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5-Bromo-2-hydroxybenzaldehyde,2-hydroxy3-ethoxybenzaldehyde,and 2-hydroxynaphthalene-1-carbaldehyde 4-(2-pyridyl) thiosemicarbazones (I–III, respectively) were synthesized and theircrystal structures were determined by X-ray diffraction. All these molecules are almost planar. The presenceof bulky substituents at the terminal nitrogen atoms of these molecules does not lead to changes in the conformation of the thiosemicarbazide moiety. Depending on the nature of substituents in the phenol rings, thecrystals are composed of either centrosymmetric dimers (I) or infinite chains (II and III. In the concentration range of 10–5–10–7 mol/L, thiosemicarbazones I–III selectively inhibit the growth of human myeloidleukemia HL60 cells