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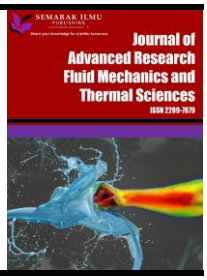

Steric Effect of Alcohol Solvent on Ternary Liquid-Liquid Equilibrium for β-Caryophyllene + Alcohol + Water Systems at 303.15 K and Atmospheric Pressure

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ABSTRACT

The objective of this study was to determine the steric effect of the alcohol solvent on the ternary liquid-liquid equilibrium for β-caryophyllene + alcohol (ethanol, tert-butanol, and 1-octanol) + water systems at 303.15 K and atmospheric pressure. Gas chromatography was used for the analysis. The experimental data obtained in this study correlated with the NRTL and UNIQUAC models. The steric effect of the solvent is an important factor in determining the suitable alcohol solvent for this ternary system. Based on the steric effect of the three alcohols used, it can be concluded that the solvent with the best correlation is ethanol.

1. Introduction

Plant essential oils are typically composed of volatile aromatic terpenes and phenylpropanoids. These lipophilic volatiles freely cross cellular membranes and play various ecological roles, such as plant-insect interactions [1,2]. The sesquiterpene β-caryophyllene is a major plant volatile found in large amounts in essential oils of many different species and food plants. β-caryophyllene is commercially used as a food additive and in cosmetics [3].

β-Caryophyllene is a pale-yellow oily liquid with an odor midway between that of cloves and turpentine [4]. β-caryophyllene in which the stereocenter adjacent to the exocyclic double bond has S configuration while the remaining stereocenter has R configuration. It is the most common form of β-caryophyllene and occurs in many essential oils, particularly cloves. It acts as a non-steroidal anti-inflammatory drug, fragrance, metabolite, and insect attractant. β-caryophyllene is an enantiomer of β-caryophyllene. β-caryophyllene insoluble on water but soluble in oils, ether, and ethanol.

In the extraction process, the thermodynamic properties of liquid-liquid phase equilibrium data systems are required to design the separation process equipment. Equilibrium is a static condition in which macroscopically, there is no change in the properties of the system over time. When the phases

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are not in equilibrium, there will be mass transfer between phases, where the transfer rate of each component depends on the driving force; in this case, the magnitude of the system deviates from equilibrium. Thus, knowledge of the liquid-liquid equilibrium for such systems is necessary for rational design and determining the optimum process conditions for the separation process.

The separation process of terpenes from oil is called deleptonization, which aims to improve flavor and aroma, increase solubility, and maintain stability during storage [2]. Deleptonization can be achieved by several methods, such as conventional methods (vacuum and steam distillation) and extraction with an organic solvent. However, in the distillation process, only a portion of the terpene component is selected, and this process occasionally causes oil degradation owing to heating [5]. Therefore, the extraction method is more widely used because it avoids degradation [4].

In the extraction process, solvent selection should consider its properties and characteristics, such as polarity, non-polarity, volatility, and toxicity. Future applications in the fields of food, cosmetics, and pharmaceuticals require the use of solvents such as alcohol and water [5]. The use of alcohol as a solvent for extraction has several advantages, including (1) high solubility in water; (2) non-toxicity; (3) increased scent of the mixture; (4) reduced oxidation reaction in the presence of alcohol; (5) selective solvent dilution of alcohol that can dissolve terpene, but slightly dissolved eugenol [6]. As a type of alcohol, methanol can be used as a solvent, but it turns out that methanol is corrosive because it can damage the extraction column. Some research has been conducted on ethanol as a solvent; however, it is not frequently used as a solvent in beverage production. This is because the selling price of ethanol as a beverage is higher than that of ethanol as a solvent. In addition to the type of solvent, another influential factor is time, where a short time during extraction will produce a small yield and a long time will consume a lot of energy, so the extraction will not be effective [7]. Therefore, research continues to identify other types of alcohols that have a lower risk of deviation. One of these was tert-butanol and 1-octanol. Tert-butanol and 1-octanol were dissolved in various concentrations of non-polar compounds. It also vaporizes rapidly and is relatively non-toxic; therefore, it is widely used as a solvent, especially for dissolving oil.

2. Methodology

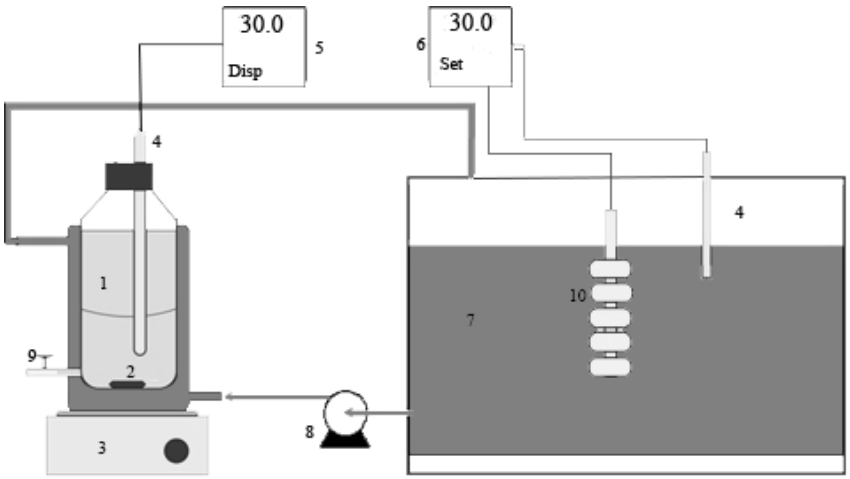
2.1 Material

β-carryophyllene with 99.9% purity was obtained from PT. Indesso Niagatama. Ethanol, 1-tert-Butanol and 1-Octanol with 99.8% purity were obtained from MERCK, and aquabidestilata was obtained from PT. Ikapharmindo Putramas. The purity of the materials was checked using Gas Chromatography. All materials used in this experiment are pure compounds.

2.2 Apparatus and Procedure

The equilibrium cell (Figure 1) is equipped with a magnetic stirrer and a jacket to maintain the temperature of equilibrium cell at desired temperature by circulating water from water bath as heating medium. The ternary mixture at certain composition was inserted to the equilibrium cell and stirred at a temperature of 303.15 K and atmospheric pressure for 4 hours, then the mixture was allowed to separate into organic and aqueous phase for about 20 hours.

The samples of each phase were collected and these compositions were analyzed using GC with TCD detector using RTX-5 column. Helium was used as carrier gas [8].



(1) Jacketed equilibrium cell
(2) Stir bar
(3) Dragon Lab MS-H280-Pro stirrer
(4) RTD Pt100
(5) Temperature display
(6) Temperature display
(7) PolyScience 9012 water bath
(8) Circulation pump
(9) Sampling port

Fig. 1. Schematic diagram of the equipment used for the experiment

2.3 Dipole Moment and Constant Dielectric

DMs (μ) were measured at 25˚C using the SH-2-11 apparatus, manufactured by the Experimental Design Office of Automation (Angarsk, Russia). The SH-2-11 apparatus allowed us to obtain the dielectric constant and density of the solutions with four-digit accuracy. The dielectric permittivity (ε) and density (ρ) were measured for dilute solutions of the tested compounds at concentrations of up to 10^{-3} mol/L. Values of molar polarization P21 of the dissolved substances were calculated using the Hedestrand method by extrapolation to infinite dilution [9].

2.4 Refractive Index

Using the DSR- refractometer which is an automatic microprocessor controlled critical angle refractometer been designed to measure the refractive index of liquid media independent of opacity, viscosity and color with high resolution 0.00001 RI/0.01 Brix [5,6]. The instrument consists of an electronic unit separated from the stainless-steel measuring unit. A sample volume of 0.3 ml is sufficient for measuring process [7,9]. The refractometer is equipped with a Peltier thermostat allowing measurement of refractive index at any selected temperature up to 80 °C.

3. Results

3.1 The Experimental Ternary LLE Data and Calculation of The Result

The experimental ternary LLE data for β-carryophyllene + alcohol + water systems at temperature of 303.15K under atmospheric pressure are presented in Table 1 and 2.

Both systems studied exhibit a ternary diagram of type-II behavior in which there are two partially miscible substances, as shown in Figure 3 and 4.

Figure 2 shows the solubility of the β-caryophyllene + tert-butanol + water system in accordance with the principle of polarity because β-caryophyllene has a non-polar tendency whereas tert-butanol has a non-polar tendency, thus β-caryophyllene is soluble with tert-butanol, while tert-butanol is not completely soluble with water and β-caryophyllene is insoluble (very little soluble) with water.

Table 1
Experimental LLE data for β-caryophyllene(1) + alcohols(2) + water(3) systems at 303.15K

System	Organic phase (I)			Aquous phase (II)		
	w_1	w_2	w_3	w_1	w_2	w_3
β-caryophyllene + tert-butanol + water	1.0000	0.0000	0.0000	0.0055	0.0000	0.9945
	0.9071	0.0881	0.0048	0.0050	0.0212	0.9737
	0.8235	0.1649	0.0116	0.0053	0.0220	0.9727
	0.7264	0.2535	0.0202	0.0055	0.0221	0.9725
	0.6097	0.3638	0.0265	0.0055	0.0239	0.9706
	0.6034	0.3660	0.0306	0.0054	0.0239	0.9707
	0.4366	0.5087	0.0548	0.0054	0.0389	0.9558
	0.0007	0.8776	0.1217	0.0051	0.0445	0.9503
β-caryophyllene + ethanol + water	1.000	0.0000	0.0000	0.0000	0.0000	1.0000
	0.9939	0.0061	0.0000	0.0000	0.0444	0.9556
	0.9856	0.0144	0.0000	0.0000	0.1343	0.8657
	0.9767	0.0233	0.0000	0.0000	0.2174	0.7188
	0.9702	0.0298	0.0000	0.0000	0.2812	0.6542
	0.9661	0.0339	0.0000	0.0014	0.3443	0.6542
	0.9576	0.0424	0.0000	0.0008	0.4272	0.5720
	0.9492	0.0508	0.0000	0.0018	0.5037	0.4945
	0.9055	0.0574	0.0000	0.0009	0.5694	0.3133
β-caryophyllene + 1-octanol + water	0.0171	0.9267	0.0563	0.0001	0.0001	0.9998
	0.2085	0.7598	0.0316	0.0001	0.0001	0.9998
	0.3759	0.6036	0.0205	0.0001	0.0001	0.9998
	0.5233	0.4666	0.0101	0.0001	0.0001	0.9998
	0.6526	0.3411	0.0064	0.0001	0.0001	0.9998
	0.7588	0.2378	0.0034	0.0001	0.0001	0.9998
	0.8523	0.1444	0.0032	0.0001	0.0001	0.9998
	0.9303	0.0656	0.0042	0.0001	0.0001	0.9998
	0.9946	0.0000	0.0054	0.0001	0.0001	0.9998

Table 2
The NRTL and UNIQUAC model parameters for β-caryophyllene(1) + alcohols(2) + water(3) systems at 303.15K

System	NRTL parameters (K)			α_{ij}	RMSD (%)
	i-j	$(g_{ij} - g_{ii})/R$	$(g_{ji} - g_{jj})/R$		
β-caryophyllene +tert-butanol + water	1-2	7723	5983	0.2	1.2
	2-3	4039	6123		
	1-3	-232	1691		
β-carryophyllene + ethanol + water	1-2	1326.90	-2165.27	0.47	1.1
	2-3	-205.01	3433.66		
	1-3	670.62	1134.83		
β-caryophyllene + 1-octanol + water	1-2	1528	1259	0.47	1.1
	2-3	15200	3680		
	1-3	56.14	82.85		
System	UNIQUAC parameters (K)				RMSD (%)
	i-j	$(u_{ij} - u_{ii})/R$	$(u_{ji} - u_{jj})/R$		
β-caryophyllene + tert-butanol + water	1-2	-215.01	6152		3.1
	2-3	121.31	1521		
	1-3	-57.63	421.4		
β-carryophyllene + ethanol + water	1-2	-17.91	-31.29		2.03
	2-3	207.66	1166.04		
	1-3	110.49	168.54		
β-caryophylenne + 1-octanol + water	1-2	-126.74	825.4		4.3
	2-3	6070.8	2908		
	1-3	299.8	1487		

Figure 3 shows the solubility of the β-caryophyllene +1- octanol + water system in accordance with the principle of polarity because β-caryophyllene has a non-polar tendency while octanol has non polar properties, so β-caryophyllene is soluble in 1-octanol, whereas Octanol tends to dissolve with water (polar) and β-caryophyllene is slightly soluble in water.

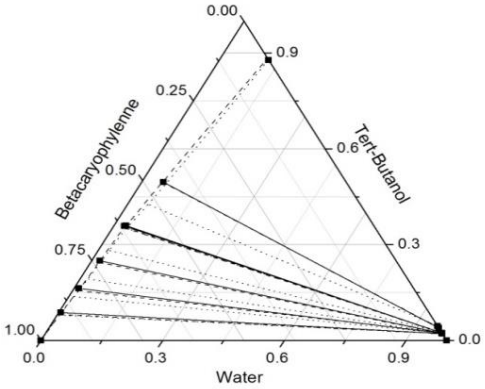


Fig. 2. Ternary liquid-liquid equilibrium for β-caryophyllene + tert-butanol + water system at 303.15K compared with (- - -) NRTL and (···) UNIQUAC equations

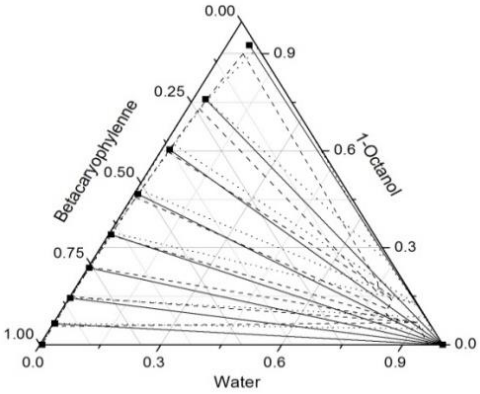


Fig. 3. Ternary liquid-liquid equilibrium for β-caryophylenne + 1-octanol + water System at 303.15K compared with (- - -) NRTL and (···) UNIQUAC equations

Figure 4 and 5 are also type-II ternary diagrams that show the solubility system of β-caryophyllene + ethanol + water, according to the principle of polarity, because β-caryophyllene has a non-polar tendency, whereas ethanol has a polar tendency (semipolar), but β-caryophyllene is soluble in ethanol with a certain composition. Ethanol can be dissolved in air.

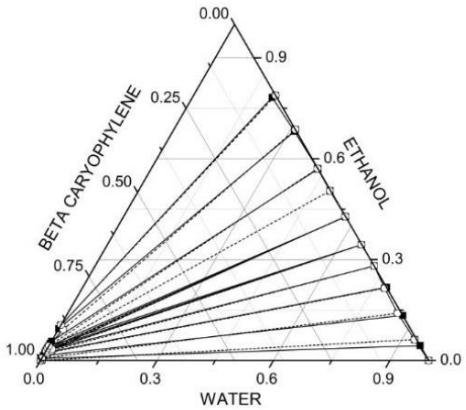


Fig. 4. Ternary liquid-liquid equilibrium for β-caryophyllene + tert-butanol + water system at 303.15K compared with experimental data (–) and (- - -) data NRTL equations.

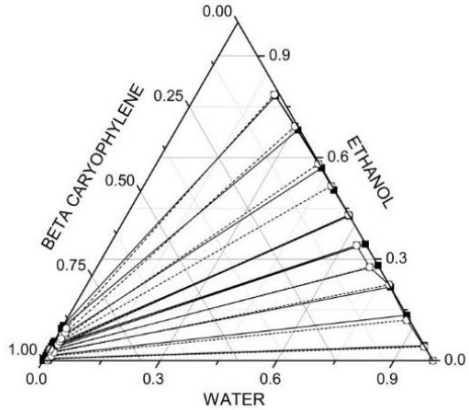


Fig. 5. Ternary liquid-liquid equilibrium for β-caryophylenne + 1-octanol + water System at 303.15K compared with experimental data (–) and (- - -) data UNIQUAC equations

3.2 Properties of β-Caryophyllene

β-Caryophyllene has physical properties, namely a high boiling point of 528.78 K, a critical temperature of 802.06 K, a density of 0.9 g/cm^3 and an index of refraction of 1.495. In terms of chemical properties, the compound is nonpolar and includes weakly basic compounds. β-

Caryophyllene is insoluble in water but will be soluble in oil and ether, can also be soluble in alcohol [10]. The β-caryophyllene molecule has a cyclic structure with the molecular formula $C_{15}H_{24}$, where there is a double bond in the molecule, owing to the shape of the structure, which causes β-caryophyllene to have non-polar properties [8]. In addition, there are several substituents, namely methyl, which have a steric effect that affects the solubility of β-caryophyllene in the solvent or affects the interaction between molecules and other compounds (refer to Table 3)**.**

Table 3
Properties of some compounds

Compound	Relative molecular mass	Dipole moment (Dbye)	Dielectric constant	Refractive index
β-caryophyllene	204	0	2.2	1.4981
Water	18	1.85	80.4	1.3333
Ethanol	46	1.69	25.7	1.3617
Tert-butanol	74	1.31	17.8	1.3954
Octanol	162	0	3.4	1.4205

3.3 Alcohol as Solvent

Chemical reactions are inseparable from the use of solutions. A solution consists of a solvent (solvent) and a solute (solute). The solvent (solvent) is generally a substance that is in solution in large quantities, whereas other substances are considered solutes. A solvent is a medium for the ionization process, which has properties and is the basic property of every type of solvent. Solvents based on this type are divided into three types: water, organic, and inorganic solvents [11].

The solvent dissolves the reactants and reagents so that they are mixed, which facilitates the combination of reactants and reagents that should occur to convert reactants into products. The concentration of a solution quantitatively expresses the composition of the solute and solvent in the solution. Concentration is generally expressed in terms of the ratio of the amount of solute to the total amount of solute in the solution, or in the ratio of the amount of solute to the amount of solvent. The solvent also acts as a temperature control, either to increase the energy of the particle collisions so that the particles can react more quickly or to absorb the heat generated during an exothermic reaction. The solvent that is widely used today is alcohol, this is because alcohol has a low price, is easy to obtain and has a low level of toxicity. The solvent was adjusted to dissolve the substance. There are several criteria for a good solvent including: The solvent must be inert to the reaction conditions, the solvent must be able to dissolve the reactants and reagents, the solvent must have the right boiling point, and be easily removed at the end of the reaction [12]. In addition, the choice of solvent can be seen from its polarity by using principles such as dissolution, where nonpolar reactants dissolve in nonpolar solvents, while polar reactants dissolve in polar solvents. Several factors determine solubility.

3.4 Relative Molecular Mass

The molecular mass of a compound affects its polarity. The greater the value of the relative molecular mass, the more non-polar the compound. In particular, for hydrocarbon compounds, the longer the carbon chain, the lower is the polarity of the molecule. This is in accordance with the β-caryophyllene compound, which has a relatively large molecular mass, so that it is non-polar, and water, which has a relatively small molecular mass, so that it is polar.

3.5 Dipole Moment

The dipole moment is a vector quantity described using the bonding moments. If the vector sum of the bond moments (dipole moment) > 0, the molecule is polar; otherwise, if the bond moment vector (dipole moment) = 0, the molecule is nonpolar [13]. Quantitatively, the dipole moment (μ) is the product of charge Q and the distance between charges r

$$\mu = Q \times r \tag{1}$$

where is the dipole moment (D, Debye), Q is the charge difference (C), and r is the distance between positive and negative charges (m).

From the available dipole moment data, β-caryophyllene has a dipole moment of 0, similar to octanol; therefore, it can be said that the two compounds are non-polar and will completely dissolve each other. Because water has a dipole moment of 1.85, which is above 0, it can be said that water has a polar nature, similar to ethanol and tert-butanol, which have a dipole moment above 0; it will be polar, the higher the value of the dipole moment, the polarity of a compound will be. more increasing. If seen from the table, the value of the dipole moment of ethanol is closer to the value of the dipole moment of water compared to the value of the dipole moment of tert-butanol, this means that the solubility of ethanol in water is higher than the solubility of tert-butanol in water. However, because there is a difference in value between the dipole moments of water and water, it can be said that the solubility of ethanol in water is limited or will dissolve at a certain composition, so ethanol is not completely soluble in water. This was similar to the solubility of tert-butanol in water.

3.6 Dielectric Constant

The dielectric constant is also a factor that determines the polarity of a compound. The lower the value of the dielectric constant, the lower the polarity; conversely, the higher the value of the dielectric constant, the more the polarity increases [14].

3.7 Refractive Index

The refractive index (RI) of a medium is dependent on its chemical composition because its composition dictates its electrical and magnetic properties under controlled conditions. The RI of a sample is defined as the ratio of the speed of light in vacuum to its speed in the sample medium. Consequently, the RI values were always greater than one. Usually, the refractive index is 1.3 and 1.7 [15]. The higher the value of the refractive index, the more nonpolar the compound. The water molecule has a refractive index of 1.3333 and the alcohol solvent, ethanol, has a refractive index whose value is close to that of water; therefore, it can be said that water and ethanol have the same polarity, and the two compounds, namely water and ethanol, dissolve each other. As for β-caryophyllene, it has a refractive index of 1.4981 which shows that β-caryophyllene has non-polar properties, from the alcohol solvent used, octanol has a refractive index value that is not much different from β-caryophyllene. Thus, it can be said that the two compounds, namely β-caryophyllene and octanol, have the same properties, namely non-polarity, and will dissolve each other.

3.8 Steric Effect

When viewed from the structure of β-caryophyllene, which is cyclic and has an alkene group, it is certain that the compound is nonpolar. Water is polar in nature because it has a hydroxyl group. Thus, alcohol solvents have the same properties as water because they have the same hydroxyl group. The hydroxyl groups possessed by the two compounds, namely alcohol and water, cause hydrogen interactions between molecules so that alcohol is more soluble or solvated by water. Figure 6-9 shows the structure of β-caryophyllene, ethanol, tert-butanol and octanol.

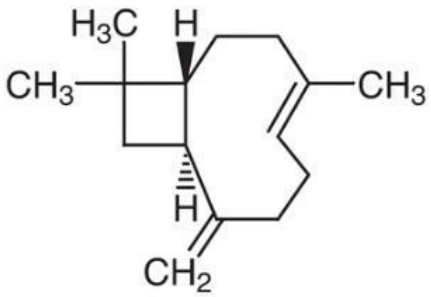


Fig. 6. β-caryophyllene structure

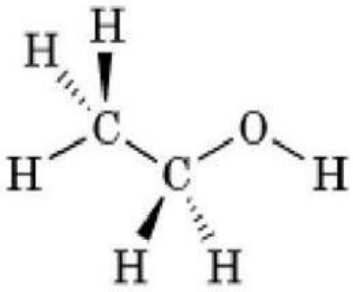


Fig. 7. Ethanol structure

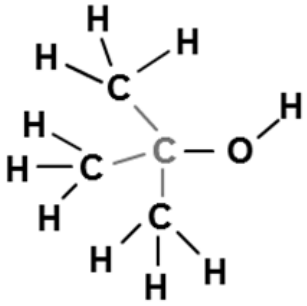


Fig. 8. Tert-butanol structure

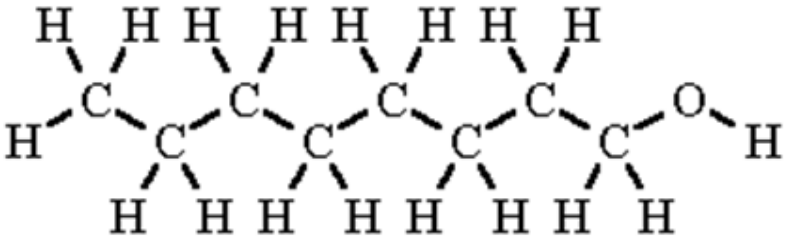


Fig. 9. Octanol structure

4. Conclusions

It can be concluded that of the three alcohol solvents used in the liquid-liquid equilibrium ternary β-caryophyllene + alcohol + water system, the best data and correlation with the NRTL and UNIQUAC models in the previous experiment was ethanol. This is because ethanol has a dual nature, namely polar, which can cause ethanol to dissolve in water, and non-polar nature, which causes ethanol to dissolve β-caryophyllene. In liquid-liquid equilibrium, the basic principle of extraction is adopted, in which there are two phases: the aqueous phase and the organic phase. Ethanol binds β-caryophyllene and brings it to the aqueous phase, and ethanol binds water and brings it to the organic phase. Thus, in both phases, there are three components: β-caryophyllene, water, and ethanol. From this, it can be determined at which composition ethanol can extract β-caryophyllene well, and will be the basis for the β-caryophyllene extraction process.

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References

[1] Russo, Antonio, Mariarita Perri, Erika Cione, Maria Luisa Di Gioia, Monica Nardi, and Maria Cristina Caroleo. "Biochemical and chemical characterization of Cynara cardunculus L. extract and its potential use as co-adjuvant therapy of chronic myeloid leukemia." *Journal of ethnopharmacology* 202 (2017): 184-191. https://doi.org/10.1016/j.jep.2017.03.026

[2] Cappello, A. R., V. Dolce, D. Iacopetta, M. Martello, M. Fiorillo, R. Curcio, L. Muto, and Dhanya Dhanyalayam. "Bergamot (Citrus bergamia Risso) flavonoids and their potential benefits in human hyperlipidemia and atherosclerosis: an overview." *Mini reviews in medicinal chemistry* 16, no. 8 (2016): 619-629. https://doi.org/10.2174/1389557515666150709110222

[3] Lawless, Julia. *The Encyclopedia of essential oils: the complete guide to the use of aromatic oils in aromatherapy, herbalism, health, and well being*. Conari Press, 2013.

[4] PS, Tagora Bangkit, and Rinaldry Sirait. "Penentuan kondisi keseimbangan unit leaching pada produksi eugenol dari daun cengkeh." *Jurnal Teknik Kimia USU* 1, no. 1 (2012): 10-14. https://doi.org/10.32734/jtk.v1i1.1399

[5] Ketaren, S. "Pengantar Teknologi Minyak dan Lemak Pangan (Indonesia." (1985).

[6] Cháfer, A., J. De La Torre, R. Muñoz, and M. C. Burguet. "Liquid–liquid equlibria of the mixture linalool+ ethanol+ water at different temperatures." *Fluid phase equilibria* 238, no. 1 (2005): 72-76. https://doi.org/10.1016/j.fluid.2005.09.009

[7] Fardhyanti, Dewi Selvia, Maharani Kusumaningrum, Nadya Alfa Cahaya Imani, Junaidah Jai, Nurul Asyikin Md Zaki, Ririn Andriyani, and Melinia Rahmahani Putri. "The Temperature Effect of Madeira Vine (Anredera Cordifolia) Leaf Oil Extraction and Its Characterization as An Additive in Health Supplement Product." *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences* 97, no. 2 (2022): 1-7. https://doi.org/10.37934/arfmts.97.2.17

[8] Sucipto, Retno Kumala Hesti, Kuswandi Kuswandi, and Gede Wibawa. "Ternary liquid-liquid equilibrium for eugenol+ tert-butanol+ water system at 303.15 and 323.15 K and atmospheric pressure." In *AIP Conference Proceedings*, vol. 1840, no. 1. AIP Publishing, 2017. https://doi.org/10.1063/1.4982330

[9] da Silva Oliveira, George Laylson, Keylla Conceição Machado, Kátia Conceição Machado, Chistiane Mendes Feitosa, and Fernanda Regina de Castro Almeida. "Non-clinical toxicity of β-caryophyllene, a dietary cannabinoid: Absence of adverse effects in female Swiss mice." *Regulatory Toxicology and Pharmacology* 92 (2018): 338-346. https://doi.org/10.1016/j.yrtph.2017.12.013

[10] Ojha, Shreesh, Hayate Javed, Sheikh Azimullah, and M. Emdadul Haque. "β-Caryophyllene, a phytocannabinoid attenuates oxidative stress, neuroinflammation, glial activation, and salvages dopaminergic neurons in a rat model of Parkinson disease." *Molecular and cellular biochemistry* 418 (2016): 59-70. https://doi.org/10.1007/s11010-016-2733-y

[11] Amiarsih, Dwi, and Sabari Sosro Diharjo. "Pengaruh jenis dan perbandingan pelarut terhadap hasil ekstraksi minyak atsiri mawar." (2006).

[12] Sa'adah, Hayatus, and Henny Nurhasnawati. "Perbandingan pelarut etanol dan air pada pembuatan ekstrak umbi bawang tiwai (Eleutherine americana Merr) menggunakan metode maserasi." *Jurnal ilmiah manuntung* 1, no. 2 (2015): 149-153. https://doi.org/10.51352/jim.v1i2.27

[13] Wilson, Grant M. "Vapor-liquid equilibrium. XI. A new expression for the excess free energy of mixing." *Journal of the American Chemical Society* 86, no. 2 (1964): 127-130. https://doi.org/10.1021/ja01056a002

[14] Mark, Richard E., and Jens Borch, eds. *Handbook of physical testing of paper*. Vol. 1. Crc Press, 2002. https://doi.org/10.1201/9781482290103

[15] Khan, Pathan Mohsin, Bakhtiyor Rasulev, and Kunal Roy. "QSPR modeling of the refractive index for diverse polymers using 2D descriptors." *ACS omega* 3, no. 10 (2018): 13374-13386. https://doi.org/10.1021/acsomega.8b01834