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The present work shows a structural study on the process of incorporation of a hydrophobic drug, Ellipticine (ELPT), into lipid model membranes for drug targeting purpose. The ELPT is an alkaloid that showed an anti proliferation activity against several types of tumour cells and against the HIV1 virus. In the context of drug targeting, there are several important processes and parameters to be studied. For instance, the drug loading efficiency into the lipid matrix, the order into the lipid system that encapsulates the drug, the lipid-carrier critical size and stability to transport the drug and the releasing mechanisms. We used the zwitterionic lipid dipalmitoylphosphatidylcholine (DPPC) and some other phopholipids with different size of head and tail and/or different net electronic charge both on a Langmuir monolayer and deposited on a solid substrate. First results appointed toward a strong increase in drug loading efficiency into DPPC lipid systems mixed with charged lipids. However, this increasing in loading efficiency was accompanied by a disturbance in the ordering of the bilayers. To characterize these systems we used Grazing Incidence X Ray Diffraction and also specular X Ray Reflectivity technique with synchrotron radiation at Troika II beamline-ESRF, France and also a rotating anode set-up at State University of Campinas, Brazil to monitor structural changes of loaded and non-loaded lipid systems.

Keywords: lipid mesophases, drug interaction, diffraction

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Crystal Structure of Chocolate from Powder Diffraction Data

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We solved the crystal structure of the β(V)-form of chocolate and cocoa butter (CB). Chocolate is a made from cocoa and sugar in a complicated process. At room temperature it consists of a well-crystallised continuous CB matrix in which fine cocoa powder and sugar particles are dispersed. In good quality consumer chocolate, the CB is crystallised in one of the two highest melting forms, β(V) or β(VI). Poor storage or improper production may result in fat bloom, the whitish layer on chocolate that is commonly associated with the phase transition from β(V) to β(VI). Any CB consists for 75% of three triacylglycerols, SOS (1,3-distearoyl-2-oleoylglycerol), POS (2-O-1-palmitoyl-3-S-glycerol) and POP. In particular SOS is known to play a major role in the β-crystallisation of CB.

The powder patterns of chocolate, CB and SOS are very similar suggesting a close structural relation. Unit cells were obtained with an indexing routine written specially for this purpose by RP. The cells of β(V)-CB and β_2-SOS are very similar and, surprisingly, so are the indexing figures of merit M_{20}. We solved SOS (63 unique non-H atoms), using the programs FOX and ORGANA. After refinement we used this structure as a starting model to solve and refine the structure of β(V)-CB, employing partial occupancies (57%) for the two end-carbon atoms of both stearin chains. Our results show a considerably different packing as postulated earlier. Moreover the crystal structure gives rise to the explanation of the mechanism of the β(V) to β(VI) phase transition of CB. This is supported by the XRD of β-POS.

Keywords: SDPD, chocolate, structure of cocoa butter

P.06.03.1

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X-ray Analysis as the Important Tool in Controlling Stereoselective Synthesis of Drugs

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Alkaloids form a group of natural heterocyclic compounds exhibiting valuable pharmacological properties: from painkilling and antihypertensive, through antidepressant and antipsychotic to anticancer. Some of them have dangerous narcotic, hallucinogenic and paralysing action. The bioactivity of compound, in great degree, depends on its stereochemical constitution and hence much effort has been made to develop new, bio mimetic methods of stereoselective synthesis of alkaloids and other heterocyclic compounds. Although the results of chemical synthesis are usually widely documented by many physicochemical methods, the final proof for stereochemistry is possible only after crystal structure determination. Here we propose a new method of synthesis using natural amino acids as building blocks which define three-dimensional structures of products. The case of 16 isoquinoline and β-carboline alkaloids and the application of X-ray methods to determine stereochemistry of products serve as an example. Quantum chemical calculations suggest thermodynamically controlled reaction.

Keywords: alkaloids, structure, modelling

P.06.03.2

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Structures of Cocrystals of Peganole with 6-Brompeganole

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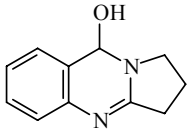
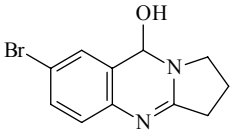
The crystal structures of two polymorphic cocrystals (I, II) of peganole (1) with 6-brompeganole (**2**) have been determined. Both forms are in the monoclinic system with space group of P2(1)/n. Cell parameters of I are a=8.232(4), b=11.768(8), c=10.156(6)Å, β=98.12(4)°, V=974.0(10) Å^3 and II are a=7.995(6) , b=15.501(8), c=8.816(6), β=112.25(5)°, V=1011.2(11) Å^3.

It is interesting to note that asymmetric unit of cell in both case consist of one molecule where this molecule at the same time can be **1** or **2**. Site occupation factors of molecules **1** and **2** are ~0.7 and ~0.3 (in I) and ~0.3 and ~0.7 (in II) respectively.

As well, tests on composition of single crystals by High-Performance Thin-Layer Chromatography (CAMAG, Switzerland) confirms the X-ray results.



1



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Keywords: cocrystals, polymorphs, small-molecule single crystals

P.06.04.1

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Crystal Structures of Fluorescent Bisazomethine Pigments

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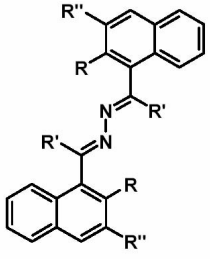
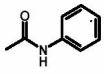
Pigment Yellow 101 (**1**) is a well-known greenish-yellow fluorescent organic pigment. The compounds **1-5** were synthesized and crystallized from DMSO, xylene and CH_3OH/C_2H_5OH mixtures



Compound	1 P.Y.101	2	3	4	5
R	OH	OCH_3	OH	H	OH
R'	H	H	CH_3	H	H
R''	H	H	H	H	
Solid state fluorescence	yes	no	yes	no	yes