

# 25<sup>th</sup> Nano Congress for Future Advancements

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12<sup>th</sup> Edition of International Conference on

## Nanopharmaceutics and Advanced Drug Delivery

August 16-18, 2018 | Dublin, Ireland



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#### Synthesis, x-ray crystal structure, emission property, and DFT calculation of monoprotonated polypyridine

A series of metal-free compounds, i.e., bpyHPF6 (1), dmbpyHPF6 (2), phenHPF6 (3) dpphenPF6 (4), bqnHPF6 (5) and ppyHPF6 (7) were newly prepared and characterized by electrospray ionization mass spectrometry, and UV-vis spectroscopy. Abbreviations used are bpy = 2,2'-bipyridine, dmbpy = 4,4'-dimethyl-2,2'-bipyridine, phen = 1,10-phenanthroline, bqn = 2,2'-biquinoline and ppy = phenylpyridine. The x-ray crystal structures of the four compounds 1, 2, 3, 4 5 and 7 were determined. Monoprotonated pyridine rings are hydrogen bonded intramolecularly to the adjacent pyridine ring in compounds 1, 2, 3, 4 and 5. The  $\pi$ - $\pi^*$  absorption bands in the UV region for 1, 2, 3, 4 and 5 in acetonitrile were red-shifted relative to those of the corresponding neutral unprotonated compounds. Density functional theory was applied to interpret the planarity in 1. The attachment of one proton to the one nitrogen in 5 leads to the remarkable emission ( $\phi = 0.10$ ). The attachment of one proton to one nitrogen in 4 also gives the large quantum yield.

#### Biography

Naokazu Yoshikawa is a researcher from 2000. He have completed PhD in 2008 from Nara Women's University and continued postdoctoral studies with Osaka University and Nara educational University. He have published more than 25 papers in reputed journals. He have an interest in iridium complexes and Ruthenium complexes. Recently he also interested in metal free emission product.

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