

## Supplementary Information for

# Triazole-based osmium(II) complexes displaying red/near-IR luminescence: antimicrobial activity and super-resolution imaging

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## Experimental Section

### General Methods

Ammonium hexachloroosmate(IV) was purchased from Alfa Aesar whilst all other reagents were obtained from either Acros Organics or Fluorochem and used as supplied. Unless otherwise stated, synthetic procedures were carried out under an atmosphere of dry N<sub>2</sub>, employing standard Schlenk line techniques. Preparative thin layer chromatography was performed utilising SiO<sub>2</sub> plates (Analtech Uniplat) of size 20 x 20 cm and 1500 μm thickness. NMR spectra were recorded on Bruker Ascend 400 and 600 MHz spectrometers, with all chemical shifts being reported relative to the residual solvent signal (MeCN: <sup>1</sup>H: δ 1.94, <sup>13</sup>C: δ 1.94, 118.26) High-resolution mass spectrometry was performed on an Agilent 6210 TOF instrument with a dual electrospray ionisation source. UV-Visible absorption spectrometers were recorded on an Agilent Cary 60 spectrometer. Luminescence measurements were performed using a Fluoromax-4 spectrophotometer. Lifetime measurements were recorded by time-correlated single photon counting using an Edinburgh instruments Mini-Tau spectrometer. Quantum yields (Φ<sub>em</sub>) are quoted relative to [Ru(bpy)<sub>3</sub>][PF<sub>6</sub>]<sub>2</sub> in aerated MeCN solution, with all analyte solutions being excited at a single wavelength with common optical density. Quantum yields are thus determined from the ratio of integrated area under the peaks. Cyclic voltammograms were recorded using a PalmSens EmStat3 potentiostat, using PSTrace electrochemical software (v4.8). Analyte solutions with a typical concentration of 1 mmoldm<sup>-3</sup> were prepared using N<sub>2</sub> saturated dry acetonitrile, freshly distilled from CaH<sub>2</sub>. All measurements were performed at room temperature (r.t.) under a stream of N<sub>2</sub> at potential scan rates of between 20 and 500 mVs<sup>-1</sup>. NBu<sub>4</sub>PF<sub>6</sub> was employed as supporting electrolyte, being recrystallized from EtOH and oven dried prior to use, with a typical solution concentration of 0.2 moldm<sup>-3</sup>. The working electrode was glassy carbon, Pt wire was used as the counter electrolyte and Ag/AgCl as the reference electrode, the latter being chemically isolated from the analyte solution by an electrolyte-containing bridge tube fitted with a porous frit. Ferrocene was employed as an internal reference, with all potentials being quoted relative to the Fc<sup>+</sup>/Fc couple.

**Synthesis of *mer*- and *fac*-[Os(pymtz)<sub>3</sub>][PF<sub>6</sub>]<sub>2</sub> (*mer*-2<sup>2+</sup> and *fac*-2<sup>2+</sup>):** [OsCl<sub>6</sub>][NH<sub>4</sub>]<sub>2</sub> (152 mg, 0.34 mmol) and pymtz (258 mg, 1.08 mmol) were combined in ethylene glycol (10 ml) and heated to 200 °C under an N<sub>2</sub> atmosphere for 2 h. The resulting solution was allowed to cool to r.t. before the addition of an aqueous solution (20 ml) of excess NH<sub>4</sub>PF<sub>6</sub> (410 mg, 2.51 mmol). After stirring for 1 h the resultant red coloured solids were collected by filtration, washed with H<sub>2</sub>O followed by Et<sub>2</sub>O and dried *in vacuo*. Purification was achieved *via* flash column chromatography (Al<sub>2</sub>O<sub>3</sub>, 8 cm pad, 1:1 MeCN / CH<sub>2</sub>Cl<sub>2</sub>), with collection of the bright red coloured eluate. Evaporation of the solvent to a minimum volume followed by dropwise addition into excess Et<sub>2</sub>O yielded bright red coloured solids which <sup>1</sup>H NMR analysis shows to be composed of a mixture of *mer*- and *fac*-isomers in a respective 2:1 ratio. Yield = 315 mg, 76%. Separation of small quantities of *mer*- and *fac*-isomers was achieved *via* preparative thin layer chromatography (SiO<sub>2</sub>, 1:1 acetone / CH<sub>2</sub>Cl<sub>2</sub>) with the upper (higher R<sub>f</sub>) band found to contain exclusively the meridional isomer. The facial isomer was obtained from the second (lower R<sub>f</sub>) red coloured band.

*mer*-2<sup>2+</sup> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.53 (s, 2H), 5.55-5.58 (m, 4H), 7.15-7.20 (m, 2H), 7.22-7.26 (m, 4H), 7.26-7.32 (m, 3H), 7.32-7.42 (m, 9H), 7.99 (dd, *J* = 1.9, 5.9 Hz, 1H), 8.06 (dd, *J* = 1.9, 6.0 Hz, 1H), 8.14 (dd, *J* = 1.9, 5.9 Hz, 1H), 8.69 (d, *J* = 1.8 Hz, 1H), 8.70 (d, *J* = 1.8 Hz, 1H), 8.72 (s, 2H), 8.73 (d, *J* = 1.9 Hz, 1H), 8.75 (s, 1H). <sup>13</sup>C NMR (CD<sub>3</sub>CN, 151 MHz): 56.49, 56.73, 56.82, 121.78, 121.89, 122.67, 128.66, 128.78, 129.20, 129.28, 129.47, 129.48, 129.90, 130.01, 130.02, 130.04, 134.27, 134.32, 134.77, 148.01, 148.06, 148.21, 157.94, 157.97, 158.10, 160.23, 160.32, 160.39, 164.58, 164.60, 164.63. HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6320 (M<sup>2+</sup>).

*fac*-2<sup>2+</sup> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.52 (s, 6H), 7.18 (dd, *J* = 2.0, 7.6 Hz, 6H), 7.26 (dd, *J* = 5.1, 5.1 Hz, 3H), 7.30-7.40 (m, 9H), 8.20 (dd, *J* = 1.9, 5.9 Hz, 3H), 8.73 (s, 3H), 8.75 (d, *J* = 1.9 Hz, 3H). <sup>13</sup>C NMR (CD<sub>3</sub>CN, 151 MHz): 56.53, 122.27, 128.84, 128.86, 129.91, 130.02, 134.74, 148.02, 158.14, 160.68, 164.74. HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6324 (M<sup>2+</sup>).

**Synthesis of *mer*- and *fac*-[Os(pyztz)<sub>3</sub>][PF<sub>6</sub>]<sub>2</sub> (*mer*-**3**<sup>2+</sup> and *fac*-**3**<sup>2+</sup>):** [OsCl<sub>6</sub>][NH<sub>4</sub>]<sub>2</sub> (143 mg, 0.33 mmol) and pyztz (243 mg, 1.03 mmol) were combined in ethylene glycol (10 ml) and heated to 200 °C under an N<sub>2</sub> atmosphere for 2 h. After cooling to room temperature, an aqueous solution (20 ml) of excess NH<sub>4</sub>PF<sub>6</sub> (386 mg, 2.37 mmol) was added followed by stirring at r.t. for a further 1.5 h. The resultant brown coloured solids were collected by filtration, washed with H<sub>2</sub>O followed by Et<sub>2</sub>O and dried *in vacuo*. Purification was achieved by flash column chromatography (Al<sub>2</sub>O<sub>3</sub>, 9 cm pad, 1:1 MeCN / CH<sub>2</sub>Cl<sub>2</sub>), with collection of the deep-red coloured eluate. Evaporation of the solvent to a minimum volume followed by dropwise addition into excess Et<sub>2</sub>O yielded brick-red coloured solids which <sup>1</sup>H NMR analysis shows to be composed of a mixture of *mer*- and *fac*- isomers in a respective 3:1 ratio. Yield = 191 mg, 49 %. Separation of small quantities of *mer*- and *fac*- isomers was achieved by preparative thin layer chromatography (SiO<sub>2</sub>, 7 % MeOH / CH<sub>2</sub>Cl<sub>2</sub>), with the upper (higher R<sub>f</sub>) red coloured band containing exclusively the *mer*-isomer. The *fac*-isomer was obtained from the second red coloured band.

*mer*-**3**<sup>2+</sup> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.51-5.63 (m, 6H), 7.21 (dd, *J* = 2.0, 7.2 Hz, 2H), 7.26-7.34 (m, 4H), 7.35-7.47 (m, 9H), 7.74 (dd, *J* = 1.0, 3.4 Hz, 1H), 7.78 (dd, *J* = 1.0, 3.4 Hz, 1H), 7.84 (dd, *J* = 1.0, 3.4 Hz, 1H), 8.26 (d, *J* = 3.4 Hz, 1H), 8.31 (d, *J* = 3.4 Hz, 1H), 8.34 (d, *J* = 3.4 Hz, 1H), 8.69 (s, 1H), 8.70 (s, 1H), 8.72 (s, 1H), 9.19 (d, *J* = 1.0 Hz, 1H), 9.20 (d, *J* = 1.0 Hz, 1H), 9.24 (d, *J* = 1.0 Hz, 1H). <sup>13</sup>C NMR (CD<sub>3</sub>CN, 101 MHz): 56.51, 56.74, 56.85, 126.84, 127.39, 127.64, 129.01, 129.55, 129.72, 129.97, 130.01, 130.05, 130.06, 130.10, 130.13, 133.84, 133.96, 134.49, 143.48, 143.57, 144.18, 146.57, 147.05, 147.11, 147.15, 147.20, 147.48, 147.99, 148.11, 148.33, 149.28, 149.56, 149.96. HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6325 (M<sup>2+</sup>).

*fac*-**3**<sup>2+</sup> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.54 (s, 6H), 7.22 (dd, *J* = 2.0, 7.6 Hz, 6H), 7.34-7.44 (m, 9H), 7.86 (dd, *J* = 1.1, 3.4 Hz, 3H), 8.28 (d, *J* = 3.4 Hz, 3H), 8.72 (s, 3H), 9.22 (d, *J* = 1.0 Hz, 3H). <sup>13</sup>C NMR (CD<sub>3</sub>CN, 101 MHz): 56.63, 127.06, 129.14, 130.06, 130.08, 134.40, 144.01, 147.05, 147.79, 147.82, 149.71. HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6323 (M<sup>2+</sup>).

## General Procedure for Counter-Ion Metathesis – Preparation of Water-Soluble Chloride Salts

The relevant Os complex as its hexafluorophosphate salt and 2.5 weight-equivalents of Amberlite chloride-form ion-exchange resin were combined in MeOH and stirred overnight, open to air in the dark, at room temperature. The resin was removed by gravity filtration and the filtrate evaporated to dryness. The resulting residue was re-dissolved in the minimum quantity of MeOH, precipitated from solution through the addition of excess Et<sub>2</sub>O and the solids collected by filtration. Successful counter-ion exchange was confirmed by the complete absence of resonances in <sup>31</sup>P and <sup>19</sup>F NMR spectra.

*mer*-[**2**]Cl<sub>2</sub> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.54-5.73 (m, 6H), 7.17-7.40 (m, 18H), 8.03 (dd, *J* = 1.8, 6.0 Hz, 1H), 8.12 (dd, *J* = 1.8, 6.0 Hz, 1H), 8.15 (dd, *J* = 1.8, 6.0 Hz, 1H), 8.68-8.71 (m, 2H), 8.75 (dd, *J* = 1.8, 4.8 Hz, 1H), 9.02 (s, 1H), 9.12 (s, 1H), 9.23 (s, 1H). HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6322 (M<sup>2+</sup>).

*fac*-[**2**]Cl<sub>2</sub> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.53 (d, *J* = 15.1 Hz, 3H), 5.59 (d, *J* = 15.1 Hz, 3H), 7.20 (dd, *J* = 1.8, 7.0 Hz, 6H), 7.27 (t, *J* = 5.4 Hz, 3H), 7.30-7.40 (m, 9H), 8.24 (dd, *J* = 1.7, 6.0 Hz, 3H), 8.74 (dd, *J* = 1.8, 5.0 Hz, 3H), 8.94 (s, 3H). HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6322 (M<sup>2+</sup>).

*mer*-[**3**]Cl<sub>2</sub> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.55-5.70 (m, 6H), 7.20-7.26 (m, 2H), 7.28-7.44 (m, 13H), 7.78 (dd, *J* = 1.1, 3.4 Hz, 1H), 7.83 (dd, *J* = 1.1, 3.4 Hz, 1H), 7.85 (dd, *J* = 1.1, 3.4 Hz, 1H), 8.24 (d, *J* = 3.4 Hz, 1H), 8.29 (d, *J* = 3.4 Hz, 1H), 8.34 (d, *J* = 3.4 Hz, 1H), 9.19 (s, 1H), 9.24 (s, 1H), 9.31 (s, 1H), 9.37 (d, *J* = 1.1 Hz, 1H), 9.42 (d, *J* = 1.1 Hz, 1H), 9.49 (d, *J* = 1.1 Hz, 1H). HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6321 (M<sup>2+</sup>).

*fac*-[**3**]Cl<sub>2</sub> <sup>1</sup>H NMR (CD<sub>3</sub>CN, 400 MHz): 5.55 (d, *J* = 15.1 Hz, 3H), 5.60 (d, *J* = 15.1 Hz, 3H), 7.24 (dd, *J* = 1.8, 6.0 Hz, 6H), 7.33-7.43 (m, 9H), 7.87 (dd, *J* = 0.7, 3.4 Hz, 3H), 8.28 (d, *J* = 3.4 Hz, 3H), 9.13 (s, 3H), 9.39 (d, *J* = 1.1 Hz, 3H). HRMS (ES); *m/z* calc'd for [OsC<sub>39</sub>H<sub>33</sub>N<sub>15</sub>]<sup>2+</sup>: 451.6323, found: 451.6324 (M<sup>2+</sup>).

## Bacterial Strain Information and General Growth Procedures

Microbiological studies were conducted with a CTX-M-15 type extended spectrum  $\beta$ -lactamase (EBSL)-producing clinical isolate *E. coli* EC958 (ST131), a clinical isolate strain (University of Surrey) of *Pseudomonas aureginosa* PA2017, a clinical isolate strain of *Acetivobacter baumannii* AB184 and a clinical isolate, methicillin resistant strain of *S. aureus* BH1CC. Bacteria were routinely grown under aseptic, aerobic conditions in autoclave-sterilised culture medium at 37 °C. Lysogeny Broth (LB) (Formedium) and Mueller-Hinton II (MH-II) (Sigma-Aldrich) were prepared as per manufacturers' instructions. Glucose defined minimal medium (GDMM) was prepared by dissolution of 4 g L<sup>-1</sup> K<sub>2</sub>PO<sub>4</sub>, 1 g L<sup>-1</sup> KH<sub>2</sub>PO<sub>4</sub>, 1 g L<sup>-1</sup> NH<sub>4</sub>Cl, 10 mg L<sup>-1</sup> CaCl<sub>2</sub> and 2.6 g L<sup>-1</sup> K<sub>2</sub>SO<sub>4</sub> in deionised H<sub>2</sub>O with supplementation of 10 mL L<sup>-1</sup> Trace Elements solution. The pH was adjusted to 7.4 by the addition of NaOH. GDMM was sterilized by autoclaving and then further supplemented with 1 mM MgCl<sub>2</sub> and 20 mM glucose prior to growth studies. Trace elements contained 5 g L<sup>-1</sup> ethylenediaminetetraacetic acid (EDTA), 0.5 g L<sup>-1</sup> Fe(III)Cl<sub>3</sub>·6H<sub>2</sub>O, 50 mg L<sup>-1</sup> ZnO, 10 mg L<sup>-1</sup> CuCl<sub>2</sub>·2H<sub>2</sub>O, 10 mg L<sup>-1</sup> CoNO<sub>3</sub>·6H<sub>2</sub>O, 10 mg L<sup>-1</sup> H<sub>3</sub>BO<sub>3</sub>, 0.12 mg L<sup>-1</sup> (NH<sub>4</sub>)<sub>2</sub>MoO<sub>4</sub> and 17 mg L<sup>-1</sup> Na<sub>2</sub>O<sub>4</sub>Se. Chemically Defined Minimal Medium (CDM). CDM solution 1: Na<sub>2</sub>HPO<sub>4</sub>·2H<sub>2</sub>O (7 g), KH<sub>2</sub>PO<sub>4</sub> (3 g), L-Aspartic acid (0.15 g), L-Alanine (0.1 g), L-Arginine (0.1 g), L-Cysteine (0.05 g), Glycine (0.1 g), L-Glutamic Acid (0.15 g), L-Histidine (0.1 g), L-Isoleucine (0.15 g), L-Lysine (0.1 g), L-Leucine (0.1 g), L-Methionine (0.1 g), L-Phenylalanine (0.1 g), L-Proline (0.15 g), L-Serine (0.1 g), L-Threonine (0.15 g), L-Tryptophan (0.1 g), L-Tyrosine (0.1 g) and L-Valine (0.15 g), dissolved in 700 mL of distilled water. CDM solution 2 (makes 1000x working concentration): Biotin (0.02 g), Nicotinic acid (0.4 g), D-Pantothenic acid (0.4 g), Thiamine HCl (0.4 g), Pyridoxal HCl (0.8 g), Pyridoxamine di-HCl (0.8 g), Riboflavin (0.4 g) dissolved in 140 mL of distilled water. CDM solution 3: Adenine sulphate (0.02 g), Guanine HCl (0.02 g) dissolved in 50 mL of 0.1 M HCl. CDM solution 4 CaCl<sub>2</sub>·6H<sub>2</sub>O (0.01 g) and (NH<sub>4</sub>)<sub>2</sub>Fe(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O (0.006 g) dissolved in 50 mL of 0.1 M HCl. CDM solution 5: Glucose (10 g) and MgSO<sub>4</sub>·7H<sub>2</sub>O (0.5 g) dissolved in 100 mL of distilled water. CDM media (1L): solution 1 (700 mL), 1x solution 2 (100 mL), solution 3 (50 mL), solution 4 (10 mL) and solution 5 (100 mL). The pH was adjusted to 7.4 by the addition of NaOH. All media was sterilised in an autoclave.

For short term storage bacterial stocks were maintained on nutrient agar plates at 4 °C for 2-3 weeks. For long-term storage, strains were stored as cell suspensions in 30 % (v/v) LB 70 % (w/v) glycerol at – 80 °C.

### **Determination of Minimum Inhibitory Concentrations (MICs) and Minimum Bactericidal Concentrations (MBCs).**

MICs and MBCs of all compounds and ampicillin (control) were determined *via* a standard broth-dilution method in 96-well micro-titre plates in either MH-II, GDMM (Gram-negative strains) or CDM (Gram-positive strains). The MIC of each compound was evaluated using 2-fold increasing concentrations of each compound between 2 to 512 µg/mL against a bacterial inoculum of  $10^7$ - $10^9$  colony forming units per mL (CFU mL<sup>-1</sup>), corresponding to an optical density at 600 nm (OD<sub>600</sub>) of 0.05-0.075. Plates were incubated at 37 °C for 20 h. After this time, the level of turbidity in each well was used to determine the extent of bacterial cell growth in the presence of the compounds. The minimal concentration of compound that did not permit bacterial growth was determined to be the MIC. For MBC determination, 10 µL samples of each well were then transferred to nutrient agar plates and further incubated at 37 °C. The lowest concentration of compound in which no CFU were observed after plating was determined to be the MBC. MIC/MBCs were determined from 3 independent biological repeats.

### **Phototoxicity**

96-well plates were made up as with the previous MIC experiment. 3 plates were made for each compound for the three different light fluences. The apparatus used to irradiate the sample was a custom made device featuring a broadband illumination source, fully contained in an empty computer base unit – Light Irradiation Source Apparatus (LISA). Plates were exposed to the light for 0, 5 and 30 minutes giving 0, 8 and 48 J cm<sup>-2</sup> fluence respectively. After light irradiation plates were incubated at 37 °C for 20 h. The MIC's after light irradiation were determined as previous.

### **Uptake by *E. coli* and *S. aureus* and Determination of Cellular Osmium and Iron levels.**

Uptake and cellular accumulation of the compounds by *E. coli* EC958 and *S. aureus* BH1CC was determined by measuring bacterial cell metal content by inductively coupled plasma-atomic emission spectroscopy (ICP-AES). Bacterial cultures were grown to midexponential phase in LB broth, washed in PBS, and then re-suspended in PBS  $\pm$  20 mM glucose to approximately  $10^8$ - $10^9$  CFU.mL. The compounds were added to the cells at MIC concentration, 20 mL samples of culture were harvested at 5, 10, 20 and 60 minutes after compound addition. Samples of non-compound treated cells were also taken for comparison. Samples were centrifuged at 5000 g for 20 min at 4 °C to obtain cell pellets and the supernatant containing unbound extracellular compound was discarded. The resultant cell pellets were then washed twice in 0.5 % (v/v) Aristar nitric acid to remove loosely bound residual complex. To prepare cell material for ICP-AES cell pellets were re-suspended in 0.5 mL Aristat nitric acid (69 % (w/v)) and then placed in a sonicator bath for 30 min to completely dissolve cells. The resulting digest was diluted to a final volume of 5 mL with diluted nitric acid, samples were analysed on a SpectroCirosCCD (Spectro Analysis) inductively-coupled plasma-atomic emission spectrophotometer. Levels of Os and Fe in the samples were determined by a calibration curve using multielement standard solutions containing 0.1, 0.2, 5 and 10 mg/L Os and Fe.

### **Single Stain Microscopy**

An overnight culture of bacteria was grown in LB. Cells were washed (x2) and re-suspended in GDMM (*E. coli*) or CDM (*S. aureus*). The cells were diluted to an OD<sub>600</sub> of 0.05 and grown to OD 0.3-0.4 in media (50 mL). One mL of culture was harvested (0 min) and the compound added at MIC concentration to the remaining culture. One mL of culture was harvested at 60 and 120 min. The bacteria were pelleted (centrifuge, 14,000 rpm, 90 s) and supernatant removed. The pellet was suspended in fixant (4 % paraformaldehyde in PBS, 1 mL) and placed on a rotary wheel at room temperature for 30 min. The samples were washed in PBS and frozen as a pellet. Coverslips were sonicated in 1 M KOH for 15 min, then coated in polylysine solution for 30 min. The pellets were suspended in 5  $\mu$ L of a SlowFade Gold Antifade Mountant (Thermo Fisher). The suspension was mounted onto the slide and



the coverslip placed on top. Slides were imaged using the structured illumination microscope (SIM) using a 1514 immersion oil, and mol\_probes microscope setting. The 450 nm laser was used to excite the compound and luminescent images were collected in the A568 channel. OMX SI reconstruction was performed on the images and processing done using the FIJI ImageJ software – the SIM plugin was used to perform a 16-bit conversion.

### **DAPI counterstain microscopy**

Initial pellets were grown and fixed as previous. After fixing, samples were washed with PBS. Cells were suspended in 300  $\mu$ L of DAPI (300 nm) in PBS. Samples were incubated on a rotary wheel at room temperature for 5 minutes. Cells were pelleted (14,000 RPM, 90 seconds) and washed with PBS (x3). Cell suspensions were mounted as previous. Laser 405 nm, emission filter DAPI. OMX SI reconstruction and OMX SI image registration were performed on the images, and the images were processed and analysed using the FIJI Image J software.

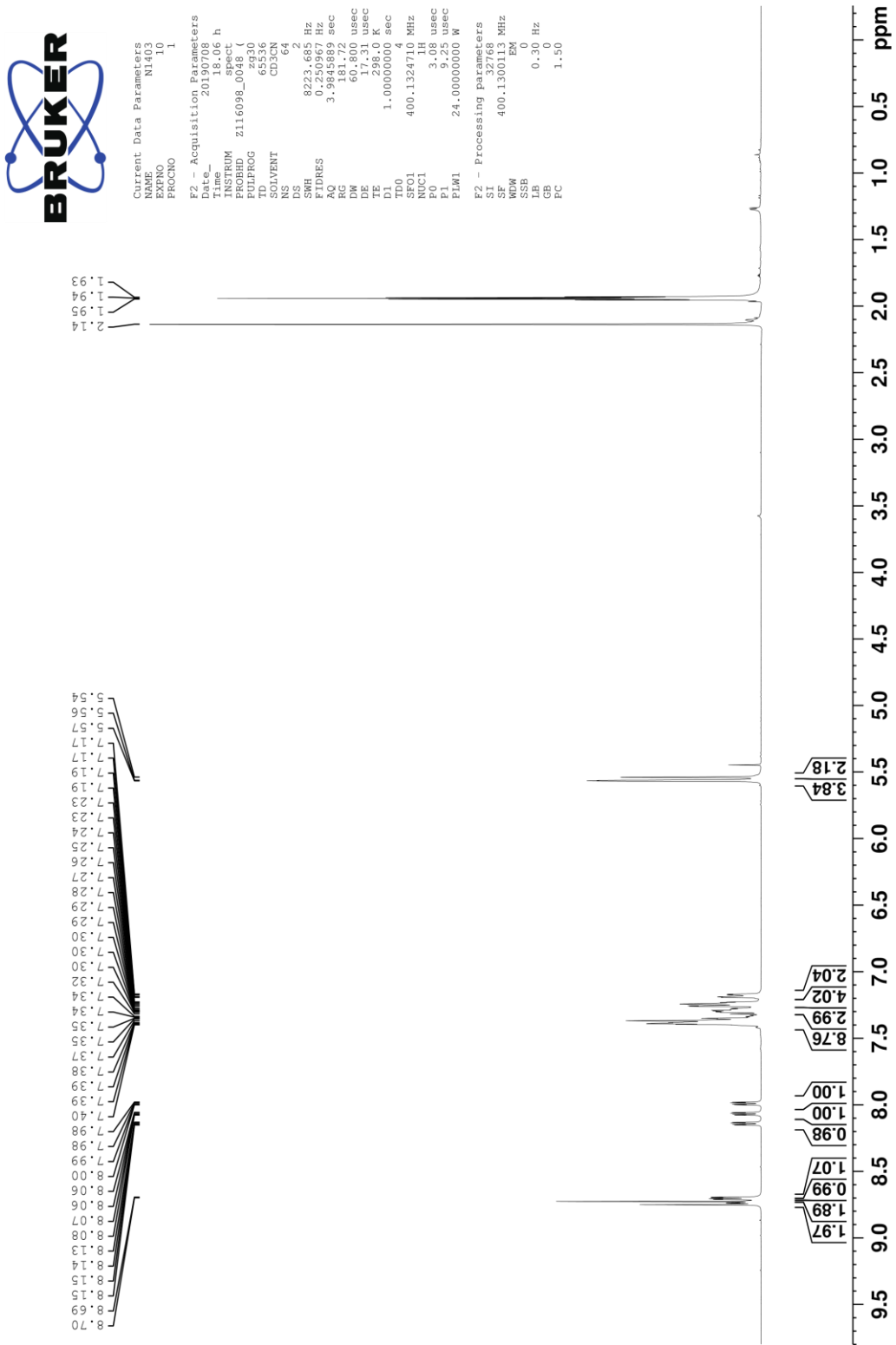


Figure S1 <sup>1</sup>H NMR spectrum (400 MHz, d<sub>3</sub>-MeCN) of *mer*-**2**<sup>2+</sup> [PF<sub>6</sub>]<sub>2</sub>



56.49  
56.73  
56.82

121.79  
121.89  
122.67  
128.66  
128.78  
129.20  
129.28  
129.48  
129.90  
130.01  
130.02  
130.04  
134.27  
134.32  
134.77  
148.01  
148.06  
148.21  
157.94  
157.97  
158.10  
160.23  
160.32  
160.39  
164.58  
164.60  
164.63

Current Data Parameters  
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PROCNO 1  
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TD 118848  
SOLVENT CD3CN  
NS 8194  
DS 4  
SWH 37037.035 Hz  
FIDRES 0.623267 Hz  
AQ 1.6044480 sec  
RG 101  
DW 13.500 usec  
DE 19.34 usec  
TE 298.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
SFO1 150.9194056 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 82.97899628 W  
SF02 600.1324005 MHz  
NUC2 1H  
CPDPRG2 waltz64  
PCPD2 80.00 usec  
PLW2 26.27899933 W  
PLW12 0.58737689 W  
PLW13 0.29439330 W  
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WDW EM  
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LB 1.00 Hz  
GB 0  
PC 1.40

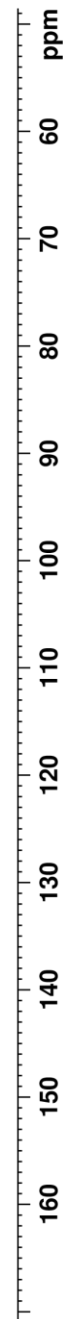


Figure S2  $^{13}\text{C}$  NMR spectrum (151 MHz,  $d_3$ -MeCN) of *mer*- $2^{2+}$   $[\text{PF}_6]_2$

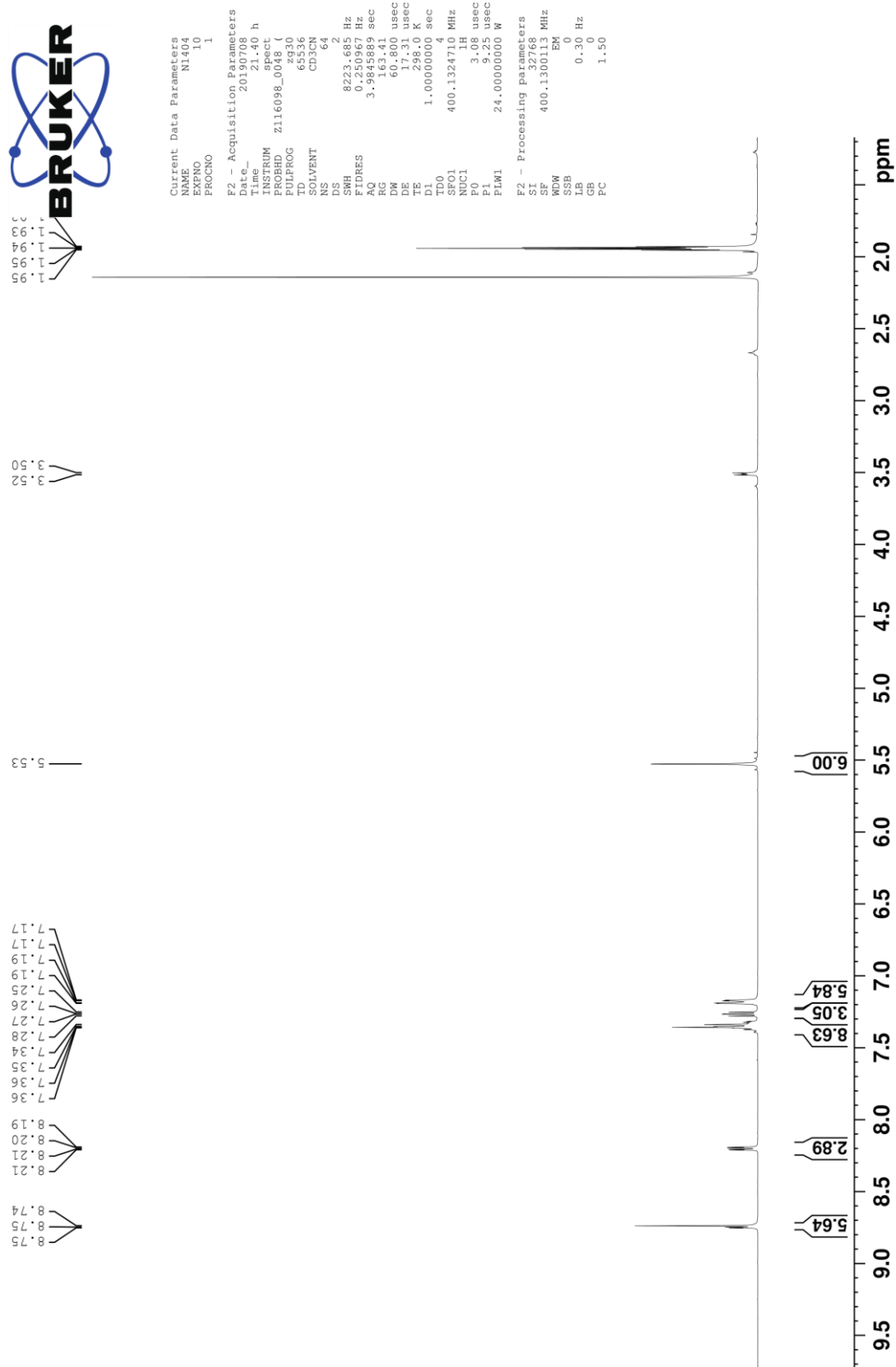


Figure S3  $^1\text{H}$  NMR spectrum (400 MHz,  $d_3$ -MeCN) of *fac*- $2^{2+}$  [ $\text{PF}_6$ ] $_2$

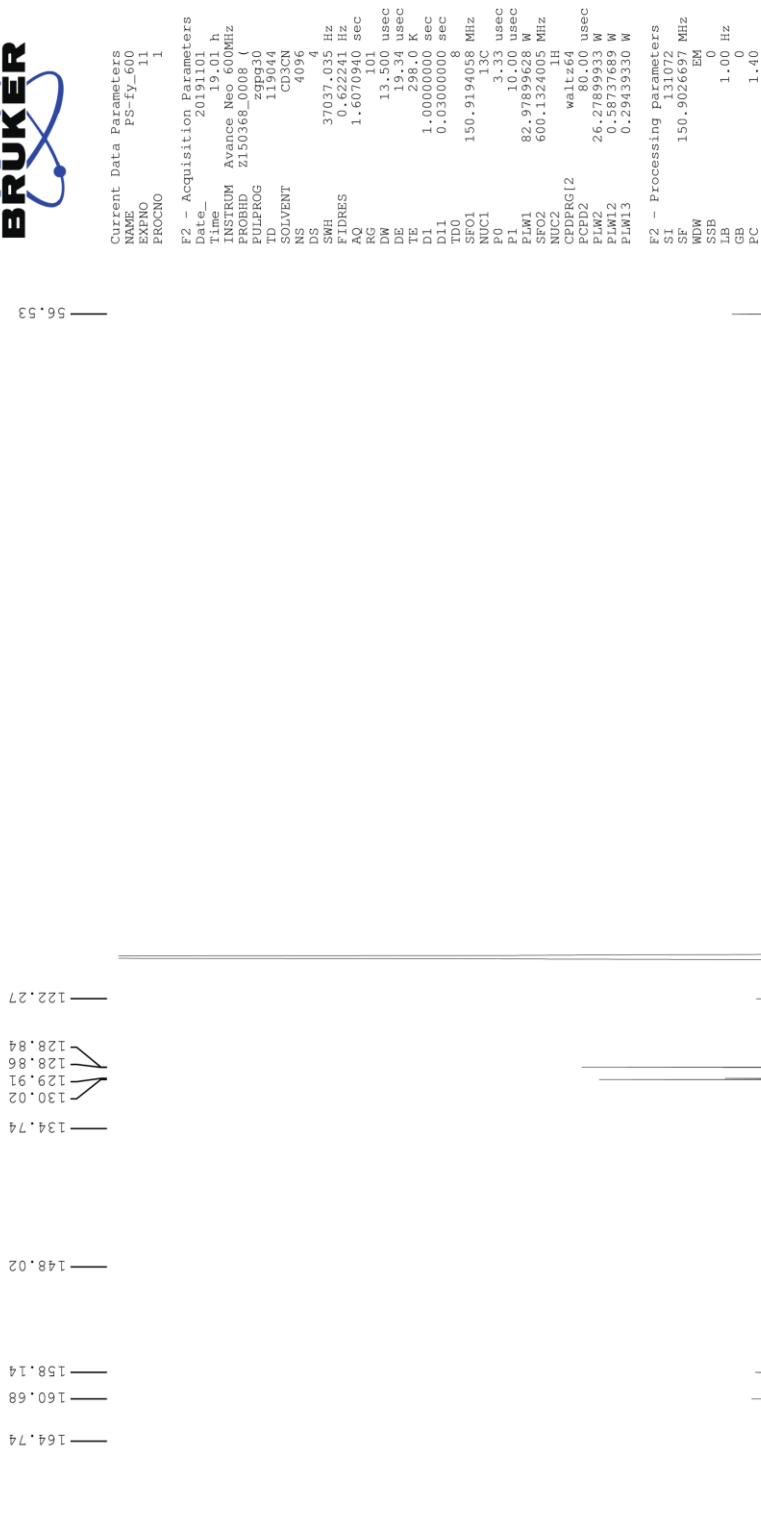


Figure S4  $^{13}\text{C}$  NMR spectrum (151 MHz,  $d_3$ -MeCN) of *fac*- $2^{2+}$   $[\text{PF}_6]_2$

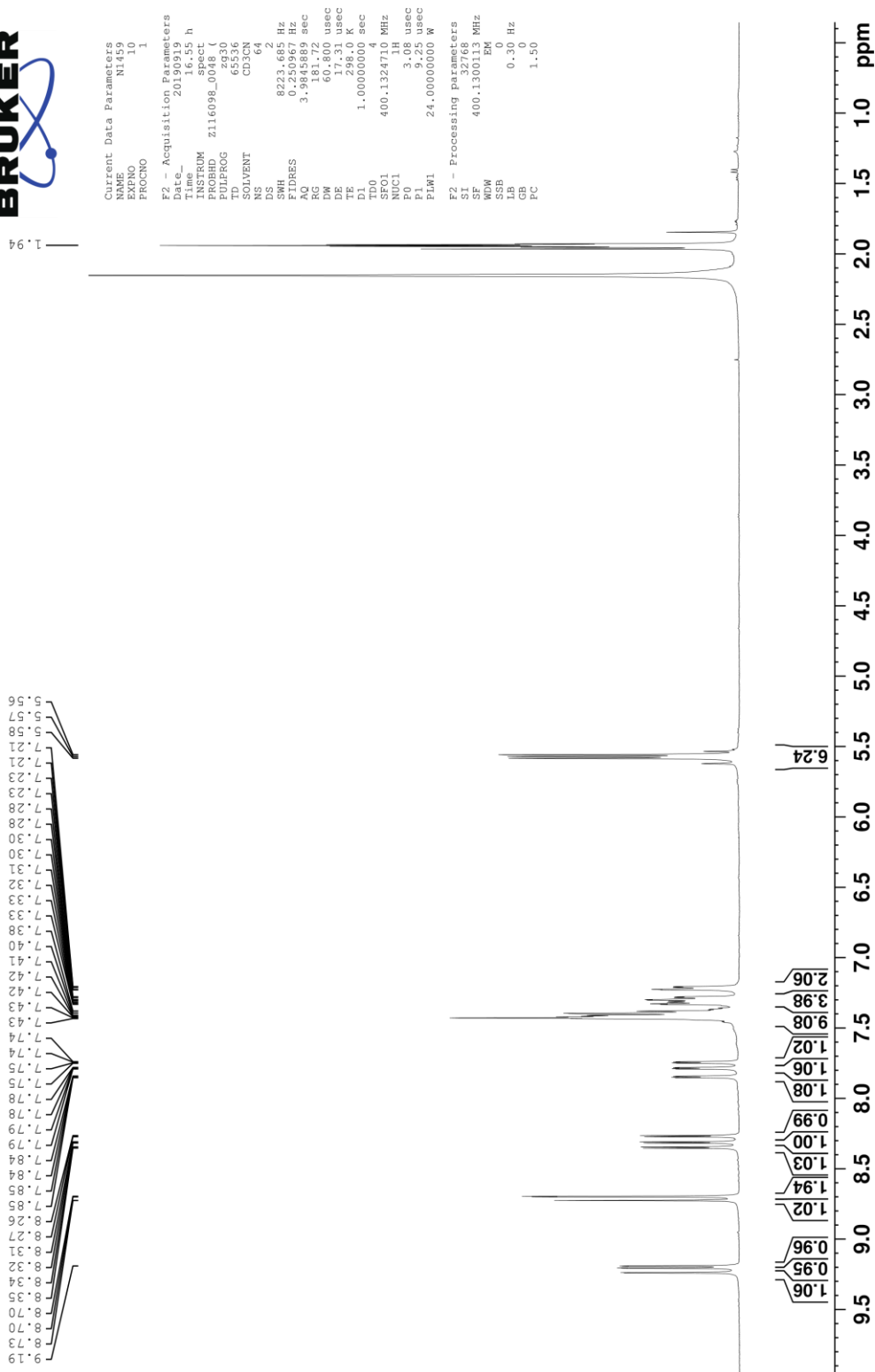


Figure S5  $^1\text{H}$  NMR spectrum (400 MHz,  $d_3$ -MeCN) of  $mer\text{-}3^{2+} [\text{PF}_6]_2$



56.85  
56.74  
56.51

149.57  
149.29  
148.34  
148.12  
147.99  
147.49  
147.21  
147.15  
147.11  
147.05  
146.58  
144.18  
143.58  
143.58  
143.49  
143.49  
134.49  
133.96  
133.84  
130.13  
130.10  
130.06  
130.06  
130.05  
130.02  
129.98  
129.72  
129.55  
129.02  
127.65  
127.40  
126.84

Current Data Parameters  
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Time 20.01 h  
INSTRUM spect  
PROBHD Z116098-0048 (zpg30)  
PULPROG zgpg30  
PROBHD 43316  
SOLVENT CD3CN  
NS 2048  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.181672 sec  
RG 181.72  
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DE 10.09 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0500000 sec  
TD 32  
SFO1 100.6228303 MHz  
NUC1 13C  
P0 3.00 usec  
PCPD2 90.00 usec  
PCPD1 90.00 usec  
F1M1 77.0000000 MHz  
SFO2 400.1316005 MHz  
NUC2 1H  
CFPRG[2] waltz16  
PCPD2 90.00 usec  
PCPD1 90.00 usec  
F1M2 0.12751999 W  
F1M3 0.12751999 W  
F2 - Processing parameters  
SI 65536  
SF 100.6126094 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Figure S6  $^{13}\text{C}$  NMR spectrum (101 MHz,  $d_3$ -MeCN) of *mer*- $3^{2+}$   $[\text{PF}_6]_2$

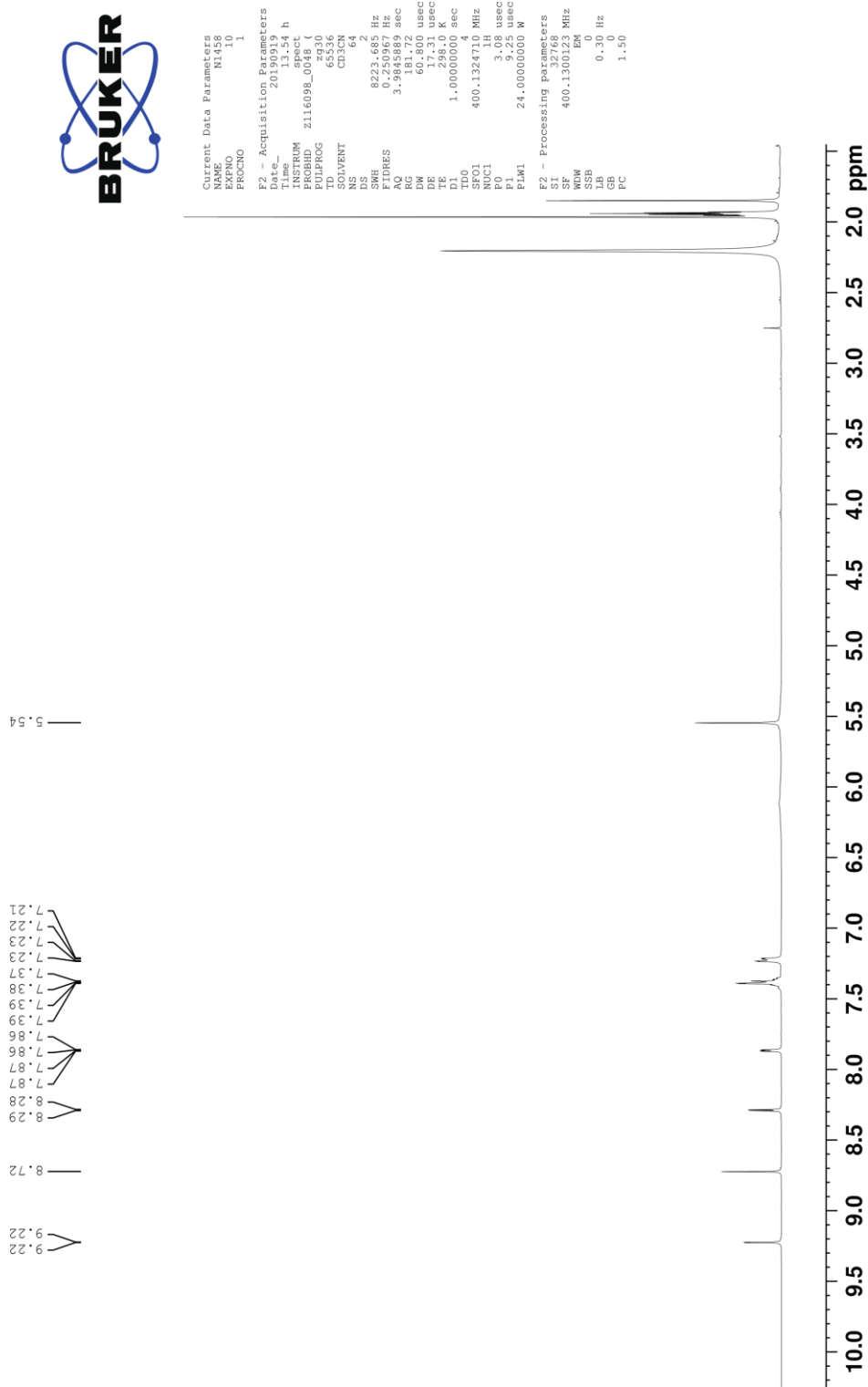


Figure S7  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{d}_3\text{-MeCN}$ ) of  $\text{fac-3}^{2+} [\text{PF}_6]_2$



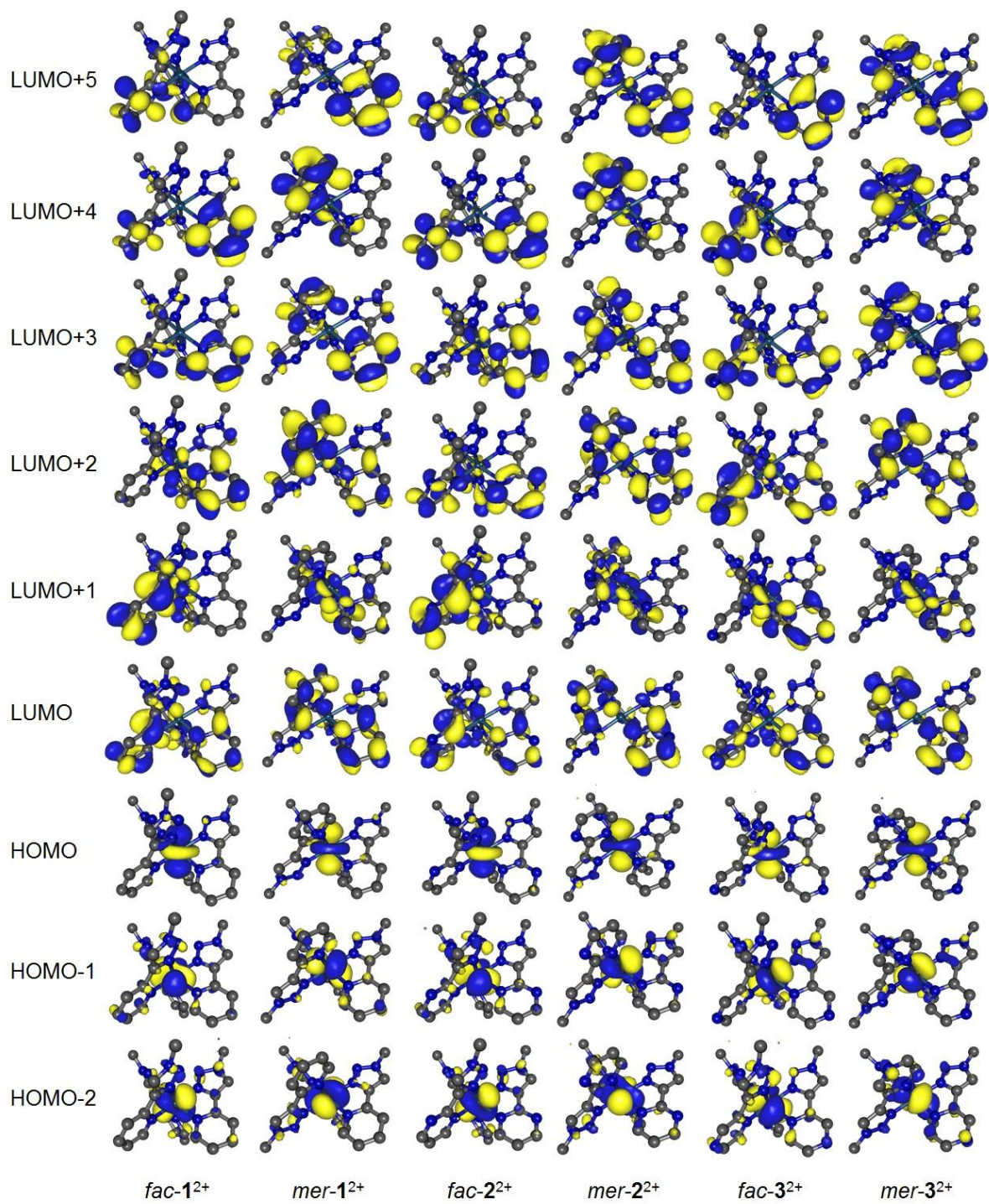


**Table S1.** UV-vis absorption data for chloride salts *mer*- and *fac*-**1**<sup>2+</sup>- **3**<sup>2+</sup> in aqueous solution.

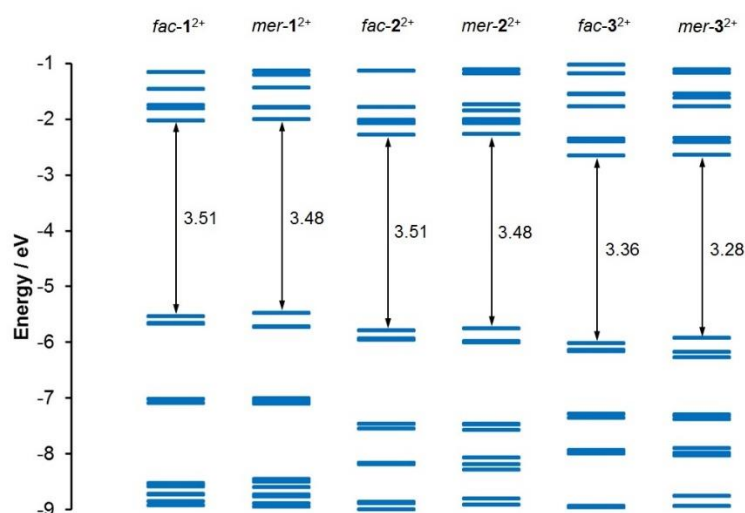
	$\lambda_{\text{abs}} / \text{nm} (\epsilon / \text{dm}^3\text{mol}^{-1}\text{cm}^{-1})$
<i>mer</i> - <b>1</b> <sup>2+</sup>	520 (3350), 472 (4220), 403 (12585), 374 (14560), 310 (10270), 272 (58210), 233 (39740)
<i>fac</i> - <b>1</b> <sup>2+</sup>	519 (2780), 478 (3390), 400 (11600), 368 (12550), 310 (8240), 272 (53400), 234 (35080)
<i>mer</i> - <b>2</b> <sup>2+</sup>	524 (3040), 473 (4050), 404 (12690), 373 (13810), 340 (12140), 306 (8200), 247 (54665)
<i>fac</i> - <b>2</b> <sup>2+</sup>	524 (2980), 473 (4030), 400 (13220), 379 (13670), 340 (11210), 299 (7575), 247 (53730)
<i>mer</i> - <b>3</b> <sup>2+</sup>	560 (3430), 534 (3955), 505 (4070), 428 (12520), 388 (11620), 277 (40290), 234 (37000)
<i>fac</i> - <b>3</b> <sup>2+</sup>	560 (3065), 510 (4025), 428 (11160), 396 (10445), 366 (8300), 281 (36625), 238 (42950)

### Computational details.

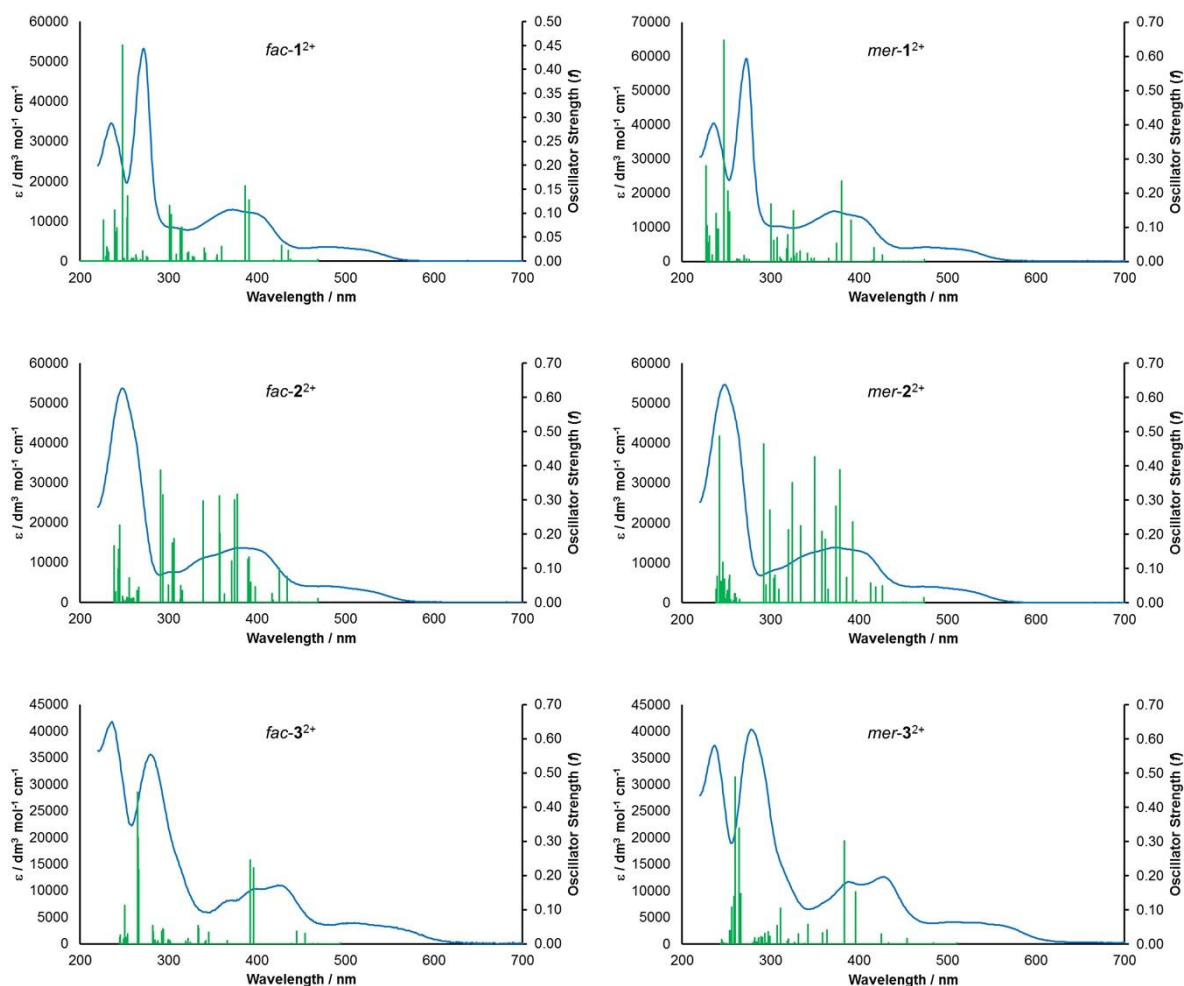
DFT calculations were carried out using Orca 4.2.1<sup>1, 2</sup> using the B3LYP hybrid functional with Grimme's D3 dispersion correction.<sup>3, 4</sup> As the benzyl substituents will have little effect on the photophysical properties these were simplified to methyl groups which also reduced computational expense. The Def2-ECP effective core potential<sup>5</sup> was used for Os with Def2-tzvp(-f) basis sets<sup>6</sup> used for all other atoms. The RIJCOSX algorithm<sup>7</sup> was employed in all calculation using the Def2/j auxiliary basis set.<sup>8</sup> Solvent effects were included in the calculations using the SMD model (water).<sup>9</sup> Ground state geometries were optimised using the keywords !tightscf and !tightopt with vibrational frequency calculations used to confirm that minima has been located. TDDFT calculations were performed at the ground state geometries using the same settings for the 50 lowest energy singlet and triplet vertical excitations. The T<sub>1</sub> geometries were optimised using unrestricted Kohn-Sham DFT by specifying a spin multiplicity of 3. Molecular orbitals were visualised and plotted using the Gabedit program.<sup>10</sup>



**Figure S9** Plots of HOMO-2 to LUMO+5 (isosurface value 0.03 a.u.) for *fac/mer-1<sup>2+</sup>-3<sup>2+</sup>*.



**Figure S10** Calculated molecular orbital energies for *fac/mer-1*<sup>2+</sup>-*3*<sup>2+</sup>.



**Figure S11** Plots of TDDFT vertical excitation spectra (green) with experimental UV-visible absorption spectra overlaid (blue) for *fac/mer-1*<sup>2+</sup>-*3*<sup>2+</sup>.

**Table S2** Data for selected TDDFT calculated singlet and triplet excitations at the ground state geometries of complexes *fac-mer-1<sup>2+</sup>-3<sup>2+</sup>*.

State	Energy / cm <sup>-1</sup>	Wavelength / nm	<i>f</i>	Composition	Character
<i>fac-1<sup>2+</sup></i>					
S <sub>1</sub>	21329	469	0.00373	H→L (98 %)	<sup>1</sup> MLCT
S <sub>4</sub>	22967	435	0.0220	H-1→L (63 %)	<sup>1</sup> MLCT
S <sub>5</sub>	23375	428	0.0330	H-2→L (63 %)	<sup>1</sup> MLCT
S <sub>7</sub>	25559	391	0.128	H-1→L+1 (27 %), H-1→L+2 (19 %), H-2→L (16 %), H-2→L+2 (15 %)	<sup>1</sup> MLCT
S <sub>8</sub>	25872	387	0.157	H-1→L+2 (24 %), H-1→L+1 (23 %), H-2→L+1 (20 %)	<sup>1</sup> MLCT
T <sub>1</sub>	19598	510		H→L (88 %)	<sup>3</sup> MLCT
T <sub>2</sub>	19703	508		H→L+1 (56 %), H-1→L (25 %)	<sup>3</sup> MLCT
T <sub>3</sub>	19950	501		H-2→L (47 %), H→L+2 (30 %)	<sup>3</sup> MLCT
T <sub>4</sub>	20708	483		H-1→L+1 (41 %), H-2→L+2 (32 %)	<sup>3</sup> MLCT
<i>mer-1<sup>2+</sup></i>					
S <sub>1</sub>	21117	474	0.00367	H→L (98 %)	<sup>1</sup> MLCT
S <sub>5</sub>	23977	417	0.0293	H-1→L (59 %), H-2→L+2 (25 %)	<sup>1</sup> MLCT
S <sub>7</sub>	25582	391	0.0874	H-2→L+2 (33 %), H-1→L+1 (28 %), H-1→L (24 %)	<sup>1</sup> MLCT
S <sub>8</sub>	26327	380	0.170	H-2→L+1 (45 %), H-1→L+2 (28 %)	<sup>1</sup> MLCT
S <sub>9</sub>	26717	374	0.0381	H→L+3 (85 %)	<sup>1</sup> MLCT
T <sub>1</sub>	18226	549		H→L (88 %)	<sup>3</sup> MLCT
T <sub>2</sub>	19249	520		H→L+2 (62 %), H→L+1 (19 %)	<sup>3</sup> MLCT
T <sub>3</sub>	18690	535		H→L+1 (67 %), H→L+2 (17 %)	<sup>3</sup> MLCT
T <sub>4</sub>	19480	513		H-2→L+2 (35 %), H-1→L (23 %), H-1→L+1 (20 %)	<sup>3</sup> MLCT
<i>fac-2<sup>2+</sup></i>					
S <sub>1</sub>	21319	469	0.00291	H→L (97 %)	<sup>1</sup> MLCT
S <sub>4</sub>	23055	434	0.0205	H-1→L (72 %)	<sup>1</sup> MLCT
S <sub>5</sub>	23531	425	0.0273	H-2→L (69 %)	<sup>1</sup> MLCT
S <sub>10</sub>	25568	391	0.0361	H-1→L+2 (32 %), H→L+4 (28 %), H→L+1 (15 %)	<sup>1</sup> MLCT
S <sub>11</sub>	25665	390	0.0344	H→L+5 (35 %), H-1→L+3 (12 %)	<sup>1</sup> MLCT
S <sub>12</sub>	26486	378	0.0862	H→L+4 (41 %)	<sup>1</sup> MLCT
S <sub>13</sub>	26729	374	0.0819	H→L+5 (22 %), H-1→L+4 (18 %), H→L+4 (12 %)	<sup>1</sup> MLCT
T <sub>1</sub>	19561	511		H→L (87 %)	<sup>3</sup> MLCT
T <sub>2</sub>	19648	509		H→L+1 (52 %)	<sup>3</sup> MLCT
T <sub>3</sub>	19837	504		H→L+3 (40 %), H-2→L (23 %)	<sup>3</sup> MLCT
T <sub>4</sub>	20819	480		H-1→L+1 (33 %), H-2→L+3 (24 %)	<sup>3</sup> MLCT
<i>mer-2<sup>2+</sup></i>					
S <sub>1</sub>	21127	473	0.00354	H→L (96 %)	<sup>1</sup> MLCT
S <sub>9</sub>	25477	393	0.0547	H-1→L+2 (36%), H-2→L+1 (24%), H-1→L (13 %)	<sup>1</sup> MLCT
S <sub>12</sub>	26440	378	0.0900	H-2→L+2 (27 %), H-1→L+1 (26 %), H-1→L+4 (19 %)	<sup>1</sup> MLCT
S <sub>13</sub>	26744	374	0.0652	H-2→L+3 (22 %), H-2→L+2 (17 %)	<sup>1</sup> MLCT
S <sub>15</sub>	27647	362	0.0429	H-1→L+5 (37 %), H-1→L+4 (34 %)	<sup>1</sup> MLCT
S <sub>16</sub>	27940	358	0.0482	H-2→L+4 (43 %), H-2→L+5 (22 %), H-1→L+4 (16 %)	<sup>1</sup> MLCT
S <sub>17</sub>	28611	350	0.0987	H-2→L+5 (42 %), H-2→L+5 (26 %), H-1→L+4 (19 %)	<sup>1</sup> MLCT
T <sub>1</sub>	17538	570		H→L (81 %)	<sup>3</sup> MLCT
T <sub>2</sub>	19975	501		H-1→L+2 (22 %), H-1→L (19 %), H-1→L+1 (19 %)	<sup>3</sup> MLCT
T <sub>3</sub>	19988	500		H→L+1 (75 %)	<sup>3</sup> MLCT
T <sub>4</sub>	20092	498		H→L+2 (42 %), H→L+3 (23 %)	<sup>3</sup> MLCT

<i>fac-3<sup>2+</sup></i>						
S <sub>1</sub>	20235	494	0.00238	H→L (95 %)	<sup>1</sup> MLCT	
S <sub>4</sub>	22032	454	0.0238	H-1→L (57 %), H→L+1 (21 %)	<sup>1</sup> MLCT	
S <sub>5</sub>	22499	445	0.0299	H-2→L (53 %), H→L+2 (17 %)	<sup>1</sup> MLCT	
S <sub>7</sub>	25235	396	0.178	H-2→L (22 %), H-2→L+1 (22 %), H-1→L+2 (22 %)	<sup>1</sup> MLCT	
S <sub>8</sub>	25511	392	0.197	H-1→L+1 (28 %), H-2→L+2 (21 %), H-1→L+2 (17 %)	<sup>1</sup> MLCT	
T <sub>1</sub>	17843	560		H→L (83 %)	<sup>3</sup> MLCT	
T <sub>2</sub>	17987	556		H→L+1 (49 %), H-1→L (31 %)	<sup>3</sup> MLCT	
T <sub>3</sub>	18240	548		H-2→L (42 %), H→L+2 (39 %)	<sup>3</sup> MLCT	
T <sub>4</sub>	19612	510		H-1→L+1 (44 %), H-2→L+2 (30 %)	<sup>3</sup> MLCT	
<i>mer-3<sup>2+</sup></i>						
S <sub>1</sub>	19578	511	0.00253	H→L (99 %)	<sup>1</sup> MLCT	
S <sub>6</sub>	23532	425	0.0218	H-2→L+1 (48 %), H-2→L (46 %)	<sup>1</sup> MLCT	
S <sub>7</sub>	25252	396	0.113	H-2→L (40 %), H-2→L+1 (28 %), H-1→L+2 (20 %)	<sup>1</sup> MLCT	
S <sub>8</sub>	26094	383	0.226	H-1→L+1 (57 %), H-2→L+2 (21 %)	<sup>1</sup> MLCT	
T <sub>1</sub>	16950	590		H→L (92 %)	<sup>3</sup> MLCT	
T <sub>2</sub>	18118	552		H→L+1 (42 %), H→L+2 (38 %)	<sup>3</sup> MLCT	
T <sub>3</sub>	18356	545		H→L+2 (47 %), H→L+1 (44 %)	<sup>3</sup> MLCT	
T <sub>4</sub>	18720	534		H-1→L+1 (53 %), H-2→L+2 (14 %)	<sup>3</sup> MLCT	

SOMO+1						
SOMO						
	<i>fac-1<sup>2+</sup></i>	<i>mer-1<sup>2+</sup></i>	<i>fac-2<sup>2+</sup></i>	<i>mer-2<sup>2+</sup></i>	<i>fac-3<sup>2+</sup></i>	<i>mer-3<sup>2+</sup></i>
Energy / eV	2.23	2.20	2.30	2.16	2.21	2.07
S <sup>2</sup>	2.0170	2.0146	2.0160	2.0129	2.0173	2.0149
Os spin dens.	0.89	0.93	0.88	0.93	0.92	0.96

**Figure S12** Plots of SOMO and SOMO+1 for the T<sub>1</sub> states *fac/mer-1<sup>2+</sup>-3<sup>2+</sup>* along with energies (quoted relative to ground state in each case), spin expectation value (S<sup>2</sup>) and Mulliken spin density for the Os atom.



Optimised geometries (XYZ coordinates) for ground and excited states of *fac/mer*-1<sup>2+</sup>-3<sup>2+</sup>.

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Coordinates from ORCA-job fac1\_gs

Os	0.09892647421814	-0.03437039543531	0.14741196656151
N	-0.90393408626642	1.61798185962373	0.98423659990891
N	0.31529021311364	1.39073078893279	-1.30807907351073
N	0.75548037046665	1.33840877719785	-2.53805296359487
N	0.47187255126340	2.53235618950266	-3.07637294859033
C	-1.51673827434519	1.64441394701093	2.18003153183338
H	-1.53988450120239	0.71587300156104	2.73021357651042
C	-2.08105964331120	2.79305847809618	2.70048230745438
H	-2.55787478759685	2.75716268003238	3.66874569818983
C	-2.01438310080255	3.97308823948112	1.96844507802294
H	-2.43500380601964	4.88916399325142	2.35925120064823
C	-1.40064013932935	3.95704291982634	0.72726025619939
H	-1.32966240282484	4.85151830630215	0.12455271008275
C	-0.86435048594209	2.7692252794720	0.25212698079607
C	-0.24497328404811	2.60854107808330	-1.04277111198229
C	-0.14149835908444	3.34828835265120	-2.19857521732195
H	-0.46031191496259	4.34142064262327	-2.45760710838341
C	0.74960441799448	2.77215287629291	-4.48529667586600
H	0.10387630804749	2.14237613091652	-5.09217716698364
H	0.54785292101761	3.81763690687281	-4.69760832036672
H	1.79144015352958	2.53913873344185	-4.69081844361664
N	-0.51134938228210	-1.40897341665953	1.62297234987799
N	-1.66943505609819	-0.73470455019843	-0.61534794749450
N	-2.34281477854998	-0.47180998238810	-1.70533252366881
N	-3.47562490016442	-1.18320248287122	-1.61260713332721
C	0.16156121372386	-1.71613264754014	2.74615551921055
H	1.11942934514951	-1.23657572344394	2.87928858647831
C	-0.33159076985018	-2.59411037686095	3.69233671906641
H	0.25502858364677	-2.80702495966278	4.57409438666641
C	-1.57543277750112	-3.18333792525690	3.48985375419878
H	-1.99111029665217	-3.86476560577984	4.21884516006646
C	-2.27548511325023	-2.88337122465975	2.33412654137750
H	-3.24153416623517	-3.32427242150218	2.13344218470982
C	-1.72605231295306	-1.99737299735439	1.41892220013107
C	-2.35527804431438	-1.61017067145689	0.17988076567240
C	-3.52984767912846	-1.89919413871018	-0.47446500464743
H	-4.36482140266980	-2.52823231456313	-0.22526652489210
C	-4.44348406173048	-1.15655863808332	-2.69835898252121
H	-4.05378520380417	-1.71283725595424	-3.54825463595039
H	-5.36030600157402	-1.61558071681668	-2.34230221564711
H	-4.63101289669930	-0.12497178001686	-2.98328941612867
N	1.95540517379227	0.44488619623637	1.01173768630036
N	1.36833398148248	-1.36118451634181	-0.75776562538733
N	1.19147613657526	-2.27165835572111	-1.67804680189023
N	2.41632209114303	-2.71240985396500	-1.99555871650752
C	2.14981232995952	1.36526857907703	1.97194048777837
H	1.26933718115907	1.86288528149662	2.34829132918362
C	3.40352326266437	1.67295005193059	2.46140183961429
H	3.50149659828574	2.42385840704163	3.23193903606959
C	4.51375187079265	1.01298061434254	1.94529018971566
H	5.50638160200242	1.24575648207763	2.30514526632044
C	4.32691705429959	0.04622987765744	0.97014984500842
H	5.16135285499672	-0.49899105286189	0.55250321554748
C	3.04035853150147	-0.22359609981563	0.52427348221285
C	2.69864111954108	-1.21085892164644	-0.47226984295151
C	3.37589257986655	-2.09171718651675	-1.28537715854763
H	4.42021100431739	-2.31343548490873	-1.41195648258188
C	2.56554456890911	-3.72221604844027	-3.03209945076111
H	2.22196068593941	-3.31543089864000	-3.98065731381255
H	3.61536996396218	-3.98901833755194	-3.09909155197861
H	1.97712848583144	-4.59650493788323	-2.76574209250215

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Coordinates from ORCA-job fac1\_t1

Os	0.00742721786467	-0.00006456650378	0.13567420395463
N	-0.93449893627093	1.59662278162553	0.99393091628201
N	0.27409690200339	1.43424683849610	-1.30981930502355
N	0.72172603093627	1.38785888822971	-2.55005148477665
N	0.53692520970426	2.61284068640088	-3.03076476547268
C	-1.61748592830890	1.62067995837936	2.18335933745360
H	-1.75919640924984	0.66399657183634	2.66521440441177
C	-2.07200922395521	2.76618082820085	2.75297751656168
H	-2.59354040378216	2.71889542223118	3.69767030400237
C	-1.84777181550138	4.02408462802631	2.09576052051161
H	-2.17885442430266	4.94696599027797	2.54987201032366
C	-1.21354196411186	4.02759734489367	0.87528644269195
H	-1.04094336606979	4.95350768641336	0.34108211927086
C	-0.77627308464639	2.83698131251470	0.29729010437121
C	-0.19965679285411	2.68496834281003	-0.98703267406259
C	-0.01546395068264	3.45183179587355	-2.13004847990042
H	-0.25714449204002	4.47119948458468	-2.36791826222327
C	0.84617641607965	2.88958308390320	-4.42727425718502
H	0.20046949826649	2.28946800857512	-5.06316975287492
H	0.66593507199437	3.94420690640010	-4.61140879945825
H	1.88750579807933	2.64457027570038	-4.62273665427247
N	-0.54556910053721	-1.41650526294872	1.60571536945087
N	-1.72673779299131	-0.75178740410571	-0.62187737434941
N	-2.40342523103191	-0.49426078064578	-1.71434851135575
N	-3.48405302892324	-1.26568568229296	-1.64956257295640
C	0.15124771277945	-1.71070413687202	2.71391562015691
H	1.08229223788774	-1.18283057281094	2.85573885584410
C	-0.29567676298163	-2.63453284240576	3.64038948005135
H	0.30218354752306	-2.83738436694715	4.51659545045116
C	-1.50901723193880	-3.27867443523261	3.42586708067347
H	-1.88772036350118	-3.99518707275440	4.14111938990432
C	-2.22969018596902	-2.99178065770209	2.27866659718374
H	-3.17159740199961	-3.47831123235462	2.07011558538381
C	-1.72708747837598	-2.05974475388640	1.38500549653198
C	-2.36673558566526	-1.68285498713407	0.14778347737881
C	-3.51668825627403	-2.01368210757910	-0.52608468910906
H	-4.32030218827186	-2.69227186785788	-0.30556228226991
C	-4.43890927683487	-1.27720182600578	-2.75029955187040
H	-4.02725884497454	-1.85336585202425	-3.57588595492011
H	-5.35534086614765	-1.73517943293932	-2.39292387024954
H	-4.62637970275364	-0.25424526278065	-3.06244228681791
N	1.89543169171357	0.53773480485936	0.92232255038191
N	1.29371680968960	-1.38134257145933	-0.73800719377345
N	1.10345073388573	-2.35985387438034	-1.58011182101133
N	2.32169587045913	-2.80657602839283	-1.89053968591416
C	2.08850971921974	1.50445726892237	1.83476775468574
H	1.20706686378076	2.01017872923221	2.19599463762985
C	3.34716481471231	1.83457718883744	2.29439020454221
H	3.45166722411539	2.61835357556910	3.03012971124804
C	4.45210738402178	1.15364480554666	1.79557163445327
H	5.44744919178772	1.40221137963393	2.13657791829272
C	4.26066378262279	0.14630093936115	0.86331845093788
H	5.09241259170575	-0.41378607484089	0.46113635573146
C	2.97131058953927	-0.14884879888753	0.44600003410633
C	2.62251569338295	-1.18946503198230	-0.49394871092045
C	3.29151738905562	-2.12406402548389	-1.25180286915942
H	4.33513296204263	-2.34557573159707	-1.38328128517198
C	2.46283905761108	-3.88493209122011	-2.85949588051765
H	2.17213013431005	-3.52142944757445	-3.84264776173261
H	3.50127217570868	-4.19962352934539	-2.86542984468073
H	1.82482976846440	-4.71169321838720	-2.56056295282512



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Coordinates from ORCA-job mer1\_gs

Os	0.00034660007922	0.05403668597587	-0.06888899964974
N	0.62313366822744	1.18672096295634	-1.72761979341680
N	-0.33855464873589	1.98662169376697	0.55741727143729
N	-0.83429718831836	2.50616467244492	1.65182173168869
N	-0.80998738606824	3.83413307390666	1.47033733848774
C	1.13096508673853	0.68076093237610	-2.86416893482719
H	1.16202462515163	-0.39551672125825	-2.94275793208225
C	1.58773453755143	1.48196824224955	-3.89271882670067
H	1.98956059166164	1.02137872628471	-4.78357680324165
C	1.52176438532464	2.86415390461172	-3.75821834923577
H	1.87212651960552	3.51326038961626	-4.54842573054840
C	0.99565875927770	3.39942981476202	-2.59419951113959
H	0.92229587694406	4.46836008542330	-2.45024212654245
C	0.56088854966393	2.54174275405158	-1.59378483668985
C	0.00684808142390	2.96883585878578	-0.33020426385756
C	-0.29783410183443	4.16833684444651	0.27087792380028
H	-0.19670850673288	5.19000246474334	-0.04838301753593
C	-1.25964033836275	4.72830756886497	2.52959600245581
H	-0.40766555449092	5.05917834166539	3.12050319995210
H	-1.75348574711187	5.58298797080374	2.07629208458722
H	-1.95885444745662	4.18450913810641	3.15759738630509
N	-0.78631457808176	-0.94186378622372	1.61101399841622
N	-1.99502932506057	-0.11293630625729	-0.54431572448225
N	-2.71013283083605	0.26487450827632	-1.57257208374849
N	-3.97063473885990	-0.09685688928319	-1.29136826534420
C	-0.07548972499649	-1.37623714283366	2.66578906389789
H	0.98143249547326	-1.15489238275889	2.65770413830001
C	-0.65209607581924	-2.06537984406115	3.71636089842244
H	-0.03155523385264	-2.39867315937588	4.53535893627903
C	-2.01912611182027	-2.31948538606475	3.69523738630584
H	-2.49495244870638	-2.85764755632355	4.50316740462301
C	-2.76361442522859	-1.87762777532061	2.61479110077261
H	-3.82708284137757	-2.06207128717880	2.55480529294172
C	-2.12536504029839	-1.19795636207604	1.58711017340159
C	-2.78214265644011	-0.71366111117156	0.39780757856207
C	-4.06619205732556	-0.70042895769220	-0.09345735225436
H	-4.99914078016029	-1.06053507558945	0.30027976538871
C	-5.03487908490906	0.14577731634168	-2.25387113461606
H	-4.84994178516671	-0.43743130991656	-3.15260631440790
H	-5.97198607696355	-0.16101442481158	-1.79978280687008
H	-5.06964925398368	1.20494740479409	-2.49690273870829
N	2.02220782606839	-0.00369496865040	0.51802902888180
N	0.61930712344031	-1.77725847375588	-0.78930049331539
N	0.00544115231907	-2.78236851802311	-1.36601247390552
N	0.93330075831331	-3.74037296641179	-1.51211647008661
C	2.66469492138216	0.95367128741019	1.20862959212338
H	2.07666562089063	1.80647119451941	1.51212339422979
C	4.00567210402639	0.86253962406106	1.53206420822338
H	4.46978196535246	1.66010611645380	2.09373575689424
C	4.72810862654029	-0.25562893170813	1.12972907950242
H	5.77659821533103	-0.35534113656308	1.37313355867487
C	4.07907349757146	-1.24727898259117	0.41429369692443
H	4.60107064344130	-2.13169290482922	0.07682244066201
C	2.73013082440653	-1.10143306211052	0.12872620095726
C	1.93379133164573	-2.08237189892098	-0.56652766451378
C	2.13320801491603	-3.35624165674282	-1.04296545153635
H	2.99567453898978	-3.99769130589395	-1.07168111661261
C	0.59991103695023	-5.01867770246774	-2.12630881362645
H	0.77400117867908	-4.97197943237808	-3.20009988261770
H	1.22871576651806	-5.78420346498466	-1.68224018386143
H	-0.44408193490636	-5.23642669346998	-1.91983753712362

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Coordinates from ORCA-job mer1\_t1

Os	0.02653630807685	0.09514550633009	-0.06834821136850
N	0.65558766112906	1.21953755693778	-1.71716857111225
N	-0.34376289646220	2.03897498426055	0.54483908737325
N	-0.84501852759583	2.56092846072893	1.63342094030345
N	-0.81369724940900	3.88287246980481	1.44689374295720
C	1.17143765841999	0.69067795665291	-2.84003263830875
H	1.23252943160978	-0.38604979431366	-2.88514527813192
C	1.59935420687999	1.48054376047190	-3.88728112973188
H	2.00791495075137	1.01278064734397	-4.77082195444668
C	1.50076619646165	2.86369889335641	-3.77902115310764
H	1.83071428027749	3.50242370571177	-4.58621716642316
C	0.97330890253164	3.41798755566311	-2.62450359491769
H	0.87869578225938	4.48797940878989	-2.50613117862298
C	0.56110732895390	2.57518553713431	-1.60441906580420
C	0.00850420640586	3.01238530165413	-0.34650216462673
C	-0.29702551812230	4.21449139818917	0.24782041549595
H	-0.18964808600562	5.23507348171408	-0.07251900425235
C	-1.26585663837900	4.78734694347056	2.49866574581529
H	-0.40399675286380	5.21794096995101	3.00383840040041
H	-1.86673609272046	5.57181073771777	2.04693548248590
H	-1.86351751551481	4.21343778344184	3.19980295017743
N	-0.75942605907977	-1.00779333755536	1.55824821701180
N	-1.99878869952806	-0.05092638350140	-0.53863970294481
N	-2.72536742510188	0.40900726600705	-1.52257628740123
N	-3.97046099434817	0.00144750721884	-1.26723064236881
C	-0.02564207269076	-1.50208962822215	2.56790881128743
H	1.02344773955636	-1.24763731801163	2.56901706948937
C	-0.58214200865255	-2.28694109679053	3.56022310957235
H	0.04796678900461	-2.66584881515087	4.35105431893036
C	-1.94072312079520	-2.57709703657961	3.51586536277009
H	-2.39937847999367	-3.19041240964323	4.27866911576240
C	-2.70276689173641	-2.07699169214763	2.47327680117164
H	-3.75907853869126	-2.29171524488914	2.39708534316734
C	-2.08849920912480	-1.29833155275271	1.50507489381013
C	-2.76069396102685	-0.74501114137399	0.35344804864269
C	-4.04897580134505	-0.70732048619848	-0.12445692693956
H	-4.97293166476269	-1.11452375904357	0.24339920256729
C	-5.04449179863675	0.28793458421867	-2.20973460606926
H	-4.88981194282644	-0.29141344539071	-3.11644815747993
H	-5.98191503706582	0.00465713057172	-1.74171899908189
H	-5.04563369124366	1.35028046479269	-2.43778229492145
N	1.98254018611784	0.04565470307689	0.56101957976251
N	0.62250289326008	-1.75036155663212	-0.77051485489431
N	-0.03251322572127	-2.78505829615140	-1.28525957790213
N	0.86893600954759	-3.75782222025525	-1.36550048749885
C	2.66607442028398	1.05168756488854	1.18408808742319
H	2.08747599084455	1.92526690608825	1.44785852036298
C	3.98812843836034	0.97152493106125	1.49457188994283
H	4.46314528764213	1.79470431962777	2.00837628185734
C	4.72985359500531	-0.20396517489101	1.13470802438265
H	5.78106417125040	-0.28519464510186	1.37200801927766
C	4.07977944235970	-1.21596551594389	0.47626192171934
H	4.60756306443819	-2.10883179811738	0.16457707236950
C	2.71481000705934	-1.11526317133162	0.18296333303600
C	1.93490642522562	-2.07737231018000	-0.49139708739871
C	2.08293113588695	-3.39372796307397	-0.91205007525026
H	2.91593515026402	-4.07236096385550	-0.90049846650301
C	0.51007723854178	-5.05595034013753	-1.92264851689852
H	0.72594752922650	-5.07253523337138	-2.98971339342388
H	1.09307344516813	-5.81857587274044	-1.41555076986524
H	-0.54841597335627	-5.22390023352858	-1.74608783162918

## Coordinates from ORCA-job fac2\_gs

Os	0.11973623922609	-0.02731790502996	0.18278206051898
N	-0.90758294665706	1.62005380961856	0.99120210508330
N	0.32676746674481	1.38514708917281	-1.28498076676626
N	0.78969403194808	1.32284893039062	-2.50263533283651
N	0.47858538758323	2.49784394576745	-3.07063553880349
C	-1.53415820433968	1.68010478828164	2.17731088991087
H	-1.54244616076302	0.78033924458840	2.77470747817711
C	-2.12972470711229	2.84503724861403	2.61279464756455
H	-2.62727125858662	2.88631789908098	3.56926360268302
C	-2.05857580753025	3.95208622062114	1.78104612061179
H	-2.49319849622932	4.89878215748174	2.07335318649021
N	-1.45818447770941	3.90760572840779	0.58898430925119
C	-0.91375592646055	2.75457960237822	0.23057351392516
C	-0.27449570153272	2.58918935251193	-1.05392978056058
C	-0.17427625805040	3.31076002816557	-2.22143147391460
H	-0.52095759328826	4.28950107438688	-2.49860742155275
C	0.78305432687513	2.71562342446071	-4.47825969499595
H	0.18019158109127	2.04336211497532	-5.08325969783762
H	0.54220306704552	3.74590831374356	-4.72113099285698
H	1.83936541261872	2.52417294204383	-4.65103246812720
N	-0.48356039039194	-1.41613640875160	1.64677921293913
N	-1.66361645161645	-0.71096274061888	-0.56689530760785
N	-2.35816138585230	-0.41163032669410	-1.63076295060300
N	-3.51187647955396	-1.08892312850327	-1.51372977915162
C	0.19308520953067	-1.78657688165074	2.74695832225819
H	1.16196049810770	-1.33580621752739	2.90239134380828
C	-0.33133662655416	-2.70144335405555	3.63553462347320
H	0.22179663760927	-2.99976194058893	4.51282540095444
C	-1.59155784725342	-3.21357409564891	3.36210407301923
H	-2.06601622812247	-3.92160659367629	4.02854949685583
N	-2.27698319064169	-2.86490629049386	2.27175416836469
C	-1.70654257087948	-1.99237651874833	1.45367078748243
C	-2.35492467297830	-1.57346340287545	0.23592085662220
C	-3.55672095510018	-1.81741547075811	-0.38565077964884
H	-4.40115282722055	-2.42427238110186	-0.11514419445279
C	-4.51479701305336	-1.00846171837875	-2.56554915701458
H	-4.17370161010479	-1.56463705211918	-3.43588509636346
H	-5.43499174999202	-1.43942013409976	-2.18437860477423
H	-4.67182629298680	0.03424893423161	-2.82718168380192
N	1.96729609060450	0.46042612677689	1.05336415910407
N	1.40627655225297	-1.34379003999585	-0.71864853725375
N	1.24277210062796	-2.24072396836453	-1.65056427370314
N	2.47522841242021	-2.66267542690671	-1.97251972996150
C	2.17722038832244	1.37383572124987	2.01552546920645
H	1.30943965946381	1.88178094004976	2.40800426245078
C	3.44760339051091	1.64835410752602	2.47360990323682
H	3.60918276682174	2.38583276309871	3.24488246666413
C	4.50099077094313	0.95051407816696	1.90015922867047
H	5.52233571181692	1.13524611082625	2.20650238081874
N	4.31176824815862	0.02263641942610	0.95801814603607
C	3.06229055242359	-0.19639975722252	0.57200070254768
C	2.73379426774713	-1.18311786359407	-0.42877638402430
C	3.42499110548429	-2.04297708897861	-1.25206246672843
H	4.47361716501290	-2.24496161325149	-1.37482534109366
C	2.63547715179319	-3.65225145524347	-3.02784212798154
H	2.29056555245685	-3.22865425855908	-3.96842522173231
H	3.68748947354999	-3.90919622463889	-3.09683107439159
H	2.05191461176979	-4.53459885796716	-2.77859704018856

## Coordinates from ORCA-job fac2\_t1

Os	0.06717152698292	0.20337658075715	0.06913916833751
N	-0.81241202189610	1.71521345345377	1.11072069901051
N	0.21742058972279	1.75806498303052	-1.27484124946510
N	0.57915135765082	1.81023847667094	-2.54192869206691
N	0.24996281338611	3.03262967178150	-2.94855205782692
C	-1.42650129867796	1.63681710276031	2.32850534328376
H	-1.43189541506563	0.66626471682906	2.80468127864279
C	-1.98034502532830	2.72462181136624	2.91901080020491
H	-2.44557688823381	2.65098323133906	3.88963603854910
C	-1.92051750616015	3.97296814147911	2.21624478978998
H	-2.32346202099081	4.87326844365372	2.66206031326599
N	-1.39166616622399	4.07955565918077	1.01288685704711
C	-0.85973231962093	2.98893408979377	0.45388809587906
C	-0.34780150180212	2.94519805038260	-0.86438274456911
C	-0.31550252936229	3.77354641796388	-1.97626106047649
H	-0.66593026250380	4.77546346530435	-2.14017188659521
C	0.41477498456957	3.39643128289444	-4.34950151917600
H	-0.27017202745946	2.80933987395316	-4.95583102620293
H	0.18511978291846	4.45263212598003	-4.45310602178472
H	1.43980957995149	3.20030808105807	-4.65320535391909
N	-0.42167638241935	-1.35445262477293	1.41900223499459
N	-1.64275646746702	-0.53901850402425	-0.73028220446257
N	-2.30346714567038	-0.23922381876093	-1.82043490234635
N	-3.27373380973821	-1.14524624171840	-1.90368192125513
C	0.28547718936158	-1.74710019230192	2.48948622502687
H	1.15715829533192	-1.16207778507517	2.74617348675898
C	-0.09676593155155	-2.85154840261377	3.22172785681013
H	0.47620424574078	-3.17430062545032	4.07704328874854
C	-1.24254923275198	-3.52345248599388	2.81899998040503
H	-1.60170494150382	-4.38889977129135	3.35914633766317
N	-1.95162126300106	-3.14951575863259	1.75131005699077
C	-1.51894216898652	-2.09064607860291	1.08673802273956
C	-2.18311504501910	-1.63046507223947	-0.11069930754917
C	-3.24977927064682	-2.02357060067050	-0.87925821003052
H	-3.95642495045736	-2.82753863556748	-0.78329950599130
C	-4.16167951452640	-1.15228712081324	-3.06072619955838
H	-3.62698067512805	-1.56087393342127	-3.91518230062740
H	-5.01883801897063	-1.77279743477513	-2.82112740680365
H	-4.47914627783025	-0.13424441659768	-3.26523721980820
N	2.00626153847905	0.68894314073271	0.78181585992492
N	1.27460227469022	-1.28838708151914	-0.75785950372966
N	0.96178867397940	-2.42185412692257	-1.32374045986881
N	2.07740984844231	-3.15721465868037	-1.29795146098090
C	2.32353089316808	1.76215074658982	1.52443104115216
H	1.51658447798409	2.41795751836374	1.81204018930854
C	3.62689845961306	1.99147932240733	1.90826595253213
H	3.88292779092743	2.85122040053607	2.50757791000145
C	4.58816147828218	1.07800206405171	1.50074291800339
H	5.62716461863897	1.20507301414855	1.77455356987694
N	4.28655489843660	0.00616812987816	0.76365503083006
C	3.01639083998581	-0.15298865578281	0.42729541428721
C	2.57699444694991	-1.28522663292318	-0.35572943479096
C	3.09985485386254	-2.50677132062926	-0.71497066082516
H	4.07270504911721	-2.94345489716849	-0.58226554459021
C	2.04065385459233	-4.53624869326118	-1.77048677598286
H	1.73020101493452	-4.55347037814442	-2.81215896394974
H	3.03686577943245	-4.95244455578593	-1.66187682557837
H	1.33719492186125	-5.09742949219995	-1.16162833925329

## Coordinates from ORCA-job mer2\_gs

Os	-0.01903790368739	0.14903434770068	-0.05269296978245
N	0.55056494590710	1.26759295168619	-1.73727464837132
N	-0.30084782960896	2.09051980506391	0.57380010235698
N	-0.65453401780396	2.61860472854695	1.71574178048412
N	-0.52998782704079	3.94578980708707	1.55958986451818
C	0.95978410028875	0.77617855335583	-2.91808608936469
H	0.99380175304863	-0.29883694661000	-3.01820016434056
C	1.31871637724614	1.61604592280861	-3.95136249068718
H	1.64511913820671	1.21582302874294	-4.89902851705304
C	1.25001826434977	2.98279991976011	-3.72452369525669
H	1.52202377541672	3.69214010632982	-4.49470478679001
N	0.84873183253341	3.49079213098283	-2.55759545248377
C	0.51139510367787	2.62464629141228	-1.61215298778085
C	0.05225433196027	3.06528039116288	-0.31772055127063
C	-0.09957160470840	4.27010366620298	0.32890595900566
H	0.06901808504272	5.28517597044017	0.01842086727190
C	-0.83062325038863	4.84159080406256	2.66733169424907
H	-0.23508479291671	4.55213507963429	3.52887135673573
H	-0.57413937774490	5.85008832266249	2.35941307010125
H	-1.88958573464209	4.78073141968975	2.90808001140143
N	-0.79089955029385	-0.88357629605152	1.61187979407944
N	-1.98835655464075	-0.11469820403925	-0.56969143141635
N	-2.69123739385052	0.20557325674332	-1.62242275332318
N	-3.90353437832643	-0.34031376772388	-1.43054138434967
C	-0.11384495826079	-1.26666078157650	2.70561130553807
H	0.90310130834542	-0.91553120503554	2.80144290489571
C	-0.69748322340846	-2.07365103951444	3.66020189066952
H	-0.14396840686949	-2.38878939137655	4.53134246100243
C	-2.01129330277524	-2.46683706110415	3.45223756077826
H	-2.52377003396012	-3.10435499439120	4.16047873277865
N	-2.70473703899107	-2.08749690124121	2.37645163551075
C	-2.07845450228204	-1.31654374883100	1.49917309503137
C	-2.73274875625758	-0.86376976388466	0.29722871035866
C	-3.97616586485694	-1.00999049750598	-0.26819206981769
H	-4.86263145317944	-1.52266093376489	0.05737121005961
C	-4.93356966508867	-0.21869806864503	-2.45175663576125
H	-4.63744305174284	-0.78455186427650	-3.33217858605702
H	-5.85523213925884	-0.62171945350597	-2.04442265186808
H	-5.06584788999671	0.82901498164790	-2.70744019899692
N	1.99651022411567	0.07723774699573	0.54519830119138
N	0.56507933267322	-1.72189371536531	-0.68637954788559
N	-0.09183248189447	-2.74114528401474	-1.17365897666596
N	0.77400397282209	-3.76726687433191	-1.17369979366750
C	2.68996554012051	1.04538013807251	1.16642474631151
H	2.16397211518490	1.95952217980540	1.39558655443708
C	4.01414244197434	0.87017203853208	1.50812858397435
H	4.56166578758898	1.65418574923905	2.00855457521332
C	4.60394023666071	-0.34525440170563	1.19139082726818
H	5.63679304740539	-0.54973884976205	1.43999475278197
N	3.93207683332796	-1.31940781605573	0.57310379195856
C	2.66483999902566	-1.08053389773178	0.27148486264854
C	1.84538861784178	-2.07980884036649	-0.37040326349473
C	1.97699449299576	-3.41011760720211	-0.69359601944991
H	2.79808074966060	-4.09785557991282	-0.60255171043866
C	0.33178871450769	-5.09756833191353	-1.57180310988904
H	0.00067395066691	-5.08085183067632	-2.60739052854871
H	1.17209463742802	-5.77488073241836	-1.45535983373629
H	-0.48477672554758	-5.40825465783329	-0.92541015406394

## Coordinates from ORCA-job mer2\_t1

Os	0.01638845876254	0.09143568804381	-0.04506302160083
N	0.65612471917950	1.18395784188408	-1.71286338842006
N	-0.33934395089425	2.05121268276077	0.52679663179182
N	-0.84891317440650	2.59665398237068	1.59767532008937
N	-0.79458452637151	3.91624727963896	1.39159641291118
C	1.17015707949057	0.65809230178750	-2.83733998348697
H	1.21862151732255	-0.41882541712944	-2.90197362626256
C	1.60641931815615	1.47533894532382	-3.85642994024983
H	2.01640254631311	1.05660439893209	-4.76241416740955
C	1.50601309231276	2.84736566776976	-3.66932734371712
H	1.83474618194488	3.53894938154868	-4.43333441581007
N	1.00525680248052	3.38397996770076	-2.55431312892263
C	0.59916095598571	2.54205426803602	-1.61719488327146
C	0.04114976196321	3.00714287861850	-0.37169041196862
C	-0.25445456071300	4.22271895975656	0.19731775081153
H	-0.12394986539076	5.23415971072547	-0.14281558385120
C	-1.25995805206371	4.84159425132017	2.42058715855351
H	-0.40361528087933	5.28179322677446	2.92633870694023
H	-1.85562090346102	5.61580600193489	1.94490682073749
H	-1.86542521243031	4.28005429441779	3.12490365763613
N	-0.73975917075727	-0.98019670717986	1.60855126597065
N	-2.00862051384726	-0.08377521513169	-0.49345559183515
N	-2.75554144982708	0.35522094275404	-1.46956417493435
N	-3.98991517299832	-0.07987270748145	-1.19927056229852
C	-0.01750810795826	-1.44711373241986	2.63910288760021
H	1.02609241519095	-1.17203811867665	2.67199253527965
C	-0.60318926958616	-2.23269606011877	3.60923088191917
H	-0.02363376784774	-2.61074024497324	4.43696103849134
C	-1.95441997299756	-2.51751171697067	3.47739505902109
H	-2.47079441663824	-3.12742692031249	4.20646677086633
N	-2.68197727662230	-2.06479578895108	2.45359459428882
C	-2.05686066872241	-1.31805536142479	1.55834909343748
C	-2.74806891033759	-0.79237289209464	0.40637515272460
C	-4.04130179844653	-0.78675845623450	-0.05554666505145
H	-4.94852002398509	-1.21699381209400	0.32731453497134
C	-5.08153239918446	0.18139957966238	-2.12964793788671
H	-4.91901208794051	-0.39056793199609	-3.03954491974944
H	-6.00505600587079	-0.13017501633884	-1.65229082513742
H	-5.11348568058283	1.24420216304593	-2.35235444237402
N	1.97424617507733	0.05397470927399	0.58499777732502
N	0.60636923058486	-1.77348714316258	-0.70032640941037
N	-0.05133583177589	-2.81172684056042	-1.20383948043436
N	0.83301175954271	-3.80300948509014	-1.22290732467383
C	2.69647401191366	1.06113093205961	1.13304609640565
H	2.17402868404083	1.98915658359470	1.31855792971588
C	4.00787928746336	0.90702903152248	1.46873925966180
H	4.56181336003110	1.71316620295706	1.92379362501736
C	4.61229120805046	-0.36564679581648	1.21706364188267
H	5.64128058245245	-0.54969729922637	1.50068338343686
N	3.96624018677793	-1.35324884452407	0.64388503137598
C	2.67725594716277	-1.15663060747799	0.30669393368780
C	1.90130641737284	-2.11871960864382	-0.36366404902492
C	2.03717273250135	-3.45054087017480	-0.73802704175087
H	2.85952742042591	-4.13882579839106	-0.67638321648649
C	0.47138076911216	-5.10796477016010	-1.76317741086864
H	0.68764009909940	-5.13632398159829	-2.82978324785569
H	1.05560378309097	-5.86287576635002	-1.24648704129070
H	-0.58700584126582	-5.27327219351075	-1.58382955651713

## Coordinates from ORCA-job fac3\_gs

Os	0.07499651930348	0.01123461213510	0.21395922707226
N	-0.88643070954082	1.68720151269699	1.01832945650426
N	0.30764130504584	1.40730001606061	-1.27524721666264
N	0.74190549497568	1.32010861192248	-2.50352850187901
N	0.46934753511654	2.50283576558010	-3.06779632349388
C	-1.49298812040885	1.78426185978195	2.21123714292015
H	-1.53847979601435	0.89741489632027	2.82508098847880
C	-2.03478958364900	2.98211178999669	2.64038621937594
H	-2.52134893607968	3.03398008728889	3.60432167179680
N	-1.97971203026298	4.10265270146675	1.91141571202838
C	-1.38728602209465	4.00613377706069	0.72503828777203
H	-1.32896992260354	4.89898158173252	0.11645762214129
C	-0.84824126422713	2.81691562963279	0.25487765987480
C	-0.24007120327385	2.63466420192330	-1.03714353449619
C	-0.13236726459093	3.34717525395839	-2.20954011663925
H	-0.44090724122805	4.33761655847858	-2.49052299775323
C	0.75037374628774	2.70830326754538	-4.48226413987629
H	0.10704899451218	2.06083475775986	-5.07221402085861
H	0.54512141006450	3.74749356878428	-4.71955367356978
H	1.79365955276620	2.47363729204494	-4.67814707878627
N	-0.52549409297412	-1.36819664411037	1.66487799168234
N	-1.68290738653200	-0.70767710161527	-0.56864400557081
N	-2.33779396846409	-0.45971987884895	-1.67050245107966
N	-3.42474899447762	-1.24055688418077	-1.62910300272001
C	0.12920952526173	-1.69651438085805	2.78962632438940
H	1.05355653392436	-1.18210843386466	3.00226053183987
C	-0.36093836190327	-2.66804293096353	3.64154713008820
H	0.19147412175988	-2.92636410764742	4.53425998773996
N	-1.50707286503779	-3.31859185987846	3.41073809865166
C	-2.16112854197535	-2.98966266975469	2.30087371854496
H	-3.08866638048227	-3.50637089948662	2.09128956796640
C	-1.69391919077493	-2.02570100577720	1.41700868552064
C	-2.33309433197396	-1.64372892135857	0.18517736372824
C	-3.46876313716838	-1.98800990410535	-0.51081024295737
H	-4.26806381847464	-2.67603281423061	-0.30330315691513
C	-4.35737436718928	-1.24549315044033	-2.74698109541664
H	-3.90052930116371	-1.74711768560727	-3.59711148028472
H	-5.25053061835463	-1.77761415091710	-2.43587635128182
H	-4.60556429860811	-0.22031849644678	-3.00682192017764
N	1.93237143331300	0.44370599912850	1.06411683218577
N	1.30650439666127	-1.35044670745094	-0.69766164807709
N	1.09865287014796	-2.25159260495502	-1.61742541767096
N	2.30730067854203	-2.72809571534909	-1.93706690050733
C	2.18582446292861	1.34804707190898	2.02275775864317
H	1.35185802397779	1.90226720893497	2.42395877006190
C	3.47372658911492	1.56313575252654	2.47538860498242
H	3.65394004349275	2.29885567843489	3.24713385447994
N	4.52859309116494	0.89663174152747	1.99223889124901
C	4.27636035399888	-0.01380557665898	1.05528272044503
H	5.11319991981681	-0.57185160527865	0.65662905957946
C	2.99445305323481	-0.26161954066016	0.58194068095938
C	2.63955444972666	-1.23925774979544	-0.41399930689142
C	3.28866250607151	-2.13860199615097	-1.23012066380864
H	4.32537386872119	-2.39144225982981	-1.35992524406167
C	2.42302160053458	-3.73788936557148	-2.97962819091497
H	2.08108015082022	-3.31608594763596	-3.92189027278999
H	3.46544326816871	-4.02916823452280	-3.05615790297228
H	1.81472625007313	-4.59732197068055	-2.71072370258900

## Coordinates from ORCA-job fac3\_t1

Os	-0.02113744544257	0.18029069889995	0.05808234026397
N	-0.93798650647018	1.73135911541855	1.02964147808877
N	0.14714992709802	1.71479176581514	-1.32162687556625
N	0.46442409382823	1.72329473907617	-2.59619961973351
N	0.18132893305911	2.95124629433803	-3.01897547448375
C	-1.34411439815905	1.73566698183703	2.34674986452040
H	-1.48007395150074	0.77683920508871	2.82433318848220
C	-1.56590379644187	2.89735127238998	3.01401946078022
H	-1.89177499940760	2.86219153450744	4.04432247230534
N	-1.41167498338804	4.14929265368962	2.45677819346101
C	-1.02767071047690	4.14619372697431	1.17026139874996
H	-0.88738044521182	5.11011220436108	0.69490943090462
C	-0.78912098965505	3.00675033383903	0.43816976100621
C	-0.34121034035793	2.93025793265063	-0.91820970688882
C	-0.31421796740221	3.73440091965309	-2.03859491839275
H	-0.62530257987887	4.74838402696454	-2.20981866085471
C	0.31880045894754	3.28181963316410	-4.43166934720315
H	-0.38085472047909	2.68316575122172	-5.00864110210938
H	0.08974864460033	4.33611867145416	-4.55331100724888
H	1.33686632641250	3.07556042726115	-4.75187503465330
N	-0.50549696266328	-1.36125287042793	1.40848587616780
N	-1.70097772055046	-0.59993588542824	-0.77288465061766
N	-2.33675937653731	-0.33001348900297	-1.88746352259320
N	-3.25181692381025	-1.28342601513421	-2.00853840303003
C	0.18398326926488	-1.71698052396136	2.49850871849738
H	1.01242872934024	-1.09354054070553	2.80017326129258
C	-0.15975376531394	-2.85675174193703	3.20576743871392
H	0.41498983190470	-3.14314473202200	4.07509714484117
N	-1.18442703183437	-3.63732752364135	2.85242346798808
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N	1.19482683264533	-1.30763784576573	-0.76475928377737
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N	4.50359352710322	1.12802344373510	1.64727457908441
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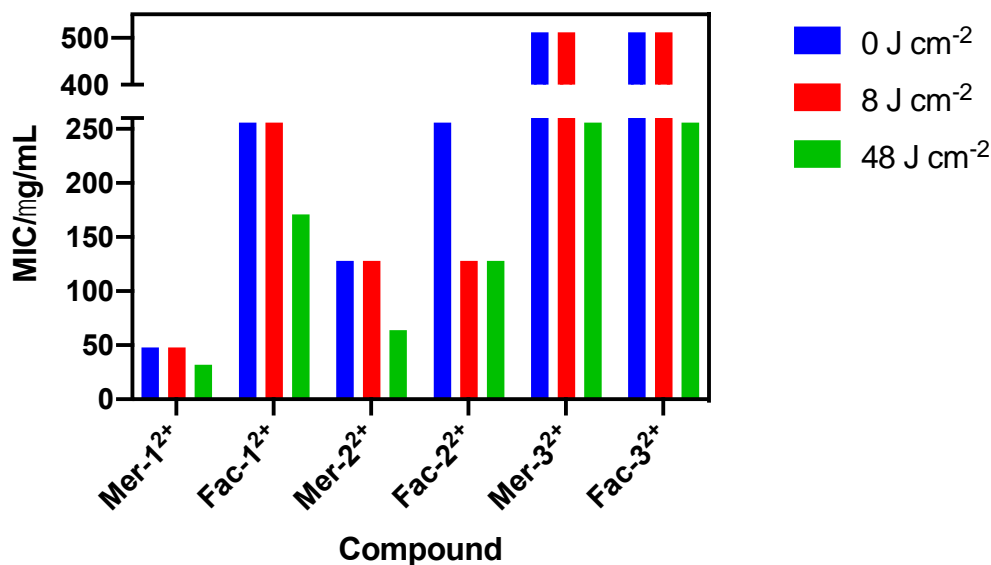


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N	-0.83642939281448	3.78646607010388	1.40948536423579
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H	1.21574376330679	-0.54061803703687	-2.89558845854362
C	1.49970614180278	1.35438203863154	-3.86963880558980
H	1.91118754735989	0.91983132363713	-4.77005596837729
N	1.38235999355878	2.68507016854417	-3.81761757397925
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H	0.76562090437596	4.26999152196936	-2.63958623832860
C	0.48927032698589	2.39917775783325	-1.62816576164717
C	-0.05352488393037	2.87324212146546	-0.38005622264600
C	-0.36364978411461	4.08798328797695	0.18573853571689
H	-0.28841428198164	5.09956733494808	-0.17060885553561
C	-1.27275481223047	4.71273296037044	2.44814093077641
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H	-1.90084005195920	4.16547020351369	3.14436185917763
N	-0.81656974808396	-1.00621581472104	1.63664702351853
N	-1.99180950063676	-0.15176816438554	-0.51641388758313
N	-2.68750556959236	0.33019109642934	-1.51067822912507
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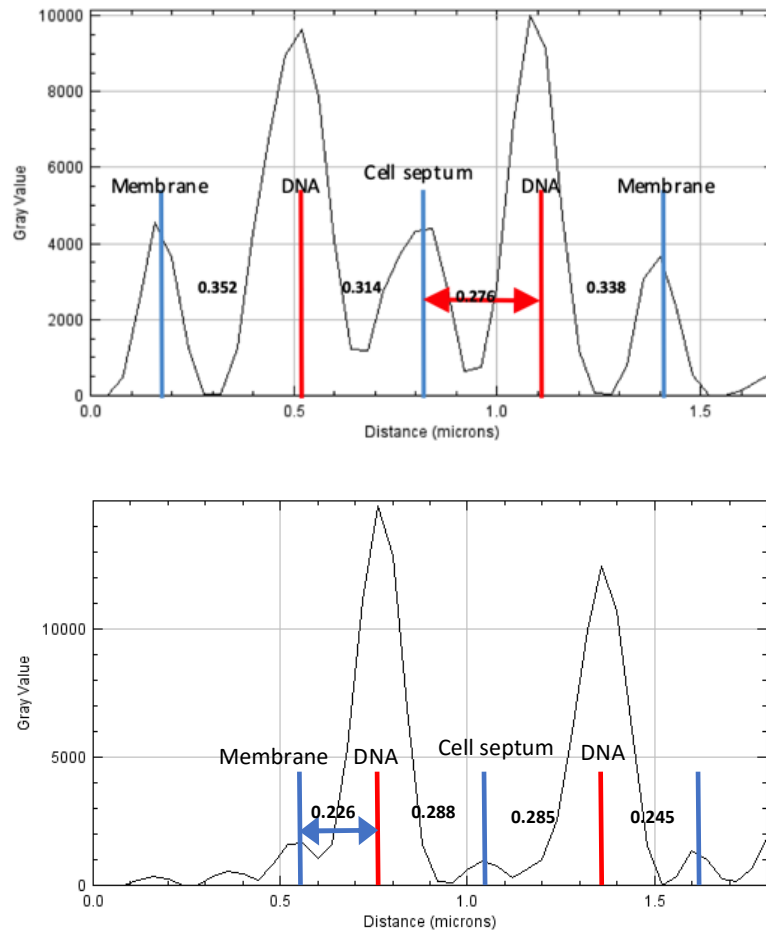
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H	2.10278240234811	0.93079050044635	-4.65763758561473
N	1.60416899219412	2.70586650503400	-3.70699018247362
C	1.06975183416863	3.23276749207535	-2.61061085103838
H	1.00532084546297	4.31085545110213	-2.54618778875256
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C	0.02211832829110	2.92362460315098	-0.33857491282955
C	-0.27089041854689	4.13733804998238	0.23627857948189
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H	-0.44682333342927	5.20363232357724	2.94628465321656
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C	-0.78642659547979	-2.36241273856114	3.57886499707801
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H	1.20259206552076	-5.91197112202543	-1.13334082360529
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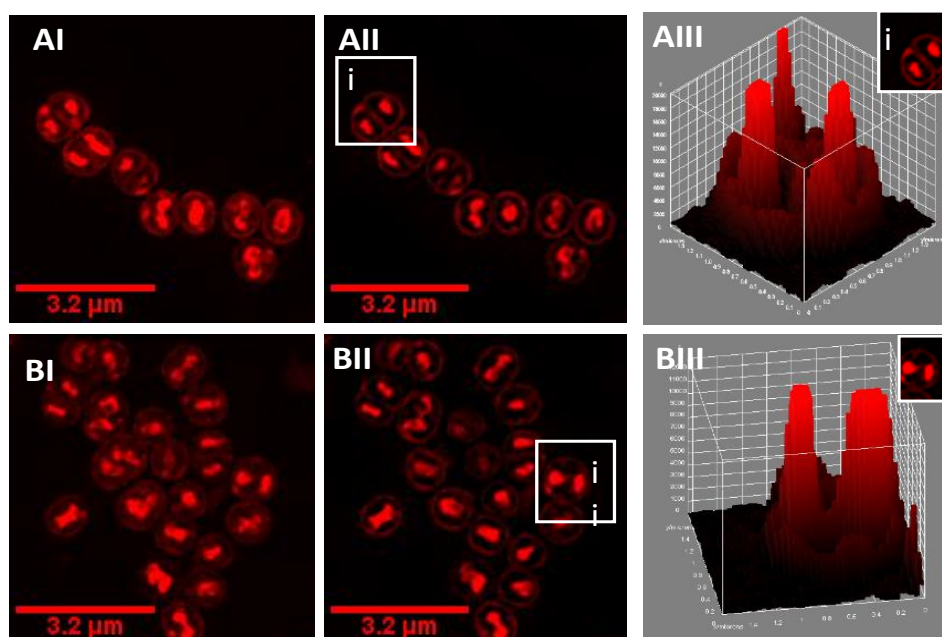


	<i>mer-1</i> <sup>2+</sup>	<i>fac-1</i> <sup>2+</sup>	<i>mer-2</i> <sup>2+</sup>	<i>fac-2</i> <sup>2+</sup>	<i>mer-3</i> <sup>2+</sup>	<i>fac-3</i> <sup>2+</sup>
PI	1.5	1.5	2	2	2	2

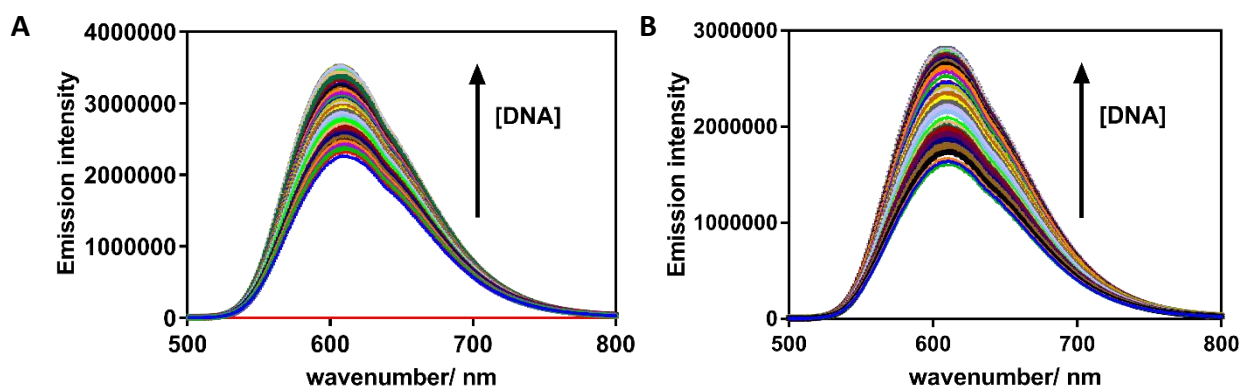
**Figure S13 Phototoxicity experiments.** A concentration range for all compounds of (0-512  $\mu\text{g/mL}$ ) was used to assess the compounds phototoxicity against the MRSA *S. aureus* cell line. Concentrations were made from a serial dilution method in 96-well plates. Experiments were conducted in MH-II media. Cells were irradiated with white light for 5 mins (red bars, 8 J cm<sup>-2</sup>) and 30 mins (green bars, 48 J cm<sup>-2</sup>) and results were compared to a control 0 mins (blue bars, 0 J cm<sup>-2</sup>). After irradiation, plates were incubated stationary overnight at 37.5 °C. MIC values were determined by eye. Phototoxic index is given for all compounds in defined medium.



**Figure S14** TOP: Peak intensity distance measurements ( $\mu\text{m}$ ) for *S. aureus* MRSA (strain) cells incubated with MIC concentrations of *mer-1*<sup>2+</sup> after 60-minute incubation. BOTTOM: Analogous experiments carried out with *fac-1*<sup>2+</sup>. Emission was collected in the A458 channel upon excitation with the 405 nm laser.



**Figure S15** Uptake of  $fac-1^{2+}$  by *S. aureus* MRSA cells monitored through SIM microscopy. *S. aureus* MRSA (strain) cells were incubated with MIC concentrations of  $fac-1^{2+}$  for 60 (A) and 120 (B) minutes. A 3D projection Z-stack is given (I), and a slice through the centre of the cell (II) where peak intensity is observed. 3D surface plots of selected cells (i, ii) show localisation of complex at the membrane and centre of the cell.



**Figure S16 DNA binding titration.** DNA binding titration showing the increase in emission intensity for  $fac-1^{2+}$  (A) and  $mer-1^{2+}$  (B) upon increasing DNA concentration. DNA binding titrations were conducted using 15 μM concentrations of complex, [DNA] = 7.14 mM was added in 5 μL increments. Excitation wavelength 480 nm.

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