ISSN PRINT 2319 1775 Online 2320 7876

Research paper UGC CARE Listed (Group -I) Journal Volume 11, Iss 12, Dec 2022

STRUCTURAL AND DOCKING STUDIES ON (2R, 3R)-2-AZANIUMYL-3-HYDROXYBUTANOATE METAL COMPLEXES

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ABSTRACT

Chemistry gives the collective behaviour of atoms in molecule, and varies accordingly with the presence of elements, form metal to non-metals. Amino acids and metal ions are the key components of life. This work is the study of blending metal ions of II A & B, Be, Mg and Zn as sulpahtes and L-threonine through the computational studies. The surfaces were obtained by Crystal Explorer/DFT/B3LYP/631G**. Computations were done through Firefly/B3LYP method using 6-31G** basis set. All the calculations were performed at 25 °C in gas phase. It was observed that hydroxyl group has poor binding ability due to the covalently and strongly held hydrogen. The metal ion stabilises the ligand in the metal complexes and metal ion can act as drug carrier. In docking the complexes have H-bond, hydrophobic, π-stacking and complex formation interaction with the proteins. It was concluded that chemistry is the chemistry of hydrogen

Keywords: azaniumyl-3-hydroxybutanoate, metal complexes, docking studies, COVID strains.

1. INTRODUCTION

Molecular dynamics (MD) is the study of physical movements and interaction of atoms and molecules on the basis of time using ab initio and molecular mechanics. MD has applications in the fields of biology, chemical reactions and physical behaviour of atoms and molecules in bulk. Molecular docking is a molecular mechanics model to predict the binding modes, site and affinity between protein and ligand. Computational chemistry helps to assist laboratory synthesis of compounds, understanding the experimental data, predict the feasibility of a reaction, spectroscopy, explore reaction mechanism, correlation between chemical structures and properties, drug design,

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catalysis, calculating the ground state, intermediate, excited state, reaction mechanism and modelling[1-6].

Amino acids are the basic building blocks for the life forming molecule the protein. A challenging aspect of life formation is the self condensation of amino acid in the ambient temperature, pressure and solvent. In order to manage and overcome the environment as well as function in the normal conditions amino acids have a self defending mechanism of forming zwitter ion. Chemistry of zwitter ion is a mysterious one and the molecule can be classified as self naturalized neutral salt and in another sense astautomeric forms of amino acid and ammonium and carboxylato. The chemistry of zwitter ion makes it to swing between active to passive molecule and kept the scientific community in achaos like Schrödinger's cat in quantum mechanics [7-11]. Many studies are going on to unearth the misty behind the chemistry of zwitter ion and this work is a *pry*.

To fulfill the above objectives, it was observed that the hydroxyl amino acid got importance and (2R,3R)-2-azaniumyl-3-hydroxybutanoate (AA-Z) has been taken for this study along with II A & B group metal ions of oxidation state two are beryllium, magnesium and zinc. The study focus on the crystallography, crystal growth, DFT, molecular dynamics, biological study and molecular docking.

DFT calculations will be performed for the amino acid, metal salts and complexes to study the Energy, Thermo chemistry, Surface scan, Structural parameters-bond length, bond angle, dihedral angle and bond order, Dipole moment, Charge density, HOMO, LUMO and orbitals, IR (Normal coordinate analysis), NMR, UV-VIS (TDDFT), Frontier molecular orbital-band gap, chemical stability, chemical potential, ionisation potential, electron affinity, and CD spectrum. The applications of the amino acid, metal salt and complexes for NLO, and Molecular Docking for COVID-7R98 and COVID-7N0R.

2. RESULTS AND DISCUSSION

2.1 Structure of metal complexes

The computational structural parameter and structure of metal complexes of Be, Mg and Zn with L-threonine (**MAA**) are given in Table 1 (a-c) and Fig.1. Due to higher computational cost through the **ZnAA** complex is of 1 : 3 ratio of Zn : AA, the 1 : 1 ratio of M : AA are chosen for the study. Here the **AA** is considered as a bidendate ligand through the carboxylato group and

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coordinate bond through the amine nitrogen. The total charge on the **MAA** complex is +1. The geometrical parameter are comparable with the literature value [12-15]. There is slight elongation in the C-O and C-N bond length due to the involvement in the complex formation process [16-19]. The order of N_3-M_{15} and O_1-M_{15} bond length is; Be > Zn > Mg. This is also the order of covalency of the complex and the Mg complex is weak and may be ionic and water stable. The bond angle O_1-M_{15}-N_{14} indicate that the complex have octahedral geometry. The dihedral angle inform that the complex is non-planar. The complexes are in ground state.

2.2 Charge density of MAAcomplexes

Table 2 and Fig.2 have the details about charge density of the compound. Due to complex formation the charge density of O_1 is reduced and increased for Be and rest of the metals by 46, 7.2 and 2.1 % respectively from Be, Mg and Zn from **AA**-N. This implies that the O_1 gets the electron from Mg and Zn, while it donates electron to Be. The order of change of O_1 is; Mg > Zn > Be. In the case of N_3, invariable of metal ion it gain electron from the metal ion. This can be accounted as proton can abstract more electrons from the nitrogen than metal ion [20-22]. In other words H^+ is more electropositive than metal ion [23-24]. The order of negative charge on N_3 is; Zn > Mg > Be. That is Zn forms a strong bond with **AA** or Zn can donate electron easily than other metal ions. At the end nitrogen can get more electron from the metal than oxygen due to the later's less electronegativity [25-27]. The electron donating ability of the metal ion is; Mg > Zn > Be. In all the above observations, Mg have a different behaviour from Be and Zn [28-29].

2.3 Dipole moment of MAA complexes

Dipole moment of the molecules is given in Table 3 and Fig. 3. The order of total dipole moment is; Mg > AA > Be > Zn. This is also the measure of bulk or molecular polarisability. The dipole moment is higher along *x*-axis. As the **AA** is studied as **AA-Z** form it has higher dipole moment. This further confirmed that proton is more electropositive than the metal ion and it may be difficult to remove the proton by metal ions but, by the change of medium to basic, it is possible [30].

2.4 Orbitals of MAAcomplexes

The MO of the complexes are given in Fig.4. In the case of Be the HOMO is contributed by the px orbital of C12 and N3 and LUMO on N3 s and Be pz. That is the metal ion can accept the electron for the nitrogen. For Mg the HOMO is on the pzcarboxylato oxygen and LUMO on the Mg

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s orbital. The Zn follows the similar trend of Mg, and in addition LUMO is on Zn p_x. Thus, the hetero atoms carboxylato oxygen and nitrogen are electron donors and metals are acceptor [31].

2.5 Docking of MAA complexes with COVID-7N0R

The docking details of the complexes with the title strain is given Table 4 and Fig. 5. The docking were obtained for MgAA and ZnAA. The docking effect is higher for MgAA over ZnAA due to the size to polarisability of Mg [32-34]. But the docking energies are comparable to each complexes. Both the complexes have H-bond, hydrophobic π-stacking and complex formation with the proteins. In the case of MgAA the strong H-bond with aspartin, hydrophobic and π-stacking with tryptophan. The Mg forms complex with protein chains. For ZnAA. The H-bond is formed with glutamic acid, salt bridge with histamine and complex with proteins.

2.6 Docking of MAA complexes with COVID-7R98

Table 5 and Fig.6 have the docking with COVID-7R98. In general the effect of complex on 7N0R is higher than 7R98 by 8.4 %. Here ZnAA has higher docking effect than MgAA. The complex-protein interactions are H-bond and complex formation. The H-bond is with leucine and complex with protein for MgAA. For ZnAA H-bond with glutamine and complex with protein. The docking energy is higher for the complex than **AA**.

3. CONCLUSION

Molecular dynamics of **MAA** the MSO_4 forms M-O bond and O---H-NH-bonds. The **AA-Z** form covalent bond with **M** through its carboxylate oxygen and H-bond with ammonium ion. In the surface scan **AA** is a monodendate ligand and the metal ion accept electron from the oxygen. **MAA** is in ground state. Mg have a different behaviour from Be and Zn. The dipole moment is higher along *x*-axis. It may be difficult to remove the proton by metal ions and can through basic medium. The hetero atoms carboxylato oxygen and nitrogen are electron donors and metals are acceptor. The complex are ionic in nature. Most of the transitions from HOMO → LUMO. All the complexes can transfer one electron and metal ions play a major role in intra and inter fragments electron transfer. The polarisation in the organic compound through it electrons donating and accepting groups. In docking complexes have H-bond, hydrophobic, π-stacking and complex formation with the proteins. The effect of complex on 7N0R is higher than 7R98.

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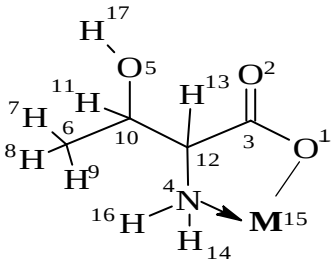

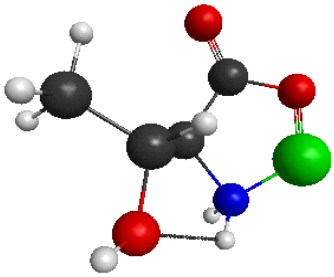

2D structure and numbering pattern **3D structure**

M-green; O-red; C-black; H-white

Figure 1: Structure of MAA complexes

Table 1(a) : Bond length of MAA complexes

Atom pair	Bond length (Å)		
	BeAA	**MgAA**	**ZnAA**
O1-O2	2.2784	2.2516	2.2467
O1-N3	2.5875	2.8248	2.8745
O1-C4	1.1921	1.2063	1.2029
N3-O5	2.5428	2.5609	2.5427
O5-C6	2.4653	2.4573	2.4593
C6-H7	1.0938	1.0938	1.0936
C6-H8	1.0926	1.0917	1.0918
C6-H9	1.0939	1.0945	1.0942
O5-C10	1.4295	1.4298	1.4289
C10-H11	1.1018	1.1050	1.1043
N3-C12	1.5474	1.5315	1.5338
C12-H13	1.0922	1.0926	1.0921
N3-H14	1.0232	1.0217	1.0218
N3-M15	1.4297	1.8423	1.8029
N3-H16	1.0366	1.0302	1.0329
O5-H17	0.9675	0.9665	0.9670

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Table 1(b) : Bond angle of MAA complexes

Atom pair	Bond angle (°)		
	BeAA	MgAA	ZnAA
O1-O2-N3	97.0729	91.5756	90.5875
O1-O2-C4	29.9530	29.2246	30.0841
O1-N3-O5	116.0724	108.9707	108.6219
N3-O5-C6	100.4965	99.8684	100.2986
O5-C6-H7	89.7085	89.9017	89.7345
C6-H7-H8	109.1501	108.7492	108.8508
C6-H7-H9	108.0052	108.2404	108.1158
N3-O5-C10	72.6081	71.0493	71.4231
O5-C10-H11	109.6863	109.3781	109.487
O1-N3-C12	123.1348	60.5733	60.0564
N3-C12-H13	108.1374	107.9476	107.8271
N3-C12-H14	110.1073	108.8539	110.3098
N3-H14-M15	34.3521	46.5365	41.241
N3-H14-H16	105.714	105.8117	106.926
O5-C10-H17	109.9774	109.8739	110.0704

Table 1(c) : Dihedral of MAA complexes

Atom pair	Dihedral (°)		
	BeAA	MgAA	ZnAA
O1-O2-N3-C4	3.2446	8.7685	8.2169
O1-O2-O5	-48.8116	-58.1022	-59.0913
O1-N3-O5-C6	41.9469	38.829	37.6462
O2-O5-C6-H7	109.4201	102.4465	101.8472
O2- C6-H7-H8	46.7016	44.9392	45.1813
C6-H7-H8-H9	-117.933	-117.8641	-117.8585
O1-N3-O5-C10	21.2178	18.8236	17.936
O5-C6-C10-H11	123.1033	121.8768	122.5002
O1-N3-C4-C12	177.6369	-13.3516	-14.2171
N3-C10-C12-H13	119.6883	119.8553	119.6278
N3- C12-H13-H14	7.4672	22.7078	22.0124
N3- C12-H14-M15	178.782	-98.3182	178.1182
N3- H14-M15-H16	42.4032	40.6463	41.2192
O5-C10-H11-H17	63.9729	73.9747	69.7213

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Table 2 :Mulliken's atomic charge density of MAA complexes

Atom	Mulliken's atomic Charge density		
	BeAA	MgAA	ZnAA
O1	-0.3168	-0.6382	-0.6076
O2	-0.3640	-0.4208	-0.3876
N3	-0.5405	-0.7270	-0.7529
C4	0.6400	0.6787	0.6379
O5	-0.5653	-0.5679	-0.5648
C6	-0.3444	-0.3454	-0.3432
H7	0.1456	0.1425	0.1473
H8	0.1723	0.1726	0.1721
H9	0.1453	0.1318	0.1392
C10	0.1580	0.1645	0.1675
H11	0.1317	0.1088	0.1178
C12	-0.0934	-0.0586	-0.0976
H13	0.2022	0.1814	0.1988
H14	0.3454	0.3341	0.3523
M15	0.5746	1.1491	1.1046
H16	0.3568	0.3506	0.3672
H17	0.3524	0.3438	0.3491

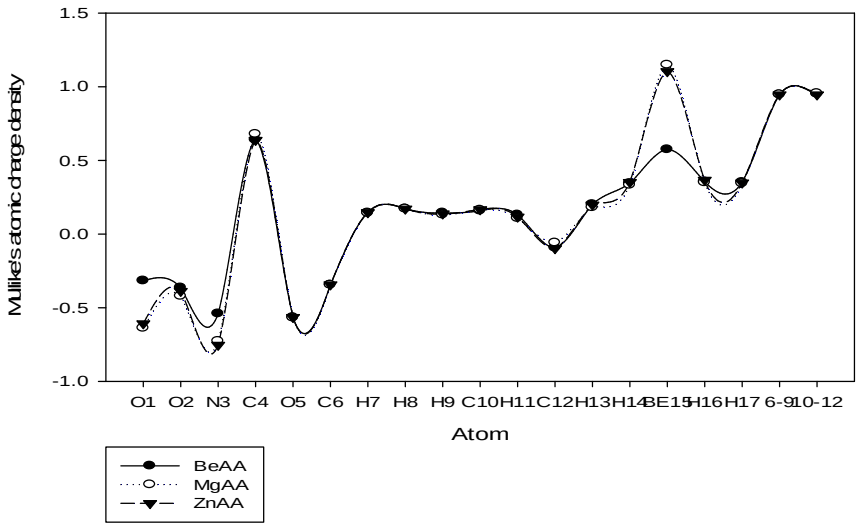

Figure 2 :Mulliken's atomic charge density of MAA complexes

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Table 3: Dipole moment of MAA complexes

Axis	Dipole moment (Debye)		
	BeAA	MgAA	ZnAA
X	6.4417	10.5035	6.4470
Y	-4.9686	-4.4748	-3.6790
Z	1.4860	-0.3716	2.6230
Total	8.2699	11.4230	7.8727

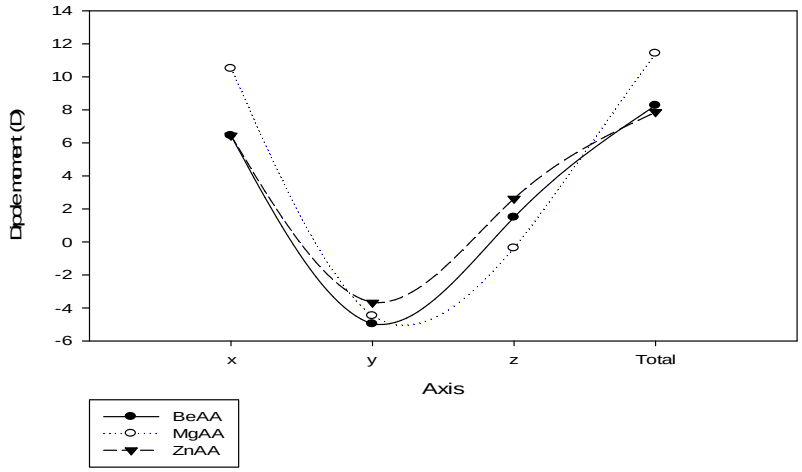

Figure 3: Dipole moment of MAA complexes

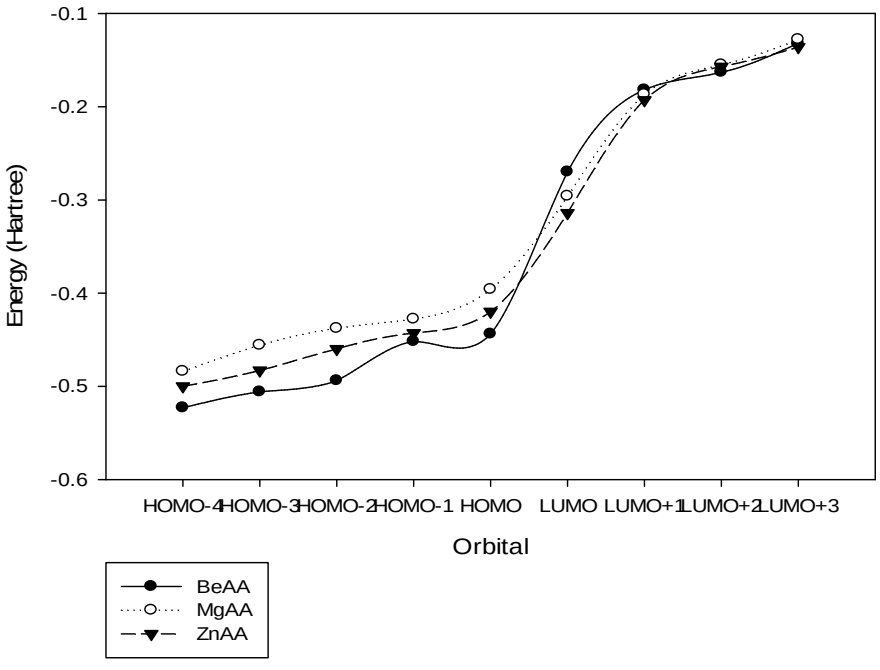

Figure 4 : Orbitals of MAA complexes (Hartree)

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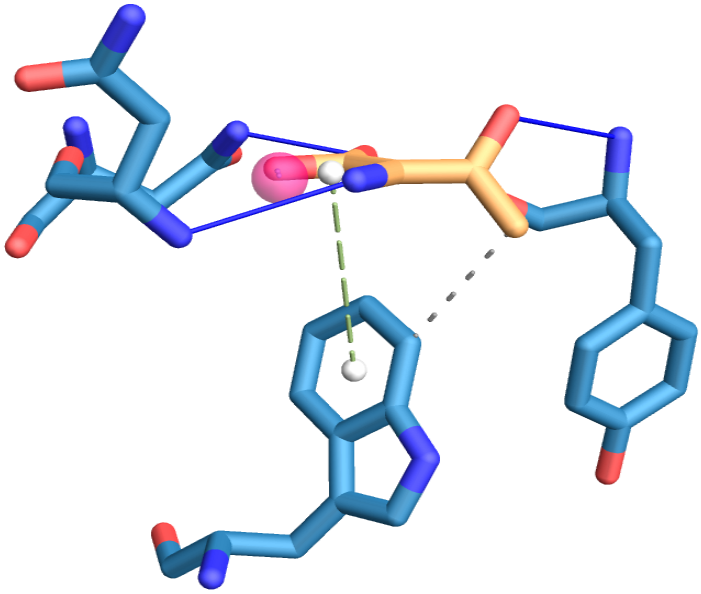
(a)



(b)

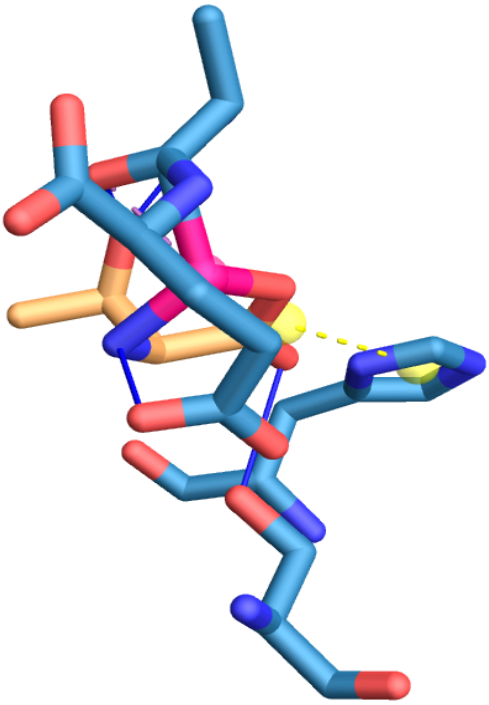


Figure 5(a): Docking of MAA (a) MgAA (b) ZnAA complexes with COVID-7N0R

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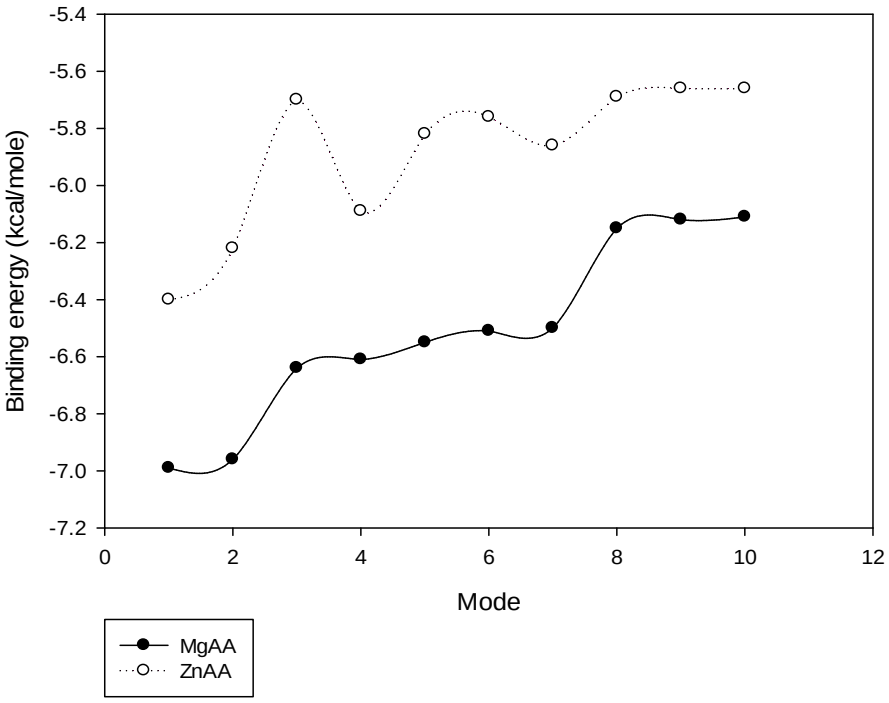

Figure 5(b): Binding energy from the Docking of MAA (a) MgAA (b) ZnAA complexes with COVID-7N0R

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Table 4 (a) : Docking of MAA (MgAA) complexes with COVID-7N0R

MgAA			
Mode	**Binding energy (kcal/mole)**	**Cluster r_{msd}**	**Reference r_{msd}**
1	-6.99	0.00	24.22
2	-6.96	0.24	24.20
3	-6.64	0.00	18.52
4	-6.61	0.12	18.56
5	-6.55	0.80	19.04
6	-6.51	1.74	19.30
7	-6.50	0.00	18.06
8	-6.15	0.00	18.75
9	-6.12	0.00	17.49
10	-6.11	0.04	17.50

Hydrophobic interaction

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	52A	TRP	3.63	4806	43

Hydrogen bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor	Side chain	Donor Atom	Acceptor Atom
1	99C	TYR	3.47	3.75	101.86	yes	no	3392 [Nam]	4808 [O3]
2	150A	ASN	2.86	3.39	121.77	yes	no	1009 [Nam]	4805 [N2]
3	154A	ASN	2.37	2.71	103.70	yes	yes	1051 [Nam]	4802 [O2

Pi-stacking

Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	52A	TRP	4.78	73.79	1.67	T	4800, 4801, 4803, 4804, 4805

Metal complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
1	1A	UNL	4804	4803	1.43	ligand
2	1A	UNL	4804	4803	1.43	protein.mainchain

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Table 4 (b) : Docking of MAA (ZnAA) complexes with COVID-7N0R

ZnAA			
Mode	**Binding energy (kcal/mole)**	**Cluster r_{msd}**	**Reference r_{msd}**
1	-6.40	0.00	28.35
2	-6.22	0.00	15.45
3	-5.70	1.66	15.05
4	-6.09	0.00	23.00
5	-5.82	1.46	23.20
6	-5.76	1.57	22.90
7	-5.86	0.00	12.80
8	-5.69	0.00	28.67
9	-5.66	0.20	28.75
10	-5.66	0.00	27.68

Hydrogen bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Side chain**	**Donor Atom**	**Acceptor Atom**
1	105A	SER	2.07	2.89	165.20	yes	yes	576 [O3]	4806 [O2]
2	173B	ALA	2.14	2.75	127.81	yes	no	2445 [Nam]	4810 [O3]
3	173B	ALA	2.25	2.65	103.63	no	no	4810 [O3]	2448 [O3]
4	174B	GLU	1.94	2.65	124.25	no	yes	4803 [N3]	2458 [O2]

Salt bridges						
Index	**Residue**	**AA**	**Distance**	**Protein positive**	**Ligand Group**	**Ligand Atoms**
1	59A	HIS	4.36	yes	Carboxylate	4800, 4806

Metal complexes						
Index	**Residue**	**AA**	**Metal**	**Target**	**Distance**	**Location**
Complex 1: Zn, square.planar (4)						
1	1A	UNL	4807	4800	1.80	ligand
2	1A	UNL	4807	4800	1.80	protein.mainchain
3	1A	UNL	4807	4810	2.99	protein.mainchain
4	173B	ALA	4807	2448	2.39	protein.mainchain

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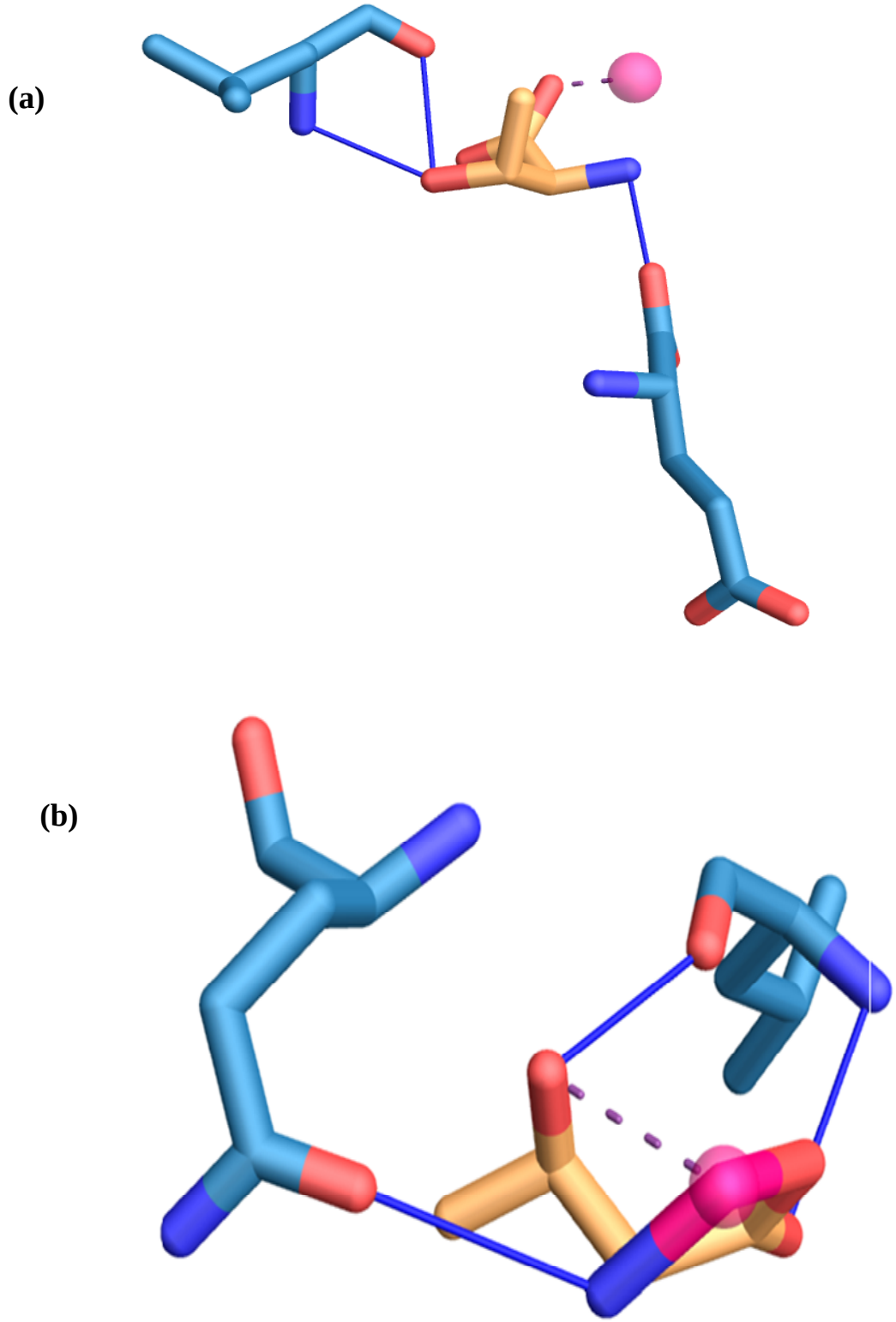

Figure 6(a) : Docking of MAA (a) MgAA (b) ZnAA complexes with COVID-7N98

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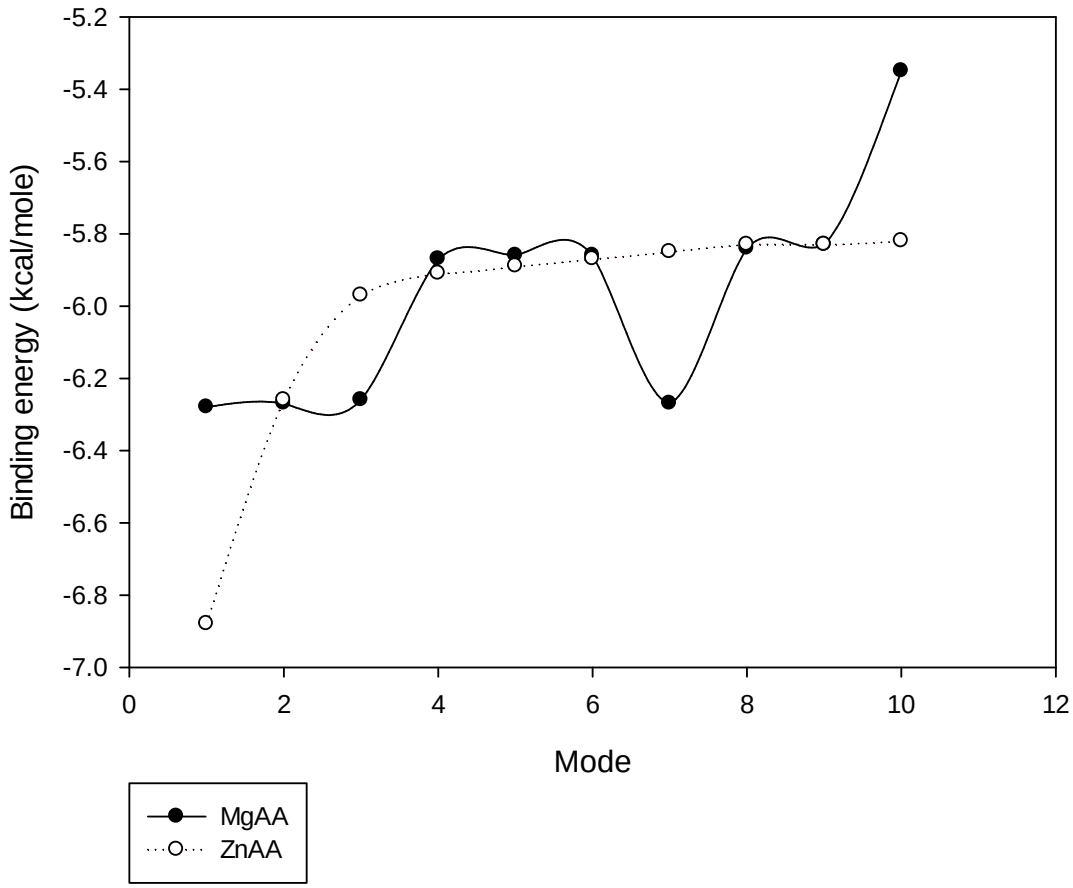

Figure 6(b) : Binding energy from Docking of MAA (a) MgAA (b) ZnAA complexes with COVID-7N98

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Table 5 (a): Docking of MAA complexes (MgAA) with COVID-7R98

MgAA			
Mode	**Binding energy (kcal/mole)**	**Cluster r_{msd}**	**Reference r_{msd}**
1	-6.28	0.00	44.31
2	-6.27	0.27	44.23
3	-6.26	0.30	44.25
4	-5.87	1.51	43.93
5	-5.86	1.32	44.47
6	-5.86	1.53	43.85
7	-6.27	0.00	37.36
8	-5.84	0.00	42.38
9	-5.83	0.08	42.35
10	-5.35	0.00	48.77

Hydrogen bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Donor Atom	Acceptor Atom
3	174B	GLU	3.21	3.91	126.82	6989 [N3]	2280 [O3]
2	161B	LEU	2.08	2.83	133.65	6996 [O3]	2163 [O2]
1	161B	LEU	1.89	2.75	171.43	2160 [Nam]	6996 [O3]

Metal complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
1	1A	UNL	6993	6986	1.84	ligand
2	1A	UNL	6993	6986	1.84	protein.mainchain

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Table 5 (b): Docking of MAA complexes (ZnAA) with COVID-7R98

ZnAA			
Mode	**Binding energy (kcal/mole)**	**Cluster r_{msd}**	**Reference r_{msd}**
1	-6.88	0.00	37.52
2	-6.26	0.00	44.22
3	-5.97	1.54	44.00
4	-5.91	1.48	43.75
5	-5.89	1.46	43.90
6	-5.87	1.59	43.76
7	-5.85	1.41	44.62
8	-5.83	1.55	43.47
9	-5.83	1.46	43.66
10	-5.82	1.43	44.67

Hydrogen bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor	Side chain	Donor Atom	Acceptor Atom
1	161B	LEU	2.13	2.66	112.83	no	no	6996 [O3]	2163 [O2]
2	161B	LEU	2.22	3.07	168.91	yes	no	2160 [Nam]	6992 [O2]
3	163B	GLN	2.31	3.29	158.71	no	yes	6989 [N3]	2183 [O2]

Metal complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Zn, trigonal.pyramidal (3)						
1	1A	UNL	6993	6986	1.80	ligand
2	1A	UNL	6993	6986	1.80	protein.mainchain
3	1A	UNL	6993	6996	2.97	protein.mainchain

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