Title of Case Study: Applications of luminescent coordination complexes

Grant Reference Number or Facility Name: Cardiff University accessing National Crystallography Service, University of Southampton

One sentence summary: Crystallography data is helping transform healthcare imaging and treatment with the development of luminescent metal-containing compounds.

One paragraph summary: Data from the University of Southampton's National Crystallography Service (NCS) is helping academics at Cardiff University develop luminescent metal-containing compounds that could transform biological imaging and help in the global fight against cancer and other medical conditions.

Key outputs in bullet points:

Data generated at NCS is enabling:

- The development of luminescent metal-containing compounds that could change real-world applications
- The development of research with the potential to transform biological imaging
- The development of molecules to help in the fight against cancer and other medical conditions
- Cardiff's research to be published in high quality journals
- Cardiff's research to be progressed to its full potential
- The formation and structure of molecules that absorb and emit light to be fully understood

Main body text

Data from the University of Southampton's National Crystallography Service (NCS) is helping academics at Cardiff University develop luminescent metal-containing compounds that could transform biological imaging and help in the global fight against cancer and other medical conditions.

The researchers at Cardiff are developing these compounds that could change the face of a wide range of real-world applications.

Biological imaging and therapeutic healthcare treatments are among the many applications that could be transformed as the team's research explores the luminescent properties of these metal-containing compounds.

Head of the Molecular Synthesis group, at Cardiff's School of Chemistry, Dr Simon Pope is leading research into understanding the formation and structure of molecules that absorb and emit light and the potential impact these molecules could have on our future society.

The targeted applications of Simon's research fall into four categories:

- The design and synthesis of new classes of luminescent metal coordination compounds based on precious metals such as rhenium, iridium, platinum and gold, to understand the factors that determine the properties of luminescence and allow the tuning of the colour of the emitted light.
- To develop metal coordination compounds for applications in bio-imaging such as optical and magnetic resonance imaging (MRI) that can offer the improved imaging quality of cells and allow the potential design of theranostic agents that can combine diagnostic and therapeutic properties in a single molecule.
- To develop and understand new therapeutic molecules based on luminescent gold compounds that are used to clinically treat inflammatory conditions such as rheumatoid arthritis.
- To generate reactive oxygen species that have significant importance in biology and catalysis, including investigating the role of iridium-containing compounds in photodynamic therapy (PDT) – a common clinical treatment for a variety of skin conditions, macular degeneration in the eye, and the potential for selective treatment of cancerous tumours by inducing cell damage.

However, in order to progress their research to its full potential Simon and his team need to understand the form, function and structure of these metal-containing compounds and their luminescent properties.

Many of the crystals Simon and his team produce are too small to be examined using the equipment at Cardiff University, so they need to access the NCS at Southampton to generate data that can effectively be used in their research.

The NCS uses X-ray crystallography to give definitive evidence of the proposed structure of the molecules and if their equipment isn't powerful enough, they have access to the more powerful synchrotron at Diamond Light Source, in Oxfordshire.

Simon said: "The data we get from the service is the most powerful technique for giving us 3D information on the structure of our molecules. Putting this data together with all our other data gives us a comprehensive picture of the structure and properties of the molecule."

Cardiff's collaboration with the NCS started about four years ago when Simon was looking for expertise in collecting and processing data.

He said: "As part of our research we are always trying to maximise the quality of the publication that we can get, so every facet of our data has to be as high quality as possible. The NCS at Southampton provides the quality of service and expertise that we require."

Over the years, NCS data has had a significant effect on the outcome of Simon's research.

He said: "We have published papers over the last year with co-authors from NCS that have been the first examples of applying gold containing compounds to biological imaging. Having the data from NCS has been a very important part of being able to publish high quality papers in this area of work."

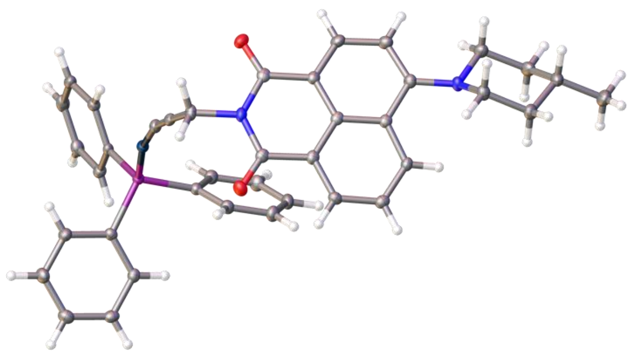

Figure 1. An example of one of the gold complexes exhibiting potential as a biological imaging agent.

NCS data also played a significant role in Cardiff's research into the use of metal-containing compounds to generate reactive oxygen species.

In one of the first papers Cardiff published with collaborators from the NCS, they showed that iridium-containing compounds were extremely efficient as photosensitisers for reactive oxygen species.

"The data we got from the NCS was absolutely crucial in understanding the structure of the complex. Without it we would have drawn the wrong conclusions about the structure," said Simon.

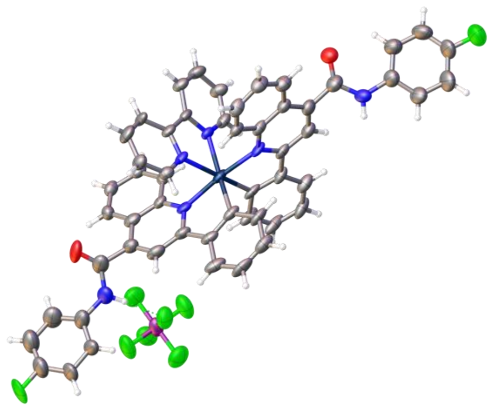

Figure 2. One of the reported iridium-based photosensitisers.

Cardiff sends up to 20 samples to the NCS each year and recognises that EPSRC-funding has allowed them to access the X-ray crystallography expertise and infrastructure available at Southampton.

“The data we have obtained by accessing this service has helped us fully characterise target compounds and facilitated the publication of our work,” said Simon.

Names of key academics and any collaborators:

Dr. Simon Pope (Cardiff University)

Dr. Peter Horton (University of Southampton)

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