

Supplementary material for the article:

Anđelković, K.; Milenković, M. R.; Pevec, A.; Turel, I.; Matić, I. Z.; Vujčić, M.; Sladić, D.; Radanović, D.; Brađan, G.; Belošević, S.; et al. Synthesis, Characterization and Crystal Structures of Two Pentagonal-Bipyramidal Fe(III) Complexes with Dihydrazone of 2,6-Diacetylpyridine and Girard's T Reagent. Anticancer Properties of Various Metal Complexes of the Same Ligand. *Journal of Inorganic Biochemistry* **2017**, *174*, 137–149.
<https://doi.org/10.1016/j.jinorgbio.2017.06.011>

Supplementary Information

Synthesis, characterization and crystal structures of two pentagonal-bipyramidal Fe(III) complexes with dihydrazone of 2,6-diacetylpyridine and Girard's T reagent. Anticancer properties of various metal complexes of the same ligand.

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Table S1. Crystal data and structure refinement details for **7** and **8**.

	7	8
formula	C ₂₂ H ₃₅ FeN ₁₀ O ₄ S ₃	C ₄₇ H ₇₂ Fe ₃ N ₂₃ O ₉ S ₉
Fw (g mol ⁻¹)	655.63	1559.36
crystal size (mm)	0.40 × 0.02 × 0.02	0.15 × 0.10 × 0.05
crystal color	green	green
crystal system	triclinic	triclinic
space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	7.5016(9)	12.1021(3)
<i>b</i> (Å)	11.8462(10)	15.9085(5)
<i>c</i> (Å)	18.2010(15)	20.0448(6)
α (°)	82.959(7)	95.611(2)
β (°)	89.790(8)	95.470(2)
γ (°)	79.031(9)	110.266(3)
<i>V</i> (Å ³)	1575.6(3)	3568.24(19)
<i>Z</i>	2	2
calcd density (g cm ⁻³)	1.382	1.451
<i>F</i> (000)	686	1618
no. of collected reflns	14602	33057
no. of independent reflns	7234	16315
<i>R</i> _{int}	0.1371	0.0453
no. of reflns observed	2972	10061
no. parameters	381	896
<i>R</i> [<i>I</i> > 2σ(<i>I</i>)] ^a	0.0696	0.0694
<i>wR</i> ₂ (all data) ^b	0.1476	0.1891

<i>Goof</i> , S^c	0.872	1.044
maximum/minimum residual	+0.64/-0.83	+2.50/-0.92
electron density ($e \text{ \AA}^{-3}$)		

^a $R = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$.

^c $S = \{ \sum [(F_o^2 - F_c^2)^2] / (n/p) \}^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

Table S2. Selected bond lengths (Å) and angles (°) for **7** and **8**.

7			
Fe1–N3	2.193(4)	O1–Fe1–N3	71.37(14)
Fe1–N4	2.208(4)	O1–Fe1–N4	140.86(16)
Fe1–N5	2.199(4)	O1–Fe1–N5	149.71(15)
Fe1–N8	2.031(4)	O1–Fe1–N8	90.44(14)
Fe1–N9	2.049(4)	O1–Fe1–N9	91.86(15)
Fe1–O1	2.079(3)	O1–Fe1–O2	78.00(13)
Fe1–O2	2.061(3)	N8–Fe1–N9	176.71(17)
8			
Fe1–N3	2.181(4)	O1–Fe1–N3	71.81(14)
Fe1–N4	2.200(3)	O1–Fe1–N4	141.57(14)
Fe1–N5	2.199(4)	O1–Fe1–N5	148.46(13)
Fe1–N8	2.039(4)	O1–Fe1–N8	90.42(15)
Fe1–N9	2.025(4)	O1–Fe1–N9	91.52(15)
Fe1–O1	2.092(3)	O1–Fe1–O2	76.81(13)
Fe1–O2	2.086(3)	N8–Fe1–N9	176.70(17)
Fe2–N12	2.197(4)	O3–Fe2–N12	71.69(14)
Fe2–N13	2.206(4)	O3–Fe2–N13	141.58(14)
Fe2–N14	2.180(4)	O3–Fe2–N14	148.41(14)
Fe2–N17	2.016(4)	O3–Fe2–N17	89.21(16)
Fe2–N18	2.043(4)	O3–Fe2–N18	92.88(14)
Fe2–O3	2.090(3)	O3–Fe2–O4	77.00(13)
Fe2–O4	2.100(3)	N17–Fe2–N18	176.28(17)
Fe3–N19	2.056(4)	N19–Fe3–O1w	90.45(17)
Fe3–O1w	2.076(4)	N21–Fe3–O1w	174.88(14)