

some volunteers. With longer echo times we obtained the following results: water (78,988/882,987), NAA (178,786/219,219), Cho (397,148/314,465), Cr in 3.03ppm (212.547/168,634) and Cr in 3.92ppm (356,235/341,296) for right hippocampus and for left hippocampus: water (81,71/84,889), NAA (154,987/210,52), Cho (373,93/353,35), Cr in 3.03ppm (113,795/165,837) and Cr in 3.92ppm (104,193/112,994) were closer of those on publications. Using short echo times that would make practical the study of metabolites with fast relaxation could have affected results in a way to cause a false impression of being shorter than they really are. Therefore calculation of T2 seems to be possible with this method and comparisons between hippocampus can be done considering the normal standard deviations.

[13/05/09 - P093]

Morphology classification of calcium oxalate monohydrate kidney calculi, EVANDRO G. BETINI, LETICIA KUPLICH, DANILO O. DE SOUZA, CINTIA G. P. ORLANDO, HUMBERTO BELICH, JANAINA B. DEPIANTI, EDNA F. MEDEIROS, MARCOS T. D. ORLANDO, (*UFES*), LUIS G. MARTINEZ, (*IPEN*), HAMILTON P. S. CORREA, (*UFMS*) ■ The composition of several kidney stones was studied by X-ray powder diffraction. Schematically kidney morphology classification is proposed to calcium oxalate monohydrate calculi $CaC_2O_4H_2O$ or COM: (I) COM papillary calculi, and (II) non-papillary COM calculi.

The first group (I) is associated to COM renal stones which appear attached to papillae. This type I (COM papillary calculi) presents a conical morphology and is formed by a core, or stone nucleus, situated in the urolith interior and a shell in its outer part grown out from the core. It was indicated the existence of four different types of papillary calculi core upon which the crystal growth occurs. Furthermore, the same authors have remarked that the fixation process of the nucleus on the papilla has been overlooked in previous works.

A second group (II), non-papillary COM calculi, presents typically ellipsoidal morphology, which is clearly different from the papillary calculi (type I). It grows in renal closed cavities and can be broadly classified into two main groups: (II-a) and (II-b). The II-a type renal calculi contain no core and their inner structures resembles the random patterns exhibited by sedimentary rocks. In this type of kidney stones the material is irregularly distributed on the inner part and may, occasionally, contain small spheres of hydroxyapatite. On another hand, the II-b calculi contain a core that is constituted mainly by organic matter that functions as a seed for the development of the stone body.

Most of the bodies of this type of stone are constituted by columnar COM crystals emerging from the core and, because of the absence of an attachment to the epithelium, they are found in renal cavities. Moreover, some authors has pointed out that these stones can be initiated by a small papillary stone accidentally detached from the papilla and trapped in the kidney cavities.

[13/05/09 - P094]

Structure-activity relationship of calcium channel blockers of type L,

FABIANA APARECIDA DE SOUZA BATISTA, MARIZA GRASSI, ANA CLAUDIA MONTEIRO CARVALHO, *UNIFEI - MG - Brasil* ■ Calcium Channel Blockers (CCB) represents a successful group of therapeutic agents directed against cardiovascular targets, including hypertension and angina. All these drugs act as antagonists of calcium channels that are responsible for cardiac and vascular smooth muscles activation. However, economical reasons lead the industry make efforts for more efficient drug development.

Theoretically, several SAR techniques have been used to propose new drugs [1-6].

The goal of the present work is the theoretical study of the structure-activity relationship of CCB used on cardiovascular diseases treatment. Electronic Indices Methodology (EIM) [7] was used in a systematic investigation of a series of molecules proposed in the literature [8]. We intend to establish a correlation between the biological activity of these molecules and their molecular structure and electronic properties.

Theoretical calculations using techniques based on semi-empirical methods (AM1), and Density Functional Theory (DFT) - BLYP and B3LYP in 6-31G basis - was made to obtain the molecular geometry and energy of formation.

Our preliminary results indicated some relationship between electronic indexes and the biological activity in the class of compounds studied. The analysis of the calculated electrostatic fields made possible the determination of the region of interest for the application of the EIM.

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[13/05/09 - P095]

A model of the homeopathic drug functioning, JOÃO DA COSTA CHAVES JUNIOR, FÁBIO GAVA AOKI, *UNESP* ■ A simple model of a cellular automata (CA) for the immune response that afford a scenery that permit some interesting conjectures about the general mechanisms of the "pharmacodynamics" underlying the action of homeopathic drugs was developed. Our model is an extension of the KUT model, named KUT revisited model. It shows several properties that mimetizes the actual immune response such as: amplification of the second dose of the immune response, high dose and low dose paralysis, and, if it shows a humoral response, the cellular response is attenuated or conversely. Both the high and low dose paralysis is