Thus when an averaging is considered, from the point of view of Molecular Modeling in Biological Systems, Quantum Chemical Calculations of optimized structures and the Chemical shift values are to be included.

It was possible to obtain **KARPLUS EQUATION** for the Dihedral dependence of the coupling constants. Hence whenever there is a motion involving such dihedral angle variations the averaging can be carried out more confidently and quickly. There does not seem to be such simple equations obtainable in general for the variation of chemical shifts with structure parameters. Each and every case has to be calculated out and considered for averaging appropriately to compare with **EXPERIMIENTAL SPECTRA**.

In order to consider the actualities at the level of details of structural variations, it was thought better to go through some exercises with calculations on certain typical dynamical events, so as to enable an appreciation of these procedures and to illustrate them in an elementary level for the beginners to pick and choose examples from actual situations they are expected to encounter.

Thus these are preliminary exercises in Computational Chemistry related to Biological contexts. Even though no detailed effort is made at this stage to critically consider the various theoretical methods, basis set variations, and appropriate options indications are provided as to the way one should be aware of the advantages or otherwise of the theoretical frame works used.

The structure of Biological molecules in solution (usually aqueous medium) depends on the interaction of the various regions of the macromolecule with the water molecules in the immediate neighborhood. Thus in this presentation a theoretical study of how the Zwitterion equilibrium of alpha amino acids get influenced by the immediately surrounding water molecules. It is thus necessary to know how the few water molecules in the vicinity get arranged favourably to interact specifically with the molecule of interest. It is in this perspective that the next two sheets display the water clusters optimized by quantum mechanical calculations indicate about the water clusters and whether any distinct NMR features can be discerned from the chemical shift calculation on these optimized cluster of water molecules. These adequately reveal the extent of complexities which will have to be addressed to by looking into the highest level of detail about the medium effects.

At this stage it is to be reiterated that there was no exhaustive efforts to increase the sophistication of the methods of calculation but rather only an approach is indicated with the quicker and faster methods available. All the calculations reported in this presentation have been obtained using the online computational machine as available at http://www.webmo.net .
The working demo of this website enables calculation of one minute duration and even with such a constraint significant results could be obtained.

The calculation of Chemical shift of carbon nuclei in standard reference compound T.M.S. and the carbon analogue T.M.M. the tetra methyl methane indicate the variations due to the quantum chemical methods in the calculated chemical shift values.