Ab-initio computational study of noncovalent interaction between peptide and alkaline metal ions on HF/6-31 G** level

by Dwi Hudiyanti

Submission date: 05-Nov-2019 06:35AM (UTC+0700)
Submission ID: 1207095360
File name: saor_aip_18.pdf (1.45M)
Word count: 3689
Character count: 19935

Ab-initio computational study of noncovalent interaction between peptide and alkaline metal ions on HF/6-31 G** level

Cite as: AIP Conference Proceedings 2049, 020053 (2018); https://doi.org/10.1063/1.5082458
Published Online: 14 December 2018

Parsaoran Siahaan, Rinaldy Christian, Anisa Nur Fauziah, Dwi Hudiyanti, and Vivitri Dewi Prasasty

Ab-initio Computational Study of Noncovalent Interaction Between Peptide and Alkaline Metal Ions on HF/6-31G** level

Parsaoran Siahaan[1, *], Rinaldy Christian[1], Anisa Nur Fauziah[1], Dwi Hudiyanti[1], Vivitri Dewi Prasasty[2]

[1]*Departement of Chemistry, Faculty of Science and Mathematics, Diponegoro University*
[2]*Faculty of Biotechnology, Atma Jaya Catholic University of Indonesia*
*Corresponding author, tel/fax: 0813-1055-3498, e-mail: siahaan.parsaoran@live.undip.ac.id; siahaan_parsaoran@yahoo.com

Abstract. Intermolecular interaction or non-covalent interaction plays an important role on the chemical processes. Intermolecular interaction also involves several phenomena that corresponding to molecular and macromolecular sciences. Intermolecular interaction phenomena become an important subject to be learned because they can explain the important process on the human body. One of the most important processes that can be learned is peptide-metal ion interaction. Peptide-metal ion interaction plays the important role for the biological process on the human body. One of the peptide-metal ion interaction that can be learned is cadherin peptide interaction with a metal ion on blood-brain barrier (BBB). Several methods were done for investigating peptide-metal ion interaction. Generally, peptide-metal ion interaction can be investigated experimentally and theoretically. The purpose of this research is to theoretically determine the structure of Ac-CA-NH_2 (Cysteine-Alanine) and Ac-VC-NH_2 (Valine-Cysteine) peptides by ab initio computational approach with a minimum energy; the interaction stability of Ac-CA-NH_2 and Ac-VC-NH_2 with potassium and sodium ions, respectively; and to understand the contribution of partial charge and Highest Occupied Molecular Orbital (HOMO) - Lowest Unoccupied Molecular Orbital(LUMO) energy on Ac-CA-NH_2 and Ac-VC-NH_2 peptide interaction with potassium and sodium ions. The calculations were carried out on HF/6-31G** including geometry optimization of peptides, geometry optimization of peptide-ion interaction, and physical and chemical properties determination such as partial charge and HOMO-LUMO energy. The results show that the most stable structure of Ac-CA-NH_2 and Ac-VC-NH_2 peptides were acquired with minimum energy -965.254 Hartree and -1043.320 Hartree, respectively, proven by their optimization convergences. The interaction energy of Ac-CA-NH_2 with sodium and potassium ion indicating the most stable configurations-1 with interaction energy -189,782 kJ/mol for sodium ion and -141.280 kJ/mol for potassium ion. Meanwhile, the interaction energy of Ac-VC-NH_2 peptide with sodium and potassium ions has the most stable configuration-1 with interaction energy -248,562 kJ/mol and -181,022 kJ/mol, respectively. The partial charge and HOMO-LUMO energy can be used for understanding the stability of peptide-metal ion interaction and also confirming the reactivity of the peptide after interacting with a metal ion.

Keyword: Ab-initio, alkaline metal ion, drug interaction, peptide, non-covalent interaction

1. Introduction

Intermolecular interaction or non-covalent interaction plays an important role on chemical process. Intermolecular chemistry also involved other phenomena that related to molecular and macromolecular fields[1]. These phenomena become essential because it can explain the process that occurred on the body. An important process such as ion interaction with peptides can be learned because it has an important role in biological process on the human body[2]. Peptide-ion interactions can be used to describe some properties like increasing the binding affinity of the peptide, explaining the selectivity of each protein or peptide to metal ion and its bonding characterization, ion regulation from protein and peptides, and figuring out the peptides or protein stability due to the presence of cofactor at protein folding reaction[3-6]. One process example regarding the peptide-ion interaction that can be learned is cadherin peptides-metal ion interaction which is occurred in blood-brain barrier (BBB).

The 3rd International Seminar on Chemistry
AIP Conf. Proc. 2049, 020053-1–020053-8; https://doi.org/10.1063/1.5082458
Published by AIP Publishing. 978-0-7354-1775-5/$30.00

BBB is biological wall that carefully regulates the environment near central nervous system[7]. The presence of calcium ion that shown affecting structure of E-Cadherin in BBB[8]. BBB can be modulated using cadherin peptide to increase its porosity. Cadherin peptides are derivatived compound from E-cadherin that usefull for modulating protein-protein interaction in BBB[9]. A few cadherin peptides like ADT-C1 (Ac-CADTPPVC-NH_2) and ADT-C5(Ac-CADTPPVC-NH_2) can be used to modulate protein-protein interactions in BBB[10]. Those cadherin peptides have an active sequence at Ac-CA-NH_2 (Cysteine-Alanine) for ADT-C1 and Ac-VC-NH_2 (Valine-Cysteine) for ADT-C5[11, 12].

ADT peptides are delivered to BBB through the paracellular pathway[13]. In the paracellular pathway, cadherin peptides will interact with a tight junction to modulate proteins in BBB[14]. Tight junction serves as a gateway for substances which going in or out on paracellular pathway[15]. Several substances like metallic ions such as sodium and potassium are through the tight junction[16]. Metallic ion on tight junction will interact with peptides that pass through paracellular pathway[17]. ADT-C1 that interacting with metallic ion will change the conformation of the peptides, so that the method is needed to know how the peptide and ions interacting in BBB[18].

Several methods were used to investigating how peptide interacting. Generally, peptide-metal ion interaction can be investigated by the experimental and theoretical approaches. In experimental approach, nuclear magnetic resonance (NMR) and infrared multiple photon dissociation (IRMPD) can be used to explain peptide-metal ion interaction[19]. NMR can be used to determine a conformation change by seeing the shape and position changing of the chemical shift on carbon or hydrogen nuclei. Moreover, NMR can be used to determine the change of peptide structure and interacting sides[20]. In addition, NMR, IRMPD can be used to determine the complex structure conformation between the peptide and metal ion[21]. However, investigating peptide-metal ion interaction using an experimental approach is quite difficult because of complex environmental from peptide and ion, solvent, and impurities on molecule[22]. On other hand, the theoretical approach can be used to investigate intermolecular interaction using the ab initio method to get the interaction energy of peptide-ion interaction.

According to the fact above, the computational approach can be used to investigate peptide-metal ion interaction. Ab initio computational method quite efficient to investigate the intermolecular interaction[23]. In this research, Ac-CA-NH_2 and Ac-VC-NH_2 that part of the sequence of ADTC1 and ADTC5 will be interacting with K^+ and Na^+ alkaline metal ion to know the interaction that occurred and physical and chemical properties of peptide sequences.

2. Computational method

2.1 Geometry Optimization

All geometry molecules were optimized using the HF method with 6-31G** basis set in the gas phase[24-26]. All calculations were performed by NWCHEM for input file X.nw contained Z-matrix[27] and output file X.out visualized by chemcraft [28]. The calculations were done using command "task scf optimize" to get the stable structure and command "property dipole" and "task scf property" to get dipole moment data.

2.2 Interaction Energy

There are two kind of configuration between peptide and metal ions calculated are called configuration-1 and configuration-2. The interaction energy, $E_{intA\ldots B}$ was obtained by calculating the energy differences of peptide-ion molecule, $E_{optA\ldots B}$, with the peptide, E_{optA}, and metal ion, E_{optB} as following, Eq. 1[29]

$$E_{intA\ldots B} = E_{optA\ldots B} - E_{optA} - E_{EoptB} \quad (1)$$

Interaction energy could be visualized in distance variation between peptide and ion by using "Scan" directive calculation from 1Å to 9Å with the increasing of 0.05Å.

2.3 HOMO-LUMO analysis

All optimized geometry of molecules was recalculated using the HF method with 6-31G** basis set. All calculation for this analysis was performed and visualized using GAMESS/Gaussian03[30] and

chemcraft[28], respectively. Using checkpoint, SP and pop=reg directive, molecular orbital diagram, and orbital coefficient can be generated. Several properties can be obtained using HOMO and LUMO from the molecular orbital diagram such as energy gap, ionization potential(IP), electron affinity(EA), and electronegativity(χ) as per Eq. 2-5[31].

$$E_{gap} = E_{LUMO} - E_{HOMO} \quad (2)$$

$$IP = -E_{HOMO} \quad (3)$$

$$EA = -E_{LUMO} \quad (4)$$

$$\chi = -(IP + EA)/2 \quad (5)$$

3. Result and Discussion

3.1 Geometry Optimization

The geometry optimization of Ac-CA-NH_2 and Ac-VC-NH_2 are performed with HF/6-31G**. All calculations were confirmed by geometry convergence to validated the structure with minimum energy. The Ac-CA-NH_2 and Ac-VC-NH_2 peptides have optimized energy at -965.254 Hartree and -1043.320 Hartree, respectively. Peptide bond of Ac-CA-NH_2 and Ac-VC-NH_2 can be determined using computation method with the distance are 1.338 Å(N6-C8) and 1.374 Å(C9-N8), respectively. The conformation of the peptide can be seen on the dihedral of the peptide bond. The stable structure of Ac-CA-NH_2 and Ac-VC-NH_2 peptide have the trans conformation based on the dihedral D(C2N6C8C9) and D(C2N8C9C10) are 170.524° and 177.172°, respectively. HOMO and LUMO can be generated to know the electron distribution of the molecule. As we can see the blue sphere represent the positive of orbital coefficient and the red sphere represent the negative value of the orbital coefficient which changed and reduced by interaction with metal ion to indicate decreasing and changing of electron density on peptide[32].

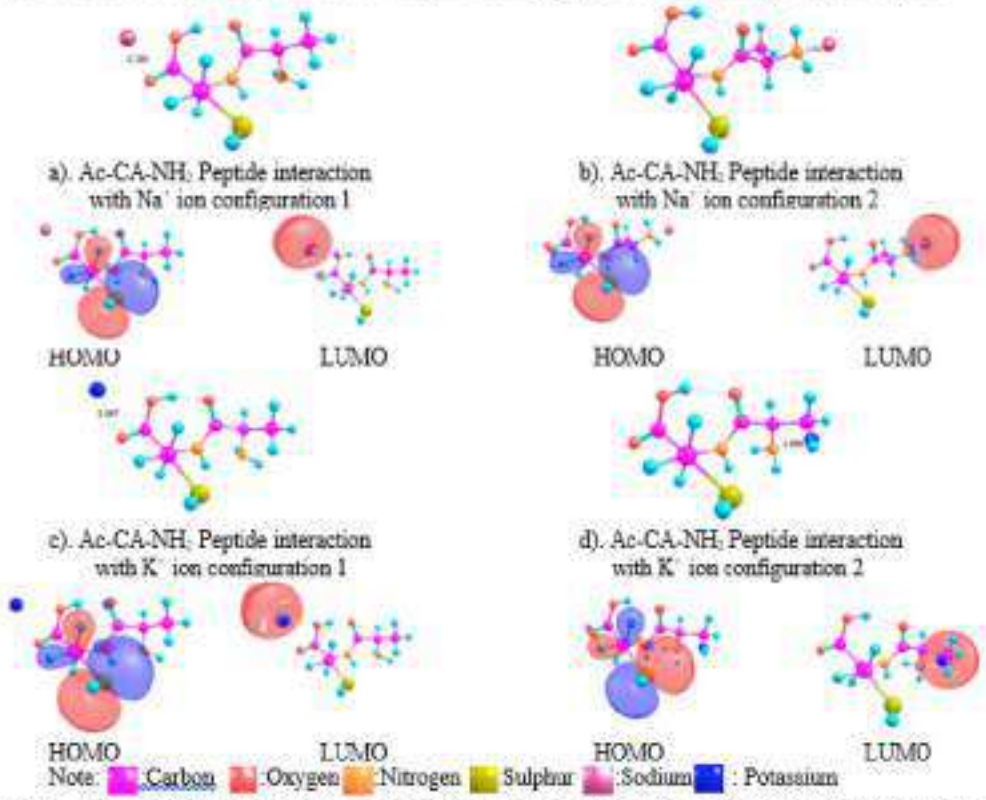


FIGURE 1. The interaction between Ac-CA-NH_2 peptide with Na^+ ion a). configuration-1 and b). configuration-2 and with K^+ ion c). configuration-1 and d). configuration-2

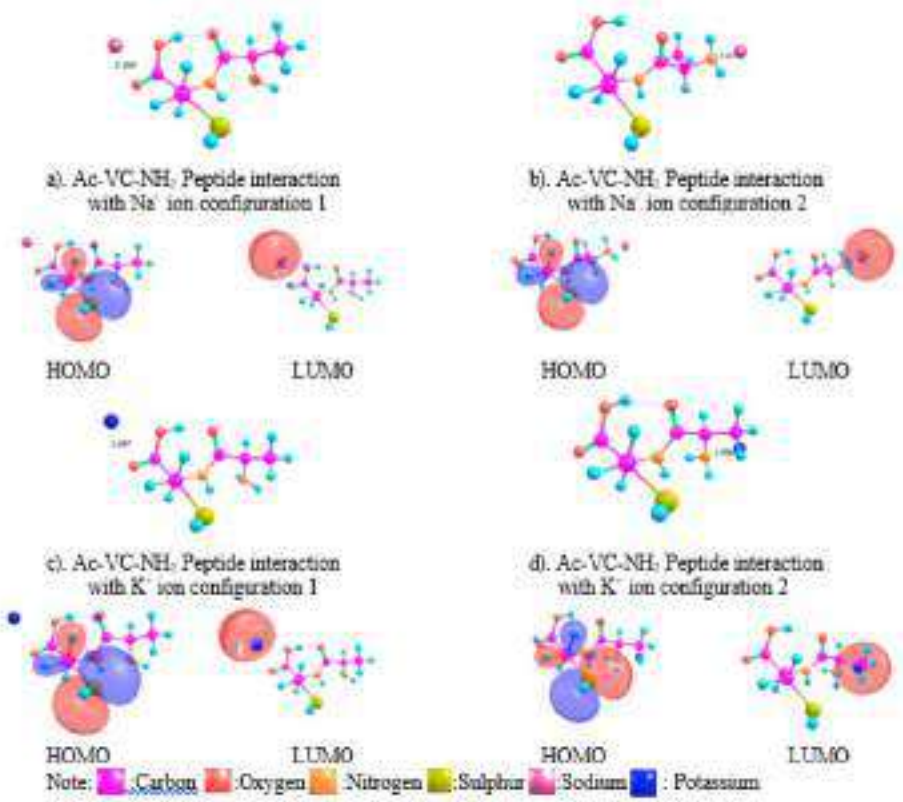


FIGURE 2. The interaction between Ac-VC-NH_2 peptide with Na^+ ion a). configuration-1 and b). configuration-2 and with K^+ ion c). configuration-1 and d). configuration-2

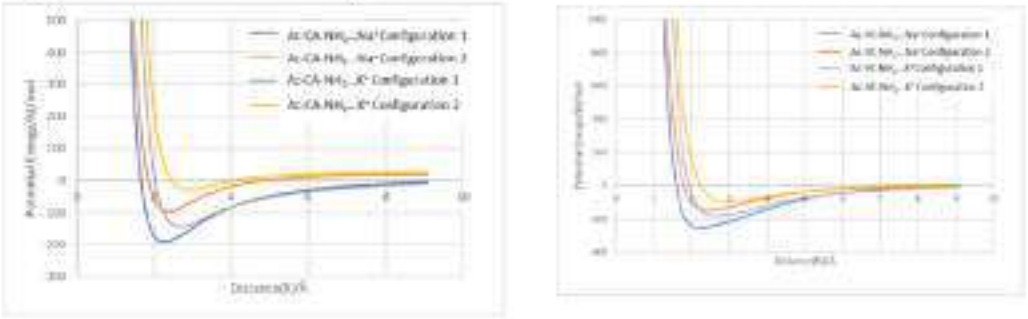
3.2 Interaction Energy

Figure 1 and Figure 2 show the interaction peptide and metal ions were on the –COOH [17]. Metal ions like Na^+ and K^+ can affect the stability and folding of peptide.[33] Lower interaction energy means that the interaction is more preferable and more stable. Table 1 shows the interaction energy between Ac-CA-NH_2 peptide with Na^+ and K^+ ions are more preferable and stable on configuration-1. Interaction between Ac-VC-NH_2 peptide with Na^+ and K^+ ions more preferable in configuration-1. The interaction energy with sodium ion is lower than potassium ion because of ionic radii of the ion. If ionic radii size is large, then the potential energy of the interaction is low. The potential energy of the interaction will affect the interaction energy. The interaction also affecting the conformation of the Ac-CA-NH_2 peptide interacting with Na^+ and K^+ ions as we can see on the change of dihedral of peptide bond after the interaction at 164.408° and 164.723° on configuration-1 and at 173.249° and 170.936° on configuration-2, respectively. The dihedral of Ac-VC-NH_2 peptide change at -177.056° and -179.367° for configuration-1 and at 175.404° and 176.282° for configuration-2 after interacting with Na^+ and K^+ ions, respectively.

TABLE 1. Interaction energy between peptide and metal ions

Peptide-Ion Interaction	Energy (kJ/mol)	
	Configuration-1	Configuration-2
Ac-CA-NH_2 Na	-189.782	-94.556
Ac-CA-NH_2 K	-141.280	-27.682
Ac-VC-NH_2 Na	-248.562	-146.414
Ac-VC-NH_2 K	-181.022	-90.568

The interaction energy can be visualized by plotting the energy with the distance variation between the Ac-CA-NH_2 and Ac-VC-NH_2 peptide and ion, Figure 3. If the distanceof the interaction is shorter, then repulsion force will dominate from attracting and resulting in the instability that causes positive energy interaction. The addition of interaction distance can reduce the repulsion from nuclear and stabilize interacting molecules. The stability of complex peptide-ion will be achieved if the potential energy reaches the deepest point on the graph. The addition of distance from the point of stability will make the attraction force dominate in the interaction. If the longer distance from the interaction even become infinity, the interaction energy will reduce until zero. As we can see on Figure 3, the interaction between Ac-CA-NH_2 and Ac-VC-NH_2 peptide with sodium and potassium ion reach the deepest of well in configuration-1. It means that configuration-1 has the most stable structure of interaction.



(a) (b)

FIGURE 3. Variation of interaction energy: (a) Ac-CA-NH_2...Na^+, Ac-CA-NH_2...K^+; b) Ac-VC-NH_2...Na^+ Ac-VC-NH_2...K^+

The partial atomic charge can be obtained from calculation. Value of partial atomic charge changed during the interaction. These can be explained by using the electronegativity parameter. Metal ion which has a positive charge tends to attract the electron and the atom that has negative charge tends to share the electron. Data of partial atomic charge on Table 2 and Table 3 can explain the reason why configuration-1 more preferable than configuration-2. There was more atomic characteristic that interacting with ion on configuration-1 than configuration-2. Steric effect also be the other factor that proposed more preferable on configuration-1 than configuration-2.

TABLE 2. The partial atomic charge of interaction between Ac-CA-NH_2 peptide with sodium and potassium ions

Atom	Before Interaction	After Interaction			
		Sodium Ion		Potassium Ion	
		Configuration 1	Configuration 2	Configuration 1	Configuration 2
O4	-0.62	-0.7	-0.61	-0.68	-0.61
O5	-0.54	-0.62	-0.51	-0.62	-0.52
N6	-0.72	-0.72	-0.73	-0.72	-0.74
S7	-0.01	0.03	-0.03	0.02	-0.03
O11	-0.69	-0.72	-0.67	-0.71	-0.65
N12	-0.74	-0.75	-0.82	-0.75	-0.8

TABLE 3. The partial atomic charge of interaction between Ac-VC-NH_2 peptide with sodium and potassium ion

Atom	Before Interaction	After Interaction			
		Sodium Ion		Potassium Ion	
		Configuration 1	Configuration 2	Configuration 1	Configuration 2
O6	-0.55	-0.64	-0.53	-0.64	-0.53
O7	-0.62	-0.56	-0.64	-0.56	-0.64
N8	-0.75	-0.73	-0.76	-0.73	-0.76
O12	-0.63	-0.72	-0.59	-0.72	-0.6
N13	-0.71	-0.75	-0.81	-0.75	-0.78
S14	0.02	0.01	-0.03	0.01	-0.08

3.3 HOMO-LUMO analysis

Other properties that can be observed in this interaction are electronic properties and chemical reactivity[34]. Electronic properties that can be observed is the energy gap. Energy gap represents the stability of the molecular system. Higher energy gap means that molecules need higher effort to excite to the excitation state. Chemical reactivity that can be observed in this interaction are ionization energy, electron affinity, and electronegativity. HOMO is described as ionization energy, and LUMO is described as electron affinity. The electronegativity is a total of ionization energy and electron affinity divided by 2. Table 4 and Table 5 show that the stability of Ac-CA-NH_2 and Ac-VC-NH_2 peptide were changed become more unstable because of decreasing of the energy gap. This decreasing of stability was supported by the increasing of electronegativity.

TABLE 4. Electronic Properties and Chemical Reactivity of interaction between Ac-CA-NH_2 peptide with sodium and potassium ions

Parameter	Before Interaction	After Interaction			
		Sodium Ion		Potassium Ion	
		Configuration 1	Configuration 2	Configuration 1	Configuration 2
HOMO	-9.992	-12.691	-12.455	-12.466	-12.28
LUMO	4.250	-3.029	-3.81	-2.729	-3.48
Energy Gap	14.242	9.662	8.645	9.737	8.8
Electronegativity	2.871	7.86	8.1325	7.5975	7.88

TABLE 5. Electronic Property and Chemical Reactivity of interaction between Ac-VC-NH_2 peptide with sodium and potassium ion

Parameter	Before Interaction	After Interaction			
		Sodium Ion		Potassium Ion	
		Configuration 1	Configuration 2	Configuration 1	Configuration 2
HOMO	-9.554	-12.380	-13.538	-12.262	-13.281
LUMO	4.552	-2.533	-3.320	-2.460	-3.074
Energy Gap	14.106	9.847	10.218	9.802	10.207
Electronegativity	2.501	7.457	8.429	7.361	8.178

The properties of interaction between Ac-CA-NH_2 and Ac-VC-NH_2 peptides with sodium and potassium ions which were obtained in this research are expected as a supplementary data for explaining the research of E-cadherin and ADT peptide interactions which were done by molecular mechanic and molecular docking [11, 35] and other peptide[33]. Furthermore, the result of this research can be used too

as a prediction to find the active side that have a conformational change. Polymer like chitin and chitosan along with their derivatives can be used to protect the peptides, thus the peptides will not have a conformational change in structure that can damage the stability of drugs that used for enhancing the porosity of BBB.[36-41] This research can be used for understanding the anion effect on amino acids and peptides conformation[22, 42].

4. Conclusion

The obtained interaction energy of Ac-CA-NH_2 peptide with sodium and potassium ions have indicated that configuration-1 was the most stable with interaction energy of -189.782 kJ/mol for sodium ion and configuration-1 with interaction energy -141.280 kJ/mol for potassium ion. Meanwhile, the interaction of Ac-VC-NH_2 peptide with sodium and potassium ions have the most stable configuration in configuration-1 with interaction energy -248.562 kJ/mol and -181.022 kJ/mol, respectively. The contribution of partial charge and HOMO-LUMO can be used for understanding the stability of peptide-metal ion interaction and also confirming the reactivity of the peptide after interacted with a metal ion.

5. Acknowledgment

Thanks to Prof. Teruna J. Siahaan, Ph.D. (Department of Pharmaceutical Chemistry, University of Kansas, US) for the valuable direction and discussion of the cells and drug delivery system. Thanks to Prof Krzysztof Kuczera, Ph.D. (Department of Chemistry, University of Kansas, US) for the in-depth discussion of a computational modeling. Thanks to the Indonesian Directorate General of Higher Education, which has funded this research and technology Funding Scheme 2013. Last but not least, Faculty of Science and Mathematics, which has funded this research through the Research Funding scheme 2017.

REFERENCE

1. P. Hobza and K. Müller-Dethlefs, *Non-covalent interactions: theory and experiment*. (Royal Society of Chemistry, 2010).
2. L. M. Teesch and J. Adams, Journal of the American Chemical Society **113** (3), 812-820 (1991).
3. A. Najafi Chermahini and Z. Jafari Chermahini, Journal of Molecular Liquids **214**, 101-110 (2016).
4. H. A. Alhazmi, M. Nachbar, H. M. Albishri, D. A. El-Hady, S. Redweik, S. El Deeb and H. Wätzig, Journal of Pharmaceutical and Biomedical Analysis **107**, 311-317 (2015).
5. J. A. Loo, International Journal of Mass Spectrometry **204** (1), 113-123 (2001).
6. N. A. Bushmarina, C. E. Blanchet, G. Vernier and V. Forge, Protein science **15** (4), 659-671 (2006).
7. C. P. Watson, E. Pazarentzos, M. Fidanboylu, B. Padilla, R. Brown and S. A. Thomas, Brain Research **1648, Part A**, 232-242 (2016).
8. O. Pertz, D. Bozic, A. W. Koch, C. Fauser, A. Brancaccio and J. Engel, The EMBO journal **18** (7), 1738-1747 (1999).
9. E. Sinaga, S. D. Jois, M. Avery, I. T. Makagiansar, U. S. Tambunan, K. L. Audus and T. J. Siahaan, Pharmaceutical research **19** (8), 1170-1179 (2002).
10. M. D. Laksitorini, P. K. Kiptoo, N. H. On, J. A. Thliveris, D. W. Miller and T. J. Siahaan, J Pharm Sci **104** (3), 1065-1075 (2015).
11. P. Siahaan, V. D. Prasasty, B. D. Simanjuntak, S. Hildayani and K. Anam, Journal of Tropical Life Science **7** (2), 138-145 (2017).
12. M. D. Laksitorini, University of Kansas, 2012.
13. P. Kiptoo, M. D. Laksitorini and T. J. Siahaan, in *Handbook of Biologically Active Peptides (Second Edition)* (Academic Press, Boston, 2013), pp. 1702-1710.

14. M. Laksitorini, V. D. Prasasty, P. K. Kiptoo and T. J. Siahaan, Ther Deliv **5** (10), 1143-1163 (2014).
15. V. W. Tang and D. A. Goodenough, Biophysical journal **84** (3), 1660-1673 (2003).
16. S. M. Krug, J. D. Schulzke and M. Fromm, presented at the Seminars in cell & developmental biology, 2014 (unpublished).
17. R. C. Dunbar, G. Berden and J. Oomens, International Journal of Mass Spectrometry **354**, 356-364 (2013).
18. A. R. Ross and S. L. Luettgen, Journal of the American Society for Mass Spectrometry **16** (9), 1536-1544 (2005).
19. A. Alaofi, E. Farokhi, V. D. Prasasty, A. Anbanandam, K. Kuczera and T. J. Siahaan, Journal of Biomolecular Structure and Dynamics **35** (1), 92-104 (2017).
20. E. Farokhi, University of Kansas, 2014.
21. R. C. Dunbar, N. C. Polfer, G. Berden and J. Oomens, International Journal of Mass Spectrometry **330**, 71-77 (2012).
22. T. M. Chang, G. Berden, J. Oomens and E. R. Williams, International Journal of Mass Spectrometry **377**, 440-447 (2015).
23. J. B. Foresman and A. Frisch, (1996).
24. P. Van Tat and U. K. Deiters, Chemical Physics (2018).
25. R. A. Evarestov, E. A. Kotomin, E. Heifets, J. Maier and G. Borstel, Solid State Communications **127** (5), 367-371 (2003).
26. M. Mian, N. M. Harrison, V. R. Saunders and W. R. Flavell, Chemical Physics Letters **257** (5), 627-632 (1996).
27. M. Valiev, E. J. Bylaska, N. Govind, K. Kowalski, T. P. Straatsma, H. J. J. Van Dam, D. Wang, J. Nieplocha, E. Apra, T. L. Windus and W. A. de Jong, Computer Physics Communications **181** (9), 1477-1489 (2010).
28. G. Andrienko, (2015).
29. Q. Wu, H. Su, H. Wang and H. Wang, Chemical Physics Letters **693**, 202-209 (2018).
30. M. Schmid, K. Baldridge, J. Boatz, S. Elbert, M. Gordon, J. Jensen, S. Koseki, N. Matsunaga, K. Nguyen and S. Su, J Comput Chem **14**, 1347-1363 (1993).
31. S. R. Pilli, T. Banerjee and K. Mohanty, Journal of Molecular Liquids **207**, 112-124 (2015).
32. B. K. Paul, A. Samanta and N. Guchhait, Journal of Molecular Structure **977** (1-3), 78-89 (2010).
33. M. J. Page and E. Di Cera, Physiological reviews **86** (4), 1049-1092 (2006).
34. P. Demir and F. Akman, Journal of Molecular Structure **1134**, 404-415 (2017).
35. A. Manna, M. D. Laksitorini, D. Hudiyanti and P. Siahaan, Jurnal Kimia Sains dan Aplikasi **20** (1), 30-36 (2017).
36. I. F. Saragih and P. Siahaan, Jurnal Kimia Sains dan Aplikasi **17** (2), 58-64 (2014).
37. A. Rahmani, T. Windarti and P. Siahaan, Jurnal Kimia Sains dan Aplikasi **14** (2), 43-47 (2011).
38. D. Yopianto, M. J. Sipangkar, R. Budiyanto and P. Siahaan, Jurnal Kimia Sains dan Aplikasi **19** (3), 118-125 (2016).
39. N. Nastiti and P. Siahaan, Jurnal Kimia Sains dan Aplikasi **18** (3), 104-109 (2015).
40. B. A. Prasojo and P. Siahaan, Jurnal Kimia Sains dan Aplikasi **18** (2), 62-66 (2015).
41. P. Siahaan, N. C. Mentari, U. O. Wiedyanto, D. Hudiyanti, S. Z. Hildayani and M. D. Laksitorini, Indonesian Journal of Chemistry **17** (2), 291-300 (2017).
42. J. T. O'Brien, J. S. Prell, G. Berden, J. Oomens and E. R. Williams, International Journal of Mass Spectrometry **297** (1-3), 116-123 (2010).

Ab-initio computational study of noncovalent interaction between peptide and alkaline metal ions on HF/6-31 G** level

ORIGINALITY REPORT

6%	1%	6%	1%
SIMILARITY INDEX	INTERNET SOURCES	PUBLICATIONS	STUDENT PAPERS

PRIMARY SOURCES

1	P Siahaan, S Wuning, A Manna, V D Prasasty, D Hudiyanti. " Probing the Interaction between Cyclic ADTC1 Ac-CADTPPVC-NH) Peptide with EC1-EC2 domain of E-cadherin using Molecular Docking Approach ", IOP Conference Series: Materials Science and Engineering, 2018 Publication	3%
2	Nurita Sari, Adid Adep Dwiatmoko, Sudiyarmanto Sudiyarmanto, Nanda Saridewi, Fauzan Aulia, Nino Rinaldi. "A preliminary study on Ru/TiO2 as heterogeneous catalyst for the depolymerization of empty fruit bunch-derived organosolv lignin", AIP Publishing, 2018 Publication	2%
3	P Siahaan, S N M Salimah, M J Sipangkar, D Hudiyanti, M C Djunaidi, M D Laksitorini. "Ab initio computational study of –N-C and –O-C bonding formation : functional group modification reaction based chitosan", IOP	1%

Conference Series: Materials Science and Engineering, 2018

Publication

4	www.nature.com Internet Source	1%

Exclude quotes	Off	Exclude matches	Off
Exclude bibliography	Off		