

Supporting Information

A Redox-Switchable Ring-Closing Metathesis Catalyst

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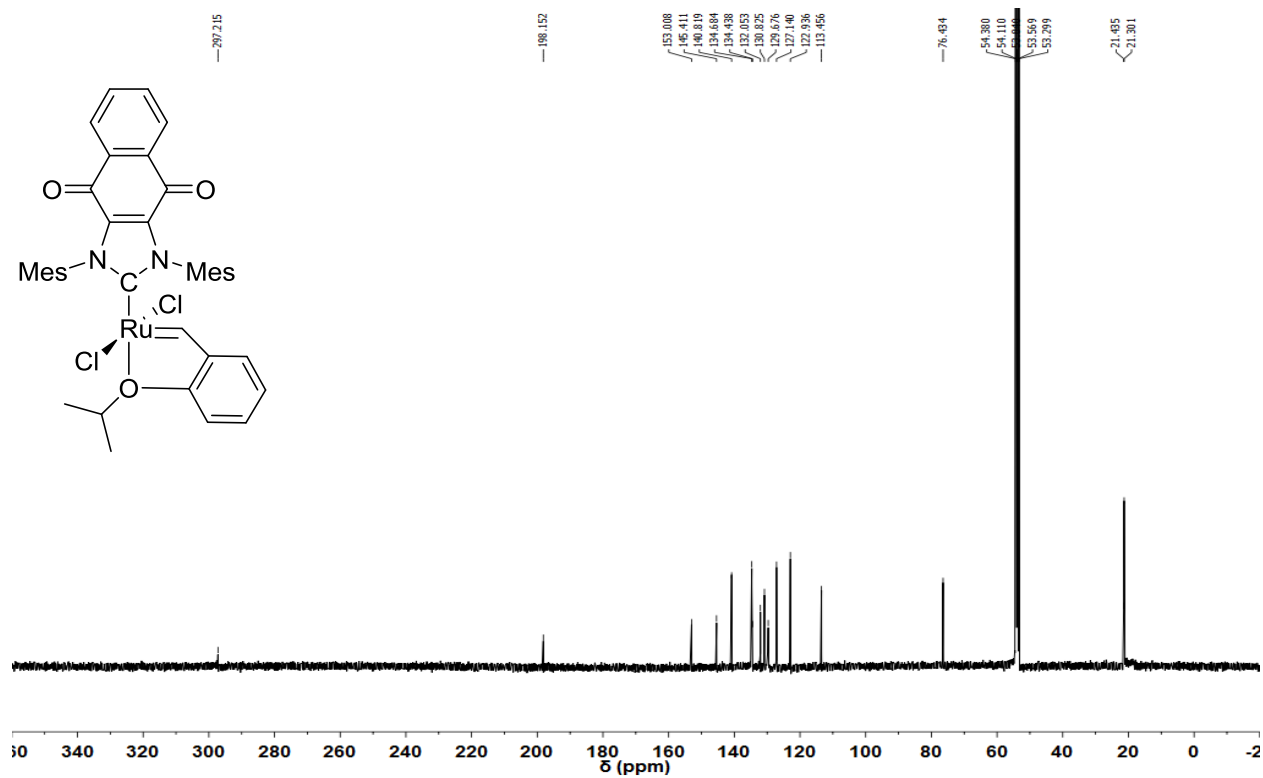
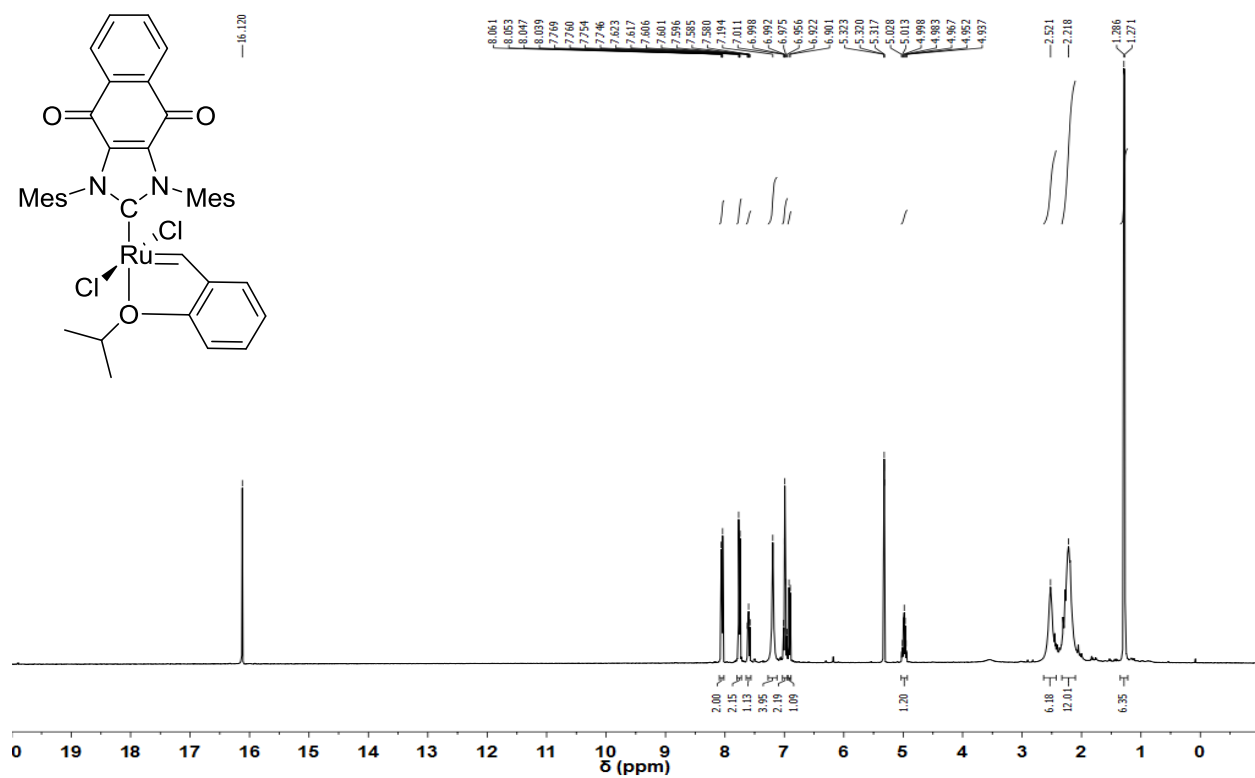
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Table S1. Summary of crystal data, data collection, and structure refinement details for **2**.

2	
Formula	C ₄₃ H ₄₆ N ₂ O ₃ Cl ₂ Ru
<i>M</i> _r	826.8
crystal size (mm ³)	0.20 × 0.20 × 0.20
crystal system	Monoclinic
space group	<i>P</i> 21
<i>a</i> (Å)	8.3800(70)
<i>b</i> (Å)	21.5800(200)
<i>c</i> (Å)	11.0723(97)
<i>α</i> (°)	90.000(0)
<i>β</i> (°)	109.143(44)
<i>γ</i> (°)	90.000(0)
<i>V</i> (Å ³)	1891.60(307)
<i>Z</i>	2
<i>ρ</i> _{calc} (g cm ⁻³)	1.45
<i>μ</i> (mm ⁻¹)	5.016
<i>F</i> (000)	856.0
<i>T</i> (K)	123(2)
scan mode	<i>ω</i>
<i>hkl</i> range	-3 → +9 -26 → +26 -13 → +13
measd reflns	40249
unique reflns [<i>R</i> _{int}]	6894 [0.097]
refinement reflns	6894
refined parameters	477
GOF on <i>F</i> ²	1.039
<i>R</i> 1 ^{<i>a</i>} (all data)	0.038 (0.052)
<i>wR</i> 2 ^{<i>b</i>} (all data)	0.081 (0.089)
<i>ρ</i> _{fin} (max/min)	0.836
(e Å ⁻³)	-0.478

$$^a R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|. \quad ^b wR2 = \{ [\Sigma w(F_o^2 - F_c^2)^2] / \Sigma w(F_o^2)^2 \}^{1/2}.$$



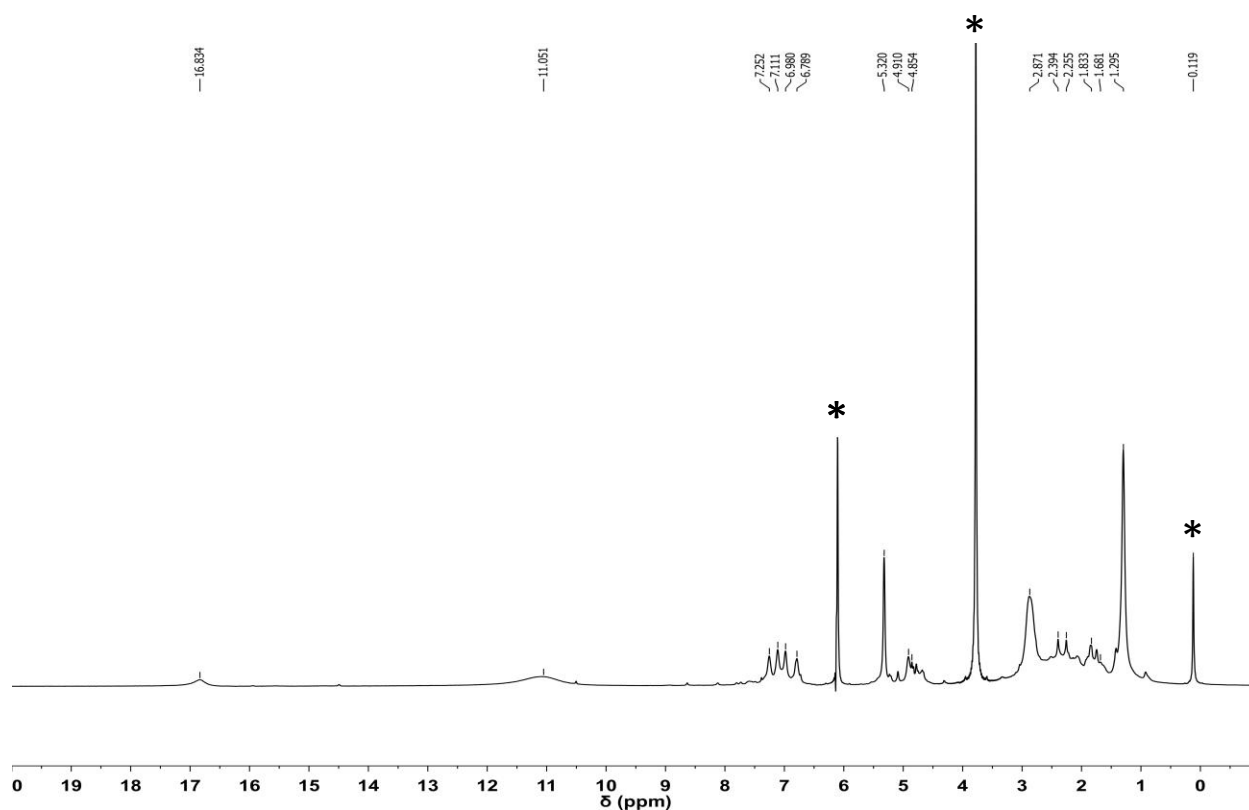


Figure S3. ^1H NMR spectrum of *in situ* generated **2_{red}**, which was recorded after adding 1.5 equiv. of CoCp_2 to a solution of **2** (CD_2Cl_2). (* = 1,3,5-trimethoxybenzene or silicone grease).

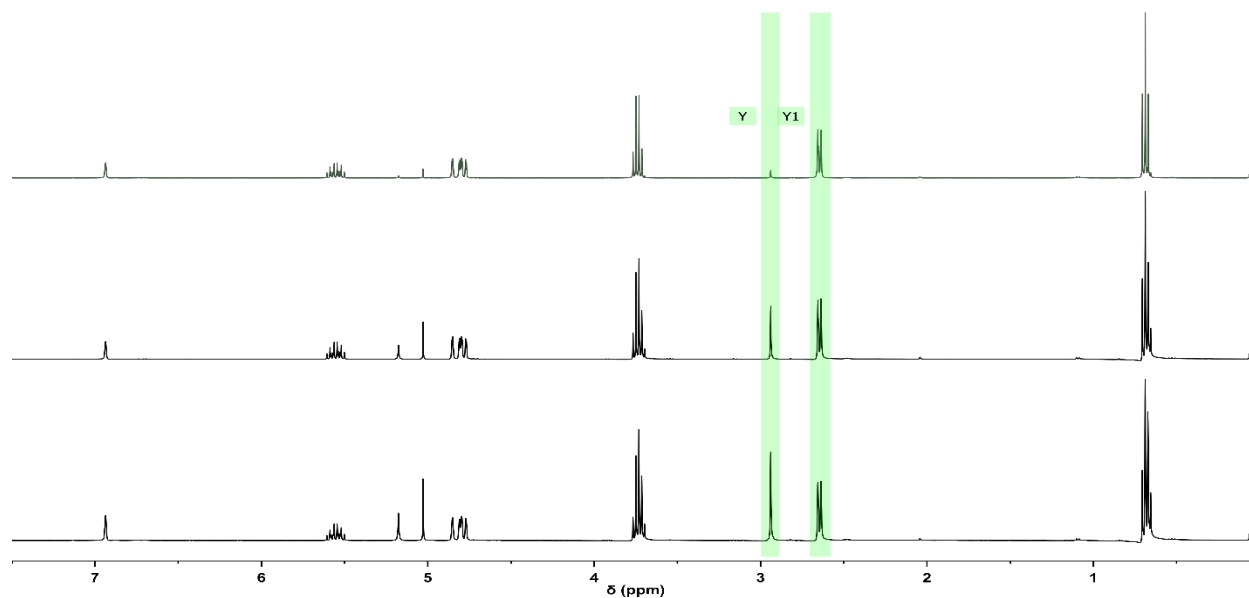


Figure S4. Representative ^1H NMR spectra of **3** in the presence of **2** recorded at $t = 134$ sec (top), 1010 sec (middle), and 2035 sec (bottom). Initial conditions: $[\mathbf{3}]_0 = 0.1$ M, $[\mathbf{3}]_0/[\mathbf{2}]_0 = 100$, 30°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S28 for more details. A complete list of integral values is provided in Table S2. Y represents an integrated region that corresponds to **4** whereas Y1 represents an integrated region that corresponds to **3**.

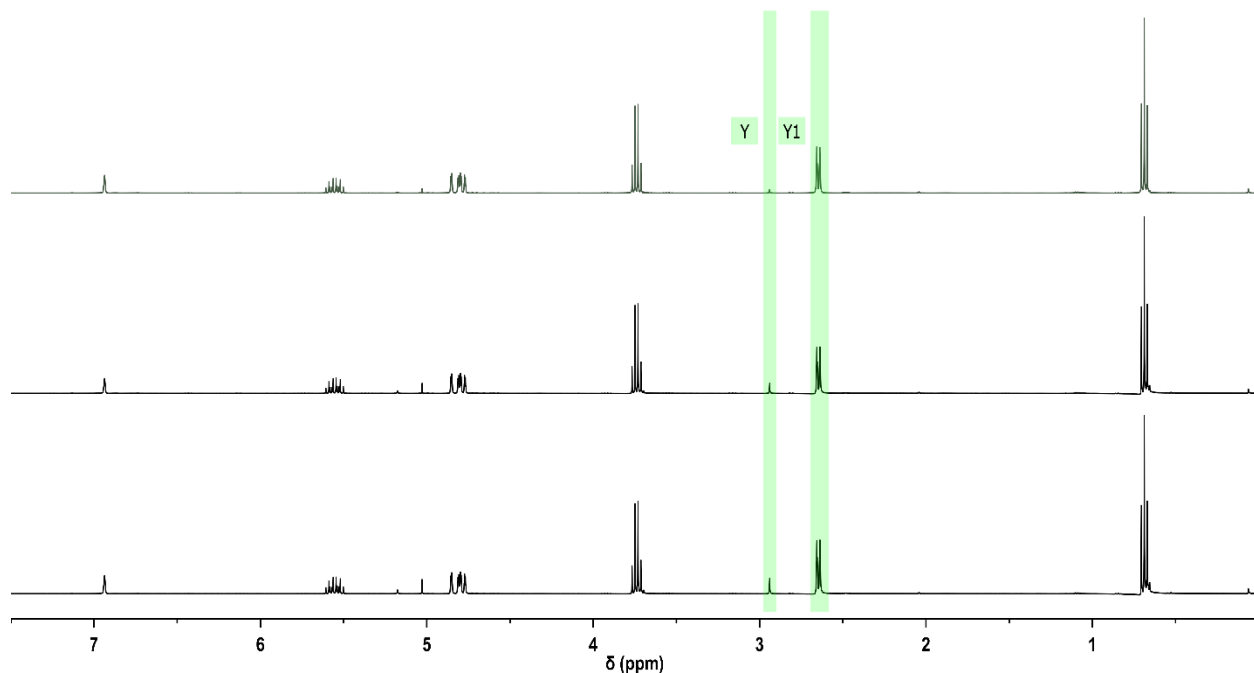


Figure S5. Representative ^1H NMR spectra of **3** in the presence of *in situ* generated **2_{red}** recorded at $t = 144$ sec (top), 1020 sec (middle), and 2041 sec (bottom). Initial conditions: $[\mathbf{3}]_0 = 0.1$ M, $[\mathbf{3}]_0/[\mathbf{2}_{\text{red}}]_0 = 100$, 30°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S29 for more details. A complete list of integral values is provided in Table S3. Y represents an integrated region that corresponds to **4** whereas Y1 represents an integrated region that corresponds to **3**.

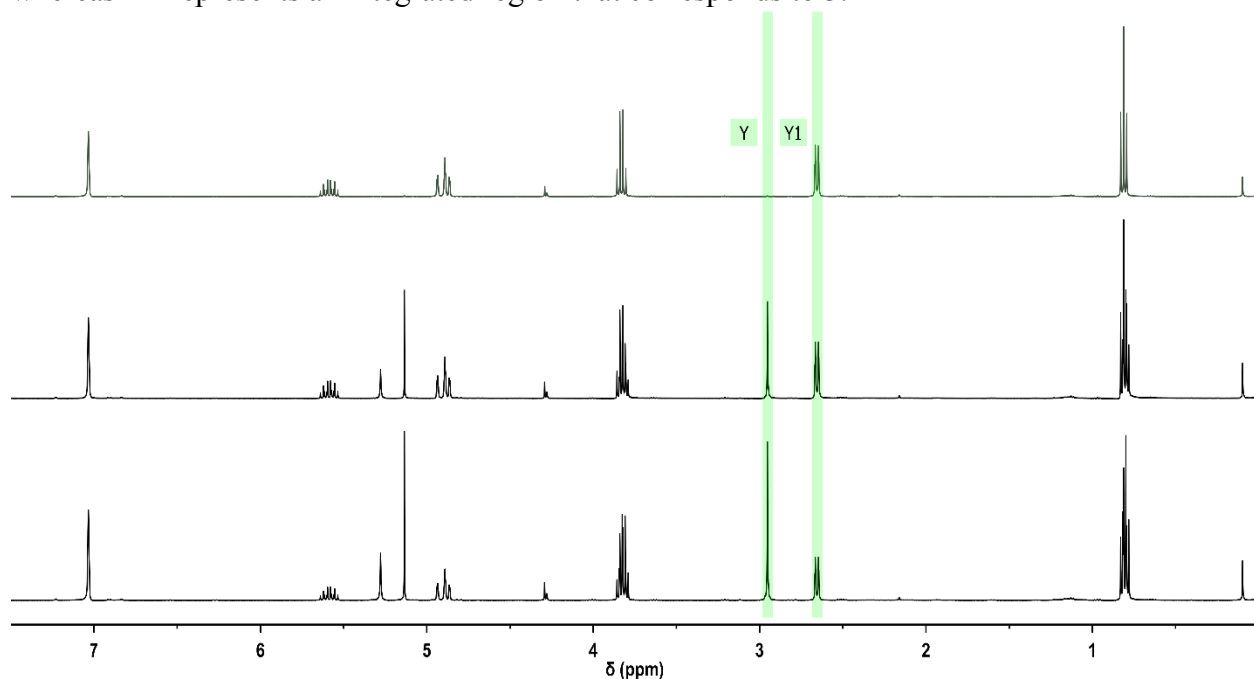


Figure S6. Representative ^1H NMR spectra of **3** in the presence of **2** recorded at $t = 157$ sec (top), 3554 sec (middle), and 7131 sec (bottom). Initial conditions: $[\mathbf{3}]_0 = 0.02$ M, $[\mathbf{3}]_0/[\mathbf{2}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S30 for more details. A complete list of integral values is provided in Table S4. Y represents an integrated region that corresponds to **4** whereas Y1 represents an integrated region that corresponds to **3**.

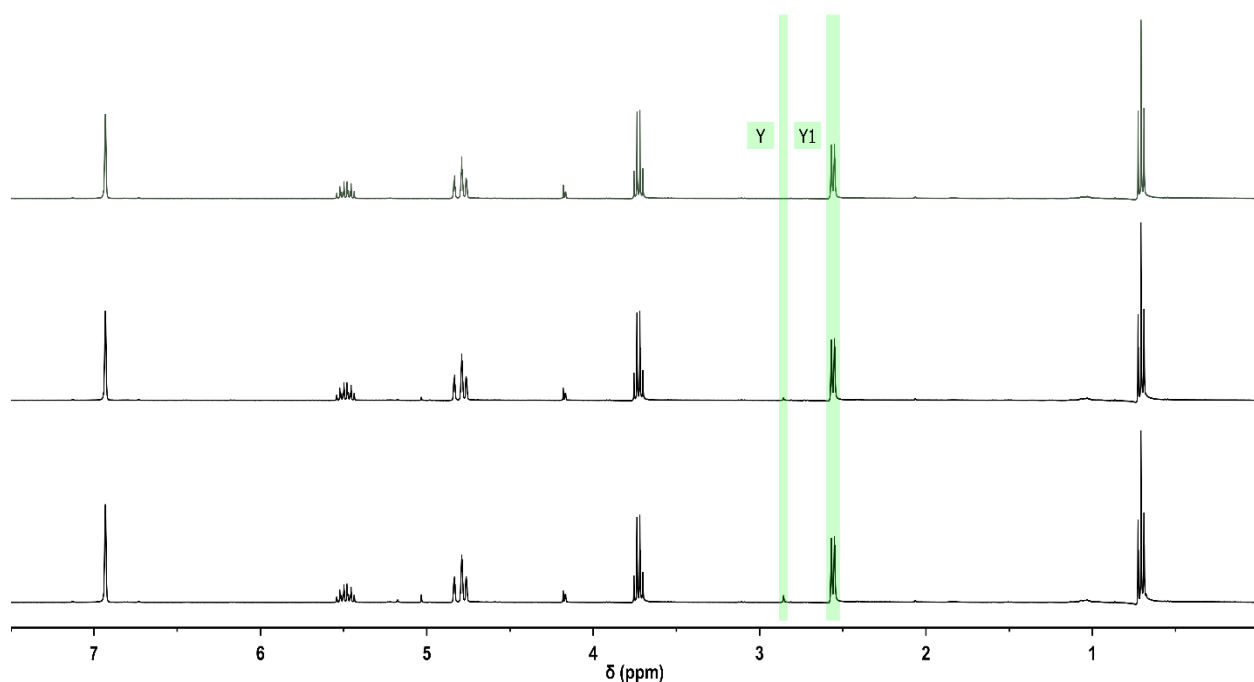


Figure S7. Representative ^1H NMR spectra of **3** in the presence of *in situ* generated **2_{red}** recorded at $t = 148$ sec (top), 3540 sec (middle), and 7168 sec (bottom). Initial conditions: $[\mathbf{3}]_0 = 0.02$ M, $[\mathbf{3}]_0/[\mathbf{2}_{\text{red}}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S31 for more details. A complete list of integral values is provided in Table S5. Y represents an integrated region that corresponds to **4** whereas Y1 represents an integrated region that corresponds to **3**.

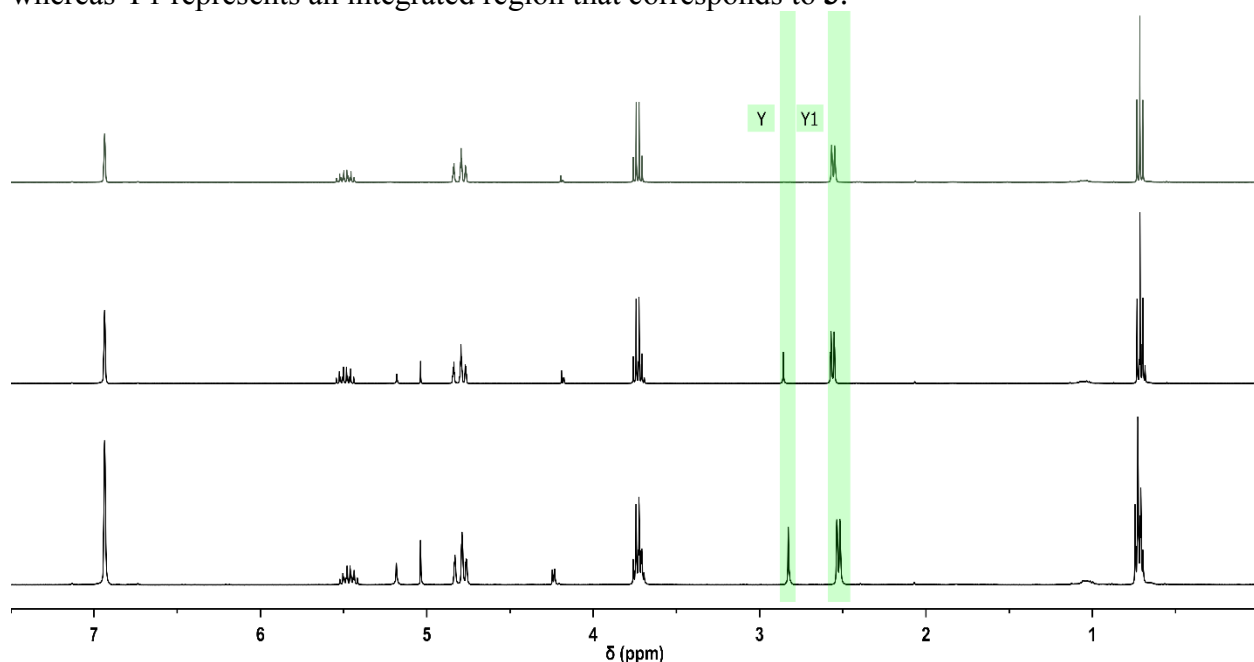


Figure S8. Representative ^1H NMR spectra of **3** in the presence of **2** recorded at $t = 107$ sec (top), 2447 sec (middle), and 7261 sec (bottom). Initial conditions: $[\mathbf{3}]_0 = 0.02$ M, $[\mathbf{3}]_0/[\mathbf{2}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S32 for more details. A complete list of integral values is provided in Table S6. Y represents an integrated region that corresponds to **4** whereas Y1 represents an integrated region that corresponds to **3**.

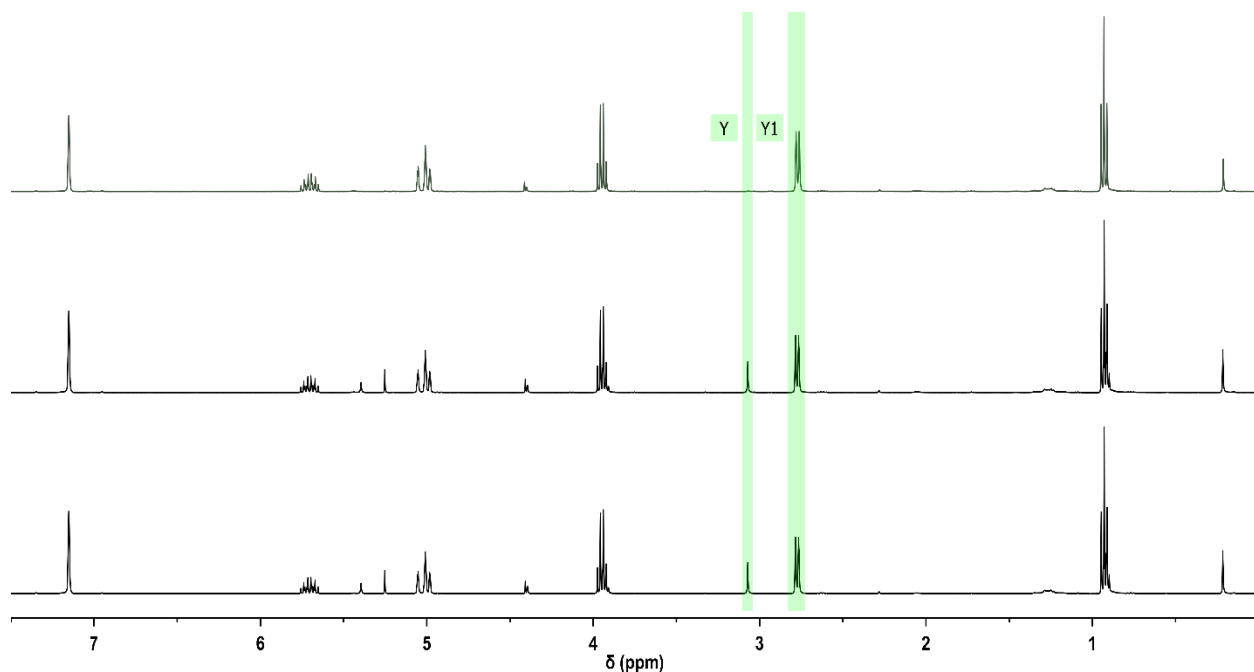


Figure S9. Representative ^1H NMR spectra of **3** in the presence of **2** recorded at $t = 123$ sec (top), 2439 sec (middle), and 7279 sec (bottom). Initial conditions: $[\mathbf{3}]_0 = 0.02$ M, $[\mathbf{3}]_0/[\mathbf{2}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S33 for more details. A complete list of integral values is provided in Table S7. Y represents an integrated region that corresponds to **4** whereas Y1 represents an integrated region that corresponds to **3**.

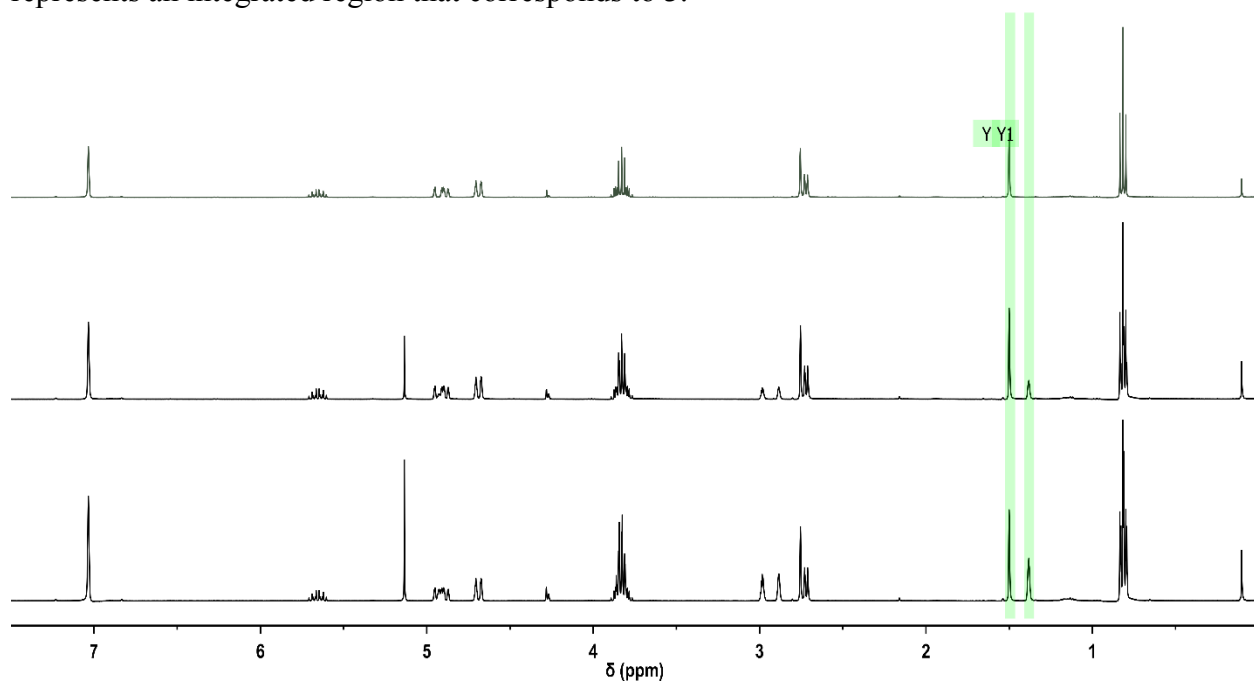


Figure S10. Representative ^1H NMR spectra of **5** in the presence of **2** recorded at $t = 84$ sec (top), 7026 sec (middle), and 14148 sec (bottom). Initial conditions: $[\mathbf{5}]_0 = 0.02$ M, $[\mathbf{5}]_0/[\mathbf{2}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S34 for more details. A complete list of integral values is provided in Table S8. Y represents an integrated region that corresponds to **5** whereas Y1 represents an integrated region that corresponds to **6**.

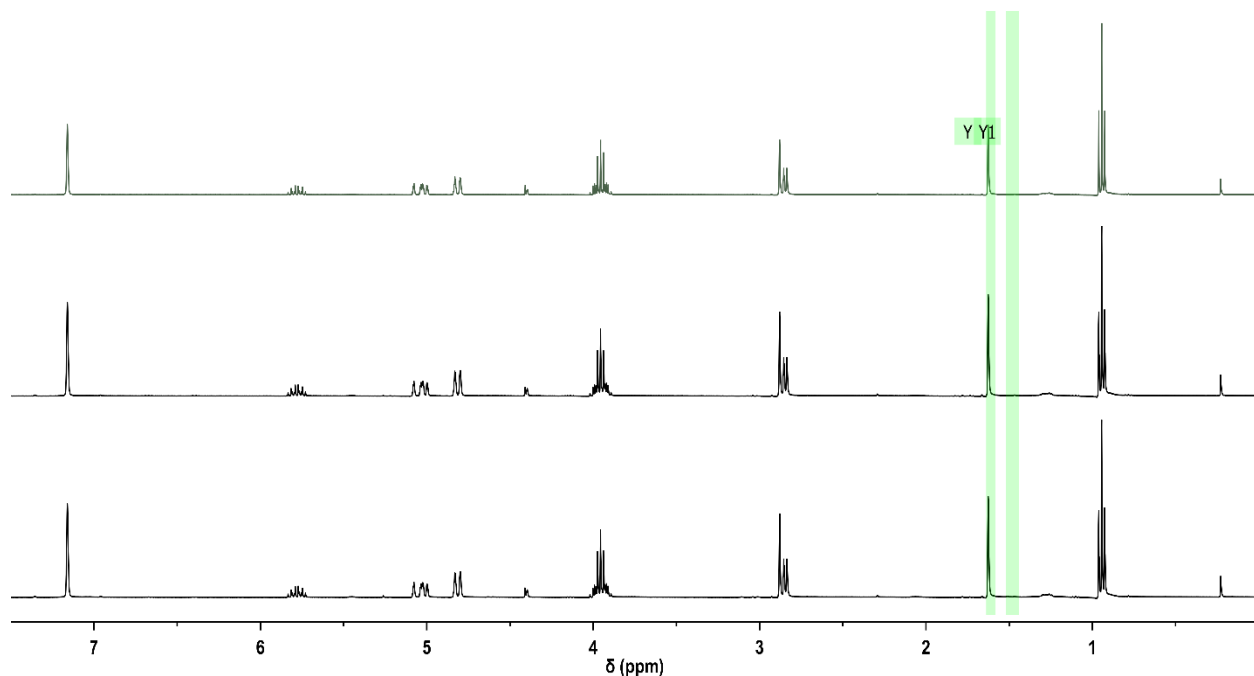


Figure S11. Representative ^1H NMR spectra of **5** in the presence of *in situ* generated **2_{red}** recorded at $t = 278$ sec (top), 7017 sec (middle), and 14153 sec (bottom). Initial conditions: $[\mathbf{5}]_0 = 0.02$ M, $[\mathbf{5}]_0/[\mathbf{2}_{\text{red}}]_0 = 100$, 20 °C, 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S35 for more details. A complete list of integral values is provided in Table S9. Y represents an integrated region that corresponds to **5** whereas Y1 represents an integrated region that corresponds to **6**.

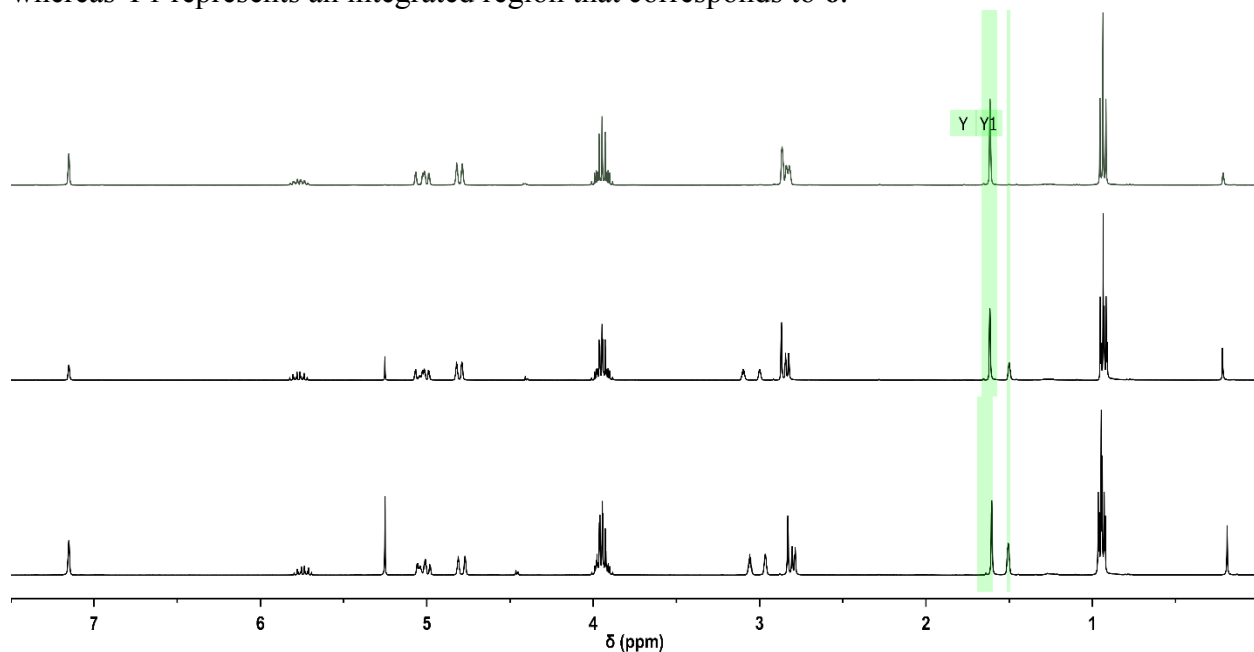


Figure S12. Representative ^1H NMR spectra of **5** in the presence of **2** recorded at $t = 147$ sec (top), 7042 sec (middle), and 13501 sec (bottom). Initial conditions: $[\mathbf{5}]_0 = 0.06$ M, $[\mathbf{5}]_0/[\mathbf{2}]_0 = 300$, 20 °C, 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S36 for more details. A complete list of integral values is provided in Table S10. Y represents an integrated region that corresponds to **5** whereas Y1 represents an integrated region that corresponds to **6**.

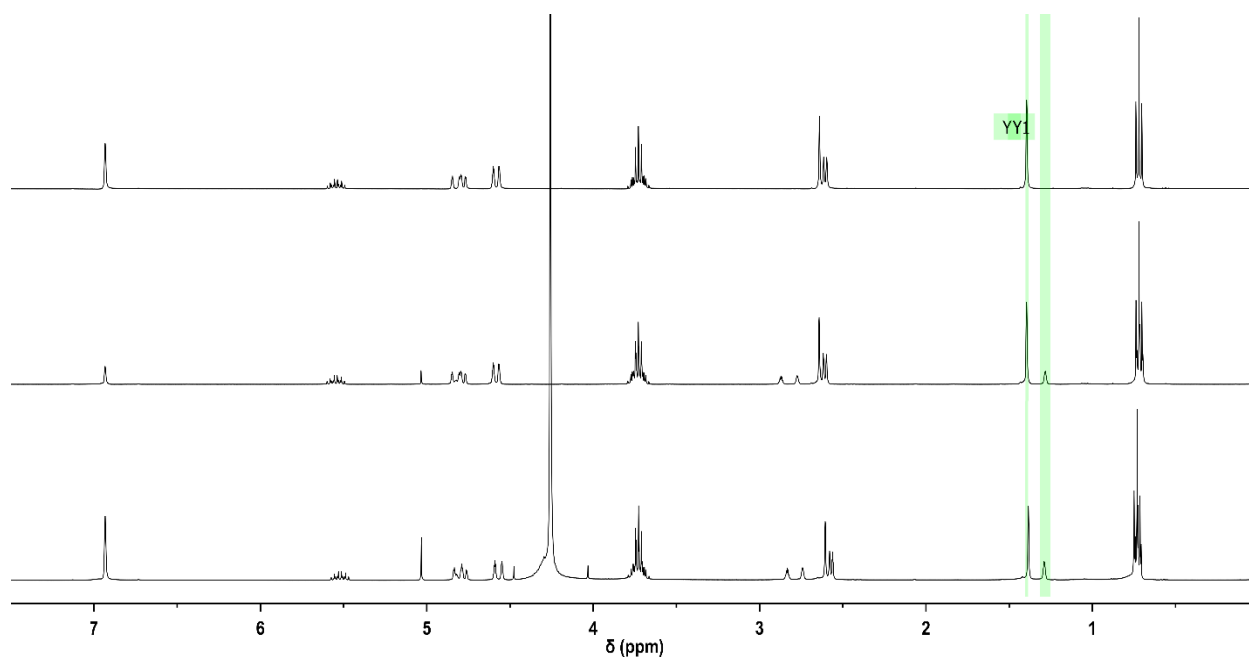


Figure S13. Representative ^1H NMR spectra of **5** in the presence of **2** recorded at $t = 140$ sec (top), 7886 sec (middle), and 15896 sec (bottom). Initial conditions: $[\mathbf{5}]_0 = 0.06$ M, $[\mathbf{5}]_0/[\mathbf{2}]_0 = 300$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S37 for more details. A complete list of integral values is provided in Table S11. Y represents an integrated region that corresponds to **5** whereas Y1 represents an integrated region that corresponds to **6**.

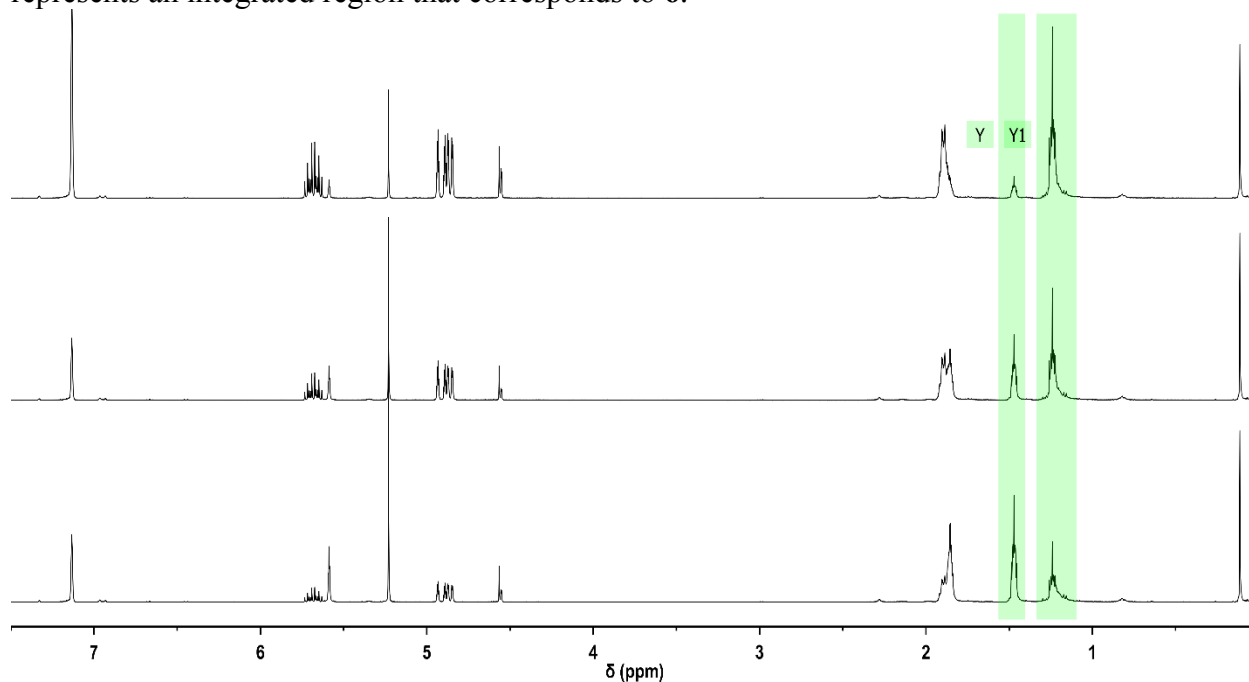


Figure S14. Representative ^1H NMR spectra of **7** in the presence of **2** recorded at $t = 182$ sec (top), 471 sec (middle), and 979 sec (bottom). Initial conditions: $[\mathbf{7}]_0 = 0.02$ M, $[\mathbf{7}]_0/[\mathbf{2}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S38 for more details. A complete list of integral values is provided in Table S12. Y represents an integrated region that corresponds to **8** whereas Y1 represents an integrated region that corresponds to **7**.

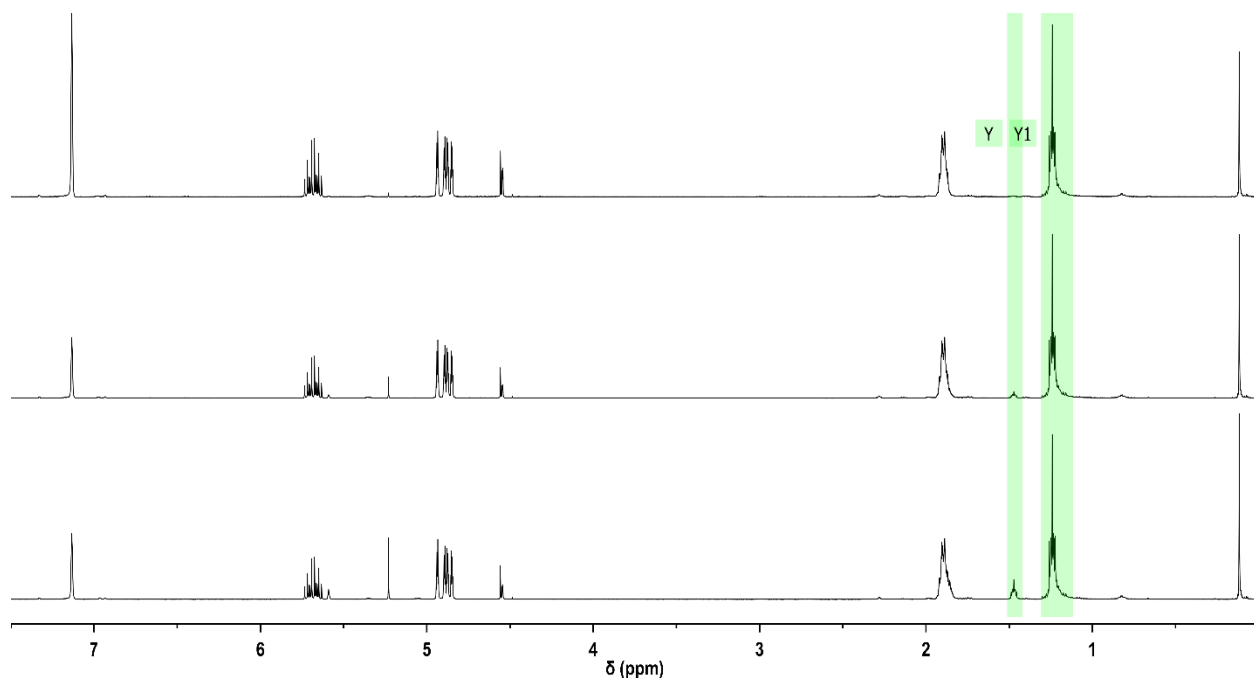


Figure S15. Representative ^1H NMR spectra of **7** in the presence of *in situ* generated **2_{red}** (see text) recorded at $t = 163$ sec (top), 478 sec (middle), and 987 sec (bottom). Initial conditions: $[\textbf{7}]_0 = 0.02$ M, $[\textbf{7}]_0/[\textbf{2}_{\text{red}}]_0 = 100$, 20 °C, 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S39 for more details. A complete list of integral values is provided in Table S13. Y represents an integrated region that corresponds to **8** whereas Y1 represents an integrated region that corresponds to **7**.

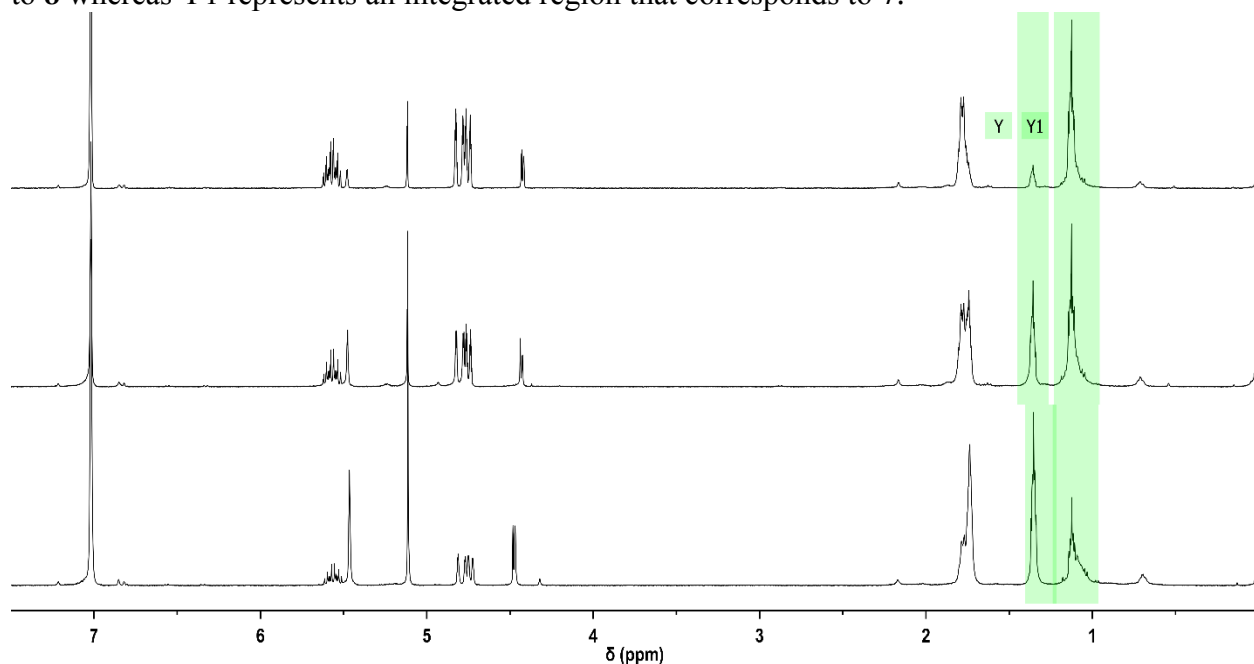


Figure S16. Representative ^1H NMR spectra of **7** in the presence of **2** recorded at $t = 163$ sec (top), 780 sec (middle), and 1982 sec (bottom). Initial conditions: $[\textbf{7}]_0 = 0.02$ M, $[\textbf{7}]_0/[\textbf{2}]_0 = 100$, 20 °C, 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S40 for more details. A complete list of integral values is provided in Table S14. Y represents an integrated region that corresponds to **8** whereas Y1 represents an integrated region that corresponds to **7**.

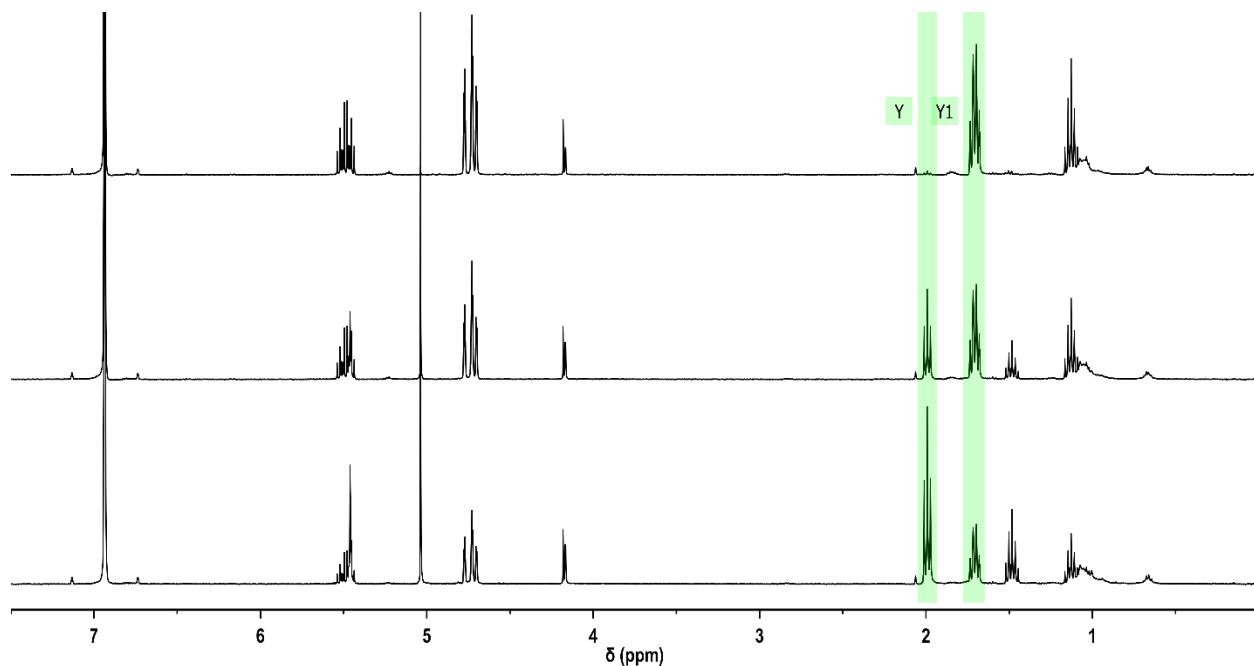


Figure S17. Representative ^1H NMR spectra of **9** in the presence of **2** recorded at $t = 122$ sec (top), 911 sec (middle), and 1862 sec (bottom). Initial conditions: $[\mathbf{9}]_0 = 0.01$ M, $[\mathbf{9}]_0/[\mathbf{2}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S41 for more details. A complete list of integral values is provided in Table S15. Y represents an integrated region that corresponds to **10** whereas Y1 represents an integrated region that corresponds to **9**.

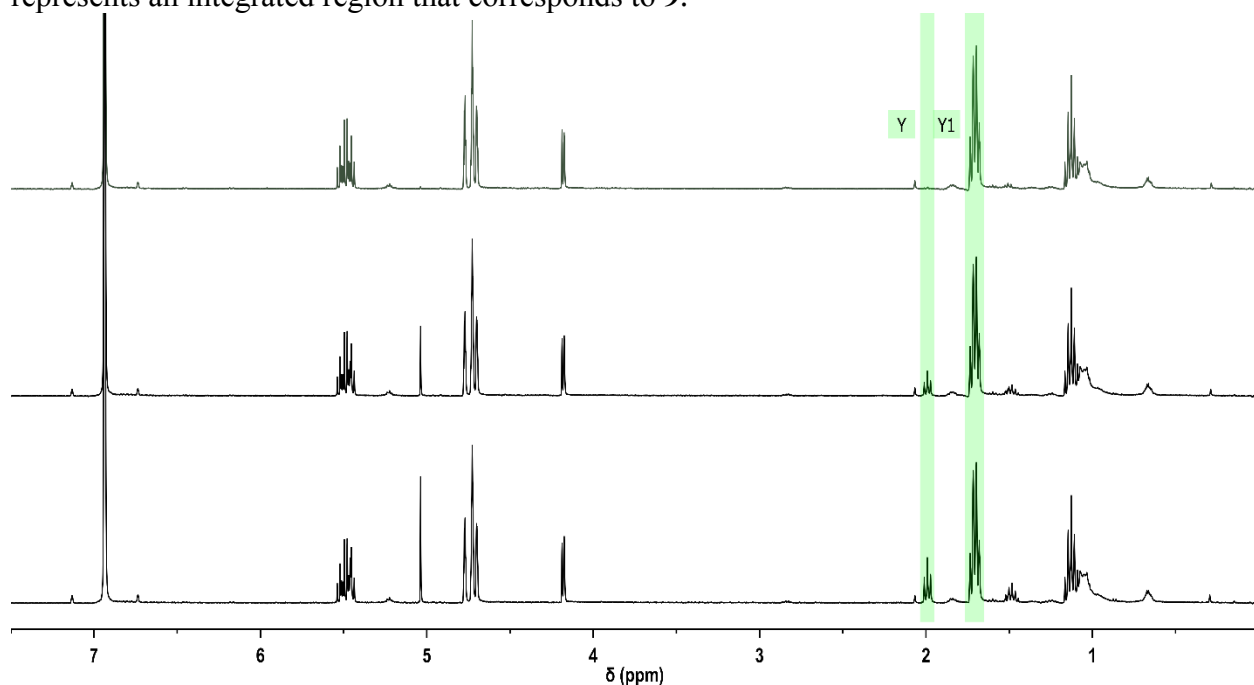


Figure S18. Representative ^1H NMR spectra of **9** in the presence of *in situ* generated **2_{red}** (see text) recorded at $t = 134$ sec (top), 923 sec (middle), and 1869 sec (bottom). Initial conditions: $[\mathbf{9}]_0 = 0.01$ M, $[\mathbf{9}]_0/[\mathbf{2}_{\text{red}}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$. See Figure S42 for more details. A complete list of integral values is provided in Table S16. Y represents an integrated region that corresponds to **10** whereas Y1 represents an integrated region that corresponds to **9**.

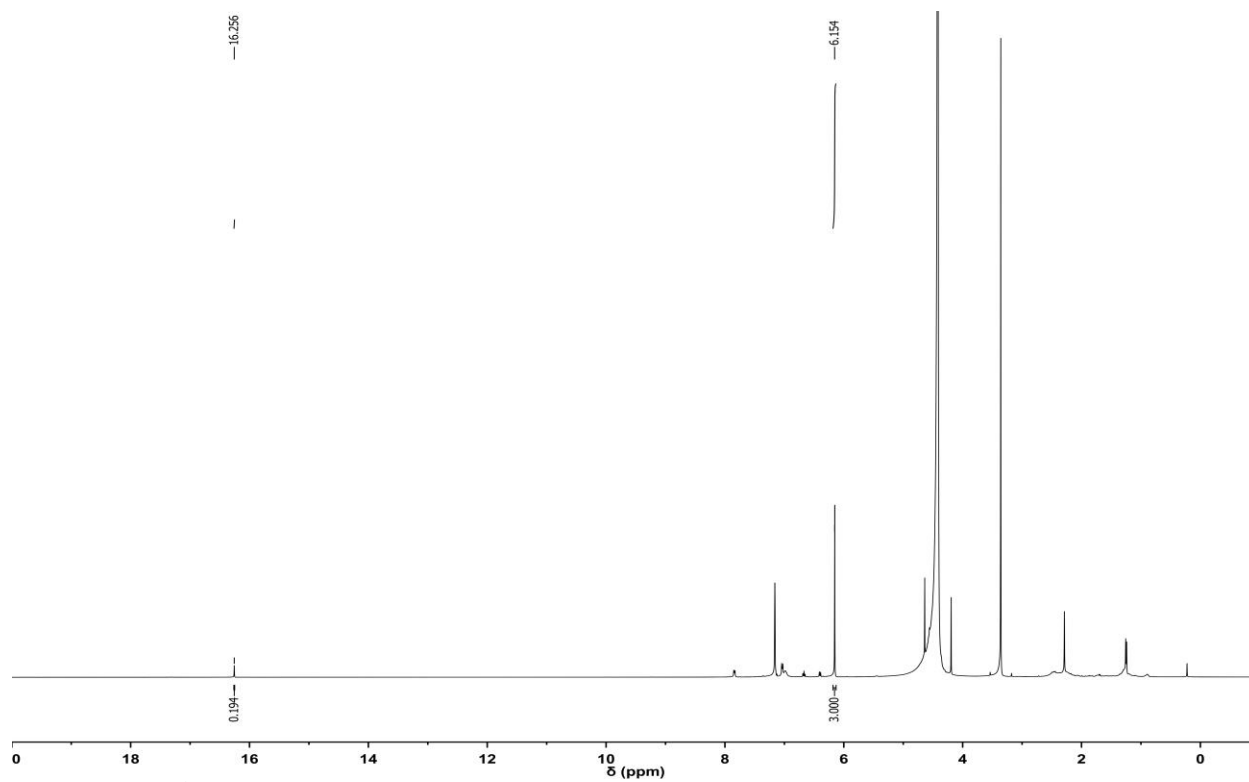


Figure S19. ^1H NMR spectrum of **2** containing 1,3,5-trimethoxybenzene as an internal standard ($\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$; Figure 3c).

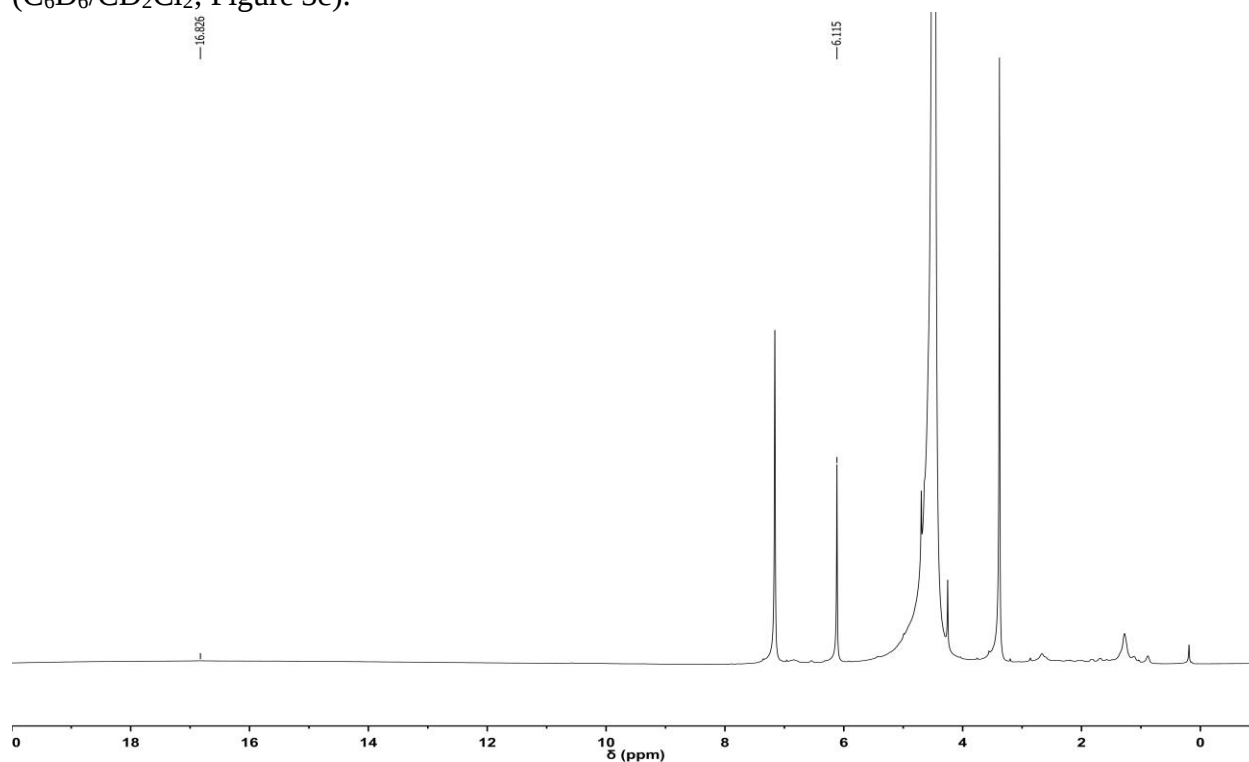


Figure S20. ^1H NMR spectrum of *in situ* generated **2_{red}**, which was recorded after adding CoCp_2 (1.5 equiv.) to a $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$ solution of **2** containing 1,3,5-trimethoxybenzene as an internal standard ($\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$; Figure 3c).

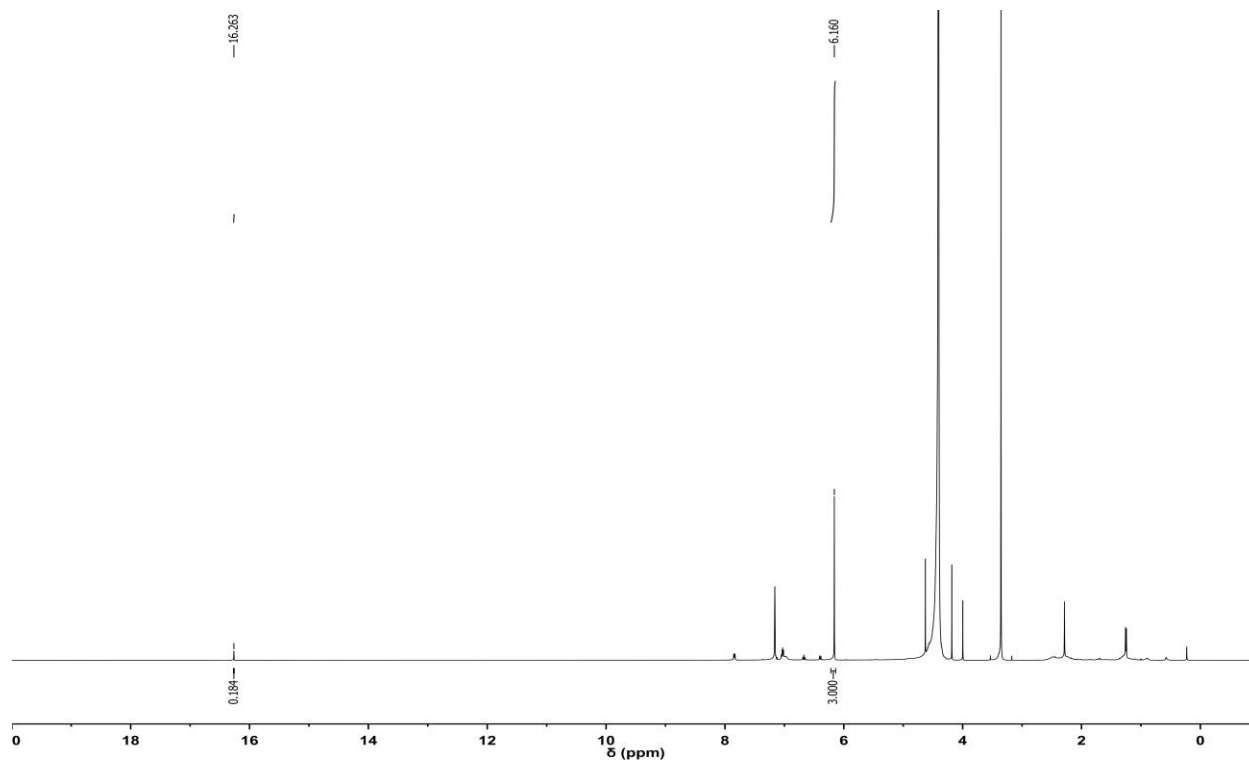


Figure S21. ^1H NMR spectrum of **2_{red-ox}**, which was recorded after adding FcPF_6 (1.5 equiv. rel. to CoCp_2) to a $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$ solution of **2_{red}** containing 1,3,5-trimethoxybenzene as an internal standard ($\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$; Figure 3c).

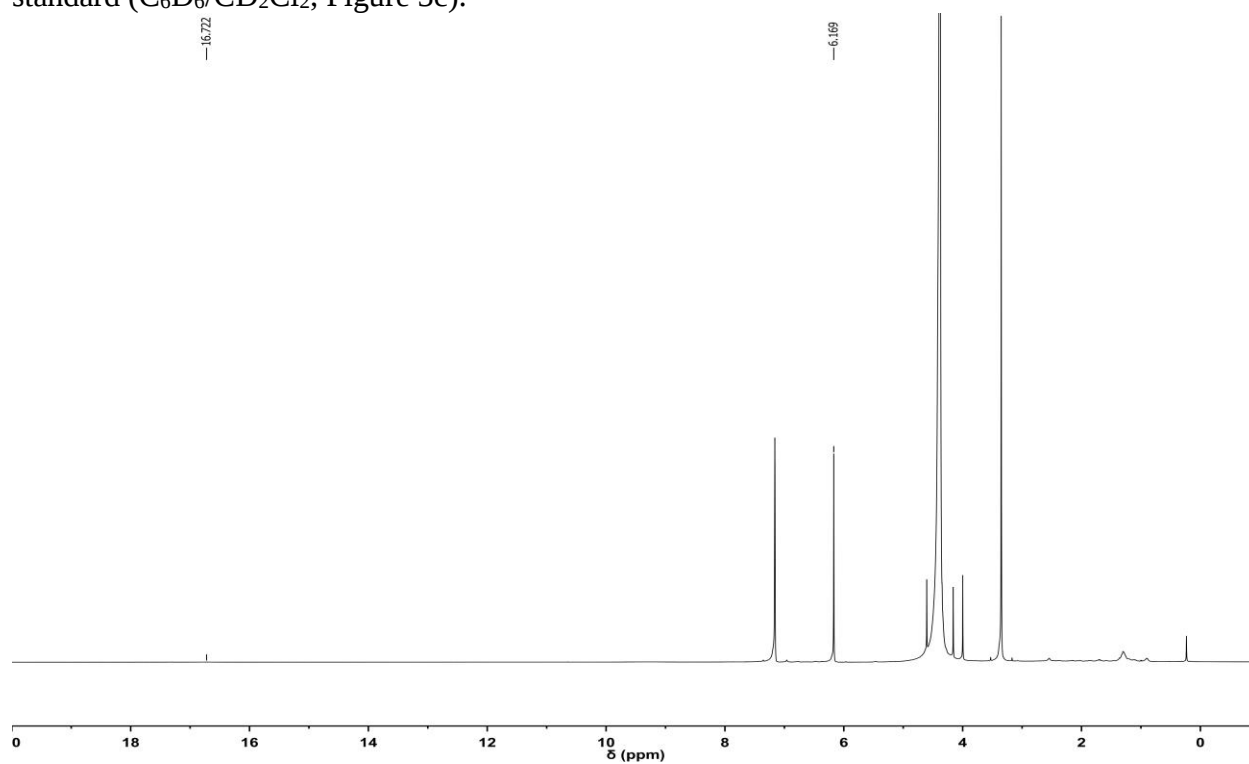


Figure S22. ^1H NMR spectrum of **2_{red-ox-red}**, which was recorded after adding CoCp_2 (1.5 equiv. rel. to FcPF_6) to a $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$ solution of **2_{red-ox}** containing 1,3,5-trimethoxybenzene as an internal standard ($\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$; Figure 3c).

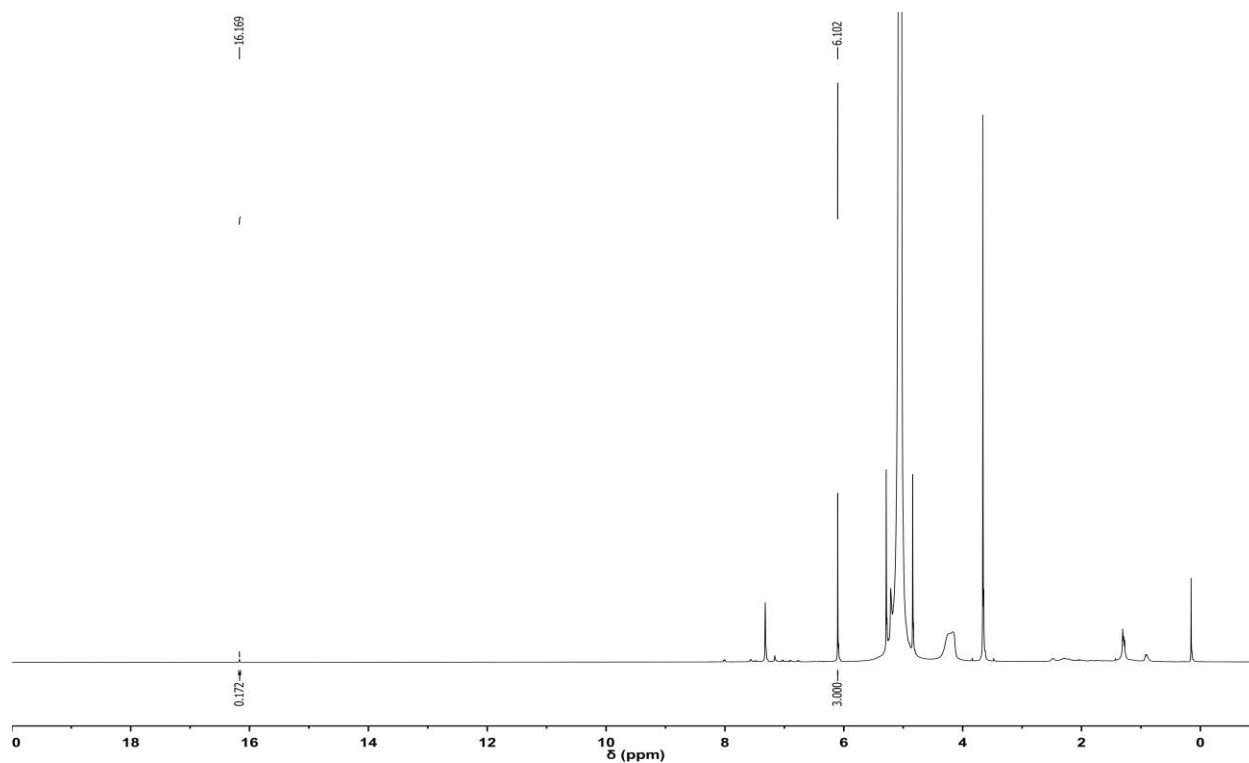


Figure S23. ^1H NMR spectrum of **2_{red-ox-red-ox}**, which was recorded after adding FcPF_6 (1.5 equiv. rel. to CoCp_2) to a $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$ solution of **2_{red-ox-red}** containing 1,3,5-trimethoxybenzene as an internal standard ($\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$; Figure 3c).

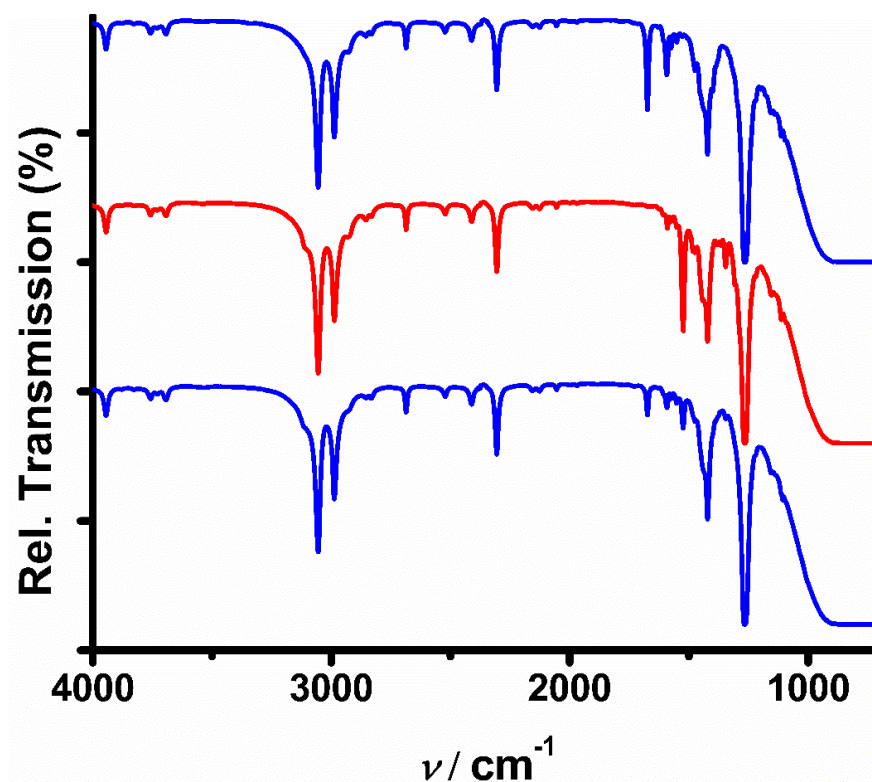


Figure S24. IR spectra of **2** (top), *in situ* generated **2_{red}** (middle), and regenerated **2** after the addition of FcPF₆ to **2_{red}** (bottom) showing the disappearance and reappearance of a ν_{CO} at 1674 cm^{-1} (CD_2Cl_2).

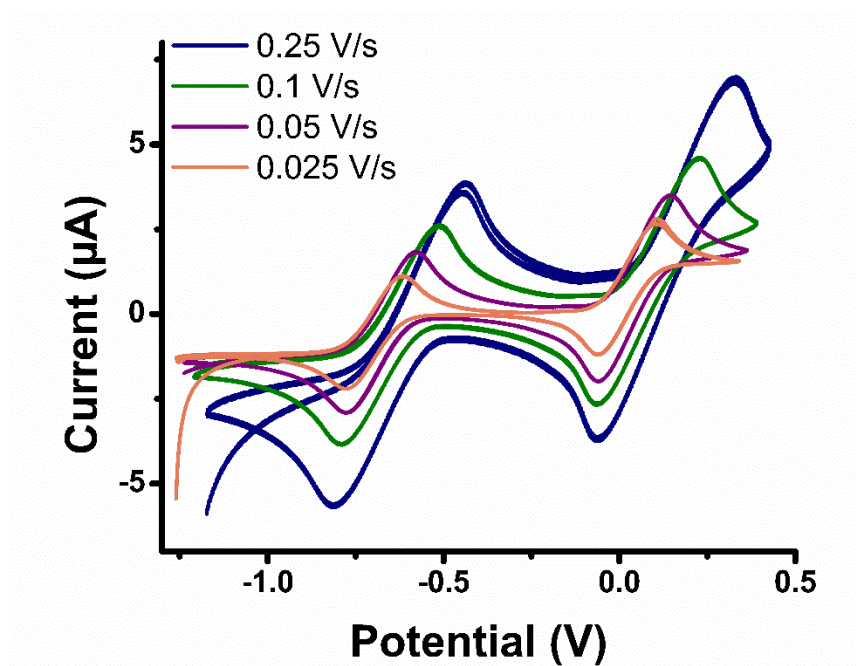


Figure S25. Cyclic voltammograms of **2** at different scan rates (indicated) in CH_2Cl_2 with 0.1 M TBAP as the electrolyte and Fc* as an internal standard. $[\mathbf{2}]_0 = 1.0 \text{ mM}$.

Summaries of Additional RCM Experiments

The ability of **2** to facilitate the RCM of diethyl 2,2-diallylmalonate (**3**) at a higher initial substrate concentration and at a lower catalyst loading than those reported in the main text was also explored. As shown in Figure S26 (left), the addition of a CD₂Cl₂ solution of **2** to a C₆D₆ solution of **3** ([**3**]₀ = 0.06 M, [**3**]₀/[**2**]₀ = 300, 5:1 v/v C₆D₆/CD₂Cl₂, 20 °C) resulted in a RCM that proceeded at a rate constant k_2 of $9.1 \times 10^{-5} \text{ s}^{-1}$, as determined by ¹H NMR spectroscopy. In contrast, a lower rate constant $k_{2\text{red}}$ of $1.2 \times 10^{-6} \text{ s}^{-1}$ ($k_2/k_{2\text{red}} = 76$) was measured using *in situ* generated **2**_{red} under otherwise identical conditions ([**3**]₀ = 0.06 M, [**3**]₀/[**2**_{red}]₀ = 300, 5:1 v/v C₆D₆/CD₂Cl₂, 20 °C).

The durability of the redox-switchable catalyst **2** was probed by alternately adding CoCp₂ and FcPF₆ multiple times over the course of a reaction (Figure S26, right). After a **2**-initiated RCM of **3** proceeded for 39 min ($k_2 = 1.2 \times 10^{-4} \text{ s}^{-1}$), the addition of CoCp₂ (1.5 equiv. rel. to added **2**) effectively inhibited the rate of the reaction ($k_{2\text{red}} = 2.6 \times 10^{-6} \text{ s}^{-1}$, $k_2/k_{2\text{red}} = 46$). The subsequent addition of FcPF₆ (1.5 equiv. rel. to added CoCp₂) restored the initial catalytic activity ($k_{2\text{red-ox}} = 1.9 \times 10^{-5} \text{ s}^{-1}$). The catalytic activity was subsequently successfully toggled again, although attenuations in the corresponding measured rate constants were observed ($k_{2\text{red-ox-red}} = 7.6 \times 10^{-7} \text{ s}^{-1}$, $k_{2\text{red-ox-red-ox}} = 2.9 \times 10^{-5} \text{ s}^{-1}$).

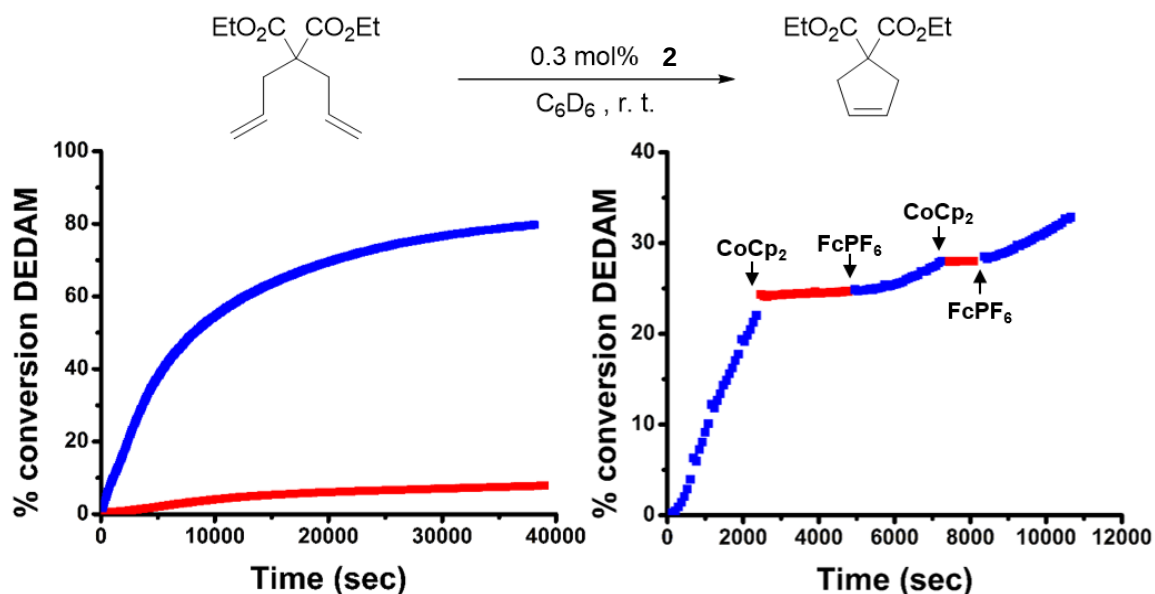


Figure S26. Plots of percent conversion of **3** vs time for (left) the RCM reaction of **3** using **2** (■) or *in situ* generated **2**_{red} (■) as the initiator, and (right) the *in situ* redox-switching of an ongoing RCM via the addition of chemical reductants and oxidants (indicated). Conditions: [**3**]₀ = 0.06 M, [**3**]₀/[**2**]₀ = 300, 20 °C, 5:1 v/v C₆D₆/CD₂Cl₂.

As shown in Figure S27, an ability to control the rate of formation of **10** during an ongoing reaction was explored via the addition of reductants and oxidants. After the RCM reaction of **9** ($[\mathbf{9}]_0 = 0.01$ M, $[\mathbf{9}]_0/[\mathbf{2}]_0 = 100$, 20 °C, 5:1 v/v C₆D₆/CD₂Cl₂) proceeded to 21% conversion at a rate constant k_2 of $3.4 \times 10^{-4} \text{ s}^{-1}$, the addition of CoCp₂ (1.5 equiv. rel. to **2**) effectively decreased the rate of the reaction ($k_{2\text{red}} = 1.1 \times 10^{-6} \text{ s}^{-1}$, $k_2/k_{2\text{red}} = 340$). The subsequent introduction of FcPF₆ (1.5 equiv. rel. to added CoCp₂) enhanced the rate of formation of **10** ($k_{2\text{red-ox}}$ of $8.8 \times 10^{-5} \text{ s}^{-1}$, $k_{2\text{red-ox}}/k_{2\text{red}} = 80$).

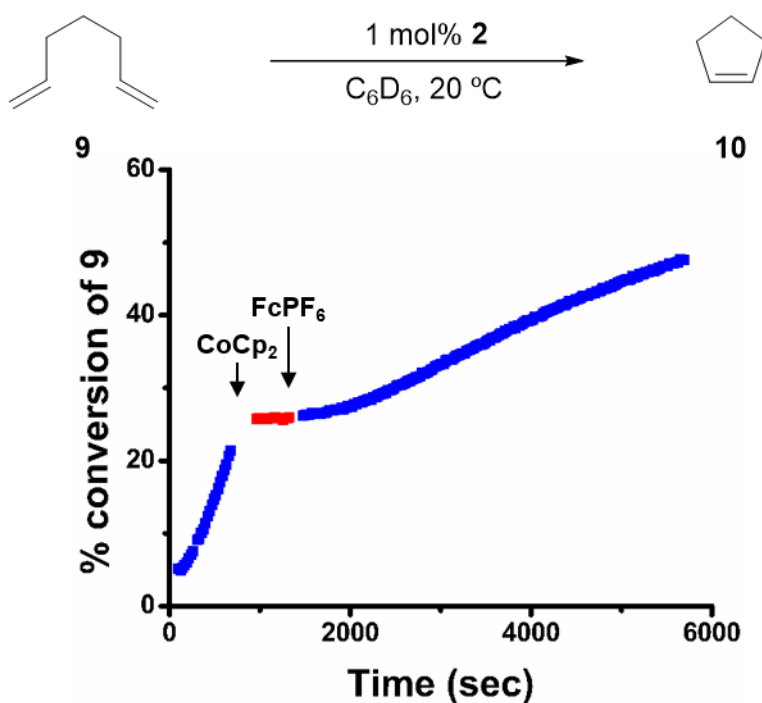
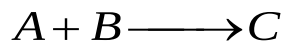


Figure S27. Plot of percent conversion of **9** vs time. Chemical reductants (CoCp₂) and oxidants (FcPF₆) were added as the reaction progressed (indicated). Conditions: $[\mathbf{9}]_0 = 0.01$ M, $[\mathbf{9}]_0/[\mathbf{2}]_0 = 100$, 20 °C, 5:1 v/v C₆D₆/CD₂Cl₂.

Kinetics Data

The ring-closing metathesis of a given substrate may be represented as:



Considering the reaction conditions employed, the substrate (A) will always be present in a large excess when compared to the catalyst (B). Assuming no side reactions, pseudo-first order kinetics may be assumed and the following rate law applies:

$$\frac{d[C]}{dt} = k[A][B]_0 = k[A]$$

The integrated form of the above equation may be written as:

$$\ln[A] = \ln[A]_0 - kt$$

Thus, plotting $-\ln [A]$ vs. t (s) should give a linear plot where k is equal to the slope of the line.

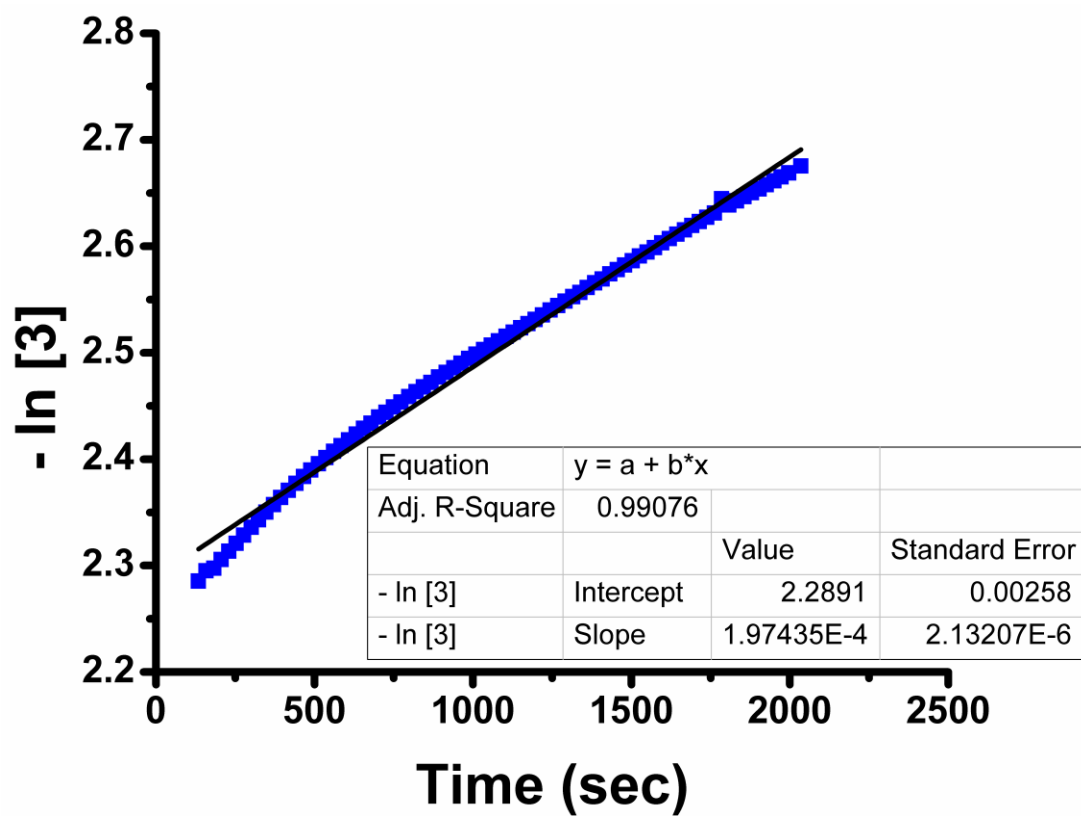


Figure S28. Plot of $-\ln [3]$ versus time using **2** (■) as the initiator. Conditions: $[3]_0 = 0.1$ M, $[3]_0/[2]_0 = 100$, 30 °C, 5:1 v/v C_6D_6/CD_2Cl_2 .

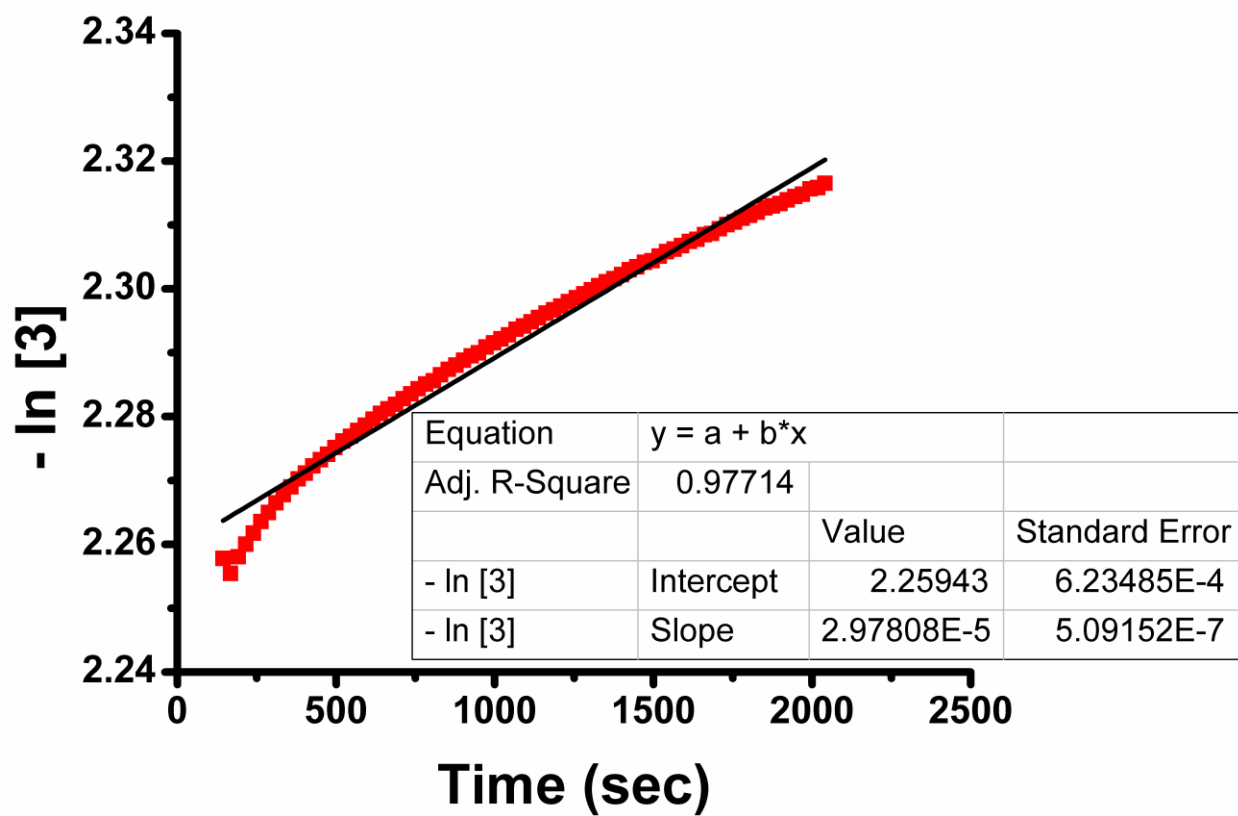


Figure S29. Plot of $-\ln [3]$ versus time using *in situ* generated 2_{red} (■) as the initiator. Conditions: $[3]_0 = 0.1 \text{ M}$, $[3]_0/[2_{\text{red}}]_0 = 100$, $30 \text{ }^\circ\text{C}$, $5:1 \text{ v/v C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

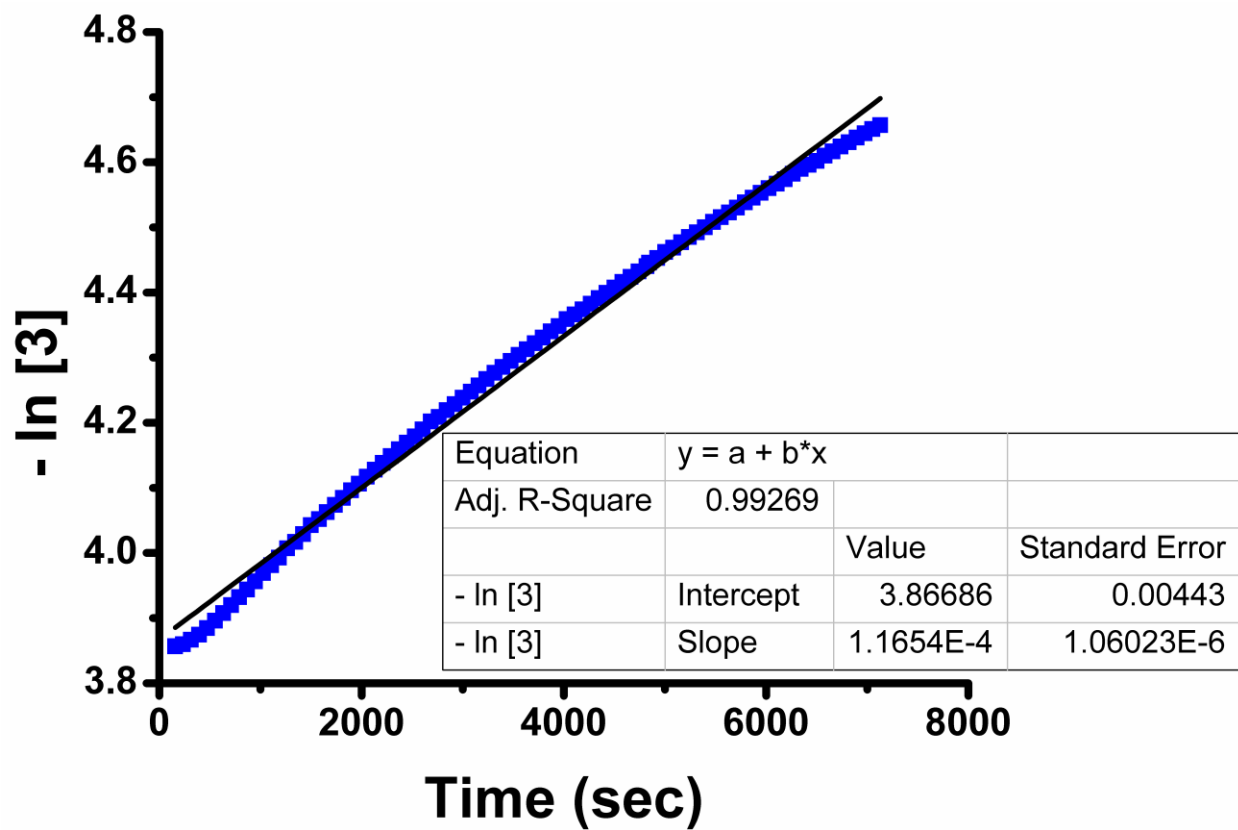


Figure S30. Plot of $-\ln [3]$ versus time using **2** (■) as the initiator. Conditions: $[3]_0 = 0.02$ M, $[3]_0/[2]_0 = 100$, 20 °C, 5:1 v/v C_6D_6/CD_2Cl_2 .

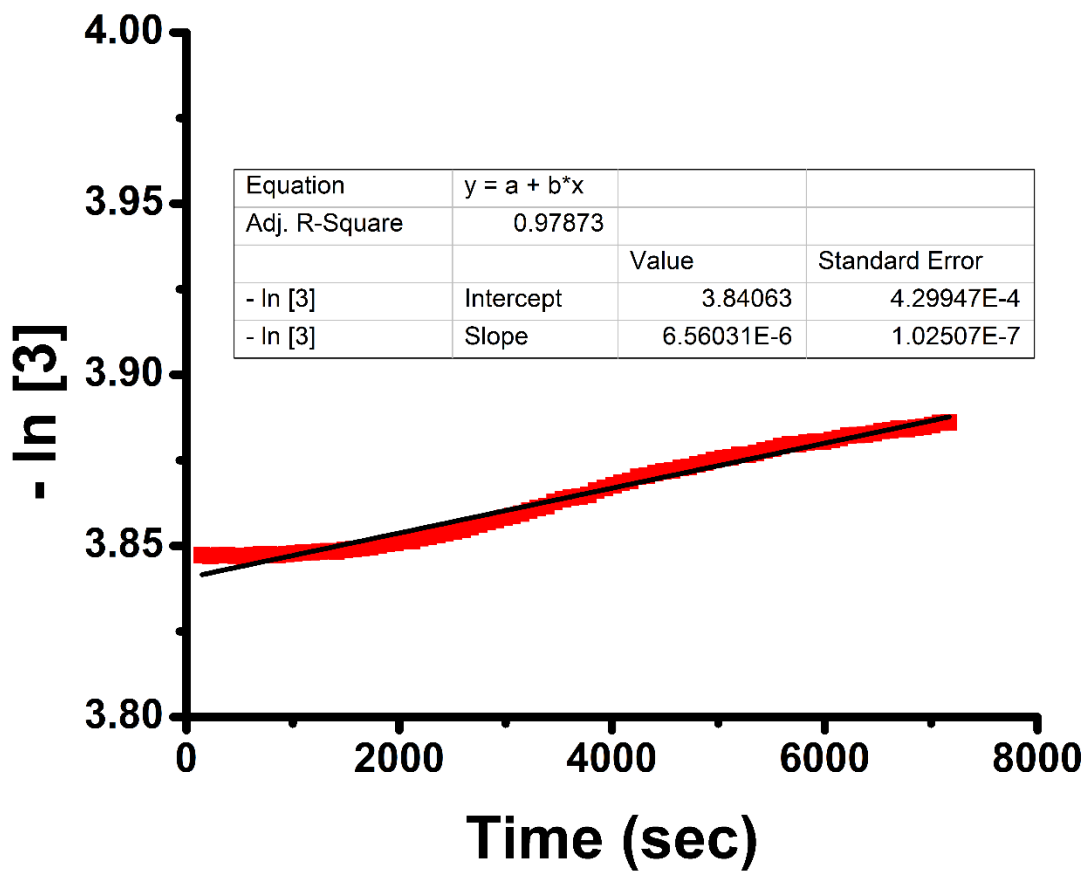


Figure S31. Plot of $-\ln [3]$ versus time using *in situ* generated 2_{red} (■) as the initiator. Conditions: $[3]_0 = 0.02$ M, $[3]_0/[2_{\text{red}}]_0 = 100$, 20 °C, 5:1 v/v C_6D_6/CD_2Cl_2 .

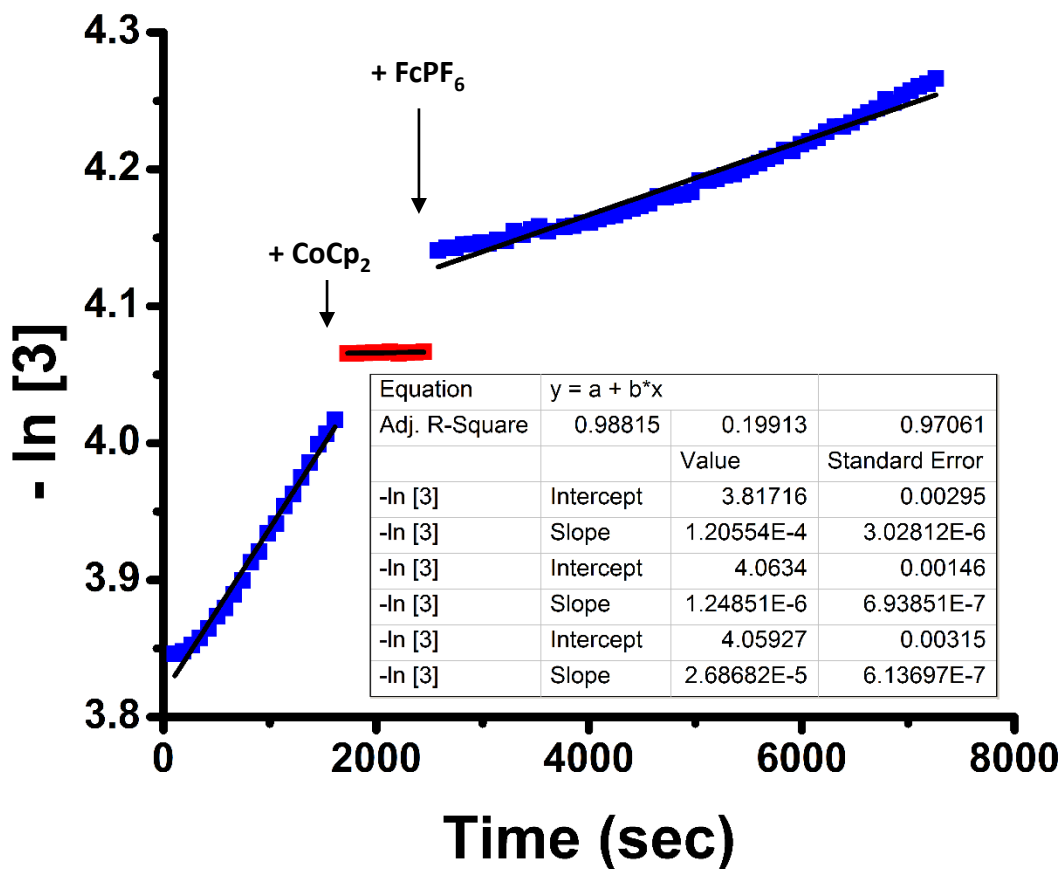


Figure S32. Plot of $-\ln [3]$ versus time using **2** (■) as the initiator followed by the reduction and re-oxidation of the catalyst using CoCp_2 (1.5 equiv. rel. to **2**) and FcPF_6 (1.5 equiv. rel. to added CoCp_2), respectively (indicated). Conditions: $[3]_0 = 0.02 \text{ M}$, $[3]_0/[2]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

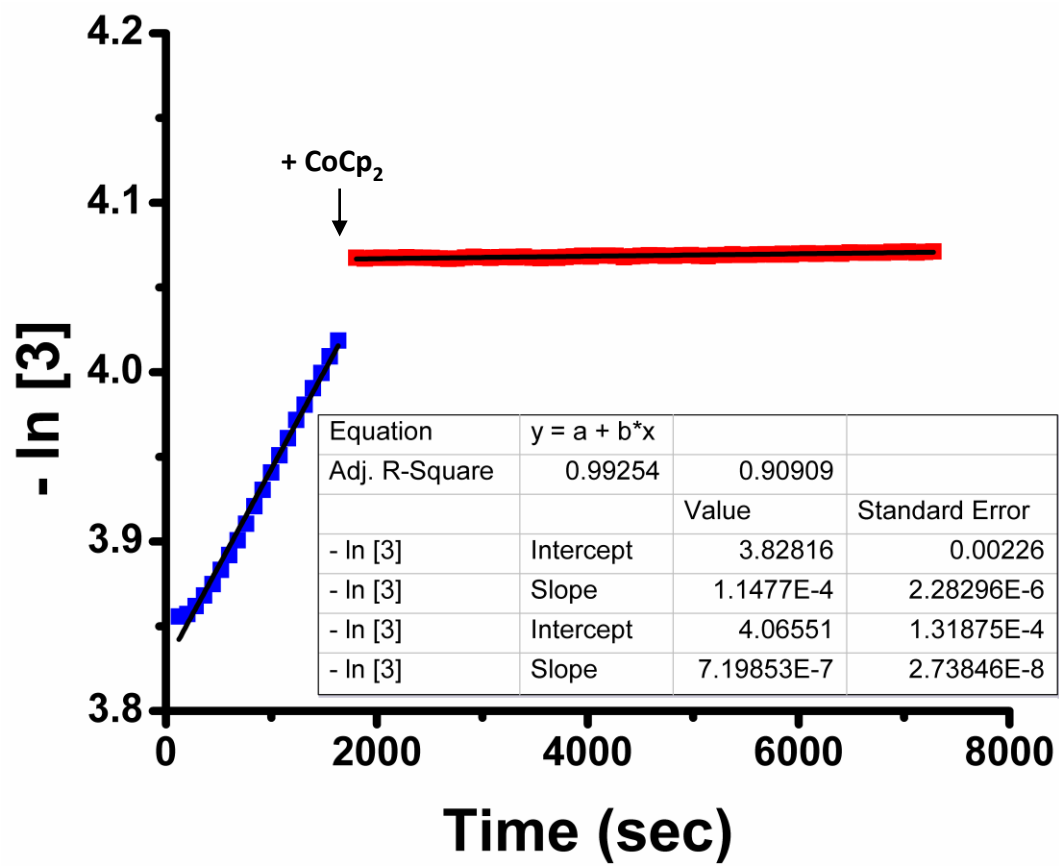


Figure S33. Plot of $-\ln [3]$ versus time using **2** (■) as the initiator followed by the reduction of the catalyst using CoCp_2 (1.5 equiv. rel. to **2**; indicated). Conditions: $[3]_0 = 0.02 \text{ M}$, $[3]_0/[2]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

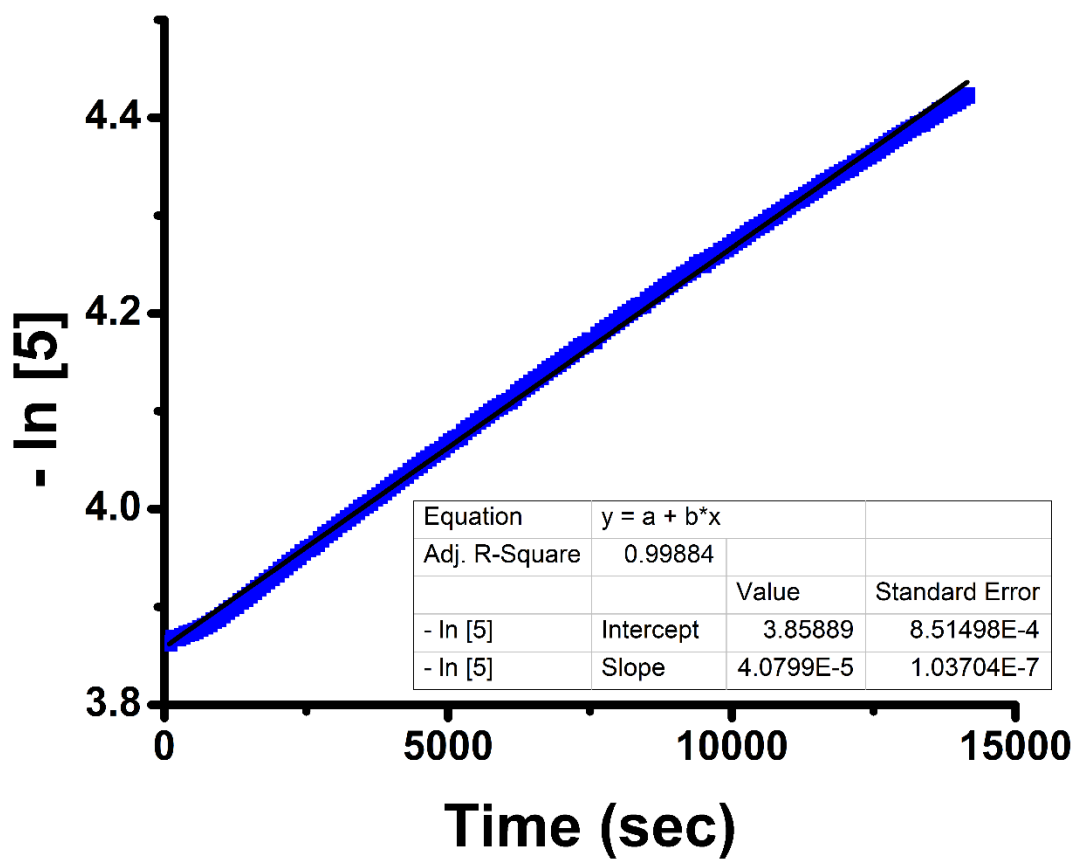


Figure S34. Plot of $-\ln [5]$ versus time using **2** (■) as the initiator. Conditions: $[5]_0 = 0.02$ M, $[5]_0/[2]_0 = 100$, 20 °C, 5:1 v/v C_6D_6/CD_2Cl_2 .

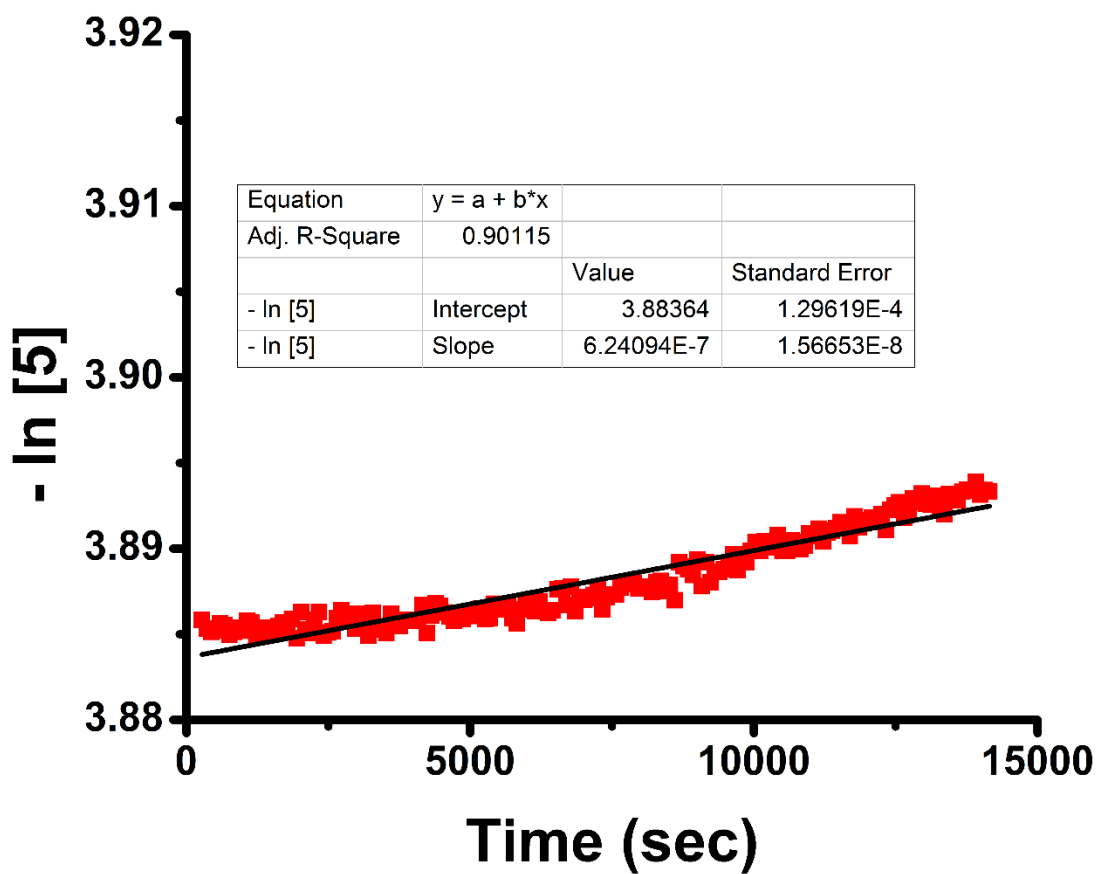


Figure S35. Plot of $-\ln [5]$ versus time using *in situ* generated 2_{red} (■) as the initiator. Conditions: $[5]_0 = 0.02 \text{ M}$, $[5]_0/[2_{\text{red}}]_0 = 100$, $20 \text{ }^\circ\text{C}$, 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

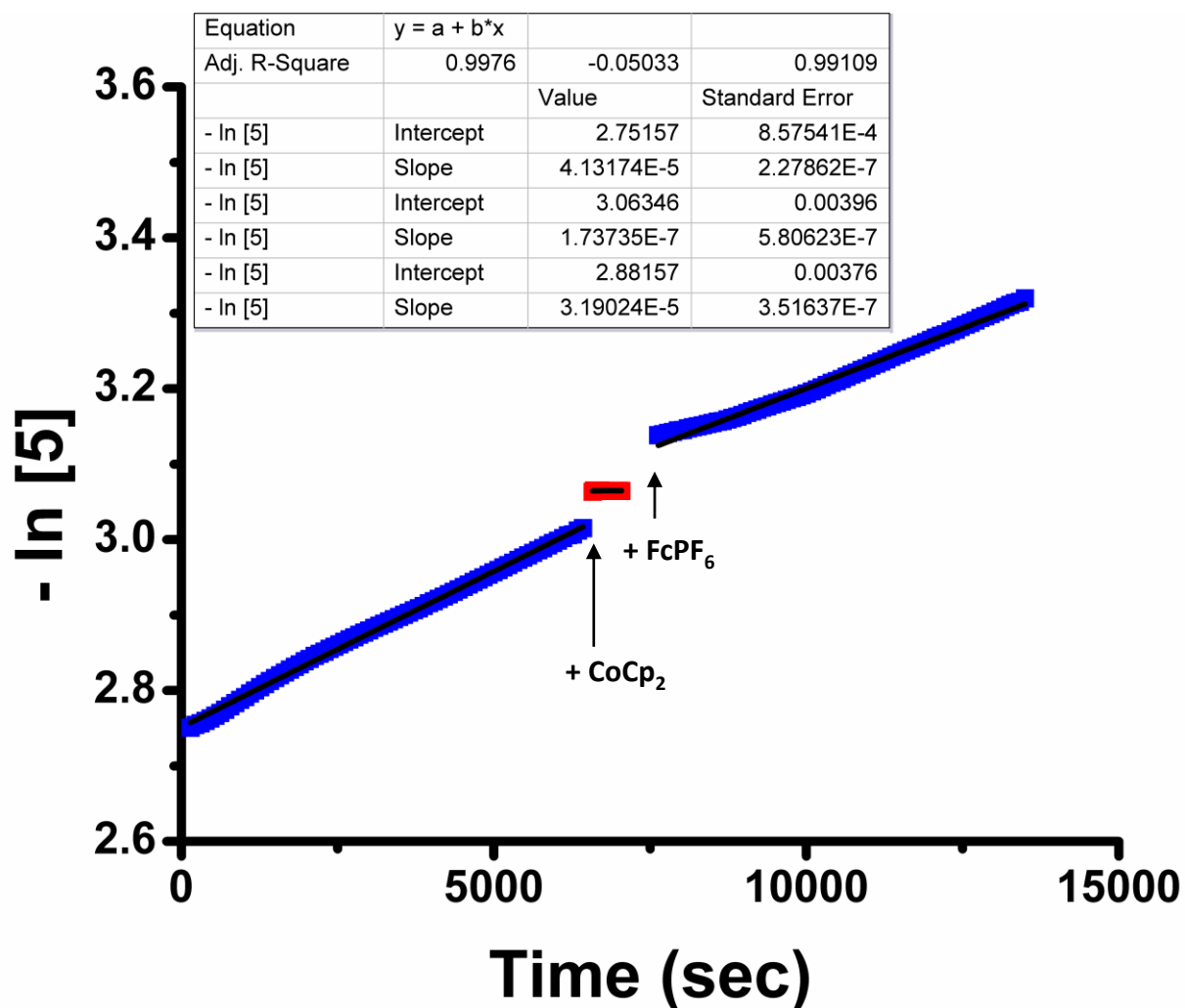


Figure S36. Plot of $-\ln [5]$ versus time using **2** (■) as the initiator followed by the reduction and re-oxidation of the catalyst using CoCp_2 (1.5 equiv. rel. to **2**) and FcPF_6 (1.5 equiv. rel. to added CoCp_2), respectively (indicated). Conditions: $[5]_0 = 0.06 \text{ M}$, $[5]_0/[2]_0 = 300$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

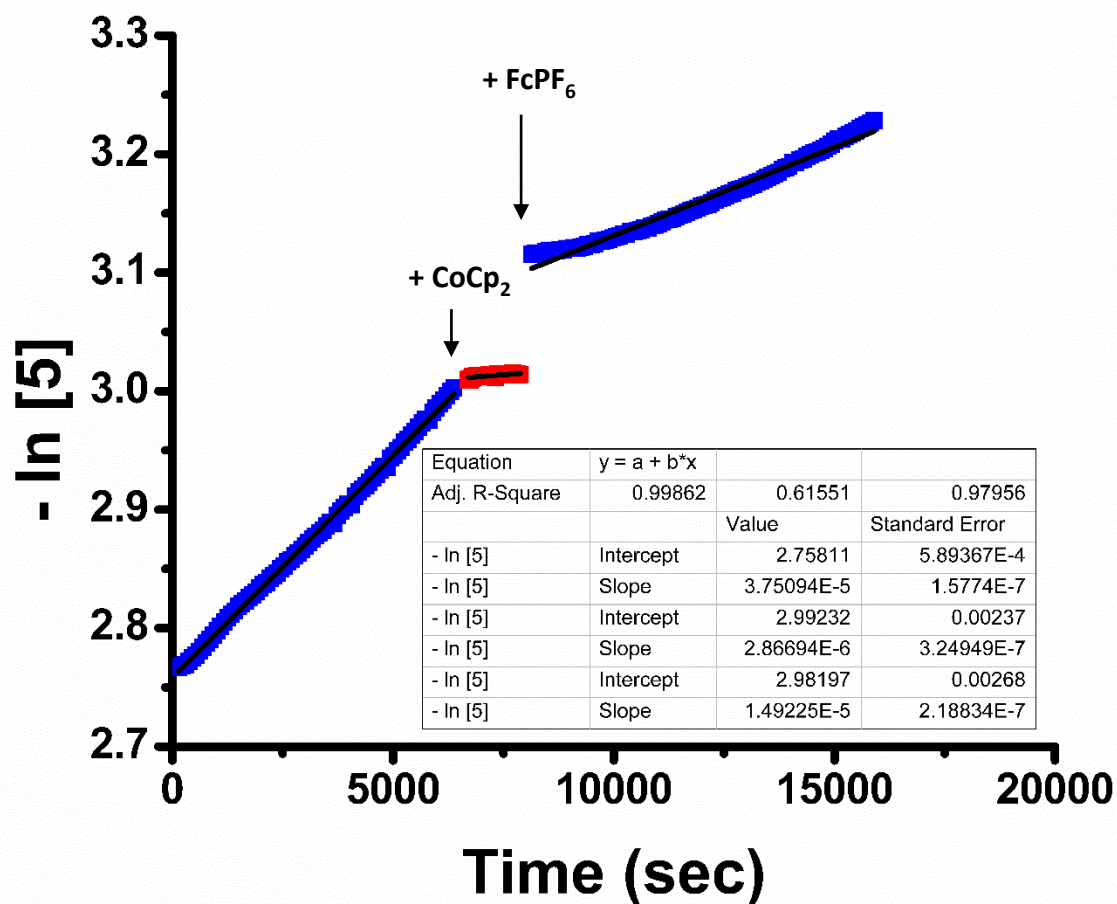


Figure S37. Plot of $-\ln [5]$ versus time using **2** (■) as the initiator followed by the reduction and re-oxidation of the catalyst using CoCp_2 (1.5 equiv. rel. to **2**) and FcPF_6 (1.5 equiv. rel. to added CoCp_2), respectively (indicated). Conditions: $[5]_0 = 0.06 \text{ M}$, $[5]_0/[2]_0 = 300$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

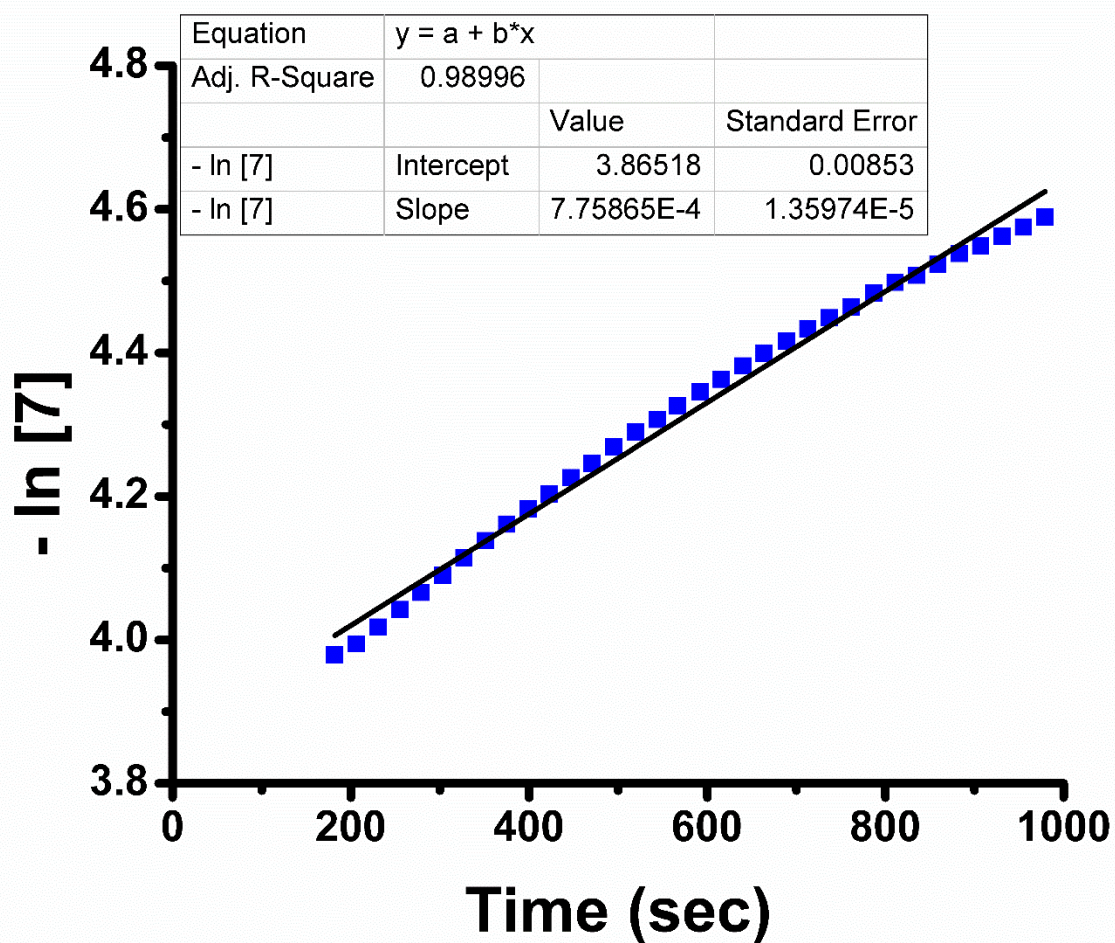


Figure S38. Plot of $-\ln [7]$ versus time using **2** (■) as the initiator. Conditions: $[7]_0 = 0.02$ M, $[7]_0/[2]_0 = 100$, 20 °C, 5:1 v/v C_6D_6/CD_2Cl_2 .

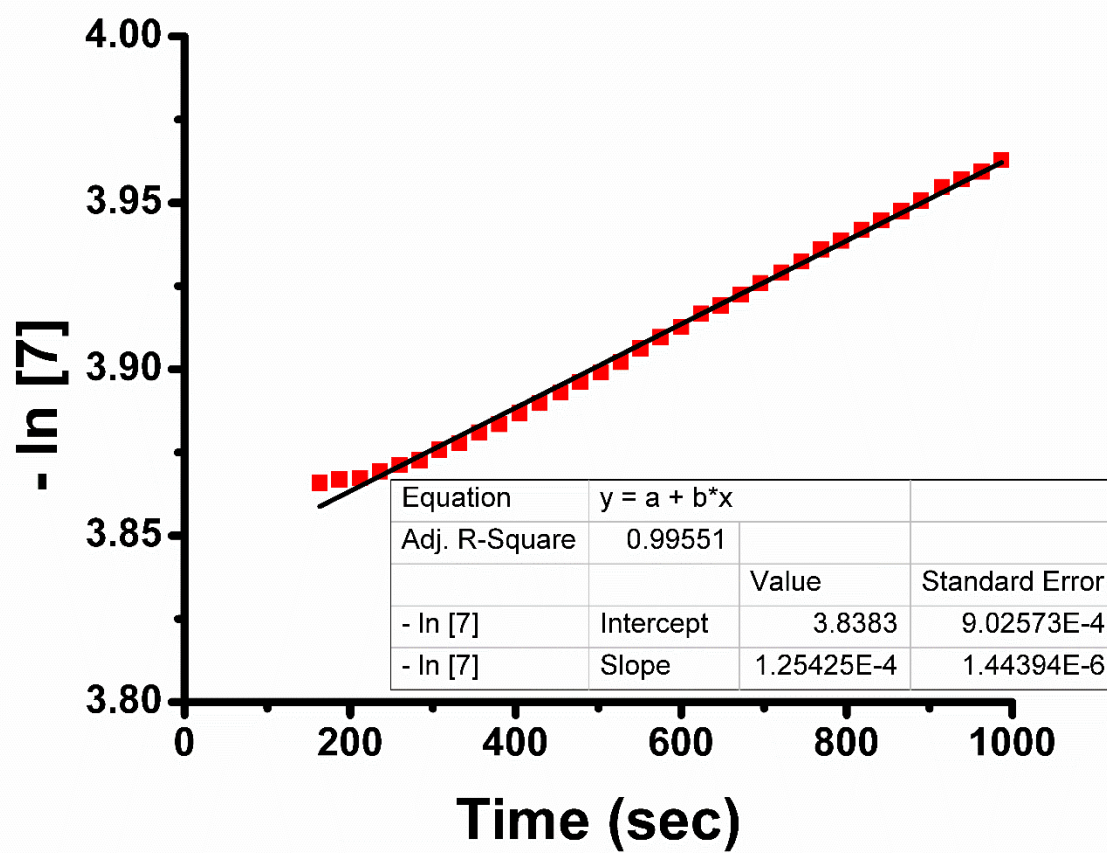


Figure S39. Plot of $-\ln [7]$ versus time using *in situ* generated 2_{red} (■) as the initiator. Conditions: $[7]_0 = 0.02$ M, $[7]_0/[2_{\text{red}}]_0 = 100$, 20 °C, 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

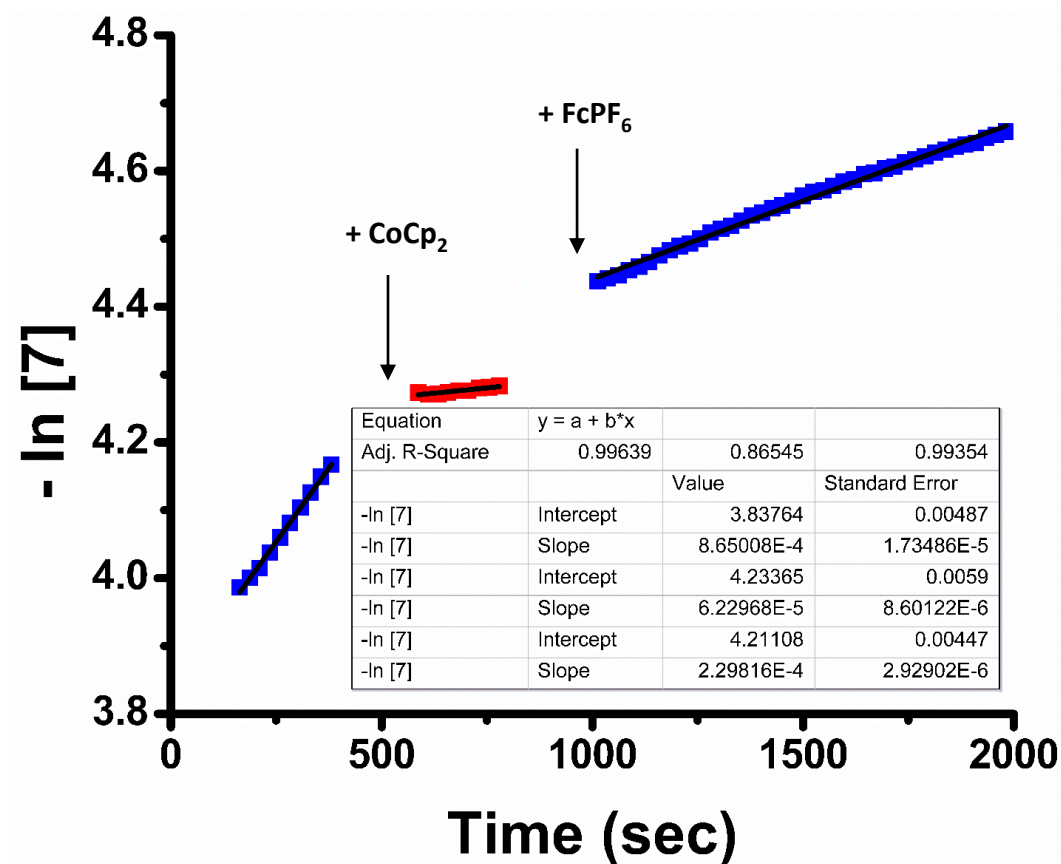


Figure S40. Plot of $-\ln [7]$ versus time using **2** (■) as the initiator followed by the reduction and re-oxidation of the catalyst using CoCp_2 (1.5 equiv. rel. to **2**) and FcPF_6 (1.5 equiv. rel. to added CoCp_2), respectively (indicated). Conditions: $[7]_0 = 0.02 \text{ M}$, $[7]_0/[2]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

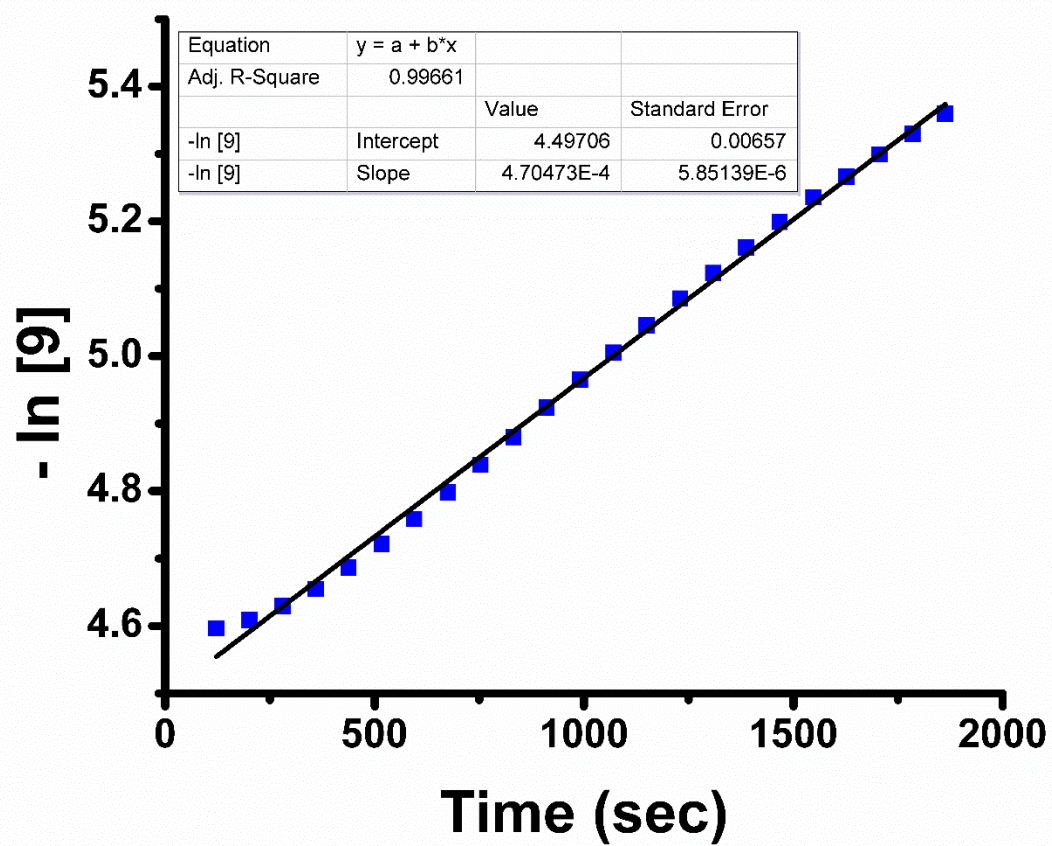


Figure S41. Plot of $-\ln [9]$ versus time using **2** (■) as the initiator. Conditions: $[9]_0 = 0.01$ M, $[9]_0/[2]_0 = 100$, 20 °C, 5:1 v/v C_6D_6/CD_2Cl_2 .

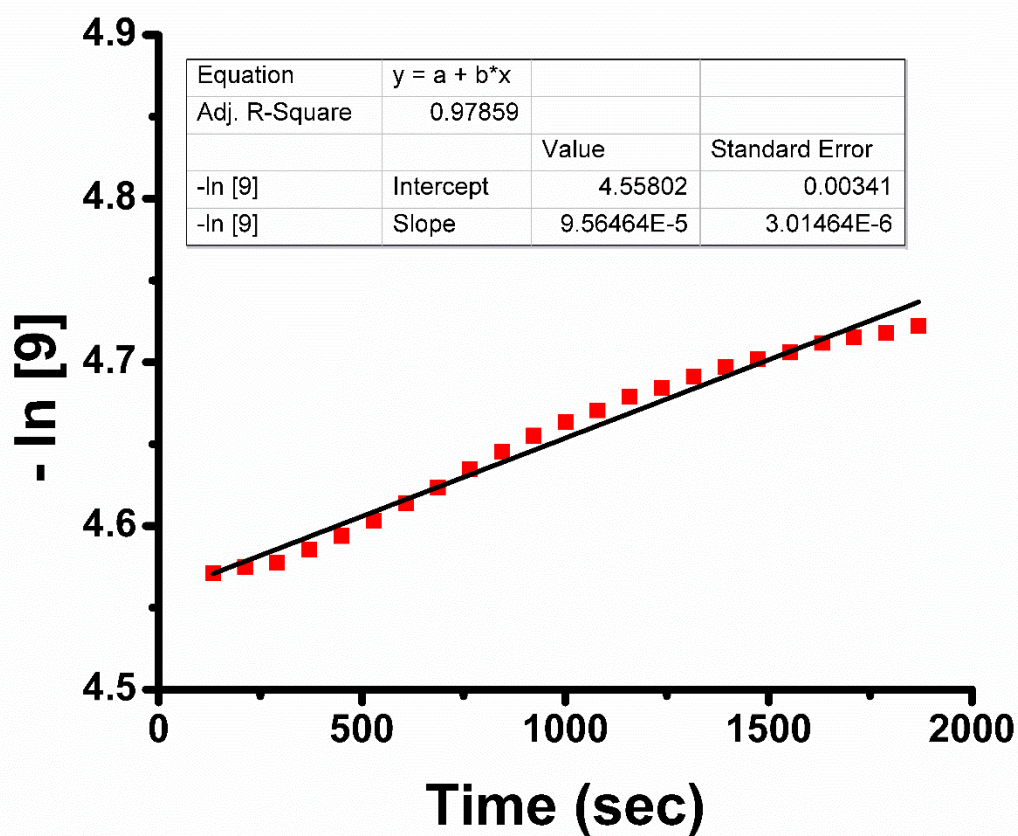


Figure S42. Plot of $-\ln [9]$ versus time using 2_{red} (■) as the initiator. Conditions: $[9]_0 = 0.01 \text{ M}$, $[9]_0/[2_{\text{red}}]_0 = 100$, 20°C , 5:1 v/v $\text{C}_6\text{D}_6/\text{CD}_2\text{Cl}_2$.

Table S2. ^1H NMR integration data for Figure S28 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
134	18215.739	325401.99
158	21351.203	322149.46
183	22001.618	320186.22
206	24657.182	317929.33
230	27163.74	315513.65
253	29424.83	312892.04
277	31815.586	310446.9
301	34089.128	308362.02
324	36301.389	306029.52
347	38441.18	303738.03
371	40563.067	301585.87
394	42626.657	299636.47
418	44603.478	297583.45
442	46568.006	295551.58
466	48456.929	293868.33
489	50217.158	291985.19
513	51984.577	290181.93
537	53655.607	288464.89
561	55317.567	286865.54
584	56824.121	285411.63
608	58395.625	283856.02
632	59913.204	282318.88
655	61470.33	280905.48
679	62804.263	279484.2
703	64429.054	277948.71
726	65640.839	276600.59
750	67069.176	275309.78
773	68343.832	273988.25
798	69762.337	272810.16
821	71000.025	271418.02
844	72203.948	270175.01
868	73379.857	269120.82
892	74723.682	267760.87
916	75897.386	266633.8
940	77071.009	265378.53
963	78173.836	264337.51
987	79370.871	263211.17
1010	80398.147	261929.11

1034	81580.128	260966.49
1058	82626.125	259796.67
1081	83663.464	258718.55
1105	84726.005	257575.74
1127	85786.741	256652.51
1151	86809.019	255612.96
1174	87812.011	254549.44
1197	88781.332	253530.59
1220	89857.952	252462.2
1244	91028.291	251283.9
1268	92096.943	250327.37
1291	93090.625	249187.88
1315	94180.733	248113.53
1338	95141.534	247155.5
1361	96271.31	246078.73
1385	97390.765	245062.25
1408	98237.843	244037.32
1432	99391.042	242934.83
1456	100409.42	241942.14
1479	101475.76	240963.49
1503	102402.71	239849.1
1526	103435.46	238853.29
1550	104320.29	237880.11
1573	105271.26	236913.5
1596	106343.92	235836.4
1620	107282.88	234823.03
1644	108248.53	233905.87
1668	109207.53	232920.09
1691	110130.85	231947.49
1715	111004.59	231065.93
1738	111923.63	230253.5
1762	112835.65	229280.88
1785	115648.82	225635.39
1808	114509.94	227464.13
1832	115399.57	226574.06
1856	116315.26	225687.49
1879	117089.01	224727.81
1903	117865.38	223987.8
1926	118780.5	223078.22
1950	119567.93	222260.36
1973	120386.16	221381.62

1997	121227.32	220601.85
2035	122813.38	219510.51

Table S3. ^1H NMR integration values for Figure S29 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
144	8860.194	325773.59
168	8107.373	327222.84
192	8961.971	326618.72
216	9645.312	327215.78
240	10246.186	327759.85
264	10859.202	327761.22
287	11341.911	327739.61
311	11849.167	327641.75
334	12267.003	327261.97
358	12661.287	326750.87
381	13083.519	326752.97
404	13388.246	326505.35
427	13748.566	326028.28
451	14068.351	325738.74
474	14348.071	325483.77
497	14686.972	325208.03
522	15018.375	324881.41
546	15275.258	324815.74
569	15562.786	324512.43
593	15830.279	324163.76
617	16135.807	323907.08
640	16433.253	323664.17
664	16664.451	323480.68
688	16894.678	323196.38
712	17177.304	322911.35
736	17430.56	322770.9
759	17684.14	322563.41
783	17924.82	322243.64
807	18087.278	322110.22
830	18392.551	321894.59
854	18665.618	321569.07
878	18879.165	321402.47
902	19119.029	321107.83
926	19351.197	321024.01
949	19499.934	320752.15

973	19787.3	320520.48
997	19995.393	320159.7
1020	20206.732	320171.65
1044	20402.069	319879.13
1068	20693.102	319724.69
1091	20850.903	319585.15
1115	21056.61	319318.27
1138	21277.814	319241.53
1162	21509.47	319069.12
1186	21673.945	318916.16
1209	21849.182	318608.35
1233	22081.358	318536.87
1258	22273.335	318199.29
1281	22458.455	317968.51
1305	22680.663	317991.47
1328	22867.281	317692.94
1352	23088.236	317710.51
1376	23234.627	317463.47
1400	23423.247	317203.07
1424	23677.477	317092.42
1448	23819.085	316858.51
1472	24053.052	316735.15
1496	24109.132	316415.02
1519	24333.831	316196.54
1542	24586.153	316226.57
1566	24692.636	315963.59
1589	24879.764	315889.55
1614	25073.185	315639.38
1638	25178.805	315508.38
1661	25404.371	315242.42
1684	25563.638	316338.11
1708	25678.554	314748.27
1732	25905.167	314767.05
1756	26033.765	314674.79
1780	26229.952	314608.23
1804	26370.334	314449.76
1828	26522.242	314191.3
1852	26736.618	314014.82
1875	26842.484	314082.14
1899	26940.794	313723.95
1922	27119.856	313512.15

1946	27322.658	313702.47
1970	27419.794	313535.25
1994	27691.188	313325.94
2018	27730.723	313019.9
2041	27950.319	312820.43

Table S4. ^1H NMR integration values for Figure S30 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
157	1057.04	65062.143
236	1255.925	64767.052
315	1696.197	64292.899
394	2211.857	63807.029
473	2848.465	63161.48
552	3557.489	62437.923
632	4277.053	61708.893
711	5018.139	60964.72
791	5787.401	60184.673
870	6473.384	59421.863
949	7214.768	58690.709
1027	7955.399	58014.185
1107	8653.069	57281.617
1185	9292.315	56524.872
1265	10121.225	55774.474
1344	10654.632	55196.5
1423	11298.694	54531.606
1501	12071.243	53823.114
1580	12553.542	53335.476
1658	13115.057	52748.04
1737	13694.737	52155.933
1816	14256.978	51576.932
1896	14853.449	50988.77
1975	15372.443	50468.346
2053	15907.438	49884.897
2132	16441.856	49371.406
2211	16950.828	48864.111
2290	17459.592	48361.858
2370	17942.3	47820.877
2448	18440.119	47340.838
2527	18869.757	46863.762
2606	19391.616	46398.734

2686	19938.232	45818.392
2765	20270.972	45496.632
2843	20723.033	45031.478
2922	21166.229	44632.357
3001	21601.18	44190.032
3080	21973.916	43743.382
3158	22419.153	43351.627
3237	22812.924	42878.581
3316	23222.861	42497.391
3395	23628.672	42132.72
3475	23985.1	41726.526
3554	24384.418	41356.521
3634	24741.451	40966.154
3713	25106.204	40606.778
3793	25435.382	40189.398
3872	25825.12	39838.679
3951	26150.801	39517.693
4030	26540.638	39027.044
4108	26830.77	38785.438
4187	27131.991	38490.291
4266	27451.54	38141.294
4345	27797.465	37831.368
4424	28098.972	37515.077
4503	28393.992	37207.149
4582	28727.575	36917.779
4661	28985.969	36596.77
4740	29301.992	36298.973
4819	29582.426	35984.603
4844	29775.321	35800.032
4924	30013.684	35515.181
5003	30333.333	35207.717
5081	30551.391	34928.956
5160	30847.101	34661.623
5239	31138.042	34392.435
5318	31357.085	34116.702
5396	31627.984	33865.776
5476	31913.53	33583.124
5554	32139.755	33326.214
5633	32366.359	33076.948
5712	32603.691	32828.916
5791	32872.283	32563.39

5870	33104.558	32333.194
5948	33361.488	32103.511
6027	33575.543	31876.149
6106	33801.443	31639.803
6185	33981.906	31398.264
6264	34269.837	31167.681
6343	34471.905	30905.215
6422	34664.923	30698.594
6501	34872.549	30542.573
6580	35077.054	30266.043
6658	35277.301	30073.374
6738	35516.203	29857.573
6817	35698.469	29643.189
6896	35895.177	29425.015
6974	36111.008	29262.934
7052	36269.201	29038.973
7131	36462.053	28883.873

Table S5. ^1H NMR integration values for Figure S31 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
148	310.091	45307.099
227	297.742	45213.187
307	305.938	45128.404
386	314.359	45109.647
464	304.124	45045.999
543	281.988	45021.65
622	313.223	45026.026
701	318.767	45104.065
780	325.186	45198.262
859	313.198	45283.679
938	326.822	45281.143
1017	330.21	45283.827
1097	342.949	45300.169
1176	350.516	45227.176
1255	354.359	45220.455
1334	362.194	45184.521
1412	360.825	45136.652
1492	381.467	45071.333
1571	393.259	45017.528
1650	403.602	44914.422

1729	414.245	44831.296
1807	436.865	44908.697
1886	461.582	44982.854
1965	467.032	45032.216
2044	491.308	45078.331
2123	500.234	45070.327
2201	537.056	45094.642
2280	554.45	45071.327
2359	573.617	45002.796
2438	598.577	44956.422
2517	617.775	44874.303
2596	641.916	44840.235
2674	674.782	44788.318
2753	710.319	44675.586
2832	740.261	44610.406
2911	769.811	44539.28
2989	794.39	44476.951
3068	819.408	44434.885
3146	851.882	44426.75
3225	895.163	44508.628
3304	924.712	44558.251
3383	954.368	44577.152
3462	1006.356	44579.449
3540	1041.01	44543.221
3619	1068.372	44480.174
3698	1078.893	44421.592
3777	1100.568	44381.984
3856	1158.313	44340.197
3934	1189.785	44249.179
4014	1221.63	44170.018
4092	1249.024	44067.533
4171	1277.865	44051.721
4250	1322.515	43892.651
4329	1339.925	43891.967
4408	1373.201	43846.163
4487	1391.491	43850.558
4566	1404.892	43881.18
4646	1443.853	43950.551
4724	1457.19	44005.535
4803	1493.064	44033.099
4882	1516.867	44067.71

4961	1549.077	44017.722
5040	1576.356	43987.894
5119	1579.327	43930.23
5198	1617.585	43893.7
5277	1614.798	43833.425
5357	1638.606	43785.835
5436	1670.946	43700.524
5515	1682.731	43597.9
5594	1722.47	43546.224
5674	1739.327	43505.984
5753	1736.521	43475.608
5830	1765.284	43540.703
5909	1781.78	43600.403
5988	1783.007	43694.484
6067	1804.912	43708.929
6145	1836.702	43722.703
6224	1862.501	43704.925
6303	1870.238	43668.558
6381	1874.435	43626.598
6460	1889.443	43597.58
6538	1921.762	43539.333
6617	1925.981	43481.54
6696	1943.861	43429.984
6775	1938.741	43404.811
6853	1950.915	43344.952
6931	1962.524	43292.587
7010	1978.5	43225.941
7089	2010.118	43190.644
7168	2017.275	43147.204

Table S6. ^1H NMR integration values for Figure S32 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
107	272.825	47339.87
187	345.154	47175.961
266	566.086	46798.131
346	818.325	46525.13
426	1137.666	46332.925
505	1539.066	45693.682
583	1822.641	45699.516
663	2276.892	45301.946

742	2748.743	44948.871
822	3301.581	43951.632
901	3686.895	44139.88
981	4235.63	43115.57
1060	4590.949	43262.733
1140	5080.145	42164.609
1219	5469.33	42048.265
1298	5937.284	41225.706
1377	6359.786	40645.215
1456	6872.474	39930.058
1535	7226.435	39911.09
1614	7676.025	39808.957
+ CoCp ₂		
1733	7668.779	37921.997
1813	7659.057	37845.943
1892	7675.171	37855.618
1971	7677.509	37816.418
2050	7678.221	37802.743
2130	7670.316	37587.217
2210	7653.248	37905.267
2289	7644.371	37643.419
2369	7645.882	37600.24
2447	7621.786	37408.59
+ FcPF ₆		
2583	6853.541	34148.336
2663	6944.449	34246.138
2743	6949.924	34271.995
2822	7075.172	34440.808
2902	7097.985	34435.516
2981	7157.326	34528.573
3060	7118.295	34499.255
3139	7225.491	34442.204
3218	7168.169	34369.116
3298	7430.29	34177.058
3377	7322.93	34230.076
3457	7467.36	34120.29
3536	7518.406	33922.981
3615	7390.354	33973.017
3773	7504.841	33931.149
3853	7550.451	33963.576
3932	7647.731	34023.23

4012	7647.481	34005.89
4092	7733.321	33931.139
4171	7820.916	33910.175
4251	7820.948	33757.802
4330	7928.531	33739.267
4409	8001.531	33634.089
4488	8055.775	33566.924
4568	8072.802	33332.84
4648	8262.151	33246.94
4726	8240.108	33241.654
4806	8274.759	33147.893
4886	8298.621	33125.106
4965	8388.981	33168.467
5044	8708.755	33128.017
5123	8709.455	33134.069
5202	8724.147	32974.748
5281	8831.235	32980.708
5361	8842.75	32838.145
5440	8947.005	32767.816
5519	9002.448	32605.315
5598	9061.448	32470.669
5677	9181.177	32401.796
5757	9212.488	32245.256
5835	9344.786	32063.614
5914	9352.257	32150.696
5993	9497.422	31978.035
6072	9561.796	31906.203
6152	9681.12	31891.119
6232	9851.252	31891.962
6311	9969.502	31776.453
6391	9958.714	31718.253
6470	10068.61	31674.223
6549	10188.8	31516.196
6629	10280.711	31383.743
6708	10369.622	31291.117
6787	10567.989	31047.282
6866	10471.569	31042.159
6945	10644.639	30896.334
7024	10686.03	30611.221
7103	10818.097	30657.061
7182	10894.621	30611.529

7261	11041.622	30583.921
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Table S7. ¹H NMR integration values for Figure S33 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
123	1115.833	72015.049
203	1213.543	71475.963
282	1548.881	71072.349
362	1993.16	70667.541
442	2460.506	70138.194
521	3051.428	69607.589
600	3654.426	68968.317
680	4253.253	68319.647
760	4912.483	67622.633
839	5609.987	66911.748
918	6250.65	66218.906
998	6923.316	65541.144
1077	7582.715	64868.468
1156	8226.368	64194.663
1236	8939.134	63664.574
1315	9486.439	62963.903
1395	10095.552	62303.533
1474	10643.428	61678.426
1554	11258.748	61194.39
1633	11810.513	60542.959
+ CoCp ₂		
1805	11987.483	58561.116
1885	11951.34	58521.555
1964	11981.731	58558.381
2043	11984.199	58507.808
2122	11977.122	58533.076
2202	11987.079	58543.132
2281	12008.495	58527.501
2360	11988.018	58526.679
2439	11976.667	58506.259
2519	11978.834	58532.957
2598	11954.321	58494.391
2678	11931.482	58518.81
2757	11949.85	58503.878
2838	11984.19	58478.193
2918	12006.213	58460.284

2998	11996.222	58461.933
3077	11964.794	58487.311
3157	11989.985	58430.413
3236	11992.141	58408.815
3315	11981.295	58449.166
3394	12014.796	58435.575
3473	11967.221	58449.874
3552	11958.63	58480.46
3632	11979.533	58419.808
3711	11965.778	58488.659
3790	11997.592	58456.005
3869	12022.837	58433.61
3948	12039.977	58401.373
4028	12007.295	58397.905
4107	12047.127	58425.261
4186	12047.372	58425.831
4265	12034.634	58373.1
4344	11974.06	58355.697
4424	12010.333	58394.058
4503	12039.594	58394.592
4582	12058.251	58394.649
4661	12051.432	58396.864
4740	12040.84	58402.993
4819	12032.188	58390.511
4898	12061.971	58394.116
4977	12063.101	58385.193
5056	12030.989	58359.155
5136	12021.88	58390.888
5214	12059.354	58354.003
5293	12057.765	58334.835
5372	12084.541	58325.158
5451	12056.565	58315.652
5530	12063.643	58336.154
5609	12078.117	58306.282
5688	12079.801	58302.115
5768	12066.737	58285.278
5847	12099.31	58283.198
5926	12064.861	58246.758
6006	12107.882	58282.119
6086	12116.246	58284.029
6165	12089.198	58257.69

6244	12098.24	58233.98
6324	12117.2	58283.258
6404	12090.284	58219.199
6484	12132.419	58180.674
6563	12134.046	58195.557
6642	12125.632	58213.738
6722	12129.392	58172.388
6802	12126.237	58208.387
6881	12156.649	58153.042
6960	12142.892	58180.637
7040	12174.441	58178.044
7120	12128.322	58173.057
7199	12144.904	58146.793
7279	12178.119	58188.992

Table S8. ^1H NMR integration values for Figure S34 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 5	Integral Value of 6
84	52248.658	1185.036
163	52306.635	1453.446
242	52280.923	1474.271
320	52202.468	1545.624
399	52034.556	1679.312
477	52016.359	1765.691
556	51931.991	1862.677
635	51805.826	1987.619
714	51690.142	2096.273
793	51511.496	2229.623
872	51387.797	2385.8
950	51235.14	2485.578
1028	51070.513	2687.905
1107	50885.703	2868.359
1186	50742.219	3038.53
1265	50567.016	3162.232
1344	50386.916	3403.452
1423	50214.613	3537.519
1502	50037.012	3724.39
1581	49874.765	3883.802
1660	49625.078	4077.372
1738	49534.918	4255.804
1817	49319.579	4429.496

1895	49159.191	4602.037
1974	48983.296	4752.86
2053	48736.693	4973.315
2132	48699.13	5144.721
2211	48404.994	5325.941
2290	48261.122	5474.816
2369	48086.262	5636.675
2448	47857.245	5831.465
2527	47687.495	6005.186
2606	47558.959	6107.138
2685	47398.251	6275.961
2764	47212.712	6465.695
2843	47037.295	6699.417
2921	46916.949	6818.022
3000	46707.075	6959.499
3079	46578.142	7173.914
3158	46407.941	7303.784
3237	46245.141	7475.991
3315	46070.864	7626.199
3394	45872.635	7780.774
3473	45695.192	7971.32
3552	45547.161	8097.754
3631	45425.683	8207.424
3711	45248.314	8423.357
3789	45135.101	8543.204
3868	44915.001	8689.747
3947	44783.923	8868.261
4026	44610.322	9004.076
4106	44496.443	9155.4
4184	44321.719	9309.206
4263	44177.157	9426.887
4342	44004.58	9640.737
4421	43826.218	9776.451
4501	43713.366	9939.118
4580	43501.132	10089.099
4659	43374.253	10195.771
4738	43237.885	10373.075
4817	43099.197	10504.39
4896	42968.985	10599.805
4975	42798.912	10812.023
5054	42634.808	10935.565

5133	42538.077	11067.917
5212	42311.195	11078.107
5291	42225.802	11351.329
5370	42050.449	11522.504
5449	41991.342	11629.886
5528	41760.547	11793.34
5606	41638.463	11937.126
5686	41514.644	12059.283
5764	41391.874	12218.294
5843	41251.377	12362.428
5922	41166.171	12451.807
6001	40955.55	12574.307
6080	40818.648	12647.973
6160	40671.239	12778.612
6239	40531.483	13013.985
6318	40402.181	13167.413
6396	40249.684	13276.437
6476	40106.905	13389.46
6554	39995.885	13551.598
6632	39855.897	13666.89
6711	39697.252	13844.813
6790	39559.491	13971.832
6868	39417.51	14067.878
6947	39308.633	14183.384
7026	39144.945	14311.741
7105	38983.313	14451.156
7183	38923.989	14553.707
7263	38771.513	14731.182
7342	38633.348	14876.519
7421	38503.853	14943.19
7500	38369.867	15091.217
7578	38274.412	15017.806
7657	38141.001	15303.141
7736	37991.815	15453.183
7815	37881.911	15595.227
7893	37768.951	15678.067
7973	37598.461	15812.634
8052	37516.331	15954.088
8131	37373.84	16081.32
8210	37255.264	16190.68
8289	37124.16	16300.079

8368	37028.11	16405.394
8447	36942.51	16439.205
8526	36843.47	16657.838
8605	36628.938	16750.251
8684	36530.648	16871.1
8763	36424.686	17018.633
8842	36304.56	17135.655
8920	36210.292	17236.969
9000	36046.348	17348.607
9079	35965.53	17436.39
9157	35837.994	17553.726
9236	35734.803	17647.663
9315	35629.708	17771.499
9394	35479.784	17915.07
9473	35407.272	18026.439
9499	35334.119	17865.823
9578	35284.303	18053.702
9657	35155.504	18198.944
9736	35075.676	18254.906
9815	34938.423	18400.319
9894	34847.983	18476.73
9973	34743.36	18601.934
10052	34568.836	18692.677
10131	34493.271	18798.42
10210	34458.332	18919.632
10289	34299.543	19009.578
10368	34167.508	19126.021
10447	34072.619	19212.576
10526	33951.72	19310.656
10605	33881.752	19415.179
10683	33747.751	19538.601
10761	33678.068	19609.752
10840	33586.636	19733.252
10919	33481.256	19847.896
10998	33386.049	19941.99
11076	33279.772	20081.051
11155	33177.067	20156.839
11234	33133.912	20226.88
11312	32952.543	20330.832
11391	32906.843	20431.881
11469	32857.85	20551.158

11548	32694.116	20625.653
11626	32591.119	20738.824
11705	32531.299	20796.854
11783	32371.896	20905.613
11863	32302.045	21017.653
11942	32186.548	21068.765
12021	32134.032	21178.236
12100	32058.256	21237.022
12179	31912.984	21356.827
12259	31868.875	21448.871
12337	31754.422	21550.181
12416	31667.349	21594.35
12494	31588.404	21695.92
12573	31512.44	21814.712
12651	31382.552	21904.621
12729	31296.521	21985.698
12808	31194.08	22096.162
12887	31115.029	22193.478
12965	31009.042	22261.958
13044	30938.022	22336.046
13122	30843.908	22445.323
13201	30778.197	22534.702
13280	30680.629	22627.923
13359	30612.969	22650.937
13438	30509.454	22726.652
13516	30409.604	22835.337
13595	30349.923	22930.337
13674	30192.932	23036.236
13753	30132.413	23105.7
13832	30067.755	23171.068
13911	30010.363	23249.335
13990	29938.403	23335.826
14068	29826.037	23432.081
14148	29750.432	23499.516
7279	12178.119	58188.992

Table S9. ^1H NMR integration values for Figure S35 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 5	Integral Value of 6
278	36211.954	1682.895
360	36231.608	1664.183

440	36231.295	1657.52
519	36235.921	1660.97
598	36175.938	1673.344
677	36155.214	1669.427
756	36134.97	1646.744
836	36086.089	1650.793
915	36064.508	1659.273
994	36046.304	1651.484
1073	36018.607	1672.597
1152	36037.827	1669.752
1232	36151.189	1646.95
1311	36179.662	1651.362
1391	36311.734	1670.595
1470	36383.323	1672.569
1549	36324.497	1659.972
1628	36307.869	1674.125
1707	36287.975	1681.381
1786	36266.929	1663.218
1865	36257.701	1686.243
1944	36174.725	1640.605
2023	36184.578	1699.526
2102	36109.495	1656.567
2181	36065.646	1646.532
2260	36033.442	1675.564
2339	36019.031	1690.968
2418	36075.069	1641.947
2498	36216.763	1655.061
2577	36265.191	1659.837
2656	36347.865	1692.82
2735	36297.827	1708.018
2815	36279.933	1699.705
2893	36301.234	1686.168
2973	36227.191	1664.741
3051	36160.888	1694.582
3131	36150.992	1679.442
3210	36059.5	1640.628
3289	36060.802	1691.309
3368	36018.437	1652.026
3448	35999.37	1652.292
3527	36000.036	1644.351
3605	36047.789	1688.839

3685	36181.745	1674.079
3765	36207.323	1669.004
3843	36176.494	1681.897
3923	36228.202	1683.714
4002	36189.492	1679.886
4081	36310.432	1688.226
4160	36253.799	1718.197
4239	36258.582	1655.777
4319	36138.88	1689.349
4398	36044.624	1711.434
4478	36120.575	1710.265
4557	36011.064	1690.051
4636	35997.354	1680.479
4716	35979.969	1669.986
4795	36084.083	1683.983
4874	36153.121	1682.992
4953	36180.015	1697.715
5033	36259.257	1693.914
5112	36217.235	1699.492
5192	36219.982	1709.005
5271	36263.168	1686.594
5351	36128.473	1682.464
5430	36199.4	1718.389
5509	36133.567	1710.841
5589	36150.71	1703.957
5668	36007.19	1707.912
5747	35998.345	1677.341
5827	36005.952	1665.397
5906	35940.18	1692.58
5986	36020.171	1712.644
6065	36056.516	1701.883
6144	36203.638	1701.998
6224	36233.075	1725.328
6383	36249.6	1700.248
6462	36245.448	1705.306
6542	36195.001	1750.43
6621	36185.719	1751.136
6701	36146.66	1713.665
6780	36129.878	1752.878
6859	35983.322	1692.063
6938	35983.374	1722.638

7017	35968.69	1715.285
7096	35994.861	1721.507
7176	36018.882	1729.021
7255	36060.819	1748.265
7334	36096.31	1700.787
7413	36085.77	1727.648
7493	36295.767	1743.764
7572	36253.467	1741.556
7651	36182.092	1753.331
7731	36246.365	1763.845
7811	36197.787	1764.764
7890	36150.713	1762.101
7970	36059.05	1744.919
8049	35918.784	1742.207
8129	35955.255	1743.277
8208	35912.512	1729.678
8287	35918.139	1752.807
8367	35947.609	1756.48
8447	35954.126	1734.849
8526	36148.684	1757.378
8606	36116.047	1721.826
8685	36152.827	1807.161
8765	36171.023	1799.994
8845	36109.184	1790.088
8924	36116.864	1777.816
9004	36164.172	1813.957
9083	36034.358	1749.183
9162	36047.634	1803.41
9241	35974.327	1754.489
9320	35969.054	1777.487
9399	35903.98	1773.574
9478	35837.648	1776.893
9557	35960.498	1793.115
9637	35955.485	1815.918
9716	36007.813	1782.682
9796	36083.458	1821.409
9875	36126.994	1806.121
9954	36136.905	1832.875
10033	36141.226	1852.504
10112	36113.856	1831.371
10191	36052.724	1848.927

10271	35966.237	1838.615
10350	36033.313	1834.082
10429	35934.543	1857.154
10507	35848.848	1816.798
10586	35777.359	1814.413
10665	35773.878	1836.167
10744	35852.074	1836.835
10823	35807.279	1819.01
10903	35921.038	1832.864
10982	35981.066	1863.486
11061	36086.924	1861.569
11141	36051.742	1877.053
11220	36088.603	1850.014
11299	36026.938	1867.887
11378	36003.148	1870.236
11457	36008.592	1876.316
11537	35952.549	1885.901
11616	35859.899	1875.514
11695	35829.981	1849.19
11774	35825.457	1892.319
11853	35770.214	1865.927
11933	35780.337	1874.693
12013	35862.85	1885.148
12092	35903.819	1893.815
12171	36031.831	1891.121
12251	35960.071	1904.622
12330	35991.789	1872.06
12410	36004.081	1916.093
12489	36044.989	1927.533
12568	35973.564	1931.295
12648	35926.699	1894.722
12727	35789.41	1899.963
12806	35791.826	1929.876
12886	35763.056	1921.246
12965	35763.907	1939.239
13044	35649.192	1911.046
13123	35708.673	1911.709
13203	35754.451	1933.544
13282	35835.286	1912.014
13361	35867.317	1899.944
13441	36017.637	1951.572

13520	35976.778	1942.11
13599	35990.929	1936.159
13678	35931.06	1952.256
13757	35920.232	1956.605
13837	35921.149	1954.322
13916	35848.779	1969.743
13995	35872.332	1942.797
14074	35791.448	1948.295
14153	35731.297	1941.725

Table S10. ^1H NMR integration values for Figure S36 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 5	Integral Value of 6
147	72155.027	645.837
227	71713.922	900.979
307	71565.945	1065.451
386	71466.468	1280.752
465	71312.205	1510.761
544	71132.132	1771.74
624	70839.992	2044.375
703	70544.176	2336.678
782	70116.63	2648.742
862	69790.311	2948.048
942	69351.342	3235.018
1021	69019.419	3500.629
1101	68569.481	3816.034
1180	68122.925	4087.285
1260	67678.468	4354.846
1340	67364.41	4657.418
1419	67063.381	4920.981
1499	66730.399	5180.208
1578	66531.556	5430.398
1658	66378.029	5678.452
1737	66271.068	5941.016
1816	66052.997	6188.409
1896	65823.495	6405.663
1975	65475.241	6666.234
2054	65204.353	6863.161
2134	64917.33	7104
2213	64694.183	7285.421
2292	64346.252	7458.557

2372	64019.928	7688.287
2451	63729.445	7853.235
2530	63477.149	8050.552
2609	63150.281	8252.699
2688	62902.559	8432.007
2768	62755.991	8616.687
2847	62621.695	8836.863
2927	62535.77	9027.082
3006	62344.906	9204.733
3086	62253.495	9433.079
3166	62034.63	9617.334
3245	61850.609	9787.196
3324	61605.934	9942.48
3403	61363.046	10120.214
3483	61121.884	10296.21
3563	60820.447	10445.595
3642	60580.793	10600.094
3722	60338.696	10776.225
3801	60037.145	10921.882
3880	59817.93	11097.162
3960	59602.227	11306.392
4039	59450.262	11477.09
4119	59382.992	11680.873
4199	59335.443	11898.823
4278	59194.349	12086.428
4358	59005.663	12271.357
4438	58789.402	12451.335
4518	58563.485	12636.093
4597	58324.041	12800.507
4676	58084.01	12990.717
4757	57809.156	13167.406
4836	57513.284	13309.762
4916	57242.118	13481.937
4995	57001.498	13659.627
5075	56675.971	13803.717
5154	56479.011	13979.575
5233	56266.836	14164.132
5312	56113.19	14339.79
5392	55993.925	14557.869
5471	55904.96	14755.167
5551	55801.571	14944.359

5630	55605.755	15119.728
5710	55404.692	15314.094
5790	55188.673	15452.925
5869	54933.47	15642.778
5948	54707.147	15798.072
6028	54475.532	15957.555
6108	54217.333	16112.684
6187	53886.257	16264.161
6266	54181.165	16448.178
6346	53427.726	16571.919
6426	53227.064	16721.842
+ CoCp ₂		
6582	51655.079	16747.601
6607	51059.091	16667.073
6631	51092.442	16658.439
6656	51105.039	16653.641
6680	51090.569	16673.141
6704	51171.489	16701.681
6728	51248.05	16677.7
6752	51167.268	16670.828
6776	51169.433	16673.962
6800	51273.526	16691.912
6824	51224.254	16708.283
6849	51275.587	16715.389
6873	51254.082	16685.425
6897	51211.151	16703.056
6921	51208.737	16684.991
6946	51261.92	16699.891
6970	51291.689	16710.088
6994	51294.666	16712.789
7018	51219.415	16684.082
7042	51246.518	16696.074
+ FcPF ₆		
7629	46623.562	14994.092
7708	46616.089	15055.949
7787	46636.109	15177.428
7867	46687.497	15275.523
7947	46685.403	15390.545
8026	46698.773	15439.432
8105	46614.957	15549.249
8185	46543.895	15608.475

8264	46460.7	15651.91
8344	46354.41	15714.123
8423	46208.277	15772.081
8502	46070.346	15812.554
8581	45916.791	15851.333
8660	45803.147	15874.936
8739	45652.279	15949.271
8819	45500.815	16005.571
8898	45451.73	16096.007
8977	45415.114	16234.69
9057	45369.312	16385.425
9136	45341.93	16503.028
9215	45317.331	16633.386
9295	45209.648	16751.674
9374	45141.279	16823.544
9453	44987.746	16924.784
9533	44863.899	17008.213
9612	44743.617	17081.029
9691	44561.151	17145.737
9770	44397.847	17217.932
9850	44217.307	17254.44
9929	44068.151	17328.867
10009	43919.794	17410.622
10089	43809.584	17534.404
10168	43725.705	17671.654
10248	43692.233	17829.887
10327	43631.281	17985.822
10407	43569.244	18143.19
10486	43475.951	18239.324
10565	43351.408	18357.256
10646	43216.736	18507.665
10725	43196.236	18667.839
10805	43111.288	18796.74
10884	43049.541	18976.909
10964	43067.375	19113.828
11043	42942.451	19281.366
11122	42853.119	19410.693
11201	42771.029	19537.612
11281	42658.462	19679.961
11360	42501.518	19804.994
11439	42396.238	19923.314

11518	42273.817	20056.088
11598	42150.37	20168.047
11677	42017.085	20275.595
11756	41913.149	20368.306
11835	41762.242	20471.821
11915	41631.097	20600.023
11994	41493.079	20711.001
12073	41380.273	20844.444
12152	41235.745	20931.441
12231	41150.067	21017.45
12311	40960.801	21156.006
12391	40881.219	21255.689
12469	40674.691	21370.275
12549	40558.315	21484.531
12628	40465.17	21596.595
12708	40330.392	21707.132
12787	40155.234	21835.291
12866	40030.305	21906.443
12946	39888.704	22011.683
13025	39777.303	22135.294
13104	39672.593	22243.01
13183	39495.973	22360.968
13263	39383.785	22483.646
13343	39295.374	22578.081
13422	39326.089	22693.257
13501	39040.509	22795.726

Table S11. ^1H NMR integration values for Figure S37 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 5	Integral Value of 6
140	60670.396	1079.219
220	60861.825	1174.304
300	60878.276	1239.689
380	60673.968	1400.761
459	60625.634	1586.844
538	60278.416	1744.546
618	59973.491	1919.468
698	59817.831	2119.157
778	59617.063	2331.179
858	59425.119	2521.41
938	59297.622	2741.882

1018	59303.626	2955.91
1098	59326.119	3205.434
1178	59380.39	3429.144
1258	59181.634	3643.255
1338	59001.234	3811.28
1418	58759.035	3979.511
1498	58570.359	4216.208
1578	58407.377	4336.541
1657	58116.893	4440.569
1737	57910.618	4630.328
1817	57636.837	4737.747
1896	57537.434	4892.734
1976	57330.271	5104.127
2057	57337.233	5279.111
2137	57206.257	5361.2
2217	57252.48	5578.321
2297	57256.666	5740.915
2377	57119.964	5862.101
2456	57072.343	6060.702
2536	56925.583	6212.635
2616	56789.082	6414.986
2695	56665.69	6528.269
2776	56407.578	6695.725
2855	56167.185	6821.834
2936	56102.447	6984.62
3015	55834.634	7138.187
3095	55620.662	7288.653
3174	55484.658	7477.839
3254	55063.572	7576.482
3334	54852.696	7721.378
3415	54772.761	7841.963
3495	54718.222	8047
3575	54706.826	8239.856
3655	54449.416	8129.344
3735	54747.36	8634.989
3818	54712.061	8831.251
3898	54620.118	9027.564
3981	54500.432	9173.63
4063	54007.188	9079.908
4144	53983.522	9528.152
4224	53732.879	9715.053

4304	53467.923	9820.371
4385	53291.97	9958.478
4465	53019.122	10107.92
4545	52756.716	10280.711
4624	52623.934	10418.227
4704	52483.594	10634.338
4784	52439.17	10820.318
4865	52186.913	10701.058
4945	52313.786	11230.01
5024	52305.876	11377.292
5104	52167.328	11613.616
5184	52142.308	11762.942
5264	51818.555	11977.089
5344	51667.909	12113.958
5423	51465.892	12273.828
5503	51276.348	12410.129
5583	50908.542	12556.142
5663	50711.396	12748.4
5743	50572.525	12902.005
5823	50079.647	12737.344
5903	50071.893	13164.766
5982	49926.607	13355.715
6063	49731.36	13520.513
6143	49662.675	13705.233
6222	49629.082	13903.469
6302	49640.907	14138.508
6382	49592.912	14341.311
+ CoCp ₂		
6707	48018.96	14276.902
6731	47852.28	14288.139
6756	47796.896	14233.974
6781	47423.164	14204.817
6806	47315.252	14271.159
6831	47331.538	14222.671
6855	47283.982	14257.031
6879	47173.924	14225.252
6904	47175.279	14256.483
6928	47138.475	14217.356
6952	47090.215	14216.674
6976	47010.449	14210.2
7001	47084.809	14205.363

7026	47077.674	14209.418
7050	47031.791	14205.569
7074	46968.222	14221.33
7099	46911.996	14161.886
7124	46875.209	14161.294
7148	46825.76	14181.257
7173	46842.691	14186.689
7197	46761.995	14181.318
7222	46797.991	14160.057
7247	46712.345	14160.689
7272	46651.193	14165.071
7296	46657.831	14134.929
7322	46516.915	13980.194
7346	46612.533	14145.562
7370	46527.09	14141.391
7394	46610.854	14142.176
7420	46586.826	14122.655
7444	46416.909	14146.774
7469	46539.684	14119.178
7493	46523.066	14130.529
7518	46440.061	14140.604
7543	46447.325	14114.958
7568	46462.876	14133
7592	46478.854	14091.479
7617	46538.502	14134.869
7642	46531.754	14104.69
7666	46635.978	14161.344
7691	46613.917	14185.713
7715	46547.558	14195.338
7740	46694.336	14163.087
7764	46815.461	14217.57
7789	46811.527	14205.41
7813	46852.514	14250.162
7838	46959.052	14258.288
7863	47072.238	14289.964
7886	46973.089	14269.655
+ FcPF ₆		
8141	38951.717	11985.844
8221	38915.213	12022.352
8301	38849.427	11990.375
8381	38785.085	11945.741

8461	38714.51	12011.003
8541	38674.902	12067.81
8621	38607.272	12004.001
8701	38496.665	11971.828
8781	38358.834	11989.318
8860	38329.043	11963.827
8940	38307.148	12027.075
9020	38232.811	12005.715
9100	38235.79	12040.073
9180	38255.302	12028.171
9260	38413.687	12108.061
9339	38477.546	12183.935
9420	38545.997	12271.495
9500	38572.364	12282.823
9579	38582.689	12312.953
9659	38528.403	12395.34
9739	38449.54	12387.478
9819	38377.568	12401.134
9899	38275.191	12399.17
9979	38216.331	12444.841
10059	38144.01	12476.025
10138	38034.687	12458.958
10218	37961.118	12518.842
10297	37872.162	12483.168
10377	37886.116	12607.259
10457	37980.896	12629.353
10537	38129.07	12737.275
10616	38174.086	12777.313
10696	38252.422	12878.9
10777	38252.061	12891.175
10856	38171.48	12951.237
10936	38137.917	12976.302
11018	38095.886	13022.9
11098	37969.901	13054.197
11178	37899.167	13118.197
11259	37818.338	13108.491
11340	37749.028	13111.763
11420	37648.263	13181.562
11500	37542.702	13182.73
11580	37407.404	13194.485
11660	37336.731	13245.289

11739	37243.104	13277.11
11819	37234.458	13313.974
11899	37246.245	13377.356
11978	37242.799	13476.815
12058	37350.629	13552.404
12138	37437.447	13627.549
12217	37395.479	13668.566
12297	37372.499	13772.639
12377	37297.295	13822.481
12457	37261.01	13850.972
12537	37185.88	13884.37
12617	37117.596	13955.541
12697	37018.332	13944.493
12777	36924.527	14028.901
12857	36817.671	14011.499
12937	36752.876	14045.82
13017	36660.001	14084.502
13097	36512.111	14084.129
13178	36465.066	14102.622
13258	36386.197	14170.887
13337	36434.565	14233.186
13417	36477.455	14355.29
13497	36500.822	14420.088
13577	36607.635	14540.053
13656	36636.08	14619.055
13736	36603.837	14676.22
13815	36527.776	14790.787
13896	36430.67	14806.64
13975	36353.75	14833.818
14055	36248.54	14955.209
14135	36142.178	14917.712
14216	35985.339	14953.437
14295	35914.455	14981.606
14375	35851.29	15072.894
14455	35726.967	15100.348
14535	35713.699	15149.925
14615	35750.433	15204.614
14695	35716.606	15265.095
14775	35879.398	15419.765
14856	35813.818	15478.871
14936	35835.392	15576.359

15016	35828.863	15713.925
15095	35781.612	15773.619
15176	35687.565	15763.701
15256	35599.882	15826.148
15336	35481.812	15838.194
15416	35427.079	15900.724
15496	35324.478	15930.928
15576	35225.685	15981.14
15655	35116.275	16019.371
15735	35050.77	16064.739
15815	34923.198	16095.108
15896	34798.611	16133.747

Table S12. ^1H NMR integration values for Figure S38 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 8	Integral Value of 7
182	10899.085	73265.343
206	11688.259	70181.677
231	13249.51	68334.097
255	14806.845	66276.096
279	16357.643	64582.671
303	17822.833	62786.132
327	19240.295	61031.838
351	20619.473	59493.188
375	21905.808	57962.781
399	23032.202	56512.234
423	24173.365	55253.101
447	25330.735	53873.171
471	26322.625	52693.455
495	27529.242	51481.784
520	28551.249	50413.812
544	29251.638	49182.325
567	30156.686	48205.022
592	31112.283	47343.554
616	31756.593	46262.16
640	32649.689	45469.985
664	33340.691	44567.102
689	34065.77	43716.03
713	34719.8	42897.167
737	35297.168	42173.938
762	35958.032	41538.049

787	36791.77	40827.973
811	37283.677	40066.071
835	37477.974	39475.88
859	38054.313	38864.923
883	38603.12	38242.865
907	38896.008	37762.133
931	39468.49	37305.49
955	39803.698	36696.9
979	40367.452	36213.12

Table S13. ^1H NMR integration values for Figure S39 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 8	Integral Value of 7
163	2029.08	78664.181
187	2079.152	77634.6
212	2101.996	77405.448
236	2258.983	77131.632
260	2403.869	76881.582
284	2517.574	76762.718
308	2758.741	76444.946
332	2901.214	76234.113
356	3147.638	76027.969
380	3334.883	75824.357
405	3593.893	75608.185
429	3811.428	75271.371
454	4051.995	75000.34
478	4278.207	74633.655
503	4498.842	74489.078
527	4710.541	74016.874
551	5013.474	73648.931
575	5261.174	73429.953
600	5498.401	73285.888
624	5774.2	72795.389
648	5939.503	72564.185
672	6173.613	72184.84
696	6423.609	72000.786
721	6648.195	71744.995
745	6874.557	71395.116
769	7136.092	71174.208
793	7316.979	70915.575
818	7557.454	70744.091

842	7722.207	70246.061
866	7911.056	69967.913
890	8133.663	69794.984
915	8432.698	69623.499
939	8575.626	69345.84
963	8728.804	69110.922
987	8970.505	68880.016

Table S14. ^1H NMR integration values for Figure S40 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 8	Integral Value of 7
163	7581.949	48293.646
188	8095.755	46688.606
211	8739.652	45926.01
235	9765.205	44736.694
260	10692.624	43565.073
283	11597.876	42524.664
308	12500.416	41427.146
332	13396.423	40499.47
357	14304.902	39509.544
381	14923.424	38578.558
+ CoCp ₂		
587	16559.232	34509.939
611	16401.397	34396.391
634	16395.902	34365.568
658	16484.473	34320.135
682	16542.938	34153.136
706	16539.159	34161.877
731	16706.351	34084.393
755	16692.942	33970.437
780	16782.449	33917.177
+ FcPF ₆		
1013	17766.878	28893.039
1037	17766.808	28556.928
1062	17868.796	28420.099
1087	18051.687	28143.383
1111	18109.836	27871.883
1135	18305.394	27677.648
1159	18566.942	27383.243
1184	18814.106	27251.24
1208	18904.417	26983.57

1232	19004.212	26856.389
1256	19147.685	26619.77
1281	19394.259	26399.509
1306	19560.707	26254.015
1330	19586.879	26062.989
1354	19791.118	25840.722
1379	20038.365	25726.632
1403	20067.087	25517.043
1427	20203.065	25319.938
1451	20334.035	25228.948
1475	20484.43	25022.19
1500	20688.754	24882.689
1525	20824.585	24732.888
1548	20820.133	24603.856
1572	20962.683	24408.229
1597	21119.923	24280.305
1621	21185.046	24185.696
1645	21387.664	24001.8
1669	21376.319	23900.007
1694	21624.716	23838.27
1717	21615.873	23686.207
1742	21758.066	23539.717
1766	21869.032	23435.144
1790	21940.339	23314.51
1814	22033.551	23163.161
1838	22167.672	23071.183
1863	22282.947	22997.247
1886	22257.544	22803.182
1910	22274.917	22749.558
1934	22505.843	22618.215
1958	22604.134	22538.365
1982	22721.832	22419.182

Table S15. ¹H NMR integration values for Figure S41 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 10	Integral Value of 9
122	1319.503	20406.85
202	1557.51	19987.552
281	1972.4	19601.528
360	2454.295	19040.78
438	3051.605	18469.572

517	3671.904	17769.608
595	4313.367	17117.482
675	4973.508	16457.552
753	5644.178	15820.899
832	6275.593	15172.198
911	6967.071	14586.088
991	7552.994	14007.297
1071	8103.632	13452.293
1150	8642.733	12915.652
1230	9127.486	12395.777
1309	9584.54	11936.541
1388	10035.067	11490.031
1468	10435.912	11042.993
1548	10829.763	10633.503
1627	11135.444	10303.857
1706	11458.833	9963.627
1785	11744.457	9653.648
1863	12021.217	9361.259

Table S16. ¹H NMR integration values for Figure S42 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 10	Integral Value of 9
134	1490.072	38737.433
213	1634.124	38639.863
292	1721.458	38372.931
371	2034.269	38198.777
450	2351.761	37882.327
529	2701.055	37461.667
608	3110.78	37139.826
687	3449.906	36703.237
766	3852.426	36247.317
845	4256.269	35966.597
923	4601.382	35610.067
1001	4883.36	35252.965
1080	5132.992	34955.85
1159	5432.803	34763.261
1237	5621.771	34541.751
1316	5845.998	34260.897
1395	6058.415	34103.978
1474	6223.995	33942.986
1553	6345.796	33746.878

1632	6554.323	33603.848
1711	6670.467	33531.972
1790	6731.052	33258.182
1869	6891.456	33253.038

Table S17. ^1H NMR integration values for Figure S26 (left, blue) as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
139	1479.81	92576.661
218	2009.279	91673.641
297	2796.472	90688.72
376	3582.429	89641.471
455	4377.828	88682.547
534	5139.477	87691.988
613	5812.401	86844.726
692	6462.948	86012.1
771	7063.951	85360.053
850	7746.467	84890.472
930	8280.855	84542.612
1008	8824.756	84310.47
1087	9394.732	84120.05
1167	9974.81	83864.708
1246	10522.164	83545.636
1325	11058.513	83077.877
1404	11608.393	82561.656
1482	12113.56	82008.365
1561	12699.444	81325.34
1641	13248.589	80610.258
1720	13748.012	79873.156
1799	14308.971	79069.307
1878	14903.282	78289.797
1958	15445.525	77472.528
2037	16024.941	76726.331
2116	16599.971	75886.589
2196	17156.147	75139.66
2275	17792.364	74364.242
2354	18412.422	73605.463
2434	19015.998	72915.225
2513	19678.115	72320.65
2592	20295.931	71903.541
2670	20982.942	71549.447

2750	21668.045	71233.063
2829	22277.772	70875.918
2909	22938.974	70476.038
2988	23485.856	70052.217
3068	24015.105	69543.215
3147	24571.589	68990.157
3226	25127.502	68321.86
3305	25569.674	67673.877
3384	26088.307	67033.017
3464	26516.016	66349.131
3543	26981.045	65647.266
3623	27419.343	64993.51
3701	27856.778	64301.656
3779	28281.711	63698.697
3858	28732.323	63048.57
3937	29138.808	62522.779
4016	29578.345	61829.184
4096	30017.998	61292.453
4174	30493.205	60868.117
4254	30995.43	60541.774
4333	31537.958	60313.062
4412	32086.489	60133.785
4491	32591.12	59938.188
4570	33068.504	59752.894
4649	33499.101	59442.27
4728	33917.583	59133.926
4807	34319.695	58712.638
4886	34582.23	58358.696
4966	34885.543	57902.178
5045	35202.548	57452.629
5124	35472.995	57020.875
5204	35752.551	56521.664
5282	36040.173	55985.952
5362	36302.407	55506.19
5442	36580.882	55051.232
5521	36807.141	54621.952
5600	37052.596	54167.528
5679	37328.815	53718.12
5759	37596.562	53330.867
5838	37957.567	52974.58
5917	38326.315	52767.164

5997	38744.609	52668.634
6076	39169.644	52590.415
6155	39643.716	52400.408
6234	40064.189	52314.225
6314	40422.318	52173.683
6394	40722	51973.149
6473	41023.372	51751.232
6553	41268.41	51428.339
6632	41527.366	51074.111
6711	41686.991	50746.68
6791	41860.533	50428.634
6870	41983.799	50147.84
6949	42106.157	49728.436
7028	42276.548	49349.065
7107	42454.591	49022.026
7186	42602.64	48677.835
7266	42823.212	48280.457
7345	43029.413	47883.663
7425	43194.677	47579.622
7504	43423.93	47342.939
7583	43742.384	47139.027
7663	44142.075	46983.725
7742	44529.274	46902.664
7822	44924.463	46858.966
7902	45294.336	46823.062
7982	45641.244	46707.994
8062	45892.524	46649.25
8141	46121.812	46413.787
8220	46335.981	46208.377
8300	46490.451	45960.203
8379	46589.381	45682.344
8458	46685.831	45454.344
8538	46821.644	45120.154
8617	46885.071	44828.976
8697	46996.233	44454.458
8776	47079.387	44199.818
8856	47194.866	43825.801
8936	47269.333	43570.001
9015	47396.492	43335.354
9095	47482.723	43106.417
9174	47658.95	42954.932

9254	47922.553	42814.193
9332	48194.003	42737.308
9412	48571.612	42690.774
9492	48914.284	42687.315
9571	49242.874	42673.815
9651	49548.918	42596.425
9730	49789.212	42521.927
9810	49969.639	42339.194
9891	50134.602	42259.247
9970	50223.566	42045.462
10049	50335.691	41796.408
10129	50406.456	41486.156
10209	50443.801	41297.368
10288	50516.971	40997.971
10368	50552.824	40681.323
10448	50608.392	40468.655
10527	50663.368	40198.259
10607	50720.032	40028.649
10686	50790.354	39751.147
10765	50835.56	39573.843
10844	51005.797	39298.92
10924	51204.648	39230.035
11004	51456.998	39125.527
11083	51804.478	39095.644
11163	52136.188	39167.33
11243	52482.572	39100.276
11322	52752.785	39079.767
11402	52959.58	39027.213
11482	53143.994	38921.941
11562	53297.551	38826.962
11641	53408.401	38594.531
11720	53413.283	38438.562
11800	53481.686	38235.312
11879	53523.316	38068.396
11959	53552.69	37830.8
12038	53599.403	37551.908
12118	53610.829	37372.977
12198	53651.49	37122.7
12277	53685.86	36907.129
12357	53713.033	36685.527
12436	53780.052	36501.421

12516	53907.634	36334.862
12596	54151.7	36236.917
12674	54358.034	36246.598
12754	54625.477	36222.276
12833	54987.668	36250.403
12912	55269.179	36272.83
12991	55515.366	36234.453
13071	55719.604	36193.541
13151	55935.142	36096.53
13230	55991.332	36037.761
13309	56078.263	35920.637
13389	56109.128	35759.708
13468	56135.189	35567.816
13547	56117.777	35426.275
13627	56129.165	35208.85
13706	56143.275	34918.171
13785	56159.453	34774.542
13864	56120.905	34549.004
13943	56102.963	34342.88
14023	56110.296	34205.422
14102	56157.529	33970.73
14182	56204.662	33829.581
14261	56378.436	33734.585
14340	56619.651	33721.776
14420	56920.69	33680.731
14498	57245.518	33719.532
14578	57519.876	33802.42
14657	57782.479	33803.678
14736	57998.412	33727.476
14815	58118.214	33689.619
14894	58241.848	33617.884
14973	58322.194	33476.788
15052	58342.989	33325.701
15132	58333.601	33183.762
15211	58362.04	33008.885
15289	58313.018	32920.9
15369	58274.676	32681.154
15448	58228.888	32511.137
15527	58241.263	32339.167
15606	58239.297	32168.431
15686	58210.914	32012.176

15765	58231.077	31863.182
15845	58308.121	31706.101
15924	58445.476	31592.511
16003	58725.902	31651.881
16082	58988.307	31671.38
16161	59298.279	31719.011
16240	59576.155	31716.057
16320	59801.337	31715.526
16399	59993.867	31687.943
16478	60151.604	31605.046
16557	60227.551	31550.678
16636	60326.24	31489.903
16715	60348.096	31270.984
16794	60328.9	31147.758
16874	60326.922	30977.18
16953	60281.991	30858.648
17032	60186.96	30673.622
17111	60157.979	30560.211
17191	60093.205	30398.349
17270	60084.049	30235.995
17350	60067.92	30014.534
17430	60090.378	29959.421
17509	60075.484	29777.426
17588	60157.359	29664.843
17667	60362.792	29627.418
17747	60615.593	29651.452
17826	60921.197	29700.812
17905	61217.142	29706.046
17984	61496.355	29739.703
18063	61745.222	29701.345
18142	61877.519	29706.744
18222	61970.619	29648.836
18301	62090.769	29560.341
18380	62066.978	29458.581
18460	62091.27	29341.953
18540	62072.624	29176.485
18619	62003.435	29053.998
18699	61941.477	28953.56
18778	61874.025	28741
18856	61791.638	28659.63
18935	61765.279	28439.996

19015	61737.224	28346.239
19094	61709.111	28212.019
19173	61719.365	28063.571
19253	61832.576	28043.607
19332	62030.96	28021.934
19412	62314.685	28048.071
19492	62589.032	28046.966
19572	62887.896	28126.163
19651	63130.956	28117.475
19730	63302.792	28120.976
19810	63453.73	28113.344
19889	63599.657	28028.792
19968	63658.21	27935.538
20048	63618.282	27858.916
20127	63598.244	27760.991
20206	63548.501	27646.122
20285	63524.417	27477.504
20365	63439.036	27356.303
20444	63358.208	27241.859
20524	63305.686	27065.818
20604	63257.394	26912.873
20684	63189.921	26796.076
20762	63138.861	26680.602
20841	63134.289	26572.797
20920	63257.71	26513.603
21000	63431.824	26527.183
21080	63702.328	26520.467
21158	63981.763	26548.622
21238	64266.889	26596.545
21317	64518.603	26636.263
21395	64707.766	26646.609
21475	64876.625	26604.303
21554	64947.581	26562.748
21634	64985.239	26482.428
21714	65025.909	26403.23
21793	64973.042	26303.796
21873	64873.001	26224.457
21952	64853.321	26087.706
22031	64753.123	25939.735
22110	64666.329	25810.94
22189	64611.761	25700.794

22269	64539.626	25597.324
22349	64469.57	25471.397
22428	64421.449	25386.314
22507	64421.449	25221.809
22587	64495.676	25152.668
22666	64672.114	25141.919
22746	64946.882	25172.612
22825	65209.714	25210.384
22904	65458.422	25254.091
22983	65734.8	25335.92
23062	65990.656	25300.114
23141	66171.322	25328.929
23220	66244.773	25278.283
23300	66306.827	25250.619
23380	66330.854	25228.314
23459	66321.526	25095.461
23538	66295.05	24973.754
23616	66231.978	24917.19
23695	66131.306	24804.28
23774	66023.178	24660.927
23854	65954.682	24545.602
23933	65839.789	24410.9
24012	65774.611	24334.181
24091	65721.448	24186.039
24171	65664.017	24098.319
24250	65696.672	24007.209
24329	65778.915	23966.696
24408	66024.713	23954.725
24487	66233.28	23976.679
24566	66554.435	24050.858
24646	66825.359	24114.008
24725	67076.861	24102.641
24804	67300.748	24175.856
24883	67392.547	24161.767
24962	67452.403	24163.267
25041	67488.292	24054.114
25120	67487.014	23951.857
25200	67441.683	23899.354
25280	67348.032	23770.215
25359	67311.2	23651.676
25438	67200.527	23600.094

25518	67062.856	23429.252
25597	66968.538	23338.01
25676	66906.343	23265.626
25756	66791.649	23127.471
25834	66772.384	23053.714
25914	66706.932	22959.796
25992	66794.314	22898.675
26071	66978.588	22906.975
26150	67153.587	22899.725
26229	67450.565	22934.355
26308	67748.05	23011.726
26386	68025.24	23026.197
26466	68194.426	23011.904
26545	68359.581	23025.893
26625	68456.994	23059.077
26704	68486.856	22995.257
26783	68487.463	22937.453
26862	68460.901	22869.607
26942	68436.934	22844.6
27022	68396.164	22828.154
27102	68454.508	22725.933
27180	68532.058	22709.919
27260	68632.048	22696.376
27339	68808.401	22659.25
27418	68924.016	22704.984
27497	69092.231	22693.071
27576	69197.466	22674.951
27655	69245.421	22594.546
27734	69269.016	22597.822
27813	69240.26	22537.357
27892	69138.299	22427.187
27971	69105.799	22350.026
28050	68993.49	22241.461
28129	69030.9	22176.083
28208	69054.356	22169.907
28289	69121.482	22119.764
28368	69248.173	22125.235
28447	69407.201	22137.684
28527	69555.697	22128.507
28606	69678.819	22143.643
28685	69716.179	22130.94

28764	69776.392	22042.639
28844	69706.262	21971.593
28924	69632.247	21897.105
29003	69649.016	21864.61
29082	69614.986	21782.003
29161	69621.896	21783.705
29240	69688.094	21754.779
29319	69756.906	21701.452
29398	69904.285	21712.407
29476	69983.315	21701.961
29555	70165.324	21697.144
29634	70298.961	21657.37
29713	70447.05	21715.049
29792	70571.735	21692.448
29872	70593.025	21635.896
29951	70554.588	21605.472
30030	70540.135	21502.588
30109	70411.725	21434.379
30189	70298.817	21377.643
30268	70252.456	21239.306
30347	70173.12	21191.648
30426	70220.097	21181.66
30506	70274.807	21084.386
30585	70405.764	21119.138
30664	70545.928	21102.847
30744	70680.594	21121.459
30823	70800.211	21101.867
30902	70883.595	21080.48
30982	70912.535	21052.617
31061	70867.978	20965.27
31140	70815.168	20931.005
31220	70772.214	20880.847
31299	70768.109	20817.822
31378	70777.761	20807.968
31457	70824.266	20815.124
31536	70898.775	20757.553
31614	71000.13	20798.678
31694	71061.98	20761.718
31773	71239.453	20827.495
31852	71338.157	20758.328
31932	71394.059	20782.005

32011	71475.461	20736.37
32091	71596.369	20746.941
32170	71569.298	20716.461
32249	71549.682	20627.908
32328	71435.681	20561.438
32408	71355.497	20450.175
32488	71250.035	20371.088
32567	71174.624	20296.132
32646	71143.73	20289.492
32726	71160.872	20205.274
32805	71284.277	20248.233
32884	71378.659	20197.346
32963	71543.559	20218.389
33042	71702.085	20207.475
33122	71821.783	20214.362
33201	71908.766	20239.221
33280	72002.768	20229.095
33359	71944.174	20151.29
33438	71874.825	20084.788
33517	71850.233	20031.616
33596	71822.491	19990.144
33675	71820.295	19988.265
33755	71885.143	20010.783
33834	71961.09	19984.869
33913	72066.338	20022.009
33993	72167.917	20026.65
34071	72220.56	20000.863
34151	72377.944	19969.839
34230	72426.66	19954.825
34309	72497.146	19953.162
34389	72511.89	19950.532
34468	72541.234	19934.634
34547	72553.89	19932.49
34627	72539.89	19690.995
34707	72438.337	19755.924
34786	72312.324	19709.189
34865	72179.594	19615.717
34944	72060.724	19544.345
35023	72000.2	19512.807
35102	72030.948	19433.342
35182	72113.19	19442.213

35261	72253.697	19431.715
35340	72402.164	19460.036
35419	72522.809	19471.625
35498	72671.521	19439.044
35577	72765.883	19545.493
35656	72765.349	19437.388
35736	72691.621	19441.714
35815	72674.835	19334.179
35895	72615.968	19316.1
35975	72578.569	19276.03
36054	72602.769	19238.952
36133	72629.335	19184.776
36212	72684.464	19231.038
36292	72788.718	19226.022
36371	72899.25	19180.929
36450	73009.814	19196.576
36529	73116.285	19229.613
36608	73172.638	19221.932
36687	73248.411	19011.104
36766	73289.613	19193.975
36845	73292.904	19234.051
36924	73232.204	19114.991
37004	73178.666	19041.892
37083	73058.794	19000.667
37162	72960.766	18891.027
37241	72812.633	18844.602
37321	72752.581	18790.838
37400	72738.784	18786.331
37480	72727.117	18796.298
37559	72833.795	18692.873
37639	72938.999	18719.613
37718	73118.579	18742.774
37797	73235.389	18765.01
37876	73319.884	18769.197
37955	73436.97	18729.512
38034	73456.396	18660.874
38114	73377.319	18669.697

Table S18. ^1H NMR integration values for Figure S26 (left, red) as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 3	Integral Value of 4
131	84933.806	382.417
211	86203.221	487.368
290	85936.162	517.559
369	85873.369	522.631
448	85873.802	538.555
527	86079.182	531.108
607	86277.149	513.102
686	86541.872	520.623
766	86993.901	522.497
845	87292.896	540.599
925	87445.922	547.233
1004	87676.511	562.006
1083	87609.109	556.648
1163	87475.939	567.552
1242	87401.276	576.993
1321	87234.999	632.062
1401	86923.775	633.195
1480	86579.781	635.571
1560	86515.821	651.554
1639	86059.144	667.793
1718	85879.299	677.895
1798	85661.694	695.945
1878	85555.297	724.472
1957	85588.363	717.928
2037	85880.075	779.053
2116	86134.583	767.143
2195	86375.246	798.048
2275	86742.147	802.341
2355	87037.849	859.779
2434	87063.159	897.512
2513	87162.018	905.397
2592	87178.917	917.513
2671	86926.938	975.243
2750	86915.914	955.014
2830	86675.375	1023.856
2910	86454.949	1040.037
2989	86064.533	1039.776
3068	85832.586	1079.335

3148	85479.397	1096.667
3227	85412.471	1095.175
3307	85199.354	1133.785
3386	85111.738	1152.275
3466	85297.129	1205.426
3545	85677.738	1224.556
3625	85884.26	1252.894
3704	86213.321	1284.843
3784	86263.116	1302.884
3863	86497.999	1378.435
3943	86807.729	1392.284
4023	86628.977	1418.194
4102	86545.577	1434.05
4182	86454.159	1476.554
4262	86219.677	1505.425
4341	85997.508	1546.921
4420	85669.666	1566.346
4500	85395.412	1567.325
4579	85081.055	1595.238
4659	84879.696	1638.594
4738	84553.448	1670.763
4817	84480.072	1676.254
4896	84616.293	1725.784
4976	84698.625	1722.322
5055	84947.744	1800.266
5134	85405.435	1844.486
5214	85601.138	1852.09
5293	85859.14	1890.522
5373	86103.698	1925.891
5452	86084.028	1976.773
5532	86031.069	2025.828
5611	86051.769	2041.634
5690	85848.772	2063.376
5768	85587.671	2073.113
5847	85358.094	2093.481
5925	85158.994	2123.661
6005	84714.216	2153.286
6085	84579.287	2187.479
6164	84244.872	2220.974
6244	84068.755	2247.225
6324	83887.046	2243.362

6404	84060.537	2317.438
6483	84321.846	2304.835
6562	84546.468	2390.369
6642	84996.432	2398.157
6721	85216.339	2478.577
6801	85395.236	2521.556
6880	85579.377	2529.733
6960	85593.699	2551.919
7039	85411.273	2588.66
7118	85409.133	2590.967
7198	85104.47	2598.819
7277	84977.053	2654.848
7357	84648.847	2639.15
7437	84323.504	2702.995
7516	83962.752	2717.146
7595	83751.637	2704.352
7675	83597.918	2730.926
7754	83420.105	2815.44
7833	83309.745	2782.354
7913	83496.116	2835.007
7992	83714.583	2882.635
8071	84018.758	2901.962
8151	84323.758	2963.93
8230	84605.957	2976.577
8310	84939.662	3051.664
8389	84851.468	3019.105
8468	84874.915	3071.966
8547	84832.375	3112.831
8627	84608.233	3116.505
8707	84464.581	3106.279
8786	84141.539	3175.719
8865	83956.606	3177.416
8945	83565.174	3185.398
9024	83276.916	3186.05
9103	83000.268	3205.35
9183	82883.019	3235.932
9263	82865.207	3222.151
9342	83018.058	3274.767
9421	83208.511	3299.563
9500	83496.957	3359.029
9580	83899.947	3392.253

9659	84067.146	3438.872
9738	84347.923	3476.224
9818	84390.76	3464.282
9897	84372.051	3514.138
9977	84300.313	3549.233
10056	84073.491	3520.498
10136	84002.934	3574.544
10215	83799.401	3579.032
10295	83368.377	3570.763
10374	83172.174	3614.37
10453	82985.083	3620.704
10532	82584.14	3613.188
10612	82487.092	3609.56
10692	82257.572	3632.565
10771	82210.128	3637.564
10851	82474.813	3689.906
10930	82700.978	3720.406
11010	82908.371	3781.779
11089	83337.315	3844.624
11169	83673.18	3855.551
11248	83665.951	3858.228
11328	83851.812	3896.567
11407	83749.208	3923.346
11486	83756.767	3913.993
11566	83491.443	3956.568
11645	83406.88	3987.928
11725	83112.976	3975.28
11804	82893.009	3966.837
11883	82641.531	3950.187
11963	82362.783	3948.511
12042	82267.031	3984.143
12121	81977.934	3982.055
12201	81894.703	4041.063
12280	81857.167	4004.213
12360	82072.525	4040.127
12439	82360.972	4092.291
12518	82628.647	4125.588
12597	82860.395	4139.468
12677	83395.245	4189.116
12757	83333.279	4206.569
12836	83475.905	4252.023

12915	83550.614	4272.341
12995	83412.634	4250.975
13074	83334.541	4279.657
13153	82898.257	4303.148
13233	82775.334	4283.444
13312	82520.826	4294.857
13392	82273.713	4300.85
13471	82138.38	4297.309
13550	81789.78	4301.286
13630	81582.974	4271.978
13709	81544.166	4303.581
13788	81765.199	4337.964
13867	82015.028	4371.398
13946	82154.511	4400.846
14026	82586.78	4456.993
14105	82871.792	4527.628
14185	83124.004	4510.074
14264	83376.27	4524.165
14343	83322.995	4542.013
14422	83381.516	4581.087
14501	83359.515	4553.719
14581	83117.856	4563.599
14661	82875.146	4551.336
14740	82715.229	4576.439
14819	82547.252	4593.559
14899	82165.047	4545.935
14978	81858.986	4604.408
15056	81740.635	4579.349
15136	81415.777	4578.529
15215	81546.721	4577.009
15294	81669.422	4606.633
15373	81797.31	4631.043
15452	82129.146	4670.404
15531	82528.207	4691.761
15611	82805.714	4701.012
15691	83022.298	4725.903
15770	83123.093	4776.428
15849	83166.075	4755.661
15929	83021.915	4824.953
16008	82971.53	4822.473
16087	82835.451	4809.445

16167	82548.903	4825.931
16246	82354.308	4808.51
16326	82244.315	4784.222
16405	81820.919	4775.917
16484	81616.493	4761.425
16563	81481.443	4776.653
16643	81327.898	4777.654
16722	81359.379	4827.743
16801	81542.417	4848.169
16881	81812.984	4877.482
16960	82154.736	4887.05
17039	82425.653	4931.746
17118	82629.8	4963.417
17198	82861.931	5002.526
17277	82986.642	4994.367
17357	82946.853	4986.137
17437	82760.417	4998.477
17516	82655.634	4998.69
17595	82464.133	4990.808
17675	82242.219	5005.898
17754	82037.273	4996.987
17834	81777.586	5004.65
17913	81401.741	4998.629
17993	81271.373	4975.84
18073	81007.534	4957.41
18152	81137.466	4982.656
18232	81009.232	4977.284
18311	81434.516	5049.779
18390	81545.397	5074.658
18469	81828.021	5099.08
18548	82221.203	5129.288
18628	82504.063	5153.448
18707	82584.884	5144.134
18787	82657.899	5163.795
18866	82656.77	5206.969
18946	82553.048	5196.456
19025	82356.26	5179.579
19105	82184.833	5198.667
19184	81995.542	5207.683
19264	81669.125	5172.701
19343	81515.48	5137.677

19422	81281.956	5172.124
19501	80971.837	5118.377
19579	80875.884	5178.487
19658	80694.251	5139.538
19737	80817.836	5152.537
19817	81221.643	5224.13
19896	81478.497	5218.937
19975	81824.513	5257.327
20054	82000.325	5278.97
20133	82273.238	5293.007
20213	82341.403	5321.372
20293	82401.687	5304.574
20372	82460.671	5357.761
20451	82271.482	5332.709
20530	82191.519	5334.631
20609	82085.041	5346.047
20689	81802.596	5311.7
20768	81515.648	5331.506
20848	81244.221	5304.854
20927	81059.892	5302.531
21006	80767.374	5306.491
21086	80586.199	5290.594
21165	80682.148	5320.574
21245	80786.138	5296.24
21325	80932.135	5337.154
21404	81331.83	5392.124
21483	81620.023	5423.663
21563	81824.942	5441.469
21643	82242.188	5470.72
21722	82377.549	5473.261
21802	82487.913	5501.867
21881	82353.878	5521.775
21960	82284.811	5504.552
22039	82079.302	5481.747
22118	81844.468	5493.6
22197	81656.916	5459.616
22277	81365.342	5475.348
22357	81171.572	5465.615
22437	80890.683	5462.678
22517	80760.48	5473.371
22595	80658.429	5448.121

22675	80798.071	5504.6
22754	80978.972	5456.137
22833	81068.792	5472.566
22912	81398.204	5541.062
22994	81842.755	5552.964
23073	82167.117	5593.884
23152	82212.618	5571.215
23232	82264.434	5614.827
23311	82225.911	5641.107
23390	82274.771	5627.981
23470	82218.41	5619.853
23549	81876.248	5626.148
23629	81721.971	5641.952
23708	81382.005	5606.984
23788	81215.116	5602.688
23868	81041.834	5595.173
23947	80612.827	5593.116
24026	80457.181	5555.317
24105	80333.734	5547.531
24185	80318.15	5591.927
24264	80497.325	5588.417
24344	80688.546	5622.23
24423	80980.425	5654.444
24503	81286.359	5645.27
24582	81607.051	5689.777
24661	81925.207	5736.43
24740	82016.088	5717.465
24819	82174.157	5756.314
24899	82037.2	5766.517
24978	82032.57	5753.764
25057	81834.737	5765.551
25137	81538.727	5748.116
25217	81262.909	5760.27
25296	81064.172	5699.62
25375	80834.467	5693.937
25455	80610.894	5707.269
25534	80267.41	5681.428
25613	80316.949	5690.877
25692	80405.723	5703.212
25772	80515.503	5704.516
25852	80682.784	5762.254

25931	80984.44	5783.681
26010	81218.418	5793.068
26089	81597.126	5828.659
26169	81853.985	5882.931
26248	81744.048	5875.148
26327	81890.087	5827.75
26407	81871.119	5857.43
26486	81856.428	5879.087
26565	81466.761	5875.658
26645	81248.335	5870.448
26724	81052.363	5858.168
26803	80870.899	5848.344
26883	80555.467	5825.045
26962	80468.802	5820.434
27042	80326.336	5834.689
27121	79945.743	5786.333
27200	80076.171	5798.12
27279	80269.125	5856.458
27358	80460.954	5876.574
27437	80873.275	5904.141
27516	81272.518	5911.455
27596	81394.58	5962.274
27675	81669.97	5994.691
27755	81883.312	5969.984
27835	81864.413	5996.68
27914	81709.938	6002.123
27993	81513.431	6008.146
28073	81391.762	6010.792
28152	81210.524	5967.332
28232	80930.412	5959.123
28311	80680.028	5937.064
28390	80544.806	5959.884
28470	80182.204	5922.102
28549	79961.261	5924.019
28628	79853.209	5889.408
28708	79830.448	5890.438
28788	79996.647	5977.695
28867	80395.166	6000.016
28946	80693.273	6029.603
29025	80938.273	6046.541
29105	81335.054	6073.655

29185	81500.061	6082.381
29264	81527.382	6096.439
29344	81619.522	6119.717
29424	81573.654	6119.877
29503	81492.495	6113.617
29582	81182.209	6086.536
29661	81091.979	6120.711
29741	80792.217	6102.945
29820	80650.521	6068.77
29899	80475.074	6023.57
29979	80151.38	6028.016
30058	80121.016	6045.897
30138	79749.007	6038.787
30217	79905.535	6055.29
30297	80080.021	6069.263
30376	80193.091	6074.026
30455	80585.604	6139.085
30534	81054.866	6164.082
30613	81135.137	6173.338
30693	81290.852	6202.478
30772	81602.396	6226.508
30851	81526.733	6229.46
30931	81448.695	6214.816
31011	81317.46	6185.259
31090	81192.61	6226.235
31170	80917.192	6199.368
31249	80755.44	6164.322
31328	80558.352	6175.955
31407	80246.6	6174.758
31487	79950.227	6199.885
31566	79857.383	6174.541
31645	79724.951	6121.351
31724	79662.209	6138.849
31804	79945.055	6196.467
31883	80079.702	6233.248
31963	80348.375	6241.204
32042	80774.379	6275.676
32121	80936.411	6263.824
32201	81073.204	6305.275
32280	81302.715	6360.697
32359	81370.742	6365.218

32439	81263.495	6389.446
32519	81168.995	6347.279
32598	81075.301	6373.798
32678	80908.606	6331.337
32757	80711.195	6291.6
32837	80372.318	6310.114
32916	80153.494	6287.733
32996	79951.154	6274.881
33075	79657.179	6311.869
33155	79627.781	6281.134
33235	79537.273	6266.158
33314	79855.588	6313.593
33393	80131.475	6330.634
33473	80368.428	6349.835
33552	80784.288	6411.73
33632	81049.581	6469.917
33711	81160.225	6442.278
33790	81278.253	6475.688
33870	81405.197	6477.448
33949	81186.404	6447.996
34028	81208.065	6482.379
34108	81083.574	6477.712
34187	80742.014	6428.419
34266	80580.184	6450.357
34345	80343.058	6404.63
34424	80044.097	6402.456
34503	79897.138	6400.891
34583	79637.358	6393.303
34662	79528.071	6433.992
34741	79657.304	6418.403
34819	79948.886	6456.138
34898	80121.698	6450.92
34977	80417.228	6497.374
35057	80807.892	6527.766
35136	80944.548	6552.661
35215	81126.195	6594.951
35295	81271.303	6633.13
35374	81224.188	6605.259
35453	81114.89	6631.093
35533	80894.316	6540.506
35612	80655.426	6536.721

35692	80554.689	6568.931
35771	80269.09	6552.176
35850	80095.495	6536.686
35930	79936.55	6516.851
36009	79730.118	6521.197
36088	79460.755	6492.153
36168	79490.529	6511.386
36247	79572.347	6530.379
36326	79753.759	6488.43
36405	80032.015	6608.771
36485	80392.038	6603.298
36565	80635.05	6638.148
36644	80947.192	6687.386
36723	81006.52	6675.091
36802	81151.603	6698.418
36882	81018.349	6696.824
36961	80860.145	6678.528
37041	80736.346	6655.658
37120	80459.545	6655.632
37199	80259.483	6689.17
37278	80212.911	6672.348
37357	79770.7	6634.386
37437	79621.558	6605.022
37516	79356.722	6623.417
37595	79404.226	6601.738
37675	79323.774	6636.479
37754	79530.024	6633.255
37833	79890.501	6685.677
37913	80093.476	6713.943
37992	80453.958	6775.012
38072	80752.845	6753.502
38151	80883.919	6817.447
38231	80968.947	6785.4
38310	81071.099	6816.647
38390	81083.764	6794.345
38470	80728.018	6811.572
38549	80706.413	6784.786
38628	78708.471	6691.352
38708	80305.653	6778.87
38787	79878.727	6777.47
38866	79555.56	6730.115

38945	79444.22	6721.454
39024	79351.163	6745.133

Table S19. ^1H NMR integration values for Figure S26 (right) as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 4	Integral Value of 3
131	351.447	135167.2
211	628.771	135534.15
290	1239.41	135449.01
370	1944.961	134581.81
449	2780.664	133366.41
528	3949.86	132257.42
608	5376.606	130893.69
687	8437.926	125112.54
765	8107.143	128062.48
845	9862.452	126390.62
924	11010.138	125337.97
1004	12394.09	123477.41
1083	13685.565	122140.27
1162	16226.804	116556
1242	15982.28	119373.66
1321	17078.103	117874.88
1400	18051.575	116818.43
1480	19301.97	115265.3
1559	20042.411	114664.2
1638	21072.681	113870.21
1717	21906.386	112969.37
1796	22987.667	111899.14
1877	24111.51	111763.68
1957	25777.149	107160.92
2035	26080.315	110163.13
2115	27001.82	109177.22
2194	27854.371	108096.77
2273	28968.888	107241.22
2353	30028.868	106302.54
+ CoCp ₂		
2471	31722.316	98663.729
2551	31566.509	98956.546
2630	31476.819	99090.2
2710	31586.901	98566.324
2790	31473.346	98398.532

2869	31497.168	98269.708
2949	31435.128	98101.986
3028	31403.826	97767.522
3107	31437.43	97525.739
3187	31427.21	97378.996
3267	31422.576	97541.428
3346	31523.773	97625.885
3426	31572.747	97569.871
3505	31643.645	97842.281
3585	31696.186	98115.526
3663	31719.799	98199.231
3743	31865.238	98134.03
3822	31806.231	98236.265
3902	32066.284	97997.235
3981	31955.924	98260.078
4060	31926.715	98603.267
4139	32001.949	98440.096
4219	32003.932	98493.543
4298	32028.586	98315.657
4377	32001.031	98397.31
4457	32000.834	98297.106
4537	32041.414	98106.208
4617	31999.76	97956.729
4696	31982.819	97577.136
4777	31929.346	97431.291
+ FcPF ₆		
4949	30401.303	91842.436
5028	30331.159	92304.229
5108	30407.834	92278.859
5187	30415.642	92382.263
5267	30579.982	92438.56
5347	30719.349	92382.916
5425	30670.89	92776.583
5504	30891.291	92696.436
5584	30952.495	92822.267
5664	31111.26	92837.075
5743	31385.291	92239.054
5821	31260.843	92673.475
5901	31348.025	92676.674
5980	31456.059	92333.896
6059	31654.674	92420.178

6139	31709.805	92009.842
6218	31791.569	91704.79
6298	31986.383	91216.375
6378	32081.592	90740.51
6457	32220.011	90391.883
6537	32277.304	90064.392
6616	32333.74	89731.285
6695	32663.289	88949.504
6774	32739.3	89138.444
6853	32879.719	89080.912
6932	33255.51	88770.094
7011	33452.913	88798.074
7090	33668.526	88804.085
7169	34018.04	88143.457
7248	34257.769	88082.215
+ CoCp ₂		
7368	32559.672	83195.505
7447	32409.069	83421.154
7525	32392.146	83416.287
7605	32344.364	83353.229
7684	32330.021	83146.256
7763	32320.362	83071.922
7842	32211.655	82832.731
7922	32165.349	82719.087
8001	32193.123	82750.979
8081	32158.571	82712.129
+ FcPF ₆		
8256	131.084	127.761
8370	30226.642	75759.775
8449	30039.149	76149.039
8527	30251.923	76160.714
8607	30344.213	76181.588
8685	30468.115	76136.394
8763	30620.841	75907.028
8842	30741.185	75811.728
8921	30804.225	75583.238
8999	30936.902	75413.482
9078	31062.351	75136.406
9156	31148.206	74905.12
9234	31505.452	74383.647
9313	31416.603	74369.477

9392	31621.041	74093.303
9471	31732.502	73958.264
9550	32027.164	73887.05
9629	32223.511	73872.005
9708	32495.678	73684.417
9786	32742.361	73639.134
9865	32803.691	73611.293
9943	33086.15	73415.328
10022	33290.201	73213.112
10101	33491.803	72958.342
10181	33605.792	72764.925
10260	33837.683	72315.182
10340	33969.025	72133.876
10420	34165.939	71761.783
10498	34521.768	71147.112
10578	34505.221	71139.412
10657	34723.068	70973.085

Table S20. ^1H NMR integration values for Figure S27 as generated using a data analysis option implemented in the Mestrelab Mnova software package (v. 9.1).

Time (s)	Integral Value of 10	Integral Value of 9
96	1027.53	18978.368
120	945.061	18068.147
144	990.054	17902.746
167	1057.584	17832.333
192	1140.643	17824.434
215	1245.832	17666.487
239	1331.39	17556.969
262	1413.511	17335.992
307	1687.487	16762.935
328	1705.948	16666.307
352	1881.389	16868.234
375	1980.528	16688.135
399	2137.065	16572.62
423	2302.109	16367.754
447	2435.289	16185.373
471	2593.733	16001.584
494	2722.788	15794.461
515	2762.105	15365.09
538	2981.618	15465.373
561	3128.458	15236.85

584	3281.041	15068.195
607	3427.327	14905.881
631	3561.437	14757.529
656	3816.336	14651.759
679	3912.187	14352.309
+ COCp ₂		
964	4428.134	12751.952
988	4452.731	12761.022
1012	4431.542	12752.036
1037	4452.878	12765.095
1060	4424.256	12720.963
1084	4393.231	12716.027
1109	4437.931	12729.856
1132	4437.65	12716.046
1157	4455.788	12702.668
1180	4431.998	12681.798
1204	4409.638	12674.713
1228	4390.741	12636.913
1252	4383.003	12708.025
1275	4428.601	12699.86
1299	4392.37	12618.783
1322	4416.511	12614.777
+ FcPF ₆		
1479	4490.943	12662.73
1503	4535.804	12733.134
1526	4559.481	12732.133
1550	4532.312	12715.137
1575	4612.495	12754.474
1599	4559.505	12688.465
1622	4559.456	12666.378
1645	4542.579	12620.552
1669	4572.244	12699.434
1692	4565.684	12597.229
1716	4590.415	12692.569
1740	4603.143	12654.218
1765	4659.245	12676.503
1789	4655.108	12637.244
1812	4633.704	12552.289
1835	4642.841	12554.096
1858	4651.561	12570.29
1881	4626.574	12489.472

1904	4663.002	12435.635
1927	4636.245	12492.114
1950	4702.763	12508.188
1973	4719.76	12441.887
1996	4705.537	12450.326
2019	4691.986	12457.402
2043	4784.663	12482.241
2066	4757.345	12373.808
2090	4805.289	12370.305
2113	4782.425	12328.063
2136	4826.72	12367.486
2160	4859.705	12346.16
2183	4870.728	12314.83
2206	4863.775	12229.562
2229	4866.98	12275.99
2253	4925.621	12238.063
2277	4945.034	12253.844
2301	4975.062	12230.987
2324	4990.6	12182.003
2348	5010.514	12128.866
2371	5018.959	12128.901
2394	5021	12069.638
2418	5095.185	12063.232
2441	5065.913	12003.8
2464	5096.695	11990.9
2487	5123.88	12013.424
2512	5196.549	11969.486
2535	5202.13	11905.456
2559	5201.651	11920.034
2583	5195.56	11840.315
2607	5247.23	11880.631
2630	5277.401	11803.263
2653	5280.918	11776.356
2677	5313.825	11748.009
2700	5349.948	11767.49
2723	5350.777	11677.073
2746	5349.351	11627.488
2770	5399.525	11667.568
2794	5501.019	11649.223
2818	5470.422	11614.844
2841	5484.112	11582.781

2864	5471.372	11532.569
2888	5546.527	11516.472
2911	5545.731	11464.41
2936	5614.134	11435.755
2960	5641.607	11432.909
2983	5650.062	11386.587
3007	5655.26	11353.67
3030	5654.885	11315.135
3054	5735.06	11276.327
3078	5784.829	11295.777
3102	5763.117	11218.19
3126	5763.901	11218.552
3149	5787.493	11153.03
3173	5858.833	11160.41
3196	5832.865	11084.437
3219	5851.538	11067.425
3243	5883.995	11078.221
3265	5870.092	11015.599
3289	5957.113	11017.335
3313	5967.677	10962.728
3337	5987.323	10970.318
3360	5998.826	10917.697
3383	6038.647	10898.918
3406	6026.202	10815.55
3430	6067.58	10830.48
3453	6078.146	10802.028
3476	6086.154	10784.631
3500	6133.318	10761.867
3524	6205.281	10763.45
3547	6153.464	10659.653
3570	6238.651	10662.448
3594	6212.261	10626.955
3617	6242.387	10610.513
3641	6308.166	10609.204
3665	6331.025	10574.778
3688	6309.556	10511.556
3711	6377.836	10488.711
3735	6393.03	10510.845
3760	6482.848	10510.181
3783	6418.782	10414.055
3807	6474.244	10356.794

3830	6429.686	10371.948
3854	6528.787	10375.065
3878	6501.857	10344.304
3902	6541.655	10289.209
3925	6567.673	10262.665
3950	6638.967	10254.052
3973	6578.153	10210.152
3996	6592.71	10180.155
4020	6617.746	10164.162
4044	6695.517	10139.998
4068	6693.353	10123.448
4091	6649.49	10058.864
4114	6685.828	10046.53
4138	6765.778	10057.292
4162	6813.472	10028.529
4186	6786.707	9984.729
4209	6794.848	9944.952
4233	6849.037	9944.279
4257	6833.949	9897.528
4280	6878.9	9884.855
4304	6885.124	9871.277
4327	6914.479	9826.183
4352	6990.586	9866.009
4375	6907.702	9768.965
4398	6961.706	9787.976
4423	7038.82	9756.403
4446	7019.222	9736.579
4470	6991.725	9679.961
4493	7052.3	9667.724
4516	7035.843	9626.795
4540	7047.512	9597.034
4563	7087.999	9584.252
4587	7118.777	9569.067
4610	7134.108	9565.997
4633	7090.175	9526.747
4657	7160.996	9517.211
4680	7170.439	9488.753
4704	7171.057	9495.506
4727	7188.191	9433.468
4751	7194.766	9416.298
4774	7253.894	9442.993

4798	7297.051	9396.541
4821	7242.18	9352.455
4845	7286.148	9371.548
4869	7340.265	9327.683
4892	7281.152	9286.846
4916	7370.034	9308.795
4939	7347.916	9275.664
4963	7408.259	9264.447
4986	7397.291	9174.443
5010	7416.821	9178.453
5034	7481.554	9207.722
5058	7485.804	9180.01
5082	7466.398	9177.034
5105	7471.839	9131.601
5129	7538.977	9075.664
5152	7493.526	9065.116
5176	7529.595	9104.708
5201	7645.28	9090.756
5225	7601.612	9055.643
5248	7594.96	9010.623
5272	7624.181	8976.134
5296	7639.301	8995.534
5319	7634.778	8950.531
5343	7658.895	8901.66
5366	7616.065	8909.045
5390	7646.137	8875.649
5413	7672.71	8842.482
5436	7680.973	8828.475
5460	7744.909	8826.777
5483	7722.61	8795.689
5507	7723.144	8808.548
5530	7790.254	8759.159
5555	7847.082	8789.291
5578	7786.424	8728.013
5602	7838.391	8737.134
5625	7815.852	8708.845
5650	7923.857	8703.342
5673	7864.247	8674.135
5696	7818.549	8618.097

Comparison of Computational Methods

The combination of using B3LYP for geometry optimization and M06 for single point energy calculations is the standard method in our recent computational studies of transition metal-catalyzed reactions. We compared the performance of this method with a few other popular methods for the computational studies of ruthenium-catalyzed olefin metathesis reactions. Changing the B3LYP geometry to BP86 with either the SVP basis set or with a mixed basis set with SDD for Ru and SVP for other atoms lead to very small changes in the $\Delta H^\ddagger$ and $\Delta G^\ddagger$ values computed with the quasiharmonic correction. Similarly, using M06L in geometry optimization also lead to very similar results. However, the $\Delta G^\ddagger$ computed without the quasiharmonic correction have much greater variation, possibly due to the error in the vibrational entropy calculations. In summary, the computed $\Delta\Delta H^\ddagger$ and $\Delta\Delta G^\ddagger$ values are not very sensitive to the choice of density functional and basis set, while the quasiharmonic correction is necessary to achieve consistent results among the methods that are tested.

Table S21. Activation energies of the rate-determining retro-[2+2] cycloaddition step computed with different levels of theories.

Method	$\Delta H^\ddagger$ (TS2)	$\Delta H^\ddagger$ (TS2 _{red})	$\Delta\Delta H^\ddagger$	Without quasiharmonic correction			With quasiharmonic correction		
				$\Delta G^\ddagger$ (TS2)	$\Delta G^\ddagger$ (TS2 _{red})	$\Delta\Delta G^\ddagger$	$\Delta G^\ddagger$ (TS2)	$\Delta G^\ddagger$ (TS2 _{red})	$\Delta\Delta G^\ddagger$
M06/SDD-6-311+G(d,p)/SMD ^a //B3LYP/SDD-6-31G(d)	11.1	11.8	-0.7	10.8	11.2	-0.4	11.0	11.7	-0.7
M06/def2TZVP/SMD ^a //B3LYP/SDD-6-31G(d)	11.8	12.5	-0.7	11.5	11.9	-0.4	11.7	12.4	-0.7
M06/SDD-6-311+G(d,p)/SMD ^a //BP86/SVP	11.1	12.1	-1.0	9.8	12.7	-2.9	10.8	11.9	-1.1
M06/def2TZVP/SMD ^a //BP86/SVP	11.7	12.7	-1.0	10.5	13.3	-2.8	11.4	12.5	-1.1
M06/SDD-6-311+G(d,p)/PCM ^a //BP86/SDD-SVP	10.6	11.6	-1.0	9.8	9.7	0.1	10.2	11.1	-0.9
M06/SDD-6-311+G(d,p)/SMD ^a //M06L/SDD-6-31G(d)/SMD ^a	11.0	11.9	-0.9	12.0	11.3	0.7	11.7	11.7	-0.6

^a Benzene was used as the solvent.

Complete Reaction Energy Profile

The reaction energy profile of the complete catalytic cycle of the RCM of 1,6-heptadiene is shown in Figure S43. The calculations indicate the rate-determining step is the retro-[2+2] cycloaddition to form the cyclopentene product (**TS2**) and the catalyst resting state is the ruthenacyclobutane intermediate **14**. The reaction employing the neutral ligand (**1**) requires 0.7 kcal/mol lower barrier for the retro-[2+2] cycloaddition than the reaction with the reduced ligand (**1_{red}**). This is in agreement with the faster reaction rate with the neutral catalyst observed in experiment, although computations underestimated the rate-difference. The experimental rate-constant ratio (100) corresponds to a Gibbs activation energy difference of about 2.7 kcal/mol. The fast reaction rate with the neutral ligand in retro-[2+2] cycloaddition is attributed to an electronic effect. The stronger donor ligand **1_{red}** stabilizes the Ru(IV) metalacyclobutane intermediate (**14_{red}**), and thus requires higher barrier for the subsequent retro-[2+2] cycloaddition.

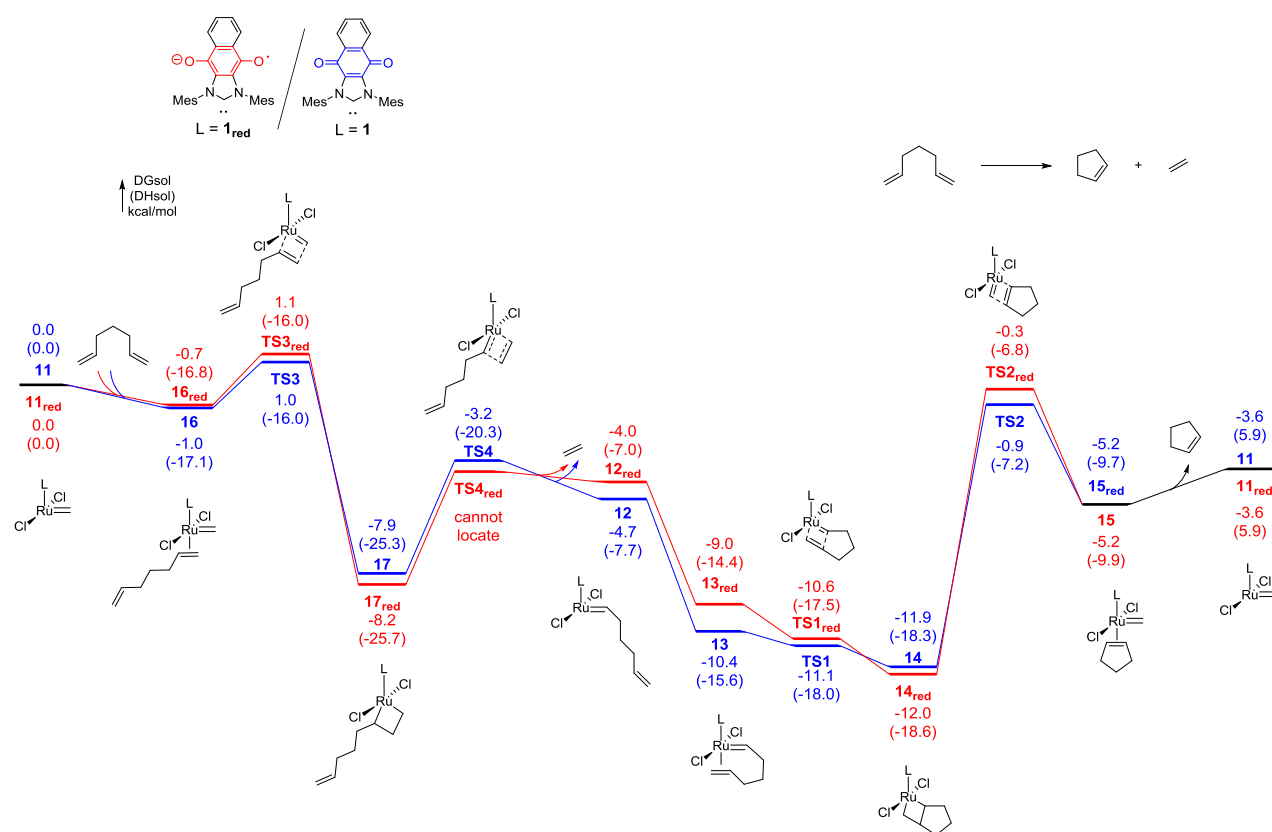


Figure S43. Computed reaction energy profile of the RCM of 1,6-heptadiene. In reactions with both catalysts, the retro-[2+2] cycloaddition (**TS2** and **TS2_{red}**) is the rate-determining step and the ruthenacyclobutane (**14** and **14_{red}**) is the catalyst resting state.

Cartesian Coordinates of the Optimized Structures

11

Three lowest frequencies (cm-1): 9.3591 25.2175 29.6666

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.327427	-2.656503	-2.242300
Cl	-1.330481	-2.657239	2.240439
Ru	-0.681884	-2.474038	-0.000456
C	-0.076509	-0.614423	-0.000031
N	1.181845	-0.040431	0.000046
N	-0.953378	0.464139	-0.000137
C	1.079962	1.343647	-0.000006
C	2.444936	-0.745147	0.000315
C	-0.252096	1.654830	-0.000125
C	-2.401622	0.349248	0.000019
C	2.153268	2.349791	0.000013
C	3.037285	-1.063877	-1.230486
C	3.036845	-1.063680	1.231381
C	-0.769237	3.033177	-0.000323
C	-3.080831	0.340352	-1.230568
C	-3.080523	0.340861	1.230939
C	1.667883	3.768508	-0.000089
O	3.344781	2.066491	0.000097
C	4.259344	-1.742779	-1.201130
C	2.381463	-0.708517	-2.542915
C	4.258918	-1.742575	1.202580
C	2.380543	-0.708129	2.543525
C	0.292534	4.090297	-0.000247
O	-1.963792	3.302740	-0.000547
C	-4.468870	0.179524	-1.199874
C	-2.377883	0.607582	-2.538652
C	-4.468443	0.180213	1.200770
C	-2.376873	0.608154	2.538637
C	2.617508	4.793367	-0.000025
C	4.886726	-2.088297	0.000863
H	4.732665	-2.005280	-2.144473
H	2.229810	0.373973	-2.635372
H	3.006177	-1.027732	-3.381898
H	1.402365	-1.190730	-2.648423
H	4.731895	-2.004921	2.146140
H	1.401294	-1.190115	2.648643
H	3.004822	-1.027470	3.382783
H	2.229097	0.374400	2.635895
C	-0.105009	5.429827	-0.000337
C	-5.176957	0.069589	0.000520
H	-5.009334	0.153124	-2.143135
H	-1.450294	0.041630	-2.639925
H	-3.020506	0.338985	-3.381507
H	-2.144477	1.677725	-2.624752
H	-5.008645	0.154417	2.144215
H	-3.019934	0.341683	3.381835
H	-1.450427	0.040377	2.640314
H	-2.141286	1.677895	2.623700

H	3.668222	4.522460	0.000092
C	2.211285	6.128336	-0.000109
C	6.225249	-2.788946	0.001182
H	-1.167081	5.652191	-0.000464
C	0.850685	6.446473	-0.000265
C	-6.670465	-0.154919	0.001140
H	2.955636	6.919447	-0.000053
H	7.048278	-2.061916	0.002527
H	6.347397	-3.420378	0.887361
H	6.348725	-3.418647	-0.886036
H	0.533976	7.485523	-0.000332
H	-7.143242	0.292816	0.881742
H	-7.140489	0.269550	-0.892266
H	-6.904818	-1.227550	0.015067
C	0.843605	-3.431876	0.000447
H	0.681257	-4.524480	0.000099
H	1.882758	-3.109195	0.001298

11red
Three lowest frequencies (cm-1): 7.8955 21.2336 29.2464

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.325792	-2.657929	-2.260761
Cl	-1.326735	-2.658333	2.259862
Ru	-0.687978	-2.473885	-0.000284
C	-0.072379	-0.584936	-0.000210
N	1.180553	-0.028113	-0.000091
N	-0.946926	0.476388	-0.000299
C	1.098333	1.378868	-0.000066
C	2.432823	-0.737786	0.000106
C	-0.250572	1.696135	-0.000194
C	-2.387876	0.354766	-0.000016
C	2.167654	2.343029	0.000033
C	3.029894	-1.062060	-1.226836
C	3.029502	-1.062091	1.227224
C	-0.776448	3.035688	-0.000273
C	-3.074201	0.345609	-1.226524
C	-3.073671	0.345535	1.226789
C	1.674283	3.733497	0.000008
O	3.390307	2.043534	0.000104
C	4.241584	-1.759712	-1.200553
C	2.387627	-0.671258	-2.534486
C	4.241204	-1.759741	1.201307
C	2.386868	-0.671278	2.534693
C	0.283599	4.060647	-0.000128
O	-2.005648	3.310487	-0.000453
C	-4.460985	0.170575	-1.198979
C	-2.370149	0.644210	-2.525574
C	-4.460463	0.170536	1.199842
C	-2.369068	0.643997	2.525575
C	2.620789	4.779705	0.000130
C	4.862779	-2.116659	0.000473
H	4.714385	-2.021880	-2.145258
H	2.260706	0.415975	-2.592684

H	3.009359	-0.987051	-3.378524
H	1.397708	-1.128176	-2.649478
H	4.713699	-2.021936	2.146156
H	1.396698	-1.127763	2.649200
H	3.008104	-0.987543	3.378921
H	2.260439	0.416007	2.593071
C	-0.097218	5.419254	-0.000138
C	-5.167784	0.051665	0.000580
H	-5.001336	0.146671	-2.143329
H	-1.457665	0.058198	-2.647748
H	-3.023737	0.430254	-3.377146
H	-2.104429	1.708889	-2.553491
H	-5.000406	0.146571	2.144425
H	-3.021874	0.428888	3.377452
H	-1.455946	0.058791	2.646799
H	-2.104304	1.708908	2.553969
H	3.669787	4.498379	0.000234
C	2.223350	6.105810	0.000123
C	6.193860	-2.833816	0.000667
H	-1.161620	5.635093	-0.000246
C	0.849895	6.428884	-0.000012
C	-6.660321	-0.187059	0.000922
H	2.968661	6.898946	0.000221
H	7.029512	-2.120296	0.000642
H	6.308648	-3.467442	0.887408
H	6.308787	-3.467662	-0.885900
H	0.536236	7.471100	-0.000018
H	-7.135821	0.247954	0.887482
H	-7.135985	0.246479	-0.886266
H	-6.892073	-1.261157	0.001850
C	0.832513	-3.434702	-0.000177
H	0.682286	-4.530814	-0.000331
H	1.869005	-3.101949	0.000004

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Three lowest frequencies (cm-1): 6.1692 13.1310 17.8639

Cartesian coordinates

ATOM	X	Y	Z
Cl	-0.953605	-2.188622	2.608654
Cl	-1.680533	-1.999848	-1.859154
Ru	-1.336171	-1.468355	0.404925
C	-2.762627	-0.401201	0.737234
H	-2.764032	0.689723	0.767709
C	-4.073154	-1.062335	1.064799
H	-4.186593	-0.985087	2.160242
H	-4.052329	-2.139536	0.843261
C	-5.304571	-0.577483	-1.150510
H	-4.365554	-0.180258	-1.563172
H	-5.317302	-1.646098	-1.399743
C	-6.475357	0.113304	-1.794788
H	-6.535039	1.192584	-1.637231
C	-7.424301	-0.486458	-2.515380
H	-7.408161	-1.558959	-2.699949
H	-8.248825	0.069296	-2.954435

C	0.155616	-0.229143	0.180186
N	0.244731	1.152490	0.154792
N	1.462422	-0.663898	-0.021373
C	1.558076	1.549024	-0.054951
C	-0.850642	2.080628	0.324222
C	2.314136	0.414086	-0.164666
C	1.864021	-2.058837	-0.060441
C	2.109878	2.908402	-0.149228
C	-1.159984	2.526631	1.617963
C	-1.545855	2.518099	-0.812693
C	3.768177	0.419669	-0.391384
C	2.276067	-2.676879	1.133293
C	1.906897	-2.719904	-1.300285
C	3.591197	2.958587	-0.378286
O	1.429526	3.922404	-0.049937
C	-2.223164	3.424342	1.755225
C	-0.388904	2.051141	2.825754
C	-2.600848	3.415379	-0.618272
C	-1.177587	2.047115	-2.198869
C	4.372259	1.787266	-0.491735
O	4.436102	-0.602054	-0.490599
C	2.610980	-4.032124	1.076143
C	2.462988	-1.903479	2.415456
C	2.249373	-4.075320	-1.296777
C	1.708654	-1.992857	-2.607514
C	4.203556	4.210238	-0.479766
C	-2.958246	3.876190	0.653520
H	-2.478123	3.782650	2.750018
H	0.673258	2.315474	2.753423
H	-0.782315	2.510523	3.737019
H	-0.452257	0.962556	2.941757
H	-3.151215	3.768378	-1.487468
H	-1.260074	0.957965	-2.292736
H	-1.836294	2.500807	-2.944924
H	-0.147508	2.325627	-2.453794
C	5.749405	1.891189	-0.703987
C	2.578212	-4.754960	-0.120323
H	2.916303	-4.530695	1.993117
H	1.626838	-1.234423	2.626770
H	2.559383	-2.586172	3.264004
H	3.383058	-1.305309	2.362062
H	2.272717	-4.606845	-2.245184
H	1.570965	-2.705673	-3.425184
H	0.837053	-1.336037	-2.594737
H	2.597113	-1.389073	-2.837793
H	3.583542	5.096183	-0.389807
C	5.579666	4.304511	-0.691525
C	-4.118595	4.827447	0.834427
H	6.328489	0.977347	-0.787709
C	6.352267	3.145693	-0.803448
C	2.896872	-6.231174	-0.140782
H	6.048536	5.281314	-0.769111
H	-4.252181	5.466633	-0.044521
H	-5.059374	4.281712	0.986369
H	-3.973640	5.473633	1.706408
H	7.423476	3.218840	-0.968085
H	3.305190	-6.540372	-1.108719

H	3.621860	-6.495742	0.636396
H	1.993716	-6.829177	0.039053
C	-5.289224	-0.402315	0.379950
H	-5.298281	0.668535	0.629192
H	-6.207056	-0.828503	0.804267

12red
Three lowest frequencies (cm-1): 8.3774 12.5902 17.4964

Cartesian coordinates

ATOM	X	Y	Z
Cl	0.876127	2.283824	2.601691
Cl	1.676323	2.022969	-1.874605
Ru	1.299743	1.521065	0.405673
C	2.732167	0.484520	0.784819
H	2.725118	-0.605032	0.854172
C	4.052213	1.137232	1.109425
H	4.167068	1.076150	2.205468
H	4.045670	2.209889	0.867219
C	5.287293	0.626167	-1.094715
H	4.331900	0.274798	-1.508966
H	5.351104	1.693631	-1.341987
C	6.424283	-0.118919	-1.737053
H	6.422474	-1.201344	-1.589085
C	7.412492	0.431438	-2.445157
H	7.457295	1.504693	-2.621828
H	8.207979	-0.166559	-2.883560
C	-0.185161	0.222397	0.176887
N	-0.230442	-1.149784	0.166936
N	-1.482877	0.631101	-0.030185
C	-1.549383	-1.602839	-0.036510
C	0.889841	-2.042066	0.308618
C	-2.340036	-0.472652	-0.167076
C	-1.907182	2.012239	-0.077132
C	-2.038133	-2.955496	-0.090949
C	1.216658	-2.526164	1.584284
C	1.603879	-2.426256	-0.836260
C	-3.760036	-0.489392	-0.398964
C	-2.349021	2.630841	1.105380
C	-1.956501	2.673376	-1.316417
C	-3.492129	-3.022211	-0.330838
O	-1.313770	-3.975173	0.055676
C	2.321689	-3.374717	1.701270
C	0.390261	-2.157696	2.790679
C	2.700890	-3.277851	-0.667926
C	1.193782	-1.955971	-2.210094
C	-4.305926	-1.856950	-0.476834
O	-4.464901	0.546876	-0.524042
C	-2.703638	3.981148	1.044463
C	-2.552977	1.845115	2.375711
C	-2.317472	4.024573	-1.322898
C	-1.757790	1.932175	-2.614119
C	-4.099210	-4.292910	-0.416090
C	3.081624	-3.754981	0.590223
H	2.584731	-3.758082	2.685427

H	-0.631693	-2.538804	2.680561
H	0.819500	-2.589880	3.700460
H	0.328902	-1.071518	2.923405
H	3.261988	-3.586392	-1.548213
H	1.265179	-0.866369	-2.304320
H	1.832268	-2.407085	-2.976745
H	0.156219	-2.239083	-2.422105
C	-5.689666	-2.015563	-0.702566
C	-2.666870	4.702386	-0.152172
H	-3.033318	4.474496	1.956742
H	-1.682470	1.237666	2.630862
H	-2.751721	2.517049	3.216581
H	-3.416856	1.178863	2.255339
H	-2.346337	4.550604	-2.275127
H	-1.713230	2.632446	-3.454381
H	-0.839186	1.342415	-2.620214
H	-2.606304	1.255051	-2.775720
H	-3.454104	-5.158885	-0.299973
C	-5.459284	-4.423803	-0.638998
C	4.287406	-4.654608	0.745706
H	-6.281287	-1.110972	-0.808650
C	-6.262843	-3.273112	-0.783749
C	-3.007867	6.174688	-0.179522
H	-5.909159	-5.412827	-0.702671
H	4.438169	-5.277565	-0.143162
H	5.208579	-4.073978	0.894452
H	4.181127	-5.319691	1.610019
H	-7.332246	-3.375089	-0.958552
H	-3.407366	6.475801	-1.154645
H	-3.751600	6.428224	0.584762
H	-2.120325	6.792967	0.013775
C	5.258429	0.449587	0.436030
H	5.235939	-0.622126	0.680940
H	6.187570	0.849011	0.864603

13

Three lowest frequencies (cm-1): 8.6414 21.9251 28.9213

Cartesian coordinates

ATOM	X	Y	Z
Ru	2.045732	0.534350	-0.020443
Cl	2.037350	0.707526	-2.440039
Cl	2.066473	0.720245	2.419330
C	2.741401	-1.152057	0.153049
H	2.439331	-1.757749	1.014868
C	0.067044	0.053425	0.011924
N	-0.618563	-1.142789	0.002231
N	-0.918713	1.023051	0.006584
C	-2.172761	0.440777	-0.007243
C	-1.987465	-0.915427	-0.009894
C	-3.494561	1.086321	-0.015667
C	-3.090773	-1.887822	-0.037404
C	-4.648117	0.129927	-0.033437
C	-4.457588	-1.269497	-0.044304
O	-3.649036	2.301305	-0.008419

O	-2.923191	-3.100817	-0.056057
C	-5.944065	0.652553	-0.040303
H	-6.064895	1.730900	-0.031968
C	-5.567674	-2.117782	-0.062328
H	-5.396947	-3.189308	-0.070977
C	-7.046407	-0.202504	-0.057616
H	-8.050962	0.210784	-0.062652
C	-6.858110	-1.587084	-0.068759
H	-7.716007	-2.253317	-0.082453
C	-0.027904	-2.465201	0.035437
C	0.166972	-3.080761	1.283394
C	0.276316	-3.103560	-1.176453
C	0.730727	-4.359453	1.291831
C	0.839598	-4.382940	-1.107998
C	1.076119	-5.025827	0.110483
H	0.897184	-4.848925	2.248859
H	1.086620	-4.892128	-2.036839
C	-0.652141	2.452864	0.020120
C	-0.581328	3.117145	1.258654
C	-0.572466	3.142299	-1.203404
C	-0.267978	4.479386	1.242885
C	-0.256743	4.504383	-1.156750
C	-0.071219	5.183606	0.050786
H	-0.196075	5.005146	2.192134
H	-0.177630	5.049768	-2.094294
C	-0.204008	-2.394668	2.575587
H	-1.272972	-2.149670	2.605254
H	0.008470	-3.046459	3.427918
H	0.355252	-1.461288	2.714512
C	-0.012145	-2.461177	-2.510575
H	0.526861	-1.515258	-2.634109
H	0.280236	-3.128531	-3.326631
H	-1.083731	-2.252643	-2.622650
C	1.649368	-6.423424	0.152098
H	2.286142	-6.570204	1.031160
H	0.850217	-7.175010	0.201361
H	2.245407	-6.639787	-0.740523
C	-0.927078	2.492763	-2.517677
H	-0.678828	3.157083	-3.350207
H	-0.394081	1.553246	-2.675832
H	-2.007285	2.298378	-2.558550
C	-0.935137	2.435146	2.556226
H	-0.361043	1.519248	2.710237
H	-0.733216	3.098463	3.401973
H	-2.005675	2.190758	2.574174
C	0.310865	6.645006	0.068928
H	-0.037562	7.162074	-0.831308
H	-0.108098	7.158075	0.941220
H	1.401368	6.766268	0.113527
C	3.828329	2.102472	0.112598
H	3.412330	2.852090	-0.558110
H	3.854778	2.339123	1.172257
C	3.848594	-1.733499	-0.667357
H	3.741611	-2.826019	-0.711779
H	3.803775	-1.339553	-1.686779
C	5.349710	0.084871	0.416764
H	5.064435	0.179759	1.469761

H	6.403226	0.393345	0.342876
C	4.519279	1.041443	-0.397422
H	4.566590	0.939999	-1.479571
C	5.235973	-1.389417	-0.044867
H	5.997210	-1.618255	-0.800390
H	5.437736	-2.043349	0.811336

13red
Three lowest frequencies (cm-1): 12.7118 22.4960 29.8840

Cartesian coordinates

ATOM	X	Y	Z
Ru	-2.040433	-0.489753	0.042622
Cl	-2.111726	-0.822347	-2.369837
Cl	-1.997382	-0.496221	2.501472
C	-2.707479	1.211806	0.111545
H	-2.359817	1.877745	0.909058
C	-0.029268	-0.036385	0.012435
N	0.672172	1.138275	0.006727
N	0.915308	-1.028808	0.008779
C	2.211188	-0.489057	0.003716
C	2.059263	0.889069	0.005467
C	3.474763	-1.175935	-0.005263
C	3.148869	1.830185	0.009975
C	4.622612	-0.251451	-0.013775
C	4.468122	1.169246	-0.006466
O	3.591904	-2.430589	-0.008724
O	3.002951	3.080493	0.032383
C	5.924298	-0.796104	-0.028649
H	6.008051	-1.878986	-0.033761
C	5.622942	1.979825	-0.012766
H	5.472726	3.055460	-0.005567
C	7.042464	0.019829	-0.036317
H	8.038393	-0.419078	-0.048344
C	6.890161	1.422637	-0.028138
H	7.768704	2.065157	-0.033841
C	0.103312	2.461956	-0.016784
C	-0.053017	3.160075	1.192996
C	-0.243558	3.032145	-1.250994
C	-0.628061	4.432342	1.144975
C	-0.814371	4.311175	-1.245161
C	-1.018546	5.024175	-0.061704
H	-0.761199	4.979848	2.076384
H	-1.089694	4.763355	-2.196281
C	0.593762	-2.439089	-0.004359
C	0.469310	-3.128440	1.215892
C	0.502161	-3.108740	-1.238130
C	0.079253	-4.471431	1.171649
C	0.113165	-4.452017	-1.226787
C	-0.133840	-5.141507	-0.036292
H	-0.031357	-5.011137	2.110288
H	0.025797	-4.975408	-2.176942
C	0.397148	2.565348	2.502920
H	1.479240	2.392049	2.486468
H	0.174313	3.247150	3.330387

H	-0.097892	1.608286	2.704210
C	0.016549	2.311640	-2.550386
H	-0.562618	1.384580	-2.625163
H	-0.245883	2.949586	-3.401052
H	1.077180	2.047995	-2.638689
C	-1.600566	6.419754	-0.083955
H	-2.262883	6.593512	0.772427
H	-0.810271	7.181868	-0.039816
H	-2.176121	6.600099	-0.998700
C	0.933762	-2.451588	-2.523628
H	0.678409	-3.080829	-3.382228
H	0.461069	-1.478627	-2.668786
H	2.022537	-2.314913	-2.506987
C	0.872679	-2.494077	2.522038
H	0.366439	-1.542022	2.694078
H	0.637374	-3.158384	3.360029
H	1.956133	-2.319622	2.515749
C	-0.595898	-6.580889	-0.054686
H	-0.226151	-7.108908	-0.941113
H	-0.250118	-7.124124	0.832262
H	-1.692580	-6.649997	-0.070190
C	-3.815753	-2.024809	0.341794
H	-3.420730	-2.825769	-0.280403
H	-3.810747	-2.180040	1.416715
C	-3.834933	1.749126	-0.716425
H	-3.720177	2.834561	-0.842836
H	-3.817259	1.281958	-1.705573
C	-5.311273	0.025789	0.537862
H	-4.984479	0.010966	1.583010
H	-6.369924	-0.277251	0.528919
C	-4.510554	-0.995913	-0.228240
H	-4.590360	-0.974399	-1.313004
C	-5.206577	1.460325	-0.038438
H	-5.989858	1.632051	-0.788241
H	-5.386122	2.178461	0.771049

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Three lowest frequencies (cm-1): 13.0332 19.9338 30.5607

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.844789	0.636600	2.604519
Cl	-2.107801	0.661532	-2.249746
C	-3.145900	2.192888	0.265510
H	-3.182534	2.747837	-0.671618
Ru	-1.977123	0.561815	0.177921
C	-4.189759	1.078715	0.397077
C	-3.592756	-0.501260	0.405125
H	-4.600265	1.137305	1.408626
H	-3.679101	-0.906464	1.415520
C	-4.380319	-1.264723	-0.654257
H	-3.841402	-1.292448	-1.603005
H	-4.553707	-2.295096	-0.325150
C	-5.242173	1.006708	-0.725519
H	-6.066797	1.695786	-0.509538

H	-4.781307	1.312903	-1.669261
H	-2.996497	2.796593	1.158898
C	0.022893	0.096270	0.054757
N	0.566228	-1.160485	0.030758
N	1.077519	0.968832	0.004153
C	1.949130	-1.071170	-0.029925
C	-0.203349	-2.394507	0.061433
C	2.268651	0.260149	-0.046257
C	0.948837	2.418796	-0.002715
C	2.946494	-2.152157	-0.072306
C	-0.594997	-2.974908	-1.156282
C	-0.468402	-2.993516	1.304390
C	3.648330	0.768435	-0.101937
C	0.869555	3.082339	-1.238780
C	0.984122	3.107071	1.222139
C	4.366865	-1.676097	-0.127492
O	2.650073	-3.339798	-0.062739
C	-1.355780	-4.146963	-1.094266
C	-0.183907	-2.401240	-2.489515
C	-1.233096	-4.164013	1.303605
C	0.080995	-2.440617	2.595773
C	4.696960	-0.302255	-0.140091
O	3.924575	1.960968	-0.114247
C	0.703683	4.470756	-1.213401
C	1.022704	2.356816	-2.552264
C	0.815362	4.494454	1.184284
C	1.264477	2.408571	2.529185
C	5.385015	-2.632420	-0.164753
C	-1.695450	-4.749219	0.120617
H	-1.676990	-4.606412	-2.026258
H	0.908282	-2.328925	-2.566798
H	-0.528860	-3.047269	-3.302052
H	-0.604211	-1.402739	-2.649738
H	-1.457963	-4.636899	2.256917
H	-0.284952	-1.428001	2.793330
H	-0.214814	-3.075415	3.435996
H	1.177875	-2.412038	2.574450
C	6.038323	0.086191	-0.188880
C	0.649975	5.191177	-0.016711
H	0.631205	5.001360	-2.159875
H	0.242476	1.603074	-2.694029
H	0.960574	3.063928	-3.384409
H	2.000282	1.861324	-2.612285
H	0.831748	5.044118	2.122589
H	1.271212	3.131011	3.350420
H	0.510174	1.649768	2.756797
H	2.249339	1.924575	2.507291
H	5.107486	-3.681393	-0.154223
C	6.721463	-2.234800	-0.213147
C	-2.490932	-6.033679	0.152976
H	6.267585	1.146773	-0.197467
C	7.047934	-0.876090	-0.224904
C	0.430806	6.685875	-0.020187
H	7.507359	-2.984113	-0.241198
H	-1.826487	-6.908039	0.165660
H	-3.121435	-6.092550	1.046535
H	-3.136352	-6.127661	-0.726483

H	8.088349	-0.566112	-0.262092
H	0.946671	7.168616	0.816779
H	0.788151	7.141423	-0.949646
H	-0.636350	6.927729	0.072687
C	-5.690187	-0.461299	-0.811672
H	-6.211362	-0.688465	-1.748304
H	-6.376782	-0.695626	0.013116

14red
 Three lowest frequencies (cm-1): 12.0288 15.7535 30.7938

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.859407	0.846584	2.570472
Cl	-2.070073	0.493599	-2.289235
C	-3.097356	2.222081	0.095645
H	-3.128766	2.704848	-0.881502
Ru	-1.950142	0.584422	0.148338
C	-4.167145	1.131804	0.308174
C	-3.593048	-0.431160	0.433759
H	-4.590042	1.288903	1.304359
H	-3.687377	-0.769619	1.468093
C	-4.377614	-1.266839	-0.575085
H	-3.827417	-1.368907	-1.512228
H	-4.563635	-2.269623	-0.174615
C	-5.212806	1.000546	-0.816275
H	-6.031813	1.713323	-0.659476
H	-4.737041	1.232619	-1.773771
H	-2.957821	2.896132	0.939735
C	0.054813	0.093460	0.061624
N	0.569753	-1.165303	0.047418
N	1.106419	0.954133	0.009356
C	1.975810	-1.110460	-0.017092
C	-0.223578	-2.373892	0.101974
C	2.316225	0.234854	-0.039391
C	0.981218	2.396475	-0.004057
C	2.919349	-2.195435	-0.062176
C	-0.577288	-3.012929	-1.099240
C	-0.567781	-2.906877	1.354480
C	3.662658	0.737860	-0.095161
C	0.874465	3.059980	-1.237770
C	1.039951	3.098887	1.211916
C	4.317025	-1.726498	-0.119426
O	2.593325	-3.411309	-0.060425
C	-1.383763	-4.151361	-1.019565
C	-0.049076	-2.536928	-2.427824
C	-1.375557	-4.050223	1.377698
C	-0.041662	-2.316269	2.638670
C	4.667926	-0.341209	-0.133659
O	3.955968	1.962104	-0.105480
C	0.695545	4.447753	-1.219220
C	1.034419	2.326537	-2.545304
C	0.858670	4.484591	1.173805
C	1.376033	2.405409	2.507044
C	5.345926	-2.690902	-0.162734

C	-1.804586	-4.677580	0.205986
H	-1.672379	-4.649669	-1.943300
H	1.043216	-2.631863	-2.447071
H	-0.458313	-3.143866	-3.242197
H	-0.310926	-1.492042	-2.617505
H	-1.655952	-4.468994	2.342422
H	-0.434294	-1.309828	2.816758
H	-0.322716	-2.946464	3.489034
H	1.052495	-2.253928	2.610278
C	6.031822	0.015840	-0.187696
C	0.660158	5.173752	-0.026165
H	0.604372	4.972799	-2.168173
H	0.274613	1.550476	-2.674947
H	0.953479	3.024233	-3.385381
H	2.022813	1.853247	-2.590313
H	0.895021	5.039232	2.109558
H	1.380914	3.123166	3.333928
H	0.654193	1.619701	2.745681
H	2.374031	1.956179	2.439135
H	5.046922	-3.734968	-0.152009
C	6.677532	-2.316291	-0.215615
C	-2.649408	-5.930877	0.258310
H	6.266151	1.076314	-0.196690
C	7.024050	-0.948627	-0.227815
C	0.427061	6.667520	-0.031597
H	7.457040	-3.075143	-0.247614
H	-2.035171	-6.832210	0.124889
H	-3.164927	-6.026733	1.220227
H	-3.407385	-5.937993	-0.533889
H	8.070713	-0.653078	-0.269167
H	0.976791	7.161871	0.777781
H	0.741806	7.118615	-0.979414
H	-0.636456	6.907735	0.106077
C	-5.677256	-0.465524	-0.807358
H	-6.190936	-0.751605	-1.733192
H	-6.377754	-0.633524	0.023315

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Three lowest frequencies (cm-1): 14.5287 19.6569 29.0980

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.964854	0.422534	2.607580
Cl	-2.123589	0.500915	-2.251791
Ru	-1.965635	0.489480	0.171396
C	-4.505881	0.971233	0.663833
C	-4.287716	-0.320991	0.280396
H	-4.258765	1.364035	1.643241
H	-3.899668	-1.085051	0.953350
C	-5.391621	1.697911	-0.322981
H	-6.364557	1.866056	0.164268
H	-5.012176	2.686054	-0.604447
C	-5.031405	-0.654776	-0.996596
H	-4.416890	-1.189371	-1.726360
H	-5.878856	-1.307771	-0.737621

C	0.012933	0.106239	0.073283
N	1.112624	0.934621	0.016989
N	0.520161	-1.174465	0.029941
C	2.272761	0.176891	-0.060105
C	1.088423	2.383434	0.046994
C	1.901092	-1.140719	-0.052878
C	-0.306230	-2.368668	0.092945
C	3.671574	0.625912	-0.134724
C	1.166549	3.033493	1.290900
C	1.061251	3.085295	-1.170294
C	2.850628	-2.261124	-0.120522
C	-0.571415	-2.938293	1.352038
C	-0.739586	-2.963269	-1.106271
C	4.674355	-0.487799	-0.200145
O	4.002265	1.804894	-0.143203
C	1.149816	4.431378	1.290356
C	1.284302	2.267354	2.584880
C	1.046751	4.482094	-1.109137
C	1.069835	2.374687	-2.500480
C	4.288727	-1.846788	-0.194818
O	2.502355	-3.435426	-0.116346
C	-1.409627	-4.056922	1.389833
C	0.080163	-2.432001	2.614530
C	-1.573314	-4.081785	-1.005204
C	-0.263840	-2.488132	-2.456069
C	6.029507	-0.154702	-0.269090
C	1.084733	5.172785	0.106156
H	1.199775	4.952094	2.243992
H	2.188409	1.645328	2.594638
H	1.350309	2.957406	3.431012
H	0.422182	1.611015	2.749428
H	1.015675	5.042499	-2.040755
H	0.199090	1.719449	-2.616486
H	1.061227	3.099549	-3.319682
H	1.972361	1.760574	-2.612692
C	5.265283	-2.844069	-0.259313
C	-1.940907	-4.627090	0.228781
H	-1.633768	-4.503947	2.355493
H	-0.154700	-1.380789	2.802405
H	-0.265577	-3.009201	3.476798
H	1.170558	-2.544308	2.556399
H	-1.924570	-4.549988	-1.921767
H	-0.715838	-3.089603	-3.250076
H	-0.525265	-1.442078	-2.637963
H	0.825287	-2.596446	-2.538316
H	6.302466	0.895517	-0.271893
C	6.997893	-1.157340	-0.332202
C	1.103434	6.683344	0.137889
H	4.944546	-3.880715	-0.254284
C	6.616133	-2.501474	-0.327613
C	-2.872702	-5.813764	0.305101
H	8.049396	-0.889881	-0.385177
H	2.133500	7.063918	0.124783
H	0.587982	7.109374	-0.729184
H	0.625236	7.071412	1.043424
H	7.369801	-3.282159	-0.377020
H	-2.784049	-6.450619	-0.581394

H	-2.667765	-6.427611	1.188517
H	-3.919901	-5.489517	0.369654
C	-1.877261	2.300943	0.179228
H	-1.946303	2.886816	-0.744273
H	-1.811605	2.870798	1.113332
C	-5.504721	0.724825	-1.526686
H	-6.520410	0.687753	-1.932246
H	-4.831613	1.048138	-2.323131

15red
 Three lowest frequencies (cm-1): 11.6219 18.3387 26.8279

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.928322	0.557771	2.616802
Cl	-2.095917	0.551986	-2.262631
Ru	-1.924440	0.568635	0.168484
C	-4.476750	1.039592	0.665045
C	-4.267474	-0.249193	0.277661
H	-4.207022	1.435798	1.636787
H	-3.852508	-1.015323	0.931846
C	-5.360693	1.775321	-0.318112
H	-6.335216	1.954016	0.163875
H	-4.967678	2.758578	-0.599427
C	-5.011838	-0.578145	-0.999473
H	-4.392315	-1.107295	-1.728925
H	-5.862781	-1.231188	-0.749108
C	0.057517	0.120384	0.081157
N	1.180206	0.896445	0.019238
N	0.489751	-1.176161	0.051776
C	2.330928	0.085065	-0.052186
C	1.212146	2.337596	0.040840
C	1.891009	-1.229847	-0.031570
C	-0.407004	-2.308446	0.107188
C	3.711919	0.481317	-0.137216
C	1.314664	2.998502	1.276996
C	1.206632	3.039964	-1.176364
C	2.745477	-2.384072	-0.088014
C	-0.741188	-2.855769	1.359833
C	-0.866217	-2.881314	-1.092869
C	4.629640	-0.673294	-0.194778
O	4.102083	1.677696	-0.163200
C	1.335777	4.396626	1.271943
C	1.433145	2.230747	2.568911
C	1.228801	4.437296	-1.125943
C	1.219882	2.315404	-2.497760
C	4.173463	-2.027756	-0.171812
O	2.321265	-3.570691	-0.069955
C	-1.674288	-3.897660	1.390297
C	-0.038416	-2.420030	2.619876
C	-1.796416	-3.922935	-1.006053
C	-0.292029	-2.476967	-2.425929
C	6.015433	-0.422622	-0.278244
C	1.286771	5.133247	0.084819
H	1.408135	4.920211	2.223525

H	2.315873	1.580657	2.546816
H	1.539418	2.918517	3.414345
H	0.554634	1.600934	2.748280
H	1.217244	4.992727	-2.062004
H	0.351559	1.656950	-2.608593
H	1.216745	3.030297	-3.327314
H	2.124694	1.701604	-2.581680
C	5.124142	-3.068598	-0.233501
C	-2.233924	-4.425226	0.222784
H	-1.946884	-4.322779	2.354316
H	-0.150123	-1.348506	2.801830
H	-0.442376	-2.953256	3.486596
H	1.030522	-2.653378	2.541067
H	-2.165289	-4.367914	-1.928196
H	-0.821382	-2.981431	-3.240895
H	-0.361862	-1.399821	-2.593531
H	0.764152	-2.771084	-2.467658
H	6.330502	0.616679	-0.294026
C	6.929704	-1.460556	-0.337164
C	1.350513	6.643912	0.107851
H	4.746268	-4.086721	-0.214905
C	6.479280	-2.797459	-0.314587
C	-3.268440	-5.525839	0.288308
H	7.994926	-1.246499	-0.401093
H	2.389840	6.999110	0.072988
H	0.829722	7.081095	-0.751655
H	0.899521	7.051033	1.019993
H	7.197290	-3.614117	-0.361217
H	-3.231501	-6.163889	-0.601987
H	-3.119924	-6.162380	1.168038
H	-4.286366	-5.116734	0.352390
C	-1.765083	2.373732	0.138241
H	-1.816180	2.944960	-0.796027
H	-1.652848	2.959012	1.058795
C	-5.477289	0.805874	-1.524824
H	-4.794638	1.125748	-2.314839
H	-6.491953	0.777423	-1.936594

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Three lowest frequencies (cm-1): 13.1049 15.1317 23.7132

Cartesian coordinates

ATOM	X	Y	Z
Cl	0.969728	-1.557071	2.733739
Cl	1.615824	-1.549967	-2.075235
Ru	1.167635	-1.528693	0.310429
C	0.254151	-3.096525	0.166226
H	0.128491	-3.606178	-0.795521
H	-0.145619	-3.617032	1.043754
C	2.846111	-3.358289	0.663926
H	2.899174	-3.963042	-0.238163
H	2.413957	-3.808552	1.550723
C	3.525765	-2.173247	0.749019
H	3.561301	-1.688964	1.725490
C	4.510233	-1.683860	-0.285293

H	5.480725	-2.127507	-0.011881
H	4.240246	-2.076188	-1.271171
C	4.650015	-0.157269	-0.340664
H	3.681430	0.275570	-0.612287
H	4.906786	0.227202	0.656245
C	5.698999	0.339131	-1.359387
H	5.622463	1.431106	-1.436325
H	5.436957	-0.064486	-2.349048
C	7.118920	-0.032407	-1.022336
H	7.361272	-1.095999	-1.037276
C	8.081586	0.836847	-0.708587
H	7.896867	1.909786	-0.688356
H	9.091019	0.515097	-0.465672
C	-0.397205	-0.254186	0.114845
N	-1.743201	-0.527237	-0.029785
N	-0.311886	1.120810	0.137450
C	-2.466216	0.655140	-0.087624
C	-2.345713	-1.841827	-0.123078
C	-1.571639	1.684873	0.019223
C	0.925844	1.876597	0.228183
C	-3.917078	0.849198	-0.241141
C	-2.824154	-2.452900	1.049222
C	-2.513614	-2.417549	-1.395467
C	-1.954192	3.105444	0.014131
C	1.387548	2.277014	1.494601
C	1.548908	2.287753	-0.964171
C	-4.349343	2.284912	-0.256482
O	-4.713384	-0.074616	-0.349471
C	-3.424454	-3.709346	0.923054
C	-2.720719	-1.782515	2.396102
C	-3.122286	-3.674183	-1.460280
C	-2.077325	-1.709203	-2.653595
C	-3.425849	3.346783	-0.136277
O	-1.147607	4.019976	0.126470
C	2.572727	3.018634	1.543075
C	0.609286	2.003875	2.757139
C	2.721745	3.040691	-0.852845
C	0.962395	1.986946	-2.321170
C	-5.711445	2.565235	-0.393104
C	-3.579249	-4.337818	-0.316698
H	-3.790850	-4.202298	1.820578
H	-3.273268	-0.834461	2.407189
H	-3.148505	-2.421903	3.173640
H	-1.679977	-1.569237	2.665130
H	-3.251282	-4.139242	-2.434995
H	-0.998409	-1.516092	-2.658520
H	-2.317540	-2.313178	-3.533315
H	-2.592343	-0.746376	-2.763011
C	-3.883095	4.667007	-0.154675
C	3.260764	3.398176	0.387257
H	2.949297	3.329949	2.514615
H	0.455343	0.933455	2.922211
H	1.141681	2.405060	3.624363
H	-0.373007	2.492230	2.717973
H	3.216615	3.367310	-1.764564
H	1.580546	2.429659	-3.107485
H	0.903788	0.909194	-2.505179

H	-0.046319	2.408003	-2.418272
H	-6.402184	1.733291	-0.483493
C	-6.158830	3.886703	-0.410906
C	-4.264538	-5.680059	-0.424585
H	-3.154973	5.465956	-0.059857
C	-5.245079	4.937161	-0.291577
C	4.549767	4.180921	0.474507
H	-7.219291	4.096562	-0.517379
H	-5.338615	-5.558257	-0.618349
H	-3.852344	-6.276083	-1.245725
H	-4.163322	-6.257451	0.500088
H	-5.593077	5.966085	-0.304807
H	4.672383	4.847776	-0.385650
H	4.589414	4.787736	1.385143
H	5.417961	3.508584	0.492663

16red
 Three lowest frequencies (cm-1): 10.9884 13.5697 22.5741

Cartesian coordinates

ATOM	X	Y	Z
Cl	0.910236	-1.682120	2.715004
Cl	1.662199	-1.425138	-2.092581
Ru	1.159041	-1.526717	0.292511
C	0.251573	-3.082200	0.033420
H	0.153811	-3.533144	-0.960683
H	-0.181802	-3.650898	0.864560
C	2.847960	-3.350716	0.632488
H	2.916901	-3.948549	-0.273385
H	2.390840	-3.803969	1.504600
C	3.518383	-2.163495	0.733871
H	3.533188	-1.680168	1.711513
C	4.514089	-1.665801	-0.287390
H	5.482258	-2.124375	-0.027936
H	4.234299	-2.032227	-1.280736
C	4.665246	-0.140007	-0.314294
H	3.694833	0.306260	-0.552214
H	4.950670	0.223053	0.682956
C	5.688096	0.371149	-1.351992
H	5.625161	1.465594	-1.396967
H	5.385535	-0.002246	-2.342067
C	7.112332	-0.031816	-1.077828
H	7.330000	-1.100560	-1.114591
C	8.107347	0.810580	-0.790934
H	7.946926	1.886637	-0.745333
H	9.118161	0.462297	-0.591726
C	-0.425824	-0.240634	0.114823
N	-1.759872	-0.513943	-0.031504
N	-0.324720	1.122241	0.142628
C	-2.503547	0.680935	-0.095066
C	-2.355409	-1.823192	-0.124408
C	-1.592592	1.719398	0.017259
C	0.915126	1.855308	0.263847
C	-3.925118	0.852361	-0.244391
C	-2.853246	-2.433943	1.040594

C	-2.501864	-2.416838	-1.390702
C	-1.935859	3.116581	0.002631
C	1.386012	2.198849	1.543720
C	1.552298	2.313019	-0.903842
C	-4.325240	2.272150	-0.265346
O	-4.743985	-0.098744	-0.343962
C	-3.432138	-3.700194	0.919221
C	-2.804014	-1.733392	2.373489
C	-3.090751	-3.684025	-1.457265
C	-2.076571	-1.697742	-2.645464
C	-3.385524	3.342010	-0.148093
O	-1.095777	4.049435	0.103424
C	2.587029	2.912602	1.629389
C	0.579241	1.912869	2.784850
C	2.741601	3.034353	-0.761441
C	0.933821	2.119805	-2.264414
C	-5.694899	2.580341	-0.406058
C	-3.555606	-4.343707	-0.316352
H	-3.813411	-4.186489	1.815222
H	-3.378613	-0.800612	2.330569
H	-3.239392	-2.365152	3.154697
H	-1.776527	-1.488433	2.662886
H	-3.202772	-4.155987	-2.431680
H	-1.005072	-1.469061	-2.641334
H	-2.293826	-2.307238	-3.528825
H	-2.621677	-0.751328	-2.743454
C	-3.858136	4.671097	-0.177766
C	3.285948	3.326539	0.492982
H	2.962619	3.180710	2.615029
H	0.396718	0.843471	2.922437
H	1.101381	2.285750	3.672220
H	-0.390223	2.422130	2.722211
H	3.240192	3.396555	-1.658549
H	1.601840	2.497034	-3.045660
H	0.730882	1.065488	-2.471282
H	-0.009572	2.675663	-2.324493
H	-6.383977	1.745301	-0.492332
C	-6.135240	3.892524	-0.432434
C	-4.225309	-5.695336	-0.421099
H	-3.119050	5.461681	-0.086485
C	-5.207111	4.948982	-0.317062
C	4.590699	4.080095	0.615810
H	-7.196031	4.110017	-0.542040
H	-5.309881	-5.591503	-0.563972
H	-3.839851	-6.270118	-1.270801
H	-4.073787	-6.289901	0.486970
H	-5.552365	5.980968	-0.337498
H	4.724560	4.786112	-0.211853
H	4.639928	4.644771	1.553660
H	5.451320	3.396749	0.602598

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Three lowest frequencies (cm-1): 10.3097 14.5374 25.0589

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.240176	-1.838316	-2.157688
Cl	-0.666128	-1.812287	2.664766
C	-0.624633	-3.733629	0.238301
H	-0.082869	-4.129867	1.095853
Ru	-0.940621	-1.792475	0.249245
H	-0.332760	-4.144225	-0.727650
C	-2.860841	-2.216048	0.598906
H	-3.098015	-2.021260	1.647412
C	-2.179424	-3.664816	0.446157
H	-2.389248	-4.163164	1.394298
H	-2.653587	-4.129640	-0.418559
C	-4.050533	-1.989071	-0.315760
H	-4.773557	-2.793630	-0.091256
H	-3.758881	-2.103983	-1.362738
C	-4.760817	-0.646639	-0.100207
H	-5.006405	-0.525058	0.965026
H	-4.092428	0.180061	-0.363844
C	-6.052674	-0.554339	-0.937313
H	-5.806301	-0.625695	-2.004897
H	-6.679166	-1.430038	-0.702602
C	-6.854563	0.692583	-0.683767
H	-7.173625	0.848749	0.348890
C	-7.204721	1.587927	-1.610171
H	-6.913884	1.473481	-2.652793
H	-7.804555	2.461254	-1.366528
C	0.375721	-0.214463	0.099399
N	0.146090	1.133231	0.138132
N	1.731985	-0.363403	-0.051321
C	1.347477	1.819135	0.013712
C	-1.149429	1.776137	0.290635
C	2.337290	0.881776	-0.105565
C	2.427609	-1.639583	-0.133664
C	1.593020	3.270980	0.001681
C	-1.582512	2.116947	1.581332
C	-1.857794	2.141551	-0.867748
C	3.763785	1.211326	-0.262146
C	2.933924	-2.210520	1.046096
C	2.642829	-2.209452	-1.400216
C	3.036474	3.648800	-0.149185
O	0.704838	4.106395	0.105550
C	-2.803377	2.792133	1.691978
C	-0.756203	1.830630	2.810293
C	-3.066419	2.820177	-0.694581
C	-1.330687	1.857377	-2.252726
C	4.057527	2.680385	-0.272483
O	4.639816	0.363920	-0.374842
C	3.567578	-3.452575	0.937878
C	2.872696	-1.500289	2.375319
C	3.284088	-3.450895	-1.445910
C	2.269415	-1.496159	-2.675568
C	3.366247	5.006660	-0.165324
C	-3.557535	3.152811	0.573655
H	-3.158054	3.062197	2.683805
H	0.217170	2.335270	2.757020
H	-1.267458	2.198698	3.704477
H	-0.575936	0.758440	2.939923

H	-3.633531	3.106140	-1.577258
H	-1.211017	0.782869	-2.429718
H	-2.017586	2.250708	-3.007654
H	-0.356349	2.336469	-2.413223
C	5.386881	3.089286	-0.409173
C	3.732016	-4.099243	-0.290665
H	3.958534	-3.914924	1.841219
H	1.842961	-1.291349	2.679617
H	3.334153	-2.114353	3.154002
H	3.422877	-0.551338	2.334841
H	3.452531	-3.911704	-2.416532
H	2.531775	-2.108665	-3.542957
H	1.196939	-1.286432	-2.725672
H	2.814608	-0.547548	-2.764200
H	2.565526	5.732645	-0.069420
C	4.696246	5.405397	-0.301608
C	-4.856251	3.909912	0.717370
H	6.153692	2.327207	-0.502446
C	5.706216	4.447215	-0.423326
C	4.388019	-5.457698	-0.371258
H	4.944557	6.462822	-0.312897
H	-4.771845	4.920889	0.298427
H	-5.665874	3.401984	0.181616
H	-5.148098	4.008394	1.767695
H	6.741723	4.757648	-0.529407
H	4.949523	-5.576636	-1.304137
H	5.076436	-5.620984	0.464449
H	3.638853	-6.259971	-0.338727

17red

Three lowest frequencies (cm-1): 8.7529 13.7947 18.9141

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.201120	-1.730761	-2.210034
Cl	-0.673457	-1.945585	2.629505
C	-0.599560	-3.729536	0.102502
H	-0.054426	-4.162282	0.940701
Ru	-0.914675	-1.793199	0.208266
H	-0.303276	-4.093344	-0.881020
C	-2.835681	-2.239839	0.508561
H	-3.095874	-2.088519	1.559568
C	-2.155897	-3.682508	0.313796
H	-2.366933	-4.220860	1.239984
H	-2.625989	-4.121503	-0.567464
C	-4.015434	-1.986153	-0.415337
H	-4.740569	-2.801793	-0.237274
H	-3.702066	-2.055720	-1.460153
C	-4.734473	-0.655364	-0.163800
H	-4.990576	-0.568248	0.902620
H	-4.068356	0.182395	-0.394316
C	-6.020198	-0.544236	-1.008400
H	-5.765094	-0.580916	-2.075852
H	-6.642812	-1.431752	-0.806225
C	-6.834806	0.687286	-0.724256

H	-7.142450	0.820982	0.315183
C	-7.203818	1.598847	-1.627149
H	-6.916038	1.513374	-2.673408
H	-7.803744	2.464649	-1.357295
C	0.393497	-0.191495	0.110685
N	0.147110	1.144017	0.150406
N	1.739560	-0.340153	-0.043103
C	1.352574	1.863869	0.013694
C	-1.145784	1.762449	0.344968
C	2.361843	0.920069	-0.108303
C	2.426207	-1.613351	-0.108641
C	1.558510	3.288711	-0.014200
C	-1.575584	2.035351	1.652920
C	-1.877779	2.178891	-0.780779
C	3.758240	1.226289	-0.270259
C	2.910002	-2.187347	1.079252
C	2.660953	-2.200985	-1.363403
C	2.981218	3.650657	-0.167966
O	0.635096	4.138467	0.075134
C	-2.808509	2.678978	1.813625
C	-0.717802	1.719732	2.852438
C	-3.099132	2.821638	-0.563916
C	-1.335680	2.009216	-2.177208
C	4.020018	2.677209	-0.288019
O	4.660100	0.355267	-0.385604
C	3.520636	-3.442897	0.995772
C	2.858011	-1.447764	2.391617
C	3.276718	-3.456435	-1.390794
C	2.353883	-1.470548	-2.645433
C	3.322781	5.019190	-0.200332
C	-3.582674	3.079616	0.723782
H	-3.153167	2.897429	2.822528
H	0.258309	2.211895	2.765744
H	-1.197643	2.081006	3.768007
H	-0.545746	0.643885	2.959189
H	-3.677269	3.147340	-1.426358
H	-1.091048	0.965100	-2.396616
H	-2.067370	2.352689	-2.915975
H	-0.424934	2.607969	-2.299116
C	5.353095	3.116222	-0.433747
C	3.690425	-4.104553	-0.223479
H	3.892358	-3.901584	1.910018
H	1.830744	-1.218159	2.687371
H	3.312375	-2.049110	3.185883
H	3.417410	-0.507765	2.313954
H	3.458236	-3.925125	-2.356220
H	2.583375	-2.102425	-3.509795
H	1.302133	-1.178902	-2.708504
H	2.971283	-0.566247	-2.710410
H	2.510798	5.734562	-0.108537
C	4.638196	5.426298	-0.342777
C	-4.888870	3.814213	0.921000
H	6.119480	2.351909	-0.523387
C	5.664049	4.464779	-0.460467
C	4.319289	-5.478221	-0.280705
H	4.881776	6.486828	-0.364495
H	-4.801789	4.866581	0.618442

H	-5.689130	3.368471	0.319124
H	-5.201260	3.798249	1.970914
H	6.698433	4.784101	-0.572803
H	4.876909	-5.624895	-1.212884
H	5.009436	-5.638055	0.555455
H	3.558977	-6.270163	-0.230097

TS1
Three lowest frequencies (cm-1): -153.4318 13.0383 20.1851

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.863441	0.772421	2.589864
Cl	-2.111476	0.720168	-2.271238
C	-3.321856	2.236462	0.227901
H	-3.322302	2.753625	-0.730168
Ru	-1.988993	0.628998	0.162185
C	-4.249563	1.126255	0.386679
C	-3.371698	-0.634510	0.386690
H	-4.600546	1.010802	1.413020
H	-3.517935	-0.977965	1.416804
C	-4.177893	-1.386092	-0.647594
H	-3.706004	-1.334711	-1.629720
H	-4.258701	-2.438103	-0.347830
C	-5.269870	0.810661	-0.701846
H	-6.176038	1.402052	-0.516973
H	-4.864150	1.110165	-1.672972
H	-3.105561	2.843040	1.104227
C	0.011547	0.102593	0.051704
N	0.551948	-1.157415	0.038406
N	1.075376	0.966840	0.001582
C	1.936060	-1.075782	-0.015928
C	-0.211620	-2.393549	0.065908
C	2.263056	0.253723	-0.039118
C	0.948432	2.416388	-0.012614
C	2.929554	-2.160868	-0.047088
C	-0.577553	-2.984974	-1.154056
C	-0.495509	-2.984305	1.307466
C	3.644439	0.755877	-0.093474
C	0.868735	3.074602	-1.252097
C	0.986247	3.112093	1.208652
C	4.352559	-1.690825	-0.101578
O	2.630325	-3.347708	-0.030196
C	-1.313888	-4.172539	-1.098575
C	-0.168960	-2.400064	-2.483375
C	-1.236744	-4.170539	1.301176
C	0.004813	-2.402025	2.606187
C	4.688989	-0.318746	-0.122115
O	3.925171	1.947564	-0.112343
C	0.697278	4.462575	-1.233436
C	1.034567	2.344576	-2.561557
C	0.811967	4.498559	1.164022
C	1.282033	2.422847	2.517147
C	5.366631	-2.651725	-0.130599
C	-1.666028	-4.772559	0.114442

H	-1.605455	-4.646359	-2.033199
H	0.921513	-2.302313	-2.555316
H	-0.495203	-3.050279	-3.300355
H	-0.609401	-1.409448	-2.641980
H	-1.467041	-4.643165	2.253319
H	-0.410696	-1.405464	2.791398
H	-0.276391	-3.046551	3.444133
H	1.098943	-2.318930	2.606791
C	6.032118	0.063643	-0.170373
C	0.640887	5.188478	-0.040213
H	0.623540	4.988366	-2.182479
H	0.265987	1.579000	-2.701876
H	0.963731	3.046430	-3.397447
H	2.020041	1.864209	-2.615692
H	0.829123	5.053147	2.099392
H	1.275354	3.147390	3.336503
H	0.543261	1.650504	2.748437
H	2.276964	1.959948	2.493420
H	5.084430	-3.699370	-0.114100
C	6.704960	-2.260319	-0.178720
C	-2.486003	-6.041706	0.140681
H	6.265906	1.123182	-0.185181
C	7.037583	-0.903192	-0.198294
C	0.414667	6.682078	-0.050481
H	7.487562	-3.013300	-0.200562
H	-2.271942	-6.638621	1.033428
H	-3.561493	-5.819344	0.147892
H	-2.289617	-6.663069	-0.739531
H	8.079452	-0.598073	-0.235360
H	0.762315	7.133973	-0.985366
H	-0.652853	6.919321	0.049780
H	0.934876	7.172003	0.779625
C	-5.560656	-0.696021	-0.690316
H	-6.144456	-1.013649	-1.561646
H	-6.138863	-0.959619	0.205944

TS1red

Three lowest frequencies (cm-1): -156.6061 14.9508 22.5004

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.919370	0.992045	2.535019
Cl	-2.070038	0.557693	-2.331629
C	-3.351974	2.246470	0.024181
H	-3.329218	2.677765	-0.975173
Ru	-1.976693	0.649765	0.115882
C	-4.261392	1.153243	0.261669
C	-3.296079	-0.650181	0.407087
H	-4.612038	1.081404	1.291739
H	-3.471056	-0.913162	1.457940
C	-4.086722	-1.472161	-0.581143
H	-3.609782	-1.471440	-1.562060
H	-4.150816	-2.506185	-0.219579
C	-5.242964	0.693117	-0.806326
H	-6.178533	1.258620	-0.691673

H	-4.830233	0.921101	-1.794037
H	-3.136641	2.920210	0.850335
C	0.032625	0.096233	0.057837
N	0.563448	-1.158701	0.049043
N	1.083707	0.961503	0.006506
C	1.970099	-1.092033	-0.010301
C	-0.200185	-2.383257	0.110973
C	2.299426	0.255619	-0.036491
C	0.939800	2.401318	-0.003982
C	2.926084	-2.167327	-0.048428
C	-0.524702	-3.047153	-1.083359
C	-0.551437	-2.902293	1.366893
C	3.640309	0.772302	-0.091103
C	0.831088	3.069344	-1.235873
C	0.984806	3.101500	1.214761
C	4.319358	-1.683809	-0.102013
O	2.615709	-3.387154	-0.044592
C	-1.284926	-4.217067	-0.995168
C	-0.027390	-2.551400	-2.416865
C	-1.312273	-4.076925	1.400203
C	-0.090441	-2.250806	2.647047
C	4.657028	-0.295222	-0.121002
O	3.919407	2.000440	-0.107477
C	0.625804	4.453708	-1.212435
C	1.031899	2.348070	-2.544493
C	0.779003	4.483737	1.181513
C	1.339190	2.409909	2.505800
C	5.358106	-2.637949	-0.137528
C	-1.694453	-4.744253	0.233556
H	-1.546158	-4.738324	-1.914459
H	1.068343	-2.579718	-2.441135
H	-0.401797	-3.187074	-3.226215
H	-0.350845	-1.523955	-2.611249
H	-1.593176	-4.487886	2.368311
H	-0.528314	-1.255334	2.780113
H	-0.371135	-2.864892	3.509349
H	1.000301	-2.139950	2.650956
C	6.017568	0.075156	-0.171772
C	0.570900	5.173750	-0.016548
H	0.532058	4.981271	-2.159733
H	0.317280	1.531648	-2.678215
H	0.914490	3.041482	-3.383788
H	2.046049	1.931958	-2.585019
H	0.803160	5.035383	2.119405
H	1.314845	3.120100	3.338774
H	0.644275	1.598061	2.734598
H	2.352873	1.997202	2.436910
H	5.069302	-3.684848	-0.123534
C	6.686209	-2.250545	-0.187089
C	-2.478195	-6.036219	0.298181
H	6.241193	1.137927	-0.184714
C	7.019440	-0.879517	-0.203985
C	0.309345	6.662815	-0.016456
H	7.473255	-3.001869	-0.212909
H	-3.166602	-6.132021	-0.549615
H	-1.810959	-6.909007	0.272460
H	-3.065824	-6.103897	1.220656

H	8.063339	-0.573866	-0.242781
H	0.853377	7.165184	0.791884
H	0.610819	7.122595	-0.964398
H	-0.757854	6.882156	0.127287
C	-5.483878	-0.816678	-0.670479
H	-6.051562	-1.021556	0.248743
H	-6.065444	-1.219196	-1.509065

TS2

Three lowest frequencies (cm-1): -207.4450 15.1631 15.6350

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.935685	0.283643	2.630616
Cl	-2.147565	0.315784	-2.236566
C	-2.538652	2.093214	0.232737
H	-2.781314	2.633827	-0.686908
Ru	-2.028475	0.326043	0.191369
C	-4.337704	0.873629	0.592910
C	-4.054329	-0.507567	0.421020
H	-4.347588	1.297707	1.592130
H	-3.864623	-1.132994	1.290768
C	-4.822958	-1.064256	-0.768498
H	-4.207213	-1.681765	-1.428408
H	-5.622228	-1.707464	-0.370020
C	-5.341870	1.328546	-0.461457
H	-6.301030	1.445445	0.064528
H	-5.116446	2.297076	-0.916882
H	-2.528492	2.677995	1.157839
C	0.011637	0.060860	0.064741
N	0.642025	-1.158389	0.032932
N	1.014869	0.997743	0.010561
C	2.014438	-0.984566	-0.038391
C	-0.060311	-2.430872	0.071150
C	2.248040	0.364524	-0.051688
C	0.825855	2.438101	0.023971
C	3.074688	-2.001471	-0.091046
C	-0.414409	-3.045178	-1.143669
C	-0.288312	-3.041629	1.317232
C	3.593975	0.956053	-0.122063
C	0.711168	3.115543	-1.200106
C	0.829125	3.106288	1.259168
C	4.462501	-1.440365	-0.159940
O	2.850493	-3.205508	-0.079342
C	-1.126834	-4.246307	-1.074007
C	0.020686	-2.493262	-2.478145
C	-1.004570	-4.242991	1.323652
C	0.280424	-2.486768	2.599307
C	4.706525	-0.048888	-0.174687
O	3.800061	2.162539	-0.137147
C	0.514477	4.499891	-1.154268
C	0.836346	2.404580	-2.524547
C	0.630564	4.490227	1.243607
C	1.076357	2.383268	2.559836
C	5.537039	-2.332179	-0.210348

C	-1.452693	-4.847928	0.145582
H	-1.414874	-4.732399	-2.003246
H	1.115715	-2.489440	-2.554217
H	-0.363879	-3.117194	-3.290045
H	-0.342497	-1.474266	-2.637903
H	-1.197382	-4.725829	2.278825
H	-0.068565	-1.469252	2.796200
H	-0.016548	-3.111275	3.446739
H	1.377453	-2.479486	2.562123
C	6.020566	0.421631	-0.240052
C	0.455459	5.202507	0.052752
H	0.420248	5.041792	-2.092543
H	0.060222	1.642140	-2.650160
H	0.746048	3.118289	-3.348625
H	1.814484	1.915544	-2.617709
H	0.627795	5.024865	2.190901
H	1.075023	3.090980	3.393986
H	0.308242	1.627710	2.756448
H	2.053108	1.882917	2.553659
H	5.324581	-3.396224	-0.197747
C	6.845638	-1.852733	-0.274921
C	-2.254886	-6.127407	0.186983
H	6.183530	1.494370	-0.250616
C	7.087244	-0.476440	-0.289839
C	0.211548	6.693622	0.072308
H	7.675992	-2.552009	-0.313516
H	-2.018943	-6.720133	1.077020
H	-3.332318	-5.916724	0.211744
H	-2.065769	-6.747247	-0.695906
H	8.105991	-0.102811	-0.340122
H	0.747686	7.176283	0.896618
H	0.531213	7.164164	-0.863296
H	-0.855316	6.918833	0.203481
C	-5.404578	0.174918	-1.493326
H	-4.783170	0.415484	-2.356436
H	-6.426844	0.003630	-1.846081

TS2red
Three lowest frequencies (cm-1): -209.4946 13.6899 14.3923

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.958169	0.314272	2.632436
Cl	-2.113410	0.339625	-2.254741
C	-2.486153	2.121492	0.209882
H	-2.716719	2.663316	-0.712997
Ru	-2.010831	0.347520	0.181914
C	-4.324586	0.894967	0.573861
C	-4.044554	-0.481064	0.386473
H	-4.327179	1.318492	1.572833
H	-3.855505	-1.120122	1.246343
C	-4.808851	-1.021308	-0.814419
H	-4.189562	-1.632504	-1.476800
H	-5.618983	-1.663126	-0.433853
C	-5.318343	1.369930	-0.480774

H	-6.285146	1.483697	0.033792
H	-5.081957	2.343242	-0.921354
H	-2.477131	2.708948	1.134097
C	0.042394	0.064177	0.066814
N	0.640251	-1.160632	0.035692
N	1.047453	0.984816	0.011697
C	2.037739	-1.025882	-0.039974
C	-0.091963	-2.406814	0.081498
C	2.297438	0.336669	-0.054546
C	0.871575	2.418884	0.032905
C	3.039523	-2.055453	-0.092074
C	-0.465041	-3.028087	-1.124195
C	-0.344782	-3.005601	1.328744
C	3.613965	0.914572	-0.126436
C	0.762602	3.112085	-1.183421
C	0.864081	3.085881	1.268300
C	4.407291	-1.510235	-0.162587
O	2.779390	-3.288191	-0.078810
C	-1.226581	-4.198841	-1.047731
C	0.024370	-2.518579	-2.455363
C	-1.108716	-4.177571	1.348564
C	0.266520	-2.468556	2.597508
C	4.678235	-0.106908	-0.178534
O	3.841208	2.152287	-0.144801
C	0.551837	4.494002	-1.132408
C	0.923669	2.408327	-2.506595
C	0.652099	4.468797	1.264419
C	1.124882	2.353225	2.559970
C	5.489022	-2.414562	-0.216452
C	-1.580206	-4.774388	0.176101
H	-1.526183	-4.685058	-1.974240
H	1.117878	-2.593837	-2.496549
H	-0.390342	-3.119946	-3.271083
H	-0.259333	-1.476683	-2.623874
H	-1.316664	-4.645924	2.308715
H	-0.032290	-1.434524	2.788782
H	-0.042547	-3.074179	3.455797
H	1.360205	-2.509348	2.526345
C	6.018914	0.326938	-0.248043
C	0.483294	5.188819	0.078556
H	0.458032	5.040567	-2.069152
H	0.181994	1.613928	-2.636453
H	0.813233	3.118081	-3.333283
H	1.922388	1.960408	-2.574600
H	0.636576	4.995410	2.217064
H	1.131771	3.053872	3.401656
H	0.362499	1.592276	2.755967
H	2.101745	1.856573	2.524078
H	5.249901	-3.473951	-0.202681
C	6.796380	-1.964681	-0.283644
C	-2.434785	-6.020531	0.228243
H	6.191865	1.399110	-0.259089
C	7.064168	-0.579338	-0.299587
C	0.291853	6.688761	0.101890
H	7.617610	-2.677836	-0.324182
H	-2.219002	-6.617045	1.121922
H	-3.505047	-5.772381	0.254026

H	-2.271107	-6.655038	-0.650322
H	8.091803	-0.224623	-0.352436
H	-0.200944	7.016329	1.024405
H	1.254669	7.215413	0.043557
H	-0.314769	7.029526	-0.745070
C	-5.372171	0.231645	-1.530005
H	-4.728493	0.480158	-2.374601
H	-6.389286	0.072974	-1.906268

TS3

Three lowest frequencies (cm-1): -152.0601 11.5867 16.2355

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.448205	1.376710	-2.219946
Cl	-1.056174	1.409119	2.636025
C	-3.397050	1.549338	0.541606
H	-3.487310	1.256480	1.587062
Ru	-1.194640	1.358267	0.203196
C	-0.770988	3.144787	0.151322
H	-0.701615	3.687250	-0.796927
H	-0.540367	3.709721	1.060030
C	-3.015658	2.881762	0.307836
H	-3.189700	3.322183	-0.670229
H	-2.929185	3.556554	1.154405
C	-4.211493	0.724192	-0.432962
H	-3.872529	-0.320149	-0.409664
H	-4.058687	1.082488	-1.454295
C	-5.709855	0.765699	-0.065023
H	-5.852568	0.436134	0.972908
H	-6.067518	1.803814	-0.113359
C	-6.562173	-0.117817	-0.997079
H	-6.222040	-1.159822	-0.927883
H	-6.387607	0.201107	-2.036104
C	-8.032969	-0.042229	-0.688991
H	-8.487550	0.945673	-0.786119
C	-8.792751	-1.068269	-0.302805
H	-8.384087	-2.071093	-0.191224
H	-9.851436	-0.949860	-0.087474
C	0.503591	0.212463	0.077109
N	0.514425	-1.160785	0.084283
N	1.820826	0.591911	-0.020407
C	1.814736	-1.629115	-0.005581
C	-0.688825	-1.971967	0.162826
C	2.632264	-0.532675	-0.072520
C	2.301072	1.961288	-0.064071
C	2.298052	-3.017006	-0.031595
C	-1.301473	-2.388711	-1.033128
C	-1.154790	-2.374422	1.427256
C	4.097133	-0.617678	-0.183736
C	2.453962	2.581977	-1.313892
C	2.653768	2.591877	1.140644
C	3.786739	-3.148111	-0.141932
O	1.552659	-3.986884	0.030681
C	-2.480596	-3.132798	-0.927284

C	-0.692046	-2.112177	-2.384796
C	-2.339640	-3.117166	1.469917
C	-0.386825	-2.091172	2.694000
C	4.632791	-2.018751	-0.213045
O	4.825892	0.363706	-0.248542
C	2.907692	3.905297	-1.325672
C	2.180843	1.854178	-2.606755
C	3.102197	3.914092	1.067516
C	2.595878	1.875636	2.467196
C	4.339885	-4.430861	-0.174386
C	-3.027657	-3.487093	0.310542
H	-2.971452	-3.458744	-1.841356
H	0.312064	-2.548982	-2.455545
H	-1.302918	-2.559454	-3.174162
H	-0.618659	-1.038919	-2.585158
H	-2.719815	-3.430549	2.439336
H	-0.280327	-1.017302	2.874809
H	-0.903372	-2.526174	3.554421
H	0.614730	-2.537387	2.648915
C	6.014923	-2.196514	-0.314998
C	3.221965	4.592733	-0.149822
H	3.029888	4.403452	-2.284692
H	1.134989	1.536348	-2.679759
H	2.397083	2.502369	-3.460951
H	2.815300	0.963518	-2.699346
H	3.378318	4.420065	1.989970
H	2.943419	2.533702	3.268918
H	1.577576	1.554320	2.711321
H	3.241969	0.988587	2.465668
H	3.669764	-5.282530	-0.118473
C	5.721268	-4.598070	-0.276545
C	-4.322053	-4.262136	0.389970
H	6.645290	-1.314871	-0.368106
C	6.558289	-3.481325	-0.346759
C	3.680867	6.031865	-0.189896
H	6.144123	-5.598330	-0.301096
H	-4.429840	-4.949352	-0.456034
H	-4.383841	-4.845887	1.314202
H	-5.188108	-3.586843	0.372364
H	7.633877	-3.610931	-0.425997
H	4.423971	6.236927	0.588381
H	4.124124	6.284439	-1.158655
H	2.841032	6.720042	-0.025138

TS3red

Three lowest frequencies (cm-1): -153.2716 10.7540 13.8833

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.471309	1.323249	-2.243621
Cl	-1.003709	1.500163	2.621590
C	-3.369632	1.562939	0.555345
H	-3.444414	1.305677	1.611401
Ru	-1.174348	1.365538	0.184205
C	-0.727155	3.141329	0.075963

H	-0.662860	3.655811	-0.888700
H	-0.479371	3.729838	0.965740
C	-3.000271	2.886386	0.268893
H	-3.182524	3.293231	-0.722201
H	-2.893193	3.591319	1.087958
C	-4.190841	0.698505	-0.380273
H	-3.854306	-0.344437	-0.313523
H	-4.035761	1.012062	-1.416067
C	-5.688703	0.760516	-0.016897
H	-5.834421	0.471119	1.032825
H	-6.042500	1.798023	-0.104745
C	-6.546000	-0.153001	-0.915197
H	-6.212236	-1.193374	-0.806839
H	-6.366823	0.125397	-1.965162
C	-8.016987	-0.056446	-0.616476
H	-8.461994	0.932846	-0.744940
C	-8.790225	-1.061268	-0.200785
H	-8.391751	-2.063649	-0.054152
H	-9.848462	-0.924238	0.008129
C	0.533226	0.204666	0.066978
N	0.517702	-1.158534	0.074770
N	1.843936	0.573995	-0.014374
C	1.825609	-1.668312	-0.001004
C	-0.698097	-1.936866	0.143160
C	2.668988	-0.568306	-0.058014
C	2.324691	1.934348	-0.071490
C	2.256695	-3.039067	-0.024601
C	-1.301568	-2.367354	-1.052359
C	-1.206848	-2.305635	1.401699
C	4.103742	-0.645953	-0.140519
C	2.461341	2.554903	-1.323332
C	2.694791	2.580241	1.119927
C	3.722661	-3.169110	-0.111545
O	1.469266	-4.021791	0.019261
C	-2.506640	-3.071120	-0.960403
C	-0.629701	-2.166981	-2.386259
C	-2.416353	-3.009134	1.437163
C	-0.435207	-2.045738	2.670470
C	4.594899	-2.037954	-0.165948
O	4.862745	0.357011	-0.182940
C	2.899956	3.883670	-1.351864
C	2.197958	1.804729	-2.604574
C	3.127372	3.907185	1.036599
C	2.685107	1.856097	2.441859
C	4.281894	-4.464113	-0.142475
C	-3.091313	-3.381619	0.271475
H	-2.984748	-3.405159	-1.879173
H	0.319427	-2.716033	-2.404664
H	-1.261918	-2.548563	-3.194595
H	-0.426693	-1.111369	-2.585167
H	-2.821943	-3.296482	2.405312
H	-0.275944	-0.977383	2.841875
H	-0.974380	-2.450805	3.533172
H	0.543261	-2.538108	2.617963
C	5.986562	-2.254928	-0.247177
C	3.221618	4.581378	-0.184967
H	3.008825	4.375293	-2.316849

H	1.157183	1.470454	-2.672273
H	2.408717	2.441071	-3.470544
H	2.843780	0.920765	-2.667731
H	3.416265	4.418543	1.953146
H	3.016431	2.522602	3.245136
H	1.685114	1.488704	2.694034
H	3.368775	0.999629	2.407053
H	3.592494	-5.302347	-0.100183
C	5.651035	-4.651624	-0.223222
C	-4.410464	-4.117310	0.339937
H	6.623212	-1.375837	-0.286151
C	6.512364	-3.535322	-0.275991
C	3.664272	6.026304	-0.238850
H	6.063571	-5.658556	-0.245660
H	-4.490072	-4.711713	1.257108
H	-5.260836	-3.420726	0.330932
H	-4.536992	-4.792575	-0.513917
H	7.589028	-3.681609	-0.339102
H	4.427878	6.239814	0.518237
H	4.080966	6.280821	-1.219775
H	2.825615	6.712037	-0.053238

TS4

Three lowest frequencies (cm-1): -69.4594 14.6978 15.9908

Cartesian coordinates

ATOM	X	Y	Z
Cl	-1.294935	-1.679061	-2.258834
Cl	-0.841260	-1.796706	2.587949
C	-1.620753	-3.723178	0.187672
H	-1.133507	-4.143893	1.062774
Ru	-1.079830	-1.609445	0.168554
H	-1.317623	-4.093002	-0.788414
C	-2.761816	-0.854663	0.454529
H	-3.036794	-0.733048	1.512079
C	-2.881316	-3.124065	0.325156
H	-3.353536	-3.105195	1.303105
H	-3.524613	-3.042422	-0.545024
C	-3.780069	-0.300859	-0.496289
H	-3.627647	-0.684620	-1.508180
H	-3.563361	0.779015	-0.543813
C	-5.235953	-0.484381	-0.024568
H	-5.484627	-1.554007	0.012844
H	-5.347578	-0.103808	0.999575
C	-6.241279	0.236106	-0.944716
H	-6.017658	1.311250	-0.961769
H	-6.099091	-0.130790	-1.972803
C	-7.670539	0.019937	-0.527356
H	-8.015243	-1.015954	-0.535616
C	-8.514771	0.979352	-0.145495
H	-8.216764	2.026123	-0.121062
H	-9.536532	0.759644	0.152533
C	0.424624	-0.197704	0.070115
N	0.388623	1.173714	0.094745
N	1.757531	-0.526704	-0.017879

C	1.677652	1.685670	0.026674
C	-0.810488	1.987524	0.144916
C	2.533172	0.619439	-0.046397
C	2.246130	-1.895081	-0.073243
C	2.122412	3.087679	0.033808
C	-1.321347	2.363089	1.397256
C	-1.368982	2.430980	-1.063999
C	3.994903	0.747283	-0.145469
C	2.619784	-2.530951	1.124945
C	2.404021	-2.506371	-1.329724
C	3.608313	3.262851	-0.075884
O	1.355507	4.038064	0.122256
C	-2.463357	3.171118	1.411294
C	-0.651284	1.955925	2.686329
C	-2.503082	3.246889	-0.989379
C	-0.775374	2.060958	-2.400930
C	4.489715	2.161847	-0.160246
O	4.748775	-0.215380	-0.213123
C	3.033750	-3.863345	1.043384
C	2.665228	-1.797484	2.441727
C	2.823354	-3.840925	-1.348209
C	2.216943	-1.748267	-2.620290
C	4.122072	4.562053	-0.093810
C	-3.070030	3.620408	0.233987
H	-2.874110	3.472875	2.372109
H	0.369915	2.354718	2.739874
H	-1.203654	2.350540	3.544086
H	-0.592465	0.866856	2.792397
H	-2.947398	3.604973	-1.915374
H	-0.790874	0.976105	-2.558928
H	-1.340221	2.530029	-3.211745
H	0.264877	2.399278	-2.485108
C	5.865780	2.382860	-0.260933
C	3.116790	-4.543568	-0.176113
H	3.315781	-4.375089	1.960633
H	1.701268	-1.348011	2.693126
H	2.931744	-2.484851	3.249595
H	3.427481	-1.007886	2.413332
H	2.940206	-4.333868	-2.310383
H	2.415946	-2.401349	-3.474784
H	1.198699	-1.363500	-2.725495
H	2.917339	-0.905045	-2.677458
H	3.426286	5.392032	-0.026980
C	5.497544	4.773065	-0.196225
C	-4.311679	4.480541	0.281148
H	6.522901	1.521579	-0.323761
C	6.369093	3.684007	-0.279836
C	3.528939	-5.996117	-0.223064
H	5.888892	5.786277	-0.210641
H	-4.371896	5.143900	-0.588007
H	-5.221362	3.864886	0.284866
H	-4.336069	5.099345	1.184261
H	7.439940	3.847938	-0.359461
H	3.958191	-6.260415	-1.194996
H	4.268264	-6.227928	0.551294
H	2.666791	-6.655307	-0.055734