

Supporting Information

Liposomal Formulation of a Gold(III) Metalloantibiotic: A Promising Strategy Against Antimicrobial Resistance.

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I. NMR Spectra

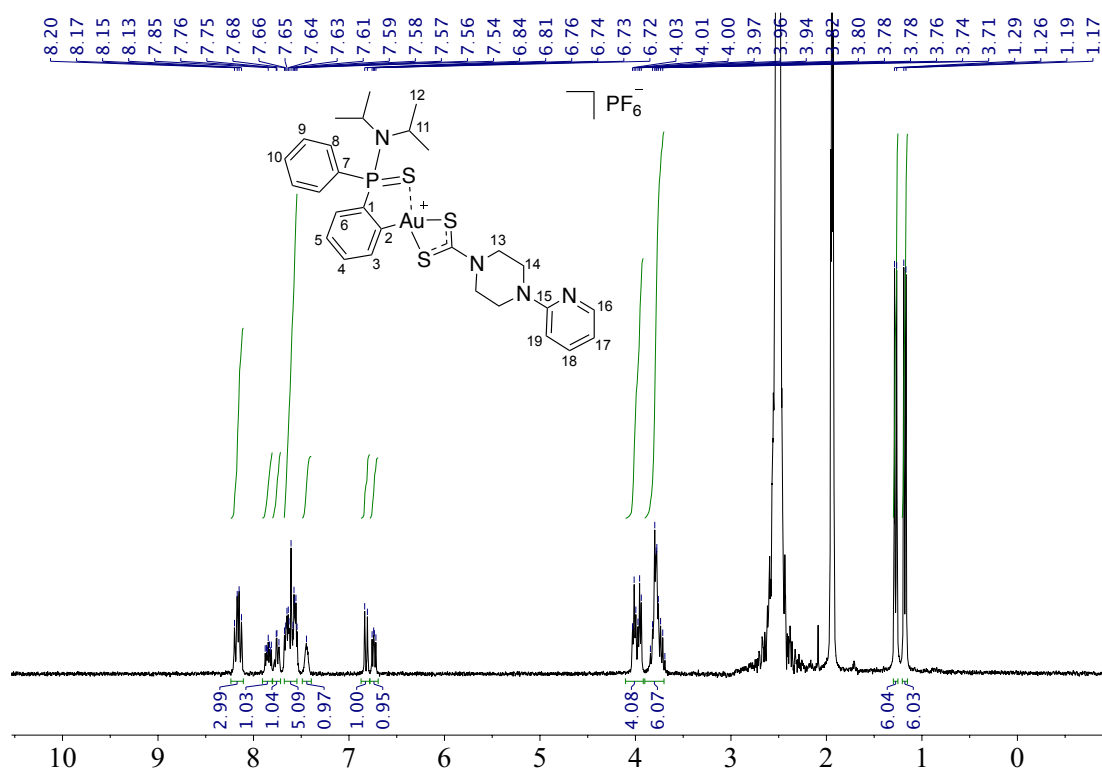


Figure S1. ¹H NMR of AuPyPZ in CD₃CN.

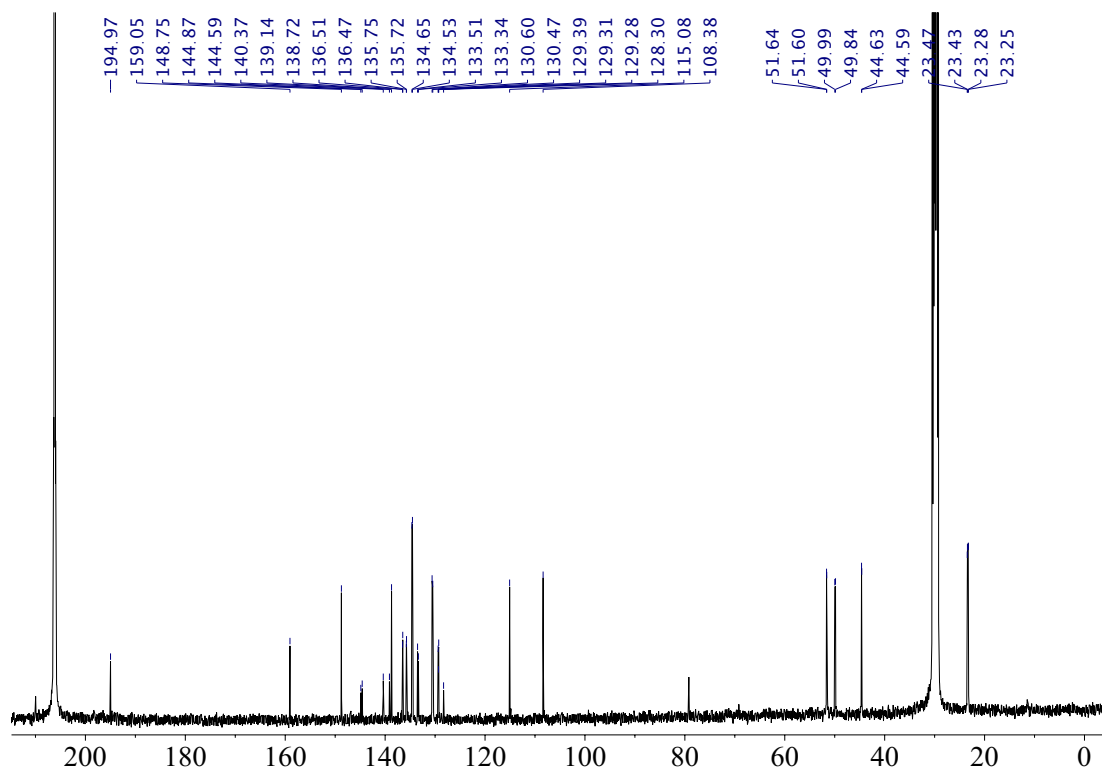


Figure S2. ¹³C NMR of AuPyPZ in (CD₃)₂CO.

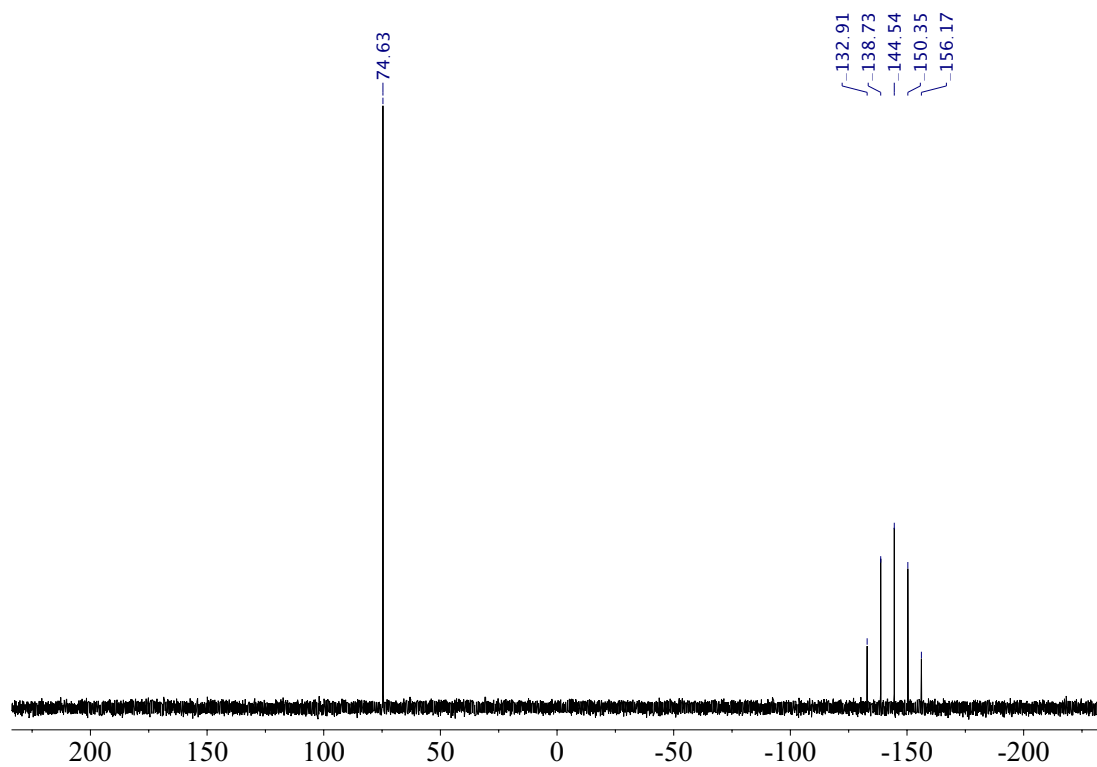


Figure S3. ^{31}P NMR of AuPyPZ in CD_3CN .

II. Antibacterial Activity

Table S1. Strains tested and minimal inhibitory concentrations obtained for AuPyPZ complex.

Entry	Strain ID	Species	Resistance	MIC (mg/L) AuPyPZ
1	162065-705	<i>S. aureus</i>	CIP, LVX, CLI, ERI, PEN	0.5
2	163501-000	<i>S. aureus</i>	CIP, CLI, ERI, LVX	0.5
3	162071-210	<i>S. aureus</i>	CIP, CLI, ERI, LVX	0.5
4	162058-967	<i>S. aureus</i>	AMK, TET, CIP, CHL, ERI, VAN	1
5	ATCC® 29213	<i>S. aureus</i>		1
6	FG22014	<i>S. epidermidis</i>	PEN, CTX, CRO, CIP, CHL, ERI	1
7	FG03015	<i>S. epidermidis</i>	OXA, PEN, CTX, CIP, ERI	1
8	FG14013	<i>S. epidermidis</i>	OXA, PEN, CTX, GEN, CIP, CHL, ERI	1
9	9510-524	<i>S. maltophilia</i>	CAZ, SXT	4
10	895	<i>S. maltophilia</i>	LVX, CAZ, CHL, SXT	4
11	166097-953	<i>P. aeruginosa</i>	TOB, GEN, CIP, AZT, LVX, IMP	16
12	30302995-242	<i>P. aeruginosa</i>	GEN, TOB, TZP, CIP, IMP, MEM, AZT, LVX, IMP, DOR	16
13	ATCC® 27853	<i>P. aeruginosa</i>		16
14	E4	<i>E. coli</i>	CHL, GEN, NAL, TET, SXT, RIF	16
15	E8	<i>E. coli</i>	CHL, GEN, CIP, NAL, TET, SXT, RIF	8
16	E11	<i>E. coli</i>	CHL, GEN, CIP, NAL, TET, SXT, RIF	8
17	ATCC® 25922	<i>E. coli</i>		8
18	AbCr17	<i>A. baumannii</i>	CST	2
19	Ab177	<i>A. baumannii</i>		2
20	Ab210	<i>A. baumannii</i>	CST	4
21	ATCC® 19606	<i>A. baumannii</i>		2

Table S2. Strains tested and minimal inhibitory concentrations (MICs) obtained for liposomal AuPyPZ complex.

Entry	Strain ID	Species	Resistance	MIC (mg/L) Liposomal AuPyPZ
1	162065-705	<i>S. aureus</i>	CIP, LVX, CLI, ERI, PEN	0.5
2	163501-000	<i>S. aureus</i>	CIP, CLI, ERI, LVX	1
3	162071-210	<i>S. aureus</i>	CIP, CLI, ERI, LVX	0.5
4	162058-967	<i>S. aureus</i>	AMK, TET, CIP, CHL, ERI, VAN	1
5	ATCC® 29213	<i>S. aureus</i>		1
6	FG22014	<i>S. epidermidis</i>	PEN, CTX, CRO, CIP, CHL, ERI	0.5
7	FG03015	<i>S. epidermidis</i>	OXA, PEN, CTX, CIP, ERI	0.5
8	FG14013	<i>S. epidermidis</i>	OXA, PEN, CTX, GEN, CIP, CHL, ERI	0.25

III. X-Ray Analysis

Table S3. Crystal data and structure refinement for **AuPyPz**.

Identification code	AuPyPz
Empirical formula	C ₅₇ H ₇₁ Au ₂ Cl ₃ F ₁₂ N ₈ P ₄ S ₆
Formula weight	1912.74
Temperature/K	273
Crystal system	triclinic
Space group	P-1
a/Å	11.5343(3)
b/Å	15.5640(3)
c/Å	21.2129(5)
α/°	95.849(2)
β/°	98.779(2)
γ/°	102.500(2)
Volume/Å ³	3638.20(15)
Z	2
ρ _{calc} /cm ³	1.746
μ/mm ⁻¹	11.566
F(000)	1884.0
Crystal size/mm ³	0.219 × 0.154 × 0.099
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	5.874 to 139.104
Index ranges	-13 ≤ h ≤ 13, -18 ≤ k ≤ 18, -23 ≤ l ≤ 25
Reflections collected	34851
Independent reflections	13442 [R _{int} = 0.0338, R _{sigma} = 0.0353]
Data/restraints/parameters	13442/921/1024
Goodness-of-fit on F ²	1.030
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0385, wR ₂ = 0.1007
Final R indexes [all data]	R ₁ = 0.0444, wR ₂ = 0.1067
Largest diff. peak/hole / e Å ⁻³	0.68/-1.19