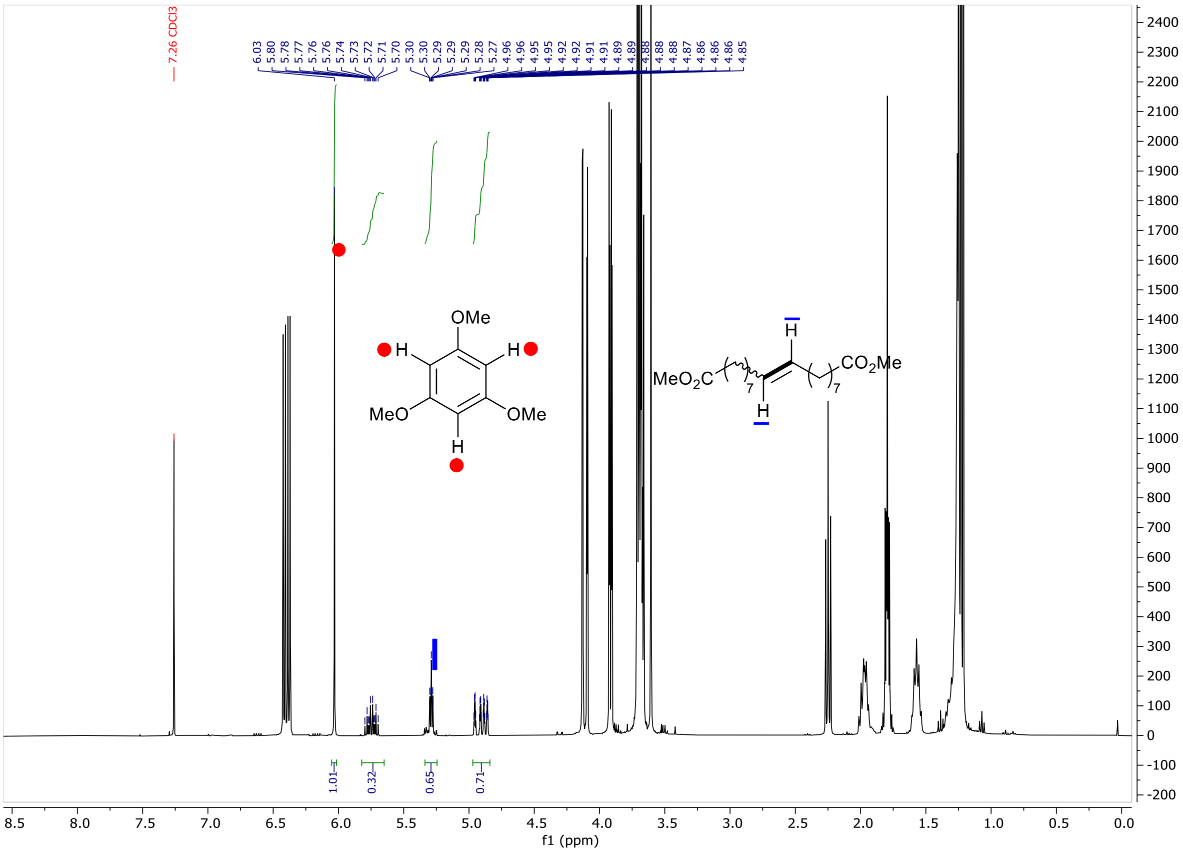
^{1}H NMR (400 MHz, CDCl$_3$) (P1c)



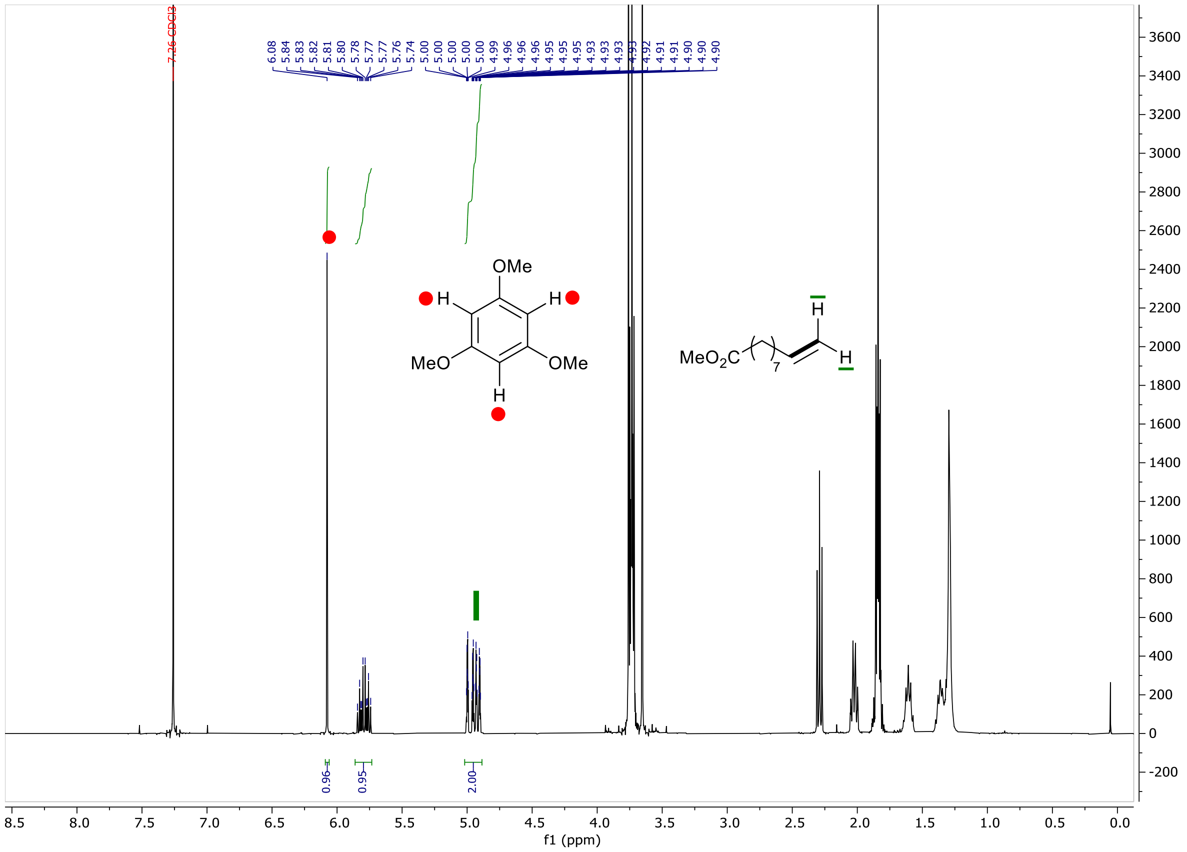
^{1}H NMR (400 MHz, CDCl$_3$) (P1d, 25 °C, 1 mol%, t0)



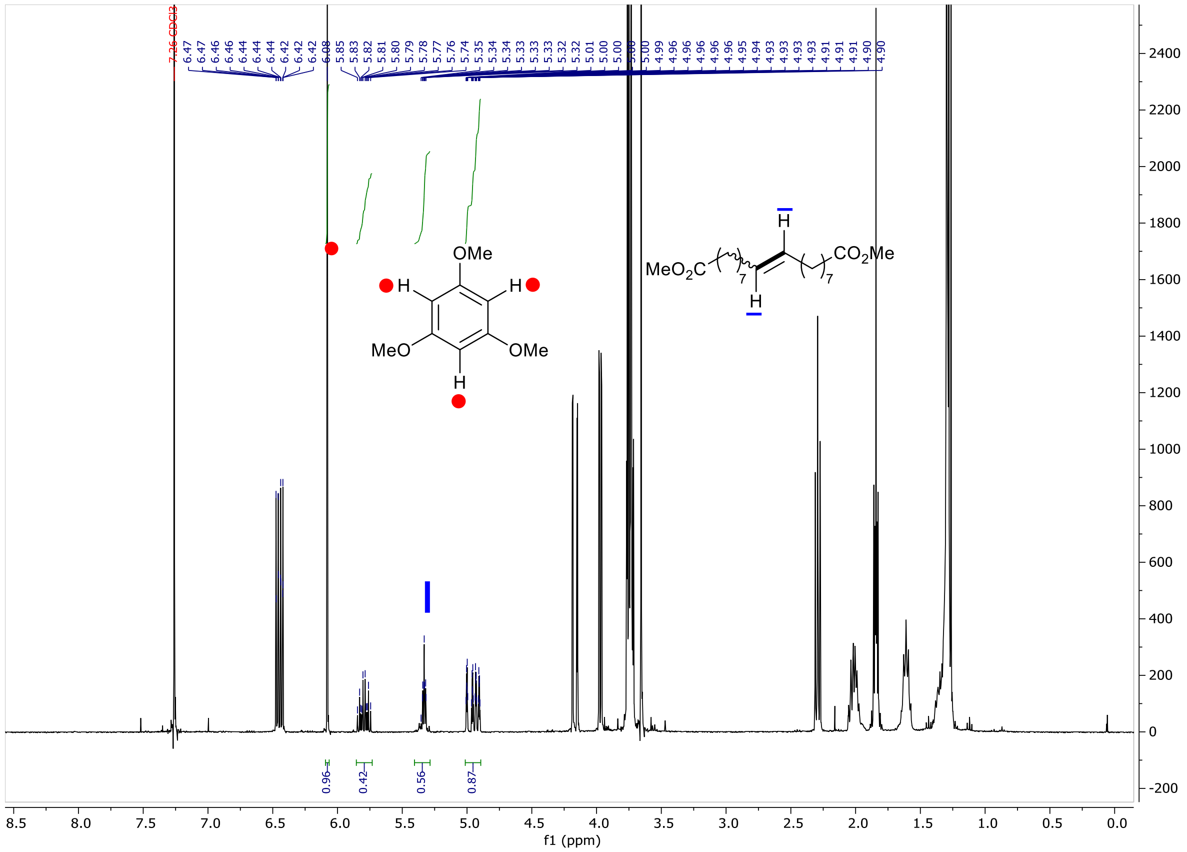
^{1}H NMR (400 MHz, CDCl$_3$) (P1d, 25 °C, 1 mol%, 32 h)



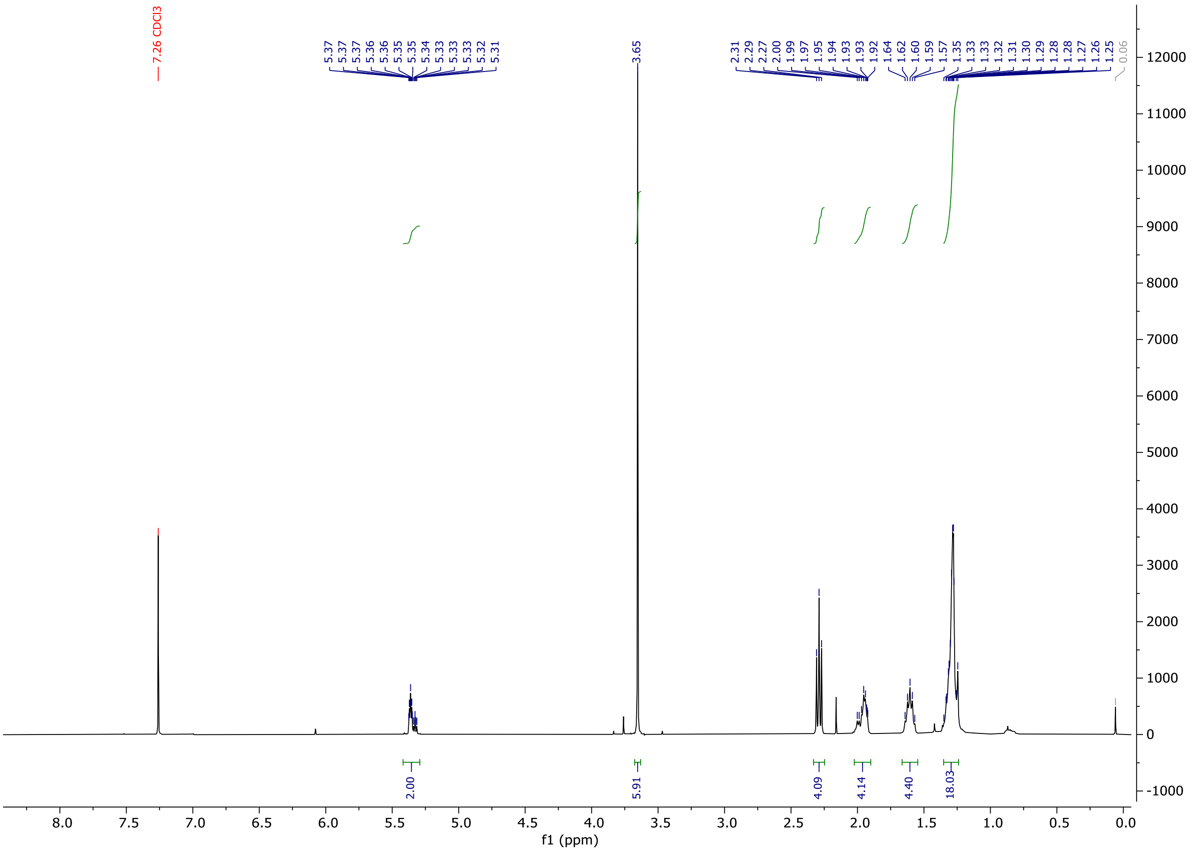
^{1}H NMR (400 MHz, CDCl$_3$) (P1d, 35 °C, 1 mol%, t0)



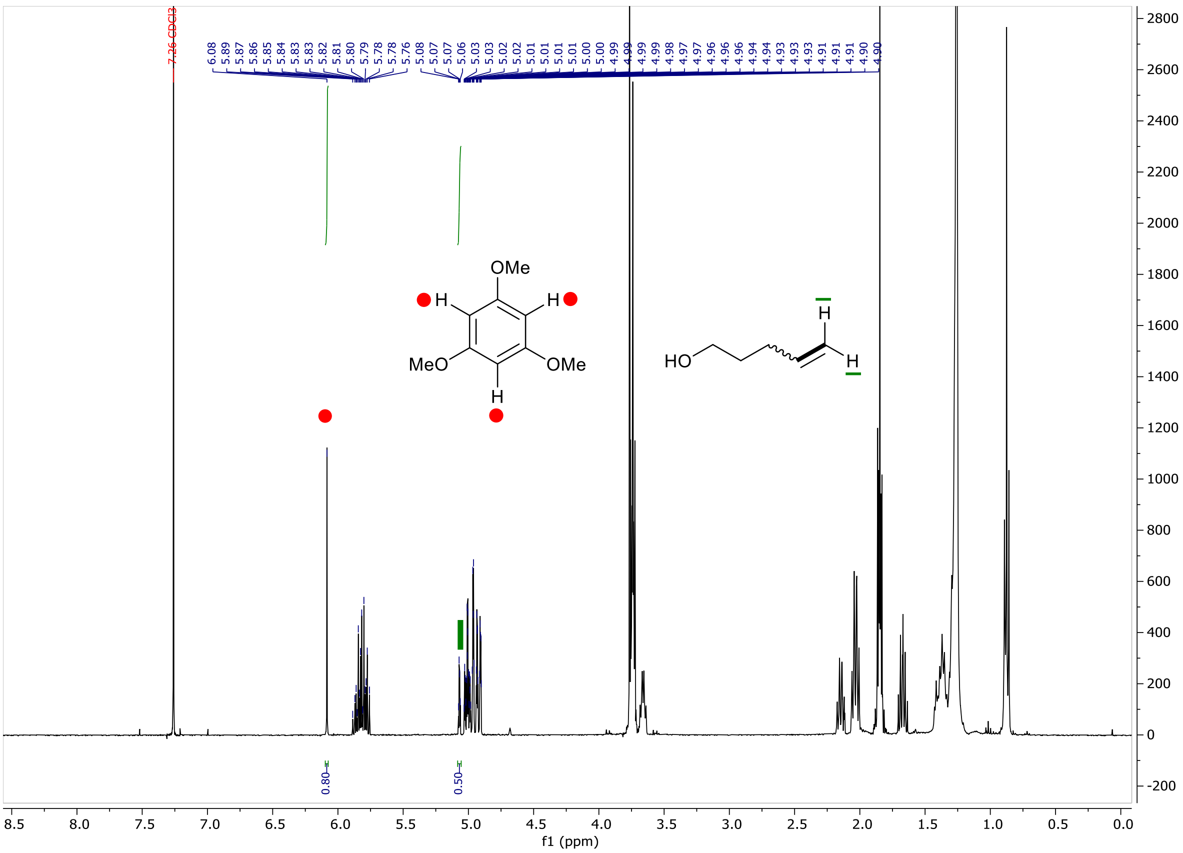
^{1}H NMR (400 MHz, CDCl$_3$) (P1d, 35 °C, 1 mol%, 16 h)



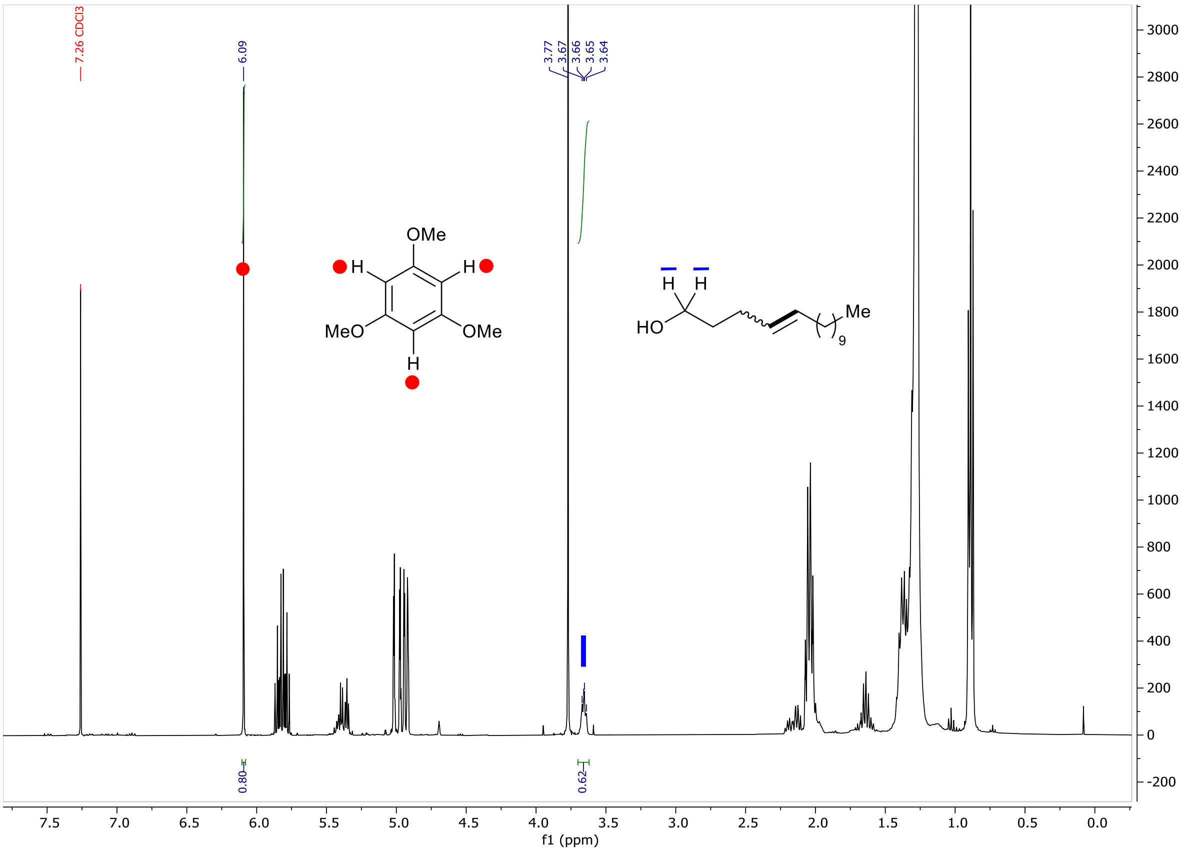
^{1}H NMR (400 MHz, CDCl$_3$) (P1d)



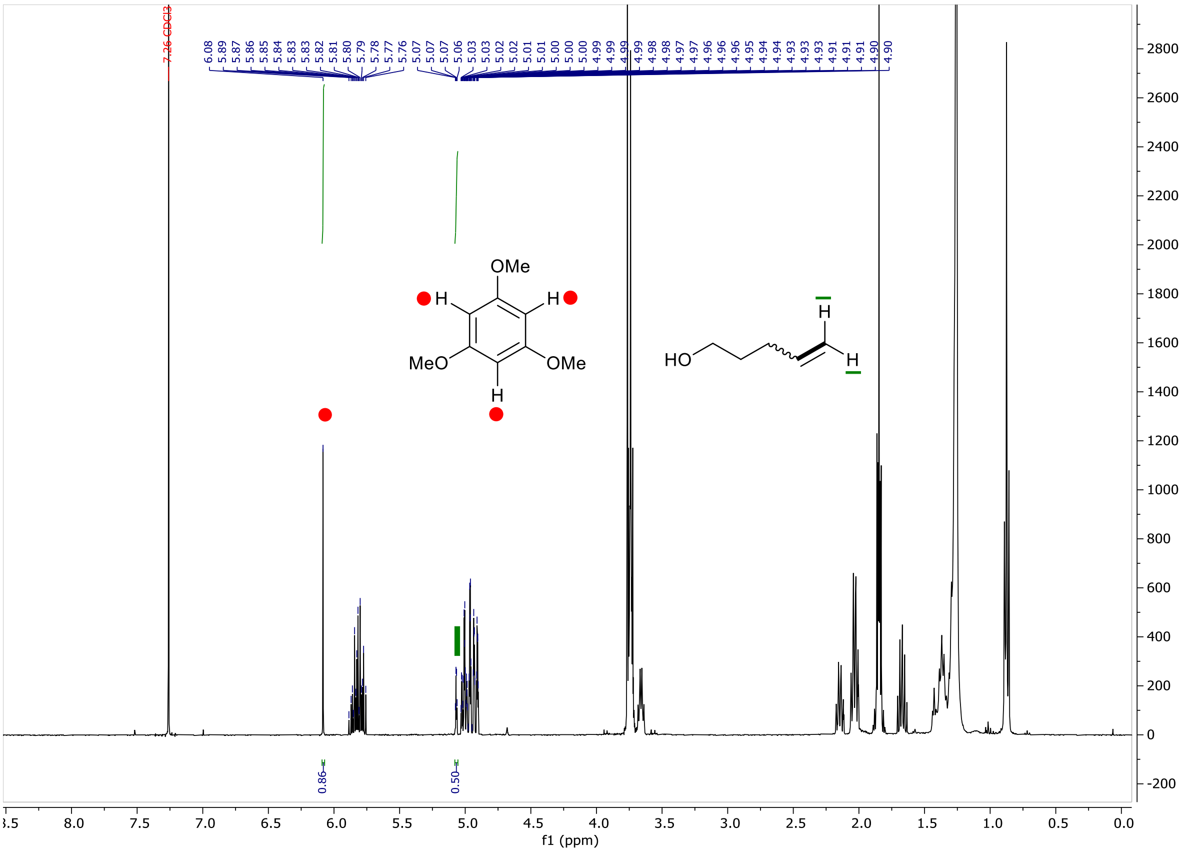
^{1}H NMR (400 MHz, CDCl$_3$) (P2a, 2 mol%, t0)



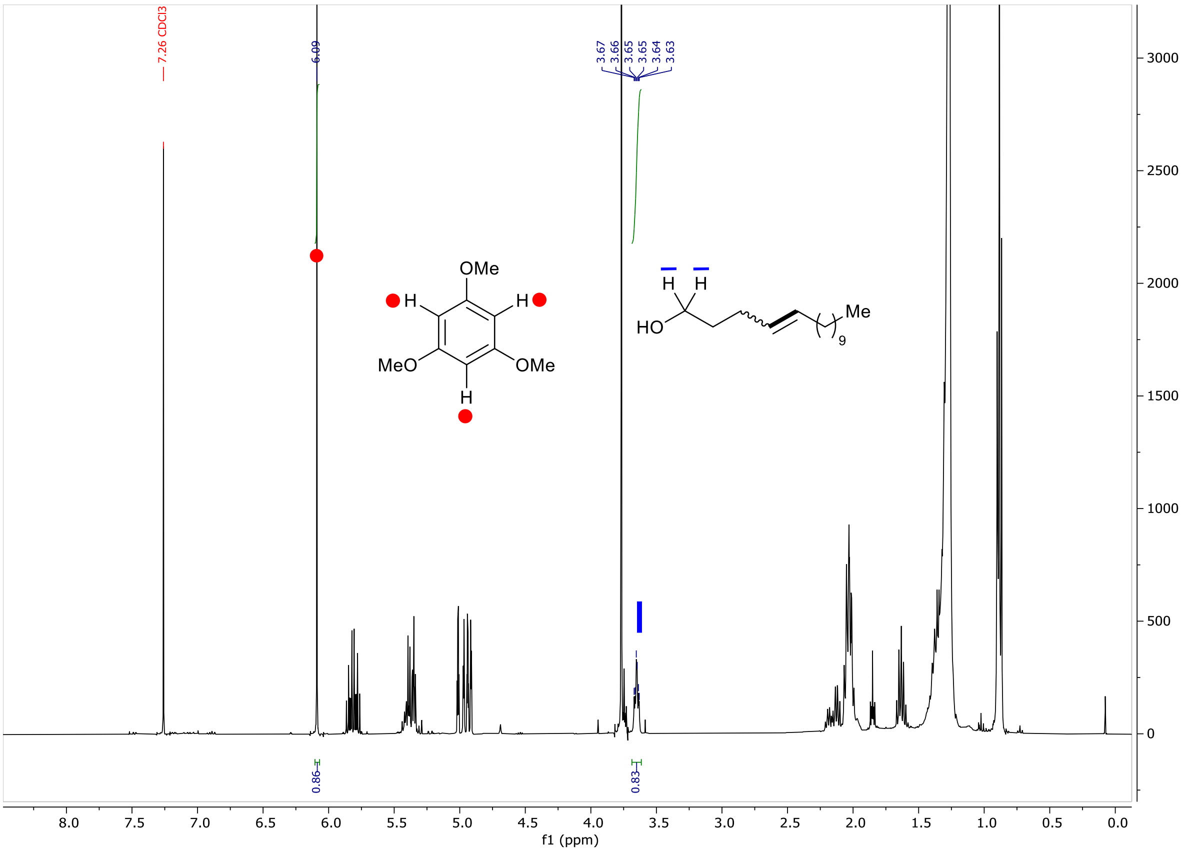
^{1}H NMR (400 MHz, $CDCl_3$) (P2a, 2 mol%, 28 h)



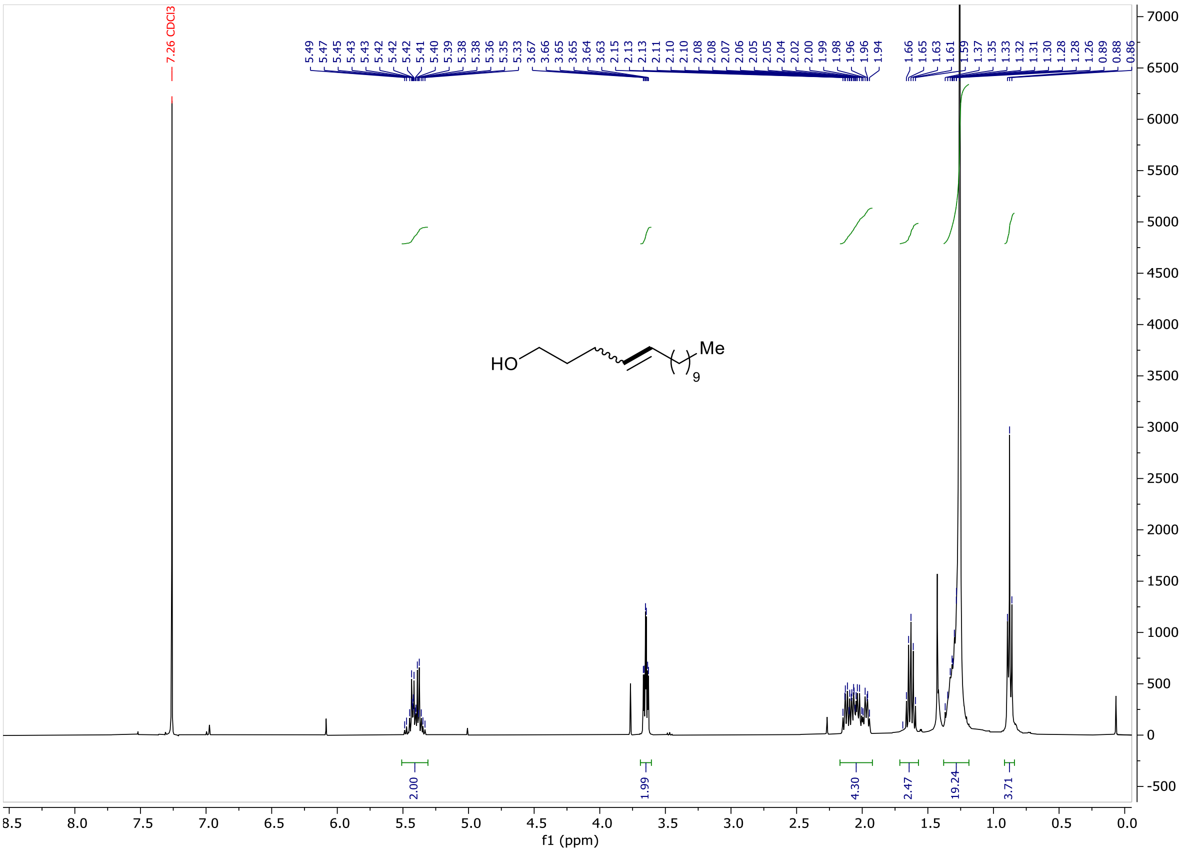
^{1}H NMR (400 MHz, $CDCl_3$) (P2a, 3 mol%, t0)



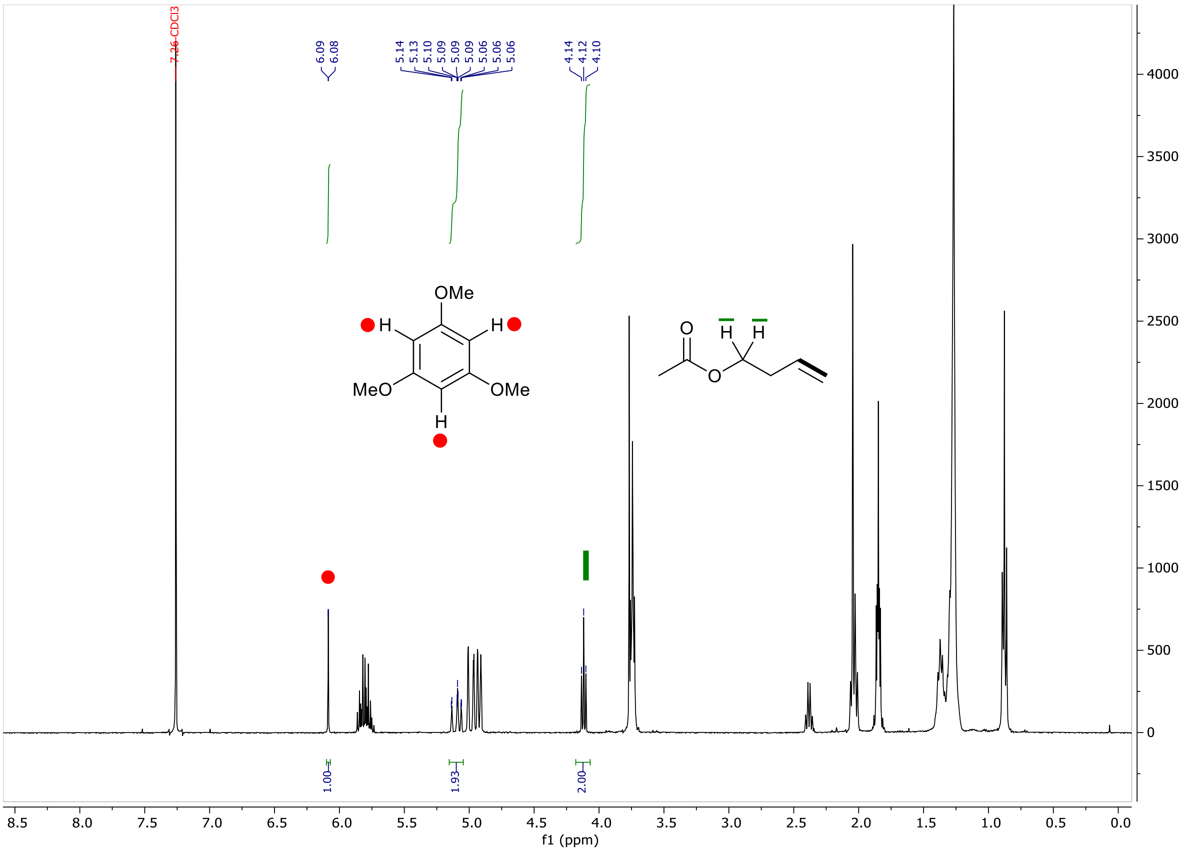
^{1}H NMR (400 MHz, CDCl$_3$) (P2a, 3 mol%, 28 h)



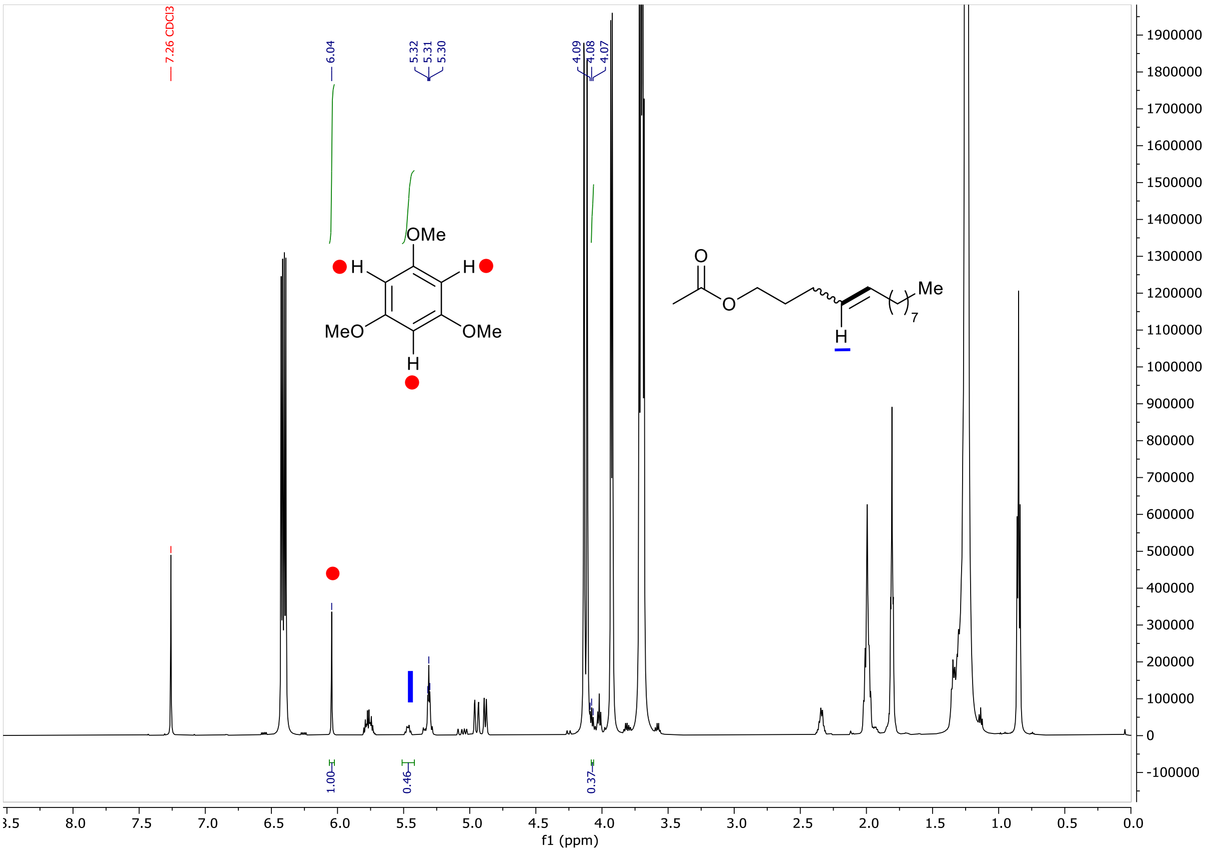
^{1}H NMR (400 MHz, CDCl$_3$) (P2a)



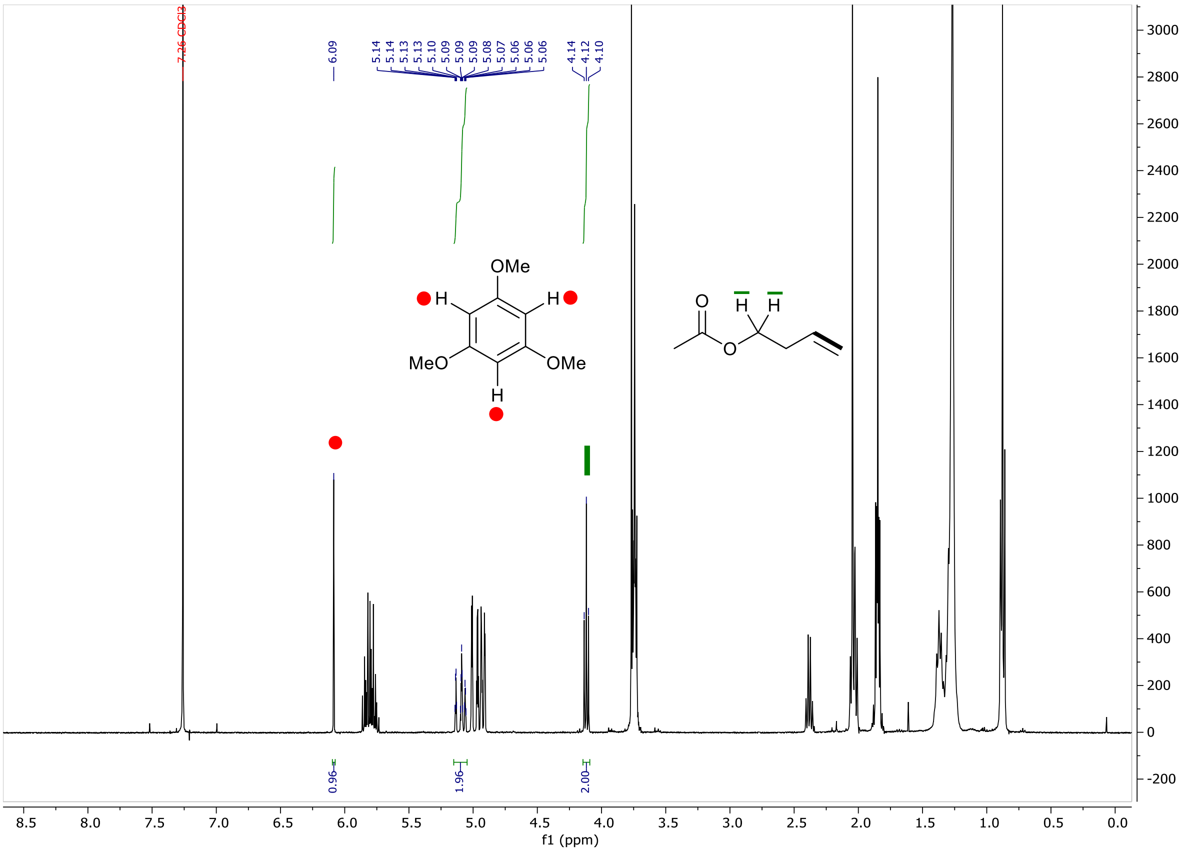
^{1}H NMR (400 MHz, CDCl$_3$) (P2b, 2 mol%, t0)



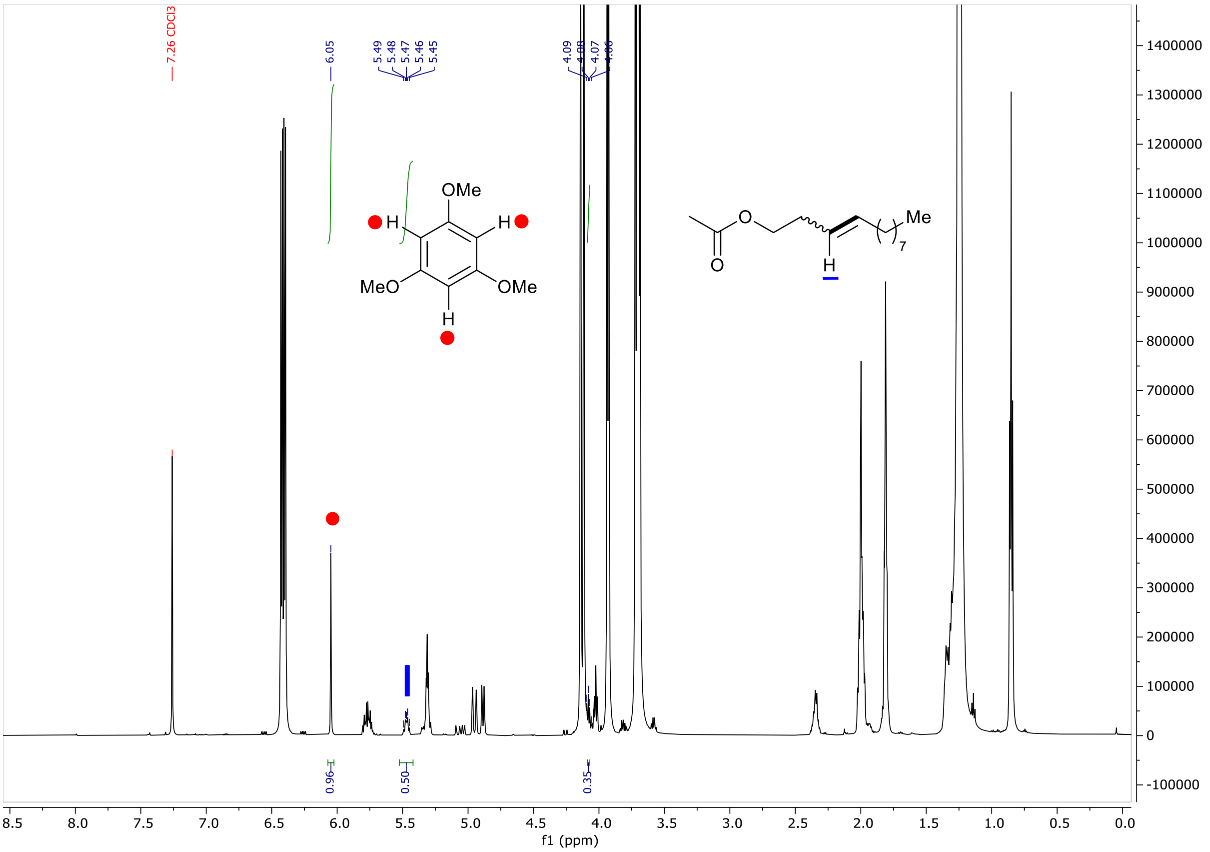
^{1}H NMR (400 MHz, CDCl$_3$) (P2b, 2 mol%, 48 h)



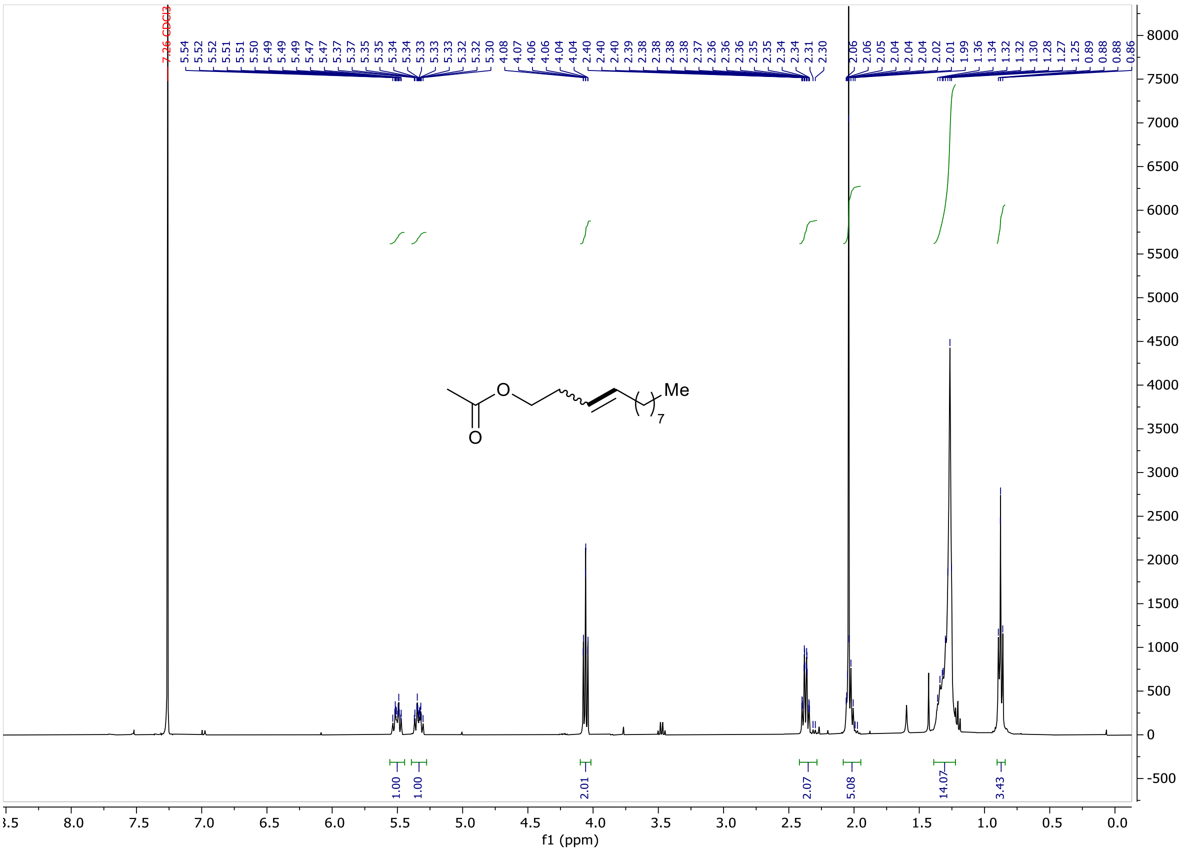
^{1}H NMR (400 MHz, $CDCl_3$) (P2b, 3 mol%, t0)



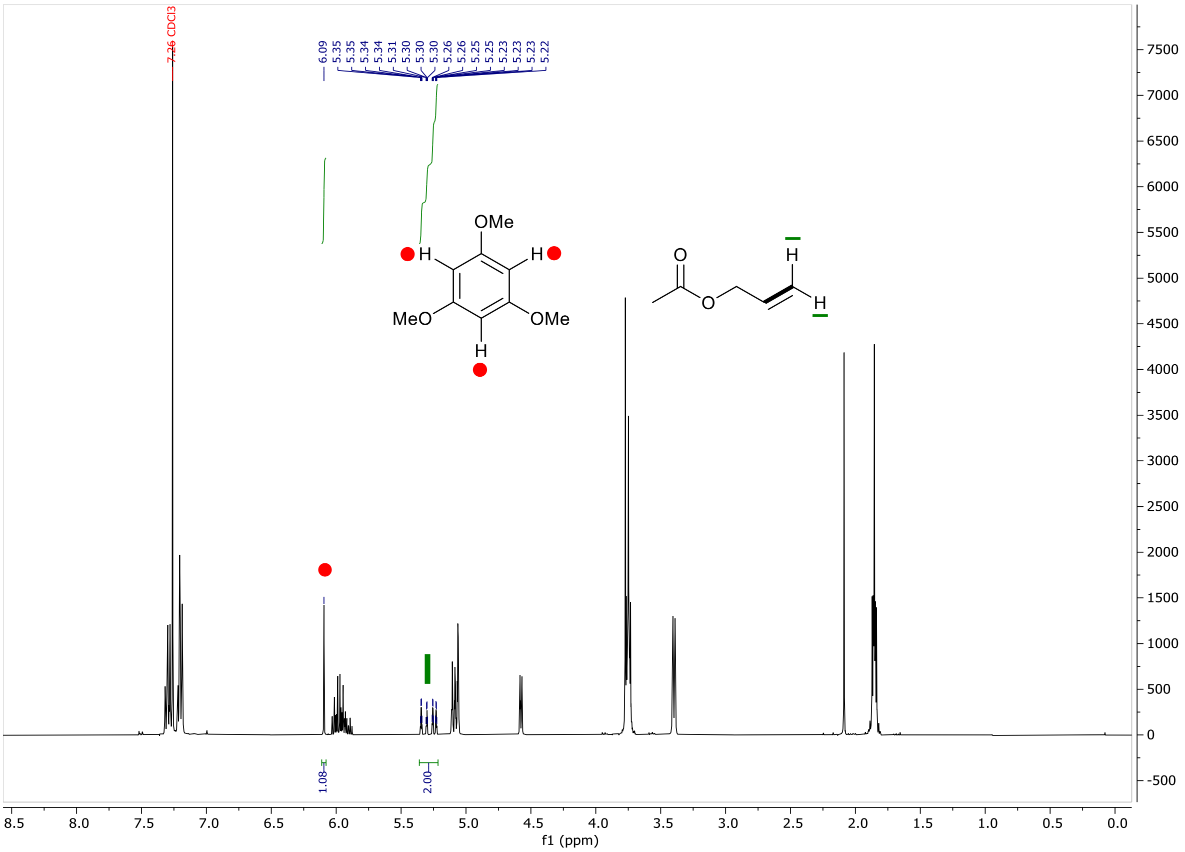
^{1}H NMR (400 MHz, $CDCl_3$) (P2b, 3 mol%, 48 h)



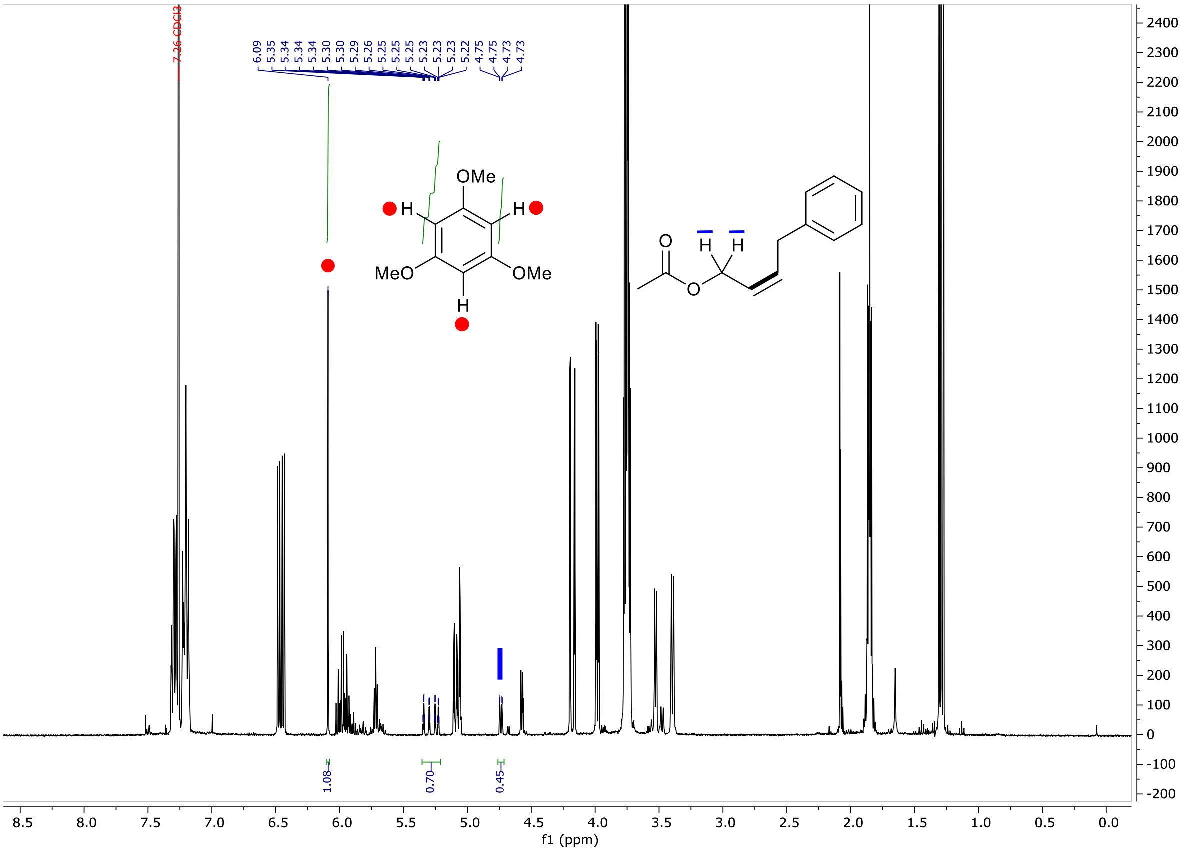
^{1}H NMR (400 MHz, $CDCl_3$) (P2b)



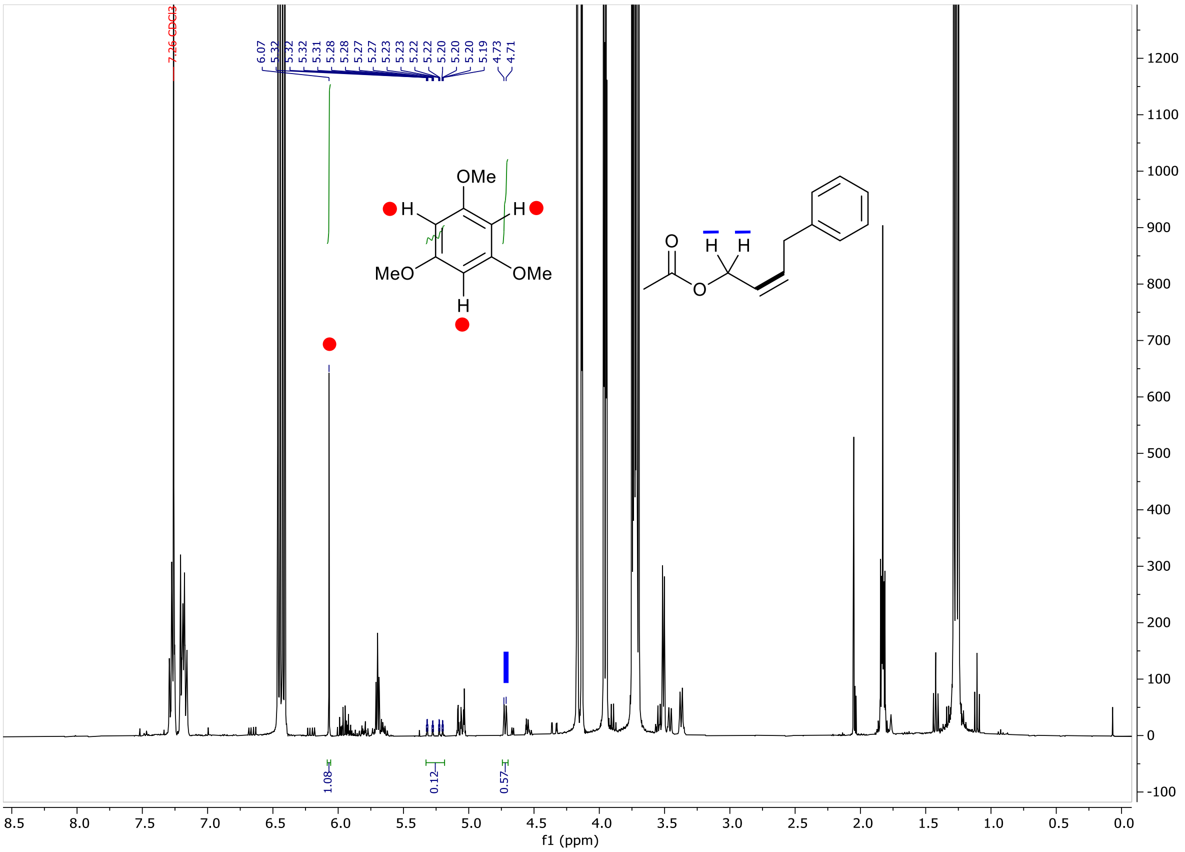
^{1}H NMR (400 MHz, $CDCl_3$) (P2c, 2 mol%, t0)



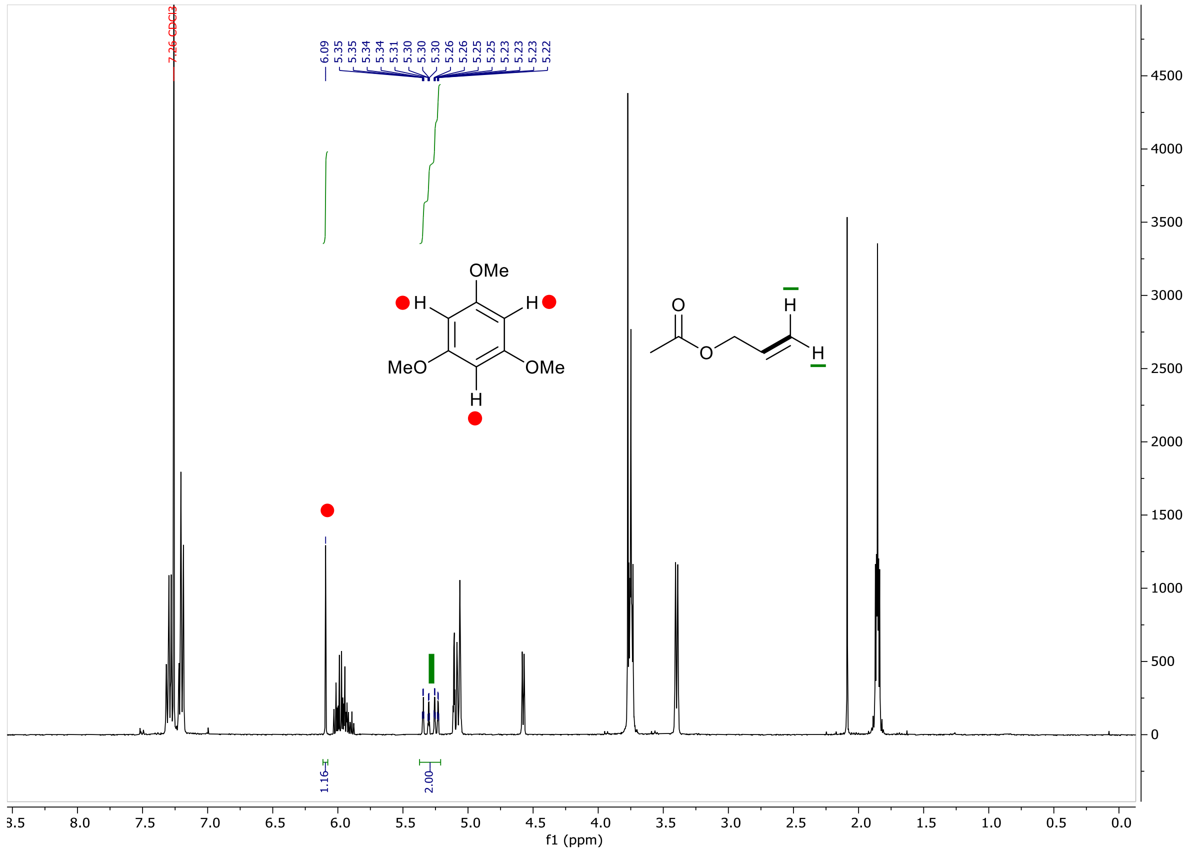
^{1}H NMR (400 MHz, CDCl$_3$) (P2c, 2 mol%, 21 h)



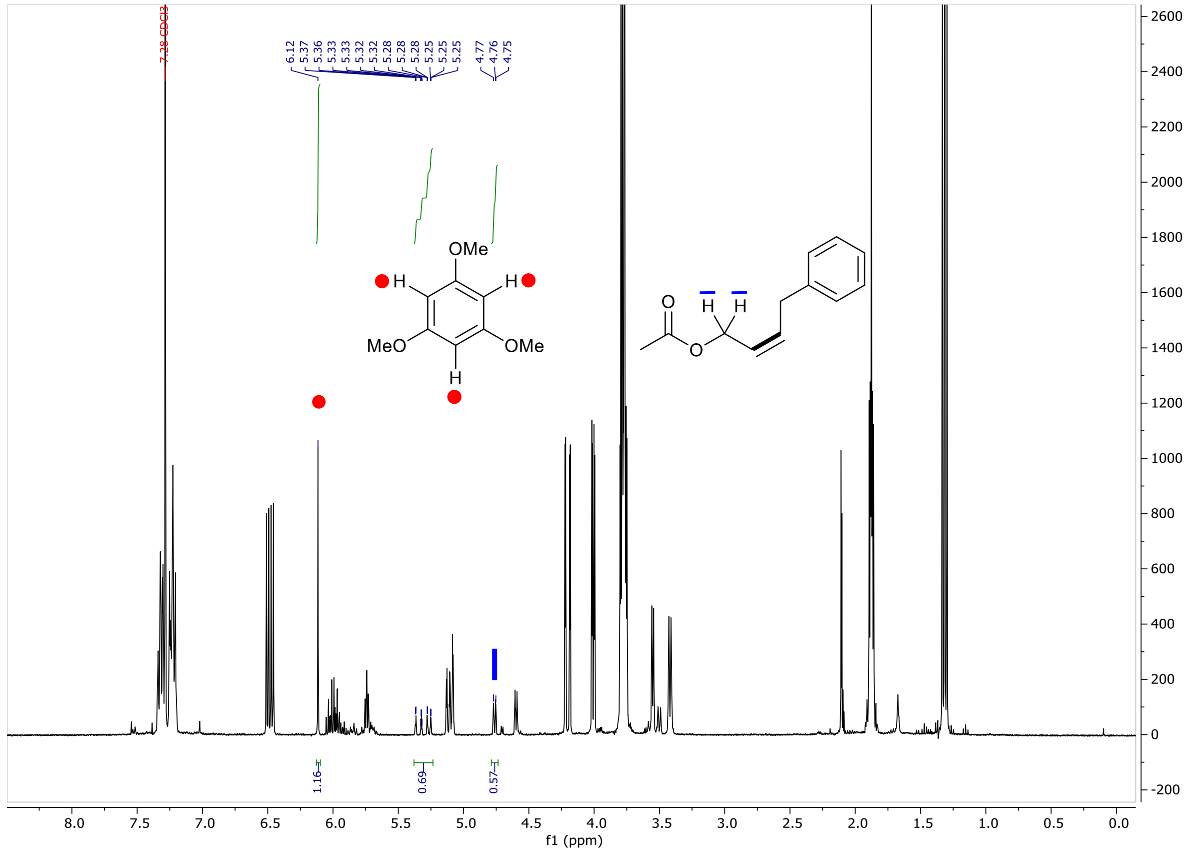
^{1}H NMR (400 MHz, CDCl$_3$) (P2c, 2 mol%, 48 h)



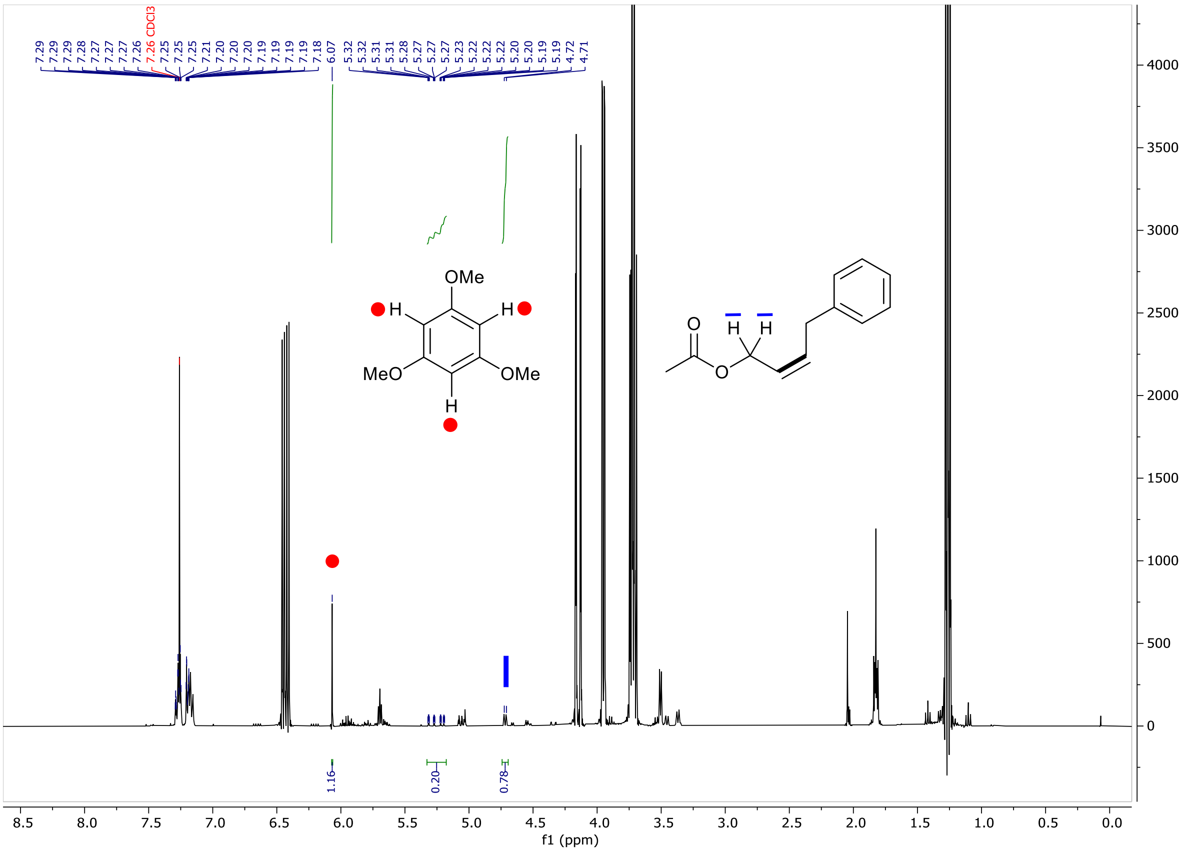
^{1}H NMR (400 MHz, CDCl$_3$) (P2c, 3 mol%, t0)



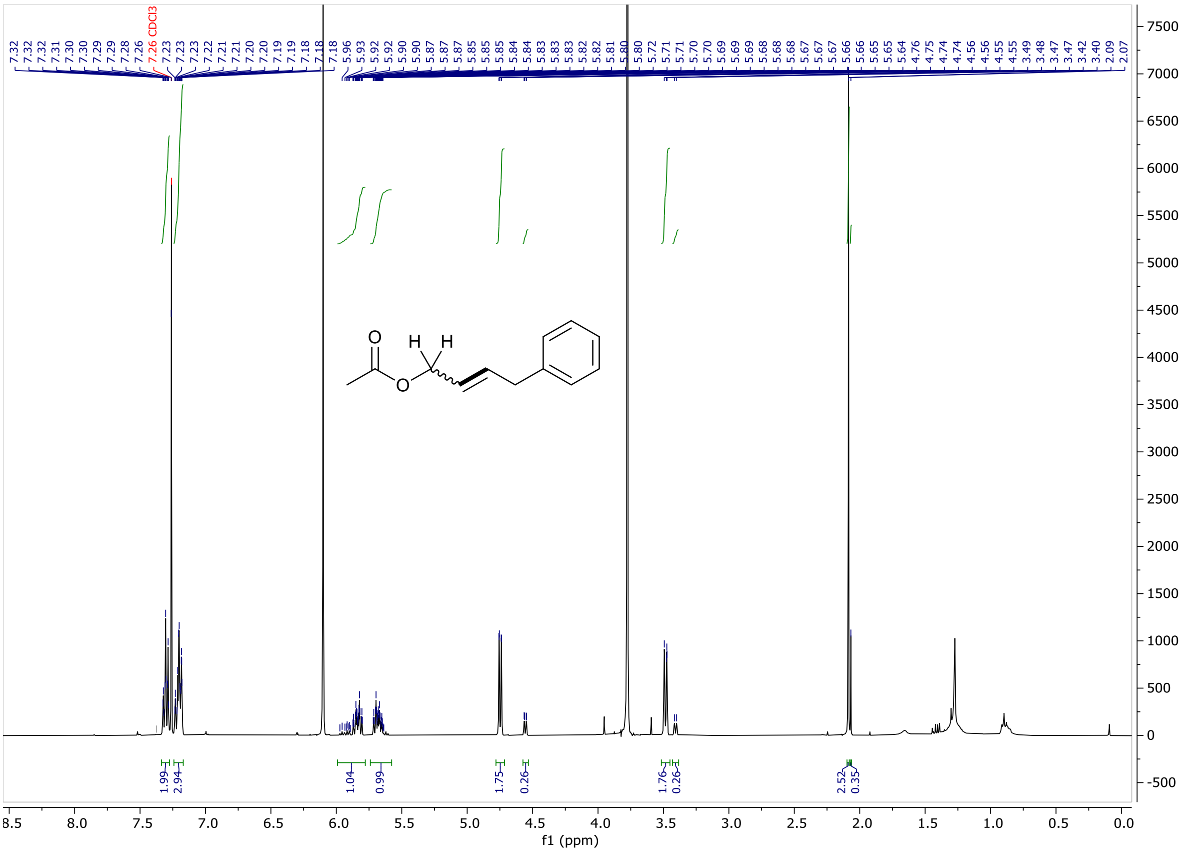
^{1}H NMR (400 MHz, CDCl$_3$) (P2c, 3 mol%, 21 h)



^{1}H NMR (400 MHz, CDCl$_3$) (P2c, 3 mol%, 48 h)

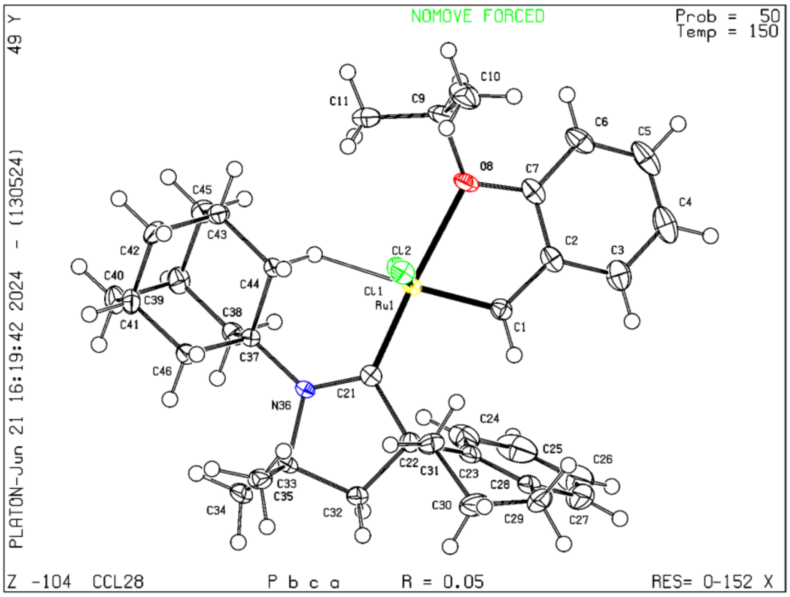


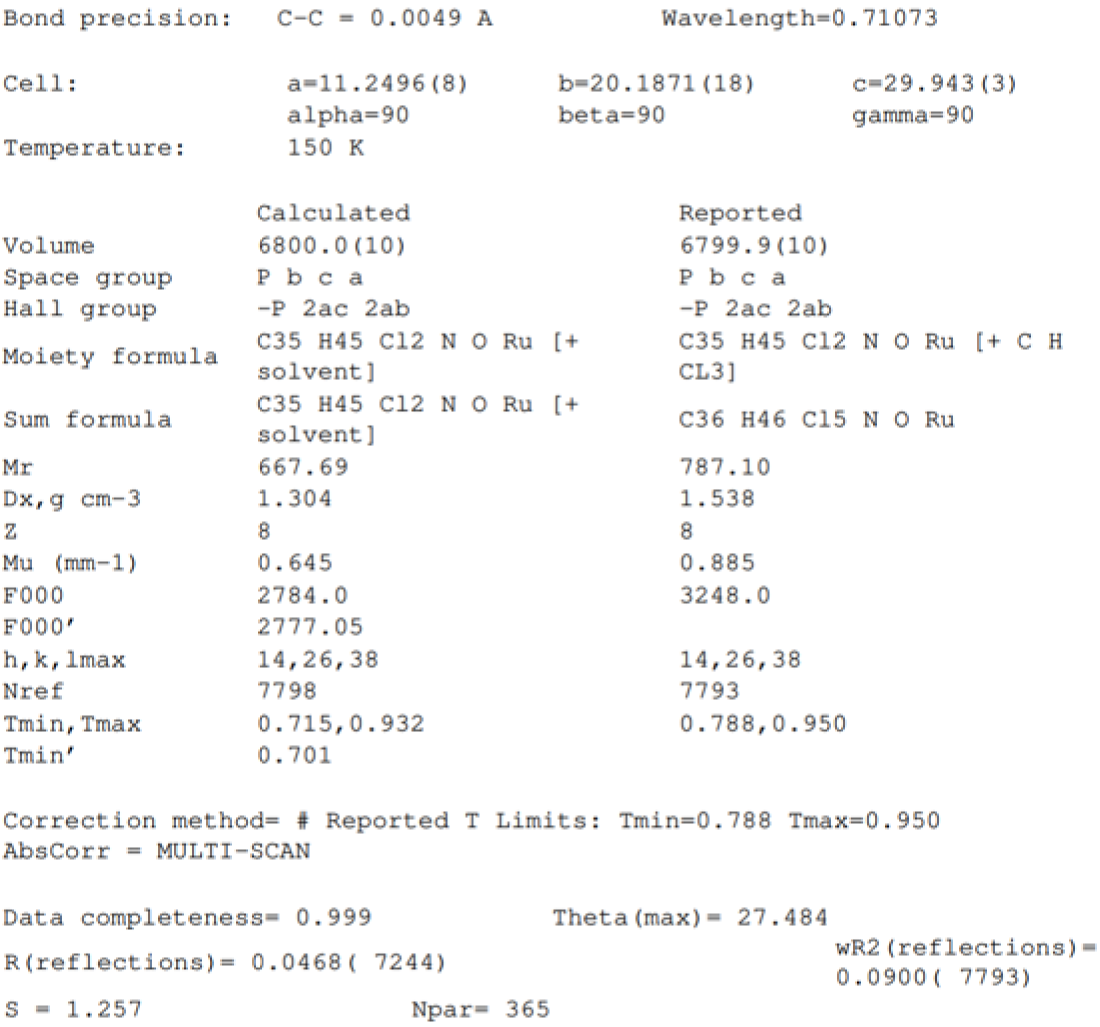
^{1}H NMR (400 MHz, CDCl$_3$) (P2c)



7. X-Ray crystallographic data

-Ru8c





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Cell:	a=11.2496(8)	b=20.1871(18)	c=29.943(3)
	alpha=90	beta=90	gamma=90
Temperature:	150 K		

	Calculated	Reported
Volume	6800.0(10)	6799.9(10)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C35 H45 Cl2 N O Ru [+ solvent]	C35 H45 Cl2 N O Ru [+ C H CL3]
Sum formula	C35 H45 Cl2 N O Ru [+ solvent]	C36 H46 Cl5 N O Ru
Mr	667.69	787.10
Dx,g cm-3	1.304	1.538
Z	8	8
Mu (mm-1)	0.645	0.885
F000	2784.0	3248.0
F000’	2777.05	
h,k,lmax	14,26,38	14,26,38
Nref	7798	7793
Tmin,Tmax	0.715,0.932	0.788,0.950
Tmin’	0.701	

Correction method= # Reported T Limits: Tmin=0.788 Tmax=0.950
AbsCorr = MULTI-SCAN

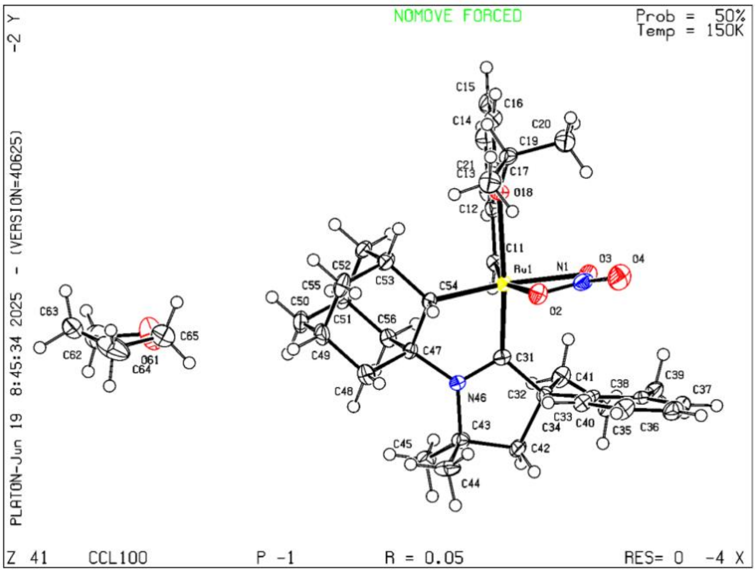
Data completeness= 0.999 Theta(max)= 27.484

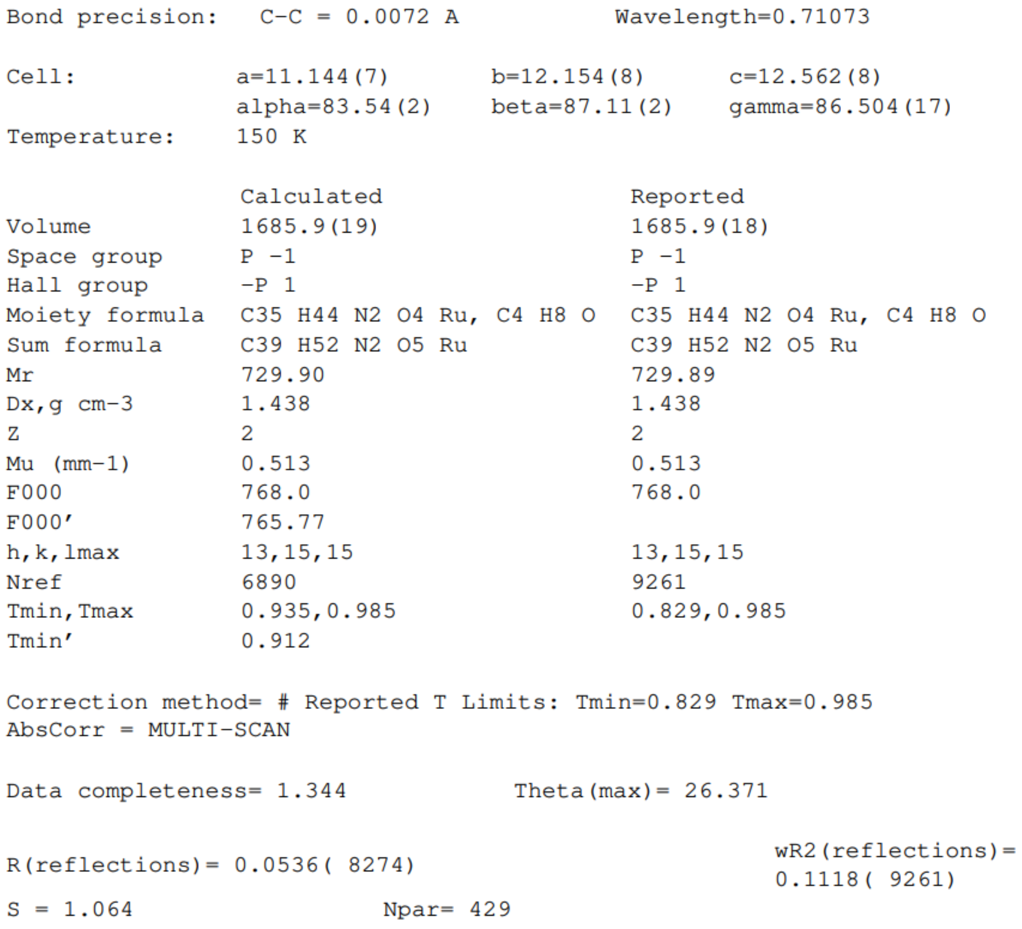
R(reflections)= 0.0468(7244) wR2(reflections)= 0.0900(7793)

S = 1.257 Npar= 365

Note : The contribution of the $CHCl_3$ disordered solvent to the calculated structure factors was estimated following the BYPASS algorithm[9], implemented as the SQUEEZE option in PLATON[10]. A new data set, free of solvent contribution, was then used in the fi\u001Cnal re\u001Cnement.

-Ru7





```
Bond precision:   C-C = 0.0072 A          Wavelength=0.71073

Cell:             a=11.144(7)       b=12.154(8)       c=12.562(8)
                  alpha=83.54(2)    beta=87.11(2)     gamma=86.504(17)
Temperature:      150 K

                  Calculated                    Reported
Volume            1685.9(19)                    1685.9(18)
Space group       P -1                          P -1
Hall group        -P 1                          -P 1
Moiety formula    C35 H44 N2 O4 Ru, C4 H8 O     C35 H44 N2 O4 Ru, C4 H8 O
Sum formula       C39 H52 N2 O5 Ru              C39 H52 N2 O5 Ru
Mr                729.90                        729.89
Dx,g cm-3         1.438                         1.438
Z                 2                             2
Mu (mm-1)         0.513                         0.513
F000              768.0                         768.0
F000'             765.77
h,k,lmax          13,15,15                      13,15,15
Nref              6890                          9261
Tmin,Tmax         0.935,0.985                   0.829,0.985
Tmin'             0.912

Correction method= # Reported T Limits: Tmin=0.829 Tmax=0.985
AbsCorr = MULTI-SCAN

Data completeness= 1.344           Theta(max)= 26.371

                                                    wR2(reflections)=
R(reflections)= 0.0536( 8274)                       0.1118( 9261)

S = 1.064                  Npar= 429
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[9] P. v.d. Sluis and A.L. Spek, *Acta Cryst.* 1990, ***A46***, 194.

[10] A.L. Spek, *Acta Cryst.* 2015, ***C71***, 9.

Note : Crystal under study has revealed the presence of twinning, with two identified domains. Diffraction frames were integrated considering these two domains and a HKLF5 final data set was generated with TWINABS software. Final crystal refinement has then been realised on a HKLF5 format data file, taking into account the presence of these two crystal domains. The proportion of this second domain has been refined to ~0.27.

TWINABS : Sheldrick, G.M. (2012). TWINABS Bruker AXS Inc., Madison, Wisconsin, USA