

Development of novel nano sized imine complexes using *Coriandrum sativum* extract: Structural elucidation, non-isothermal kinetic study, theoretical investigation and pharmaceutical applications

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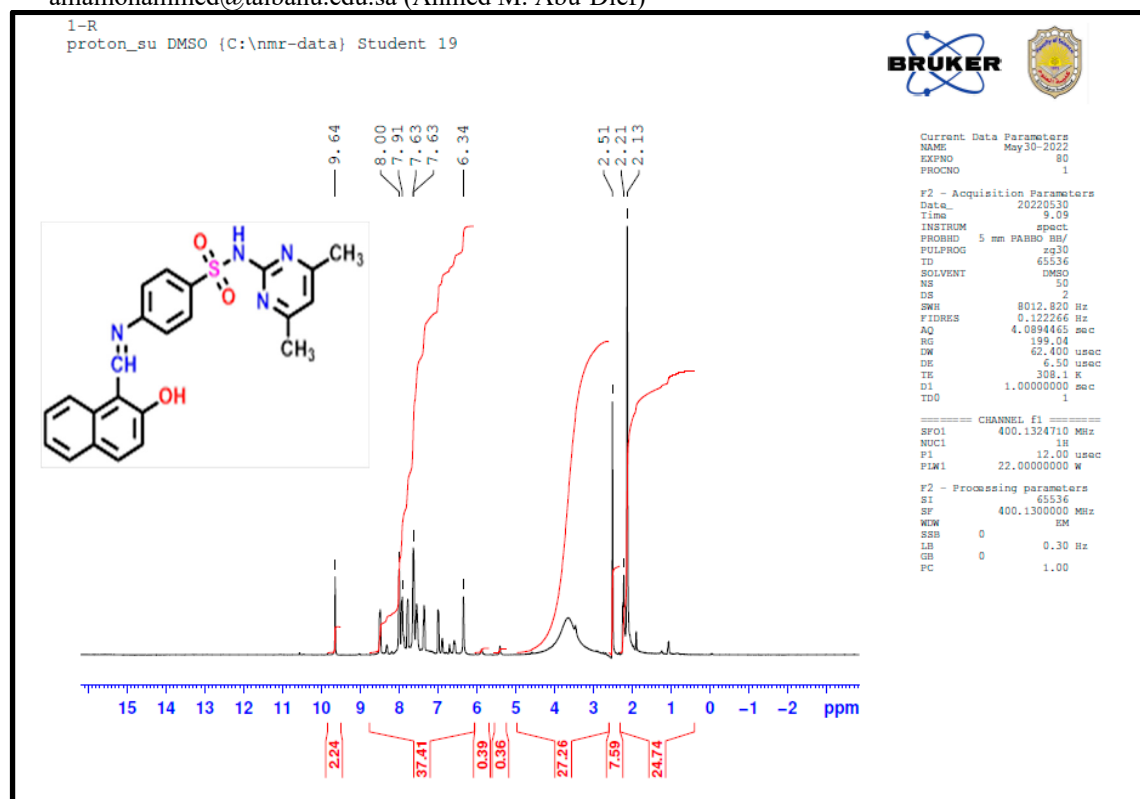
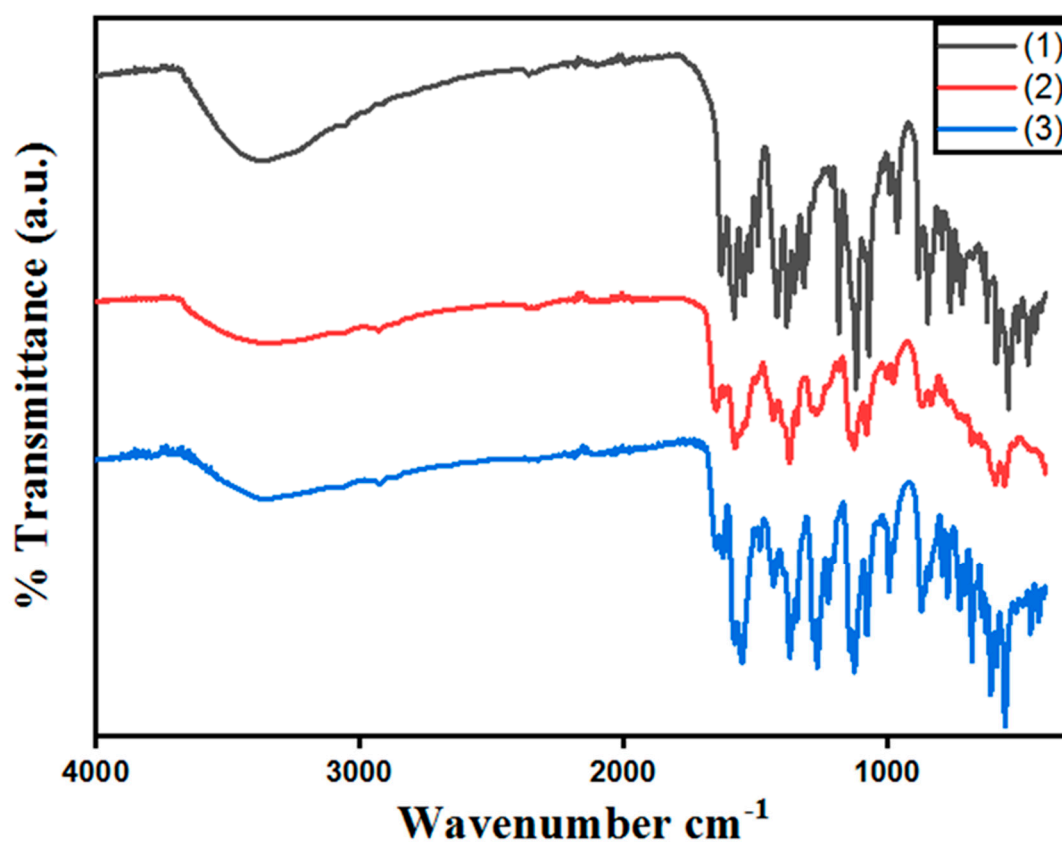


Figure S1. ¹H NMR spectrum of H₂L in DMSO

Table S1 Essential vibrational frequencies (cm^{-1}) of H_2L and its micro-complexes

| IR bands (cm^{-1}) | | | | | | | | |
|-------------------------------|--|--------------------------|--|--------------------------------|--------------------------------|------------------------------|--------------------------|--------------------------|
| No | Compound | $\nu(\text{C}=\text{N})$ | $\nu(\text{O}-\text{H})$); $\nu(\text{NH})$ | $\nu_{\text{as}}(\text{SO}_2)$ | $\nu_{\text{sy}}(\text{SO}_2)$ | $\delta(\text{H}_2\text{O})$ | $\nu(\text{M}-\text{O})$ | $\nu(\text{M}-\text{N})$ |
| I | H_2L | 1633 | 3200;3457 | 1384 | 1156 | ----- | ----- | ----- |
| II | $[\text{NiL}_2] \cdot 1.5\text{H}_2\text{O}$ | 1602 | ;3453 | 1384 | 1152 | 970 | 585 | 549 |
| III | CdL_2 | 1624 | ;3458 | 1384 | 1157 | ----- | 566 | 544 |

**Figure S2.** FT-IR spectra of H_2L (1), Ni (II) complex(2) and Cd(II) complex(3)

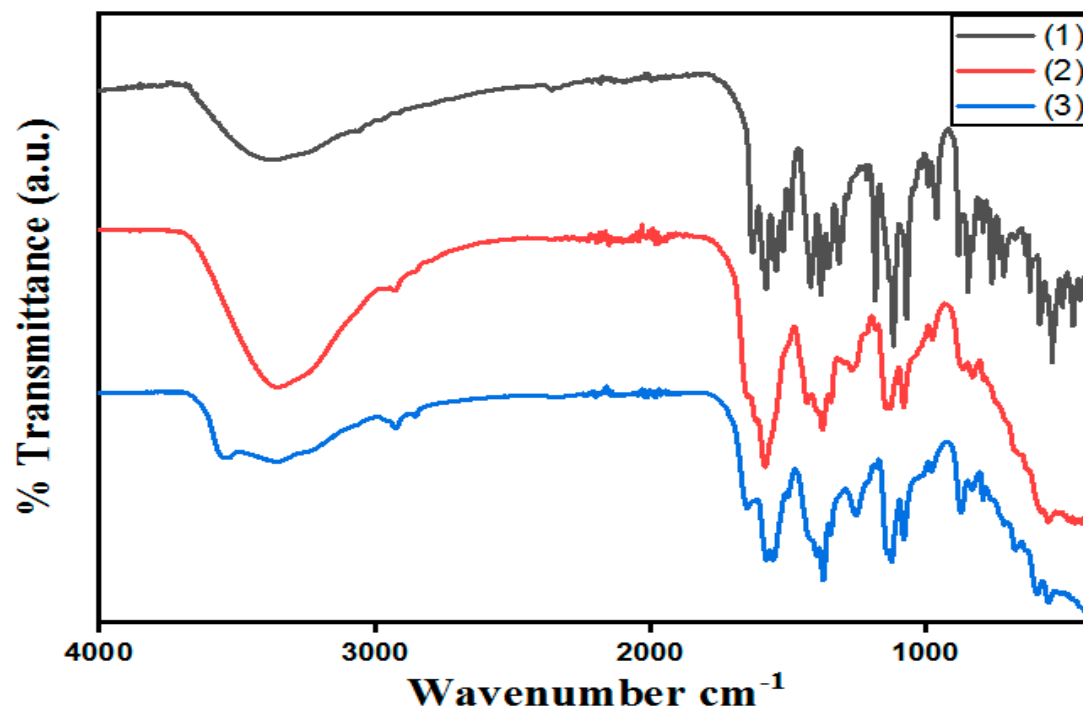
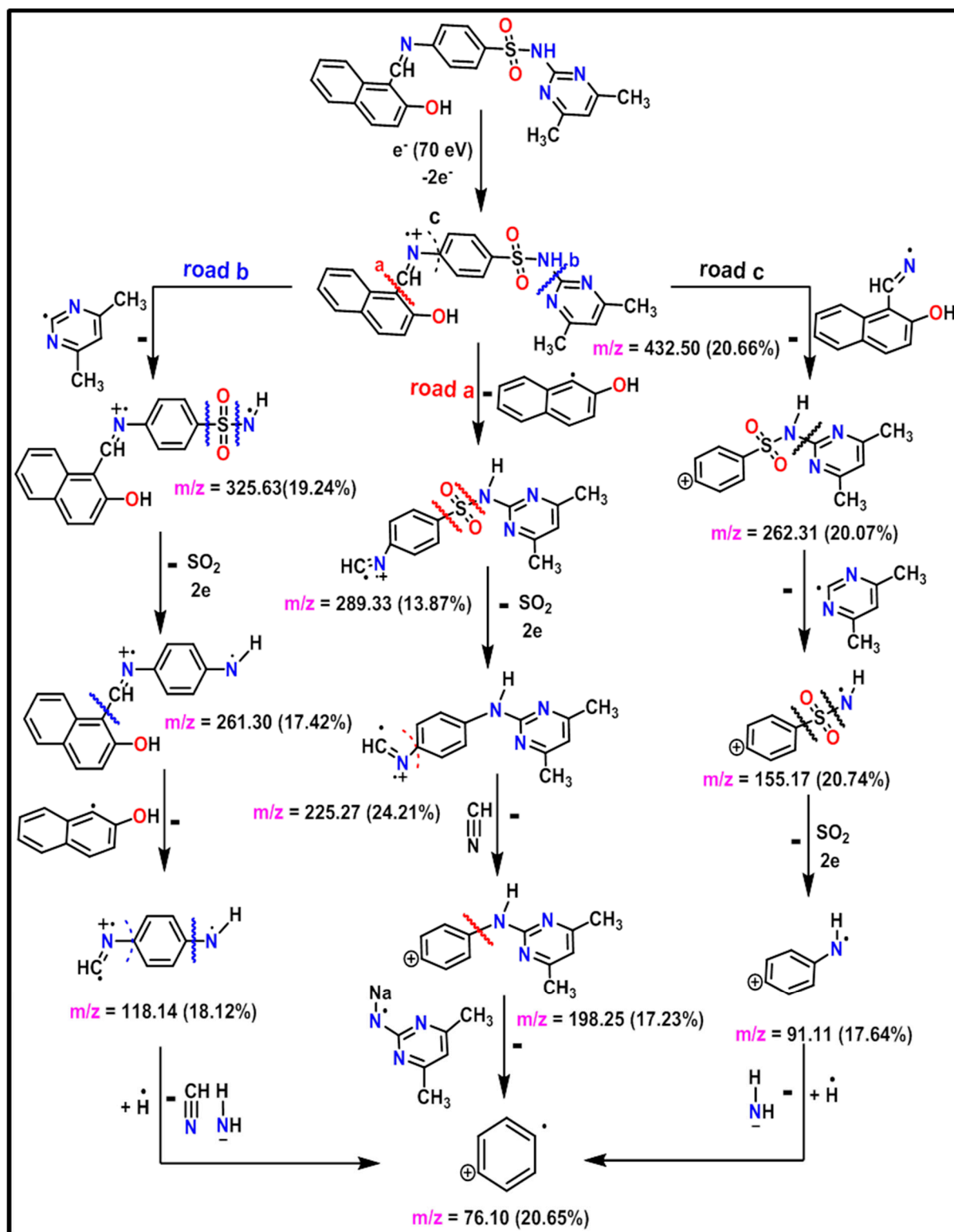


Figure S3. FT-IR spectra of H_2L (1), Ni nano complex (2) and Cd nano complex(3)



Scheme S1 Suggested MS fragmentation pattern of Schiff base ligand

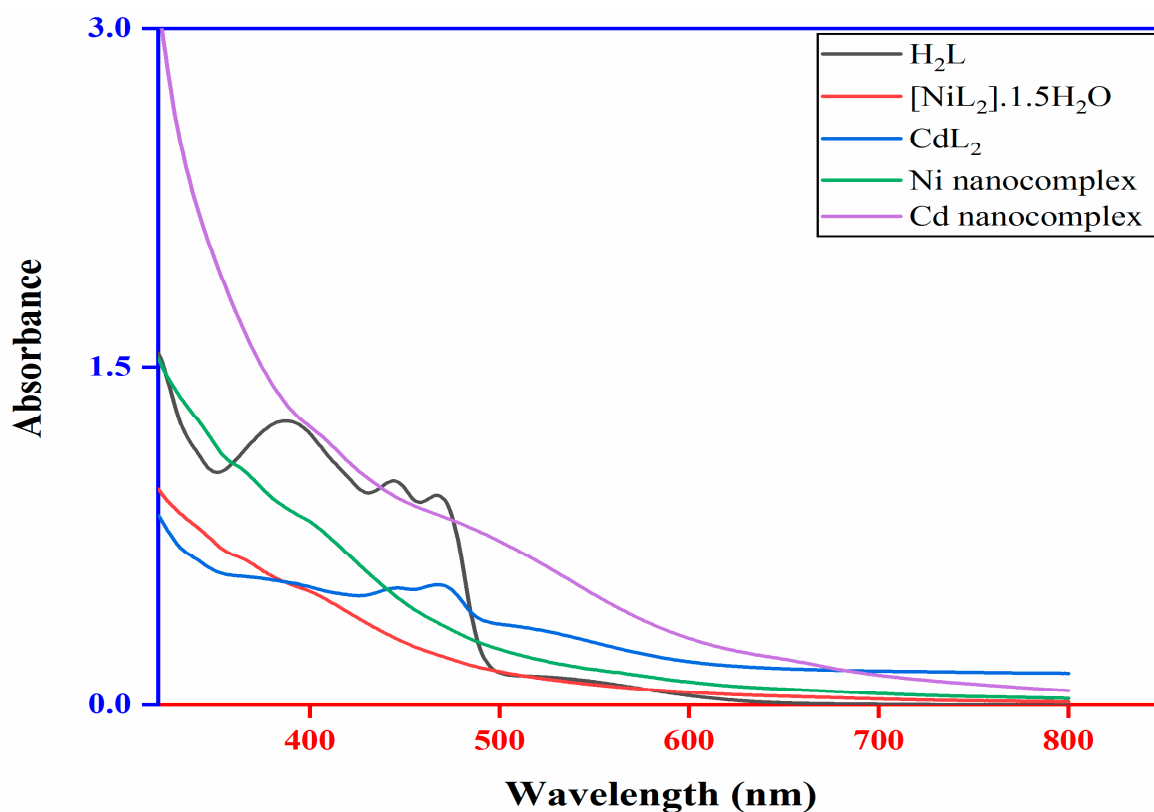


Figure S4. UV-Vis absorption spectra in 10^{-4} DMF solution

Section S1: Materials and equipment's

All chemicals used were obtained from Aldrich or BDH. They included 2-Hydroxy-1-naphthaldehyde, sulfamethazine, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ or $\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O}$ and LiOH . The solvents, such as absolute ethyl alcohol and Dimethylformamide (DMF) were used as received without pretreatment.

The characterization of ligand H_2L and their corresponding micro/nano Ni(II) , and Cd(II) complexes was carried out utilizing the various spectroscopic techniques: Elemental analyses (C, H, Cl, and N) were performed by Micro analytical unit of the Cairo University, Egypt. ^1H NMR spectra in deuterated dimethyl sulfoxide $d_6\text{-DMSO}$ were recorded using a 300 MHz Varian NMR spectrometer. The chemical shift was measured relative to the solvent peak. Mass spectrum for ligand and metal complexes was run on Shimadzu-QP 2010 plus Mass Spectrometer, Microanalytical Laboratory, Faculty of Science, Cairo University, Egypt. The Fourier transform infrared absorption spectra of solid ligand and micro/nano complexes was performed by Micro analytical unit at Cairo University, Egypt, in the wavelength range ($4000\text{-}400\text{ cm}^{-1}$) using KBr discs using a Nenexeus-Nicolidite -640-MSA FT-IR infrared

spectrophotometer. The electronic spectra (ultraviolet/visible) were recorded using a Perkin Elmer Lambda 330 spectrophotometer. The electronic spectra of Dimethyl Formamide (DMF) solution of both the ligand and micro/nano complexes were recorded in 1cm quartz cells. The molar conductivity measurements were determined in N, N' Dimethyl- formamide (DMF) solution at (10^{-3}M) using a tacussel conductimeter type CD6N.

Thermal Analyzer with a heating rate of $10\text{ }^{\circ}\text{C}/\text{min}$ in a nitrogen atmosphere with a following rate of $20\text{ mL}/\text{min}$ in the ambient temperature range up to $800\text{ }^{\circ}\text{C}$ using platinum crucibles. X-ray powder diffraction analyses of solid samples were measured using APD 2000 PROModel GNR-X-ray Diffractometer at (Central lab., Tanta University, Egypt). X-ray diffractograms give computer control formally finished by PHILIPS®MPDX'PERT X-ray diffractometer ready with Cu radiation $\text{CuK}\alpha$ ($\lambda=1.540\text{ }56\text{ \AA}$). The x'pertdiffractometer has the Bragg-Brentano geometry. The x-ray tube was a copper tube operating at 40 KV and 30 mA . The scanning range (2θ) was $5\text{--}90^{\circ}$ with a step size of 0.050° and a counting time of $2\text{ s}/\text{step}$. Quartz was used as the standard material to accurate for the instrumental expansion. This identification of the nano complexes was done by a known method. From the fit identified Scherrer formula, the average crystallite size (D) is $D = (K\lambda / \beta \cos \theta)$ Where: λ is the X- ray wavelength in the nanometer, K is a factor related to crystallite shape, with a value of about 0.9 and β is the peak width at half maximum height. The value of β in the 2θ axis of diffraction shape must be in radians. The θ is the Bragg angle and can be in radians since the $\cos \theta$ compatible with the same number. The surface morphological and particle size study was recorded by TEM micrographs were executed using JEOL JEM-1200 EX II, Japan at $60\text{--}70\text{ kV}$.