# A Simple and Practical Preparation of an Efficient Water Soluble Olefin Metathesis Catalyst

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## Supporting Information
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# General Experimental Information

## General Considerations

Manipulation of organometallic compounds was performed using standard Schlenk techniques under an atmosphere of dry nitrogen or in a nitrogen-filled drybox.

## Instrumentation

Melting points (m.p.) were determined using a Reichert hot-stage melting point apparatus and are uncorrected.

Infrared spectra (IR) spectra were recorded on a Perkin-Elmer 1600 series Fourier Transform infrared spectrophotometer as thin films of liquid (neat) between sodium chloride plates. IR absorptions ($\nu_{max}$) are reported in wavenumbers ($cm^{-1}$) with the relative intensities expressed as s (strong), m (medium) or prefixed b (broad).

Proton nuclear magnetic resonance ($^{1}$H-NMR) spectra were recorded on Bruker DPX300 or DRX400 spectrometers operating at 300 or 400 MHz respectively, as solutions in deuterated solvents as specified. Each resonance was assigned according to the following convention: chemical shift; multiplicity; observed coupling constants (*J* Hz); number of protons. Chemical shifts (δ), measured in parts per million (ppm), are reported relative to the residual proton peak in the solvent used as specified. Multiplicities are denoted as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), multiplet (m) or prefixed broad (b), or a combination where necessary.

Carbon-13 nuclear magnetic resonance ($^{13}$C-NMR) spectra were recorded on Bruker DPX300 or DRX400 spectrometers operating at 75 or 100 MHz respectively, as solutions in deuterated solvents as specified. Chemical shifts (δ), measured in parts per million (ppm), are reported relative to the residual proton peak in the deuterated solvent (as specified).

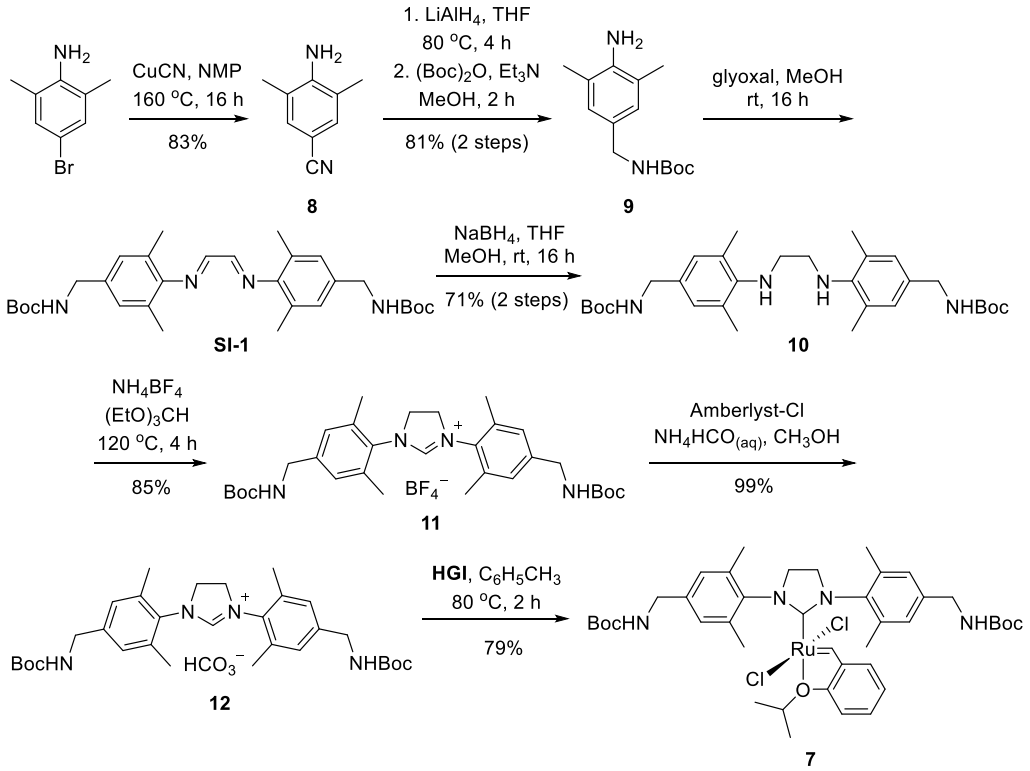
Low resolution electrospray ionisation (ESI) mass spectra were recorded on a Micromass Platform Electrospray mass spectrometer (QMS-quadrupole mass spectrometry) as solutions in specified solvents. Spectra were recorded in positive and negative modes ($ESI^{+}$ and $ESI^{-}$) as specified. High resolution electrospray mass spectra (HRMS) were recorded on a Bruker BioApex 47e Fourier Transform mass spectrometer (4.7 Tesla magnet) fitted with an analytical electrospray source. The mass spectrometer was calibrated with an internal standard solution of sodium iodide in $CH_3OH$.

## Solvents and Reagents

Dichloromethane ($CH_2Cl_2$) was supplied by Merck and distilled over $CaH_2$ prior to use. Diethyl ether ($Et_2O$), tetrahydrofuran (THF) and toluene ($C_6H_5CH_3$) were supplied by Merck and distilled over potassium prior to use. Acetic acid (AcOH), ethyl acetate (EtOAc), hexane, methanol ($CH_3OH$) and triethylamine ($Et_3N$) were used as supplied by Merck. 4-Bromo-2,6-dimethylaniline, cuprous cyanide (CuCN), lithium aluminum hydride ($LiAlH_4$), di-*tert*-butyl dicarbonate ($(Boc)_2O$), glyoxal solution 40 wt.% in $H_2O$, sodium borohydride ($NaBH_4$), ammonium tetrafluoroborate ($NH_4BF_4$), triethyl orthoformate ($(EtO)_3CH$), ammonium bicarbonate ($NH_4HCO_3$) and dichloro(*o*-isopropoxyphenylmethylene)(tricyclohexylphosphine)ruthenium(II) (**HGI**) were used as

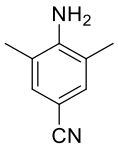
supplied by Sigma-Aldrich. $D_2O$ was purchased from Cambridge Isotopes Laboratory and degassed by bubbling with Ar (30 minutes).

# Experimental Procedures




**Scheme S1: Preparation of Ru-alkylidene 7**

## 4-Amino-3,5-dimethylbenzonitrile 8

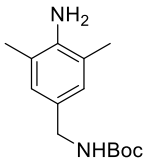



**8**

Compound **8** was prepared following a modified procedure developed by Gerritz and coworkers.[1] A magnetically stirred solution of 4-bromo-2,6-dimethylaniline (30.0 g, 150 mmol) and CuCN (26.7 g, 300 mmol) in NMP (400 mL) was heated to 160 °C for 16 h. After cooling to room temperature, water (150 mL) and ammonium hydroxide (150 mL) were added and the mixture stirred for a further 0.5 h. During this period, a grey precipitate formed, and the mixture was filtered. The filtrate was extracted with EtOAc (3x200 mL) and the combined organic extracts washed with brine (200 mL), dried ($Na_2SO_4$), filtered and concentrated under reduced pressure to afford **7** (18.2 g, 83%) as a colourless solid, m.p. 106.0-107.5 °C. IR $\nu_{max}$ 3476m, 3384m, 2205s, 1631s, 1599s, 1487s, 1431s, 1323s $cm^{-1}$.

$^{1}$H-NMR (400 MHz, $CDCl_3$): δ 7.20 (s, 2H), 4.16 (br s, 2H), 2.17 (s, 6H). $^{13}$C-NMR (100 MHz, $CDCl_3$): δ 147.0, 132.2, 121.8, 120.6, 99.8, 17.4. All data was consistent with that previously reported.[1]

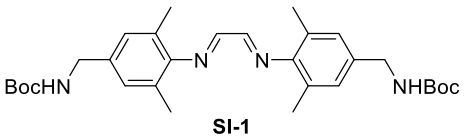
## *tert*-Butyl (4-amino-3,5-dimethylbenzyl)carbamate 9




**9**

A solution of benzonitrile **8** (17.5 g, 120 mmol) in THF (500 mL) was added dropwise to a magnetically stirred suspension of $LiAlH_4$ (9.31 g, 245 mmol). The mixture was stirred at reflux for 4 h then cooled to room temperature. The reaction was quenched by careful addition of $H_2O$ (5 mL) and 1 M NaOH (5 mL) and stirred for 0.5 h. The mixture was dried ($NaSO_4$), filtered and the filtrate concentrated under reduced pressure to afford the amine as a clear colourless oil. To this residue was added $CH_3OH$ (250 mL) and $Et_3N$ (25 mL). The mixture was cooled to 0 °C and a solution of $(Boc)_2O$ (26.2 g, 120 mmol) in $CH_3OH$ (40 mL) was added over 2 minutes. The reaction was stirred for 2 h at room temperature. The mixture was diluted with $Et_2O$ (200 mL) and washed with $H_2O$ (2x150 mL) followed by brine (200 mL). The organic layer was dried ($Na_2SO_4$), filtered and concentrated under reduced pressure to afford **9** (24.3 g, 81%) as a colourless solid, m.p. 100.2-101.3 °C, which was used without further purification. IR $\nu_{max}$ 3383m, 3347m, 2927m, 1673s, 1622m, 1515s, 1490s, 1155s cm$^{-1}$. $^{1}$H-NMR (400 MHz, $CDCl_3$): δ 6.86 (s, 2H), 4.76 (br s, 1H), 4.15 (d, $J$ = 5.2 Hz, 2H), 3.57 (br s, 2H), 2.16 (s, 6H), 1.46 (s, 9H). $^{13}$C-NMR (100 MHz, $CDCl_3$): δ 155.9, 142.1, 128.1, 127.9, 121.9, 79.2, 44.5, 28.5, 17.6. HRMS (ESI$^+$, MeOH): *m/z* 251.1749 $[M + H]^+$, $C_{14}H_{23}N_2O_2^+$ requires 251.1754.

## Di-*tert*-butyl (((ethane-1,2-diylidenebis(azanylylidene))bis(3,5-dimethyl-4,1-phenylene))bis(methylene))dicarbamate SI-1

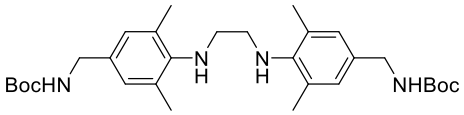



**SI-1**

The intermediate diimine **SI-1** was prepared following a modified procedure of Hintermann.[2] To a magnetically stirred solution of carbamate **9** (20 g, 79.9 mmol) in $CH_3OH$ (50 mL) at 50 °C was added a solution of glyoxal (5.80 g, 40 wt.% in $H_2O$, 40 mmol) and acetic acid (0.1 mL). The mixture was stirred at room temperature for 16 h. The product precipitated from the solution and the suspension was filtered. The resultant yellow solid was washed with $CH_3OH$ (2x15 mL) and dried to constant weight under reduced pressure to afford pure **SI-1**. The filtrate was concentrated under reduced pressure to a volume of 30 mL and set aside for a second crystallisation. Total yield of **SI-1**: 15.7 g (75%) as a yellow

solid, m.p. 185.9-187.5 °C. IR $\nu_{max}$ 3339m, 2973m, 2932m, 1708s, 1519m, 1246m, 1158s, 1124m $cm^{-1}$. $^1$H-NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 2H), 7.00 (s, 4H), 4.86 (br s, 2H), 4.24 (d, *J* = 7.6 Hz, 4H), 2.16 (s, 12H), 1.47 (s, 18H). $^{13}$C-NMR (100 MHz, $CDCl_3$): δ 163.6, 156.0, 149.1, 135.4, 127.6, 126.9, 79.6, 44.4, 28.6, 18.4. HRMS ($ESI^+$, MeOH): *m/z* 523.3286 $[M + H]^+$, $C_{30}H_{43}N_4O_4^+$ requires 523.3279.

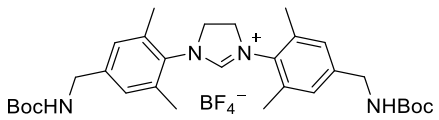
## Di-tert-butyl (((ethane-1,2-diylbis(azanediyl))bis(3,5-dimethyl-4,1-phenylene))bis(methylene))dicarbamate 10




**10**

Compound **10** was prepared following a modified procedure of Nolan and coworkers.[3] To magnetically a stirred solution of diimine **SI-1** (15.0 g, 28.7 mmol) in THF (100 mL) and $CH_3OH$ (50 mL) at 0 °C was carefully added $NaBH_4$ (6.54 g, 172 mmol) in small portions. The mixture was stirred at room temperature for 16 h. The reaction was quenched with sat. $NH_4Cl_{(aq)}$ (20 mL). The product was extracted with $Et_2O$ (3x50 mL) and the combined organic extracts was washed brine (50 mL), dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The crude material was purified by column chromatography (1:1, EtOAc : hexane) to afford **10** (14.4 g, 95%) as a colourless solid, m.p. 107.8-108.7 °C. IR $\nu_{max}$ 3339m, 3230m, 2969m, 1687s, 1538m, 1480m, 1271m, 1250m, 1155m, 1133m $cm^{-1}$. $^1$H-NMR (400 MHz, $CDCl_3$): δ 6.92 (s, 4H), 4.81 (br s, 2H), 4.18 (d, *J* = 5.2 Hz, 4H), 3.35 (br s, 2H), 3.19 (s, 4H), 2.29 (s, 12H), 1.47 (s, 18H). $^{13}$C-NMR (100 MHz, $CDCl_3$): δ 156.0, 144.9, 132.6, 129.9, 128.3, 79.4, 49.0, 44.4, 28.5, 18.7. HRMS ($ESI^+$, MeOH): *m/z* 527.3596 $[M + H]^+$, $C_{30}H_{47}N_4O_4^+$ requires 527.3592.

## 1,3-Bis(4-(((*tert*-butoxycarbonyl)amino)methyl)-2,6-dimethylphenyl)-4,5-dihydro-1*H*-imidazol-3-ium tetrafluoroborate 11

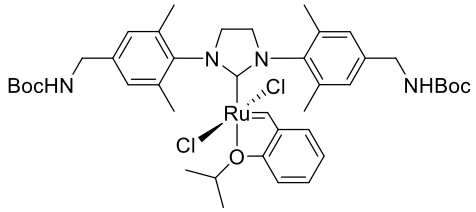



**11**

To a solution of diamine **10** (12.5 g, 23.7 mmol) in $(EtO)_3CH$ (35 mL) was added $NH_4BF_4$ (2.48 g, 23.7 mmol). The mixture was stirred at 120 °C for 16 h. The reaction was cooled to room temperature and the product precipitated from solution. The mixture was filtered and the solid was washed with $CH_2Cl_2$ (10 mL), $Et_2O$ (10 mL) and dried under reduced pressure to afford imidazolinium salt **11** (12.6 g, 85%) as a colourless solid, m.p. 240.3 (decomp.). IR $\nu_{max}$ 3333m, 2976m, 1690s, 1637s, 1260s, 1169m, 1046s $cm^{-1}$. $^1$H-NMR (400 MHz, $CD_3OD$): δ 8.87 (s, 1H), 7.18 (s, 4H), 4.53 (s, 4H), 4.20 (s, 4H), 2.43 (s,

12H), 1.45 (s, 18H). $^{13}$C-NMR (100 MHz, $CD_3OD$): δ 162.1, 158.4, 143.9, 137.0, 133.1, 129.1, 80.5, 52.6, 44.6, 28.8, 17.8. $^{19}$F-NMR (282 MHz, $CD_3OD$): δ -154.7. HRMS (ESI$^+$, MeOH): *m/z* 537.3449 $[M + H]^+$, $C_{31}H_{45}N_4O_4^+$ requires 537.3435.

## Ru-alkylidene complex 7




**7**

A glass column (2 cm diameter) packed with 5.0 g of Amberlite resin IRA-400 ($Cl^-$) was washed with $H_2O$ (30 mL). A solution of sat. $NH_4HCO_3$(aq) (50 mL) was passed slowly through the resin. The resin was washed with $H_2O$ (30 mL) followed by $H_2O/CH_3OH$ mixture (1:1) (30 mL) then finally $CH_3OH$ (30 mL). A solution of imidazolinium $BF_4$ salt **11** (1.29 g, 2.07 mmol) dissolved in minimal $CH_3OH$ (15 mL) was loaded onto the resin, and eluted with $CH_3OH$ (25 mL). The combined eluent was concentrated and rigourlessly dried under reduced pressure to afford imidazolinium $HCO_3$ salt **12** (1.22 g, 99%) as a colourless solid. To the vessel containing **12** (1.22 g, 2.04 mmol) was added **HGI** (919 mg, 1.53 mmol) and a stir bar. The vessel was evacuated and backfilled with $N_2$ (three times). Toluene (30 mL) was added to the vessel *via* syringe and the mixture stirred at 80 °C for 2 h. The mixture was cool to room temperature and concentrated under reduced pressure. The residue was purified by silica column chromatography (1:1 $Et_2O$ : hexane → 20:1 $Et_2O$ : hexane) (green band was collected) to afford Ru-alkylidene **7** (1.04 g, 79%) as a green solid, m.p. 158.1 °C (decomp.). IR $\nu_{max}$ 3361m, 2971m, 1697s, 1515m, 1482m, 1365m, 1259s, 1165s cm$^{-1}$. $^1$H-NMR (400 MHz, $C_6D_6$): δ 16.6 (s, 1H), 7.24 (d, *J* = 6.4 Hz, 1H), 7.11 (t, *J* = 6.4 Hz, 1H), 6.96 (s, 4H), 6.79 (t, *J* = 6.4 Hz, 1H), 6.31 (d, *J* = 6.4 Hz, 1H), 4.52 (br s, 2H), 4.51 (sept, *J* = 5.2 Hz, 1H), 4.23 (d, *J* = 4.4 Hz, 4H), 3.37 (s, 4H), 1.50 (s, 18H), 1.31 (d, *J* = 5.2 Hz, 6H). $^{13}$C-NMR (100 MHz, $C_6D_6$): δ 292.5, 213.1, 155.9, 152.7, 145.9, 140.4, 139.9, 129.1, 128.2, 127.9, 122.7, 122.4, 113.2, 79.0, 75.2, 51.2, 44.5, 30.2, 28.6, 21.4. HRMS (ESI$^+$, MeOH): *m/z* 857.3165 – 867.3336 (cluster) $[M + H]^+$, $C_{41}H_{57}Cl_2N_4O_5Ru^+$ requires 857.2744. Elemental analysis found: C, 56.6; H, 6.8; N, 6.3. $C_{41}H_{56}Cl_2N_4O_5Ru$ requires C, 57.5; H, 6.6; N, 6.5% $C_{41}H_{56}Cl_2N_4O_5Ru$ + $H_2O$ requires C, 56.3; H, 6.7; N, 6.4%.

## Substrate Preparation

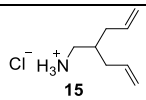
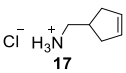
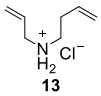
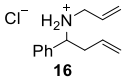
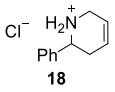
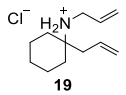
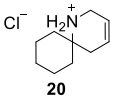
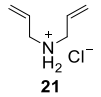
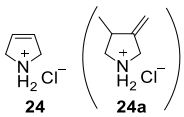
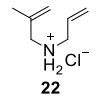
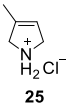
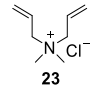
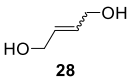
*N*,*N*-Diallylamine hydrochloride (**21**), diallyldimethylammonium chloride (**23**), allyl alcohol (**27**), butenylammonium chloride (**37**), and allylammonium chloride (**41**) were used as supplied by Sigma-

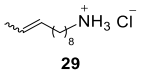
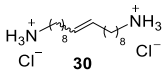
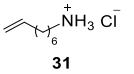
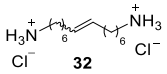
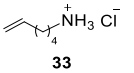
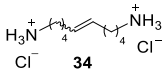
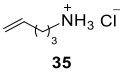
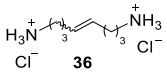
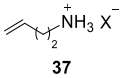
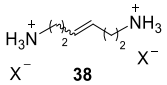
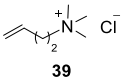
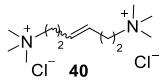
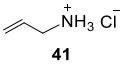
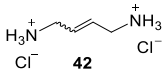
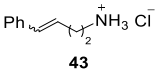
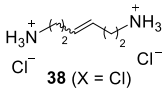
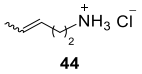
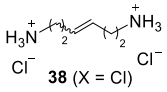
Aldrich. Substrates **15**,[4] **13**,[5] **16**,[6] **19**,[7] **22**,[4] **31**,[8] **33**,[9] **35**,[10] **39**,[11] **43**[12] and **44**[13] were prepared according to previous literature reports.

## General Procedure for Olefin Metathesis in Water

Trifluoroacetic acid (0.50 mL) was added dropwise to a stirred and cooled (0 °C.) solution of **7** (10.0 mg, 0.012 mmol, 5 mol%) in $CH_2Cl_2$ (1.0 mL). The mixture was stirred for 1 h at 0 °C. The mixture was then concentrated under reduced pressure to afford **6** as a green solid. To **6** was added fresh $CH_2Cl_2$ (2.0 mL) and the resultant suspension was concentrated under reduced pressure to remove remaining traces to trifluoroacetic acid. Pre-catalyst **6** was dried under reduced pressure and a solution of the substrate (0.23 mmol) in $D_2O$ (2.3 mL) was added. The homogeneous mixture was stirred at 80 °C for 1 h. The reaction mixture was analysed by $^1$H-NMR spectroscopy. Isolation of metathesis products was performed on selected substrates. For isolation, the reaction mixture was cooled to r.t. and diluted with $H_2O$ (5 ml). The aqueous phase was washed with $Et_2O$ (5 mL) and the organic phase discarded. The aqueous phase was basified with 1 M NaOH solution (2 mL) and the free amine extracted with $Et_2O$ (3 x 10 mL). The combined organic extracts were dried ($Na_2SO_4$), filtered and to the filtrate was added a saturated solution of HCl in $Et_2O$ (2 mL). The resultant cloudy suspension was then concentrated in vacuo to afford the corresponding ammonium hydrochloride salt.

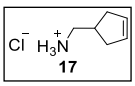
**Table 1.** Olefin metathesis reaction catalyzed by pre-catalyst **6** in $D_2O$

| Entry | Substrate | Product | Conversion | Reference[d] |
|---|---|---|---|---|
| 1 |  **15** |  **17** | 95%[c]<br>91%[b] | Figure S1 |
| 2 |  **13** |  **14** | >95%<br>88%[c] | Figure S2 |
| 3 |  **16** |  **18** | >95%<br>94%[c] | Figure S3 |
| 4 |  **19** |  **20** | 56% | Figure S4 |
| 5 |  **21** |  **24** **24a** | 61% (29%) | Figure S5 |
| 6 |  **22** |  **25** | 47% | Figure S6 |
| 7 |  **23** |  **26** | 25% | Figure S7 |
| 8 |  **27** |  **28** | >95% | Figure S8 |

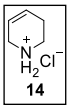
| | | | | |
|---|---|---|---|---|
| 9 |  **29** |  **30** | >95% | Figure S9 |
| 10 |  **31** |  **32** | >95%<br>92%[c] | Figure S10 |
| 11 |  **33** |  **34** | >95%<br>90%[c] | Figure S11 |
| 12 |  **35** |  **36** | 0% | Figure S12 |
| 13 |  **37**<br>X = Cl, $BF_4$, OTf, $SO_2$ |  **38** | 0% | Figure S13 |
| 14 |  **39** |  **40** | 0% | Figure S14 |
| 15 |  **41** |  **42** | 0% | Figure S15 |
| 16 |  **43** |  **38** (X = Cl) | 0% | Figure S16 |
| 17 |  **44** |  **38** (X = Cl) | 33% | Figure S17 |

[a] Metathesis reactions were performed using 5 mol% **6** in $D_2O$ at 80 °C for 1 h. The initial substrate concentration was 0.1 M in $D_2O$. Conversions were determined by $^1$H-NMR spectroscopy. [b] Reaction performed using 0.1 mol% precatalyst **6**. [c] Isolated yield. [d] See Spectral Data section below.

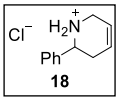
## Isolated Product Characterisation


**17**

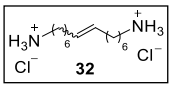
Prepared following general procedure in 91% yield. $^1$H-NMR (400 MHz, $D_2O$): δ 5.75 (s, 2H), 3.04 (d, $J$ = 6.0 Hz, 2H), 2.63-2.56 (m, 3H), 2.15-2.08 (m, 2H). $NH_3$ protons not observed due to deuterium exchange. $^{13}$C-NMR (75 MHz, $D_2O$): δ 129.8, 44.6, 36.3, 35.3. HRMS (ESI$^+$, MeOH): *m/z* 98.0966 $[M + H]^+$, $C_6H_{12}N^+$ requires 98.0965.


**14**

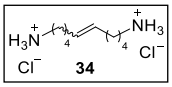
Prepared following general procedure in 88% yield. $^1$H-NMR (400 MHz, $D_2O$): δ 6.02-5.96 (m, 1H), 5.79-5.73 (m, 1H), 3.67 (t, $J$ = 2.4 Hz, 2H), 3.34 (t, $J$ = 6.2 Hz, 2H), 2.42-2.36 (m, 2H). $NH_2$ protons not observed due to deuterium exchange. HRMS (ESI$^+$, MeOH): *m/z* 84.0807 $[M + H]^+$, $C_5H_{10}N^+$ requires 85.0808. All data was consistent with that previously reported.[4]


**18**

Prepared following general procedure in 94% yield. $^1$H-NMR (400 MHz, $D_2O$): δ 7.56-7.54 (m, 5H), 6.17-6.13 (m, 1H), 5.92-5.89 (m, 1H), 4.56 (dd, $J$ = 10.4 & 4.8 Hz, 1H), 3.97 (d, $J$ = 16.8 Hz, 1H), 3.81 (d, $J$ = 16.8 Hz, 1H), 2.82-2.65 (m, 2H). $NH_2$ protons not observed due to deuterium exchange. $^{13}$C-NMR (100 MHz, $D_2O$): δ 136.4, 129.9, 129.7, 127.3, 126.2, 119.8, 57.0, 43.4, 29.4. HRMS (ESI$^+$, MeOH): *m/z* 160.1120 $[M + H]^+$, $C_{11}H_{14}N^+$ requires 160.1121.




Prepared following general procedure in 92% yield. $^{1}$H-NMR (400 MHz, $D_2O$): δ 5.44-5.41 (m, 2H), 2.88 (t, *J* = 7.6 Hz, 4H), 1.98-1.86 (m, 4H), 1.57-1.51 (m, 4H), 1.31-1.18 (m, 12H). $NH_3$ protons not observed due to deuterium exchange. $^{13}$C-NMR (100 MHz, $D_2O$): δ 131.0, 39.6, 31.7, 28.5, 27.7, 26.7, 25.4. HRMS (ESI$^+$, MeOH): *m/z* 227.2481 $[M + H]^+$, $C_{14}H_{31}N_2^+$ requires 227.2481.




Prepared following general procedure in 90% yield. $^{1}$H-NMR (400 MHz, $D_2O$): δ 5.57-5.54 (m, 2H), 3.02 (t, *J* = 7.6 Hz, 4H), 2.10-2.06 (m, 4H), 1.73-1.65 (m, 4H), 1.47 (p, *J* = 7.6 Hz, 4H). $NH_3$ protons not observed due to deuterium exchange. $^{13}$C-NMR (100 MHz, $D_2O$): δ 130.6, 39.4, 31.2, 26.2, 25.5. HRMS (ESI$^+$, MeOH): *m/z* 171.1857 $[M + H]^+$, $C_{10}H_{23}N_2^+$ requires 171.1856.

## References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## Spectra Data

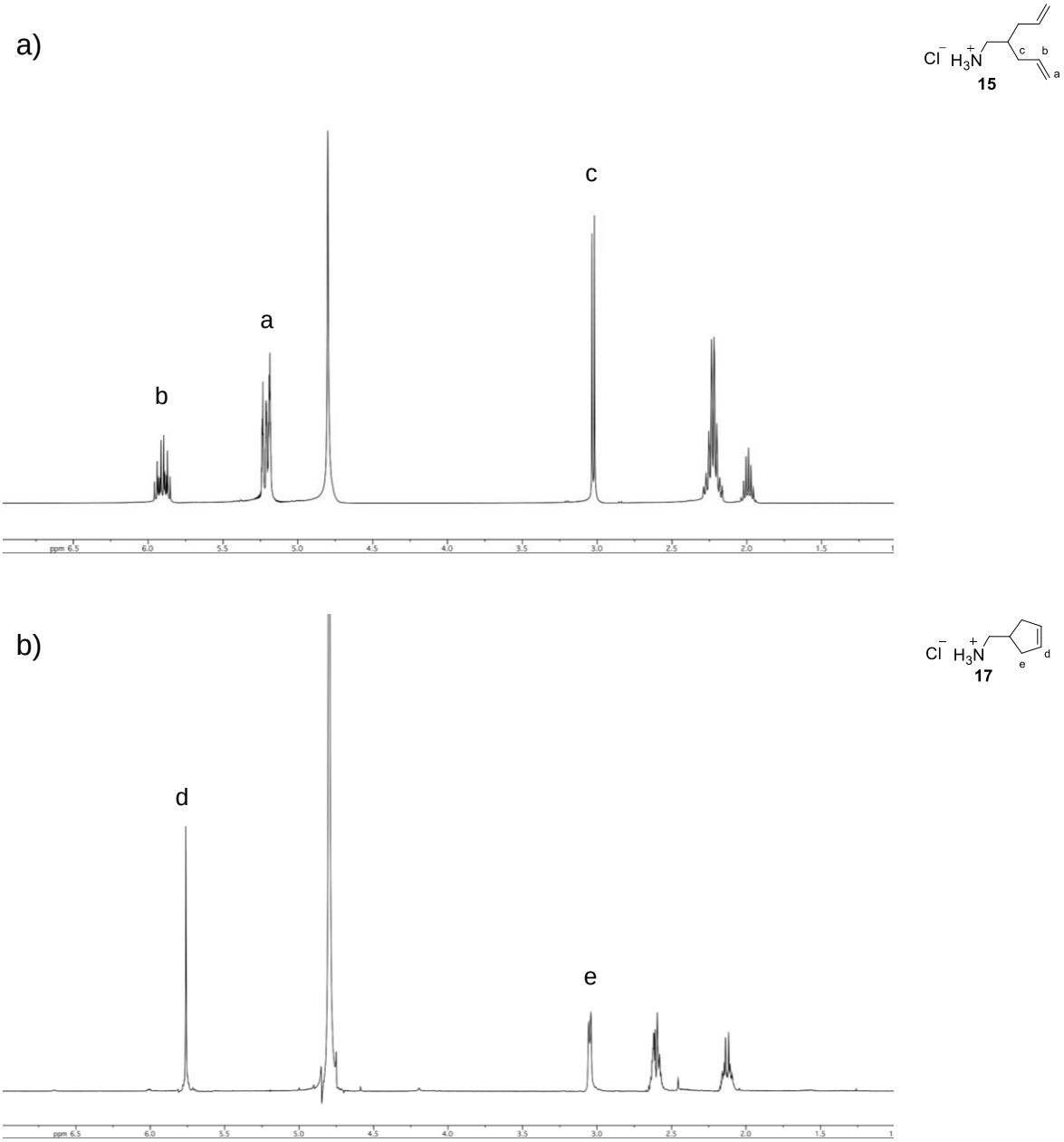



**Figure S1.** [1]H-NMR spectrum of a) starting substrate **15** and b) crude reaction mixture after olefin metathesis in water

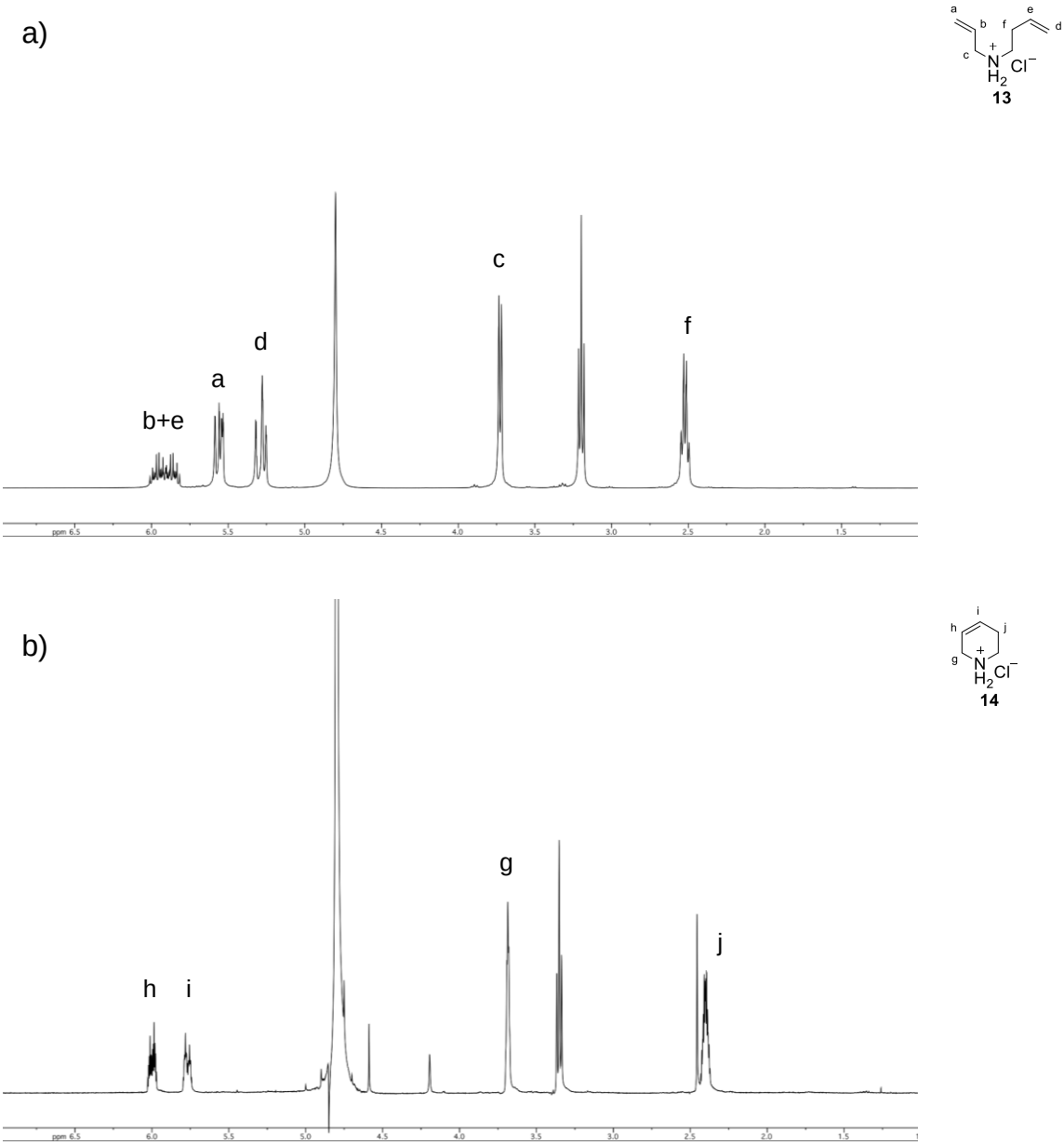



**Figure S2.** [1]H-NMR spectrum of a) starting substrate **13** and b) crude reaction mixture after olefin metathesis in water

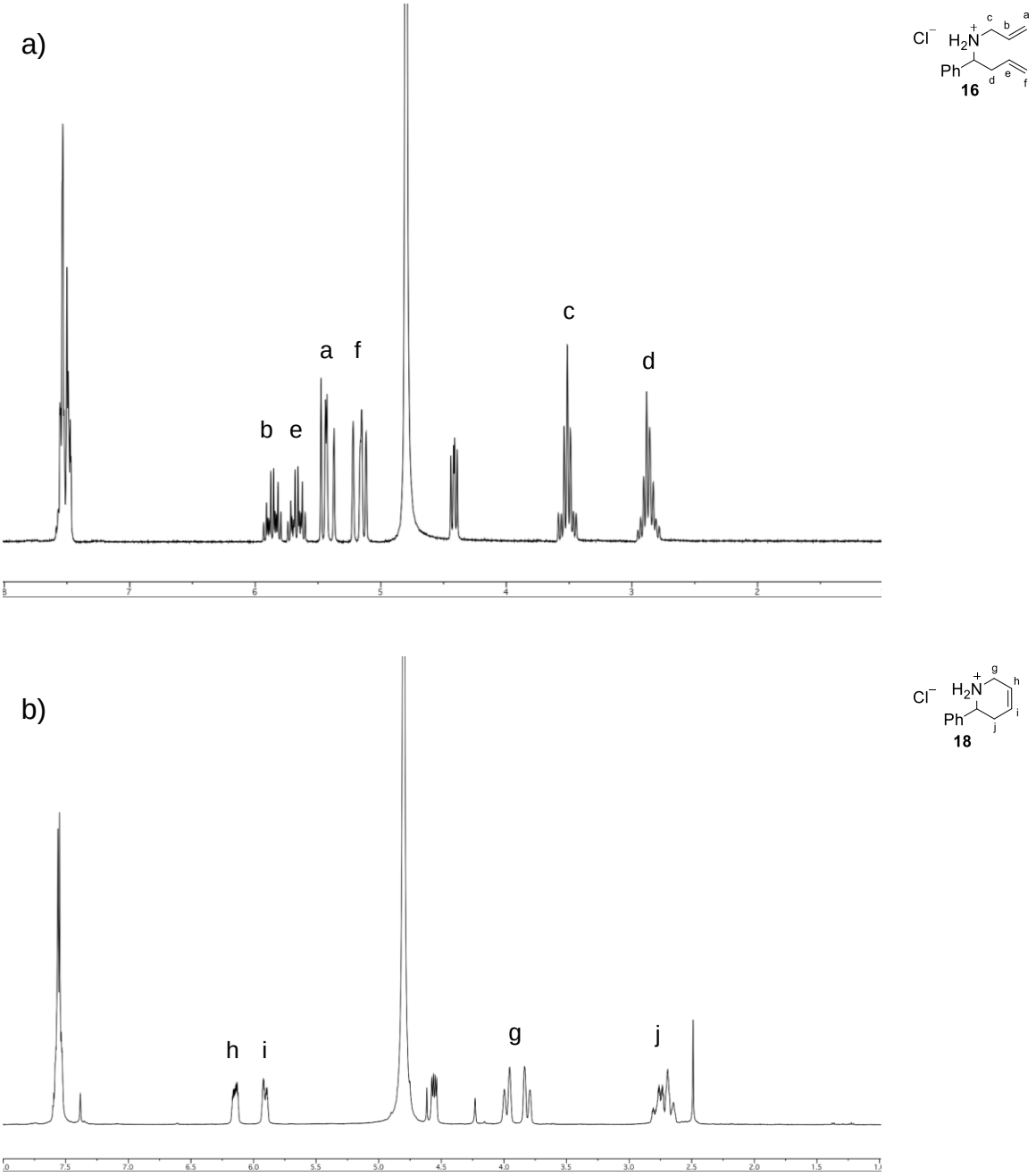



**Figure S3.** $^{1}$H-NMR spectrum of a) starting substrate **16** and b) crude reaction mixture after olefin metathesis in water

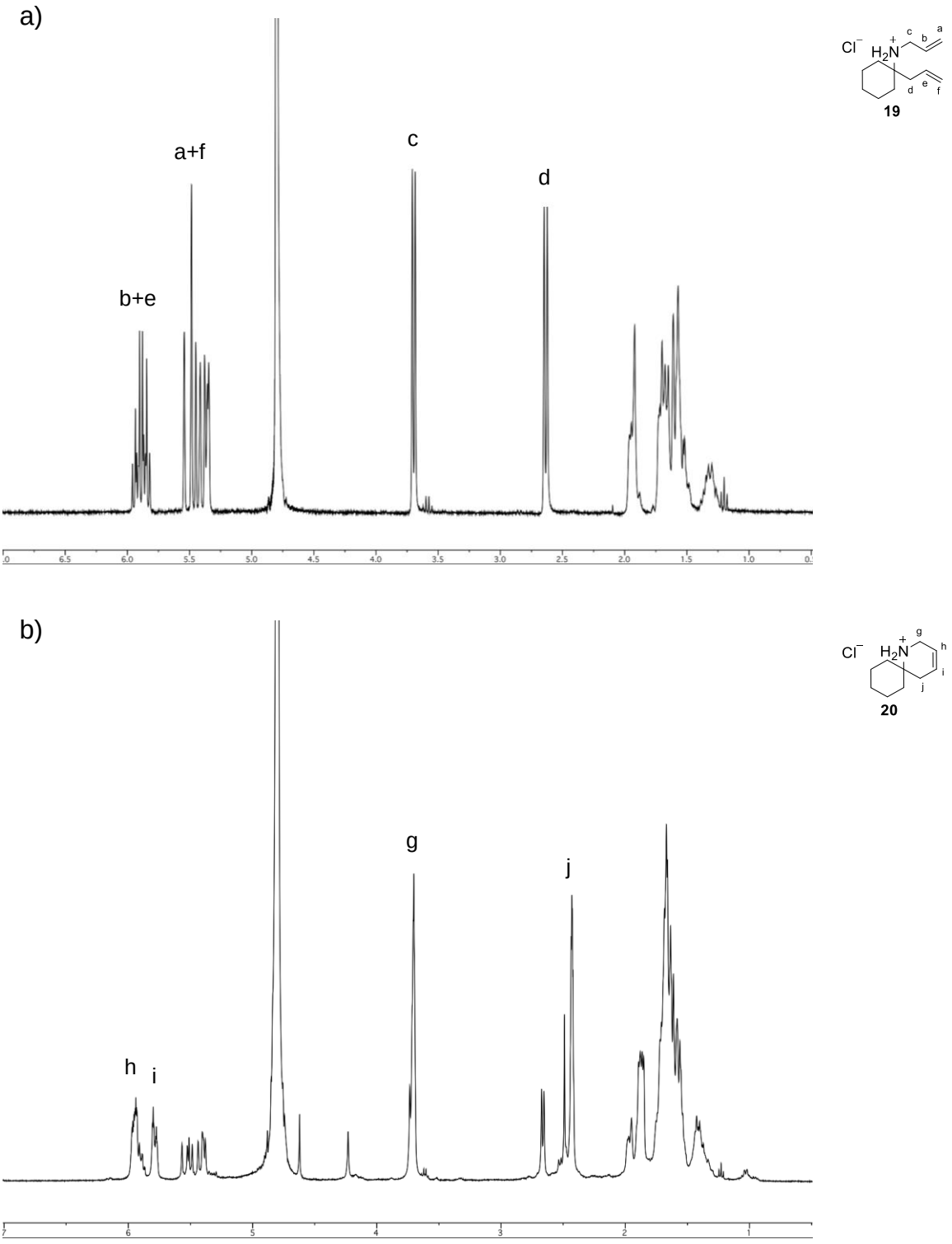



**Figure S4.** [1]H-NMR spectrum of a) starting substrate **19** and b) crude reaction mixture after olefin metathesis in water

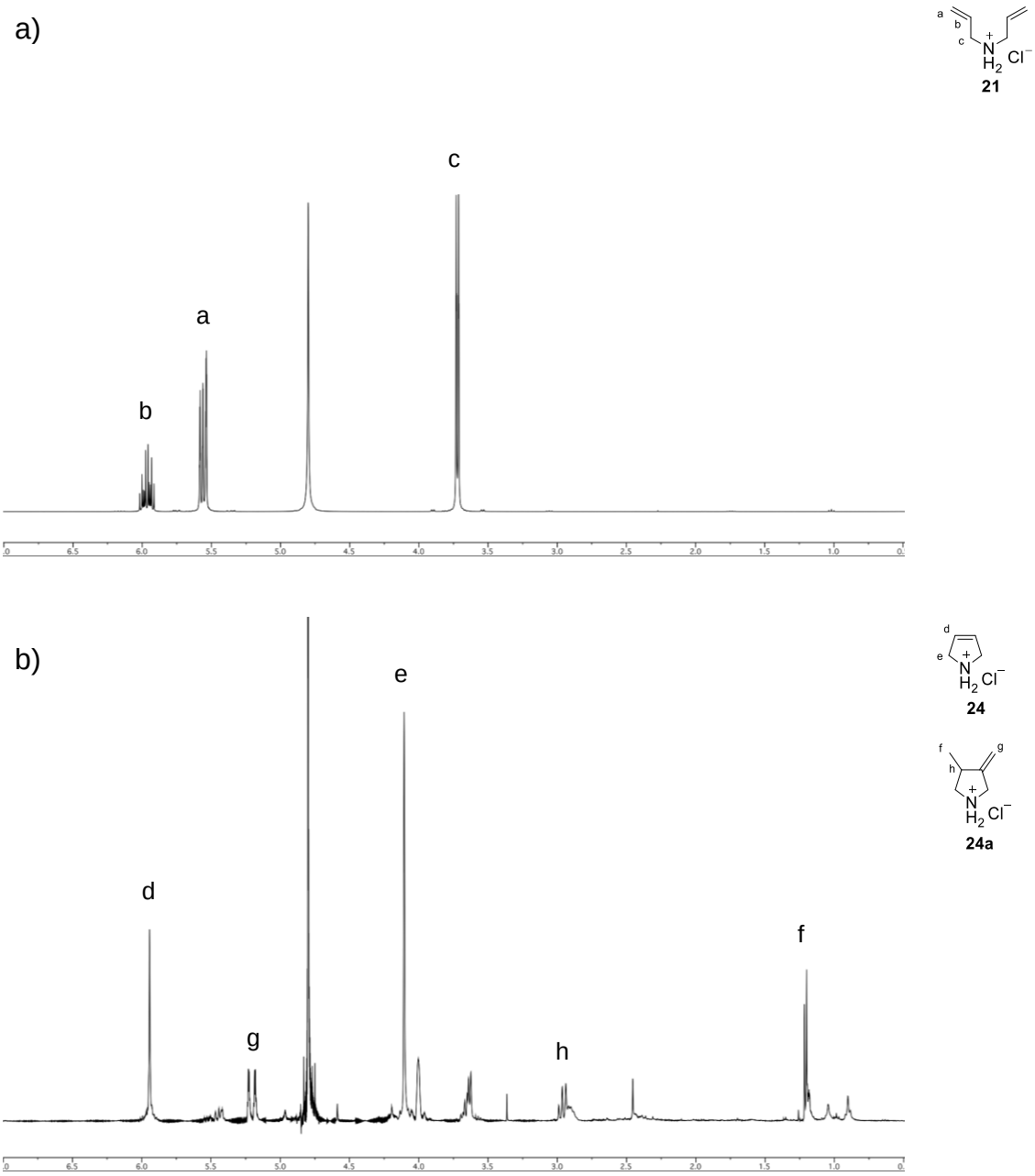



**Figure S5.** [1]H-NMR spectrum of a) starting substrate **21** and b) crude reaction mixture after olefin metathesis in water

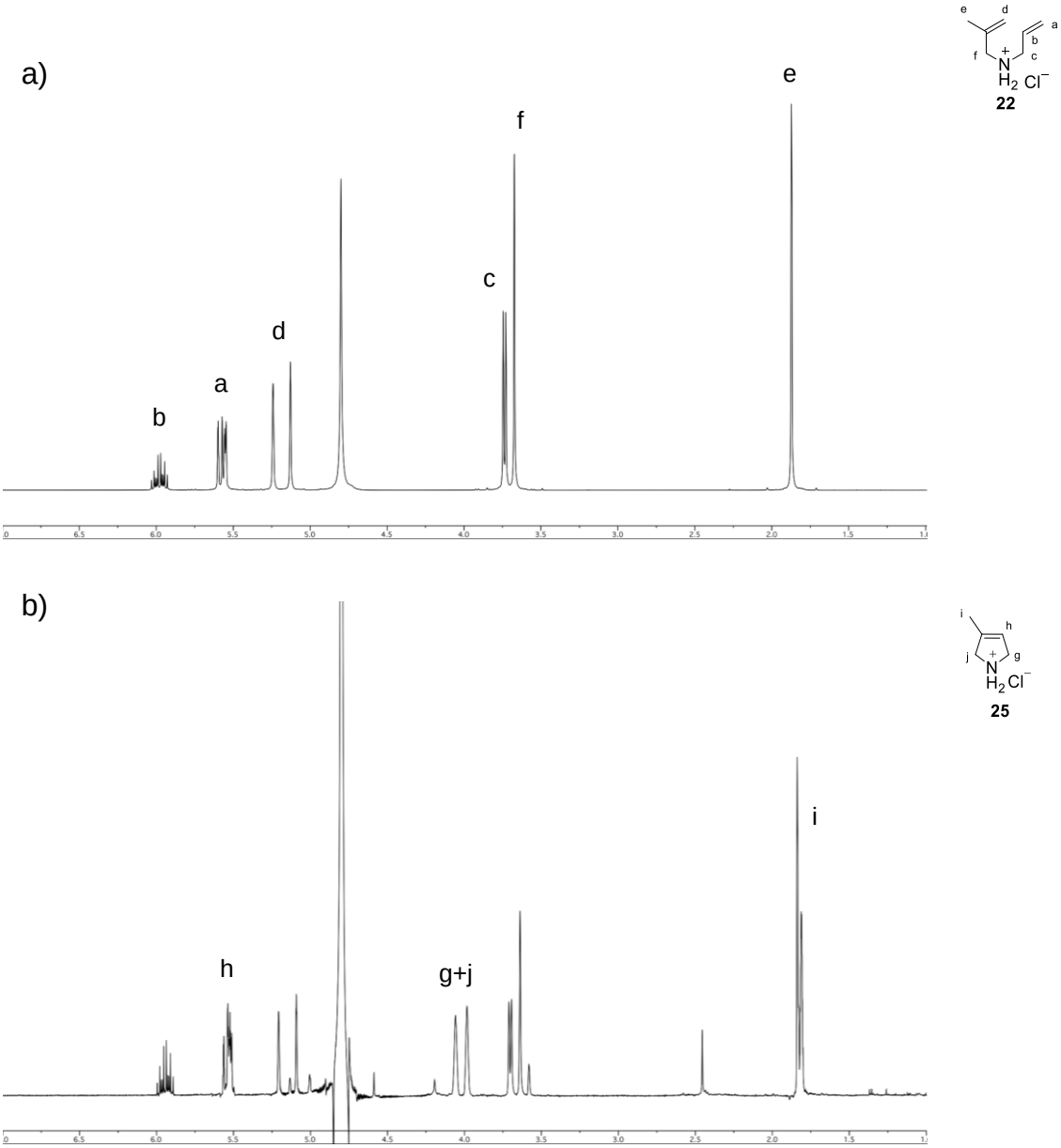



**Figure S6.** $^{1}$H-NMR spectrum of a) starting substrate **22** and b) crude reaction mixture after olefin metathesis in water

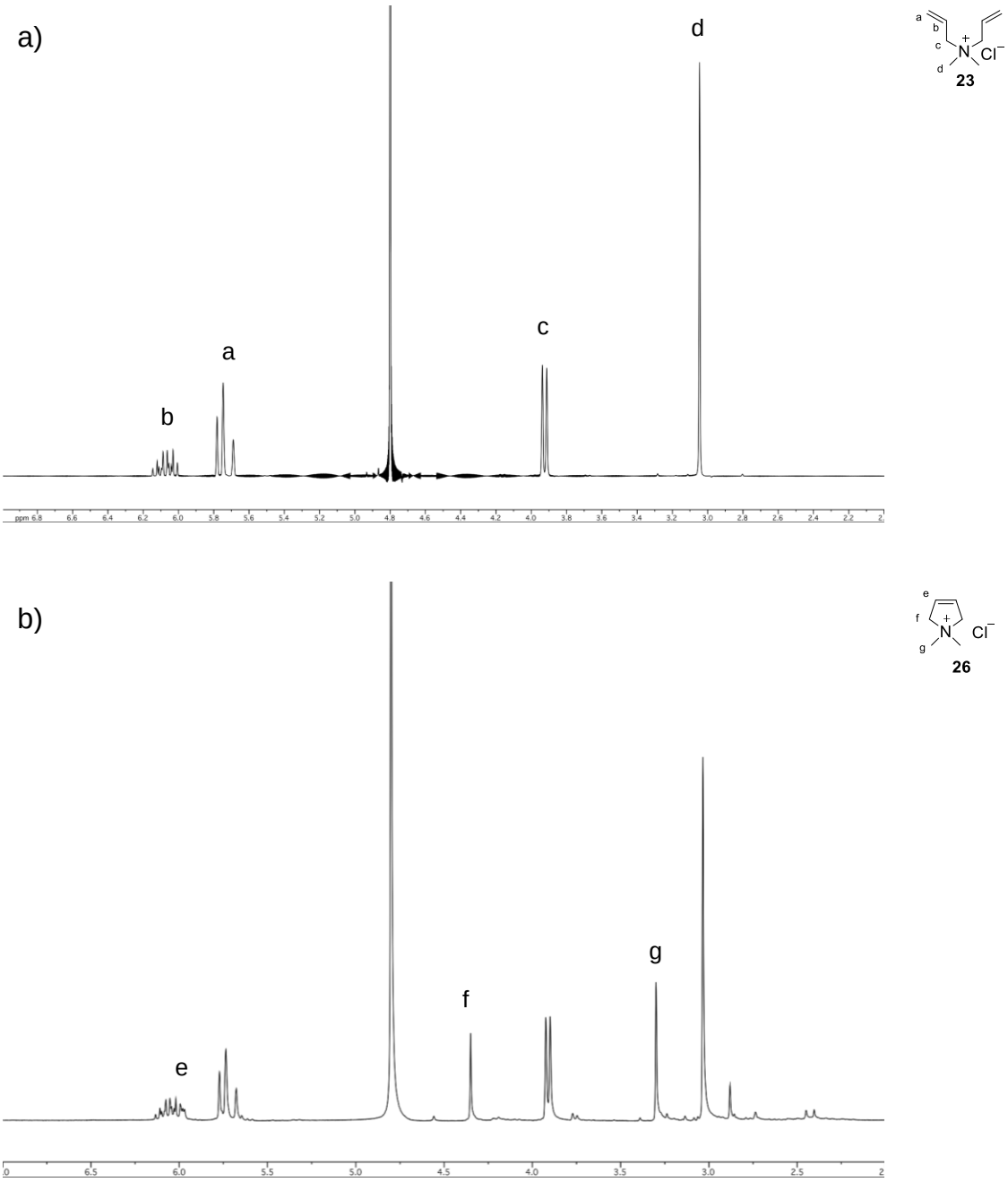



**Figure S7.** [1]H-NMR spectrum of a) starting substrate **23** and b) crude reaction mixture after olefin metathesis in water

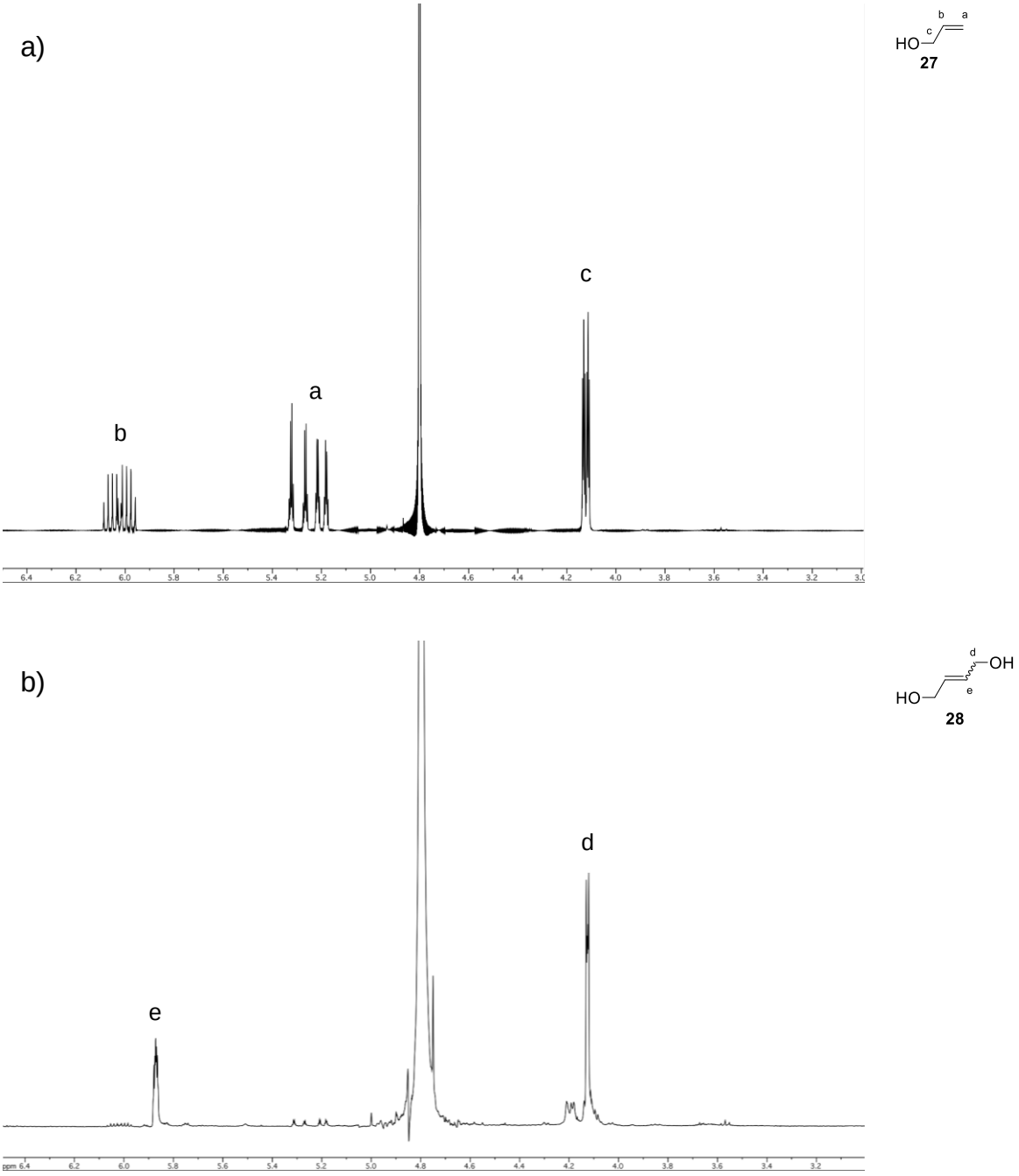



**Figure S8.** $^{1}$H-NMR spectrum of a) starting substrate **27** and b) crude reaction mixture after olefin metathesis in water

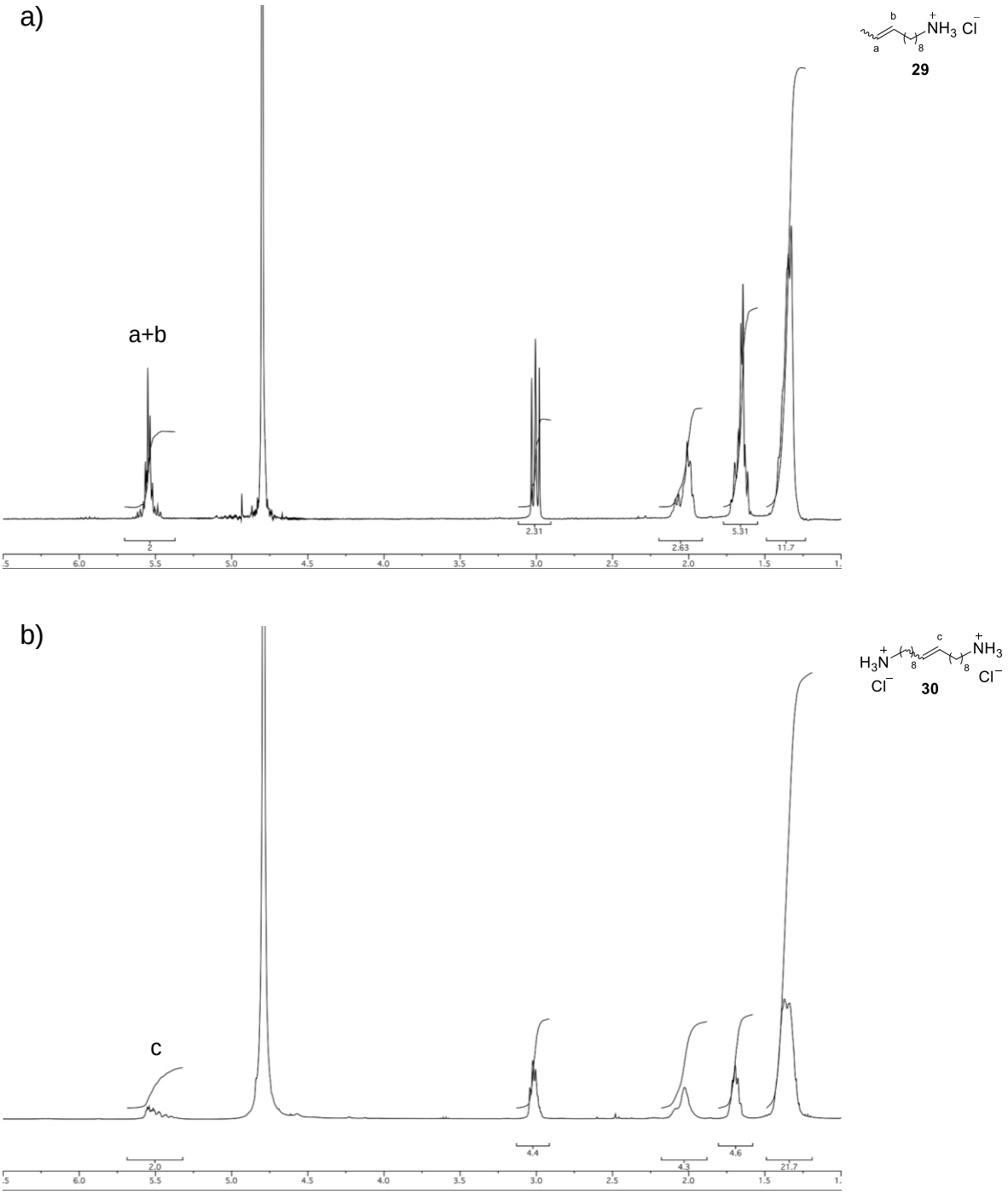



**Figure S9.** [1]H-NMR spectrum of a) starting substrate **29** and b) crude reaction mixture after olefin metathesis in water

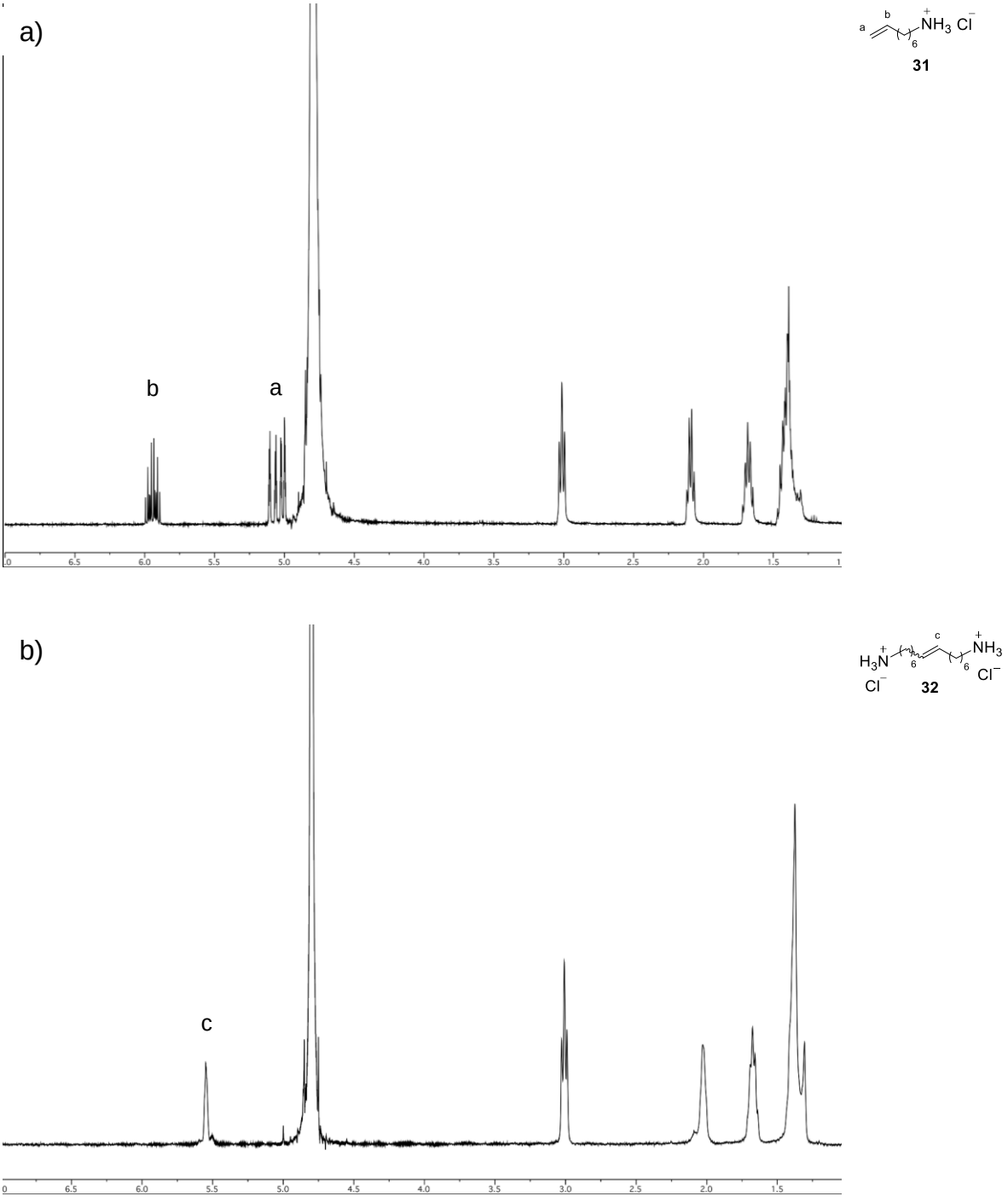
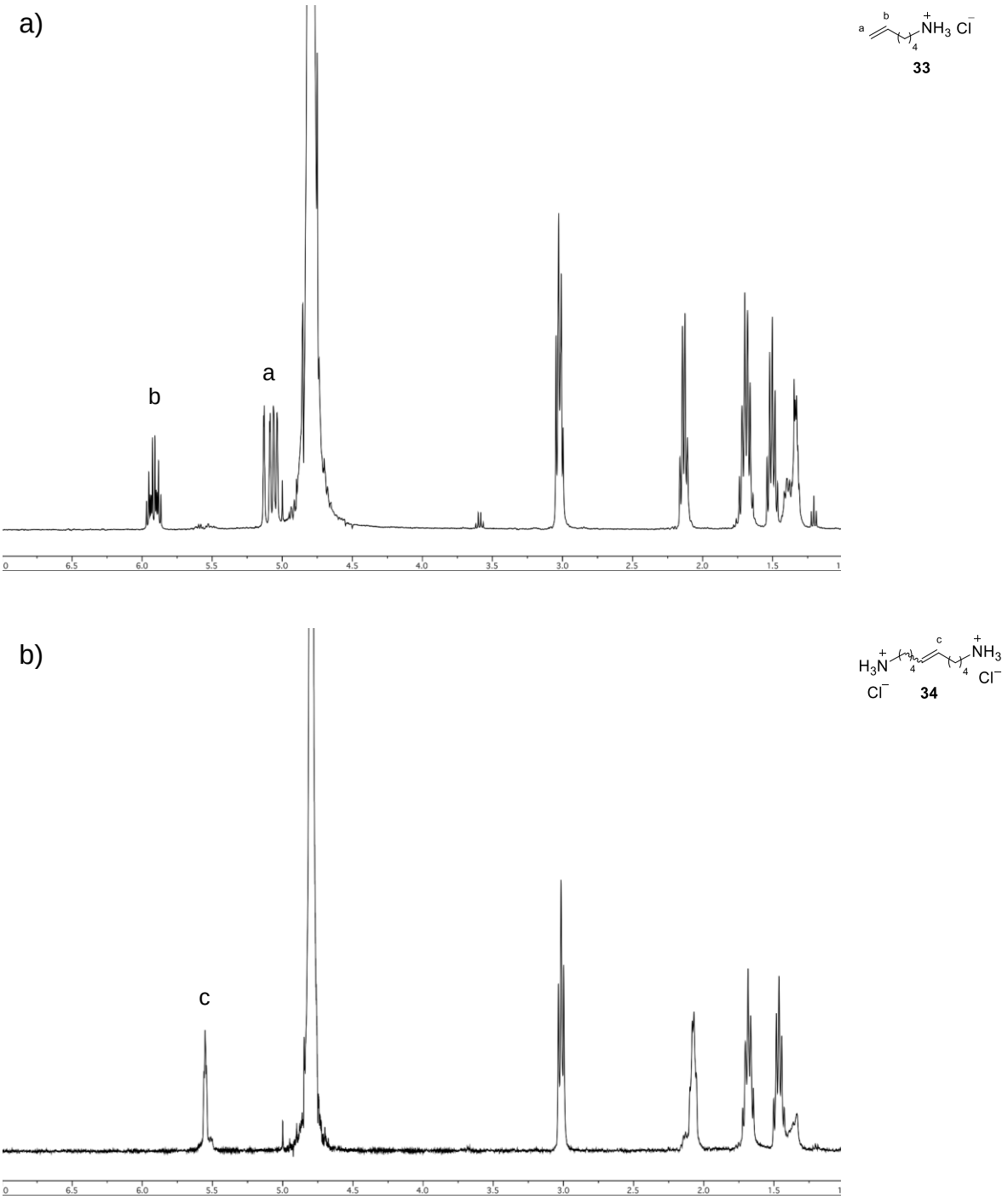


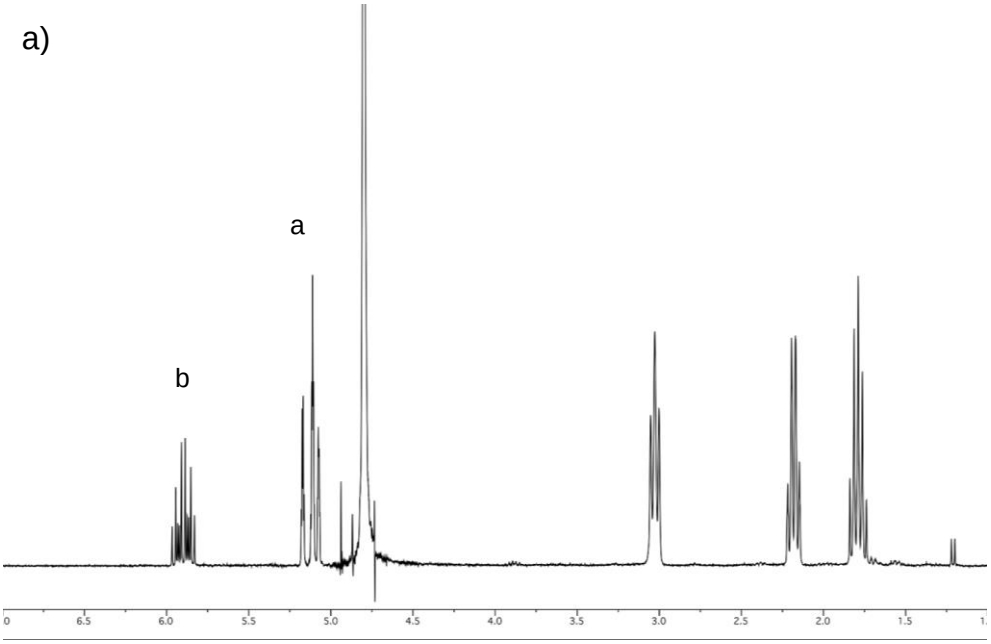

**Figure S10.** $^{1}$H-NMR spectrum of a) starting substrate **31** and b) crude reaction mixture after olefin metathesis in water

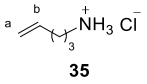



**33**

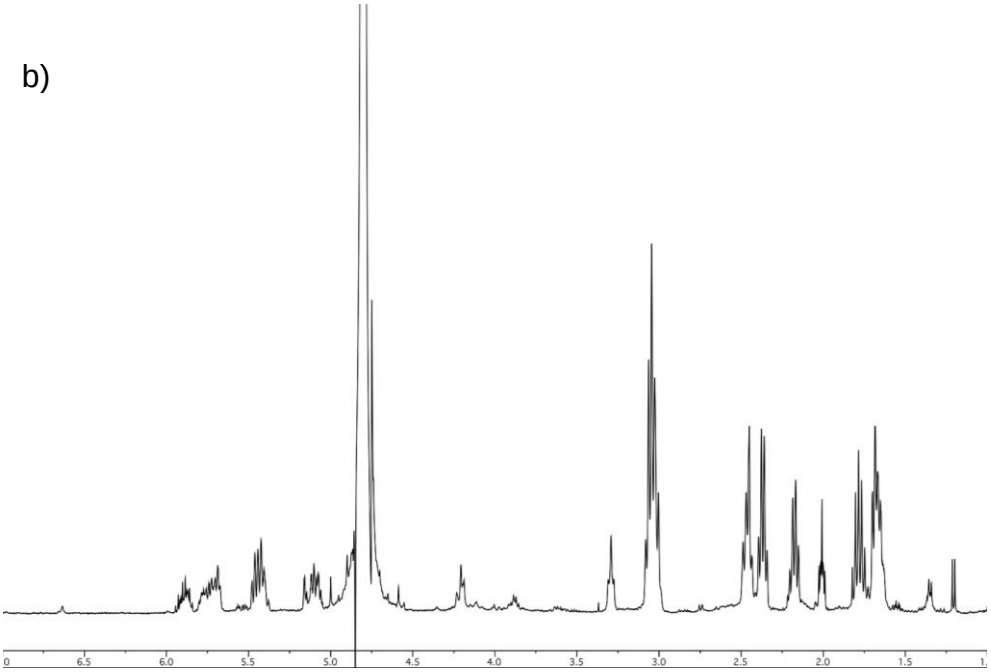
**34**

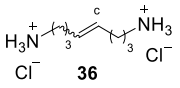
**Figure S11.** [1]H-NMR spectrum of a) starting substrate **33** and b) crude reaction mixture after olefin metathesis in water




**35**



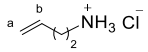




**36**

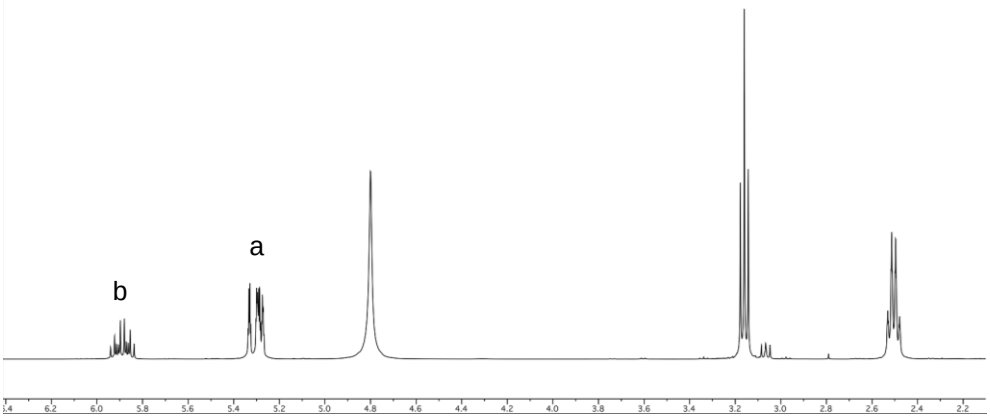
(not observed)

**Figure S12.** [1]H-NMR spectrum of a) starting substrate **35** and b) crude reaction mixture after olefin metathesis in water

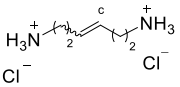
a)




**37** (X = Cl)

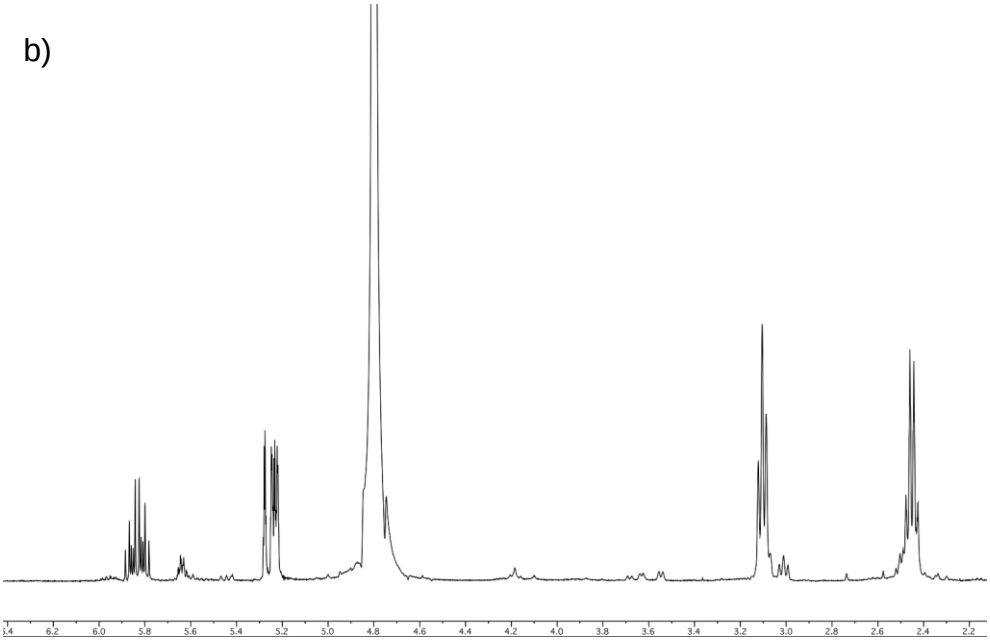


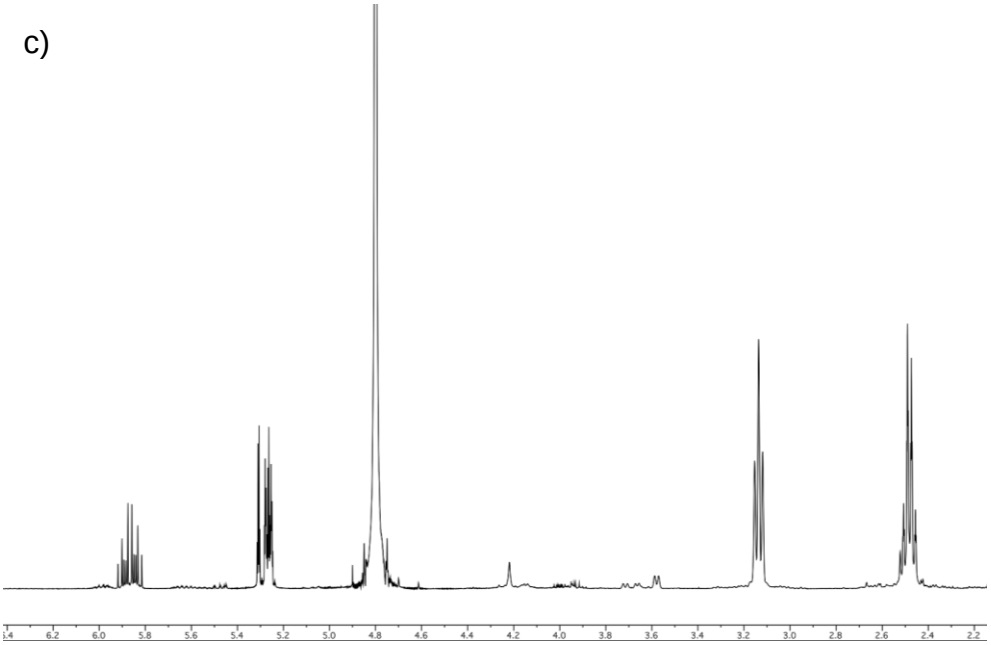

b)




**38** (X = Cl)

(not observed)





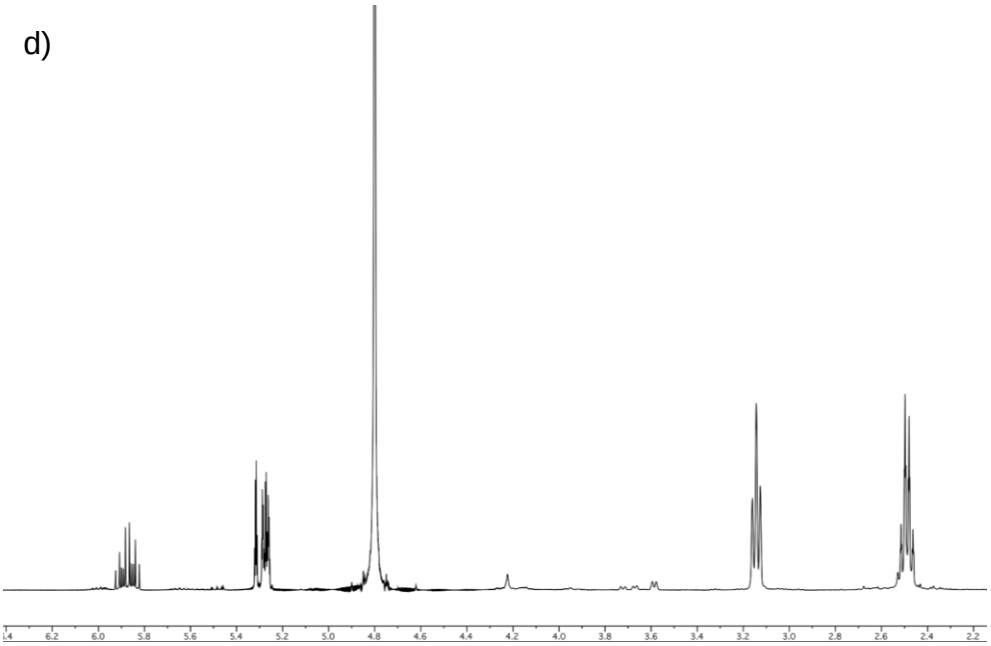
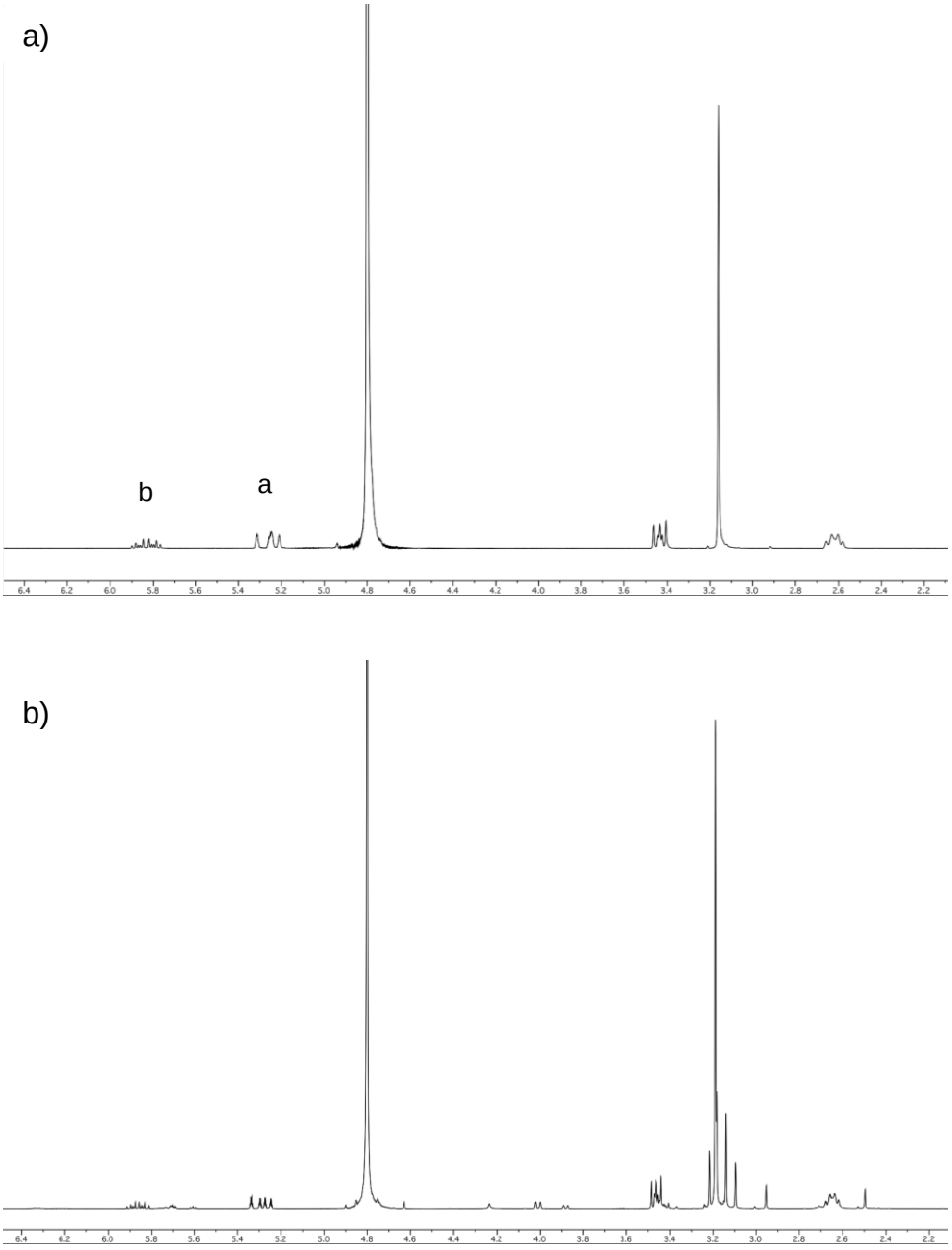




**Figure S13.** [1]H-NMR spectrum of a) starting substrate **37** and b-d) crude reaction mixtures after olefin metathesis in water



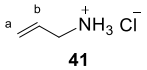

**39**

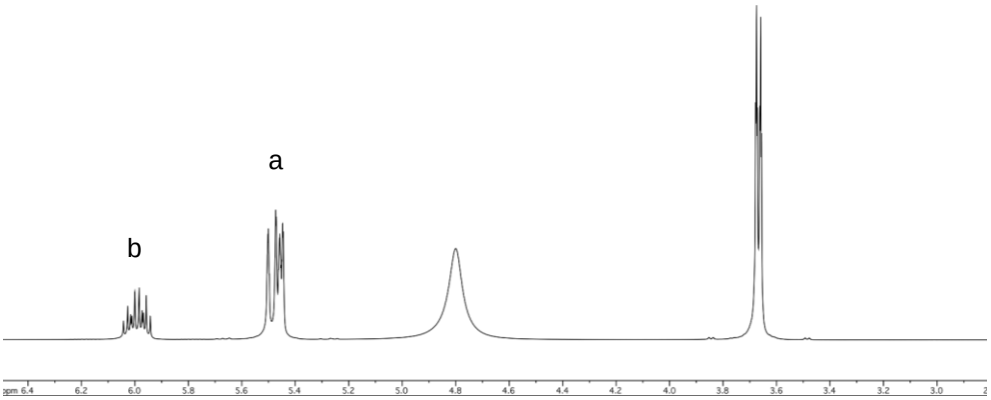
**40**

(not observed)

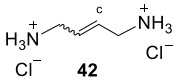
**Figure S14.** $^{1}$H-NMR spectrum of a) starting substrate **39** and b) crude reaction mixture after olefin metathesis in water

a)




b)




(not observed)

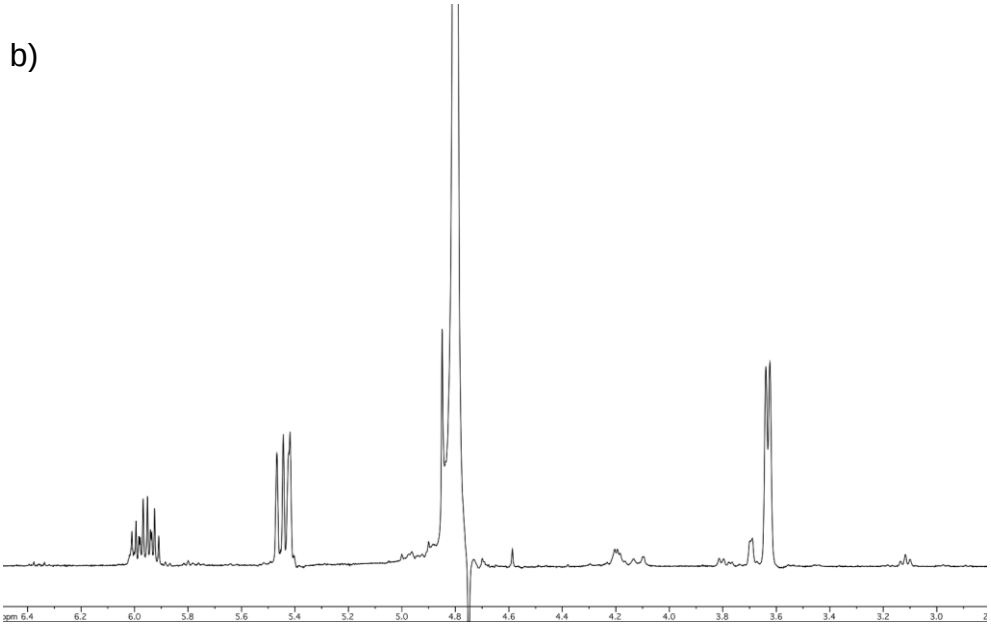


**Figure S15.** [1]H-NMR spectrum of a) starting substrate **41** and b) crude reaction mixture after olefin metathesis in water

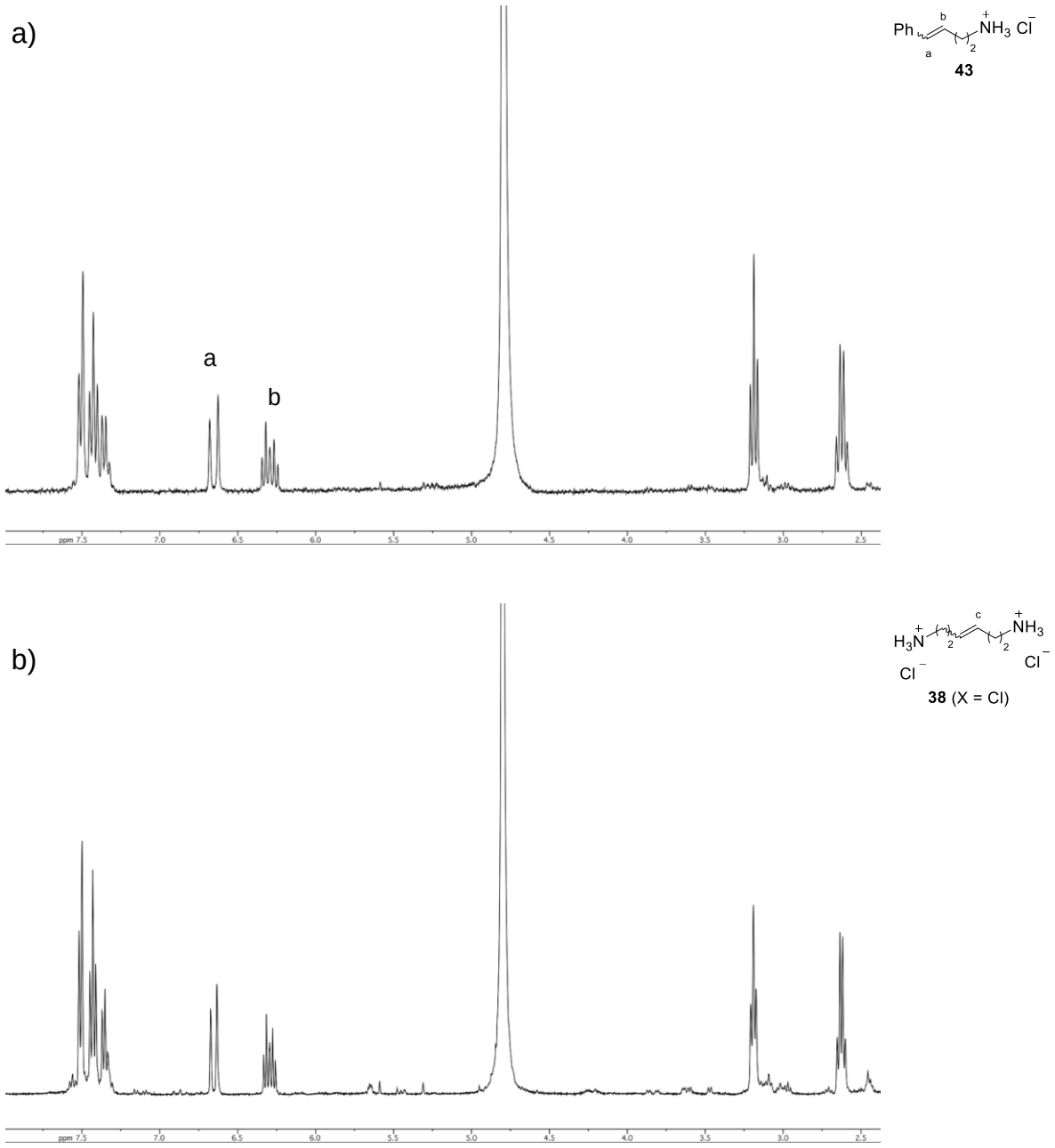



**Figure S16.** [1]H-NMR spectrum of a) starting substrate **43** and b) crude reaction mixture after olefin metathesis in water

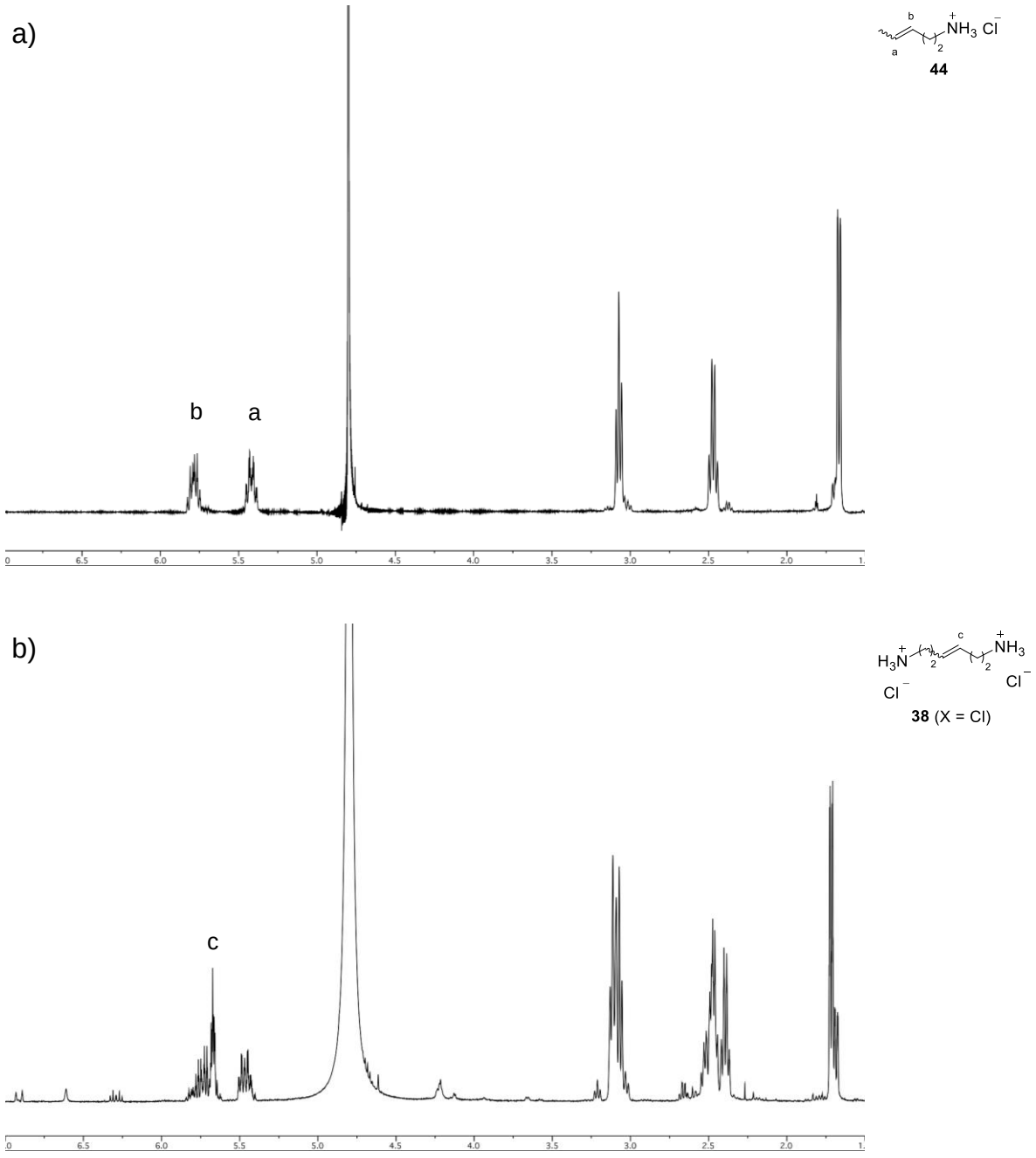
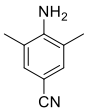
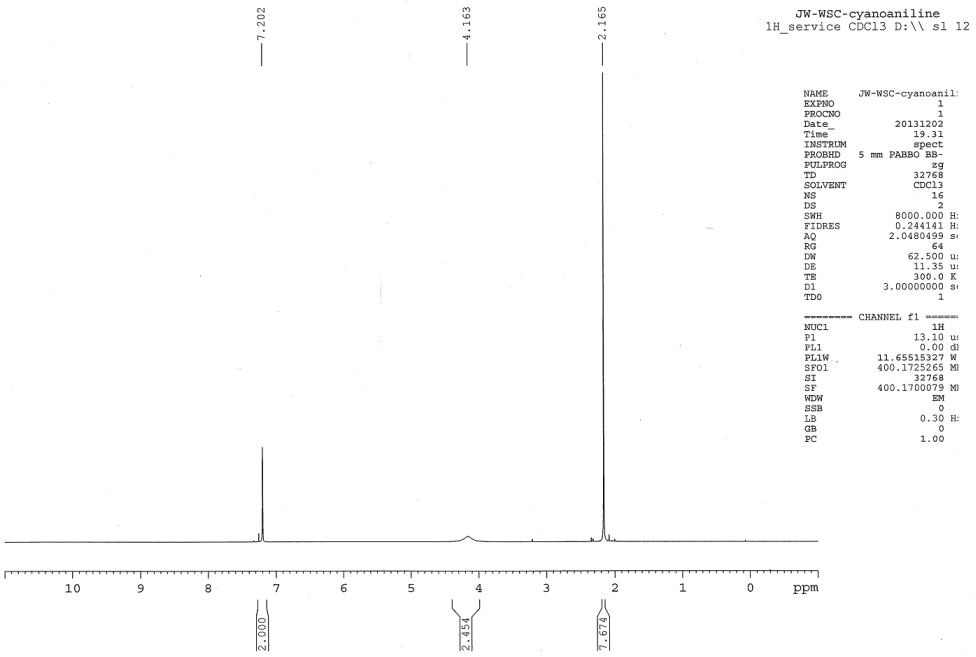
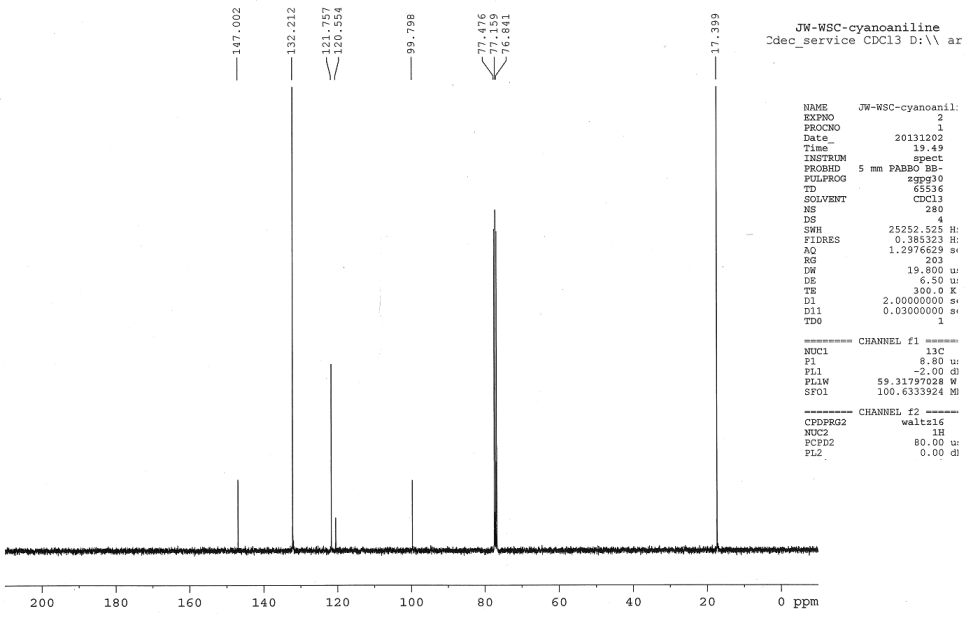


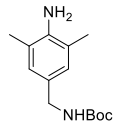

**Figure S17.** [1]H-NMR spectrum of a) starting substrate **44** and b) crude reaction mixture after olefin metathesis in water


NH2
CN

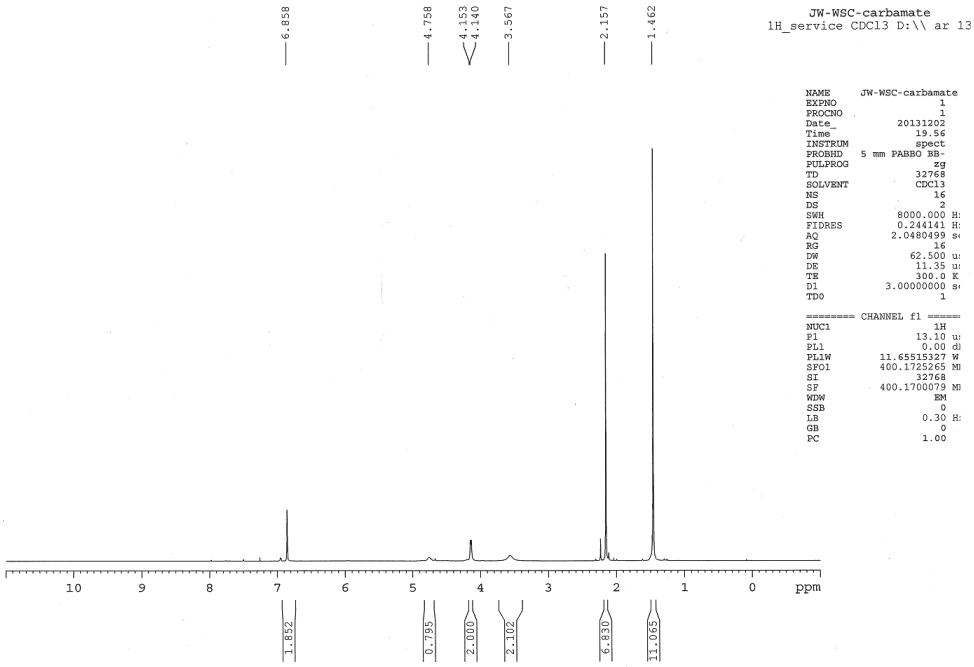
**7**

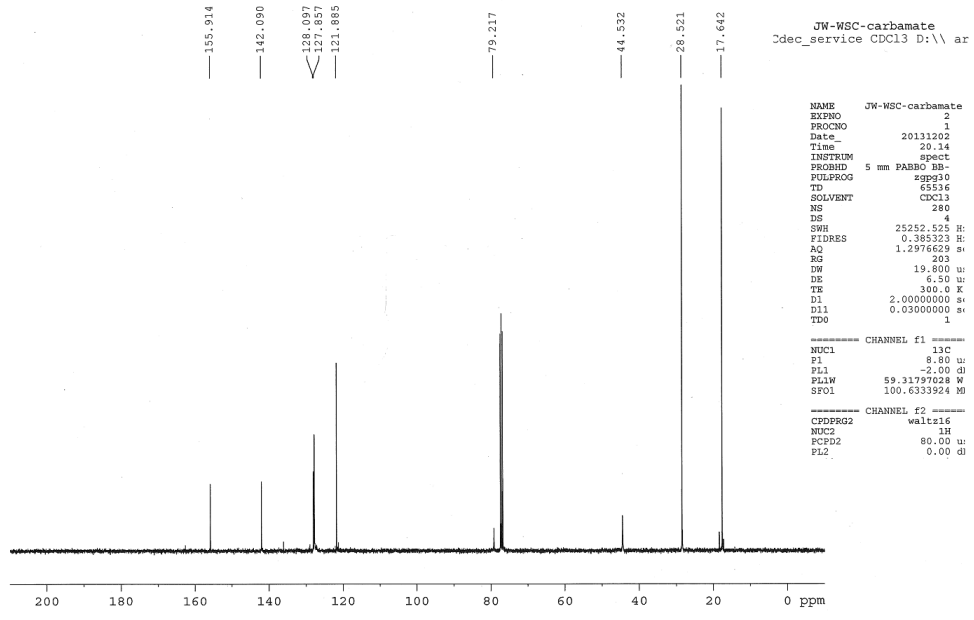

7.202
4.163
2.165
JW-WSC-cyanoaniline
1H_service CDCl3 D:\\ sl 12
NAME JW-WSC-cyanoanil
EXPNO 1
PROCNO 1
Date_ 20131202
Time 19.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8000.000 H
FIDRES 0.244141 H
AQ 2.0480499 s
RG 64
DW 62.500 u
DE 11.35 u
TE 300.0 K
D1 3.00000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.10 u
PL1 0.00 dB
PL1W 11.65515327 W
SFO1 400.1725265 M
SI 32768
SF 400.1700079 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
2.000
2.454
7.674

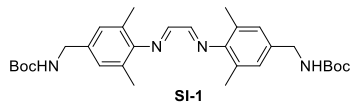

147.002
132.212
121.757
120.554
99.798
77.476
77.159
76.841
17.399
JW-WSC-cyanoaniline
2dec_service CDCl3 D:\\ ar
NAME JW-WSC-cyanoanil
EXPNO 2
PROCNO 1
Date_ 20131202
Time 19.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 280
DS 4
SWH 25252.525 H
FIDRES 0.385323 H
AQ 1.2976629 s
RG 203
DW 19.800 u
DE 6.50 u
TE 300.0 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 8.80 u
PL1 -2.00 dB
PL1W 59.31797028 W
SFO1 100.6333924 M
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 dB
200 180 160 140 120 100 80 60 40 20 0 ppm


NH2
NHBoc

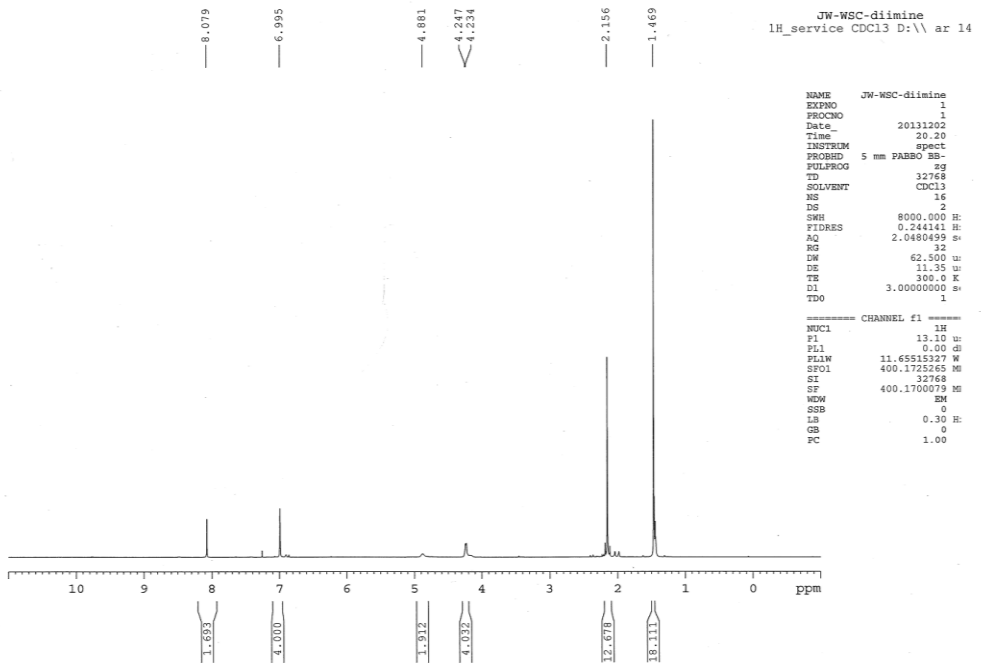
**9**

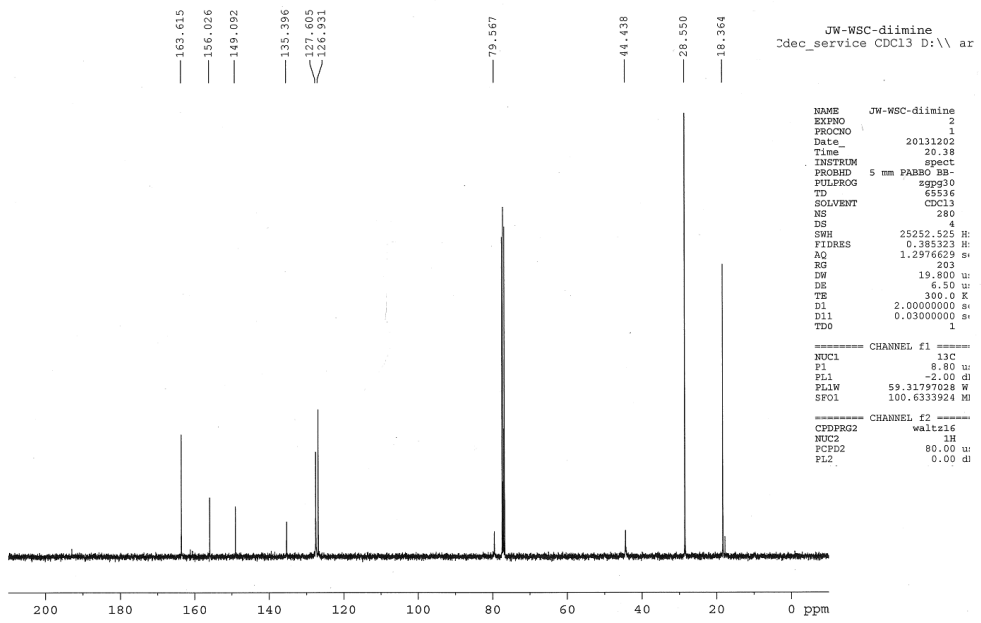

6.858
4.758
4.153
4.140
3.567
2.157
1.462
JW-WSC-carbamate
1H_service CDCl3 D:\\ ar 13
NAME JW-WSC-carbamate
EXPNO 1
PROCNO 1
Date_ 20131202
Time 19.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8000.000 H
FIDRES 0.244141 H
AQ 2.0480499 s
RG 16
DW 62.500 u
DE 11.35 u
TE 300.0 K
D1 3.00000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.10 u
PL1 0.00 d
PL1W 11.65515327 W
SFO1 400.1725265 M
SI 32768
SF 400.1700079 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
1.852
0.795
2.000
2.102
6.830
11.065

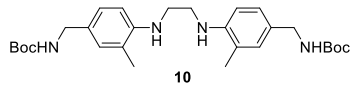

155.914
142.090
128.097
127.857
121.885
79.217
44.532
28.521
17.642
JW-WSC-carbamate
Cdec_service CDCl3 D:\\ ar
NAME JW-WSC-carbamate
EXPNO 2
PROCNO 1
Date_ 20131202
Time 20.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 280
DS 4
SWH 25252.525 H
FIDRES 0.385323 H
AQ 1.2976629 s
RG 203
DW 19.800 u
DE 6.50 u
TE 300.0 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 8.80 u
PL1 -2.00 d
PL1W 59.31797028 W
SFO1 100.6333924 M
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
200 180 160 140 120 100 80 60 40 20 0 ppm


BocHN
N
N
NHBoc

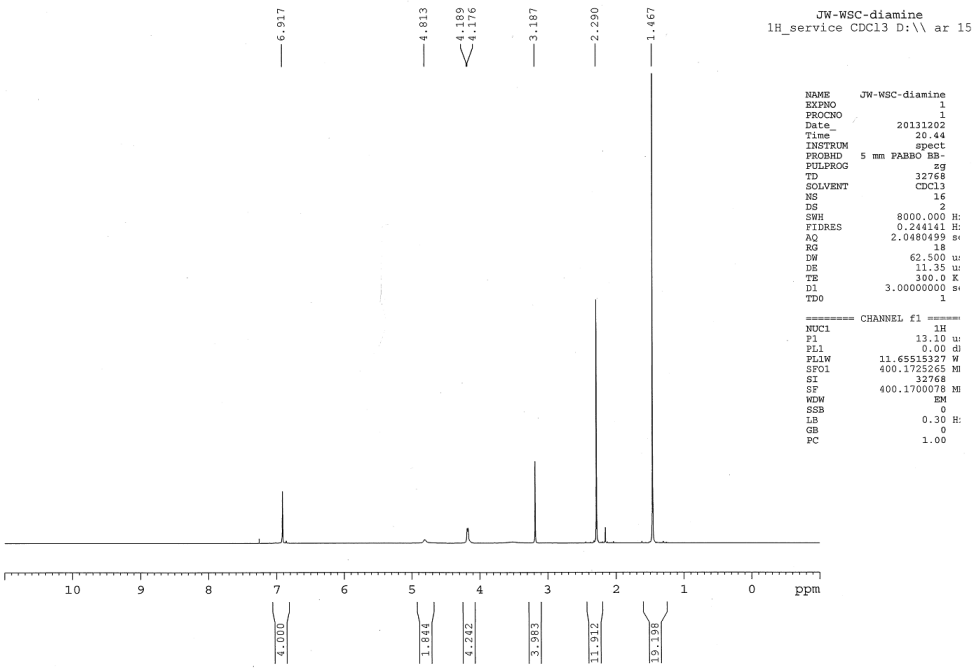
**SI-1**

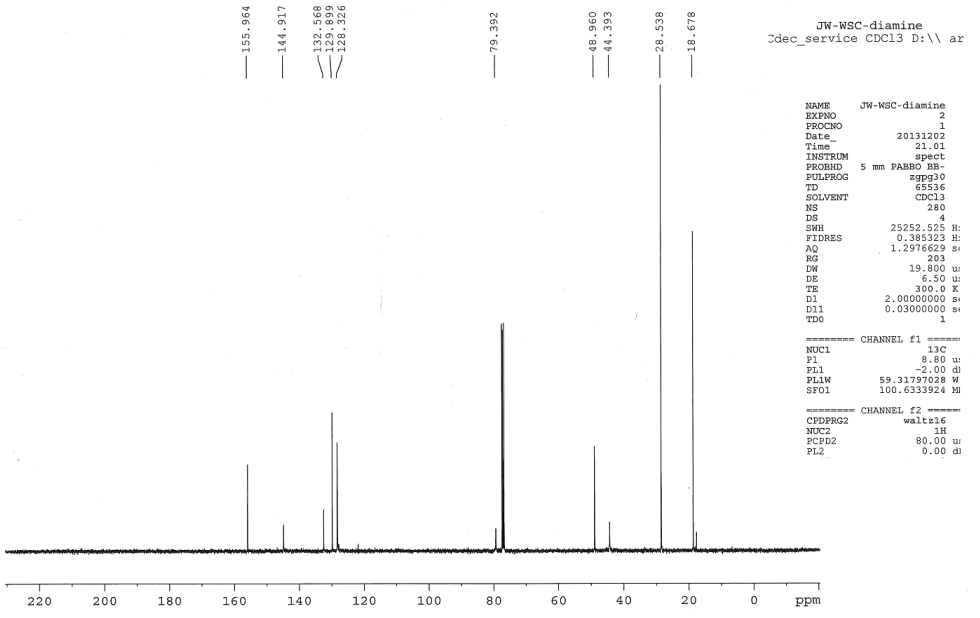

8.079
6.995
4.881
4.247
4.234
2.156
1.469
JW-WSC-diimine
1H_service CDCl3 D:\\ ar 14
NAME JW-WSC-diimine
EXPNO 1
PROCNO 1
Date_ 20131202
Time 20.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8000.000 H
FIDRES 0.244141 H
AQ 2.0480499 s
RG 32
DW 62.500 u
DE 11.35 u
TE 300.0 K
D1 3.00000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.10 u
PL1 0.00 d
PL1W 11.65515327 W
SFO1 400.1725265 M
SI 32768
SF 400.1700079 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.693
4.000
1.912
4.032
12.678
18.111

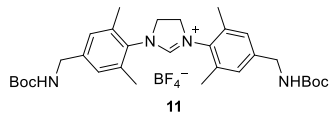

163.615
156.026
149.092
135.396
127.605
126.931
79.567
44.438
28.550
18.364
JW-WSC-diimine
Cdec_service CDCl3 D:\\ ar
NAME JW-WSC-diimine
EXPNO 2
PROCNO 1
Date_ 20131202
Time 20.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 280
DS 4
SWH 25252.525 H
FIDRES 0.385323 H
AQ 1.2976629 s
RG 203
DW 19.800 u
DE 6.50 u
TE 300.0 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
========== CHANNEL f1 ======
NUC1 13C
P1 8.80 u
PL1 -2.00 d
PL1W 59.31797028 W
SFO1 100.6333924 M
========== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
200
180
160
140
120
100
80
60
40
20
0 ppm


BocHN
N
H
N
H
NHBoc

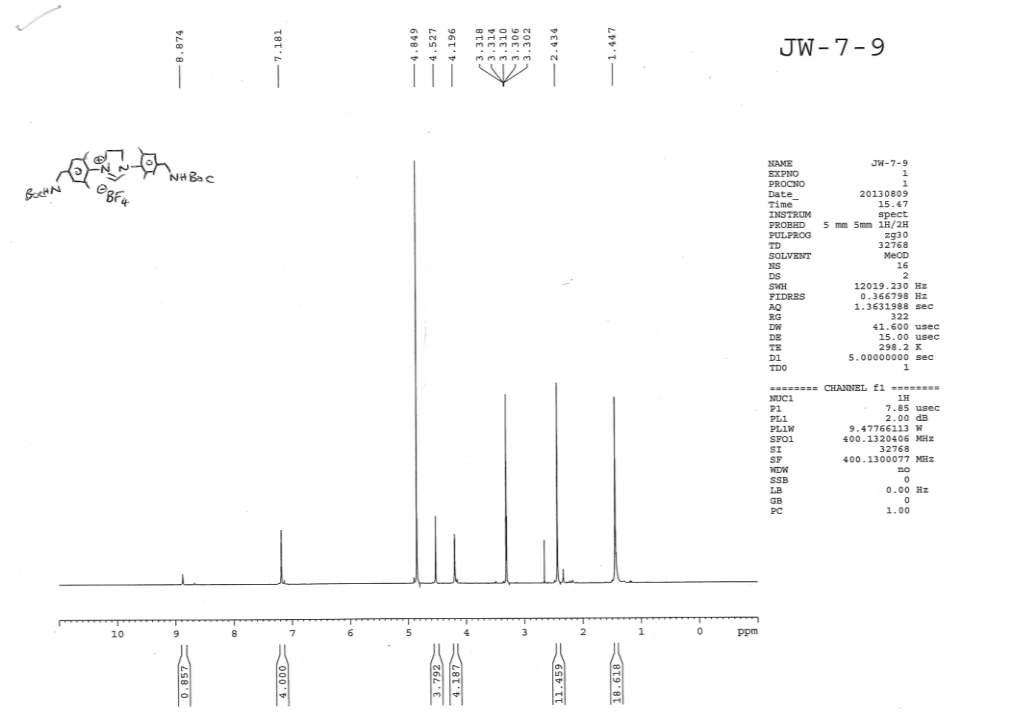
**10**

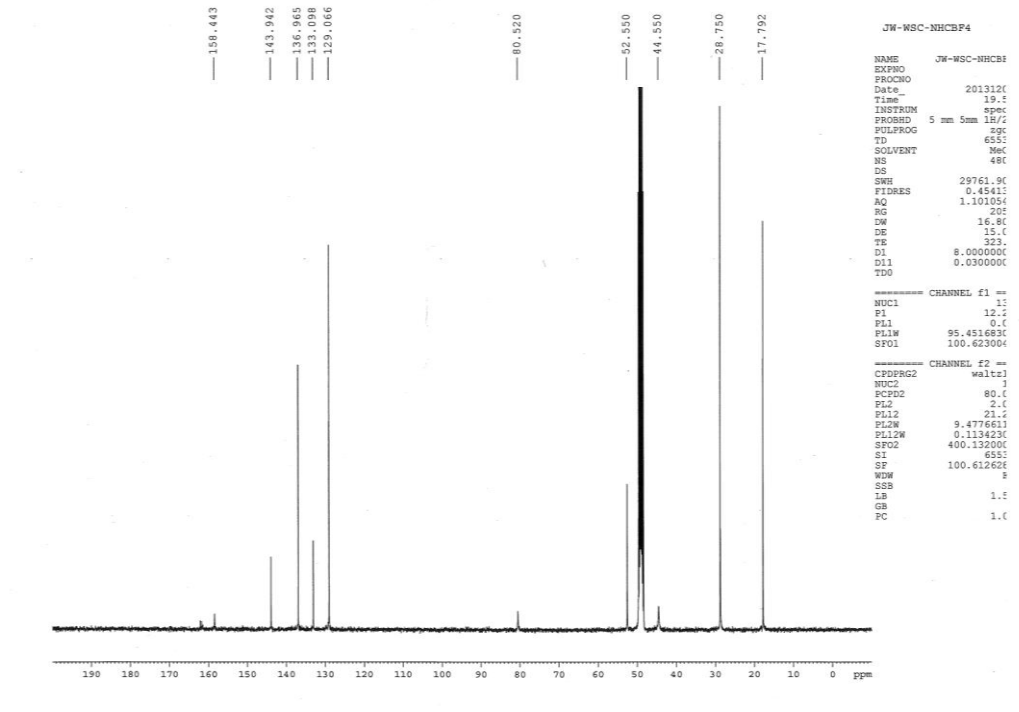

6.917
4.813
4.189
4.176
3.187
2.290
1.467
JW-WSC-diamine
1H_service CDCl3 D:\\ ar 15
NAME JW-WSC-diamine
EXPNO 1
PROCNO 1
Date_ 20131202
Time 20.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8000.000 H
FIDRES 0.244141 H
AQ 2.0480495 s
RG 18
DW 62.500 u
DE 11.35 u
TE 300.0 K
D1 3.00000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.10 u
PL1 0.00 d
PL1W 11.65515327 W
SFO1 400.1725265 M
SI 32768
SF 400.1700078 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
4.000
1.844
4.242
3.983
11.912
19.198

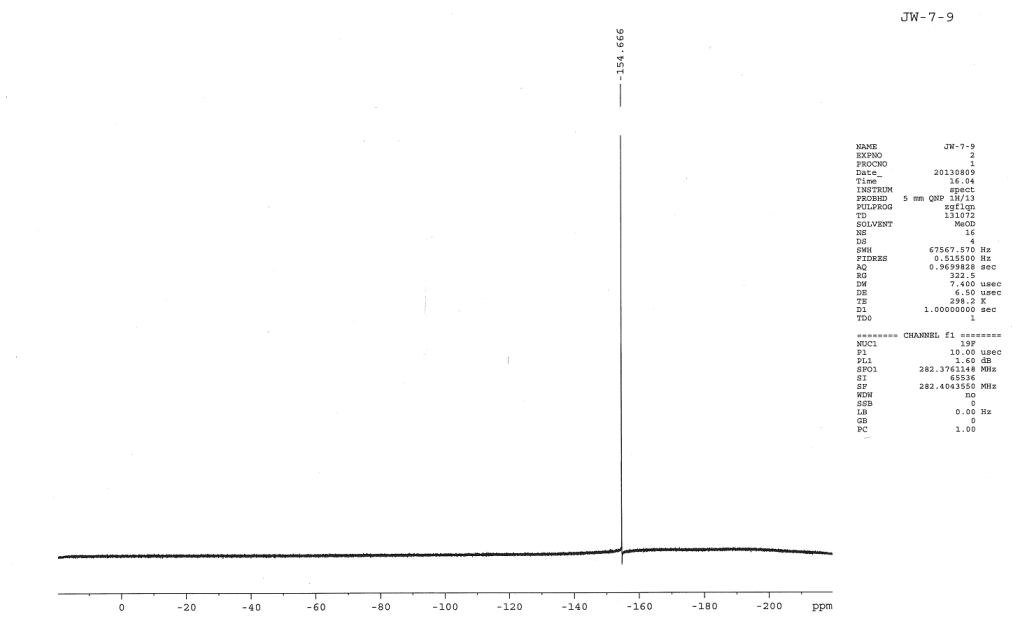

155.964
144.917
132.568
129.899
128.326
79.392
48.960
44.393
28.538
18.678
JW-WSC-diamine
Cdec_service CDCl3 D:\\ ar
NAME JW-WSC-diamine
EXPNO 2
PROCNO 1
Date_ 20131202
Time 21.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 280
DS 4
SWH 25252.525 H
FIDRES 0.385323 H
AQ 1.2976629 s
RG 203
DW 19.800 u
DE 6.50 u
TE 300.0 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 8.80 u
PL1 -2.00 d
PL1W 59.31797028 W
SFO1 100.6333924 M
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
220 200 180 160 140 120 100 80 60 40 20 0 ppm

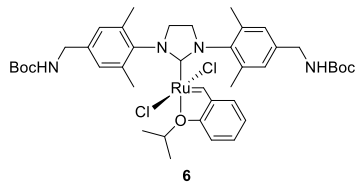

BocHN
$BF_4^-$
NHBoc

11

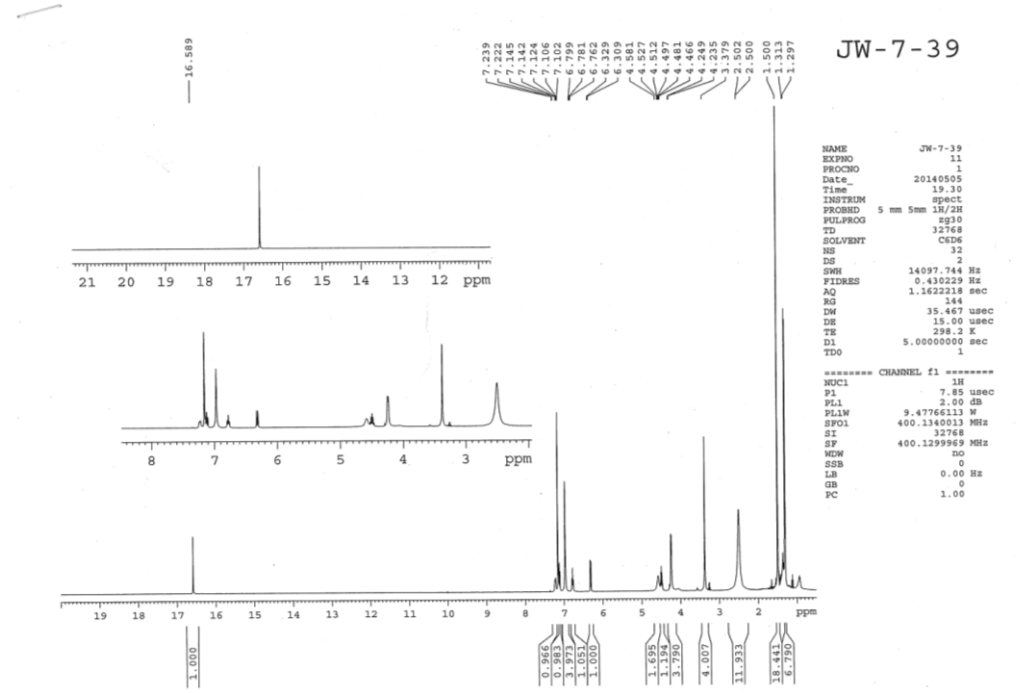

JW-7-9
8.874
7.181
4.849
4.527
4.196
3.318
3.314
3.310
3.305
3.302
2.434
1.447
NAME JW-7-9
EXPNO 1
PROCNO 1
Date_ 20130809
Time 15.47
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 322
DW 41.600 usec
DE 15.00 usec
TE 298.2 K
D1 5.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.85 usec
PL1 2.00 dB
PL1W 9.47766113 W
SFO1 400.1320406 MHz
SI 32768
SF 400.1300077 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
0.857
4.000
3.792
4.187
11.459
18.618

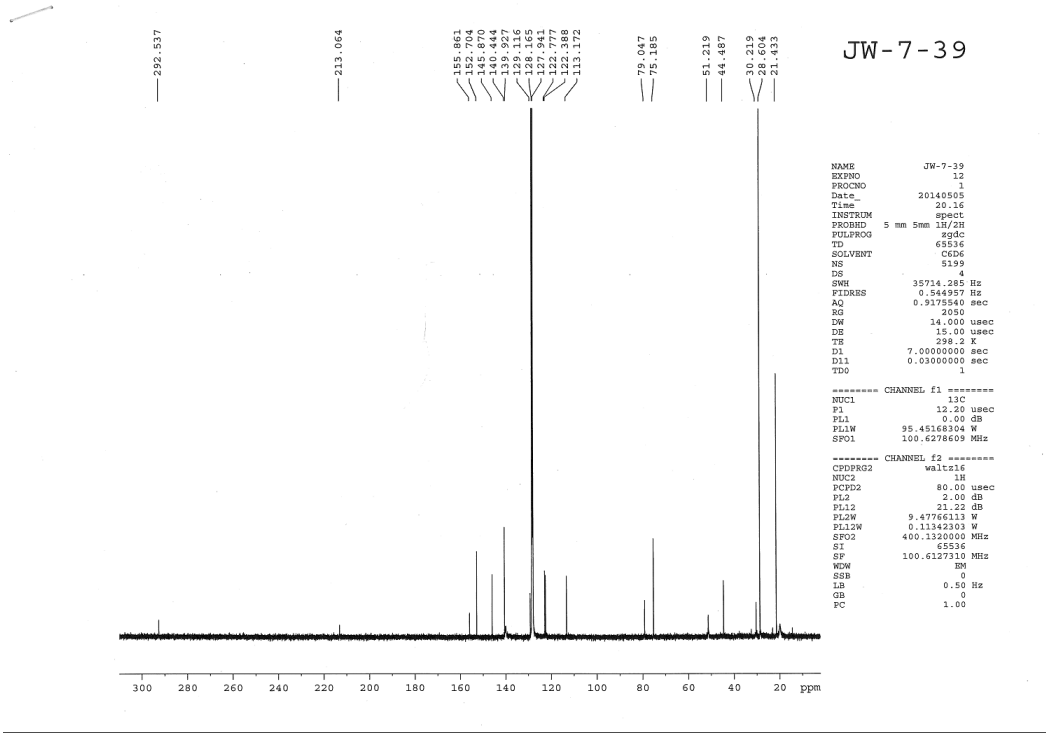

158.443
143.942
136.965
133.098
129.066
80.520
52.550
44.550
28.750
17.792
JW-WSC-NHCBF4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

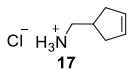

JW-7-9
-154.666
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
NAME JW-7-9
EXPNO 2
PROCNO 1
Date_ 20130809
Time 16.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgflqn
TD 131072
SOLVENT MeOD
NS 16
DS 4
SWH 67567.570 Hz
FIDRES 0.515500 Hz
AQ 0.9699828 sec
RG 322.5
DW 7.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.00 usec
PL1 1.60 dB
SFO1 282.3761148 MHz
SI 65536
SF 282.4043550 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00


BocHN
NHBoc
N
N
Cl
Cl
Ru
O

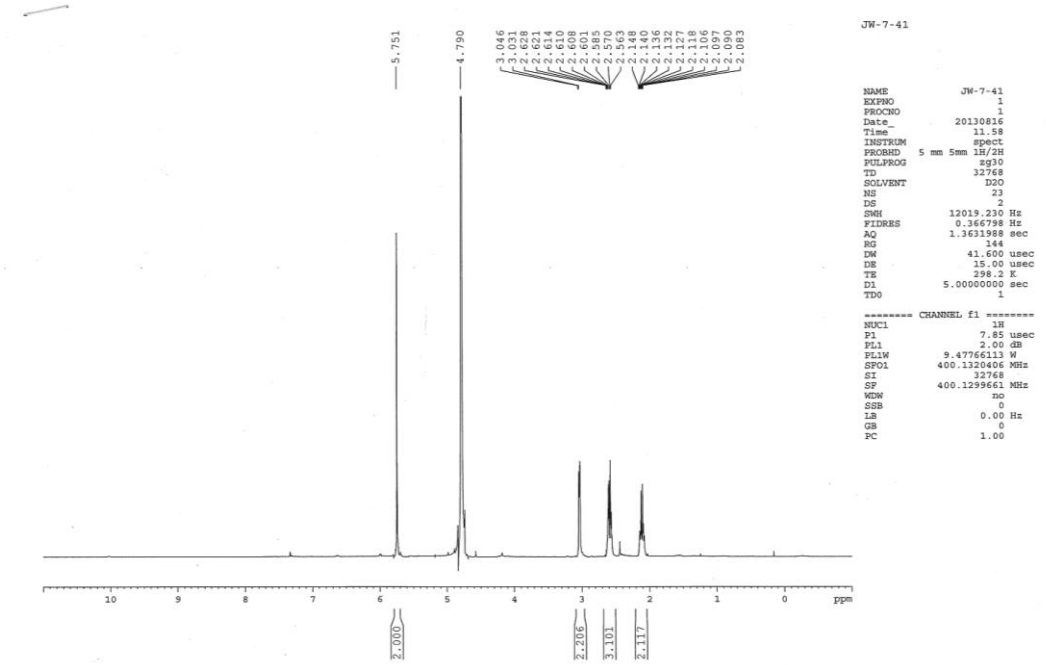
**6**

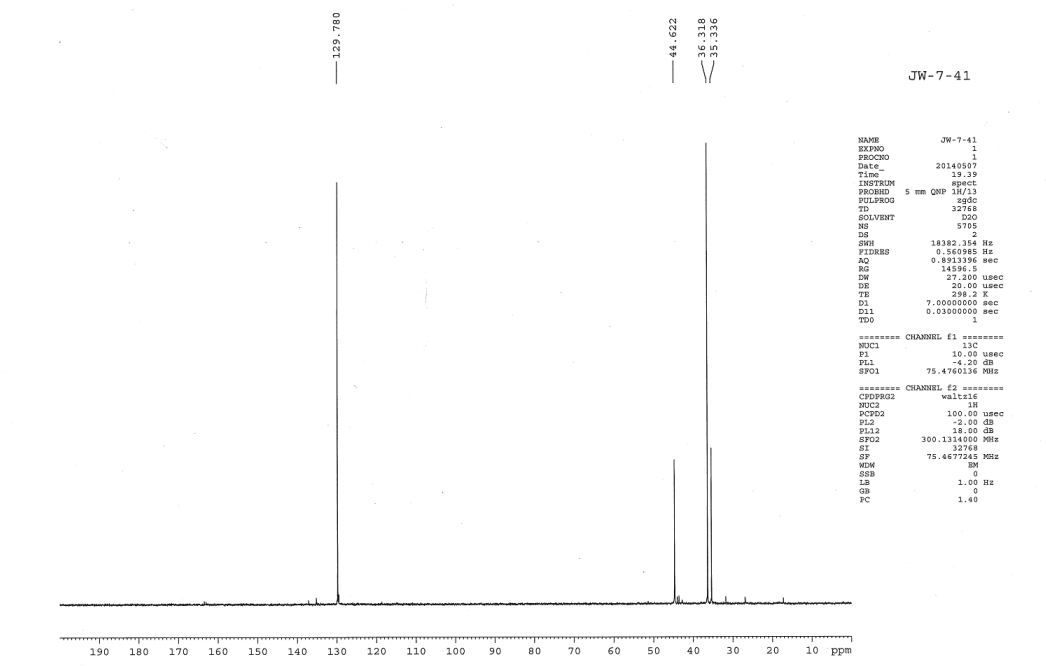

JW-7-39
16.589
7.239
7.222
7.155
7.142
7.124
7.106
7.102
6.799
6.781
6.762
6.329
6.309
4.581
4.527
4.512
4.487
4.481
4.466
4.249
4.235
3.379
2.502
2.500
1.500
1.333
1.297
NAME JW-7-39
EXPNO 11
PROCNO 1
Date_ 20140505
Time 19.30
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zg30
TD 32768
SOLVENT C6D6
NS 32
DS 2
SWH 14097.744 Hz
FIDRES 0.430229 Hz
AQ 1.1622218 sec
RG 144
DW 35.467 usec
DE 15.00 usec
TE 298.2 K
D1 5.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.85 usec
PL1 2.00 dB
PL1W 9.47766113 W
SFO1 400.1340013 MHz
SI 32768
SF 400.1299969 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1.000
0.966
0.983
3.973
1.051
1.000
1.698
1.194
3.790
4.007
11.933
18.441
6.790
ppm

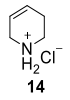

JW-7-39
292.537
213.064
155.861
152.704
145.870
140.444
139.927
129.116
128.165
127.941
127.277
122.388
113.172
79.047
75.185
51.219
44.487
30.219
28.604
21.433
NAME JW-7-39
EXPNO 12
PROCNO 1
Date_ 20140505
Time 20.16
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zgdc
TD 65536
SOLVENT C6D6
NS 5199
DS 4
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 15.00 usec
TE 298.2 K
D1 7.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 12.20 usec
PL1 0.00 dB
PL1W 95.45168304 W
SFO1 100.6276609 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 21.22 dB
PL2W 9.47766113 W
PL12W 0.11342303 W
SFO2 400.1320000 MHz
SI 65536
SF 100.6127310 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
ppm



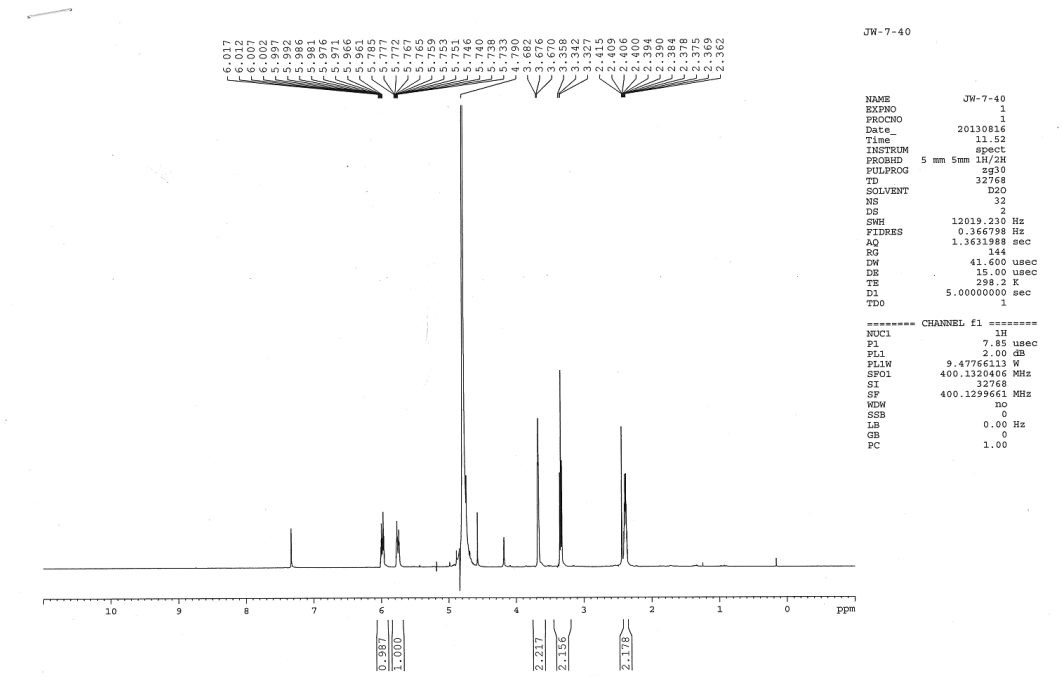
**17**


JW-7-41
5.751
4.790
3.046
3.031
2.628
2.621
2.614
2.610
2.608
2.601
2.585
2.570
2.563
2.148
2.140
2.136
2.132
2.127
2.118
2.106
2.097
2.090
2.083
NAME JW-7-41
EXPNO 1
PROCNO 1
Date_ 20130816
Time 11.58
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zg30
TD 32768
SOLVENT D2O
NS 23
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 41.600 usec
DE 15.00 usec
TE 298.2 K
D1 5.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.85 usec
PL1 2.00 dB
PL1W 9.47766113 W
SFO1 400.1320406 MHz
SI 32768
SF 400.1299661 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
2.000
2.206
3.101
2.117


129.780
44.622
36.318
35.336
JW-7-41
NAME JW-7-41
EXPNO 1
PROCNO 1
Date_ 20140507
Time 19.39
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT D2O
NS 5705
DS 2
SWH 18382.354 Hz
FIDRES 0.560985 Hz
AQ 0.8913396 sec
RG 14596.5
DW 27.200 usec
DE 20.00 usec
TE 298.2 K
D1 7.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -4.20 dB
SFO1 75.4760136 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.00 dB
SFO2 300.1314000 MHz
SI 32768
SF 75.4677245 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

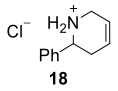


**14**

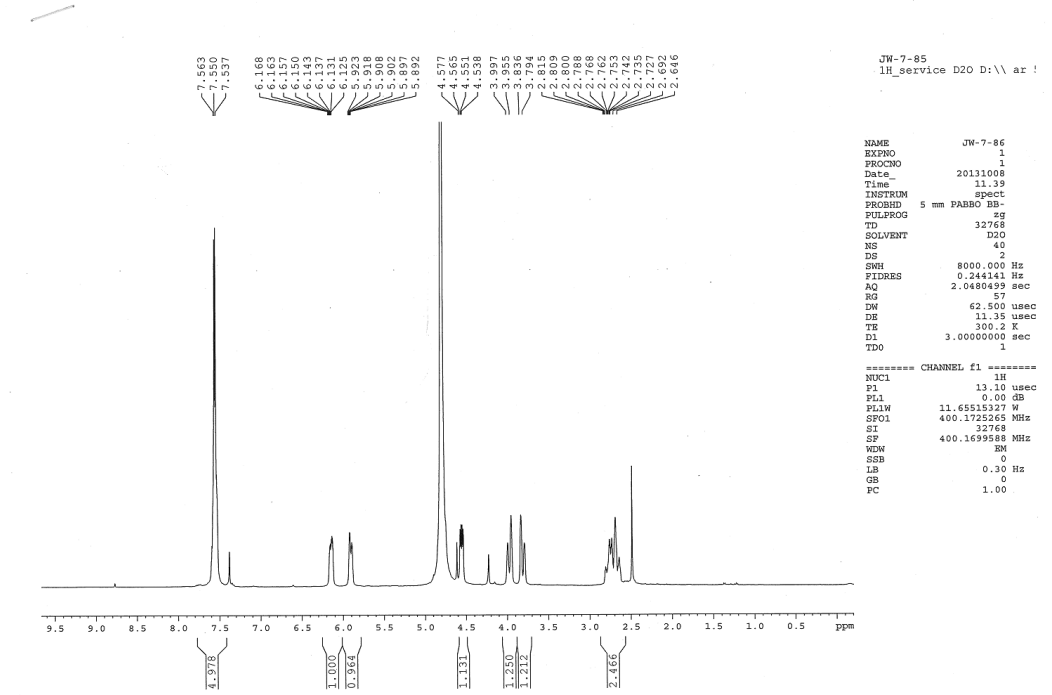


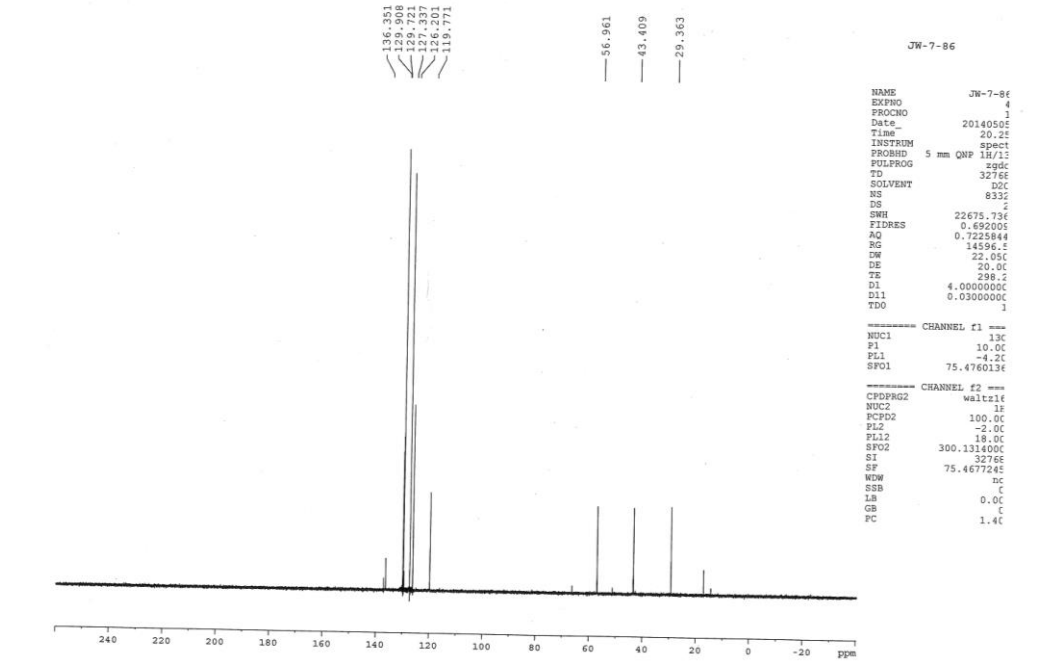

JW-7-40

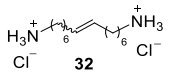
| | |
|---|---|
| NAME | JW-7-40 |
| EXPNO | 1 |
| PROCNO | 1 |
| Date_ | 20130816 |
| Time | 11.52 |
| INSTRUM | spect |
| PROBHD | 5 mm 5mm 1H/2H |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | D2O |
| NS | 32 |
| DS | 2 |
| SWH | 12019.230 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3631988 sec |
| RG | 144 |
| DW | 41.600 usec |
| DE | 15.00 usec |
| TE | 298.2 K |
| D1 | 5.00000000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| NUC1 | 1H |
| P1 | 7.85 usec |
| PL1 | 2.00 dB |
| PL1W | 9.47766113 W |
| SFO1 | 400.1320406 MHz |
| SI | 32768 |
| SF | 400.1299661 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |


Cl⁻
H2N+
Ph

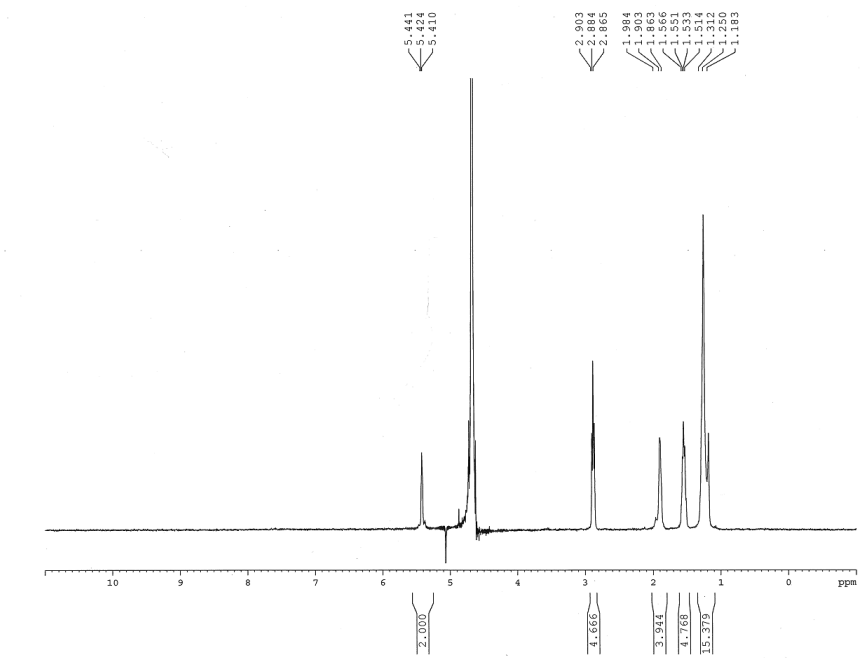
**18**

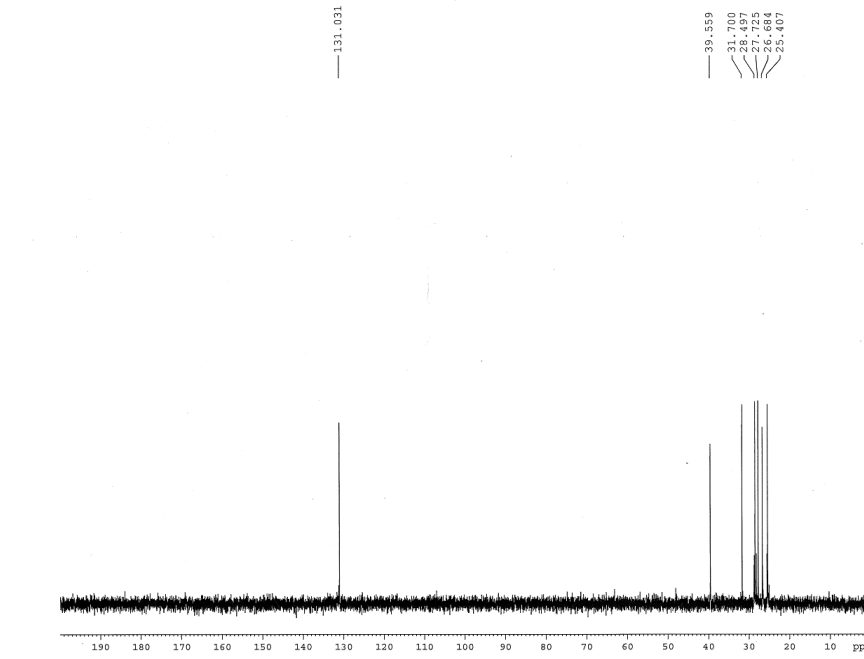

7.563
7.550
7.537
6.168
6.163
6.157
6.150
6.143
6.137
6.131
6.125
5.923
5.918
5.908
5.902
5.897
5.892
4.577
4.565
4.551
4.538
3.997
3.955
3.936
3.894
2.815
2.809
2.800
2.788
2.768
2.762
2.753
2.742
2.735
2.727
2.692
2.646
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.978
1.000
0.964
1.131
1.250
1.212
2.466
JW-7-85
1H_service D2O D:\\ ar !
NAME JW-7-86
EXPNO 1
PROCNO 1
Date_ 20131008
Time_ 11.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT D2O
NS 40
DS 2
SWH 8000.000 Hz
FIDRES 0.244141 Hz
AQ 2.0480499 sec
RG 57
DW 62.500 usec
DE 11.35 usec
TE 300.2 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.10 usec
PL1 0.00 dB
PL1W 11.65515327 W
SFO1 400.1725265 MHz
SI 32768
SF 400.1699588 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

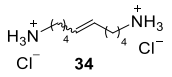

136.351
129.908
129.721
127.337
126.201
119.771
56.961
43.409
29.363
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 ppm
JW-7-86
NAME JW-7-8
EXPNO 4
PROCNO 1
Date_ 2014050
Time_ 20.2
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgdc
TD 3276
SOLVENT D2C
NS 833
DS 2
SWH 22675.73
FIDRES 0.692005
AQ 0.7225844
RG 14596.
DW 22.05
DE 20.0
TE 298.
D1 4.0000000
D11 0.0300000
TD0 1
======== CHANNEL f1 ===
NUC1 13
P1 10.0
PL1 -4.2
SFO1 75.476013
======== CHANNEL f2 ===
CPDPRG2 waltz1
NUC2 1
PCPD2 100.0
PL2 -2.0
PL12 18.0
SFO2 300.131400
SI 3276
SF 75.467724
WDW nc
SSB
LB 0.0
GB
PC 1.4



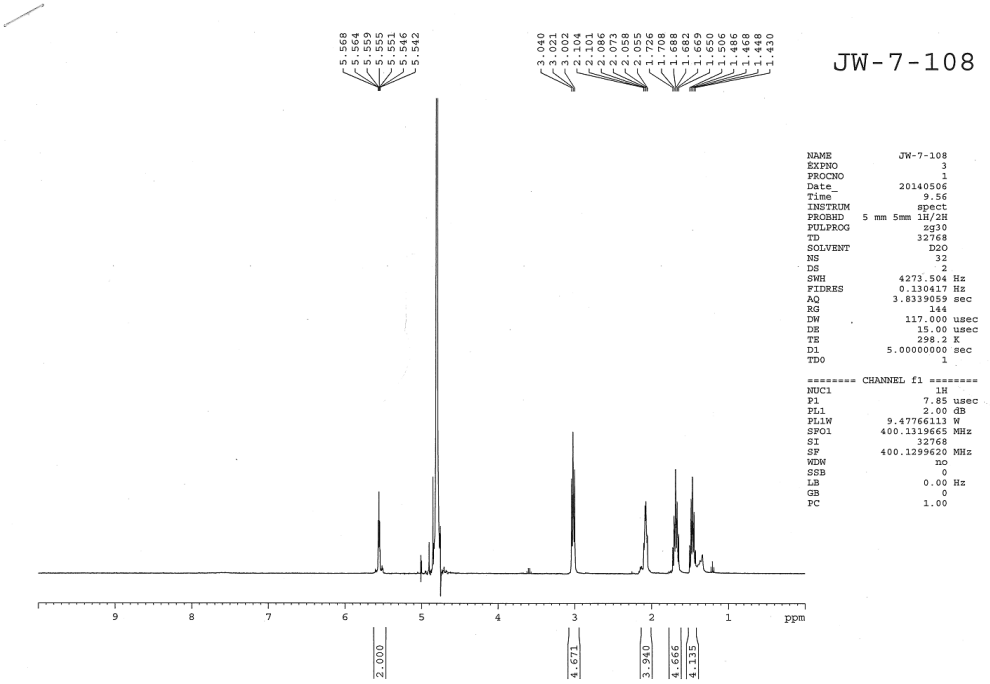
**32**

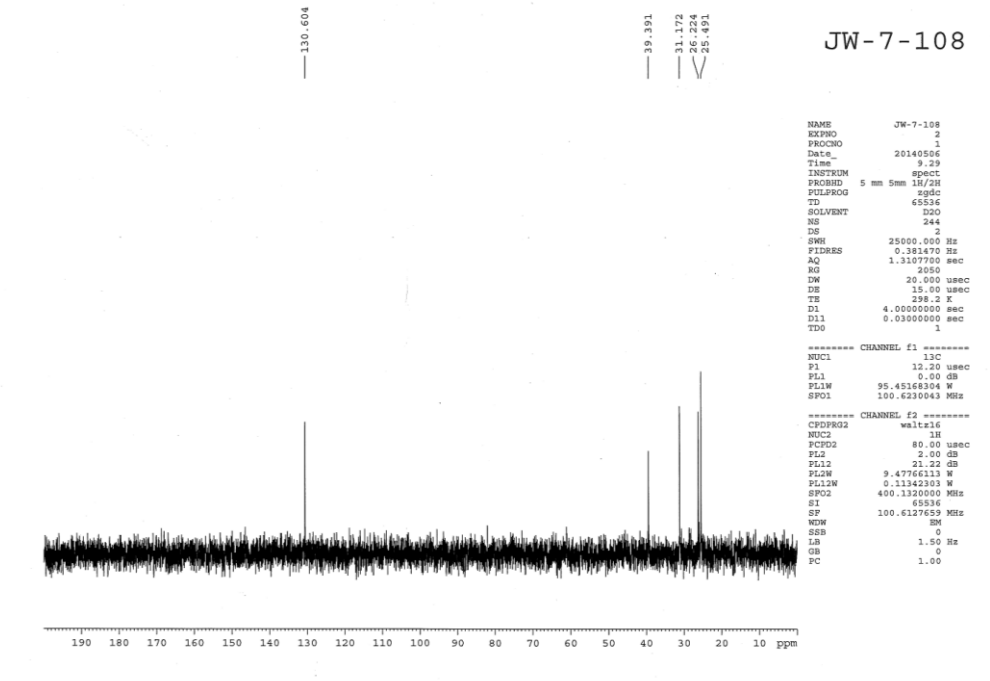

5.441
5.424
5.410
2.903
2.884
2.865
1.984
1.903
1.863
1.566
1.551
1.533
1.514
1.312
1.250
1.183
JW-7-107
NAME JW-7-107
EXPNO 2
PROCNO 1
Date_ 20140410
Time 18.53
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zg30
TD 32768
SOLVENT D2O
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 1150
DW 41.600 usec
DE 15.00 usec
TE 298.2 K
D1 5.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.85 usec
PL1 2.00 dB
PL1W 9.47766113 W
SFO1 400.1320406 MHz
SI 32768
SF 400.1300120 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
2.000
4.666
3.944
4.768
15.379


131.031
39.559
31.700
28.497
27.785
27.688
25.407
JW-7-107
NAME JW-7-107(1)
EXPNO 2
PROCNO 1
Date_ 20140507
Time 7.56
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zgdc
TD 65536
SOLVENT D2O
NS 500
DS 4
SWH 25000.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 2050
DW 20.000 usec
DE 15.00 usec
TE 298.2 K
D1 4.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 12.20 usec
PL1 0.00 dB
PL1W 95.45168304 W
SFO1 100.6230043 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 21.22 dB
PL2W 9.47766113 W
PL12W 0.11342303 W
SFO2 400.1320000 MHz
SI 65536
SF 100.6127659 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



**34**


JW-7-108
5.568
5.564
5.559
5.555
5.551
5.546
5.542
3.040
3.021
3.002
2.104
2.101
2.086
2.073
2.058
2.055
2.026
1.708
1.688
1.682
1.669
1.650
1.506
1.466
1.448
1.430
NAME JW-7-108
EXPNO 3
PROCNO 1
Date_ 20140506
Time 9.56
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zg30
TD 32768
SOLVENT D2O
NS 32
DS 2
SWH 4273.504 Hz
FIDRES 0.130417 Hz
AQ 3.8339059 sec
RG 144
DW 117.000 usec
DE 15.00 usec
TE 298.3 K
D1 5.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.85 usec
PL1 2.00 dB
PL1W 9.47766113 W
SFO1 400.1319665 MHz
SI 32768
SF 400.1299620 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 ppm
2.000
4.671
3.940
4.666
4.135


JW-7-108
130.604
39.391
31.172
26.224
25.491
NAME JW-7-108
EXPNO 2
PROCNO 1
Date_ 20140506
Time 9.29
INSTRUM spect
PROBHD 5 mm 5mm 1H/2H
PULPROG zgdc
TD 65536
SOLVENT D2O
NS 244
DS 2
SWH 25000.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 2050
DW 20.000 usec
DE 15.00 usec
TE 298.2 K
D1 4.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 12.20 usec
PL1 0.00 dB
PL1W 95.45168304 W
SFO1 100.6230043 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 21.22 dB
PL2W 9.47766113 W
PL12W 0.11342303 W
SFO2 400.1320000 MHz
SI 65536
SF 100.6127659 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm