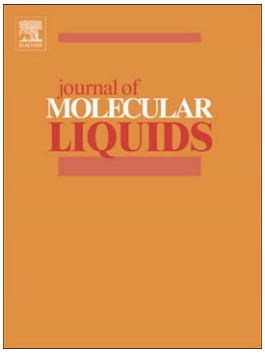


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# Molecular Dynamics Simulation Studies of Dopamine Aqueous Solution

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**Abstract**

The structure, transport properties and hydrogen bond dynamics of aqueous dopamine solution were calculated via molecular dynamics simulations. The impact of ascorbic acid and uric acid on the structure of water was also investigated. With increasing the concentration of dopamine, the coordination number, tetrahedral order parameter and self-diffusion coefficient decreasing. The coordination number obtained by our simulation is in agreement with the available experimental data. A hydration shell of dopamine and shorter H-bond lifetimes with respect to the water-water system is observed.

**Keywords：** Aqueous dopamine solution; Tetrahedral structure; Hydrogen bond dynamics; Molecular dynamics simulations

## 1. Introduction

Dopamine (DA) is one of the most important catecholamine neurotransmitters which plays a vital role in the function of central nervous, cardiovascular, renal and hormonal systems [1-3]. Due to DA contacts the nervous system, its deficiency in biological fluids may lead to neurological disorders such as Parkinsonism [4-6]. DA also exhibits a number of significant conformations which provided an opportunity to study the conformational properties of the flexible molecule [7]. Both experiments and theoretical calculations have been performed to analyze the conformational forms of neutral, protonated and deprotonated dopamine at different pH [8-12]. However,