

This data folder is associated with the following publication in the Journal of Photochemistry and Photobiology: Biology B:

Spectrally resolved infrared microscopy and chemometric tools to reveal the interaction between blue light (470 nm) and methicillin-resistant *Staphylococcus aureus*

The paper has been published by E. Aboulizadeh, et al. in February 2017. You can access the paper via the following link:

<https://doi.org/10.1016/j.jphotobiol.2016.12.030>

When using the data, please cite the publication. Here is the abstract of the publication:

“**Blue light** inactivates methicillin-resistant *Staphylococcus aureus* (MRSA), a **Gram-positive antibiotic** resistant bacterium that leads to fatal infections; however, the mechanism of bacterial death remains unclear. In this paper, to uncover the mechanism underlying the **bactericidal** effect of blue light, a combination of Fourier transform infrared (FTIR) spectroscopy and **chemometric** tools is employed to detect the photoreactivity of **MRSA** and its distinctive pathway toward **apoptosis** after treatment. The mechanism of action of UV light and **vancomycin** against MRSA is also investigated to support the findings. Principal component analysis followed by linear discriminant analysis (PCA- LDA) is employed to reveal clustering of five groups of MRSA samples, namely untreated (control I), untreated and incubated at ambient air (control II), irradiated with 470 nm blue light, irradiated with 253.5 UV light, and vancomycin-treated MRSA. Loadings plot from PCA-LDA analysis reveals important functional groups in proteins (1683, 1656, 1596, 1542 cm^{-1}), **lipids** (1743, 1409 cm^{-1}), and **nucleic acids** region of the spectrum (1060, 1087 cm^{-1}) that are responsible for the classification of blue light irradiated spectra and control spectra. Cluster vector plots and scores plot reveals that UV light-irradiated spectra are the most biochemically similar to blue light- irradiated spectra; however, some **wavenumbers** experience a shift. The shifts between blue light and UV light irradiated loadings plot at $\nu_{\text{asym}} \text{PO}_2^-$ band (from 1228 to 1238 cm^{-1}), DNA backbone (from 970 to 966 cm^{-1}) and base pairing vibration of DNA (from 1717 to 1712 cm^{-1}) suggest distinctive changes in DNA conformation in response to irradiation. Our findings indicate that irradiation of MRSA with 470 nm light induces A-DNA cleavage and that B-DNA is more resistant to damage by blue light. Blue light and UV light treatment of MRSA are complementary and distinct from the known antimicrobial effect of vancomycin. Moreover, it is known that UV-induced cleavage of DNA predominantly targets B-DNA, which is in agreement with the **FTIR** findings. Overall the results suggest that the combination of light and vancomycin could be a more robust approach in treating MRSA infections. “

The data folder contains all the data that has been included in this publication. The data files are stored as .dpt files, which contain FT-IR spectra from alive, blue-light irradiated, UV-irradiated, and vancomycin-treated MRSA.

Please feel free to contact either Dr. Carol Hirschmugl (cjhirsch@uwm.edu) or Dr. Ebrahim Aboulizadeh (eabouali@ur.rochester.edu) for any question or concerns regarding this data.