



SUPPLEMENTARY MATERIAL TO

**Synthesis, characterization and antimicrobial activity of the
isothiocyanato Fe(III) Girard's T hydrazone complex**

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CHARACTERISATION DATA

HLCl [(E)-N,N,N-trimethyl-2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)ethan-1-aminium chloride]. Anal. Calcd. for C₁₂H₁₉ClN₄O: C, 53.23; H, 7.07; N, 20.69 %. Found: C, 53.36; H, 7.26; N, 20.43 %; IR (ATR, cm⁻¹): 3387 (w), 3127 (m), 3090 (m), 3049 (m), 3016 (m), 2950 (s), 1700 (vs), 1612 (w), 1549 (s), 1485 (m), 1400 (m), 1300 (w), 1253 (w), 1200 (s), 1153 (w), 1135 (m), 1095 (w), 1073 (m), 975 (w), 944 (w), 914 (m), 748 (w), 683 (w); ¹H-NMR (500 MHz, DMSO-d₆, δ / ppm): 11.41 (1H, s, N-H), 11.66 (0.4H, s, N-H), 4.92 (2H, s, C10-H), 4.86 (0.8H, s, C10-H), 3.35 (9H, s, C11-H), 3.31 (3.6H, s, C11-H), 2.37 (3H, s, C8-H), 2.49 (1.2H, s, C8-H), 8.62 (1.4H, m, C3-H), 7.45 (1.4H, m, C4-H), 7.91 (1H, td, ³J = 10.0 Hz & ⁴J = 5.0 Hz, C5-H), 7.88 (0.4 H, td, ³J = 10.0 Hz & ⁴J = 5.0 Hz, C5-H), 8.12 (1H, d, ³J = 10 Hz, C6-H), 8.05 (0.4H, d, ³J = 10.0 Hz, C6-H); ¹³C-NMR (125 MHz, DMSO-d₆, δ / ppm): 63.2 & 63.9 (C10), 53.7 & 53.9 (C11), 13.9 & 12.7 (C8), 149.2 & 149.1 (C3), 124.9 & 124.8 (C4), 137.2 & 137.1 (C5), 120.8 & 120.9 (C6), 155.3 & 155.1 (C2), 154.9 & 151.4 (C7), 167.1 & 161.3 (C9).

Fe(III) complex (I). Anal. Calcd. for C₁₅H₁₈FeN₇OS₃: C, 38.80; H, 3.91; N, 21.11; S, 20.71 %. Found: C, 38.96; H, 4.17; N, 20.96; S, 20.42 %; IR (ATR, cm⁻¹): 3072 (w), 2964 (w), 2036 (s), 2024 (s), 1620 (m), 1598 (m), 1566 (m),

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1521 (*m*), 1464 (*m*), 1393 (*m*), 1327 (*m*), 1260 (*w*), 1166 (*w*), 1144 (*w*), 1109 (*w*), 1073 (*w*), 1023 (*w*), 968 (*w*), 906 (*w*), 806 (*w*), 776 (*w*), 675 (*w*).

CRYSTAL STRUCTURE ANALYSIS

Crystal structure analysis for 1. C₁₅H₁₈FeN₇OS₃, *M*: 464.39 g mol⁻¹, triclinic, *P*-1, *a* = 8.5770(3) Å, *b* = 9.2198(3) Å, *c* = 14.1558(4) Å, α = 108.577(2)°, β = 91.249(2)°, γ = 90.930(2)°, *V* = 1060.52(6) Å³, *Z* = 2, $\rho_{\text{calcd.}}$ = 1.454 g cm⁻³, *F*(000) = 478, 8298 reflections measured, 4803 were independent of symmetry, of which 3579 were observed (*I* > 2σ(*I*)), *R*₁ = 0.0622, *wR*₂ (all data) = 0.2178, 248 parameters.

ANTIMICROBIAL ACTIVITY

TABLE S-I. Antimicrobial activity (*MIC* / μg mL⁻¹) of ligand **HLCl** and complex **1**; n.t. – not tested

Microorganism	HLCl	1	Fe(NO ₃)·9H ₂ O	NH ₄ SCN	Mero- penem	Amikacin	Ampho- tericin
<i>S. aureus</i> ATCC 6538	>1000	>1000	>1000	>1000	8	5	n.t.
<i>B. subtilis</i> ATCC 6633	1000	>1000	>1000	>1000	0.25	0.5	n.t.
<i>E. coli</i> ATCC 8739	500	>1000	>1000	>1000	0.06	1	n.t.
<i>K. pneumoniae</i> ATCC 13883	1000	>1000	>1000	>1000	0.06	0.25	n.t.
<i>S. enterica</i> <i>subsp. enterica</i> <i>serovar</i> <i>Typhimurium</i> ATCC 14028	1000	>1000	>1000	>1000	0.06	2	n.t.
<i>P. aeruginosa</i> ATCC 9027	1000	1000	>1000	>1000	1	2	n.t.
<i>C. albicans</i> ATCC 10231	1000	500	>1000	>1000	n.t.	n.t.	0.82