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Concomitant study of three factors that affect the size of AuNPs, with chemometrics approaches (and/ or Box-Behenken design)

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Background and Aims: Gold nanoparticles are promising nanocarriers for therapeutics due to their unique optical, chemical, and biological properties.Since the properties of gold nanoparticles(e.g.,toxicity, permeation through tissues) can be affected by their sizes and shapes, production of gold nanoparticles with suitable size and shape is usefull.
Methods: AuNPs were prepared as described in previous literatures. Briefly, 85 ml of filtrated deionized water was refluxed in250 ml flask on a hot plate. Five milliliters of 5 mM of HAuCl4 (2 mg/ml) was added to the above solution and heated up to boiling point. Five milliliters of different concentration of sodium citrate solution was quickly added to the boiling solution and stirred for 30 min until the color was turned to wine red. Study of relationship between characteristics of a material and their properties, often done experimentally, while mathematical models can be also used for study of relationship between these factors and the size of nanoparticles. The chemometric approach was applied for this study. The effect of three experimental parameters on size was investigated by mean of multivariant analysis. The Factors considered were concentration of sodium citrate solution(SC.Conc), stirrer speed(St.R) and ionic straight of the media(IS).
Results: The experiments were performed according to Box-Behnken experimental design. The obtained regression model was characterized by both descriptive and predictive ability. The method was optimized with respect to Z average diameter as a response. The equation resulted for the relationship between these factors and the size of AuNPs is " 114.578 + (-28.696 × (SC.Con×SC.Con)) + (-38.281× (St.R×SC.Con)) + (28.956 (×St.R×IS)) + (39.756× (SC.Con×IS))+(27.379× (St.R×St.R×IS))+(12.546× (SC.Con×SC.Con×St.R))+(27.301× (SC.Con×SC.Con×IS))".
Conclusions: It can be concluded that the Box-Behnken experimental design provides a suitable means of optimizing and testing the robustness of gold nanoparticles preparation method. With the equation given from this study we can predict the size of AuNPs produced in different conditions regarding these three factors.

Keywords: Nanoparticles; Gold; Box-Behnken experimental design; Optimization