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# A highly sensitive and selective thiosemicarbazone chemosensor for detection of $Co^{2+}$ in aqueous environments using RSM and TD/DFT approaches

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## Abstract

Chemosensor using organic based compound offering superior alternative method in recognizing metal ion in environmental water. The optimization process strongly affected the performance of the designed sensor. In this study, a highly sensitive and selective colorimetric sensor system utilizing an organic compound, namely thiosemicarbazone-linked acetylpyrazine (TLA), to recognize $Co^{2+}$ ions in different environmental water samples was successfully developed using the response surface methodology (RSM) approach. The developed model was optimized successfully and had statistically significant independent variables ($p < 0.05$), with optimum recognition occurring in 8:2 v/v DMSO/water at a pH of 5.3, a 100:70 μM TLA/$Co^{2+}$ concentration, and 15 min of reaction time. Under optimum conditions, the TLA sensor recognized $Co^{2+}$ ions at concentrations as low as 1.637 μM, which is lower than the detection limit of

flame atomic absorption spectroscopy (FAAS). Theoretical approaches supported the experimental data as well as characterized and predicted the mechanistic non-covalent interactions of TLA-$Co^{2+}$ within the chemosensing system. Finally, all the positive results produced in this study point to TLA as an alternative and comparable probe for recognizing $Co^{2+}$ pollution in water that is cost effective, movable and easy-to-handle, requires no special training and ecofriendly. © 2021, The Author(s).

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