

SUPPORTING INFORMATION

## Mono- and Bimetallic Homo- and Heterodinuclear Pd and Pt Complexes Bridged by Diphosphines: Synthesis, Characterisation and Cytotoxicity

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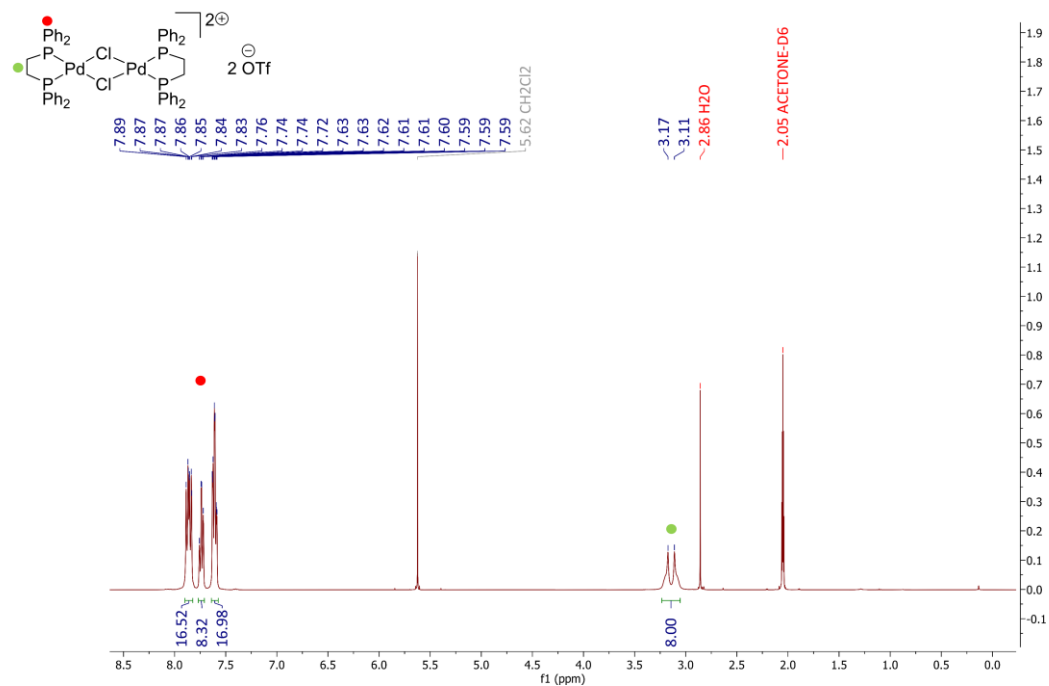
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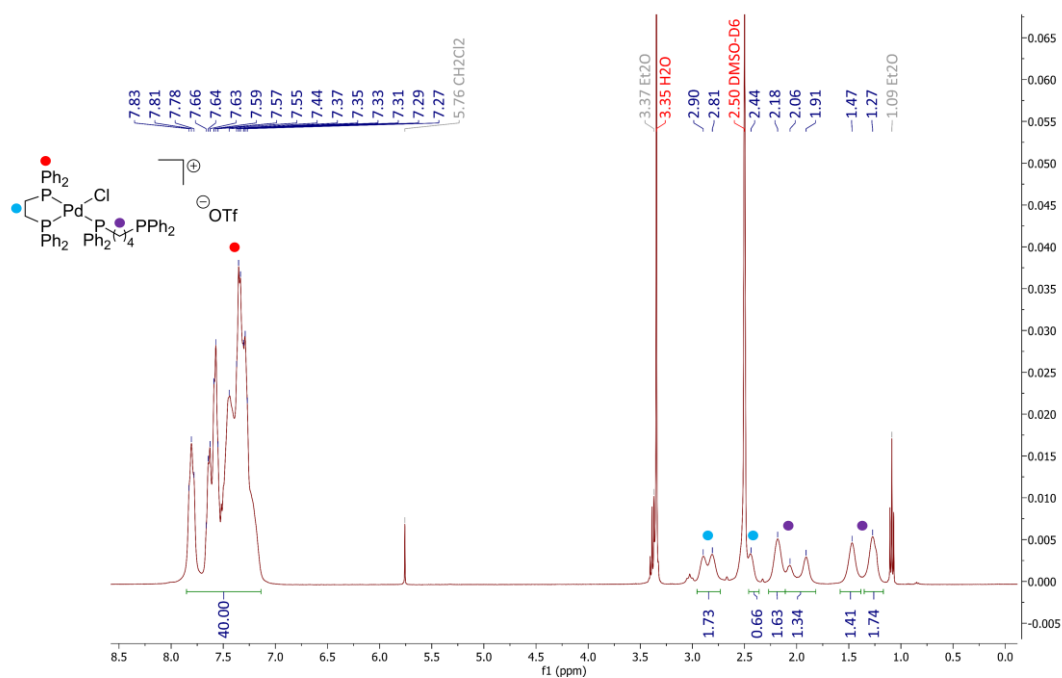
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1.  $^1\text{H}$  NMR spectra



**Fig. S1.**  $^1\text{H}$  NMR spectrum of **PdPd-0** in acetone- $d_6$  at 298 K



**Fig. S2.**  $^1\text{H}$  NMR spectrum of **Pd-1** in DMSO- $d_6$  at 298 K

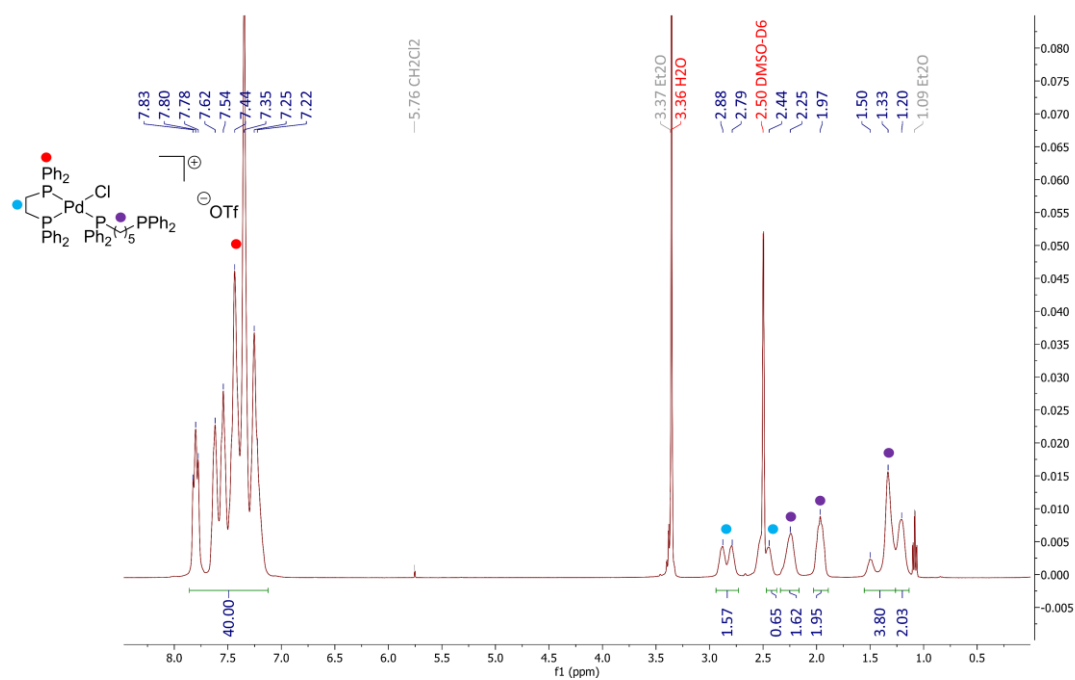


Fig. S3. <sup>1</sup>H NMR spectrum of Pd-2 in DMSO-d<sub>6</sub> at 298 K

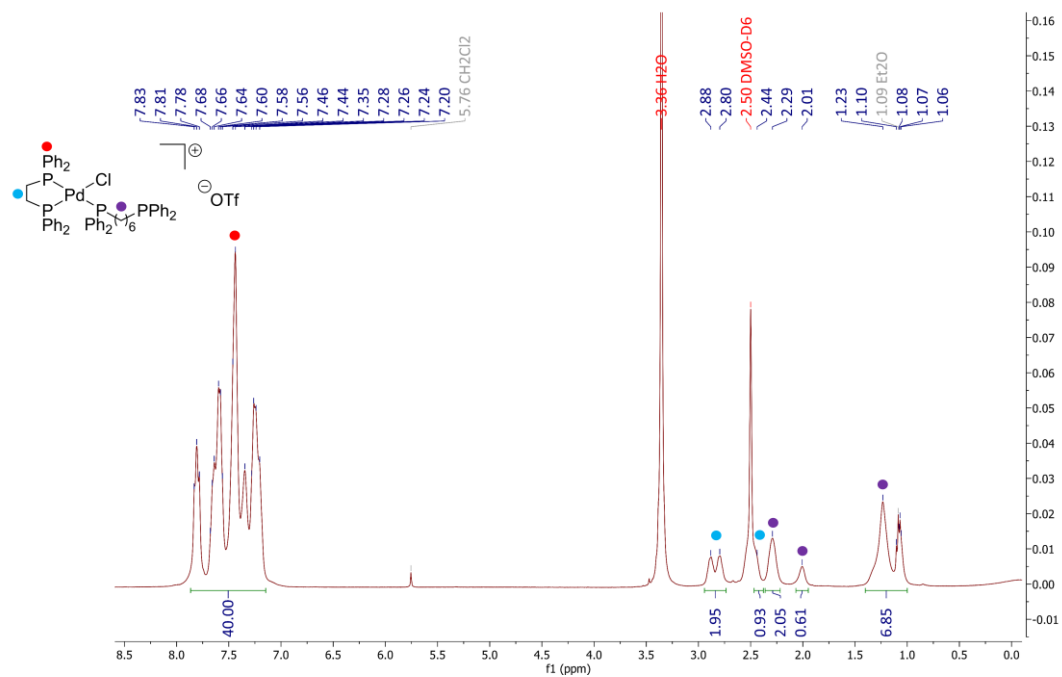


Fig. S4. <sup>1</sup>H NMR spectrum of Pd-3 in DMSO-d<sub>6</sub> at 298 K

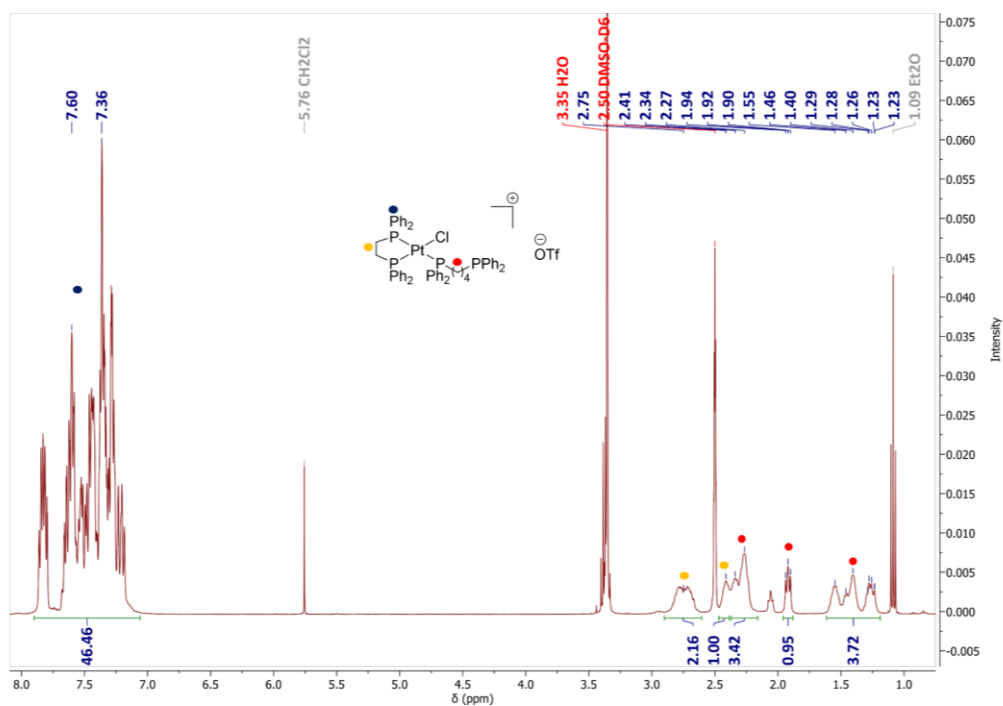


Fig. S5. <sup>1</sup>H NMR spectrum of Pt-1 in DMSO-*d*<sub>6</sub> at 298 K

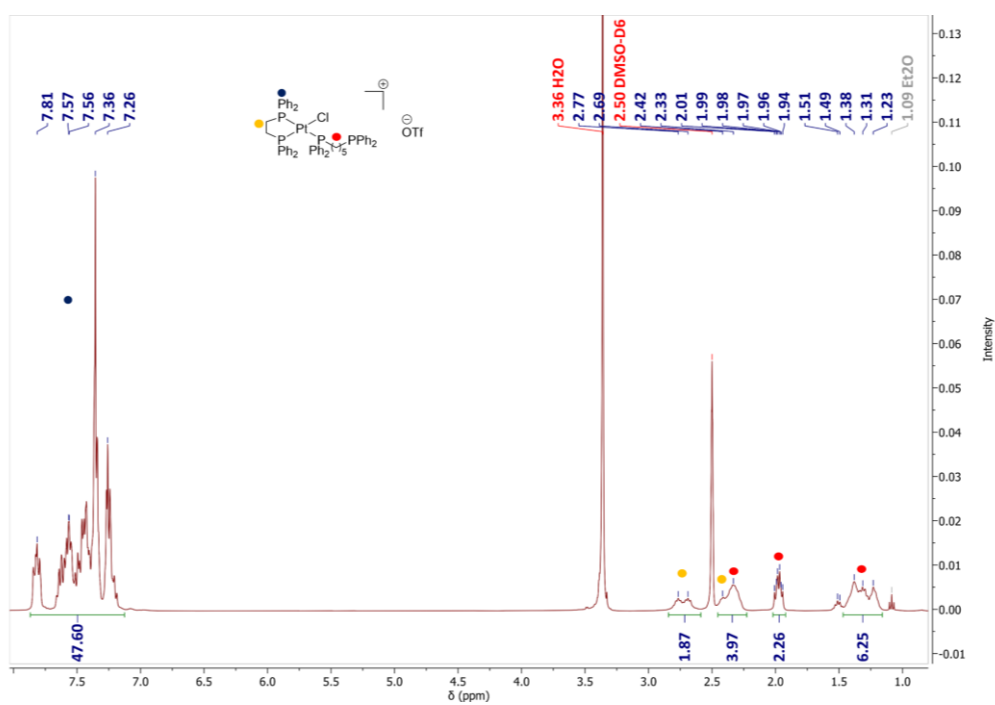


Fig. S6. <sup>1</sup>H NMR spectrum of Pt-2 in DMSO-*d*<sub>6</sub> at 298 K



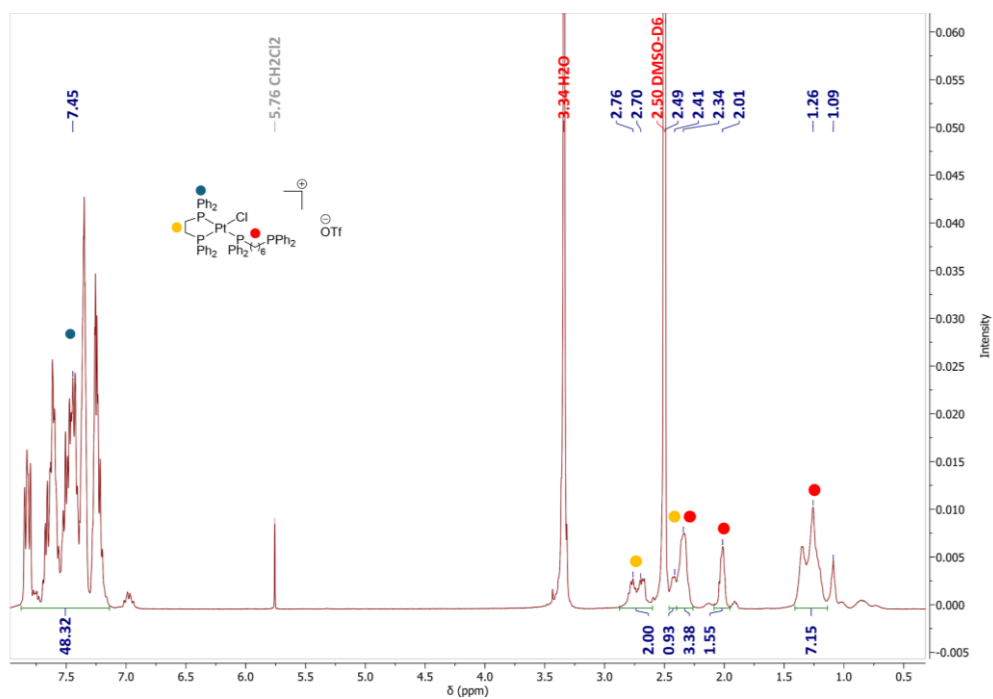


Fig. S7. <sup>1</sup>H NMR spectrum of **Pt-3** in DMSO-*d*<sub>6</sub> at 298 K

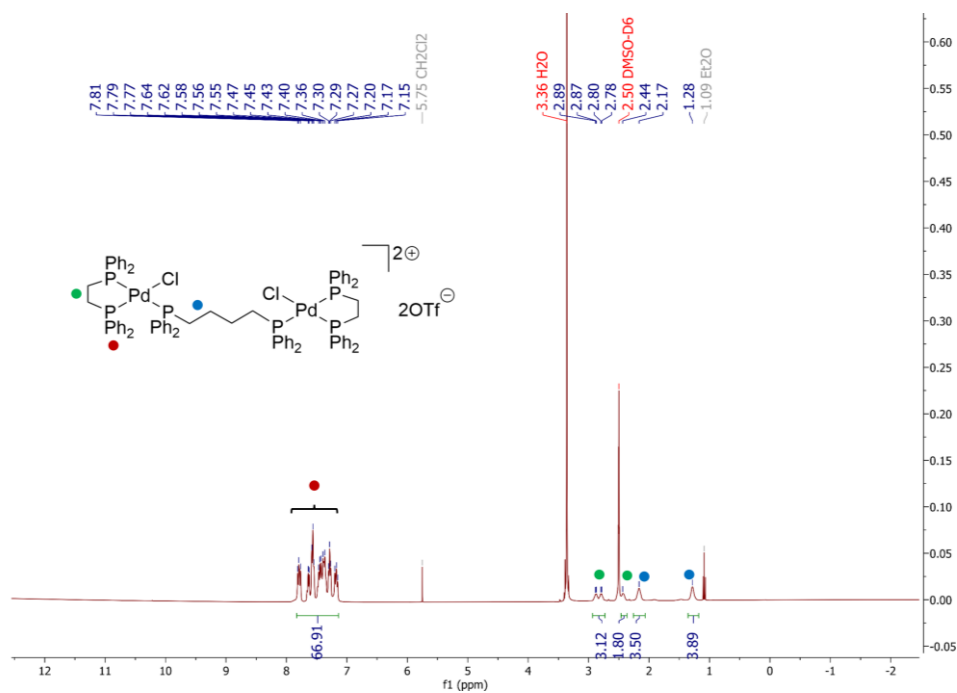


Fig. S8. <sup>1</sup>H NMR spectrum of **PdPd-1** in DMSO-*d*<sub>6</sub> at 298 K

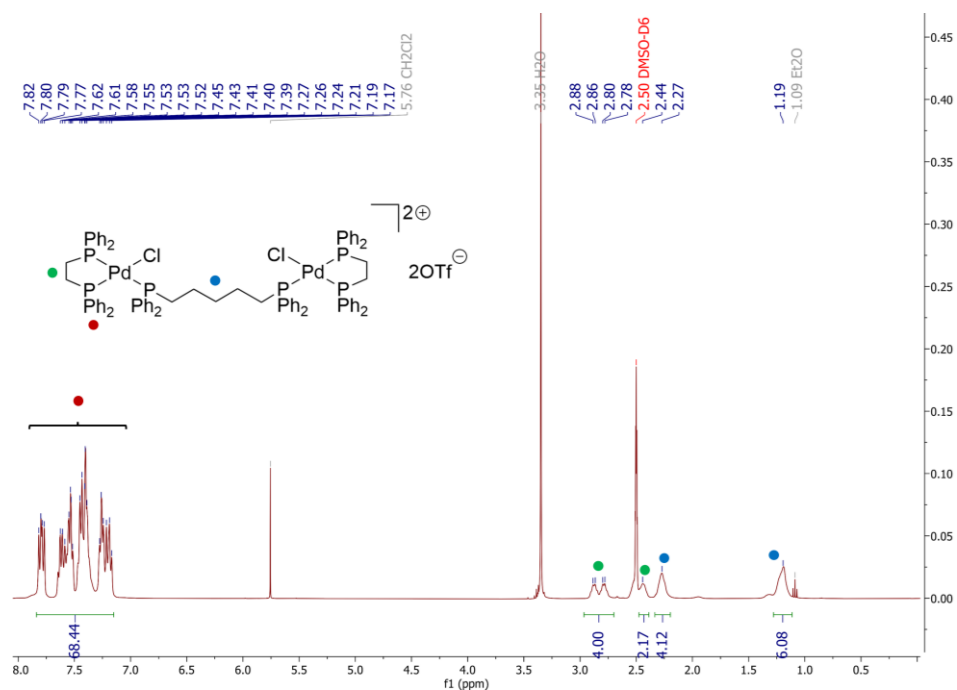


Fig. S9. <sup>1</sup>H NMR spectrum of PdPd-2 in DMSO-*d*<sub>6</sub> at 298 K

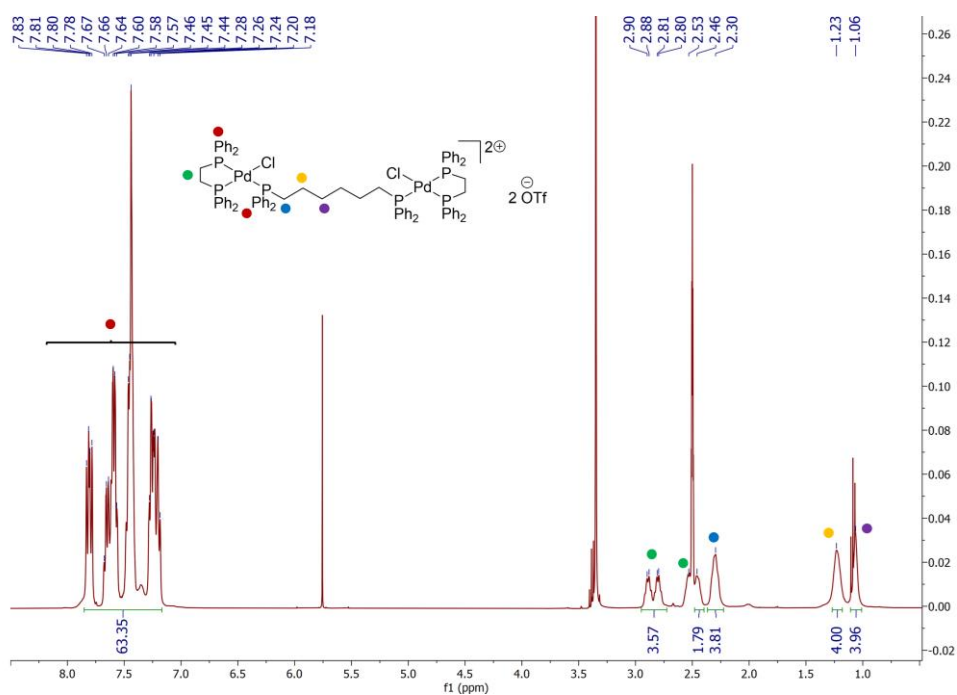
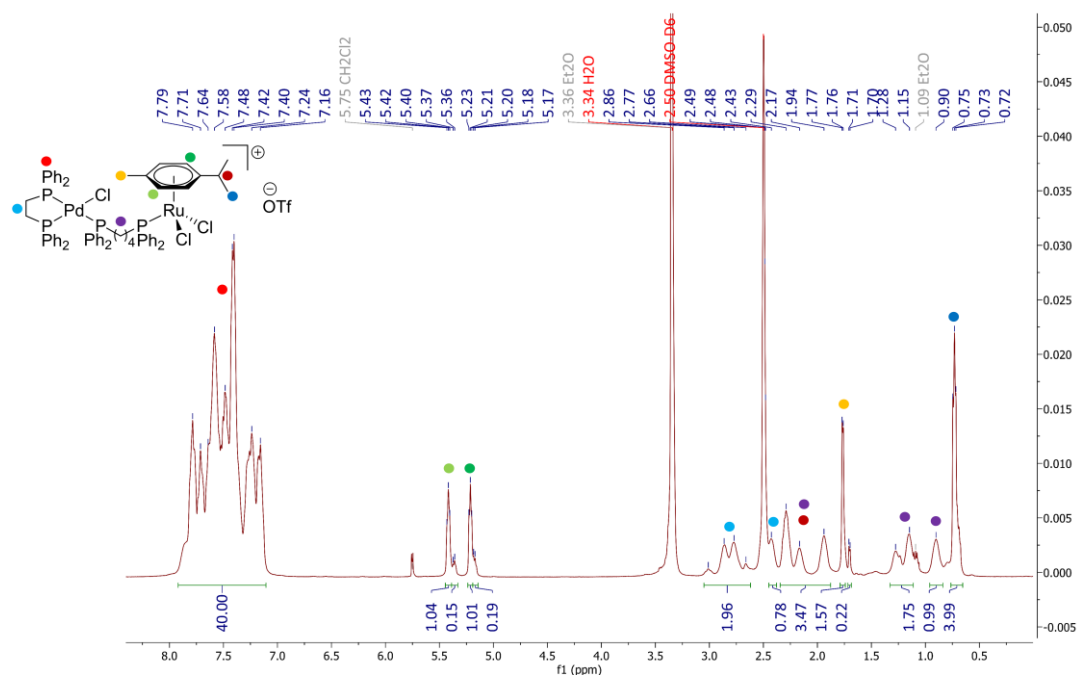
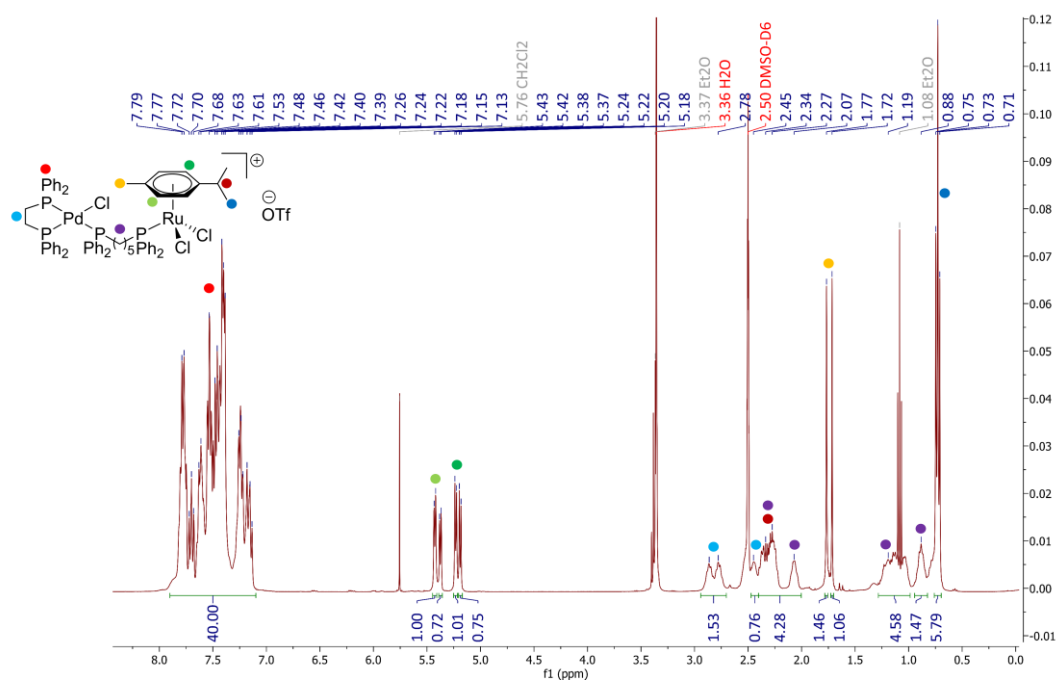


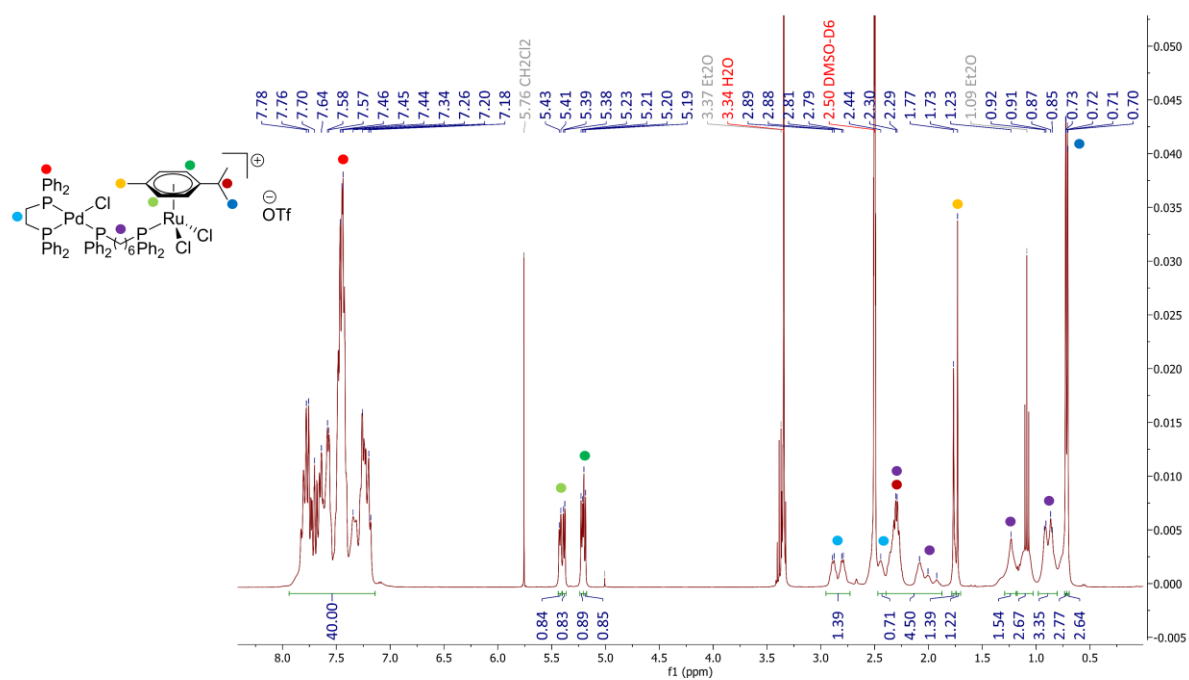
Fig. S10. <sup>1</sup>H NMR spectrum of PdPd-3 in DMSO-*d*<sub>6</sub> at 298 K



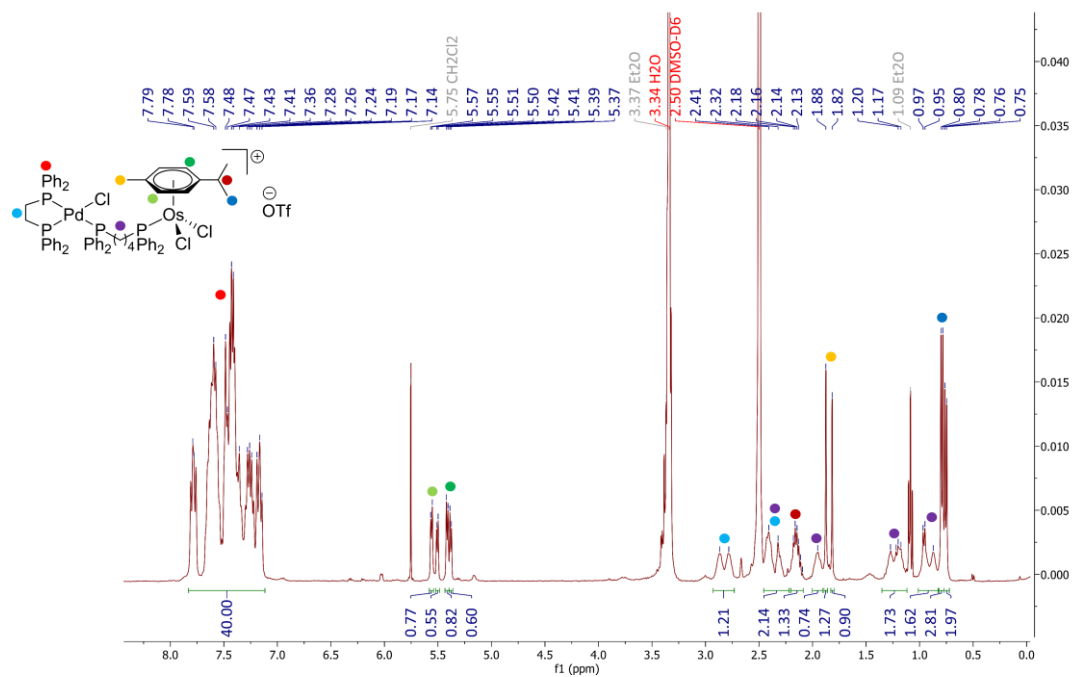
**Fig. S11.** <sup>1</sup>H NMR spectrum of **PdRu-1** in DMSO-d<sub>6</sub> at 298 K



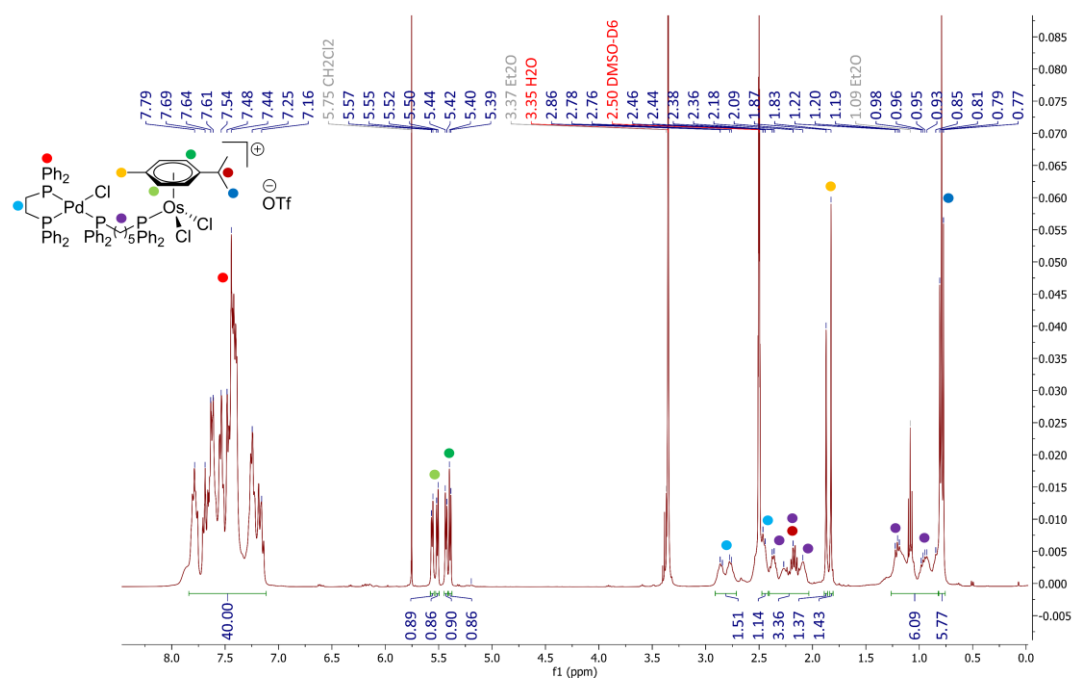
**Fig. S12.** <sup>1</sup>H NMR spectrum of **PdRu-2** in DMSO-d<sub>6</sub> at 298 K



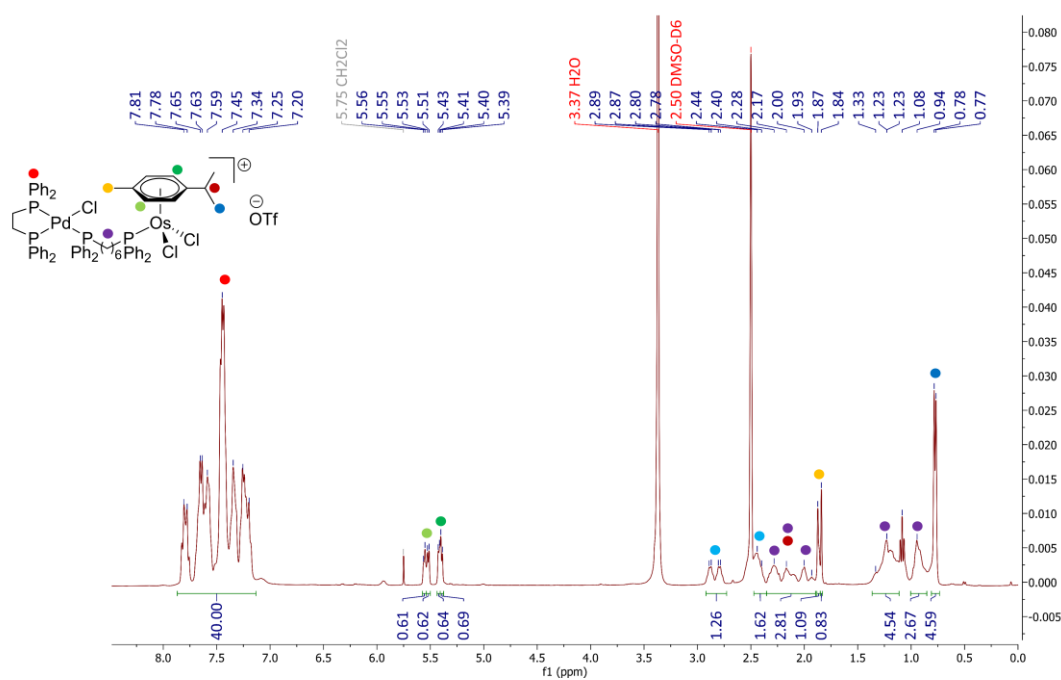
**Fig. S13.** <sup>1</sup>H NMR spectrum of **PdRu-3** in DMSO-*d*<sub>6</sub> at 298 K



**Fig. S14.** <sup>1</sup>H NMR spectrum of **PdOs-1** in DMSO-*d*<sub>6</sub> at 298 K



**Fig. S15.** <sup>1</sup>H NMR spectrum of PdOs-2 in DMSO-*d*<sub>6</sub> at 298 K



**Fig. S16.** <sup>1</sup>H NMR spectrum of PdOs-3 in DMSO-*d*<sub>6</sub> at 298 K

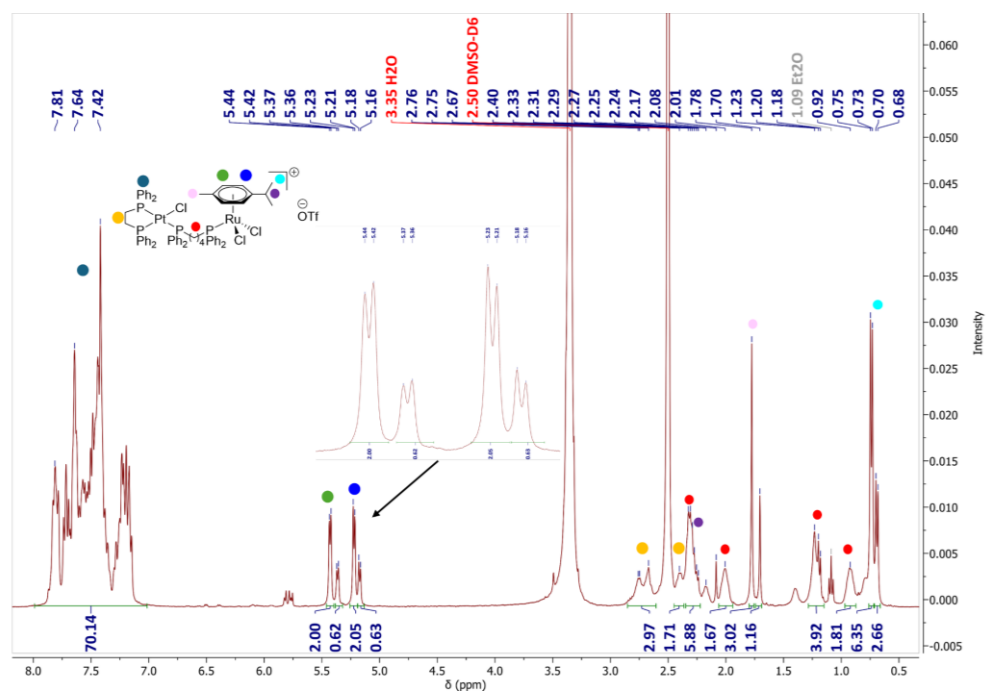


Fig. S17. <sup>1</sup>H NMR spectrum of PtRu-1 in DMSO-*d*<sub>6</sub> at 298 K

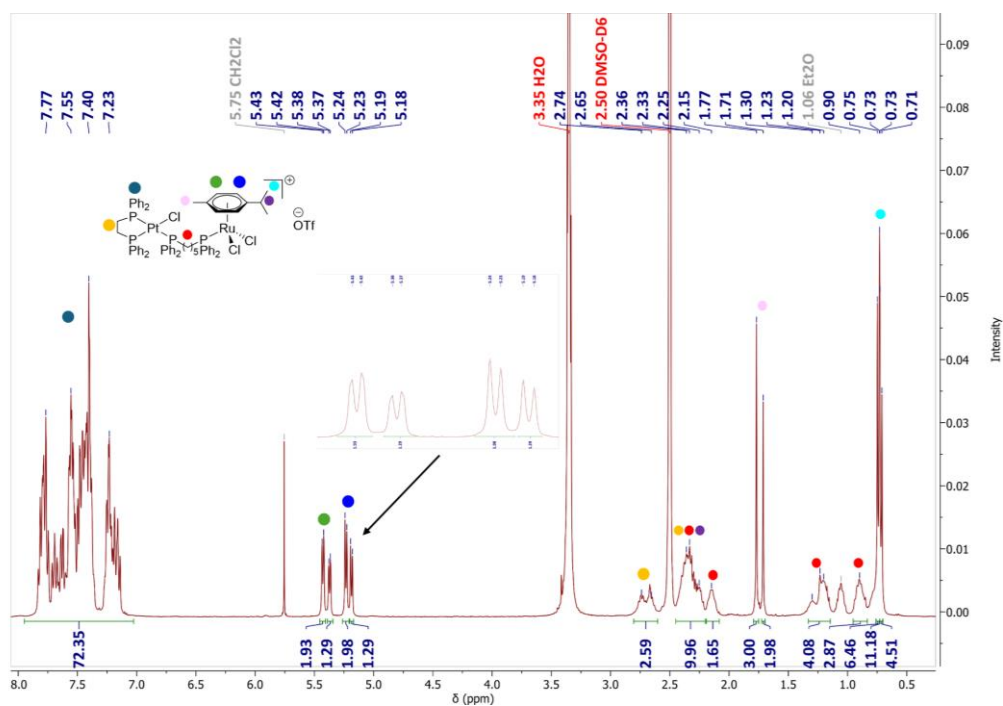


Fig. S18. <sup>1</sup>H NMR spectrum of PtRu-2 in DMSO-*d*<sub>6</sub> at 298 K

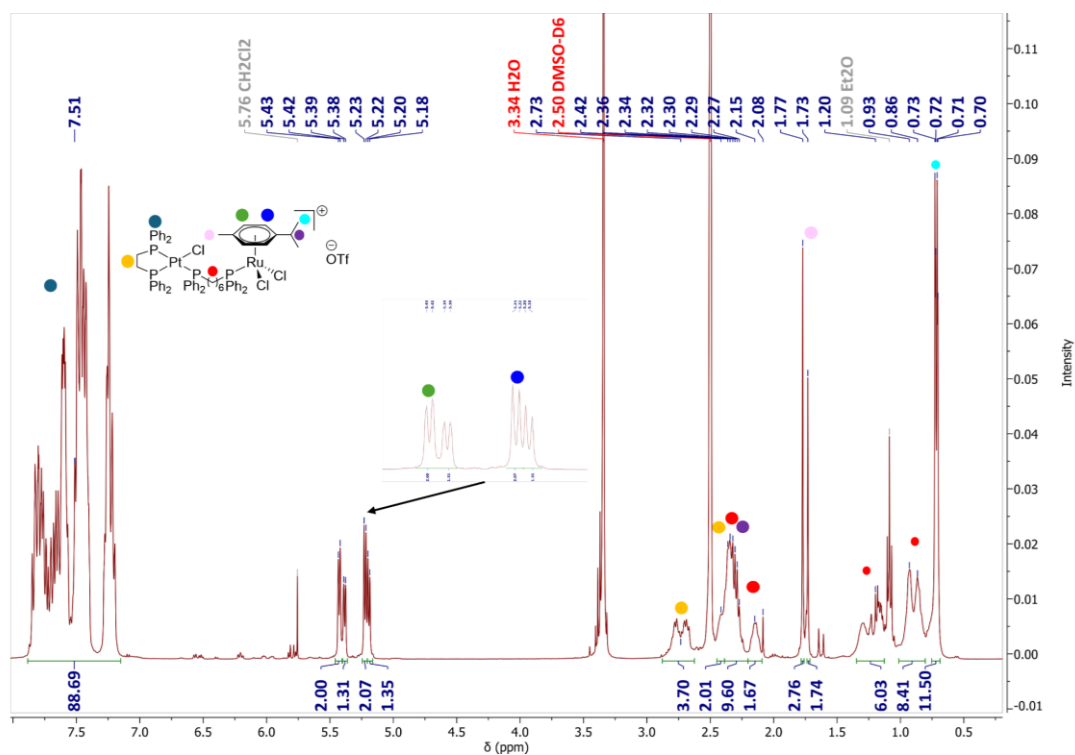


Fig. S19. <sup>1</sup>H NMR spectrum of PtRu-3 in DMSO-*d*<sub>6</sub> at 298 K

## 2. <sup>13</sup>C{<sup>1</sup>H} NMR spectra

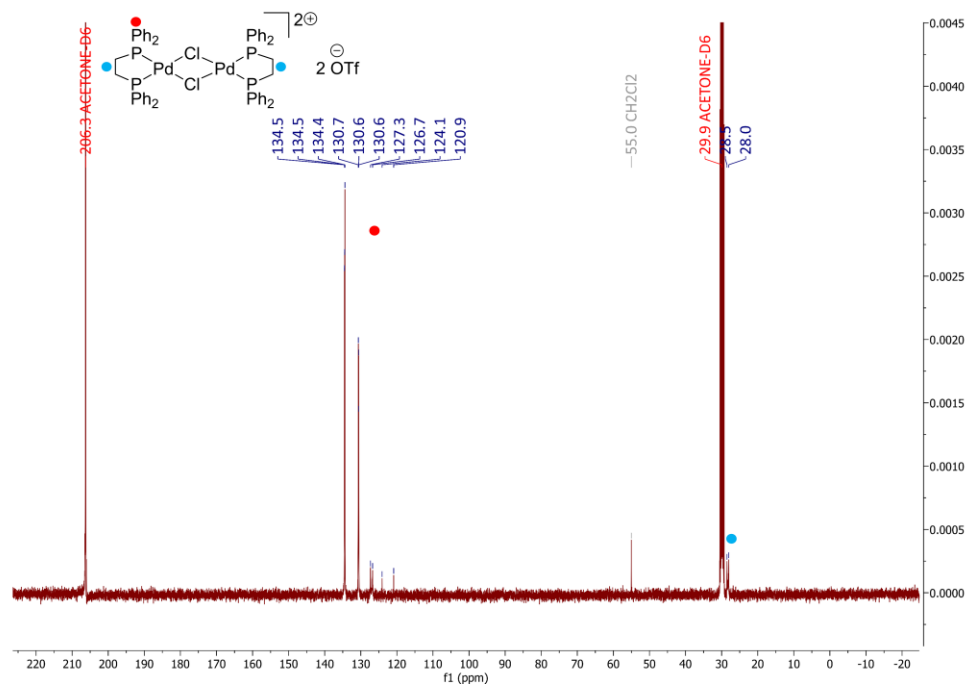
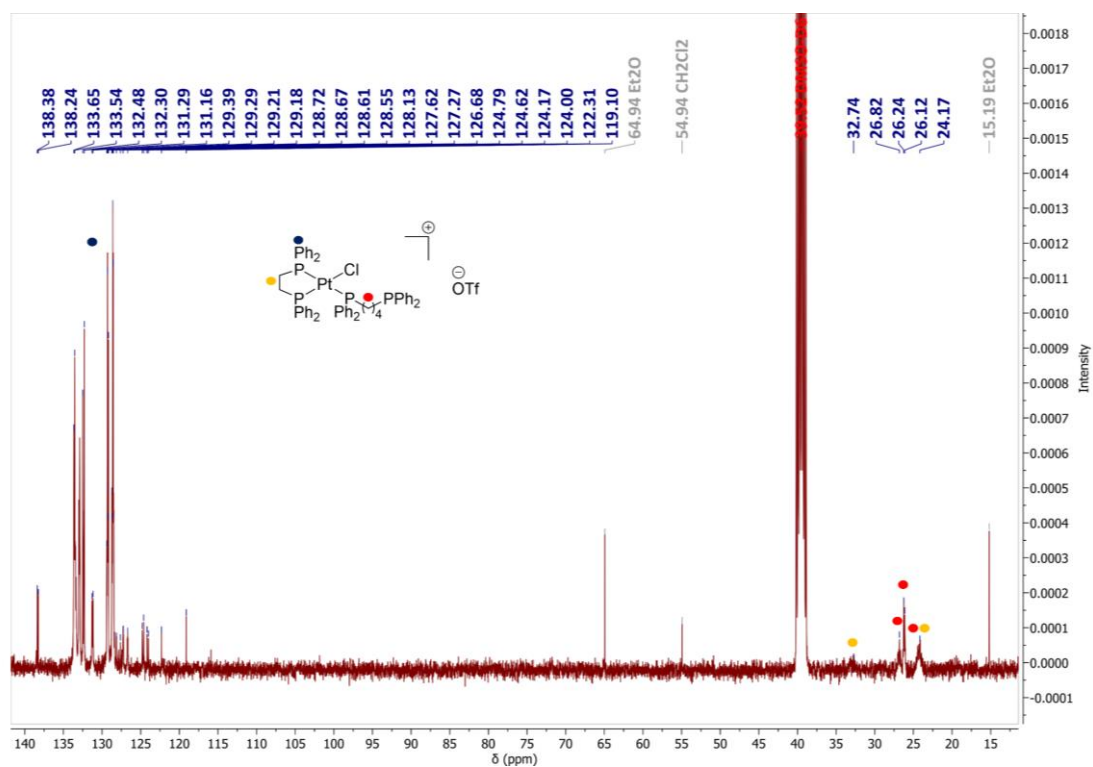
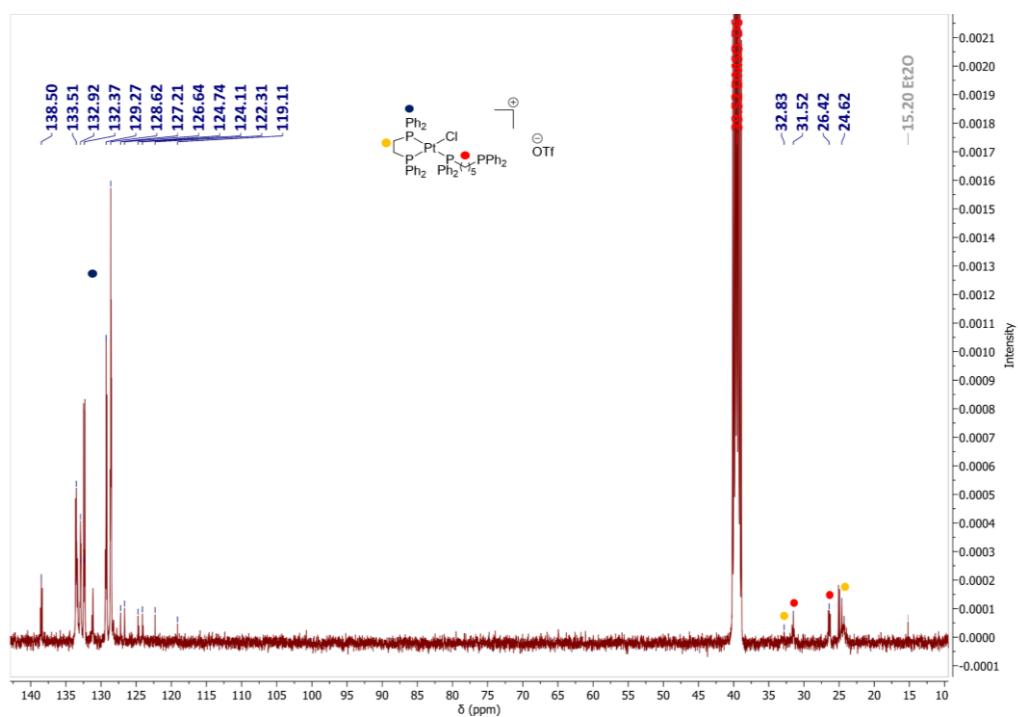


Fig. S20. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of PdPd-0 in acetone-*d*<sub>6</sub> at 298 K

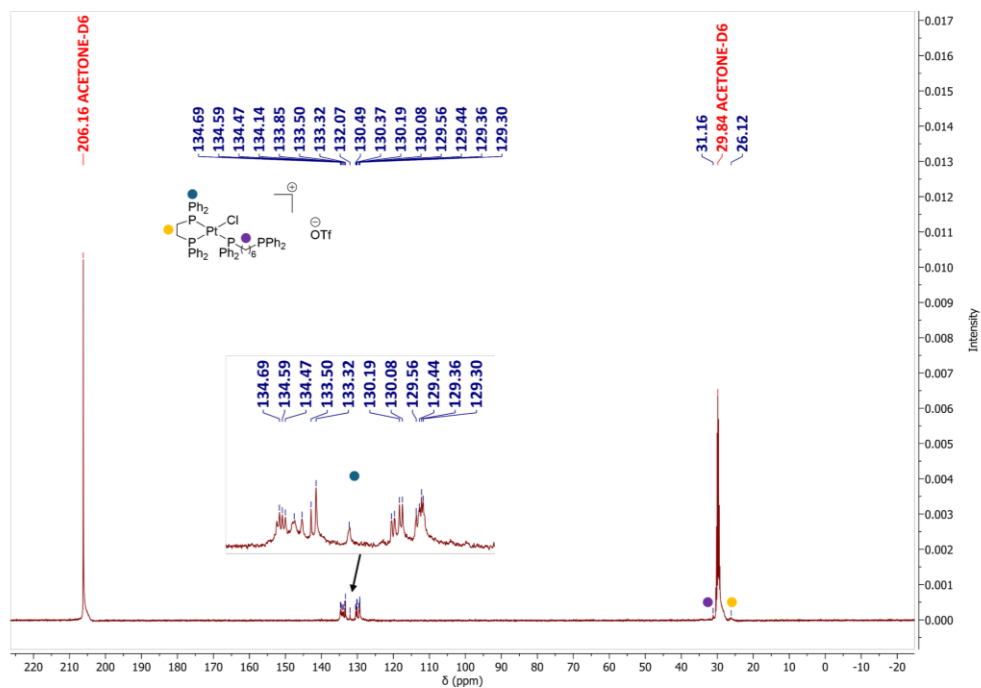


**Fig. S21.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **Pt-1** in  $\text{DMSO-}d_6$  at 298 K

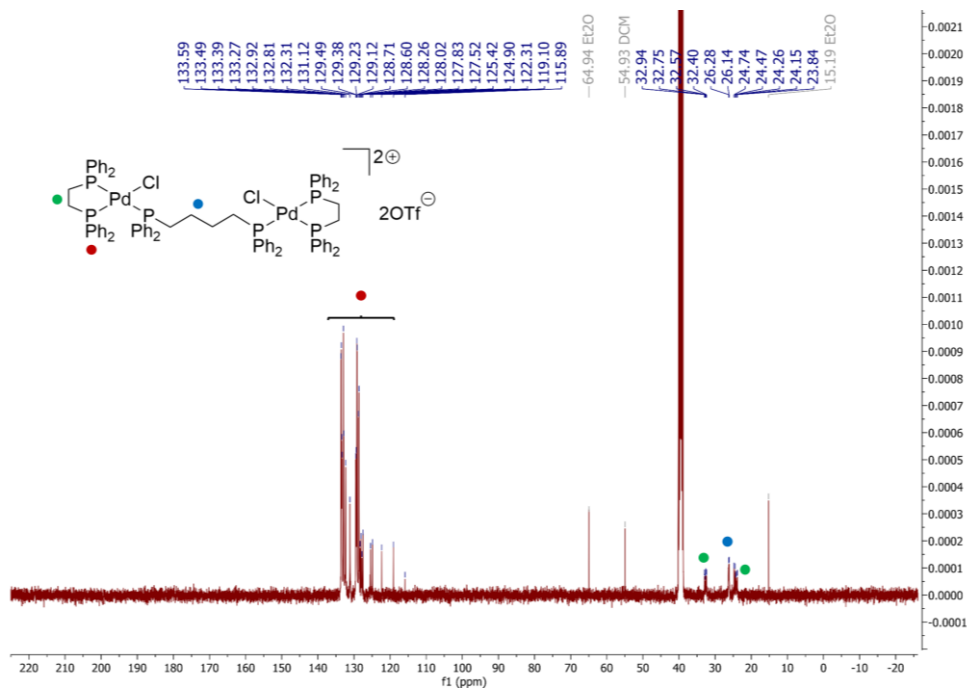


**Fig. S22.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **Pt-2** in  $\text{DMSO-}d_6$  at 298 K

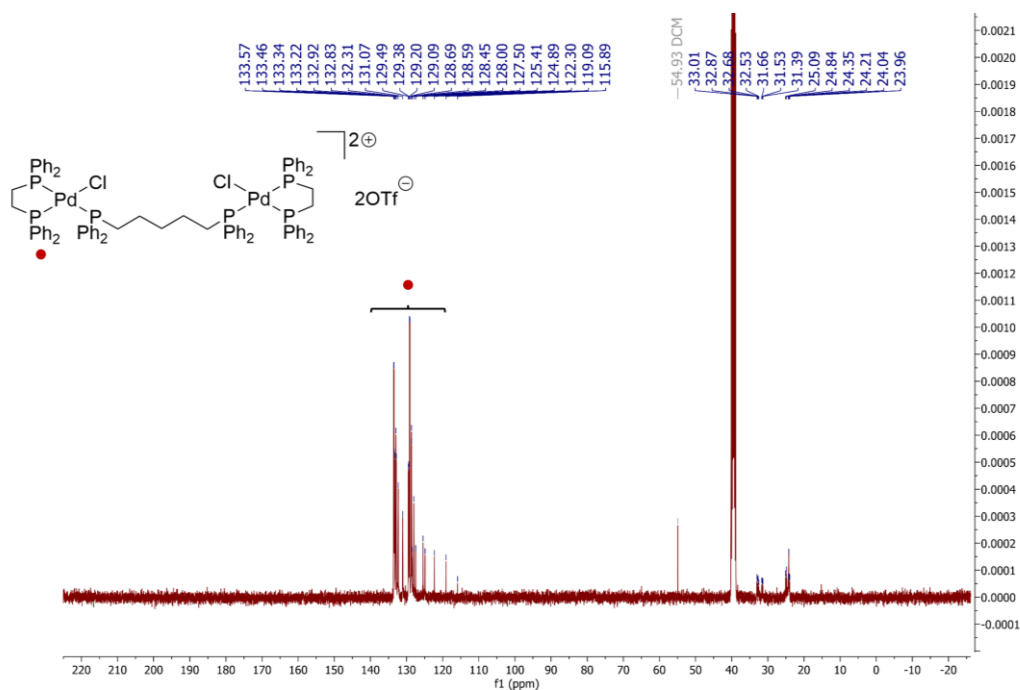




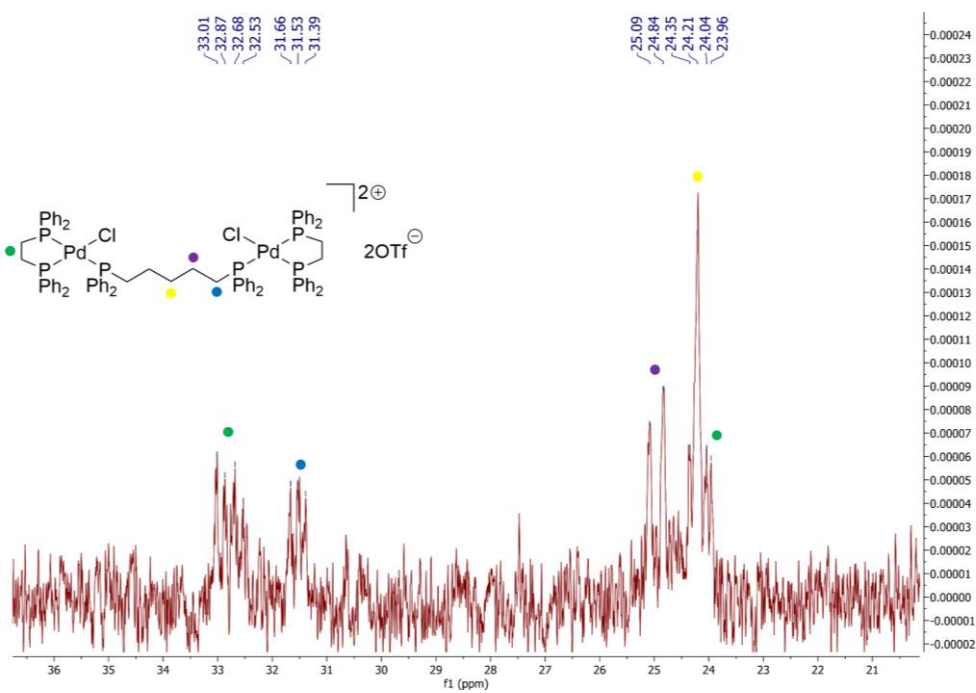
**Fig. S23.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **Pt-3** in acetone- $d_6$  at 298 K



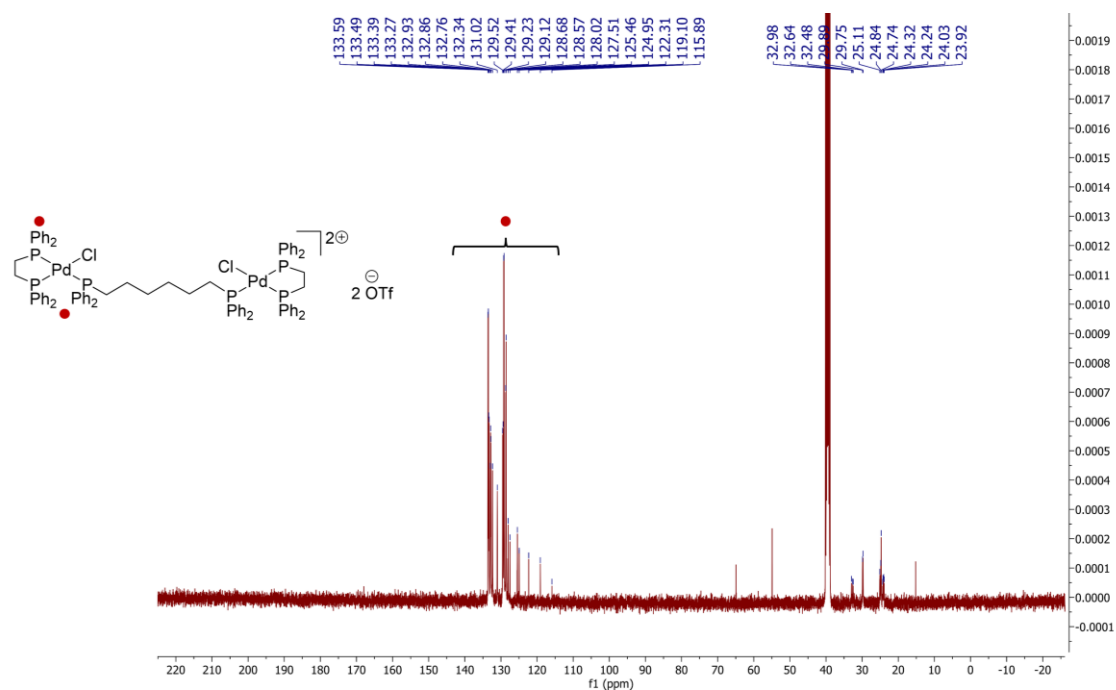
**Fig. S24.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdPd-1** in DMSO- $d_6$  at 298 K



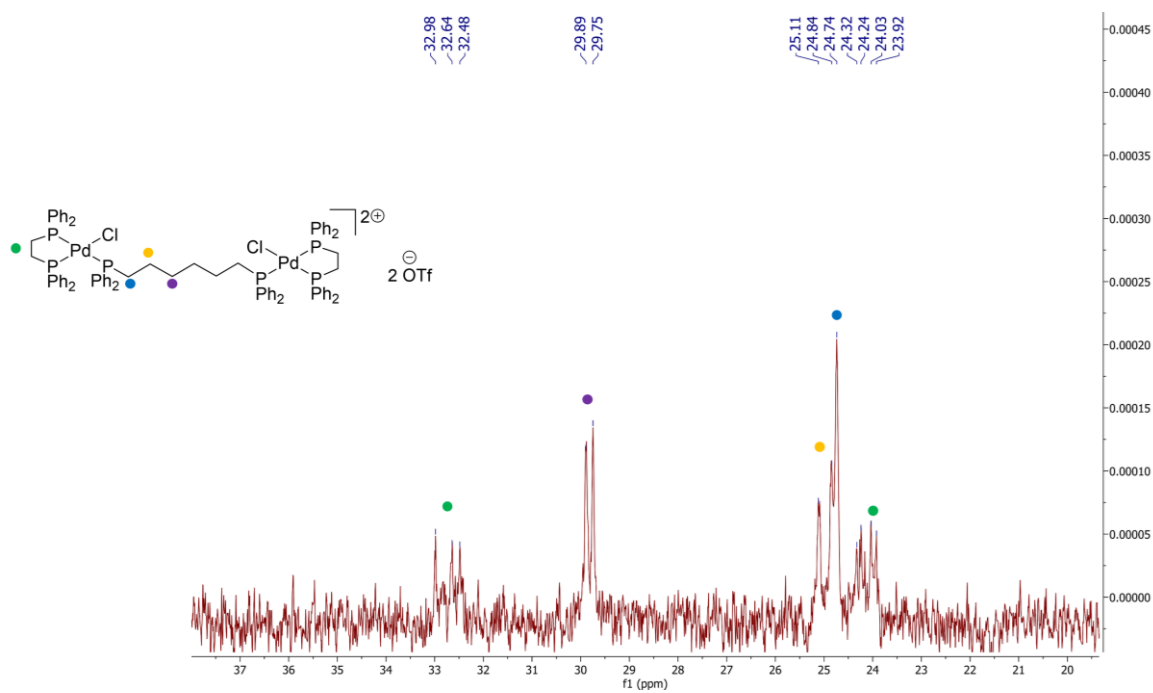
**Fig. S25.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdPd-2** in  $\text{DMSO-}d_6$  at 298 K



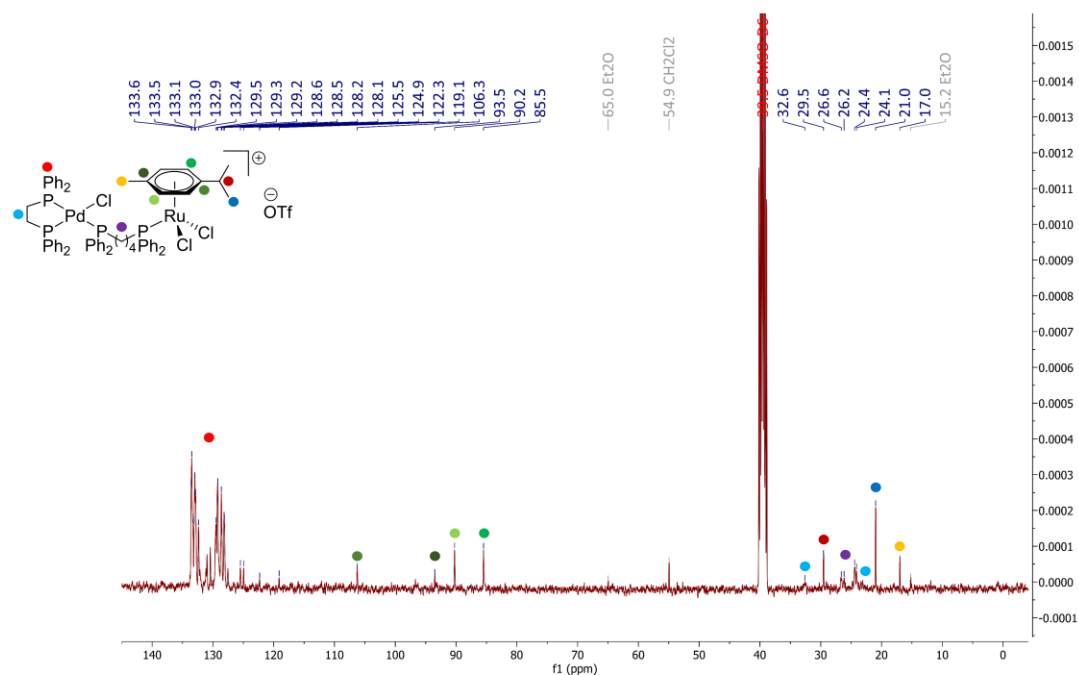
**Fig. S26.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdPd-2** (aliphatic region) in  $\text{DMSO-}d_6$  at 298 K

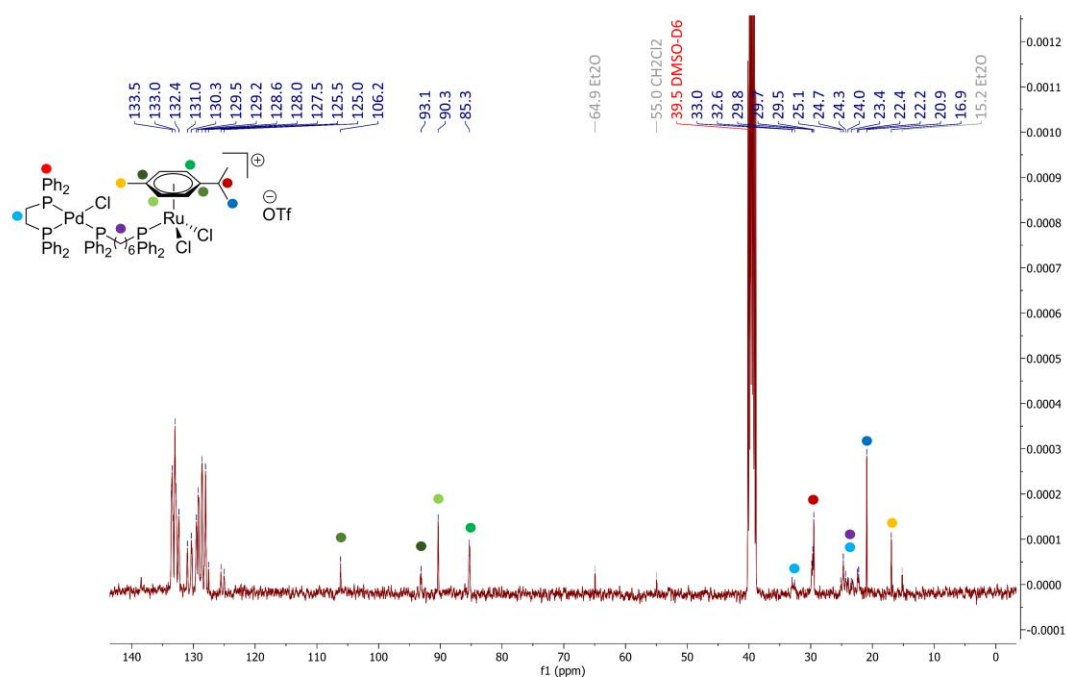


**Fig. S27.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdPd-3** in  $\text{DMSO}-d_6$  at 298 K

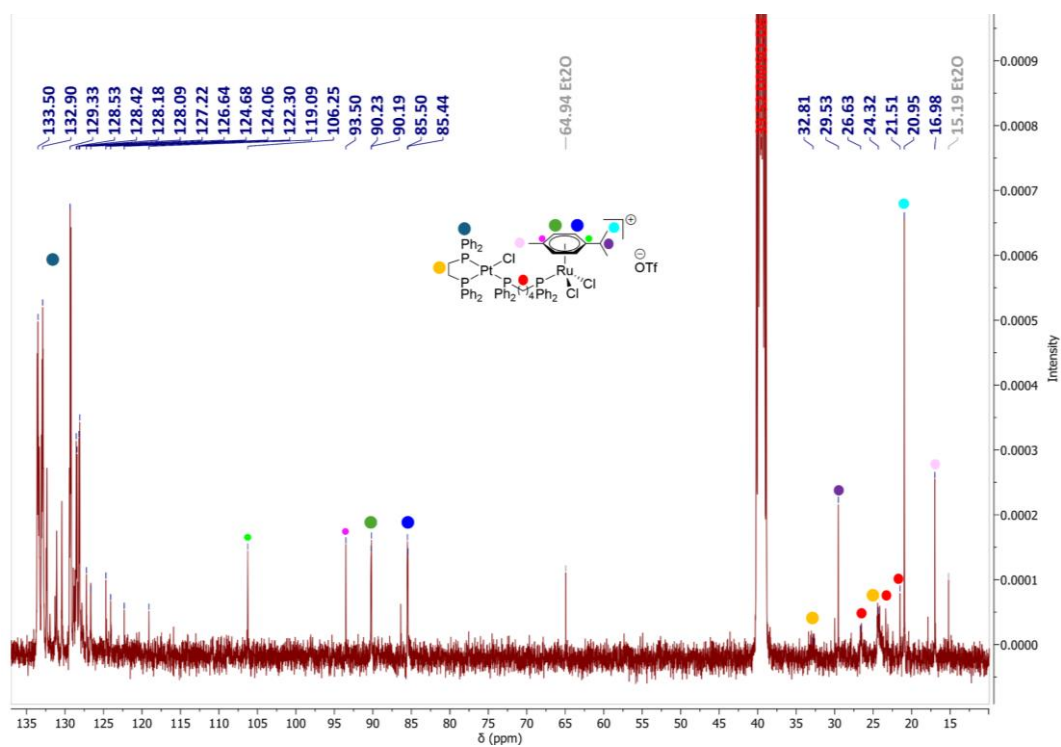


**Fig. S28.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdPd-3** (aliphatic region) in  $\text{DMSO}-d_6$  at 298 K

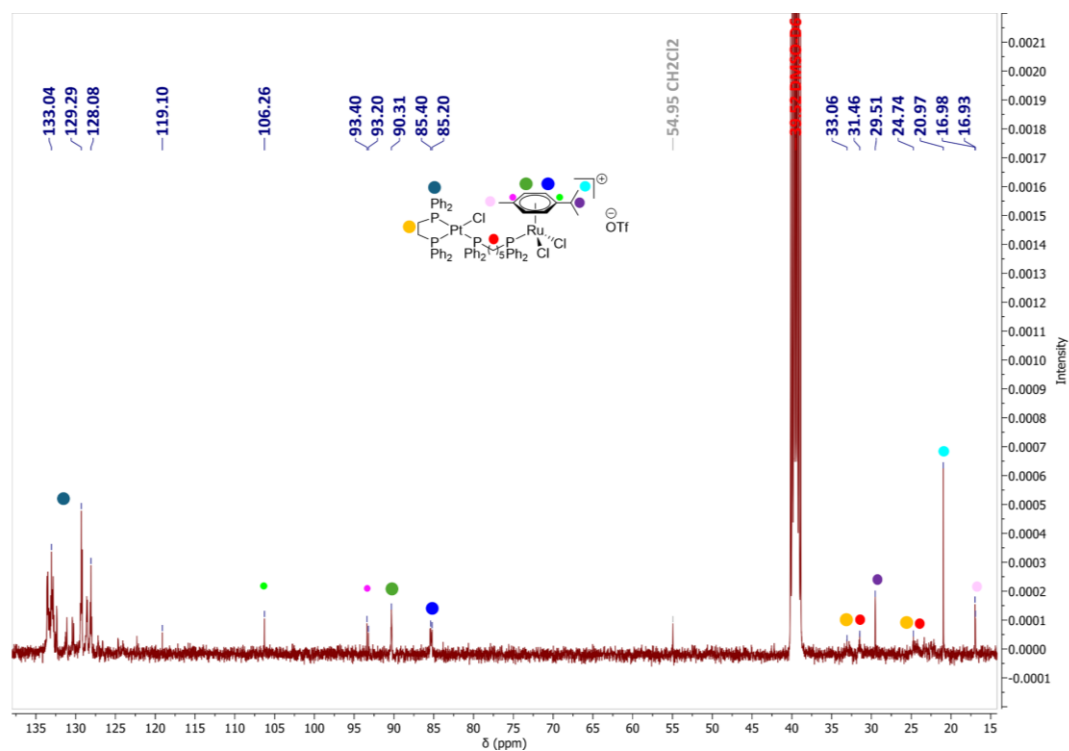




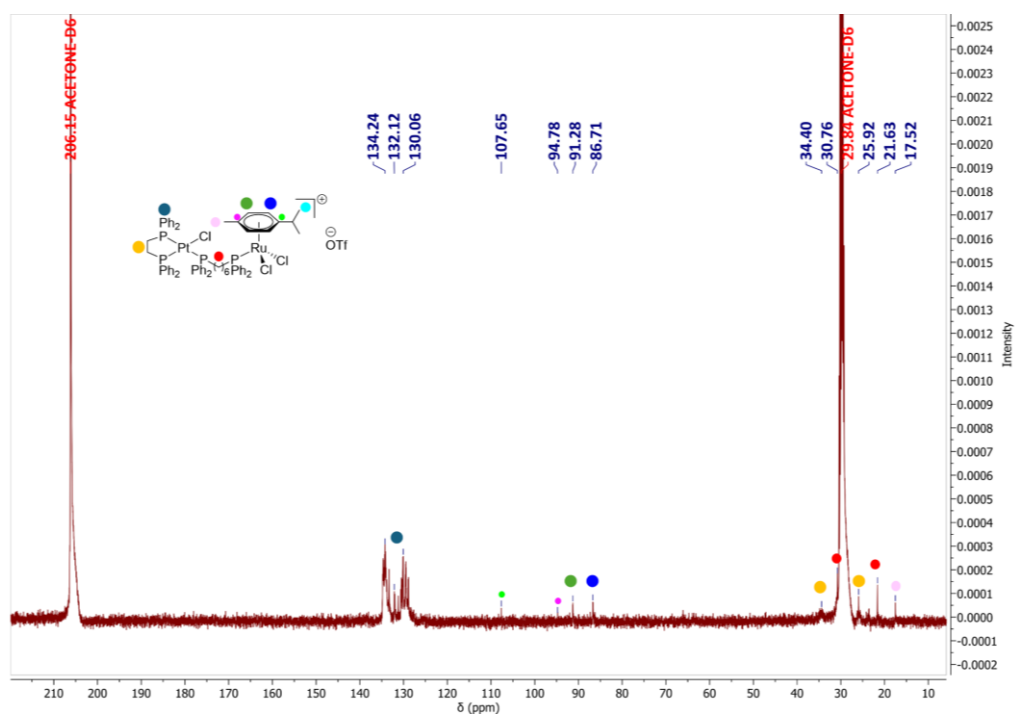
**Fig. S31.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdRu-3** in DMSO- $d_6$  at 298 K



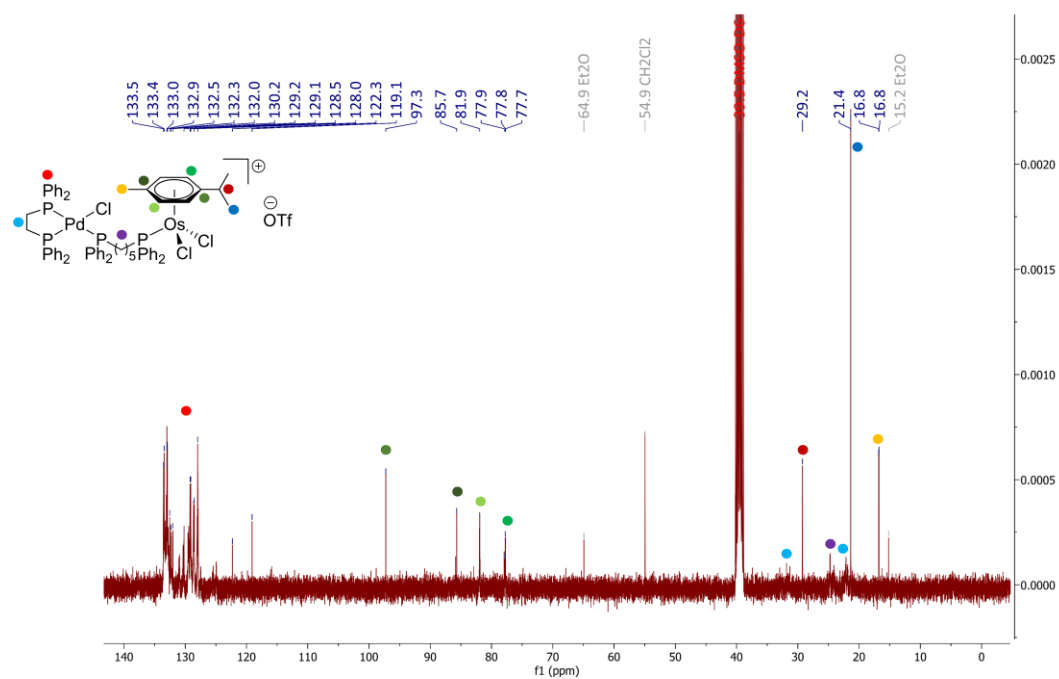
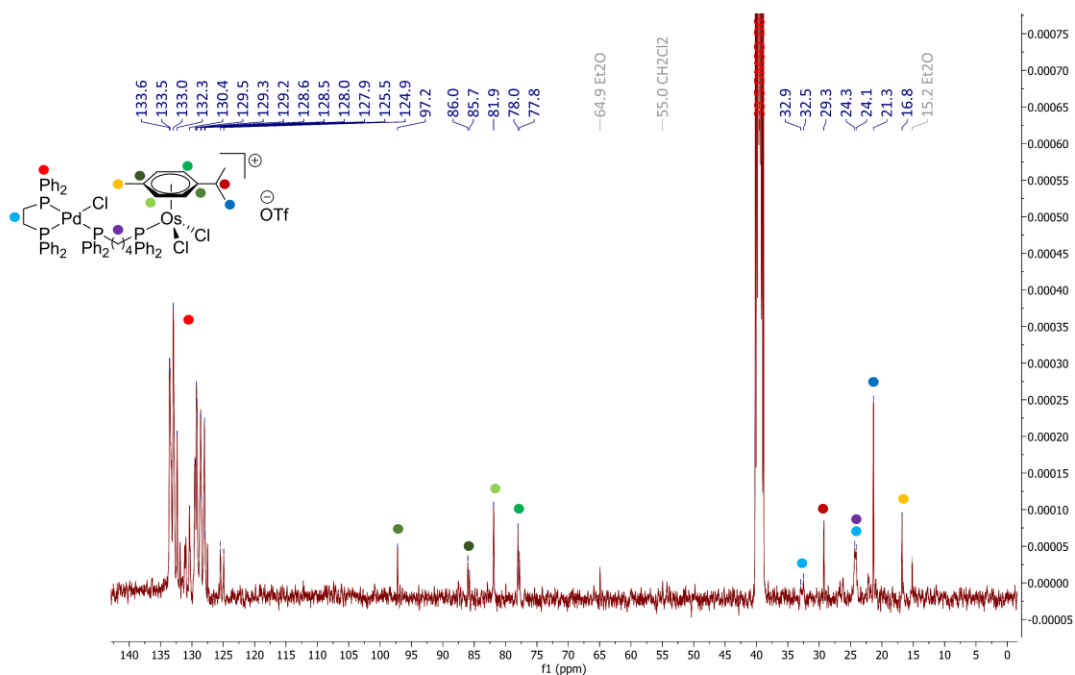
**Fig. S32.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PtRu-1** in DMSO- $d_6$  at 298 K

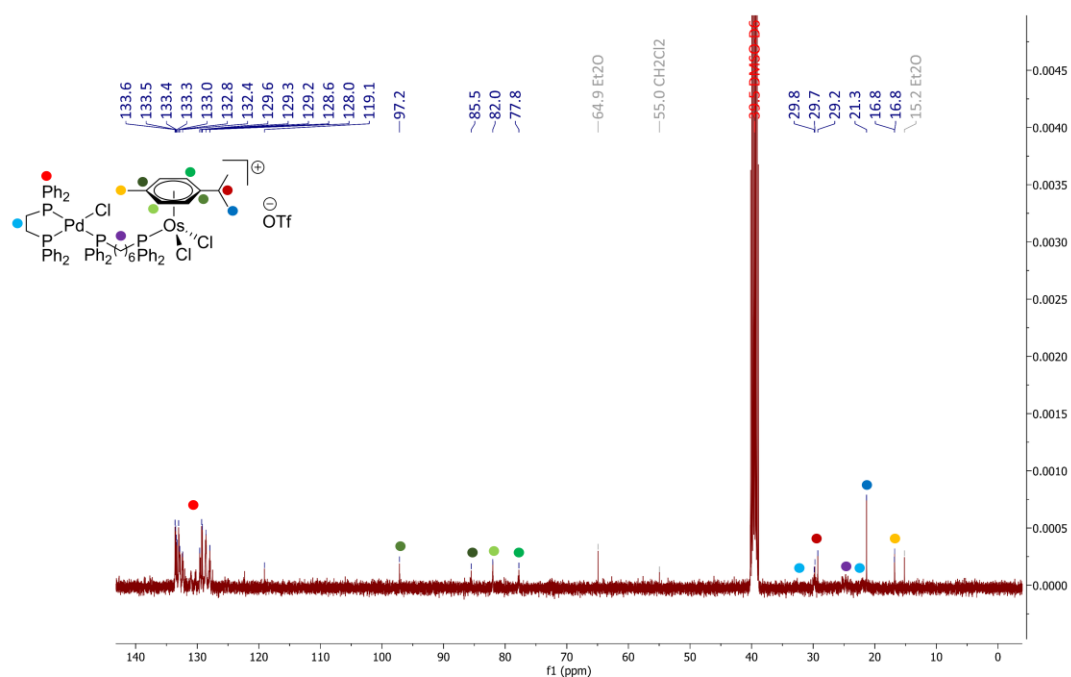


**Fig. S33.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PtRu-2** in  $\text{DMSO-}d_6$  at 298 K



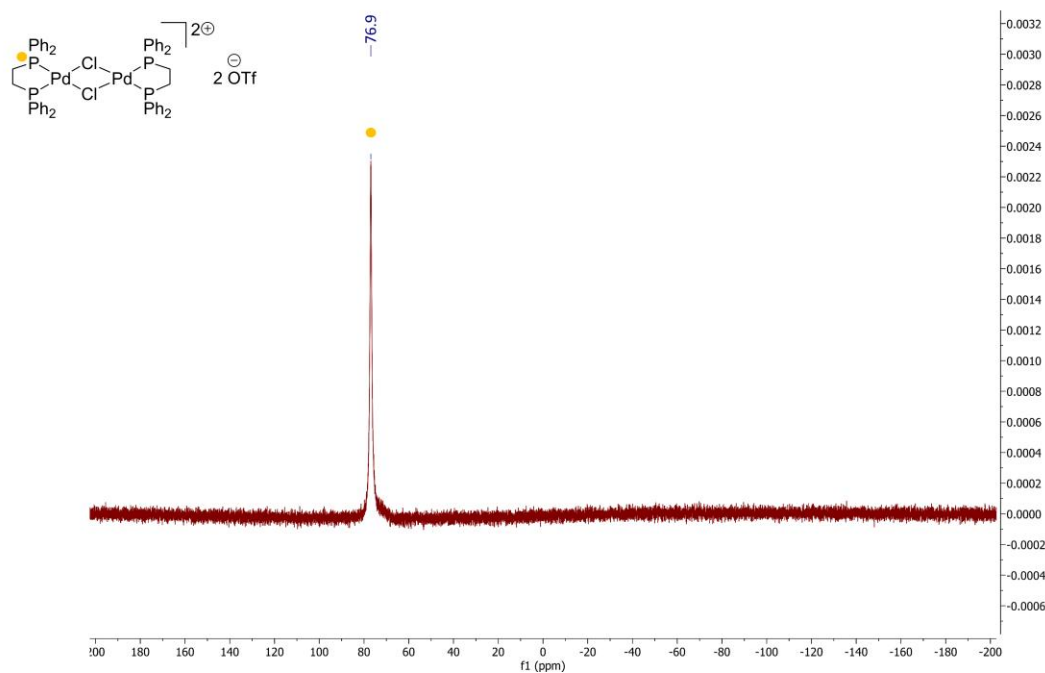
**Fig. S34.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PtRu-3** in  $\text{acetone-}d_6$  at 298 K





**Fig. S37.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **PdOs-3** in  $\text{DMSO-}d_6$  at 298 K

### 3. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra



**Fig. S38.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **PdPd-0** in  $\text{acetone-}d_6$  at 298 K



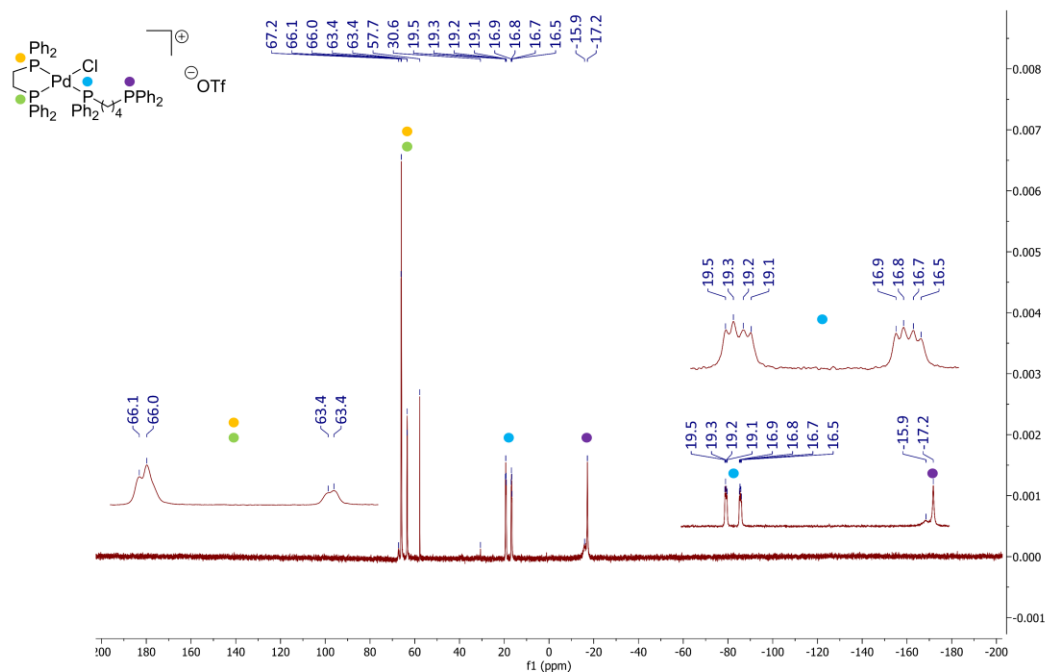


Fig. S39.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of Pd-1 in  $\text{DMSO-}d_6$  at 298 K

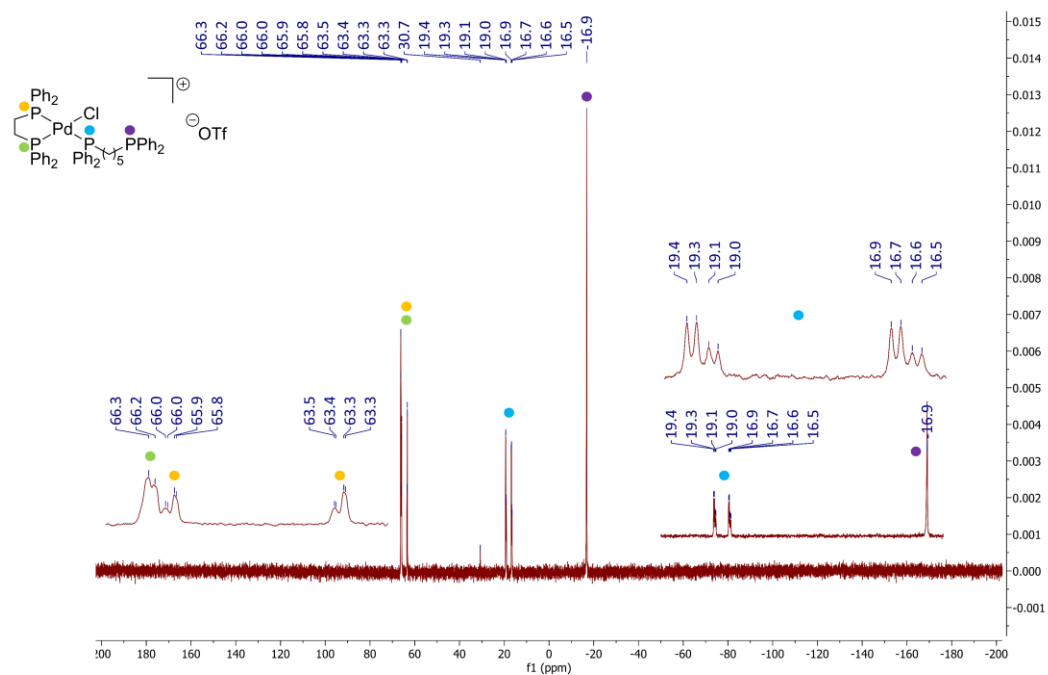
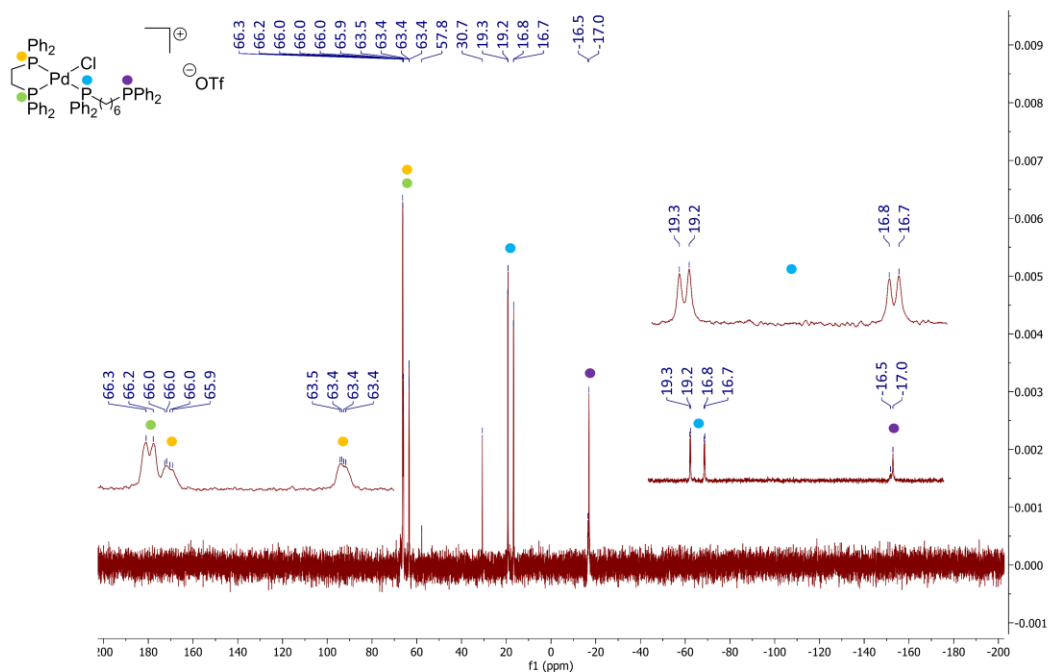
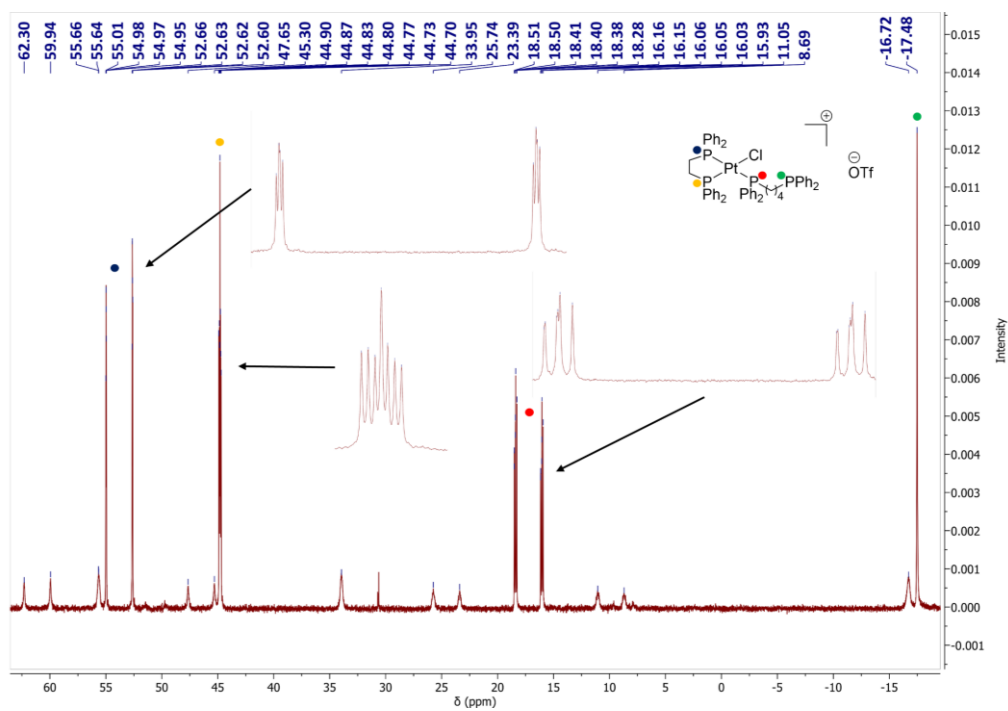


Fig. S40.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of Pd-2 in  $\text{DMSO-}d_6$  at 298 K



**Fig. S41.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **Pd-3** in  $\text{DMSO}-d_6$  at 298 K



**Fig. S42.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **Pt-1** in  $\text{DMSO}-d_6$  at 298 K

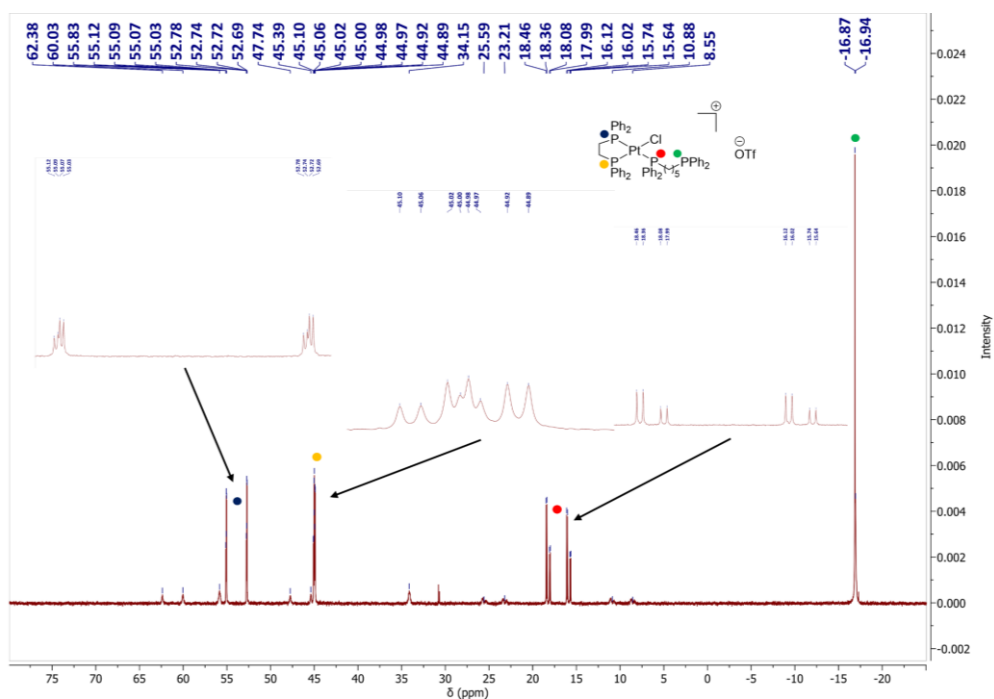


Fig. S43.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of Pt-2 in DMSO- $d_6$  at 298 K

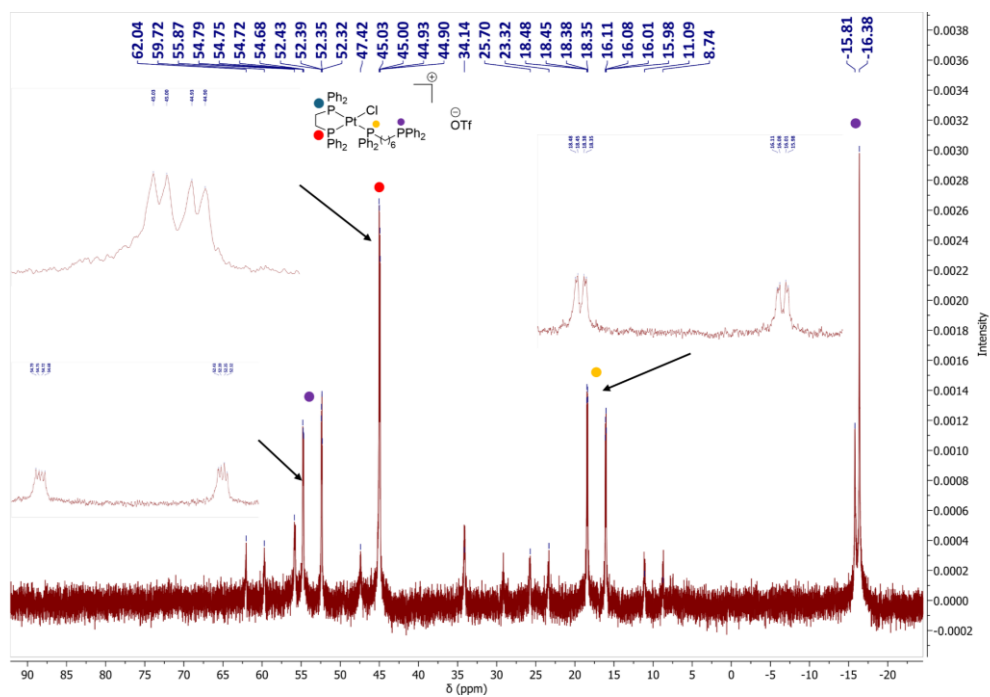
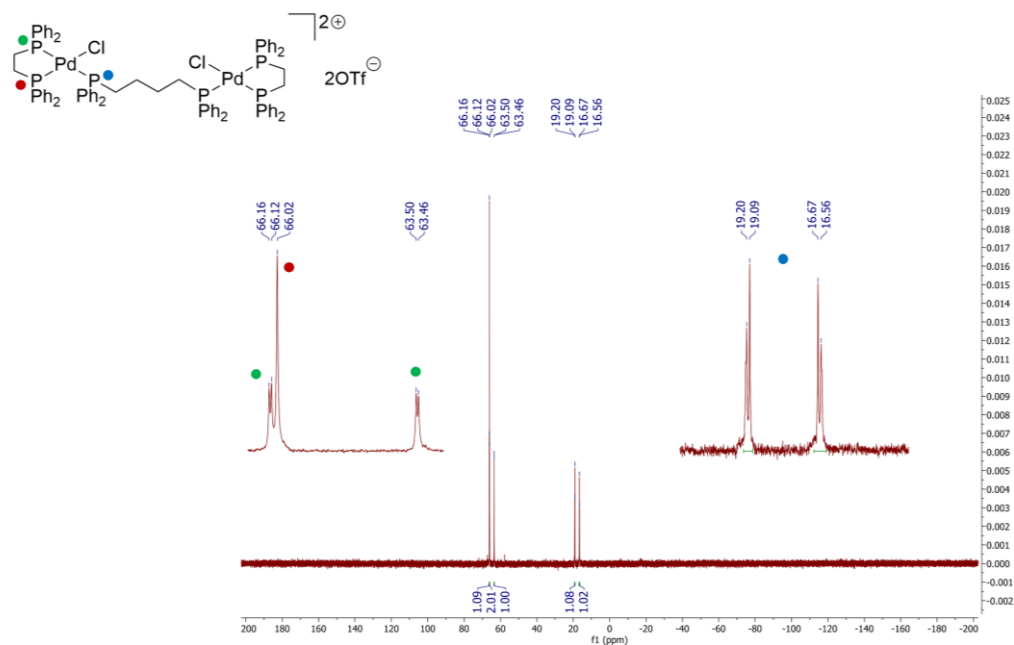
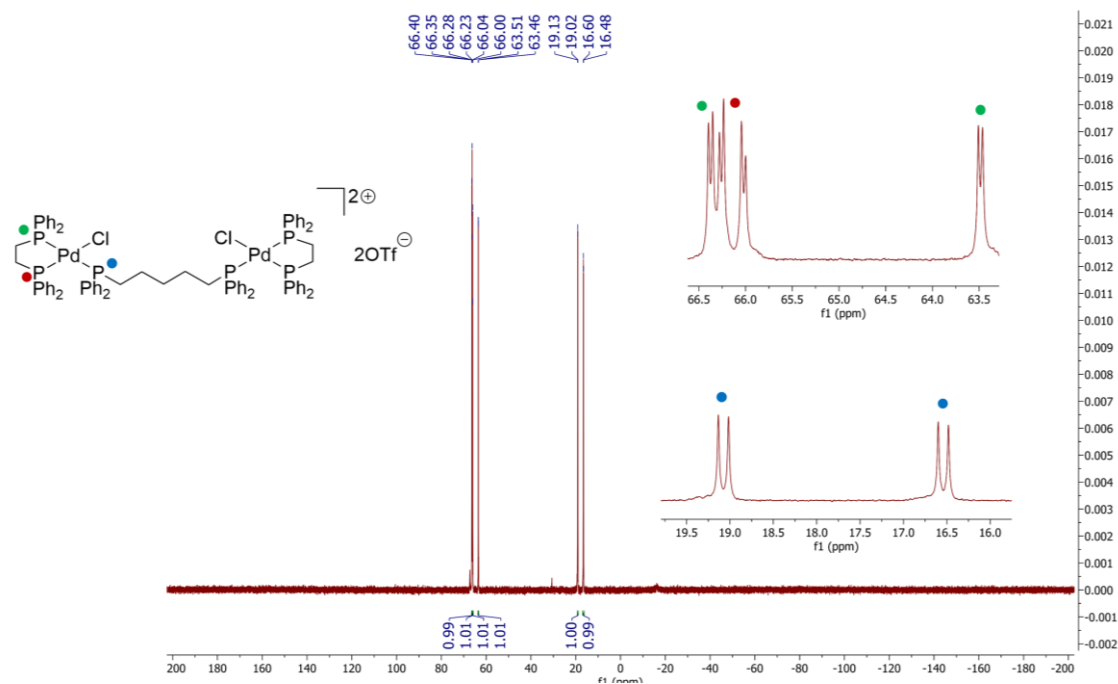


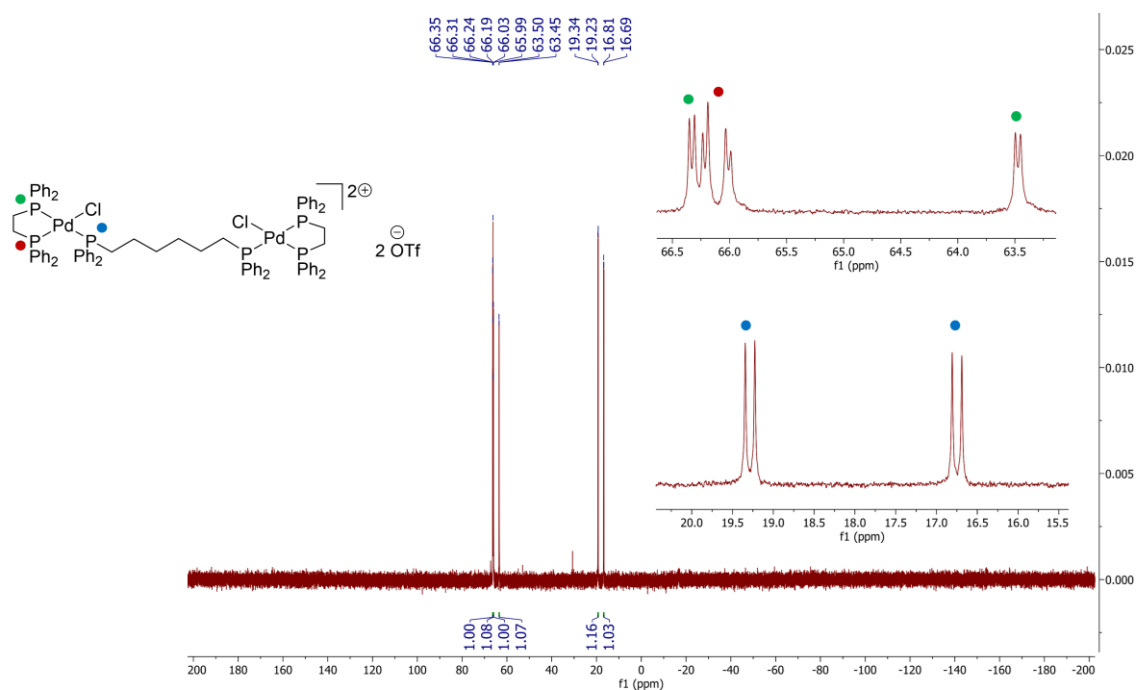
Fig. S44.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of Pt-3 in acetone- $d_6$  at 298 K



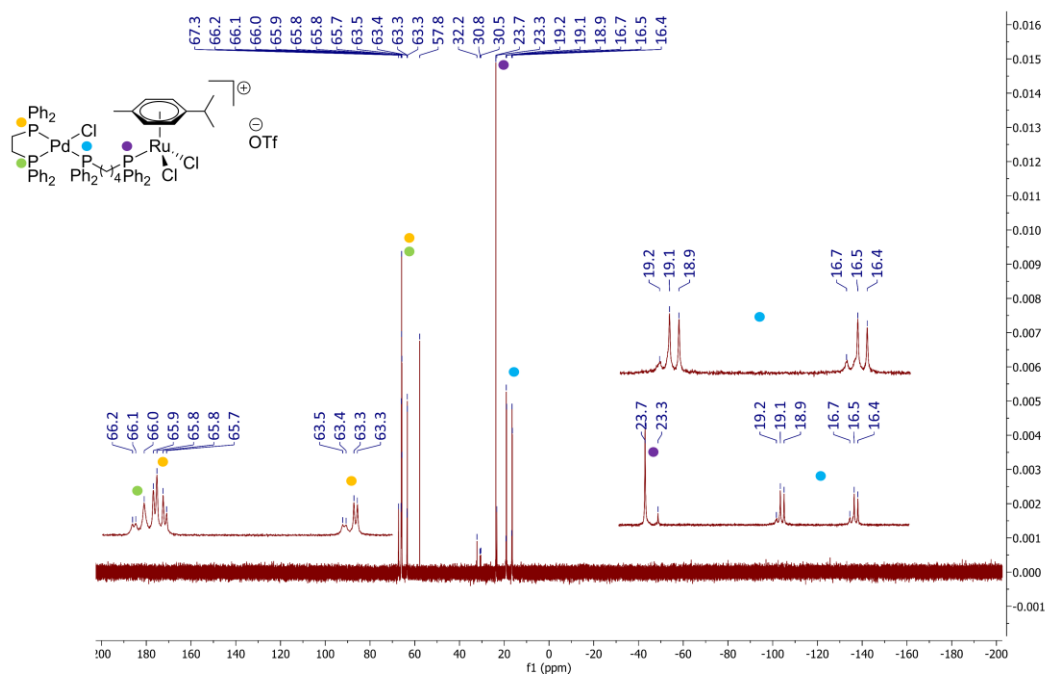
**Fig. S45.** <sup>31</sup>P{<sup>1</sup>H} NMR spectrum of **PdPd-1** in DMSO-*d*<sub>6</sub> at 298 K



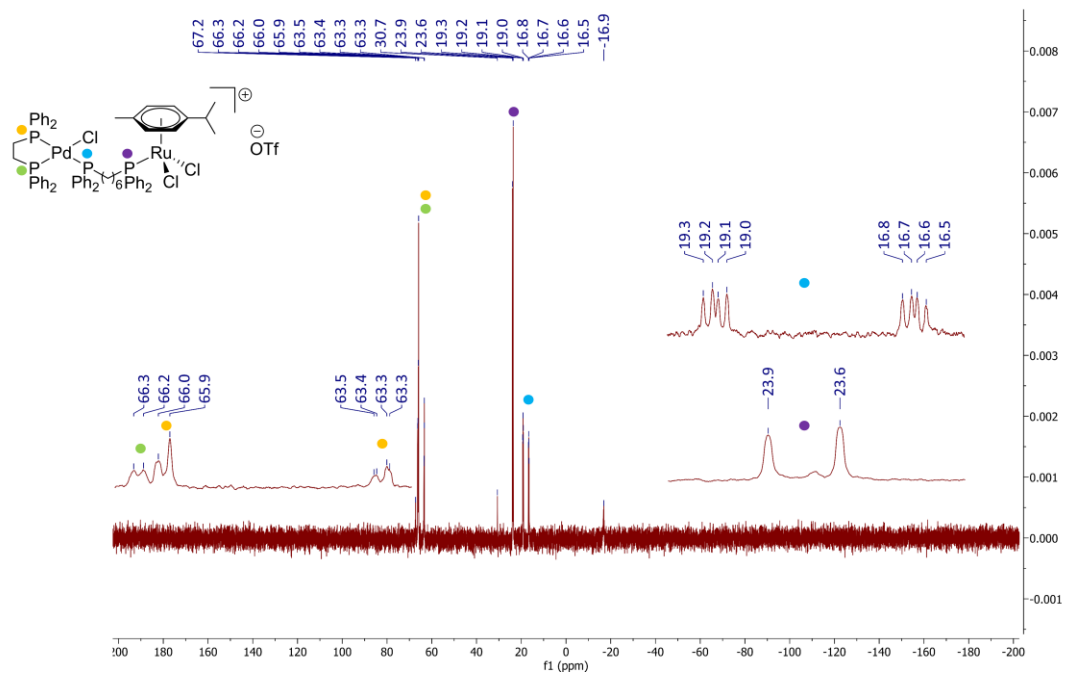
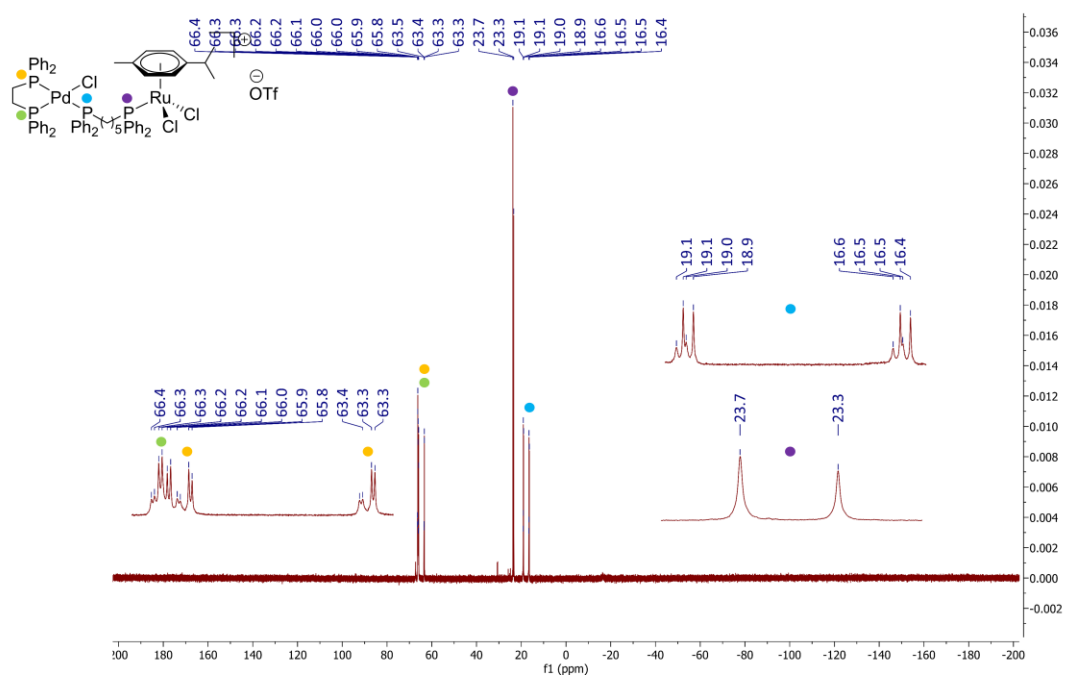
**Fig. S46.** <sup>31</sup>P{<sup>1</sup>H} NMR spectrum of **PdPd-2** in DMSO-*d*<sub>6</sub> at 298 K

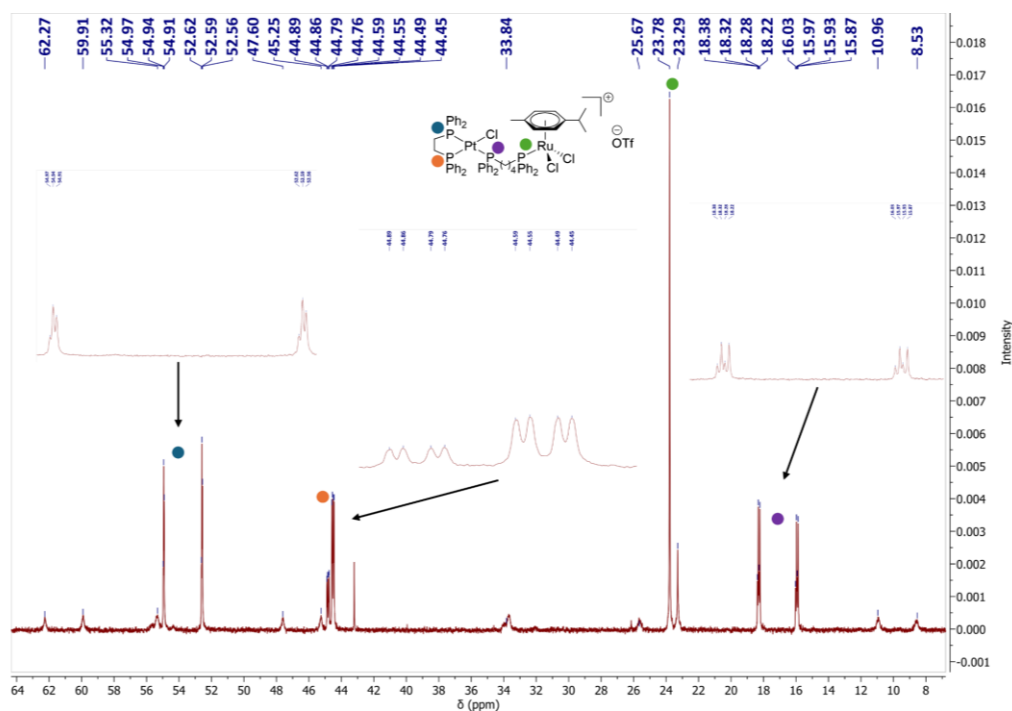


**Fig. S47.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **PdPd-3** in DMSO- $d_6$  at 298 K

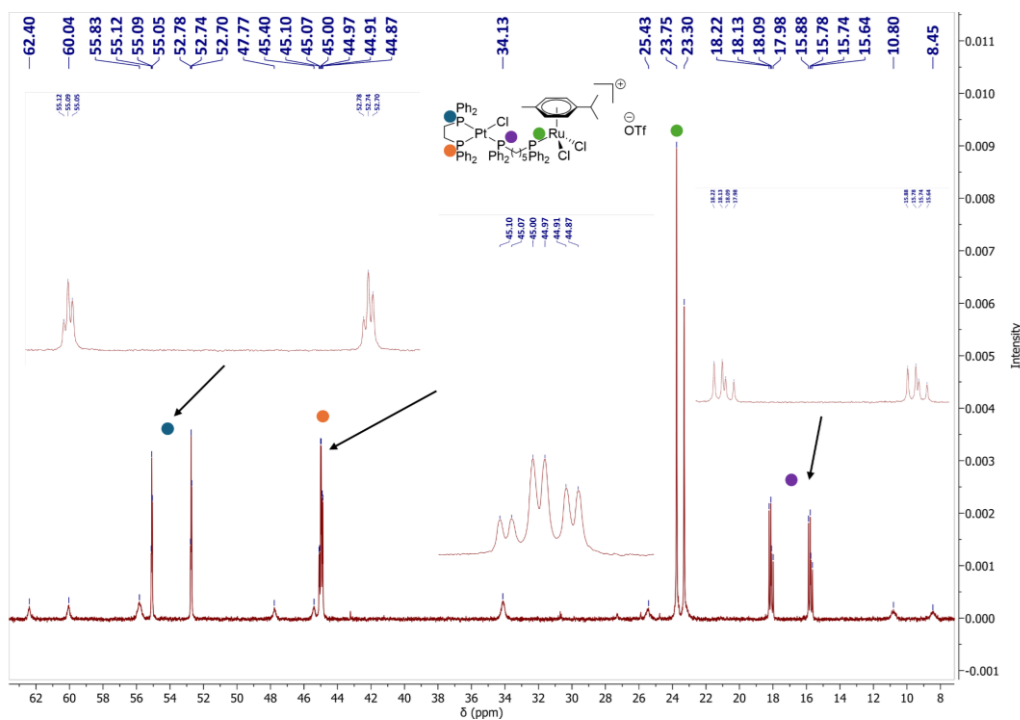


**Fig. S48.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **PdRu-1** in DMSO- $d_6$  at 298 K





**Fig. S51.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of PtRu-1 in DMSO- $d_6$  at 298 K



**Fig. S52.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of PtRu-2 in DMSO- $d_6$  at 298 K

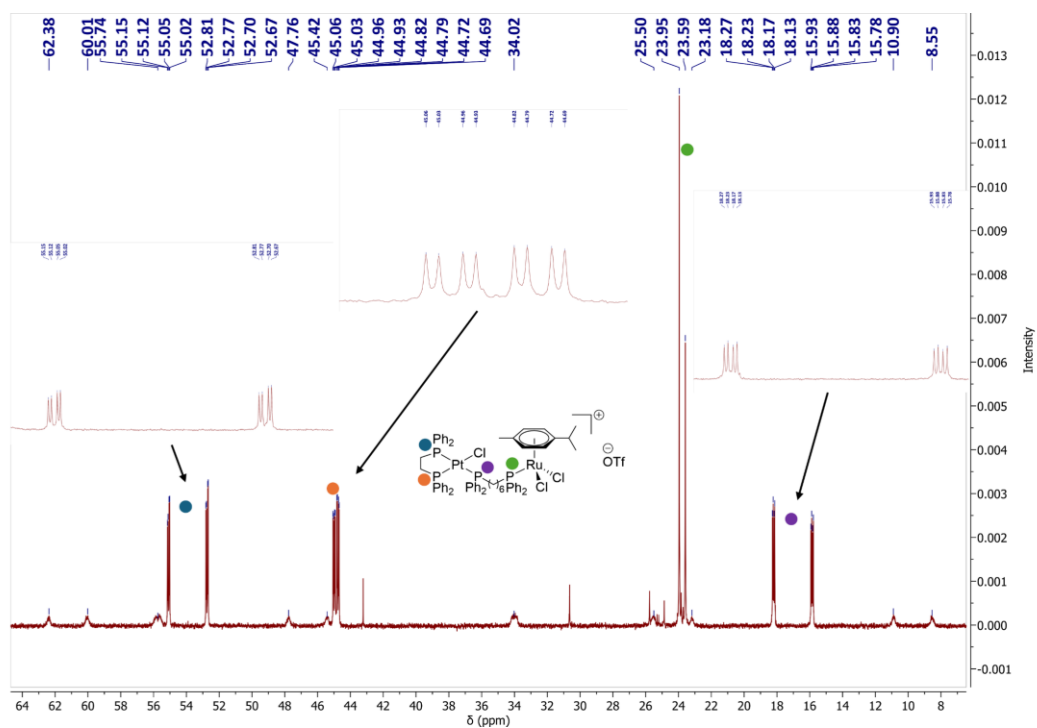


Fig. S53.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of PtRu-3 in DMSO- $d_6$  at 298 K

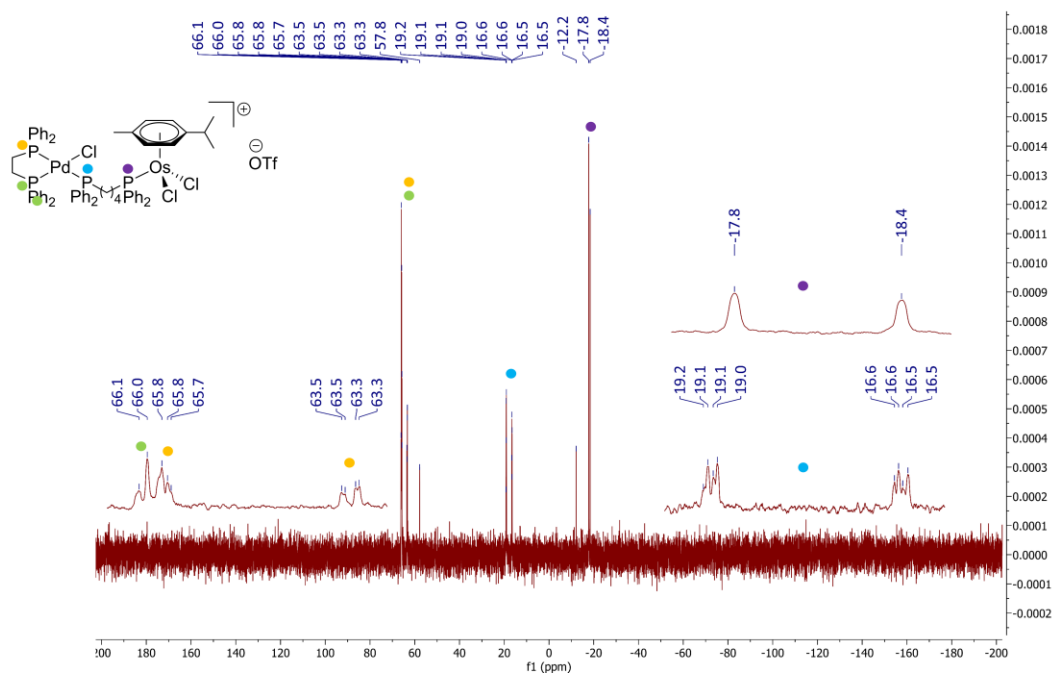
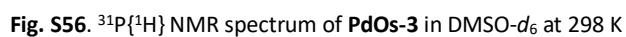
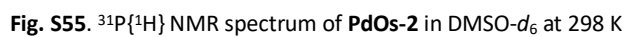


Fig. S54.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of PdOs-1 in DMSO- $d_6$  at 298 K





#### 4. 2D NMR spectra

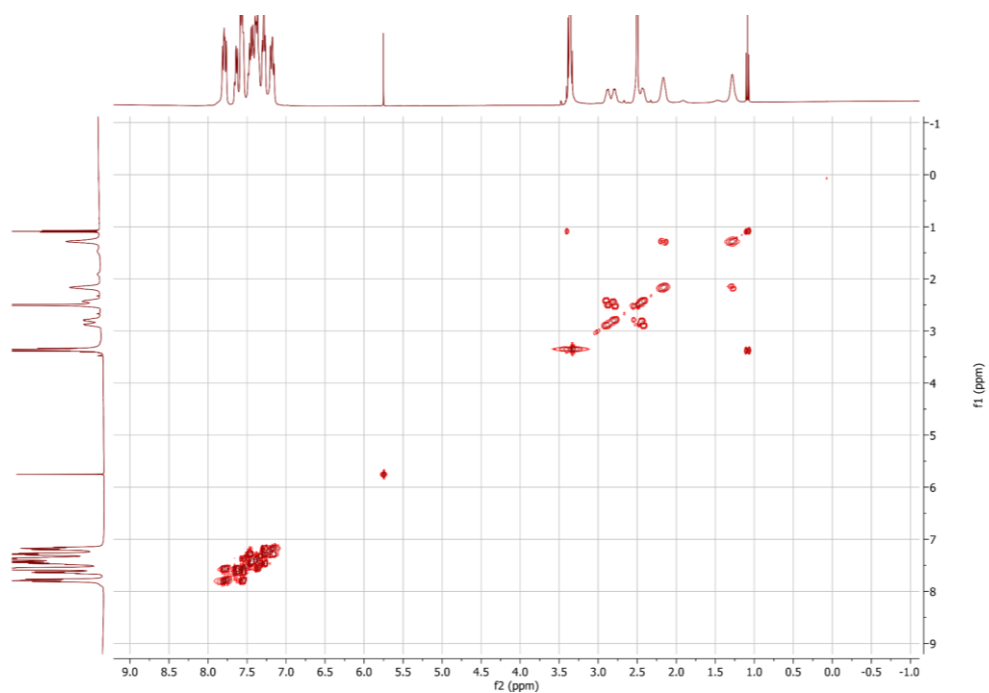


Fig. S57.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **PdPd-1** in  $\text{DMSO-}d_6$  at 298 K

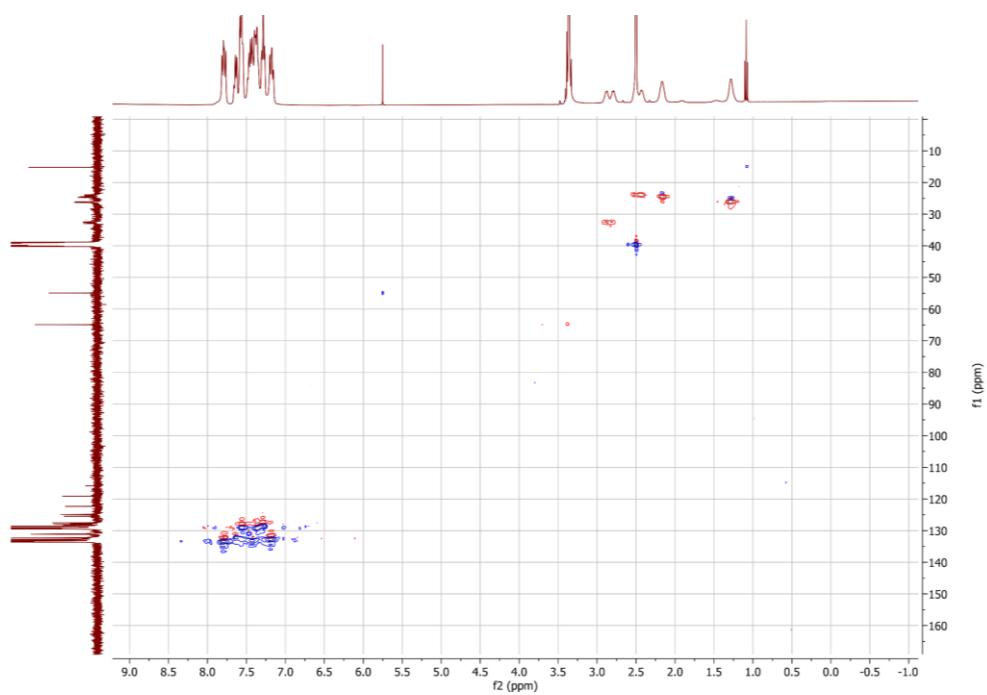
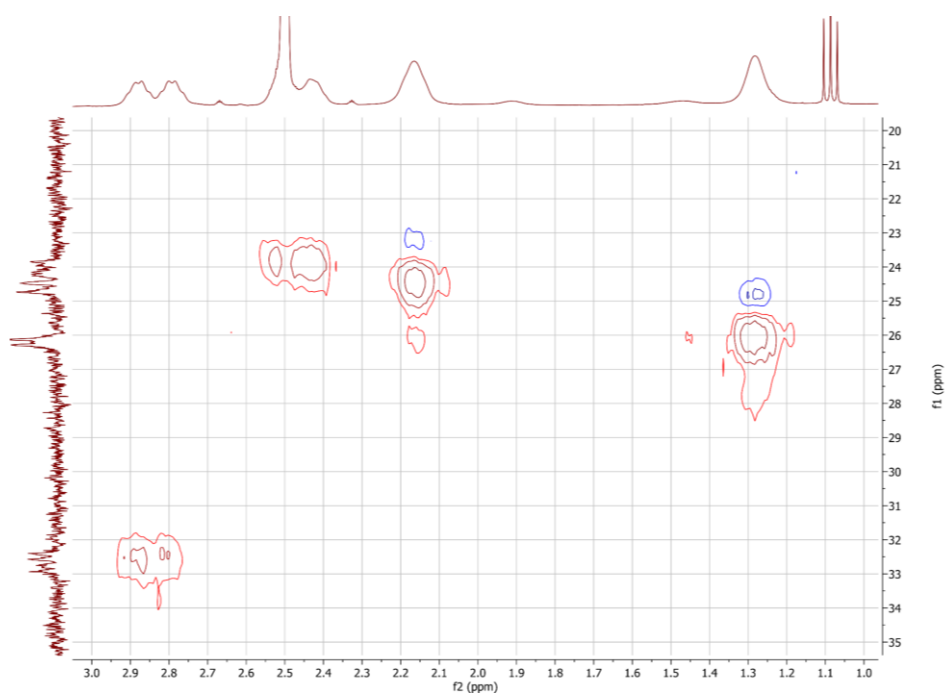
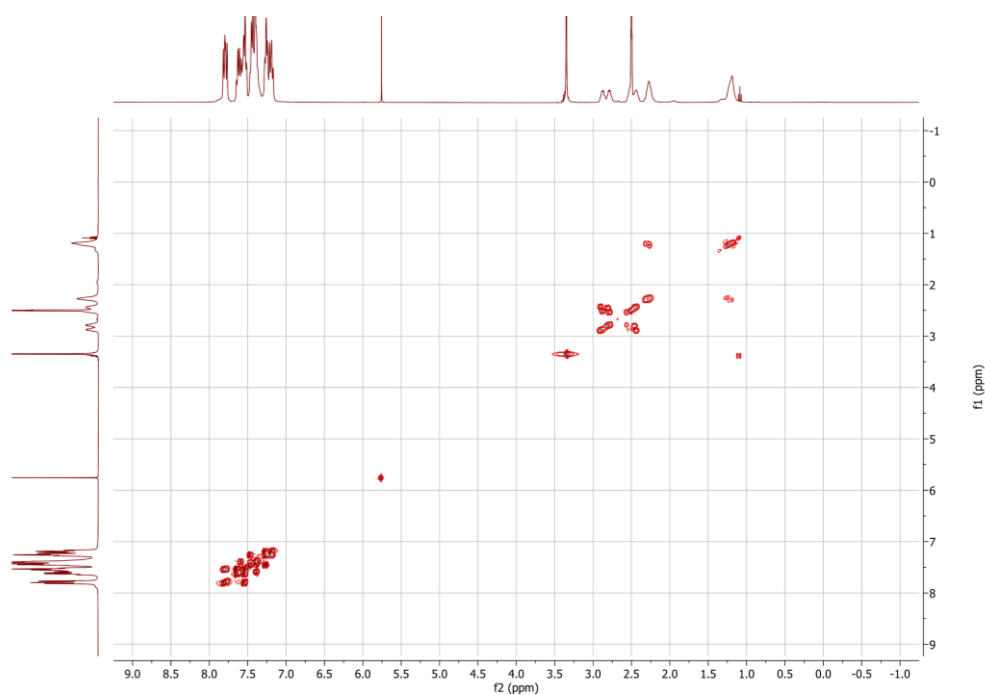


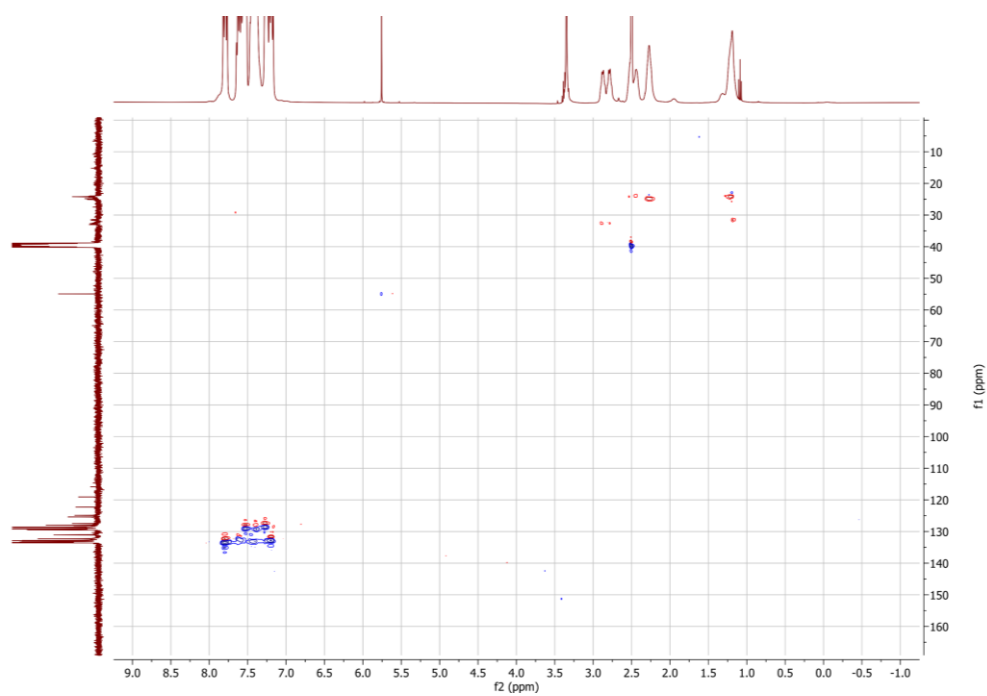
Fig. S58.  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **PdPd-1** in  $\text{DMSO-}d_6$  at 298 K



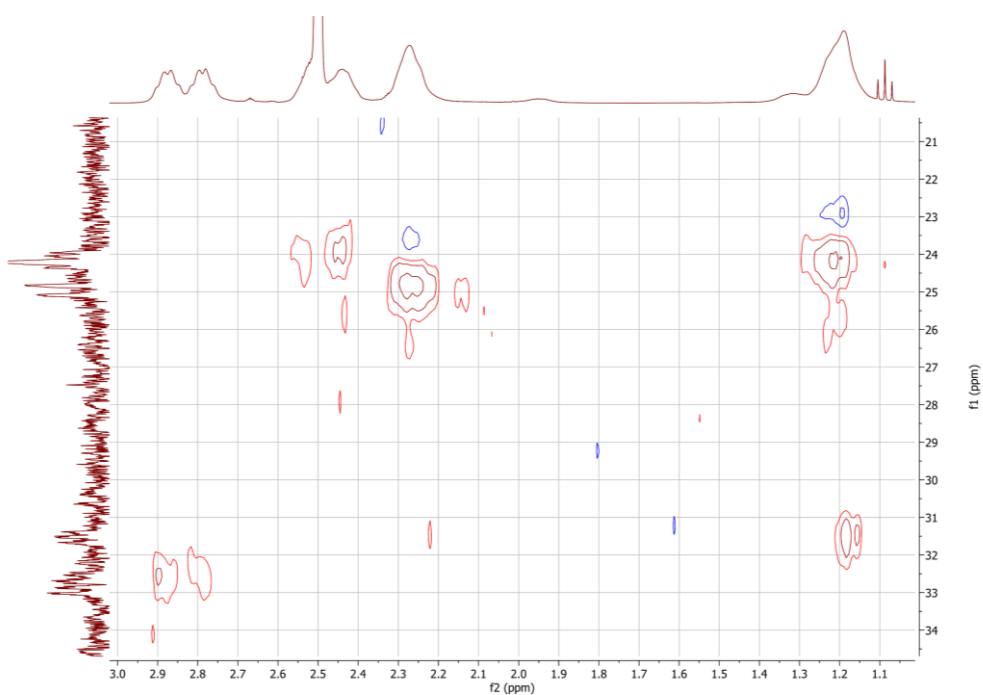
**Fig. S59.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **PdPd-1** (zoom in aliphatic region) in  $\text{DMSO}-d_6$  at 298 K



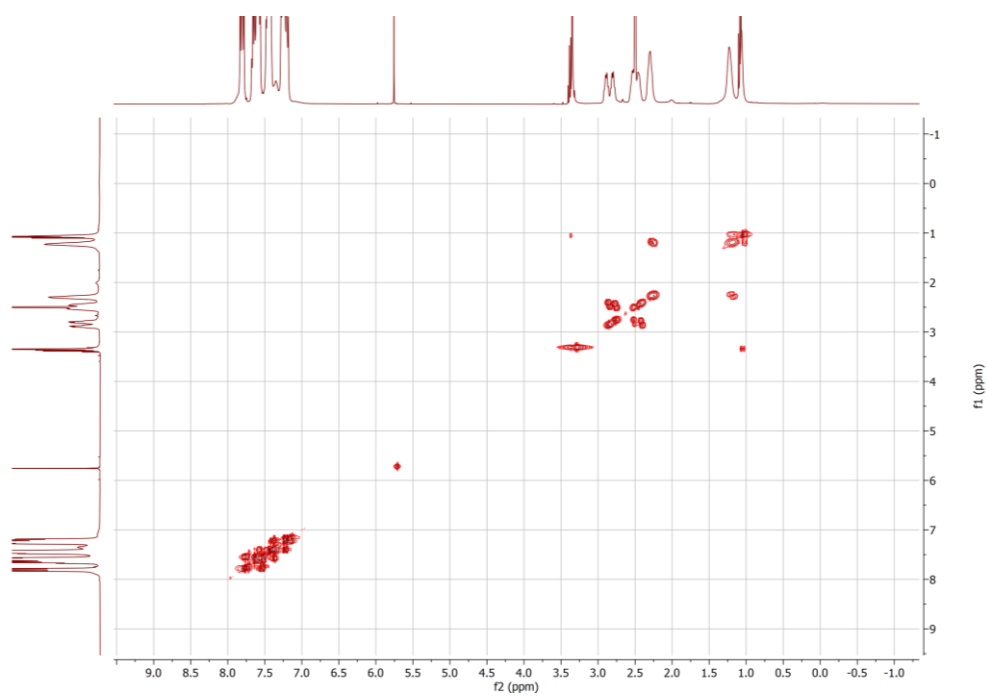
**Fig. S60.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **PdPd-2** in  $\text{DMSO}-d_6$  at 298 K



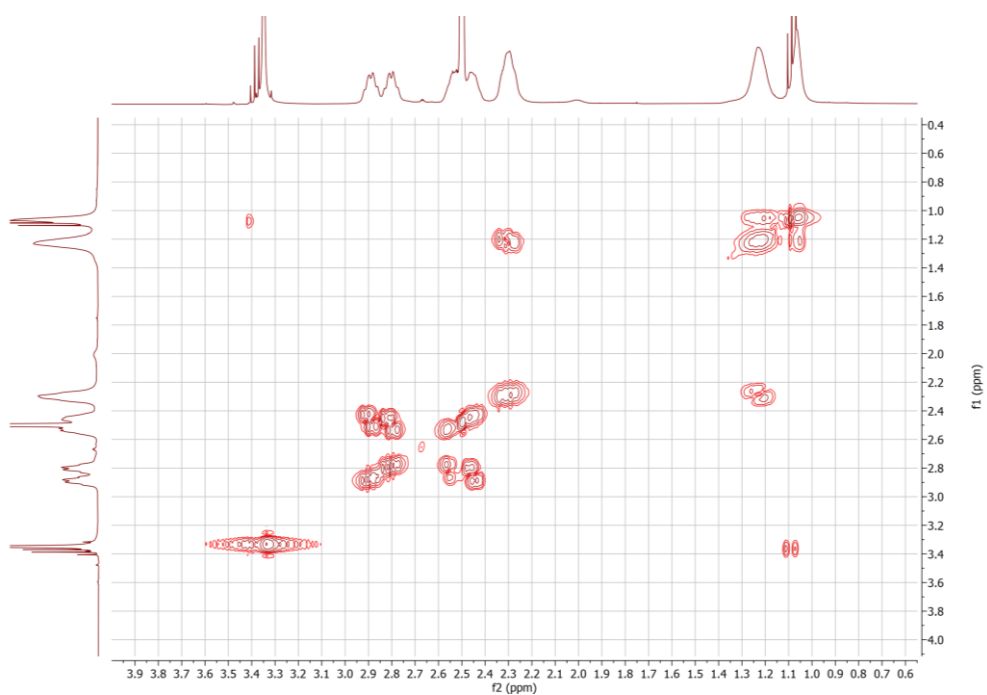
**Fig. S61.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **PdPd-2** in  $\text{DMSO}-d_6$  at 298 K



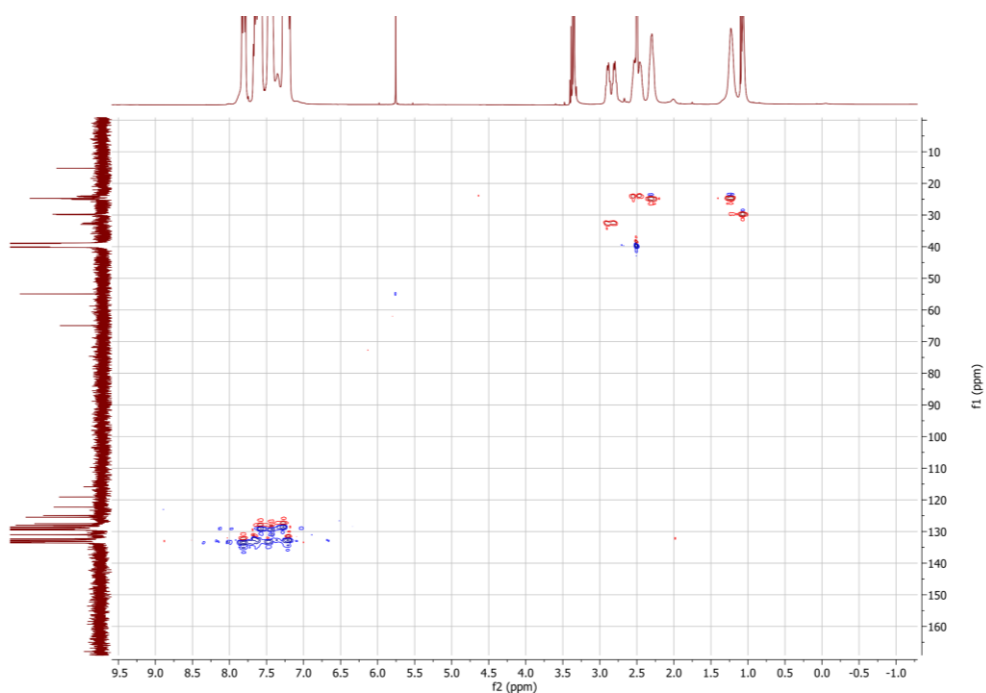
**Fig. S62.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **PdPd-2** in  $\text{DMSO}-d_6$  at 298 K



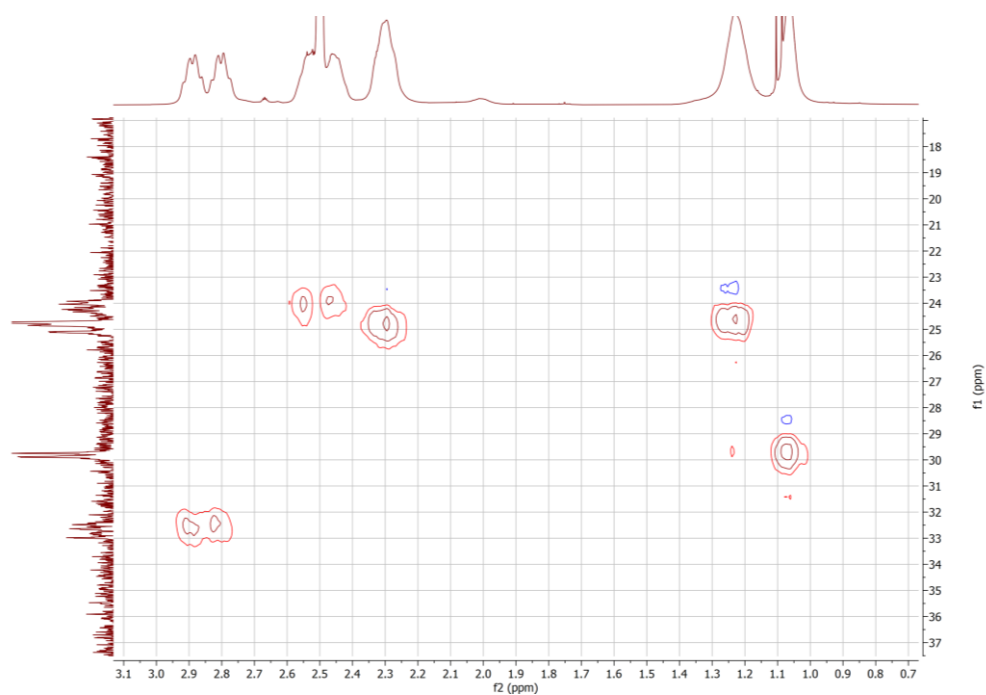
**Fig. S63.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **PdPd-3** in  $\text{DMSO}-d_6$  at 298 K



**Fig. S64.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **PdPd-3** (zoom in aliphatic region) in  $\text{DMSO}-d_6$  at 298 K

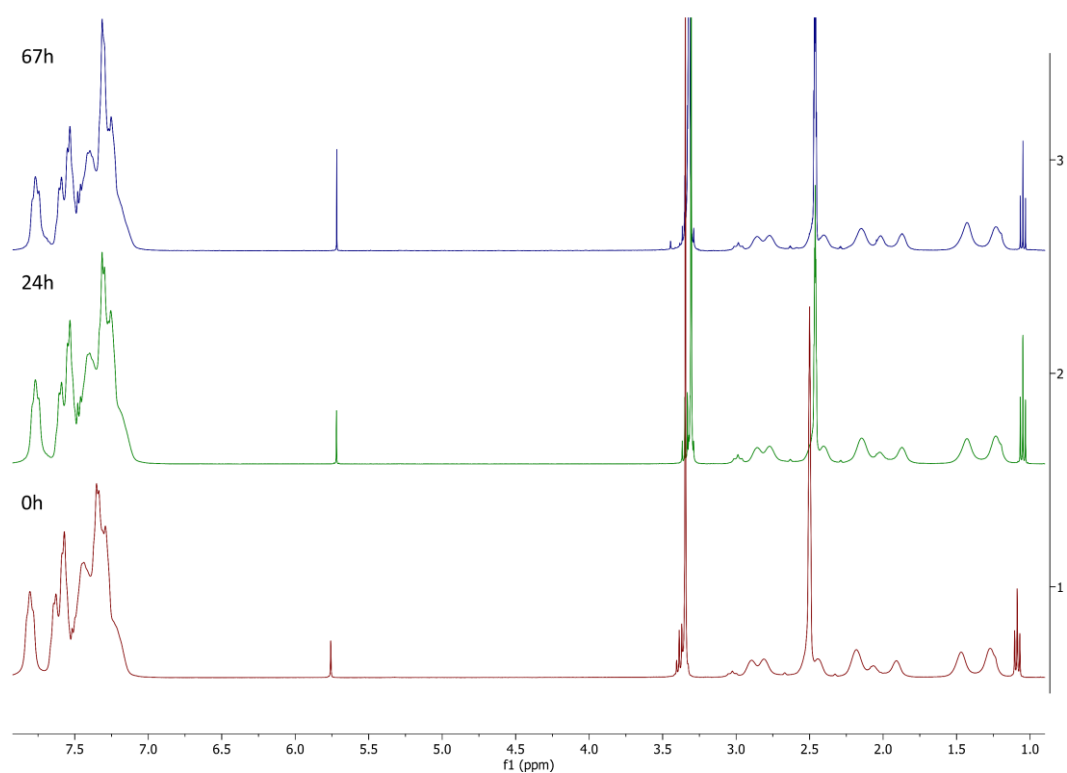


**Fig. S65.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **PdPd-3** in  $\text{DMSO}-d_6$  at 298 K

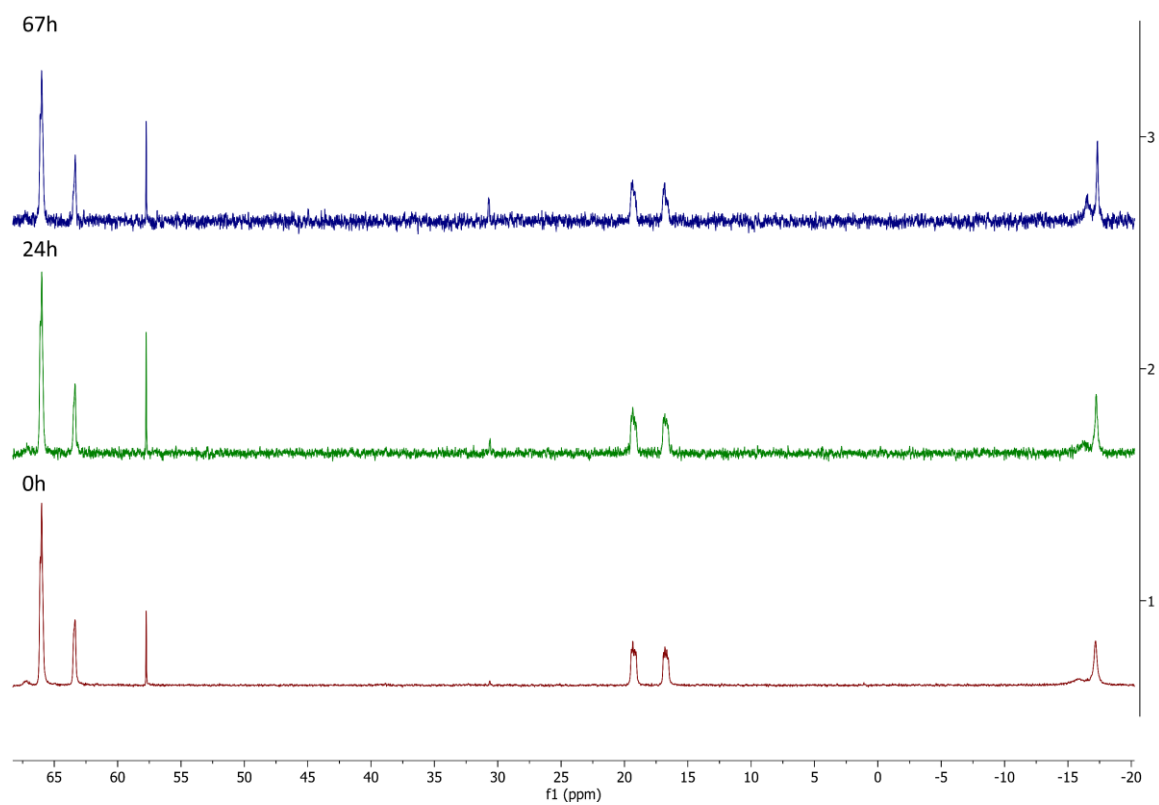


**Fig. S66.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **PdPd-3** (zoom in aliphatic region) in  $\text{DMSO}-d_6$  at 298 K

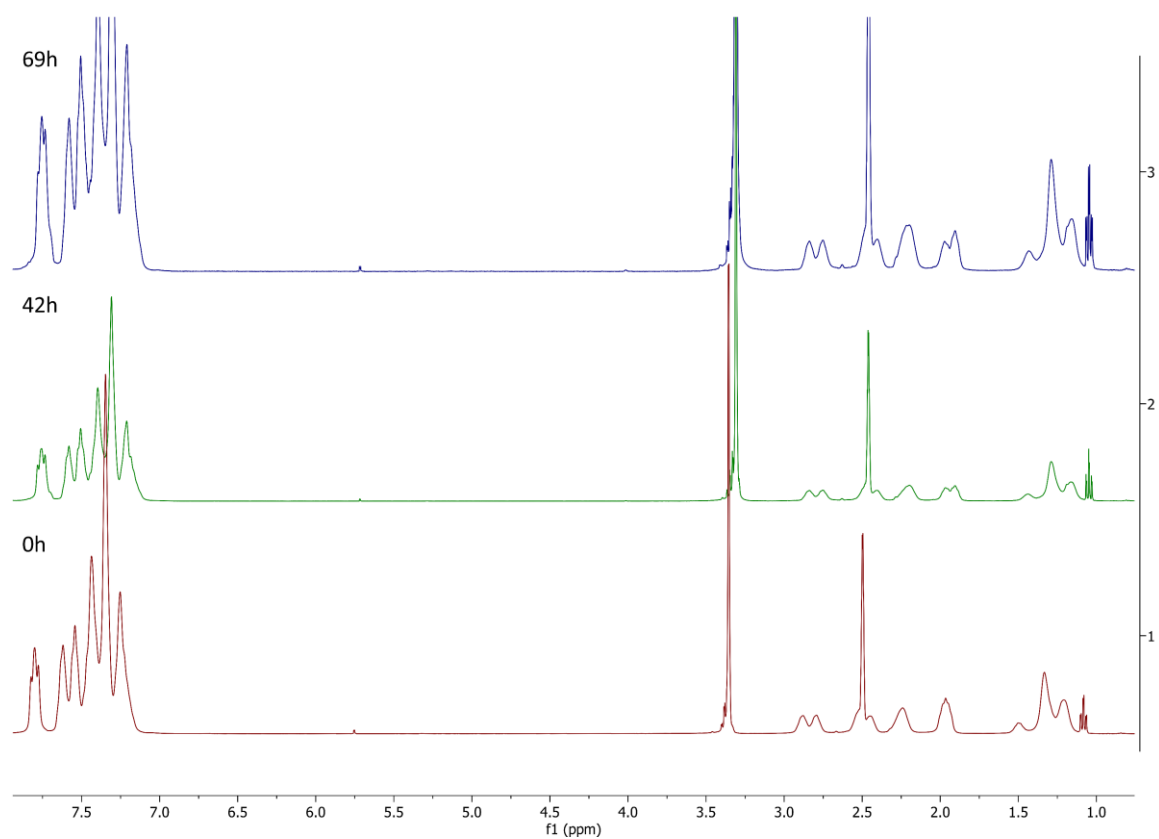
## 5. DMSO stability studies



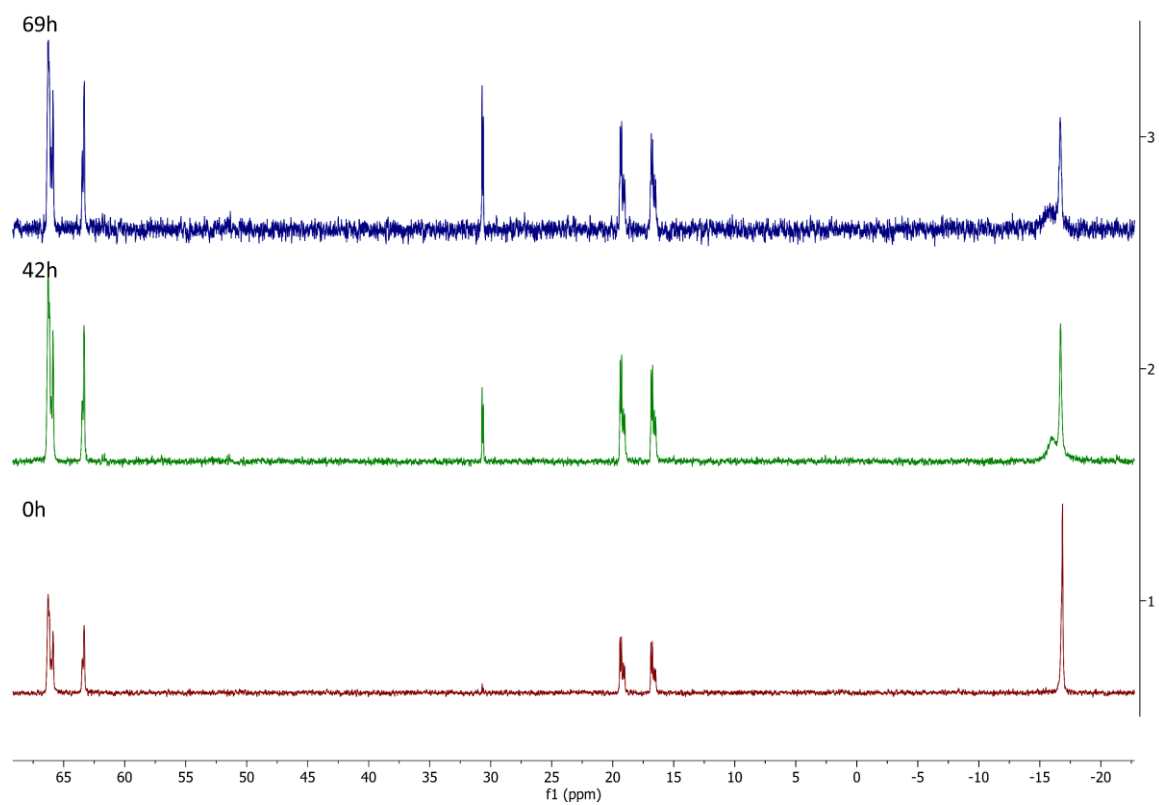
**Fig. S67.**  $\text{DMSO-}d_6$  stability studies of **Pd-1** ( $^1\text{H}$  NMR spectra, 298 K)



**Fig. S68.**  $\text{DMSO-}d_6$  stability studies of **Pd-1** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)

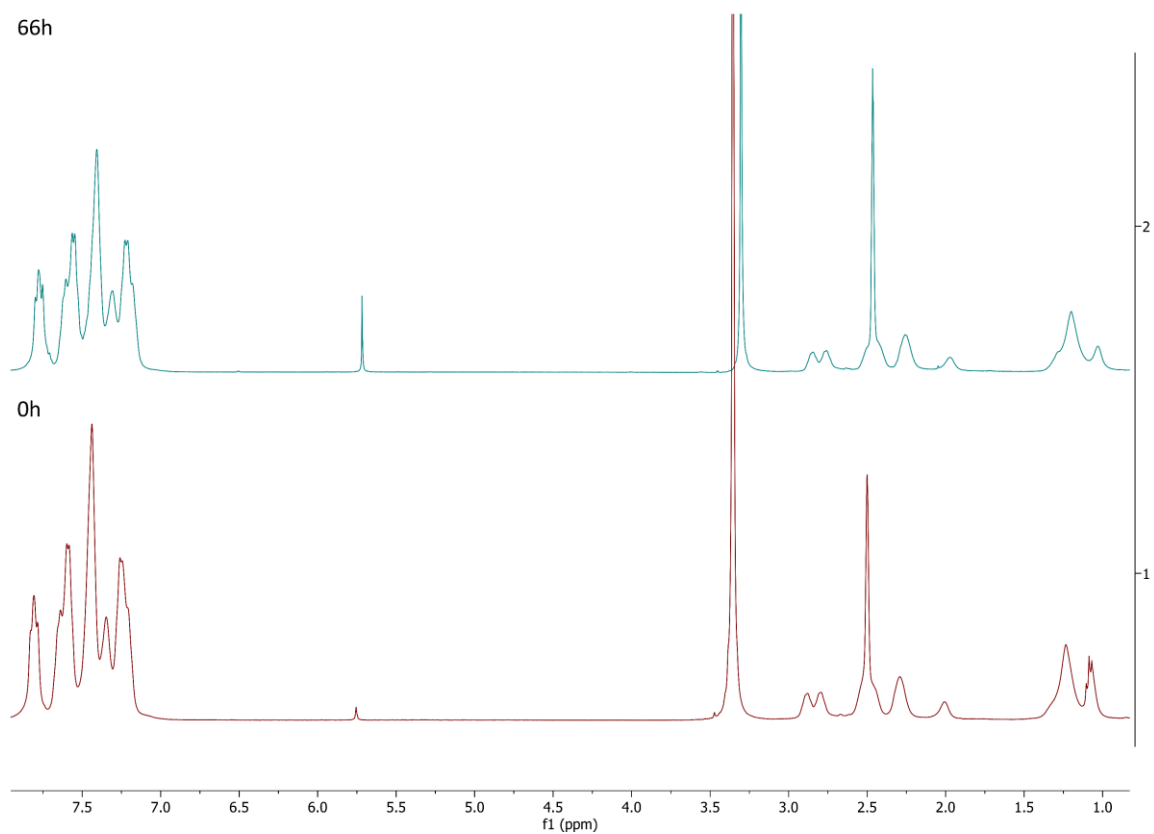


**Fig. S69.** DMSO- $d_6$  stability studies of **Pd-2** ( $^1\text{H}$  NMR spectra, 298 K)

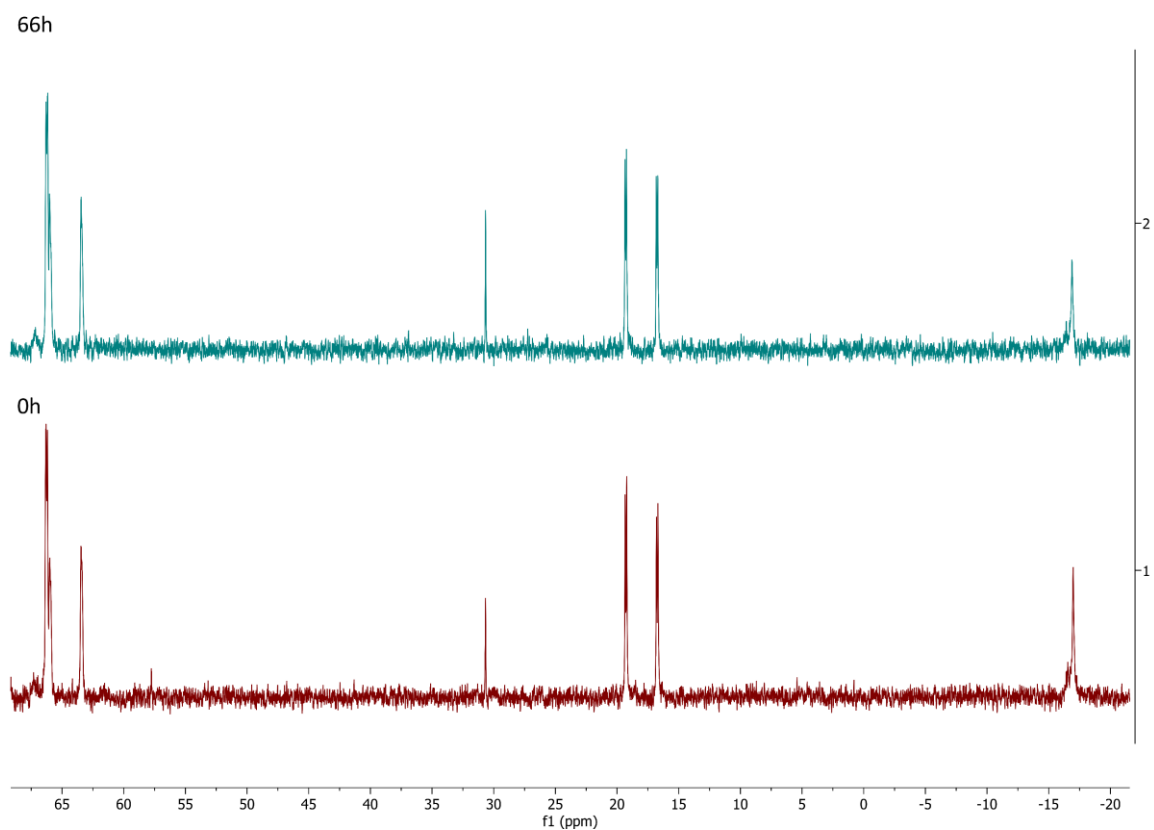


**Fig. S70.** DMSO- $d_6$  stability studies of **Pd-2** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)

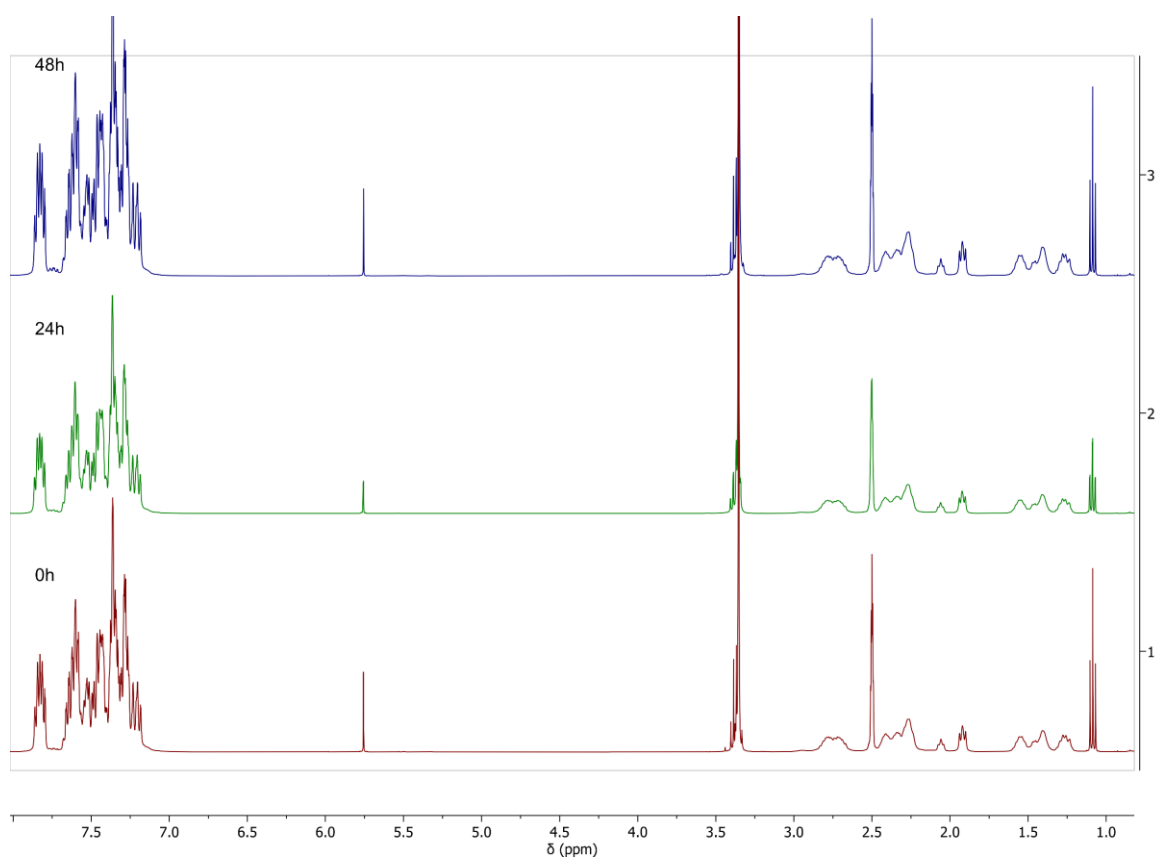




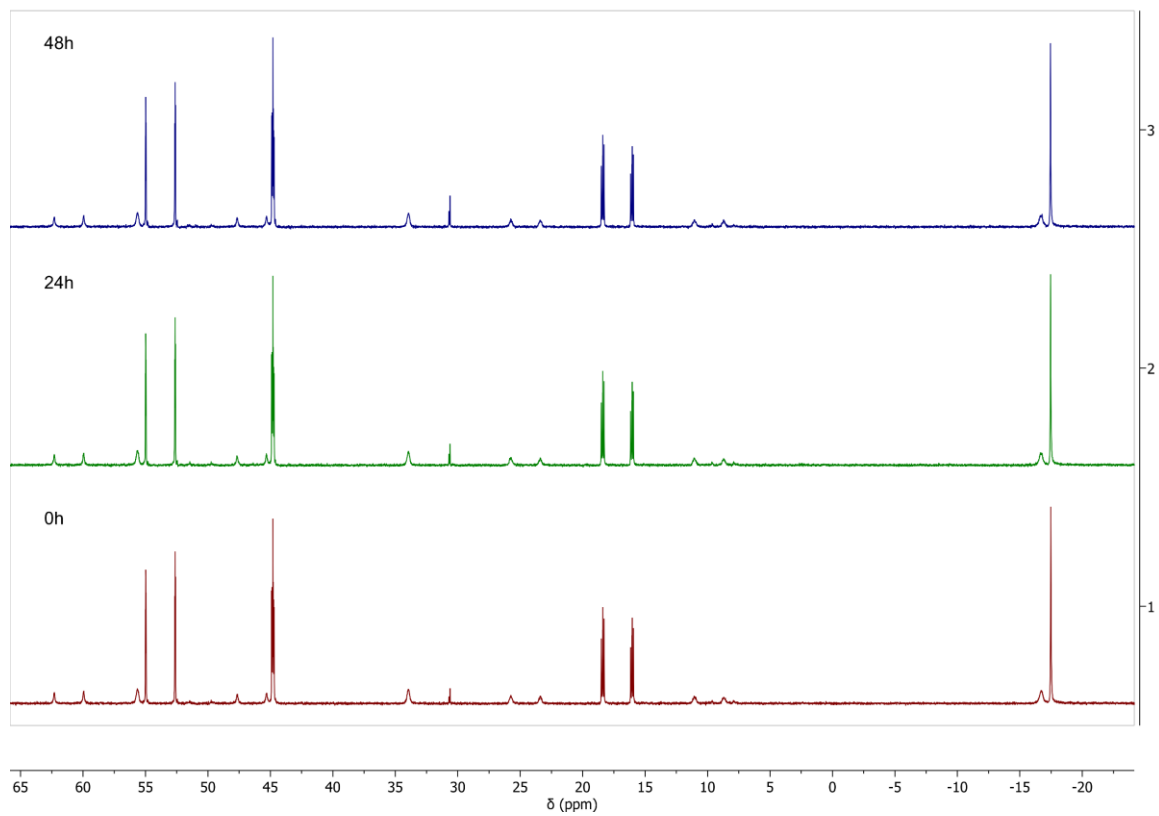
**Fig. S71.** DMSO- $d_6$  stability studies of **Pd-3** ( $^1\text{H}$  NMR spectra, 298 K)



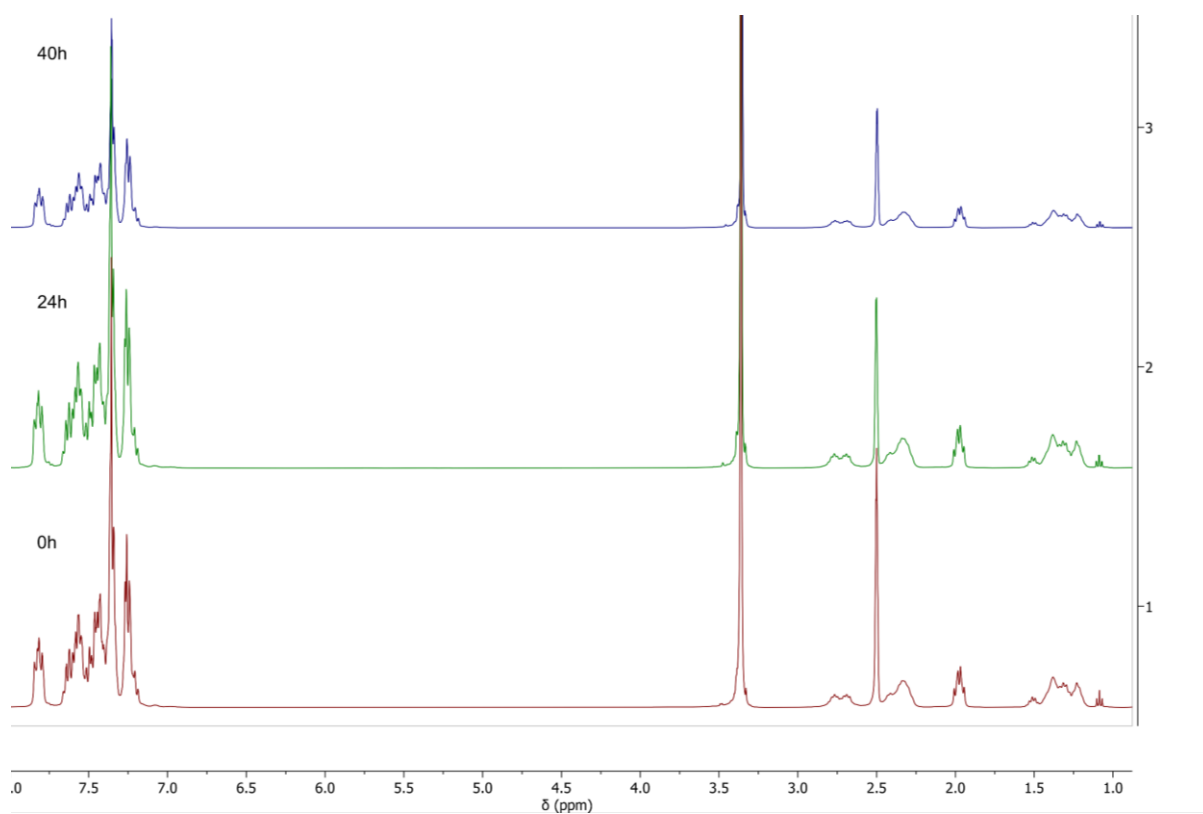
**Fig. S72.** DMSO- $d_6$  stability studies of **Pd-3** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



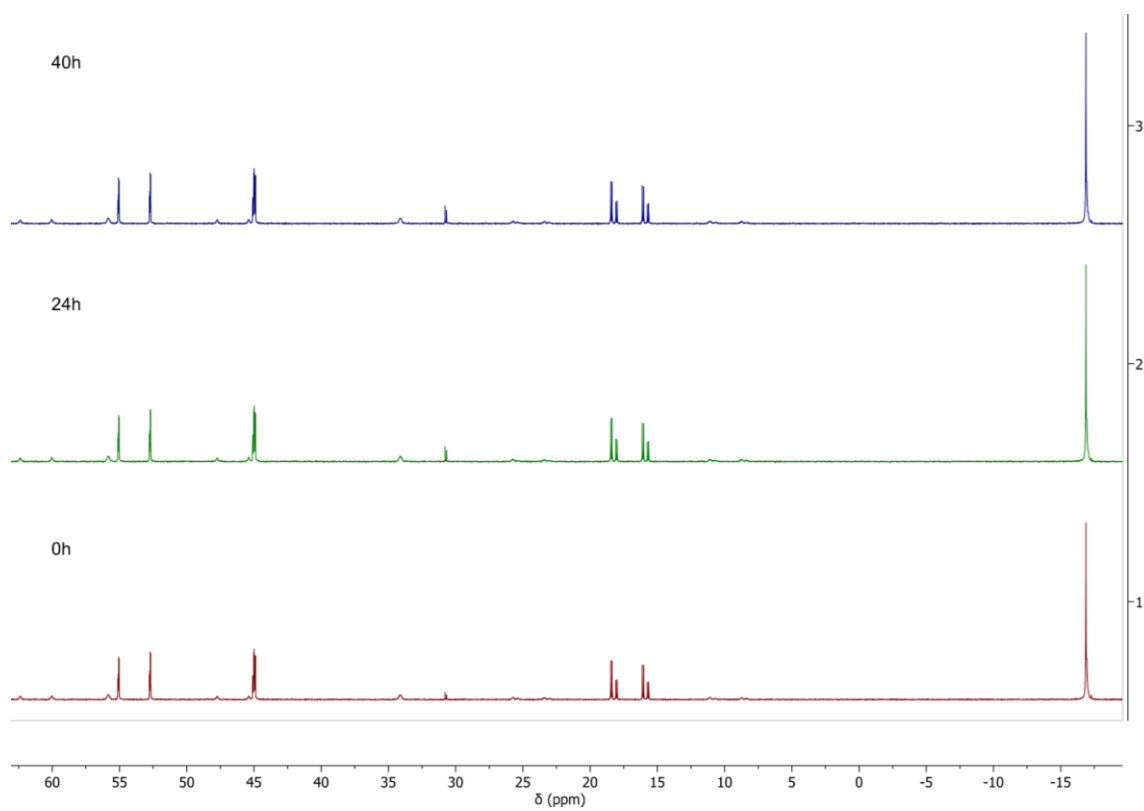
**Fig. S73.**  $\text{DMSO-}d_6$  stability studies of **Pt-1** ( $^1\text{H}$  NMR spectra, 298 K)



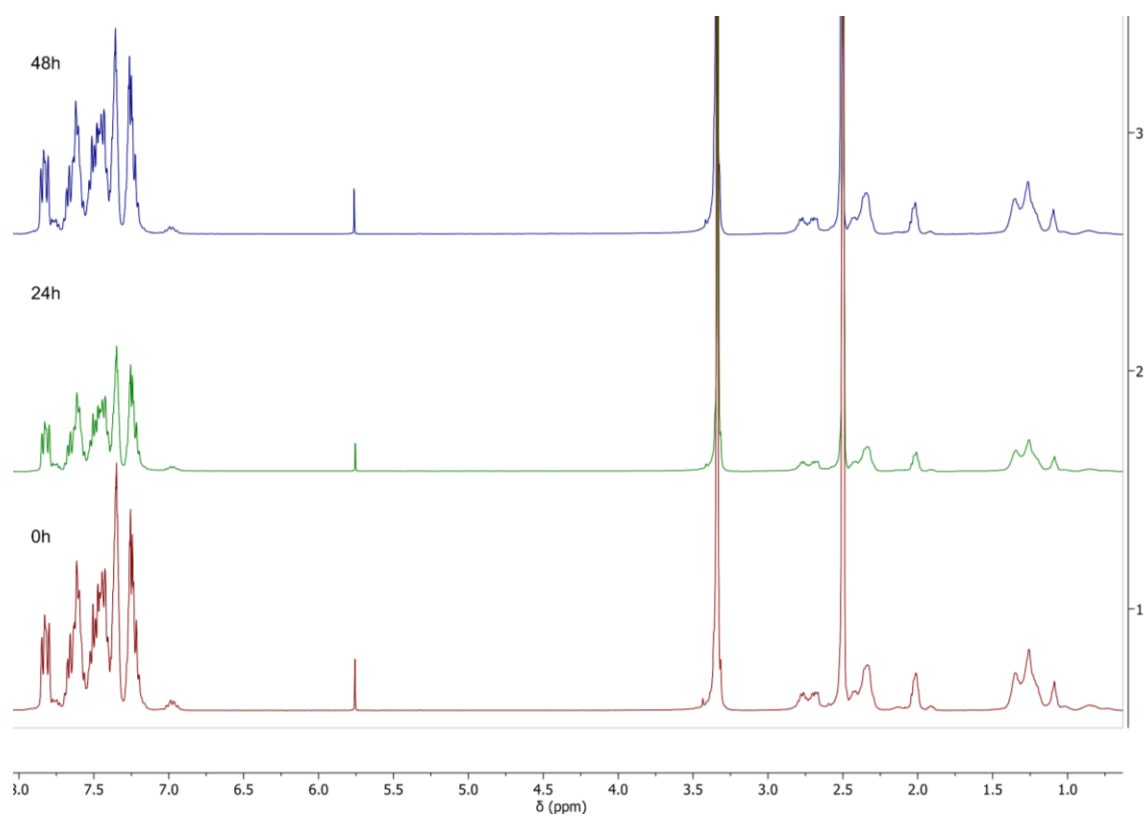
**Fig. S74.**  $\text{DMSO-}d_6$  stability studies of **Pt-1** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



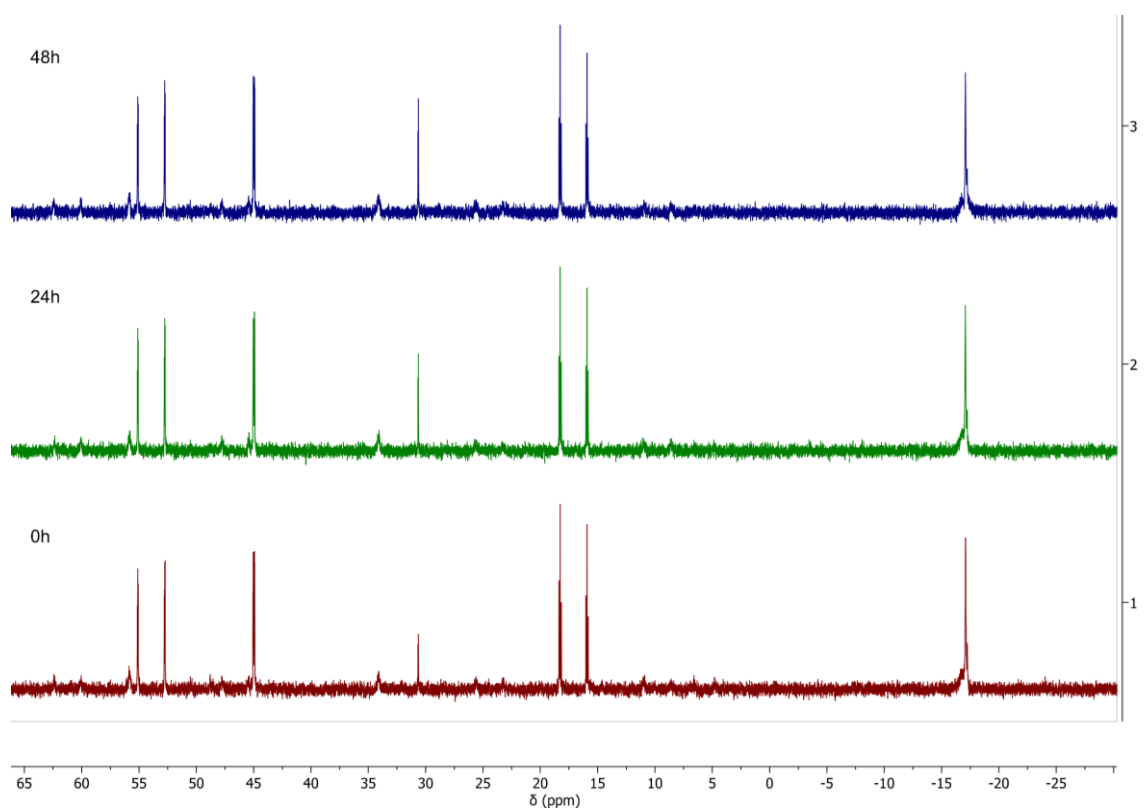
**Fig. S75.** DMSO- $d_6$  stability studies of **Pt-2** ( $^1\text{H}$  NMR spectra, 298 K)



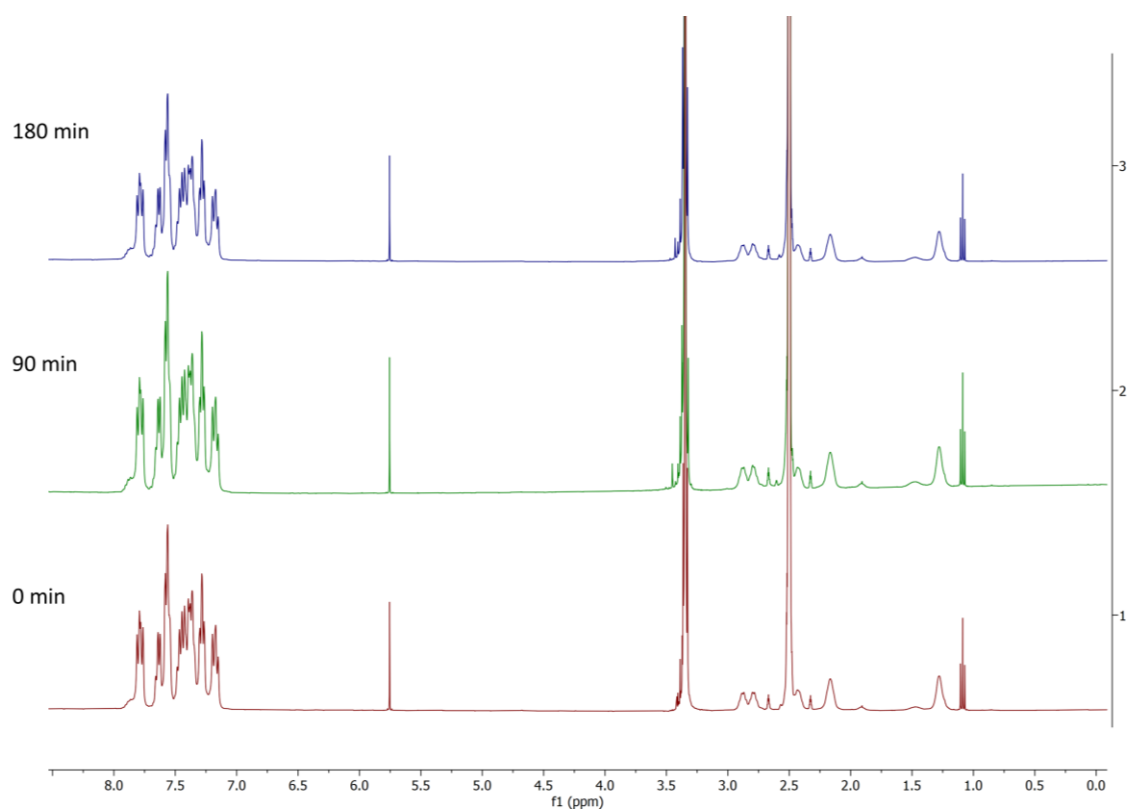
**Fig. S76.** DMSO- $d_6$  stability studies of **Pt-2** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



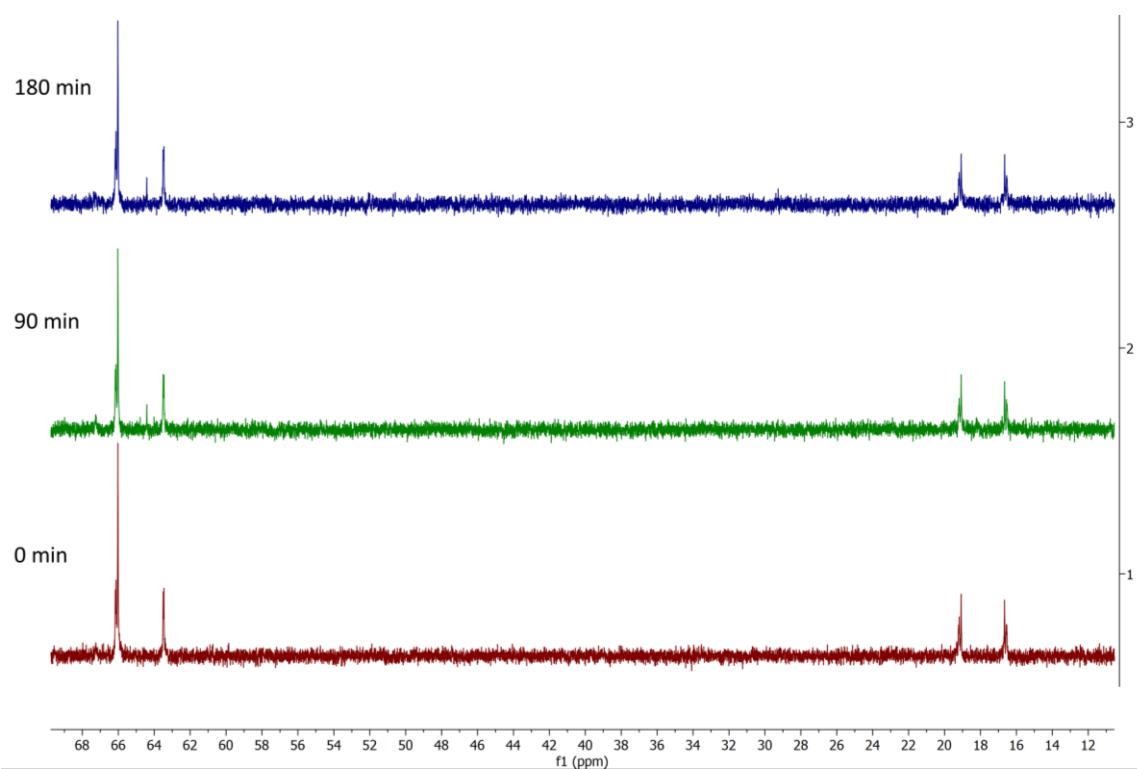
**Fig. S77.** DMSO- $d_6$  stability studies of **Pt-3** ( $^1\text{H}$  NMR spectra, 298 K)



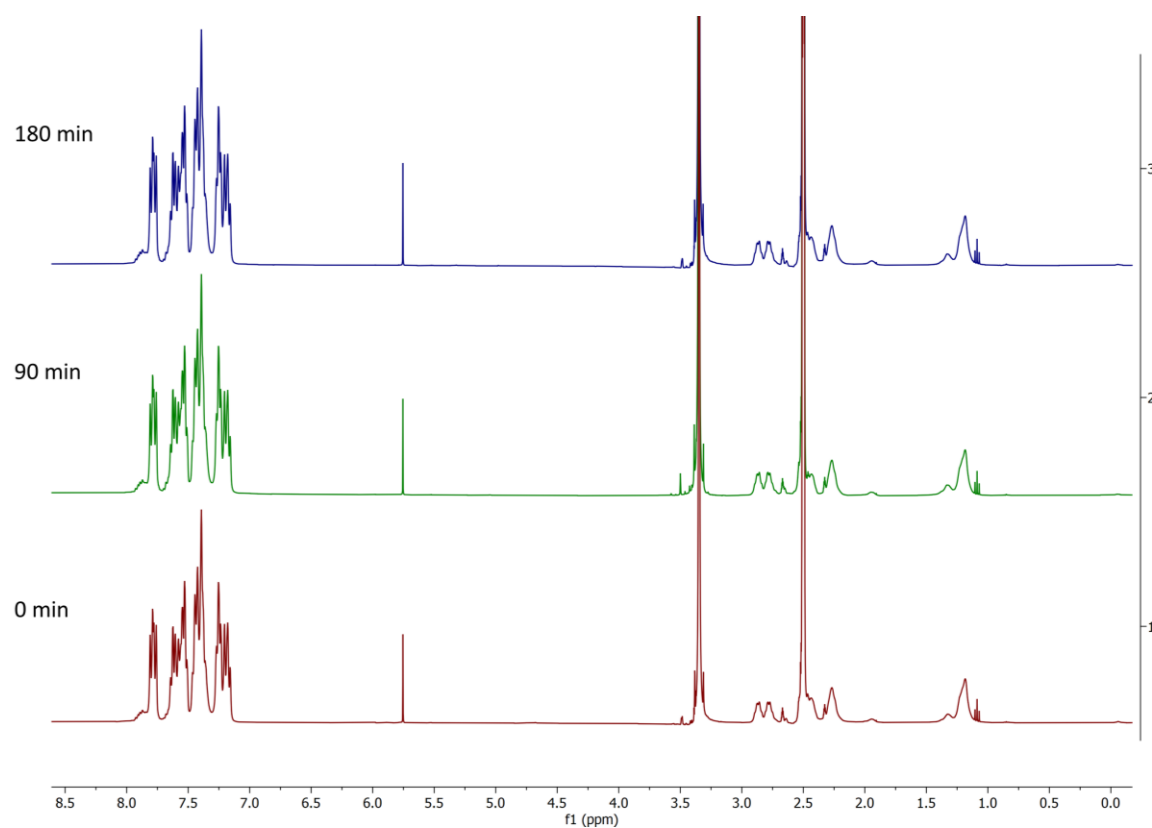
**Fig. S78.** DMSO- $d_6$  stability studies of **Pt-3** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



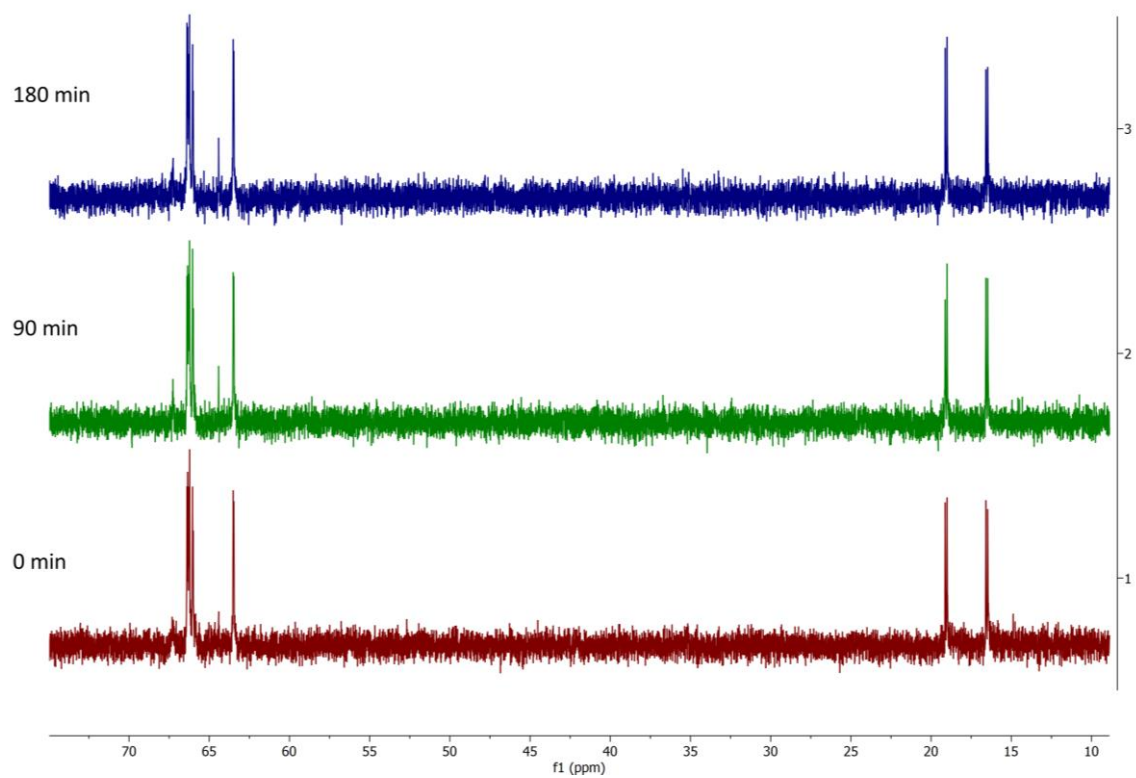
**Fig. S79.** DMSO- $d_6$  stability studies of **PdPd-1** ( $^1\text{H}$  NMR spectra, 298 K)



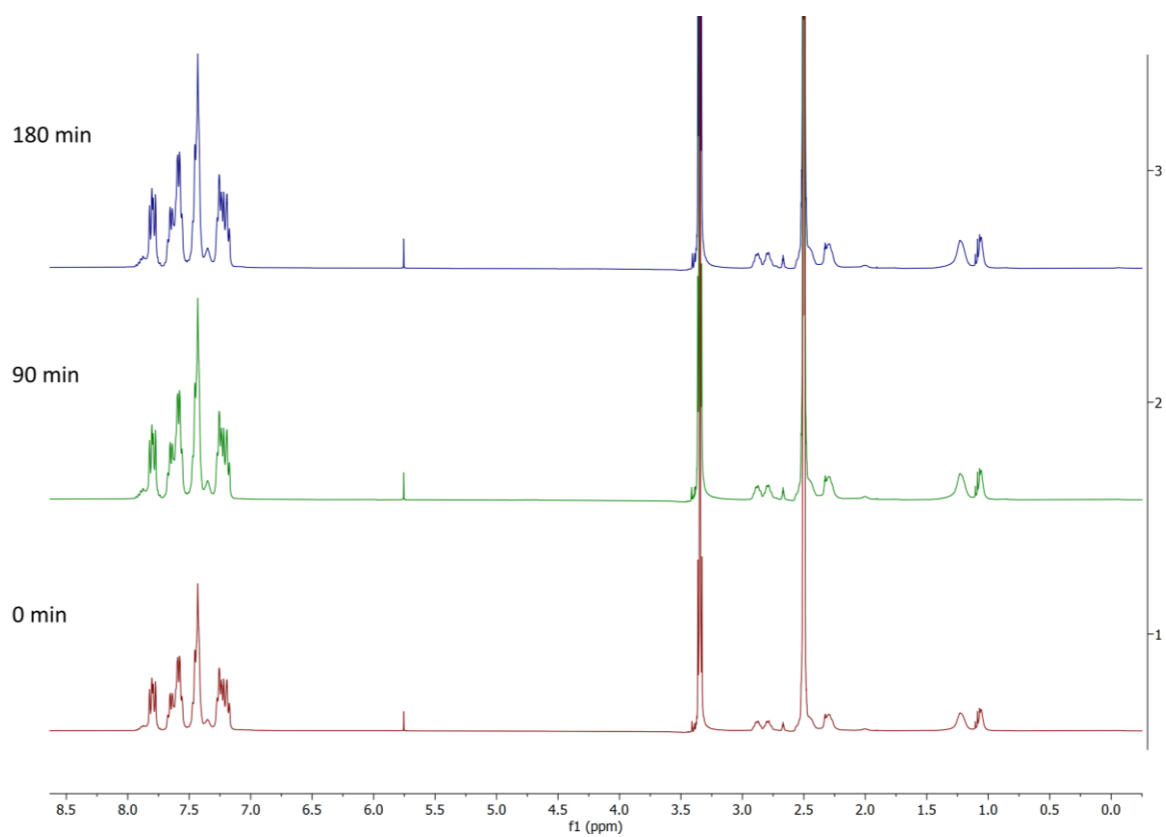
**Fig. S80.** DMSO- $d_6$  stability studies of **PdPd-1** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



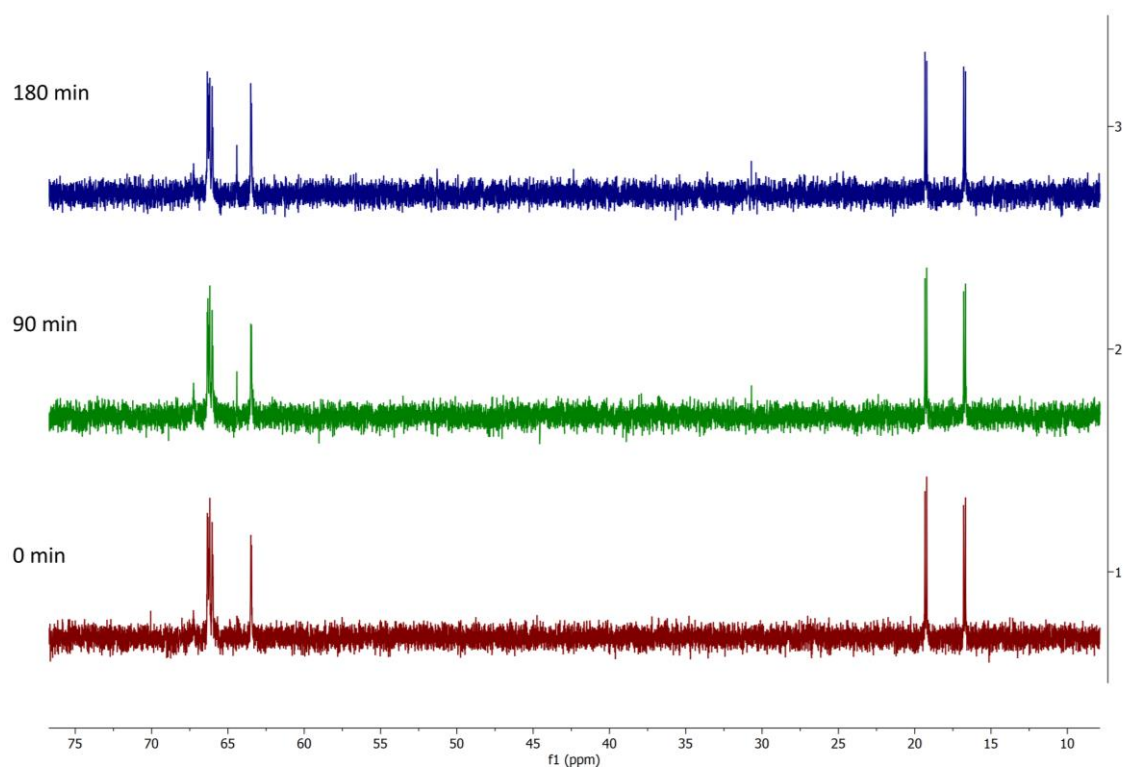
**Fig. S81.**  $\text{DMSO-}d_6$  stability studies of **PdPd-2** ( $^1\text{H}$  NMR spectra, 298 K)



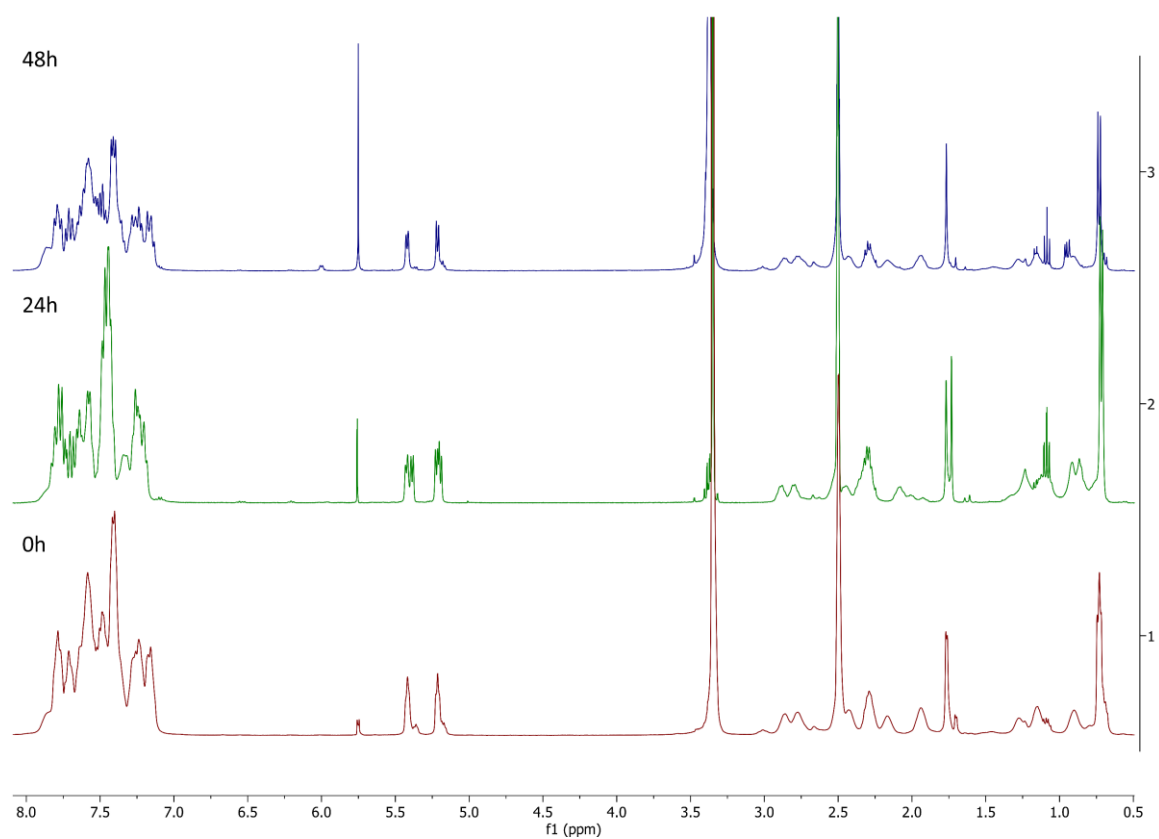
**Fig. S82.**  $\text{DMSO-}d_6$  stability studies of **PdPd-2** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



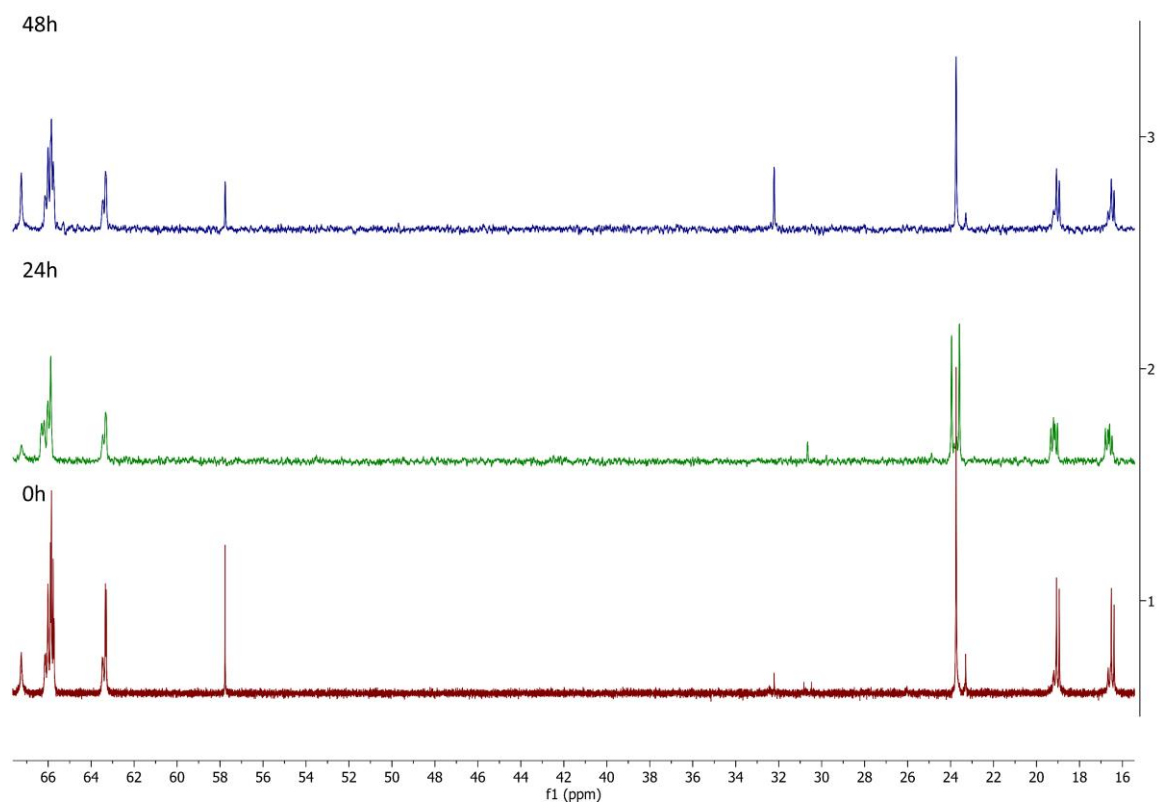
**Fig. S83.** DMSO- $d_6$  stability studies of **PdPd-3** ( $^1\text{H}$  NMR spectra, 298 K)



**Fig. S84.** DMSO- $d_6$  stability studies of **PdPd-3** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)

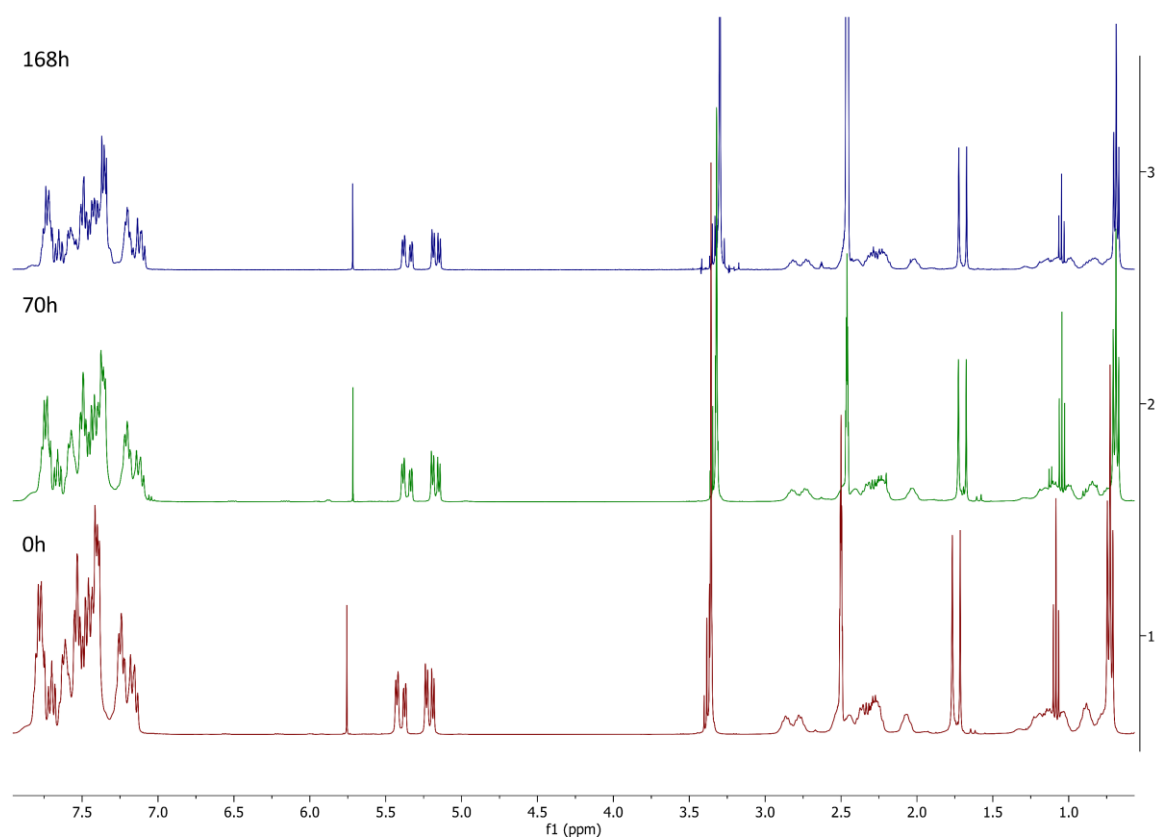


**Fig. S85.** DMSO- $d_6$  stability studies of **PdRu-1** ( $^1\text{H}$  NMR spectra, 298 K)

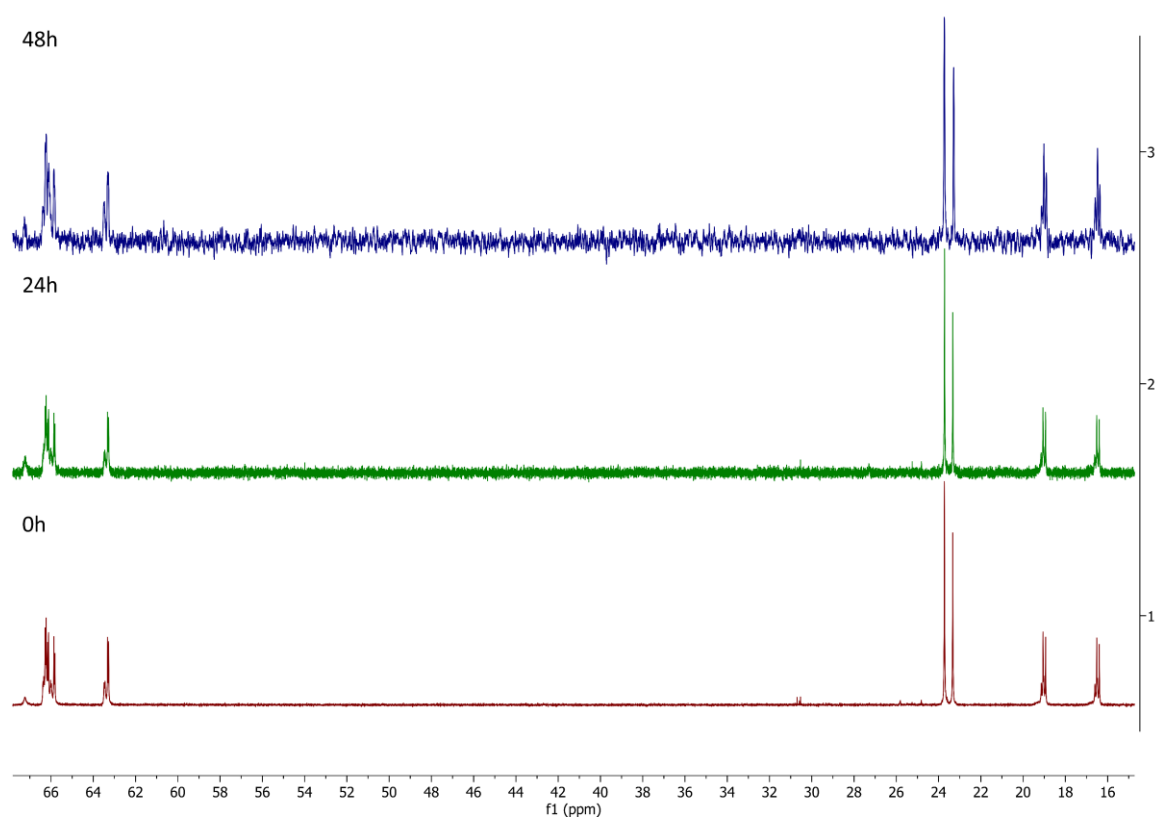


**Fig. S86.** DMSO- $d_6$  stability studies of **PdRu-1** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)

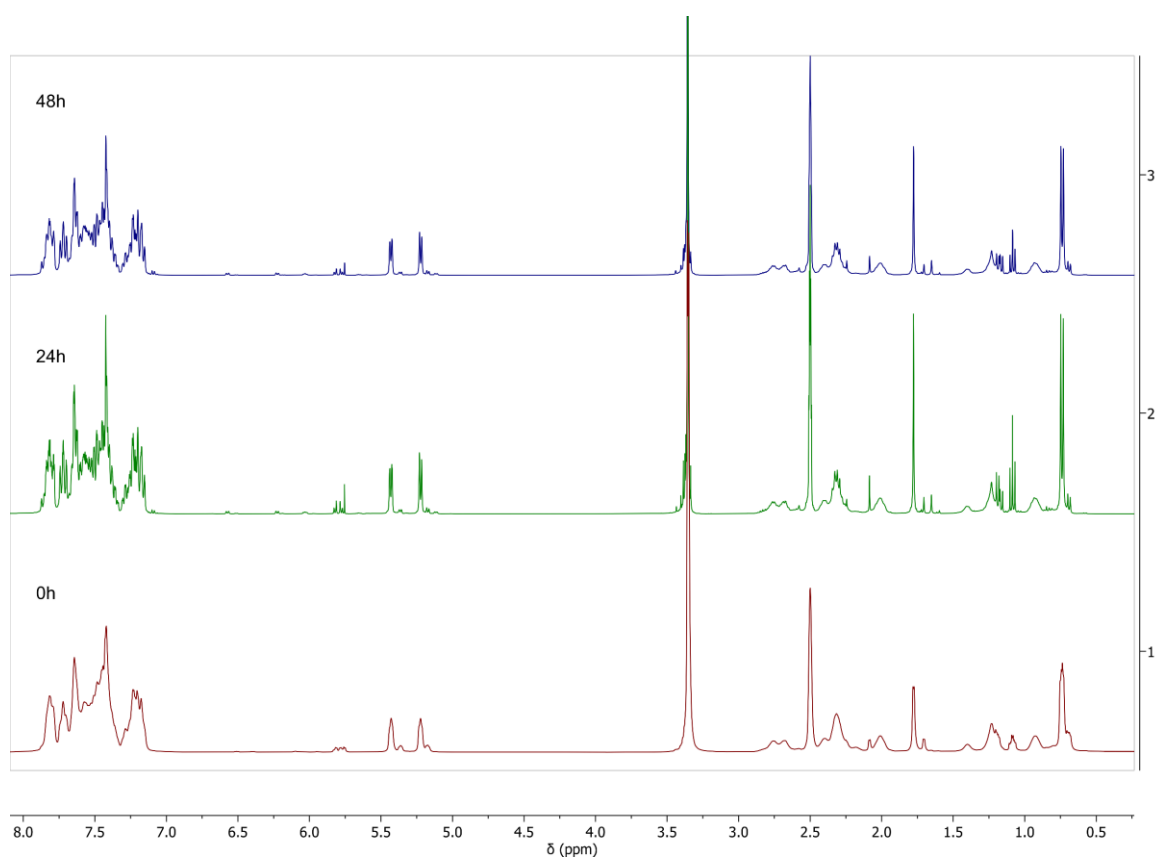




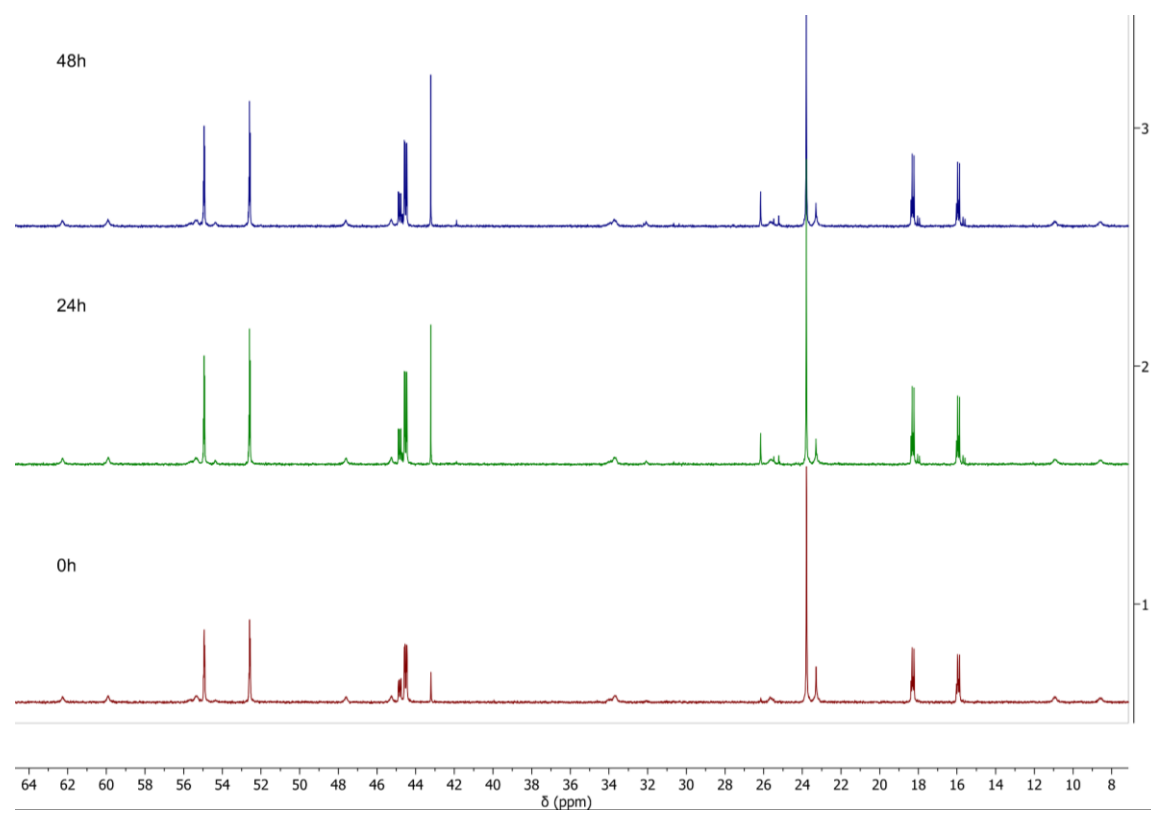
**Fig. S87.** DMSO- $d_6$  stability studies of **PdRu-2** ( $^1\text{H}$  NMR spectra, 298 K)



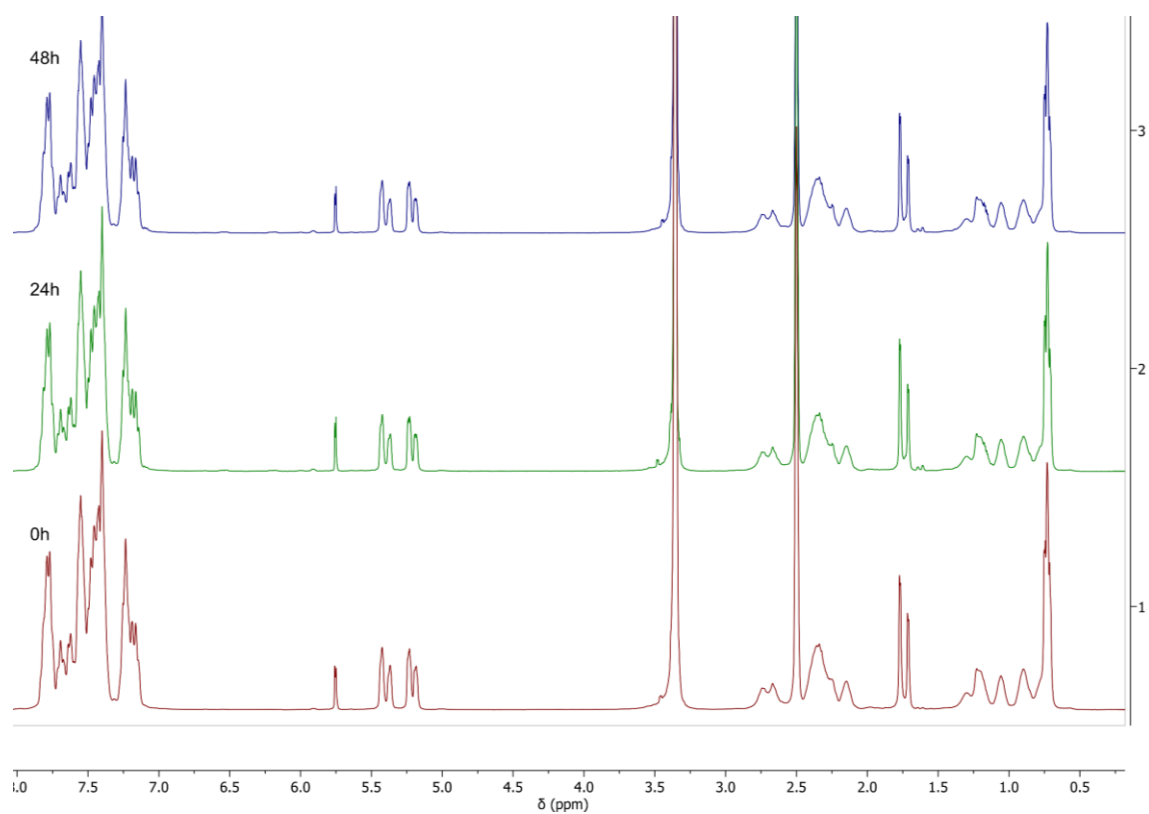
**Fig. S88.** DMSO- $d_6$  stability studies of **PdRu-2** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



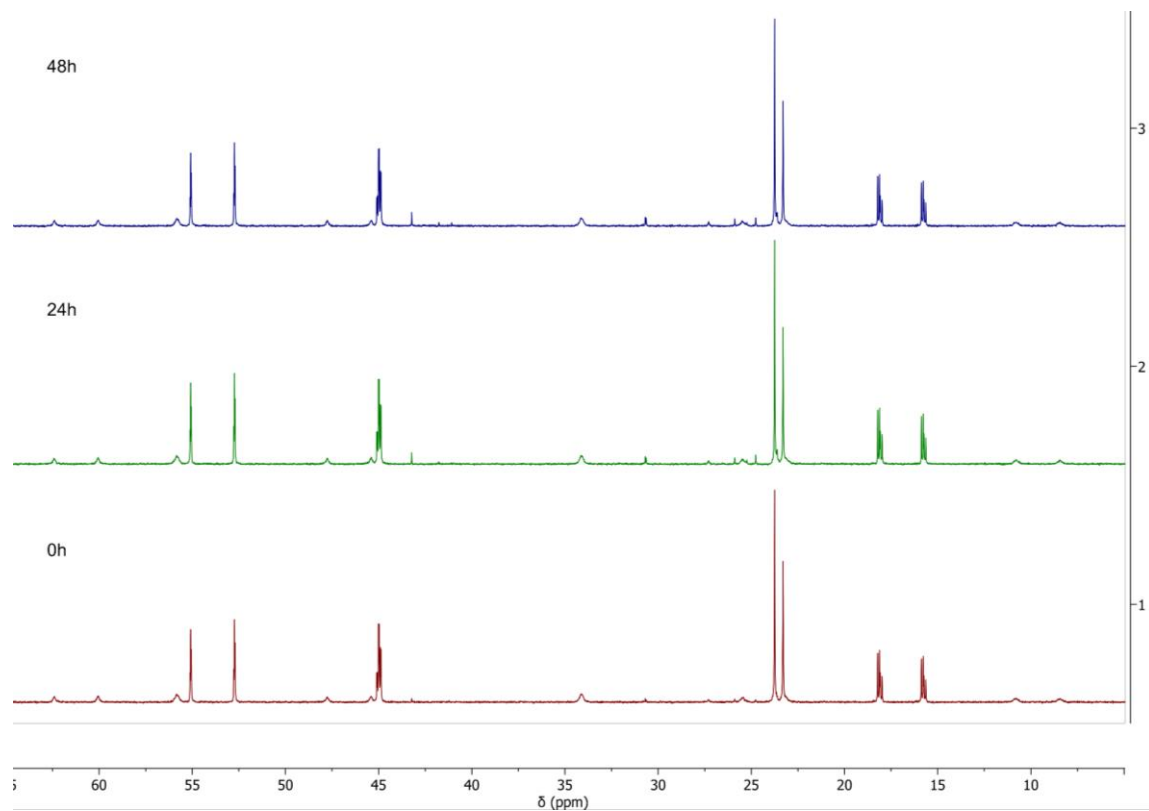
**Fig. S89.** DMSO- $d_6$  stability studies of **PtRu-1** ( $^1\text{H}$  NMR spectra, 298 K)



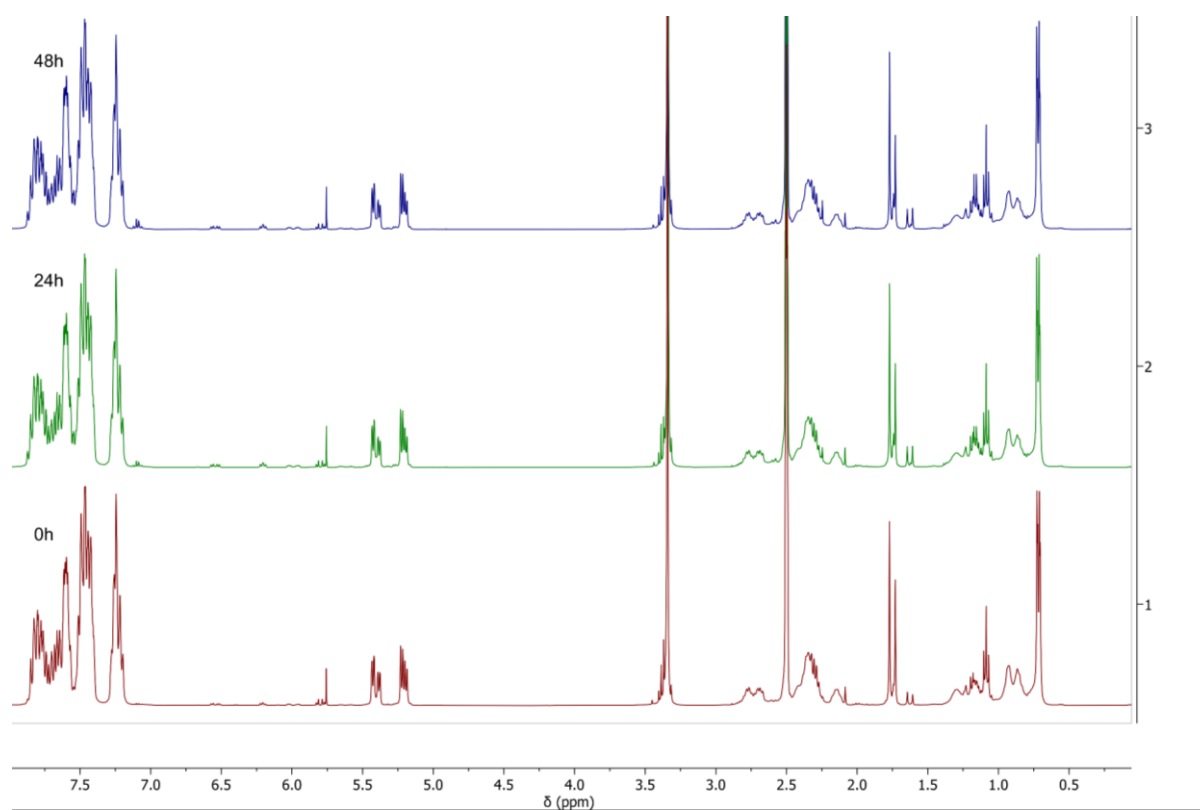
**Fig. S90.** DMSO- $d_6$  stability studies of **PtRu-1** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



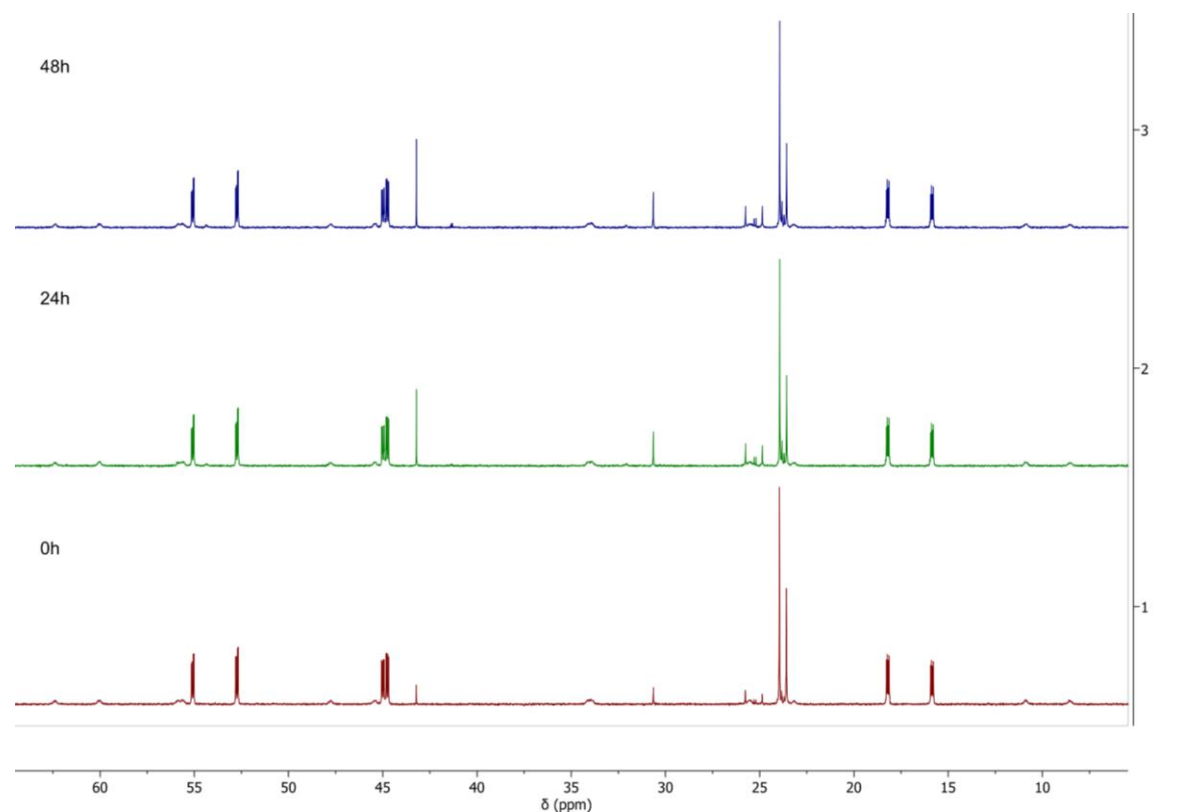
**Fig. S91.**  $\text{DMSO-}d_6$  stability studies of PtRu-2 ( $^1\text{H}$  NMR spectra, 298 K)



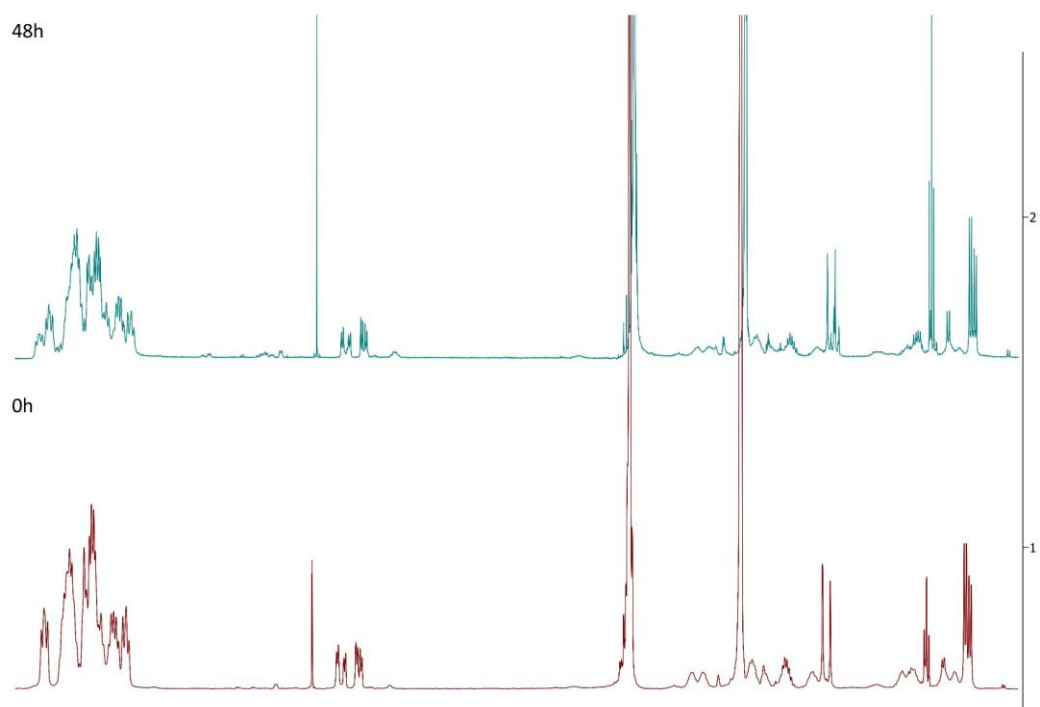
**Fig. S92.**  $\text{DMSO-}d_6$  stability studies of PtRu-2 ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



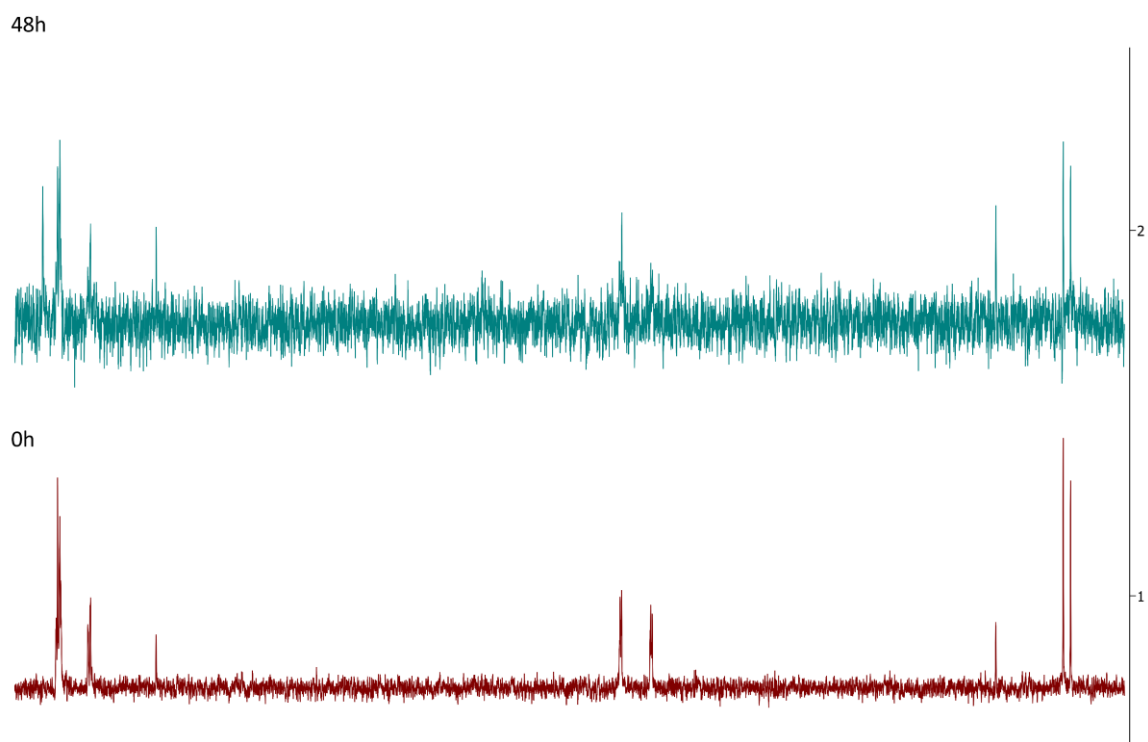
**Fig. S93.** DMSO- $d_6$  stability studies of **PtRu-3** ( $^1\text{H}$  NMR spectra, 298 K)



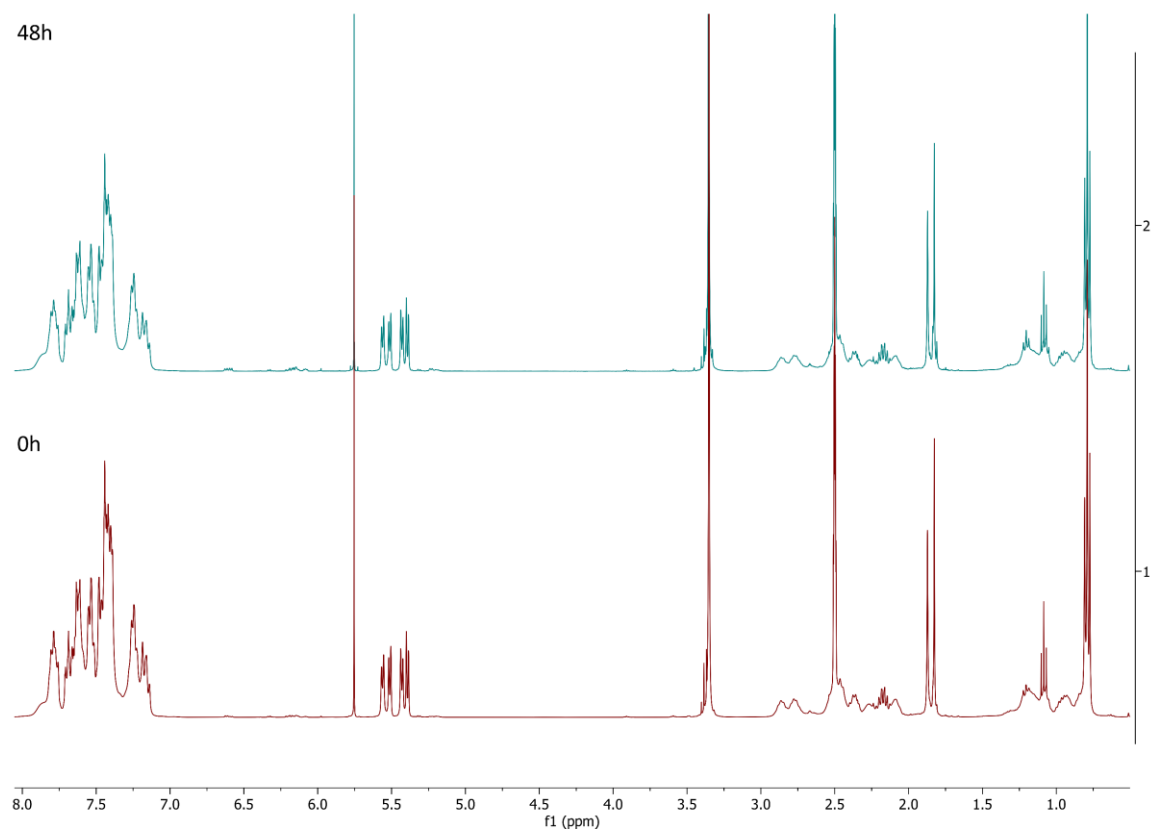
**Fig. S94.** DMSO- $d_6$  stability studies of **PtRu-3** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



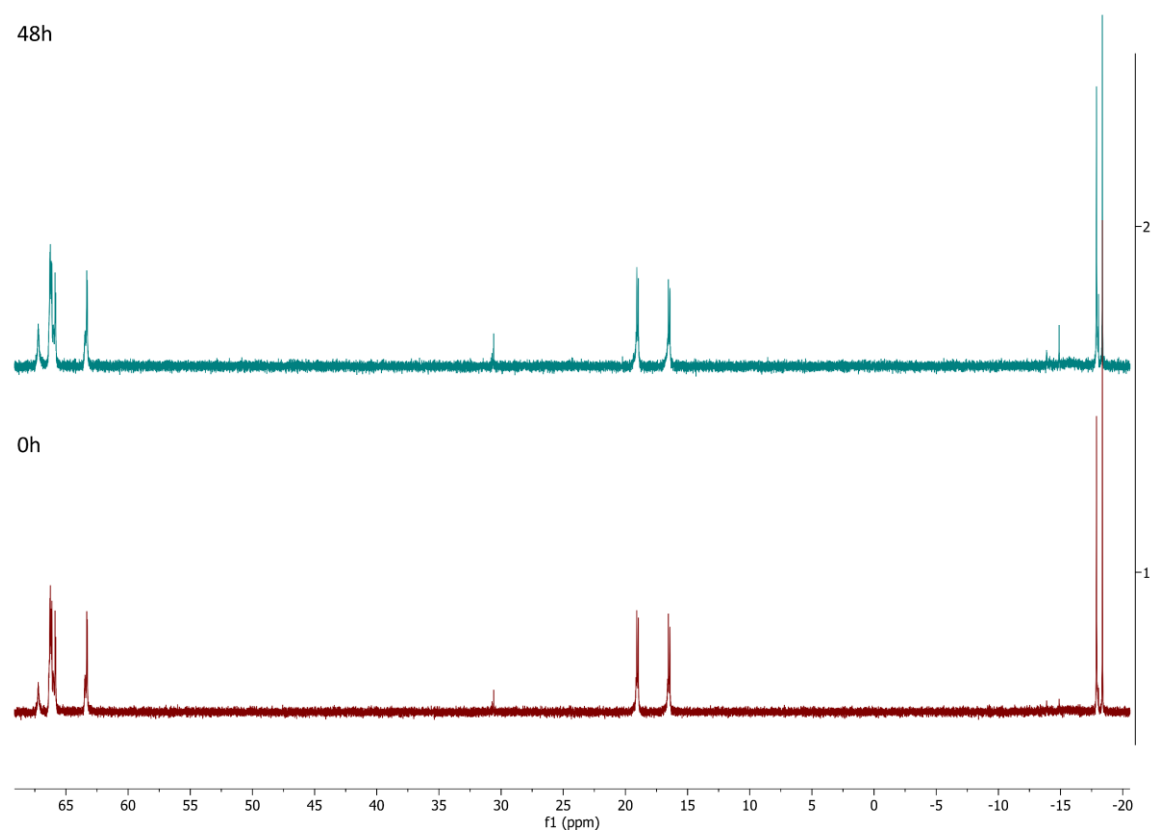
**Fig. S95.** DMSO- $d_6$  stability studies of **PdOs-1** ( $^1\text{H}$  NMR spectra, 298 K)



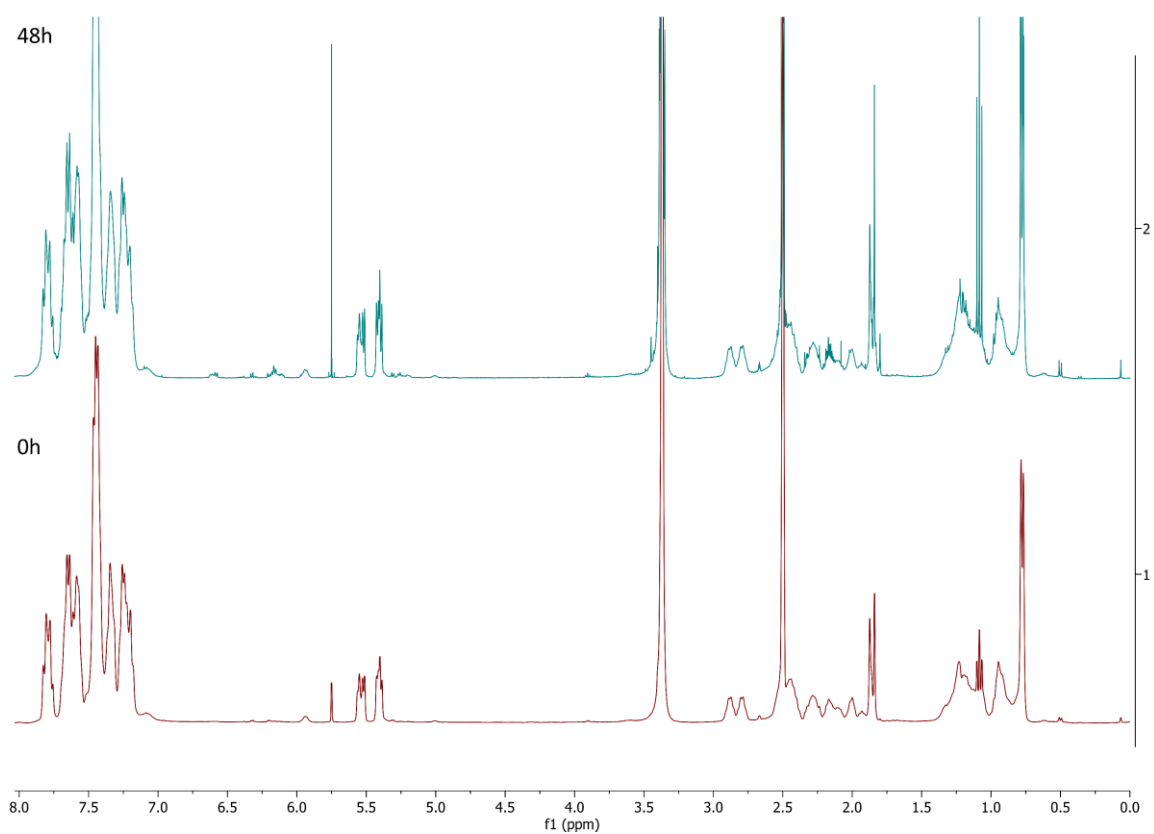
**Fig. S96.** DMSO- $d_6$  stability studies of **PdOs-1** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)



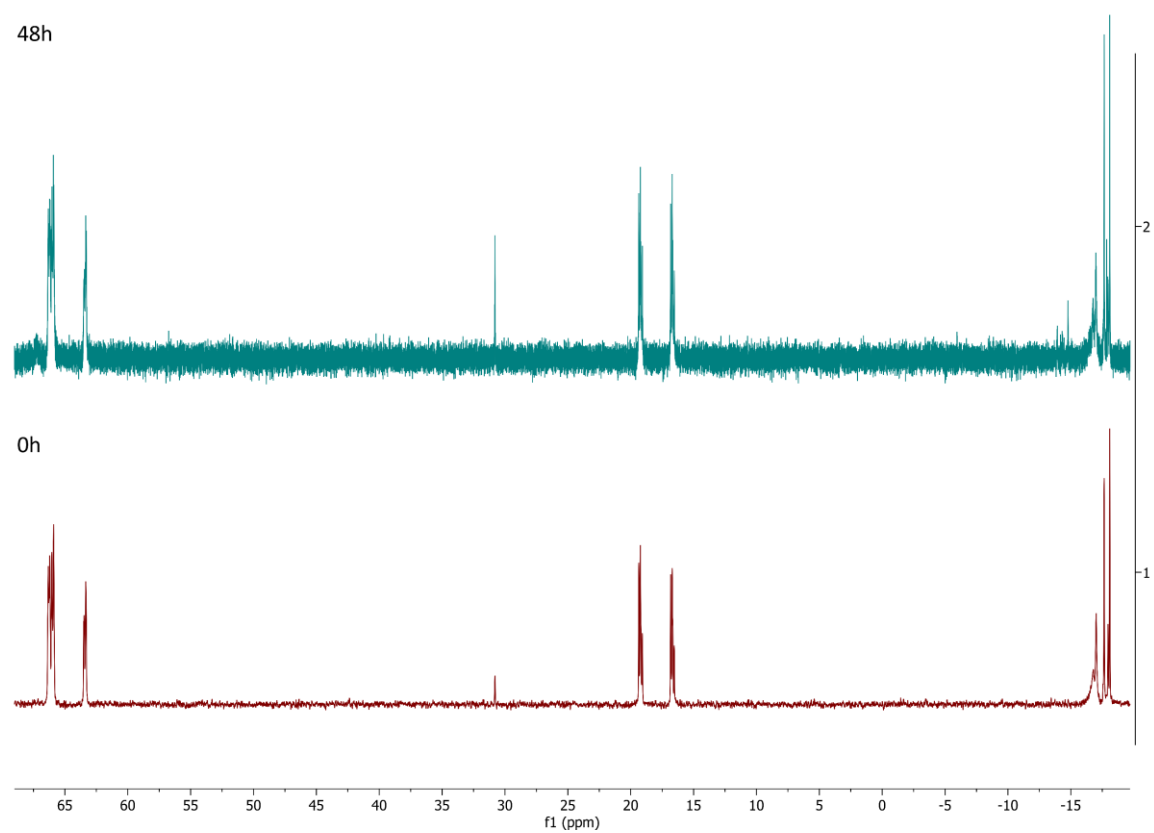
**Fig. S97.** DMSO- $d_6$  stability studies of **PdOs-2** ( $^1\text{H}$  NMR spectra, 298 K)



**Fig. S98.** DMSO- $d_6$  stability studies of **PdOs-2** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)

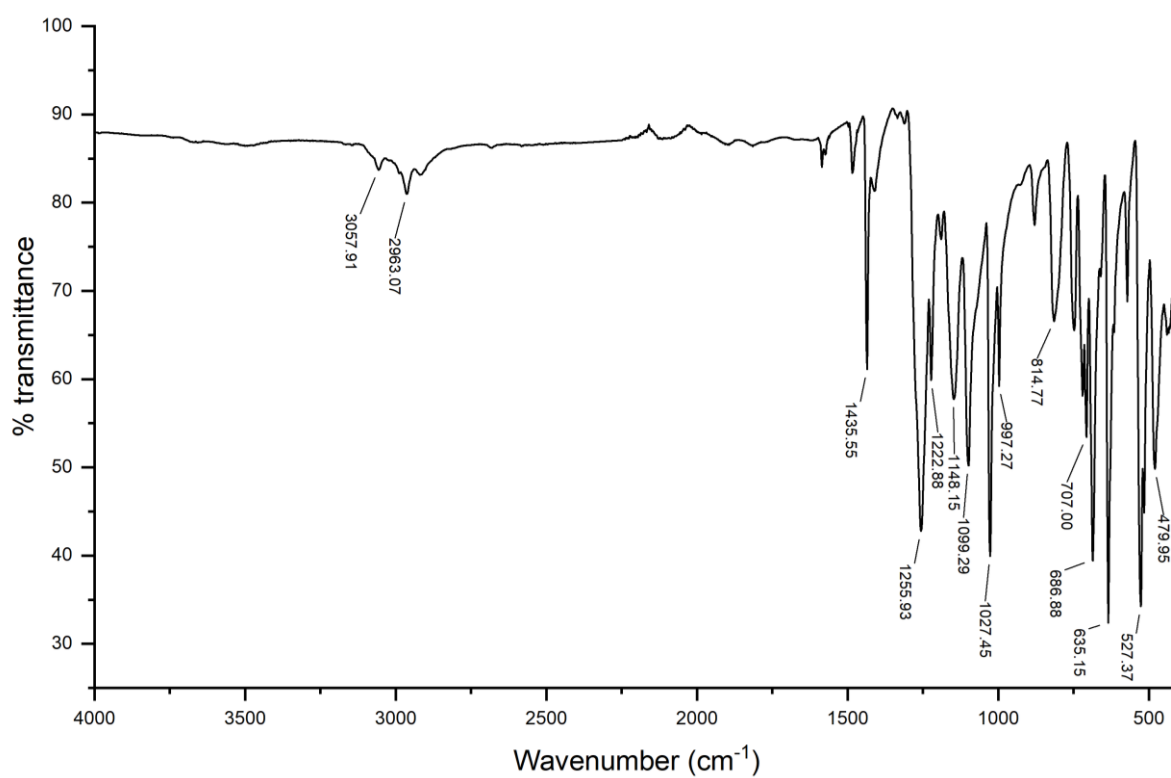


**Fig. S99.** DMSO- $d_6$  stability studies of **PdOs-3** ( $^1\text{H}$  NMR spectra, 298 K)

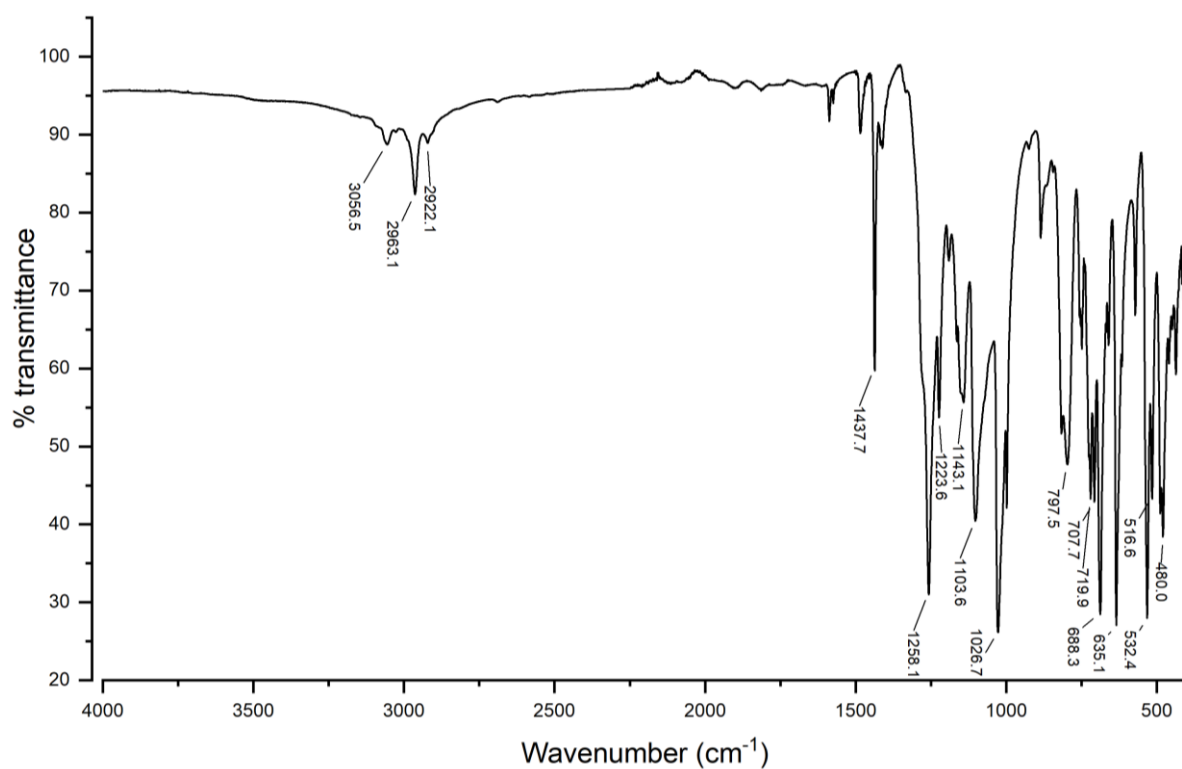


**Fig. S100.** DMSO- $d_6$  stability studies of **PdOs-3** ( $^{31}\text{P}\{^1\text{H}\}$  NMR spectra, 298 K)

## 6. FT-IR spectra

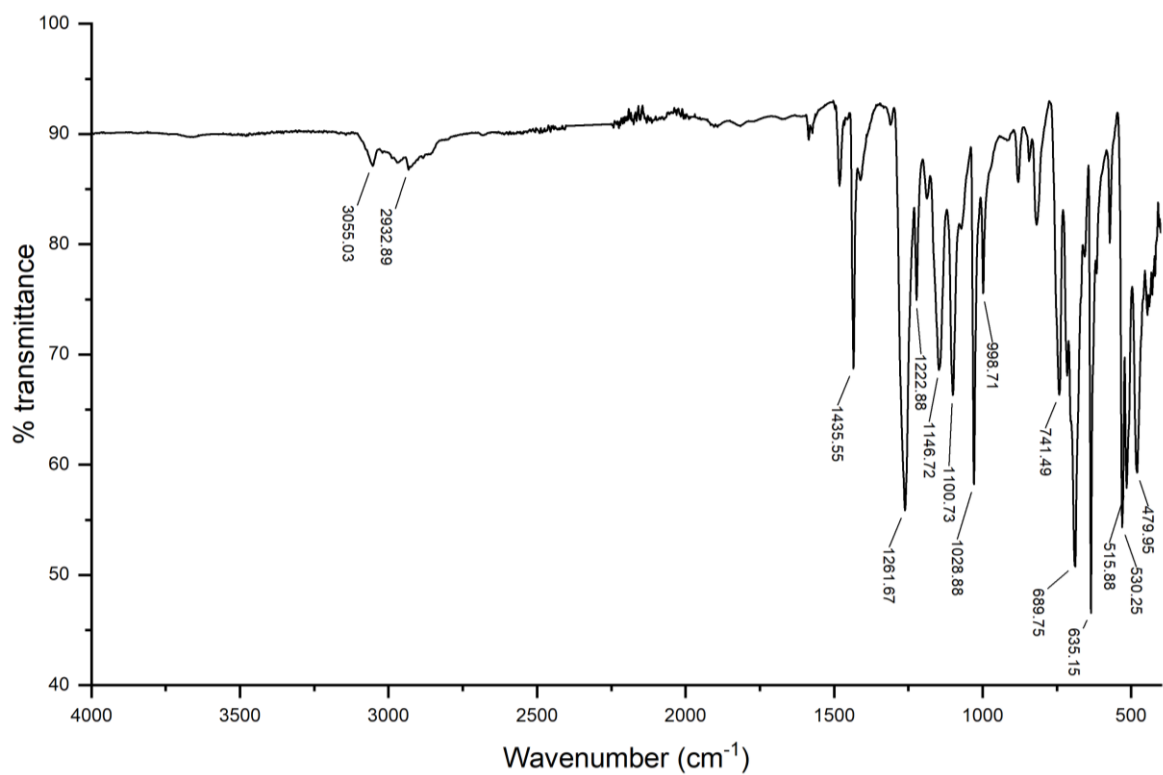


**Fig. S101.** FT-IR spectrum of PdPd-0

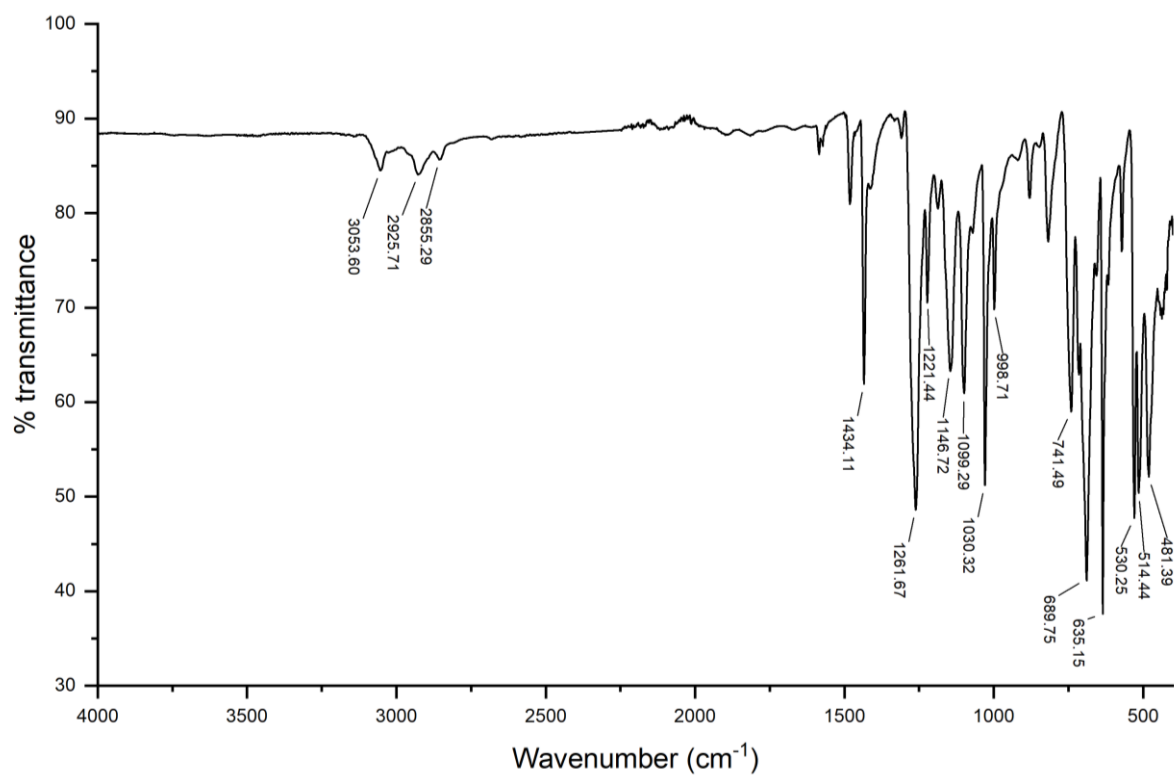


**Fig. S102.** FT-IR spectrum of PtPt-0

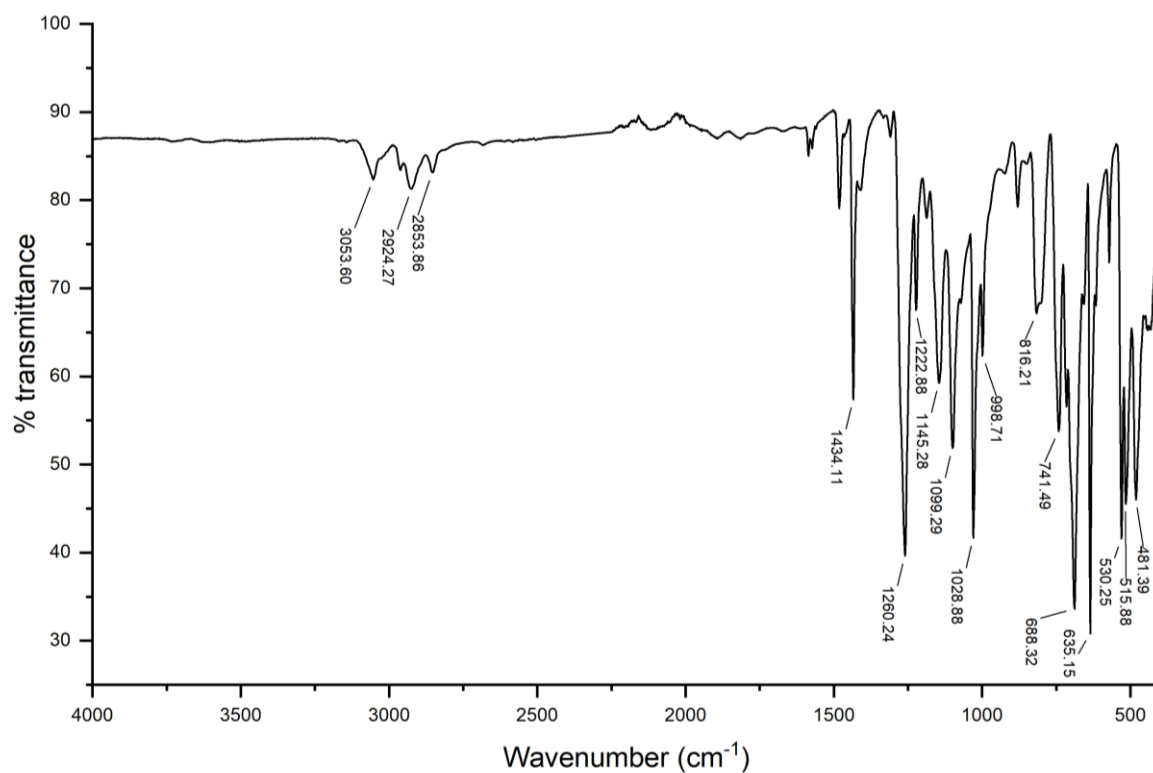




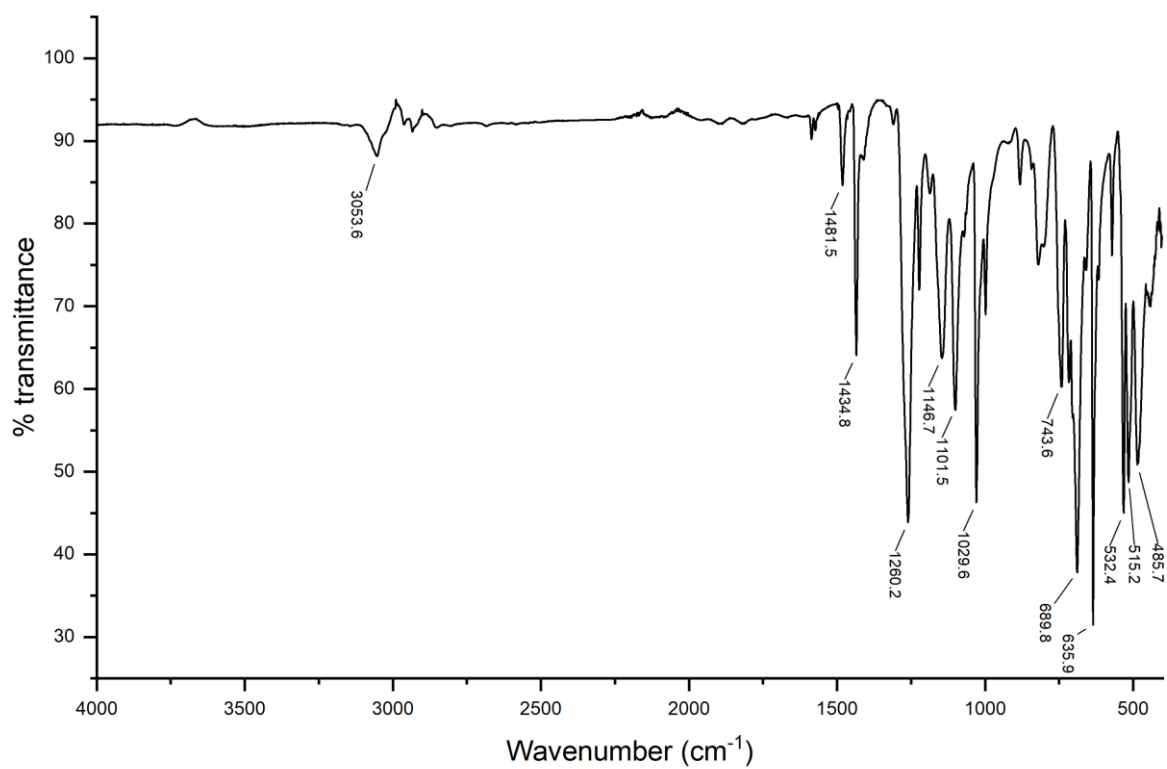
**Fig. S103.** FT-IR spectrum of **Pd-1**



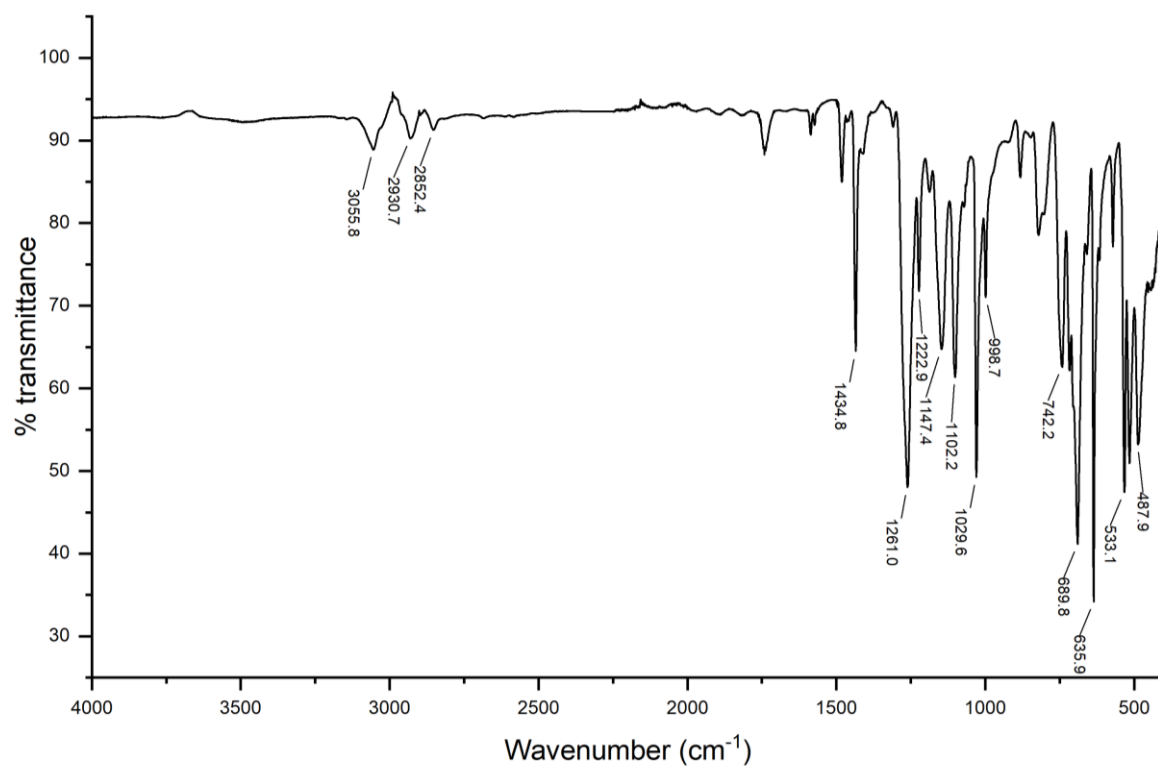
**Fig. S104.** FT-IR spectrum of **Pd-2**



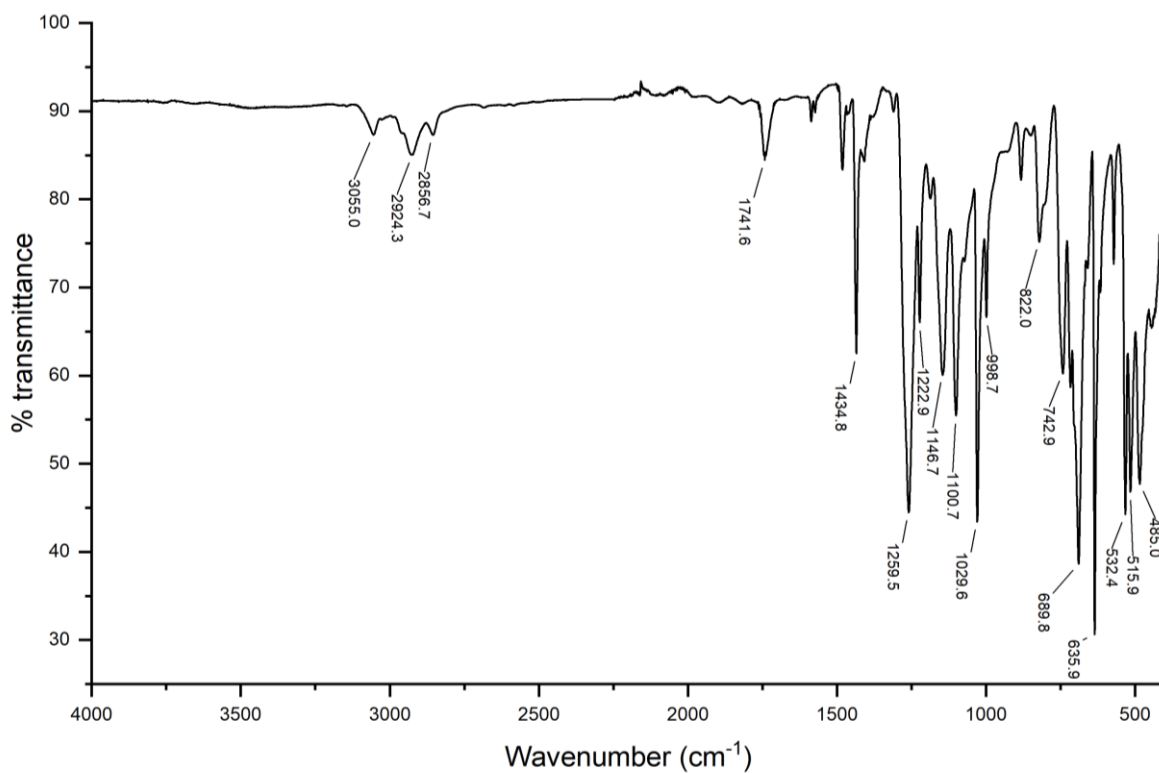
**Fig. S105.** FT-IR spectrum of **Pd-3**



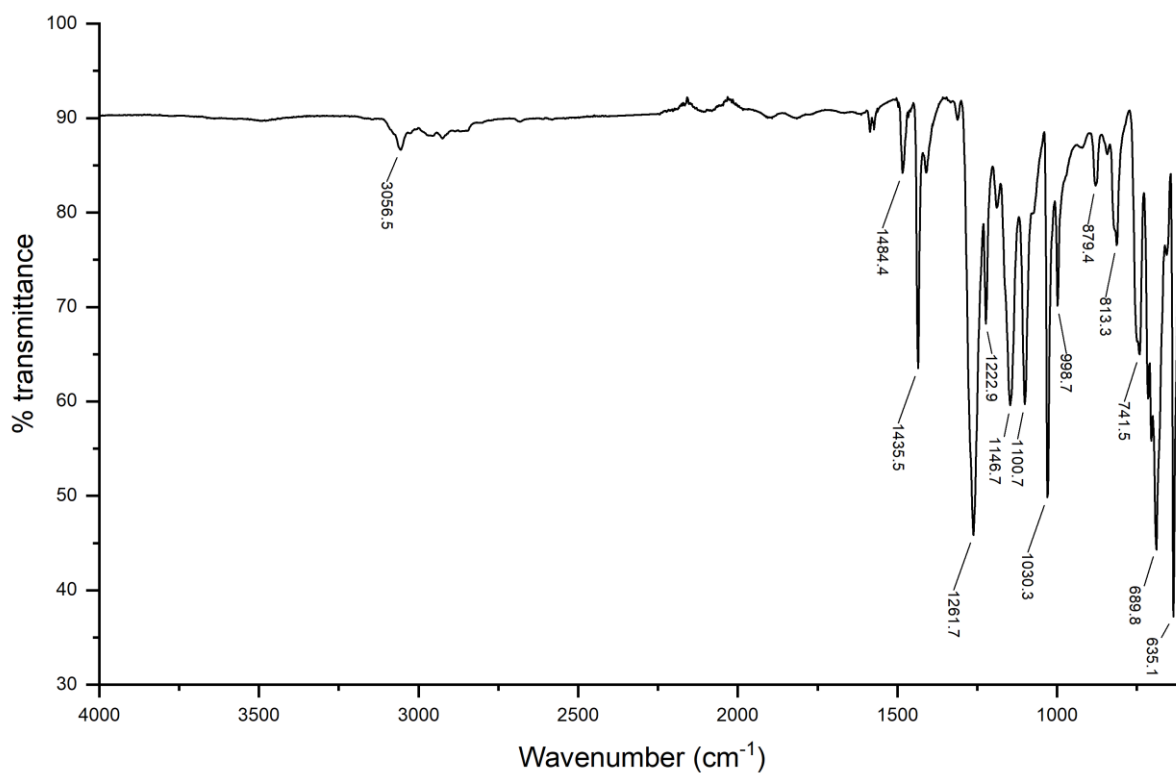
**Fig. S106.** FT-IR spectrum of **Pt-1**



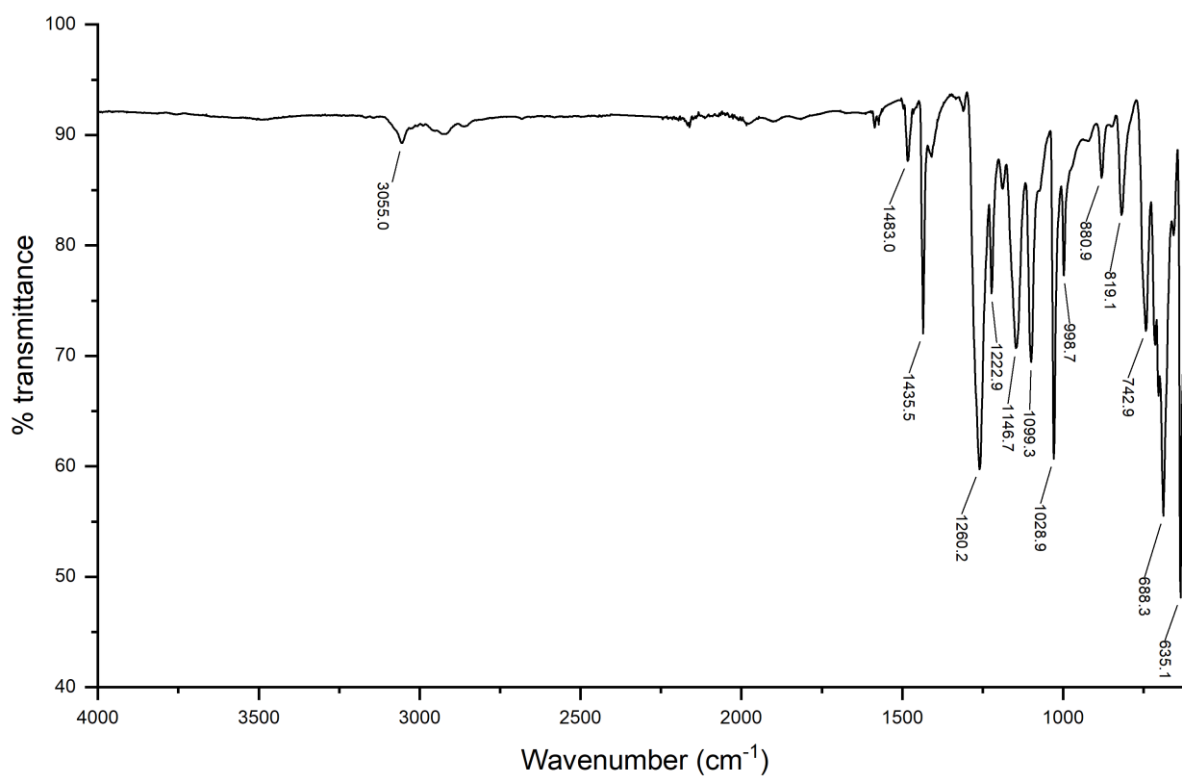
**Fig. S107.** FT-IR spectrum of **Pt-2**



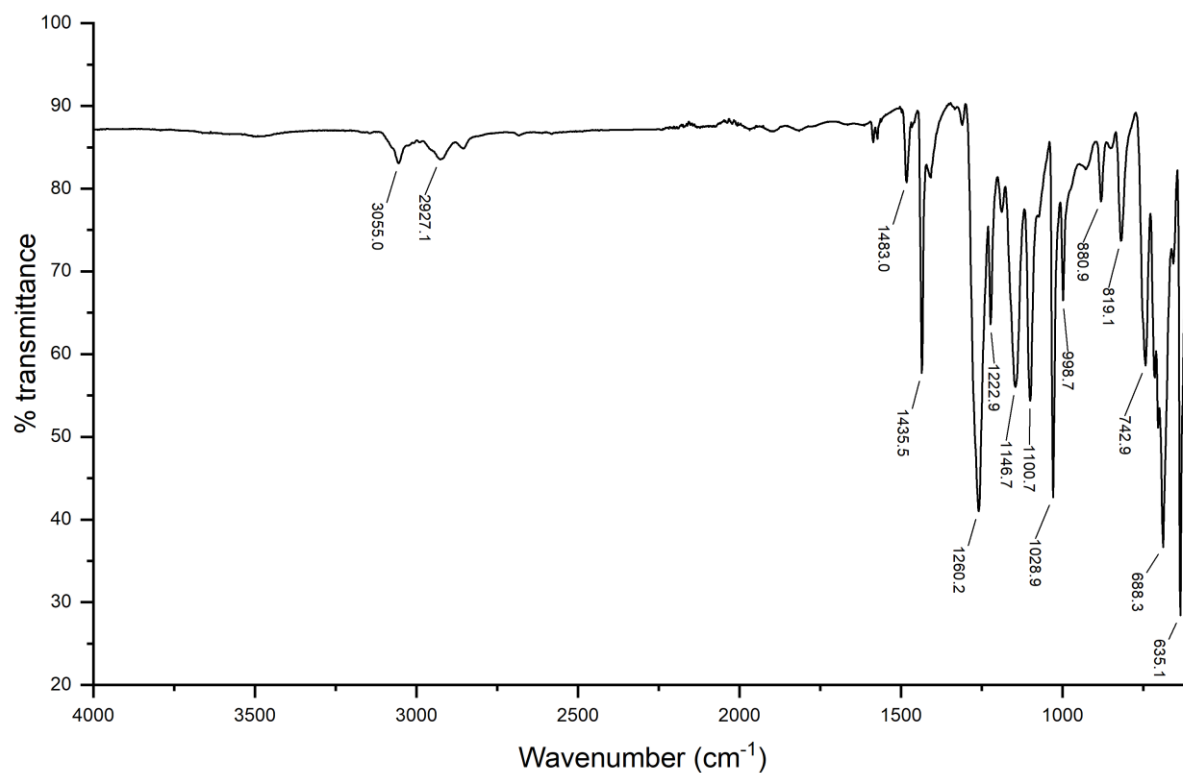
**Fig. S108.** FT-IR spectrum of **Pt-3**



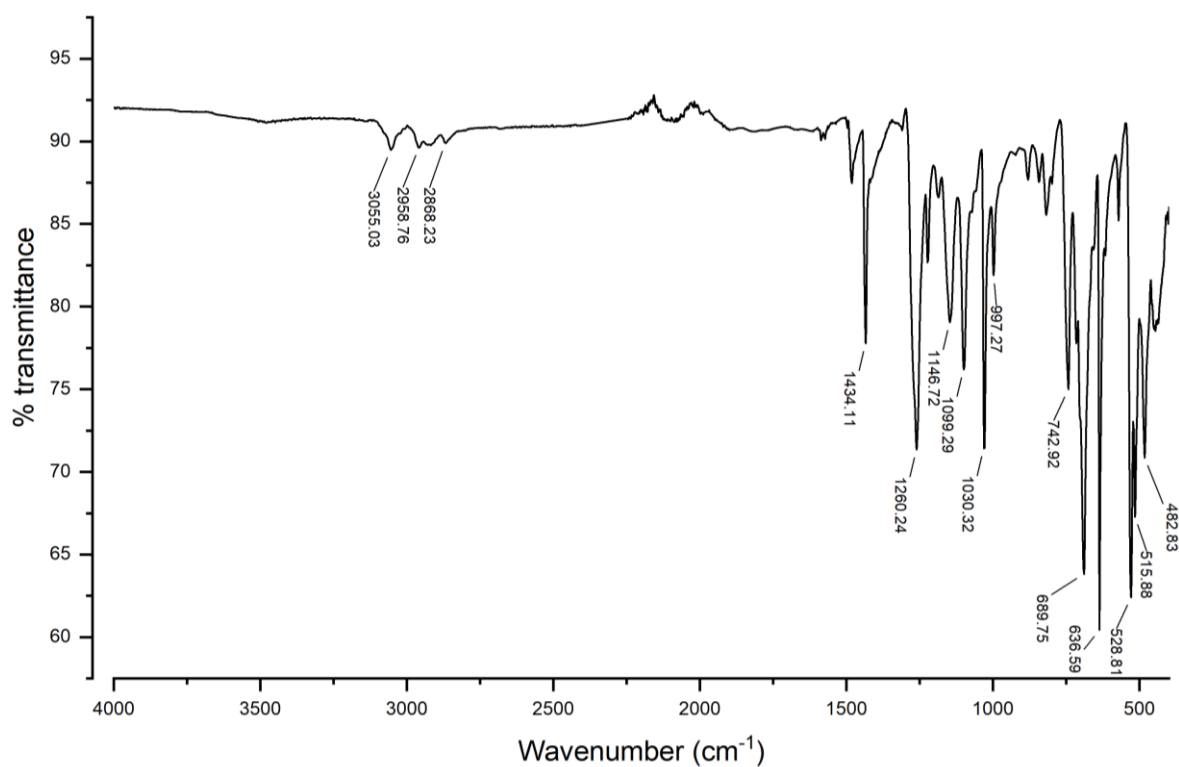
**Fig. S109.** FT-IR spectrum of PdPd-1



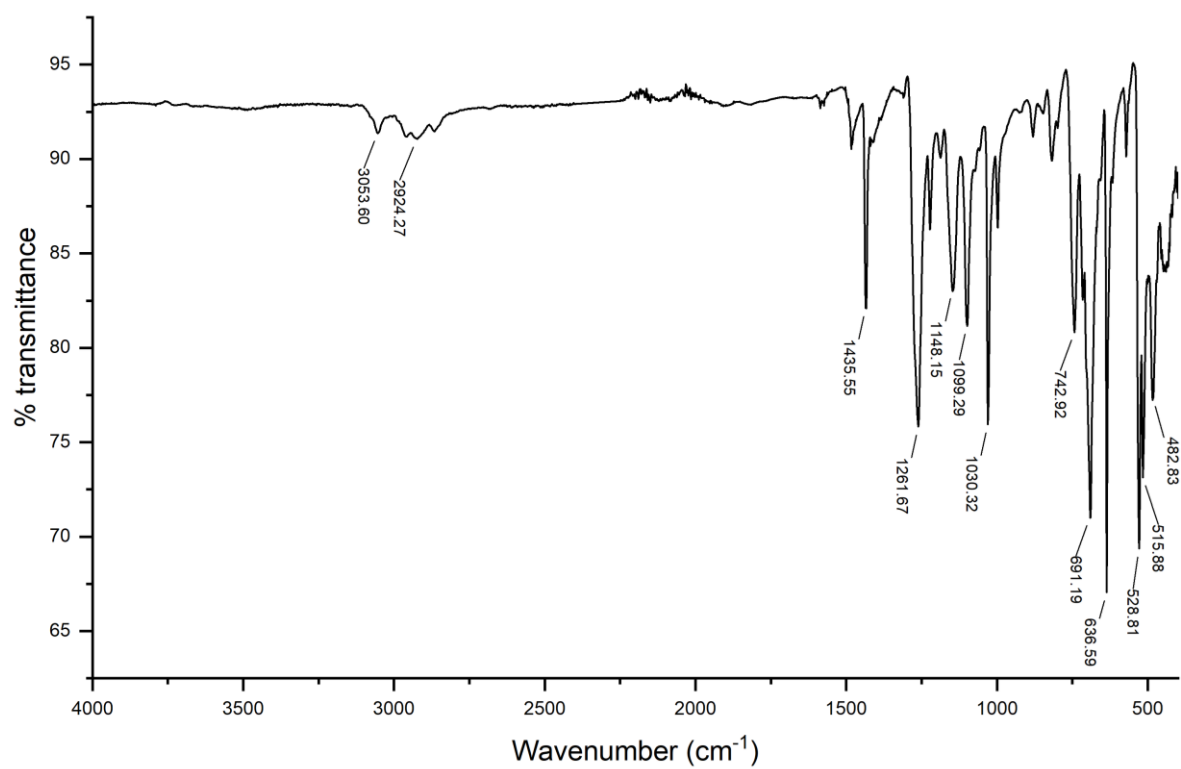
**Fig. S110.** FT-IR spectrum of PdPd-2



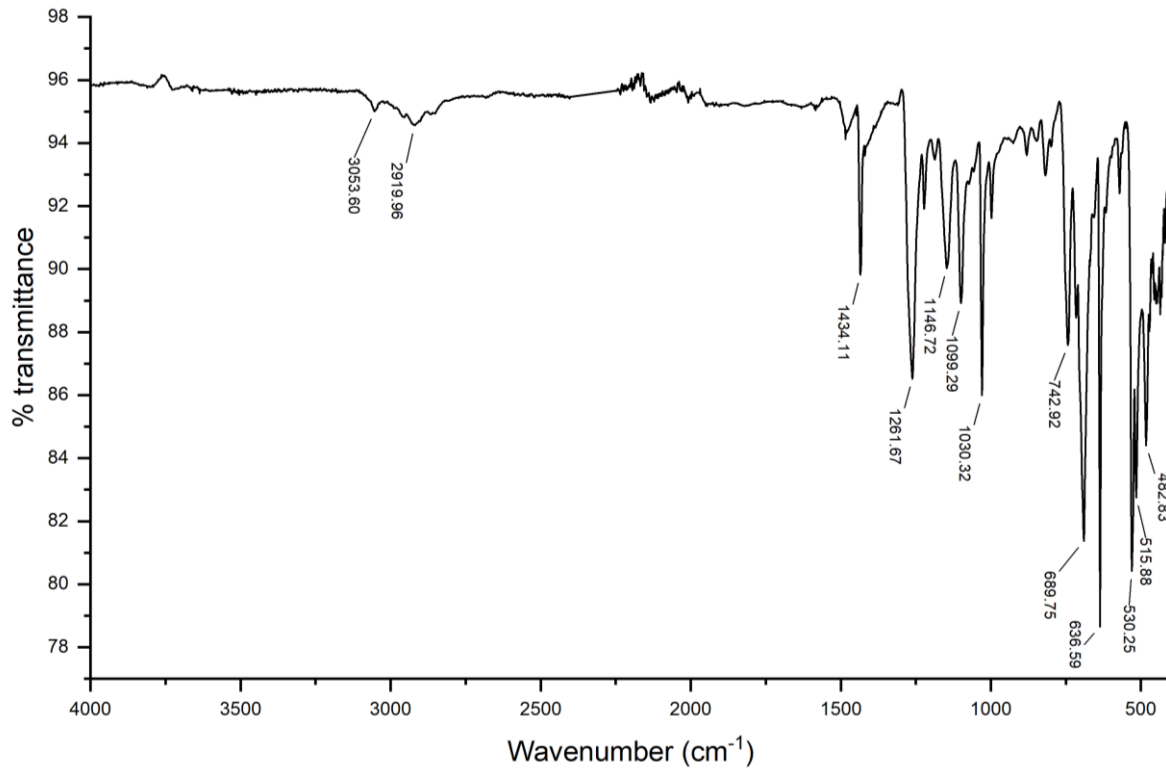
**Fig. S111.** FT-IR spectrum of **PdPd-3**



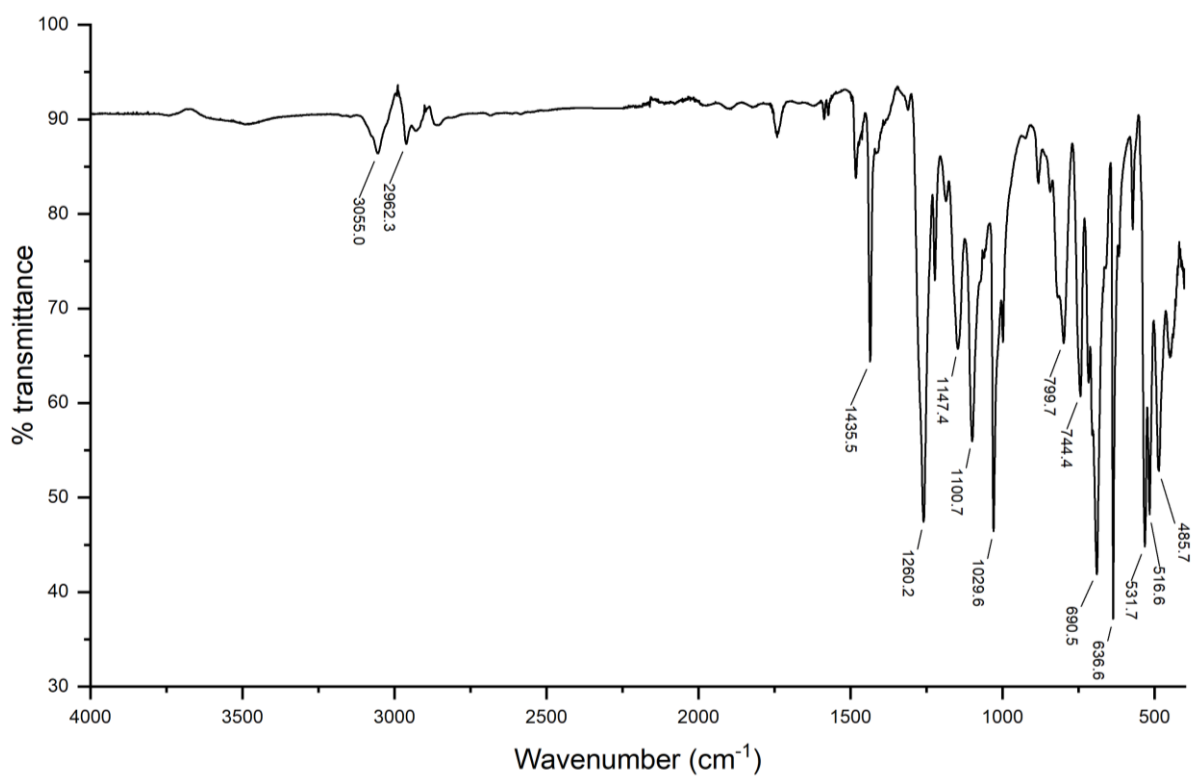
**Fig. S112.** FT-IR spectrum of **PdRu-1**



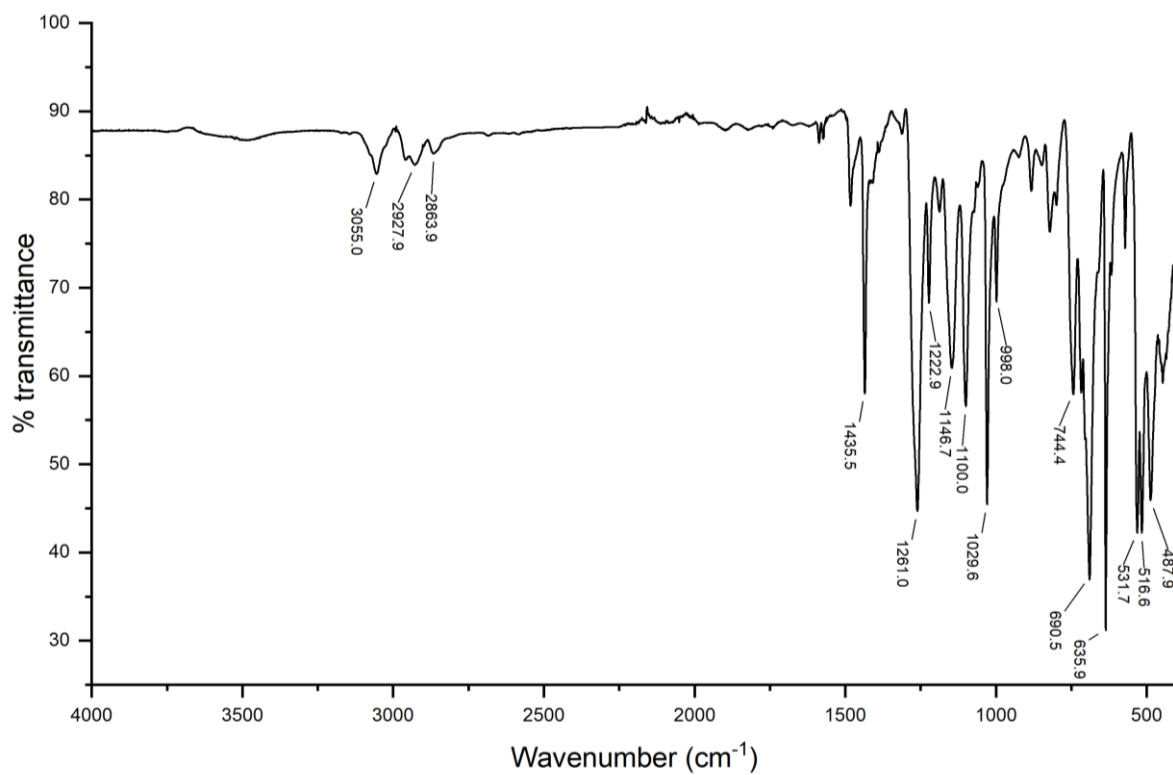
**Fig. S113.** FT-IR spectrum of **PdRu-2**



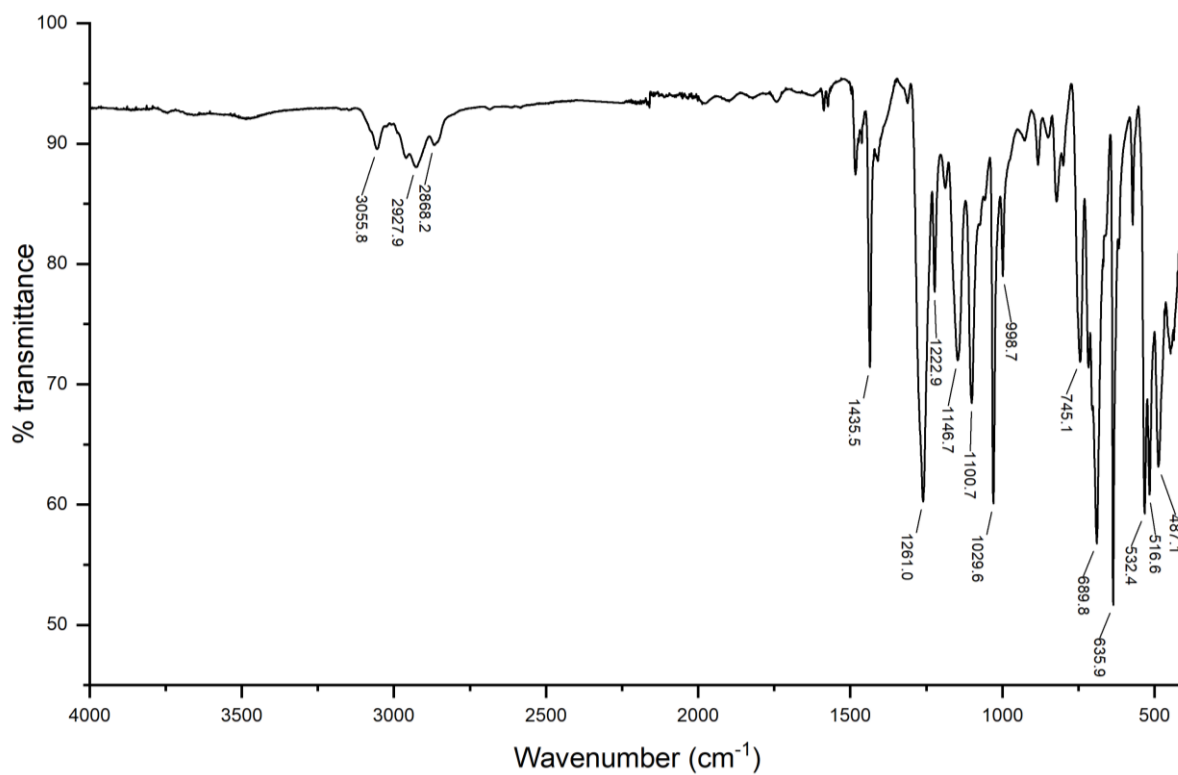
**Fig. S114.** FT-IR spectrum of **PdRu-3**



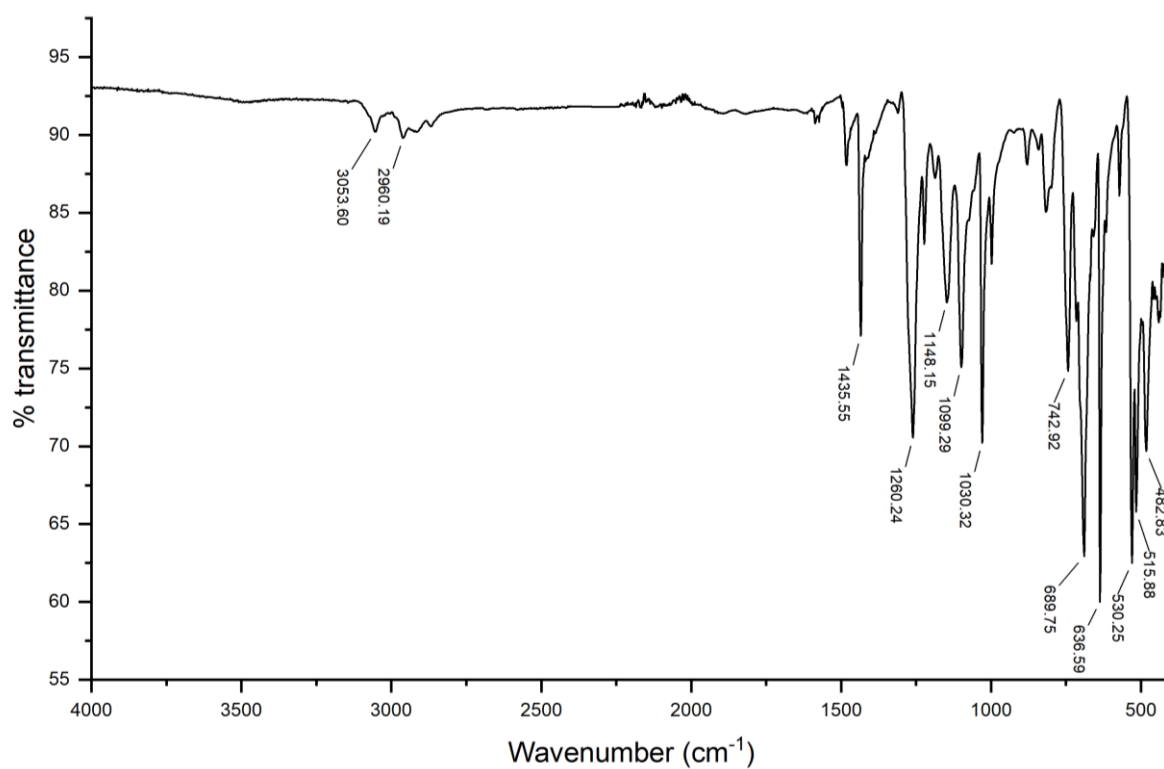
**Fig. S115.** FT-IR spectrum of PtRu-1



**Fig. S116.** FT-IR spectrum of PtRu-2

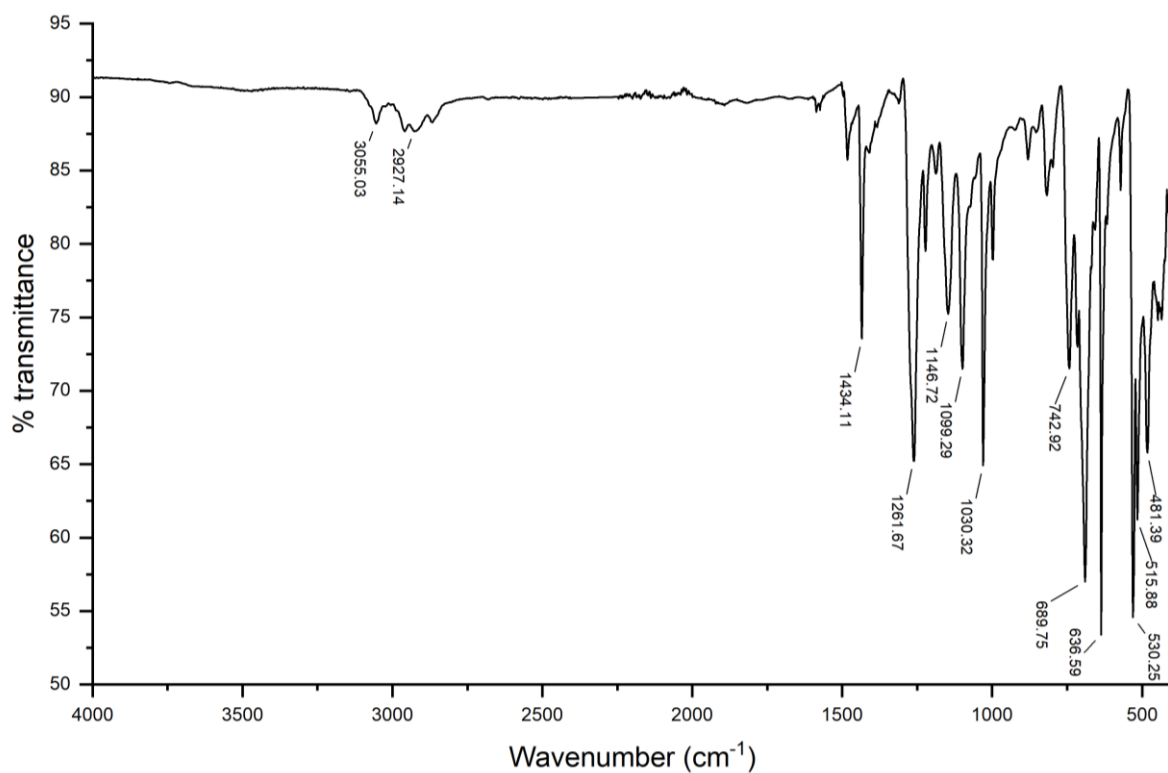


**Fig. S117.** FT-IR spectrum of PtRu-3

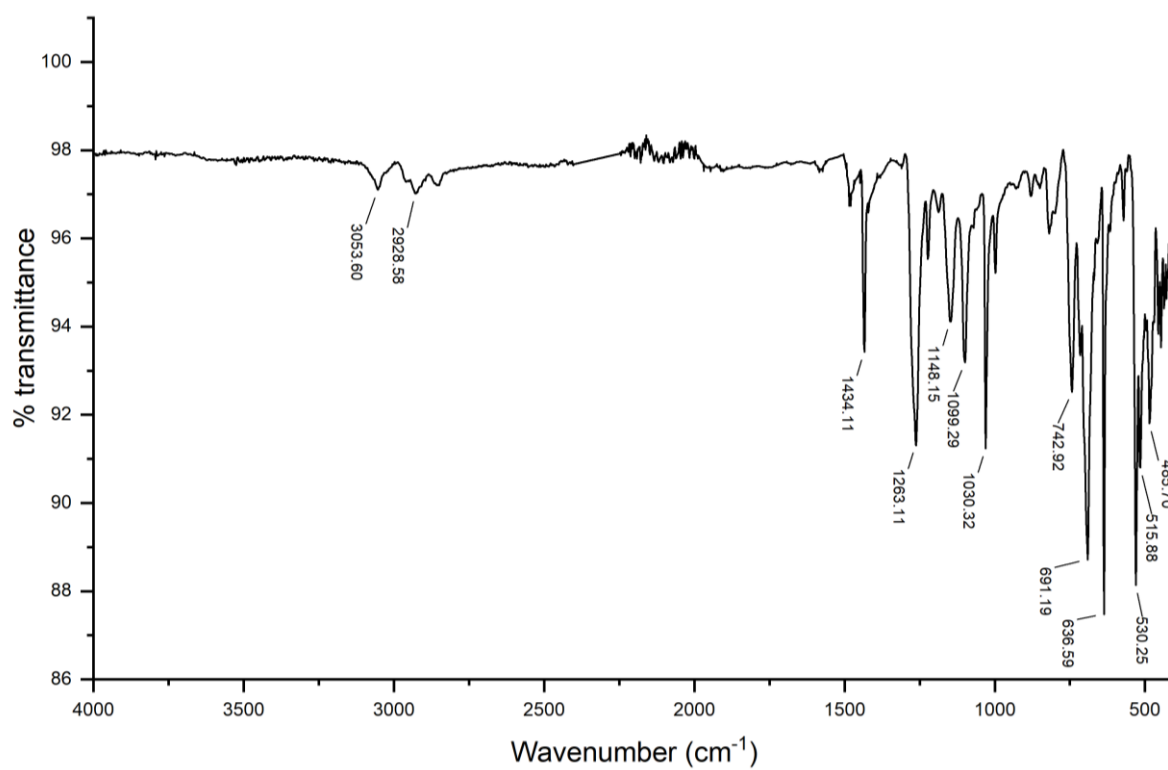


**Fig. S118.** FT-IR spectrum of PdOs-1



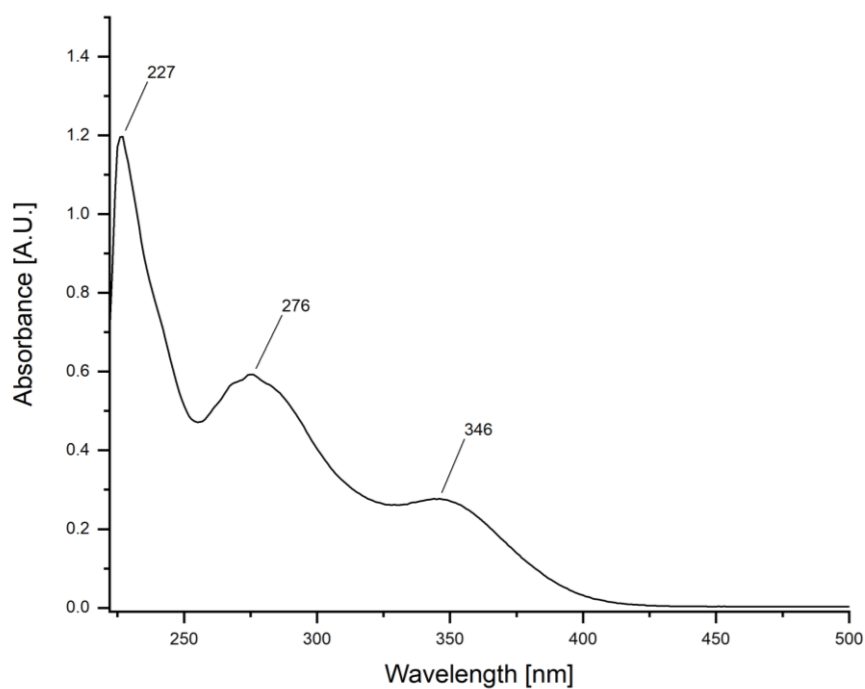


**Fig. S119.** FT-IR spectrum of PdOs-2

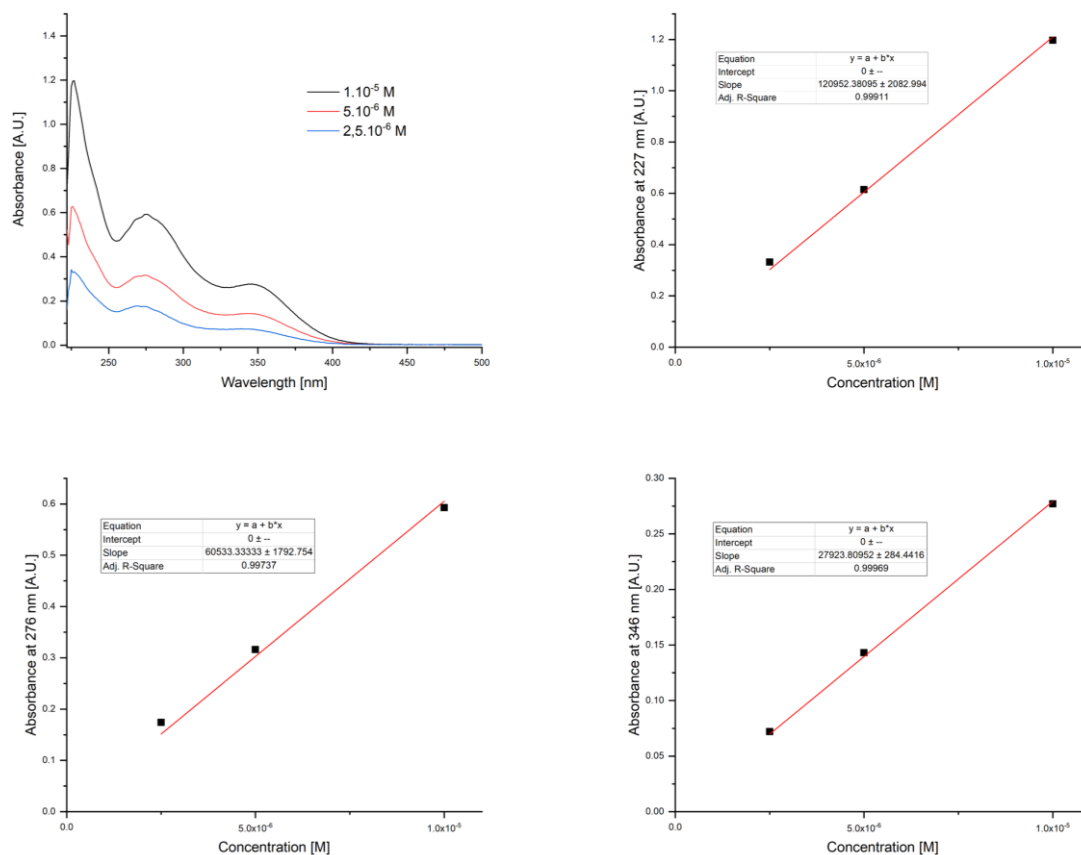


**Fig. S120.** FT-IR spectrum of PdOs-3

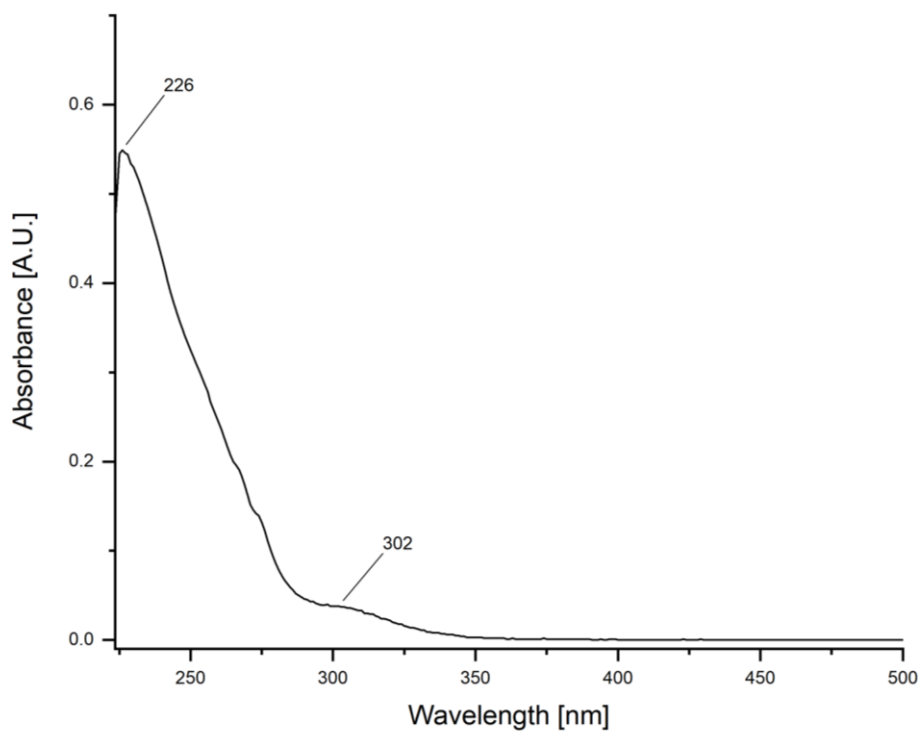
## 7. UV-Vis spectra



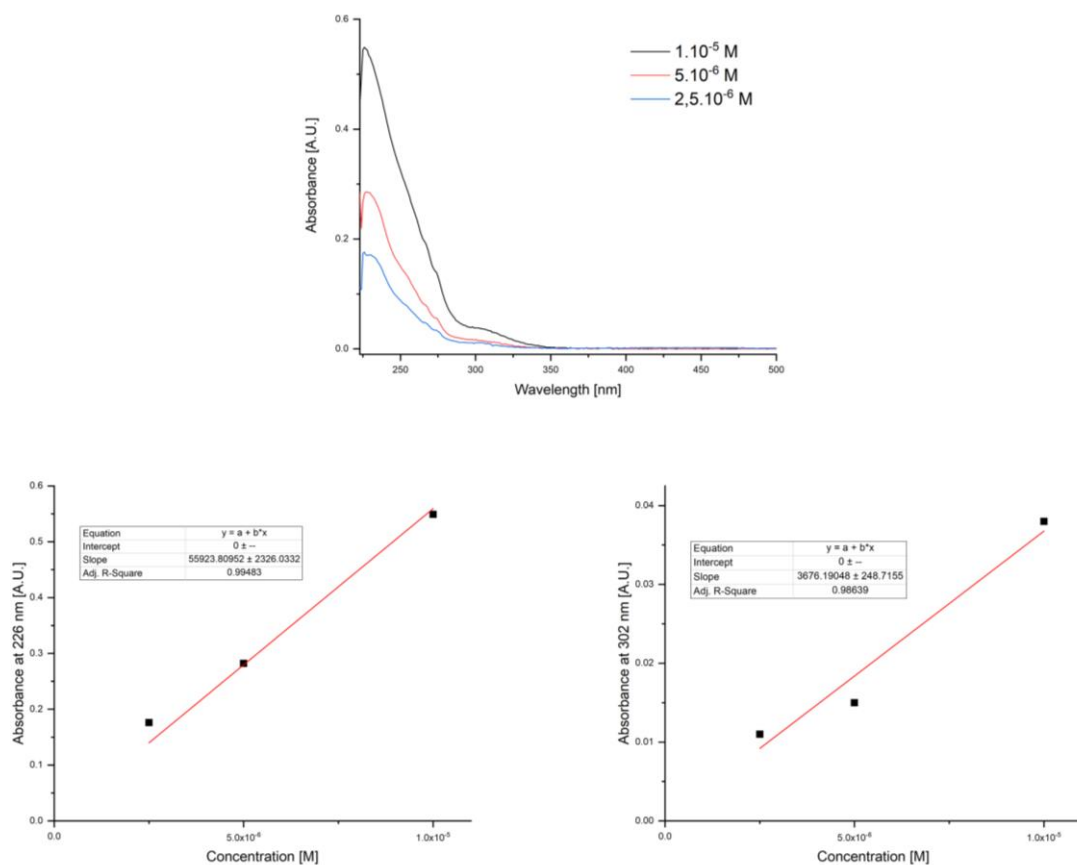
**Fig. S121.** UV-Vis spectrum of **PdPd-0** ( $1 \cdot 10^{-5}$  M, dichloromethane, 298 K)



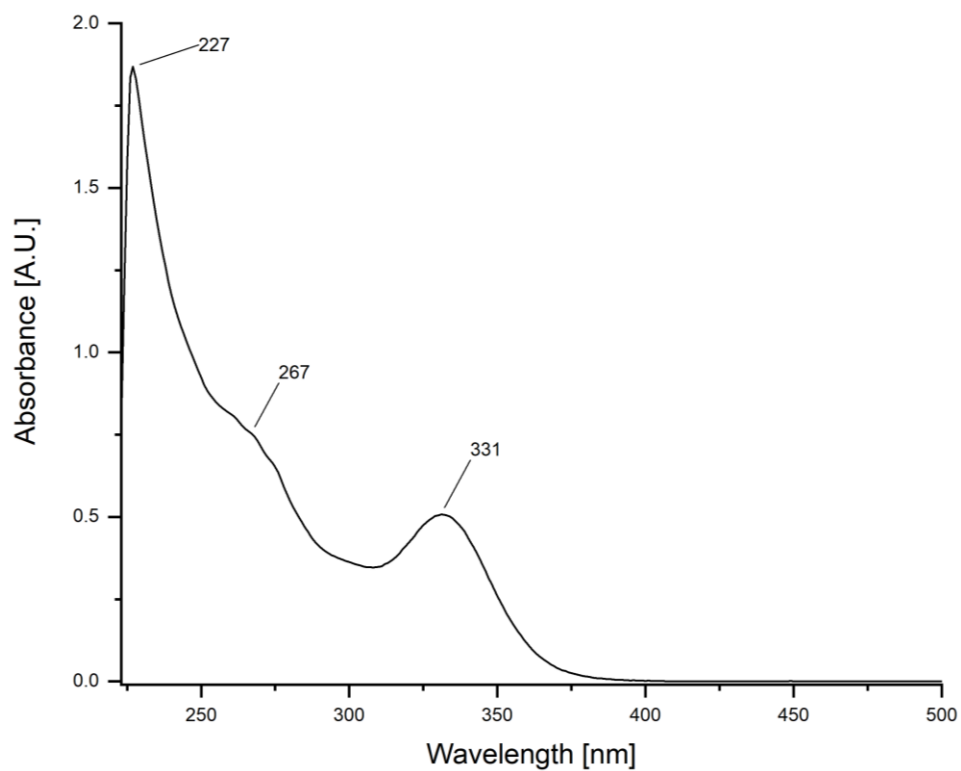
**Fig. S122.** Variable concentration UV-Vis spectra of **PdPd-0** (top left), and plots of absorptions at the respective maxima for given concentrations



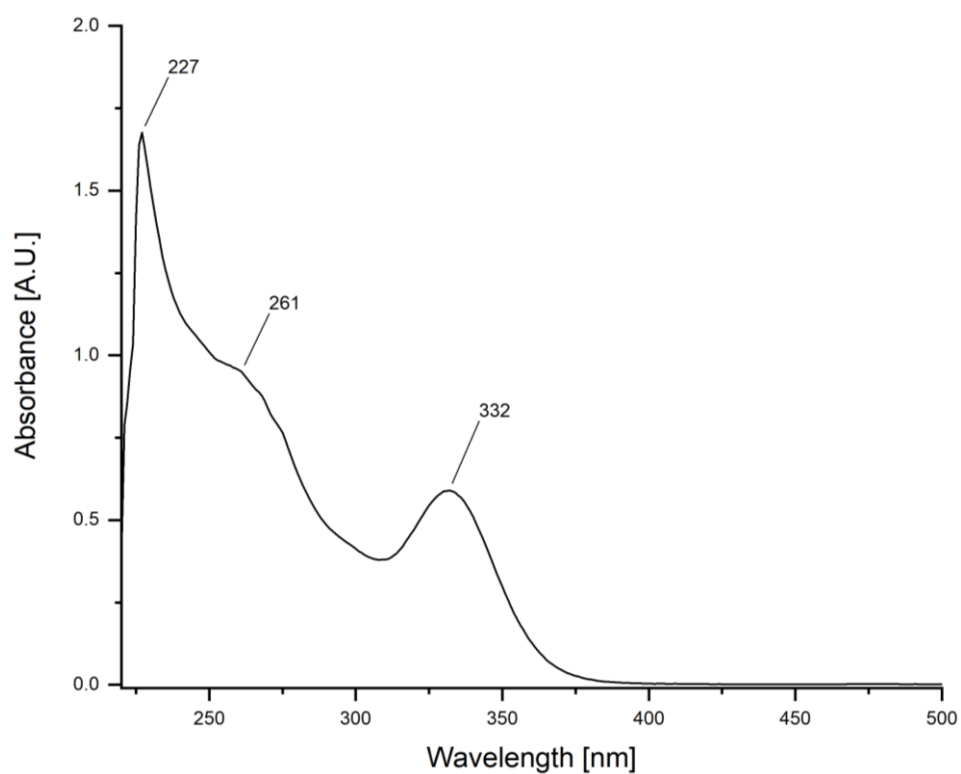
**Fig. S123.** UV-Vis spectrum of **PtPt-0**, recorded in DCM at 298 K



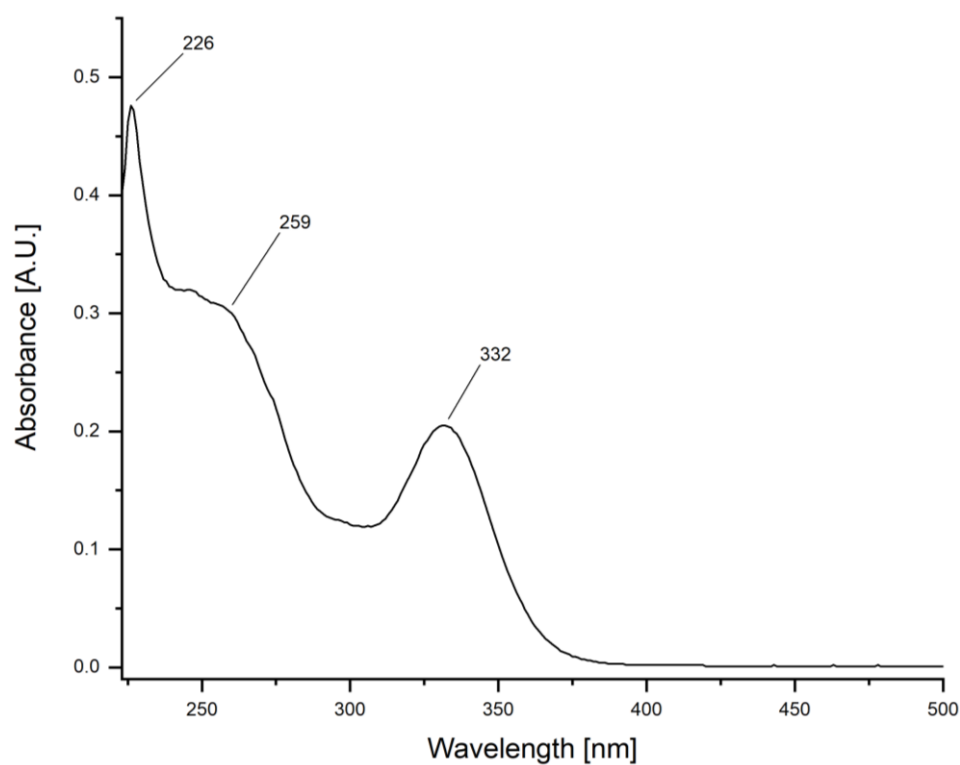
**Fig. S124.** Variable concentration UV-Vis spectra of **PtPt-0** (top), and plots of absorptions at the respective maxima for given concentrations



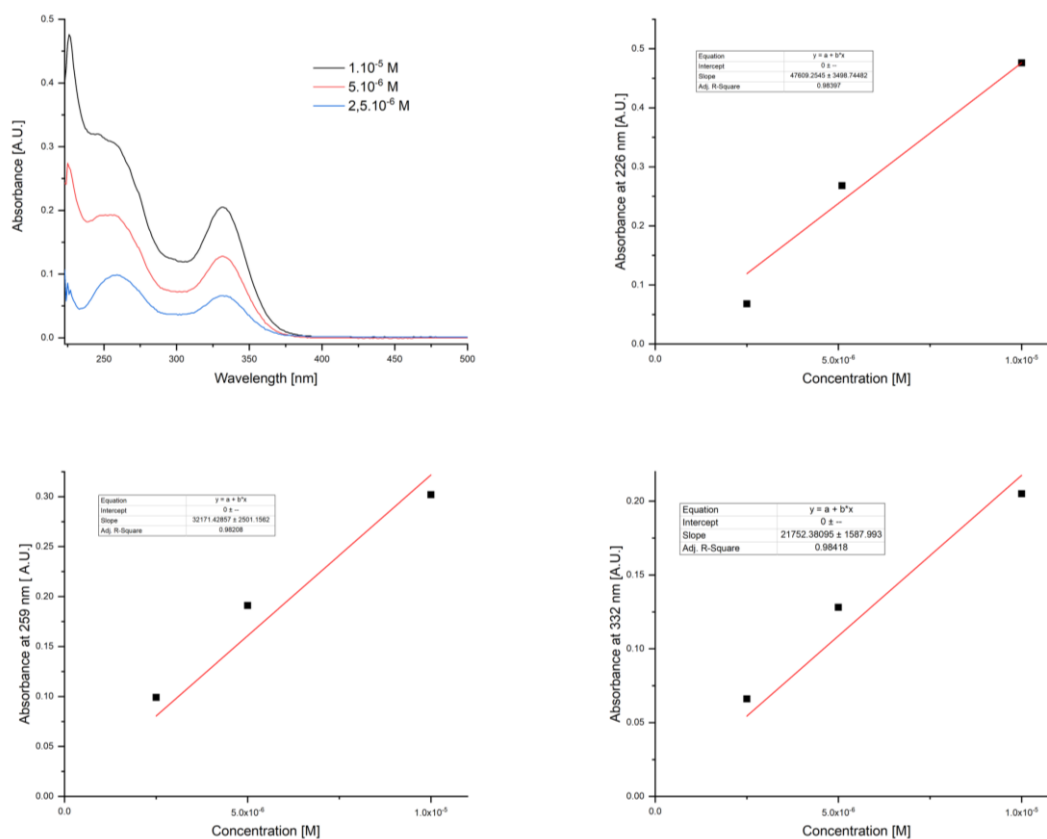
**Fig. S125.** UV-Vis spectrum of **Pd-1** (dichloromethane, 298 K)



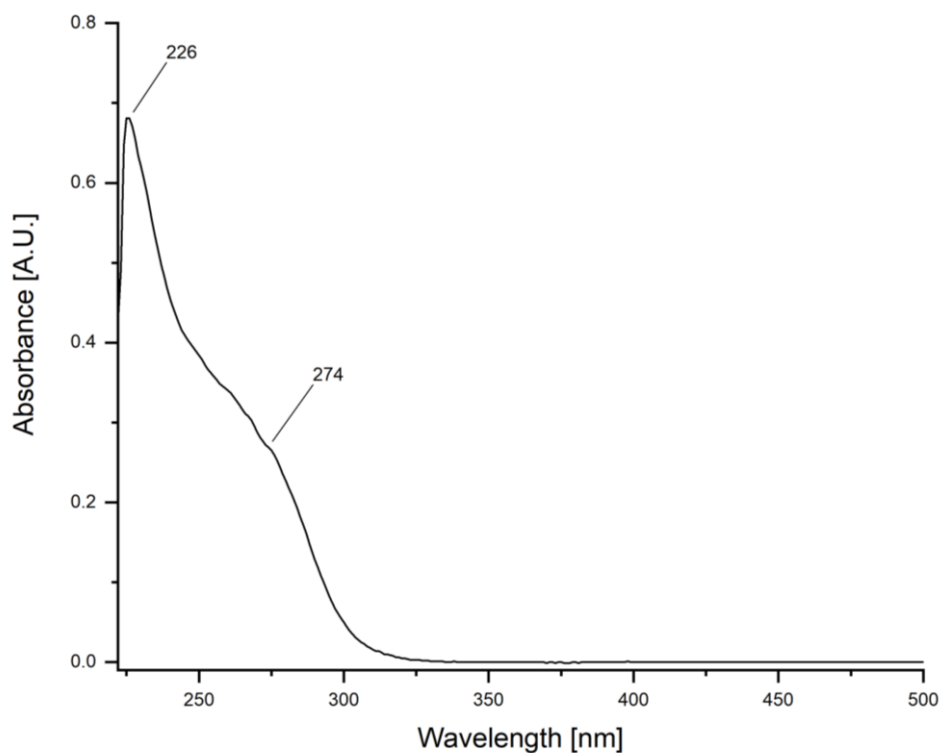
**Fig. S126.** UV-Vis spectrum of **Pd-2** (dichloromethane, 298 K)



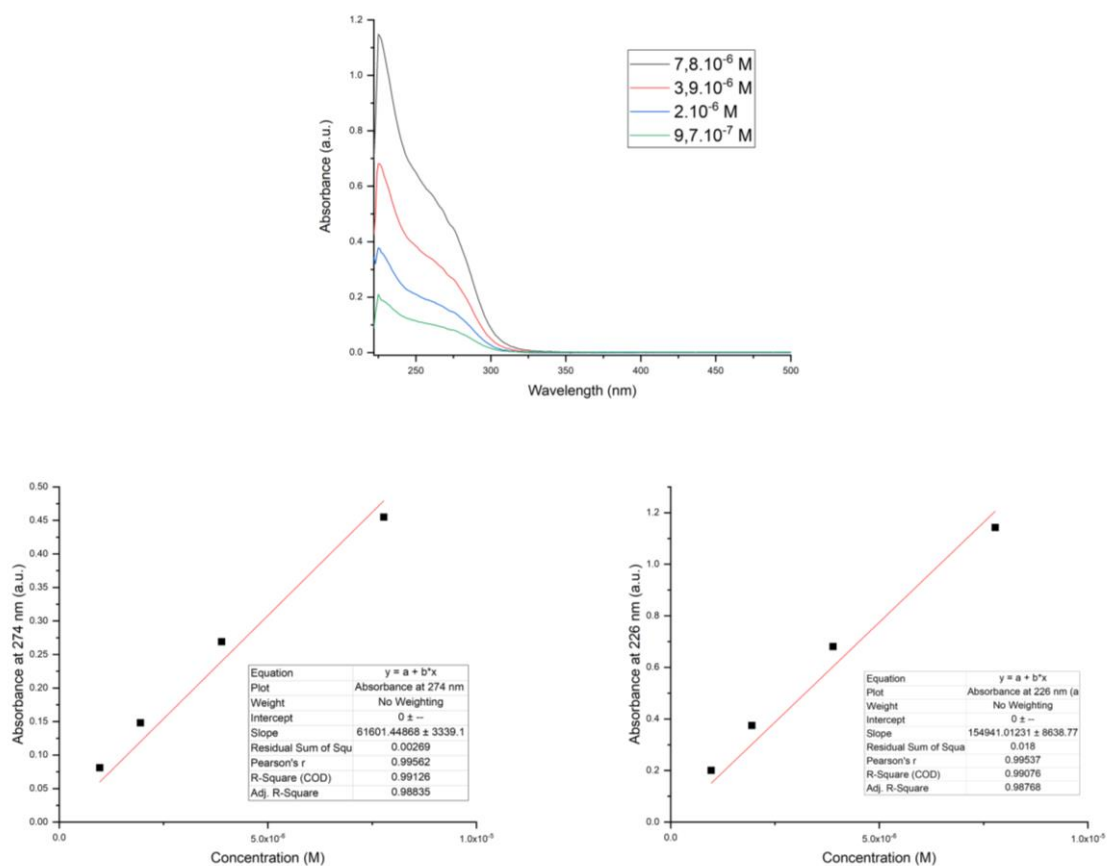
**Fig. S127.** UV-Vis spectrum of **Pd-3** ( $1.10^{-5}$  M, dichloromethane, 298 K)



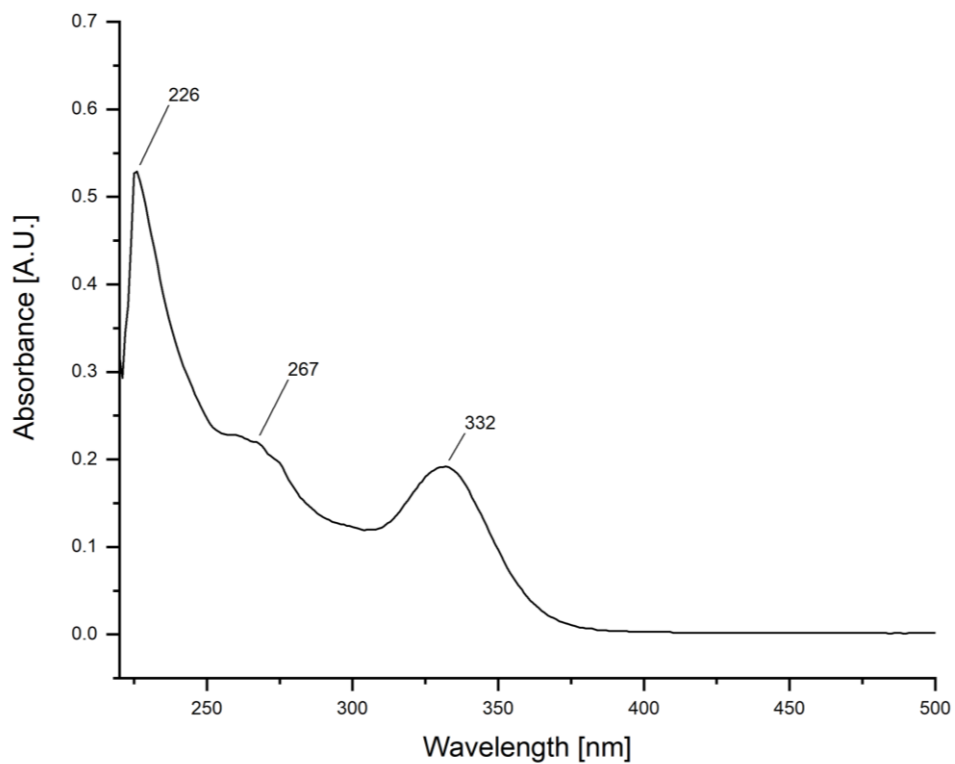
**Fig. S128.** Variable concentration UV-Vis spectra of **Pd-3** (top left), and plots of absorptions at the respective maxima for given concentrations



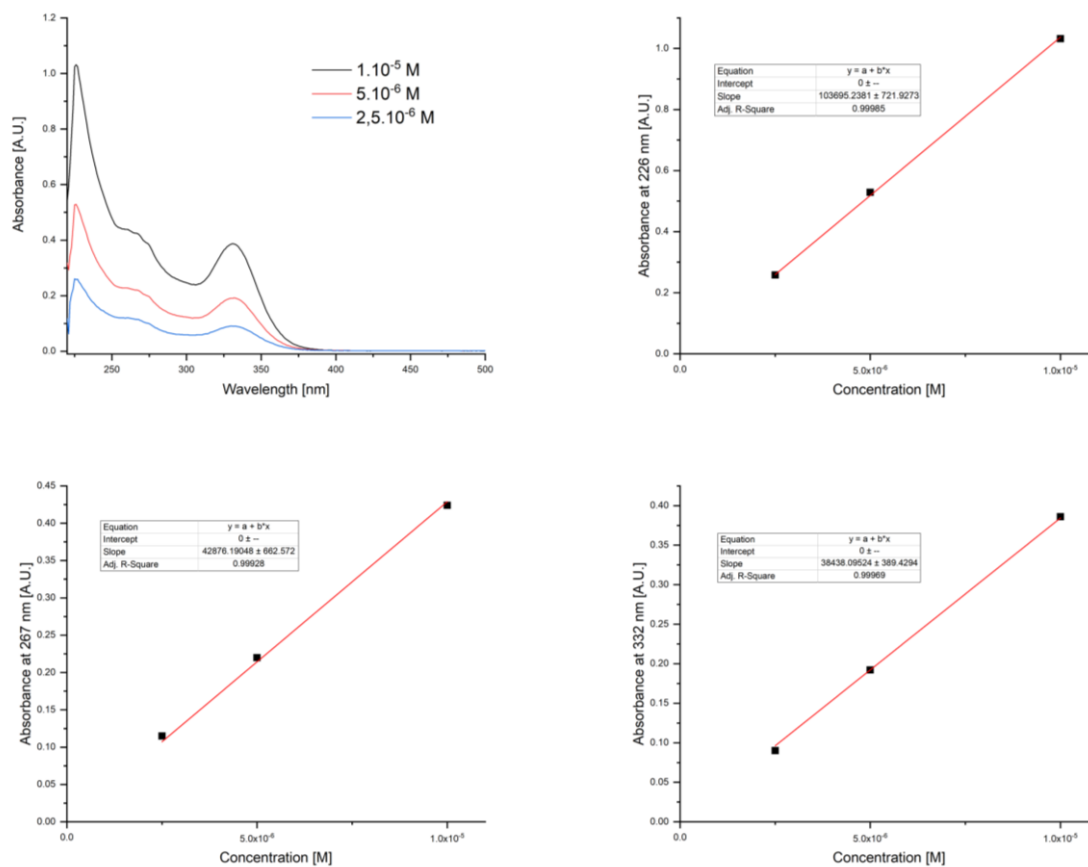
**Fig. S129.** UV-Vis spectrum of **Pt-3**, recorded in DCM at 298 K



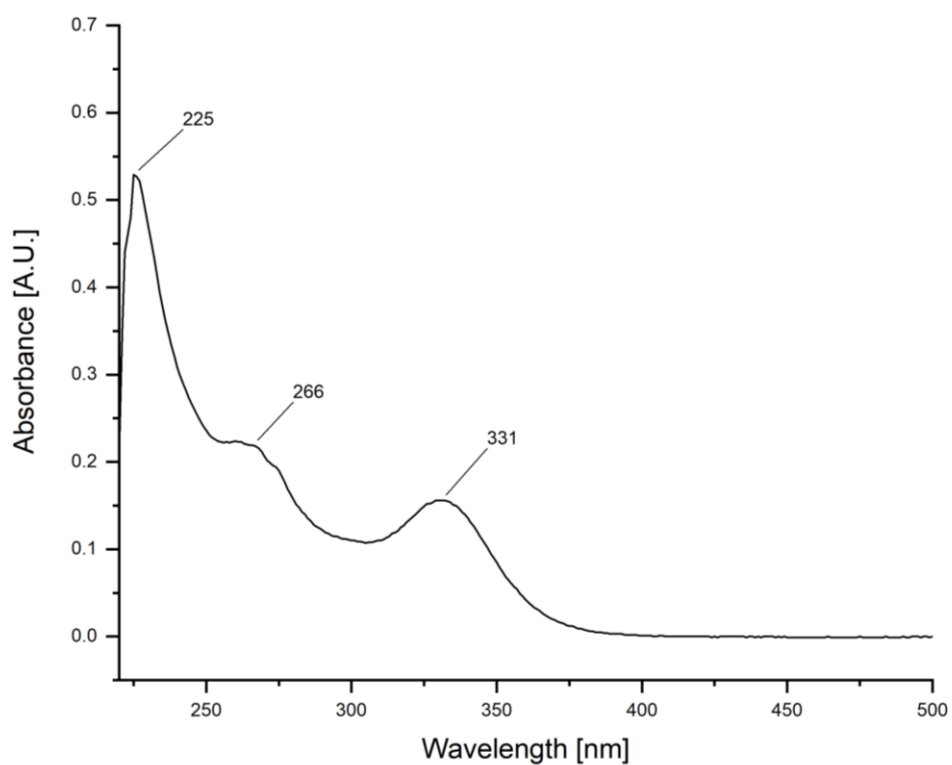
**Fig. S130.** Variable concentration UV-Vis spectra of **Pt-3** (top), and plots of absorptions at the respective maxima for given concentrations



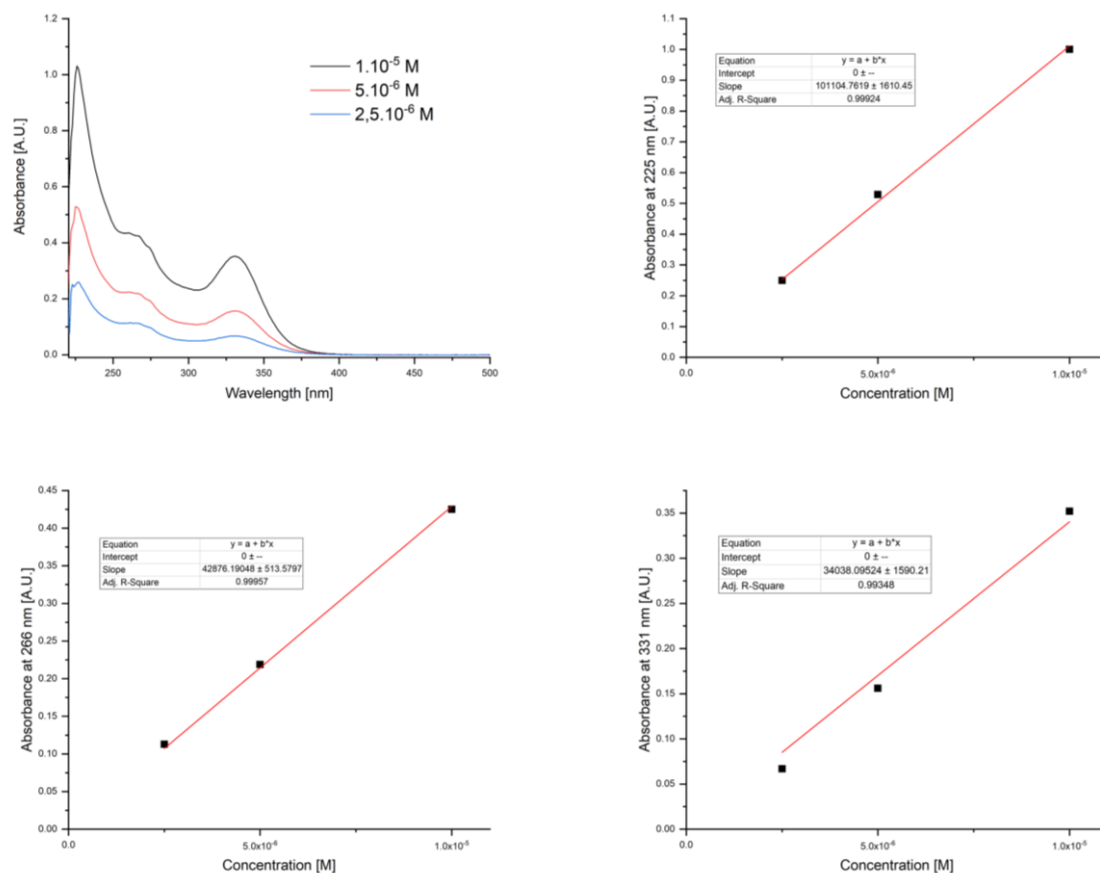
**Fig. S131.** UV-Vis spectrum of **PdPd-1**, ( $5 \cdot 10^{-6}$  M, dichloromethane, 298 K)



**Fig. S132.** Variable concentration UV-Vis spectra of **PdPd-1** (top left), and plots of absorptions at the respective maxima for given concentrations

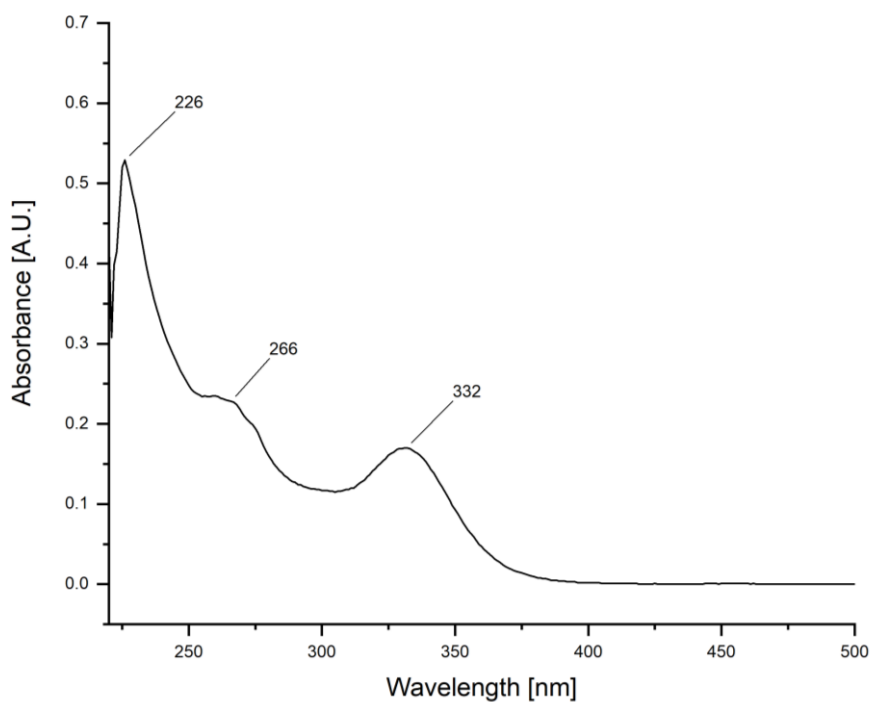


**Fig. S133.** UV-Vis spectrum of **PdPd-2**, recorded in DCM at 298 K

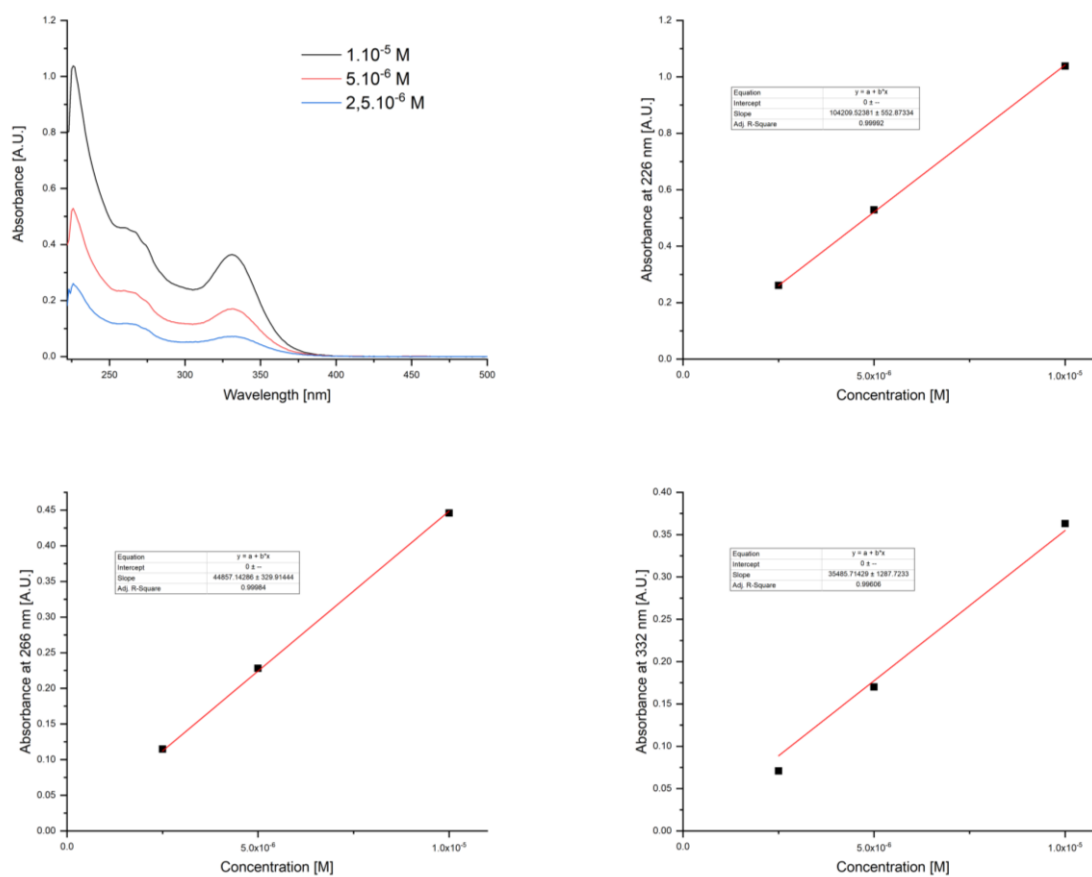


**Fig. S134.** Variable concentration UV-Vis spectra of **PdPd-2** (top left), and plots of absorptions at the respective maxima for given concentrations

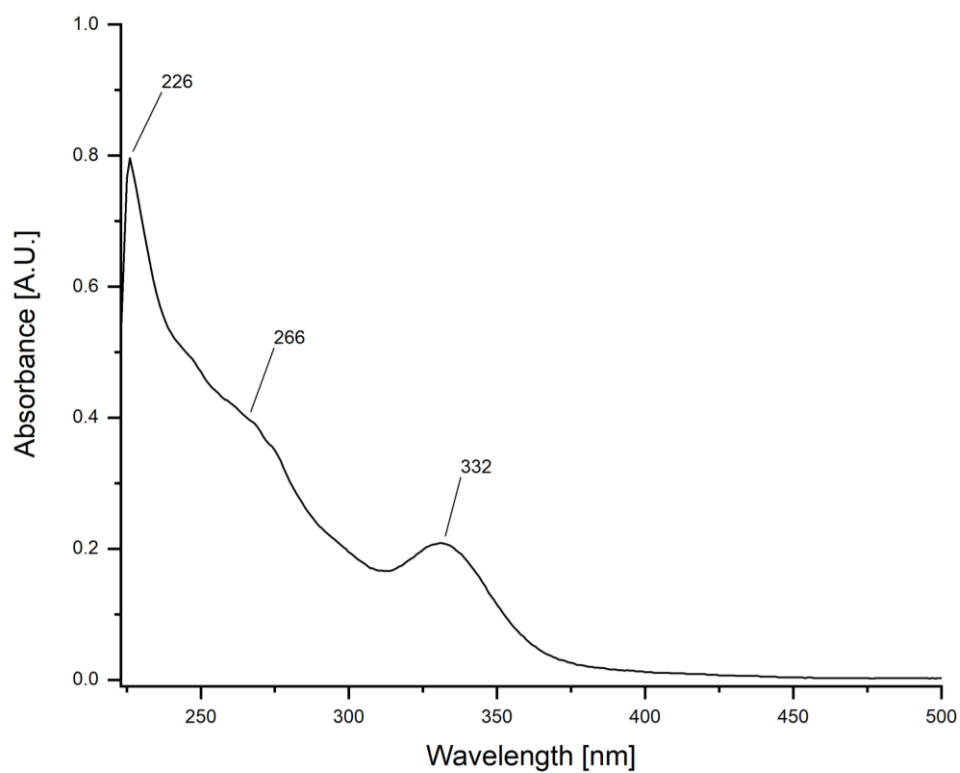




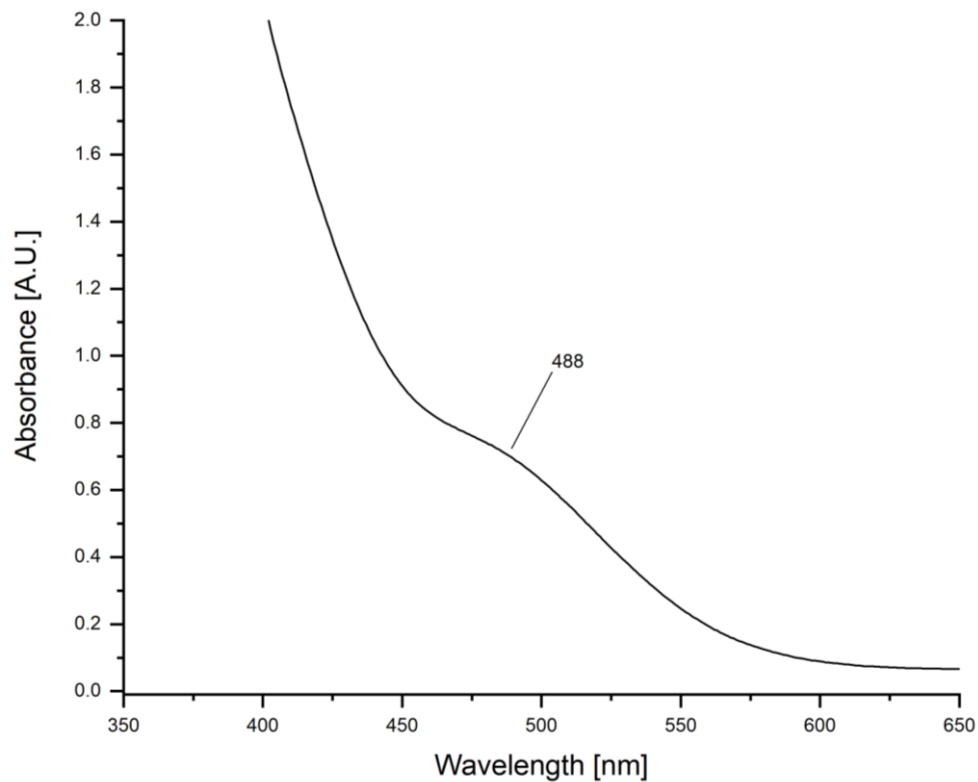
**Fig. S135.** UV-Vis spectrum of **PdPd-3** ( $5.10^{-6}$  M), recorded in  $\text{CH}_2\text{Cl}_2$  at 298 K



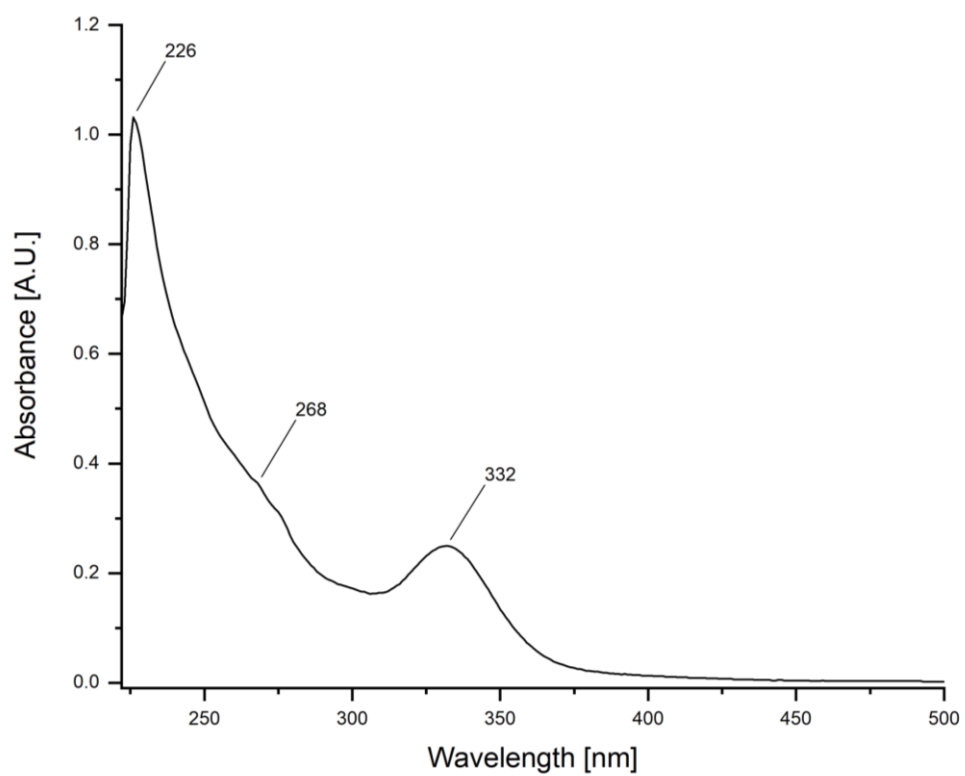
**Fig. S136.** Variable concentration UV-Vis spectra of **PdPd-3** (top left), and plots of absorptions at the respective maxima for given concentrations



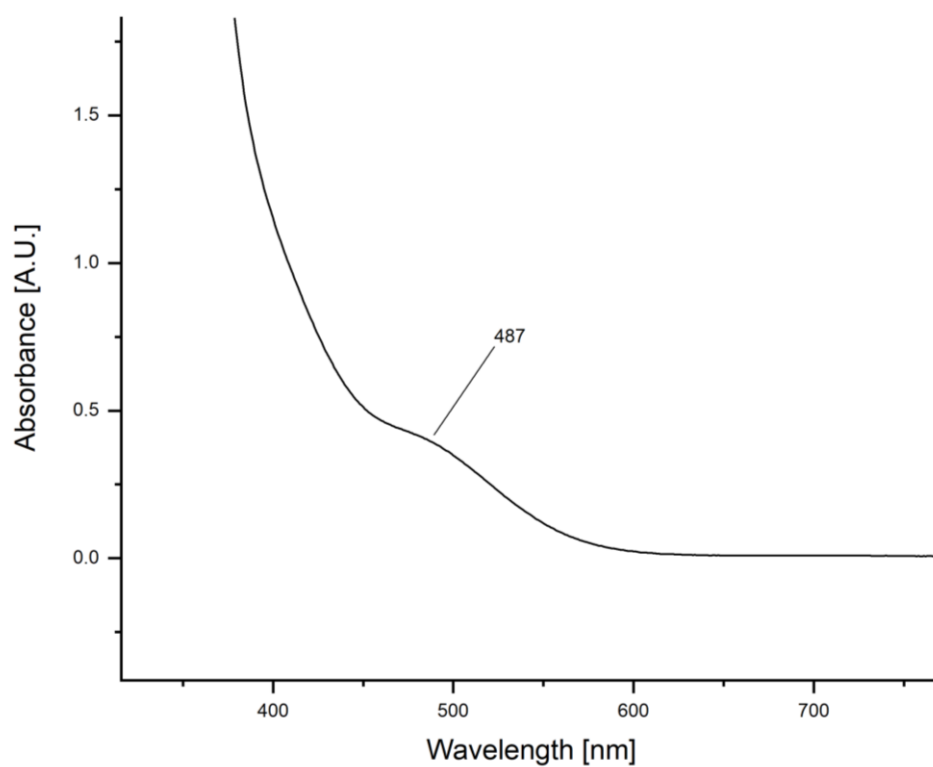
**Fig. S137.** UV-Vis spectrum of **PdRu-1** (1.10<sup>-5</sup> M, dichloromethane, 298 K)



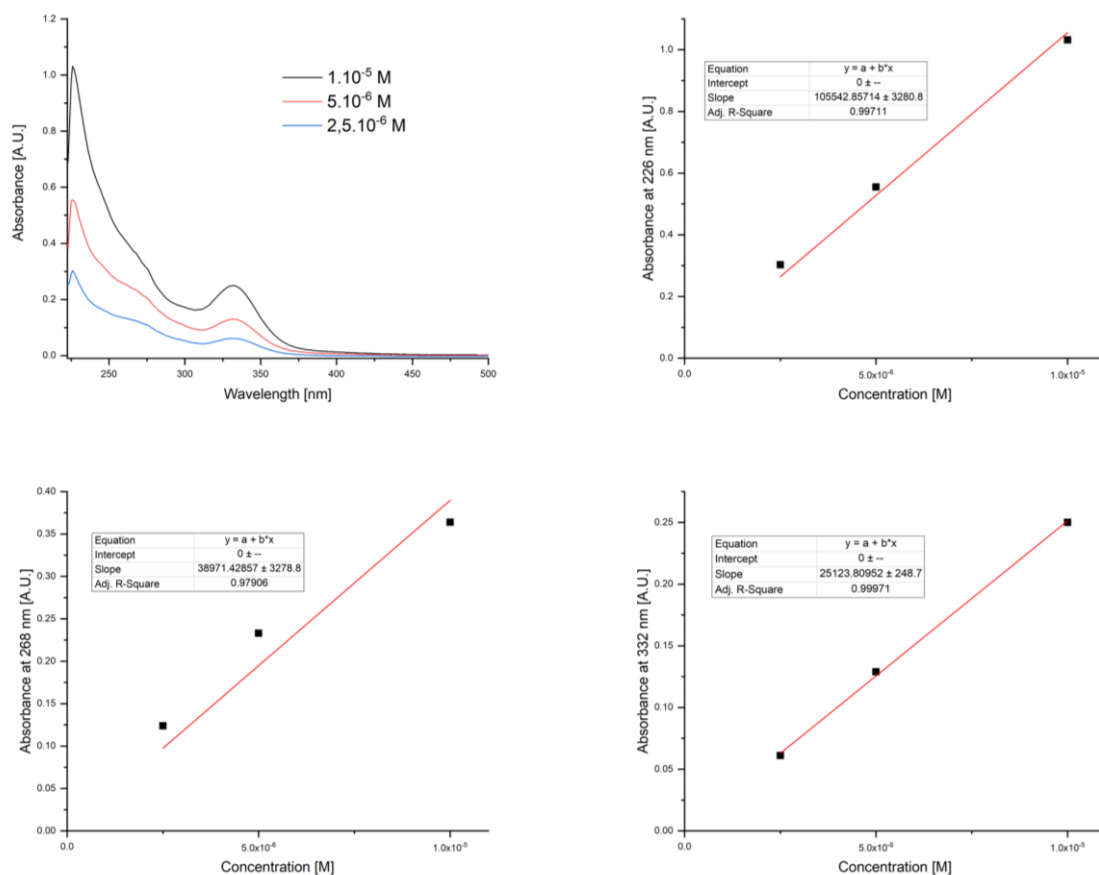
**Fig. S138.** UV-Vis spectrum of **PdRu-1** (1.10<sup>-4</sup> M, dichloromethane, 298 K)



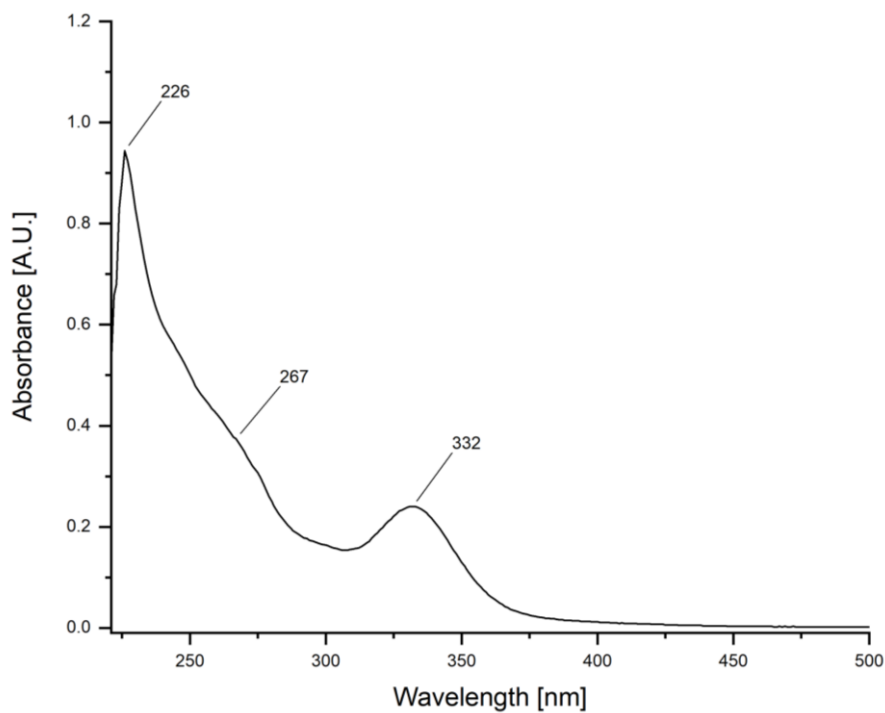
**Fig. S139.** UV-Vis spectrum of **PdRu-2** (1.10<sup>-5</sup> M, dichloromethane, 298 K)



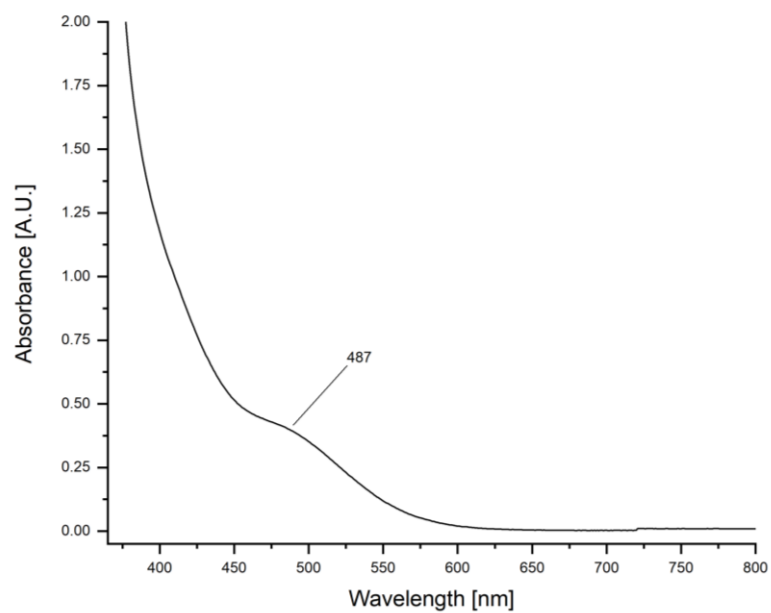
**Fig. S140.** UV-Vis spectrum of **PdRu-2** (1.10<sup>-4</sup> M, dichloromethane, 298 K)



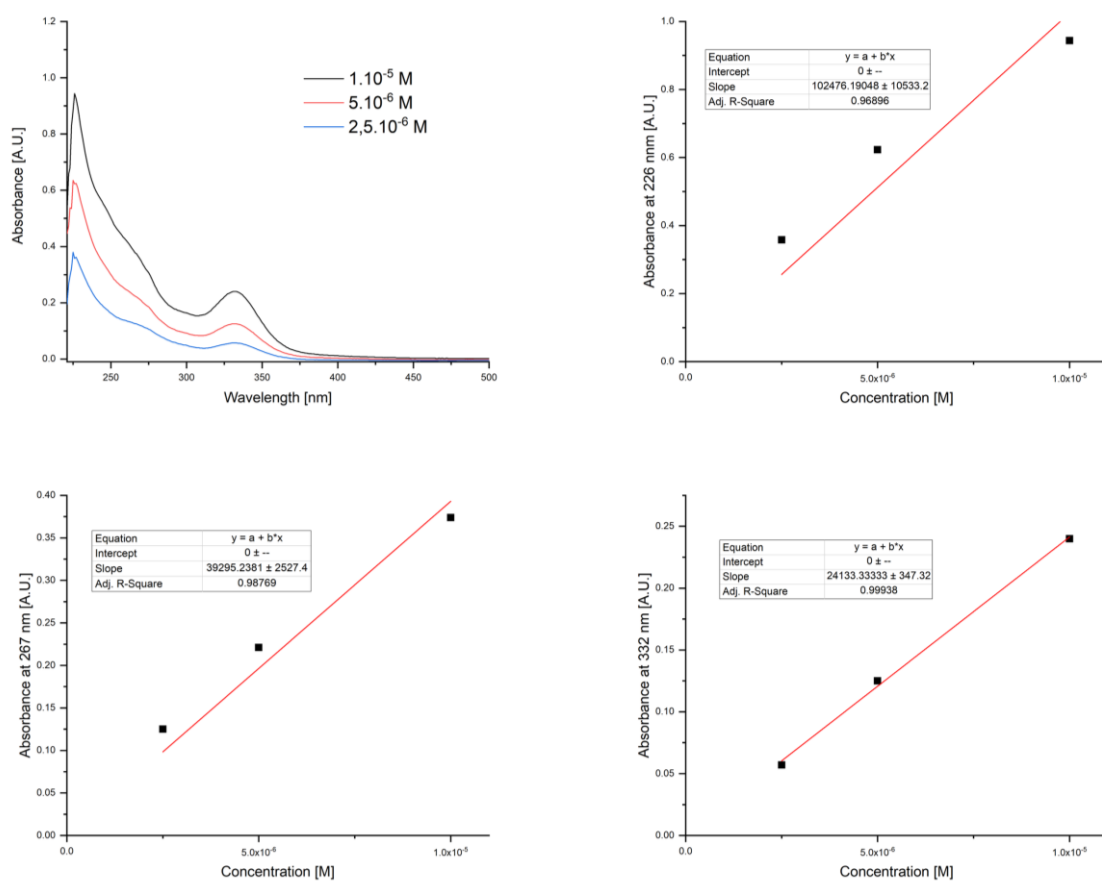
**Fig. S141.** Variable concentration UV-Vis spectra of **PdRu-2** (top left), and plots of absorptions at the respective maxima for given concentrations



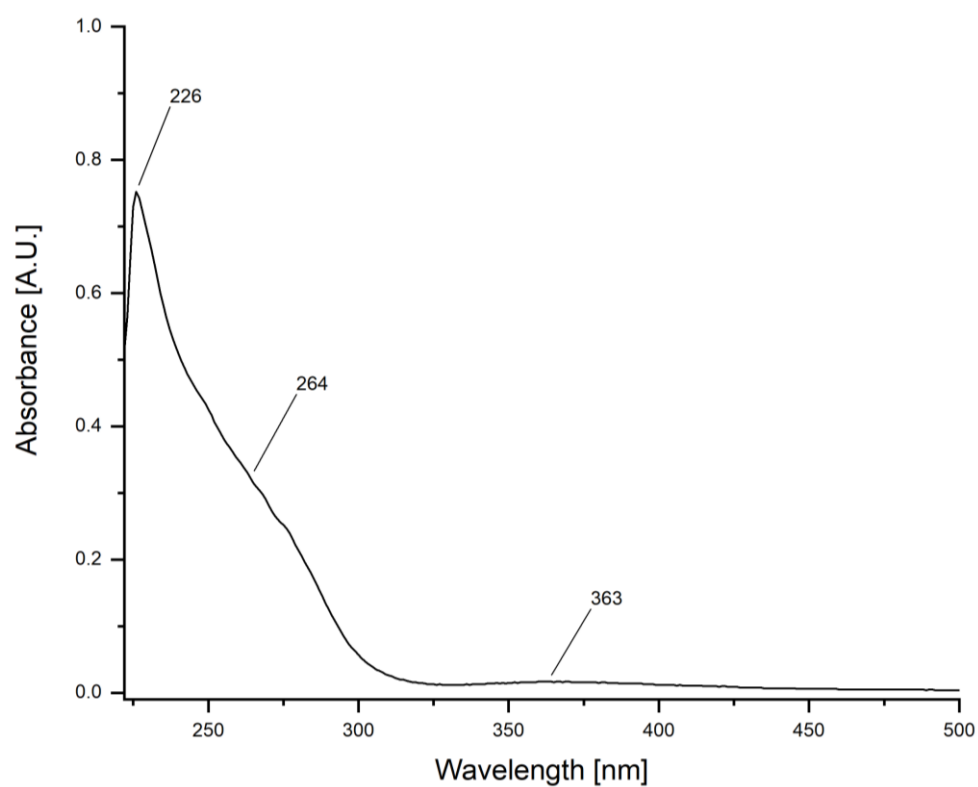
**Fig. S142.** UV-Vis spectrum of **PdRu-3** (1.10<sup>-5</sup> M, dichloromethane, 298 K)



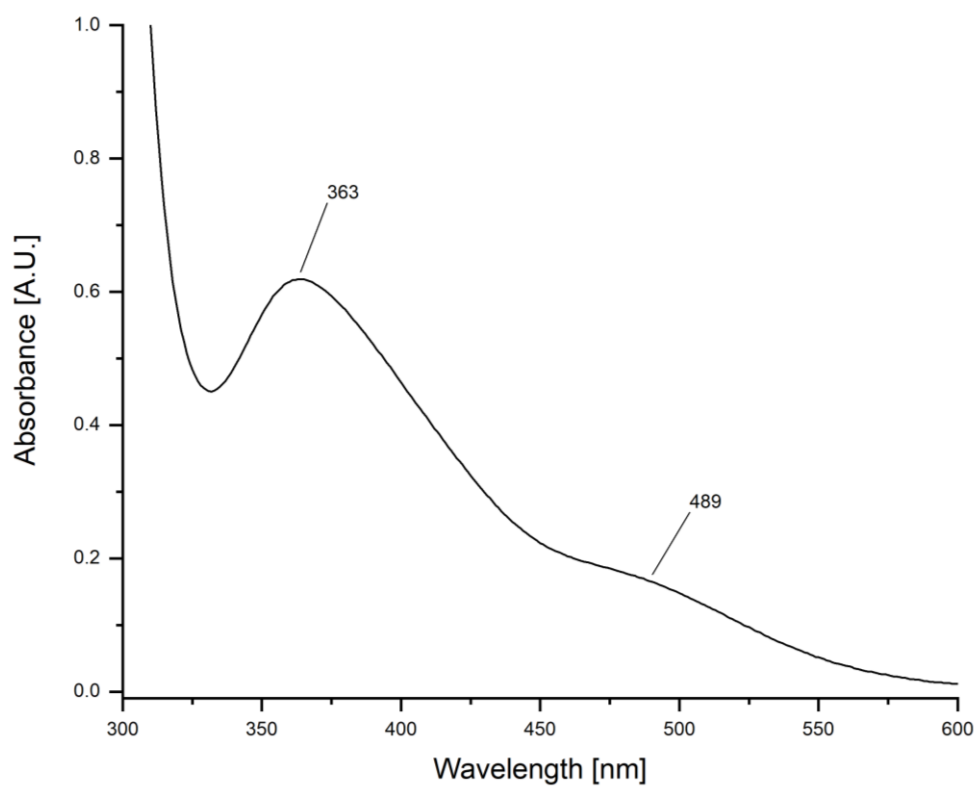
**Fig. S143.** UV-Vis spectrum of PdRu-3 (1.10<sup>-4</sup> M, dichloromethane, 298 K)



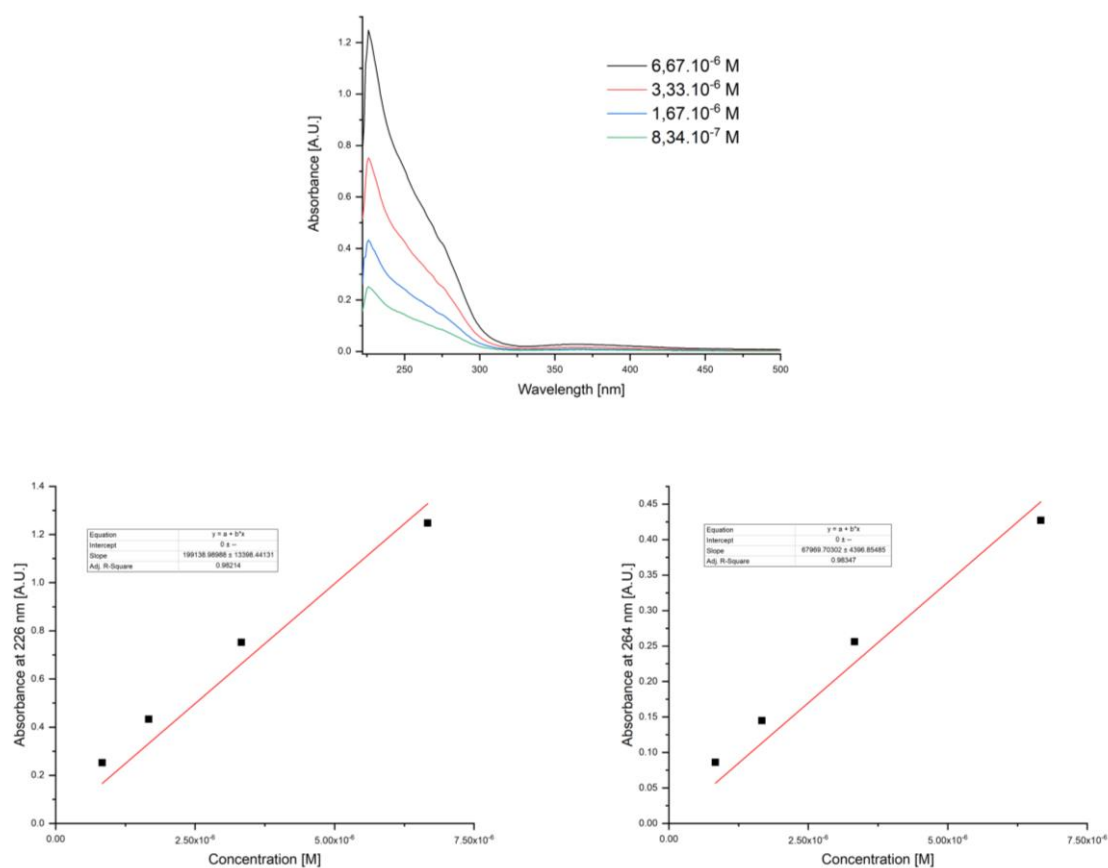
**Fig. S144.** Variable concentration UV-Vis spectra of PdRu-3 (top left), and plots of absorptions at the respective maxima for given concentrations



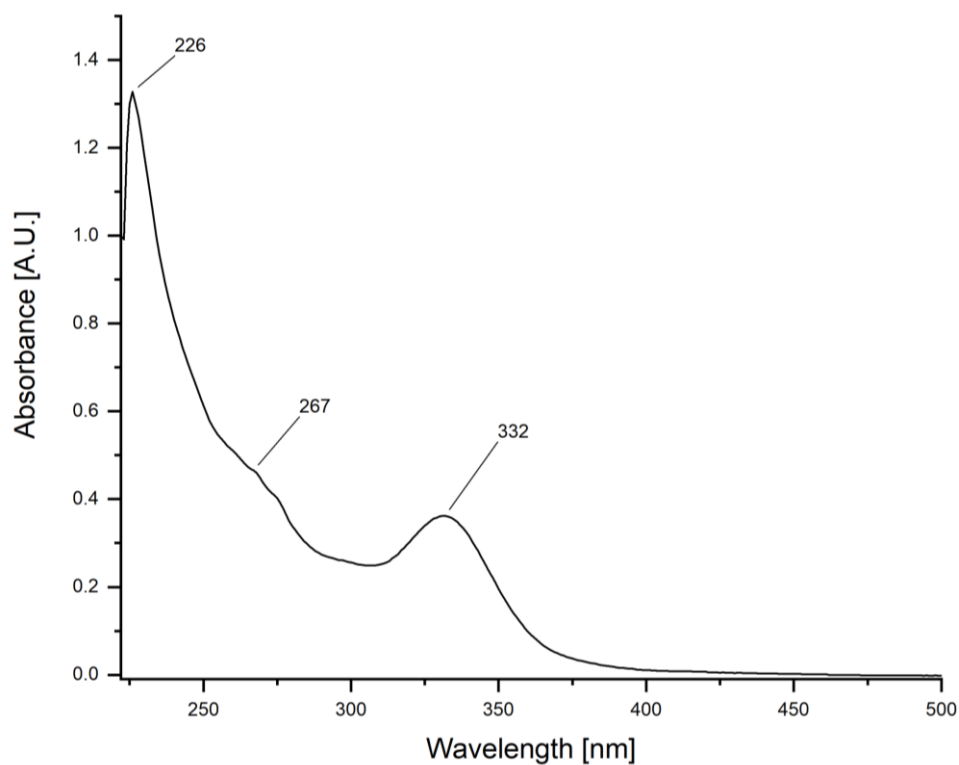
**Fig. S145.** UV-Vis spectrum of **PtRu-3** ( $3.33 \cdot 10^{-6}$  M, dichloromethane, 298 K)



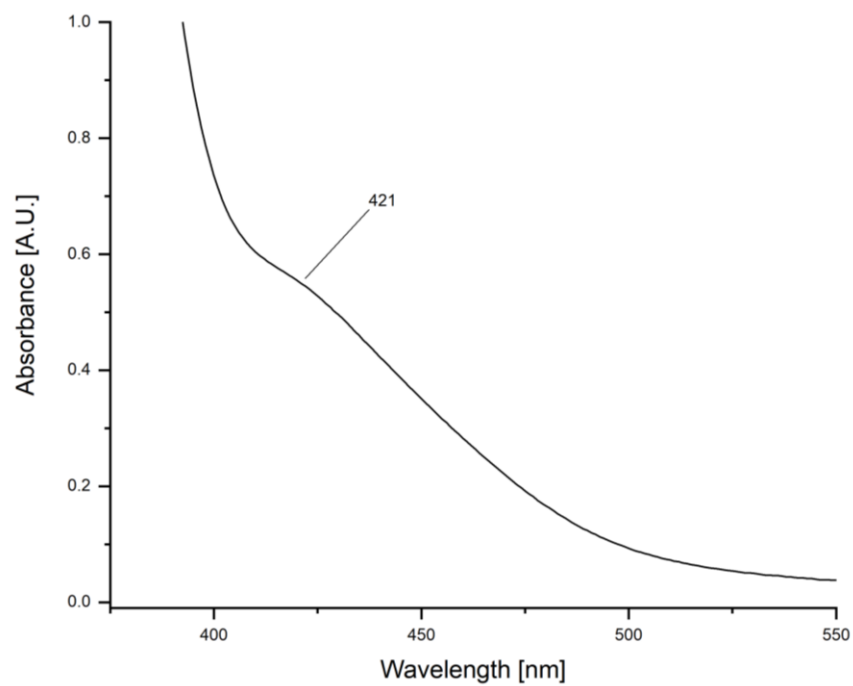
**Fig. S146.** UV-Vis spectrum of **PtRu-3** ( $4.27 \cdot 10^{-4}$  M, dichloromethane, 298 K)



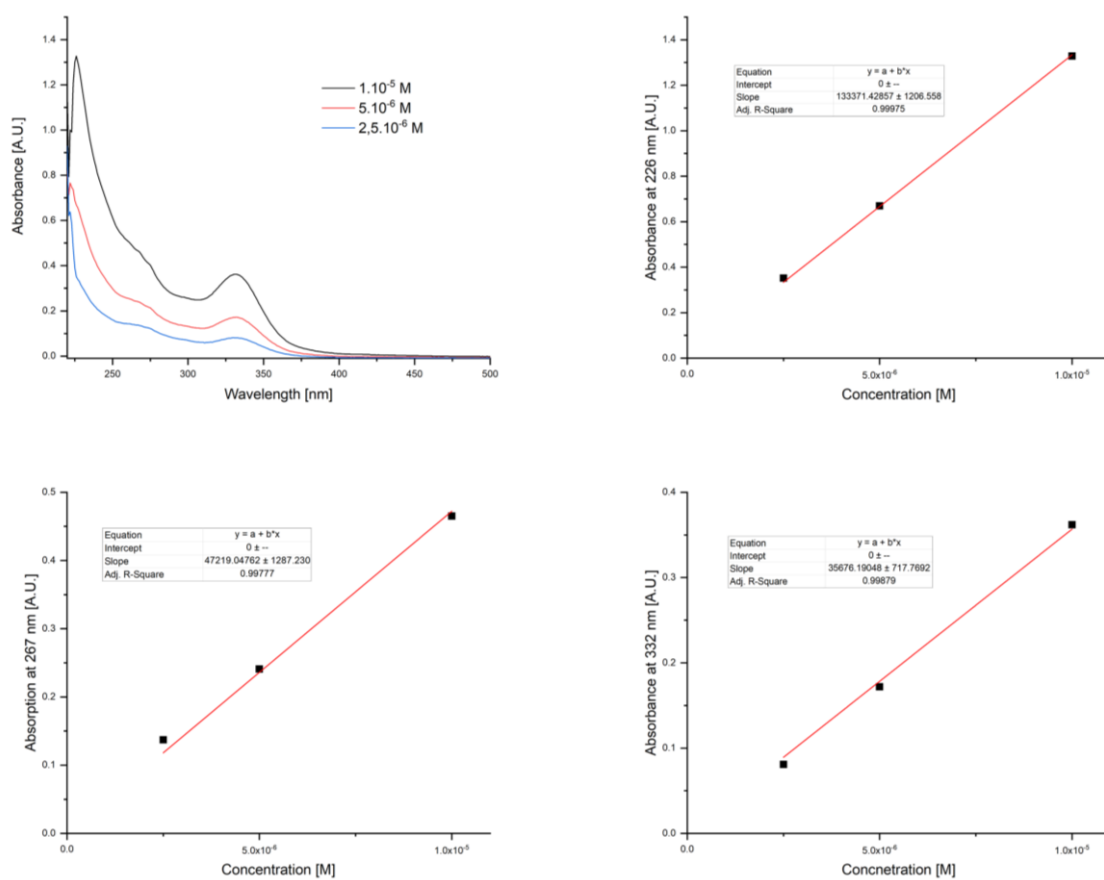
**Fig. S147.** Variable concentration UV-Vis spectra of **PtRu-3** (top), and plots of absorptions at the respective maxima for given concentrations



**Fig. S148.** UV-Vis spectrum of **PdOs-1** ( $1 \cdot 10^{-5}$  M, dichloromethane, 298 K)

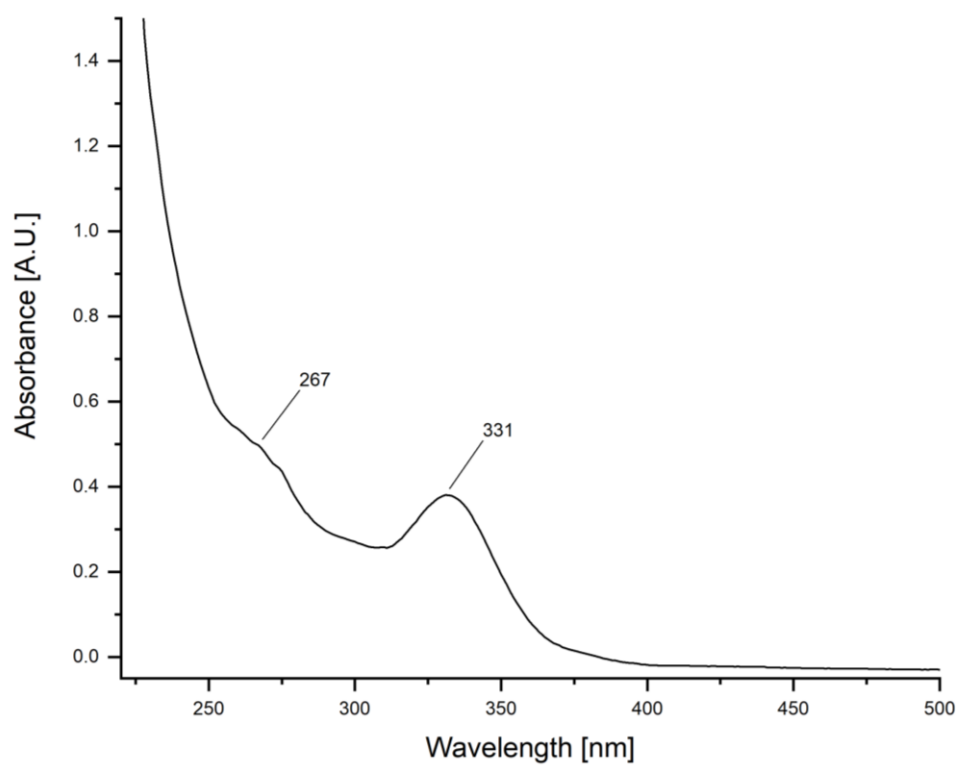


**Fig. S149.** UV-Vis spectrum of PdOs-1 (1.10<sup>-4</sup> M, dichloromethane, 298 K)

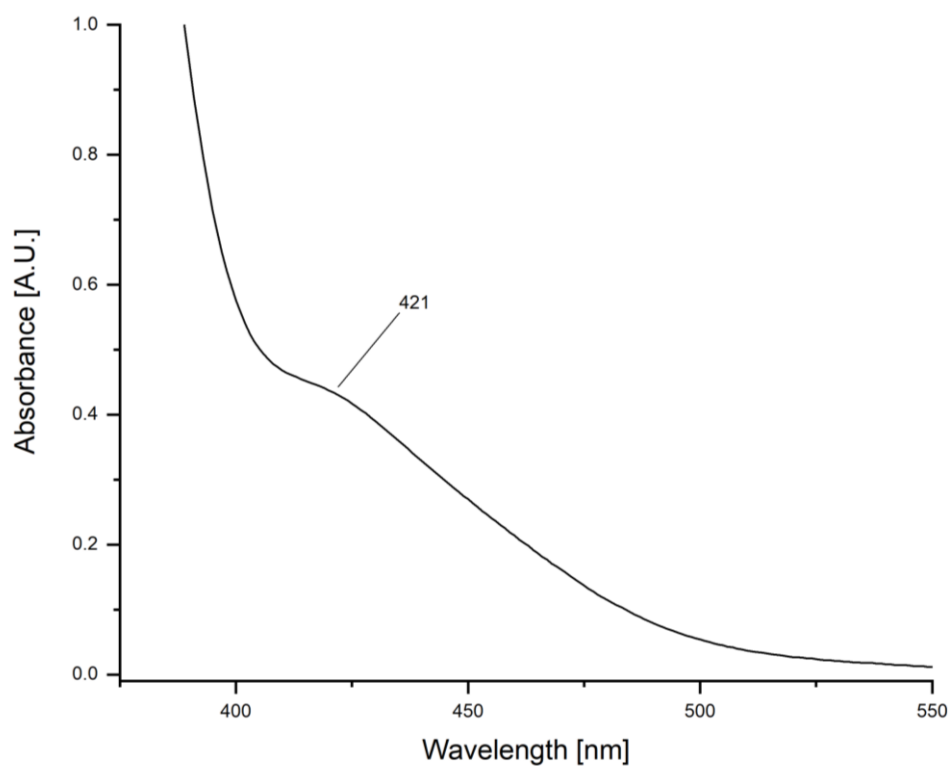


**Fig. S150.** Variable concentration UV-Vis spectra of PdOs-1 (top left), and plots of absorptions at the respective maxima for given concentrations

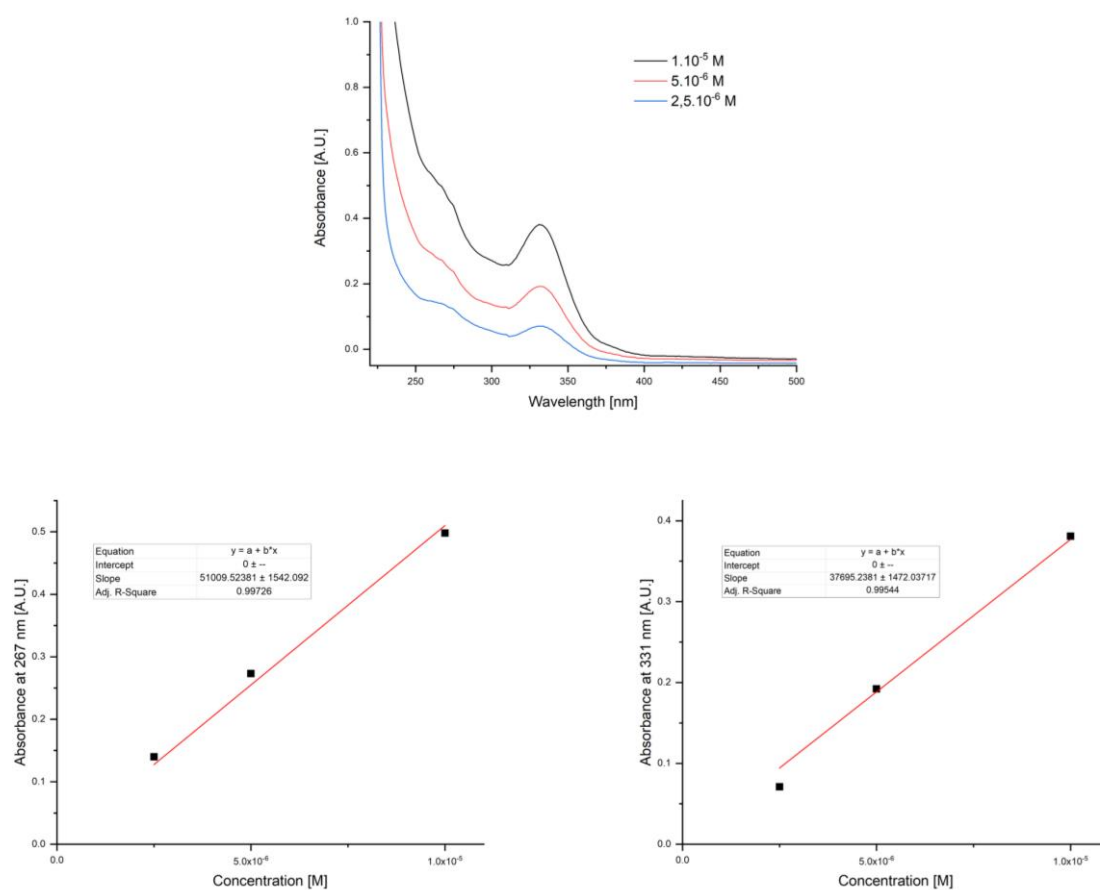




**Fig. S151.** UV-Vis spectrum of PdOs-3 (1.10<sup>-5</sup> M, dichloromethane, 298 K)

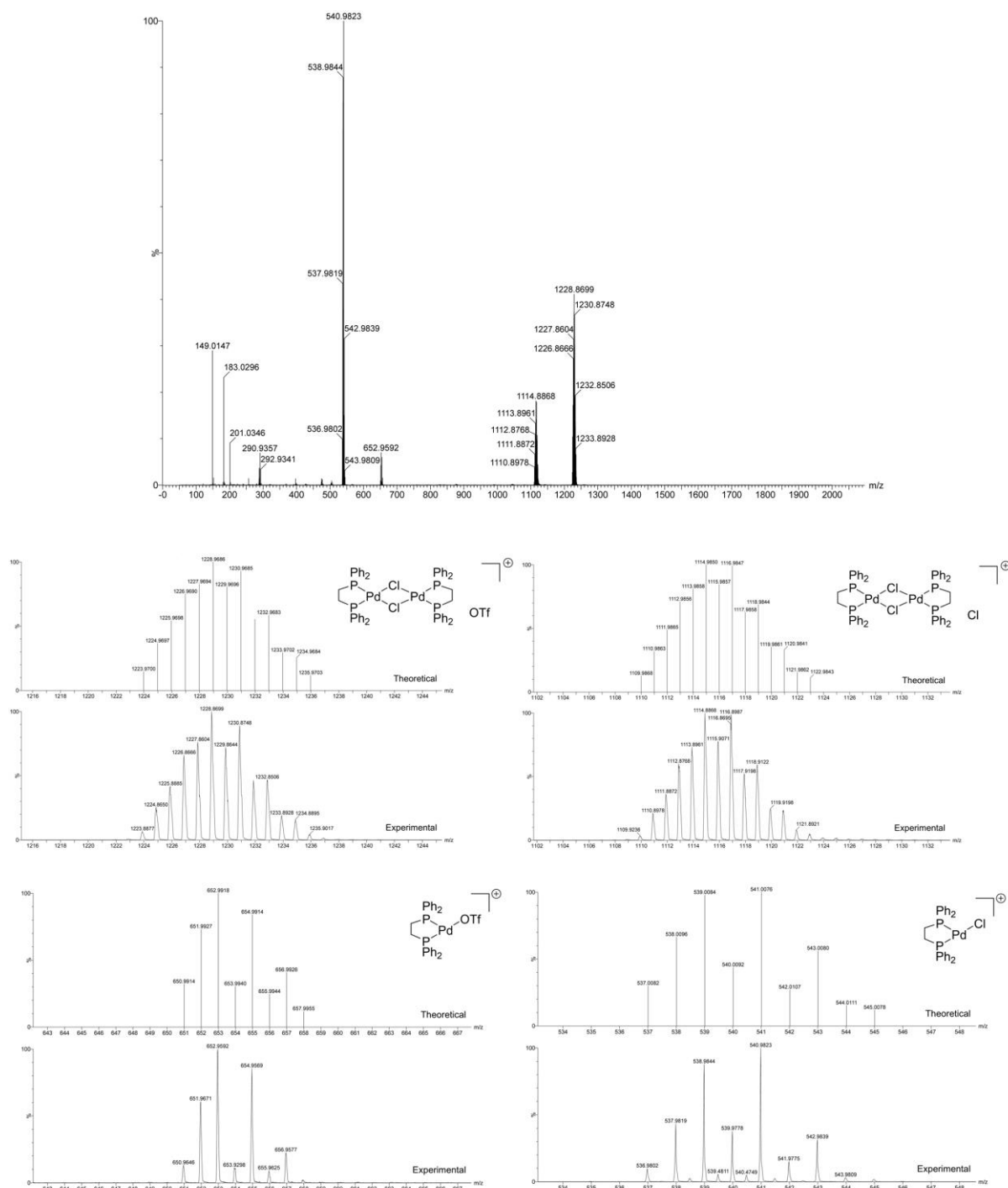


**Fig. S152.** UV-Vis spectrum of PdOs-3 (1.10<sup>-4</sup> M, dichloromethane, 298 K)

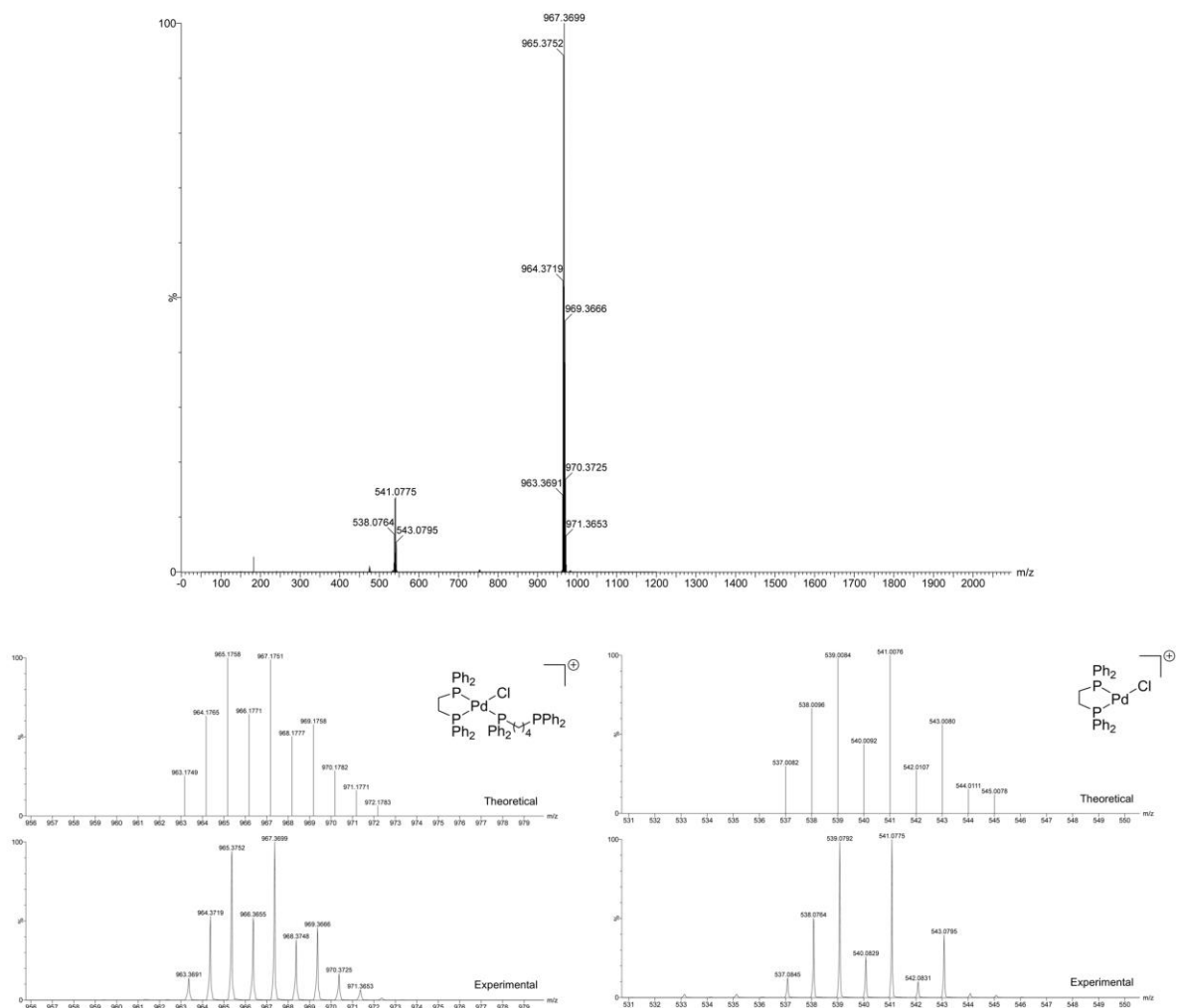


**Fig. S153.** Variable concentration UV-Vis spectra of **PdOs-3** (top), and plots of absorptions at the respective maxima for given concentrations

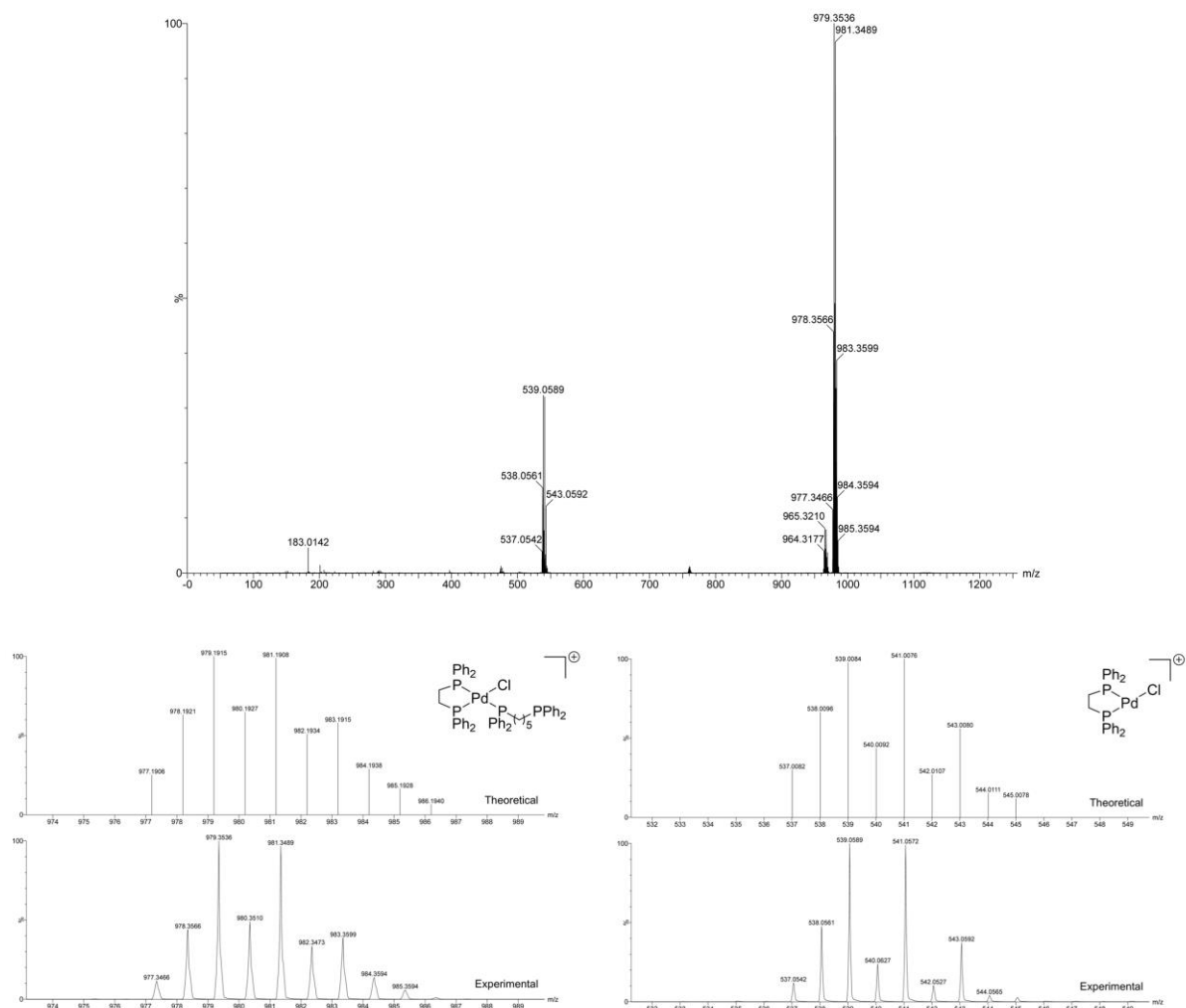
## 8. Individual mass spectra



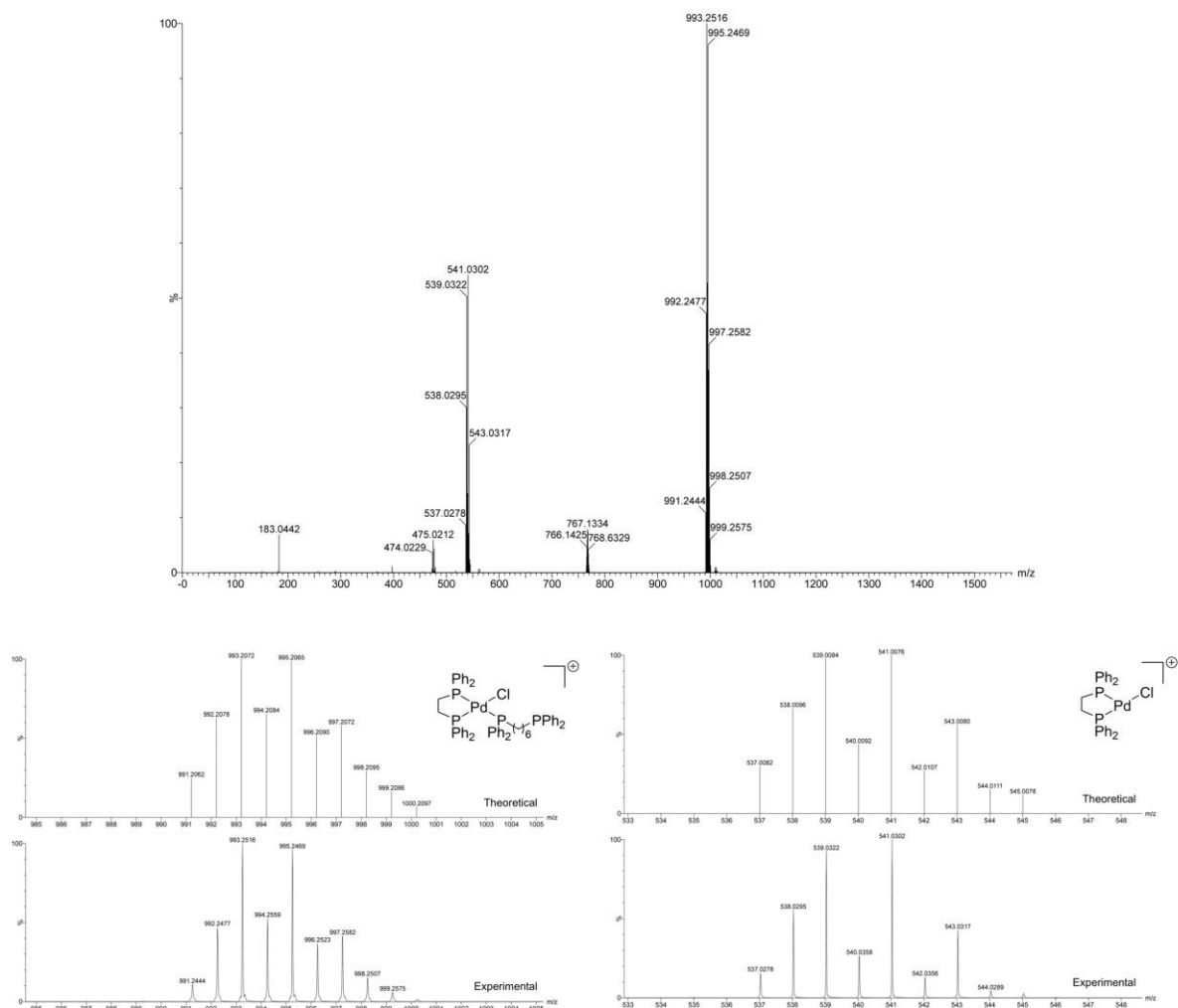
**Fig. S154.** Mass spectrum of **PdPd-0**, including relevant fragments together with their respective theoretical isotope pattern

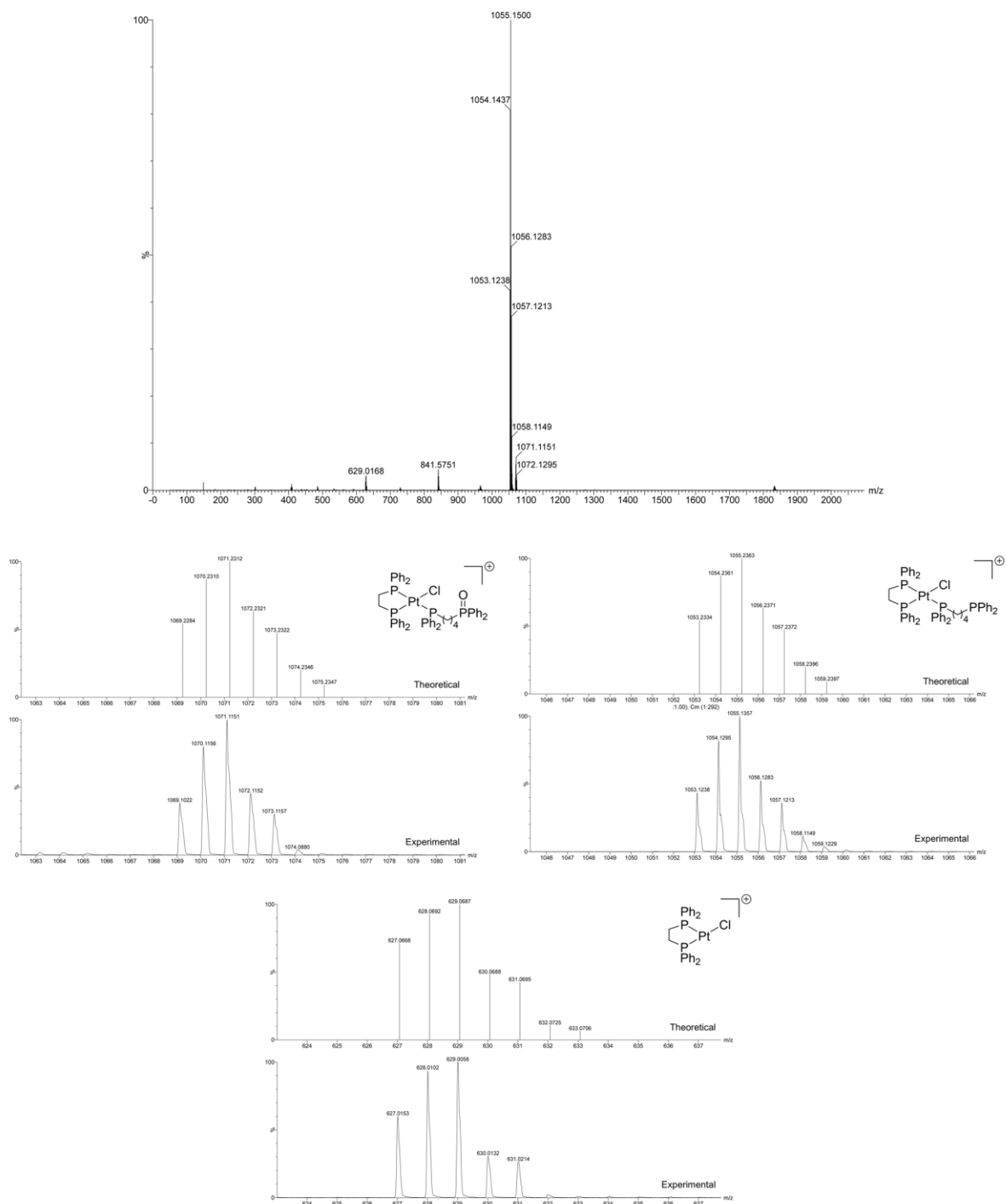


**Fig. S155.** Mass spectrum of Pd-1, including relevant fragments together with their respective theoretical isotope pattern



**Fig. S156.** Mass spectrum of Pd-2, including relevant fragments together with their respective theoretical isotope pattern



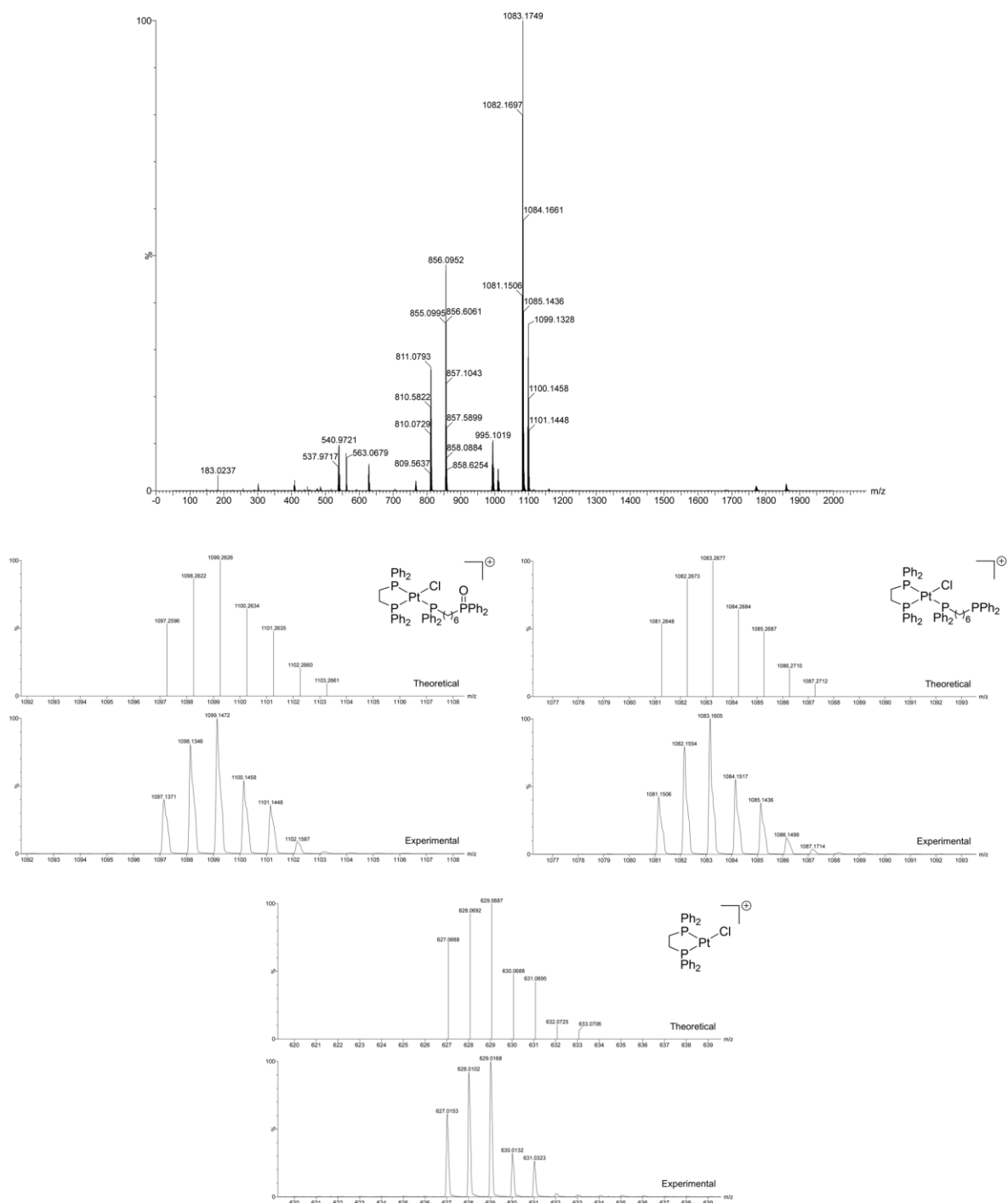


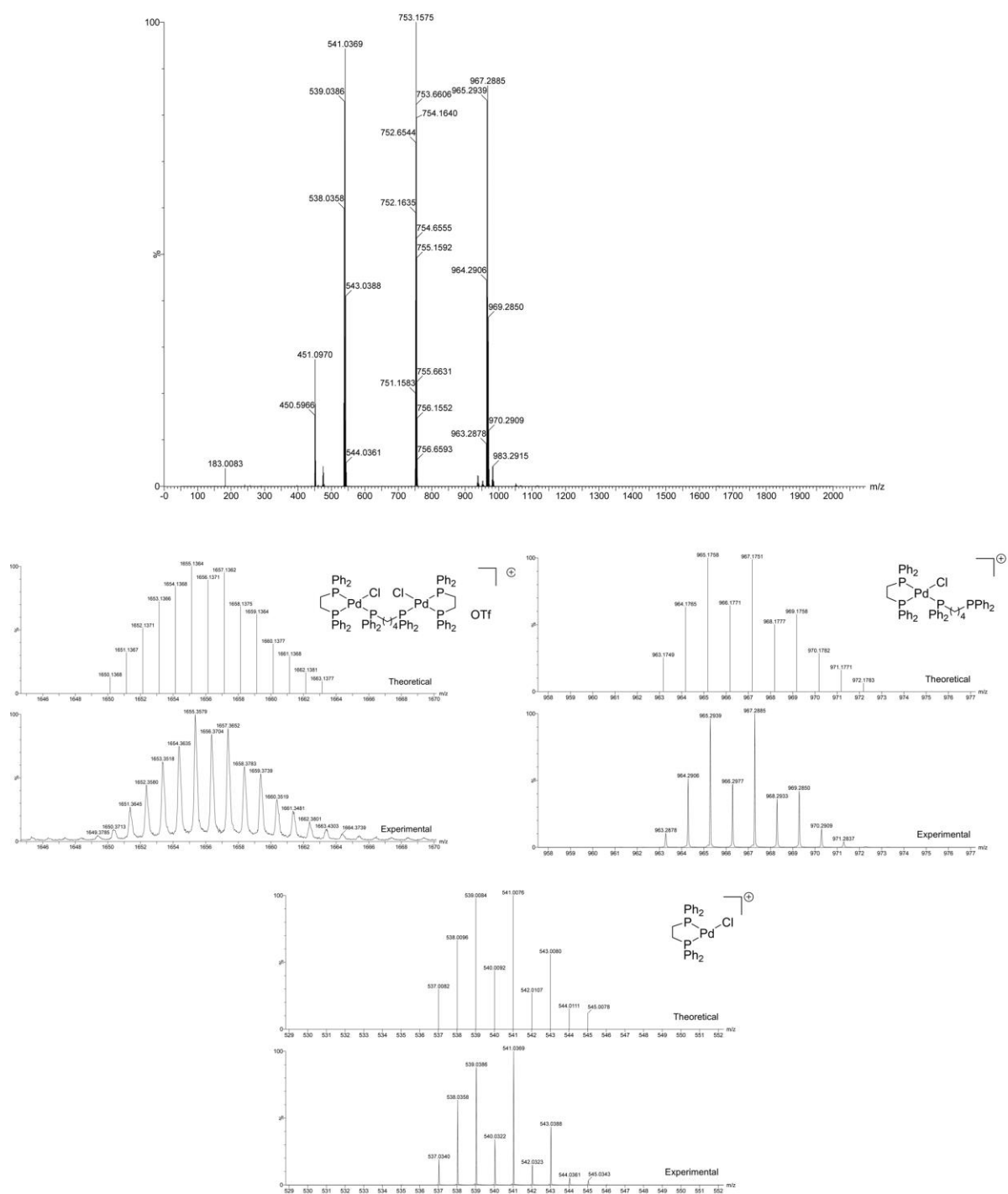
**Fig. S158.** Mass spectrum of Pt-1, including relevant fragments together with their respective theoretical isotope pattern

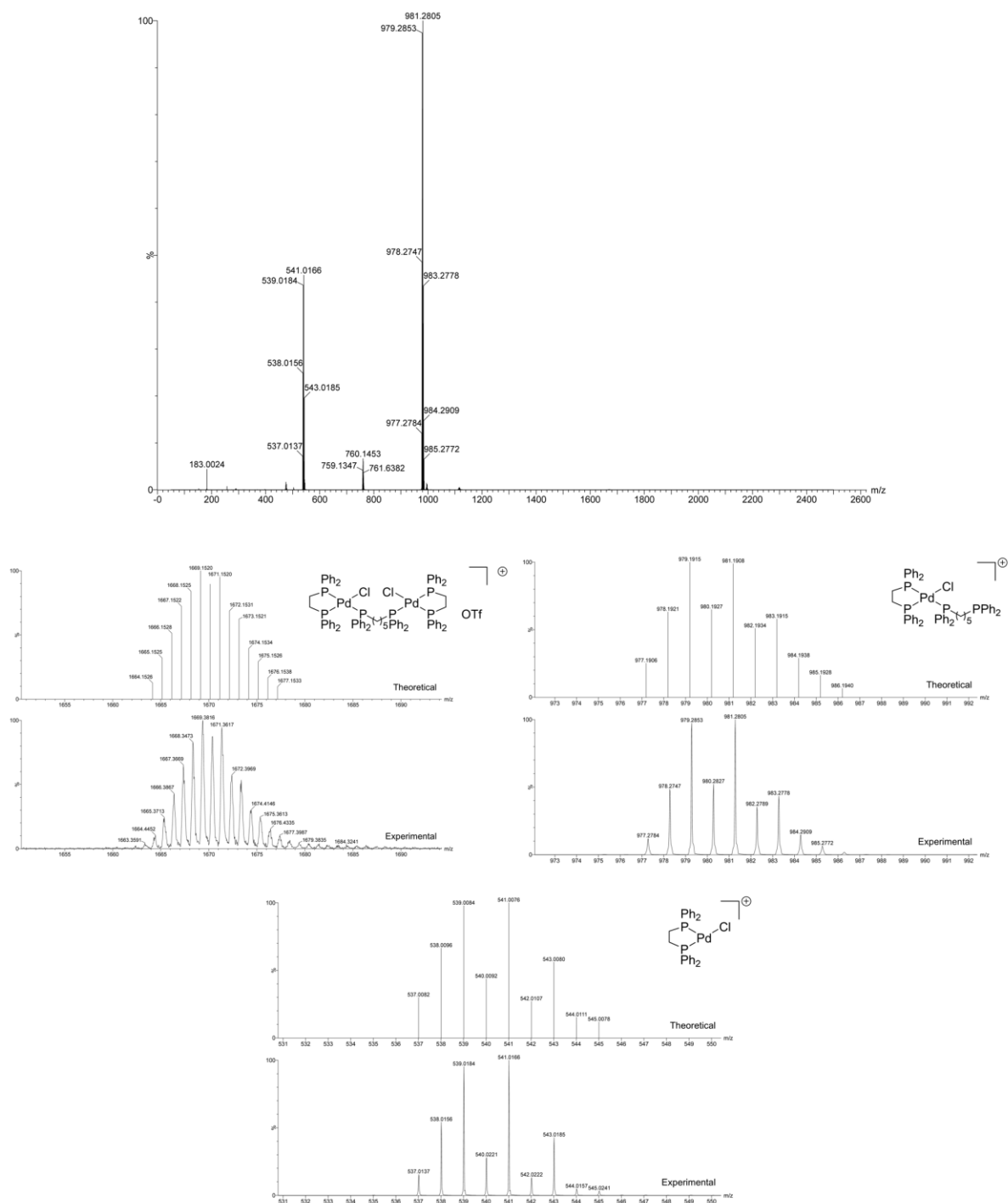


**Fig. S159.** Mass spectrum of Pt-2, including relevant fragments together with their respective theoretical isotope pattern

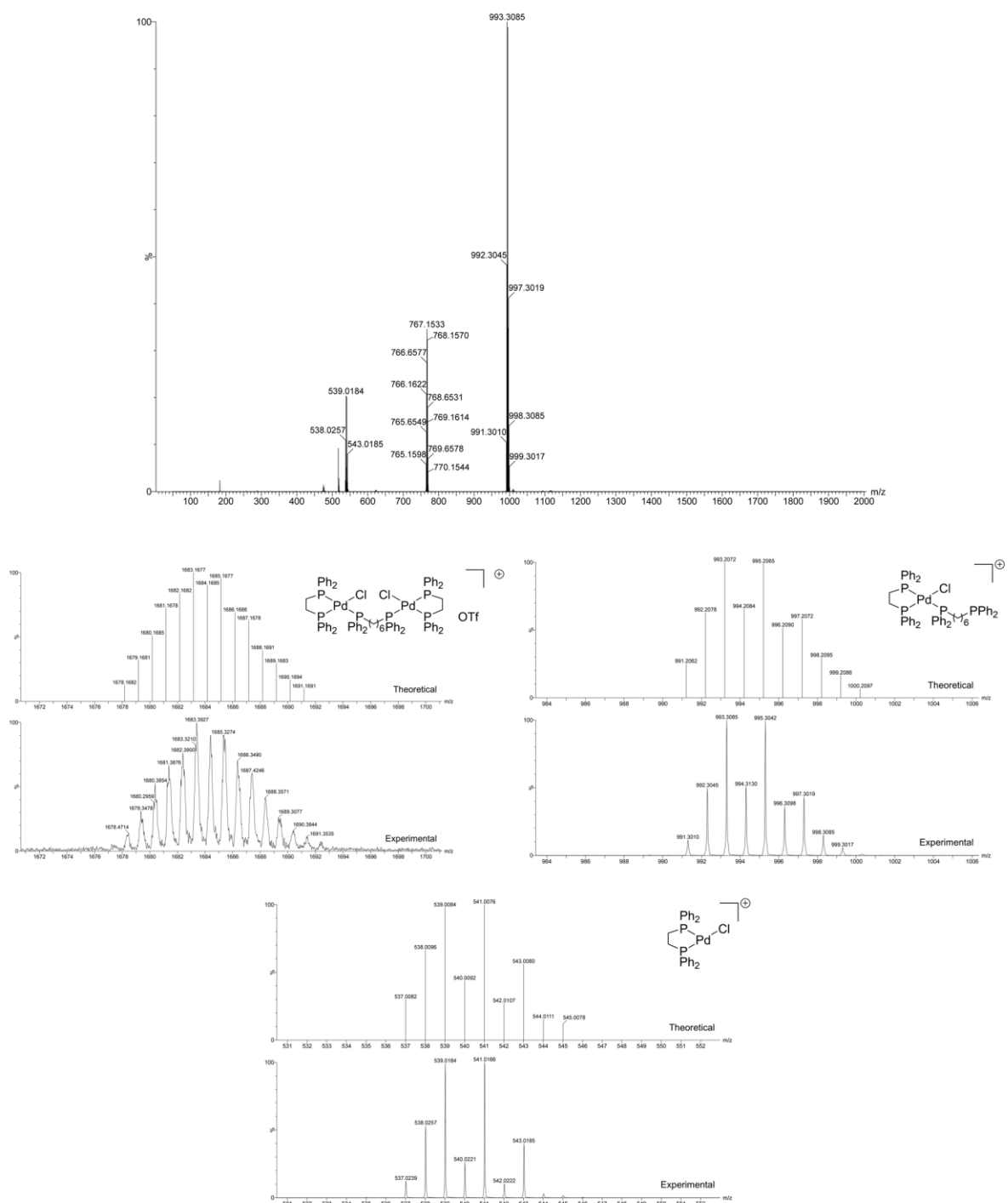




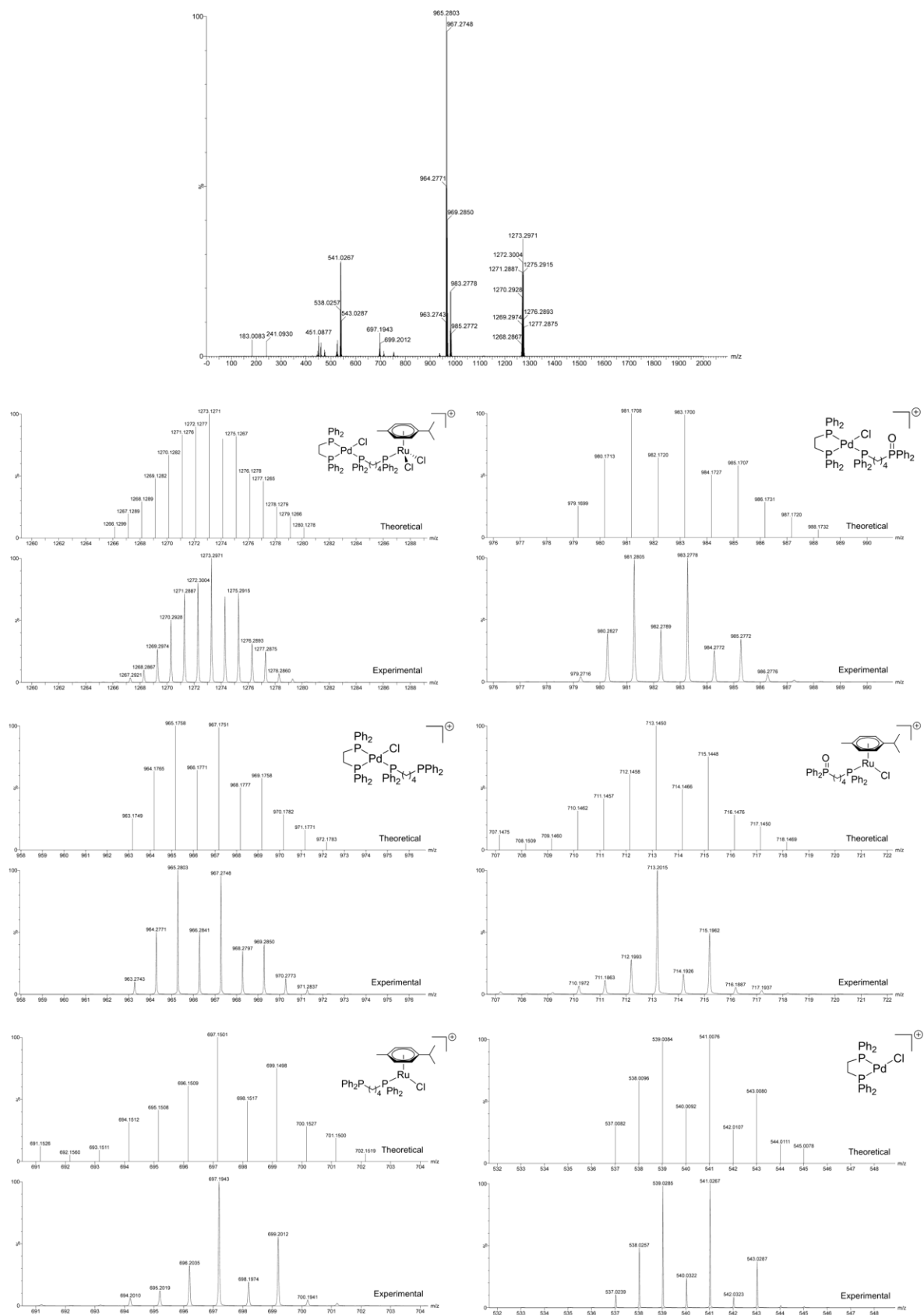




**Fig. S162.** Mass spectrum of **PdPd-2**, including relevant fragments together with their respective theoretical isotope pattern

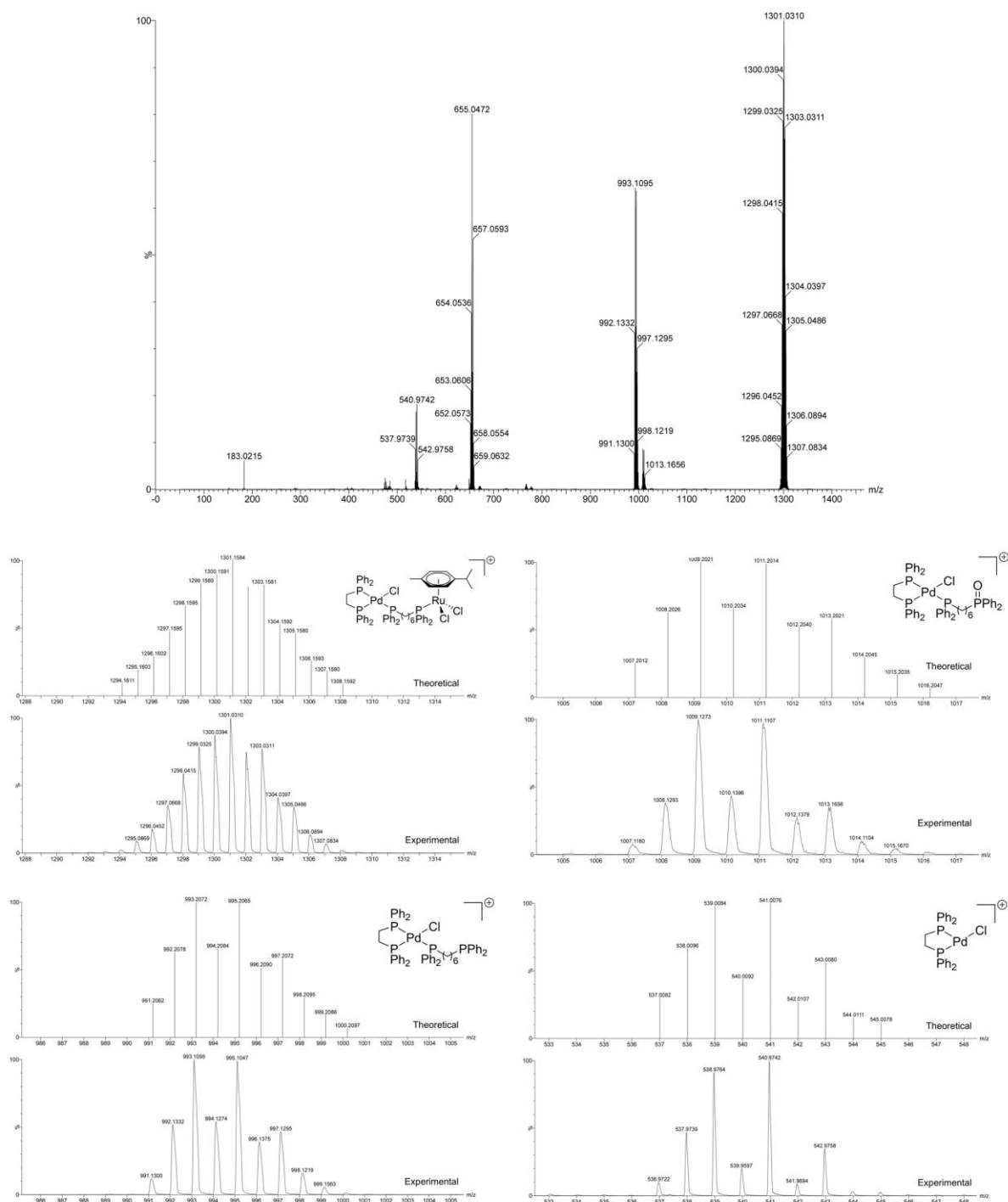


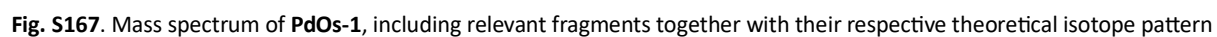
**Fig. S163.** Mass spectrum of **PdPd-3**, including relevant fragments together with their respective theoretical isotope pattern



**Fig. S164.** Mass spectrum of **PdRu-1**, including relevant fragments together with their respective theoretical isotope pattern

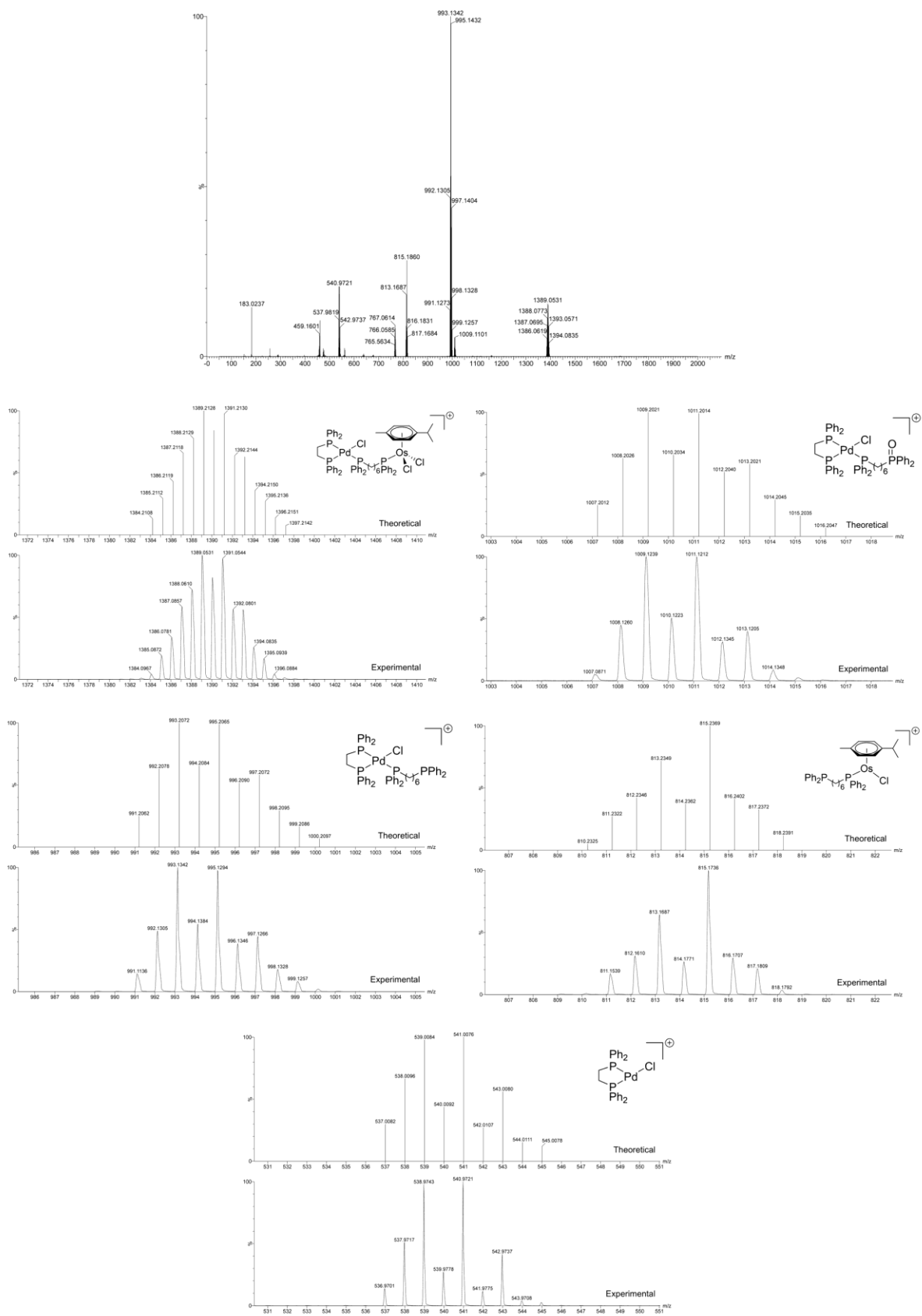




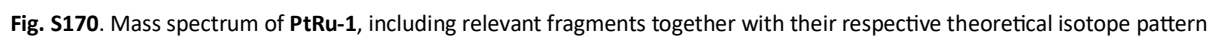


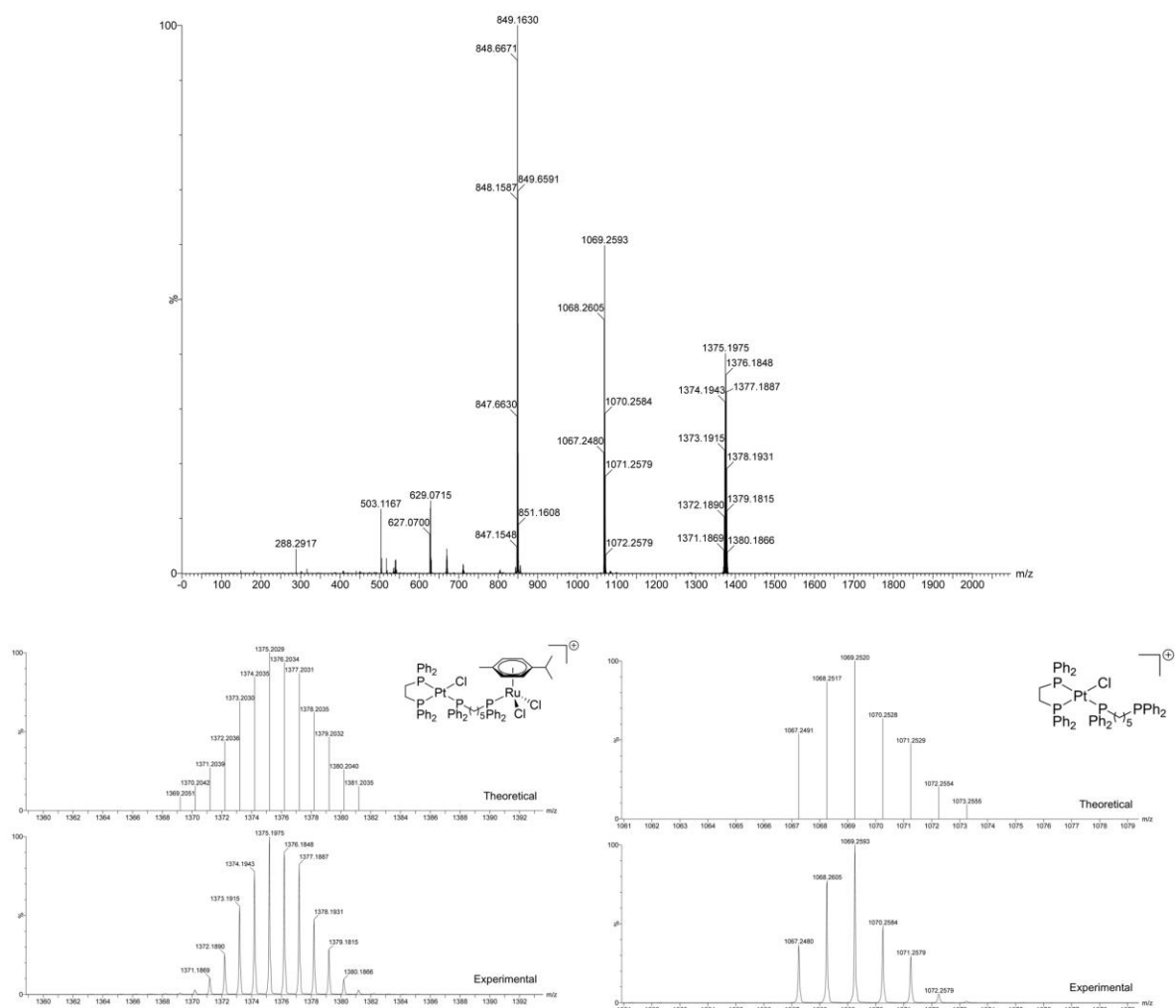




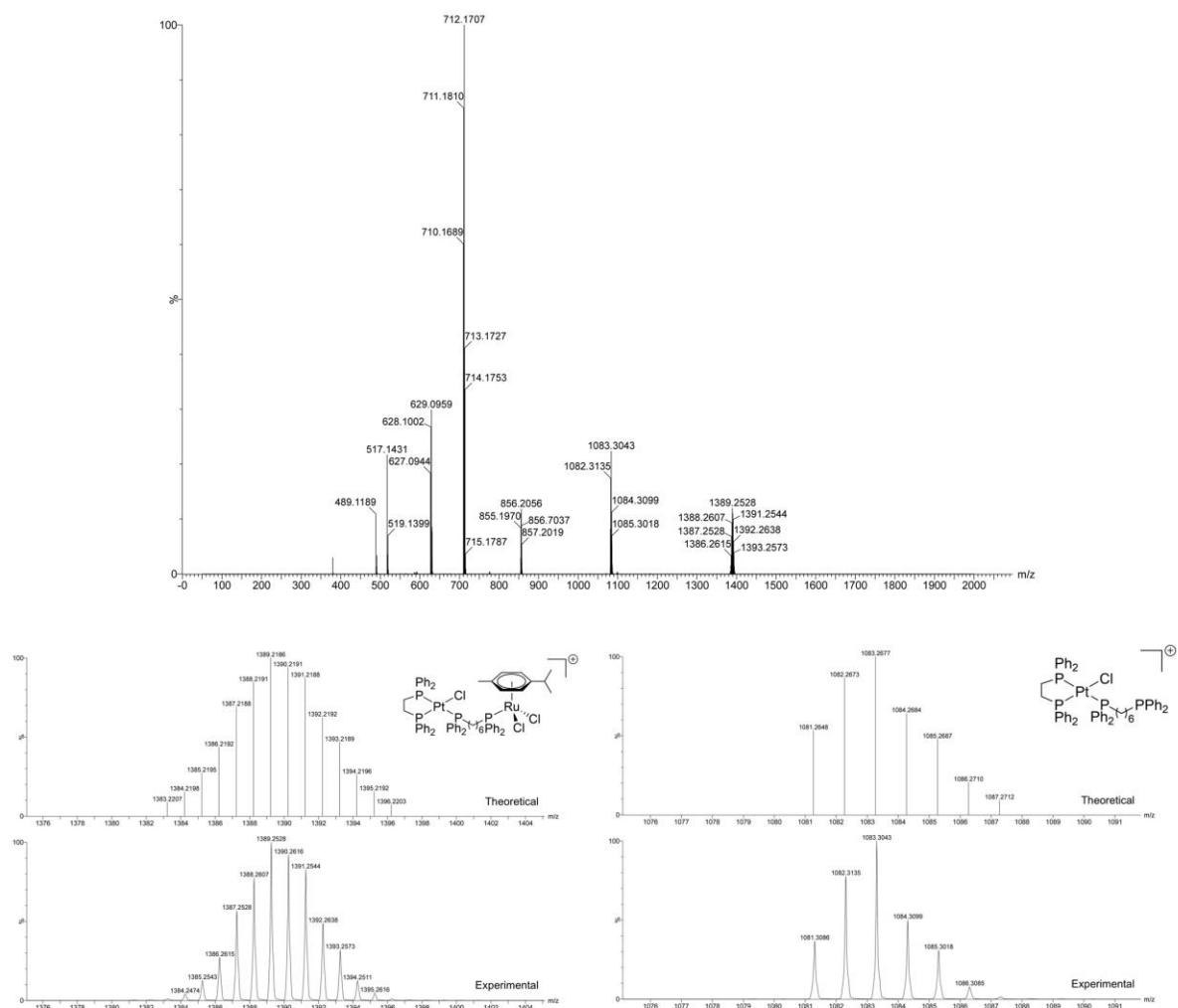


**Fig. S169.** Mass spectrum of **PdOs-3**, including relevant fragments together with their respective theoretical isotope pattern

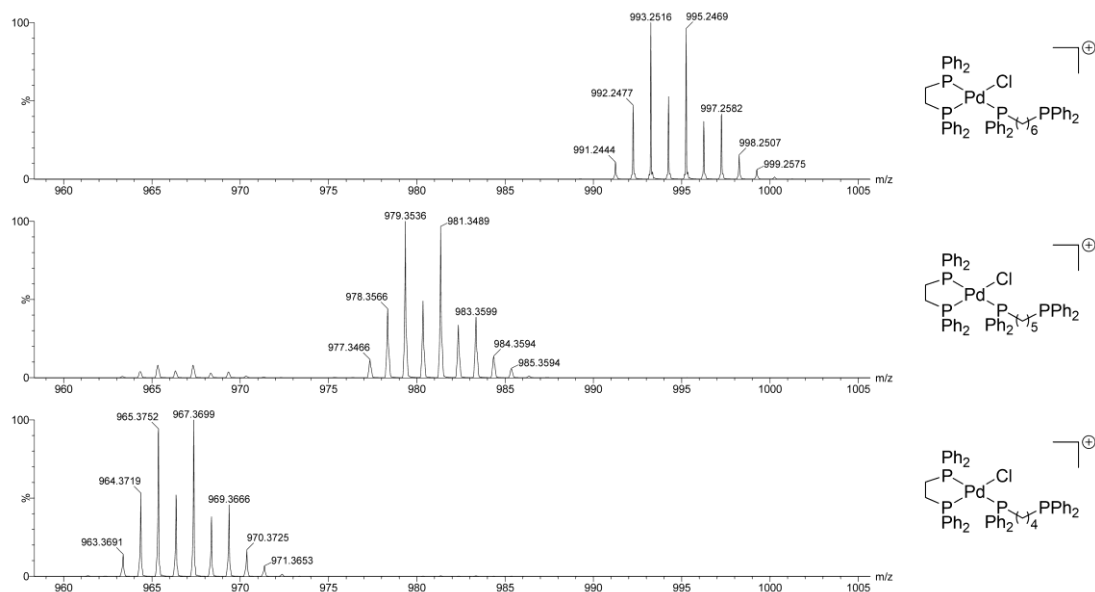




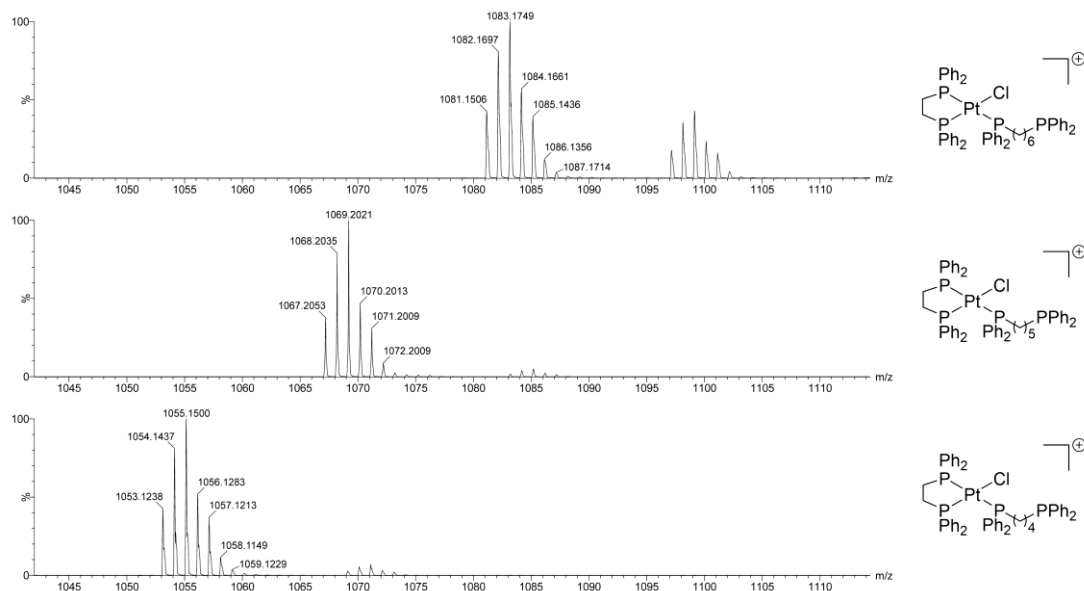
**Fig. S171.** Mass spectrum of PtRu-2, including relevant fragments together with their respective theoretical isotope pattern



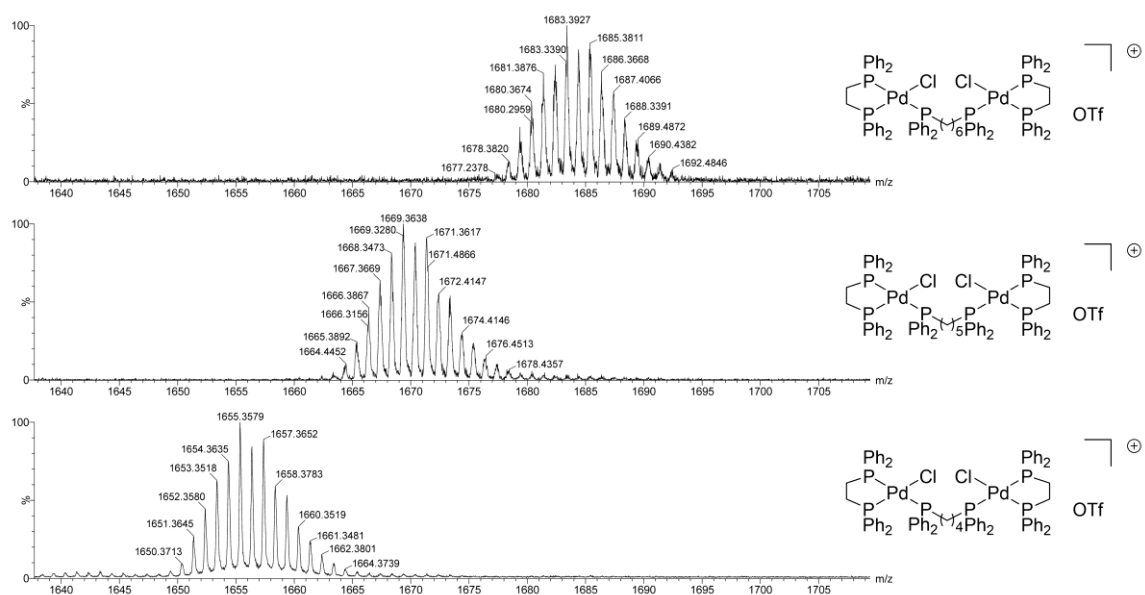
## 9. Stacked Mass Spectra for Each Homologous Series



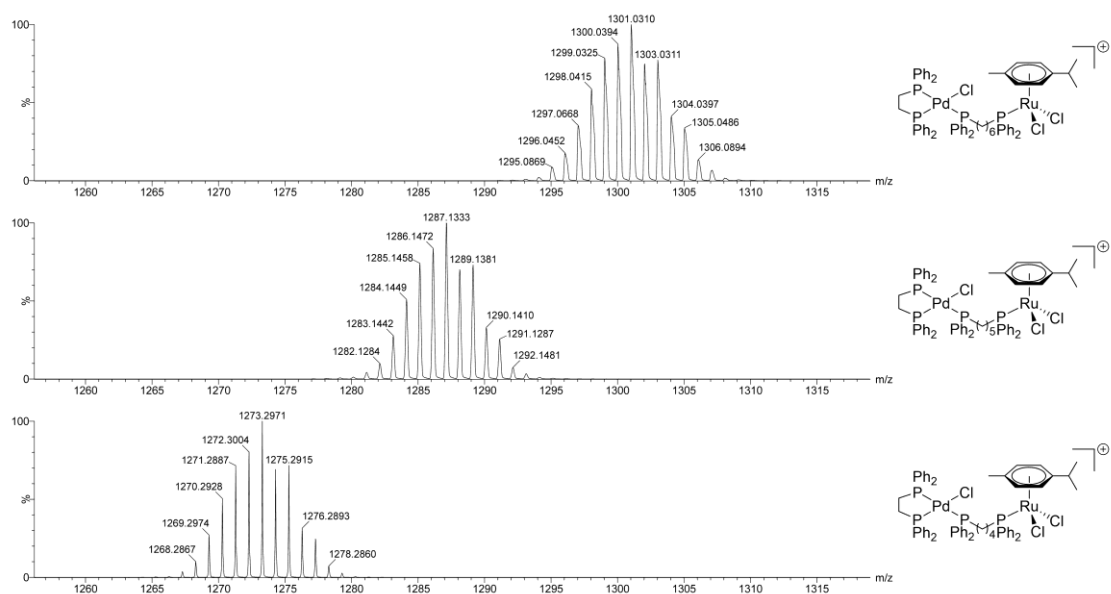
**Fig. S173.** Stacked Mass Spectra of **Pd-1** (bottom), **Pd-2** (middle) and **Pd-3** (top), zoomed in on the  $[M]^+$  peaks.



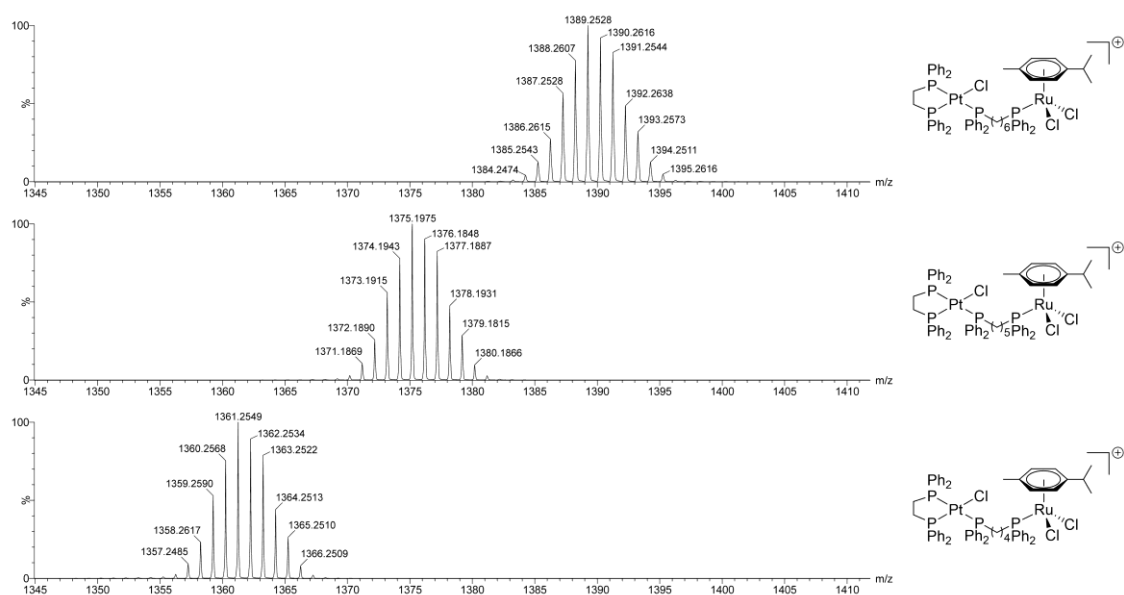
**Fig. S174.** Stacked Mass Spectra of **Pt-1** (bottom), **Pt-2** (middle) and **Pt-3** (top), zoomed in on the  $[M]^+$  peaks.



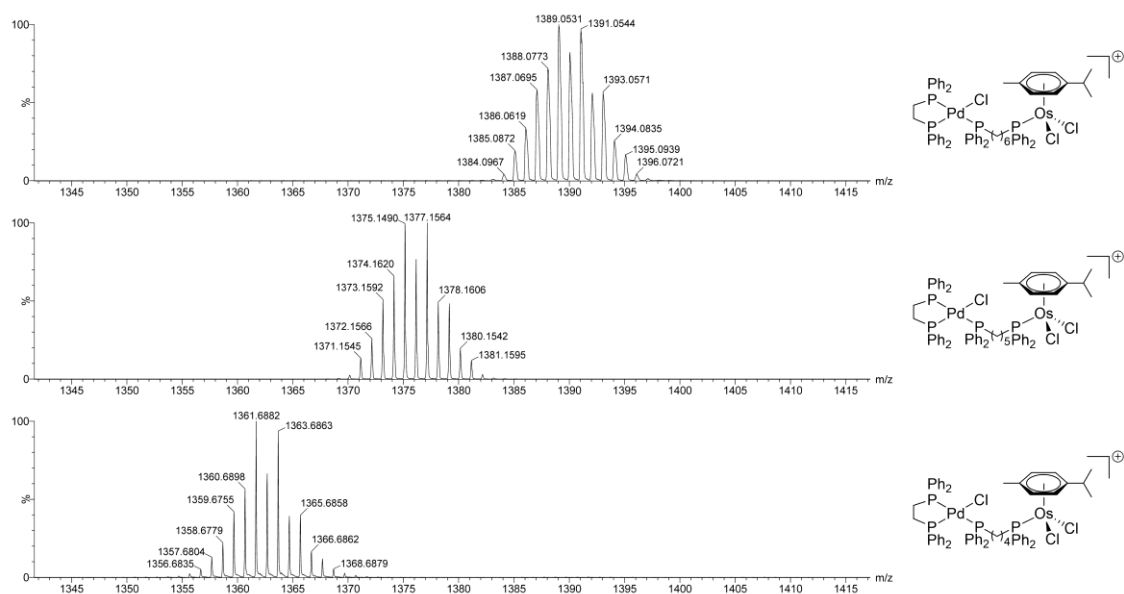
**Fig. S175.** Stacked Mass Spectra of **PdPd-1** (bottom), **PdPd-2** (middle) and **PdPd-3** (top), zoomed in on the  $[M]^+$  peaks.



**Fig. S176.** Stacked Mass Spectra of **PdRu-1** (bottom), **PdRu-2** (middle) and **PdRu-3** (top), zoomed in on the  $[M]^+$  peaks.



**Fig. S177.** Stacked Mass Spectra of **PtRu-1** (bottom), **PtRu-2** (middle) and **PtRu-3** (top), zoomed in on the  $[M]^+$  peaks.



**Fig. S178.** Stacked Mass Spectra of **PdOs-1** (bottom), **PdOs-2** (middle) and **PdOs-3** (top), zoomed in on the  $[M]^+$  peaks.



## 10. Cell viability studies

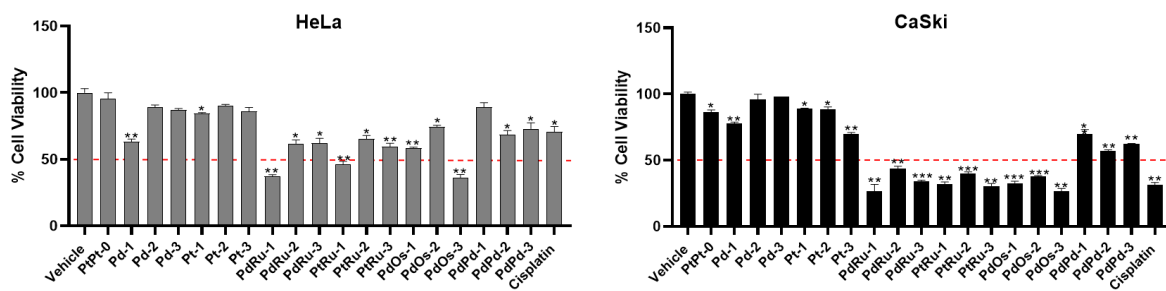


Fig. S179. Single dose treatments at 10µM in cervical cancer cell lines

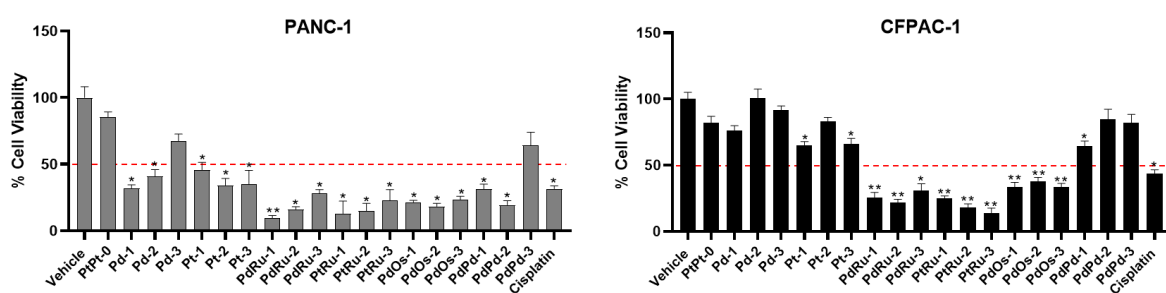


Fig. S180. Single dose treatments at 10µM in pancreatic cancer cell lines

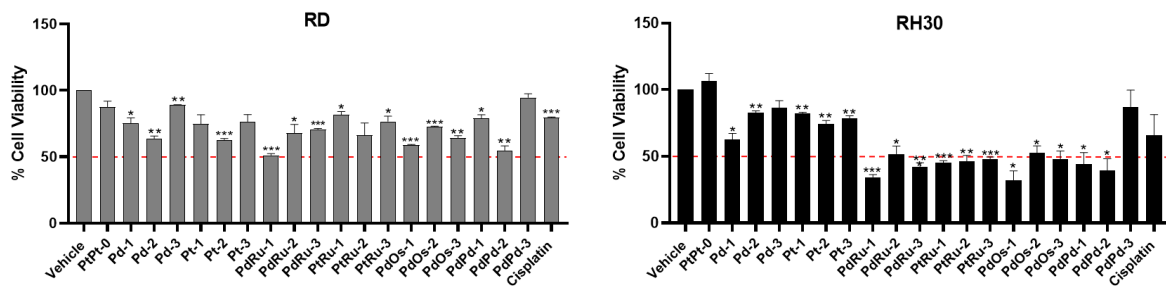


Fig. S181. Single dose treatments at 10µM in rhabdomyosarcoma cell lines

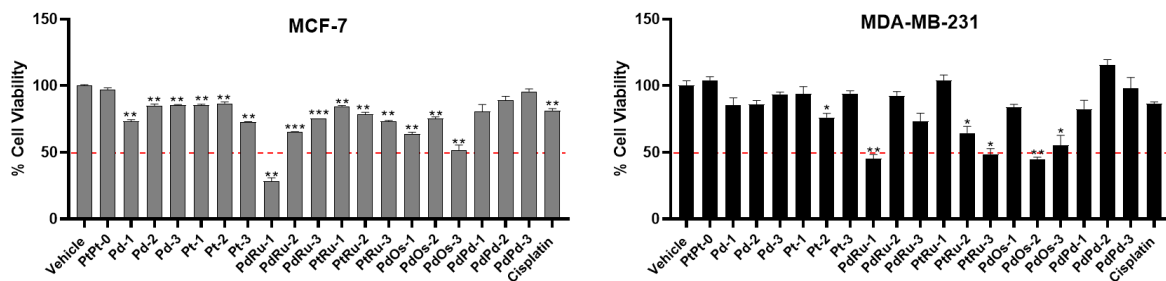
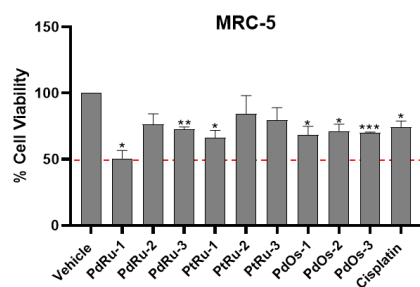
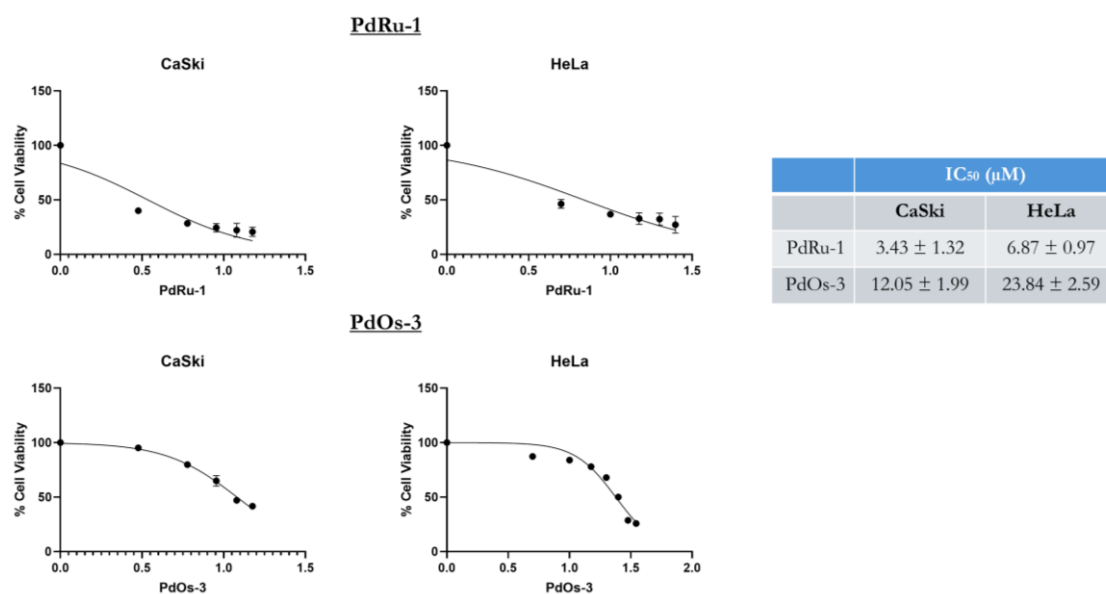


Fig. S182. Single dose treatments at 10µM in breast cancer cell lines

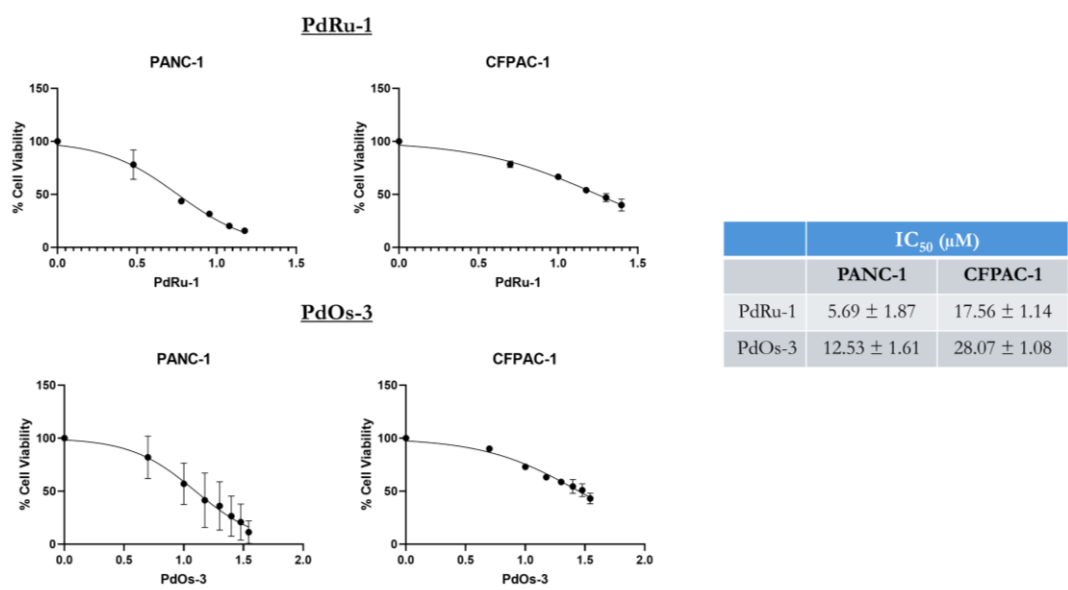


**Fig. S183.** Single dose treatments at 10 $\mu$ M in non-malignant cell line MRC-5

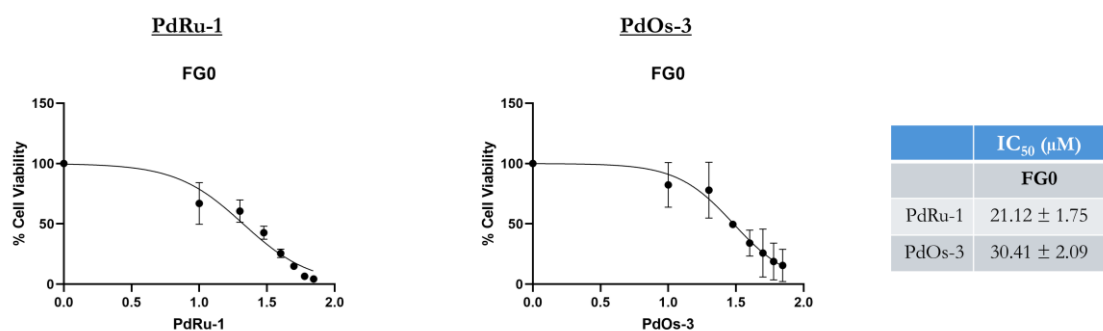
## 11. IC<sub>50</sub> plots



**Fig. S184.** Concentration plots on cervical cancer cell lines for **PdRu-1** (top) and **PdOs-3** (bottom), and derived IC<sub>50</sub> values (right)

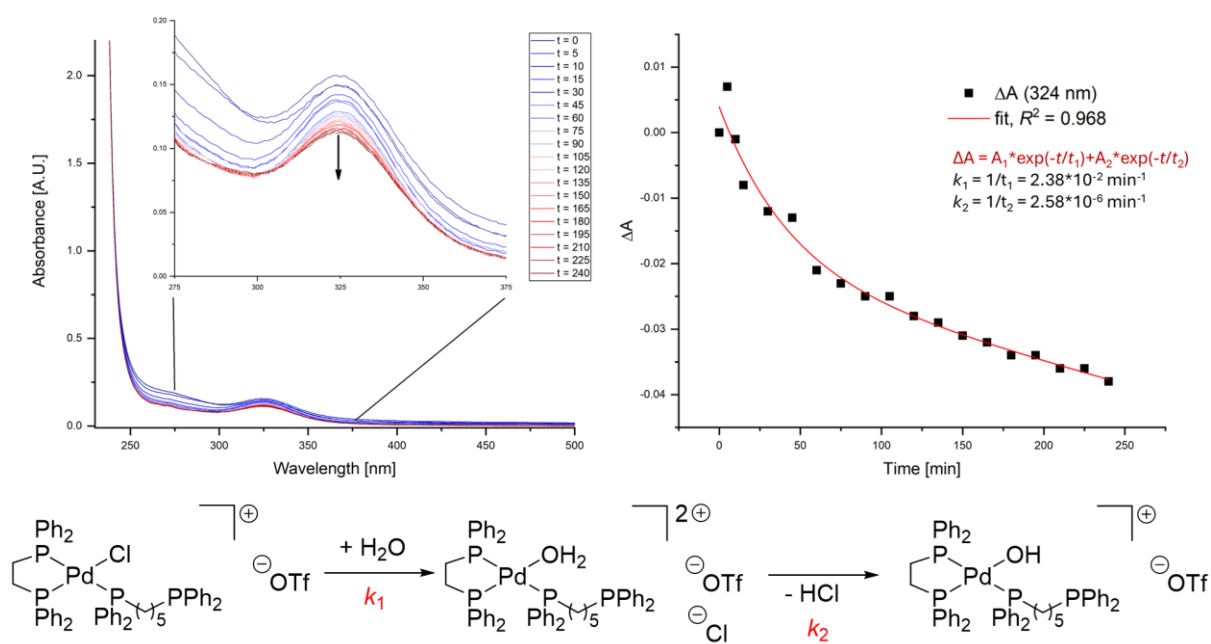


**Fig. S185.** Concentration plots on pancreatic cancer cell lines for **PdRu-1** (top) and **PdOs-3** (bottom), and derived IC<sub>50</sub> values (right)

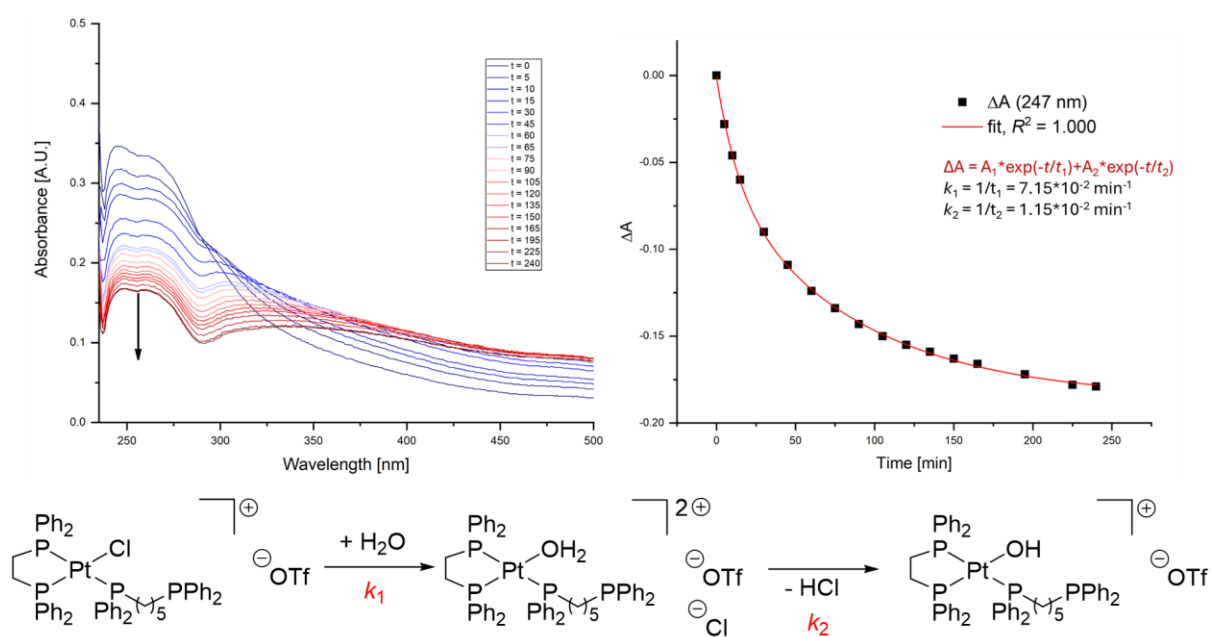


**Fig. S186.** Concentration plots on healthy cell line FG0 for **PdRu-1** (left) and **PdOs-3** (middle), and derived IC<sub>50</sub> values (right)

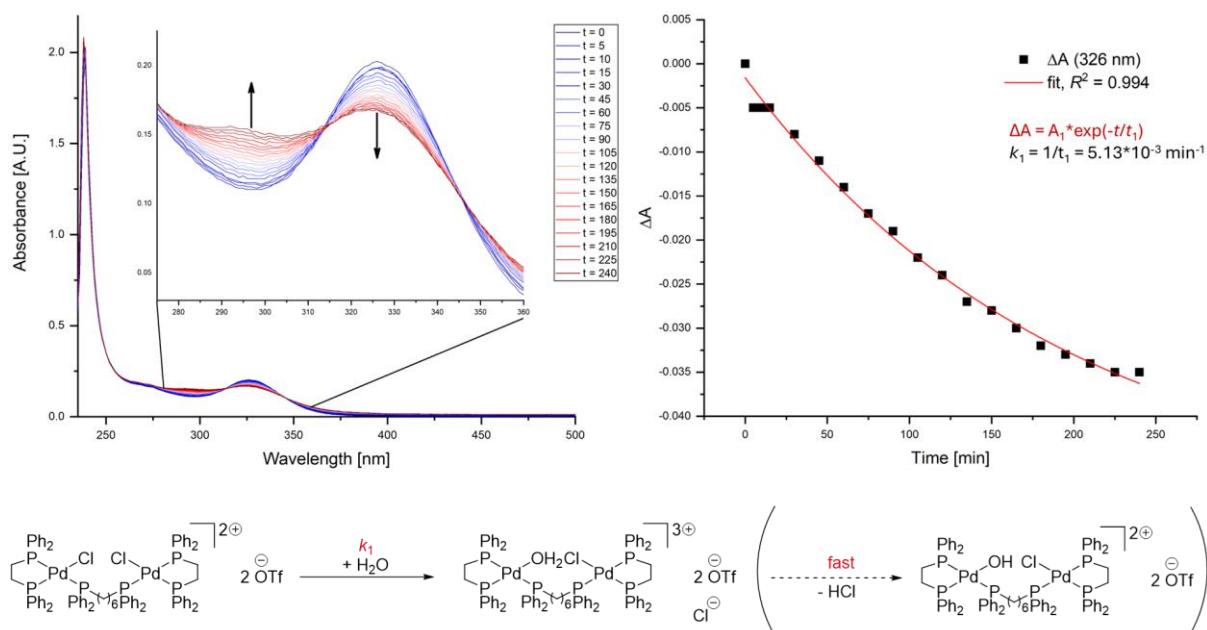
## 12. Aquations studies



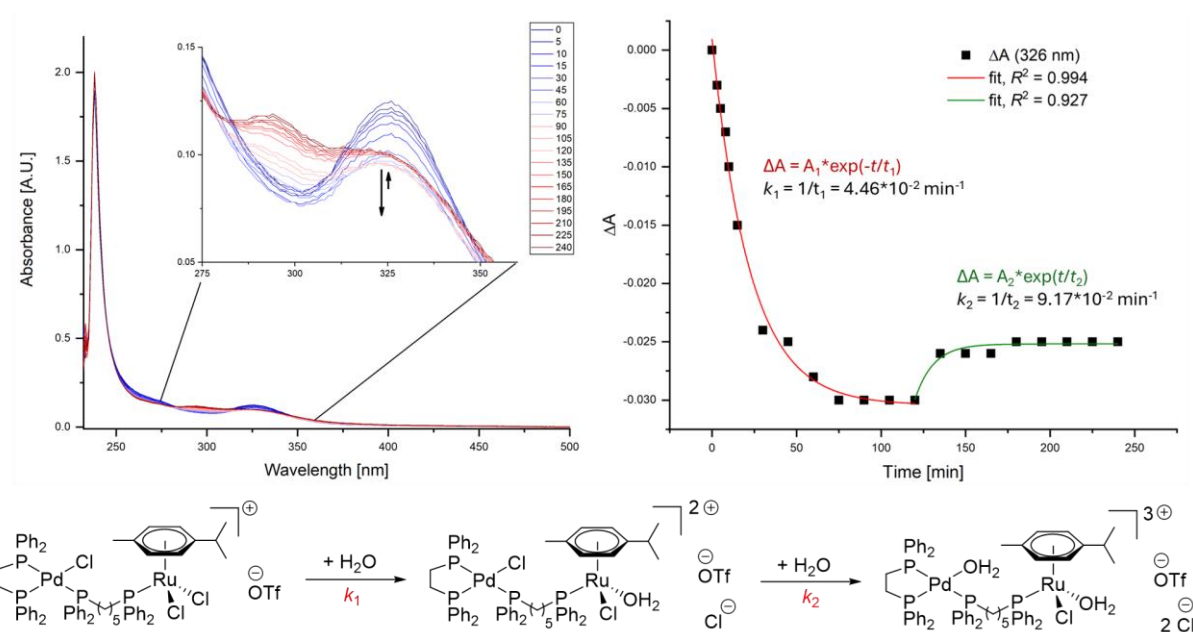
**Fig. S187.** UV-Vis spectral changes over time of **Pd-2** ( $C = 5 \cdot 10^{-6} \text{ M}$ ) in a 90:10 PBS buffer (pH = 7.45):DMSO solution at 37°C (top left), plot of the change in absorbance over time at 324 nm (top right), and hypothesised mechanism (bottom).



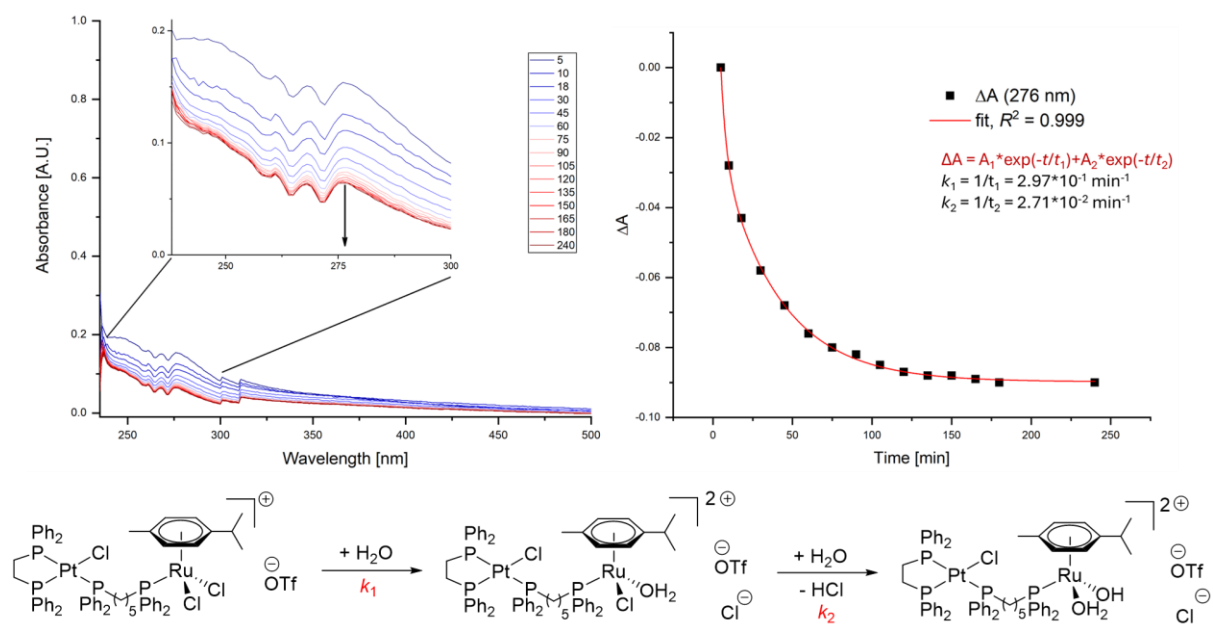
**Fig. S188.** UV-Vis spectral changes over time of **Pt-2** ( $C = 5 \cdot 10^{-6} \text{ M}$ ) in a 90:10 PBS buffer (pH = 7.45):DMSO solution at 37°C (top left), plot of the change in absorbance over time at 247 nm (top right), and hypothesised mechanism (bottom).



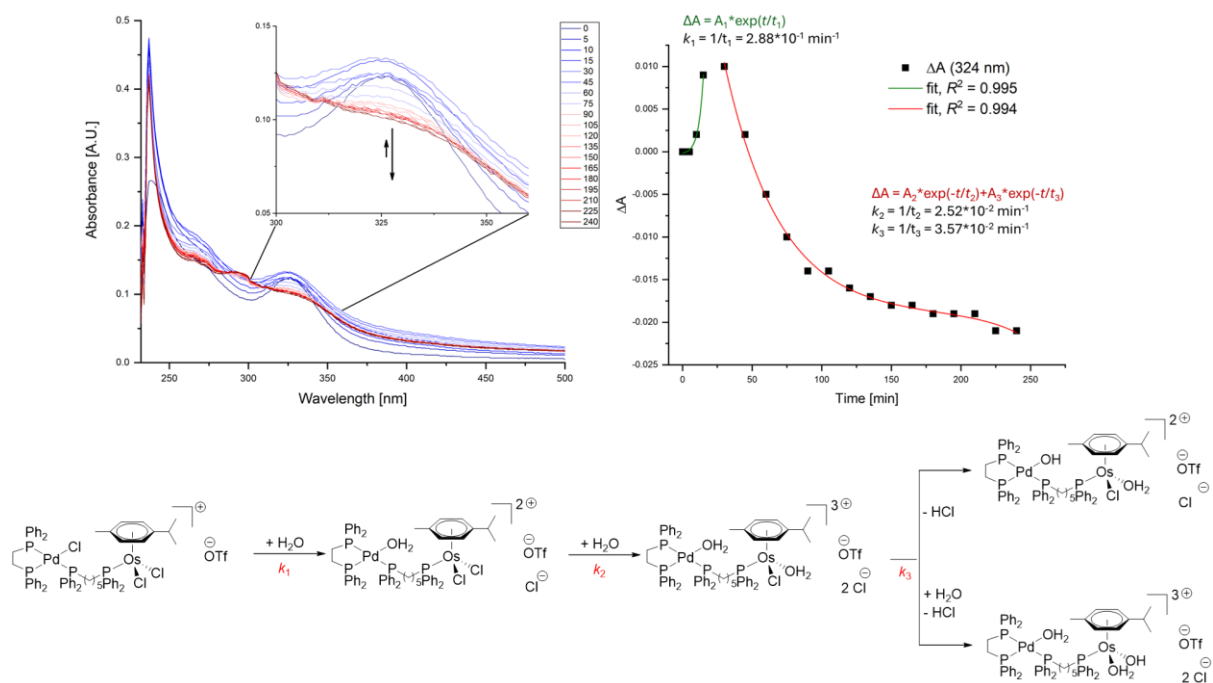
**Fig. S189.** UV-Vis spectral changes over time of **PdPd-3** ( $C = 5.10^{-6}$  M) in a 90:10 PBS buffer (pH = 7.45):DMSO solution at 37°C (top left), plot of the change in absorbance over time at 326 nm (top right), and hypothesised mechanism (bottom).



**Fig. S190.** UV-Vis spectral changes over time of **PdRu-2** ( $C = 5.10^{-6}$  M) in a 90:10 PBS buffer (pH = 7.45):DMSO solution at 37°C (top left), plot of the change in absorbance over time at 326 nm (top right), and hypothesised mechanism (bottom).

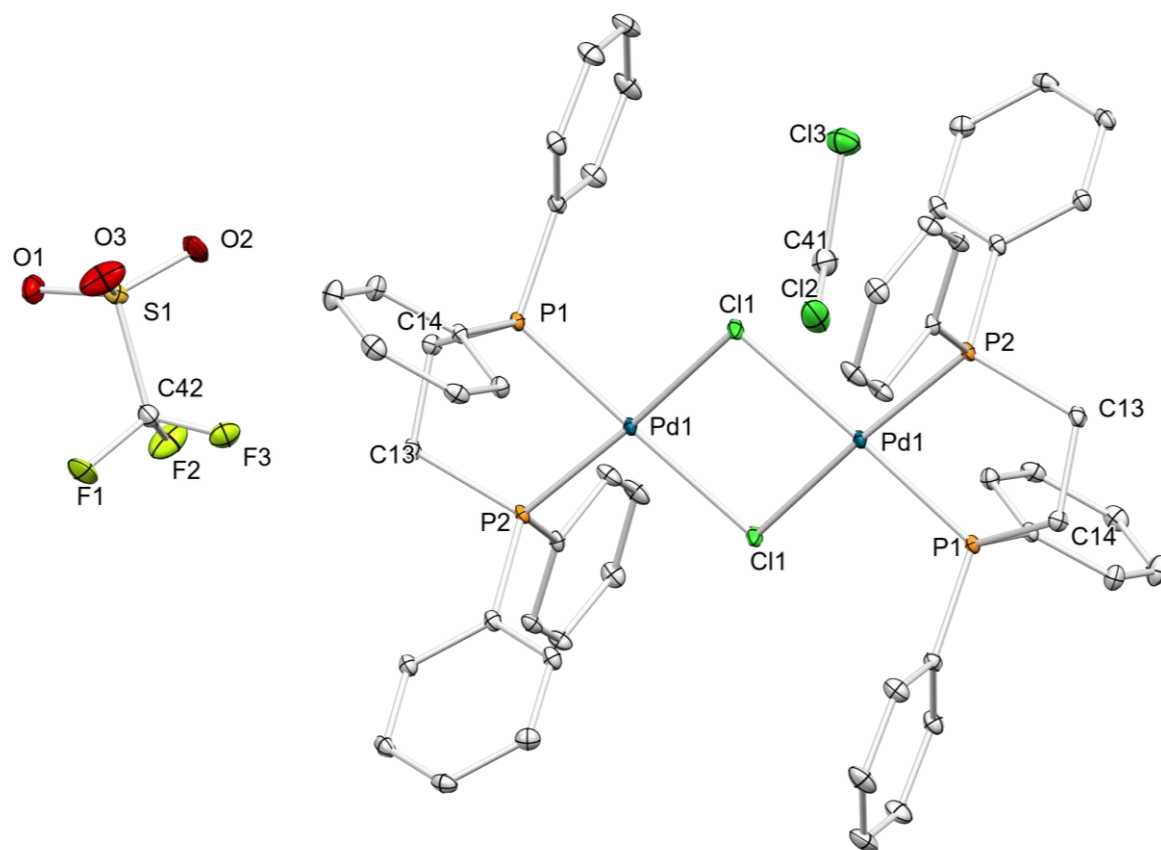


**Fig. S191.** UV-Vis spectral changes over time of PtRu-2 (C =  $5.10^{-6}$  M) in a 90:10 PBS buffer (pH = 7.45):DMSO solution at 37°C (top left), plot of the change in absorbance over time at 276 nm (top right), and hypothesised mechanism (bottom).



**Fig. S192.** UV-Vis spectral changes over time of PdOs-2 (C =  $5.10^{-6}$  M) in a 90:10 PBS buffer (pH = 7.45):DMSO solution at 37°C (top left), plot of the change in absorbance over time at 324 nm (top right), and hypothesised mechanism (bottom).

### 13. Single crystal X-ray diffraction analyses



**Fig. S193.** ORTEP representation of **PdPd-O-CH<sub>2</sub>Cl<sub>2</sub>** in the solid state determined by single crystal X-ray diffraction analysis. Thermal ellipsoids represented at the 30% probability level. H atoms omitted for clarity.

**Table S1 Crystal data and structure refinement for PdPd-O**

|                                    |                                                                                                  |
|------------------------------------|--------------------------------------------------------------------------------------------------|
| Empirical formula                  | C <sub>28</sub> H <sub>26</sub> Cl <sub>3</sub> F <sub>3</sub> O <sub>3</sub> P <sub>2</sub> PdS |
| Formula weight                     | 774.298                                                                                          |
| Temperature/K                      | 99.99(10)                                                                                        |
| Crystal system                     | triclinic                                                                                        |
| Space group                        | P-1                                                                                              |
| a/Å                                | 10.12541(6)                                                                                      |
| b/Å                                | 13.02540(9)                                                                                      |
| c/Å                                | 13.97395(11)                                                                                     |
| α/°                                | 117.4073(7)                                                                                      |
| β/°                                | 104.6035(6)                                                                                      |
| γ/°                                | 95.7305(5)                                                                                       |
| Volume/Å <sup>3</sup>              | 1532.45(2)                                                                                       |
| Z                                  | 2                                                                                                |
| ρ <sub>calc</sub> /cm <sup>3</sup> | 1.678                                                                                            |
| μ/mm <sup>-1</sup>                 | 9.344                                                                                            |
| F(000)                             | 782.8                                                                                            |
| Crystal size/mm <sup>3</sup>       | 0.3 × 0.21 × 0.11                                                                                |
| Radiation                          | Cu Kα (λ = 1.54184 Å)                                                                            |
| 2θ range for data collection/°     | 7.58 to 155.08                                                                                   |
| Index ranges                       | -12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17                                                         |
| Reflections collected              | 47101                                                                                            |

|                                                |                                                                  |
|------------------------------------------------|------------------------------------------------------------------|
| Independent reflections                        | 6435 [ $R_{\text{int}} = 0.0533$ , $R_{\text{sigma}} = 0.0246$ ] |
| Data/restraints/parameters                     | 6435/0/371                                                       |
| Goodness-of-fit on $F^2$                       | 1.035                                                            |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1 = 0.0297$ , $wR_2 = 0.0737$                                 |
| Final R indexes [all data]                     | $R_1 = 0.0299$ , $wR_2 = 0.0739$                                 |
| Largest diff. peak/hole / $e \text{ \AA}^{-3}$ | 0.80/-1.23                                                       |

**Table S2 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdPd-0.**  
 $U_{\text{eq}}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$  tensor.

| Atom | x           | y           | z           | $U(\text{eq})$ |
|------|-------------|-------------|-------------|----------------|
| Pd1  | 9051.04(15) | 8551.32(12) | 8957.23(12) | 9.34(6)        |
| Cl1  | 11495.0(5)  | 9613.4(4)   | 9892.3(5)   | 15.40(12)      |
| P1   | 6775.8(6)   | 7601.1(5)   | 8070.6(5)   | 10.07(11)      |
| P2   | 9420.6(6)   | 6754.4(5)   | 7916.0(5)   | 10.12(11)      |
| C1   | 6157(2)     | 7114.8(19)  | 8927.4(19)  | 11.2(4)        |
| C2   | 4849(3)     | 6303(2)     | 8456(2)     | 17.2(5)        |
| C3   | 4355(3)     | 5962(2)     | 9131(2)     | 23.8(5)        |
| C4   | 5160(3)     | 6424(2)     | 10273(2)    | 19.6(5)        |
| C5   | 6466(3)     | 7216(2)     | 10739(2)    | 16.6(5)        |
| C6   | 6973(2)     | 7567(2)     | 10070.6(19) | 14.2(4)        |
| C7   | 5679(2)     | 8494.5(19)  | 7779.7(19)  | 13.0(4)        |
| C8   | 5855(3)     | 8844(2)     | 7002(2)     | 18.6(5)        |
| C9   | 5058(3)     | 9566(2)     | 6782(2)     | 25.5(6)        |
| C10  | 4097(3)     | 9948(2)     | 7343(2)     | 26.4(6)        |
| C11  | 3932(3)     | 9616(2)     | 8128(2)     | 24.4(5)        |
| C12  | 4723(3)     | 8889(2)     | 8350(2)     | 17.0(5)        |
| C13  | 7713(2)     | 5653(2)     | 7003(2)     | 14.0(4)        |
| C14  | 6590(2)     | 6270(2)     | 6721.9(19)  | 13.6(4)        |
| C21  | 10342(2)    | 6140(2)     | 8731.6(19)  | 12.8(4)        |
| C22  | 11129(3)    | 6876(2)     | 9895(2)     | 15.3(4)        |
| C23  | 11806(3)    | 6389(2)     | 10520(2)    | 18.1(5)        |
| C24  | 11709(3)    | 5168(2)     | 9991(2)     | 17.7(5)        |
| C25  | 10930(3)    | 4433(2)     | 8835(2)     | 16.8(5)        |
| C26  | 10242(2)    | 4907(2)     | 8204(2)     | 15.0(4)        |
| C27  | 10358(2)    | 6806.2(19)  | 6988.4(18)  | 11.5(4)        |
| C28  | 10099(3)    | 7571(2)     | 6557(2)     | 17.7(5)        |
| C29  | 10773(3)    | 7623(2)     | 5824(2)     | 21.5(5)        |
| C30  | 11720(3)    | 6936(2)     | 5534(2)     | 17.9(5)        |
| C31  | 11961(3)    | 6161(2)     | 5948(2)     | 17.1(5)        |
| C32  | 11285(2)    | 6092(2)     | 6676(2)     | 14.7(4)        |
| Cl2  | 9741.6(9)   | 10754.7(7)  | 7618.2(6)   | 42.5(2)        |
| Cl3  | 8068.7(8)   | 11513.4(7)  | 6156.5(7)   | 36.50(17)      |
| C41  | 9439(3)     | 10817(3)    | 6344(2)     | 27.8(6)        |
| S1   | 3008.2(6)   | 2894.9(5)   | 5935.6(5)   | 17.63(13)      |
| F1   | 4869(2)     | 1893.7(19)  | 6615(2)     | 60.6(7)        |
| F2   | 5518.7(19)  | 2765.1(19)  | 5765.1(16)  | 44.0(5)        |
| F3   | 5562.5(17)  | 3791.2(15)  | 7483.7(13)  | 28.4(3)        |
| O1   | 2412(2)     | 1785.6(17)  | 4869.6(17)  | 27.5(4)        |
| O2   | 3228(2)     | 3935.4(18)  | 5814.2(19)  | 36.8(5)        |
| O3   | 2457(2)     | 3018(3)     | 6816.7(19)  | 45.0(6)        |
| C42  | 4821(3)     | 2828(2)     | 6469(2)     | 22.1(5)        |



**Table S3 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdPd-0. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\dots]$ .**

| Atom | $U_{11}$  | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|------|-----------|----------|----------|----------|----------|----------|
| Pd1  | 11.45(10) | 5.78(9)  | 10.45(9) | 2.42(6)  | 5.41(6)  | 2.91(7)  |
| Cl1  | 13.1(2)   | 7.9(2)   | 20.4(3)  | 2.82(19) | 7.9(2)   | 2.3(2)   |
| P1   | 12.1(3)   | 8.4(2)   | 9.8(3)   | 2.7(2)   | 4.8(2)   | 4.0(2)   |
| P2   | 13.6(3)   | 6.9(2)   | 10.6(3)  | 3.9(2)   | 5.8(2)   | 3.7(2)   |
| C1   | 13.5(10)  | 10.0(10) | 12.0(10) | 3.6(8)   | 6.5(9)   | 6.0(8)   |
| C2   | 17.4(11)  | 16.9(11) | 14.4(11) | -0.4(9)  | 4.5(9)   | 7.0(9)   |
| C3   | 22.4(13)  | 23.7(13) | 24.8(13) | -1.9(10) | 9.9(11)  | 12.3(11) |
| C4   | 25.9(13)  | 21.3(12) | 21.3(12) | 9.4(10)  | 14.6(11) | 14.5(10) |
| C5   | 23.2(12)  | 18.3(11) | 13.0(11) | 9.9(10)  | 7.7(10)  | 9.7(9)   |
| C6   | 16.5(11)  | 12.4(10) | 12.8(11) | 2.4(9)   | 4.6(9)   | 5.9(9)   |
| C7   | 16.3(11)  | 9.6(10)  | 11.8(10) | 4.0(8)   | 3.9(9)   | 4.6(9)   |
| C8   | 25.5(13)  | 18.8(12) | 18.4(12) | 10.3(10) | 12.0(10) | 11.6(10) |
| C9   | 40.2(16)  | 22.6(13) | 24.7(14) | 14.8(12) | 14.0(12) | 17.7(11) |
| C10  | 34.8(15)  | 21.7(13) | 29.9(14) | 17.6(12) | 11.4(12) | 16.3(12) |
| C11  | 27.7(14)  | 21.3(13) | 29.2(14) | 14.7(11) | 14.3(12) | 12.6(11) |
| C12  | 22.1(12)  | 13.9(11) | 16.5(12) | 6.2(9)   | 9.6(10)  | 7.0(9)   |
| C13  | 15.9(11)  | 9.3(10)  | 14.2(11) | 3.3(8)   | 6.1(9)   | 3.4(9)   |
| C14  | 15.9(11)  | 13.3(10) | 9.3(10)  | 3.9(9)   | 4.1(9)   | 4.0(9)   |
| C21  | 15.2(11)  | 11.8(10) | 14.4(11) | 3.9(8)   | 7.7(9)   | 7.3(9)   |
| C22  | 20.1(12)  | 11.7(10) | 15.2(11) | 5.1(9)   | 8.5(9)   | 6.3(9)   |
| C23  | 19.3(12)  | 21.5(12) | 16.2(12) | 6.4(10)  | 6.7(10)  | 10.9(10) |
| C24  | 17.8(11)  | 23.8(12) | 25.0(13) | 10.3(10) | 11.8(10) | 19.5(11) |
| C25  | 19.5(12)  | 14.3(11) | 24.3(13) | 6.5(9)   | 11.5(10) | 13.1(10) |
| C26  | 17.3(11)  | 11.9(10) | 16.3(11) | 4.4(9)   | 7.0(9)   | 6.7(9)   |
| C27  | 15.4(11)  | 8.4(9)   | 8.8(10)  | 2.0(8)   | 4.5(8)   | 2.9(8)   |
| C28  | 24.9(13)  | 16.4(11) | 21.7(12) | 13.0(10) | 14.1(10) | 12.6(10) |
| C29  | 34.6(14)  | 19.8(12) | 24.1(13) | 14.2(11) | 16.9(11) | 17.0(11) |
| C30  | 24.5(12)  | 18.6(11) | 17.8(12) | 7.5(10)  | 13.4(10) | 11.2(10) |
| C31  | 21.9(12)  | 17.2(11) | 17.3(12) | 10.8(10) | 11.2(10) | 9.0(10)  |
| C32  | 19.1(11)  | 14.4(11) | 14.4(11) | 7.5(9)   | 6.0(9)   | 9.4(9)   |
| Cl2  | 55.3(5)   | 26.1(3)  | 24.9(4)  | 5.5(3)   | -10.0(3) | 9.2(3)   |
| Cl3  | 37.8(4)   | 41.6(4)  | 44.6(4)  | 17.1(3)  | 14.5(3)  | 31.3(4)  |
| C41  | 27.7(14)  | 22.8(13) | 26.3(14) | 6.7(11)  | 6.8(12)  | 8.2(11)  |
| S1   | 21.7(3)   | 18.7(3)  | 13.4(3)  | 9.8(2)   | 6.7(2)   | 7.5(2)   |
| F1   | 38.7(11)  | 39.2(11) | 113(2)   | 10.9(9)  | 2.3(12)  | 56.8(13) |
| F2   | 28.2(9)   | 57.3(12) | 30.2(9)  | 6.3(9)   | 16.1(8)  | 7.2(9)   |
| F3   | 25.8(8)   | 35.2(9)  | 20.8(8)  | 6.6(7)   | 2.9(6)   | 14.1(7)  |
| O1   | 26.6(10)  | 17.7(9)  | 24.8(10) | 3.2(8)   | 6.9(8)   | 1.6(8)   |
| O2   | 44.5(13)  | 18.8(10) | 36.1(12) | 7.8(9)   | -6.3(10) | 15.4(9)  |
| O3   | 28.8(11)  | 82.5(19) | 25.8(11) | 13.3(12) | 15.0(9)  | 26.2(12) |
| C42  | 23.5(13)  | 17.1(12) | 29.3(14) | 7.4(10)  | 9.9(11)  | 13.5(11) |

**Table S4 Bond Lengths for PdPd-0.**

| Atom Atom            | Length/ $\text{\AA}$ | Atom Atom | Length/ $\text{\AA}$ |
|----------------------|----------------------|-----------|----------------------|
| Pd1 Cl1              | 2.4014(5)            | C13 C14   | 1.530(3)             |
| Pd1 Cl1 <sup>1</sup> | 2.4040(5)            | C21 C22   | 1.398(3)             |
| Pd1 P1               | 2.2257(6)            | C21 C26   | 1.404(3)             |
| Pd1 P2               | 2.2471(5)            | C22 C23   | 1.389(3)             |
| P1 C1                | 1.796(2)             | C23 C24   | 1.391(3)             |
| P1 C7                | 1.794(2)             | C24 C25   | 1.389(4)             |

|     |     |          |     |     |            |
|-----|-----|----------|-----|-----|------------|
| P1  | C14 | 1.828(2) | C25 | C26 | 1.387(3)   |
| P2  | C13 | 1.839(2) | C27 | C28 | 1.397(3)   |
| P2  | C21 | 1.806(2) | C27 | C32 | 1.394(3)   |
| P2  | C27 | 1.810(2) | C28 | C29 | 1.388(3)   |
| C1  | C2  | 1.394(3) | C29 | C30 | 1.385(3)   |
| C1  | C6  | 1.397(3) | C30 | C31 | 1.390(3)   |
| C2  | C3  | 1.385(3) | C31 | C32 | 1.390(3)   |
| C3  | C4  | 1.391(4) | Cl2 | C41 | 1.771(3)   |
| C4  | C5  | 1.383(4) | Cl3 | C41 | 1.761(3)   |
| C5  | C6  | 1.391(3) | S1  | O1  | 1.4359(19) |
| C7  | C8  | 1.399(3) | S1  | O2  | 1.444(2)   |
| C7  | C12 | 1.396(3) | S1  | O3  | 1.427(2)   |
| C8  | C9  | 1.387(3) | S1  | C42 | 1.826(3)   |
| C9  | C10 | 1.389(4) | F1  | C42 | 1.327(3)   |
| C10 | C11 | 1.390(4) | F2  | C42 | 1.327(3)   |
| C11 | C12 | 1.389(3) | F3  | C42 | 1.336(3)   |

<sup>12</sup>-X,2-Y,2-Z

**Table S5 Bond Angles for PdPd-0.**

| Atom | Atom | Atom             | Angle/°     | Atom | Atom | Atom | Angle/°    |
|------|------|------------------|-------------|------|------|------|------------|
| P1   | Pd1  | Cl1              | 178.38(2)   | C11  | C12  | C7   | 119.6(2)   |
| P1   | Pd1  | Cl1 <sup>1</sup> | 91.661(19)  | C14  | C13  | P2   | 110.08(15) |
| P2   | Pd1  | Cl1 <sup>1</sup> | 174.967(19) | C13  | C14  | P1   | 106.52(15) |
| P2   | Pd1  | Cl1              | 96.039(19)  | C22  | C21  | P2   | 120.66(17) |
| P2   | Pd1  | P1               | 84.80(2)    | C26  | C21  | P2   | 119.90(18) |
| C1   | P1   | Pd1              | 109.62(8)   | C26  | C21  | C22  | 119.4(2)   |
| C7   | P1   | Pd1              | 113.64(8)   | C23  | C22  | C21  | 120.2(2)   |
| C7   | P1   | C1               | 108.34(10)  | C24  | C23  | C22  | 120.2(2)   |
| C14  | P1   | Pd1              | 108.29(8)   | C25  | C24  | C23  | 119.9(2)   |
| C14  | P1   | C1               | 107.65(10)  | C26  | C25  | C24  | 120.5(2)   |
| C14  | P1   | C7               | 109.13(10)  | C25  | C26  | C21  | 119.9(2)   |
| C13  | P2   | Pd1              | 109.31(7)   | C28  | C27  | P2   | 117.80(17) |
| C21  | P2   | Pd1              | 115.36(7)   | C32  | C27  | P2   | 122.25(17) |
| C21  | P2   | C13              | 104.72(10)  | C32  | C27  | C28  | 119.9(2)   |
| C27  | P2   | Pd1              | 110.47(7)   | C29  | C28  | C27  | 119.9(2)   |
| C27  | P2   | C13              | 107.74(10)  | C30  | C29  | C28  | 120.3(2)   |
| C27  | P2   | C21              | 108.85(10)  | C31  | C30  | C29  | 119.8(2)   |
| C2   | C1   | P1               | 119.85(17)  | C32  | C31  | C30  | 120.4(2)   |
| C6   | C1   | P1               | 120.03(17)  | C31  | C32  | C27  | 119.6(2)   |
| C6   | C1   | C2               | 120.1(2)    | Cl3  | C41  | Cl2  | 110.92(16) |
| C3   | C2   | C1               | 119.6(2)    | O2   | S1   | O1   | 114.26(13) |
| C4   | C3   | C2               | 120.2(2)    | O3   | S1   | O1   | 115.83(14) |
| C5   | C4   | C3               | 120.3(2)    | O3   | S1   | O2   | 115.69(16) |
| C6   | C5   | C4               | 120.0(2)    | C42  | S1   | O1   | 103.09(12) |
| C5   | C6   | C1               | 119.7(2)    | C42  | S1   | O2   | 101.31(12) |
| C8   | C7   | P1               | 118.16(17)  | C42  | S1   | O3   | 103.88(13) |
| C12  | C7   | P1               | 121.62(18)  | F1   | C42  | S1   | 111.61(19) |
| C12  | C7   | C8               | 120.1(2)    | F2   | C42  | S1   | 111.87(19) |
| C9   | C8   | C7               | 119.8(2)    | F2   | C42  | F1   | 108.2(2)   |
| C10  | C9   | C8               | 119.8(2)    | F3   | C42  | S1   | 112.41(17) |
| C11  | C10  | C9               | 120.5(2)    | F3   | C42  | F1   | 106.2(2)   |
| C12  | C11  | C10              | 120.0(2)    | F3   | C42  | F2   | 106.2(2)   |

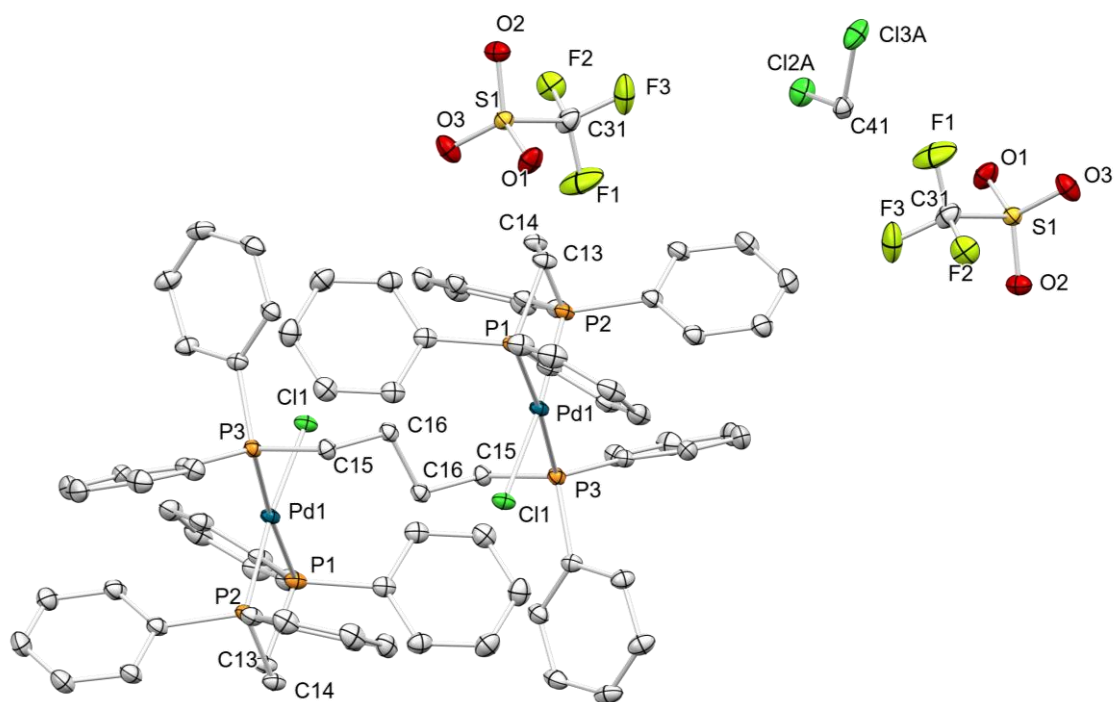
<sup>12</sup>-X,2-Y,2-Z

Table S6 Torsion Angles for PdPd-0.

| A  | B   | C   | D   | Angle/°     | A   | B   | C   | D   | Angle/° |
|----|-----|-----|-----|-------------|-----|-----|-----|-----|---------|
| P1 | C1  | C2  | C3  | -177.8(2)   | C7  | C8  | C9  | C10 | 0.5(3)  |
| P1 | C1  | C6  | C5  | 177.88(17)  | C7  | C12 | C11 | C10 | -0.2(3) |
| P1 | C7  | C8  | C9  | -178.0(2)   | C8  | C9  | C10 | C11 | 0.3(3)  |
| P1 | C7  | C12 | C11 | 177.7(2)    | C9  | C10 | C11 | C12 | -0.5(3) |
| P1 | C14 | C13 | P2  | -46.77(13)  | C21 | C22 | C23 | C24 | 0.2(3)  |
| P2 | C21 | C22 | C23 | 178.48(18)  | C21 | C26 | C25 | C24 | 0.6(3)  |
| P2 | C21 | C26 | C25 | -178.90(17) | C22 | C23 | C24 | C25 | -0.1(3) |
| P2 | C27 | C28 | C29 | -178.73(19) | C23 | C24 | C25 | C26 | -0.3(3) |
| P2 | C27 | C32 | C31 | 179.18(19)  | C27 | C28 | C29 | C30 | -1.1(3) |
| C1 | C2  | C3  | C4  | -0.2(3)     | C27 | C32 | C31 | C30 | 0.1(3)  |
| C1 | C6  | C5  | C4  | 0.0(3)      | C28 | C29 | C30 | C31 | 2.2(3)  |
| C2 | C3  | C4  | C5  | -0.7(3)     | C29 | C30 | C31 | C32 | -1.6(3) |
| C3 | C4  | C5  | C6  | 0.8(3)      |     |     |     |     |         |

Table S7 Hydrogen Atom Coordinates ( $\text{\AA} \times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdPd-0.

| Atom | x        | y        | z           | U(eq)   |
|------|----------|----------|-------------|---------|
| H2   | 4301(3)  | 5985(2)  | 7675(2)     | 20.7(6) |
| H3   | 3463(3)  | 5412(2)  | 8814(2)     | 28.5(7) |
| H4   | 4811(3)  | 6193(2)  | 10734(2)    | 23.5(6) |
| H5   | 7017(3)  | 7521(2)  | 11517(2)    | 20.0(6) |
| H6   | 7870(2)  | 8111(2)  | 10389.3(19) | 17.1(5) |
| H8   | 6519(3)  | 8586(2)  | 6625(2)     | 22.3(6) |
| H9   | 5168(3)  | 9799(2)  | 6250(2)     | 30.6(7) |
| H10  | 3549(3)  | 10440(2) | 7189(2)     | 31.7(7) |
| H11  | 3277(3)  | 9885(2)  | 8512(2)     | 29.3(7) |
| H12  | 4613(3)  | 8663(2)  | 8887(2)     | 20.4(6) |
| H13a | 7801(2)  | 5033(2)  | 6286(2)     | 16.7(5) |
| H13b | 7427(2)  | 5258(2)  | 7405(2)     | 16.7(5) |
| H14a | 5636(2)  | 5731(2)  | 6391.1(19)  | 16.3(5) |
| H14b | 6737(2)  | 6495(2)  | 6162.7(19)  | 16.3(5) |
| H22  | 11201(3) | 7710(2)  | 10258(2)    | 18.3(5) |
| H23  | 12337(3) | 6891(2)  | 11310(2)    | 21.8(6) |
| H24  | 12174(3) | 4837(2)  | 10420(2)    | 21.3(6) |
| H25  | 10869(3) | 3600(2)  | 8475(2)     | 20.2(6) |
| H26  | 9703(2)  | 4399(2)  | 7415(2)     | 18.0(5) |
| H28  | 9463(3)  | 8055(2)  | 6765(2)     | 21.3(6) |
| H29  | 10583(3) | 8133(2)  | 5520(2)     | 25.8(6) |
| H30  | 12203(3) | 6995(2)  | 5053(2)     | 21.5(6) |
| H31  | 12592(3) | 5674(2)  | 5733(2)     | 20.6(6) |
| H32  | 11453(2) | 5561(2)  | 6958(2)     | 17.6(5) |
| H41a | 10313(3) | 11268(3) | 6377(2)     | 33.4(7) |
| H41b | 9187(3)  | 9997(3)  | 5680(2)     | 33.4(7) |



**Fig. S194.** ORTEP representation of **PdPd-1·CH<sub>2</sub>Cl<sub>2</sub>** in the solid state determined by single crystal X-ray diffraction analysis. Thermal ellipsoids represented at the 30% probability level. H atoms omitted for clarity.

**Table S8 Crystal data and structure refinement for PdPd-1·CH<sub>2</sub>Cl<sub>2</sub>.**

|                                             |                                                                                                         |
|---------------------------------------------|---------------------------------------------------------------------------------------------------------|
| Empirical formula                           | C <sub>41.5</sub> H <sub>39.87</sub> Cl <sub>2.5</sub> F <sub>3</sub> O <sub>3</sub> P <sub>3</sub> PdS |
| Formula weight                              | 963.59                                                                                                  |
| Temperature/K                               | 100.00(10)                                                                                              |
| Crystal system                              | monoclinic                                                                                              |
| Space group                                 | P2 <sub>1</sub> /c                                                                                      |
| a/Å                                         | 14.08760(10)                                                                                            |
| b/Å                                         | 15.34030(10)                                                                                            |
| c/Å                                         | 19.8791(2)                                                                                              |
| α/°                                         | 90                                                                                                      |
| β/°                                         | 105.1110(10)                                                                                            |
| γ/°                                         | 90                                                                                                      |
| Volume/Å <sup>3</sup>                       | 4147.49(6)                                                                                              |
| Z                                           | 4                                                                                                       |
| ρ <sub>calc</sub> /cm <sup>3</sup>          | 1.543                                                                                                   |
| μ/mm <sup>-1</sup>                          | 7.096                                                                                                   |
| F(000)                                      | 1957.0                                                                                                  |
| Crystal size/mm <sup>3</sup>                | 0.11 × 0.06 × 0.01                                                                                      |
| Radiation                                   | Cu Kα (λ = 1.54184 Å)                                                                                   |
| 2θ range for data collection/°              | 8.688 to 155.13                                                                                         |
| Index ranges                                | -17 ≤ h ≤ 17, -19 ≤ k ≤ 19, -24 ≤ l ≤ 25                                                                |
| Reflections collected                       | 69734                                                                                                   |
| Independent reflections                     | 8768 [R <sub>int</sub> = 0.0608, R <sub>sigma</sub> = 0.0278]                                           |
| Data/restraints/parameters                  | 8768/76/603                                                                                             |
| Goodness-of-fit on F <sup>2</sup>           | 1.045                                                                                                   |
| Final R indexes [I ≥ 2σ(I)]                 | R <sub>1</sub> = 0.0341, wR <sub>2</sub> = 0.0824                                                       |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0359, wR <sub>2</sub> = 0.0837                                                       |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.96/-0.84                                                                                              |

**Table S9 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdPd-1-CH<sub>2</sub>Cl<sub>2</sub>. U<sub>eq</sub> is defined as 1/3 of the trace of the orthogonalised U<sub>ij</sub> tensor.**

| Atom | x          | y          | z          | U(eq)     |
|------|------------|------------|------------|-----------|
| Pd1  | 4366.7(2)  | 4504.0(2)  | 6510.9(2)  | 21.50(6)  |
| Cl1  | 4945.5(4)  | 5940.7(3)  | 6698.2(3)  | 28.04(12) |
| P1   | 5658.1(5)  | 4070.5(4)  | 7415.7(3)  | 25.49(13) |
| P2   | 4004.8(4)  | 3065.0(4)  | 6382.4(3)  | 23.89(12) |
| P3   | 3122.1(4)  | 4975.1(4)  | 5527.2(3)  | 22.42(12) |
| C00G | 2782.4(17) | 6121.6(15) | 5548.0(12) | 26.3(5)   |
| C00H | 2030(2)    | 7799.0(18) | 5544.2(16) | 40.3(6)   |
| C00I | 1920.6(18) | 4456.3(15) | 5318.2(13) | 26.8(5)   |
| C00J | 1458.9(19) | 4163.5(18) | 4645.9(14) | 32.9(5)   |
| C00N | 2717.1(19) | 6673.3(17) | 4982.0(14) | 32.1(5)   |
| C00S | 2497.7(19) | 6431.0(17) | 6126.1(13) | 32.1(5)   |
| C00W | 2351(2)    | 7512.8(18) | 4984.6(16) | 39.5(6)   |
| C00X | 523(2)     | 3793.7(19) | 4506.1(17) | 41.6(6)   |
| C1   | 5822(2)    | 4625.1(16) | 8244.1(13) | 30.1(5)   |
| C01C | 60(2)      | 3707(2)    | 5036.5(19) | 45.0(7)   |
| C01G | 515(2)     | 3996(2)    | 5700.1(18) | 42.7(7)   |
| C2   | 6730(2)    | 4598.7(18) | 8733.4(14) | 37.1(6)   |
| C3   | 6820(2)    | 4933(2)    | 9399.3(14) | 42.3(7)   |
| C4   | 6018(2)    | 5302.7(19) | 9563.1(14) | 41.1(7)   |
| C5   | 5122(2)    | 5348.1(18) | 9069.5(15) | 39.5(6)   |
| C6   | 5013(2)    | 5006.6(17) | 8404.8(13) | 33.8(5)   |
| C7   | 6836.7(19) | 4151.0(17) | 7209.4(12) | 29.4(5)   |
| C8   | 7321(2)    | 3421.3(18) | 7049.4(14) | 35.8(6)   |
| C9   | 8212(2)    | 3521(2)    | 6883.0(16) | 43.6(7)   |
| C010 | 2110(2)    | 7263.0(19) | 6118.4(15) | 38.7(6)   |
| C10  | 8627(2)    | 4330(2)    | 6882.7(16) | 43.1(7)   |
| C11  | 8150(2)    | 5062.8(19) | 7045.9(14) | 37.4(6)   |
| C12  | 7254(2)    | 4979.2(18) | 7202.1(13) | 32.4(5)   |
| C13  | 5471(2)    | 2923.2(16) | 7603.2(12) | 29.1(5)   |
| C14  | 5029.7(19) | 2431.3(15) | 6922.8(12) | 28.3(5)   |
| C15  | 3567.6(17) | 4857.6(16) | 4752.0(12) | 26.8(5)   |
| C015 | 1436(2)    | 4380.6(17) | 5842.9(15) | 32.8(5)   |
| C16  | 4572.9(17) | 5302.0(16) | 4840.4(12) | 26.9(5)   |
| C17  | 4598(2)    | 2283.7(19) | 4576.5(14) | 38.3(6)   |
| C21  | 2958.1(19) | 2764.9(16) | 6699.4(13) | 30.0(5)   |
| C22  | 2466(2)    | 1975.8(17) | 6524.6(14) | 35.2(6)   |
| C23  | 1666(2)    | 1786(2)    | 6787.9(16) | 42.7(7)   |
| C24  | 1383(2)    | 2363(2)    | 7240.1(17) | 45.5(7)   |
| C25  | 1893(2)    | 3128(2)    | 7433.7(15) | 41.3(6)   |
| C26  | 2676(2)    | 3333.3(18) | 7162.4(14) | 34.7(6)   |
| C27  | 3845.8(18) | 2644.9(15) | 5506.7(12) | 26.4(5)   |
| C28  | 2923(2)    | 2498.5(16) | 5056.7(13) | 30.7(5)   |
| C29  | 2844(2)    | 2246.1(19) | 4371.0(13) | 37.8(6)   |
| C30  | 3676(2)    | 2138(2)    | 4134.8(14) | 41.8(7)   |
| C32  | 4688(2)    | 2535.6(16) | 5264.1(13) | 30.7(5)   |
| Cl2A | 613.1(9)   | 1180.9(8)  | 5051.5(6)  | 47.4(4)   |
| Cl2B | -180(20)   | 1270(20)   | 3558(5)    | 107(5)    |
| Cl3A | 28(4)      | 1510(4)    | 3566(3)    | 50.6(19)  |
| Cl3B | -56(12)    | 132(8)     | 4683(9)    | 160(8)    |
| C41  | 534(4)     | 752(4)     | 4237(2)    | 32.3(10)  |
| S1   | 7605.3(6)  | 652.5(5)   | 6759.0(4)  | 27.36(15) |

|      |            |          |            |          |
|------|------------|----------|------------|----------|
| F1   | 9435(2)    | 295(2)   | 7375(2)    | 92.7(12) |
| F3   | 9253.6(19) | 1273(2)  | 6579.1(16) | 72.0(9)  |
| O1   | 7629(3)    | -24(2)   | 6267(2)    | 45.4(8)  |
| O2   | 7144(3)    | 1447(4)  | 6465(2)    | 39.5(9)  |
| O3   | 7349(3)    | 358(3)   | 7378.0(19) | 46.3(8)  |
| C31  | 8890(3)    | 965(3)   | 7091(2)    | 44.3(8)  |
| F2   | 9015(4)    | 1586(3)  | 7577(3)    | 49.3(10) |
| S1A  | 8227(4)    | 860(3)   | 7119(2)    | 50.4(10) |
| F1A  | 8926(10)   | 834(8)   | 6037(6)    | 74(3)    |
| F2A  | 9378(10)   | -254(9)  | 6715(6)    | 76(3)    |
| F3A  | 7935(12)   | -196(10) | 6085(7)    | 70(4)    |
| O1A  | 7888(17)   | 186(11)  | 7482(10)   | 71(5)    |
| O2A  | 9010(30)   | 1370(20) | 7460(17)   | 84(10)   |
| O3A  | 7394(19)   | 1405(15) | 6726(12)   | 67(5)    |
| C31A | 8641(14)   | 292(11)  | 6455(9)    | 52(4)    |

**Table S10 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdPd-1-CH<sub>2</sub>Cl<sub>2</sub>. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$ .**

| Atom | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>23</sub> | U <sub>13</sub> | U <sub>12</sub> |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Pd1  | 30.29(10)       | 17.62(9)        | 16.66(9)        | 0.73(5)         | 6.26(6)         | -0.10(6)        |
| Cl1  | 36.9(3)         | 19.5(2)         | 25.3(3)         | -0.1(2)         | 3.7(2)          | -2.0(2)         |
| P1   | 37.0(3)         | 20.2(3)         | 17.5(3)         | 0.0(2)          | 4.0(2)          | 1.3(2)          |
| P2   | 35.2(3)         | 18.1(3)         | 19.0(3)         | -0.2(2)         | 8.3(2)          | -1.0(2)         |
| P3   | 26.7(3)         | 22.1(3)         | 19.0(3)         | 1.8(2)          | 7.1(2)          | -0.4(2)         |
| C00G | 27.5(11)        | 22.7(11)        | 26.9(11)        | 0.6(9)          | 3.6(9)          | -1.0(9)         |
| C00H | 37.6(14)        | 23.5(13)        | 51.9(17)        | -3.8(12)        | -2.2(12)        | 2.2(10)         |
| C00I | 27.9(11)        | 21.6(11)        | 31.2(12)        | 2.8(9)          | 8.4(9)          | 1.3(9)          |
| C00J | 32.0(12)        | 32.8(13)        | 31.4(13)        | 0.4(10)         | 3.9(10)         | -2.9(10)        |
| C00N | 33.2(12)        | 30.3(13)        | 32.5(13)        | 6.7(10)         | 7.9(10)         | -1.6(10)        |
| C00S | 35.7(13)        | 30.2(13)        | 28.1(12)        | 0.0(10)         | 4.1(10)         | 4.4(10)         |
| C00W | 37.5(14)        | 31.0(14)        | 45.5(16)        | 14.4(12)        | 3.0(12)         | -2.3(11)        |
| C00X | 34.6(14)        | 37.1(15)        | 46.2(16)        | 0.9(12)         | -1.7(12)        | -5.9(11)        |
| C1   | 48.8(15)        | 20.0(11)        | 20.9(11)        | 1.3(9)          | 7.9(10)         | -1.5(10)        |
| C01C | 27.0(13)        | 37.0(15)        | 70(2)           | 6.3(14)         | 10.2(13)        | -4.5(11)        |
| C01G | 37.3(14)        | 39.0(15)        | 58.3(18)        | 5.2(13)         | 23.9(13)        | -1.9(12)        |
| C2   | 51.0(16)        | 31.2(13)        | 25.7(13)        | -1.9(10)        | 4.0(11)         | 0.2(11)         |
| C3   | 60.5(18)        | 38.1(15)        | 23.2(12)        | -4.0(11)        | 1.8(12)         | -2.5(13)        |
| C4   | 71(2)           | 30.4(13)        | 21.7(12)        | -2.2(10)        | 11.1(12)        | -8.5(13)        |
| C5   | 62.1(18)        | 28.9(13)        | 32.8(14)        | -2.8(11)        | 22.0(13)        | -1.1(12)        |
| C6   | 51.4(15)        | 25.2(12)        | 25.5(12)        | 2.2(10)         | 11.2(11)        | -1.3(11)        |
| C7   | 38.5(13)        | 28.1(12)        | 19.4(10)        | -1.4(9)         | 3.8(9)          | 0.7(10)         |
| C8   | 43.1(14)        | 31.1(13)        | 32.0(13)        | -3.9(11)        | 7.7(11)         | 2.4(11)         |
| C9   | 47.2(16)        | 40.8(16)        | 43.7(16)        | -9.8(13)        | 13.3(13)        | 5.6(13)         |
| C010 | 40.5(14)        | 34.0(14)        | 36.8(14)        | -8.9(11)        | 1.4(11)         | 6.0(11)         |
| C10  | 42.9(15)        | 52.1(18)        | 36.6(15)        | -7.8(13)        | 14.5(12)        | -1.4(13)        |
| C11  | 42.9(14)        | 38.6(15)        | 29.9(13)        | -2.0(11)        | 7.8(11)         | -4.2(12)        |
| C12  | 39.1(13)        | 31.5(13)        | 24.1(11)        | -0.9(10)        | 4.0(10)         | 0.9(10)         |
| C13  | 42.0(13)        | 22.5(11)        | 20.6(11)        | 1.8(9)          | 4.1(9)          | 0.4(10)         |
| C14  | 40.4(13)        | 20.6(11)        | 22.9(11)        | -0.5(9)         | 6.4(9)          | 1.2(9)          |
| C15  | 29.3(11)        | 29.5(12)        | 22.6(11)        | -0.5(9)         | 8.7(9)          | -2.1(9)         |
| C015 | 36.0(13)        | 27.3(12)        | 39.2(14)        | 2.5(10)         | 17.2(11)        | 0.4(10)         |
| C16  | 30.7(12)        | 28.5(12)        | 23.1(11)        | 3.1(9)          | 9.9(9)          | -1.3(10)        |
| C17  | 51.4(16)        | 37.9(14)        | 30.2(13)        | -1.7(11)        | 18.7(12)        | -3.7(12)        |

|      |          |          |          |           |           |           |
|------|----------|----------|----------|-----------|-----------|-----------|
| C21  | 39.0(13) | 25.9(12) | 26.3(11) | 3.8(9)    | 10.6(10)  | -1.0(10)  |
| C22  | 46.8(15) | 26.9(13) | 34.2(13) | 4.3(10)   | 14.6(11)  | -3.3(11)  |
| C23  | 50.0(16) | 36.6(15) | 44.3(16) | 7.3(12)   | 17.0(13)  | -8.7(12)  |
| C24  | 48.4(16) | 50.0(18) | 45.7(16) | 12.1(14)  | 26.0(14)  | 0.3(14)   |
| C25  | 53.9(17) | 39.7(15) | 36.3(14) | 8.0(12)   | 22.6(13)  | 5.3(13)   |
| C26  | 49.0(15) | 28.9(13) | 29.0(12) | 2.2(10)   | 15.5(11)  | 0.8(11)   |
| C27  | 38.7(12) | 20.2(11) | 20.5(10) | 0.7(8)    | 8.0(9)    | -2.2(9)   |
| C28  | 41.2(13) | 25.2(12) | 25.6(12) | 0.7(9)    | 8.8(10)   | -2.0(10)  |
| C29  | 48.1(15) | 37.9(15) | 23.6(12) | -1.9(11)  | 2.5(11)   | -7.0(12)  |
| C30  | 64.8(19) | 41.0(15) | 20.7(12) | -4.8(11)  | 13.4(12)  | -6.7(13)  |
| C32  | 40.1(13) | 28.0(12) | 25.5(12) | -0.7(9)   | 11.5(10)  | -4.9(10)  |
| Cl2A | 46.3(7)  | 56.6(8)  | 38.0(6)  | -10.2(5)  | 8.6(5)    | -1.0(5)   |
| Cl2B | 66(7)    | 194(12)  | 50(3)    | -34(5)    | -5(3)     | 54(9)     |
| Cl3A | 40.1(18) | 74(4)    | 35.5(15) | -5.6(16)  | 5.5(13)   | 19.9(14)  |
| Cl3B | 183(13)  | 117(10)  | 229(17)  | 35(9)     | 142(13)   | 7(8)      |
| C41  | 35(3)    | 35(3)    | 30(2)    | -4(2)     | 13(2)     | 0(2)      |
| S1   | 29.1(4)  | 26.5(4)  | 26.8(4)  | -1.5(3)   | 7.8(3)    | -0.5(3)   |
| F1   | 44.7(14) | 61.3(17) | 141(3)   | -14.2(19) | -31.1(17) | 18.7(13)  |
| F3   | 48.7(14) | 101(2)   | 77.7(19) | -30.4(16) | 37.4(13)  | -28.8(14) |
| O1   | 39.6(16) | 45.7(19) | 50(2)    | -20.5(14) | 10.9(13)  | 0.3(13)   |
| O2   | 41.0(16) | 31.6(17) | 42(2)    | 3.5(16)   | 4.3(14)   | 2.6(12)   |
| O3   | 59(2)    | 50(2)    | 32.4(14) | 0.7(13)   | 16.4(16)  | -17.7(16) |
| C31  | 30.6(19) | 43(2)    | 56(2)    | -9.5(19)  | 5.2(17)   | 1.3(16)   |
| F2   | 48.7(15) | 52(2)    | 41(2)    | -13.3(18) | 0.2(13)   | -13.5(14) |
| S1A  | 82(4)    | 32.9(19) | 43(2)    | -7.1(16)  | 28(2)     | -16(2)    |
| F1A  | 108(9)   | 73(7)    | 55(6)    | 24(6)     | 47(7)     | 24(7)     |
| F2A  | 90(8)    | 90(9)    | 49(6)    | 12(6)     | 16(6)     | 33(7)     |
| F3A  | 85(11)   | 59(8)    | 52(8)    | -18(6)    | -3(7)     | 6(7)      |
| O1A  | 131(16)  | 46(8)    | 58(10)   | 0(6)      | 62(12)    | -24(9)    |
| O2A  | 121(14)  | 100(20)  | 42(10)   | -37(11)   | 35(9)     | -62(14)   |
| O3A  | 100(14)  | 27(7)    | 84(15)   | 6(10)     | 43(10)    | -3(10)    |
| C31A | 71(11)   | 42(8)    | 37(8)    | 5(7)      | 3(7)      | 13(8)     |

**Table S11 Bond Lengths for PdPd-1·CH<sub>2</sub>Cl<sub>2</sub>.**

| Atom | Atom | Length/Å  | Atom | Atom | Length/Å  |
|------|------|-----------|------|------|-----------|
| Pd1  | Cl1  | 2.3458(5) | C25  | C26  | 1.385(4)  |
| Pd1  | P1   | 2.2980(6) | C27  | C28  | 1.391(4)  |
| Pd1  | P2   | 2.2651(6) | C27  | C32  | 1.403(3)  |
| Pd1  | P3   | 2.3734(6) | C28  | C29  | 1.393(4)  |
| P1   | C1   | 1.814(3)  | C29  | C30  | 1.382(4)  |
| P1   | C7   | 1.815(3)  | Cl2A | Cl3B | 1.912(16) |
| P1   | C13  | 1.832(2)  | Cl2A | C41  | 1.724(5)  |
| P2   | C14  | 1.837(3)  | Cl2B | C41  | 1.664(11) |
| P2   | C21  | 1.808(3)  | Cl3A | C41  | 1.773(7)  |
| P2   | C27  | 1.815(2)  | Cl3B | C41  | 1.662(9)  |
| P3   | C00G | 1.826(2)  | S1   | O1   | 1.432(3)  |
| P3   | C00I | 1.818(2)  | S1   | O2   | 1.432(5)  |
| P3   | C15  | 1.818(2)  | S1   | O3   | 1.443(4)  |
| C00G | C00N | 1.392(3)  | S1   | C31  | 1.821(4)  |
| C00G | C00S | 1.395(4)  | S1   | S1A  | 1.026(5)  |
| C00H | C00W | 1.377(4)  | S1   | F3A  | 2.007(14) |
| C00H | C010 | 1.387(4)  | S1   | O1A  | 1.562(18) |
| C00I | C00J | 1.399(4)  | S1   | O3A  | 1.19(2)   |

|      |                  |          |     |      |           |
|------|------------------|----------|-----|------|-----------|
| C00I | C015             | 1.393(3) | S1  | C31A | 1.806(19) |
| C00J | C00X             | 1.395(4) | F1  | C31  | 1.319(5)  |
| C00N | C00W             | 1.388(4) | F1  | S1A  | 1.859(6)  |
| C00S | C010             | 1.387(4) | F1  | F2A  | 1.544(13) |
| C00X | C01C             | 1.383(5) | F1  | O2A  | 1.77(4)   |
| C1   | C2               | 1.391(4) | F1  | C31A | 1.879(17) |
| C1   | C6               | 1.390(4) | F3  | C31  | 1.339(6)  |
| C01C | C01G             | 1.381(5) | F3  | S1A  | 2.110(5)  |
| C01G | C015             | 1.385(4) | F3  | F1A  | 1.252(14) |
| C2   | C3               | 1.395(4) | F3  | C31A | 1.720(19) |
| C3   | C4               | 1.376(5) | O1  | S1A  | 2.161(5)  |
| C4   | C5               | 1.384(5) | O1  | F3A  | 0.684(15) |
| C5   | C6               | 1.392(4) | O1  | C31A | 1.46(2)   |
| C7   | C8               | 1.390(4) | O2  | S1A  | 1.947(7)  |
| C7   | C12              | 1.402(4) | O2  | O3A  | 0.55(2)   |
| C8   | C9               | 1.388(4) | O3  | S1A  | 1.650(6)  |
| C9   | C10              | 1.371(5) | O3  | O1A  | 0.78(2)   |
| C10  | C11              | 1.391(4) | C31 | F2   | 1.335(6)  |
| C11  | C12              | 1.382(4) | C31 | S1A  | 0.963(6)  |
| C13  | C14              | 1.532(3) | C31 | O2A  | 0.94(3)   |
| C15  | C16              | 1.540(3) | C31 | C31A | 1.600(18) |
| C16  | C16 <sup>1</sup> | 1.520(5) | F2  | S1A  | 1.666(6)  |
| C17  | C30              | 1.382(4) | S1A | O1A  | 1.415(15) |
| C17  | C32              | 1.394(4) | S1A | O2A  | 1.38(3)   |
| C21  | C22              | 1.393(4) | S1A | O3A  | 1.49(2)   |
| C21  | C26              | 1.399(4) | S1A | C31A | 1.801(18) |
| C22  | C23              | 1.391(4) | F1A | C31A | 1.31(2)   |
| C23  | C24              | 1.392(5) | F2A | C31A | 1.33(2)   |
| C24  | C25              | 1.377(5) | F3A | C31A | 1.31(2)   |

<sup>1</sup>1-X,1-Y,1-Z

**Table S12 Bond Angles for PdPd-1·CH<sub>2</sub>Cl<sub>2</sub>.**

| Atom | Atom | Atom | Angle/°    | Atom | Atom | Atom | Angle/°   |
|------|------|------|------------|------|------|------|-----------|
| Cl1  | Pd1  | P3   | 89.78(2)   | O3A  | O2   | S1   | 53(3)     |
| P1   | Pd1  | Cl1  | 88.64(2)   | O3A  | O2   | S1A  | 28(3)     |
| P1   | Pd1  | P3   | 175.60(2)  | S1   | O3   | S1A  | 38.01(18) |
| P2   | Pd1  | Cl1  | 172.88(2)  | O1A  | O3   | S1   | 83.7(13)  |
| P2   | Pd1  | P1   | 85.14(2)   | O1A  | O3   | S1A  | 58.9(12)  |
| P2   | Pd1  | P3   | 96.18(2)   | F1   | C31  | S1   | 111.2(3)  |
| C1   | P1   | Pd1  | 117.51(9)  | F1   | C31  | F3   | 107.7(4)  |
| C1   | P1   | C7   | 105.42(12) | F1   | C31  | F2   | 107.1(4)  |
| C1   | P1   | C13  | 104.88(11) | F1   | C31  | C31A | 79.5(6)   |
| C7   | P1   | Pd1  | 112.81(8)  | F3   | C31  | S1   | 111.0(3)  |
| C7   | P1   | C13  | 107.44(12) | F3   | C31  | C31A | 71.0(7)   |
| C13  | P1   | Pd1  | 108.11(8)  | F2   | C31  | S1   | 112.4(3)  |
| C14  | P2   | Pd1  | 109.29(8)  | F2   | C31  | F3   | 107.2(4)  |
| C21  | P2   | Pd1  | 112.88(9)  | F2   | C31  | C31A | 173.4(7)  |
| C21  | P2   | C14  | 104.45(12) | S1A  | C31  | S1   | 24.5(3)   |
| C21  | P2   | C27  | 109.64(12) | S1A  | C31  | F1   | 108.0(5)  |
| C27  | P2   | Pd1  | 114.97(8)  | S1A  | C31  | F3   | 132.2(5)  |
| C27  | P2   | C14  | 104.76(11) | S1A  | C31  | F2   | 91.4(5)   |
| C00G | P3   | Pd1  | 114.60(8)  | S1A  | C31  | C31A | 85.5(8)   |



|                  |      |      |            |      |     |      |           |
|------------------|------|------|------------|------|-----|------|-----------|
| C00I             | P3   | Pd1  | 119.92(8)  | O2A  | C31 | S1   | 115(2)    |
| C00I             | P3   | C00G | 101.12(11) | O2A  | C31 | F1   | 102(3)    |
| C00I             | P3   | C15  | 105.63(11) | O2A  | C31 | F3   | 109(2)    |
| C15              | P3   | Pd1  | 108.91(8)  | O2A  | C31 | F2   | 5(3)      |
| C15              | P3   | C00G | 105.38(11) | O2A  | C31 | S1A  | 93(2)     |
| C00N             | C00G | P3   | 122.00(19) | O2A  | C31 | C31A | 178(3)    |
| C00N             | C00G | C00S | 119.1(2)   | C31A | C31 | S1   | 63.3(7)   |
| C00S             | C00G | P3   | 118.66(19) | C31  | F2  | S1A  | 35.3(2)   |
| C00W             | C00H | C010 | 120.2(3)   | S1   | S1A | F1   | 126.9(3)  |
| C00J             | C00I | P3   | 122.15(19) | S1   | S1A | F3   | 108.2(3)  |
| C015             | C00I | P3   | 118.3(2)   | S1   | S1A | O1   | 34.10(17) |
| C015             | C00I | C00J | 119.5(2)   | S1   | S1A | O2   | 45.6(3)   |
| C00X             | C00J | C00I | 120.0(3)   | S1   | S1A | O3   | 60.0(3)   |
| C00W             | C00N | C00G | 120.5(3)   | S1   | S1A | F2   | 156.2(4)  |
| C010             | C00S | C00G | 120.1(2)   | S1   | S1A | O1A  | 77.8(10)  |
| C00H             | C00W | C00N | 120.0(3)   | S1   | S1A | O2A  | 161.4(17) |
| C01C             | C00X | C00J | 119.8(3)   | S1   | S1A | O3A  | 52.8(10)  |
| C2               | C1   | P1   | 119.8(2)   | S1   | S1A | C31A | 73.7(6)   |
| C6               | C1   | P1   | 119.2(2)   | F1   | S1A | F3   | 65.1(2)   |
| C6               | C1   | C2   | 120.7(2)   | F1   | S1A | O1   | 93.7(2)   |
| C01G             | C01C | C00X | 120.2(3)   | F1   | S1A | O2   | 154.2(3)  |
| C01C             | C01G | C015 | 120.7(3)   | F3   | S1A | O1   | 88.22(19) |
| C1               | C2   | C3   | 119.5(3)   | O2   | S1A | F3   | 92.5(2)   |
| C4               | C3   | C2   | 119.9(3)   | O2   | S1A | O1   | 71.9(3)   |
| C3               | C4   | C5   | 120.4(3)   | O3   | S1A | F1   | 113.8(3)  |
| C4               | C5   | C6   | 120.6(3)   | O3   | S1A | F3   | 165.5(3)  |
| C1               | C6   | C5   | 118.8(3)   | O3   | S1A | O1   | 77.4(2)   |
| C8               | C7   | P1   | 121.9(2)   | O3   | S1A | O2   | 84.5(3)   |
| C8               | C7   | C12  | 119.7(2)   | O3   | S1A | F2   | 126.0(3)  |
| C12              | C7   | P1   | 118.4(2)   | O3   | S1A | C31A | 114.6(7)  |
| C9               | C8   | C7   | 119.6(3)   | C31  | S1A | S1   | 132.5(5)  |
| C10              | C9   | C8   | 120.8(3)   | C31  | S1A | F1   | 42.4(4)   |
| C00S             | C010 | C00H | 120.1(3)   | C31  | S1A | F3   | 28.1(3)   |
| C9               | C10  | C11  | 120.0(3)   | C31  | S1A | O1   | 104.2(4)  |
| C12              | C11  | C10  | 120.1(3)   | C31  | S1A | O2   | 119.1(4)  |
| C11              | C12  | C7   | 119.8(3)   | C31  | S1A | O3   | 155.9(5)  |
| C14              | C13  | P1   | 109.90(16) | C31  | S1A | F2   | 53.2(4)   |
| C13              | C14  | P2   | 109.39(16) | C31  | S1A | O1A  | 127.8(11) |
| C16              | C15  | P3   | 111.70(16) | C31  | S1A | O2A  | 42.9(15)  |
| C01G             | C015 | C00I | 119.9(3)   | C31  | S1A | O3A  | 121.4(10) |
| C16 <sup>1</sup> | C16  | C15  | 112.5(2)   | C31  | S1A | C31A | 62.3(7)   |
| C30              | C17  | C32  | 119.9(3)   | F2   | S1A | F1   | 74.3(3)   |
| C22              | C21  | P2   | 122.2(2)   | F2   | S1A | F3   | 68.3(3)   |
| C22              | C21  | C26  | 119.8(2)   | F2   | S1A | O1   | 156.4(4)  |
| C26              | C21  | P2   | 117.9(2)   | F2   | S1A | O2   | 110.6(3)  |
| C23              | C22  | C21  | 119.1(3)   | F2   | S1A | C31A | 115.3(7)  |
| C22              | C23  | C24  | 120.5(3)   | O1A  | S1A | F1   | 85.7(10)  |
| C25              | C24  | C23  | 120.4(3)   | O1A  | S1A | F3   | 147.9(9)  |
| C24              | C25  | C26  | 119.7(3)   | O1A  | S1A | O1   | 80.1(8)   |
| C25              | C26  | C21  | 120.5(3)   | O1A  | S1A | O2   | 111.7(10) |
| C28              | C27  | P2   | 122.35(19) | O1A  | S1A | O3   | 28.2(9)   |
| C28              | C27  | C32  | 119.5(2)   | O1A  | S1A | F2   | 118.3(9)  |
| C32              | C27  | P2   | 117.93(19) | O1A  | S1A | O3A  | 110.8(14) |
| C27              | C28  | C29  | 119.8(2)   | O1A  | S1A | C31A | 103.8(9)  |
| C30              | C29  | C28  | 120.5(3)   | O2A  | S1A | F1   | 64.5(16)  |

|      |      |      |           |      |      |      |           |
|------|------|------|-----------|------|------|------|-----------|
| C29  | C30  | C17  | 120.3(2)  | O2A  | S1A  | F3   | 60.8(14)  |
| C17  | C32  | C27  | 120.1(2)  | O2A  | S1A  | O1   | 147.1(14) |
| C41  | Cl2A | Cl3B | 54.1(4)   | O2A  | S1A  | O2   | 117.1(17) |
| C41  | Cl3B | Cl2A | 57.2(4)   | O2A  | S1A  | O3   | 132.9(14) |
| Cl2A | C41  | Cl3A | 111.7(4)  | O2A  | S1A  | F2   | 10.9(16)  |
| Cl2B | C41  | Cl2A | 117.1(7)  | O2A  | S1A  | O1A  | 119.8(18) |
| Cl2B | C41  | Cl3A | 15.2(15)  | O2A  | S1A  | O3A  | 111.2(19) |
| Cl3B | C41  | Cl2A | 68.7(7)   | O2A  | S1A  | C31A | 105.2(16) |
| Cl3B | C41  | Cl2B | 115.1(16) | O3A  | S1A  | F1   | 161.4(10) |
| Cl3B | C41  | Cl3A | 128.1(7)  | O3A  | S1A  | F3   | 96.7(9)   |
| O1   | S1   | O3   | 114.3(2)  | O3A  | S1A  | O1   | 81.3(10)  |
| O1   | S1   | C31  | 103.9(2)  | O3A  | S1A  | O2   | 10.1(11)  |
| O1   | S1   | F3A  | 12.5(5)   | O3A  | S1A  | O3   | 82.7(10)  |
| O1   | S1   | O1A  | 104.6(7)  | O3A  | S1A  | F2   | 103.5(10) |
| O1   | S1   | C31A | 52.0(6)   | O3A  | S1A  | C31A | 104.5(11) |
| O2   | S1   | O1   | 115.2(3)  | C31A | S1A  | F1   | 61.8(6)   |
| O2   | S1   | O3   | 115.2(3)  | C31A | S1A  | F3   | 51.4(6)   |
| O2   | S1   | C31  | 103.1(2)  | C31A | S1A  | O1   | 42.0(6)   |
| O2   | S1   | F3A  | 116.0(5)  | C31A | S1A  | O2   | 94.7(6)   |
| O2   | S1   | O1A  | 138.2(7)  | F3   | F1A  | C31A | 84.4(10)  |
| O2   | S1   | C31A | 116.4(6)  | C31A | F2A  | F1   | 81.3(10)  |
| O3   | S1   | C31  | 102.7(2)  | O1   | F3A  | S1   | 27.1(10)  |
| O3   | S1   | F3A  | 121.3(5)  | O1   | F3A  | C31A | 88.5(16)  |
| O3   | S1   | O1A  | 29.7(7)   | C31A | F3A  | S1   | 61.9(10)  |
| O3   | S1   | C31A | 126.4(5)  | O3   | O1A  | S1   | 66.6(14)  |
| C31  | S1   | F3A  | 91.8(5)   | O3   | O1A  | S1A  | 93.0(16)  |
| S1A  | S1   | O1   | 122.2(3)  | S1A  | O1A  | S1   | 39.9(5)   |
| S1A  | S1   | O2   | 103.5(3)  | C31  | O2A  | F1   | 46.6(17)  |
| S1A  | S1   | O3   | 82.0(3)   | C31  | O2A  | S1A  | 44.3(14)  |
| S1A  | S1   | C31  | 22.9(3)   | S1A  | O2A  | F1   | 71.0(14)  |
| S1A  | S1   | F3A  | 111.2(5)  | S1   | O3A  | S1A  | 43.4(8)   |
| S1A  | S1   | O1A  | 62.3(8)   | O2   | O3A  | S1   | 105(4)    |
| S1A  | S1   | O3A  | 83.8(12)  | O2   | O3A  | S1A  | 142(4)    |
| S1A  | S1   | C31A | 73.2(6)   | S1   | C31A | F1   | 90.0(8)   |
| O1A  | S1   | C31  | 78.3(8)   | F3   | C31A | S1   | 95.9(8)   |
| O1A  | S1   | F3A  | 105.7(8)  | F3   | C31A | F1   | 73.1(7)   |
| O1A  | S1   | C31A | 97.7(9)   | F3   | C31A | S1A  | 73.6(7)   |
| O3A  | S1   | O1   | 135.7(11) | O1   | C31A | S1   | 50.7(6)   |
| O3A  | S1   | O2   | 21.8(11)  | O1   | C31A | F1   | 122.9(11) |
| O3A  | S1   | O3   | 103.6(12) | O1   | C31A | F3   | 138.3(12) |
| O3A  | S1   | C31  | 88.5(12)  | O1   | C31A | C31  | 114.5(12) |
| O3A  | S1   | F3A  | 133.7(12) | O1   | C31A | S1A  | 82.3(9)   |
| O3A  | S1   | O1A  | 119.7(13) | C31  | C31A | S1   | 64.3(7)   |
| O3A  | S1   | C31A | 119.4(13) | C31  | C31A | F1   | 43.6(5)   |
| C31A | S1   | C31  | 52.3(6)   | C31  | C31A | F3   | 47.4(6)   |
| C31A | S1   | F3A  | 39.6(7)   | C31  | C31A | S1A  | 32.2(4)   |
| C31  | F1   | S1A  | 29.5(2)   | S1A  | C31A | S1   | 33.0(4)   |
| C31  | F1   | F2A  | 99.6(5)   | S1A  | C31A | F1   | 60.6(6)   |
| C31  | F1   | O2A  | 31.2(11)  | F1A  | C31A | S1   | 115.2(12) |
| C31  | F1   | C31A | 56.8(6)   | F1A  | C31A | F1   | 114.4(14) |
| S1A  | F1   | C31A | 57.6(6)   | F1A  | C31A | F3   | 46.4(9)   |
| F2A  | F1   | S1A  | 100.4(5)  | F1A  | C31A | O1   | 119.3(13) |
| F2A  | F1   | O2A  | 130.0(12) | F1A  | C31A | C31  | 92.9(12)  |
| F2A  | F1   | C31A | 44.4(7)   | F1A  | C31A | S1A  | 111.6(12) |
| O2A  | F1   | S1A  | 44.5(11)  | F1A  | C31A | F2A  | 108.1(16) |

|      |    |      |           |     |          |           |
|------|----|------|-----------|-----|----------|-----------|
| O2A  | F1 | C31A | 88.0(12)  | F2A | C31A S1  | 132.8(13) |
| C31  | F3 | S1A  | 19.8(2)   | F2A | C31A F1  | 54.3(8)   |
| C31  | F3 | C31A | 61.6(6)   | F2A | C31A F3  | 100.6(13) |
| F1A  | F3 | C31  | 109.6(6)  | F2A | C31A O1  | 120.1(15) |
| F1A  | F3 | S1A  | 97.3(6)   | F2A | C31A C31 | 96.4(12)  |
| F1A  | F3 | C31A | 49.2(8)   | F2A | C31A S1A | 112.9(12) |
| C31A | F3 | S1A  | 55.0(6)   | F3A | C31A S1  | 78.5(12)  |
| S1   | O1 | S1A  | 23.68(17) | F3A | C31A F1  | 136.2(14) |
| S1   | O1 | C31A | 77.3(7)   | F3A | C31A F3  | 149.5(14) |
| F3A  | O1 | S1   | 140.4(15) | F3A | C31A O1  | 27.9(8)   |
| F3A  | O1 | S1A  | 119.0(15) | F3A | C31A C31 | 142.4(16) |
| F3A  | O1 | C31A | 63.5(15)  | F3A | C31A S1A | 110.2(14) |
| C31A | O1 | S1A  | 55.7(7)   | F3A | C31A F1A | 108.7(15) |
| S1   | O2 | S1A  | 30.82(14) | F3A | C31A F2A | 105.1(15) |

<sup>1</sup>1-X,1-Y,1-Z

**Table S13 Torsion Angles for PdPd-1-CH<sub>2</sub>Cl<sub>2</sub>.**

| A    | B    | C    | D                | Angle/°     | A   | B   | C        | D | Angle/°    |
|------|------|------|------------------|-------------|-----|-----|----------|---|------------|
| Pd1  | P1   | C1   | C2               | -159.75(18) | C31 | F1  | C31A S1  |   | -51.1(5)   |
| Pd1  | P1   | C1   | C6               | 25.8(2)     | C31 | F1  | C31A F3  |   | 45.1(4)    |
| Pd1  | P1   | C7   | C8               | -103.6(2)   | C31 | F1  | C31A O1  |   | -92.1(13)  |
| Pd1  | P1   | C7   | C12              | 75.3(2)     | C31 | F1  | C31A S1A |   | -35.3(3)   |
| Pd1  | P1   | C13  | C14              | 37.33(19)   | C31 | F1  | C31A F1A |   | 66.8(12)   |
| Pd1  | P2   | C14  | C13              | 36.36(18)   | C31 | F1  | C31A F2A |   | 162.2(13)  |
| Pd1  | P2   | C21  | C22              | 164.25(19)  | C31 | F1  | C31A F3A |   | -124(2)    |
| Pd1  | P2   | C21  | C26              | -19.0(2)    | C31 | F3  | F1A C31A |   | -13.0(11)  |
| Pd1  | P2   | C27  | C28              | -101.2(2)   | C31 | F3  | C31A S1  |   | 46.6(5)    |
| Pd1  | P2   | C27  | C32              | 73.4(2)     | C31 | F3  | C31A F1  |   | -41.6(3)   |
| Pd1  | P3   | C00G | C00N             | 131.38(19)  | C31 | F3  | C31A O1  |   | 79.2(17)   |
| Pd1  | P3   | C00G | C00S             | -54.3(2)    | C31 | F3  | C31A S1A |   | 22.0(3)    |
| Pd1  | P3   | C00I | C00J             | -131.21(19) | C31 | F3  | C31A F1A |   | 166.1(11)  |
| Pd1  | P3   | C00I | C015             | 51.2(2)     | C31 | F3  | C31A F2A |   | -88.9(10)  |
| Pd1  | P3   | C15  | C16              | -52.19(18)  | C31 | F3  | C31A F3A |   | 124(3)     |
| P1   | C1   | C2   | C3               | -172.2(2)   | C31 | F2  | S1A S1   |   | -113.4(11) |
| P1   | C1   | C6   | C5               | 173.2(2)    | C31 | F2  | S1A F1   |   | 41.7(4)    |
| P1   | C7   | C8   | C9               | 178.8(2)    | C31 | F2  | S1A F3   |   | -27.3(4)   |
| P1   | C7   | C12  | C11              | -179.9(2)   | C31 | F2  | S1A O1   |   | -19.9(8)   |
| P1   | C13  | C14  | P2               | -46.8(2)    | C31 | F2  | S1A O2   |   | -111.7(5)  |
| P2   | C21  | C22  | C23              | 179.9(2)    | C31 | F2  | S1A O3   |   | 150.0(7)   |
| P2   | C21  | C26  | C25              | -178.6(2)   | C31 | F2  | S1A O1A  |   | 117.8(12)  |
| P2   | C27  | C28  | C29              | 174.5(2)    | C31 | F2  | S1A O2A  |   | 17(9)      |
| P2   | C27  | C32  | C17              | -174.7(2)   | C31 | F2  | S1A O3A  |   | -119.2(11) |
| P3   | C00G | C00N | C00W             | 172.7(2)    | C31 | F2  | S1A C31A |   | -5.8(7)    |
| P3   | C00G | C00S | C010             | -171.3(2)   | C31 | S1A | O1A S1   |   | -135.1(8)  |
| P3   | C00I | C00J | C00X             | -178.0(2)   | C31 | S1A | O1A O3   |   | 177.8(12)  |
| P3   | C00I | C015 | C01G             | 179.4(2)    | C31 | S1A | O2A F1   |   | -46.5(14)  |
| P3   | C15  | C16  | C16 <sup>1</sup> | 88.4(3)     | C31 | S1A | O3A S1   |   | 122.1(8)   |
| C00G | P3   | C00I | C00J             | 101.7(2)    | C31 | S1A | O3A O2   |   | 80(6)      |
| C00G | P3   | C00I | C015             | -75.9(2)    | C31 | S1A | C31A S1  |   | -161.6(7)  |
| C00G | P3   | C15  | C16              | 71.22(19)   | C31 | S1A | C31A F1  |   | 48.4(5)    |
| C00G | C00N | C00W | C00H             | -1.3(4)     | C31 | S1A | C31A F3  |   | -31.1(5)   |
| C00G | C00S | C010 | C00H             | -1.9(4)     | C31 | S1A | C31A O1  |   | -176.8(9)  |

|      |      |      |      |             |     |     |      |      |            |
|------|------|------|------|-------------|-----|-----|------|------|------------|
| C00I | P3   | C00G | C00N | -98.1(2)    | C31 | S1A | C31A | F1A  | -58.3(13)  |
| C00I | P3   | C00G | C00S | 76.2(2)     | C31 | S1A | C31A | F2A  | 63.7(14)   |
| C00I | P3   | C15  | C16  | 177.77(17)  | C31 | S1A | C31A | F3A  | -179.2(14) |
| C00I | C00J | C00X | C01C | -0.9(4)     | F2  | C31 | S1A  | S1   | 149.8(6)   |
| C00J | C00I | C015 | C01G | 1.7(4)      | F2  | C31 | S1A  | F1   | -108.5(5)  |
| C00J | C00X | C01C | C01G | 0.9(5)      | F2  | C31 | S1A  | F3   | 114.9(7)   |
| C00N | C00G | C00S | C010 | 3.2(4)      | F2  | C31 | S1A  | O1   | 171.9(3)   |
| C00S | C00G | C00N | C00W | -1.6(4)     | F2  | C31 | S1A  | O2   | 94.9(5)    |
| C00W | C00H | C010 | C00S | -1.1(4)     | F2  | C31 | S1A  | O3   | -97.3(12)  |
| C00X | C01C | C01G | C015 | 0.4(5)      | F2  | C31 | S1A  | O1A  | -99.8(11)  |
| C1   | P1   | C7   | C8   | 126.9(2)    | F2  | C31 | S1A  | O2A  | -5(3)      |
| C1   | P1   | C7   | C12  | -54.2(2)    | F2  | C31 | S1A  | O3A  | 83.5(12)   |
| C1   | P1   | C13  | C14  | 163.48(18)  | F2  | C31 | S1A  | C31A | 174.1(7)   |
| C1   | C2   | C3   | C4   | -1.4(4)     | F2  | C31 | O2A  | F1   | -177(28)   |
| C01C | C01G | C015 | C00I | -1.7(4)     | F2  | C31 | O2A  | S1A  | 74(29)     |
| C2   | C1   | C6   | C5   | -1.2(4)     | F2  | S1A | O1A  | S1   | 161.2(7)   |
| C2   | C3   | C4   | C5   | -0.3(4)     | F2  | S1A | O1A  | O3   | 114.1(16)  |
| C3   | C4   | C5   | C6   | 1.2(4)      | F2  | S1A | O2A  | F1   | 154(10)    |
| C4   | C5   | C6   | C1   | -0.5(4)     | F2  | S1A | O2A  | C31  | -160(11)   |
| C6   | C1   | C2   | C3   | 2.1(4)      | F2  | S1A | O3A  | S1   | 177.1(6)   |
| C7   | P1   | C1   | C2   | -33.1(2)    | F2  | S1A | O3A  | O2   | 135(6)     |
| C7   | P1   | C1   | C6   | 152.5(2)    | F2  | S1A | C31A | S1   | -156.4(5)  |
| C7   | P1   | C13  | C14  | -84.69(19)  | F2  | S1A | C31A | F1   | 53.6(6)    |
| C7   | C8   | C9   | C10  | 0.8(4)      | F2  | S1A | C31A | F3   | -25.9(7)   |
| C8   | C7   | C12  | C11  | -0.9(4)     | F2  | S1A | C31A | O1   | -171.6(5)  |
| C8   | C9   | C10  | C11  | -0.4(5)     | F2  | S1A | C31A | C31  | 5.2(6)     |
| C9   | C10  | C11  | C12  | -0.6(4)     | F2  | S1A | C31A | F1A  | -53.1(14)  |
| C010 | C00H | C00W | C00N | 2.7(4)      | F2  | S1A | C31A | F2A  | 68.9(15)   |
| C10  | C11  | C12  | C7   | 1.3(4)      | F2  | S1A | C31A | F3A  | -173.9(10) |
| C12  | C7   | C8   | C9   | -0.1(4)     | S1A | S1  | O1   | F3A  | -31(3)     |
| C13  | P1   | C1   | C2   | 80.2(2)     | S1A | S1  | O1   | C31A | -22.3(7)   |
| C13  | P1   | C1   | C6   | -94.3(2)    | S1A | S1  | O2   | O3A  | -26(4)     |
| C13  | P1   | C7   | C8   | 15.4(2)     | S1A | S1  | O3   | O1A  | -45.4(15)  |
| C13  | P1   | C7   | C12  | -165.65(19) | S1A | S1  | C31  | F1   | 87.1(8)    |
| C14  | P2   | C21  | C22  | -77.1(2)    | S1A | S1  | C31  | F3   | -153.0(8)  |
| C14  | P2   | C21  | C26  | 99.6(2)     | S1A | S1  | C31  | F2   | -32.9(7)   |
| C14  | P2   | C27  | C28  | 138.8(2)    | S1A | S1  | C31  | O2A  | -28(3)     |
| C14  | P2   | C27  | C32  | -46.5(2)    | S1A | S1  | C31  | C31A | 152.7(10)  |
| C15  | P3   | C00G | C00N | 11.7(2)     | S1A | S1  | O1A  | O3   | 127.2(16)  |
| C15  | P3   | C00G | C00S | -174.02(19) | S1A | S1  | O3A  | O2   | 155(4)     |
| C15  | P3   | C00I | C00J | -7.9(2)     | S1A | S1  | C31A | F1   | 25.8(5)    |
| C15  | P3   | C00I | C015 | 174.52(19)  | S1A | S1  | C31A | F3   | -47.2(6)   |
| C015 | C00I | C00J | C00X | -0.4(4)     | S1A | S1  | C31A | O1   | 160.4(6)   |
| C21  | P2   | C14  | C13  | -84.68(19)  | S1A | S1  | C31A | C31  | -10.8(4)   |
| C21  | P2   | C27  | C28  | 27.2(2)     | S1A | S1  | C31A | F1A  | -91.4(14)  |
| C21  | P2   | C27  | C32  | -158.11(19) | S1A | S1  | C31A | F2A  | 63.2(18)   |
| C21  | C22  | C23  | C24  | -2.3(4)     | S1A | S1  | C31A | F3A  | 163.2(11)  |
| C22  | C21  | C26  | C25  | -1.8(4)     | S1A | F1  | C31  | S1   | -25.8(3)   |
| C22  | C23  | C24  | C25  | -0.2(5)     | S1A | F1  | C31  | F3   | -147.7(7)  |
| C23  | C24  | C25  | C26  | 1.6(5)      | S1A | F1  | C31  | F2   | 97.3(6)    |
| C24  | C25  | C26  | C21  | -0.6(4)     | S1A | F1  | C31  | O2A  | 97(2)      |
| C26  | C21  | C22  | C23  | 3.2(4)      | S1A | F1  | C31  | C31A | -81.7(9)   |
| C27  | P2   | C14  | C13  | 160.06(17)  | S1A | F1  | F2A  | C31A | 14.9(11)   |
| C27  | P2   | C21  | C22  | 34.7(3)     | S1A | F1  | O2A  | C31  | -44.2(14)  |
| C27  | P2   | C21  | C26  | -148.6(2)   | S1A | F1  | C31A | S1   | -15.8(3)   |

|      |      |      |      |            |     |     |      |      |            |
|------|------|------|------|------------|-----|-----|------|------|------------|
| C27  | C28  | C29  | C30  | 0.1(4)     | S1A | F1  | C31A | F3   | 80.3(5)    |
| C28  | C27  | C32  | C17  | 0.1(4)     | S1A | F1  | C31A | O1   | -56.8(11)  |
| C28  | C29  | C30  | C17  | -0.3(4)    | S1A | F1  | C31A | C31  | 35.3(3)    |
| C30  | C17  | C32  | C27  | -0.3(4)    | S1A | F1  | C31A | F1A  | 102.0(13)  |
| C32  | C17  | C30  | C29  | 0.3(4)     | S1A | F1  | C31A | F2A  | -162.6(13) |
| C32  | C27  | C28  | C29  | -0.1(4)    | S1A | F1  | C31A | F3A  | -89(2)     |
| Cl2A | Cl3B | C41  | Cl2B | -110.9(11) | S1A | F3  | C31  | S1   | 14.7(5)    |
| Cl2A | Cl3B | C41  | Cl3A | -101.5(7)  | S1A | F3  | C31  | F1   | 136.8(9)   |
| Cl3B | Cl2A | C41  | Cl2B | 108.2(18)  | S1A | F3  | C31  | F2   | -108.3(7)  |
| Cl3B | Cl2A | C41  | Cl3A | 123.9(7)   | S1A | F3  | C31  | O2A  | -113(3)    |
| S1   | O1   | F3A  | C31A | 9(3)       | S1A | F3  | C31  | C31A | 64.9(9)    |
| S1   | O1   | C31A | F1   | 58.0(10)   | S1A | F3  | F1A  | C31A | -28.9(10)  |
| S1   | O1   | C31A | F3   | -43.8(15)  | S1A | F3  | C31A | S1   | 24.6(3)    |
| S1   | O1   | C31A | C31  | 8.8(8)     | S1A | F3  | C31A | F1   | -63.6(5)   |
| S1   | O1   | C31A | S1A  | 10.6(3)    | S1A | F3  | C31A | O1   | 57.2(16)   |
| S1   | O1   | C31A | F1A  | -99.9(14)  | S1A | F3  | C31A | C31  | -22.0(3)   |
| S1   | O1   | C31A | F2A  | 122.7(15)  | S1A | F3  | C31A | F1A  | 144.1(11)  |
| S1   | O1   | C31A | F3A  | -174.1(18) | S1A | F3  | C31A | F2A  | -110.9(12) |
| S1   | O2   | O3A  | S1A  | 28(3)      | S1A | F3  | C31A | F3A  | 102(3)     |
| S1   | O3   | S1A  | F1   | -120.2(3)  | S1A | O1  | F3A  | S1   | -13.5(11)  |
| S1   | O3   | S1A  | F3   | -37.6(13)  | S1A | O1  | F3A  | C31A | -4.5(17)   |
| S1   | O3   | S1A  | O1   | -31.72(18) | S1A | O1  | C31A | S1   | -10.6(3)   |
| S1   | O3   | S1A  | O2   | 41.0(3)    | S1A | O1  | C31A | F1   | 47.4(9)    |
| S1   | O3   | S1A  | C31  | -128.4(12) | S1A | O1  | C31A | F3   | -54.5(14)  |
| S1   | O3   | S1A  | F2   | 152.4(6)   | S1A | O1  | C31A | C31  | -1.9(6)    |
| S1   | O3   | S1A  | O1A  | -124.2(18) | S1A | O1  | C31A | F1A  | -110.5(16) |
| S1   | O3   | S1A  | O2A  | 163(2)     | S1A | O1  | C31A | F2A  | 112.0(16)  |
| S1   | O3   | S1A  | O3A  | 50.9(10)   | S1A | O1  | C31A | F3A  | 175.3(18)  |
| S1   | O3   | S1A  | C31A | -51.7(6)   | S1A | O2  | O3A  | S1   | -28(3)     |
| S1   | O3   | O1A  | S1A  | 30.8(8)    | S1A | O3  | O1A  | S1   | -30.8(8)   |
| S1   | C31  | F2   | S1A  | 13.0(3)    | S1A | C31 | O2A  | F1   | 109.1(8)   |
| S1   | C31  | S1A  | F1   | 101.7(7)   | S1A | C31 | C31A | S1   | 11.0(4)    |
| S1   | C31  | S1A  | F3   | -34.9(11)  | S1A | C31 | C31A | F1   | -109.3(5)  |
| S1   | C31  | S1A  | O1   | 22.1(4)    | S1A | C31 | C31A | F3   | 137.7(5)   |
| S1   | C31  | S1A  | O2   | -54.9(6)   | S1A | C31 | C31A | O1   | 3.5(10)    |
| S1   | C31  | S1A  | O3   | 112.9(14)  | S1A | C31 | C31A | F1A  | 127.6(11)  |
| S1   | C31  | S1A  | F2   | -149.8(6)  | S1A | C31 | C31A | F2A  | -123.8(12) |
| S1   | C31  | S1A  | O1A  | 110.4(12)  | S1A | C31 | C31A | F3A  | 1(2)       |
| S1   | C31  | S1A  | O2A  | -154(2)    | F1A | F3  | C31  | S1   | -39.1(7)   |
| S1   | C31  | S1A  | O3A  | -66.3(13)  | F1A | F3  | C31  | F1   | 82.9(7)    |
| S1   | C31  | S1A  | C31A | 24.3(9)    | F1A | F3  | C31  | F2   | -162.1(7)  |
| S1   | C31  | O2A  | F1   | 120.5(15)  | F1A | F3  | C31  | S1A  | -53.8(9)   |
| S1   | C31  | O2A  | S1A  | 11.4(10)   | F1A | F3  | C31  | O2A  | -167(3)    |
| S1   | C31  | C31A | F1   | -120.3(5)  | F1A | F3  | C31  | C31A | 11.1(9)    |
| S1   | C31  | C31A | F3   | 126.6(5)   | F1A | F3  | C31A | S1   | -119.5(12) |
| S1   | C31  | C31A | O1   | -7.5(7)    | F1A | F3  | C31A | F1   | 152.3(12)  |
| S1   | C31  | C31A | S1A  | -11.0(4)   | F1A | F3  | C31A | O1   | -86.9(18)  |
| S1   | C31  | C31A | F1A  | 116.6(11)  | F1A | F3  | C31A | C31  | -166.1(11) |
| S1   | C31  | C31A | F2A  | -134.8(13) | F1A | F3  | C31A | S1A  | -144.1(12) |
| S1   | C31  | C31A | F3A  | -10(2)     | F1A | F3  | C31A | F2A  | 104.9(15)  |
| S1   | S1A  | O1A  | O3   | -47.1(15)  | F1A | F3  | C31A | F3A  | -42(3)     |
| S1   | S1A  | O2A  | F1   | -132(4)    | F2A | F1  | C31  | S1   | 68.4(6)    |
| S1   | S1A  | O2A  | C31  | -85(5)     | F2A | F1  | C31  | F3   | -53.5(7)   |
| S1   | S1A  | O3A  | O2   | -42(5)     | F2A | F1  | C31  | F2   | -168.4(7)  |
| S1   | S1A  | C31A | F1   | -150.0(6)  | F2A | F1  | C31  | S1A  | 94.3(7)    |

|    |     |      |      |            |     |    |      |      |            |
|----|-----|------|------|------------|-----|----|------|------|------------|
| S1 | S1A | C31A | F3   | 130.5(6)   | F2A | F1 | C31  | O2A  | -169(2)    |
| S1 | S1A | C31A | O1   | -15.2(5)   | F2A | F1 | C31  | C31A | 12.6(9)    |
| S1 | S1A | C31A | C31  | 161.6(7)   | F2A | F1 | S1A  | S1   | 24.5(7)    |
| S1 | S1A | C31A | F1A  | 103.3(13)  | F2A | F1 | S1A  | F3   | -70.2(6)   |
| S1 | S1A | C31A | F2A  | -134.7(15) | F2A | F1 | S1A  | O1   | 16.1(6)    |
| S1 | S1A | C31A | F3A  | -17.6(11)  | F2A | F1 | S1A  | O2   | -38.3(9)   |
| S1 | F3A | C31A | F1   | 77.8(18)   | F2A | F1 | S1A  | O3   | 93.9(6)    |
| S1 | F3A | C31A | F3   | -82(3)     | F2A | F1 | S1A  | C31  | -91.1(8)   |
| S1 | F3A | C31A | O1   | 4.7(14)    | F2A | F1 | S1A  | F2   | -143.2(6)  |
| S1 | F3A | C31A | C31  | 8.9(18)    | F2A | F1 | S1A  | O1A  | 95.8(10)   |
| S1 | F3A | C31A | S1A  | 9.7(6)     | F2A | F1 | S1A  | O2A  | -138.2(17) |
| S1 | F3A | C31A | F1A  | -112.9(14) | F2A | F1 | S1A  | O3A  | -57(3)     |
| S1 | F3A | C31A | F2A  | 131.5(14)  | F2A | F1 | S1A  | C31A | -12.3(9)   |
| F1 | C31 | F2   | S1A  | -109.4(6)  | F2A | F1 | O2A  | C31  | 15(3)      |
| F1 | C31 | S1A  | S1   | -101.7(7)  | F2A | F1 | O2A  | S1A  | 59(2)      |
| F1 | C31 | S1A  | F3   | -136.7(8)  | F2A | F1 | C31A | S1   | 146.8(14)  |
| F1 | C31 | S1A  | O1   | -79.7(5)   | F2A | F1 | C31A | F3   | -117.1(13) |
| F1 | C31 | S1A  | O2   | -156.7(4)  | F2A | F1 | C31A | O1   | 105.7(16)  |
| F1 | C31 | S1A  | O3   | 11.2(14)   | F2A | F1 | C31A | C31  | -162.2(13) |
| F1 | C31 | S1A  | F2   | 108.5(5)   | F2A | F1 | C31A | S1A  | 162.6(13)  |
| F1 | C31 | S1A  | O1A  | 8.7(12)    | F2A | F1 | C31A | F1A  | -95.4(17)  |
| F1 | C31 | S1A  | O2A  | 104(2)     | F2A | F1 | C31A | F3A  | 73(2)      |
| F1 | C31 | S1A  | O3A  | -168.0(12) | F3A | S1 | O1   | S1A  | 31(3)      |
| F1 | C31 | S1A  | C31A | -77.4(7)   | F3A | S1 | O1   | C31A | 8(2)       |
| F1 | C31 | O2A  | S1A  | -109.1(8)  | F3A | S1 | O2   | S1A  | -122.1(6)  |
| F1 | C31 | C31A | S1   | 120.3(5)   | F3A | S1 | O2   | O3A  | -148(4)    |
| F1 | C31 | C31A | F3   | -113.0(5)  | F3A | S1 | O3   | S1A  | 110.1(6)   |
| F1 | C31 | C31A | O1   | 112.8(11)  | F3A | S1 | O3   | O1A  | 64.6(16)   |
| F1 | C31 | C31A | S1A  | 109.3(5)   | F3A | S1 | C31  | F1   | -61.7(6)   |
| F1 | C31 | C31A | F1A  | -123.1(11) | F3A | S1 | C31  | F3   | 58.2(5)    |
| F1 | C31 | C31A | F2A  | -14.5(10)  | F3A | S1 | C31  | F2   | 178.2(6)   |
| F1 | C31 | C31A | F3A  | 111(2)     | F3A | S1 | C31  | S1A  | -148.8(8)  |
| F1 | S1A | O1A  | S1   | -129.2(4)  | F3A | S1 | C31  | O2A  | -177(3)    |
| F1 | S1A | O1A  | O3   | -176.3(16) | F3A | S1 | C31  | C31A | 3.8(8)     |
| F1 | S1A | O2A  | C31  | 46.5(14)   | F3A | S1 | S1A  | F1   | -22.0(7)   |
| F1 | S1A | O3A  | S1   | 96(3)      | F3A | S1 | S1A  | F3   | 50.2(6)    |
| F1 | S1A | O3A  | O2   | 54(8)      | F3A | S1 | S1A  | O1   | -6.8(6)    |
| F1 | S1A | C31A | S1   | 150.0(6)   | F3A | S1 | S1A  | O2   | 125.3(6)   |
| F1 | S1A | C31A | F3   | -79.5(6)   | F3A | S1 | S1A  | O3   | -120.6(5)  |
| F1 | S1A | C31A | O1   | 134.8(9)   | F3A | S1 | S1A  | C31  | 33.7(9)    |
| F1 | S1A | C31A | C31  | -48.4(5)   | F3A | S1 | S1A  | F2   | 127.6(11)  |
| F1 | S1A | C31A | F1A  | -106.7(14) | F3A | S1 | S1A  | O1A  | -97.1(9)   |
| F1 | S1A | C31A | F2A  | 15.3(11)   | F3A | S1 | S1A  | O2A  | 101(5)     |
| F1 | S1A | C31A | F3A  | 132.5(14)  | F3A | S1 | S1A  | O3A  | 134.7(13)  |
| F1 | F2A | C31A | S1   | -48.3(18)  | F3A | S1 | S1A  | C31A | 11.4(8)    |
| F1 | F2A | C31A | F3   | 60.1(9)    | F3A | S1 | O1A  | O3   | -126.7(13) |
| F1 | F2A | C31A | O1   | -110.9(14) | F3A | S1 | O1A  | S1A  | 106.1(7)   |
| F1 | F2A | C31A | C31  | 12.3(9)    | F3A | S1 | O3A  | O2   | 41(4)      |
| F1 | F2A | C31A | S1A  | -16.5(12)  | F3A | S1 | O3A  | S1A  | -113.6(13) |
| F1 | F2A | C31A | F1A  | 107.5(14)  | F3A | S1 | C31A | F1   | -137.4(13) |
| F1 | F2A | C31A | F3A  | -136.6(14) | F3A | S1 | C31A | F3   | 149.6(13)  |
| F3 | C31 | F2   | S1A  | 135.3(5)   | F3A | S1 | C31A | O1   | -2.8(9)    |
| F3 | C31 | S1A  | S1   | 34.9(11)   | F3A | S1 | C31A | C31  | -174.0(13) |
| F3 | C31 | S1A  | F1   | 136.7(8)   | F3A | S1 | C31A | S1A  | -163.2(11) |
| F3 | C31 | S1A  | O1   | 57.0(7)    | F3A | S1 | C31A | F1A  | 105.4(17)  |

|    |     |      |      |            |     |     |      |      |            |
|----|-----|------|------|------------|-----|-----|------|------|------------|
| F3 | C31 | S1A  | O2   | -20.0(8)   | F3A | S1  | C31A | F2A  | -100(2)    |
| F3 | C31 | S1A  | O3   | 147.9(9)   | F3A | O1  | C31A | S1   | 174.1(18)  |
| F3 | C31 | S1A  | F2   | -114.9(7)  | F3A | O1  | C31A | F1   | -128(2)    |
| F3 | C31 | S1A  | O1A  | 145.4(10)  | F3A | O1  | C31A | F3   | 130(2)     |
| F3 | C31 | S1A  | O2A  | -120(2)    | F3A | O1  | C31A | C31  | -177(2)    |
| F3 | C31 | S1A  | O3A  | -31.4(14)  | F3A | O1  | C31A | S1A  | -175.3(18) |
| F3 | C31 | S1A  | C31A | 59.2(8)    | F3A | O1  | C31A | F1A  | 74(2)      |
| F3 | C31 | O2A  | F1   | -114.0(13) | F3A | O1  | C31A | F2A  | -63(2)     |
| F3 | C31 | O2A  | S1A  | 136.9(11)  | O1A | S1  | O1   | S1A  | -66.1(9)   |
| F3 | C31 | C31A | S1   | -126.6(5)  | O1A | S1  | O1   | F3A  | -97(3)     |
| F3 | C31 | C31A | F1   | 113.0(5)   | O1A | S1  | O1   | C31A | -88.5(10)  |
| F3 | C31 | C31A | O1   | -134.2(11) | O1A | S1  | O2   | S1A  | 63.3(12)   |
| F3 | C31 | C31A | S1A  | -137.7(5)  | O1A | S1  | O2   | O3A  | 37(4)      |
| F3 | C31 | C31A | F1A  | -10.0(9)   | O1A | S1  | O3   | S1A  | 45.4(15)   |
| F3 | C31 | C31A | F2A  | 98.5(12)   | O1A | S1  | C31  | F1   | 43.9(7)    |
| F3 | C31 | C31A | F3A  | -136(2)    | O1A | S1  | C31  | F3   | 163.8(7)   |
| F3 | S1A | O1A  | S1   | -104.9(15) | O1A | S1  | C31  | F2   | -76.2(8)   |
| F3 | S1A | O1A  | O3   | -152.0(10) | O1A | S1  | C31  | S1A  | -43.2(10)  |
| F3 | S1A | O2A  | F1   | -74.5(9)   | O1A | S1  | C31  | O2A  | -72(3)     |
| F3 | S1A | O2A  | C31  | -28.0(11)  | O1A | S1  | C31  | C31A | 109.5(9)   |
| F3 | S1A | O3A  | S1   | 107.8(7)   | O1A | S1  | S1A  | F1   | 75.1(8)    |
| F3 | S1A | O3A  | O2   | 66(6)      | O1A | S1  | S1A  | F3   | 147.2(9)   |
| F3 | S1A | C31A | S1   | -130.5(6)  | O1A | S1  | S1A  | O1   | 90.2(8)    |
| F3 | S1A | C31A | F1   | 79.5(6)    | O1A | S1  | S1A  | O2   | -137.7(8)  |
| F3 | S1A | C31A | O1   | -145.7(9)  | O1A | S1  | S1A  | O3   | -23.5(8)   |
| F3 | S1A | C31A | C31  | 31.1(5)    | O1A | S1  | S1A  | C31  | 130.8(11)  |
| F3 | S1A | C31A | F1A  | -27.2(10)  | O1A | S1  | S1A  | F2   | -135.3(14) |
| F3 | S1A | C31A | F2A  | 94.8(15)   | O1A | S1  | S1A  | O2A  | -162(5)    |
| F3 | S1A | C31A | F3A  | -148.0(15) | O1A | S1  | S1A  | O3A  | -128.3(14) |
| F3 | F1A | C31A | S1   | 73.1(12)   | O1A | S1  | S1A  | C31A | 108.5(10)  |
| F3 | F1A | C31A | F1   | -29.2(11)  | O1A | S1  | O3A  | O2   | -152(3)    |
| F3 | F1A | C31A | O1   | 130.5(14)  | O1A | S1  | O3A  | S1A  | 53.1(12)   |
| F3 | F1A | C31A | C31  | 10.2(8)    | O1A | S1  | C31A | F1   | -32.1(9)   |
| F3 | F1A | C31A | S1A  | 37.2(12)   | O1A | S1  | C31A | F3   | -105.1(9)  |
| F3 | F1A | C31A | F2A  | -87.5(13)  | O1A | S1  | C31A | O1   | 102.5(8)   |
| F3 | F1A | C31A | F3A  | 158.9(14)  | O1A | S1  | C31A | C31  | -68.7(8)   |
| O1 | S1  | O2   | S1A  | -136.0(3)  | O1A | S1  | C31A | S1A  | -57.9(8)   |
| O1 | S1  | O2   | O3A  | -162(4)    | O1A | S1  | C31A | F1A  | -149.3(14) |
| O1 | S1  | O3   | S1A  | 121.8(3)   | O1A | S1  | C31A | F2A  | 5(2)       |
| O1 | S1  | O3   | O1A  | 76.4(15)   | O1A | S1  | C31A | F3A  | 105.3(12)  |
| O1 | S1  | C31  | F1   | -58.4(4)   | O1A | O3  | S1A  | S1   | 124.2(18)  |
| O1 | S1  | C31  | F3   | 61.5(3)    | O1A | O3  | S1A  | F1   | 4.1(18)    |
| O1 | S1  | C31  | F2   | -178.5(4)  | O1A | O3  | S1A  | F3   | 87(2)      |
| O1 | S1  | C31  | S1A  | -145.5(7)  | O1A | O3  | S1A  | O1   | 92.5(17)   |
| O1 | S1  | C31  | O2A  | -174(3)    | O1A | O3  | S1A  | O2   | 165.2(18)  |
| O1 | S1  | C31  | C31A | 7.2(7)     | O1A | O3  | S1A  | C31  | -4(2)      |
| O1 | S1  | S1A  | F1   | -15.2(5)   | O1A | O3  | S1A  | F2   | -83.4(18)  |
| O1 | S1  | S1A  | F3   | 57.0(4)    | O1A | O3  | S1A  | O2A  | -73(3)     |
| O1 | S1  | S1A  | O2   | 132.1(4)   | O1A | O3  | S1A  | O3A  | 175(2)     |
| O1 | S1  | S1A  | O3   | -113.8(3)  | O1A | O3  | S1A  | C31A | 72.6(18)   |
| O1 | S1  | S1A  | C31  | 40.5(8)    | O1A | S1A | O2A  | F1   | 68.4(16)   |
| O1 | S1  | S1A  | F2   | 134.4(10)  | O1A | S1A | O2A  | C31  | 115.0(19)  |
| O1 | S1  | S1A  | O1A  | -90.2(8)   | O1A | S1A | O3A  | S1   | -55.1(13)  |
| O1 | S1  | S1A  | O2A  | 108(5)     | O1A | S1A | O3A  | O2   | -97(6)     |
| O1 | S1  | S1A  | O3A  | 141.5(12)  | O1A | S1A | C31A | S1   | 72.7(11)   |

|    |     |      |      |            |     |     |      |      |            |
|----|-----|------|------|------------|-----|-----|------|------|------------|
| O1 | S1  | S1A  | C31A | 18.2(6)    | O1A | S1A | C31A | F1   | -77.4(11)  |
| O1 | S1  | O1A  | O3   | -113.8(13) | O1A | S1A | C31A | F3   | -156.9(11) |
| O1 | S1  | O1A  | S1A  | 119.1(4)   | O1A | S1A | C31A | O1   | 57.5(12)   |
| O1 | S1  | O3A  | O2   | 24(5)      | O1A | S1A | C31A | C31  | -125.8(12) |
| O1 | S1  | O3A  | S1A  | -131.1(12) | O1A | S1A | C31A | F1A  | 176.0(15)  |
| O1 | S1  | C31A | F1   | -134.6(9)  | O1A | S1A | C31A | F2A  | -62.1(18)  |
| O1 | S1  | C31A | F3   | 152.4(10)  | O1A | S1A | C31A | F3A  | 55.1(16)   |
| O1 | S1  | C31A | C31  | -171.1(8)  | O2A | F1  | C31  | S1   | -123(2)    |
| O1 | S1  | C31A | S1A  | -160.4(6)  | O2A | F1  | C31  | F3   | 115(2)     |
| O1 | S1  | C31A | F1A  | 108.3(15)  | O2A | F1  | C31  | F2   | 0(2)       |
| O1 | S1  | C31A | F2A  | -97(2)     | O2A | F1  | C31  | S1A  | -97(2)     |
| O1 | S1  | C31A | F3A  | 2.8(9)     | O2A | F1  | C31  | C31A | -179(2)    |
| O1 | S1A | O1A  | S1   | -34.69(19) | O2A | F1  | S1A  | S1   | 162.7(17)  |
| O1 | S1A | O1A  | O3   | -81.8(16)  | O2A | F1  | S1A  | F3   | 68.0(16)   |
| O1 | S1A | O2A  | F1   | -53(3)     | O2A | F1  | S1A  | O1   | 154.3(16)  |
| O1 | S1A | O2A  | C31  | -6(4)      | O2A | F1  | S1A  | O2   | 99.9(17)   |
| O1 | S1A | O3A  | S1   | 20.7(6)    | O2A | F1  | S1A  | O3   | -127.9(16) |
| O1 | S1A | O3A  | O2   | -21(6)     | O2A | F1  | S1A  | C31  | 47.1(17)   |
| O1 | S1A | C31A | S1   | 15.2(5)    | O2A | F1  | S1A  | F2   | -5.0(18)   |
| O1 | S1A | C31A | F1   | -134.8(9)  | O2A | F1  | S1A  | O1A  | -126.0(18) |
| O1 | S1A | C31A | F3   | 145.7(9)   | O2A | F1  | S1A  | O3A  | 81(3)      |
| O1 | S1A | C31A | C31  | 176.8(9)   | O2A | F1  | S1A  | C31A | 125.9(18)  |
| O1 | S1A | C31A | F1A  | 118.5(15)  | O2A | F1  | F2A  | C31A | -23(2)     |
| O1 | S1A | C31A | F2A  | -119.5(17) | O2A | F1  | C31A | S1   | -50.4(13)  |
| O1 | S1A | C31A | F3A  | -2.4(9)    | O2A | F1  | C31A | F3   | 45.7(13)   |
| O1 | F3A | C31A | S1   | -4.7(14)   | O2A | F1  | C31A | O1   | -91.5(16)  |
| O1 | F3A | C31A | F1   | 73(2)      | O2A | F1  | C31A | C31  | 0.6(12)    |
| O1 | F3A | C31A | F3   | -87(3)     | O2A | F1  | C31A | S1A  | -34.6(12)  |
| O1 | F3A | C31A | C31  | 4(3)       | O2A | F1  | C31A | F1A  | 67.4(17)   |
| O1 | F3A | C31A | S1A  | 5.0(19)    | O2A | F1  | C31A | F2A  | 162.8(15)  |
| O1 | F3A | C31A | F1A  | -117.6(19) | O2A | F1  | C31A | F3A  | -124(2)    |
| O1 | F3A | C31A | F2A  | 126.9(18)  | O2A | C31 | F2   | S1A  | -107(29)   |
| O2 | S1  | O1   | S1A  | 127.1(4)   | O2A | C31 | S1A  | S1   | 154(2)     |
| O2 | S1  | O1   | F3A  | 96(2)      | O2A | C31 | S1A  | F1   | -104(2)    |
| O2 | S1  | O1   | C31A | 104.8(7)   | O2A | C31 | S1A  | F3   | 120(2)     |
| O2 | S1  | O3   | S1A  | -101.2(3)  | O2A | C31 | S1A  | O1   | 177(2)     |
| O2 | S1  | O3   | O1A  | -146.7(15) | O2A | C31 | S1A  | O2   | 100(2)     |
| O2 | S1  | C31  | F1   | -179.0(4)  | O2A | C31 | S1A  | O3   | -93(3)     |
| O2 | S1  | C31  | F3   | -59.0(4)   | O2A | C31 | S1A  | F2   | 5(3)       |
| O2 | S1  | C31  | F2   | 61.0(5)    | O2A | C31 | S1A  | O1A  | -95(3)     |
| O2 | S1  | C31  | S1A  | 93.9(7)    | O2A | C31 | S1A  | O3A  | 88(3)      |
| O2 | S1  | C31  | O2A  | 66(3)      | O2A | C31 | S1A  | C31A | 179(3)     |
| O2 | S1  | C31  | C31A | -113.4(7)  | O2A | S1A | O1A  | S1   | 173.5(19)  |
| O2 | S1  | S1A  | F1   | -147.2(4)  | O2A | S1A | O1A  | O3   | 126(2)     |
| O2 | S1  | S1A  | F3   | -75.1(3)   | O2A | S1A | O3A  | S1   | 169.0(16)  |
| O2 | S1  | S1A  | O1   | -132.1(4)  | O2A | S1A | O3A  | O2   | 127(6)     |
| O2 | S1  | S1A  | O3   | 114.2(3)   | O2A | S1A | C31A | S1   | -160.7(18) |
| O2 | S1  | S1A  | C31  | -91.6(7)   | O2A | S1A | C31A | F1   | 49.3(18)   |
| O2 | S1  | S1A  | F2   | 2.3(11)    | O2A | S1A | C31A | F3   | -30.2(18)  |
| O2 | S1  | S1A  | O1A  | 137.7(8)   | O2A | S1A | C31A | O1   | -175.9(18) |
| O2 | S1  | S1A  | O2A  | -24(5)     | O2A | S1A | C31A | C31  | 0.9(18)    |
| O2 | S1  | S1A  | O3A  | 9.4(13)    | O2A | S1A | C31A | F1A  | -57(2)     |
| O2 | S1  | S1A  | C31A | -113.9(6)  | O2A | S1A | C31A | F2A  | 65(2)      |
| O2 | S1  | O1A  | O3   | 48(2)      | O2A | S1A | C31A | F3A  | -178(2)    |
| O2 | S1  | O1A  | S1A  | -79.0(11)  | O3A | S1  | O1   | S1A  | 117.6(18)  |



|    |     |      |      |            |      |     |      |      |            |
|----|-----|------|------|------------|------|-----|------|------|------------|
| O2 | S1  | O3A  | S1A  | -155(4)    | O3A  | S1  | O1   | F3A  | 87(3)      |
| O2 | S1  | C31A | F1   | 122.9(5)   | O3A  | S1  | O1   | C31A | 95.3(19)   |
| O2 | S1  | C31A | F3   | 49.9(8)    | O3A  | S1  | O2   | S1A  | 26(4)      |
| O2 | S1  | C31A | O1   | -102.5(6)  | O3A  | S1  | O3   | S1A  | -81.6(12)  |
| O2 | S1  | C31A | C31  | 86.3(6)    | O3A  | S1  | O3   | O1A  | -127.0(19) |
| O2 | S1  | C31A | S1A  | 97.1(4)    | O3A  | S1  | C31  | F1   | 164.6(12)  |
| O2 | S1  | C31A | F1A  | 5.7(16)    | O3A  | S1  | C31  | F3   | -75.4(11)  |
| O2 | S1  | C31A | F2A  | 160.2(17)  | O3A  | S1  | C31  | F2   | 44.6(12)   |
| O2 | S1  | C31A | F3A  | -99.7(10)  | O3A  | S1  | C31  | S1A  | 77.5(13)   |
| O2 | S1A | O1A  | S1   | 31.2(5)    | O3A  | S1  | C31  | O2A  | 49(3)      |
| O2 | S1A | O1A  | O3   | -15.9(19)  | O3A  | S1  | C31  | C31A | -129.8(13) |
| O2 | S1A | O2A  | F1   | -151.2(5)  | O3A  | S1  | S1A  | F1   | -156.6(12) |
| O2 | S1A | O2A  | C31  | -104.7(18) | O3A  | S1  | S1A  | F3   | -84.5(12)  |
| O2 | S1A | O3A  | S1   | 42(5)      | O3A  | S1  | S1A  | O1   | -141.5(12) |
| O2 | S1A | C31A | S1   | -41.0(3)   | O3A  | S1  | S1A  | O2   | -9.4(13)   |
| O2 | S1A | C31A | F1   | 169.0(4)   | O3A  | S1  | S1A  | O3   | 104.8(12)  |
| O2 | S1A | C31A | F3   | 89.5(5)    | O3A  | S1  | S1A  | C31  | -101.0(13) |
| O2 | S1A | C31A | O1   | -56.2(7)   | O3A  | S1  | S1A  | F2   | -7.1(16)   |
| O2 | S1A | C31A | C31  | 120.6(5)   | O3A  | S1  | S1A  | O1A  | 128.3(14)  |
| O2 | S1A | C31A | F1A  | 62.3(13)   | O3A  | S1  | S1A  | O2A  | -34(5)     |
| O2 | S1A | C31A | F2A  | -175.7(14) | O3A  | S1  | S1A  | C31A | -123.3(13) |
| O2 | S1A | C31A | F3A  | -58.6(12)  | O3A  | S1  | O1A  | O3   | 63(2)      |
| O3 | S1  | O1   | S1A  | -96.0(3)   | O3A  | S1  | O1A  | S1A  | -63.9(16)  |
| O3 | S1  | O1   | F3A  | -127(2)    | O3A  | S1  | C31A | F1   | 98.4(14)   |
| O3 | S1  | O1   | C31A | -118.3(7)  | O3A  | S1  | C31A | F3   | 25.4(15)   |
| O3 | S1  | O2   | S1A  | 87.4(3)    | O3A  | S1  | C31A | O1   | -127.0(13) |
| O3 | S1  | O2   | O3A  | 62(4)      | O3A  | S1  | C31A | C31  | 61.8(14)   |
| O3 | S1  | C31  | F1   | 61.0(4)    | O3A  | S1  | C31A | S1A  | 72.6(13)   |
| O3 | S1  | C31  | F3   | -179.1(3)  | O3A  | S1  | C31A | F1A  | -19(2)     |
| O3 | S1  | C31  | F2   | -59.1(4)   | O3A  | S1  | C31A | F2A  | 136(2)     |
| O3 | S1  | C31  | S1A  | -26.1(7)   | O3A  | S1  | C31A | F3A  | -124.2(15) |
| O3 | S1  | C31  | O2A  | -54(3)     | O3A  | S1A | O1A  | S1   | 42.0(11)   |
| O3 | S1  | C31  | C31A | 126.6(7)   | O3A  | S1A | O1A  | O3   | -5(2)      |
| O3 | S1  | S1A  | F1   | 98.6(4)    | O3A  | S1A | O2A  | F1   | -160.3(11) |
| O3 | S1  | S1A  | F3   | 170.8(3)   | O3A  | S1A | O2A  | C31  | -114(2)    |
| O3 | S1  | S1A  | O1   | 113.8(3)   | O3A  | S1A | C31A | S1   | -43.5(10)  |
| O3 | S1  | S1A  | O2   | -114.2(3)  | O3A  | S1A | C31A | F1   | 166.5(10)  |
| O3 | S1  | S1A  | C31  | 154.3(7)   | O3A  | S1A | C31A | F3   | 87.0(11)   |
| O3 | S1  | S1A  | F2   | -111.8(11) | O3A  | S1A | C31A | O1   | -58.7(12)  |
| O3 | S1  | S1A  | O1A  | 23.5(8)    | O3A  | S1A | C31A | C31  | 118.1(11)  |
| O3 | S1  | S1A  | O2A  | -139(5)    | O3A  | S1A | C31A | F1A  | 59.8(17)   |
| O3 | S1  | S1A  | O3A  | -104.8(12) | O3A  | S1A | C31A | F2A  | -178.2(16) |
| O3 | S1  | S1A  | C31A | 132.0(6)   | O3A  | S1A | C31A | F3A  | -61.0(16)  |
| O3 | S1  | O1A  | S1A  | -127.2(16) | C31A | S1  | O1   | S1A  | 22.3(7)    |
| O3 | S1  | O3A  | O2   | -125(3)    | C31A | S1  | O1   | F3A  | -8(2)      |
| O3 | S1  | O3A  | S1A  | 80.2(4)    | C31A | S1  | O2   | S1A  | -77.8(7)   |
| O3 | S1  | C31A | F1   | -40.4(10)  | C31A | S1  | O2   | O3A  | -104(4)    |
| O3 | S1  | C31A | F3   | -113.4(6)  | C31A | S1  | O3   | S1A  | 62.2(8)    |
| O3 | S1  | C31A | O1   | 94.2(6)    | C31A | S1  | O3   | O1A  | 16.8(17)   |
| O3 | S1  | C31A | C31  | -77.0(7)   | C31A | S1  | C31  | F1   | -65.6(7)   |
| O3 | S1  | C31A | S1A  | -66.2(6)   | C31A | S1  | C31  | F3   | 54.4(7)    |
| O3 | S1  | C31A | F1A  | -157.6(10) | C31A | S1  | C31  | F2   | 174.4(8)   |
| O3 | S1  | C31A | F2A  | -3(2)      | C31A | S1  | C31  | S1A  | -152.7(10) |
| O3 | S1  | C31A | F3A  | 97.0(10)   | C31A | S1  | C31  | O2A  | 179(3)     |
| O3 | S1A | O1A  | S1   | 47.1(15)   | C31A | S1  | S1A  | F1   | -33.4(7)   |

|     |     |      |      |            |         |     |     |            |
|-----|-----|------|------|------------|---------|-----|-----|------------|
| O3  | S1A | O2A  | F1   | 99.6(16)   | C31AS1  | S1A | F3  | 38.8(6)    |
| O3  | S1A | O2A  | C31  | 146.2(11)  | C31AS1  | S1A | O1  | -18.2(6)   |
| O3  | S1A | O3A  | S1   | -57.6(7)   | C31AS1  | S1A | O2  | 113.9(6)   |
| O3  | S1A | O3A  | O2   | -99(6)     | C31AS1  | S1A | O3  | -132.0(6)  |
| O3  | S1A | C31A | S1   | 45.0(4)    | C31AS1  | S1A | C31 | 22.3(8)    |
| O3  | S1A | C31A | F1   | -105.0(5)  | C31AS1  | S1A | F2  | 116.2(12)  |
| O3  | S1A | C31A | F3   | 175.5(4)   | C31AS1  | S1A | O1A | -108.5(10) |
| O3  | S1A | C31A | O1   | 29.9(8)    | C31AS1  | S1A | O2A | 89(5)      |
| O3  | S1A | C31A | C31  | -153.4(6)  | C31AS1  | S1A | O3A | 123.3(13)  |
| O3  | S1A | C31A | F1A  | 148.4(11)  | C31AS1  | O1A | O3  | -166.4(14) |
| O3  | S1A | C31A | F2A  | -89.7(15)  | C31AS1  | O1A | S1A | 66.4(8)    |
| O3  | S1A | C31A | F3A  | 27.5(14)   | C31AS1  | O3A | O2  | 88(4)      |
| C31 | S1  | O1   | S1A  | 15.1(3)    | C31AS1  | O3A | S1A | -66.8(9)   |
| C31 | S1  | O1   | F3A  | -16(3)     | C31AF1  | C31 | S1  | 55.9(8)    |
| C31 | S1  | O1   | C31A | -7.2(7)    | C31AF1  | C31 | F3  | -66.0(8)   |
| C31 | S1  | O2   | S1A  | -23.6(3)   | C31AF1  | C31 | F2  | 179.0(9)   |
| C31 | S1  | O2   | O3A  | -49(4)     | C31AF1  | C31 | S1A | 81.7(9)    |
| C31 | S1  | O3   | S1A  | 10.0(3)    | C31AF1  | C31 | O2A | 179(2)     |
| C31 | S1  | O3   | O1A  | -35.4(15)  | C31AF1  | S1A | S1  | 36.8(8)    |
| C31 | S1  | S1A  | F1   | -55.7(7)   | C31AF1  | S1A | F3  | -57.9(7)   |
| C31 | S1  | S1A  | F3   | 16.5(5)    | C31AF1  | S1A | O1  | 28.4(7)    |
| C31 | S1  | S1A  | O1   | -40.5(8)   | C31AF1  | S1A | O2  | -26.0(10)  |
| C31 | S1  | S1A  | O2   | 91.6(7)    | C31AF1  | S1A | O3  | 106.2(8)   |
| C31 | S1  | S1A  | O3   | -154.3(7)  | C31AF1  | S1A | C31 | -78.8(8)   |
| C31 | S1  | S1A  | F2   | 93.9(12)   | C31AF1  | S1A | F2  | -130.9(7)  |
| C31 | S1  | S1A  | O1A  | -130.8(11) | C31AF1  | S1A | O1A | 108.1(10)  |
| C31 | S1  | S1A  | O2A  | 67(5)      | C31AF1  | S1A | O2A | -125.9(18) |
| C31 | S1  | S1A  | O3A  | 101.0(13)  | C31AF1  | S1A | O3A | -45(3)     |
| C31 | S1  | S1A  | C31A | -22.3(8)   | C31AF1  | O2A | C31 | -1(2)      |
| C31 | S1  | O1A  | O3   | 144.7(15)  | C31AF1  | O2A | S1A | 43.2(13)   |
| C31 | S1  | O1A  | S1A  | 17.5(4)    | C31AF3  | C31 | S1  | -50.2(7)   |
| C31 | S1  | O3A  | O2   | 132(3)     | C31AF3  | C31 | F1  | 71.8(7)    |
| C31 | S1  | O3A  | S1A  | -22.5(3)   | C31AF3  | C31 | F2  | -173.3(8)  |
| C31 | S1  | C31A | F1   | 36.6(4)    | C31AF3  | C31 | S1A | -64.9(9)   |
| C31 | S1  | C31A | F3   | -36.4(4)   | C31AF3  | C31 | O2A | -178(3)    |
| C31 | S1  | C31A | O1   | 171.1(8)   | C31AO1  | F3A | S1  | -9(3)      |
| C31 | S1  | C31A | S1A  | 10.8(4)    | C31AC31 | S1A | S1  | -24.3(9)   |
| C31 | S1  | C31A | F1A  | -80.6(14)  | C31AC31 | S1A | F1  | 77.4(7)    |
| C31 | S1  | C31A | F2A  | 73.9(18)   | C31AC31 | S1A | F3  | -59.2(8)   |
| C31 | S1  | C31A | F3A  | 174.0(13)  | C31AC31 | S1A | O1  | -2.2(6)    |
| C31 | F1  | S1A  | S1   | 115.6(7)   | C31AC31 | S1A | O2  | -79.2(7)   |
| C31 | F1  | S1A  | F3   | 20.8(5)    | C31AC31 | S1A | O3  | 88.6(13)   |
| C31 | F1  | S1A  | O1   | 107.2(5)   | C31AC31 | S1A | F2  | -174.1(7)  |
| C31 | F1  | S1A  | O2   | 52.8(8)    | C31AC31 | S1A | O1A | 86.1(12)   |
| C31 | F1  | S1A  | O3   | -175.0(6)  | C31AC31 | S1A | O2A | -179(3)    |
| C31 | F1  | S1A  | F2   | -52.1(5)   | C31AC31 | S1A | O3A | -90.6(13)  |
| C31 | F1  | S1A  | O1A  | -173.1(10) | C31AS1A | O1A | S1  | -69.6(7)   |
| C31 | F1  | S1A  | O2A  | -47.1(17)  | C31AS1A | O1A | O3  | -116.7(16) |
| C31 | F1  | S1A  | O3A  | 34(3)      | C31AS1A | O2A | F1  | -47.7(12)  |
| C31 | F1  | S1A  | C31A | 78.8(9)    | C31AS1A | O2A | C31 | -1(2)      |
| C31 | F1  | F2A  | C31A | -15.1(11)  | C31AS1A | O3A | S1  | 56.0(11)   |
| C31 | F1  | O2A  | S1A  | 44.2(14)   | C31AS1A | O3A | O2  | 14(6)      |

<sup>1</sup>1-X,1-Y,1-Z

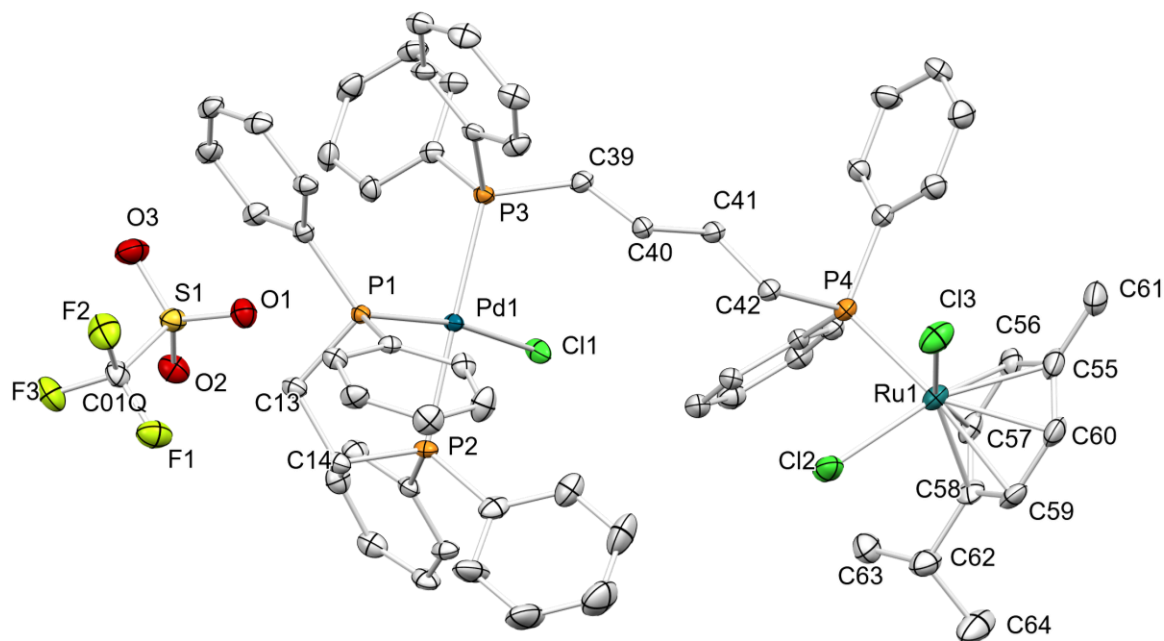
**Table S14 Hydrogen Atom Coordinates ( $\text{\AA} \times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdPd-1-CH<sub>2</sub>Cl<sub>2</sub>.**

| Atom | x       | y       | z        | U(eq) |
|------|---------|---------|----------|-------|
| H00H | 1753.66 | 8364.88 | 5537.07  | 48    |
| H00J | 1782.9  | 4216.53 | 4284.38  | 39    |
| H00N | 2924.84 | 6473.78 | 4590.88  | 38    |
| H00S | 2569.61 | 6071.43 | 6525.32  | 39    |
| H00W | 2321.35 | 7889.8  | 4600.53  | 47    |
| H00X | 204.86  | 3602.37 | 4048.35  | 50    |
| H01C | -573.51 | 3447.06 | 4944.01  | 54    |
| H01G | 194.25  | 3930.72 | 6062.1   | 51    |
| H2   | 7284.49 | 4354.59 | 8614.67  | 44    |
| H3   | 7433.72 | 4906.23 | 9739.64  | 51    |
| H4   | 6080.5  | 5527.86 | 10017.78 | 49    |
| H5   | 4577.02 | 5614.8  | 9185.26  | 47    |
| H6   | 4396.51 | 5033.76 | 8067     | 41    |
| H8   | 7042.95 | 2857.64 | 7053.92  | 43    |
| H9   | 8539.22 | 3023.27 | 6767.93  | 52    |
| H010 | 1898.67 | 7466.27 | 6506.95  | 46    |
| H10  | 9239.54 | 4389.27 | 6771.06  | 52    |
| H11  | 8440.81 | 5622.2  | 7050.08  | 45    |
| H12  | 6922.33 | 5481.4  | 7304.16  | 39    |
| H13A | 6107.88 | 2656.63 | 7847.39  | 35    |
| H13B | 5023.14 | 2881.38 | 7911.48  | 35    |
| H14A | 4790.97 | 1852.71 | 7027     | 34    |
| H14B | 5539.12 | 2341.21 | 6667.99  | 34    |
| H15A | 3627.09 | 4230.27 | 4653.28  | 32    |
| H15B | 3085.27 | 5118.39 | 4348.9   | 32    |
| H015 | 1735.69 | 4592.26 | 6297.79  | 39    |
| H16A | 4631.28 | 5501.88 | 4379.37  | 32    |
| H16B | 4609.8  | 5821.65 | 5141.52  | 32    |
| H17  | 5168.07 | 2212.05 | 4411.68  | 46    |
| H22  | 2673.38 | 1572.33 | 6229.39  | 42    |
| H23  | 1310.95 | 1259.75 | 6658.31  | 51    |
| H24  | 834.83  | 2228.78 | 7416.23  | 55    |
| H25  | 1707.95 | 3513.62 | 7751.74  | 50    |
| H26  | 3024.26 | 3863.49 | 7291.73  | 42    |
| H28  | 2347.99 | 2570.23 | 5216.47  | 37    |
| H29  | 2213.14 | 2147.48 | 4063.52  | 45    |
| H30  | 3615.19 | 1963.48 | 3666.93  | 50    |
| H32  | 5321.06 | 2633.39 | 5568.63  | 37    |
| H41C | 118.23  | 222.05  | 4170.48  | 39    |
| H41D | 1198.26 | 579.01  | 4205.87  | 39    |
| H41A | 997.97  | 379.62  | 4068.2   | 39    |
| H41B | 927.41  | 1188.77 | 4558.2   | 39    |

**Table S15 Atomic Occupancy for PdPd-1-CH<sub>2</sub>Cl<sub>2</sub>.**

| Atom | Occupancy | Atom | Occupancy | Atom | Occupancy |
|------|-----------|------|-----------|------|-----------|
| Cl2A | 0.638(4)  | Cl2B | 0.31(3)   | Cl3A | 0.42(3)   |
| Cl3B | 0.162(6)  | C41  | 0.5       | H41C | 0.77(7)   |
| H41D | 0.62(9)   | H41A | 0.17(9)   | H41B | 0.48(7)   |
| S1   | 0.8       | F1   | 0.8       | F3   | 0.8       |

|      |     |     |     |     |     |
|------|-----|-----|-----|-----|-----|
| O1   | 0.8 | O2  | 0.8 | O3  | 0.8 |
| C31  | 0.8 | F2  | 0.8 | S1A | 0.2 |
| F1A  | 0.2 | F2A | 0.2 | F3A | 0.2 |
| O1A  | 0.2 | O2A | 0.2 | O3A | 0.2 |
| C31A | 0.2 |     |     |     |     |



**Fig. S195.** ORTEP representation of **PdRu-1** in the solid state determined by single crystal X-ray diffraction analysis. Thermal ellipsoids represented at the 30% probability level. H atoms omitted for clarity.

**Table S16 Crystal data and structure refinement for PdRu-2.**

|                                      |                                                                                                    |
|--------------------------------------|----------------------------------------------------------------------------------------------------|
| Empirical formula                    | C <sub>65</sub> H <sub>66</sub> Cl <sub>3</sub> F <sub>3</sub> O <sub>3</sub> P <sub>4</sub> PdRuS |
| Formula weight                       | 1421.93                                                                                            |
| Temperature/K                        | 99.99(10)                                                                                          |
| Crystal system                       | monoclinic                                                                                         |
| Space group                          | P2 <sub>1</sub> /n                                                                                 |
| a/Å                                  | 10.29070(10)                                                                                       |
| b/Å                                  | 17.9374(2)                                                                                         |
| c/Å                                  | 34.5299(5)                                                                                         |
| α/°                                  | 90                                                                                                 |
| β/°                                  | 97.9880(10)                                                                                        |
| γ/°                                  | 90                                                                                                 |
| Volume/Å <sup>3</sup>                | 6311.97(13)                                                                                        |
| Z                                    | 4                                                                                                  |
| ρ <sub>calc</sub> /g/cm <sup>3</sup> | 1.496                                                                                              |
| μ/mm <sup>-1</sup>                   | 7.110                                                                                              |
| F(000)                               | 2896.0                                                                                             |
| Crystal size/mm <sup>3</sup>         | 0.59 × 0.1 × 0.03                                                                                  |
| Radiation                            | Cu Kα (λ = 1.54184 Å)                                                                              |
| 2θ range for data collection/°       | 5.564 to 159.884                                                                                   |
| Index ranges                         | -13 ≤ h ≤ 12, -22 ≤ k ≤ 20, -43 ≤ l ≤ 42                                                           |
| Reflections collected                | 61163                                                                                              |

Independent reflections 13330 [ $R_{\text{int}} = 0.0765$ ,  $R_{\text{sigma}} = 0.0492$ ]  
 Data/restraints/parameters 13330/0/734  
 Goodness-of-fit on  $F^2$  1.071  
 Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0881$ ,  $wR_2 = 0.2255$   
 Final R indexes [all data]  $R_1 = 0.0931$ ,  $wR_2 = 0.2292$   
 Largest diff. peak/hole /  $e \text{ \AA}^{-3}$  1.51/-1.86

**Table S17 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdRu-2.**  
 $U_{\text{eq}}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$  tensor.

| Atom | x           | y          | z         | $U(\text{eq})$ |
|------|-------------|------------|-----------|----------------|
| Pd1  | 1039.3(5)   | 4703.7(3)  | 3257.2(2) | 21.79(14)      |
| Ru1  | 4496.8(7)   | 2049.6(4)  | 5255.5(2) | 36.15(18)      |
| Cl3  | 5537(3)     | 3226.9(15) | 5448.9(7) | 57.4(6)        |
| P1   | 383.6(17)   | 5864.4(9)  | 3079.8(5) | 21.1(3)        |
| Cl1  | 1309.1(19)  | 3438.2(10) | 3412.4(7) | 37.6(4)        |
| Cl2  | 2482(3)     | 2726.3(14) | 5068.6(7) | 52.6(6)        |
| P2   | -1064.6(17) | 4585.2(10) | 3408.5(6) | 25.5(4)        |
| P3   | 3183.3(17)  | 4757.4(10) | 3097.6(5) | 24.5(4)        |
| P4   | 4872(2)     | 2300.1(11) | 4614.2(6) | 30.0(4)        |
| C6   | 1835(7)     | 7007(4)    | 2779(2)   | 29.6(15)       |
| C38  | 2048(8)     | 4353(4)    | 2352(2)   | 33.5(17)       |
| C1   | 1052(7)     | 6366(4)    | 2702(2)   | 27.2(14)       |
| C2   | 776(9)      | 6096(4)    | 2320(2)   | 33.9(17)       |
| C33  | 3210(8)     | 4420(4)    | 2606(2)   | 28.5(15)       |
| C50  | 4270(9)     | 959(5)     | 4198(3)   | 35.7(17)       |
| C32  | 4518(7)     | 5973(4)    | 2807(3)   | 30.9(16)       |
| C40  | 4236(8)     | 4106(5)    | 3842(2)   | 31.7(16)       |
| C44  | 6941(8)     | 1865(5)    | 4190(3)   | 38.5(19)       |
| C5   | 2290(9)     | 7367(4)    | 2468(3)   | 38.4(19)       |
| C7   | 339(7)      | 6468(4)    | 3494(2)   | 25.9(14)       |
| C42  | 4513(8)     | 3252(5)    | 4434(2)   | 32.9(16)       |
| C21  | -1901(7)    | 3779(4)    | 3180(2)   | 27.5(15)       |
| C58  | 3360(10)    | 1072(5)    | 5405(3)   | 44(2)          |
| C26  | -2510(8)    | 3256(4)    | 3389(3)   | 32.0(16)       |
| C35  | 4391(9)     | 3952(5)    | 2099(3)   | 38.7(19)       |
| C14  | -2043(7)    | 5395(4)    | 3210(2)   | 30.9(16)       |
| C49  | 3881(7)     | 1688(4)    | 4262(2)   | 28.1(15)       |
| C53  | 1861(9)     | 1463(5)    | 3831(3)   | 38.5(18)       |
| C3   | 1245(9)     | 6471(5)    | 2016(3)   | 39.2(19)       |
| C27  | 4099(7)     | 5634(4)    | 3134(2)   | 26.9(14)       |
| C45  | 8256(9)     | 1840(6)    | 4138(3)   | 46(2)          |
| C52  | 2237(9)     | 734(5)     | 3773(3)   | 40.7(19)       |
| C22  | -1945(8)    | 3692(5)    | 2772(2)   | 32.7(16)       |
| C9   | -600(9)     | 7569(5)    | 3768(3)   | 37.3(18)       |
| C56  | 5598(10)    | 1015(5)    | 5263(3)   | 43(2)          |
| C46  | 9218(8)     | 2108(6)    | 4422(3)   | 43(2)          |
| C54  | 2662(8)     | 1932(5)    | 4076(2)   | 31.9(16)       |
| C43  | 6573(8)     | 2167(5)    | 4527(2)   | 32.4(16)       |
| C36  | 3225(11)    | 3897(5)    | 1846(3)   | 46(2)          |
| C15  | -1215(9)    | 4557(5)    | 3920(3)   | 40(2)          |
| C28  | 4411(9)     | 5980(5)    | 3501(3)   | 36.3(18)       |
| C25  | -3206(8)    | 2684(5)    | 3193(3)   | 36.4(18)       |
| C29  | 5164(9)     | 6610(5)    | 3542(3)   | 40.0(19)       |
| C59  | 3800(10)    | 1473(5)    | 5765(3)   | 44(2)          |
| C37  | 2052(10)    | 4099(5)    | 1966(2)   | 42(2)          |

|      |           |            |            |          |
|------|-----------|------------|------------|----------|
| C48  | 7549(9)   | 2457(6)    | 4810(3)    | 42(2)    |
| C10  | -226(10)  | 7273(5)    | 4136(3)    | 45(2)    |
| C31  | 5256(8)   | 6625(5)    | 2852(3)    | 37.2(18) |
| C20  | -238(12)  | 4245(6)    | 4184(3)    | 52(2)    |
| C30  | 5577(9)   | 6942(5)    | 3215(3)    | 42(2)    |
| C23  | -2619(9)  | 3113(5)    | 2584(3)    | 37.9(18) |
| C47  | 8864(11)  | 2426(7)    | 4758(3)    | 52(2)    |
| C60  | 5163(11)  | 1628(6)    | 5862(3)    | 48(2)    |
| C24  | -3272(9)  | 2609(5)    | 2792(3)    | 38.4(19) |
| C51  | 3467(9)   | 489(5)     | 3956(3)    | 38.6(18) |
| C41  | 4785(8)   | 3378(5)    | 4017(3)    | 35.8(18) |
| C4   | 1995(9)   | 7106(5)    | 2095(3)    | 39(2)    |
| C13  | -1357(7)  | 5758(4)    | 2887(2)    | 30.2(16) |
| C8   | -320(7)   | 7162(4)    | 3441(2)    | 29.6(15) |
| C57  | 4246(10)  | 850(5)     | 5170(3)    | 41(2)    |
| C39  | 4272(8)   | 4115(4)    | 3397(2)    | 32.7(16) |
| C12  | 747(8)    | 6208(4)    | 3868(2)    | 32.2(16) |
| C34  | 4388(8)   | 4209(4)    | 2477(3)    | 34.8(17) |
| C63  | 1449(11)  | 716(7)     | 4895(3)    | 57(3)    |
| C11  | 457(12)   | 6613(5)    | 4194(3)    | 48(2)    |
| C16  | -2308(10) | 4871(8)    | 4058(3)    | 63(3)    |
| C61  | 7477(12)  | 1576(8)    | 5712(3)    | 66(3)    |
| C55  | 6087(11)  | 1404(6)    | 5608(3)    | 50(2)    |
| C62  | 1867(11)  | 950(7)     | 5316(3)    | 54(3)    |
| C64  | 1399(15)  | 431(10)    | 5602(4)    | 93(6)    |
| C19  | -340(17)  | 4236(8)    | 4582(3)    | 77(4)    |
| C18  | -1434(16) | 4532(9)    | 4717(4)    | 79(4)    |
| C17  | -2411(14) | 4836(11)   | 4459(4)    | 89(5)    |
| S1   | -1808(2)  | 4581.8(12) | 1709.7(6)  | 36.3(4)  |
| F1   | -3541(6)  | 5206(4)    | 2095.7(18) | 54.6(14) |
| F3   | -4002(6)  | 5312(4)    | 1467.4(19) | 59.1(16) |
| F2   | -2464(7)  | 5981(3)    | 1785(2)    | 62.7(17) |
| O1   | -982(6)   | 4618(4)    | 2081.2(19) | 42.9(14) |
| O2   | -2597(7)  | 3912(4)    | 1646(2)    | 46.3(15) |
| O3   | -1210(7)  | 4837(5)    | 1384(2)    | 58(2)    |
| C01Q | -3036(9)  | 5296(5)    | 1766(3)    | 38.8(19) |

**Table S18 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for PdRu-2. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$ .**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$  |
|------|----------|----------|----------|----------|----------|-----------|
| Pd1  | 18.5(2)  | 19.3(2)  | 28.4(3)  | 2.95(18) | 6.37(18) | 0.74(17)  |
| Ru1  | 45.0(4)  | 35.4(3)  | 29.6(3)  | 5.6(2)   | 10.7(3)  | -3.3(3)   |
| Cl3  | 80.3(18) | 50.7(13) | 42.9(12) | -3.7(10) | 15.0(12) | -15.6(13) |
| P1   | 18.7(8)  | 19.4(7)  | 25.7(8)  | 1.7(6)   | 4.6(6)   | 0.9(6)    |
| Cl1  | 27.6(9)  | 21.0(8)  | 63.9(13) | 9.5(8)   | 5.9(8)   | 1.3(7)    |
| Cl2  | 51.3(13) | 56.4(13) | 55.7(13) | 16.0(11) | 27.0(11) | 15.5(11)  |
| P2   | 20.4(8)  | 26.1(8)  | 31.1(9)  | -0.1(7)  | 7.9(7)   | -5.0(7)   |
| P3   | 20.7(8)  | 22.6(8)  | 31.4(9)  | 3.9(7)   | 7.8(7)   | 2.8(6)    |
| P4   | 31.0(10) | 31.4(9)  | 28.2(9)  | 6.9(7)   | 5.8(8)   | -1.4(8)   |
| C6   | 26(4)    | 24(3)    | 41(4)    | 2(3)     | 11(3)    | 3(3)      |
| C38  | 34(4)    | 32(4)    | 34(4)    | 5(3)     | 3(3)     | 9(3)      |
| C1   | 26(3)    | 25(3)    | 32(4)    | 2(3)     | 6(3)     | 5(3)      |
| C2   | 40(4)    | 26(4)    | 38(4)    | 2(3)     | 16(4)    | 6(3)      |

|     |       |         |       |        |        |        |
|-----|-------|---------|-------|--------|--------|--------|
| C33 | 30(4) | 21(3)   | 36(4) | 3(3)   | 11(3)  | 2(3)   |
| C50 | 35(4) | 34(4)   | 39(4) | 9(3)   | 11(3)  | 2(3)   |
| C32 | 22(3) | 29(4)   | 44(4) | 6(3)   | 14(3)  | -2(3)  |
| C40 | 24(4) | 34(4)   | 37(4) | 11(3)  | 5(3)   | 3(3)   |
| C44 | 26(4) | 54(5)   | 34(4) | 0(4)   | 2(3)   | 2(4)   |
| C5  | 37(4) | 22(4)   | 59(5) | 11(4)  | 20(4)  | 2(3)   |
| C7  | 19(3) | 29(4)   | 31(4) | 2(3)   | 6(3)   | -5(3)  |
| C42 | 28(4) | 33(4)   | 38(4) | 10(3)  | 6(3)   | -1(3)  |
| C21 | 19(3) | 26(3)   | 37(4) | 3(3)   | 3(3)   | -1(3)  |
| C58 | 45(5) | 34(4)   | 52(5) | 16(4)  | 6(4)   | -18(4) |
| C26 | 29(4) | 26(4)   | 44(4) | 4(3)   | 16(3)  | -3(3)  |
| C35 | 42(5) | 32(4)   | 47(5) | 1(4)   | 25(4)  | 4(3)   |
| C14 | 23(3) | 26(4)   | 45(4) | -2(3)  | 8(3)   | -1(3)  |
| C49 | 24(3) | 37(4)   | 25(3) | 6(3)   | 5(3)   | 1(3)   |
| C53 | 32(4) | 47(5)   | 38(4) | 9(4)   | 9(3)   | 3(4)   |
| C3  | 41(5) | 41(4)   | 39(4) | 7(4)   | 20(4)  | 14(4)  |
| C27 | 17(3) | 28(3)   | 37(4) | 2(3)   | 9(3)   | 3(3)   |
| C45 | 34(5) | 53(5)   | 55(6) | 1(4)   | 17(4)  | 3(4)   |
| C52 | 43(5) | 46(5)   | 34(4) | -4(4)  | 10(4)  | -5(4)  |
| C22 | 28(4) | 33(4)   | 37(4) | -2(3)  | 4(3)   | -10(3) |
| C9  | 40(5) | 33(4)   | 42(4) | -3(3)  | 16(4)  | 7(3)   |
| C56 | 51(5) | 33(4)   | 45(5) | 13(4)  | 5(4)   | 9(4)   |
| C46 | 22(4) | 56(5)   | 52(5) | 4(4)   | 2(4)   | -1(4)  |
| C54 | 26(4) | 37(4)   | 33(4) | 5(3)   | 7(3)   | 2(3)   |
| C43 | 30(4) | 35(4)   | 33(4) | 11(3)  | 5(3)   | -1(3)  |
| C36 | 63(6) | 46(5)   | 34(4) | 3(4)   | 20(4)  | 9(4)   |
| C15 | 42(5) | 39(4)   | 40(5) | -3(4)  | 9(4)   | -20(4) |
| C28 | 43(5) | 31(4)   | 38(4) | 0(3)   | 17(4)  | 1(3)   |
| C25 | 25(4) | 29(4)   | 56(5) | 3(4)   | 6(4)   | -9(3)  |
| C29 | 34(4) | 36(4)   | 50(5) | -11(4) | 9(4)   | -3(3)  |
| C59 | 57(6) | 47(5)   | 32(4) | 10(4)  | 22(4)  | 0(4)   |
| C37 | 48(5) | 45(5)   | 30(4) | 8(4)   | 1(4)   | 15(4)  |
| C48 | 37(5) | 54(5)   | 35(4) | 2(4)   | 7(4)   | -4(4)  |
| C10 | 54(6) | 41(5)   | 42(5) | -11(4) | 10(4)  | 2(4)   |
| C31 | 30(4) | 30(4)   | 53(5) | 4(4)   | 14(4)  | 2(3)   |
| C20 | 72(7) | 43(5)   | 41(5) | 6(4)   | 9(5)   | -4(5)  |
| C30 | 38(5) | 32(4)   | 57(5) | -8(4)  | 9(4)   | -11(4) |
| C23 | 39(4) | 37(4)   | 36(4) | -6(3)  | 0(3)   | 0(4)   |
| C47 | 44(5) | 73(7)   | 38(5) | 6(5)   | -1(4)  | -12(5) |
| C60 | 60(6) | 58(6)   | 27(4) | 16(4)  | 3(4)   | -6(5)  |
| C24 | 33(4) | 27(4)   | 55(5) | -7(4)  | 7(4)   | -2(3)  |
| C51 | 45(5) | 36(4)   | 36(4) | 1(3)   | 11(4)  | -3(4)  |
| C41 | 29(4) | 38(4)   | 42(4) | 13(4)  | 12(3)  | 3(3)   |
| C4  | 45(5) | 32(4)   | 46(5) | 17(4)  | 23(4)  | 11(4)  |
| C13 | 24(4) | 25(3)   | 42(4) | 1(3)   | 8(3)   | 1(3)   |
| C8  | 26(4) | 28(4)   | 35(4) | -3(3)  | 5(3)   | 0(3)   |
| C57 | 62(6) | 28(4)   | 32(4) | 6(3)   | 5(4)   | -5(4)  |
| C39 | 32(4) | 31(4)   | 37(4) | 9(3)   | 11(3)  | 0(3)   |
| C12 | 33(4) | 28(4)   | 34(4) | -2(3)  | -1(3)  | -4(3)  |
| C34 | 31(4) | 31(4)   | 45(5) | 0(3)   | 15(4)  | -1(3)  |
| C63 | 46(6) | 69(7)   | 52(6) | 8(5)   | -4(5)  | -8(5)  |
| C11 | 73(7) | 40(5)   | 29(4) | -3(4)  | 3(4)   | 3(5)   |
| C16 | 34(5) | 115(10) | 43(5) | -14(6) | 17(4)  | -13(6) |
| C61 | 59(7) | 86(9)   | 46(6) | 25(6)  | -11(5) | -4(6)  |
| C55 | 56(6) | 51(5)   | 40(5) | 22(4)  | -3(4)  | -6(5)  |

|      |          |          |          |         |        |         |
|------|----------|----------|----------|---------|--------|---------|
| C62  | 51(6)    | 63(6)    | 48(5)    | 5(5)    | 12(5)  | -17(5)  |
| C64  | 84(10)   | 137(14)  | 54(7)    | 20(8)   | -8(7)  | -71(10) |
| C19  | 112(12)  | 79(9)    | 36(5)    | 15(6)   | -1(6)  | -6(8)   |
| C18  | 95(11)   | 106(11)  | 39(6)    | 2(6)    | 19(7)  | -12(9)  |
| C17  | 56(7)    | 173(17)  | 44(6)    | 3(8)    | 23(6)  | -22(9)  |
| S1   | 30.9(10) | 44.6(11) | 33.8(10) | -3.7(8) | 5.8(8) | -5.8(8) |
| F1   | 48(3)    | 64(4)    | 54(3)    | -14(3)  | 16(3)  | -6(3)   |
| F3   | 39(3)    | 68(4)    | 65(4)    | -3(3)   | -12(3) | 2(3)    |
| F2   | 65(4)    | 39(3)    | 81(4)    | 4(3)    | -2(3)  | -6(3)   |
| O1   | 41(3)    | 45(3)    | 41(3)    | -2(3)   | -2(3)  | -2(3)   |
| O2   | 42(4)    | 42(3)    | 54(4)    | -10(3)  | 4(3)   | -4(3)   |
| O3   | 50(4)    | 87(6)    | 41(4)    | -4(4)   | 16(3)  | -16(4)  |
| C01Q | 32(4)    | 42(5)    | 38(4)    | 0(4)    | -7(3)  | -8(4)   |

**Table S19 Bond Lengths for PdRu-2.**

| Atom | Atom | Length/Å   | Atom | Atom | Length/Å  |
|------|------|------------|------|------|-----------|
| Pd1  | P1   | 2.2472(17) | C58  | C57  | 1.362(14) |
| Pd1  | Cl1  | 2.3401(18) | C58  | C62  | 1.540(14) |
| Pd1  | P2   | 2.3065(18) | C26  | C25  | 1.375(12) |
| Pd1  | P3   | 2.3493(18) | C35  | C36  | 1.385(14) |
| Ru1  | Cl3  | 2.419(3)   | C35  | C34  | 1.386(12) |
| Ru1  | Cl2  | 2.412(3)   | C14  | C13  | 1.547(11) |
| Ru1  | P4   | 2.344(2)   | C49  | C54  | 1.398(11) |
| Ru1  | C58  | 2.208(8)   | C53  | C52  | 1.385(13) |
| Ru1  | C56  | 2.173(9)   | C53  | C54  | 1.380(12) |
| Ru1  | C59  | 2.242(8)   | C3   | C4   | 1.381(14) |
| Ru1  | C60  | 2.242(9)   | C27  | C28  | 1.407(11) |
| Ru1  | C57  | 2.182(9)   | C45  | C46  | 1.381(14) |
| Ru1  | C55  | 2.224(10)  | C52  | C51  | 1.403(13) |
| P1   | C1   | 1.798(8)   | C22  | C23  | 1.363(11) |
| P1   | C7   | 1.799(8)   | C9   | C10  | 1.381(13) |
| P1   | C13  | 1.832(8)   | C9   | C8   | 1.405(11) |
| P2   | C21  | 1.808(8)   | C56  | C57  | 1.415(14) |
| P2   | C14  | 1.845(8)   | C56  | C55  | 1.412(14) |
| P2   | C15  | 1.795(9)   | C46  | C47  | 1.386(15) |
| P3   | C33  | 1.806(8)   | C43  | C48  | 1.399(12) |
| P3   | C27  | 1.829(8)   | C36  | C37  | 1.378(14) |
| P3   | C39  | 1.825(8)   | C15  | C20  | 1.379(15) |
| P4   | C42  | 1.837(8)   | C15  | C16  | 1.399(15) |
| P4   | C49  | 1.838(8)   | C28  | C29  | 1.367(12) |
| P4   | C43  | 1.832(8)   | C25  | C24  | 1.383(13) |
| C6   | C1   | 1.408(11)  | C29  | C30  | 1.395(13) |
| C6   | C5   | 1.388(11)  | C59  | C60  | 1.424(15) |
| C38  | C33  | 1.387(11)  | C48  | C47  | 1.390(14) |
| C38  | C37  | 1.407(12)  | C10  | C11  | 1.378(14) |
| C1   | C2   | 1.398(11)  | C31  | C30  | 1.373(13) |
| C2   | C3   | 1.389(11)  | C20  | C19  | 1.393(15) |
| C33  | C34  | 1.399(11)  | C23  | C24  | 1.384(13) |
| C50  | C49  | 1.394(11)  | C60  | C55  | 1.437(16) |
| C50  | C51  | 1.380(13)  | C12  | C11  | 1.404(12) |
| C32  | C27  | 1.403(10)  | C63  | C62  | 1.517(15) |
| C32  | C31  | 1.393(11)  | C16  | C17  | 1.404(15) |
| C40  | C41  | 1.515(11)  | C61  | C55  | 1.459(16) |



|     |     |           |     |      |           |
|-----|-----|-----------|-----|------|-----------|
| C40 | C39 | 1.540(11) | C62 | C64  | 1.485(15) |
| C44 | C45 | 1.390(12) | C19 | C18  | 1.38(2)   |
| C44 | C43 | 1.384(12) | C18 | C17  | 1.36(2)   |
| C5  | C4  | 1.366(14) | S1  | O1   | 1.439(6)  |
| C7  | C8  | 1.418(11) | S1  | O2   | 1.450(7)  |
| C7  | C12 | 1.385(11) | S1  | O3   | 1.432(7)  |
| C42 | C41 | 1.522(11) | S1  | C01Q | 1.830(10) |
| C21 | C26 | 1.385(10) | F1  | C01Q | 1.324(11) |
| C21 | C22 | 1.412(11) | F3  | C01Q | 1.330(10) |
| C58 | C59 | 1.452(14) | F2  | C01Q | 1.359(10) |

**Table S20 Bond Angles for PdRu-2.**

| Atom | Atom | Atom | Angle/°   | Atom | Atom | Atom | Angle/°  |
|------|------|------|-----------|------|------|------|----------|
| P1   | Pd1  | Cl1  | 169.33(7) | C59  | C58  | C62  | 115.2(9) |
| P1   | Pd1  | P2   | 83.77(6)  | C57  | C58  | Ru1  | 70.9(5)  |
| P1   | Pd1  | P3   | 98.87(6)  | C57  | C58  | C59  | 119.9(9) |
| Cl1  | Pd1  | P3   | 90.46(7)  | C57  | C58  | C62  | 124.9(9) |
| P2   | Pd1  | Cl1  | 86.79(7)  | C62  | C58  | Ru1  | 127.8(7) |
| P2   | Pd1  | P3   | 177.03(7) | C25  | C26  | C21  | 119.4(8) |
| Cl2  | Ru1  | Cl3  | 88.03(11) | C36  | C35  | C34  | 120.1(8) |
| P4   | Ru1  | Cl3  | 88.21(8)  | C13  | C14  | P2   | 108.6(5) |
| P4   | Ru1  | Cl2  | 84.21(8)  | C50  | C49  | P4   | 121.3(6) |
| C58  | Ru1  | Cl3  | 149.0(3)  | C50  | C49  | C54  | 118.7(8) |
| C58  | Ru1  | Cl2  | 89.9(3)   | C54  | C49  | P4   | 119.8(6) |
| C58  | Ru1  | P4   | 122.4(3)  | C54  | C53  | C52  | 120.6(8) |
| C58  | Ru1  | C59  | 38.1(4)   | C4   | C3   | C2   | 119.5(8) |
| C58  | Ru1  | C60  | 67.5(4)   | C32  | C27  | P3   | 121.9(6) |
| C58  | Ru1  | C55  | 80.3(4)   | C32  | C27  | C28  | 118.6(7) |
| C56  | Ru1  | Cl3  | 122.1(3)  | C28  | C27  | P3   | 119.4(6) |
| C56  | Ru1  | Cl2  | 149.4(3)  | C46  | C45  | C44  | 120.7(9) |
| C56  | Ru1  | P4   | 91.2(3)   | C53  | C52  | C51  | 118.9(9) |
| C56  | Ru1  | C58  | 67.2(4)   | C23  | C22  | C21  | 120.1(8) |
| C56  | Ru1  | C59  | 79.7(4)   | C10  | C9   | C8   | 118.5(8) |
| C56  | Ru1  | C60  | 67.0(4)   | C57  | C56  | Ru1  | 71.4(5)  |
| C56  | Ru1  | C57  | 37.9(4)   | C55  | C56  | Ru1  | 73.2(6)  |
| C56  | Ru1  | C55  | 37.4(4)   | C55  | C56  | C57  | 121.2(9) |
| C59  | Ru1  | Cl3  | 111.3(3)  | C45  | C46  | C47  | 119.5(9) |
| C59  | Ru1  | Cl2  | 94.9(3)   | C53  | C54  | C49  | 120.8(8) |
| C59  | Ru1  | P4   | 160.4(3)  | C44  | C43  | P4   | 124.6(6) |
| C59  | Ru1  | C60  | 37.0(4)   | C44  | C43  | C48  | 118.6(8) |
| C60  | Ru1  | Cl3  | 88.3(3)   | C48  | C43  | P4   | 116.5(7) |
| C60  | Ru1  | Cl2  | 124.0(3)  | C37  | C36  | C35  | 120.7(8) |
| C60  | Ru1  | P4   | 151.4(3)  | C20  | C15  | P2   | 120.5(8) |
| C57  | Ru1  | Cl3  | 159.6(3)  | C20  | C15  | C16  | 119.1(9) |
| C57  | Ru1  | Cl2  | 112.3(3)  | C16  | C15  | P2   | 120.4(8) |
| C57  | Ru1  | P4   | 95.3(2)   | C29  | C28  | C27  | 120.9(8) |
| C57  | Ru1  | C58  | 36.1(4)   | C26  | C25  | C24  | 120.9(8) |
| C57  | Ru1  | C59  | 66.8(3)   | C28  | C29  | C30  | 120.1(8) |
| C57  | Ru1  | C60  | 79.0(4)   | C58  | C59  | Ru1  | 69.7(4)  |
| C57  | Ru1  | C55  | 68.0(4)   | C60  | C59  | Ru1  | 71.5(5)  |
| C55  | Ru1  | Cl3  | 92.3(3)   | C60  | C59  | C58  | 118.6(9) |
| C55  | Ru1  | Cl2  | 161.5(3)  | C36  | C37  | C38  | 119.2(9) |
| C55  | Ru1  | P4   | 114.3(3)  | C47  | C48  | C43  | 120.8(9) |

|     |     |     |          |     |      |      |           |
|-----|-----|-----|----------|-----|------|------|-----------|
| C55 | Ru1 | C59 | 67.8(4)  | C11 | C10  | C9   | 122.4(8)  |
| C55 | Ru1 | C60 | 37.5(4)  | C30 | C31  | C32  | 120.6(8)  |
| C1  | P1  | Pd1 | 122.1(2) | C15 | C20  | C19  | 120.6(12) |
| C1  | P1  | C7  | 109.2(3) | C31 | C30  | C29  | 120.1(8)  |
| C1  | P1  | C13 | 104.0(4) | C22 | C23  | C24  | 120.1(8)  |
| C7  | P1  | Pd1 | 112.4(2) | C46 | C47  | C48  | 119.9(9)  |
| C7  | P1  | C13 | 102.7(3) | C59 | C60  | Ru1  | 71.5(5)   |
| C13 | P1  | Pd1 | 104.1(2) | C59 | C60  | C55  | 121.0(9)  |
| C21 | P2  | Pd1 | 112.4(2) | C55 | C60  | Ru1  | 70.6(5)   |
| C21 | P2  | C14 | 105.5(4) | C25 | C24  | C23  | 119.8(8)  |
| C14 | P2  | Pd1 | 109.0(2) | C50 | C51  | C52  | 120.5(8)  |
| C15 | P2  | Pd1 | 115.9(3) | C40 | C41  | C42  | 113.5(7)  |
| C15 | P2  | C21 | 107.8(4) | C5  | C4   | C3   | 121.0(7)  |
| C15 | P2  | C14 | 105.6(4) | C14 | C13  | P1   | 107.6(5)  |
| C33 | P3  | Pd1 | 110.1(3) | C9  | C8   | C7   | 120.1(7)  |
| C33 | P3  | C27 | 106.1(3) | C58 | C57  | Ru1  | 73.0(5)   |
| C33 | P3  | C39 | 103.5(4) | C58 | C57  | C56  | 121.5(9)  |
| C27 | P3  | Pd1 | 120.7(2) | C56 | C57  | Ru1  | 70.7(5)   |
| C39 | P3  | Pd1 | 111.3(3) | C40 | C39  | P3   | 118.3(6)  |
| C39 | P3  | C27 | 103.5(4) | C7  | C12  | C11  | 120.2(8)  |
| C42 | P4  | Ru1 | 116.5(3) | C35 | C34  | C33  | 120.3(8)  |
| C42 | P4  | C49 | 105.4(4) | C10 | C11  | C12  | 119.3(8)  |
| C49 | P4  | Ru1 | 111.1(2) | C15 | C16  | C17  | 119.4(12) |
| C43 | P4  | Ru1 | 114.6(3) | C56 | C55  | Ru1  | 69.3(5)   |
| C43 | P4  | C42 | 102.6(4) | C56 | C55  | C60  | 117.7(10) |
| C43 | P4  | C49 | 105.6(4) | C56 | C55  | C61  | 122.3(11) |
| C5  | C6  | C1  | 118.6(8) | C60 | C55  | Ru1  | 71.9(6)   |
| C33 | C38 | C37 | 120.7(8) | C60 | C55  | C61  | 119.9(10) |
| C6  | C1  | P1  | 122.6(6) | C61 | C55  | Ru1  | 130.3(7)  |
| C2  | C1  | P1  | 117.6(6) | C63 | C62  | C58  | 111.9(9)  |
| C2  | C1  | C6  | 119.8(7) | C64 | C62  | C58  | 111.3(10) |
| C3  | C2  | C1  | 120.0(8) | C64 | C62  | C63  | 112.8(10) |
| C38 | C33 | P3  | 119.9(6) | C18 | C19  | C20  | 120.3(13) |
| C38 | C33 | C34 | 119.0(8) | C17 | C18  | C19  | 119.7(11) |
| C34 | C33 | P3  | 121.1(7) | C18 | C17  | C16  | 120.9(13) |
| C51 | C50 | C49 | 120.5(8) | O1  | S1   | O2   | 115.0(4)  |
| C31 | C32 | C27 | 119.7(8) | O1  | S1   | C01Q | 101.8(4)  |
| C41 | C40 | C39 | 110.4(7) | O2  | S1   | C01Q | 102.5(4)  |
| C43 | C44 | C45 | 120.5(9) | O3  | S1   | O1   | 114.9(4)  |
| C4  | C5  | C6  | 121.0(8) | O3  | S1   | O2   | 115.9(4)  |
| C8  | C7  | P1  | 119.5(6) | O3  | S1   | C01Q | 103.8(5)  |
| C12 | C7  | P1  | 120.1(6) | F1  | C01Q | S1   | 111.4(6)  |
| C12 | C7  | C8  | 119.5(7) | F1  | C01Q | F3   | 109.2(8)  |
| C41 | C42 | P4  | 113.8(6) | F1  | C01Q | F2   | 106.7(7)  |
| C26 | C21 | P2  | 122.5(6) | F3  | C01Q | S1   | 112.6(6)  |
| C26 | C21 | C22 | 119.5(7) | F3  | C01Q | F2   | 106.9(7)  |
| C22 | C21 | P2  | 118.0(6) | F2  | C01Q | S1   | 109.7(6)  |
| C59 | C58 | Ru1 | 72.2(5)  |     |      |      |           |

**Table S21 Torsion Angles for PdRu-2.**

| A   | B  | C  | D  | Angle/°   | A   | B  | C   | D   | Angle/°  |
|-----|----|----|----|-----------|-----|----|-----|-----|----------|
| Pd1 | P1 | C1 | C6 | -112.8(6) | C49 | P4 | C42 | C41 | -56.6(7) |
| Pd1 | P1 | C1 | C2 | 66.8(7)   | C49 | P4 | C43 | C44 | 18.6(8)  |

|                 |            |                 |           |
|-----------------|------------|-----------------|-----------|
| Pd1 P1 C7 C8    | -166.1(5)  | C49 P4 C43 C48  | -167.5(6) |
| Pd1 P1 C7 C12   | 3.1(7)     | C49 C50 C51 C52 | -0.9(12)  |
| Pd1 P1 C13 C14  | 56.5(5)    | C53 C52 C51 C50 | 2.1(13)   |
| Pd1 P2 C21 C26  | 128.2(6)   | C27 P3 C33 C38  | -116.4(6) |
| Pd1 P2 C21 C22  | -52.8(7)   | C27 P3 C33 C34  | 64.9(7)   |
| Pd1 P2 C14 C13  | 19.8(6)    | C27 P3 C39 C40  | 84.2(7)   |
| Pd1 P2 C15 C20  | -32.1(8)   | C27 C32 C31 C30 | -0.1(12)  |
| Pd1 P2 C15 C16  | 145.9(8)   | C27 C28 C29 C30 | 3.4(13)   |
| Pd1 P3 C33 C38  | 15.8(7)    | C45 C44 C43 P4  | 174.9(7)  |
| Pd1 P3 C33 C34  | -162.8(6)  | C45 C44 C43 C48 | 1.2(13)   |
| Pd1 P3 C27 C32  | -117.8(6)  | C45 C46 C47 C48 | 1.4(16)   |
| Pd1 P3 C27 C28  | 62.9(7)    | C52 C53 C54 C49 | 1.6(12)   |
| Pd1 P3 C39 C40  | -47.0(7)   | C22 C21 C26 C25 | -3.5(12)  |
| Ru1 P4 C42 C41  | 179.7(5)   | C22 C23 C24 C25 | -1.9(13)  |
| Ru1 P4 C49 C50  | -80.7(6)   | C9 C10 C11 C12  | -2.3(16)  |
| Ru1 P4 C49 C54  | 94.3(6)    | C54 C53 C52 C51 | -2.4(13)  |
| Ru1 P4 C43 C44  | 141.3(7)   | C43 P4 C42 C41  | 53.7(7)   |
| Ru1 P4 C43 C48  | -44.9(7)   | C43 P4 C49 C50  | 44.1(7)   |
| Ru1 C58 C59 C60 | -54.1(8)   | C43 P4 C49 C54  | -140.8(6) |
| Ru1 C58 C57 C56 | 53.6(7)    | C43 C44 C45 C46 | 0.7(15)   |
| Ru1 C58 C62 C63 | 78.7(12)   | C43 C48 C47 C46 | 0.4(16)   |
| Ru1 C58 C62 C64 | -154.0(10) | C36 C35 C34 C33 | -0.5(13)  |
| Ru1 C56 C57 C58 | -54.6(8)   | C15 P2 C21 C26  | -0.7(8)   |
| Ru1 C56 C55 C60 | 55.0(8)    | C15 P2 C21 C22  | 178.3(6)  |
| Ru1 C56 C55 C61 | -125.3(9)  | C15 P2 C14 C13  | 145.0(6)  |
| Ru1 C59 C60 C55 | -52.3(8)   | C15 C20 C19 C18 | 1(2)      |
| Ru1 C60 C55 C56 | -53.7(7)   | C15 C16 C17 C18 | 3(2)      |
| Ru1 C60 C55 C61 | 126.6(9)   | C28 C29 C30 C31 | -1.7(14)  |
| P1 C1 C2 C3     | 178.6(6)   | C59 C58 C57 Ru1 | -55.0(7)  |
| P1 C7 C8 C9     | 166.8(6)   | C59 C58 C57 C56 | -1.4(13)  |
| P1 C7 C12 C11   | -166.3(7)  | C59 C58 C62 C63 | 165.1(9)  |
| P2 C21 C26 C25  | 175.5(6)   | C59 C58 C62 C64 | -67.7(13) |
| P2 C21 C22 C23  | -176.9(7)  | C59 C60 C55 Ru1 | 52.7(8)   |
| P2 C14 C13 P1   | -48.0(6)   | C59 C60 C55 C56 | -1.0(14)  |
| P2 C15 C20 C19  | 178.7(9)   | C59 C60 C55 C61 | 179.3(9)  |
| P2 C15 C16 C17  | 179.4(11)  | C37 C38 C33 P3  | 179.3(6)  |
| P3 C33 C34 C35  | -180.0(6)  | C37 C38 C33 C34 | -2.0(12)  |
| P3 C27 C28 C29  | 175.9(7)   | C10 C9 C8 C7    | -0.4(13)  |
| P4 C42 C41 C40  | 168.3(6)   | C31 C32 C27 P3  | -177.5(6) |
| P4 C49 C54 C53  | -175.5(6)  | C31 C32 C27 C28 | 1.7(11)   |
| P4 C43 C48 C47  | -176.0(8)  | C20 C15 C16 C17 | -2.6(18)  |
| C6 C1 C2 C3     | -1.7(12)   | C20 C19 C18 C17 | 0(2)      |
| C6 C5 C4 C3     | -0.6(13)   | C51 C50 C49 P4  | 175.1(6)  |
| C38 C33 C34 C35 | 1.4(12)    | C51 C50 C49 C54 | 0.0(11)   |
| C1 P1 C7 C8     | 55.2(7)    | C41 C40 C39 P3  | 159.1(6)  |
| C1 P1 C7 C12    | -135.7(6)  | C13 P1 C1 C6    | 130.3(6)  |
| C1 P1 C13 C14   | -174.7(5)  | C13 P1 C1 C2    | -50.1(7)  |
| C1 C6 C5 C4     | -0.4(12)   | C13 P1 C7 C8    | -54.8(6)  |
| C1 C2 C3 C4     | 0.7(12)    | C13 P1 C7 C12   | 114.4(6)  |
| C2 C3 C4 C5     | 0.4(13)    | C8 C7 C12 C11   | 2.9(12)   |
| C33 P3 C27 C32  | 8.3(7)     | C8 C9 C10 C11   | 2.8(15)   |
| C33 P3 C27 C28  | -171.0(6)  | C57 C58 C59 Ru1 | 54.4(7)   |
| C33 P3 C39 C40  | -165.3(6)  | C57 C58 C59 C60 | 0.3(13)   |
| C33 C38 C37 C36 | 1.7(13)    | C57 C58 C62 C63 | -13.2(14) |
| C50 C49 C54 C53 | -0.4(11)   | C57 C58 C62 C64 | 114.0(12) |

|                 |           |                 |           |
|-----------------|-----------|-----------------|-----------|
| C32 C27 C28 C29 | -3.4(12)  | C57 C56 C55 Ru1 | -55.1(7)  |
| C32 C31 C30 C29 | 0.0(14)   | C57 C56 C55 C60 | -0.1(13)  |
| C44 C45 C46 C47 | -2.0(16)  | C57 C56 C55 C61 | 179.5(9)  |
| C44 C43 C48 C47 | -1.7(14)  | C39 P3 C33 C38  | 134.9(6)  |
| C5 C6 C1 P1     | -178.8(6) | C39 P3 C33 C34  | -43.7(7)  |
| C5 C6 C1 C2     | 1.6(11)   | C39 P3 C27 C32  | 116.9(6)  |
| C7 P1 C1 C6     | 21.2(7)   | C39 P3 C27 C28  | -62.4(7)  |
| C7 P1 C1 C2     | -159.2(6) | C39 C40 C41 C42 | -167.3(7) |
| C7 P1 C13 C14   | -60.9(6)  | C12 C7 C8 C9    | -2.4(11)  |
| C7 C12 C11 C10  | -0.6(15)  | C34 C35 C36 C37 | 0.2(14)   |
| C42 P4 C49 C50  | 152.2(6)  | C16 C15 C20 C19 | 0.6(16)   |
| C42 P4 C49 C54  | -32.7(7)  | C55 C56 C57 Ru1 | 56.0(7)   |
| C42 P4 C43 C44  | -91.5(8)  | C55 C56 C57 C58 | 1.4(13)   |
| C42 P4 C43 C48  | 82.3(7)   | C62 C58 C59 Ru1 | -124.0(8) |
| C21 P2 C14 C13  | -101.0(6) | C62 C58 C59 C60 | -178.2(9) |
| C21 P2 C15 C20  | 94.8(8)   | C62 C58 C57 Ru1 | 123.3(9)  |
| C21 P2 C15 C16  | -87.2(9)  | C62 C58 C57 C56 | 176.9(8)  |
| C21 C26 C25 C24 | 2.2(13)   | C19 C18 C17 C16 | -2(3)     |
| C21 C22 C23 C24 | 0.6(13)   | O1 S1 C01Q F1   | -50.4(7)  |
| C58 C59 C60 Ru1 | 53.2(7)   | O1 S1 C01Q F3   | -173.5(6) |
| C58 C59 C60 C55 | 0.9(14)   | O1 S1 C01Q F2   | 67.6(7)   |
| C26 C21 C22 C23 | 2.2(12)   | O2 S1 C01Q F1   | 68.9(7)   |
| C26 C25 C24 C23 | 0.6(13)   | O2 S1 C01Q F3   | -54.2(7)  |
| C35 C36 C37 C38 | -0.8(14)  | O2 S1 C01Q F2   | -173.1(6) |
| C14 P2 C21 C26  | -113.2(7) | O3 S1 C01Q F1   | -170.0(6) |
| C14 P2 C21 C22  | 65.8(7)   | O3 S1 C01Q F3   | 66.8(7)   |
| C14 P2 C15 C20  | -152.9(7) | O3 S1 C01Q F2   | -52.1(7)  |
| C14 P2 C15 C16  | 25.2(9)   |                 |           |

**Table S22 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for PdRu-2.**

| Atom | x        | y       | z       | U(eq) |
|------|----------|---------|---------|-------|
| H6   | 2047.82  | 7189.78 | 3038.54 | 36    |
| H38  | 1240.41  | 4480.04 | 2438.94 | 40    |
| H2   | 268.62   | 5655.75 | 2268.27 | 41    |
| H50  | 5095.25  | 784.17  | 4322.83 | 43    |
| H32  | 4298.43  | 5757.14 | 2554.58 | 37    |
| H40A | 4759.56  | 4527.07 | 3965.41 | 38    |
| H40B | 3320.24  | 4167.33 | 3893.79 | 38    |
| H44  | 6290.86  | 1674.05 | 3992.85 | 46    |
| H5   | 2814.18  | 7802.16 | 2516.04 | 46    |
| H42A | 3578.46  | 3363.46 | 4447.77 | 39    |
| H42B | 5048.57  | 3606.84 | 4609.11 | 39    |
| H26  | -2445.77 | 3292.08 | 3665.84 | 38    |
| H35  | 5193.88  | 3812.44 | 2012.8  | 46    |
| H14A | -2938.88 | 5233.28 | 3100.85 | 37    |
| H14B | -2115.34 | 5760.67 | 3421.38 | 37    |
| H53  | 1046.27  | 1641.34 | 3701.77 | 46    |
| H3   | 1051.26  | 6292.23 | 1755.04 | 47    |
| H45  | 8494.22  | 1636.66 | 3903.48 | 55    |
| H52  | 1671.42  | 406.05  | 3613.16 | 49    |
| H22  | -1504.61 | 4039.31 | 2628.17 | 39    |
| H9   | -1036.52 | 8035.91 | 3736.12 | 45    |
| H56  | 6188.1   | 861.36  | 5089.54 | 52    |

|      |          |         |         |     |
|------|----------|---------|---------|-----|
| H46  | 10116.66 | 2074.24 | 4387.87 | 52  |
| H54  | 2380.82  | 2425.89 | 4118.34 | 38  |
| H36  | 3234.39  | 3719.39 | 1587.61 | 55  |
| H28  | 4093.86  | 5771.92 | 3723.17 | 44  |
| H25  | -3649.36 | 2334.29 | 3335.1  | 44  |
| H29  | 5406.18  | 6822.4  | 3794.1  | 48  |
| H59  | 3191.64  | 1629.06 | 5931.56 | 53  |
| H37  | 1256.42  | 4066.84 | 1791.2  | 50  |
| H48  | 7309.65  | 2678.81 | 5039.36 | 50  |
| H10  | -447.44  | 7534.72 | 4356.57 | 54  |
| H31  | 5540.23  | 6853.74 | 2630.35 | 45  |
| H20  | 512.59   | 4034.89 | 4093.74 | 62  |
| H30  | 6080.09  | 7387.64 | 3243.11 | 50  |
| H23  | -2639.86 | 3053.56 | 2310.17 | 45  |
| H47  | 9517.68  | 2621.55 | 4952.66 | 63  |
| H60  | 5467.11  | 1883.58 | 6098.26 | 58  |
| H24  | -3763.05 | 2214.34 | 2660.17 | 46  |
| H51  | 3748.42  | -3.92   | 3911.22 | 46  |
| H41A | 5745.46  | 3371.36 | 4013.92 | 43  |
| H41B | 4400.49  | 2960.93 | 3851.45 | 43  |
| H4   | 2310.28  | 7364.16 | 1886.5  | 47  |
| H13A | -1751.52 | 6250.78 | 2814.39 | 36  |
| H13B | -1457.56 | 5438.45 | 2650.72 | 36  |
| H8   | -572.72  | 7353.26 | 3185.38 | 36  |
| H57  | 3949.28  | 578.14  | 4938.5  | 49  |
| H39A | 4071.19  | 3604.73 | 3297.28 | 39  |
| H39B | 5182.24  | 4228.86 | 3354.54 | 39  |
| H12  | 1225.26  | 5754.72 | 3905.61 | 39  |
| H34  | 5188.49  | 4241.62 | 2650.31 | 42  |
| H63A | 1842.76  | 1051.43 | 4720.25 | 85  |
| H63B | 490.55   | 739.37  | 4835.29 | 85  |
| H63C | 1743.02  | 204.09  | 4858.18 | 85  |
| H11  | 728.37   | 6433.31 | 4451.03 | 57  |
| H16  | -2974.89 | 5106.57 | 3881.91 | 76  |
| H61A | 7897.31  | 1185.47 | 5884.39 | 98  |
| H61B | 7571.14  | 2057.08 | 5848.05 | 98  |
| H61C | 7895.38  | 1602.06 | 5474.48 | 98  |
| H62  | 1444.04  | 1443.38 | 5350.47 | 64  |
| H64A | 1780.68  | -63.68  | 5574.78 | 140 |
| H64B | 439.69   | 396.45  | 5551.39 | 140 |
| H64C | 1666.89  | 617.19  | 5867.67 | 140 |
| H19  | 344.34   | 4025.64 | 4761.83 | 92  |
| H18  | -1503.55 | 4523.71 | 4988.19 | 95  |
| H17  | -3172.38 | 5026.49 | 4551.27 | 107 |