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## The Study of Stability and Structure of the Interaction Between $\beta$ -Carotene Compounds with Methanol, Ethanol, Acetone, Chloroform, Carbon Tetrachloride, Cyclohexane, and N-Hexane using the Hartree-Fock and the Density Functional Theory Method

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**Abstract.** The purpose of this study was to determine the stability and structure on the interaction between  $\beta$ -carotene compounds with methanol, ethanol, acetone, chloroform, carbon tetrachloride, cyclohexane, and n-hexane compounds. This research is a molecular modeling using computational chemistry calculations with the function/ basis set RHF/3-21G and B3LYP/3-21G. The computational chemistry calculations used Gaussian 09 Revision D 01 and visualization used the Jmol and Avogadro software. The data obtained from computational chemistry calculations with the function/ basis set RHF/3-21G on the interaction between  $\beta$ -carotene -methanol compounds are  $\Delta E = -11.899$  kJ / mol,  $\beta$ -carotene -ethanol  $\Delta E = -12.256$  kJ/mol,  $\beta$ -carotene -acetone  $\Delta E = -9.276$  kJ/mol,  $\beta$ -carotene -chloroform  $\Delta E = 5.262$  kJ/mol,  $\beta$ -carotene -carbon tetrachloride  $\Delta E = 3.747$  kJ/mol,  $\beta$ -carotene-cyclohexane  $\Delta E = 2.691$  kJ/mol,  $\beta$ -carotene-n-hexane  $\Delta E = 6.453$  kJ/mol. The data obtained with the function/basis set B3LYP/3-21G on the interaction between  $\beta$ -carotene-methanol compounds are  $\Delta E = -24.588$  kJ/mol,  $\beta$ -carotene -ethanol  $\Delta E = -25.123$  kJ/mol,  $\beta$ -carotene -acetone  $\Delta E = -18.140$  kJ/mol,  $\beta$ -carotene -chloroform  $\Delta E = 2.255$  kJ/mol,  $\beta$ -carotene -carbon tetrachloride  $\Delta E = -1.187$  kJ/mol,  $\beta$ -carotene-cyclohexane  $\Delta E = -0.801$  kJ/mol,  $\beta$ -carotene -hexane  $\Delta E = -0.412$  kJ/mol. Based on the analysis of thermodynamic data from computational chemistry calculations with the function / basis set UHF/3-21G and B3LYP/3-21G, it was found that  $\beta$ -carotene-ethanol and  $\beta$ -carotene-methanol mixtures had very stable mixtures.

**Key words:**  $\beta$ -carotene, solvent, interactions, and computational chemistry.

### 4 Introduction

Palm oil is the largest source of vegetable oil needed by many industries in the world. In addition, the world demand for palm oil continues to grow by 5 percent per year. The fulfillment of world palm oil



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demand is dominated by Indonesian production. Indonesia produces about 43 percent of the total production of crude palm oil (CPO) in the world. The growth of palm oil production in Indonesia, which is 7.8 percent per year, is also better than Malaysia's which is 4.2 percent per year. Sumatra makes a very large contribution as a producer of palm oil, where 70% of palm oil production is produced on the island of Sumatra, followed by Kalimantan at 26% and the remaining 4% is produced from Sulawesi, Papua and Java. Seeing the mapping of oil palm producers, it is still possible to increase the amount of production, in addition to increasing the added value from the sale of palm oil products. So far, the products exported by Indonesia are still in the form of CPO, where the CPO can still be processed into semi-finished or finished materials [1].

Oil palm has a variety of uses to meet various human needs. One of the benefits of palm oil is palm oil, which is one of the most needed foodstuffs by humans. Palm oil has several advantages, including beta carotene as pro-vitamin A and vitamin E [2, 3]. Quantitatively palm oil contains 96.2% neutral lipids; 2.4% phospholipids; 1.4% glycolipid and also contains unsophisticated fraction which is rich in carotenoids and tocopherols. Carotenoids can function as provitamin A and antioxidants, while tocopherol has activity as vitamin E and is an antioxidant substance [4]. Carotenoid compounds are very useful in human life [5].

In an effort to optimize the use of CPO,  $\beta$ -carotene and  $\alpha$ -tocopherol were separated by extraction method. An important step in the extraction of  $\beta$ -carotene and  $\alpha$ -tocopherol is the determination of the suitable solvent for these compounds. Several solvent extraction methods on the partition coefficient of carotenoids and tocopherols [6]. Prá [7] extracted bioactive compounds from palm oil press fibers using different compressed fluids. Supercritical fluid extraction of tocopherol compounds from crude palm oil using CO<sub>2</sub> solvents [8,9]. Extraction methods of carotene ( $\alpha$ - and  $\beta$ -carotene) and tocopherols ( $\alpha$ -tocopherol,  $\alpha$ -,  $\gamma$ -, and  $\delta$ -tocotrienol) from crude palm oil olein using ethyl lactate (EL) and ethanol (EtOL) in a temperature controlled mixer system -settler [10,11]. Pressurized liquid extraction (PLE) together with normal phase liquid chromatography (NPLC) was evaluated as a new approach for the determination of carotene and vitamin E isomers in residual oil obtained from palm compressed fiber (PPF) [12]. One method that can be done is using computational chemical methods through molecular modeling. The results obtained from this computational chemistry method are interaction data between molecules in the form of thermodynamic data. In this research, computational chemical calculations will be carried out on the interaction of several solvents with  $\beta$ -carotene and  $\alpha$ -tocopherol compounds. The solvents that will be used are ethanol, methanol, acetone, chloroform, n-hexane, cyclohexane, and carbon tetrachloride.

Simulations of calculating the amount of molecular energy using a computer program are usually done by calculating the energy of the molecules regardless of their environment. In reality, there is never a single molecule in a single state but the number is very large and surrounded by other molecules as a solvent. In order to get closer to the real conditions, various efforts were made, including by considering the influence of the solvent. Several computer simulation studies to date have taken into account the presence of solvents in calculating molecular energies.

Yin [13] has determined the amount of energy involving the solvent as the environment of the reaction using a hybrid approach between Quantum Mechanics (QM) and Molecular Mechanics (MM). In the calculation, the Potential Energy Surface (PES) method using Quasi Trajectory (QCT) and Time-Dependent Wave Packet (TDWP) was used by Jorfi [14]. Theoretical studies of the energy in the molecules that form clusters have been carried out based on the *ab initio* molecular orbital theory using the Hartree-Fock theory (HF) and Møller-Plesset perturbation theory [15].

Based on research conducted by Tewari[16], the effect of solvation and solvent polarization was calculated using the Polarizable Continuum Model (PCM) and the Self-Consistent Isodensity Polarizable Continuum Model (SCI-PCM). To describe the interaction between anions and water molecules using the Crooks fluctuation relationship to determine the effect of quantum on the free energy of dissociation in  $I-(H_2O)$  ions and the average force of  $Na^+(H_2O)_{12}$  evaluated using the Jurzinsky theorem [17].

## 2. Method

This research is a theoretical study using quantum mechanical theory on the interactions between molecules through molecular modeling. Computational chemistry calculations using Gaussian 09 Revision D 01[18]. Computational chemistry calculations are used to determine the amount of molecular energy and energy in the interactions between molecules. The results of computational chemistry calculations were visualized using Jmol [19] software. The method used in computational chemistry calculations is the HF (UHF) and DFT (B3LYP) method with the basis set 3-21G. The association models observed were: ethanol -  $\beta$ -carotene; methanol -  $\beta$ -carotene; acetone -  $\beta$ -carotene; chloroform -  $\beta$ -carotene; n-hexane -  $\beta$ -carotene; cyclohexane -  $\beta$ -carotene; carbon tetrachloride -  $\beta$ -carotene.

## 3. Result and Discussion

### 3.1. Determination of the interaction between $\beta$ -carotene compounds and solvents.

Based on the results of computational chemistry calculations using the RHF / 3-21G function / basis set, energy data is obtained, so that energy changes can be calculated in the interaction process between the two molecules. The smallest energy change of -12.256 kJ / mol is the interaction between  $\beta$ -carotene and ethanol, while the largest energy change is 6,453 kJ / mol is the interaction between  $\beta$ -carotene and n-hexane. This fact shows that the most stable pair is  $\beta$ -carotene and ethanol. The amount of total energy (E) calculated by computational chemistry with the function/basis set UHF/3-21G is shown in Table 1.

**Table 1.** The total energy (E) calculated by computational chemistry using UHF / 3-21G

No	Solvent Type	Energy (Ht)				Energy Difference ( $\Delta E$ ) kJ/ mol
		Solvent	$\beta$ -carotene	Solvent - $\beta$ -carotene	Energy Difference ( $\Delta E$ )	
1	Methanol	-114.340	-1537.663	-1652.008	-0.005	-11.899
2	Ethanol	-153.133	-1537.663	-1690.801	-0.005	-12.256
3	Acetone	-190.792	-1537.663	-1728.459	-0.004	-9.276
4	Chloroform	-1410.059	-1537.663	-2947.720	0.002	5.262
5	Carbon tetrachloride	-1866.757	-1537.663	-3404.418	0.001	3.747
6	Cyclohexane	-232.729	-1537.663	-1770.391	0.001	2.691
7	n-hexane	-233.860	-1537.663	-1771.521	0.002	6.453

Based on the results of computational chemistry calculations using the function/basis set B3LYP/3-21G, energy data is obtained, so that energy changes can be calculated in the interaction process between the two molecules. The smallest energy change of -24,588 kJ/mol is the interaction between  $\beta$ -carotene and ethanol, while the largest energy change is 2.255 kJ/mol, which is the interaction between  $\beta$ -carotene and chloroform. This fact shows that the most stable pair is  $\beta$ -carotene and ethanol. The amount of total energy (E) calculated by computational chemistry with the function/basis set B3LYP/3-21G is shown in Table 2.

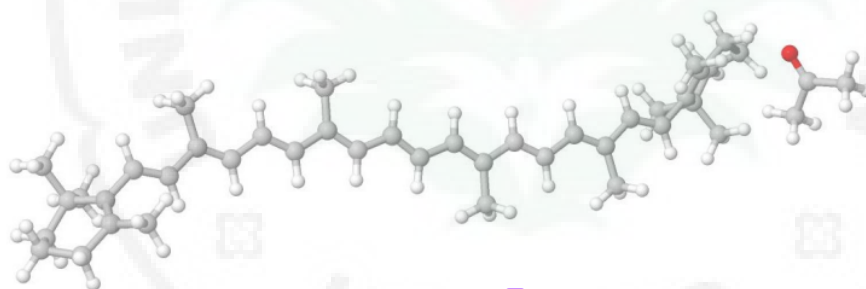


**Table 2.** The total energy (E) calculated by computational chemistry using B3LYP/ 3-21G

No	Solvent Type	Energy (Ht)				Energy Difference ( $\Delta E$ ) kJ/ mol
		Solvent	$\beta$ -carotene	Solvent - $\beta$ -carotene	Energy Difference ( $\Delta E$ )	
1	Methanol	-115.020	-1548.505	-1663.534	-0.009	-24.588
2	Ethanol	-154.098	-1548.505	-1702.613	-0.010	-25.123
3	Acetone	-192.003	-1548.505	-1740.515	-0.007	-18.140
4	Chloroform	-1412.430	-1548.505	-2960.935	0.001	2.255
5	Carbon tetrakloride	-1869.814	-1548.505	-3418.320	0.000	-1.187
6	Cyclohexane	-234.430	-1548.505	-1782.935	0.000	-0.801
7	n-hexane	-235.606	-1548.505	-1784.112	0.000	-0.412

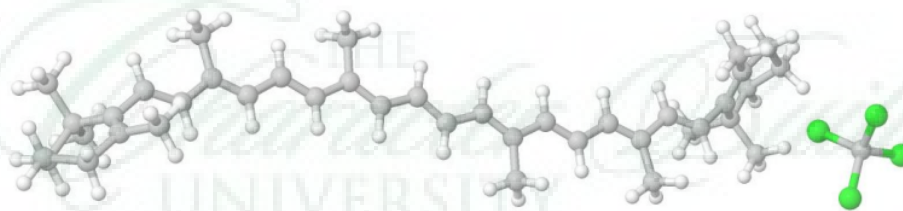
### 3.2. The structure of the interaction between $\beta$ -carotene compounds and solvents.

In addition to obtaining thermodynamic data, computational chemistry calculations obtain the structure of the visualization of computational chemistry calculations. This section describes the structure of the visualization results on the interaction between  $\beta$ -carotene compounds and solvents. The structure of the visualization results using Jmol software for interactions between  $\beta$ -carotene-acetone compounds is presented in Figure 1.



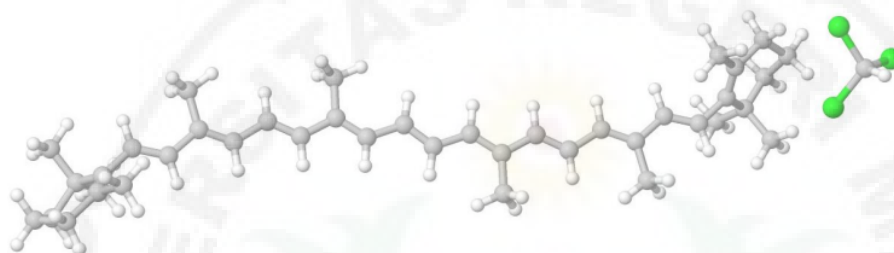
**Figure 1.** The structure of the visualization results on the interaction between  $\beta$ -carotene-acetone compounds

In the Figure, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and acetone. In the figure, it can be seen that the carbonyl group (C = O) approaches the H atom of the  $\beta$ -carotene compound. The structure of the visualization results using Jmol software for interactions between  $\beta$ -carotene-CCl<sub>4</sub> compounds is presented in Figure 2.



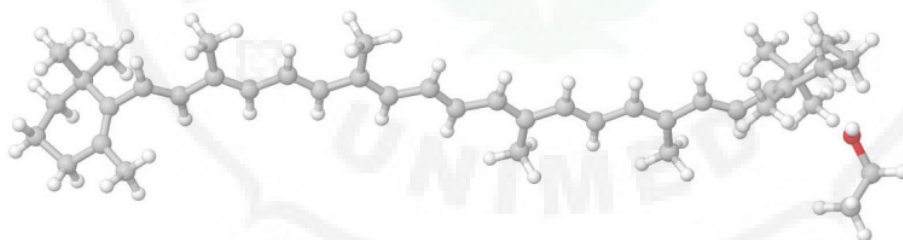
**Figure 2.** The structure of the visualization results on the interaction between  $\beta$ -carotene-CCl<sub>4</sub> compounds

In the Figure 2, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and carbontetrachloride. Although the carbon tetrachloride compound is non-polar, it can be seen in the figure that the Cl group of carbon tetra chloride approaches the H atom of the  $\beta$ -carotene compound. The structure of the visualization results using Jmol software for the interaction between  $\beta$ -carotene -CHCl<sub>3</sub> compounds is presented in Figure 3.



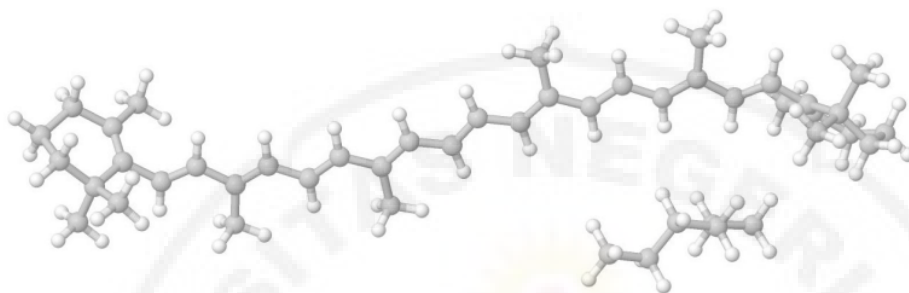
**Figure 3.** The structure of the visualization results on the interaction between  $\beta$ -carotene -CHCl<sub>3</sub> compounds

The Figure 3, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and chloroform compounds. In the figure, it can be seen that the Cl group of chloroform approaches the H atom of the  $\beta$ -carotene compound. The structure of the visualization results using Jmol software for the interaction between  $\beta$ -carotene-ethanol compounds is presented in Figure 4.



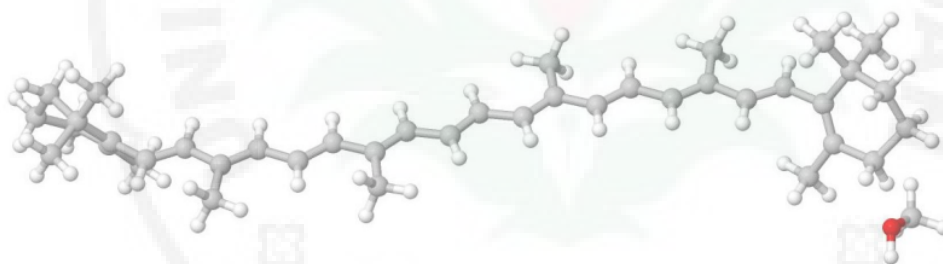
**Figure 4.** The structure of the visualization results on the interaction between  $\beta$ -carotene -ethanol compounds

The Figure 4, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and ethanol. In the figure, it can be seen that the O atom group of ethanol approaches the H atom of the  $\beta$ -carotene compound. The structure of the visualization results using Jmol software for interactions between  $\beta$ -carotene -hexane compounds is presented in Figure 5.



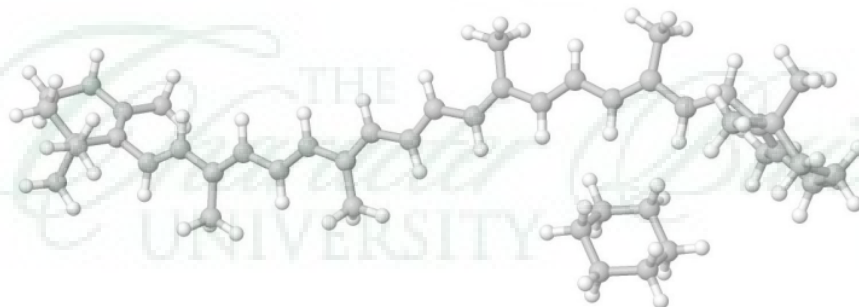
**Figure 5.** The structure of the visualization results on the interaction between  $\beta$ -carotene-n-hexane compounds

In the Figure, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and n-hexane. In the figure, it can be seen that the n-hexane compound is closer to the carbon chain of the  $\beta$ -carotene compound. This happens because n-hexane is non-polar and prefers to interact with non-polar carbon chains. The structure of the visualization results using Jmol software for the interaction between  $\beta$ -carotene -methanol compounds is presented in Figure 6.



**Figure 6.** The structure of the visualization results on the interaction between  $\beta$ -carotene-methanol compounds.

In the Figure, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and methanol. In the figure, it can be seen that the O atom group of methanol approaches the H atom of the  $\beta$ -carotene compound. The structure of the visualization results using Jmol software for interactions between  $\beta$ -carotene -cyclohexane compounds is presented in Figure 7.



**Figure 7.** The structure of the visualization results on the interaction between  $\beta$ -carotene-cyclohexane compounds



The Figure 7, a visualization of the results of computational chemistry calculations on the interaction between  $\beta$ -carotene and cyclohexane. In the figure, it can be seen that the cyclohexane compound is closer to the carbon chain of the  $\beta$ -carotene compound. This happens because cyclohexane is non-polar and prefers to interact with non-polar carbon chains.

#### 4. Conclusion

The data obtained from computational chemistry calculations with the function/basis set RHF/3-21G on the interaction between  $\beta$ -carotene -methanol compounds are  $\Delta E = -11.899$  kJ/mol;  $\beta$ -carotene -ethanol  $\Delta E = -12.256$  kJ/mol;  $\beta$ -carotene -acetone  $\Delta E = -9.276$  kJ/mol;  $\beta$ -carotene -chloroform  $\Delta E = 5.262$  kJ/mol;  $\beta$ -carotene -carbon tetrachloride  $\Delta E = 3.747$  kJ/mol;  $\beta$ -carotene-cyclohexane  $\Delta E = 2.691$  kJ/mol;  $\beta$ -carotene -hexane  $\Delta E = 6.453$  kJ/mol. The data obtained with the hybrid function/basis set B3LYP/3-21G on the interaction between  $\beta$ -carotene -methanol compounds are  $\Delta E = -24.588$  kJ/mol;  $\beta$ -carotene -ethanol  $\Delta E = -25.123$  kJ/mol;  $\beta$ -carotene -acetone  $\Delta E = -18.140$  kJ/mol;  $\beta$ -carotene -chloroform  $\Delta E = 2.255$  kJ/mol;  $\beta$ -carotene -carbon tetrachloride  $\Delta E = -1.187$  kJ/mol;  $\beta$ -carotene-cyclohexane  $\Delta E = -0.801$  kJ/mol;  $\beta$ -carotene n--hexane  $\Delta E = -0.412$  kJ/mol. Based on the analysis of thermodynamic data from computational chemistry calculations with the function/basis set UHF/3-21G and B3LYP/3-21G, it was found that  $\beta$ -carotene-ethanol and  $\beta$ -carotene-methanol mixtures had very stable mixtures.

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#### References

- [1] Kementerian Koordinator Bidang Perekonomian, 2011, Kementerian Perencanaan Pembangunan Nasional/ Badan Perencanaan Pembangunan Nasional, Masterplan Percepatan dan Perluasan Pembangunan Ekonomi Indonesia (MP3EI) 2011 – 2025, cet.1, Jakarta.
- [2] Choo, Yuen-May, Soon-Chee Yap, Cheng-Keat Ooi, Ah-Ngan Ma, Swee-Hock Goh, and Augustine Soon-Hock Ong, 1996, Recovered Oil from Palm-Pressed Fiber: A Good Source of Natural Carotenoids, Vitamin E, and Sterols, *JAOCS*, **73**,5, 599-602.
- [3] Chuang Meng-Han and Gerd Brunner, 2006, Concentration of minor components in crude palm oil, *J. of Supercritical Fluids*, **37**, 151–156.
- [4] Damanik, M and M. Murkovic, 2018, The stability of palm oils during heating in a rancimat European Food Research and Technology, <https://doi.org/10.1007/s00217-018-3044-1>
- [5] Amorim-Carrilho, K.T., A. Cepeda, C. Fente, P. Regal, 2014, Review of methods for analysis of carotenoids, *Trends in Analytical Chemistry*, **56**, 49–73
- [6] Goncalves, Cintia B., Pedro A. Pessoa Filho, Antonio J.A. Meirelles, 2007, Partition of nutraceutical compounds in deacidification of palm oil by solvent extraction, *Journal of Food Engineering*, **81**, 21–26
- [7] Prá, Valéria Dal, Juliana Ferreira Soares, Debora Luana Monego, Raquel Guidetti Vendruscolo, Denise M. Guimarães Freire, Maria Alexandri, Apostolis Koutinas, Roger Wagner, Marcio A. Mazutti, Marcelo Barcellos da Rosa, 2016, Extraction of bioactive compounds from palm (*Elaeis guineensis*) pressed fiber using different compressed fluids, *The Journal of Supercritical Fluids*, <http://dx.doi.org/10.1016/j.supflu.2016.02.011>
- [8] Davarnejad, Reza, Zainal Ahmad, Suhairi A. Sata, Mostafa Keshavarz Moraveji, and Farzaneh Ahmadloo, 2010, Mutual Solubility Study in Supercritical Fluid Extraction of Tocopherols from Crude Palm Oil Using CO<sub>2</sub> Solvent, *Int. J. Mol. Sci.*, **11**, 3649-3659.
- [9] Lau, Harrison Lik Nang, Yuen May Choo, Ah Ngan Ma, and Cheng Hock Chuah, 2008, Selective extraction of palm carotene and vitamin E from fresh palm-pressed mesocarp fiber (*Elaeis guineensis*) using supercritical CO<sub>2</sub>, *Journal of Food Engineering*, **84**, 289–296
- [10] Kua, Yin Leng, Suyin Gan, Andrew Morris, and Hoon Kiat Ng, 2018, Optimization of

- simultaneous carotenes and vitamin E (tocols) extraction from crude palm olein using response surface methodology, *Chemical Engineering Communications*, **205**, 5, 596–609
- [11] Setapar, Siti Hamidah Mohd, Asma Khatoun, Akil Ahmad, Mohd-Azizi Che Yunus And Muhammad Abbas Ahmad Zaini, 2014, Use of Supercritical CO<sub>2</sub> and R134a as Solvent for Extraction of b-Carotene and a-Tocopherols from Crude Palm Oil, *Asian Journal of Chemistry*; **26**, 18, 5911-5916
- [12] Sanagi, M. Marsin, H.H. See, Wan Aini Wan Ibrahim, and Ahmedy Abu Naim, 2005, Determination of carotene, tocopherols and tocotrienols in residue oil from palm pressed fiber using pressurized liquid extraction-normal phase liquid chromatography, *Analytica Chimica Acta*, **538**, 71–76
- [13] Yin Hongyun, Donyou Wang, and Marat Valiev, 2011, Hybrid Quantum Mechanical/Molecular Mechanics Study of the SN<sub>2</sub> Reaction of CH<sub>3</sub>Cl+OH<sup>-</sup> in Water, *The Journal of Physical Chemistry A*, **115**, 12047 – 12052
- [14] Jorfi, M., 2011, State-to-State Quantum Dynamics Calculations of the C+OH Reaction on the Second Excited Potential Energy Surface, *The Journal of Physical Chemistry A*, **115**, 8791-8796
- [15] Zygmunt, SA, L A Curtiss, L E Iton, and M K Erhardt, 1996, Computational Studies of Water Adsorption in the Zeolite H-ZSM-5, *J. Phys. Chem.*, **100**, 16, 6663-6671
- [16] Tewari B. Yadu, Jiangang Chen, Marcia J Holden, Kendall N Houk, and Robert N Goldberg, 1998, Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyrupate + 4-Hydroxybenzoate), *J Phys Chem. B*, **102**, 43, 8634 – 8639.
- [17] de la Pena, Lisandro Hernandez and Gilles H. Peslherbe, 2010, Quantum Effect on the Free Energy of Ionic Aqueous Clusters Evaluated by Nonequilibrium Computational Methods, *J Phys Chem. B*, **114**, 16, 5404 – 5411
- [18] Frisch M. J., G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013. Frisch M. J., G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
- [19] Jmol: an open-source Java viewer for chemical structures in 3D. <http://www.jmol.org/>

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