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Homology Modelling and Molecular Docking Study of Voltage Gated Ion Channels for their Role in Plant Abiotic Stress

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ABSTRACT

Voltage-gated ion channels (VGICs) are responsible for generation of electrical signals in cell membranes. They exist mainly in three major forms namely, VGKC (Voltage-gated potassium channel), VGCC (Voltage-gated calcium channel), and VGSC (Voltage-gated sodium channel). VGICs have been studied extensively in animal system, especially for their role in electrical signalling during nerve conduction. Their existence in plant system has been related from very early period of evolution but their role in plant system has not been studied intensively and is a less explored area. Therefore, the present study was undertaken to investigate the role of VGICs in plant stress response, abiotic stress in particular, using *in-silico* tool of docking simulation. No solved crystal structure of plant VGICs were available at Protein Databank for the purpose of docking studies. Therefore, 3D-structures of three different VGICs (VGCC, VGKC and VGSC) were constructed using homology modelling tool of SWISS-MODEL and were selected after structure evaluation. These structures were subjected to docking simulation against major soil salts and fertilizers. While conducting molecular docking simulation studies, it was observed that VGICs seems to have negligible role in simple salts physiology like NaCl or KCl, while VGKC showed good binding pattern with ammonium nitrate and ammonium sulfate, reflecting its significant role in ammonium -ion physiology. Also, phosphoric acid binding was found significant towards VGKC. Superphosphate ions and Calcium nitrate showed a good binding pattern towards VGCC while VGSC showed good affinity for nitrate, phosphate, sodium and ammonium–ions. Also, during simulated annealing docking, it was observed that binding of phosphoric acid (or phosphate ion) increased at both extreme temperature ends (lower and higher). The study has provided a good platform for further investigation to establish the role of VGICs in plant stress response and correlated to other living systems like animals, fungi, etc.

1. INTRODUCTION

Voltage gated ion channel have a crucial role in excitable cells, allowing a rapid and co-ordinated depolarization in response to triggering voltage change [1]. The first voltage-dependent ion channel that was isolated and purified was extracted from the eel electroplax where there is a large concentration of Na channels [2]. Several years later, the sequence of the eel Na channel was deduced from its mRNA [3]. The first K^+ channel sequence was deduced from the *Shaker* mutant of *Drosophila melanogaster* [4]. These initial sequences were the basis to subsequent cloning of a large number of Na, K and Ca channels in many different species. VGICs are of great importance in plants as they are involved in many activities for instance like voltage gated calcium channel (VGCC) are involved in maintaining cellular homeostasis, signal transduction etc. Salinisation of agricultural land threatens world food production because it exposes crops to low water potential and high concentration of toxic ions in the soil. In particular, all major crops are sensitive to high concentrations of sodium (Na^+) [5]. Due to the negative electrical potential inside cells Na^+ influx into plant roots can occur through ion channels or other membrane transport proteins that facilitate passive diffusion of Na^+ across the plasma membrane.

The combined evidence suggests that cytoplasmic Na^+ concentrations are generally in the low millimolar range. This is in accordance with the notion that cytoplasmic Na^+ concentrations above 100 mM are toxic due to the detrimental effects of a high Na^+ environment to protein stability [6] and displacement of K^+ from essential co-factor binding sites on K^+-dependent enzymes [7]. Numerous pharmacological and cell biological studies have suggested that voltage-dependent Ca^{2+} channels in the plasma membrane are important for initiation of plant responses to environmental, hormonal, and pathogenic signals [8].

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Direct measurements of such channels in plant cells have been reported recently in patch clamp studies [9], radioactive tracer flux studies using plasma membrane vesicles [10,11], and reconstitution studies [12]. These plant Ca^{2+} channels are activated by membrane depolarization, a characteristic typical of voltage-dependentCa^{2+} channels in other systems. Voltage gated potassium channels (VGKC) are involved in regulation of cell volume and the flow of salt across epithelia. Moreover (VGCC) are also involved in opening and closure of stomatal aperture in response to stress conditions [13].

Voltage-gated Ca^{2+}channel from guard cells are involved in early events of plant hormone-induced responses [14-16]. VGCC from Arabidopsis roots and *Daucus carota* suspension protoplasts have been shown to be involved in cation uptake, maintaining appropriate electrochemical gradients important for the transport of other ions and cell volume regulation and signalling mechanisms and priming the cell for response [17, 18].

The abiotic stress is considered as the inappropriate condition for the living organism in its environment caused by non-living factors or "environmental factors". In plants, these factors confer an adverse affect on the growth rate and the productivity of the crops. It is, thus important to study the role of abiotic stress in plant system [19]. So the present study was carried out to investigate plant VGICs structures and their functional correlation in abiotic stress in plant system using *in-silico* tool of molecular docking simulation.

2. MATERIALS AND METHODS

2.1 Collection of protein sequence data of plant VGICs

The protein sequence of plant VGICs was collected from NCBI [20]. A total of 15 different sequence entries for VGKC were found and retrieved, out of which the sequence of AtKAT1 *Arabidopsis thaliana*gi| 44888080| sp| Q39128.2| KAT1_ARATH was selected for further studies. Similarly 8 different protein sequence for VGCC were retrieved out of which AtTPC1 *Arabidopsis thaliana* gi|75166464|sp|Q94KI8.1| was selected and 4 different protein sequence for VGSC were found and retrieved out of which VGSC superfamily *Micromonaspusilla* CCMP1545 gi|303285434|ref|XP_003062007.1| was selected for further studies.

2.2 Homology modelling

Homology modelling of the VGIC-proteins was done since no native solved crystal structure of the plant VGICs was available in PDB. The structures of the VGKCs, VGCCs and VGSCs, selected above, were generated using the SWISS MODEL [21] in auto-template mode. The generated models were evaluated using WHAT IF online server [22] for each of the protein models. The different evaluated models, each for VGKCs, VGCCs and VGSCs were selected thus obtained were energy minimised using UCSF-Chimera [23].

2.3 Docking analysis of VGICs with soil salts and fertilisers

For the docking analysis, the structures of the ligands namely the salts- KCl and NaCl and fertilisers namely- $(NH_4)_2SO_4$, urea, NH_4NO_3, single super phosphate, triple super phosphate (TSP), H_3PO_4, $Ca(NO_3)_2$, KNO_3, mono-ammonium phosphate, diammonium phosphate monocalcium phosphate and K_2SO_4 were constructed and energy minimized using the Chemsketch [24] software.

After structure optimization, these structures were converted in .pdb file format using Open Babel [25] software and further energy minimized using UCSF-Chimera. These energy minimized ligands were docked against the modelled protein namely AtKat1 (VGKC of *A. thaliana*), AtTpc1 (VGCC of *A. thaliana*) and Mpccmp1545 (VGSC of *M. pusilla*) and the interacting residues and the binding energy were noted. For this Autodock 4.2 [26] was used to prepare, run and analyse the docking simulations.

Lamarckian model of genetics, were used in which environmental adaptations of an individual's phenotypes are reverse transcribed into its genotype and become heritable traits. Only polar hydrogen was added to the protein and Kollman and Gastegier charges were assigned. The spacing between grid points was set to default value of 0.375Å. The grid box was set to 480 $\times$ 260 $\times$ 280 (x, y and z axis) to include all the amino acid residues that were present in protein. A total of 50 independent runs were performed with a step sizes of 0.2 Å for translations and 5^0 for orientations and torsions. The maximum number of generations was set to 1000 and maximum number of top individuals that automatically survived was set to 1 with mutation rate of 0.02, crossover rate of 0.8, cluster tolerance 0.5 Å, external grid energy 1000.0.

2.4 Simulated annealing using Autodock was done at different temperatures

The docking simulation was performed for selected ligands against all the three modelled VGICs, as referred above, using simulated annealing method for analysing the effect of temperature on binding pattern of these proteins for ligands. The selection of ligands was made on the basis of lower binding energies obtained when docked using Lamarckian model of genetics. For this purpose, NaCl, H_3PO_4, TSP, $(NH_4)_2SO_4$ and NH_4NO_3 were selected as ligands while the simulated annealing docking studies were done at 8 different temperatures- 10°C, 15°C, 25°C, 30°C, 35°C, 40°C, 45°C and 50°C and the binding energy were noted.

3. RESULTS AND DISCUSSION

3.1 Homology modelling

The structures of the selected VGICs, namely VGKC (AtKAT1 *Arabidopsis thaliana*gi| 44888080| sp| Q39128.2|), VGCC (AtTPC1 *Arabidopsis thaliana* gi|75166464|sp|Q94KI8.1|) and VGSC (*Micromonaspusilla* CCMP1545 gi|303285434 |ref|XP_003062007.1|) were generated using the SWISS MODEL

in auto-template mode. These models (Figure 1a-c), when evaluated using online WHAT-IF server, showed the Q-mean score, Z-score Ramachandran and Z-score that reflects the acceptability of the models (Table 1). Hence they were used for further docking studies after energy minimization and dockprep using UCSF-Chimera.

3.2 Docking analysis of VGICs with soil salts and fertilizers

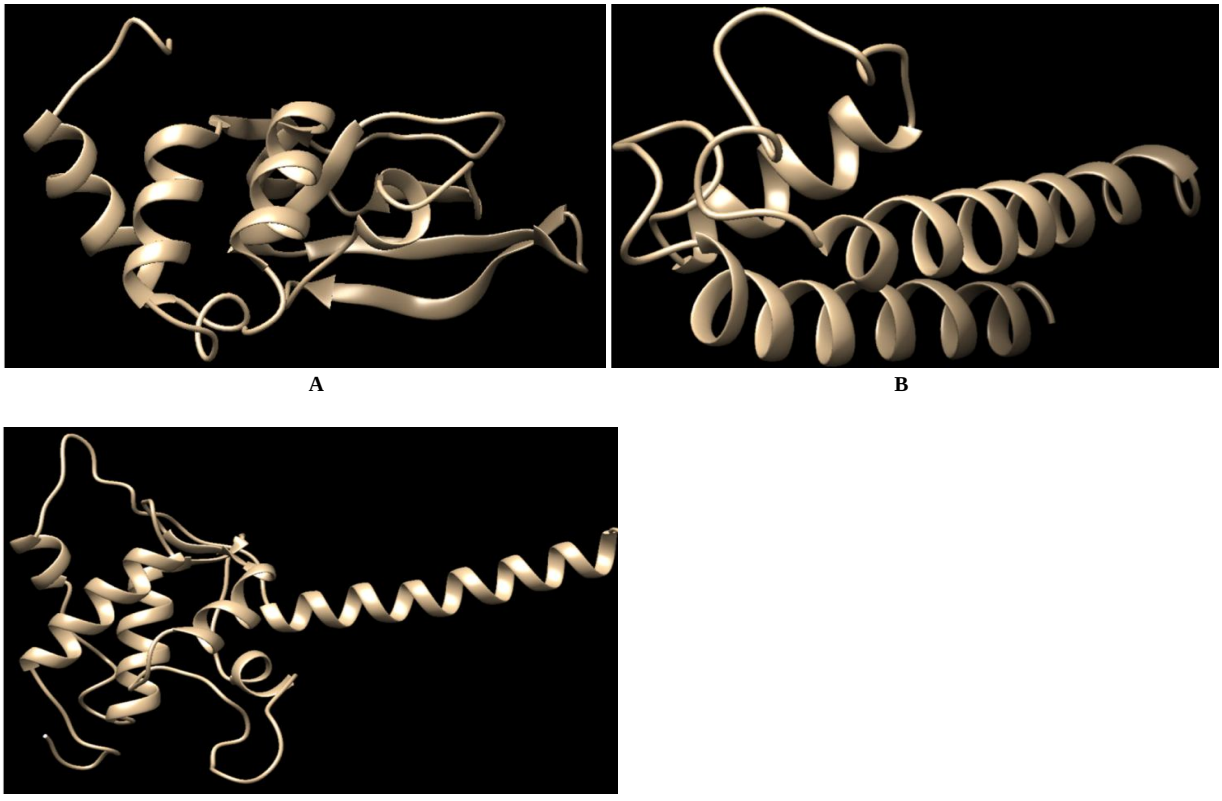
To investigate the role of plant VGICs in plant stress response, abiotic stress in particular, the modelled VGICs were individually docked against different soil salts and fertilizers. The docking analysis revealed that the binding energy (B.E.) of VGKC ranged from -0.9kCal/mol to -4.57kCal/mol while that of VGCC and VGSC range from -0.86kCal/mol to -3.67kCal/mol and from -0.83kCal/mol to -4.6kCal/mol, respectively (Table 2-4). The docking results reflect that VGICs seems to have negligible role in simple salts physiology like NaCl or KCl, while VGKC showed good binding pattern with ammonium nitrate and ammonium sulfate, reflecting its significant role in ammonium-ion physiology. Also, phosphoric acid binding was found significant towards VGKC. Superphosphate ions and Calcium nitrate showed a good binding pattern towards VGCC while VGSC showed good affinity for nitrate, phosphate, sodium and ammonium –ions. Also, arginine was observed to be important in binding of salts to VGKC while aromatic amino acid tyrosine/phenyl alanine was observed to be commonly important for binding of salts to VGCC. Lysine/serine/Leucine was observed to be important in binding of salts to VGSC (Figure 2a-c).

3.3 Simulated annealing using Autodock was done at different temperatures.

Simulated annealing was performed for the selected ligands against all the three modelled proteins for the analysis of effect of different temperatures on the binding pattern of the proteins with the ligands at different temperatures. During simulated annealing docking, it was observed that binding of phosphoric acid (or phosphate ion) increased at both extreme temperature ends (lower and higher) as reflected in Table 5-7.

Table. 1: Parametric evaluation of models if VGICs generated by SWISS MODEL.

Model name	Template used	Q-mean	Z- score	Ramachandran Plot Z-Score
VGKC of *A. thaliana* (AtKat1)	411O	0.5	-3.29	-0.461
VGKC of *A. thaliana* (AtKat1)	4f41	0.24	-4.68	-1.607
VGSC of *M. pusilla* (Mpccmp1545)	4dck	0.44	-3.93	-0.343



A **B**

C

Fig. 1: a-c: Homology Models of VGICs of plant systems [a: VGKC of *A. thaliana* (AtKat1); b: VGCC of *A. thaliana* (AtTpc1); c: VGSC of *M. pusilla* (Mpccmp1545)]

Table. 2: Docking analysis of VGKC of *A. thaliana* (AtKat1) against different soil salts and fertilizers.

S.No.	Salt name	B.E. (kCal/mol)	Ki	Interacting residues	H-Bond forming residues
1	Urea	-3.93	1.31mM	Ile404, Ile405, Glu409, Thr412, Tyr415	Glu409, Thr412, Tyr415
2	NH_4NO_3	-4.39	605.53uM	Lys357, Arg360	Lys357, Arg360
3	SSP	-4.05	1.08mM	Arg307, Arg310, Arg314, Tyr397	Arg305, Arg310, Arg314
4	H_3PO_4	-5.05	197.24uM	Arg305, Lys347, Asp394, Ala393, Glu390	Lys347, Ala 395
5	NaCl	-0.96	198.17mM	Ile375, Leu377, Thr443, Leu493, Lys496	-
6	KCl	-0.9	217.08mM	Ile375,Leu377,Thr443,Leu493, Lys496	-
7	$Ca(NO_3)_2$	-4.57	445.14uM	Arg305, Arg307, Arg310, Arg314	Arg307, Arg310, Arg314
8	TSP	-4.54	4.52.88uM	Arg305, Arg307, Arg310, Asp311, Tyr397	Arg305, Arg307
9	KNO_3	-3.72	1.88mM	Gln348, Gln349, Glu350, Asp392, Ser471	Asp392, Ser471
10	$(NH_4)_2SO_4$	-4.03	1.11mM	Gln344, Glu350, Ser391, Asp392, Asp394	Gln349, Asp392, Asp394
11	$NaNO_3$	-3.91	1.36mM	Arg305, Arg310, Arg314	Arg310, Arg314
12	MAP	-3.21	4.44mM	Arg305, Thr306, Arg307, Arg310, Arg314	Arg305, Arg307, Arg310, Arg314
13	DAP	-3.6	2.28mM	Arg305, Thr306, Arg307, Arg310, Asp311, Arg314	Arg305, Arg307, Arg310, Arg314
14	MCP	-3.89	1.41mM	Ile405, Ala410, Pro411, Thr412, Tyr415	Ala410, Thr412, Tyr415

SSP: Single Sugar Phosphate; TSP: Triple Sugar Phosphate; MAP: monoammonium phosphate;
DAP: Diammonium phosphate; MCP: Monocalcium phospate

Table. 3: Docking analysis of VGCC of *A. thaliana* (AtTpc1) against different soil salts and fertilizers.

S.No.	Salt name	BE (kCal/mol)	Ki	Interacting residues	H-Bond forming residues
1	Urea	-3.15	4.87mM	Phe238, Thr241, Gln242, Ser277, Ser278	Ser278, Glu242
2	NH_4NO_3	-2.22	23.49mM	Asn267, Phe285, Val289	Asn267
3	SSP	-3.54	2.56mM	Asn267, Pro268, Val270, Ala274, Tyr275	Val270, Tyr275
4	H_3PO_4	-3.07	5.66mM	Tyr275, Ser277, Arg279	Ser277, Arg279
5	NaCl	-1.05	169.67mM	Leu227, Ser231, Leu255, Met258	-
6	KCl	-0.86	233.82mM	Trp223, Phe226, Ile291, Gly292, Phe295	-
7	$Ca(NO_3)_2$	-3	6.37mM	Pro244, Pro268, Val270, Pro273, Ala274, Tyr275, Lys276	Tyr275, Lys276
8	TSP	-3.67	2.05mM	Pro268, Asp269, Val270, Ile272, Ala274, Tyr275, Ser 281, Ser282	Val270, Tyr275
9	KNO_3	-3.17	4.78mM	Phe238, Glu239, Asp240, Thr241	Asp240
10	$(NH_4)_2SO_4$	-3.58	2.38mM	Pro268, Asp269, Val270, Ile272, Pro273	Val270, Ile272
11	$NaNO_3$	-2.89	7.61mM	Tyr275, Lys276, Arg279	Lys276
12	MAP	-2.69	10.59mM	Thr215, Tyr216, Ala302, Tyr305, Asp306	Tyr216,Tyr305, Asp306
13	DAP	-3.05	5.83mM	Tyr216	Tyr216
14	MCP	-3.17	4.71mM	Ala410, Thr412, Tyr415	Pro268, Val270

SSP: Single Sugar Phosphate; TSP: Triple Sugar Phosphate; MAP: monoammonium phosphate;
DAP: Diammonium phosphate; MCP: Monocalcium phospate

Table. 4: Docking analysis of VGSC of *A. thaliana* (Mpccmp1545) against different soil salts and fertilizers.

S.No.	Salt name	BE (kCal/mol)	Ki	Interacting residues	H-Bond forming residues
1	Urea	-3.36	3.42mM	Lys1680, Asp1682, Ser1684, Asp1685	Lys1680, Asp1682, Ser1684
2	NH_4NO_3	-4.6	422.13uM	Leu1627, Lys1628, Asn 1629, Lys 1630	Lys1628, Lys1630
3	SSP	-3.54	2.56mM	Tyr1595, Phe1639, Gln1640, Arg 1642, Ile1643, His1644, Phe 1687	Tyr275
4	H_3PO_4	-3.5	2.71mM	Lys1630, Arg1655, Glu1570	Glu1570, Lys1630, Arg1655
5	NaCl	-0.99	186.80mM	Trp1585, Met1596, Ile1643, Thr1648	-
6	KCl	-0.83	247.63m	Trp1585, Met1596, Leu1601, Ile1643, Thr1648	-
7	$Ca(NO_3)_2$	-4.39	601.5uM	Asn1638, Phe1639, Gly1641, Ser1684, Lys1688, Tyr1697	Asn1638, Gly1641, Lys1688, Ser1689
8	TSP	-4.46	537.44uM	Phe1639, Gln1640, Arg1642, His1644, Asp1647, Lys1668, Asp1685	Asp1547, Lys1668, Asp168
9	KNO_3	-3.2	4.53mM	Tyr1594, Trp1675, Lys1676, Phe1677, Glu1873	Asn1681
10	$(NH_4)_2SO_4$	-3.06	5.76mM	His1644, Asn 1671, Asn1681, Glu1683, Ser1684	Gln349, Asp392, Asp394
11	$NaNO_3$	-3.77	1.74mM	Lys1688, Ser1689, Ser1694, Tyr1697	Lys1688
12	MAP	-2.82	8.59mM	Phe1687, Lys1688	Phe1687, Lys1688
13	DAP	-2.9	7.53mM	Asn1629, Lys1630, Ser1633	Asn1629, Lys1630
14	MCP	-3.97	1.29mM	Tyr1595, Phe1639, Gln1640, Arg 1642, His1644	Asp1685

SSP: Single Sugar Phosphate; TSP: Triple Sugar Phosphate; MAP: monoammonium phosphate;
DAP: Diammonium phosphate; MCP: Monocalcium phospate

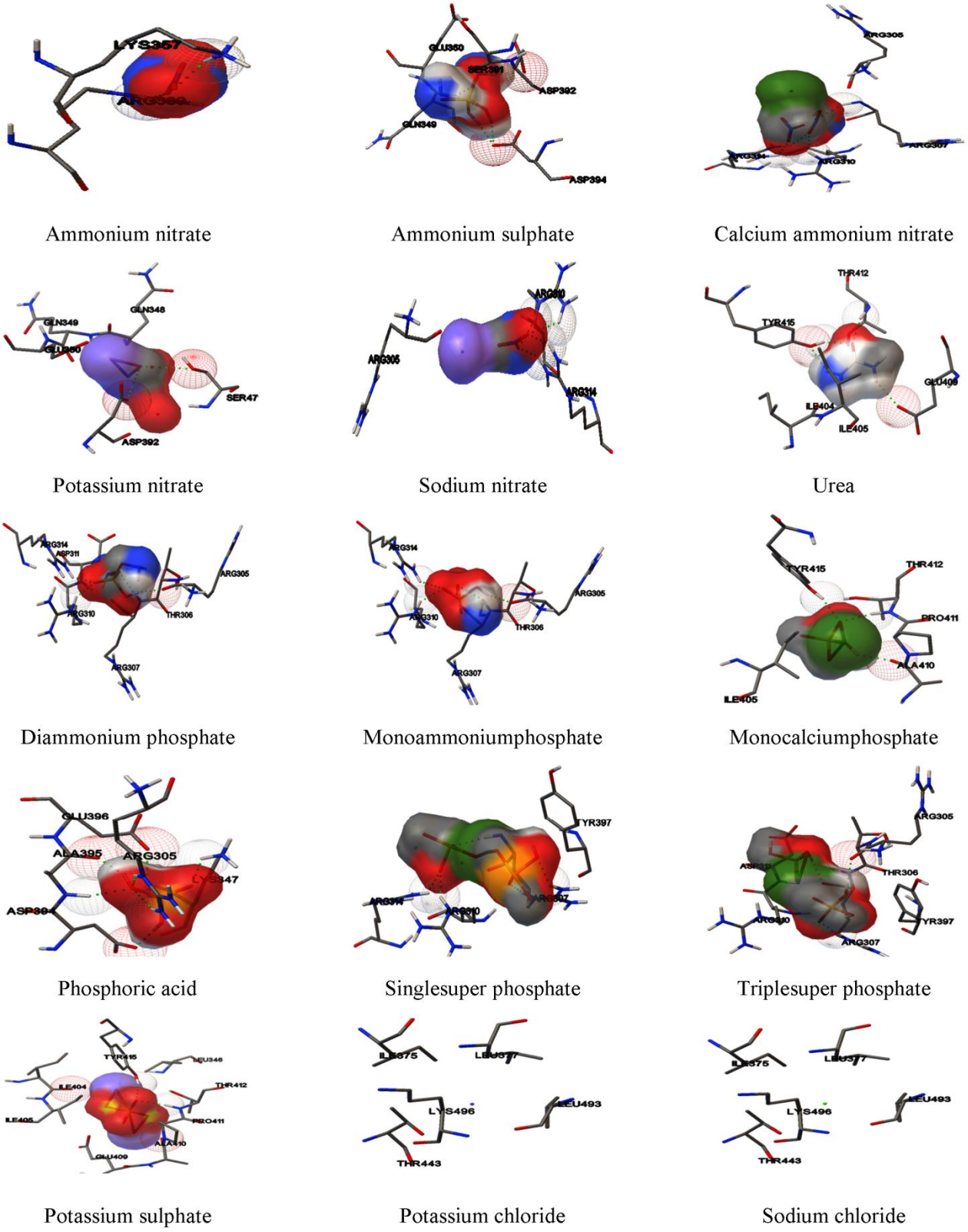


Fig. 2a: Docking results showing interaction of VGKC(AtKat1) with different fertilizers

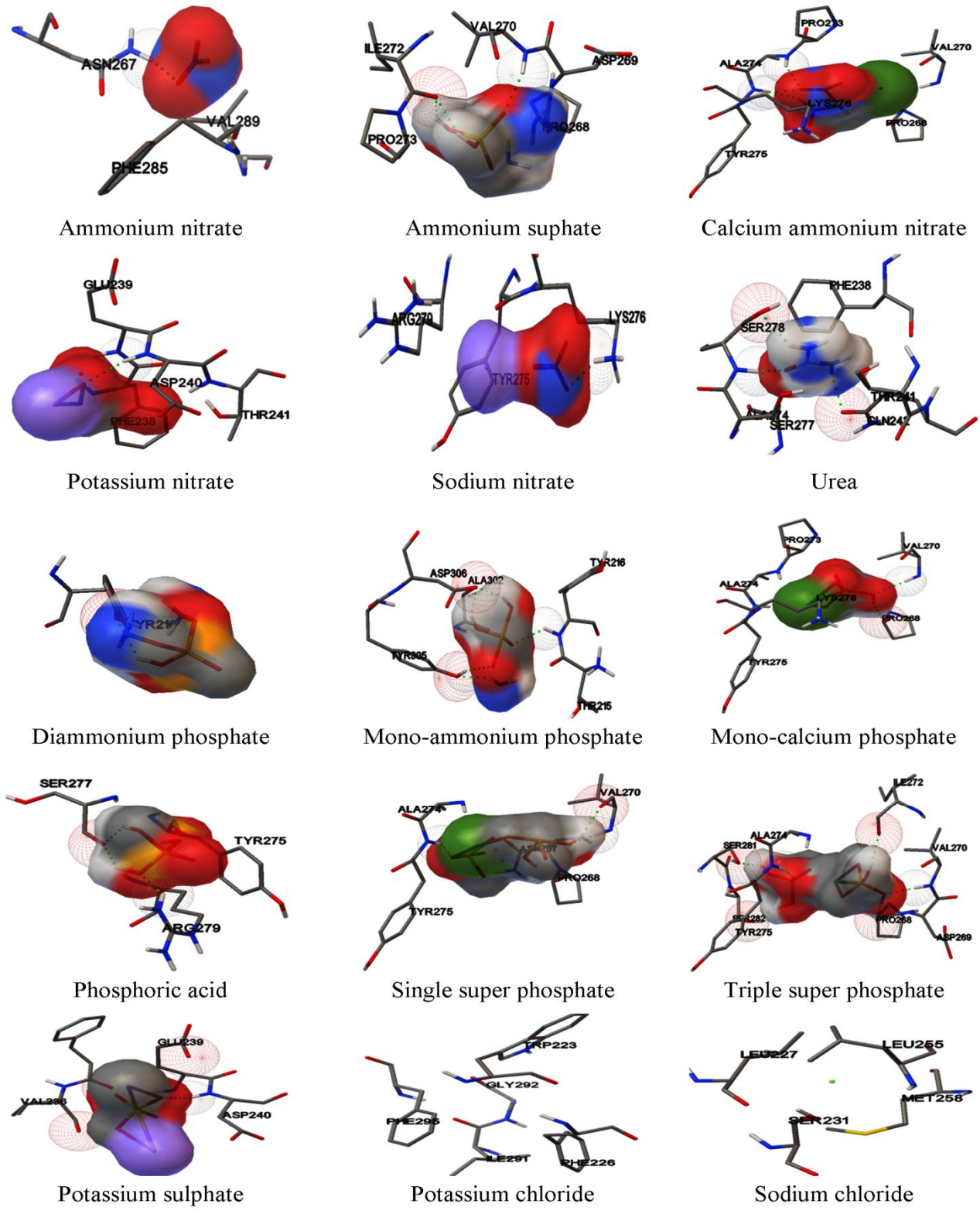


Fig. 2b: Docking results showing interaction of VGCC(AtTpc1) with different fertilizers

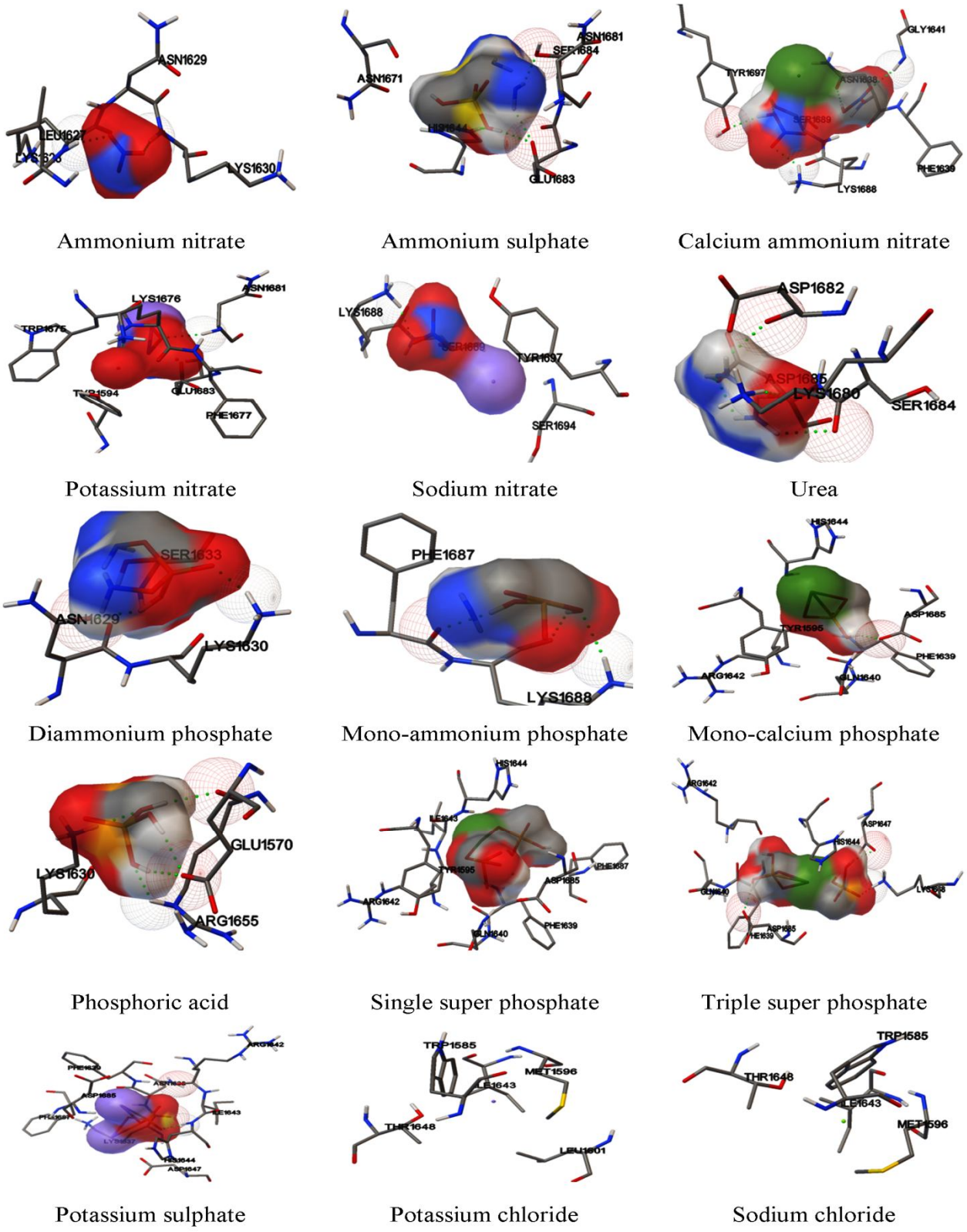


Fig. 2c: Docking results showing interaction of VGSC(Mpccmp1545) with different fertilizers.

Table. 5: Docking analysis of VGKC of *A. thaliana* (AtKat1) against selected soil salts and fertilizers at different temperature.

S.No.	Salt name	Binding Energy (kCal/mol)							
		10^0C	15^0C	25^0C	30^0C	35^0C	40^0C	45^0C	50^0C
1	NH_4NO_3	-4.26	-4.29	-4.24	-4.25	-4.3	-4.3	-4.3	-4.26
2	H_3PO_4	-3.16	-3.29	-3.53	-3.1	-2.78	-2.89	-2.49	-4.26
3	NaCl	-1.01	-1.01	-1.01	-1.01	-1.01	-1.01	-1.01	-1.01
4	Triple super phosphate	-2.52	-2.86	-2.97	-2.69	-2.69	-2.92	-2.94	-2.69
5	$(NH_4)_2SO_4$	-2.26	-2.23	-1.91	-2.17	-2.24	-2.19	-2.42	-2.22

Table. 6: Docking analysis of VGCC of *A. thaliana* (AtTpc1) against selected soil salts and fertilizers at different temperature.

S.No.	Salt name	Binding Energy (kCal/mol)							
		10^0C	15^0C	25^0C	30^0C	35^0C	40^0C	45^0C	50^0C
1	NH_4NO_3	-3.23	-3.17	-3.22	-3.25	-3.25	-3.22	-3.22	-3.23
2	H_3PO_4	-2.2	-2.02	-2.18	-2.1	-2.03	-2.34	-2.15	-3.22
3	NaCl	-1.05	-1.05	-1.05	-1.05	-1.05	-1.05	-1.05	-1.05
4	Triple super phosphate	-2.43	-2.17	-2.46	2.46	-2.13	-2.35	-2.45	-2.44
5	$(NH_4)_2SO_4$	-2.29	-2.01	-1.54	-1.98	-1.81	-2.04	-1.88	-2.00

Table. 7: Docking analysis of VGSC of *A. thaliana* (Mpccmp1545) against selected soil salts and fertilizers at different temperature.

S.No.	Salt name	Binding Energy (kCal/mol)							
		10^0C	15^0C	25^0C	30^0C	35^0C	40^0C	45^0C	50^0C
1	NH_4NO_3	-1.75	-1.73	-1.74	-1.75	-1.74	-1.75	-1.76	-1.75
2	H_3PO_4	-2.25	-2.25	-2.21	-2.19	-2.15	2.51	-2.35	-3.75
3	NaCl	-1	-1	-1	-1	-1	-1	-1	-1
4	Triple super phosphate	-3.49	-2.8	-2.5	-2.72	-2.94	-2.7	-2.87	-2.22
5	$(NH_4)_2SO_4$	-1.93	-1.71	-1.42	-1.57	-1.73	-1.49	-2.17	-1.79

4. CONCLUSION

The present study is novel in itself being probably the first comprehensive study about role of VGICs in plant system with special reference to abiotic stress (salinity and temperature) response. The study has provided a good platform for further investigation to establish the role of VGICs in plant stress response and correlated to other living systems like animals, fungi, etc.

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