GCMS analysis, Pharmacokinetics and Drug-likeness properties of phytoconstituents of medicinal plant "*Aloe vera* (L.) Burm. f."

Kiran[1], A. K. Giri[1], Bhupendra Kumar*[2]
[1]Institute of Environment & Development Studies, Bundelkhand University, Jhansi, India
[2]Department of Biotechnology, ITS-IHAS, Ghaziabad, India

Abstract: *The present chemical analysis deals with the GC MS analysis of methanol leaf extract of the medicinal plant Aloe vera to understand the bio molecules present in it. The plant leaves was collected from IDES, Bhundelkhnad University, Jhansi. The phytochemical compound screened by GC-MS method. The peak components were identified based on the NIST Library. The total 24 bioactive photochemical compounds were identified in the methanolic extract of Aloe vera. Some important constituents such as cis-11-Eicosenoic acid, i-Propyl 9-octadecenoate, Octadec-9-enoic acid, 9,12,15-Octadecatrienoic acid, (Z,Z,Z),Gamolenic Acid, (E,Z,Z)-2,4,7-Tridecatrienal etc. were shown in the GC MS analysis results. The bioactive compounds from the leaves of Aloe vera screen the antimicrobial, antioxidant, and anti-inflammatory activity. All compounds in the extract of Aloe vera studies using SwissADME. SwissADME method used to understand the ADME properties of the compounds present in Aloe vera phytoconstituents. The ADME analysis results indicated that Aloe vera extracts could be developed as traditional medicine.*

Key words: GCMS, Phytochemical, *Aloe Vera*, SwissADME, Pharmacokinetics, Drug-likeness.

*corresponding author-genuinebhupendra@gmail.com

Introduction: Herbal medicines have been used for ancient time to present day for human diseases (Arokiyaraj et al., 2008). Medicinal plants have played an important role in medicine and its cultivation help in reclamation of degraded land (Kiran et al., 2020; Kiran et al., 2009) Medicinal plants are equipped from a diversity of plant materials as leaves, stems, roots, barks, inflorescence etc. (Gordon, 2001) Medicinal plants contain biologically active principles with specific therapeutic effects. The soil of Bundelkhand region was slight or moderate alkaline in nature and scarcity of water in this region (Kiran et al., 2018). *Aloe vera* (L.) Burm. f. is a perennial succulent xerophyte, which develops water storage tissue in the leaves to survive in dry areas of low or erratic rainfall. The innermost part of the leaf is a clear, soft, moist, and slippery tissue that consists of large thin-walled parenchyma cells in which water is held in the form of viscous mucilage (Dabai, 2007). Therefore, the thick fleshy leaves of aloe plants contain not only cell wall carbohydrates such as cellulose and hemicellulose but also storage carbohydrates such as acetylated mannans(Ferro et al., 2003). Many of the medicinal effects of aloe leaf extracts have been attributed to the polysaccharides found in the inner leaf parenchymatous tissue (Boutagy and Harvey, 1979; Rice-Evans, 2003), but it is believed that these biological activities should be assigned to a synergistic action of the compounds contained therein rather than a single chemical substance (Scalbert and Williamson, 2000). *Aloe vera* is the most commercialized aloe species.

The determination of phytochemical constituents is mostly performed by the moderately expensive and often laborious techniques such as gas chromatography (GC) and liquid chromatography (LC) combined with specific detection schemes (Eisenhauer et al., 2009). In the past few years, GC-MS has become strongly established as a key technological metabolic profiling in both plant and non-plant species (Sivakumar and Gajalakshmi, 2014; Janakiraman et al., 2012). The crude extracts and medicines manufactured of the principles of

biological active compounds even by pharmaceutical companies could be lead to large scale exposure of humans to natural products.

In-silico studies and bioinformatics are releasing a considerable role in the design, screening, and discovery of drugs with a fast time and low cost (Prabhu et al., 2018). At present, computer-assisted computations of ADME (Absorption, Distribution, Metabolism, and Excretion) of drugs are being considered for applying an anticipatory and reliable complement of data to experimental accessions. This computational model predicts the pharmacokinetic, physicochemical, and drug properties of small molecules for drugs (Sliwoski et al., 2014). This study aimed to evaluate the chemical profiles of *Aloe vera* using Gas Chromatography-Mass Spectrometry (GC-MS) and predict its biological activity using computational analysis (Absorption, Distribution, Metabolism, and Excretion -ADME).

Materials and Methods:

Collection of plant material: The plant material (leaves) of cultivated medicinal plant *Aloe vera (L.) Burm. f.* were collected from IDES, Bundelkhand University Campus Jhansi. The plant authenticated and verified by the CCRAS, Regional Ayurveda Research Institute, Ministry of AYUSH, Govt. of India, Gwalior Road, Jhansi-284003. The moisture content of the samples was 23.71% (Kiran et al., 2021). The *Aloe vera* leaves was washed and shade dried for 2 weeks. After drying, the homogenate was transformed into a fine powder by using an electric mixer.

Prepration of plant Extract: A portion of dried leaves (100 g) of *Aloe vera* was placed in a Soxhlet apparatus. Extraction was performed with 500 ml of methanol for 12h at 64 °C. The extract was filtered through a Whatmann filter paper. The resulting solution was stored it in refrigerator for further analysis and for the separation of pure mixture from solvent using Rota-evaporator for separation.

GC-MS analysis: GC-MS analysis was carried out on GC Clarus 500 Perkin Elmer system comprising an AOC-20i auto sampler and Gas Chromatograph interfaced to a Mass Spectrophotometer (GC-MS) to study the phytochemical components present in the extract.The identification of the compound was obtained by comparing the retention time with the original compound with spectral data obtained from the appropriate compound data library. The number of compounds is represented as a percentage of the relative area originating from the integrator (Kumaresan et al., 2015). The chemical structure profile screening was based on analysis of the mass spectrum fragmentation pattern compared with the mass spectrum in the National Institute of Standards and Technology (NIST).

Computational analysis: The Computational analysis was (ADME- Absorption, Distribution, Metabolism, and Excretion) through SwissADME. SwissADME compute physicochemical properties of bioactive compounds, as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry.

Results and Discussion:

GC-MS Analysis: The bioactive fraction upon GC-MS analysis revealed a chromatogram showing four major peaks with 8.14% Peak area in figure 1. *Aloe vera* leaves methanolic extract was found to possess 24 compounds (table 1). Most of which are bioactive compounds which may act as good antimicrobial, antioxidant, anti-inflammatory agents and used commercially in Agrochemicals , Herbicides, Insecticides, Other substances, Repellents, Adjuvants, Fungicides, Cosmetics, skin conditioning, softener and conditioner, preparation of

oleates and lotions, and as a pharmaceutical solvent. Biocompounds such as RT 27.09–3.29% PA; cis-11-Eicosenoic acid have hair conditioning properties (NCBI 2021, CID-5282768), i-Propyl 9-octadecenoate used for skin conditioning, softener and conditioner (NCBI 2021, CID-66981), Octadec-9-enoic acid - used commercially in the preparation of oleates and lotions, and as a pharmaceutical solvent (NCBI 2021, CID-965), RT 22.11–1.84% PA; 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- have Cosmetics, Antistatic; Cleansing; Emollient; Emulsifying; Hair conditioning; Skin conditioning; Surfactant (NCBI 2021, CID-5280934), and (E,Z,Z)-2,4,7-Tridecatrienal used as Flavouring Agents (NCBI 2021, CID-6421281).

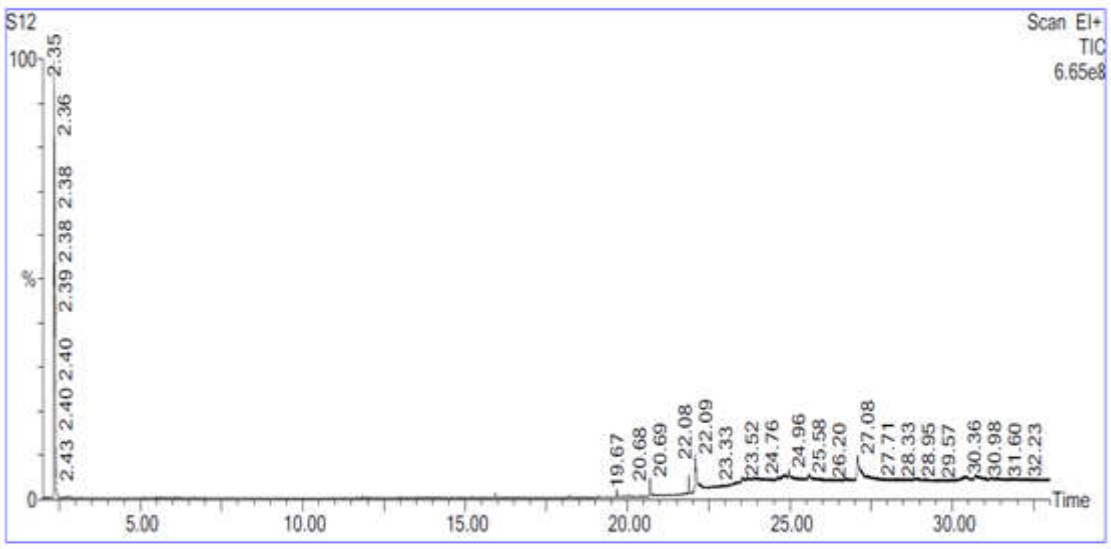

Figure 1. GC-MS chromatogram for leaf methanolic extract of *Aloe vera*

Table 1. GC-MS spectral analysis of leaf methanolic extract of *Aloe vera*

S. No.	RT	Peak%	Compounds Name	Formula
1	27.09	3.29	Cis-13-Eicosenoic acid	$C_{20}H_{38}O_2$
2			Cis-13-Octadecenoic acid	$C_{18}H_{34}O_2$
3			n-Propyl 11-octadecenoate	$C_{21}H_{40}O_2$
4			Cis-11-Eicosenoic acid	$C_{20}H_{38}O_2$
5			Trans-13-Octadecenoic acid	$C_{18}H_{34}O_2$
6			i-Propyl 9-octadecenoate	$C_{21}H_{40}O_2$
7			Cis-10-Nonadecenoic acid	$C_{19}H_{36}O_2$
8			Octadec-9-enoic acid	$C_{18}H_{34}O_2$
9	22.11	1.84	Z,Z,Z-4,6,9-Nonadecatriene	$C_{19}H_{34}$
10			9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	$C_{18}H_{30}O_2$
11			9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	$C_{21}H_{36}O_4$
12			5,8,11-Heptadecatrien-1-ol	$C_{17}H_{30}O$
13			Exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	$C_{10}H_{18}O$
14			Gamolenic Acid	$C_{18}H_{30}O_2$
15			6-Hexadecen-4-yne, (E)-	$C_{16}H_{28}$
16			(E,Z,Z)-2,4,7-Tridecatrienal	$C_{13}H_{20}O$
17	22.09	1.75	Oleic Acid	$C_{18}H_{34}O_2$
18			Cis-10-Heptadecenoic acid	$C_{17}H_{32}O_2$
19			Cis-9-Hexadecenoic acid	$C_{16}H_{30}O_2$
20	24.97	1.26	Dasycarpidan-1-methanol, acetate (ester)	$C_{20}H_{26}N_2O_2$
21			15-Hexenoic acid, 14-hydroxy-14-methyl-	$C_{17}H_{32}O_3$
22			Hexadecanedioic acid, dimethyl ester	$C_{18}H_{34}O_4$
23			Strychane, 1-acetyl-20à-hydroxy-16-methylene	$C_{21}H_{26}N_2O_2$
24			17-Pentatriacontene	$C_{35}H_{70}$

Computational analysis:

Physicochemical properties: The physicochemical properties of the phytoconstituents of *Aloe vera* presented in table 2. The molecular and physicochemical properties such as molecular weight, number of heavy atoms, number of aromatic heavy atoms, number of rotatable bonds, number of H-bond acceptors, number of H-bond donors, molar refractivity, and topological polar surface area (TPSA).Molecular polar surface area (PSA) i.e., surface belonging to polar atoms, is a descriptor that was shown to correlate well with passive molecular transport through membranes and, therefore, allows prediction of transport properties of drugs. The PSA is computed using a fragmental technque known as topological polar surface area (TPSA). The topological polar surface area considering sulfur and phosphorus as polar atoms (Ertl et al., 2000). General characteristics of the phytoconstituents of *Aloe vera* revealed all the compounds having molecular weight less than 500 Da, which is a prime property to be called as drug likeness of the small molecules.

Table 2. Physicochemical properties of the phytoconstituents of *Aloe vera*

S. No.	Compounds Name	MW	HA	AHA	RB	HBA	HBD	MR	TPSA
1	Cis-13-Eicosenoic acid	310.5	22	0	17	2	1	99.55	37.3
2	Cis-13-Octadecenoic acid	282.5	20	0	15	2	1	89.94	37.3
3	n-Propyl 11-octadecenoate	324.5	23	0	18	2	0	103.9	26.3
4	cis-11-Eicosenoic acid	310.5	22	0	17	2	1	99.55	37.3
5	Trans-13-Octadecenoic acid	282.5	20	0	15	2	1	89.94	37.3
6	i-Propyl 9-octadecenoate	324.5	23	0	17	2	0	103.9	26.3
7	Cis-10-Nonadecenoic acid	296.5	21	0	16	2	1	94.74	37.3
8	Octadec-9-enoic acid	282.5	20	0	15	2	1	89.94	37.3
9	Z,Z,Z-4,6,9-Nonadecatriene	262.5	19	0	13	0	0	92.03	0
10	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	278.4	20	0	13	2	1	88.99	37.3
11	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	352.5	25	0	17	4	2	105.3	66.76
12	5,8,11-Heptadecatrien-1-ol	250.4	18	0	12	1	1	83.57	20.23
13	Exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	154.3	11	0	0	1	1	46.9	20.23
14	Gamolenic Acid	278.4	20	0	13	2	1	88.99	37.3
15	6-Hexadecen-4-yne, (E)-	220.4	16	0	9	0	0	76.71	0
16	(E,Z,Z)-2,4,7-Tridecatrienal	192.3	14	0	8	1	0	63.38	17.07
17	Oleic Acid	282.5	20	0	15	2	1	89.94	37.3
18	Cis-10-Heptadecenoic acid	268.4	19	0	14	2	1	85.13	37.3
19	Cis-9-Hexadecenoic acid	254.4	18	0	13	2	1	80.32	37.3
20	Dasycarpidan-1-methanol, acetate (ester)	326.4	24	9	4	3	1	100.2	45.33
21	15-Hexenoic acid, 14-hydroxy-14-methyl-	284.4	20	0	14	3	2	86.33	57.53
22	Hexadecanedioic acid, dimethyl ester	314.5	22	0	17	4	0	91.21	52.6
23	Strychane, 1-acetyl-20à-hydroxy-16-methylene	338.4	25	6	2	3	1	105.4	43.78
24	17-Pentatriacontene	490.9	35	0	31	0	0	169.9	0

MW - molecular weight (g/mol); HA – number heavy atoms; AHA – number aromatic heavy atoms; RB – number rotatable bonds; HBA – number hydrogen bond acceptor; HBD – number hydrogen bound donor; MR - molar refractivity (m3/mol); TPSA - topology polar surface area (Å²)

Lipophilicity characteristics: The lipophilicity characteristics of the phytoconstituents of *Aloe vera* studies via SwissADME (table 3), which provides five freely available models to evaluate the lipophilicity character of a compound, namely XLOGP3, WLOGP, MLOGP, SILICOS-IT, and iLOGP(Cheng et al., 2007). XLOGP3, an atomistic approach with corrective factors and a knowledge-based library. WLOGP is a purely atomistic method that is applied to a fragmental system (Wildman et al., 1999). MLOGP an archetype of the topological method is based on a linear relationship with 13 molecular descriptors

implemented (Moriguchi et al., 1992 and Moriguchi et al., 1994). SILICOS-IT is a hybrid method that relies on 27 fragments and seven topological descriptors. iLOGP is a physics-based method that uses the generalized-born and solvent accessible surface area (GB/SA) model to calculate solvation free energies in n-octanol and water. The arithmetic mean of the values predicted by the five proposed methods is the consensus log P o/w. (Diana et al., 2017).

Table 3. Lipophilicity characteristics of the phytoconstituents of *Aloe vera*

S. No.	Compounds Name	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
1	Cis-13-Eicosenoic acid	4.26	8.72	6.89	5.03	6.83	6.34
2	Cis-13-Octadecenoic acid	3.93	7.64	6.11	4.57	5.95	5.64
3	n-Propyl 11-octadecenoate	5.32	8.43	6.98	5.25	7.42	6.68
4	Cis-11-Eicosenoic acid	4.7	8.72	6.89	5.03	6.83	6.43
5	Trans-13-Octadecenoic acid	3.93	7.64	6.11	4.57	5.95	5.64
6	i-Propyl 9-octadecenoate	5.45	8.25	6.98	5.25	7.25	6.64
7	Cis-10-Nonadecenoic acid	4.45	8.18	6.5	4.8	6.39	6.06
8	Octadec-9-enoic acid	4.27	7.64	6.11	4.57	5.95	5.71
9	Z,Z,Z-4,6,9-Nonadecatriene	5.24	8.45	6.99	5.89	7	6.71
10	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	3.36	6.46	5.66	4.38	5.59	5.09
11	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	4.81	5.11	4.47	3.33	5.76	4.7
12	5,8,11-Heptadecatrien-1-ol	3.96	5.53	5.18	4.35	5.56	4.91
13	Exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	2.42	2.3	2.19	2.45	2.27	2.33
14	Gamolenic Acid	3.98	6.58	5.66	4.38	5.59	5.24
15	6-Hexadecen-4-yne, (E)-	4.54	7.26	5.57	6.18	5.71	5.85
16	(E,Z,Z)-2,4,7-Tridecatrienal	3.24	4.19	3.82	3.25	4.1	3.72
17	Oleic Acid	4.27	7.64	6.11	4.57	5.95	5.71
18	Cis-10-Heptadecenoic acid	3.9	7.1	5.72	4.33	5.51	5.31
19	Cis-9-Hexadecenoic acid	3.53	6.58	5.33	4.09	5.07	4.92
20	Dasycarpidan-1-methanol, acetate (ester)	3.12	3.21	3.14	2.82	3.51	3.16
21	15-Hexenoic acid, 14-hydroxy-14-methyl-	3.59	5.31	4.69	3.45	4.79	4.37
22	Hexadecanedioic acid, dimethyl ester	4.29	6.25	4.79	3.65	5.46	4.89
23	Strychane, 1-acetyl-20à-hydroxy-16-methylene	3.17	1.71	1.7	2.72	2.48	2.36
24	17-Pentatriacontene	9.06	18.24	13.68	10.23	14.45	13.13

Water solubility: The water solubility characteristics of the phytoconstituents of *Aloe vera* were showed in table 4. Most of the compounds were moderately poorly soluble, with 70.83%, and the remaining was pooraly soluble. SwissADME to predict water solubility, one of which was adopted from Ali et al. 2012, i.e. Solubility class: Log S Scale: Insoluble < -10 poorly <-6, moderately, < -4 soluble, < -2 very, < 0 highly. The solubility of a compound is strongly influenced by the solvent used and the ambient temperature and pressure. The saturation concentration is defined as the point at which adding more solute does not increase its concentration in the solution (Lachman et al., 1986 and Savjani et al., 2012).

Table 4. Water solubility characteristics of the phytoconstituents of *Aloe vera*

S. No.	Compounds Name	ESOL Log S	Solubility (mg/ml)	Solubility (mol/l)	ESOL Class
1	Cis-13-Eicosenoic acid	-6.14	2.27E-04	7.30E-07	Poorly soluble
2	Cis-13-Octadecenoic acid	-5.41	1.09E-03	3.85E-06	Moderately soluble
3	n-Propyl 11-octadecenoate	-5.98	3.44E-04	1.06E-06	Moderately soluble
4	Cis-11-Eicosenoic acid	-6.14	2.27E-04	7.30E-07	Poorly soluble
5	Trans-13-Octadecenoic acid	-5.41	1.09E-03	3.85E-06	Moderately soluble
6	i-Propyl 9-octadecenoate	-5.93	3.83E-04	1.18E-06	Moderately soluble
7	Cis-10-Nonadecenoic acid	-5.78	4.97E-04	1.68E-06	Moderately soluble
8	Octadec-9-enoic acid	-5.41	1.09E-03	3.85E-06	Moderately soluble
9	Z,Z,Z-4,6,9-Nonadecatriene	-5.93	3.06E-04	1.17E-06	Moderately soluble
10	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	-4.78	4.64E-03	1.67E-05	Moderately soluble
11	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	-4.12	2.66E-02	7.54E-05	Moderately soluble
12	5,8,11-Heptadecatrien-1-ol	-4.08	2.06E-02	8.23E-05	Moderately soluble
13	Exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	-2.25	8.77E-01	5.68E-03	Soluble
14	Gamolenic Acid	-4.85	3.90E-03	1.40E-05	Moderately soluble
15	6-Hexadecen-4-yne, (E)-	-5.19	1.44E-03	6.51E-06	Moderately soluble
16	(E,Z,Z)-2,4,7-Tridecatrienal	-3.14	1.38E-01	7.18E-04	Soluble
17	Oleic Acid	-5.41	1.09E-03	3.85E-06	Moderately soluble
18	Cis-10-Heptadecenoic acid	-5.05	2.37E-03	8.85E-06	Moderately soluble
19	Cis-9-Hexadecenoic acid	-4.7	5.02E-03	1.97E-05	Moderately soluble
20	Dasycarpidan-1-methanol, acetate (ester)	-3.9	4.11E-02	1.26E-04	Soluble
21	15-Hexenoic acid, 14-hydroxy-14-methyl-	-4.02	2.69E-02	9.45E-05	Moderately soluble
22	Hexadecanedioic acid, dimethyl ester	-4.61	7.81E-03	2.48E-05	Moderately soluble
23	Strychane, 1-acetyl-20à-hydroxy-16-methylene	-3.06	2.94E-01	8.68E-04	Soluble
24	17-Pentatriacontene	-12.33	2.30E-10	4.69E-13	Insoluble

Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Pharmacokinetic and Drug-likeness: The pharmacokinetic, bioavailability and drug-likeness of the phytoconstituents of *Aloe vera* were showed in table 5. The 17 compounds of the *Aloe vera* had high values for GI absorption. This is directly proportional to the permeant BBB, where 12 compounds of the *Aloe vera*. This means that most of the compounds in the *Aloe vera* have very good absorption, which is helpful for drug discovery and development (Di et al., 2012 and Brito et al., 2015). A set of rules and guidelines for determining the structural properties is preferred for initial screening of drug-likeness of compound. Some such Drug-likeness rules are Lipinski's rule, MDDR-like rule, Veber's rule, Ghose filter, Egan rule, Muegge rule, Lipophilicity (iLOGP, WLOGP, XLOGP3, MLOGP, Log Po/w), water solubility (Log S (SILICOSIT)), etc. (Hammed et al., 2021). According to Lipinski's rule (Pfizer's rule or simply the rule of five (RO5)), any chemical compound can be used as an orally active drug if and only if it will not violate that set of rules (Lipinski et al., 2004). The compounds which simply obey RO5 will have more chances for being orally used for human consumption and reach the markets. The mentioned rules preliminarily justify whether the compound is ideal for drug synthesis or not. Some of the rules like molecular weight < 500, hydrogen-bond donors < 5, hydrogen-bond acceptor < 10, MLOGP (noctanol–water partition coefficient) < 4.15, molar refractivity should be between 40 and 130, log P ranging between − 0.4 to + 5.6, solubility (log S) > − 5.7, also help us to preliminary test the suitable

drug molecule. All these preclinical tests help in differentiating between druglike and non-drug-like structure (Giacomini et al., 2010).

Table 5. Pharmacokinetics, Bioavailability and Druglikeness of the phytoconstituents of *Aloe vera.*

S. No.	Compounds Name	GI absorption	BBB permeant	Bioavailability Score	Lipinski #violations
1	Cis-13-Eicosenoic acid	Low	No	0.85	Yes; 1 violation: MLOGP>4.15
2	Cis-13-Octadecenoic acid	High	No	0.85	Yes; 1 violation: MLOGP>4.15
3	n-Propyl 11-octadecenoate	Low	No	0.55	Yes; 1 violation: MLOGP>4.15
4	Cis-11-Eicosenoic acid	Low	No	0.85	Yes; 1 violation: MLOGP>4.15
5	Trans-13-Octadecenoic acid	High	No	0.85	Yes; 1 violation: MLOGP>4.15
6	i-Propyl 9-octadecenoate	Low	No	0.55	Yes; 1 violation: MLOGP>4.15
7	Cis-10-Nonadecenoic acid	High	No	0.85	Yes; 1 violation: MLOGP>4.15
8	Octadec-9-enoic acid	High	No	0.85	Yes; 1 violation: MLOGP>4.15
9	Z,Z,Z-4,6,9-Nonadecatriene	Low	No	0.55	Yes; 1 violation: MLOGP>4.15
10	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	High	Yes	0.85	Yes; 1 violation: MLOGP>4.15
11	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	High	Yes	0.55	Yes; 0 violation
12	5,8,11-Heptadecatrien-1-ol	High	Yes	0.55	Yes; 1 violation: MLOGP>4.15
13	Exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	High	Yes	0.55	Yes; 1 violation: MLOGP>4.15
14	Gamolenic Acid	High	Yes	0.85	Yes; 1 violation: MLOGP>4.15
15	6-Hexadecen-4-yne, (E)-	Low	No	0.55	Yes; 1 violation: MLOGP>4.15
16	(E,Z,Z)-2,4,7-Tridecatrienal	High	Yes	0.55	Yes; 0 violation
17	Oleic Acid	High	No	0.85	Yes; 1 violation: MLOGP>4.15
18	Cis-10-Heptadecenoic acid	High	Yes	0.85	Yes; 1 violation: MLOGP>4.15
19	Cis-9-Hexadecenoic acid	High	Yes	0.85	Yes; 0 violation
20	Dasycarpidan-1-methanol, acetate (ester)	High	Yes	0.55	Yes; 0 violation
21	15-Hexenoic acid, 14-hydroxy-14-methyl-	High	Yes	0.85	Yes; 0 violation
22	Hexadecanedioic acid, dimethyl ester	High	Yes	0.55	Yes; 0 violation
23	Strychane, 1-acetyl-20à-hydroxy-16-methylene	High	Yes	0.55	Yes; 0 violation
24	17-Pentatriacontene	Low	No	0.55	Yes; 1 violation: MLOGP>4.15

GI absorption - Gastrointestinal absorption; BBB permeant – blood brain barrier permeation

Conclusion: Traditional plants have been considered as the rich source of ailments for various diseases. For this study, we have considered some phytochemicals extracted from a specific plant *Aloe vera*, which is aproven medicinal plant since ancient times. The main aim of these studies was to determine bioactive compounds in *Aloe vera* leaf extracts using gas chromatographic technique and to investigate their drug-likeness potential using ADME studies. *Aloe vera* contains some very important bio-molecules which have significant medicinal properties. The potential biological activity of the phytoconstituents of *Aloe vera* was antimicrobial, antioxidant, anti-inflammatory, antibacterial etc. The computational analysis on the pharmacokinetics and drug likeness parameters of *Aloe vera* has confirmed the safety of the compound for oral administration. All compounds in the extract of *Aloe vera* met the druglikeness according to Lipisnki's rules. The ADME analysis results indicated that *Aloe vera* could be developed as traditional medicine.

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