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Computation Study of Jatropha Curcas L. Leaves

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ABSTRACT

Fever is a condition when the body temperature increases to more than 380C. Fever indicates the presence of a disease or other condition in the body. Fever generally occurs as a reaction of the immune system to fight viral, bacterial, fungal, or parasitic infections that cause disease. Some of the diseases that often cause fever are flu, sore throat, and urinary tract infections. Fever can happen to anyone, starting frombaby, children, to adults. This disease can be cured by using drugs that contain antipyretics, analgesics and anti-inflammatory. Jatropha leaves contain active compounds in the form of flavonoids which contain antipyretics, analgesics, and anti-inflammatory properties. Here will be explained about the content of jatropha leaves which can be used as a medicine for fever.

Keywords: fever, flavonoids, antipyretics, analgesics, anti-inflammatory

1. INTRODUCTION

Fever is an increase in body temperature characterized by an increase in the threshold point for heat regulation of the hypothalamus[1][2]. The hypothalamus heat regulation/regulatory center controls body temperature by balancing signals from peripheral neuronal receptors for cold and heat[3][5]. Fever occurs when various infectious and non-infectious processes interact with the host's defense mechanisms. Fever in most children is caused by a recognized microbiological agent and fever disappears after a short period [7][8][9].

Limit values or degrees of fever with measurements in various parts of the body as follows: axillary/axillary temperature above 37.2°C, oral/mouth temperature above 37.8°C, rectal/anus temperature above 38.0°C, forehead temperature above 38.0°C, the temperature in the ear membrane is above 38.0°C [10][12]. Meanwhile, it is said to have a high fever if the body temperature is above 39.5°C and hyperpyrexia if the temperature is above 41.1°C [13].

The most accurate measurement is to carefully place the tip of the thermometer in the anal canal or commonly called the rectum in children [14]. Four types of fever: a) Intermittent Fever Body temperature changes in regular intervals, between periods of fever and normal periods abnormally[21][22]. b) Remittance Fever There is a wide range of temperature fluctuations (more than 2°C) and the body temperature is above normal for 24 hours [15][16]. c) Recurrent Fever Short febrile period of several days interspersed with periods of normal temperature of 1-2 days [17][18]. d) Constant Fever. Body temperature will fluctuate slightly, but above normal temperature[19][23]. Etiology of Fever Broadly speaking, there are two categories of fever that often affects children, namely non-infectious fever and infectious fever[20][24].

Jatropha leaves contain saponins, flavonoids such as kaempferol, nicotoflorine, quercitin, astragalin, ricinin and vitamin C [25]. One of the secondary metabolites that can be used as fever-reducing drugs is flavonoids[26]. Flavonoids exhibit more than a hundred different bioactivities. Bioactivity shown includes antipyretic, analgesic and anti-inflammatory effects [27].

2. LITERATURE REVIEW

Fever or pyrexia is a symptom of a disease. The negative effects of fever include dehydration, lack of oxygen, nerve damage, and discomfort such as headaches, decreased appetite (anorexia), weakness, and muscle aches [28]. To reduce these negative effects, fever can be treated with antipyretics. An antipyretic drug that is often used to treat fever is paracetamol [29].

Several research results on paracetamol recently found that although it is quite safe, paracetamol has many side effects[11]. In addition, there is a possible similarity in the structure of paracetamol with flavonoids[4]. Because of the side effects that appear in long-term use of paracetamol and in large doses, it is necessary to think about alternative ways to reduce the appearance of these side effects, including through the use of traditional plants for fever therapy. Based on this description, jatropha leaves containing flavonoids are expected to have antipyretic activity that can reduce fever[30].

3. EXPERIMENTAL

3.1 Compuound and protein target preparation

Flavonoid chemical compounds that refer to previous research. The compound samples were obtained from PubChemhttps://pubchem.ncbi.nlm.nih.gov/, from Phytochem https://phytochem.nal.usda.gov/, from Switzerland the target http://swisstargetprediction.ch/, from chemdraw and chem3d

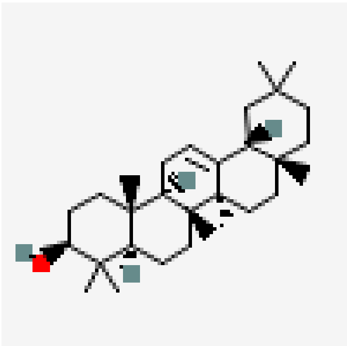
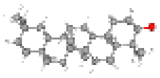
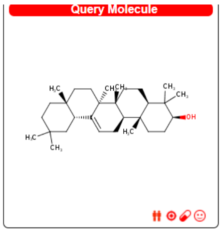
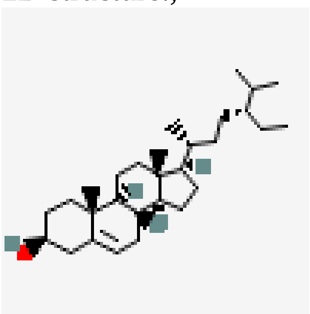
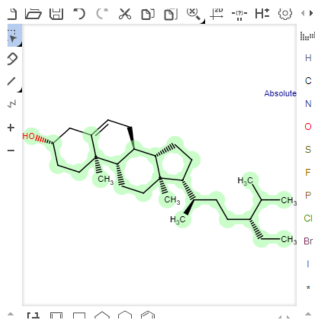
3.2 Druglikeness analysis

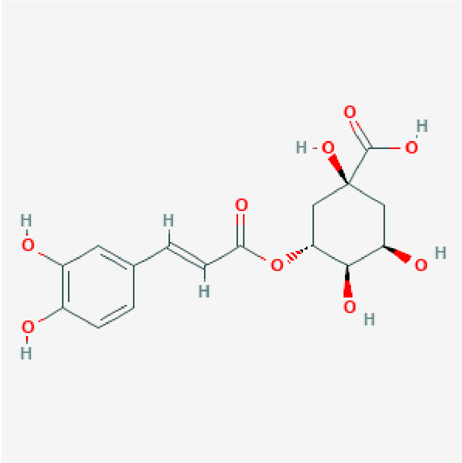
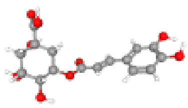
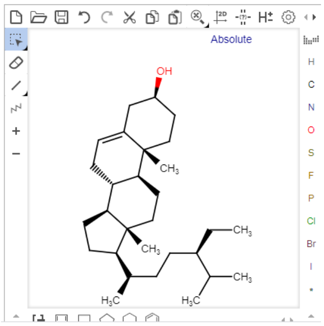
Senayawa that we got earlier from Pubchem, earlier, was analyzed in the form of checking its structure and content through phtochem, Swiss target, chemdraw, and chem3d.

3.3 Stages

The chemical compounds from the Jatropha leaves, see the content and active compounds in the phytochem, in the phytochhem we will use the active sentawa in the leaves, which include flavonoids, the active compounds we got earlier we checked their structure, properties, and smiles through pubchem, swiss target, and chemdraw and chem3d applications

4. RESULTS AND DISCUSSION

No.	Active Compounds		
1.	Beta-Amyrin (Leaf) Analgesic Antiedemic IC27 = 40 mg / kg ipr rat Antiinflammatory Antinociceptive Antiulcer Gastroprotective Hepatoprotective Larvicide Mosquitocide	2D structure:  3D structure: 	
2.	beta-Sitosterol (Root)	2D structure:;  3D structure: 	

3.	Chlorogenic-acid	2D structure:  3D structure: 	

Picture 1. Obtained Data

Target	Common name	Uniprot ID
Androgen Receptor	AR	P10275
Protein-tyrosine phosphatase 1B	PTPN1	P18031
Estrogen receptor alpha	ESR1	P03372
Muscarinic acetylcholine receptor M2	CHRM2	P08172
Acetylcholinesterase	ACHE	P22303
Serotonin transporter	SLC6A4	P31645
Cytochrome P450 2C19	CYP2C19	P33261
Nuclear receptor subfamily 1 group I member 3 (by homology)	NR1I3	Q14994
Norepinephrine transporter	SLC6A2	P23975
Cytochrome P450 19A1	CYP19A1	P11511
Butyrylcholinesterase	BCHE	P06276
HMG-CoA reductase	HMGCR	P04035
Cytochrome P450 51 (by homology)	CYP51A1	Q16850
Niemann-Pick C1-like protein 1	NPC1L1	Q9UHC9
Sterol regulatory element-binding protein 2	SREBF2	Q12772
Estrogen receptor beta	ESR2	Q92731

Picture 2. The data obtained from Beta-Amyrin

Target	Common name	Uniprot ID
Niemann-Pick C1-like protein 1	NPC1L1	Q9UHC9
LXR-alpha	NR1H3	Q13133
The nuclear receptor ROR-gamma	RORC	P51449
HMG-CoA reductase	HMGCR	P04035
Testis-specific androgen-binding protein	SHBG	P04278
Cytochrome P450 51 (by homology)	CYP51A1	Q16850
Cytochrome P450 17A1	CYP17A1	P05093
Cytochrome P450 19A1	CYP19A1	P11511
Sterol regulatory element-binding protein 2	SREBF2	Q12772
Androgen Receptor	AR	P10275
The nuclear receptor ROR-alpha	RORA	P35398
Estrogen receptor alpha	ESR1	P03372
Estrogen receptor beta	ESR2	Q92731
Protein-tyrosine phosphatase 1B	PTPN1	P18031
Cytochrome P450 2C19	CYP2C19	P33261
Norepinephrine transporter	SLC6A2	P23975
Acetylcholinesterase	ACHE	P22303
Corticosteroid binding globulin	SERPINA6	P08185
Glucose-6-phosphate 1-dehydrogenase	G6PD	P11413
Butyrylcholinesterase	BCHE	P06276
Serotonin transporter	SLC6A4	P31645
Muscarinic acetylcholine receptor M2	CHRM2	P08172
Nuclear receptor subfamily 1 group I member 3 (by homology)	NR1I3	Q14994
LXR-beta	NR1H2	P55055
Anti-estrogen binding site (AEBS) (by homology)	DHCR7	Q9UBM7
Prostanoid EP1 receptor (by homology)	PTGER1	P34995
Prostanoid EP2 receptor (by homology)	PTGER2	P43116
Vitamin D receptors	VDR	P11473
Thromboxane-A synthase	TBXAS1	P24557
Prostaglandin E synthase	PTGES	O14684
Peroxisome proliferator-activated receptor delta	PPARD	Q03181
Carboxylesterase 2	CES2	O00748
11-beta-hydroxysteroid dehydrogenase 1	HSD11B1	P28845
Squalene monooxygenase	SQLE	Q14534
Protein-tyrosine phosphatase 1C	PTPN6	P29350
T-cell protein-tyrosine phosphatase	PTPN2	P17706
Glycine receptor alpha-1 subunit	GLRA1	P23415
Nitric oxide synthase, inducible (by homology)	NOS2	P35228

Picture 3. The data obtained from beta-sitosterol

Target	Common name	Uniprot ID
Niemann-Pick C1-like protein 1	NPC1L1	Q9UHC9
LXR-alpha	NR1H3	Q13133
The nuclear receptor ROR-gamma	RORC	P51449
HMG-CoA reductase	HMGCR	P04035
Testis-specific androgen-binding protein	SHBG	P04278
Cytochrome P450 51 (by homology)	CYP51A1	Q16850
Cytochrome P450 17A1	CYP17A1	P05093
Cytochrome P450 19A1	CYP19A1	P11511
Sterol regulatory element-binding protein 2	SREBF2	Q12772
Androgen Receptor	AR	P10275
The nuclear receptor ROR-alpha	RORA	P35398
Estrogen receptor alpha	ESR1	P03372
Estrogen receptor beta	ESR2	Q92731
Protein-tyrosine phosphatase 1B	PTPN1	P18031
Cytochrome P450 2C19	CYP2C19	P33261
Norepinephrine transporter	SLC6A2	P23975
Acetylcholinesterase	ACHE	P22303
Corticosteroid binding globulin	SERPINA6	P08185
Glucose-6-phosphate 1-dehydrogenase	G6PD	P11413
Butyrylcholinesterase	BCHE	P06276
Serotonin transporter	SLC6A4	P31645
Muscarinic acetylcholine receptor M2	CHRM2	P08172
Nuclear receptor subfamily 1 group I member 3 (by homology)	NR1I3	Q14994
LXR-beta	NR1H2	P55055
Anti-estrogen binding site (AEBS) (by homology)	DHCR7	Q9UBM7
Prostanoid EP1 receptor (by homology)	PTGER1	P34995
Prostanoid EP2 receptor (by homology)	PTGER2	P43116
Vitamin D receptors	VDR	P11473
Thromboxane-A synthase	TBXAS1	P24557
Prostaglandin E synthase	PTGES	O14684
Peroxisome proliferator-activated receptor delta	PPARD	Q03181
Carboxylesterase 2	CES2	O00748
11-beta-hydroxysteroid dehydrogenase 1	HSD11B1	P28845
Squalene monooxygenase	SQLE	Q14534
Protein-tyrosine phosphatase 1C	PTPN6	P29350
T-cell protein-tyrosine phosphatase	PTPN2	P17706
Glycine receptor alpha-1 subunit	GLRA1	P23415
Nitric oxide synthase, inducible (by homology)	NOS2	P35228
Peroxisome proliferator-activated receptor gamma	PPARG	P37231
UDP-glucuronosyltransferase 2B7	UGT2B7	P16662

DNA polymerase beta (by homology)	POLB	P06746
Prolyl endopeptidase	PREP	P48147
Dynamin-1	DNM1	Q05193
Glucocorticoid receptor	NR3C1	P04150
Prostanoid EP4 receptor (by homology)	PTGER4	P35408
Indoleamine 2,3-dioxygenase	IDO1	P14902
Smoothened homolog	SMO	Q99835
Potassium-transporting ATPase alpha chain 2	ATP12A	P54707
Prostanoid IP receptors	PTGIR	P43119
p53-binding protein Mdm-2	MDM2	Q00987
Sigma opioid receptor	SIGMAR1	Q99720
Anti-estrogen binding site (AEBS)	DHCR7 EBP	Q9UBM7 Q15125
Isoprenylcysteine carboxyl methyltransferase	ICMT	O60725
Fatty acid binding protein adipocyte	FABP4	P15090
Telomerase reverse transcriptase	TERT	O14746
Fatty acid binding muscle protein	FABP3	P05413
Epidermal fatty acid binding protein	FABP5	Q01469
Fatty acid-binding protein, liver	FABP1	P07148
Phosphodiesterase 4A	PDE4A	P27815
Phosphodiesterase 4B	PDE4B	Q07343
Phosphodiesterase 4C	PDE4C	Q08493
11-beta-hydroxysteroid dehydrogenase 2	HSD11B2	P80365
Dopamine transporter	SLC6A3	Q01959
MAP kinase ERK1	MAPK3	P27361
Beta protein kinase	PRKCH	P24723
Protein-tyrosine phosphatase 2C	PTPN11	Q06124
Aldo-keto reductase family 1 member B10	AKR1B10	O60218
Methionine aminopeptidase 1	METAP1	P53582
Receptor-type tyrosine-protein phosphatase F (LAR)	PTPRF	P10586
Phospholipase A2 group 1B	PLA2G1B	P04054
Low molecular weight phosphotyrosine protein phosphatase	ACP1	P24666
Dopamine D2 receptor	DRD2	P14416
Sphingosine 1-phosphate receptor Edg-3	S1PR3	Q99500
Sphingosine 1-phosphate receptor Edg-1	S1PR1	P21453
CXC chemokine receptor type 3	CXCR3	P49682
Vitamin D-binding protein	GC	P02774

Picture 4. The data obtained from Chlorogenic-acid

From the data we get, there are 3 active compounds contained in Jatropha leaves, the data above is data obtained from 3 different links, namely phytochem, pubchem, Swiss target prediction, and chemdraw and chem3d applications.

5. CONCLUSION

Jatropha leaves contain flavonoids which flavonoids containantipyretic, analgesic and anti-inflammatory so it is very well used in treating fever and this jatropha leaf is safer than paracetamol.

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