hydrogen bonds system (intra- and intermolecular ones) and crystal packing are also discussed. The crystal packing are stabilized by π-π-interactions between benzene rings and/or triazole heterocycles. The packing coefficient and solvent accessible potential area in crystal were also analyzed.
Keywords: triazoles, X-ray structure, tautomerism

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An Investigation of Interactions in Barakol Complexes
Pitiporn Chimsook[a], Nattaya Ngamrojnavanich[a], Chaiyo Chaichantipyuth[b], Narongsak Chaichit[c], Palangpon Kongsaeree[d], Surachai Pornpakakul[a], Amorn Petsom[a], Nongnuj Muangsin[a], *[a]Dept. of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand. [b]Dept. of Pharmacognosy, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok 10330, Thailand. [c]Dept. of Physics, Faculty of Science and Technology, Thammasart University, Bangkok 12121, Thailand. [d]Dept. of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.* E-mail: Pitiporn.C@student. chula.ac.th

Barakol has various interactions that contribute to its biological activities. This work presents the first successful crystal structure determination of anhydrobarakol and its analogues. Anhydrobarakol and anhydrobarakol hydrochloride were crystallized in a monoclinic system, space group $P2_1/c$ and $P2_1/n$, $Z = 4$ with unit cell parameters a = 13.2280(7), b= 6.8738(2) , c = 19.7879(9) Å, β = 127.013(2)° and a = 12.2547(2), b = 8.051(2) , c = 12.8133(2) Å, β = 99.514(1)°, respectively. The novel 1:1 molecular complexes of barakol and carboxylic acid (phthalic acid and 3-hydroxybenzoic acid) were synthesized and charactherized by spectroscopic and X-ray crystallographic techniques. Electrostatic effects, electron delocalization, and intermolecular interactions in the barakol ring system were investigated. The X-ray crystallographic studies revealed that the barakol-phthalate complex exists in an ion-pair complex. The formation of barakol-phthalate ion-pair complex is stabilized by the complementary of ion-ion interaction,π-π interaction and hydrogen bonding. The barakol-3-hydroxybenzoic acid complex is a π-π molecular complex. The co-crystallization of barakol- 3-hydroxybenzoic acid complex is solely stabilized by π-π interactions. The spectroscopic studies including IR, ^{1}H-NMR and UV-visible are consistent with the results from the X-ray analysis.
Keywords: barakol, X-ray diffraction, spectroscopic method

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Amino Acids at High Pressure
Patricia Lozano-Casal, D. R. Allan, S. Parsons, C. Morrison, *School of Chemistry, University of Edinburgh King's Buildings, West Mains Road, EH9 3JJ, Edinburgh, Scotland, United Kingdom.* E-mail: P.Lozano-Casal@ed.ac.uk

The use of pressure to perform structural studies has been of important use to many areas of research, from Physics to Geochemistry. However, pressure studies have become a new notable tool in Chemistry and Biology to study the structure of small compounds. The main reason for this is the necessity of a better understanding of different processes, which happen even at extreme conditions of pressure, such as the existence of life in the deep ocean. Thus, small molecules may play important roles in these biological processes and therefore, a good knowledge of their structural features could be essential to explain how they happen.

In this work we are exploring the behaviour of amino acids structures at high pressure. Changes in pressure have been known to induce conformational changes in small molecules. We are trying to extend this research to the larger amino acids.

We have been working, principally, with L-glutamine, L-asparagine monohydrate, L- glutamic acid and L-aspartic acid. It was found that by applying pressure the cell parameters were reduced but no structural rearrangement was found up to pressures of 50-60 kbar. *Ab initio* computational studies were then performed to establish a possible relationship between the energetics of the hydrogen bonding with their compressibility.
Keywords: high-pressure crystallography, amino acids, *ab initio* calculations

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Structural Studies on ST1481, Gimatecan, a 7-substituted Camptothecin with Anti-tumor Activity
Miriam Rossi[a], Christine Phillips[a], Genevieve Lidoff[a], Francesco Caruso[b], Franco Zunino[c], *[a]Department of Chemistry, Vassar College, Poughkeepsie, NY 12604-0484, USA. [b]ICB-CNR, Ple. Aldo Moro 5, Roma, Italy. [c]Istituto Nazionale Tumori, Via Venezian 1, Milano, Italy.* E-mail: rossi@vassar.edu

Camptothecins are a class of of active antitumor agents that target the nuclear enzyme DNA topoisomerase I, inhibiting single strand religation. Several camptothecin derivatives are in clinical trials [1]. The substitution of position 7 by lipophilic side chains seems to be important as it increases cytotoxic potency, helps in the drug delivery and in stabilizing the DNA-topoisomerase I cleavable complex that forms in ST1481 presence and is is as part of its mechanism of action. Of 44 compounds synthesized [1] the most potent derivative contains a $CH{=}NOC(CH_3)_3$ substituent and its X-ray crystal structure has been determined. The unit cell parameters are space group: $\boldsymbol{P2_1}$, a = 12.131(8)Å, b = 6.712(5)Å, c = 13.817(8)Å, β = 96.05(3). This derivative (gimatecan) is orally administered, and thus, represents a significant advantage compared to other camptothecins. *Ab initio* studies have been performed using Density Functional Theory to analyze the lactone ring opening, a critical step in the interaction with topoisomerase I.

[1] Dallavalle S., Ferrari A., Biasotti B., Merlini L., Penco S., Gallo G., Marzi M., Tinti M. O., Martinelli R., Pisano C., Carminati P., Carenini N., Beretta G., Perego P., De Cesare M., Pratesi G., Zunino F., *J. Med. Chem.*, 2001, **44**, 3264.
Keywords: camptothecin, anti-tumor, topoisomerase I inhibitor

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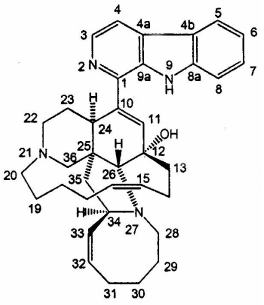
Hydrogen Bonding and Absolute Configuration in Manzamine Alkaloids
Frank R. Fronczek[a], M. Donia[b], M. Reddy[b], K. V. Rao[b], J. Peng[b], M. T. Hamann[b], *[a]Dept. of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA. [b]Dept. of Pharmacognosy and NCNPR, The University of Mississippi, University, MS 38677, USA.* E-mail: ffroncz@lsu.edu

The manzamines, a class of sponge-derived alkaloids, have a complex polycyclic system with 5, 6, 8, and 13-membered rings and a β-carboline substituent. They show promising antibacterial, antitumor, and antimalarial activities, and moderate activity against HIV-1. Manzamine A (**1**) forms solvates with MeOH and acetone. Formation of the hydrochloride of 8-OH manzamine A (**2**) by N27 protonation allows absolute configuration determination. The Cl^- accepts hydrogen bonds from all four donors of one cation. Manzamine F (**3**) also has an 8-OH group and C31=O rather than C32=C33, and forms a mixed solvate with H_2O and MeCN. Ircinol A (**4**) lacks the β-carboline group, but has CH_2OH at C10, and crystallizes with Z'=3.



Keywords: marine natural products, absolute structure, hydrogen bonding

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The Structure of Protocyanin, a Complex Pigment from Blue Cornflower
Masaaki Shiono[a], Naohiro Matsugaki[b], Kosaku Takeda[c], *[a]Department of Physics, Kyushu University, Fukuoka, Japan. [b]Photon Factory,*