# The Structural Effect of Methyl Substitution on the Binding of Polypyridyl Ru-dppz Complexes to DNA

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**Supplementary Information**

**Contents**

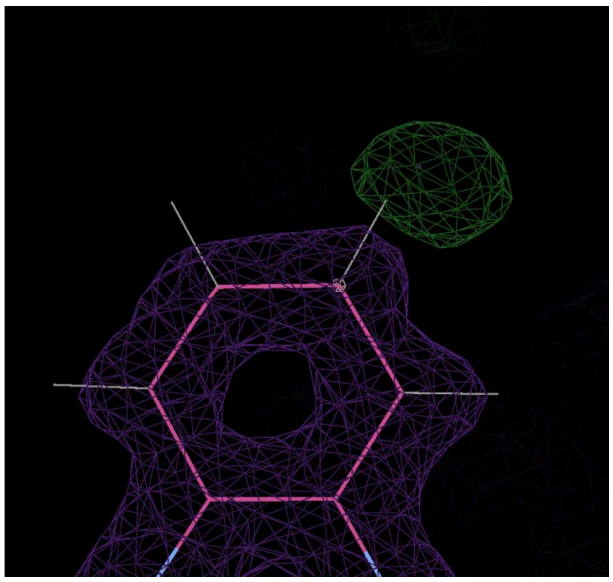

Figure S1 – The assignment of the methyl group position for structure 2 was on the basis of a positive (6σ) peak in the $F_o$-$F_c$ electron density difference map when the complex was modelled as $[Ru(TAP)_2(dppz)]^{2+}$. The peak is illustrated in green with the $2F_o$-$F_c$ electron density map for the complex in purple.

Table S1 – Full data collection, data processing and refinement statistics

| **Crystallization Parameters** | **1** | 2 | 3 | **4** |
|---|---|---|---|---|
| DNA Sequence | d(TCGGCGCCGA) | d(TCGGCGCCGA) | d(TCGGCGCCGA) | d(TCGGCGCCGA) |
| Complex | $[Ru(TAP)_2(dppz\text{-}10\text{-}Me)]^{2+}$ | $[Ru(TAP)_2(dppz\text{-}11\text{-}Me)]^{2+}$ | $[Ru(TAP)_2(dppz\text{-}10,12\text{-}Me_2)]^{2+}$ | Λ-$[Ru(TAP)_2(dppz\text{-}11,12\text{-}Me_2)]^{2+}$ |
| Crystallization temperature, °C | 4 | 18 | 18 | 4 |
| Crystal size, µm | 80x80x80 | 80x80x30 | 100x60x60 | 100x30x50 |
| Growth time (weeks) | 1 | 1 | 1 | 2 |
| **Data Collection** | | | | |
| Beamline | I02 | I02 | I02 | I02 |
| Radiation wavelength, Å | 0.8856 | 0.7749 | 0.7749 | 0.9795 |
| Temperature, K | 100 | 100 | 100 | 100 |
| Oscillation angle, ° | 0.1 | 0.1 | 0.1 | 1.3 |
| Number of images | 900 | 900 | 900 | 103 |
| Wedge collected, ° | 90 | 90 | 90 | 133.9 |
| Exposure time, s | 0.1 | 0.1 | 0.1 | 0.5 |
| Detector | Pilatus 6M | Pilatus 6M | Pilatus 6M | ADSC Q315r |
| **Data Processing** | | | | |
| Structure Solution Method | Molecular Replacement | SAD | SAD | Molecular Replacement |
| Molecular Replacement Model | **3QRN** | N/A | N/A | **3QRN** |
| Space group | $P4_32_12$ | $P43212$ | $P4_32_12$ | $P4_32_12$ |
| Cell Dimensions, Å | 42.2, 42.2, 39.6 | 42.1, 42.1, 39.2 | 42.2, 42.2, 39.6 | 42.4, 42.4, 39.6 |
| Resolution, Å | 21.14-0.97 (1.00-0.97) | 28.70-1.05 (1.08-1.05) | 17.05-0.89 (0.91-0.89) | 42.4-1.24 (1.27-1.24) |
| $R_{merge}$ | 0.032 (0.498) | 0.035 (0.800) | 0.030 (0.723) | 0.066 (0.631) |
| $R_{pim}$ | 0.018 (0.273) | 0.020 (0.504) | 0.018 (0.344) | 0.026 (0.217) |
| I/σI | 24.2 (2.6) | 21.8 (2.1) | 23.5 (2.2) | 20.2 (3.5) |
| Completeness, % | 95.9 (98.7) | 99.1 (97.7) | 98.5 (95.9) | 99.9 (100) |
| Multiplicity | 6.3 (4.8) | 6.2 (6.3) | 6.2 (6.1) | 10 (10.2) |
| **Refinement** | | | | |
| No. Reflections | 19713 | 15996 | 26155 | 10212 |
| $R_{work}/R_{free}$ | 0.08/0.09 | 0.09/0.10 | 0.09/0.10 | 0.10/0.12 |
| **No. Atoms** | | | | |
| DNA | 315 | 315 | 315 | 202 |
| Ligands | 78 | 78 | 80 | 55 |
| Water | 115 | 77 | 92 | 101 |
| **Average B factors, Å$^2$** | | | | |
| DNA | 13.73 | 15.6 | 12.19 | 15.8 |
| Ligands | 12.27 | 13.76 | 11.08 | 13.76 |
| Water | 31.11 | 30.58 | 28.01 | 31 |
| **rmsd** | | | | |
| Bond Lengths, Å | 0.03 | 0.038 | 0.04 | 0.038 |
| Bond Angles, ° | 2.54 | 2.81 | 2.75 | 2.84 |
| **PDB ID** | **4MJ9** | **4X18** | **4X1A** | **4E8S** |

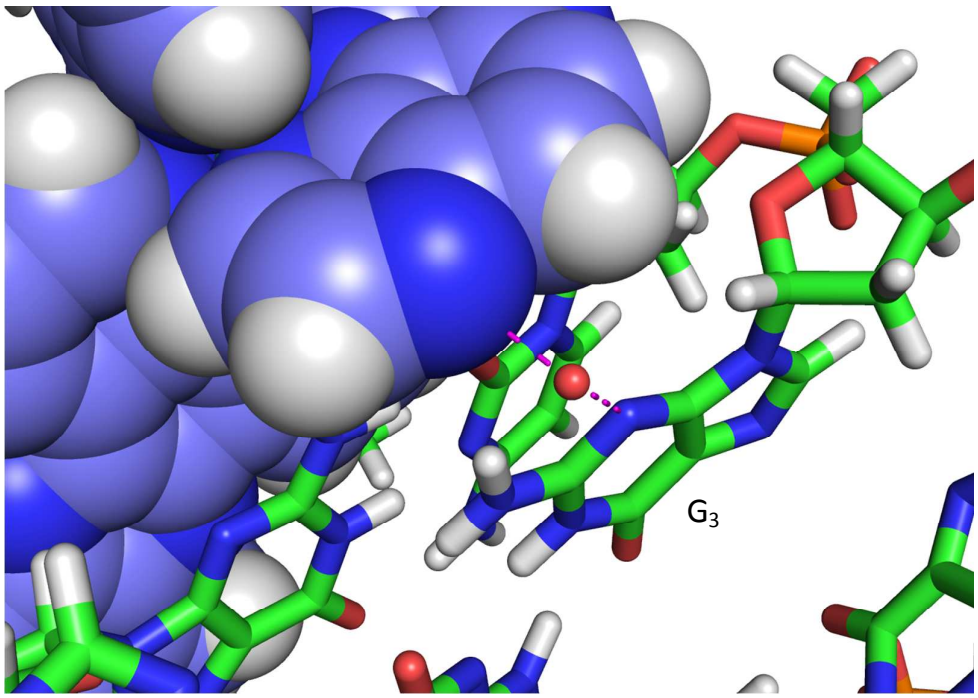


Figure S2: A water-mediated TAP-$G_3(N_3)$ hydrogen bond in structure1. The water molecule is displayed as a red sphere. It forms a bridging hydrogen bond with a nitrogen on TAP 2 and atom N3 on G3. The hydrogen bonds are illustrated in magenta. Elements are coloured according to type with nitrogen in blue, oxygen in red, phosphorus in orange and hydrogen in white. The DNA carbon atoms are in green with the complex carbon atoms in purple.