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An Investigation of Several Methodologies for Predicting the Solubility of Organic Compounds

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ABSTRACT:

One of the most important factors in achieving the desired concentration of drug in the systemic circulation for the desired pharmacological reaction is solubility, which is the process of solute in solvent to give a homogenous framework. Inadequate permeability solubility may be the cause of the bioavailability problem. The solubility problems affect the majority of mixed solutions. Therefore, as synthetic science advances, there is an increasing need for improved drug inventions. Homogeneous liquid phases with factor proportions of solute and solvent are expressed by the solute-solvent interaction mechanisms. The medication property, the retention site, and the necessary measurement structure attribute all influence the choice of solubility improvement technique.

Introduction

The greatest solute that can dissolve in a specific amount of solvent is referred to as "solubility." It is defined quantitatively as the solute concentration in a soaking solution at a certain temperature. One definition of solubility is the spontaneous combination of two or more homogeneous molecular dispersions.[1]

Resolving

The process of solubilisation involves adding one or more extra components to a substance that is ordinarily insoluble or only marginally soluble in a given solvent to create a thermodynamically stable isotropic solution.[2]

Pressure and temperature are the two direct parameters that impact solubility. Pressure only has an impact on the solubility of gases; temperature affects both the Gas solubility. Based on an immediate release product's maximum dose strength, solubility is determined. When the maximum dose strength of a medicine dissolves in 250 millilitres or less of aqueous medium within the pH range of 1 to 7.5, the drug is said to be very soluble.

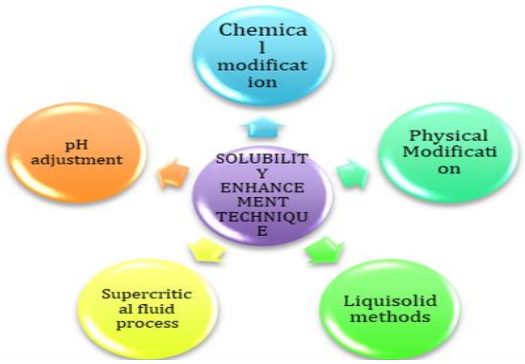

Figure : 01 Different solubility enhancement techniques

Expression of Solubility

Quantitative expressions of solubility include %, molality, and molarity.

Molarity is the number of moles (gramme molecular weight) of solute dissolved in 1000 g of solvent, whereas molality is the number of moles of solute dissolved in 1000 g of solvent. In the pharmaceutical industry, three terminology are used to describe concentration.

These are as follows: % w/w indicates how many grammes of solute are dissolved in 100 grammes of solution.

The amount of solute dissolved in 100 grammes of solution is expressed as % v/v.[3]

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The solute's grammes dissolved in 100 millilitres of solution is expressed as % w/v.

Any instrumental method of analysis, including gravimetric and titrimetric methods, can be used to determine the concentration.[3]

Procedure:

A) For Physical Solubility

A few drops of various solvents are added to separate test tubes.

A few drops of the organic sample solution are added to this and thoroughly mixed.

After letting the test tubes stand for roughly five minutes, observations are made.[4]

B) By Gravimetric Method

1. approximately 50 ml of water and a conical flask are filled with progressively more sodium chloride while being shaken, until the solution is saturated and some solid remains undissolved (approximately 20 g of sodium chloride is needed).
2. After filtering the mixture, 10 millilitres of the filtrate are pipetted into an evaporating dish that has been preweighed and tared.
3. Weigh the dish that holds the 10 millilitre filtrate.
4. The filtrate is dried in an oven at around 100°C after being evaporated to the point of dryness.
5. It is then weighed after cooling. Drying is carried out until a steady weight is achieved.

Observations:

(i) Empty dish weight in grammes: w 1

(ii) Dish weight + 10 ml solution in grammes: w 2

(iii) Dry solution + dish weight in grammes: w 3

Estimate:

Solute weight in 10 millilitres of solution (g) = w3–w 1

Solvent weight in 10 millilitres of solution (g) = w2-w 3

Solvent Weight x Solvent Volume in millilitres, Solvent density (water) = w2−w 3 /Water density

The number of solvent parts needed for each solute component is known as solubility.

(w3–w1) g of solute is needed, and w2−w 3/ Water density per millilitre.

For every 1 g of solute, (w3–w1)* w2−w3/water density in millilitres.[5]

1. Water solubility:

On six test tubes indicate the name of the hydrocarbon to be tested, then place about 1 mL
in each tube.

Add dropwise about 0.5 mL of water into each tube.

Is the obtained mixture homogenous or heterogeneous?

Which substance is on the top and which one is on the bottom?

Mix the content of each tube, then observe. What happens when it allowed to settle?

Conclude about the density of the hydrocarbons relatively to the water?

Take notes and save the solutions for the next part.

2. Solubility in Petroleum ether:

On six test tubes indicate the name of the hydrocarbon to be tested, then place about 1 mL
in each tube.

Add dropwise about 0.5 mL of ligroin (non polar solvent) into each test tube.

Is the mixture homogenous? If not which layer is on the top?

Results

By Physical Solubility

S. NO	SOLVENT / COMPOUNDS	HCL	H2SO4	WATER	ACETONE	ALCOHOL
1	BENZOIC ACID	Insoluble	Insoluble	Insoluble	Soluble	Soluble
2	ACETANILIDE	Insoluble	Soluble	Insoluble	Soluble	Insoluble
3	BENZALDEHYDE	Insoluble	Insoluble	Insoluble	Soluble	Soluble
4	D-GLUCOSE	Soluble	Insoluble	Insoluble	Insoluble	Insoluble
5	RESORCINOL	Soluble	Soluble	Soluble	Insoluble	Soluble

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Figure: 02 Physical solubility determination

B) By Gravimetric Method

The solubility of sodium benzoate in distilled water at room temperature was 0.04

Figure : 03 After drying at room temperature

Conclusion

It can be concluded that solubility of different types of organic compounds can be determined by both method. Physical method was easy to determined and short time consuming process while gravimetric method was time taking process. Accuracy could be calculated by gravimetric method only.

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