Supplementary materials

Bimetallic *bis*-Aroyldihydrazone-Isatin Complexes of High O=V(IV) and Low Cu(II) Valent Ions as Effective Biological Reagents for Antimicrobial and Anticancer Assays

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2.1. Devices and methodologies

The essential materials used in the current study (without rehandling) were obtained from various suppliers (BDH, Sigma-Aldrich and Merck). In particular, the main element percentages of C, H and N in H_2Lph, VOLph and CuLph were estimated at an ambient temperature within the V2.3 model of the GMBH varioEI device. For the determination of the melting and/or decomposition points, a Gallenkamp–Sanyo-type apparatus was utilized. Also, at 25 ºC, the molar conducting power of VOLph and CuLph (with concentration = 1.0×10^{-3} mol dm^{-3}) was studied in polar medium of *N*,*N*-dimethylformamide (DMF) or dimethyl sulfoxide (DMSO) using a Jenway conductivity meter apparatus. Studying the nuclear magnetic resonance spectroscopy (^{1}H- and ^{13}C-nuclei) for the ligand H_2Lph in DMSO-d_6 at 25 °C was achieved using an FT-NMR Bruker multinuclear spectrophotometric device (ARX400 model), in which the field magnetism for ^{1}H- and ^{13}C-nuclei was employed at 400.1 and 100.6 MHz, respectively. At 25 °C, FTIR spectra for H_2Lph, VOLph and CuLph (as solid samples) were studied using a FT-IR spectrophotometer from Agilent Technology (Cary-630 model). The electronic spectrometric titrations for the solutions in DMF with concentrations of 1.0×10^{-6} mol dm^{-3} for H_2Lph, VOLph and CuLph were examined at 25 °C using a Shimadzu spectrophotometer (UV-1800 model). MS (m/z) mass spectra for H_2Lph, VOLph and CuLph in DMF were obtained using a mass spectrometric machine (model of Qtof Micro YA263). Magnetic features of the studied complexes were evaluated based on a magnetic susceptibility balance (Sherwood Scientific).

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Table S1. Activity index (%) of the antibacterial assay for H_2Lph, VOLph and CuLph reagents.

	Activity index (%)		
Comp.	S. Marcescence (-ve)	E. Coli (-ve)	S. Aureus (+ve)
H_2Lph	47.5	48.7	41.3
VOLph	90.0	81.1	84.8
CuLph	87.5	78.4	82.6

Table S2. Activity index (%) of the antifungal assay for H_2Lph, VOLph and CuLph reagents.

	Activity index (%)		
Comp.	C. albicans	A. flavus	T. rubrum
H_2Lph	45.9	52.0	51.6
VOLph	67.6	80.0	90.3
CuLph	70.3	80.0	87.1

Table S3. *IC*$_{50}$, the antiproliferative index of H_2Lph, VOLph and CuLph reagents versus the current human cancer cell lines.

	IC$_{50}$ (μM)			
Comp.	HCT-116	MCF-7	HepG-2	WI-38
H_2Lph	67.56±0.12	43.00±0.55	56.75±0.50	128.15±0.25
VOLph	38.30±0.72	25.10±0.36	38.05±0.25	92.70±0.90
CuLph	39.09±0.64	25.25±0.45	37.80±0.45	117.36±0.33
Vinblastine	13.30±0.11	4.12±0.14	7.50±0.10	--

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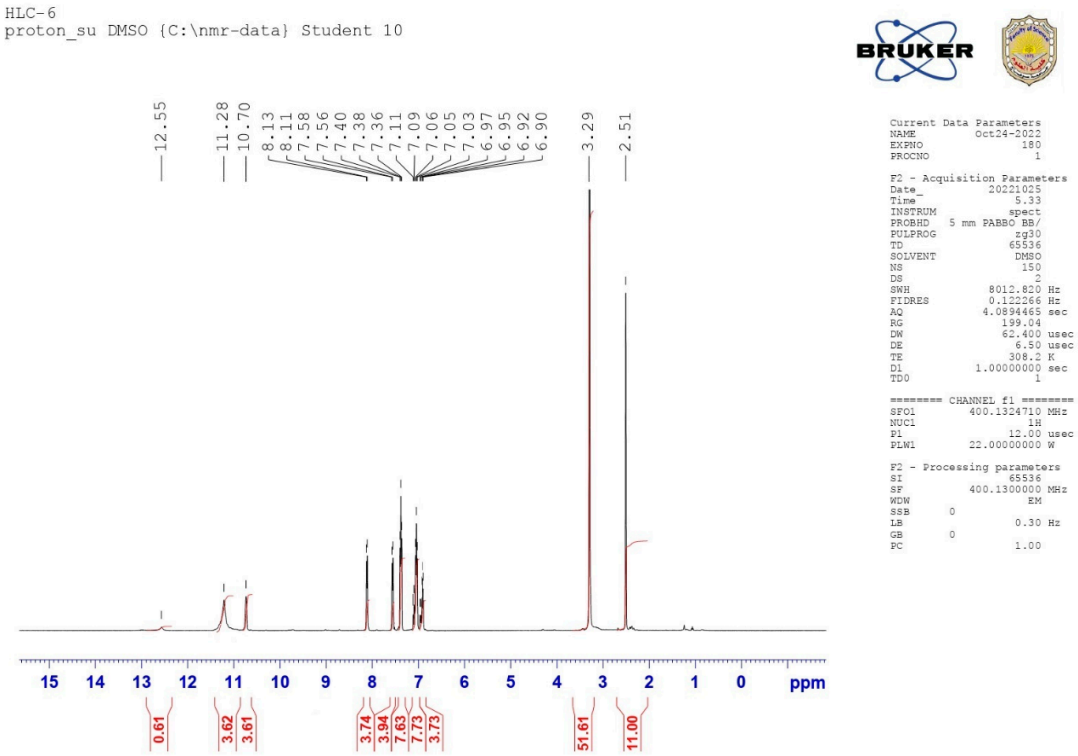
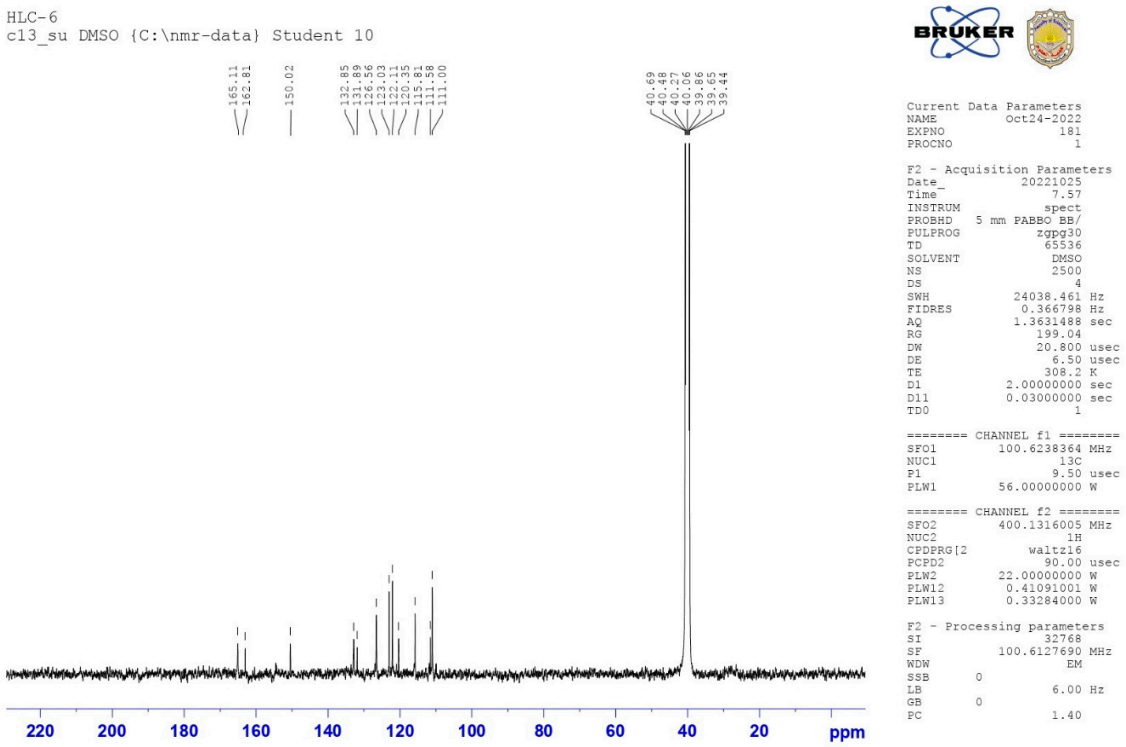


Figure S1. ^{1}HNMR spectrum of H_2Lph in DMSO-d_6 at 25 °C.

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PROCNO                 1

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DS                     4
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TD0                    1

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PLW12        0.41091001 W
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Figure S2. ^{13}CNMR spectrum of H_2Lph in DMSO-d_6 at 25 °C.

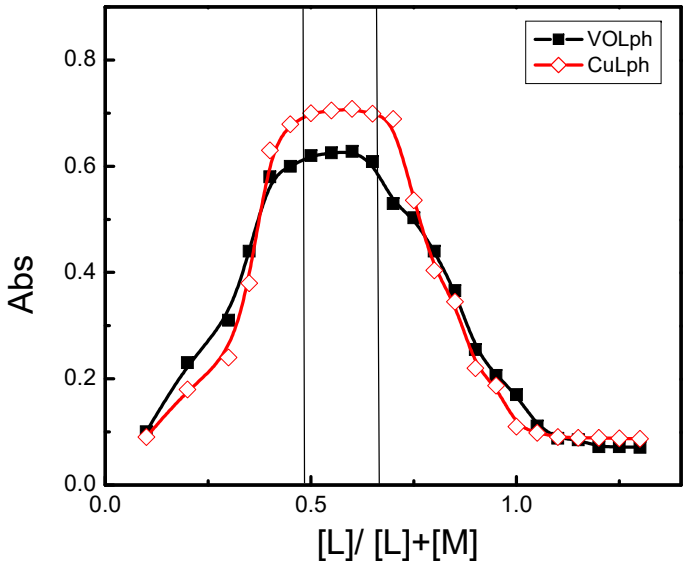

Figure S3. Continuous variation plot for the stoichiometric molar ratios for VOLph and CuLph complexation formed with H_2Lph in DMF media at [L] = [VO^{2+}] or [Cu^{2+}] = 1 × 10^{-5} mol dm^{-3} and 25 °C.

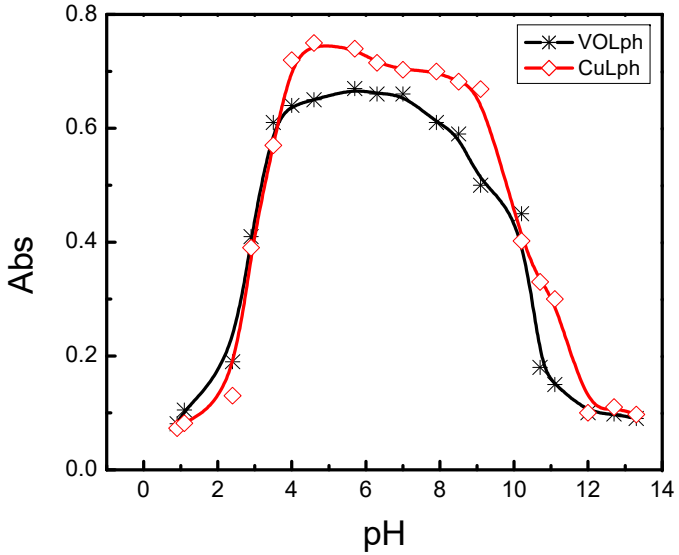

Figure S4. pH effect stability of an DMF solution of VOLph and CuLph complexes.

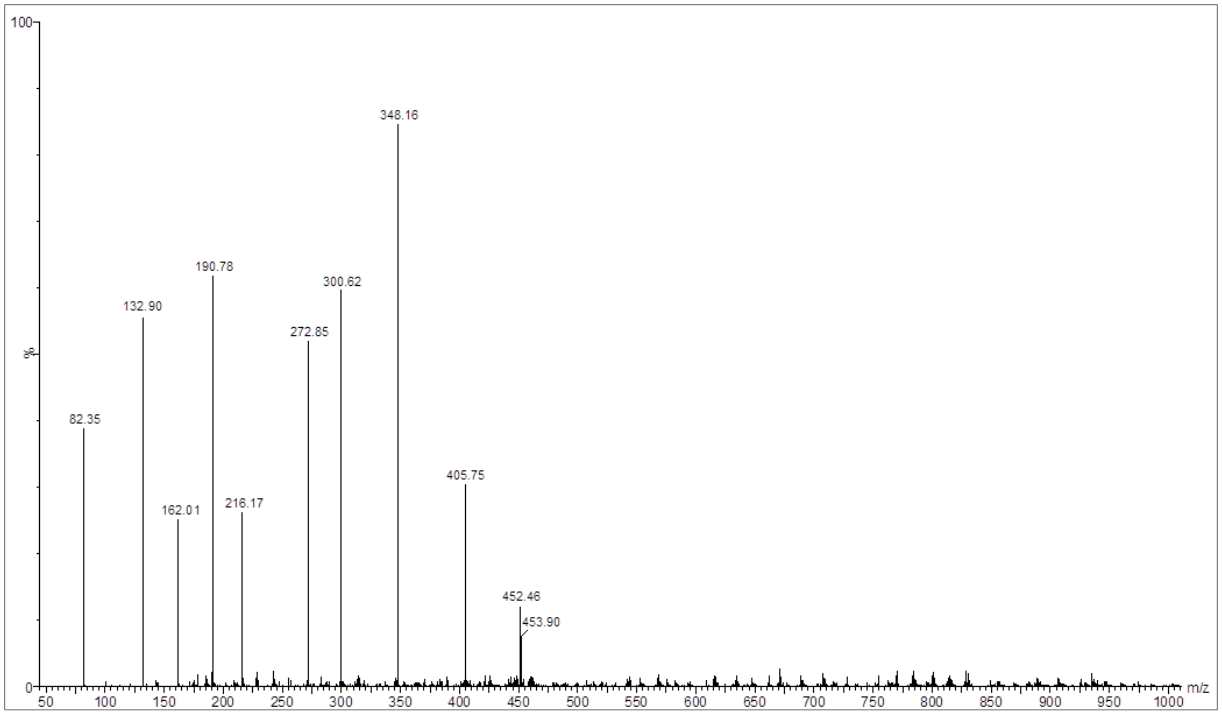

Figure S5. EI-Mass spectrum of H_2Lph in DMF media at 25 °C.

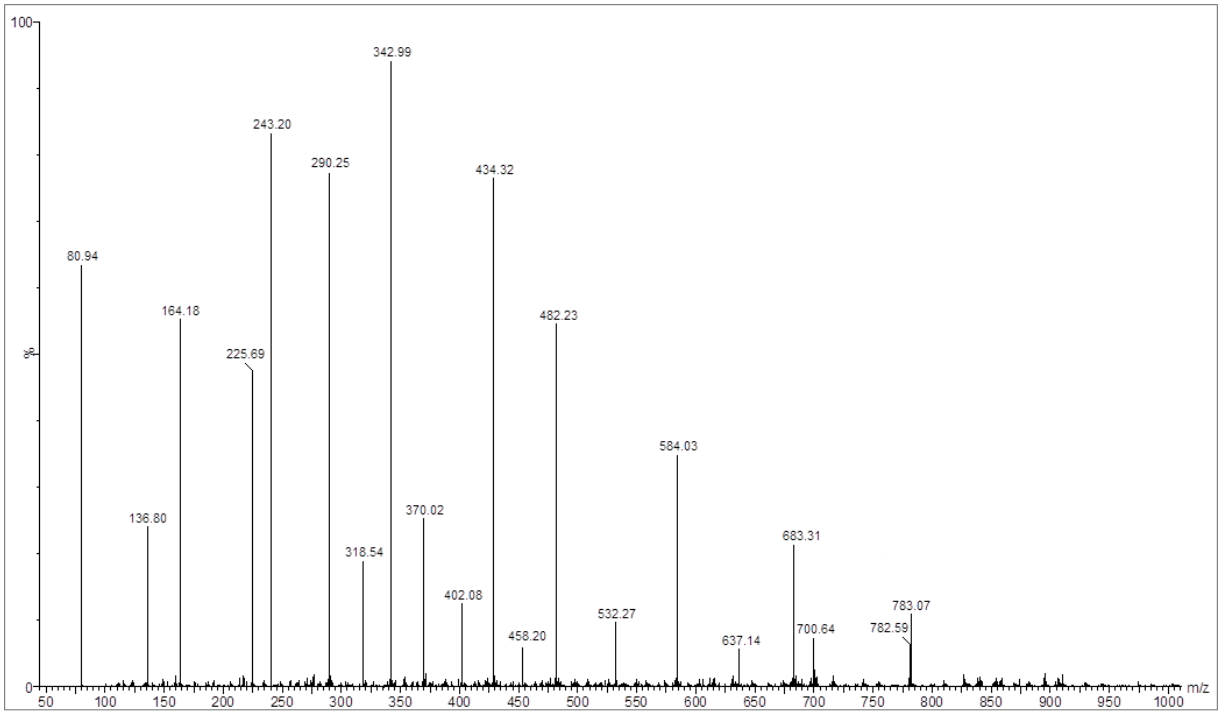

Figure S6. EI-Mass spectrum of VOLph in DMF media at 25 °C.

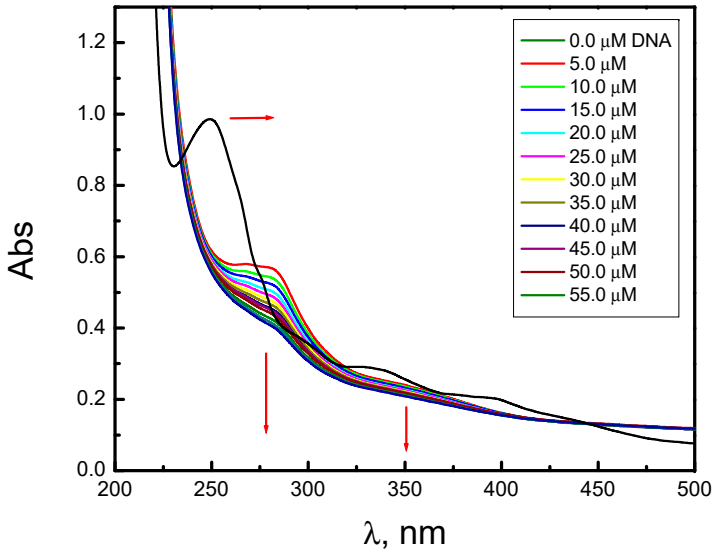

Figure S7. The spectral changes for the electronic transitions for H_2Lph solutions with [DNA] of different *ct*DNA concentrations in DMSO, in μM (at 25 °C).