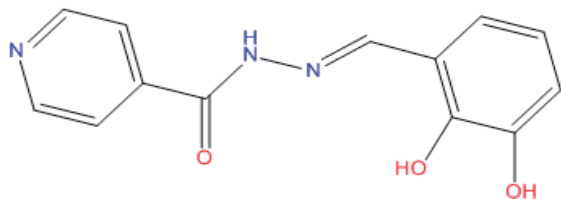


bases play an important role in inorganic chemistry as they easily form stable complexes with most transition metal ions. The development of the field of bioinorganic chemistry has increased the interest in Schiff base complexes, since it has been recognized that many of these complexes may serve as models for biologically important species [1], [2].



[1] S. Khlood, Abou-Melha, *Spectrochimica Acta A* **2008**, *70*, 162–170. [2] Z.H. Chohan, S.K. Sheazi, A. Synth. React. *Inorg. Met-Org. Chem.* **1999**, *29*, 105.

Keywords: single-crystal X-ray study, isonicotinic acid

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Preparation and Evaluation of Anti-inflammatory Potential of Some Sesquiterpene lactones: X-ray Structure of Psilostachyin

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The natural sesquiterpene lactones (SLs) have displayed a diverse range of bioactivities from antiinflammatory to antibacterial, ameobicidal to anticancer, therefore, they constitute interesting targets for further investigations in the area of drug development. The spiro lactone psilostachyin (**1**) and acetylated pseudoguaianolides (**2**, **3**) are the SLs isolated from *Ambrosia psilostachya* and *Parthenium hysterophorus* respectively (Fig.1).

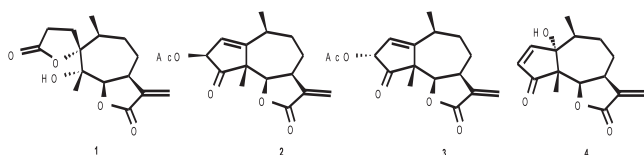


Fig.1 Naturally occurring sesquiterpene lactones

In continuity to our research programme of isolation and structural modifications of natural products to develop bioactive lead molecules particularly in the area of inflammation and cancer, we report the semi-synthesis of naturally occurring acetylated pseudoguaianolides (**2** and **3**) and spiro lactone psilostachyin (**1**) including their analogues from the major pseudoguaianolide parthenin from *Parthenium hysterophorus* for the evaluation of their anti-inflammatory potential estimated through *in vitro* expression of TNF- α , IL-1 β and IL-6 in murine neutrophils. The structure of semi-synthetic psilostachyin was also confirmed by X-ray crystallography.

Keywords: sesquiterpenes lactones, Parthenin, crystal structure

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Crystal structures of novel CB[6] complexes with *p*-Xylylenediammine derivatives

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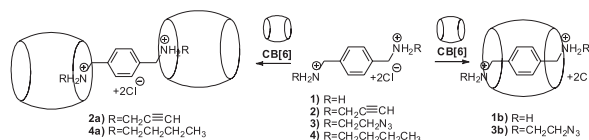
The ability of cucurbit[6]uril, **CB[6]**, to form host-guest complex with diammonium salts, in particular with linear aliphatic diammonium salts, has been widely used for the construction of pseudorotaxanes and rotaxanes that exhibited interesting dynamic, structural and functional properties. By contrast, the ability of **CB[6]** to host aromatic compounds has been less obvious. It has been shown that **CB[6]** and the dihydrochloride salt of bis-1,4-(allylaminomethyl)benzene, form only [3] pseudorotaxane. This mode of binding with two molecules of **CB[6]** hosting the allylic side chains of the guest was led to the interpretation that the aromatic moiety is too big to be encapsulated in the cavity of **CB[6]**. [1] However, it has already been reported that **CB[6]** and *p*-xylylenediammonium salt, **1**, form a stable inclusion complex, **1b**. [2] Furthermore, 4-aminobipyridine, and 4-(2-pyridyl)aniline, form strong, 1:1 inclusion complexes with **CB[6]**, whereas the bifunctional analog forms strong 1:2 complex with **CB[6]**, exhibiting remarkably large enhancements of fluorescence intensity and quantum yields. [3] These led us to speculate that the encapsulation of aromatic guest molecules, within the inner cavity of **CB[6]** can be thermodynamically favored but their formation may involve unexpectedly high kinetic barriers.

Novel pseudorotaxane compounds based on **CB[6]** and *p*-xylylenediammonium salts derivatives, **1**, **3-4**, were obtained by crystallization from aqueous solutions that contain a mixture of each diammonium guest and **CB[6]** at room temperature. The X-ray diffraction analysis of their complexes, **1b**, **3b** and **4a** was also supported by ¹H NMR in solution. The 1:2 complex of guest **2**, namely **2a**, was evident by NMR, but suitable for X-ray analysis single crystal were not be able to obtain. Nevertheless, upon heating and crystallization, the 1:1 complex, **2b**, was obtained.

Further support for these two different binding modes was obtained from ITC measurements at room temperature.

Each 1:1 complex exhibits two types of hydrogen bonding between the portal oxygen atoms and the guest. The more obvious bonds are formed with the ammonium hydrogen atoms (NH...O=C, 1.980(3)–2.420(3)Å), The less obvious, but quite visible from the solid state structure, are the hydrogen bonding between the carbonyl oxygens of **CB[6]** and the benzylic methylene hydrogens of the guest: CH...O=C, 2.317(3)–2.508(2) Å. Complex **4a** exhibited two distinguished hydrogen bond interactions: one corresponds to donor water molecule that is bridged by carbonyl oxygen of each cucurbituril unit (C=O(10)..O_w..(6A)O=C, 2.84-- 2.97Å); second, where two water molecules formed a string bridge between the two cucurbituril units. These strong interactions (C=O(8)..O_w..(O4A)O=C, 2.73-2.88Å) could explain the asymmetry observed in the structure of **4a** where the **CB** units are obviously attracted to one another, creating an angle of 42.56° between them.

Our results show that 2:1 host-guest complexes, **2a** and **4a**, are kinetic products, which may be converted to the thermodynamic products upon prolonged heating.



[1] S.Y. Kim, J.W. Lee, S.C. Han, K. Kim, *Bull. Korean Chem. Soc.* **2005**, *26*,