We studied the structure and dynamics of several very different chemical systems in which the association of molecules with hydrogen bonds plays an important role in their properties. We used a combination of experimental and theoretical research approaches in conjunction with the X-ray scattering method and molecular dynamics simulations. The structure was studied in terms of molecular conformations, preferred orientation and spatial organization of molecules, and their association to clusters at the supramolecular level. Using the theoretical *complemented system approach*, the results of the molecular dynamics simulations were used to calculate the scattering intensities of the modelled systems, which were then compared with the experimental X-ray scattering data. In this way, the simulations provided us with a direct insight into the structure and dynamics of the model systems, as the laboratory experiment served as a criterion for assessing the correctness of the model used. The system's dynamics was studied in terms of the molecular self diffusion coefficients and the lifetime of the different types of hydrogen bonds in the system. Similarly, the rheological properties or viscosity trends were investigated using the results of the nonequilibrium molecular dynamics simulations and the experimental literature data. Our studies of various chemical systems began with a study of a relatively simple pure liquid *n*-butanol, continued with two studies of the more complex 1,4-butanediol, and a study of a homologous series of terminal diols from ethylene glycol to 1,5-pentanediol. This was followed by a study of a rather complex binary aqueous mixture of hydrotropic tert-butanol over the entire concentration range with very versatile structural and dynamic behaviour and structural segments on the order of a few nanometres. Finally, a study of macromolecular systems with the non-ionic surfactant Brij 35 in organic and aqueous-organic media was also successfully completed. The results demonstrate that the methodology used provides a comprehensive insight into the relationships between the structure and the rheological-dynamic properties of fluid systems at intra-, inter- and supramolecular levels of detail, even for quite complex chemical systems with large structural segments and even macromolecules.