

ABSTRACT

Synthesis and Characterization of Chemosensors and their Screening against Metals and Pharmaceuticals

Selective chemosensors for determination and quantification of various types of molecular target analyte are very important in many fields including chemistry, medicine, and biology. Chemosensors for the sensing of metal ions (Hg(II), Fe(III) & Pd(II) and pharmaceuticals (cephradine & pefloxacin mesylate) was explored. Synthesis of two new sulfonate and sulfonamide based fluorescent chemosensors, their characterization by ESI-MS and ^1H NMR and synthesis of gold nanoparticles and silver nanoparticles stabilized Schiff bases have been explained. The synthesized nanoparticles have been characterized by UV-vis spectrophotometric, FTIR and AFM techniques. The average size of synthesized silver and gold nanoparticles were found to be 20-30 and 11 nm respectively, and were polydispersed as evidenced by AFM. To ascertain the potential for in vivo application, the stability of all synthesized nanoparticles was investigated as a function of pH, time, temperature and salt concentration. The water suspension of gold nanoparticles were found to be stable for several days at a temperature up to 100 $^{\circ}\text{C}$, a pH range of 2-10 and salt (NaCl) concentration 5mM-0.01mM, however gold nanoparticles showed instability at higher salt concentration. The main goal was to achieve sensing in water, which is a prerequisite for application to real samples. The first analyte of choice was heavy metal ion i.e. Hg. The already synthesized probe **218** exhibited marked selectivity for **Pb(II)** and **Hg(II)** over 10 other selected metal ions under physiological buffer condition. Owing to **Hg(II)** undesirable effects on the environment and the health concerns associated with Hg exposure, this fluorescent probe represents an appealing target and efficient chemosensor for **Hg(II)**. The fluorescence of each solution was measured and the resultant intensity is plotted against concentration of Hg(II) added which shows linear relationship from 10 to 6 μM with a limit of detection of Hg(II) was 0.05 μM . A novel supramolecular molecular tweezers based on a **biphenyl bis-triazolehexahydroquinoline** system was used for highly sensitive and selective fluorescent probe for recognizing and detecting **cephradine** in the presence of other drugs at pH 7.7. The detection limit was calculated to be 2.25 μM with a regression coefficient of 0.99. The competitiveness study, pH sensitivity of the sensor was also studied. The chemosensor allowed the detection of cephradine in tap water also.

Among the nanoparticles synthesized, the main attention was paid to the gold nanoparticles chemosensing properties. A **pyraziniumthioacetate stabilized** gold nanoparticles have been synthesized and were found an excellent sensor for heavy metal **Fe(III)** and **Pd(II)** ions in water, without any particular pretreatment. The detection method for **Fe(III)** by using gold nanoparticles was elegantly applicable over a wide range of pH (2-13) and concentrations (1-100 μM). The regression constant (R^2) calculated 0.9813, while the limit of detection (LOD) and the limit of quantification (LOQ) for **Fe(III)** ions was found to be 4.3 μM and 13.19 μM , respectively. The same **pyraziniumthioacetate stabilized** gold nanoparticles showed colorimetric change from win-red to grey in the presence of **Pd(II)**. LOD and LOQ for **Pd(II)** ions was found to be 4.23 μM and 12.83 μM , respectively. **Schiff base stabilized** gold nanoparticles displayed great selectivity and exhibited best chemosensor properties for **pefloxacin** in aqueous solution, A linear relationship was almost found when the concentration of **pefloxacin** was between 80 μM to 0.01 μM with a linear regression equation of $y=0.0015x + 0.0373$ with $R^2 = 0.99$. LOD was calculated 13.88 μM and LOQ 42.06 μM . The competitiveness study, pH sensitivity of the sensor was studied. These gold nanoparticles were found to be potent colorimetric sensor and display a very high selectivity for **Fe(III)**, **Pd(II)** and **pefloxacin**. The nanoparticle used for the drug sensing allowed the detection of pefloxacin in human serum by simple UV-vis spectroscopic measurements.