

**LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU *PEER REVIEW*
KARYA ILMIAH: PROSIDING**

Judul Publikasi Ilmiah (Artikel) : Ab-initio computational study of noncovalent interaction between peptide and alkaline metal ions on HF/6-31 G** level

Jumlah Penulis : 5 orang

Status Pengusul : penulis anggota

Identitas Jurnal Ilmiah

a. Nama Jurnal Ilmiah: : AIP Conference Proceedings, Volume 2049, 020053, ISSN 0094-243X

b. Nomor ISBN /ISSN : ISSN:0094-243X dan E-ISSN:1551-7616

c. Volume, Nomor, Bulan, Tahun : Volume 2049, 14 December 2018, Article number 020053

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f. Alamat web jurnal : <https://aip.scitation.org/toc/apc/2049/1>

g. Terindeks di [SCOPUS](#) (CiteScore is 0.37), [Scimago journal Rank](#) (H-index 60, SJR 0.18), Google Scholar, dll

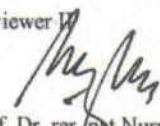
e. Jumlah Halaman : 8 halaman

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Hasil Penilaian *Peer Review*

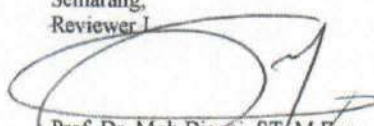
Komponen Yang Dinilai	Nilai Reviewer		Nilai Rata-rata
	Reviewer I	Reviewer II	
a. Kelengkapan unsur isi prosiding (10%)	3	2,4	2,7
b. Ruang lingkup dan kedalaman pembahasan (30%)	8	9	8,5
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9	9	9
d. Kelengkapan unsur dan kualitas penerbit (30%)	9	9	9
Total = (100%)	29	29,4	29,2
Nilai Pengusul= (60%)	2,9	2,94	2,92

Reviewer II


Prof. Dr. rer. nat Nuryono, M.S.
NIP. 196407141988111001

Unit kerja : Universitas Gadjah Mada Yogyakarta
Jabatan Fungsional : Guru Besar
Bidang ilmu : Kimia

Semarang,
Reviewer I


Prof. Dr. Moh Djaeni, ST, M.Eng
NIP. 197102071995121001

Unit Kerja : Universitas Diponegoro Semarang
Jabatan Fungsional : Guru Besar
Bidang Ilmu : Teknik Kimia

LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
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Hasil Penilaian Peer Review

Komponen Yang Dinilai	Nilai Maksimal Jurnal Ilmiah			Nilai Akhir yang diperoleh
	Internasional Bereputasi (prosiding)	Nasional Terakreditasi	Nasional	
	(30)			
a. Kelengkapan unsur isi prosiding (10%)	3			3
b. Ruang lingkup dan kedalaman pembahasan (30%)	9			8
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9			9
d. Kelengkapan unsur dan kualitas penerbit (30%)	9			9
Total = (100 %)	30			29
Nilai Pengusul = (40% x 29)/4 = 2.9				2.9

Catatan Penilaian artikel oleh Reviewer :

1. Kesesuaian dan kelengkapan unsur isi artikel:

Artikel sangat lengkap, dimana analisis tentang studi komputasi Ab-initio tentang interaksi nonkovalen antara ion logam peptida dan alkali pada tingkat HF / 6-31 G ** disajikan dengan terperinci, disitasi dan dibahas. Topik dan materi sesuai dengan jurnal yang bersangkutan. Tata penulisan tersaji dengan sangat baik.

Ruang lingkup dan kedalaman pembahasan:

Artikel ini membahas tentang studi komputasi Ab-initio tentang interaksi nonkovalen antara ion logam peptida dan alkali pada tingkat HF / 6-31 G **. Energi interaksi Ac-CA-NH₂ dengan ion natrium dan kalium menunjukkan yang paling stabil konfigurasi-1 dengan energi interaksi -189.782 kJ / mol untuk ion natrium dan -141.280 kJ / mol untuk ion kalium. Secara teknis pembahasan cukup jelas, hanya ada beberapa struktur molekul yang perlu dilengkapi citasi.

2. Kecukupan dan kemutakhiran data/informasi dan metodologi:

Referensi yang dicitasi dalam artikel ini ada 42 dimana 30 Baru (dalam 10 tahun terakhir). Nilai novelty/kebaruan artikel sangat baik. Analisa dengan singkat dan cukup jelas.

3. Kelengkapan unsur dan kualitas terbitan:

Penerbit adalah AIP Publishing dan terindeks Scopus, SJR 0.19, H-index 24. Nilai similaritas artikel berdasarkan Turnitin hanya 6%, sehingga orisinalitas sangat baik.

Semarang, November 2019
Reviewer

Prof. Dr. Moh. Djaeni, ST, M.Eng
NIP 197102071995121001

Unit Kerja : Universitas Diponegoro
Jabatan Fungsional : Guru Besar
Bidang Ilmu : Teknik Kimia

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Hasil Penilaian Peer Review

Komponen Yang Dinilai	Nilai Maksimal Jurnal Ilmiah			Nilai Akhir yang diperoleh
	Internasional Bereputasi (prosiding)	Nasional Terakreditasi	Nasional	
	(30)			
a. Kelengkapan unsur isi prosiding (10%)	3			2,4
b. Ruang lingkup dan kedalaman pembahasan (30%)	9			9,0
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9			9,0
d. Kelengkapan unsur dan kualitas penerbit (30%)	9			9,0
Total = (100 %)	30			29,4

Nilai Pengusul = $(40\% \times 29,4)/4 = 2,94$

Catatan Penilaian artikel oleh Reviewer:

- a. Kelengkapan unsur isi Prosiding:**
 Prosiding diterbitkan dalam AIP Conference Proceedings 2049, 020053 (2018). Komponen dalam artikel sangat lengkap. Penulisan kurang sistematis; abstract terlalu panjang, ditemui beberapa kesalahan gramatika. Similaritas artikel berdasarkan Turnitin hanya 6%, originalitas tinggi.
- b. Ruang lingkup dan kedalaman pembahasan:**
 Pembahasan dalam artikel ini memiliki ruang lingkup yang sesuai dan selaras dengan dengan topik riset, yaitu membahas studi komputasi Ab-initio tentang interaksi nonkovalen antara ion logam peptida dan alkali pada tingkat HF / 6-31 G **. Pembahasan disajikan secara mendalam dan detail, disertai dengan referensi pendukung.
- c. Kecukupan dan kemutakhiran data/informasi dan metodologi:**
 Data riset yang disajikan sangat mencukupi untuk prosiding dan memiliki nilai kebaruan tinggi. Kemutakhiran dari aspek referensi, sebanyak 42 referensi disitasi, dan 29 (67%) terbit dalam 10 tahun terakhir. Metode disajikan dengan tahapan yang jelas untuk penelitian dengan pendekatan komputasi.
- d. Kelengkapan unsur dan kualitas penerbit:**
 Penerbit adalah AIP Publishing (bereputasi), prosiding terindeks Scopus, SJR 0.19, H-index 24.

Yogyakarta, November 2019

Reviewer



Prof. Dr. nat Nuryono, M.S.

NIP. 196407141988111001

Bidang ilmu/Unit kerja :

Departemen Kimia pada Fakultas MIPA UGM Yogyakarta



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AIP Conference Proceedings

Volume 2049, 14 December 2018, Article number 020053

3rd International Seminar on Chemistry: Green Chemistry and Its Role for Sustainability, ISOC 2018; Sheraton Surabaya Hotel and Towers Surabaya; Indonesia; 18 July 2018 through 19 July 2018; Code 143205

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

Siahaan, P.^a ✉, Christian, R.^a, Fauziah, A.N.^a, Hudiayanti, D.^a, Prasasty, V.D.^b 👤

🔖 Save all to author list

^aDepartement of Chemistry, Faculty of Science and Mathematics, Diponegoro University, Indonesia

^bFaculty of Biotechnology, Atma Jaya Catholic University of Indonesia, Indonesia

Abstract

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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-NH₂ (Cysteine-Alanine) and Ac-VC-NH₂ (Valine-Cysteine) peptides by ab initio computational approach with a minimum energy; the interaction stability of Ac-CA-NH₂ and Ac-VC-NH₂ 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-NH₂ and Ac-VC-NH₂ 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-NH₂ and Ac-VC-NH₂ 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-NH₂ 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-NH₂ 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. © 2018 Author(s).

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Probing of interaction mode between linier and cyclic ADTC6 (Ac-CDTPPC-NH₂) with E-cadherin protein using molecular docking approach

Siahaan, P., Kaswanda, J.A., Budiayanto, R. (2019) *IOP Conference Series: Materials Science and Engineering*

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References (42)

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- ☐ 1 Hobza, P., Müller-Dethlefs, K.
(2010) *Non-covalent Interactions: Theory and Experiment*. Cited 335 times.
(Royal Society of Chemistry)

- ☐ 2 Teesch, L.M., Adams, J.
Fragmentations of Gas-Phase Complexes between Alkali Metal Ions and Peptides: Metal Ion Binding to Carbonyl Oxygens and Other Neutral Functional Groups

(1991) *Journal of the American Chemical Society*, 113 (3), pp. 812-820. Cited 168 times.
doi: 10.1021/ja00003a013

[View at Publisher](#)

- ☐ 3 Najafi Chermahini, A., Jafari Chermahini, Z.
Comparing the ion affinity of two ionophores: Theoretical study of alkali earth metal ion-nano tubular cyclic peptide complexes

(2016) *Journal of Molecular Liquids*, 214, pp. 101-110. Cited 4 times.
doi: 10.1016/j.molliq.2015.12.024

[View at Publisher](#)

- ☐ 4 Alhazmi, H.A., Nachbar, M., Albishri, H.M., El-Hady, D.A., Redweik, S., El Deeb, S., Wätzig, H.
A comprehensive platform to investigate protein-metal ion interactions by affinity capillary electrophoresis

(2015) *Journal of Pharmaceutical and Biomedical Analysis*, 107, pp. 311-317. Cited 28 times.
www.elsevier.com/locate/jpba
doi: 10.1016/j.jpba.2015.01.017

[View at Publisher](#)

- ☐ 5 Loo, J.A.
Probing protein-metal ion interactions by electrospray ionization mass spectrometry: Enolase and nucleocapsid protein
(2001) *International Journal of Mass Spectrometry*, 204 (1-3), pp. 113-123. Cited 36 times.
doi: 10.1016/S1387-3806(00)00334-1
[View at Publisher](#)
-
- ☐ 6 Bushmarina, N.A., Blanchet, C.E., Vernier, G., Forge, V.
Cofactor effects on the protein folding reaction: Acceleration of α -lactalbumin refolding by metal ions
(2006) *Protein Science*, 15 (4), pp. 659-671. Cited 39 times.
<http://www.proteinscience.org/cgi/reprint/15/4/659>
doi: 10.1110/ps.051904206
[View at Publisher](#)
-
- ☐ 7 Watson, C.P., Pazarentzos, E., Fidanboyu, M., Padilla, B., Brown, R., Thomas, S.A.
The transporter and permeability interactions of asymmetric dimethylarginine (ADMA) and L-arginine with the human blood-brain barrier in vitro ([Open Access](#))
(2016) *Brain Research, Part A* 1648, pp. 232-242. Cited 7 times.
www.elsevier.com/locate/bri
doi: 10.1016/j.brainres.2016.07.026
[View at Publisher](#)
-
- ☐ 8 Pertz, O., Bozic, D., Koch, A.W., Fauser, C., Brancaccio, A., Engel, J.
A new crystal structure, Ca^{2+} dependence and mutational analysis reveal molecular details of E-cadherin homoassociation
(1999) *EMBO Journal*, 18 (7), pp. 1738-1747. Cited 329 times.
[View at Publisher](#)
-
- ☐ 9 Sinaga, E., Jois, S.D.S., Avery, M., Makagiansar, I.T., Tambunan, U.S.F., Audus, K.L., Siahaan, T.J.
Increasing paracellular porosity by E-cadherin peptides: Discovery of bulge and groove regions in the EC1-domain of E-cadherin
(2002) *Pharmaceutical Research*, 19 (8), pp. 1170-1179. Cited 42 times.
doi: 10.1023/A:1019850226631
[View at Publisher](#)
-
- ☐ 10 Laksitorini, M.D., Kiptoo, P.K., On, N.H., Thliveris, J.A., Miller, D.W., Siahaan, T.J.
Modulation of intercellular junctions by cyclic-ADT peptides as a method to reversibly increase blood-brain barrier permeability
(2015) *Journal of Pharmaceutical Sciences*, 104 (3), pp. 1065-1075. Cited 20 times.
www.interscience.wiley.com/jpages/0022-3549
doi: 10.1002/jps.24309
[View at Publisher](#)
-
- ☐ 11 Siahaan, P., Prasasty, V.D., Simanjuntak, B.D., Hildayani, S., Anam, K.
(2017) *Journal of Tropical Life Science*, 7 (2), pp. 138-145. Cited 3 times.

- ☐ 12 Laksitorini, M.D.
(2012) *University of Kansas*
-
- ☐ 13 Kiptoo, P., Laksitorini, M.D., Siahaan, T.J.
Peptide Delivery
(2013) *Handbook of Biologically Active Peptides*, pp. 1702-1710. Cited 7 times.
<http://www.sciencedirect.com/science/book/9780123850959>
ISBN: 978-012385095-9
doi: 10.1016/B978-0-12-385095-9.00233-5

View at Publisher
-
- ☐ 14 Laksitorini, M., Prasasty, V.D., Kiptoo, P.K., Siahaan, T.J.
Pathways and progress in improving drug delivery through the intestinal mucosa and blood-brain barriers
(2014) *Therapeutic Delivery*, 5 (10), pp. 1143-1163. Cited 40 times.
<http://www.future-science.com/loi/tde>
doi: 10.4155/tde.14.67

View at Publisher
-
- ☐ 15 Tang, V.W., Goodenough, D.A.
Paracellular ion channel at the tight junction (Open Access)
(2003) *Biophysical Journal*, 84 (3), pp. 1660-1673. Cited 148 times.
<http://www.sciencedirect.com/science/journal/00063495>
doi: 10.1016/S0006-3495(03)74975-3

View at Publisher
-
- ☐ 16 Krug, S.M., Schulzke, J.D., Fromm, M.
(2014) *Present. at the Seminars in Cell Developmental Biology*
(unpublished)
-
- ☐ 17 Dunbar, R.C., Berden, G., Oomens, J.
How does a small peptide choose how to bind a metal ion? IRMPD and computational survey of CS versus Iminol binding preferences
(2013) *International Journal of Mass Spectrometry*, 354-355, pp. 356-364. Cited 28 times.
doi: 10.1016/j.ijms.2013.07.017

View at Publisher
-
- ☐ 18 Ross, A.R.S., Luetzggen, S.L.
Speciation of cyclo(Pro-Gly)₃ and its divalent metal-ion complexes by electrospray ionization mass spectrometry (Open Access)
(2005) *Journal of the American Society for Mass Spectrometry*, 16 (9), pp. 1536-1544. Cited 12 times.
doi: 10.1016/j.jasms.2005.05.002

View at Publisher
-

- ☐ 19 Alaofi, A., Farokhi, E., Prasasty, V.D., Anbanandam, A., Kuczera, K., Siahaan, T.J.
Probing the interaction between cHAVc3 peptide and the EC1 domain of E-cadherin using NMR and molecular dynamics simulations
(2017) *Journal of Biomolecular Structure and Dynamics*, 35 (1), pp. 92-104. Cited 10 times.
<http://www.tandfonline.com/loi/tbsd20>
doi: 10.1080/07391102.2015.1133321
[View at Publisher](#)
-
- ☐ 20 Farokhi, E.
(2014)
University of Kansas
-
- ☐ 21 Dunbar, R.C., Polfer, N.C., Berden, G., Oomens, J.
Metal ion binding to peptides: Oxygen or nitrogen sites?
(2012) *International Journal of Mass Spectrometry*, 330-332, pp. 71-77. Cited 40 times.
doi: 10.1016/j.ijms.2012.10.006
[View at Publisher](#)
-
- ☐ 22 Chang, T.M., Berden, G., Oomens, J., Williams, E.R.
Halide anion binding to Gly₃, Ala₃ and Leu₃
(2015) *International Journal of Mass Spectrometry*, 377 (1), pp. 440-447. Cited 7 times.
<http://www.journals.elsevier.com/international-journal-of-mass-spectrometry/>
doi: 10.1016/j.ijms.2014.02.019
[View at Publisher](#)
-
- ☐ 23 Foresman, J.B., Frisch, A.
(1996)
-
- ☐ 24 Van Tat, P., Deiters, U.K.
(2018) *Chemical Physics*
-
- ☐ 25 Evarestov, R.A., Kotomin, E.A., Heifets, E., Maier, J., Borstel, G.
Ab initio Hartree-Fock calculations of LaMnO₃ (1 1 0) surfaces
(2003) *Solid State Communications*, 127 (5), pp. 367-371. Cited 23 times.
doi: 10.1016/S0038-1098(03)00440-X
[View at Publisher](#)
-
- ☐ 26 Mian, M., Harrison, N.M., Saunders, V.R., Flavell, W.R.
An ab initio Hartree-Fock investigation of galena (PbS)
(1996) *Chemical Physics Letters*, 257 (5-6), pp. 627-632. Cited 32 times.
<http://www.elsevier.com/locate/cplonline>
doi: 10.1016/0009-2614(96)00591-X
[View at Publisher](#)
-

- 27 Valiev, M., Bylaska, E.J., Govind, N., Kowalski, K., Straatsma, T.P., Van Dam, H.J.J., Wang, D., (...), De Jong, W.A.
NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations
(2010) *Computer Physics Communications*, 181 (9), pp. 1477-1489. Cited 2530 times.
doi: 10.1016/j.cpc.2010.04.018
[View at Publisher](#)
-
- 28 Andrienko, G.
(2015)
-
- 29 Wu, Q., Su, H., Wang, H., Wang, H.
Ab initio calculations, structure, NBO and NCI analyses of X–H···TT interactions
(2018) *Chemical Physics Letters*, 693, pp. 202-209. Cited 6 times.
<http://www.elsevier.com/locate/cplonline>
doi: 10.1016/j.cplett.2018.01.015
[View at Publisher](#)
-
- 30 Schmidt, M.W., Baldridge, K.K., Boatz, J.A., Elbert, S.T., Gordon, M.S., Jensen, J.H., Koseki, S., (...), Montgomery, J.A.
General atomic and molecular electronic structure system
(1993) *Journal of Computational Chemistry*, 14 (11), pp. 1347-1363. Cited 17173 times.
doi: 10.1002/jcc.540141112
[View at Publisher](#)
-
- 31 Pilli, S.R., Banerjee, T., Mohanty, K.
HOMO-LUMO energy interactions between endocrine disrupting chemicals and ionic liquids using the density functional theory: Evaluation and comparison
(2015) *Journal of Molecular Liquids*, 207, art. no. 4714, pp. 112-124. Cited 16 times.
doi: 10.1016/j.molliq.2015.03.019
[View at Publisher](#)
-
- 32 Paul, B.K., Samanta, A., Guchhait, N.
Influence of chlorine substitution on intramolecular hydrogen bond energy and ESPT barrier: Experimental and theoretical measurements on the photophysics of 3,5-dichlorosalicylic acid
(2010) *Journal of Molecular Structure*, 977 (1-3), pp. 78-89. Cited 28 times.
doi: 10.1016/j.molstruc.2010.05.018
[View at Publisher](#)
-
- 33 Page, M.J., Di Cera, E.
Role of Na⁺ and K⁺ in enzyme function
(2006) *Physiological Reviews*, 86 (4), pp. 1049-1092. Cited 193 times.
<http://physrev.physiology.org/cgi/reprint/86/4/1049>
doi: 10.1152/physrev.00008.2006
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-

- 34 Demir, P., Akman, F.
Molecular structure, spectroscopic characterization, HOMO and LUMO analysis of PU and PCL grafted onto PEMA-co-PHEMA with DFT quantum chemical calculations
(2017) *Journal of Molecular Structure*, 1134, pp. 404-415. Cited 16 times.
www.elsevier.com/locate/jmolstruc
doi: 10.1016/j.jmolstruc.2016.12.101
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-
- 35 Manna, A., Laksitorini, M.D., Hudiyanti, D., Siahaan, P.
(2017) *Jurnal Kimia Sains Dan Aplikasi*, 20 (1), pp. 30-36.
-
- 36 Saragih, I.F., Siahaan, P.
(2014) *Jurnal Kimia Sains Dan Aplikasi*, 17 (2), pp. 58-64.
-
- 37 Rahmani, A., Windarti, T., Siahaan, P.
(2011) *Jurnal Kimia Sains Dan Aplikasi*, 14 (2), pp. 43-47.
-
- 38 Yopianto, D., Sipangkar, M.J., Budiyanto, R., Siahaan, P.
(2016) *Jurnal Kimia Sains Dan Aplikasi*, 19 (3), pp. 118-125.
-
- 39 Nastiti, N., Siahaan, P.
(2015) *Jurnal Kimia Sains Dan Aplikasi*, 18 (3), pp. 104-109.
-
- 40 Prasajo, B.A., Siahaan, P.
(2015) *Jurnal Kimia Sains Dan Aplikasi*, 18 (2), pp. 62-66.
-
- 41 Siahaan, P., Mentari, N.C., Wiedyanto, U.O., Hudiyanti, D., Hildayani, S.Z., Laksitorini, M.D.
The optimum conditions of carboxymethyl chitosan synthesis on drug delivery application and its release of kinetics study ([Open Access](#))
(2017) *Indonesian Journal of Chemistry*, 17 (2), pp. 291-300. Cited 6 times.
<http://pdm-mipa.ugm.ac.id/ojs/index.php/ijc/article/download/1272/1291>
doi: 10.22146/ijc.24252
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-
- 42 O'Brien, J.T., Prell, J.S., Berden, G., Oomens, J., Williams, E.R.
Effects of anions on the zwitterion stability of Glu, His and Arg investigated by IRMPD spectroscopy and theory
(2010) *International Journal of Mass Spectrometry*, 297 (1-3), pp. 116-123. Cited 39 times.
doi: 10.1016/j.ijms.2010.07.003
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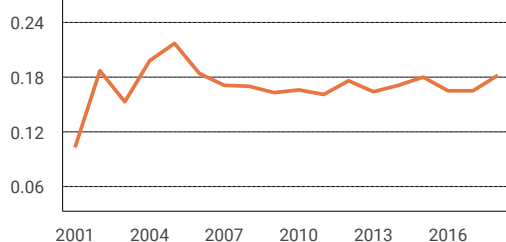
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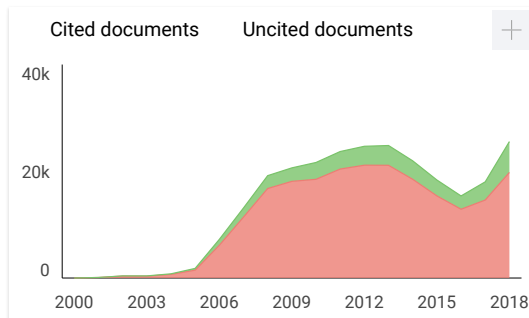
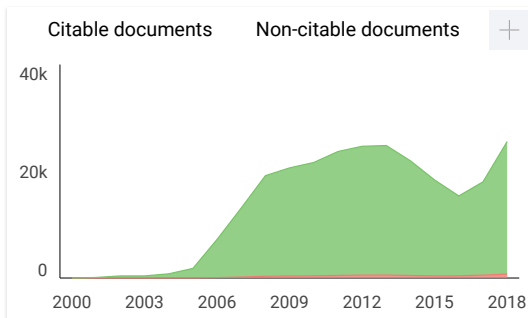
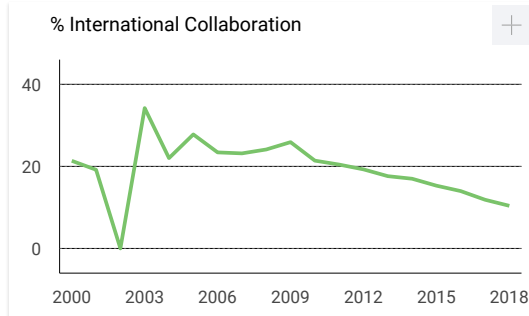
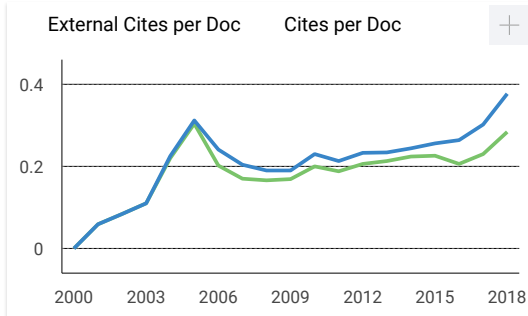
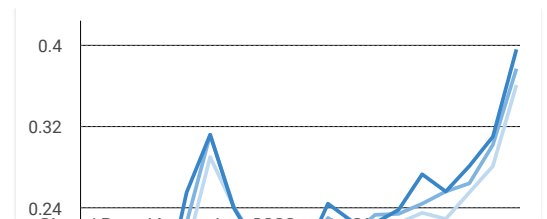
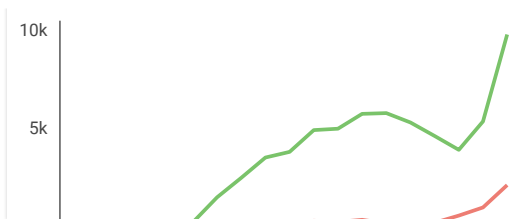
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The 3rd International Seminar on Chemistry

Green Chemistry and its Role
for Sustainability



Surabaya, Indonesia

18–19 July 2018

Editors

Yuly Kusumawati, Sri Fatmawati, Adi Setyo Purnomo, Fredy Kurniawan
and Hendro Juwono

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Wednesday, 18 July 2018

Keynote speaker dari 4 negara

Time

07.30 - 08.30	Registration
08.30 - 08.45	Opening Ceremony: Welcoming Remarks of Rector of Institut Teknologi Sepuluh Nopember Surabaya (Prof. Ir. Joni Hermana, M.Sc.Es., Ph.D.)
08.45 - 09.25	Keynote 1: Searching for Bioactive Compounds from Thai Plants (Prof. Dr. Warinthorn Chavasiri from Chulalongkorn University - Thailand)
09.25 - 10.05	Keynote 2: Integrated fungal fermentation for the conversion of woody biomass by the multifunctional fungus (Prof. Ichiro Kamei from University of Miyazaki - Japan)
10.05 - 10.20	Coffee Break
10.20 - 11.00	Keynote 3: Modified Magnesium fluoride as a potential heterogeneous catalyst in some organic reactions (Prof. Dr. Irminda Kris Murwani from ITS Surabaya - Indonesia)
11.00 - 11.40	Keynote 4: Templated carbons - Synthesis and Applications (Prof. Takashi Kyotani from Tohoku University - Japan)
11.40 - 12.20	Keynote 5: Challenges in structure-activity correlation in Titania catalysis and photocatalysis (Prof. Hadi Nur from Universiti Teknologi Malaysia - Malaysia)
12.20 - 13.20	Lunch and Poster Session
ORAL SESSION	

	ROOM 1 (Medicine) Ballroom 1	ROOM 2 (Medicine) Ballroom 2	ROOM 3 (Medicine) Ballroom 3	ROOM 4 (Material) Singasari	ROOM 5 (Environment) Mataram	ROOM 6 (Medicine /Material) Kahuripan	ROOM 7 (Food) Jenggala	ROOM 8 (Organic) Daha
13.20 - 13.35	1054	1129	1003	1005	1001	1121	1018	1010
13.35 - 13.50	1057	1142	1006	1008	1022	1133	1045	1011
13.50 - 14.05	1058	1146	1009	1017	1026	1169	1056	1016
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Thursday, 19 July 2018

Time

07.30 - 08.00	Registration
08.00 - 08.10	Welcoming Remarks of Dean of Faculty of Science - ITS (Prof. Dr. rer.nat. Agus Rubiyanto)
08.10 - 08.20	Welcoming Remarks of The President of OWSD Indonesia National Chapter and Brief overview of OWSD – Indonesia National Chapter (Sri Fatmawati, PhD)
08.20 - 08.30	Welcoming Remarks Delegation of the secretariat OWSD – Italy, by The vice president of Asia Pacific Region (Dr. Atya Kapley)*
08.30 - 09.00	Honorary Speech: Women in science empowerment in Indonesia by The First Lady of Indonesia (Hj. Iriana Joko Widodo, SE, MM)*
09.00 - 09.30	Best practice of women empowerment in Surabaya by Mayor of Surabaya (Dr.HC. Tri Rismaharini)*
09.30 - 09.40	Launching OWSD – Indonesia National Chapter, “beating with Javanese gong and photo session”
09.40 - 09.50	Coffee Break
09.50 - 10.20	Invited 1: Selective Synthesis of Phenylpropanoid Sucrose Esters (Prof. Zaher Judeh from Nanyang Technological University -
10.20 - 10.50	Invited 2: Reuse of Mother Liquor in the Synthesis of UiO-66 using Solvothermal Method (Ratna Ediati Ph.D from Institut Teknologi Sepuluh Nopember - Indonesia)
10.50 - 11.20	Invited 3: Carbon dot-and Boronic Acid-Modified Nanoparticle as Selestive Targeting on Cancer Cell and HIV Virus (Moch. Zakki Fahmi, Ph.D from Airlangga University - Indonesia)
11.20 - 12.30	Lunch and Poster Session

ORAL SESSION

	ROOM 1 (Material) Ballroom 1	ROOM 2 (Material) Ballroom 2	ROOM 3 (Material) Ballroom 3	ROOM 4 (Education / Material)	ROOM 5 (Environmenta l) Kahuripan	ROOM 6 (Energy) Jenggala
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Optimization of Biomass-Based Electrochemical Capacitor Performance

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Abstract. The electrochemical capacitor (EC) from various carbon materials, i.e., carbon nanosheet from gelam wood, carbon nanotube from sesame oil, carbon honeycomb-like from sengon wood used as electrodes were studied, as well as the solvent used, i.e., dimethylsulphoxide, ethyleneglycol, propylene carbonate and the electrolytes, i.e., disodiumtetraboratdecahydrate (DSTB) and sodiumdiethyldithiocarbamate (SDEDTC). Their performance were optimized for three factors by using full factorial design of experiment technique. The three factors chosen for experiments were the controllable variables that have key role to play in the EC performance, i.e., carbon types applied in electrodes, organic solvent that dispersed electrolytes, and electrolytes. Types of carbon has highest effect on capacitance value and carbon from gelam wood bark has the best capacitance value. There exist strong interaction effect between type of carbon and solvent as well as between type of carbon and electrolyte contribute capacitance of ECs. Operating voltage of EC from the beginning cycle until cycle-2000 is about 1.2 to 1.4 volts, i.e., using CNS electrode with 20% SDEDTC electrolyte and DMSO as solvent.

Keywords: supercapacitor, voltammetry, galvanostatic, electrodes, full-factorial, capacitance, ESR

INTRODUCTION

Human activities and machinery are always need supply energy to proceed. Research about energy conversion and storage run simultaneously to achieve energy security. Energy storage device, such as electrochemical capacitor (EC), also known as supercapacitor must have characters, i.e., long cycle life, high efficiency, high power density an environmental friendly[1].

Biomass based carbon materials have gained considerable attention in the last few years due to their high chemical and thermal stability, tunable pore size distribution, and high specific surface areas, which lead to become a choice in support EC manufacture [2]. The facts are biomass based carbon is cheap and its availability, make the perfect substitute for polymer-based carbon electrodes in EC [3]. However, the usage the carbons in EC are very limited because of their distinct crystallographies and morphologies or allotropes [4].

It should be noted, however, that the information comes up from the “one variable at time” (OVAT) observations do not have satisfactory. Such observations do not analyzed simultaneously and reduce a part observations that normally must do. This method does not count the possibility of intervariable action that affect the outcome or parameter [5]. The whole pictures of a system can be unify, by deconvulated the effects of each variable from possible variable interactions that contribute to the same observed effects [6]. Some additional observations must be provided in order to achieve good understanding of the contribution of the each variables [7].

Factorial design is the method for such situation and has been used as Design of Experiment (DOE). The three factors observation is chosen for the experiment. The controllable variables that have key role to play in the

Ion-Molecule Reactions of Organic Molecules with Noble Metal Atoms in Superfluid Helium Droplets

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Abstract. Superfluid helium droplets (HeDs) provide a unique environment for the study of physical and chemical phenomena at a very low temperature. Properties of HeDs include the very low temperature (0.37 K), superfluidity and the ability to capture a wide variety of atoms and molecules. Subsequently, the molecules isolated in HeDs can be studied by mass spectrometry and/or spectroscopy. In this work, dissociative ion-molecule reactions of metal-organic complexes formed in superfluid HeDs are reported. Two organic molecules, 1-pentanol and 1,9-decadiene, and two noble metals, gold (Au) and silver (Ag), were employed to form binary metal-organic complexes by sequential addition of organic molecules and metal atoms to superfluid HeDs. The resulting complexes were then investigated by mass spectrometry. Electron impact of a doped HeDs first creates a He^+ ion, which ionizes the embedded molecules through resonance charge transfer. This highly energetic process delivers excess energy to the molecular clusters, leading to dissociative ion-molecule reactions. The mass spectra show softening effects and caging effects induced by the superfluid helium for both 1-pentanol and 1,9-decadiene, and the co-addition of Ag or Au has been found to have minor influence to the fragmentation patterns, except for the 1,9-decadiene-Au complex. This is attributed to the different ionization energy of the selected molecules and metals, which influences the overall energy delivered to the organic molecules studied and thus the degree of fragmentation.

Keywords : Binary Complex, Ion-molecule reaction, Mass Spectrometry, Superfluid Helium Droplets

INTRODUCTION

Helium droplets (HeDs) are large clusters of superfluid helium typically composed of 10^3 - 10^{11} helium atoms [1,2,3]. Having remarkable properties as a superfluid, HeDs provide a means to study molecules and molecular clusters in isolated nanoreactors. Due to the superfluidity and the very low steady-state temperature, HeDs have an ultrahigh cooling rate for the species captured, *i.e.*, by evaporation of weakly bound helium atoms. Doping of single or multiple atoms/molecules to a droplet is possible, which can be achieved by collision(s) between the droplet and gas-phase atoms/molecules. This process is highly “sticky”, with a near unity pickup probability upon each collision event [4]. When different types of molecules/atoms are added to HeDs, binary clusters can be obtained, which can be investigated, for example, by mass spectrometry and spectroscopy [5].

Electron-impact (EI) mass spectrometry is one of the most commonly used methods for studying the molecules or clusters embedded in HeDs. The ionization process starts with the creation of a He^+ ion near the surface of the droplet, which then transfer its charge to the dopants *via* a charge transfer process proposed by Atkins [6]. If the He^+ ion reaches an impurity after a small number of hops, it can transfer its charge to the dopant [7,8] resulting in ionization and subsequent ion-molecule reactions due to the large ionization energy of the helium atom. Otherwise, it may terminate by the formation of He_n^+ ions by self-trapping, predominantly leading to the formation of He_2^+ . A combination of experimental and associated theoretical model showed that the number of hops is about 10 before

Influence of Nanocellulose in The Emulsion System of Resiprene-35 Containing Lutrol F127 and Tween80

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Abstract

The research focusing on the influence of surfactant and nanocellulose type to the emulsion stability of resiprene-35 has been conducted. The prepared emulsion has 30:30:10 ratio of resiprene-35, water, and surfactant, respectively. Emulsion system also contained nanocellulose (NCC and LCNF, both concentration is 1%) with 2.1-28.6% of fibril dosages. The homogenization process of emulsion system is conducted with ultrasonic treatment. Emulsion system with the addition of Lutrol F127 showed lower result on stability than Tween80. The emulsion system with Tween80 in the presence of NCC showed higher ESI value than the emulsion system that contained LCNF. On 1st day of observation, emulsion system of resiprene-35/ Tween80 showed 100% of ESI. The value decreased to 70-100% of ESI at the 28th days with trend increasing of fibril dosage.

Keywords: Emulsion, resiprene-35, NCC, LCNF, stability, ESI

INTRODUCTION

Resiprene-35 is one of the obtainable materials from natural rubber by cyclization process using Lewis acid (e.g. AlCl₃, SnCl₄, etc.) [1–4]. Resiprene-35 as binder (paint) vessel has also many advantages than the other type of commercial binder, such as resistance to chemicals and water as well as an excellent resin for application in environments that are susceptible to corrosion.

Nowadays, nanocellulose (NC) material has become popular in many research field because of its promising properties that can act as filler or reinforcing agent for improving the mechanical properties of material [5–7]. Many references referred cellulose and its derivatives, e.g. microcrystalline cellulose, hydrophobic modification of cellulose, cellulose whisker, BC-TEMPO modified, are able to be used for stabilizing agent of W/O and O/W emulsion [8–11]. The other references also report that nanocrystalline cellulose (NCC) and lignocellulose nanofiber (LCNF) have been used as a reinforcing additive in the waterborne, solvent base two component polyurethane lacquer coating and inkjet printing [12–15]. However, no studies could be found yet on the effect of surfactants to the emulsion stability of resiprene-35 in the presence of NC. The stability of emulsion is affected by the wettability of particle surface. Many researches have been conducted to improve the emulsion stability using biomass-nanoparticle, such as using soy protein, keratin, starch, cellulose and chitin [16–19]. The utilization of NCs as emulsion stabilizer is expected to be advantageous than inorganic nanoparticles when cost issue, biodegradability and biocompatibility are considered.

In this study, the influence of NC into the resiprene-35 emulsion system containing two commercial surfactants, Tween80 and Lutrol F127 was investigated. In other words, this work is quite new about designing resiprene-35 emulsions that supported by a mixture of surfactants-NC. The NCC and LCNF were used as NC resources, the different on the morphology of those NCs will give a different effect on the emulsion stability of

Antioxidant Activity against Hydrogen Peroxide-Induced Cytotoxicity of *Euphorbia Hirta* L.

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Abstract. *Euphorbia hirta* L. has been proved a medicinally important plant. This study aimed to investigate the antioxidant capacities of fractioned extracts and some isolated compounds from *Euphorbia hirta* L. on pancreatic β -cells MIN6 exposed to hydrogen peroxide-oxidative stress conditions. Four pure compounds were isolated from ethyl acetate and methanol extracts and identified as quercitrin (**1**), luteolin (**2**), quercetin (**3**) and caffeic acid (**4**). The results showed that the ethyl acetate extract as well as quercetin possess strong protective effects with the cell viability of 81% and 82% at the dose of 0.1 mg/mL. This proves that *E. hirta* L. is a potentially natural antioxidative plant and worth testing for further pharmacological potential in the treatment of oxidative stress which may be related to neurodegenerative diseases.

Keywords: *Euphorbia hirta* L., antioxidant activity, MIN6

INTRODUCTION

Euphorbia hirta L., belonging to genus *Euphorbia*, family Euphorbiaceae, is frequently seen to occupy open waste spaces and grasslands, road side and pathways in many parts of the world. It has been widely used as a traditional medicinal herb in many tropical countries. The leaves of *E. hirta* L. are found to contain flavonoids, polyphenols, tannins, sterols, alkaloids, glycosides and triterpenoids [1, 2]. There were several researches on pharmaceutical application of *E. hirta* L. in the world. The whole plant is commonly applied to cure various diseases, especially gastrointestinal disorders, affections of the skin and mucous membranes, and respiratory system [3, 4]. Recently, pharmacological investigations have shown that *E. hirta* L. and its active components possessed wide range of bioactivities such as anti-inflammatory, antifungal, antibacterial, antidiarrheal, antioxidant activities [5 -7]. This last activity is most often determined in solution but less on living cells. Furthermore, there are only a few reports on the chemical compositions and the antioxidant capacity of this species from Vietnam. Therefore, we analyzed in this paper the antioxidant activity against H_2O_2 -induced cytotoxicity of fractioned extracts and some isolated compounds from a sample of *E. hirta* L. from Vietnam.

EXPERIMENTAL

Chemicals and reagents

Solvents utilized including *n*-hexane, chloroform, ethyl acetate, *n*-butanol, methanol (purity $\geq$ 99.0%), and ethanol 96% were purchased from Chemsol company (Vietnam). Silica gel 60 (0.063–0.200mm, Merck) and Bondesil C-18 were used for column chromatograph. TLC F₂₅₄ plate (Merck) and TLC RP-18 F₂₅₄ plate (Merck) were used for thin layer chromatography.

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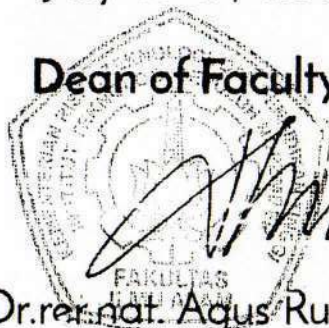
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