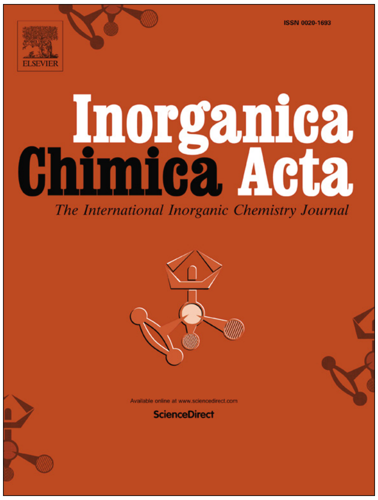

Research paper

Self-Assembly of Pt(II) based Nanoscalar Ionic Hexagons and Their Anticancer Potencies

Achintya Jana, Sourav Bhowmick, Santosh Kumar, Khushwant Singh, Pankaj Garg, Neeladri Das

PII: S0020-1693(18)31140-X
DOI: https://doi.org/10.1016/j.ica.2018.09.009
Reference: ICA 18467

To appear in: *Inorganica Chimica Acta*

Received Date: 23 July 2018
Revised Date: 4 September 2018
Accepted Date: 4 September 2018

Please cite this article as: A. Jana, S. Bhowmick, S. Kumar, K. Singh, P. Garg, N. Das, Self-Assembly of Pt(II) based Nanoscalar Ionic Hexagons and Their Anticancer Potencies, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.09.009

Self-Assembly of Pt(II) based Nanoscalar Ionic Hexagons and Their Anticancer Potencies

Achintya Jana, [a] Sourav Bhowmick,[a] Santosh Kumar,[b] Khushwant Singh,[a] Pankaj Garg,*[c]
Neeladri Das*[a]

[a]*Department of Chemistry, Indian Institute of Technology Patna, Patna 801106, Bihar, India*

[b]*Department of Organic and Nano System Engineering, Konkuk University, Seoul 05029, South Korea*

[c]*Department of Biosystems & Biomaterials Science and Engineering, Seoul National University, Seoul 151921, South Korea*

Abstract

Two nanoscalar and supramolecular metallacycles were self-assembled by employing a predesigned pyrazine based molecular "acceptor" clip with two different ditopic pyridyl "donor" tectons. The platina macrocycles were characterized by multinuclear NMR spectroscopy, mass spectrometry (ESI-MS), and elemental analyses. Molecular modelling using PM6 semiempirical molecular orbital method suggested these metallacycles having nanoscalar dimensions with hexagonal cavities. Additionally, interactions of these macrocycles were studied with three carcinoma cell lines. Results suggest that anticancer properties of supramolecular metallacycles were higher than their organometallic precursor. The nanoscalar supramolecular metallacycles were capable of efficiently reducing cell proliferation of different cancer lines (A549, HepG2, HeLa). The anticancer activity of the larger of the two macrocycles was higher even at lower concentrations and IC_{50} values are comparable with that of cisplatin. TUNEL assay suggested that macrocycles induces apoptotic cell death. These results suggest that the nanoscalar supramolecular metallacycles could find potential biomedical applications as therapeutic agents.

Keywords: Platinum; Self-assembly; Metallamacrocycles; cancer cells; Cytotoxicity; proliferation assay

1. Introduction

Supramolecular chemistry is an interdisciplinary research area that has been nurtured by organic, inorganic and physical chemistry. The origin of supramolecular chemistry started with design of covalent macrocycles bearing a central cavity that could bind guest species using non-covalent (*aka* supramolecular) interactions. Cyclic organic molecules explored for host-guest chemistry include but are not limited to calixarenes, crown ethers, cryptands, cyclophanes and others.[1] Guest(s) were trapped/ encapsulated using supramolecular interactions such as H-bonding, ion-dipole and others. Syntheses of these organic cyclic molecules (*aka* macrocycles) using conventional multi-step organic chemistry resulted in poor yields of the target molecules. In this context, coordination-driven self-assembly protocol was developed as a new strategy to yield macrocyclic compounds.[2] This protocol was developed by Stang,[3] Fujita[4] and others to construct metal containing supramolecules of various shapes and sizes ranging from two-dimensional (2-D) macrocyles to three-dimensional (3-D) frameworks such as prisms, boxes, cages and