Viva Biotech, headquartered in the pharma-valley of Shanghai, China, is a premium preclinical drug discovery service provider to pharmaceutical and biotech companies worldwide. Viva is privately owned and financed by a leading US private equity fund. It currently employs 200 scientists working in a state-of-the-art research center spanning 65,000 square feet. The research center includes cell culture/biochemistry/crystallography laboratories, medicinal chemistry/bioanalytical laboratories, and animal facilities.

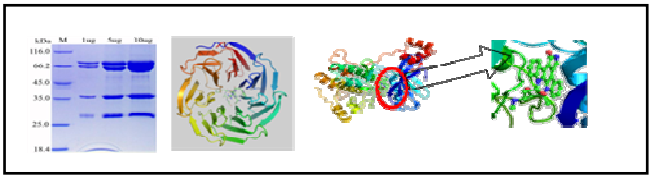
Viva is one of the very few CROs that integrate those technologies with X-RAY, MS, NMR and SPR platform, thereby providing a full line of drug discovery services to pharmaceutical and biotech companies. With this integrated technology platform, Viva's scientists team has involved in the preparation of several hundreds of drug targets and determined several hundreds of crystal structures every year to most of big pharmaceutical companies as well as dozens of biotech companies.

Viva has taken the protein and structure services to a new height by successfully providing GPCR protein crystallography to clients.

Building on the success of the aforementioned gene-to-protein and gene-to-structure services, Viva has expanded services to the structure-based drug discovery with strong in-house capabilities in medicinal chemistry and computational chemistry. With the addition of antibody research, bioanalytical and in vivo pharmacology platforms, Viva is well positioned to provide an integrated drug discovery service capable of executing from hit generation to lead optimization programs for clients.

In summary, Viva has expertise and large technical base in each of the following areas:

1. Gene-2-structure and gene-2-protein with preparation of several thousands of proteins and several hundreds of crystal structures each year, and with world class expertise in GPCR protein crystallography.
2. Structure-based drug discovery (hit generation to lead optimization)
3. Unmatched experience and expertise in biophysics techniques including: X-ray, NMR, MS, and SPR
4. High-level medicinal chemistry
5. Fragment-based drug discovery preclinic structure-based drug discovery (hit generation to lead optimization)
6. Antibody research platform with phage display library
7. In vivo disease models in CNS, oncology and inflammation



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Acta Cryst. (2011) A**67,** C822

The molecular weight of proteins from a single SAXS measurement on a relative scale

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An important step in the characterization of proteins is the determination of their molecular weights and their multimeric state in solution. Accuracies of classical methodologies for the determination of the molecular weight of proteins in dilute solution were recently evaluated by Mylonas & Svergun [1]. These authors demostrate that the molecular weight of a protein can be obtained by comparing the experimental SAXS curve produced by the protein in dilute solution *(i)* to another experimental SAXS curve corresponding to a standard protein with known molecular weight, or *(ii)* to a SAXS curve corresponding to pure water leading in this case to the determination of SAXS intensity of the studied protein in an absolute scale. Both of these procedures require the determination of at least two SAXS curves. In addition, the first procedure requires the precise knowledge of the protein concentration, which is frequently not known with high accuracy, and the second method needs the determination of the SAXS intensity by water with a considerable precision, which implies in rather long counting times. Both methodologies yield the molecular weight of proteins with an error of about 10% provided the solute concentration is measured with an accuracy of 5 – 10 %, which might not always be straightforward. A novel procedure for the determination of the molecular weight of proteins in diluted solution from a single SAXS curve measured on a relative scale is avaiable, which uses experimental data of a single small angle X-ray scattering (SAXS) curve measured on a relative scale [2]. This procedure does not require the measurement of SAXS intensity on an absolute scale and does not involve a comparison with another SAXS curve determined from a known standard protein. The proposed procedure can be applied to monodisperse systems of proteins in dilute solution, either in monomeric or multimeric state, and it was successfully tested by applying it to SAXS data measured for 22 proteins with known molecular weights. The molecular weights determined by using this novel method of all the measured set deviate from their known values by less than 10 % and the average discrepancy was 5.6 %. Importantly, this method allows for a simple and unambiguous determination of the multimeric state of proteins with known monomeric molecular weight.

Work supported by FAPESP and LNLS, Brazil.

[1] E. Mylonas and D. I. Svergun *J. Appl. Cryst*. **2007,** 40, 245–249. [2] H. Fischer, M. Oliveira Neto,H.B. Napolitano,I. Polikarpov and A.F. Craievich *J. Appl. Cryst*. **2010**, 43, 101-109.

Keywords: SAXS, Protein, Molecular weight

L.A.35

Acta Cryst. (2011) A**67,** C822-823

Parallel alignment interactions of water and aryl rings at large displacements

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Water plays an essential role in nature. Its geometry, small size, and high polarity govern its capabilities and the complexity of its behavior. Most important is its ability to form strong hydrogen bonds with polar molecules and builds strong networks with itself. In addition to these strong intermolecular interactions, water molecules also have important weaker interactions with less polar molecule. The water–benzene complex has been the subject of extensive investigation.

Recently, we recognized the parallel alignment interactions of water and aromatic rings [1]. These important new geometric features were discovered by examining crystal structures from the Cambridge Structural Database (CSD) and analyzed by ab initio calculations of the water–benzene dimer including coupled cluster electron correlation treatment (CCSD(T)) and complete basis set extrapolation.

Analysis of crystal structures from the Cambridge Structural Database (CSD) revealed the existence of orientation where the whole water molecule (A set) or one of its O–H bonds (B set) is

parallel to the aromatic ring plane. Attractive interaction energies, obtained from ab initio calculations, are significant and consistent with the observed crystal structures. The most stable parallel alignment interactions are not above C-H region of the aromatic ring, but for larger offset distances.

The most stable model system of all those considered has one O–H bond parallel to benzene ring at horizontal displacement of 2.6 Å (B set), $\Delta E_{CCSD(T)(limit)}$= -2.45 kcal/mol. These interactions are somewhat weaker than O-H···π (-3.19 kcal/mol) but quite stronger than C-H···O interactions (-1.41 kcal/mol). The calculated energies of the parallel alignment interactions are comparable with the energy for the slipped-parallel benzene-benzene dimmer ($\Delta E_{CCSD(T)(limit)}$= -2.45 kcal/mol).

[1] G. V. Janjić, D. Ž. Veljković, S.D. Zarić, *Crystal Growth & Design*, 2010, submitted.

Keywords: Water/aromatic interactions, Crystal structures, Ab initio calculations.

L.A.36

Acta Cryst. (2011) A**67,** C823

A Copper(II) Complex with Neutral Carboxylic Acid Ligand

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A large number of dimeric copper(II) carboxylate adducts, $[Cu(RCOO)_2 \cdot L]_2$, were studied and characterized the structure being copper(II) acetate type by many groups.[1] When $Cu(OH)_2$ (0.99 g, 10 mmol) were added to ethanol solution (20 ml) of pivalic acid (Hpiv: 2,2-dimethylpropnoic acid) (3.27 g, 32 mmol) and kept for a week in a refrigerator, deep green crystals were grown from the solution, in which the axial position of square-pyramidal cooridination geometry around the Cu is occupied by an O atom at C=O of the neutral pivalic acid molecule. Thus the formula is $[Cu(piv)_2 \cdot Hpiv]_2$. The O-H group of the pivalic acid molecule forms an intramolecular H-bond (O...O distance of 2.692(5) Å).

X-ray structure determination showed that the crystal exhibits disorder in the position of tertial butyl group at one of the bridging ligands at ambient temperature. However, at 123K, all the carbon atoms can fixed at suitable positions.

Crystal data . $[Cu_2(C_5H_9O_2)_4(C_5H_{10}O_2)_2]$, Mr = 735.86

For 296K: monoclinic, $P2_1/c$, a = 9.505(5), b = 17.965(12), c = 11.642(8) Å, β = 99.42(2)°, V = 1961.2(21) $Å^3$, Z = 2, D_x = 1.246 Mg m^{-3}.

For 123K: monoclinic, $P2_1/c$, a = 9.561(5), b = 17.514(11), c = 11.323(6) Å, β =99.739(19)°, V = 1868.7(18) $Å^3$, Z = 2, D_x = 1.308 Mg m^{-3}.

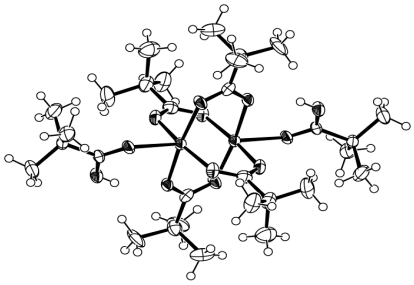

Fig. 1. Molecular structure of $[Cu_2(\mu\text{-piv})_4(Hpiv)_2]$ at 123 K.

[1] For exapmle, Y. Kani, M. Tsuchimoto, S. Ohba, H. Matsushima, & T. Tokii. (2000), *Acta Cryst*. C56, 923-925.

Keywords: copper(II)_carboxylate**,** intramolecular_H-bond