

Synthesis and characterization of trimethylbenzene and chlorobenzene derivatized platinum complexes towards biological applications

K. W. G. K. P. Yasarathna^{1,2}, I. C. Perera³, F. R. Fronczek⁴, N. T. Perera^{1*}

¹ Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura, Sri Lanka.

² Department of Pharmacy, Faculty of Allied Health Sciences, University of Ruhuna, Sri Lanka.

³ Department of Zoology and Environment Sciences, University of Colombo, Sri Lanka.

⁴ Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803.

*Corresponding author: theshi@sjp.ac.lk

Synthesis of metal-based complexes as potential therapeutic agents for diseases like cancer, arthritis is a recent topic of interest. With the intention of identifying novel drug leads with potential biological applications, novel platinum complexes; {[Pt(N(SO₂trimethylbenzene)dpa)Cl₂] (C1) and [Pt(N(SO₂chlorobenzene)dpa)Cl₂] (C2)}, derived from sulfonamide ligands; {N(SO₂trimethylbenzene)dpa (L1) and N(SO₂chlorobenzene)dpa (L2)} were synthesized. These compounds were characterized by ¹H NMR, X-ray crystallography, FT-IR, UV-Vis and fluorescence spectroscopic methods. Biological target prediction was carried out using 'SwissTargetPrediction' and 'SwissADME' servers and 'Pyrx 0.9.4' software was used for molecular docking. Structural data confirm the formation of the compounds and the S-N bond length for L1 was 1.6273 Å whereas for the C1 it was 1.6461 Å. In ¹H NMR data, the peaks of L1 were de-shielded upon binding with the metal and the singlet peak observed at 4.53 ppm for methylene protons appeared as two

doublets (5.08 ppm, 6.09 ppm) in the spectrum of C1. Similarly, in L2, a singlet peak observed at 4.56 ppm for methylene protons appeared as two doublets (5.23 ppm, 6.02 ppm) in the spectrum of C2. L1 shows high energy absorption bands at 205 nm and 227 - 295 nm due to intraligand π-π* and n-π* transitions whereas C1 displays absorption bands at 205 nm, 229 nm and 275 nm. L2 shows high energy absorption bands at 204 nm, 237 nm and 254 nm and C2 shows absorption bands at 204 nm and 275 nm. Both L1 and L2 display high fluorescence intensities in the visible range which have lowered in corresponding platinum complexes. *In silico* analysis of drug-likeness indicates that ligands comply with the Lipinski rule of five and they are predicted to bind with Cyclooxygenase-2 and L1 is predicted to bind with a calculated binding affinity of -6.9 kcal/mol showing their potential to be used as anti-inflammatory drug leads.

Keywords:

Anti-inflammatory, chlorobenzene, platinum, trimethylbenzene

The effect of the metal ion composition on the decarboxylation percentage of metal basic soap and level of unsaturation in producing green diesel

U S K Weliwegamage*, M K S Jayasinghe, G W C S Perera

College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka.

*Corresponding author: weliwegama@ichemc.edu.lk

The growing demand for fossil fuels has led to their depletion, causing higher fuel prices and threatening the sustainability of industrialized countries. Biodiesel is a renewable fuel produced through the trans-esterification of fatty acids, however, it has several technical issues such as lower energy density and less oxidation stability compared to petroleum diesel. Green diesel, an

oxygen-free hydrocarbon-like fuel, produced through deoxygenation, solves the inefficiency issue of biodiesel. Deoxygenation techniques such as decarboxylation and decarbonylation are preferred to hydrodeoxygenation from an economic perspective. The decarboxylation of metal basic soap (MBS) is a promising method of deoxygenation for green diesel production, and the

metals introduced during the saponification process play a direct role as catalysts during the reaction. This research investigated the effect of metal ion composition on the decarboxylation percentage of MBS and the level of unsaturation in producing green diesel. The results showed that composition of the metal mixture certainly affects the liquid product of metal basic soap as observed by the analysis of percentage decarboxylation results. Out of the three Mg-Zn basic soaps produced, the metal basic soap prepared with the 9:3 mole ratio of Mg to Zn was observed to archive a higher percentage of

decarboxylation with 31.26%. Except Mg, the quantity of the other metal used; in this instance Zn, seemed to affect the level of unsaturation of fatty acid chains as the peaks observed on the FTIR spectra of liquid products seem to diminish. The findings indicate that controlling the metal ion composition can help optimize the decarboxylation process and enhance the alkane to alkene fraction of green diesel production.

Key words:

Green diesel, Metal basic soap, Decarboxylation, Unsaturation, Metal ion

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Electropolymerization of EDOT (3,4-Ethylenedioxythiophene) with Berberine isolated from *Coscinium fenestratum*

R. M. G. Rajapakse^{1*}, M. G. S. A. M. E. W. D. D. K. Egodawele¹, J. M. Susanthi Jayasinghe¹, V. N. Seneviratne¹, Sajith Vijayan², Davita. L. Watkins², H. M. N. P. Gunarathna¹, A. U. Malikaramage¹, W. H. M. R. N. K. Herath¹, Shane Wylie¹, P. G. P. R. Abewardana¹, V. M. Y. S. U. Bandara¹ and W. V. N. S. Bowaththa¹

¹ Department of Chemistry, Faculty of Science, University of Peradeniya, Sri Lanka

² Department of Chemistry and Biochemistry, University of Mississippi.

*Corresponding author: rmgr@pdn.ac.lk

D-A type polymers (Donor –Acceptor) are the third generation of the ECPs (Electronically Conducting Polymers) and used in optoelectronic devices and bio imaging techniques. Electropolymerization has become a convenient method for synthesizing and characterizing them and leads to synthesize stoichiometrically controlled block copolymers. Currently available D-A type ECPs utilize synthetic D and A materials although there are many naturally available materials that fulfil requirements as A or D units and it would open up horizon of a novel area of materials designed. This study extended to form acceptors isolated from natural products and chemically modified to attach suitable donor segments which is beneficial in bypassing tedious chemical synthesis strategies involving expensive and hazardous chemicals. Berberine (9,10-dimethoxy-5,6-dihydro-2H-7λ5- [1,3] dioxolo[4,5-g] isoquinolino[3,2-a] isoquinolin-7-ylum) which is an extendedly conjugated cation with an electron-rich methylenedioxy and methoxy donor (D) moieties and electron-deficient isoquinolium acceptor (A) moieties, was isolated from methanolic extract of the stem of *Coscinium fenestratum* and the structure

was confirmed by 1H-NMR spectroscopic data. Electro polymerization with ethylenedioxythiophene (EDOT) give novel D-A type polymers. In the investigated potential range irreversible peaks which are lower potential than the monomer was observed at +0.8 V and +1.7 V in the first scan. During successive scans, their height was found to increase through the next cycles. The morphological structure of the polymer confirmed that the structure of polymer is different than monomer structure. The advanced functional materials thus derived from natural products will be important as future optronic and photonic devices for myriad of applications in optical, electronic, bio-imaging, disease diagnosis and treatment technologies.

Keywords:

Berberine, *Coscinium fenestratum*, electro-polymerization, 3,4-Ethylenedioxythiophene, advanced functional materials