



## Original Article

# Voltammetric Analysis of Lead Nitrate with Various Ligands in Aqueous Solutions at 302.15 K

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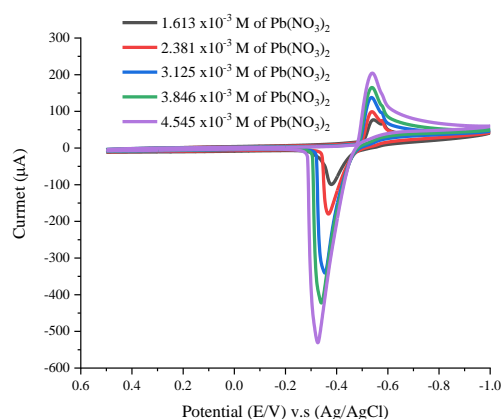
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## ABSTRACT

The cyclic voltammetry of different concentrations of lead nitrate was studied in 0.1 M NaCl as aqueous solution in absence and presence of Favipiravir or Fuchsine at 302.15 K using (glassy carbon electrode, GCE) as a working electrode. Favipiravir and Fuchsin were used as complex materials. The effect of different scan speed was studied and the evaluated data were discussed. The different solvation, kinetic and thermodynamic parameters were also evaluated from the cyclic voltammograms to find weak interaction between Favipiravir with lead ions than that of Fuchsin.

## GRAPHICAL ABSTRACT



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## Introduction

Electro-voltammetry is an electrochemical technique that involves the application of a potential waveform to study the redox behavior of a species in solution. It provides information about the electrochemical properties of a substance such as oxidation, reduction potentials, diffusion coefficients, and electron transfer kinetics [1, 2].

Lead ions ( $\text{Pb}^{2+}$ ) can be studied by cyclic voltammetry to understand their redox behavior and electrochemical properties. Lead (II) is a hard acceptor; it forms stronger complexes with nitrogen and oxygen electron-donating ligands [3-6]. The cyclic voltammetry of lead ions typically shows two well-defined peaks corresponding to the oxidation and reduction reactions. The importance of lead ions cyclic voltammetry is the investigation of redox potentials of lead species, the kinetics of electron processes, and the mechanism of redox reactions. Furthermore, the aim of environmental monitors lead toxic heavy metal that contaminates water. By measuring the current response of lead ions at different potentials, it is possible to determine the lead concentration and assess the level of environmental pollution. This information aids to monitor and control lead contamination. Cyclic voltammetry can be employed to evaluate the performance of different electrode materials for lead ion detection. Electrochemical energy batteries can also applied to investigate the electrochemical behavior of lead-based electrodes. There are many applications can be used from applying cyclic voltammetry of lead ions.

It can be initially used in environmental analysis as waste water or soil for monitoring contamination levels and assessing potential health risks. Secondly, in electrodeposition was carried out to optimize electrodeposition processes for lead-based materials. By studying the reduction behavior of lead ions, suitable deposition conditions can be determined as potential range and deposition time to achieve desired material properties. Thirdly, it is used in corrosion studies to investigate the corrosion behavior of lead-based materials to assess the

corrosion resistance and stability of some materials.

Fourthly, in batteries which provides insights into the electrochemical performance and degradation mechanisms of the batteries by studying the redox reactions involving lead ions. Fifthly, in the analytical chemistry study to determine trace amounts of lead ions by comparing the peak currents or potential obtained from sample with those of known standard; therefore, the corresponding concentration of lead ions can be estimated. Overall cyclic voltammetry is a versatile technique that can be applied to study the electrochemical behavior of lead ions [7-16]. Overall, cyclic voltammetry offers a powerful approach to investigate the electrochemical properties of mercuric chloride and has numerous applications in environmental monitoring, material characterization and analytical chemistry. New applications for cyclic voltammetry as using Silver nanoparticles decorated functionalized multiwalled carbon nanotubes modified screen printed as sensor for the voltammetric determination of butorphanol [17]. Recent work in cyclic voltammetry is preparation of new electrochemical sensor for the detection of ketoconazole using carbon paste electrode modified with sheaf-like Ce-BTC MOF nanostructure and ionic liquid [18]. New work about voltammetric determination of hydrochlorothiazide at a modified carbon paste electrode with polypyrrole nanotubes was done [19]. New voltammetric determination of vitamin B6 in the presence of vitamin C based on zinc ferrite nano-particles modified screen-printed graphite electrode was done recently [20]. Application of electrochemical sensor for determination of butylated hydroxyanisole in real samples using glassy carbon electrode modified by  $[\text{Co}(\text{HL})_2\text{Cl}_2]$  nano-complex application was done [21].  $\text{CuFe}_2\text{O}_4$  nanoparticles-based was prepared as electrochemical sensor for sensitive determination of the anticancer drug 5-fluorouracil [22].

Favipiravir is an antiviral medication and has been approved to treat influenza in Japan [23]. It

has been also studied to treat a number of other viral infections as SARS-CoV-2 [24]. Coronavir is the brand name of favipiravir that used in Russia and it has been approved for the treatment of COVID-19 in several countries as Turkey, Japan, India, Thailand, and Serbia under emergency provisions [25-28].

Fuchsine has been used to stain bacteria and sometimes as a disinfectant. It becomes magenta when dissolved in water to form dark green crystals.

By dying textiles, combustible at high temperature, slightly explosive around open flames and sparks. It has been well established that production of fuchsine results in development of bladder cancers by production workers. Magenta production is listed as a circumstance known to result in cancer [29-33].

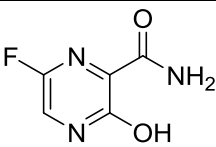
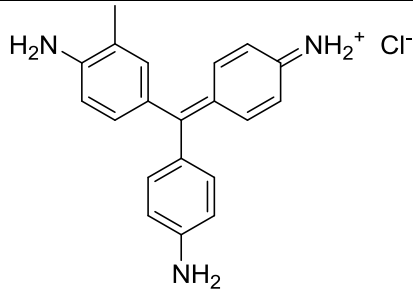
In this work, the cyclic voltammetry of different concentrations of lead nitrate was studied in 0.1 M NaCl as aqueous solution in absence and presence of Favipiravir or Fuchsine as complex materials at 302.15 K using (glassy carbon electrode, GCE) as a working electrode.

## Experimental

### Materials and Solvents

Pure lead nitrate salt  $\text{Pb}(\text{NO}_3)_2$  from Merck Company was used in the present study, Favipiravir and Fuchsine from Oxford Laboratory were used as ligands, pure sodium chloride salt (NaCl) from Adwic Company as a supporting electrolyte and prepared bi-distilled water with conductivity of  $3.2 \mu\text{S cm}^{-1}$  (Table 1).

**Table 1:** Structure of Favipiravir and Fuchsine

	Favipiravir	Fuchsine
Structure		
Formula	$\text{C}_5\text{H}_4\text{FN}_3\text{O}_2$	$\text{C}_{20}\text{H}_{19}\text{N}_3\cdot\text{HCl}$
Molar mass	157.104 g/mol	337.86 g/mol

### Cyclic voltammetric analysis (CV)

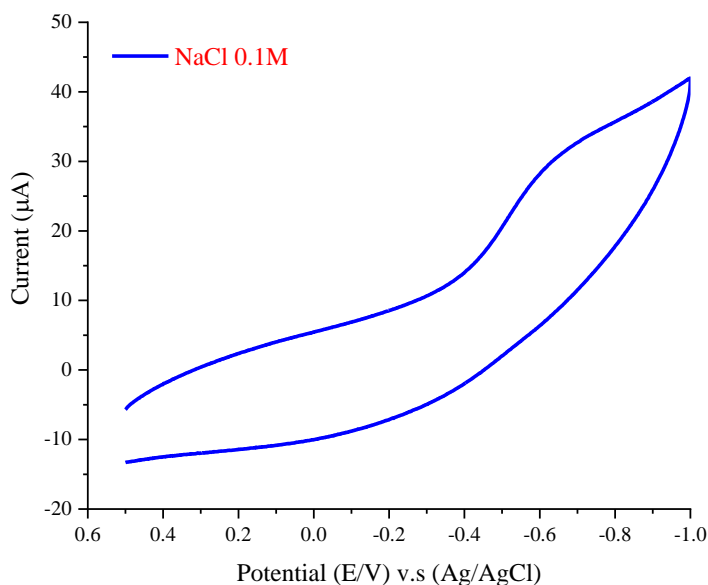
DY2000 multichannel potentiometer from USA was used for cyclic voltammetric studies. It was connected to a cell of three electrodes, reference electrode (silver/silver chloride put in saturated KBr solution), working electrode (glassy carbon electrode, GCE), and auxiliary electrode (platinum wire). Area of the working electrode was  $0.3 \text{ cm}^2$ . The system was applied from (0.5 to -1) V potential window and different scan rates (0.1, 0.05, 0.02, and 0.01) V/sec at 302.15 K. Finally, origin software was used to analyze data.

## Results and Discussion

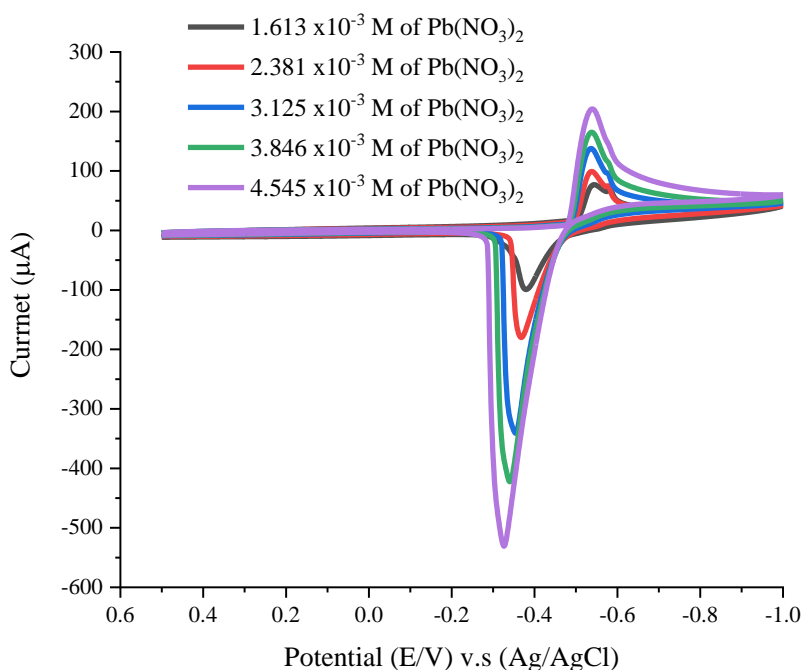
### Electrochemical behavior of lead ions alone at 302.15 K

### Cyclic voltammetric studies of different lead ions concentrations

First, cyclic voltammogram of 30 ml NaCl (0.1) M as a supporting electrolyte was measured from (0.5 to -1) V of potential window and scan rate 0.1 V/S at 302.15 K, as displayed in Figure 1, and then the lead nitrate solution  $\text{Pb}(\text{NO}_3)_2$  is added step wisely from 1 ml ( $1.613 \times 10^{-3}$ ) M to reach till 3 ml ( $4.545 \times 10^{-3}$ ) M, as depicted in Figure 2.



**Figure1:** Cyclic voltammogram of NaCl 0.1M at 302.15 K



**Figure 2:** Cyclic voltammogram of different  $\text{Pb}(\text{NO}_3)_2$  concentrations in NaCl 0.1M at 302.15 K

The redox mechanism of the used lead nitrate is happened through two electron mechanism for the reduction of lead ion  $\text{Pb}^{2+}$  to lead zero and the oxidation is the opposite one giving the oxidation mechanism. The observed waves were at -0.55 V for the reduction and at 0.3 V approximately for the reverse oxidation. Two electrons were used for the electro-behavior in this medium. The

electrochemical redox behavior of lead ions at the GCE was studied at the steady state current of the ions examined [34-43]. The calculated different solvation cyclic voltammetry and kinetic parameters of lead ions at 302.15 K using scan speed 0.1 V/S were presented in Table 2. It was observed increased of the analysis data by

increasing in lead ion concentrations supporting the diffusion effect.

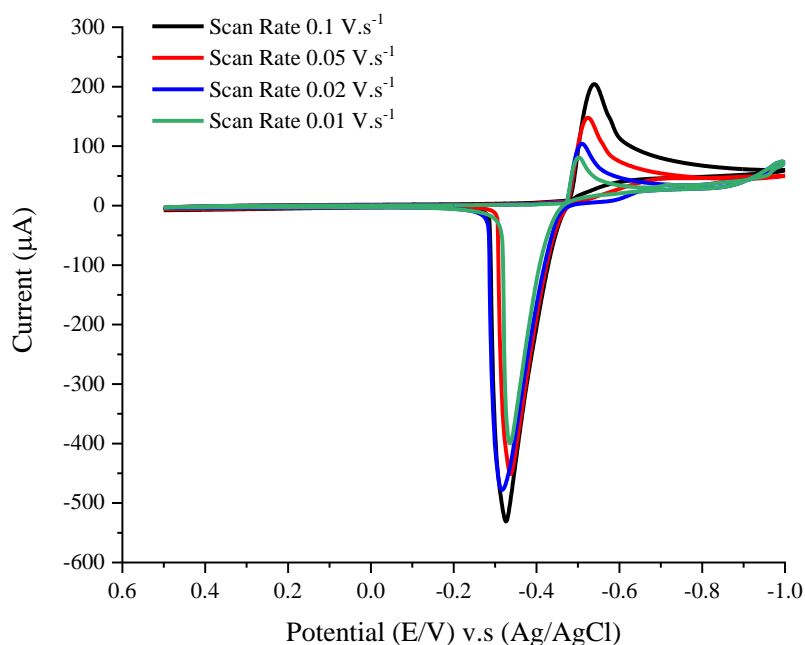
**Table 2:** Cyclic voltammogram of different  $\text{Pb}(\text{NO}_3)_2$  concentrations in NaCl 0.1M at 302.15 K

$[\text{M}] \times 10^{-3}$ (mol.Lit <sup>-1</sup> )	$E_{pa}$ (V)	$E_{pc}$ (V)	$(-)\text{I}_{pa}$ ( $\mu\text{A}$ )	$\text{I}_{pc}$ ( $\mu\text{A}$ )	$D_a \times 10^{-12}$ ( $\text{cm}^2.\text{s}^{-1}$ )	$D_c \times 10^{-13}$ ( $\text{cm}^2.\text{s}^{-1}$ )
1.613	-0.375	-0.542	123.10	68.04	1.135	3.470
2.381	-0.363	-0.541	194.60	92.07	1.303	2.916
3.125	-0.353	-0.537	306.80	125.30	1.879	3.133
3.846	-0.340	-0.536	416.10	160.50	2.283	3.398
4.545	-0.321	-0.531	507.70	192.30	2.433	3.490
$[\text{M}] \times 10^{-3}$ (mol.Lit <sup>-1</sup> )	$k_s \times 10^{-5}$ ( $\text{cm}.\text{s}^{-1}$ )	$\Gamma_a \times 10^{-9}$ (mol/ $\text{cm}^2$ )	$\Gamma_c \times 10^{-10}$ (mol/ $\text{cm}^2$ )	$(-)\text{Q}_a \times 10^{-4}$ (coulomb)	$(+)\text{Q}_c \times 10^{-5}$ (coulomb)	
1.613	1.327	1.107	6.120	0.641	3.543	
2.381	1.508	1.751	8.282	1.014	4.794	
3.125	1.760	2.759	11.27	1.597	6.522	
3.846	2.312	3.743	14.44	2.167	8.360	
4.545	3.080	4.567	17.30	2.644	10.01	

#### Study of different scan speed

The redox behavior of lead ions was studied in different scan speed (0.1, 0.05, 0.02, and 0.01) V/S at 302.15 K, as demonstrated in Figure 3. It

was observed that the solvation and kinetic parameters of different scan speed of lead ions were increased by decreasing in scan speed indicating diffusion controlled reaction, as presented in Table 3.



**Figure 3:** Different scan rate studies of  $(4.545 \times 10^{-3} \text{M}) \text{Pb}(\text{NO}_3)_2$  at 302.15K

**Table 3:** The solvation and kinetic parameters of different scan speed of  $(4.545 \times 10^{-3})$  M  $\text{Pb}(\text{NO}_3)_2$  at 302.15 K

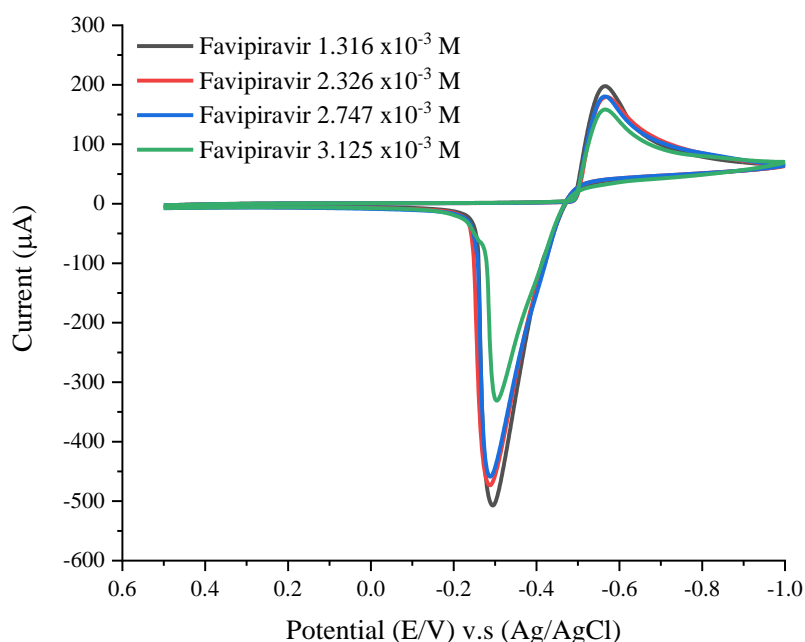
$\nu$	$E_{pa}$ (V)	$E_{pc}$ (V)	$(-I)_{pa}$ ( $\mu\text{A}$ )	$I_{pc}$ ( $\mu\text{A}$ )	$D_a \times 10^{-12}$ ( $\text{cm}^2.\text{s}^{-1}$ )	$D_c \times 10^{-13}$ ( $\text{cm}^2.\text{s}^{-1}$ )
0.1	-0.321	-0.531	507.70	192.30	2.433	3.490
0.05	-0.342	-0.523	395.70	140.50	2.956	3.726
0.02	-0.346	-0.512	347.00	97.80	5.682	4.521
0.01	-0.348	-0.502	327.90	73.16	10.15	5.052
$\nu$	$k_s \times 10^{-5}$ ( $\text{cm}.\text{s}^{-1}$ )	$\Gamma_a \times 10^{-8}$ ( $\text{mol}/\text{cm}^2$ )	$\Gamma_c \times 10^{-9}$ ( $\text{mol}/\text{cm}^2$ )	$(-) Q_a \times 10^{-3}$ (coulomb)	$(+) Q_c \times 10^{-4}$ (coulomb)	
0.1	3.080	0.457	1.730	0.264	1.001	
0.05	1.301	0.712	2.527	0.412	1.463	
0.02	0.687	1.560	4.402	0.903	2.548	
0.01	0.410	2.950	6.581	1.708	3.810	

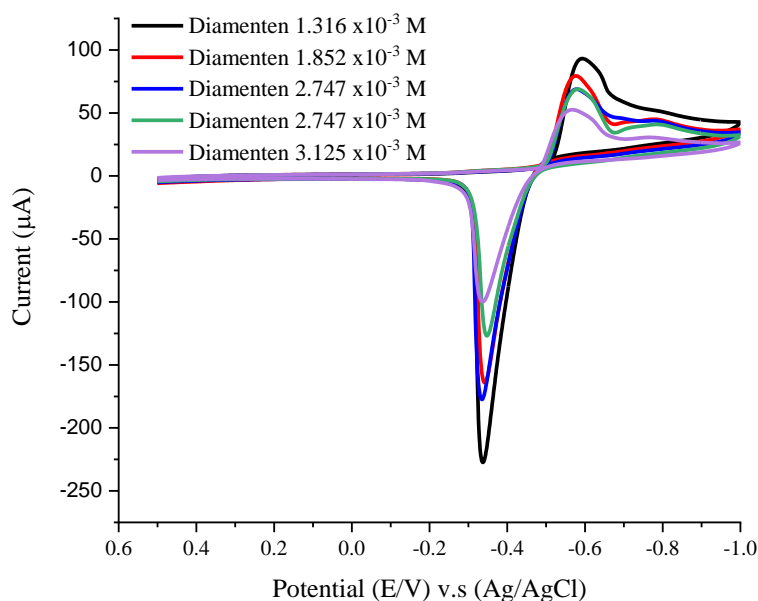
### Electrochemical behavior of lead ions in presence of ligand (Favipiravir or Fuchsine) at 302.15 K

The electrochemical behavior of the complexation between lead ions and Favipiravir or Fuchsine as complex materials in the supporting electrolyte NaCl (0.1) M at 302.15 K from (0.5 to -1) V potential windows and scan speed 0.1 V/S were studied, as shown in Figures 4 and 5. It was observed the formation of the

complex appear in decreasing the anodic and cathodic peak beside the potential shifts to new values.

The solvation and kinetic parameters of interaction of lead ions and different concentrations of Favipiravir or Fuchsine at 302.15 K and scan speed 0.1 V/S were decreased due to the complexation behavior, as listed in Tables 4 and 5.

**Figure 4:** Cyclic voltammograms for the interaction of lead ions and different concentrations of Favipiravir at 302.15K



**Figure 5:** Cyclic voltammograms for the interaction of lead ions and different concentrations of Fuchsin at 302.15 K

The great area under most figures especially Figure 5 for lead ions in presence of Fuchsin or

Favipiravir ligands indicate their uses for energy storage materials.

**Table 4:** The solvation and kinetic parameters of lead ions and different concentrations of Favipiravir at 302.15K

[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	E <sub>pa</sub> (V)	E <sub>pc</sub> (V)	(-)I <sub>pa</sub> (μA)	I <sub>pc</sub> (μA)	D <sub>a</sub> x10 <sup>-13</sup> (cm <sup>2</sup> .s <sup>-1</sup> )	D <sub>c</sub> x10 <sup>-14</sup> (cm <sup>2</sup> .s <sup>-1</sup> )
3.947	1.316	-0.297	-0.571	482.50	193.10	29.14	46.69
3.488	2.326	-0.290	-0.569	442.80	176.90	31.42	50.15
3.297	2.747	-0.289	-0.565	404.90	176.50	29.42	55.87
3.125	3.125	-0.287	-0.564	304.20	152.60	18.48	46.53
[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	k <sub>s</sub> Cx10 <sup>-5</sup> (cm.s <sup>-1</sup> )	Γ <sub>a</sub> x10 <sup>-9</sup> (mol/cm <sup>2</sup> )	Γ <sub>c</sub> x10 <sup>-10</sup> (mol/cm <sup>2</sup> )	(-) Q <sub>a</sub> x10 <sup>-4</sup> (coulomb)	(+) Q <sub>c</sub> x10 <sup>-5</sup> (coulomb)	
3.947	1.316	11.84	4.340	17.37	2.513	10.06	
3.488	2.326	13.55	3.983	15.91	2.306	9.212	
3.297	2.747	13.54	3.642	15.87	2.109	9.189	
3.125	3.125	12.63	2.736	13.73	1.584	7.948	

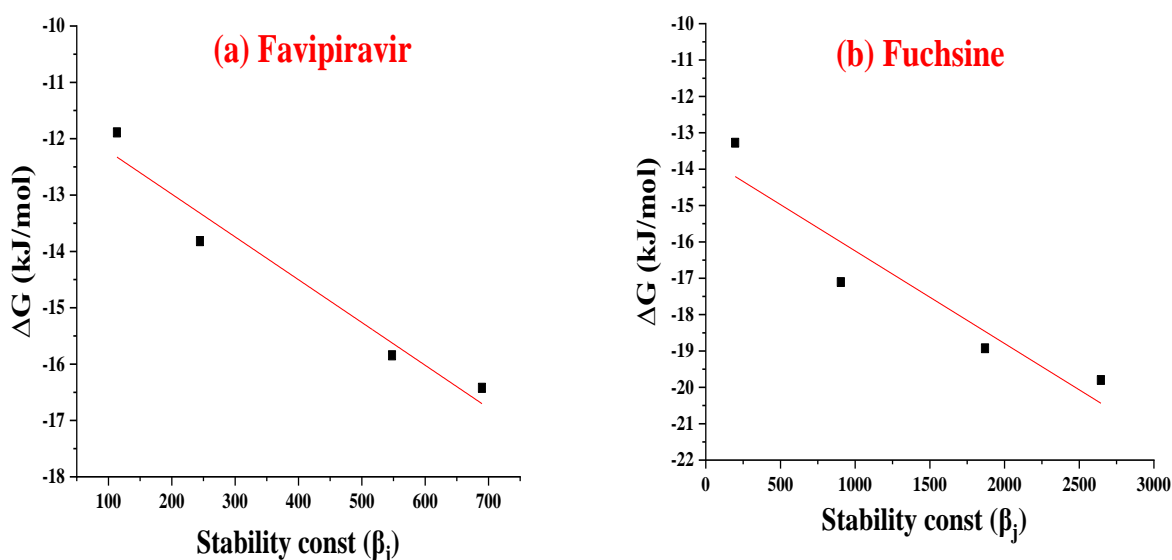
### Complexation functions

Different complexation parameters as the association, complexation stability constants (**B<sub>j</sub>**) and Gibbs Free energies (**ΔG**) of complexation were estimated following different literature references [44-48]. By drawing the relation between Gibbs free energy against stability constant of lead complexes, straight lines were

obtained, as illustrated in Figure 6. It was observed that the evaluated thermodynamic data greater for the interaction between Fuchsin with lead nitrate than that for the interaction between Favipiravir with lead nitrate indicating greater complex interaction for the first, as listed in Tables 6 and 7.

**Table 5:** The solvation and kinetic parameters of interaction of lead ions and different concentrations of Fuchisine at 302.15K

[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	E <sub>pa</sub> (V)	E <sub>pc</sub> (V)	(-)I <sub>pa</sub> (μA)	I <sub>pc</sub> (μA)	D <sub>a</sub> x10 <sup>-13</sup> (cm <sup>2</sup> .s <sup>-1</sup> )	D <sub>c</sub> x10 <sup>-14</sup> (cm <sup>2</sup> .s <sup>-1</sup> )
3.947	1.316	-0.341	-0.591	213.70	85.55	5.714	9.160
3.488	2.326	-0.347	-0.577	146.00	64.20	3.414	6.605
3.297	2.747	-0.348	-0.572	121.70	60.58	2.657	6.586
3.125	3.125	-0.339	-0.568	93.30	52.19	1.737	5.440
[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	k <sub>s</sub> Cx10 <sup>-5</sup> (cm.s <sup>-1</sup> )	Γ <sub>a</sub> x10 <sup>-9</sup> (mol/cm <sup>2</sup> )	Γ <sub>c</sub> x10 <sup>-10</sup> (mol/cm <sup>2</sup> )	(-) Q <sub>a</sub> x10 <sup>-4</sup> (coulomb)	(+) Q <sub>c</sub> x10 <sup>-5</sup> (coulomb)	
3.947	1.316	3.245	1.922	7.695	1.113	4.455	
3.488	2.326	1.901	1.313	5.774	0.760	3.343	
3.297	2.747	1.690	1.095	5.449	0.634	3.155	
3.125	3.125	1.715	8.389	4.695	0.486	2.718	

**Figure 6:** The relation between Gibbs free energy ( $\Delta G$ ) against stability constant ( $\beta_j$ ) in case of (a) lead complex with Favipiravir (b) lead complex with Fuchisine at 302.15K and scan rate 0.1 V/S**Table 6:** Thermodynamic parameters (Formal potential  $E^\circ$ , stability constant  $\beta_j$  and Gibbs free energy  $\Delta G$ ) for (1:1) lead ions complex with Favipiravir at 302.15K

[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	E <sup>o</sup> Metal (V)	E <sup>o</sup> complex (V)	j	Log[L]	Log $\beta_j$	$\beta_j$	$\Delta G$ (kJ/mol)
3.947	1.316	0.429	0.434	0.333	-2.881	1.127	13.4	-6.520
3.947	2.326	0.429	0.430	0.667	-2.633	1.772	59.2	-10.253
3.947	2.747	0.429	0.427	0.833	-2.561	2.068	116.8	-11.961
3.947	3.125	0.429	0.426	1.000	-2.505	2.388	244.6	-13.818

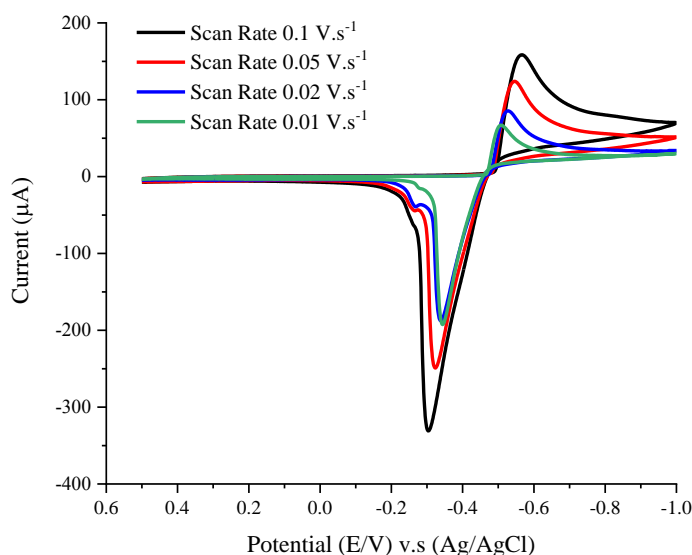
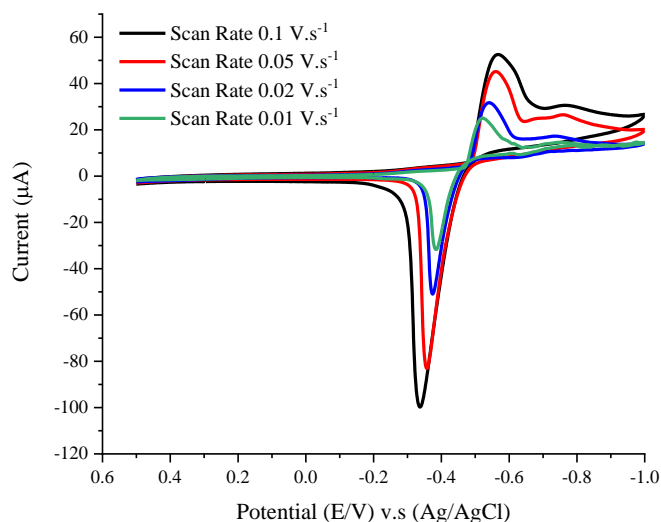
**Table 7:** Thermodynamic functions (Formal potential  $E^\circ$ , stability constant  $\beta_{MX}$  and Gibbs free energy  $\Delta G$ ) for (1:1) lead ions complex with Fuchsine at 302.15K

[M] $\times 10^{-3}$ (mol.Lit $^{-1}$ )	[L] $\times 10^{-3}$ (mol.Lit $^{-1}$ )	$E^\circ_{\text{Metal}}$ (V)	$E^\circ_{\text{complex}}$ (V)	j	Log[L]	Log $\beta_j$	$\beta_j$	$\Delta G$ (kJ/mol)
3.947	1.316	0.426	0.466	0.333	-2.881	2.294	197.0	-13.274
3.947	2.326	0.426	0.462	0.667	-2.633	2.956	904.6	-17.104
3.947	2.747	0.426	0.460	0.833	-2.561	3.272	1869.2	-18.928
3.947	3.125	0.426	0.454	1.000	-2.505	3.422	2645.0	-19.800

*Different scan speed study for (1:1) complex*

The effect of different scan speed on the interaction between lead ions and Favipiravir or Fuchsine was studied in different scan speed (0.1, 0.05, 0.02, and 0.01) V/S at 302.15 K, as illustrated in Figures 7 and 8. The solvation and

kinetic parameters of different scan speed for (1:1) complex were shown increase in their values by decreasing of the scan speed favoring more diffusion mechanism, as provided in Tables 8 and 9.

**Figure 7:** Different scan rate for (1:1) lead ions complex with Favipiravir at 302.15 K**Figure 8:** Different scan rate for (1:1) lead ions complex with Fuchsine at 302.15 K

**Table 8:** Different scan rate studies for (1:1) lead ions complex with Favipiravir at 302.15K

υ	[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	Ep <sub>a</sub> (v)	Ep <sub>c</sub> (v)	(-)Ip <sub>a</sub> (μA)	Ip <sub>c</sub> (μA)	D <sub>a</sub> x10 <sup>-13</sup> (cm <sup>2</sup> .s <sup>-1</sup> )	D <sub>c</sub> x10 <sup>-14</sup> (cm <sup>2</sup> .s <sup>-1</sup> )
0.1	3.125	3.125	-0.287	-0.564	304.20	152.60	18.48	46.53
0.05	3.125	3.125	-0.325	-0.548	233.10	121.30	21.71	58.80
0.02	3.125	3.125	-0.322	-0.527	174.40	82.61	30.36	68.14
0.01	3.125	3.125	-0.305	-0.507	167.60	64.50	56.12	83.08
υ	[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	k <sub>s</sub> C x10 <sup>-5</sup> (cm.s <sup>-1</sup> )	Γ <sub>a</sub> x10 <sup>-9</sup> (mol/cm <sup>2</sup> )	Γ <sub>c</sub> x10 <sup>-10</sup> (mol/cm <sup>2</sup> )	(-) Q <sub>a</sub> x10 <sup>-4</sup> (coulomb)	(+) Q <sub>c</sub> x10 <sup>-5</sup> (coulomb)	
0.1	3.125	3.125	12.63	2.736	13.73	1.584	7.950	
0.05	3.125	3.125	3.595	4.194	21.83	2.428	12.64	
0.02	3.125	3.125	1.759	7.842	37.15	4.540	21.51	
0.01	3.125	3.125	1.341	15.08	58.02	8.729	33.59	

**Table 9:** Different scan rate studies for (1:1) lead ions complex with Fuchsine complex at 302.15K

υ	[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	Ep <sub>a</sub> (v)	Ep <sub>c</sub> (v)	(-)Ip <sub>a</sub> (μA)	Ip <sub>c</sub> (μA)	D <sub>a</sub> x10 <sup>-13</sup> (cm <sup>2</sup> .s <sup>-1</sup> )	D <sub>c</sub> x10 <sup>-14</sup> (cm <sup>2</sup> .s <sup>-1</sup> )
0.1	3.125	3.125	-0.339	-0.568	92.20	45.48	1.697	4.130
0.05	3.125	3.125	-0.360	-0.559	77.10	38.05	2.376	5.783
0.02	3.125	3.125	-0.373	-0.540	42.90	26.52	1.838	7.022
0.01	3.125	3.125	-0.386	-0.519	23.90	21.21	1.143	8.985
υ	[M] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	[L] x10 <sup>-3</sup> (mol.Lit <sup>-1</sup> )	k <sub>s</sub> C x10 <sup>-5</sup> (cm.s <sup>-1</sup> )	Γ <sub>a</sub> x10 <sup>-9</sup> (mol/cm <sup>2</sup> )	Γ <sub>c</sub> x10 <sup>-10</sup> (mol/cm <sup>2</sup> )	(-) Q <sub>a</sub> x10 <sup>-4</sup> (coulomb)	(+) Q <sub>c</sub> x10 <sup>-5</sup> (coulomb)	
0.1	3.125	3.125	1.491	0.829	4.091	0.480	2.368	
0.05	3.125	3.125	0.704	1.388	6.845	0.803	3.963	
0.02	3.125	3.125	0.269	1.929	11.93	1.117	6.905	
0.01	3.125	3.125	0.114	2.152	19.08	1.246	11.05	

### Molecular docking of Favipiravir drug with viral protein 8JOP

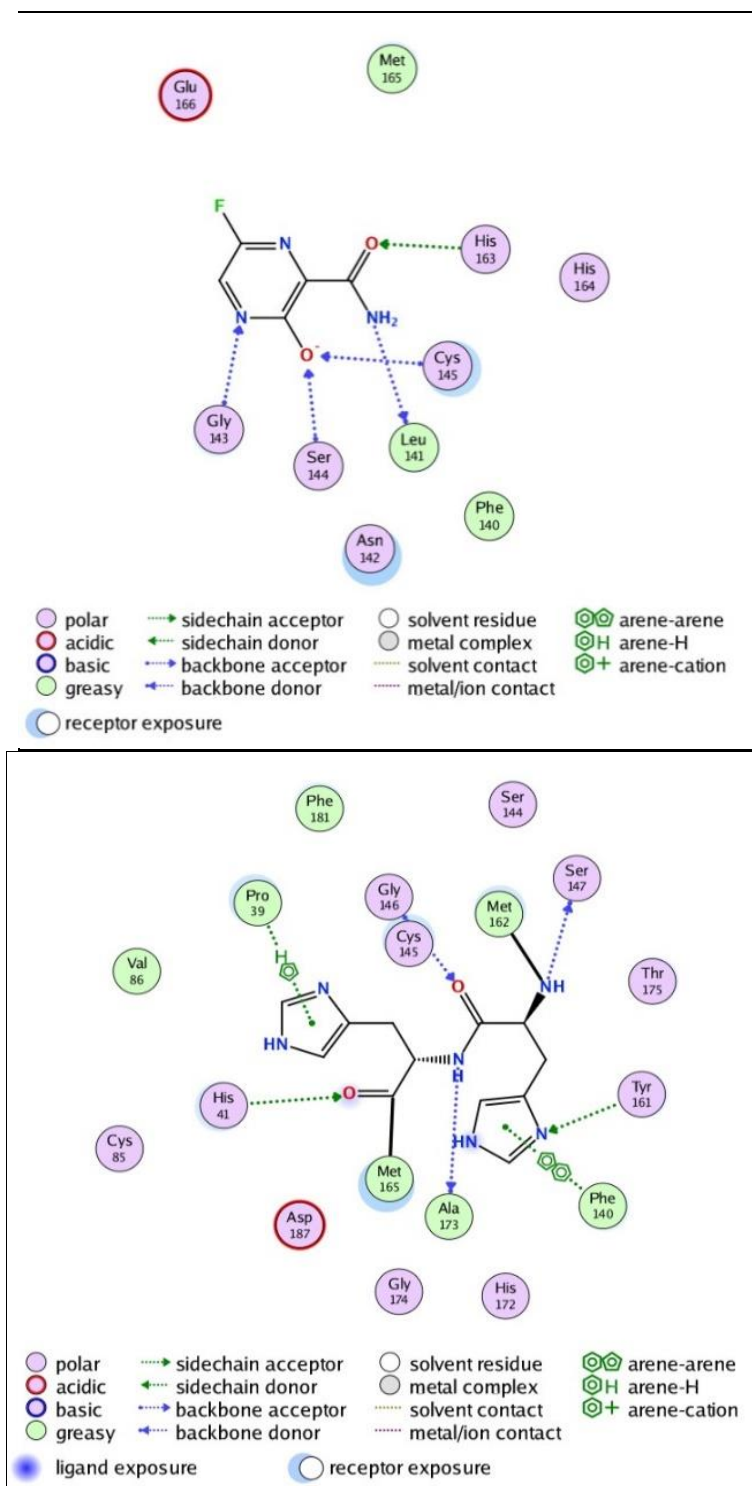
Since Favipiravir drug is an antiviral medication so, it can be used as an application for theoretical docking study with viral proteins as the spike protein of SARS-CoV-2 (8JOP) which causes COVID-19.

Docking with viral protein (8JOP) is a computational technique used to predict the binding interactions between the viral protein and potential drug molecules. This approach plays a crucial role in drug discovery and development, as it helps researchers to identify potential therapeutic compounds that can inhibit the function of viral proteins replication. Some of the uses of docking with viral protein (8JOP) are in the drug discovery to screen large databases of small molecules, natural compounds or existing drugs to identify potential candidates that can

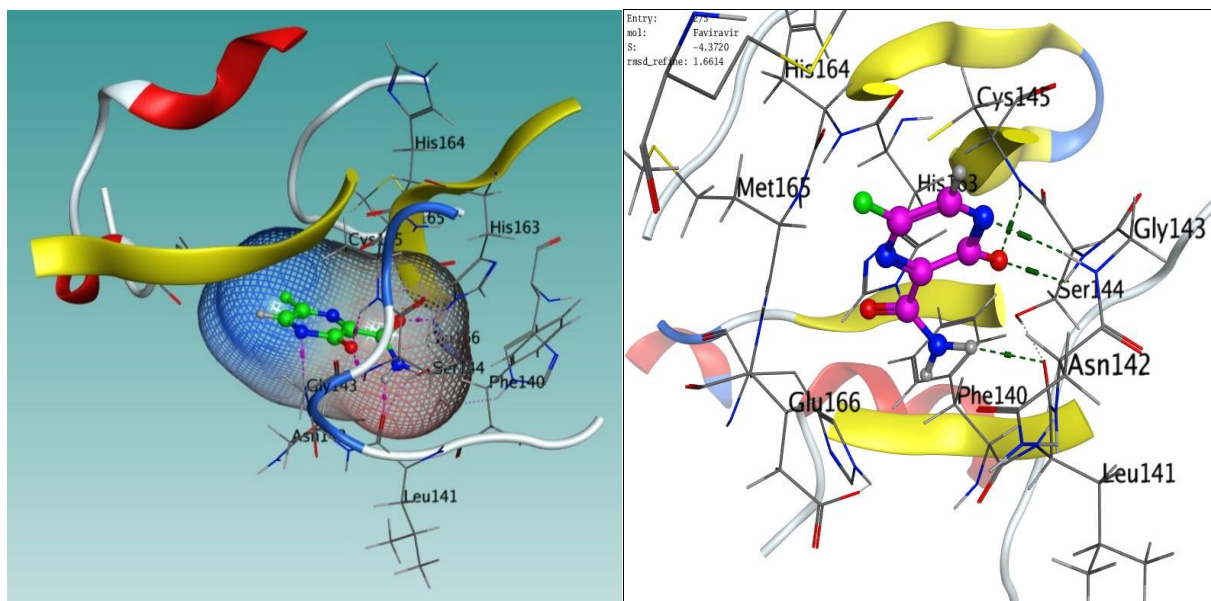
bind to the protein and interfere with its function. Secondly in virtual screening, since docking can be used to virtually screen large libraries of compounds to identify those with the highest binding affinity to the spike protein. This enables researchers to select the more promising compounds for further testing. Thirdly in binding mode analysis, since docking provides insights into the binding modes and interactions between the spike protein and potential inhibitors. Fourthly in structurebased drug design, since the three-dimensional structure of spike protein obtained from experimental techniques like x-ray crystallography can be used for docking studies. This allows researchers to design and optimize drug structure. Fifthly in vaccine design, since docking studies can aid in vaccine design by predicting the binding interactions between the spike proteins and neutralizing antibodies.

Molecular Operating Environment (MOE) [48, 49] was performed to rationalize the interaction between Favipiravir drug and (8JOP) receptor, as depicted in Figure 9. The binding modes between Favipiravir drug and active sites of different proteins of SARS-CoV-2 (8JOP) were also

predicted using MOE, as shown in Figure 10. The docking of Favipiravir drug with active sites of SARS-CoV-2 (8JOP) revealed forming of H-acceptor bonds of the type electrostatic energy giving good energy values till -1.9 kcal/mol, as presented in Table 10.



**Figure 9:** The 2D interaction between Favipiravir drug and (8JOP) receptor



**Figure 10:** The binding modes (3D) between Favipiravir drug and different proteins of SARS-CoV-2 (8JOP)

**Table 10:** Interaction parameters between Favipiravir drug and active sites of the spike protein of SARS-CoV-2 (8JOP)

Ligand		Receptor		Interaction	Distance	E (kcal/mol)
N	6	O	LEU 141	H-donor	3.15	-0.8
O	2	N	SER 144	H-acceptor	2.92	-1.7
O	2	N	CYS 145	H-acceptor	3.12	-1.9
O	3	NE2	HIS 163	H-acceptor	3.04	-1.0
N	4	N	GLY 143	H-acceptor	3.45	-1.5

## Conclusion

- 1- Solvation parameters for lead nitrate increased by increasing its concentrations due to the diffusion and pre-concentration reaction.
- 2- Sharp detection of reduction and oxidation peaks for lead nitrate alone and in presence of the used ligands indicating selective lead ion waves.
- 3- Effect of different Favipiravir and Fuchsine concentrations on lead nitrate were studied cyclic voltammetrically to find decrease in most solvation parameters by increasing ligand concentrations indicating complexation reactions.
- 4- Effect of different scan speed on interaction between lead nitrate and Favipiravir or Fuchsine were studied decreased by increasing in scan speed indicating reversibility of the waves.
- 5- The stability constants and Gibbs free energies of complexation are found to be greater for interaction of Fuchsine with lead nitrate than that

for interaction of Favipiravir with lead nitrate favoring more complexation for the first one.

- 6- Molecular docking of Favipiravir drug with active sites of SARS-CoV-2 (8JOP) revealed forming of H- acceptor bonds of the type electrostatic energy giving good energy values.
- 7- The great area of all figures here indicate their uses for energy storage for lead ions in the presence of the two ligands used.

## Highlights

- 1- Estimation of the cyclic voltammetry data for redox reaction of lead nitrate alone and in presence of ligand Favipiravir or Fuchsine.
- 2- Study the different scan speed for lead nitrate in 0.1 M NaCl alone and in presence of ligands Favipiravir or Fuchsine.
- 3- Estimation of the stability constants and Gibbs free energies of complexation for (1:1) complexes for metal to ligand.

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