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GC-MS ANALYSIS AND *IN-SILICO* ADMET ANALYSIS OF THE AQUEOUS METHANOL LEAF EXTRACT OF *ISODON TERNIFOLIUS* (D. DON) KUDO

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Keywords:

Isodon ternifolius (D. Don) Kudo, Phytocompound, Gas chromatography-mass spectrometry (GC-MS), Drug-likeness, ADMET property

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ABSTRACT: Medicinal plants contain phytocompounds which are of medicinal value. Scientific evaluation of these compounds that may serve as potential drugs is important in validating the medicinal plants. The leaf extract of the medicinal plant, *Isodon ternifolius* (D. Don) Kudo was prepared by the maceration method using 80% aqueous methanol as the extraction solvent. The resulting extract was subjected to gas chromatography-mass spectrometry (GC-MS) analysis. The mass spectra of all the major phytocompounds obtained were compared with the standard mass spectra found in the NIST and Wiley libraries, and the phytocompounds were identified. All these identified phytocompounds were characterized biocomputationally with respect to their pharmacologically relevant physicochemical properties, *viz.* molecular weight, number of heavy atoms, number of heavy aromatic atoms, fraction Csp^3, rotatable bond, hydrogen bond acceptor, hydrogen bond donor, molar refractivity and topological polar surface area. Further, drug-likeness, bioavailability, and ADMET properties of each of the phytocompounds were also characterised. The results obtained may be useful in further *in-vitro* and *in-vivo* experimentation that might lead to the discovery of drugs from the concerned traditional medicinal plant.

INTRODUCTION: Plants having applications in the traditional health care system are important from a human health point of view [1]. They are the sources of various active phytocompounds having therapeutic properties [2]. These phytocompounds may also be the precursors for the semi-synthesis of drugs currently employed in modern therapy [3].

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This is mainly due to the general perception that traditional medicine has no scientific basis [4]. Besides, detailed information regarding the safety of most herbal treatments vis-a-vis synthetic drug treatments is lacking [5].

Therefore, isolation and scientific evaluation of the phytocompounds from the traditional medicinal plants that may serve as potential drugs are important in validating traditional herbal medicine [6]. At this juncture, it must be mentioned that the appropriate plant parts and the availability of the required quantity of the concerned traditional medicinal plant are important determinants for herbal medicine. The roots, leaves, rhizomes, barks, stems, flowers, fruits, grains, or seeds of

medicinal plants are the sources of herbal medicine, and they are used in the management or therapy of various diseases [7]. The phytocompounds obtained from the medicinal plants are either primary or secondary metabolites or their derivatives. The drugs derived from plant secondary metabolites contribute more than 25% of the currently available drugs [8]. Systematic profiling of phytocompounds derived from traditional medicinal plants is, therefore, necessary for discovering new drugs that may help manage or cure various diseases. In the present study, GC-MS analysis of the 80% aqueous methanol leaf extract from a traditional medicinal plant *Isodon ternifolius* (D. Don) Kudo followed by *in-silico* ADMET analysis of all the identified major phytocompounds was carried out.

MATERIALS AND METHODS:

Plant Material: In the present investigation, GC-MS and ADMET analyses of the phytocompounds present in the extract from the leaf of the traditional medicinal plant, *Isodon ternifolius (D.Don) Kudo* were carried out. The plant, shown in **Fig. 1** along with its systematic position, is a shrub mainly found in tropical and subtropical countries [9].

FIG.1: *ISODON TERNIFOLIUS* (D. DON) KUDO

It is locally known as "Khoiju" in Manipuri and the leaves required for the investigation were collected from the plant grown in the *"Chiru Hill"* of Manipur, India, and authenticated by Dr. Biseshwori Thongam, Scientist-E, the Institute of Bioresources and Sustainable Development, IBSD, Department of Biotechnology, Government of India, Takyelpat, Imphal, Manipur, India. A voucher specimen bearing No. IBSD/M-281 has been stored at the institute.

The systemic position of the plant:

Kingdom: Plantae

Phylum: Tracheophyta

Class: Magnoliopsida

Order: Lamiales

Family: Lamiaceae

Genus: Isodon

Species: *Isodon ternifolius* (D.Don) Kudo

Preparation of the Leaf Extract: 24 Kg of the leaves of the plant *Isodon ternifolius (D.Don) Kudo* at the flowering stage was collected and thoroughly washed with tap water and then shade dried at room temperature for two weeks with intermittent shuffling [10]. 5 Kg of the resulting dried leaves was pulverized into a coarse powder using a kitchen blender at low speed, soaked with 36 L of 80% aqueous methanol for 3 days in a sealed round-bottom flask, and then the resulting suspension was strained through a plastic strainer. The marc obtained was collected for further extraction, and the resulting filtrate was further filtered through ordinary filter paper and then concentrated using a rotary vacuum evaporator at 40°C to collect the viscous extract. The above extraction procedure was repeated, taking the resulting marc and distillate as the extraction solvent. This repeated procedure was carried out until the extraction solvent became colourless. The concentrated viscous leaf extracts were pooled together to obtain a greenish-brown semi-solid mass weighing 583g.

GC-MS Analysis:

Sample Preparation: 80 mg of the leaf extract was dissolved in 1mL of HPLC grade methanol and filtered through a 0.2 µm membrane (PVDF) filter before it was subjected to GC-MS analysis at the Advanced Instrumentation Research Facility at Jawaharlal Nehru University, New Delhi.

GC-MS Running Conditions: 2µL of the sterile leaf extract was taken as the sample for the GC-MS analysis in a Shimadzu QP-2010 Plus instrument with a GC Capillary Column Rtx-5MS of 30 m length, 0.25 mm internal diameter, and 0.25 m film thickness. The injector port temperature, the

column oven temperature, and pressure were maintained at 260°C, 50°C, and 69.0kpa, respectively. The total and column flow rates were kept constant at 16.3 and 1.21 mL/min, respectively. Helium gas was employed as the carrier gas. The total runtime was 60.32 min. The sample was scanned fully at 40 to 650 m/z, and then a GC-MS chromatogram was obtained.

Identification of Phytocompounds: The mass spectra obtained by GC-MS analysis were compared with the spectral data found in Wiley and NIST libraries using a library search program, according to Bano and Deora [11]. The relative amount of each phytocompounds was determined by comparing the average peak area with the total area according to Shettima*et al* (2013) [12].

ADMET Profiling of the Phytocompounds: The canonical SMILES strings of all the compounds except 8-acetyl-7A-[(acetyloxy) methyl]-5B-hydroxy-5A-methyl-3-oxo-1a, 3, 4, 5, 5a, 5b, 6, 7, 9, 10, 10a, 10b, 10c-tetradeca -hydro-7ah –cyclopental [1,2] phenanthro [9,10-b]oxiren-6-yl acetate were obtained with the help of the PubChem server.

As the structure of 8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy - 5A - methyl – 3 -oxo-1a, 3, 4, 5, 5a, 5b, 6, 7, 9, 10, 10a, 10b, 10c-tetradeca -hydro-7ah –cyclopental [1,2] phenanthro [9,10-b] oxiren-6-yl acetate was not found in PubChem server, and therefore, the structure of the compound was drawn using ChemSketch, a software for drawing chemical structure.

The canonical SMILES string of the compound was then obtained. ADMET profiling of all the phytocompounds was conducted using SwissADME and pkCSM server tools.

RESULTS AND DISCUSSION: The phytocompounds present in the leaf extract from the plant *Isodon ternifolius* (D. Don) GC-MS detected Kudo, and their ADMET properties were analysed by *in-silico* method.

The corresponding total ion chromatogram is shown in **Fig. 2**. One hundred and four peaks characterized the chromatogram. However, these peaks were found to represent only 82 different compounds after analyzing the corresponding GC-MS data.

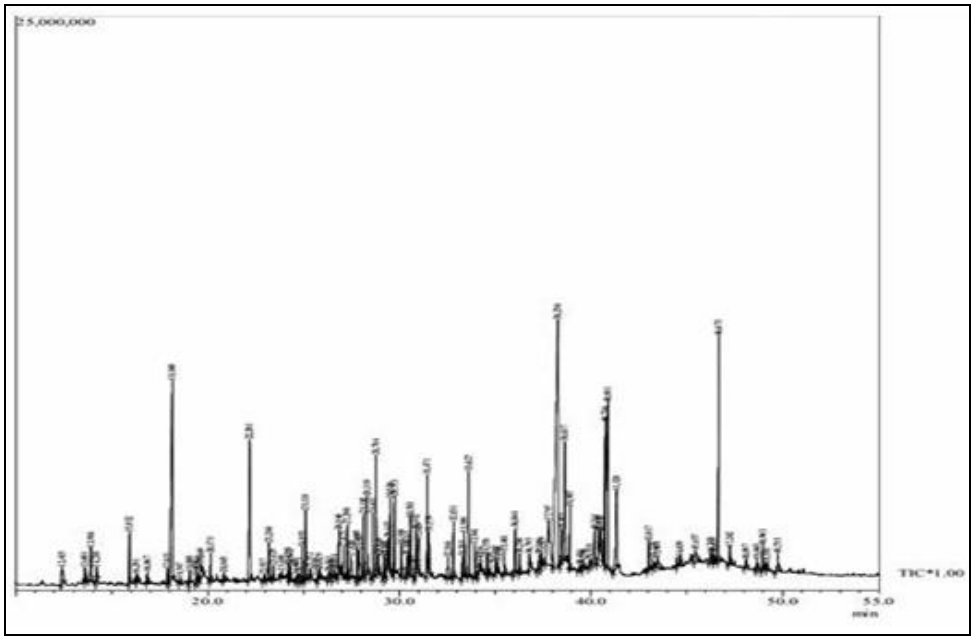

FIG. 2: THE TOTAL ION CHROMATOGRAM OF THE AQUEOUS METHANOL LEAF EXTRACT FROM *ISODON TERNIFOLIUS* (D.DON) KUDO

The concentration of each of the phytocompounds in the extract was estimated in terms of area percentage. The area percent and the retention time (RT) of all the phytocompounds detected by GC-MS are given in **Table 1**. Thus, the current investigation revealed the major phytocompounds present in the leaf extract of the medicinal plant, *Isodon ternifolius* (D. Don) Kudo.

TABLE 1: THE PHYTOCOMPOUNDS PRESENT IN AQUEOUS METHANOL LEAF EXTRACT FROM THE MEDICINAL PLANT *ISODON TERNIFOLIUS* (D. DON) KUDO IDENTIFIED BY GC-MS ANALYSIS

Peak	R. Time (min)	Area%	Name
1	12.415	0.65	2-propenal,3–phenyl-
2	13.601	0.37	2,3-dihydro-benzofuran
3	13.916	1.01	3-hexene-2,5-dione
4	14.210	0.29	3-hexene-2,5-dione
5	15.932	1.04	2-methoxy-4-vinylphenol
6	16.219	0.23	1-penten-3-one,1-phenyl-
7	16.867	0.34	Biphenylene,1,2,3,6,7,8,8a,8b-octahydro-,trans-
8	17.915	0.29	1H-Indene,1-ethylideneoctahydro-,trans-
9	18.160	7.03	1,4-Diacetoxy-1,3-butadiene
10	18.547	0.07	2,6-heptanedione,3-acetyl-
11	19.068	0.19	1,3-decadiene-7,9-dione
12	19.409	0.08	11-oxatetracyclo[5.3.2.0(2,7).0(2,8)]dodecan-9-one
13	19.490	0.21	2-(3,3-dimethyl-1-butynyl)-1,1,3-trimethylcyclopropane
14	19.669	0.67	2,6-cresotaldehyde
15	20.173	0.69	2-tert-butyl-5-methyl-1,4-benzoquinone
16	20.845	0.17	4-penten-2-one,3-cyclohexyl-
17	22.201	3.42	Aceticacid,(1,2-dimethyl-1-propenyl)ester
18	22.937	0.14	1-hexen-5-on,3-methyl-4-henyl-(Diastereomeres2)
19	23.204	0.70	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl
20	23.429	0.26	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl
21	23.848	0.10	6-[1-hydroxymethyl)Vinyl]-4,8A-dimethyl-
22	24.210	0.24	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl
23	24.312	0.24	3-methyl-3-phenyl-2-oxiranecarbonitrile
24	24.615	0.10	2,5-monoformal-l-rhamnitoltriacetate
25	24.773	0.25	3-buten-2-one,4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-
26	24.955	0.63	3-octen-2-one,8-phenyl-
27	25.118	1.34	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl
28	25.352	0.16	3-octen-2-one,8-phenyl-
29	25.757	0.07	Adamantane-1-carboxylicacid,(4-acetylaminofurazan-3-yl)amide
30	25.829	0.18	3-acetylbicyclo[3.3.1]non-6-ene
31	26.311	0.19	4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol
32	26.490	0.08	3-phenylpropionicacid,2-tetrahydrofurylmethylester
33	26.634	0.12	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one
34	26.846	0.72	2,4-oxazolidinedione,5-ethyl-3,5-dimethyl-
35	27.075	0.58	2-hexanol,3,3,5-trimethyl-2-(3-methylphenyl)-
36	27.290	0.95	Adamantane-1-carboxylic acid
37	27.489	0.66	2,6,8-trimethylbicyclo[4.2.0]oct-2-ene-11,8-diol
38	27.805	0.57	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl
39	27.907	0.81	3-pentanone,2-methyl-4-phenyl-
40	28.140	1.33	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one
41	28.319	1.69	Neophytadiene
42	28.632	1.21	Hotrienyl acetate
43	28.784	2.65	Hotrienyl acetate
44	28.939	0.42	Hotrienyl acetate
45	29.192	0.56	2-hexadecen-1-ol, 3, 7, 11, 15-tetramethyl-[R-[R
46	29.363	0.18	5-methyl-2(2-oxo-4-heptyl)furan
47	29.437	0.38	2, 2, 9, 9-tetramethyl-5-decene-3, 7-diyne
48	29.753	1.49	9,12,15-Octadecatrienoic acid, 2,3-bis(acetyloxy)propyl ester, (Z,Z,Z)-
49	29.753	1.48	2,5-heptanedione,3,3,6-trimethyl-
50	30.106	0.42	Hexadecanoic, methylester
51	30.378	0.35	Propanoic acid, 2-methyl-3-Phenyl-2-propyl ester
52	30.517	0.26	1,3-pentanedione,2,4-dimethyl-1-phenyl-
53	30.583	0.71	Propanoic acid, 2-methyl-, 3-phenyl-2-propyl ester
54	30.797	0.05	Propanoic acid, 2-methyl-, 3-phenyl-2-propyl ester
55	30.882	0.60	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-tetradeca -hydro-cyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate

56	31.028	1.10	Hexadecanoic acid
57	31.471	1.74	Propanoic acid,2-methyl-,3-phenyl-2-propenyl ester
58	31.559	0.61	Menthylacetate
59	32.546	0.67	2-pentanone,5-(2-methylenecyclohexyl)-,stereoisomer
60	32.831	1.06	2,5-heptanedione,3,3,6-trimethyl-
61	33.285	0.36	9, 12-octadecadienoic acid (Z, Z)-methyl ester
62	33.399	0.95	9, 12, 15-octadecatrienoic acid, methyl ester (Z, Z, Z)
63	33.627	2.06	2-hexadecen-1-ol,3,7,11,15-tetramethyl-[R-[R
64	33.941	0.66	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-tetradeca -hydro-7ahcyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate
65	34.130	0.10	2-undecen-4-ol
66	34.234	0.29	8-tetradecyn-1-ol
67	34.570	0.34	Cyclohexanol,1-methyl-,acetate
68	34.698	0.17	Octadecanoic acid
69	35.032	0.28	1, 5-dodecadiene
70	35.161	0.23	Estran-3-one, 17-(acetyloxy)-2-methyl, (2alpha, 5alpha, 17beta)
71	35.461	0.56	Phytol, acetate
72	36.044	1.18	1, 1-diacetoxy-9, 9-diformylnona-2,4,6,8-tetraene
73	36.266	0.38	Z-(13, 14-epoxy) tetradec-11-en-1-ol acetate
74	36.795	0.20	Methyl (9Z)-12-hydroxy-9-octadecenoate
75	37.304	0.48	1-(1H-imidazol-2-yl)ethenone
76	37.424	0.29	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester
77	37.797	3.05	2-hexenoicacid,3,4,4-trimethyl-5-oxo-,(E)-
78	38.256	13.13	3,5-heptanedione,2,2,6,6-tetramethyl
79	38.485	0.89	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester
80	38.637	3.34	3,5-heptanedione,2,2,6,6-tetramethyl
81	38.907	1.29	Estran-3-one,17-(acetyloxy)-2-methyl,(2alpha,5alpha,17beta)
82	39.431	0.14	Nonanoic acid
83	39.596	0.15	3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol
84	39.938	0.20	4, 6-nonanedione,5-(3-butanon-1-yl)-2,8-dimethyl-
85	40.211	1.37	Acetic acid, 2-(2-acetyl-3-oxoisoxazolidin-5-yl)-1-methylethyl ester
86	40.420	0.65	3,5-dimethyl-cyclohexanol
87	40.533	0.63	5,7-dodecadiene-4,9-dione,6,7-dihydroxy-2,11-dimethyl-
88	40.736	3.81	1,2-benzenedicarboxylic acid
89	40.881	6.12	3,5-heptanedione,2,2,6,6-tetramethyl
90	41.328	2.20	3,5-heptanedione,2,2,6,6-tetramethyl
91	43.017	0.65	Hexanal,4,4-dimethyl-
92	43.226	0.17	5,7-dodecadiene-4,9-dione,6,7-dihydroxy-2,11-dimethyl-
93	43.468	0.34	2-monolinolenin
94	44.639	0.51	1-(2-hydroxy-7,9a,11b-trimethylhexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-9-yl)ethanone
95	45.457	0.52	1-(1-heptadecynyl)cyclopentanol
96	46.242	0.25	3.beta.-acetoxy-17.alpha.-methyl-d-homoandrostane-17a-one
97	46.417	0.17	2,4,7,14-tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol
98	46.673	4.87	4,4-dimethyl-3,7-dioxoandrost-5-en-17-yl acetate
99	47.242	0.43	Ergost-7,22-dien-9,11-epoxy-3-ol,acetate(ester)
100	48.097	0.21	4-(2,2,6-trimethylbicyclo[4.1.0]Hept-1-yl)-2-butanone
101	48.663	0.27	5-cholestene-3-ol,24-methyl-
102	48.963	0.56	Stigmasta-5,22-dien-3-ol
103	49.193	0.14	1H-3A,7-methanozulen-6-ol,octahydro3,6,8,8-tetramethyl
104	49.755	0.56	gamma.-sitosterol
Total area %	100		

The chemical profiling of the plant reported herewith is a first of its kind as far as our knowledge is concerned based on the latest literature survey. The canonical SMILES and molecular formulae of all the 82 phytocompounds, including the 20 major compounds mentioned above are given in **Table 2.**

TABLE 2: THE MOLECULAR FORMULAE AND CANONICAL SMILES OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT ISODON TERNIFOLIUS (D. DON) KUDO IDENTIFIED BY GC-MS ANALYSIS

Compd. no.	Compounds	Molecular formula	Canonical SMILES
1	3–phenyl-2-propenal,	C_9H_8O	C1=CC=C(C=C1)C=CC=O
2	2,3-dihydro-benzofuran	C_8H_8O	C1COC2=CC=CC=C21
3	3-hexene-2,5-dione	$C_6H_8O_2$	CC(=O)C=CC(=O)C
4	2-methoxy-4-vinylphenol	$C_9H_{10}O_2$	COC1=C(C=CC(=C1)C=C)O
5	1-penten-3-one,1-phenyl-	$C_{11}H_{12}O$	CCC(=O)C=CC1=CC=CC=C1
6	Biphenylene,1,2,3,6,7,8,8a,8b-octahydro-, trans-	$C_{12}H_{16}$	C1CC=C2C(C1)C3C2=CCCC3
7	1H-Indene,1-ethylideneoctahydro-,trans-	$C_{11}H_{18}$	CC=C1CCC2C1CCCC2
8	1,4-Diacetoxy-1,3-butadiene	$C_8H_{10}O_4$	CC (=O) CCC (C(=O)C) C(=O) C
9	2,6-Heptanedione,3-acetyl-	$C_9H_{14}O_3$	CC(=O)CC(=O)CCC=CC=C
10	1,3-Decadiene-7,9-dione	$C_{10}H_{14}O_2$	C1CCC23C4CC(=O)C2C3(C1)CO4
11	11-Oxatetracyclo[5.3.2.0(2,7).0(2,8)]dodecan-9-one	$C_{11}H_{14}O_2$	CC1C(C1(C)C)C#CC(C)(C)C
12	2-(3,3-dimethyl-1-butynyl)-1,1,3-trimethylcyclopropane	$C_{12}H_{20}$	CC1=C(C(=CC=C1)O)C=O
13	2,6-cresotaldehyde	$C_8H_8O_2$	CC1=CC(=O)C(=CC1=O)C(C)(C)C
14	2-tert-butyl-5-methyl-1,4-benzoquinone	$C_{11}H_{14}O_2$	CC(=O)C(C=C)C1CCCCC1
15	4-penten-2-one,3-cyclohexyl-	$C_{11}H_{18}O$	CC(=C(C)OC(=O)C)C
16	Aceticacid,(1,2-dimethyl-1-propenyl)ester	$C_7H_{12}O_2$	CCC(C1=CC=CC=C1)(C(C)C=C)O
17	1-hexen-5-on,3-methyl-4-henyl-	$C_{13}H_{18}O$	CC(=O)OCC(CC1=CC=CC=C1)(COC(=O)C)[N+](=O)[O-]
18	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl	$C_{14}H_{17}NO_6$	CC1=C2CC(CCC2(CC(C1=O)OC(=O)C)C)C(=C)CO
19	6-[1-hydroxymethyl)Vinyl]-4,8A-dimethyl-	$C_{17}H_{24}O_4$	CC1(C(O1)C#N)C2=CC=CC=C2
20	3-methyl-3-phenyl-2-oxiranecarbonitrile	$C_{10}H_9NO$	CC1C(C(C(OC(=O)O1)COC(=O)C)OC(=O)C)OC(=O)C
21	2,5-monoformal-l-rhamnitoltriacetate	$C_{13}H_{18}O_9$	CC(=O)C=CC1C(CCCC1(C)O)(C)C
22	3-buten-2-one,4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-	$C_{13}H_{22}O_2$	CC(=O)C=CCCCCC1=CC=CC=C1
23	3-octen-2-one,8-phenyl-	$C_{14}H_{18}O$	CC(=O)NC1=NON=C1NC(=O)C23CC4CC(C2)CC(C4)C3
24	Adamantane-1-carboxylicacid,(4-acetylaminofurazan-3-yl)amide	$C_{15}H_{20}N_4O_3$	CC(=O)C1CC2CC=CC(C2)C1
25	3-acetylbicyclo[3.3.1]non-6-ene	$C_{11}H_{16}O$	COC1=C(C=CC(=C1)C=CCO)O
26	4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol	$C_{10}H_{12}O_3$	C1CC(OC1)COC(=O)CCC2=CC=CC=C2
27	3-phenylpropionicacid,2-tetrahydrofurylmethylester	$C_{14}H_{18}O_3$	CC(=O)C1=CCC2C1(CCC3(C2CC=C4C3(CCC(C4)O)C)O)C
28	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one	$C_{21}H_{30}O_3$	CCC1(C(=O)N(C(=O)O1)C)C
29	2,4-oxazolidinedione,5-ethyl-3,5-dimethyl-	$C_7H_{11}NO_3$	CC1=CC(=CC=C1)C(C)(C(C)(C)CC(C)C)O
30	2-hexanol,3,3,5-trimethyl-2-(3-methylphenyl)-	$C_{16}H_{26}O$	CC1=CCCC2(C1(C(C2)(C)O)O)C
31	2,6,8-trimethylbicyclo[4.2.0]oct-2-ene-11,8-diol	$C_{11}H_{18}O_2$	CC(C)C(=O)C(C)C1=CC=CC=C1
32	3-pentanone,2-methyl-4-phenyl-	$C_{12}H_{16}O$	CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C
33	Neophytadiene	$C_{20}H_{38}$	O=C(C)OC(C)(C/C=C/C(C)=C)C=C
34	Hotrienyl acetate	$C_{12}H_{18}O_2$	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C
35	2-hexadecen-1-ol, 3, 7, 11, 15-tetramethyl-[R-[R	$C_{20}H_{40}O$	CCCC(CC(=O)C)C1=CC=C(O1)C

36	5-methyl-2(2-oxo-4-heptyl)furan	$C_{12}H_{18}O_2$	CC(C)(C)C#CC=CC#CC(C)(C)C
37	2, 2, 9, 9-tetramethyl-5-decene-3, 7-diyne	$C_{14}H_{20}$	CCC=CCC=CCC=CCCCCCCCC(=O)OCC(COC(=O)C)OC(=O)C
38	9,12,15-Octadecatrienoic acid, 2,3-bis(acetyloxy)propyl ester, (Z,Z,Z)-	$C_{25}H_{40}O_6$	CC(C)C(=O)CC(C)(C)C(=O)C
39	2,5-heptanedione,3,3,6-trimethyl-	$C_{10}H_{18}O_2$	CCCCCCCCCCCCCCCC(=O)OC
40	Hexadecanoic, methylester	$C_{17}H_{34}O_2$	CC(C)C(=O)OCC=CC1=CC=CC=C1
41	Propanoic acid, 2-methyl-3-Phenyl-2-propenyl ester	$C_{13}H_{16}O_2$	CC(C)C(=O)C(C)C(=O)C1=CC=CC=C1
42	1,3-pentanedione,2,4-dimethyl-1-phenyl-	$C_{13}H_{16}O_2$	CC(=O)C1CCC2C3C(C(OC(C)=O)C(O)C12COC(C) = O) C1CCC (=O) CC1C1OC13
43	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-1a,3,4,5,5a,5b,6,7,9,10,10a,10b,10c-tetradeca -hydro-7ah -cyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate	C24H32O8	CCCCCCCCCCCCCCCC(=O)O
44	Hexadecanoic acid	$C_{16}H_{32}O_2$	CC1CCC(C(C1)OC(=O)C)C(C)C
45	Menthylacetate	$C_{12}H_{22}O_2$	CC(=O)CCCC1CCCCC1=C
46	2-pentanone,5-(2-methylenecyclohexyl)-,stereoisomer	$C_{12}H_{20}O$	CCCCCC=CCC=CCCCCCCCC(=O)OC
47	9, 12-octadecadienoic acid (Z, Z)-methyl ester	$C_{19}H_{34}O_2$	CCC=CCC=CCC=CCCCCCCCC(=O)OC
48	9, 12, 15-octadecatrienoic acid, methyl ester (Z, Z, Z)	$C_{19}H_{32}O_2$	CCCCCCCC(C=CC)O
49	2-Undecen-4-ol	C11H22O	CCCCCC#CCCCCCCCO
50	8-tetradecyn-1-ol	$C_{14}H_{26}O$	CC(=O)OC1(CCCCC1)C
51	Cyclohexanol,1-methyl-,acetate	$C_9H_{16}O_2$	CCCCCCCCCCCCCCCCCC(=O)O
52	Octadecanoic acid	$C_{18}H_{36}O_2$	CCCCCCC=CCCC=C
53	1, 5-dodecadiene	$C_{12}H_{22}$	CC1CC2C(CCC3C2CCC4(C3CCC4OC(=O)C)C)CC1=O
54	Estran-3-one, 17-(acetyloxy)-2-methyl, (2alpha, 5alpha, 17beta)	$C_{21}H_{32}O_3$	CC(C)CCCC(C)CCCC(C)CCCC(=CCOC(=O)C)C
55	Phytol,acetate	$C_{22}H_{42}O_2$	CC(=O)OC(C=CC=CC=CC=C(C=O)C=O)OC(=O)C
56	1, 1-diacetoxy-9, 9-diformylnona-2,4,6,8-tetraene	$C_{15}H_{16}O_6$	CC(=O)OCCCCCCCCCCC=CC1CO1
57	Z-(13, 14-epoxy) tetradec-11-en-1-ol acetate	$C_{16}H_{28}O_3$	CCCCCCC(CC=CCCCCCCCC(=O)OC)O
58	Methyl (9Z)-12-hydroxy-9-octadecenoate	$C_{19}H_{36}O_3$	CC(=O)C1=NC=CN1
59	1-(1H-imidazol-2-yl)ethanone	$C_5H_6N_2O$	CC(=O)C(CC1=CC=C(C=C1)OC(=O)C)NC(=O)C
60	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester	$C_{14}H_{17}NO_4$	CC(=CC(=O)O)C(C)(C)C(=O)C
61	2-hexenoicacid,3,4,4-trimethyl-5-oxo-,(E)-	$C_9H_{14}O_3$	CC(C)C(=O)C(C)C(=O)C(C)(C)C
62	3,5-heptanedione,2,2,6,6-tetramethyl	$C_11H_{20}O_2$	CCCCCCCCC(=O)O
63	Nonanoic acid	$C_9H_{18}O_2$	CC(=O)OC1C(COC1COC)OC
64	3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol	$C_9H_{16}O_5$	CC(C)CC(=O)C(CCC(=O)C)C(=O)CC(C)C
65	4, 6-nonanedione,5-(3-butanon-1-yl)-2,8-dimethyl-	$C_{15}H_{26}O_3$	CC(CC1CC(=O)N(O1)C(=O)C)OC(=O)C
66	Acetic acid, 2-(2-acetyl-3-oxoisoxazolidin-5-yl)-1-methyl ethyl ester	$C_{10}H_{15}NO_5$	CC1CC(CC(C1)O)C
67	3,5-dimethyl-cyclohexanol	$C_8H_{16}O$	CC(C)CC(=O)C=C(C(=CC(=O)CC(C)C)O)O
68	5,7-dodecadiene-4,9-dione,6,7-	$C_{14}H_{22}O_4$	C1=CC=C(C(=C1)C(=O)O)C(=O)O

	dihydroxy-2,11-dimethyl-		
69	1,2-benzenedicarboxylic acid	$C_8H_6O_4$	CCC(C)(C)CCC=O
70	Hexanal,4,4-dimethyl-	$C_8H_{16}O$	CCC=CCC=CCC=CCCCCCCCC(=O)OC(CO)CO
71	2-monolinolenin	$C_{21}H_{36}O_4$	CC1CC(C2(C1C3CC4C5(O4)CCC(CC5(C3CC2)C)O)C)C(=O)C
72	1-(2-hydroxy-7,9a,11b-trimethylhexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-9-yl)ethanone	$C_{22}H_{34}O_3$	CCCCCCCCCCCCCCCC#CC1(CCCC1)O
73	1-(1-heptadecynyl)cyclopentanol	$C_{22}H_{40}O$	CC1CCC2C3CCC4CC(CCC4(C3CCC2(C1=O)C)C)OC(=O)C
74	3.beta.-acetoxy-17.alpha.-methyl-d-homoandrostane-17a-one	$C_{23}H_{36}O_3$	CC1CCC23CCCC2C1(C(CC(CC3C)(C)C=C)O)C
75	2,4,7,14-tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	$C_{20}H_{34}O$	CC(=O)OC1CCC2C1(CCC3C2C(=O)C=C4C3(CCC(=O)C4(C)C)C)C
76	4,4-dimethyl-3,7-dioxoandrost-5-en-17-yl acetate	$C_{23}H_{32}O_4$	CC(C)C(C)C=CC(C)C1CCC2C1(CC3C4(C2=CCC5C4(CCC(C5)OC(=O)C)C)O3)C
77	Ergost-7,22-dien-9,11-epoxy-3-ol,acetate(ester)	$C_{30}H_{46}O_3$	CC(=O)CCC12CC1(CCCC2(C)C)C
78	4-(2,2,6-trimethylbicyclo[4.1.0]Hept-1-yl)-2-butanone	$C_{14}H_{24}O$	CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
79	5-cholestene-3-ol,24-methyl-	$C_{28}H_{48}O$	CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
80	Stigmasta-5,22-dien-3-ol	$C_{29}H_{48}O$	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O
81	1H-3A,7-methanozulen-6-ol,octahydro3,6,8,8-tetramethyl	$C_{15}H_{26}O$	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
82	Gamma.-sitosterol	$C_{29}H_{50}O$	C1=CC=C(C=C1)C=CC=O

*Simplified molecular-input line-entry system (SMILES) is a chemical notation that allows a user to represent a chemical structure of an organic compound in a way that can be used by the computer.

In the current investigation ADMET analysis of all the phytocompounds was carried out using SwissADME and pkCSM server tools. The *in-silico* ADMET analysis was conducted as it saves time and cost of drug discovery and development. It also provided dependable data very quickly, reducing the chance of failure in the clinical trial phase. These could predict the pharmacokinetic properties of various compounds [13, 14]. The physicochemical properties of the phytocompounds identified by GC-MS analysis of the extract were evaluated using the SwissADME server tool. The results of the evaluation are given in **Table 3.**

TABLE 3: PHYSICOCHEMICAL PROPERTIES OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT *ISODON TERNIFOLIUS* (D. DON) KUDO

Compd. no.	Compounds	MW	HA	AHA	FC	RB	HBA	HBD	MR	TPSA
1	3–phenyl- 2-propenal	132.16	10	6	0.00	2	1	0	41.54	17.07
2	2,3-dihydro-benzofuran	120.15	9	6	0.25	0	1	0	35.79	9.23
3	3-hexene-2,5-dione	112.13	8	0	0.33	2	2	0	30.88	34.14
4	2-methoxy-4-vinylphenol	150.17	11	6	0.11	2	2	1	45.05	29.46
5	1-penten-3-one,1-phenyl-	160.21	12	6	0.18	3	1	0	51.15	17.07
6	Biphenylene,1,2,3,6,7,8,8a,8b-octahydro-,trans-	160.26	12	0	0.67	0	0	0	52.51	0.00
7	1H-Indene,1-ethylideneoctahydro, trans-	150.26	11	0	0.82	0	0	0	50.29	0.00
8	1,4-Diacetoxy-1,3-butadiene	170.16	12	0	0.25	5	4	0	42.19	52.60
9	2,6-heptanedione,3-acetyl-	170.21	12	0	0.67	5	3	0	45.98	51.21
10	1,3-decadiene-7,9-dione	166.22	12	0	0.40	6	2	0	49.64	34.14
11	11-oxatetracyclo[5.3.2.0(2,7).0(2,8)]dodecan-9-one	178.23	13	0	0.91	0	2	0	47.30	26.30
12	2-(3,3-dimethyl-1-butynyl)-	164.29	12	0	0.83	0	0	0	55.33	0.00

	1,1,3-trimethylcyclopropane									
13	2,6-cresotaldehyde	136.15	10	6	0.12	1	2	1	38.82	37.30
14	2-tert-butyl-5-methyl-1,4-benzoquinone	178.23	13	0	0.45	1	2	0	52.07	34.14
15	4-penten-2-one,3-cyclohexyl-	166.26	12	0	0.73	3	1	0	52.60	17.07
16	Aceticacid,(1,2-dimethyl-1-propenyl)ester	128.17	9	0	0.57	2	2	0	36.57	26.30
17	1-hexen-5-on,3-methyl-4-henyl-	190.28	14	6	0.38	4	1	1	60.82	20.23
18	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl	295.29	21	6	0.43	9	6	0	75.77	98.42
19	6-[1-hydroxymethyl)Vinyl]-4,8A-dimethyl-	292.37	21	0	0.65	4	4	1	81.04	63.60
20	3-methyl-3-phenyl-2-oxiranecarbonitrile	159.18	12	6	0.30	1	2	0	44.43	36.32
21	2,5-monoformal-l-rhamnitoltriacetate	318.28	22	0	0.69	7	9	0	69.11	114.43
22	3-buten-2-one,4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-	210.31	15	0	0.77	2	2	1	63.16	37.30
23	3-octen-2-one,8-phenyl-	202.29	15	6	0.36	6	1	0	64.78	17.07
24	Adamantane-1-carboxylicacid,(4-acetylaminofurazan-3-yl)amide	304.34	22	5	.73	5	5	2	79.58	97.12
25	3-acetylbicyclo[3.3.1]non-6-ene	164.24	12	0	0.73	1	1	0	50.49	17.07
26	4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol	180.20	13	6	0.20	3	3	2	51.02	49.69
27	3-phenylpropionicacid,2-tetrahydrofurylmethylester	234.29	17	6	0.50	6	3	0	65.31	35.53
28	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one	330.46	24	0	0.76	1	3	2	95.70	57.53
29	2,4-oxazolidinedione,5-ethyl-3,5-dimethyl-	157.17	11	0	0.71	1	3	0	42.37	46.61
30	2-hexanol,3,3,5-trimethyl-2-(3-methylphenyl)-	234.38	17	6	0.62	4	1	1	75.61	20.23
31	2,6,8-trimethylbicyclo[4.2.0]oct-2-ene-11,8-diol	182.26	13	0	0.82	0	2	2	52.43	40.46
32	3-pentanone,2-methyl-4-phenyl-	176.25	13	6	0.42	3	1	0	55.64	17.07
33	Neophytadiene	278.52	20	0	0.80	0	0	0	97.31	0.00
34	Hotrienyl acetate	194.27	14	0	0.42	6	2	0	59.70	26.30
35	2-hexadecen-1-ol, 3, 7, 11, 15-tetramethyl-[R-[R	296.53	21	0	0.90	13	1	1	98.94	20.23
36	5-methyl-2(2-oxo-4-heptyl)furan	194.27	14	5	0.58	5	2	0	57.68	30.21
37	2, 2, 9, 9-tetramethyl-5-decene-3, 7-diyne	188.31	14	0	0.57	0	0	0	64.74	0.00
38	9,12,15-Octadecatrienoic acid, 2,3-bis(acetyloxy)propyl ester, (Z,Z,Z)-	436.58	31	0	0.64	21	6	0	124.72	78.90
39	2,5-heptanedione,3,3,6-trimethyl-	170.25	12	0	.80	4	2	0	50.32	34.14
40	Hexadecanoic, methylester	270.45	19	0	0.94	15	2	0	85.12	26.30
41	Propanoic acid, 2-methyl-3-Phenyl-2-propenyl ester	204.26	15	6	0.31	5	2	0	61.85	26.30
42	1,3-pentanedione,2,4-dimethyl-1-phenyl-	204.26	15	6	0.38	4	2	0	60.87	34.14
43	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-1a,3,4,5,5a,5b,6,7,9,10,10a,10b, 10c-tetradeca -hydro-7ah -	448.51	32	0	0.83	6	8	1	111.87	119.50

	cyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate									
44	Hexadecanoic acid	256.42	18	0	0.94	14	2	1	80.80	37.30
45	Menthylacetate	198.30	14	0	0.92	3	2	0	58.97	26.30
46	2-pentanone,5-(2-methylenecyclohexyl)-,stereoisomer	180.29	13	0	0.75	4	1	0	57.41	17.07
47	9, 12-octadecadienoic acid (Z, Z)-methyl ester	294.47	12	0	0.74	15	2	0	93.78	26.30
48	9, 12, 15-octadecatrienoic acid, methyl ester (Z, Z, Z)	292.46	21	0	0.63	14	2	0	93.31	26.30
49	2-Undecen-4-ol	170.29	12	0	0.82	7	1	1	55.68	20.23
50	8-tetradecyn-1-ol	210.36	15	0	0.86	9	1	1	68.74	20.23
51	Cyclohexanol,1-methyl-,acetate	156.22	11	0	0.89	2	2	0	44.59	26.30
52	Octadecanoic acid	284.48	20	0	0.94	16	2	1	90.41	37.30
53	1, 5-dodecadiene	166.30	12	0	0.67	8	0	0	58.85	0.00
54	Estran-3-one, 17-(acetyloxy)-2-methyl, (2alpha, 5alpha, 17beta)	332.48	24	0	0.90	2	3	0	95.83	43.37
55	Phytol,acetate	338.57	20	0	0.86	15	2	0	108.68	26.30
56	1, 1-diacetoxy-9, 9-diformylnona-2,4,6,8-tetraene	108.68	21	0	0.20	10	6	0	75.29	86.74
57	Z-(13, 14-epoxy) tetradec-11-en-1-ol acetate	268.39	19	0	0.81	13	3	0	78.81	38.83
58	Methyl (9Z)-12-hydroxy-9-octadecenoate	312.49	22	0	0.84	16	3	1	95.42	46.53
59	1-(1H-imidazol-2-yl)ethanone	110.11	8	5	0.20	1	2	1	28.78	45.75
60	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester	263.29	19	6	0.36	7	4	1	70.14	72.47
61	2-hexenoicacid,3,4,4-trimethyl-5-oxo-,(E)-	170.21	12	0	0.56	3	3	1	46.61	54.37
62	3,5-heptanedione,2,2,6,6-tetramethyl	184.28	13	0	0.82	4	2	0	55.13	34.14
63	Nonanoic acid	158.24	11	0	0.89	7	2	1	47.15	37.30
64	3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol	204.22	14	0	0.89	5	5	0	47.80	53.99
65	4, 6-nonanedione,5-(3-butanon-1-yl)-2,8-dimethyl-	254.37	18	0	0.80	9	3	0	74.82	51.21
66	Acetic acid, 2-(2-acetyl-3-oxoisoxazolidin-5-yl)-1-methyl ethyl ester	229.23	16	0	0.70	5	5	0	57.65	72.91
67	3,5-dimethyl-cyclohexanol	128.21	9	0	1.0	0	1	1	39.62	20.23
68	5,7-dodecadiene-4,9-dione,6,7-dihydroxy-2,11-dimethyl-	254.32	18	0	0.57	7	4	2	72.01	74.60
69	1,2-benzenedicarboxylic acid	166.13	12	6	0.00	2	4	2	40.36	74.60
70	Hexanal,4,4-dimethyl-	128.21	9	0	0.88	4	1	0	40.51	17.07
71	2-monolinolenin	352.51	25	0	0.67	17	4	2	105.25	66.76
72	1-(2-hydroxy-7,9a,11b-trimethylhexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-9-yl)ethanone	346.50	25	0	0.95	1	3	1	99.26	49.83
73	1-(1-heptadecynyl)cyclopentanol	320.55	23	0	0.91	13	1	1	105.12	20.23
74	3.beta.-acetoxy-17.alpha.-methyl-d-homoandrostane-17a-one	360.53	26	0	0.91	2	3	0	105.18	43.37
75	2,4,7,14-tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	290.48	21	0	0.90	1	1	1	91.82	20.23
76	4,4-dimethyl-3,7-dioxoandrost-5-en-17-yl acetate	372.50	27	0	0.78	2	4	0	104.65	60.44

77	Ergost-7,22-dien-9,11-epoxy-3-ol,acetate(ester)	454.68	33	0	0.83	6	3	0	136.69	38.83
78	4-(2,2,6-trimethylbicyclo[4.1.0]Hept-1-yl)-2-butanone	208.34	15	0	0.93	3	1	0	64.60	17.07
79	5-cholestene-3-ol,24-methyl-	400.68	29	0	0.93	5	1	1	128.42	20.23
80	Stigmasta-5,22-dien-3-ol	412.69	30	0	0.86	5	1	1	132.75	20.23
81	1H-3A,7-methanozulen-6-ol,octahydro3,6,8,8-tetramethyl	222.37	16	0	1.0	0	1	1	68.56	20.23
82	gamma.-sitosterol	414.71	30	0	0.93	6	1	1	133.23	20.23

*MW- Molecular Weight, HA- Number of Heavy Atoms, AHA- Number of Aromatic Heavy Atoms, FC- Fraction Csp^3, RB- Rotatable Bond, HBA- Hydrogen Bond Acceptor, HBD- Hydrogen Bond Donor, MR- Molar Refractivity, TPSA- Topological Polar Surface Area.

Molecular weight (MW), number of heavy atoms (HA), number of heavy atoms in aromatic ring (AHA), number of rotatable bonds (RB), number of hydrogen bond acceptors (HBA), number of hydrogen bond donors (HBD), molar refractivity (MR), and topological surface area (TPSA) are included in the table. The molecular weight of the compounds varies from 110.11 to 454.68 Da. Using the SwissADME server tool, the hydrophobicity characteristics of the compounds were evaluated, and the result is given in **Table 4.**

TABLE 4: LIPOPHILICITY CHARACTERISTICS OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT ISODONTERNIFOLIUS (D. DON) KUDO

Compd. no.	Compounds	iLOGP	XLOGP3	WLOGP	MLOGP	SILICOS-IT	Consensus Log $P_{o/w}$
1	3-phenyl-2-propenal	1.65	1.90	1.79	2.01	2.48	1.97
2	2,3-dihydro-benzofuran	1.89	2.14	1.62	1.75	2.62	2.00
3	3-hexene-2,5-dione	1.43	-0.13	0.72	0.26	0.90	0.64
4	2-methoxy-4-vinylphenol	2.14	2.81	1.93	1.71	2.13	2.14
5	1-penten-3-one,1-phenyl-	2.26	2.54	2.57	2.61	3.03	2.60
6	Biphenylene,1,2,3,6,7,8,8a,8b-octahydro-,trans-	2.76	3.09	3.45	3.84	3.16	3.26
7	1H-Indene,1-ethylideneoctahydro-,trans-	2.81	3.75	3.53	4.58	3.30	3.59
8	1,4-Diacetoxy-1,3-butadiene	2.05	0.65	1.14	0.75	0.81	1.08
9	2,6-heptanedione,3-acetyl-	1.20	-0.15	1.15	0.38	1.80	0.88
10	1,3-decadiene-7,9-dione	1.82	1.48	2.06	1.47	2.60	1.89
11	11-oxatetracyclo[5.3.2.0(2,7).0(2,8)]dodecan-9-one	2.04	0.98	1.53	1.67	2.58	1.76
12	2-(3,3-dimethyl-1-butynyl)-1,1,3-trimethylcyclopropane	3.24	4.17	3.41	4.86	3.24	3.78
13	2,6-cresotaldehyde	1.67	1.94	1.51	1.12	1.96	1.64
14	2-tert-butyl-5-methyl-1,4-benzoquinone	2.13	2.59	2.06	1.37	2.52	2.13
15	4-penten-2-one,3-cyclohexyl-	2.52	3.47	2.96	2.49	3.13	2.91
16	Aceticacid,(1,2-dimethyl-1-propenyl)ester	2.19	1.84	1.86	1.52	1.01	1.68
17	1-hexen-5-on,3-methyl-4-henyl-	2.69	3.22	3.00	3.25	3.30	3.09
18	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl	2.36	1.62	1.37	1.15	0.50	1.40
19	6-[1-hydroxymethyl)Vinyl]-4,8A-dimethyl-	2.43	2.57	2.56	2.02	3.17	2.55
20	3-methyl-3-phenyl-2-oxiranecarbonitrile	2.00	1.39	1.72	1.08	2.56	1.75
21	2,5-monoformal-l-rhamnitoltriacetate	1.98	0.60	0.34	-0.16	0.19	0.59
22	3-buten-2-one,4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-	2.52	2.24	2.71	2.11	2.94	2.50
23	3-octen-2-one,8-phenyl-	2.88	3.71	3.54	3.42	4.17	3.55

24	Adamantane-1-carboxylicacid,(4-acetylaminofurazan-3-yl)amide	1.94	1.35	1.80	2.01	1.15	1.65
25	3-acetylbicyclo[3.3.1]non-6-ene	2.24	2.15	2.57	2.49	2.28	2.35
26	4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol	2.16	1.79	1.30	1.13	1.71	1.62
27	3-phenylpropionicacid,2-tetrahydrofurylmethylester	2.92	2.41	2.34	2.12	3.24	2.61
28	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one	2.87	2.50	3.55	3.07	3.38	3.07
29	2,4-oxazolidinedione,5-ethyl-3,5-dimethyl-	1.84	0.83	0.38	0.21	0.68	0.79
30	2-hexanol,3,3,5-trimethyl-2-(3-methylphenyl)-	3.25	4.50	4.17	4.10	4.31	4.07
31	2,6,8-trimethylbicyclo[4.2.0]oct-2-ene-1,8-diol	2.20	0.71	1.62	1.67	2.01	1.64
32	3-pentanone,2-methyl-4-phenyl-	2.47	3.16	3.02	2.97	3.24	2.97
33	Neophytadiene	5.05	9.62	7.17	6.21	7.30	7.07
34	Hotrienyl acetate	3.06	3.36	3.02	2.86	2.97	3.05
35	2-hexadecen-1-ol, 3, 7, 11, 15-tetramethyl-[R-[R	4.71	8.19	6.36	5.25	6.57	6.22
36	5-methyl-(2-oxo-4-heptyl)furan	2.78	2.57	3.45	1.70	3.65	2.83
37	2, 2, 9, 9-tetramethyl-5-decene-3, 7-diyne	3.88	5.07	3.80	5.58	3.84	4.44
38	9,12,15-Octadecatrienoic acid, 2,3-bis(acetyloxy)propyl ester, (Z,Z,Z)-	4.97	6.07	5.61	4.00	6.98	5.53
39	2,5-heptanedione,3,3,6-trimethyl-	2.27	1.51	2.22	1.66	2.29	1.99
40	Hexadecanoic, methylester	4.41	7.38	5.64	4.44	5.84	5.54
41	Propanoic acid, 2-methyl-3-Phenyl-2-propenyl ester	2.98	3.30	2.79	3.04	3.16	3.06
42	3-pentanedione,2,4-dimethyl-1-phenyl-	2.02	3.15	2.73	2.23	3.17	2.66
43	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-1a,3,4,5,5a,5b,6,7,9,10,10a,10b,10c-tetradeca -hydro-7ah -cyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate	2.99	0.34	1.46	1.17	2.02	1.60
44	Hexadecanoic acid	3.85	7.17	5.55	4.19	5.25	5.20
45	Menthylacetate	2.73	4.00	3.01	2.76	2.49	3.00
46	2-pentanone,5-(2-methylenecyclohexyl)-,stereoisomer	2.69	2.96	3.49	2.77	3.67	3.12
47	9, 12-octadecadienoic acid (Z, Z)-methyl ester	4.61	6.82	5.97	4.70	6.36	5.69
48	9, 12, 15-octadecatrienoic acid, methyl ester (Z, Z, Z)	4.94	6.29	5.75	4.61	6.18	5.55
49	2-Undecen-4-ol	3.16	3.87	3.28	2.99	3.10	3.28
50	8-tetradecyn-1-ol	3.80	5.23	3.98	3.80	4.45	4.25
51	Cyclohexanol,1-methyl-,acetate	2.48	2.11	2.27	1.88	2.24	2.20
52	Octadecanoic acid	4.30	8.23	6.33	4.67	6.13	5.93
53	1, 5-dodecadiene	3.57	5.27	4.48	4.23	4.25	4.36
54	Estran-3-one, 17-(acetyloxy)-2-methyl, (2alpha, 5alpha, 17beta)	3.19	4.52	4.39	3.98	3.64	3.94
55	Phytol,acetate	5.01	8.76	6.93	5.47	7.19	6.67
56	1, 1-diacetoxy-9, 9-diformylnona-2,4,6,8-tetraene	2.65	1.50	1.43	1.17	2.61	1.87
57	Z-(13, 14-epoxy) tetradec-11-en-1-ol acetate	3.80	4.51	4.02	2.81	5.03	4.03
58	Methyl (9Z)-12-hydroxy-9-octadecenoate	4.45	5.92	5.17	3.92	5.80	5.05

59	1-(1H-imidazol-2-yl)ethanone	1.04	0.08	0.61	-1.03	1.26	0.39
60	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester	2.07	1.04	1.25	1.34	2.24	1.59
61	2-hexenoicacid,3,4,4-trimethyl-5-oxo-,(E)-	1.29	1.42	1.63	1.19	1.16	1.34
62	3,5-heptanedione,2,2,6,6-tetramethyl	2.07	2.81	2.46	1.95	2.55	2.37
63	Nonanoic acid	2.30	3.42	2.82	2.28	2.20	2.60
64	3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol	1.83	-0.35	-0.02	-0.68	0.51	0.26
65	4, 6-nonanedione,5-(3-butanon-1-yl)-2,8-dimethyl-	2.70	2.38	3.20	2.05	4.05	2.88
66	Acetic acid, 2-(2-acetyl-3-oxoisoxazolidin-5-yl)-1-methyl ethyl ester	1.53	0.00	0.03	0.64	0.47	0.53
67	3,5-dimethyl-cyclohexanol	2.17	2.23	1.80	1.83	1.56	1.92
68	5,7-dodecadiene-4,9-dione,6,7-dihydroxy-2,11-dimethyl-	2.59	3.02	3.10	0.85	2.41	2.39
69	1,2-benzenedicarboxylic acid	0.60	0.73	1.08	1.20	0.61	0.84
70	Hexanal,4,4-dimethyl-	2.01	2.28	2.40	2.07	2.12	2.18
71	2-monolinolenin	4.73	4.99	4.47	3.33	5.76	4.66
72	1-(2-hydroxy-7,9a,11b-trimethylhexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-9-yl)ethanone	3.24	3.71	3.97	3.49	3.86	3.65
73	1-(1-heptadecynyl)cyclopentanol	5.36	8.70	6.86	5.30	7.51	6.75
74	3.beta.-acetoxy-17.alpha.-methyl-d-homoandrostane-17a-one	3.53	5.56	5.17	4.41	4.38	4.61
75	2,4,7,14-tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	3.62	6.59	5.19	4.86	4.63	4.98
76	4,4-dimethyl-3,7-dioxoandrost-5-en-17-yl acetate	3.33	3.45	4.27	3.37	4.33	3.75
77	Ergost-7,22-dien-9,11-epoxy-3-ol,acetate(ester)	4.89	6.90	7.11	5.73	6.81	6.29
78	4-(2,2,6-trimethylbicyclo[4.1.0]Hept-1-yl)-2-butanone	2.80	3.91	3.96	3.41	4.28	3.67
79	5-cholestene-3-ol,24-methyl-	4.92	8.80	7.63	6.54	6.63	6.90
80	Stigmasta-5,22-dien-3-ol	5.01	8.56	7.80	6.62	6.86	6.97
81	1H-3A,7-methanozulen-6-ol,octahydro3,6,8,8-tetramethyl	3.03	3.88	3.61	3.81	3.40	3.55
82	gamma.-sitosterol	4.79	9.34	8.02	6.73	7.04	7.19

Table 4 provides information regarding hydrophobicity classes, XLOGP3, WLOGP, MLOGP, SILICOS-IT, and the concensuslogP o/w (average hydrophobicity) values. The concensus logP o/w values of the compounds range from 0.26 to 7.19. 3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol and gamma-sitosterol have the lowest and highest log average hydrophobicity values, respectively. Hydrophobicity of the identified phytocompounds greatly influences the solubility, permeability, selectivity, potency and promiscuity of the phytocompounds [15]. The water solubility (LogS) of all the phytocompounds were also determined by using the SwissADME server tool. Water solubility values, solubility, and classes of solubility are all illustrated in **Table 5.**

TABLE 5: WATER SOLUBILITY CHARACTERISTICS OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT *ISODONTERNIFOLIUS* (D. DON) KUDO

Compd. no.	Compounds	ESOL				Ali				SILICOS-IT			
		Log S	Solubility		C	Log S	Solubility		C	Log S	Solubility		C
			mg/mL	mol/L			mg/mL	mol/L			mg/mL	mol/L	
1	2-propenal,3–phenyl-	-2.17	8.97e-01	6.79e-03	S	-1.88	1.74e+00	1.31e-02	VS	-2.40	5.26e-01	3.98e-03	S

2	2,3-dihydro-benzofuran	-2.43	4.50e-01	3.75e-03	S	-1.97	1.30e+00	1.08e-02	VS	-2.64	2.76e-01	2.30e-03	S
3	3-hexene-2,5-dione	-0.32	5.35e+01	4.77e-01	VS	-0.13	8.25e+01	7.36e-01	VS	-0.58	2.94e+01	2.62e-01	S
4	2-methoxy-4-vinylphenol	-2.81	2.31e-01	1.54e-03	S	-3.09	1.23e-01	8.21e-04	S	-2.38	6.30e-01	4.20e-03	S
5	1-penten-3-one,1-phenyl-	-2.61	3.97e-01	2.48e-03	S	-2.55	4.56e-01	2.85e-03	S	-3.22	9.74e-02	6.08e-04	S
6	Biphenylene,1,2,3,6,7,8,8a,8b-octahydro-,trans-	-2.78	2.66e-01	1.66e-03	S	-2.76	2.80e-01	1.75e-03	S	-2.24	9.31e-01	5.81e-03	S
7	1H-Indene,1-ethylideneoctahydro-,trans-	-3.13	1.10e-01	7.34e-04	S	-3.44	5.42e-02	3.61e-04	S	-2.31	7.29e-01	4.85e-03	S
8	1,4-Diacetoxy-1,3-butadiene	-0.97	1.80e+01	1.06e-01	VS	-1.33	7.95e+00	4.67e-02	VS	-0.21	1.06e+02	6.21e-01	S
9	2,6-heptanedione,3-acetyl-	-0.47	5.76e+01	3.38e-01	VS	-0.47	5.75e+01	3.38e-01	VS	-1.74	3.10e+00	1.82e-02	S
10	1,3-decadiene-7,9-dione	-1.41	6.51e+00	3.92e-02	VS	-1.80	2.61e+00	1.57e-02	VS	-1.91	2.06e+00	1.24e-02	S
11	11-oxatetracyclo[5.3.2.0(2,7).0(2,8)]dodecan-9-one	-1.56	4.88e+00	2.74e-02	VS	-1.12	1.35e+01	7.58e-02	VS	-2.06	1.54e+00	8.63e-03	S
12	2-(3,3-dimethyl-1-butynyl)-1,1,3-trimethylcyclopropane	-3.49	5.37e-02	3.27e-04	S	-3.88	2.17e-02	1.32e-04	S	-2.68	3.41e-01	2.07e-03	S
13	2,6-cresotaldehyde	-2.28	7.07e-01	5.20e-03	S	-2.35	6.11e-01	4.49e-03	S	-2.13	1.02e+00	7.46e-03	S
14	2-tert-butyl-5-methyl-1,4-benzoquinone	-2.51	5.50e-01	3.09e-03	S	-2.96	1.97e-01	1.11e-03	S	-2.42	6.74e-01	3.78e-03	S
15	4-penten-2-one,3-cyclohexyl-	-2.86	2.30e-01	1.38e-03	S	-3.51	5.13e-02	3.09e-04	S	-2.14	1.21e+00	7.26e-03	S
16	Aceticacid,(1,2-dimethyl-1-propenyl)ester	-1.66	2.79e+00	2.18e-02	VS	-2.01	1.24e+00	9.71e-03	S	-1.17	8.69e+00	6.78e-02	S
17	1-hexen-5-on,3-methyl-4-henyl-	-3.10	1.51e-01	7.92e-04	S	-3.32	9.16e-02	4.81e-04	S	-3.55	5.40e-02	2.84e-04	S
18	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl	-2.31	1.45e+00	4.91e-03	S	-3.30	1.48e-01	5.02e-04	S	-3.19	1.93e-01	6.53e-04	S
19	6-[1-hydroxymethyl)Vinyl]-4,8A-dimethyl-	-3.01	2.87e-01	9.82e-04	S	-3.55	8.17e-02	2.79e-04	S	-3.16	2.01e-01	6.89e-04	S
20	3-methyl-3-phenyl-2-oxiranecarbonitrile	-2.01	1.57e+00	9.85e-03	S	-1.76	2.79e+00	1.75e-02	VS	-2.91	1.97e-01	1.24e-03	S
21	2,5-monoformal-l-rhamnitoltriacetate	-1.73	5.94e+00	1.87e-02	VS	-2.58	8.43e-01	2.65e-03	S	-0.72	6.09e+01	1.91e-01	S
22	3-buten-2-one,4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-	-2.42	7.94e-01	3.77e-03	S	-2.66	4.61e-01	2.19e-03	S	-2.31	1.02e+00	4.86e-03	S
23	3-octen-2-one,8-phenyl-	-3.33	9.43e-02	4.66e-04	S	-3.76	3.52e-02	1.74e-04	S	-4.45	7.23e-03	3.57e-05	MD
24	Adamantane-1-carboxylicacid,(4-acetylaminofurazan-3-yl)amide	-2.42	1.17e+00	3.84e-03	S	-2.99	3.10e-01	1.02e-03	S	-3.31	1.50e-01	4.92e-04	S
25	3-acetylbicyclo[3.3.1]non-6-ene	-2.15	1.17e+00	7.13e-03	S	-2.14	1.19e+00	7.23e-03	S	-1.54	4.69e+00	2.86e-02	S
26	4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol	-2.23	1.06e+00	5.91e-03	S	-2.45	6.36e-01	3.53e-03	S	-1.87	2.44e+00	1.35e-02	S

27	3-phenylpropionicacid,2-tetrahydrofurylmethylester	-2.68	4.94e-01	2.11e-03	S	-2.80	3.73e-01	1.59e-03	S	-3.93	2.77e-02	1.18e-04	S
28	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one	-3.40	1.32e-01	4.00e-04	S	-3.35	1.46e-01	4.43e-04	S	-3.31	1.64e-01	4.95e-04	S
29	2,4-oxazolidinedione,5-ethyl-3,5-dimethyl-	-1.27	8.41e+00	5.35e-02	VS	-1.39	6.38e+00	4.06e-02	VS	-1.11	1.23e+01	7.83e-02	S
30	2-hexanol,3,3,5-trimethyl-2-(3-methylphenyl)-	-4.13	1.76e-02	7.49e-05	MS	-4.65	5.30e-03	2.26e-05	MS	-4.70	4.64e-03	1.98e-05	MS
31	2,6,8-trimethylbicyclo[4.2.0]oct-2-ene-11,8-diol	-1.42	6.97e+00	3.83e-02	VS	-1.14	1.33e+01	7.28e-02	VS	-1.83	2.72e+00	1.49e-02	S
32	3-pentanone,2-methyl-4-phenyl-	-3.07	1.51e-01	8.57e-04	S	-3.19	1.14e-01	6.47e-04	S	-3.60	4.42e-02	2.51e-04	S
33	Neophytadiene	-6.77	4.74e-05	1.70e-07	PS	-9.53	8.15e-08	2.93e-10	PS	-6.11	2.18e-04	7.82e-07	PS
34	Hotrienyl acetate	-2.77	3.34e-01	1.72e-03	S	-3.59	4.99e-02	2.57e-04	S	-2.17	1.31e+00	6.76e-03	S
35	2-hexadecen-1-ol, 3, 7, 11, 15-tetramethyl-[R-[R	-2.77	3.34e-01	1.72e-03	S	-3.59	4.99e-02	2.57e-04	S	-2.17	1.31e+00	6.76e-03	S
36	5-methyl-2(2-oxo-4-heptyl)furan	-2.60	4.90e-01	2.52e-03	S	-2.85	2.73e-01	1.40e-03	S	-3.99	2.00e-02	1.03e-04	S
37	2, 2, 9, 9-tetramethyl-5-decene-3, 7-diyne	-4.20	1.18e-02	6.29e-05	MS	-4.81	2.90e-03	1.54e-05	MS	-2.56	5.21e-01	2.77e-03	S
38	9,12,15-Octadecatrienoic acid, 2,3-bis(acetyloxy)propyl ester, (Z,Z,Z)-	-4.98	4.52e-03	1.04e-05	MS	-7.51	1.36e-05	3.11e-08	PS	-5.17	2.92e-03	6.70e-06	MS
39	2,5-heptanedione,3,3,6-trimethyl-	-1.58	4.45e+00	2.61e-02	VS	-1.84	2.49e+00	1.46e-02	VS	-2.21	1.05e+00	6.17e-03	S
40	Hexadecanoic, methylester	-5.18	1.80e-03	6.67e-06	MS	-7.76	4.68e-06	1.73e-08	PS	-6.01	2.64e-04	9.75e-07	PS
41	Propanoic acid, 2-methyl-3-Phenyl-2-propenyl ester	-3.15	1.44e-01	7.06e-04	S	-3.53	6.06e-02	2.97e-04	S	-3.41	7.95e-02	3.89e-04	S
42	1,3-pentanedione,2,4-dimethyl-1-phenyl-	-3.12	1.54e-01	7.53e-04	S	-3.54	5.93e-02	2.90e-04	S	-3.56	5.64e-02	2.76e-04	S
43	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-1a,3,4,5,5a,5b,6,7,9,10,10a,10b,10c-tetradeca - hydro-7ah - cyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate	-2.44	1.63e+00	3.64e-03	S	-2.41	1.73e+00	3.86e-03	S	-2.10	3.60e+00	8.02e-03	S
44	Hexadecanoic acid	-5.02	2.43e-03	9.49e-06	MS	-7.77	4.31e-06	1.68e-08	PS	-5.31	1.25e-03	4.88e-06	MS
45	Menthylacetate	-3.39	8.05e-02	4.06e-04	S	-4.25	1.10e-02	5.57e-05	MS	-2.15	1.41e+00	7.13e-03	S
46	2-pentanone,5-(2-methylenecyclohexyl)-,stereoisomer	-2.56	4.98e-01	2.76e-03	S	-2.98	1.88e-01	1.04e-03	S	-3.25	1.01e-01	5.60e-04	S
47	9, 12-octadecadienoic acid (Z, Z)-methyl ester	-4.97	3.14e-03	1.07e-05	MS	-7.18	1.94e-05	6.60e-08	PS	-5.37	1.25e-03	4.25e-06	MS
48	9, 12, 15-octadecatrienoic acid,	-4.69	5.94e-03	2.03e-05	MS	-6.63	6.85e-05	2.34e-07	PS	-4.65	6.49e-03	2.22e-05	MS

	methyl ester (Z, Z, Z)												
49	2-Undecen-4-ol	-2.87	2.29e-01	1.34e-03	S	-3.99	1.73e-02	1.02e-04	S	-2.64	3.89e-01	2.29e-03	S
50	8-tetradecyn-1-ol	-3.85	3.01e-02	1.43e-04	S	-5.40	8.31e-04	3.95e-06	MS	-4.23	1.23e-02	5.83e-05	MS
51	Cyclohexanol,1-methyl-,acetate	-2.01	1.54e+00	9.87e-03	S	-2.29	7.96e-01	5.09e-03	S	-1.99	1.62e+00	1.04e-02	S
52	Octadecanoic acid	-5.73	5.26e-04	1.85e-06	MS	-8.87	3.80e-07	1.33e-09	PS	-6.11	2.19e-04	7.71e-07	PS
53	1, 5-dodecadiene	-3.66	3.61e-02	2.17e-04	S	-5.02	1.59e-03	9.55e-06	MS	-3.63	3.91e-02	2.35e-04	S
54	Estran-3-one, 17-(acetyloxy)-2-methyl, (2alpha, 5alpha, 17beta)	-4.62	8.03e-03	2.42e-05	MS	-5.15	2.34e-03	7.04e-06	MS	-3.68	6.91e-02	2.08e-04	S
55	Phytol,acetate	-6.47	1.15e-04	3.40e-07	PS	-9.19	2.17e-07	6.40e-10	PS	-6.14	2.43e-04	7.18e-07	PS
56	1, 1-diacetoxy-9, 9-diformylnona-2,4,6,8-tetraene	-1.94	3.38e+00	1.16e-02	VS	-2.93	3.44e-01	1.18e-03	S	-0.33	1.36e+02	4.67e-01	S
57	Z-(13, 14-epoxy) tetradec-11-en-1-ol acetate	-3.49	8.74e-02	3.26e-04	S	-5.05	2.41e-03	8.98e-06	MS	-4.16	1.87e-02	6.98e-05	MS
58	Methyl (9Z)-12-hydroxy-9-octadecenoate	-4.45	1.11e-02	3.54e-05	MS	-6.67	6.66e-05	2.13e-07	PS	-5.15	2.20e-03	7.05e-06	MS
59	1-(1H-imidazol-2-yl) ethanone	-0.97	1.18e+01	1.07e-01	VS	-0.59	2.80e+01	2.54e-01	VS	-1.51	3.42e+00	3.10e-02	S
60	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester	-1.90	3.32e+00	1.26e-02	VS	-2.15	1.85e+00	7.04e-03	S	-3.65	5.85e-02	2.22e-04	S
61	2-hexenoicacid,3,4,4-trimethyl-5-oxo-,(E)-	-1.59	4.36e+00	2.56e-02	VS	-2.17	1.16e+00	6.82e-03	S	-0.88	2.22e+01	1.31e-01	S
62	3,5-heptanedione,2,2,6,6-tetramethyl	-2.49	5.98e-01	3.24e-03	S	-3.18	1.21e-01	6.55e-04	S	-2.25	1.04e+00	5.66e-03	S
63	Nonanoic acid	-2.51	4.85e-01	3.06e-03	S	-3.88	2.07e-02	1.31e-04	S	-2.46	5.46e-01	3.45e-03	S
64	3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol	-0.56	5.68e+01	2.78e-01	VS	-0.32	9.73e+01	4.77e-01	VS	-0.78	3.38e+01	1.66e-01	S
65	4, 6-nonanedione,5-(3-butanon-1-yl)-2,8-dimethyl-	-2.32	1.21e+00	4.76e-03	S	-3.10	2.04e-01	8.01e-04	S	-3.43	9.41e-02	3.70e-04	S
66	Acetic acid, 2-(2-acetyl-3-oxoisoxazolidin-5-yl)-1-methyl ethyl ester	-0.93	2.69e+01	1.17e-01	VS	-1.08	1.90e+01	8.27e-02	VS	-0.71	4.51e+01	1.97e-01	
67	3,5-dimethyl-cyclohexanol	-2.04	1.17e+00	9.12e-03	S	-2.29	6.57e-01	5.13e-03	S	-1.01	1.24e+01	9.66e-02	S
68	5,7-dodecadiene-4,9-dione,6,7-dihydroxy-2,11-dimethyl-	-2.86	3.53e-01	1.39e-03	S	-4.25	1.42e-02	5.60e-05	MS	-1.27	1.37e+01	5.40e-02	S
69	1,2-benzenedicarboxylic acid	-1.57	4.49e+00	2.70e-02	VS	-1.88	2.21e+00	1.33e-02	VS	-1.14	1.21e+01	7.29e-02	S
70	Hexanal,4,4-dimethyl-	-1.81	2.00e+00	1.56e-02	VS	-2.28	6.80e-01	5.30e-03	S	-2.21	7.83e-01	6.11e-03	S
71	2-monolinolenin	-4.05	3.16e-02	8.97e-05	MS	-6.13	2.61e-04	7.39e-07	PS	-3.94	4.04e-02	1.15e-04	S
72	1-(2-hydroxy-7,9a,11b-trimethylhexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-9-	-4.26	1.91e-02	5.50e-05	MS	-4.45	1.24e-02	3.57e-05	MS	-3.57	9.41e-02	2.72e-04	S

	yl)ethanone												
73	1-(1-heptadecynyl)cyclopentanol	-6.45	1.14e-04	3.54e-07	PS	-9.00	3.18e-07	9.91e-10	PS	-6.80	5.12e-05	1.60e-07	PS
74	3.beta.-acetoxy-17.alpha.-methyl-d-homoandrostane-17a-one	CCCC	1.29e-03	3.58e-06	MS	-6.23	2.12e-04	5.87e-07	PS	-4.55	1.02e-02	2.83e-05	MS
75	2,4,7,14-tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	-5.73	5.45e-04	1.88e-06	MS	-6.81	4.45e-05	1.53e-07	PS	-4.22	1.74e-02	6.00e-05	MS
76	4,4-dimethyl-3,7-dioxoandrost-5-en-17-yl acetate	-4.19	2.40e-02	6.44e-05	MS	-4.40	1.48e-02	3.98e-05	MS	-4.74	6.83e-03	1.83e-05	MS
77	Ergost-7,22-dien-9,11-epoxy-3-ol,acetate(ester)	-6.61	1.12e-04	2.45e-07	PS	-7.53	1.35e-05	2.97e-08	PS	-5.40	1.82e-03	4.00e-06	MS
78	4-(2,2,6-trimethylbicyclo[4.1.0]Hept-1-yl)-2-butanone	-3.40	8.35e-02	4.01e-04	S	-3.97	2.25e-02	1.08e-04	S	-4.10	1.66e-02	7.98e-05	MS
79	5-cholestene-3-ol,24-methyl-	-7.54	1.16e-05	2.90e-08	PS	-9.11	3.13e-07	7.80e-10	PS	-5.79	6.42e-04	1.60e-06	MS
80	Stigmasta-5,22-dien-3-ol	-7.46	1.43e-05	3.46e-08	PS	-8.86	5.71e-07	1.38e-09	PS	-5.47	1.40e-03	3.39e-06	MS
81	1H-3A,7-methanozulen-6-ol,octahydro3,6,8,8-tetramethyl	-3.66	4.83e-02	2.17e-04	S	-4.00	2.21e-02	9.95e-05	MS	-3.18	1.46e-01	6.55e-04	S
82	gamma.-sitosterol	-7.90	5.23e-06	1.26e-08	PS	-9.67	8.90e-08	2.15e-10	PS	-6.19	2.69e-04	6.49e-07	PS

*C- Solubility class, PS- Poorly soluble, MS- Moderately soluble, S- soluble and VS- Very soluble.

Drug-likeness of all the phytocompounds was also evaluated by SwissADME analysis based on the five rules, *viz.*Lipinski, Ghose, Veber, Egan and Muegge rules. Drug-likeness qualitatively evaluates the probability for a molecule to become an oral drug with respect to bioavailability. Bioavailability scores of all the phytocompounds were similarly determined by SwissADME analysis. Bioavailability score is the parameter that determines the extent and rate at which compounds enter and eventually reaches the target sites upon administration [16, 17, 18]. The drug-likeness and bioavailability scores are given together in the **Table 6.**

TABLE 6: DRUGLIKENESS AND BIOAVAILABILITY SCORES VALUES OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT *ISODONTERNIFOLIUS* (D. DON) KUDO

Compd. no.	Compounds	Lipinski	Ghose	Veber	Egan	Muegge	BS
1	3-phenyl-2-propenal	yes	No; 2 violations: MW<160, #atoms<20	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
2	2,3-dihydro-benzofuran	yes	No; 3 violations: MW<160, MR<40, #atoms<20	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
3	3-hexene-2,5-dione	yes	No; 3 violations: MW<160, MR<40, #atoms<20	yes	yes	No; 1 violation: MW<200	0.55
4	2-methoxy-4-vinylphenol	yes	No; 1 violation: MW<160	yes	yes	No; 1 violation: MW<200	0.55
5	1-penten-3-one,1-phenyl-	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
6	Biphenylene,1,2,3,6,7,8,8a,8b-octahydro-,trans-	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55

7	1H-Indene,1-ethylideneoctahydro-, trans-	Yes; 1 violation: MLOGP >4.15	No; 1 violation: MW<160	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
8	1,4-Diacetoxy-1,3-butadiene	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
9	3-acetyl-2,6-heptanedione	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
10	1,3-decadiene-7,9-dione	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
11	11-oxatetracyclo[5.3.2.0(2,7).0(2,8)]dodecan-9-one	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
12	2-(3,3-dimethyl-1-butynyl)-1,1,3-trimethylcyclopropane	Yes; 1 violation: MLOGP >4.15	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
13	2,6-cresotaldehyde	yes	No; 3 violations: MW<160, MR<40, #atoms<20	yes	yes	No; 1 violation: MW<200	0.55
14	2-tert-butyl-5-methyl-1,4-benzoquinone	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
15	4-penten-2-one,3-cyclohexyl-	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
16	Aceticacid,(1,2-dimethyl-1-propenyl)ester	yes	No; 2 violations: MW<160, MR<40	yes	yes	No; 1 violation: MW<200	0.55
17	1-hexen-5-on,3-methyl-4-henyl-	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
18	Acetate,3-(acetyloxy)-2-nitro-2-benzylpropyl	yes	yes	yes	yes	yes	0.55
19	6-[1-hydroxymethyl)Vinyl]-4,8A-dimethyl-	yes	yes	yes	yes	yes	0.55
20	3-methyl-3-phenyl-2-oxiranecarbonitrile	yes	No; 1 violation: MW<160	yes	yes	No; 1 violation: MW<200	0.55
21	2,5-monoformal-l-rhamnitoltriacetate	yes	yes	yes	yes	yes	0.55
22	3-buten-2-one,4-(2-hydroxy-2,6,6-trimethylcyclohexyl)-	yes	yes	yes	yes	yes	0.55
23	8-phenyl-3-octen-2-one	yes	yes	yes	yes	No; 1 violation: Heteroatoms<2	0.55
24	Adamantane-1-carboxylicacid,(4-acetylaminofurazan-3-yl)amide	yes	yes	yes	yes	yes	0.55
25	3-acetylbicyclo[3.3.1]non-6-ene	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
26	4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
27	3-phenylpropionicacid, 2-	yes	yes	yes	yes	yes	0.55

	tetrahydrofurylmethyl ester						
28	Pregna-5,16-dien-3.beta,9.alpha.-diol-20-one	yes	yes	yes	yes	yes	0.55
29	5-ethyl-3,5-dimethyl-2,4-oxazolidinedione	yes	No; 1 violation: MW<160	yes	yes	No; 1 violation: MW<200	0.55
30	3,3,5-trimethyl-2-(3-methylphenyl)-2-hexanol	yes	yes	yes	yes	No; 1 violation: Heteroatoms<2	0.55
31	2,6,8-trimethylbicyclo[4.2.0]oct-2-ene-1,8-diol	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
32	2-methyl-4-phenyl-3-pentanone	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
33	Neophytadiene	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
34	Hotrienyl acetate	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
35	2-hexadecen-1-ol, 3, 7, 11, 15-tetramethyl-[R-[R	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
36	5-methyl-2-(2-oxo-4-heptyl)furan	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
37	2, 2, 9, 9-tetramethyl-5-decene-3, 7-diyne	Yes; 1 violation: MLOGP >4.15	yes	yes	yes	No; 3 violations: MW<200, XLOGP3>5, Heteroatoms<2	0.55
38	9,12,15-Octadecatrienoic acid, 2,3-bis(acetyloxy)propyl ester, (Z,Z,Z)-	yes	No; 2 violations: WLOGP>5.6, #atoms>70	No; 1 violation: Rotors >10	yes	No; 2 violations: XLOGP3>5, Rotors>15	0.55
39	3,3,6-trimethyl-2,5-heptanedione	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
40	Hexadecanoic, methylester	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	yes	No; 1 violation: XLOGP3>5	0.55
41	Propanoic acid, 2-methyl-3-Phenyl-2-propenyl ester	yes	yes	yes	yes	yes	0.55
42	2,4-dimethyl-1-phenyl-1,3-pentanedione	yes	yes	yes	yes	yes	0.55
43	8-acetyl-7A-[(acetyloxy)methyl]-5B-hydroxy-5A-methyl-3-oxo-1a,3,4,5,5a,5b,6,7,9,10,10a,10b,10c-tetradeca -hydro-7ah-	yes	yes	yes	yes	yes	0.55

	cyclopental[1,2]phenanthro[9,10-b]oxiren-6-yl acetate						
44	Hexadecanoic acid	Yes; 1 violation: MLOGP >4.15	yes	No; 1 violation: Rotors >10	yes	No; 1 violation: XLOGP3>5	0.85
45	Menthylacetate	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
46	2-pentanone,5-(2-methylenecyclohexyl)-,stereoisomer	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
47	9, 12-octadecadienoic acid (Z, Z)-methyl ester	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	No; 1 violation: WLOGP>5.88	No; 1 violation: XLOGP3>5	0.55
48	9, 12, 15-octadecatrienoic acid, methyl ester (Z, Z, Z)	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	yes	No; 1 violation: XLOGP3>5	0.55
49	2-Undecen-4-ol	yes	yes	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
50	8-tetradecyn-1-ol	yes	yes	yes	yes	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
51	Cyclohexanol,1-methyl-,acetate	yes	No; 1 violation: MW<160	yes	yes	No; 1 violation: MW<200	0.55
52	Octadecanoic acid	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Rotors>15	0.85
53	1, 5-dodecadiene	Yes; 1 violation: MLOGP >4.15	yes	yes	yes	No; 3 violations: MW<200, XLOGP3>5, Heteroatoms<2	0.55
54	Estran-3-one, 17-(acetyloxy)-2-methyl, (2alpha, 5alpha, 17beta)	yes	yes	Yes	yes	yes	0.55
55	Phytol,acetate	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	No; 1 violation: WLOGP>5.88	No; 1 violation: XLOGP3>5	0.55
56	1, 1-diacetoxy-9, 9-diformylnona-2,4,6,8-tetraene	yes	yes	yes	yes	yes	0.55
57	Z-(13, 14-epoxy) tetradec-11-en-1-ol acetate	yes	yes	No; 1 violation: Rotors >10	yes	yes	0.55
58	Methyl (9Z)-12-hydroxy-9-octadecenoate	yes	yes	No; 1 violation:	yes	No; 2 violations: XLOGP3>5, Rotors>15	0.55

				Rotors >10			
59	1-(1H-imidazol-2-yl)ethanone	yes	No; 3 violations: MW<160, MR<40, #atoms<20	yes	yes	No; 1 violation: MW<200	0.55
60	Aceticacid,4-[2-(acetylamino)-3-oxobutyl]phenylester	yes	yes	yes	yes	yes	0.55
61	2-hexenoicacid,3,4,4-trimethyl-5-oxo-,(E)-	yes	yes	yes	yes	No; 1 violation: MW<200	0.85
62	3,5-heptanedione,2,2,6,6-tetramethyl	yes	yes	yes	yes	No; 1 violation: MW<200	0.55
63	Nonanoic acid	yes	No; 1 violation: MW<160	yes	yes	No; 1 violation: MW<200	0.85
64	3-O-acetyl-1,4-anhydro-2,5-di-O-methyl-D-xylitol	yes	yes	yes	yes	yes	0.55
65	5-(3-butanon-1-yl)-2,8-dimethyl-4, 6-nonanedione	yes	yes	yes	yes	yes	0.55
66	Acetic acid, 2-(2-acetyl-3-oxoisoxazolidin-5-yl)-1-methyl ethyl ester	yes	yes	yes	yes	yes	0.55
67	3,5-dimethyl-cyclohexanol	yes	No; 2 violations: MW<160, MR<40	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
68	6,7-dihydroxy-2,11-dimethyl-5,7-dodecadiene-4,9-dione	yes	yes	yes	yes	yes	0.85
69	1,2-benzenedicarboxylic acid	yes	No; 1 violation: #atoms<20	yes	yes	No; 1 violation: MW<200	0.85
70	4,4-dimethyl-hexanal	yes	No; 1 violation: MW<160	yes	yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
71	2-monolinolenin	yes	yes	No; 1 violation: Rotors >10	yes	No; 1 violation: Rotors>15	0.55
72	1-(2-hydroxy-7,9a,11b-trimethylhexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-9-yl)ethanone	yes	yes	yes	yes	yes	0.55
73	1-(1-heptadecynyl)cyclopentanol	Yes; 1 violation: MLOGP >4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors >10	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
74	3.beta.-acetoxy-17.alpha.-methyl-d-homoandrostane-17a-one	Yes; 1 violation: MLOGP >4.15	yes	yes	yes	No; 1 violation: XLOGP3>5	0.55
75	2,4,7,14-tetramethyl-4-	Yes; 1	yes	yes	yes	No; 2 violations:	0.55

	vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	violation: MLOGP >4.15				XLOGP3>5, Heteroatoms<2	
76	4,4-dimethyl-3,7-dioxoandrost-5-en-17-yl acetate	yes	yes	yes	yes	yes	0.55
77	Ergost-7,22-dien-9,11-epoxy-3-ol,acetate(ester)	Yes; 1 violation: MLOGP >4.15	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	yes	No; 1 violation: WLOGP>5.88	No; 1 violation: XLOGP3>5	0.55
78	4-(2,2,6-trimethylbicyclo[4.1.0]Hept-1-yl)-2-butanone	yes	yes	yes	yes	No; 1 violation: Heteroatoms<2	0.55
79	24-methyl-5-cholestene-3-ol	Yes; 1 violation: MLOGP >4.15	No; 2 violations: WLOGP>5.6, #atoms>70	yes	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
80	Stigmasta-5,22-dien-3-ol	Yes; 1 violation: MLOGP >4.15	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	yes	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
81	1H-3A,7-methanozulen-6-ol,octahydro3,6,8,8-tetramethyl	yes	yes	yes	yes	No; 1 violation: Heteroatoms<2	0.55
82	gamma.-sitosterol	Yes; 1 violation: MLOGP >4.15	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	yes	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55

* BS: Bioavailability score.

All the phytocompounds follow RO5 or Lipinski Rule of 5. However, only twenty-five phytocompounds, i.e., compounds 18, 19, 21, 22, 24, 25, 26, 27, 28, 41, 42, 43, 50, 51, 53, 54, 56, 57, 60, 64, 65, 66, 68, 72, and 76, follow all the five drug-likeness rules, namely, Lipinski, Ghose, Veber, Egen, and Muegge. Regarding the bioavailibilty, all the phytocompounds have bioavailability score of 0.55 and above indicating good pharmacokinetic properties. Using the SMILE string, the ADMET properties each of the 82 phytocompounds was predicted using pkCSM online tool (http://biosig.unimelb.edu.au/pkcsm/prediction).

The absorptional and distributional characteristics of the phytocompounds obtained are given in the **Table 7.**

TABLE 7: THE ABSORPTION AND DISTRIBUTION CHARACTERISTICS OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT ISODONTERNIFOLIUS (D. DON) KUDO

	Absorption						Distribution			
Compd. no.	**Caco2 permeability (log Papp in 10^{-6} cm/s)**	**HIA (% Absorbed)**	**Log Kp(cm/s)**	**Pgp substrate**	**Pgp ι i**	**Pgpui**	**VDsslog L/kg**	**Fu**	**log BB**	**log PS**
1	1.634	95.015	-2.355	No	No	No	0.266	0.3	0.436	-1.582
2	1.39	96.926	-1.995	No	No	No	0.236	0.381	0.452	-1.901
3	1.413	100	-2.71	No	No	No	-0.23	0.698	-0.193	-2.464
4	1.338	94.645	-2.735	No	No	No	0.008	0.704	0.216	-2.783
5	1.426	97.254	-1.695	No	No	No	0.295	0.237	0.479	-1.661
6	1.388	95.858	-1.904	No	No	No	0.695	0.413	0.78	-2.459

7	1.397	95.384	-1.587	No	No	No	0.564	0.21	0.804	-1.325
8	1.235	100	-2.804	No	No	No	-0.366	0.653	-0.273	-2.906
9	1.219	97.722	-2.643	No	No	No	-0.227	0.627	-0.212	-2.877
10	1.112	97.424	-2.005	No	No	No	-0.039	0.489	0.227	-2.236
11	1.324	98.614	-2.792	No	No	No	0.35	0.436	0.046	-2.204
12	1.426	96.202	-1.29	No	No	No	0.449	0.255	0.784	-1.437
13	1.716	93.307	-2.192	No	No	No	0.131	0.502	-0.192	-2.076
14	1.248	98.909	-2.403	No	No	No	-0.026	0.463	0.339	-2.109
15	1.21	96.485	-1.632	No	No	No	0.207	0.327	0.664	-1.836
16	1.625	96.389	-2.715	No	No	No	-0.151	0.649	0.132	-2.615
17	1.625	92.682	-1.592	No	No	No	0.626	0.195	0.568	-1.972
18	0.571	82.963	-2.771	No	Yes	No	-0.378	0.211	-0.832	-2.868
19	1.07	95.73	-3.33	No	Yes	No	0.019	0.29	-0.156	-2.29
20	1.491	96.936	-2.877	No	No	No	0.145	0.372	0.279	-2.134
21	0.306	81.748	-2.514	No	No	No	-0.21	0.595	-1.305	-3.068
22	1.219	94.291	-2.657	No	No	No	0.056	0.481	0.112	-2.753
23	1.387	96.225	-1.762	No	No	No	0.462	0.112	0.659	-1.495
24	0.734	90.658	-3.317	Yes	No	No	0.039	0.199	0.121	-2.288
25	1.239	97.392	-2.005	No	No	No	0.307	0.413	0.646	-2.149
26	1.227	91.734	-2.848	No	No	No	-0.125	0.292	-0.182	-2.569
27	1.708	97.729	-2.563	No	No	No	0.197	0.252	0.646	-2.341
28	1.338	95.227	-3.784	No	No	No	0.367	0.296	0.054	-2.857
29	1.208	98.477	-3.603	No	No	No	-0.106	0.704	-0.216	-3.014
30	1.658	93.658	-1.626	No	No	No	0.845	0.07	0.518	-1.913
31	1.576	94.58	-3.635	No	No	No	0.052	0.618	0.354	-3.168
32	1.401	97.754	-1.772	No	No	No	0.336	0.195	0.503	-1.57
33	1.425	92.85	-2.518	No	No	Yes	0.692	0	0.983	-1.299
34	1.82	96.202	-1.915	No	No	No	0.062	0.432	0.552	-2.414
35	1.515	90.71	-2.576	No	No	Yes	0.468	0	0.806	-1.563
36	1.584	94.781	-1.865	No	No	No	0.214	0.373	0.45	-2.585
37	1.461	95.863	-1.706	No	No	No	0.268	0.11	0.806	-0.6
38	0.52	94.463	-2.718	No	Yes	Yes	-0.315	0.059	-0.97	-3.116
39	1.429	96.618	-2.147	No	No	No	-0.091	0.511	0.361	-2.236
40	1.6	92.335	-2.595	No	No	No	0.334	0.074	0.749	-1.678
41	1.699	96.779	-1.763	No	No	No	0.238	0.151	0.325	-1.561
42	1.196	97.399	-2.251	No	No	No	0.091	0.215	0.287	-1.744
43	0.883	94.418	-3.064	Yes	Yes	No	-0.015	0.27	-0.777	-3.004
44	1.558	92.004	-2.717	No	No	No	-0.543	0.101	-0.111	-1.816
45	1.698	96.497	-2.208	No	No	No	0.125	0.439	0.539	-2.39
46	1.238	95.585	-1.558	No	No	No	0.25	0.265	0.673	-1.768
47	1.612	92.66	-2.719	No	No	Yes	0.272	0.028	0.767	-1.463
48	1.619	93.166	-2.675	No	No	Yes	0.246	0.029	0.757	-1.41
49	1.485	92.414	-1.371	No	No	No	0.287	0.356	0.666	-2.064
50	1.486	92.303	-1.765	No	No	No	0.357	0.198	0.737	-1.687
51	1.602	96.442	-2.69	No	No	No	0.078	0.614	0.216	-2.997
52	1.556	91.317	-2.726	No	No	No	-0.528	0.051	-0.195	-1.707
53	1.385	93.402	-1.214	No	No	No	0.542	0.214	0.864	-1.582
54	1.413	97.238	-3.175	No	Yes	No	0.298	0.061	0.234	-2.203
55	1.174	92.822	-2.753	No	No	Yes	0.364	0	0.766	-1.603
56	0.862	98.346	-2.616	No	Yes	No	-0.479	0.388	-0.753	-3.095
57	1.661	95.058	-4.38	No	Yes	No	0.198	0.179	-0.034	-2.242
58	1.534	90.69	-2.769	No	No	Yes	0.1	0.114	0.101	-1.892
59	1.602	100	-2.735	Yes	No	No	0.012	0.683	0.606	-2.107
60	0.585	79.827	-3.307	No	No	No	-0.268	0.359	-0.339	-2.745
61	1.22	97.609	-2.734	No	No	No	-0.899	0.576	-0.115	-2.885
62	1.092	97.63	-2.061	No	No	No	-0.142	0.398	0.246	-1.814
63	1.565	94.409	-2.687	No	No	No	-0.734	0.419	0.184	-2.198
64	1.189	100	-3.219	No	No	No	-0.261	0.731	-0.29	-3.025
65	1.558	98.547	-2.457	No	Yes	No	-0.146	0.248	-0.393	-2.485
66	0.921	100	-2.703	No	No	No	-0.221	0.665	-0.602	-3.001

67	1.49	94.385	-2.582	Yes	No	No	0.134	0.617	0.154	-2.652
68	1.49	94.385	-2.582	Yes	No	No	0.134	0.617	0.154	-2.888
69	0.641	75.609	-2.735	No	No	No	-1.775	0.497	-0.038	-2.891
70	1.503	95.799	-1.749	No	No	No	0.098	0.524	0.629	-2.231
71	0.444	91.109	-2.811	No	Yes	Yes	-0.381	0.151	-0.267	-3.174
72	1.227	95.156	-3.553	No	Yes	No	0.259	0.123	-0.078	-1.799
73	1.478	89.887	-2.729	No	No	Yes	0.514	0	0.805	-1.769
74	1.18	98.151	-3.219	No	Yes	Yes	0.31	0.002	-0.124	-2.327
75	1.521	94.297	-2.569	No	No	No	0.541	0.011	0.65	-1.957
76	1.468	99.173	-3.454	No	Yes	Yes	0.187	0.09	-0.273	-1.592
77	1.193	97.003	-3.464	No	Yes	Yes	0.43	0	0.207	-2.333
78	1.352	95.368	-1.823	No	No	No	0.378	0.207	0.676	-1.917
79	1.223	94.543	-2.86	No	Yes	Yes	0.427	0	0.774	-1.758
80	1.213	94.97	-2.783	No	Yes	Yes	0.178	0	0.771	-1.652
81	1.496	93.844	-2.163	No	No	No	0.572	0.249	0.627	-2.216
82	1.201	94.464	-2.783	No	Yes	Yes	0.193	0	0.781	-1.705

*HIA: Human intestinal absorption, Pgp: P-Glycoprotein, Fu: Fraction unbound.

Caco-2 cell line, which was composed of human epithelial colorectal adenocarcinoma cells, is widely used to predict the absorption of orally administered drugs. The Caco2 permeability values of the phytocompounds from the aqueous methanolic leaf extract from the medicinal plant *Isodonternifolius* (D. Don) Kudo. varies from 0.306 to 1.82, indicating that the phytocompounds are poorly permeable through Caco2. According to the US Food and Drug Administration, Papp values of $<1 \times 10^{-6}$cm/s and $>10 \times 10^{-6}$cm/s indicate poor and high permeabilities, respectively.

The intestine is the primary site for the absorption of orally administered drugs. Human intestinal absorption of a compound is one of the most important parameters to be ascertained during drug development. A molecule with less than 30% absorption is considered as poorly absorbed. The absorption percentages of all the phytocompounds under consideration through the human intestine range from 75.6 to 100%. LogKp (Skin permeability) is an important parameter for monitoring drug efficacy, particularly for the one administered through transdermal route. Log Kp value > -2.5 cm/h indicates a low skin permeability.

A molecule barely penetrates the skin if its log Kp is more than -2.5 cm/h [19]. The Log Kp values of the phytocompounds in the current investigation were found to range from -4.38 to -1.21 cm/h. Out of the total 82 phytocompounds, 30 were found to have a log Kp> -2.5, indicating that they have low skin permeability. P-glycoprotein (Pgp) is a transporter protein that plays an important role in expelling molecules out of the cell. Modulation of Pgp mediated transport has significant pharmacokinetic implications for Pgp substrates, which may be exploited for specific therapeutic advantages or result in contraindications. Four out of the total 82 phytocompounds, *viz.* compound 24, 43, 59, 67 and 68, were Pgp substrates. A total of sixteen compounds, *viz.* compounds 18, 19, 38, 43, 54, 56, 57, 65, 71, 72, 74, 76, 77, 79, 80, and 82, were predicted to be the inhibitors of Pgp I. Fifteen compounds, *viz.* Compounds 33, 35, 37, 47, 48, 55, 58, 71, 73, 74, 76, 77, 79, 80, and 82 were predicted as inhibitors of Pgp II.

The volume of distribution (VD) is the theoretical volume that the total drug dose would need to be distributed to give the same concentration as in blood plasma. The higher the VD is, the larger the amount of a drug is distributed to tissue rather than plasma. This model is established by estimating the steady-state volume of distribution (VDss), which is then revealed as log L/kg. VDss higher than 2.81 L/kg (log VDss> 0.45) is categorized as high, whereas VDss lower than 0.71 L/kg (log VDss< -0.15) is categorized as low [20].

The pharmacokinetic parameter, Steady State Volume of Distribution (VD_{ss}), determines drug distribution within tissues. Compounds having higher VDss value are distributed more into a tissue rather than plasma. Log VD_{ss} values above 0.45 and below 0.15 are considered as high and low VD_{ss}. Eleven compounds (6, 7, 17, 23, 30, 33, 35, 53, 73, 75, and 81) were highly distributed with log Vd_{ss} values ranging between 0.462 and 0.845. And the other seventeen phytocompounds (3, 8, 9, 16, 18, 21, 39, 44, 52, 56, 60, 61, 63, 64, 66, 69, and 71)

were predicted to be poorly distributed with log VD_{ss} values ranging from-0.21 to-1.775. On the other hand, the remaining phytocompounds were found to be moderately distributed. The fraction unbound (fu) is one factor determining a drug's efficacy in pharmacodynamic and pharmacokinetic analysis. Most of the drugs in plasma exist in equilibrium between an unbound state and a bound state in which the drug is bound to the serum proteins. Generally, the unbound fraction of a drug is able to diffuse between plasma and tissues and interact with the target proteins, *viz.*, receptors, channels, and enzymes. The hepatic metabolism and glomerular filtration are also greatly influenced by fu [21].

The fraction of the unbound state of the phytocompounds ranges from 0 to 0.731. LogBB, or blood brain permeability, is an important parameter to assess a drug's side effects, toxicities, and efficacy. LogBB values of the phytocompounds range from -1.305 to 0.983. Thirty-four phytocompounds (1, 2, 5, 7, 12, 15, 17, 23, 30, 32, 33, 35, 37, 40, 41, 42, 44, 46, 47, 48, 50, 52, 53, 55, 58, 62, 72, 73, 75, 76, 78, 79, 80, and 82) out of the total of eighty-two phytocompounds were predicted to readily cross the blood brain barrier (BBB).

Only one phytocompound (21) having a LogBB value of -1.305 was found to cross the BBB membrane poorly, while the other remaining phytocompounds could diffuse moderately into the brain. LogPS (permeability surface-area product) is a commonly used descriptor of BBB permeability, which measures the initial permeability rate and considering BBB penetration, it is more appropriate and informative than logBB.

This enables a direct measurement of BBB apparent permeability, thereby eliminating serum binding effects of the compound in question. It is measured in ml/min/g of brain. It is the pharmacokinetic uptake clearance across the BBB into the brain [22].

Regarding CNS permeability, compounds with a log PS greater than -2 and less than -3 are classified as able to and unable to penetrate the CNS. The Log PS values of the phytocompounds under the present study range from -3.16 to -0.6. As the fate of a given drug is greatly influenced by its metabolism, metabolic prediction of compounds is crucial during drug discovery. The detoxification enzyme cytochrome P-450, found primarily in the liver, facilitates the excretion of xenobiotics from the body by carrying out oxidation. The cytochrome P-450 can activate or deactivate many drugs and is responsible for drug metabolism inside our body. It is important to evaluate whether the drug is a cytochrome P450 substrate or inhibitor, as the drug's pharmacokinetics may be altered dramatically by P450 inhibitors. There are two main isoforms of cytochrome, *viz.* P3A4 cytochrome (CYP3A4) and P2D6 cytochrome (CYP2D6) play vital roles in drug metabolism [23].

None of the phytocompounds were predicted as the substrate of CYP2D6. Thirty-five phytocompounds (18, 19, 23, 24, 27, 28, 30, 33, 35, 37, 38, 40, 43, 44, 47, 48, 50,52, 54, 55, 56, 57, 58, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81 and 82) out of the total eighty-two phytocompounds were found to be CYP3A4 substrate. And twenty-five phytocompounds (1, 5, 6, 7, 17, 20, 23, 27, 30, 32, 33, 35, 37, 40, 41, 42, 47, 48, 50, 52, 55, 58, 73, 75 and 81) were CYP1A2 inhibitors.

Out of the total phytocompounds, four (27, 54, 75 and 81) were predicted as CYP2C19 inhibitors. Only one compound (75) was found to be CYP2C9 inhibitor. None of the compounds were predicted as the inhibitors of CYP2D6 and CYP3A4. OCT2 or organic cation transporter 2 plays an important role in disposition and renal clearance of drugs and endogenous compounds.

The excretion profiles of all the phytocompounds were predicted based on total clearance, which is a combination of hepatic and renal clearance. Total clearance of all the phytocompounds ranges from -8.021 to 2.217 log mL/min/kg. Compound numbers 71 and 4 showed the highest and lowest total clearance of the phytocompounds.

Only five compounds (19, 57, 65, 72 and 76) were predicted to be the substrate of OCT2 or organic cation transporter 2. The characteristics regarding the metabolism and excretion of the compounds are given in **Table 8.**

TABLE 8: METABOLISM AND EXCRETION CHARACTERISTICS OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT FROM THE MEDICINAL PLANT ISODONTERNIFOLIUS (D. DON) KUDO

	Metabolism							Excretion	
Com. no.	**CYP2D6 substrate**	**CYP3A4 substrate**	**CYP1A2 inhibitior**	**CYP2C19 inhibitior**	**CYP2C9 inhibitior**	**CYP2D6 inhibitior**	**CYP3A4 inhibitior**	**Total Clearance (log ml/min/kg)**	**Renal OCT2 substrate**
1	No	No	Yes	No	No	No	No	0.203	No
2	No	No	No	No	No	No	No	0.26	No
3	No	No	No	No	No	No	No	0.734	No
4	No	No	No	No	No	No	No	-8.021	No
5	No	No	Yes	No	No	No	No	0.311	No
6	No	No	Yes	No	No	No	No	0.052	No
7	No	No	Yes	No	No	No	No	1.243	No
8	No	No	No	No	No	No	No	0.929	No
9	No	No	No	No	No	No	No	0.807	No
10	No	No	No	No	No	No	No	0.453	No
11	No	No	No	No	No	No	No	0.173	No
12	No	No	Yes	No	No	No	No	0.232	No
13	No	No	No	No	No	No	No	0.156	No
14	No	No	No	No	No	No	No	0.159	No
15	No	No	No	No	No	No	No	0.271	No
16	No	No	No	No	No	No	No	0.788	No
17	No	No	Yes	No	No	No	No	0.406	No
18	No	Yes	No	No	No	No	No	0.707	No
19	No	Yes	No	No	No	No	No	1.238	Yes
20	No	No	Yes	No	No	No	No	0.22	No
21	No	No	No	No	No	No	No	1.236	No
22	No	No	No	No	No	No	No	1.237	No
23	No	Yes	Yes	No	No	No	No	0.262	No
24	No	Yes	No	No	No	No	No	0.519	No
25	No	No	No	No	No	No	No	0.095	No
26	No	No	Yes	No	No	No	No	0.233	No
27	No	Yes	Yes	Yes	No	No	No	0.417	No
28	No	Yes	No	No	No	No	No	0.703	No
29	No	No	No	No	No	No	No	0.571	No
30	No	Yes	Yes	No	No	No	No	1.101	No
31	No	No	No	No	No	No	No	1.097	No
32	No	No	Yes	No	No	No	No	0.368	No
33	No	Yes	Yes	No	No	No	No	1.764	No
34	No	No	No	No	No	No	No	0.706	No
35	No	Yes	Yes	No	No	No	No	1.686	No
36	No	No	No	No	No	No	No	1.387	No
37	No	Yes	Yes	No	No	No	No	0.467	No
38	No	Yes	No	No	No	No	No	2.184	No
39	No	No	No	No	No	No	No	0.484	No
40	No	Yes	Yes	No	No	No	No	1.861	No
41	No	No	Yes	No	No	No	No	0.302	No
42	No	No	Yes	No	No	No	No	0.343	No
43	No	Yes	No	No	No	No	No	0.622	No
44	No	Yes	No	No	No	No	No	1.763	No
45	No	No	No	No	No	No	No	1.207	No
46	No	No	No	No	No	No	No	1.348	No
47	No	Yes	Yes	No	No	No	No	2.032	No
48	No	Yes	Yes	No	No	No	No	2.086	No
49	No	No	No	No	No	No	No	1.738	No
50	No	Yes	Yes	No	No	No	No	1.791	No
51	No	No	No	No	No	No	No	1.227	No
52	No	Yes	Yes	No	No	No	No	1.832	No

53	No	No	No	No	No	No	No	1.844	No
54	No	Yes	No	Yes	No	No	No	0.629	No
55	No	Yes	Yes	No	No	No	No	1.684	No
56	No	Yes	No	No	No	No	No	0.686	No
57	No	Yes	No	No	No	No	No	1.652	Yes
58	No	Yes	Yes	No	No	No	No	2.005	No
59	No	No	No	No	No	No	No	-0.07	No
60	No	No	No	No	No	No	No	0.466	No
61	No	No	No	No	No	No	No	0.897	No
62	No	No	No	No	No	No	No	0.394	No
63	No	No	No	No	No	No	No	1.516	No
64	No	No	No	No	No	No	No	0.785	No
65	No	No	No	No	No	No	No	1.569	Yes
66	No	No	No	No	No	No	No	1.51	No
67	No	No	No	No	No	No	No	0.143	No
68	No	No	No	No	No	No	No	0.558	No
69	No	No	No	No	No	No	No	0.682	No
70	No	No	No	No	No	No	No	0.424	No
71	No	Yes	No	No	No	No	No	2.217	No
72	No	Yes	No	No	No	No	No	0.525	Yes
73	No	Yes	Yes	No	No	No	No	1.703	No
74	No	Yes	No	No	No	No	No	0.548	No
75	No	Yes	Yes	Yes	Yes	No	No	0.852	No
76	No	Yes	No	No	No	No	No	0.415	Yes
77	No	Yes	No	No	No	No	No	0.392	No
78	No	Yes	No	No	No	No	No	0.921	No
79	No	Yes	No	No	No	No	No	0.572	No
80	No	Yes	No	No	No	No	No	0.618	No
81	No	Yes	Yes	Yes	No	No	No	0.837	No
82	No	Yes	No	No	No	No	No	0.628	No

Assessment of the toxicity of compounds is also an important step in the process of drug discovery [24]. Therefore, the toxicity profile of all the phytocompounds under consideration was assessed, and the values are given in **Table 9.**

TABLE 9: TOXICITY PROFILING OF THE PHYTOCOMPOUNDS FROM THE AQUEOUS METHANOLIC LEAF EXTRACT OF THE MEDICINAL PLANT *ISODONTERNIFOLIUS* (D. DON) KUDO

	Toxicity									
Com. no.	**AMES toxicity**	**Max. tolerated dose (human) (log mg/kg/ day)**	**hERG I inhibitor**	**hERG II inhibitor**	**LD50 (mol/ kg)**	**LOAEL (log mg/kg_bw/day)**	**Hepatot-oxicity**	**Skin Sensiti-sation**	**T.Pyriformis toxicity (log µg/L)**	**Minnow toxicity (log mM)**
1	No	0.876	No	No	1.88	1.944	No	Yes	0.665	1.605
2	Yes	0.907	No	No	1.887	1.907	No	Yes	0.236	1.59
3	No	1.076	No	No	1.851	2.379	No	Yes	-0.709	2.321
4	Yes	0.429	No	No	2.482	3.388	No	No	0.285	6.485
5	Yes	1.048	No	No	1.92	2.09	No	Yes	0.875	0.714
6	No	0.48	No	No	1.797	2.317	No	No	0.652	1.193
7	No	-0.04	No	No	1.56	2.46	No	No	1.09	0.542
8	No	0.973	No	No	2.737	2.462	No	Yes	-0.367	2.204
9	No	0.87	No	No	1.867	2.553	No	Yes	-0.197	1.849
10	No	0.851	No	No	1.726	2.413	Yes	No	0.422	1.281
11	No	0.338	No	No	1.715	2.218	No	Yes	0.512	1.595
12	No	0.223	No	No	1.382	2.28	No	No	1.09	0.644
13	No	0.527	No	No	2.06	2.314	No	Yes	0.041	1.882
14	No	0.851	No	No	1.67	2.343	No	Yes	0.329	1.682
15	No	0.573	No	No	1.653	2.082	No	Yes	0.708	1.024
16	No	1.057	No	No	1.967	2.234	No	Yes	-0.248	2.074
17	No	0.934	No	No	2.086	1.26	No	Yes	1.057	0.865
18	No	0.645	No	No	2.329	1.844	No	No	0.883	-0.038

19	No	0.046	No	No	1.975	1.701	No	No	1.156	1.473
20	Yes	0.809	No	No	1.857	1.775	No	Yes	0.527	1.822
21	No	0.772	No	No	3.056	1.119	No	No	0.255	4.36
22	No	0.567	No	No	1.911	1.9	No	Yes	0.663	1.763
23	No	0.797	No	No	1.781	1.2	No	Yes	2.059	-0.414
24	No	-0.683	No	No	2.091	1.362	Yes	No	0.315	1.138
25	No	0.544	No	No	1.759	1.94	No	Yes	0.482	1.354
26	No	1.338	No	No	2.029	1.884	No	No	0.385	2.066
27	No	0.913	No	No	2.193	1.68	No	No	1.028	-0.023
28	No	-0.162	No	No	1.763	1.553	No	No	0.672	1.556
29	No	1.069	No	No	2.313	2.295	Yes	No	-0.629	2.283
30	No	0.947	No	No	2.019	1.199	No	Yes	2.091	-0.848
31	No	0.979	No	No	1.713	2.494	No	Yes	-0.394	2.169
32	No	1.169	No	No	1.896	1.465	No	Yes	1.186	0.419
33	No	0.272	No	Yes	1.473	1.158	No	Yes	1.65	-2.039
34	No	0.618	No	No	1.785	2.163	No	Yes	1.18	0.974
35	No	0.05	No	Yes	1.607	1.043	No	Yes	1.884	-1.504
36	No	0.643	No	No	2.209	1.139	No	Yes	1.128	1.085
37	No	-0.258	No	No	1.189	1.598	No	Yes	1.274	0.075
38	No	0.328	No	No	1.83	0.507	No	No	0.477	-0.835
39	No	0.859	No	No	1.748	2.126	No	Yes	0.377	1.328
40	No	0.178	No	No	1.635	2.998	No	Yes	1.935	-1.373
41	No	1.102	No	No	1.771	2.222	No	Yes	1.823	-0.596
42	No	1.324	No	No	1.584	2.451	No	Yes	1.276	0.408
43	Yes	-0.661	No	No	3.797	2.292	No	No	0.288	3.47
44	No	-0.708	No	No	1.44	3.181	No	Yes	0.84	-1.083
45	No	0.747	No	No	1.823	2.04	No	Yes	0.877	1.335
46	No	0.33	No	No	1.673	1.335	No	Yes	1.19	0.62
47	No	-0.019	No	No	1.617	3.004	No	Yes	1.603	-1.6
48	No	-0.078	No	No	1.596	2.932	No	Yes	1.668	-1.473
49	No	0.522	No	No	1.6	2.191	No	Yes	1.427	0.557
50	No	0.028	No	No	1.437	1.232	No	Yes	2.316	-0.075
51	No	0.76	No	No	2.155	2.002	Yes	Yes	-0.388	1.825
52	No	-0.791	No	No	1.406	3.33	No	Yes	0.65	-1.565
53	No	0.292	No	No	1.485	2.658	No	Yes	1.834	-0.204
54	No	-0.808	No	No	1.829	1.75	No	No	1.022	0.124
55	No	0.094	No	No	1.664	2.929	No	Yes	1.604	-2.113
56	No	0.417	No	No	1.784	0.801	No	No	0.374	1.283
57	No	0.164	No	No	1.607	2.351	No	Yes	2.09	-1.287
58	No	0.199	No	No	1.581	2.852	No	Yes	1.394	-1.23
59	Yes	0.324	No	No	2.482	4.008	No	No	0.285	4.367
60	No	0.744	No	No	2.146	1.473	No	No	0.632	2.189
61	No	0.725	No	No	1.765	2.679	No	No	0.102	1.922
62	No	0.889	No	No	1.675	2.182	No	Yes	0.452	0.856
63	No	0.1	No	No	1.54	2.68	No	Yes	0.499	0.762
64	Yes	0.852	No	No	2.175	0.852	No	Yes	-0.709	2.923
65	No	0.712	No	No	1.616	2.174	No	No	1.116	0.165
66	Yes	0.504	No	No	2.636	0.991	No	No	-0.326	1.895
67	No	1.038	No	No	1.921	1.82	No	Yes	-0.526	2.098
68	No	0.778	No	No	1.739	2.34	No	No	0.809	1.309
69	No	0.582	No	No	1.449	2.165	No	No	0.281	2.378
70	No	0.85	No	No	1.815	2.011	No	Yes	0.157	1.249
71	No	-0.005	No	No	1.593	2.656	No	Yes	0.562	-0.587
72	No	-0.734	No	No	1.978	1.598	No	No	0.618	0.778
73	No	-0.407	No	Yes	1.707	0.914	No	Yes	1.682	-1.411
74	No	-0.89	No	No	1.851	1.749	No	No	0.995	-0.035
75	No	-0.607	No	Yes	1.841	1.183	Yes	No	1.619	-0.139
76	No	-0.499	No	No	2.035	1.297	No	No	0.597	0.428
77	No	-0.302	No	No	1.705	1.956	No	No	0.504	-1.311
78	No	0.068	No	No	1.728	1.196	No	Yes	1.399	0.714

79	No	-0.458	No	Yes	2.08	0.892	No	No	0.631	-1.94
80	No	-0.664	No	Yes	2.54	0.872	No	No	0.433	-1.675
81	No	-0.036	No	No	1.666	1.254	No	Yes	1.363	0.851
82	No	-0.621	No	Yes	2.552	0.855	No	No	0.43	-1.802

By the toxicity analysis of the phytocompounds by pkCSM, eight phytocompounds (2, 4, 5, 20, 43, 59, 64 and 66) were predicted to be mutagenic as per AMES test result. The toxic dose threshold of the phytocompounds in humans was also estimated based on maximum recommended tolerated dose (MRTD). MRTD is considered as low and high if it is less than or equal to 0.477 log (mg/kg/day) and greater than 0.477 log (mg/kg/day). From the analysis, MRTD of the phytocompounds under investigation was found to range from -0.89 to 1.338 log (mg/kg/day).

More than 53% of the phytocompounds *i.e*, forty four phytocompounds (1, 2, 3, 5, 6, 8, 9, 10, 13, 14, 15, 16, 17, 18, 20, 21, 22, 23, 25, 26, 27, 29, 30, 31, 32, 34, 36, 39, 41, 42, 45, 49, 51, 60, 61, 62, 64, 65, 66, 67, 68, 69, 70 and 74) were predicted to have high MRTD. All the phytocompounds were not inhibitors of Herg I. Only seven phytocompounds of the total identified phytocompounds (33, 35, 73, 75, 79, 80 and 82) were predicted as inhibitors of heRG II. LD_{50} or lethal dosage values are a standard measurement of acute toxicity and are used to assess the relative toxicity of different molecules. The LD_{50} values of the phyto-compounds range from 1.406 to 3.797mol/kg. The predicted lowest dose of a compound observed adverse effect (LOAEL) values of the phytocompounds under study range from log 0.507 to 4.008 log mg/kgbw/day. Regarding hepato-toxicity of the phytocompounds under study, only five phytocompounds (10, 24, 29, 51 and 75) were predicted as hepatotoxic. Fifty phytocompounds among the phytocompounds under study were predicted to be associated with skin sensitization. From the toxicity analysis, *T. pyriformis* toxicity values of the phytocompounds were found to range from -0.709 to 2.316log µg/L.

T. pyriformis toxicity values greater than -0.5 log µg/L is considered as toxic. Except for three phytocompounds (Nos. 3, 64 and 67) all other phytocompounds were found to have pIGC50 (negative logarithm of the concentration required to inhibit 50% growth in log µg/L) values greater than -0.5 log µg/L indicating that they have antibacterial property. LC_{50} (lethal concentration) values of all the phytocompounds were also evaluated. LC_{50} value is the compound concentration necessary to cause the death of 50% of the Flathead Minnows. Thirty-two phytocompounds (18, 23, 27, 30, 32, 33, 35, 37, 38, 40, 41, 42, 44, 47, 48, 50, 52, 53, 54, 55, 57, 58, 65, 71, 73, 74, 75, 76, 77, 79, 80 and 82) among the total eighty-two phytocompounds were predicted as high or acute toxic compounds as their LC_{50} values fall below 0.5mM.

CONCLUSION: In the present study, eighty-two (82) different phytocompounds were identified in the methanolic extract from the medicinal plant leaf, *Isodon ternifolius* (D. Don) Kudo by GC-MS analysis.

The physicochemical properties of all the phytocompounds were predicted using the SwissADME web tool, and their ADMET properties were also predicted using the pkCSM online server tool. Out of the phytocompounds, twenty-five were found to follow all the five drug-likeness rules, *viz.,* Lipinski, Ghose, Veber, Egen, and Muegge. These results may be useful in further *in-vitro* and *in-vivo* experimentation that might lead to the discovery of drugs from the concerned traditional medicinal plant.

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CONFLICTS OF INTEREST: Nil

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