Phytochemical characterization of medicinal plants-*Houttuynia cordata* and *Potentilla fulgens* Wall. Ex Sims using *in vitro* and *in silico* methods

Careen Liza Pakyntein[1], Daiahun Thabah[1], Donkupar Syiem[*]

[*,1] Department of Biochemistry, School of Life Sciences, North-Eastern Hill University, Shillong-793022, Meghalaya, India

INTRODUCTION: India is a land of immense biodiversity with over 6000 plants used in traditional,folk, and herbal medicine, representing about 75% of the medicinal needs of the Third World countries. Several substances derived from plants are currently used as drugs. However, the pharmacological properties of many of these metabolites are still unknown. Therefore, in-depth phytochemical screening and evaluation of these plants are valuable to understand the complete action of the plant as a whole.

MATERIALS AND METHODS:*Houttuynia cordata* and *Potentilla fulgens* were collected from Meghalaya, India and extracted with 10 volumes solvent and the crude powder obtained was used for HPTLC, GCMS/MS and FTIR profiling. Compounds identified were then characterized for their adsorption, distribution, metabolism, excretion, and toxicity properties.

RESULTS:

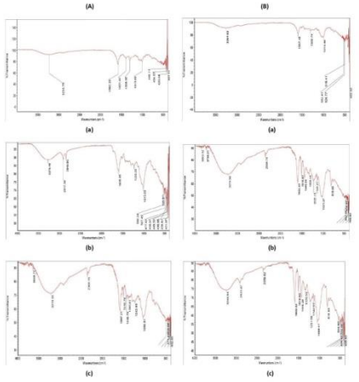

Fig1. FTIR Spectrum of (A) *Houttuynia cordata* (HC), and (B) *Potentilla fulgens* (PF)

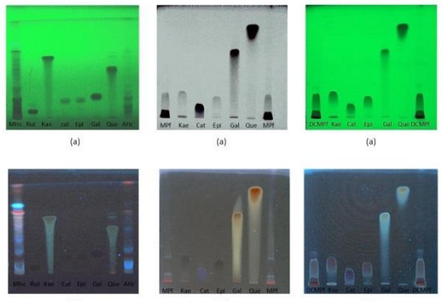

Fig2. HPTLC profiles of (A) Aqueous extract of HC (AHC), (B).Methanolic extract of HC (MHC) and (C) Dichloromethane extract of PF (DCMPF)

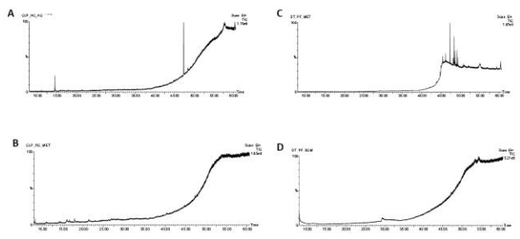

Fig3. GCMS chromatogram of HC and PF

Table 1: Compounds identified from HC using GCMS/MS

Sl. No.	Compounds	Molecular formula	Molecular weight(gms)
1	1R,-Alpha,-pinene	$C_{10}H_{16}$	136
2	3-carene	$C_{10}H_{16}$	136
3	Alpha,-pinene	$C_{10}H_{16}$	136
4	Bicyclo[3.1.0]hex-2-ene,2-methyl-5-(1-methylethyl)-	$C_{10}H_{16}$	136
5	D-Limonene	$C_{10}H_{16}$	136
6	Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)-	$C_{10}H_{16}$	136
7	Hexanedioic acid, bis (2-ethylhexyl)ester	$C_{22}H_{42}O_4$	370
8	Hexanedioic acid, mono(2-ethylhexyl)ester	$C_{14}H_{26}O_4$	258
9	2-ethylpiperidine	$C_7H_{15}N$	113
10	Cyclohexylamine, N-ethyl-	$C_8H_{17}N$	127
11	4-piperidinecarboxylic acid hydrazide	$C_6H_{13}ON_3$	143
12	Piperidine, 1-acetyl-	$C_7H_{13}ON$	127
13	1-ethyl-2-pyrrolidinone	$C_6H_{11}ON$	113
14	Heptane, 1,1'-oxybis-	$C_{14}H_{30}O$	214
15	1-propanamine, 2- methyl –n-(3- methylbutylidene)-	$C_9H_{19}N$	141
16	1-butanmine, 2-methyl-n-(2- methylbutylidene)-	$C_{10}H_{21}N$	155
17	Piperidin-4-one, 1-ethyl-2,3-dimethyl-	$C_9H_{17}ON$	155
18	N-(5,5-dimethyl-7-oxo-4,5,6,7-tetrahydro-benothiazn	$C_{13}H_{15}O_2N_3S$	321
19	Cyclohexane, 2-hexyl-1,1,4-trimethyl-, cis-	$C_{15}H_{30}$	182
20	ISOPULEGOL	$C_{10}H_{18}O$	154
21	(Z)-3,7-dimethyl-2,7-octadien-1-ol, propanoate(ester)	$C_{13}H_{22}O_2$	210
22	Cis-1,2-dihydrocatechol	$C_6H_8O_2$	112
23	2,5-Cyclohexadiene-1,4-diol	$C_6H_8O_2$	112
24	Exo-norbornyl alcohol	$C_7H_{12}O$	112
25	1,2- Cyclohexanedione	$C_6H_8O_2$	112
26	Cyclohexanone, 4-methyl-	$C_7H_{12}O$	112
27	2-ethyl-5-propylcyclopentanone	$C_{10}H_{18}O$	154
28	Cyclohexanone, 2-methyl-	$C_7H_{12}O$	112
29	Cycloheptanone	$C_7H_{12}O$	112

Table 2: Compounds identified from PF using GCMS/MS

Sl. No.	Compounds	Molecular formula	Molecular weight (gms)
1	cis-13-eicosenoic acid 5312518	$C_{20}H_{38}O_2$	310
2	cis-11-eicosenoic acid 5282768	$C_{20}H_{38}O_2$	310
3	Cis-10-nonadecenoic acid	$C_{19}H_{36}O_2$	296
4	Trans-2-methyl-4-n-pentylthiane-x,x-dioxide	$C_{11}H_{22}O_2S$	218
5	Hexanedioic acid mono(2-ethylhexyl)ester	$C_{14}H_{26}O_4$	258
6	Hexanedioic acid bis(2-ethylhexyl)ester	$C_{22}H_{42}O_4$	370
7	oleyl alcohol trifluoroacetate 88368751	$C_{20}H_{35}O_2F_3$	364
8	oleyl alcohol heptafluorobutyrate 91754008	$C_{22}H_{35}O_2F_7$	464
9	oleyl alcohol 5284499	$C_{18}H_{36}O$	268
10	(z)-14-tricosenyl formate 5364716	$C_{24}H_{46}O_2$	366
11	9-octadecenoic acid-1,2,3-propanetriyl ester (E,E,E)-	$C_{57}H_{104}O_6$	884
12	6-octadecenoic acid 5282754	$C_{18}H_{34}O_2$	282
13	Hexanedioic acid (Z)-2-hydroxy-1-(hydroxymethyl)ethyl ester	$C_{13}H_{24}O_6$	356
14	n-propyl-11-octadecenoate 87131822	$C_{21}H_{40}O_2$	324
15	1-propyl-9,12-octadecenadienoate	$C_{21}H_{38}O_2$	322
16	cis-9-hexadecenal 5364643	$C_{16}H_{30}O$	238
17	13-octadecenal, (z)- 5364497	$C_{18}H_{34}O$	266
18	oleic acid 445639	$C_{18}H_{34}O_2$	282
19	butyl-9-hexadecenoate 14325762	$C_{20}H_{38}O_2$	310
20	17-octadecynoic acid 1449	$C_{18}H_{32}O_2$	280
21	Cis-Hexadecenal	$C_{16}H_{30}O$	238

Table3: ADME properties of Compounds identified from HC and PF.

Compounds	Pubchem Id	GI Absorption	Blood-Brain Barrier	# Lipinski's violation
Alpha Pinene	6654	Low	Yes	1
Bicyclo[3.1.0]hex-2-ene, 2-Methyl-5-(1-Methylethyl)-	17868	Low	Yes	1
3-carene	26049	Low	Yes	1
D-Limonene	440917	Low	Yes	0
Cyclohexene,1-methyl-5-(1-methylethenyl)-, (R)	12304570	Low	Yes	0
Hexanedioic acid, bis(2-ethylhexyl) ester	40468165	High	No	1
Hexanedioic acid, mono(2-ethylhexyl) ester	20342	High	Yes	0
2-ethylpiperidine	94205	High	Yes	0
Cyclohexylamine, N-ethyl-	21609	High	Yes	0
4-piperidinecarboxylic acid hydrazide	456704	High	Yes	0
Piperidine, 1-acetyl-	12858	High	No	0
1-ethyl-2-pyrrolidinone	17595	High	No	0
1-propanamine,2-methyl-n-(3-methylbutylidene)	567295	High	Yes	0
1-butanamine, 2-methyl-n-(2-methylbutylidene)-	521517	High	Yes	0
Cyclobutane,2-hexyl-1,1,4-trimethyl-, cis	91695418	Low	No	1
Isopulegol	24585	High	Yes	0
(Z)-3,7-dimethyl-2,7-octadien-1-ol, propanoate	5365067	High	Yes	0
cis-1,2-dihydrocatechol	176951	High	No	0
2,5-cyclohexadiene-1,4-diol	548773	High	No	0
Exo-norbornyl alcohol	79028	High	Yes	0
1,2-cyclohexanedione	13006	High	Yes	0
Cyclohexanone, 4-methyl-	11525	High	Yes	0
Cyclohexanone, 2-methyl-	11419	High	Yes	0
Cycloheptanone	10400	High	Yes	0
cis-13-eicosenoic acid	5312518	Low	No	1
cis-11-eicosenoic acid	5282768	Low	No	1
oleyl alcohol trifluoroacetate	88368751	Low	No	1
oleyl alcohol heptafluorobutyrate	91754008	Low	No	1
oleyl alcohol	5284499	High	No	1
(z)-14-tricosenyl formate	5364716	Low	No	1
6-octadecenoic acid	5282754	High	No	1
n-propyl-11-octadecenoate	87131822	Low	No	1
cis-9-hexadecenal	5364643	High	Yes	1
13-octadecenal, (z)-	5364497	Low	No	1
oleic acid	445639	High	No	1
butyl-9-hexadecenoate	14325762	Low	No	1
17-octadecynoic acid	1449	High	Yes	1

Table 4: Toxicity properties of compounds from HC and PF.

Compounds	Mutagenicity	Tumorigenicity	Reproductive Effectiveness	Irritant	Toxicity	Druglikeness Score
Alpha Pinene	None	None	None	High	Toxic	-1.7952
Bicyclo[3.1.0]hex-2-ene, 2- Methyl-5-(1- Methylethyl)-	None	None	None	Low	Toxic	-2.3721
3-carene	None	High	None	High	Toxic	-2.9036
D-Limonene	None	None	None	Low	Toxic	-21.855
Cyclohexene,1-methyl-5-(1-methylethenyl)-, (R)	None	None	None	None	Non-Toxic	-21.802
Hexanedioic acid, bis(2-ethylhexyl) ester	None	High	High	Low	Toxic	-17.046
Hexanedioic acid, mono(2-ethylhexyl) ester	None	High	High	Low	Toxic	-17.917
2-ethylpiperidine	None	None	None	None	Non-Toxic	-6.14521
Cyclohexylamine, N-ethyl-	None	None	None	High	Toxic	-6.8375
4-piperidinecarboxylic acid hydrazide	None	High	None	None	Toxic	-1.8604
Piperidine, 1-acetyl-	None	None	Low	None	Toxic	-1.4705
1-ethyl-2-pyrrolidinone	None	None	None	High	Toxic	4.939
1-propanamine,2-methyl-n-(3-methylbutylidene)	None	None	None	None	Non-Toxic	-0.79564
1-butanamine, 2-methyl-n-(2-methylbutylidene)-	None	None	None	None	Non-Toxic	1.7567
Cyclobutane,2-hexyl-1,1,4-trimethyl-, cis	None	None	None	High	Toxic	-17.134
Isopulegol	None	None	None	None	Non-Toxic	-21.978
(Z)-3,7-dimethyl-2,7-octadien-1-ol, propanoate	None	None	None	High	Toxic	-18.751
cis-1,2-dihydrocatechol	Low	Low	None	None	Toxic	-3.2639
2,5-cyclohexadiene-1,4-diol	None	None	None	None	Non-Toxic	-3.2045
Exo-norbornyl alcohol	None	None	None	None	Non-Toxic	-1.4207
1,2-cyclohexanedione	None	None	None	None	Non-Toxic	-13.941
Cyclohexanone, 4-methyl-	None	None	High	None	Toxic	-5.1881
Cyclohexanone, 2-methyl-	None	None	None	Low	Toxic	-7.6665
Cycloheptanone	None	None	None	None	Toxic	-9.0322
cis-13-eicosenoic acid	None	None	None	None	Non-Toxic	-26.101
cis-11-eicosenoic acid	None	None	None	None	Non-Toxic	-28.971
oleyl alcohol trifluoroacetate	None	None	None	Low	Toxic	-64.617
oleyl alcohol heptafluorobutyrate	High	None	None	Low	Toxic	-126.4
oleyl alcohol	None	None	None	Low	Toxic	-35.866
(z)-14-tricosenyl formate	None	None	None	None	Non-Toxic	-26.596
6-octadecenoic acid	None	None	None	None	Non-Toxic	-27.751
n-propyl-11-octadecenoate	None	None	None	None	Non-Toxic	-27.394
cis-9-hexadecenal	None	None	None	High	Toxic	-23.152
13-octadecenal, (z)-	None	None	None	High	Toxic	-17.802
oleic acid	High	None	None	High	Toxic	-28.971
butyl-9-hexadecenoate	None	None	None	None	Toxic	-30.127
17-octadecynoic acid	None	None	None	None	Non-Toxic	-15.577

CONCLUSION: As per the FTIR (Fig.1), HPTLC (Fig.2), and GCMS/MS analysis(Fig.3),several phytochemicals were found to bepresent in *H.cordata* and *P.fulgens.* These metabolites have been associated with numerous pharmacological functions such as antibacterial, antiprotozoal, antitumor,anti-inflammatory, antiallergic, antiviral, cytoprotective, vasoactive, hypolipidaemic, antiplatelet, antispasmodic, and antihypertensive. The compounds also had positive pharmocological properties which justifies their use as medicinal plants.

ACKNOWLEDGEMENT:

We thank Guwahati Biotech Park, Guwahati, Assam for the FTIR and GCMS analysis; UGC funded UPE program for NEHU, DRS program in Biochemistry, DST through FIST, and the Department of Biochemistry, North-Eastern Hill University, Shillong, India for providing facilities.

REFERENCES

Dubey NK, Kumar R, Tripathi P. *Curr Sci.* 2004;86(1):37-40

Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. *Adv Drug Deliv Rev*. 2001; 46:3–26.

Patel K, Patel DK. 2019. Academic Press. 457-479p.

Bondia-Pons I, Aura AM, Vuorela S, Kolehmainen M, Mykkänen H, Poutanen K. *J Cereal Sci.* 2009**;** 49(3):323-36.