

Supplementary Information

Catechol Oxidase, Phosphatase-Like Activity, DNA/BSA Binding Studies of Ru^{II} Complexes of S-Allyldithiocarbamate: Synthesis and Spectral Studies

*Ponnusamy Selvakumar,^a Ramaswamy Narayanasamy,^{*b} Nanjan Nanjundan,^b
Krishnaswamy Velmurugan^c and Raju Nandhakumar^c*

^a*Department of Chemistry, SVS College of Engineering, 642 109 Coimbatore, India*

^b*Department of Chemistry, Coimbatore Institute of Technology, 641 014 Coimbatore, India*

^c*Department of Chemistry, Karunya University, 641 114 Karunya Nagar Coimbatore, India*

*e-mail: narayanasamycit@gmail.com

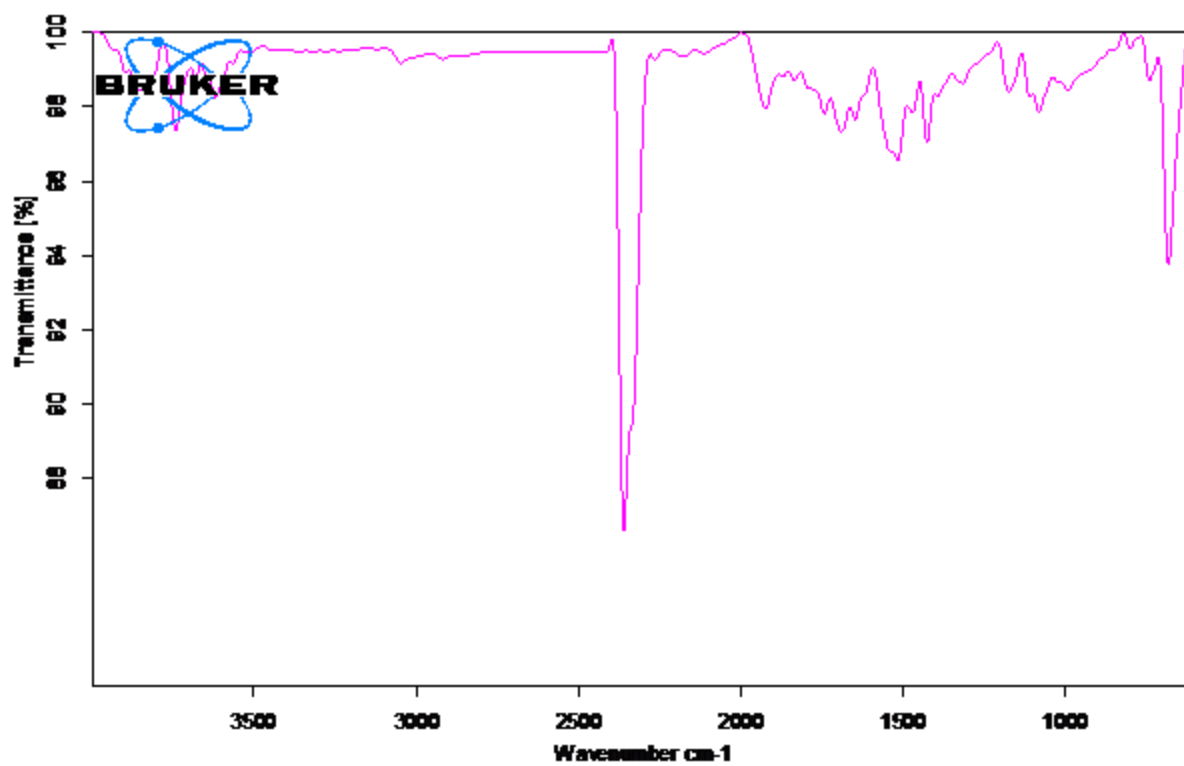
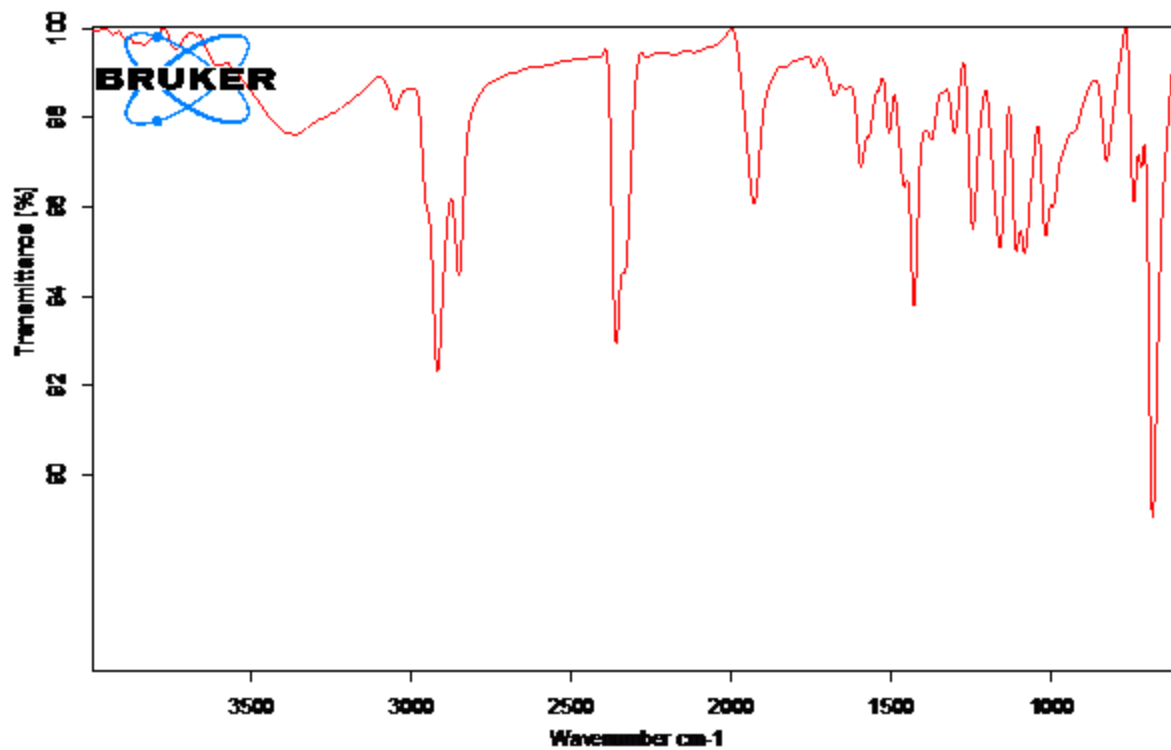


Figure S1. IR spectra (KBr) of complexes 1 (top) and 2 (bottom).

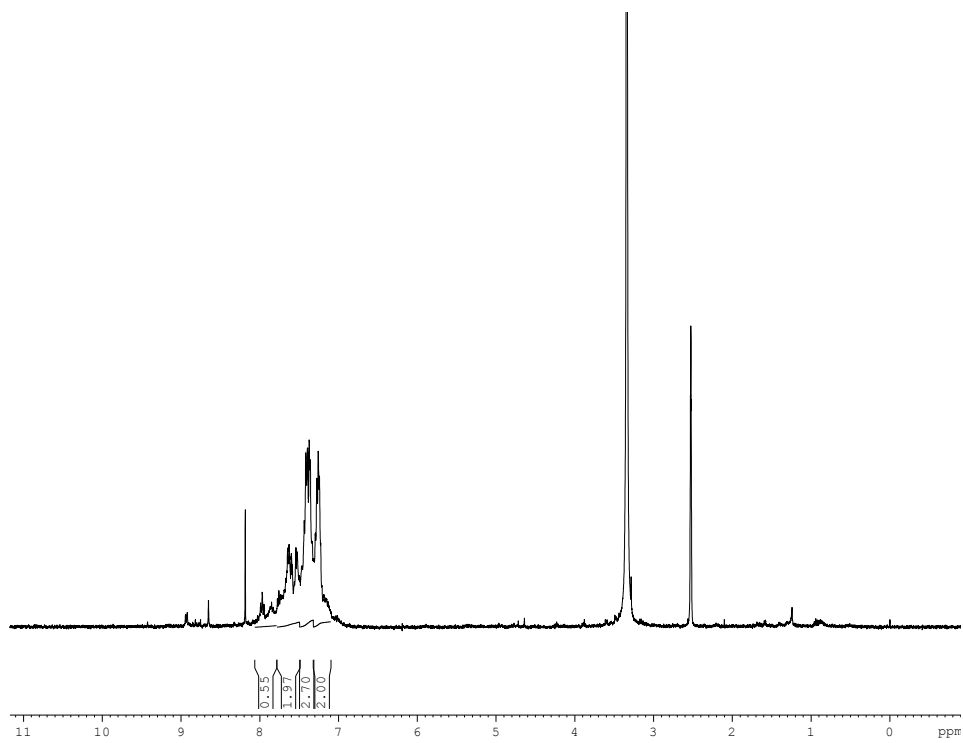
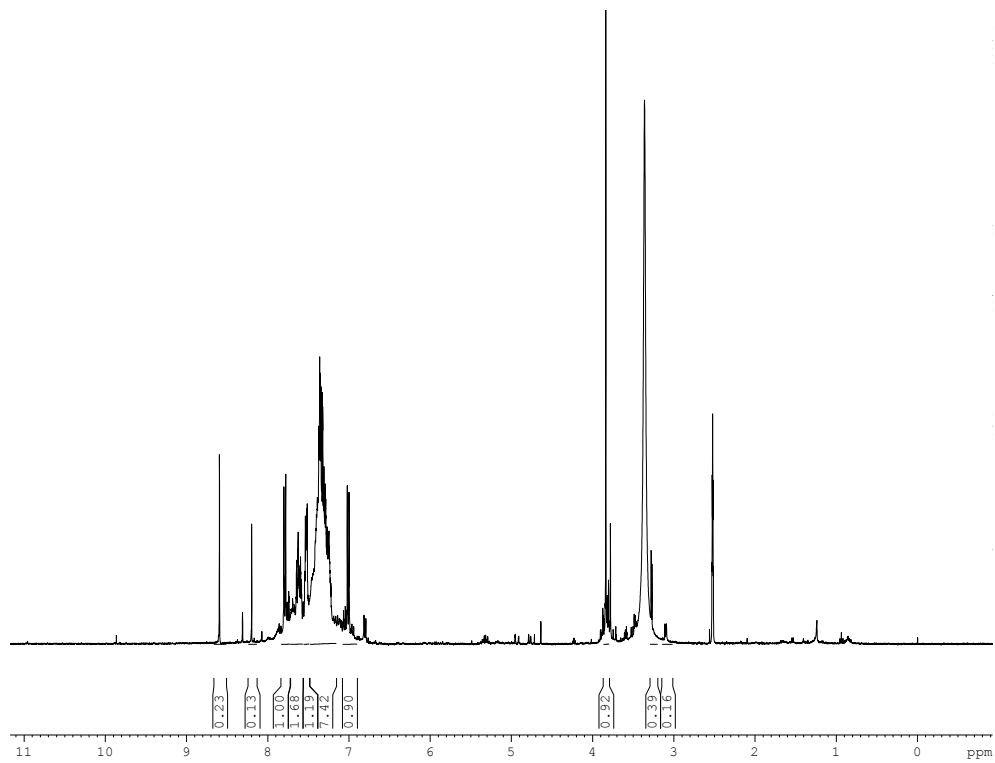


Figure S2. ¹H or ¹³C NMR (frequency, solvent) spectra of complexes **1** (top) and **2** (bottom).

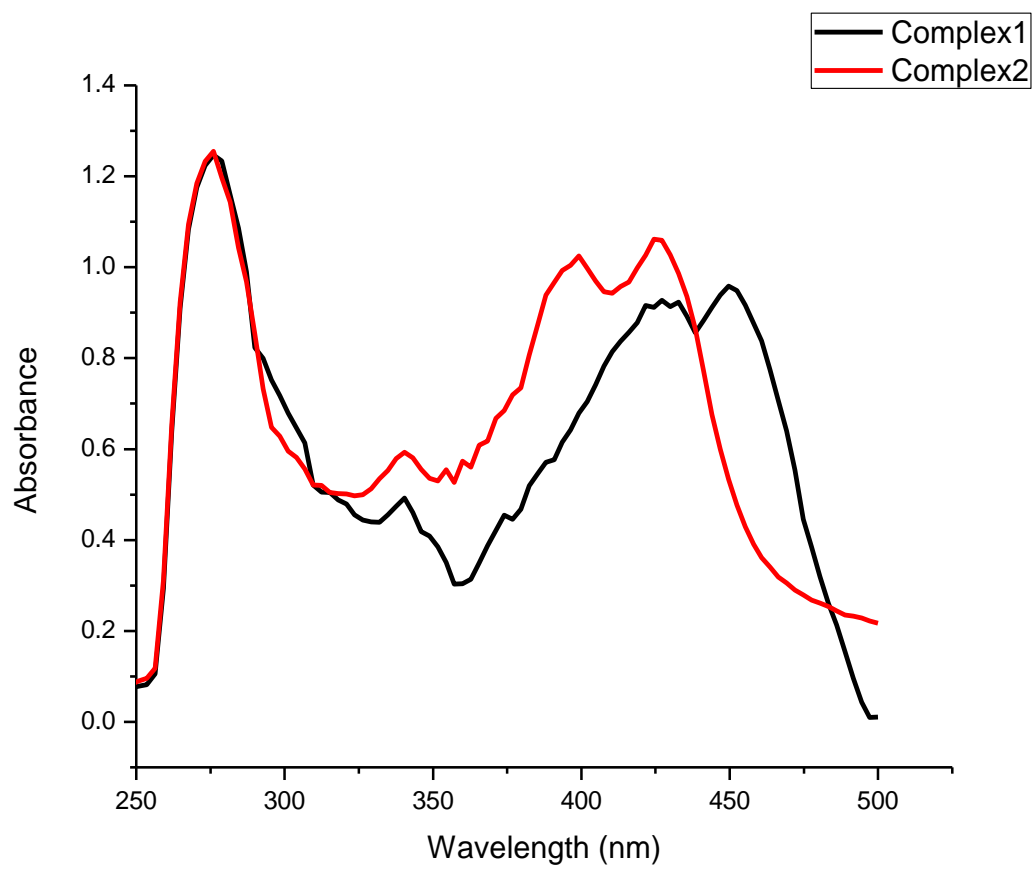


Figure S3. UV-Vis spectra of complexes **1** and **2**.

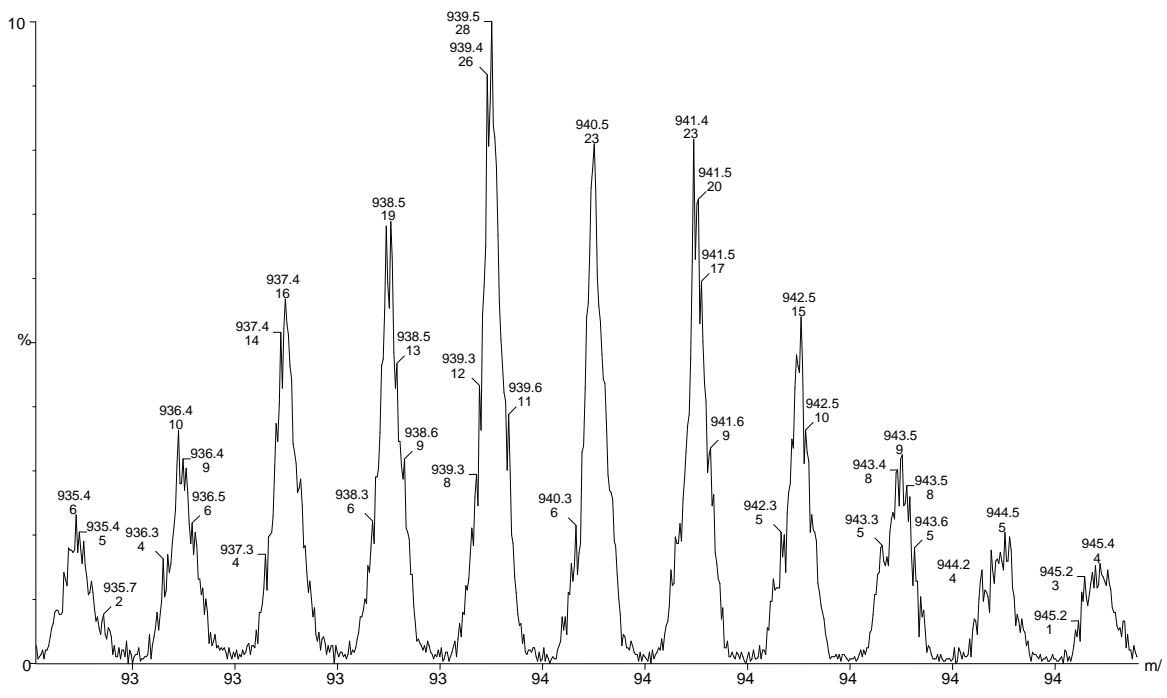
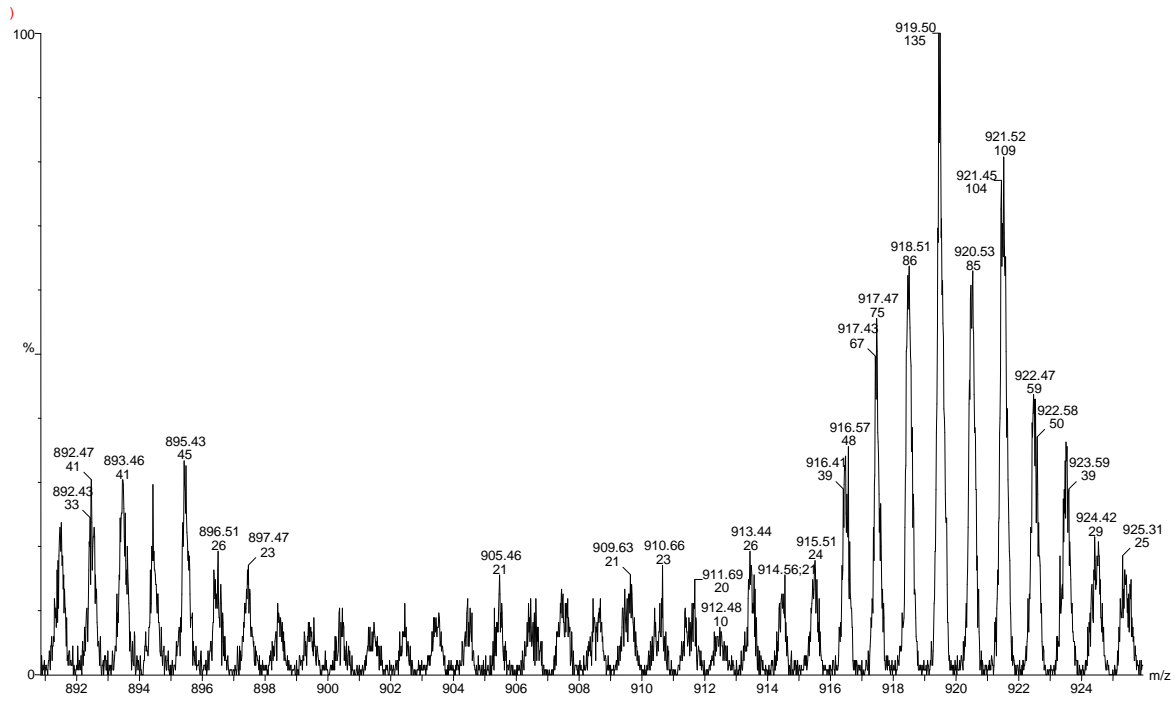


Figure S4. LC-MS spectra of complexes 1 (top) and 2 (bottom).

Table S1. CT-DNA binding constant (K_b), quenching constant (K_{sv}) and apparent binding constant (K_{app}) values for complexes **1** and **2**

Compound	K_b / mol^{-1}	K_{sv} / mol^{-1}	$K_{app} / \text{mol}^{-1}$
1	5.0×10^3	8.0×10^3	9.35×10^5
2	3.0×10^3	7.0×10^3	1.071×10^4

Table S2. Quenching constant (K_q), binding constant (K_{bin}), and number of binding sites (n) for the interactions of complexes with BSA

Compound	K_b / mol^{-1}	K_{sv} / mol^{-1}	K_q / mol^{-1}	'n' value
1	8.3×10^5	1.156×10^6	1.156×10^{14}	2.306
2	6.16×10^5	1.060×10^6	1.060×10^{14}	2.264

Table S3. Kinetic parameters for complexes **1** and **2** in DMSO solution

Catalyst	$K_m / (\text{mol L}^{-1})$	$V_{max} / (\text{mol S}^{-1})$	K_{cat} / h^{-1}
1	105.08×10^{-4}	5.58×10^{-4}	105
2	104.64×10^{-4}	2.46×10^{-4}	104

Table S4. Phosphate hydrolysis kinetic parameters for complexes **1** and **2**

Catalyst	$K_m / (\text{mol L}^{-1})$	$V_{max} / (\text{mol S}^{-1})$	K_{cat} / h^{-1}
1	155.89×10^{-3}	1.605×10^{-3}	3117
2	52.07×10^{-3}	1.919×10^{-3}	1041

Table S5. *In vitro* cytotoxicity of the complexes in normal and HeLa cancer cell line

Complex	IC ₅₀ / μM^{a}	
	Vero	HeLa
1	52.31 \pm 2.41	18.74 \pm 2.14
2	54.24 \pm 3.65	22.34 \pm 2.42
Cisplatin ^b	–	13.00 \pm 2.01

^aFifty percent inhibitory concentration after exposure for 24 h in the MTT assay.