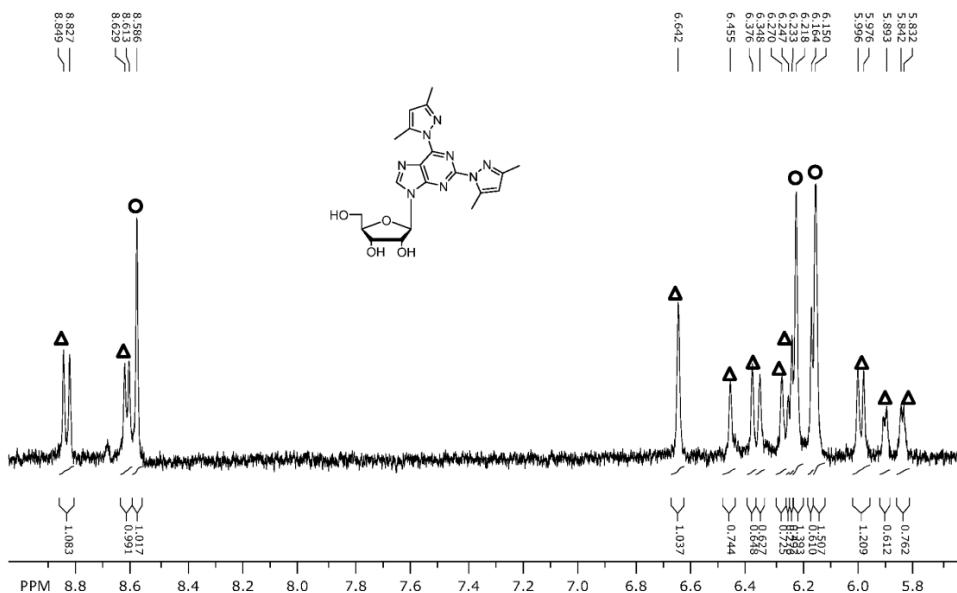
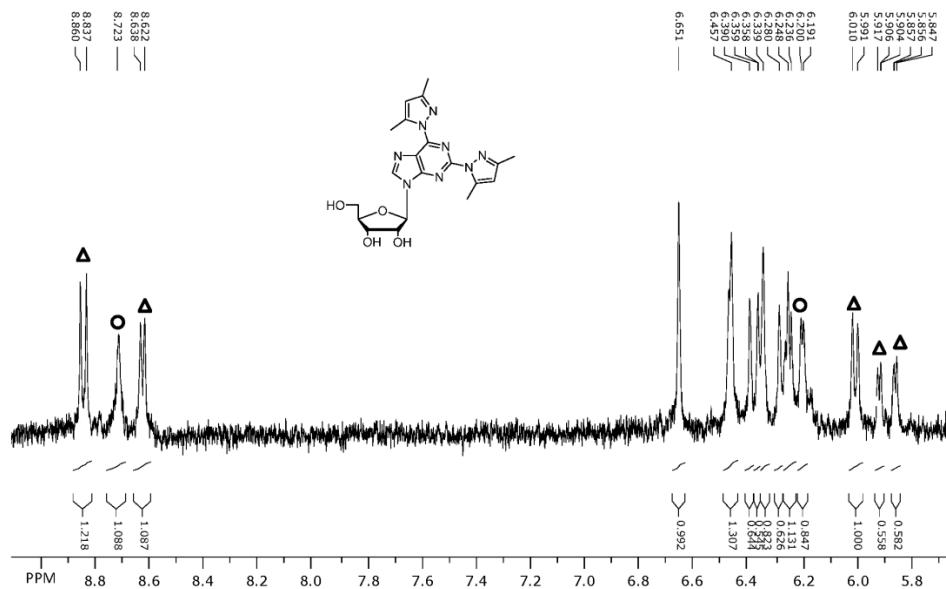


# Supplementary Materials

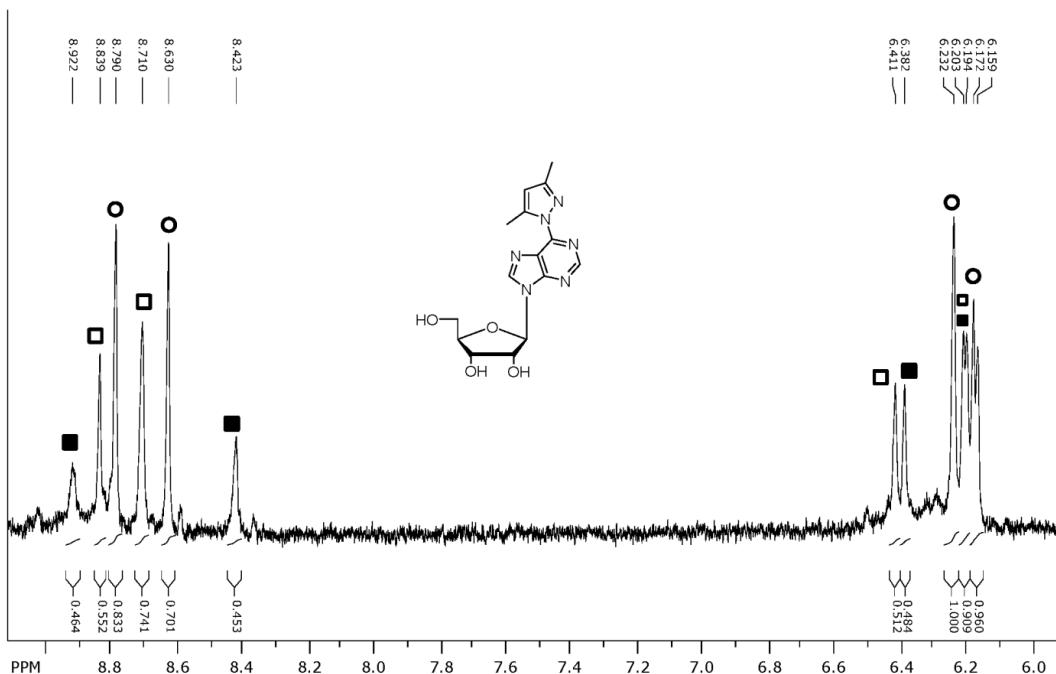
**Figure S1.** Aromatic and anomeric proton signals for the mixture of 2,6-bis(3,5-dimethylpyrazol-1-yl)-9- $\beta$ -D-ribofuranosylpurine (**1**, 5.0 mmol·L<sup>-1</sup>) and K<sub>2</sub>PdCl<sub>4</sub> (2.0 mmol·L<sup>-1</sup>) in D<sub>2</sub>O (phosphate buffer 0.12 mol·L<sup>-1</sup>, pD 7.6, 25 °C). Notation: Open circles refer to uncomplexed **1** and triangles to a 1:2 complex (Pd:**1**).



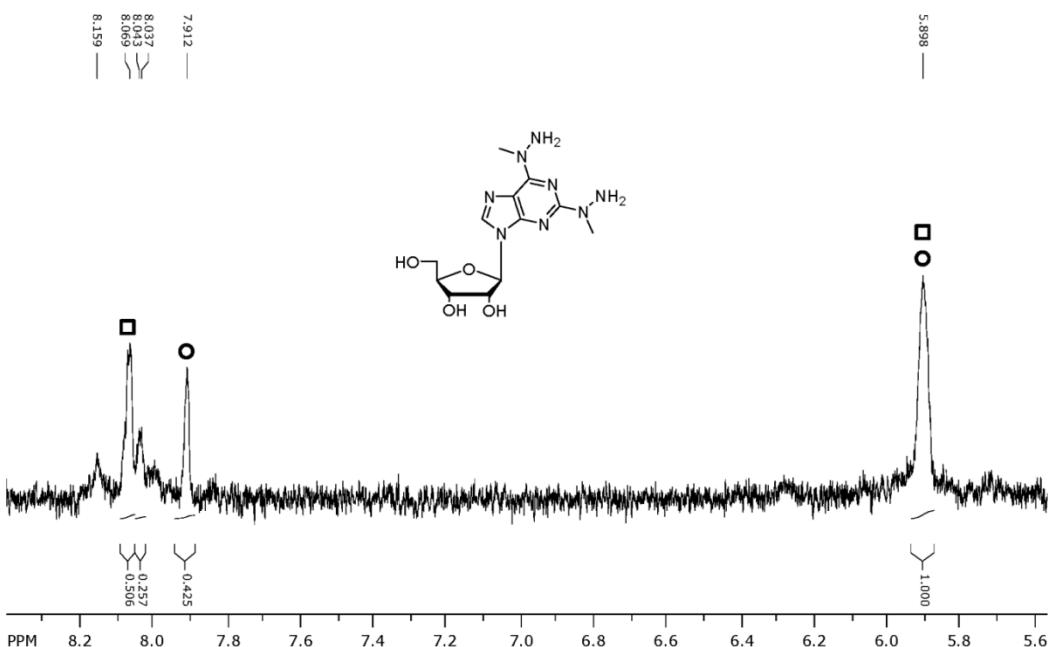
**Figure S2.** Aromatic and anomeric proton signals for the mixture of 2,6-bis(3,5-dimethylpyrazol-1-yl)-9- $\beta$ -D-ribofuranosylpurine (**1**, 5.0 mmol·L<sup>-1</sup>) and K<sub>2</sub>PdCl<sub>4</sub> (4.0 mmol·L<sup>-1</sup>) in D<sub>2</sub>O (phosphate buffer 0.12 mol·L<sup>-1</sup>, pD 7.6, 25 °C). Notation: Open circles refer to a 1:1 and triangles to a 1:2 complex (Pd:**1**).



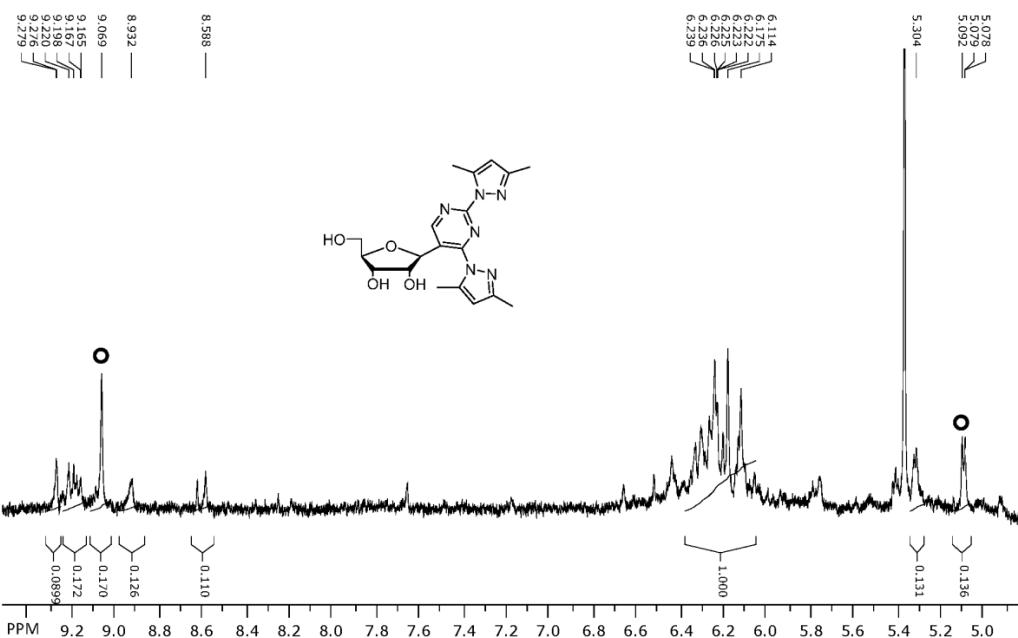
**Figure S3.** Aromatic and anomeric proton signals for the mixture of 6-(3,5-dimethylpyrazol-1-yl)-9- $\beta$ -D-ribofuranosylpurine (**3**, 5.0 mmol·L<sup>-1</sup>) and K<sub>2</sub>PdCl<sub>4</sub> (5.0 mmol·L<sup>-1</sup>) in D<sub>2</sub>O (phosphate buffer 0.12 mol L<sup>-1</sup>, pD 7.6, 25 °C). Notation: Open circles refer to uncomplexed **3** and open and filled squares to two different 1:1 complexes (Pd:**3**).



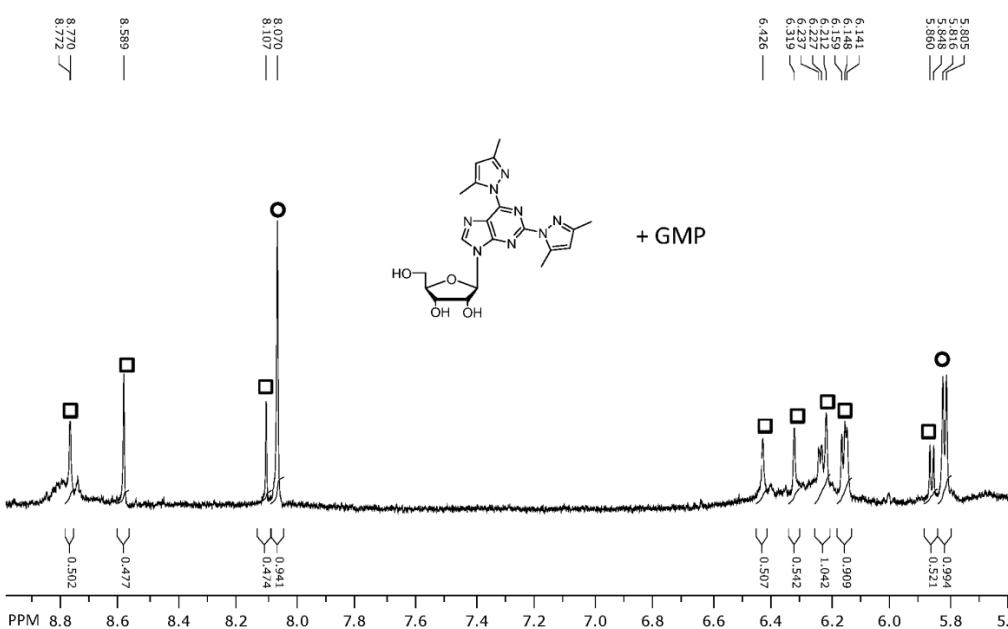
**Figure S4.** Aromatic and anomeric proton signals for the mixture of 2,6-bis(1-methylhydrazinyl)-9- $\beta$ -D-ribofuranosylpurine (**2**, 5.0 mmol·L<sup>-1</sup>) and K<sub>2</sub>PdCl<sub>4</sub> (5.0 mmol·L<sup>-1</sup>) in D<sub>2</sub>O (phosphate buffer 0.12 mol·L<sup>-1</sup>, pD 7.6, 25 °C). Notation: Open circles refer to uncomplexed **2** and open squares to a 1:1 complex (Pd:**2**).



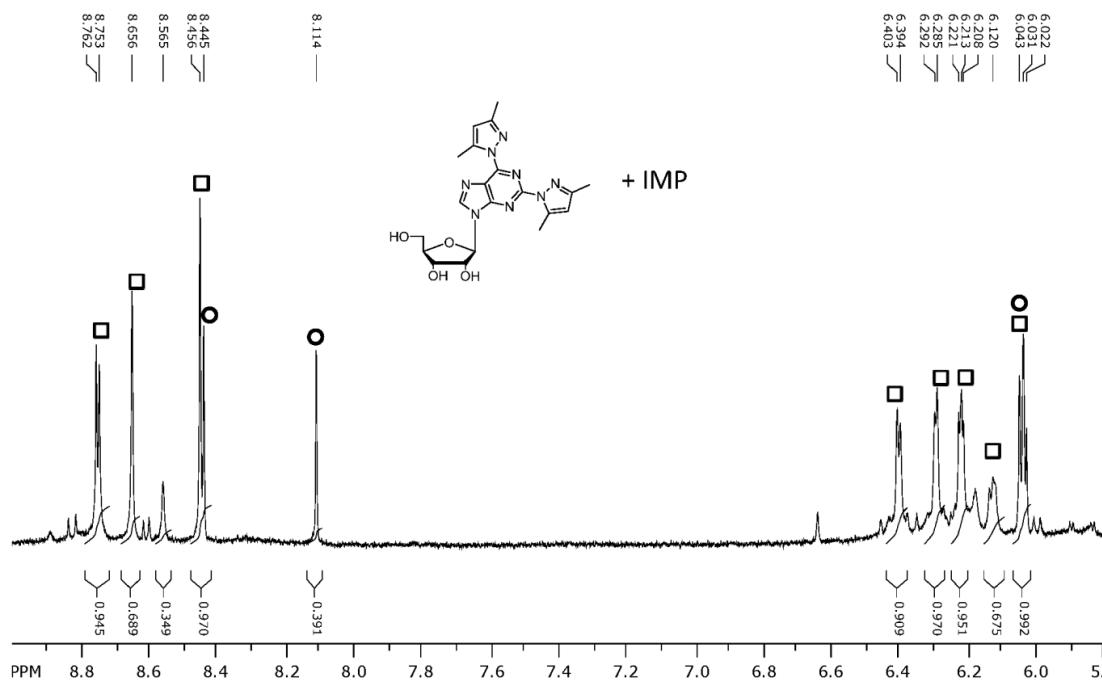
**Figure S5.** Aromatic and anomeric proton signals for the mixture of 2,4-bis(3,5-dimethylpyrazol-1-yl)-5-( $\beta$ -D-ribofuranosyl)-pyrimidine (**4**, 5.0 mmol·L<sup>-1</sup>) and K<sub>2</sub>PdCl<sub>4</sub> (5.0 mmol·L<sup>-1</sup>) in D<sub>2</sub>O (phosphate buffer 0.12 mol·L<sup>-1</sup>, pD 7.6, 25 °C). Notation: Open circles refer to uncomplexed **4** and the rest of the signals to numerous Pd<sup>2+</sup> containing species.



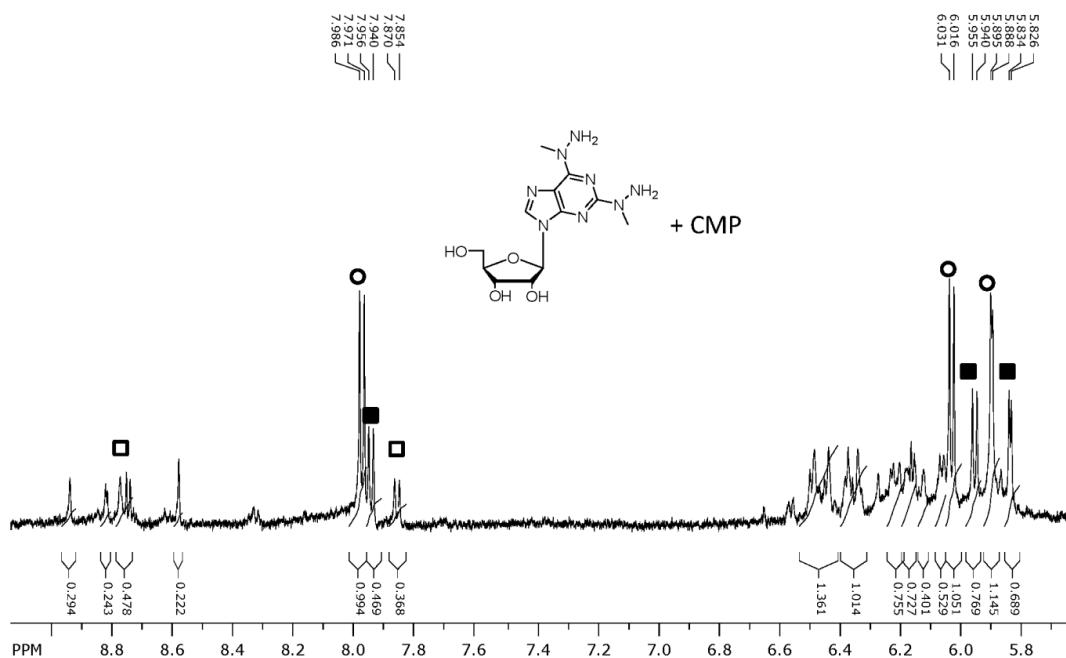
**Figure S6.** Aromatic and anomeric proton signals for the mixture of GMP (5 mmol·L<sup>-1</sup>), 2,6-bis(3,5-dimethylpyrazol-1-yl)-9-β-D-ribofuranosylpurine (**1**, 3.0 mmol·L<sup>-1</sup>) and K<sub>2</sub>PdCl<sub>4</sub> (3.0 mmol·L<sup>-1</sup>) in D<sub>2</sub>O (phosphate buffer 0.12 mol·L<sup>-1</sup>, pH 7.6, 25 °C). Notation: Open circles refer to uncomplexed GMP and squares to 1:1:1 complexes (**1**:Pd:GMP).



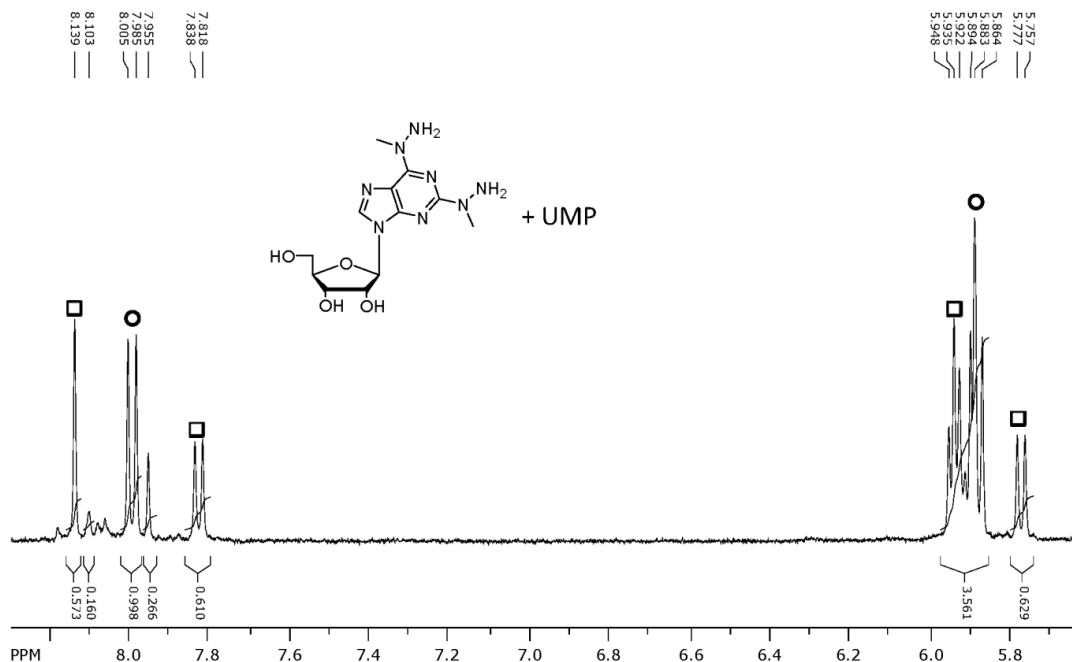
**Figure S7.** Aromatic and anomeric proton signals for the mixture of IMP ( $5 \text{ mmol}\cdot\text{L}^{-1}$ ), 2,6-bis(3,5-dimethylpyrazol-1-yl)-9- $\beta$ -D-ribofuranosylpurine (**1**,  $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) and  $\text{K}_2\text{PdCl}_4$  ( $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) in  $\text{D}_2\text{O}$  (phosphate buffer  $0.12 \text{ mol}\cdot\text{L}^{-1}$ ,  $\text{pD } 7.6$ ,  $25^\circ\text{C}$ ). Notation: Open circles refer to uncomplexed IMP and squares to 1:1:1 complexes (**1**:Pd:IMP).



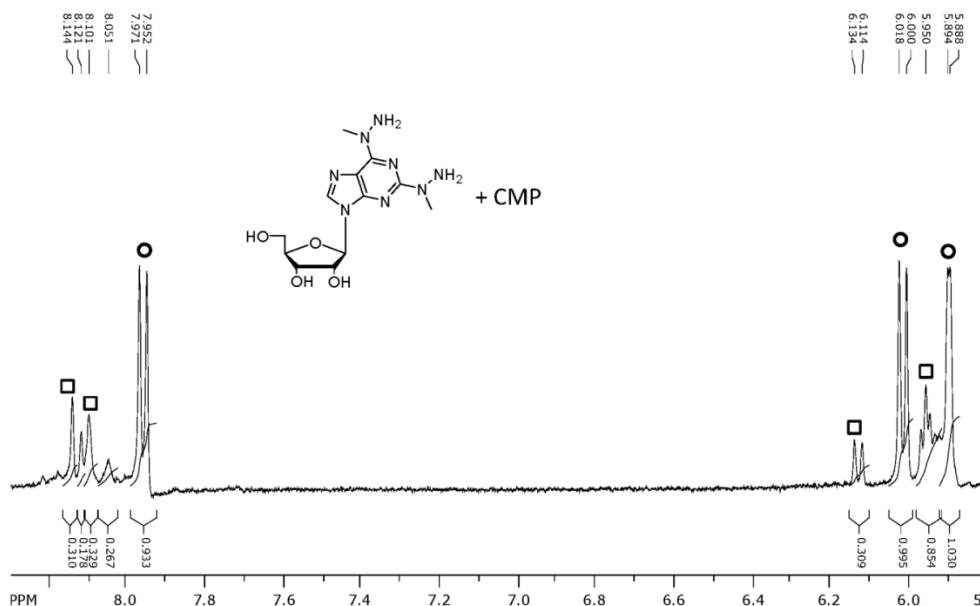
**Figure S8.** Aromatic and anomeric proton signals for the mixture of CMP ( $5 \text{ mmol}\cdot\text{L}^{-1}$ ), 2,6-bis(3,5-dimethylpyrazol-1-yl)-9- $\beta$ -D-ribofuranosylpurine (**1**,  $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) and  $\text{K}_2\text{PdCl}_4$  ( $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) in  $\text{D}_2\text{O}$  (phosphate buffer  $0.12 \text{ mol}\cdot\text{L}^{-1}$ ,  $\text{pD } 7.6$ ,  $25^\circ\text{C}$ ). Notation: Open circles refer to uncomplexed CMP, filled squares to the binary complex  $(\text{CMP})\text{Pd}^{2+}$  complex and open squares to the mixed ligand complex **(1)**Pd(CMP).



**Figure S9.** Aromatic and anomeric proton signals for the mixture of UMP ( $5 \text{ mmol}\cdot\text{L}^{-1}$ ), 2,6-bis(1-methylhydrazinyl)-9- $\beta$ -D-ribofuranosylpurine (**2**,  $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) and  $\text{K}_2\text{PdCl}_4$  ( $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) in  $\text{D}_2\text{O}$  (phosphate buffer  $0.12 \text{ mol}\cdot\text{L}^{-1}$ , pD 7.6,  $25^\circ\text{C}$ ). Notation: Open circles refer to uncomplexed UMP and open squares to the mixed ligand complex (**2**Pd(UMP)).



**Figure S10.** Aromatic and anomeric proton signals for the mixture of CMP ( $5 \text{ mmol}\cdot\text{L}^{-1}$ ), 2,6-bis(1-methylhydrazinyl)-9- $\beta$ -D-ribofuranosylpurine (**2**,  $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) and  $\text{K}_2\text{PdCl}_4$  ( $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) in  $\text{D}_2\text{O}$  (phosphate buffer  $0.12 \text{ mol}\cdot\text{L}^{-1}$ , pD 7.6,  $25^\circ\text{C}$ ). Notation: Open circles refer to uncomplexed CMP and open squares to the mixed ligand complex (**2**Pd(CMP)).



**Figure S11.** Aromatic and anomeric proton signals for the mixture of GMP ( $5 \text{ mmol}\cdot\text{L}^{-1}$ ), 2,6-bis(1-methylhydrazinyl)-9- $\beta$ -D-ribofuranosylpurine (**2**,  $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) and  $\text{K}_2\text{PdCl}_4$  ( $4.0 \text{ mmol}\cdot\text{L}^{-1}$ ) in  $\text{D}_2\text{O}$  (phosphate buffer  $0.12 \text{ mol}\cdot\text{L}^{-1}$ , pD 7.6,  $25^\circ\text{C}$ ). Notation: Open circles refer to uncomplexed GMP and open squares to the mixed ligand complex (**2**Pd(GMP).

