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New zinc(II), copper(II), nickel(II), iron(III), and cobalt(III) coordination compounds, [Zn(HL)₂] (1), [Cu(HL)Cl₂] (2), [Cu(HL)Br₂] (3), {[Cu(HL)NO₃]_nNO₃}_n (4), [Ni(HL)₂](NO₃)₂ (5), [Fe(L)₂]NO₃ (6), [Co(L)₂]NO₃ (7), and [Co(L)₂]Cl·H₂O (8), were obtained with 2-acetylpyridine N⁴-allyl-S-methylisothiosemicarbazone (HL). The isothiosemicarbazone proligand was characterized by nuclear magnetic resonance (NMR) (¹H and ¹³C), infrared (IR) spectroscopy, and X-ray diffraction. All the coordination compounds were characterized by elemental analysis, IR, UV–Vis spectroscopy, molar conductivity, and magnetic susceptibility measurements. Single-crystal X-ray diffraction analysis elucidated the structure of the cationic form of the proligand in the salt [H₂L]⁺ and compounds 1–4 and 8 and demonstrated an unusual way of coordination through methylated sulfur atom in 1 and 3. Nevertheless, the electron paramagnetic resonance (EPR) and UV–Vis investigations showed that this way of coordination quickly changes upon dissolution of coordination compounds in dimethyl sulfoxide (DMSO). The antiproliferative properties of these compounds towards human cervical epithelial HeLa, human epithelial pancreatic adenocarcinoma BxPC-3, human muscle rhabdomyosarcoma spindle, large multinucleated RD cancer cell lines, and normal kidney epithelial MDCK cell line have been investigated. Copper coordination compounds (2–4) show promising anticancer activity with high selectivity (selectivity index [SI] = 10–18) towards BxPC-3 cell line. They also possess significant antibacterial and antifungal activity, which is useful for cancer treatment.