

EXPERIMENTAL INVESTIGATION OF THE SEPARATION OF 4-HYDROXYBENZOIC ACID EMPLOYING NATURAL AND CONVENTIONAL SOLVENTS

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4-hydroxybenzoic acid (4-HBA) has a wide range of applications in various chemicals, cosmetics, pharmaceuticals, wines and the polymer industries. In the present study, 4-HBA was extracted from the aqueous phase utilizing natural and conventional solvents (NACS) at a constant temperature of 298 K. The natural solvents used were corn oil and cottonseed oil, while the conventional solvents used were isoamyl alcohol, ethyl acetate and diethyl carbonate. Five different concentrations, 0.005 to 0.035 mol/liter, were prepared and applied in the batch experiment. Various extraction parameters were investigated, including the distribution coefficient (K_{DHBA}), extraction efficiency ($\%E_{HBA}$), partition coefficient (P) and dimerization coefficient (D). The experimental results revealed the attractive association between the solute and solvent based on their various physicochemical properties. The highest extraction efficiency was obtained for isoamyl alcohol (58.98%) and the lowest for corn oil (39.48%). The order of distribution coefficients was experimentally obtained as follows: isoamyl alcohol (1.438) > ethyl acetate (0.986) > diethyl carbonate (0.961) > cottonseed oil (0.677) > corn oil (0.652). Natural solvents have the potential to avoid toxicity and could be explored for large-scale applications.

Keywords: 4-hydroxybenzoic acid, separation, natural solvents, conventional solvents, distribution coefficient, extraction efficiency

1. Introduction

Phenolic acids are valuable chemicals due to their various applications as antibacterial, antifungal and antioxidation compounds in the pharmaceutical industry, preservatives in the food and cosmetic industries, as well as esters in various biorefineries and polymer industries, etc. [1]-[6]. 4-hydroxybenzoic acid (4-HBA) is naturally present in coconuts, gooseberries, raspberries, fennel, etc. [1]-[2]. 4-HBA is found in very low concentrations (<0.035 mol/liter) in effluent streams of several food-preparation units from the pulp and paper industry, olive oil mills and wine industry [7]-[11]. The extremely slow biodegradation rate of 4-HBA directly affects the soil quality when disposed of on land. With exceptional physiological characteristics and several appealing uses, it is necessary to separate 4-HBA from wastewater and fermentation broth to improve the environment and sustainable economy. The standard methods for recovering 4-HBA are adsorption, reactive distillation, precipitation and the Fenton process with UV light [12]-[18]. These methods have several drawbacks,

including low conversion rates, prolonged processing durations, poor efficacy in diluted solutions, high energy requirements, high costs and the production of hazardous chemicals as by-products. Extractive separation has overcome these challenges and provides a better level of efficiency than existing methods. The extractive separation of 2-hydroxypropanoic acid, pyridine-2-carboxylic acid, ethanecarboxylic acid, 2-hydroxyethanoic acid, 4-oxopentanoic acid and other carboxylic acids have been reported in the literature [19]-[26]. Studies have also reported using different types of eco-friendly solvents in the extractive separation of carboxylic acids such as ionic liquids (ILs), supercritical fluids (SCF) and non-toxic organic solvents [22,27-35]. The choice of solvents poses a considerable difficulty because of the existence of microorganisms in the fermentation broth. The most valued attributes of solvents include non-toxicity, accessibility, inability to mix with the water phase and strong solvation properties. Some of the most important literature data on extraction of hydroxybenzoic acid with natural solvents are summarized in *Table 1* [13,30,32].

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Table 1: Comparative analysis of the existing literature on the extraction of hydroxybenzoic acid with natural solvents

Ref.	Author and year of publication	Hydroxybenzoic acid	Natural solvent used	Maximum extraction efficiency (%E)	Distribution coefficient (K_D)
[32]	Joshi et al. 2022	4-hydroxybenzoic acid	Canola Oil	18.85	0.23
			Mustard Oil	20.45	0.25
			Sunflower Oil	21.00	0.27
			Soyabean Oil	25.06	0.34
[16]	Joshi et al. 2021	4-hydroxybenzoic acid	Sesame Oil	33.24	0.49
			Canola Oil	18.85	0.23
[12]	De et al. 2018	3,4-dihydroxybenzoic acid	Canola Oil	7.41	0.08
			Soyabean Oil	6.56	0.07
			Groundnut Oil	6.18	0.07
			Sesame Oil	6.17	0.07
			Sunflower Oil	4.70	0.05

The present work focuses on investigating the extraction of 4-HBA from an aqueous phase. Five different solvents were used to study the extraction efficiency in batch experiments at a constant temperature of 298 K. Corn and Cottonseed oils were used as two harmless natural solvents, while isoamyl alcohol (IAA), ethyl acetate (EA) and diethyl carbonate (DEC) were used as three conventional solvents. According to the literature [16],[32], the extraction of 4-HBA in the presence of these solvents has not yet been reported.

The complete experimental analysis elaborates on the interaction between the solute and solvents in terms of polarity, dipole moment and other physicochemical properties. The extraction efficiency of conventional and natural solvents was also investigated as well as the effect of the initial solute concentration on the value of the distribution coefficient.

2. Experimental

2.1. Samples and measurements

The chemicals and solvents used in the experiment were as follows: 4-hydroxybenzoic acid (98%) was bought from HiMedia Laboratories Pvt. Ltd., India. Isoamyl alcohol (98%), ethyl acetate (98%) and diethyl carbonate (98%) were purchased from S D Fine Chem Pvt. Ltd., India. Corn oil was procured from Kush Proteins Pvt. Ltd., India and cottonseed oil from Eywa Seeds & Exports Pvt Ltd., India.

2.2. Methods

In the extraction experiment, 4-HBA as a solute was prepared in distilled water at varying concentrations (0.005-0.035 mol/liter). Considering its maximum availability (<5%) in fermentation broths or industrial effluent streams, the highest concentration (0.035 mol/liter) of the aqueous solute (4-HBA) was chosen for experimental analysis and an equilibrium time of 4 hours achieved at a constant temperature of 298 K. 10 milliliters of the aqueous solute phase and 10 milliliters of the solvent were mixed in a conical flask. The volume ratio remained constant at 1:1. Next, the conical flask was placed in an orbital shaking incubator (SE-363 Science Enterprises, India) at 298 K and 200 rpm for 4 hours. The sample obtained after shaking was kept in a centrifuge for 5 minutes at 4000 rpm to separate the aqueous and organic phases. The aqueous phase was examined in a UV-Vis spectrophotometer (Shimadzu UV-1800) at a wavelength of 255 nm. The solute concentration in the organic phase was calculated by a mass balance. The experimental process is presented in Figure 1.

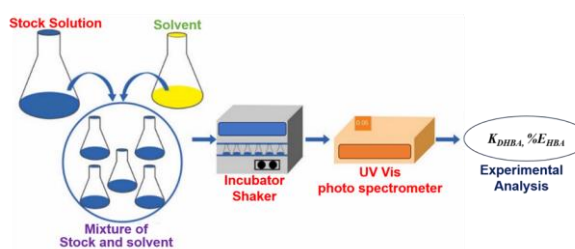


Figure 1: Flow diagram of the experimental process for extracting 4-HBA

2.2.1. Statistical analysis of uncertainty

Experimental uncertainties due to instrument errors and various random variations may be present which can be computed as:

$$\theta = \sqrt{\frac{\sum_{i=0}^n (x_i - \bar{x})^2}{n-1}} \quad (1)$$

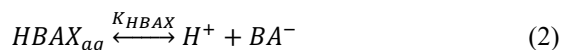
The mean experimental value is denoted by \bar{x}_j and the values of experimental observations by x_j , while n represents the total number of observations. The uncertainties from the experiment fell within the range of $x \pm 0.002$.

2.2.2. Extraction of 4-HBA

4-HBA was extracted in the presence of three conventional solvents, namely IAA, EA, DEC, as well as two natural solvents, that is, corn oil and cottonseed oil. Since the attraction between the acid and water as a result of hydrogen bonding is stronger than that of 4-HBA itself, 4-HBA remained as a monomer. 4-HBA appears as dimers in the organic phase because the identical solute molecules form hydrogen-hydrogen bonds in the organic phase due to either low- or non-polar solvents [30]. The physical separation of 4-HBA from the aqueous phase was accomplished in three steps: acid detachment, partition of the undissociated 4-HBA molecule and dimerization of 4-HBA.

2.2.3. Detachment of the solute

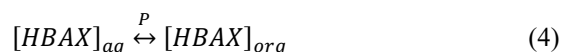
Detachment of the solute 4-HBA in the aqueous phase is represented in the following equations:



$$K_{HBAX} = \frac{[H^+][BA^-]}{[HBAX]_{aq}} \quad (3)$$

K_{HBAX} represents the dissociation constant and $HBAX$ the 4-HBA concentration in moles/liter.

2.2.4. Partition Coefficient of undissociated 4-HBA



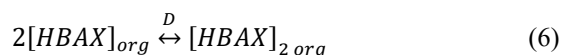
The partition coefficient of the solute (4-HBA) is denoted by P :

$$P = \frac{[HBAX]_{org}}{[HBAX]_{aq}} \quad (5)$$

where $[HBAX]_{aq}$ and $[HBAX]_{org}$ are the solute concentrations in the aqueous and organic phases in moles per liter, respectively.

2.2.5. Dimerization constant of 4-HBA

In the organic phase, the 4-HBA molecules are not in their dissociated form. Due to the stronger attraction between solute molecules than between the solute and solvent as a result of hydrogen bonding, dimer molecules were formed. The process is described by the following equation:



Mathematically, the dimerization constant (D) in liters/mol can be determined using Equation 6 as follows:

$$D = \frac{[HBAX]_{2org}}{[HBAX]_{org}^2} \quad (7)$$

From a physical extraction perspective, one crucial parameter is the overall distribution coefficient (K_{DHBA}).

$$K_{DHBA} = \frac{[HBAX]_{org}^{tot}}{[HBAX]_{aq}^{tot}} = \frac{[HBAX]_{org} + 2[HBAX]_{2org}}{[HBAX]_{aq} + [BA^-]} \quad (8)$$

$$K_{DHBA} = \frac{P[HBAX]_{aq} + 2D[HBAX]_{org}^2}{[HBAX]_{aq} + \frac{K_{HBAX}[HBAX]_{aq}}{[H^+]}} \quad (9)$$

$$K_{DHBA} = \frac{P[HBAX]_{aq} + 2DP^2[HBAX]_{aq}^2}{[HBAX]_{aq} \cdot \left[1 + \frac{K_{HBAX}}{[H^+]}\right]} \quad (10)$$

$$K_{DHBA} = \frac{P + 2DP^2[HBAX]_{aq}}{\left[1 + \frac{K_{HBAX}}{[H^+]}\right]} \quad (11)$$

4-HBA is considered to be a weak acid due to its low pK_a (4.54) [30]. The pH values of dilute solutions were measured (3.3 to 3.8) and it was found that pK_a was less than 4.54. For dilute solutions with a pH significantly lower than the pK_a of acid, the denominator of Equation 11 may be neglected because the numerical value of the $K_{HBAX}/[H^+]$ ratio is very low. Therefore, K_{DHBA} is calculated from Equation 11 as the ratio of $[HBAX]_{org}^{tot}$ to $[HBAX]_{aq}^{tot}$. The relationship between extraction and the equilibrium is determined by the concentrations of the solute in the organic and aqueous phases. The distribution coefficient K_{DHBA} can be calculated based on this connection.

In the following equation, the partition coefficient (P) is predicted as the intercept and the dimerization coefficient (D) as the gradient.

$$K_{DHBA} = P + 2P^2D[HBAX]_{aq} \quad (12)$$

These two important parameters of physical extraction determine the extraction capacity of the solvent.

Additionally, the distribution coefficient (K_{DHBA}) is used to calculate the percentage of extraction efficiency ($\%E_{HBA}$) as follows:

$$\%E_{HBA} = \left(\frac{K_{DHBA}}{1 + K_{DHBA}}\right) \times 100 \quad (13)$$

2.2.6. Solvent regeneration

Recovery of the solute from the organic phase and solvent regeneration constitute the second stage of the process. Back extraction and solvent regeneration have been reported by numerous researchers [14-15,21]. A variety of techniques have been described, including the use of HCl, trimethylamine (TMA), temperature swing, solvent swing and NaOH. Based on available research, the most effective method for solvent regeneration is to use TMA instead of any other method [14]-[15].

Table 2: Physicochemical properties of the used chemicals [1,2,29,36-39]

Chemical	ρ (g/m ³)	μ (cP)	S (g/L)	MP (K)	MW (g/mol)	BP (K)	RI	ε	D_m (Debye)	E_T
4-hydroxybenzoic acid	1460	-	5	487.6	138.12	607.2	1.46	-	2.76	-
Isoamyl alcohol	810	3.692	28	156.0	88.15	404.2	1.41	15.60	1.70	47.0
Ethyl acetate	902	0.426	64	189.6	88.11	350.2	1.37	6.02	1.88	38.1
Diethyl carbonate	975	0.969	0.019	230.0	118.13	399.0	1.38	3.10	1.07	36.2
Corn oil	918	51.44	Insoluble	255.2	-	511.2	1.47	3.60	1.85	-
Cottonseed oil	926	62	Insoluble	268.1	-	505.2	1.47	2.90	-	-

ρ : density, μ : viscosity, S : solubility in water, MP : melting point, MW : molecular weight, BP : boiling point, RI : refractive index, ε : dielectric constant, D_m : dipole moment, E_T : solvent polarity parameter

Table 3: Extraction of 4-HBA using the conventional solvent isoamyl alcohol at 298±1 K

$[HBAX]_0$ (mol/L)	$[HBAX]_{aq}$ (mol/L)	$[HBAX]_{org}$ (mol/L)	K_{DHBA}	$\%E_{HBA}$	pH_0	pH_{aq}
0.005	0.0041	0.0009	0.228	18.59	3.8	3.9
0.010	0.0060	0.0033	0.558	35.81	3.7	3.8
0.020	0.0096	0.0091	0.949	48.68	3.6	3.7
0.030	0.0128	0.0165	1.292	56.37	3.4	3.6
0.035	0.0144	0.0207	1.438	58.98	3.3	3.4

Table 4: Extraction of 4-HBA using the conventional solvent ethyl acetate at 298±1 K

$[HBAX]_0$ (mol/L)	$[HBAX]_{aq}$ (mol/L)	$[HBAX]_{org}$ (mol/L)	K_{DHBA}	$\%E_{HBA}$	pH_0	pH_{aq}
0.005	0.0045	0.0005	0.110	9.90	3.8	3.9
0.010	0.0070	0.0023	0.332	24.93	3.7	3.8
0.020	0.0111	0.0077	0.691	40.88	3.6	3.7
0.030	0.0156	0.0138	0.885	46.96	3.5	3.6
0.035	0.0176	0.0174	0.986	49.65	3.4	3.5

Table 5: Extraction of 4-HBA using the conventional solvent diethyl carbonate at 298±1 K

$[HBAX]_0$ (mol/L)	$[HBAX]_{aq}$ (mol/L)	$[HBAX]_{org}$ (mol/L)	K_{DHBA}	$\%E_{HBA}$	pH_0	pH_{aq}
0.005	0.0044	0.0006	0.140	12.31	3.7	3.9
0.010	0.0071	0.0022	0.305	23.40	3.6	3.8
0.020	0.0115	0.0073	0.636	38.89	3.5	3.7
0.030	0.0158	0.0136	0.859	46.21	3.4	3.6
0.035	0.0179	0.0172	0.961	49.00	3.4	3.5

Table 6: Extraction of 4-HBA using the natural solvent corn oil at 298±1 K

$[HBAX]_0$ (mol/L)	$[HBAX]_{aq}$ (mol/L)	$[HBAX]_{org}$ (mol/L)	K_{DHBA}	$\%E_{HBA}$	pH_0	pH_{aq}
0.005	0.0048	0.0002	0.048	4.56	3.8	3.9
0.010	0.0076	0.0017	0.221	18.09	3.7	3.8
0.020	0.0131	0.0056	0.431	30.12	3.6	3.7
0.030	0.0184	0.0110	0.596	37.33	3.5	3.6
0.035	0.0212	0.0138	0.652	39.48	3.4	3.5

Table 7: Extraction of 4-HBA using the natural solvent cottonseed oil at 298±1 K

$[HBAX]_0$ (mol/L)	$[HBAX]_{aq}$ (mol/L)	$[HBAX]_{org}$ (mol/L)	K_{DHBA}	$\%E_{HBA}$	pH_0	pH_{aq}
0.005	0.0047	0.0003	0.065	6.11	3.7	3.9
0.010	0.0077	0.0017	0.217	17.81	3.6	3.8
0.020	0.0134	0.0054	0.403	28.70	3.5	3.7
0.030	0.0187	0.0106	0.569	36.28	3.4	3.6
0.035	0.0209	0.0141	0.677	40.38	3.4	3.5

3. Results and discussion

The separation of 4-HBA from its aqueous solution was accomplished using three conventional and two natural solvents. The physicochemical properties of the solvents used are presented in Table 2.

The impacts of different solvents such as IAA, EA, DEC, corn oil and cottonseed oil on the extraction efficiency and distribution coefficient are displayed in Tables 3-7, respectively. A comparative analysis regarding the physical extraction of 4-HBA was conducted based on various parameters such as the partition coefficient, dimerization constant, extraction efficiency of solvents and distribution coefficient as presented in Table 8.

Table 8: Parametric comparison of the extraction of 4-HBA using different solvents

Solvent used	Range of K_{DHBA}	Avg. K_{DHBA}	Range of %E _{HBA}	Avg. %E _{HBA}	P	D (L/mol)
Isoamyl alcohol	0.228-1.438	0.893	18.59-58.98	43.69	0.186	1664.41
Ethyl Acetate	0.110-0.986	0.600	9.90-49.65	34.46	0.139	1719.37
Diethyl carbonate	0.140-0.961	0.580	12.31-49.00	33.96	0.123	2090.25
Corn oil	0.048-0.652	0.389	4.56-39.48	25.92	0.084	2597.38
Cottonseed oil	0.065-0.677	0.386	6.11-40.38	25.86	0.085	2489.36

The distribution coefficient which shows the affinity of the solute between two phases was measured. The term distribution coefficient refers to the proportion of acid content in the aqueous and organic phases as well as denotes the degree of selectivity of the solvent or organic phase compared to in water or an aqueous phase. K_{DHBA} fell within the range of 0.228-1.438 for isoamyl alcohol, 0.110-0.986 for ethyl acetate, 0.140-0.961 for diethyl carbonate, 0.048-0.652 for corn oil and 0.065-0.677 for cottonseed oil. The equilibrium curve presenting the extraction of 4-HBA is shown in Figure 2, revealing that as the solute concentration increases in the aqueous phase, the solute concentration increases in the organic phase. The conventional solvent IAA is highly polarizable in nature, leading to a better extraction efficiency and distribution coefficient, followed by the aprotic polar solvent EA and aprotic solvent DEC. A polar solvent has high values for some physicochemical properties (such as dielectric constant, dipole moment, solvent polarity) and low viscosity, as shown in Table 2.

A high dielectric constant causes a high degree of polarization, moreover, stronger interactions between the solvent and solute tend to result in a higher extraction efficiency. The polar solvent tends to donate hydrogen atoms which attach to O-(O-H) groups [14]-[21]. The highest extraction efficiency, that is, 58.98%, was achieved when IA was used as a conventional solvent as shown in Table 3, while the lowest of 39.48% was recorded by corn oil as shown in Table 6. The distribution coefficient with an initial concentration of 4-HBA is

shown in Figure 3, which reveals the interaction between the solvent and solute molecules. As the initial solute concentration increased, the distribution coefficient increased for each solvent as shown in Figure 3. However, the highest distribution coefficient, that is, 1.43, was achieved for IA due to its better physicochemical properties with regard to the interaction between solute and solvent molecules when compared to other solvents. Another conventional solvent, ethyl acetate, was used to extract 4-HBA from the aqueous phase. EA is polar and aprotic in nature. An extraction efficiency and distribution coefficient of 49.65% and 0.986, respectively, were achieved by this solvent (Table 4). The dielectric constant and dipole moment for EA (Table 2) play a crucial role regarding the interaction between the solute and solvent. A low degree of dimerization and high partition coefficient are observed in Figure 4, confirming that the solute-solute interaction is less significant than the solute-solvent interaction. 4-HBA was also extracted with diethyl carbonate (Table 5). DEC is aprotic in nature and yielded the lowest extraction efficiency among the conventional solvents used due to its structural properties. This aprotic solvent does not accept the proton and donates it, causing C-H bonds to not be sufficiently polarized, therefore, the interaction between the solvent and solute molecules is weaker so acts as a poor anionic solvator, resulting in a lower distribution coefficient and extraction efficiency as presented in Figures 3 and 5, respectively.

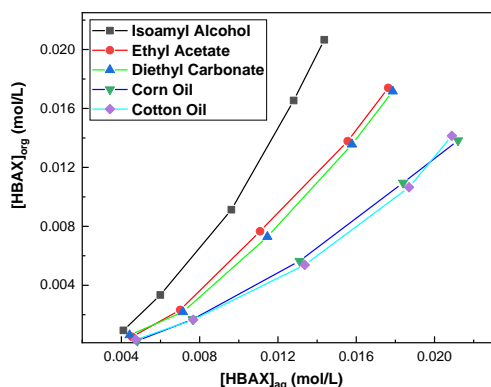


Figure 2: Extraction equilibrium of 4-HBA in terms of the concentration of the solute in the aqueous $[HBAX]_{aq}$ and organic $[HBAX]_{org}$ phases using different solvents

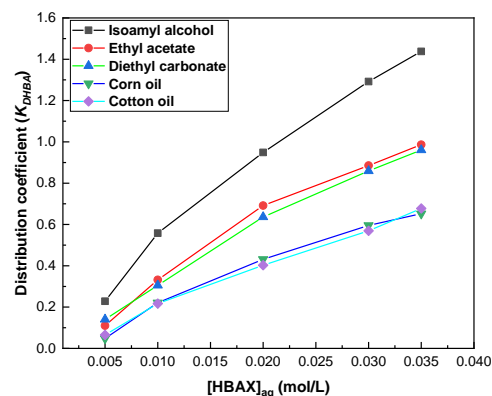


Figure 3: Distribution coefficient at different initial concentrations of 4-HBA

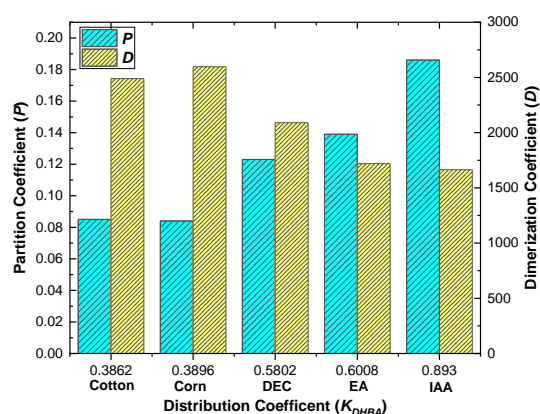


Figure 4: Comparative analysis of the partition and dimerization coefficients with regard to the distribution coefficient for different solvents such as cottonseed oil, corn oil, diethyl carbonate (DEC), ethyl acetate (EA) and isoamyl alcohol (IAA)

DEC contains an oxygen double bond where two adjacent oxygen atoms bond together, leading to strong steric repulsion. This affects the interaction between the solute and solvent. A high degree of dimerization and low partition coefficient represented in Figure 4 also confirm that the solute-solute interaction is stronger than the solute-solvent interaction.

The OH functional group present in 4-HBA has a tendency to hydrogen bond with oxygen atoms present in EA and DEC. However, EA has a stronger tendency to hydrogen bond with 4-HBA due to its methyl group being closer to an oxygen double bond compared to DEC. Therefore, the extraction efficiency is higher in EA compared to DEC. 4-HBA was successfully physically extracted using non-toxic natural solvents, namely corn oil and cottonseed oil. These oils are non-toxic compared to the conventional solvents [37]-[38]. The extraction efficiencies of corn oil (39.48%) and cottonseed oil (40.38%) are shown in Tables 6 and 7, respectively. The distribution coefficients for corn oil and cottonseed oil were 0.652 and 0.677, respectively. The non-polar nature of natural solvents as well as their low dipole moments and minimal dielectric constants led to low extraction efficiencies and distribution coefficients as shown in Figures 3 and 5.

The large oil molecules cause a rotating rigid structure, the high density and viscosity of oil as well as the immiscibility of oil with the aqueous phase. Therefore, oils are expected to yield low extraction efficiencies and distribution coefficients. However, the high percentages of unsaturated fatty acids in corn and cottonseed oil - e.g. 27 and 20% of the monounsaturated fatty acid, oleic acid, as well as 52 and 54% of the polyunsaturated fatty acid, linoleic acid, respectively - make them important solvents. The unsaturated fatty acid, linoleic acid, contains a hydroxyl group (OH), which interacts with solute molecules and bonds to them. Therefore, natural solvents are emerging as competitive alternatives to traditional solvents with moderate extraction efficiencies and their non-toxic nature. The extraction efficiencies using different solvents were obtained in the following order: IA (58.98%) > EA

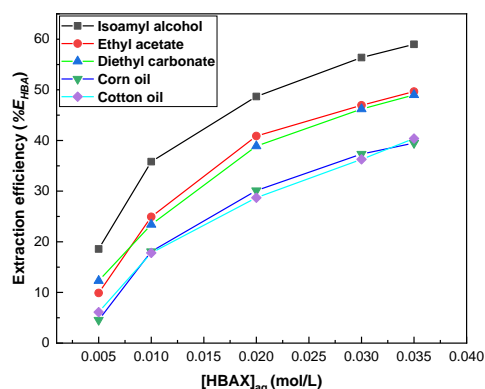


Figure 5: Extraction efficiency at different initial concentrations of 4-HBA

(49.65%) > DEC (49.00%) > cottonseed oil (40.38%) > corn oil (39.48%). From Equation 12, the intercept and gradient were calculated to determine the partition coefficient and dimerization coefficient, respectively. The partition coefficient and dimerization coefficient of each solvent are shown in Figure 4 and Table 8. The highest partition coefficient and lowest dimerization coefficient were obtained for IA due to its strong solute-solvent interactions, while the lowest ones were obtained for DEC and corn oil due to their weak solute-solvent interactions as presented in Figure 4 and Table 8. As the distribution coefficient increases, the partition coefficient increases, while the opposite trend is observed with regard to the dimerization coefficient, meaning that the solute-solvent interaction is stronger than the solute-solute equivalent. The dimerization and partition coefficients are presented in Table 8. The dimerization and partition coefficients for different solvents range from 1664.41 to 2597.38, while their partition coefficients range from 0.186 to 0.085.

4. Conclusion

4-HBA was extracted using different natural and conventional solvents. Isoamyl alcohol yielded the best extraction efficiency (58.98%) and distribution coefficient (0.186) among all the solvents used. However, a problem posed by conventional solvents is their toxicity, especially when separated from the fermentation broth. Nevertheless, conventional solvents exhibit very hazardous and toxic characteristics so cannot be used in many pharmaceutical and food industries due to their adverse effects on the process and product yield. Natural oils like corn and cottonseed oil may be used to overcome this problem due to their non-toxic characteristics. Cottonseed oil as a natural solvent yielded the highest extraction efficiency of 21.48%, higher than in the literature [16] when compared to other natural solvents. The extraction efficiency and distribution coefficient with regard to the initial concentration of the solute were determined, moreover,

the solvent-solute interaction was investigated based on the various physicochemical properties of solvents. The results obtained affirm the use of natural oils as alternative solvents instead of conventional ones, where toxicity is a primary concern in the food and pharmaceutical sectors.

SYMBOLS

4-HBA	4-hydroxybenzoic acid
IAA	Isoamyl alcohol
EA	Ethyl acetate
DEC	Diethyl carbonate
$[HBAX]_0$	Initial concentration of 4-HBA (mol/L)
$[HBAX]_{aq}$	Concentration of 4-HBA in the aqueous phase (mol/L)
$[HBAX]_{org}$	Concentration of 4-HBA in the organic phase (mol/L)
pH_0	Initial pH value of 4-HBA
pH_{aq}	Final pH value of the aqueous phase
K_{DHBA}	Distribution coefficient
$\%E_{HBA}$	Extraction efficiency of the solvent
P	Partition coefficient
D	Dimerization coefficient

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