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IN-SILICO BIOAVAILABILITY AND PHARMACOKINETIC STUDY OF SOME HERBAL MUCILAGES

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ABSTRACT

Herbal excipients are a better choice instead of synthetic one. The developing interest and awareness about herbal excipients, which are of natural in origin, the pharmaceutical industries are tending to use them in development of various formulations. Nowadays preferences are given to herbal excipients as they involves fewer regulatory issues and being stable during the formulation process as well as in the finished formulation in comparison with synthetic excipients. The current study enlists various herbal excipients along with their major chemical constituents and their uses in pharmaceutical preparations. Software based pharmacokinetic and bioavailability study of some selected chemical constituents was performed. Generated data (for solubility, skin permeability, gastrointestinal absorption, cytochrome P450 activity, Bioavailability etc.) was studied for suitability of that particular excipient for specific type dosage form.

KEYWORDS

Excipients, Bioavailability, Pharmacokinetics and Herbal mucilage.

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INTRODUCTION

The substances used as a medium in the preparation of medicament or formulation are called as "excipients"[1,2]. In pharmaceutical formulations, excipients aid to develop drug delivery systems. They contribute towards various pharmacokinetic attributes such as solubility, stability, patient acceptance and bioavailability. Excipients are used to provide safety, effectiveness during storage and use of pharmaceutical formulations[3].

Excipients can be categorized based on their applications and uses in formulation. The reported categories are Binders, Diluents, Lubricants,

Glidants, Disintegrants, Coating agents, Polishing Film formers, Plasticizers, Coloring agents, Suspending agents, Preservatives, Antioxidants, Flavouring agents, Sweetening agents, Taste enhancers, Printing inks and Dispersing agents[4].

Merits and Demerits of Herbal Excipients

The major benefits to be considered during selection of excipients during formulation are summarized below[5,6]

- Herbal excipients are biodegradable and do not show any adverse effects towards environment and living organisms.
- Herbal excipients are carbohydrates and thus non-toxic and biocompatible.
- When compared to synthetic counterparts, they are economic with low production cost.
- They offer ease of availability.

In addition to this some limitations restrict the use of herbal excipients. These are as follows[6,7],

- On exposure to environment, they may get contaminated by microorganisms.
- Production is dependent on environmental factors.
- The chemical composition may vary depending on region, species and climate as well as cultivation time.
- Generally, natural polymers have slow production rate.
- These are contaminated by heavy metal impurities and need to be purified.

Various major categories of herbal excipients and the constituents are presented in tabular form (Table No.1). In the present work, a concise report has been prepared on various categories of herbal excipients followed by computational studies of their physicochemical and pharmacokinetic properties.

Bioavailability and other Pharmacokinetic studies

Among different routes of drug administration, oral route is highly favoured for the comfort and compliance of patient. Oral bioavailability estimation of drug in early stage, i.e., the fraction of the drug that reaches the systemic circulation after oral administration, is an important decisive factor at various steps of the discovery process. Bioavailability is primarily driven by gastrointestinal absorption. Water soluble drugs are suitable candidates for oral dosage forms. Gastrointestinal (GI) absorption of drugs is directly related to the availability of drug in systemic circulation. It means GI absorption of drugs leads to better bioavailability.

Lipophilicity is an important criterion for topical formulations. Lipophilic drugs easily get absorbed through skin and impart great therapeutic action. Enzyme cytochrome P450 is responsible for metabolism of a number of drugs. This family of isoenzymes (containing more than 50 enzymes) and mainly found in the liver, catalyzes various bio transformational reactions (primarily oxidation) of drugs[64]. Inhibition or induction of this isoenzyme family may alter the basic biotransformation pathways and leads to altered pharmacological response[65].

Mucilages are widely used in sustained release drug delivery system as they form a matrix system when comes in the contact of solvent (mostly water). This matrix entraps the drug and hinders the immediate release of drug from the system due to formation of slimy mass of the mucilage and slows down the release of drug by porous matrix-controlled system. Dosing frequency can be reduced by using such type of natural sustained release agents. Modulation of drug release by mucilages is as shown in Figure No.1.

For the selected constituents from herbal sources *in-silico* pharmacokinetic studies were performed using website http://www.swissadme.ch/index.php (Table No.2).

Herbal excipients shows lack of toxicity, are easily available and economical as compared to their synthetic counterparts. To cross lipoidal membrane, log p value should lie between 1-2 and most of the above chemicals (Table No.2) show the value within the range. As per the absorption concern, these chemicals show good GI absorption and hence suitable for oral dosage form. Most of them do not inhibit cytochome P450 and thus do not show any

interference with the biotransformation of other constituents present in the body. These chemicals also show good skin permeability and thus a suitable topical formulation of drug can be prepared using these mucilages as a carrier. Bioavailability is also good for these chemicals, so these mucilages can be used as a suitable drug carrier for various types of dosage forms[66].

Table No.1: Herbal excipients with their chemical constituents and uses

S.No	Excipients	Source	Active constituents	Category/Uses	Ref
1	Agar	*Gelidium amansii* (Gelidaceae)	Galactan	Laxative, Emulsifying agent, Suspending agent, Gelling agent, Disintegrates, Lubricant, Medium for bacterial culture, Supporting medium for immune-electrophoresis and immune-diffusion	8, 9
2	Tragacanth	*Astragalus gummifer* (Leguminosae)	Tragacanthin, Bassorin	Demulcent, Suspending agent, Emulsifying agent, Thickening agent, Emollient in cosmetics, Sustained release agent	10
3	Aloe mucilage	Aloe species (Liliaceae)	Glucomannan acemannan Aloe-emodin, aloetic-acid, anthranol, barbaloin, is obarbaloin, emodin, ester of cinnamic acid	Sustained release agent, Gelling agent	11, 12
4	Satavari mucilage	*Asparagus racemosus* (Aapocynaceae)	Sarsapogenin, Saponins A-4 to A-7, Shatavarin I to IV, Sitosterol, Glycosides of quercetin, Stigmasterol, Asparagamine A and Sitosterol 7	Binding agent, Sustaining agent	13
5	Bavchi mucilage	*Ocimum canum* (Gigarginaceae)	Glucose, rhamnose, glucuronic acid	Emulsifying agent Suspending agent	14
6	Gum acacia	*Acacia arabica* (Combretaceae)	Arabinogalactan	Suspending agent, Emulsifying agent, Demulcent, binder, Emollient	15

7	Gum Ghatti	*Anogeissus latifolia* (Combretaceae)	L-arabinose, D-galactose, D-mannose, Xylose, D-glucuronic acid, methylpentons, aldobioronic, galacturonic acid, pentosan,	Binder, Emulsifier, Suspending agent	16
8	Albizia gum	*Albizia zygia* (Leguminoseae)	Galactose and arabinose	Binding agent, Drug targeting	17, 18
9	Gellan gum	*Pseudomonas elodea* (Leguminoseae)	Glucose, rhamnose, glucuronic acid	Disintegrating agent, Binding agent	19
10	Khaya gum	*Khaya grandifolia* (Labiatae)	Galactose, rhamnose, galacturonic acid	Binding agent, Drug release modifier, Thickener, emulsifier	20, 21
11	Tamarind seeds	*Tamarindus indica* (Leguminoseae)	Polysaccharides, β-1,4-connected glucose molecules together with xylose (alpha-1,6) and galactose	Binding agent, Emulsifying agent	22
12	Cassia tora	*Cassia tora* Linn. (Leguminoseae)	Heteropolysaccharide of galactose and mannose (galactomannans)	Binding agent	23
13	Abelmoschus Gum (Orka gum)	*Abelmoschus esculentus* (Malvaceae)	Cellulose, hemicelluloses, lignin, pectic matter	Suspending agent, Disintegrant in low concentrations (4%), sustained release, microbially triggered material for colon targeting	24
14	Locust Bean Gum (Carob gum)	*Ceratonia siliqua* (Leguminosae)	D-galacto Dmannoglycan, pentane, proteins and cellulose	Controlled-release agent, Super disintegrant	25, 26, 27
15	Almond gum	*Prunus amygdalus* (Rosaceae)	arabinose, xylitol, galactose and uronic acid, rhamnose, mannose and glucose	Emulsifying, Thickening agent, Suspending agent, adhesive, glazing, and stabilizing properties. Drug release increased	28
16	Neem Gum	*Azadirachta indica* (Meliaceae)	L-arabinose, L-fucose, D-galactose and D-glucoronic acid, glucose, fructose, mannose and xylose, alanine, aminobutyric acid, arginine, asparagines, aspartic acid, glycine, norvaline, praline	Controlled and sustained release agent, binding agent	29, 30
17	Cashew Gum	*Anacardium occidentale* (Anacardiaceae)	L-arabinose, L-rhamnose, D-galactose, glucuronic acid	Gelling property, Controlled release agent	31, 32

18	Fenugreek Mucilage	*Trigonella foenum-graceum* (Leguminosae)	Galactomannan (monosaccharides mannose and galactose units)	Suspending agent, Sustained release agent	33
19	Hibiscus Mucilage	Fresh leaves of *Hibiscus rosasinensis* (Malvaceae)	L□rhamnose, D□galactose, D□galactouronic acid, and D□glucuronic acid	Sustained release agent	34
20.	Cactus mucilage	*Opuntia ficus-indica* (Cactaceae)	Rhamnose, arabinose, galactose, Xylose	Gelling agent in sustained drug delivery	35
21	Menthol	*Mentha piperita* (Labiatae)	Menthol	Penetration enhancer	36
22	Caraway oil	*Carum carvi* (Umbelliferae)	R-carvone, D-limonene, β-myrcene, γ-terpinene, thymol, o-cymene, trim ethylene dichloride	Controlled release agent	37
23	Alginates	Brown sea weed (Phaeophyceae)	binary, linear copolymers of (1 → 4) linked ß-d-mannuronic acid and α-l-guluronic acid	Sodium salt of alginic acid is used as matrix, GI transit modulator, in drug targeting, bioadhesive, etc.	38, 39
24	Pectins	Plants cell wall	galacturonic acid, homogalacturonans, D-galactose, L-arabinose, D-xylose	Pectin with ethyl cellulose for colon specific drug delivery system	40
25	Starches	Seeds and underground organs of green plants (eg. (*Zea mays, Oryza sativa, Triticum aestivum, Solanum tuberosum* etc.)	Amylose, amylopectin	Starch acetate based delivery system as controlled drug delivery	41
26	Xanthum gum	*Xanthomonas campestris* (using microbial fermentation) (Xanthomonadaceae)	Glucose units, cellulose, beta-D-glucuronic acid, beta-D-mannose, alpha-D-mannose and alpha-D-glucoronic acid, beta-D-glucose	Hydrophilic matrixing agent (release modifier)	42, 43
27	Kanjac glucomannan	From tubers of *Amorphophallus konjac* (Araceae)	Polysaccharide chain of β-1,4-linked glucose and mannose	In controlled drug delivery system	44
28	Mimosa pudica mucilage	From seeds of *Mimosa pudica* (Fabaceae)	d-xylose and d-glucuronic acid, tubulin, gallic acid, calcium oxalate crystals, C-glycosylflavones	Sustained drug release	45
29	Bhara gum	Bark of *Terminalia bellerica*	ß-sitosterol, gallic acid, ellagic acid, ethyl gallate,	Film forming agent, emulgent, sustained drug release,	46, 47

		(Combretaceae)	galloyl glucose and chebulaginic acid	microencapsulation	
30	Grewia gum	Inner bark of the edible plant *Grewia mollis* (Tiliaceae)	Glucose, rhamnose, galacturonic acid	Binding agent, sustained drug release,	48, 49
31	Gum Damar	*Shorea wiesneri* (Dipterocarpaceae)	alpha-resin, beta-resin, dammarol acid	Sustained drug release	50
32	Rosin	From pine trees (eg. *Pinus soxburghui, Pinus longifolium, Pinus toeda* etc. (Pinaceae)	Abietic acid	Film former Sustained drug release	51
33	Cordial gum	*Cordia obliqua willed* (Boraginaecae)	xylose, arabinose, rhamnose and galacturonic acids	Novel oral sustained release matrix forming agent in tablets	52
34	Mucuna gum	*Mucuna flagillepes* (Papillionaceae)	Galactomannans	Microencapsulating agent	53
35	Gaur gum	Endosperm of the seeds of *Cyamopsis tetragonolobus* L. (Leguminosae)	Galactomannans (Galactose and mannose)	Site specific drug delivery, sustained drug release	54
36	Tara gum	Endosperm of seed of *Caesalpinia spinosa* (Leguminosae or Fabaceae)	Galactomannans (ratio of mannose to galactose in tara gum is 3:1)	Gastro retentive, controlled release	55, 56
37	Gum copal	Natural resinous material of plant *Bursera bipinnata* (Burseraceae)	Agathic acid along with ciscommunic acid, transcommunic acid, polycommunic acid, sandaracopimaric acid, agathalic acid, monomethyl ester of agathalic acid, agatholic acid and acetoxy agatholic acid	Sustained release drug delivery	57, 58
38	Moi gum	Leaves, stems, fruits, and bark of the stem *Lannea coromandelica* (Anacardiaceae)	Ellagic acid, quercetin, and quercetin-3 arabinoside, is oquercetin and morin, beta-sitosterol, leucocyanidin and leucodelphinidin	Sustained drug release	59
39	Moringa oleifera Gum	Exudes of stem of *Moringa oleifera* (Moringaceae)	Arabinose, galactose, and glucuronic acid	Gelling, binding agent	60, 61
40	Grewia gum	Inner bark of the edible plant *Grewia mollis* (Tiliaceae)	Glucose, rhamnose, galacturonic acid	Control drug release	62, 63

Table No.2: Chemical constituents with their pharmacokinetics and bioavailability parameters

S.No	Chemical constituent	Log *P*	Solubility	GI absorption	BBB Permeation	Cytochrome P450 inhibitor					Log Kp (Skin permeability	Bioavailability score
						CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor		
1	Aloe-emodin	0.76	1.87e+00mg/ml; 6.87e-03 mol/l	High	No	No	No	No	No	No	-7.42cm/s	0.55
2	Emodin	2.72	5.74e-02mg/ml; 2.12e-04 mol/l	High	No	Yes	No	No	No	Yes	-6.02 cm/s	0.55
3	Anthranol	4.19	8.20e-03mg/ml;4.22e-05 mol/l	High	Yes	Yes	Yes	No	No	No	-4.51 cm/s	0.55
4	Glucuronic acid	-2.34	8.58e+02mg/ml, 5.71e+00 mol/l	Low	No	No	No	No	No	No	-9.15 cm/s	0.56
5	Arabinose	-2.32	8.58e+02 mg/ml, 5.71e+00 mol/l	Low	No	No	No	No	No	No	-8.86 cm/s	0.55
6	Rhamnose	-2.09	4.72e+02mg/ml, 2.88e+00 mol/l	High	No	No	No	No	No	No	-8.79 cm/s	0.55
7	Xylitol	*-2.48*	1.68e+03mg/ml, 1.10e+01 mol/l	Low	No	No	No	No	No	No	-8.99 cm/s	0.55
8	Menthol	3.40	2.04e-01mg/ml, 1.30e-03 mol/l	High	Yes	No	No	No	No	No	-4.85 cm/s	0.55
9	Carvone	2.71	5.81e-01mg/ml, 3.87e-03 mol/l	High	Yes	No	No	No	No	No	-5.29 cm/s	0.55
10	Limonene	4.57	4.33e-02 mg/ml, 3.18e-04 mol/l	Low	Yes	No	No	Yes	No	No	-3.89 cm/s	0.55
11	Myrcene	4.17	1.22e-01mg/ml, 8.96e-04 mol/l	Low	Yes	No	No	No	No	No	-4.17 cm/s	- 0.55
12	Thymol	3.30	9.74e-02mg/ml, 6.49e-04 mol/l	High	Yes	Yes	No	No	No	No	-4.87 cm/s	0.55
13	Cymene	4.38	2.08e-02 mg/ml, 1.55e-04 mol/l	Low	Yes	No	No	No	Yes	No	-4.01 cm/s	0.55
14	Gallic acid	0.70	3.90e+00mg/ml, 2.29e-02 mol/l	High	Low	No	No	No	No	Yes	-6.84 cm/sec	0.56
15	Abietic acid	4.78	7.69e-03mg/ml, 2.54e-05 mol/l	High	Yes	No	Yes	Yes	No	No	-4.75 cm/s	0.56

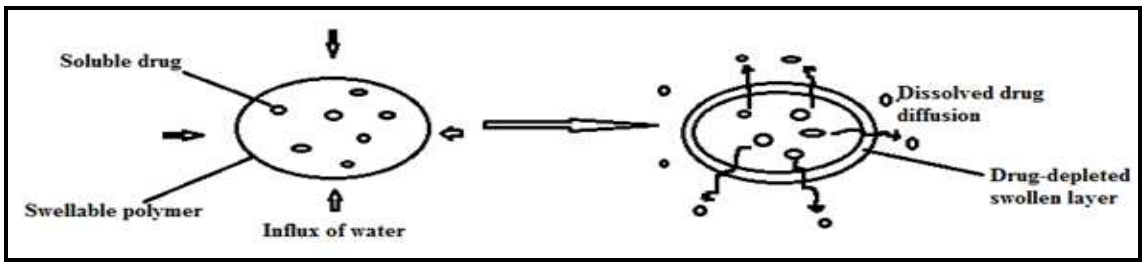

Figure No.1: Drug release by matrix-controlled system

CONCLUSION

Herbal excipients play an important role in formulating various dosage forms. These are useful in preparing conventional to advanced formulations like site specific, controlled and sustained release drug delivery. A wide range of applications for these excipents are reported by eminent researchers. Stringent regulations are imposed on the excipients which have been employed for the first time in any of the drug delivery systems before their use. Futuristic applications of herbal excipients offer a safer and effective drug delivery system.

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CONFLICT OF INTEREST

We declare that we have no conflict of interest.

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