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HASIL PENILAIAN SEJAWAT SEBIDANG ATAU *PEER REVIEW*
KARYA ILMIAH : JURNAL ILMIAH

Judul Jurnal Ilmiah (Artikel)	:	Ab-Initio Computational Study : The Activation Energy Changes and Steric Effects In Peptide Synthesis Of Ac-AA-NH2 and Ac-AP-NH2		
Jumlah Penulis	:	3 orang (Indah Pratiwi, **Bambang Cahyono**, Parsaoran Siahaan)		
Status Pengusul	:	penulis ke-2		
Identitas Jurnal Ilmiah	:	a. Nama Jurnal	:	Molekul
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		c. Vol, No., Bln Thn	:	Vol. 16 No. 2 (2021)
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		f. Alamat web jurnal	:	https://ojs.jmolekul.com/ojs/index.php/jm/article/view/723
		Alamat Artikel	:	https://ojs.jmolekul.com/ojs/index.php/jm/article/view/723/370
		g. Terindex	:	Scopus, Q3 SJR: 0.26 (2021) https://www.scopus.com/sourceid/21100926576

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Semarang, Mei 2022

Reviewer 2

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2. Ruang lingkup dan kedalaman pembahasan: Artikel ini membahas tentang mekanisme reaksi terpadu dan membandingkan efek sterik terhadap reaksi yang diberikan oleh rantai samping yang berbeda dari alanin (A) dan prolin (P). penelitian dilakukan menggunakan Ab-Initio Computational Study (in silico). Data dan pembahasan cukup berkontribusi pada pengembangan keilmuan. Namun demikian temuan utama yang diperoleh belum tersampaikan dengan jelas. Judul yang diberikan belum secara explisit menggambarkan topik dan temuan yang dibahas.

3. Kecukupan dan kemutakhiran data/informasi dan metodologi: referensi sebanyak 34 dengan 26 referen yang disitasi baru (10 tahun terakhir). Beberapa referen bukan merupakan sumber primer. Nilai kebaruan artikel cukup baik. Metode dan analisis disajikan cukup jelas.

4. Kelengkapan unsur dan kualitas terbitan: Penerbit adalah Universitas Jenderal Soedirman. Jurnal Molekul merupakan jurnal internasional bereputasi (terindeks Scopus, SJR 2021: 0,26, Q3), ISSN 19079761, dengan cakupan bidang kimia. Masih ditemukan beberapa typo, misal pada acknowledgments. Nilai SI berdasarkan turnitin adalah 6% sehingga nilai orisinalitas baik.

Semarang, 31 Mei 2022
Reviewer 1

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2. **Ruang lingkup dan kedalaman pembahasan:**
   Lingkup artikel ini adalah tinjauan komputasi ikatan peptida antara asam amino sejenis (alanin) dan dua asam amino tak sejenis (alanin dan proline), terlihat dan bisa dibuktikan dalam artikel ini ikatan peptida lebih mungkin terjadi dari asam amino yang berbeda. Tinjauan diperoleh dari perhitungan energi, sudut ikatan, panjang ikatan, entropi dan sebagainya, energi aktifasi, HOMO LUMO. (11,5)
3. **Kecukupan dan kemutakhiran data/informasi dan metodologi:**
   Metode yang digunakan cukup memadai yaitu komputasi menggunakan software NWChem 6.8. Reference yang dirujuk cukup banyak 13 dari 35 references (kurang dari 50% merupakan reference yang terbit sebelum 5 tahun terbitnya artikel jurnal ini (Juli 2022). (11,5)
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Semarang, Mei 2022
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Ab-initio computational study: The activation energy and steric effects in peptide synthesis of ac-aa-nh$_2$ and ac-ap-nh$_2$

Pratiwi, Indah; Cahyono, Bambang; Siahaan, Parsaoran

Save all to author list

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Abstract

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Abstract

Ab-Initio computational method can be used for simulating reaction mechanisms, such as concerted reaction mechanism on peptide synthesis. The concerted reaction is one of many possible pathways on how peptide can be synthesized. The purpose of this study are probing the concerted reaction mechanism and comparing the steric effect to the reaction, given by different side-chain of alanine (A) and proline (P). Two dipeptides formed from alanine and proline were computed at HF-SCF/6-31G** theory level: Ac-AA-NH2 and Ac-AP-NH2. The res.lts show the activation energy of Ac-AA-NH2 and Ac-AP-NH2 forming via concerted pathway are 167.541 kJ/mol and 161.044 kJ/mol, respectively. The steric difference in side-chain affects the dihedral angle of the structure, and also gives difference to the entropy value of reaction.

Author keywords

Ab-initio; Activation energy; Peptides; Reaction mechanism

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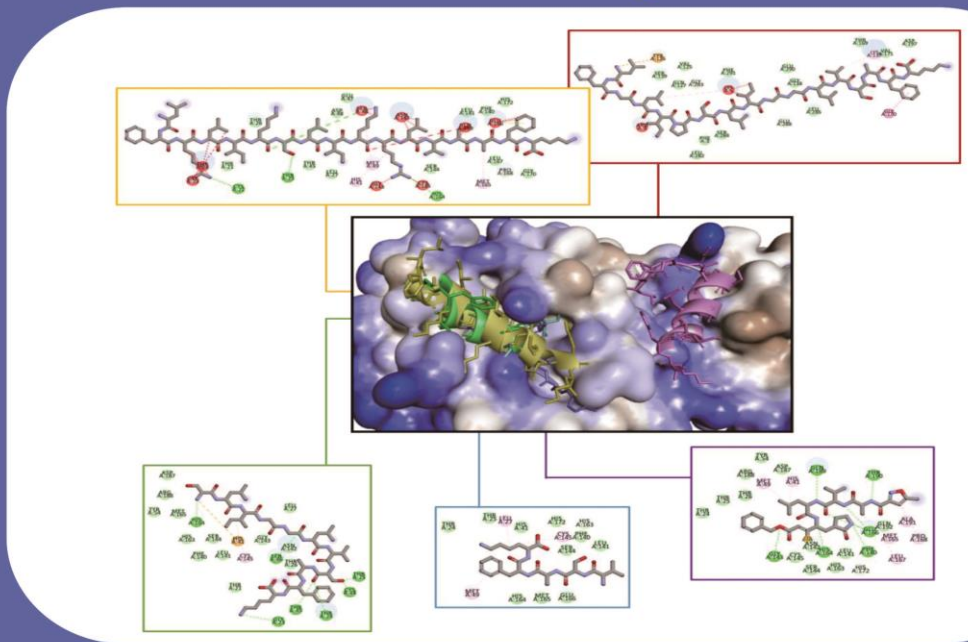

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Ab-Initio Computational Study : The Activation Energy and Steric Effects in Peptide Synthesis of Ac-AA-NH_2 and Ac-AP-NH_2

Indah Pratiwi[1], Bambang Cahyono[1], Parsaoran Siahaan[1]*

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Received November 05, 2020; **Accepted** April 21, 2021; **Available online** July 20, 2021

ABSTRACT. Ab-Initio computational method can be used for simulating reaction mechanisms, such as concerted reaction mechanism on peptide synthesis. The concerted reaction is one of many possible pathways on how peptide can be synthesized. The purpose of this study are probing the concerted reaction mechanism and comparing the steric effect to the reaction, given by different side-chain of alanine (A) and proline (P). Two dipeptides formed from alanine and proline were computed at HF-SCF/6-31G** theory level: Ac-AA-NH_2 and Ac-AP-NH_2. The res.lts show the activation energy of Ac-AA-NH_2 and Ac-AP-NH_2 forming via concerted pathway are 167.541 kJ/mol and 161.044 kJ/mol, respectively. The steric difference in side-chain affects the dihedral angle of the structure, and also gives difference to the entropy value of reaction.

Keywords: ab-initio; activation energy; peptides; reaction mechanism

INTRODUCTION

Condensation of amino acids is a crucial reaction in protein chemistry as it represents a key reaction for all life processes. An essential structural element of all proteins is a peptide bond (C–N), which is formed because of the conjugation between the α-amino group of one amino acid and the α-carboxylic group of another amino acid (Santos et al., 2014). The detailed knowledge of the peptide bond formation mechanism is vital for understanding of various biological processes, and it is a subject of intensive investigations as such.

Non-catalyzed reaction of peptide bond formation has been studied by Bhunia et al. (2016) and Monajemi et al. (2012). Concerted reaction mechanism is one of possible mechanism propose. It also has been studied using molecular dynamics approach by Trobro and Aqvist (2005) and further by Wallin and Aqvist (2010), as a process of peptides synthesis occurring at cell level. Ribosome transforms genetic information, expressing genes into proteins (Ramkumar & Ramakrishnan, 2010; Yonath, 2010). Briefly, a peptide formation reaction is a reaction between two active groups: the amine (-NH_2) group and the carboxylic group (-COOH) from two different amino acids. The reaction mechanism involves the nucleophilic attack of the nitrogen atom from amine group to the carbon of the carboxylic group. Furthermore, a hydrogen atom of the amine group will be attracted to the oxygen atom (hydroxyl group of carboxylic), out in the molecular form of H_2O and the dipeptide will be produced (Anslyn & Dougherty, 2006a; Konwar et al., 2016; Solomons et al., 2014). The peptide bond forming reaction according to concerted mechanism shown in **Figure 1**.

The kind of mechanism in term of the topology of the potential energy surface, the nature of the transition states, the presence or absence of intermediates. Reactants progress over transition states on to intermediates, perhaps through multiple intermediates and ending at products. This type of scenario analysis has a long successful story for studying organic reactions (Dai et al., 2018; Gale et al., 2020; Singh et al., 2020; Trinchillo et al., 2016).

Besides of only studying the pathway from thermodynamics and kinetics, the steric effect also studied as well in some previous studies. It can be seen from the bulky steric structure, bond torsions, or the size of atom attached to the particular chain of organic compound (Elias et al., 2020; Ghosh et al., 2007; Mukherjee et al., 2019). Steric effect relates on how electron are occupied in space and reaction mechanism itself tells how electron go through particular reaction pathway which we desired. However, steric can affect the electron, and finally, can affect on how reaction occurs.

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Articles

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Two Limonoids from The Seeds of *Chisocheton Macrophyllus* and Their Cytotoxic Activity Against Mcf-7 Breast Cancer Cells

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Received October 07, 2020; **Accepted** May 30, 2021; **Available online** July 20, 2021

ABSTRACT. Limonoids (tetranortriterpenoids) are triterpenoid compounds that lose four terminals in their structural framework. These compounds have a wide variety of structures and interesting activities including anti-inflammatory, anti-cancer, anti-tumor and anti-malarial properties. The purpose of this study was to find limonoid compounds from the Indonesian *Chisocheton* plant, and one of which is *Chisocheton macrophyllus*. The dried and powdered seeds of *C. macrophyllus* (4.5 kg) were extracted with methanol and partitioned successively with *n*-hexane, ethyl acetate and *n*-butanol. Evaporation of each extract resulted in the crude extracts of *n*-hexane (346.6 g), ethyl acetate (60.8 g) and *n*-butanol (14.6 g). The *n*-hexane fraction was subjected to a silica gel vacuum-liquid chromatography (VLC) column packed with silica gel 60 using gradient of *n*-hexane, ethyl acetate and methanol (10% stepwise) to afford thirteen fractions (A-M). Fraction F (4.4 g) was subjected to silica gel column chromatography using gradient of *n*-hexane and ethyl acetate (5% stepwise). Subfraction F5 (1.2 g) was chromatographed on a column of silica gel eluted with *n*-hexane: CH_2Cl_2: EtOAc (2:7.5:0.5) to give compound **1** (19.7 mg) and fraction H (1.8 g) was subjected to silica gel column chromatography using gradient of *n*-hexane and ethyl acetate (5% stepwise) as eluting solvent to give **2** (12.0 mg). Chemical structures of **1** and **2** were elucidated by spectroscopic methods and determined as 6α-acetoxyepoxyazadiradione (**1**) and Dysobinin(**2**). Dysobinin (**2**) showed weak cytotoxic activity against MCF-7 breast cancer cells with an IC_{50} value of 228.15 µM

Keywords: 6α-acetoxyepoxyazadiradione, *C. macrophyllus*, dysobinin, limonoid, MCF-7

INTRODUCTION

Limonoids are a class of tetranortriterpenoids that are formed through the loss of four terminal carbons of side chain of euphane (20-*S*) or tirucallane (20-*R*) skeleton that are followed by a cyclization to form a 17β-furan ring (Tan, & Luo, 2011; Shi et al., 2020). Limonoids are classified into ten classes based on the differences on A, B, C, D, and furan ring of the limonoid skeleton and can be identified by their biosynthetic relationships (Fang, Di, & Hao, 2011; Tan & Luo, 2011; Shi *et al*., 2020). Ten classes of limonoid include protolimonoids, apoeuphol skeleton, D-ring *seco*, B, D-ring *seco*, A-ring *seco*, A,B-ring *seco*, C-ring *seco*, A,D-ring *seco* and B-ring *seco* limonoids.

Limonoids occur mainly in the plant order of Rutales and most of them are found in Meliaceae and Rutaceae families (Li, Peng, & Zheng, 2016). Limonoids isolated from species of the family of Meliaceae have been of interest due to their diverse structures and their biological activities, including antifeedant, anticancer, antimicrobial, antimalarial, and antiviral properties (Tan, & Luo, 2011; Wong et al., 2011; Gualdani, Cavalluzzi, Lentini, & Habtemariam, 2016; Shilpi et al., 2016; Chong et al., 2019; Supratman et al., 2020). Nimbolide is a major limonoid isolated from the leaves of *Azadirachta indica* A. Juss or known as neem tree. Nimbolide as a neem limonoid is widely used for anti-malaria, antibacterial activity against *S. aureus* and *S. coagulase*, anti-feedant and insecticidal activity (Kumar & Navaratnam, 2013; Bodduluru, Kasala, Thota, Barua & Sistla, 2014; Wang et al., 2016; Sophia et al., 2018). Nimbolide was presumed to be a more potent anticancer. Nimbolide shows anticancer activity throughout selective modulation of signaling pathways linked to inflammation, survival, growth, invasion, angiogenesis and metastasis. Nimbolide was reported to induce apoptosis by disruption of Mitochondrial Outer Membrane Potential (MOMP) and inhibits tumor cell proliferation through alterations of cyclins, cdks, PCNA and p53 levels. In addition, nimbolide also reducing the nuclear