Abstract: Three different projects were carried out in this thesis, which contain, as a primary theme, the application of quantum chemical methods to biochemical problems and the collaboration between theory and experiment. The first investigation focused on the toxicity of ozone and was performed in collaboration with experiment. The abstraction of H atoms from organic substrates by ozone was found to lead in solution to the formation of the HOOO anion, which initiates a radical reaction by decomposition into the OH anion and singlet $O_2(^1\Delta)$. This project exemplified the need for the consideration of environmental effects such as solvation (specific and non-specific). - The second project focused on the development of the J-**OC**-PSP2 method to analyze measured and calculated NMR spin-spin coupling constants (SSCC) in terms of Ramsey densities and orbital contributions. The orbitals contribute to the SSCC in an active or passive manner representing specific electronic interactions: (1) Ramsey distortion; (2) steric exchange interaction; (3) echo effect; (4) spin transport. Interactions (1) and (2) are primarily associated with active orbitals and dominate short-range spin-spin coupling whereas (3) and (4) result from passive orbital contributions, which play an important role for long-range coupling. For example, long-range spin-spin coupling in polyenes is exclusively transported by the passive contributions of the π-orbitals. - By applying J-**OC**-PSP2 it could also be demonstrated that through-space coupling always involves steric exchange interactions between two orbitals and that it can occur both inter- and intramolecularly, where in the latter case we distinguish between a framework (mediated by orbital back lobes) and a non-framework mechanism. The coupling mechanism across a typical H-bond (N-H$\cdots$O=C) in the protein ubiquitin was investigated and the covalent nature of the H-bond could be described by the dependence of coupling on either interactions (1) or (2). - The NMR-DFT-SSCC method was outlined, which as a hybrid method combines NMR measurements and SSCC calculations to determine electronic structure, geometry, and conformation of molecules. - In the third project, a new strategy for the deisgn of a potent, non-toxic antitumor drug was successfully implemented. The strategy is concerned with decreasing the toxicity of the naturally occurring enediynes. By appropriate substitution of the head group, a double bond, present in natural enediynes is removed, and renders the molecule inactive. At the pH of tumor cells, protonation of the headgroup results in the reformation of the double bond and the biological activity of the drug. The importance of the appropriate triggering and docking of the drug to the receptor was demonstrated. In this connection, the use of models in a self consistent rather than *ad hoc* fashion was stressed. The importance of global shape parameters reflecting the handedness of a ligand when binding to a receptor was illustrated. The biological activity of the drug was found to depend highly on the modulation of strain effects transported by conformational changes.