SUPPORTING INFORMATION

Cyclic Alkyl Amino Carbene Ruthenium Complexes – Efficient Catalysts for Macrocyclization and Acrylonitrile Cross Metathesis.

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1. Materials and methods

NMR spectra were acquired on Bruker spectrometer (NMR Avance III HD 500 MHz). High-resolution mass spectrometry was performed at the Mass Spectrometry Facility, Institute of Organic Chemistry, Polish Academy of Sciences. Elemental analyses were performed by analytical laboratory at the Institute of Organic Chemistry, Polish Academy of Sciences. Gas Chromatography analyses were conducted using an PerkinElmer Clarus 680 GC equipped with GL Sciences InertCap® 5MS/NP column. Analytical thin-layer chromatography (TLC) was performed using silica gel 60 F254 precoated plates (0.25 mm thickness) with a fluorescent indicator. Visualization of TLC plates was performed by UV light (254 nm) and $KMnO_4$ water solution. The column chromatography was performed using silica gel 60 (230–400 mesh).

Ethyl 10-undecenoate (Sigma-Aldrich >=97%) was distilled under reduced pressure and further purified by filtration through pad of activated neutral alumina, degassed, purged with argon and stored over activated neutral alumina (2 wt%). Methyl 9-decenoate (obtained by ethenolysis of methyl oleate)[1] was distilled under reduced pressure and further purified by filtration through pad of activated neutral alumina, degassed, purged with argon and stored over activated neutral alumina (2 wt%). Acrylonitrile (Sigma-Aldrich >=99%; stabilized with 35-45 ppm of monomethyl ether hydroquinone) was purged with argon and stored over 3Å molecular sieves.

Ruthenium complexes **3b**,[2] **6b**,[3] **14**,[4] salts **13**, **29-31**[5], ligand **15**[6], diene **10**[7] and **28**[8] were prepared according to the methods reported in the literature. Ruthenium complex **5** was purchased from Strem Chemicals Inc.

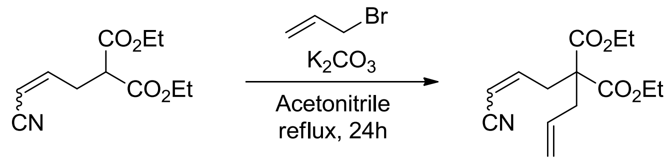
Substrates **10**, **23** and **25** were distilled under reduced pressure and further purified by filtration through pad of activated neutral alumina, degassed, purged with argon and stored over activated neutral alumina (2 wt%).

Green crystals of **16a**, **16b** and **17b** were obtained from the dichloromethane/methanol solution. The X-ray data for all reported structures were collected at 293(2) K with an Oxford Sapphire CCD diffractometer using MoKα radiation λ = 0.71073 Å and ω-2θ method. Structures were solved by direct methods and refined with the full-matrix least-squares method on F^2 with the use of SHELX2014 program packages.[9] The analytical absorption corrections were applied (CrysAlis Pro Software System).[10] Positions of hydrogen atoms have been found from the electron density maps and hydrogen atoms were constrained with the appropriate model as implemented in SHELX during refinement. The absolute configuration for **16a** was determined by the Flack method.[11] The data collection and refinement processes are summarized in Table S1, whereas selected bond lengths and angles for in Table S2.

Preparation of catalysts was carried out under Ar in pre-dried glassware using Schlenk techniques. All work-up and purification procedures were carried out with reagent grade solvents in air. Toluene was washed with citric acid (2.5 wt% in water) and water, filtered through activated neutral alumina, degassed by purging with argon and stored over activated 4Å molecular sieves. Dichloromethane was degassed by purging with argon and stored over activated 4Å molecular sieves. All other reagents were purchased from Sigma-Aldrich and used without further purification.

Before GC analysis or distillation, metathesis reactions were quenched with 1,4-Bis(3-isocyanopropyl)piperazine [SnatchCat, CAS: 51641-96-4] (4.4 equivalents relative to catalyst) or ethyl vinyl ether.

2. Synthesis of 25



Mixture of **28** (11.60 g, 51.5 mmol), allyl bromide (6.7 mL, 77.0 mmol, 1.5 equiv) and K_2CO_3 (10.68 g, 77.0 mmol, 1.5 equiv) in acetonitrile (170 mL) was refluxed for 24h. After that time the reaction mixture was cooled down to rt and insoluble material was filtered off. Filtrate was concentrated in vacuum. Reaction product was isolated by silica gel column chromatography (eluent: ethyl acetate/cyclohexane 1:9). After evaporation of solvents and drying in vacuum product **25** was obtained as colorless oil (10.5 g, 77%). Mixture of isomers *Z*/*E* = 5.5:1.

^{1}H NMR ($CDCl_3$, 500 MHz): δ = 6.63 (dt, *J* = 16.1, 7.7 Hz, 1H, *E*), 6.47 (dt, *J* = 11.0, 7.7 Hz, 1H, *Z*), 5.70-5.62 (m, 1H, *Z*), 5.62-5.53 (m, 1H, *E*), 5.41 (dt, *J* = 11.0, 1.4 Hz, 1H, *Z*), 5.38 (dt, *J* = 16.3, 1.4 Hz, 1H, *E*), 5.16 (t, *J* = 1.2 Hz, 1H, *Z*), 5.15-5.12 (m, 1H, *Z+E*), 5.12-5.10 (m, 1H, *E*), 4.24-4.16 (m, 4H, *Z+E*), 2.97-2.93 (m, 2H, *Z*), 2.74-2.71 (m, 2H, *E*), 2.67-2.62 (m, 2H, *Z+E*), 1.28-1.23 (m, 6H, *Z+E*).

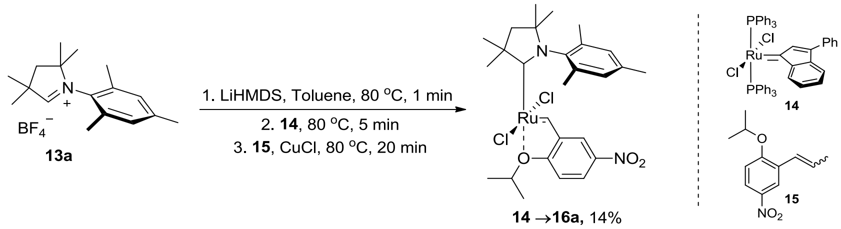
^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.9 (*Z*), 169.8 (*E*), 150.2 (*E*), 149.1 (*Z*), 131.4 (*Z+E*), 120.1 (*Z*), 120.0 (*E*), 116.8 (*E*), 115.4 (*Z*), 103.1 (*E*), 102.4 (*Z*), 61.8 (*Z+E*), 56.8 (*Z*), 56.7 (*E*), 37.8 (*Z*), 37.7 (*E*), 36.6 (*E*), 34.9 (*Z*), 14.0 (*Z+E*).

HRMS-ESI (*m/z*): calcd for $C_{14}H_{19}NO_4Na$ $[M+Na]^+$: 288.1212; found 288.1211.

Anal. calcd for $C_{14}H_{19}NO_4$: C 63.38; H 7.22; N 5.28; found: C 63.53; H 7.11; N 5.21.

3. Synthesis of complexes 16-19

3.1. Synthesis of 16a



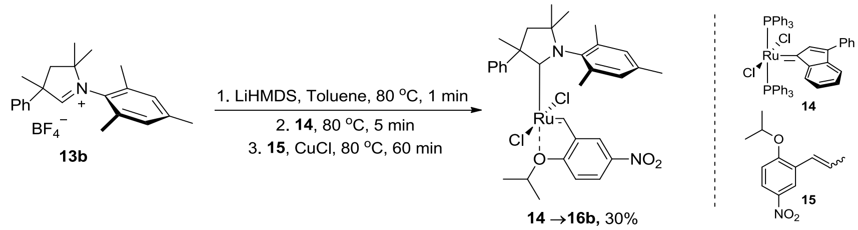
Dry deoxygenated toluene (20 mL) was added under argon atmosphere to salt **13a** (1.66 g, 5.0 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 5.0 mL, 5.0 mmol, 2 equiv). After 1 minute solid **14** was added (2.22 g, 2.5 mmol, 1 equiv). The mixture was stirred at 80 °C for 2 minutes and then **15** (0.664 g, 3.0 mmol, 1.2 equiv) and CuCl (0.866 g, 8.75 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 30 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **16a** (0.215 g, 14%).

^{1}H NMR (CD_2Cl_2, 500 MHz): δ = 16.12 (s, 1H), 8.48 (dd, *J* = 9.1; 2.7 Hz, 1H), 7.75 (d, *J* = 2.8 Hz, 1H), 7.20 (s, 2H), 7.08 (d, *J* = 9.1 Hz, 1H), 5.25 (septet, *J* = 6.1 Hz, 1H), 2.54 (s, 3H), 2.21 (s, 2H), 2.19 (s, 6H), 2.05 (s, 6H), 1.74 (d, *J* = 6.2 Hz, 6H), 1.43 (s, 6H).

^{13}C NMR (CD_2Cl_2, 125 MHz): δ = 292.6, 264.1, 156.7, 144.2, 143.3, 139.7, 138.5, 137.9, 131.2, 125.7, 118.6, 113.7, 79.6, 78.1, 56.5, 52.4, 29.7, 29.3, 22.3, 21.2, 20.9.

HRMS-ESI (*m/z*): calcd for $C_{27}H_{36}N_2O_3NaCl_2Ru$ $[M+Na]^+$: 631.1044; found: 631.1028.
Anal. calcd for $C_{27}H_{36}N_2Cl_2O_3Ru$: C 53.29; H 5.96; N 4.60; Cl 11.65; found: C 53.21; H 5.93; N 4.53; Cl 11.61.

3.2. Synthesis of 16b



Dry deoxygenated toluene (56 mL) was added under argon atmosphere to salt **13b** (5.51 g, 14.0 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 14.0 mL, 14.0 mmol, 2 equiv). After 1 minute solid **14** was added (6.21 g, 7.0 mmol, 1 equiv). The mixture was stirred at 80 °C for 5 minutes and then **15** (1.86 g, 8.4 mmol, 1.2 equiv) and CuCl (2.42 g, 24.5 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 60 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene -> ethyl acetate/cyclohexane 1:5). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of methanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold methanol and dried in vacuum to give green crystalline solid **16b** (1.43 g, 30%). Mixture of isomers.

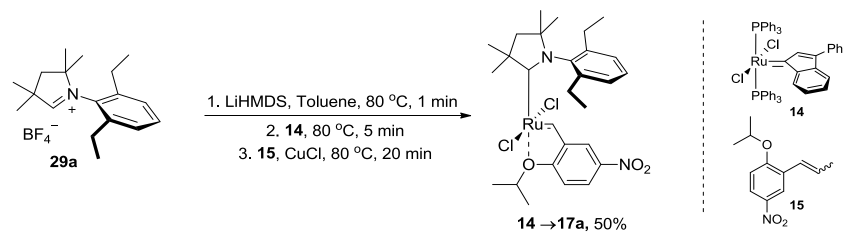
^{1}H NMR (CD_2Cl_2, 500 MHz): δ = [17.71 (s), 16.22 (s), 1H], 8.46 (dd, *J* = 9.3, 2.6 Hz, 1H), 8.30-7.30 (m, 6H), 7.14 (s, 2H), 7.01 (d, *J* = 9.1 Hz, 1H), 5.05 (septet, *J* = 6.2 Hz, 1H), 2.75-1.80 (m, 14H), 1.70-1.20 (m, 12H).

^{13}C NMR (CD_2Cl_2, 125 MHz): δ = 268.1, 157.8, 144.2, 143.2, 139.6, 137.9, 136.3, 132.4, 131.0, 129.2, 127.5, 125.8, 113.8, 78.0, 64.2, 58.1, 49.1, 30.1, 28.6, 25.5, 24.9, 21.8, 21.1.

HRMS-ESI (*m/z*): calcd for $C_{32}H_{38}N_2O_3NaCl_2Ru$ $[M+Na]^+$: 693.1201; found: 693.1179.

Anal. calcd for $C_{32}H_{38}N_2Cl_2O_3Ru$: C 57.31; H 5.71; N 4.18; Cl 10.57; found: C 57.43; H 5.72; N 4.14; Cl 10.42.

3.3. Synthesis of 17a



Dry deoxygenated toluene (40 mL) was added under argon atmosphere to salt **29a** (3.45 g, 10.0 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 10.0 mL, 10.0 mmol, 2 equiv). After 1 minute solid **14** was added (4.43 g, 5.0 mmol, 1 equiv). The mixture was stirred at 80 °C for 5 minutes and then **15** (1.33 g, 6.0 mmol, 1.2 equiv) and CuCl (1.73 g, 17.5 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 20 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **17a** (1.57 g, 50%).

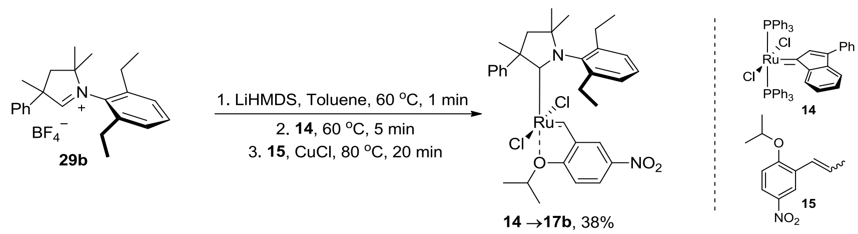
^1H NMR (CD_2Cl_2, 500 MHz): δ = 16.29 (s, 1H), 8.46 (dd, *J* = 9.1; 2.7 Hz, 1H), 7.72-7.65 (m, 2H), 7.51 (d, *J* = 7.7 Hz, 2H), 7.08 (d, *J* = 8.7 Hz, 1H), 5.26 (septet, *J* = 6.1 Hz, 1H), 2.61-2.49 (m, 4H), 2.21 (s, 2H), 2.07 (s, 6H), 1.77 (d, *J* = 6.2 Hz, 6H), 1.33 (s, 6H), 0.91 (t, *J* =7.4 Hz, 6H).

^{13}C NMR (CD_2Cl_2, 125 MHz): δ = 290.4, 263.8, 165.6, 157.1, 143.7, 143.4, 138.8, 129.9, 127.7, 125.7, 118.3, 113.7, 79.4, 78.2, 56.5, 52.3, 29.9, 28.9, 25.3, 22.4, 14.9.

HRMS-ESI (*m/z*): calcd for $C_{28}H_{39}N_2O_3Ru$ $[M-2Cl+H]^+$: 553.2006; found: 553.2004.

Anal. calcd for $C_{28}H_{38}N_2Cl_2O_3Ru$: C 54.02; H 6.15; N 4.50; Cl 11.39; found: C 54.18; H 6.09; N 4.42; Cl 11.20.

3.4. Synthesis of 17b



Dry deoxygenated toluene (24 mL) was added under argon atmosphere to salt **29b** (2.44 g, 6.0 mmol, 2 equiv). Resulted suspension was heated up to 60 °C and solution of LiHMDS in toluene was added (1M, 6.0 mL, 6.0 mmol, 2 equiv). After 1 minute solid **14** was added (2.66 g, 3.0 mmol, 1 equiv). The mixture was stirred at 60 °C for 5 minutes and then **15** (0.797 g, 3.6 mmol, 1.2 equiv) and CuCl (1.04 g, 10.5 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 20 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **17b** (0.780 g, 38%). Mixture of isomers.

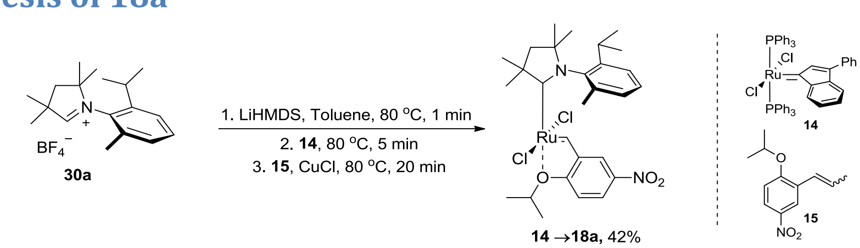
^{1}H NMR (C_6D_6, 500 MHz): δ = [17.73 (s), 16.37 (s), 1H], 8.27 (br. s, 1H), 7.89 (dd, *J* = 9.1; 2.7 Hz, 1H), 7.78 (br. s, 1H), 7.48 (br. s, 1H), 7.36-7.16 (m, 6H), 6.03 (d, *J* = 9.1 Hz, 1H), 4.43-4.33 (m, 1H), 2.95-1.80 (m, 8H), 1.50-0.60 (m, 19H).

^{13}C NMR (C_6D_6, 125 MHz): δ =292.2, 262.4, 157.0, 144.0, 143.4, 139.1, 130.0, 129.7, 127.9, 127.6, 125.5, 118.2, 113.4, 78.4, 77.3, 63.7, 49.2, 31.1, 27.9, 27.6, 26.3, 25.9, 24.9, 22.5, 15.5, 14.9.

HRMS-ESI (*m/z*): calcd for $C_{33}H_{40}N_2O_3ClRu$ $[M-Cl]^+$: 649.1771; found: 649.1746.

Anal. calcd for $C_{33}H_{40}N_2Cl_2O_3Ru$: C 57.89; H 5.89; N 4.09; Cl 10.36; found: C 57.98; H 5.99; N 4.08; Cl 10.44.

3.5. Synthesis of 18a



Dry deoxygenated toluene (20 mL) was added under argon atmosphere to salt **30a** (1.73 g, 5.0 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 5.0 mL, 5.0 mmol, 2 equiv). After 1 minute solid **14** was added (2.22 g, 2.5 mmol, 1 equiv). The mixture was stirred at 80 °C for 5 minutes and then **15** (0.664 g, 3.0 mmol, 1.2 equiv) and CuCl (0.866 g, 8.75 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 20 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **18a** (0.663 g, 42%).

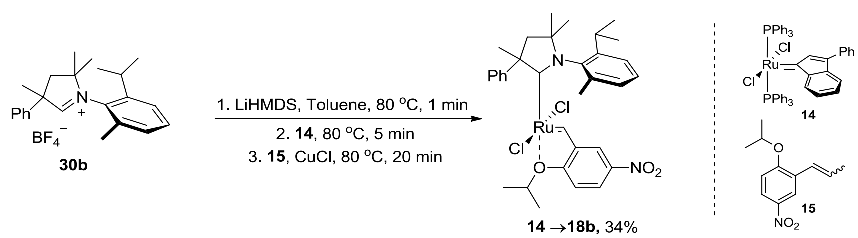
^{1}H NMR (CD_2Cl_2, 500 MHz): δ = 16.19 (s, 1H), 8.45 (dd, *J* = 9.1; 2.7 Hz, 1H), 7.70 (d, *J* = 2.7 Hz, 1H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.55 (dd, *J* = 8.0; 1.5 Hz, 1H), 7.35 (ddd, *J* = 7.5; 1.6; 0.7 Hz, 1H), 7.08 (d, *J* = 8.9 Hz, 1H), 5.26 (sept, *J* = 6.2 Hz, 1H), 2.97 (sept, *J* = 6.7 Hz, 1H), 2.26-2.19 (m, 5H), 2.13 (s, 3H), 2.03 (s, 3H), 1.77 (dd, *J* = 16.1; 6.1 Hz, 6H), 1.43 (s, 3H), 1.38 (s, 3H), 1.30 (d, *J* = 6.6 Hz, 3H), 0.68 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (CD_2Cl_2, 125 MHz): δ = 290.2, 264.6, 157.2, 149.1, 143.5, 143.4, 138.5, 138.4, 130.4, 130.0, 126.5, 125.8, 118.4, 113.7, 79.4, 78.2 56.6, 52.3, 29.9, 29.7, 29.6, 29.1, 28.9, 26.3, 24.3, 22.4, 22.3, 21.8.

HRMS-ESI (*m/z*): calcd for $C_{28}H_{38}ClN_2O_3Ru$ $[M-Cl]^+$: 587.1613; found: 587.1636.

Anal. calcd for $C_{28}H_{38}N_2Cl_2O_3Ru$: C 54.02; H 6.15; N 4.50; Cl 11.39; found: C 54.19; H 6.18; N 4.37; Cl 11.21.

3.6. Synthesis of 18b



Dry deoxygenated toluene (8 mL) was added under argon atmosphere to salt **30b** (0.815 g, 2.0 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 2.0 mL, 2.0 mmol, 2 equiv). After 1 minute solid **14** was added (0.887 g, 1.0 mmol, 1 equiv). The mixture was stirred at 80 °C for 5 minutes and then **15** (0.266 g, 1.2 mmol, 1.2 equiv) and CuCl (0.346 g, 3.50 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 20 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **18b** (0.235 g, 34%). Mixture of isomers.

^{1}H NMR (C_6D_6, 500 MHz): δ = [16.28 (br. s), 16.25 (s), 1H], 8.35-8.15 (m, 2H), 7.87 (dd, *J* = 9.1; 2.8 Hz, 1H), 7.77 (dd, *J* = 19.6; 2.7 Hz, 1H), 7.52 (t, *J* = 7.9 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.35-7.20 (m, 2H), 7.14 (s, 1H), 7.08-6.88 (m, 1H), 6.10-5.98 (m, 1H), 4.46-4.31 (m, 1H), 3.09 (septet, *J* = 6.9 Hz, 1H), 2.88-2.67 (m, 1H), 2.44 (s, 1H), 2.34 (s, 3H), 2.21 (s, 2H), 1.93-1.86 (m, 1H), 1.48-1.33 (m, 3H), 1.32-1.20 (m, 2H), 1.18-1.14 (m, 3H), 1.10-0.97 (m, 8H).

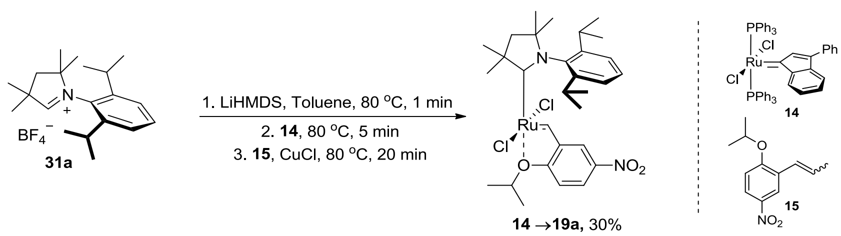
^{13}C NMR (C_6D_6, 125 MHz): δ = 292.6, 291.6, 262.9, 157.0, 149.5, 149.3, 144.0, 143.6, 143.3, 142.3, 138.9, 138.8 (2C), 138.6, 130.7, 130.5 (2C), 130.1 (2C), 129.9, 129.6 (2C), 128.0, 127.9, 126.9, 126.4, 125.7, 125.5, 118.6, 118.4, 113.5, 78.4, 78.3, 77.4, 77.3, 64.2, 64.0, 63.5, 49.9, 49.1, 31.8, 31.4, 29.3, 28.8, 28.6, 28.4, 27.5, 27.4, 27.3, 26.2, 25.9, 24.5, 23.1, 22.5, 22.3, 21.9.

HRMS-ESI (*m/z*): calcd for $C_{33}H_{40}N_2O_3NaCl_2Ru$ $[M+Na]^+$: 707.1357; found: 707.1360.

Anal. calcd for $C_{34.5}H_{44}N_2Cl_2O_{3.5}Ru$ [M+0.5C_3H_8O (2-propanol solvate)]:

C 57.98; H 6.21; N 3.92; Cl 9.92; found C 58.08; H 6.04; N 3.89; Cl 10.12.

3.7. Synthesis of 19a



Dry deoxygenated toluene (20 mL) was added under argon atmosphere to salt **31a** (1.87 g, 5.0 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 5.0 mL, 5.0 mmol, 2 equiv). After 1 minute solid **14** was added (2.22 g, 2.5 mmol, 1 equiv). The mixture was stirred at 80 °C for 5 minutes and then **15** (0.664 g, 3.0 mmol, 1.2 equiv) and CuCl (0.866 g, 8.75 mmol, 3.5 equiv) were added. The mixture was stirred at 80 °C for 20 min and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in ethyl acetate, filtered and evaporated. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **19a** (0.490 g, 30%).

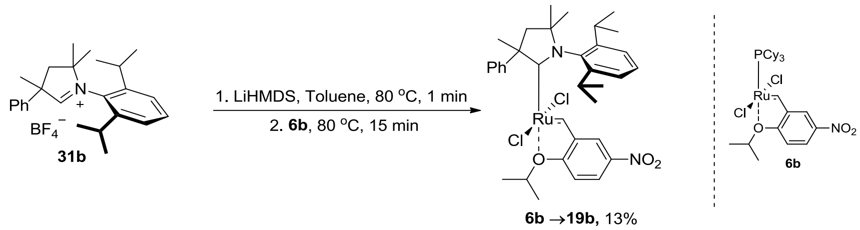
^{1}H NMR (CD_2Cl_2, 500 MHz): δ = 16.31 (s, 1H), 8.42 (dd, *J* = 9.1; 2.7 Hz, 1H), 7.73 (t, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 2.7 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.09 (d, *J* = 9.1 Hz, 1H), 5.27 (septet, *J* = 6.2 Hz, 1H), 2.96 (septet, *J* = 6.5 Hz, 2H), 2.20 (s, 2H), 2.09 (s, 6H), 1.79 (d, *J* = 6.2 Hz, 6H), 1.36 (s, 6H), 1.28 (d, *J* = 6.7 Hz, 6H), 0.66 (d, *J* = 6.4 Hz, 6H).

[13]C NMR (CD_2Cl_2, 125 MHz): δ = 288.0, 287.7, 264.8, 157.5, 148.7, 143.3, 142.7 (2C), 136.7, 130.4, 126.5, 125.7, 118.3, 113.8, 79.1, 78.3, 56.7, 51.9, 30.2, 29.5, 29.0, 27.8, 25.7, 24.6, 22.4.

HRMS-ESI (*m/z*): calcd for $C_{30}H_{42}N_2O_3ClRu$ $[M-Cl]^+$: 615.1927; found: 615.1918.

Anal. calcd for $C_{30}H_{42}N_2Cl_2O_3Ru$: C 55.38; H 6.51; N 4.31; Cl 10.90; found: C 55.15; H 6.45; N 4.15; Cl 10.86.

3.8. Synthesis of 19b



Dry deoxygenated toluene (3.2 mL) was added under argon atmosphere to salt **31b** (0.348 g, 0.8 mmol, 2 equiv). Resulted suspension was heated up to 80 °C and solution of LiHMDS in toluene was added (1M, 0.8 mL, 0.8 mmol, 2 equiv). After 1 minute solid **6b** was added (0.258 g, 0.4 mmol, 1 equiv). The mixture was stirred at 80 °C for 15 minutes and then cooled down to room temperature. Crude reaction product was isolated by silica gel column chromatography (eluent: toluene). Green fraction was collected and evaporated to dryness. Residue was dissolved in CH_2Cl_2 and excess of 2-propanol was added. CH_2Cl_2 was slowly evaporated under reduced pressure. Precipitate formed during evaporation was filtered, washed with a minimal amount of cold 2-propanol and dried in vacuum to give green crystalline solid **19b** (0.037 g, 13%).

[1]H NMR (CD_2Cl_2, 500 MHz): δ = 16.49 (s, 1H), 8.40 (dd, *J* = 9.1; 2.7 Hz, 1H), 8.24-8.20 (m, 2H), 7.74 (t, *J* = 7.8 Hz, 1H), 7.59-7.49 (m 5H), 7.40-7.35 (m, 1H), 7.00 (d, *J* = 9.1 Hz, 1H), 5.05 (septet, *J* = 6.1 Hz, 1H), 3.15 (d, *J* = 12.9 Hz, 1H), 3.04 (septet, *J* = 6.6 Hz, 1H), 2.93 (septet, *J* = 6.5 Hz, 1H), 2.38 (d, *J* = 12.8 Hz, 1H), 2.33 (s, 3H), 1.57 (d, *J* = 6.1 Hz, 3H), 1.53 (s, 3H), 1.43-1.40 (m, 6H), 1.36 (d, *J* = 6.6 Hz, 3H), 1.27 (d, *J* = 6.6 Hz, 3H), 0.80 (d, *J* = 6.5 Hz, 3H), 0.48 (d, *J* = 6.4 Hz, 3H).

[13]C NMR (CD_2Cl_2, 125 MHz): δ = 291.8, 291.4, 262.2, 157.4, 148.8, 148.5, 143.2 (2C), 142.9, 137.0, 130.5, 129.8, 129.6, 128.0, 126.8, 126.6, 125.9, 118.6, 113.9, 78.7, 77.9, 63.6, 48.6, 33.0, 29.4, 29.0, 28.8, 28.1, 27.5, 26.5, 24.7, 24.6, 22.7, 22.6.

HRMS-ESI (*m/z*): calcd for $C_{35}H_{44}N_2O_3NaCl_2Ru$ $[M+Na]^+$: 735.1670; found: 735.1639.

Anal. calcd for $C_{38}H_{50}N_2Cl_2O_3Ru$ [M+0.5C_6H_{12} (cyclohexane solvate)]:

C 60.47; H 6.68; N 3.71; Cl 9.39 ; found: C 60.20; H 6.52; N 3.77; Cl 9.48.

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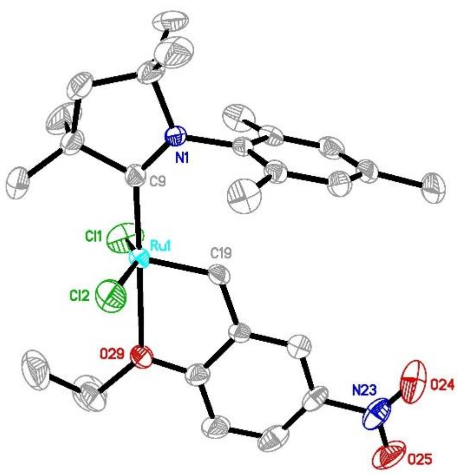
4. X-ray crystallography

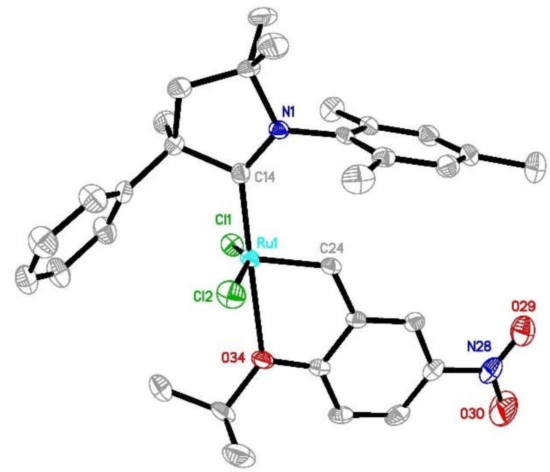
*Crystal structure of **16a, 16b** and **17b**.*

The asymmetric unit of **16a**, **16b** and **17b** contain of the ruthenium CAAC-benzylidene complex molecule. For these structures, the distorted square pyramidal coordination sphere of Ru(II) is formed by two chloride ions, carbon atom of CAAC ligand, and benzylidene ligand *via* their oxygen and carbon atoms, with its carbon atom in the apical position (Figure S1). For complexes **16a** and **17b**, Ru-Cl, Ru-O, and Ru-$C_{carbene}$ distances are very similar. For **16b** these distances are the longest among the structures described here. While, the Ru-$C_{benzylidene}$ distance (1.816(5) Å) is the shortest for **17b** (Table S2). These geometry parameters (Ru-Cl, Ru-$C_{carbene}$, and Ru-$C_{benzylidene}$) are very similar to those reported for the CAAC-benzylidene complexes (e.g. **7**).[12] Contrary, in such complexes the analogous Ru-O distances (e.g. **7**, 2.301(4) Å) are significantly shorter than these found in **16a**, **16b** and **17b**. Whereas in the ruthenium bis-CAAC-indenylidene catalysts (e.g. **9**) the Ru-Cl and Ru-$C_{carbene}$ distances are significantly longer than these found in **16a**, **16b** and **17b**.[1]

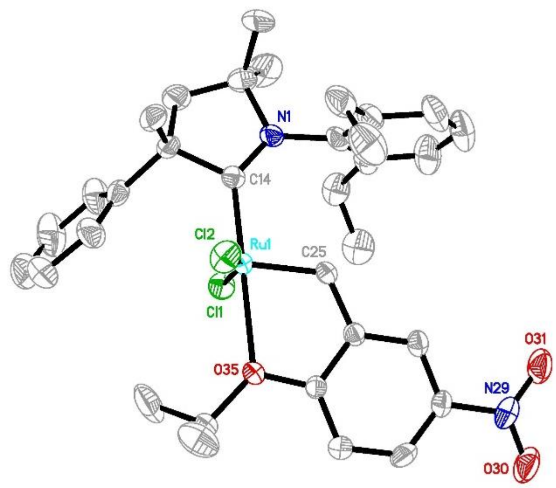
Among the structures described here, the longest distance between the Ru ion and the $Cl_2OC_{carbene}$ best plane is observed for **16a** (0.251 Å), while in **16b** and **17b** distance is shorter, 0.206 Å and 0.213 Å, respectively. The architecture of all structures is very similar, the N-aryl group is on the same side as benzylidene ligand with respect to the $RuCl_2OC_{carbene}$ best plane. For **16a** and **16b** the aromatic ring of benzylidene ligand and aromatic ring of N-aryl group are situated almost perpendicularly. The dihedral angles measured between best planes of these two rings are 87.1(4), and 89.3(3)° for **16a**, and **16b**, respectively. However in complex **17b**, the corresponding dihedral angle decreases to 76.8(3)°. Analysis of crystal packing in **16a** and **16b** structures revealed the intramolecular Ru-C…π interactions between carbon atom of benzylidene ligand and the N-TMP moiety of CAAC ligands, with C19…π and C24…π distance of 3.304(10)° and 3.213(6) Å, respectively. Also, in **17b** such intramolecular interactions are found, with Ru-C…$\pi_{(N\text{-}DEP)}$ distance of 3.516(5) Å.



16a



16b



17b

Figure S1. X-ray crystal structure of **16a**, **16b** and **17b**. Ellipsoids are drawn at the 30% probability level. Hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for **16a**, **16b**, and **17b**.

Empirical formula	**16a**	**16b**	**17b**
CCDC	1530952	1530953	1530951
Chemical formula	$C_{27}H_{36}N_2O_3Cl_2Ru$	$C_{32}H_{38}N_2O_3Cl_2Ru$	$C_{33}H_{40}N_2O_3Cl_2Ru$
Formula weight	608.55	670.61	684.64
Crystal system, space group	Monoclinic, P2(1)	Monoclinic, P2(1)/c	Monoclinic, P2(1)/n
a [Å]	8.6064(15)	10.0685(7)	16.3803(14)
b [Å]	9.9045(16)	16.6797(11)	12.7318(8)
c [Å]	16.722(3)	18.7168(13)	17.4287(17)
β [°]	98.138(15)	98.979(8)	114.581(11)
V [$Å^3$]	1411.1(4)	3104.8(4)	3305.4(5)
Z, ρ_{calcd} [mg m^{-3}]	2, 1.432	4, 1.435	4, 1.376
Absorption coefficient; mm^{-1}	0.775	0.712	0.670
F(000)	628	1384	1416
Crystal size [mm]	0.66 x 0.24 x 0.20	0.51 x 0.41 x 0.16	0.44 x 0.13 x 0.09
Theta range for data collection [°]	2.391 to 28.399	2.384 to 28.570	2.052 to 28.451
hkl range	-10 ≤h≤ 10, -12≤ k≤ 12 -19≤ l ≤21	-13 ≤h≤ 12, -20≤ k≤ 20, -24≤ l ≤24	-21 ≤h≤ 21, -16≤ k≤ 16, -23≤ l ≤23
Reflections collected/unique	9721 / 5904 [R(int) = 0.0377]	21831 / 7072 [R(int) = 0.0401]	22729 / 7554 [R(int) = 0.1088]
Completeness to theta	25.24, 99.9 %	25.00, 99.9 %	25.00, 100.0 %
Max. and min. transmission	0.875 and 0.600	0.918 and 0.723	0.952 and 0.770
Data/restraints/parameters	5904 / 1 / 316	7072 / 0 / 361	7554 / 0 / 370
Goodness-of-fit on F^2	1.072	1.177	1.037
Final R indices [I > 2σ(I)]	R1 = 0.0522, wR2 = 0.1110	R1 = 0.0698, wR2 = 0.1534	R1 = 0.0693, wR2 = 0.1576
R indices (all data)	R1 = 0.0635, wR2 = 0.1203	R1 = 0.0805, wR2 = 0.1585	R1 = 0.1169, wR2 = 0.1949
Absolute structure parameter	-0.07(3)	n/a	n/a
Residual peaks [$eÅ^{-3}$]	0.814 and -0.613	3.151 and -1.317	1.994 and -1.671

Table S2. Bond lengths [Å] and angles [°] within the coordination sphere for **16a**, **16b**, and **17b**.

16a		**16b**		**17b**	
		Bond length [Å]			
Ru1-Cl1	2.303(3)	Ru1-Cl1	2.3641(14)	Ru1-Cl1	2.3252(14)
Ru1-Cl2	2.333(3)	Ru1-Cl2	2.3318(14)	Ru1-Cl2	2.3314(14)
Ru1-C9$_{carbene}$	1.925(9)	Ru1-C14$_{carbene}$	1.943(5)	Ru1-C14$_{carbene}$	1.924(5)
Ru1-C19$_{benzylidene}$	1.823(6)	Ru1-C24$_{benzylidene}$	1.824(5)	Ru1-C25$_{benzylidene}$	1.816(5)
Ru1-O29	2.353(6)	Ru1-O34	2.389(3)	Ru1-O35	2.367(3)
		Angle [°]			
C19-Ru1-O29	77.5(3)	C24-Ru1-O34	76.56(18)	C25-Ru1-O35	77.62(17)
C19-Ru1-C9	103.7(4)	C24-Ru1-C14	102.5(2)	C25-Ru1-C14	102.4(2)
O29-Ru1-C9	176.7(3)	O34-Ru1-C14	177.98(18)	O35-Ru1-C14	176.23(17)
C19-Ru1-Cl2	99.8(3)	C24-Ru1-Cl2	101.32(18)	C25-Ru1-Cl2	97.90(16)
O29-Ru1-Cl2	86.2(2)	O34-Ru1-Cl2	86.92(10)	O35-Ru1-Cl2	86.69(13)
C9-Ru1-Cl2	90.5(3)	C14-Ru1-Cl2	91.51(15)	C14-Ru1-Cl2	89.94(13)
C19-Ru1-Cl1	101.6(3)	C24-Ru1-Cl1	97.23(18)	C25-Ru1-Cl1	93.83(15)
O29-Ru1-Cl1	85.8(2)	O34-Ru1-Cl1	84.51(10)	O35-Ru1-Cl1	86.04(10)
C9-Ru1-Cl1	96.9(2)	C14-Ru1-Cl1	97.41(15)	C14-Ru1-Cl1	90.03(14)
Cl2-Ru1-Cl1	154.94(13)	Cl2-Ru1-Cl1	157.14(6)	Cl2-Ru1-Cl1	157.55(6)

5. Metathesis reactions

5.1. Conversion, selectivity, yield and TON calculation

For CM reactions of **20**, **22** and **11** with acrylonitrile conversion was calculated by GC using methyl stearate as internal standard. Selectivity was calculated using Response factors (see representative example below).

Response factors calculation (for CM of 20 with acrylonitrile)

To a vial were precisely weighed following substances:

Substance	m [mg]	purity by GC [%]	Corr. mass [mg]
20	23.66	98.4	23.28
21	27.01	99.0	26.74
22	24.83	98.8	24.53

The mixture was dissolved in 10 mL of toluene and analyzed by GC (5 injections). The average area for each substance was divided by mass of the substance to give absolute Response factors and then (with assumption that for **20** Response factor = 1.0) were transformed to relative Response factors.

Inj.	GC Area 20	GC Area 21	GC Area 22
1	87300.0	103645.2	97226.6
2	85575.0	102433.3	96638.0
3	82764.4	99483.8	94880.7
4	83946.6	100074.9	94345.1
5	85088.6	99712.7	94808.3
Av. area	84934.9	101070.0	95579.8
mass	23.28	26.74	24.53
Av. area / mass	3648.4	3779.7	3896.4
Response factor	1.0	1.04	1.07

In further calculations GC areas of each component were transformed using Response factors. Conversion, selectivity, yield and TON were calculated from following equations:

$$Conversion = 100 \times \left(1 - \frac{A_{\mathbf{20}} \times A_{IS}^{0}}{A_{\mathbf{20}}^{0} \times A_{IS}}\right)$$

$$Selectivity = 100 \times \frac{n_{\mathbf{21}}}{n_{\mathbf{21}} + 2 \times n_{\mathbf{22}}}$$

$$Yield = \frac{Conversion \times Selectivity}{100}$$

$$TON = \frac{Yield \times n_{\mathbf{20}}^{0}/n_{\mathbf{cat}}^{0}}{100}$$

A_{20}, A_{IS}: GC area of ethyl 10-undecenoate (**20**) and internal standard (methyl stearate) at the end of the reaction

A^0_{20}, A^0_{IS}: GC area of ethyl 10-undecenoate (**20**) and internal standard (methyl stearate) before the reaction

n_{21}, n_{22}: moles of product **21** and diester **22**

n^0_{20}, n^0_{cat}: initial moles of ethyl 10-undecenoate (**20**) and moles of catalyst used

Representative example of calculations (Entry 4 Table 1 in main text; 300 ppm of 17b):

GC Area	20	21	22	Int. std.
Before rxn	174610.5	0	0	22901.1
End of rxn	36434.0	281210.7	9288.9	37934.7
Resp. factor	1.0	1.04	1.07	
M [g/mol]	212.33	237.34	396.60	
Area/Resp. factor/M	171.6	1139.3	21.9	

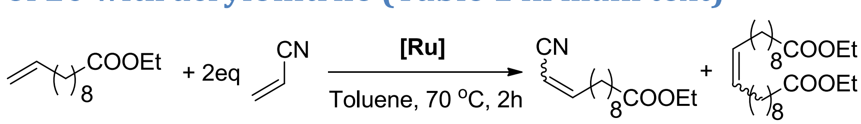
$$Conversion = 100 \times \left(1 - \frac{36434.0 \times\ 22901.1}{174610.5 \times 37934.7}\right) = 87.4\%$$

$$Selectivity = 100 \times \frac{1139.3}{1139.3 + 2 \times (21.9)} = 96.3\%$$

$$Yield = \frac{87.4\ \times 96.3}{100} = 84.2\%$$

$$TON = \frac{84.2\ \times \frac{1.578\, mmol}{0.0004734\, mmol}}{100} = 2807$$

5.2. CM of 20 with acrylonitrile (Table 1 in main text)



20 **21** **22**

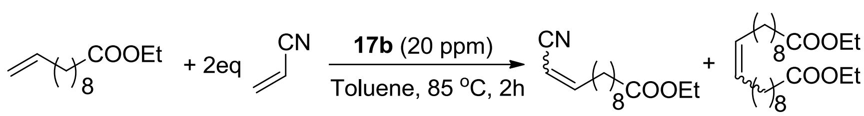
Reactions with 300 ppm of (pre)catalysts:

To a solution of **20** (0.355 g, 1.58 mmol, 1 equiv), acrylonitrile (0.207 mL, 3.16 mmol, 2 equiv) and methyl stearate (ca. 10 mg, internal standard) in toluene (15.5 mL, C_{16}^{0}=0.1 M) at 70 °C under argon atmosphere of argon (pre)catalyst **16a/b-19a/b** was added in 4 portions (75 ppm in 50 µL of toluene) every 5 min (300 ppm in 200 µL toluene total). The mixture was stirred for 2h at 70 °C under argon atmosphere. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and was analyzed by GC.

Reactions with 25 ppm of (pre)catalysts:

To a solution of **20** (1.606 g, 7.56 mmol, 1 equiv), acrylonitrile (0.495 mL, 7.56 mmol, 1 equiv) and methyl stearate (ca. 40 mg, internal standard) in toluene (30 mL, C_{20}^{0}=0.25 M) at 70 °C under argon atmosphere of argon (pre)catalyst **3b**, **16b** or **17b** (25 ppm in 1 mL) and acrylonitrile (0.495 mL, 7.56 mmol, 1 equiv) were added dropwise over 1 hour. The mixture was stirred for additional 1h at 70 °C under argon atmosphere. From the beginning of the reaction argon was bubbled through the reaction mixture to actively remove ethylene. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and analyzed by GC.

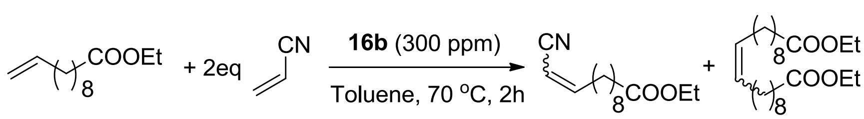
Reaction with 20 ppm of (pre)catalyst 11b:



To a solution of **20** (1.606 g, 7.56 mmol, 1 equiv), acrylonitrile (0.495 mL, 7.56 mmol, 1 equiv) and methyl stearate (ca. 40 mg, internal standard) in toluene (30 mL, C_{20}^{0}=0.25 M) at 85 °C under argon atmosphere of argon (pre)catalyst **17b** (25 ppm in 1 mL) and acrylonitrile (0.495 mL, 7.56 mmol, 1 equiv) were added dropwise over 1 hour. The mixture was stirred for additional 1h at 85 °C under argon atmosphere. From the beginning of the reaction argon was bubbled through the reaction mixture to actively remove ethylene. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and analyzed by GC.

5.3. Optimization of CM of 20 with acrylonitrile

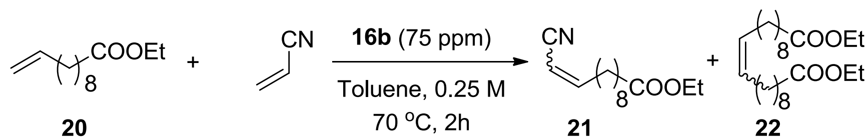
Concentration effect



To a solution of **20** (0.335 g, 1.58 mmol, 1 equiv), acrylonitrile (0.207 mL; 3.16 mmol; 2 equiv) and methyl stearate (ca. 10 mg, internal standard) in a suitable amount of toluene at 70 °C under argon atmosphere (pre)catalyst **16b** (300 ppm) in toluene (50 µL) was added in one portion. The mixture was stirred for 2h at 70 °C under argon atmosphere. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and was analyzed by GC .

C^{0}_{20} [M]	Conversion [%]	**21** [%]	**22** [%]	Selectivity to **21** [%]	TON_{21}
0.1	86	83	3	97	2770
0.25	95	92	3	97	3070
1	87	82	5	94	2730

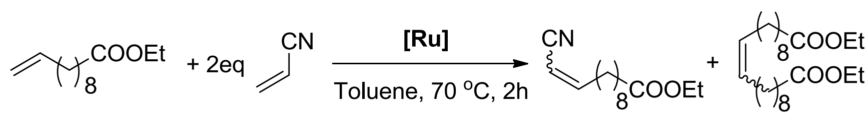
Acrylonitrile equivalents



To a solution of **20** (0.335 g, 1.58 mmol, 1 equiv), acrylonitrile (1,1 or 2 or 4 equiv) and methyl stearate (ca. 10 mg, internal standard) in toluene (C^0_{20}=0.25 M)at 70 °C under argon atmosphere (pre)catalyst **16b** (75 ppm) in toluene (50 µL) was added in one portion. The mixture was stirred for 2h at 70 °C under argon atmosphere. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and was analyzed by GC .

Equivalents of acrylonitrile	Conversion [%]	**21** [%]	**22** [%]	Selectivity to **21** [%]	TON_{21}
1.1	87	81	6	93	10800
2	84	80	4	95	10670
4	75	72	3	97	9600

Different mode of addition of catalyst and different concentration

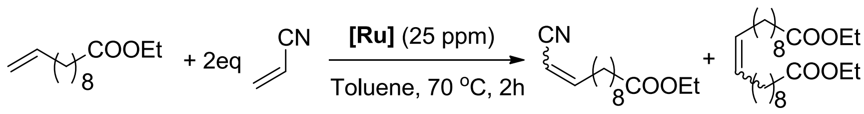


To a solution of **20** (1.606 g, 7.56 mmol, 1 equiv), acrylonitrile (0.991 mL; 15.13 mmol; 2 equiv) and methyl stearate (ca.50 mg, internal standard) in a suitable amount of toluene (C^0_{20}=0.1 or 0.25 M) at 70 °C under argon atmosphere (pre)catalyst **16b** or **17b** in toluene was added. For a reactions were 150 ppm of (pre)catalyst s was used, (pre)catalyst was added in 4 portions (1 portion, 37,5 ppm each 5 min). For a reactions were 75 ppm of (pre)catalyst was used catalyst was added dropwise during 1h via syringe. For a reaction were 25 ppm of **16b** was used, catalyst was added via syringe pump over 1h, additionally in this case, argon was bubbled through reaction mixture. The mixture was stirred at 70 °C under argon atmosphere (total reaction time 2h). Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and was analyzed by GC.

(Pre)catalyst (loading ppm)	C^0_{20} [M]	Conversion [%]	**21** [%]	**22** [%]	Selectivity to **21** [%]	TON_{21}
16b (150)	0.1	88	85	3	97	5670
16b (150)	0.25	93	90	3	97	6000
16b (75)	0.1	82	78	4	95	10400
16b (75)	0.25	84	80	4	95	10670
17b (75)	0.25	86	81	5	94	10800
16b (25)[a]	0.25	48	43	5	90	17200

[a]Argon was bubbled through reaction mixture.

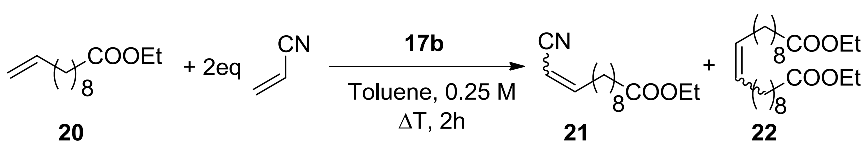
Slow addition of catalyst and acrylonitrile



To a solution of **20** (1.606 g, 7.56 mmol, 1 equiv), acrylonitrile (0.495 mL; 7.56 mmol; 1 equiv) and methyl stearate (ca.50 mg, internal standard) in toluene (23.8 mL) at 70 °C under argon atmosphere (pre)catalyst **16b** or **17b** (25 ppm) in toluene (3 mL) and acrylonitrile (0.495 mL, 7.56 mmol, 1 equiv) in toluene (3 mL) were added via syringe pump during 1h. The mixture was stirred at 70 °C under argon atmosphere (total reaction time 2h), during the course of the reaction argon was bubbled through reaction mixture. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and was analyzed by GC

(Pre)catalyst (loading ppm)	$C^{0}_{\mathbf{20}}$ [M]	Conversion [%]	**21** [%]	**22** [%]	Selectivity to **21** [%]	TON_{21}
16b (25)	0.25	63	56	7	89	22400
17b (25)	0.25	73	62	11	84	24800

Temperature effect

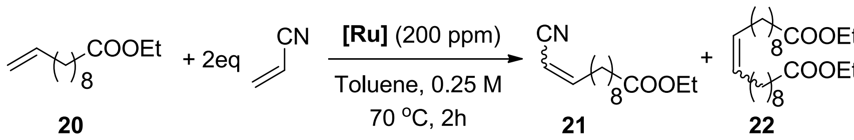


To a solution of **20** (1.606 g, 7.56 mmol, 1 equiv), acrylonitrile (0.495 mL; 7.56 mmol; 1 equiv) and methyl stearate (ca.50 mg, internal standard) in toluene (23.8 mL) at suitable temperature under argon atmosphere (pre)catalyst **17b** (50 or 20 ppm) in toluene (3 mL) and acrylonitrile (0.495 mL, 7.56 mmol, 1 equiv) in toluene (3 mL) were added via syringe pump during 1h. The mixture was stirred at suitable temperature under argon atmosphere (total reaction time 2h). In case where 20 ppm of **17b** was used argon was bubbled through reaction mixture during the course of the reaction. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and was analyzed by GC

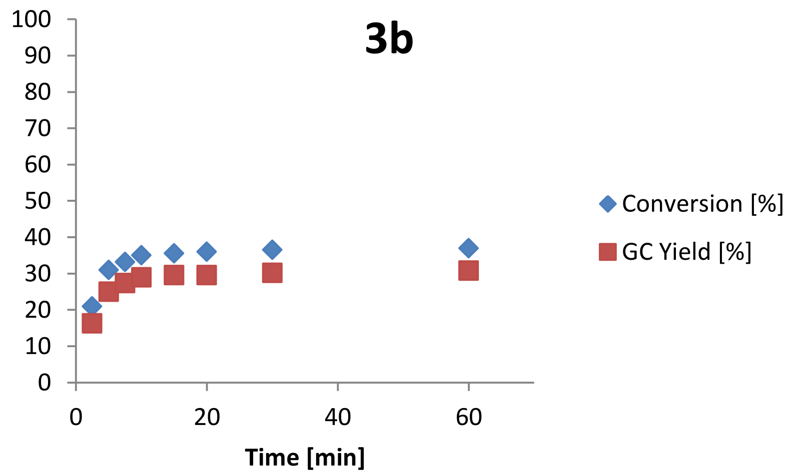
(Pre)catalyst (loading ppm)	Temperature [°C]	Conversion [%]	**21** [%]	**22** [%]	Selectivity to **21** [%]	TON_{21}
17b (50)	70	69	60	9	87	12000
17b (50)	85	79	69	10	88	13800
17b (50)	100	3	2	1	60	400
17b (20)[a]	85	71	57	14	80	28500

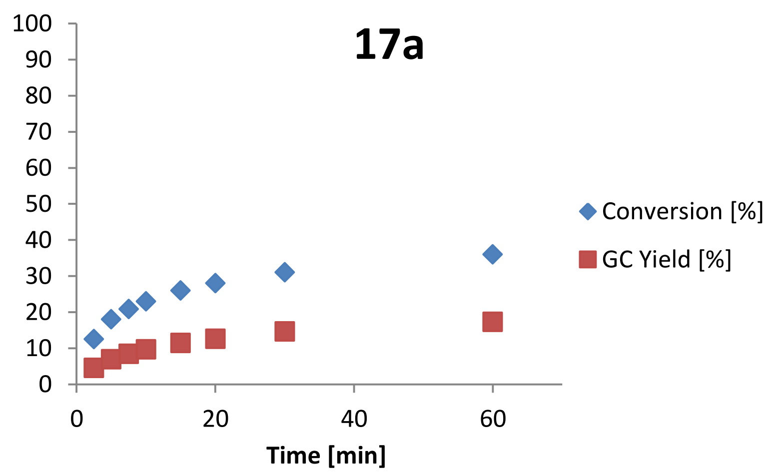
[a]Argon was bubbled through reaction mixture.

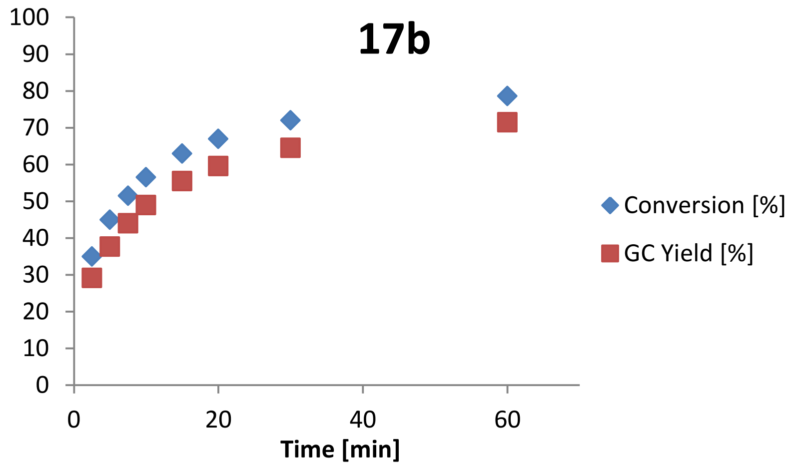
5.4. Reaction profiles for CM of 20 with acrylonitrile



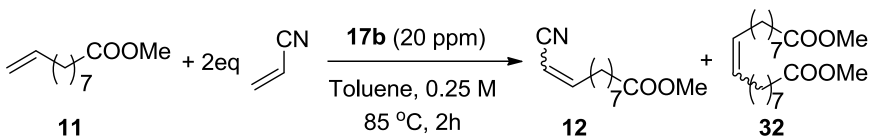
To a solution of **20** (0.355 g, 1.58 mmol, 1 equiv), acrylonitrile (0.207 mL, 3.16 mmol, 2 equiv) and methyl stearate (ca. 10 mg, internal standard) in toluene (5.8 mL, C_{16}^{0}=0.25 M) at 70 °C under argon atmosphere of argon (pre)catalyst **3b**, or **17a** or **17b** (200 ppm in 50 μL of toluene) was added in one portion. The mixture was stirred for 2h at 70 °C under argon atmosphere. Samples of the reaction mixture were taken in appropriate time intervals. The samples were quenched by addition of ethyl vinyl ether (3 drops) and were analyzed by GC.







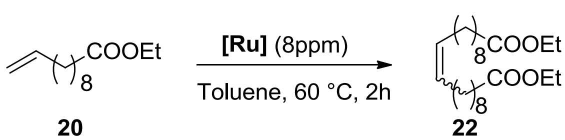
5.5. CM of 11 with acrylonitrile



To a solution of **11** (3.46 g, 18.78 mmol, 1 equiv), acrylonitrile (1.23 mL; 18.78 mmol; 1 equiv) and methyl stearate (ca. 100 mg, internal standard) in toluene (69 mL) at 85 °C under argon atmosphere (pre)catalyst **17b** (20 ppm) in toluene (3 mL) and acrylonitrile (1.23 mL, 18.78 mmol, 1 equiv) in toluene (3 mL) were added via syringe pump during 1h. The mixture was stirred at 85 °C under argon atmosphere (total reaction time 2h). Argon was bubbled through reaction mixture during the course of the reaction. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and analyzed by GC.

Conversion [%]	**12** [%]	**32** [%]	Selectivity to **12** [%]	TON_{12}
71	60	11	84	30000

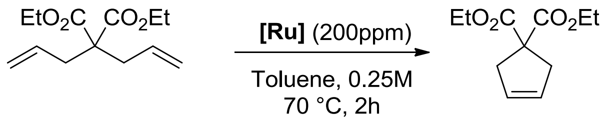
5.6. Dimerization of 20 to 22



To a **20** (3.0 g, 14.13 mmol) and methyl stearate (ca. 100 mg, internal standard) at 60 °C under argon atmosphere (pre)catalyst **17a/b** was added in portions (2+2+1+1+1+1 ppm; 8 ppm total; 15 min between portions). The mixture was stirred for 2h (total time))at 60 °C under argon atmosphere. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and analyzed by GC.

[Ru]	Conversion [%]	**22** [%]	Selectivity to **22** [%]	TON_{22}
17a	82	77	94	48125
17b	75	67	89	41875

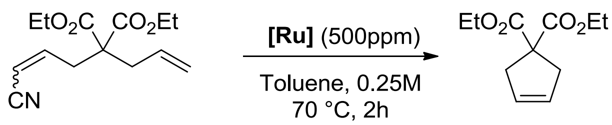
5.7. RCM of DEDAM (23) in the presence of additives



23 **24**

To a solution of **23** (0.410 g, 1.71 mmol, 1 equiv) in toluene (6 mL, C^0_{23}=0.25 M) at 70 °C under argon atmosphere acrylonitrile (0.174 mL, 3.41 mmol, 2 equiv) or acetonitrile (0.178 mL, 3.41 mmol, 2equiv) or DMSO (0.127 mL, 3.41 mmol, 2 equiv) were added optionally followed by addition of (pre)catalyst **3b**, **17a** or **17b** (200 ppm in 0.1 mL of toluene). The mixture was stirred for 2h at 70 °C under argon atmosphere. Samples of the reaction mixture (taken after 5 min and 2h) were quenched by addition of ethyl vinyl ether (3 drops) and were analyzed by GC.

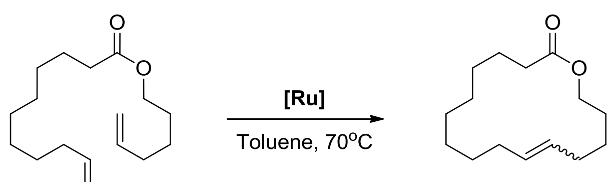
5.8. RCM of 25



25 **24**

To a solution of **25** (0.262 g, 0.988 mmol) in toluene (3.6 mL, C^0_{25}=0.25 M) at 70 °C under argon atmosphere (pre)catalyst **3b**, **17a** or **17b** (500 ppm in 0.1 mL of toluene) was added in one portion. The mixture was stirred for 2h at 70 °C under argon atmosphere. Sample of the reaction mixture was quenched by addition of ethyl vinyl ether (3 drops) and analyzed by GC.

5.9. Macrocyclization of 10



10 **27**

To a solution of **10** (0.184 g, 0.691 mmol) in toluene (138 mL, C^0_{10}=0.005 M or 69 mL, C^0_{10}=0.010 M or 34.5 mL, C^0_{10}=0.020 M) at 70 °C under argon atmosphere 30 ppm or 15 ppm or 10 ppm of (pre)catalyst in toluene (50 µL) was added in one portion. The mixture was stirred for additional 20 min at 70 °C under argon atmosphere. Reaction mixture was intensively purged with argon during the course of the reaction (efficient condensers were installed on reaction vessel to avoid evaporation of toluene). Sample of the reaction mixture (1.5 mL) was quenched by addition of SnatchCat (4.4 eq in relation to catalyst) and analyzed by GC (external standard was used for calculations). The identity of product was confirmed by comparison of retention time with sample previously authenticated by NMR.[13]

5.10. Analytical data of metathesis reaction products

Ethyl 11-cyano-10-undecenoate (21):

Isomer *Z*: ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 6.46 (dt, *J* = 10.9; 7.7 Hz, 1H), 5.29 (dt, *J* = 10.9; 1.4 Hz, 1H), 4.10 (q, *J* = 7.1 Hz, 2H), 2.40 (qd, *J* = 7.6; 1.4 Hz, 2H), 2.26 (t, *J* = 7.5 Hz, 2H), 1.64-1.54 (m, 2H), 1.49-1.38 (m, 2H), 1.35-1.25 (m, 8H), 1.23 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ = 173.8, 156.0 (*E*), 155.1 (*Z*), 117.5 (*E*), 116.0 (*Z*), 99.6 (*E*), 99.4 (*Z*), 60.1 (2C, *E*+*Z*), 34.3 (*Z*), 34.2 (*E*), 33.2 (*E*), 31.8 (*Z*), 29.0 (6C, *E*+*Z*), 28.9 (*Z*), 28.8 (*E*), 28.1 (*Z*), 27.5 (*E*), 24.9 (*Z*), 24.8 (*E*), 14.2

HRMS-ESI (*m/z*): Calcd for $C_{14}H_{23}NO_2Na$ $[M+Na]^+$: 260.1626; found: 260.1623 .

Anal. Calcd for $C_{14}H_{23}NO_2$: C 70.85; H 9.77; N 5.90; found: C 70.89; H 9.84; N 5.92.

Diethyl 10-eicosene-1,20-dioate (22):

^{1}H NMR ($CDCl_3$, 600 MHz): δ = 5.41-5.30 (m, 2H), 4.12 (q, *J* = 7.1 Hz, 4H), 2.28 (t, *J* = 7.6 Hz, 4H), 2.02-1.90 (m, 4H), 1.64-1.56 (m, 4H), 1.35-1.21 (m, 26H).

^{13}C NMR ($CDCl_3$, 150 MHz): δ = 173.8, 130.3, 60.1, 34.4, 32.5, 29.6, 29.3, 29.2, 29.1, 29.0, 24.9, 14.2.

HRMS-EI (*m/z*): Calcd for $C_{24}H_{44}O_4$ $[M^{\cdot}]^+$: 396.3240; found: 396.3248.

Anal. Calcd for $C_{24}H_{44}O_4$: C 72.68; H 11.18; found: C 72.58; H 11.10.

Methyl 10-cyano-9-decenoate (12) :

Z isomer: ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 6.46 (dt, *J* = 10.9; 7.7 Hz, 1H), 5.29 (dt, *J* = 10.9; 1.3 Hz, 1H), 3.65 (s, 3H), 2.40 (dq, *J* = 7.6; 1.3 Hz, 2H), 2.29 (t, *J* = 7.5 Hz, 2H), 1.64-1.54 (m, 2H), 1.50-1.39 (m, 2H), 1.36-1.26 (m, 6H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ = 174.12 (*Z*), 174.08 (*E*), 156.0 (*E*), 155.0 (*Z*), 117.5 (*E*), 116.0 (*Z*), 99.6 (*E*), 99.5 (*Z*), 51.39 (*E*), 51.37 (*Z*), 33.95 (*Z*), 33.92 (*E*), 33.2 (*E*) 31.7 (*Z*), 28.87 (*Z*), 28.85 (*E*), 28.83 (*Z*+*E*), 28.72 (*Z*), 28.68 (*E*), 28.1 (*Z*), 27.5 (*E*), 24.77 (*Z*), 24.75 (*E*).

Anal. Calcd for $C_{12}H_{19}NO_2$: C 68.87; H 9.15; N 6.69; found: C 68.95; H 9.29; N 6.56.

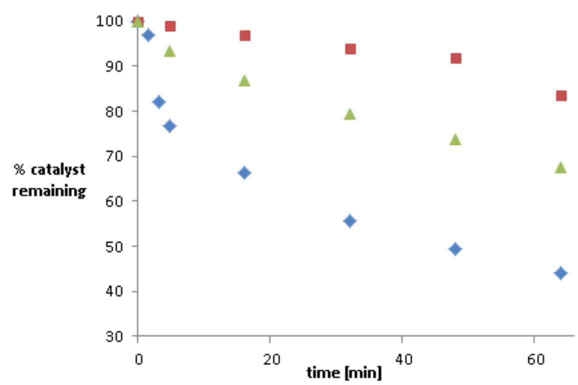
Dimethyl 9-octadecene-1,18-dioate (32):

^{1}H NMR ($CDCl_3$, 500 MHz): δ = 5.36 (ddd, *J* = 5.3; 3.7; 1.6 Hz, 2H, *E*), 5.32 (ddd, *J* = 5.7; 4.3; 1.1 Hz, 2H, *Z*), 3.65 (s, 6H), 2.29 (t, *J* = 7.5 Hz, 4H), 2.03-1.90 (m, 4H), 1.68-1.56 (m, 4H), 1.35-1.23 (m, 16H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ = 174.25 (*E*), 174.24 (*Z*), 130.3 (*E*), 129.8 (*Z*), 51.4, 34.1, 32.5, 29.6 (*Z*), 29.5 (*E*), 29.12 (*Z*), 29.08 (*E*), 29.07 (*E*), 29.05 (*Z*), 28.9, 27.1(*Z*), 24.9 (*E*).

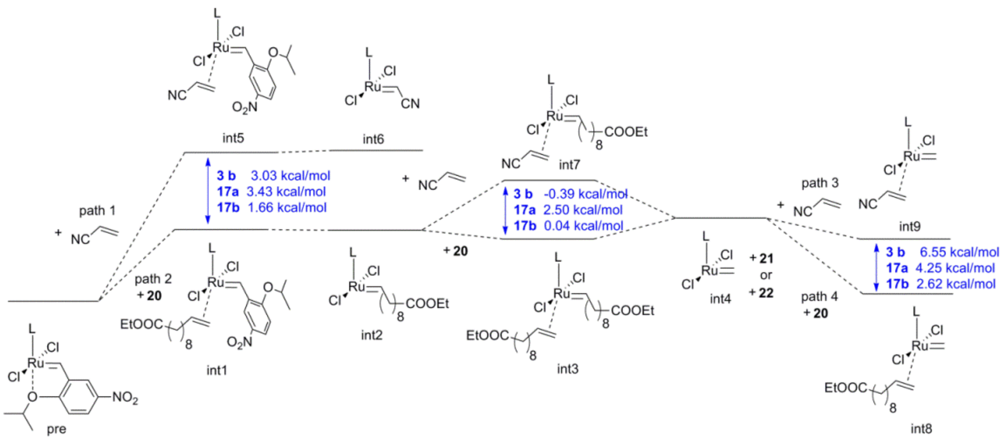
6. NMR study of reaction between 3b, 17a, 17b and acrylonitrile

Solution of dimethyl carbonate (internal standard, 0.9 mg) in toluene-d_8 (0.1 mL) was added under nitrogen to the solution of complex **3b**/**17a**/**17b** (0.02 mmol) in toluene-d_8 (0.6 mL, final $C_{[Ru]}$ 0.025 M). Mixture was transferred to the NMR tube which was placed in the spectrometer at 50°C. ^{1}H NMR spectra was recorded (time=0). NMR tube was removed from spectrometer, acrylonitrile (4.31 mg, 0,08 mmol, 4 equiv) in toluene-d_8 (0.1 mL) was added and NMR tube was immediately placed in spectrometer at 50°C The ^{1}H NMR spectra was recorded after each 1.5 min over a time period of about 65 min. Disappearance of (pre)catalysts was calculated basing on integrations of characteristic proton of **3b** (s, 16.31 ppm)/**17a** (sept, 4.62 ppm)/**17b** (sept, 4.47 ppm) and dimethyl carbonate (s, 3.38 ppm). Stability of complexes is shown on Figure below (■ - **17a**; ▲ - **3b**; ◆ - **17b**).



7. DFT results for CM of ethyl 10-undecenoate (20)with acrylonitrile

To further explore the CM reaction of ethyl 10-undecenoate with acrylonitrile using DFT computational approach we additionally considered other events occurring later in the catalytic cycle. Upon formation of methylidene intermediate (int4) the catalytic cycle can follow either path 3 (similar to path 1) started with the association of acrylonitrile or path 4 (similar to path 2) commenced with the association of 10-undecenoate (see Scheme S1). Our calculations suggest that for all computationally studied systems (**3b**, **17a** and **17b**) path 4 is the most likely option. In the case of **3b** the Gibbs free energy difference of 6.55 kcal/mol in favour of path 4 implies that path 3 has absolutely no practical meaning. The Gibbs free energy difference for **17a** is lower (4.25 kcal/mol), but still large enough to almost completely favour path 4. On the other hand the 2.62 kcal/mol Gibbs free energy difference found for **17b** indicates that path 3 is more likely than in the case of **17a** and **3b**, yet still less important than path 4. It is also worth noting that during the entire catalytic cycle the boomerang mechanism is also a viable possibility,[14] so the final ratio of CM products **21** and **22** depends on the relative likelihood of formation of int1 vs int5, int3 versus int7 and int8 versus int9 as well as regeneration of (pre)catalyst. Nevertheless the results obtained in the DFT part of this investigation are in good agreement with the experimental findings.



Scheme S1. Schematic representation of essential intermediates in the CM of ethyl 10-undecenoate (**20**) with acrylonitrile.

Computational details

In this study we used density functional theory (DFT) calculations to study the structures of investigated complexes and intermediates in the metathesis catalytic cycle. The calculations have been performed using a computational protocol similar to our previous studies.[15] We have used an all-atom model for all studied catalysts and olefins apart from ethyl 10-undecenoate, which was modelled as 1-pentene. Starting models for precatalyst **17a** and **17b** were prepared on the basis of crystal structures of **16a** and **16b** described in this study, while the starting model of **3b** was prepared on the basis of crystal structures of the well-known nitro Grela catalyst.[3] All structures were modelled using the M06-D3 density functional with the 6-31G** basis set for all atoms except the Ru atom, which was described by the Los Alamos angular momentum projected effective core potential (ECP) using the double-ζ contraction of valence functions (denoted as LACVP**). We have chosen M06 functional, since it was also shown to perform particularly well for ruthenium-based catalysts, giving accurate energies for a number of Grubbs and Hoveyda systems.[16] Since the M06 functional has already medium-range dispersion implemented, M06-D3 may overestimate the effect of dispersion due to double-counting of these effects.[17] On the other hand the addition of D3 correction to M06 was shown to improve the results for many organic reactions when calculating the differences in relative energies.[18] We have used the standard energy convergence criterion of $5 \cdot 10^{-5}$ Hartree. For each structure frequencies were calculated to verify the nature of each stationary point. Energies discussed in this work for stationary points are Gibbs free energies, calculated as the sum of electronic energies, zero-point energy corrections, internal energies, pV and the negative product of temperature and entropy (all at 343.15 K). All quantum chemical calculations have been performed in Jaguar v. 8.7 software (Schrodinger, Inc., New York, NY, 2015.).[19]

Table S3. Total energy values (E) and components of the Gibbs free energy values (G; as defined above) for all the stationary points / intermediates studied in this work.

complex	structure	SCF E	zero-point E correction (kcal/mol)	internal E (kcal/mol)	entropy (cal/mol)	G (Hartrees)
3b	pre	-2842.347410	498.412	39.289	300.679	-2841.653868
	int1	-3038.731231	585.074	45.361	335.991	-3037.909218
	int2	-2331.835150	442.063	33.946	274.045	-2331.225356
	int3	-2528.238115	530.005	38.712	296.766	-2527.493004
	int4	-2213.968332	388.719	30.455	248.529	-2213.435155
	int5	-3013.054660	531.738	43.844	330.963	-3012.317310
	int6	-2306.157826	388.632	31.840	260.381	-2305.629063
	int7	-2502.570478	475.828	36.690	281.650	-2501.906550
	int8	-2410.381476	476.199	27.998	254.353	-2409.697894
	int9	-2384.701618	423.018	26.230	244.892	-2384.101108
17a	pre	-2438.286766	384.417	31.612	254.413	-2437.761820
	int1	-2634.663798	471.457	37.532	287.930	-2634.009037
	int2	-1927.777628	328.383	25.287	215.011	-1927.330510
	int3	-2124.175390	415.168	31.339	250.384	-2123.599671
	int4	-1809.910982	275.036	21.836	190.027	-1809.540715
	int5	-2608.988861	417.553	35.593	276.119	-2608.416635
	int6	-1902.099700	274.869	23.243	202.167	-1901.734103
	int7	-2098.503957	361.818	29.001	235.078	-2098.008610
	int8	-2006.312449	362.031	27.894	228.672	-2005.815024
	int9	-1980.636591	308.382	25.858	216.355	-1980.221171
17b	pre	-2629.874148	417.859	33.521	264.147	-2629.298189
	int1	-2826.250475	505.021	40.051	304.024	-2825.547015
	int2	-2119.363530	361.935	27.850	232.528	-2118.868439
	int3	-2315.760485	449.037	33.762	267.765	-2315.136434
	int4	-2001.496181	308.459	24.456	208.276	-2001.078454
	int5	-2800.580580	451.074	37.549	286.122	-2799.957287
	int6	-2093.685195	308.317	25.830	220.399	-2093.272134
	int7	-2290.090901	395.376	31.760	256.312	-2289.549292
	int8	-2197.901417	395.665	30.316	243.046	-2197.354394
	int9	-2172.226344	341.835	28.483	234.102	-2171.763135

8. References

[1] Gawin, R.; Kozakiewicz, A.; Guńka, P. A.; Dąbrowski, P.; Skowerski, K. *Angew. Chem. Int. Ed.* **2017**, *56*, 981-986.

[2] Courchay, F. C.; Sworen, J. C.; Coronado, A.; Wagener, K. B. *J. Mol. Catal. A-Chem.* **2006**, *254*, 111-117.

[3] Michrowska, A.; Bujok, R.; Harutyunyan, S.; Sashuk, V.; Dolgonos, G.; Grela, K. *J. Am. Chem. Soc*. **2004**, *126*, 9318-9325.

[4] a) Shaffer, E. A.; Chen, C.-L.; Beatty, A. M.; Valente, E. J.; Schanz, H.-J. *J. Organomet. Chem.* **2007**, *692*, 5221–5233; b) Harlow, K. J.; Hill, A. F.; Wilton-Ely, J. D. E. T. *J. Chem. Soc., Dalton Trans.* **1999**, 285-292; c) Fürstner, A.; Grabowski, J.; Lehmann, C. W. *J. Org. Chem.* **1999**, *64*, 8275-8280; d) Schanz, H.-J.; Jafarpour, L.; Stevens, E. D.; Nolan, S. P. *Organometallics*, **1999**, *18*, 5187-5190.

[5] Jazzar, R.; Dewhurst, R. D.; Bourg, J.-B.; Donnadieu, B.; Canac, Y.; Bertrand, G. *Angew. Chem. Int. Ed*. **2007**, *46*, 2899–2902; *Angew. Chem*. **2007**, *119*, 2957–2960.

[6] Bieniek, M.; Michrowska, A.; Gułajski, Ł.; Grela, K. *Organometallics*, **2007**, *26*, 1096-1099.

[7] Kadyrov, R. *Chem. Eur. J*. **2013**, *19*, 1002-1012.

[8] Grela, K.; Harutyunyan, S.; Michrowska, A. ; *Angew. Chem. Int. Ed*. **2002**, *41*, 4038–4040; *Angew. Chem.* **2002**, *114*, 4210-4212.

[9] Sheldrick, G. M. *Acta Crystallogr*. **2015,** C71, 3-8.

[10] CrysAlis Pro Software System ver. 171.38.43, Rigaku, Oxford Diffraction, **2015**.

[11] Spek, A. L. *Acta Cryst.* **2015**, C71, 9-19.

[12] a) Marx, V. M.; Sullivan, A. H.; Melaimi, M.; Virgil, S. C.; Keitz, B. K.; Weinberger, D. S.; Bertrand, G.; Grubbs, R. H. *Angew. Chem. Int. Ed.* **2015**, *54*, 1919-1923; b) Anderson, D. R.; Lavallo, V.; O'Leary, D. J.; Bertrand, G.; Grubbs, R. H. *Angew. Chem. Int. Ed.* **2007**, *46*, 7262-7265.

[13] Skowerski, K.; Kasprzycki, P.; Bieniek, M.; Olszewski, T. K. *Tetrahedron*, **2013**, *69*, 7408-7415.

[14] Bates, J. M.; Lummiss, J. A. M.; Bailey, G. A.; Fogg, D. E. *ACS Catal.* **2014**, *4*, 2387-2394.

[15] a) Trzaskowski, B.; Grela, K. *Catal. Commun.* **2016**, *86*, 133-138; b) Trzaskowski, B.; Ostrowska, K. *RSC Adv.* **2016**, *6*, 21423-21429; c) Pazio, A.; Woźniak, K.; Grela, K.; Trzaskowski, B. *Dalton Trans.* **2015**, *44*, 20021-20026; d) Pazio, A.; Woźniak, K.; Grela, K.; Trzaskowski, B. *Organometallics* **2015**, *34*, 563-570; e) Trzaskowski, B.; Grela, K. *Organometallics* **2013**, *32*, 3625-3630; f) Żukowska, K.; Szadkowska, A.; Trzaskowski, B.; Pazio, A.; Pączek, Ł.; Woźniak, K.; Grela, K. *Organometallics* **2013**, *32*, 2192-2198.

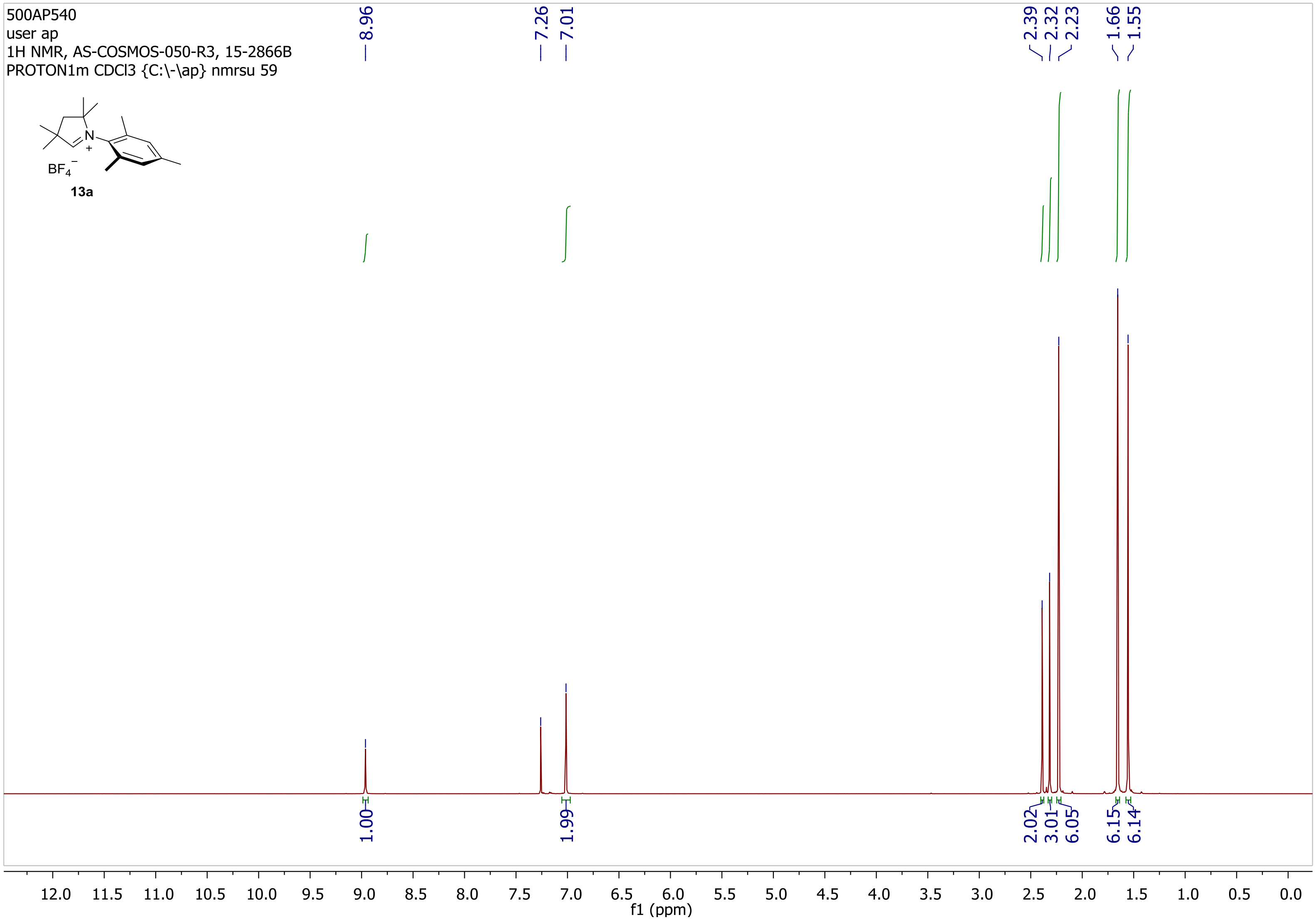
[16] a) Benitez, D.; Tkatchouk, E.; Goddard, W. A. *Chem. Commun.* **2008**, 6194-6196; b) Benitez, D.; Tkatchouk, E.; Goddard, W. A. *Organometallics* **2009**, *28*, 2643-2645; c) Minenkov, Y.; Occhipinti, G.; Jensen, V. R. *Organometallics* **2013**, *32*, 2099-2111.

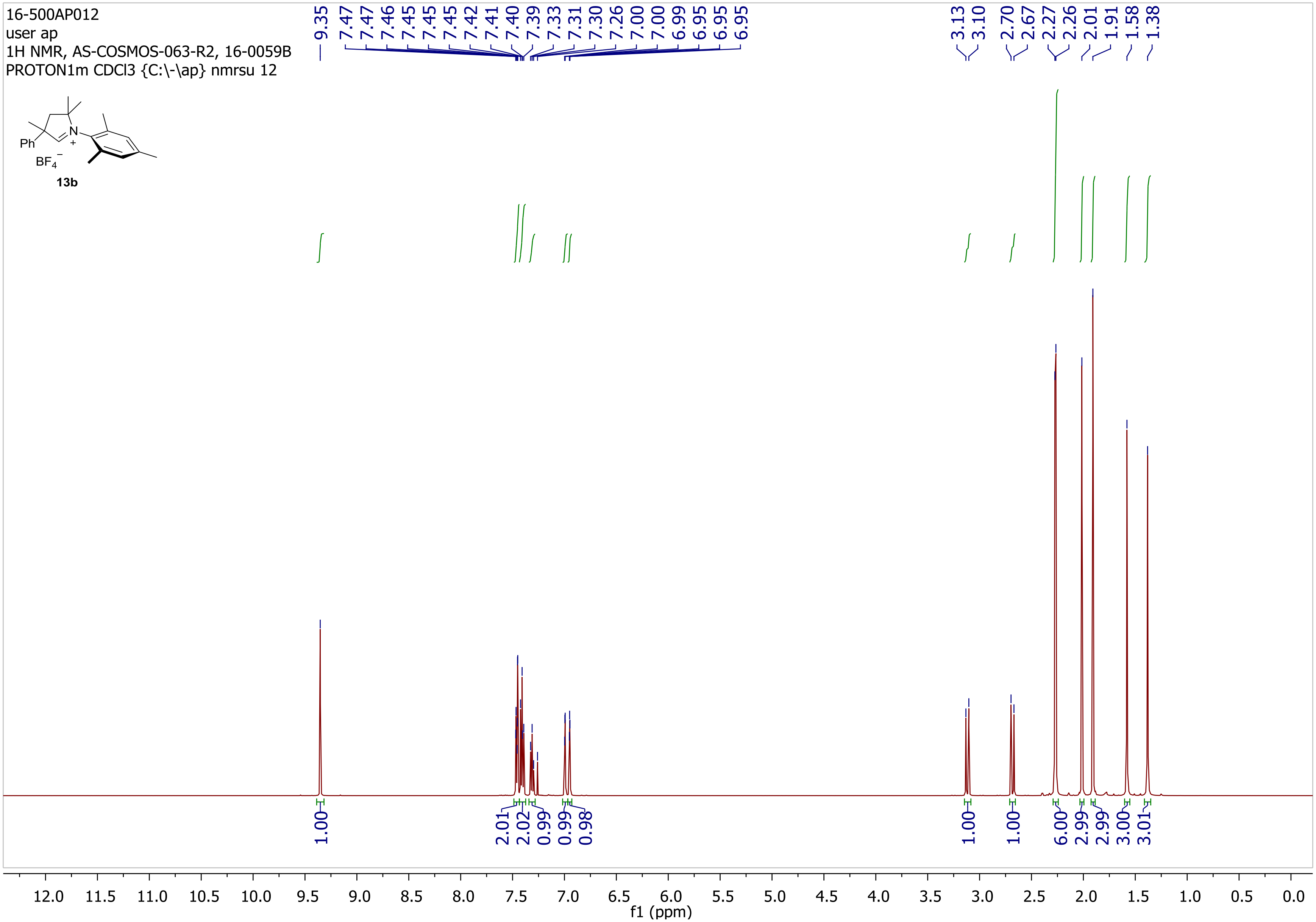
[17] Goerikg, L. *J. Phys. Chem. Lett.* **2015**, *6*, 3891-3896.

[18] Luo, S.; Zhao, Y.; Truhlar, D. G. *Phys. Chem. Chem. Phys*. **2011**, *13*, 13683-13689.

[19] Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A. *Int. J. Quantum Chem.* **2013**, *113*, 2110-2142.

9. NMR Spectra of salts 13, 29-31




16-500AP012
user ap
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PROTON1m CDCl3 {C:\-\ap} nmrsu 12
Ph
N
+
BF4−
13b
9.35
7.47
7.47
7.46
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7.39
7.33
7.31
7.30
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2.27
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2.01
1.91
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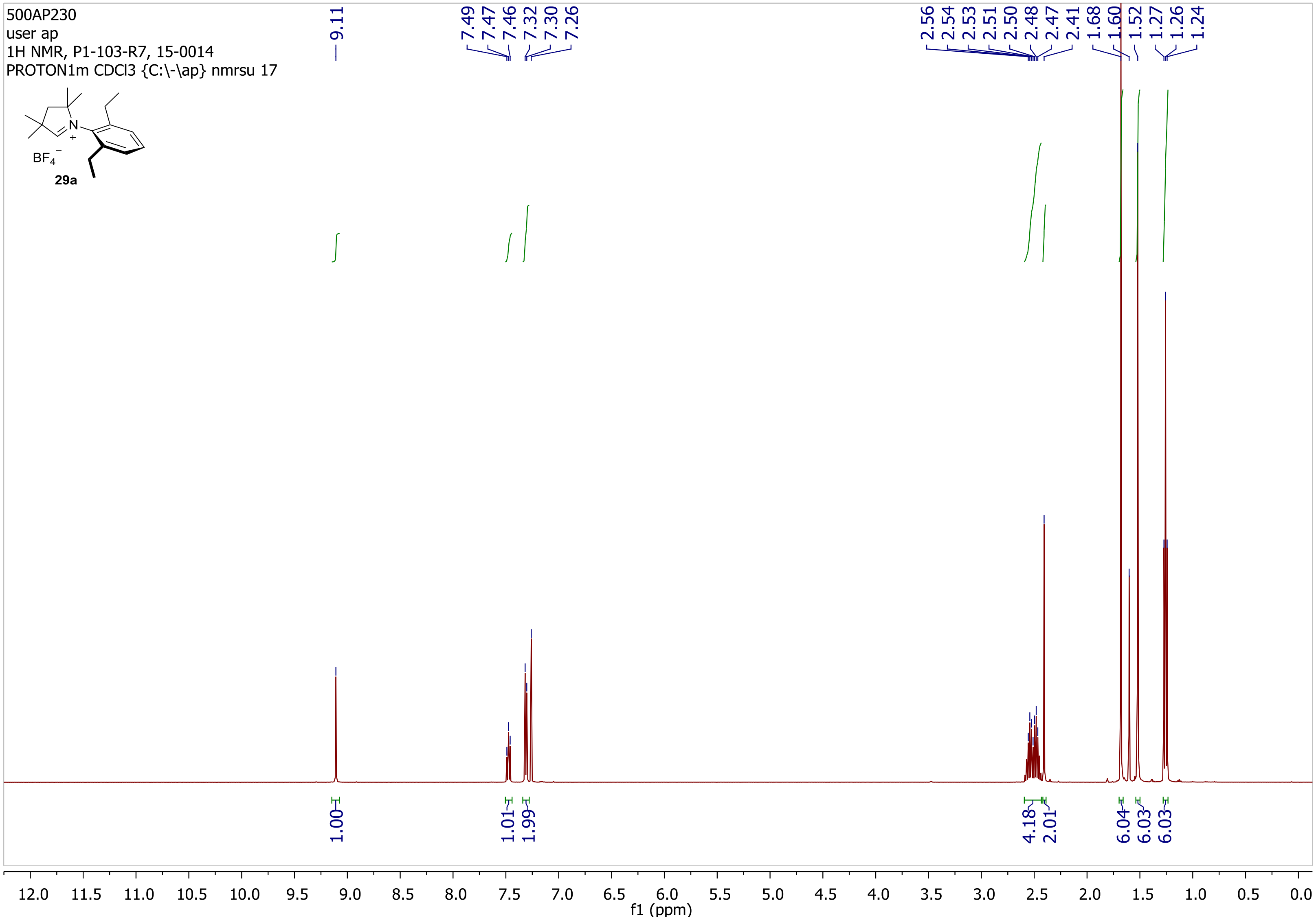
f1 (ppm)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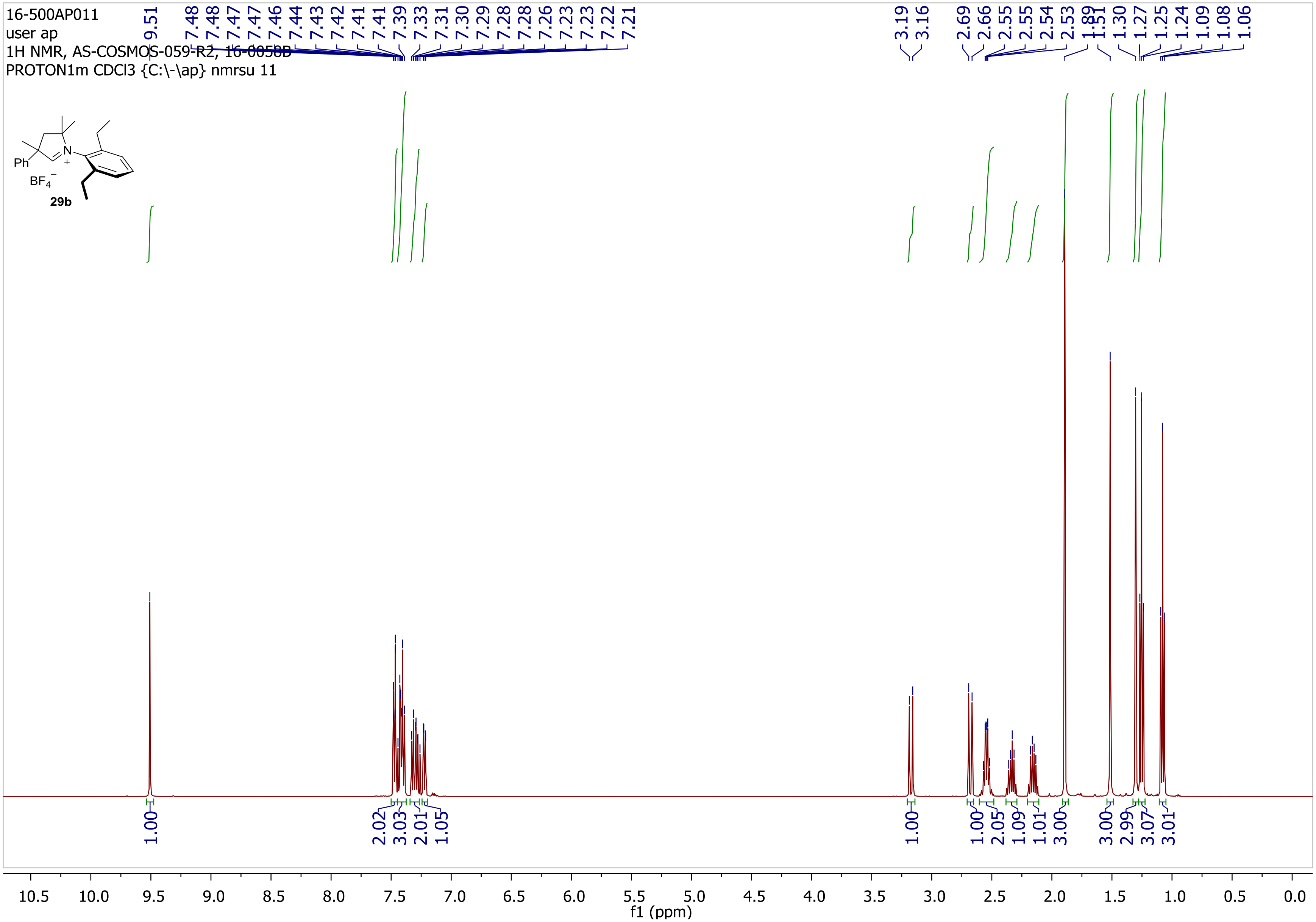
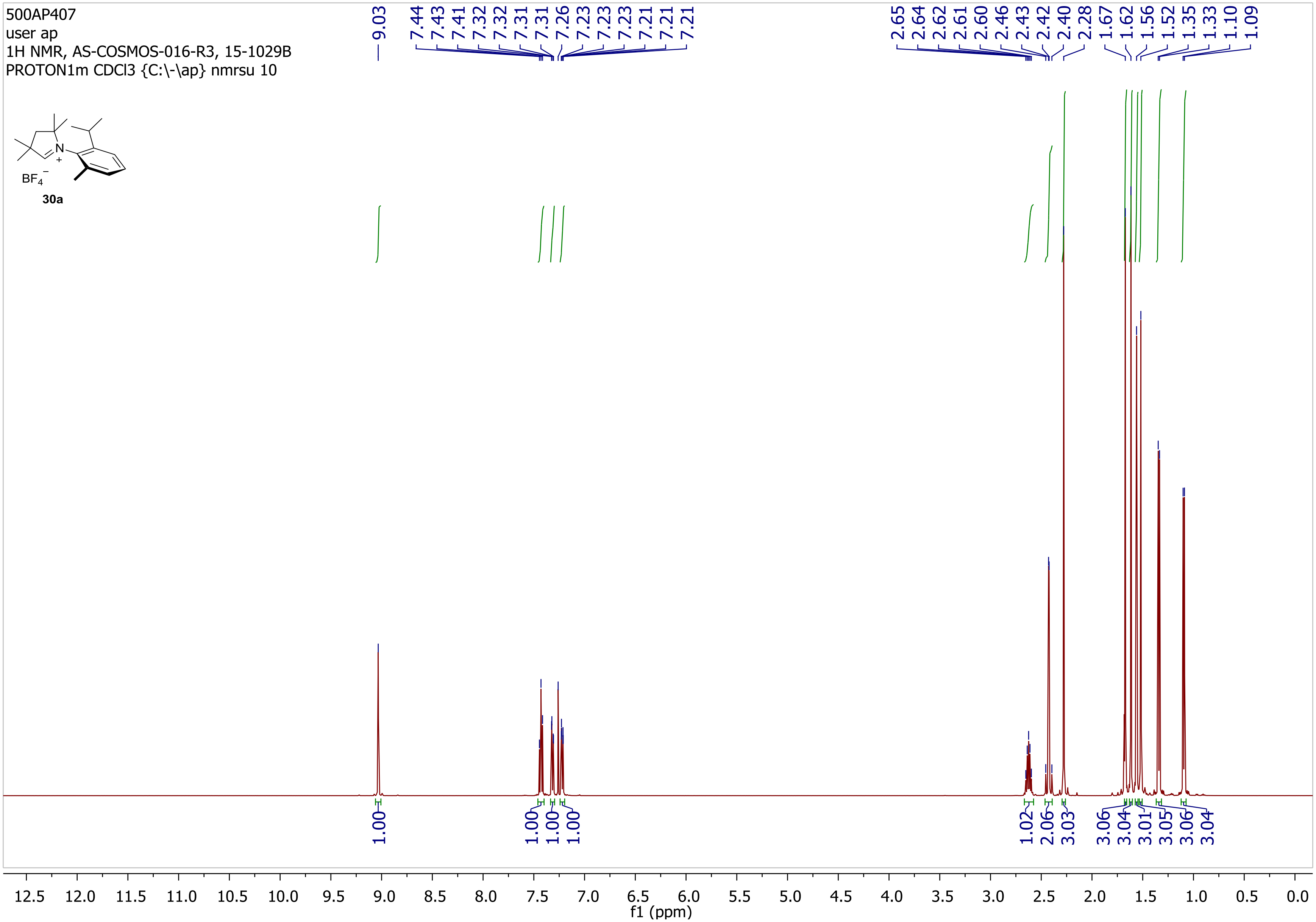
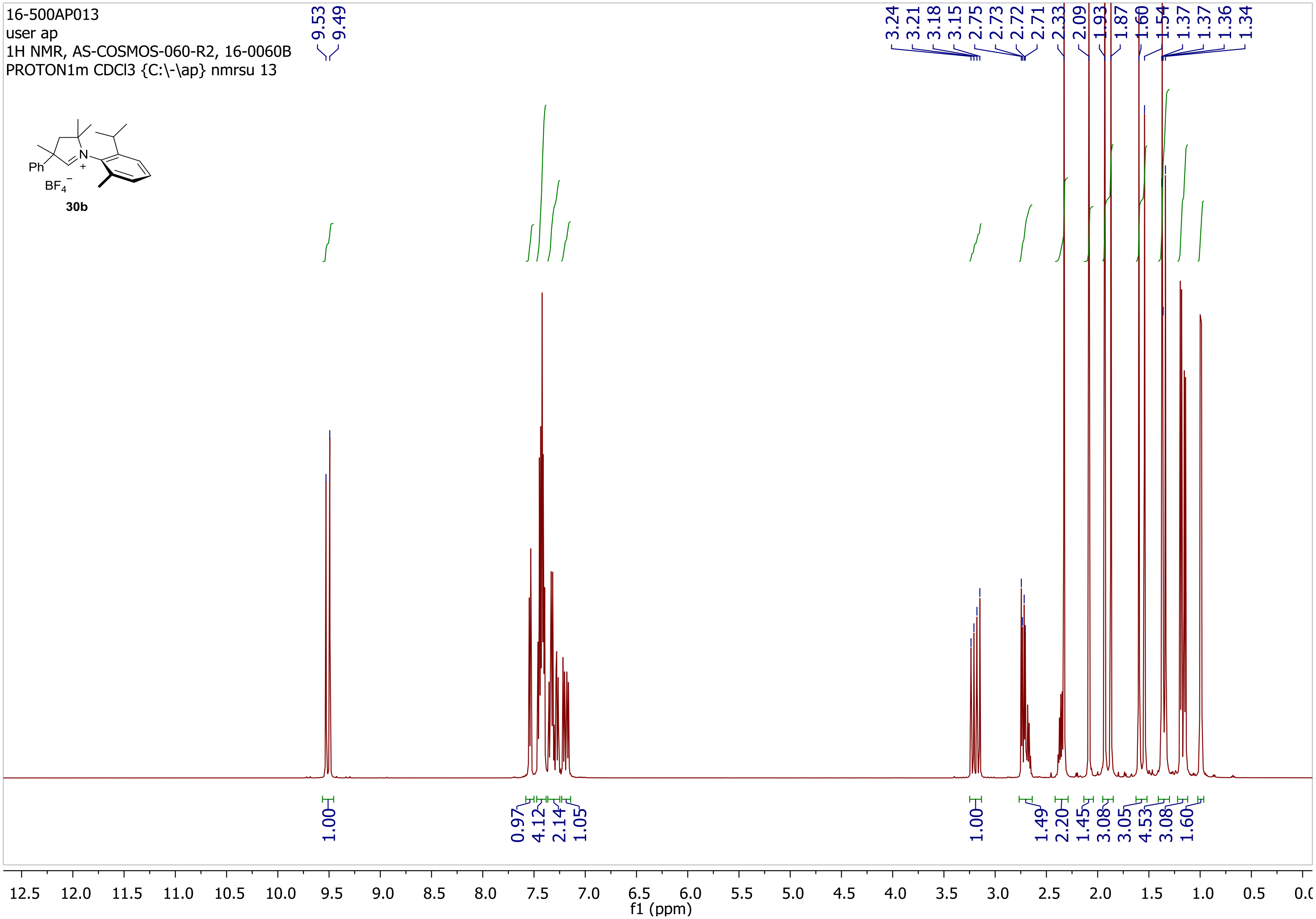
BF4−
29a
9.11
7.49
7.47
7.46
7.32
7.30
7.26
2.56
2.54
2.53
2.51
2.50
2.48
2.47
2.41
1.68
1.60
1.52
1.27
1.26
1.24
1.00
1.01
1.99
4.18
2.01
6.04
6.03
6.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

16-500AP011
user ap
1H NMR, AS-COSMOS-059-R2, 16-0050B
PROTON1m CDCl3 {C:\-\ap} nmrsu 11



29b


500AP407
user ap
1H NMR, AS-COSMOS-016-R3, 15-1029B
PROTON1m CDCl3 {C:\-\ap} nmrsu 10
9.03
7.44 7.43 7.41 7.32 7.32 7.31 7.31 7.26 7.23 7.23 7.23 7.21 7.21 7.21
2.65 2.64 2.62 2.61 2.60 2.46 2.43 2.42 2.40 2.28 1.67 1.62 1.56 1.52 1.35 1.33 1.10 1.09
BF4−
30a
1.00
1.00 1.00 1.00
1.02 2.06 3.03 3.06 3.04 3.01 3.05 3.06 3.04
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


16-500AP013
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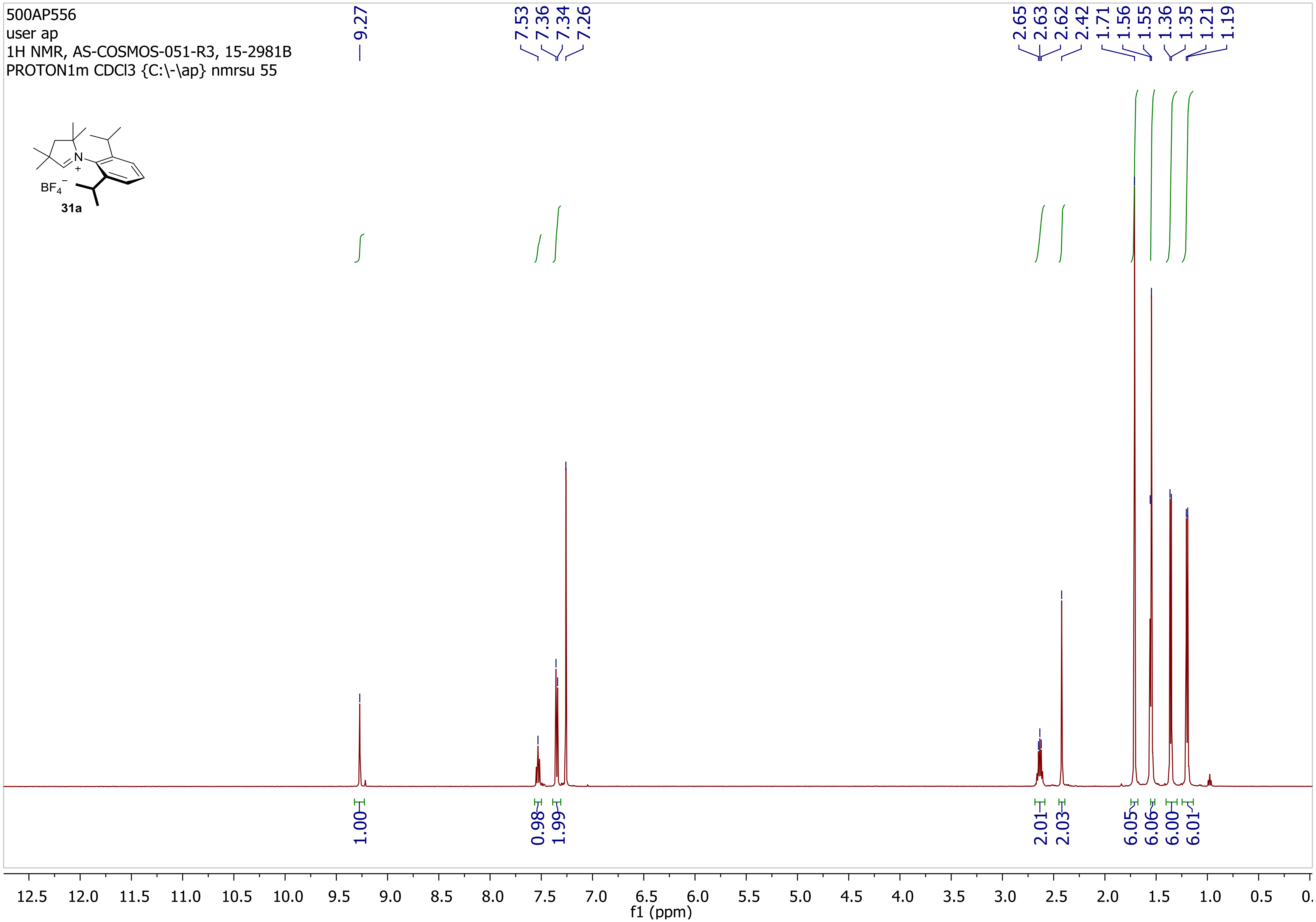
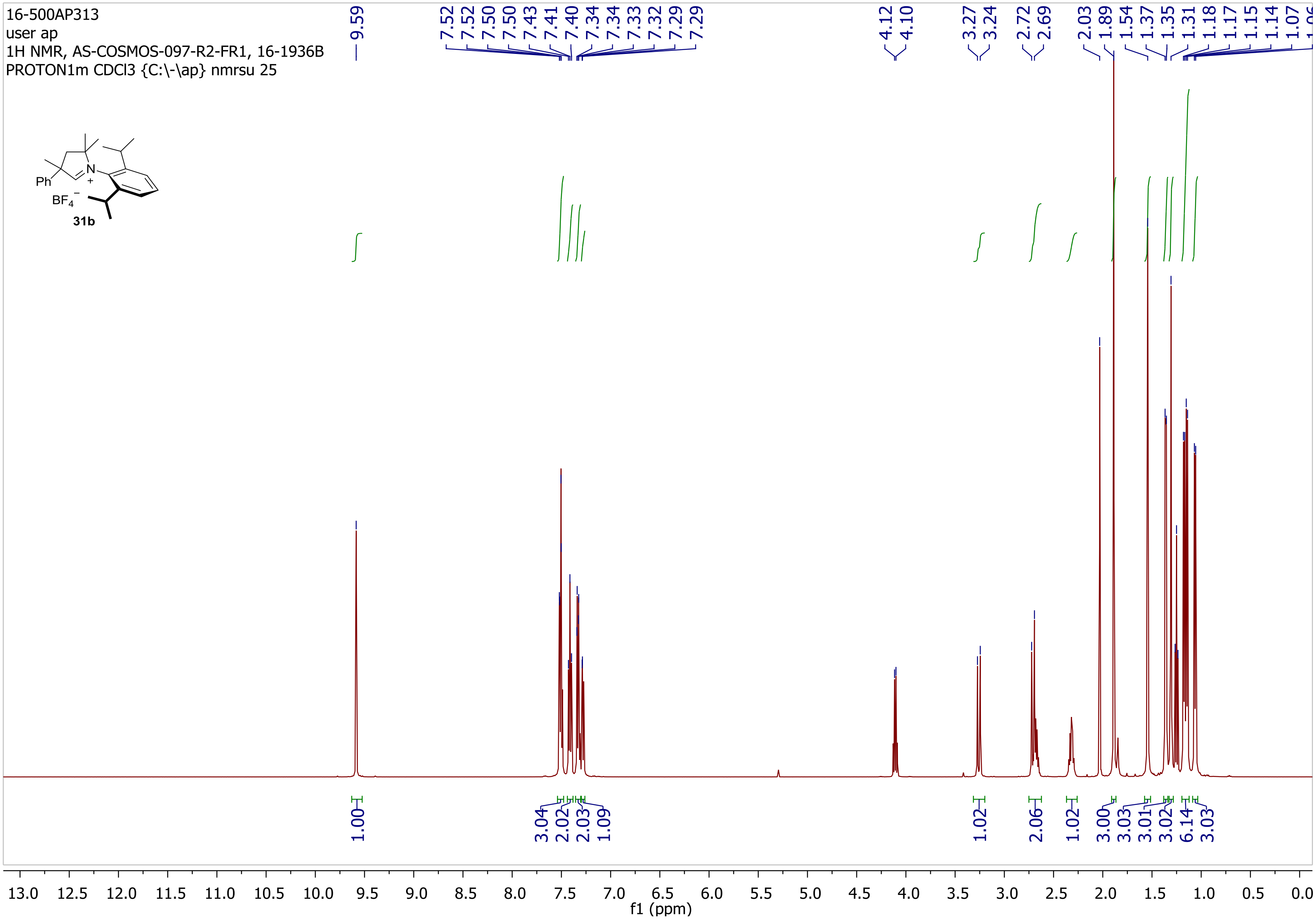
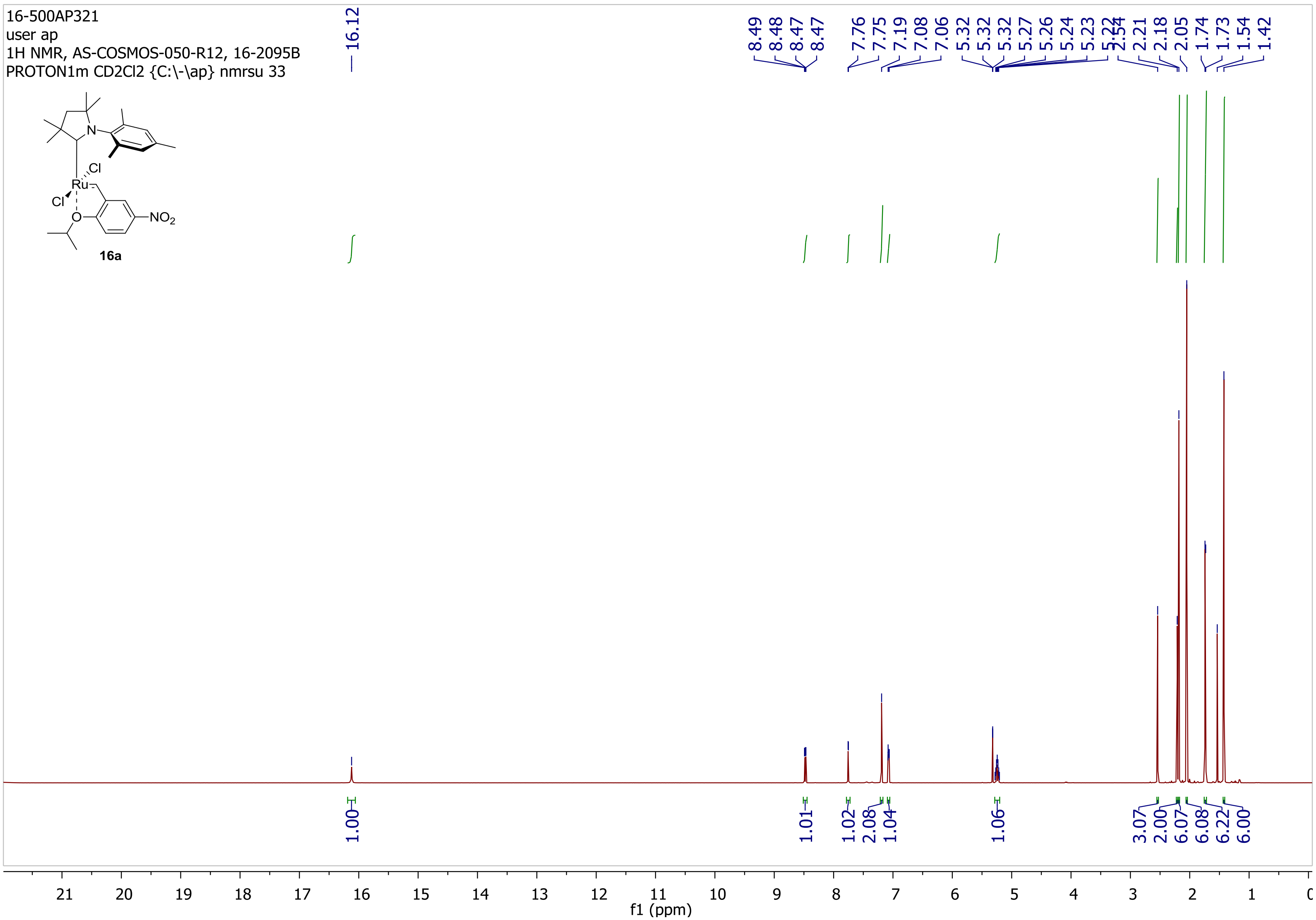
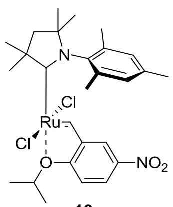
1H NMR, AS-COSMOS-060-R2, 16-0060B
PROTON1m CDCl3 {C:\-\ap} nmrsu 13
9.53
9.49
3.24
3.21
3.18
3.15
2.75
2.73
2.72
2.71
2.33
2.09
1.93
1.87
1.60
1.54
1.37
1.37
1.36
1.34
Ph
N
+
BF4
30b
1.00
0.97
4.12
2.14
1.05
1.00
1.49
2.20
1.45
3.08
3.05
4.53
3.08
1.60
f1 (ppm)


500AP556
user ap
1H NMR, AS-COSMOS-051-R3, 15-2981B
PROTON1m CDCl3 {C:\-\ap} nmrsu 55
9.27
7.53
7.36
7.34
7.26
2.65
2.63
2.62
2.42
1.71
1.56
1.55
1.36
1.35
1.21
1.19
BF4
31a
1.00
0.98
1.99
2.01
2.03
6.05
6.06
6.00
6.01
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)


16-500AP313
user ap
1H NMR, AS-COSMOS-097-R2-FR1, 16-1936B
PROTON1m CDCl3 {C:\-\ap} nmrsu 25
Ph
N
+
BF_4^-
31b
f1 (ppm)

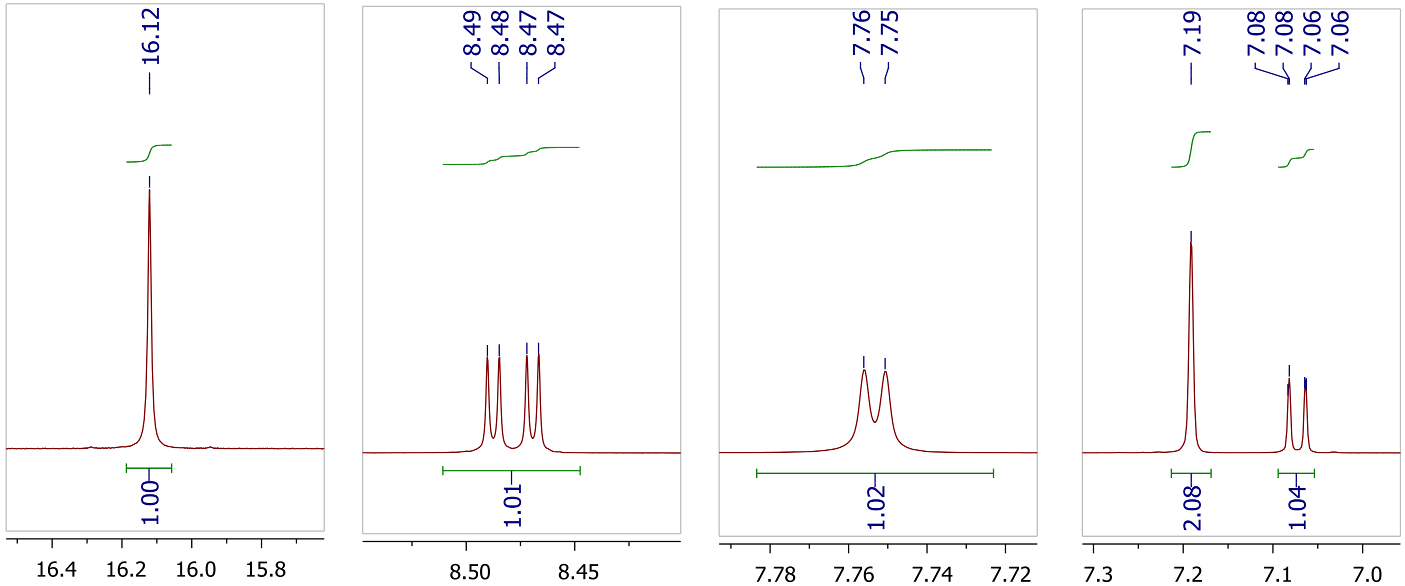
10. NMR Spectra of complexes 16-19



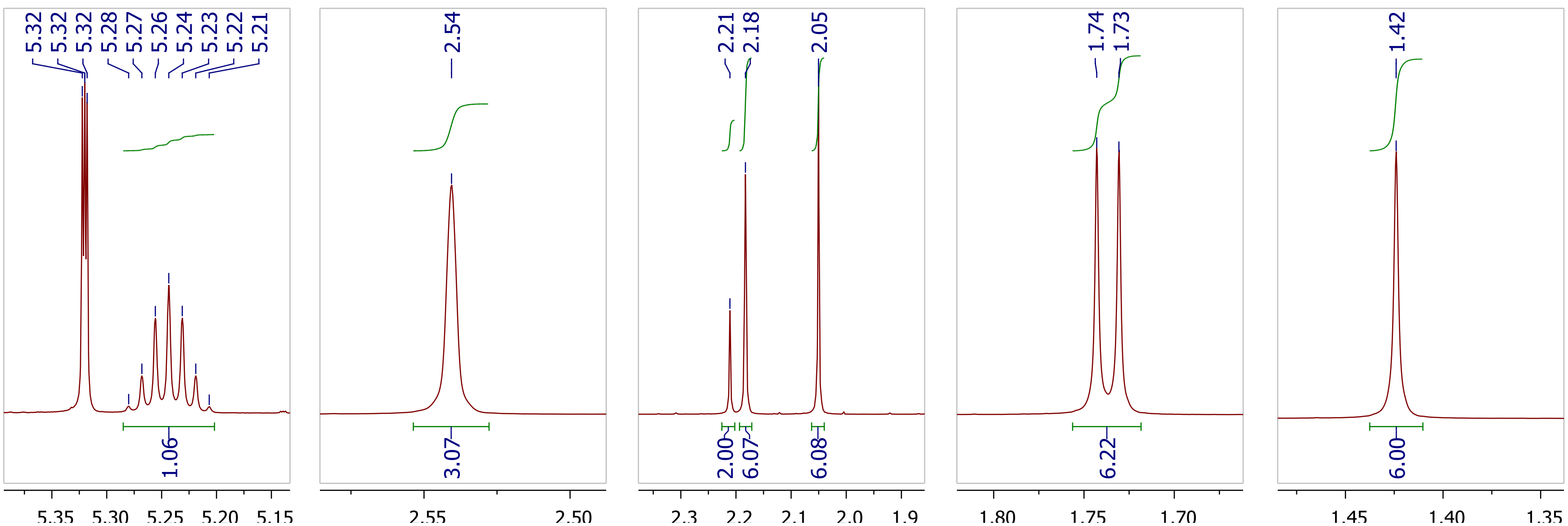


Cl
Ru
Cl
N
O
NO2

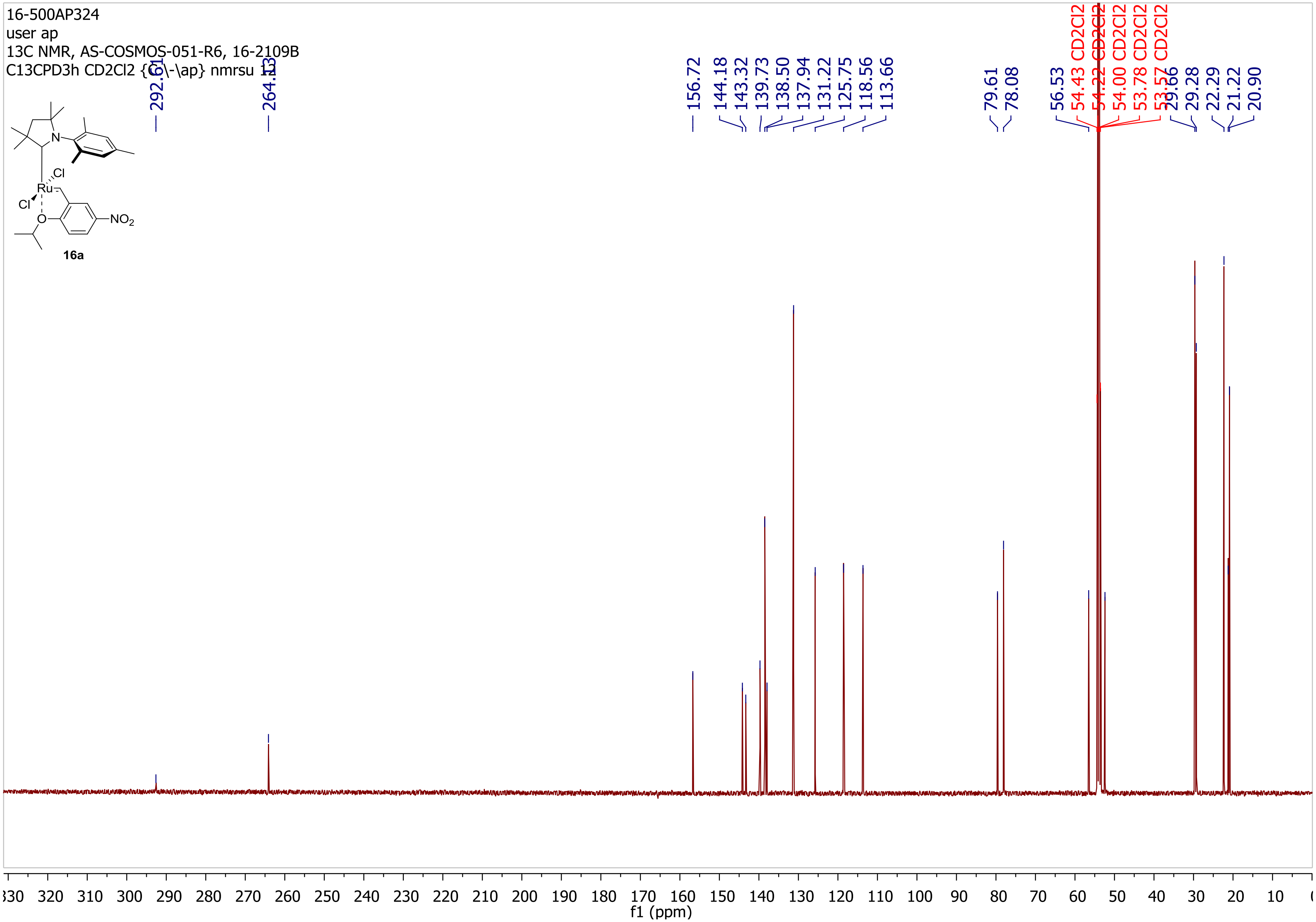
16a

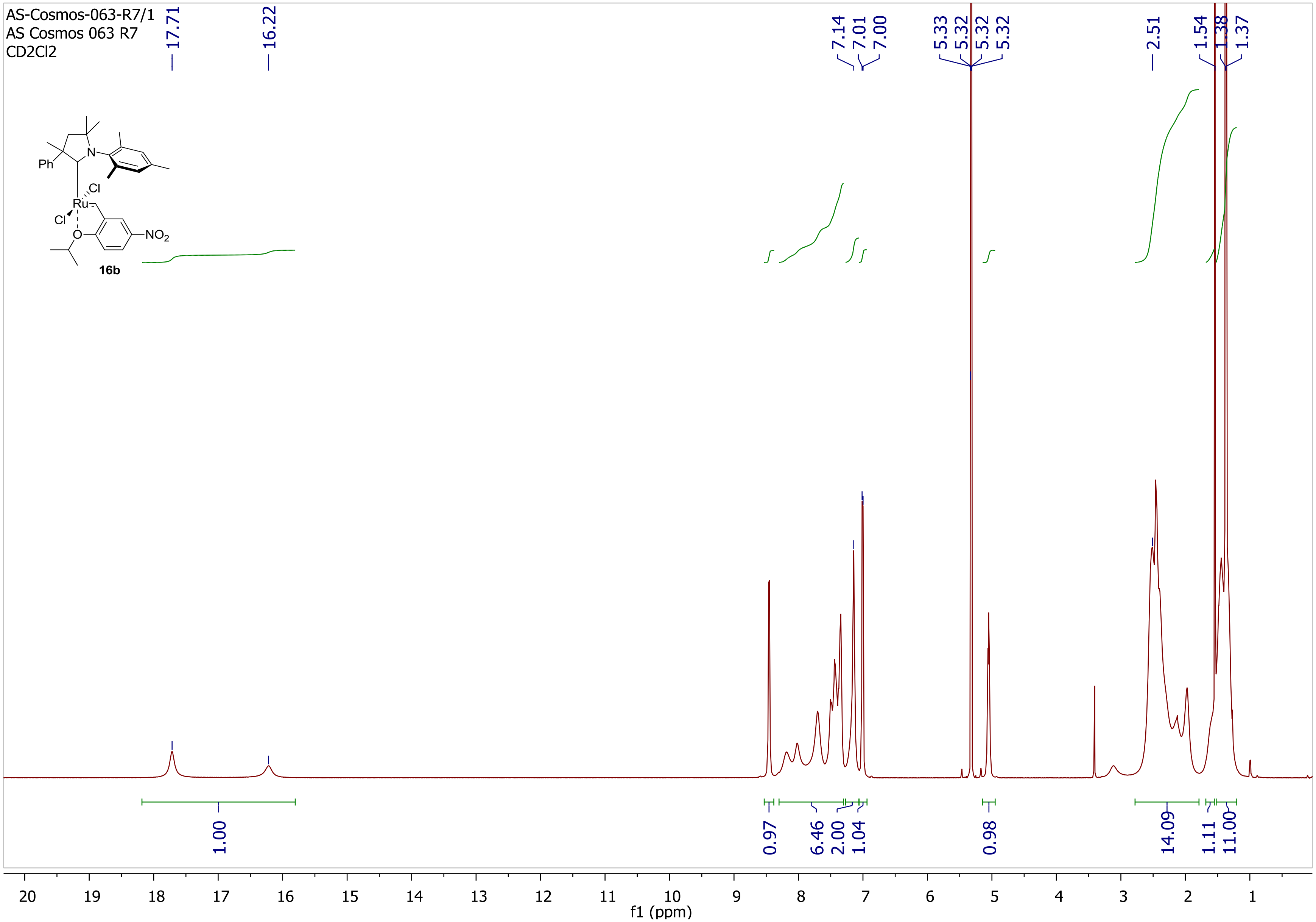


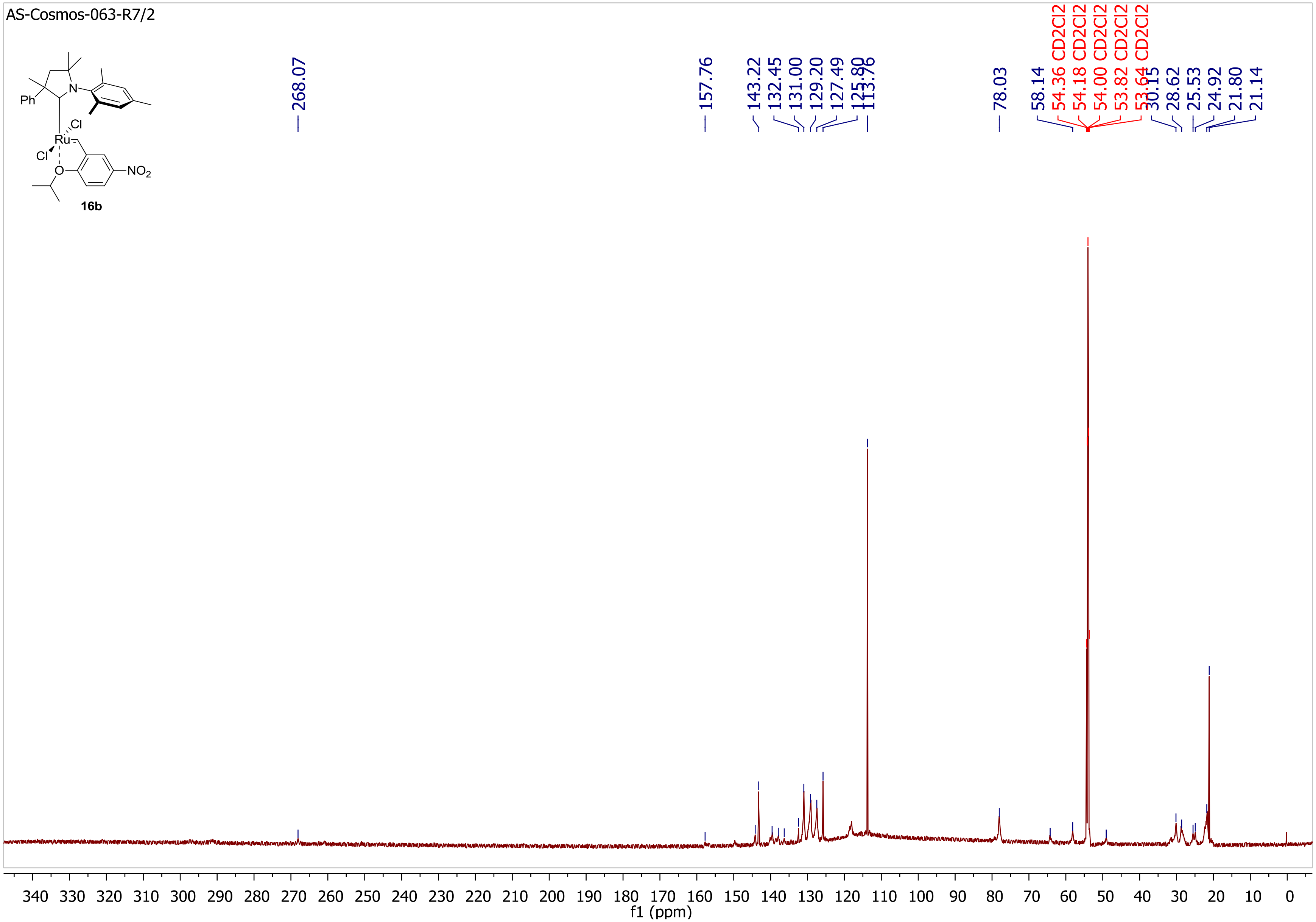
16.12
1.00
16.4 16.2 16.0 15.8
8.49 8.48 8.47 8.47
1.01
8.50 8.45
7.76 7.75
1.02
7.78 7.76 7.74 7.72
7.19 7.08 7.08 7.06 7.06
2.08 1.04
7.3 7.2 7.1 7.0

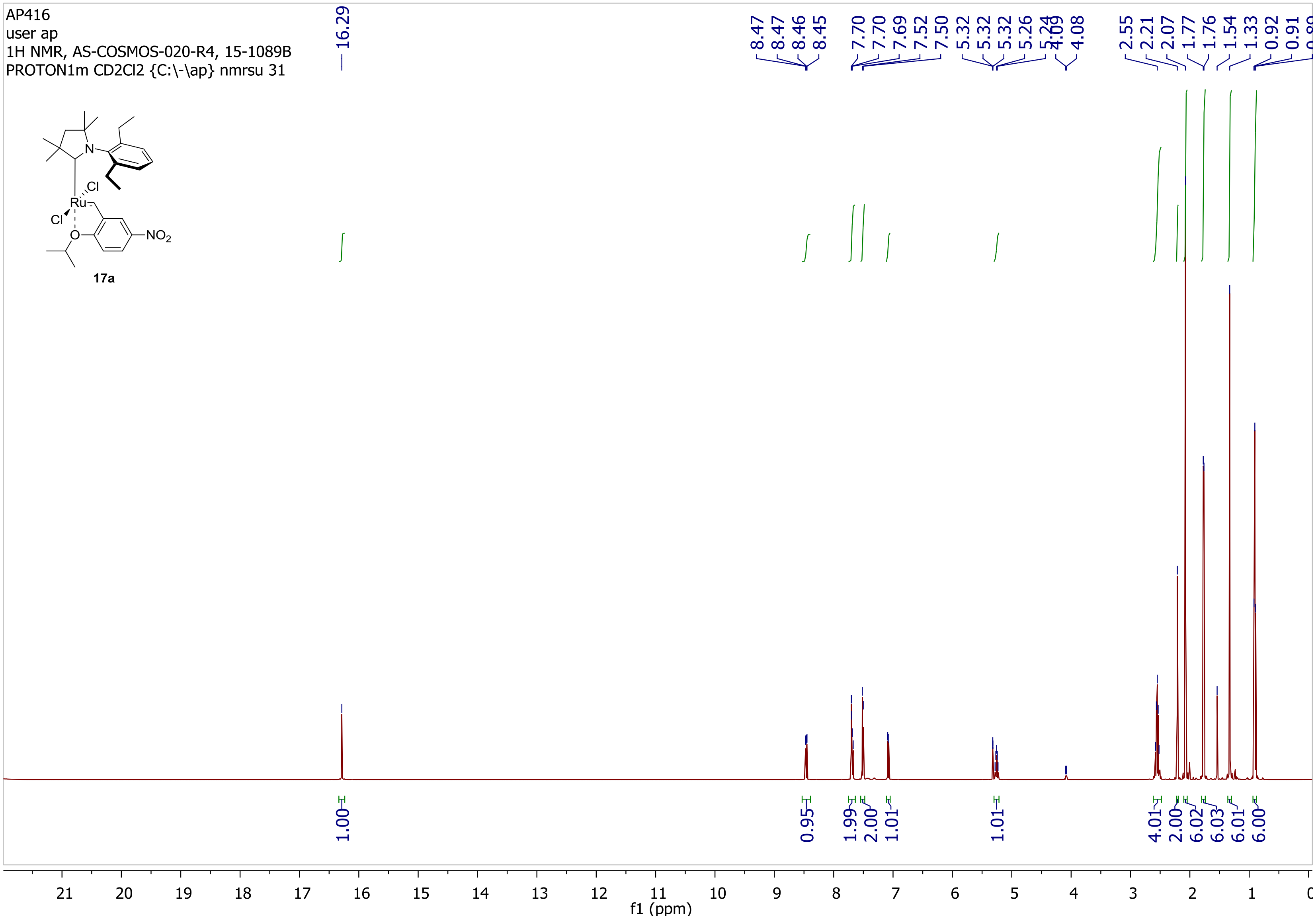


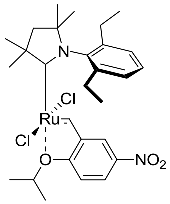
5.32 5.32 5.32 5.28 5.27 5.26 5.24 5.23 5.22 5.21
1.06
5.35 5.30 5.25 5.20 5.15
2.54
3.07
2.55 2.50
2.21 2.18 2.05
2.00 6.07 6.08
2.3 2.2 2.1 2.0 1.9
1.74 1.73
6.22
1.80 1.75 1.70
1.42
6.00
1.45 1.40 1.35


16-500AP324
user ap
13C NMR, AS-COSMOS-051-R6, 16-2109B
C13CPD3h CD2Cl2 {C\-\ap} nmrsu 12
292.61
264.13
156.72
144.18
143.32
139.73
138.50
137.94
131.22
125.75
118.56
113.66
79.61
78.08
56.53
54.43 CD2Cl2
54.22 CD2Cl2
54.00 CD2Cl2
53.78 CD2Cl2
53.57 CD2Cl2
29.66
29.28
22.29
21.22
20.90
Cl
Ru
Cl
O
N
NO2
16a
330 320 310 300 290 280 270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

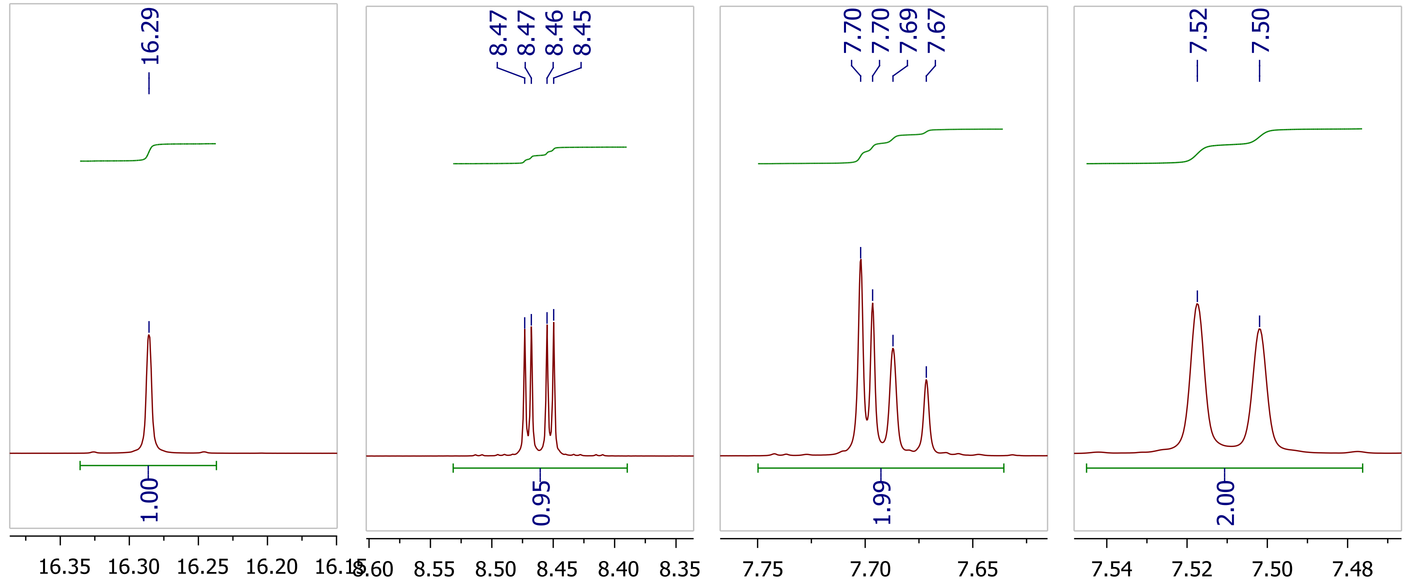

AS-Cosmos-063-R7/1
AS Cosmos 063 R7
CD2Cl2
17.71
16.22
7.14
7.01
7.00
5.33
5.32
5.32
5.32
2.51
1.54
1.38
1.37
Ph
N
Cl
Ru
Cl
O
NO2
16b
1.00
0.97
6.46
2.00
1.04
0.98
14.09
1.11
11.00
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1
f1 (ppm)

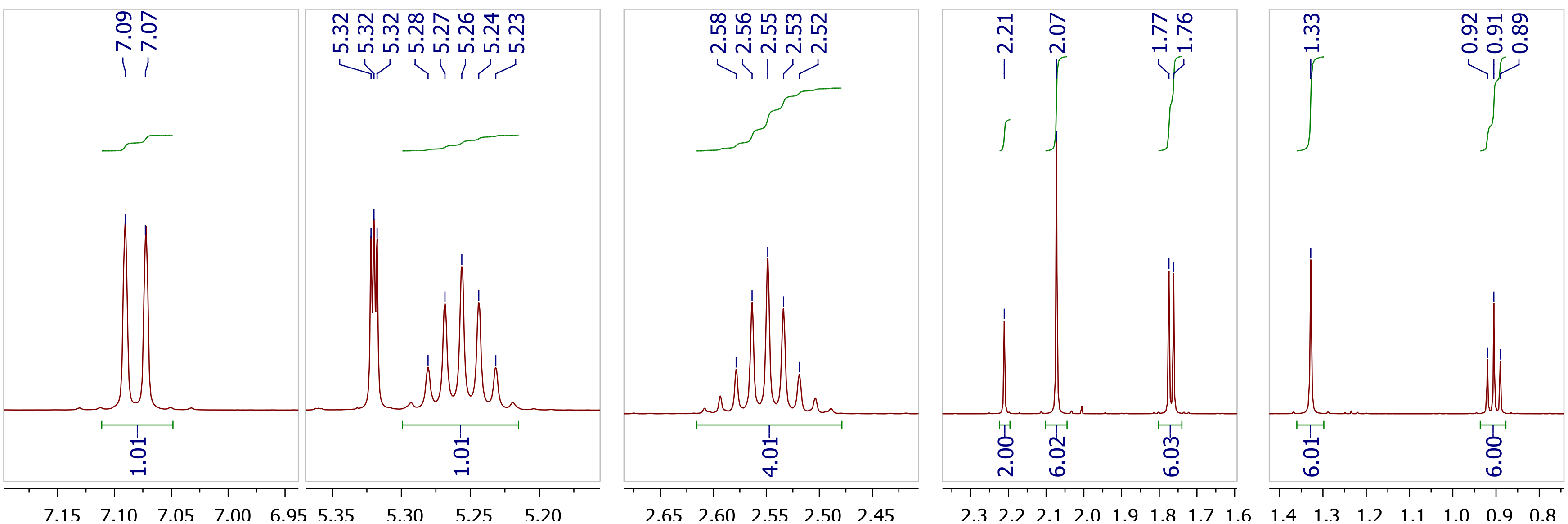

AS-Cosmos-063-R7/2
Ph
N
Cl
Ru
Cl
O
NO2
16b
268.07
157.76
143.22
132.45
131.00
129.20
127.49
125.80
113.76
78.03
58.14
54.36 CD2Cl2
54.18 CD2Cl2
54.00 CD2Cl2
53.82 CD2Cl2
53.64 CD2Cl2
30.15
28.62
25.53
24.92
21.80
21.14
340 330 320 310 300 290 280 270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

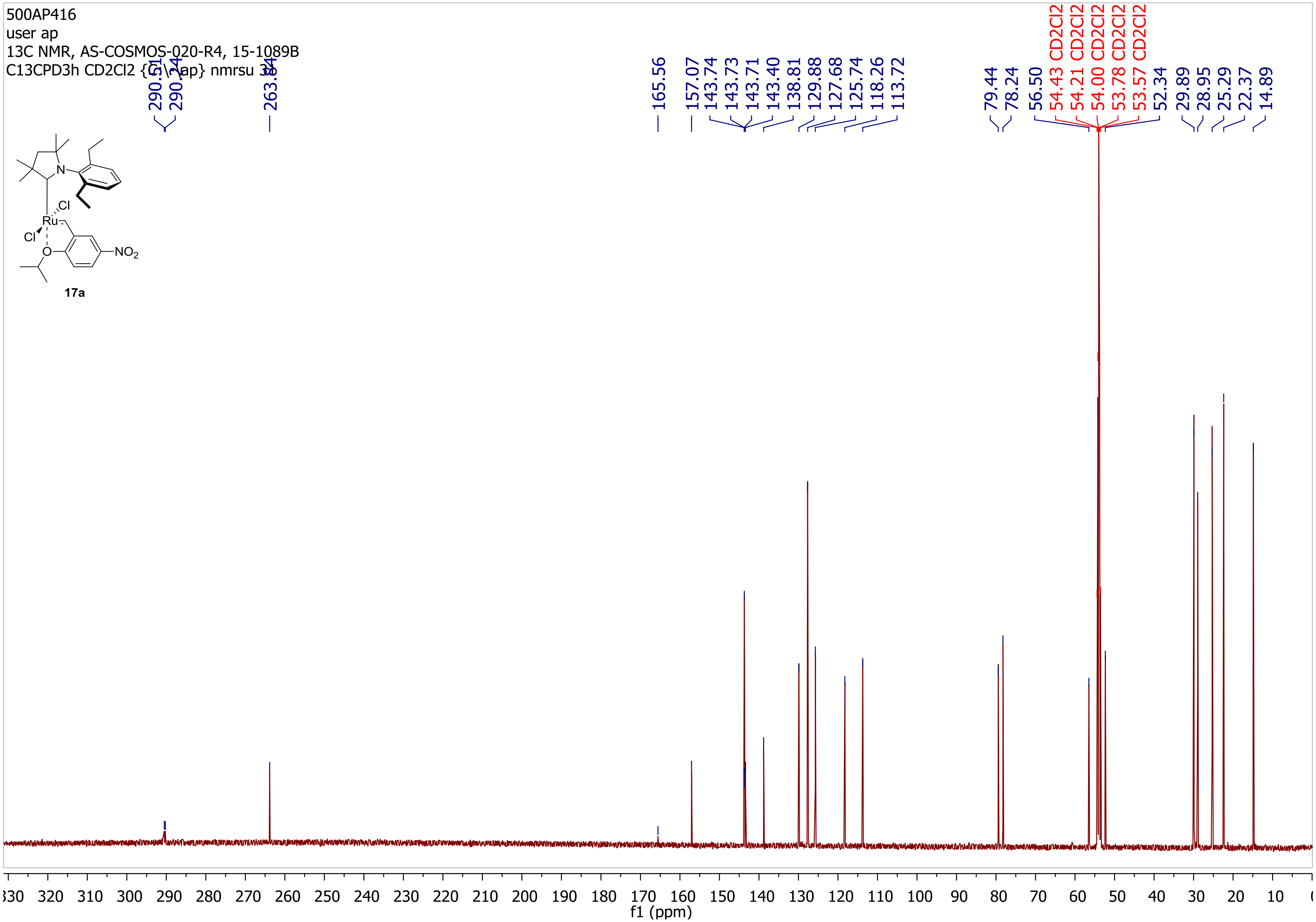

AP416
user ap
1H NMR, AS-COSMOS-020-R4, 15-1089B
PROTON1m CD2Cl2 {C:\-\ap} nmrsu 31
16.29
8.47 8.47 8.46 8.45
7.70 7.70 7.69 7.52 7.50
5.32 5.32 5.32 5.26 5.24
4.09 4.08
2.55 2.21 2.07 1.77 1.76 1.54 1.33 0.92 0.91
N
Cl
Ru
Cl
O
NO2
17a
1.00
0.95
1.99 2.00 1.01
1.01
4.01 2.00 6.02 6.03 6.01 6.00
21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1
f1 (ppm)

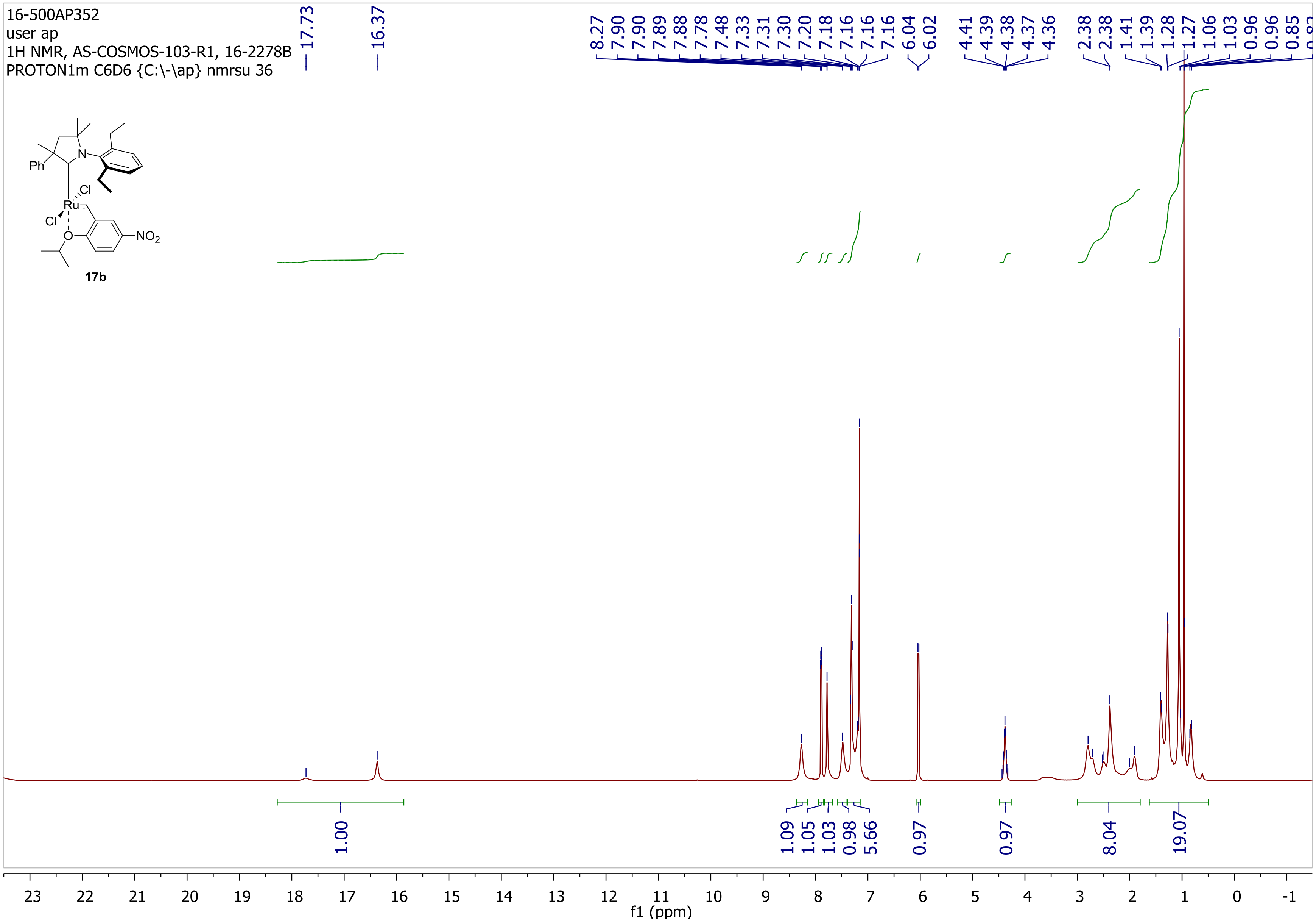

N
Cl
Ru
Cl
O
NO_2

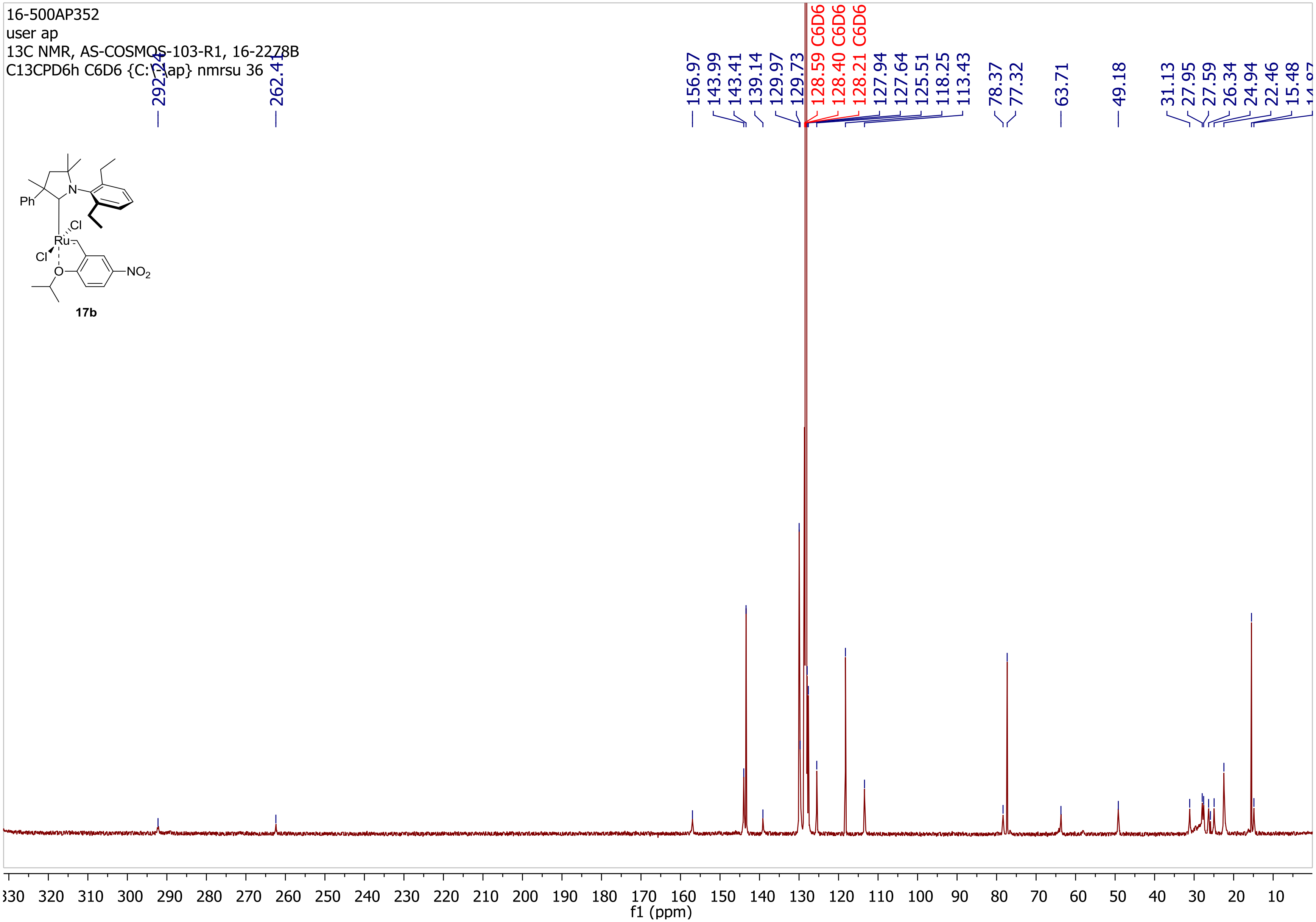
17a


16.29
1.00
16.35 16.30 16.25 16.20 16.15
8.47 8.47 8.46 8.45
0.95
8.60 8.55 8.50 8.45 8.40 8.35
7.70 7.70 7.69 7.67
1.99
7.75 7.70 7.65
7.52 7.50
2.00
7.54 7.52 7.50 7.48


7.09 7.07
1.01
7.15 7.10 7.05 7.00 6.95
5.32 5.32 5.32 5.28 5.27 5.26 5.24 5.23
1.01
5.35 5.30 5.25 5.20
2.58 2.56 2.55 2.53 2.52
4.01
2.65 2.60 2.55 2.50 2.45
2.21 2.07 1.77 1.76
2.00 6.02 6.03
2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
1.33 0.92 0.91 0.89
6.01 6.00
1.4 1.3 1.2 1.1 1.0 0.9 0.8


500AP416
user ap
13C NMR, AS-COSMOS-020-R4, 15-1089B
C13CPD3h CD2Cl2 {C:\ ap} nmrsu 33
290.51
290.44
263.44
165.56
157.07
143.74
143.73
143.71
143.40
138.81
129.88
127.68
125.74
118.26
113.72
79.44
78.24
56.50
54.43 CD2Cl2
54.21 CD2Cl2
54.00 CD2Cl2
53.78 CD2Cl2
53.57 CD2Cl2
52.34
29.89
28.95
25.29
22.37
14.89
Cl
Ru
Cl
O
N
NO2
17a
f1 (ppm)


16-500AP352
user ap
1H NMR, AS-COSMOS-103-R1, 16-2278B
PROTON1m C6D6 {C:\-\ap} nmrsu 36
17.73
16.37
8.27 7.90 7.90 7.89 7.88 7.78 7.48 7.33 7.31 7.30 7.20 7.18 7.16 7.16 7.16 6.04 6.02
4.41 4.39 4.38 4.37 4.36 2.38 2.38 2.38 1.41 1.39 1.28 1.27 1.06 1.03 0.96 0.96 0.85
Ph
N
Cl
Ru
Cl
O
NO2
17b
1.00
1.09 1.05 1.03 0.98 5.66
0.97
0.97
8.04
19.07
f1 (ppm)


16-500AP352
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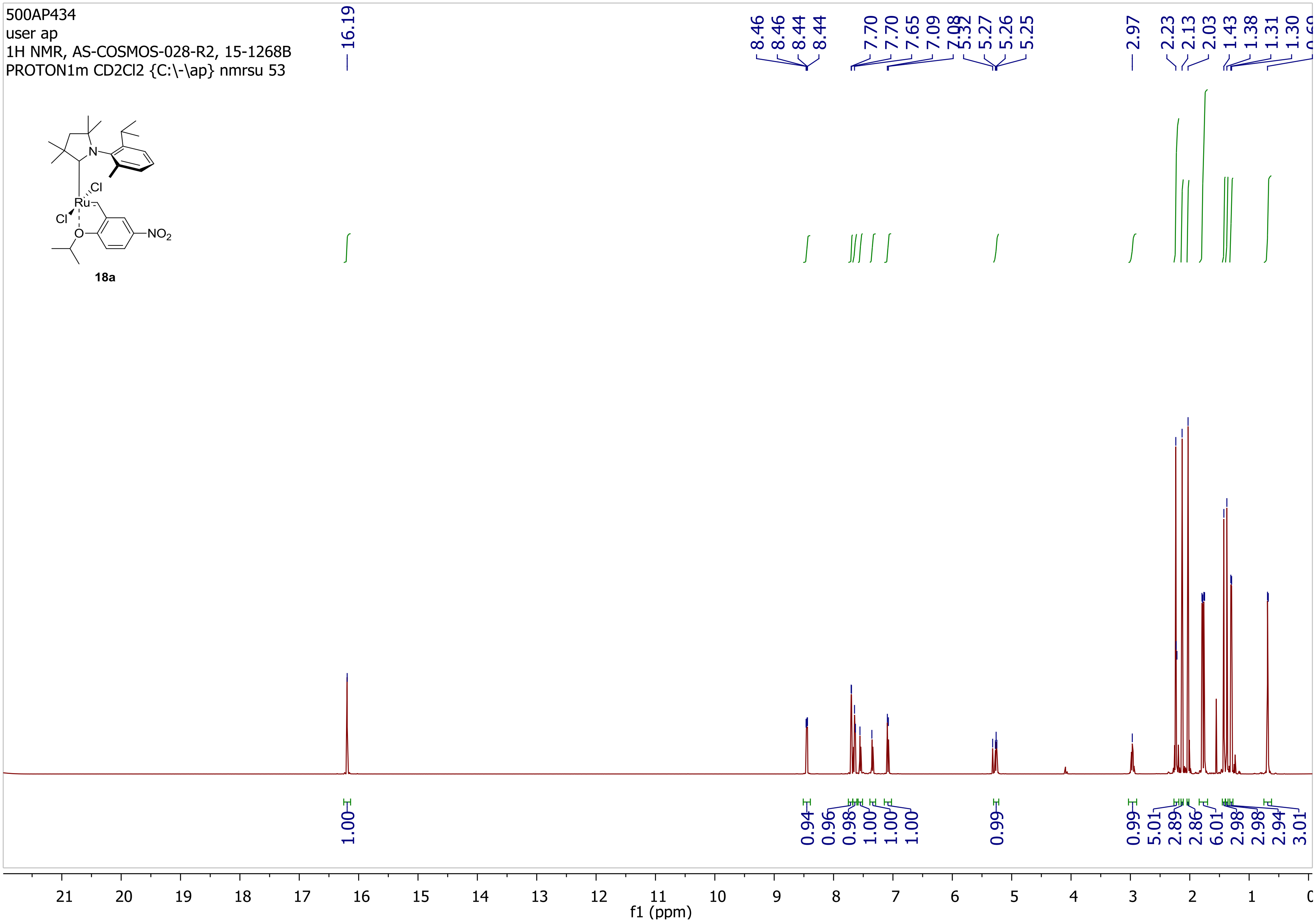
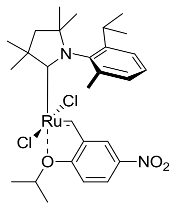
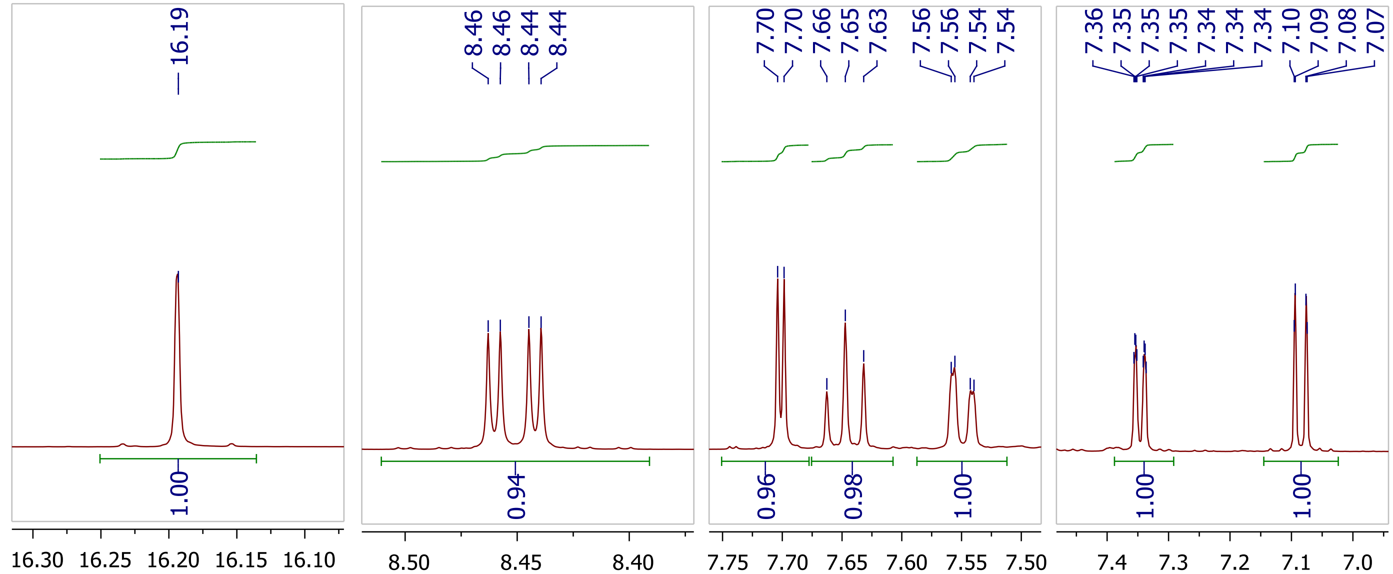
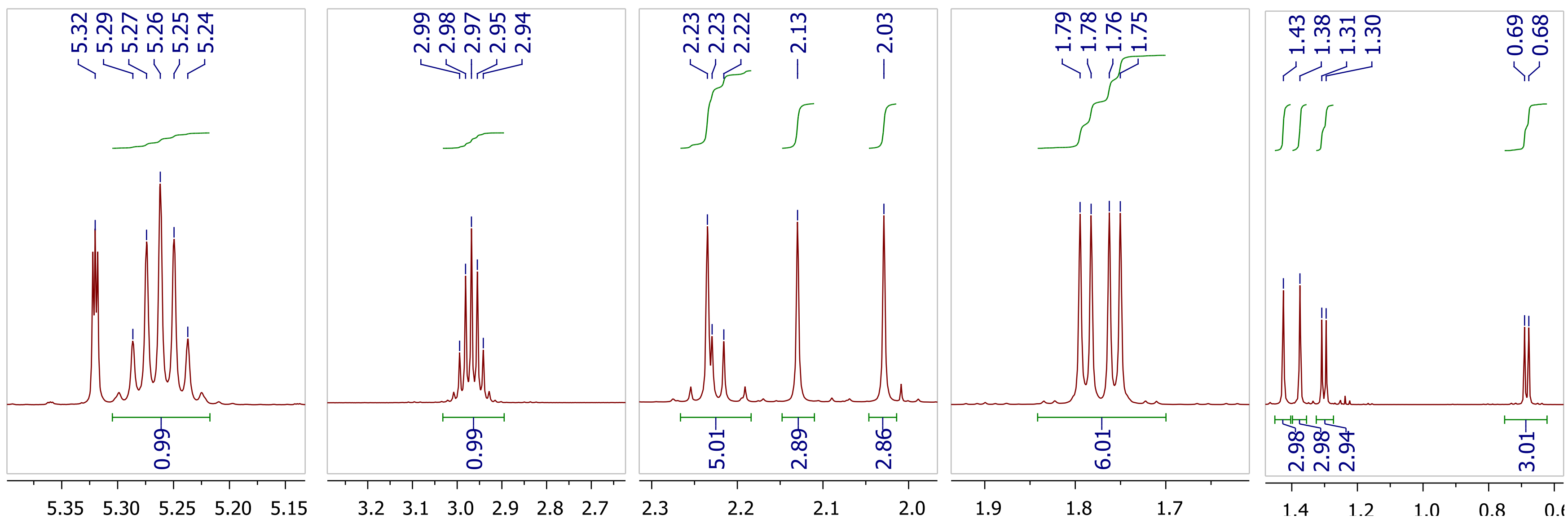
13C NMR, AS-COSMOS-103-R1, 16-2278B
C13CPD6h C6D6 {C:\ap} nmrsu 36
292.74
262.41
156.97
143.99
143.41
139.14
129.97
129.73
128.59 C6D6
128.40 C6D6
128.21 C6D6
127.94
127.64
125.51
118.25
113.43
78.37
77.32
63.71
49.18
31.13
27.95
27.59
26.34
24.94
22.46
15.48
Ph
N
Cl
Ru
Cl
O
NO2
17b
f1 (ppm)

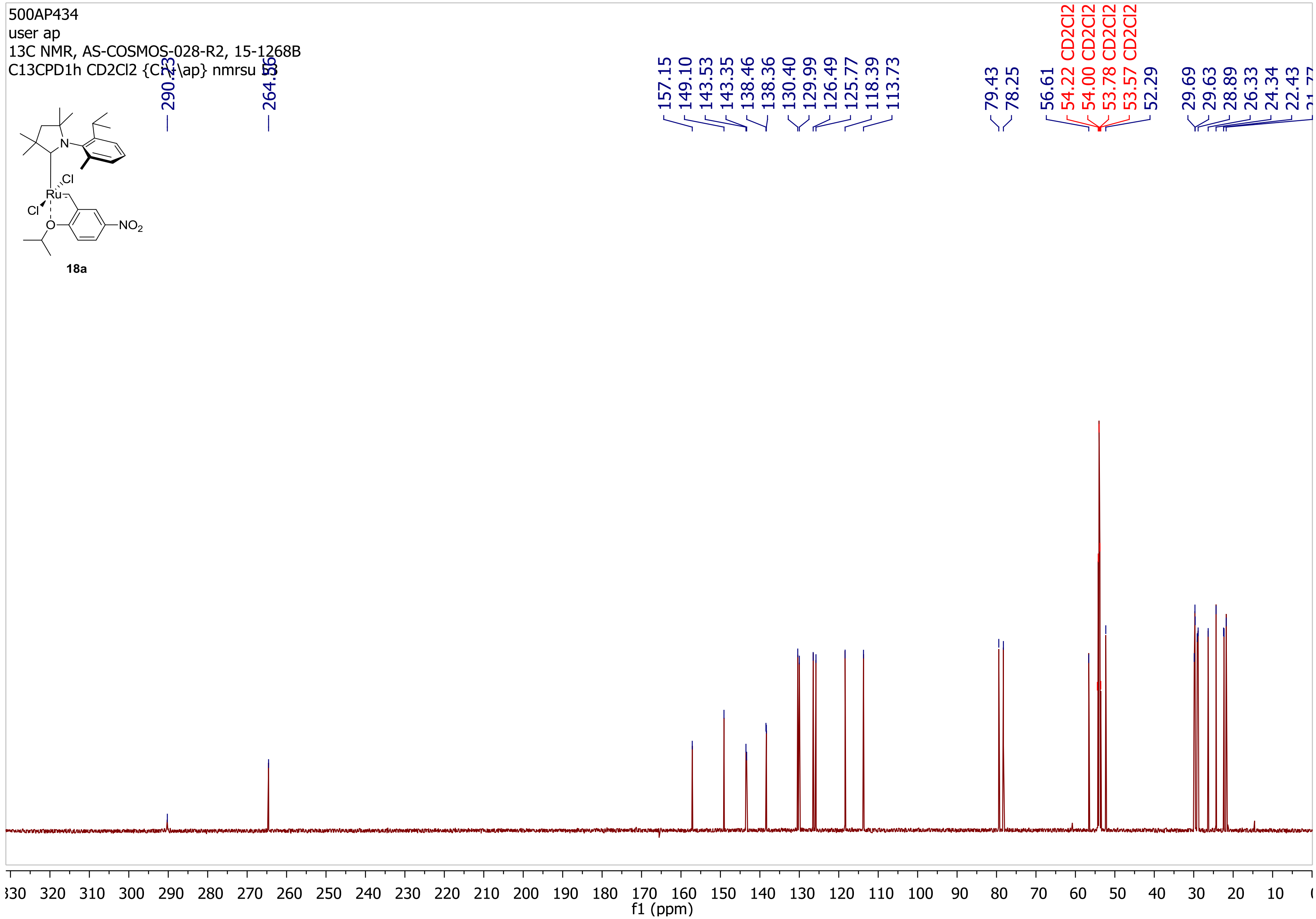

500AP434
user ap
1H NMR, AS-COSMOS-028-R2, 15-1268B
PROTON1m CD2Cl2 {C:\-\ap} nmrsu 53
Cl
Ru
Cl
O
N
NO2
18a
16.19
8.46
8.46
8.44
8.44
7.70
7.70
7.65
7.09
7.08
5.32
5.27
5.26
5.25
2.97
2.23
2.13
2.03
1.43
1.38
1.31
1.30
1.00
0.94
0.96
0.98
1.00
1.00
1.00
0.99
0.99
5.01
2.89
2.86
6.01
2.98
2.98
2.94
3.01
f1 (ppm)

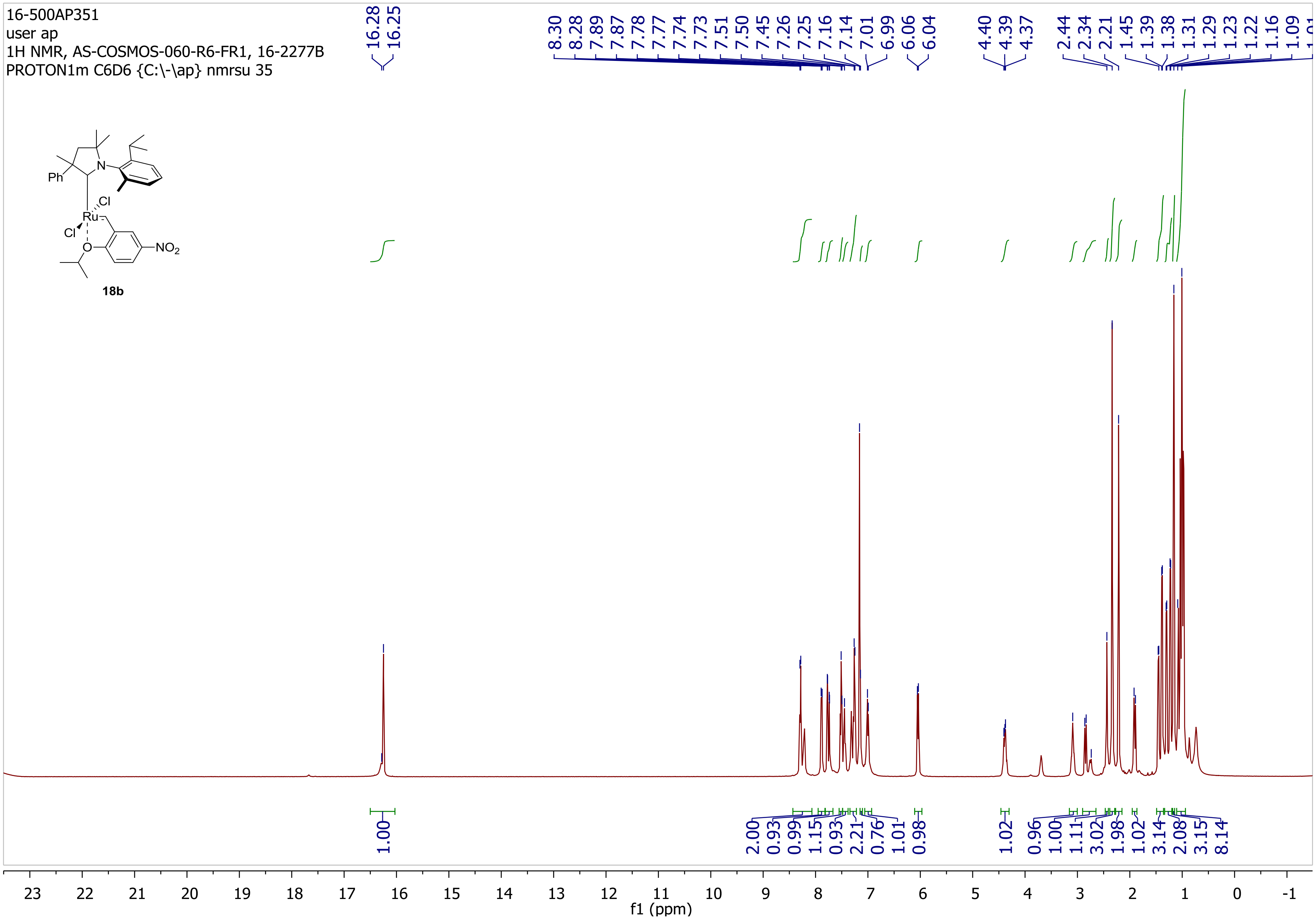

N
Cl
Ru
Cl
O
NO2

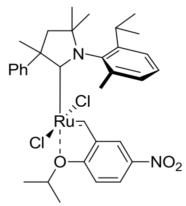
18a


16.19
1.00
16.30 16.25 16.20 16.15 16.10
8.46 8.46 8.44 8.44
0.94
8.50 8.45 8.40
7.70 7.70 7.66 7.65 7.63 7.56 7.56 7.54 7.54
0.96 0.98 1.00
7.75 7.70 7.65 7.60 7.55 7.50
7.36 7.35 7.35 7.35 7.34 7.34 7.34 7.10 7.09 7.08 7.07
1.00 1.00
7.4 7.3 7.2 7.1 7.0


5.32 5.29 5.27 5.26 5.25 5.24
0.99
5.35 5.30 5.25 5.20 5.15
2.99 2.98 2.97 2.95 2.94
0.99
3.2 3.1 3.0 2.9 2.8 2.7
2.23 2.23 2.22 2.13 2.03
5.01 2.89 2.86
2.3 2.2 2.1 2.0
1.79 1.78 1.76 1.75
6.01
1.9 1.8 1.7
1.43 1.38 1.31 1.30 0.69 0.68
2.98 2.98 2.94 3.01
1.4 1.2 1.0 0.8

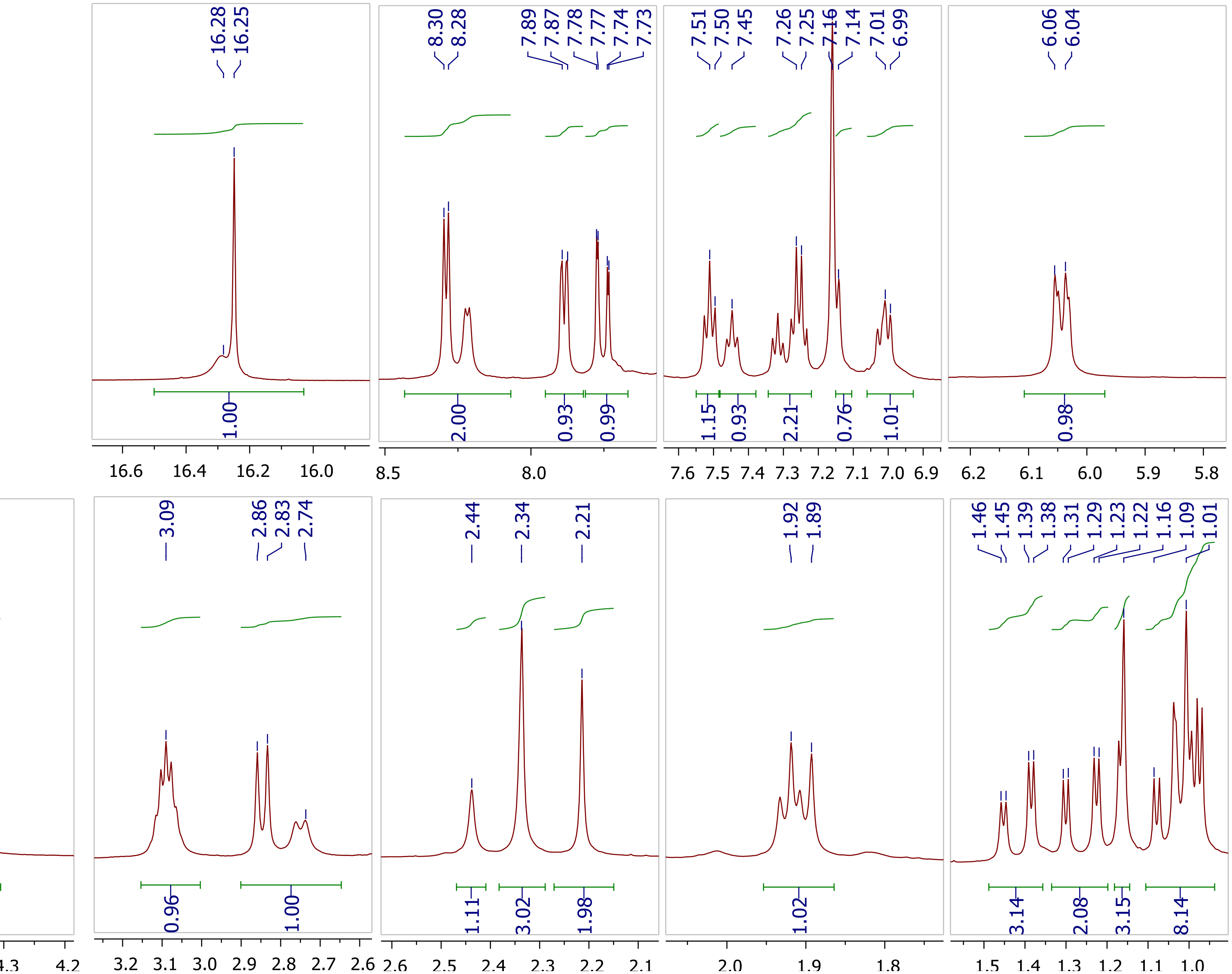

500AP434
user ap
13C NMR, AS-COSMOS-028-R2, 15-1268B
C13CPD1h CD2Cl2 {C:\ap} nmrsu 53
18a
NO2
Cl
Ru
O
N
290.33
264.56
157.15
149.10
143.53
143.35
138.46
138.36
130.40
129.99
126.49
125.77
118.39
113.73
79.43
78.25
56.61
54.22 CD2Cl2
54.00 CD2Cl2
53.78 CD2Cl2
53.57 CD2Cl2
52.29
29.69
29.63
28.89
26.33
24.34
22.43
f1 (ppm)


16-500AP351
user ap
1H NMR, AS-COSMOS-060-R6-FR1, 16-2277B
PROTON1m C6D6 {C:\-\ap} nmrsu 35
18b
16.28
16.25
8.30
8.28
7.89
7.87
7.78
7.77
7.74
7.73
7.51
7.50
7.45
7.26
7.25
7.16
7.14
7.01
6.99
6.06
6.04
4.40
4.39
4.37
2.44
2.34
2.21
1.45
1.39
1.38
1.31
1.29
1.23
1.22
1.16
1.09
1.00
2.00
0.93
0.99
1.15
0.93
2.21
0.76
1.01
0.98
1.02
0.96
1.00
1.11
3.02
1.98
1.02
3.14
2.08
3.15
8.14
f1 (ppm)

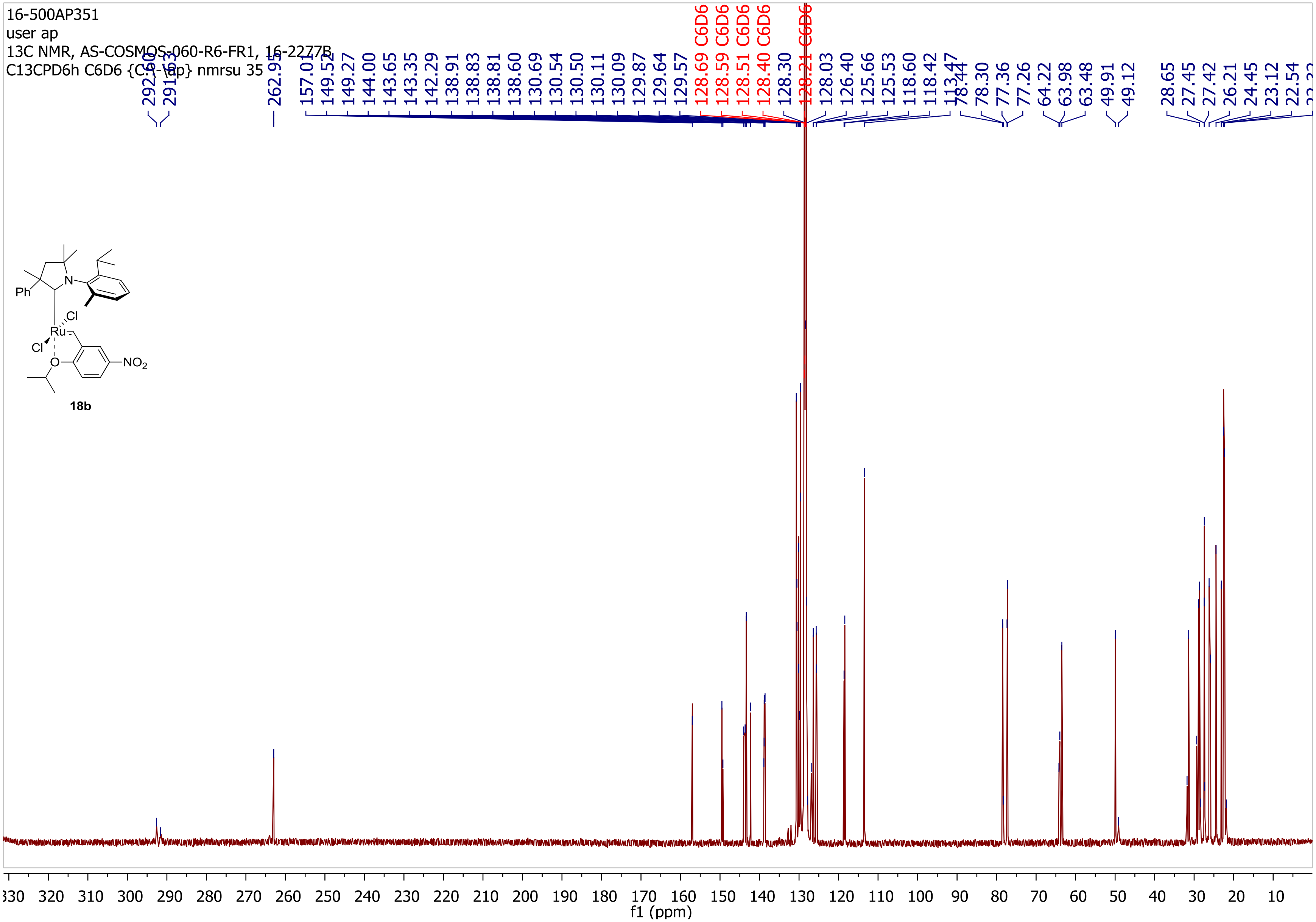


Ph
N
Cl
Ru
Cl
O
NO2

18b



16.28
16.25
1.00
16.6 16.4 16.2 16.0
8.30
8.28
7.89
7.87
7.78
7.77
7.74
7.73
2.00
0.93
0.99
8.5 8.0
7.51
7.50
7.45
7.26
7.25
7.16
7.14
7.01
6.99
1.15
0.93
2.21
0.76
1.01
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
6.06
6.04
0.98
6.2 6.1 6.0 5.9 5.8
4.40
4.39
4.37
1.02
4.6 4.5 4.4 4.3 4.2
3.09
2.86
2.83
2.74
0.96
1.00
3.2 3.1 3.0 2.9 2.8 2.7 2.6
2.44
2.34
2.21
1.11
3.02
1.98
2.6 2.5 2.4 2.3 2.2 2.1
1.92
1.89
1.02
2.0 1.9 1.8
1.46
1.45
1.39
1.38
1.31
1.29
1.23
1.22
1.16
1.09
1.01
3.14
2.08
3.15
8.14
1.5 1.4 1.3 1.2 1.1 1.0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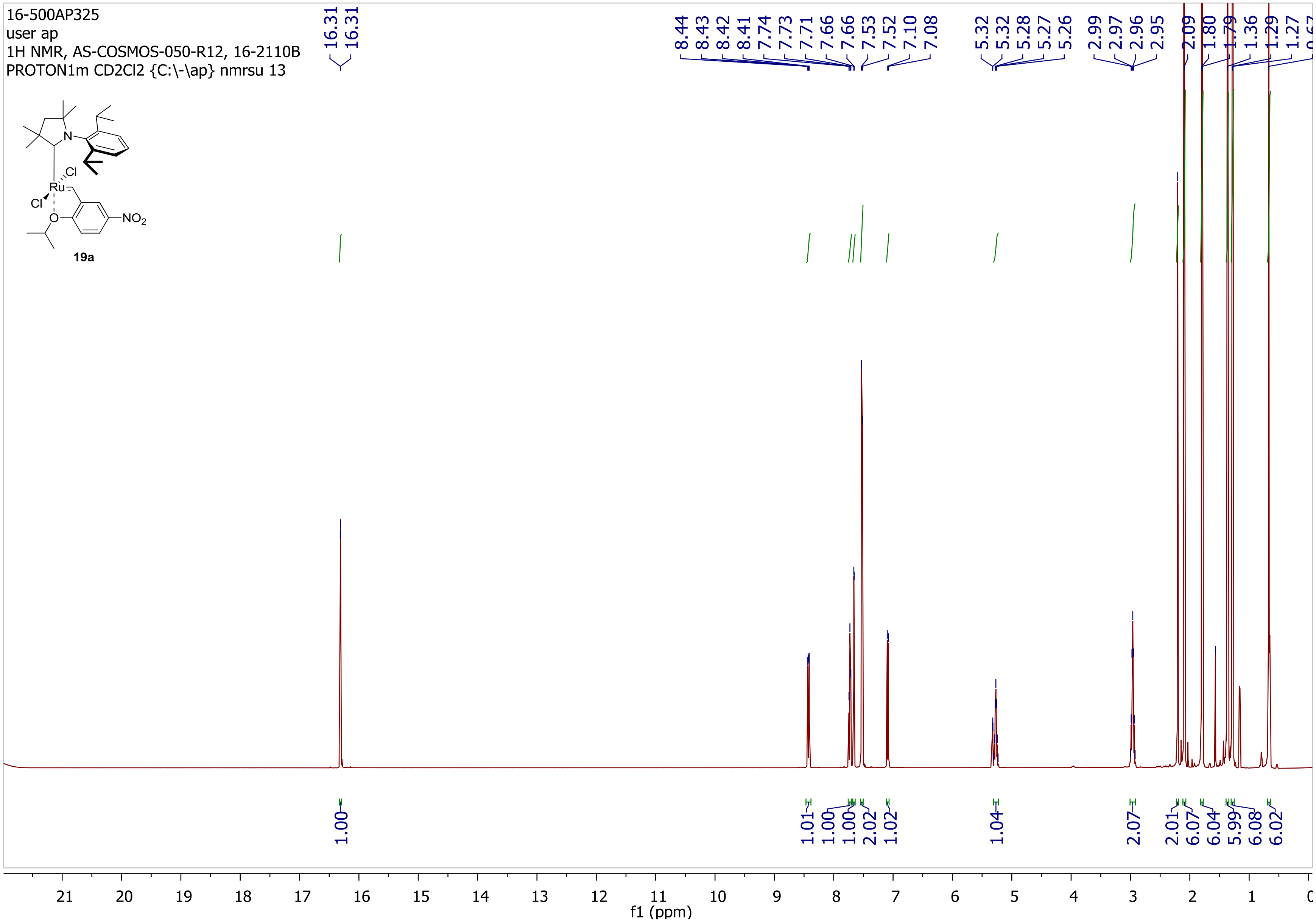
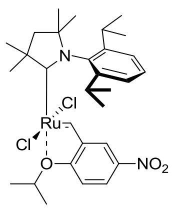
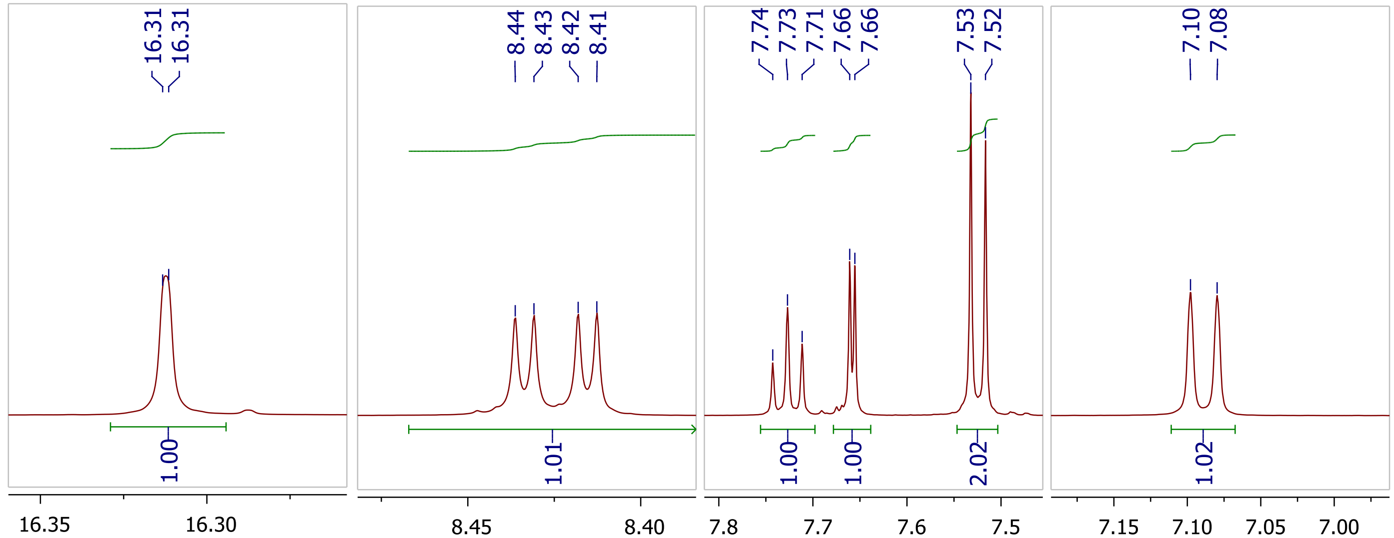
C13CPD6h C6D6 {C:\ap} nmrsu 35
262.95
157.01
149.52
149.27
144.00
143.65
143.35
142.29
138.91
138.83
138.81
138.60
130.69
130.54
130.50
130.11
130.09
129.87
129.64
129.57
128.69 C6D6
128.59 C6D6
128.51 C6D6
128.40 C6D6
128.30
128.21 C6D6
128.03
126.40
125.66
125.53
118.60
118.42
113.47
78.44
78.30
77.36
77.26
64.22
63.98
63.48
49.91
49.12
28.65
27.45
27.42
26.21
24.45
23.12
22.54
Ph
N
Cl
Ru
Cl
O
NO2
18b
f1 (ppm)

16-500AP325
user ap
1H NMR, AS-COSMOS-050-R12, 16-2110B
PROTON1m CD2Cl2 {C:\-\ap} nmrsu 13




N
Cl
Ru
Cl
O
NO2

19a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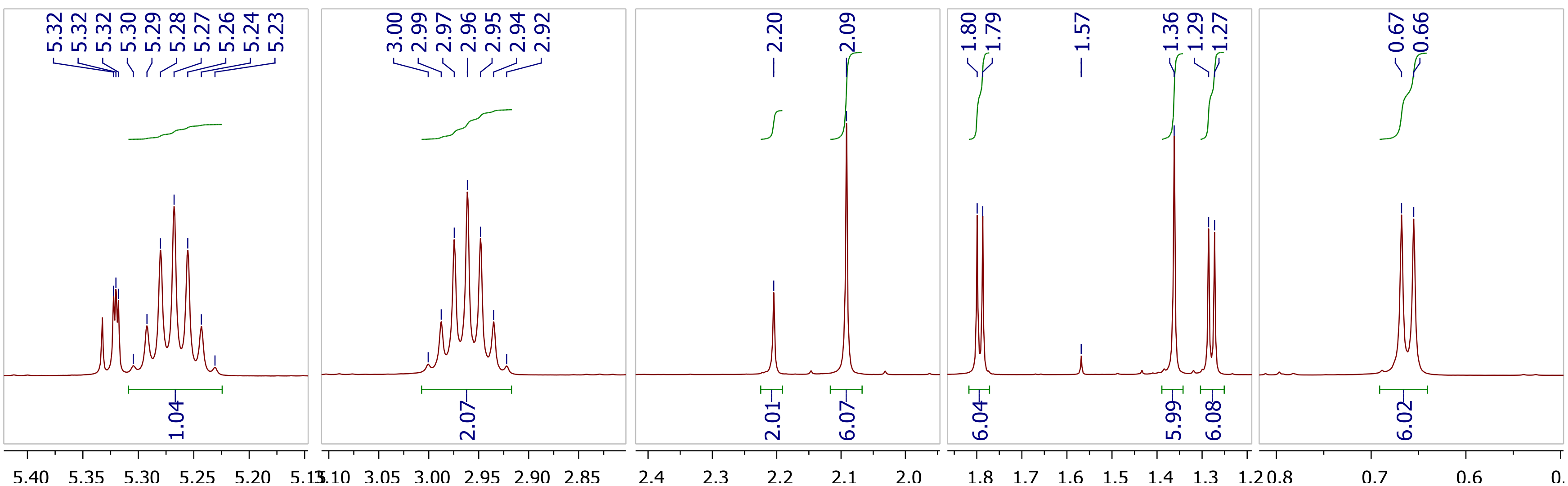
16.30
8.44
8.43
8.42
8.41
1.01
8.45
8.40
7.74
7.73
7.71
7.66
7.66
7.53
7.52
1.00
1.00
2.02
7.8
7.7
7.6
7.5
7.10
7.08
1.02
7.15
7.10
7.05
7.00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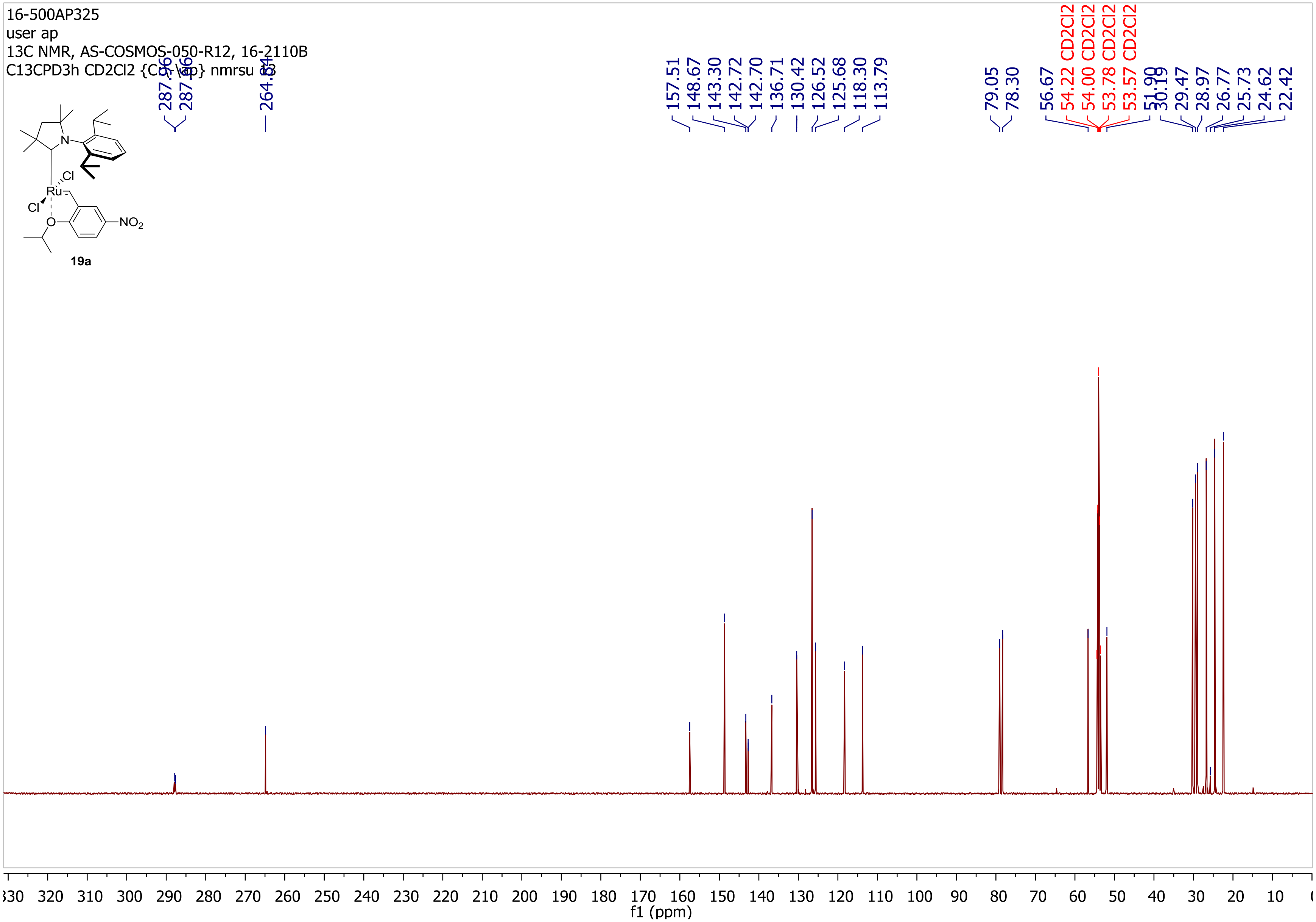
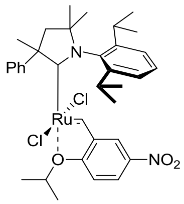
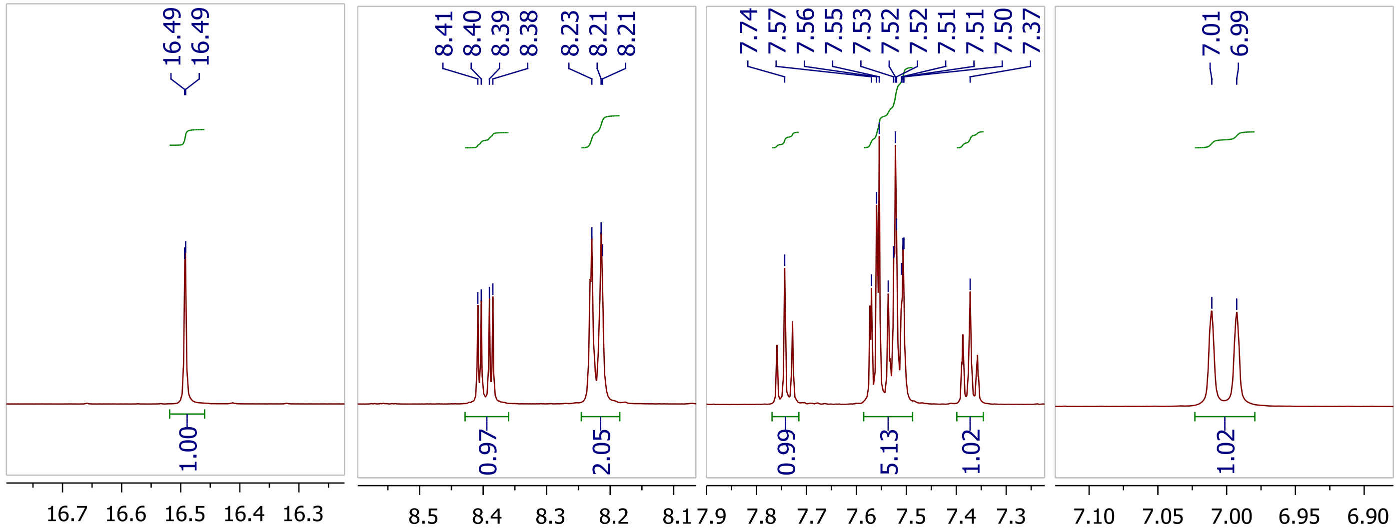
5.32
5.32
5.30
5.29
5.28
5.27
5.26
5.24
5.23
1.04
5.40
5.35
5.30
5.25
5.20
3.00
2.99
2.97
2.96
2.95
2.94
2.92
2.07
3.10
3.05
3.00
2.95
2.90
2.85
2.20
2.09
2.01
6.07
2.4
2.3
2.2
2.1
2.0
1.80
1.79
1.57
1.36
1.29
1.27
6.04
5.99
6.08
1.8
1.7
1.6
1.5
1.4
1.3
1.2
0.67
0.66
6.02
0.8
0.7
0.6


16-500AP325
user ap
13C NMR, AS-COSMOS-050-R12, 16-2110B
C13CPD3h CD2Cl2
N
Cl
Ru
Cl
O
NO2
19a
157.51
148.67
143.30
142.72
142.70
136.71
130.42
126.52
125.68
118.30
113.79
79.05
78.30
56.67
54.22 CD2Cl2
54.00 CD2Cl2
53.78 CD2Cl2
53.57 CD2Cl2
51.90
30.19
29.47
28.97
26.77
25.73
24.62
22.42
f1 (ppm)


16-500AP336
user ap
1H NMR, AS-COSMOS-097-R14, 16-2149B
PROTON1m CD2Cl2 {C:\-\ap} nmrsu 21
Ph
N
Cl
Ru
Cl
O
NO2
19b
f1 (ppm)


Ph
N
Cl
Ru
Cl
O
NO_2

19b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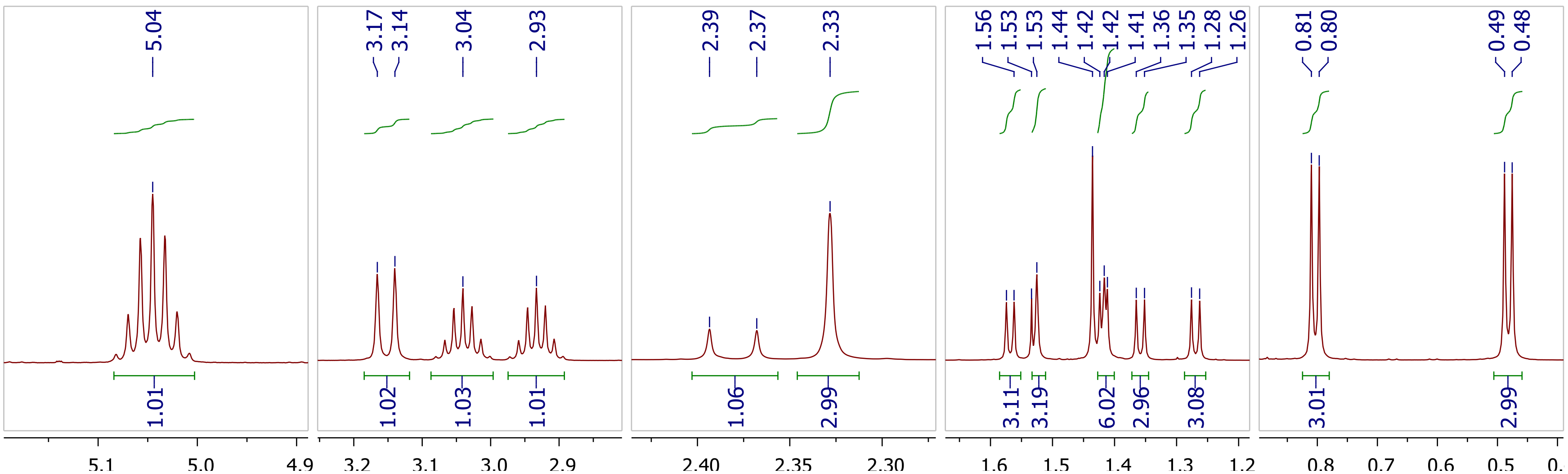
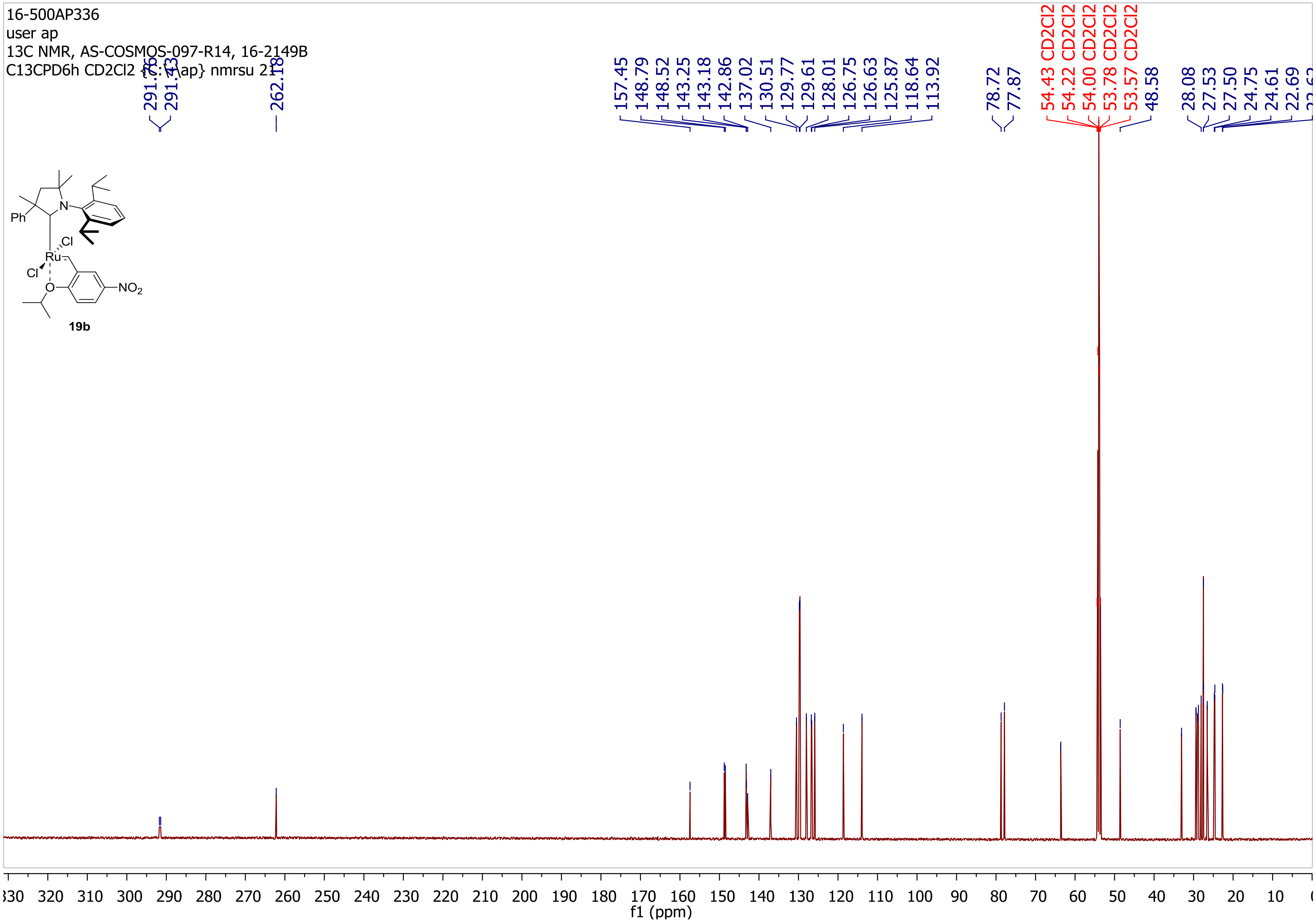
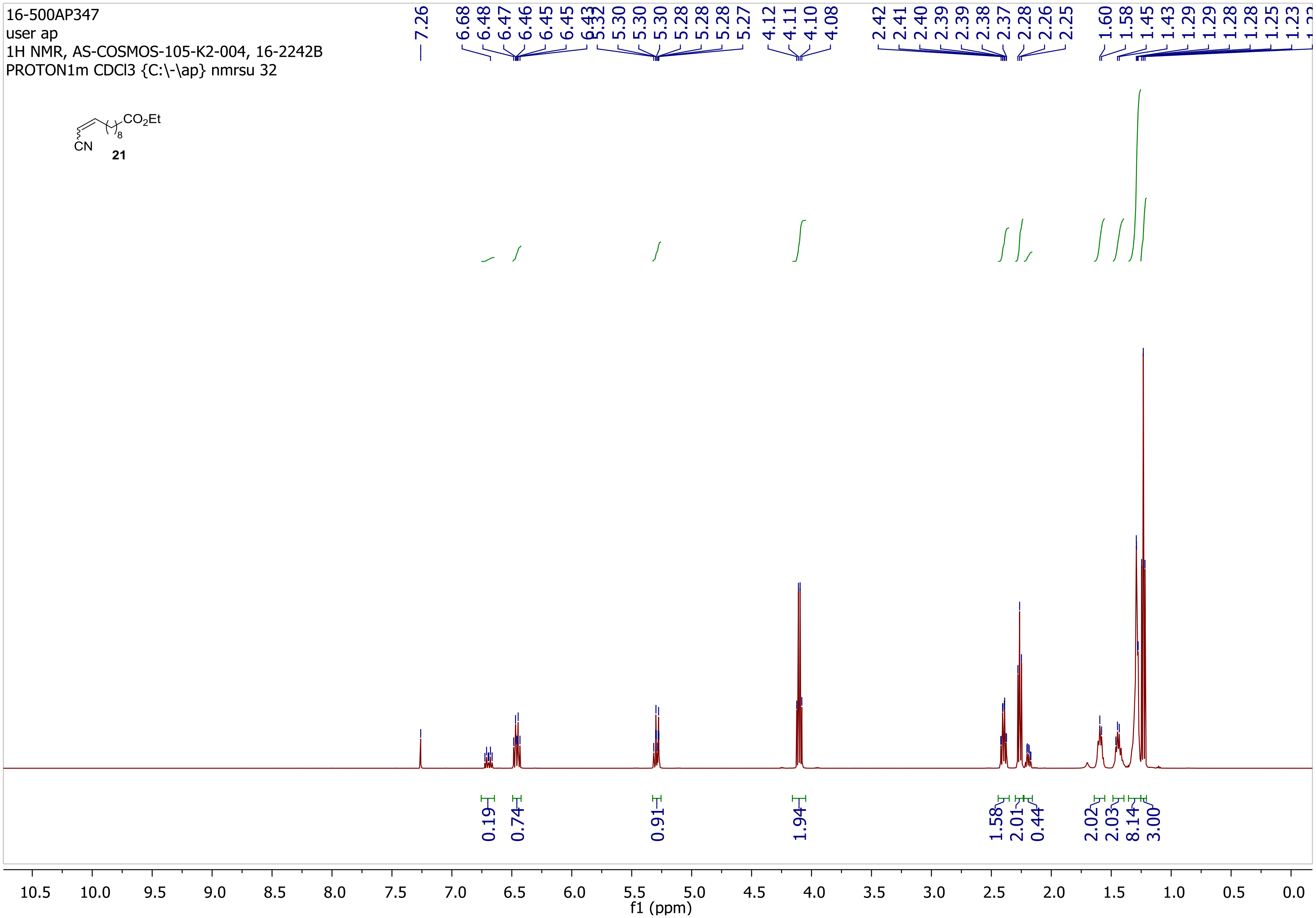
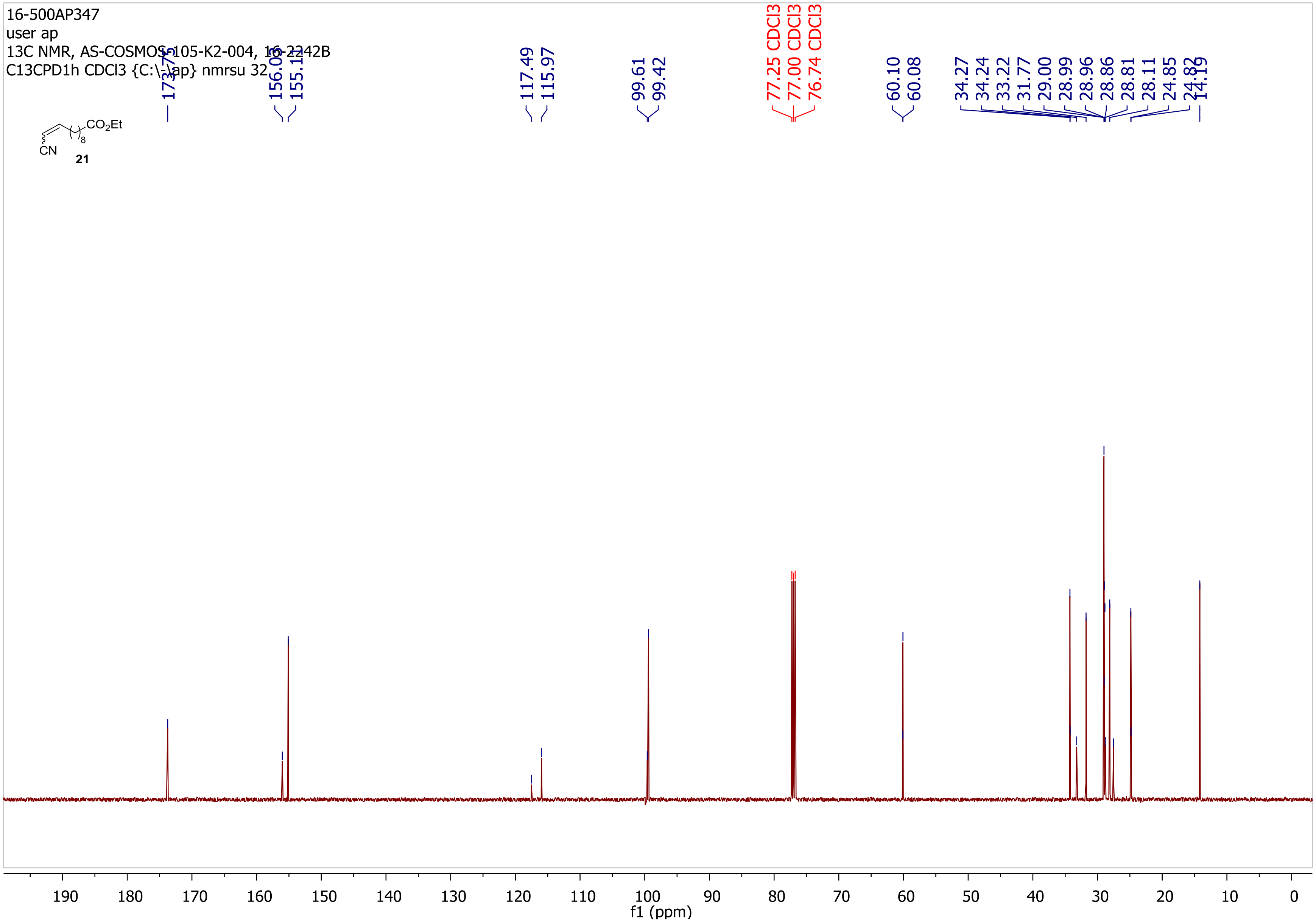
1.00
16.7 16.6 16.5 16.4 16.3
8.41 8.40 8.39 8.38 8.23 8.21 8.21
0.97 2.05
8.5 8.4 8.3 8.2 8.1
7.74 7.57 7.56 7.55 7.53 7.52 7.52 7.51 7.51 7.50 7.37
0.99 5.13 1.02
7.9 7.8 7.7 7.6 7.5 7.4 7.3
7.01 6.99
1.02
7.10 7.05 7.00 6.95 6.90


5.04
1.01
5.1 5.0 4.9
3.17 3.14 3.04 2.93
1.02 1.03 1.01
3.2 3.1 3.0 2.9
2.39 2.37 2.33
1.06 2.99
2.40 2.35 2.30
1.56 1.53 1.53 1.44 1.42 1.42 1.41 1.36 1.35 1.28 1.26
3.11 3.19 6.02 2.96 3.08
1.6 1.5 1.4 1.3 1.2
0.81 0.80 0.49 0.48
3.01 2.99
0.8 0.7 0.6 0.5


16-500AP336
user ap
13C NMR, AS-COSMOS-097-R14, 16-2149B
C13CPD6h CD2Cl2 {C:\ap} nmrsu 21
262.18
157.45
148.79
148.52
143.25
143.18
142.86
137.02
130.51
129.77
129.61
128.01
126.75
126.63
125.87
118.64
113.92
78.72
77.87
54.43 CD2Cl2
54.22 CD2Cl2
54.00 CD2Cl2
53.78 CD2Cl2
53.57 CD2Cl2
48.58
28.08
27.53
27.50
24.75
24.61
22.69
Ph
N
Cl
Ru
Cl
O
NO2
19b
f1 (ppm)

11. NMR spectra of metathesis reaction products




16-500AP347
user ap
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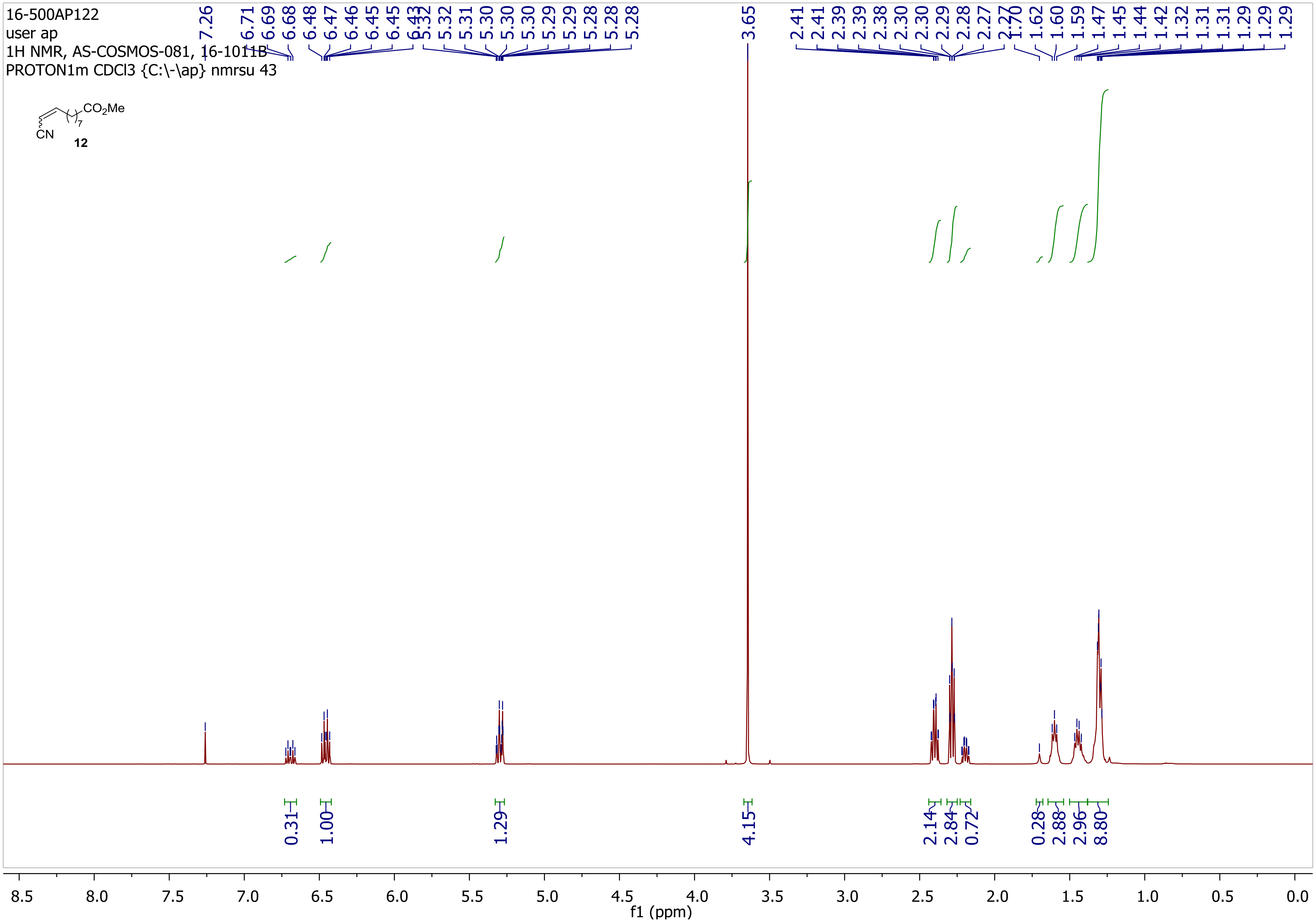
C13CPD1h CDCl3 {C:\-\ap} nmrsu 32
CO2Et
8
CN
21
173.75
156.03
155.11
117.49
115.97
99.61
99.42
77.25 CDCl3
77.00 CDCl3
76.74 CDCl3
60.10
60.08
34.27
34.24
33.22
31.77
29.00
28.99
28.96
28.86
28.81
28.11
24.85
24.82
14.19
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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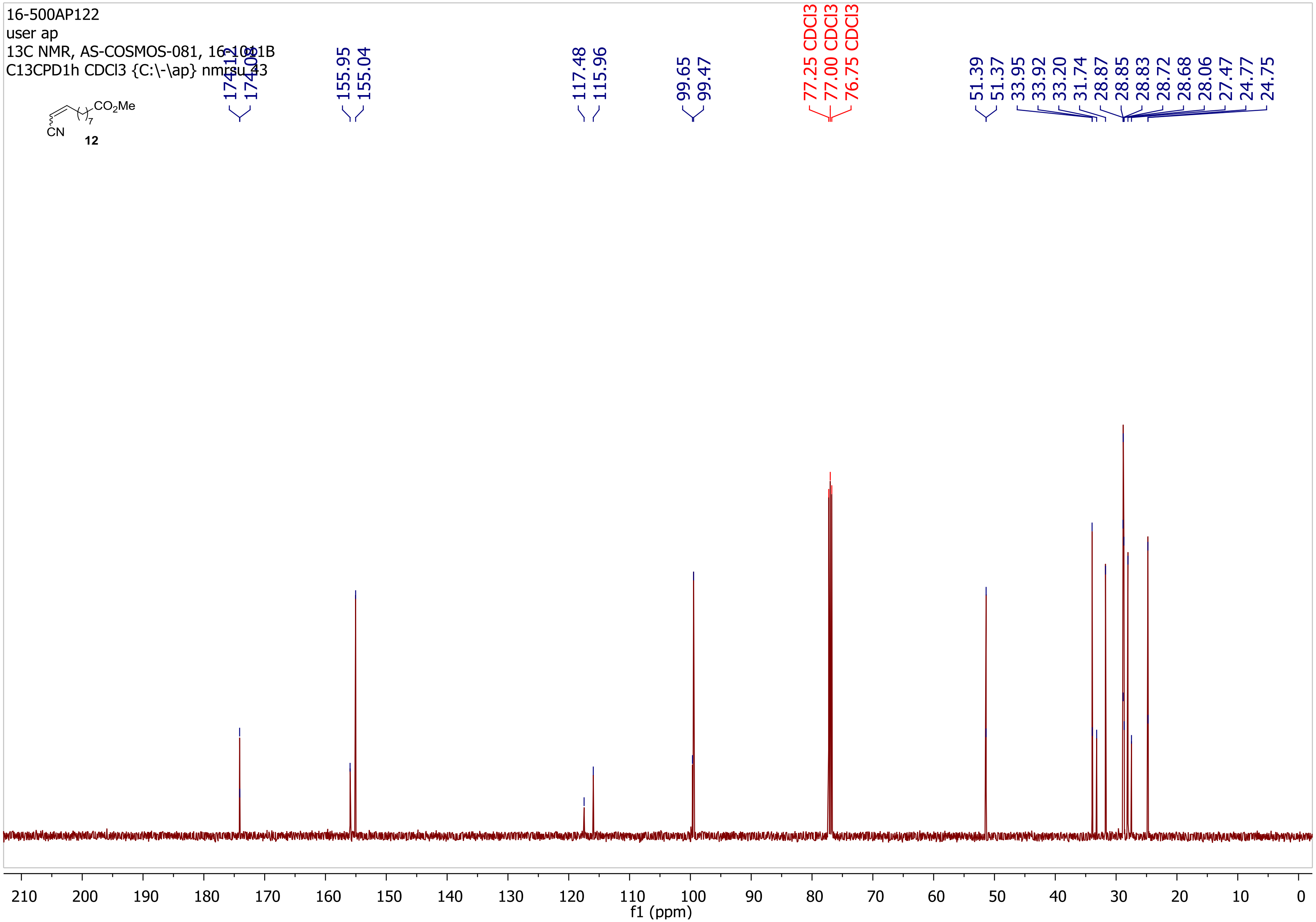
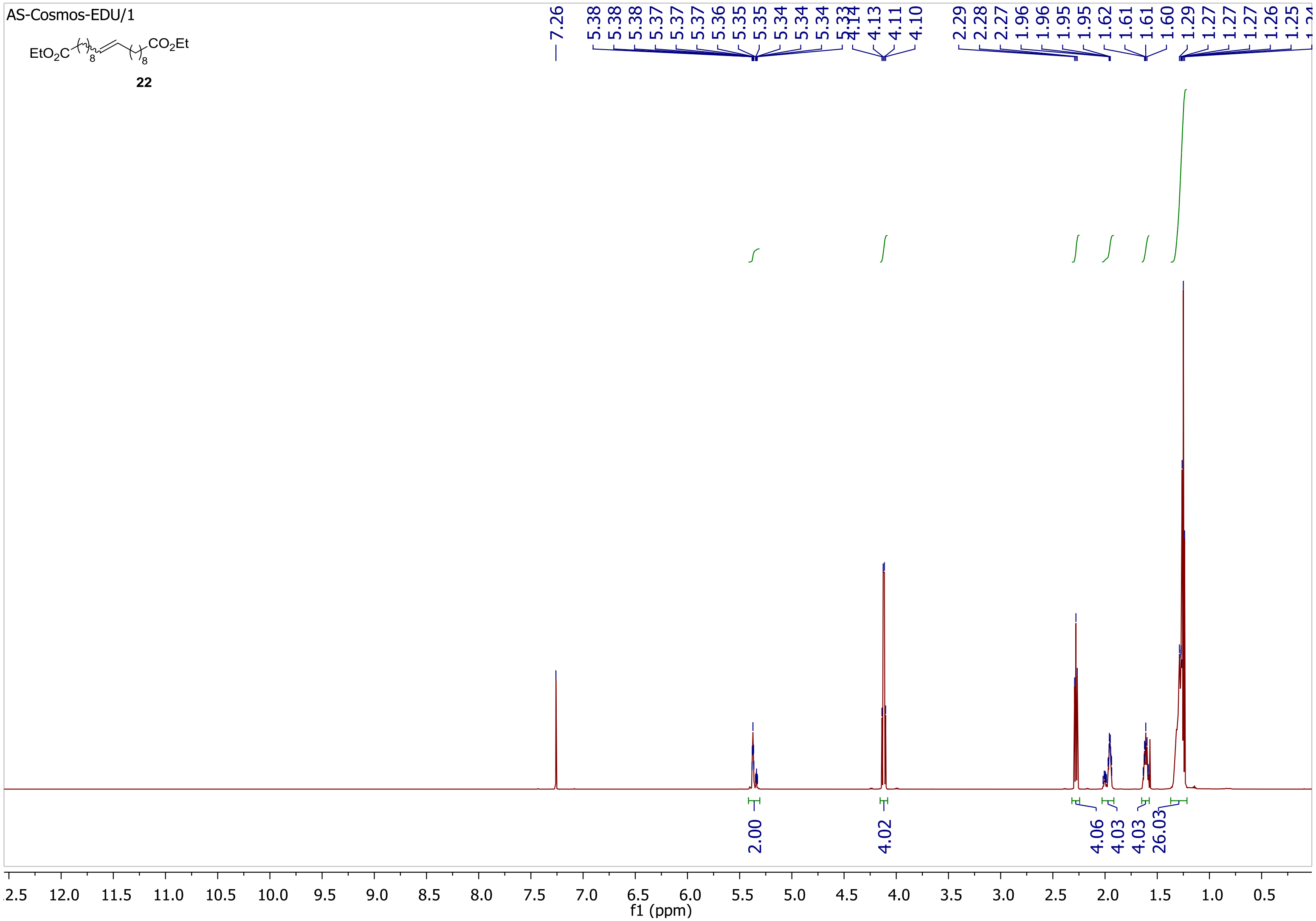
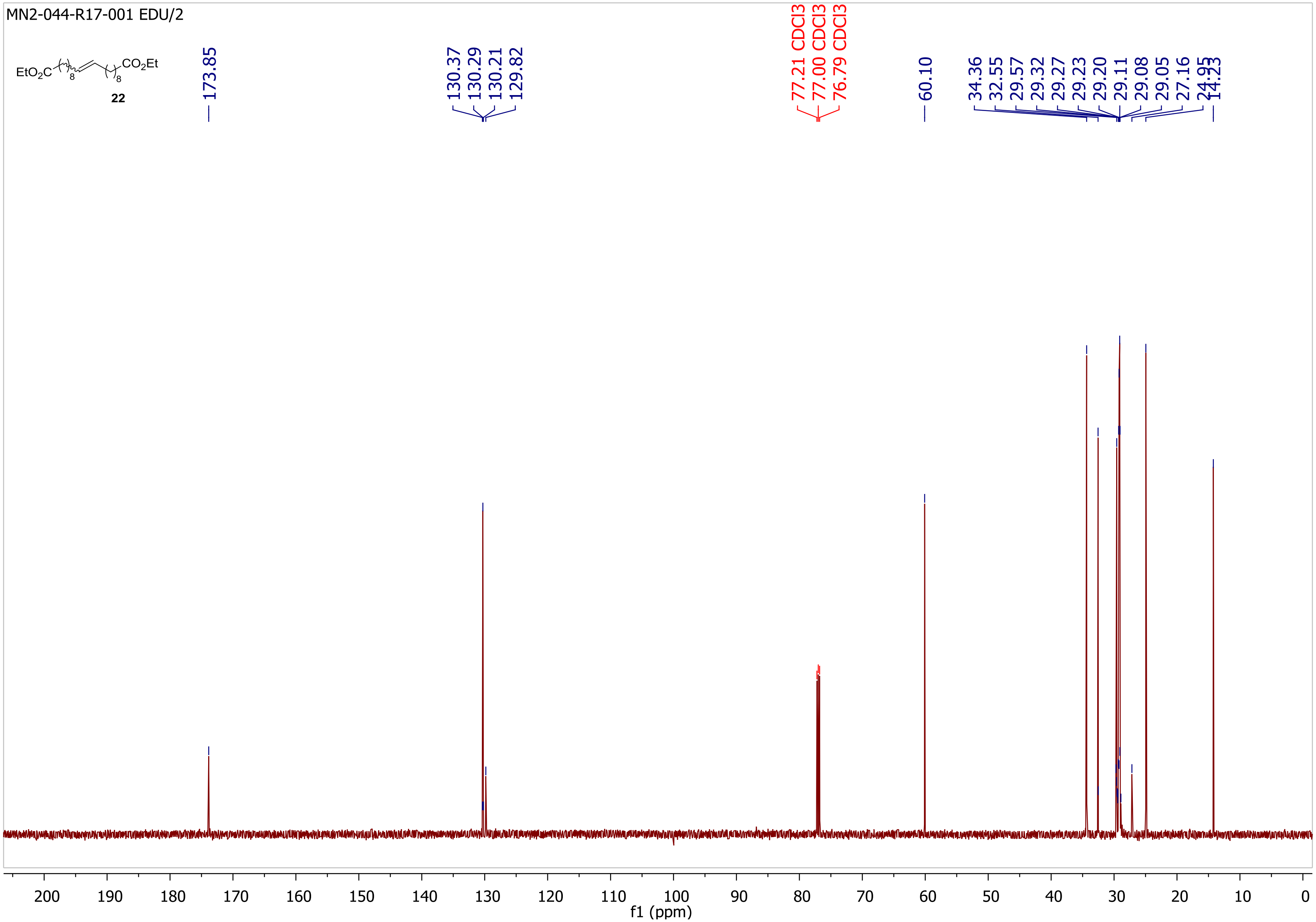
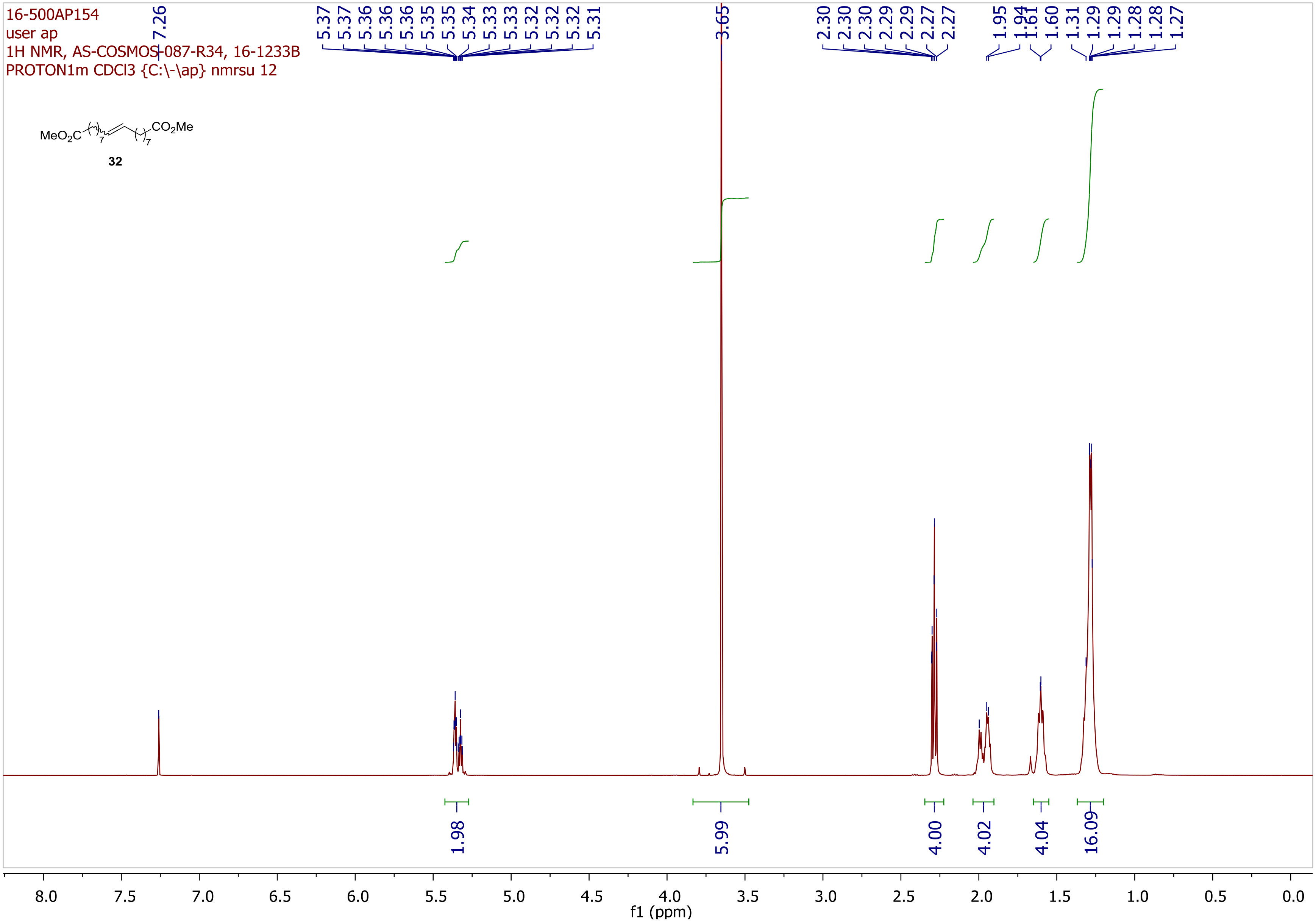
PROTON1m CDCl3 {C:\-\ap} nmrsu 43
CO2Me
7
CN
12
7.26
6.71 6.69 6.68 6.48 6.47 6.46 6.45 6.45 6.43
5.32 5.32 5.31 5.30 5.30 5.30 5.29 5.29 5.28 5.28 5.28
3.65
2.41 2.41 2.39 2.39 2.38 2.30 2.30 2.29 2.28 2.27 2.27
1.70 1.62 1.60 1.59 1.47 1.45 1.44 1.42 1.32 1.31 1.31 1.29 1.29 1.29
0.31 1.00 1.29 4.15 2.14 2.84 0.72 0.28 2.88 2.96 8.80
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



16-500AP122
user ap
13C NMR, AS-COSMOS-081, 16-1011B
C13CPD1h CDCl3 {C:\-\ap} nmrsu 43
CO2Me
CN
7
12
174.12
174.08
155.95
155.04
117.48
115.96
99.65
99.47
77.25 CDCl3
77.00 CDCl3
76.75 CDCl3
51.39
51.37
33.95
33.92
33.20
31.74
28.87
28.85
28.83
28.72
28.68
28.06
27.47
24.77
24.75
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


AS-Cosmos-EDU/1
EtO2C
CO2Et
8
8
22
f1 (ppm)
2.00
4.02
4.06
4.03
4.03
26.03


MN2-044-R17-001 EDU/2
EtO2C CO2Et
8 8
22
173.85
130.37
130.29
130.21
129.82
77.21 CDCl3
77.00 CDCl3
76.79 CDCl3
60.10
34.36
32.55
29.57
29.32
29.27
29.23
29.20
29.11
29.08
29.05
27.16
24.95
14.23
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


16-500AP154
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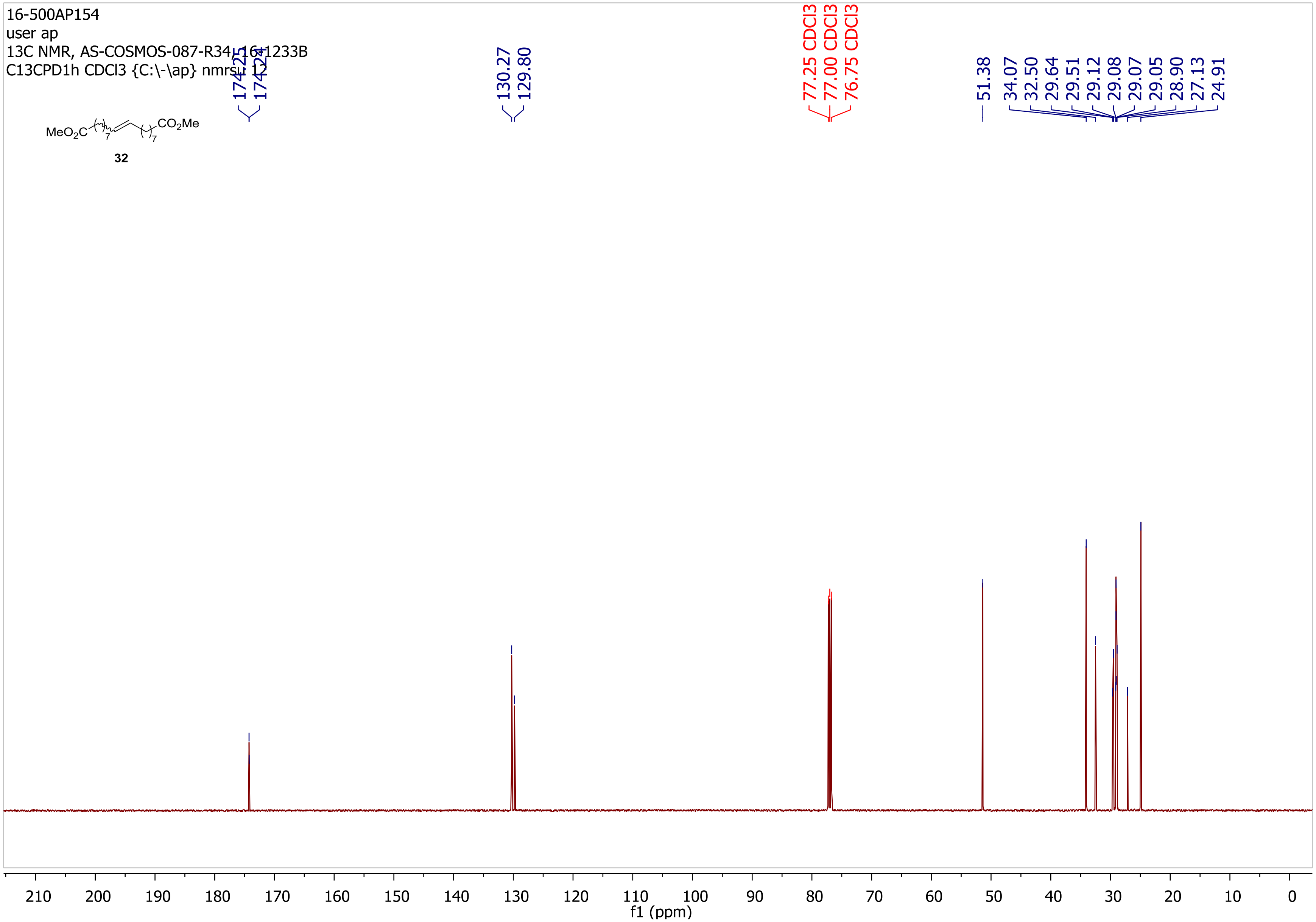
1H NMR, AS-COSMOS-087-R34, 16-1233B
PROTON1m CDCl3 {C:\-\ap} nmrsu 12
32
7.26
5.37 5.37 5.36 5.36 5.36 5.35 5.35 5.34 5.33 5.33 5.32 5.32 5.32 5.31
3.65
2.30 2.30 2.30 2.29 2.29 2.27 2.27
1.95 1.94 1.61 1.60 1.31 1.29 1.29 1.28 1.28 1.27
1.98
5.99
4.00
4.02
4.04
16.09
f1 (ppm)


16-500AP154
user ap
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174.24
130.27
129.80
77.25 CDCl3
77.00 CDCl3
76.75 CDCl3
51.38
34.07
32.50
29.64
29.51
29.12
29.08
29.07
29.05
28.90
27.13
24.91
32
f1 (ppm)

12. Cartesian coordinates of optimized geometries of all intermediates

```
95
3b - pre
Ru2 8.342 3.486 31.637
Cl5 9.107 4.608 33.587
O73 8.374 8.375 26.930
O72 10.445 8.335 26.294
O71 10.466 3.946 30.730
N27 9.518 7.950 26.991
C55 7.882 -0.030 33.421
C54 7.273 1.193 33.748
N26 5.301 3.362 31.739
N25 6.336 1.784 32.837
C49 4.437 5.745 29.046
C34 8.770 6.441 28.775
C51 4.935 5.767 33.335
C45 4.954 4.572 31.071
C50 4.774 4.548 29.678
C38 10.339 4.901 29.794
C47 4.447 6.914 31.150
C43 4.218 2.496 32.220
C59 7.496 1.830 34.992
C44 4.980 1.255 32.645
C46 4.773 5.741 31.830
C48 4.286 6.919 29.771
C56 8.767 -0.589 34.346
C35 9.799 6.902 27.970
C57 9.033 0.041 35.550
C37 11.366 5.385 28.983
C32 7.986 4.902 30.541
C62 6.745 3.084 35.400
H29 9.731 -0.406 36.255
C53 4.970 3.292 28.855
C60 7.551 -0.787 32.153
H32 4.037 7.845 29.257
C33 9.031 5.432 29.700
C58 8.398 1.234 35.869
C42 6.519 2.959 32.170
C36 11.090 6.390 28.067
C40 11.808 2.199 29.696
C39 11.682 3.154 30.864
C41 11.575 2.439 32.190
Cl2 8.221 1.757 29.984
H34 7.768 6.854 28.677
H36 11.864 6.787 27.418
H37 12.373 4.988 29.056
H47 4.322 7.840 31.711
H49 4.305 5.760 27.965
H58 8.607 1.709 36.825
H56 9.250 -1.537 34.114
H51a 5.184 4.750 33.666
H43a 3.685 2.989 33.051
H43b 3.499 2.309 31.414
H44a 4.987 0.494 31.849
H44b 4.606 0.793 33.566
H32a 7.021 5.414 30.478
H62a 6.709 3.745 34.526
H53b 5.318 2.492 29.524
H60b 7.079 -0.084 31.457
H40a 10.945 1.523 29.683
H40b 11.847 2.715 28.731
H40c 12.725 1.609 29.805
H39 12.517 3.870 30.897
H41a 11.417 3.143 33.012
H41b 10.736 1.729 32.178
H41c 12.495 1.872 32.370
C72 5.315 2.751 35.832
H73 4.766 3.671 36.076
H74 4.747 2.220 35.060
H75 5.323 2.117 36.729
C75 7.420 3.882 36.508
H76 6.896 4.838 36.636
H77 7.376 3.362 37.475
H78 8.464 4.103 36.267
C78 6.572 -1.921 32.464
H79 6.277 -2.442 31.544
H80 7.031 -2.660 33.135
H81 5.661 -1.558 32.957
C81 8.788 -1.335 31.449
H82 8.507 -1.760 30.478
H83 9.521 -0.541 31.261
H84 9.274 -2.132 32.027
C84 3.654 2.855 28.214
H85 3.786 1.912 27.670
H86 2.863 2.710 28.960
H87 3.294 3.604 27.497
C87 6.054 3.485 27.796
H88 6.207 2.555 27.236
H89 5.783 4.270 27.078
H90 7.015 3.746 28.256
C90 3.632 6.166 34.025
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H91 3.750 6.123 35.115
H92 3.339 7.192 33.767
H93 2.804 5.504 33.744
C93 6.085 6.676 33.761
H94 6.222 6.631 34.850
H95 7.033 6.370 33.301
H96 5.887 7.723 33.494
110
3b - int1
Ru1 8.285 4.652 31.847
Cl2 7.400 6.646 32.973
O3 5.452 7.520 26.488
O4 6.367 6.791 24.665
O5 10.185 4.262 28.891
N6 6.305 6.888 25.883
C7 7.719 1.263 34.133
C8 7.202 2.565 34.316
N9 5.285 4.033 31.659
N10 6.259 3.086 33.367
C11 4.752 3.818 28.007
C12 7.233 6.174 28.040
C13 4.077 6.652 31.193
C14 4.976 4.419 30.319
C15 5.240 3.509 29.275
C16 9.242 4.835 28.157
C17 3.805 5.875 28.815
C18 4.168 3.647 32.538
C19 7.467 3.311 35.479
C20 4.844 2.711 33.513
C21 4.287 5.623 30.100
C22 4.023 4.978 27.780
C23 8.569 0.756 35.115
C24 7.320 6.192 26.662
C25 8.868 1.492 36.254
C26 9.302 4.868 26.751
C27 7.797 5.447 30.247
C28 6.813 4.648 35.759
H29 9.528 1.074 37.012
C30 6.010 2.227 29.515
C31 7.315 0.368 32.979
H32 3.645 5.200 26.783
C33 8.154 5.470 28.835
C34 8.315 2.750 36.435
C35 6.486 3.820 32.250
C36 8.348 5.528 26.004
C37 10.628 2.120 27.834
C38 11.213 3.442 28.291
C39 12.268 3.253 29.355
Cl40 9.208 2.530 31.144
H41 6.396 6.685 28.508
H42 8.390 5.546 24.920
H43 10.114 4.371 26.232
H44 3.272 6.803 28.612
H45 4.945 3.136 27.180
H46 8.539 3.311 37.341
H47 8.995 -0.238 34.988
H48 4.629 6.323 32.086
H49 3.764 4.542 33.037
H50 3.367 3.179 31.954
H51 4.708 1.654 33.242
H52 4.520 2.849 34.550
H54 6.959 6.139 30.411
H55 6.379 5.026 34.824
H56 6.736 2.405 30.318
H57 6.918 1.005 32.178
H58 10.184 1.610 28.697
H59 9.851 2.241 27.071
H60 11.420 1.489 27.415
H61 11.647 4.001 27.446
H62 12.652 4.216 29.711
H63 11.841 2.703 30.202
H64 13.107 2.679 28.946
C65 5.691 4.484 36.786
H66 5.178 5.440 36.949
H67 4.941 3.748 36.468
H68 6.087 4.146 37.753
C69 7.815 5.696 36.234
H70 7.332 6.678 36.293
H71 8.215 5.460 37.230
H72 8.653 5.789 35.534
C73 6.223 -0.610 33.428
H74 5.870 -1.208 32.578
H75 6.620 -1.303 34.182
H76 5.355 -0.112 33.877
C77 8.476 -0.435 32.396
H78 8.180 -0.858 31.427
H79 9.357 0.192 32.233
H80 8.752 -1.277 33.046
C81 5.072 1.103 29.953
H82 5.642 0.184 30.151
H83 4.519 1.359 30.867
H84 4.334 0.882 29.169
C85 6.834 1.785 28.312
H86 7.524 0.989 28.619
H87 6.209 1.388 27.500
H88 7.434 2.614 27.910
C89 2.595 6.790 31.540
H90 2.456 7.483 32.378
H91 2.027 7.184 30.686
H92 2.143 5.828 31.814

C93 4.664 8.007 30.799
H94 4.493 8.740 31.597
H95 5.750 7.944 30.653
H96 4.213 8.399 29.877
C97 10.333 6.082 31.435
C98 10.506 5.516 32.655
H99 10.058 6.028 33.515
H101 10.815 5.670 30.551
H102 9.802 7.027 31.337
C102 11.419 4.372 32.956
H104 11.547 3.759 32.055
H105 12.413 4.784 33.205
C105 10.942 3.503 34.112
H106 10.925 4.097 35.040
H107 9.903 3.187 33.928
C108 11.806 2.266 34.278
H109 11.723 1.627 33.387
H110 12.865 2.529 34.405
H111 11.498 1.671 35.144
82
3b - int2
Ru1 8.755 4.504 32.032
Cl2 8.247 2.241 32.445
C3 4.974 4.631 31.683
C4 5.551 4.441 32.947
N5 8.241 6.268 34.397
N6 6.435 5.435 33.480
C7 11.584 7.735 34.976
C8 9.377 4.198 36.107
C9 9.580 6.430 34.862
C10 10.296 7.569 34.465
C11 11.408 5.683 36.222
C12 7.142 6.812 35.204
C13 5.247 3.325 33.751
C14 5.943 6.536 34.315
C15 10.121 5.464 35.732
C16 12.133 6.807 35.849
C17 4.125 3.633 31.201
C18 3.842 2.508 31.960
C19 10.481 4.558 32.548
C20 5.771 3.178 35.165
H21 3.179 1.741 31.565
C22 9.716 8.595 33.516
C23 5.172 5.909 30.899
H24 13.138 6.957 36.239
C25 4.385 2.365 33.230
C26 7.795 5.412 33.446
Cl27 8.651 6.451 30.677
H28 11.854 4.952 36.895
H29 12.167 8.607 34.681
H30 4.140 1.487 33.825
H31 3.670 3.749 30.219
H32 8.512 4.105 35.441
H33 7.085 6.285 36.171
H34 7.305 7.878 35.400
H35 5.697 7.401 33.678
H36 5.043 6.235 34.862
H37 6.590 3.896 35.295
H38 8.789 8.179 33.096
H39 6.056 6.424 31.300
C40 4.686 3.538 36.183
H41 5.093 3.515 37.203
H42 4.266 4.537 36.008
H43 3.855 2.823 36.136
C44 6.338 1.794 35.466
H45 6.783 1.783 36.470
H46 5.557 1.022 35.454
H47 7.107 1.516 34.737
C48 3.957 6.818 31.092
H49 4.105 7.778 30.582
H50 3.051 6.353 30.681
H51 3.764 7.022 32.154
C52 5.434 5.665 29.418
H53 5.691 6.608 28.922
H54 6.273 4.974 29.272
H55 4.553 5.253 28.908
C56 9.379 9.887 34.260
H57 8.912 10.613 33.584
H58 8.692 9.713 35.098
H59 10.285 10.350 34.674
C60 10.649 8.872 32.341
H61 10.159 9.534 31.618
H62 11.580 9.359 32.662
H63 10.901 7.943 31.816
C64 8.862 4.259 37.545
H65 8.268 3.365 37.779
H66 9.695 4.304 38.260
H67 8.231 5.140 37.720
C68 10.216 2.941 35.887
H69 9.607 2.049 36.078
H70 10.572 2.874 34.851
H71 11.084 2.900 36.557
H72 10.872 4.910 33.511
C73 11.471 4.112 31.532
H75 12.047 3.266 31.949
H76 10.971 3.725 30.625
C76 12.410 5.265 31.158
H77 11.810 6.055 30.685
H78 12.825 5.699 32.081
C79 13.525 4.814 30.230

H80 14.140 4.034 30.697
H81 13.117 4.400 29.300
H82 14.186 5.645 29.962
97
3b - int3
Ru1 -6.977 -2.008 -2.662
Cl2 -5.011 -0.575 -2.264
C3 -9.102 -1.174 0.219
C4 -8.441 -0.185 -0.532
N5 -8.716 0.206 -4.056
N6 -8.844 0.075 -1.884
C7 -8.896 -0.658 -7.646
C8 -6.189 1.371 -4.954
C9 -8.337 0.060 -5.426
C10 -9.227 -0.601 -6.292
C11 -6.862 0.562 -7.248
C12 -9.667 1.266 -3.670
C13 -7.404 0.608 0.009
C14 -10.037 0.842 -2.265
C15 -7.141 0.647 -5.883
C16 -7.728 -0.080 -8.122
C17 -8.642 -1.418 1.515
C18 -7.587 -0.692 2.045
C19 -6.332 -2.264 -4.348
C20 -6.816 1.786 -0.746
H21 -7.238 -0.902 3.054
C22 -10.530 -1.213 -5.814
C23 -10.350 -1.863 -0.290
H24 -7.488 -0.136 -9.182
C25 -6.986 0.320 1.306
C26 -8.210 -0.412 -2.976
Cl27 -9.073 -3.241 -3.168
H28 -5.945 1.006 -7.632
H29 -9.567 -1.165 -8.339
H30 -6.176 0.897 1.747
H31 -9.129 -2.181 2.119
H32 -6.290 0.938 -3.951
H33 -9.161 2.243 -3.691
H34 -10.516 1.293 -4.358
H35 -10.921 0.184 -2.257
H36 -10.212 1.675 -1.576
H37 -6.776 1.520 -1.811
H38 -10.517 -1.225 -4.715
H39 -10.346 -1.809 -1.386
C40 -7.710 3.018 -0.584
H41 -7.289 3.869 -1.134
H42 -8.730 2.856 -0.952
H43 -7.783 3.303 0.474
C44 -5.397 2.145 -0.322
H45 -4.977 2.867 -1.034
H46 -5.375 2.619 0.669
H47 -4.747 1.266 -0.317
C48 -11.580 -1.128 0.251
H49 -12.502 -1.555 -0.163
H50 -11.631 -1.214 1.345
H51 -11.563 -0.056 0.012
C52 -10.431 -3.342 0.069
H53 -11.314 -3.788 -0.404
H54 -9.558 -3.892 -0.300
H55 -10.522 -3.503 1.151
C56 -11.720 -0.380 -6.296
H57 -12.658 -0.767 -5.880
H58 -11.635 0.678 -6.017
H59 -11.802 -0.416 -7.391
C60 -10.697 -2.664 -6.262
H61 -11.637 -3.068 -5.866
H62 -10.734 -2.756 -7.355
H63 -9.888 -3.295 -5.878
C64 -6.519 2.862 -4.874
H65 -5.864 3.356 -4.144
H66 -6.369 3.348 -5.848
H67 -7.557 3.049 -4.573
C68 -4.724 1.195 -5.339
H69 -4.088 1.567 -4.529
H70 -4.467 0.140 -5.495
H71 -4.466 1.751 -6.251
H72 -5.394 -1.716 -4.555
C73 -6.817 -3.135 -5.454
H75 -6.930 -4.169 -5.089
H76 -7.843 -2.831 -5.710
C76 -5.930 -3.081 -6.694
H77 -5.795 -2.028 -6.988
H78 -4.928 -3.466 -6.452
C79 -6.539 -3.863 -7.846
H80 -6.684 -4.917 -7.578
H81 -7.524 -3.453 -8.109
H82 -5.911 -3.829 -8.743
C97 -5.611 -3.287 -1.175
C98 -6.619 -4.152 -1.492
H99 -7.527 -4.136 -0.884
H100 -4.636 -3.343 -1.655
H101 -5.686 -2.609 -0.325
C102 -6.494 -5.315 -2.422
H103 -7.333 -5.304 -3.134
H104 -5.560 -5.237 -3.001
C105 -6.526 -6.633 -1.645
H106 -5.695 -6.654 -0.925
H107 -7.450 -6.666 -1.048
C108 -6.461 -7.840 -2.565
H109 -7.303 -7.840 -3.270

H110 -5.537 -7.837 -3.157
H111 -6.495 -8.781 -2.006
73
3b - int4
Ru1 8.685 4.741 31.869
Cl2 8.301 2.438 32.078
C3 4.845 4.566 31.908
C4 5.580 4.328 33.077
N5 8.272 6.207 34.448
N6 6.446 5.347 33.594
C7 11.489 7.946 34.962
C8 9.734 4.093 35.834
C9 9.627 6.447 34.821
C10 10.194 7.692 34.509
C11 11.612 5.767 35.979
C12 7.212 6.608 35.385
C13 5.450 3.136 33.817
C14 5.962 6.329 34.571
C15 10.324 5.460 35.544
C16 12.188 6.999 35.696
C17 4.019 3.542 31.442
C18 3.908 2.344 32.130
C19 10.437 4.883 32.239
C20 6.139 2.926 35.150
H21 3.261 1.557 31.748
C22 9.452 8.736 33.704
C23 4.856 5.911 31.218
H24 13.196 7.218 36.044
C25 4.604 2.151 33.316
C26 7.797 5.424 33.453
Cl27 8.231 6.778 30.759
H28 12.177 5.025 36.541
H29 11.956 8.903 34.732
H30 4.491 1.215 33.860
H31 3.445 3.695 30.529
H32 8.852 3.962 35.195
H33 7.271 6.004 36.305
H34 7.330 7.663 35.657
H35 5.607 7.229 34.044
H36 5.134 5.915 35.155
H37 6.905 3.704 35.258
H38 8.512 8.288 33.348
H39 5.728 6.473 31.578
C40 5.147 3.103 36.301
H41 5.663 3.034 37.268
H42 4.630 4.071 36.261
H43 4.376 2.322 36.276
C44 6.850 1.581 35.264
H45 7.394 1.526 36.217
H46 6.141 0.743 35.252
H47 7.562 1.440 34.443
C48 3.594 6.690 31.596
H49 3.611 7.694 31.154
H50 2.693 6.177 31.234
H51 3.493 6.798 32.684
C52 4.992 5.800 29.704
H53 5.116 6.796 29.264
H54 5.869 5.204 29.428
H55 4.105 5.344 29.245
C56 9.117 9.952 34.566
H57 8.533 10.683 33.994
H58 8.539 9.679 35.458
H59 10.030 10.455 34.912
C60 10.242 9.145 32.464
H61 9.650 9.832 31.848
H62 11.178 9.654 32.728
H63 10.480 8.271 31.845
C64 9.287 3.984 37.292
H65 8.801 3.016 37.475
H66 10.145 4.062 37.972
H67 8.578 4.775 37.568
C68 10.689 2.957 35.478
H69 10.187 1.991 35.613
H70 11.008 3.017 34.430
H71 11.584 2.954 36.113
H72 10.933 5.198 33.162
H73 11.086 4.597 31.392
102
3b - int5
Ru1 8.310 4.418 31.810
Cl2 7.956 6.482 33.086
O3 5.609 7.792 26.698
O4 6.393 7.064 24.814
O5 10.097 4.019 28.797
N6 6.384 7.117 26.035
C7 8.194 1.753 34.439
C8 7.274 2.812 34.321
N9 5.331 3.612 31.451
N10 6.346 2.844 33.225
C11 4.357 4.382 27.973
C12 7.317 6.243 28.126
C13 4.553 6.418 31.781
C14 4.938 4.360 30.300
C15 4.892 3.694 29.065
C16 9.206 4.725 28.118
C17 3.957 6.325 29.334
C18 4.308 2.822 32.160
C19 7.187 3.844 35.283
C20 5.161 1.987 33.090
C21 4.485 5.687 30.455

C22 3.882 5.677 28.107
C23 9.119 1.814 35.483
C24 7.364 6.310 26.749
C25 9.107 2.863 36.387
C26 9.239 4.831 26.715
C27 7.883 5.366 30.270
C28 6.049 4.849 35.279
H29 9.846 2.898 37.185
C30 5.390 2.275 28.887
C31 8.111 0.517 33.570
H32 3.473 6.201 27.246
C33 8.200 5.428 28.856
C34 8.137 3.855 36.302
C35 6.480 3.654 32.147
C36 8.321 5.600 26.032
C37 10.233 1.894 27.600
C38 10.996 3.086 28.144
C39 11.990 2.680 29.206
Cl40 8.674 2.255 30.762
H41 6.542 6.801 28.647
H42 8.336 5.669 24.948
H43 9.996 4.297 26.152
H44 3.610 7.353 29.415
H45 4.314 3.890 27.002
H46 8.116 4.649 37.044
H47 9.861 1.024 35.582
H48 5.289 5.907 32.416
H49 3.631 3.499 32.705
H50 3.721 2.233 31.448
H51 5.446 1.028 32.628
H52 4.701 1.786 34.063
H54 7.120 6.121 30.503
H55 5.837 5.120 34.237
H56 5.854 1.953 29.830
H57 7.632 0.802 32.626
H58 9.736 1.376 28.427
H59 9.472 2.174 26.863
H60 10.935 1.204 27.118
H61 11.514 3.628 27.336
H62 12.551 3.542 29.585
H63 11.469 2.204 30.044
H64 12.709 1.967 28.788
C65 4.790 4.219 35.880
H66 3.964 4.941 35.876
H67 4.457 3.328 35.336
H68 4.971 3.920 36.922
C69 6.358 6.142 36.024
H70 5.571 6.878 35.816
H71 6.379 5.988 37.111
H72 7.310 6.574 35.703
C73 7.250 -0.532 34.282
H74 7.118 -1.418 33.649
H75 7.733 -0.855 35.215
H76 6.256 -0.152 34.548
C77 9.468 -0.080 33.216
H78 9.336 -0.879 32.476
H79 10.140 0.670 32.787
H80 9.959 -0.529 34.091
C81 4.236 1.329 28.556
H82 4.591 0.294 28.492
H83 3.441 1.368 29.313
H84 3.778 1.584 27.591
C85 6.479 2.201 27.820
H86 6.853 1.173 27.730
H87 6.112 2.515 26.833
H88 7.328 2.837 28.096
C89 3.203 6.398 32.499
H90 3.295 6.856 33.493
H91 2.454 6.968 31.932
H92 2.811 5.382 32.629
C93 5.041 7.857 31.644
H94 5.202 8.285 32.641
H95 6.001 7.918 31.117
H96 4.316 8.492 31.119
C97 10.542 5.531 31.427
C98 10.561 4.755 32.550
H99 10.241 5.180 33.507
C100 11.249 3.507 32.629
H101 10.961 5.175 30.491
H102 10.185 6.554 31.498
N103 11.852 2.521 32.763
74
3b - int6
Ru1 8.652 4.806 31.764
Cl2 8.235 2.522 31.883
C3 4.832 4.577 31.885
C4 5.585 4.327 33.040
N5 8.290 6.202 34.393
N6 6.454 5.345 33.560
C7 11.524 7.933 34.841
C8 9.791 4.071 35.714
C9 9.655 6.442 34.739
C10 10.214 7.689 34.426
C11 11.674 5.740 35.822
C12 7.248 6.577 35.361
C13 5.478 3.123 33.762
C14 5.981 6.297 34.574
C15 10.371 5.442 35.427
C16 12.245 6.974 35.536
C17 4.008 3.553 31.416

C18 3.917 2.344 32.087
C19 10.427 4.942 32.161
C20 6.199 2.893 35.075
H21 3.271 1.558 31.703
C22 9.454 8.746 33.655
C23 4.825 5.928 31.207
H24 13.265 7.183 35.851
C25 4.632 2.139 33.259
C26 7.797 5.440 33.396
Cl27 8.167 6.854 30.734
H28 12.255 4.988 36.353
H29 11.988 8.890 34.607
H30 4.537 1.193 33.790
H31 3.421 3.714 30.513
H32 8.887 3.949 35.103
H33 7.337 5.957 36.268
H34 7.362 7.628 35.647
H35 5.596 7.200 34.076
H36 5.176 5.854 35.169
H37 6.946 3.689 35.193
H38 8.511 8.300 33.305
H39 5.684 6.502 31.579
C40 5.228 3.005 36.252
H41 5.767 2.921 37.205
H42 4.684 3.959 36.252
H43 4.479 2.203 36.218
C44 6.951 1.566 35.129
H45 7.511 1.491 36.071
H46 6.267 0.709 35.094
H47 7.654 1.475 34.294
C48 3.550 6.686 31.582
H49 3.555 7.692 31.146
H50 2.658 6.162 31.212
H51 3.441 6.785 32.670
C52 4.974 5.828 29.693
H53 5.088 6.829 29.259
H54 5.859 5.244 29.417
H55 4.096 5.364 29.226
C56 9.125 9.940 34.549
H57 8.532 10.682 34.002
H58 8.559 9.644 35.442
H59 10.041 10.437 34.896
C60 10.222 9.189 32.412
H61 9.613 9.879 31.817
H62 11.154 9.708 32.674
H63 10.469 8.333 31.773
C64 9.392 3.938 37.184
H65 8.913 2.967 37.368
H66 10.273 4.006 37.836
H67 8.692 4.725 37.495
C68 10.733 2.939 35.310
H69 10.236 1.972 35.452
H70 11.019 3.008 34.254
H71 11.649 2.928 35.914
H72 10.901 5.208 33.107
C73 11.244 4.642 31.045
N74 11.864 4.387 30.088
89
3b - int7
Ru1 8.594 4.006 32.048
Cl2 8.467 2.170 33.681
C3 5.053 4.773 31.705
C4 5.610 4.523 32.972
N5 8.425 6.229 34.317
N6 6.541 5.456 33.539
C7 11.726 7.867 34.611
C8 9.729 4.357 36.151
C9 9.797 6.444 34.665
C10 10.434 7.592 34.161
C11 11.706 5.914 36.014
C12 7.377 6.959 35.062
C13 5.255 3.396 33.746
C14 6.166 6.720 34.190
C15 10.417 5.584 35.591
C16 12.354 7.042 35.532
C17 4.196 3.807 31.173
C18 3.885 2.660 31.887
C19 10.391 4.036 32.400
C20 5.714 3.227 35.182
H21 3.221 1.915 31.453
C22 9.756 8.555 33.206
C23 5.247 6.095 30.993
H24 13.360 7.277 35.874
C25 4.393 2.467 33.166
C26 7.883 5.316 33.502
Cl27 8.672 6.129 30.805
H28 12.210 5.270 36.732
H29 12.245 8.748 34.236
H30 4.116 1.576 33.724
H31 3.756 3.966 30.190
H32 8.947 4.048 35.447
H33 7.267 6.516 36.064
H34 7.645 8.014 35.167
H35 6.052 7.506 33.426
H36 5.225 6.622 34.739
H37 6.731 3.633 35.263
H38 8.832 8.082 32.844
H39 6.176 6.548 31.363
C40 4.801 4.012 36.128
H41 5.142 3.900 37.165

H42 4.770 5.084 35.902
H43 3.771 3.634 36.070
C44 5.774 1.776 35.645
H45 6.292 1.722 36.611
H46 4.770 1.354 35.795
H47 6.323 1.150 34.936
C48 4.069 7.016 31.326
H49 4.217 8.009 30.885
H50 3.133 6.605 30.924
H51 3.930 7.139 32.408
C52 5.394 5.970 29.482
H53 5.639 6.948 29.052
H54 6.208 5.289 29.210
H55 4.471 5.622 29.002
C56 9.405 9.861 33.924
H57 8.839 10.526 33.261
H58 8.808 9.698 34.831
H59 10.315 10.393 34.232
C60 10.605 8.858 31.973
H61 10.053 9.521 31.296
H62 11.544 9.363 32.235
H63 10.841 7.947 31.412
C64 9.074 4.655 37.501
H65 8.521 3.777 37.857
H66 9.832 4.907 38.255
H67 8.372 5.497 37.451
C68 10.668 3.162 36.285
H69 10.085 2.262 36.511
H70 11.216 2.970 35.355
H71 11.399 3.299 37.094
H72 10.710 3.243 33.099
C73 11.467 4.895 31.861
H74 11.585 4.653 30.787
H75 11.135 5.943 31.863
C76 12.788 4.730 32.608
H77 12.610 4.854 33.687
H78 13.163 3.705 32.469
C79 13.819 5.743 32.143
H80 14.021 5.642 31.069
H81 13.458 6.766 32.317
H82 14.769 5.630 32.676
C83 8.487 3.235 29.919
C84 8.222 2.192 30.799
H85 7.192 1.943 31.051
H86 8.970 1.442 31.040
H87 7.678 3.812 29.472
C88 9.761 3.377 29.290
N89 10.803 3.484 28.783
88
3b - int8
Ru1 8.226 4.619 31.864
Cl2 7.391 6.594 33.021
C3 7.703 1.284 34.208
C4 7.166 2.569 34.428
N5 5.280 3.897 31.695
N6 6.219 3.094 33.493
C7 5.036 3.900 28.008
C8 4.204 6.581 31.294
C9 5.060 4.357 30.362
C10 5.339 3.472 29.298
C11 4.210 6.003 28.841
C12 4.144 3.534 32.555
C13 7.420 3.291 35.607
C14 4.813 2.683 33.615
C15 4.503 5.630 30.154
C16 4.471 5.149 27.781
C17 8.522 0.744 35.198
C18 8.791 1.444 36.366
C19 7.727 5.340 30.276
C20 6.787 4.637 35.890
H21 9.429 1.001 37.129
C22 5.944 2.103 29.546
C23 7.371 0.449 32.988
H24 4.238 5.460 26.765
C25 8.248 2.704 36.566
C26 6.463 3.750 32.337
Cl27 9.217 2.741 30.684
H28 3.776 6.984 28.650
H29 5.246 3.247 27.164
H30 8.461 3.243 37.487
H31 8.954 -0.244 35.051
H32 4.710 6.202 32.194
H33 3.699 4.443 32.986
H34 3.374 3.008 31.980
H35 4.721 1.605 33.414
H36 4.446 2.880 34.629
H37 7.273 6.340 30.210
H38 6.332 5.006 34.960
H39 6.673 2.204 30.361
H40 6.917 1.108 32.234
C41 5.692 4.496 36.949
H42 5.190 5.457 37.114
H43 4.930 3.761 36.659
H44 6.111 4.167 37.909
C45 7.818 5.676 36.319
H46 7.341 6.658 36.420
H47 8.275 5.426 37.286
H48 8.611 5.777 35.569
C49 6.364 -0.647 33.350
H50 6.074 -1.214 32.456

H51 6.808 -1.355 34.062
H52 5.452 -0.254 33.814
C53 8.604 -0.186 32.350
H54 8.332 -0.625 31.381
H55 9.385 0.558 32.165
H56 9.012 -0.993 32.973
C57 4.875 1.094 29.971
H58 5.334 0.115 30.166
H59 4.347 1.400 30.883
H60 4.126 0.963 29.179
C61 6.727 1.557 28.360
H62 7.272 0.657 28.670
H63 6.074 1.276 27.522
H64 7.471 2.277 28.003
C65 2.696 6.651 31.546
H66 2.479 7.277 32.421
H67 2.180 7.092 30.684
H68 2.255 5.661 31.715
C69 4.763 7.980 31.050
H70 4.592 8.606 31.934
H71 5.845 7.953 30.883
H72 4.282 8.473 30.196
C73 10.216 5.944 31.121
C74 10.431 5.537 32.403
H75 10.097 6.202 33.206
H76 10.615 5.377 30.280
H77 9.773 6.917 30.920
C78 11.292 4.378 32.796
H79 11.417 3.701 31.940
H80 12.291 4.772 33.048
C81 10.754 3.608 33.996
H82 10.681 4.279 34.867
H83 9.725 3.266 33.789
C84 11.614 2.399 34.317
H85 11.581 1.678 33.490
H86 12.663 2.687 34.468
H87 11.268 1.887 35.221
H89 7.934 4.817 29.329
80
3b - int9
Ru1 8.270 4.400 31.788
Cl2 7.372 6.457 32.756
C3 8.170 1.610 34.185
C4 7.318 2.731 34.241
N5 5.212 3.693 31.540
N6 6.265 2.879 33.274
C7 4.854 4.065 27.874
C8 4.129 6.406 31.432
C9 4.936 4.279 30.262
C10 5.122 3.484 29.113
C11 4.187 6.123 28.929
C12 4.152 3.132 32.402
C13 7.454 3.727 35.234
C14 4.951 2.213 33.301
C15 4.446 5.594 30.194
C16 4.399 5.373 27.782
C17 9.245 1.568 35.075
C18 9.451 2.586 35.995
C19 7.958 5.131 30.165
C20 6.392 4.782 35.468
H21 10.307 2.543 36.667
C22 5.528 2.026 29.200
C23 7.879 0.427 33.290
H24 4.197 5.809 26.806
C25 8.553 3.639 36.089
C26 6.397 3.621 32.158
Cl27 8.703 2.290 30.605
H28 3.814 7.142 28.845
H29 4.998 3.481 26.967
H30 8.701 4.404 36.848
H31 9.930 0.724 35.043
H32 4.696 5.979 32.271
H33 3.676 3.948 32.969
H34 3.390 2.625 31.803
H35 5.042 1.200 32.877
H36 4.563 2.138 34.321
H37 7.623 6.173 30.079
H38 5.946 5.042 34.501
H39 6.110 1.885 30.120
H40 7.334 0.796 32.410
C41 5.304 4.207 36.378
H42 4.510 4.946 36.542
H43 4.843 3.300 35.968
H44 5.725 3.941 37.357
C45 6.928 6.072 36.077
H46 6.147 6.841 36.057
H47 7.222 5.937 37.126
H48 7.781 6.459 35.510
C49 6.998 -0.565 34.055
H50 6.712 -1.406 33.412
H51 7.544 -0.971 34.918
H52 6.082 -0.102 34.442
C53 9.127 -0.283 32.780
H54 8.847 -1.026 32.025
H55 9.820 0.421 32.309
H56 9.649 -0.820 33.583
C57 4.282 1.139 29.269
H58 4.565 0.082 29.354
H59 3.639 1.384 30.124
H60 3.674 1.253 28.361

C61 6.421 1.578 28.049
H62 6.805 0.571 28.250
H63 5.878 1.537 27.096
H64 7.287 2.240 27.935
C65 2.631 6.317 31.735
H66 2.391 6.849 32.664
H67 2.050 6.778 30.925
H68 2.282 5.281 31.833
C69 4.553 7.866 31.317
H70 4.420 8.368 32.283
H71 5.610 7.952 31.046
H72 3.950 8.412 30.580
C73 10.473 4.103 32.073
C74 10.175 5.360 32.581
H75 9.956 5.503 33.640
H76 10.502 3.242 32.740
H77 10.930 3.974 31.096
H79 8.125 4.545 29.252
C80 10.477 6.548 31.844
N81 10.761 7.505 31.246
74
17a - pre
Ru1 -6.657 -2.051 -3.147
Cl1 -8.075 -3.937 -2.832
Cl2 -4.982 -0.500 -2.442
N1 -8.422 0.259 -3.913
C2 -9.273 1.354 -3.302
C3 -10.723 1.251 -3.763
H3A -11.204 0.315 -3.472
H3B -11.296 2.074 -3.320
H3C -10.791 1.350 -4.853
C4 -8.754 2.734 -3.678
H4A -7.713 2.873 -3.372
H4B -8.837 2.923 -4.755
H4C -9.362 3.484 -3.159
C5 -9.062 1.067 -1.814
H5A -8.221 1.676 -1.450
H5B -9.947 1.320 -1.215
C6 -8.683 -0.415 -1.704
C7 -9.919 -1.318 -1.569
H7A -10.612 -1.237 -2.413
H7B -9.628 -2.370 -1.492
H7C -10.462 -1.033 -0.659
C8 -7.777 -0.679 -0.505
H8A -7.488 -1.739 -0.448
H8B -6.864 -0.077 -0.538
H8C -8.324 -0.449 0.419
C9 -8.005 -0.673 -3.056
C10 -8.207 0.248 -5.335
C11 -9.078 -0.509 -6.143
C12 -10.117 -1.462 -5.603
H12B -10.190 -1.381 -4.515
H12C -11.102 -1.181 -6.005
C13 -8.913 -0.448 -7.528
H13A -9.588 -1.022 -8.162
C14 -7.906 0.315 -8.097
H36 -7.796 0.357 -9.179
C16 -7.021 1.005 -7.282
H16A -6.207 1.572 -7.729
C17 -7.138 0.977 -5.891
C18 -6.066 1.648 -5.068
H18A -6.138 2.739 -5.196
H18B -6.217 1.438 -4.003
C19 -6.294 -2.137 -4.938
H19A -6.880 -1.630 -5.710
C20 -5.157 -2.888 -5.411
C21 -4.762 -2.832 -6.748
H21A -5.320 -2.228 -7.461
C22 -3.644 -3.541 -7.154
N23 -3.225 -3.477 -8.552
O24 -3.885 -2.781 -9.307
O25 -2.241 -4.125 -8.877
C26 -2.907 -4.314 -6.261
H26A -2.039 -4.853 -6.627
C27 -3.287 -4.385 -4.930
H27A -2.707 -4.990 -4.240
C28 -4.405 -3.670 -4.500
O29 -4.867 -3.629 -3.240
C30 -4.320 -4.494 -2.206
H30A -3.224 -4.427 -2.282
C31 -4.768 -3.913 -0.887
H31A -4.477 -2.861 -0.803
H31B -5.859 -3.995 -0.792
H31C -4.309 -4.477 -0.067
C32 -4.814 -5.908 -2.423
H32A -4.430 -6.561 -1.631
H32B -5.910 -5.916 -2.390
H32C -4.496 -6.320 -3.387
C68 -4.663 1.182 -5.443
H69 -3.918 1.653 -4.793
H70 -4.568 0.097 -5.307
H71 -4.405 1.422 -6.481
C71 -9.810 -2.915 -5.960
H72 -10.587 -3.581 -5.570
H73 -9.749 -3.065 -7.045
H74 -8.860 -3.234 -5.513
89
17a - int1
Ru1 -6.798 -2.145 -3.187
Cl2 -4.996 -0.592 -2.556

O3 -5.217 -0.203 -9.392
O4 -5.679 -1.747 -10.841
O5 -6.839 -4.806 -5.529
N6 -5.578 -1.331 -9.695
C7 -5.895 -1.803 -7.310
C8 -6.585 -3.989 -6.542
C9 -5.920 -2.250 -8.616
C10 -6.602 -4.416 -7.884
C11 -6.305 -1.932 -4.959
C12 -6.259 -2.632 -6.235
C13 -6.284 -3.557 -8.917
C14 -8.813 -6.066 -6.173
C15 -7.358 -6.137 -5.753
C16 -7.186 -6.877 -4.448
Cl17 -8.632 -3.746 -3.293
H18 -5.622 -0.767 -7.124
H19 -6.302 -3.885 -9.952
H20 -6.867 -5.439 -8.123
H21 -5.881 -0.930 -5.098
H22 -9.386 -5.560 -5.386
H23 -8.956 -5.517 -7.110
H24 -9.210 -7.078 -6.307
H25 -6.740 -6.620 -6.526
H26 -6.137 -6.892 -4.134
H27 -7.786 -6.390 -3.669
H28 -7.525 -7.913 -4.562
C29 -4.868 -3.837 -3.219
C30 -5.317 -3.851 -1.941
H31 -4.947 -3.071 -1.266
H32 -5.149 -4.621 -3.920
H33 -4.137 -3.099 -3.539
N35 -8.393 0.366 -3.863
C36 -9.259 1.441 -3.224
C37 -10.708 1.306 -3.684
H38 -11.141 0.327 -3.466
H39 -11.315 2.065 -3.178
H40 -10.787 1.484 -4.764
C41 -8.792 2.848 -3.562
H42 -7.762 3.026 -3.241
H43 -8.875 3.066 -4.634
H44 -9.436 3.556 -3.028
C45 -9.032 1.125 -1.749
H46 -8.181 1.720 -1.388
H47 -9.905 1.375 -1.133
C48 -8.666 -0.364 -1.670
C49 -9.913 -1.239 -1.470
H50 -10.629 -1.170 -2.295
H51 -9.649 -2.296 -1.377
H52 -10.419 -0.915 -0.551
C53 -7.706 -0.623 -0.512
H54 -7.425 -1.684 -0.442
H55 -6.785 -0.040 -0.609
H56 -8.205 -0.362 0.431
C57 -8.033 -0.620 -3.047
C58 -8.152 0.454 -5.281
C59 -9.028 -0.201 -6.166
C60 -10.094 -1.181 -5.743
H61 -10.102 -1.308 -4.655
H62 -11.077 -0.773 -6.024
C63 -8.893 0.056 -7.533
H64 -9.576 -0.431 -8.227
C65 -7.922 0.918 -8.014
H66 -7.836 1.114 -9.080
C67 -7.031 1.509 -7.129
H68 -6.240 2.150 -7.515
C69 -7.112 1.284 -5.755
C70 -6.063 1.914 -4.867
H71 -6.210 3.005 -4.870
H72 -6.179 1.572 -3.832
C73 -4.632 1.611 -5.305
H74 -3.922 2.134 -4.656
H75 -4.407 0.542 -5.212
H76 -4.432 1.917 -6.339
C77 -9.911 -2.559 -6.372
H78 -10.765 -3.204 -6.137
H79 -9.809 -2.513 -7.464
H80 -9.021 -3.042 -5.957
C81 -6.111 -4.959 -1.325
H82 -6.659 -5.496 -2.110
H83 -5.395 -5.679 -0.892
C84 -7.077 -4.518 -0.234
H85 -6.521 -4.011 0.571
H86 -7.775 -3.783 -0.659
C87 -7.875 -5.687 0.315
H88 -8.477 -6.141 -0.484
H89 -7.218 -6.468 0.721
H90 -8.560 -5.378 1.111
61
17a - int2
C19 -6.373 -2.154 -5.010
H72 -6.851 -1.565 -5.803
C73 -5.392 -3.195 -5.420
H75 -4.536 -2.691 -5.904
H76 -4.978 -3.720 -4.540
C76 -6.021 -4.209 -6.381
H77 -6.851 -4.711 -5.864
H78 -6.464 -3.668 -7.231
C79 -5.007 -5.230 -6.869
H80 -4.177 -4.744 -7.398
H81 -4.579 -5.789 -6.028

H82 -5.461 -5.954 -7.552
Ru5 -6.696 -2.026 -3.238
Cl6 -8.085 -3.913 -2.930
Cl7 -4.844 -0.741 -2.523
N8 -8.404 0.331 -3.837
C9 -9.242 1.403 -3.173
C10 -10.704 1.304 -3.597
H11 -11.170 0.356 -3.318
H12 -11.270 2.109 -3.113
H13 -10.804 1.435 -4.681
C14 -8.743 2.797 -3.524
H15 -7.696 2.938 -3.240
H16 -8.854 3.014 -4.593
H17 -9.344 3.528 -2.970
C18 -8.993 1.075 -1.699
H19 -8.148 1.679 -1.338
H20 -9.863 1.307 -1.072
C21 -8.604 -0.410 -1.636
C22 -9.831 -1.319 -1.473
H23 -10.548 -1.230 -2.297
H24 -9.535 -2.371 -1.417
H25 -10.348 -1.047 -0.544
C26 -7.642 -0.688 -0.485
H27 -7.352 -1.747 -0.449
H28 -6.729 -0.089 -0.563
H29 -8.139 -0.456 0.466
C30 -7.974 -0.629 -3.016
C31 -8.185 0.374 -5.255
C32 -9.068 -0.326 -6.098
C33 -10.130 -1.278 -5.606
H34 -10.209 -1.242 -4.515
H35 -11.106 -0.960 -6.002
C36 -8.900 -0.194 -7.477
H37 -9.586 -0.720 -8.141
C38 -7.882 0.584 -8.006
H39 -7.775 0.685 -9.084
C40 -6.984 1.214 -7.156
H41 -6.162 1.793 -7.573
C42 -7.102 1.112 -5.769
C43 -6.029 1.728 -4.905
H44 -6.103 2.825 -4.961
H45 -6.181 1.449 -3.855
C46 -4.624 1.294 -5.310
H47 -3.883 1.718 -4.626
H48 -4.528 0.203 -5.252
H49 -4.365 1.612 -6.327
C50 -9.850 -2.721 -6.022
H51 -10.661 -3.381 -5.698
H52 -9.745 -2.820 -7.109
H53 -8.930 -3.086 -5.550

76
17a - int3
C1 -6.061 -2.175 -4.677
H2 -5.695 -1.207 -5.056
C3 -5.938 -3.293 -5.650
H4 -4.948 -3.756 -5.480
H5 -6.674 -4.081 -5.428
C6 -6.010 -2.828 -7.104
H7 -6.952 -2.286 -7.266
H8 -5.207 -2.098 -7.290
C9 -5.911 -3.994 -8.071
H10 -4.978 -4.555 -7.928
H11 -6.742 -4.696 -7.920
H12 -5.942 -3.660 -9.114
Ru13 -6.594 -2.197 -2.930
Cl14 -8.253 -3.949 -3.208
Cl15 -4.847 -0.587 -2.333
N16 -8.303 0.144 -3.894
C17 -9.235 1.226 -3.375
C18 -10.659 1.007 -3.873
H19 -11.069 0.034 -3.590
H20 -11.307 1.783 -3.449
H21 -10.707 1.097 -4.965
C22 -8.790 2.614 -3.808
H23 -7.774 2.836 -3.469
H24 -8.841 2.744 -4.895
H25 -9.465 3.349 -3.352
C26 -9.064 1.038 -1.869
H27 -8.281 1.722 -1.511
H28 -9.986 1.263 -1.318
C29 -8.595 -0.407 -1.654
C30 -9.779 -1.363 -1.447
H31 -10.493 -1.345 -2.276
H32 -9.446 -2.402 -1.347
H33 -10.311 -1.070 -0.533
C34 -7.673 -0.496 -0.441
H35 -7.336 -1.525 -0.254
H36 -6.781 0.127 -0.564
H37 -8.224 -0.172 0.452
C38 -7.892 -0.732 -2.981
C39 -8.041 0.107 -5.309
C40 -8.901 -0.638 -6.140
C41 -9.918 -1.630 -5.626
H42 -9.818 -1.753 -4.543
H43 -10.930 -1.240 -5.812
C44 -8.780 -0.467 -7.521
H45 -9.457 -1.010 -8.179
C46 -7.813 0.365 -8.063
H47 -7.742 0.489 -9.141
C48 -6.916 1.014 -7.228

H49 -6.129 1.632 -7.657
C50 -7.006 0.902 -5.840
C51 -5.981 1.605 -4.981
H52 -6.189 2.686 -4.986
H53 -6.066 1.269 -3.939
C54 -4.542 1.383 -5.437
H55 -3.850 1.834 -4.718
H56 -4.298 0.315 -5.488
H57 -4.340 1.824 -6.420
C58 -9.780 -3.009 -6.264
H59 -10.529 -3.693 -5.851
H60 -9.909 -2.985 -7.353
H61 -8.798 -3.441 -6.038
C62 -4.756 -3.954 -2.703
C63 -5.237 -3.851 -1.443
H64 -4.860 -3.033 -0.817
H65 -5.058 -4.788 -3.337
H66 -3.978 -3.284 -3.062
C67 -6.109 -4.870 -0.783
H68 -6.611 -5.476 -1.550
H69 -5.447 -5.551 -0.220
C70 -7.141 -4.293 0.177
H71 -6.635 -3.685 0.944
H72 -7.802 -3.616 -0.384
C73 -7.985 -5.377 0.823
H74 -8.536 -5.937 0.056
H75 -7.364 -6.093 1.377
H76 -8.718 -4.960 1.522
52
17a - int4
C1 -6.358 -2.130 -5.031
H2 -6.822 -1.571 -5.849
Ru3 -6.675 -2.022 -3.263
Cl4 -8.044 -3.900 -2.909
Cl5 -4.893 -0.685 -2.486
N6 -8.396 0.324 -3.860
C7 -9.237 1.397 -3.195
C8 -10.697 1.306 -3.629
H9 -11.171 0.360 -3.356
H10 -11.260 2.113 -3.147
H11 -10.789 1.440 -4.714
C12 -8.730 2.790 -3.537
H13 -7.684 2.925 -3.249
H14 -8.837 3.013 -4.606
H15 -9.330 3.520 -2.982
C16 -8.997 1.060 -1.723
H17 -8.150 1.657 -1.355
H18 -9.869 1.293 -1.098
C19 -8.616 -0.427 -1.664
C20 -9.851 -1.330 -1.526
H21 -10.552 -1.238 -2.361
H22 -9.562 -2.383 -1.461
H23 -10.384 -1.053 -0.606
C24 -7.680 -0.716 -0.495
H25 -7.390 -1.776 -0.462
H26 -6.766 -0.115 -0.544
H27 -8.202 -0.495 0.445
C28 -7.972 -0.635 -3.040
C29 -8.186 0.369 -5.281
C30 -9.078 -0.330 -6.114
C31 -10.131 -1.287 -5.609
H32 -10.190 -1.258 -4.517
H33 -11.114 -0.966 -5.984
C34 -8.931 -0.189 -7.495
H35 -9.623 -0.713 -8.152
C36 -7.922 0.597 -8.031
H37 -7.830 0.705 -9.110
C38 -7.014 1.224 -7.191
H39 -6.200 1.809 -7.615
C40 -7.114 1.114 -5.803
C41 -6.032 1.731 -4.949
H42 -6.095 2.828 -5.022
H43 -6.185 1.470 -3.895
C44 -4.634 1.272 -5.350
H45 -3.885 1.708 -4.681
H46 -4.549 0.182 -5.264
H47 -4.379 1.559 -6.376
C48 -9.861 -2.728 -6.040
H49 -10.651 -3.392 -5.675
H50 -9.813 -2.826 -7.131
H51 -8.915 -3.089 -5.619
H52 -5.594 -2.879 -5.304
81
17a - int5
Ru1 -6.840 -2.190 -3.287
Cl2 -5.073 -0.605 -2.610
O3 -5.405 -0.348 -9.582
O4 -5.868 -1.951 -10.964
O5 -6.743 -4.885 -5.537
N6 -5.742 -1.495 -9.837
C7 -5.982 -1.897 -7.430
C8 -6.555 -4.093 -6.579
C9 -6.018 -2.388 -8.719
C10 -6.588 -4.561 -7.906
C11 -6.347 -1.986 -5.069
C12 -6.279 -2.712 -6.323
C13 -6.331 -3.720 -8.968
C14 -8.706 -6.214 -6.078
C15 -7.242 -6.240 -5.689
C16 -7.015 -6.912 -4.356

Cl17 -8.640 -3.788 -3.432
H18 -5.756 -0.844 -7.282
H19 -6.360 -4.078 -9.993
H20 -6.815 -5.602 -8.106
H21 -5.999 -0.959 -5.234
H22 -9.277 -5.699 -5.297
H23 -8.881 -5.699 -7.030
H24 -9.079 -7.240 -6.173
H25 -6.632 -6.738 -6.460
H26 -5.951 -6.933 -4.093
H27 -7.561 -6.382 -3.567
H28 -7.372 -7.946 -4.399
C29 -4.849 -3.805 -3.360
C30 -5.363 -3.784 -2.101
H31 -5.023 -3.021 -1.397
C32 -6.130 -4.852 -1.542
H33 -5.090 -4.604 -4.055
H34 -4.119 -3.053 -3.647
N35 -6.703 -5.722 -1.025
N37 -8.420 0.337 -3.944
C38 -9.257 1.404 -3.253
C39 -10.698 1.361 -3.754
H40 -11.183 0.395 -3.604
H41 -11.284 2.120 -3.221
H42 -10.738 1.603 -4.823
C43 -8.722 2.806 -3.495
H44 -7.693 2.918 -3.143
H45 -8.774 3.091 -4.552
H46 -9.347 3.509 -2.931
C47 -9.067 0.987 -1.795
H48 -8.189 1.512 -1.391
H49 -9.934 1.246 -1.174
C50 -8.783 -0.521 -1.808
C51 -10.082 -1.340 -1.731
H52 -10.735 -1.209 -2.598
H53 -9.870 -2.409 -1.655
H54 -10.634 -1.021 -0.837
C55 -7.893 -0.950 -0.642
H56 -7.688 -2.032 -0.677
H57 -6.940 -0.412 -0.632
H58 -8.421 -0.768 0.303
C59 -8.099 -0.692 -3.171
C60 -8.164 0.466 -5.357
C61 -9.034 -0.167 -6.265
C62 -10.115 -1.148 -5.879
H63 -10.164 -1.274 -4.793
H64 -11.087 -0.738 -6.195
C65 -8.875 0.107 -7.627
H66 -9.554 -0.363 -8.337
C67 -7.885 0.961 -8.082
H68 -7.778 1.164 -9.145
C69 -7.000 1.527 -7.176
H70 -6.193 2.159 -7.541
C71 -7.107 1.288 -5.806
C72 -6.055 1.880 -4.896
H73 -6.185 2.973 -4.866
H74 -6.183 1.509 -3.872
C75 -4.626 1.567 -5.333
H76 -3.914 2.013 -4.631
H77 -4.436 0.487 -5.326
H78 -4.397 1.949 -6.335
C79 -9.910 -2.525 -6.504
H80 -10.761 -3.178 -6.281
H81 -9.792 -2.477 -7.595
H82 -9.021 -3.002 -6.077
53
17a - int6
C1 -6.315 -2.148 -4.970
H2 -6.834 -1.650 -5.791
C3 -5.272 -3.055 -5.274
N4 -4.401 -3.811 -5.464
Ru5 -6.623 -1.994 -3.177
Cl6 -7.930 -3.870 -2.719
Cl7 -4.912 -0.578 -2.435
N8 -8.382 0.292 -3.904
C9 -9.248 1.380 -3.294
C10 -10.697 1.255 -3.751
H11 -11.167 0.317 -3.448
H12 -11.276 2.076 -3.313
H13 -10.771 1.345 -4.842
C14 -8.745 2.762 -3.683
H15 -7.705 2.917 -3.382
H16 -8.837 2.942 -4.760
H17 -9.360 3.508 -3.166
C18 -9.029 1.102 -1.806
H19 -8.197 1.724 -1.446
H20 -9.915 1.346 -1.206
C21 -8.631 -0.376 -1.683
C22 -9.857 -1.291 -1.539
H23 -10.539 -1.244 -2.394
H24 -9.556 -2.336 -1.421
H25 -10.416 -0.984 -0.645
C26 -7.715 -0.611 -0.486
H27 -7.406 -1.663 -0.413
H28 -6.814 0.008 -0.530
H29 -8.264 -0.373 0.434
C30 -7.960 -0.623 -3.039
C31 -8.154 0.282 -5.324
C32 -9.026 -0.467 -6.137
C33 -10.072 -1.417 -5.605

H34 -10.148 -1.342 -4.517
H35 -11.054 -1.126 -6.007
C36 -8.859 -0.386 -7.520
H37 -9.534 -0.950 -8.163
C38 -7.853 0.388 -8.078
H39 -7.746 0.446 -9.158
C40 -6.966 1.065 -7.254
H41 -6.153 1.639 -7.694
C42 -7.083 1.018 -5.864
C43 -6.018 1.684 -5.028
H44 -6.093 2.776 -5.149
H45 -6.179 1.469 -3.965
C46 -4.609 1.228 -5.395
H47 -3.873 1.701 -4.737
H48 -4.505 0.144 -5.270
H49 -4.345 1.480 -6.429
C50 -9.779 -2.872 -5.970
H51 -10.569 -3.529 -5.593
H52 -9.711 -3.016 -7.055
H53 -8.837 -3.208 -5.521
68
17a - int7
C1 -5.632 -4.389 -2.680
C2 -5.630 -3.623 -1.551
C3 -6.649 -2.434 -4.784
H4 -7.580 -2.755 -5.283
C5 -5.475 -2.365 -5.676
H6 -5.499 -1.342 -6.099
H7 -4.527 -2.431 -5.127
C8 -5.547 -3.371 -6.825
H9 -5.547 -4.393 -6.418
H10 -6.504 -3.241 -7.355
C11 -4.382 -3.190 -7.781
H12 -4.380 -2.175 -8.202
H13 -3.429 -3.339 -7.260
H14 -4.423 -3.900 -8.614
Ru15 -6.823 -2.148 -2.974
Cl16 -8.765 -3.639 -2.894
Cl17 -4.800 -0.809 -2.784
N18 -8.348 0.301 -3.951
C19 -9.232 1.431 -3.458
C20 -10.695 1.127 -3.765
H21 -11.012 0.147 -3.399
H22 -11.328 1.889 -3.296
H23 -10.877 1.167 -4.846
C24 -8.884 2.767 -4.091
H25 -7.870 3.087 -3.843
H26 -8.996 2.745 -5.182
H27 -9.578 3.522 -3.702
C28 -8.895 1.404 -1.968
H29 -8.062 2.098 -1.781
H30 -9.742 1.723 -1.348
C31 -8.441 -0.028 -1.645
C32 -9.602 -0.891 -1.133
H33 -10.419 -0.987 -1.855
H34 -9.273 -1.908 -0.901
H35 -10.001 -0.429 -0.220
C36 -7.332 -0.031 -0.594
H37 -7.014 -1.053 -0.342
H38 -6.444 0.514 -0.933
H39 -7.710 0.429 0.329
C40 -7.936 -0.528 -3.003
C41 -8.032 0.167 -5.352
C42 -8.833 -0.662 -6.166
C43 -9.964 -1.494 -5.607
H44 -9.744 -1.761 -4.565
H45 -10.881 -0.887 -5.574
C46 -8.523 -0.733 -7.525
H47 -9.116 -1.373 -8.173
C48 -7.464 -0.014 -8.059
H49 -7.244 -0.079 -9.122
C50 -6.672 0.770 -7.235
H51 -5.827 1.309 -7.657
C52 -6.924 0.869 -5.865
C53 -5.986 1.688 -5.008
H54 -6.248 2.752 -5.115
H55 -6.128 1.428 -3.951
C56 -4.511 1.512 -5.347
H57 -3.897 2.061 -4.625
H58 -4.216 0.459 -5.279
H59 -4.258 1.888 -6.345
C60 -10.259 -2.779 -6.369
H61 -10.972 -3.388 -5.805
H62 -10.691 -2.595 -7.360
H63 -9.354 -3.386 -6.505
H64 -6.477 -3.700 -0.866
H65 -4.745 -3.075 -1.237
H66 -6.496 -5.006 -2.929
C67 -4.479 -4.532 -3.506
N68 -3.561 -4.679 -4.205
67
17a - int8
C1 -6.373 -2.217 -4.734
H2 -5.565 -1.615 -5.176
Ru3 -6.701 -2.210 -2.953
Cl4 -8.484 -3.844 -3.249
Cl5 -4.780 -0.788 -2.524
N6 -8.390 0.136 -3.823
C7 -9.385 1.172 -3.339
C8 -10.801 0.789 -3.755

H9 -11.076 -0.222 -3.442
H10 -11.510 1.492 -3.301
H11 -10.918 0.858 -4.843
C12 -9.088 2.560 -3.883
H13 -8.108 2.923 -3.560
H14 -9.136 2.590 -4.978
H15 -9.845 3.252 -3.497
C16 -9.150 1.095 -1.832
H17 -8.414 1.859 -1.546
H18 -10.068 1.287 -1.262
C19 -8.567 -0.299 -1.540
C20 -9.660 -1.295 -1.132
H21 -10.453 -1.380 -1.883
H22 -9.264 -2.305 -0.988
H23 -10.113 -0.955 -0.192
C24 -7.516 -0.205 -0.433
H25 -7.094 -1.182 -0.170
H26 -6.679 0.438 -0.730
H27 -7.984 0.208 0.470
C28 -7.947 -0.694 -2.883
C29 -8.006 0.085 -5.210
C30 -8.730 -0.730 -6.105
C31 -9.847 -1.644 -5.660
H32 -9.731 -1.872 -4.594
H33 -10.808 -1.120 -5.766
C34 -8.360 -0.703 -7.451
H35 -8.900 -1.325 -8.161
C36 -7.314 0.090 -7.895
H37 -7.048 0.098 -8.950
C38 -6.594 0.858 -6.993
H39 -5.757 1.457 -7.346
C40 -6.912 0.870 -5.635
C41 -6.065 1.691 -4.691
H42 -6.396 2.740 -4.741
H43 -6.228 1.355 -3.659
C44 -4.571 1.635 -4.979
H45 -4.021 2.156 -4.188
H46 -4.213 0.600 -4.987
H47 -4.306 2.109 -5.932
C48 -9.921 -2.967 -6.410
H49 -10.661 -3.620 -5.935
H50 -10.210 -2.846 -7.461
H51 -8.961 -3.496 -6.374
C52 -5.034 -4.154 -3.154
C53 -5.259 -4.003 -1.825
H54 -4.642 -3.277 -1.287
H55 -5.570 -4.908 -3.730
H56 -4.233 -3.605 -3.643
C57 -6.170 -4.861 -1.005
H58 -6.868 -5.395 -1.664
H59 -5.560 -5.620 -0.489
C60 -6.947 -4.056 0.030
H61 -6.248 -3.595 0.746
H62 -7.450 -3.226 -0.489
C63 -8.000 -4.881 0.746
H64 -8.733 -5.265 0.024
H65 -7.553 -5.742 1.260
H66 -8.542 -4.289 1.492
H68 -6.930 -2.885 -5.409
59
17a - int9
C1 -4.771 -3.559 -2.775
C2 -5.551 -3.592 -1.659
H3 -4.022 -2.779 -2.905
C4 -6.565 -2.300 -4.851
H5 -6.925 -1.579 -5.593
Ru6 -6.853 -2.108 -3.067
Cl7 -8.444 -3.889 -2.869
Cl8 -5.273 -0.386 -2.427
N9 -8.517 0.301 -3.966
C10 -9.317 1.448 -3.363
C11 -10.746 1.459 -3.895
H12 -11.303 0.547 -3.669
H13 -11.285 2.300 -3.443
H14 -10.754 1.606 -4.982
C15 -8.683 2.793 -3.682
H16 -7.652 2.852 -3.323
H17 -8.703 3.011 -4.757
H18 -9.263 3.573 -3.173
C19 -9.190 1.118 -1.875
H20 -8.326 1.660 -1.463
H21 -10.080 1.418 -1.308
C22 -8.921 -0.389 -1.785
C23 -10.228 -1.196 -1.721
H24 -10.902 -1.002 -2.560
H25 -10.027 -2.271 -1.702
H26 -10.757 -0.918 -0.799
C27 -8.098 -0.748 -0.550
H28 -7.910 -1.831 -0.498
H29 -7.139 -0.221 -0.525
H30 -8.669 -0.487 0.351
C31 -8.203 -0.663 -3.114
C32 -8.308 0.282 -5.393
C33 -9.223 -0.438 -6.188
C34 -10.278 -1.368 -5.643
H35 -10.332 -1.307 -4.552
H36 -11.261 -1.051 -6.023
C37 -9.103 -0.341 -7.575
H38 -9.814 -0.881 -8.199
C39 -8.103 0.419 -8.160

H40 -8.035 0.493 -9.243
C41 -7.173 1.063 -7.358
H42 -6.363 1.628 -7.816
C43 -7.243 1.000 -5.966
C44 -6.123 1.622 -5.169
H45 -6.122 2.710 -5.332
H46 -6.273 1.451 -4.099
C47 -4.760 1.047 -5.546
H48 -3.975 1.490 -4.924
H49 -4.738 -0.036 -5.371
H50 -4.506 1.229 -6.596
C51 -10.021 -2.822 -6.032
H52 -10.803 -3.473 -5.626
H53 -9.997 -2.957 -7.119
H54 -9.067 -3.175 -5.619
H55 -6.228 -4.420 -1.465
H56 -5.381 -2.862 -0.870
C57 -4.790 -4.589 -3.757
N58 -4.795 -5.378 -4.612
H59 -6.048 -3.188 -5.245
81
17b - pre
Ru1 1.632 11.970 2.304
Cl1 -0.023 11.802 0.585
Cl2 2.482 11.728 4.519
N1 3.000 14.628 1.933
C2 2.863 16.104 2.231
C3 2.869 16.932 0.951
H3A 3.812 16.807 0.406
H3B 2.046 16.682 0.276
H3C 2.775 17.992 1.215
C4 4.002 16.584 3.119
H4A 4.973 16.514 2.615
H4B 3.828 17.638 3.369
H4C 4.046 16.017 4.055
C5 1.529 16.141 2.985
H5A 0.927 17.010 2.694
H5B 1.721 16.234 4.058
C6 0.796 14.825 2.660
C7 -0.135 15.077 1.462
H7A 0.397 15.597 0.659
H7B -0.541 14.156 1.037
H7C -0.959 15.723 1.788
C8 0.041 14.239 3.849
C9 0.609 14.259 5.127
H9A 1.606 14.672 5.274
C10 -0.048 13.706 6.216
H10A 0.425 13.727 7.195
C11 -1.292 13.105 6.050
H11A -1.808 12.668 6.902
C12 -1.861 13.055 4.784
H12A -2.827 12.576 4.635
C13 -1.201 13.616 3.694
H13A -1.664 13.552 2.712
C14 1.934 13.880 2.224
C15 4.197 14.172 1.277
C16 4.204 14.099 -0.130
C17 2.978 14.271 -0.996
H17A 3.158 15.089 -1.711
H17C 2.114 14.567 -0.395
C18 5.397 13.748 -0.763
H18A 5.420 13.699 -1.851
C19 6.537 13.448 -0.032
H43 7.459 13.181 -0.543
C21 6.487 13.458 1.354
H21A 7.370 13.179 1.925
C22 5.321 13.804 2.039
C23 5.305 13.673 3.543
H23A 5.925 14.467 3.987
H23B 4.286 13.809 3.922
C24 3.045 11.328 1.334
H24A 3.838 11.947 0.912
C25 3.152 9.922 1.044
C26 4.142 9.445 0.186
H26A 4.856 10.130 -0.265
C27 4.201 8.090 -0.093
N28 5.234 7.593 -0.997
O29 6.005 8.411 -1.477
O30 5.264 6.392 -1.217
C31 3.298 7.192 0.468
H31A 3.383 6.138 0.221
C32 2.311 7.647 1.329
H32A 1.612 6.939 1.763
C33 2.230 9.012 1.615
O34 1.318 9.590 2.409
C35 0.390 8.796 3.201
H35A -0.021 8.026 2.530
C36 -0.711 9.734 3.628
H36A -1.473 9.173 4.180
H36B -0.313 10.515 4.290
H36C -1.179 10.211 2.760
C37 1.129 8.184 4.372
H37A 0.432 7.603 4.987
H37B 1.940 7.519 4.056
H37C 1.559 8.986 4.983
C75 5.806 12.311 4.016
H76 5.698 12.223 5.102
H77 5.213 11.506 3.567
H78 6.861 12.143 3.769
C78 2.621 12.995 -1.758

H79 1.750 13.163 -2.400
H80 3.446 12.649 -2.392
H81 2.353 12.187 -1.066
96
17b - int1
N1 2.855 14.547 1.858
C2 2.781 15.986 2.345
C3 2.665 16.970 1.184
H4 3.545 16.910 0.533
H5 1.771 16.821 0.575
H6 2.625 17.986 1.593
C7 4.004 16.374 3.163
H8 4.918 16.392 2.558
H9 3.843 17.385 3.555
H10 4.149 15.703 4.015
C11 1.546 15.918 3.234
H12 0.970 16.852 3.220
H13 1.859 15.740 4.271
C14 0.705 14.725 2.742
C15 -0.242 15.182 1.622
H16 0.300 15.518 0.735
H17 -0.903 14.375 1.296
H18 -0.840 16.026 1.985
C19 -0.079 14.134 3.909
C20 0.614 13.564 4.981
H21 1.699 13.481 4.938
C22 -0.056 13.056 6.086
H23 0.514 12.588 6.886
C24 -1.442 13.148 6.166
H25 -1.971 12.761 7.035
C26 -2.144 13.744 5.125
H27 -3.228 13.828 5.173
C28 -1.471 14.222 4.004
H29 -2.054 14.653 3.193
C30 1.788 13.793 2.132
C31 3.991 14.187 1.039
C32 3.882 14.312 -0.361
C33 2.601 14.619 -1.099
H34 2.738 15.564 -1.647
H35 1.775 14.775 -0.401
C36 5.034 14.144 -1.134
H37 4.960 14.256 -2.215
C38 6.256 13.854 -0.550
H39 7.146 13.733 -1.162
C40 6.333 13.681 0.824
H41 7.286 13.406 1.273
C42 5.215 13.827 1.645
C43 5.377 13.550 3.123
H44 5.950 14.370 3.580
H45 4.397 13.527 3.612
C46 6.083 12.231 3.421
H47 6.126 12.066 4.502
H48 5.533 11.382 2.998
H49 7.110 12.203 3.036
C50 2.189 13.518 -2.071
H51 1.340 13.845 -2.681
H52 3.004 13.229 -2.748
H53 1.862 12.632 -1.517
Ru54 1.432 11.851 1.988
Cl55 2.786 11.383 4.003
O56 7.418 10.929 -0.875
O57 7.207 10.186 -2.900
O58 1.277 9.913 -0.994
N59 6.754 10.498 -1.807
C60 4.743 10.782 -0.432
C61 2.570 10.082 -1.230
C62 5.319 10.348 -1.609
C63 3.186 9.650 -2.419
C64 2.936 11.354 1.024
C65 3.357 10.707 -0.212
C66 4.544 9.789 -2.618
C67 0.123 10.586 -3.018
C68 0.374 9.465 -2.030
C69 -0.892 9.038 -1.326
Cl70 -0.248 12.196 0.267
H71 5.385 11.230 0.321
H72 5.017 9.462 -3.538
H73 2.590 9.197 -3.203
H74 3.833 11.607 1.601
H75 -0.302 11.444 -2.484
H76 1.038 10.915 -3.524
H77 -0.589 10.255 -3.783
H78 0.825 8.590 -2.523
H79 -0.693 8.251 -0.590
H80 -1.336 9.900 -0.813
H81 -1.609 8.651 -2.058
C82 1.167 9.271 2.099
C83 0.155 9.744 2.863
H84 0.383 10.009 3.902
H85 0.991 8.941 1.078
H86 2.155 9.116 2.526
C88 -1.284 9.788 2.462
H89 -1.361 9.837 1.368
H90 -1.758 8.841 2.774
C91 -2.028 10.955 3.093
H92 -2.017 10.851 4.189
H93 -1.479 11.881 2.872
C94 -3.448 11.092 2.580
H95 -3.448 11.268 1.495
H96 -4.038 10.186 2.771

H97 -3.967 11.934 3.053
68
17b - int2
Ru1 1.608 12.086 1.907
Cl2 -0.288 12.031 0.479
Cl3 2.651 11.366 3.896
N4 2.950 14.746 1.709
C5 2.877 16.171 2.203
C6 2.730 17.157 1.049
H7 3.582 17.093 0.363
H8 1.810 17.005 0.477
H9 2.706 18.174 1.457
C10 4.128 16.533 2.990
H11 5.026 16.521 2.360
H12 4.011 17.549 3.387
H13 4.280 15.855 3.837
C14 1.648 16.120 3.118
H15 1.019 17.010 2.992
H16 1.971 16.108 4.163
C17 0.865 14.840 2.760
C18 -0.242 15.212 1.762
H19 0.161 15.830 0.952
H20 -0.712 14.340 1.300
H21 -1.005 15.802 2.284
C22 0.325 14.095 3.976
C23 1.104 13.973 5.131
H24 2.104 14.406 5.165
C25 0.653 13.258 6.229
H26 1.284 13.172 7.111
C27 -0.585 12.626 6.190
H28 -0.937 12.056 7.047
C29 -1.360 12.715 5.042
H30 -2.326 12.216 4.992
C31 -0.912 13.445 3.945
H32 -1.536 13.494 3.056
C33 1.917 13.969 2.048
C34 4.039 14.347 0.862
C35 3.875 14.453 -0.532
C36 2.567 14.794 -1.205
H37 2.715 15.682 -1.838
H38 1.808 15.061 -0.465
C39 4.967 14.148 -1.345
H40 4.859 14.239 -2.426
C41 6.171 13.727 -0.801
H42 7.015 13.504 -1.449
C43 6.289 13.568 0.572
H44 7.223 13.199 0.992
C45 5.228 13.857 1.432
C46 5.383 13.562 2.905
H47 6.045 14.314 3.362
H48 4.411 13.646 3.406
C49 5.933 12.167 3.178
H50 5.945 11.969 4.255
H51 5.293 11.404 2.720
H52 6.955 12.036 2.802
C53 2.026 13.643 -2.051
H54 1.114 13.948 -2.576
H55 2.752 13.305 -2.800
H56 1.760 12.790 -1.415
C57 2.837 11.486 0.722
H58 3.602 12.093 0.224
C59 2.803 10.040 0.376
H60 3.736 9.583 0.754
H61 1.977 9.521 0.892
C62 2.693 9.834 -1.139
H63 1.746 10.274 -1.484
H64 3.498 10.398 -1.634
C65 2.760 8.365 -1.518
H66 3.706 7.914 -1.194
H67 1.946 7.800 -1.047
H68 2.676 8.225 -2.601
83
17b - int3
Ru1 1.466 11.781 2.000
Cl2 -0.233 11.938 0.270
Cl3 2.961 11.292 3.881
N4 2.869 14.475 1.714
C5 2.780 15.952 2.065
C6 2.556 16.826 0.833
H7 3.348 16.677 0.089
H8 1.587 16.659 0.354
H9 2.589 17.877 1.143
C10 4.039 16.443 2.762
H11 4.913 16.423 2.099
H12 3.877 17.484 3.069
H13 4.255 15.859 3.661
C14 1.600 15.937 3.025
H15 0.994 16.850 2.959
H16 1.974 15.864 4.054
C17 0.770 14.677 2.699
C18 -0.284 14.980 1.623
H19 0.169 15.186 0.650
H20 -0.961 14.135 1.469
H21 -0.862 15.864 1.916
C22 0.124 14.188 3.986
C23 0.925 13.628 4.985
H24 1.985 13.463 4.799
C25 0.384 13.238 6.203
H26 1.028 12.776 6.949
C27 -0.966 13.443 6.464

H28 -1.392 13.149 7.421
C29 -1.768 14.028 5.492
H30 -2.826 14.197 5.684
C31 -1.230 14.391 4.261
H32 -1.888 14.821 3.509
C33 1.829 13.724 2.082
C34 3.977 14.051 0.898
C35 3.799 14.035 -0.502
C36 2.433 14.169 -1.129
H37 1.803 14.806 -0.506
H38 1.924 13.191 -1.087
C39 4.922 13.816 -1.299
H40 4.818 13.823 -2.382
C41 6.165 13.572 -0.734
H42 7.030 13.409 -1.373
C43 6.299 13.509 0.643
H44 7.269 13.278 1.080
C45 5.214 13.743 1.492
C46 5.416 13.608 2.983
H47 5.954 14.492 3.358
H48 4.441 13.583 3.486
C49 6.185 12.354 3.380
H50 6.206 12.259 4.471
H51 5.692 11.456 2.991
H52 7.222 12.367 3.027
C53 2.415 14.698 -2.552
H54 1.384 14.863 -2.880
H55 2.954 15.652 -2.631
H56 2.868 14.000 -3.266
C57 2.791 11.239 0.855
H58 3.829 11.488 1.134
C59 2.680 10.357 -0.340
H60 2.917 9.340 0.030
H61 1.650 10.322 -0.716
C62 3.666 10.680 -1.463
H63 3.406 11.652 -1.904
H64 4.678 10.798 -1.046
C65 3.654 9.607 -2.539
H66 3.955 8.633 -2.132
H67 2.649 9.489 -2.964
H68 4.337 9.851 -3.360
C82 1.018 9.233 2.092
C83 0.143 9.725 2.997
H84 0.512 9.928 4.009
H85 0.682 8.967 1.090
H86 2.036 8.983 2.382
C88 -1.319 9.913 2.763
H89 -1.517 9.961 1.683
H90 -1.848 9.025 3.150
C91 -1.850 11.160 3.455
H92 -1.749 11.052 4.546
H93 -1.213 12.013 3.181
C94 -3.283 11.479 3.074
H95 -3.356 11.683 1.998
H96 -3.957 10.643 3.303
H97 -3.653 12.362 3.610
59
17b - int4
Ru1 1.632 12.068 1.898
Cl2 -0.278 12.030 0.507
Cl3 2.640 11.423 3.921
N4 2.965 14.728 1.695
C5 2.897 16.156 2.188
C6 2.746 17.138 1.032
H7 3.600 17.077 0.347
H8 1.829 16.982 0.458
H9 2.718 18.156 1.438
C10 4.153 16.518 2.967
H11 5.047 16.504 2.333
H12 4.037 17.534 3.363
H13 4.308 15.841 3.814
C14 1.673 16.108 3.111
H15 1.046 17.000 2.990
H16 2.003 16.094 4.153
C17 0.884 14.832 2.753
C18 -0.221 15.213 1.755
H19 0.183 15.838 0.952
H20 -0.691 14.346 1.286
H21 -0.984 15.798 2.282
C22 0.333 14.093 3.969
C23 1.087 13.994 5.142
H24 2.080 14.440 5.196
C25 0.622 13.283 6.237
H26 1.234 13.216 7.134
C27 -0.605 12.630 6.176
H28 -0.967 12.063 7.030
C29 -1.355 12.696 5.011
H30 -2.311 12.181 4.944
C31 -0.893 13.424 3.918
H32 -1.498 13.455 3.015
C33 1.933 13.959 2.039
C34 4.051 14.334 0.842
C35 3.881 14.450 -0.551
C36 2.564 14.773 -1.215
H37 2.685 15.681 -1.826
H38 1.799 15.002 -0.467
C39 4.978 14.174 -1.367
H40 4.869 14.275 -2.446
C41 6.189 13.768 -0.827
H42 7.037 13.567 -1.478

C43 6.310 13.591 0.544
H44 7.250 13.232 0.959
C45 5.246 13.855 1.407
C46 5.404 13.548 2.877
H47 6.078 14.289 3.335
H48 4.436 13.639 3.385
C49 5.940 12.144 3.135
H50 5.969 11.942 4.211
H51 5.283 11.392 2.684
H52 6.953 12.003 2.740
C53 2.052 13.631 -2.089
H54 1.111 13.911 -2.574
H55 2.769 13.361 -2.874
H56 1.850 12.738 -1.485
C57 2.858 11.480 0.717
H58 3.635 12.038 0.186
H59 2.802 10.395 0.514
88
17b - int5
N1 2.982 14.613 1.834
C2 2.955 16.034 2.372
C3 2.872 17.050 1.235
H4 3.792 17.031 0.638
H5 2.031 16.887 0.558
H6 2.775 18.055 1.662
C7 4.198 16.358 3.187
H8 5.107 16.353 2.574
H9 4.080 17.368 3.599
H10 4.326 15.666 4.024
C11 1.728 15.966 3.289
H12 1.182 16.918 3.322
H13 2.084 15.753 4.302
C14 0.853 14.821 2.762
C15 -0.118 15.383 1.704
H16 0.382 16.093 1.041
H17 -0.557 14.603 1.077
H18 -0.920 15.920 2.224
C19 0.066 14.041 3.820
C20 0.430 14.021 5.170
H21 1.305 14.563 5.518
C22 -0.288 13.278 6.096
H23 0.027 13.277 7.137
C24 -1.391 12.529 5.699
H25 -1.953 11.950 6.428
C26 -1.767 12.531 4.364
H27 -2.624 11.952 4.026
C28 -1.045 13.278 3.432
H29 -1.370 13.258 2.395
C30 1.888 13.907 2.093
C31 4.078 14.231 0.974
C32 3.910 14.363 -0.419
C33 2.597 14.671 -1.100
H34 2.697 15.629 -1.633
H35 1.792 14.799 -0.369
C36 5.028 14.181 -1.238
H37 4.913 14.298 -2.314
C38 6.268 13.871 -0.705
H39 7.131 13.742 -1.354
C40 6.398 13.683 0.664
H41 7.362 13.386 1.072
C42 5.315 13.838 1.529
C43 5.526 13.522 2.992
H44 6.201 14.275 3.426
H45 4.577 13.581 3.536
C46 6.115 12.133 3.234
H47 6.287 11.980 4.305
H48 5.419 11.346 2.918
H49 7.067 11.979 2.712
C50 2.174 13.578 -2.079
H51 1.259 13.869 -2.606
H52 2.948 13.364 -2.827
H53 1.947 12.655 -1.535
Ru54 1.416 11.996 2.050
Cl55 2.702 11.767 4.140
O56 7.352 10.909 -0.899
O57 7.066 10.167 -2.915
O58 1.232 9.807 -0.755
N59 6.655 10.476 -1.806
C60 4.691 10.782 -0.370
C61 2.501 10.014 -1.061
C62 5.229 10.320 -1.553
C63 3.077 9.563 -2.264
C64 2.913 11.403 1.102
C65 3.314 10.695 -0.099
C66 4.423 9.723 -2.517
C67 -0.024 10.365 -2.764
C68 0.288 9.298 -1.734
C69 -0.932 8.889 -0.946
Cl70 -0.163 12.284 0.226
H71 5.353 11.265 0.346
H72 4.868 9.380 -3.447
H73 2.460 9.073 -3.009
H74 3.818 11.707 1.642
H75 -0.455 11.238 -2.261
H76 0.862 10.692 -3.319
H77 -0.752 9.975 -3.485
H78 0.739 8.410 -2.204
H79 -0.689 8.119 -0.204
H80 -1.355 9.754 -0.424
H81 -1.690 8.479 -1.622

C82 1.276 9.464 2.351
C83 0.211 10.041 2.971
H84 0.304 10.402 3.998
C85 -1.118 9.964 2.453
H86 1.174 9.009 1.369
H87 2.216 9.370 2.887
N88 -2.221 9.863 2.097
60
17b - int6
Ru1 1.551 12.038 1.976
Cl2 -0.380 11.977 0.648
Cl3 2.553 11.451 3.998
N4 2.917 14.679 1.679
C5 2.872 16.121 2.138
C6 2.724 17.073 0.957
H7 3.569 16.982 0.265
H8 1.797 16.915 0.398
H9 2.714 18.102 1.337
C10 4.142 16.480 2.895
H11 5.029 16.437 2.253
H12 4.046 17.508 3.267
H13 4.295 15.823 3.757
C14 1.656 16.113 3.071
H15 1.035 17.005 2.925
H16 1.993 16.132 4.111
C17 0.851 14.833 2.763
C18 -0.266 15.196 1.773
H19 0.130 15.798 0.947
H20 -0.754 14.323 1.334
H21 -1.015 15.801 2.298
C22 0.318 14.127 4.006
C23 1.081 14.071 5.176
H24 2.069 14.530 5.211
C25 0.633 13.383 6.293
H26 1.252 13.349 7.187
C27 -0.585 12.713 6.259
H28 -0.933 12.164 7.130
C29 -1.345 12.738 5.098
H30 -2.294 12.209 5.053
C31 -0.901 13.442 3.982
H32 -1.515 13.443 3.085
C33 1.883 13.935 2.056
C34 3.993 14.253 0.826
C35 3.813 14.338 -0.567
C36 2.495 14.660 -1.231
H37 2.624 15.547 -1.869
H38 1.739 14.924 -0.485
C39 4.899 14.024 -1.385
H40 4.781 14.096 -2.465
C41 6.108 13.614 -0.844
H42 6.946 13.381 -1.497
C43 6.239 13.470 0.529
H44 7.176 13.106 0.946
C45 5.186 13.770 1.395
C46 5.352 13.484 2.869
H47 6.053 14.212 3.304
H48 4.395 13.614 3.388
C49 5.852 12.069 3.142
H50 5.892 11.884 4.220
H51 5.170 11.326 2.712
H52 6.854 11.893 2.735
C53 1.958 13.501 -2.069
H54 1.019 13.783 -2.557
H55 2.664 13.197 -2.850
H56 1.744 12.627 -1.442
C57 2.794 11.438 0.776
H58 3.527 12.020 0.214
C59 2.770 10.037 0.577
N60 2.719 8.877 0.443
75
17b - int7
Ru1 1.520 12.096 1.844
Cl2 -0.309 12.301 0.273
Cl3 2.939 11.603 3.756
N4 3.078 14.740 1.646
C5 3.091 16.118 2.286
C6 3.056 17.227 1.240
H7 3.925 17.166 0.574
H8 2.151 17.218 0.627
H9 3.101 18.195 1.754
C10 4.341 16.305 3.133
H11 5.253 16.307 2.523
H12 4.274 17.276 3.638
H13 4.424 15.528 3.900
C14 1.843 16.055 3.176
H15 1.287 17.001 3.160
H16 2.144 15.878 4.213
C17 0.982 14.896 2.642
C18 0.003 15.451 1.595
H19 0.510 16.136 0.910
H20 -0.460 14.663 0.994
H21 -0.778 16.024 2.110
C22 0.250 14.117 3.732
C23 0.906 13.781 4.922
H24 1.952 14.047 5.060
C25 0.265 13.057 5.917
H26 0.807 12.797 6.823
C27 -1.054 12.648 5.745
H28 -1.558 12.081 6.524
C29 -1.718 12.962 4.565

H30 -2.745 12.639 4.411
C31 -1.071 13.686 3.567
H32 -1.606 13.898 2.645
C33 2.003 14.004 1.919
C34 4.128 14.385 0.718
C35 3.902 14.627 -0.654
C36 2.594 15.109 -1.236
H37 2.784 16.044 -1.786
H38 1.882 15.356 -0.445
C39 4.930 14.339 -1.551
H40 4.768 14.532 -2.611
C41 6.134 13.808 -1.119
H42 6.926 13.594 -1.833
C43 6.321 13.540 0.227
H44 7.260 13.103 0.561
C45 5.330 13.812 1.174
C46 5.594 13.443 2.613
H47 6.280 14.182 3.054
H48 4.661 13.487 3.184
C49 6.179 12.047 2.789
H50 6.261 11.807 3.854
H51 5.521 11.292 2.343
H52 7.177 11.945 2.347
C53 1.938 14.093 -2.170
H54 1.046 14.524 -2.635
H55 2.615 13.775 -2.972
H56 1.608 13.201 -1.622
C57 2.748 11.655 0.554
H58 3.039 12.466 -0.124
C59 3.387 10.382 0.170
H60 4.479 10.532 0.278
H61 3.115 9.536 0.813
C62 3.079 10.079 -1.306
H63 1.988 10.051 -1.445
H64 3.458 10.911 -1.920
C65 3.693 8.763 -1.747
H66 4.780 8.758 -1.592
H67 3.266 7.928 -1.179
H68 3.504 8.571 -2.808
C69 0.954 9.568 2.251
C70 0.054 10.411 2.825
H71 -0.903 10.613 2.350
H72 0.218 10.772 3.839
H73 1.869 9.300 2.778
C74 0.682 8.872 1.037
N75 0.497 8.262 0.063
74
17b - int8
Ru1 1.436 11.842 2.001
Cl2 -0.079 12.026 0.100
Cl3 2.868 11.291 3.894
N4 2.797 14.517 1.681
C5 2.718 16.003 1.970
C6 2.466 16.806 0.699
H7 3.289 16.675 -0.013
H8 1.528 16.544 0.202
H9 2.420 17.870 0.959
C10 3.993 16.527 2.613
H11 4.857 16.439 1.943
H12 3.852 17.591 2.839
H13 4.211 16.012 3.552
C14 1.556 16.037 2.958
H15 0.945 16.941 2.849
H16 1.952 16.028 3.981
C17 0.727 14.756 2.725
C18 -0.369 14.997 1.677
H19 0.051 15.223 0.693
H20 -1.004 14.116 1.542
H21 -0.984 15.851 1.982
C22 0.146 14.287 4.050
C23 1.003 13.772 5.026
H24 2.061 13.638 4.803
C25 0.521 13.373 6.265
H26 1.207 12.943 6.991
C27 -0.829 13.518 6.567
H28 -1.210 13.212 7.539
C29 -1.688 14.055 5.616
H30 -2.746 14.176 5.840
C31 -1.206 14.430 4.365
H32 -1.906 14.823 3.631
C33 1.763 13.791 2.110
C34 3.892 14.002 0.895
C35 3.733 13.885 -0.502
C36 2.436 14.148 -1.226
H37 1.676 14.513 -0.532
H38 2.031 13.186 -1.571
C39 4.821 13.434 -1.251
H40 4.708 13.322 -2.328
C41 6.024 13.110 -0.647
H42 6.862 12.765 -1.248
C43 6.152 13.205 0.731
H44 7.091 12.920 1.201
C45 5.097 13.636 1.534
C46 5.278 13.645 3.034
H47 5.775 14.580 3.332
H48 4.294 13.638 3.516
C49 6.081 12.469 3.575
H50 6.041 12.465 4.670
H51 5.656 11.518 3.236
H52 7.137 12.509 3.285

C53 2.560 15.098 -2.410
H54 1.579 15.265 -2.867
H55 2.959 16.074 -2.109
H56 3.220 14.704 -3.191
C57 2.787 11.390 0.879
H58 3.783 11.113 1.254
C59 1.119 9.310 1.698
C60 0.288 9.682 2.704
H61 0.689 9.676 3.722
H62 0.761 9.234 0.672
H63 2.127 8.967 1.919
C64 -1.175 9.958 2.564
H65 -1.423 10.124 1.506
H66 -1.732 9.066 2.896
C67 -1.603 11.157 3.400
H68 -1.436 10.949 4.468
H69 -0.950 12.015 3.166
C70 -3.041 11.563 3.139
H71 -3.168 11.866 2.091
H72 -3.731 10.731 3.331
H73 -3.343 12.403 3.775
H75 2.611 11.296 -0.203
66
17b - int9
Ru1 1.365 12.197 1.863
Cl2 -0.135 12.529 -0.015
Cl3 2.758 11.492 3.729
N4 2.986 14.755 1.686
C5 3.004 16.193 2.166
C6 2.856 17.162 0.999
H7 3.702 17.068 0.306
H8 1.929 17.015 0.439
H9 2.858 18.187 1.387
C10 4.296 16.523 2.895
H11 5.169 16.446 2.235
H12 4.237 17.559 3.251
H13 4.445 15.876 3.764
C14 1.810 16.201 3.133
H15 1.249 17.141 3.066
H16 2.179 16.124 4.160
C17 0.927 14.996 2.757
C18 -0.175 15.468 1.796
H19 0.240 16.114 1.017
H20 -0.681 14.645 1.285
H21 -0.908 16.053 2.365
C22 0.358 14.201 3.931
C23 1.086 14.039 5.113
H24 2.068 14.497 5.222
C25 0.606 13.250 6.146
H26 1.196 13.135 7.053
C27 -0.610 12.584 6.014
H28 -0.985 11.963 6.824
C29 -1.332 12.709 4.836
H30 -2.277 12.186 4.705
C31 -0.853 13.511 3.800
H32 -1.449 13.598 2.894
C33 1.897 14.079 2.021
C34 4.026 14.222 0.841
C35 3.815 14.223 -0.558
C36 2.523 14.700 -1.181
H37 2.549 15.795 -1.275
H38 1.688 14.469 -0.509
C39 4.838 13.731 -1.368
H40 4.700 13.714 -2.446
C41 6.018 13.251 -0.822
H42 6.805 12.878 -1.474
C43 6.187 13.222 0.552
H44 7.102 12.810 0.971
C45 5.196 13.689 1.418
C46 5.402 13.555 2.909
H47 6.003 14.404 3.268
H48 4.431 13.610 3.415
C49 6.081 12.258 3.330
H50 6.066 12.168 4.421
H51 5.545 11.390 2.930
H52 7.128 12.204 3.009
C53 2.197 14.098 -2.539
H54 1.185 14.390 -2.836
H55 2.882 14.428 -3.328
H56 2.217 13.002 -2.504
C57 2.652 11.659 0.689
H58 3.634 11.301 1.033
C59 0.879 9.707 1.537
C60 0.070 10.191 2.521
H61 0.414 10.192 3.557
C62 -1.317 10.478 2.322
H63 0.524 9.614 0.513
H64 1.854 9.309 1.801
N65 -2.462 10.669 2.245
H67 2.460 11.626 -0.394