

Electronic Supplementary Information (ESI) for

# Dinuclear Nitrido-Bridged Ruthenium Complexes Bearing Diimine Ligands

Julie Urgiles, Sarah R. Nathan, Samantha N. MacMillan, and Justin J. Wilson\*

*Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853, USA*

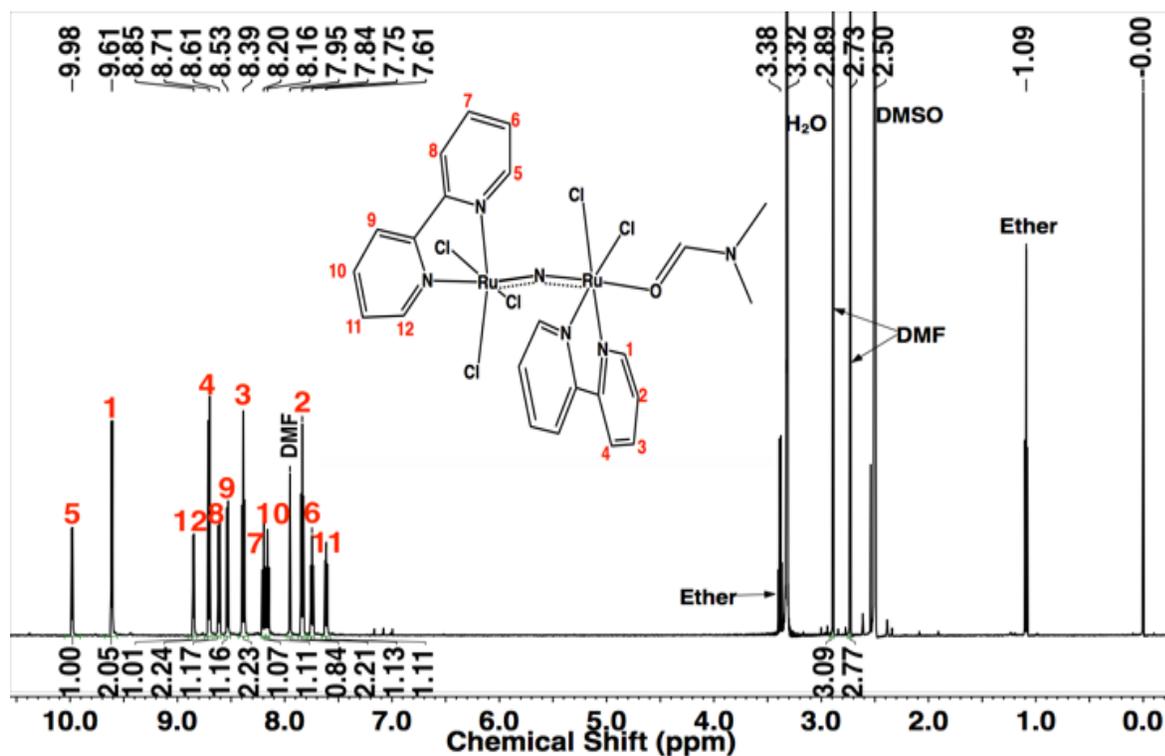
\*E-mail: jjw275@cornell.edu

## Contents:

|                 |   |
|-----------------|---|
| <b>Table S1</b> | UV-vis absorbance peak maxima and extinction coefficients.                  |
| <b>Fig. S1</b>  | $^1\text{H}$ NMR spectrum of <b>1</b> in DMSO- $d_6$ .                      |
| <b>Fig. S2</b>  | $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>1</b> in DMSO- $d_6$ .     |
| <b>Fig. S3</b>  | $^1\text{H}$ NMR spectrum of <b>2</b> in DMSO- $d_6$ .                      |
| <b>Fig. S4</b>  | $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>2</b> in DMSO- $d_6$ .     |
| <b>Fig. S5</b>  | $^1\text{H}$ NMR spectrum of <b>3</b> in DMSO- $d_6$ .                      |
| <b>Fig. S6</b>  | $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>3</b> in DMSO- $d_6$ .     |
| <b>Fig. S7</b>  | FT-IR spectrum of <b>1</b> .  |
| <b>Fig. S8</b>  | FT-IR spectrum of <b>2</b> .  |
| <b>Fig. S9</b>  | FT-IR spectrum of <b>3</b> .  |
| <b>Fig. S10</b> | Mitochondrial calcium uptake in permeabilized cells treated with <b>1</b> . |
| <b>Fig. S11</b> | Mitochondrial calcium uptake in permeabilized cells treated with <b>2</b> . |
| <b>Fig. S12</b> | Mitochondrial calcium uptake in permeabilized cells treated with <b>3</b> . |

**Table S1.** UV-vis absorbance maxima and extinction coefficients for **1–3** in DMSO.

| UV-Vis   |                             |   |
|----------|-----------------------------|---|
|          | $\lambda_{\text{max}}$ (nm) | $\epsilon$ ( $\text{M}^{-1}\cdot\text{cm}^{-1}$ ) |
| <b>1</b> | 299                         | $29000 \pm 200$                                   |
|          | 381                         | $8200 \pm 100$                                    |
| <b>2</b> | 298                         | $20400 \pm 800$                                   |
|          | 376                         | $6000 \pm 300$                                    |
| <b>3</b> | 292                         | $35000 \pm 4000$                                  |
|          | 368                         | $10200 \pm 900$                                   |



**Fig. S1.**  $^1\text{H}$  NMR of **1** in  $\text{DMSO}-d_6$  at  $25\text{ }^\circ\text{C}$  and  $600\text{ MHz}$ .

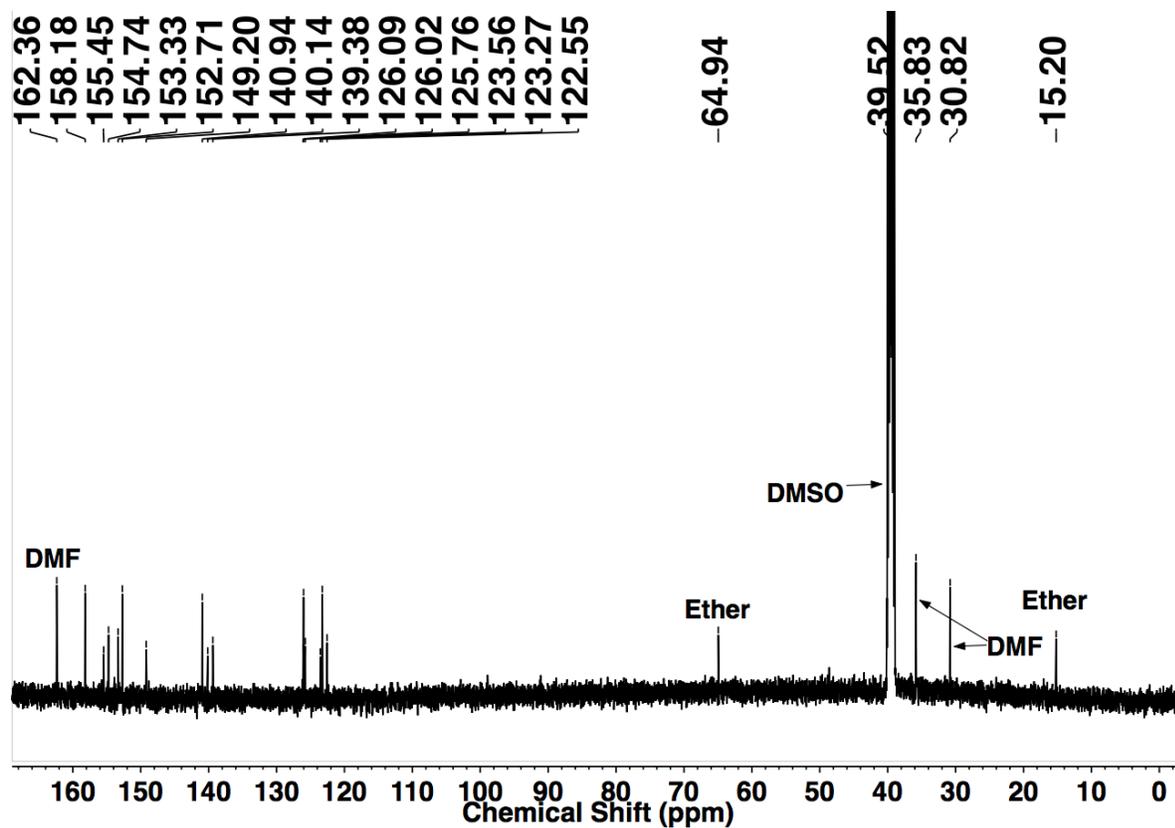


Fig. S2.  $^{13}\text{C}\{^1\text{H}\}$  NMR of **1** in  $\text{DMSO-}d_6$  at  $25\text{ }^\circ\text{C}$  and 125 MHz.

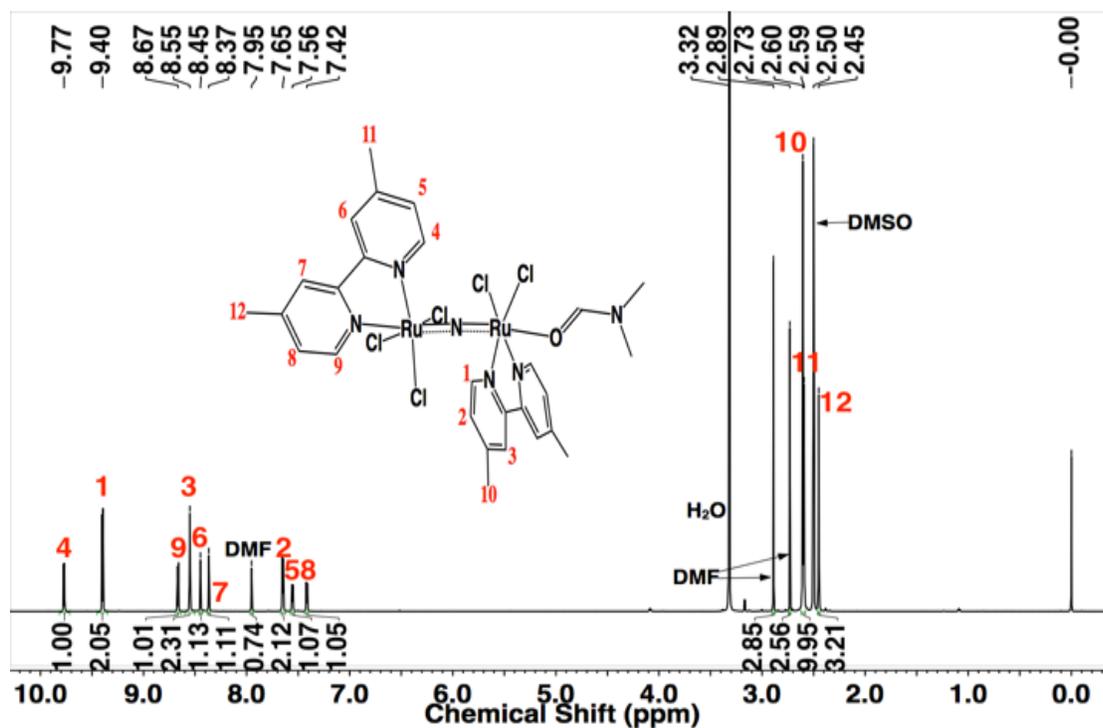


Fig. S3.  $^1\text{H}$  NMR of **2** in  $\text{DMSO-}d_6$  at  $25\text{ }^\circ\text{C}$  and 600 MHz.

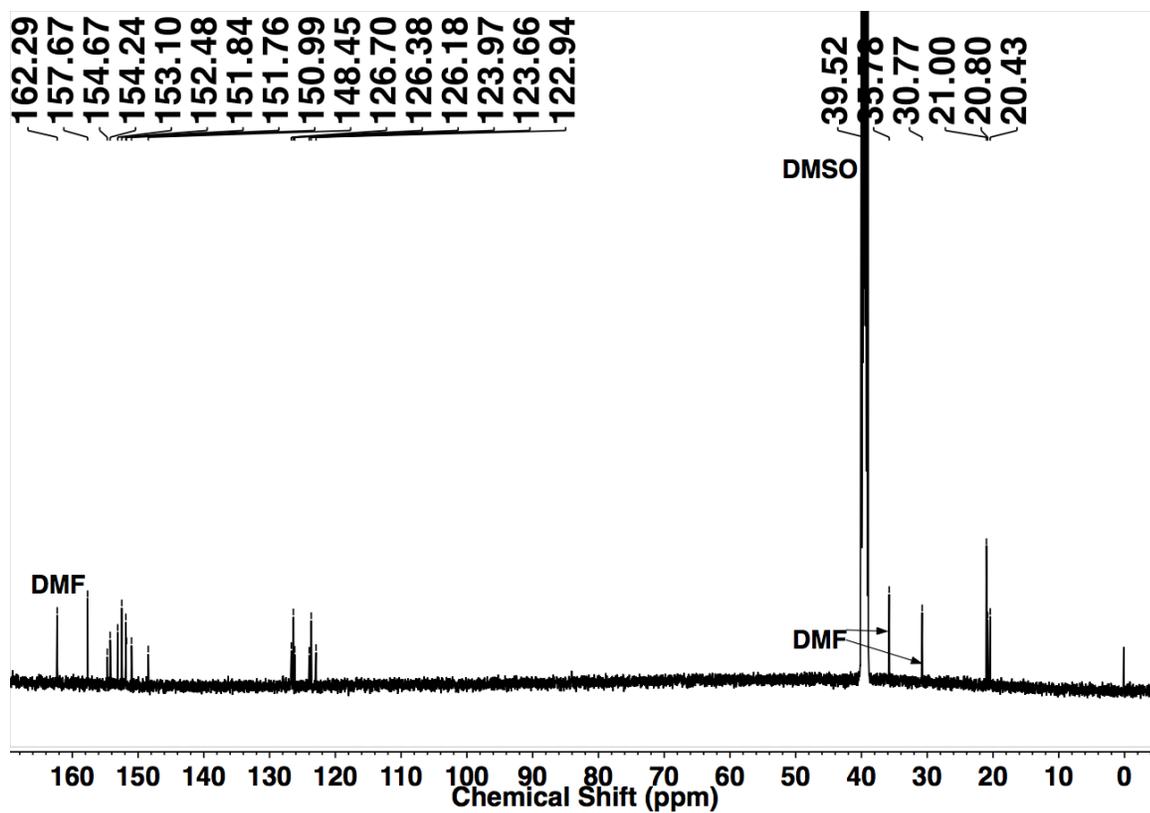


Fig. S4.  $^{13}\text{C}\{^1\text{H}\}$  NMR of **2** in  $\text{DMSO-}d_6$  at  $25^\circ\text{C}$  and 125 MHz.

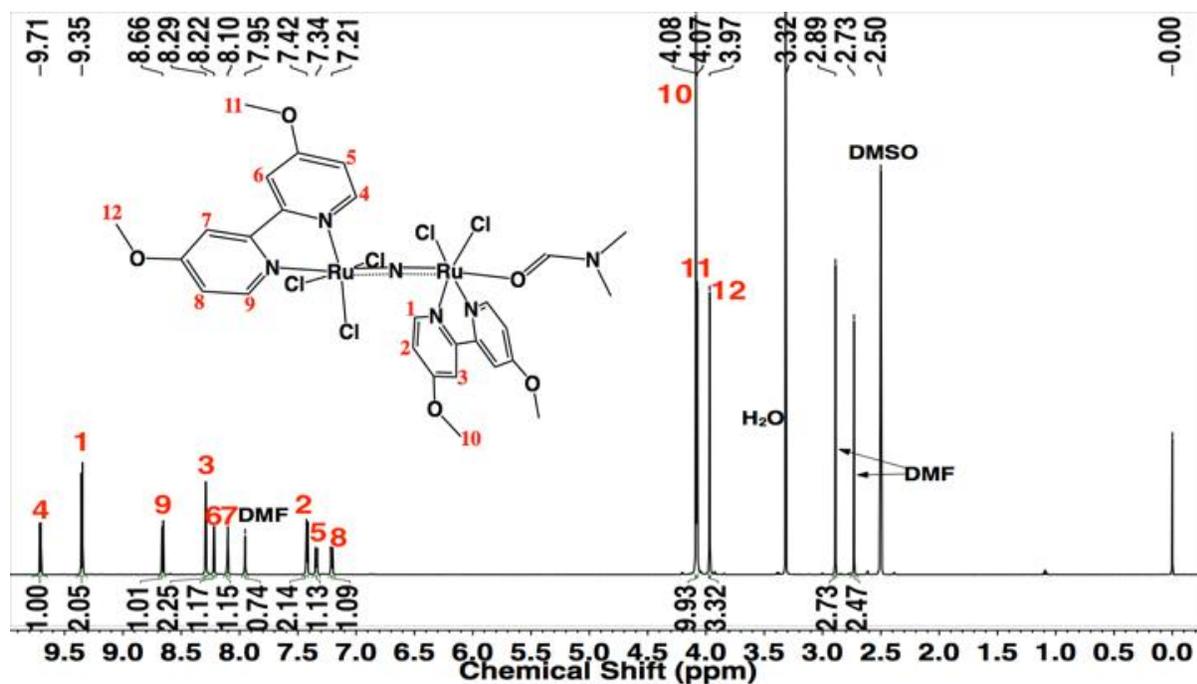


Fig. S5.  $^1\text{H}$  NMR of **3** in  $\text{DMSO-}d_6$  at  $25^\circ\text{C}$  and 600 MHz

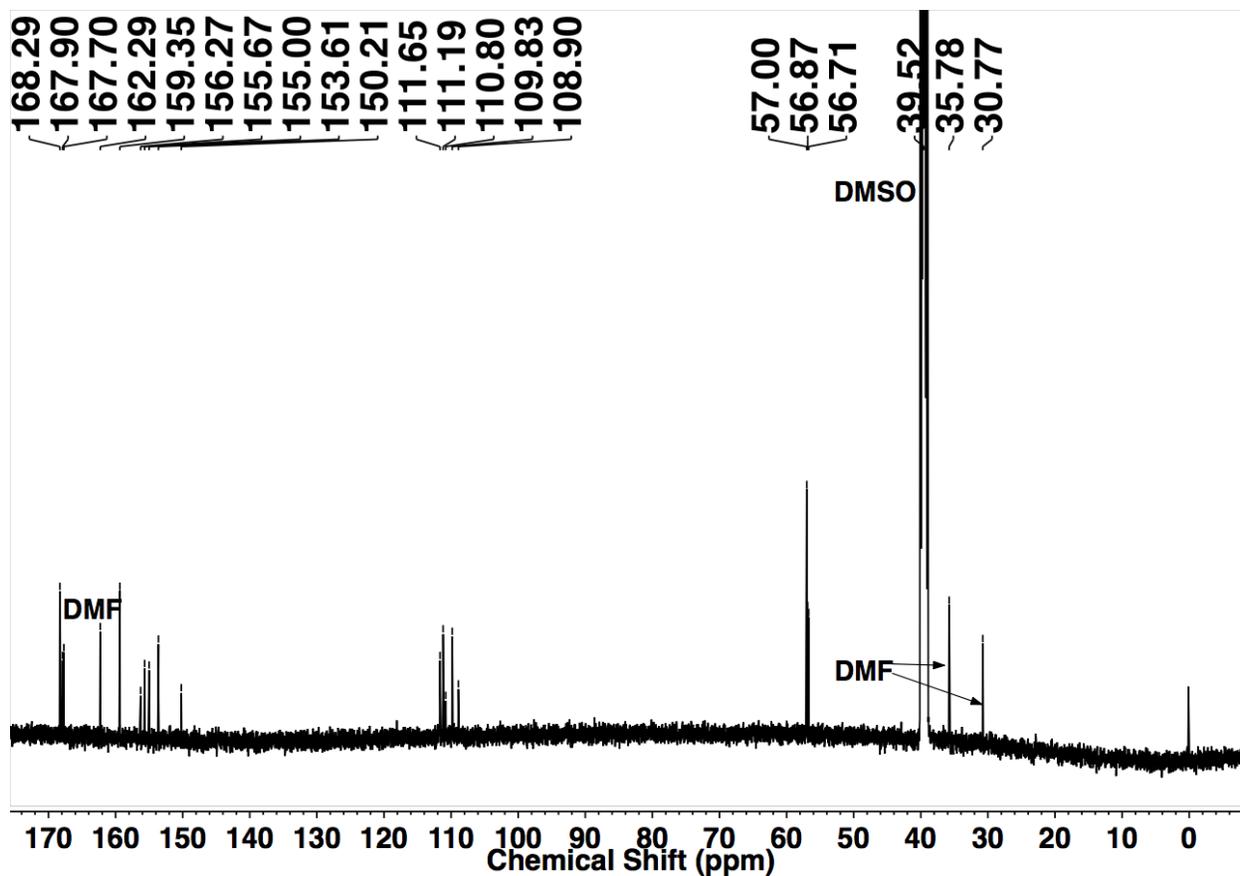


Fig. S6.  $^{13}\text{C}\{^1\text{H}\}$  NMR of **3** in  $\text{DMSO-}d_6$  at 25 °C and 125 MHz.

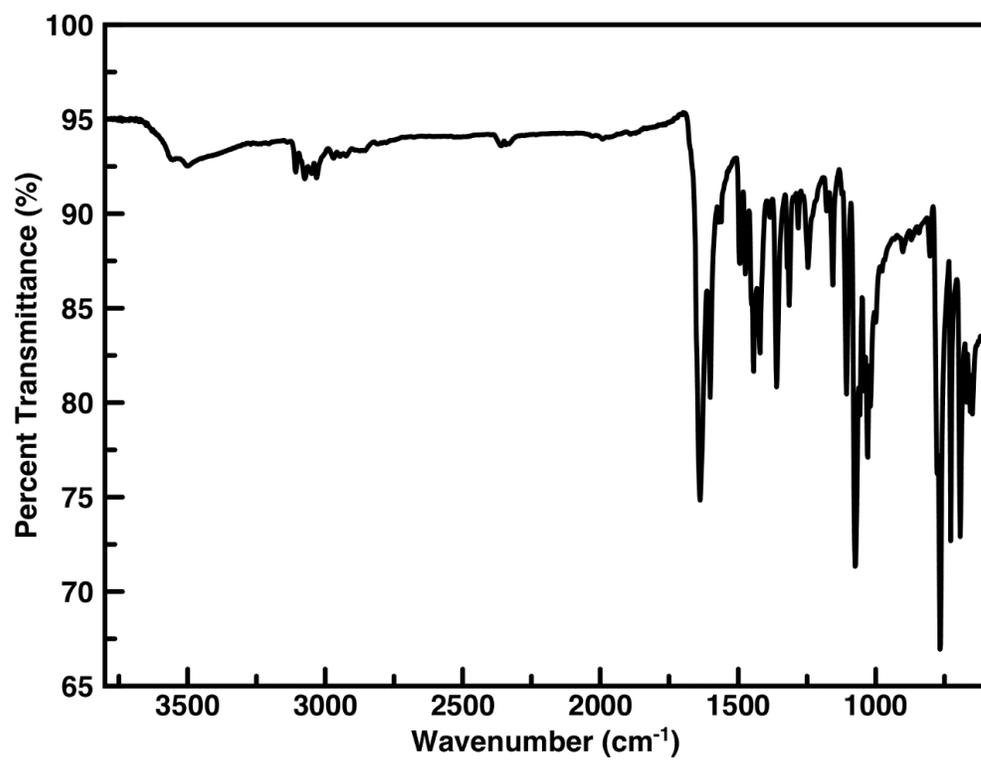


Fig. S7. IR spectrum of 1.

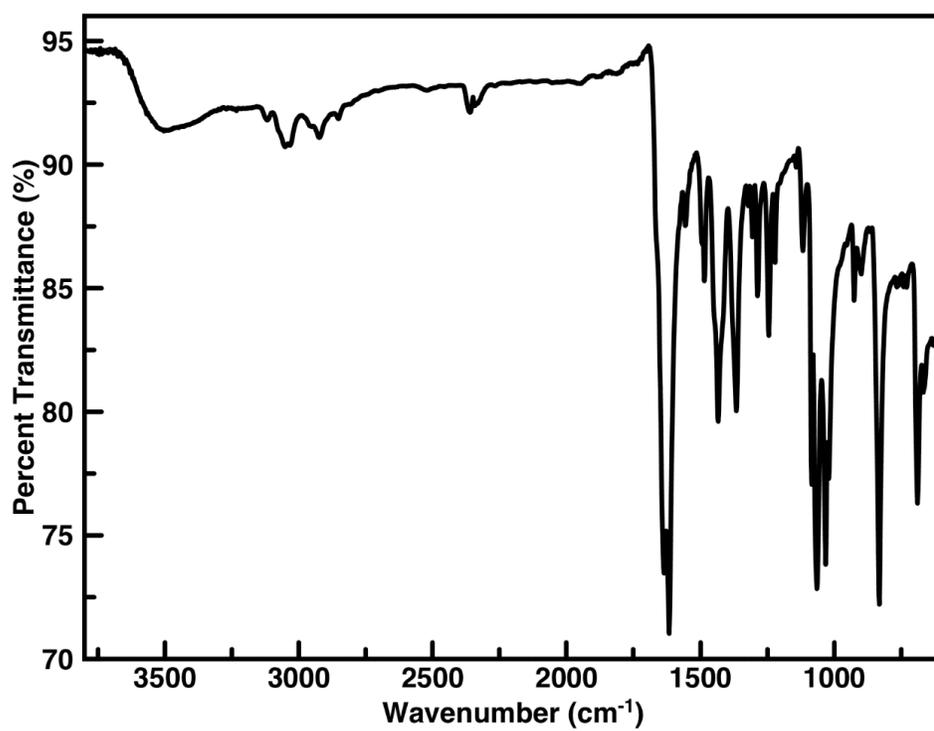
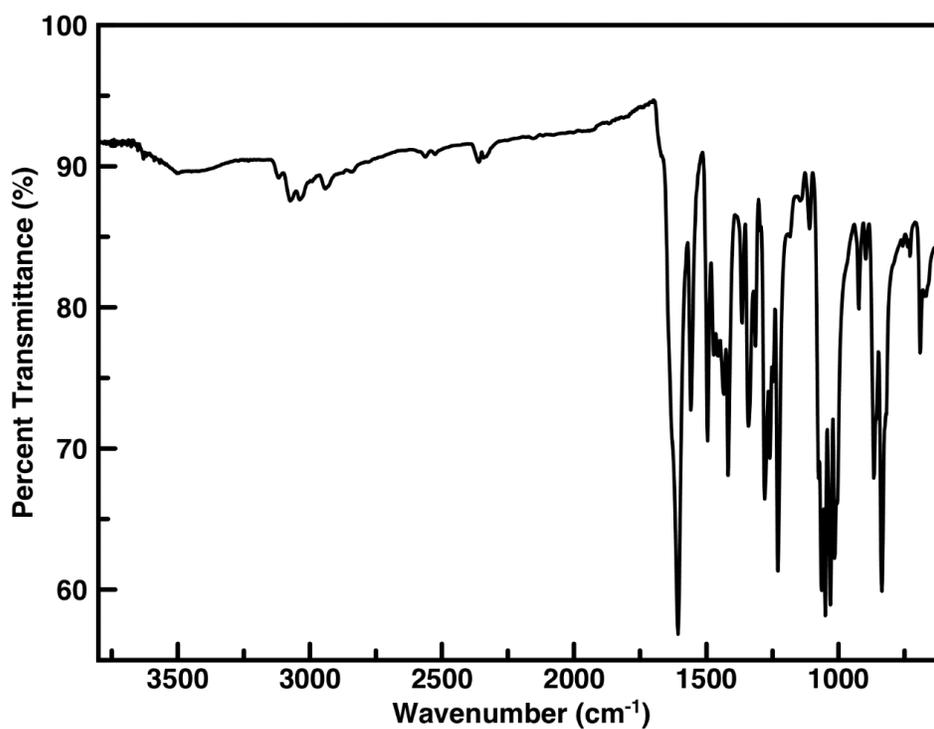
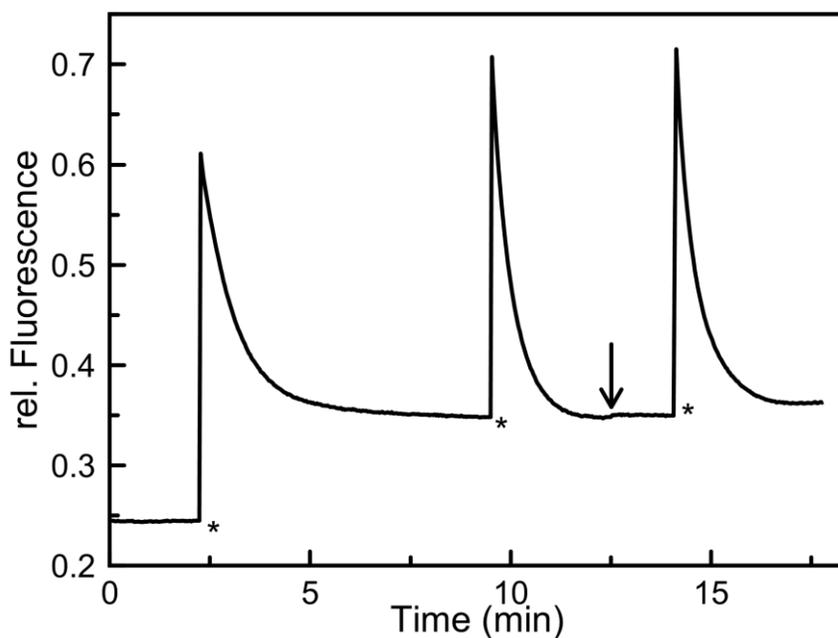


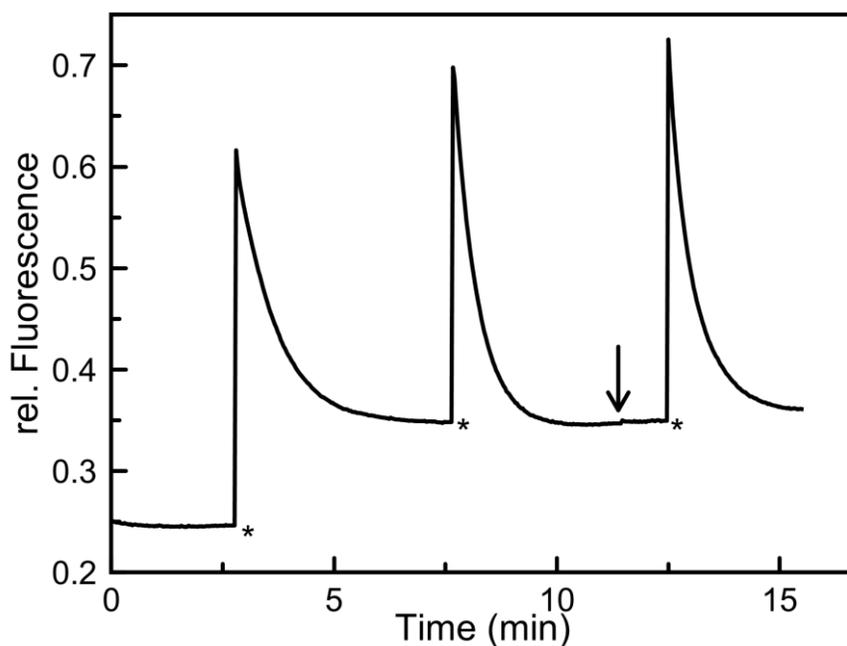
Fig. S8. IR spectrum of 2.



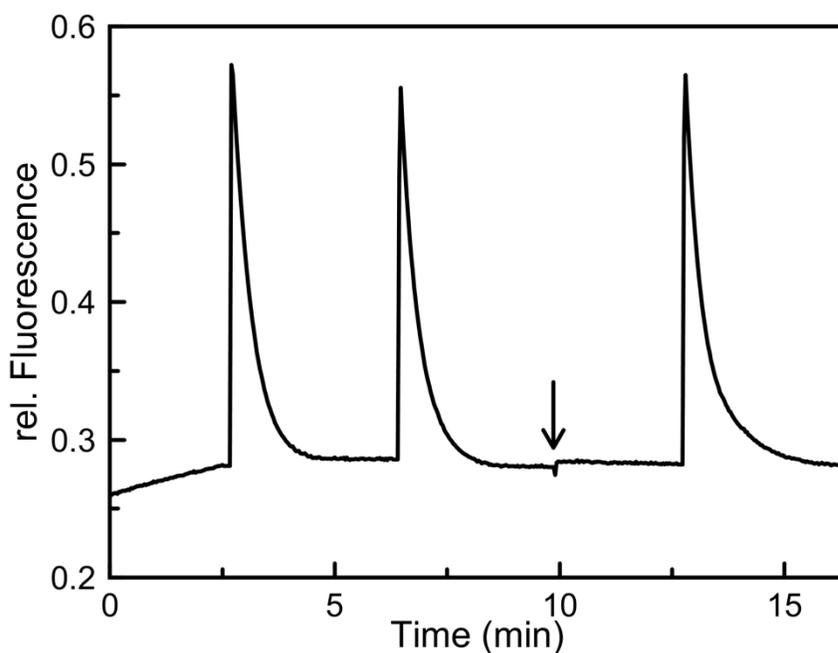
**Fig. S9.** IR spectrum of **3**.



**Fig. S10.** Mitochondrial calcium uptake in permeabilized cells treated with **1**. The asterisk indicates when a bolus of  $\text{Ca}^{2+}$  ions ( $7.5 \mu\text{M}$ ) was added. The arrow indicates when **1** ( $5 \mu\text{M}$ ) was added. The fluorescence was re-normalized after addition of the ruthenium compound.



**Fig. S11.** Mitochondrial calcium uptake in permeabilized cells treated with **2**. The asterisk indicates when a bolus of  $\text{Ca}^{2+}$  ions ( $7.5 \mu\text{M}$ ) was added. The arrow indicates when **2** ( $5 \mu\text{M}$ ) was added. The fluorescence was re-normalized after addition of the ruthenium compound.



**Fig. S12.** Mitochondrial calcium uptake in permeabilized cells treated with **3**. The asterisk indicates when a bolus of  $\text{Ca}^{2+}$  ions ( $7.5 \mu\text{M}$ ) was added. The arrow indicates when **3** ( $5 \mu\text{M}$ ) was added. The fluorescence was re-normalized after addition of the ruthenium compound.